



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 08:23 PM EST

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.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) : 2.40

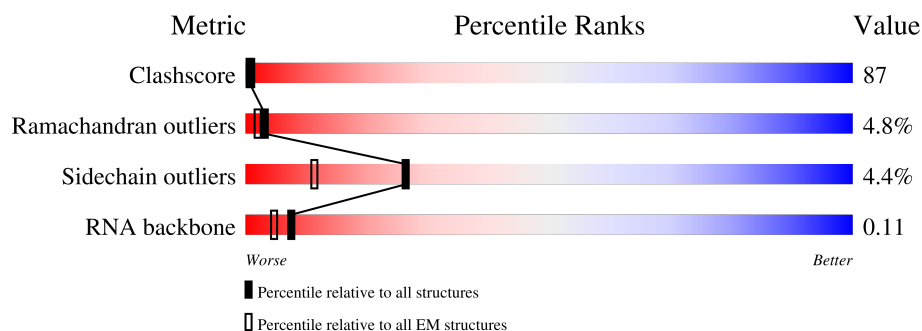
1 Overall quality at a glance

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.





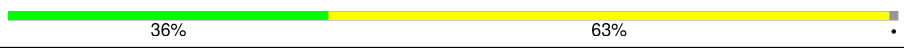
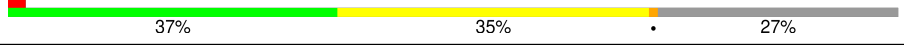
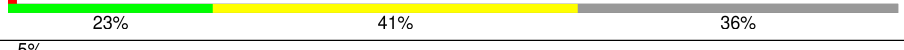


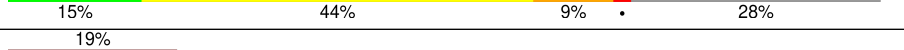
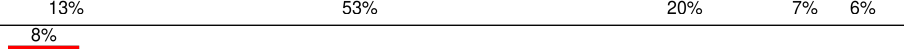
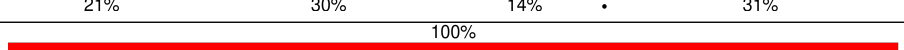

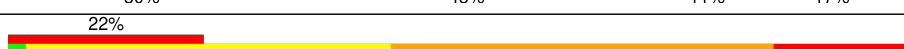
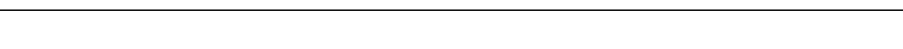
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1664	
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

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
1	A	1461	Total	C	N	O	S	0	0
			11542	7292	2004	2184	62		

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

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

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

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

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

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

- 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
			670	428	114	125	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	103	Total	C	N	O	S	0	0
			810	506	132	167	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	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

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

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

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

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

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

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

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

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

- Molecule 18 is a RNA chain called RNA.

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

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

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

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

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

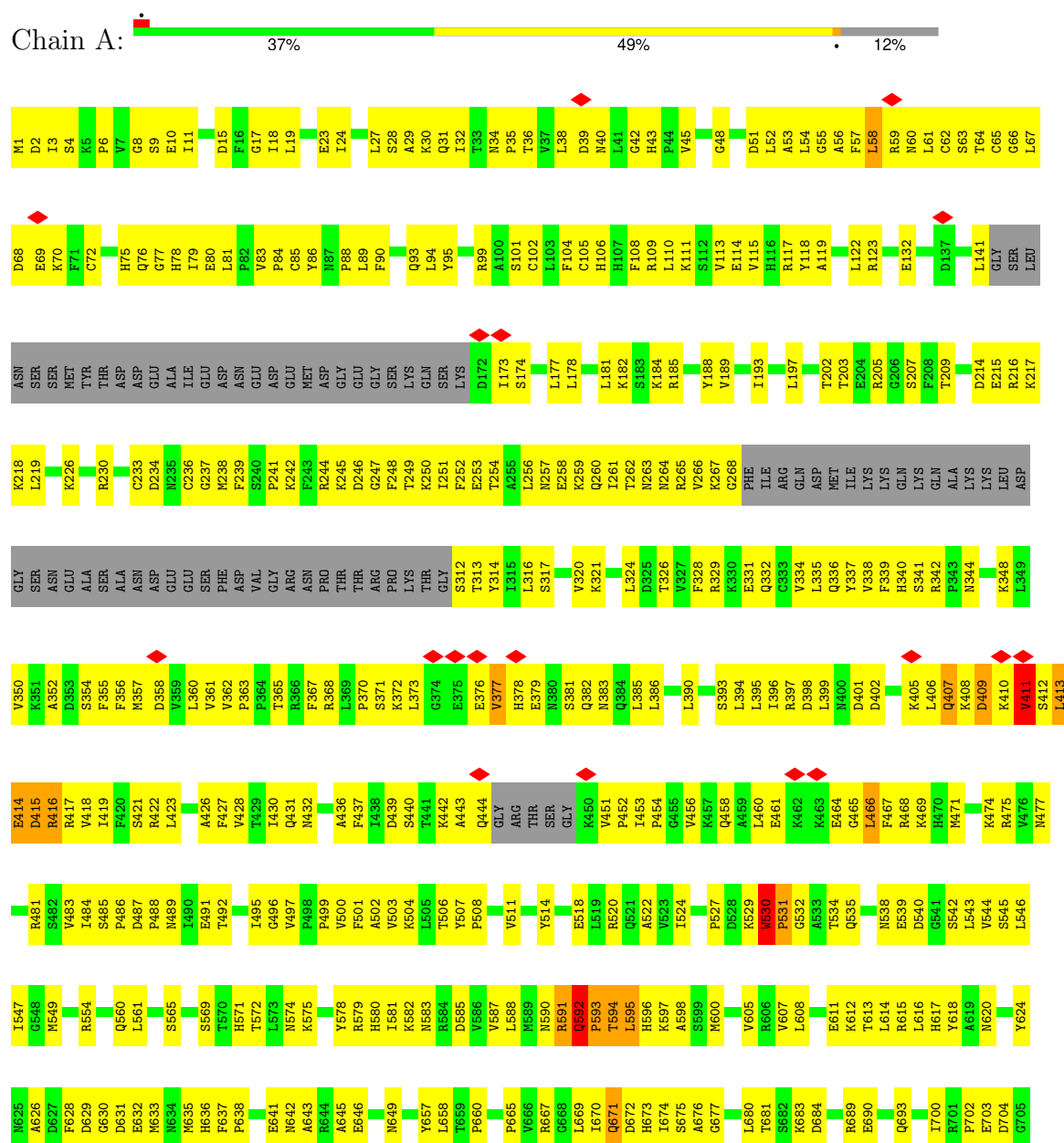
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

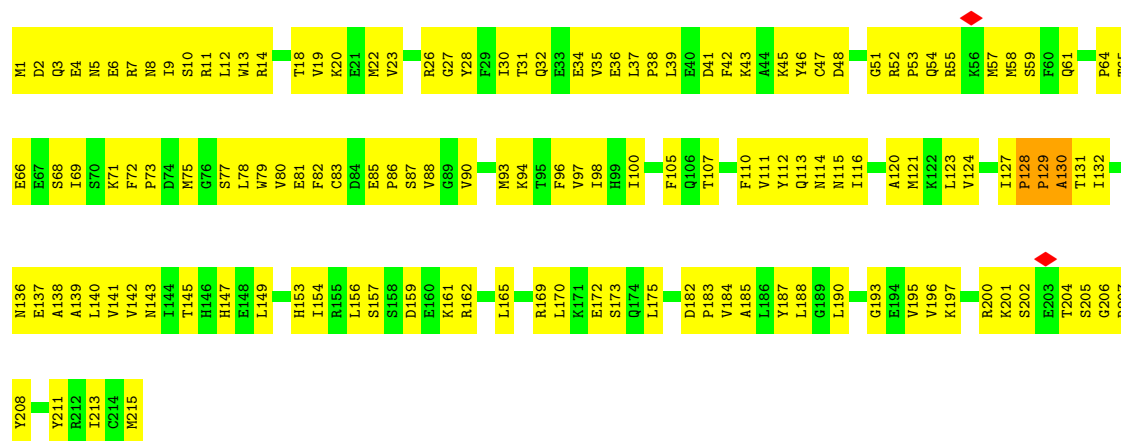
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



