



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:36 AM UTC

PDB ID : 7ML2 / pdb_00007ml2
EMDB ID : EMD-23906
Title : RNA polymerase II pre-initiation complex (PIC3)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 3.40 Å(reported)
Based on initial model : 5OQJ

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:

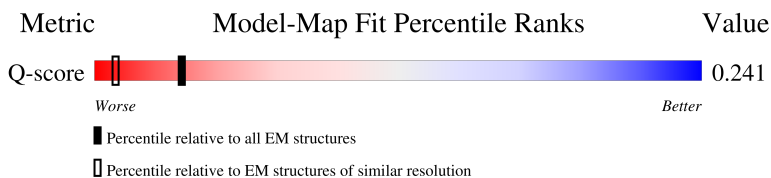
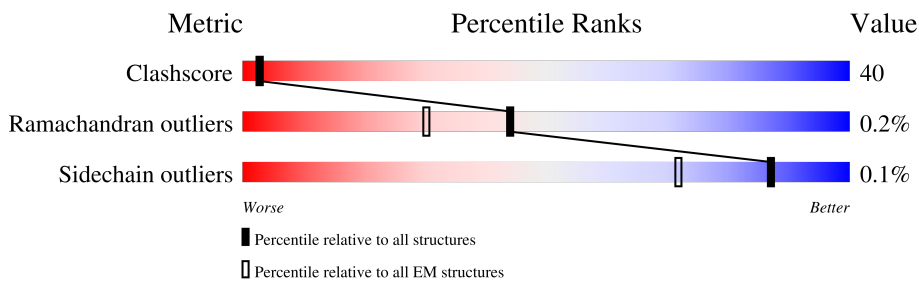
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1733	<p>34% 46% 19%</p>
2	B	1224	<p>43% 51% 6%</p>
3	C	318	<p>33% 49% 18%</p>
4	D	221	<p>19% 57% 52% 29%</p>


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Mol	Chain	Length	Quality of chain
5	E	215	41% 58%
6	F	155	18% 35% 46%
7	G	171	26% 74%
8	H	146	10% 22% 70% 7%
9	I	122	21% 30% 65% 5%
10	J	70	23% 66% 7%
11	K	120	13% 32% 60% 7%
12	L	70	16% 19% 37% 9%
13	M	345	24% 25% 55% 19%
14	Q	735	8% 12% 80%
15	R	400	13% 26% 22% 52%
16	U	286	16% 7% 9% 84%
17	V	122	36% 14% 26% 60%
18	W	482	23% 19% 21% 60%
19	X	328	20% 33% 14% 52%
20	T	56	14% 39% 61%
21	N	56	18% 27% 73%
22	O	240	10% 35% 40% 25%
23	1	542	23% 42% 25% 32%
24	4	338	11% 42% 42% 16%
25	0	778	27% 36% 60%
26	6	461	13% 35% 41% 24%
27	2	513	24% 50% 40% 10%
28	5	72	33% 35% 57% 8%
29	7	843	28% 31% 43% 25%

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Mol	Chain	Length	Quality of chain
30	3	321	

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
33	SF4	0	801	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 64550 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10997	6931	1927	2078	61	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1152	9178	5807	1608	1708	55	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

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

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1340	861	222	249	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	136	1089	686	184	215	4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	944	581	172	181	10	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	65	532	339	93	94	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	112	904	580	154	168	2	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

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

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	279	2175	1382	373	403	17	0	0

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	46	Total	C	N	O	S	0	0
			383	242	67	71	3		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	49	Total	C	N	O	S	0	0
			381	241	63	74	3		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	56	Total	C	N	O	P	0	0
			1140	550	188	346	56		

- Molecule 21 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	N	56	1156	552	222	326	56	0	0

- Molecule 22 is a protein called BJ4_G0004860.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	180	1416	921	242	247	6	0	0

- Molecule 23 is a protein called Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	1	367	2411	1536	438	430	7	0	0

- Molecule 24 is a protein called Tfb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	4	284	2041	1310	343	376	12	0	0

- Molecule 25 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	754	6108	3891	1032	1147	38	0	0

- Molecule 26 is a protein called General transcription and DNA repair factor IIIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	6	351	2527	1590	454	456	27	0	0

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	2	460	3011	1856	562	584	9	0	0

- Molecule 28 is a protein called General transcription and DNA repair factor IIIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 30 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

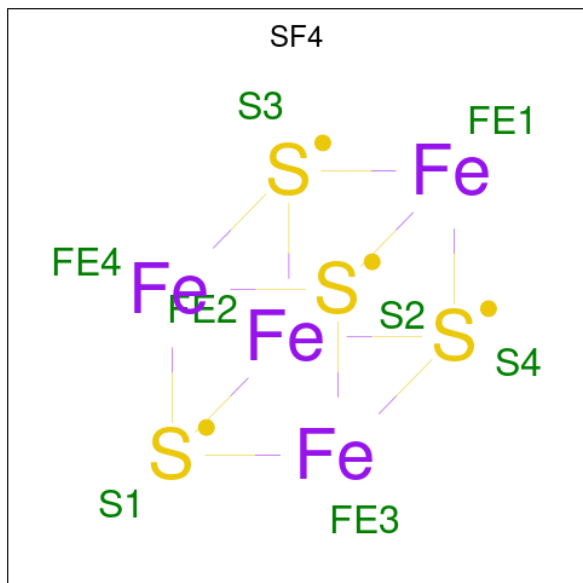
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	W	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	
31	3	2	Total	Zn	0
			2	2	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Mg	0
			1	1	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

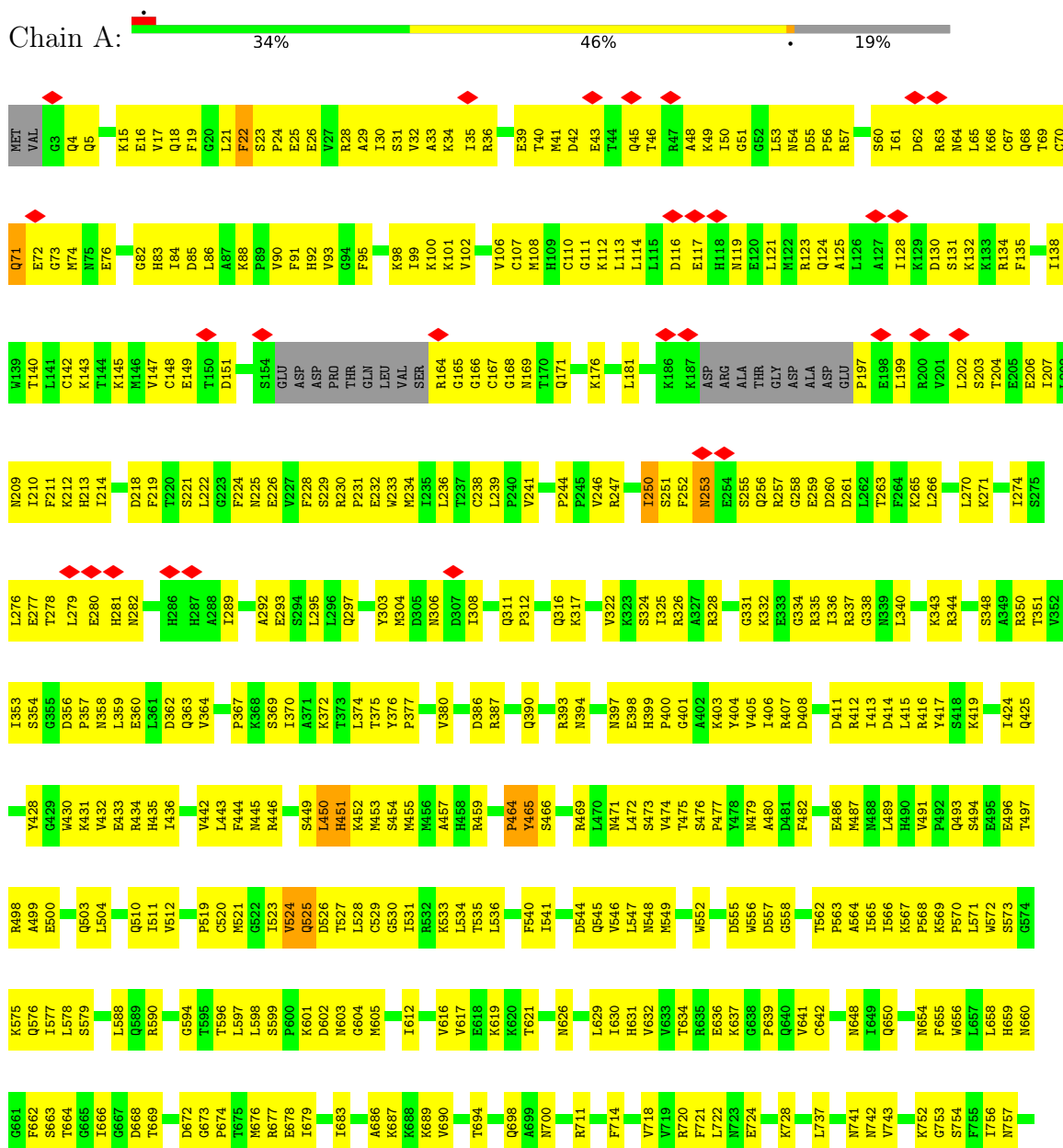


Mol	Chain	Residues	Atoms			AltConf
33	0	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots i

