



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2025 – 04:04 pm GMT

PDB ID : 9S3G / pdb\_00009s3g  
EMDB ID : EMD-54537  
Title : State 1 MAP3 RNA Pol II activated elongation complex with SETD2 and upstream hexasome  
Authors : Walshe, J.L.; Ochmann, M.; Dienemann, C.; Cramer, P.  
Deposited on : 2025-07-24  
Resolution : 6.40 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.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

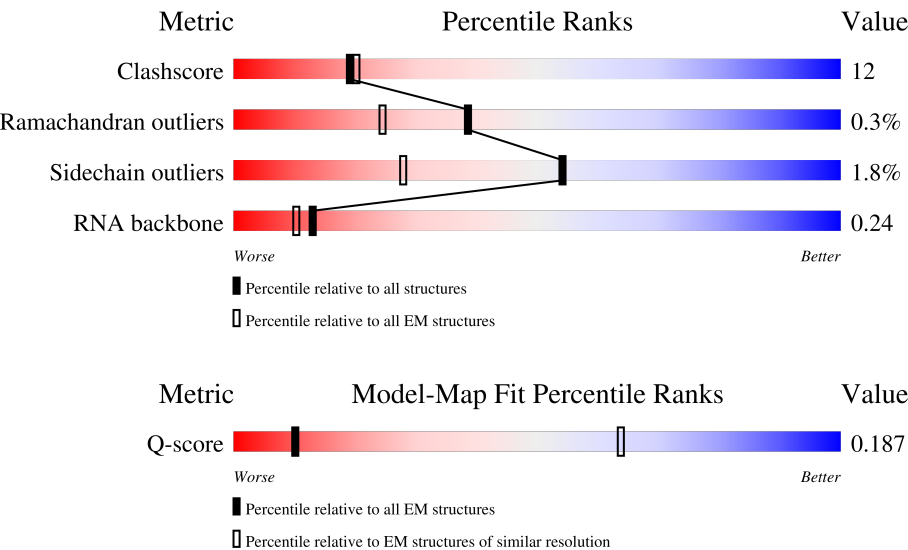


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.40 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	544 ( 5.90 - 6.90 )

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  $\geq 3$ , 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	1970	<div><div>8%</div><div>52%</div><div>20%</div><div>•</div><div>27%</div></div>
2	B	1174	<div><div>8%</div><div>62%</div><div>33%</div><div>• •</div></div>
3	C	275	<div><div>11%</div><div>72%</div><div>21%</div><div>•</div><div>6%</div></div>

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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	1729	
14	N	184	
15	O	1133	
16	P	21	
17	Q	1179	
18	R	713	
19	S	304	
20	T	184	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	103	
28	f	103	
29	g	135	
30	h	126	
31	j	1049	
32	k	709	



## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 75297 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
1	A	1444	Total	C	N	O	S	0	0
			11455	7198	2046	2137	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1136	Total	C	N	O	S	0	0
			9088	5745	1597	1682	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	N	O	S	0	0
			2072	1300	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	N	O	S	0	0
			1014	634	170	206	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	N	O	S	0	0
			1721	1089	300	324	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	N	O	S	0	0
			627	401	106	115	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	N	O	S	0	0
			1343	871	217	247	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	N	O	S	0	0
			1198	759	195	239	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			950	587	169	183	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	N	O	S	0	0
			524	339	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	N	O	S	0	0
			920	593	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	N	O	S	0	0
			398	246	77	69	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	852	Total	C	N	O	S	0	0
			7001	4440	1219	1308	34		

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	55	Total	C	N	O	P	0	0
			1130	535	197	343	55		

- Molecule 15 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	152	Total	C	N	O	S	0	0
			1228	772	209	241	6		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			436	195	66	154	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	892	Total	C	N	O	S	0	0
			7240	4587	1266	1355	32		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1177	TYR	-	expression tag	UNP Q6PD62
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	220	Total	C	N	O	S	0	0
			1694	1063	312	312	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-262	SER	-	expression tag	UNP Q92541
R	-261	ASN	-	expression tag	UNP Q92541
R	-260	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	99	Total	C	N	O	S	0	0
			795	484	147	158	6		

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	67	Total	C	N	O	P	0	0
			1369	645	273	384	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	179	Total	C	N	O	S	0	0
			1469	919	262	282	6		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	281	Total	C	N	O	S	0	0
			2310	1461	390	447	12		

- Molecule 23 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	305	Total	C	N	O	S	0	0
			2374	1507	399	463	5		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	53	Total	C	N	O	0	0
			434	268	85	81		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	116	Total	C	N	O	S	0	0
			912	570	159	174	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 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	498	Total	C	N	O	S	0	0
			3976	2529	702	728	17		

- Molecule 27 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	96	Total	C	N	O	S	0	0
			789	497	152	138	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	76	Total	C	N	O	S	0	0
			615	390	115	108	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	MET	LYS	engineered mutation	UNP Q71DI3
a	111	ALA	CYS	engineered mutation	UNP Q71DI3
e	37	MET	LYS	engineered mutation	UNP Q71DI3
e	111	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
28	f	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	g	91	Total	C	N	O	0	0
			710	444	141	125		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-4	SER	-	expression tag	UNP P04908
g	-3	ASN	-	expression tag	UNP P04908
g	-2	ALA	-	expression tag	UNP P04908
g	-1	PRO	-	expression tag	UNP P04908
g	0	TRP	-	expression tag	UNP P04908

- Molecule 30 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	94	Total	C	N	O	S	0	0
			734	461	132	139	2		

- Molecule 31 is a protein called FACT complex subunit SPT16.



Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	497	Total	C	N	O	S	0	0
			4050	2560	686	787	17		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 32 is a protein called FACT complex subunit SSRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	423	Total	C	N	O	S	0	0
			3446	2206	590	635	15		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	A	2	Total	Zn	0
			2	2	
33	B	1	Total	Zn	0
			1	1	
33	C	1	Total	Zn	0
			1	1	
33	I	2	Total	Zn	0
			2	2	
33	J	1	Total	Zn	0
			1	1	
33	L	1	Total	Zn	0
			1	1	
33	Y	1	Total	Zn	0
			1	1	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

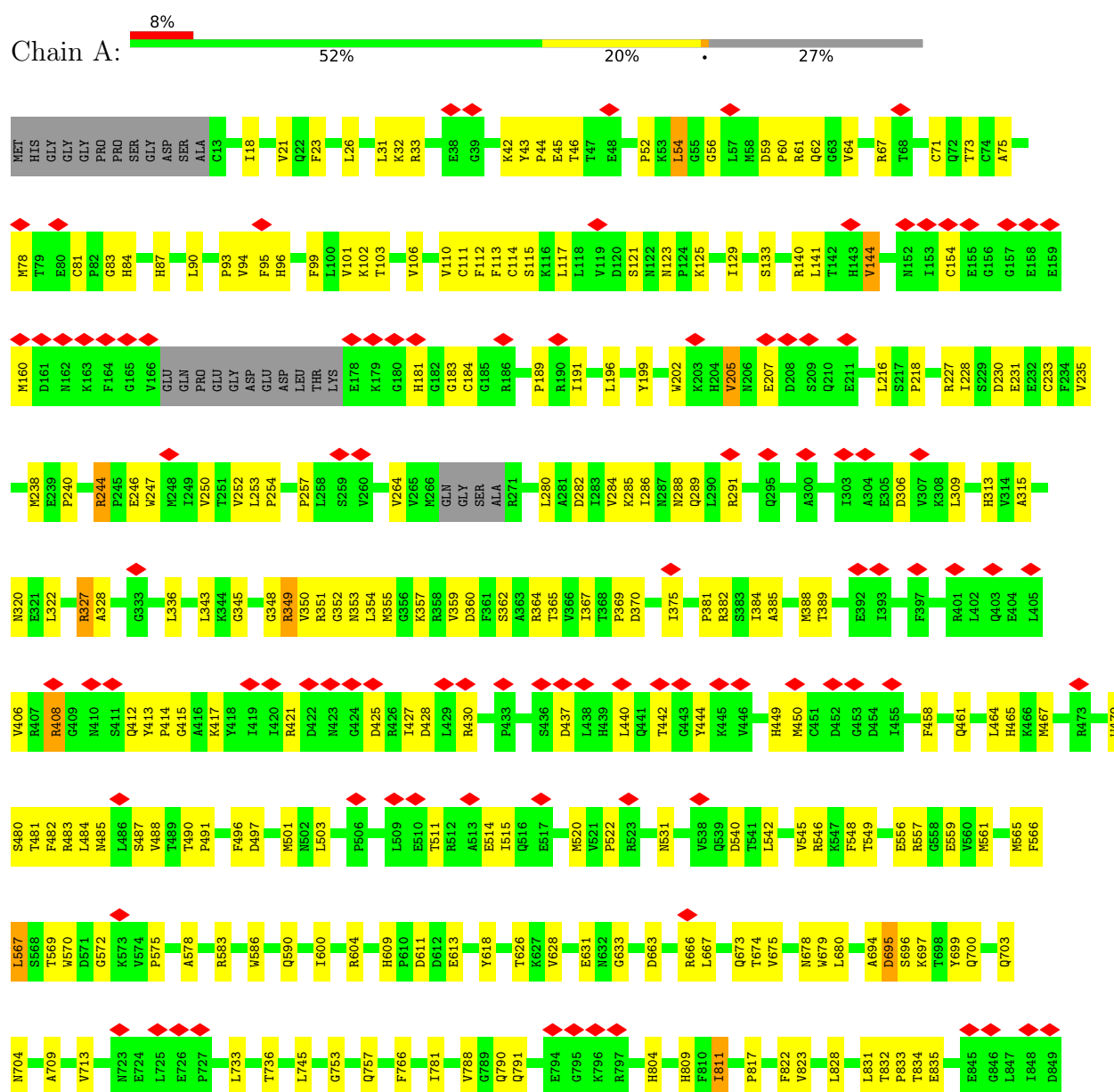
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Mg	0
			1	1	



### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit



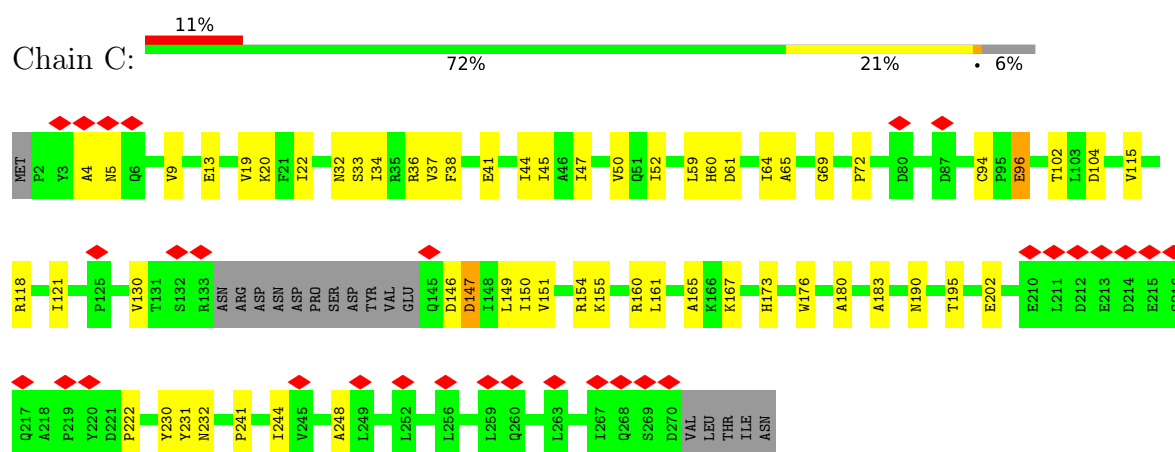




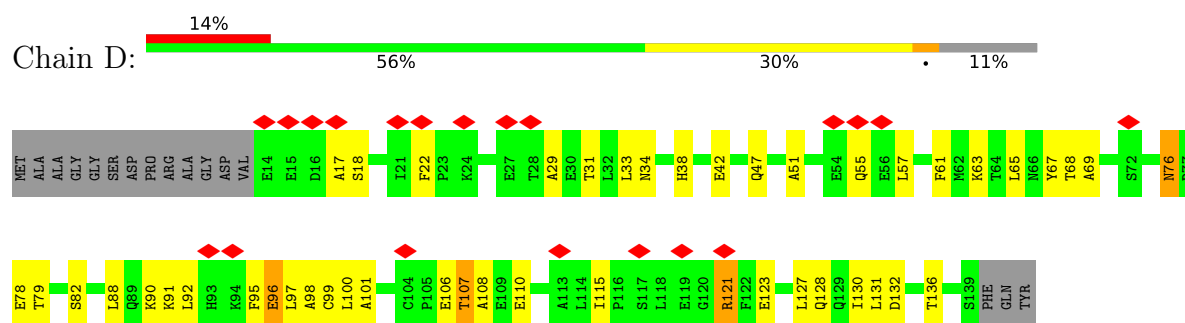




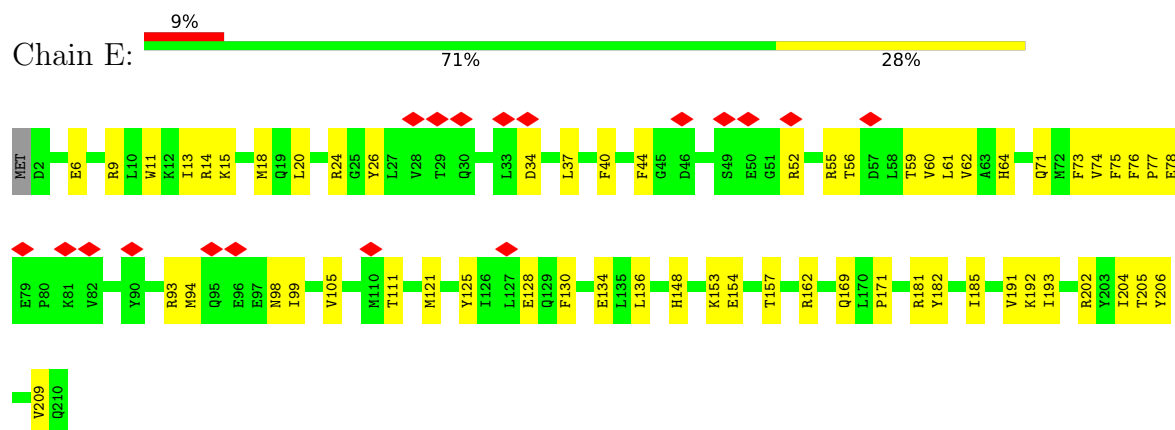




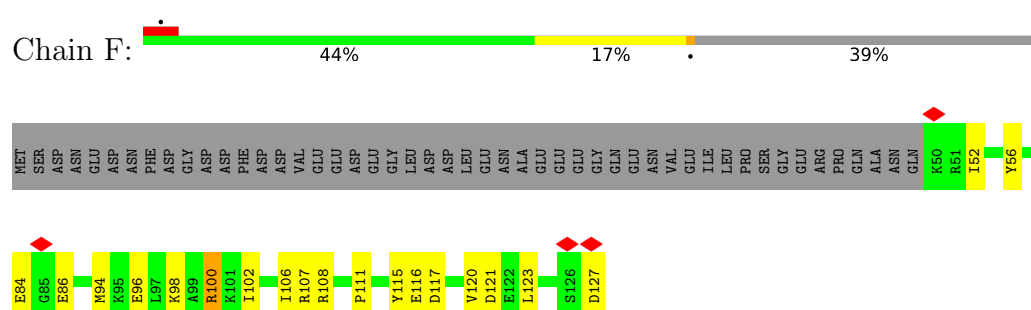
• Molecule 4: RNA polymerase II subunit D



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

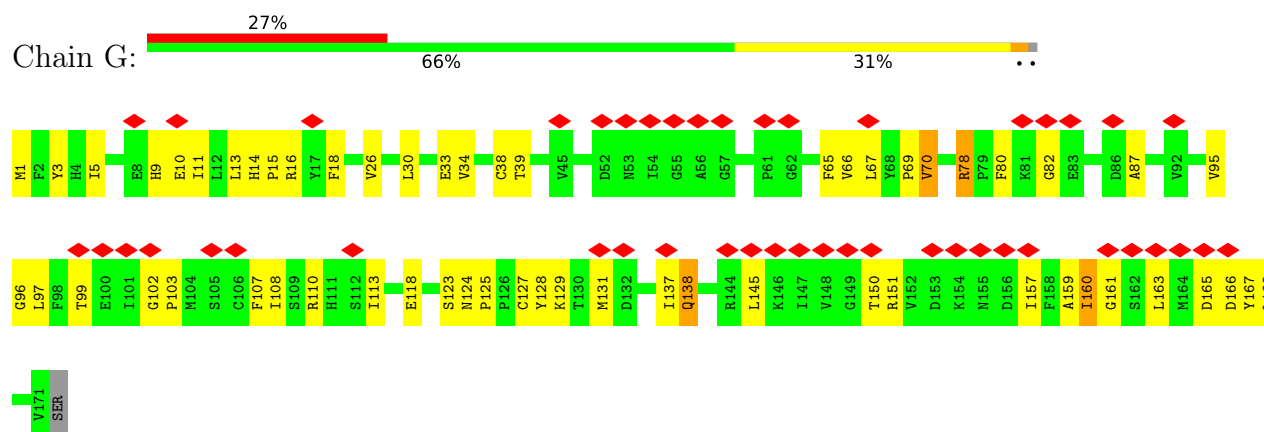


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

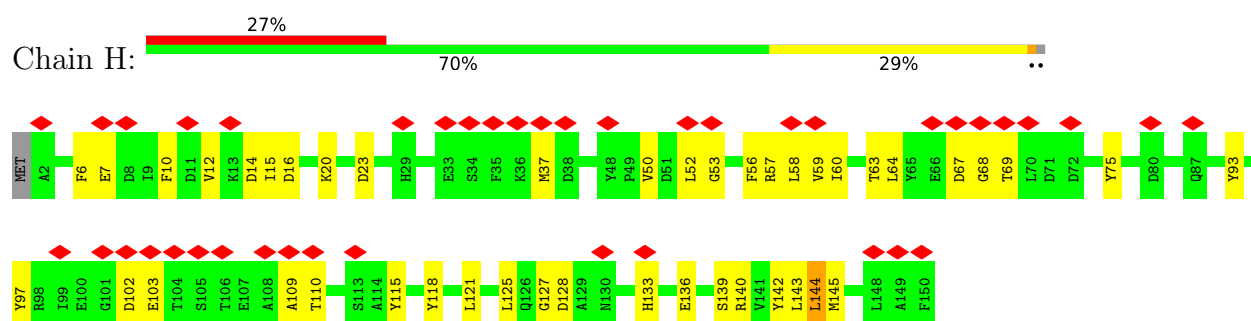




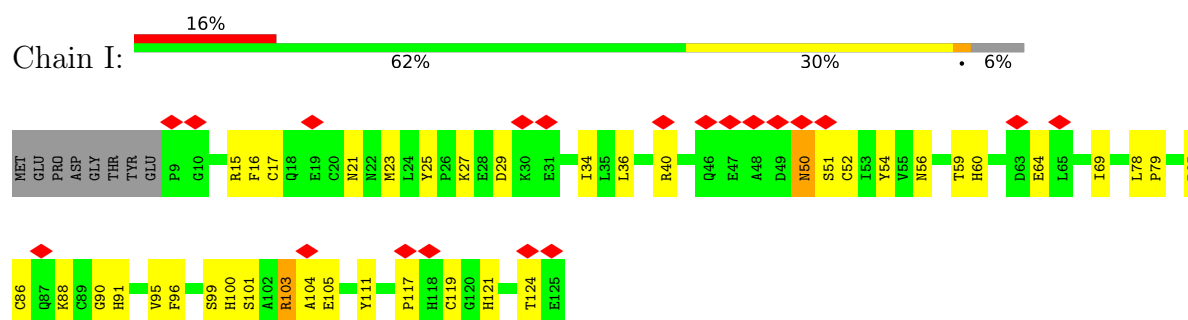
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



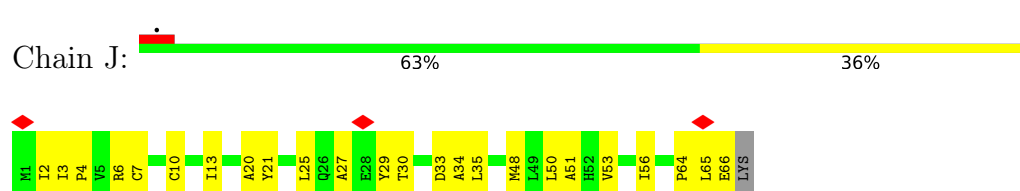
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



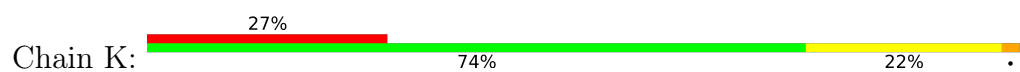
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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



