Full wwPDB EM Validation Report

Feb 25, 2023 – 01:42 PM EST

PDB ID	:	7UIF
EMDB ID	:	EMD-26544
Title	:	Mediator-PIC Early (Core B)
Authors	:	Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on	:	2022-03-29
Resolution	:	4.60 Å(reported)

This is a Full wwPDB EM Validation 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:

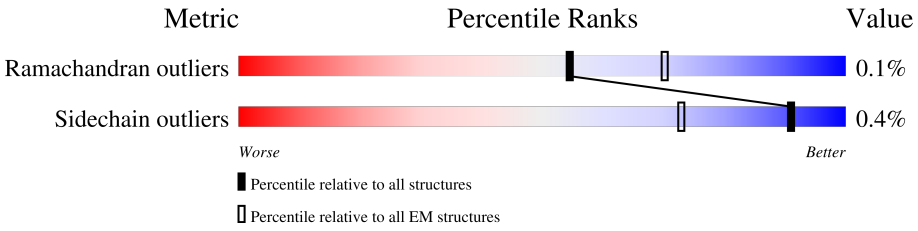
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1733	8% 84% 16%
1	z	1733	99%
2	B	1224	22% 96%
3	C	318	12% 85% 15%
4	D	221	17% 76% 24%
5	E	215	100%
6	F	155	55% 45%
7	G	171	16% 99%
8	H	146	97%

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Mol	Chain	Length	Quality of chain
9	I	122	17% 95% 5%
10	J	70	27% 100%
11	K	120	97%
12	L	70	11% 61% 39%
13	M	345	10% 90%
14	P	735	14% 86%
15	Q	400	13% 31% 69%
16	S	309	9% 58% 41%
17	a	566	26% 63% 36%
18	d	284	21% 60% 40%
19	f	295	28% 57% 43%
20	g	222	33% 75% 24%
21	h	223	22% 61% 39%
22	i	149	5% 55% 44%
23	j	157	65% 93% 7%
24	k	115	16% 94% 6%
25	n	1082	16% 57% 42%
26	q	687	15% 75% 25%
27	r	307	8% 82% 18%
28	s	220	35% 37% 63%
29	t	210	8% 100%
30	u	140	21% 84% 13%
31	v	121	24% 89% 10%
32	w	127	44% 81% 19%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 63137 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1453	Total	C	N	O	S	0	0
			11425	7192	1995	2176	62		
1	z	25	Total	C	N	O		0	0
			184	116	25	43			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	141	Total	C	N	O	S	0	0
			1126	706	189	226	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			943	580	171	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 16 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	169	Total	C	N	O	S	0	0
			1409	903	238	263	5		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	h	136	Total	C	N	O	S	0	0
			1126	709	199	215	3		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	83	Total	C	N	O	S	0	0
			709	444	130	134	1		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	j	146	Total	C	N	O	S	0	0
			1173	725	206	239	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	k	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	n	625	Total	C	N	O	S	0	0
			5139	3318	884	913	24		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

- Molecule 27 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	t	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 30 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	u	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 31.

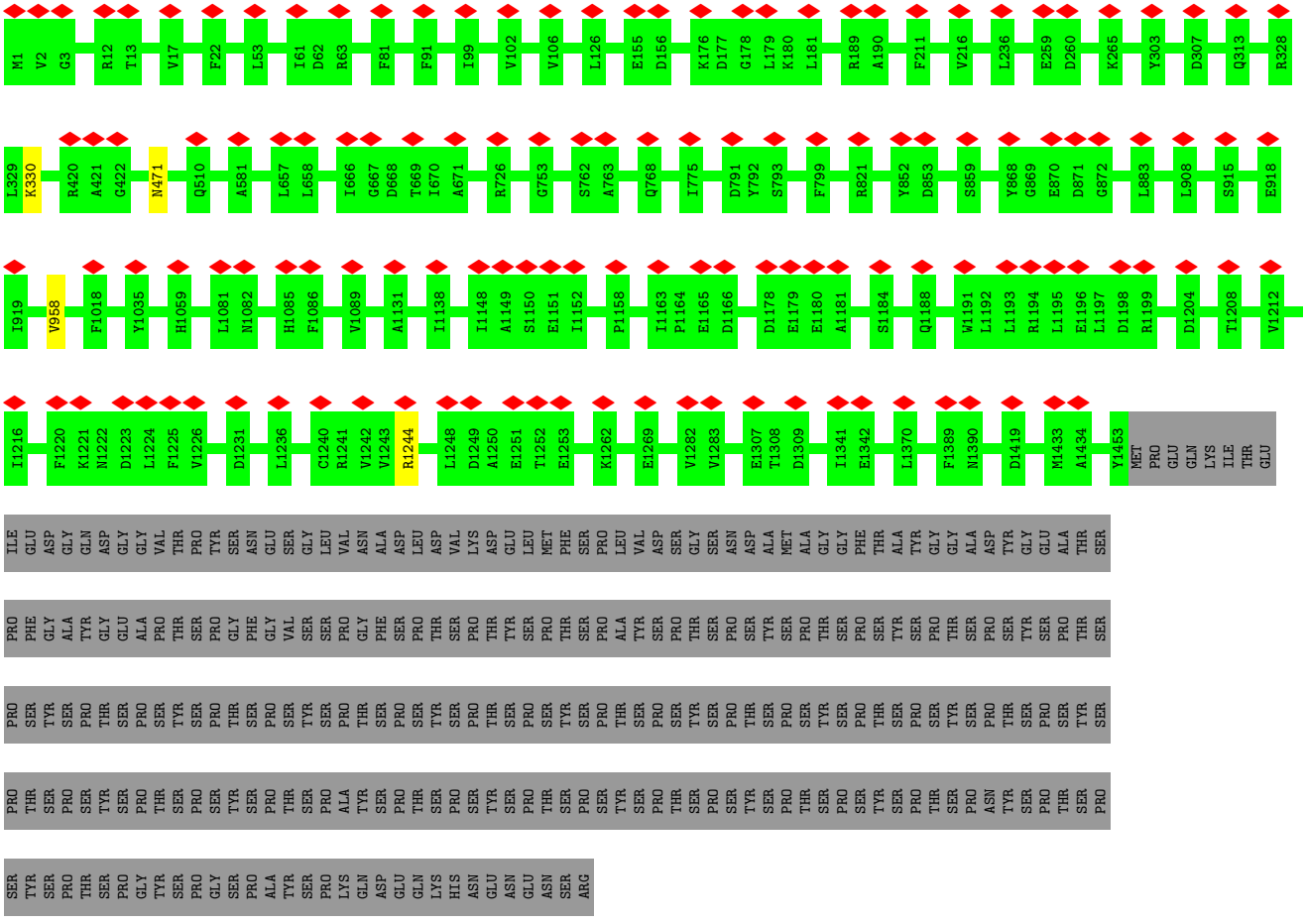
Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

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.

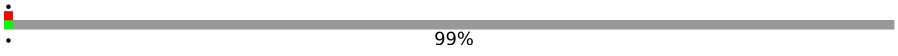
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain z:



ILE ASP ARG ASN LEU LYS CYS GLN THR CYS GLN GLU GLY MET ASN GLU CYS PRO GLY HIS PHE GLY HIS ILE ASP LEU ALA LYS PRO VAL PHE HIS VAL GLY PHE ILE ALA LYS ILE LYS LYS VAL CYS GLU CYS VAL CYS MET HIS CYS GLY LYS LEU LEU LEU ASP GLU HIS ASN GLU

LEU MET ARG GLN ALA LEU ALA ILE LYS ASP SER LYS LYS ARG PHE ALA ALA ILE TRP THR LEU CYS LYS THR LYS MET VAL CYS GLU THR ASP VAL PRO SER GLU ASP ASP PRO THR GLN LEU VAL SER ARG GLY GLY CYS GLY ASN THR GLN PRO THR ILE ARG LYS ASP GLY LEU LYS

LEU VAL GLY SER TRP LYS LYS ASP ARG ALA THR GLY ASP ALA ASP GLU PRO GLU LEU ARG VAL LEU SER THR GLU GLU ILE LEU ASN ILE PHE LYS HIS ILE SER VAL LYS ASP PHE THR SER LEU GLY PHE ASN GLU VAL PHE SER ARG PRO GLU TRP MET ILE LEU THR CYS LEU PRO

VAL PRO PRO PRO PRO VAL ARG PRO SER ILE SER PHE ASN GLU SER GLN ARG GLY GLU ASP ASP LEU THR PHE LYS LEU ALA ASP ILE LEU LYS ALA ASN ILE SER LEU GLU THR LEU GLU HIS ASN GLY ALA PRO HIS HIS ALA ILE GLU GLU ALA GLU SER LEU LEU GLN PHE HIS VAL

ALA THR TYR MET ASP ASN ASP ILE ALA GLY GLN PRO GLN ALA LEU GLN LYS SER GLY ARG PRO VAL LYS SER ILE ARG ALA ARG LEU LYS GLY LYS GLU GLY ARG ILE ARG GLY ASN LEU MET GLY LYS ARG VAL ASP PHE SER ALA ARG THR VAL ILE SER GLY ASP PRO ASN LEU GLU

LEU ASP GLN VAL GLY VAL PRO LYS SER ILE ALA LYS THR LEU THR TYR PRO GLU VAL VAL THR PRO TYR ASN ILE ASP ARG LEU THR GLN LEU VAL ARG ASN GLY PRO ASN GLU HIS PRO GLY ALA LYS TYR VAL ILE ARG ASP SER GLY ASP ARG ILE ASP LEU ARG TYR SER LYS ARG

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

ASP PHE ASP GLY ASP GLU MET ASN LEU HIS VAL PRO GLN SER GLU GLU THR ARG ALA GLU LEU SER GLN LEU CYS ALA VAL PRO LEU GLN ILE VAL SER PRO GLN SER ASN LYS PRO CYS MET GLY ILE VAL GLN ASP THR LEU CYS GLY ILE ARG LYS LEU THR LEU ARG ASP THR PHE

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

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

GLY PHE SER THR GLY ILE GLY ASP THR ILE ALA ASP GLY PRO THR MET ARG GLU ILE THR GLU THR ILE ALA GLU ALA LYS LYS LYS VAL LEU ASP VAL THR LYS GLU ALA GLN ALA ASN LEU LEU THR ALA LYS HIS GLY MET THR LEU ARG GLU SER PHE GLU ASP ASN VAL VAL ARG

PHE LEU ASN GLU ALA ARG ASP LYS ALA GLY ARG LEU ALA GLU VAL ASN LEU LYS ASP LEU ASN ASN VAL LYS GLN MET VAL MET ALA GLY SER LYS GLY SER PHE ILE ASN ILE ALA GLN MET SER ALA CYS VAL GLY GLN GLN SER VAL GLU GLY LYS ARG ILE ALA PHE GLY PHE VAL

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

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

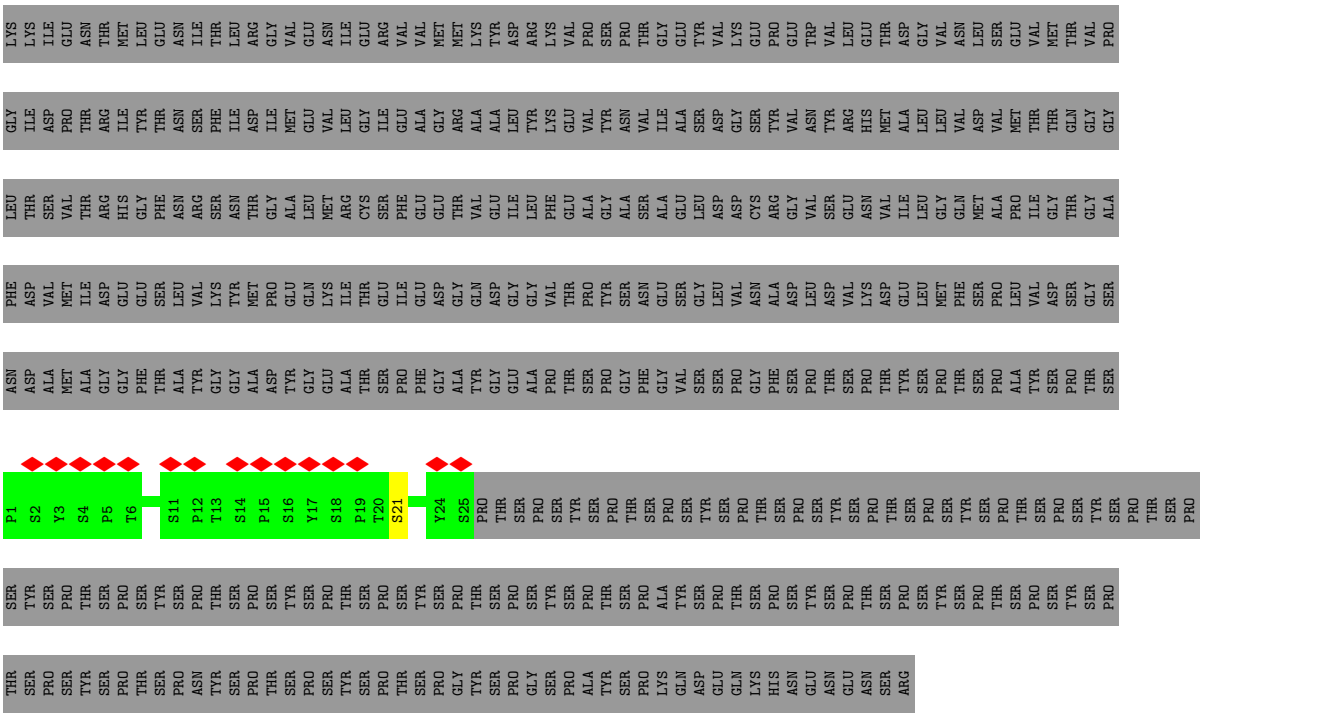
ARG ARG ILE ILE GLN ASN ALA GLN GLN THR PHE HIS ILE ASP HIS THR LYS PRO SER ASP LEU THR ILE LYS ASP ILE VAL LEU GLY VAL LYS ASP LEU GLN GLU ASN LEU LEU VAL LEU ARG GLY LYS ASN GLU ILE ILE GLN ASN ALA GLN ARG ASP ALA VAL THR LEU PHE CYS CYS