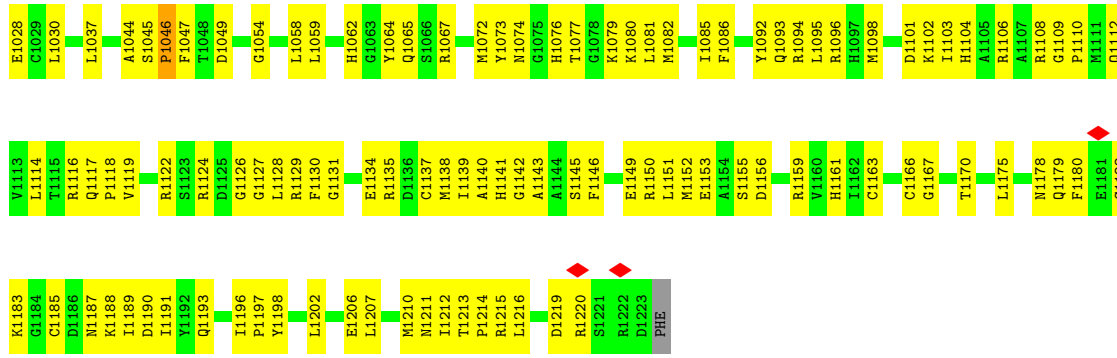
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

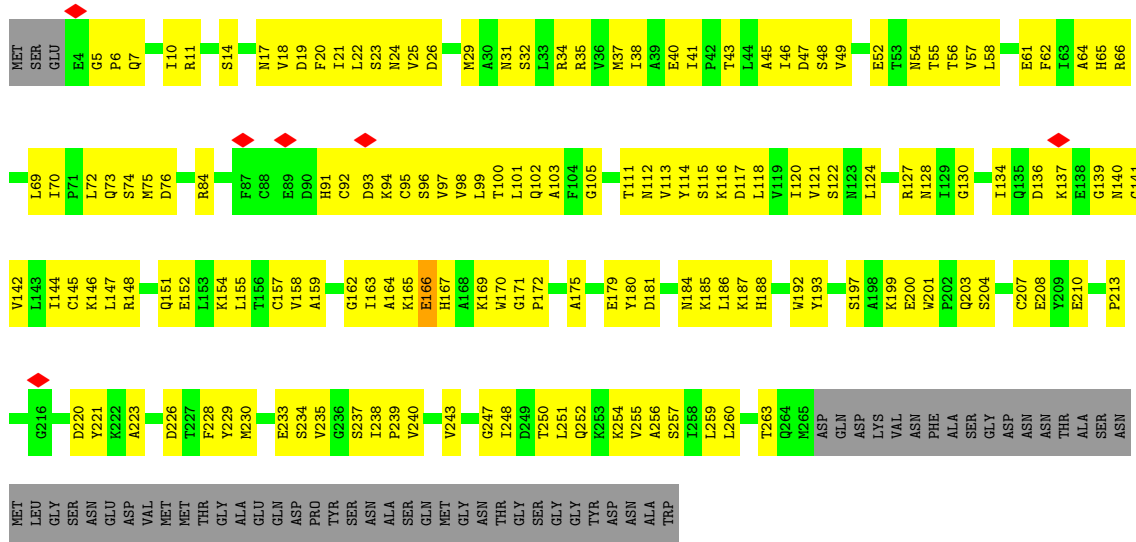




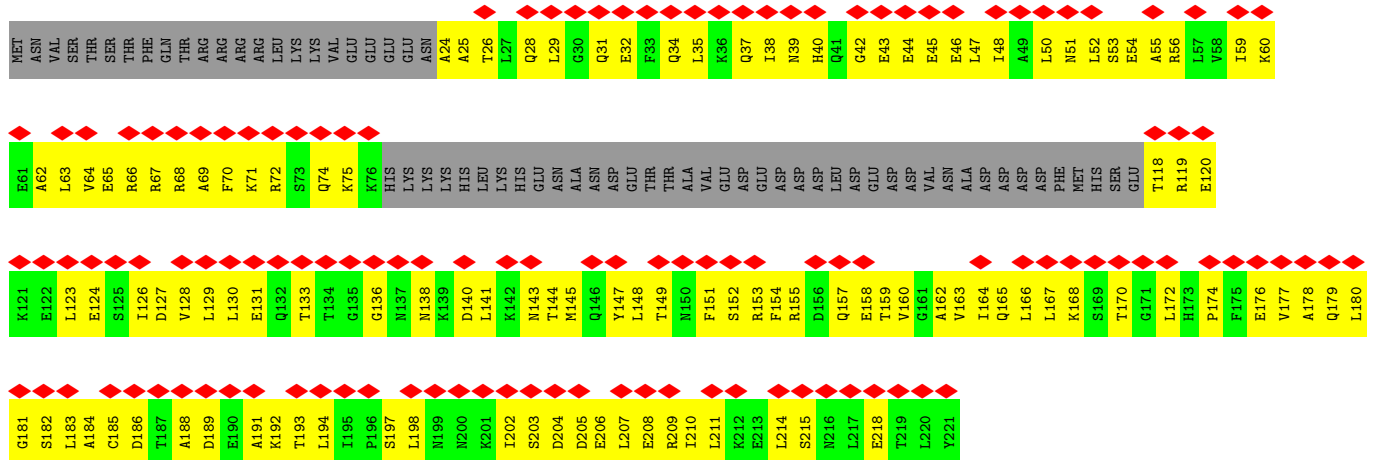
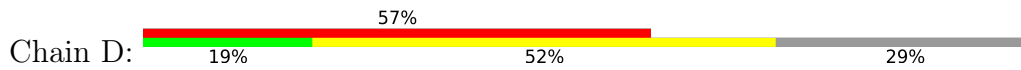
MET	SER	ASP	LEU	ALA	ASN	SER	GLU	LYS	TYR	ASN	GLU	ASP	PRO	TYR	GLY	PHE	D20	E21	S22	A23	P24	Y96	L25	T26	
Q73	L74	A75	HIS	THR	THR	GLU	SER	ASP	ASN	TRP	S84	S85	R86	R87	R88	R89	G93	R94	R95	A23	Y96	Y97	T98	R99	
ALA	ILE	ASP	VAL	GLY	ARG	GLU	L147	K148	L149	E150	L151	ILE	ALA	GLU	GLU	SER	GLU	ASP	ASP	GLU	SER	G163	R169	P170	
V211	L212	I213	A214	Q215	R216	R217	S218	A219	I222	L223	A230	P231	S232	P233	I234	S235	H236	V237	A238	R241	L244	E245	P100	P171	
F286	R287	I292	P293	D294	C295	E296	L297	E299	H300	I301	C302	Y303	D304	Y305	M306	Q309	M310	L311	G312	M313	L314	V318	L170	P171	
I385	E389	L361	P362	H363	L364	T365	L367	F370	E371	S372	R373	K374	A375	F376	F377	L378	G379	Y380	R384	L385	L386	A389	D320	G321	
A439	M443	K444	K445	I448	K451	T454	L457	K488	A460	G467	GLN	LYS	LYS	ALA	S474	S475	V479	S480	Q481	V482	M484	R485	L406	L407	
B511	R512	Q513	M516	T517	H518	M519	G520	V521	G523	P524	Q531	M532	C533	M538	L539	S540	L541	I545	D550	P551	M552	P553	I554	F557	
L600	R604	I609	M610	P611	V612	V613	S614	M615	I616	R617	D618	D619	I620	E621	K622	E623	I626	T628	D629	A630	G631	R632	V633	I634	
Q667	D668	ILE	GLU	GLY	PHE	GLU	D675	V676	Y679	T680	W681	L684	L689	V690	E691	Y692	I693	D694	E697	E698	E699	S700	I701	L702	
A735	T736	G738	T739	H740	P745	I748	L749	A753	S754	I755	I756	P757	F758	P759	D760	H761	I693	D694	E697	E698	E699	S700	I701	L702	
R815	E816	Q821	I824	V825	A826	I827	A828	C829	Y830	S831	C832	Y833	M834	Q835	E836	D837	S838	M839	I840	M841	N842	Q843	S844	S845	
K866	H867	G888	T889	Y890	D891	K892	L893	D894	A895	F896	C897	L898	G899	S900	R904	V905	S906	G907	E908	H909	D909	M910	Q911	I912	T915
Q951	V952	L953	T956	L961	K962	F963	V964	K965	L966	R967	T976	F980	A981	S982	R983	H984	G988	I989	G991	I992	T993	Y994	R995	R996	
V1007	P1008	D1009	L1010	I1011	I1012	P1014	H1015	A1016	I1017	P1018	S1019	I1020	M1021	T1022	P1023	A1024	V1007	Q927	R928	T929	A930	Y931	H932	S933	
E1004	G926	Q927	R928	T929	A930	Y931	H932	S933	K934	R935	D936	A937	S938	T939	R940	L941	R942	S943	T944	E945	N946	V1007	Q927	R928	
V1007	P1008	D1009	L1010	I1011	I1012	P1014	H1015	A1016	I1017	P1018	S1019	I1020	M1021	T1022	P1023	A1024	V1007	Q927	R928	T929	A930	Y931	H932	S933	



• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



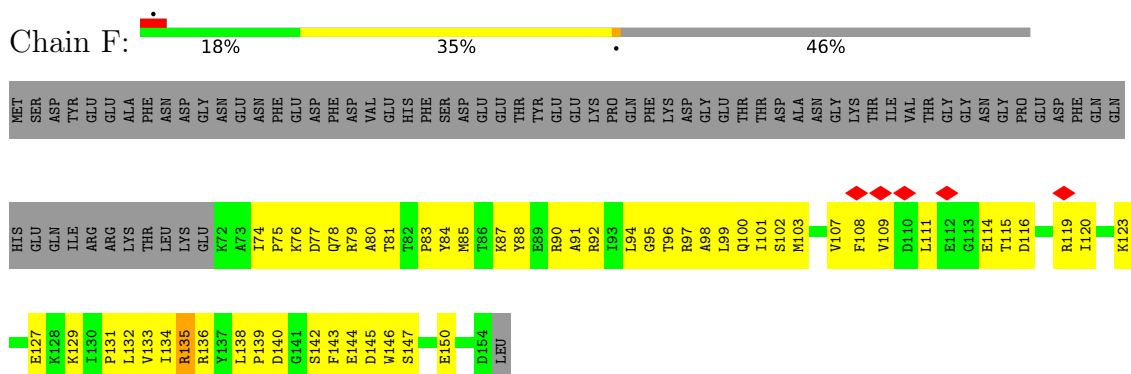
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