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



















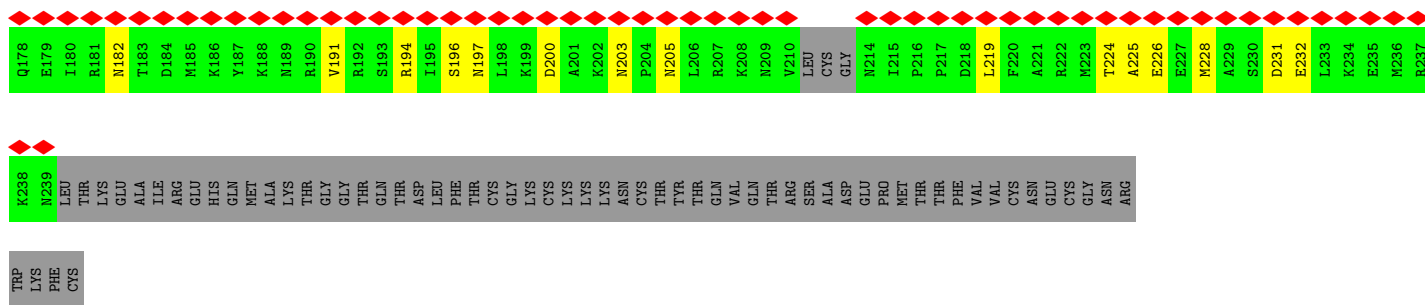


- Molecule 18: RNA polymerase-associated protein RTF1 homolog

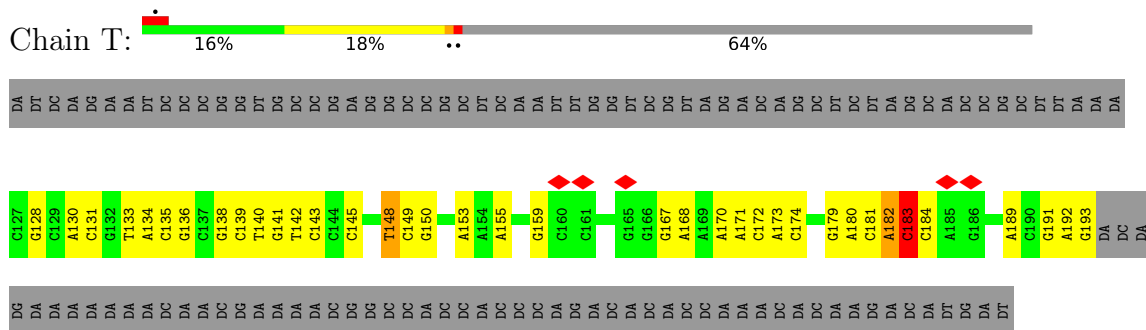




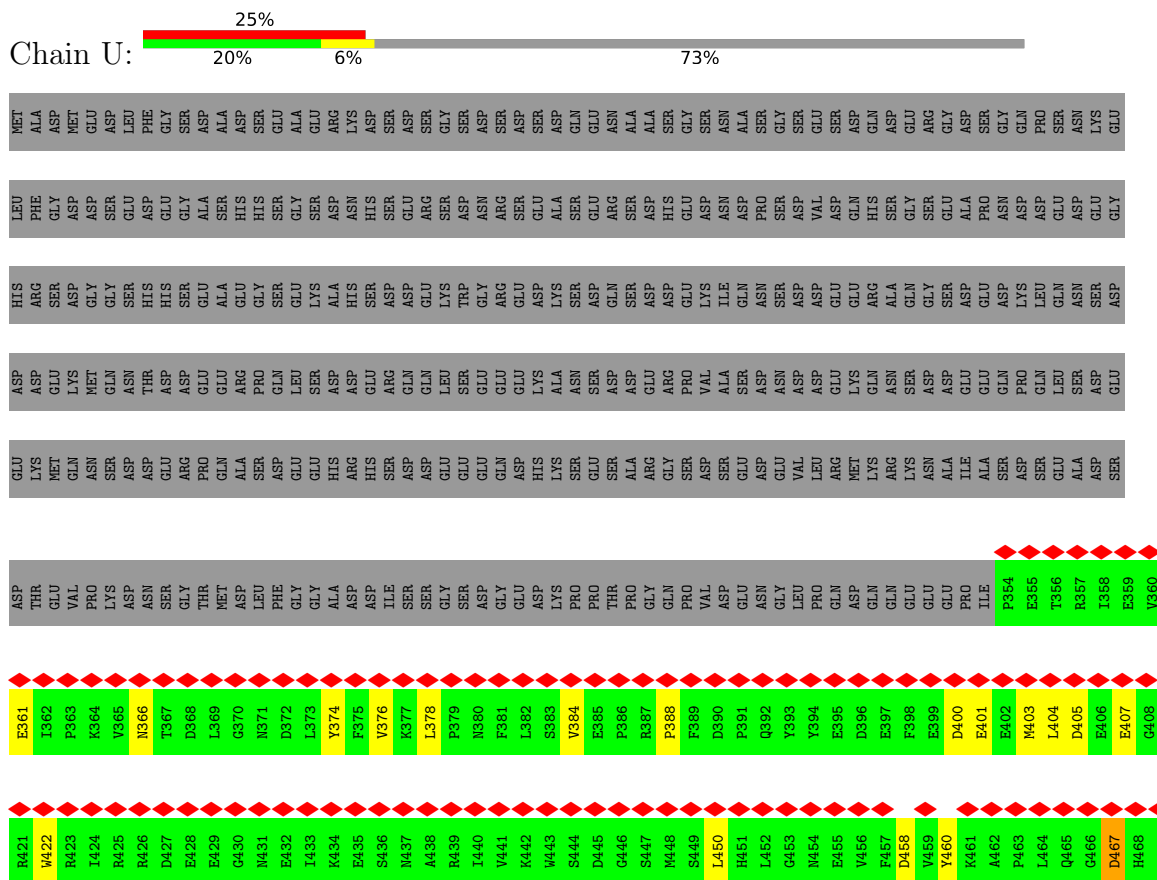




- Molecule 20: Template DNA



- Molecule 21: RNA polymerase-associated protein LEO1







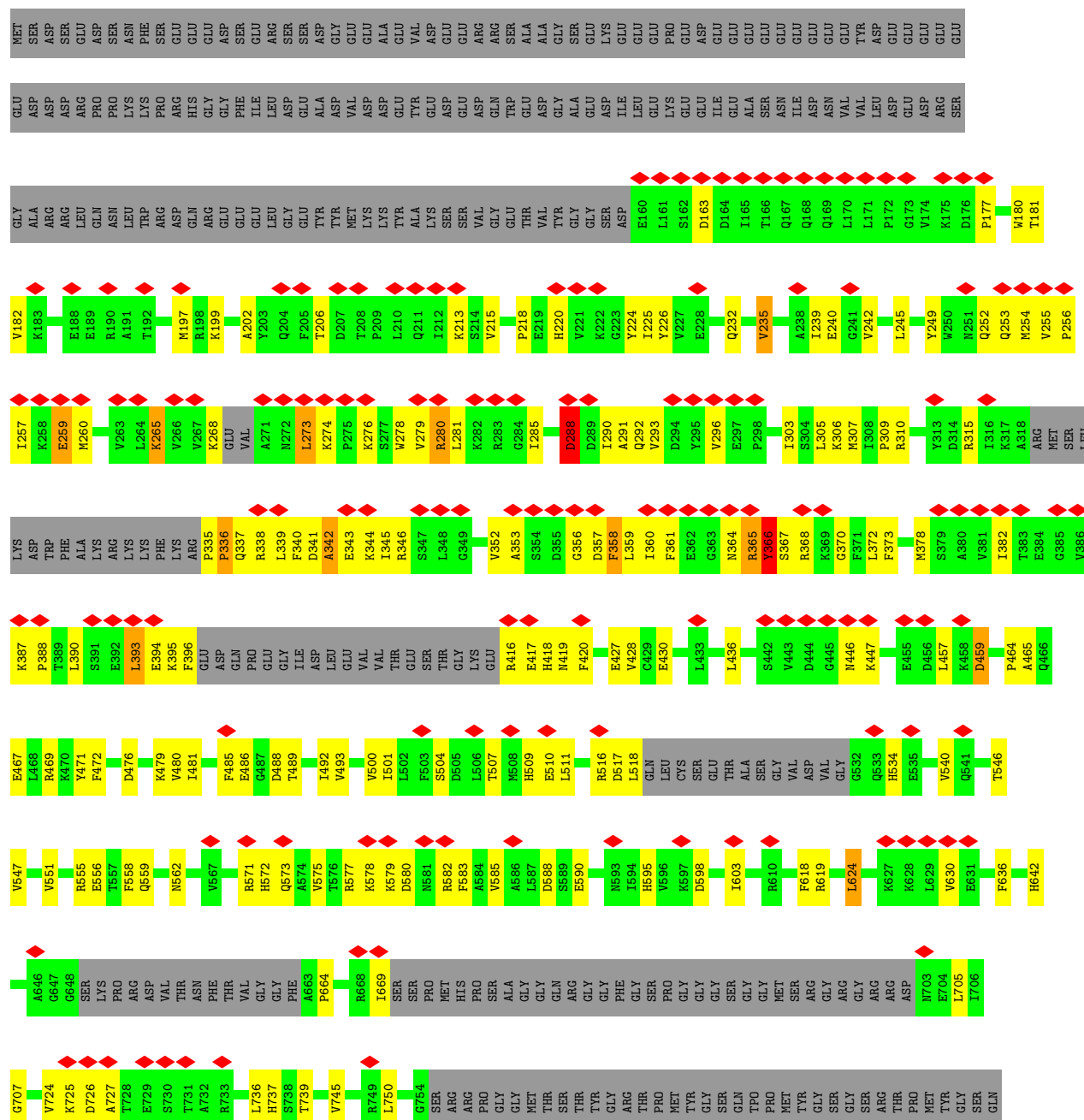








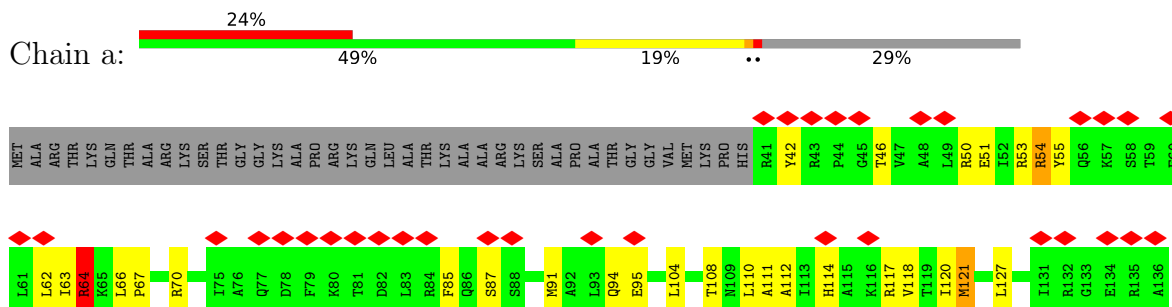
Chain Z:  14% 30% 15% 41%



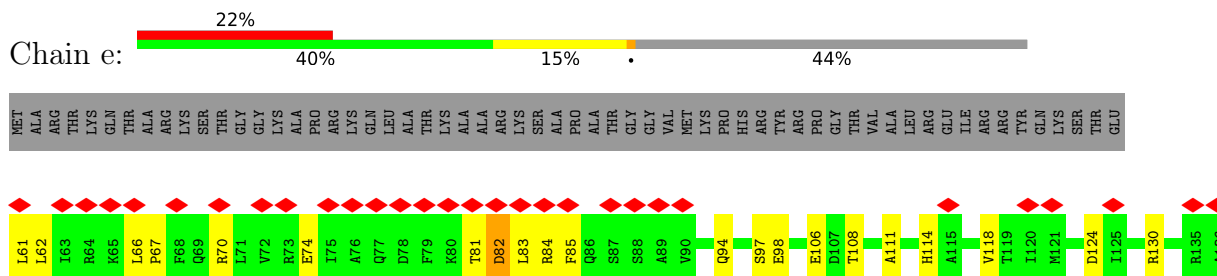




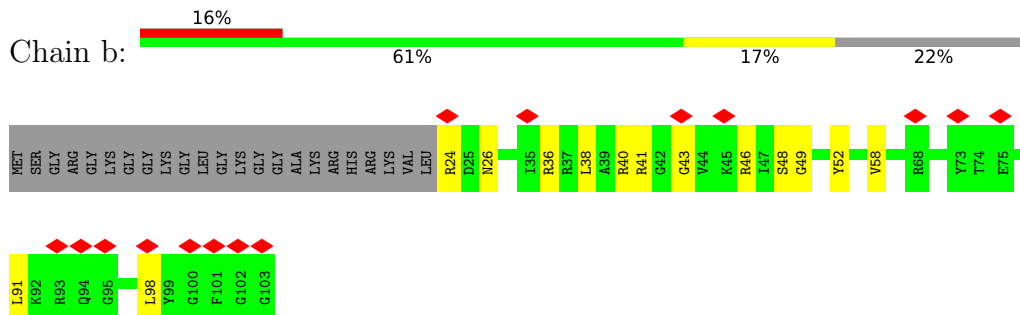
- Molecule 27: Histone H3.2



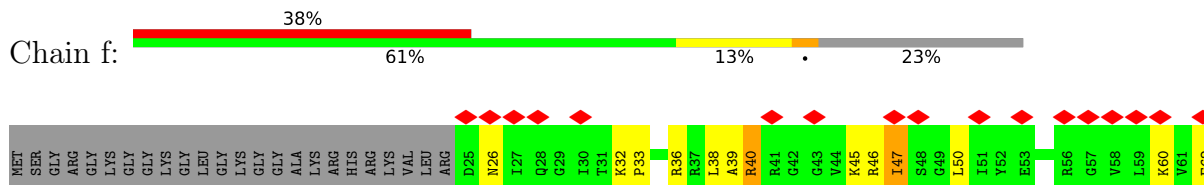
- Molecule 27: Histone H3.2



- Molecule 28: Histone H4



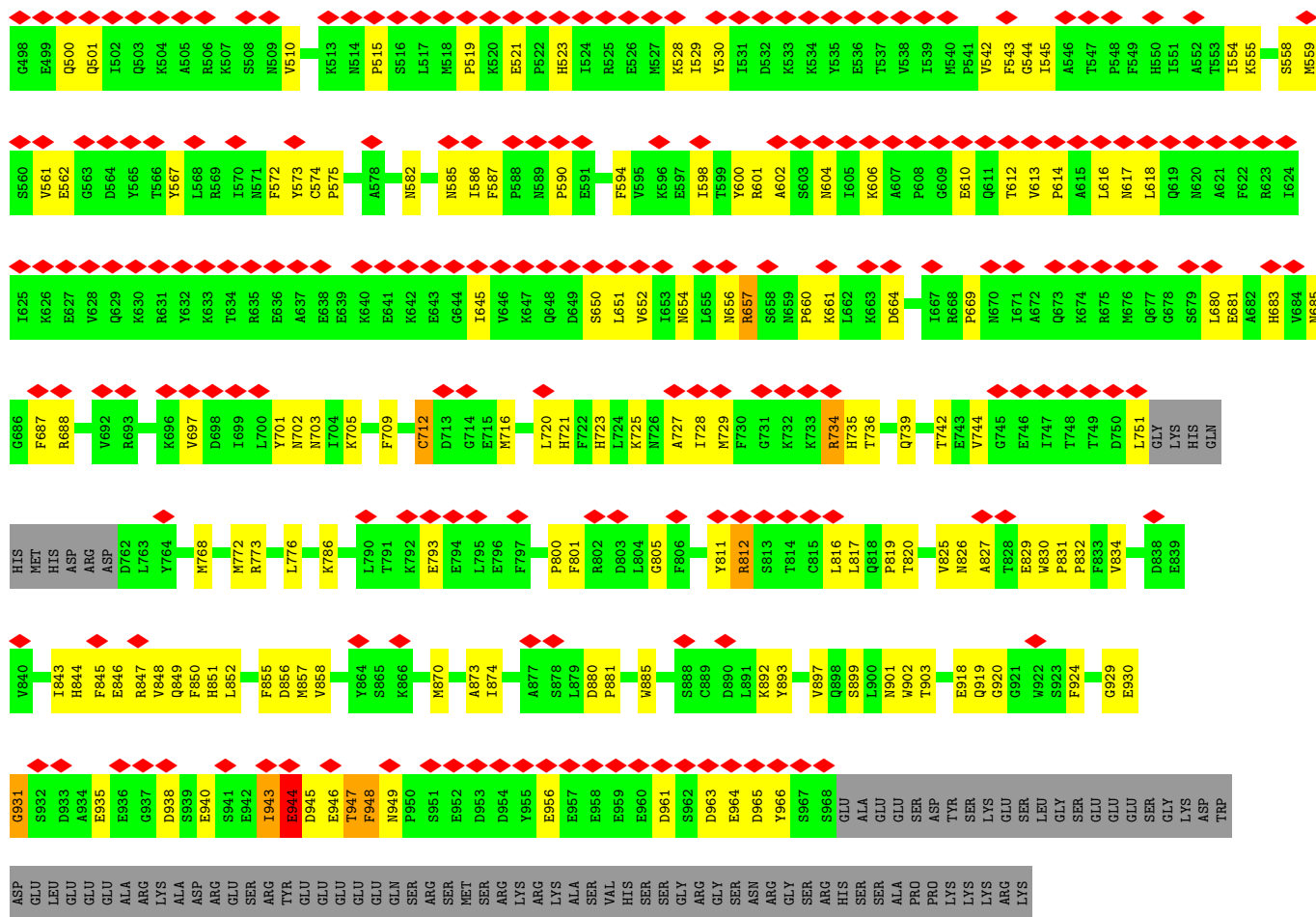
- Molecule 28: Histone H4



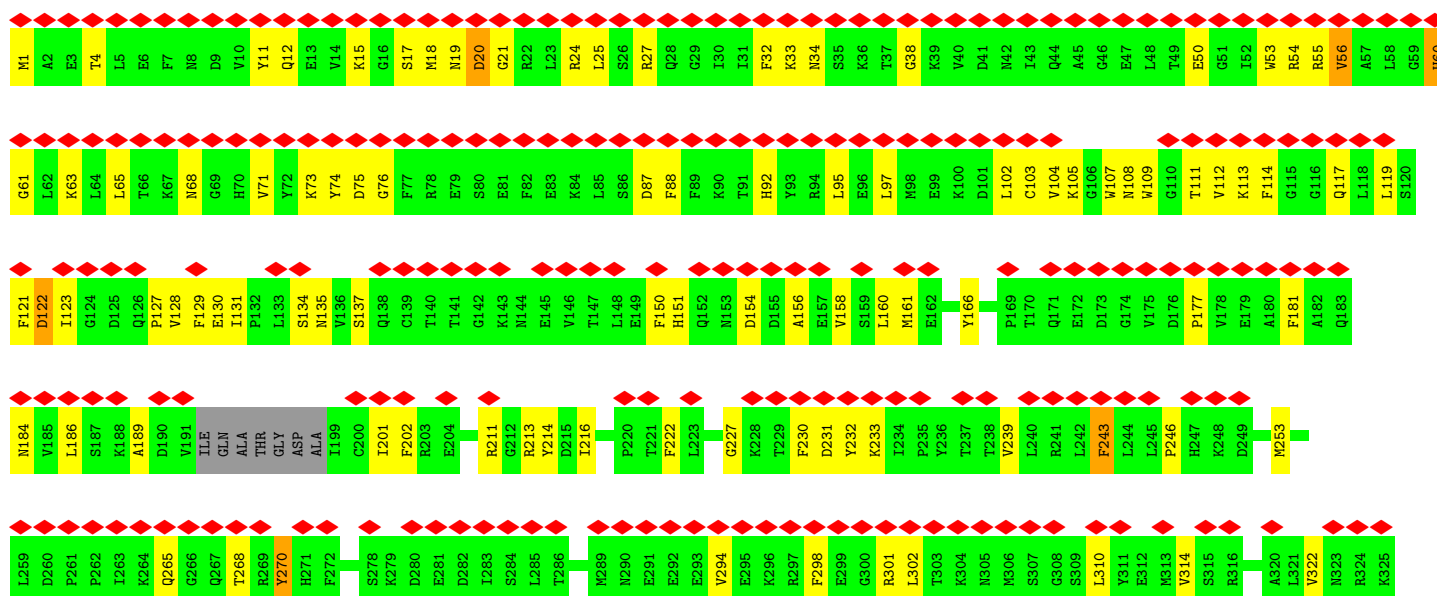








• Molecule 32: FACT complex subunit SSRP1





[illegible]



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112302	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 ( $e^-/\text{\AA}^2$ )	39.83	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0075	Depositor
Map size ( $\text{\AA}$ )	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: 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	0.44	0/11663	0.96	6/15739 (0.0%)
2	B	0.40	0/9269	0.95	7/12512 (0.1%)
3	C	0.35	0/2115	0.86	0/2873
4	D	0.48	0/1027	1.03	1/1381 (0.1%)
5	E	0.43	0/1752	0.99	0/2366
6	F	0.49	0/637	0.92	0/859
7	G	0.43	0/1374	0.97	3/1865 (0.2%)
8	H	0.37	0/1220	0.80	0/1644
9	I	0.39	0/973	0.92	0/1316
10	J	0.33	0/533	0.88	0/719
11	K	0.38	0/939	0.77	0/1271
12	L	0.42	0/404	0.98	0/536
13	M	0.73	3/7131 (0.0%)	1.20	32/9607 (0.3%)
14	N	0.75	0/1262	1.31	10/1946 (0.5%)
15	O	0.79	0/1243	1.51	5/1672 (0.3%)
16	P	0.94	8/483 (1.7%)	1.08	1/748 (0.1%)
17	Q	0.35	0/7379	0.85	0/9945
18	R	0.34	0/1717	0.96	1/2303 (0.0%)
19	S	0.31	0/800	0.64	0/1068
20	T	0.67	0/1540	1.23	7/2370 (0.3%)
21	U	0.40	0/1498	0.98	3/2018 (0.1%)
22	V	0.38	0/2360	0.94	0/3188
23	W	0.29	0/2433	0.73	0/3311
24	X	0.34	0/438	0.87	0/587
25	Y	0.37	0/928	1.01	0/1250
26	Z	0.43	0/4045	1.15	19/5445 (0.3%)
27	a	0.78	0/799	1.20	1/1070 (0.1%)
27	e	0.37	0/622	0.91	0/833
28	b	0.59	0/645	1.11	0/862
