



wwPDB EM Validation Summary Report ⓘ

Jan 7, 2025 – 04:35 PM EST

PDB ID : 8T1L
EMDB ID : EMD-40971
Title : Atomic model of the mammalian mouse Mediator complex with CKM module
Authors : Zhao, H.; Asturias, F.
Deposited on : 2023-06-02
Resolution : 4.83 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) : 2.40

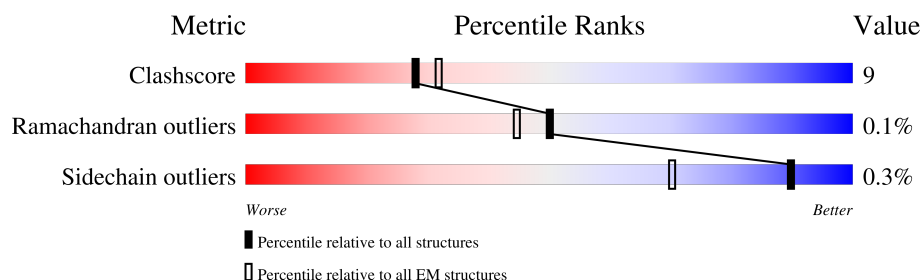
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.83 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	E	268	<div> <div>35%</div> <div>66%</div> <div>33%</div> </div>
2	A	1575	<div> <div>29%</div> <div>70%</div> </div>
3	B	270	<div> <div>16%</div> <div>59%</div> <div>41%</div> </div>
4	C	246	<div> <div>43%</div> <div>67%</div> <div>28%</div> </div>
5	D	233	<div> <div>41%</div> <div>69%</div> <div>31%</div> </div>
6	F	142	<div> <div>11%</div> <div>51%</div> <div>49%</div> </div>
7	G	135	<div> <div>87%</div> <div>90%</div> <div>10%</div> </div>
8	H	117	<div> <div>14%</div> <div>79%</div> <div>8%</div> <div>10%</div> </div>

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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	O	212	
15	P	144	
16	Q	200	
17	R	1367	
18	S	987	
19	T	745	
20	V	311	
21	W	178	
22	X	199	
23	Y	178	
24	Z	131	
25	a	20	
26	9	2171	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49460 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 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	179	Total	C	N	O	0	0
			888	530	179	179		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	472	Total	C	N	O	0	0
			2339	1395	472	472		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	176	Total	C	N	O	0	0
			963	584	193	186		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

- 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
			582	352	117	112	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	1111	Total	C	N	O	S	0
			6892	4356	1276	1240	20	0

- 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
			1171	748	217	200	6	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	732	Total	C	N	O	S	0
			5051	3258	906	863	24	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	559	Total	C	N	O	S	0
			3424	2155	645	621	3	0

- 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
			1140	725	217	197	1	0

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	114	Total	C	N	O		0	0
			568	340	114	114			

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	1299	Total	C	N	O	S	0	0
			9771	6312	1684	1722	53		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	913	Total	C	N	O	S	0	0
			5934	3785	1074	1048	27		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	197	Total	C	N	O	S	0	0
			1287	814	226	241	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	278	Total	C	N	O	S	0	0
			1726	1097	313	313	3		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	119	Total	C	N	O	S	0	0
			778	489	146	141	2		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	127	Total	C	N	O	S	0	0
			859	540	154	162	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	154	Total	C	N	O	S	0	0
			994	616	198	177	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	103	Total	C	N	O		0	0
			513	307	103	103			

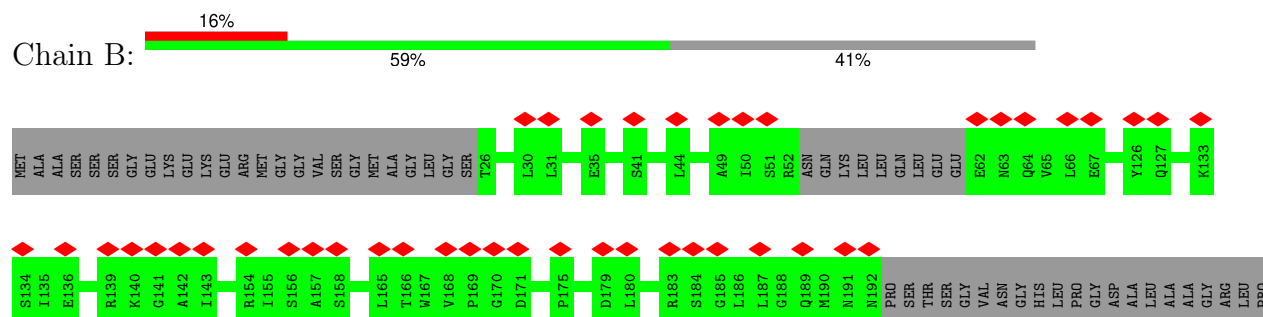
- Molecule 25 is a protein called Unknown.

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

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 13.

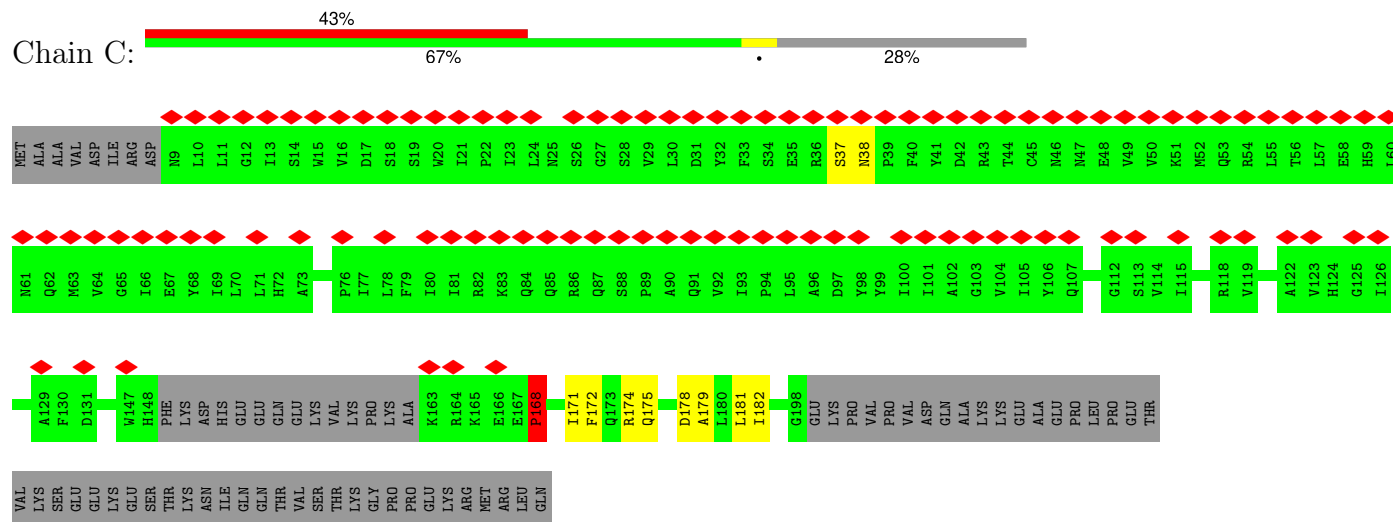
Mol	Chain	Residues	Atoms					AltConf	Trace
26	9	19	Total	C	N	O		0	0
			160	107	26	27			

- Molecule 3: Mediator of RNA polymerase II transcription subunit 4

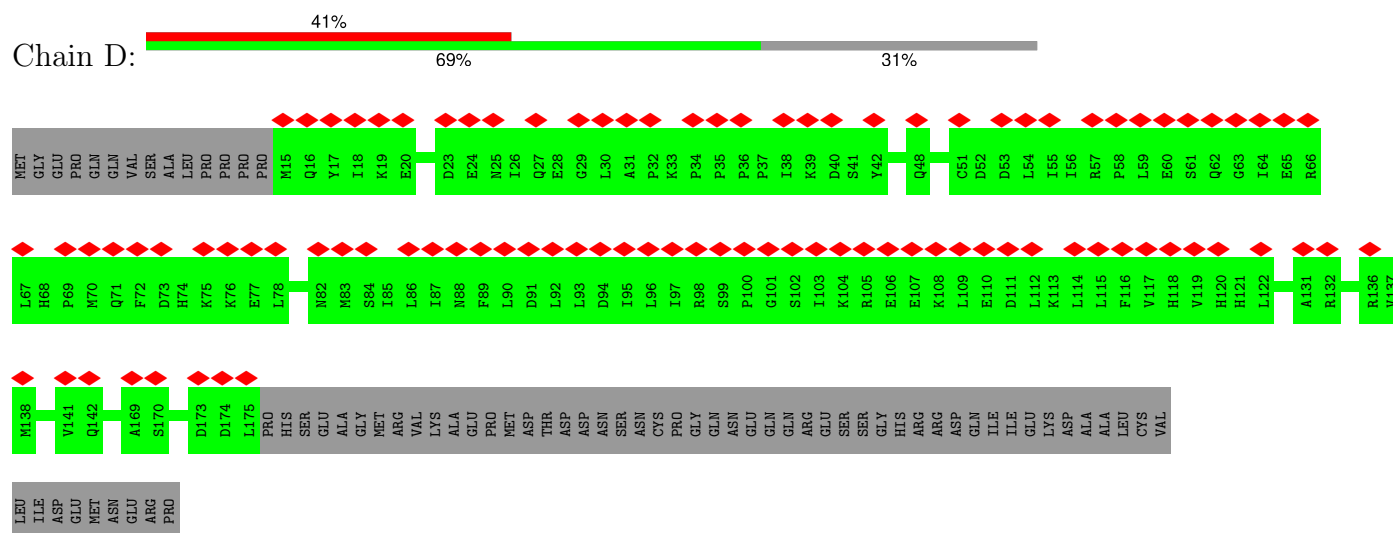


ASP VAL LEU ALA VAL PRO GLN TYR PRO TRP GLN SER ASN ASP MET VAL VAL MET MET MET LEU PRO PRO HIS SER SER ASP PHE LEU LEU GLU PRO PRO GLY HIS ASN ASN LYS LYS LYS ASP ASP VAL VAL MET MET THR THR ASP SER SER SER SER SER SER ASP ASP

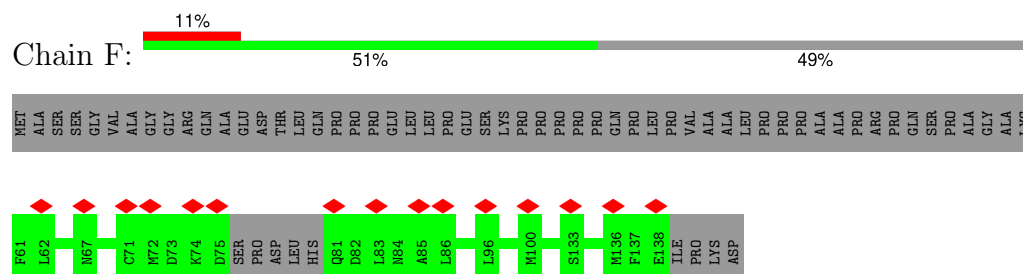
• Molecule 4: Mediator of RNA polymerase II transcription subunit 6



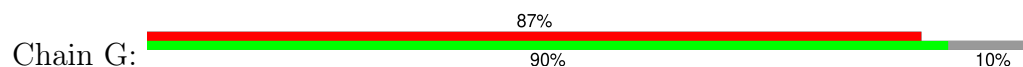
• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

