



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 08:57 PM UTC

PDB ID : 8A3Y / pdb_00008a3y
EMDB ID : EMD-15127
Title : Structure of mammalian Pol II-DSIF-SPT6-PAF1-TFIIS-hexasome elongation complex
Authors : Farnung, L.; Ochmann, M.; Garg, G.; Vos, S.M.; Cramer, P.
Deposited on : 2022-06-09
Resolution : 3.30 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:

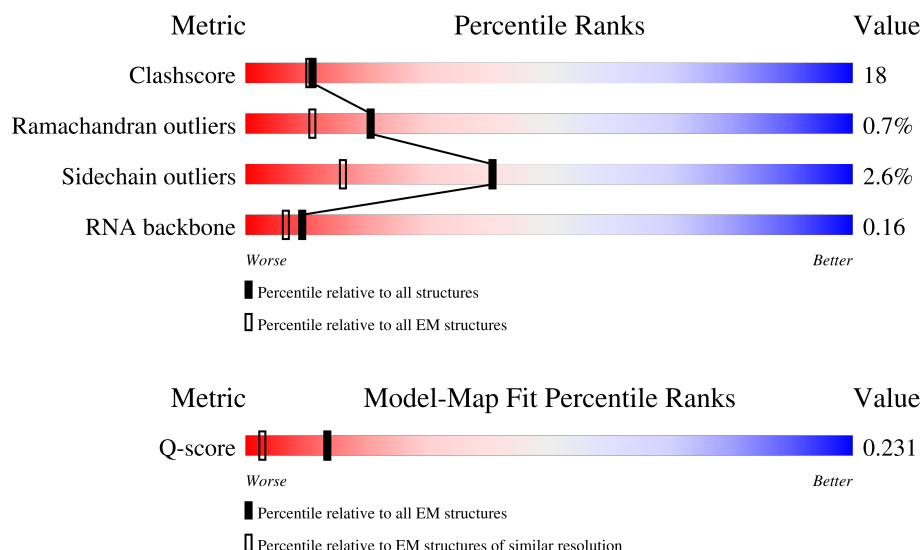
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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

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

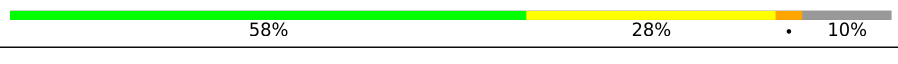
The reported resolution of this entry is 3.30 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1984	
2	B	1251	
3	C	270	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1002	
14	N	127	
15	P	28	
16	Q	1845	
16	U	1845	
17	R	248	
18	T	138	
19	V	311	
20	W	305	
21	X	531	
22	Y	121	
23	Z	1087	
24	a	136	
24	e	136	
25	b	103	
25	f	103	

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Mol	Chain	Length	Quality of chain
26	c	103	 65%27%8%
27	d	95	 58%35%6% •

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 125225 atoms, of which 59820 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
1	A	1426	Total	C	H	N	O	P	S	0	0
			22642	7074	11387	2014	2095	2	70		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1122	Total	C	H	N	O	S	0	0
			18007	5684	9027	1576	1656	64		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	258	Total	C	H	N	O	S	0	0
			4097	1300	2025	356	410	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	126	Total	C	H	N	O	S	0	0
			1985	630	981	170	200	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3458	1089	1738	300	323	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	78	Total	C	H	N	O	S	0	0
			1284	401	658	106	114	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2654	866	1321	214	245	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	149	Total	C	H	N	O	S	0	0
			2354	759	1157	195	238	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	116	Total	C	H	N	O	S	0	0
			1822	582	880	168	181	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1068	339	544	88	91	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			786	240	396	77	67	6		

- Molecule 13 is a protein called SPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	1002	Total	C	H	N	O	S	0	0
			7015	2583	2278	1071	1076	7		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	127	Total	C	H	N	O	P	0	0
			4051	1239	1420	507	758	127		

- Molecule 15 is a RNA chain called RNA, Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	28	Total	C	H	N	O	P	0	0
			911	271	307	120	185	28		

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	890	Total	C	H	N	O	S	0	0
			14396	4579	7170	1264	1352	31		
16	U	125	Total	C	H	N	O	S	0	0
			1524	534	672	151	166	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	linker	UNP Q6PD62
Q	1175	ASN	-	linker	UNP Q6PD62
Q	1176	LEU	-	linker	UNP Q6PD62
Q	1177	TYR	-	linker	UNP Q6PD62
Q	1178	PHE	-	linker	UNP Q6PD62
Q	1179	GLN	-	linker	UNP Q6PD62
U	-5	GLU	-	linker	UNP Q6PD62
U	-4	ASN	-	linker	UNP Q6PD62
U	-3	LEU	-	linker	UNP Q6PD62
U	-2	TYR	-	linker	UNP Q6PD62
U	-1	PHE	-	linker	UNP Q6PD62
U	0	GLN	-	linker	UNP Q6PD62

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	244	Total	C	H	N	O	S	0	0
			3523	1148	1691	340	337	7		

- Molecule 18 is a DNA chain called RNA, Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	138	Total	C	H	N	O	P	0	0
			4353	1331	1550	502	833	137		

- Molecule 19 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	244	Total	C	H	N	O	S	0	0
			3136	1061	1433	305	333	4		

- Molecule 20 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	W	300	Total	C	H	N	O	S	0	0
			4581	1483	2248	392	454	4		

- Molecule 21 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	43	Total	C	H	N	O	0	0
			725	220	372	69	64		

- Molecule 22 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Y	116	Total	C	H	N	O	S	0	0
			1819	570	908	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP Q4R941
Y	-2	PRO	-	expression tag	UNP Q4R941
Y	-1	GLY	-	expression tag	UNP Q4R941
Y	0	SER	-	expression tag	UNP Q4R941

- Molecule 23 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
23	Z	510	Total	C	H	N	O	P	S	0	0
			8063	2550	4040	709	745	1	18		

- Molecule 24 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	97	Total	C	H	N	O	S	0	0
			1643	506	841	155	138	3		
24	e	97	Total	C	H	N	O	S	0	0
			1640	504	839	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 25 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	b	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
25	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

- Molecule 26 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	c	103	Total	C	H	N	O		0	0
			1644	501	849	155	139			

- Molecule 27 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d	95	Total	C	H	N	O	S	0	0
			1521	469	776	134	140	2		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Zn	0
			2	2	
28	B	1	Total	Zn	0
			1	1	
28	C	1	Total	Zn	0
			1	1	
28	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
28	J	1	Total 1	Zn 1	0
28	L	1	Total 1	Zn 1	0
28	Y	1	Total 1	Zn 1	0

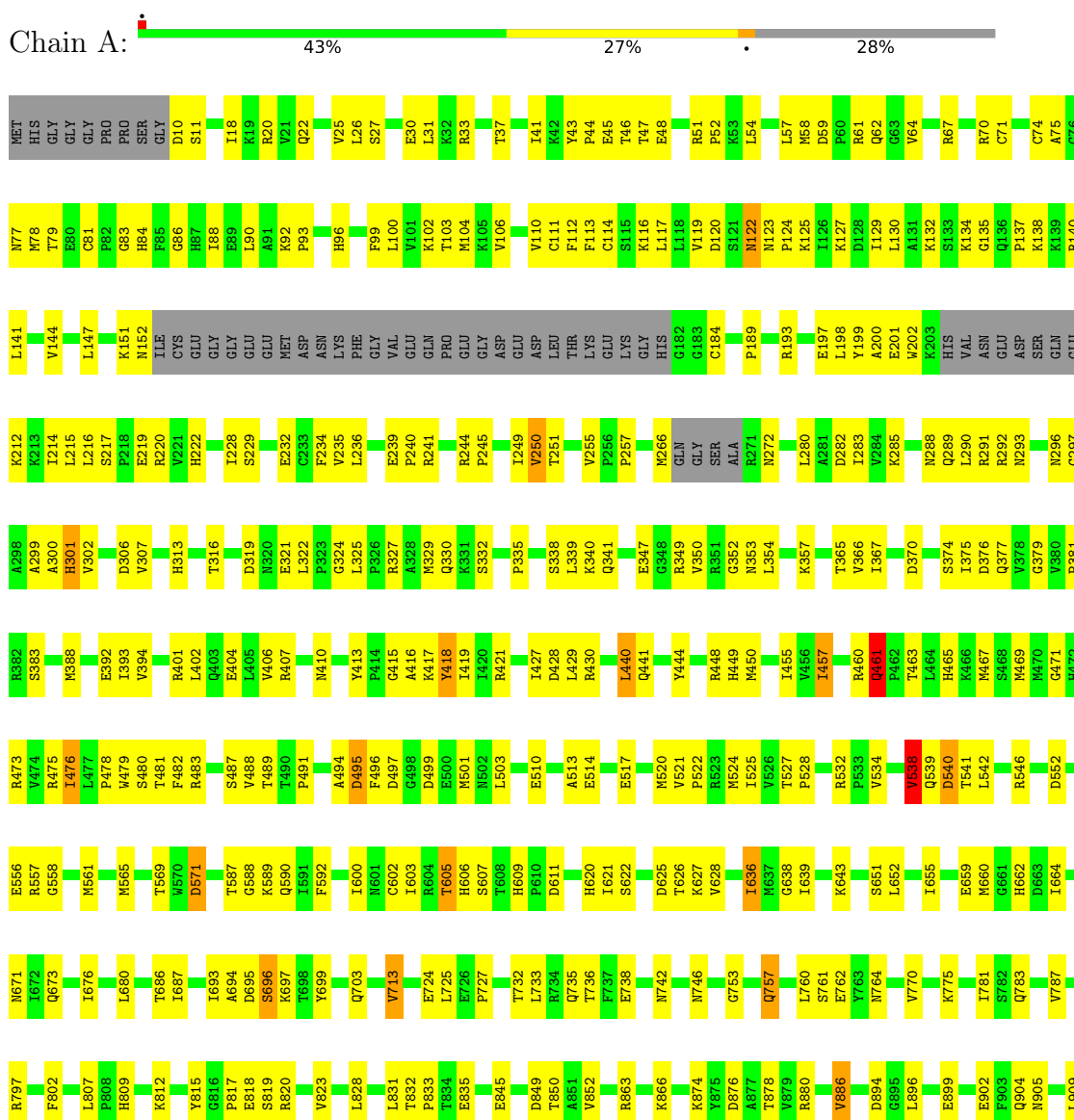
- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
29	P	1	Total 1	Mg 1	0

3 Residue-property plots

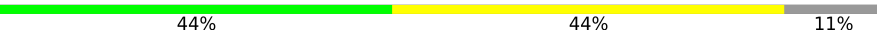
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

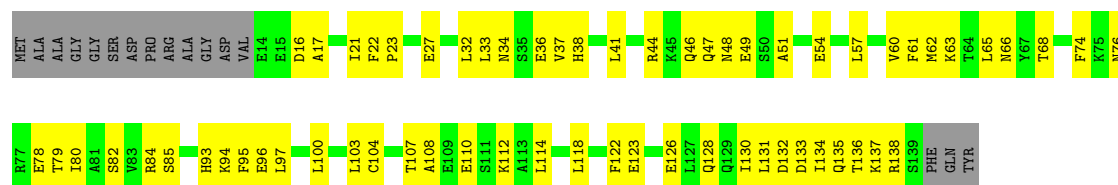
• Molecule 1: DNA-directed RNA polymerase subunit