28	f	0.33	0/634	0.99	3/848 (0.4%)
29	g	0.29	0/718	0.89	0/966
30	h	0.39	0/745	0.92	1/1000 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	j	0.40	0/4133	0.97	6/5573 (0.1%)
32	k	0.41	0/3523	0.99	3/4746 (0.1%)
All	All	0.47	11/76982 (0.0%)	1.00	109/104437 (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	7
2	B	0	8
4	D	0	1
6	F	0	1
7	G	0	2
9	I	0	1
10	J	0	1
12	L	0	2
13	M	0	16
14	N	0	9
16	P	0	3
17	Q	0	1
18	R	0	2
20	T	0	10
21	U	0	1
24	X	0	2
25	Y	0	2
26	Z	0	6
27	a	0	1
29	g	0	2
30	h	0	2
31	j	0	4
32	k	0	2
All	All	0	86

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	-20	C	C1'-N1	6.79	1.58	1.48
13	M	1037	ILE	CA-C	6.67	1.60	1.52
16	P	-6	U	C1'-N1	6.62	1.58	1.48
16	P	-1	A	P-OP1	6.48	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1013	SER	CA-C	-5.96	1.45	1.52

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1038	ASP	CA-CB-CG	13.18	125.78	112.60
13	M	685	TYR	N-CA-C	11.09	125.55	111.24
13	M	1036	LYS	CA-C-N	9.22	132.44	122.11
13	M	1036	LYS	C-N-CA	9.22	132.44	122.11
13	M	968	GLU	CB-CA-C	-9.18	95.25	110.85

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	349	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	583	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11455	0	11554	347	0
2	B	9088	0	9112	307	0
3	C	2072	0	2020	49	0
4	D	1014	0	988	45	0
5	E	1721	0	1737	46	0
6	F	627	0	657	18	0
7	G	1343	0	1340	50	0
8	H	1198	0	1156	29	0
9	I	950	0	879	33	0
10	J	524	0	540	21	0
11	K	920	0	942	25	0
12	L	398	0	401	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	7001	0	6979	248	0
14	N	1130	0	619	60	0
15	O	1228	0	1260	11	0
16	P	436	0	222	33	0
17	Q	7240	0	7186	67	0
18	R	1694	0	1626	23	0
19	S	795	0	798	29	0
20	T	1369	0	740	84	0
21	U	1469	0	1441	37	0
22	V	2310	0	2247	29	0
23	W	2374	0	2290	46	0
24	X	434	0	444	4	0
25	Y	912	0	904	30	0
26	Z	3976	0	4048	160	0
27	a	789	0	827	35	0
27	e	615	0	646	24	0
28	b	638	0	676	23	0
28	f	627	0	663	28	0
29	g	710	0	750	21	0
30	h	734	0	756	18	0
31	j	4050	0	3970	134	0
32	k	3446	0	3418	87	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	I	2	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	Y	1	0	0	0	0
34	A	1	0	0	0	0
All	All	75297	0	73836	1853	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 12.