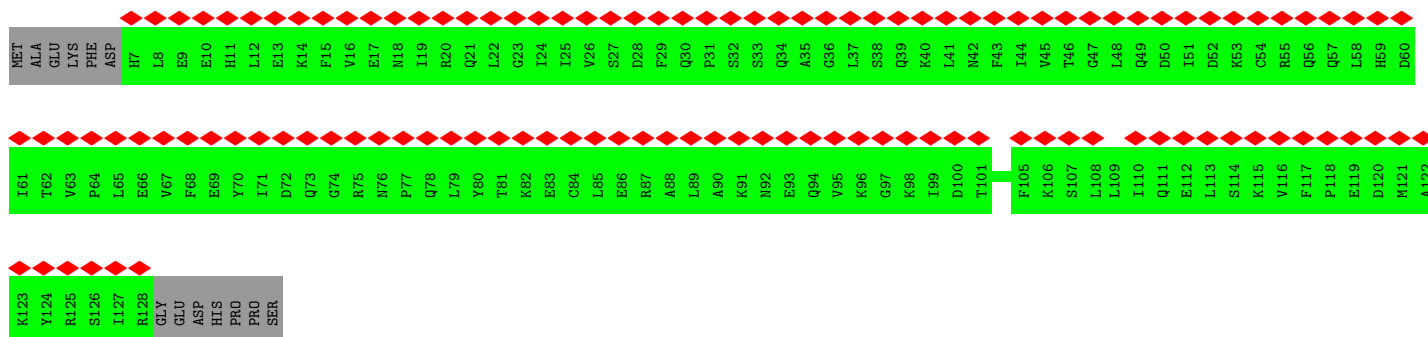


• Molecule 6: Mediator of RNA polymerase II transcription subunit 9

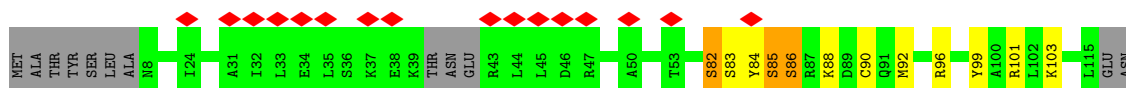
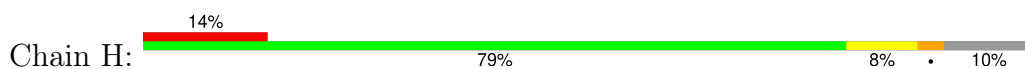


• Molecule 7: Mediator of RNA polymerase II transcription subunit 10

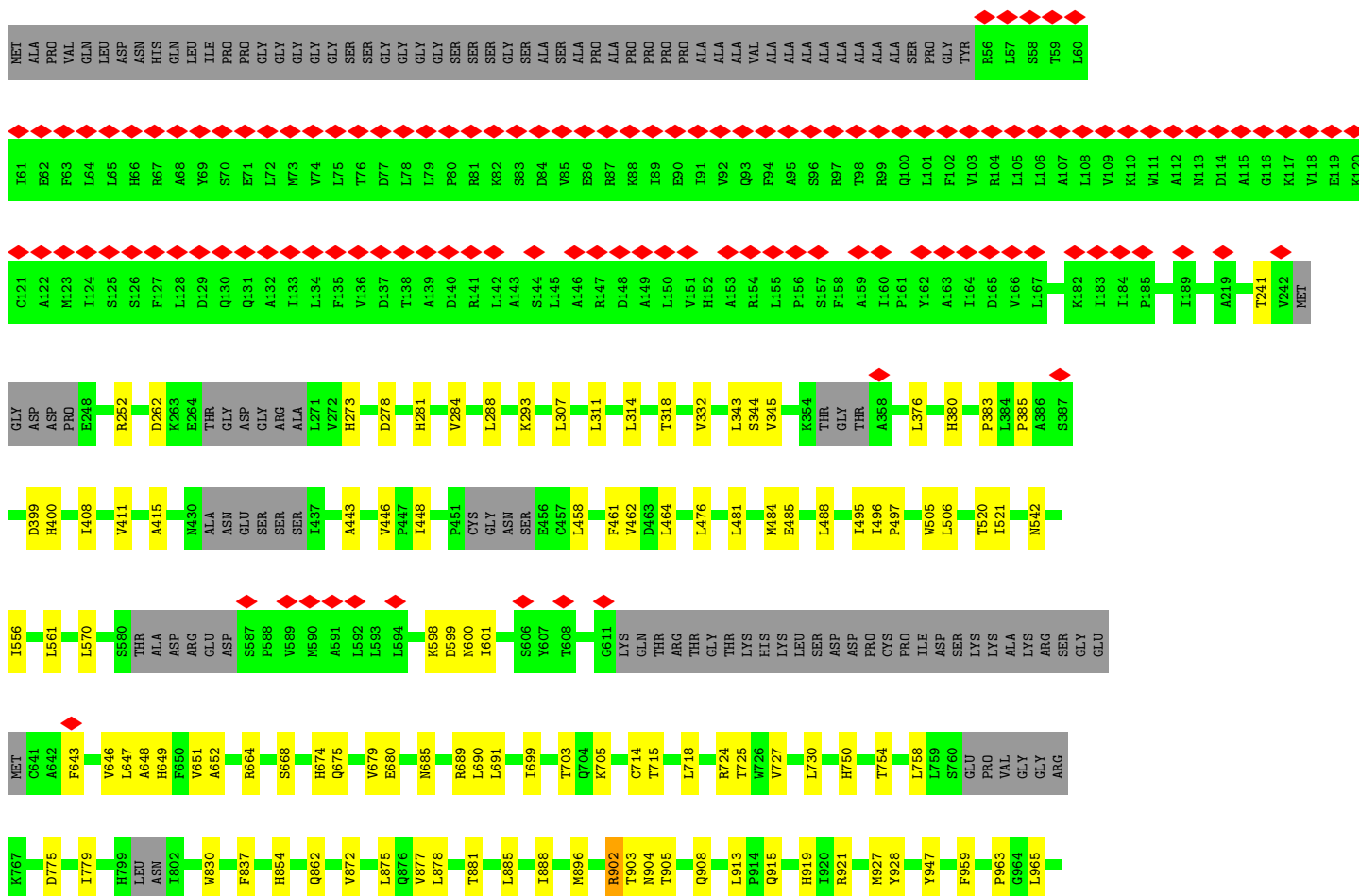




- Molecule 8: Mediator of RNA polymerase II transcription subunit 11

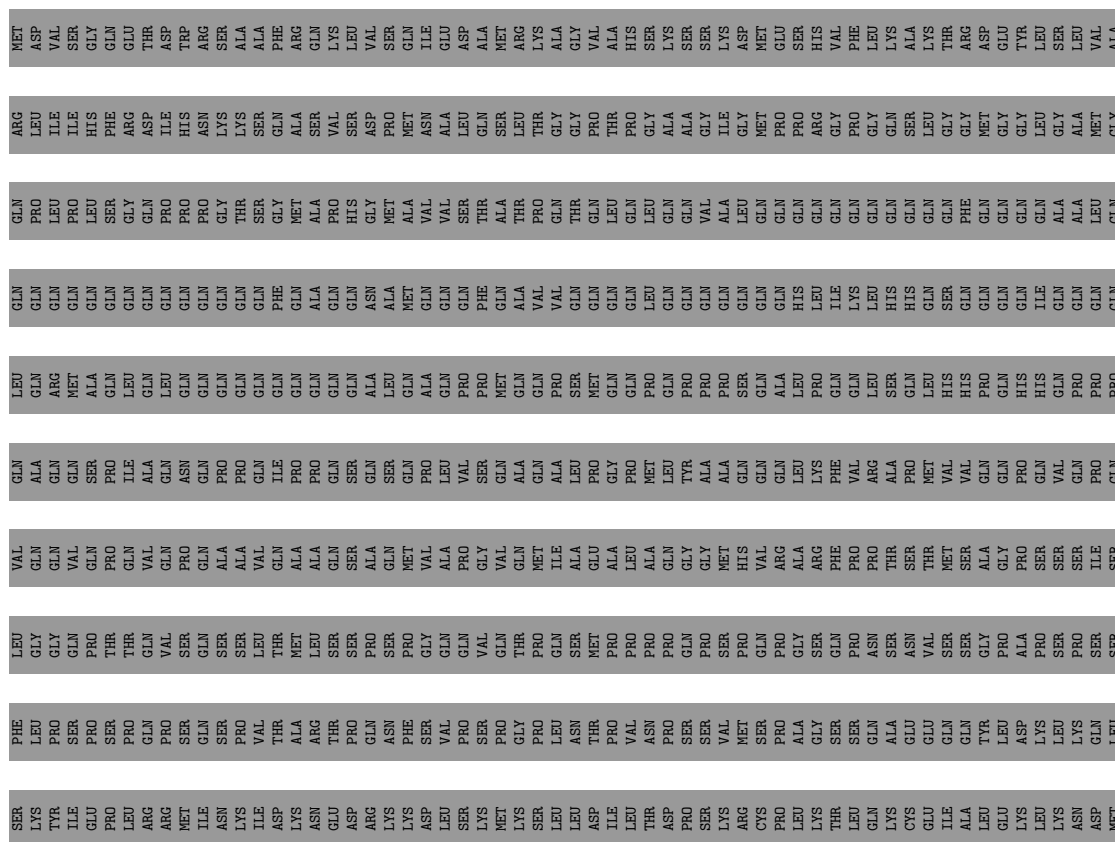


- Molecule 9: Mediator of RNA polymerase II transcription subunit 14



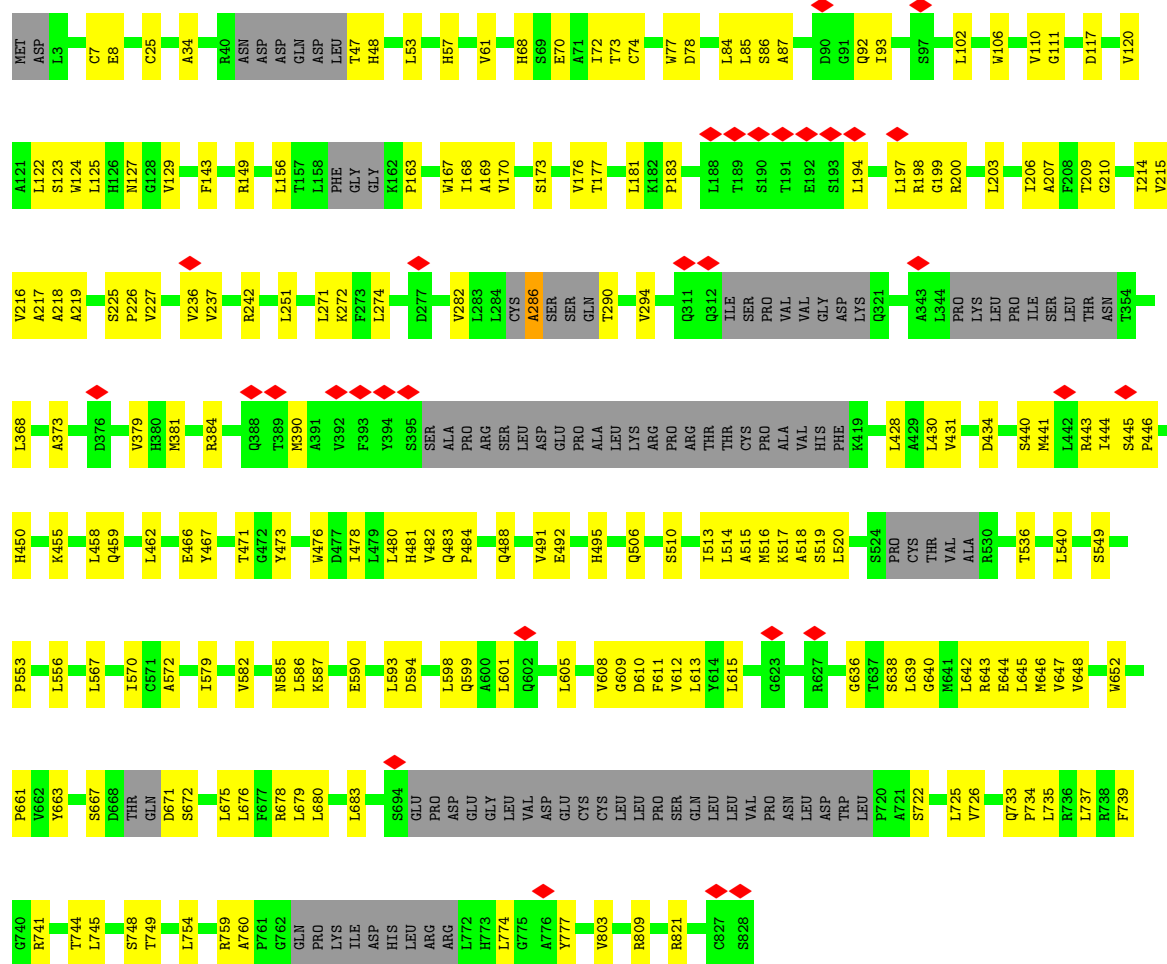
- Molecule 10: Mediator of RNA polymerase II transcription subunit 15