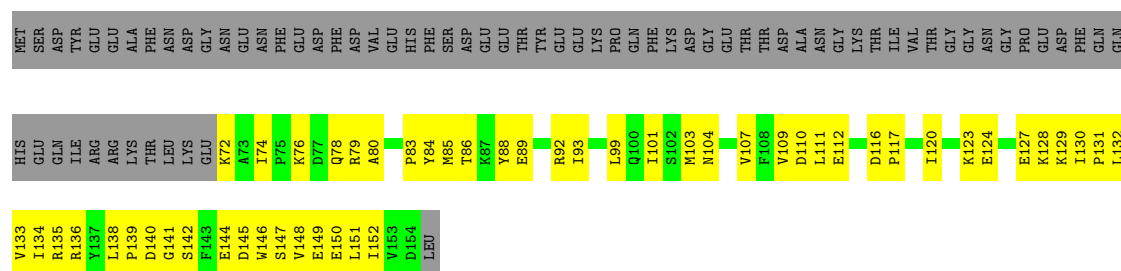


Q979	D980	S981	I985	F986	N987	E988	P992	F996	Q999	L1000	A1001	K1002	A1003	G1004	Y1005	G1009	N1010	E1011	M1013	S1015	G1016	E1021	D1025	I1026	Y1027	V1028	V1031	Y1032	Y1033	Q1034	R1035	L1036	R1037	H1038	M1039	V1040	N1041	D1042	K1043	F1044	Q1045	V1046	R1047	S1048	T1049	G1050	P1051	V1052	N1053				
E642	D843	P846	Y847	I848	Y851	V852	E853	E854	P857	L858	C859	A860	Y861	F862	D863	D864	N867	K868	T869	K870	L871	K872	T873	Y874	H875	S876	P879	A880	Y881	L882	E883	E884	L887	I888	Q889	D890	E891	S892	K893	K894	F895	Q896	E897	L898	Q899	T900	I903	X904	Y905	R906	I907	A908	
R909	T910	P911	Q912	I913	G914	D915	K916	R920	R921	G922	Q923	K924	G925	Y926	S927	S928	R929	K930	N931	P932	T933	I934	R935	P936	F937	F938	S939	E940	T941	G942	I943	Q944	P945	D946	I947	I948	I949	N950	P951	H952	A953	F954	P955	S956	N957	T959	F963	Y964	E965	K970	L974	I977	A978
V772	V773	S777	Y778	T779	G780	Y781	D782	M783	D784	A785	A786	H787	N790	K791	S792	A793	D794	E795	R796	F797	F798	M803	Y804	K805	T806	D810	L811	A812	L813	N814	R815	N816	R817	G818	P819	P820	T822	Q823	H824	F825	G826	F827	G828	N829	D830	E831	W832	P833	F834	E835	W836	L840	D841
N884	H888	H889	I896	L897	S898	P899	L900	A701	N702	P705	F709	N710	Y628	Q711	S712	N715	M716	Y717	Q718	Q719	Q720	K723	Q724	Y725	M726	V731	A732	L733	C734	H735	K736	S737	P657	L658	D659	K660	V664	E668	Q669	N672	A675	V676	T677	P678	Q679	E680	F681	Q682	N683				
E523	C529	P530	V531	H532	Q536	S537	P538	C539	G540	L541	L542	H547	K548	Q554	Q555	V558	I561	P562	S563	L564	L565	Y566	S567	L568	G569	V570	A571	P572	A573	A574	H575	L576	F577	A578	P581	C585	I588	D589	G590	K591	L592	I593	G594	W595	Q600	K604	I605	D606					
M451	R452	Y453	M454	E455	M456	S459	K460	M461	Q462	Y463	F464	L465	G468	M469	L470	V471	S472	L478	Q479	Q480	V481	S482	Y484	Y487	K490	L491	M492	F493	Y494	R495	F496	H499	F500	R501	M502	R505	G506	S507	F508	F509	A510	Q511	L512	K513	K443	Y445	M446	K519	L520	P522			
F371	R372	M373	L374	L375	F376	K377	K380	L384	V385	S390	Q398	E401	L404	G405	G406	Y409	T424	M411	L412	L413	K414	E415	K416	L421	Q422	M423	N424	L425	L426	Q427	Y428	R429	L432	G435	M436	A437	L438	M439	F440	K441	D442	K443	R444	Y445	M446	K519	L520	P522					
V297	K298	D299	S300	F301	R305	L306	E307	L308	L309	L310	G312	F313	K314	K315	R316	Y317	L320	Q321	N322	R323	T324	Q325	V326	Q328	L330	F334	R335	F338	Q339	A340	P342	D343	D346	V349	E352	V353	L354	D355	R356	L359	V360	H361	L362	Q368	D369	K370							
Y229	Y232	Q235	I236	E237	R237	S238	V239	R240	P241	L242	Q243	T244	Q245	T247	M248	V249	L250	H251	Y252	L253	Q257	V258	T259	R261	P262	S263	W264	L277	K278	L280	C281	H282	T283	S284	D285	R286	E287	I218	F289	D290	G291	I292	I293	G294	N295	D296							
K77	P78	N80	S86	G87	S88	G89	Y90	L91	N93	K94	M96	L95	V97	S98	I99	E100	Q101	V102	P107	M108	S109	N110	D111	G112	V113	S114	S115	A116	V117	E118	K119	K120	V121	V122	Q128	R129	L130	T131	S132	Y133	K134	G135	K136	L137	L138	L139	F141	G142					
MET	SER	LYS	VAL	ILE	LYS	PRO	PRO	GLY	GLN	ALA	R12	D15	F16	R21	E22	S23	R24	F25	I26	P29	S33	A34	F35	P36	L37	V42	Q43	P44	F49	M50	A51	L52	T53	E54	D57	L60	L61	M62	L63	G64	V65	I68	G69	E70	K71	V72	I73	L139	F74	D75	G76		



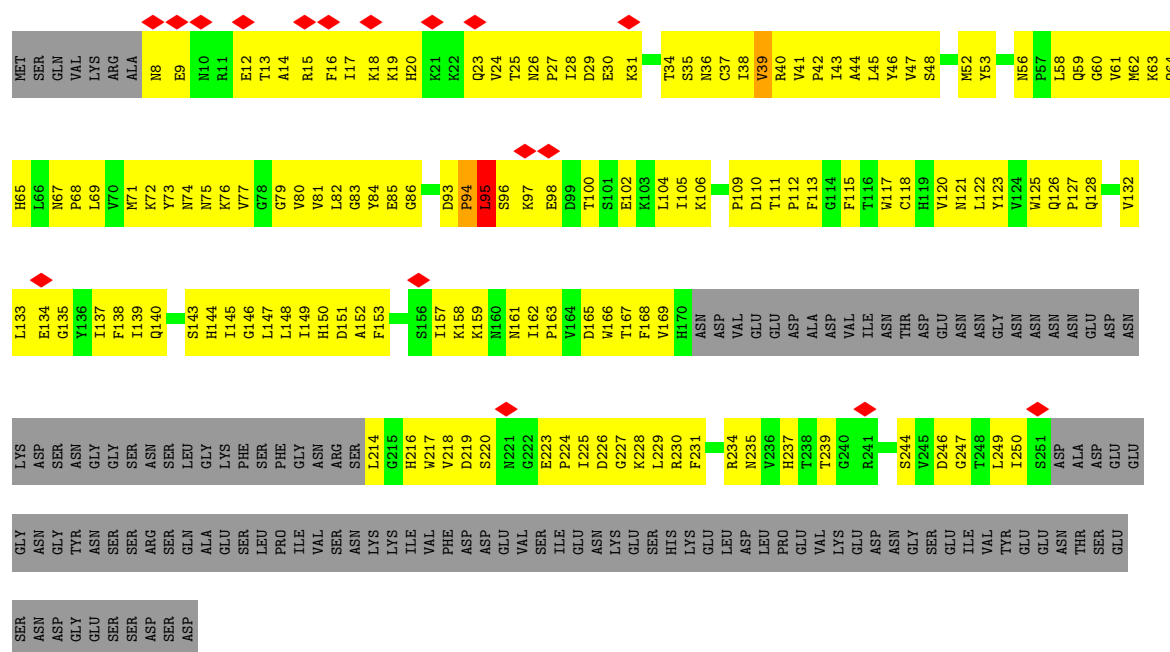
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 20% 34% 46%

