



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 05:58 AM EDT

PDB ID : 8T1I
EMDB ID : EMD-40968
Title : Atomic model of the mammalian Mediator complex with MED26 subunit
Authors : Zhao, H.; Asturias, F.
Deposited on : 2023-06-02
Resolution : 4.68 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.dev113
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) : 2.39

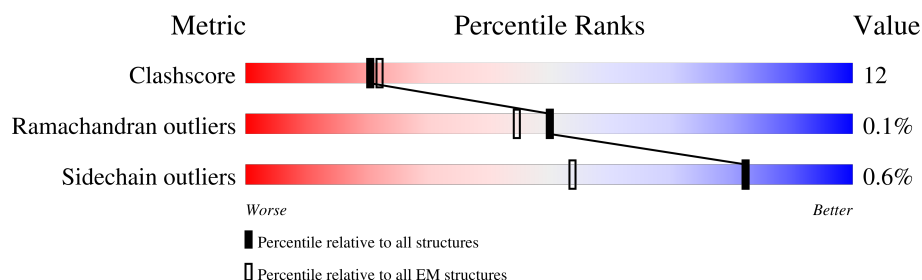
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.68 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.








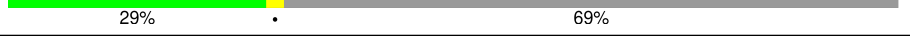
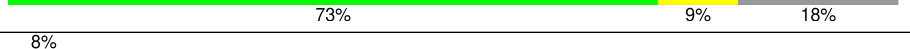
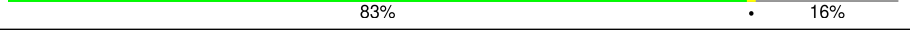
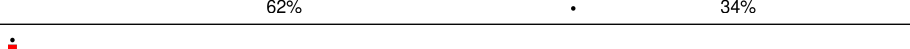
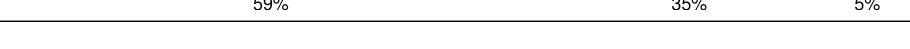


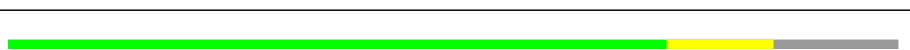

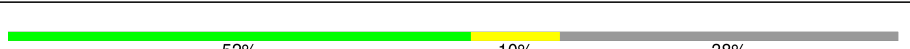




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1575	
2	B	270	
3	C	246	
4	D	233	
5	E	268	
6	F	142	
7	G	135	
8	H	117	

Continued on next page...

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Mol	Chain	Length	Quality of chain
9	I	1459	
10	J	789	
11	K	828	
12	L	649	
13	M	208	
14	N	240	
15	O	212	
16	P	144	
17	Q	200	
18	R	1367	
19	S	987	
20	T	745	
21	U	588	
22	V	311	
23	W	178	
24	X	199	
25	Y	178	
26	Z	131	
27	a	20	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 49568 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 Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	467	Total	C	N	O	0	0
			2314	1380	467	467		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	158	Total	C	N	O	0	0
			784	468	158	158		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	157	Total	C	N	O	0	0
			785	471	157	157		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	161	Total	C	N	O	0	0
			801	479	161	161		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	165	Total	C	N	O	0	0
			837	506	166	165		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	73	Total	C	N	O	0	0
			363	217	73	73		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	122	Total	C	N	O	0	0
			605	361	122	122		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	105	Total	C	N	O	S	0	0
			578	349	116	112	1		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1086	Total	C	N	O	S	0	0
			6772	4287	1254	1211	20		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1171	748	217	200	6		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	738	Total	C	N	O	S	0	0
			5085	3283	912	867	23		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	544	Total	C	N	O	S	0	0
			3335	2093	628	611	3		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	180	Total	C	N	O	S	0	0
			1140	725	217	197	1		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	75	Total	C	N	O	S	0	0
			475	293	85	95	2		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	174	Total	C	N	O	S	0	0
			1013	640	177	192	4		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	121	Total	C	N	O		0	0
			602	360	121	121			

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	131	Total	C	N	O		0	0
			754	463	145	146			

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	1295	Total	C	N	O	S	0	0
			9744	6296	1680	1715	53		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	901	Total	C	N	O	S	0	0
			5875	3750	1062	1036	27		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	192	Total	C	N	O	S	0	0
			1299	837	222	235	5		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	97	Total	C	N	O	0	0
			481	287	97	97		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	266	Total	C	N	O	S	0	0
			1657	1053	301	300	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	118	Total	C	N	O	S	0	0
			773	486	145	140	2		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	123	Total	C	N	O	S	0	0
			839	528	150	158	3		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	132	Total	C	N	O	S	0	0
			843	527	168	145	3		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	109	Total	C	N	O	0	0
			543	325	109	109		

- Molecule 27 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	20	Total	C	N	O	0	0
			100	60	20	20		

[illegible]

- Molecule 2: Mediator of RNA polymerase II transcription subunit 4

Chain B:  58% 41%

[illegible]

- Molecule 3: Mediator of RNA polymerase II transcription subunit 6

Chain C:  23% 59% 36%

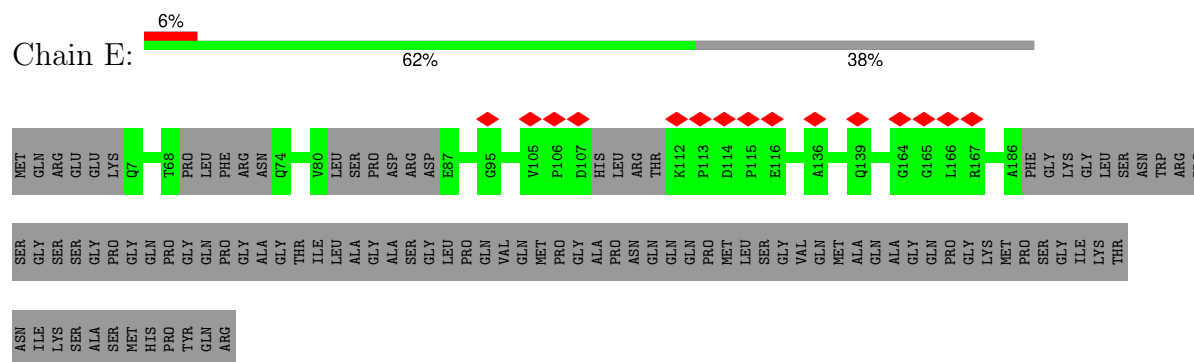
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Q61	Q62	Q63	Q64	Q65	Q66	E75	P76	I77	L78	S142	LYS	GLY	TVR	V16	TRP	TRP	HIS	PHE	LYS	ASP	HIS	GLU	GLU	GLN	GLN	LYS	VAL	LYS	PRO	ALA	ARG	Q165																											
MET	ALA	ALA	VAL	ASP	ILE	ARG	ASP	N9	L10	L11	GLI2	I13	S14	W15	V16	D17	S18	S19	W20	I21	P22	I23	L24	W25	S26	Q27	S28	V29	L30	D31	Y32	F33	S34	E35	R36	S37	N38	F39	F40	Y41	D42	R43	T44	C45	N46	N47	F48	W49	Y50	K51	W52	Q53	R54	L55	T56	L57	E58	H59	L60

- Molecule 4: Mediator of RNA polymerase II transcription subunit 7

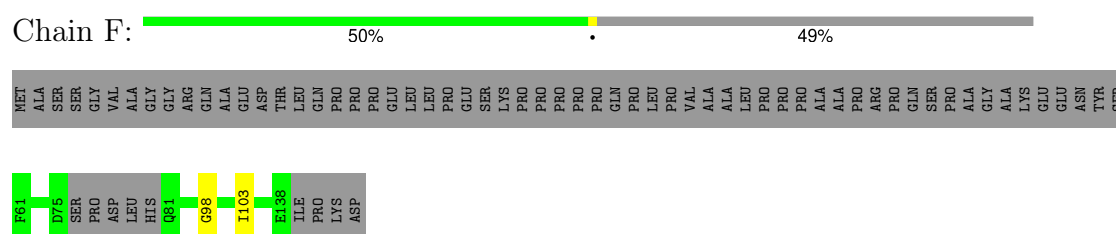
Chain D:  66% 31%

ASN	GLU	GLN	GLN	ARG	GLU	SER	SER	GLY	HIS	ARG	ARG	ASP	GLN	ILE	GLU	LYS	ASP	ALA	ALA	LEU	CYS	VAL	LEU	ILE	ASP	GLU	MET	ASN	GLU	ARG	PRO																						
MET	GLY	GLU	PRO	GLN	GLN	VAL	SER	ALA	PRO	PRO	PRO	PRO	PRO	MIS	E107	E110	E111	L112	F116	H121	L122	L123	M124	E126	Y126	R127	P172	L175	PRO	HIS	SER	SER	GLU	ALA	ALA	GLY	MET	ARG	VAL	VAL	LYS	ALA	ALA	GLU	PRO	MET	ASP	THR	ASP	ASN	ASN	CYS	GLY

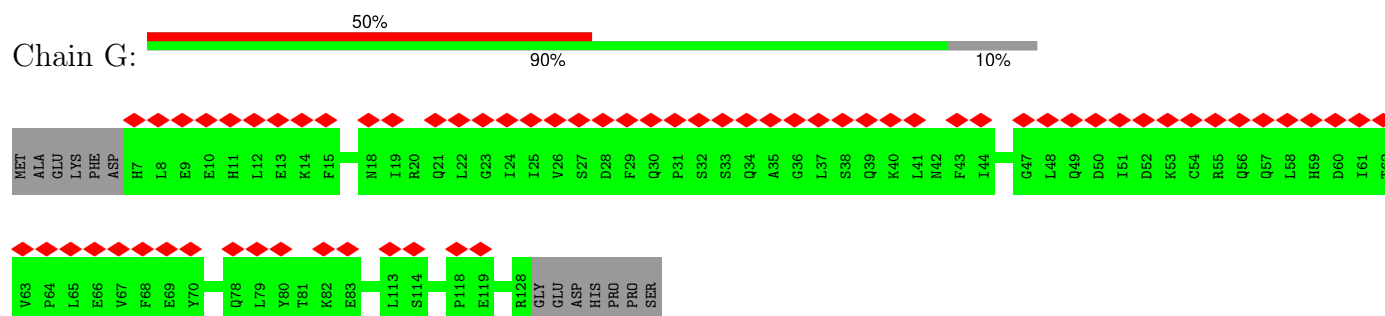
- Molecule 5: Mediator of RNA polymerase II transcription subunit 8



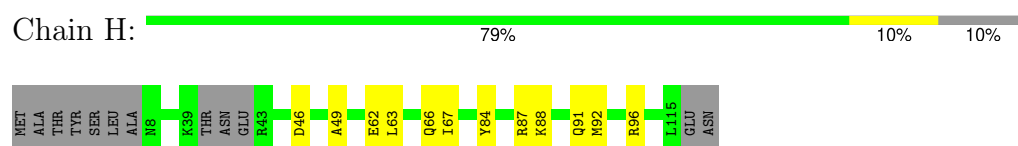
- Molecule 6: Mediator of RNA polymerase II transcription subunit 9



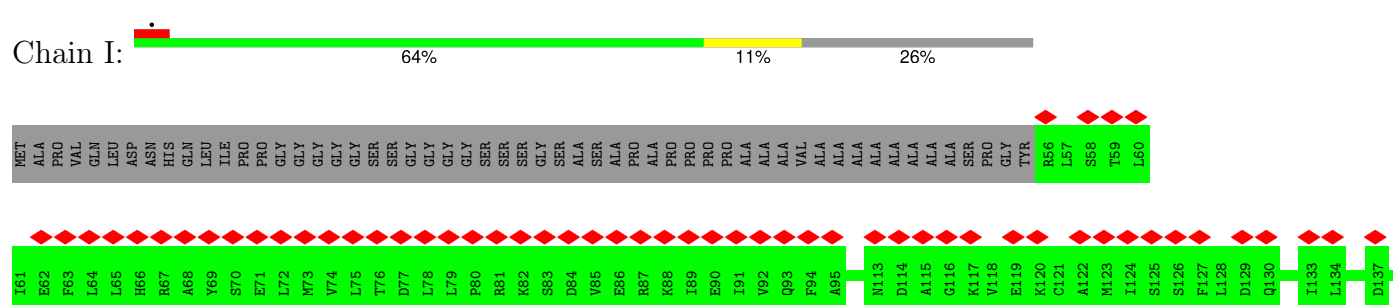
- Molecule 7: Mediator of RNA polymerase II transcription subunit 10