The worst 5 of 1853 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)
14:N:-6:DT:OP1	27:a:64:ARG:HD2	1.25	1.25
20:T:173:DA:OP1	28:f:45:LYS:NZ	1.68	1.25
14:N:1:DT:OP1	31:j:582:ASN:ND2	1.69	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:ASN:CB	19:S:228:MET:HG3	1.67	1.23
20:T:173:DA:P	28:f:45:LYS:NZ	2.12	1.22

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	1436/1970 (73%)	1368 (95%)	65 (4%)	3 (0%)	44	78
2	B	1130/1174 (96%)	1052 (93%)	77 (7%)	1 (0%)	48	83
3	C	254/275 (92%)	239 (94%)	13 (5%)	2 (1%)	16	55
4	D	124/142 (87%)	123 (99%)	1 (1%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
8	H	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	19	56
9	I	115/125 (92%)	106 (92%)	9 (8%)	0	100	100
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
13	M	832/1729 (48%)	792 (95%)	37 (4%)	3 (0%)	30	68
15	O	148/1133 (13%)	140 (95%)	8 (5%)	0	100	100
17	Q	890/1179 (76%)	877 (98%)	13 (2%)	0	100	100
18	R	214/713 (30%)	208 (97%)	6 (3%)	0	100	100
19	S	95/304 (31%)	90 (95%)	5 (5%)	0	100	100
21	U	175/666 (26%)	166 (95%)	8 (5%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	V	275/531 (52%)	264 (96%)	11 (4%)	0	100	100
23	W	303/305 (99%)	295 (97%)	8 (3%)	0	100	100
24	X	51/531 (10%)	50 (98%)	0	1 (2%)	6	31
25	Y	114/121 (94%)	106 (93%)	7 (6%)	1 (1%)	14	51
26	Z	484/1087 (44%)	457 (94%)	24 (5%)	3 (1%)	22	60
27	a	94/136 (69%)	88 (94%)	6 (6%)	0	100	100
27	e	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
28	b	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
28	f	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
29	g	89/135 (66%)	86 (97%)	3 (3%)	0	100	100
30	h	92/126 (73%)	90 (98%)	1 (1%)	1 (1%)	12	47
31	j	493/1049 (47%)	447 (91%)	35 (7%)	11 (2%)	5	29
32	k	419/709 (59%)	392 (94%)	26 (6%)	1 (0%)	44	78
All	All	8877/15383 (58%)	8445 (95%)	403 (4%)	29 (0%)	38	72

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	Z	342	ALA
26	Z	393	LEU
30	h	105	GLY
31	j	948	PHE
31	j	963	ASP

### 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	1274/1747 (73%)	1253 (98%)	21 (2%)	58	73
2	B	996/1027 (97%)	968 (97%)	28 (3%)	38	57
3	C	235/252 (93%)	231 (98%)	4 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	112/126 (89%)	109 (97%)	3 (3%)	40	58
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	65 (96%)	3 (4%)	24	45
7	G	149/153 (97%)	145 (97%)	4 (3%)	40	58
8	H	130/131 (99%)	127 (98%)	3 (2%)	45	64
9	I	105/112 (94%)	102 (97%)	3 (3%)	37	56
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	102 (98%)	2 (2%)	52	69
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	758/1524 (50%)	743 (98%)	15 (2%)	50	68
15	O	143/1017 (14%)	142 (99%)	1 (1%)	81	87
17	Q	763/1011 (76%)	758 (99%)	5 (1%)	81	87
18	R	163/625 (26%)	162 (99%)	1 (1%)	84	88
19	S	86/268 (32%)	84 (98%)	2 (2%)	45	64
21	U	163/590 (28%)	162 (99%)	1 (1%)	84	88
22	V	255/462 (55%)	251 (98%)	4 (2%)	58	73
23	W	260/260 (100%)	259 (100%)	1 (0%)	89	91
24	X	48/467 (10%)	47 (98%)	1 (2%)	48	66
25	Y	102/105 (97%)	100 (98%)	2 (2%)	50	68
26	Z	438/939 (47%)	426 (97%)	12 (3%)	40	58
27	a	82/110 (74%)	78 (95%)	4 (5%)	21	42
27	e	64/110 (58%)	63 (98%)	1 (2%)	58	73
28	b	65/79 (82%)	64 (98%)	1 (2%)	60	75
28	f	64/79 (81%)	62 (97%)	2 (3%)	35	54
29	g	72/104 (69%)	71 (99%)	1 (1%)	62	75
30	h	80/105 (76%)	80 (100%)	0	100	100
31	j	446/929 (48%)	438 (98%)	8 (2%)	54	71
32	k	380/631 (60%)	370 (97%)	10 (3%)	41	59
All	All	7895/13483 (59%)	7752 (98%)	143 (2%)	54	71

5 of 143 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
26	Z	624	LEU
27	a	121	MET
31	j	938	ASP
2	B	1157	LEU
2	B	1118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
31	j	710	GLN
32	k	70	HIS
11	K	29	ASN
9	I	41	ASN
32	k	92	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	20/21 (95%)	8 (40%)	5 (25%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-20	C
16	P	-17	C
16	P	-16	U
16	P	-13	G
16	P	-12	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	-21	U
16	P	-13	G
16	P	-11	G
16	P	-10	G
16	P	-9	U



## 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 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](#)

There are no chain breaks in this entry.



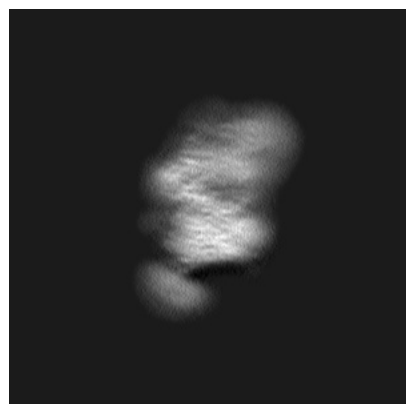
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54537. These allow visual inspection of the internal detail of the map and identification of artifacts.

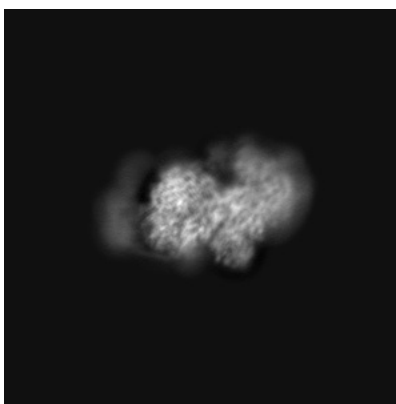
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