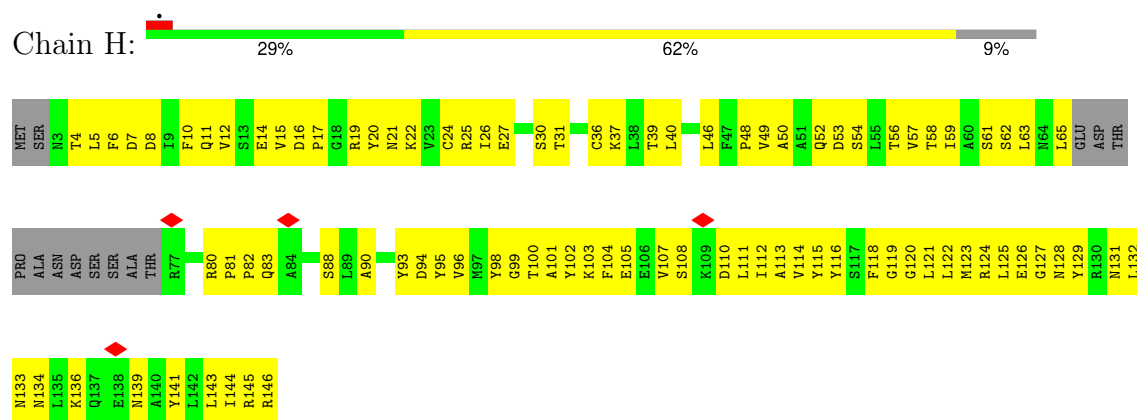


• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

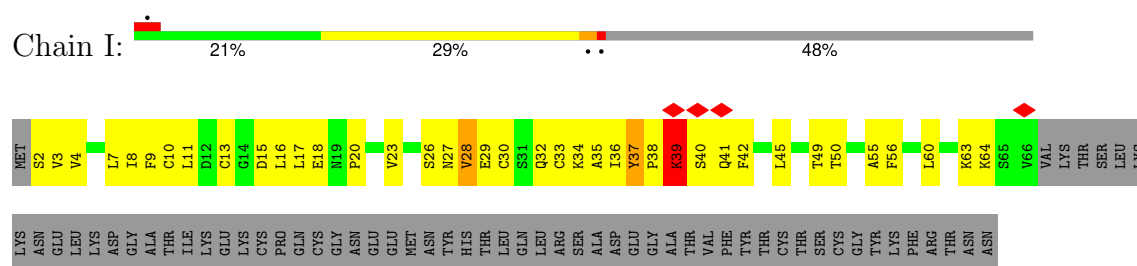
Chain G: 5% 17% 44% 38%



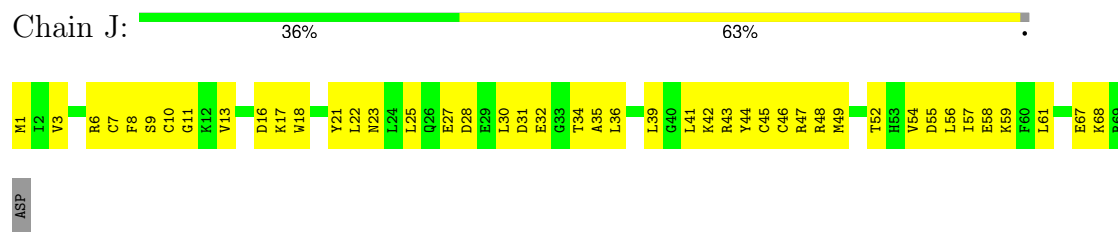
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



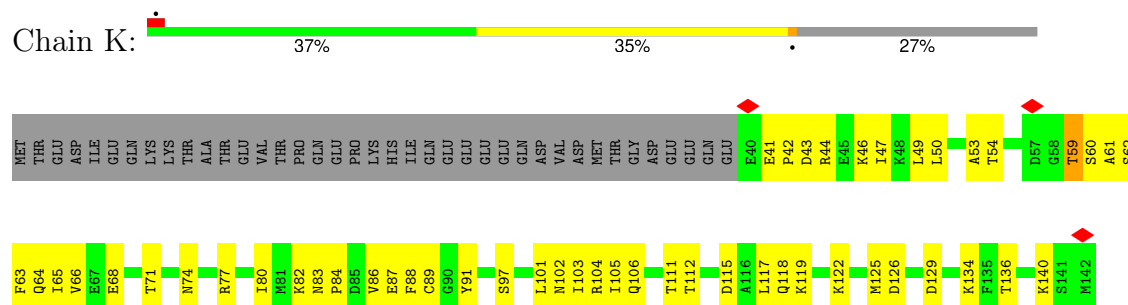
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



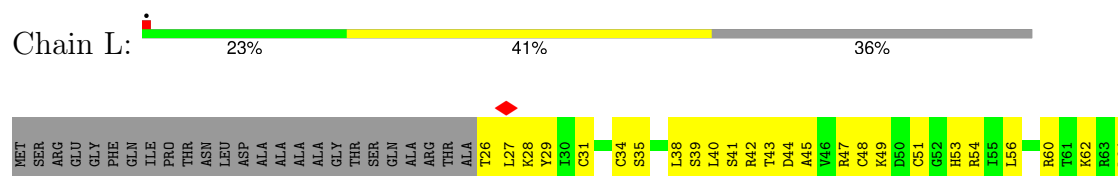
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