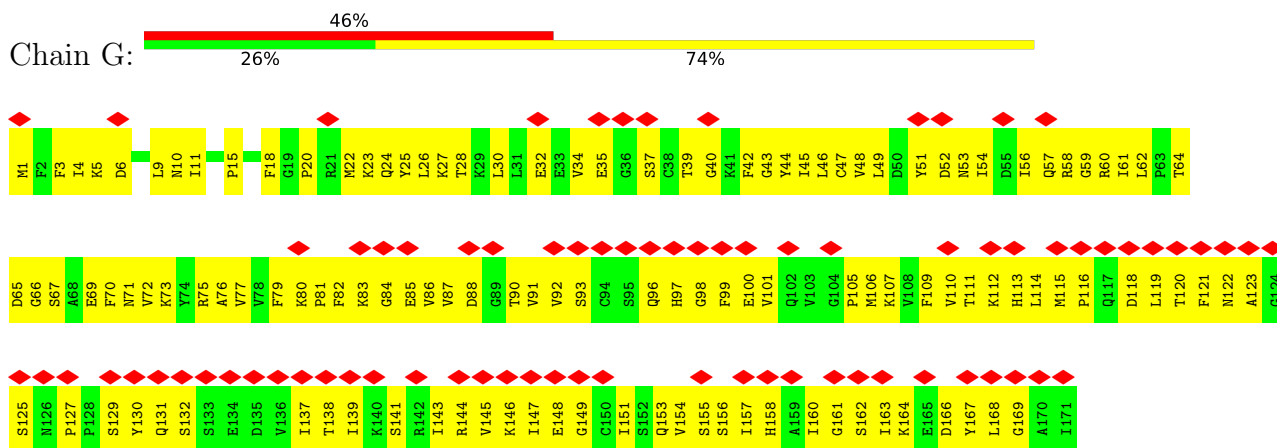
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

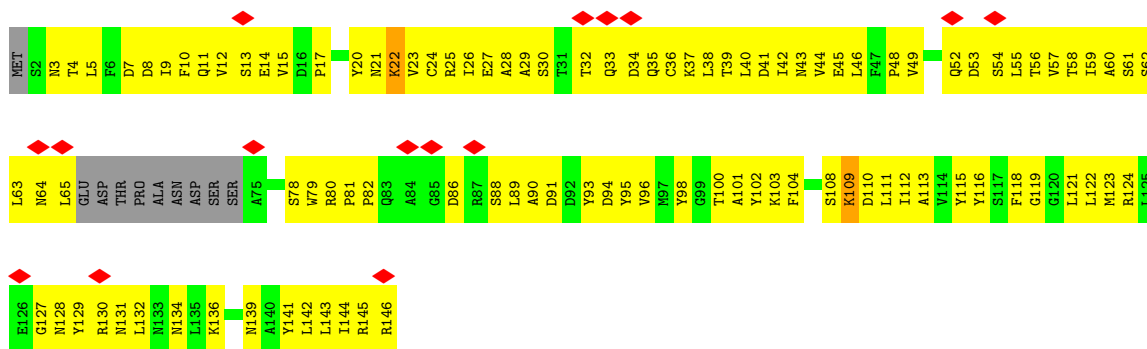


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

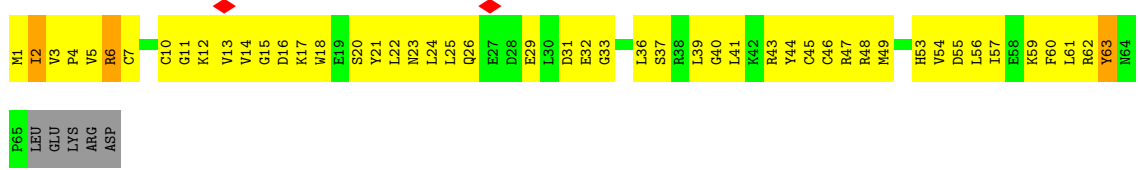




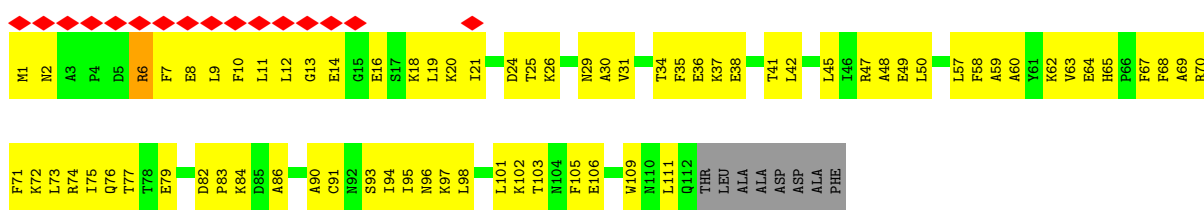
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



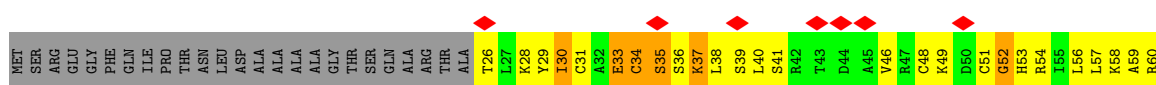
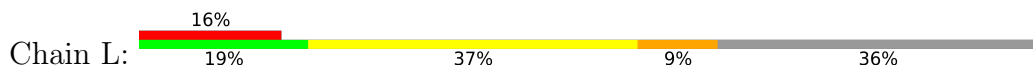
• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

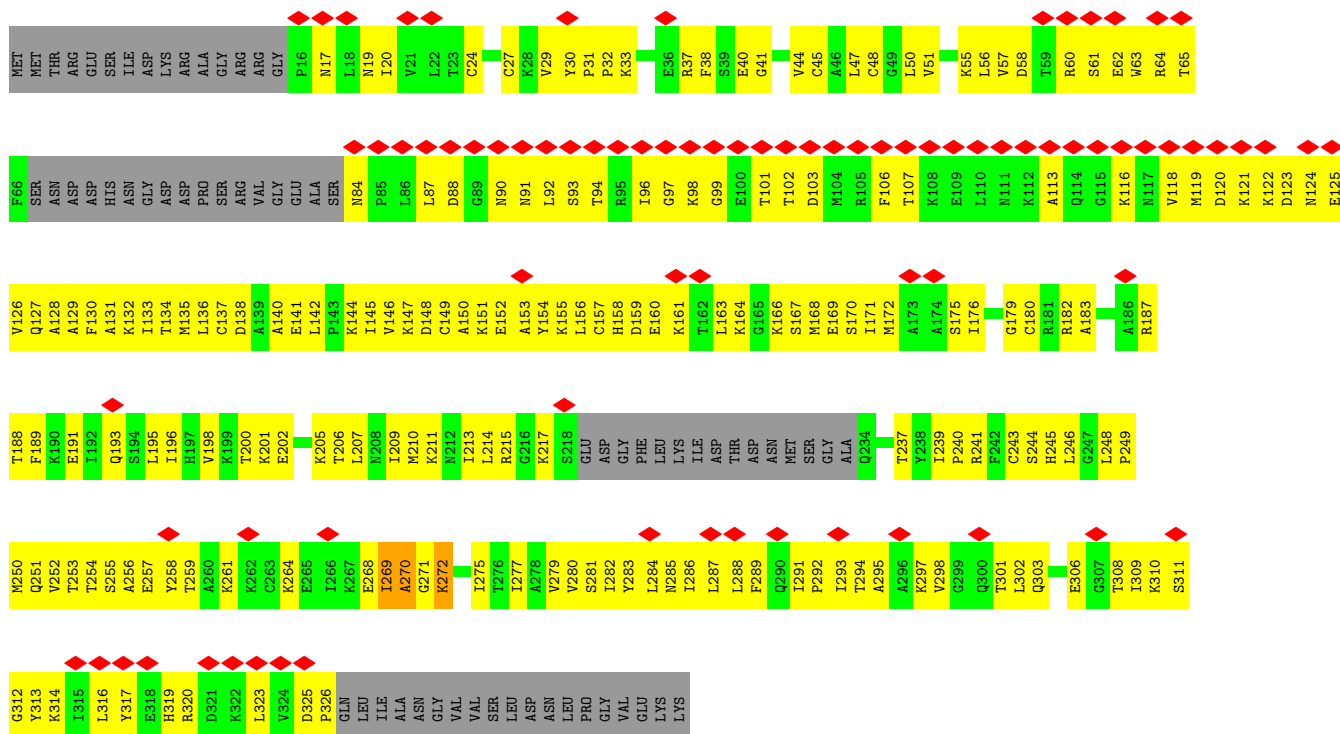


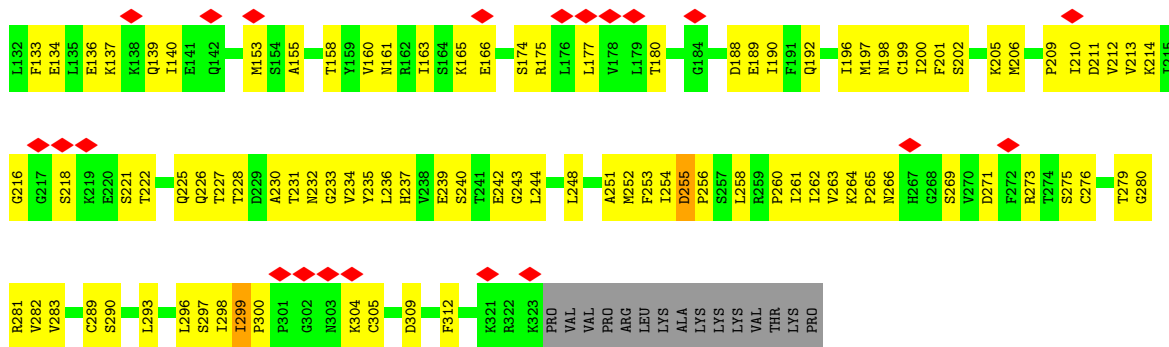
• Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