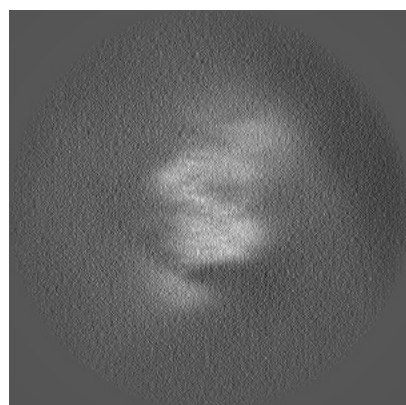


Y

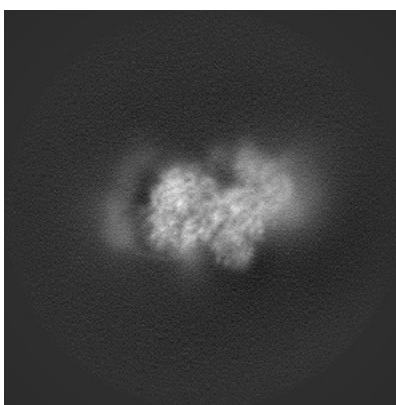


Z

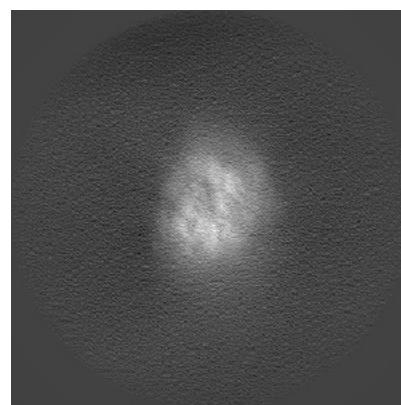
#### 6.1.2 Raw map



X



Y



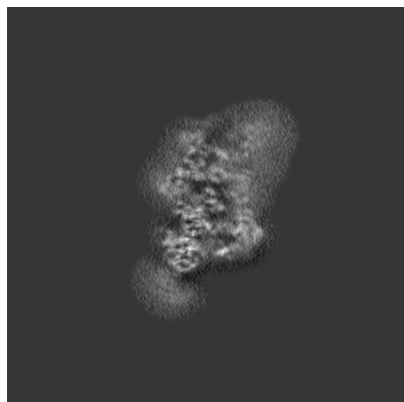
Z

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

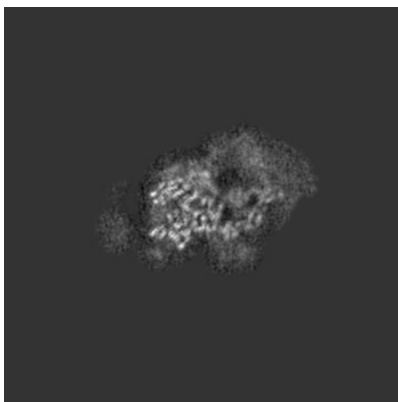


## 6.2 Central slices [i](#)

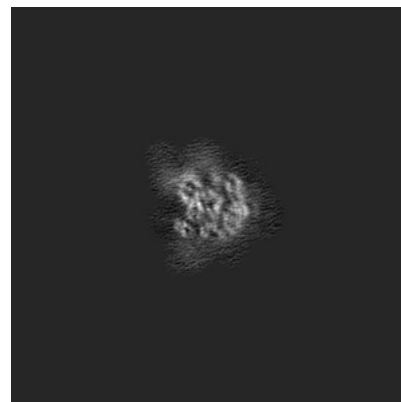
### 6.2.1 Primary map



X Index: 256

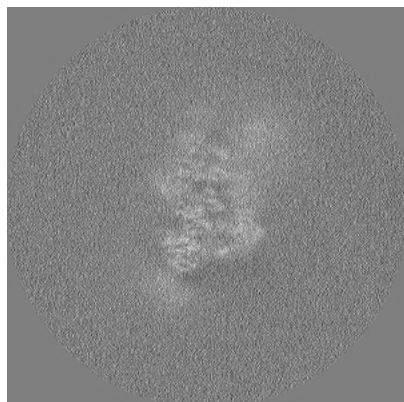


Y Index: 256

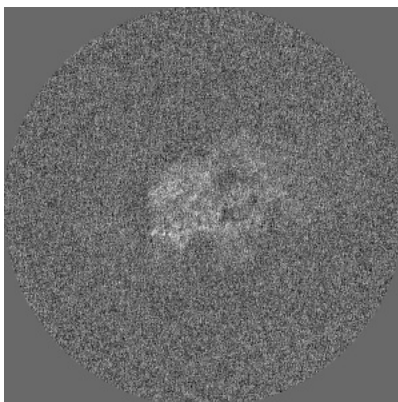


Z Index: 256

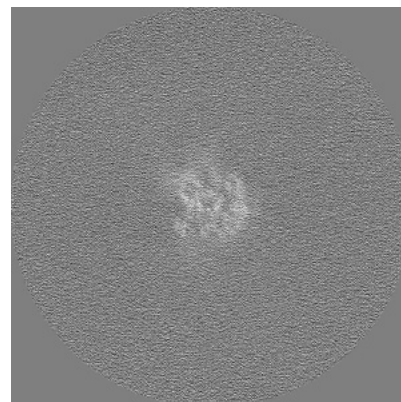
### 6.2.2 Raw map



X Index: 256



Y Index: 256



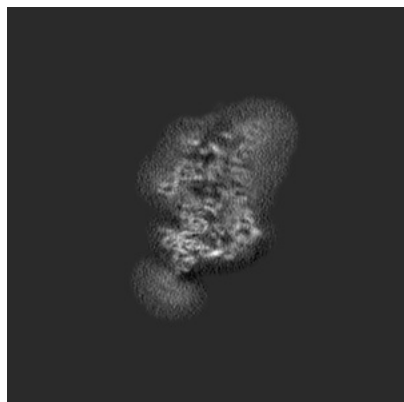
Z Index: 256

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

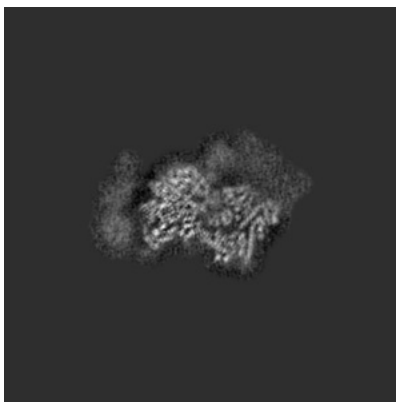


## 6.3 Largest variance slices [i](#)

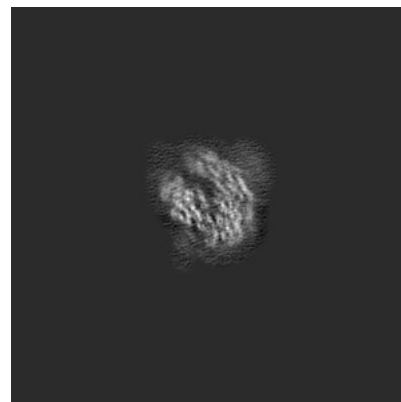
### 6.3.1 Primary map



X Index: 260

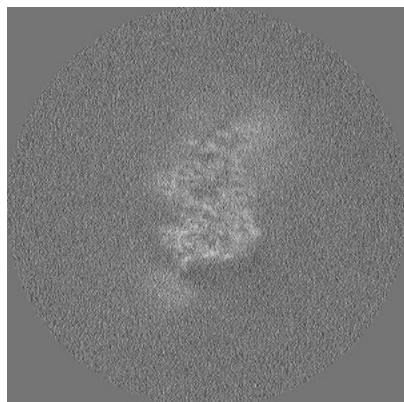


Y Index: 234

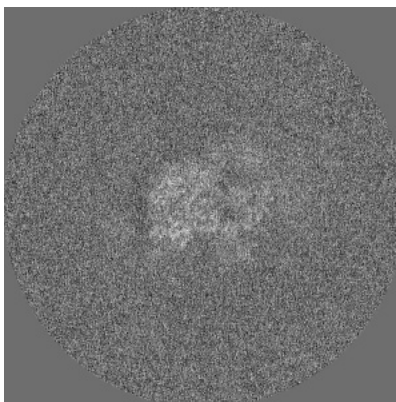


Z Index: 219

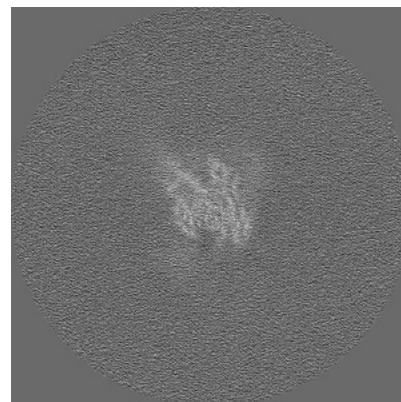
### 6.3.2 Raw map



X Index: 262



Y Index: 254



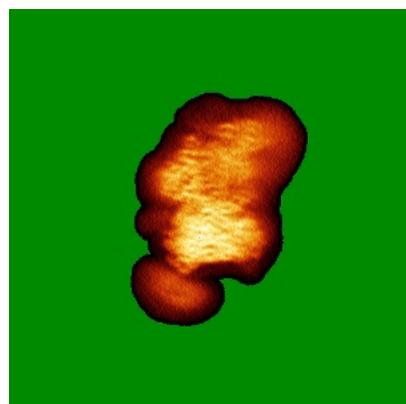
Z Index: 232

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

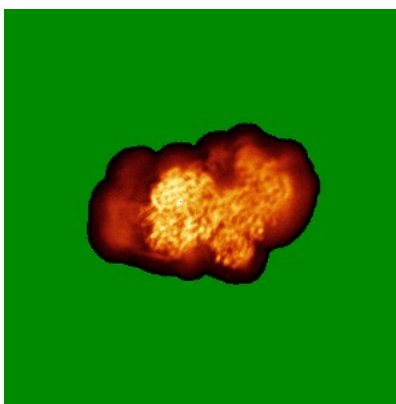


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

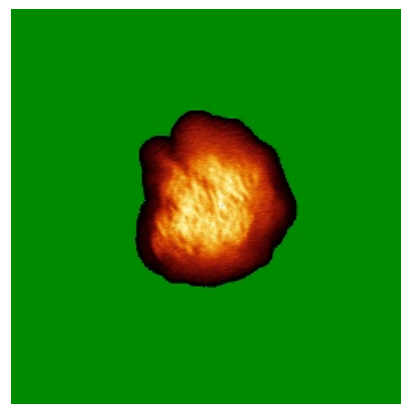
### 6.4.1 Primary map



X

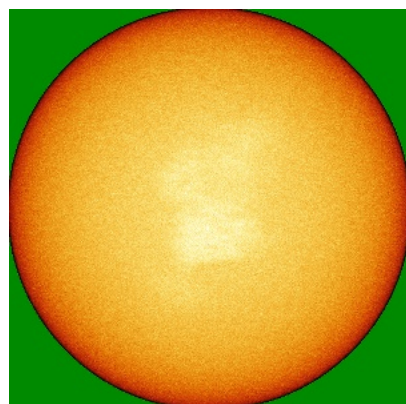


Y

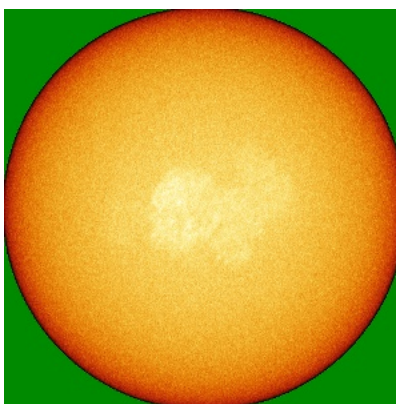


Z

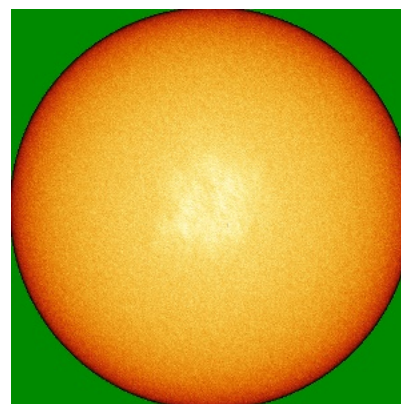
### 6.4.2 Raw map



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



X



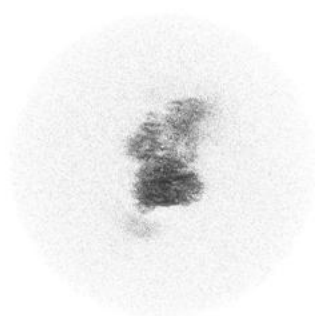
Y



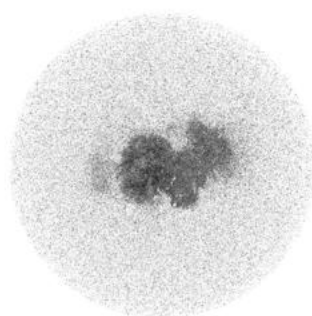
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

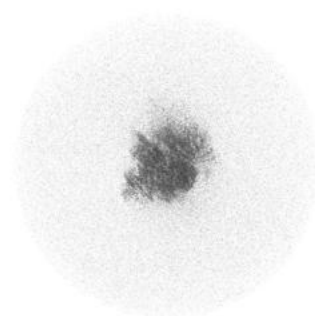
### 6.5.2 Raw map



X



Y



Z

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](#)

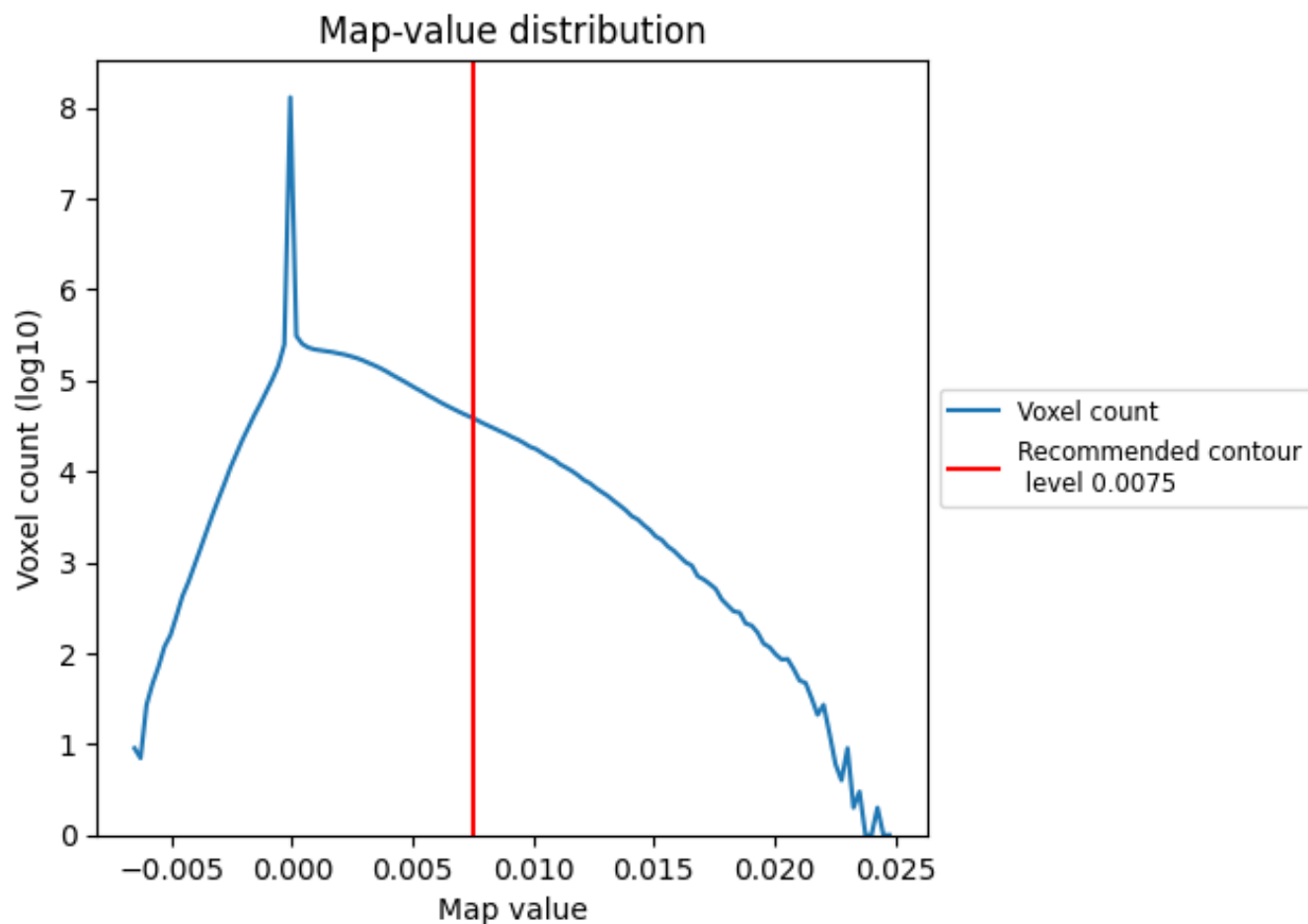
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