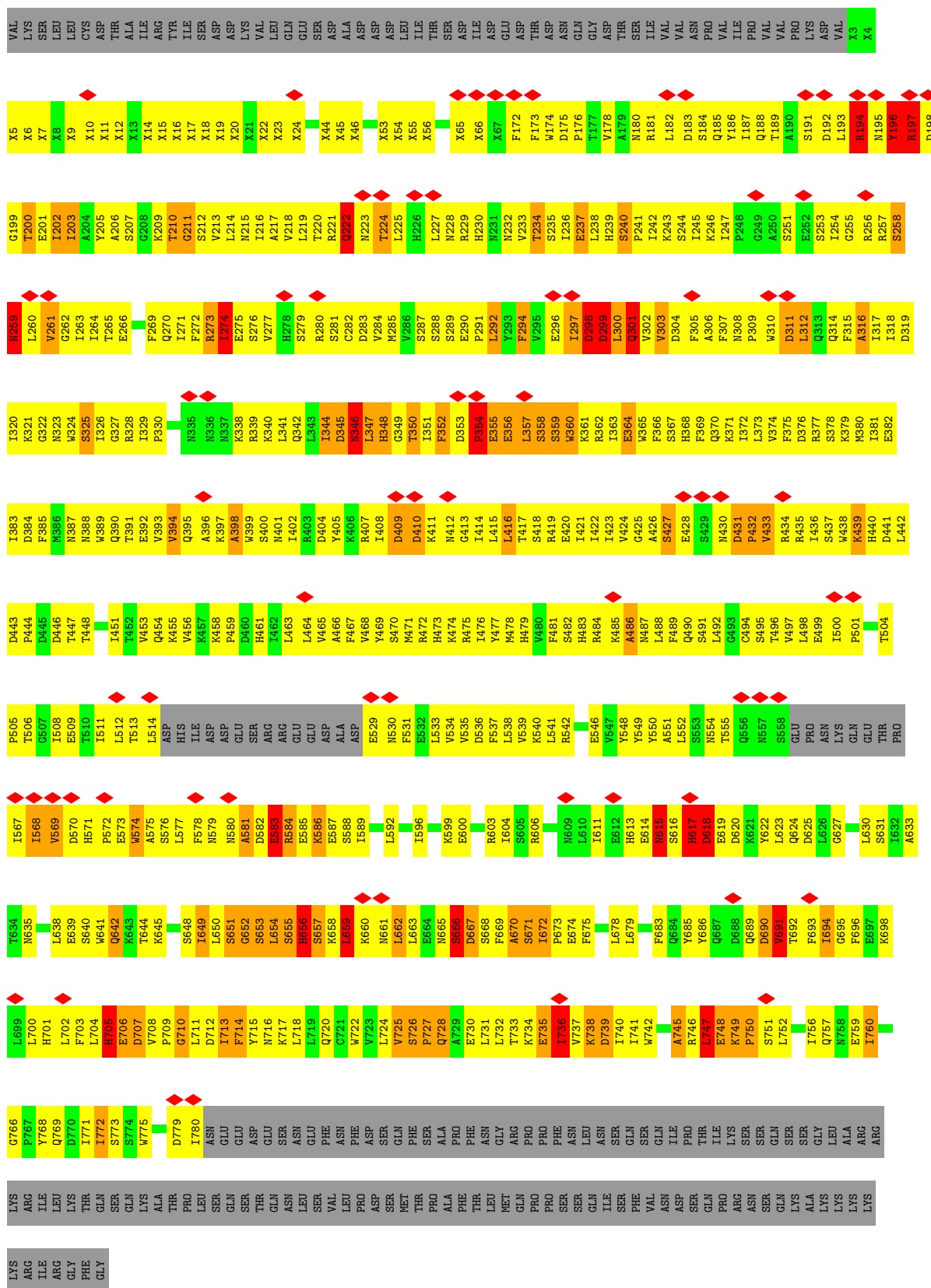


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

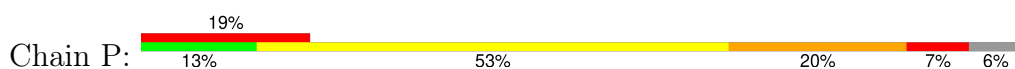


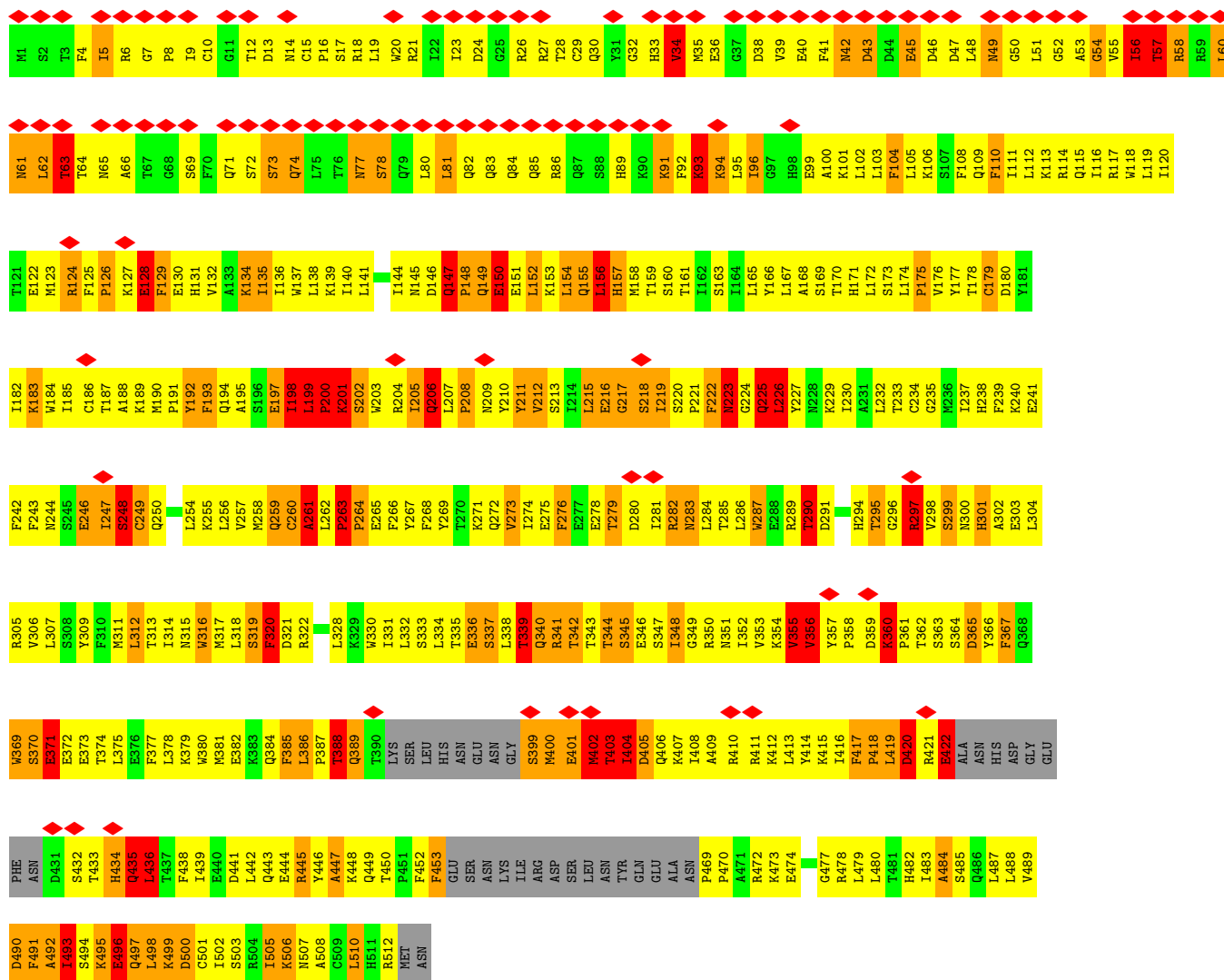
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



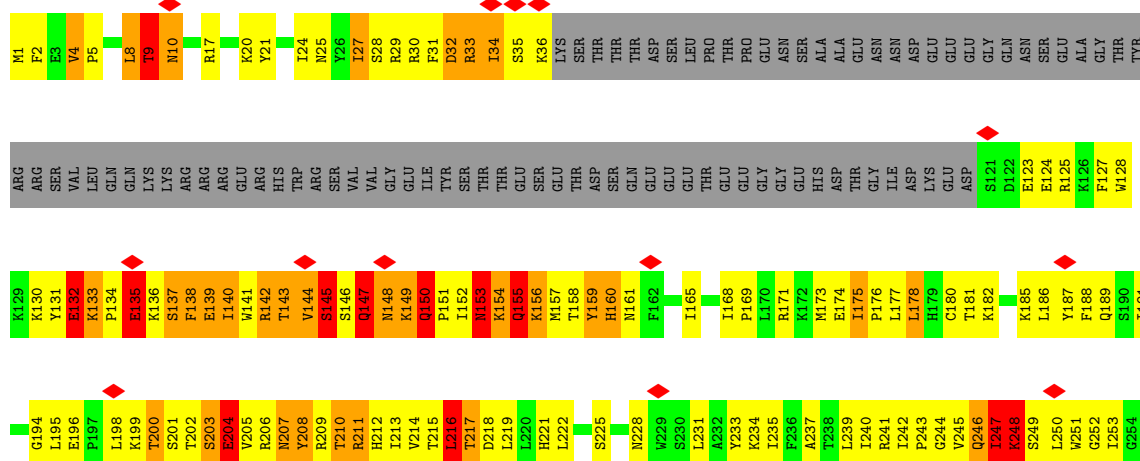


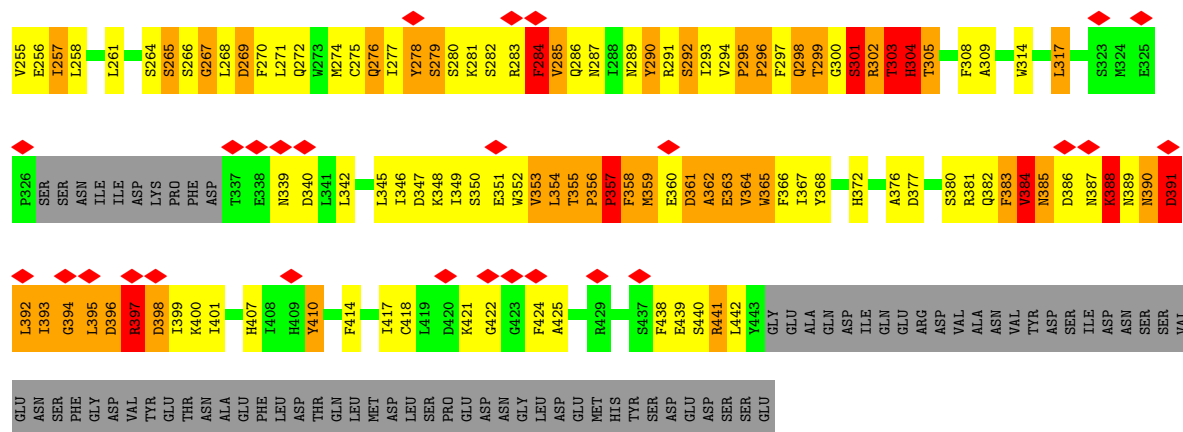
• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN7





• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN11





• 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 (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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...

Continued from previous page...

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

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

Continued on next page...