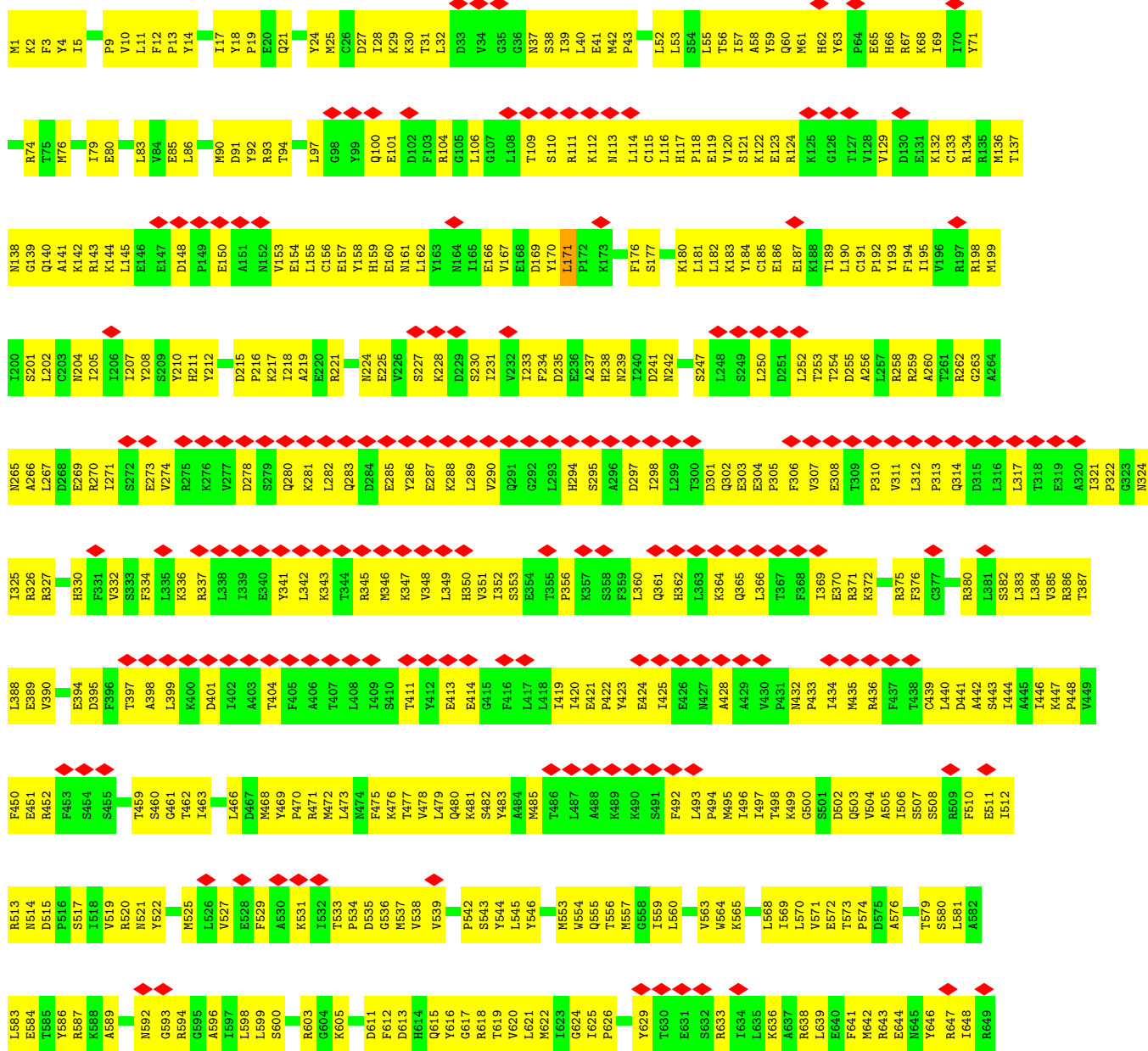


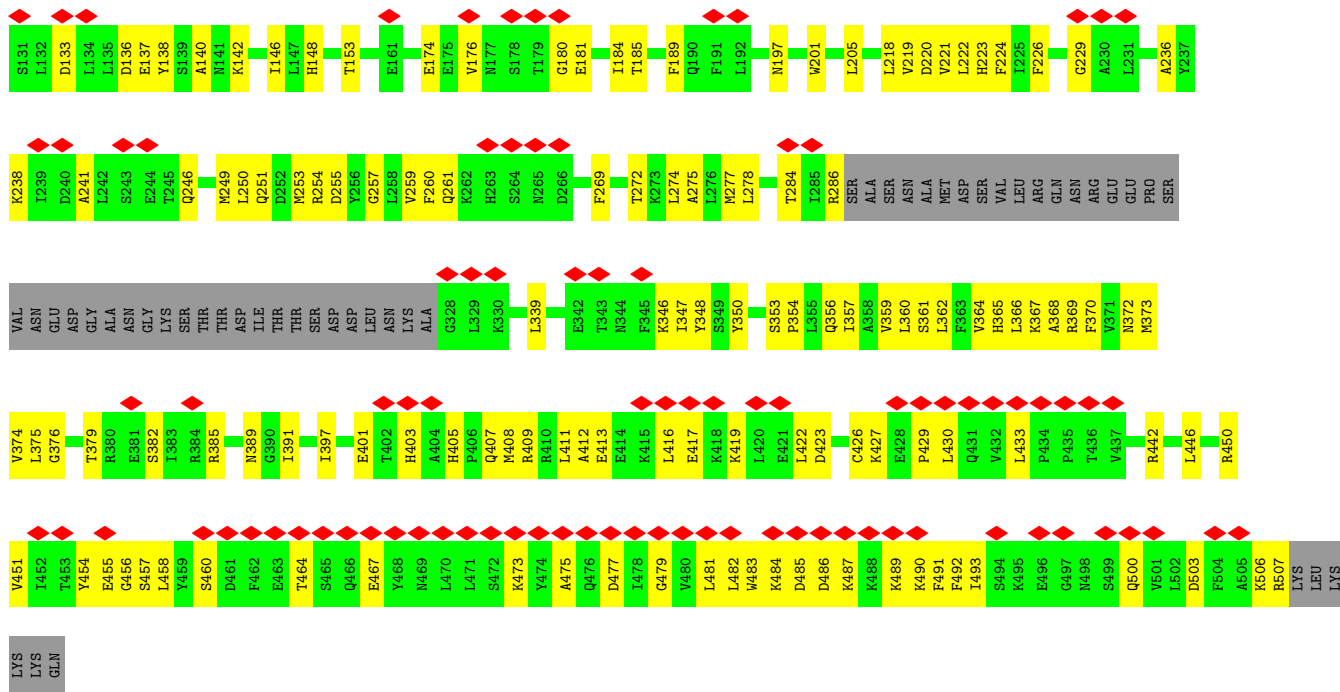
• Molecule 13: Transcription initiation factor IIB



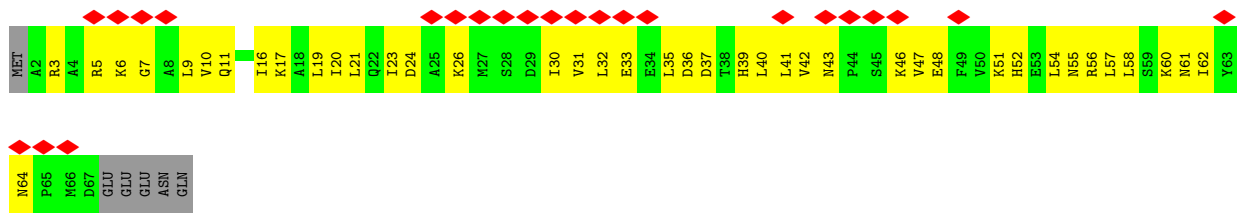
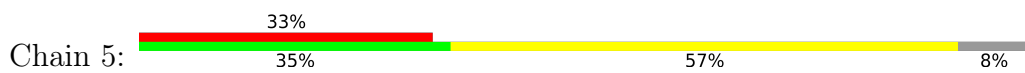


• Molecule 25: General transcription and DNA repair factor IIH helicase subunit XPD