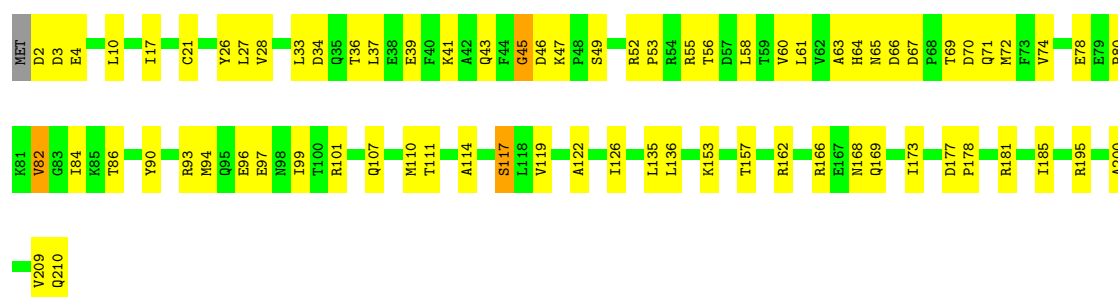
- Molecule 4: RNA polymerase II subunit D

Chain D: 



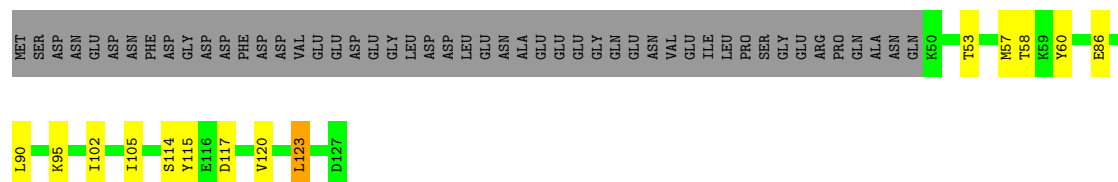
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 



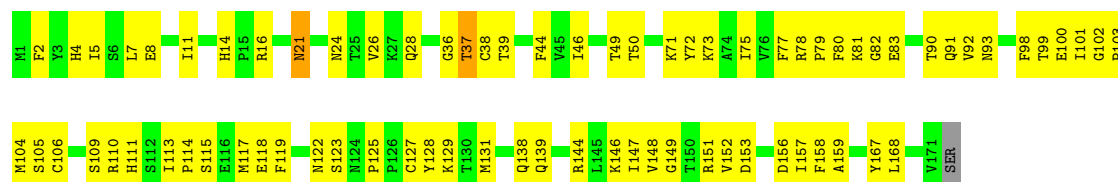
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



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

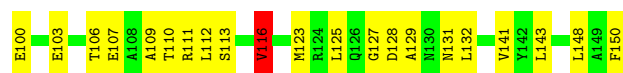
Chain G: 



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

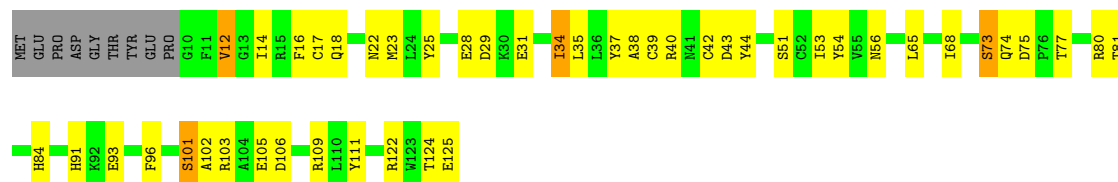
Chain H: 





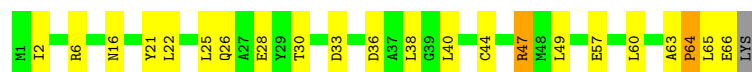
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 56% 34% 7%



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

Chain J: 66% 30% 2%



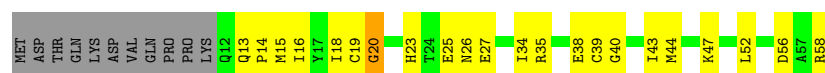
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 74% 23% 3%



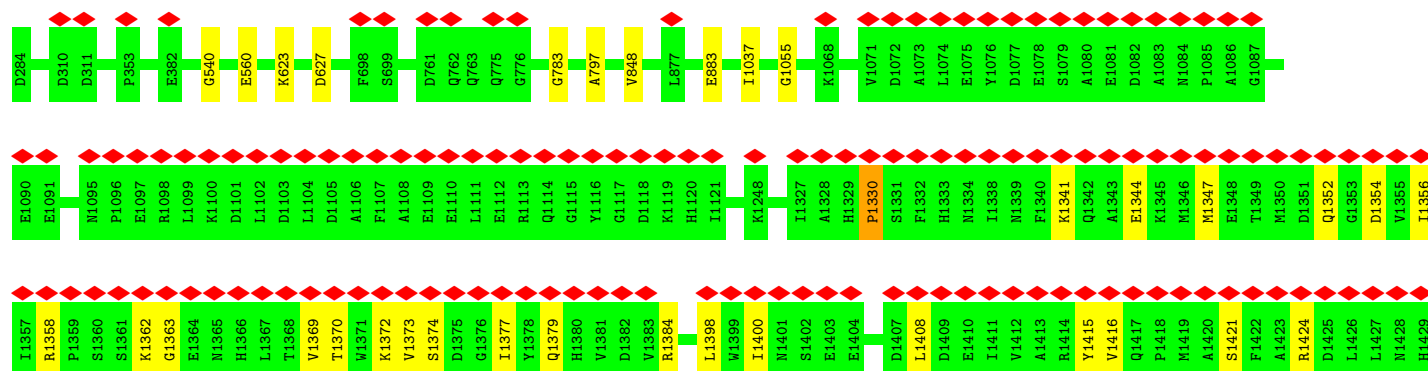
- Molecule 12: RNA polymerase II subunit K

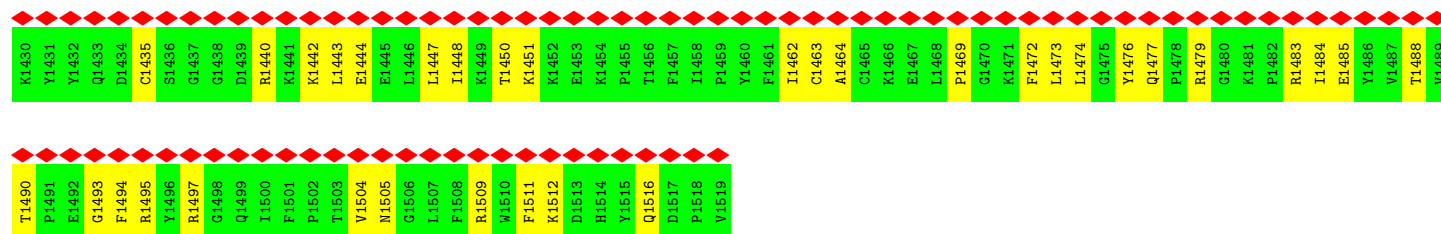
Chain L: 43% 36% 19%



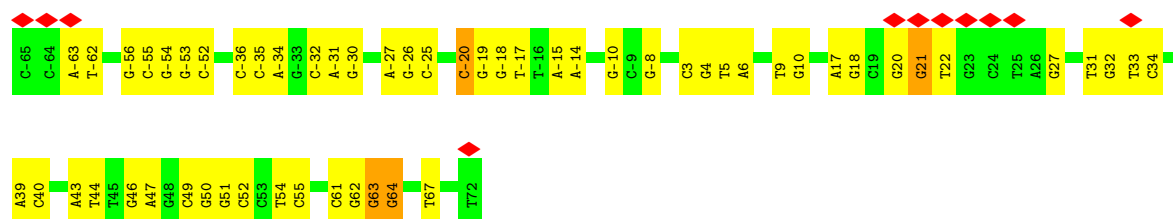
- Molecule 13: SPT6

Chain M: 23% 93% 7%

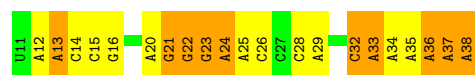
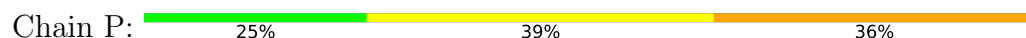




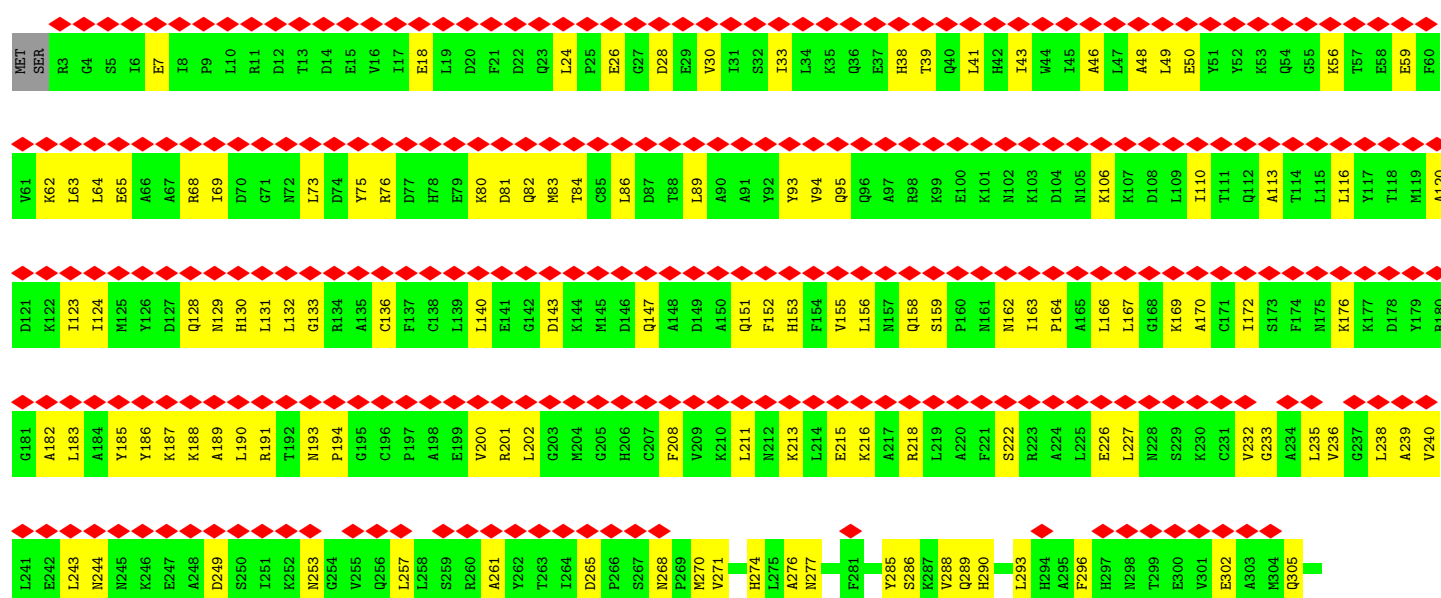
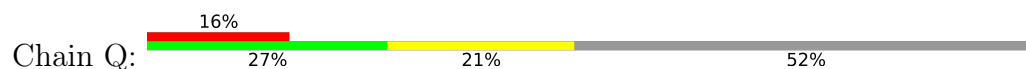
• Molecule 14: Non-template DNA