Chain J: 17% 79%




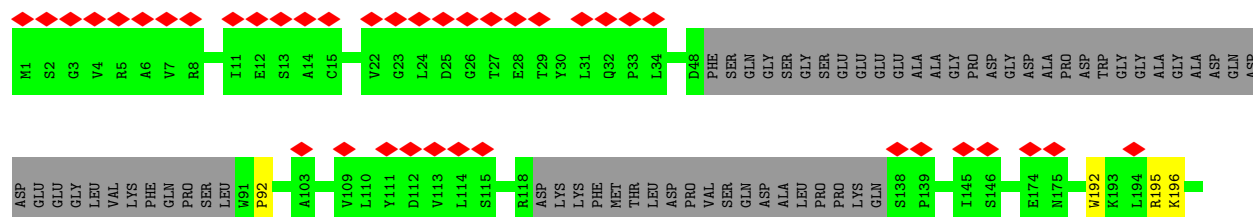
- Molecule 11: Mediator of RNA polymerase II transcription subunit 16

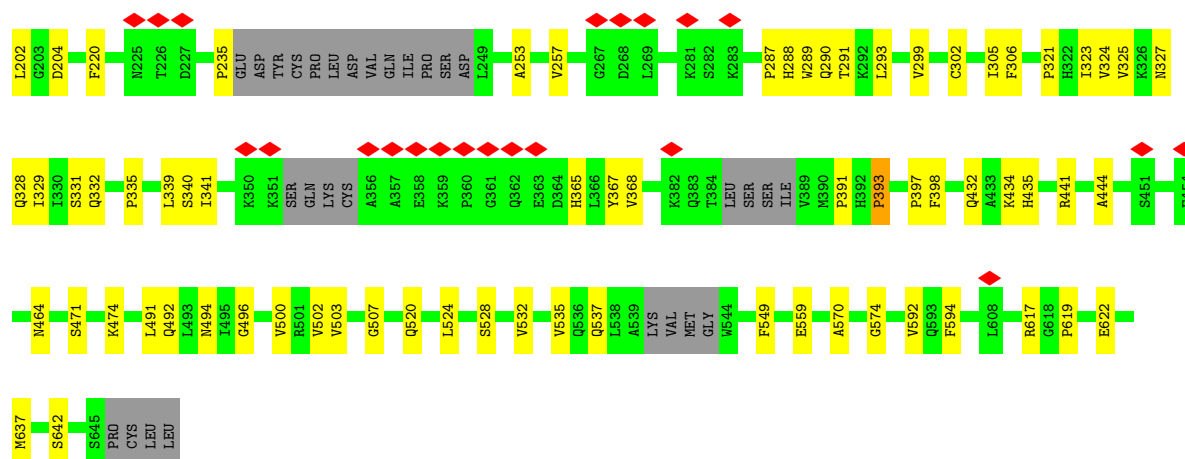
Chain K:  65% 23% 12%



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

Chain L: 





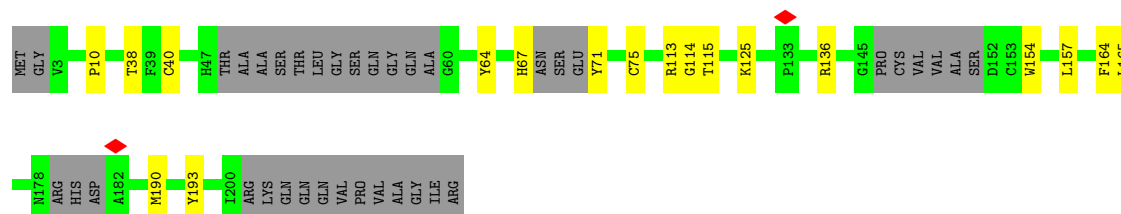
- Molecule 13: Mediator of RNA polymerase II transcription subunit 18

Chain M: 73% 13% 13%



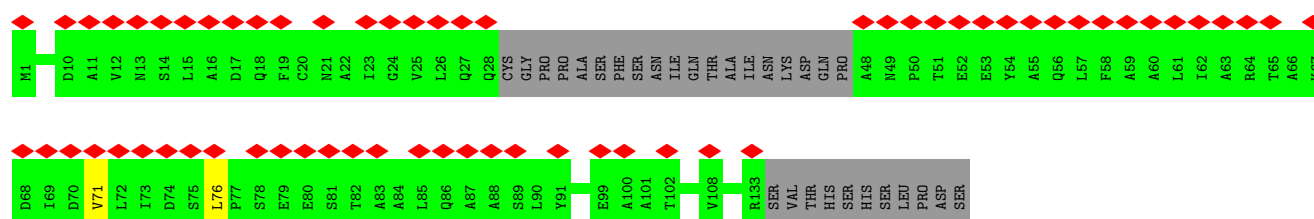
- Molecule 14: Mediator of RNA polymerase II transcription subunit 20

Chain O: 74% 8% 18%



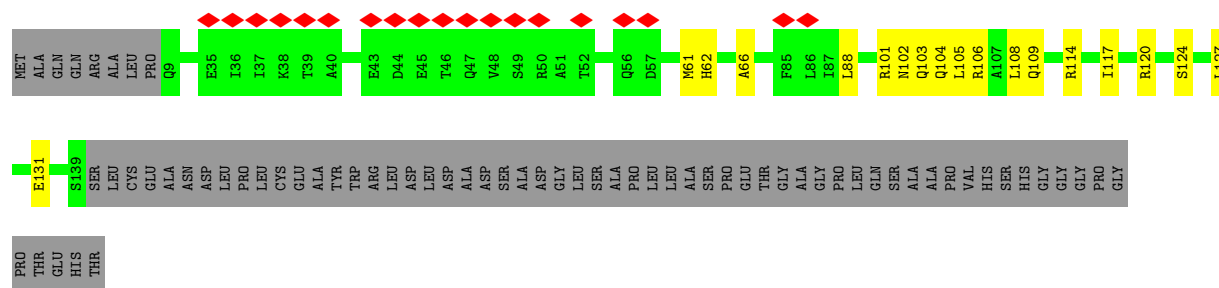
- Molecule 15: Mediator of RNA polymerase II transcription subunit 21

Chain P: 44% 78% 21%

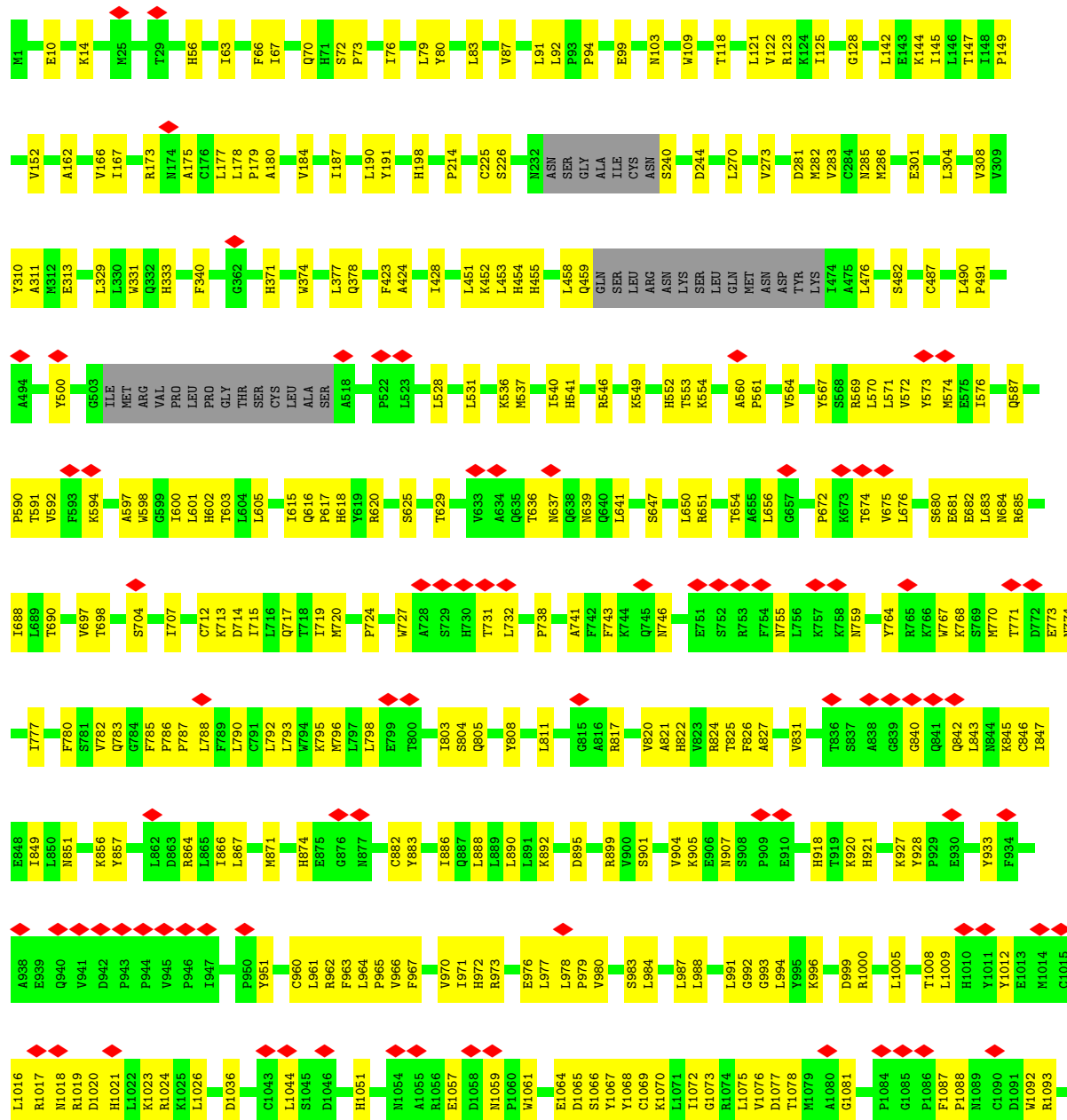


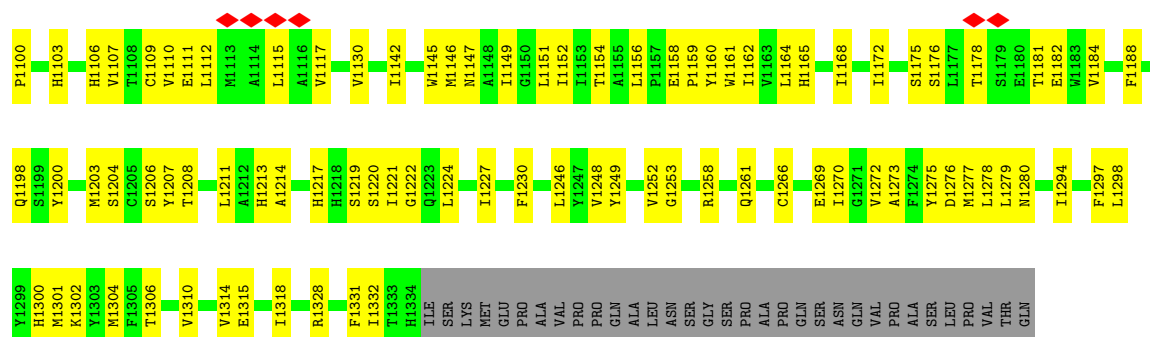
- Molecule 16: Mediator of RNA polymerase II transcription subunit 22