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

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

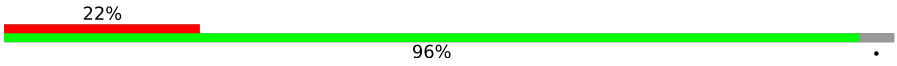
THR THR LEU LYS SER VAL THR ILE ALA SER GLU ILE TYR TYR ASP PRO ASP PRO ARG SER THR VAL ILE PRO GLU ASP GLU GLU ILE ILE GLN LEU HIS PHE SER LEU LEU ASP GLU GLU ALA GLU GLN SER PHE ASP GLN GLN SER PRO TRP LEU LEU ARG LEU GLU LEU ASP ARG ALA

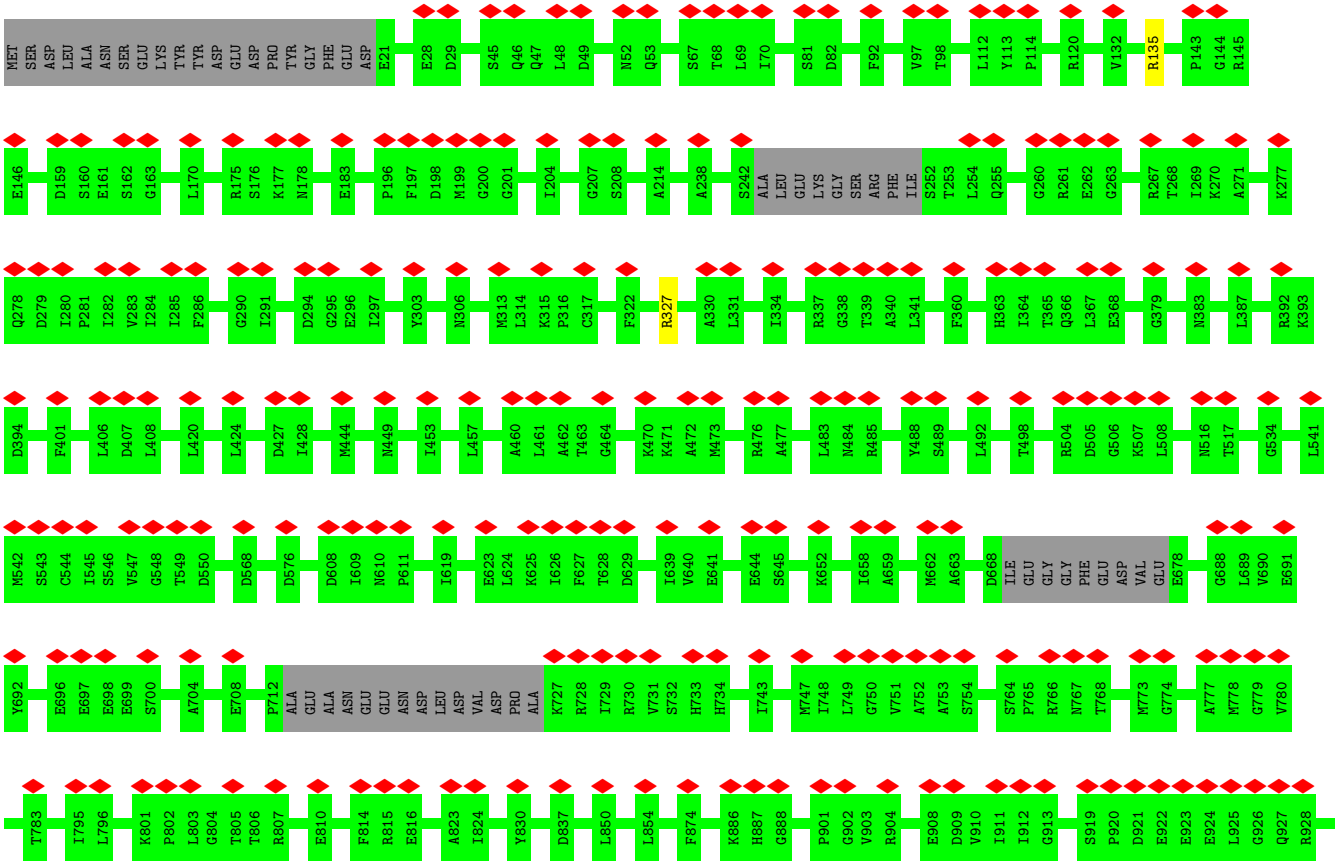
ALA MET ASN ASP LYS ASP LEU THR MET GLY GLN VAL GLY GLU ARG ILE LYS GLN THR PHE LYS ASN ASP LEU PHE VAL ILE TRP SER GLU ASP ASN ASP GLU LYS LEU ILE ILE ARG CYS ARG VAL VAL ARG PRO LYS SER LEU ASP ALA GLU THR GLU ALA GLU GLU ASP HIS MET LEU

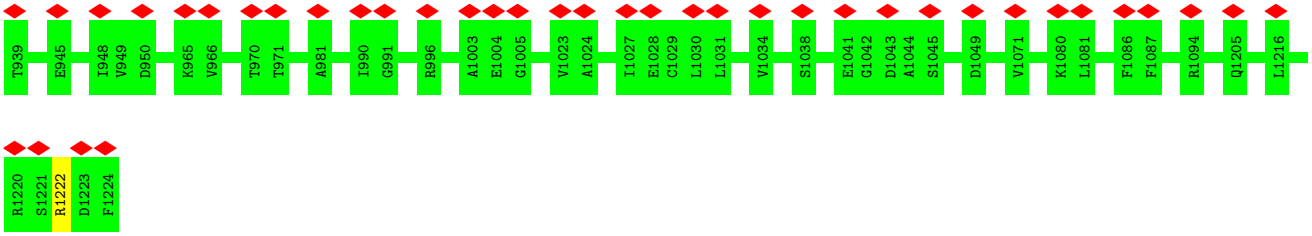


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

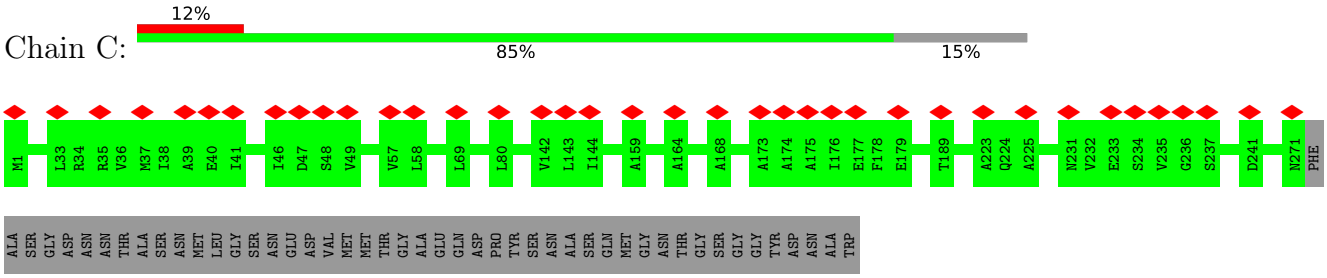
Chain B:



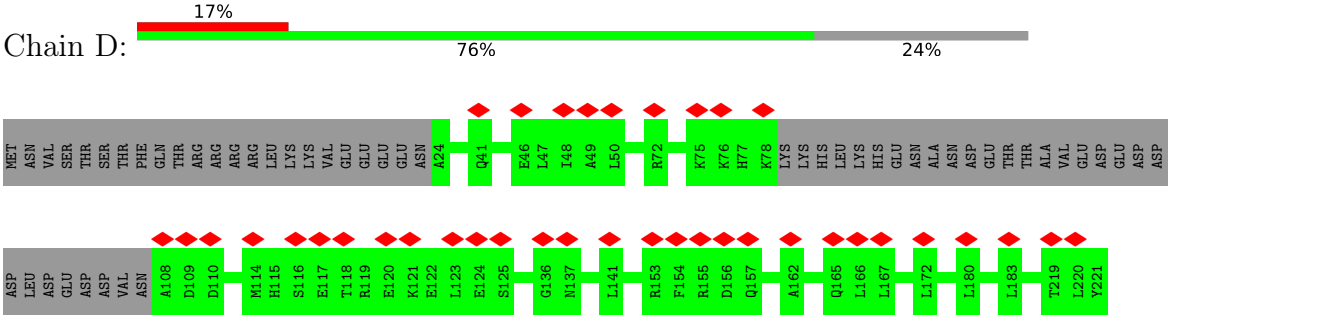




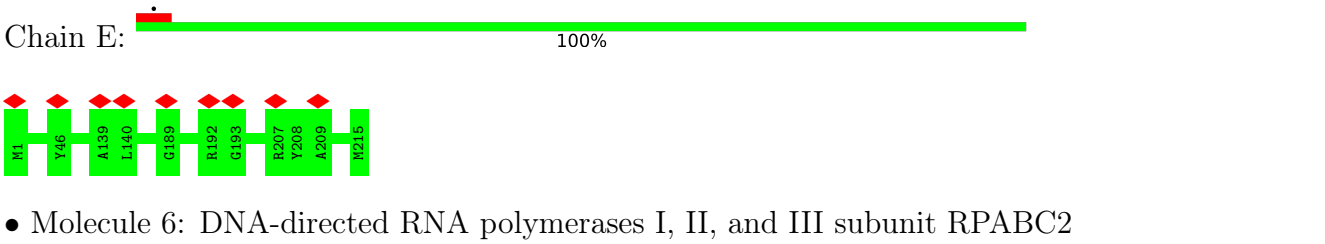
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



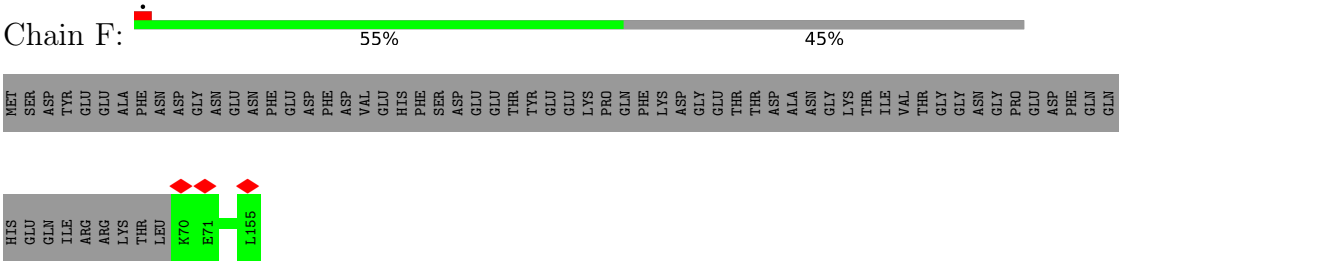
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



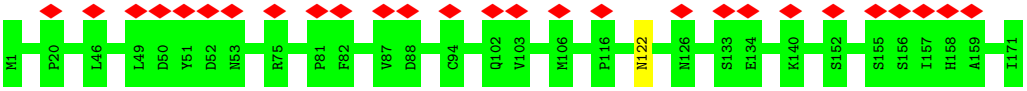
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

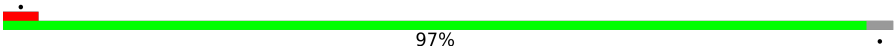


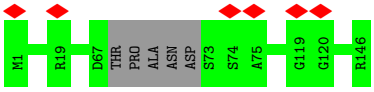
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

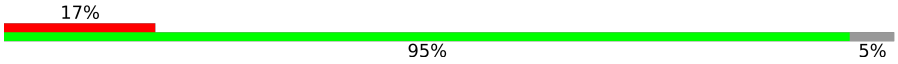
Chain H:

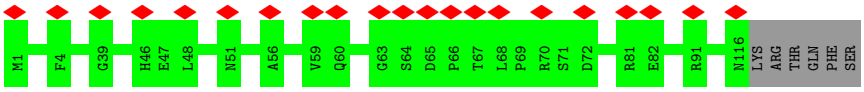




• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

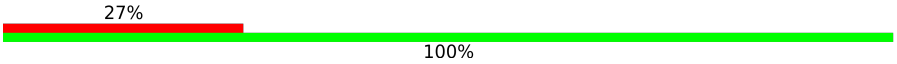
Chain I:

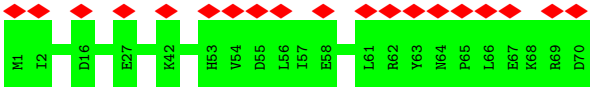




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

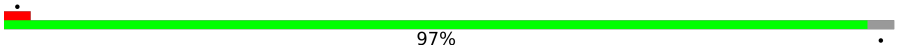
Chain J:

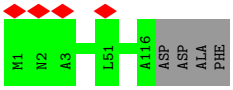




• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

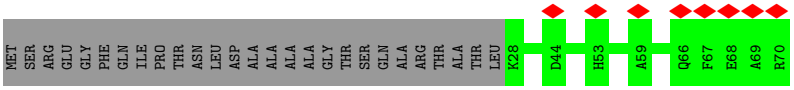
Chain K:





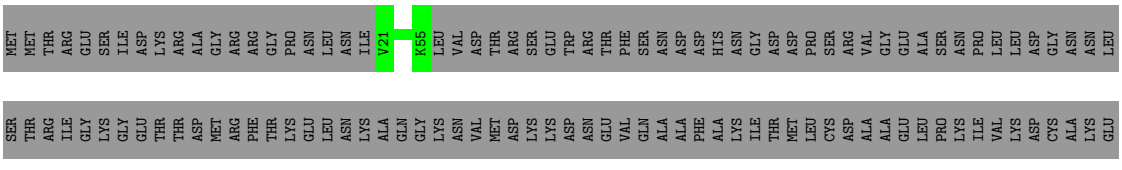
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

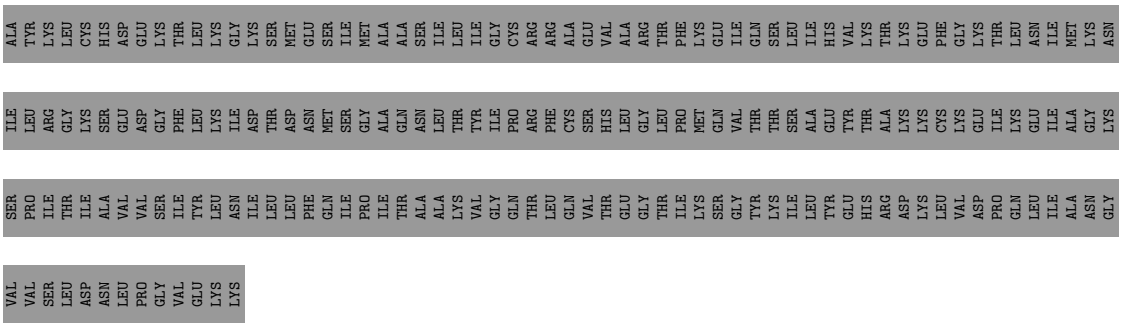
Chain L:



• Molecule 13: Transcription initiation factor IIB

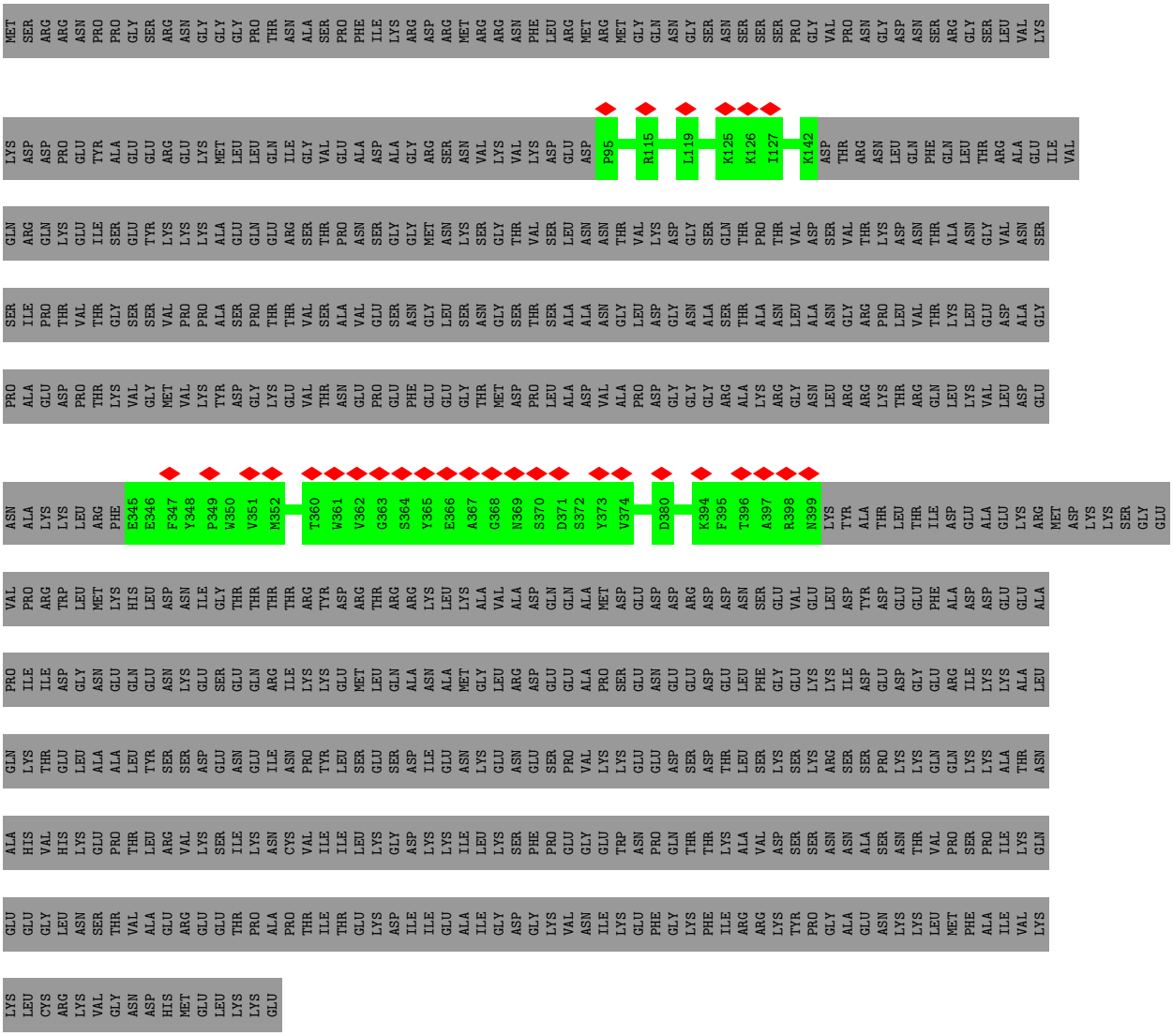
Chain M:





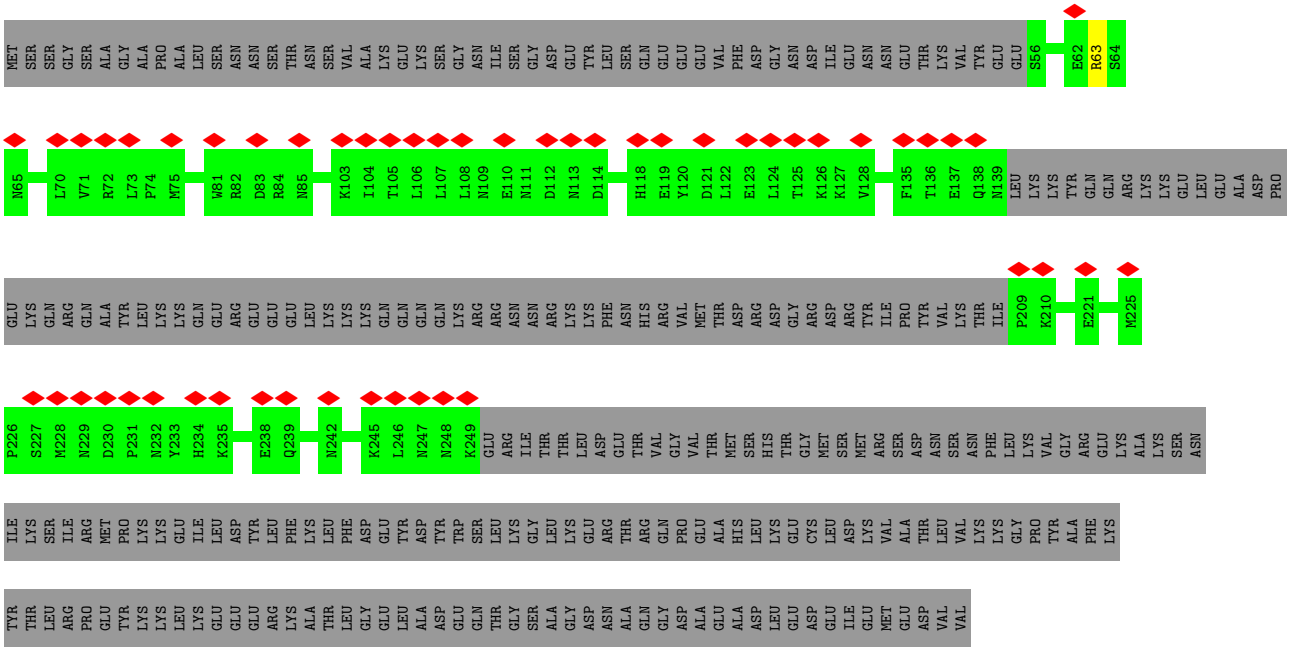
• Molecule 14: Transcription initiation factor IIF subunit alpha

Chain P:

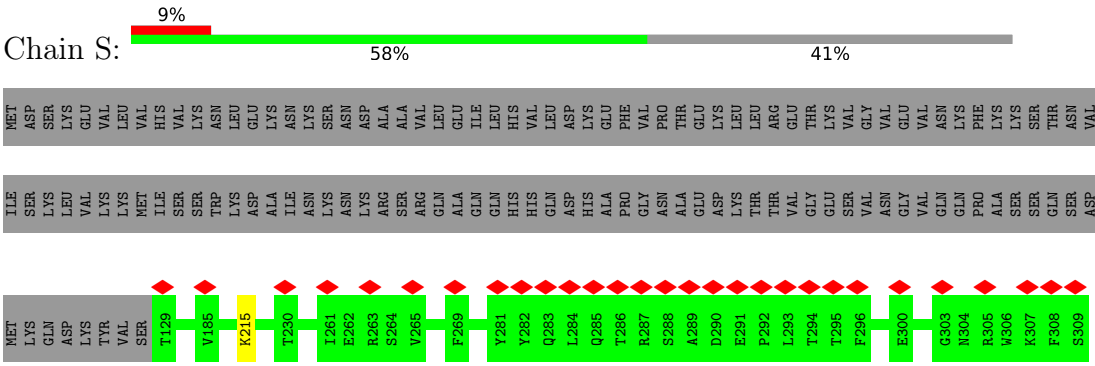


• Molecule 15: Transcription initiation factor IIF subunit beta

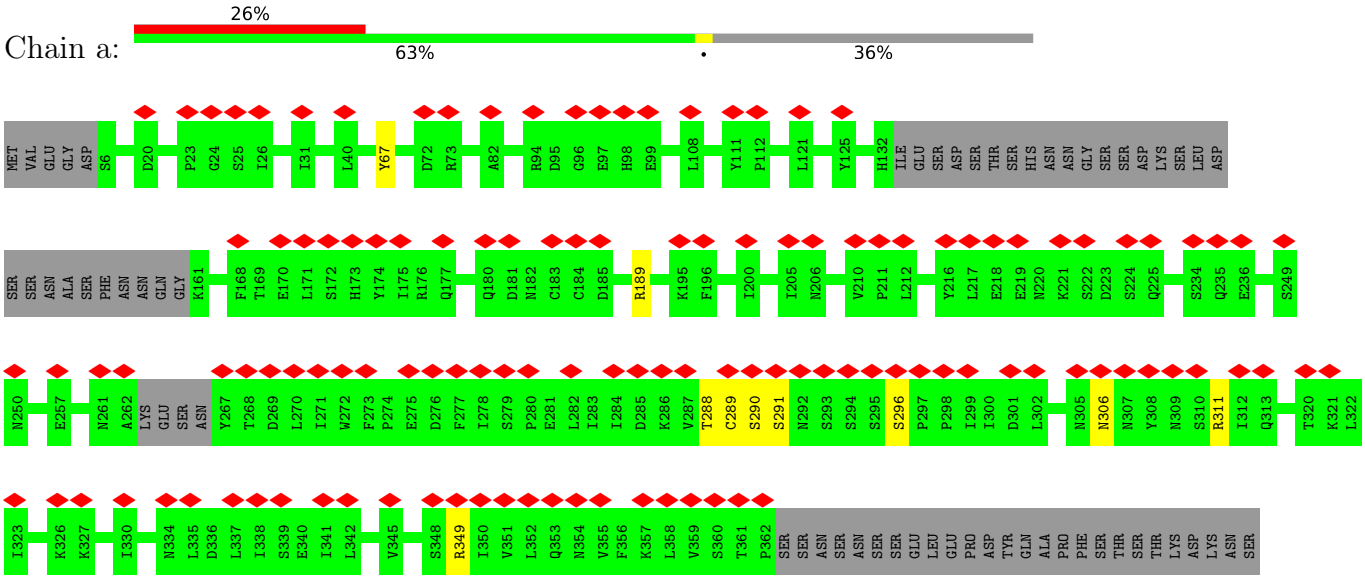
Chain Q:

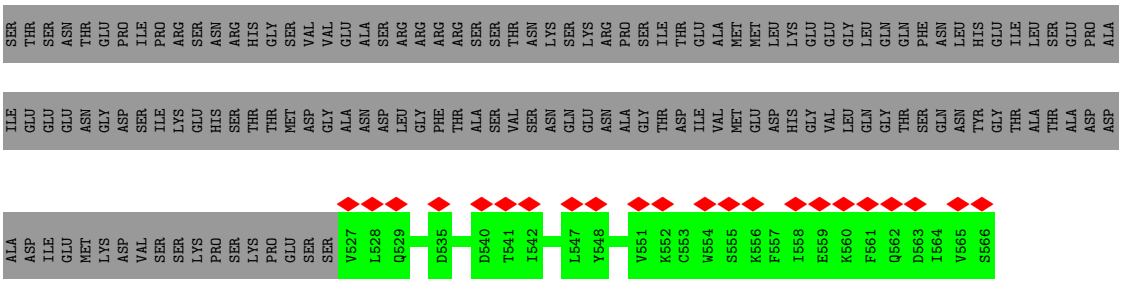


• Molecule 16: Transcription elongation factor S-II



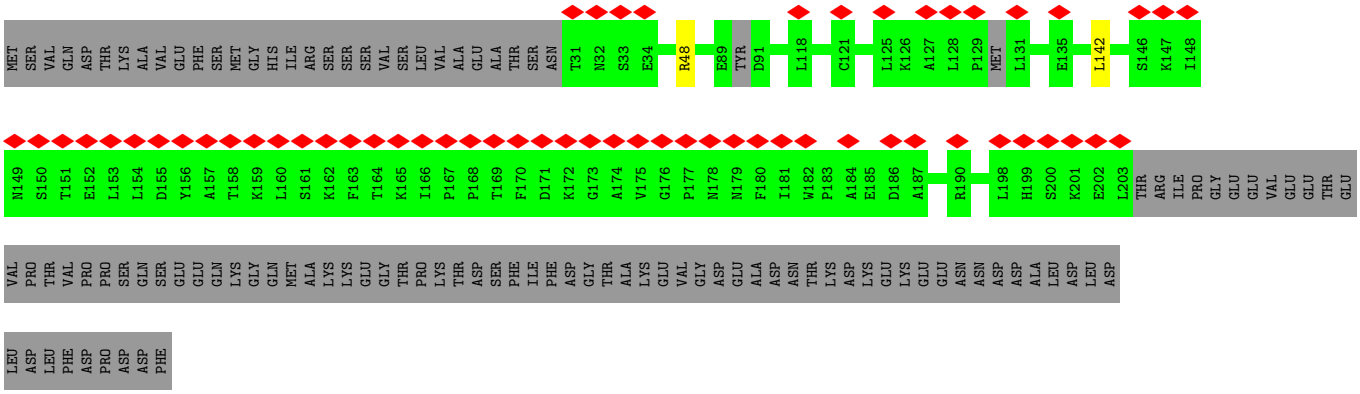
• Molecule 17: Mediator of RNA polymerase II transcription subunit 1





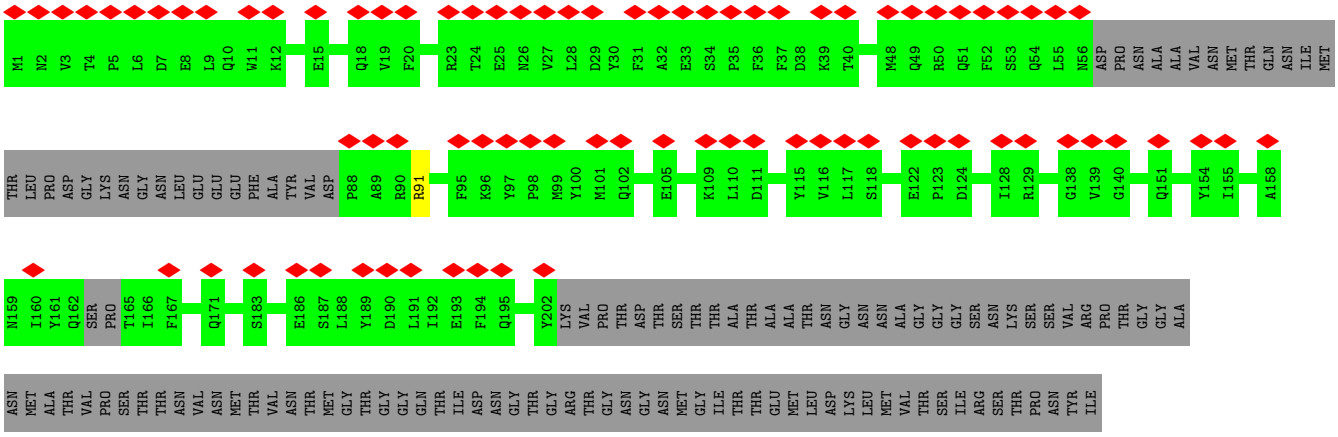
• Molecule 18: Mediator of RNA polymerase II transcription subunit 4

Chain d:



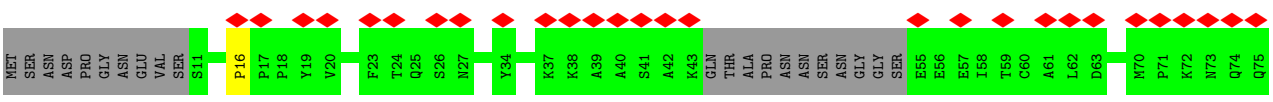
• Molecule 19: Mediator of RNA polymerase II transcription subunit 6

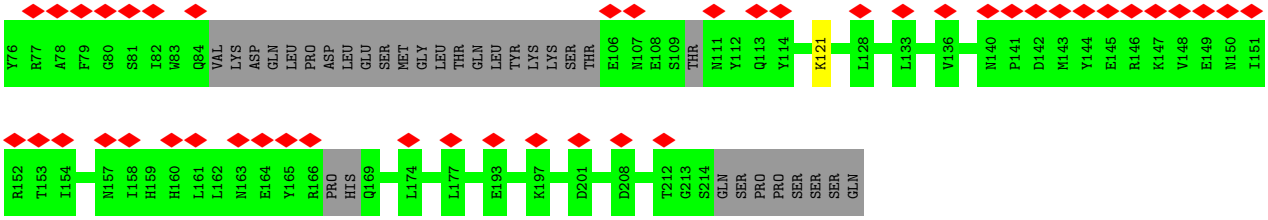
Chain f:



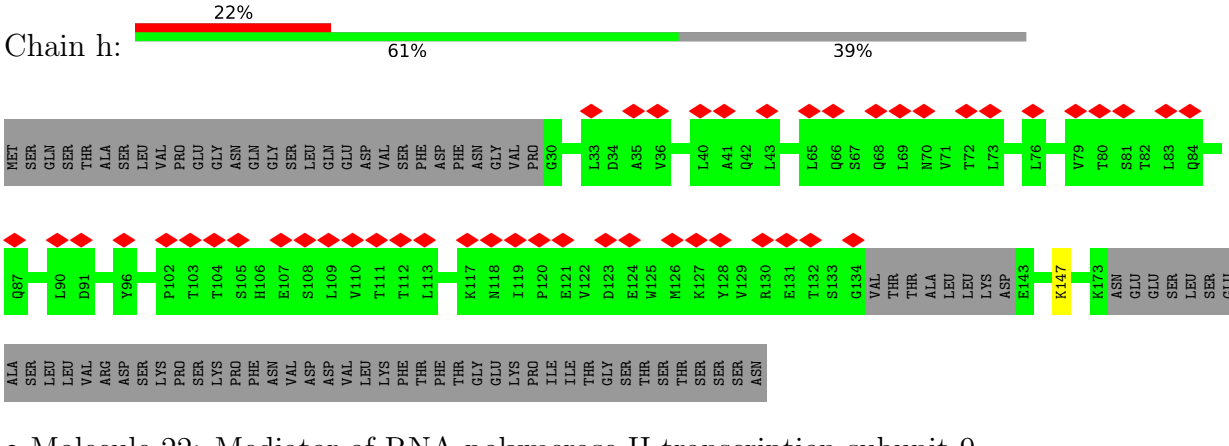
• Molecule 20: Mediator of RNA polymerase II transcription subunit 7

Chain g:

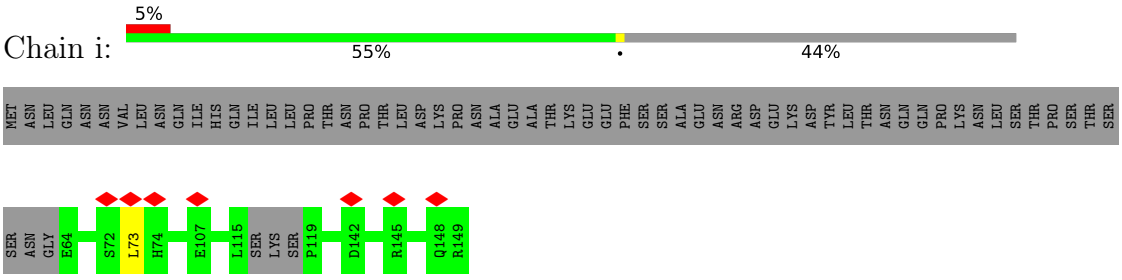




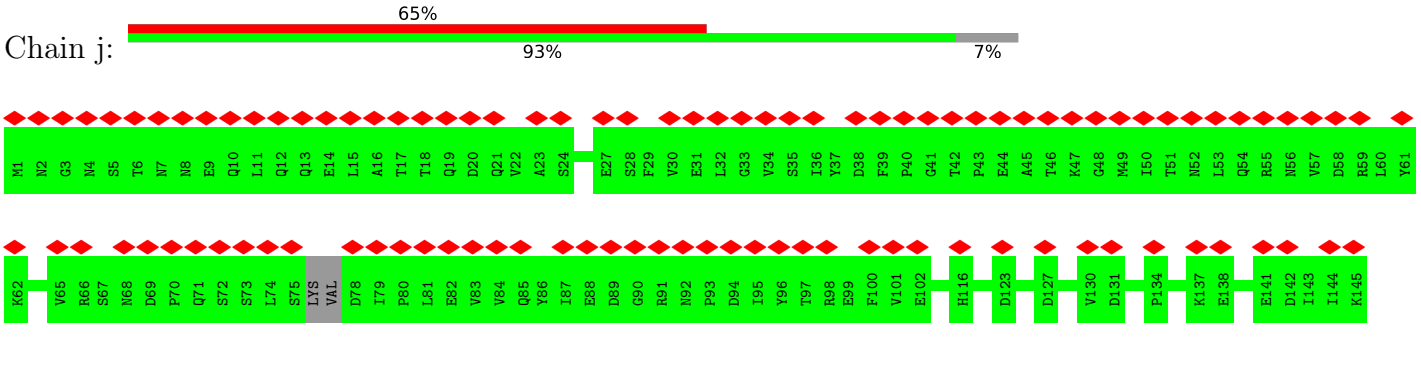
• Molecule 21: Mediator of RNA polymerase II transcription subunit 8



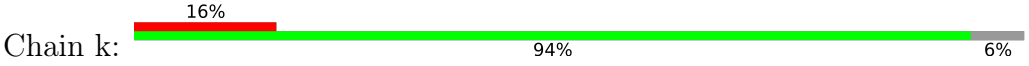
• Molecule 22: Mediator of RNA polymerase II transcription subunit 9

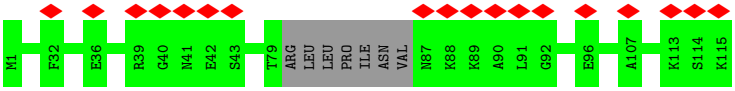


• Molecule 23: Mediator of RNA polymerase II transcription subunit 10



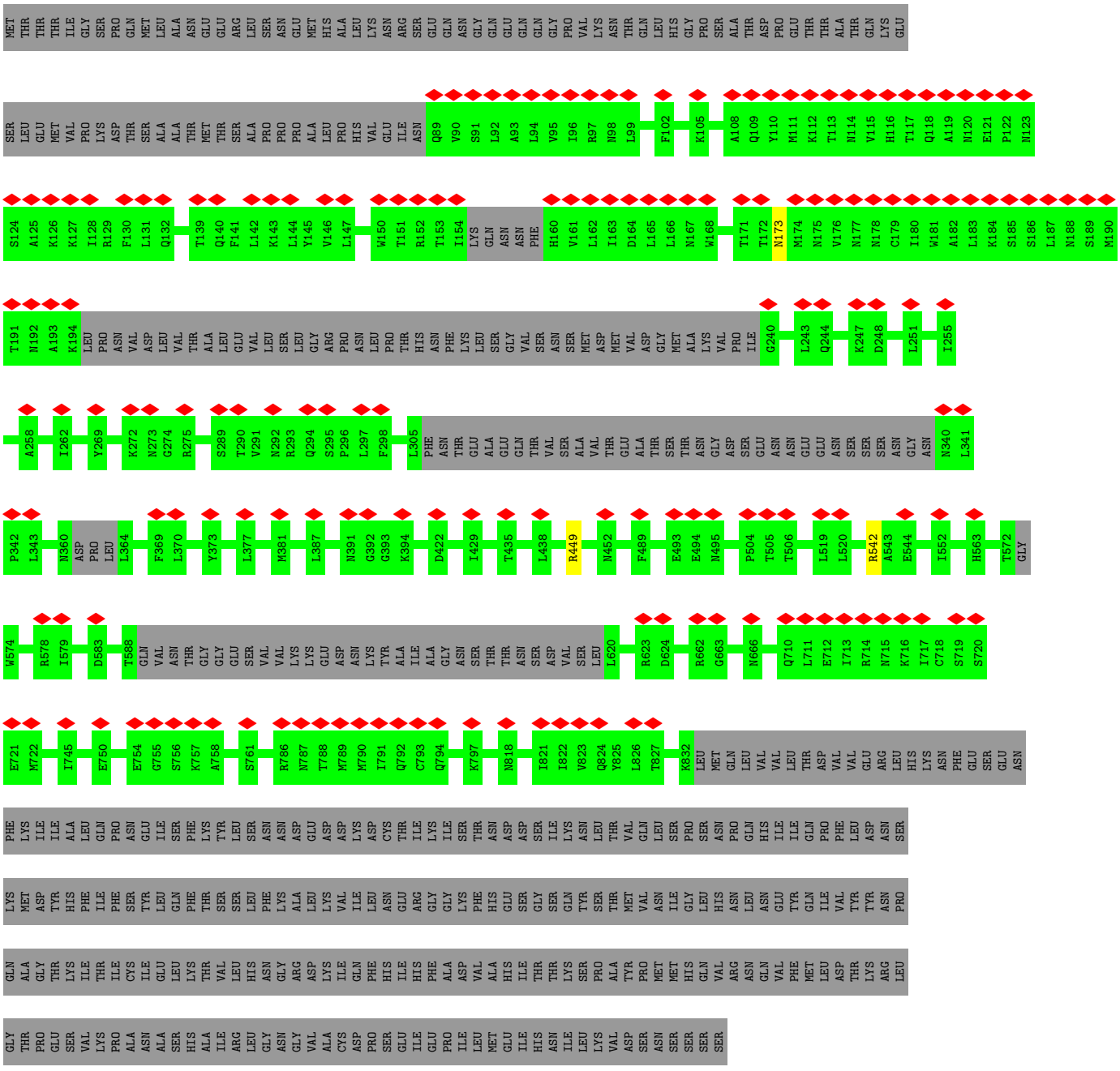
• Molecule 24: Mediator of RNA polymerase II transcription subunit 11





