wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 04:37 PM UTC

PDB ID	:	7UIO / pdb_00007uio
EMDB ID	:	EMD-26551
Title	:	Mediator-PIC Early (Composite Model)
Authors	:	Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on	:	2022-03-29
Resolution	:	3.30 Å(reported)
Based on initial models	:	7UIL, 7UI9, 7UIK

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 (i) 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 (1)) were used in the production of this report:

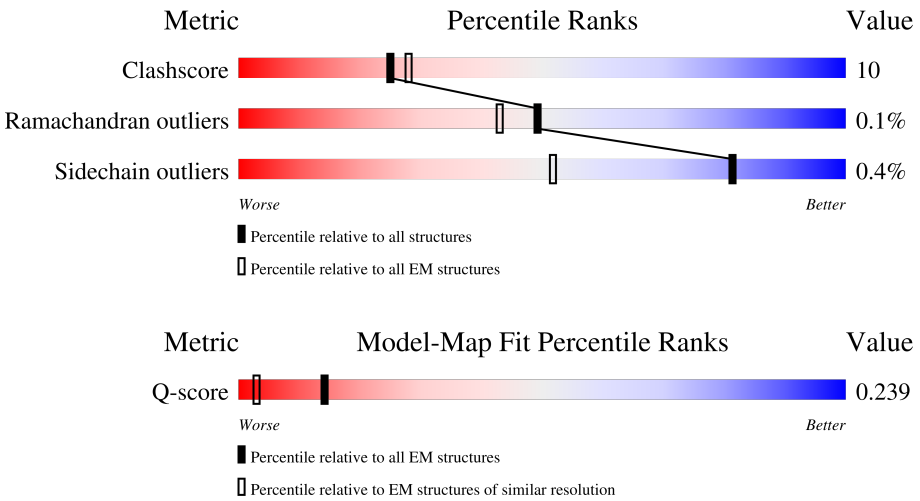
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	38	42%; 5%, 89%, 5%
2	B	37	49%; 14%, 73%, 14%
3	Ao	1081	•; 8%, •, 90%
3	Bo	1081	•; 8%, •, 90%

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Mol	Chain	Length	Quality of chain
4	Ab	431	11% • 85%
4	Bb	431	10% 5% 85%
5	Ac	397	• 18% 10% 72%
5	Bc	397	• 18% 9% 73%
6	An	1082	36% 61% 18% 22%
6	Bn	1082	36% 61% 17% 22%
7	Ae	1132	7% 49% 15% 36%
7	Be	1132	7% 50% 14% 36%
8	Ap	974	12% 71% 21% 8%
8	Bp	974	12% 70% 22% 8%
9	GA	147	35% 17% 30% 10% • 39%
9	GB	147	35% 18% 26% 12% 5% 39%
10	At	210	• 84% 16%
10	Bt	210	• 84% 16%
11	Ag	222	37% 51% 26% 23%
11	Bg	222	38% 51% 26% 23%
12	Ah	223	12% 47% 17% • 35%
12	Bh	223	12% 47% 17% • 35%
13	Ai	149	19% 40% 17% • 42%
13	Bi	149	19% 40% 17% • 42%
14	Aj	157	92% 78% 15% • 6%
14	Bj	157	92% 78% 16% • 6%
15	Ak	115	16% 77% 22% •
15	Bk	115	17% 77% 22% •
16	Aq	687	17% 54% 20% 25%

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Mol	Chain	Length	Quality of chain
16	Bq	687	16% 55% 20% 25%
17	Ar	307	• 71% 12% 18%
17	Br	307	• 70% 12% 18%
18	As	220	36% 31% 6% 63%
18	Bs	220	37% 30% 7% 63%
19	Au	140	36% 59% 28% 13%
19	Bu	140	35% 58% 29% 13%
20	Av	120	17% 59% 32% 9%
20	Bv	120	16% 61% 30% 9%
21	Aw	127	14% 58% 23% 19%
21	Bw	127	13% 58% 23% 19%
22	Az	25	40% 76% 20% •
22	Bz	25	40% 76% 20% •
23	AA	1453	6% 82% 18%
23	BA	1453	5% 82% 18%
24	AB	1224	11% 74% 21% •
24	BB	1224	10% 74% 21% •
25	AC	318	• 69% 16% 15%
25	BC	318	• 70% 15% 15%
26	AD	221	48% 64% 12% 24%
26	BD	221	48% 65% 12% 24%
27	AE	215	• 84% 16%
27	BE	215	• 84% 16%
28	AF	155	• 49% 6% 45%
28	BF	155	• 49% 6% 45%

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Mol	Chain	Length	Quality of chain
29	AG	171	42% 80% 20%
29	BG	171	41% 80% 20%
30	AH	146	5% 81% 16% •
30	BH	146	5% 79% 17% •
31	AI	122	10% 75% 20% 5%
31	BI	122	11% 75% 20% 5%
32	AJ	70	9% 70% 30%
32	BJ	70	9% 70% 30%
33	AK	120	• 85% 12% •
33	BK	120	• 86% 11% •
34	AL	70	11% 46% 16% 39%
34	BL	70	11% 43% 19% 39%
35	AM	345	9% • 90%
35	BM	345	9% • 90%
36	AP	735	12% 11% • 86%
36	BP	735	13% 11% • 86%
37	AQ	400	28% 22% 9% 69%
37	BQ	400	29% 23% 8% 69%
38	AS	309	23% 43% 16% 41%
38	BS	309	23% 42% 17% 41%
39	Aa	566	50% 58% 6% 36%
39	Ba	566	50% 58% 6% 36%
40	Ad	284	22% 34% 26% 40%
40	Bd	284	20% 34% 26% 40%
41	Af	295	25% 36% 21% 43%

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Mol	Chain	Length	Quality of chain
41	Bf	295	24% 37% 20% 43%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
42	ZN	A	1001	-	-	X	-

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 164116 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 DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	38	774	367	146	224	37	0	0

- Molecule 2 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	37	761	359	142	223	37	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ao	111	894	558	161	169	6	0	0
3	Bo	111	894	558	161	169	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Ab	65	516	328	82	102	4	0	0
4	Bb	65	516	328	82	102	4	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Ac	110	891	560	155	172	4	0	0
5	Bc	107	871	549	152	166	4	0	0

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	An	846	6927	4460	1187	1247	33	0	0
6	Bn	846	6927	4460	1187	1247	33	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ae	729	5916	3826	956	1120	14	0	0
7	Be	729	5916	3826	956	1120	14	0	0

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Ap	895	7247	4668	1202	1342	35	0	0
8	Bp	895	7247	4668	1202	1342	35	0	0

- Molecule 9 is a protein called Regulatory protein GAL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	GA	89	727	459	130	130	8	0	0
9	GB	89	727	459	130	130	8	0	0

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	At	210	1609	1016	270	317	6	0	0
10	Bt	210	1609	1016	270	317	6	0	0

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Ag	171	1426	914	242	265	5	0	0
11	Bg	171	1426	914	242	265	5	0	0

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Ah	144	1185	747	208	227	3	0	0
12	Bh	144	1185	747	208	227	3	0	0

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Ai	86	730	456	134	139	1	0	0
13	Bi	86	730	456	134	139	1	0	0

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Aj	148	1189	736	209	241	3	0	0
14	Bj	148	1189	736	209	241	3	0	0

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Ak	115	933	584	160	185	4	0	0
15	Bk	115	933	584	160	185	4	0	0

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 17.

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

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

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Ar	253	1995	1271	331	383	10	0	0
17	Br	253	1995	1271	331	383	10	0	0

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	As	81	657	415	109	132	1	0	0
18	Bs	81	657	415	109	132	1	0	0

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Au	122	978	611	163	199	5	0	0
19	Bu	122	978	611	163	199	5	0	0

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Av	109	869	540	143	180	6	0	0
20	Bv	109	869	540	143	180	6	0	0

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Aw	103	871	575	135	155	6	0	0
21	Bw	103	871	575	135	155	6	0	0

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	Az	25	185	116	25	44	0	0
22	Bz	25	185	116	25	44	0	0

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AA	1453	11426	7192	1995	2177	62	0	0
23	BA	1453	11426	7192	1995	2177	62	0	0

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AB	1172	9336	5895	1637	1748	56	0	0
24	BB	1172	9336	5895	1637	1748	56	0	0

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	AD	169	1353	838	237	275	3	0	0
26	BD	169	1353	838	237	275	3	0	0

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	AE	215	1760	1116	310	322	12	0	0
27	BE	215	1760	1116	310	322	12	0	0

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AF	86	697	445	118	131	3	0	0
28	BF	86	697	445	118	131	3	0	0

- Molecule 29 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AG	171	1340	861	222	249	8	0	0
29	BG	171	1340	861	222	249	8	0	0

- Molecule 30 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AH	141	1126	706	189	226	5	0	0
30	BH	141	1126	706	189	226	5	0	0

- Molecule 31 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AI	116	943	580	171	181	11	0	0
31	BI	116	943	580	171	181	11	0	0

- Molecule 32 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

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

- Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	AK	116	929	596	158	173	2	0	0
33	BK	116	929	596	158	173	2	0	0

- Molecule 34 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AL	43	344	211	69	60	4	0	0
34	BL	43	344	211	69	60	4	0	0

- Molecule 35 is a protein called Transcription initiation factor IIB.

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

- Molecule 36 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AP	103	861	554	142	162	3	0	0
36	BP	103	861	554	142	162	3	0	0

- Molecule 37 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AQ	125	1033	644	189	195	5	0	0
37	BQ	125	1033	644	189	195	5	0	0

- Molecule 38 is a protein called Transcription elongation factor S-II.

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

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Aa	365	3008	1932	478	588	10	0	0
39	Ba	365	3008	1932	478	588	10	0	0

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Ad	171	1388	875	233	276	4	0	0
40	Bd	171	1388	875	233	276	4	0	0

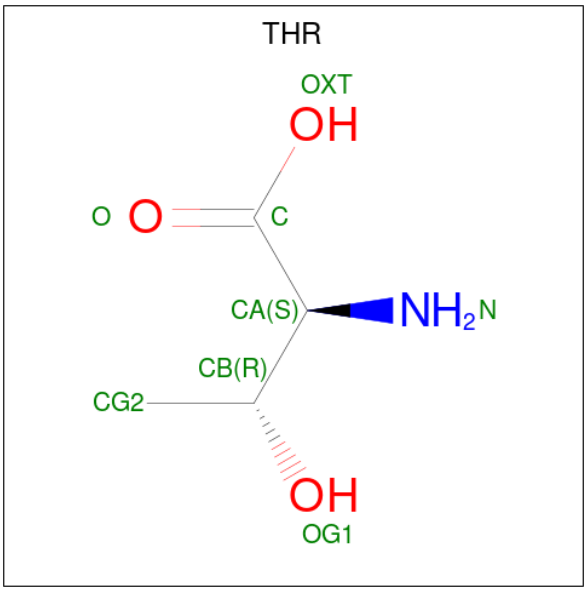
- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Af	169	1407	905	234	262	6	0	0
41	Bf	169	1407	905	234	262	6	0	0

- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

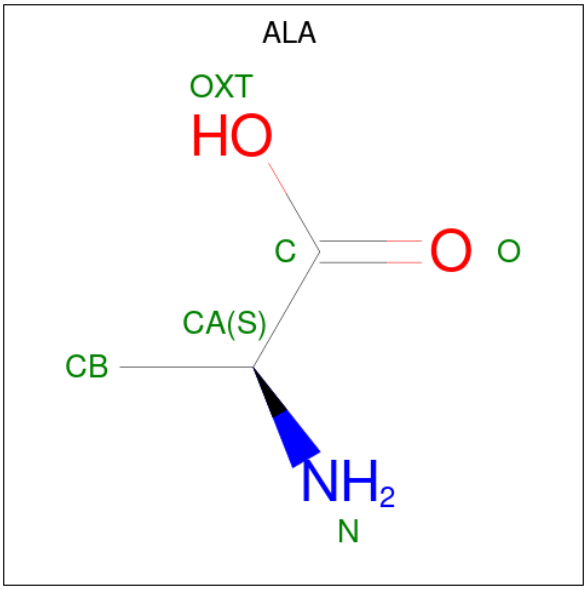
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
42	A	2	2	2	0
42	B	2	2	2	0

- Molecule 43 is THREONINE (CCD ID: THR) (formula: $C_4H_9NO_3$).



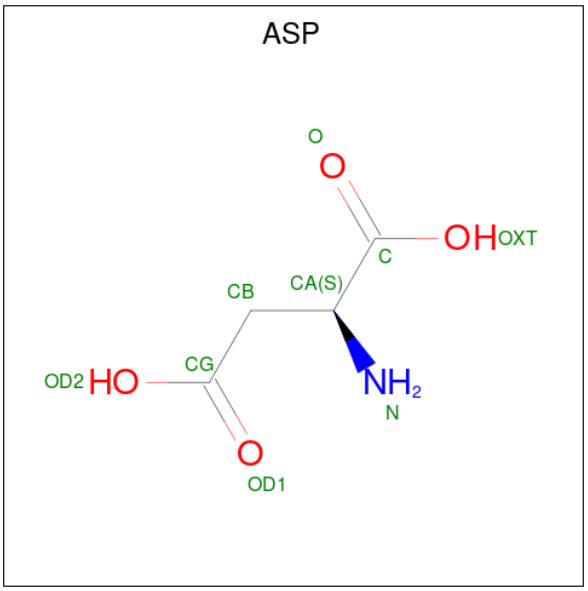
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
43	Bc	1	7	4	1	2	0

- Molecule 44 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
44	Bc	1	5	3	1	1	0

- Molecule 45 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



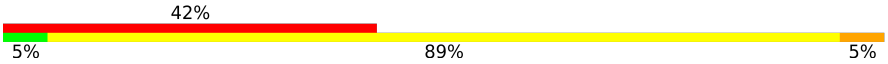
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
45	Bc	1	9	4	1	4	0

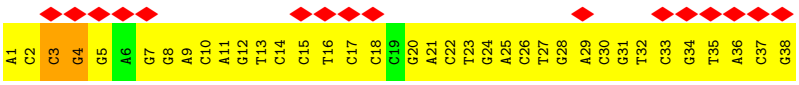
3 Residue-property plots (i)

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 (38-MER)

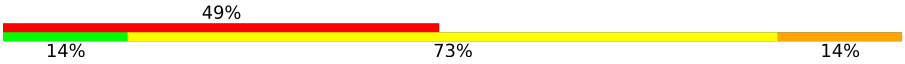
Chain A:





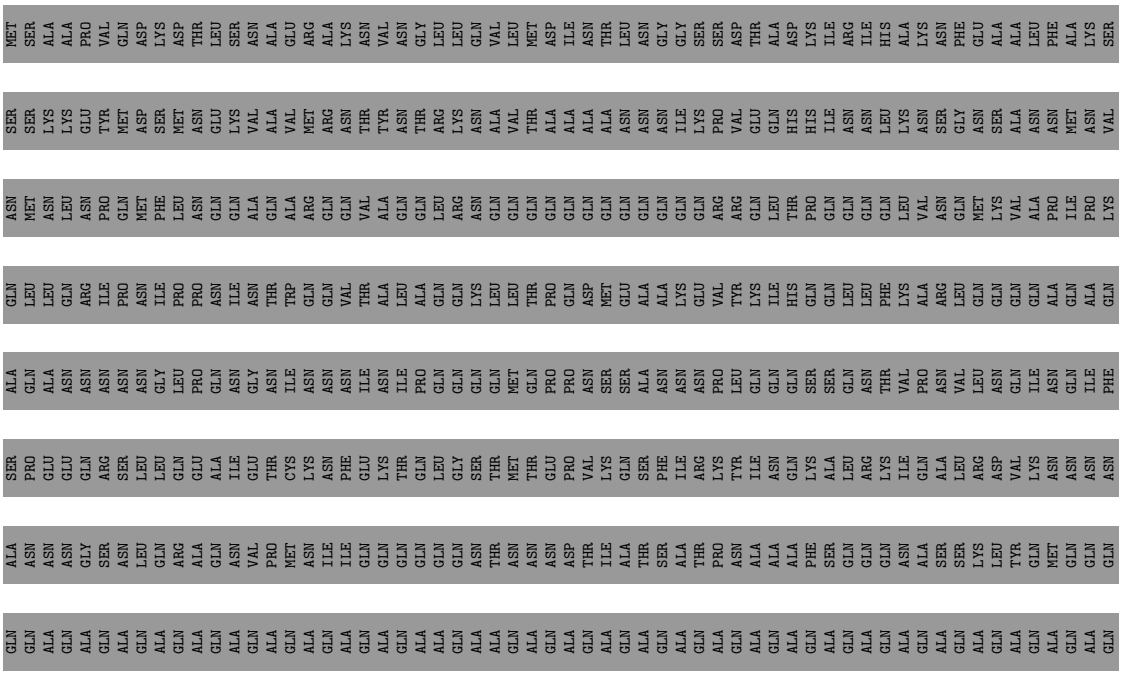
- Molecule 2: DNA (37-MER)

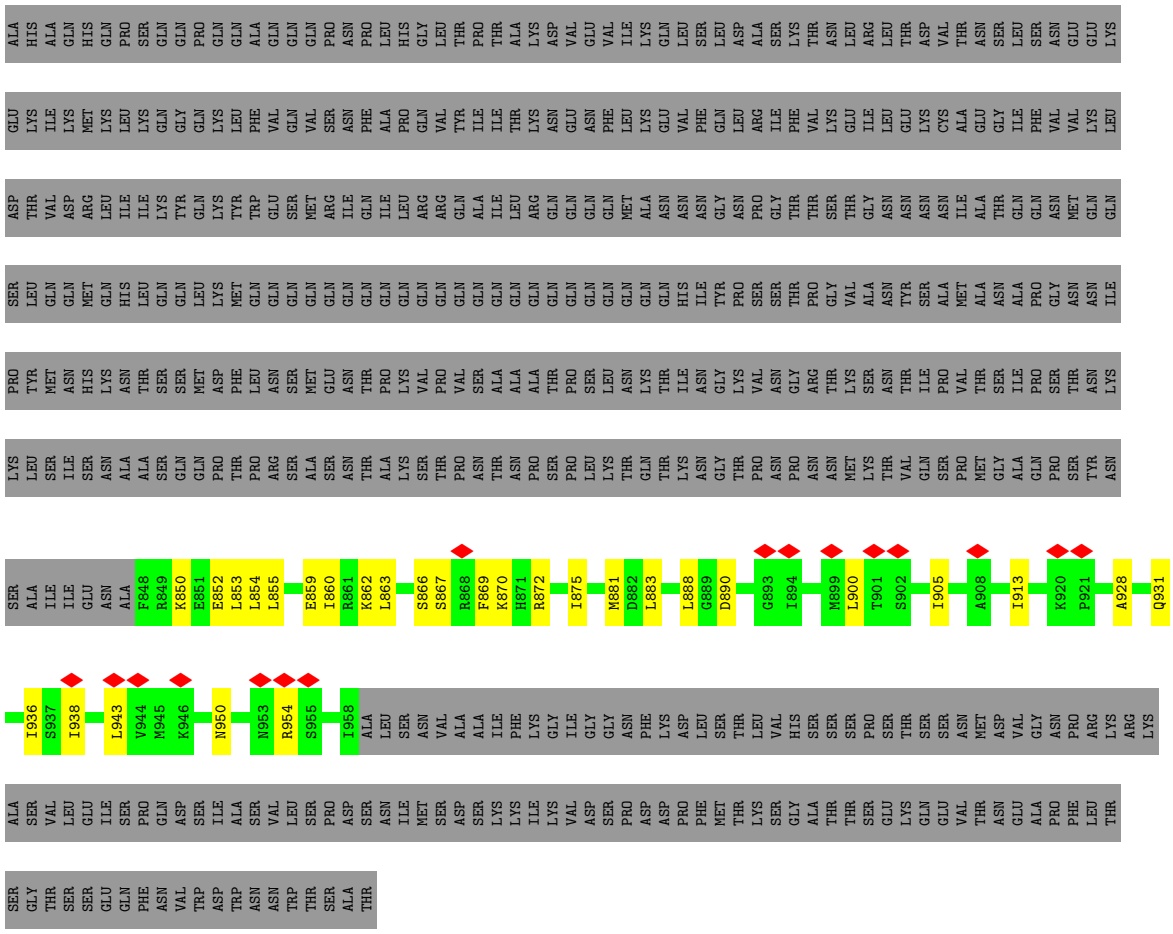
Chain B:



- Molecule 3: Mediator of RNA polymerase II transcription subunit 15

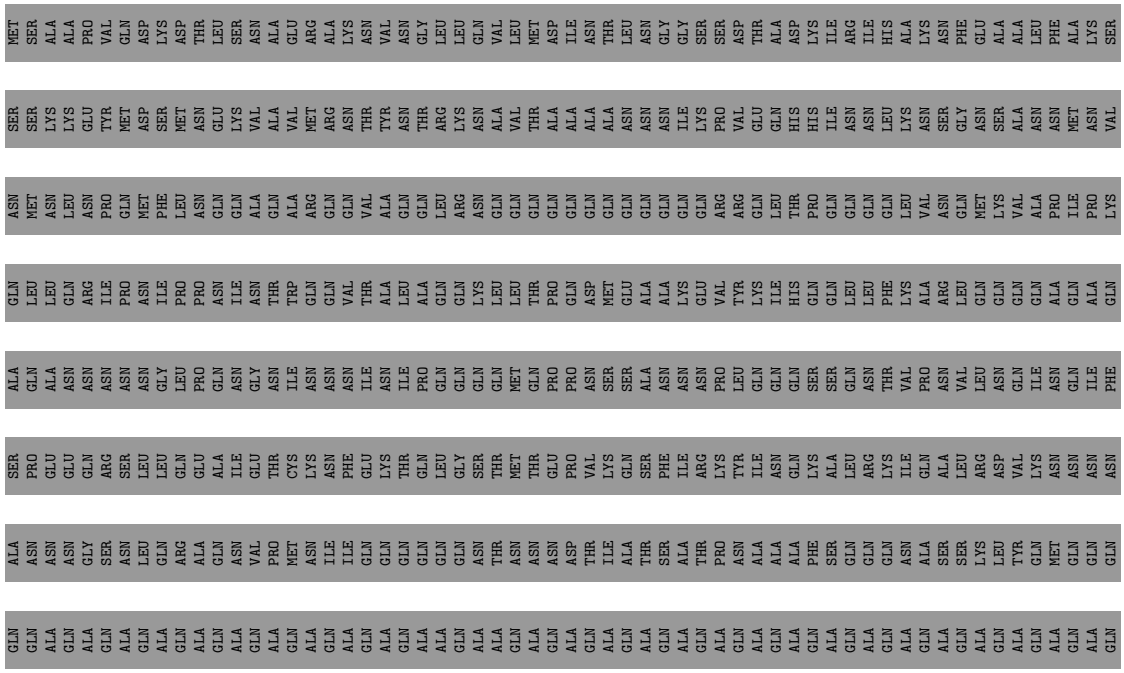
Chain Ao:

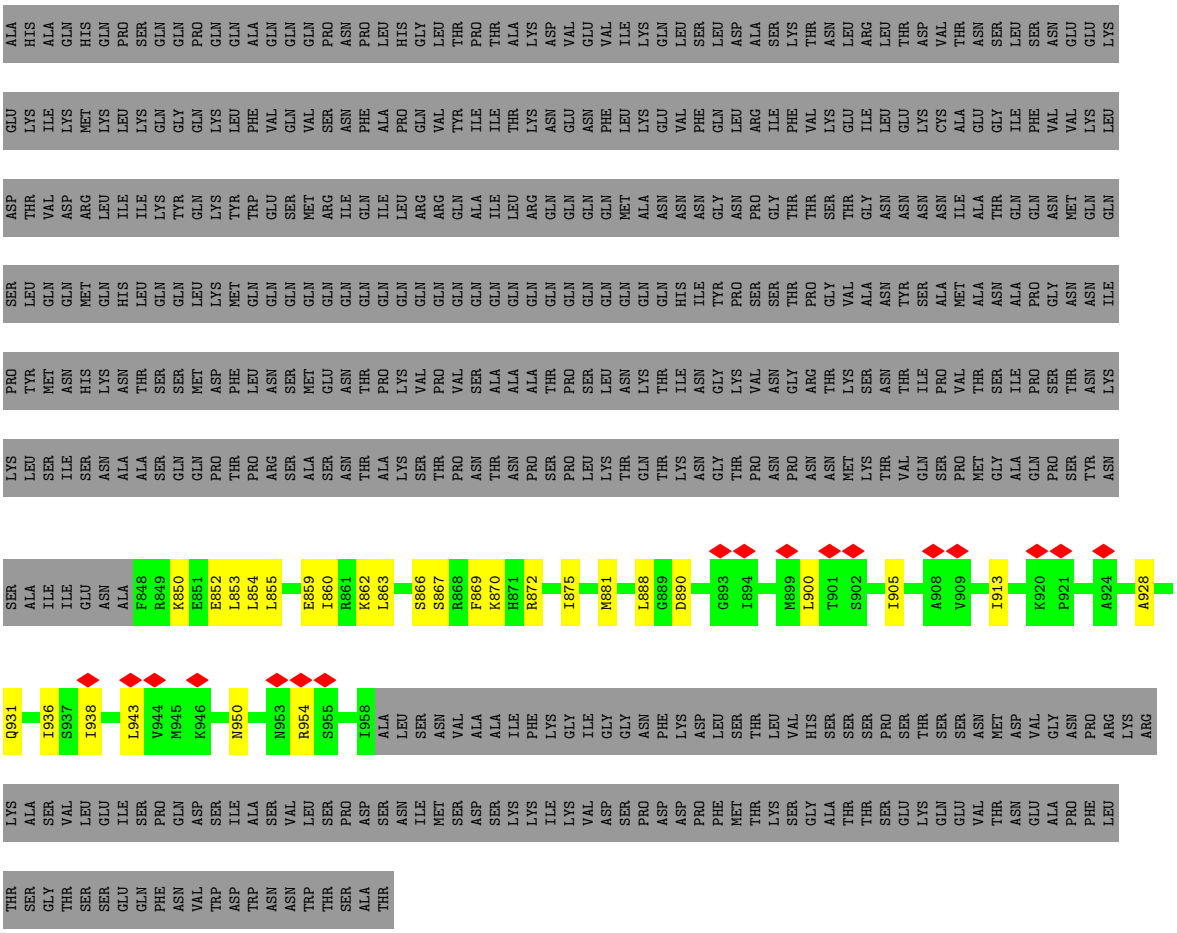




• Molecule 3: Mediator of RNA polymerase II transcription subunit 15

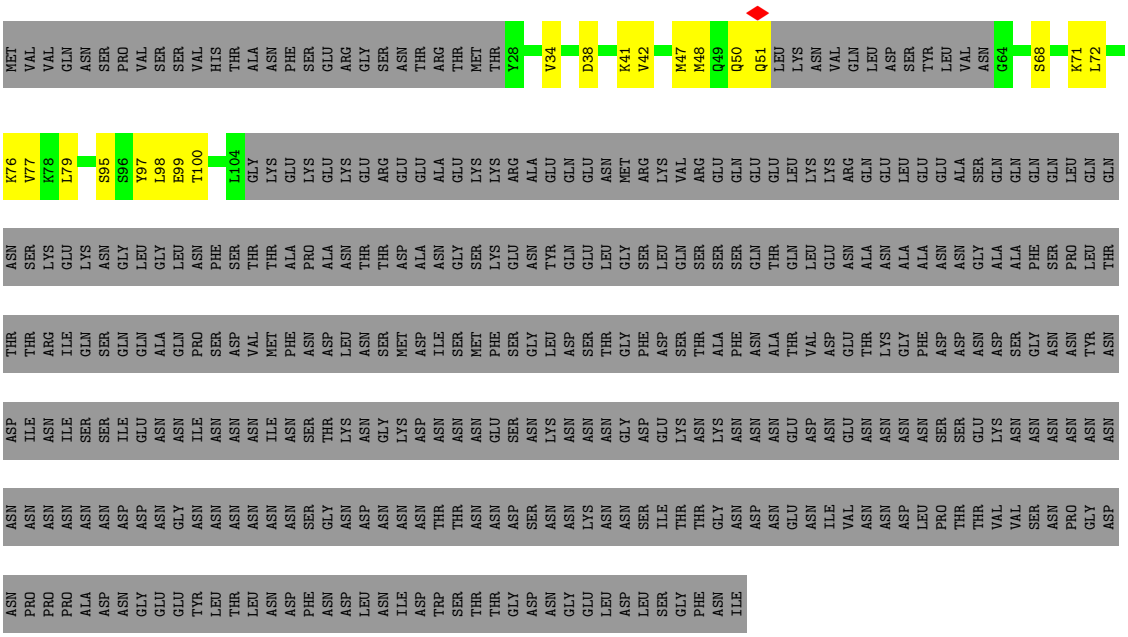
Chain Bo:





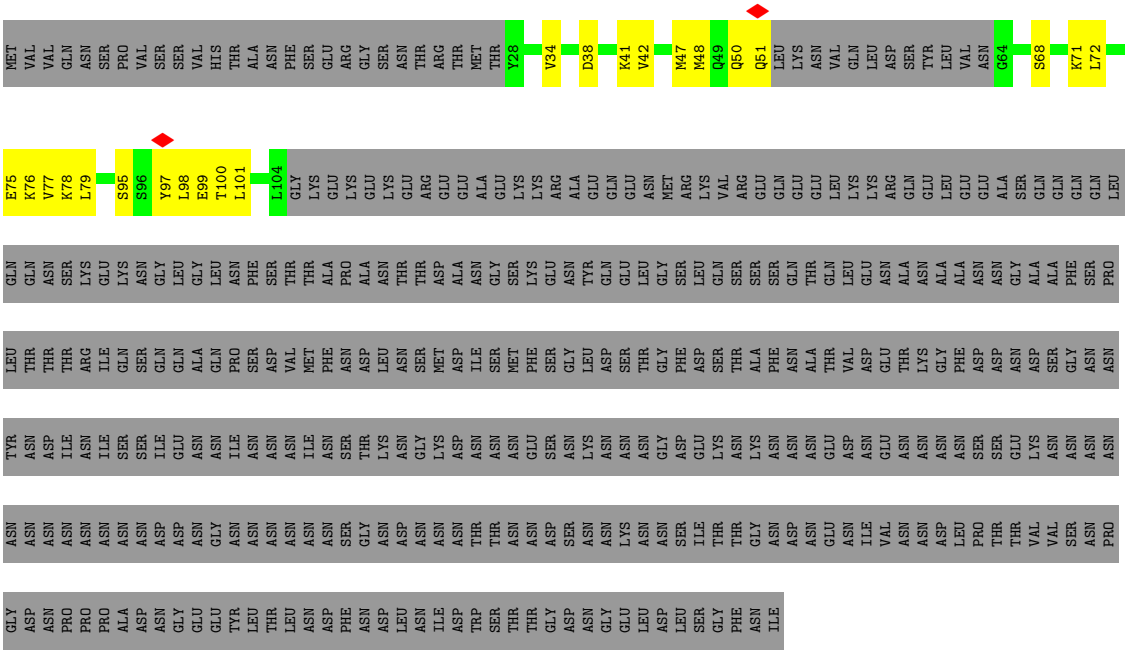
• Molecule 4: Mediator of RNA polymerase II transcription subunit 2

Chain Ab: 11% 85%



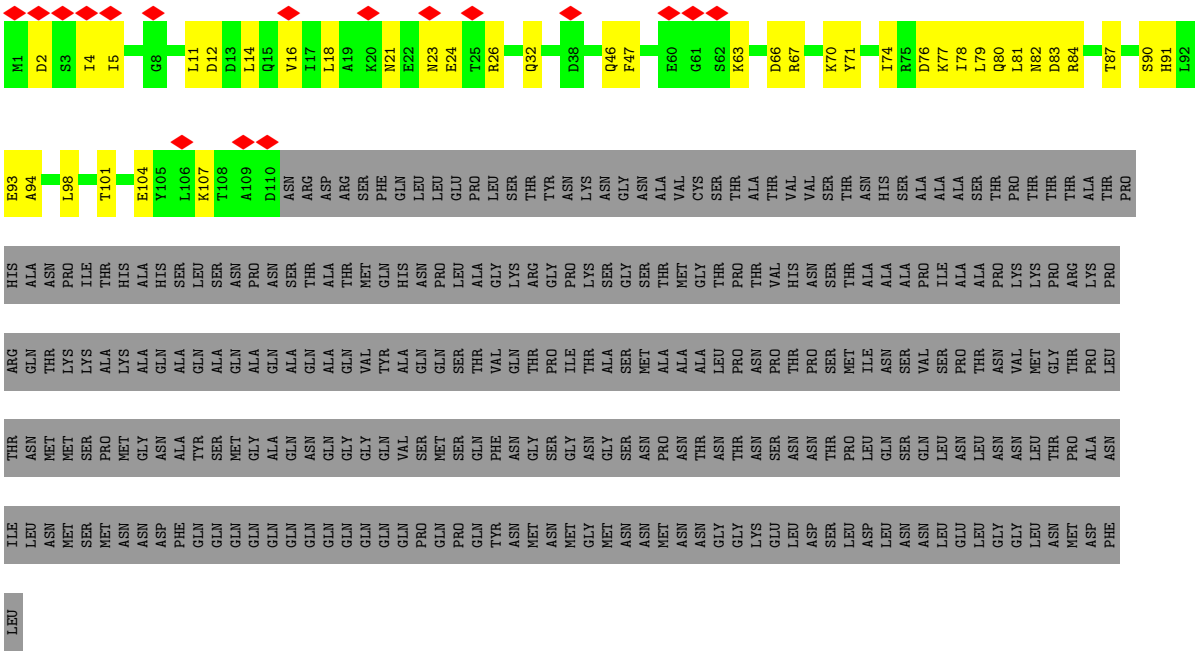
• Molecule 4: Mediator of RNA polymerase II transcription subunit 2

Chain Bb: 10% 5% 85%



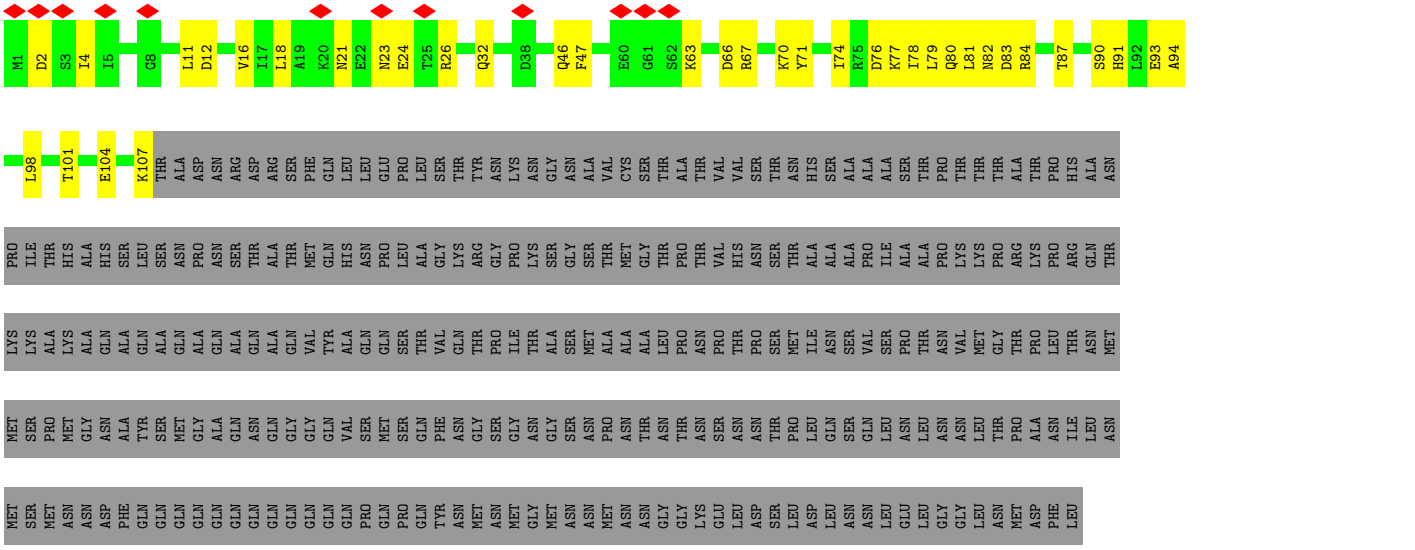
• Molecule 5: Mediator of RNA polymerase II transcription subunit 3

Chain Ac: 18% 10% 72%



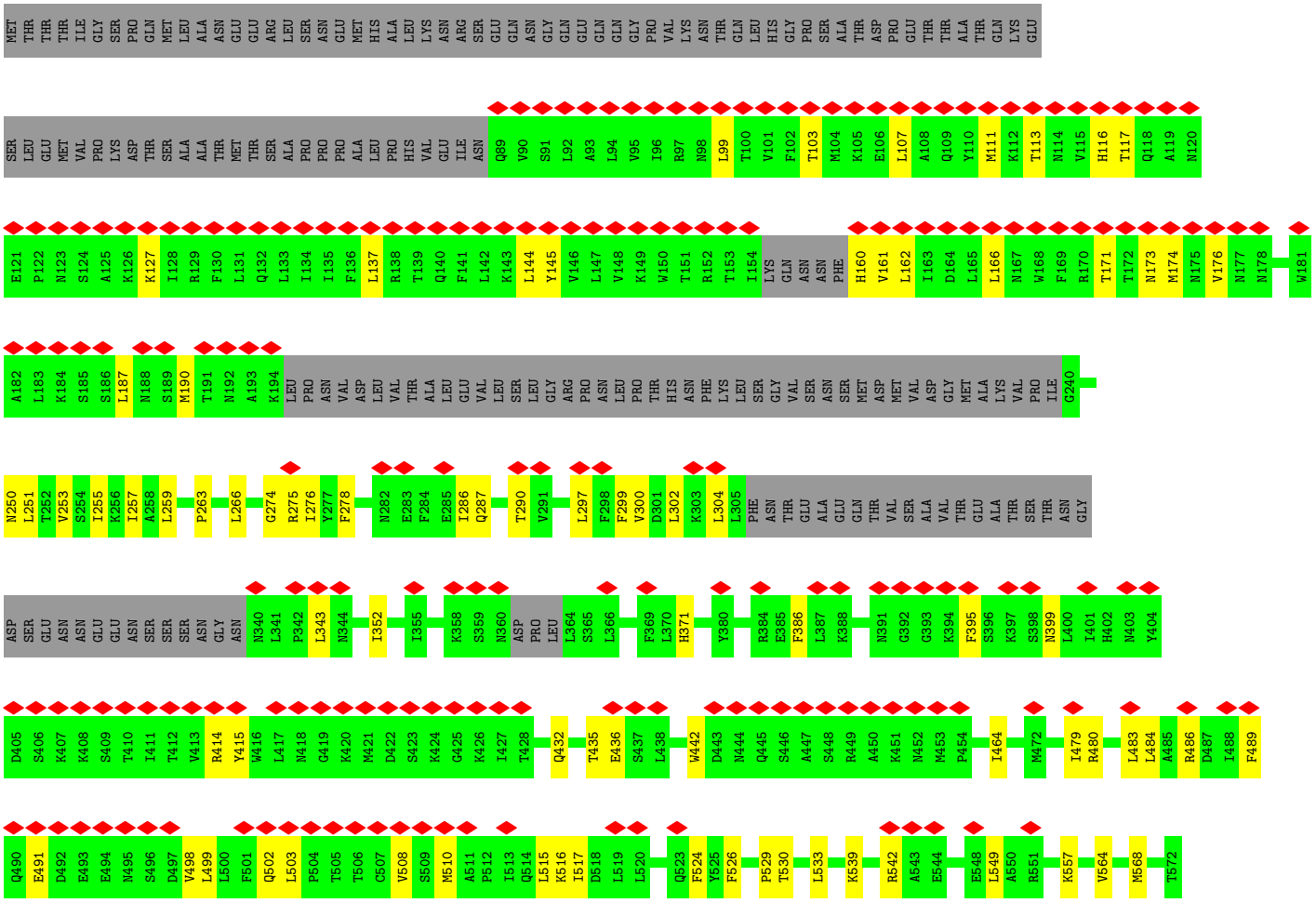
• Molecule 5: Mediator of RNA polymerase II transcription subunit 3

Chain Bc: 18% 9% 73%



- Molecule 6: Mediator of RNA polymerase II transcription subunit 14

Chain An:



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W665 N666 L670 D671 N672 S673 N674 E681 M689 R693 I699 M703 L704 I705 D706 S707 L708 N709 Q710 L711 E712 I713 R714 N715 K716 I717 C718 S719 S720 E721 M722 I723 N724 E725 Q726 K727 L728 P729 Q730 Y731 I732 I733 Q734 G735 S736 N737 T738 N739 D740 N741 I742 S743 I744 I745

T746 L747 E748 L749 E750 S751 F752 L753 E754 G755 S756 K757 A758 I759 N760 S761 I762 L763 E764 S765 S766 M767 F768 L769 R770 I771 D772 Y773 S774 N775 S776 Q777 I778 R779 L780 Y781 A782 K783 F784 K785 R786 N787 T788 M789 M790 I791 Q792 C793 Q794 I795 D796 K797 L798 Y799 I800 H801 F802 V803 Q804 E805

E806 P807 L808 A809 F810 Y811 L812 E813 E814 S815 F816 T817 N818 L819 G820 I821 I822 V823 Q824 Y825 L826 T827 K828 F829 R830 Q831 K832 L833 M834 Q835 L836 V837 V838 L839 T840 L846 H847 K848 N849 F850 F855 K856 I857 I858 A859 L860 Q861 P862 I865 S866 F867 K868 Y869 L870 S871 N872 N873

D874 E875 D876 D877 K878 D879 I882 K883 I884 S885 T886 N887 D888 D889 S890 I891 L894 T895 V896 N902 P903 Q904 H905 I906 I907 Q908 P909 N913 S914 K915 F927 F932 K933 A934 L935 K936 L939 N940 E941 R942 F946 H947 E948 S949 V957 L961 Y971 P974

K979 I980 T981 T988 V989 L990 H991 N992 G993 R994 D995 K996 I997 Q998 F999 H1002 A1007 H1008 I1009 T1010 T1011 K1012 S1013 Y1016 M1019 H1020 Q1021 Q1025 V1026 F1027 MET LEU ASP THR LYS ARG LEU GLY THR PRO GLU SER VAL LYS PRO ALA ASN ALA SER HIS ALA I1049 R1050

L1051 G1054 V1055 D1058 P1059 I1062 E1063 P1064 I1065 L1066 M1067 E1068 I1069 H1070 N1071 I1072 L1073 K1074 VAL ASP SER ASN SER SER SER SER

- Molecule 6: Mediator of RNA polymerase II transcription subunit 14

Chain Bn:

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

SER LEU GLU MET VAL PRO LYS ASP THR SER ALA ALA THR MET THR SER ALA ALA PRO PRO PRO ALA LEU PRO HIS VAL GLU ILE ASN Q89 V90 S91 L92 A93 L94 V95 I96 R97 N98 L99 T100 V101 F102 T103 M104 K105 E106 L107 A108 Q109 Y110 M111 K112 T113 N114 V115 H116 T117 Q118 A119 N120

E121 P122 N123 S124 A125 K126 K127 I128 R129 F130 L131 Q132 L133 I134 I135 F136 L137 R138 T139 Q140 F141 L142 K143 L144 Y145 V146 L147 V148 K149 W150 T151 R152 T153 I154 LYS GLN ASN ASN PHE H160 V161 L162 I163 D164 L165 L166 N167 W168 F169 R170 T171 T172 N173 M174 N175 V176 N177 N178 C179 I180

W181 A182 L183 K184 S185 S186 L187 N188 S189 M190 T191 N192 A193 K194 LEU PRO ASN VAL ASP LEU VAL THR ALA LEU GLU VAL LEU SER LEU GLY ARG PRO ASN LEU PRO THR HIS ASN PHE LYS LEU SER GLY VAL SER ASN SER MET ASP MET VAL ASP GLY MET ALA LYS VAL PRO ILE G240

N250 L251 T252 V253 S254 I255 K256 I257 A258 L259 P263 L266 I271 G274 R275 I276 Y277 F278 N282 E285 I286 Q287 T290 V291 L297 F298 F299 V300 D301 L302 K303 L304 L305 PHE ASN THR GLU ALA GLU GLN THR VAL SER ALA VAL THR GLU ALA THR SER THR

ASN GLY ASP SER GLU ASN ASN GLU GLU ASN SER SER SER ASN GLY ASN N340 L341 P342 L343 N344 I355 K358 S359 N360 ASP PRO LEU L364 S365 L366 F369 L370 H371 Y380 R384 E385 F386 L387 K388 L389 A390 N391 G392 G393 K394 F395 S396 K397 S398 N399 L400 I401 H402 N403

Y404 D405 S406 K407 K408 S409 T410 I411 T412 V413 R414 Y415 W416 L417 N418 G419 K420 M421 D422 S423 K424 G425 K426 I427 T428 I429 E436 S437 L438 W442 D443 N444 Q445 S446 A447 S448 R449 A450 K451 N452 M453 P454 I464 I479 R480 L483 L484 A485 R486 D487 I488 F489 Q490 E491 D492

E493 E494 N495 S496 D497 V498 L499 L500 F501 Q502 L503 P504 T505 T506 C507 V508 S509 M510 A511 P512 I513 Q514 L515 K516 I517 D518 L519 L520 Q523 F524 Y525 F526 P529 T530 L533 K539 R542 A543 E544 E548 L549 A550 R551 K557 V564 M568 T572 GLY W574

I582 D583 K584 P585 I586 R587 T588 GLN VAL ASN THR GLY GLY GLU SER VAL VAL LYS LYS GLU ASP ASN LYS TYR ALA ILE ALA GLY ASN SER THR THR ASN SER ASP VAL SER LEU L620 L621 Q622 R623 D624 L629 W632 K646 E652 K653 R654 S660 Q661 R662 W665 N666

L670 D671 N672 S673 N674 E681 M689 R693 D706 S707 L708 N709 Q710 L711 E712 I713 R714 N715 K716 I717 C718 S719 S720 E721 M722 I723 N724 E725 Q726 K727 L728 P729 Q730 Y731 I732 I733 Q734 G735 S736 N737 T738 N739 D740 N741 I742 S743 I744 I745 T746 L747 E748 L749 E750 S751 F752

L753 E754 G755 S756 K757 A758 L759 N760 S761 I762 L763 E764 S765 S766 M767 F768 L769 R770 I771 D772 Y773 S774 N775 S776 Q777 I778 R779 L780 Y781 A782 K783 F784 K785 R786 N787 T788 M789 M790 I791 Q792 C793 Q794 I795 D796 K797 L798 Y799 I800 H801 F802 V803 Q804 E805 E806 P807 L808 A809 F810 Y811 L812

E813 E814 S815 F816 T817 N818 L819 G820 I821 I822 V823 Q824 Y825 L826 T827 K828 F829 R830 Q831 K832 L833 M834 Q835 L836 V837 V838 L839 T840 L846 H847 K848 N849 F850 F855 K856 I857 I858 A859 L860 Q861 P862 I865 S866 Y869 L870 S871 N872 N873 D874 E875 D876 D877 K878 D879 I882

K883 I884 S885 T886 N887 D888 D889 S890 I891 L894 T895 V896 N902 P903 Q904 H905 I906 I907 Q908 P909 N913 S914 K915 F927 F932 K933 A934 L935 K936 L939 N940 E941 R942 F946 H947 E948 S949 V957 L961 Y971 P974 K979 I980 T981 T988 V989 L990

H991 N992 G993 R994 D995 K996 I997 Q998 F999 H1002 A1007 H1008 I1009 T1010 T1011 K1012 S1013 Y1016 M1019 H1020 Q1021 Q1025 V1026 F1027 MET LEU ASP THR LYS ARG LEU GLY THR PRO GLU SER VAL LYS PRO ALA ASN ALA SER HIS ALA I1049 R1050 L1051 G1054 V1055 D1058 P1059

I1062 E1063 P1064 I1065 L1066 M1067 E1068 I1069 H1070 N1071 I1072 L1073 K1074 VAL ASP SER ASN SER SER SER SER

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

Chain Ae: 7% 49% 15% 36%

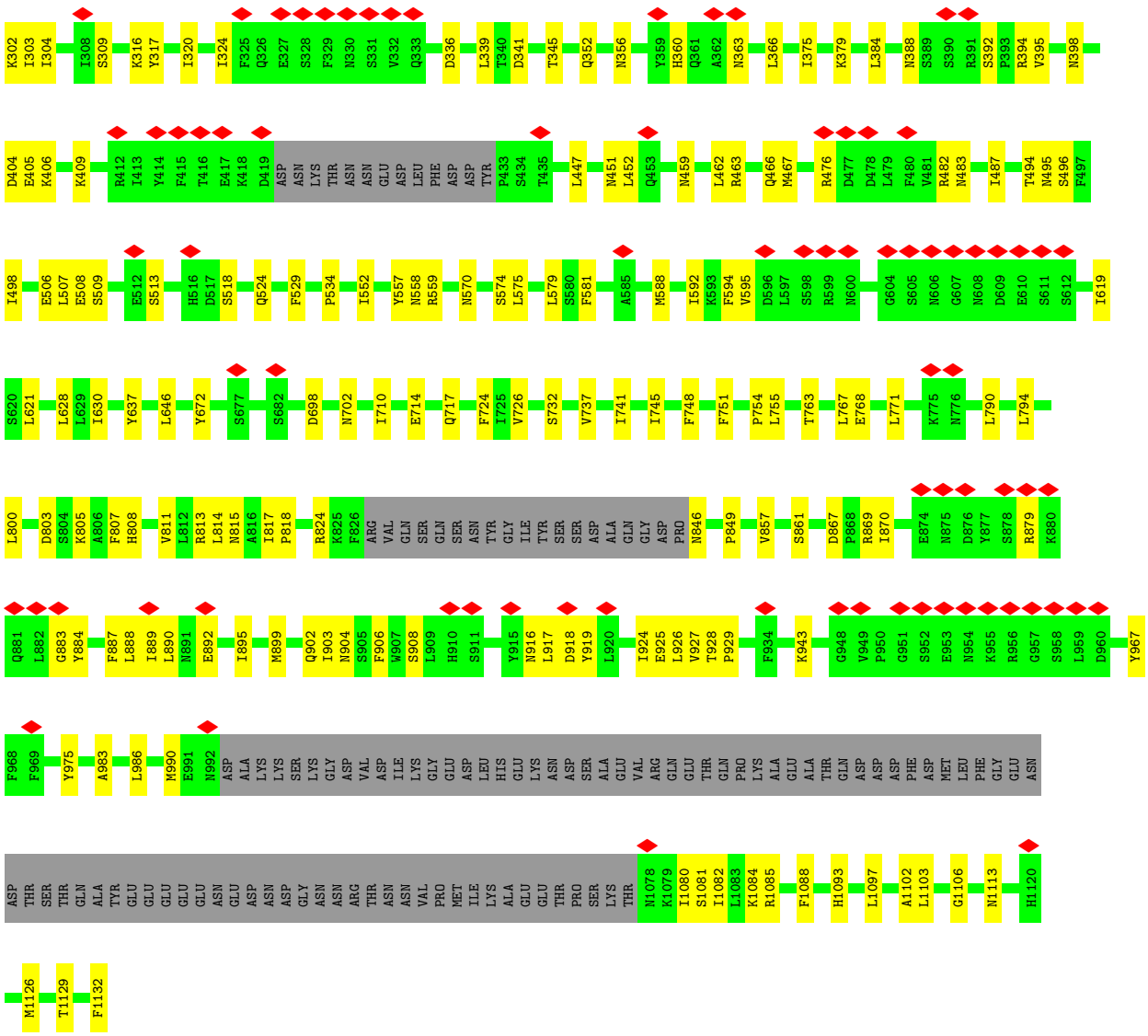
MET GLU LYS GLU SER VAL TYR ASN LEU ALA LEU LYS CYS ALA GLU ARG GLN LEU THR SER MET GLU PHE SER ASN LEU LEU TYR LYS GLU PHE PHE ASN GLU LYS PHE PRO SER LEU ILE GLN GLU GLU GLU GLU ASP THR THR THR THR ALA ASN ILE ASN GLU VAL LYS LYS ALA SER ASP

LEU VAL ASP THR PRO SER ASN ASN THR ALA ALA THR ALA ASP THR THR HIS LEU HIS GLU ALA LEU ASP ILE VAL CYS SER ASP PHE VAL LYS ILE LEU ASN LEU GLU LYS PRO LEU ILE LEU ALA ASP TYR ILE VAL GLU VAL LEU LEU VAL ASN TYR ASN SER ASP MET ILE LYS CYS