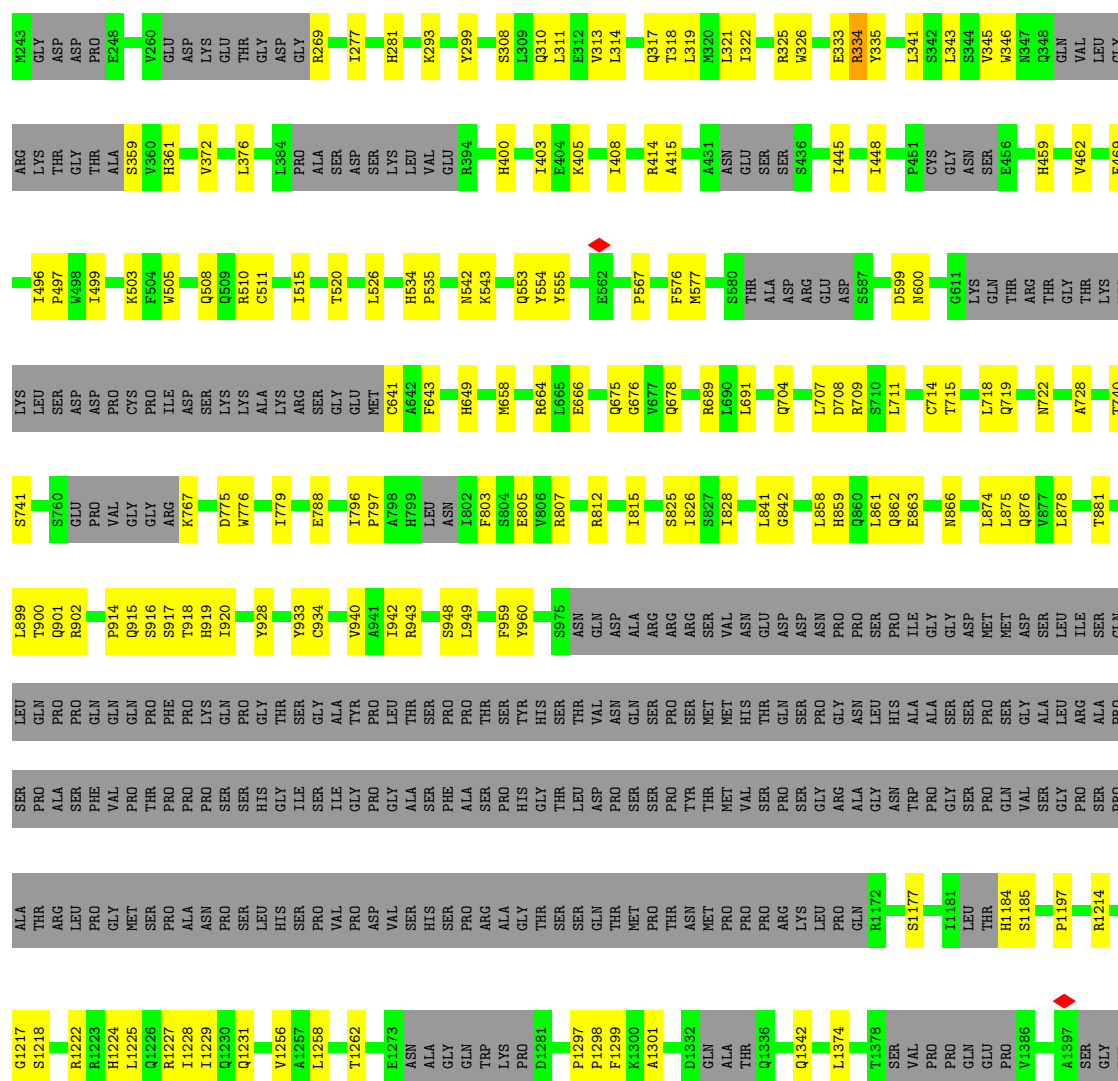


- Molecule 8: Mediator of RNA polymerase II transcription subunit 11



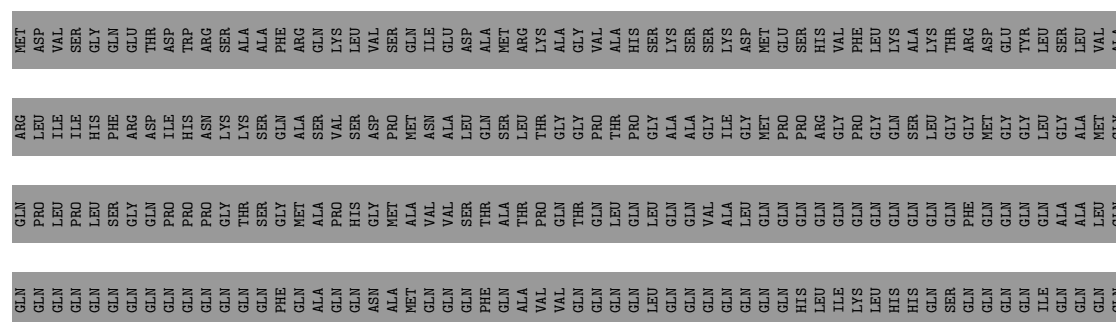
- Molecule 9: Mediator of RNA polymerase II transcription subunit 14

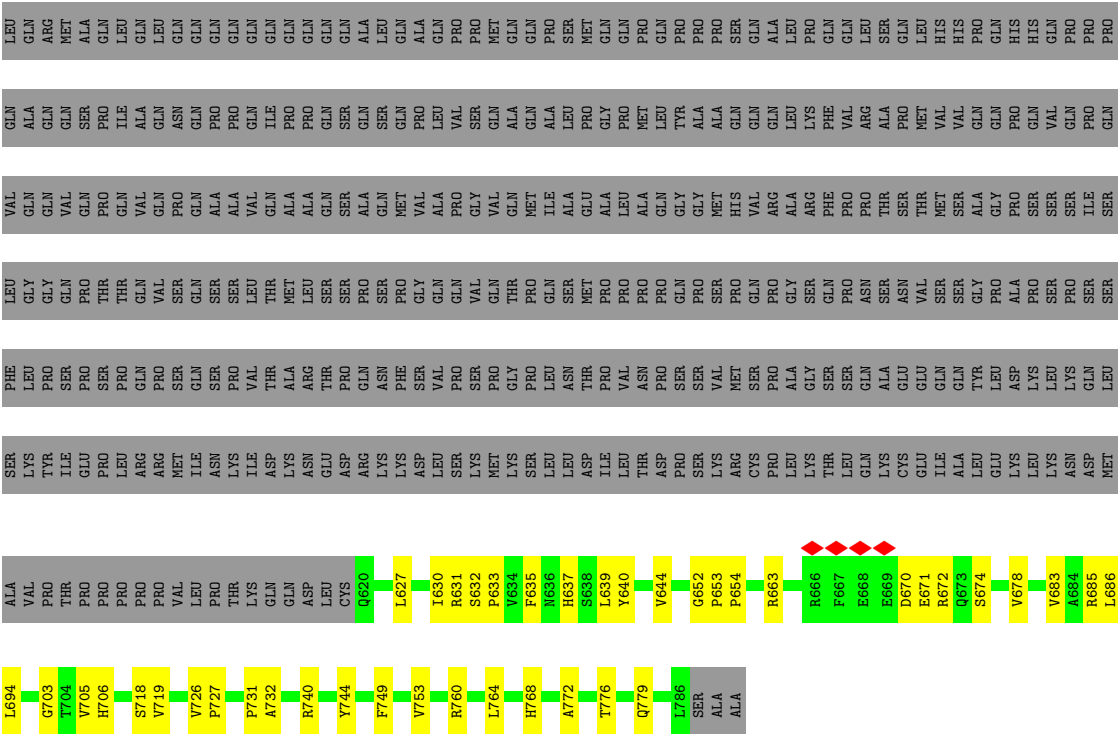




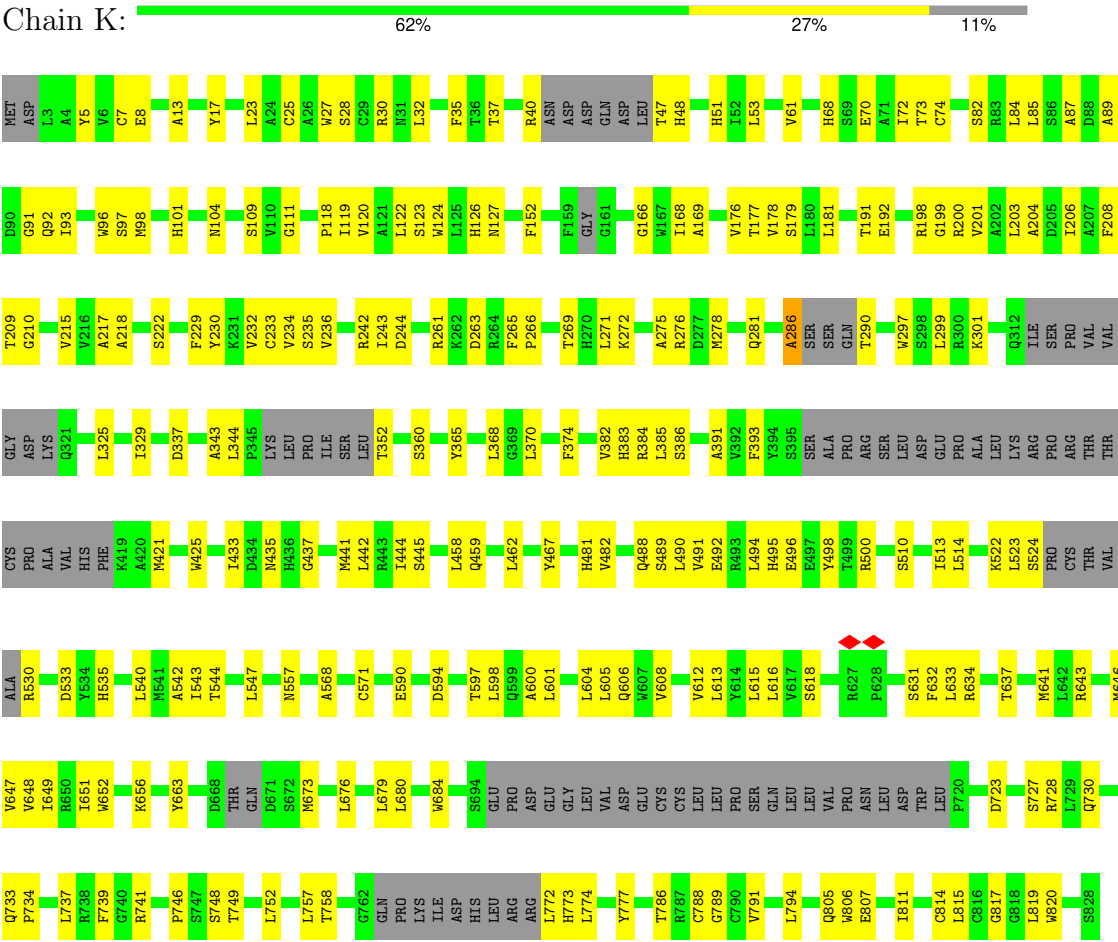
• Molecule 10: Mediator of RNA polymerase II transcription subunit 15

