



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 06:33 PM UTC

PDB ID : 9RTT / pdb_00009rtt
EMDB ID : EMD-54251
Title : Activated Elongation Complex with IWS1 and ELOF1
Authors : Walshe, J.L.; Cramer, P.
Deposited on : 2025-07-03
Resolution : 4.01 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:

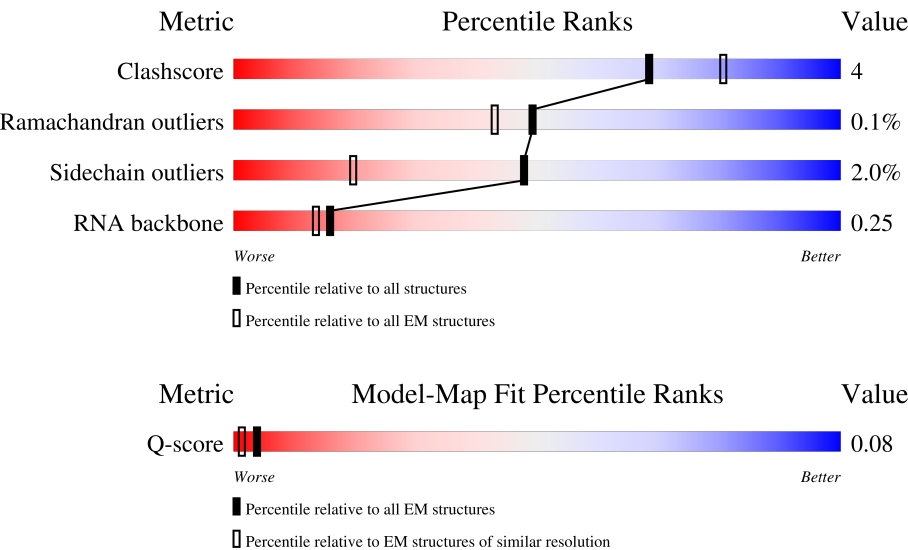
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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

The reported resolution of this entry is 4.01 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	6765 (3.51 - 4.51)

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	D	142	
2	E	210	
3	F	127	

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Mol	Chain	Length	Quality of chain
4	G	172	
5	H	150	
6	I	125	
7	J	67	
8	K	117	
9	L	58	
10	P	21	
11	Q	1179	
12	T	257	
13	W	305	
14	Y	121	
15	b	85	
16	A	1970	
17	B	1174	
18	C	275	
19	M	1729	
20	N	247	
21	U	666	
22	V	531	
23	X	531	
24	Z	1087	
25	a	821	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 64867 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 RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	126	Total	C	N	O	S	0	0
			1014	634	170	206	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1343	871	217	247	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	149	Total	C	N	O	S	0	0
			1198	759	195	239	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 9 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	21	Total	C	N	O	P	0	0
			439	196	68	154	21		

- Molecule 11 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 12 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	43	Total	C	N	O	P	0	0
			881	417	171	250	43		

- Molecule 13 is a protein called Superskiller complex protein 8.

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

- Molecule 14 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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 P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 15 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	67	Total	C	N	O	S	0	0
			523	322	84	110	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-1	SER	-	expression tag	UNP P60002
b	0	ASN	-	expression tag	UNP P60002
b	1	ALA	-	expression tag	UNP P60002

- Molecule 16 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	A	1473	Total	C	N	O	P	S	0	0
			11651	7315	2076	2183	2	75		

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	1136	Total	C	N	O	S	0	0
			9088	5745	1597	1682	64		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	1074	Total	C	N	O	S	0	0
			8835	5613	1536	1644	42		

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 20 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	31	Total	C	N	O	P	0	0
			633	302	106	194	31		

- 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 Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	227	Total	C	N	O	S	0	0
			1881	1207	340	329	5		

- Molecule 24 is a protein called Transcription elongation factor SPT5.

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

- Molecule 25 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	232	Total	C	N	O	S	0	0
			1878	1183	340	340	15		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

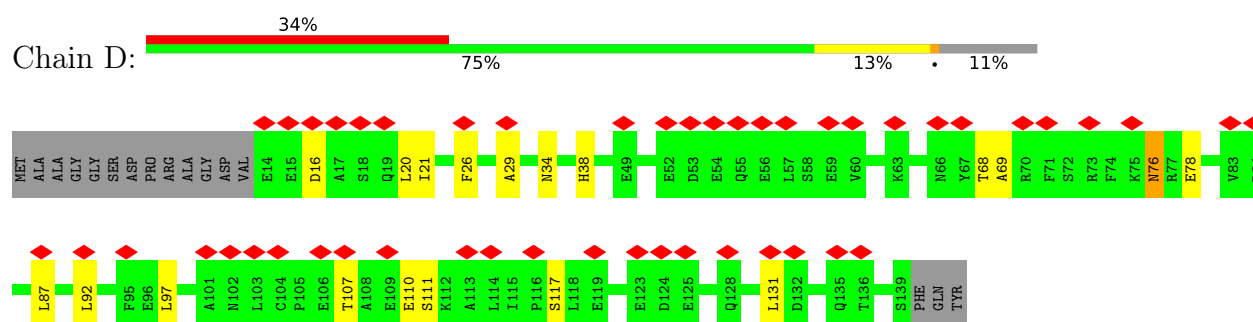
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

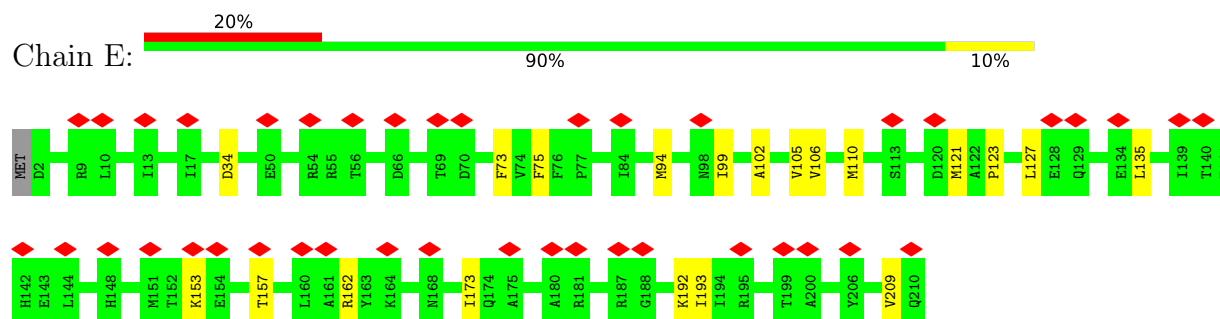
3 Residue-property plots [i](#)

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

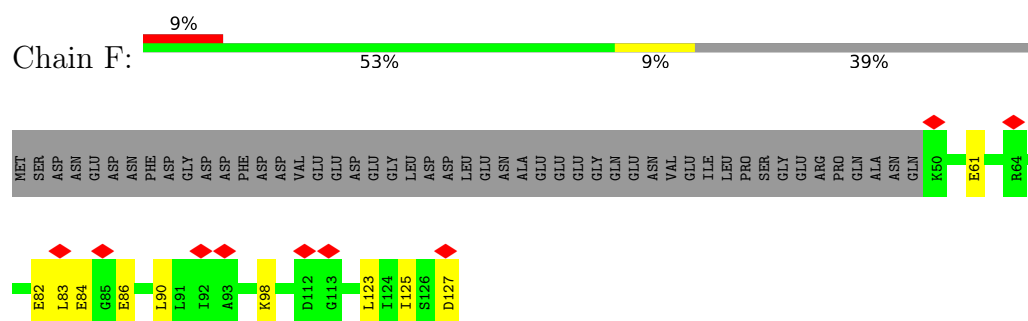
- Molecule 1: RNA polymerase II subunit D



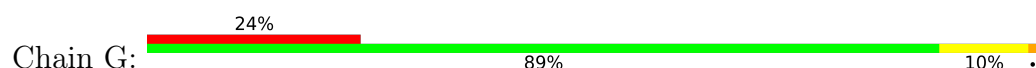
- Molecule 2: DNA-directed RNA polymerase II subunit E

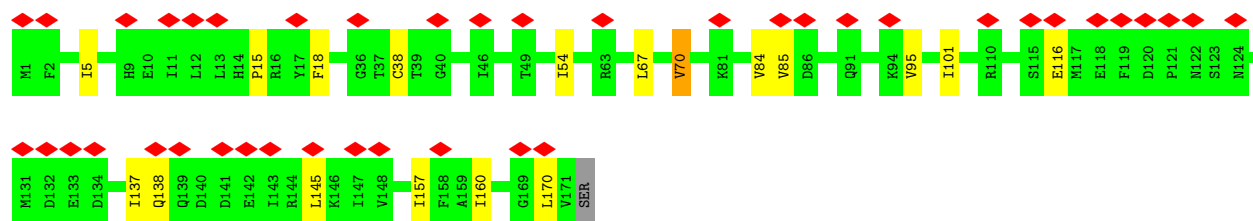


- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2



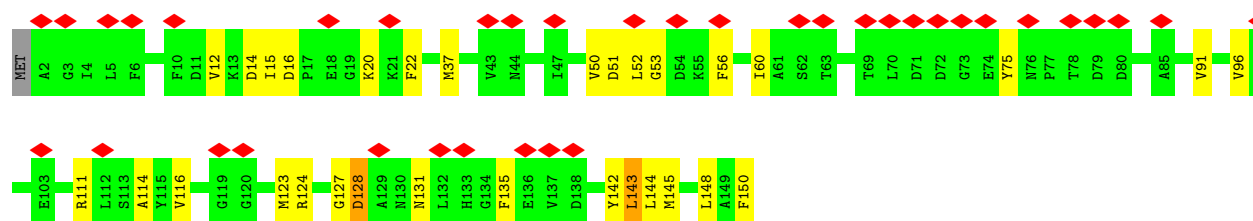
- Molecule 4: DNA-directed RNA polymerase II subunit RPB7





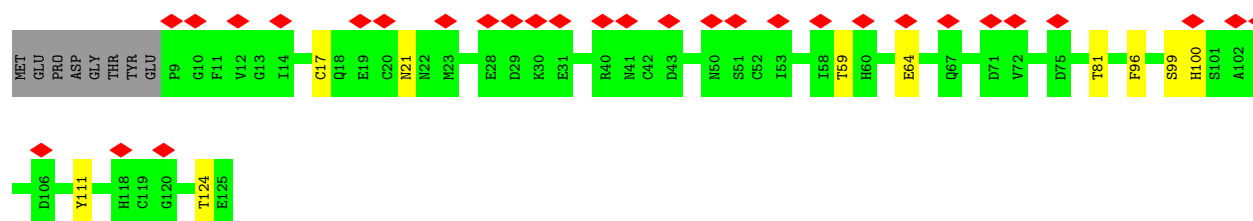
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



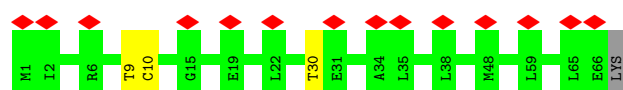
- Molecule 6: DNA-directed RNA polymerase II subunit RPB9

Chain I:



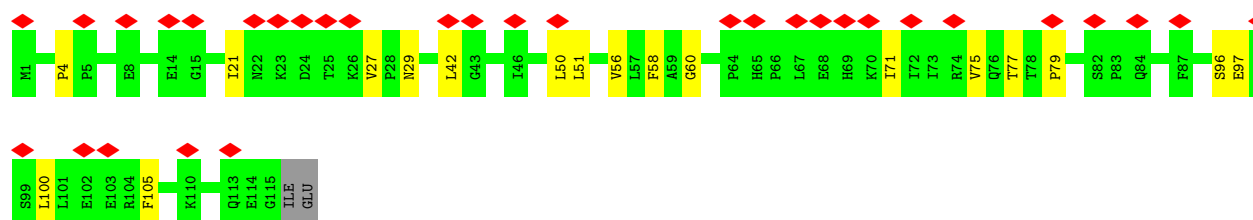
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