• Molecule 28: General transcription and DNA repair factor IIIH subunit TFB5



LEU
THR
GLU
ALA
PHE
MET
GLY
LEU
GLY
CYS
VAL
ILE
SER
GLU
GLU
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69513	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	474.87997, 501.37997, 473.81998	wwPDB
Map dimensions	448, 473, 447	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: SF4, MG, 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	0.46	1/11192 (0.0%)	0.71	8/15128 (0.1%)
2	B	0.48	1/9357 (0.0%)	0.70	1/12618 (0.0%)
3	C	0.53	1/2099 (0.0%)	0.76	0/2845
4	D	0.31	0/1262	0.65	0/1693
5	E	0.41	0/1780	0.69	0/2395
6	F	0.59	1/682 (0.1%)	0.89	0/922
7	G	0.32	0/1368	0.62	0/1844
8	H	0.47	0/1107	0.79	0/1499
9	I	0.40	0/962	0.83	0/1295
10	J	0.55	0/541	1.03	3/727 (0.4%)
11	K	0.53	0/922	0.88	2/1244 (0.2%)
12	L	0.39	0/360	0.94	0/478
13	M	0.32	0/2204	0.69	0/2963
14	Q	0.26	0/1168	0.52	0/1579
15	R	0.24	0/1312	0.51	0/1777
16	U	0.16	0/389	0.47	0/523
17	V	0.18	0/384	0.39	0/518
18	W	0.21	0/1490	0.47	0/2014
19	X	0.17	0/993	0.47	0/1357
20	T	0.41	0/1273	0.55	0/1962
21	N	0.42	0/1301	0.60	0/2006
22	O	0.24	0/1443	0.49	0/1942
23	1	0.20	0/1896	0.48	0/2543
24	4	0.26	0/2062	0.58	0/2805
25	0	0.26	0/6226	0.57	1/8407 (0.0%)
26	6	0.25	0/2506	0.56	0/3402
27	2	0.23	0/3057	0.53	1/4071 (0.0%)
28	5	0.23	0/502	0.53	0/677
29	7	0.32	0/4521	0.67	4/6036 (0.1%)
30	3	0.49	1/870 (0.1%)	0.71	2/1190 (0.2%)
All	All	0.38	5/65229 (0.0%)	0.65	22/88460 (0.0%)

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	7
2	B	0	4
8	H	0	3
9	I	0	1
10	J	0	1
13	M	0	3
18	W	0	1
19	X	0	1
24	4	0	2
25	0	0	2
26	6	0	1
29	7	0	8
30	3	0	2
All	All	0	36

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	61	LYS	CE-NZ	-6.75	1.29	1.49
1	A	1074	GLU	CD-OE2	-5.86	1.14	1.25
6	F	135	ARG	CA-CB	-5.54	1.39	1.53
3	C	166	GLU	CA-CB	-5.31	1.44	1.53
2	B	112	LEU	C-N	-5.14	1.23	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	501	VAL	N-CA-C	-11.57	101.38	112.83
27	2	70	GLY	N-CA-C	-8.83	103.97	114.48
10	J	63	TYR	CA-C-N	-8.14	108.93	120.49
10	J	63	TYR	C-N-CA	-8.14	108.93	120.49
10	J	6	ARG	N-CA-C	7.68	121.11	110.35

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	250	ILE	Peptide
1	A	450	LEU	Peptide
1	A	465	TYR	Peptide
1	A	71	GLN	Peptide

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	10997	0	11081	837	0
2	B	9178	0	9195	650	0
3	C	2061	0	2029	162	0
4	D	1253	0	1275	133	0
5	E	1744	0	1772	126	0
6	F	670	0	690	66	0
7	G	1340	0	1357	138	0
8	H	1089	0	1062	129	0
9	I	944	0	899	106	0
10	J	532	0	542	65	0
11	K	904	0	911	93	0
12	L	358	0	383	39	0
13	M	2175	0	2283	231	0
14	Q	1144	0	1034	115	0
15	R	1303	0	1110	125	0
16	U	383	0	384	25	0
17	V	381	0	388	35	0
18	W	1469	0	1432	112	0
19	X	984	0	722	60	0
20	T	1140	0	641	73	0
21	N	1156	0	631	87	0
22	O	1416	0	1493	105	0
23	1	2411	0	1881	126	0
24	4	2041	0	1954	147	0
25	0	6108	0	6168	577	0
26	6	2527	0	2321	226	0
27	2	3011	0	2600	229	0
28	5	498	0	506	59	0
29	7	4447	0	3905	498	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	860	0	623	103	0
31	3	2	0	0	0	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	W	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	3	0
All	All	64550	0	61272	5031	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 40.

The worst 5 of 5031 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)
12:L:48:CYS:SG	12:L:53:HIS:HB3	1.70	1.32
12:L:34:CYS:SG	12:L:36:SER:OG	1.98	1.18
2:B:649:LYS:NZ	2:B:736:THR:O	1.83	1.11
25:0:162:LEU:HD22	25:0:194:PHE:HB3	1.27	1.09
1:A:253:ASN:HA	2:B:935:ARG:HH12	1.17	1.07

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	1386/1733 (80%)	1192 (86%)	189 (14%)	5 (0%)	30	59
2	B	1136/1224 (93%)	987 (87%)	146 (13%)	3 (0%)	36	65
3	C	260/318 (82%)	214 (82%)	46 (18%)	0	100	100
4	D	153/221 (69%)	135 (88%)	18 (12%)	0	100	100
5	E	211/215 (98%)	193 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	69 (85%)	12 (15%)	0	100	100
7	G	169/171 (99%)	152 (90%)	17 (10%)	0	100	100
8	H	132/146 (90%)	106 (80%)	24 (18%)	2 (2%)	8	30
9	I	114/122 (93%)	94 (82%)	20 (18%)	0	100	100
10	J	63/70 (90%)	44 (70%)	19 (30%)	0	100	100
11	K	110/120 (92%)	95 (86%)	15 (14%)	0	100	100
12	L	43/70 (61%)	33 (77%)	7 (16%)	3 (7%)	1	6
13	M	273/345 (79%)	221 (81%)	52 (19%)	0	100	100
14	Q	140/735 (19%)	120 (86%)	20 (14%)	0	100	100
15	R	176/400 (44%)	163 (93%)	13 (7%)	0	100	100
16	U	44/286 (15%)	38 (86%)	6 (14%)	0	100	100
17	V	45/122 (37%)	44 (98%)	1 (2%)	0	100	100
18	W	189/482 (39%)	182 (96%)	7 (4%)	0	100	100
19	X	152/328 (46%)	136 (90%)	16 (10%)	0	100	100
22	O	178/240 (74%)	167 (94%)	11 (6%)	0	100	100
23	1	256/542 (47%)	234 (91%)	19 (7%)	3 (1%)	10	35
24	4	279/338 (82%)	222 (80%)	57 (20%)	0	100	100
25	0	752/778 (97%)	670 (89%)	82 (11%)	0	100	100
26	6	336/461 (73%)	298 (89%)	36 (11%)	2 (1%)	21	50
27	2	456/513 (89%)	390 (86%)	66 (14%)	0	100	100
28	5	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
29	7	630/843 (75%)	539 (86%)	90 (14%)	1 (0%)	43	71
30	3	136/321 (42%)	105 (77%)	31 (23%)	0	100	100
All	All	7964/11371 (70%)	6901 (87%)	1044 (13%)	19 (0%)	44	71

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
2	B	364	ILE
8	H	110	ASP
26	6	411	PRO
29	7	349	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1221/1520 (80%)	1221 (100%)	0	100	100
2	B	1000/1061 (94%)	1000 (100%)	0	100	100
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	11
13	M	245/299 (82%)	245 (100%)	0	100	100
14	Q	109/641 (17%)	109 (100%)	0	100	100
15	R	107/363 (30%)	107 (100%)	0	100	100
16	U	42/260 (16%)	42 (100%)	0	100	100
17	V	46/108 (43%)	46 (100%)	0	100	100
18	W	155/429 (36%)	155 (100%)	0	100	100
19	X	62/295 (21%)	62 (100%)	0	100	100
22	O	152/205 (74%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1	169/395 (43%)	169 (100%)	0	100	100
24	4	198/298 (66%)	198 (100%)	0	100	100
25	0	686/707 (97%)	686 (100%)	0	100	100
26	6	247/406 (61%)	247 (100%)	0	100	100
27	2	258/468 (55%)	258 (100%)	0	100	100
28	5	53/66 (80%)	53 (100%)	0	100	100
29	7	414/737 (56%)	414 (100%)	0	100	100
30	3	53/303 (18%)	53 (100%)	0	100	100
All	All	6432/9989 (64%)	6426 (100%)	6 (0%)	87	89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	35	SER
12	L	38	LEU
12	L	40	LEU
12	L	33	GLU
12	L	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
25	0	224	ASN
27	2	500	GLN
25	0	699	GLN
26	6	249	GLN
29	7	589	GLN

5.3.3 RNA [i](#)

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 19 ligands modelled in this entry, 18 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
33	SF4	0	801	25	0,12,12	-	-	-		

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
33	SF4	0	801	25	-	-	0/6/5/5

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	3	0

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
23	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.96
1	1	519:UNK	C	537:GLU	N	11.53
1	1	355:UNK	C	368:UNK	N	10.44

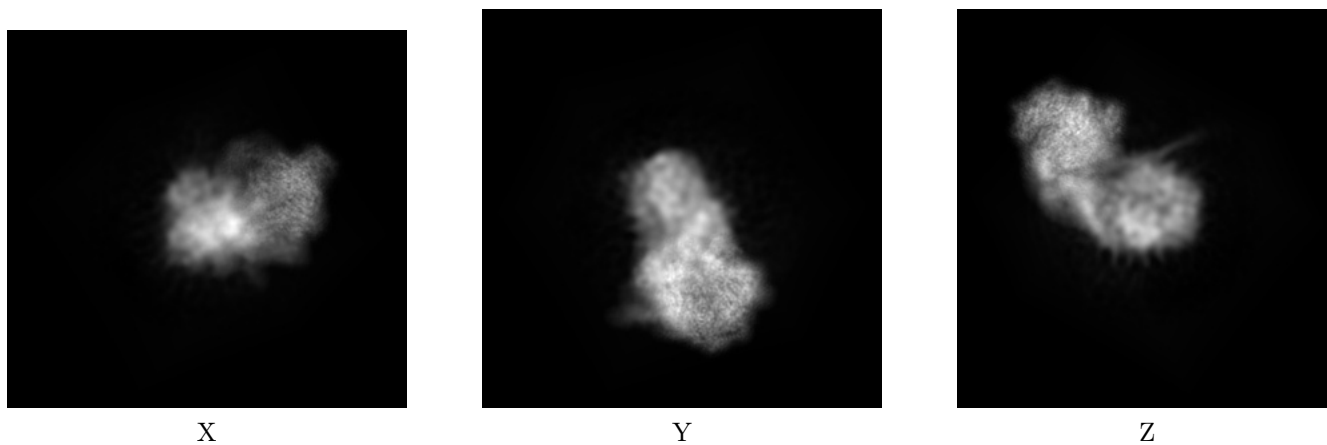
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23906. 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](#)