Chain J: 16% 5% 79%

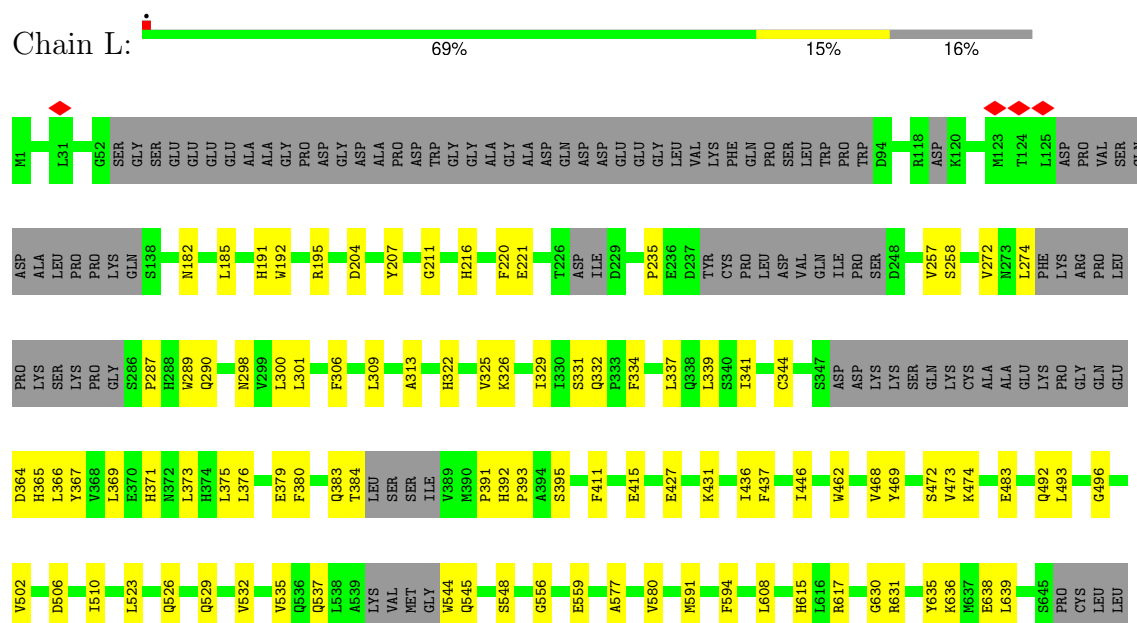




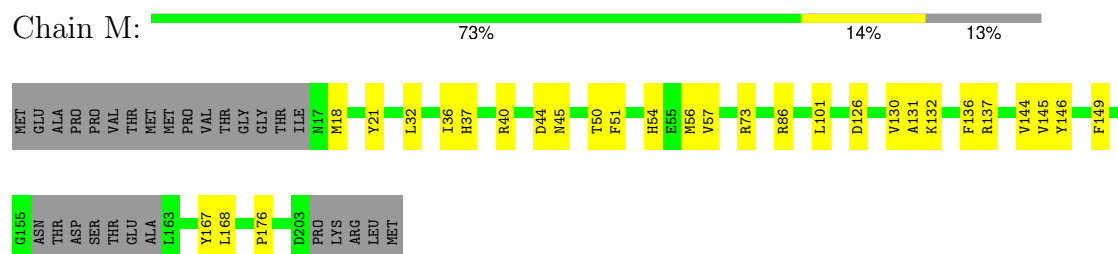
● Molecule 11: Mediator of RNA polymerase II transcription subunit 16



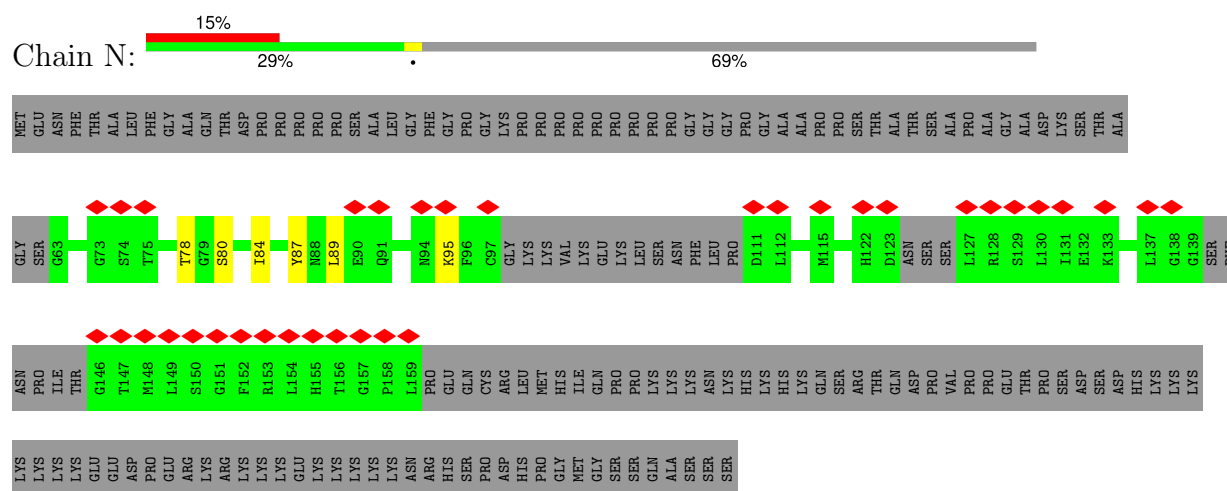
- Molecule 12: Mediator of RNA polymerase II transcription subunit 17



- Molecule 13: Mediator of RNA polymerase II transcription subunit 18

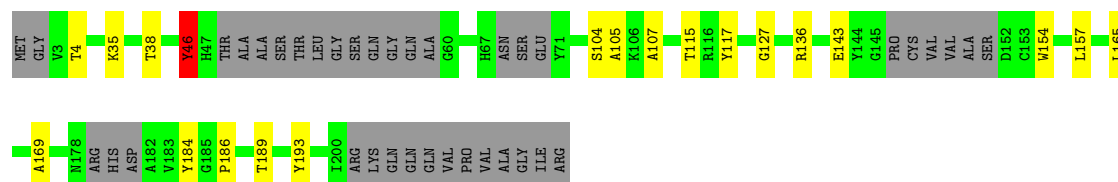


- Molecule 14: Mediator of RNA polymerase II transcription subunit 19

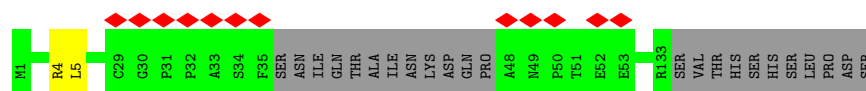
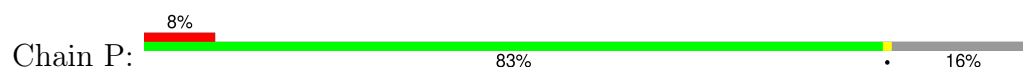


- Molecule 15: Mediator of RNA polymerase II transcription subunit 20

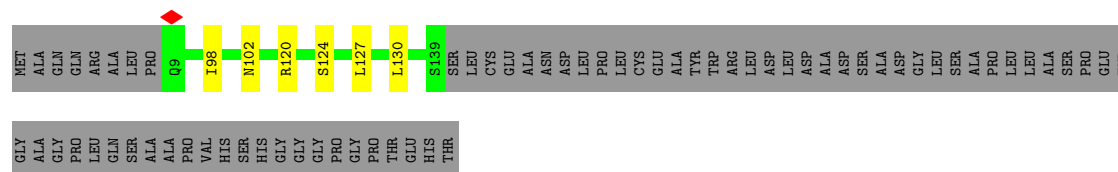




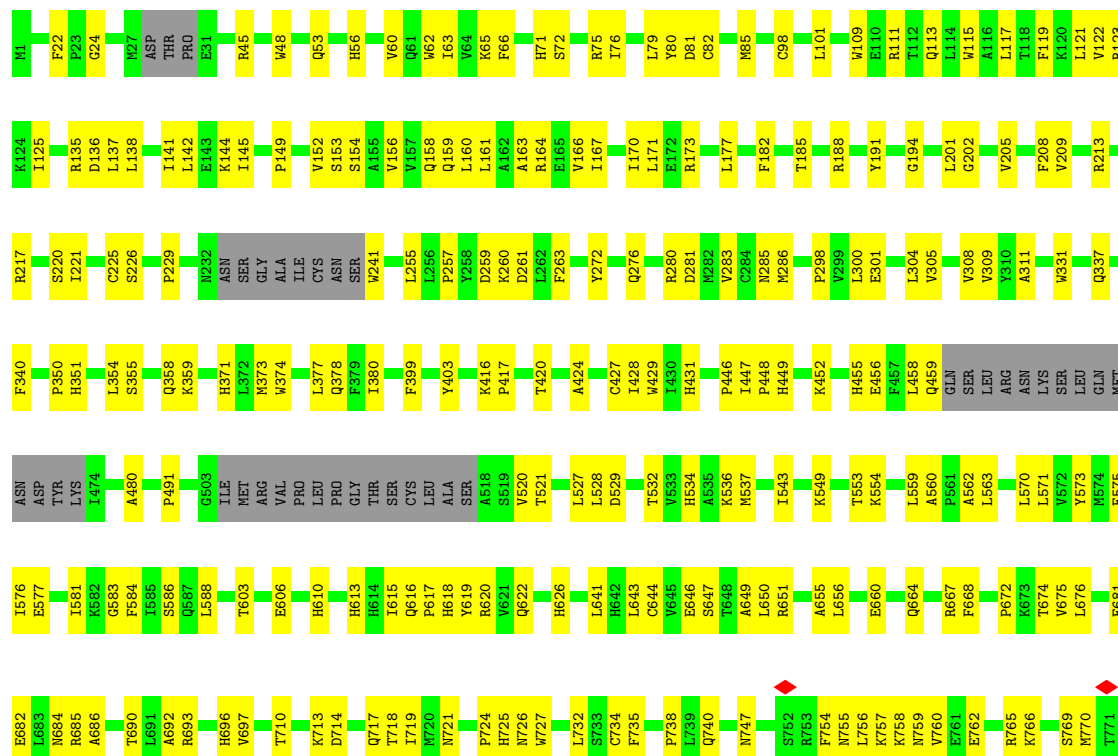
- Molecule 16: Mediator of RNA polymerase II transcription subunit 21