Chain Q: 10% 56% 9% 34%

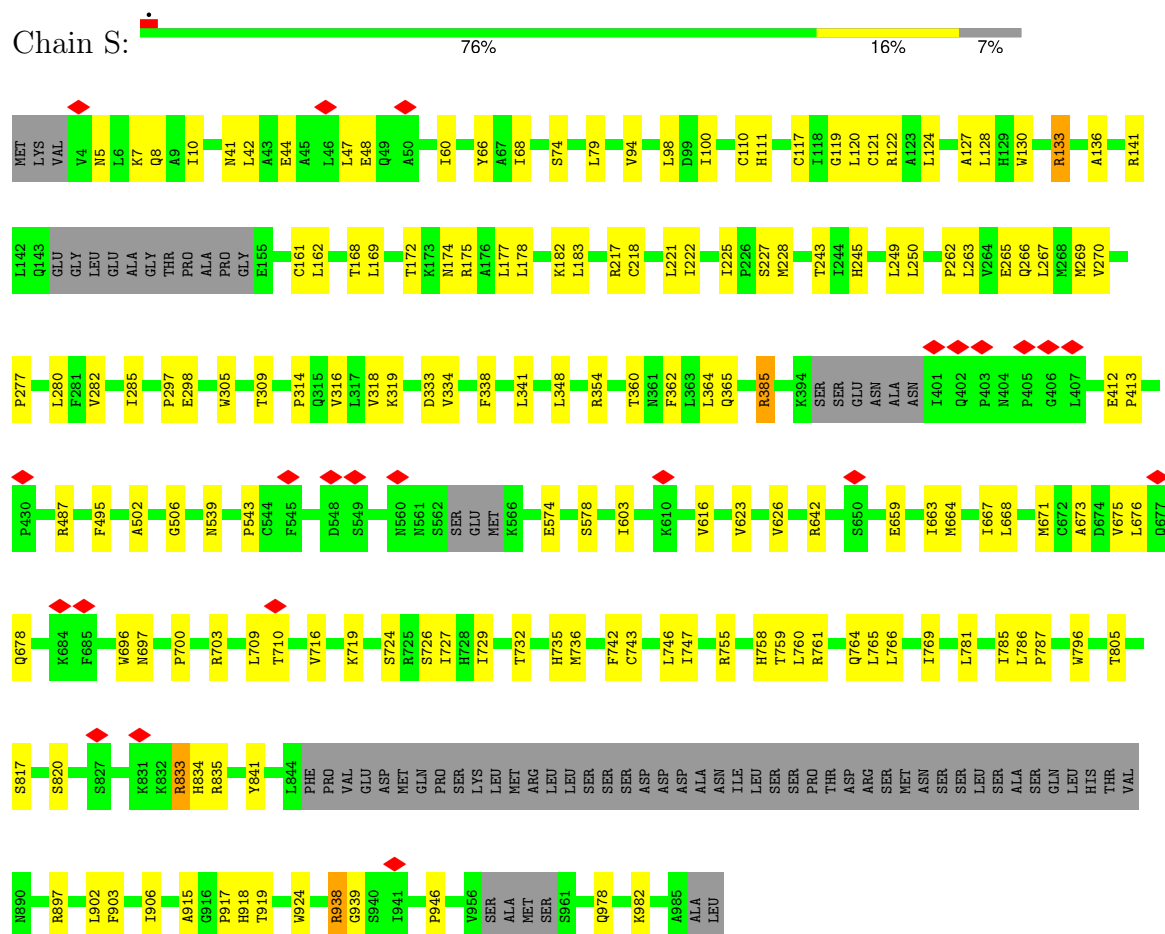


• Molecule 17: Mediator of RNA polymerase II transcription subunit 23

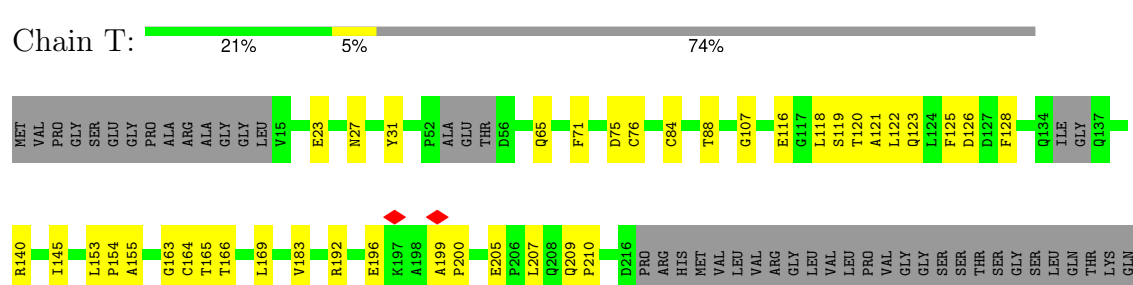


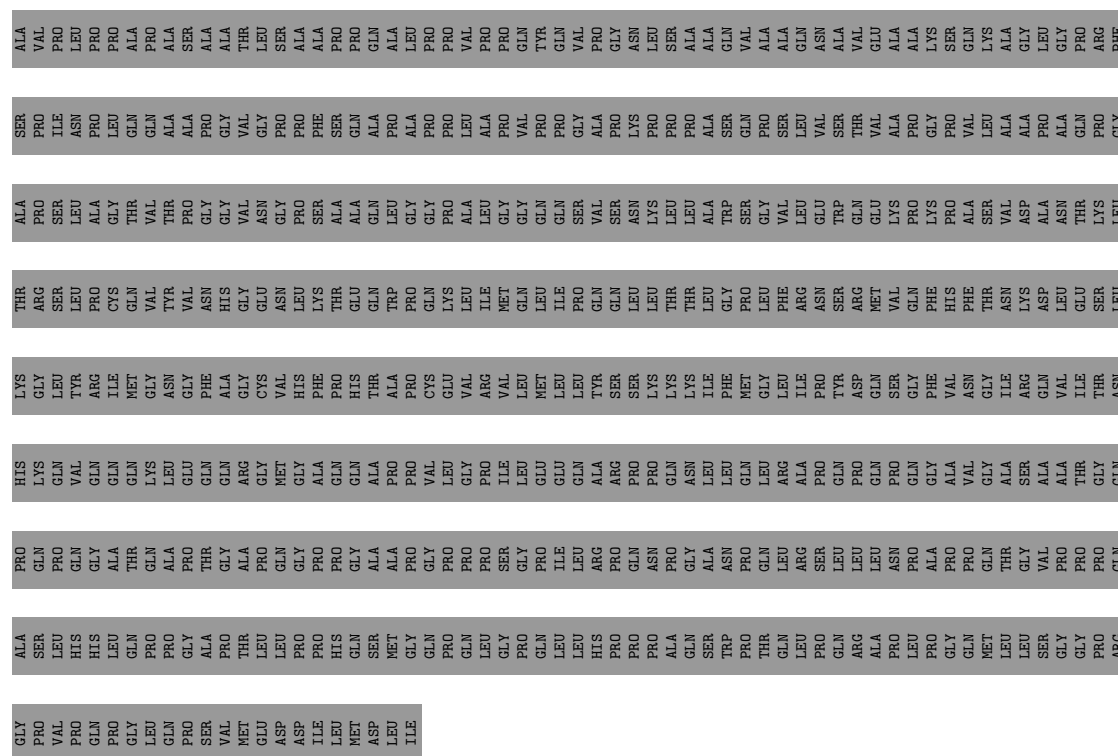


• Molecule 18: Mediator of RNA polymerase II transcription subunit 24

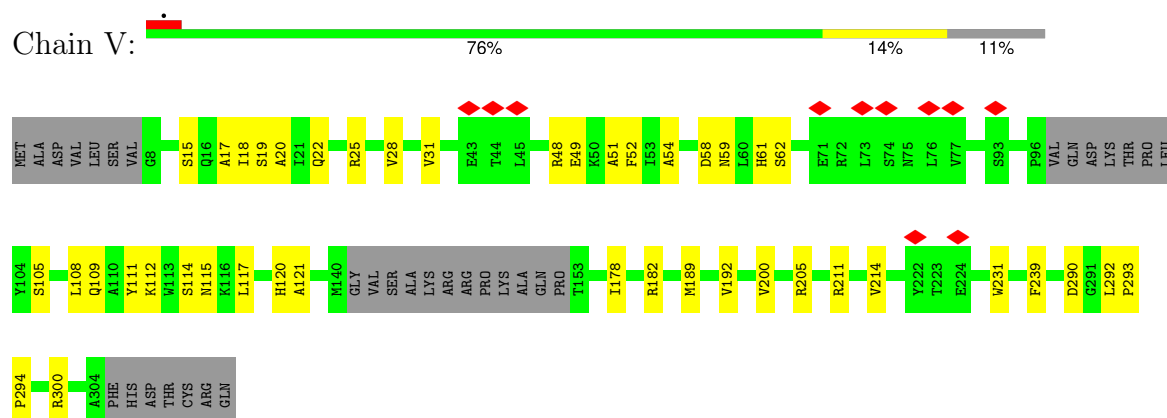


• Molecule 19: Mediator of RNA polymerase II transcription subunit 25

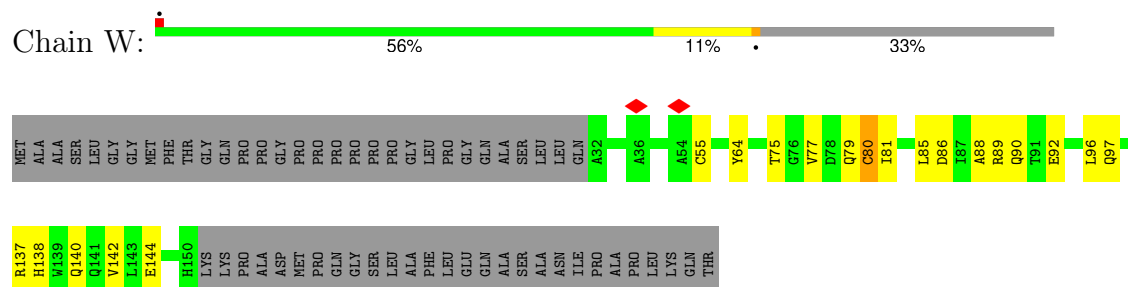




- Molecule 20: Mediator of RNA polymerase II transcription subunit 27



- Molecule 21: Mediator of RNA polymerase II transcription subunit 28



- Molecule 22: Mediator of RNA polymerase II transcription subunit 29





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111331	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	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.621	Depositor
Minimum map value	-0.346	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	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 [i](#)

5.1 Standard geometry [i](#)

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	E	0.23	0/885	0.37	0/1230
2	A	0.23	0/2334	0.41	0/3247
3	B	0.23	0/782	0.34	0/1088
4	C	0.26	0/967	0.49	1/1333 (0.1%)
5	D	0.23	0/800	0.34	0/1116
6	F	0.22	0/361	0.33	0/501
7	G	0.23	0/604	0.33	0/841
8	H	0.22	0/584	0.43	0/802
9	I	0.24	0/7018	0.42	1/9683 (0.0%)
10	J	0.24	0/1207	0.42	0/1668
11	K	0.23	0/5165	0.47	1/7090 (0.0%)
12	L	0.24	0/3482	0.42	1/4795 (0.0%)
13	M	0.23	0/1163	0.42	0/1593
14	O	0.24	0/1027	0.39	0/1412
15	P	0.22	0/566	0.30	0/788
16	Q	0.24	0/758	0.38	0/1046
17	R	0.24	0/10024	0.41	0/13697
18	S	0.24	0/6059	0.40	0/8332
19	T	0.25	0/1320	0.43	0/1813
20	V	0.24	0/1765	0.41	0/2441
21	W	0.24	0/790	0.40	0/1083
22	X	0.24	0/872	0.41	0/1197
23	Y	0.25	0/1007	0.36	0/1375
24	Z	0.22	0/512	0.40	0/714
26	9	0.28	0/165	0.45	0/220
All	All	0.24	0/50217	0.41	4/69105 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	168	PRO	CA-N-CD	-8.23	99.97	111.50
9	I	385	PRO	N-CA-CB	6.10	110.62	103.30
12	L	92	PRO	N-CA-CB	6.04	110.55	103.30
11	K	286	ALA	C-N-CA	6.02	136.75	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	82	SER	Peptide
8	H	85	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	888	0	392	2	0
2	A	2339	0	1005	10	0
3	B	784	0	357	0	0
4	C	963	0	554	8	0
5	D	801	0	327	0	0
6	F	363	0	146	0	0
7	G	605	0	256	0	0
8	H	582	0	352	10	0
9	I	6892	0	5009	92	0
10	J	1171	0	1010	27	0
11	K	5051	0	4492	128	0
12	L	3424	0	2463	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1140	0	832	17	0
14	O	1013	0	663	9	0
15	P	568	0	286	1	0
16	Q	754	0	448	13	0
17	R	9771	0	9126	269	0
18	S	5934	0	4713	105	0
19	T	1287	0	992	23	0
20	V	1726	0	1220	26	0
21	W	778	0	609	17	0
22	X	859	0	708	18	0
23	Y	994	0	777	16	0
24	Z	513	0	225	0	0
25	a	100	0	23	0	0
26	9	160	0	170	1	0
All	All	49460	0	37155	810	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 9.