• Molecule 15: RNA, Template DNA



• Molecule 16: RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein LEO1

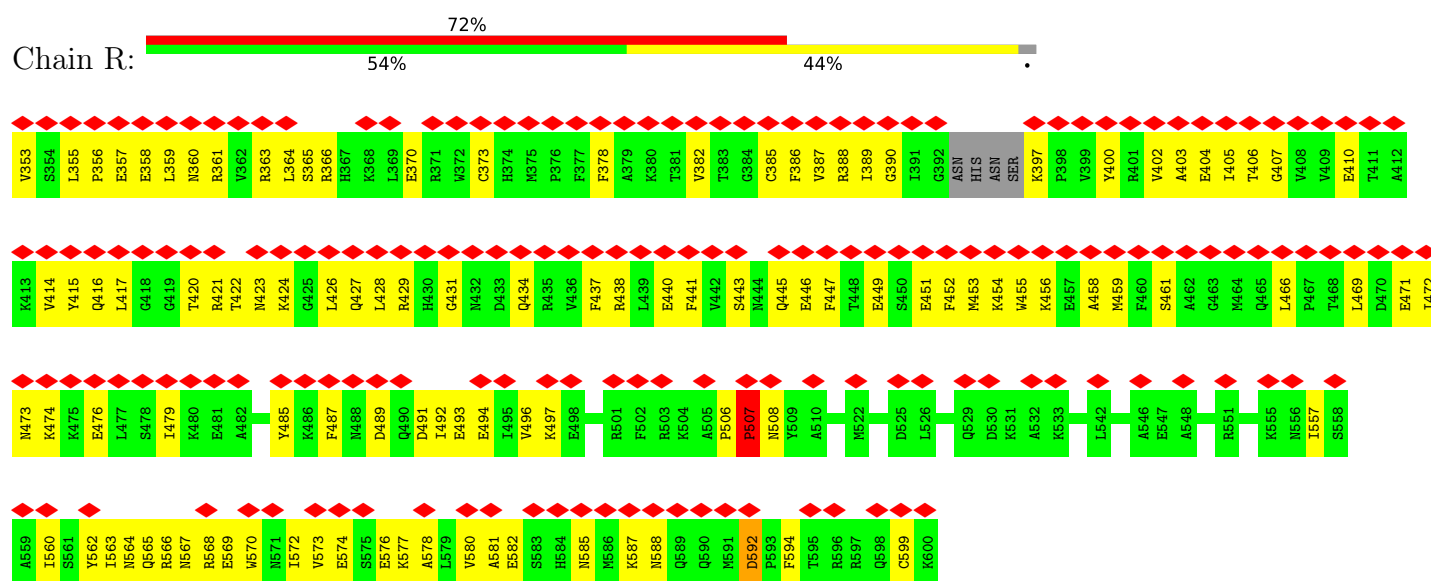




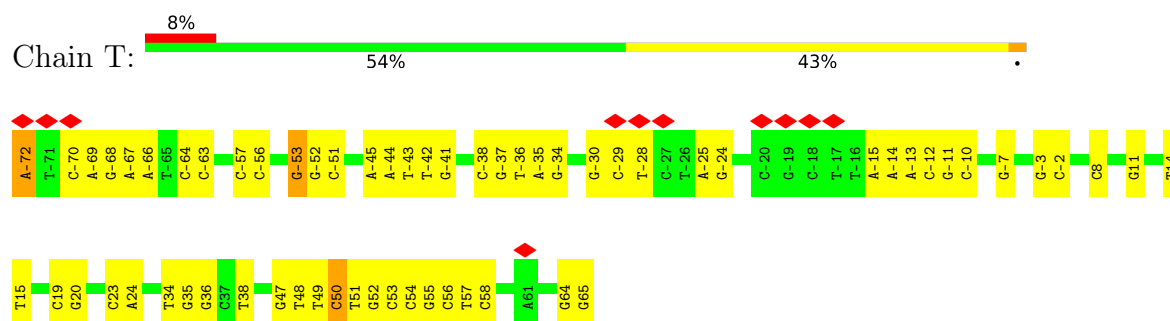
- Molecule 16: RNA polymerase-associated protein CTR9 homolog, RNA polymerase-associated protein LEO1

[illegible]

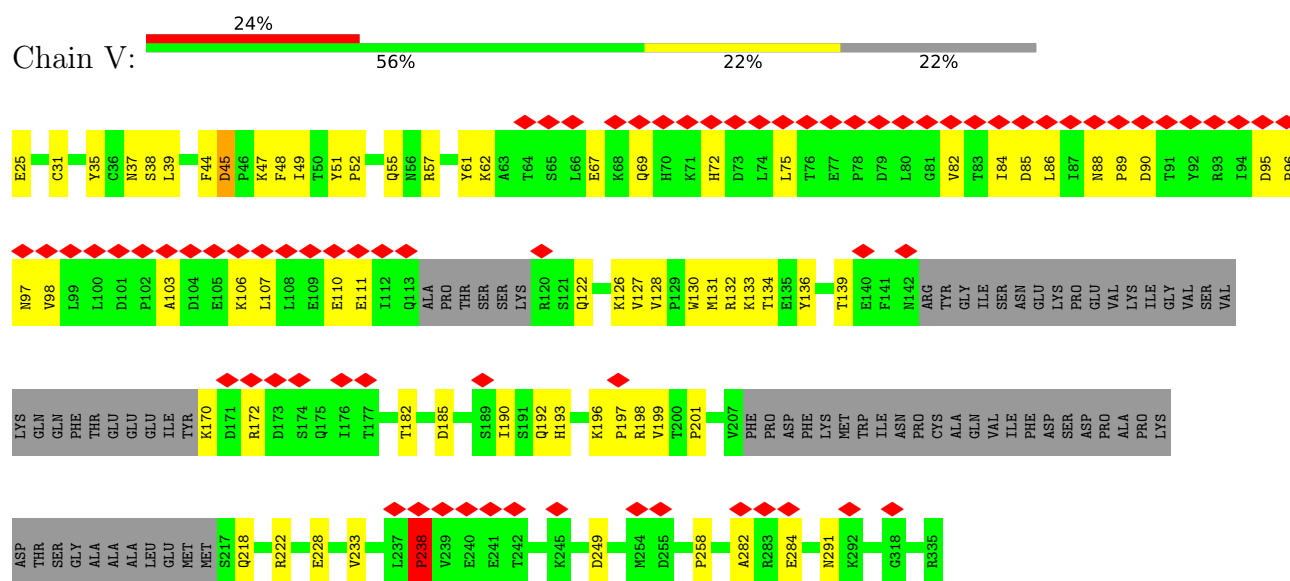
- Molecule 17: RNA polymerase-associated protein RTF1 homolog



• Molecule 18: RNA, Template DNA

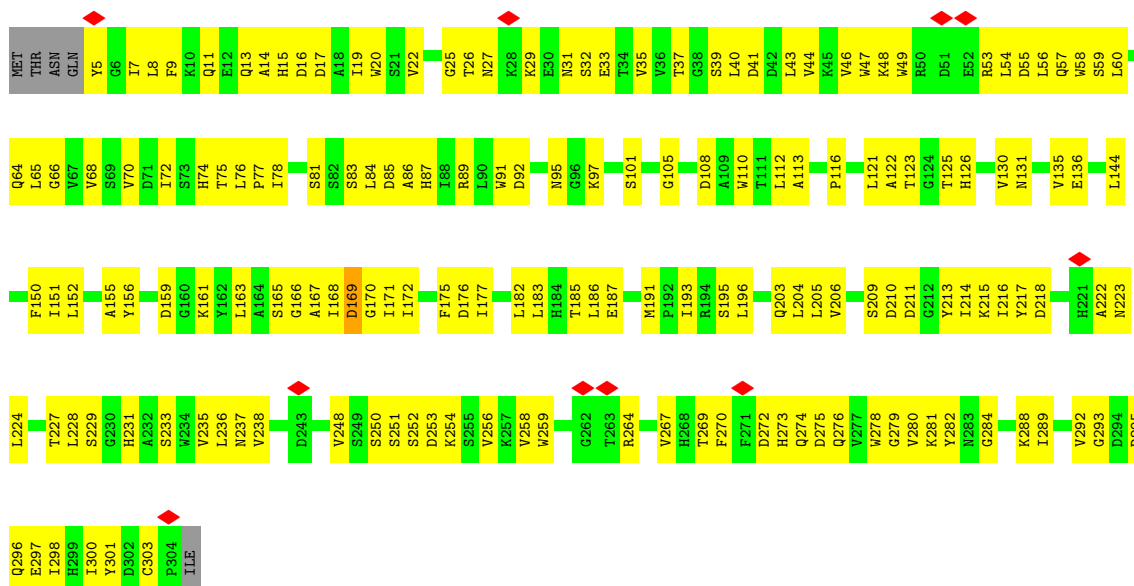


• Molecule 19: RNA polymerase II-associated factor 1 homolog



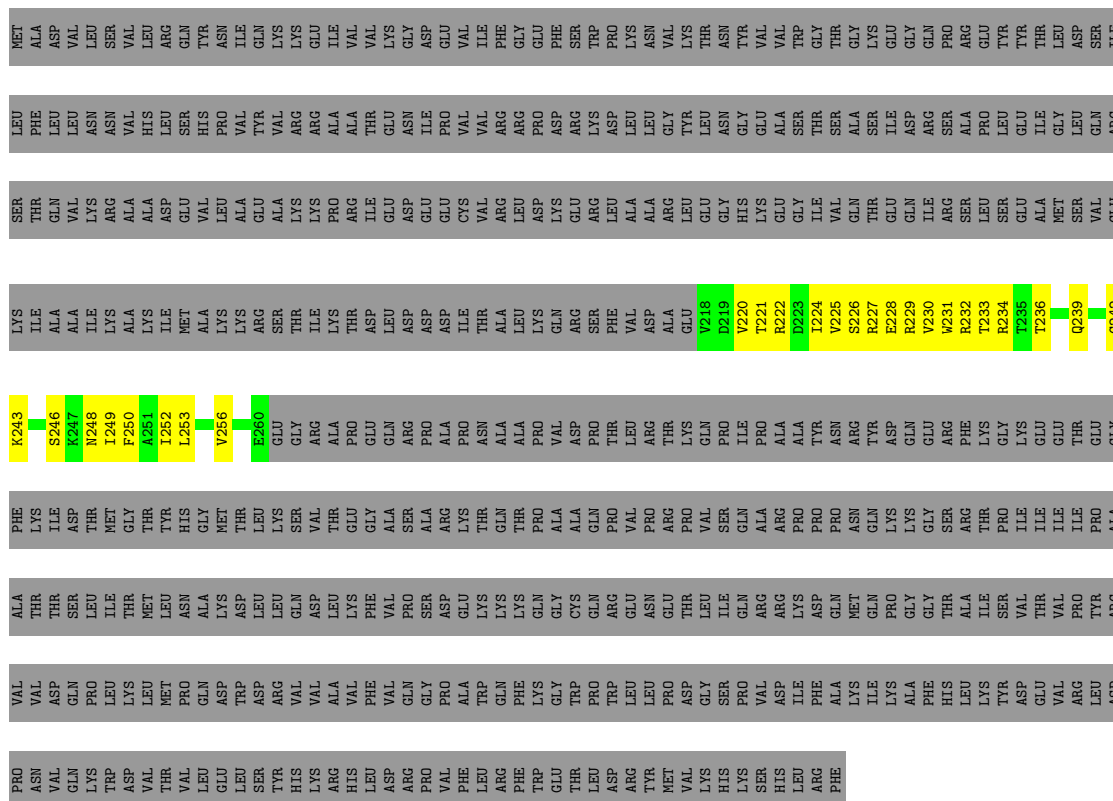
• Molecule 20: WD repeat-containing protein 61