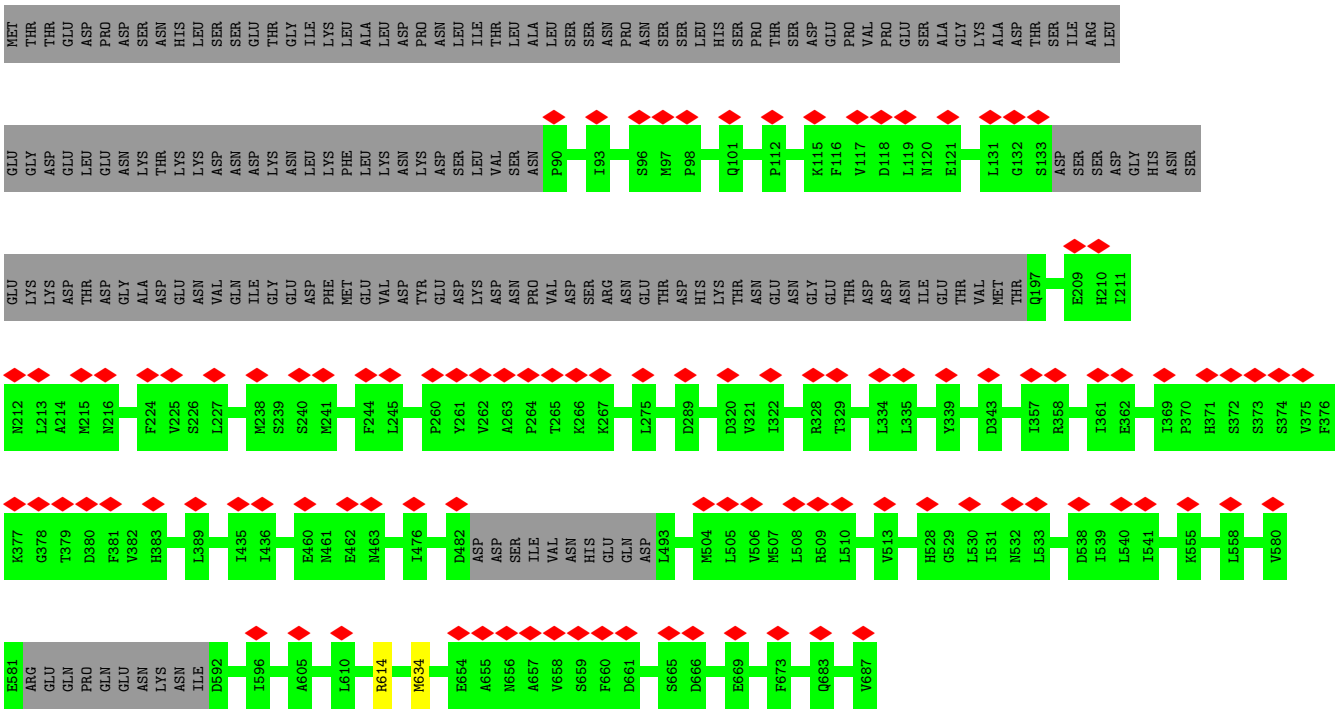
• Molecule 25: Mediator of RNA polymerase II transcription subunit 14

Chain n:



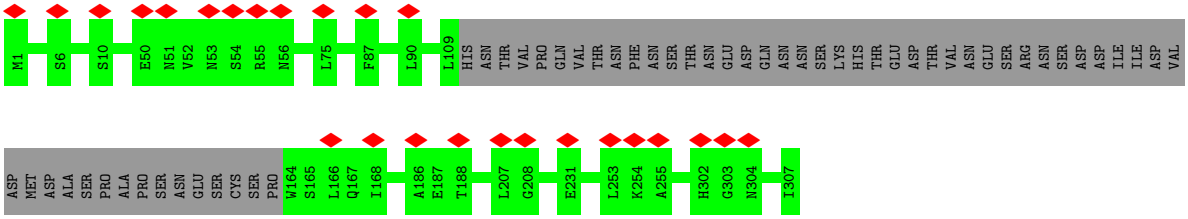
• Molecule 26: Mediator of RNA polymerase II transcription subunit 17

Chain q:



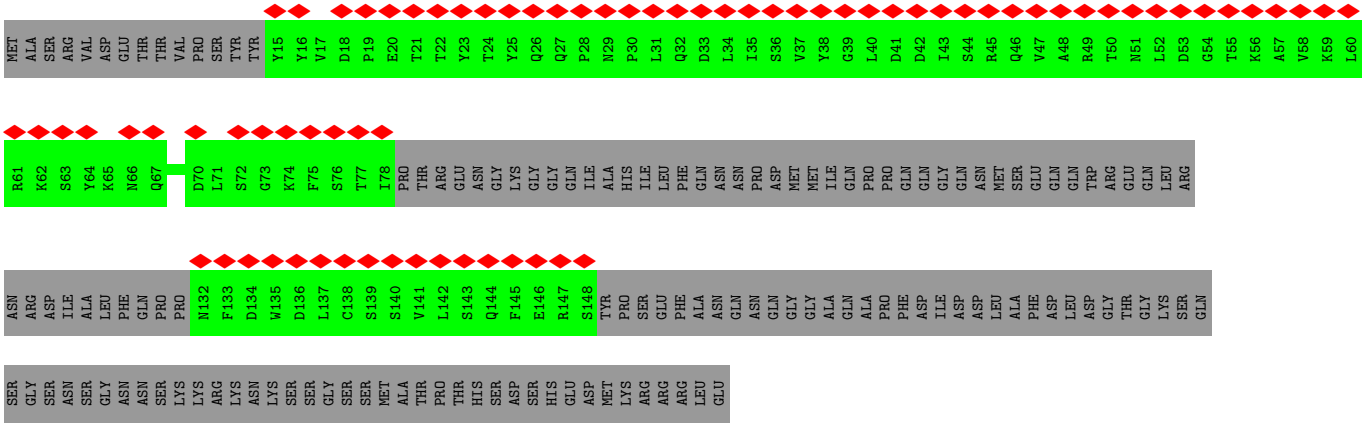
• Molecule 27: Mediator of RNA polymerase II transcription subunit 18

Chain r:



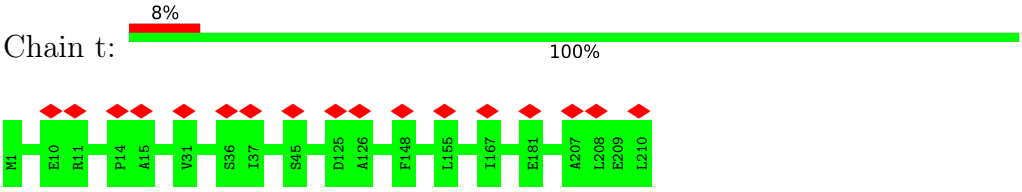
• Molecule 28: Mediator of RNA polymerase II transcription subunit 19

Chain s:



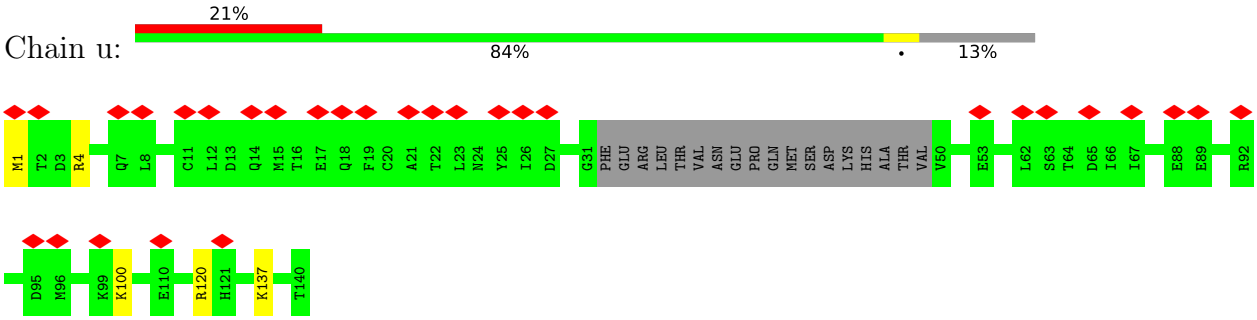
• Molecule 29: Mediator of RNA polymerase II transcription subunit 20

Chain t:



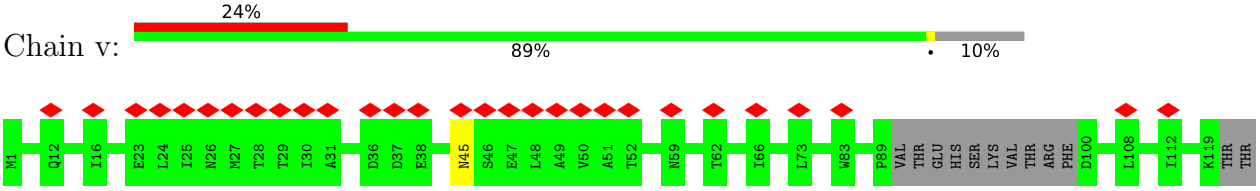
• Molecule 30: Mediator of RNA polymerase II transcription subunit 21

Chain u:



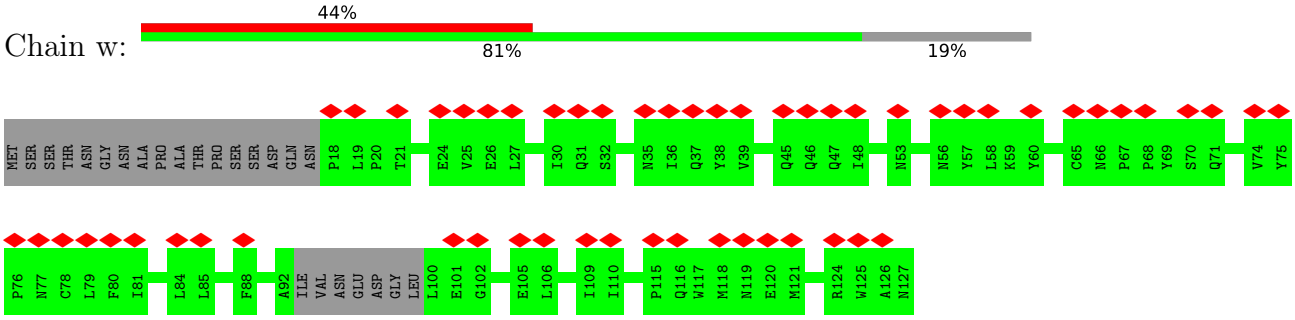
• Molecule 31: Mediator of RNA polymerase II transcription subunit 22

Chain v:



• Molecule 32: Mediator of RNA polymerase II transcription subunit 31

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	A	0.28	0/11632	0.51	0/15735
1	z	0.25	0/194	0.40	0/270
2	B	0.27	0/9520	0.52	0/12839
3	C	0.27	0/2171	0.50	0/2941
4	D	0.24	0/1365	0.44	0/1831
5	E	0.26	0/1796	0.49	0/2416
6	F	0.27	0/709	0.50	0/956
7	G	0.26	0/1368	0.49	0/1844
8	H	0.28	0/1144	0.53	0/1548
9	I	0.25	0/961	0.55	0/1294
10	J	0.29	0/587	0.57	0/786
11	K	0.28	0/947	0.51	0/1279
12	L	0.25	0/346	0.61	0/457
13	M	0.26	0/267	0.47	0/362
14	P	0.25	0/886	0.47	0/1198
15	Q	0.24	0/1049	0.48	0/1413
16	S	0.25	0/1462	0.48	0/1973
17	a	0.65	0/3067	0.86	4/4148 (0.1%)
18	d	0.27	0/1405	0.58	1/1889 (0.1%)
19	f	0.27	0/1440	0.50	0/1946
20	g	0.28	0/1434	0.50	1/1930 (0.1%)
21	h	0.26	0/1147	0.55	0/1552
22	i	0.26	0/720	0.63	1/965 (0.1%)
23	j	0.24	0/1188	0.45	0/1604
24	k	0.27	0/885	0.49	0/1183
25	n	0.24	0/5226	0.46	0/7051
26	q	0.26	0/4245	0.49	0/5702
27	r	0.26	0/2030	0.50	0/2747
28	s	0.24	0/669	0.43	0/906
29	t	0.26	0/1635	0.50	0/2215
30	u	0.28	0/984	0.58	0/1317
31	v	0.26	0/873	0.51	0/1177
32	w	0.26	0/897	0.42	0/1219
All	All	0.30	0/64249	0.53	7/86693 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	349	ARG	NE-CZ-NH1	7.26	123.93	120.30
17	a	67	TYR	CB-CG-CD2	-6.29	117.23	121.00
17	a	189	ARG	NE-CZ-NH1	6.23	123.41	120.30
22	i	73	LEU	CA-CB-CG	5.85	128.76	115.30
17	a	311	ARG	NE-CZ-NH1	5.41	123.01	120.30
20	g	16	PRO	CA-N-CD	-5.25	104.16	111.50
18	d	142	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1451/1733 (84%)	1407 (97%)	43 (3%)	1 (0%)	51 85
1	z	23/1733 (1%)	21 (91%)	1 (4%)	1 (4%)	2 25
2	B	1164/1224 (95%)	1132 (97%)	32 (3%)	0	100 100
3	C	269/318 (85%)	261 (97%)	8 (3%)	0	100 100
4	D	165/221 (75%)	163 (99%)	2 (1%)	0	100 100
5	E	213/215 (99%)	210 (99%)	3 (1%)	0	100 100
6	F	84/155 (54%)	83 (99%)	1 (1%)	0	100 100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
9	I	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
10	J	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
11	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
12	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
13	M	33/345 (10%)	33 (100%)	0	0	100	100
14	P	99/735 (14%)	98 (99%)	1 (1%)	0	100	100
15	Q	121/400 (30%)	121 (100%)	0	0	100	100
16	S	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
17	a	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	19	60
18	d	165/284 (58%)	164 (99%)	1 (1%)	0	100	100
19	f	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
20	g	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
21	h	132/223 (59%)	129 (98%)	3 (2%)	0	100	100
22	i	79/149 (53%)	79 (100%)	0	0	100	100
23	j	142/157 (90%)	137 (96%)	5 (4%)	0	100	100
24	k	104/115 (90%)	104 (100%)	0	0	100	100
25	n	611/1082 (56%)	607 (99%)	4 (1%)	0	100	100
26	q	505/687 (74%)	500 (99%)	5 (1%)	0	100	100
27	r	249/307 (81%)	244 (98%)	5 (2%)	0	100	100
28	s	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
29	t	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
30	u	116/140 (83%)	115 (99%)	1 (1%)	0	100	100
31	v	105/121 (87%)	105 (100%)	0	0	100	100
32	w	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
All	All	7715/12992 (59%)	7560 (98%)	150 (2%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	z	21	SER
17	a	291	SER
17	a	306	ASN