The worst 5 of 810 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)
17:R:620:ARG:HH21	17:R:656:LEU:HD22	1.45	0.81
18:S:117:CYS:O	18:S:120:LEU:HB3	1.82	0.80
11:K:203:LEU:HA	11:K:218:ALA:HB3	1.64	0.79
12:L:494:ASN:HA	12:L:500:VAL:HG12	1.66	0.78
12:L:393:PRO:HG2	12:L:397:PRO:HD2	1.65	0.77

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	E	173/268 (65%)	160 (92%)	13 (8%)	0	100	100
2	A	462/1575 (29%)	420 (91%)	42 (9%)	0	100	100
3	B	154/270 (57%)	152 (99%)	2 (1%)	0	100	100
4	C	172/246 (70%)	152 (88%)	18 (10%)	2 (1%)	11	44
5	D	159/233 (68%)	156 (98%)	3 (2%)	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%)	89 (88%)	9 (9%)	3 (3%)	3	22
9	I	1075/1459 (74%)	943 (88%)	132 (12%)	0	100	100
10	J	165/789 (21%)	136 (82%)	29 (18%)	0	100	100
11	K	710/828 (86%)	578 (81%)	132 (19%)	0	100	100
12	L	545/649 (84%)	463 (85%)	81 (15%)	1 (0%)	44	78
13	M	176/208 (85%)	160 (91%)	16 (9%)	0	100	100
14	O	164/212 (77%)	153 (93%)	11 (7%)	0	100	100
15	P	110/144 (76%)	106 (96%)	4 (4%)	0	100	100
16	Q	129/200 (64%)	117 (91%)	12 (9%)	0	100	100
17	R	1291/1367 (94%)	1116 (86%)	175 (14%)	0	100	100
18	S	901/987 (91%)	811 (90%)	90 (10%)	0	100	100
19	T	191/745 (26%)	166 (87%)	25 (13%)	0	100	100
20	V	272/311 (88%)	231 (85%)	40 (15%)	1 (0%)	30	68
21	W	117/178 (66%)	110 (94%)	7 (6%)	0	100	100
22	X	123/199 (62%)	117 (95%)	6 (5%)	0	100	100
23	Y	150/178 (84%)	133 (89%)	17 (11%)	0	100	100
24	Z	101/131 (77%)	99 (98%)	2 (2%)	0	100	100
26	9	17/2171 (1%)	13 (76%)	4 (24%)	0	100	100
All	All	7647/13742 (56%)	6766 (88%)	874 (11%)	7 (0%)	50	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	86	SER
4	C	168	PRO
8	H	83	SER
8	H	85	SER

Continued on next page...

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Mol	Chain	Res	Type
20	V	293	PRO

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	
4	C	25/223 (11%)	25 (100%)	0	100	100
8	H	13/98 (13%)	13 (100%)	0	100	100
9	I	387/1276 (30%)	386 (100%)	1 (0%)	91	92
10	J	100/693 (14%)	99 (99%)	1 (1%)	73	82
11	K	419/729 (58%)	418 (100%)	1 (0%)	92	94
12	L	182/572 (32%)	182 (100%)	0	100	100
13	M	61/183 (33%)	61 (100%)	0	100	100
14	O	44/177 (25%)	44 (100%)	0	100	100
16	Q	23/173 (13%)	23 (100%)	0	100	100
17	R	952/1231 (77%)	952 (100%)	0	100	100
18	S	395/867 (46%)	390 (99%)	5 (1%)	65	77
19	T	90/598 (15%)	90 (100%)	0	100	100
20	V	96/279 (34%)	96 (100%)	0	100	100
21	W	52/153 (34%)	51 (98%)	1 (2%)	52	70
22	X	65/164 (40%)	65 (100%)	0	100	100
23	Y	61/157 (39%)	61 (100%)	0	100	100
26	9	19/1912 (1%)	19 (100%)	0	100	100
All	All	2984/9485 (32%)	2975 (100%)	9 (0%)	90	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	938	ARG
21	W	80	CYS

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Mol	Chain	Res	Type
18	S	133	ARG
18	S	385	ARG
18	S	487	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
17	R	1165	HIS
20	V	109	GLN
17	R	1320	ASN
18	S	370	GLN
20	V	252	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

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](#)

There are no chain breaks in this entry.

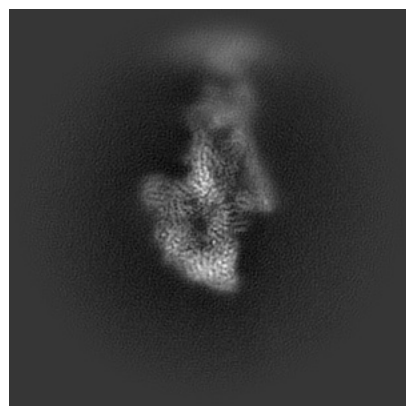
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40971. These allow visual inspection of the internal detail of the map and identification of artifacts.

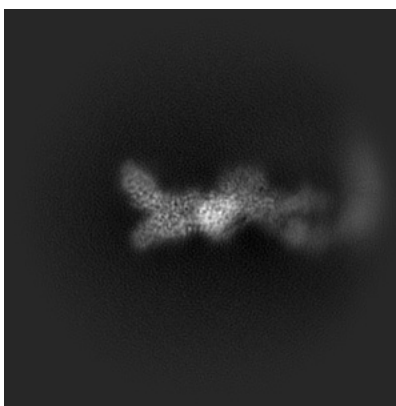
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

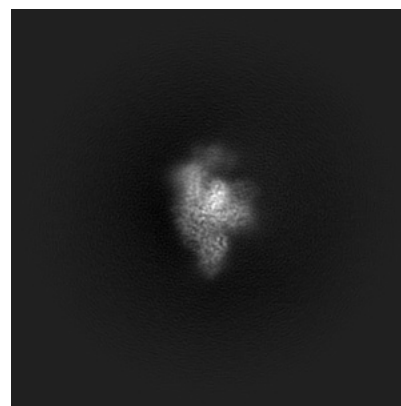
6.1.1 Primary map



X

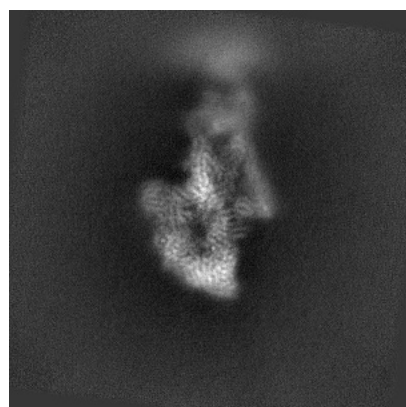


Y

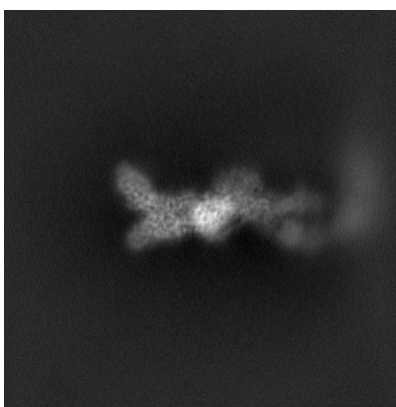


Z

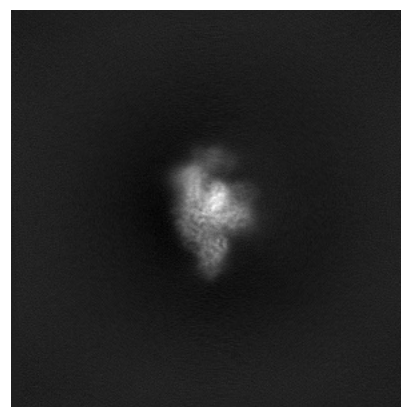
6.1.2 Raw map



X



Y

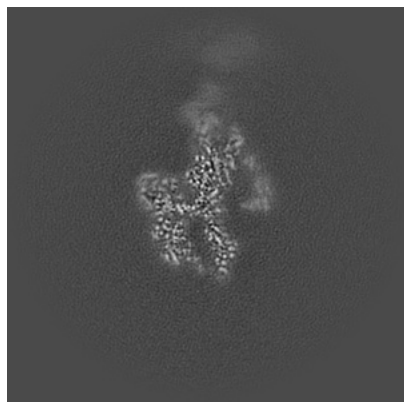


Z

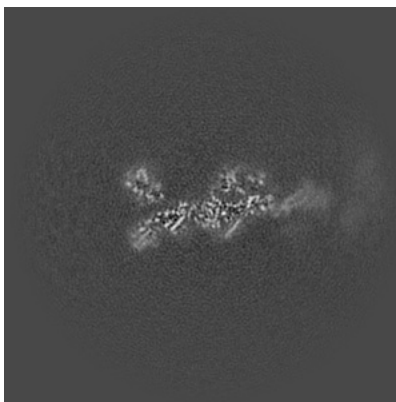
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

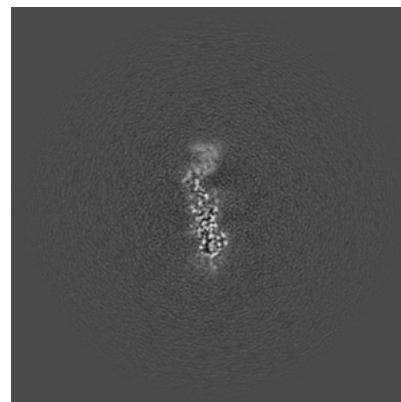
6.2.1 Primary map



X Index: 280

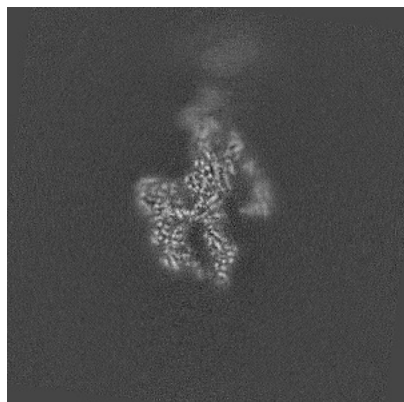


Y Index: 280



Z Index: 280

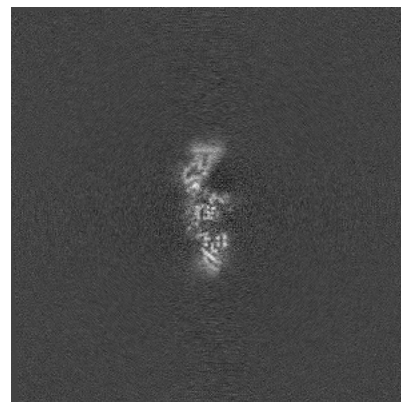
6.2.2 Raw map



X Index: 280



Y Index: 280

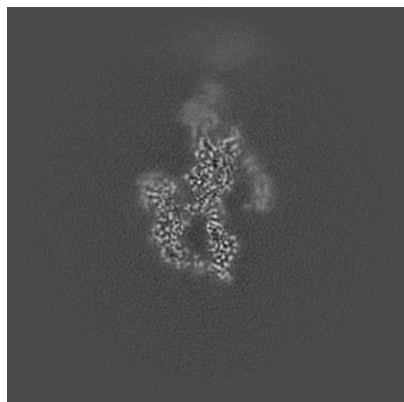


Z Index: 280

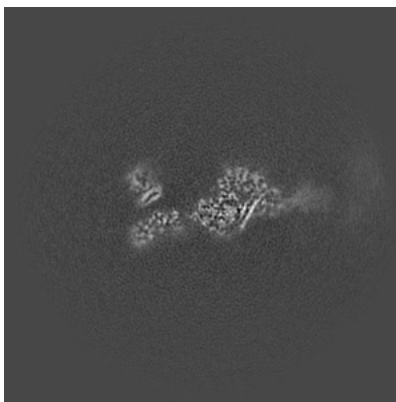
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

