



## wwPDB EM Validation Summary Report ⓘ

Feb 1, 2025 – 12:32 PM EST

PDB ID : 9EH2  
EMDB ID : EMD-48044  
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-SETD2-FACT nucleosome upstream  
Authors : Markert, J.; Farnung, L.  
Deposited on : 2024-11-21  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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

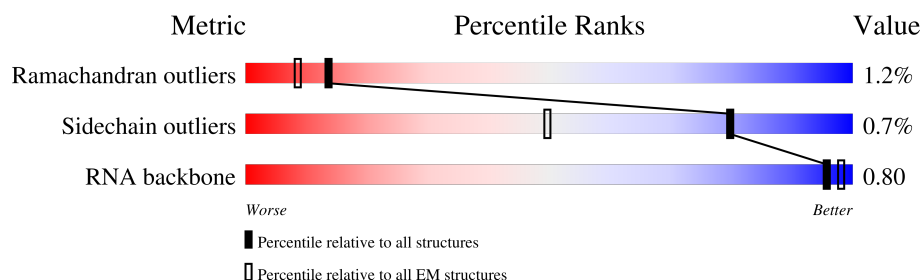


# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	205	
15	O	821	
16	P	11	
17	Q	1179	
18	R	713	
19	S	304	
20	T	215	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	
28	b	103	
28	f	103	
29	g	130	
30	h	123	
31	l	1133	

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Mol	Chain	Length	Quality of chain
32	x	1049	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>44%</div><div>54%</div></div>
33	y	709	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>8%</div><div>59%</div><div>40%</div></div>



## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 148010 atoms, of which 72095 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
			22643	7074	11388	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
			4096	1300	2024	356	410	6		

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

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 RNA polymerase II subunit J.

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
			803	246	406	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	1172	Total	C	H	N	O	S	0	0
			18977	6063	9394	1658	1815	47		

There are 3 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	54	Total	C	N	O	P	0	0
			1106	526	182	344	54		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	132	Total	C	H	N	O	S	0	0
			2143	663	1097	181	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	11	Total	C	N	O	P	0	0
			232	103	35	83	11		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	890	Total	C	H	N	O	S	0	0
			14396	4579	7170	1264	1352	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	283	Total	C	H	N	O	S	0	0
			4222	1349	2056	409	400	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	161	Total	C	H	N	O		0	0
			858	334	201	161	162			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	65	Total	C	N	O	P		0	0
			1335	627	279	364	65			

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	125	Total	C	H	N	O	S	0	0
			1540	538	684	151	166	1		



- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	244	Total	C	H	N	O	S	0	0
			3150	1065	1443	305	333	4		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	300	Total	C	H	N	O	S	0	0
			4582	1483	2249	392	454	4		

- Molecule 24 is a protein called Parafibromin.

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

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	116	Total	C	H	N	O	S	0	0
			1820	570	909	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 P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
26	Z	510	Total	C	H	N	O	P	S	0	0
			8071	2552	4046	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	76	Total	C	H	N	O	S	0	0
			1237	391	621	112	110	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
27	e	75	Total	C	H	N	O	S	0	0
			1225	387	617	111	107	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	78	Total	C	H	N	O	S	0	0
			1283	393	661	120	108	1		
28	f	72	Total	C	H	N	O	S	0	0
			1195	361	619	114	100	1		

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	g	90	Total	C	H	N	O		0	0
			1425	441	721	140	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	h	89	Total	C	H	N	O	S	0	0
			1387	438	693	122	132	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	3	MET	-	initiating methionine	UNP P02281
h	32	THR	SER	engineered mutation	UNP P02281



- Molecule 31 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	23	Total	C	H	N	O	0	0
			395	119	200	35	41		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	1432	SER	-	expression tag	UNP Q9BYW2
l	1433	ASN	-	expression tag	UNP Q9BYW2
l	1434	ALA	-	expression tag	UNP Q9BYW2
l	1962	LEU	PRO	conflict	UNP Q9BYW2

- Molecule 32 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	x	483	Total	C	H	N	O	S	0	0
			7818	2506	3870	682	743	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-1	SER	-	expression tag	UNP Q9Y5B9
x	0	ASN	-	expression tag	UNP Q9Y5B9

- Molecule 33 is a protein called FACT complex subunit SSRP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	y	422	Total	C	H	N	O	S	0	0
			6842	2201	3406	585	635	15		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

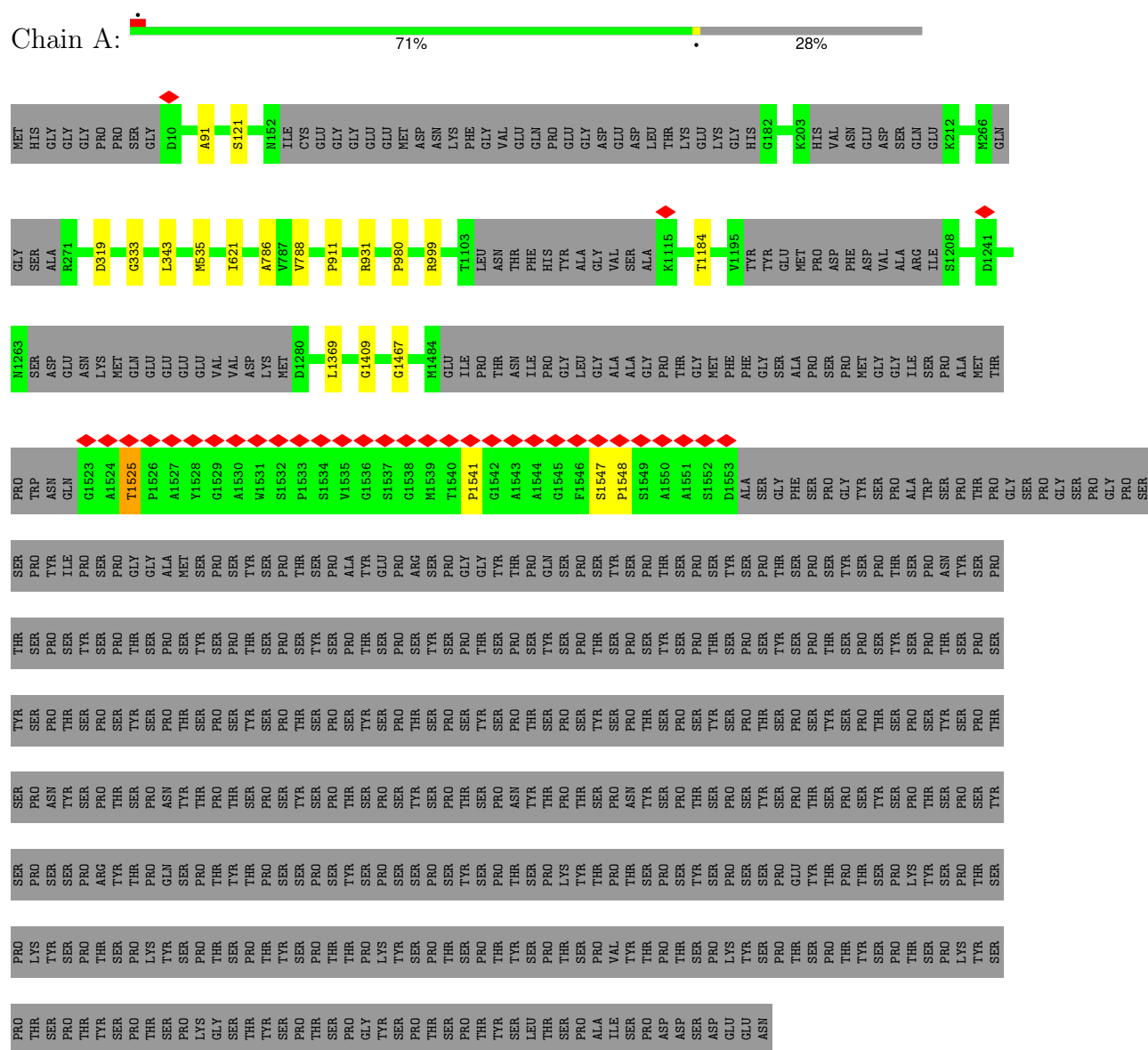
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total 1	Mg 1	0



### 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.

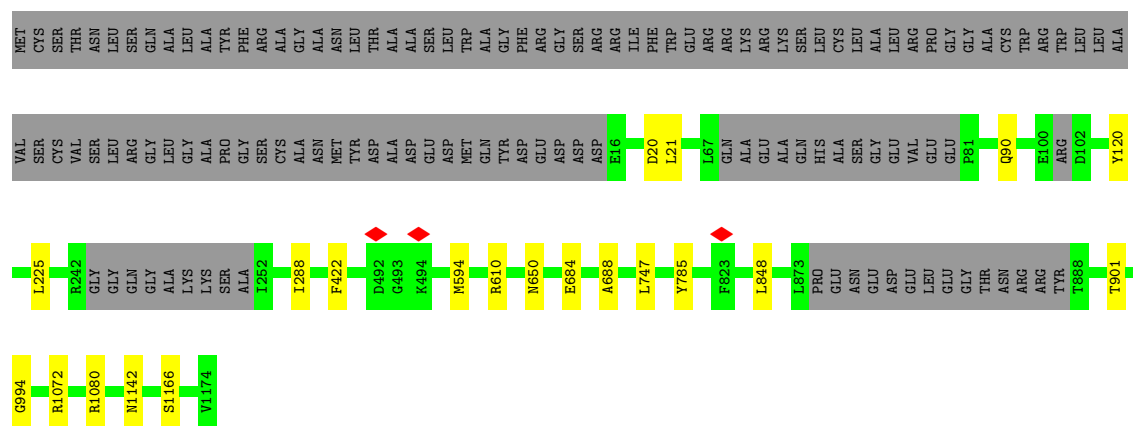
- Molecule 1: DNA-directed RNA polymerase subunit