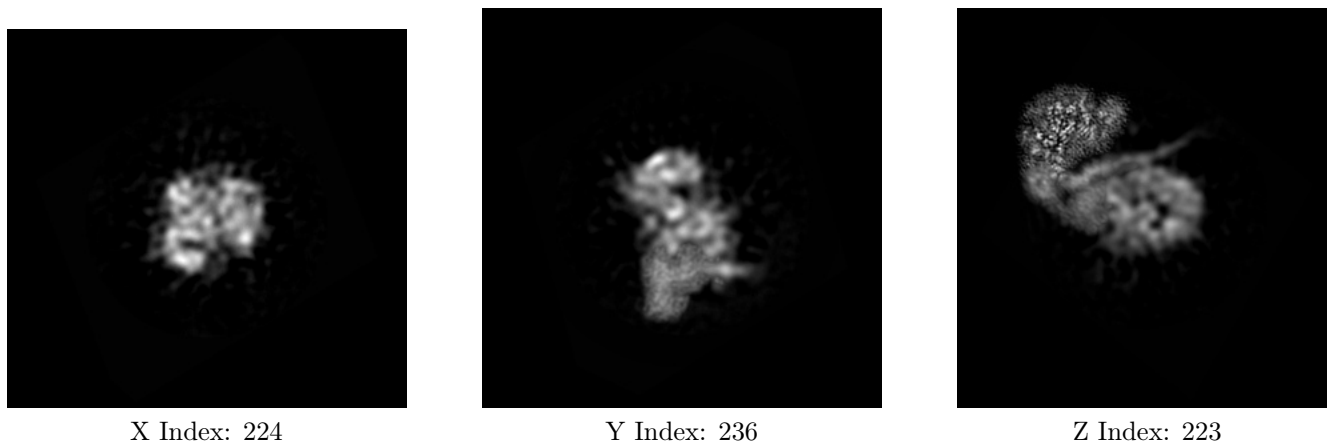
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



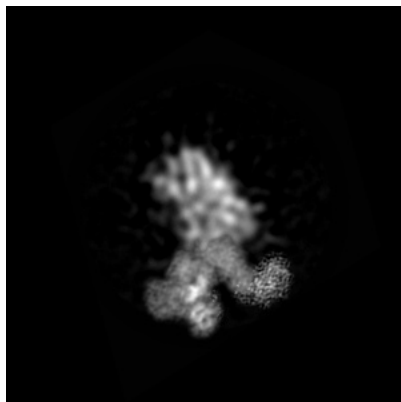
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

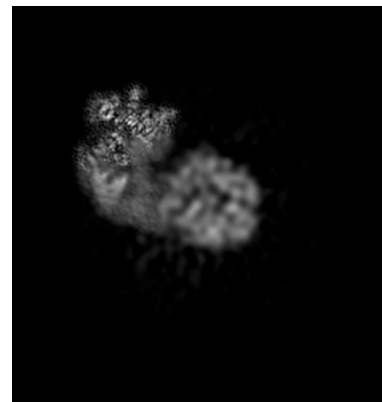
6.3.1 Primary map



X Index: 152



Y Index: 263

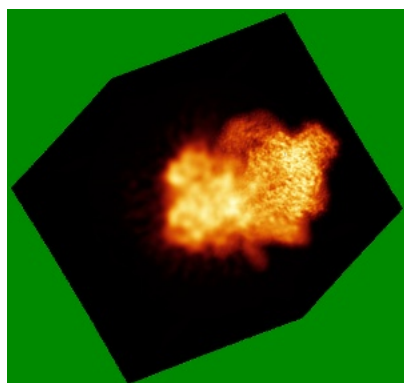


Z Index: 210

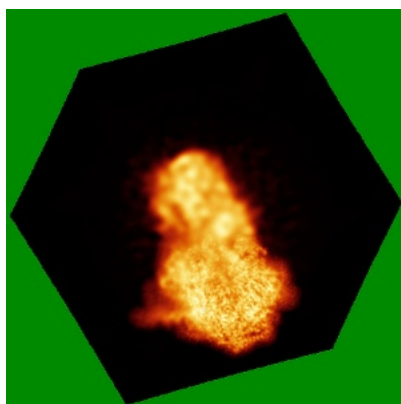
The images above show the largest variance slices of the map in three orthogonal directions.

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

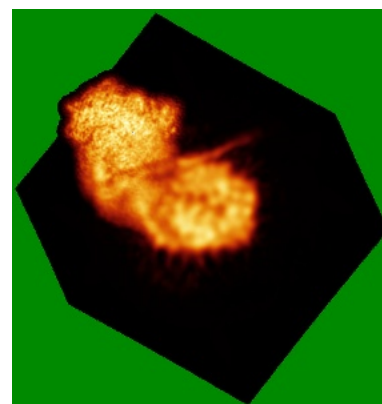
6.4.1 Primary map



X



Y

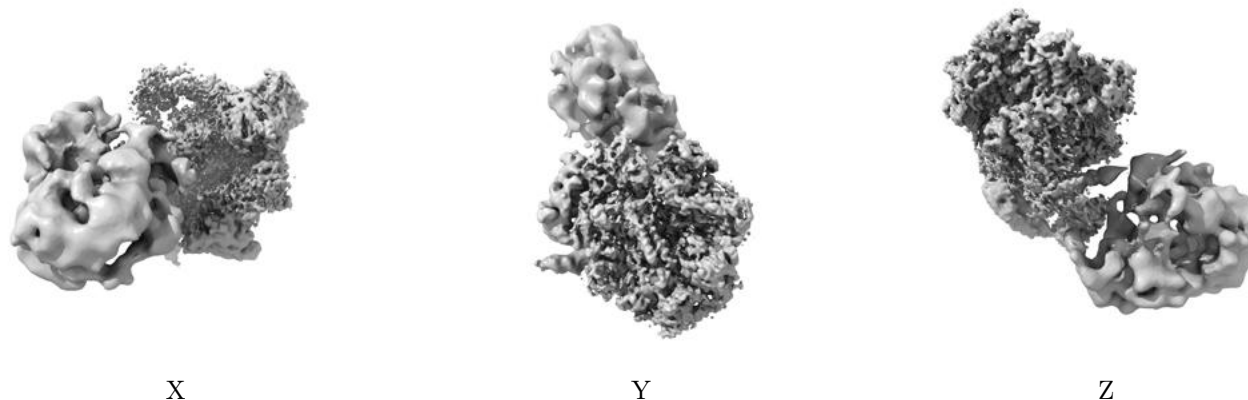


Z

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

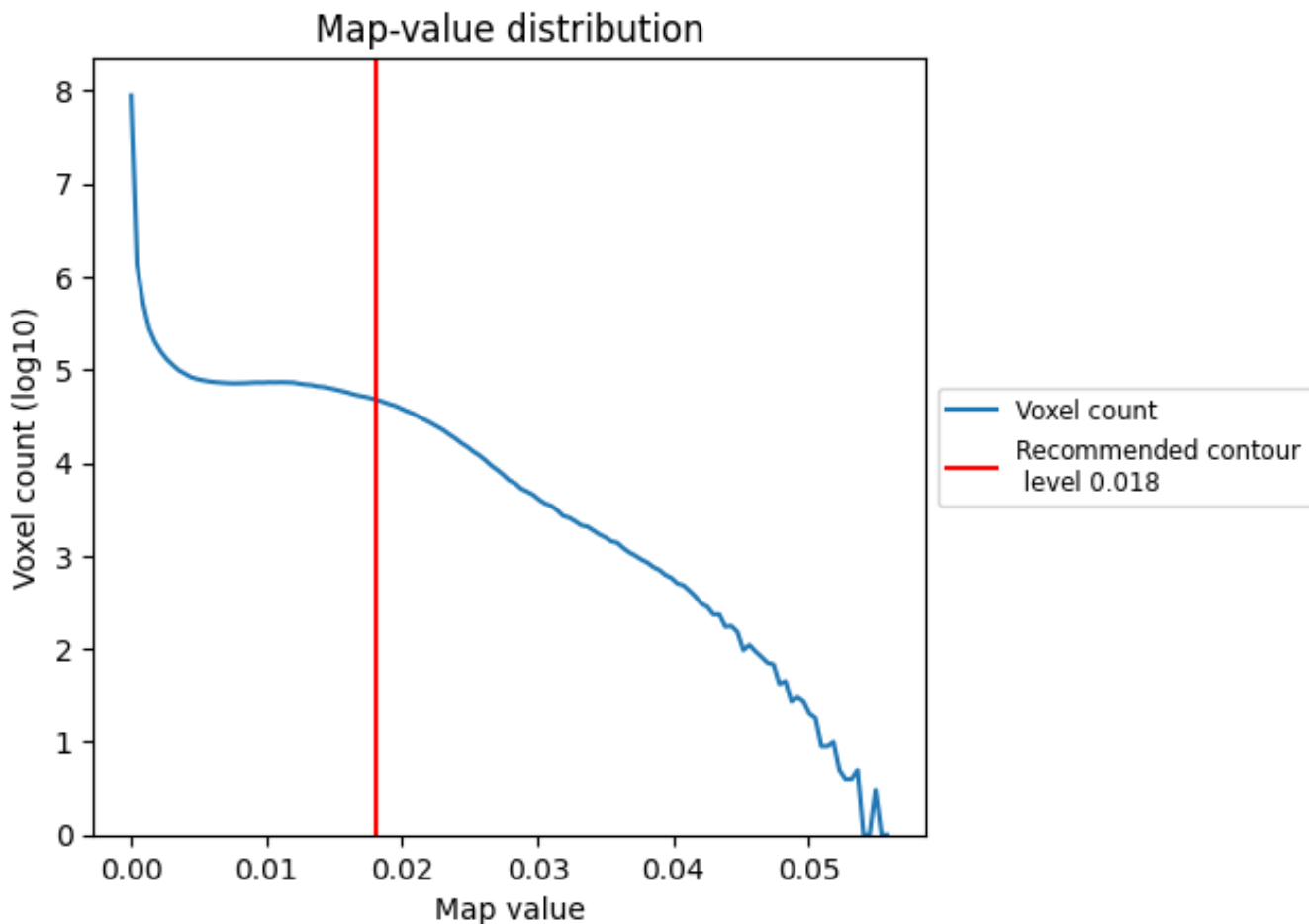
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