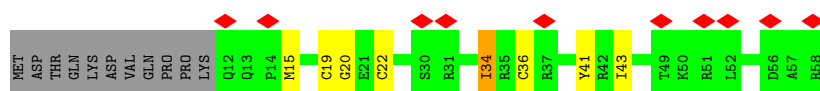


- Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a

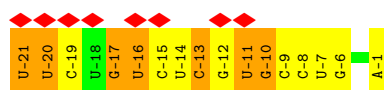
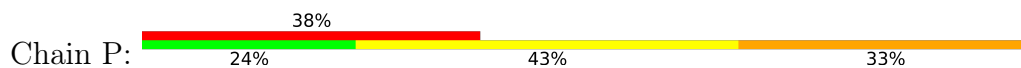
Chain K:



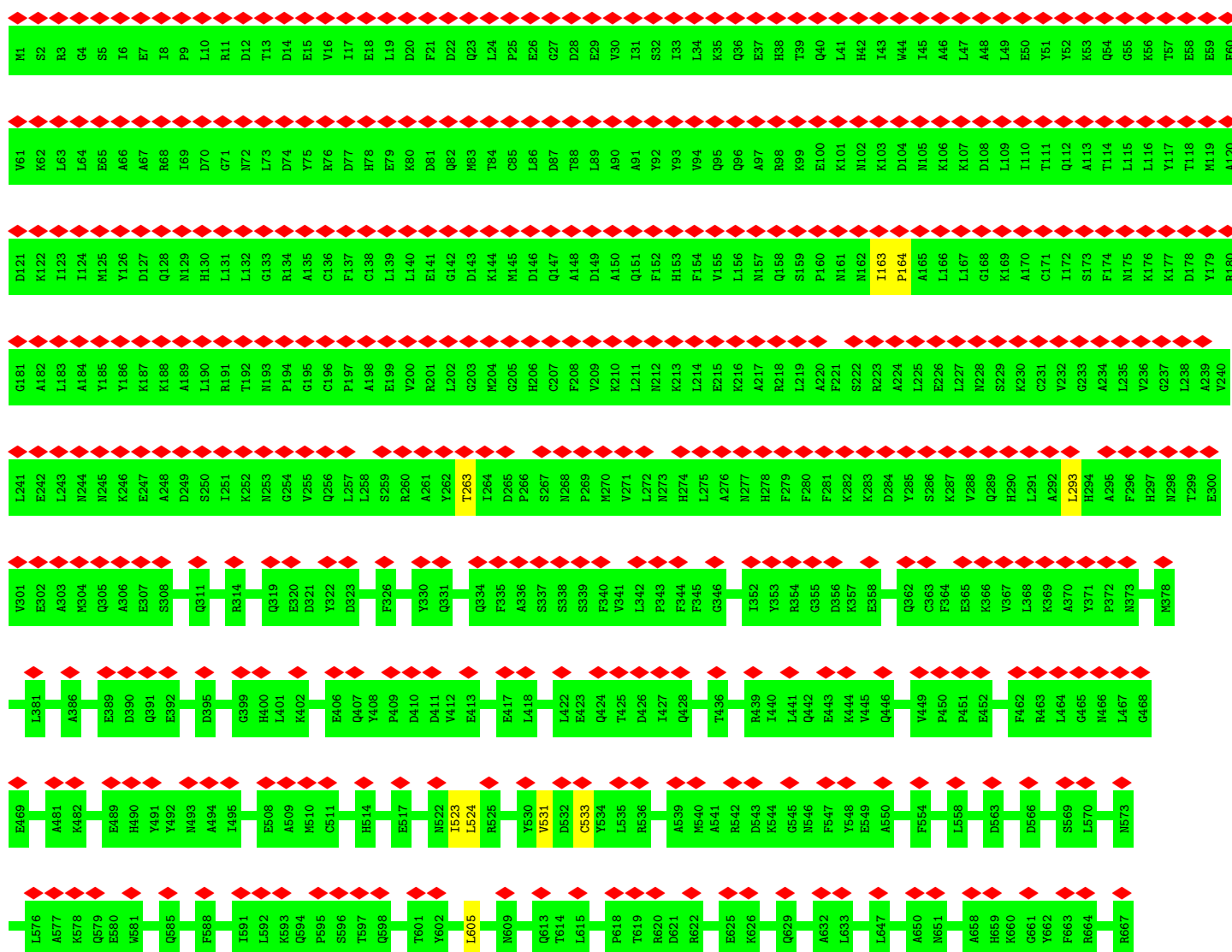
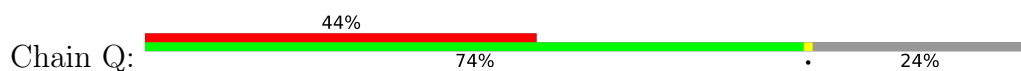
- Molecule 9: RNA polymerase II subunit K

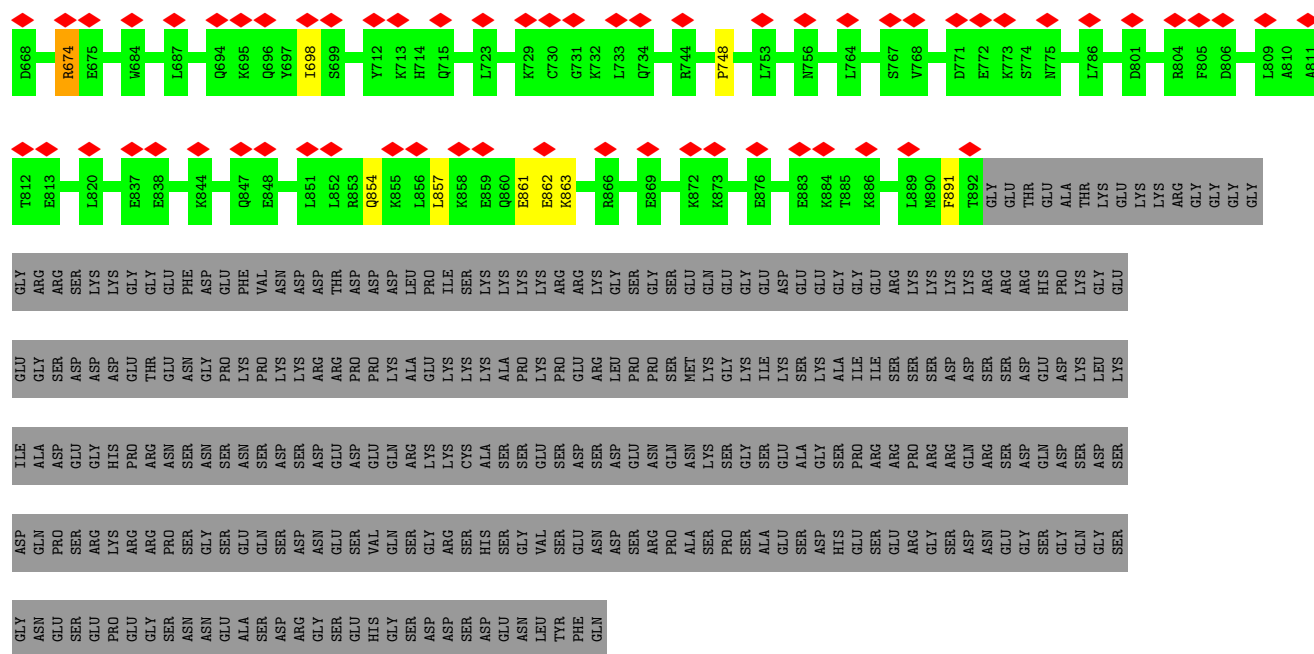


• Molecule 10: RNA

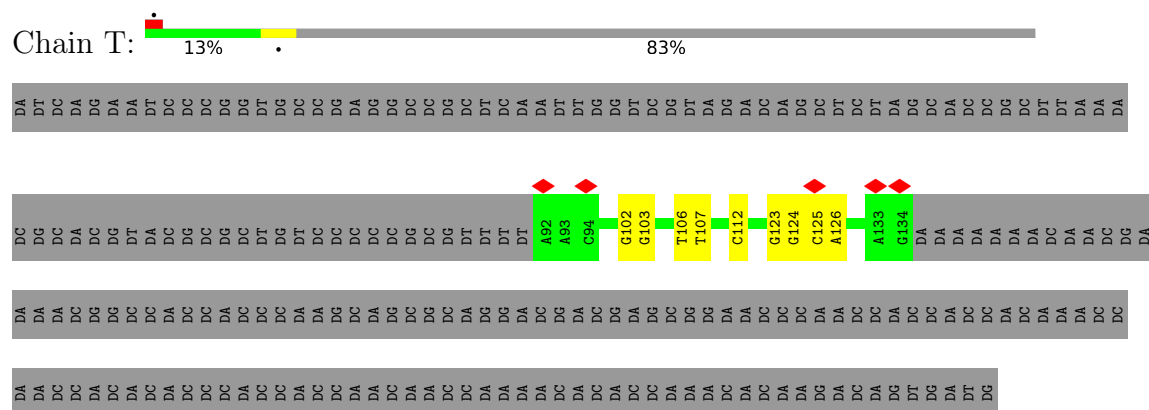


• Molecule 11: RNA polymerase-associated protein CTR9 homolog

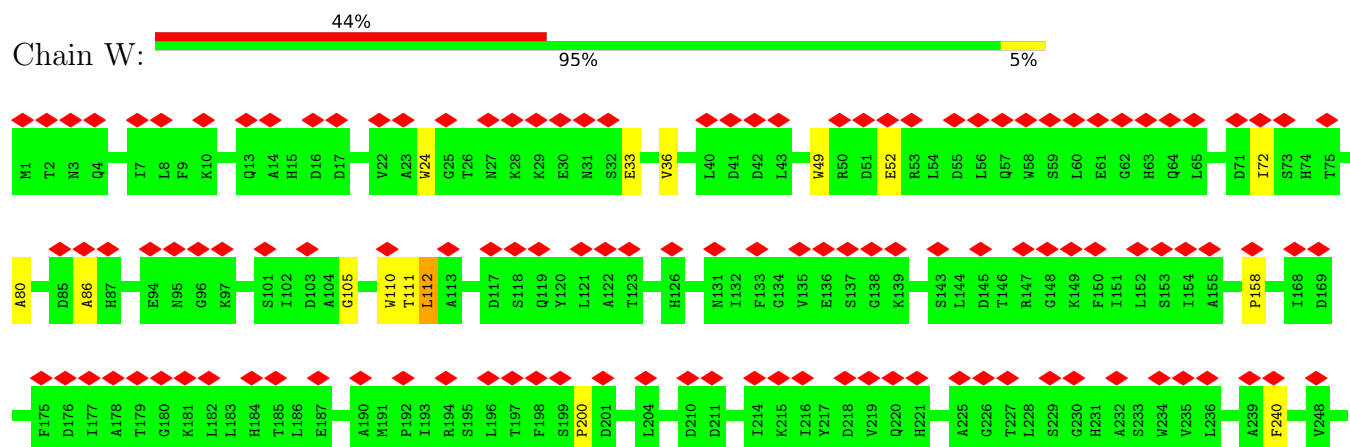


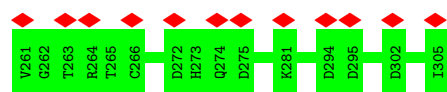


• Molecule 12: Template DNA

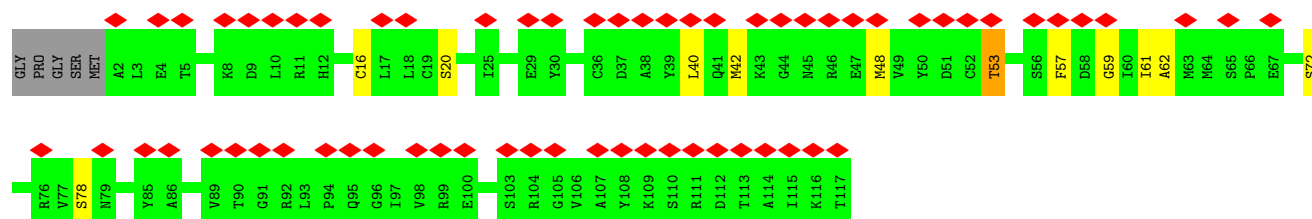
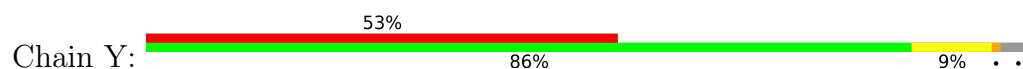