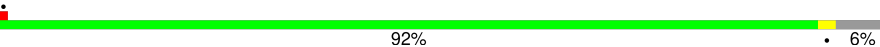
- Molecule 2: DNA-directed RNA polymerase subunit beta



Chain B:  88% • 10%




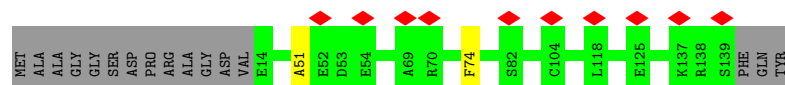
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:  92% • 6%



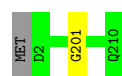
- Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D:  7% 87% • 11%



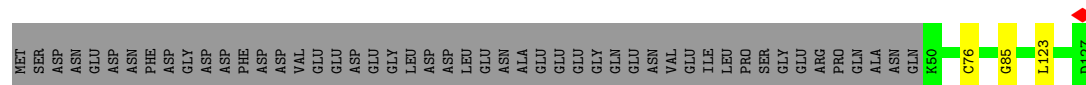
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  99%



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

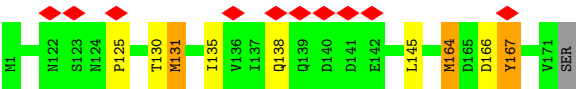
Chain F:  59% • 39%



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

Chain G:  6% 94% • • •

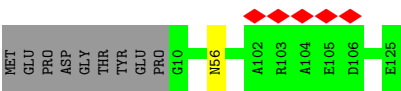
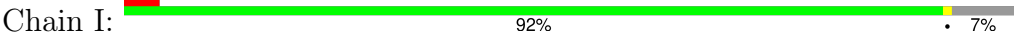




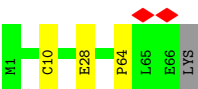
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



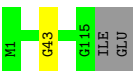
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



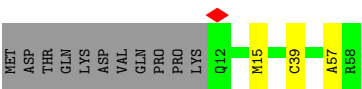
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



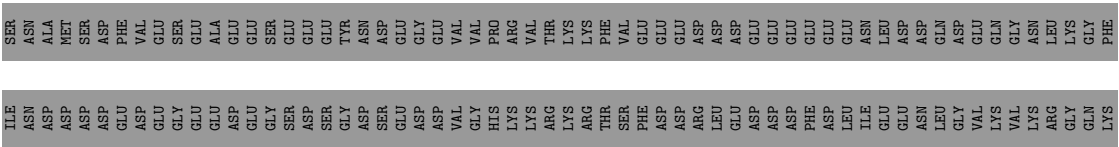
- Molecule 11: RNA polymerase II subunit J



- Molecule 12: RNA polymerase II subunit K



- Molecule 13: Transcription elongation factor SPT6



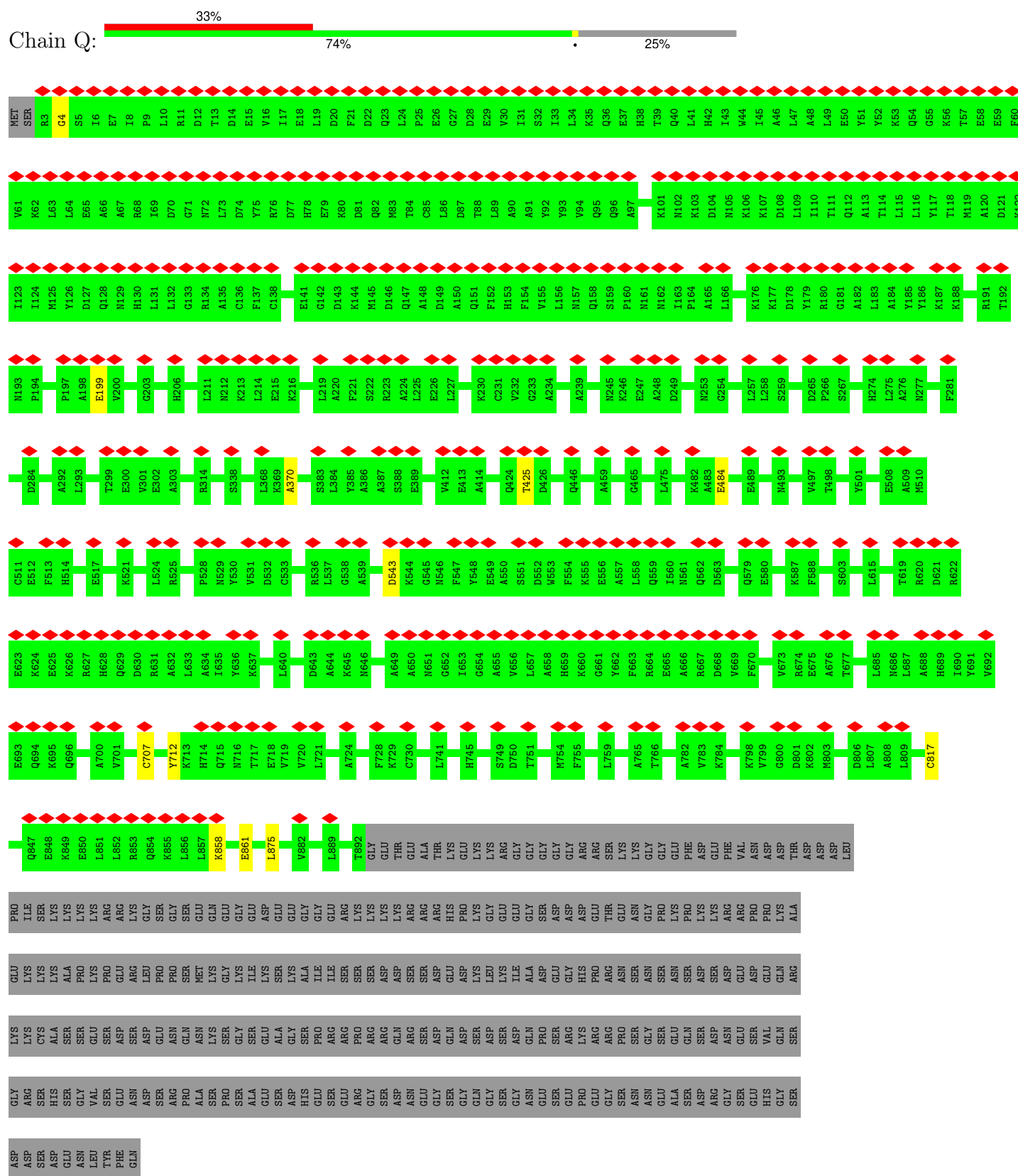












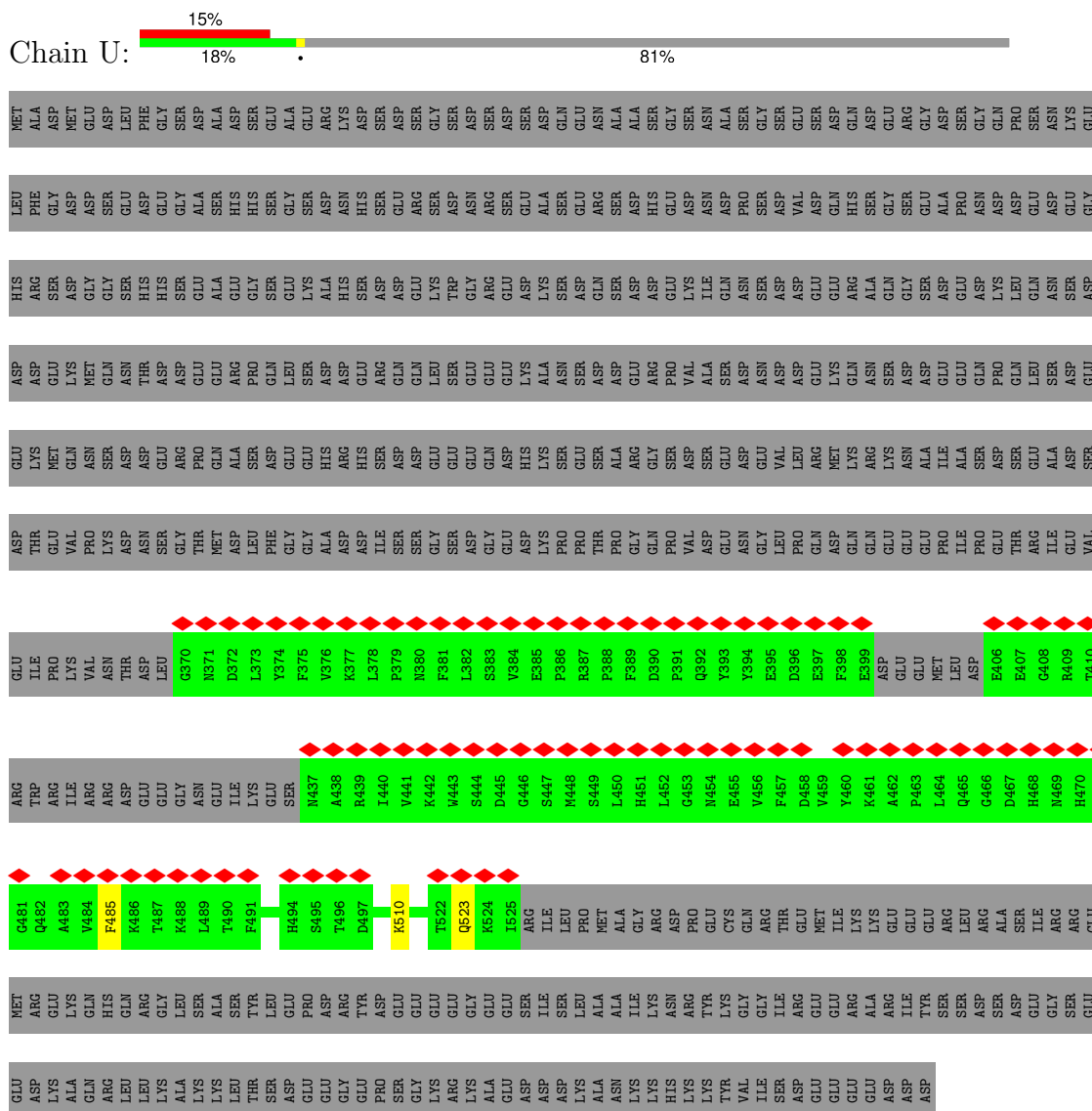
- Molecule 18: RNA polymerase-associated protein RTF1 homolog