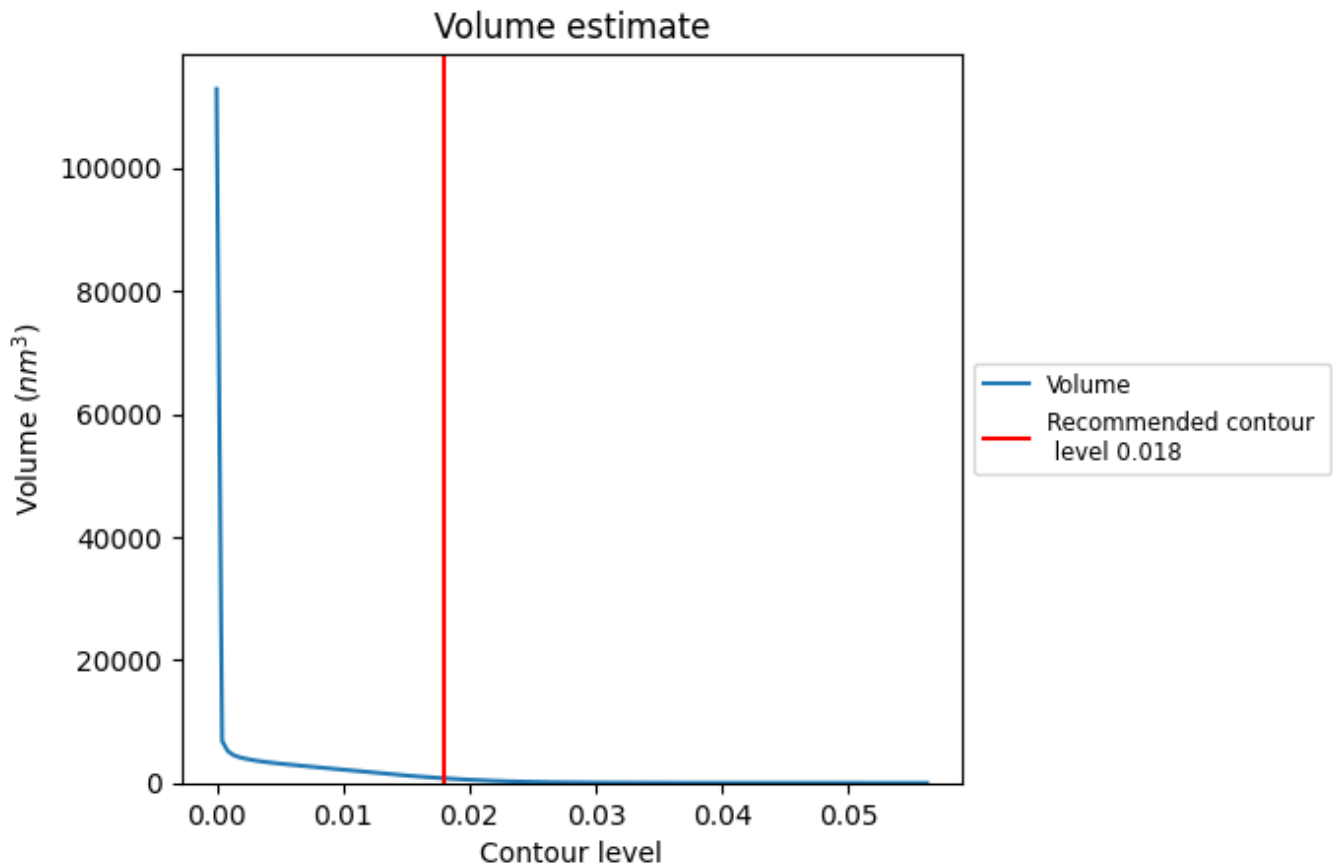
This section contains the results of statistical analysis of the map.

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 762 nm^3 ; this corresponds to an approximate mass of 688 kDa.

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

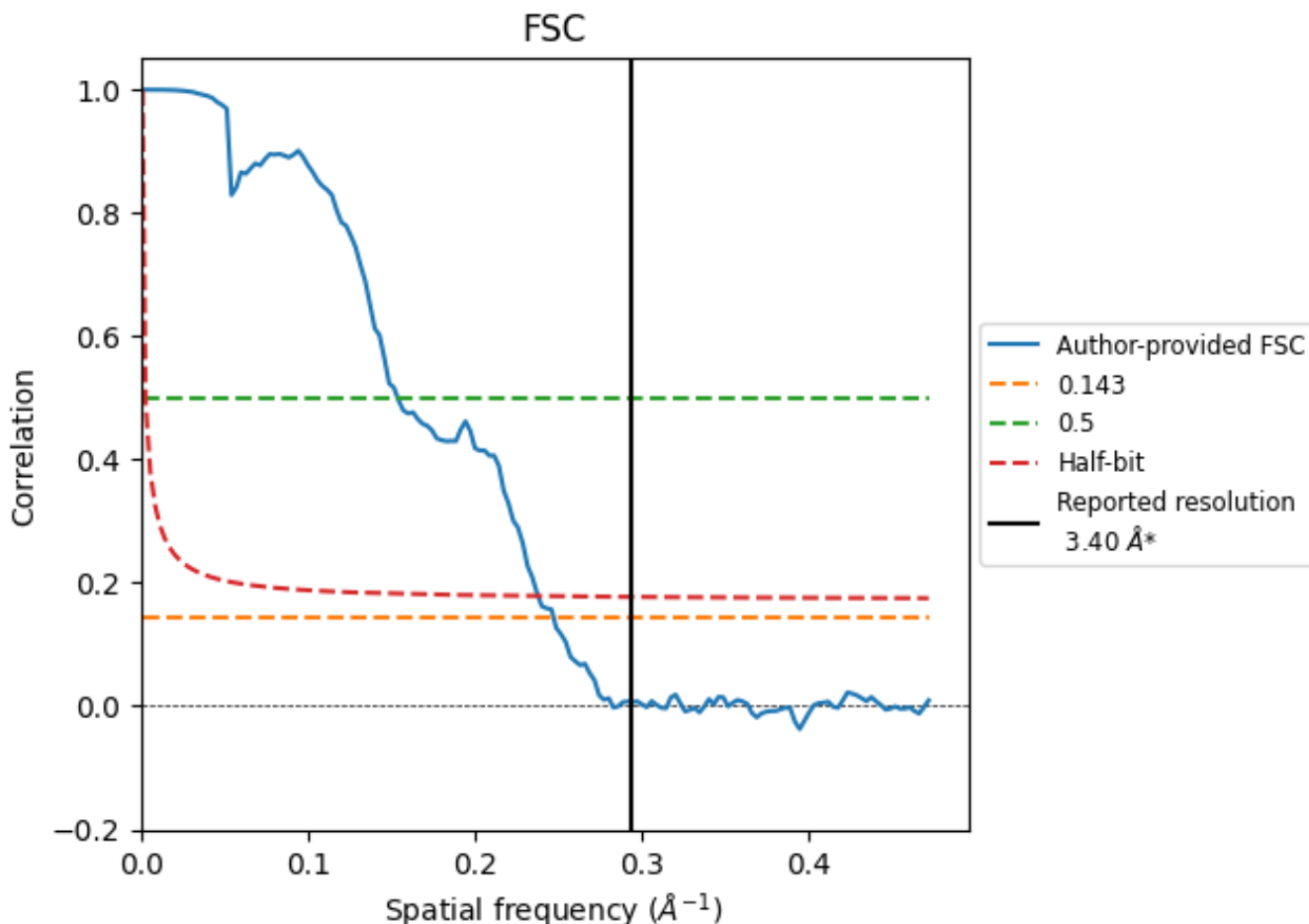
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