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

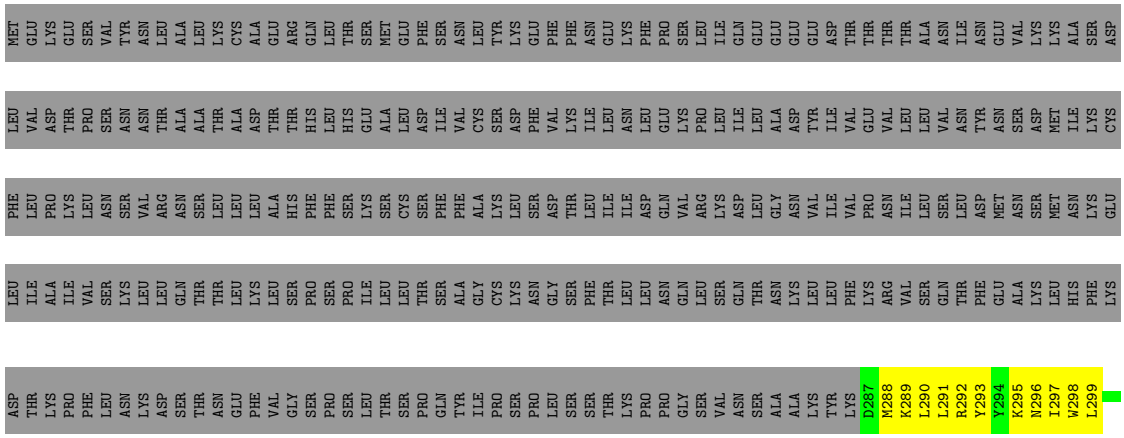
LEU ILE ALA ILE VAL SER LYS LEU LEU GLN THR THR LEU LYS LEU SER PRO SER PRO ILE LEU LEU THR SER ALA ALA GLY CYS LYS ASN GLY SER PHE THR LEU LEU ASN GLN LEU SER GLN THR ASN LYS LEU LEU PHE LYS ARG VAL SER GLN THR PHE GLU ALA LYS LEU HIS PHE LYS

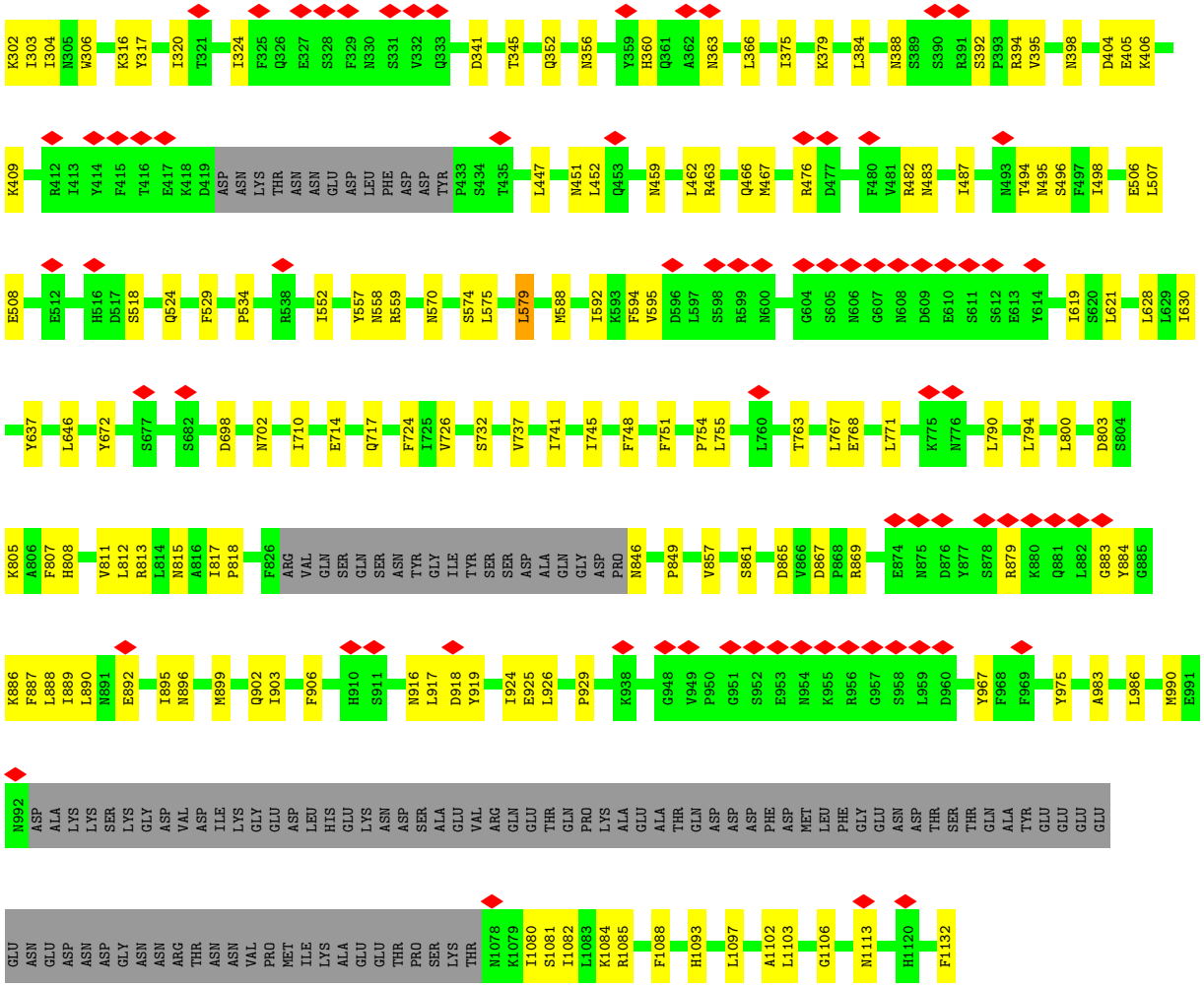
ASP THR LYS PRO PHE LEU ASN LYS ASP SER THR ASN GLU PHE VAL GLY SER PRO SER LEU THR SER PRO GLN TYR ILE PRO SER PRO LEU SER SER THR LYS PRO PRO GLY SER VAL ASN SER ALA ALA LYS TYR LYS D287 M288 K289 L290 L291 R292 Y293 Y294 K295 N296 I297 W298 L299



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

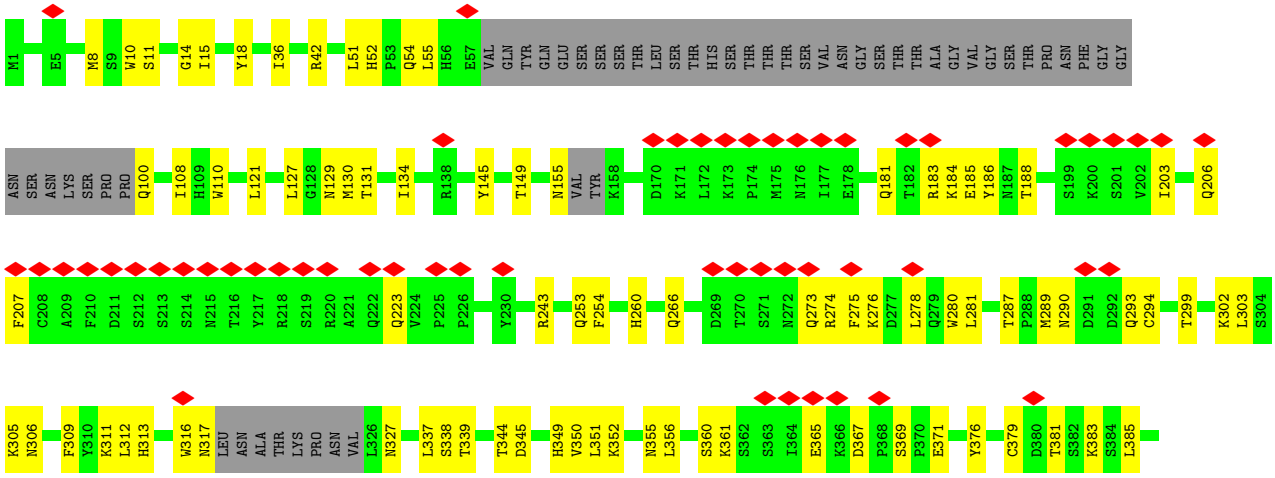
Chain Be:

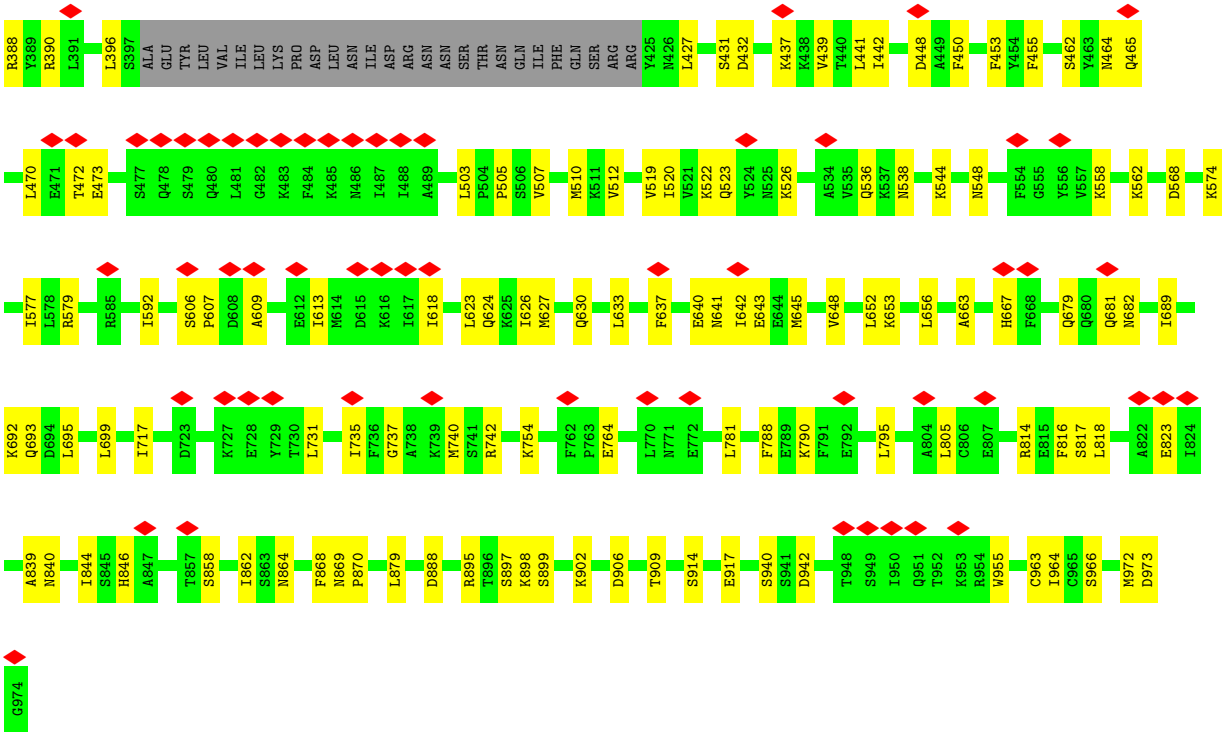




- Molecule 8: Mediator of RNA polymerase II transcription subunit 16

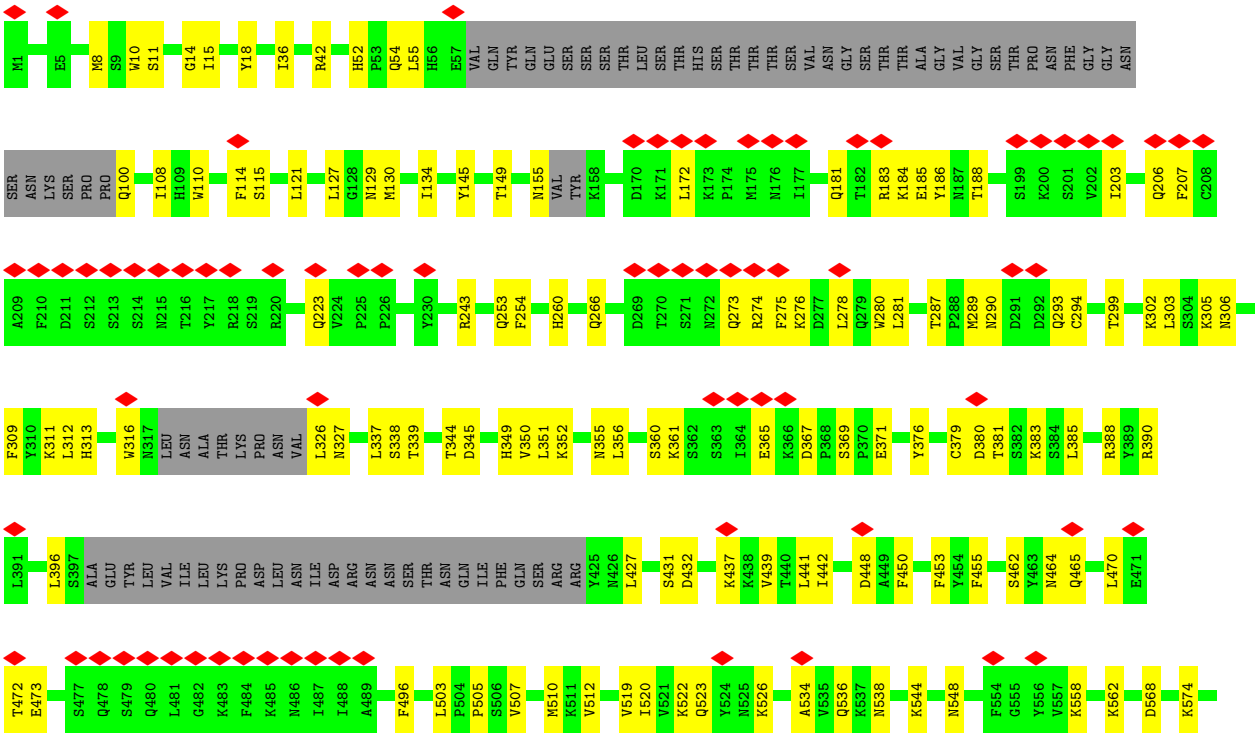
Chain Ap:

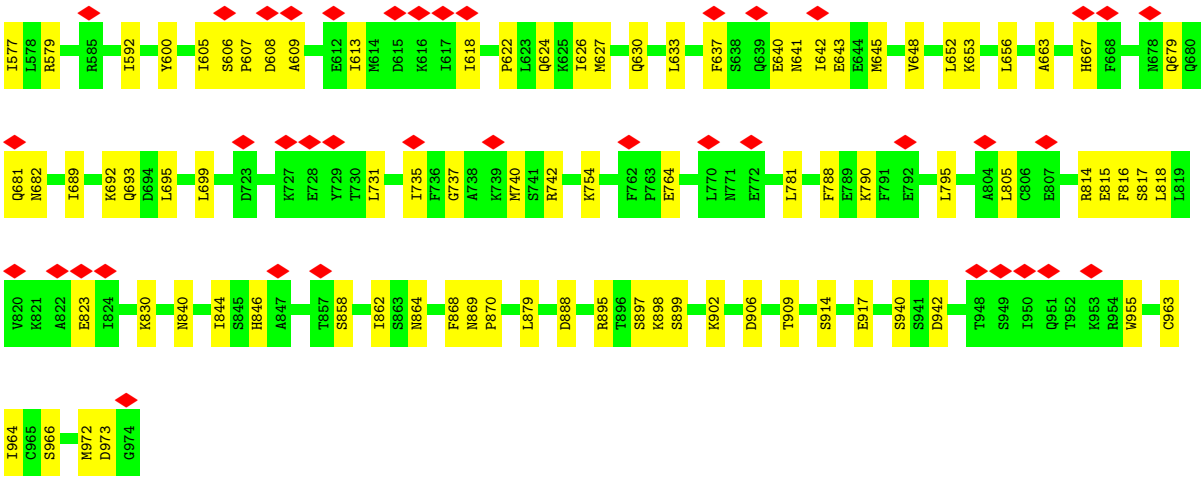




• Molecule 8: Mediator of RNA polymerase II transcription subunit 16

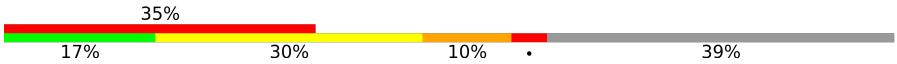
Chain Bp:

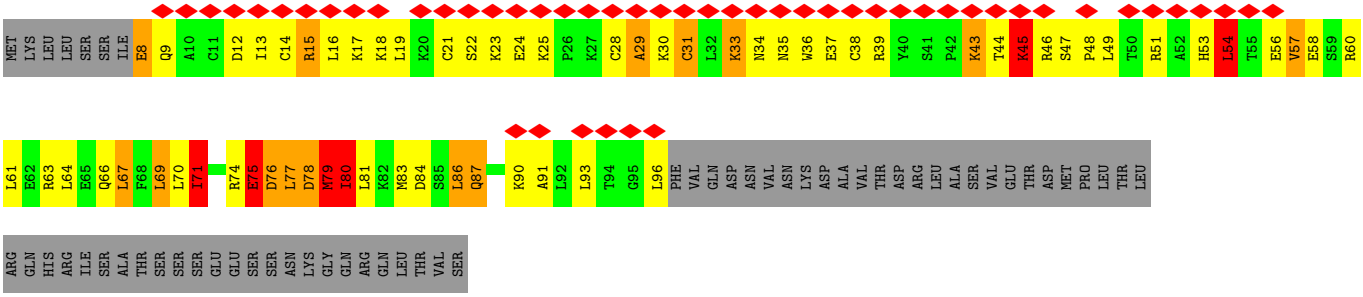




- Molecule 9: Regulatory protein GAL4

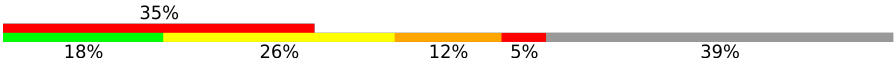
Chain GA:

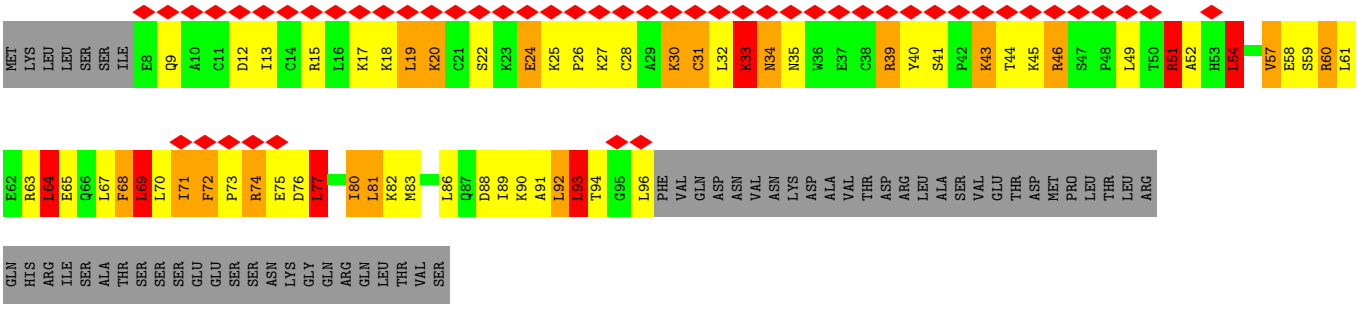




- Molecule 9: Regulatory protein GAL4

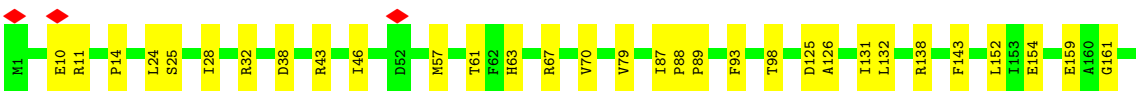
Chain GB:

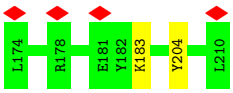




- Molecule 10: Mediator of RNA polymerase II transcription subunit 20

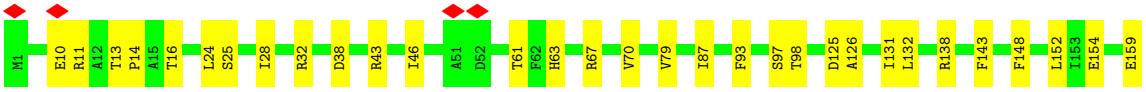
Chain At:

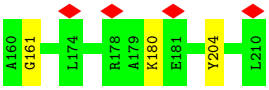




• Molecule 10: Mediator of RNA polymerase II transcription subunit 20

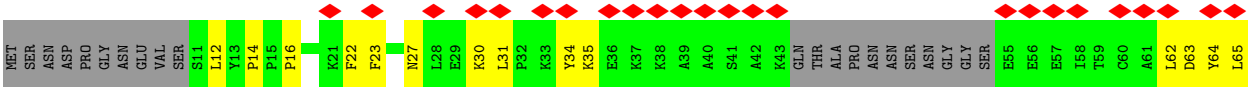
Chain Bt:

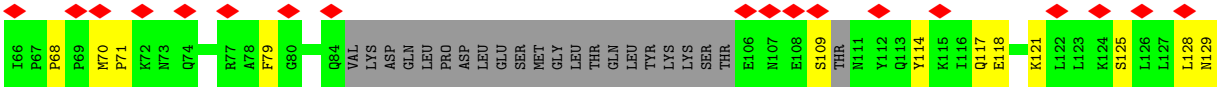


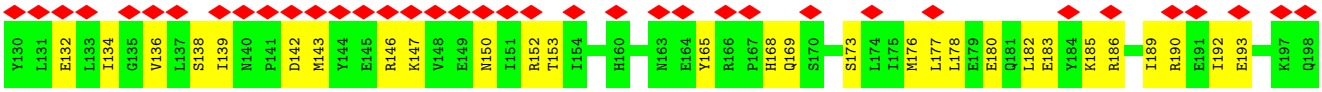


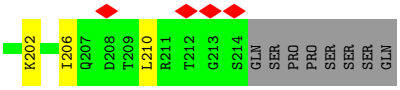
• Molecule 11: Mediator of RNA polymerase II transcription subunit 7

Chain Ag:



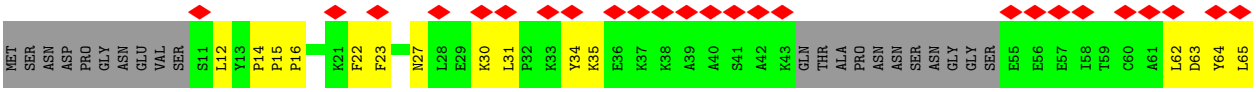


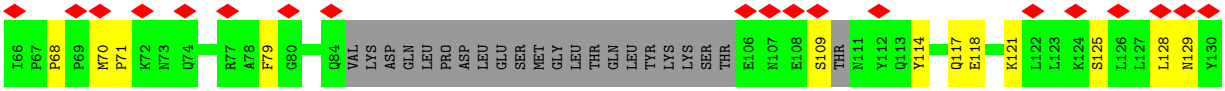


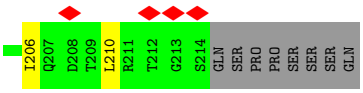


• Molecule 11: Mediator of RNA polymerase II transcription subunit 7

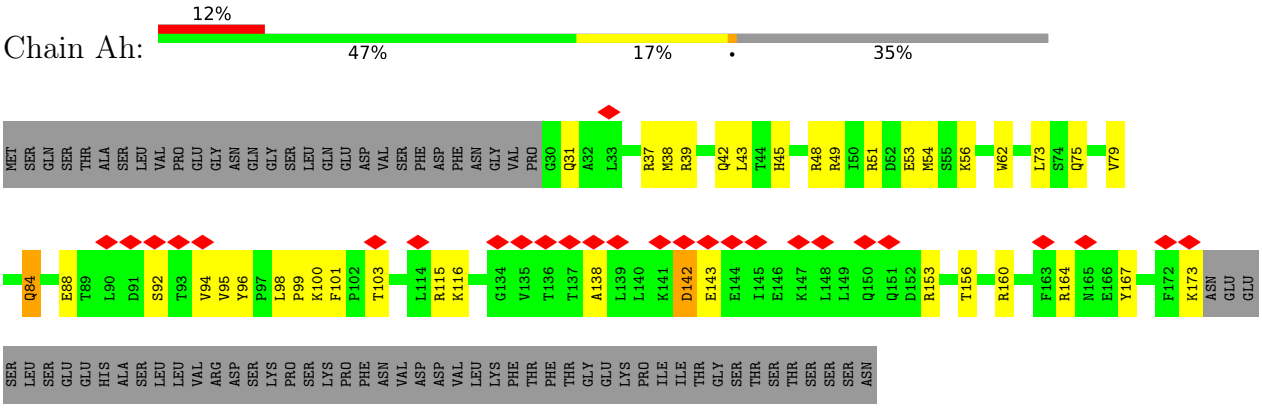
Chain Bg:



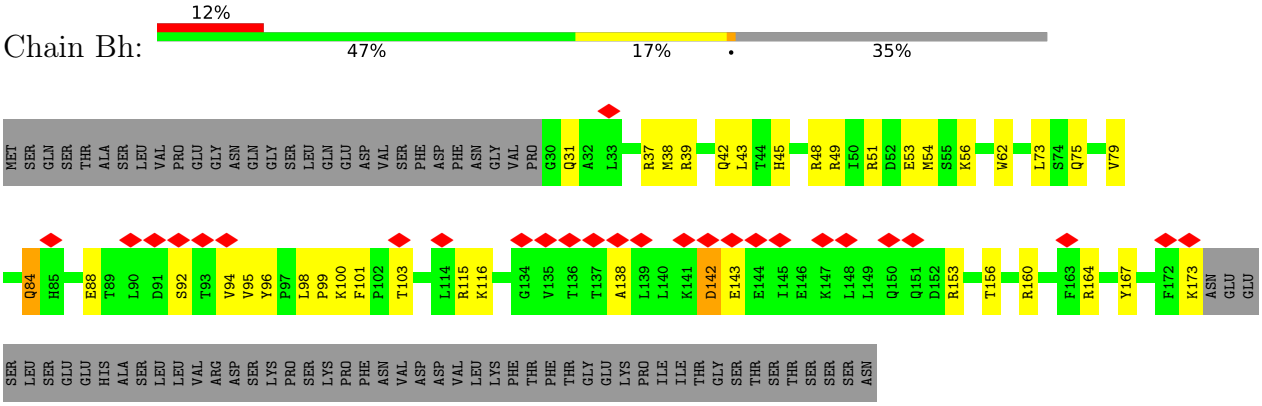




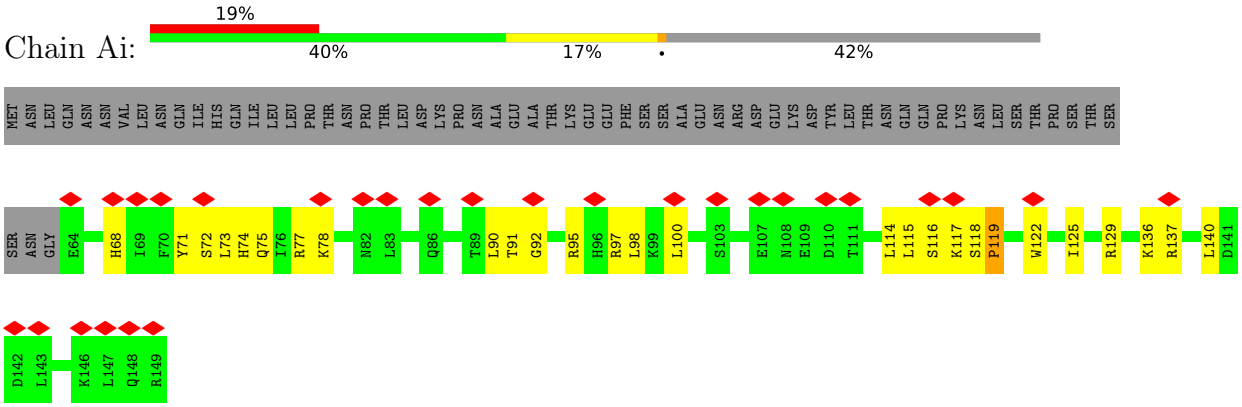
• Molecule 12: Mediator of RNA polymerase II transcription subunit 8



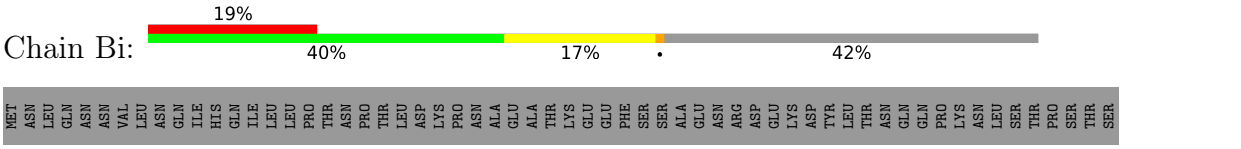
• Molecule 12: Mediator of RNA polymerase II transcription subunit 8

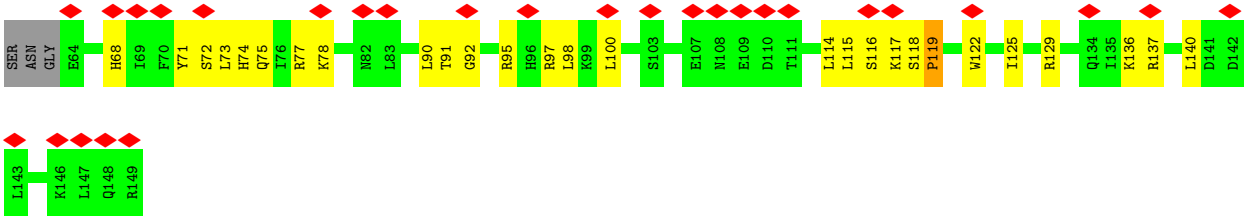


• Molecule 13: Mediator of RNA polymerase II transcription subunit 9



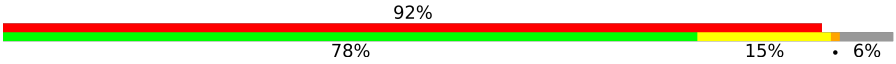
• Molecule 13: Mediator of RNA polymerase II transcription subunit 9

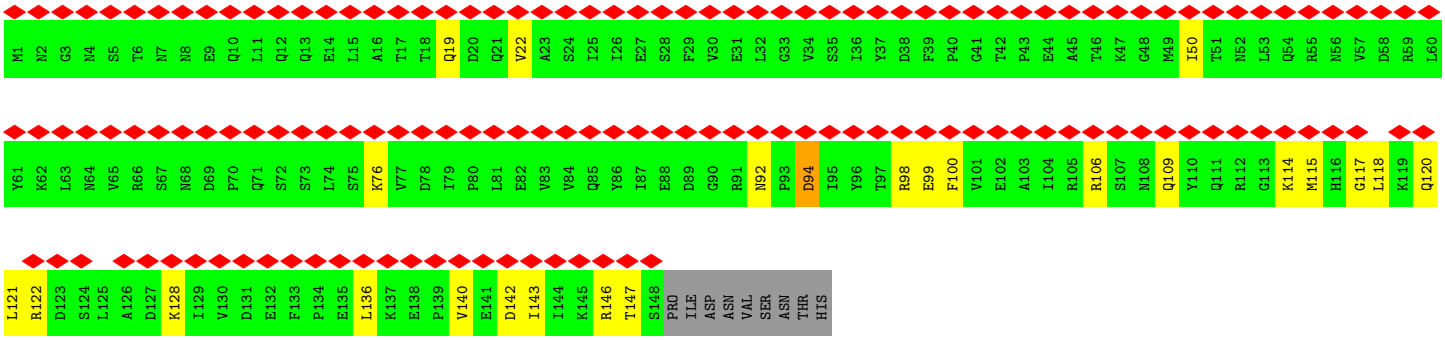




• Molecule 14: Mediator of RNA polymerase II transcription subunit 10

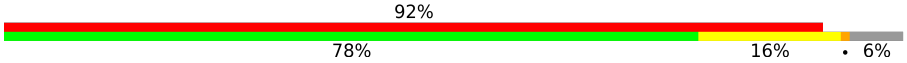
Chain Aj:

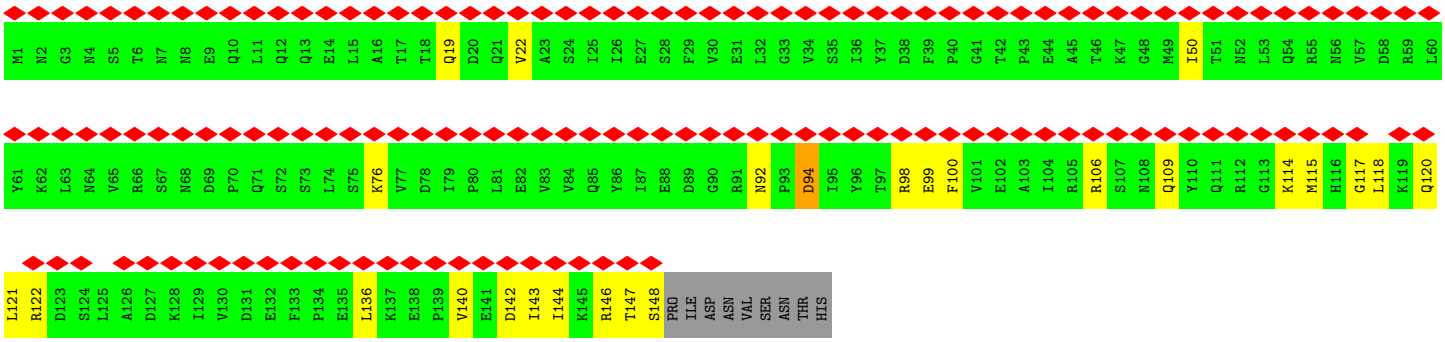




• Molecule 14: Mediator of RNA polymerase II transcription subunit 10

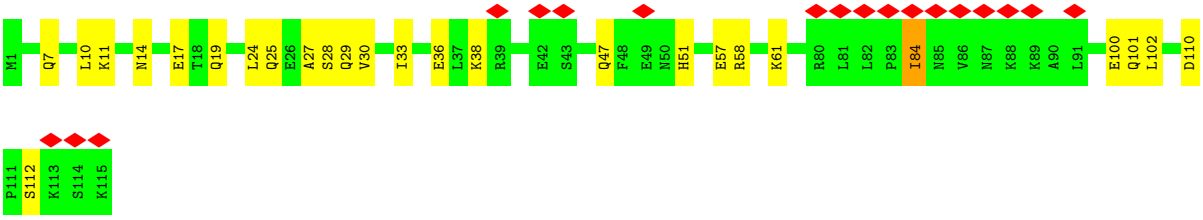
Chain Bj:





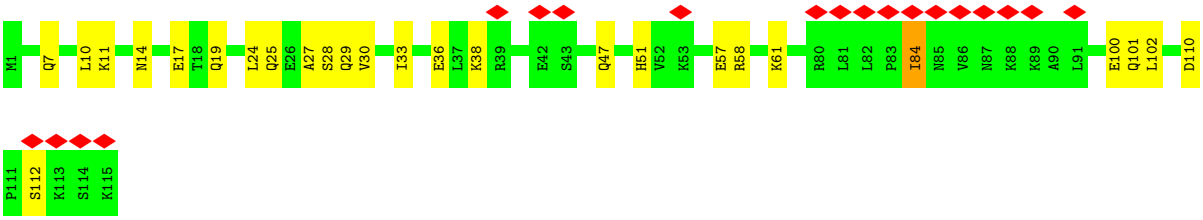
• Molecule 15: Mediator of RNA polymerase II transcription subunit 11

Chain Ak:



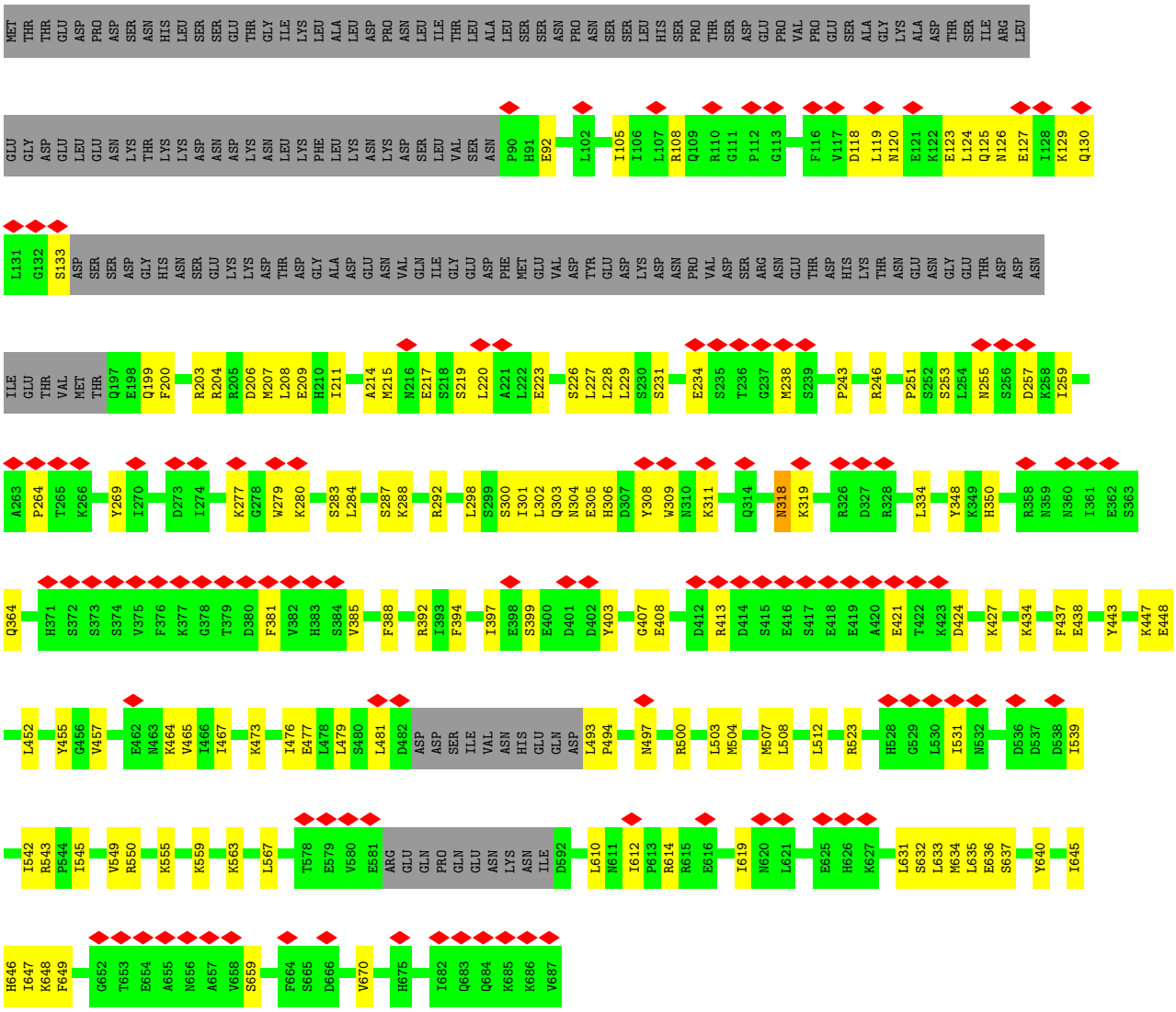
• Molecule 15: Mediator of RNA polymerase II transcription subunit 11

Chain Bk: 17% 77% 22%



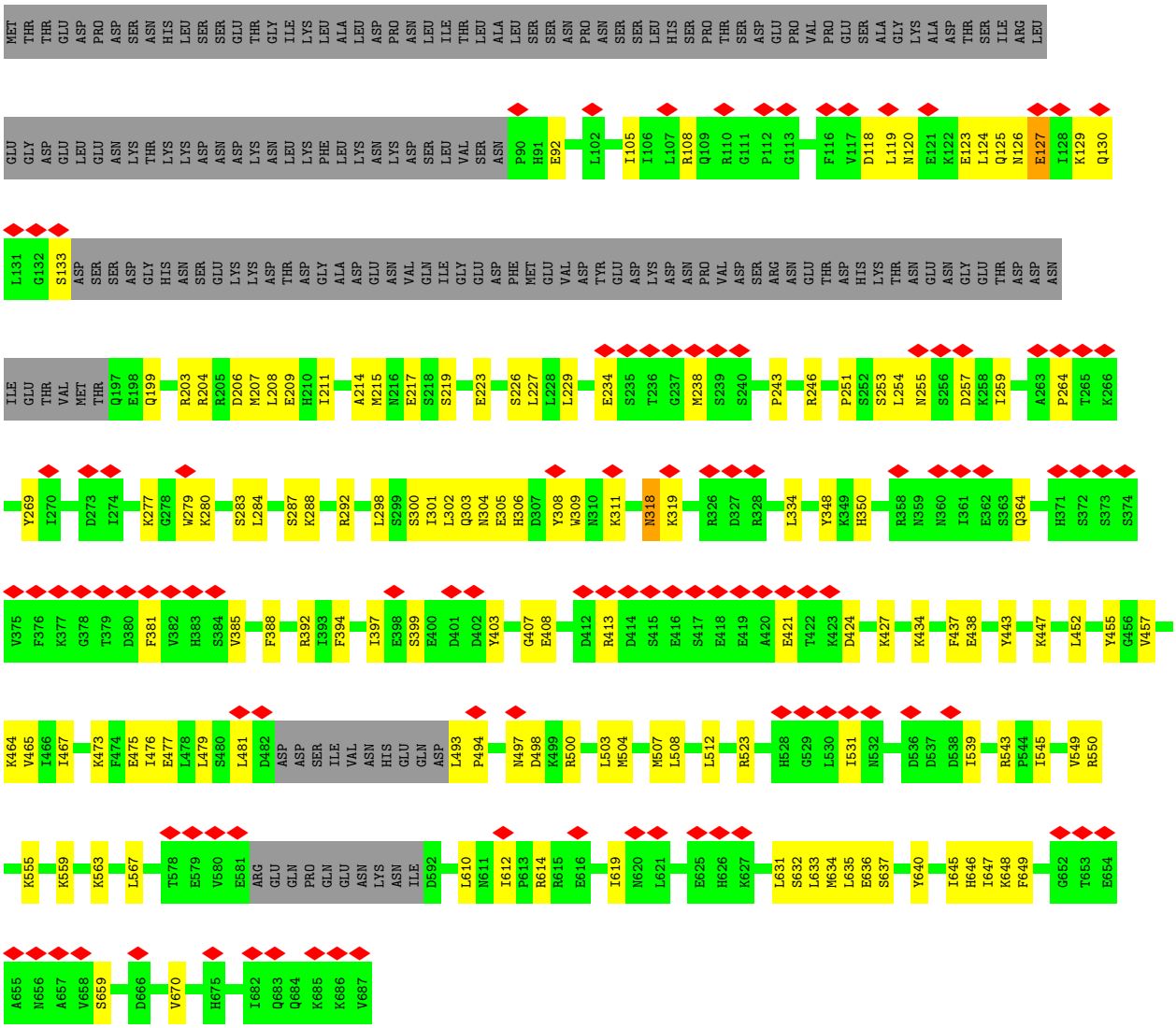
- Molecule 16: Mediator of RNA polymerase II transcription subunit 17

Chain Aq: 17% 54% 20% 25%



- Molecule 16: Mediator of RNA polymerase II transcription subunit 17

Chain Bq: 16% 55% 20% 25%

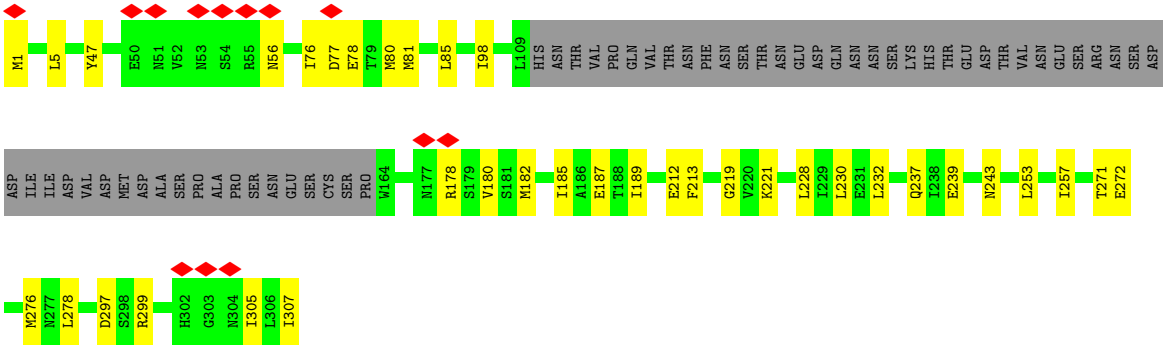


• Molecule 17: Mediator of RNA polymerase II transcription subunit 18

Chain Ar:

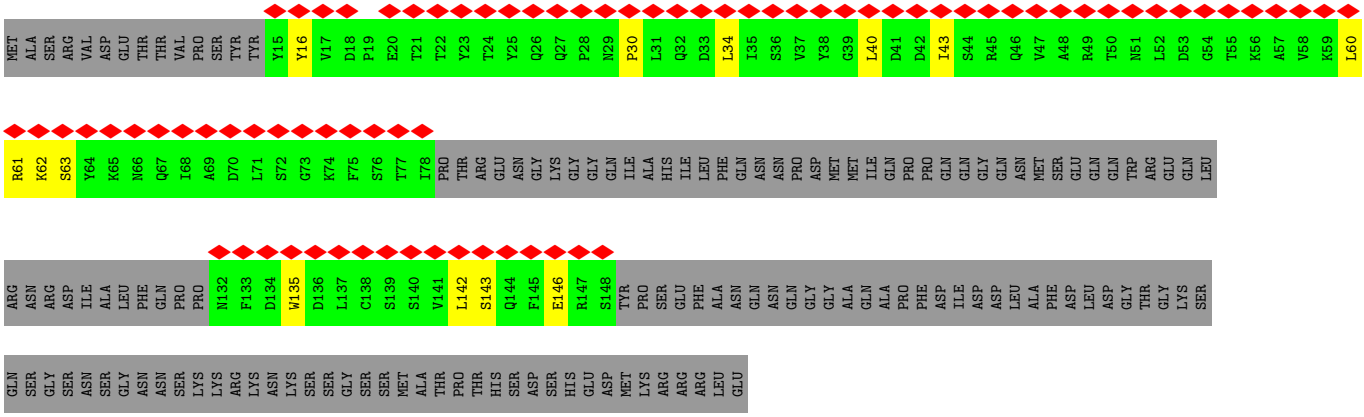
• Molecule 17: Mediator of RNA polymerase II transcription subunit 18

Chain Br:



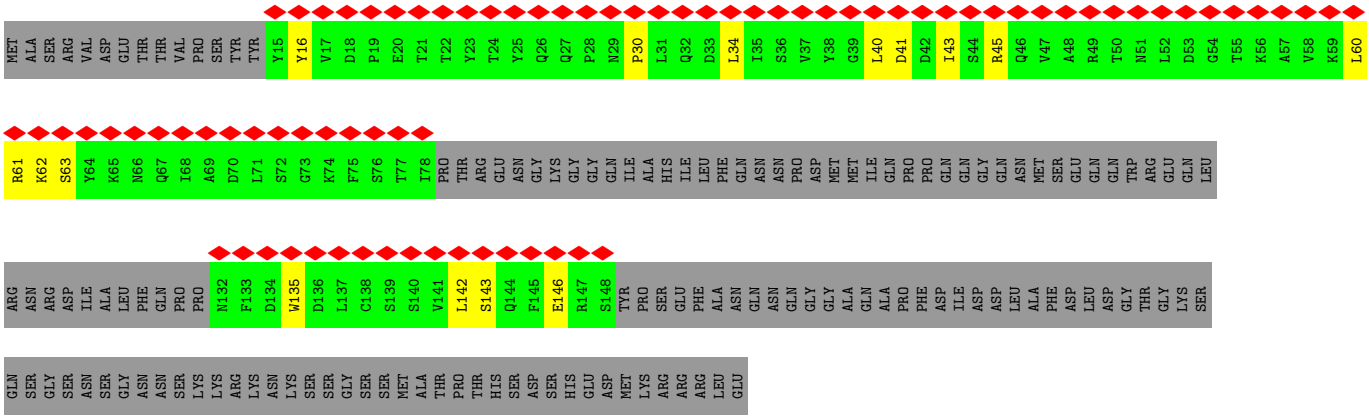
- Molecule 18: Mediator of RNA polymerase II transcription subunit 19

Chain As:



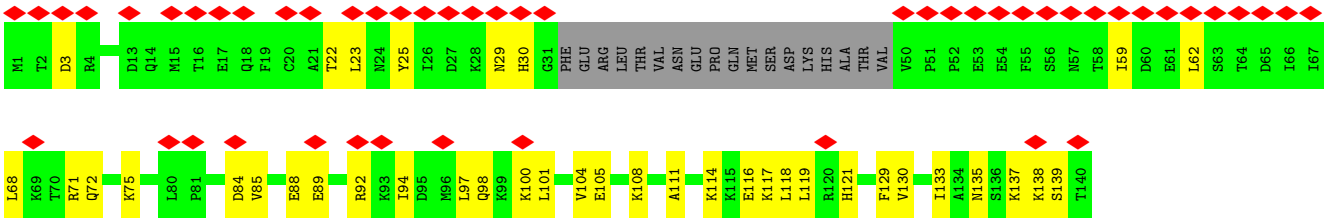
- Molecule 18: Mediator of RNA polymerase II transcription subunit 19

Chain Bs:



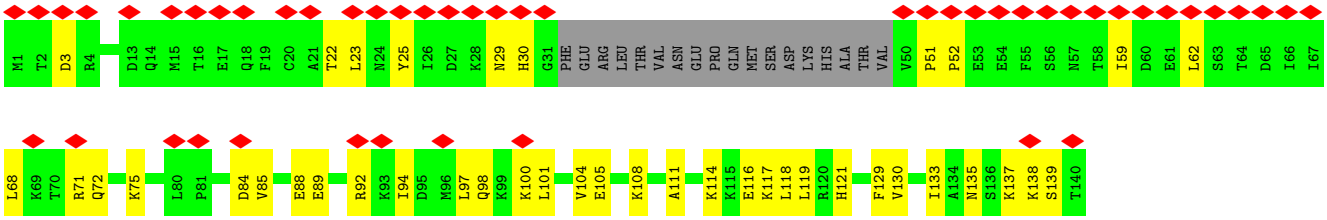
- Molecule 19: Mediator of RNA polymerase II transcription subunit 21

Chain Au:



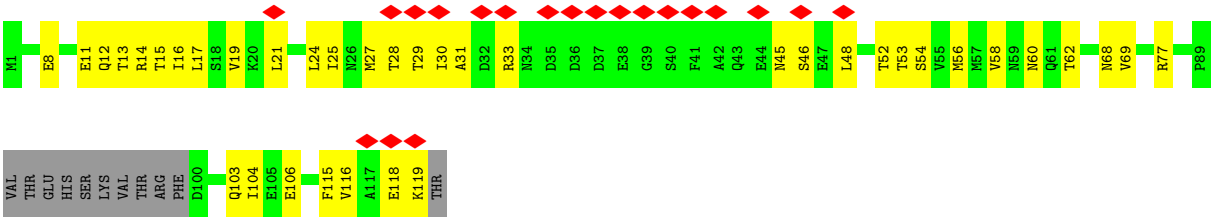
• Molecule 19: Mediator of RNA polymerase II transcription subunit 21

Chain Bu:



• Molecule 20: Mediator of RNA polymerase II transcription subunit 22

Chain Av:

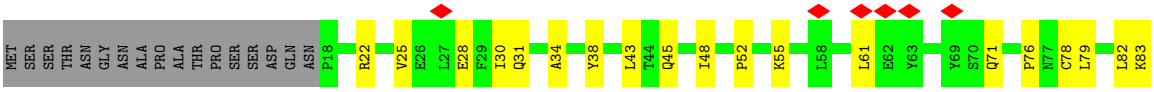


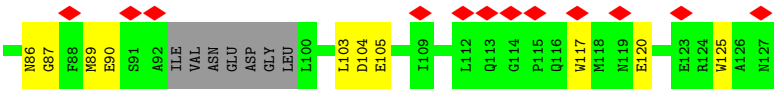
• Molecule 20: Mediator of RNA polymerase II transcription subunit 22

Chain Bv:

• Molecule 21: Mediator of RNA polymerase II transcription subunit 31

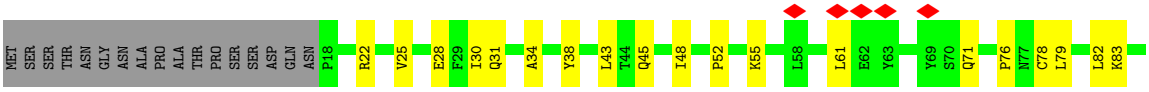
Chain Aw:

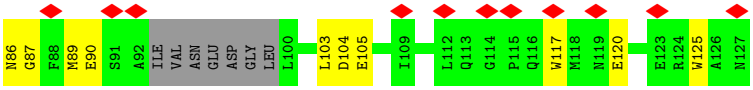




• Molecule 21: Mediator of RNA polymerase II transcription subunit 31

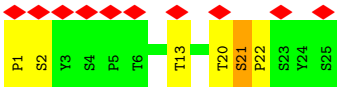
Chain Bw:





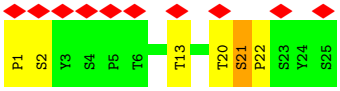
• Molecule 22: DNA-directed RNA polymerase II subunit RPB1

Chain Az:



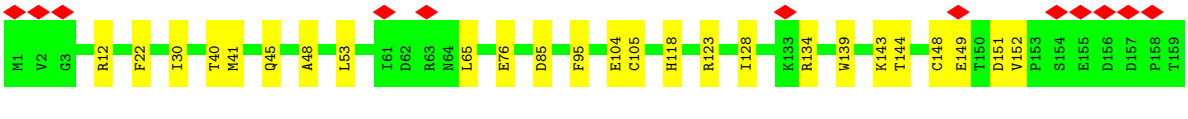
• Molecule 22: DNA-directed RNA polymerase II subunit RPB1

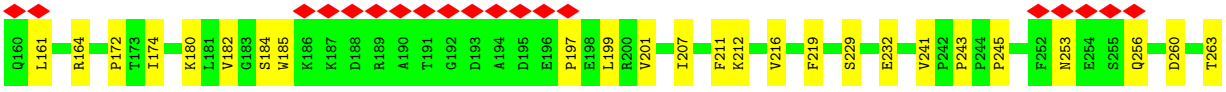
Chain Bz:

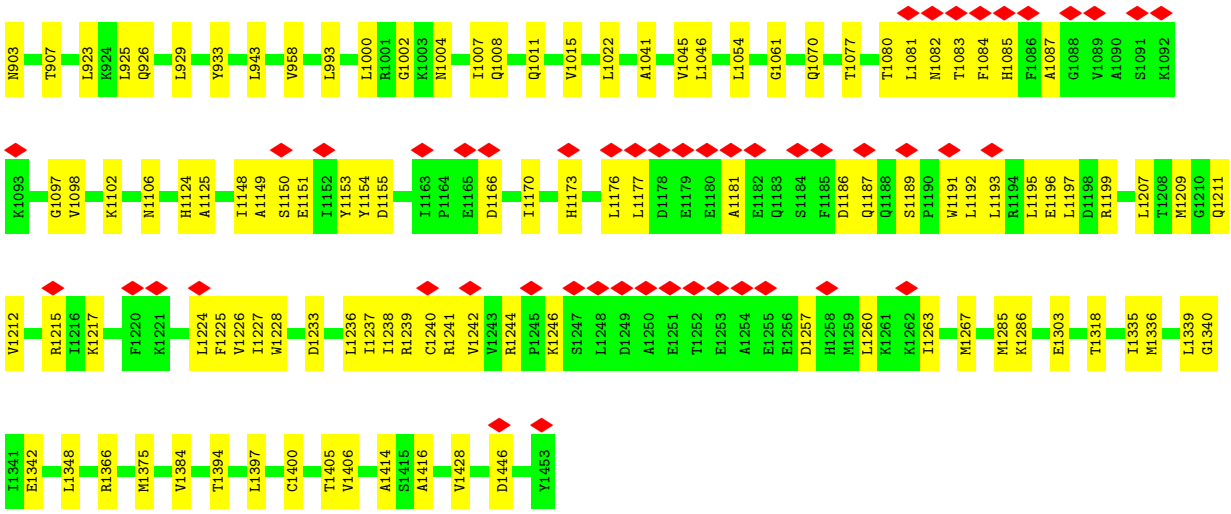


• Molecule 23: DNA-directed RNA polymerase II subunit RPB1

Chain AA:

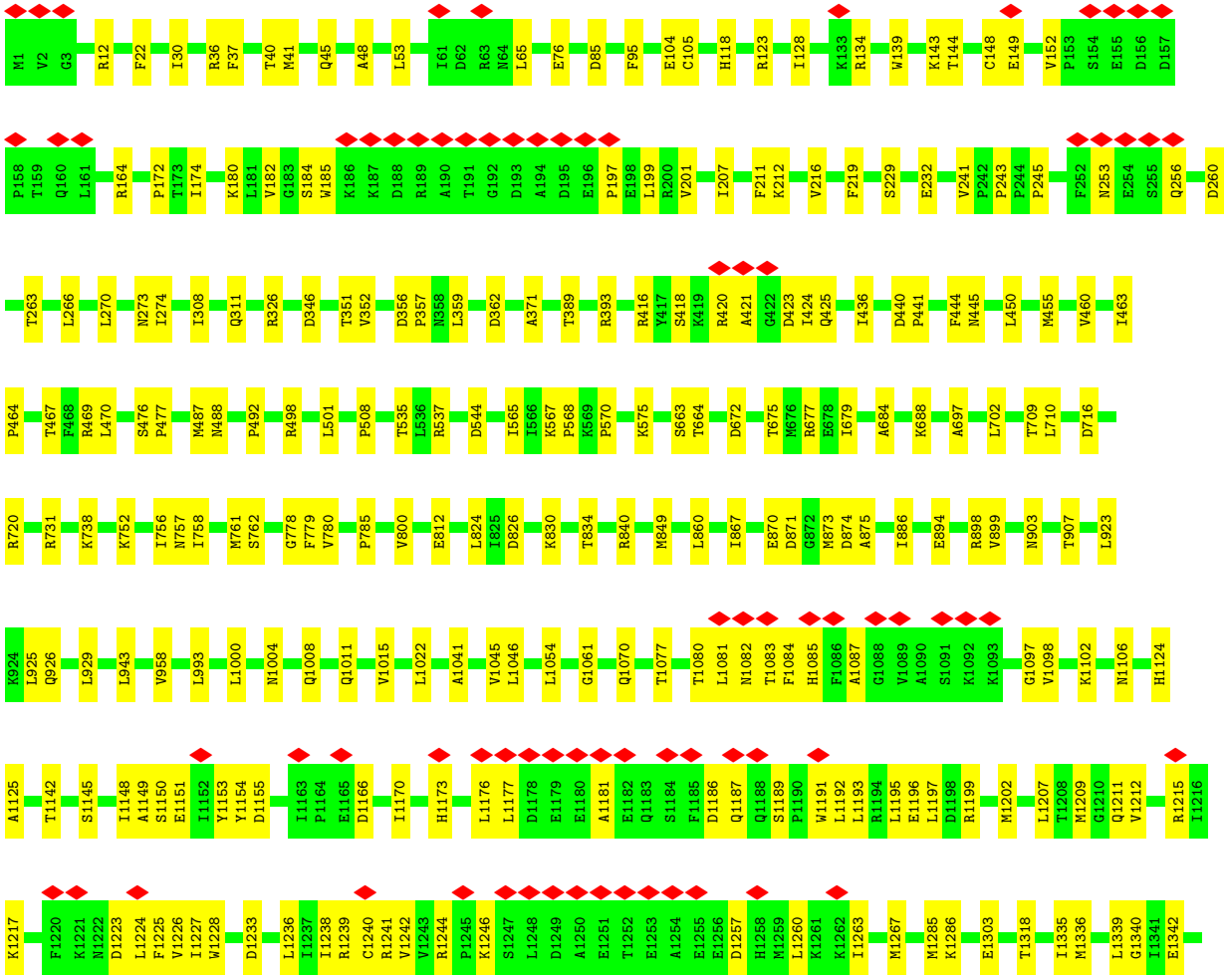


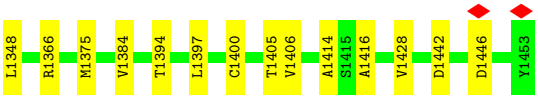




- Molecule 23: DNA-directed RNA polymerase II subunit RPB1

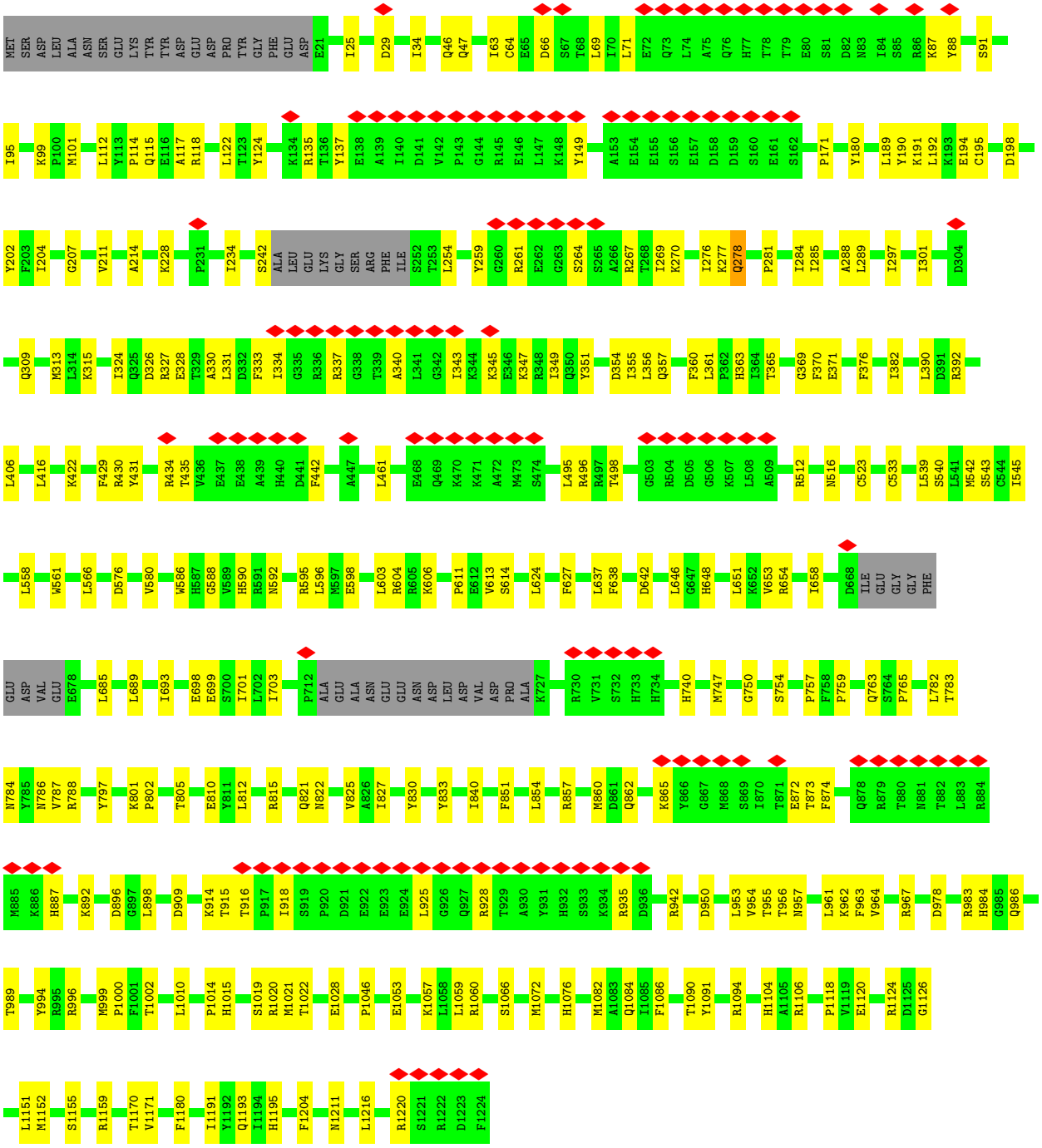
Chain BA:





• Molecule 24: DNA-directed RNA polymerase II subunit RPB2

Chain AB:



• Molecule 24: DNA-directed RNA polymerase II subunit RPB2

Chain BB: 10% 74% 21% •

MET SER ASP LEU ALA ASN SER GLU LYS TYR TYR ASP GLU ASP PRO TYR GLY PHE GLU ASP E21 I25 D29 V33 I34 Q46 Q47 I63 C64 S67 T68 L69 I70 L71 E72 Q73 L74 A75 Q76 H77 T78 T79 E80 S81 D82 N83 I84 S85 R86 K87 Y88 S91

I95 T98 K99 P100 M101 L112 Y113 P114 Q115 E116 A117 R118 L122 T123 Y124 S125 S126 R135 T136 Y137 E138 A139 I140 D141 V142 P143 G144 R145 E146 L147 K148 Y149 A153 E154 E155 S156 E157 D158 D159 S160 E161 S162 P171 Y180 L189 Y190 K191 L192 K193 E194 C195

D198 Y202 F203 I204 G207 V211 A214 K228 I234 S242 ALA LEU GLU LYS GLY SER ARG PHE ILE S252 T253 L254 Y259 G260 R261 E262 G263 S264 S265 A266 R267 T268 I269 K270 I276 K277 Q278 P281 I284 I285 A288 L289 I297 I301 D304

D307 W308 Q309 M310 M313 L314 K315 I324 Q325 D326 R327 E328 T329 A330 L331 D332 F333 I334 G335 R336 R337 G338 T339 A340 L341 G342 I343 K344 K345 E346 K347 R348 I349 Q350 Y351 D354 I355 L356 Q357 F360 L361 P362 H363 I364 T365 G369 F370 E371 F376 I382 L390

D391 R392 F429 R430 Y431 R434 T435 V436 E437 E438 A439 H440 D441 F442 A447 L461 E468 Q469 K470 K471 A472 M473 S474 L495 R496 R497 T498 G503 R504 D505 G506 K507 L508 A509 R512 N516 C523 C533 L539 S540 L541 M542 S543 L558 W561

L566 D576 V580 W586 H587 G588 V589 H590 R591 N592 R595 L596 M597 E598 T602 L603 R604 R605 K606 P611 E612 V613 S614 L624 F627 L637 F638 D642 L646 G647 H648 L651 K652 V653 R654 I658 D668 ILE GLU GLY GLY GLY PHE GLU ASP VAL GLU

E678 L685 L689 I693 E698 E699 S700 I701 L702 I703 P712 ALA GLU ALA ASN GLU GLU ASN ASP LEU ASP VAL ASP PRO ALA K727 R730 V731 S732 H733 H734 H740 C741 M747 G750 S754 P757 F758 P759 Q763 S764 P765 L782 T783 N784 Y785 N786

V787 R788 Y797 K801 E810 Y811 L812 R815 Q821 N822 V825 A826 I827 Y830 Y833 I840 F851 L854 R857 M860 D861 Q862 E863 K864 K865 Y866 G867 M868 S869 I870 T871 E872 T873 F874 Q878 R879 T880 N881 T882 L883 R884 M885 K886 H887 D896

G897 L898 K914 T915 T916 P917 I918 S919 P920 D921 E922 E923 E924 L925 G926 Q927 R928 T929 A930 Y931 H932 S933 K934 R935 D936 R942 S943 D950 L953 V954 T955 T956 N957 L961 K962 F963 V964 R967 D978 R983 H984 G985 Q986 Y994 R995 R996 M999 P1000 F1001 T1002

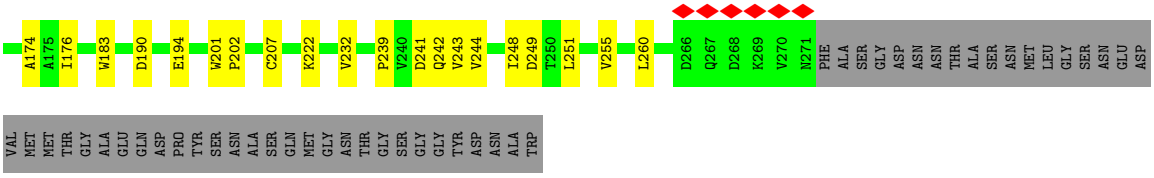
L1010 P1014 H1015 S1019 R1020 M1021 T1022 E1028 P1046 E1053 K1067 L1068 L1059 R1060 S1066 M1072 H1076 M1082 A1083 Q1084 I1085 F1086 T1090 Y1091 R1094 H1104 A1105 R1106 P1118 V1119 E1120 R1124 D1125 G1126 L1151 M1152 S1155 R1159 T1170 V1171

F1180 I1191 Y1192 Q1193 I1194 H1195 F1204 N1211 L1216 R1220 S1221 R1222 D1223 F1224

• Molecule 25: DNA-directed RNA polymerase II subunit RPB3

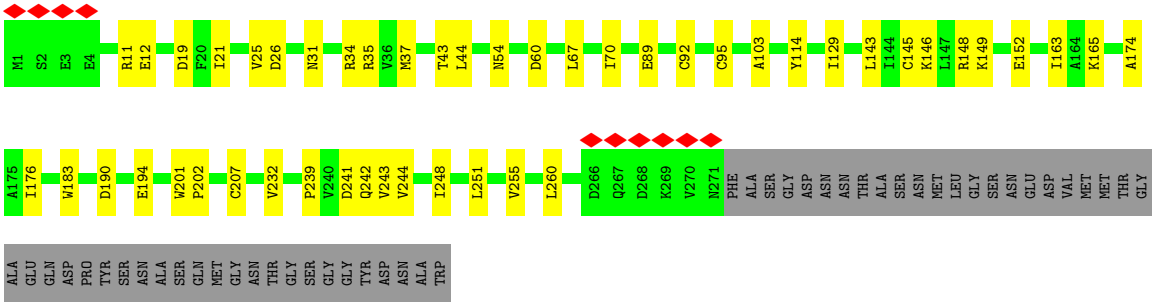
Chain AC: • 69% 16% 15%

M1 S2 E3 E4 R11 E12 D19 F20 I21 V25 D26 N31 R34 R35 V36 M37 T43 L44 N54 D60 L67 I70 E89 C92 C95 A103 E108 Y114 I129 L143 I144 C145 K146 L147 R148 K149 E152 I163 A164 K165



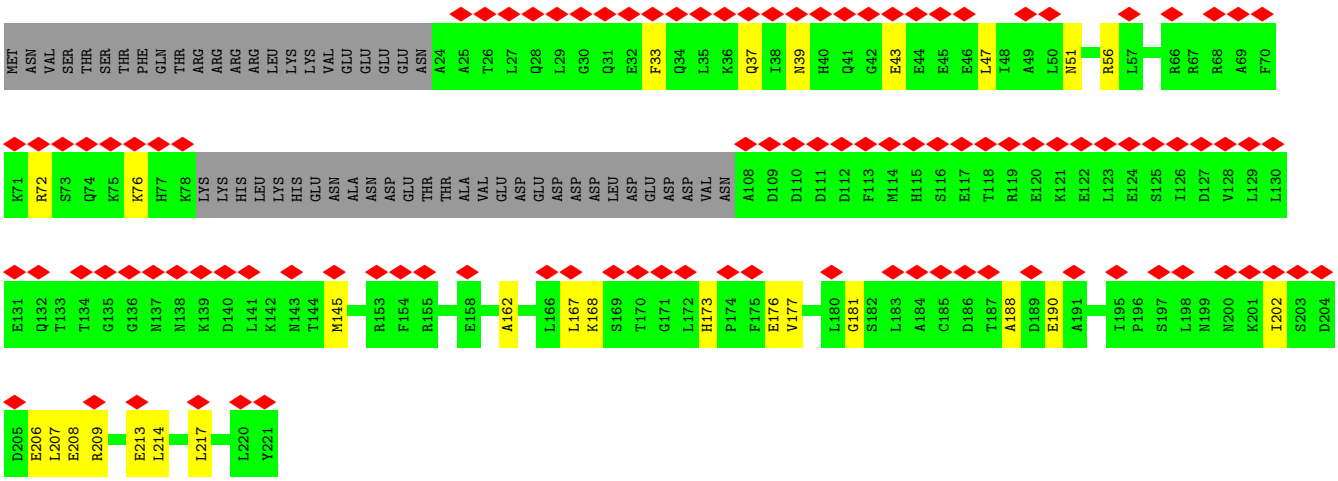
• Molecule 25: DNA-directed RNA polymerase II subunit RPB3

Chain BC:



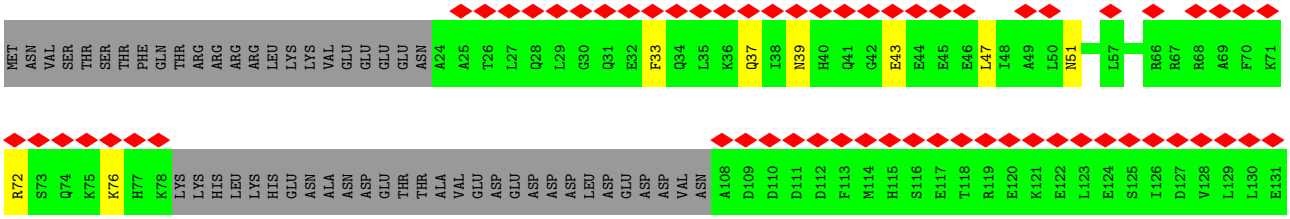
• Molecule 26: DNA-directed RNA polymerase II subunit RPB4

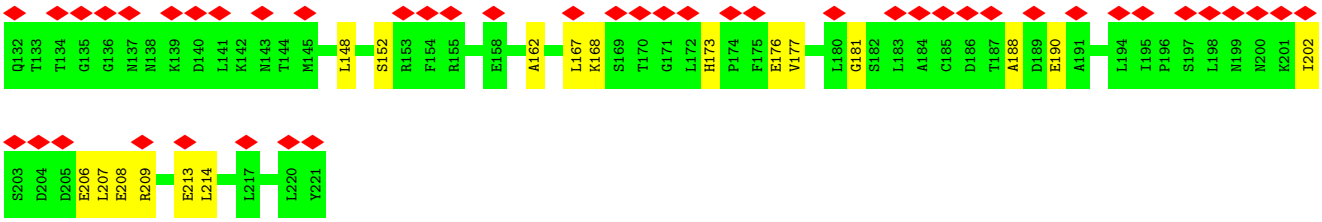
Chain AD:



• Molecule 26: DNA-directed RNA polymerase II subunit RPB4

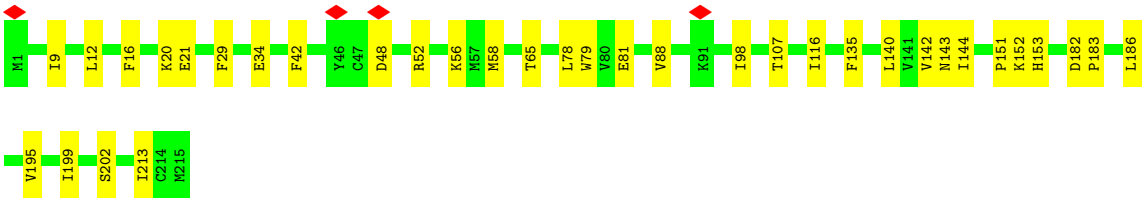
Chain BD:





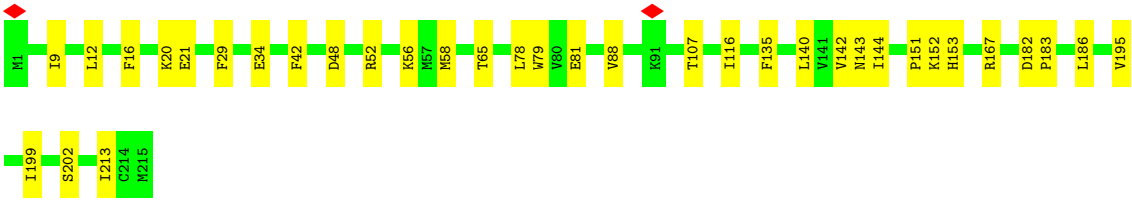
• Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain AE:



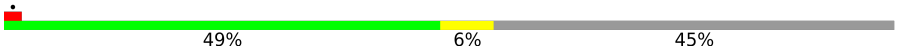
• Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC1

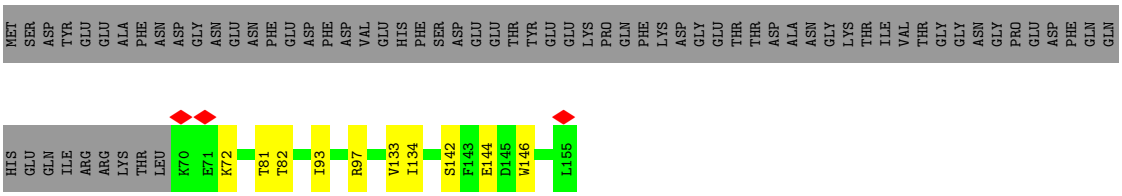
Chain BE:



• Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC2

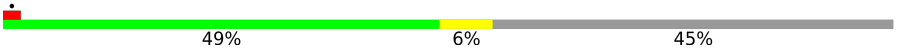
Chain AF:

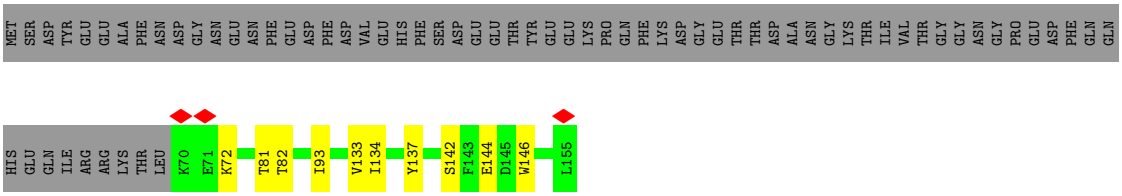




• Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC2

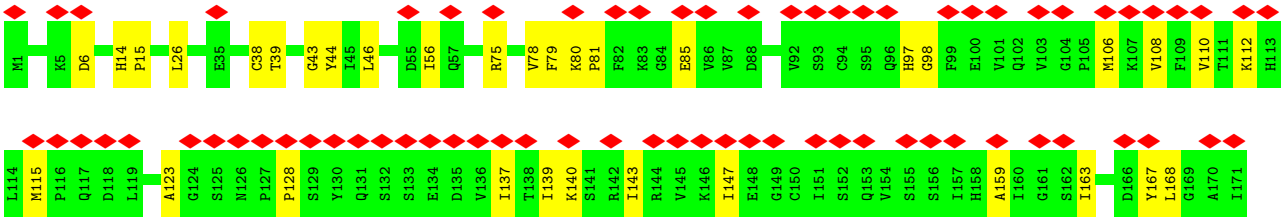
Chain BF:





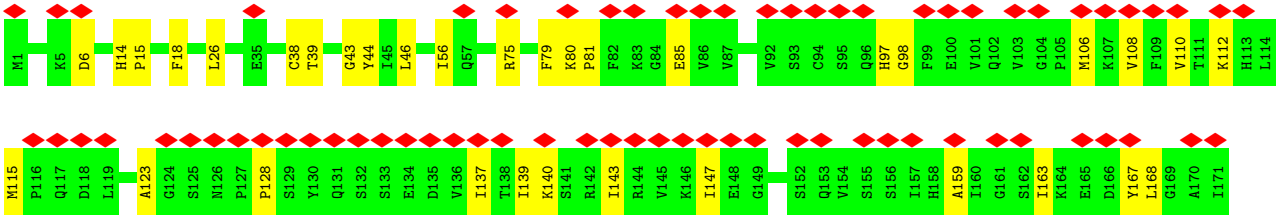
• Molecule 29: DNA-directed RNA polymerase II subunit RPB7

Chain AG: 42% 80% 20%



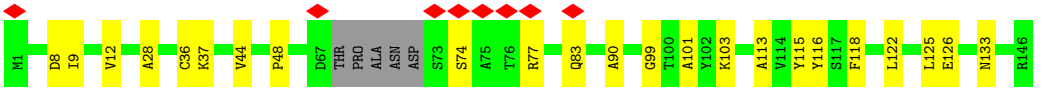
- Molecule 29: DNA-directed RNA polymerase II subunit RPB7

Chain BG: 41% 80% 20%



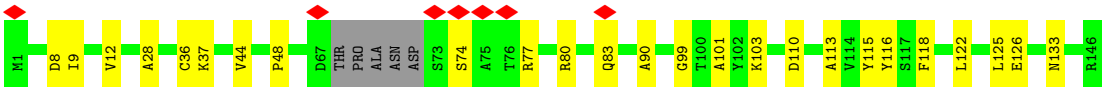
- Molecule 30: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain AH: 5% 81% 16%



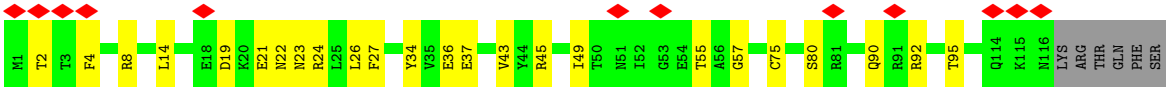
- Molecule 30: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain BH: 5% 79% 17%



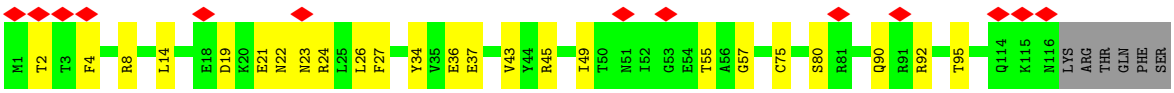
- Molecule 31: DNA-directed RNA polymerase II subunit RPB9

Chain AI: 10% 75% 20% 5%



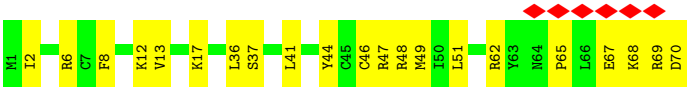
- Molecule 31: DNA-directed RNA polymerase II subunit RPB9

Chain BI: 11% 75% 20% 5%



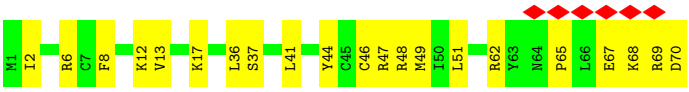
• Molecule 32: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain AJ:



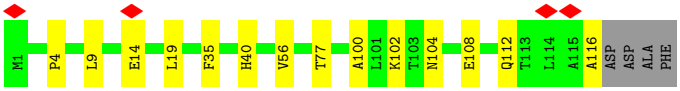
• Molecule 32: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain BJ:



• Molecule 33: DNA-directed RNA polymerase II subunit RPB11

Chain AK:

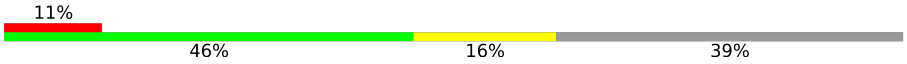


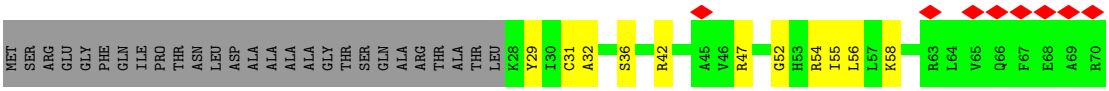
• Molecule 33: DNA-directed RNA polymerase II subunit RPB11

Chain BK:

• Molecule 34: DNA-directed RNA polymerases I, II, and III subunit RPABC4

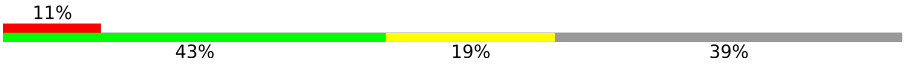
Chain AL:

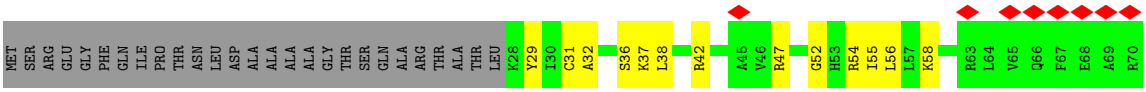




• Molecule 34: DNA-directed RNA polymerases I, II, and III subunit RPABC4

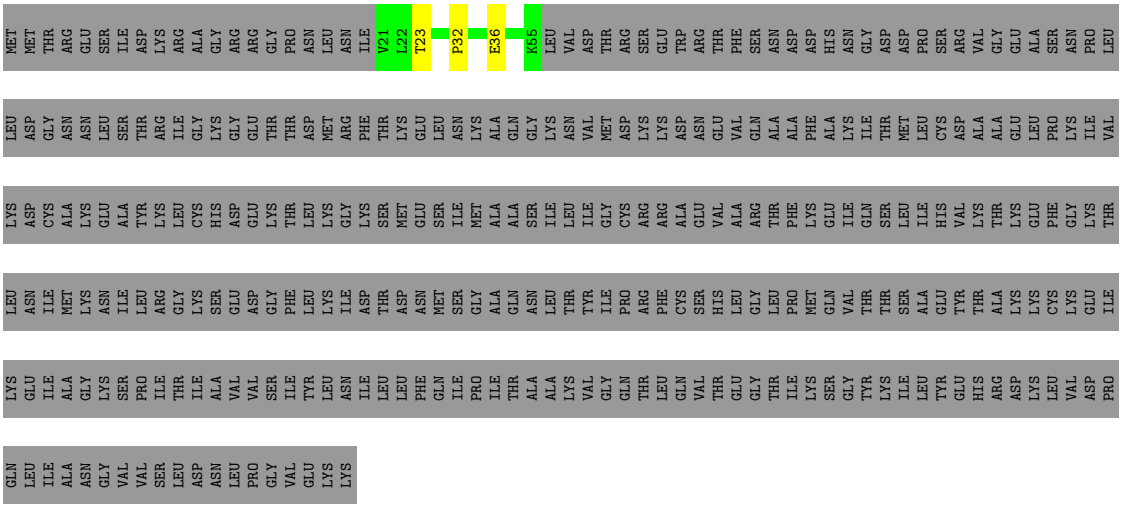
Chain BL:





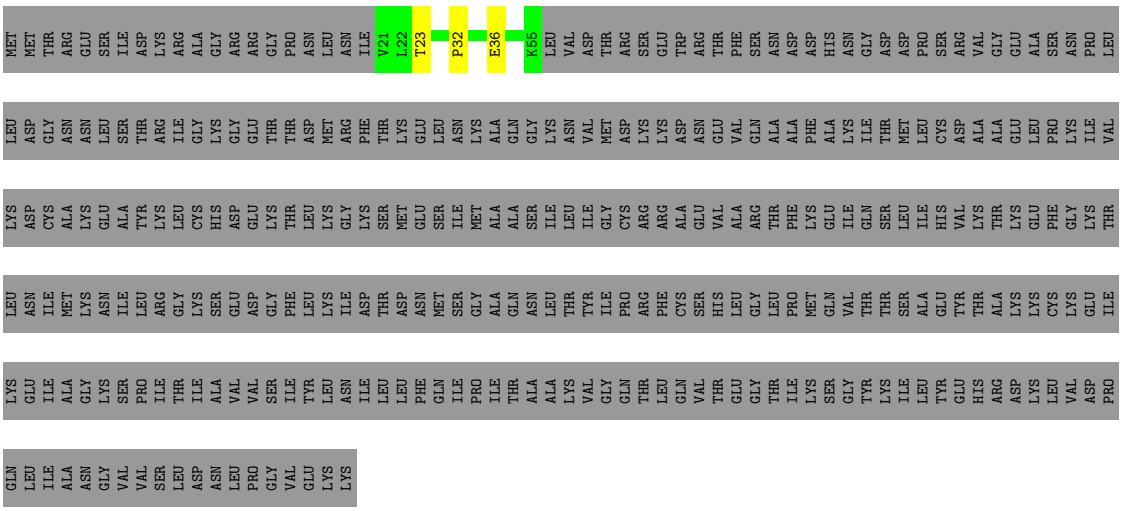
• Molecule 35: Transcription initiation factor IIB

Chain AM:



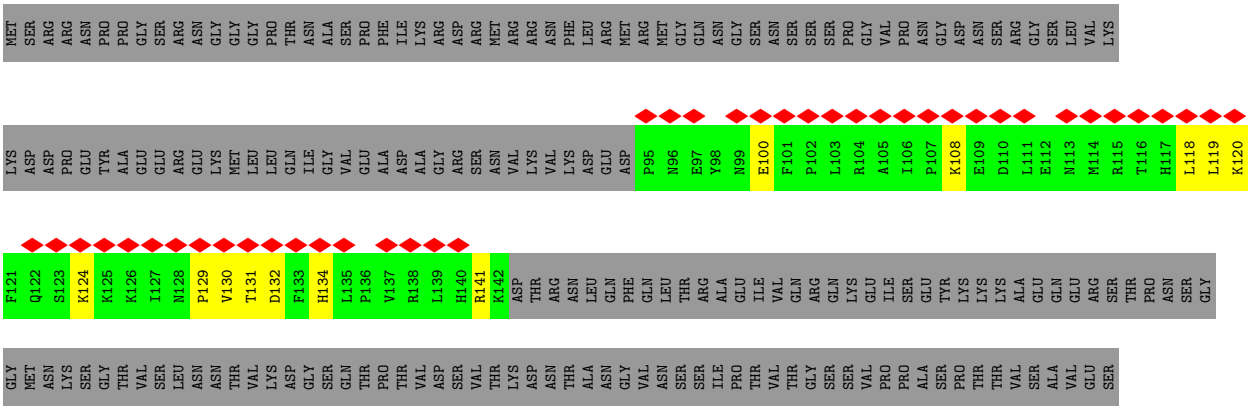
• Molecule 35: Transcription initiation factor IIB

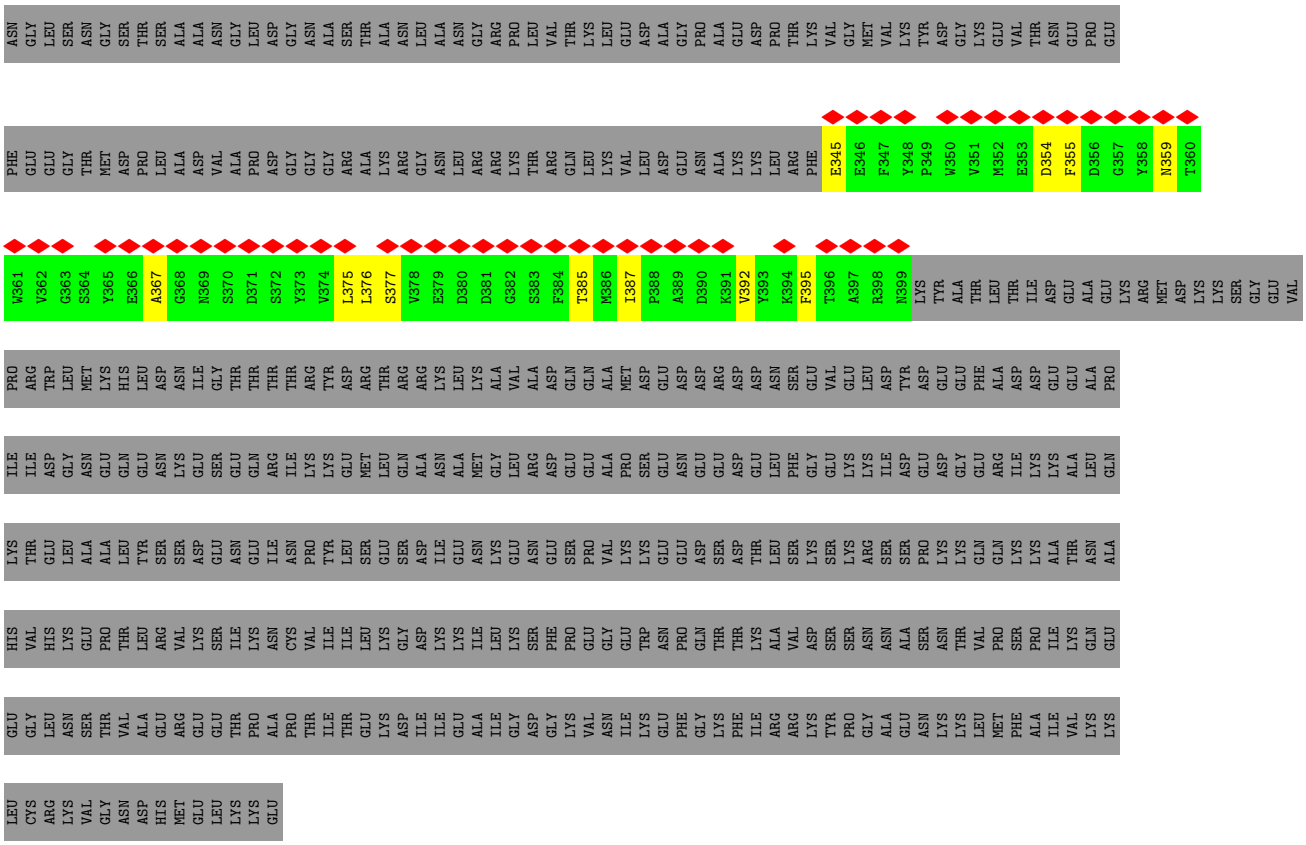
Chain BM: 9% • 90%



• Molecule 36: Transcription initiation factor IIF subunit alpha

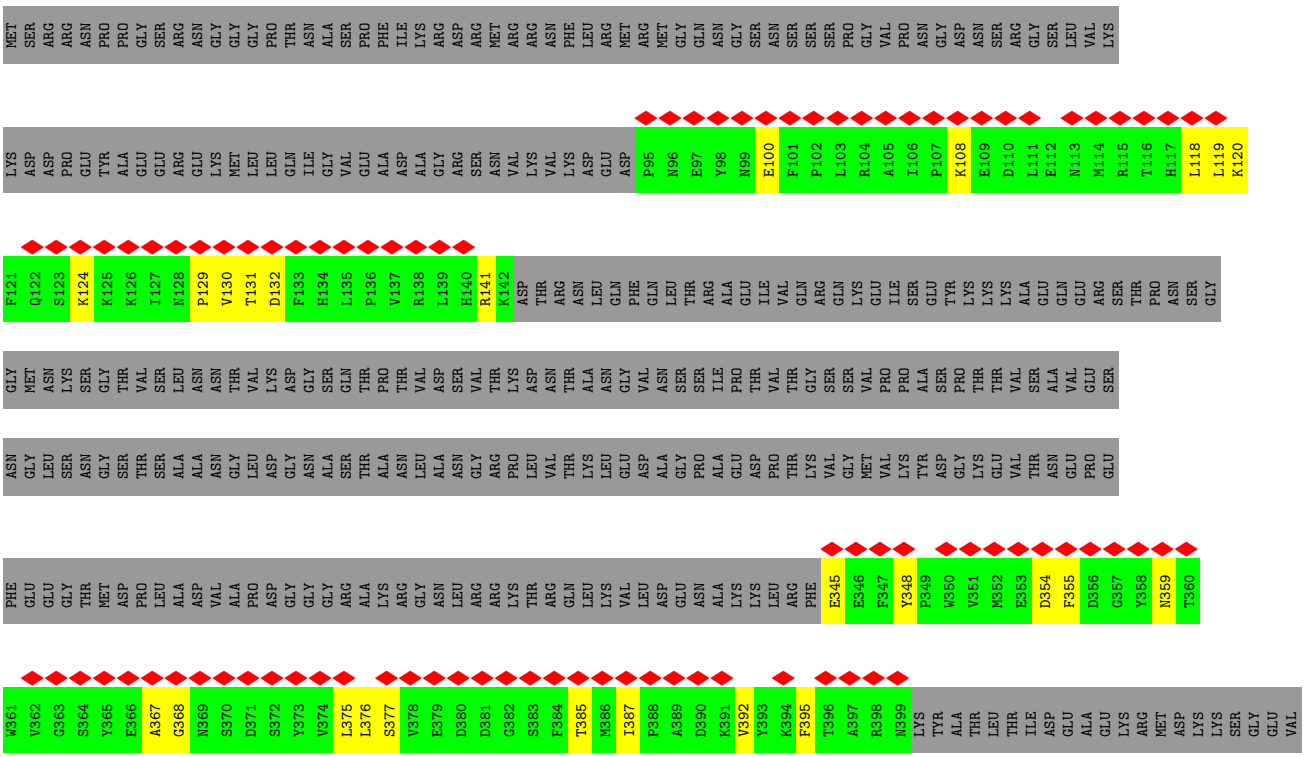
Chain AP: 12% 11% • 86%





- Molecule 36: Transcription initiation factor IIF subunit alpha

Chain BP: 13% 11% 86%



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

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

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

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

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

LEU CYS ARG LYS VAL GLY ASN ASP HIS MET GLU LEU LYS LYS GLU

- Molecule 37: Transcription initiation factor IIF subunit beta

Chain AQ: 28% 22% 9% 69%

MET SER SER GLY SER ALA GLY ALA PRO ALA LEU SER ASN ASN SER THR ASN SER VAL ALA LYS GLU LYS SER GLY ASN ILE SER GLY ASP GLU TYR LEU SER GLN GLU GLU GLU VAL PHE ASP GLY ASN ASP ILE GLU ASN ASN GLU THR LYS VAL TYR GLU GLU S56 L57 D58 L59 D60

L61 E62 R63 S64 N65 R66 Q67 V68 W69 L70 V71 R72 L73 P74 M75 F76 L77 A78 E79 K80 W81 R82 D83 R84 N85 N86 L87 H88 E91 L92 G93 K94 I95 R96 I97 N98 K99 D100 G101 S102 K103 I104 T105 L106 L107 L108 N109 E110 N111 D112 N113 D114 S115 I116 P117 H118 E119 Y120 D121

L122 E123 L124 T125 K126 K127 V128 V129 E130 N131 E132 Y133 V134 F135 T136 E137 Q138 N139 LEU LYS LYS TYR GLN GLN ARG LYS LYS GLU LEU GLU ALA ASP PRO GLU LYS GLN ARG GLN ALA TYR LEU LYS LYS GLN GLU ARG GLU GLU GLU LEU LYS LYS LYS GLN GLN GLN LYS ARG ARG

ASN ASN ARG LYS LYS PHE ASN HIS ARG VAL MET THR ASP ARG ASP GLY ARG ASP ARG TYR ILE PRO TYR VAL LYS THR ILE P209 K210 K211 T212 A213 I214 V215 G216 T217 V218 C219 H220 E221 C222 Q223 V224 M225 P226 S227 M228 N229 D230 Y233 H234 K235 I236 V237 E238 Q239 R240 R241 N242

I243 V244 K245 L246 N247 N248 K249 GLU ARG ILE THR THR LEU ASP GLU THR VAL GLY VAL THR MET SER HIS THR GLY MET SER MET ARG SER ASP ASN SER ASN PHE LEU LYS VAL GLY ARG GLU LYS ALA LYS SER ASN ILE LYS SER ILE ARG MET PRO LYS LYS GLU ILE LEU ASP TYR

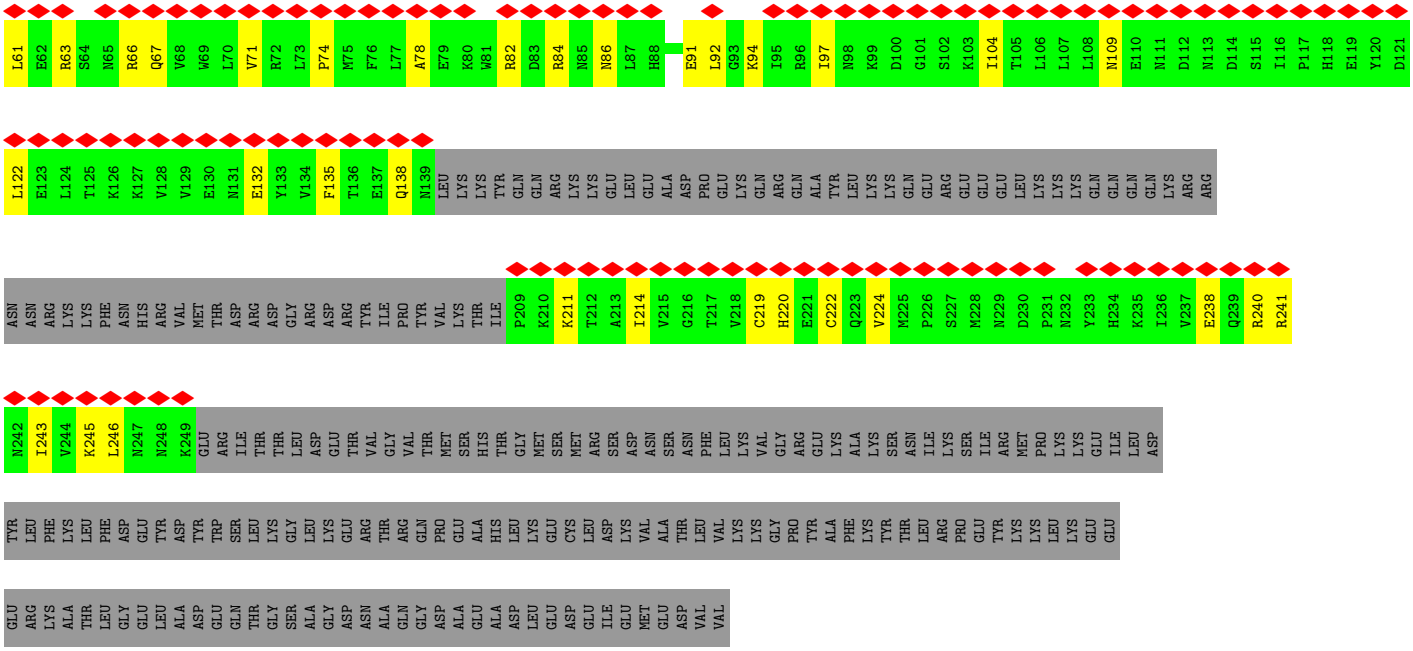
LEU PHE LYS LEU PHE ASP GLU TYR ASP TYR TRP SER LEU LYS GLY LEU LYS GLU ARG THR ARG GLN PRO GLU ALA HIS LEU LYS GLU CYS LEU ASP LYS VAL ALA THR LEU VAL LYS LYS GLY PRO TYR ALA PHE LYS TYR THR LEU ARG PRO GLU TYR TYR LYS LYS LEU LYS GLU GLU GLU

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

- Molecule 37: Transcription initiation factor IIF subunit beta

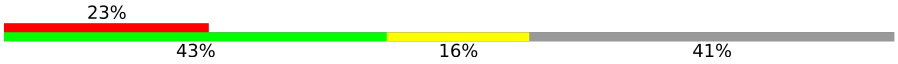
Chain BQ: 29% 23% 8% 69%

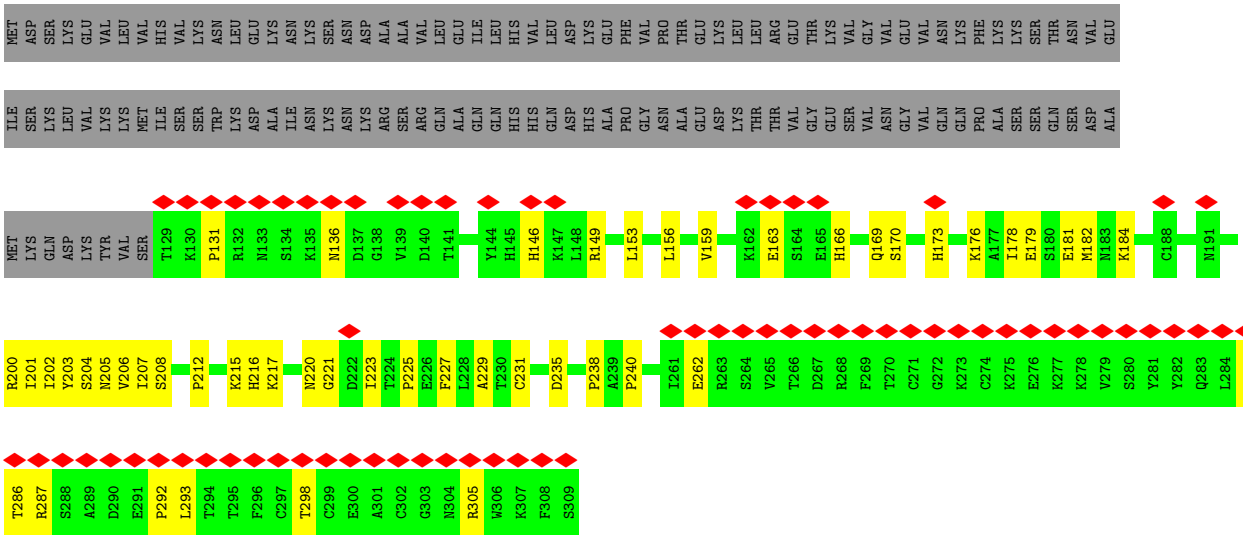
MET SER SER GLY SER ALA GLY ALA PRO ALA LEU SER ASN ASN SER THR ASN SER VAL ALA LYS GLU LYS SER GLY ASN ILE SER GLY ASP GLU TYR LEU SER GLN GLU GLU GLU VAL PHE ASP GLY ASN ASP ILE GLU ASN ASN GLU THR LYS VAL TYR GLU GLU S56 L57 D58 L59 D60