• Molecule 13: Superskiller complex protein 8

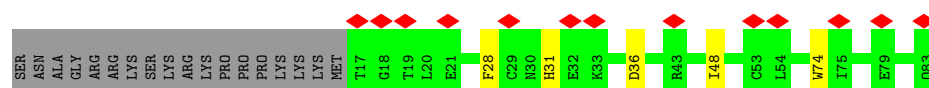




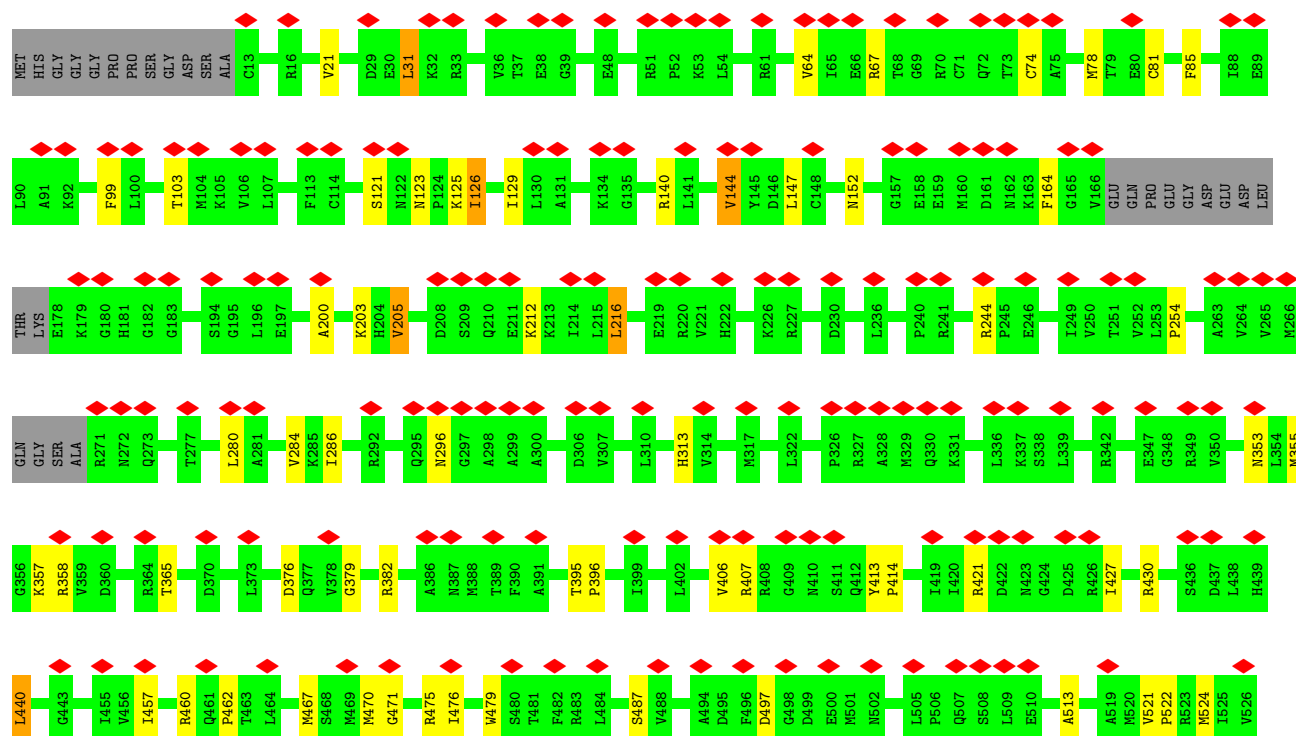
• Molecule 14: Transcription elongation factor SPT4

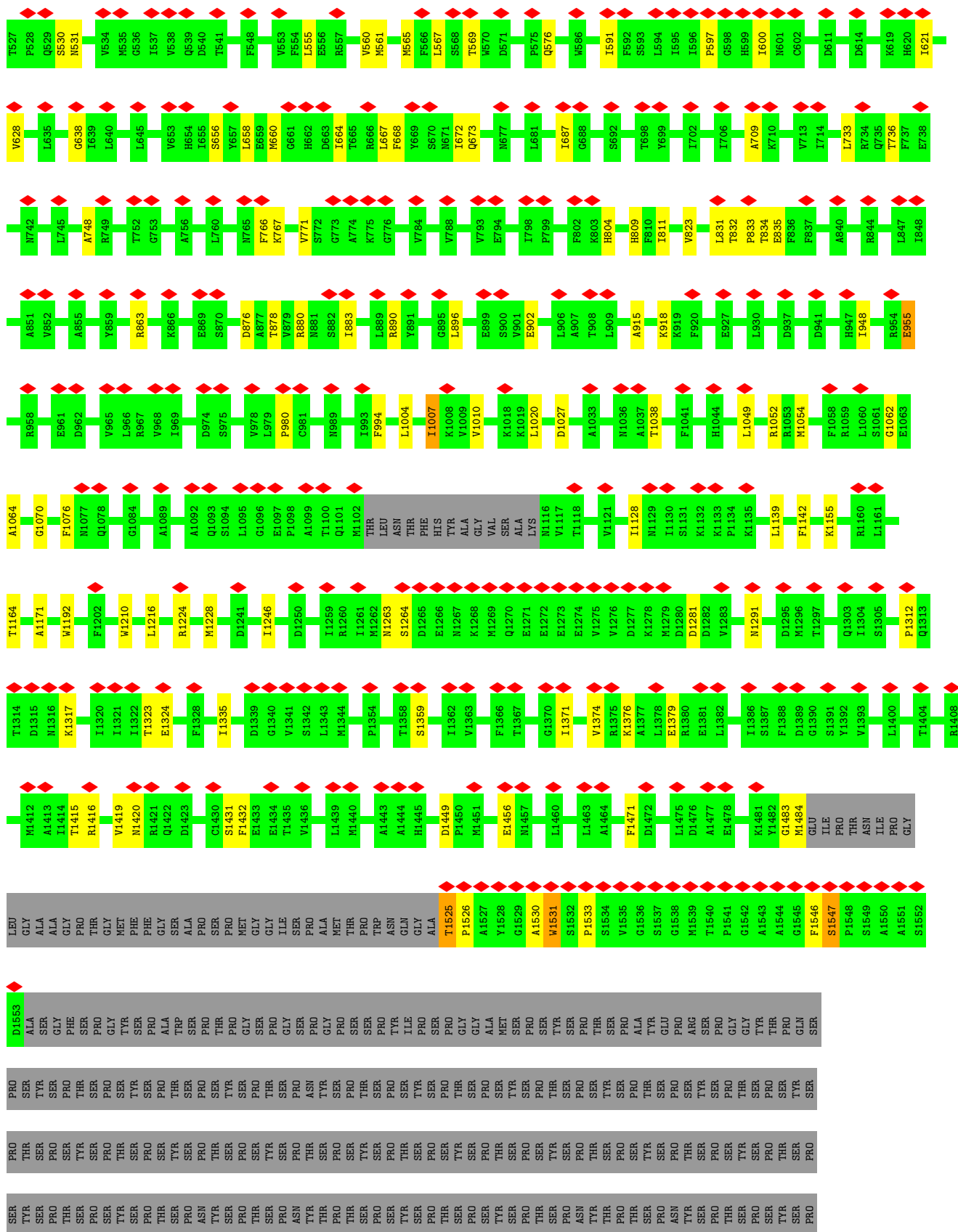


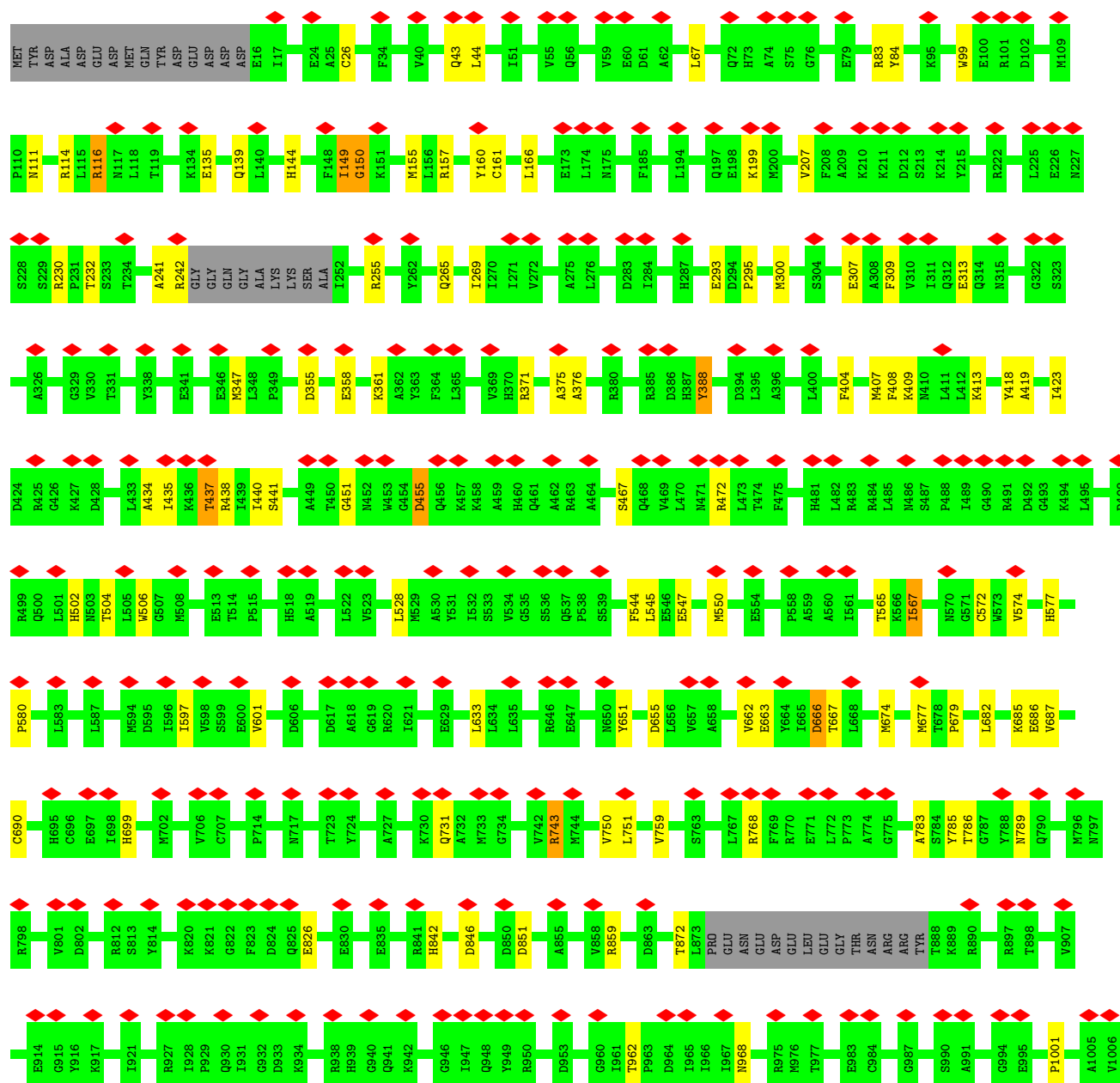
• Molecule 15: Transcription elongation factor 1 homolog