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%)	8	37
2	B	1172/1203 (97%)	1078 (92%)	71 (6%)	23 (2%)	6	32
3	C	304/335 (91%)	286 (94%)	13 (4%)	5 (2%)	8	37
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	203 (95%)	7 (3%)	3 (1%)	9	40
6	F	81/155 (52%)	73 (90%)	7 (9%)	1 (1%)	11	43
7	G	197/326 (60%)	182 (92%)	12 (6%)	3 (2%)	8	39
8	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
9	I	63/125 (50%)	55 (87%)	6 (10%)	2 (3%)	3	22
10	J	67/70 (96%)	60 (90%)	6 (9%)	1 (2%)	8	39
11	K	101/142 (71%)	94 (93%)	7 (7%)	0	100	100
12	L	43/70 (61%)	38 (88%)	4 (9%)	1 (2%)	5	29
13	M	104/415 (25%)	97 (93%)	5 (5%)	2 (2%)	6	33
14	N	156/233 (67%)	129 (83%)	21 (14%)	6 (4%)	2	20
15	O	581/894 (65%)	408 (70%)	111 (19%)	62 (11%)	0	6
16	P	473/514 (92%)	320 (68%)	74 (16%)	79 (17%)	0	2
17	Q	343/507 (68%)	234 (68%)	56 (16%)	53 (16%)	0	2
All	All	5527/7151 (77%)	4772 (86%)	491 (9%)	264 (5%)	3	17

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 ⓘ

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%)	67	79
2	B	1030/1053 (98%)	1009 (98%)	21 (2%)	50	69
3	C	270/296 (91%)	269 (100%)	1 (0%)	89	91
4	D	56/116 (48%)	56 (100%)	0	100	100
5	E	197/197 (100%)	196 (100%)	1 (0%)	86	90
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	179/291 (62%)	175 (98%)	4 (2%)	47	66
8	H	117/128 (91%)	116 (99%)	1 (1%)	75	83
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%)	70	80
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	96/371 (26%)	92 (96%)	4 (4%)	25	48
14	N	146/220 (66%)	143 (98%)	3 (2%)	48	67
15	O	545/778 (70%)	496 (91%)	49 (9%)	8	25
16	P	445/476 (94%)	379 (85%)	66 (15%)	2	13
17	Q	331/474 (70%)	276 (83%)	55 (17%)	2	11
All	All	5031/6364 (79%)	4810 (96%)	221 (4%)	26	47

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 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

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

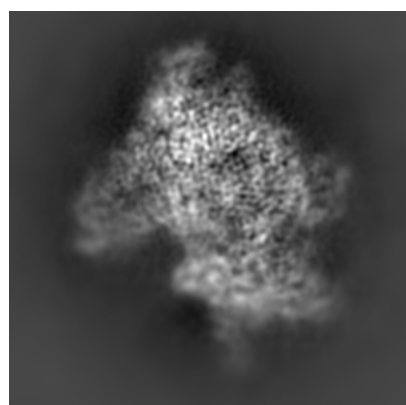
6 Map visualisation [i](#)

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.

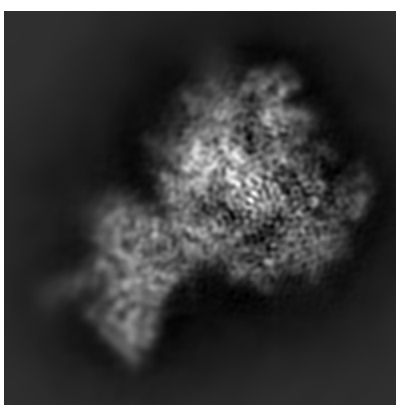
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

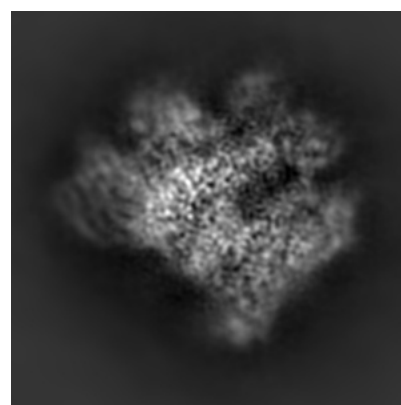
6.1.1 Primary map



X



Y

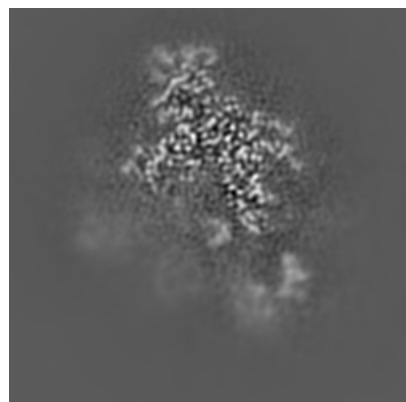


Z

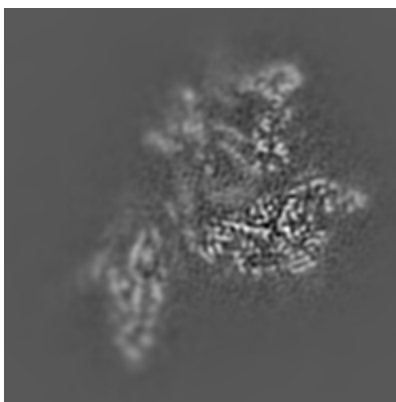
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

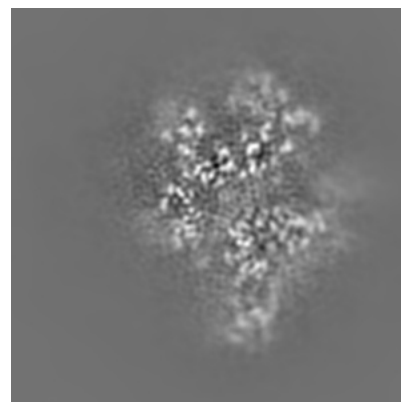
6.2.1 Primary map



X Index: 96



Y Index: 96

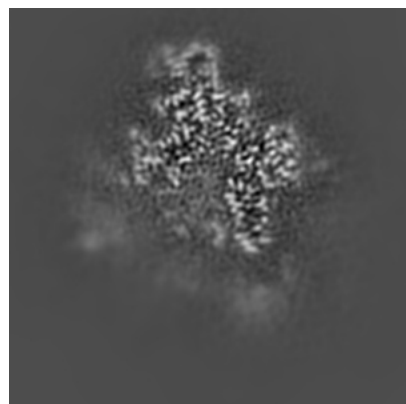


Z Index: 96

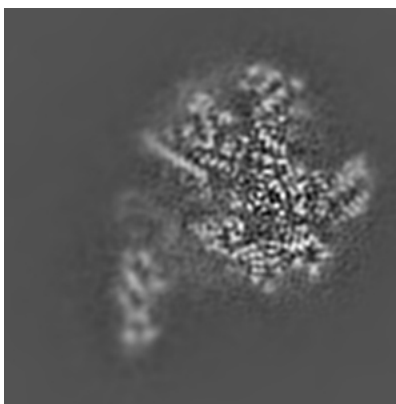
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

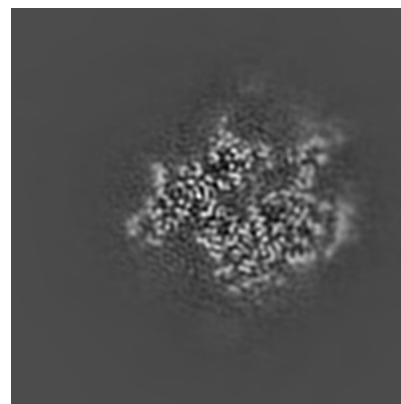
6.3.1 Primary map



X Index: 100



Y Index: 87

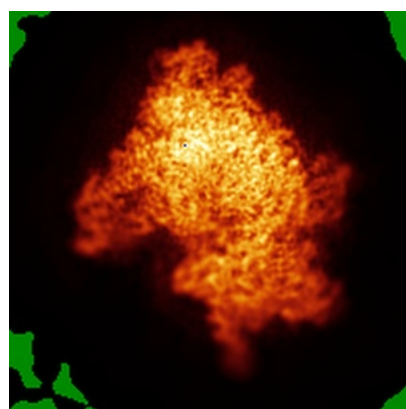


Z Index: 127

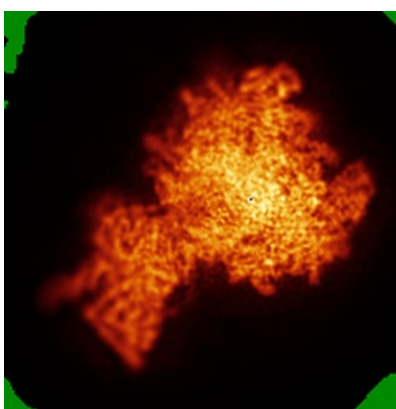
The images above show the largest variance slices of the map in three orthogonal directions.

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

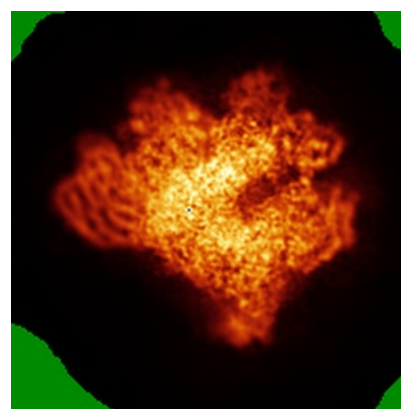
6.4.1 Primary map



X



Y

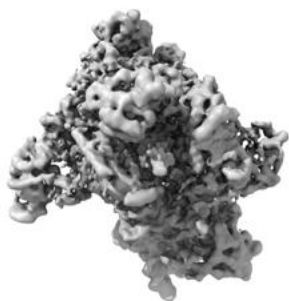


Z

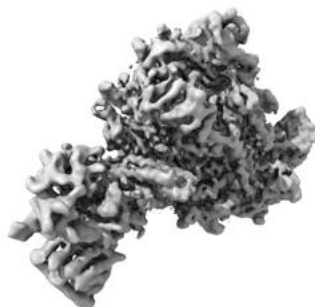
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

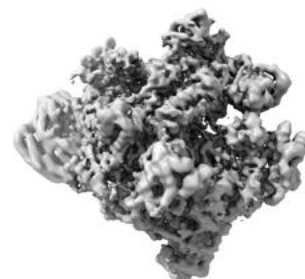
6.5.1 Primary map



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.