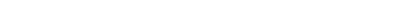


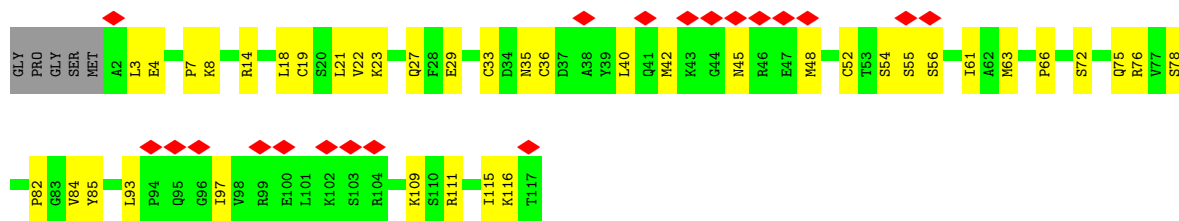
- Molecule 21: Parafibromin

Chain X: 5% 92%

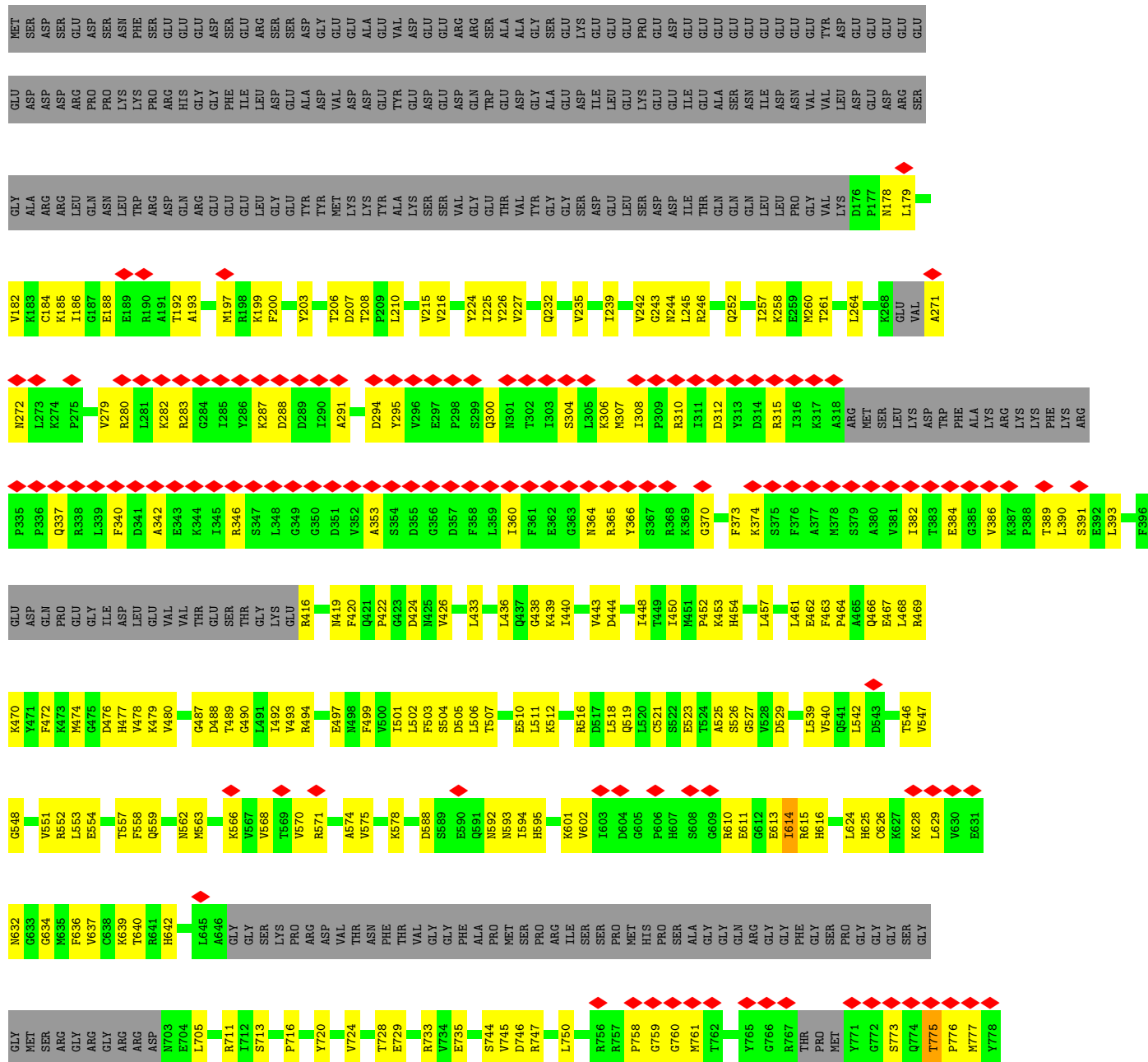
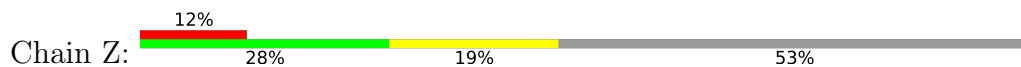


- Molecule 22: Transcription elongation factor SPT4

Chain Y:  17% 64% 32%

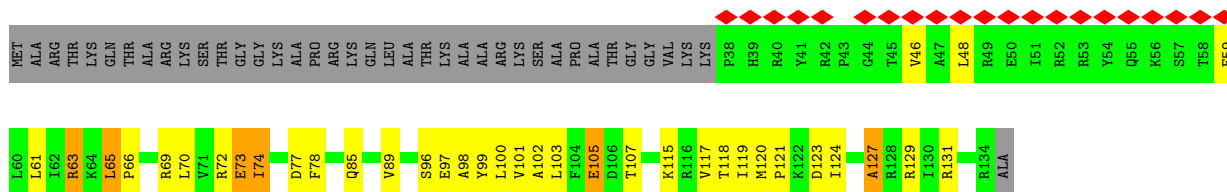
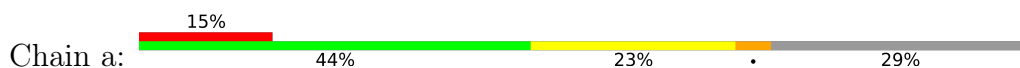


• Molecule 23: Transcription elongation factor SPT5

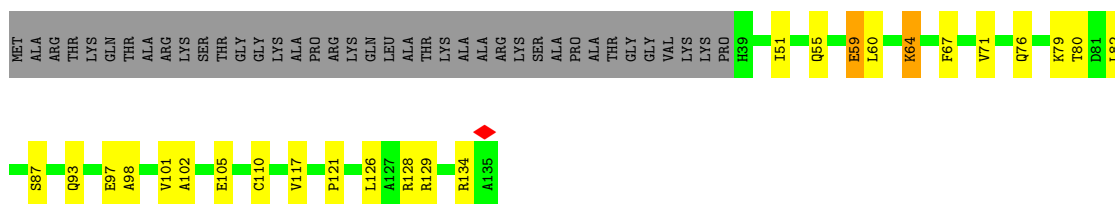




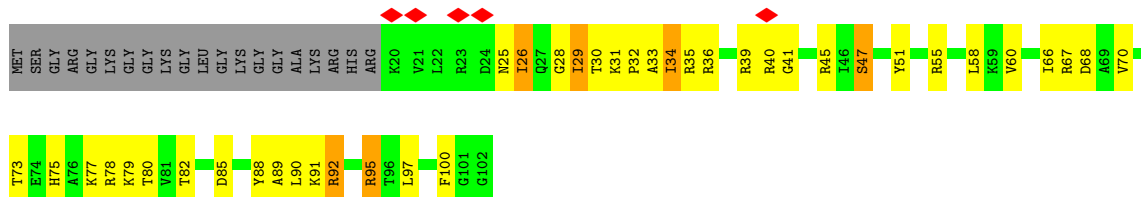
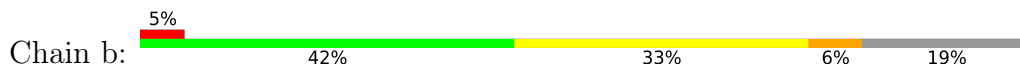
- Molecule 24: Histone H3.2



- Molecule 24: Histone H3.2

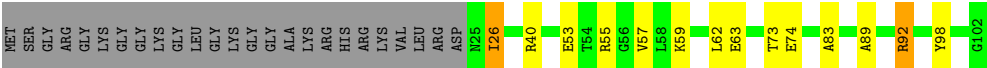


- Molecule 25: Histone H4

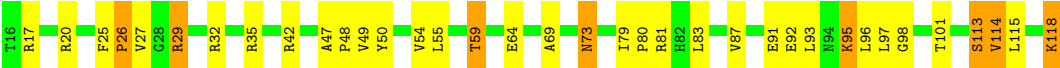


- Molecule 25: Histone H4

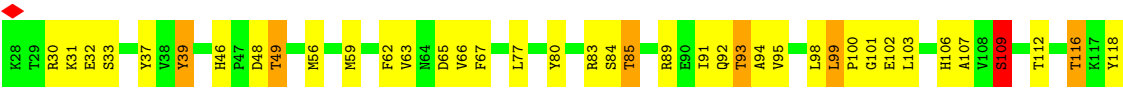




● Molecule 26: Histone H2A



● Molecule 27: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.036	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, SEP, 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	1.41	9/11437 (0.1%)	0.97	12/15433 (0.1%)
2	B	1.57	8/9158 (0.1%)	1.07	20/12360 (0.2%)
3	C	1.69	3/2115 (0.1%)	1.06	5/2873 (0.2%)
4	D	0.40	0/1017	0.51	0/1368
5	E	1.23	0/1751	0.87	0/2366
6	F	1.62	1/636 (0.2%)	0.97	0/859
7	G	0.68	0/1364	0.66	0/1853
8	H	1.59	2/1219 (0.2%)	0.98	0/1644
9	I	1.13	0/964	0.88	0/1305
10	J	1.75	1/533 (0.2%)	1.00	0/719
11	K	1.69	1/939 (0.1%)	0.94	0/1271
12	L	1.40	0/395	1.11	1/525 (0.2%)
13	M	0.20	0/4763	0.43	1/6084 (0.0%)
14	N	0.44	0/2957	1.02	11/4566 (0.2%)
15	P	0.58	0/678	0.76	1/1055 (0.1%)
16	Q	0.31	0/7365	0.50	0/9927
16	U	0.36	0/864	0.75	3/1173 (0.3%)
17	R	0.36	0/1860	0.60	2/2509 (0.1%)
18	T	0.60	1/3137 (0.0%)	0.97	5/4835 (0.1%)
19	V	0.31	0/1728	0.65	2/2357 (0.1%)
20	W	0.32	0/2392	0.50	0/3257
21	X	0.33	0/356	0.54	0/478
22	Y	0.17	0/927	0.40	0/1250
23	Z	0.41	0/4081	0.52	1/5493 (0.0%)
24	a	0.83	1/814 (0.1%)	1.04	3/1092 (0.3%)
24	e	0.65	0/812	1.05	2/1088 (0.2%)
25	b	0.81	0/669	1.16	2/894 (0.2%)
25	f	0.68	0/626	1.01	0/837
26	c	0.58	0/805	0.97	1/1088 (0.1%)
27	d	0.60	0/756	1.02	2/1015 (0.2%)
All	All	1.04	27/67118 (0.0%)	0.85	74/91574 (0.1%)

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	2
2	B	0	3
14	N	0	9
17	R	0	1
18	T	0	6
All	All	0	21

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-13.39	1.20	1.53
2	B	94	SER	C-N	-8.44	1.07	1.33
3	C	104	ASP	CA-CB	-8.21	1.40	1.53
18	T	-72	DA	O5'-C5'	7.53	1.65	1.42
1	A	418	TYR	CA-CB	-6.89	1.43	1.53

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	20	DG	O3'-P-O5'	-15.18	81.22	104.00
14	N	20	DG	OP2-P-O3'	-8.28	83.17	108.00
3	C	224	GLY	CA-C-N	8.13	147.27	121.98
3	C	224	GLY	C-N-CA	8.13	147.27	121.98
19	V	258	PRO	N-CA-CB	7.97	110.87	103.46

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide

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	11255	11387	11374	462	0
2	B	8980	9027	9019	320	0
3	C	2072	2025	2019	43	0
4	D	1004	981	980	53	0
5	E	1720	1738	1737	77	0
6	F	626	658	657	11	0
7	G	1333	1321	1321	83	0
8	H	1197	1157	1156	45	0
9	I	942	880	873	41	0
10	J	524	544	541	19	0
11	K	920	942	942	26	0
12	L	390	396	397	13	0
13	M	4737	2278	2262	49	0
14	N	2631	1420	1421	48	0
15	P	604	307	307	30	0
16	Q	7226	7170	7169	367	0
16	U	852	672	668	31	0
17	R	1832	1691	1687	123	0
18	T	2803	1550	1550	55	0
19	V	1703	1433	1426	88	0
20	W	2333	2248	2246	154	0
21	X	353	372	371	30	0
22	Y	911	908	908	27	0
23	Z	4023	4040	4035	184	0
24	a	802	841	841	21	0
24	e	801	839	838	16	0
25	b	662	710	709	37	0
25	f	619	660	659	10	0
26	c	795	849	846	26	0
27	d	745	776	773	39	0
28	A	2	0	0	0	0
28	B	1	0	0	0	0
28	C	1	0	0	0	0
28	I	2	0	0	0	0
28	J	1	0	0	0	0
28	L	1	0	0	0	0
28	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	P	1	0	0	0	0
All	All	65405	59820	59732	2267	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 18.