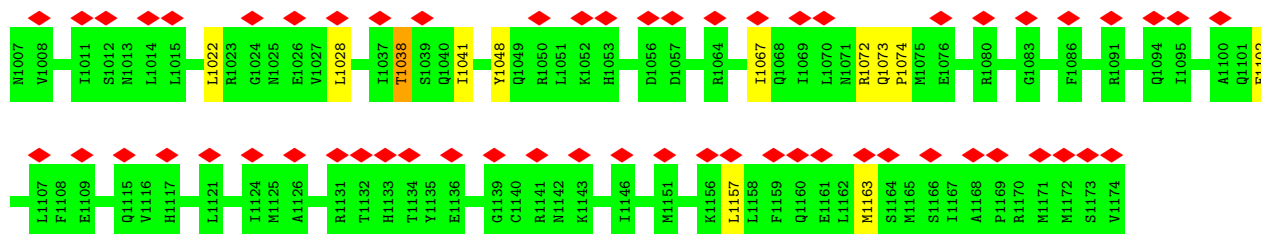


• Molecule 16: DNA-directed RNA polymerase subunit

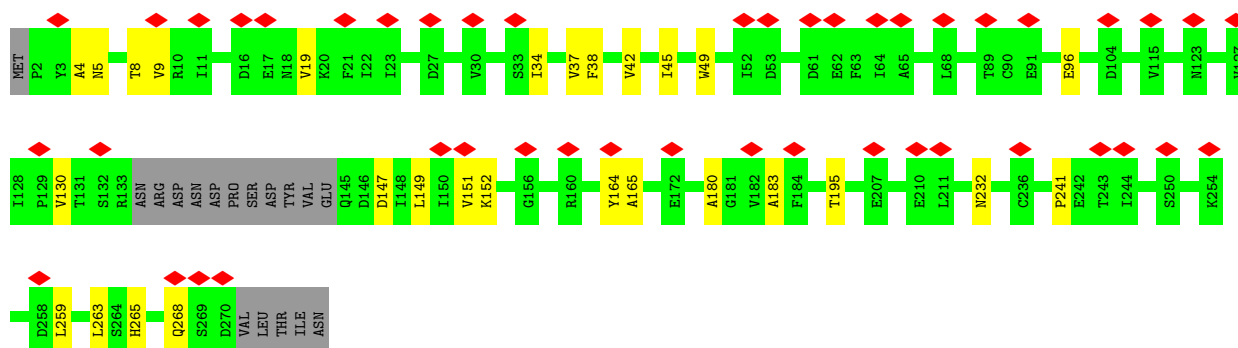
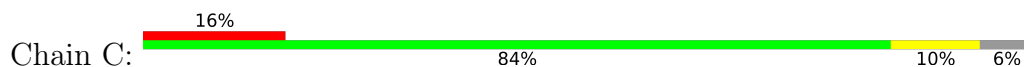




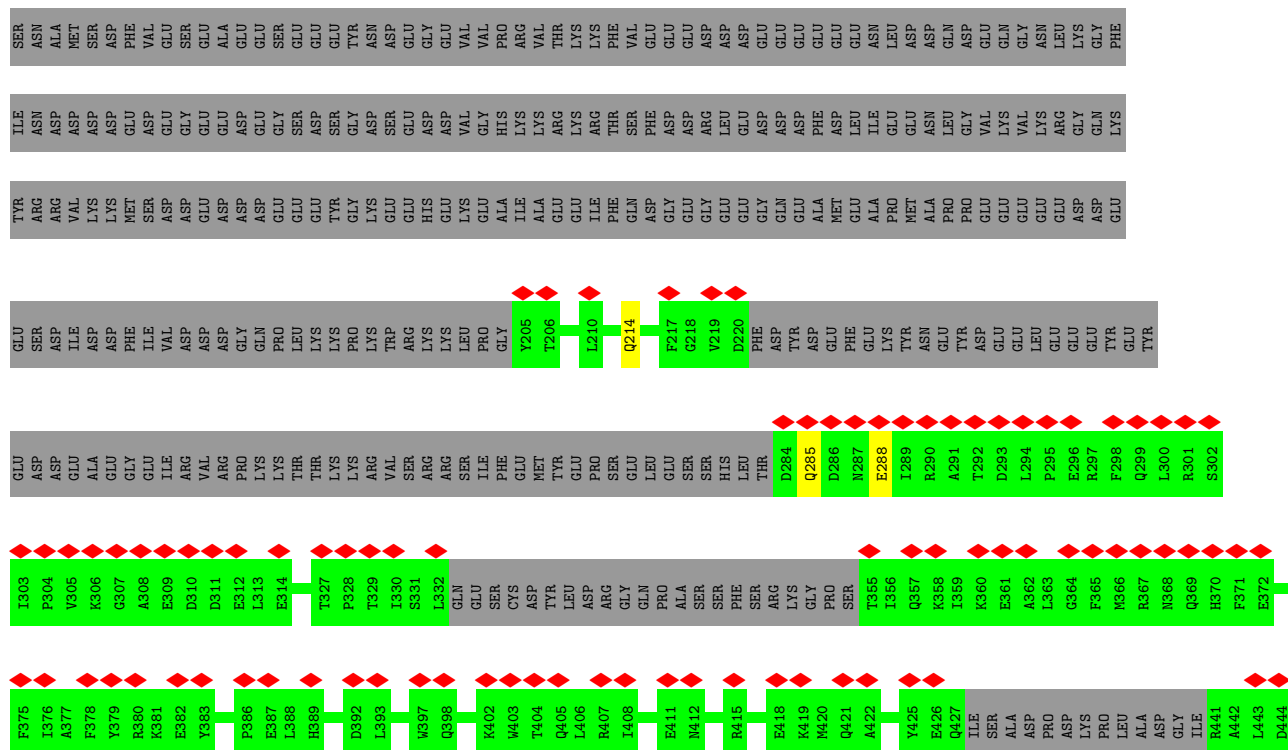




• Molecule 18: DNA-directed RNA polymerase II subunit RPB3



• Molecule 19: Transcription elongation factor SPT6









Chain a: 14% 28% 72%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1837	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 ($e^-/\text{\AA}^2$)	40.03	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	0.608	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SEP, ZN, TPO

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	D	0.27	0/1027	0.74	0/1381
2	E	0.23	0/1752	0.77	0/2366
3	F	0.31	0/637	0.84	0/859
4	G	0.21	0/1374	0.77	0/1865
5	H	0.26	0/1220	0.77	1/1644 (0.1%)
6	I	0.28	0/973	0.82	0/1316
7	J	0.26	0/533	0.75	0/719
8	K	0.30	0/939	0.85	0/1271
9	L	0.62	0/404	0.92	0/536
10	P	0.89	8/487 (1.6%)	0.95	0/755
11	Q	0.26	0/7379	0.68	0/9945
12	T	0.50	1/990 (0.1%)	1.06	0/1524
13	W	0.22	0/2433	0.64	0/3311
14	Y	0.28	0/928	0.87	1/1250 (0.1%)
15	b	0.26	0/533	0.78	0/725
16	A	0.26	0/11844	0.76	0/15984
17	B	0.76	6/9269 (0.1%)	0.93	15/12512 (0.1%)
18	C	0.25	0/2115	0.71	0/2873
19	M	0.28	0/9010	0.81	0/12135
20	N	0.35	0/705	1.06	0/1084
21	U	0.40	0/1498	0.99	10/2018 (0.5%)
22	V	0.24	0/2360	0.78	0/3188
23	X	0.38	0/1926	1.04	4/2606 (0.2%)
24	Z	0.26	0/4045	0.84	0/5445
25	a	0.23	0/1907	0.69	0/2547
All	All	0.39	15/66288 (0.0%)	0.81	31/89859 (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
9	L	0	1
12	T	0	2
16	A	0	6
17	B	0	4
19	M	0	5
20	N	0	2
21	U	0	2
22	V	0	1
23	X	0	3
24	Z	0	2
All	All	0	28

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	-14	U	C1'-N1	6.62	1.58	1.48
10	P	-1	A	P-OP1	6.51	1.61	1.48
12	T	112	DC	P-OP1	6.49	1.61	1.48
10	P	-11	U	C1'-N1	6.41	1.57	1.47
10	P	-15	C	C1'-N1	6.38	1.58	1.48

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	111	ASN	CA-CB-CG	-8.84	103.76	112.60
17	B	743	ARG	NE-CZ-NH2	8.72	127.05	119.20
17	B	455	ASP	CA-CB-CG	7.44	120.04	112.60
17	B	114	ARG	NE-CZ-NH2	7.43	125.89	119.20
17	B	144	HIS	CA-CB-CG	-6.55	107.25	113.80

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	A	152	ASN	Mainchain
16	A	203	LYS	Mainchain
9	L	41	TYR	Sidechain
12	T	123	DG	Sidechain
12	T	124	DG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1014	0	988	12	0
2	E	1721	0	1737	10	0
3	F	627	0	657	9	0
4	G	1343	0	1340	9	0
5	H	1198	0	1156	22	0
6	I	950	0	879	7	0
7	J	524	0	540	2	0
8	K	920	0	942	16	0
9	L	398	0	402	6	0
10	P	439	0	222	4	0
11	Q	7240	0	7186	10	0
12	T	881	0	480	3	0
13	W	2374	0	2290	9	0
14	Y	912	0	904	10	0
15	b	523	0	484	3	0
16	A	11651	0	11722	114	0
17	B	9088	0	9112	61	0
18	C	2072	0	2019	17	0
19	M	8835	0	8777	72	0
20	N	633	0	354	10	0
21	U	1469	0	1441	9	0
22	V	2310	0	2247	15	0
23	X	1881	0	1919	66	0
24	Z	3976	0	4048	35	0
25	a	1878	0	1957	4	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	Y	1	0	0	0	0
27	A	1	0	0	0	0
All	All	64867	0	63803	471	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 4.