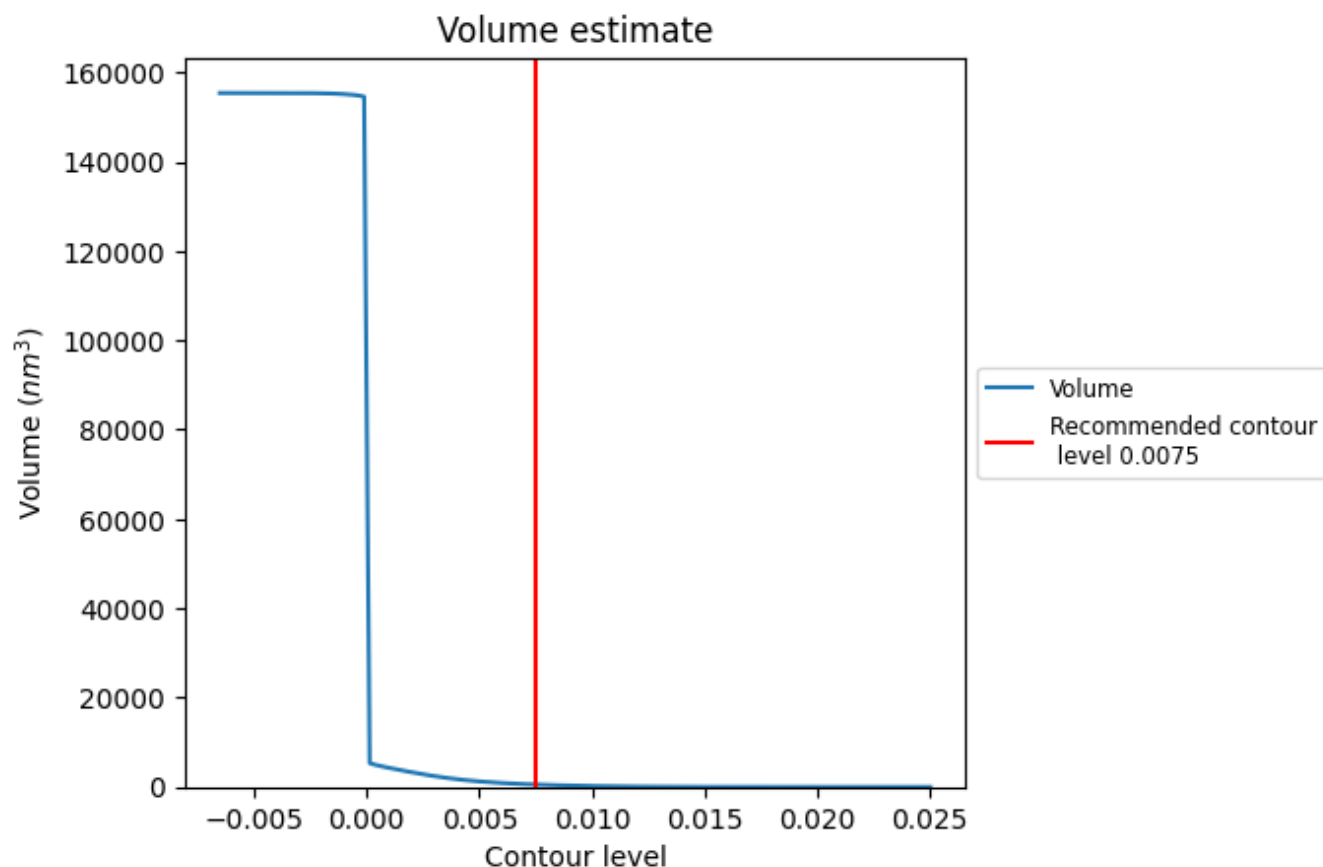
### 7.1 Map-value distribution [i](#)



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](#)

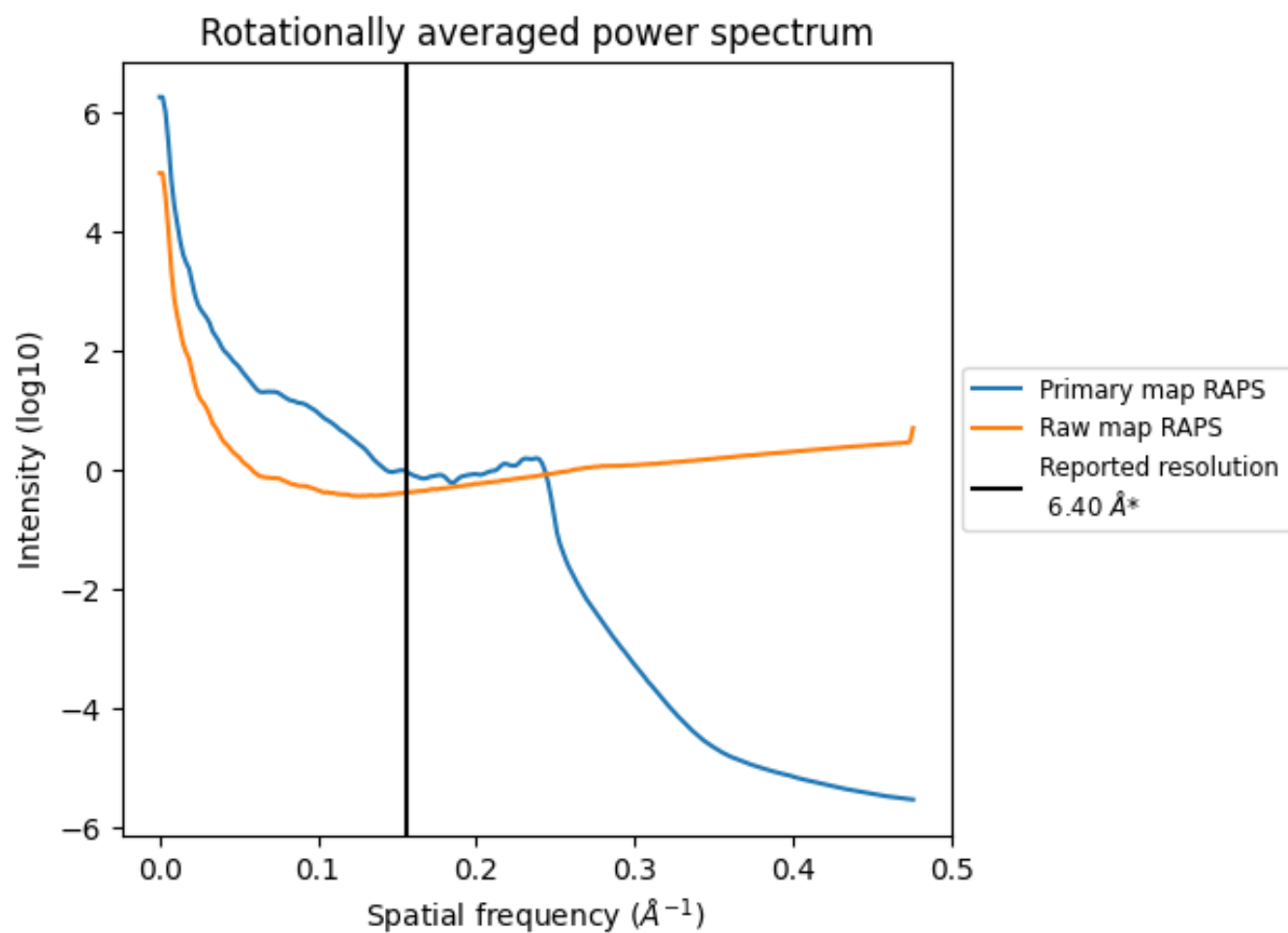


The volume at the recommended contour level is 539 nm<sup>3</sup>; this corresponds to an approximate mass of 487 kDa.

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 ⓘ



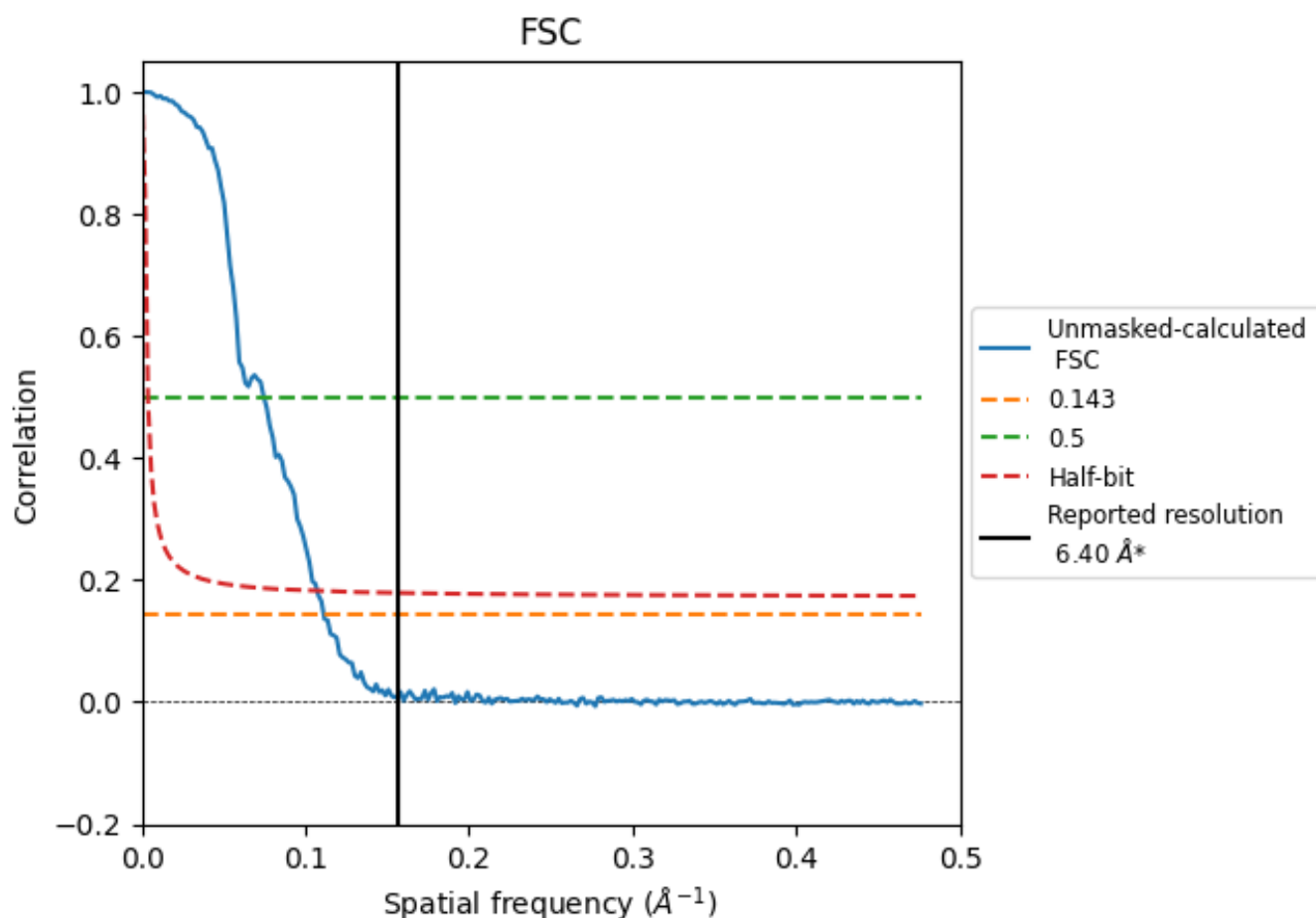
\*Reported resolution corresponds to spatial frequency of 0.156  $\text{\AA}^{-1}$