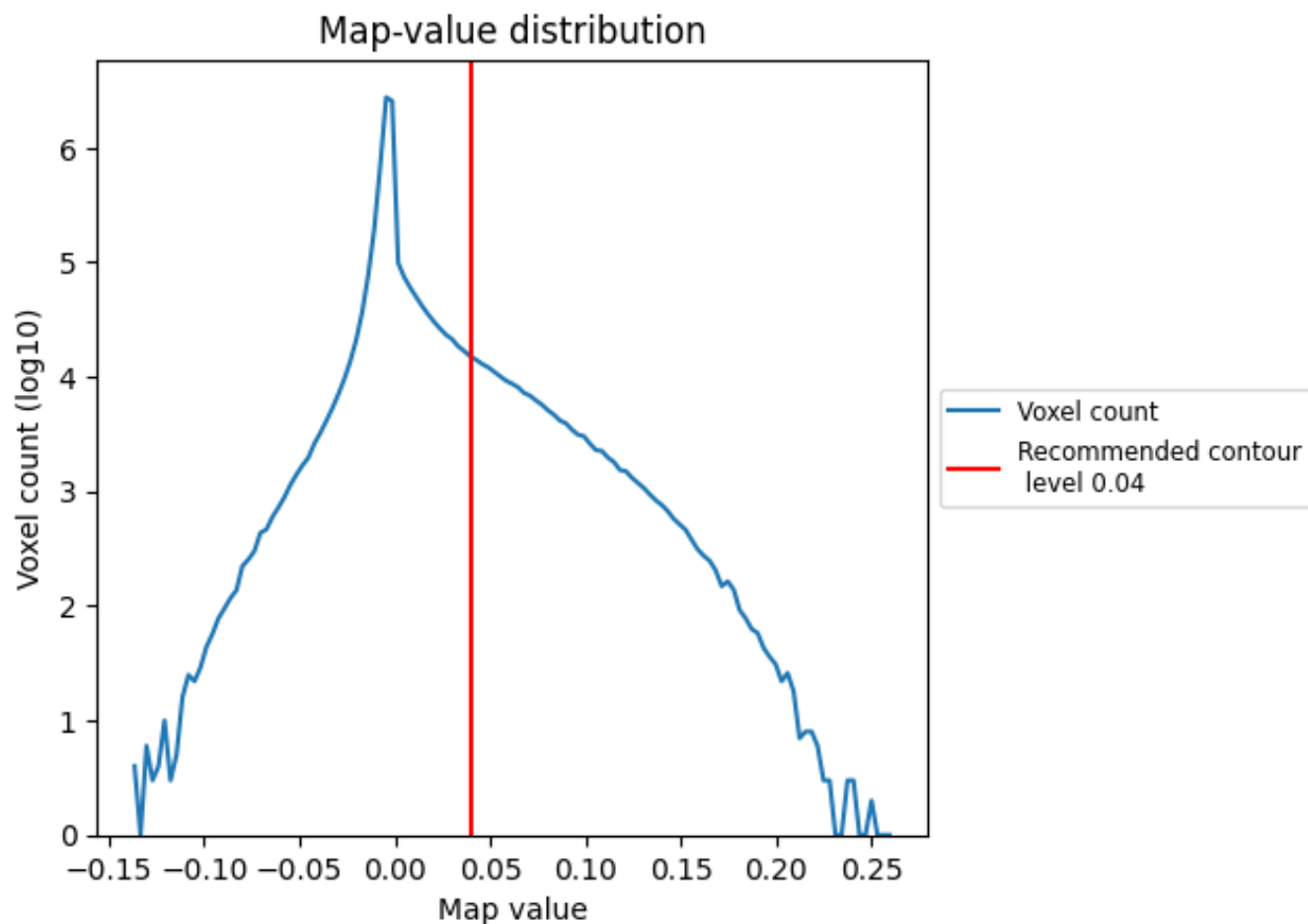
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

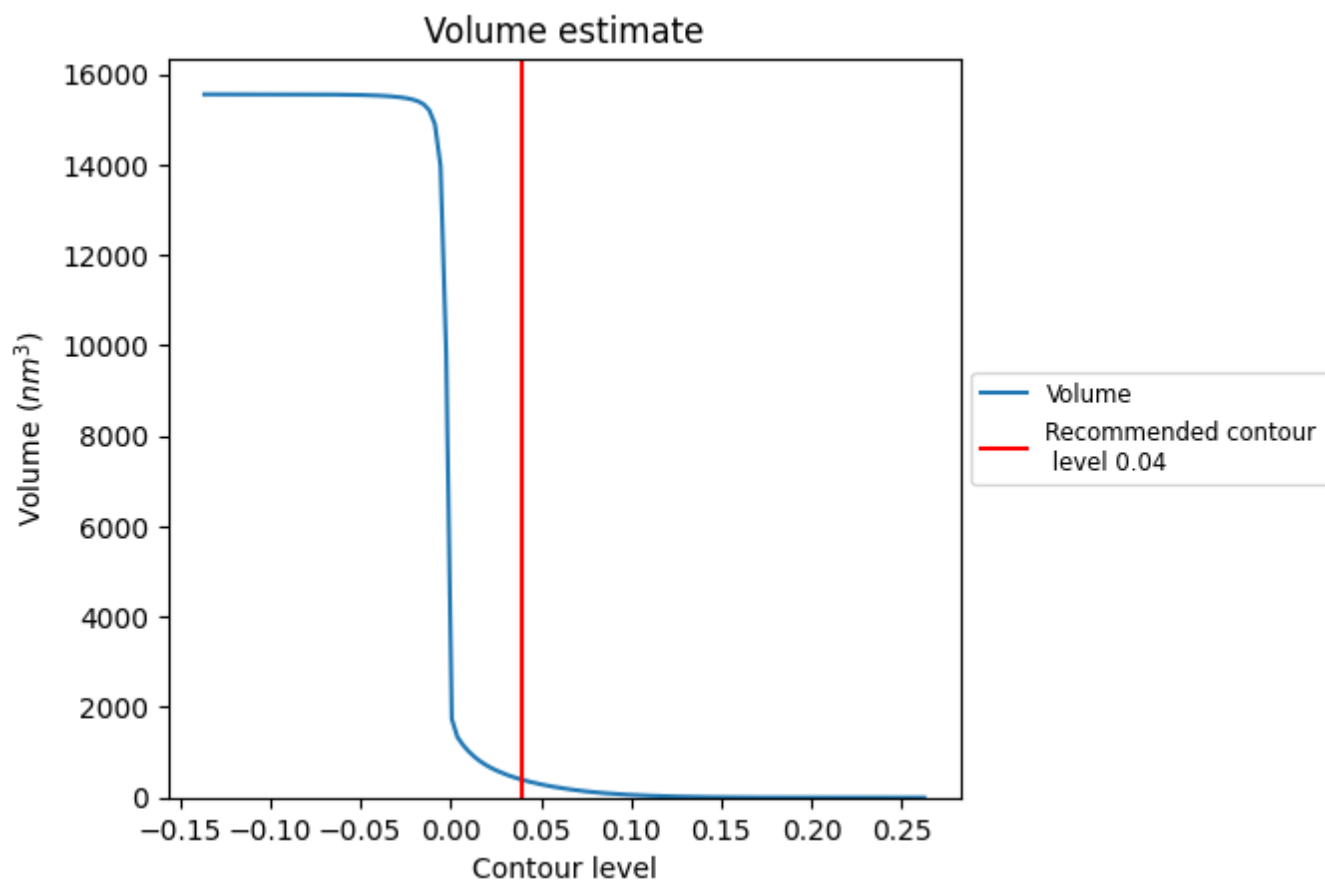
This section contains the results of statistical analysis of the map.

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.