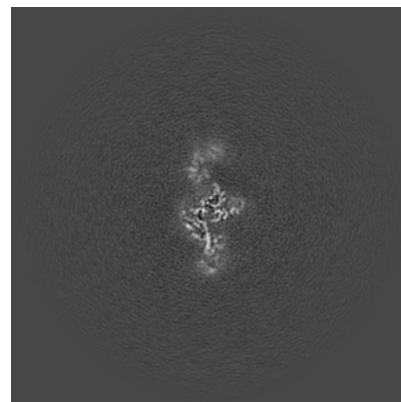
6.3.1 Primary map



X Index: 284

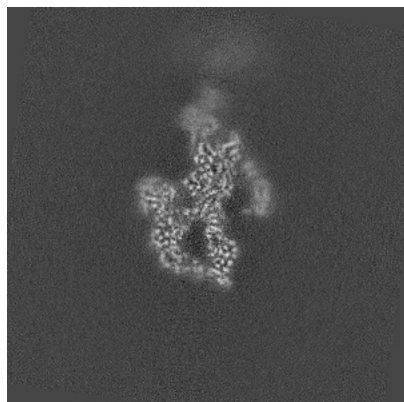


Y Index: 274

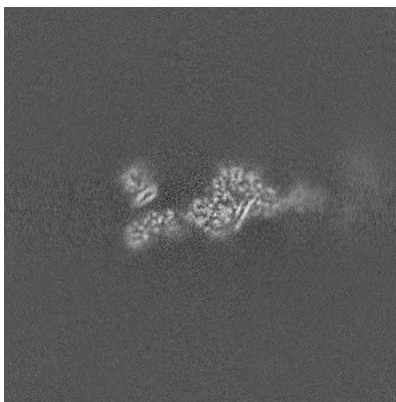


Z Index: 303

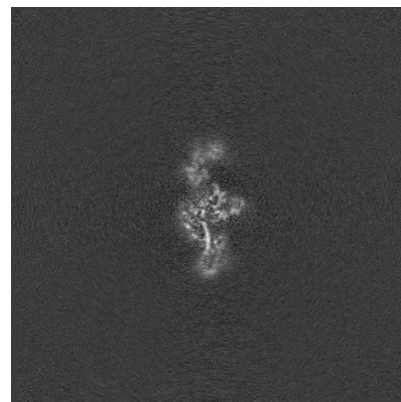
6.3.2 Raw map



X Index: 284



Y Index: 273

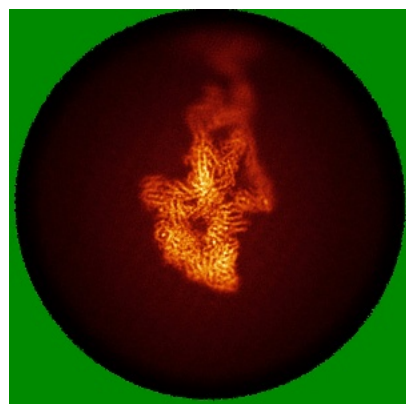


Z Index: 295

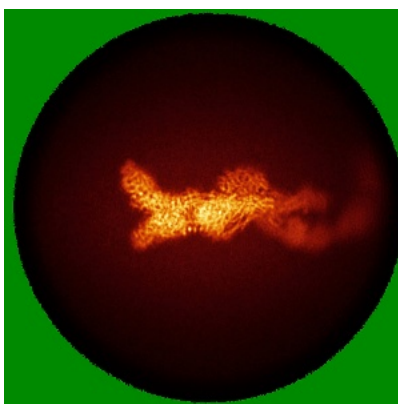
The images above show the largest variance slices of the map in three orthogonal directions.

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

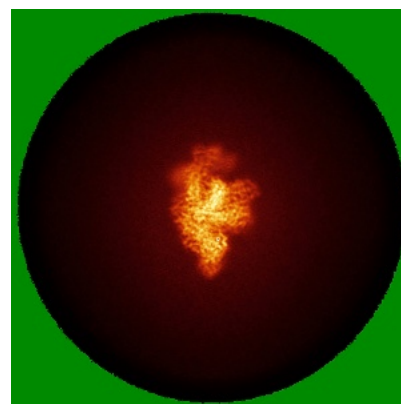
6.4.1 Primary map



X

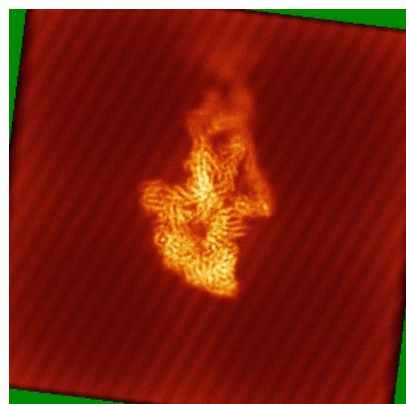


Y

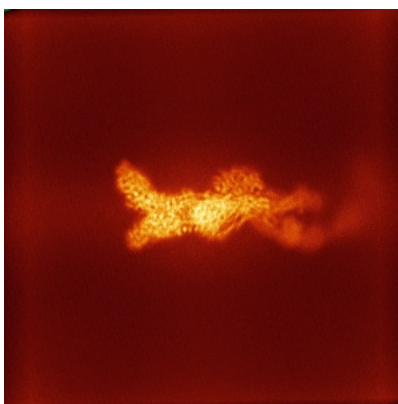


Z

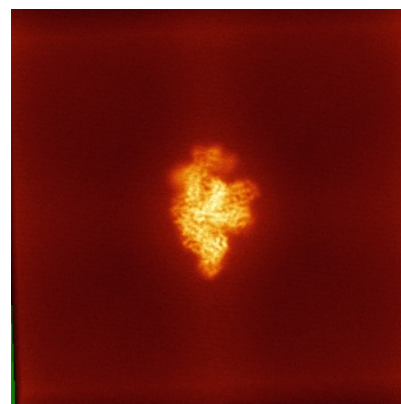
6.4.2 Raw map



X



Y

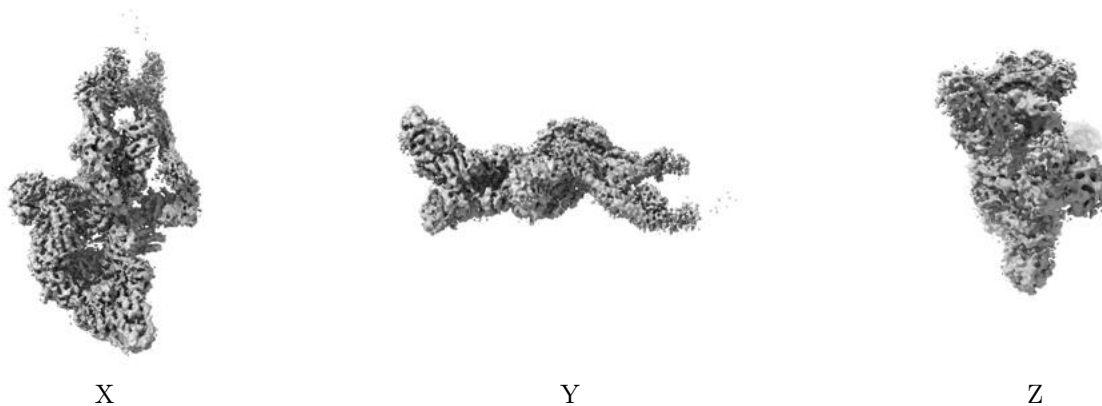


Z

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.

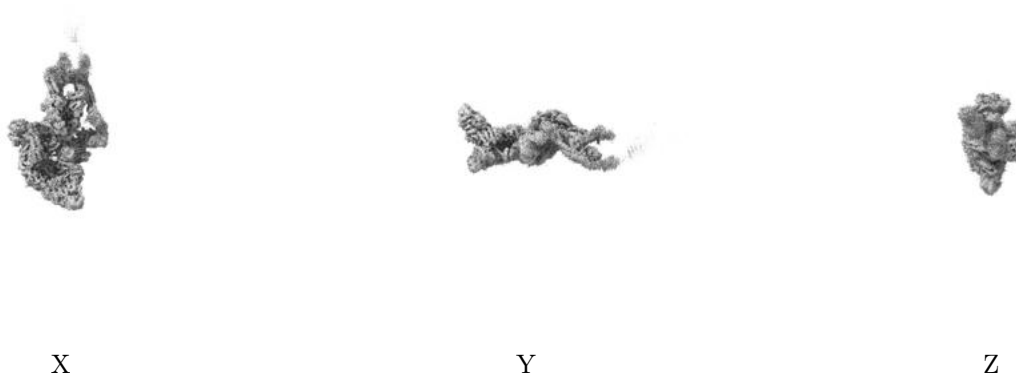
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