- Molecule 38: Transcription elongation factor S-II

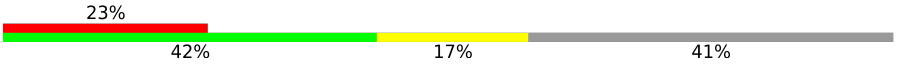
Chain AS:

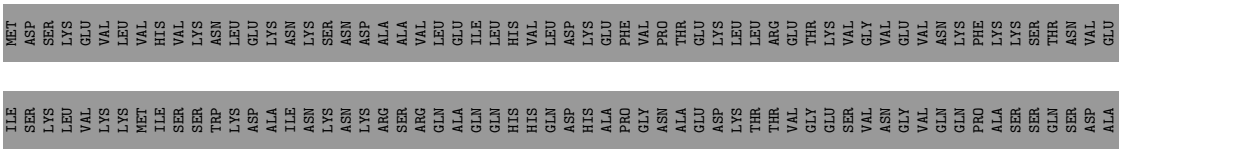


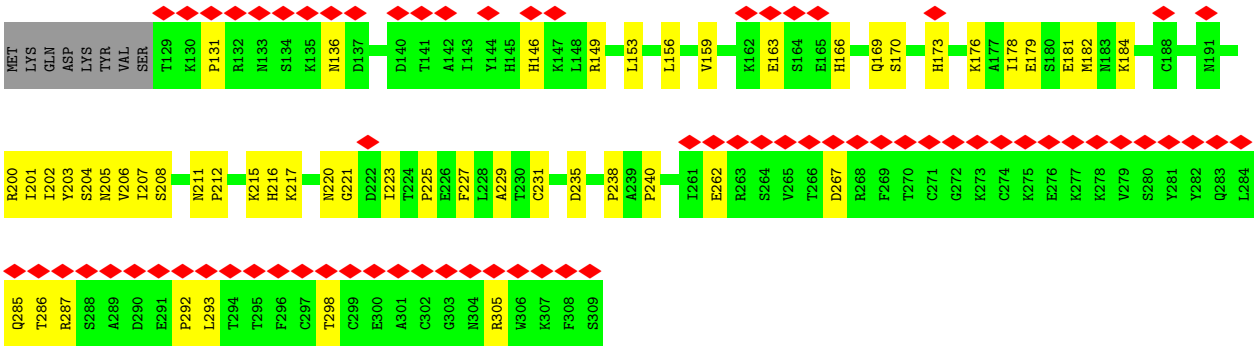


- Molecule 38: Transcription elongation factor S-II

Chain BS:

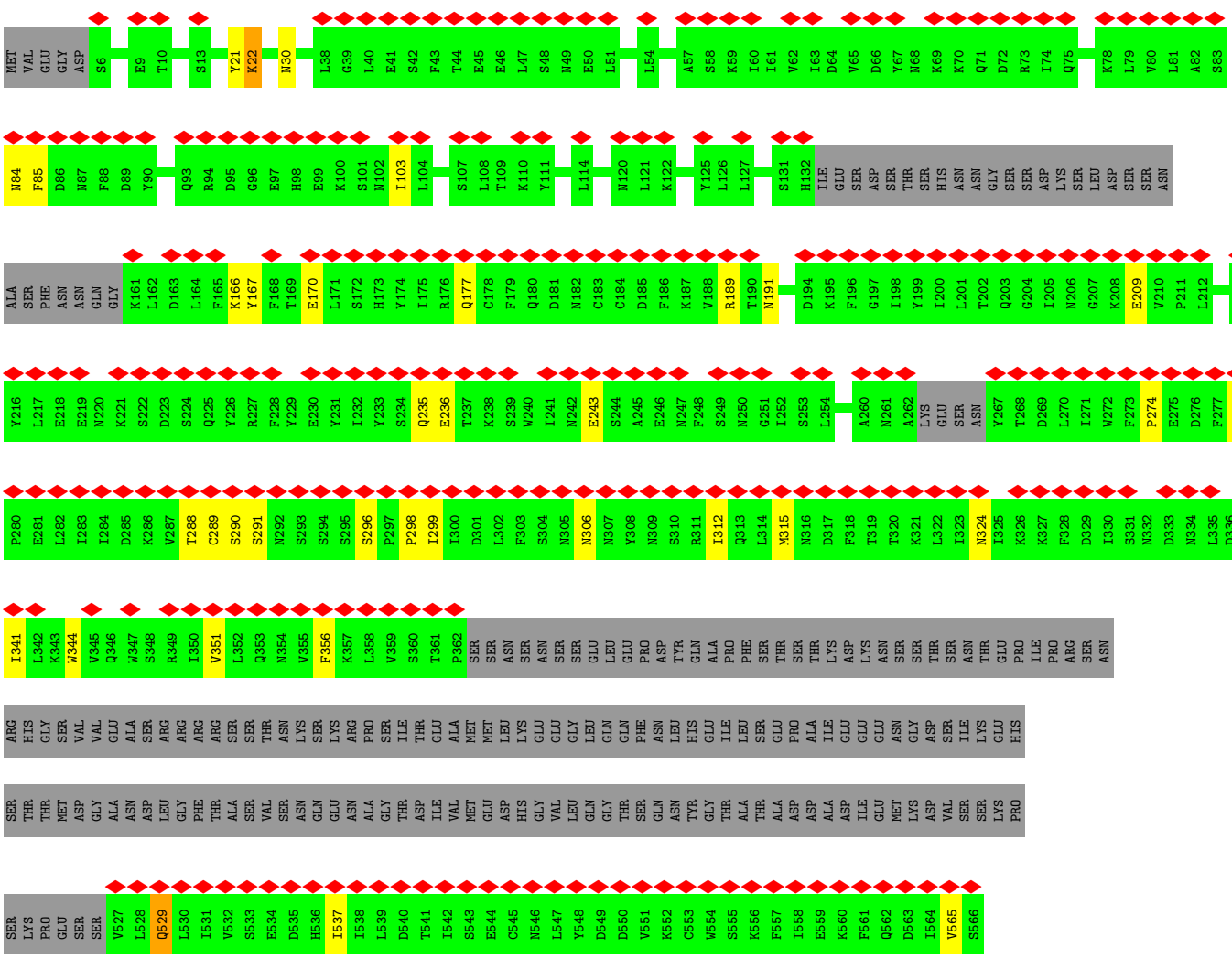






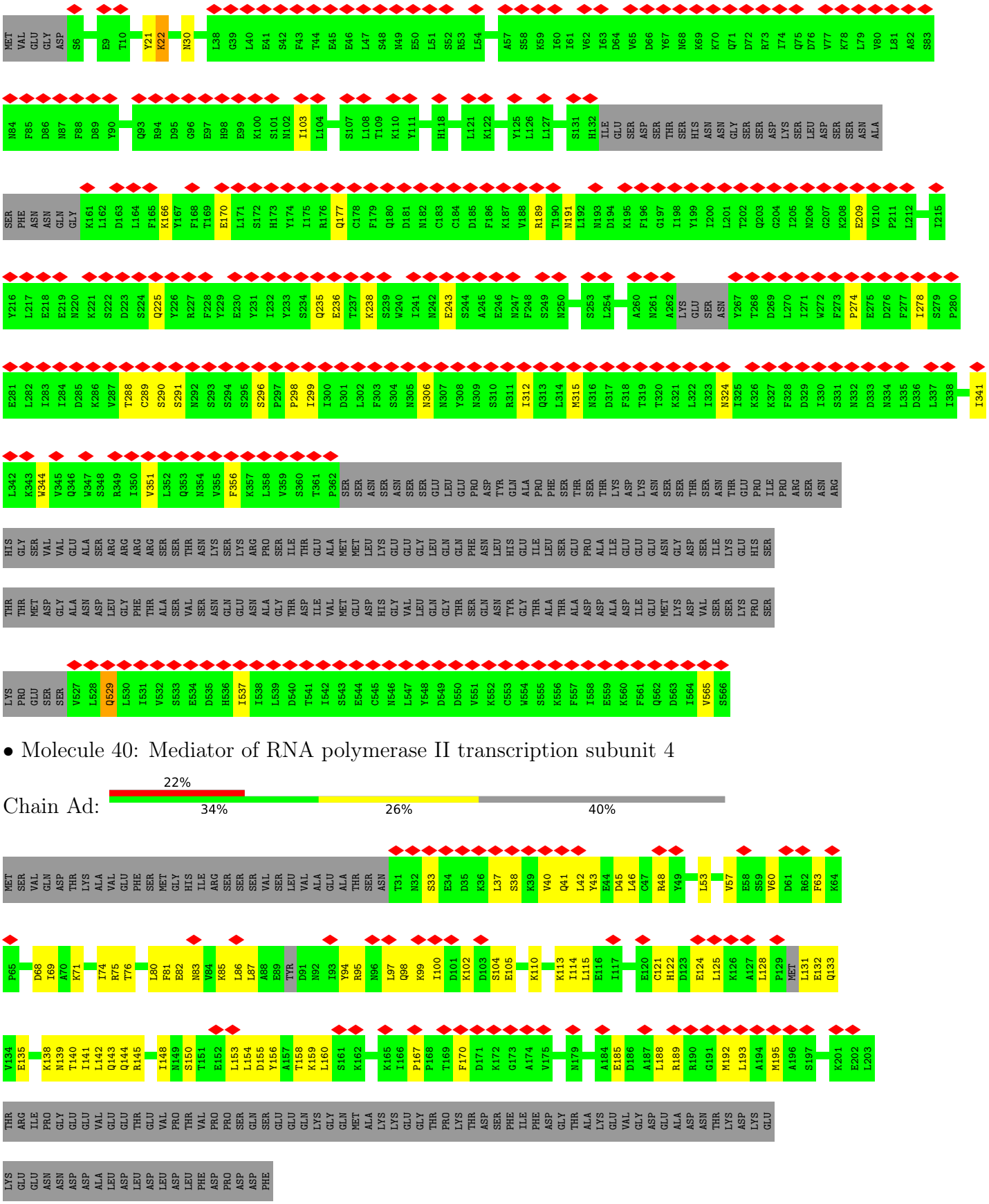
• Molecule 39: Mediator of RNA polymerase II transcription subunit 1

Chain Aa:



• Molecule 39: Mediator of RNA polymerase II transcription subunit 1

Chain Ba:

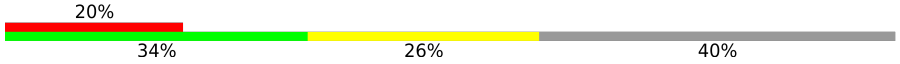


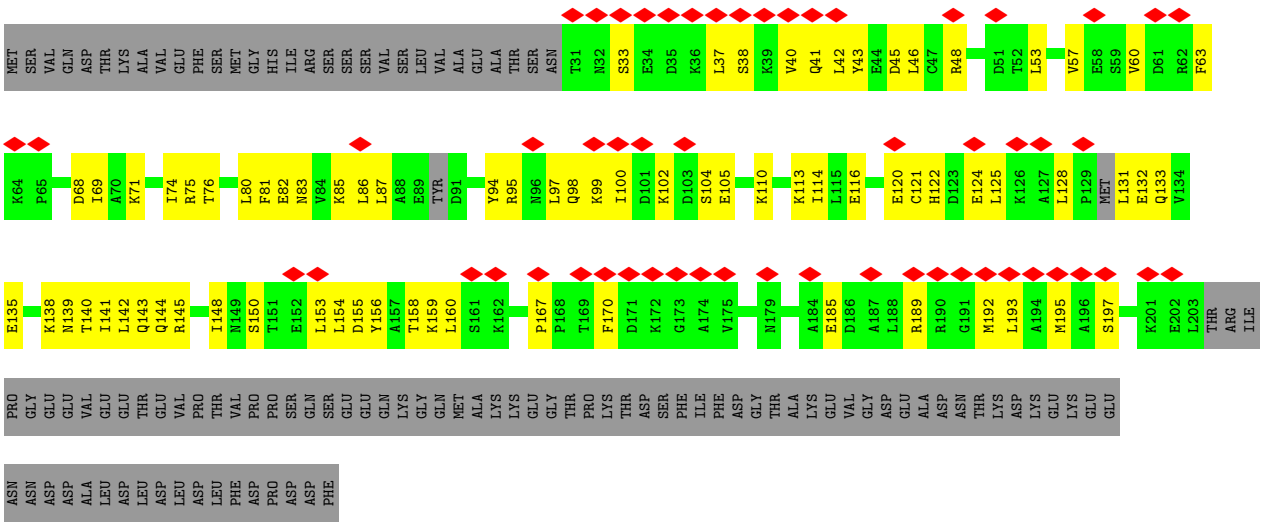
• Molecule 40: Mediator of RNA polymerase II transcription subunit 4

Chain Ad:

• Molecule 40: Mediator of RNA polymerase II transcription subunit 4

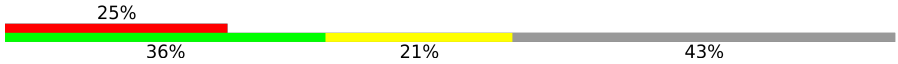
Chain Bd:

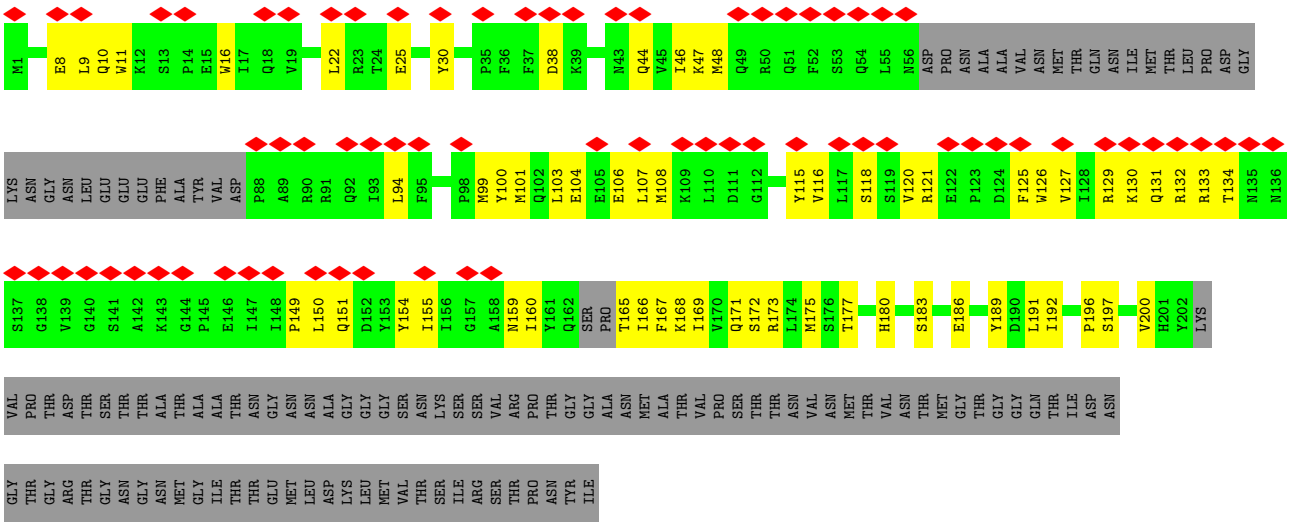




• Molecule 41: Mediator of RNA polymerase II transcription subunit 6

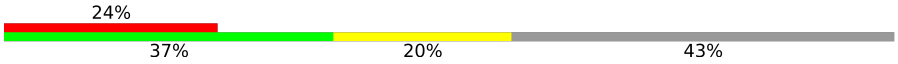
Chain Af:

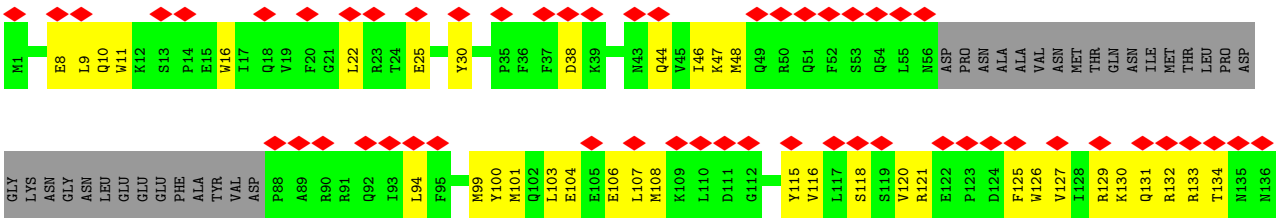


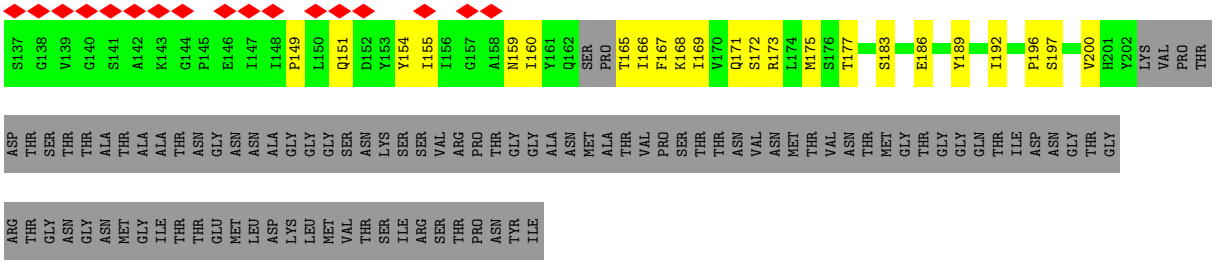


• Molecule 41: Mediator of RNA polymerase II transcription subunit 6

Chain Bf:






S137 G138 V139 G140 S141 A142 K143 G144 P145 E146 I147 I148 P149 L150 Q151 D152 Y153 Y154 I155 I156 G157 A158 N159 I160 Y161 Q162 SER PRO T165 I166 F167 K168 I169 V170 Q171 S172 R173 L174 M175 S176 T177 S183 E186 Y189 I192 P196 S197 V200 H201 Y202 LYS VAL PRO THR
ASP THR SER THR THR ALA THR ALA ALA THR ASN GLY ASN ASN ALA GLY GLY GLY SER ASN LYS SER SER VAL ARG PRO THR GLY GLY ALA ASN MET ALA THR VAL PRO SER THR THR ASN VAL ASN MET THR VAL ASN THR MET GLY THR GLY GLY GLN THR ILE ASP ASN GLY THR GLY
ARG THR GLY ASN GLY ASN MET GLY ILE THR THR GLU MET LEU ASP LYS LEU MET VAL THR SER ILE ARG SER THR PRO ASN TYR ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1102984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.857	Depositor
Minimum map value	-0.168	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	852.84, 891.48, 832.14	wwPDB
Map dimensions	618, 646, 603	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)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.78	1/868 (0.1%)	1.45	17/1337 (1.3%)
2	B	0.78	0/853	1.53	25/1315 (1.9%)
3	Ao	0.13	0/904	0.42	0/1202
3	Bo	0.13	0/904	0.42	0/1202
4	Ab	0.13	0/520	0.38	0/693
4	Bb	0.14	0/520	0.38	0/693
5	Ac	0.15	0/902	0.45	0/1215
5	Bc	0.16	0/882	0.46	0/1187
6	An	0.32	0/7053	0.60	2/9524 (0.0%)
6	Bn	0.33	0/7053	0.60	2/9524 (0.0%)
7	Ae	0.11	0/6033	0.31	0/8183
7	Be	0.11	0/6033	0.31	0/8183
8	Ap	0.10	0/7413	0.30	0/10031
8	Bp	0.11	0/7413	0.30	0/10031
9	GA	1.79	11/736 (1.5%)	1.86	15/983 (1.5%)
9	GB	1.86	17/736 (2.3%)	1.81	20/983 (2.0%)
10	At	0.17	0/1635	0.39	0/2215
10	Bt	0.17	0/1635	0.39	0/2215
11	Ag	0.43	0/1453	0.78	1/1957 (0.1%)
11	Bg	0.43	0/1453	0.78	1/1957 (0.1%)
12	Ah	0.60	1/1207 (0.1%)	1.31	7/1636 (0.4%)
12	Bh	0.60	1/1207 (0.1%)	1.31	7/1636 (0.4%)
13	Ai	0.55	0/741	1.05	1/992 (0.1%)
13	Bi	0.55	0/741	1.05	1/992 (0.1%)
14	Aj	0.48	0/1204	0.82	1/1625 (0.1%)
14	Bj	0.48	0/1204	0.82	1/1625 (0.1%)
15	Ak	0.57	0/943	0.98	1/1263 (0.1%)
15	Bk	0.57	0/943	0.98	1/1263 (0.1%)
16	Aq	0.25	0/4246	0.53	2/5705 (0.0%)
16	Bq	0.25	0/4246	0.53	3/5705 (0.1%)
17	Ar	0.28	0/2030	0.51	0/2747
17	Br	0.28	0/2030	0.51	0/2747

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	As	0.31	0/669	0.51	1/906 (0.1%)
18	Bs	0.31	0/669	0.51	1/906 (0.1%)
19	Au	0.45	0/985	0.91	1/1321 (0.1%)
19	Bu	0.46	0/985	0.91	1/1321 (0.1%)
20	Av	0.31	0/873	0.71	0/1177
20	Bv	0.31	0/873	0.71	0/1177
21	Aw	0.16	0/897	0.39	0/1219
21	Bw	0.16	0/897	0.39	0/1219
22	Az	0.26	0/195	0.45	0/270
22	Bz	0.26	0/195	0.45	0/270
23	AA	0.20	0/11633	0.43	0/15735
23	BA	0.20	0/11633	0.43	0/15735
24	AB	0.19	0/9520	0.45	2/12839 (0.0%)
24	BB	0.20	0/9520	0.45	2/12839 (0.0%)
25	AC	0.19	0/2171	0.40	0/2941
25	BC	0.19	0/2171	0.40	0/2941
26	AD	0.13	0/1365	0.32	0/1831
26	BD	0.14	0/1365	0.32	0/1831
27	AE	0.16	0/1796	0.40	0/2416
27	BE	0.16	0/1796	0.40	0/2416
28	AF	0.18	0/709	0.43	0/956
28	BF	0.18	0/709	0.43	0/956
29	AG	0.15	0/1368	0.37	0/1844
29	BG	0.15	0/1368	0.37	0/1844
30	AH	0.18	0/1144	0.42	0/1548
30	BH	0.18	0/1144	0.42	0/1548
31	AI	0.17	0/961	0.48	0/1294
31	BI	0.17	0/961	0.48	0/1294
32	AJ	0.21	0/587	0.55	0/786
32	BJ	0.21	0/587	0.56	0/786
33	AK	0.21	0/947	0.42	0/1279
33	BK	0.21	0/947	0.42	0/1279
34	AL	0.17	0/346	0.48	0/457
34	BL	0.17	0/346	0.48	0/457
35	AM	0.16	0/267	0.32	0/362
35	BM	0.16	0/267	0.32	0/362
36	AP	0.14	0/886	0.33	0/1198
36	BP	0.14	0/886	0.33	0/1198
37	AQ	0.14	0/1049	0.38	0/1413
37	BQ	0.15	0/1049	0.38	0/1413
38	AS	0.16	0/1462	0.39	0/1973
38	BS	0.16	0/1462	0.39	0/1973
39	Aa	0.67	0/3067	1.14	6/4148 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	Ba	0.67	0/3067	1.13	7/4148 (0.2%)
40	Ad	0.18	0/1405	0.51	0/1889
40	Bd	0.18	0/1405	0.51	0/1889
41	Af	0.15	0/1440	0.35	0/1946
41	Bf	0.15	0/1440	0.35	0/1946
All	All	0.33	31/167225 (0.0%)	0.59	129/226062 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	GA	0	2
11	Ag	0	1
11	Bg	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	GA	44	THR	CA-C	8.97	1.64	1.52
12	Ah	142	ASP	C-N	8.77	1.46	1.33
12	Bh	142	ASP	C-N	8.69	1.45	1.33
9	GB	51	ARG	N-CA	-8.63	1.35	1.46
9	GB	57	VAL	C-O	-8.09	1.14	1.24

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Ah	142	ASP	O-C-N	-26.49	87.36	122.59
12	Bh	142	ASP	O-C-N	-26.46	87.39	122.59
12	Bh	142	ASP	CA-C-N	17.82	155.57	121.54
12	Bh	142	ASP	C-N-CA	17.82	155.57	121.54
12	Ah	142	ASP	CA-C-N	17.79	155.52	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	Ag	165	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	Bg	165	TYR	Sidechain
9	GA	74	ARG	Peptide
9	GA	75	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	774	0	425	27	0
2	B	761	0	414	24	0
3	Ao	894	0	930	19	0
3	Bo	894	0	930	18	0
4	Ab	516	0	527	14	0
4	Bb	516	0	527	16	0
5	Ac	891	0	907	31	0
5	Bc	871	0	891	32	0
6	An	6927	0	7151	140	0
6	Bn	6927	0	7151	135	0
7	Ae	5916	0	5956	173	0
7	Be	5916	0	5954	162	0
8	Ap	7247	0	7292	142	0
8	Bp	7247	0	7292	152	0
9	GA	727	0	770	69	0
9	GB	727	0	768	79	0
10	At	1609	0	1626	22	0
10	Bt	1609	0	1626	24	0
11	Ag	1426	0	1448	56	0
11	Bg	1426	0	1448	54	0
12	Ah	1185	0	1193	67	0
12	Bh	1185	0	1193	61	0
13	Ai	730	0	735	72	0
13	Bi	730	0	735	76	0
14	Aj	1189	0	1178	26	0
14	Bj	1189	0	1178	25	0
15	Ak	933	0	953	19	0
15	Bk	933	0	953	19	0
16	Aq	4182	0	4325	103	0
16	Bq	4182	0	4325	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ar	1995	0	2018	26	0
17	Br	1995	0	2018	28	0
18	As	657	0	636	13	0
18	Bs	657	0	636	13	0
19	Au	978	0	1005	47	0
19	Bu	978	0	1005	46	0
20	Av	869	0	881	42	0
20	Bv	869	0	881	40	0
21	Aw	871	0	857	22	0
21	Bw	871	0	857	21	0
22	Az	185	0	163	9	0
22	Bz	185	0	163	8	0
23	AA	11426	0	11482	212	0
23	BA	11426	0	11482	209	0
24	AB	9336	0	9341	213	0
24	BB	9336	0	9341	212	0
25	AC	2133	0	2096	39	0
25	BC	2133	0	2096	37	0
26	AD	1353	0	1352	21	0
26	BD	1353	0	1352	20	0
27	AE	1760	0	1788	23	0
27	BE	1760	0	1788	23	0
28	AF	697	0	720	8	0
28	BF	697	0	720	7	0
29	AG	1340	0	1357	23	0
29	BG	1340	0	1357	23	0
30	AH	1126	0	1094	14	0
30	BH	1126	0	1094	16	0
31	AI	943	0	906	18	0
31	BI	943	0	906	18	0
32	AJ	578	0	593	31	0
32	BJ	578	0	593	30	0
33	AK	929	0	939	12	0
33	BK	929	0	939	11	0
34	AL	344	0	367	10	0
34	BL	344	0	367	11	0
35	AM	263	0	273	2	0
35	BM	263	0	273	2	0
36	AP	861	0	819	21	0
36	BP	861	0	819	22	0
37	AQ	1033	0	1036	26	0
37	BQ	1033	0	1036	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	AS	1436	0	1428	35	0
38	BS	1436	0	1428	37	0
39	Aa	3008	0	2952	74	0
39	Ba	3008	0	2952	78	0
40	Ad	1388	0	1400	128	0
40	Bd	1388	0	1400	128	0
41	Af	1407	0	1385	83	0
41	Bf	1407	0	1385	76	0
42	A	2	0	0	2	0
42	B	2	0	0	0	0
43	Bc	7	0	6	0	0
44	Bc	5	0	5	0	0
45	Bc	9	0	4	0	0
All	All	164116	0	164592	3447	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 10.