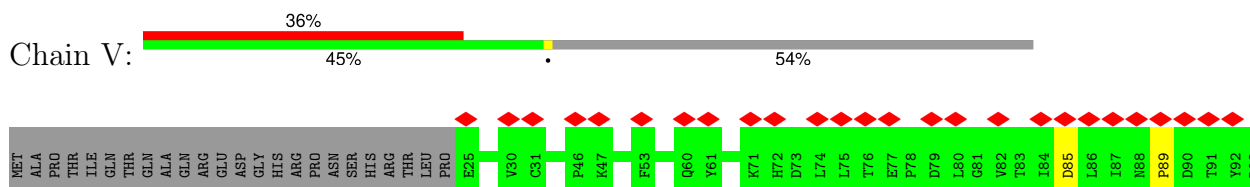




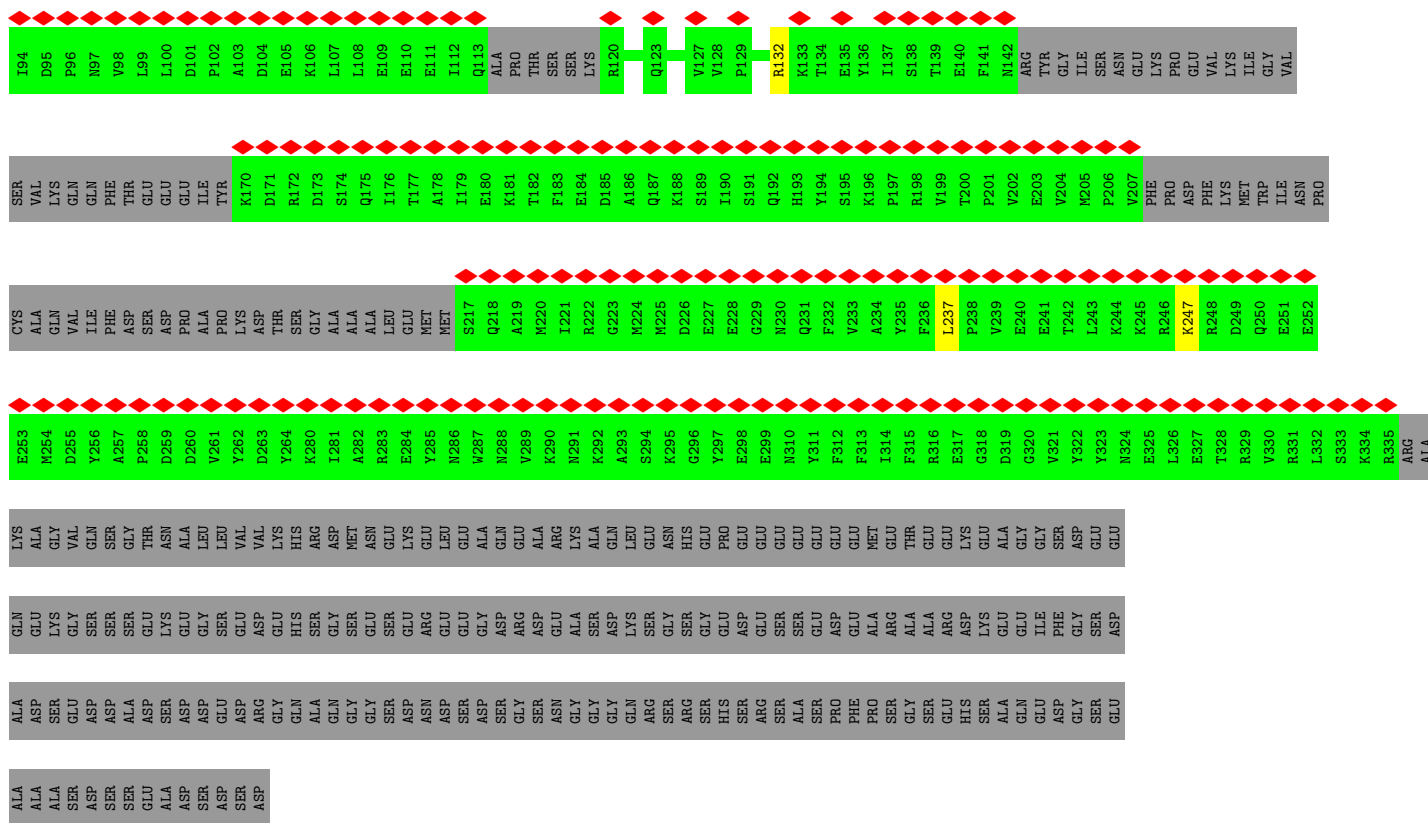
- Molecule 21: RNA polymerase-associated protein LEO1



- Molecule 22: RNA polymerase II-associated factor 1 homolog



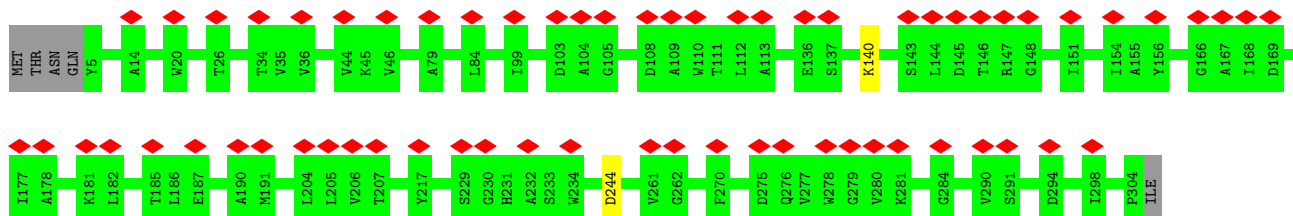




- Molecule 23: WDR61



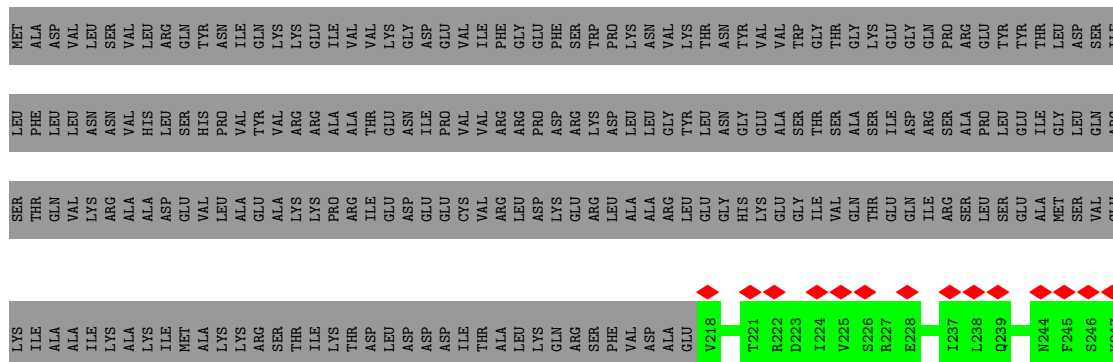
Chain W:



- Molecule 24: Parafibromin



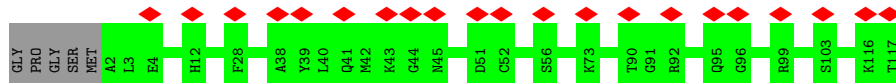
Chain X:



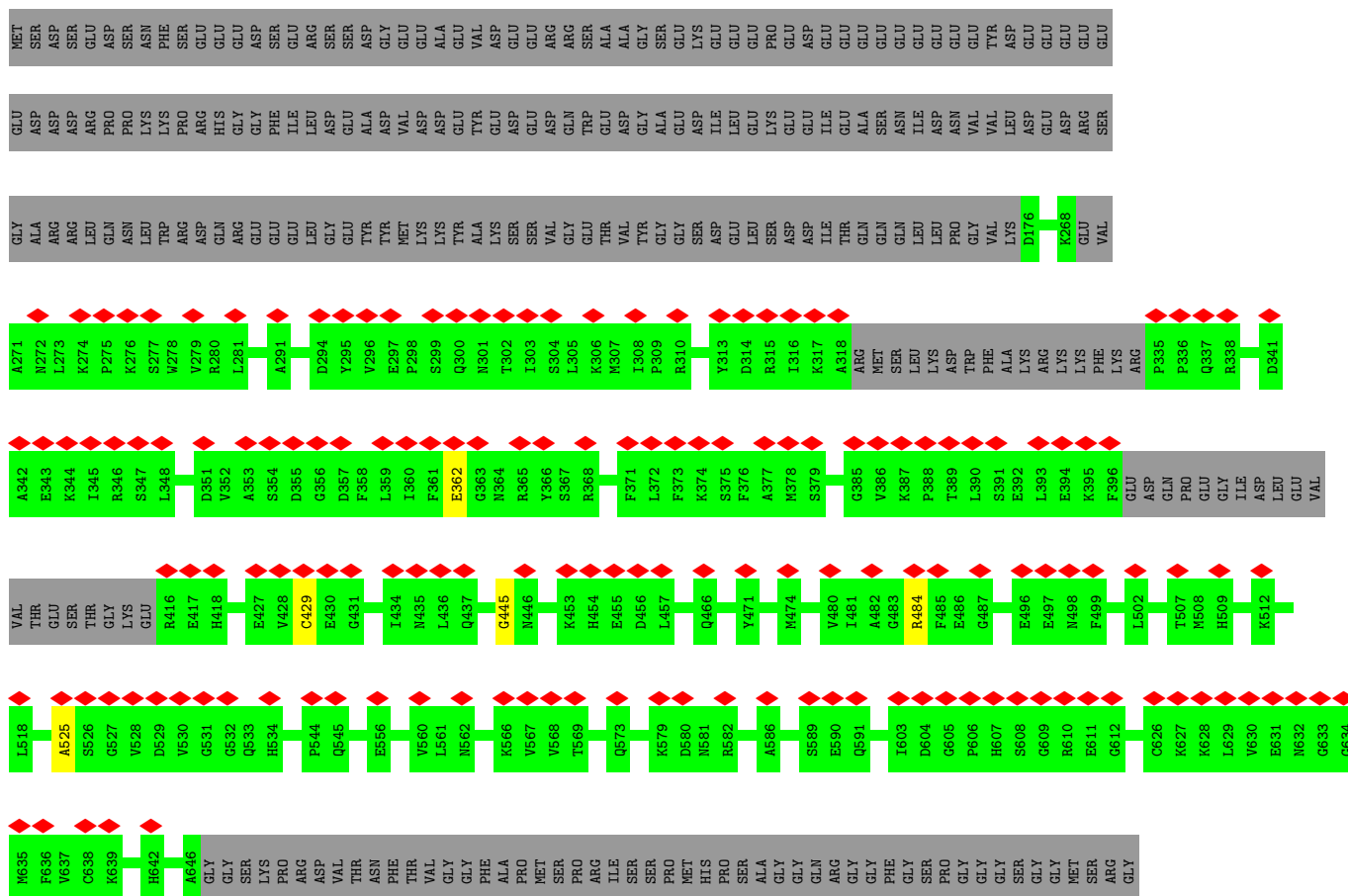




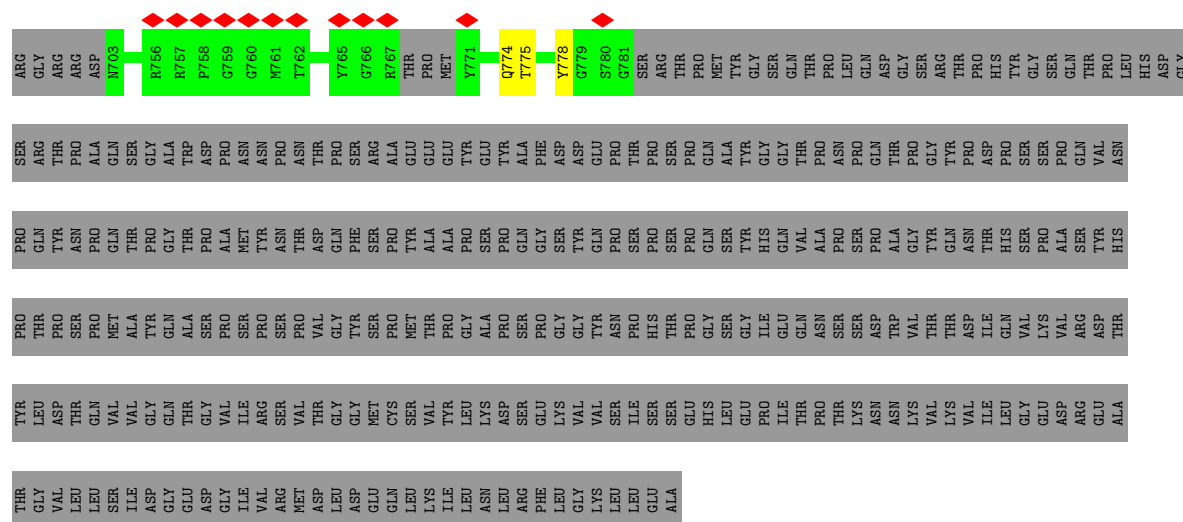
- Molecule 25: Transcription elongation factor SPT4



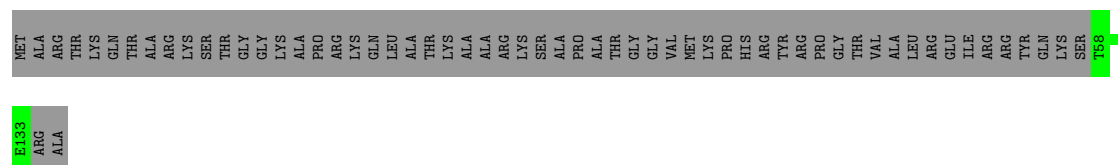
- Molecule 26: Transcription elongation factor SPT5