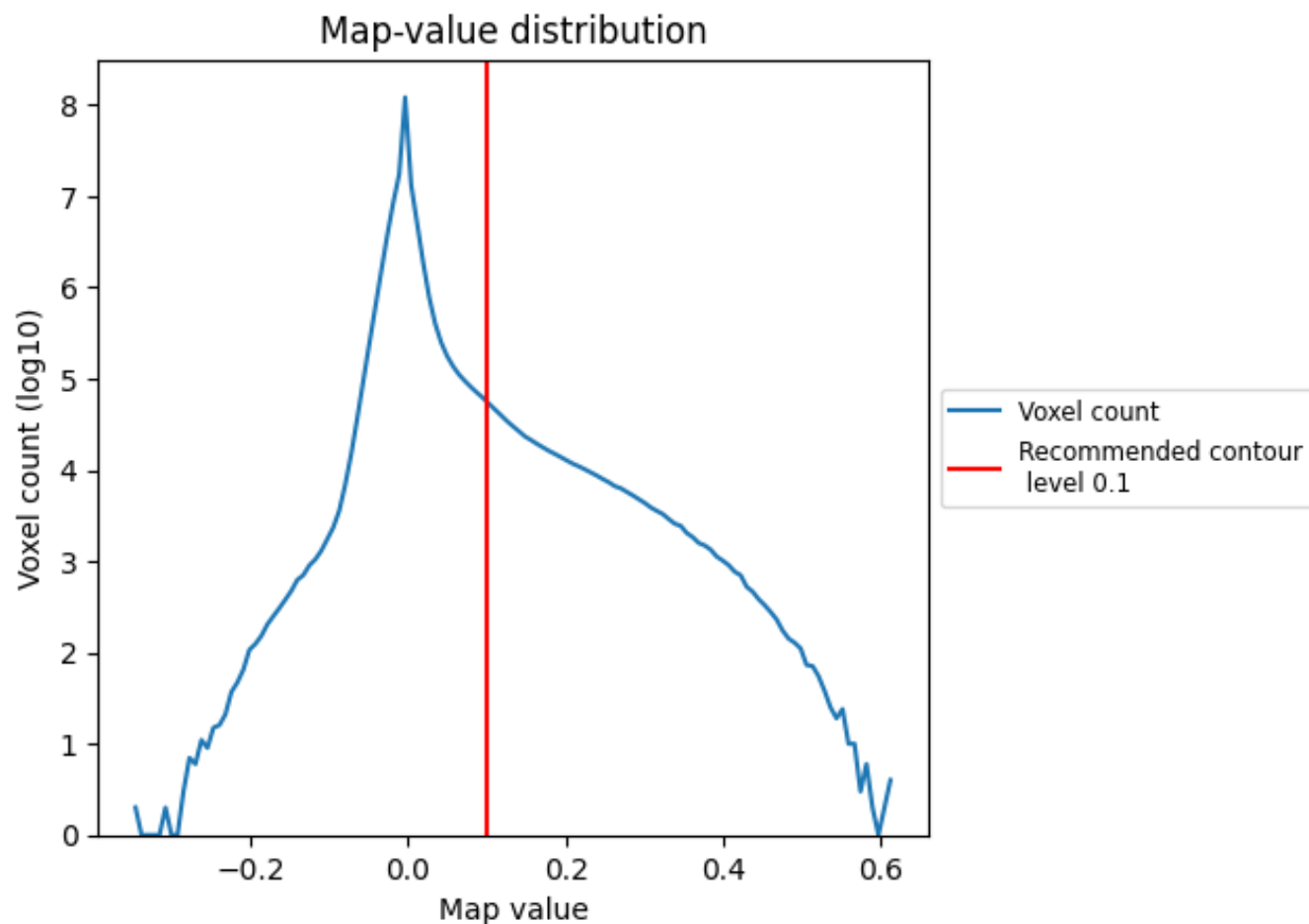
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

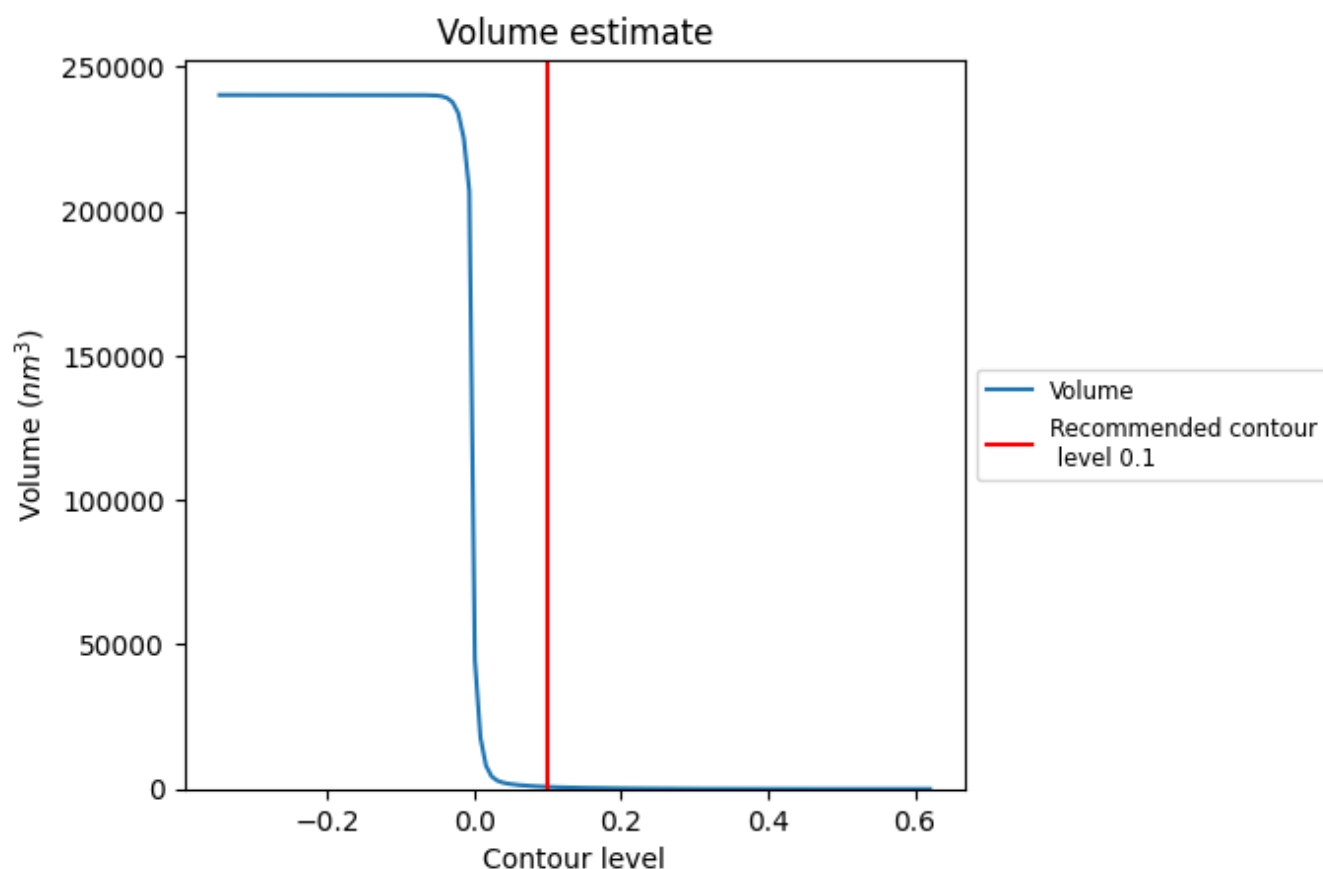
This section contains the results of statistical analysis of the map.

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.

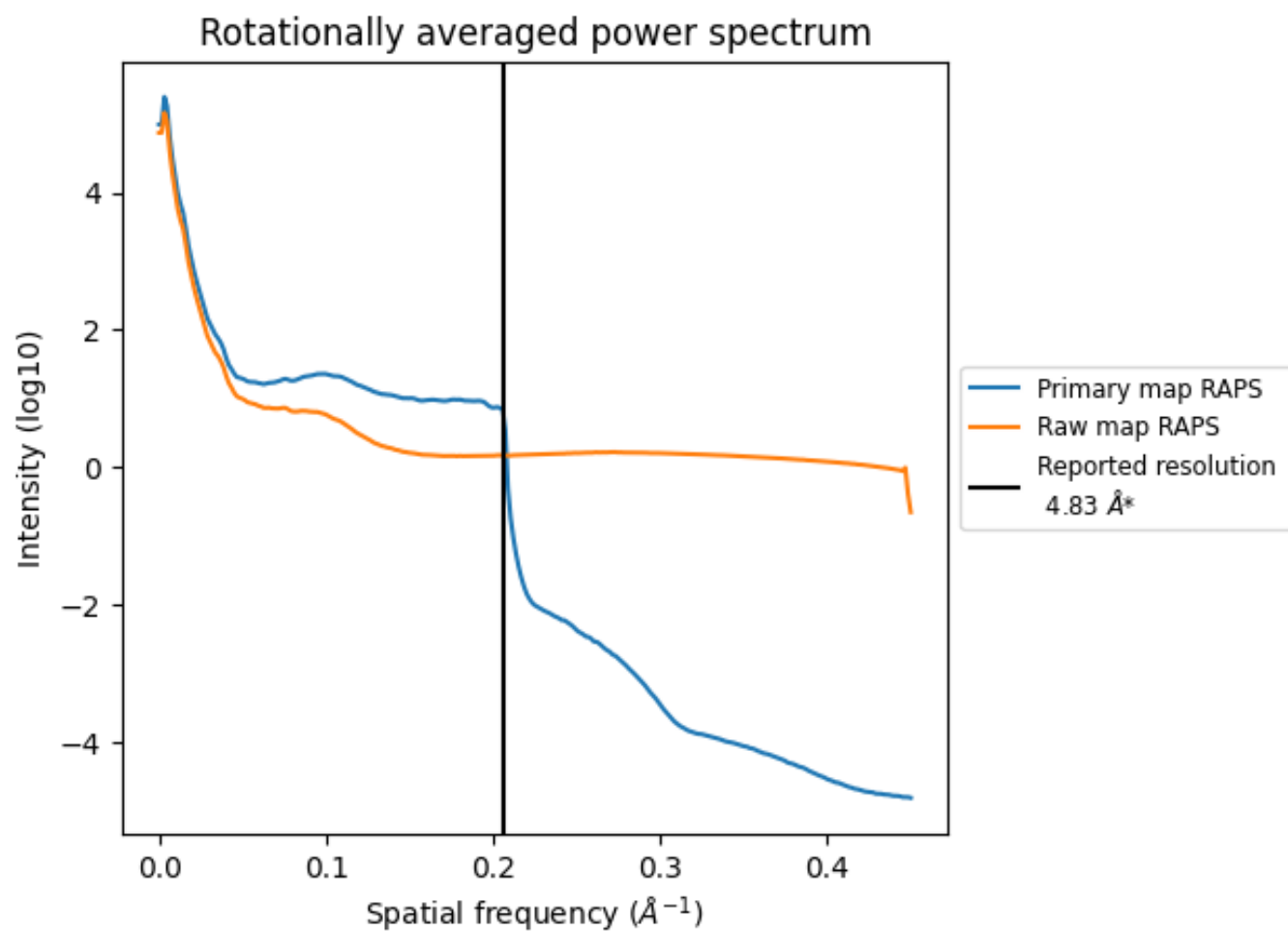
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718 nm³; this corresponds to an approximate mass of 648 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 ⓘ