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Mol	Chain	Res	Type
17	a	289	CYS
1	A	958	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1268/1520 (83%)	1265 (100%)	3 (0%)	93 96
1	z	25/1520 (2%)	25 (100%)	0	100 100
2	B	1018/1061 (96%)	1015 (100%)	3 (0%)	92 95
3	C	239/274 (87%)	239 (100%)	0	100 100
4	D	150/200 (75%)	150 (100%)	0	100 100
5	E	197/197 (100%)	197 (100%)	0	100 100
6	F	76/137 (56%)	76 (100%)	0	100 100
7	G	152/152 (100%)	151 (99%)	1 (1%)	84 90
8	H	124/128 (97%)	124 (100%)	0	100 100
9	I	110/116 (95%)	110 (100%)	0	100 100
10	J	65/65 (100%)	65 (100%)	0	100 100
11	K	99/102 (97%)	99 (100%)	0	100 100
12	L	38/57 (67%)	38 (100%)	0	100 100
13	M	32/299 (11%)	32 (100%)	0	100 100
14	P	95/641 (15%)	95 (100%)	0	100 100
15	Q	119/363 (33%)	118 (99%)	1 (1%)	81 89
16	S	158/274 (58%)	157 (99%)	1 (1%)	86 92
17	a	350/528 (66%)	347 (99%)	3 (1%)	78 87
18	d	158/258 (61%)	157 (99%)	1 (1%)	86 92
19	f	158/259 (61%)	157 (99%)	1 (1%)	86 92
20	g	160/208 (77%)	159 (99%)	1 (1%)	86 92
21	h	128/207 (62%)	127 (99%)	1 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	i	82/144 (57%)	82 (100%)	0	100	100
23	j	134/145 (92%)	134 (100%)	0	100	100
24	k	101/108 (94%)	101 (100%)	0	100	100
25	n	591/1001 (59%)	588 (100%)	3 (0%)	88	93
26	q	482/642 (75%)	480 (100%)	2 (0%)	91	94
27	r	228/280 (81%)	228 (100%)	0	100	100
28	s	75/195 (38%)	75 (100%)	0	100	100
29	t	178/178 (100%)	178 (100%)	0	100	100
30	u	115/132 (87%)	110 (96%)	5 (4%)	29	54
31	v	101/113 (89%)	100 (99%)	1 (1%)	76	86
32	w	97/117 (83%)	97 (100%)	0	100	100
All	All	7103/11621 (61%)	7076 (100%)	27 (0%)	91	94

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	LYS
1	A	471	ASN
1	A	1244	ARG
2	B	135	ARG
2	B	327	ARG
2	B	1222	ARG
7	G	122	ASN
15	Q	63	ARG
16	S	215	LYS
17	a	288	THR
17	a	290	SER
17	a	296	SER
18	d	48	ARG
19	f	91	ARG
20	g	121	LYS
21	h	147	LYS
25	n	173	ASN
25	n	449	ARG
25	n	542	ARG
26	q	614	ARG
26	q	634	MET
30	u	1	MET

Continued on next page...

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Mol	Chain	Res	Type
30	u	4	ARG
30	u	100	LYS
30	u	120	ARG
30	u	137	LYS
31	v	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	445	ASN
1	A	811	GLN
1	A	1211	GLN
7	G	122	ASN
7	G	131	GLN
14	P	359	ASN
16	S	166	HIS
17	a	177	GLN
17	a	235	GLN
19	f	10	GLN
21	h	150	GLN
24	k	19	GLN
25	n	715	ASN
30	u	9	GLN
30	u	98	GLN

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 monosaccharides 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
26	q	1
30	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	C	319:LYS	N	5.82
1	u	80:LEU	C	81:PRO	N	3.17

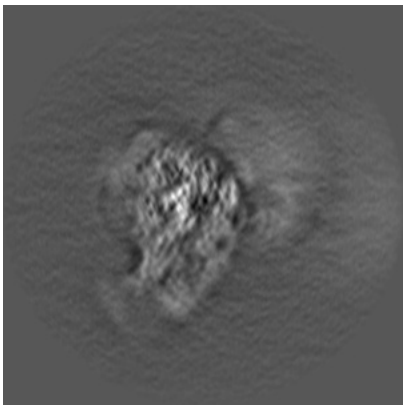
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26544. These allow visual inspection of the internal detail of the map and identification of artifacts.

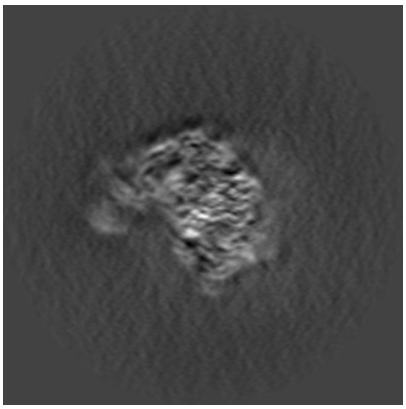
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

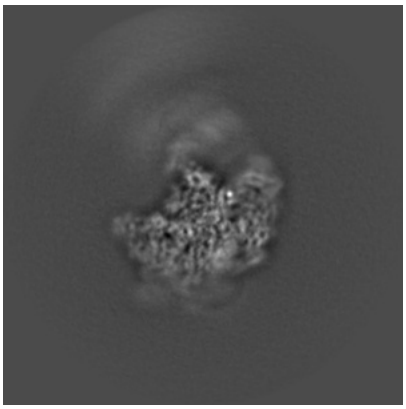
6.1.1 Primary map



X

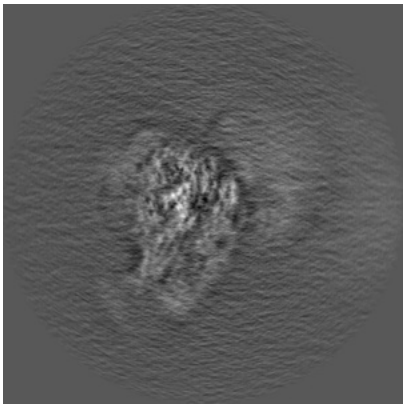


Y

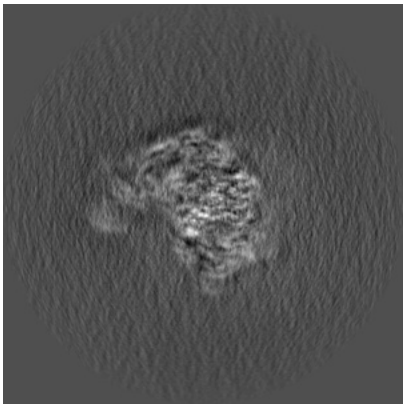


Z

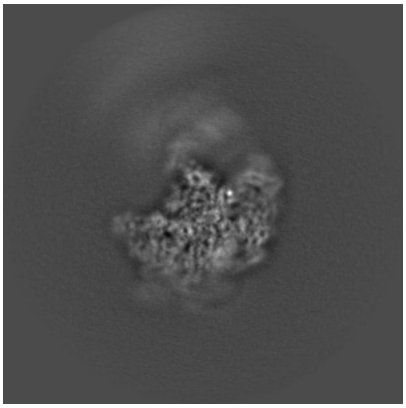
6.1.2 Raw map



X



Y

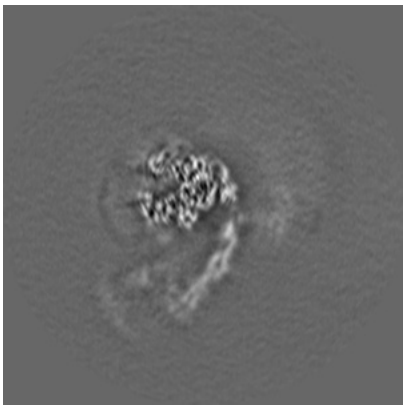


Z

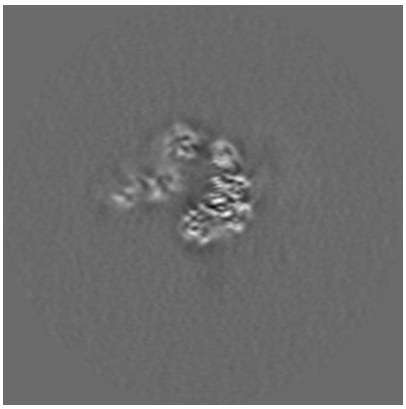
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

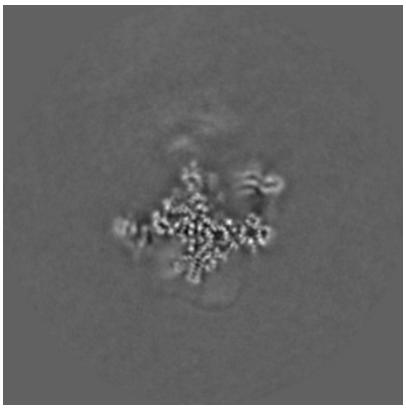
6.2.1 Primary map



X Index: 180

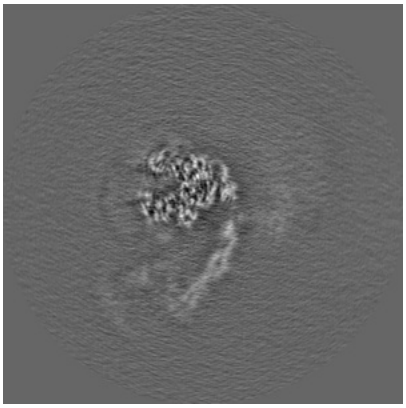


Y Index: 180

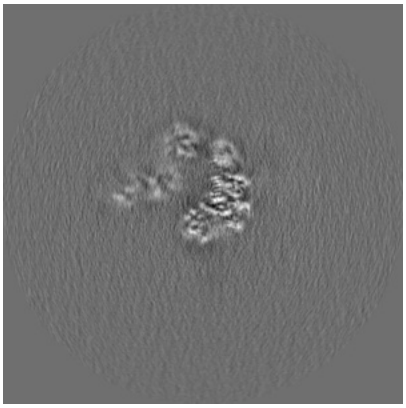


Z Index: 180

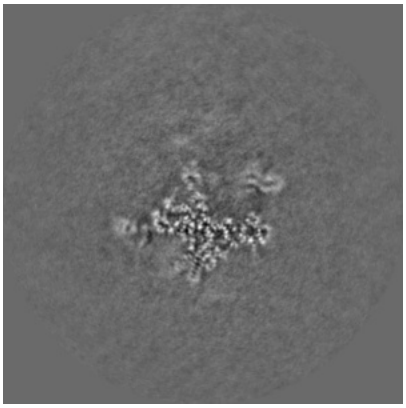
6.2.2 Raw map



X Index: 180



Y Index: 180

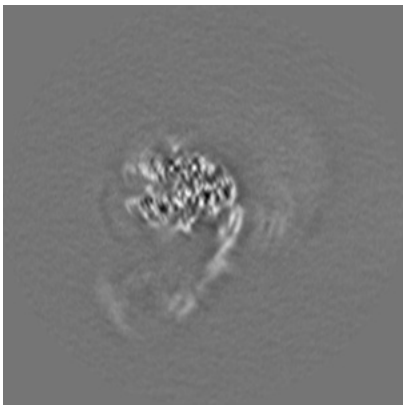


Z Index: 180

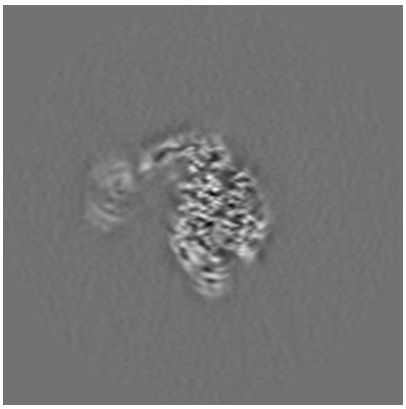
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