The worst 5 of 471 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)
24:Z:181:THR:HG22	24:Z:226:TYR:CE2	2.14	0.82
23:X:364:ILE:HG23	23:X:427:VAL:HG12	1.63	0.80
16:A:834:THR:HG23	17:B:677:MET:HE3	1.63	0.78
19:M:1487:VAL:HG13	19:M:1495:ARG:O	1.89	0.73
23:X:364:ILE:CG2	23:X:427:VAL:HG12	2.20	0.71

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	D	124/142 (87%)	124 (100%)	0	0	100	100
2	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
3	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
4	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	H	147/150 (98%)	135 (92%)	12 (8%)	0	100	100
6	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
7	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
8	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
9	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
11	Q	890/1179 (76%)	877 (98%)	13 (2%)	0	100	100
13	W	303/305 (99%)	296 (98%)	7 (2%)	0	100	100
14	Y	114/121 (94%)	108 (95%)	6 (5%)	0	100	100
15	b	65/85 (76%)	62 (95%)	3 (5%)	0	100	100
16	A	1462/1970 (74%)	1389 (95%)	72 (5%)	1 (0%)	48	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	B	1130/1174 (96%)	1063 (94%)	65 (6%)	2 (0%)	43	75
18	C	254/275 (92%)	240 (94%)	13 (5%)	1 (0%)	30	65
19	M	1050/1729 (61%)	1007 (96%)	42 (4%)	1 (0%)	48	81
21	U	175/666 (26%)	169 (97%)	6 (3%)	0	100	100
22	V	275/531 (52%)	266 (97%)	9 (3%)	0	100	100
23	X	223/531 (42%)	211 (95%)	10 (4%)	2 (1%)	14	48
24	Z	484/1087 (44%)	461 (95%)	23 (5%)	0	100	100
25	a	224/821 (27%)	218 (97%)	6 (3%)	0	100	100
All	All	7709/11642 (66%)	7385 (96%)	317 (4%)	7 (0%)	49	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	424	PRO
17	B	150	GLY
19	M	1515	TYR
16	A	1530	ALA
23	X	242	GLY

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	D	112/126 (89%)	110 (98%)	2 (2%)	51	68
2	E	191/192 (100%)	189 (99%)	2 (1%)	68	76
3	F	68/111 (61%)	65 (96%)	3 (4%)	25	48
4	G	149/153 (97%)	144 (97%)	5 (3%)	32	55
5	H	130/131 (99%)	125 (96%)	5 (4%)	29	51
6	I	105/112 (94%)	104 (99%)	1 (1%)	68	76
7	J	55/56 (98%)	54 (98%)	1 (2%)	51	68
8	K	104/106 (98%)	102 (98%)	2 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L	44/55 (80%)	43 (98%)	1 (2%)	44	64
11	Q	763/1011 (76%)	755 (99%)	8 (1%)	68	76
13	W	260/260 (100%)	258 (99%)	2 (1%)	73	78
14	Y	102/105 (97%)	101 (99%)	1 (1%)	68	76
15	b	61/77 (79%)	60 (98%)	1 (2%)	55	69
16	A	1290/1747 (74%)	1268 (98%)	22 (2%)	53	68
17	B	996/1027 (97%)	964 (97%)	32 (3%)	34	56
18	C	235/252 (93%)	230 (98%)	5 (2%)	47	65
19	M	954/1524 (63%)	943 (99%)	11 (1%)	63	73
21	U	163/590 (28%)	162 (99%)	1 (1%)	78	81
22	V	255/462 (55%)	247 (97%)	8 (3%)	35	57
23	X	208/467 (44%)	196 (94%)	12 (6%)	18	42
24	Z	438/940 (47%)	427 (98%)	11 (2%)	42	62
25	a	211/737 (29%)	211 (100%)	0	100	100
All	All	6894/10241 (67%)	6758 (98%)	136 (2%)	48	66

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	390	ASP
23	X	443	VAL
24	Z	457	LEU
16	A	955	GLU
16	A	883	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
19	M	1151	ASN
19	M	1336	HIS
24	Z	300	GLN
15	b	31	HIS
14	Y	12	HIS

5.3.3 RNA

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

5 of 8 RNA backbone outliers are listed below:

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

All (5) RNA pucker outliers are listed below:

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

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

2 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	$\# Z > 2$
16	TPO	A	1525	16	8,10,11	2.64	1 (12%)	10,14,16	1.29	1 (10%)
16	SEP	A	1547	16	8,9,10	1.54	1 (12%)	7,12,14	2.64	2 (28%)

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
16	TPO	A	1525	16	-	1/9/11/13	-
16	SEP	A	1547	16	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1525	TPO	P-OG1	7.29	1.72	1.59
16	A	1547	SEP	P-O1P	3.30	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1547	SEP	OG-CB-CA	6.22	114.20	108.14
16	A	1547	SEP	O3P-P-OG	2.56	113.33	106.67
16	A	1525	TPO	OG1-P-O1P	-2.27	101.23	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	1547	SEP	N-CA-CB-OG
16	A	1547	SEP	C-CA-CB-OG
16	A	1525	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1525	TPO	1	0
16	A	1547	SEP	2	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](#)

There are no chain breaks in this entry.

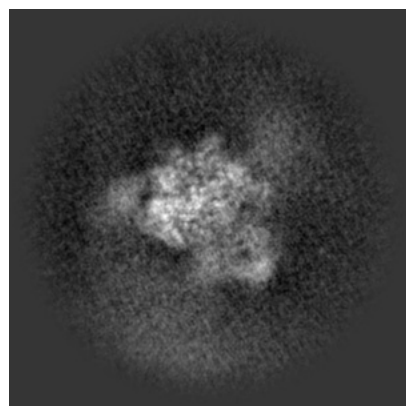
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54251. These allow visual inspection of the internal detail of the map and identification of artifacts.

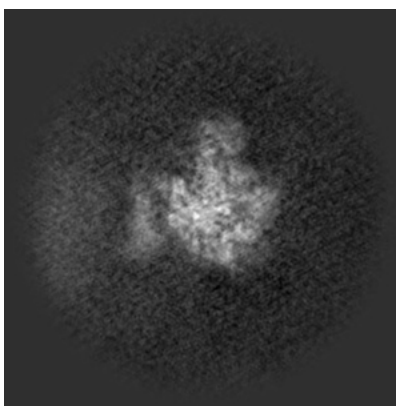
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

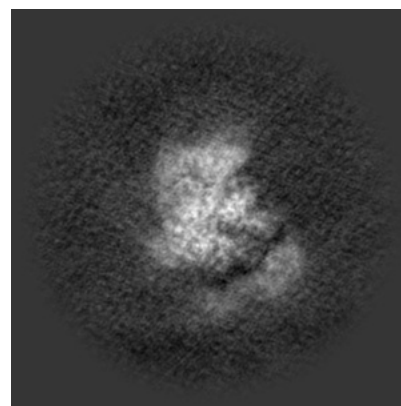
6.1.1 Primary map



X

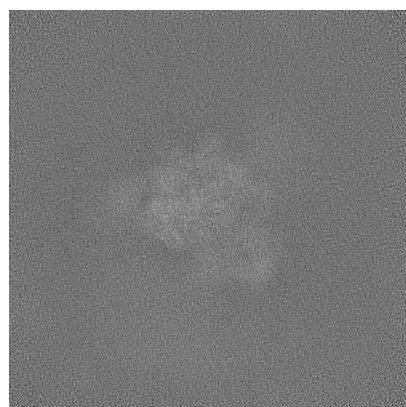


Y

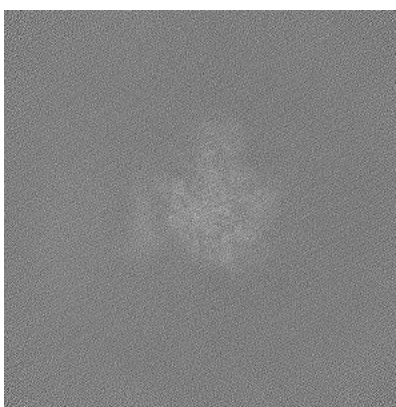


Z

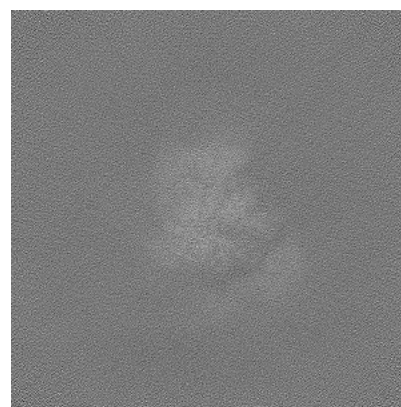
6.1.2 Raw map



X



Y

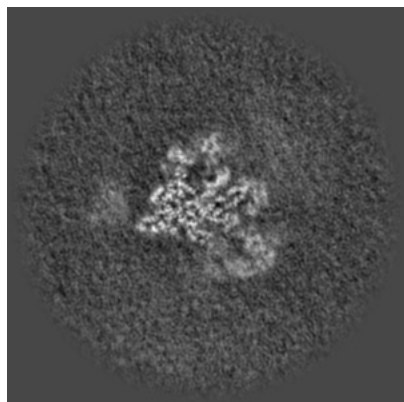


Z

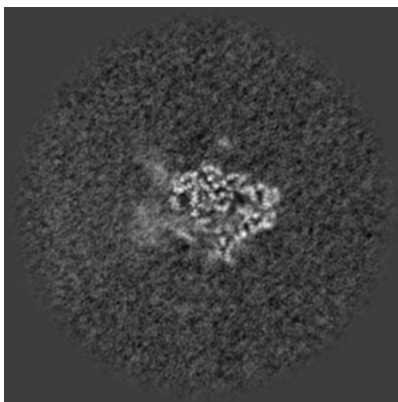
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

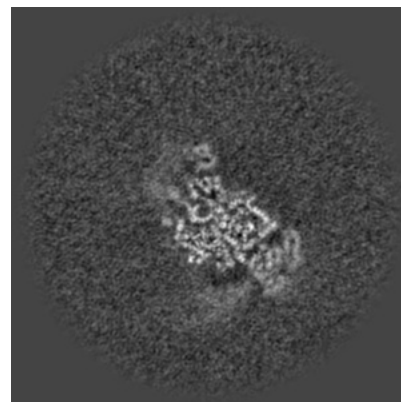
6.2.1 Primary map



X Index: 220

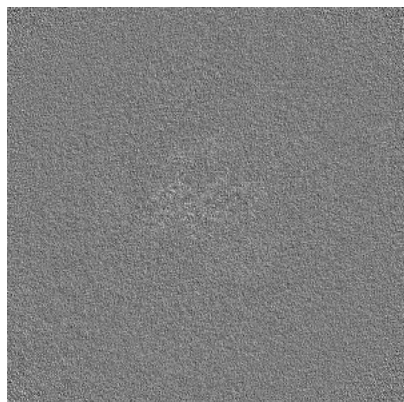


Y Index: 220

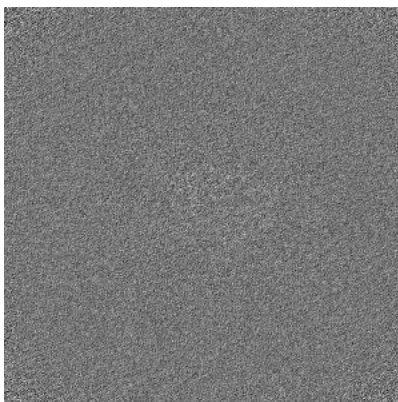


Z Index: 220

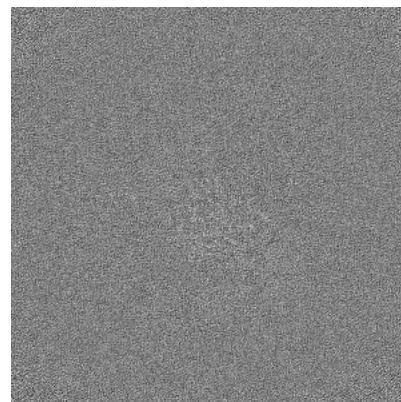
6.2.2 Raw map



X Index: 220



Y Index: 220

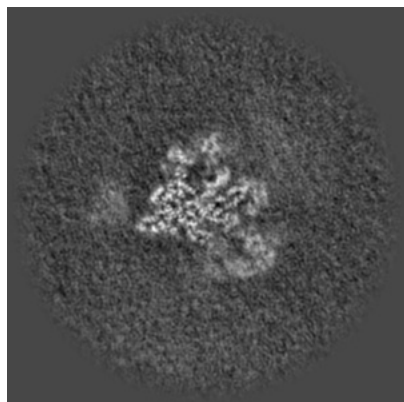


Z Index: 220

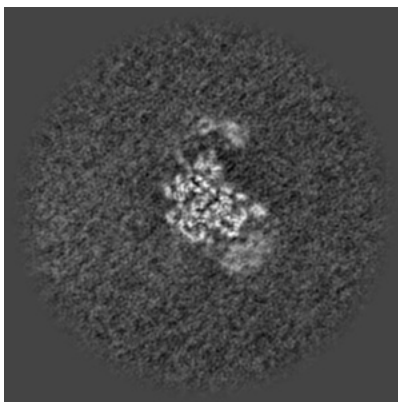
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