The worst 5 of 2267 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)
18:T:-72:DA:C5'	18:T:-72:DA:O5'	1.65	1.42
25:b:75:HIS:CD2	27:d:93:THR:HG21	1.58	1.38
25:b:75:HIS:HD2	27:d:93:THR:CG2	1.55	1.19
2:B:953:ASP:OD1	3:C:36:ARG:NH1	1.96	0.98
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.43	0.96

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	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	18	49
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	16	45
3	C	254/270 (94%)	232 (91%)	19 (8%)	3 (1%)	10	37
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24	55
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	3	20
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1002 (97%)	903 (92%)	72 (7%)	1 (0%)	48	75
16	Q	888/1845 (48%)	836 (94%)	52 (6%)	0	100	100
16	U	117/1845 (6%)	88 (75%)	21 (18%)	8 (7%)	1	7
17	R	240/248 (97%)	225 (94%)	14 (6%)	1 (0%)	30	60
19	V	234/311 (75%)	197 (84%)	33 (14%)	4 (2%)	7	30
20	W	298/305 (98%)	269 (90%)	29 (10%)	0	100	100
21	X	41/531 (8%)	41 (100%)	0	0	100	100
22	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
23	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	43	71
24	a	95/136 (70%)	83 (87%)	9 (10%)	3 (3%)	3	19
24	e	95/136 (70%)	87 (92%)	8 (8%)	0	100	100
25	b	81/103 (79%)	70 (86%)	8 (10%)	3 (4%)	2	17
25	f	76/103 (74%)	67 (88%)	9 (12%)	0	100	100
26	c	101/103 (98%)	88 (87%)	9 (9%)	4 (4%)	2	15
27	d	93/95 (98%)	82 (88%)	9 (10%)	2 (2%)	5	26
All	All	7779/12644 (62%)	7099 (91%)	627 (8%)	53 (1%)	20	49

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE

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	1245/1761 (71%)	1214 (98%)	31 (2%)	42	64
2	B	986/1084 (91%)	939 (95%)	47 (5%)	23	52
3	C	235/247 (95%)	232 (99%)	3 (1%)	61	74
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	188 (98%)	3 (2%)	55	72
6	F	68/111 (61%)	66 (97%)	2 (3%)	37	62
7	G	146/153 (95%)	144 (99%)	2 (1%)	59	73
8	H	130/131 (99%)	122 (94%)	8 (6%)	16	45
9	I	104/112 (93%)	100 (96%)	4 (4%)	29	57
10	J	55/56 (98%)	54 (98%)	1 (2%)	51	70
11	K	104/106 (98%)	102 (98%)	2 (2%)	50	68
12	L	43/55 (78%)	39 (91%)	4 (9%)	8	30
13	M	154/894 (17%)	154 (100%)	0	100	100
16	Q	761/1601 (48%)	759 (100%)	2 (0%)	86	86
16	U	63/1601 (4%)	63 (100%)	0	100	100
17	R	168/222 (76%)	167 (99%)	1 (1%)	78	81
19	V	144/285 (50%)	143 (99%)	1 (1%)	76	80
20	W	255/260 (98%)	253 (99%)	2 (1%)	73	79
21	X	40/467 (9%)	40 (100%)	0	100	100
22	Y	102/105 (97%)	101 (99%)	1 (1%)	68	76
23	Z	434/939 (46%)	432 (100%)	2 (0%)	81	83
24	a	85/111 (77%)	76 (89%)	9 (11%)	6	24
24	e	84/111 (76%)	81 (96%)	3 (4%)	31	58
25	b	68/79 (86%)	62 (91%)	6 (9%)	9	32
25	f	63/79 (80%)	60 (95%)	3 (5%)	23	52
26	c	82/82 (100%)	74 (90%)	8 (10%)	7	28
27	d	81/81 (100%)	70 (86%)	11 (14%)	3	16
All	All	6000/11051 (54%)	5844 (97%)	156 (3%)	41	64

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Z	720	TYR
27	d	84	SER
24	a	63	ARG
25	b	95	ARG
24	e	59	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
20	W	27	ASN
20	W	268	HIS
23	Z	616	HIS
4	D	19	GLN
3	C	262	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	27/28 (96%)	14 (51%)	5 (18%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	13	A
15	P	14	C
15	P	15	C
15	P	16	G
15	P	21	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	13	A
15	P	21	G
15	P	23	G
15	P	34	A
15	P	36	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
23	TPO	Z	775	23	8,10,11	1.60	1 (12%)	10,14,16	2.21	1 (10%)
1	SEP	A	1547	1	8,9,10	1.55	1 (12%)	7,12,14	1.12	1 (14%)
1	TPO	A	1525	1	8,10,11	1.66	1 (12%)	10,14,16	2.02	1 (10%)

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
23	TPO	Z	775	23	-	1/9/11/13	-
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.57	1.61	1.50
23	Z	775	TPO	P-O1P	3.50	1.61	1.50
1	A	1547	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	775	TPO	P-OG1-CB	-6.55	105.53	123.33
1	A	1525	TPO	P-OG1-CB	-5.57	108.20	123.33
1	A	1547	SEP	OG-CB-CA	2.03	110.12	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
23	Z	775	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Z	775	TPO	2	0
1	A	1547	SEP	1	0
1	A	1525	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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
13	M	12
2	B	3
14	N	1
16	U	1
19	V	1
1	A	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	1287:MET	C	1327:ILE	N	37.43
1	N	-52:DC	O3'	-40:DG	P	31.66
1	M	477:LYS	C	538:LYS	N	28.32
1	U	497:ASP	C	505:SER	N	25.85
1	M	430:ALA	C	440:ILE	N	16.17

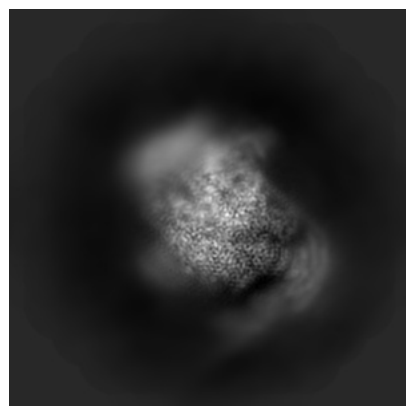
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15127. These allow visual inspection of the internal detail of the map and identification of artifacts.

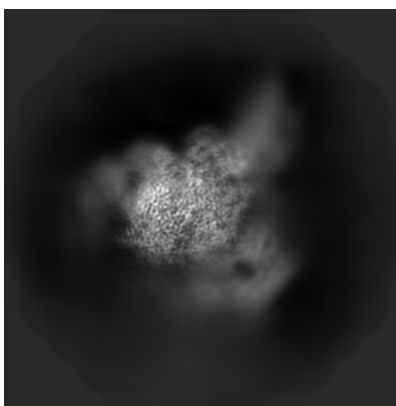
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

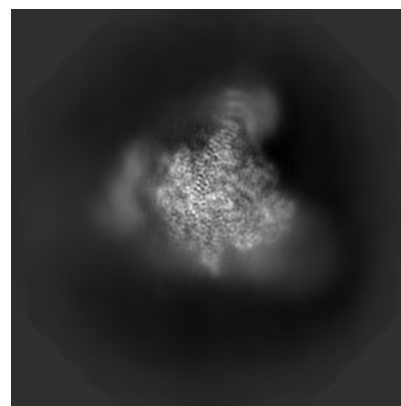
6.1.1 Primary map



X

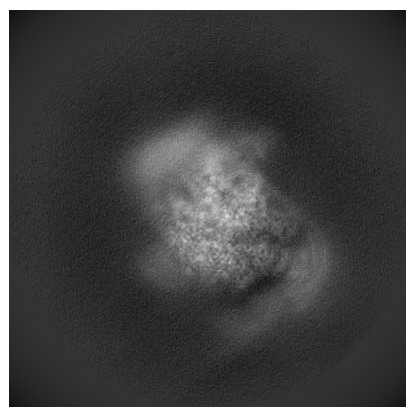


Y

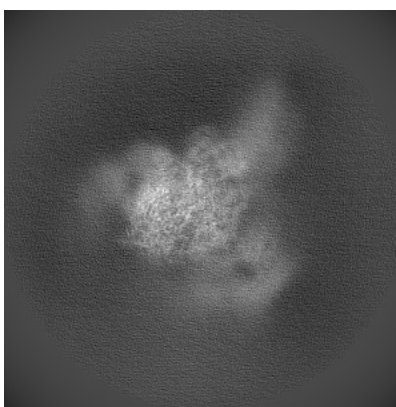


Z

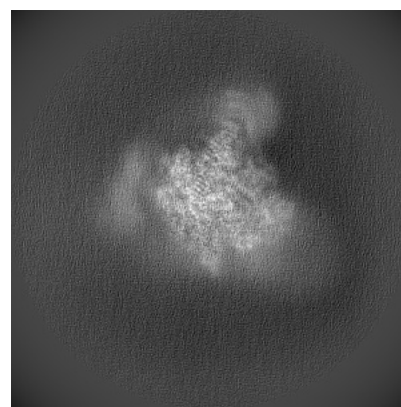
6.1.2 Raw map



X



Y

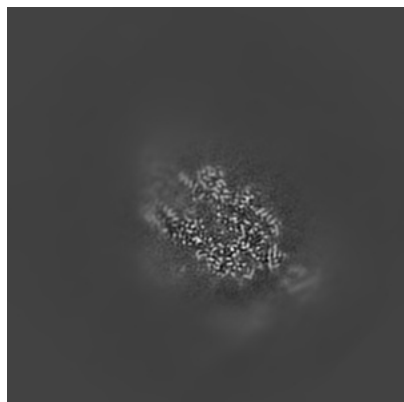


Z

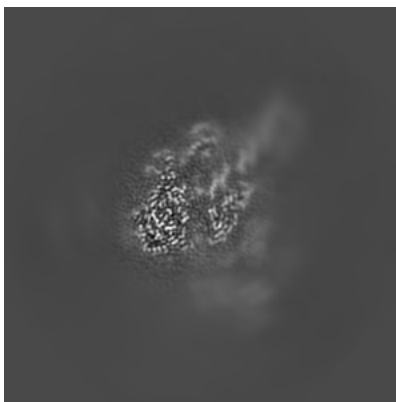
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