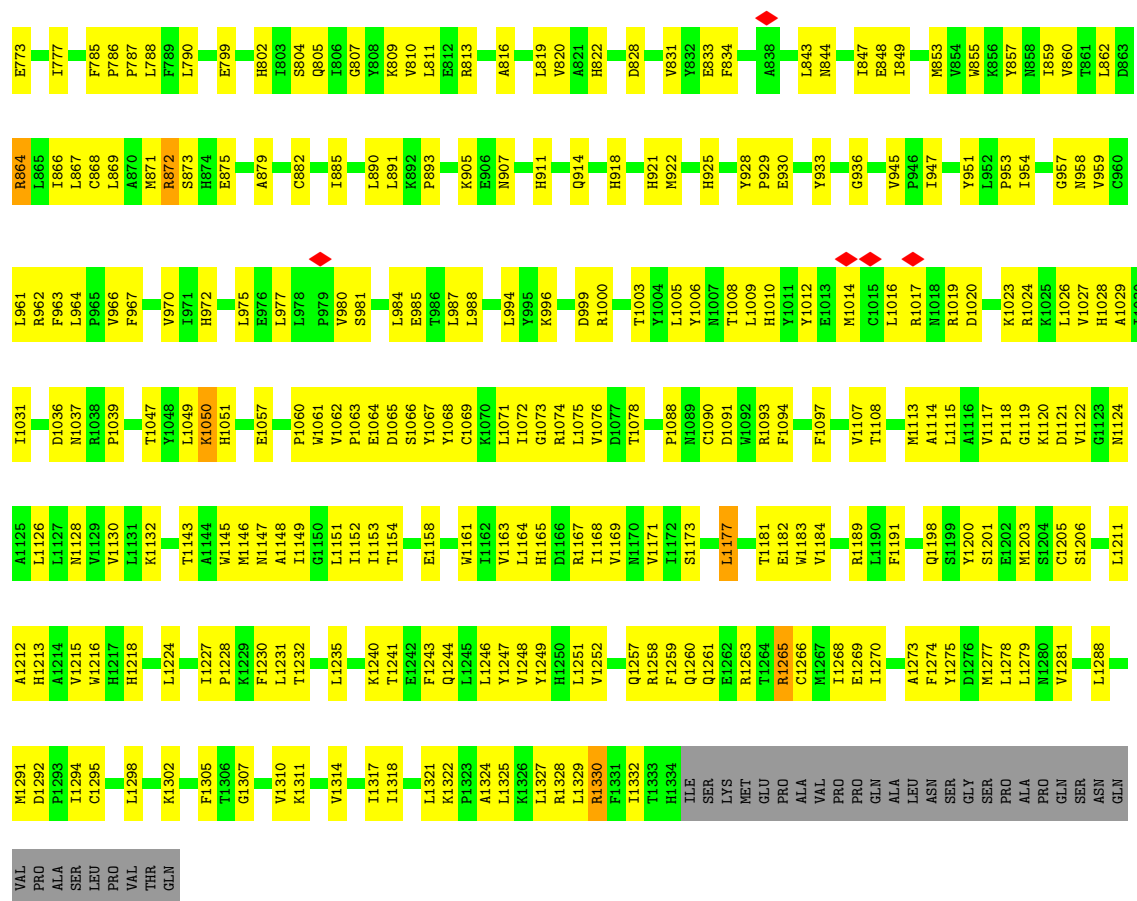


- Molecule 17: Mediator of RNA polymerase II transcription subunit 22



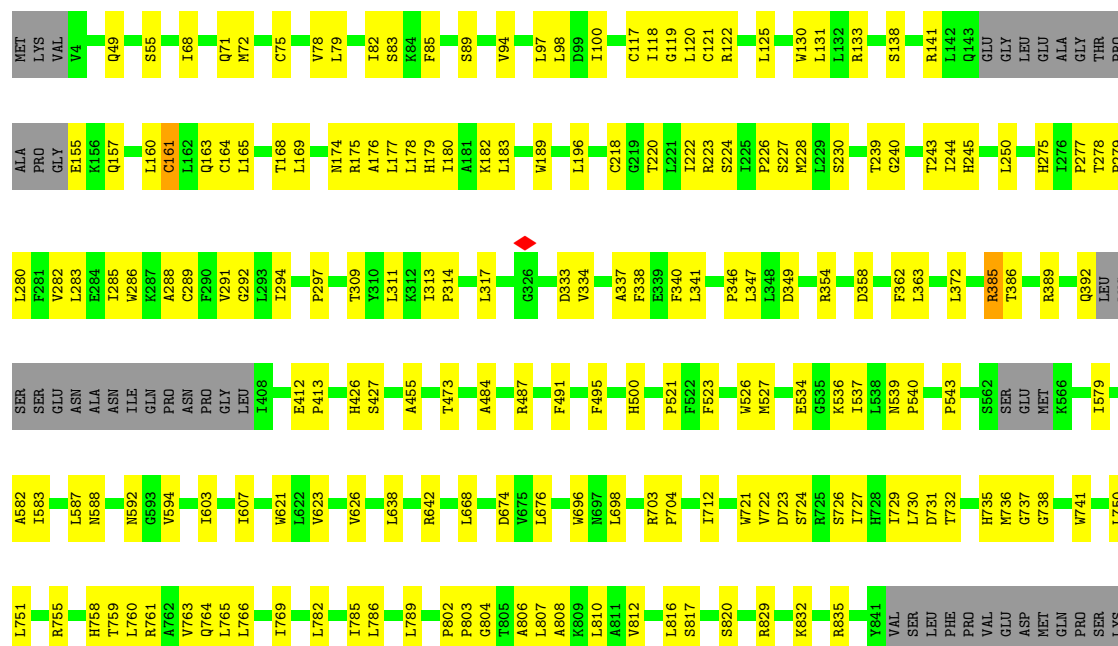
- Molecule 18: Mediator of RNA polymerase II transcription subunit 23





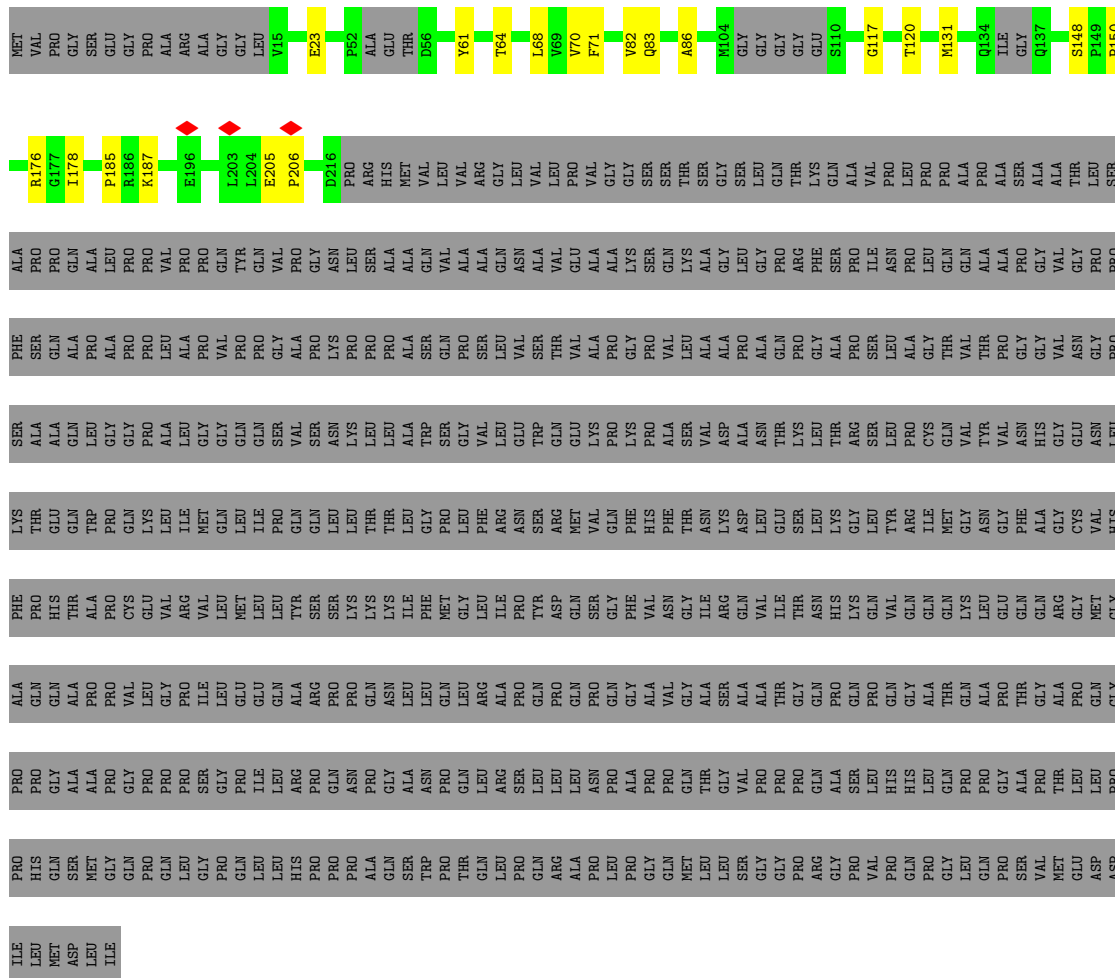
• Molecule 19: Mediator of RNA polymerase II transcription subunit 24

Chain S: 71% 20% 9%



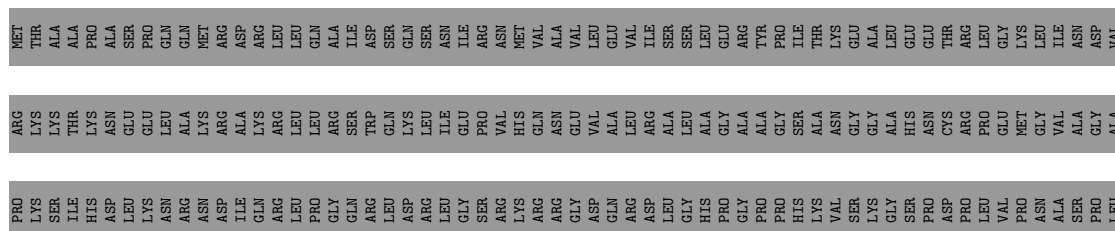
- Molecule 20: Mediator of RNA polymerase II transcription subunit 25

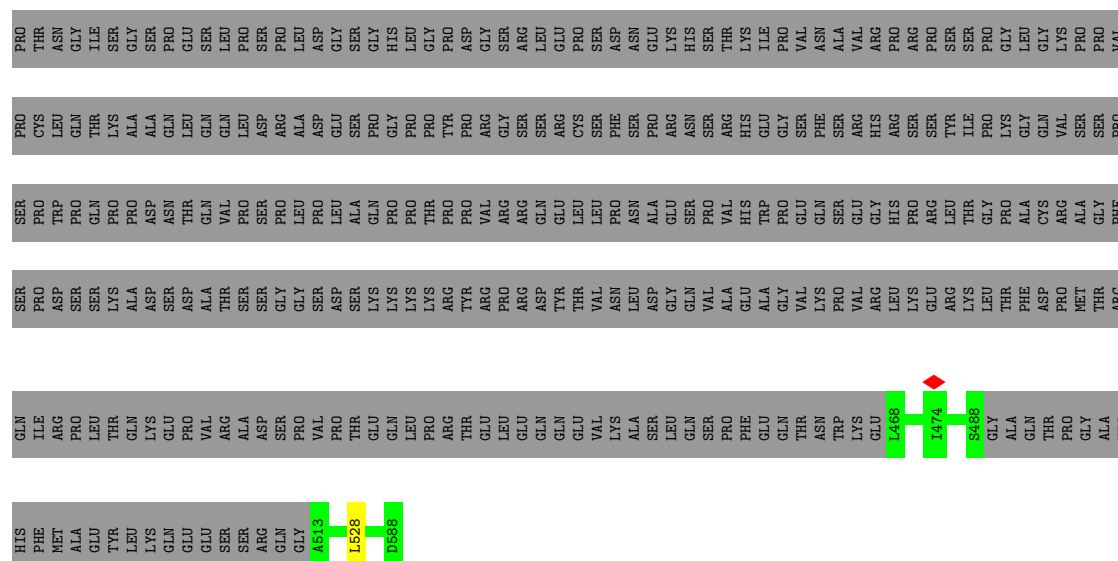
Chain T:  23% 1% 74%



- Molecule 21: Mediator of RNA polymerase II transcription subunit 26

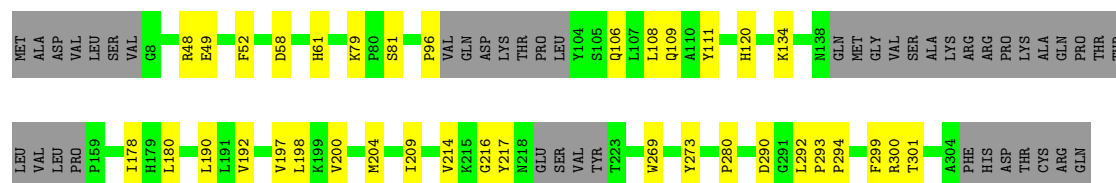
Chain U: 16% 84%





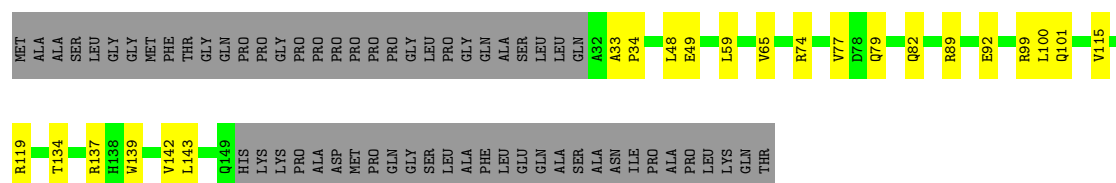
• Molecule 22: Mediator of RNA polymerase II transcription subunit 27

Chain V: 74% 12% 14%



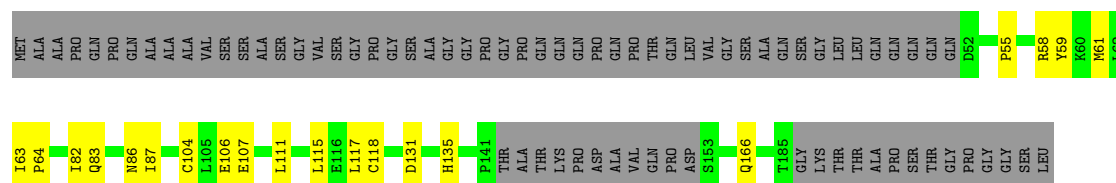
• Molecule 23: Mediator of RNA polymerase II transcription subunit 28

Chain W: 54% 12% 34%



• Molecule 24: Mediator of RNA polymerase II transcription subunit 29

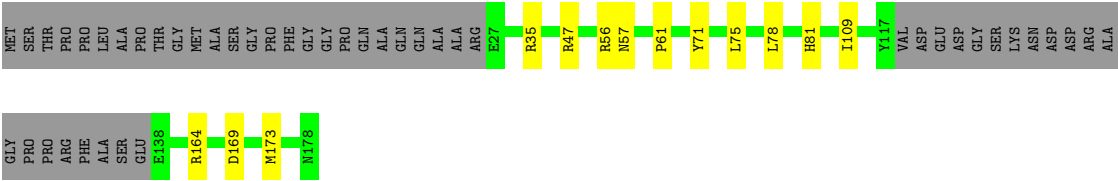
Chain X: 52% 10% 38%



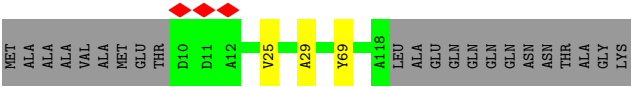
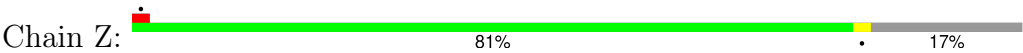
• Molecule 25: Mediator of RNA polymerase II transcription subunit 30