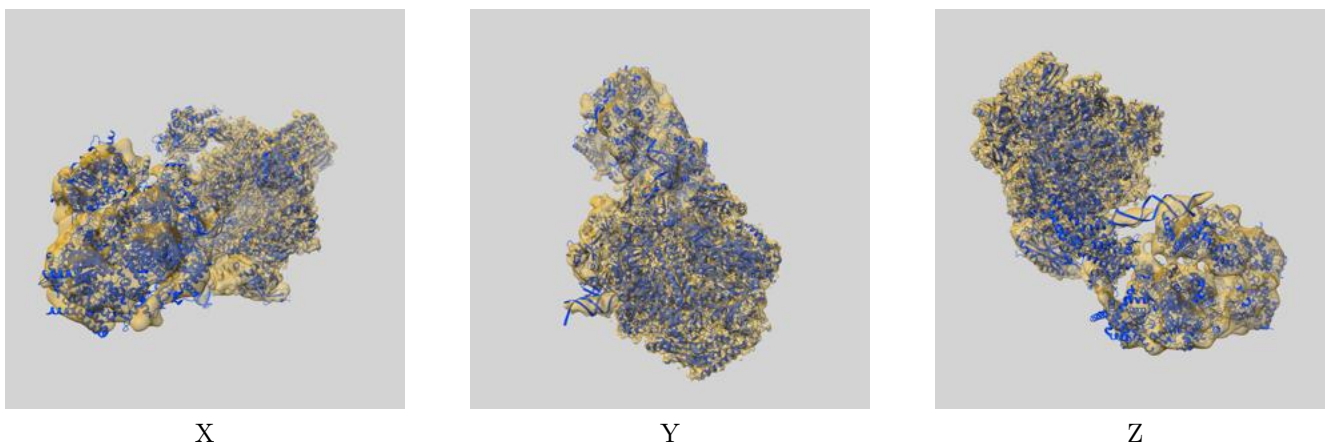
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	4.05	6.50	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

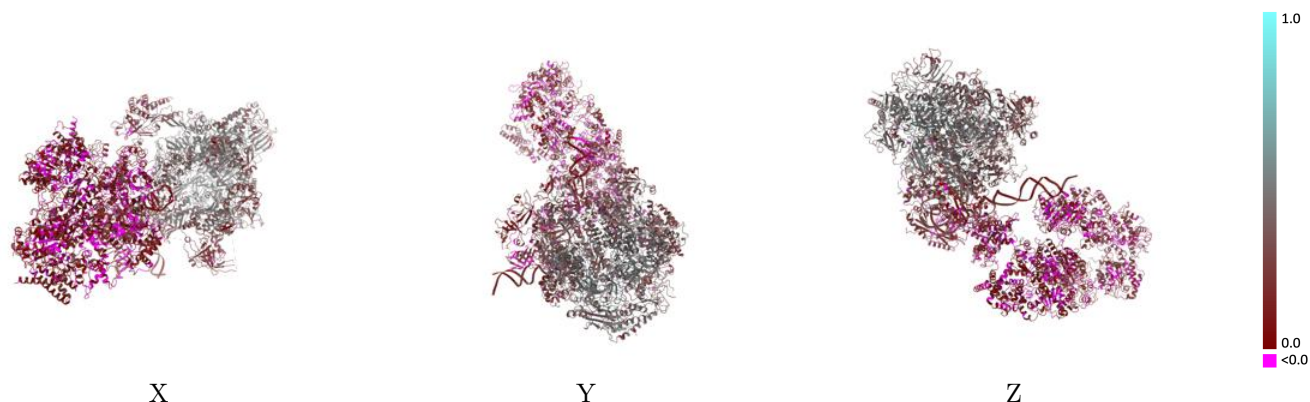
This section contains information regarding the fit between EMDB map EMD-23906 and PDB model 7ML2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



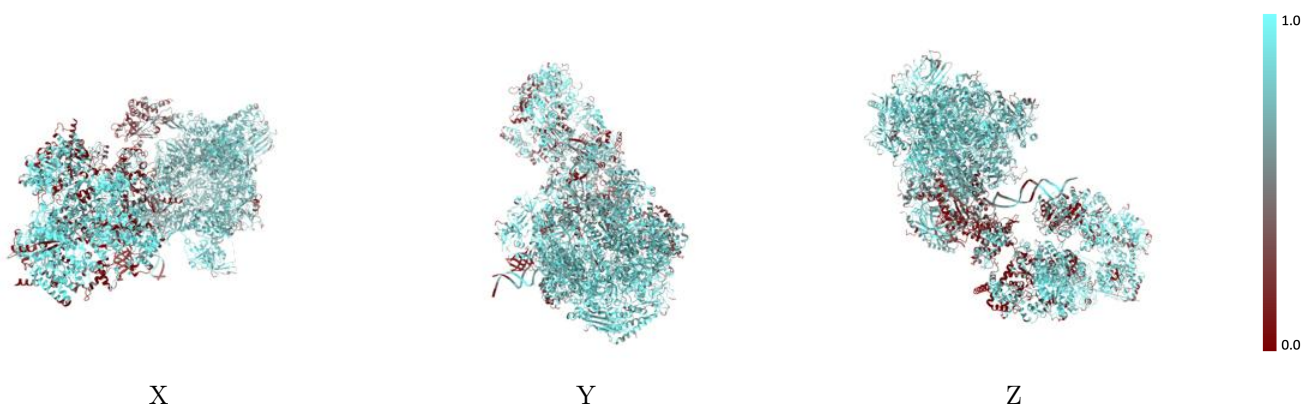
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



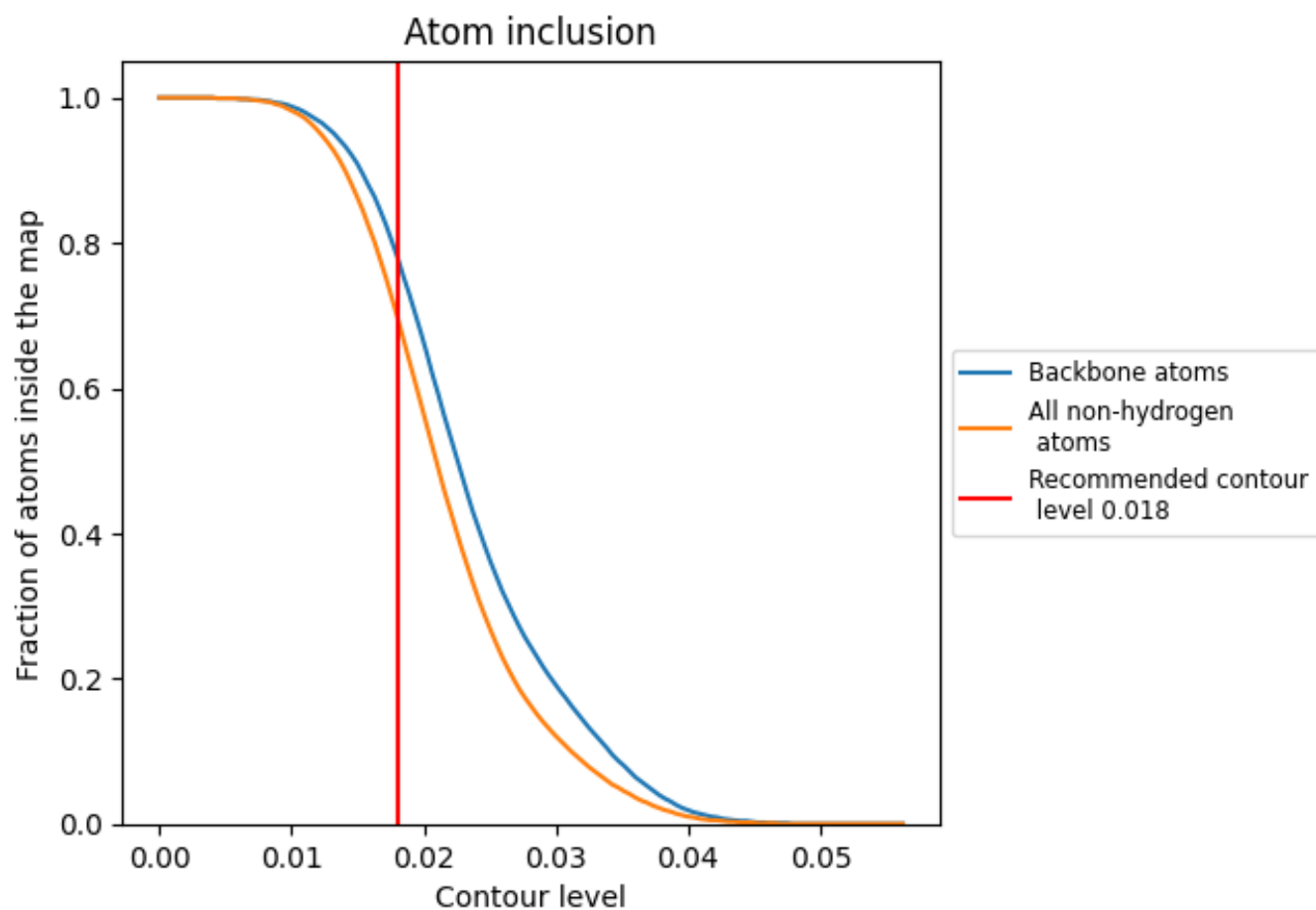
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.2410
0	 0.6760	 0.0760
1	 0.6300	 0.0700
2	 0.6610	 0.0730
3	 0.3780	 0.0870
4	 0.8350	 0.0840
5	 0.6360	 0.0880
6	 0.8020	 0.0860
7	 0.5850	 0.0670
A	 0.7980	 0.4070
B	 0.8270	 0.4220
C	 0.8410	 0.4250
D	 0.2470	 0.2040
E	 0.7770	 0.3820
F	 0.7930	 0.3810
G	 0.4360	 0.2550
H	 0.7370	 0.3440
I	 0.6100	 0.2690
J	 0.8380	 0.4100
K	 0.7150	 0.3710
L	 0.6970	 0.2880
M	 0.5480	 0.2340
N	 0.6980	 0.1450
O	 0.7610	 0.1580
Q	 0.8080	 0.2110
R	 0.6770	 0.1820
T	 0.7070	 0.1650
U	 0.0290	 0.0510
V	 0.1140	 0.0470
W	 0.4040	 0.0900
X	 0.5360	 0.0920