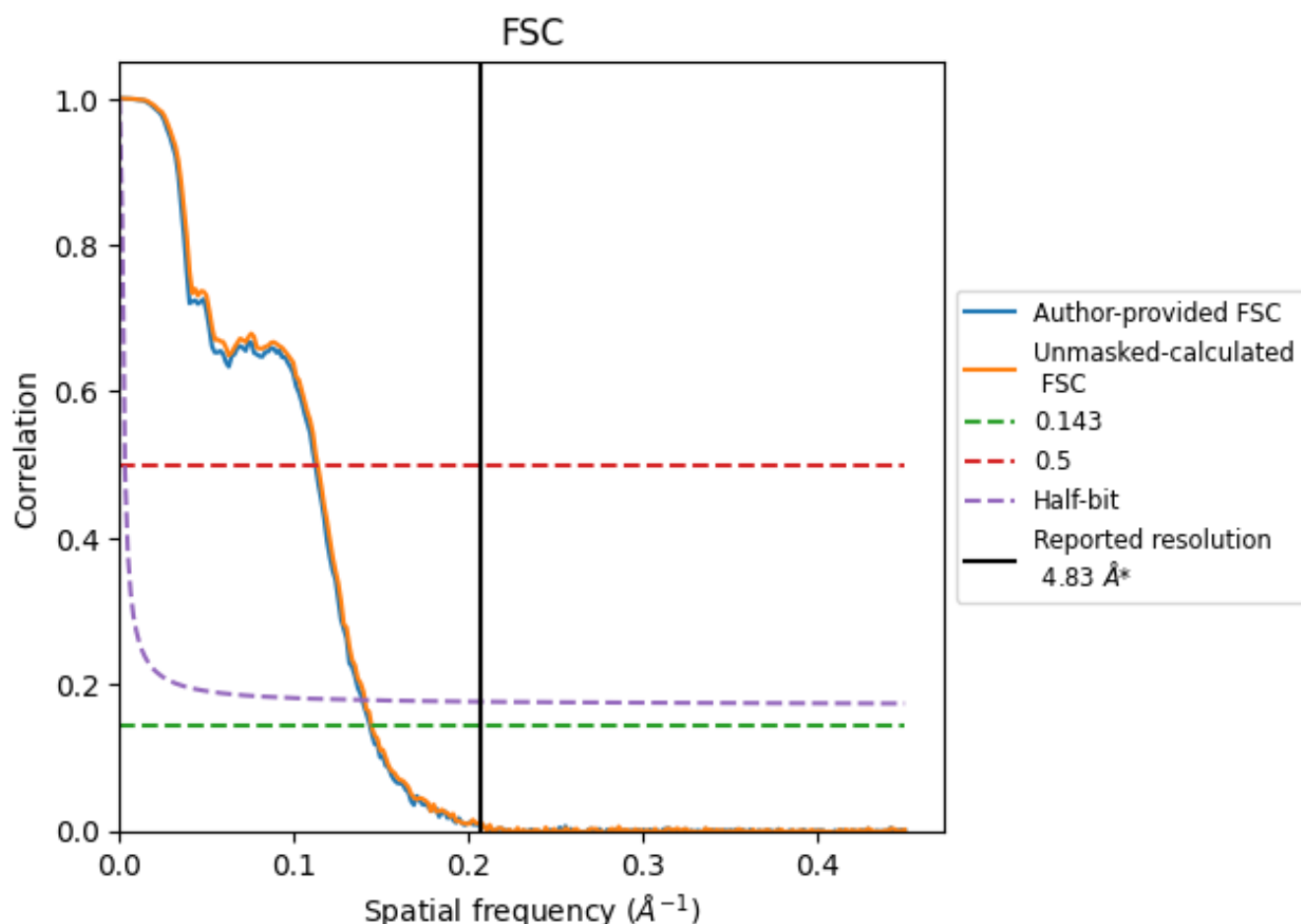


*Reported resolution corresponds to spatial frequency of 0.207\AA^{-1}

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 0.207 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.83	-	-
Author-provided FSC curve	6.96	8.90	7.18
Unmasked-calculated*	6.92	8.80	7.11

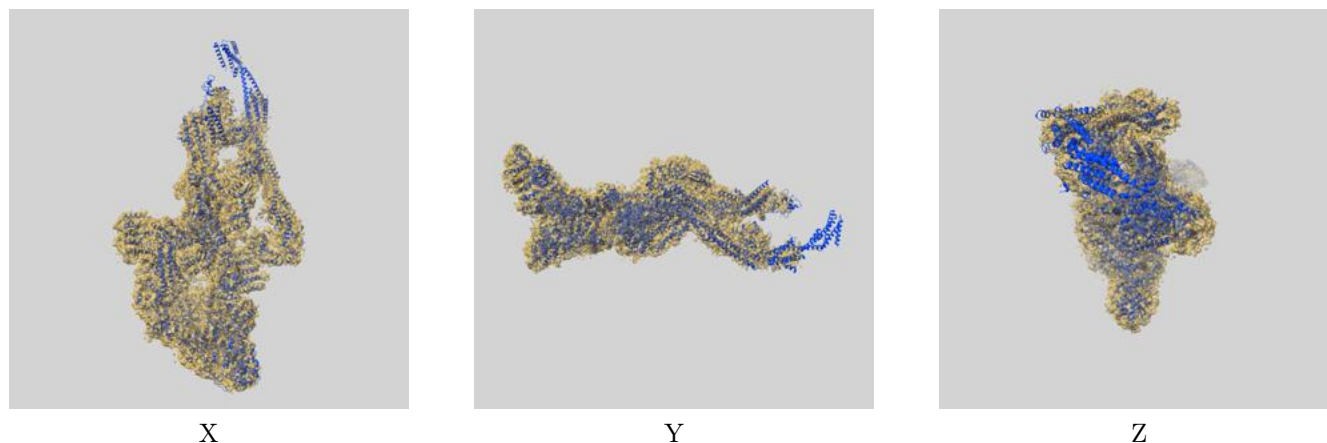
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 4.83 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.92 differs from the reported value 4.83 by more than 10 %

9 Map-model fit [i](#)

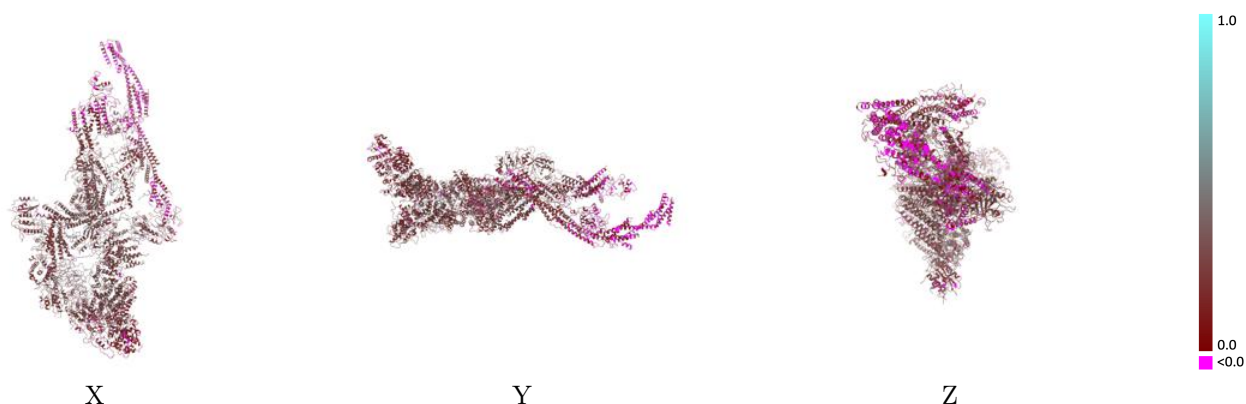
This section contains information regarding the fit between EMDB map EMD-40971 and PDB model 8T1L. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



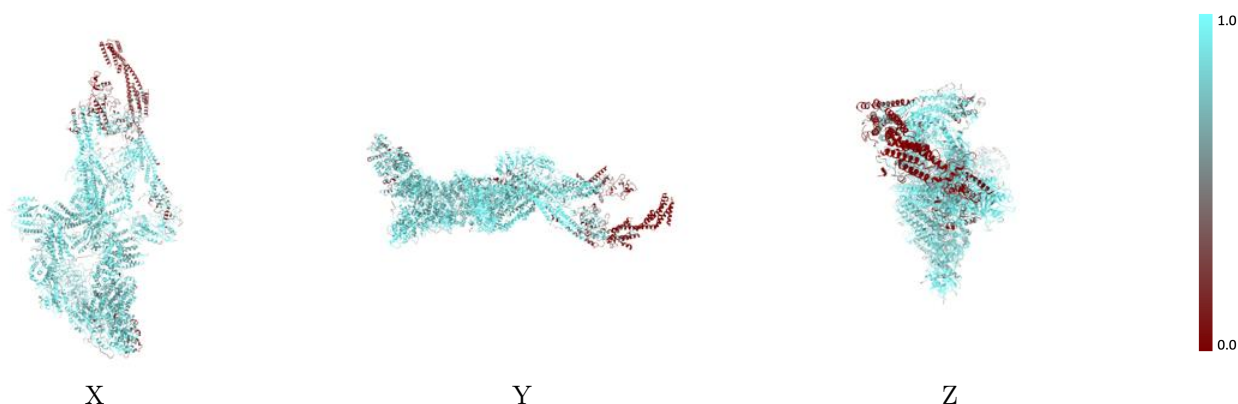
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



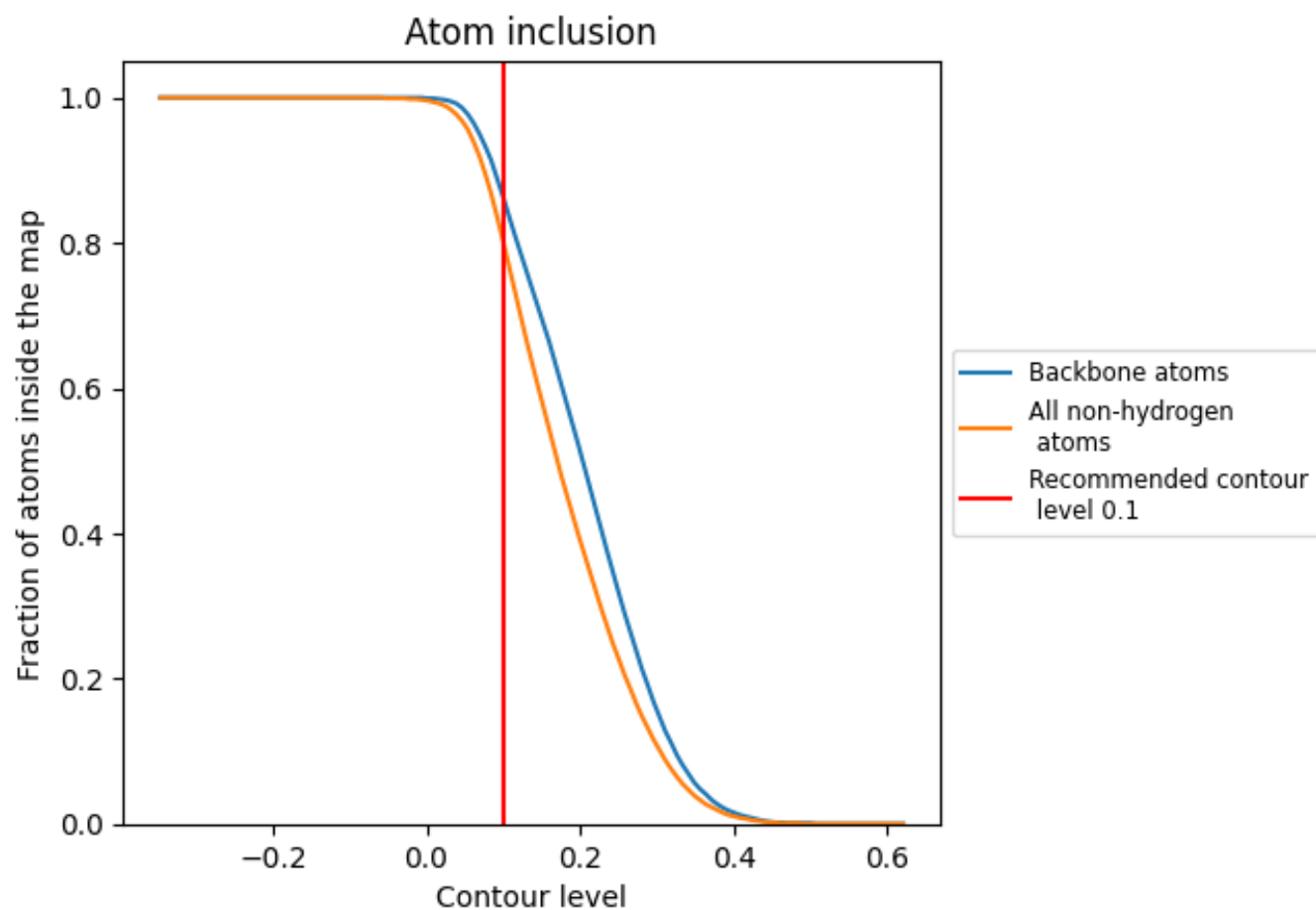
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.2470
9	 0.4750	 0.1650
A	 0.8390	 0.2250
B	 0.6940	 0.1400
C	 0.4310	 0.1550
D	 0.4160	 0.0960
E	 0.4980	 0.1370
F	 0.7490	 0.1570
G	 0.0430	 0.0540
H	 0.7920	 0.2050
I	 0.8130	 0.2680
J	 0.8700	 0.2860
K	 0.8660	 0.2830
L	 0.8260	 0.2780
M	 0.9250	 0.2940
O	 0.9420	 0.3050
P	 0.4470	 0.1080
Q	 0.8040	 0.2150
R	 0.8090	 0.2300
S	 0.8670	 0.2700
T	 0.8990	 0.2750
V	 0.9020	 0.3150
W	 0.8860	 0.2840
X	 0.8740	 0.2650
Y	 0.8510	 0.2470
Z	 0.6300	 0.1590
a	 0.8900	 0.2320