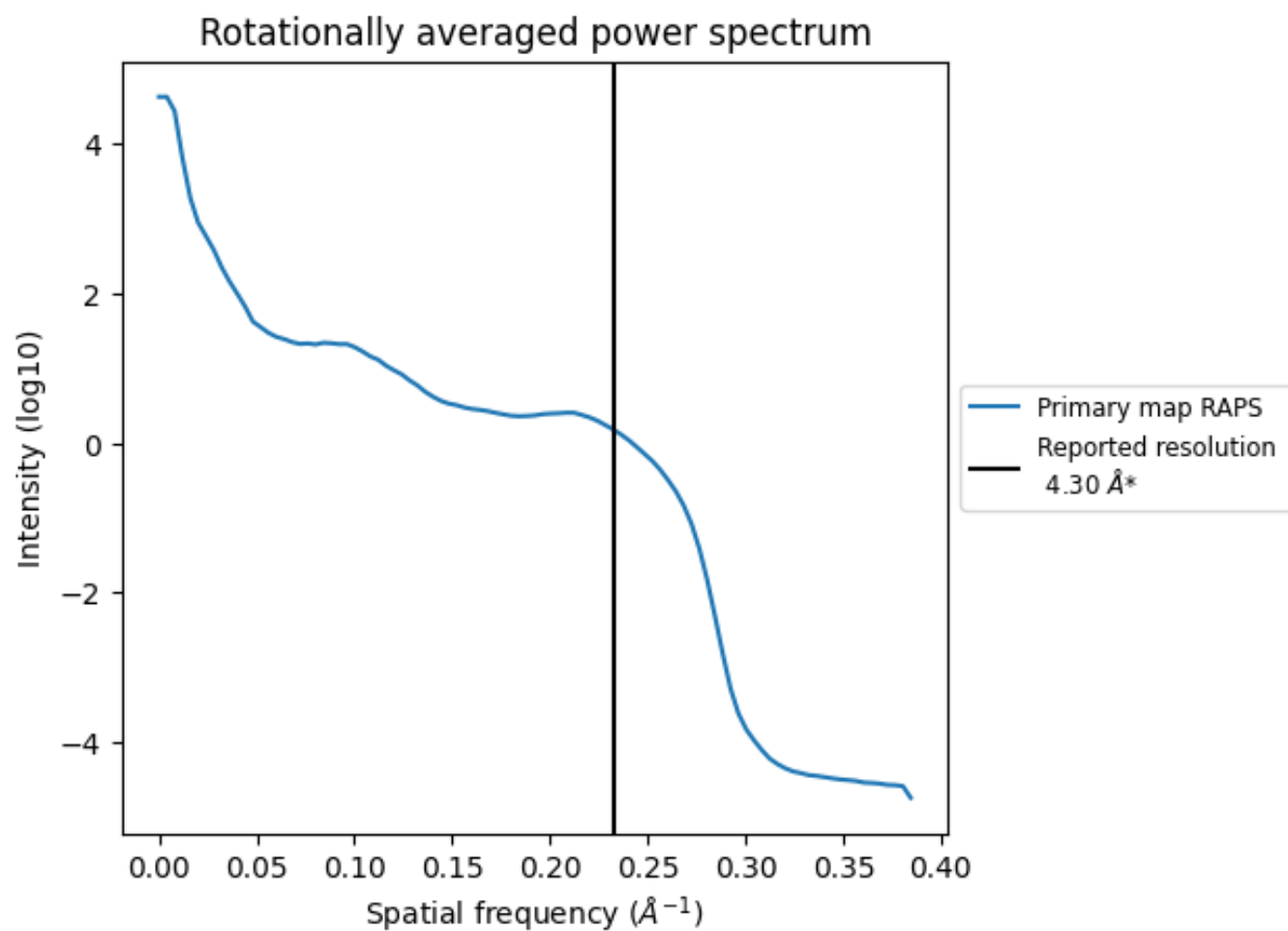
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm^3 ; 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 ⓘ

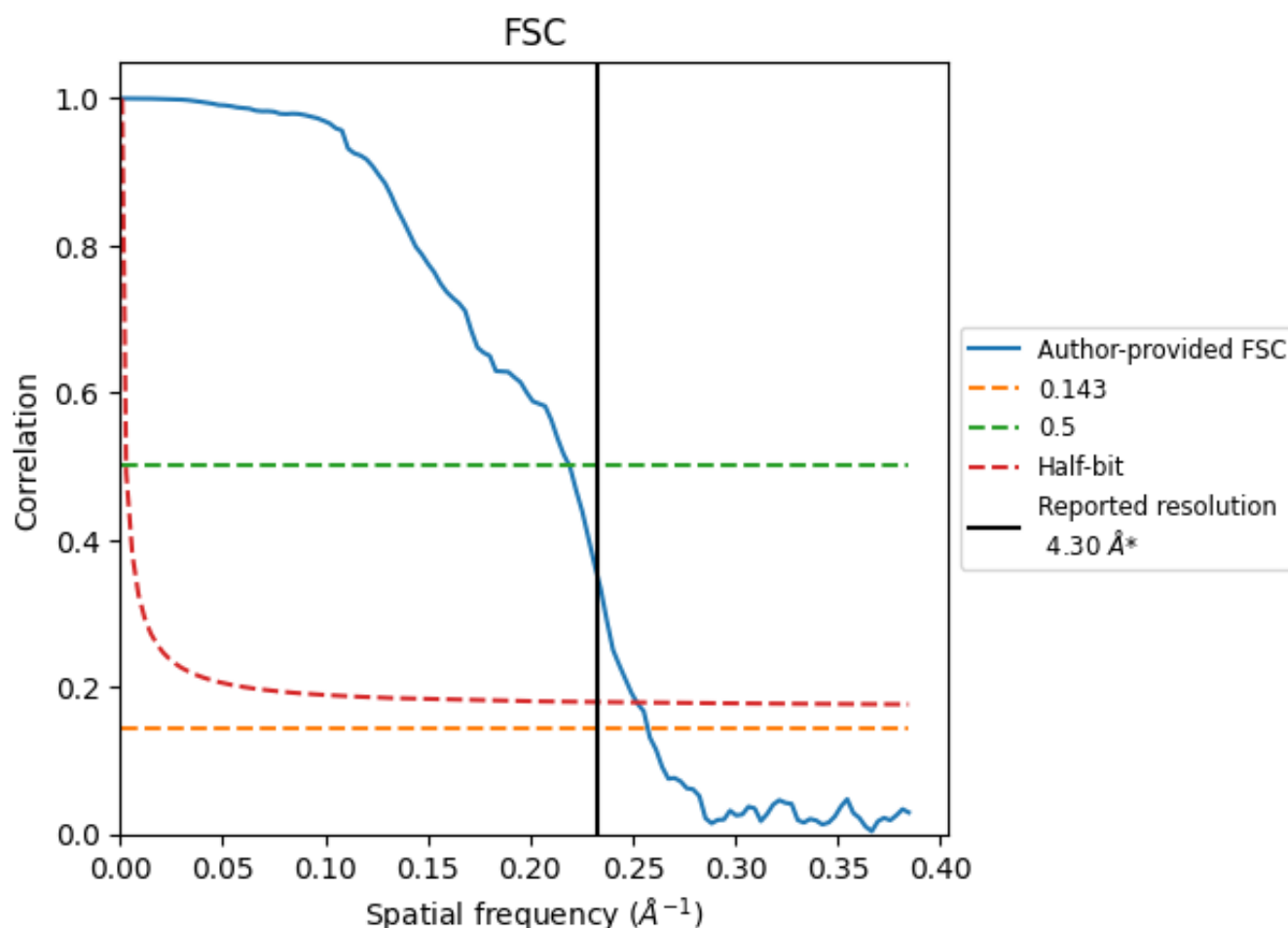


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

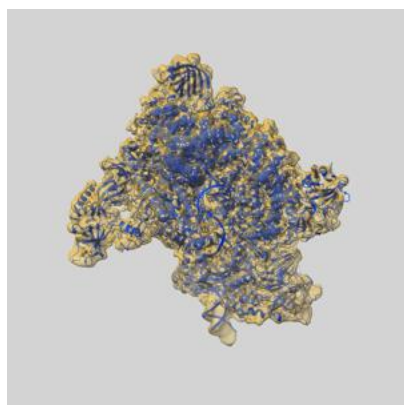
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	3.89	4.56	3.97
Unmasked-calculated*	-	-	-

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

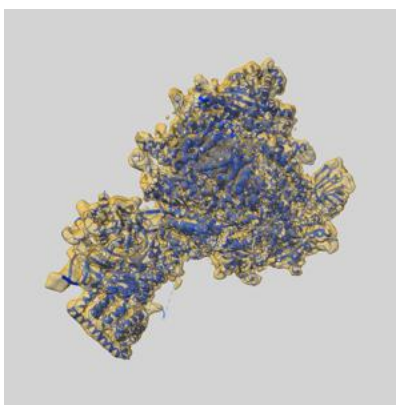
9 Map-model fit [i](#)

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](#).