## 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 0.156 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.00	13.42	9.33

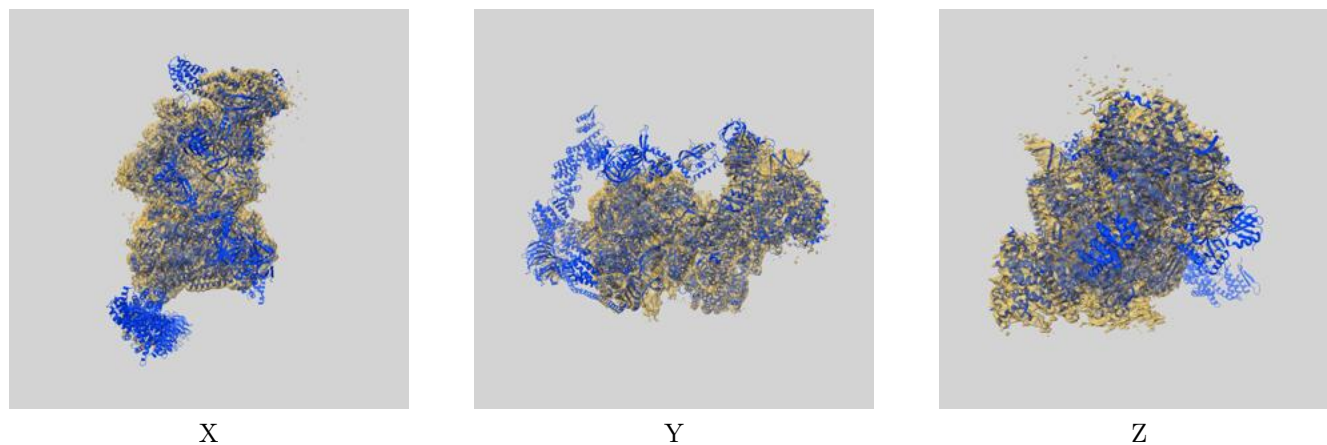
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.00 differs from the reported value 6.4 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-54537 and PDB model 9S3G. Per-residue inclusion information can be found in section [3](#) on page [12](#).

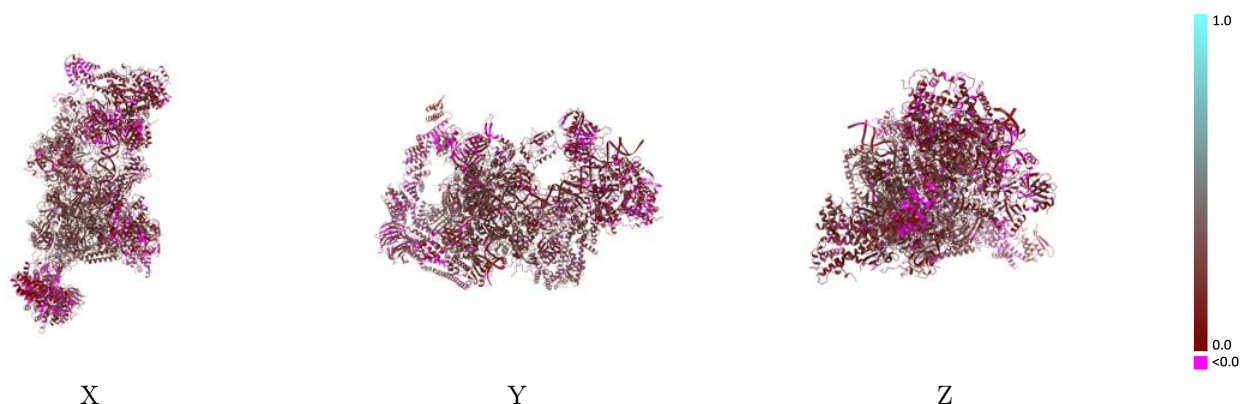
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0075 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.

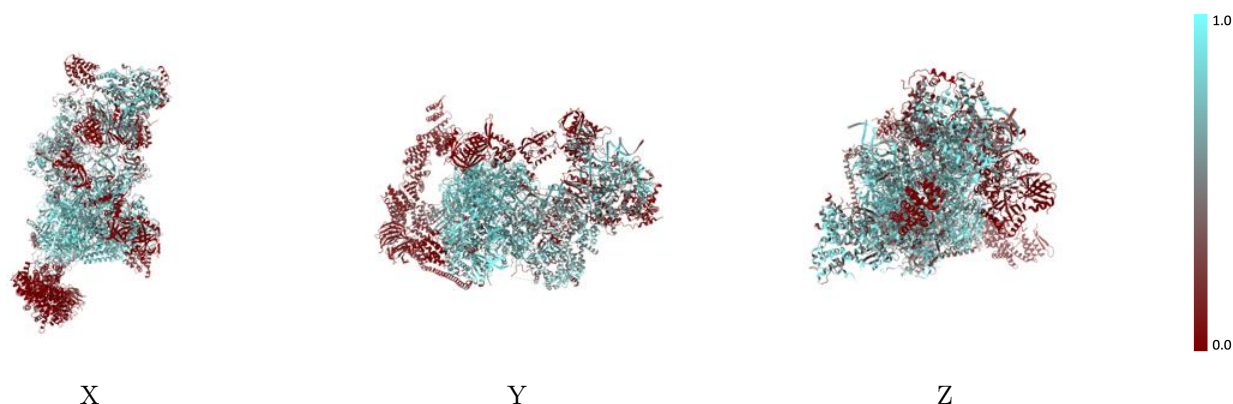


## 9.2 Q-score mapped to coordinate model [i](#)



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.

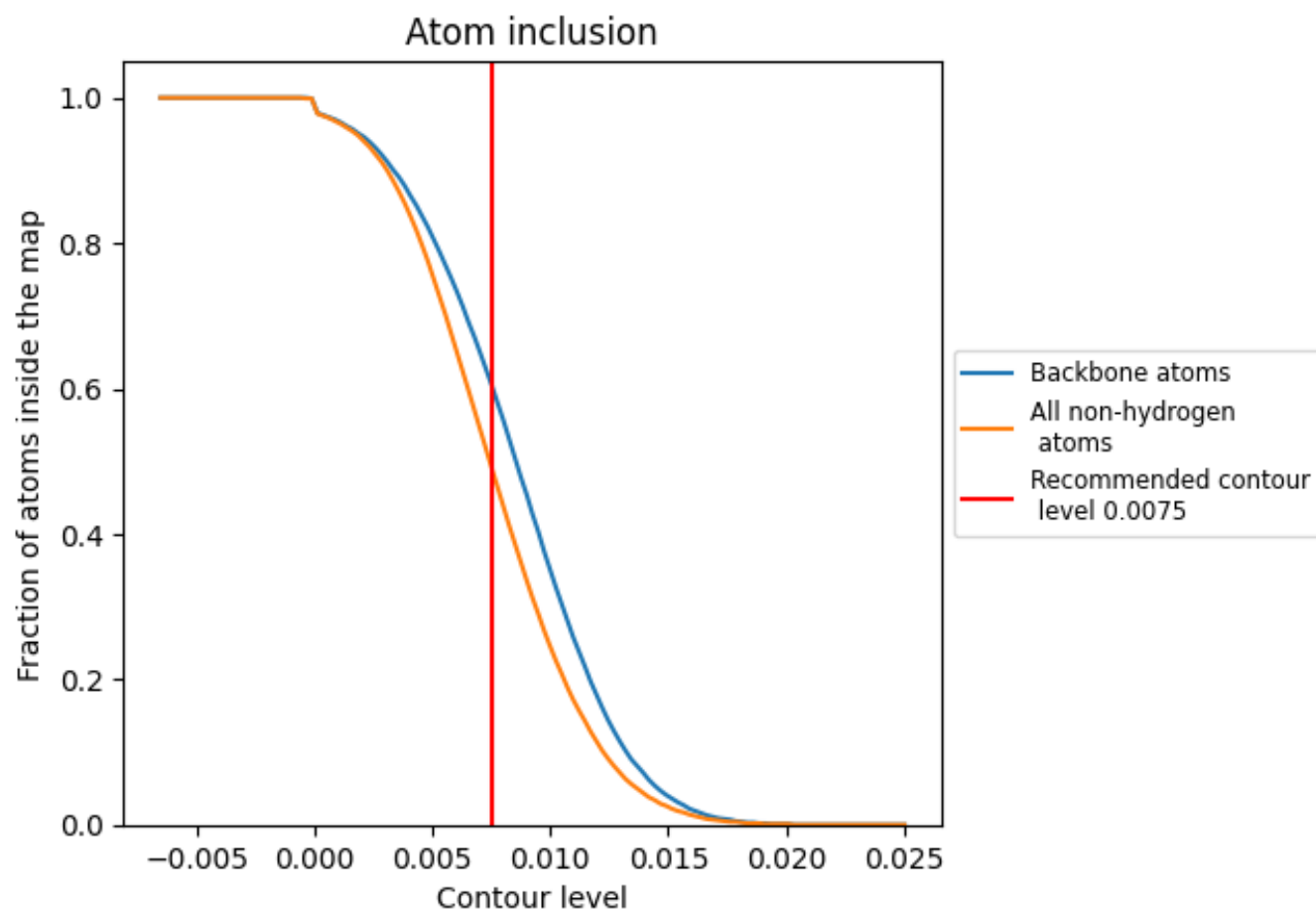
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0075).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 61% of all backbone atoms, 49% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4920	 0.1870
A	 0.7390	 0.2670
B	 0.7600	 0.2350
C	 0.7600	 0.2460
D	 0.6450	 0.2200
E	 0.7590	 0.2360
F	 0.7860	 0.2840
G	 0.5810	 0.2380
H	 0.5710	 0.2990
I	 0.6930	 0.2060
J	 0.8610	 0.2190
K	 0.6350	 0.2560
L	 0.7120	 0.1990
M	 0.6220	 0.2070
N	 0.7560	 0.1580
O	 0.0230	 0.0020
P	 0.7250	 0.2130
Q	 0.0240	 0.1120
R	 0.1120	 0.1590
S	 0.0050	 0.0430
T	 0.7810	 0.1630
U	 0.0480	 0.1170
V	 0.0060	 0.1050
W	 0.0130	 0.1270
X	 0.0190	 0.1540
Y	 0.3710	 0.1640
Z	 0.5420	 0.2020
a	 0.5380	 0.1330
b	 0.5830	 0.1500
e	 0.4330	 0.1230
f	 0.4050	 0.1280
g	 0.4670	 0.1040
h	 0.4520	 0.1130
j	 0.4520	 0.1520
k	 0.2270	 0.1030