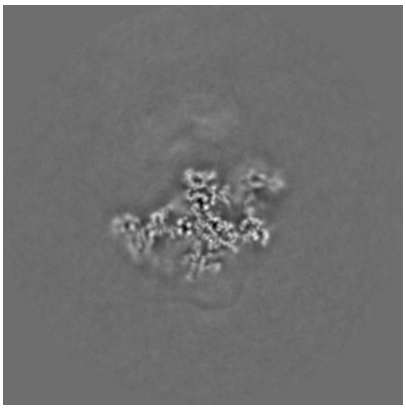
6.3.1 Primary map



X Index: 176

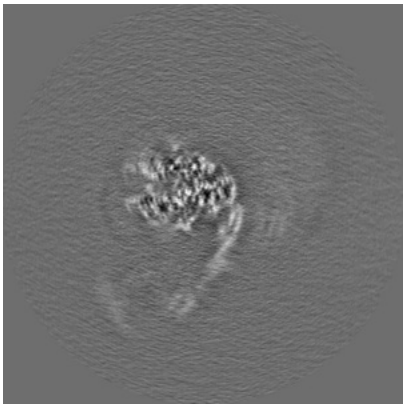


Y Index: 160

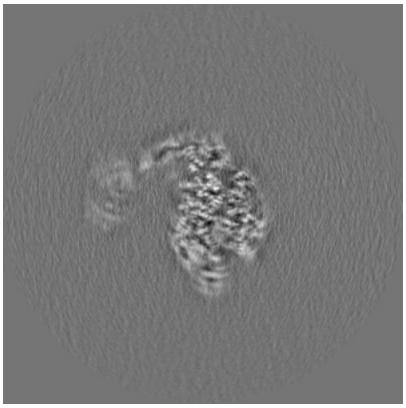


Z Index: 187

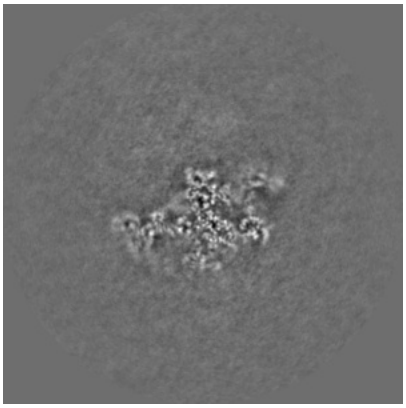
6.3.2 Raw map



X Index: 176



Y Index: 160



Z Index: 188

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

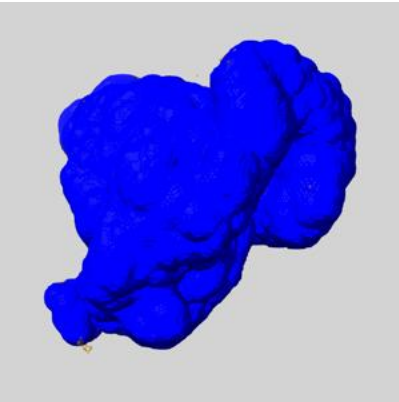
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

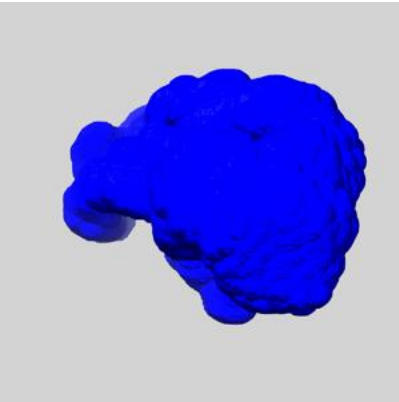
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

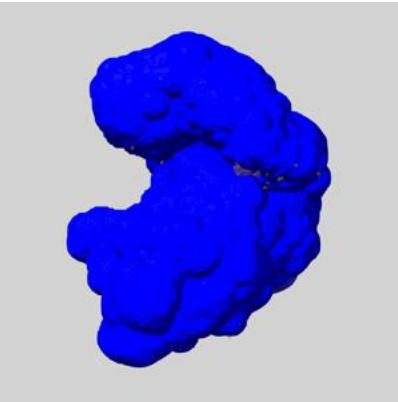
6.5.1 emd_26544_msk_1.map (i)



X



Y

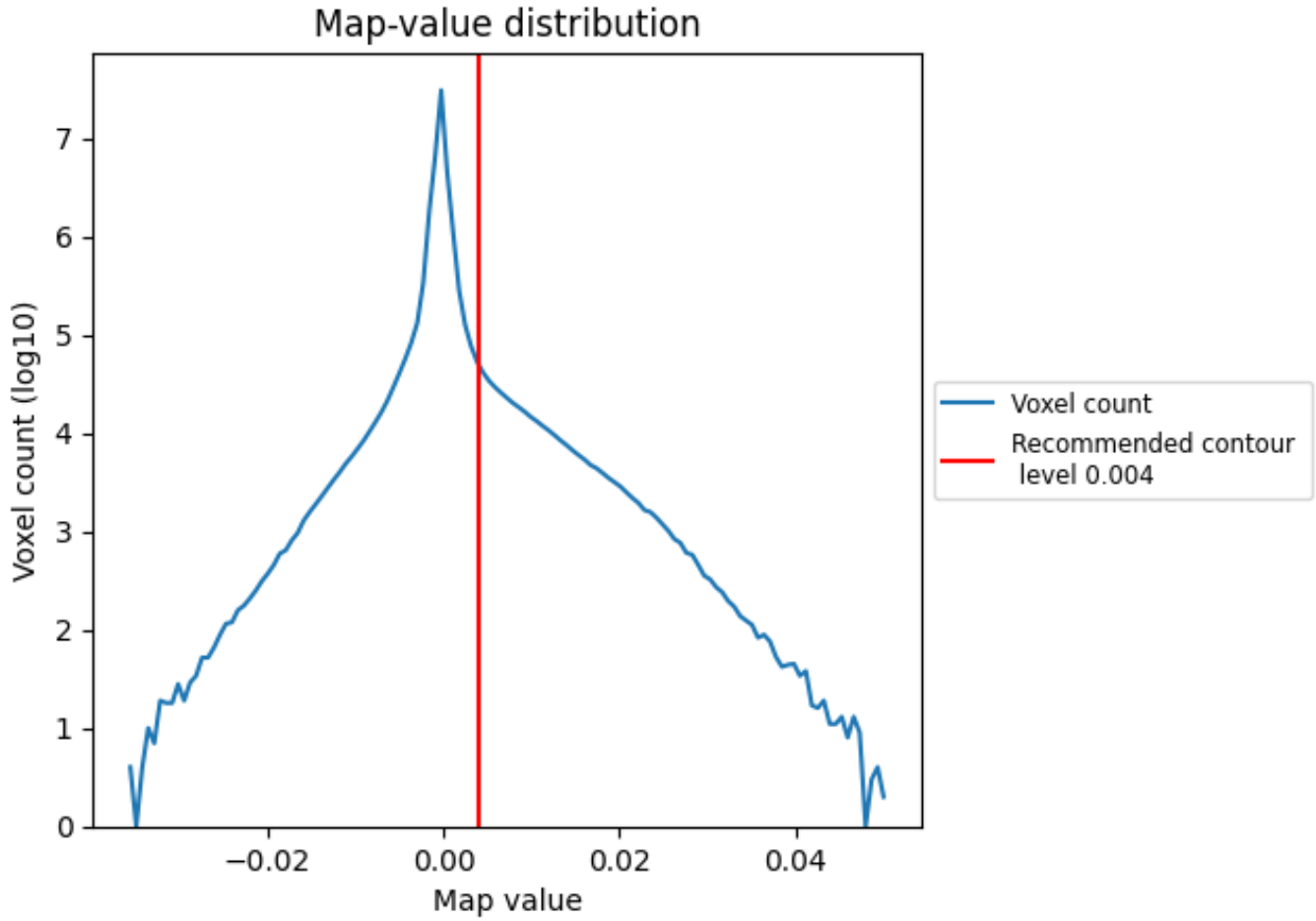


Z

7 Map analysis

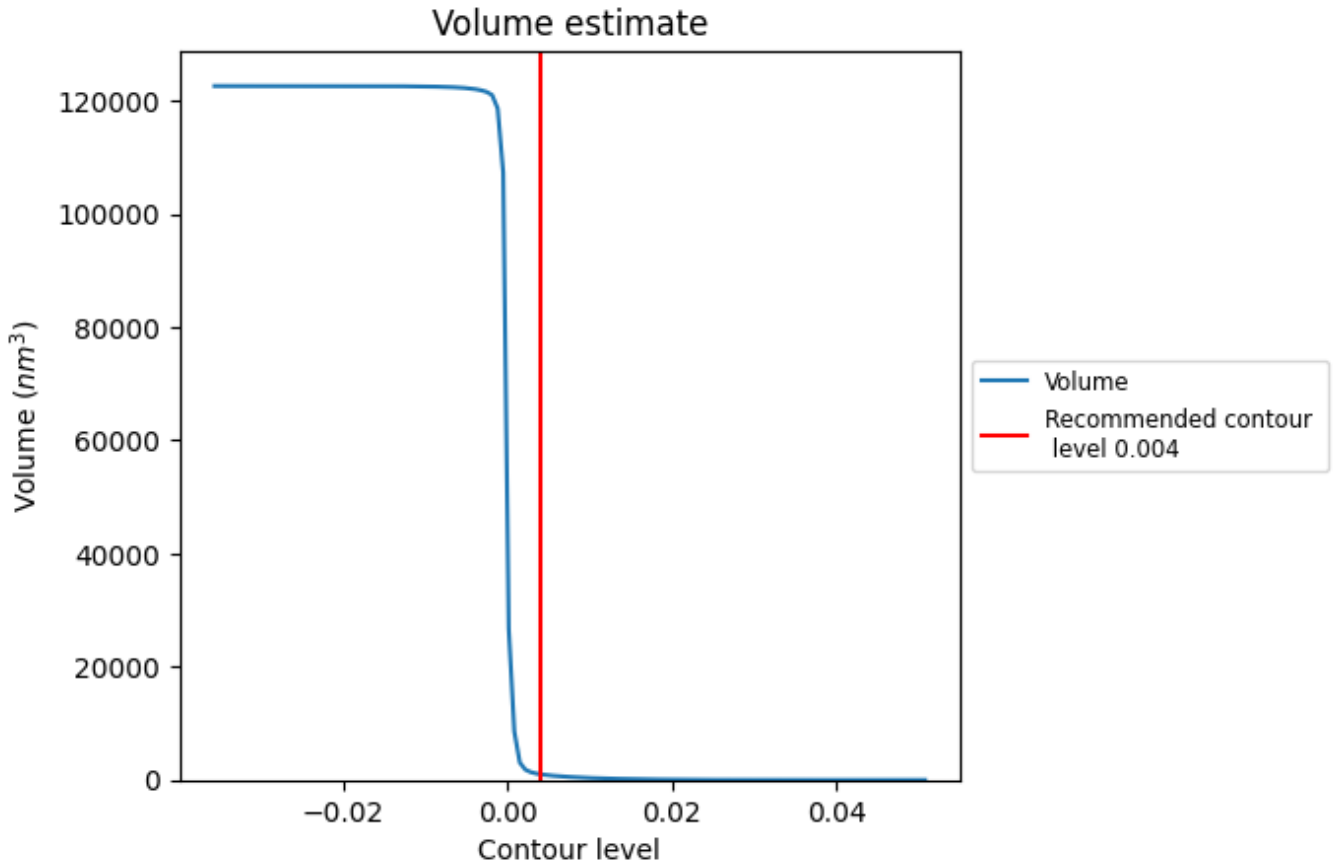
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

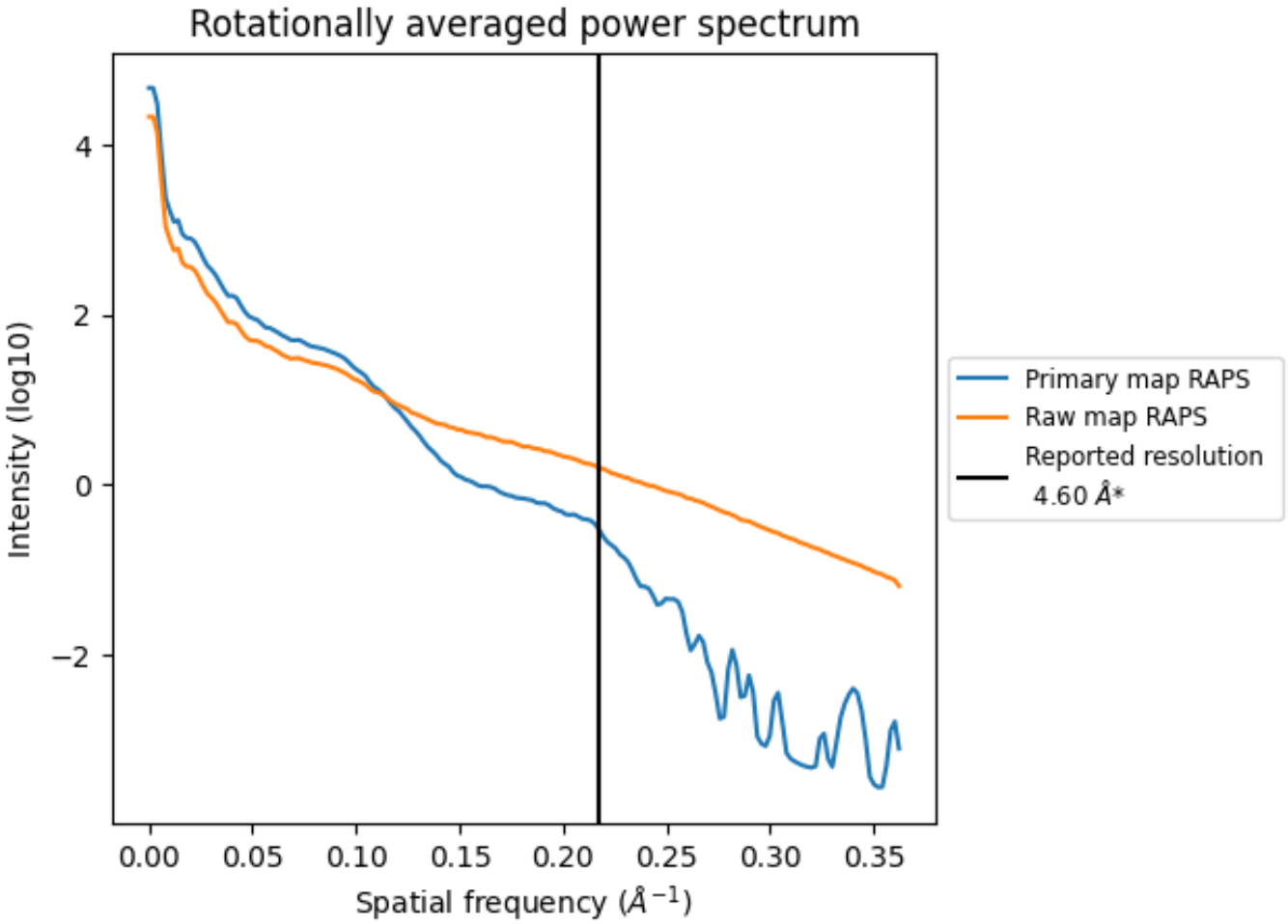
7.2 Volume estimate



The volume at the recommended contour level is 1005 nm^3; this corresponds to an approximate mass of 908 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 (i)