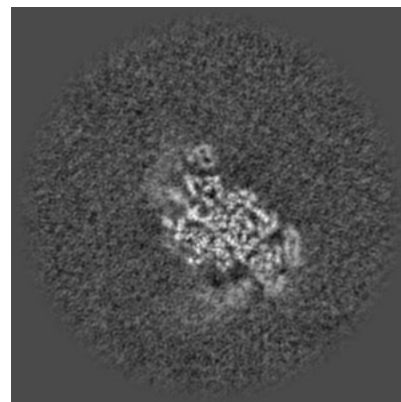
6.3.1 Primary map



X Index: 220

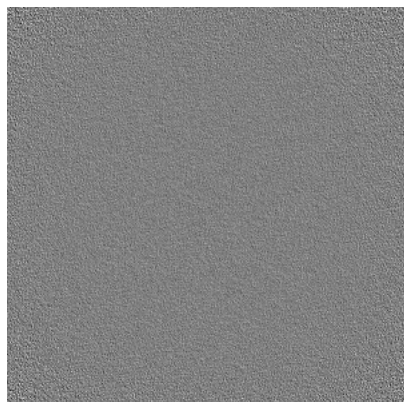


Y Index: 180

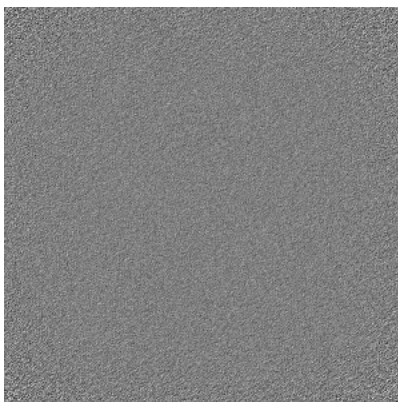


Z Index: 222

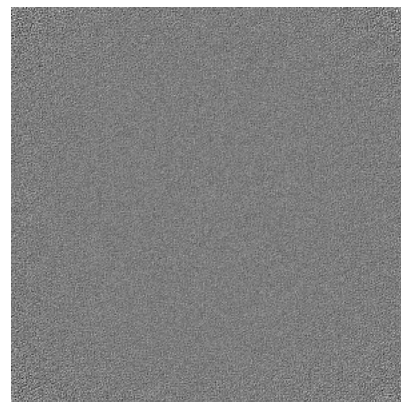
6.3.2 Raw map



X Index: 0



Y Index: 0

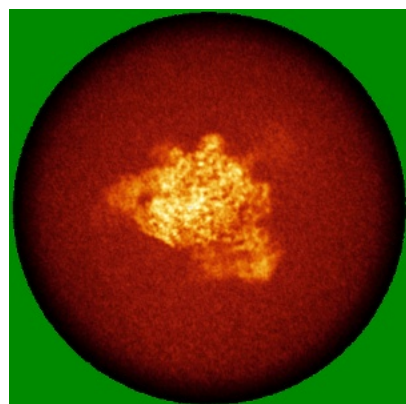


Z Index: 0

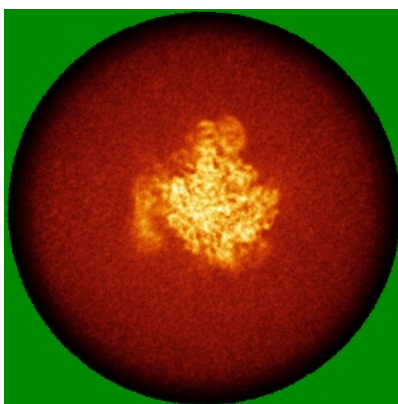
The images above show the largest variance slices of the map in three orthogonal directions.

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

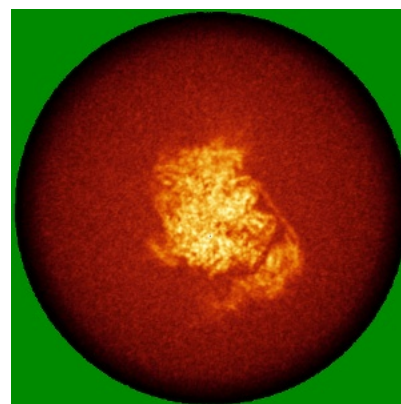
6.4.1 Primary map



X

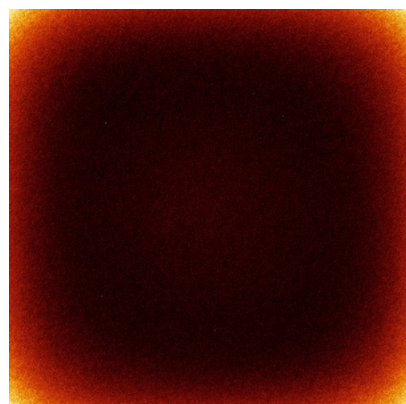


Y

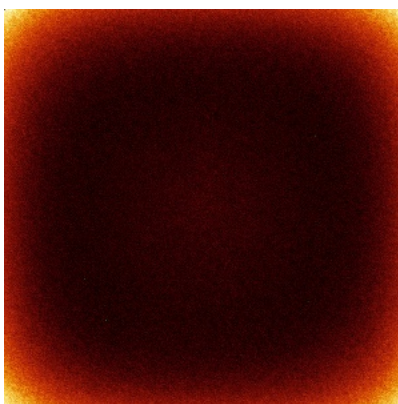


Z

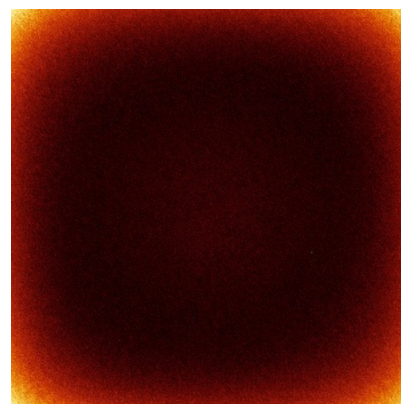
6.4.2 Raw map



X



Y

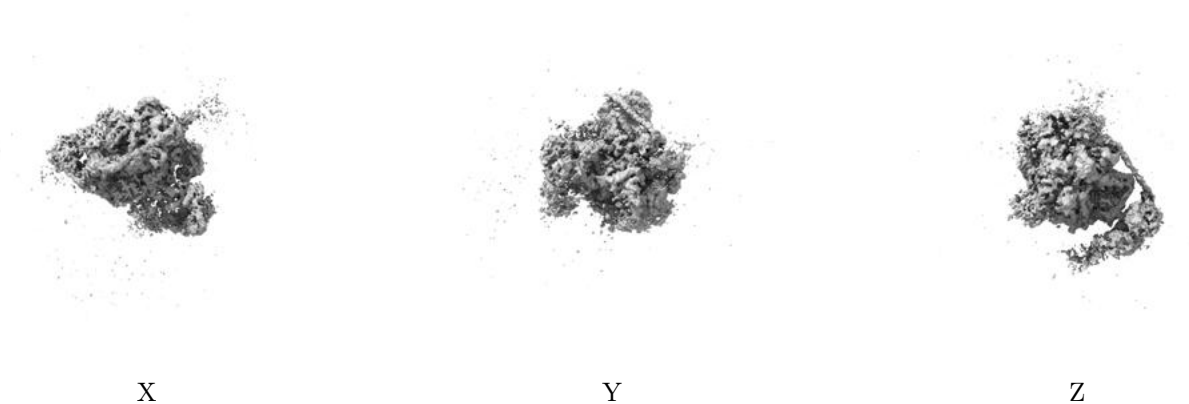


Z

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.

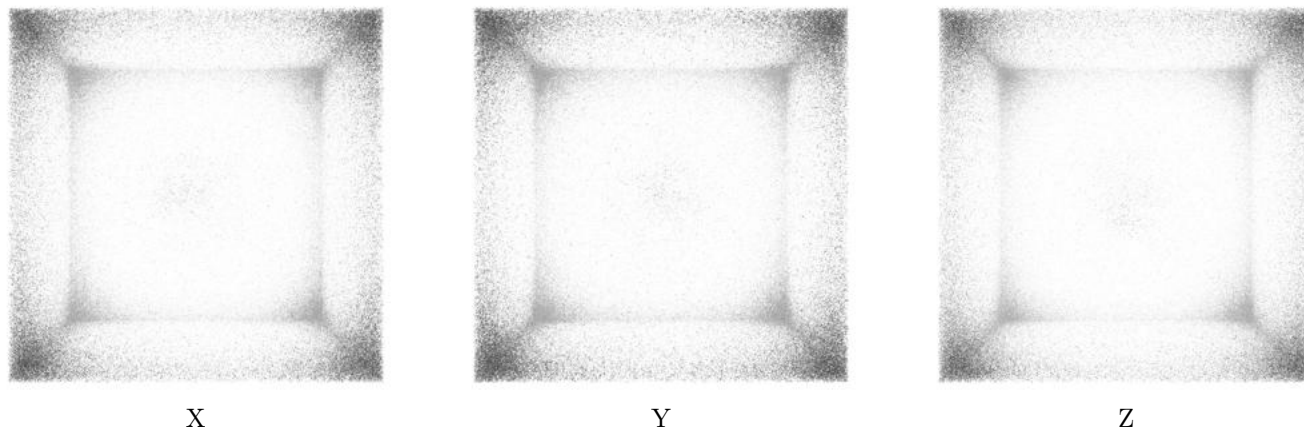
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

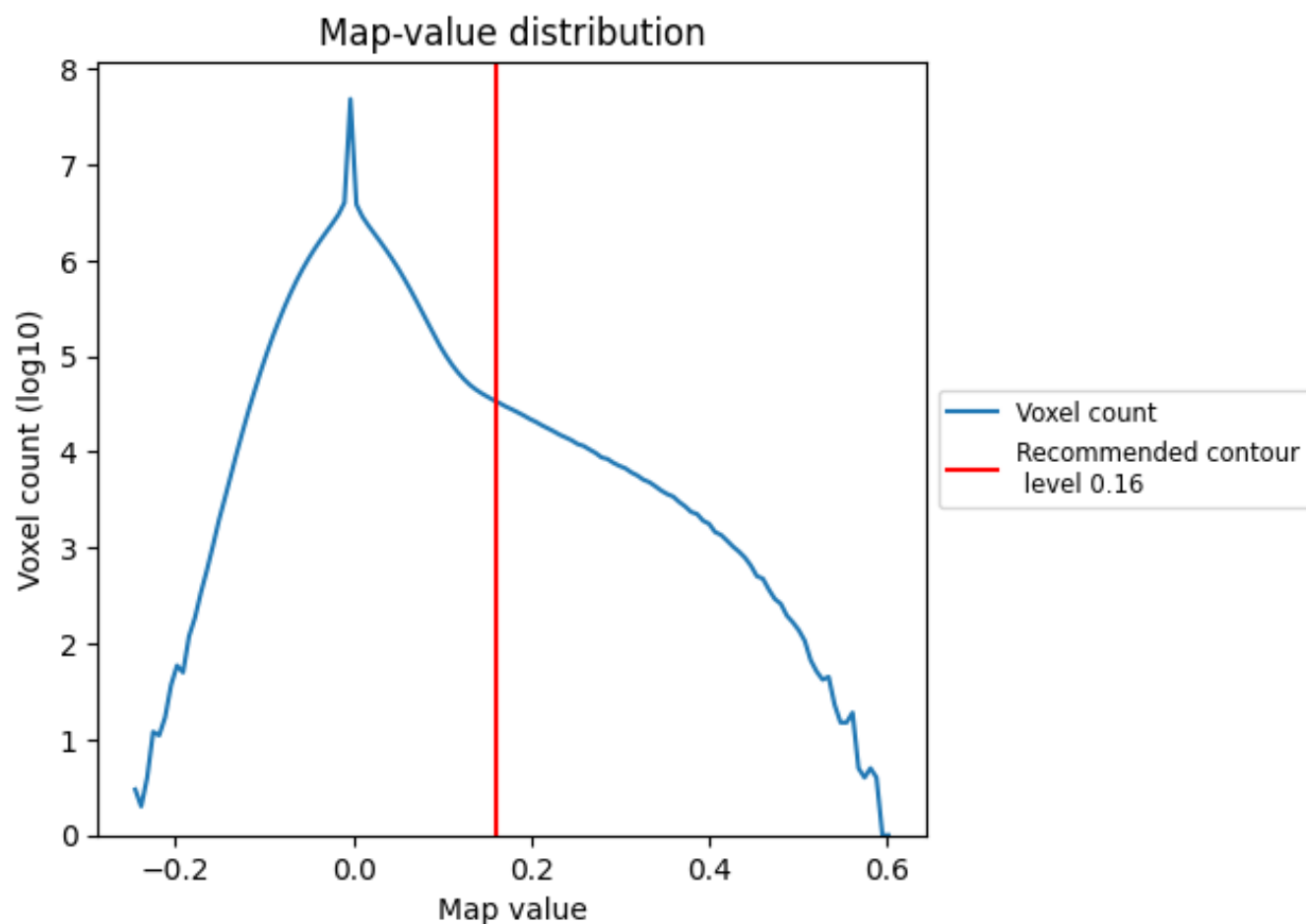
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