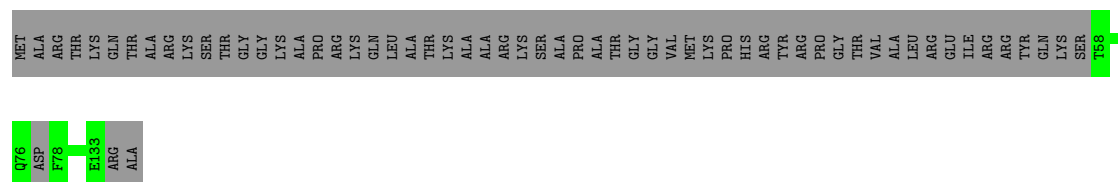




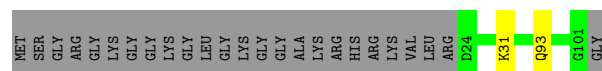
- Molecule 27: Histone H3



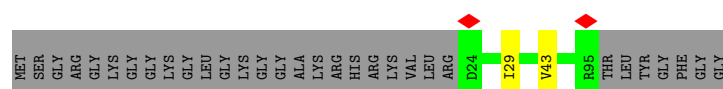
- Molecule 27: Histone H3



- Molecule 28: Histone H4



- Molecule 28: Histone H4



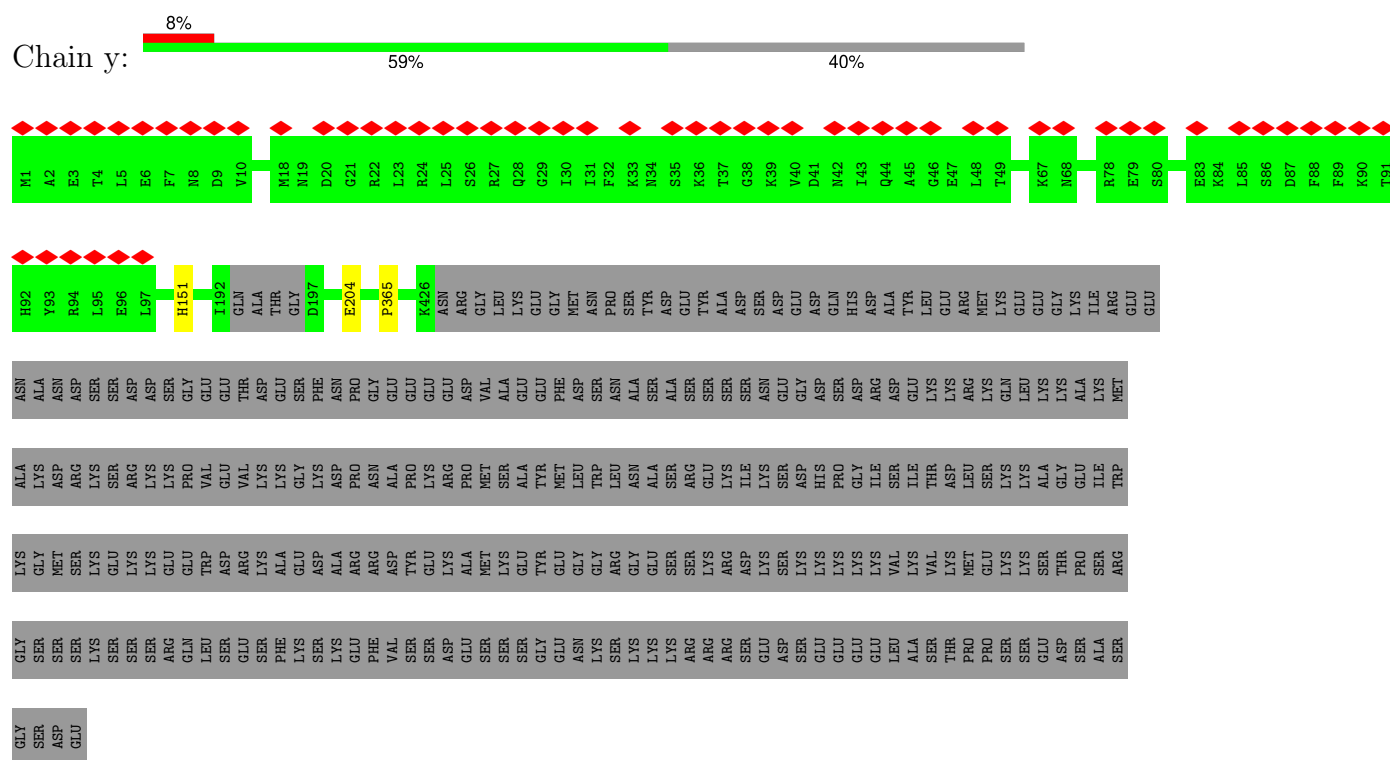














## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74820	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.008	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	535.5, 535.5, 535.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, 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	0.36	0/11437	0.58	0/15433
2	B	0.38	0/9158	0.58	0/12360
3	C	0.36	0/2115	0.56	0/2873
4	D	0.30	0/1017	0.51	0/1368
5	E	0.36	0/1751	0.58	0/2366
6	F	0.38	0/636	0.60	0/859
7	G	0.36	0/1364	0.61	0/1853
8	H	0.38	0/1219	0.60	0/1644
9	I	0.34	0/964	0.55	0/1305
10	J	0.39	0/533	0.55	0/719
11	K	0.34	0/939	0.52	0/1271
12	L	0.42	0/403	0.67	0/536
13	M	0.33	0/9783	0.52	0/13201
14	N	0.79	0/1232	1.04	0/1900
15	O	0.23	0/1062	0.41	0/1428
16	P	0.61	0/257	1.03	0/398
17	Q	0.26	0/7365	0.45	0/9927
18	R	0.25	0/2195	0.47	0/2947
19	S	0.23	0/659	0.45	0/827
20	T	0.90	0/1506	0.87	0/2318
21	U	0.25	0/870	0.45	0/1183
22	V	0.25	0/1734	0.48	0/2367
23	W	0.26	0/2392	0.47	0/3257
24	X	0.25	0/356	0.54	0/478
25	Y	0.27	0/927	0.51	0/1250
26	Z	0.27	0/4084	0.51	0/5498
27	a	0.34	0/623	0.57	0/837
27	e	0.34	0/615	0.57	0/826
28	b	0.31	0/629	0.59	0/843
28	f	0.29	0/581	0.59	0/778
29	g	0.32	0/712	0.58	0/959
30	h	0.32	0/705	0.49	0/951



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	l	0.29	0/196	0.50	0/261
32	x	0.35	0/4033	0.55	2/5438 (0.0%)
33	y	0.31	0/3513	0.52	0/4734
All	All	0.36	0/77565	0.56	2/105193 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	x	463	ARG	NE-CZ-NH1	7.09	123.85	120.30
32	x	463	ARG	N-CA-C	-5.04	97.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1525	TPO	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	1244 (88%)	148 (10%)	16 (1%)	12	39
2	B	1112/1251 (89%)	972 (87%)	123 (11%)	17 (2%)	8	33
3	C	254/275 (92%)	221 (87%)	28 (11%)	5 (2%)	6	26
4	D	124/142 (87%)	111 (90%)	12 (10%)	1 (1%)	16	48
5	E	207/210 (99%)	187 (90%)	19 (9%)	1 (0%)	25	58
6	F	76/127 (60%)	69 (91%)	5 (7%)	2 (3%)	4	21
7	G	169/172 (98%)	143 (85%)	20 (12%)	6 (4%)	3	16
8	H	147/150 (98%)	125 (85%)	22 (15%)	0	100	100
9	I	114/125 (91%)	98 (86%)	16 (14%)	0	100	100
10	J	64/67 (96%)	55 (86%)	6 (9%)	3 (5%)	2	12
11	K	113/117 (97%)	105 (93%)	7 (6%)	1 (1%)	14	45
12	L	45/58 (78%)	39 (87%)	3 (7%)	3 (7%)	1	6
13	M	1154/1729 (67%)	1045 (91%)	93 (8%)	16 (1%)	9	34
15	O	130/821 (16%)	124 (95%)	5 (4%)	1 (1%)	16	48
17	Q	888/1179 (75%)	804 (90%)	78 (9%)	6 (1%)	19	51
18	R	277/713 (39%)	256 (92%)	21 (8%)	0	100	100
19	S	157/304 (52%)	149 (95%)	6 (4%)	2 (1%)	10	36
21	U	117/666 (18%)	95 (81%)	18 (15%)	4 (3%)	3	17
22	V	234/531 (44%)	194 (83%)	37 (16%)	3 (1%)	10	36
23	W	298/305 (98%)	259 (87%)	37 (12%)	2 (1%)	19	51
24	X	41/531 (8%)	38 (93%)	3 (7%)	0	100	100
25	Y	114/121 (94%)	98 (86%)	16 (14%)	0	100	100
26	Z	497/1087 (46%)	422 (85%)	70 (14%)	5 (1%)	13	42
27	a	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
27	e	73/136 (54%)	70 (96%)	3 (4%)	0	100	100
28	b	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
28	f	70/103 (68%)	65 (93%)	3 (4%)	2 (3%)	3	20
29	g	88/130 (68%)	85 (97%)	3 (3%)	0	100	100
30	h	87/123 (71%)	81 (93%)	6 (7%)	0	100	100
31	l	21/1133 (2%)	19 (90%)	2 (10%)	0	100	100
32	x	479/1049 (46%)	427 (89%)	40 (8%)	12 (2%)	4	22
33	y	418/709 (59%)	386 (92%)	29 (7%)	3 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9126/16287 (56%)	8130 (89%)	885 (10%)	111 (1%)	14	38

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	130	THR
7	G	167	TYR
12	L	39	CYS
13	M	570	ALA
13	M	1057	ARG

### 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%)	1242 (100%)	3 (0%)	92	96
2	B	986/1084 (91%)	982 (100%)	4 (0%)	89	94
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/126 (86%)	108 (99%)	1 (1%)	75	88
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	67 (98%)	1 (2%)	60	80
7	G	146/153 (95%)	140 (96%)	6 (4%)	26	57
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	104/112 (93%)	103 (99%)	1 (1%)	73	86
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	1037/1524 (68%)	1020 (98%)	17 (2%)	58	79
15	O	118/737 (16%)	116 (98%)	2 (2%)	56	78
17	Q	761/1011 (75%)	755 (99%)	6 (1%)	79	89
18	R	205/625 (33%)	203 (99%)	2 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	4/268 (2%)	4 (100%)	0	100	100
21	U	65/590 (11%)	65 (100%)	0	100	100
22	V	146/462 (32%)	144 (99%)	2 (1%)	62	81
23	W	255/260 (98%)	255 (100%)	0	100	100
24	X	40/467 (9%)	40 (100%)	0	100	100
25	Y	102/105 (97%)	102 (100%)	0	100	100
26	Z	435/939 (46%)	433 (100%)	2 (0%)	86	92
27	a	66/111 (60%)	66 (100%)	0	100	100
27	e	65/111 (59%)	65 (100%)	0	100	100
28	b	64/79 (81%)	62 (97%)	2 (3%)	35	63
28	f	60/79 (76%)	60 (100%)	0	100	100
29	g	71/102 (70%)	70 (99%)	1 (1%)	62	81
30	h	76/103 (74%)	75 (99%)	1 (1%)	65	82
31	l	23/1017 (2%)	23 (100%)	0	100	100
32	x	431/929 (46%)	426 (99%)	5 (1%)	67	83
33	y	379/631 (60%)	379 (100%)	0	100	100
All	All	7820/14289 (55%)	7764 (99%)	56 (1%)	80	90

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	1153	LEU
32	x	828	THR
17	Q	543	ASP
32	x	504	LYS
29	g	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	775	ASN
32	x	617	ASN
18	R	264	ASN
23	W	273	HIS
32	x	949	ASN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/11 (100%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	52	G
16	P	54	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	51	G
16	P	53	C

## 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$
26	TPO	Z	775	26	8,10,11	1.13	0	10,14,16	1.91	1 (10%)
1	SEP	A	1547	1	8,9,10	1.61	1 (12%)	7,12,14	1.35	1 (14%)
1	TPO	A	1525	1	8,10,11	1.09	0	10,14,16	2.97	3 (30%)

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
26	TPO	Z	775	26	-	2/9/11/13	-
1	SEP	A	1547	1	-	0/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	1525	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.52	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	CG2-CB-CA	-6.50	100.60	113.26
1	A	1525	TPO	P-OG1-CB	-5.65	107.96	123.33
26	Z	775	TPO	P-OG1-CB	-5.29	108.96	123.33
1	A	1525	TPO	O-C-CA	-3.11	116.77	124.77
1	A	1547	SEP	OG-CB-CA	2.97	111.04	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	O-C-CA-CB
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

## 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.05
1	V	299:GLU	C	310:ASN	N	12.58
1	M	1334:ASN	C	1338:ILE	N	9.04



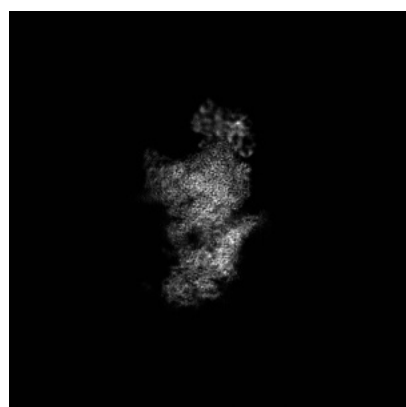
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48044. These allow visual inspection of the internal detail of the map and identification of artifacts.