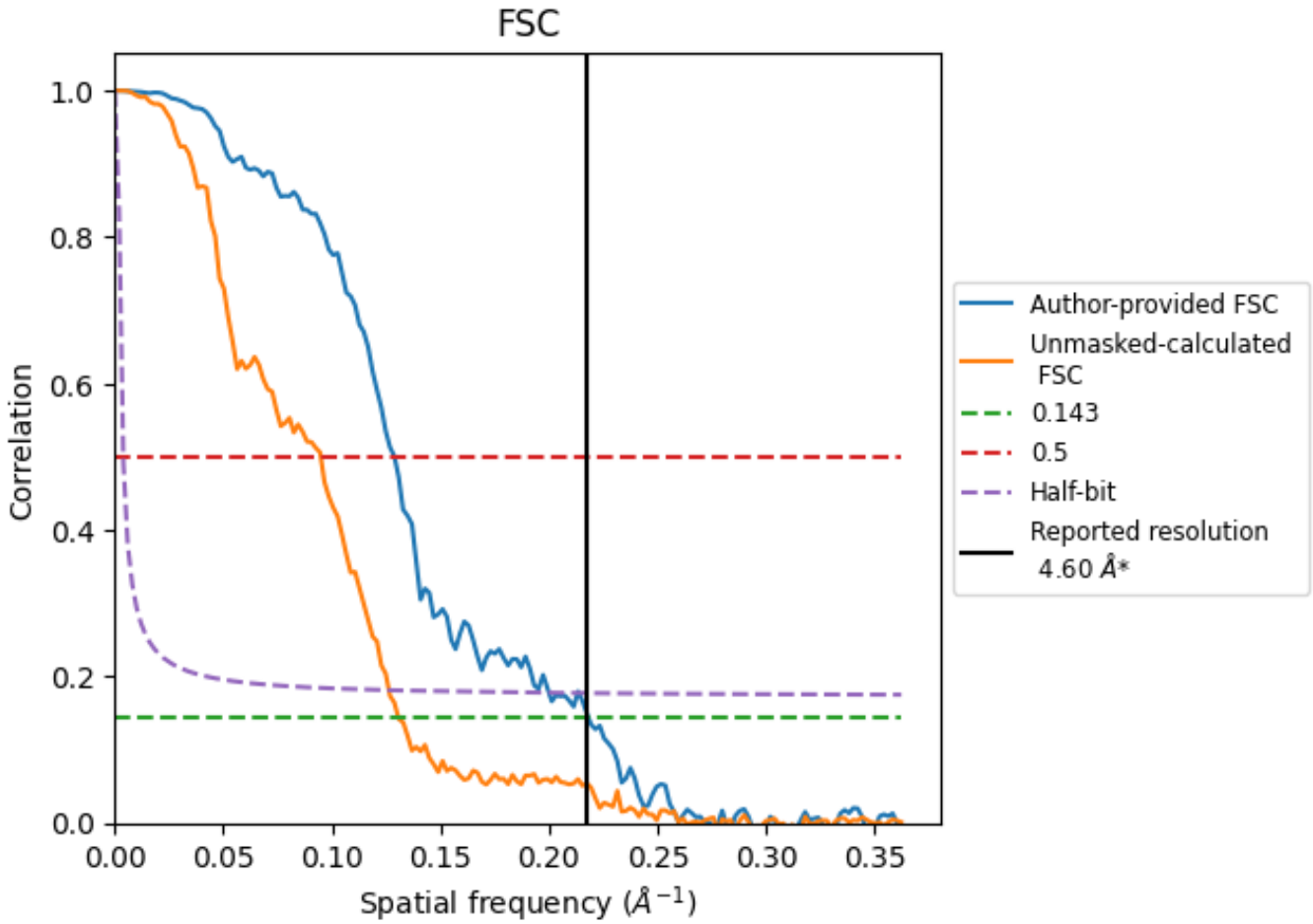


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

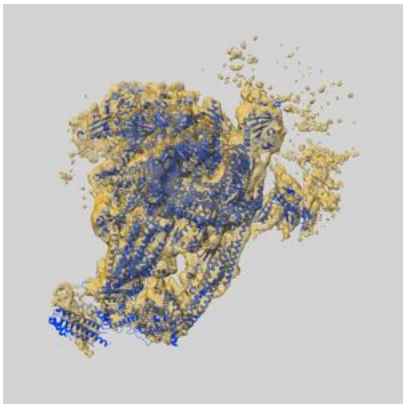
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	7.76	5.00
Unmasked-calculated*	7.65	10.54	7.92

*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 7.65 differs from the reported value 4.6 by more than 10 %

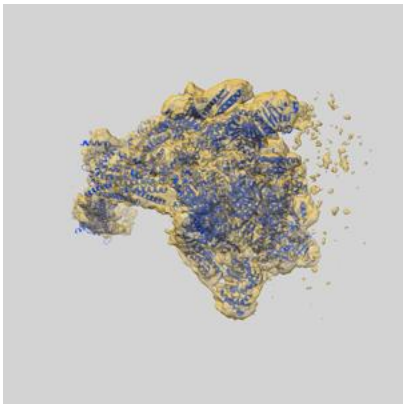
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26544 and PDB model 7UIF. Per-residue inclusion information can be found in section 3 on page 9.

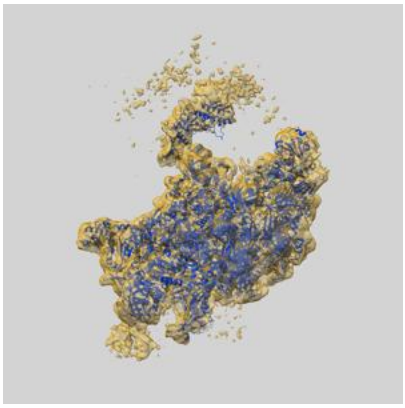
9.1 Map-model overlay



X



Y



Z

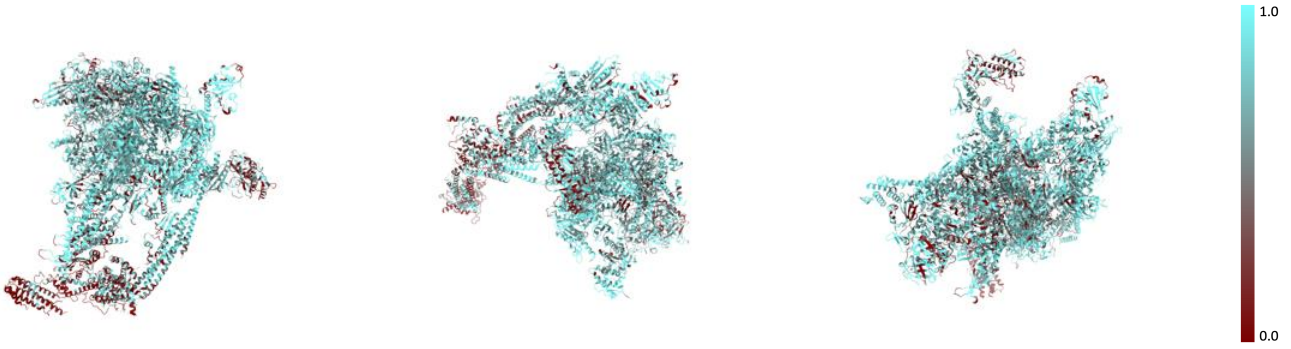
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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.

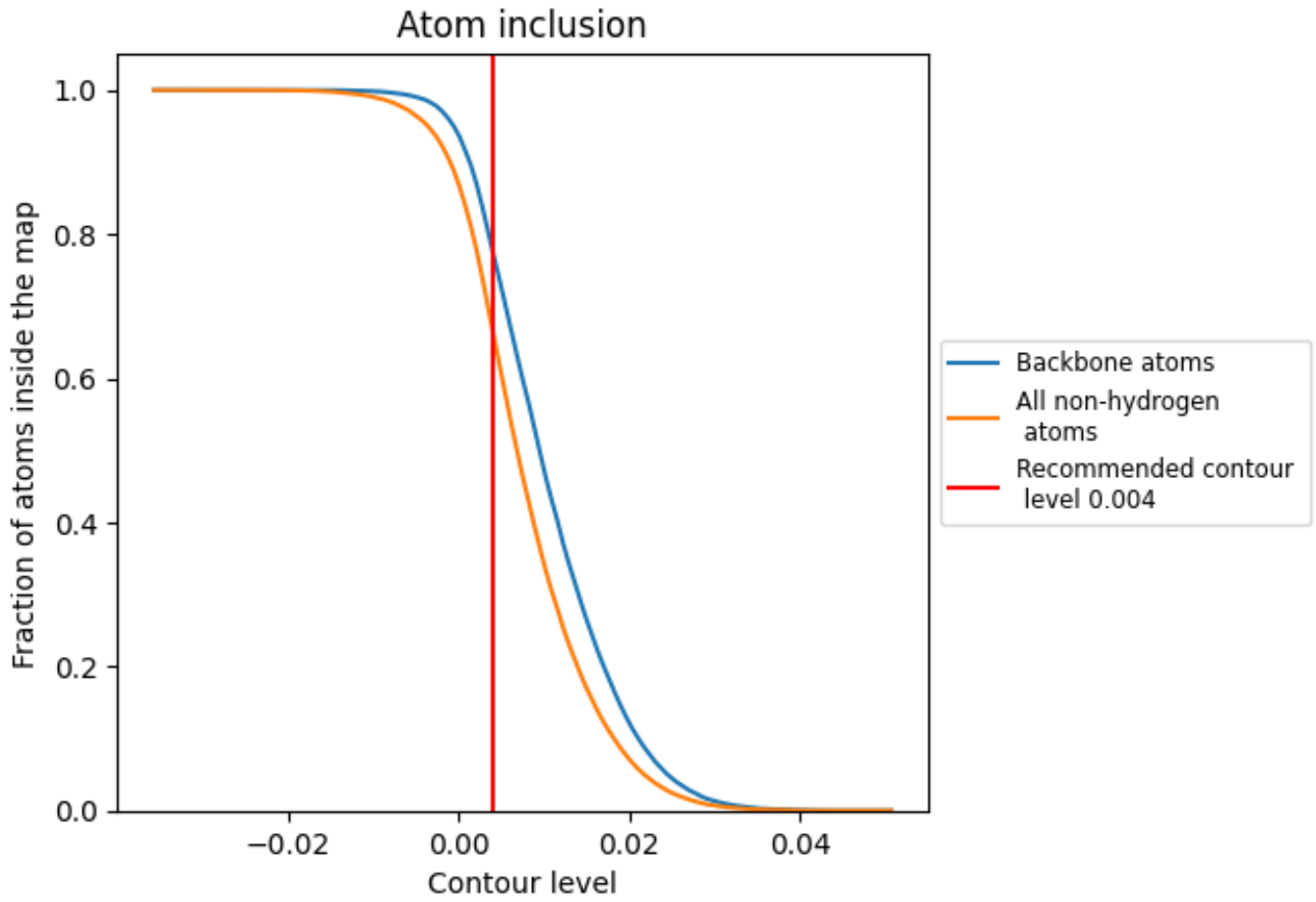
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6664	0.1270
A	0.7457	0.2120
B	0.6401	0.1190
C	0.7501	0.1590
D	0.6819	0.0850
E	0.8276	0.1850
F	0.7776	0.2120
G	0.7345	0.1250
H	0.8206	0.2300
I	0.7462	0.1490
J	0.5929	0.0660
K	0.7784	0.2310
L	0.6828	0.0900
M	0.7962	0.2840
P	0.6524	0.0890
Q	0.5049	0.0270
S	0.7264	0.1410
a	0.5298	0.0480
d	0.5984	0.0650
f	0.4644	0.0360
g	0.5344	0.0110
h	0.5951	0.0450
i	0.7775	0.1330
j	0.2831	0.0210
k	0.7529	0.1220
n	0.6591	0.0750
q	0.6909	0.1120
r	0.7734	0.2220
s	0.0888	0.0160
t	0.7816	0.2000
u	0.6687	0.0670
v	0.6411	0.0800
w	0.4042	-0.0340
z	0.3333	0.0140