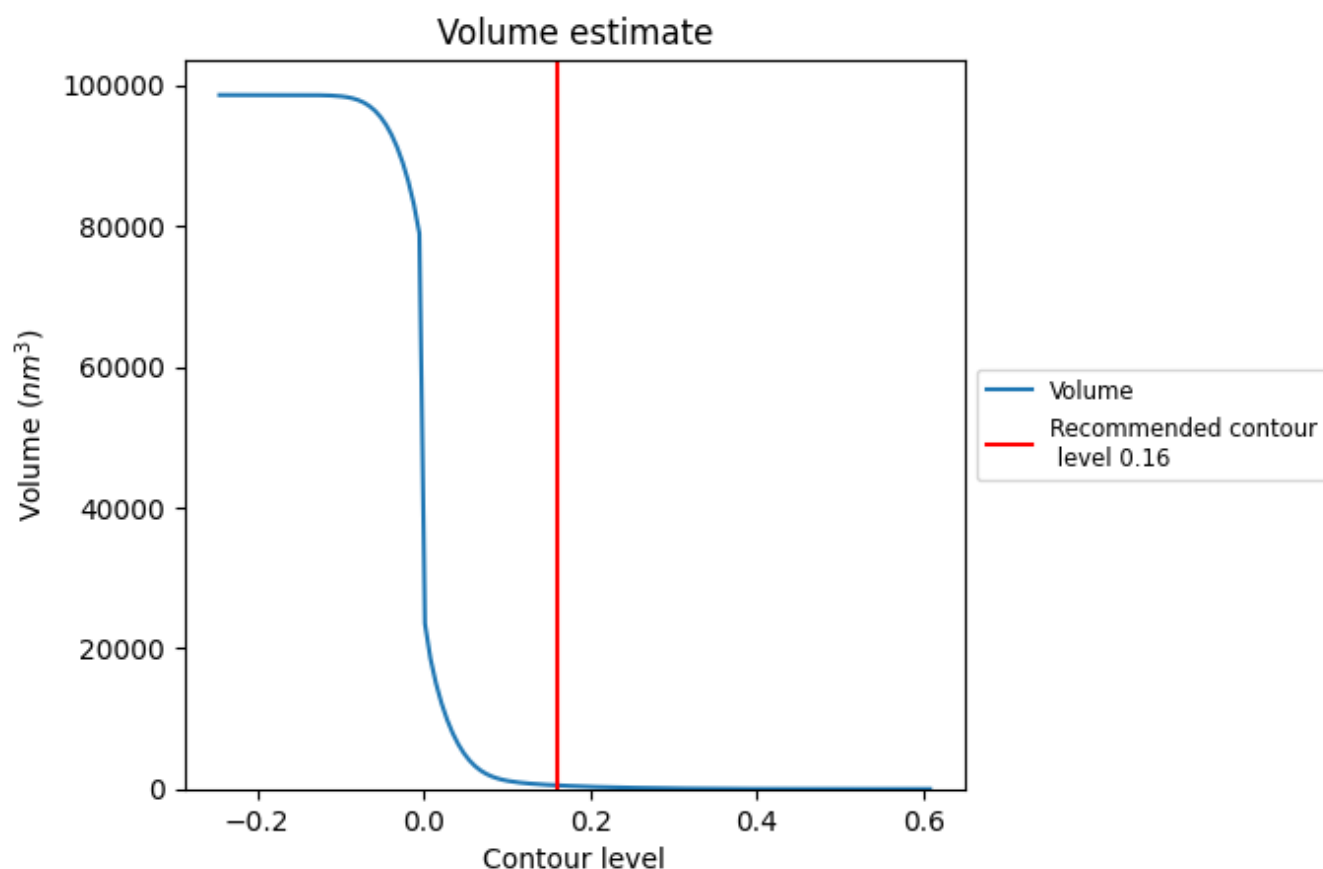
This section contains the results of statistical analysis of the map.

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.

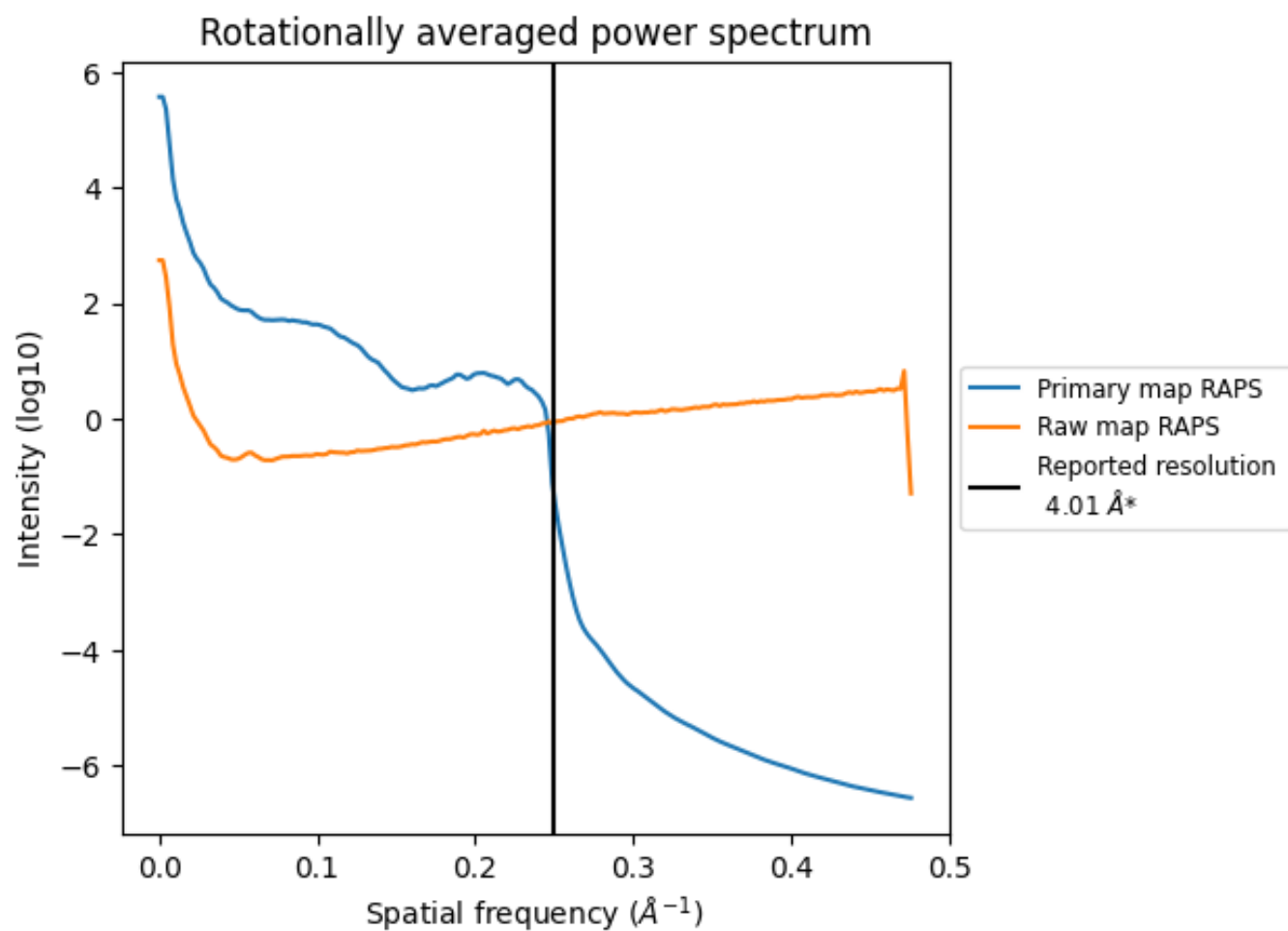
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm^3 ; this corresponds to an approximate mass of 467 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 ⓘ