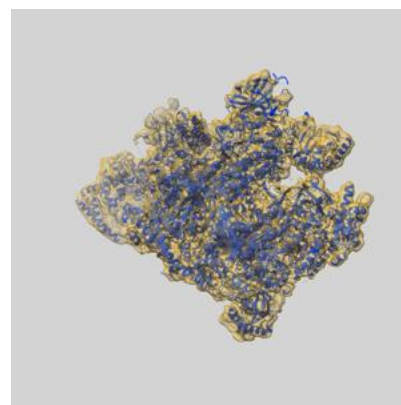
9.1 Map-model overlay [i](#)



X



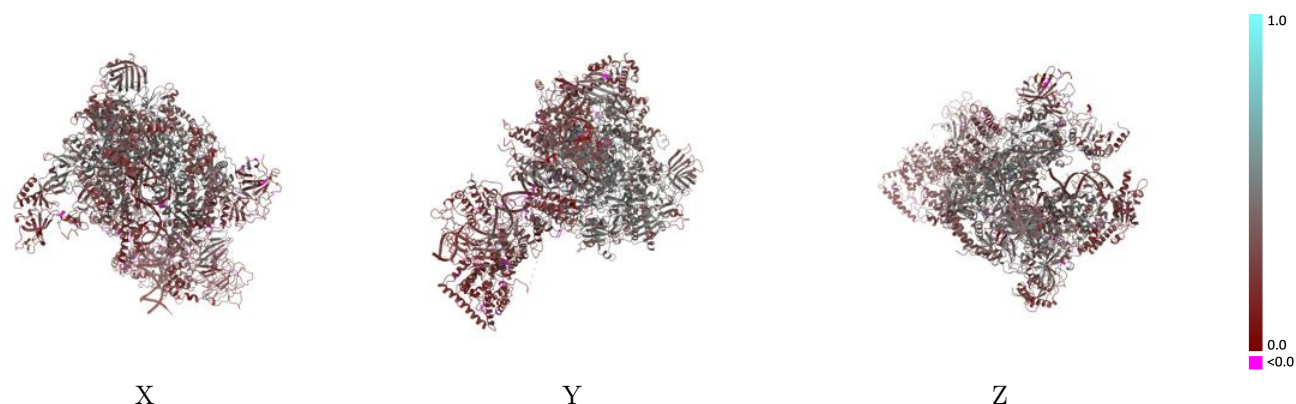
Y



Z

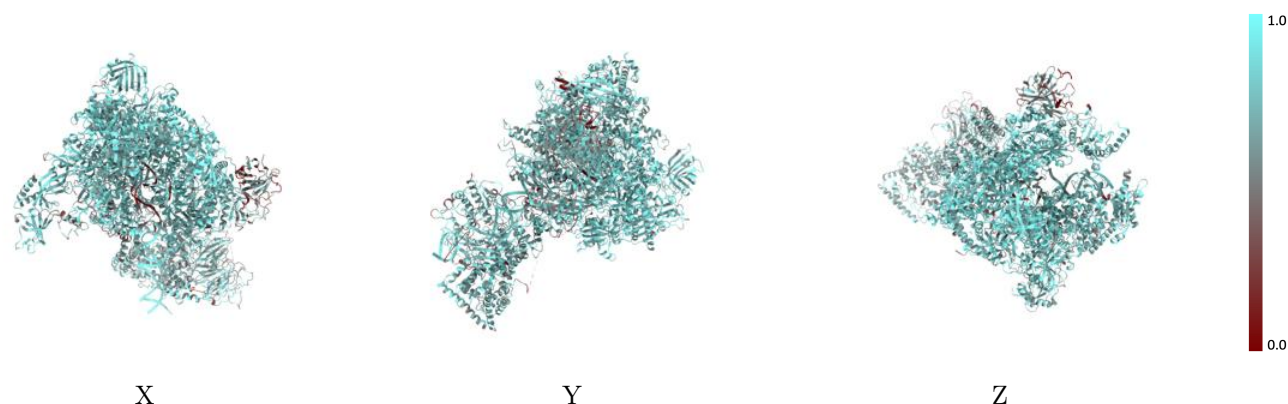
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



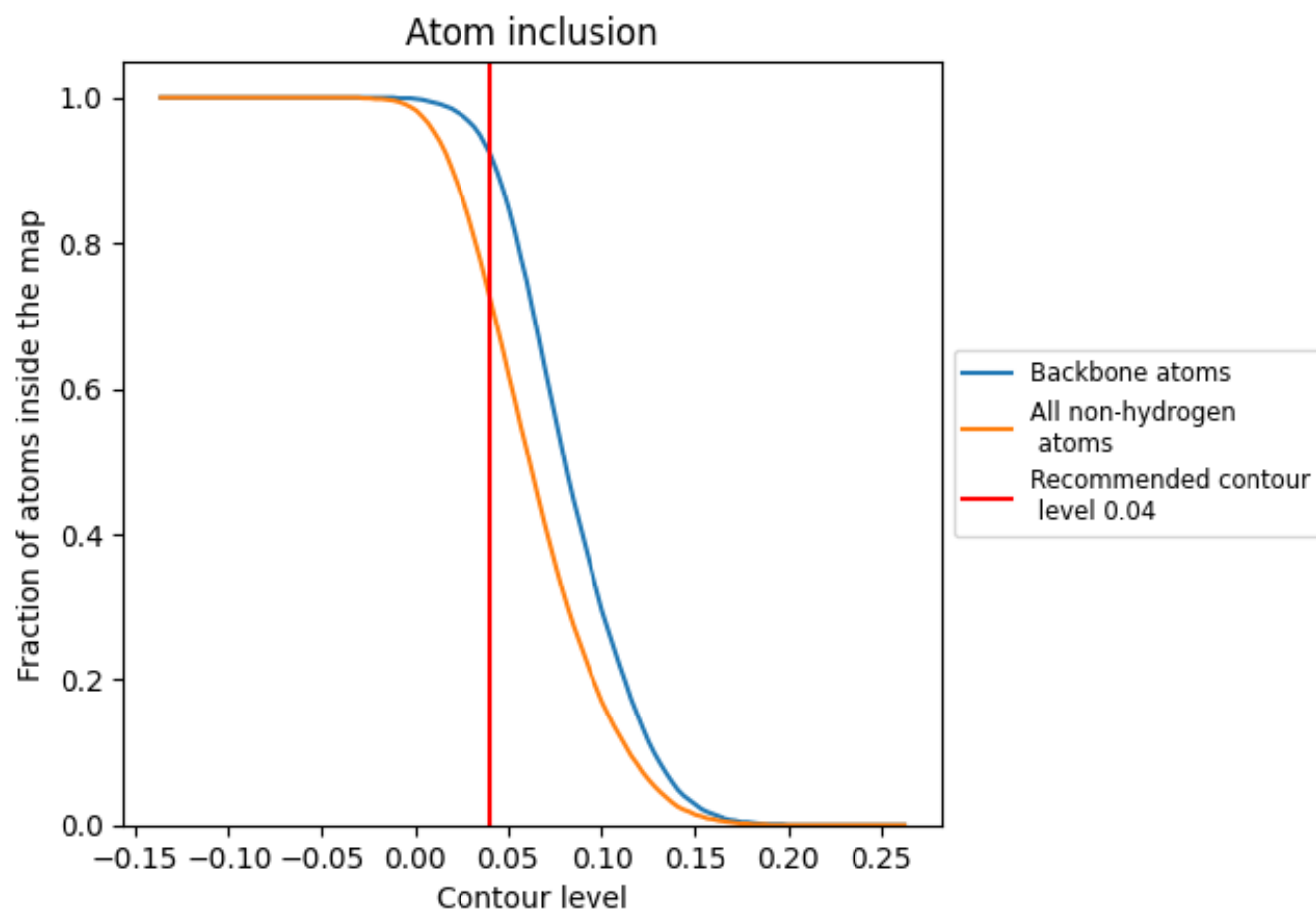
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.7280	 0.3360
A	 0.7790	 0.3860
B	 0.7960	 0.4230
C	 0.8230	 0.4070
D	 0.6870	 0.2640
E	 0.7660	 0.3280
F	 0.8210	 0.4130
G	 0.7170	 0.2790
H	 0.7950	 0.3690
I	 0.7000	 0.3270
J	 0.8440	 0.4440
K	 0.7700	 0.3980
L	 0.8090	 0.4350
M	 0.5360	 0.2680
N	 0.4700	 0.2770
O	 0.6650	 0.2350
P	 0.5810	 0.1930
Q	 0.6560	 0.2550
R	 0.1180	 0.1490
S	 0.7560	 0.2550
T	 0.6540	 0.2300