Chain Y: 67% 7% 26%





● Molecule 26: Mediator of RNA polymerase II transcription subunit 31



● Molecule 27: Unknown Peptide



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.071	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.054	Depositor
Map size (\AA)	621.60004, 621.60004, 621.60004	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/2308	0.42	0/3209
2	B	0.23	0/782	0.34	0/1088
3	C	0.24	0/784	0.50	0/1090
4	D	0.23	0/800	0.39	0/1116
5	E	0.23	0/840	0.38	0/1170
6	F	0.22	0/361	0.34	0/501
7	G	0.22	0/604	0.34	0/841
8	H	0.23	0/580	0.33	0/798
9	I	0.25	0/6899	0.43	0/9516
10	J	0.26	0/1207	0.45	0/1668
11	K	0.25	0/5202	0.48	1/7144 (0.0%)
12	L	0.25	0/3385	0.43	0/4658
13	M	0.25	0/1163	0.43	0/1593
14	N	0.24	0/479	0.40	0/648
15	O	2.77	6/1026 (0.6%)	0.51	0/1409
16	P	0.23	0/600	0.36	0/835
17	Q	0.24	0/758	0.36	0/1046
18	R	0.25	0/9995	0.44	0/13654
19	S	0.25	0/6000	0.41	0/8250
20	T	0.26	0/1336	0.42	0/1836
21	U	0.34	0/480	0.45	0/666
22	V	0.25	0/1694	0.42	0/2338
23	W	0.25	0/785	0.42	0/1076
24	X	0.25	0/852	0.42	0/1169
25	Y	0.23	0/853	0.37	0/1167
26	Z	0.22	0/542	0.39	0/756
All	All	0.47	6/50315 (0.0%)	0.43	1/69242 (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
3	C	0	3
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	46	TYR	CD2-CE2	49.40	2.13	1.39
15	O	46	TYR	CD1-CE1	47.38	2.10	1.39
15	O	46	TYR	CE1-CZ	31.17	1.79	1.38
15	O	46	TYR	CE2-CZ	31.14	1.79	1.38
15	O	46	TYR	CG-CD2	24.77	1.71	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	286	ALA	C-N-CA	6.22	137.26	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	THR	Peptide
3	C	46	ASN	Peptide
3	C	50	VAL	Peptide
3	C	58	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2314	0	992	18	0
2	B	784	0	357	1	0
3	C	785	0	344	9	0
4	D	801	0	327	8	0
5	E	837	0	402	0	0
6	F	363	0	146	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	605	0	256	0	0
8	H	578	0	341	8	0
9	I	6772	0	4972	109	0
10	J	1171	0	1010	33	0
11	K	5085	0	4509	159	0
12	L	3335	0	2395	73	0
13	M	1140	0	832	21	0
14	N	475	0	349	4	0
15	O	1013	0	662	36	0
16	P	602	0	302	7	0
17	Q	754	0	448	4	0
18	R	9744	0	9105	371	0
19	S	5875	0	4690	142	0
20	T	1299	0	1022	11	0
21	U	481	0	202	0	0
22	V	1657	0	1170	24	0
23	W	773	0	607	16	0
24	X	839	0	700	16	0
25	Y	843	0	639	11	0
26	Z	543	0	240	2	0
27	a	100	0	23	0	0
All	All	49568	0	37042	1030	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 1030 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)
15:O:46:TYR:CZ	15:O:46:TYR:CE1	1.79	1.66
15:O:46:TYR:CZ	15:O:46:TYR:CE2	1.79	1.63
15:O:46:TYR:CE1	15:O:46:TYR:CD1	2.10	1.39
15:O:46:TYR:CE2	15:O:46:TYR:CD2	2.13	1.35
15:O:46:TYR:CD1	15:O:105:ALA:N	1.97	1.33

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	455/1575 (29%)	426 (94%)	28 (6%)	1 (0%)	44	78
2	B	154/270 (57%)	150 (97%)	4 (3%)	0	100	100
3	C	153/246 (62%)	123 (80%)	30 (20%)	0	100	100
4	D	159/233 (68%)	147 (92%)	12 (8%)	0	100	100
5	E	157/268 (59%)	144 (92%)	13 (8%)	0	100	100
6	F	69/142 (49%)	66 (96%)	3 (4%)	0	100	100
7	G	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
8	H	101/117 (86%)	94 (93%)	7 (7%)	0	100	100
9	I	1050/1459 (72%)	901 (86%)	149 (14%)	0	100	100
10	J	165/789 (21%)	135 (82%)	30 (18%)	0	100	100
11	K	718/828 (87%)	574 (80%)	143 (20%)	1 (0%)	48	83
12	L	524/649 (81%)	457 (87%)	67 (13%)	0	100	100
13	M	176/208 (85%)	160 (91%)	16 (9%)	0	100	100
14	N	67/240 (28%)	63 (94%)	4 (6%)	0	100	100
15	O	162/212 (76%)	134 (83%)	28 (17%)	0	100	100
16	P	117/144 (81%)	107 (92%)	10 (8%)	0	100	100
17	Q	129/200 (64%)	126 (98%)	3 (2%)	0	100	100
18	R	1285/1367 (94%)	1105 (86%)	179 (14%)	1 (0%)	48	83
19	S	889/987 (90%)	790 (89%)	99 (11%)	0	100	100
20	T	184/745 (25%)	163 (89%)	21 (11%)	0	100	100
21	U	93/588 (16%)	84 (90%)	8 (9%)	1 (1%)	12	46
22	V	258/311 (83%)	216 (84%)	42 (16%)	0	100	100
23	W	116/178 (65%)	109 (94%)	7 (6%)	0	100	100
24	X	119/199 (60%)	116 (98%)	3 (2%)	0	100	100
25	Y	128/178 (72%)	112 (88%)	16 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	107/131 (82%)	96 (90%)	11 (10%)	0	100	100
All	All	7655/12399 (62%)	6717 (88%)	934 (12%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	SER
18	R	1177	LEU
21	U	528	LEU
11	K	97	SER

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	
3	C	1/223 (0%)	1 (100%)	0	100	100
5	E	6/226 (3%)	6 (100%)	0	100	100
8	H	12/98 (12%)	12 (100%)	0	100	100
9	I	387/1276 (30%)	385 (100%)	2 (0%)	86	90
10	J	100/693 (14%)	100 (100%)	0	100	100
11	K	418/729 (57%)	415 (99%)	3 (1%)	81	87
12	L	180/572 (32%)	180 (100%)	0	100	100
13	M	61/183 (33%)	61 (100%)	0	100	100
14	N	32/205 (16%)	31 (97%)	1 (3%)	35	55
15	O	44/177 (25%)	43 (98%)	1 (2%)	45	64
17	Q	23/173 (13%)	23 (100%)	0	100	100
18	R	949/1231 (77%)	942 (99%)	7 (1%)	81	87
19	S	395/867 (46%)	392 (99%)	3 (1%)	79	85
20	T	94/598 (16%)	94 (100%)	0	100	100
21	U	1/510 (0%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	V	92/279 (33%)	91 (99%)	1 (1%)	70	80
23	W	52/153 (34%)	52 (100%)	0	100	100
24	X	65/164 (40%)	65 (100%)	0	100	100
25	Y	47/157 (30%)	47 (100%)	0	100	100
All	All	2959/8514 (35%)	2941 (99%)	18 (1%)	82	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	72	MET
22	V	48	ARG
19	S	385	ARG
18	R	864	ARG
18	R	1330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	759	ASN
18	R	1283	GLN
23	W	90	GLN
18	R	851	ASN
18	R	1054	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	104:SER	C	105:ALA	N	2.41

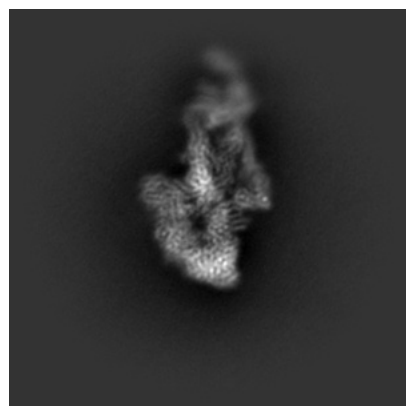
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40968. These allow visual inspection of the internal detail of the map and identification of artifacts.

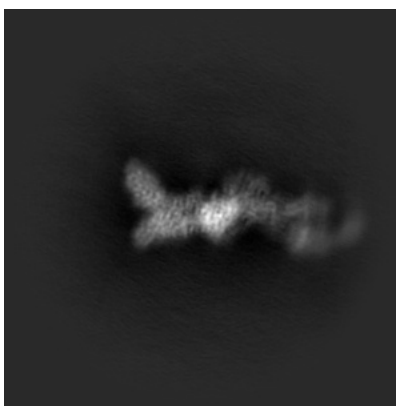
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

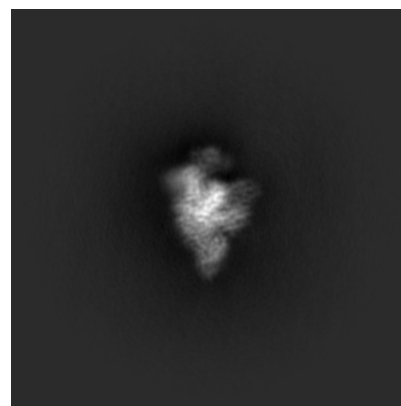
6.1.1 Primary map



X

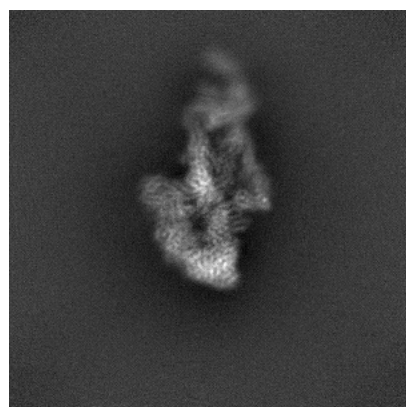


Y

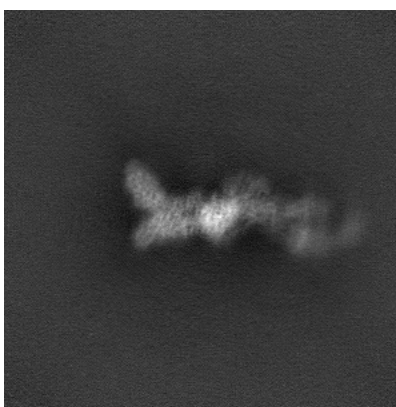


Z

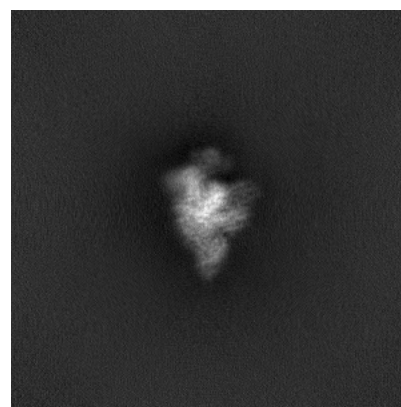
6.1.2 Raw map



X



Y

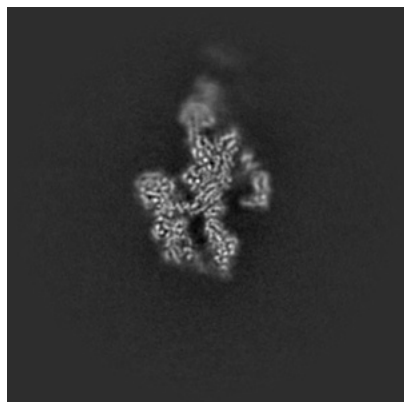


Z

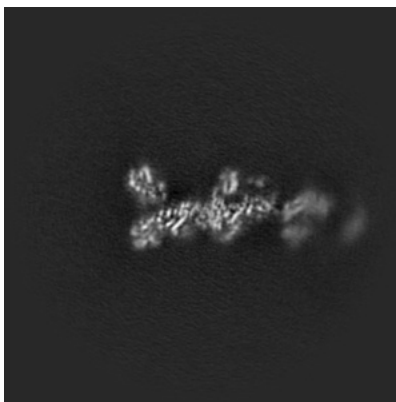
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