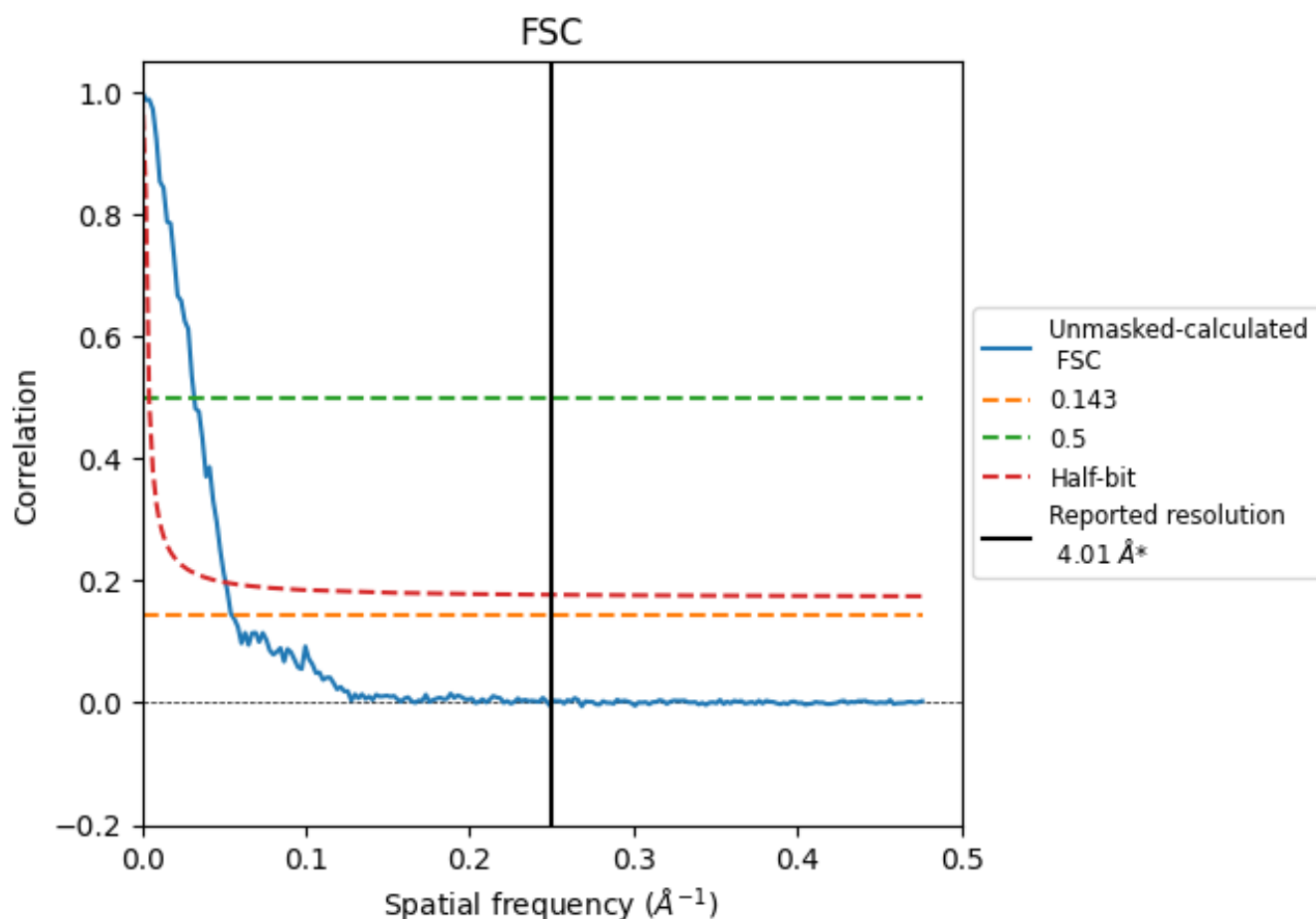


*Reported resolution corresponds to spatial frequency of 0.249 $\text{\AA}^{-1}$

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 0.249 Å⁻¹

8.2 Resolution estimates [i](#)

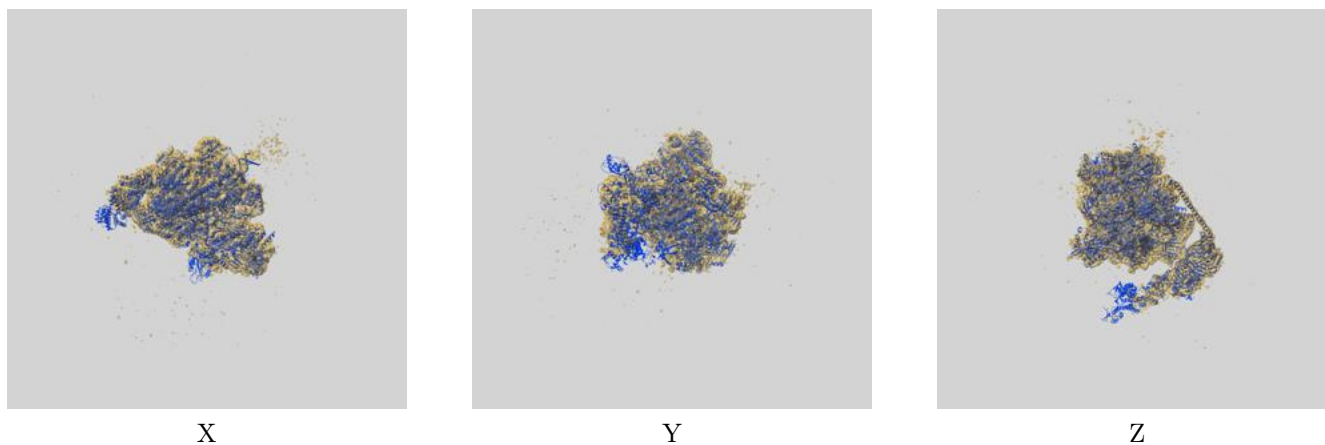
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	18.28	31.55	19.61

*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 18.28 differs from the reported value 4.01 by more than 10 %

9 Map-model fit [i](#)

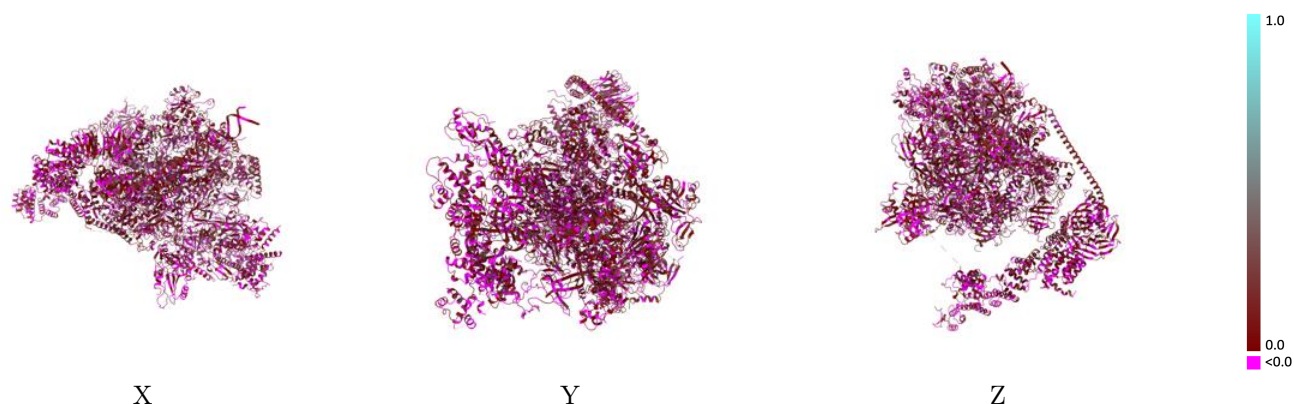
This section contains information regarding the fit between EMDB map EMD-54251 and PDB model 9RTT. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



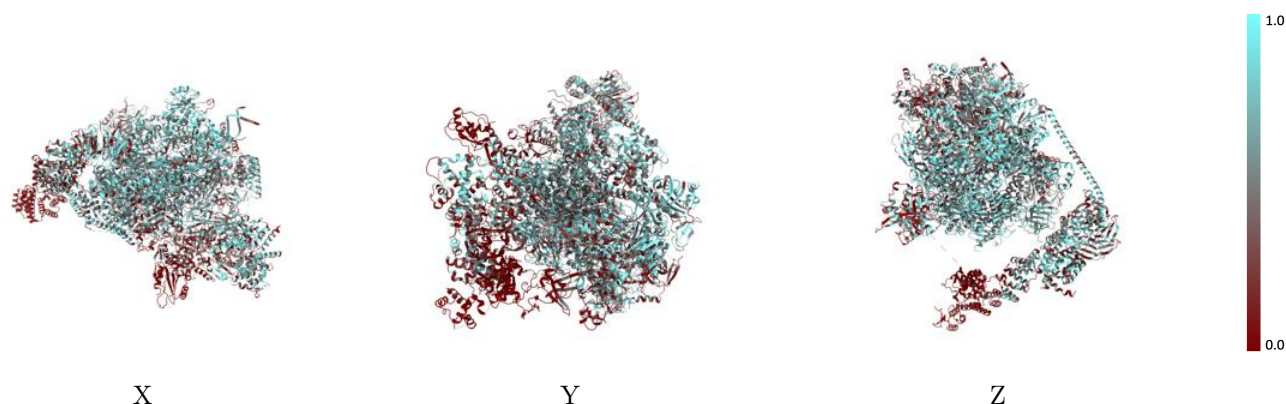
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



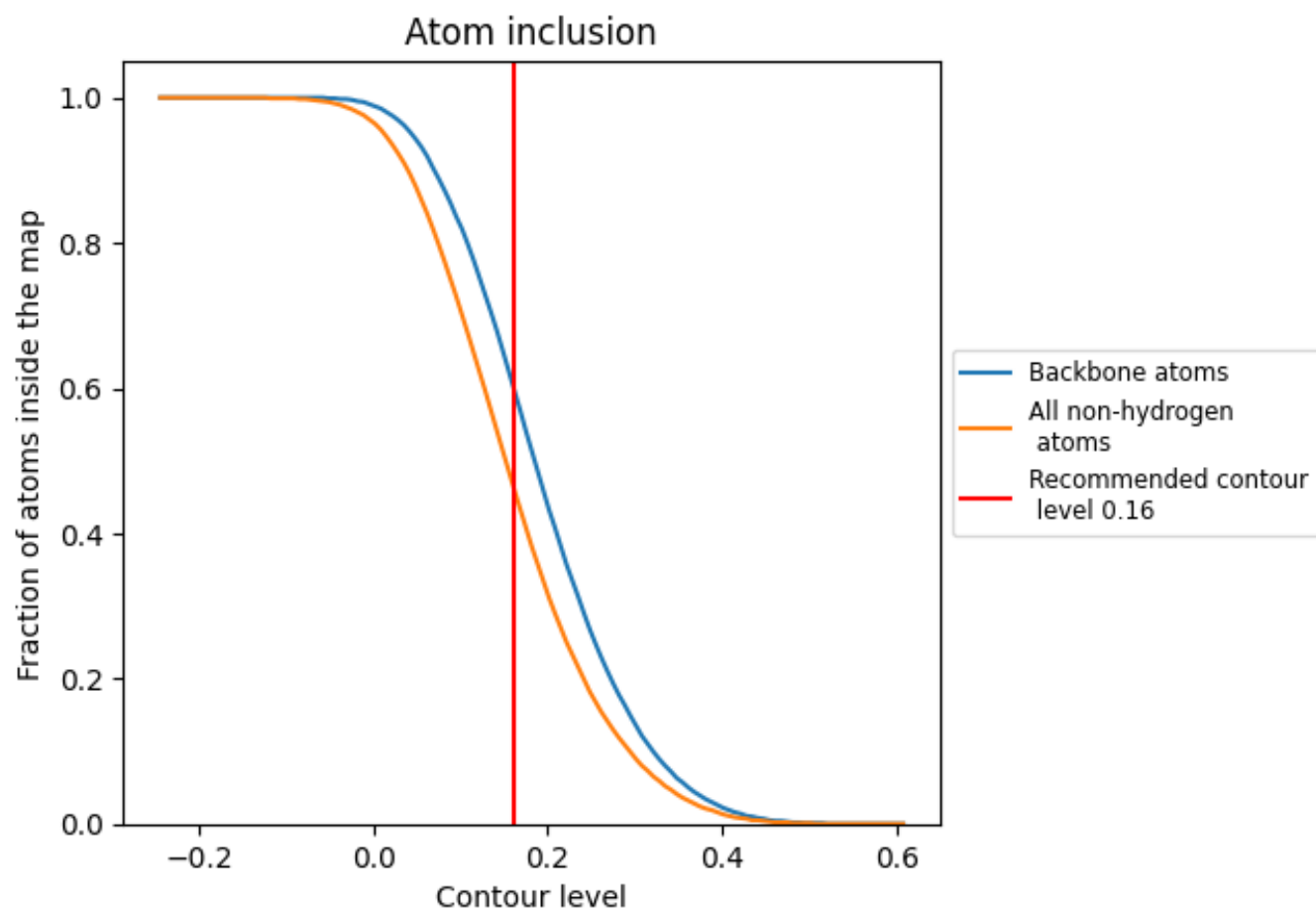
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 47% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4660	 0.0800
A	 0.5760	 0.0970
B	 0.5840	 0.0960
C	 0.6610	 0.1030
D	 0.5300	 0.0620
E	 0.6680	 0.1170
F	 0.6580	 0.1140
G	 0.5840	 0.0940
H	 0.5850	 0.0840
I	 0.6400	 0.0930
J	 0.6270	 0.0780
K	 0.5840	 0.1040
L	 0.6470	 0.1420
M	 0.2420	 0.0380
N	 0.5810	 0.1170
P	 0.5120	 0.1400
Q	 0.3480	 0.0560
T	 0.6530	 0.1400
U	 0.3590	 0.0770
V	 0.3030	 0.0640
W	 0.4860	 0.0650
X	 0.2900	 0.1100
Y	 0.3740	 0.0570
Z	 0.3230	 0.0530
a	 0.4290	 0.0860
b	 0.6800	 0.1110