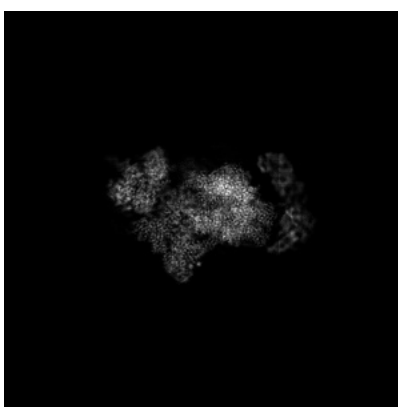
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

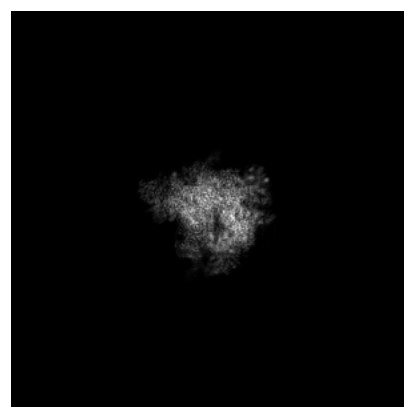
#### 6.1.1 Primary map



X



Y



Z

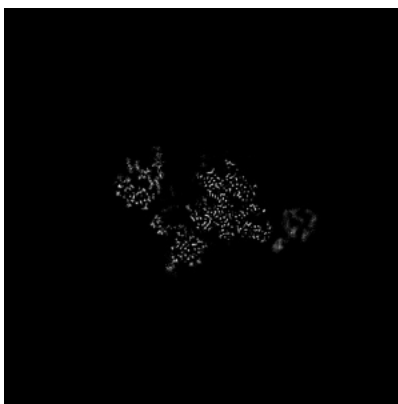
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 225



Y Index: 225



Z Index: 225



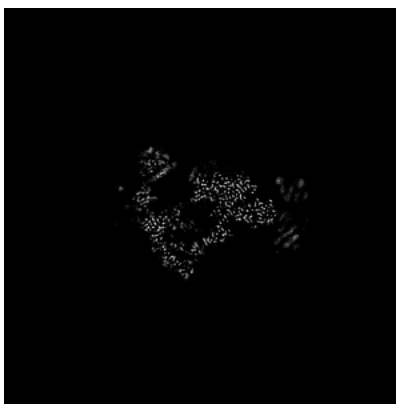
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 251



Y Index: 238

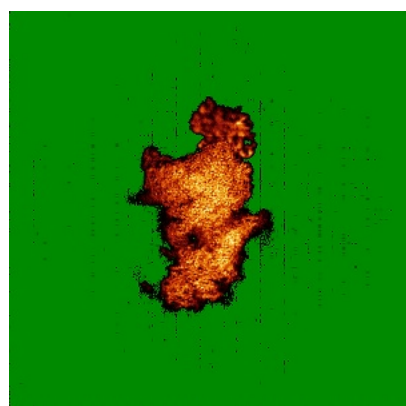


Z Index: 250

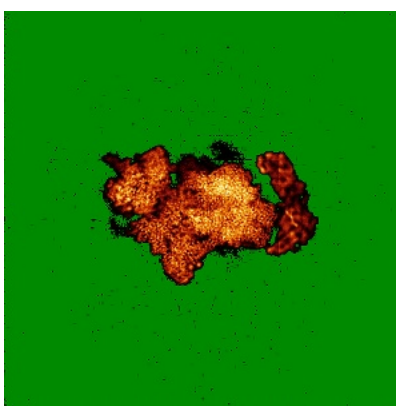
The images above show the largest variance slices of the map in three orthogonal directions.

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

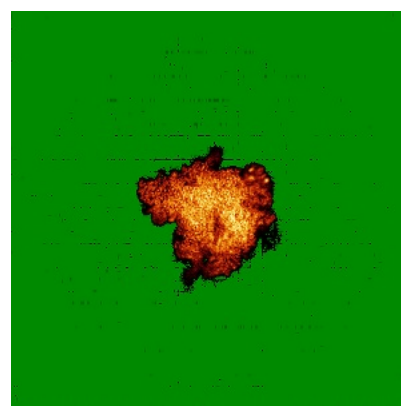
### 6.4.1 Primary map



X



Y



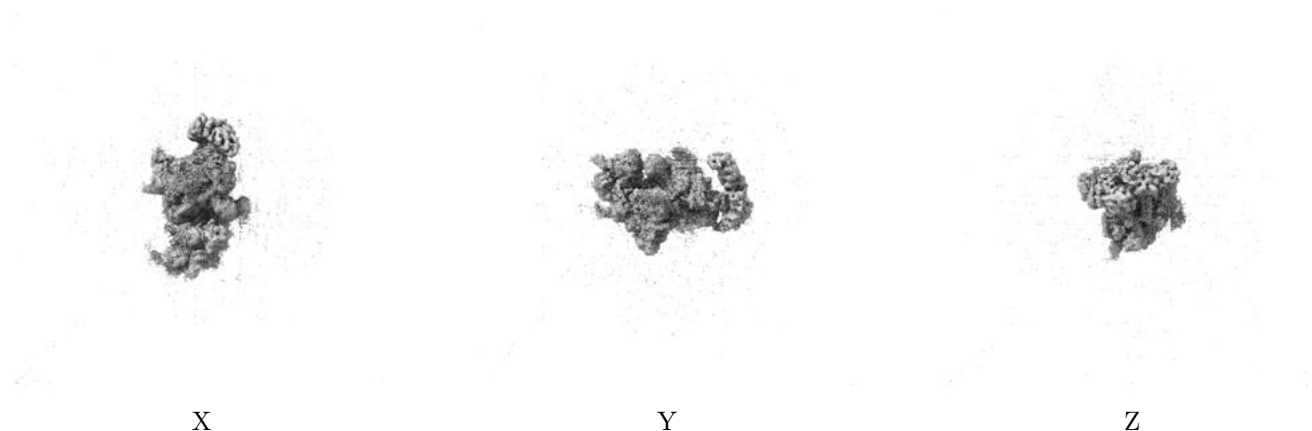
Z

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 0.01. 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](#)

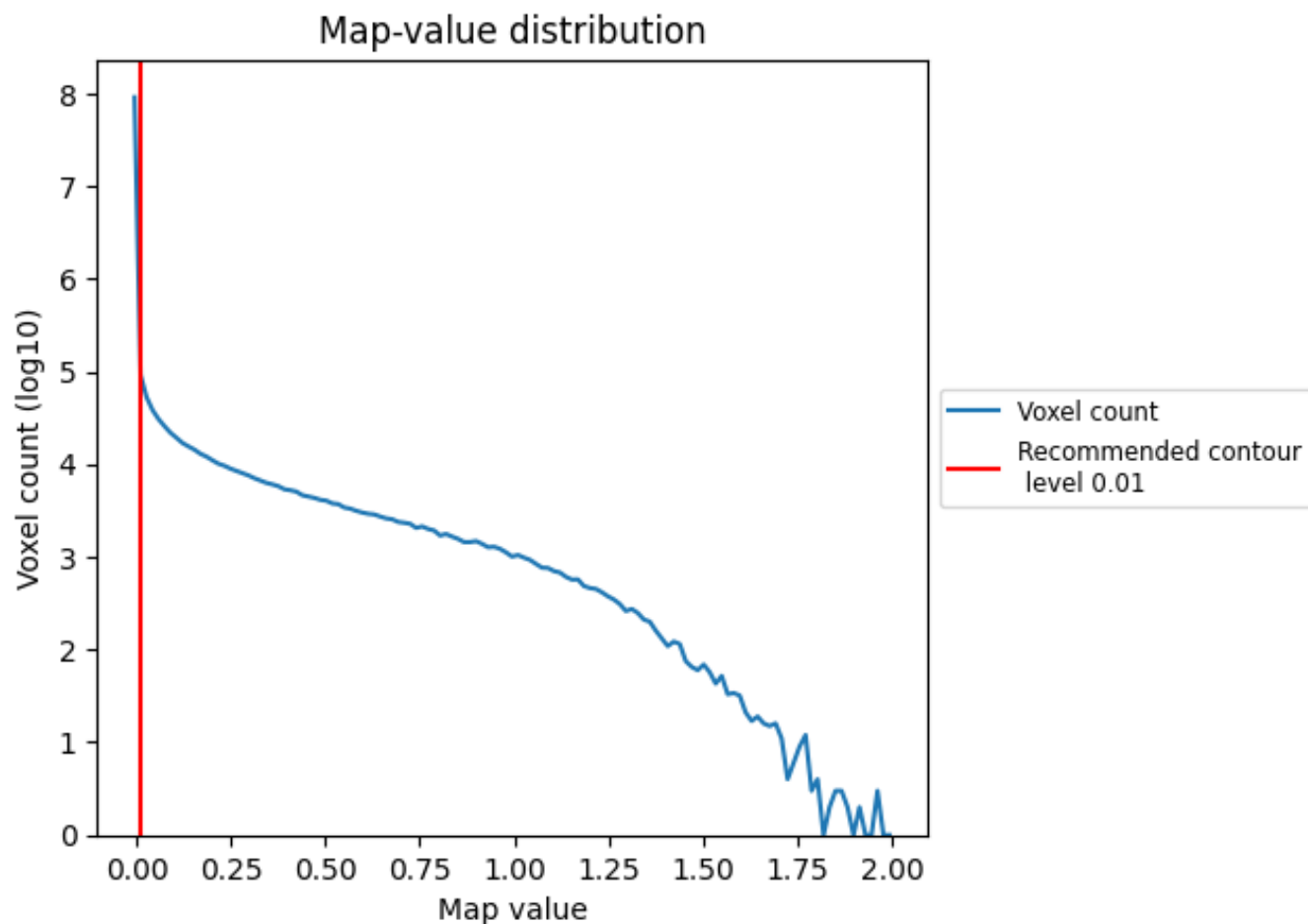
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