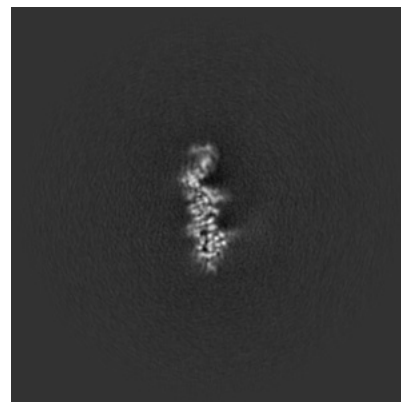
6.2.1 Primary map



X Index: 280

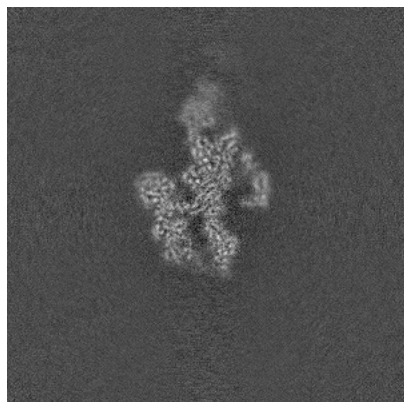


Y Index: 280

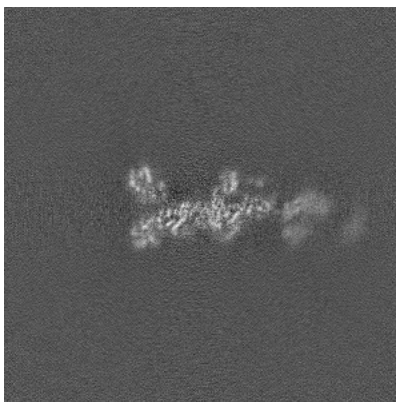


Z Index: 280

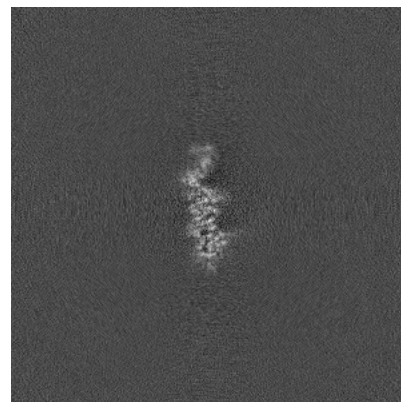
6.2.2 Raw map



X Index: 280



Y Index: 280

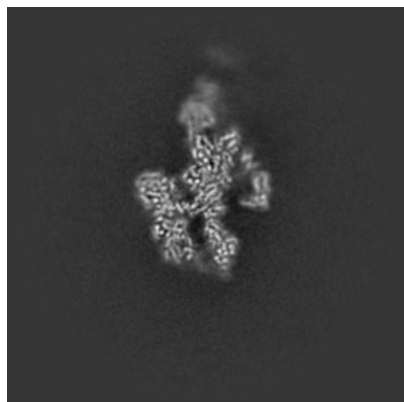


Z Index: 280

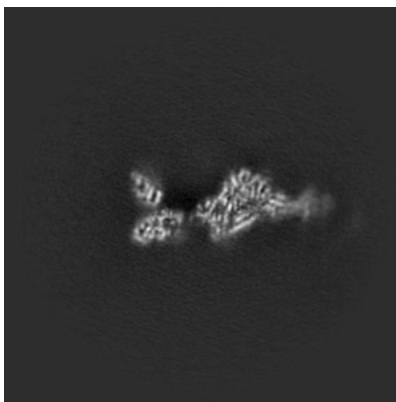
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

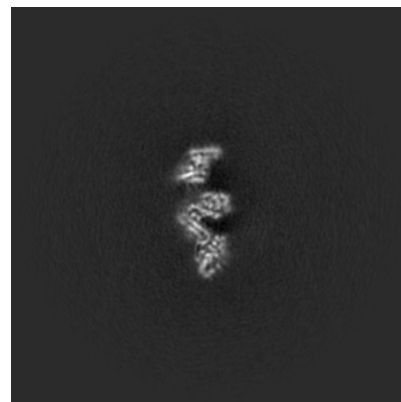
6.3.1 Primary map



X Index: 279

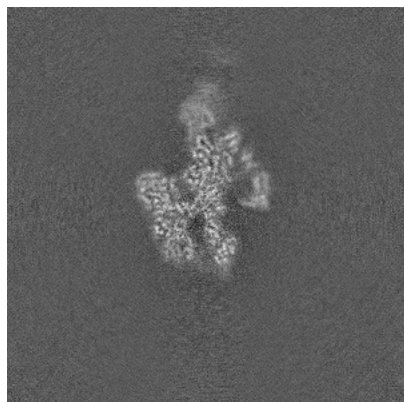


Y Index: 266

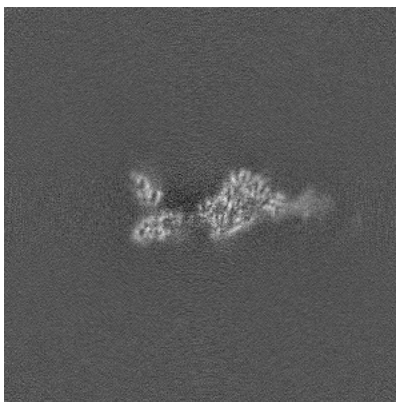


Z Index: 296

6.3.2 Raw map



X Index: 278



Y Index: 267



Z Index: 295

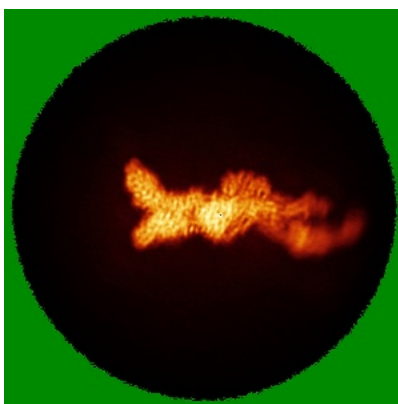
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

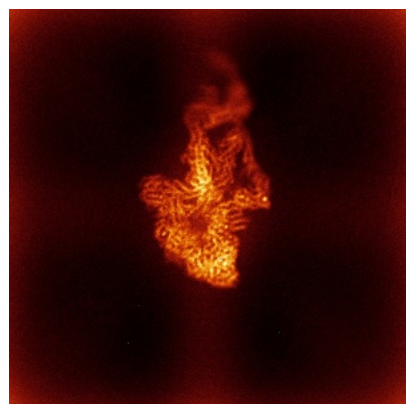


Y

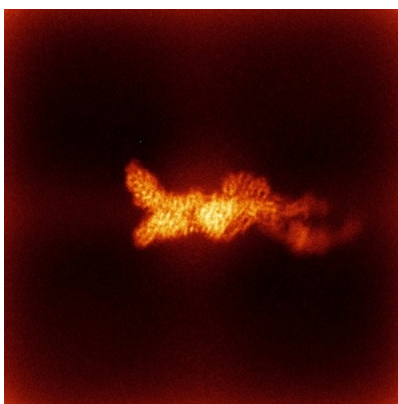


Z

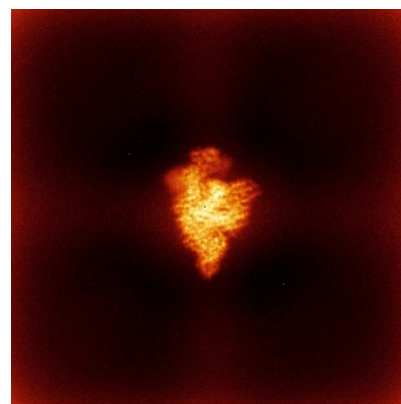
6.4.2 Raw map



X



Y

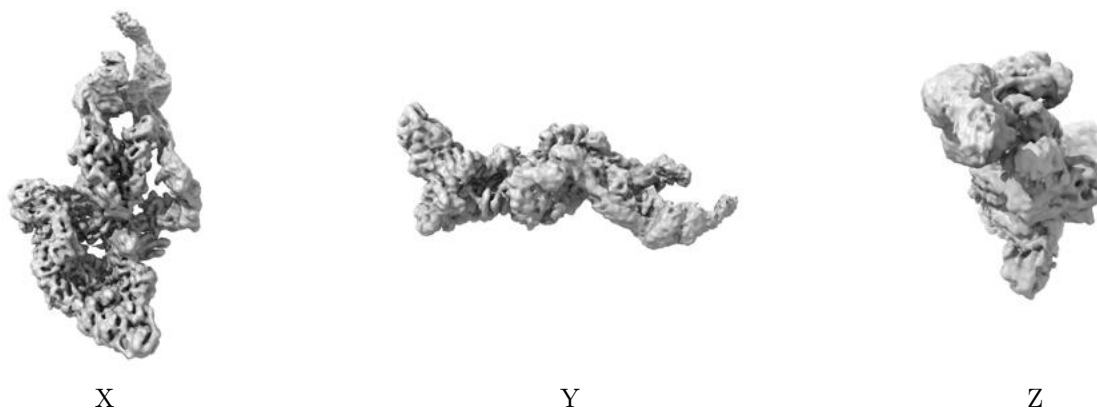


Z

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.

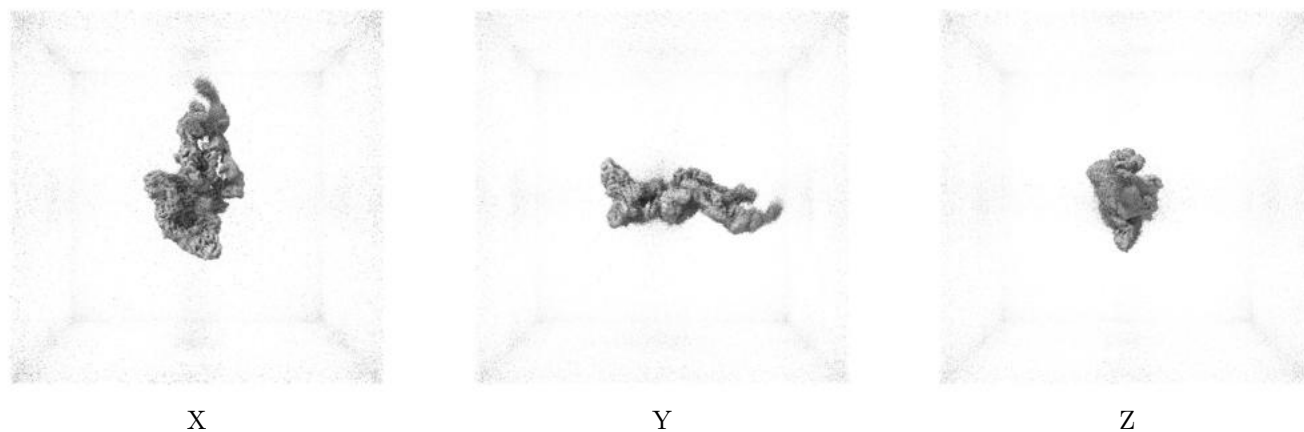
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. 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.