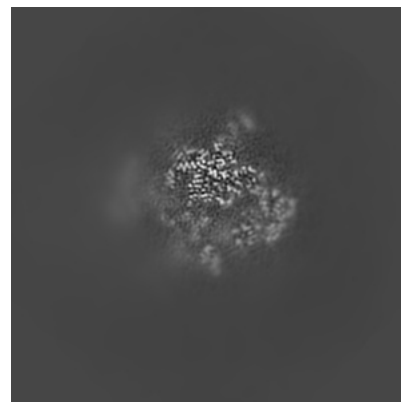
6.2.1 Primary map



X Index: 180

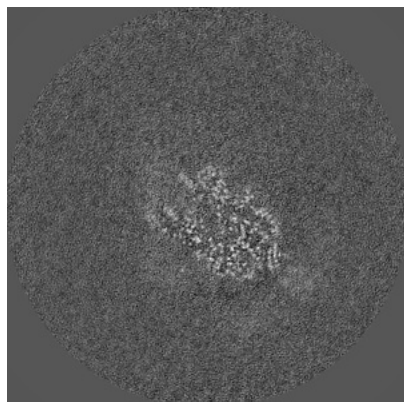


Y Index: 180

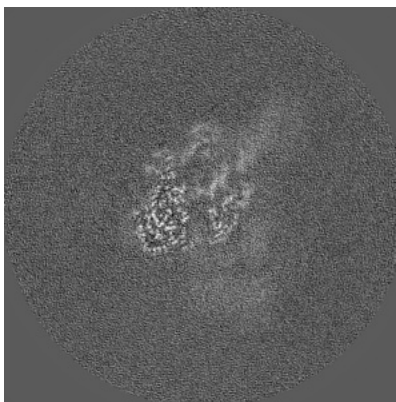


Z Index: 180

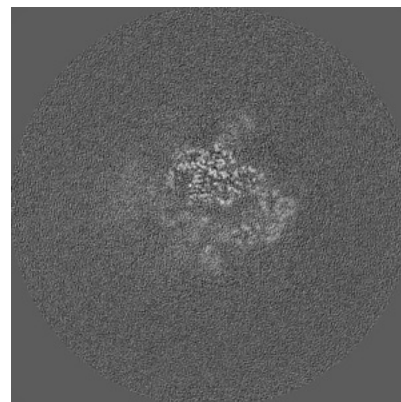
6.2.2 Raw map



X Index: 180



Y Index: 180

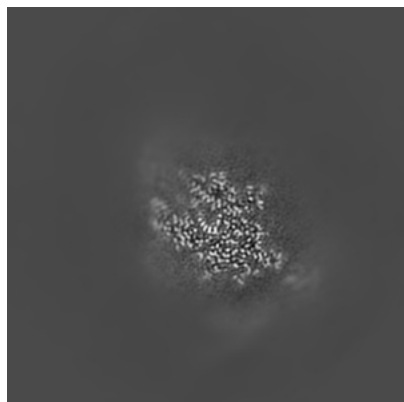


Z Index: 180

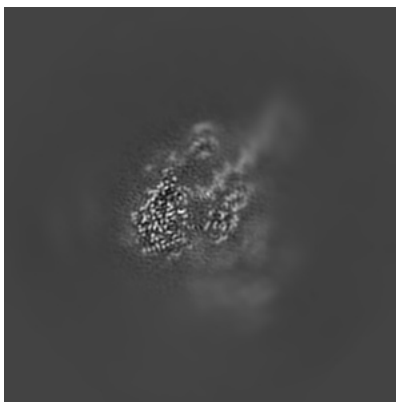
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

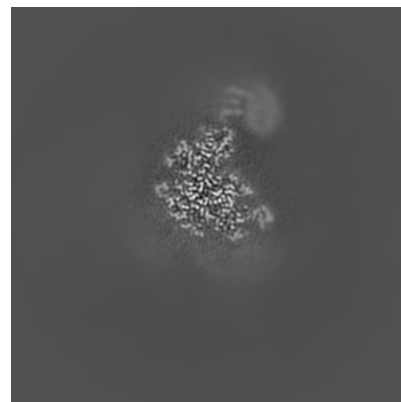
6.3.1 Primary map



X Index: 175

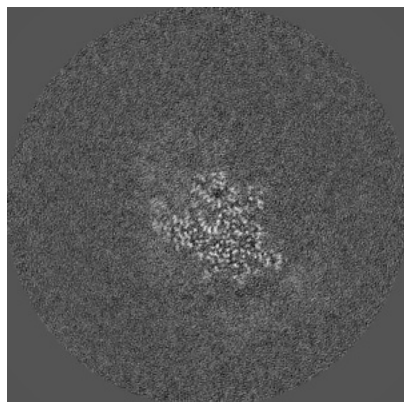


Y Index: 182

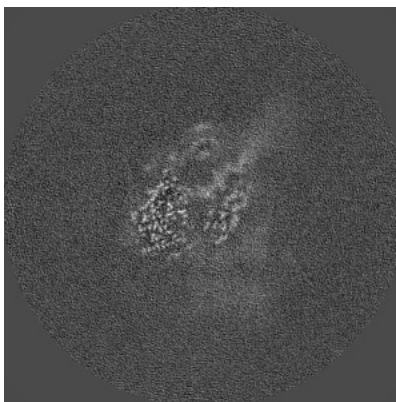


Z Index: 138

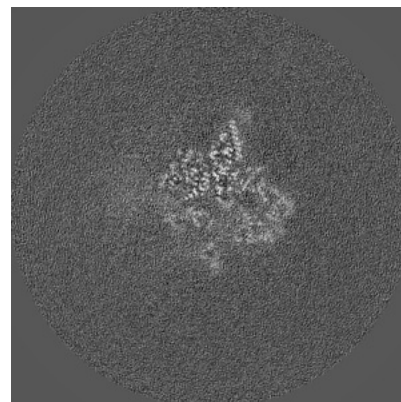
6.3.2 Raw map



X Index: 175



Y Index: 182

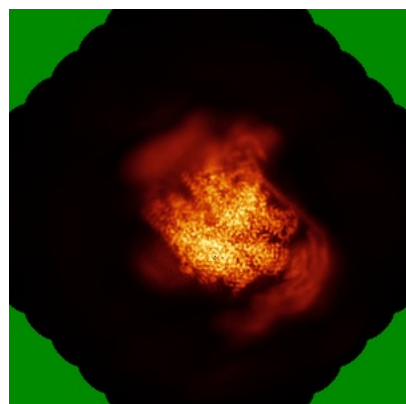


Z Index: 175

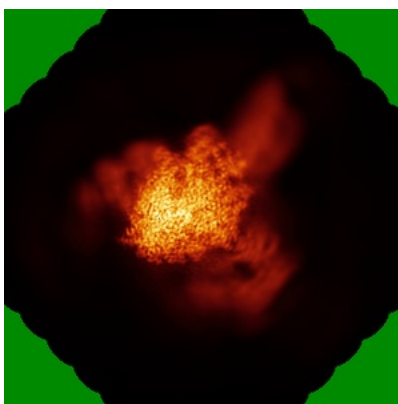
The images above show the largest variance slices of the map in three orthogonal directions.

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

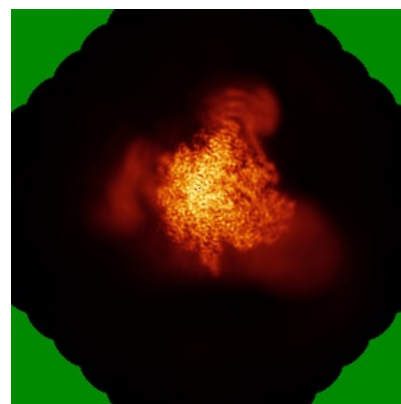
6.4.1 Primary map



X

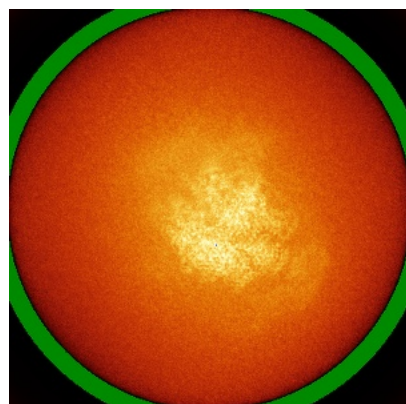


Y

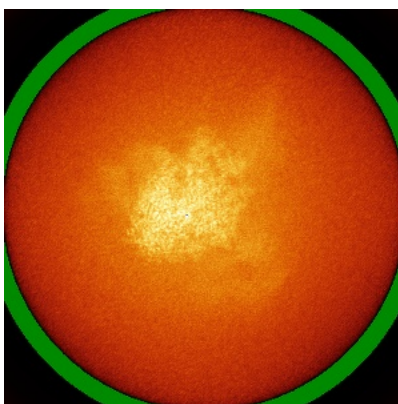


Z

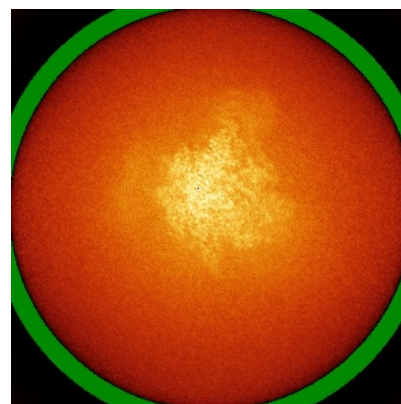
6.4.2 Raw map



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.

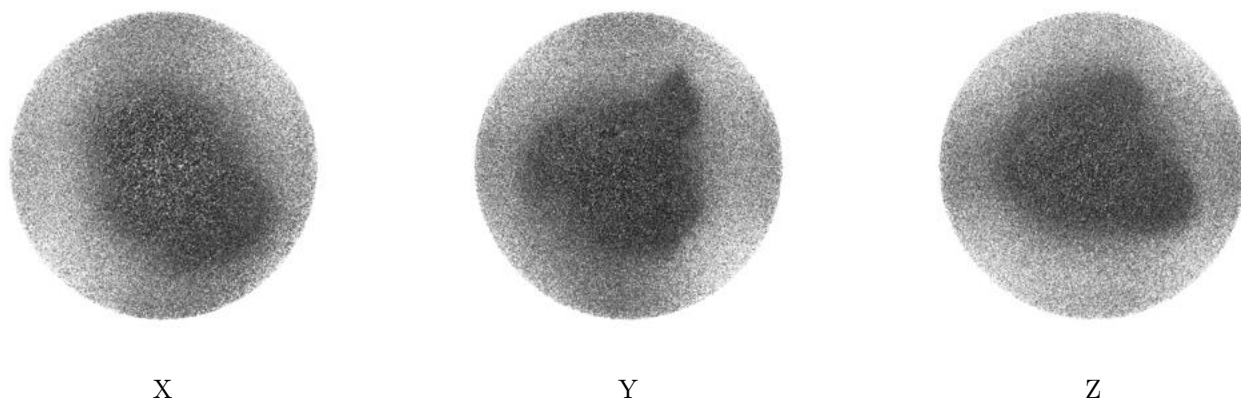
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