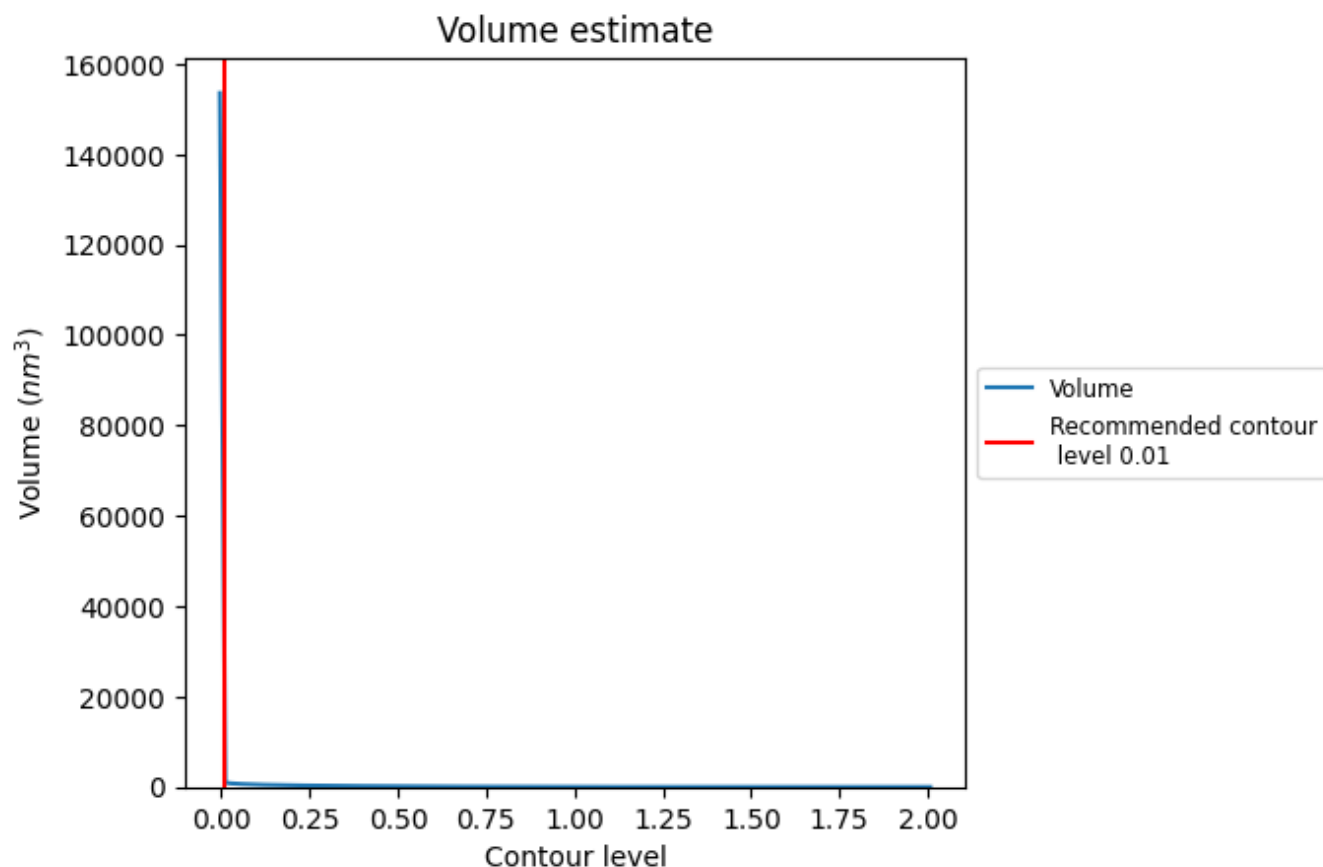
### 7.1 Map-value distribution [i](#)



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](#)

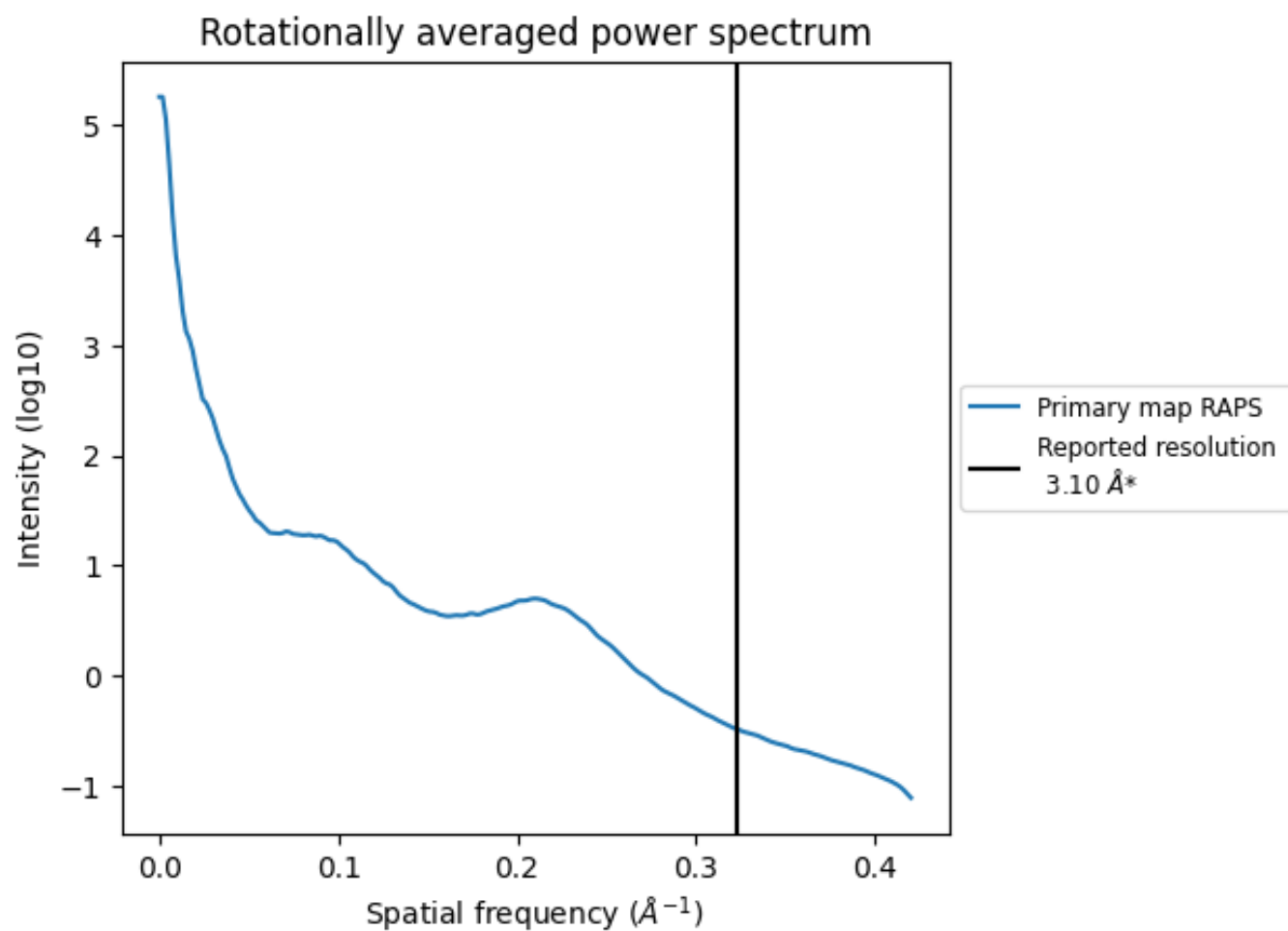


The volume at the recommended contour level is 14275  $\text{nm}^3$ ; this corresponds to an approximate mass of 12895 kDa.

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 0.323 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

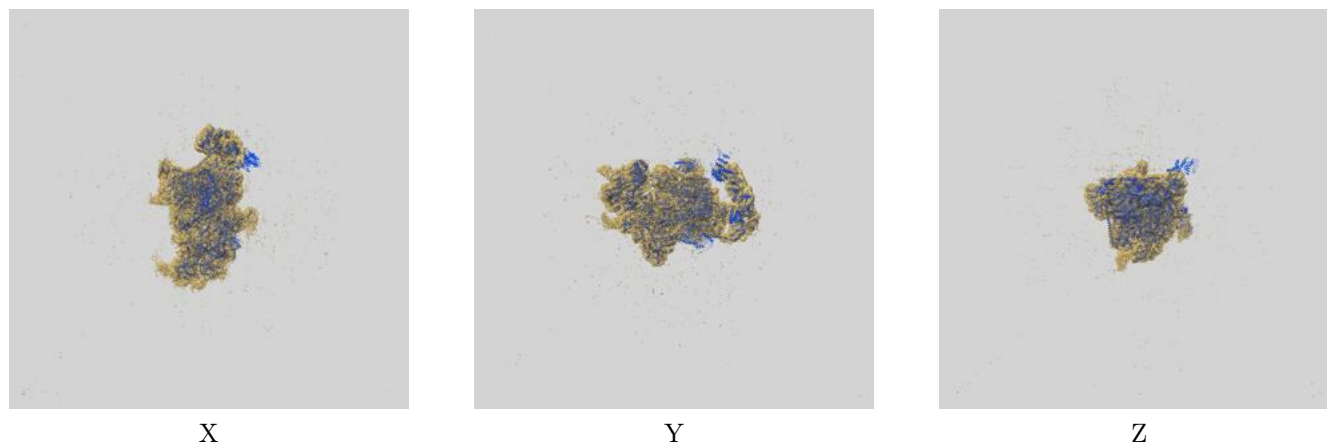
This section was not generated. No FSC curve or half-maps provided.