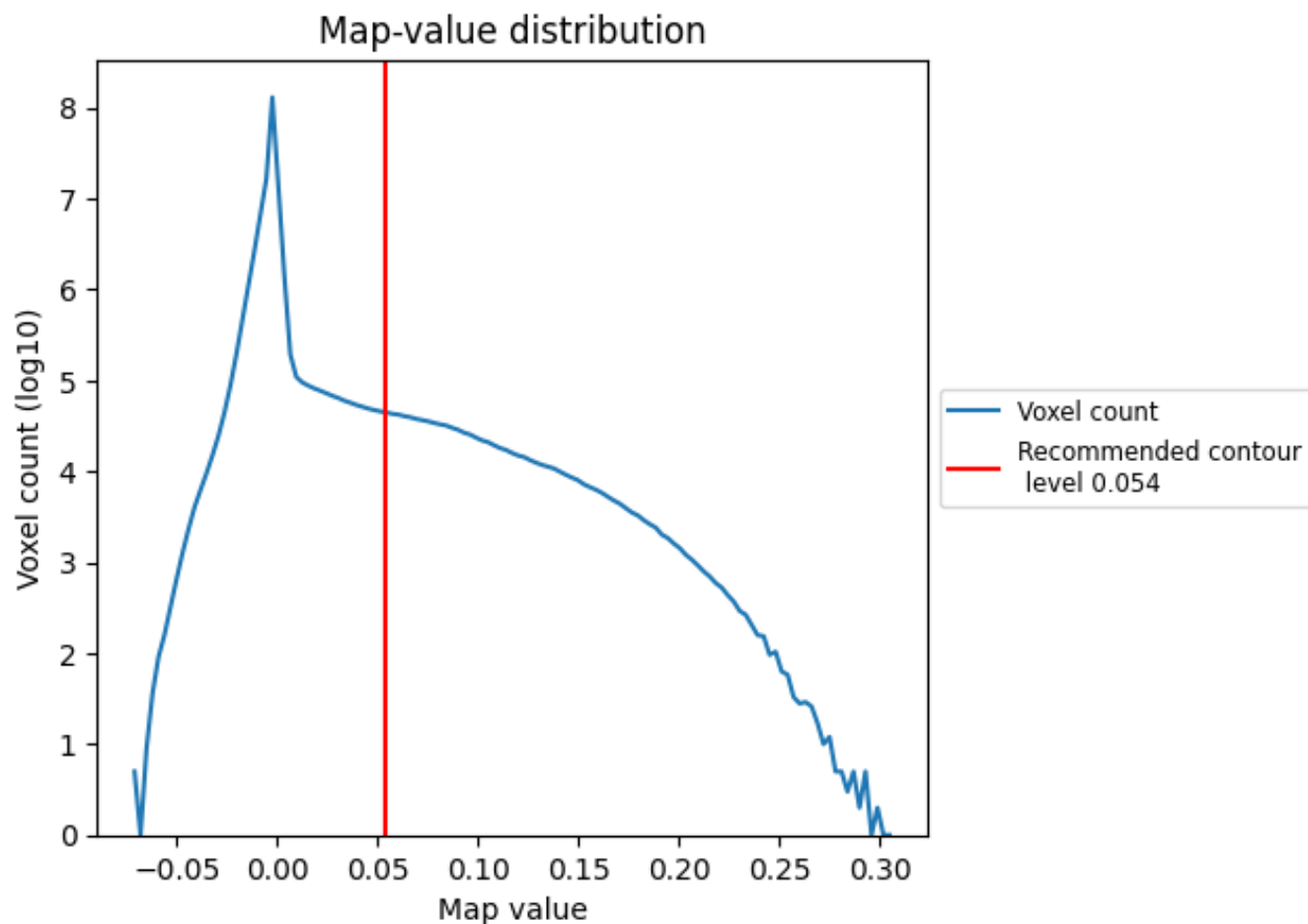
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

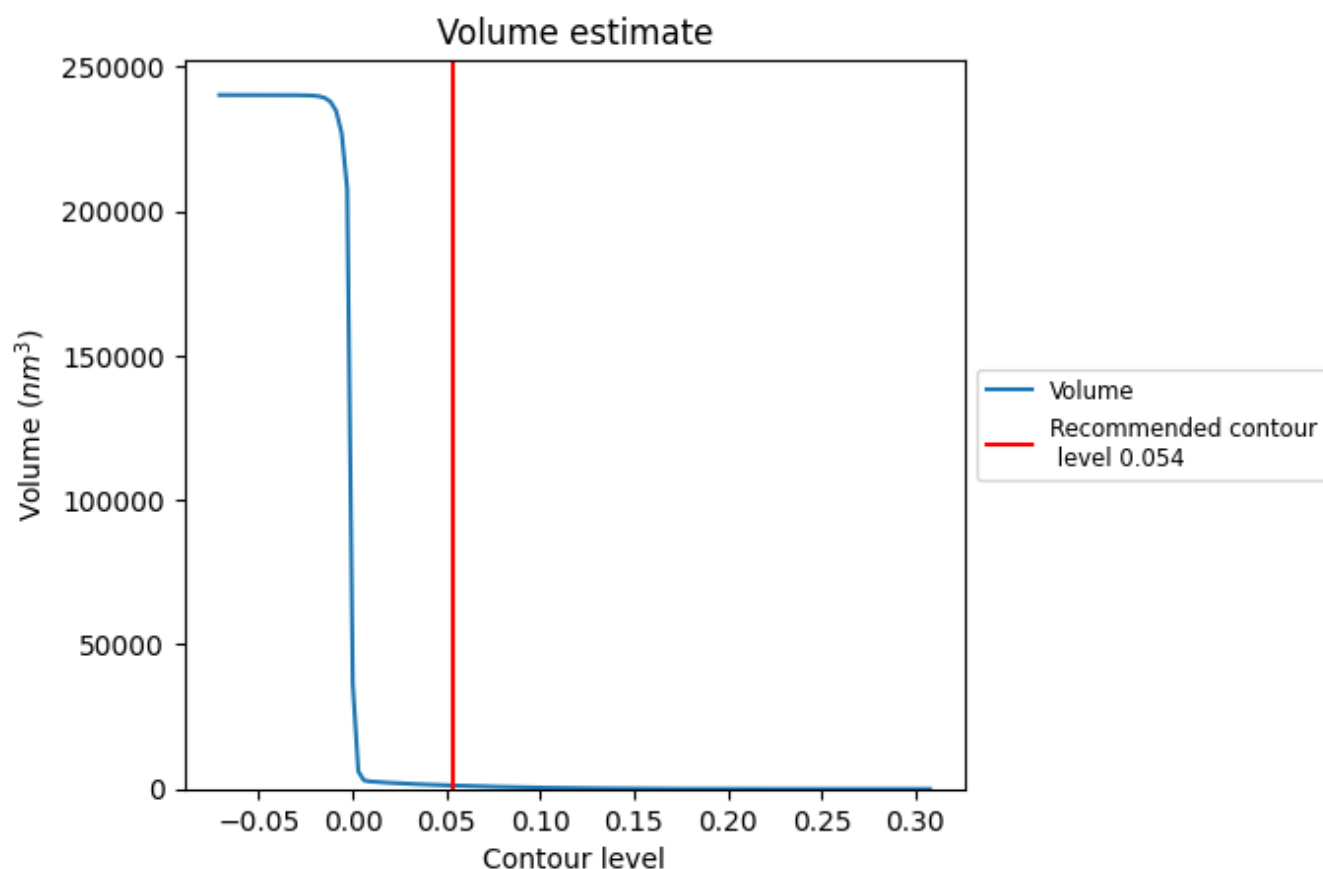
This section contains the results of statistical analysis of the map.

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.

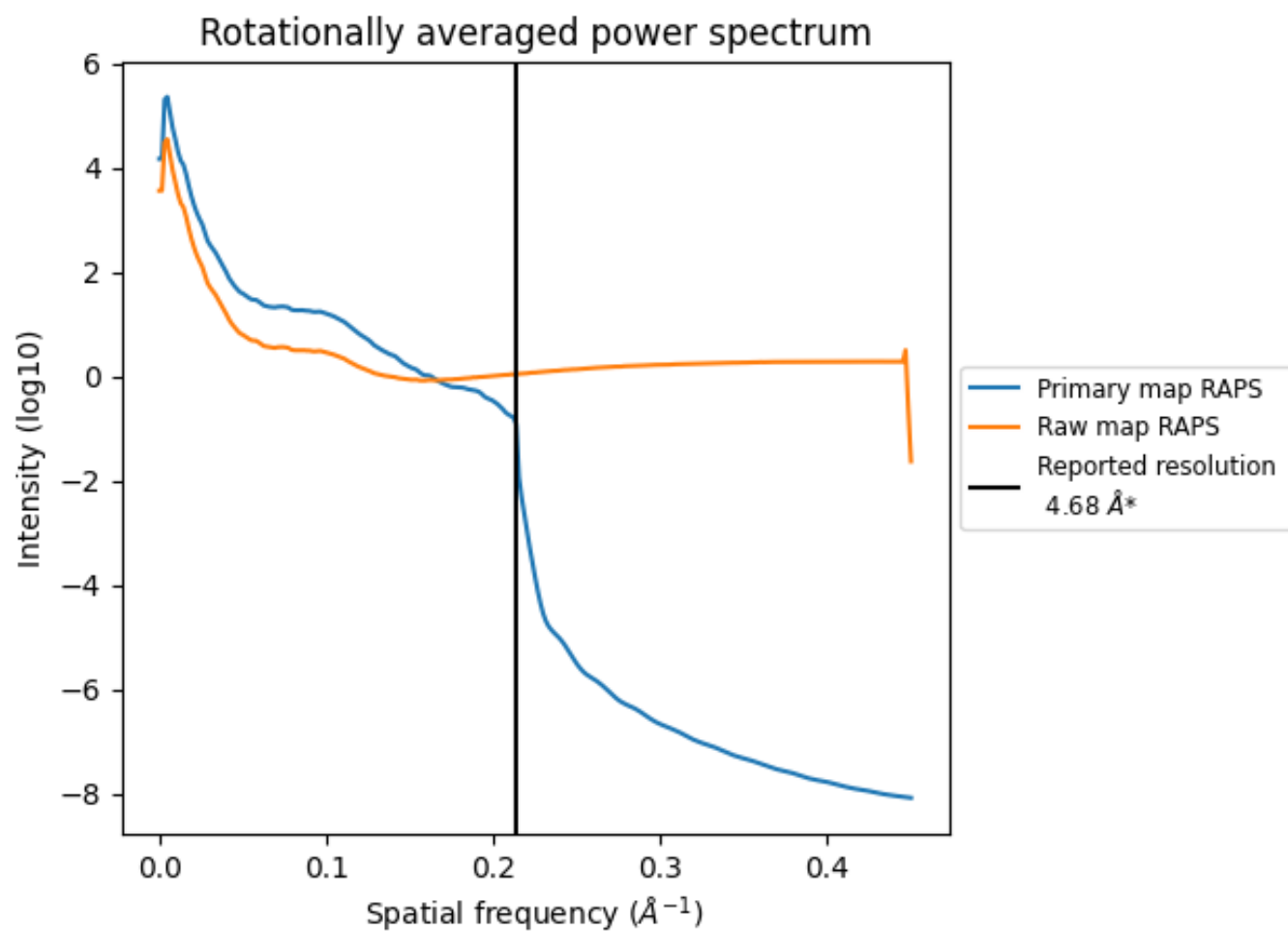
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192 nm^3 ; this corresponds to an approximate mass of 1076 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 ⓘ