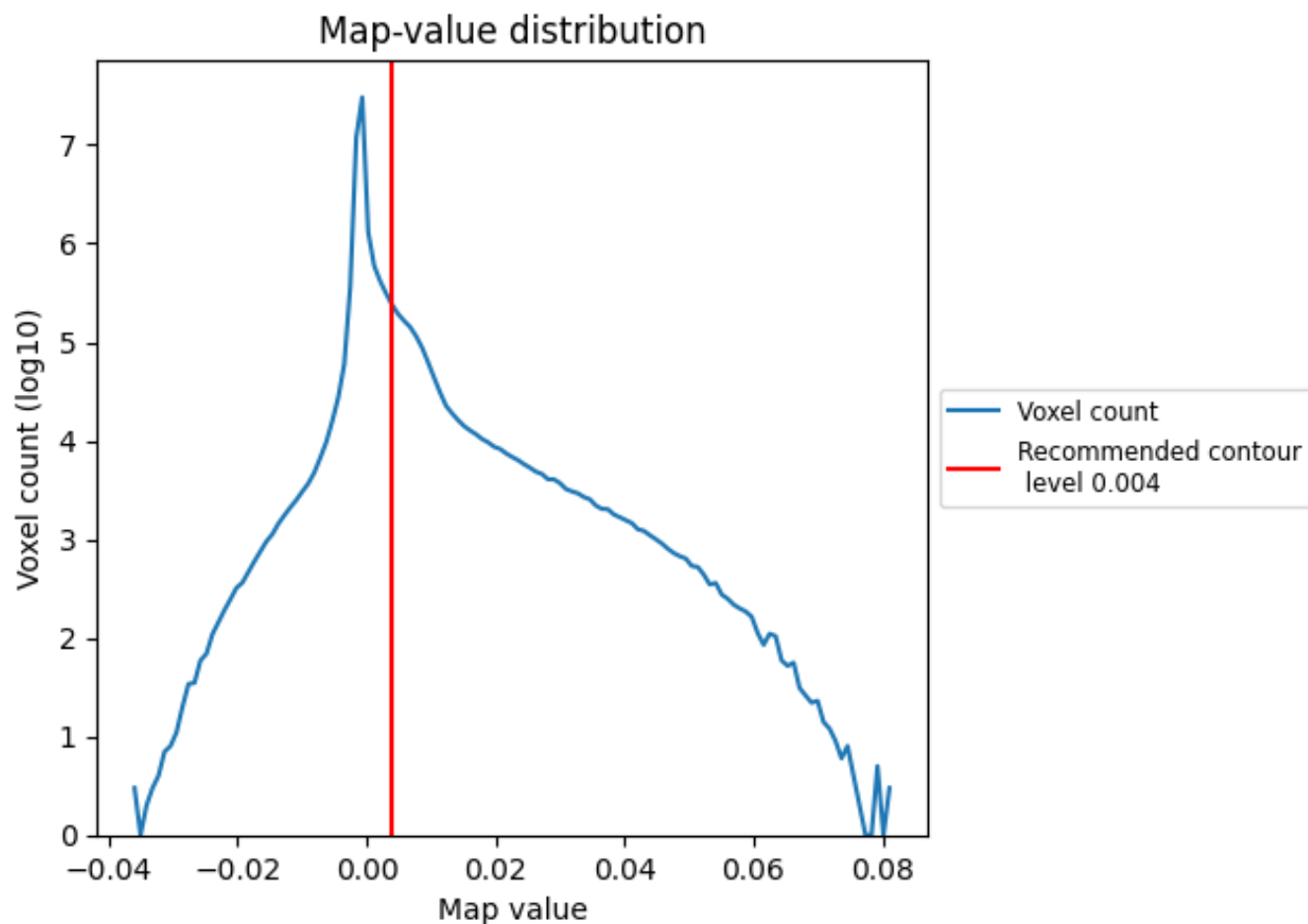
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

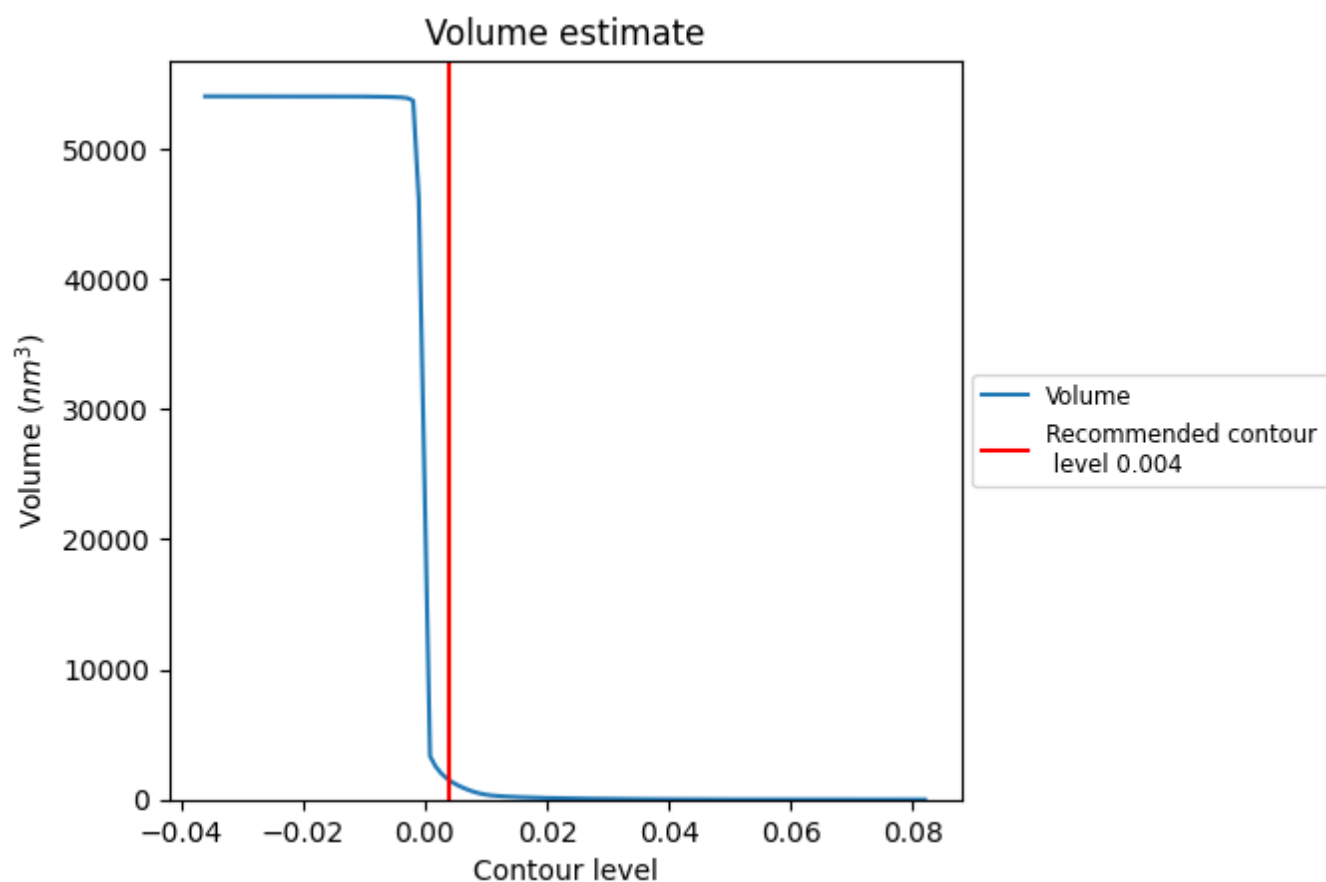
This section contains the results of statistical analysis of the map.

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.

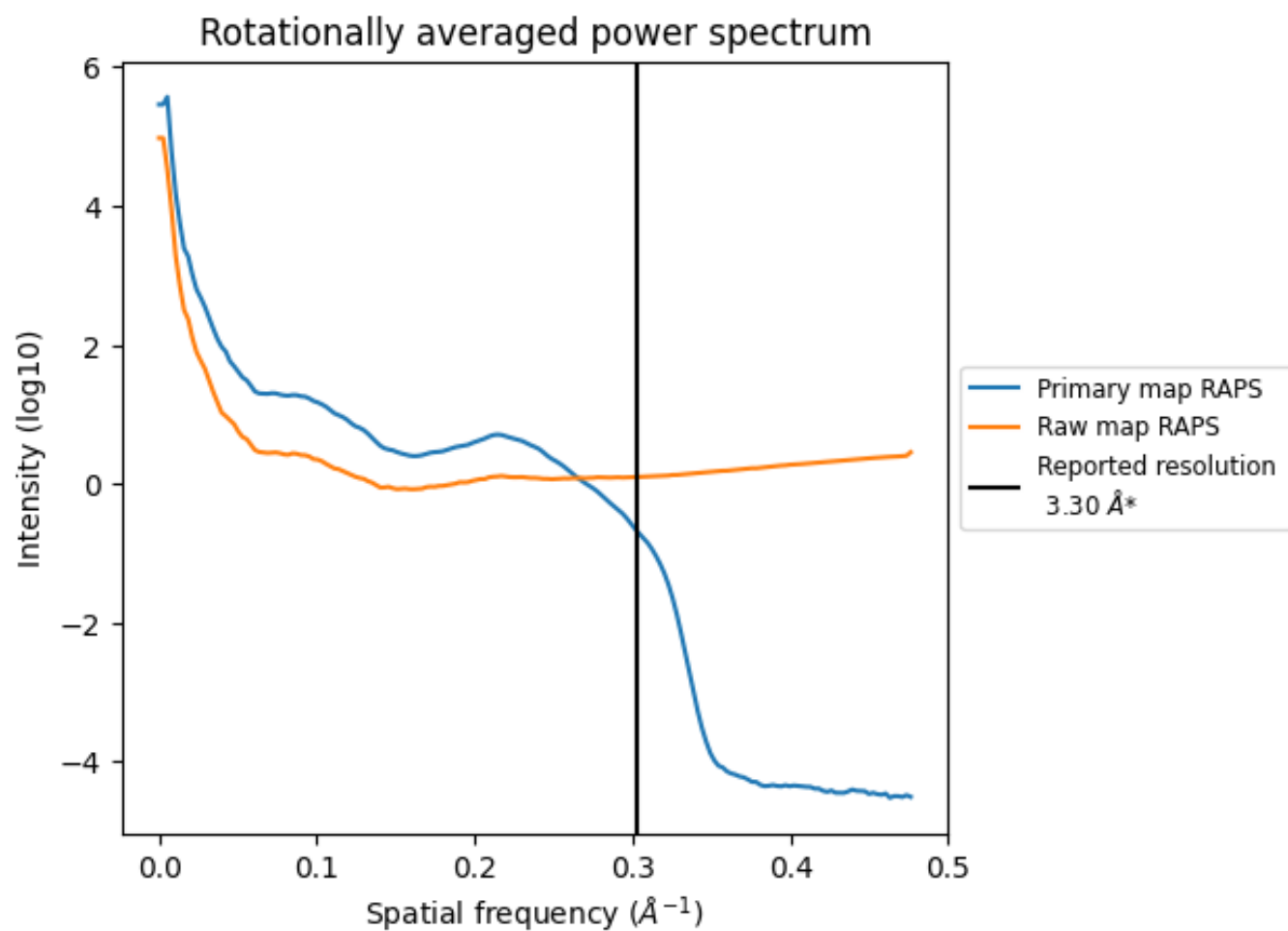
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1502 nm^3 ; this corresponds to an approximate mass of 1357 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 ⓘ