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

This section contains information regarding the fit between EMDB map EMD-48044 and PDB model 9EH2. Per-residue inclusion information can be found in section [3](#) on page [13](#).

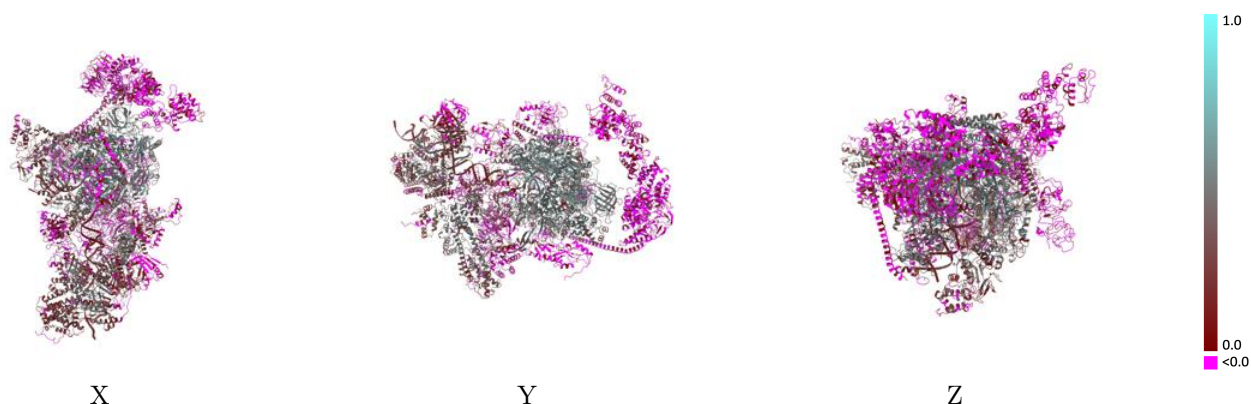
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

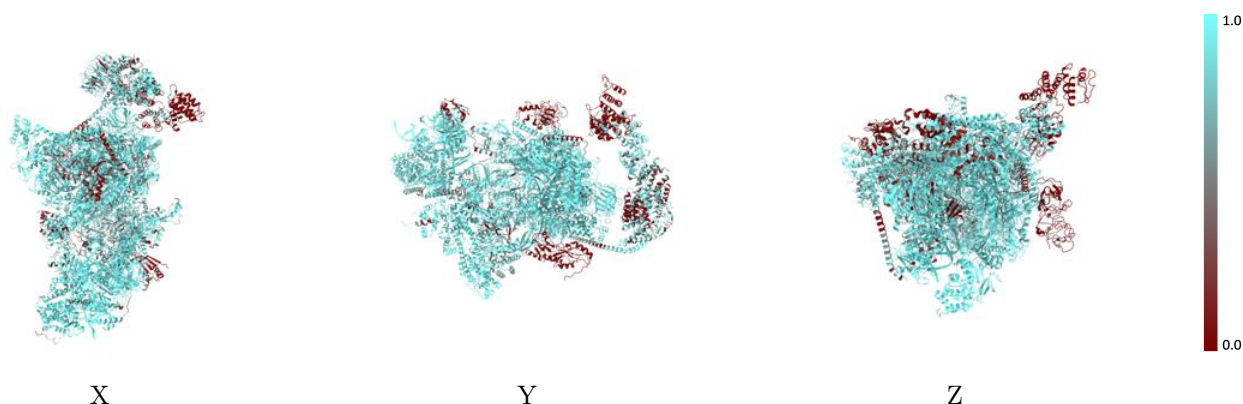


## 9.2 Q-score mapped to coordinate model [i](#)



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.

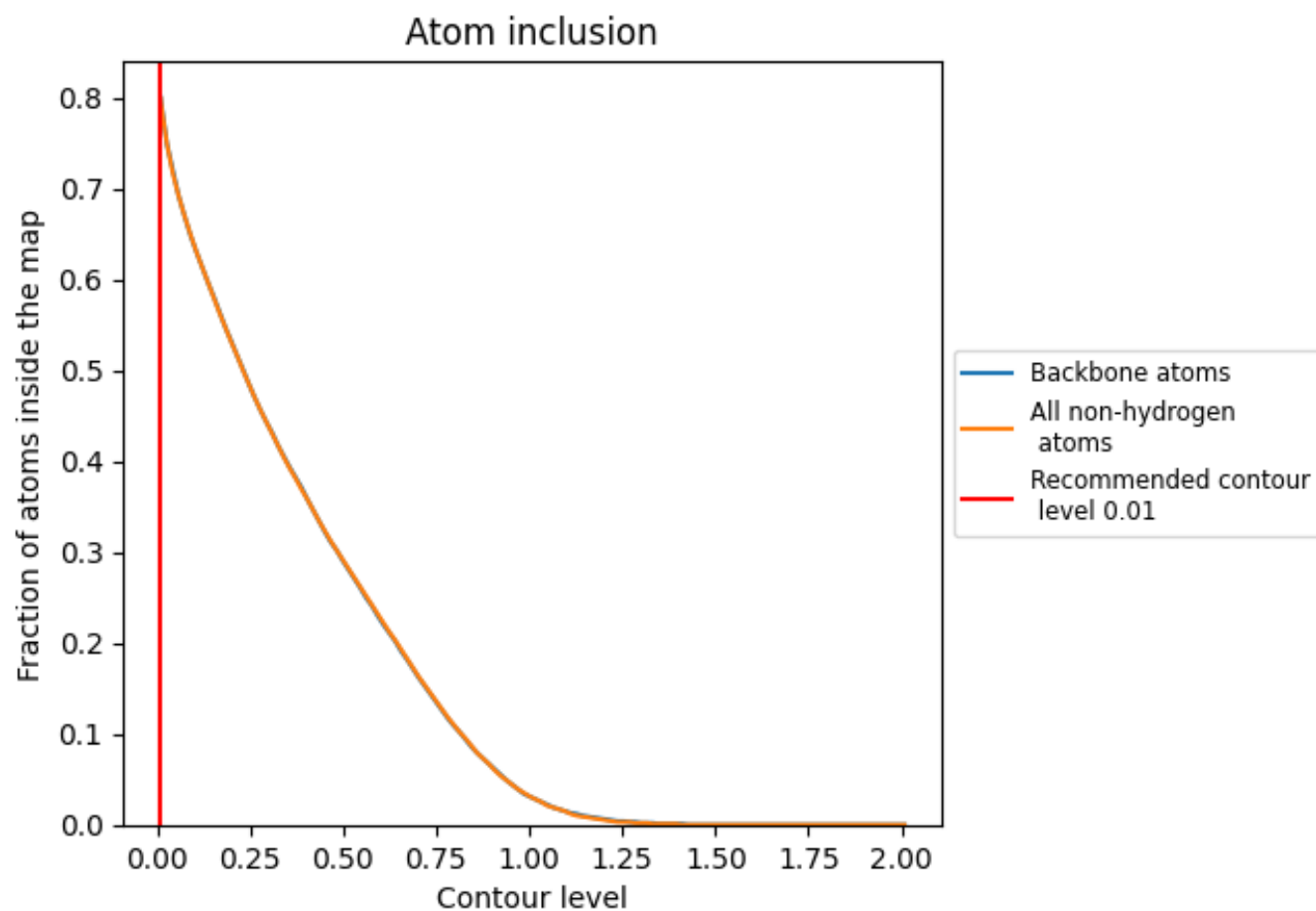
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.01).



## 9.4 Atom inclusion [i](#)










































































At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.2520
A	 0.9480	 0.4280
B	 0.9690	 0.4570
C	 0.9700	 0.4850
D	 0.7800	 0.0450
E	 0.9630	 0.3890
F	 0.9700	 0.4810
G	 0.8570	 0.1550
H	 0.9660	 0.4480
I	 0.9210	 0.3110
J	 0.9610	 0.4770
K	 0.9800	 0.4840
L	 0.9530	 0.3820
M	 0.8100	 0.2810
N	 0.9540	 0.2330
O	 0.3770	 -0.0500
P	 0.8970	 0.4270
Q	 0.5000	 -0.0160
R	 0.6270	 0.0260
S	 0.7320	 0.1500
T	 0.9550	 0.2770
U	 0.1730	 -0.0050
V	 0.2400	 -0.0400
W	 0.7210	 -0.0180
X	 0.3560	 -0.0690
Y	 0.7060	 -0.0260
Z	 0.5910	 0.0250
a	 0.9530	 0.3440
b	 0.9480	 0.3340
e	 0.9440	 0.3440
f	 0.9080	 0.2680
g	 0.9430	 0.2710
h	 0.9490	 0.2770
l	 0.6530	 0.1300
x	 0.8930	 0.2660
y	 0.8260	 0.2110