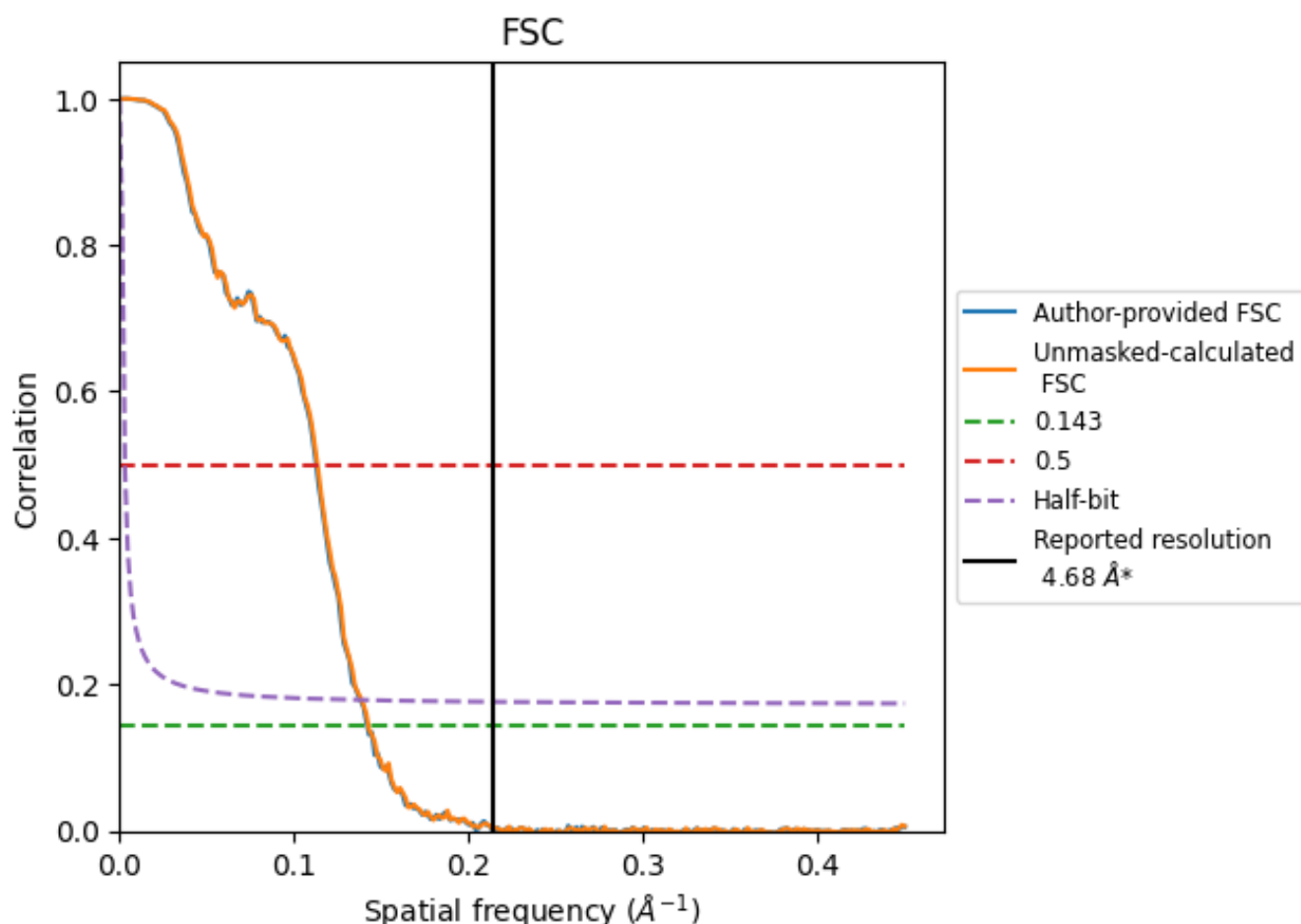


*Reported resolution corresponds to spatial frequency of 0.214 Å⁻¹

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 0.214 Å⁻¹

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.68	-	-
Author-provided FSC curve	7.04	8.87	7.24
Unmasked-calculated*	7.00	8.80	7.20

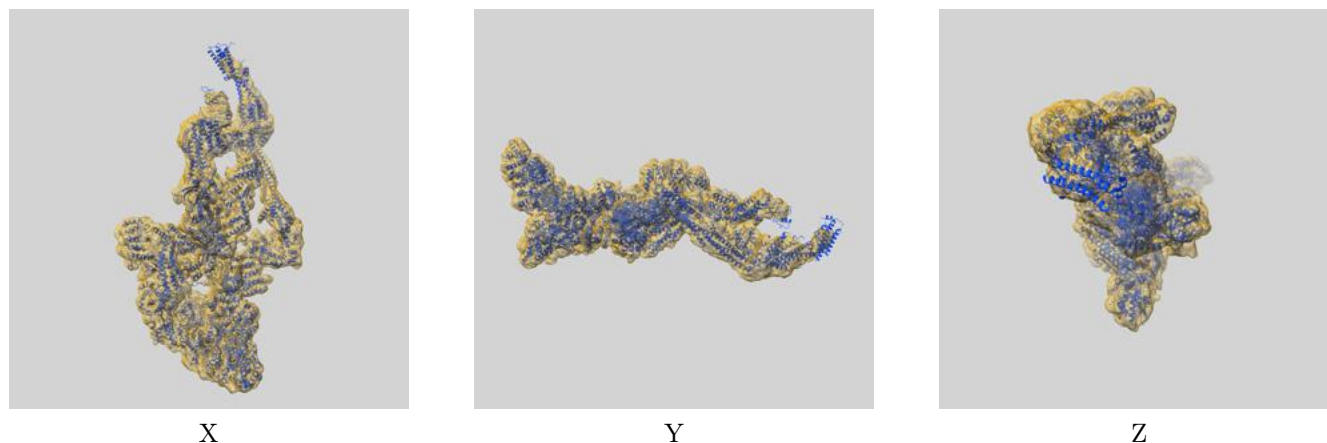
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.04 differs from the reported value 4.68 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 4.68 by more than 10 %

9 Map-model fit [i](#)

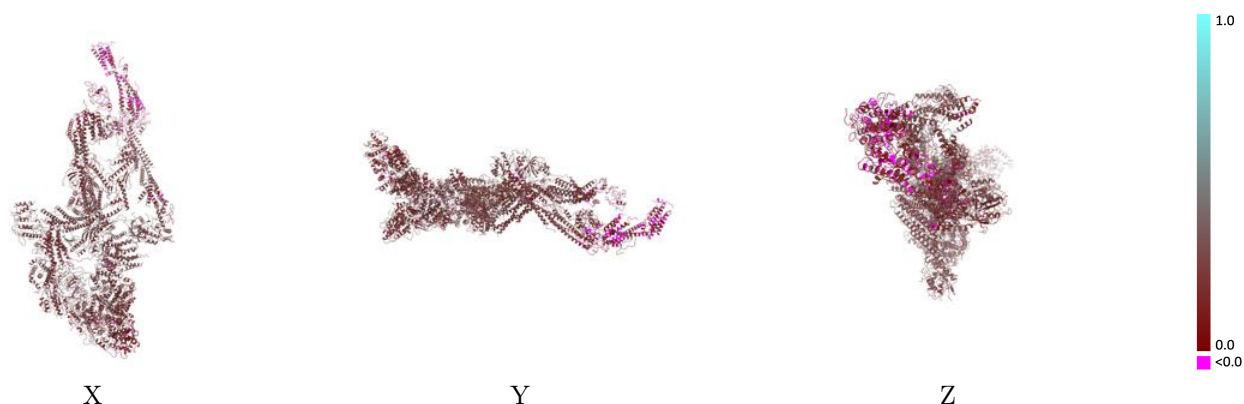
This section contains information regarding the fit between EMDB map EMD-40968 and PDB model 8T1I. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



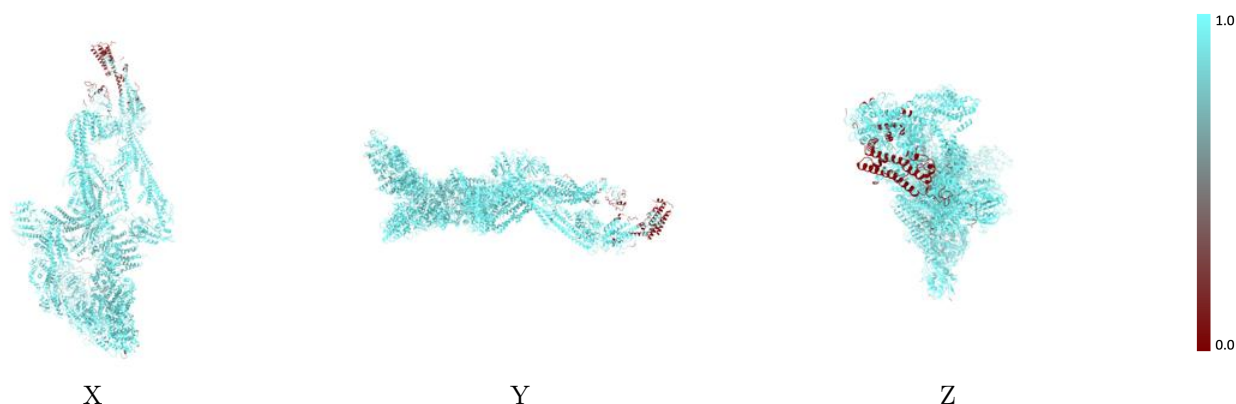
The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



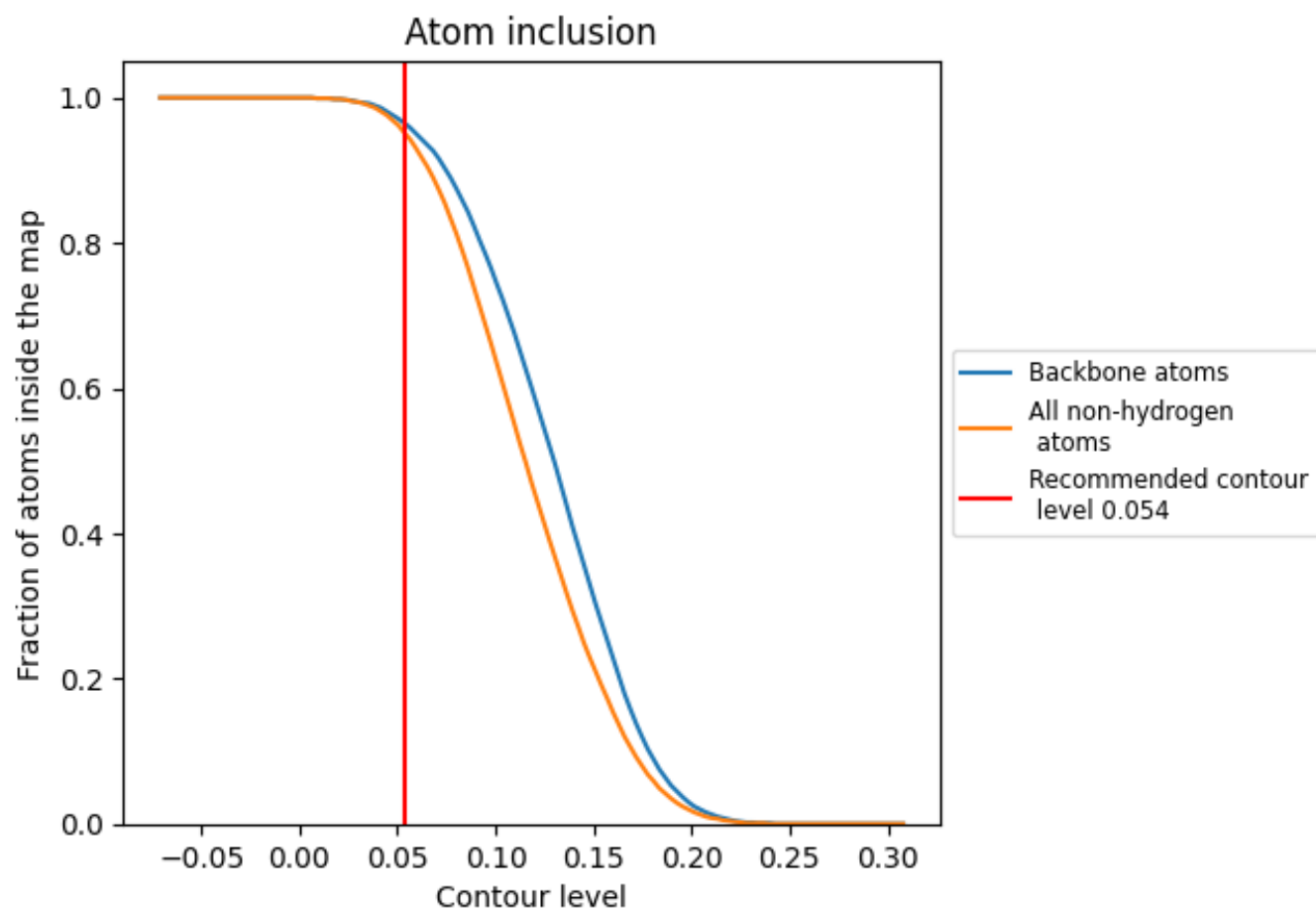
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.054).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.2380
A	 0.9950	 0.2750
B	 0.9940	 0.1950
C	 0.6480	 0.1630
D	 0.9760	 0.1820
E	 0.8900	 0.2080
F	 0.9970	 0.2470
G	 0.4300	 0.0860
H	 0.9970	 0.2420
I	 0.9340	 0.2580
J	 0.9390	 0.2720
K	 0.9820	 0.2550
L	 0.9700	 0.2640
M	 0.9900	 0.2400
N	 0.5570	 0.0880
O	 0.9940	 0.2680
P	 0.9000	 0.1290
Q	 0.9840	 0.2220
R	 0.9650	 0.2220
S	 0.9760	 0.2530
T	 0.9200	 0.2340
U	 0.9540	 0.1250
V	 0.9880	 0.2870
W	 0.9670	 0.2440
X	 0.9890	 0.2470
Y	 0.9820	 0.2480
Z	 0.9760	 0.1780
a	 1.0000	 0.3010