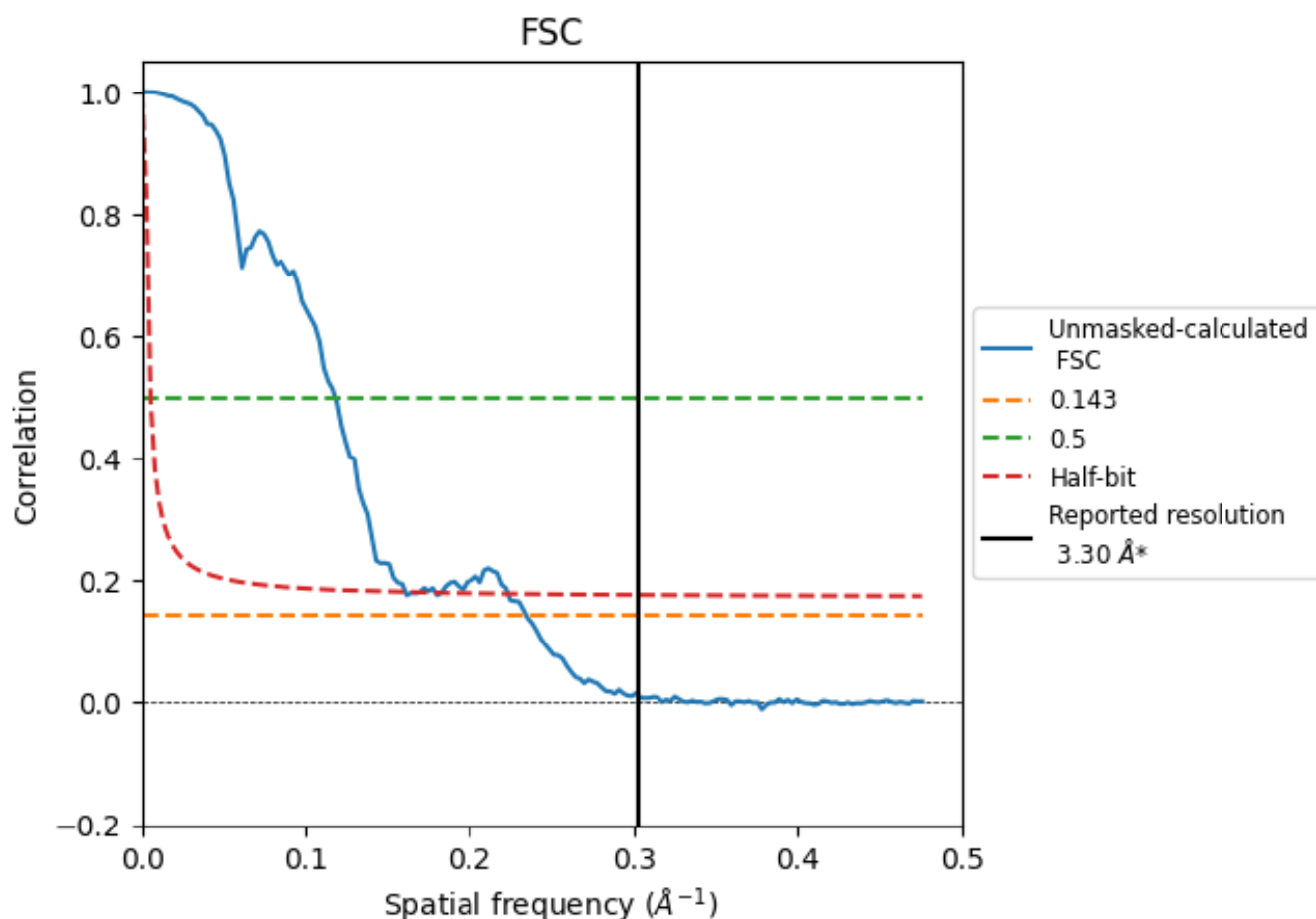


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

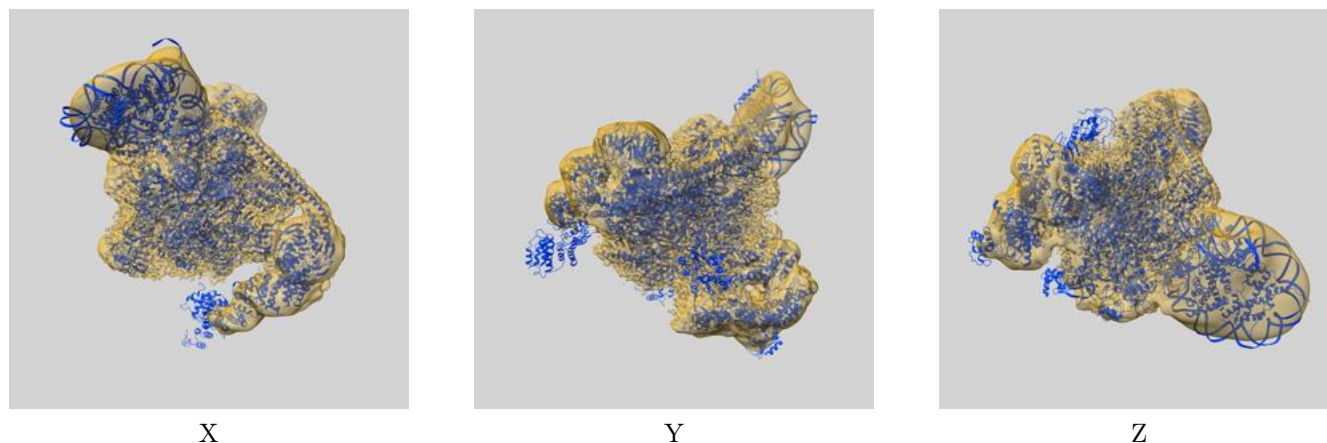
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	8.47	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

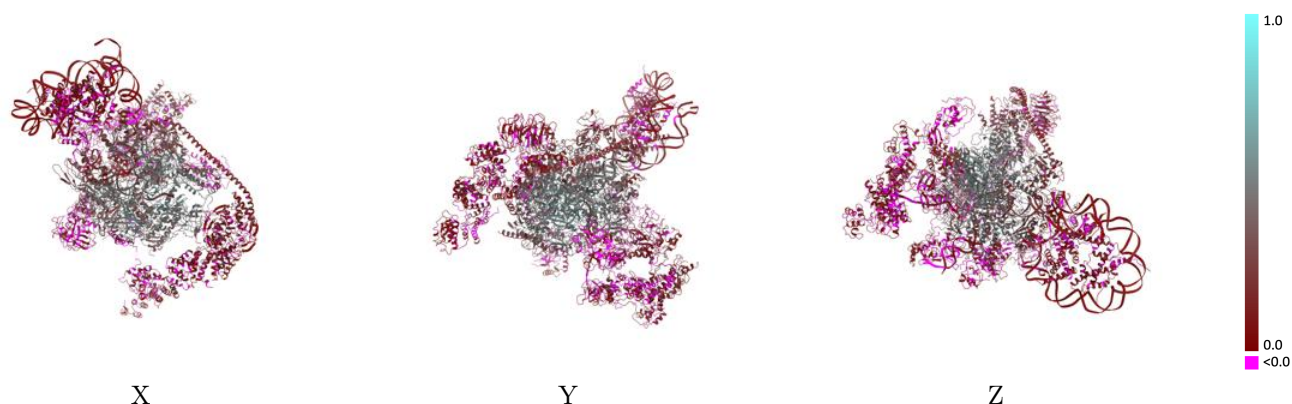
This section contains information regarding the fit between EMDB map EMD-15127 and PDB model 8A3Y. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



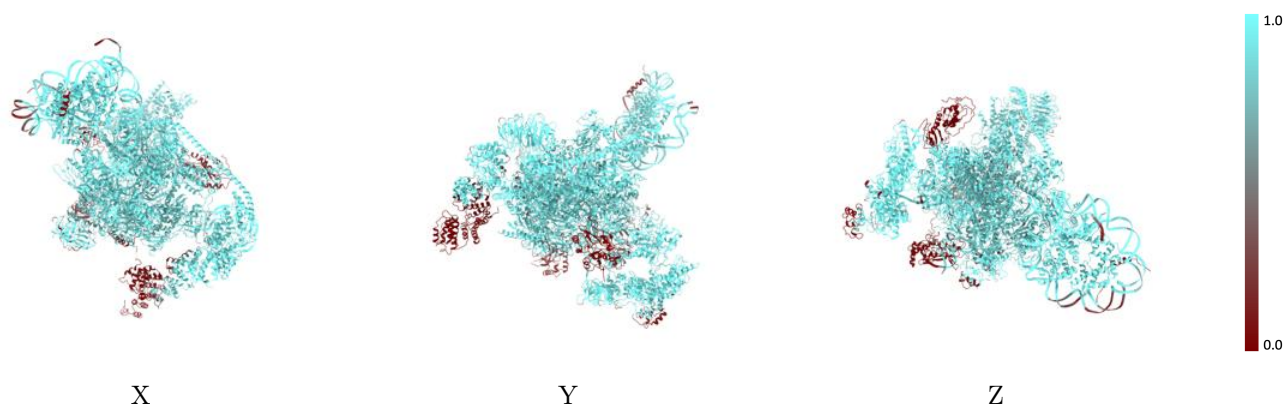
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



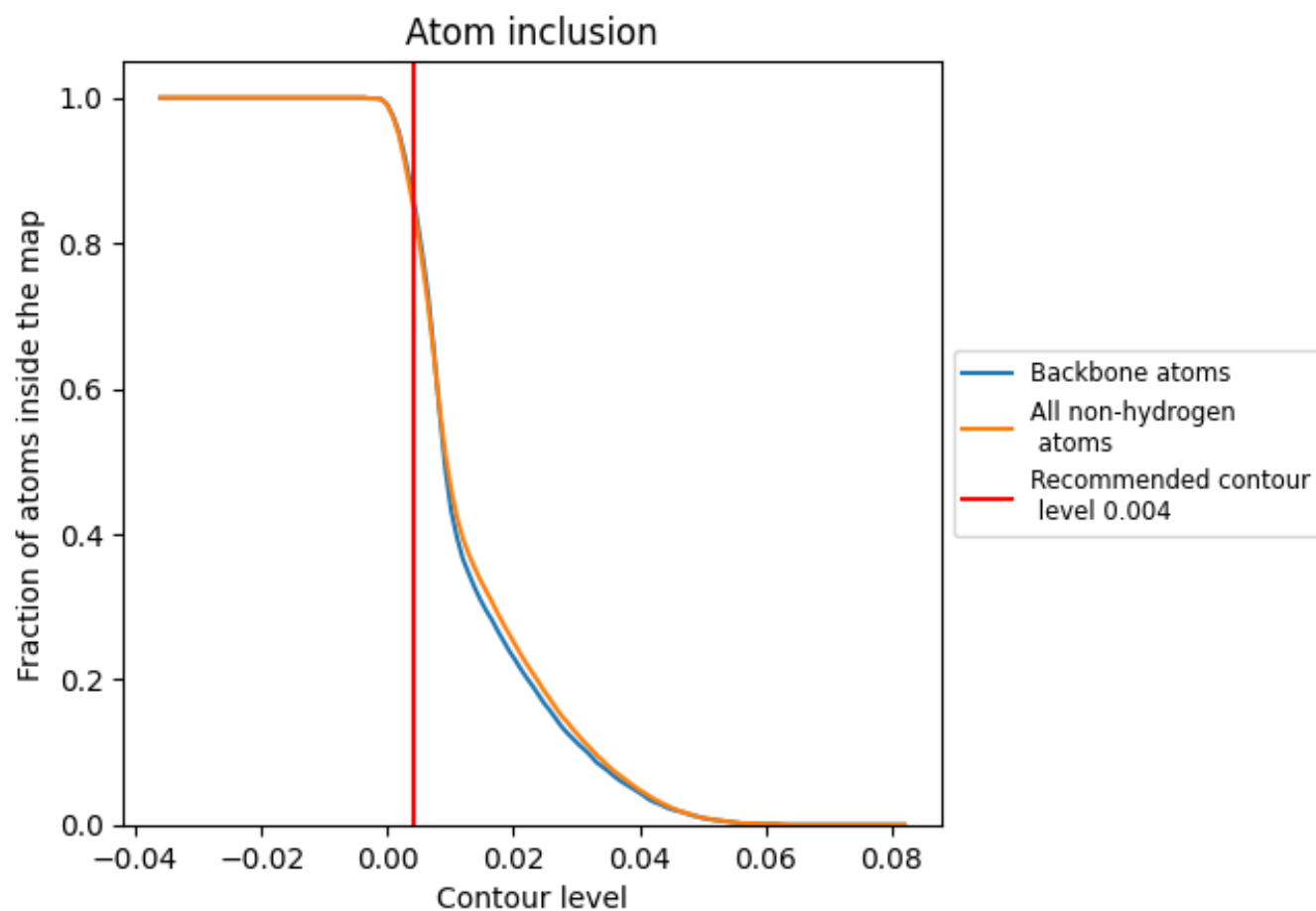
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.2310
A	 0.9610	 0.4150
B	 0.9810	 0.4340
C	 0.9720	 0.4110
D	 0.9750	 0.1460
E	 0.9850	 0.3490
F	 0.9750	 0.4570
G	 0.9780	 0.2040
H	 0.9540	 0.4170
I	 0.9730	 0.2390
J	 0.9790	 0.4590
K	 0.9470	 0.4140
L	 0.9790	 0.3900
M	 0.6510	 0.0520
N	 0.8830	 0.1140
P	 0.9840	 0.2390
Q	 0.6500	 0.1010
R	 0.2380	 0.0400
T	 0.8720	 0.1360
U	 0.8490	 0.0610
V	 0.6360	 0.0580
W	 0.9410	 0.0870
X	 0.9740	 0.1480
Y	 0.8040	 0.0610
Z	 0.7260	 0.0840
a	 0.7730	 0.0370
b	 0.9130	 0.0720
c	 1.0000	 0.0690
d	 0.9900	 0.0620
e	 0.9880	 0.0240
f	 0.9980	 0.0480