The worst 5 of 3447 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)
39:Aa:236:GLU:CG	39:Ba:166:LYS:HD3	1.28	1.64
39:Aa:236:GLU:HG3	39:Ba:166:LYS:CD	1.31	1.57
39:Aa:236:GLU:CG	39:Ba:166:LYS:CD	1.83	1.47
7:Ae:409:LYS:NZ	7:Be:409:LYS:HD3	1.22	1.47
39:Aa:21:TYR:CE1	40:Ad:74:ILE:HG21	1.49	1.45

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	
3	Ao	109/1081 (10%)	109 (100%)	0	0	100	100
3	Bo	109/1081 (10%)	109 (100%)	0	0	100	100
4	Ab	61/431 (14%)	61 (100%)	0	0	100	100
4	Bb	61/431 (14%)	61 (100%)	0	0	100	100
5	Ac	108/397 (27%)	107 (99%)	1 (1%)	0	100	100
5	Bc	105/397 (26%)	104 (99%)	1 (1%)	0	100	100
6	An	830/1082 (77%)	817 (98%)	12 (1%)	1 (0%)	48	75
6	Bn	830/1082 (77%)	818 (99%)	11 (1%)	1 (0%)	48	75
7	Ae	721/1132 (64%)	711 (99%)	10 (1%)	0	100	100
7	Be	721/1132 (64%)	712 (99%)	9 (1%)	0	100	100
8	Ap	885/974 (91%)	877 (99%)	8 (1%)	0	100	100
8	Bp	885/974 (91%)	875 (99%)	10 (1%)	0	100	100
9	GA	87/147 (59%)	72 (83%)	10 (12%)	5 (6%)	1	9
9	GB	87/147 (59%)	76 (87%)	8 (9%)	3 (3%)	3	18
10	At	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
10	Bt	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
11	Ag	161/222 (72%)	159 (99%)	2 (1%)	0	100	100
11	Bg	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
12	Ah	142/223 (64%)	135 (95%)	5 (4%)	2 (1%)	9	33
12	Bh	142/223 (64%)	135 (95%)	5 (4%)	2 (1%)	9	33
13	Ai	82/149 (55%)	80 (98%)	2 (2%)	0	100	100
13	Bi	82/149 (55%)	80 (98%)	2 (2%)	0	100	100
14	Aj	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
14	Bj	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
15	Ak	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
15	Bk	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
16	Aq	507/687 (74%)	498 (98%)	7 (1%)	2 (0%)	30	60
16	Bq	507/687 (74%)	498 (98%)	7 (1%)	2 (0%)	30	60
17	Ar	249/307 (81%)	245 (98%)	4 (2%)	0	100	100
17	Br	249/307 (81%)	245 (98%)	4 (2%)	0	100	100
18	As	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
18	Bs	77/220 (35%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Au	118/140 (84%)	117 (99%)	1 (1%)	0	100	100
19	Bu	118/140 (84%)	117 (99%)	1 (1%)	0	100	100
20	Av	105/120 (88%)	103 (98%)	2 (2%)	0	100	100
20	Bv	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
21	Aw	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
21	Bw	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
22	Az	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	14
22	Bz	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	14
23	AA	1451/1453 (100%)	1405 (97%)	45 (3%)	1 (0%)	48	75
23	BA	1451/1453 (100%)	1406 (97%)	44 (3%)	1 (0%)	48	75
24	AB	1164/1224 (95%)	1131 (97%)	33 (3%)	0	100	100
24	BB	1164/1224 (95%)	1131 (97%)	33 (3%)	0	100	100
25	AC	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
25	BC	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
26	AD	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
26	BD	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
27	AE	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
27	BE	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
28	AF	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
28	BF	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
29	AG	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
29	BG	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
30	AH	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
30	BH	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
31	AI	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
31	BI	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
32	AJ	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
32	BJ	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
33	AK	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
33	BK	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
34	AL	41/70 (59%)	39 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BL	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
35	AM	33/345 (10%)	33 (100%)	0	0	100	100
35	BM	33/345 (10%)	33 (100%)	0	0	100	100
36	AP	99/735 (14%)	99 (100%)	0	0	100	100
36	BP	99/735 (14%)	99 (100%)	0	0	100	100
37	AQ	121/400 (30%)	121 (100%)	0	0	100	100
37	BQ	121/400 (30%)	121 (100%)	0	0	100	100
38	AS	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
38	BS	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
39	Aa	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	45
39	Ba	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	45
40	Ad	165/284 (58%)	163 (99%)	2 (1%)	0	100	100
40	Bd	165/284 (58%)	163 (99%)	2 (1%)	0	100	100
41	Af	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
41	Bf	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
All	All	19863/30330 (66%)	19446 (98%)	389 (2%)	28 (0%)	49	75

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	GA	29	ALA
9	GA	75	GLU
9	GA	76	ASP
12	Ah	142	ASP
16	Aq	319	LYS

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	
3	Ao	103/944 (11%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Bo	103/944 (11%)	103 (100%)	0	100	100
4	Ab	60/389 (15%)	60 (100%)	0	100	100
4	Bb	60/389 (15%)	60 (100%)	0	100	100
5	Ac	100/339 (30%)	100 (100%)	0	100	100
5	Bc	98/339 (29%)	98 (100%)	0	100	100
6	An	797/1001 (80%)	796 (100%)	1 (0%)	88	90
6	Bn	797/1001 (80%)	796 (100%)	1 (0%)	88	90
7	Ae	684/1053 (65%)	684 (100%)	0	100	100
7	Be	684/1053 (65%)	683 (100%)	1 (0%)	88	90
8	Ap	826/897 (92%)	826 (100%)	0	100	100
8	Bp	826/897 (92%)	826 (100%)	0	100	100
9	GA	84/138 (61%)	63 (75%)	21 (25%)	0	3
9	GB	84/138 (61%)	62 (74%)	22 (26%)	0	2
10	At	178/178 (100%)	178 (100%)	0	100	100
10	Bt	178/178 (100%)	178 (100%)	0	100	100
11	Ag	162/208 (78%)	162 (100%)	0	100	100
11	Bg	162/208 (78%)	162 (100%)	0	100	100
12	Ah	135/207 (65%)	134 (99%)	1 (1%)	76	80
12	Bh	135/207 (65%)	134 (99%)	1 (1%)	76	80
13	Ai	85/144 (59%)	85 (100%)	0	100	100
13	Bi	85/144 (59%)	85 (100%)	0	100	100
14	Aj	136/145 (94%)	134 (98%)	2 (2%)	57	72
14	Bj	136/145 (94%)	134 (98%)	2 (2%)	57	72
15	Ak	108/108 (100%)	107 (99%)	1 (1%)	70	78
15	Bk	108/108 (100%)	107 (99%)	1 (1%)	70	78
16	Aq	482/642 (75%)	481 (100%)	1 (0%)	87	88
16	Bq	482/642 (75%)	481 (100%)	1 (0%)	87	88
17	Ar	228/280 (81%)	228 (100%)	0	100	100
17	Br	228/280 (81%)	228 (100%)	0	100	100
18	As	75/195 (38%)	74 (99%)	1 (1%)	61	74
18	Bs	75/195 (38%)	74 (99%)	1 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Au	115/132 (87%)	114 (99%)	1 (1%)	70	78
19	Bu	115/132 (87%)	114 (99%)	1 (1%)	70	78
20	Av	101/112 (90%)	100 (99%)	1 (1%)	68	76
20	Bv	101/112 (90%)	100 (99%)	1 (1%)	68	76
21	Aw	97/117 (83%)	97 (100%)	0	100	100
21	Bw	97/117 (83%)	97 (100%)	0	100	100
22	Az	25/25 (100%)	25 (100%)	0	100	100
22	Bz	25/25 (100%)	25 (100%)	0	100	100
23	AA	1268/1268 (100%)	1267 (100%)	1 (0%)	88	90
23	BA	1268/1268 (100%)	1267 (100%)	1 (0%)	88	90
24	AB	1018/1061 (96%)	1018 (100%)	0	100	100
24	BB	1018/1061 (96%)	1018 (100%)	0	100	100
25	AC	239/274 (87%)	239 (100%)	0	100	100
25	BC	239/274 (87%)	239 (100%)	0	100	100
26	AD	150/200 (75%)	150 (100%)	0	100	100
26	BD	150/200 (75%)	150 (100%)	0	100	100
27	AE	197/197 (100%)	197 (100%)	0	100	100
27	BE	197/197 (100%)	197 (100%)	0	100	100
28	AF	76/137 (56%)	76 (100%)	0	100	100
28	BF	76/137 (56%)	76 (100%)	0	100	100
29	AG	152/152 (100%)	152 (100%)	0	100	100
29	BG	152/152 (100%)	152 (100%)	0	100	100
30	AH	124/128 (97%)	124 (100%)	0	100	100
30	BH	124/128 (97%)	124 (100%)	0	100	100
31	AI	110/116 (95%)	110 (100%)	0	100	100
31	BI	110/116 (95%)	110 (100%)	0	100	100
32	AJ	65/65 (100%)	65 (100%)	0	100	100
32	BJ	65/65 (100%)	65 (100%)	0	100	100
33	AK	99/102 (97%)	99 (100%)	0	100	100
33	BK	99/102 (97%)	99 (100%)	0	100	100
34	AL	38/57 (67%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BL	38/57 (67%)	38 (100%)	0	100	100
35	AM	32/299 (11%)	32 (100%)	0	100	100
35	BM	32/299 (11%)	32 (100%)	0	100	100
36	AP	95/641 (15%)	95 (100%)	0	100	100
36	BP	95/641 (15%)	95 (100%)	0	100	100
37	AQ	119/363 (33%)	119 (100%)	0	100	100
37	BQ	119/363 (33%)	119 (100%)	0	100	100
38	AS	158/274 (58%)	158 (100%)	0	100	100
38	BS	158/274 (58%)	158 (100%)	0	100	100
39	Aa	350/528 (66%)	347 (99%)	3 (1%)	70	78
39	Ba	350/528 (66%)	347 (99%)	3 (1%)	70	78
40	Ad	158/258 (61%)	158 (100%)	0	100	100
40	Bd	158/258 (61%)	158 (100%)	0	100	100
41	Af	158/259 (61%)	158 (100%)	0	100	100
41	Bf	158/259 (61%)	158 (100%)	0	100	100
All	All	18372/27266 (67%)	18302 (100%)	70 (0%)	81	84

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Be	579	LEU
14	Bj	76	LYS
20	Bv	45	ASN
9	GB	24	GLU
9	GB	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
8	Bp	313	HIS
23	BA	510	GLN
8	Bp	630	GLN
15	Bk	101	GLN
23	BA	1232	ASN

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)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	THR	Bc	108	-	5,6,7	0.58	0	5,7,9	0.87	0
44	ALA	Bc	109	-	3,4,5	0.75	0	2,4,6	1.13	0
45	ASP	Bc	110	-	7,8,8	1.15	1 (14%)	6,10,10	1.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	THR	Bc	108	-	-	1/5/6/8	-
44	ALA	Bc	109	-	-	0/1/2/4	-
45	ASP	Bc	110	-	-	4/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Bc	110	ASP	OXT-C	-2.23	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	Bc	108	THR	O-C-CA-CB
45	Bc	110	ASP	O-C-CA-N
45	Bc	110	ASP	OXT-C-CA-N
45	Bc	110	ASP	N-CA-CB-CG
45	Bc	110	ASP	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	Aj	1
14	Bj	1
15	Ak	1
15	Bk	1
13	Ai	1
13	Bi	1
11	Ag	1
11	Bg	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Aj	77:VAL	C	78:ASP	N	3.28
1	Bj	77:VAL	C	78:ASP	N	3.28
1	Ak	86:VAL	C	87:ASN	N	3.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bk	86:VAL	C	87:ASN	N	3.04
1	Ai	118:SER	C	119:PRO	N	2.69

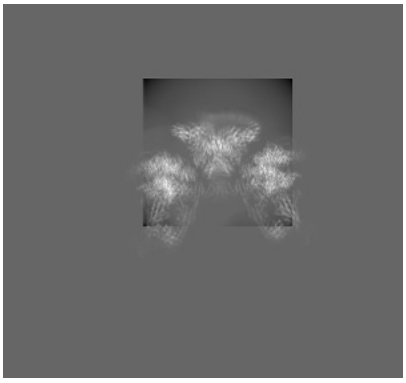
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26551. These allow visual inspection of the internal detail of the map and identification of artifacts.

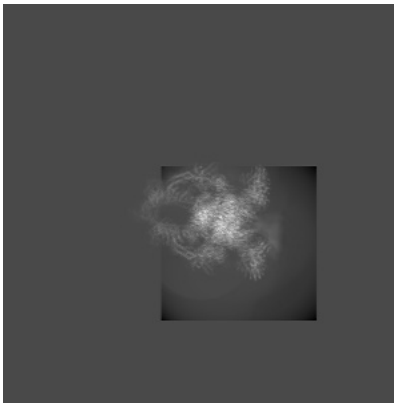
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

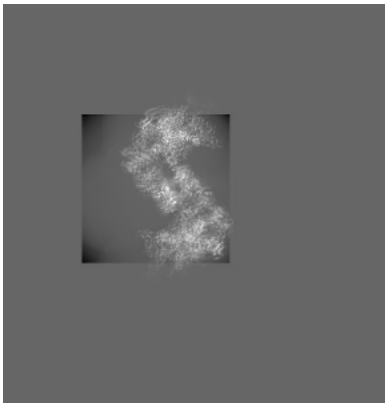
6.1.1 Primary map



X



Y

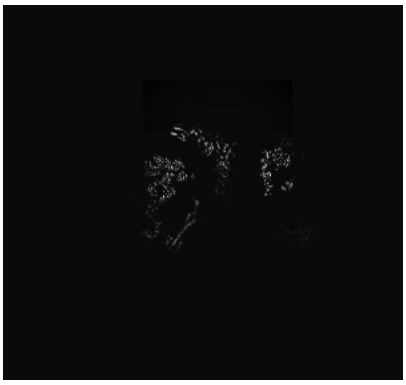


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 309

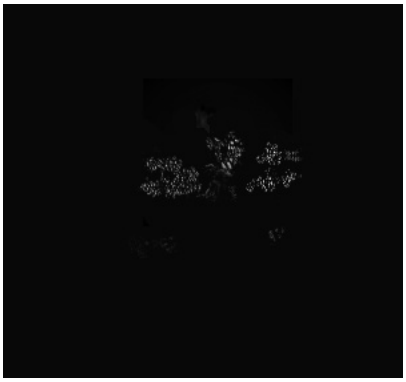
Y Index: 323

Z Index: 301

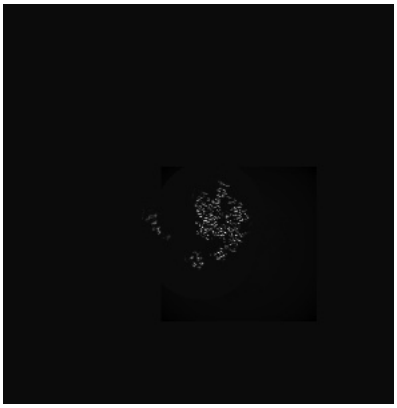
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 291



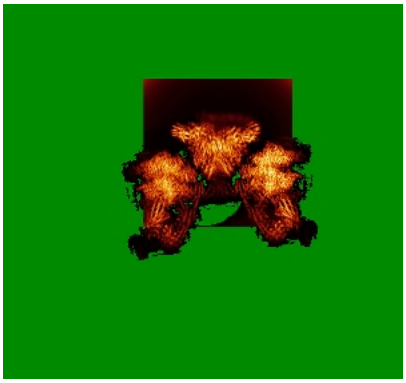
Y Index: 431

Z Index: 351

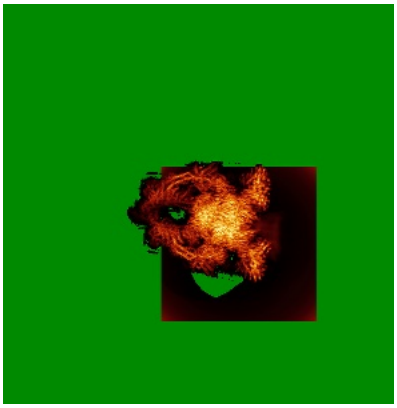
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

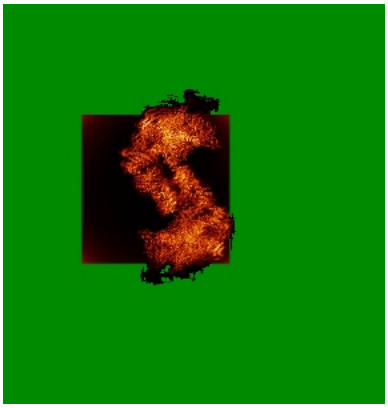
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

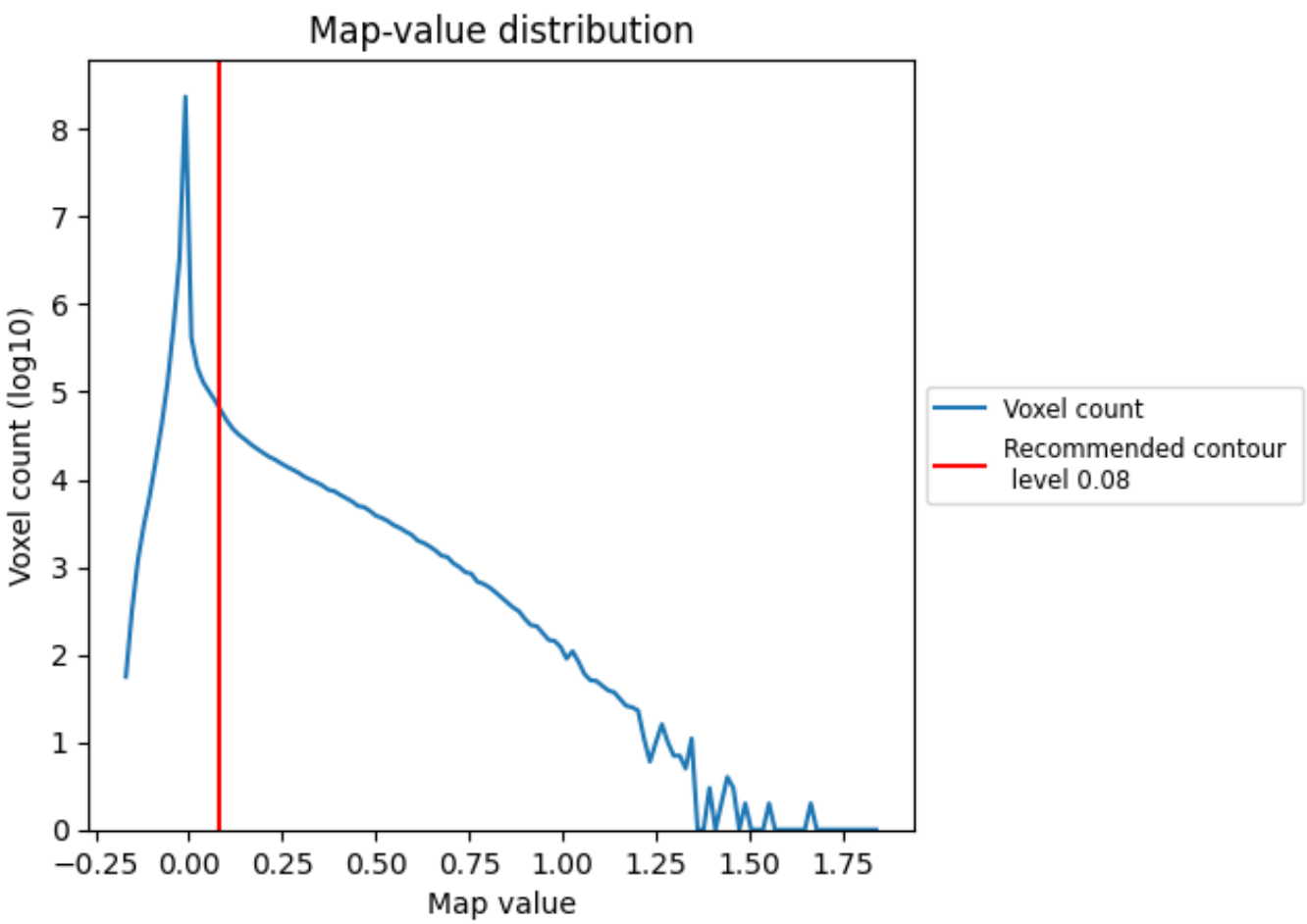
6.6 Mask visualisation (i)

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

7 Map analysis (i)

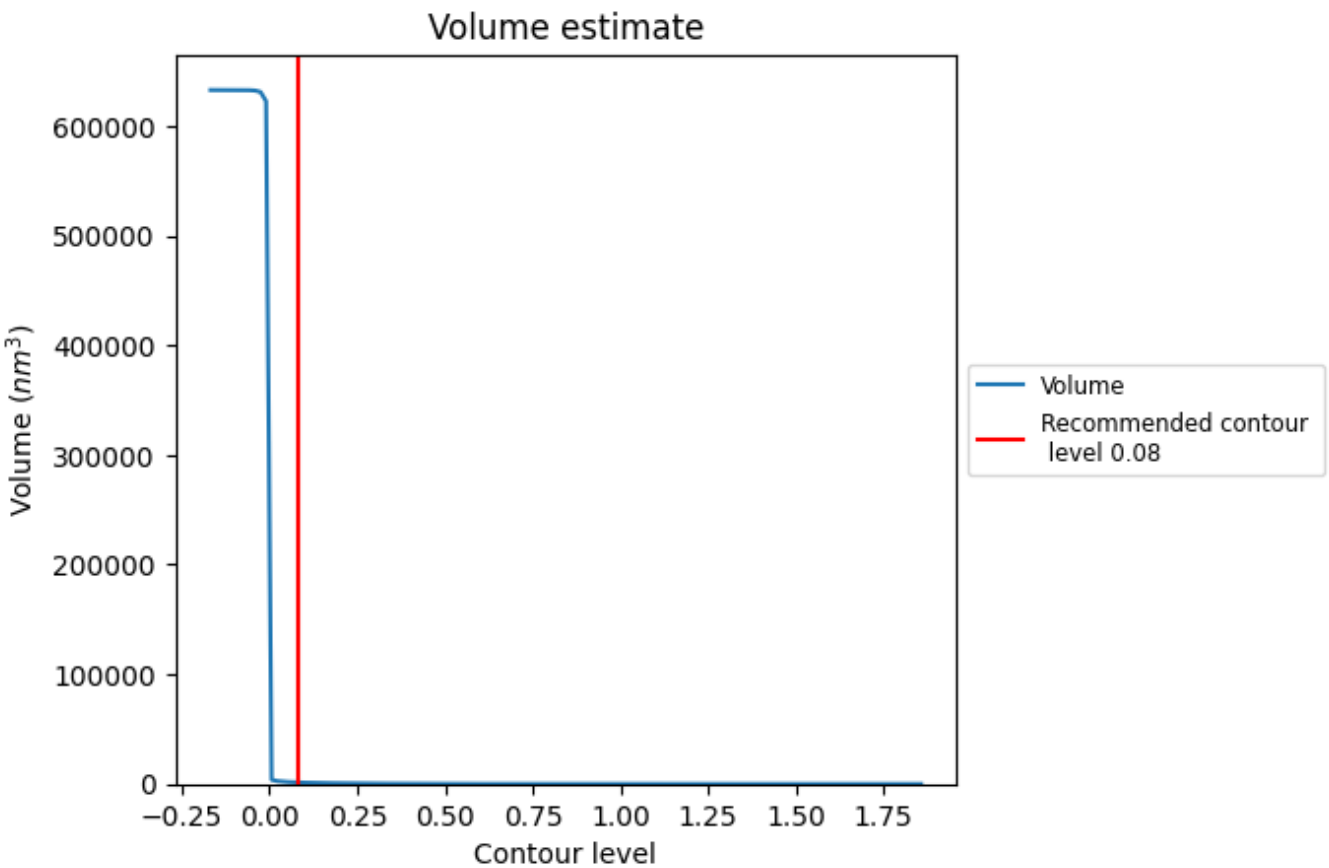
This section contains the results of statistical analysis of the map.

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 1377 nm^3; this corresponds to an approximate mass of 1244 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

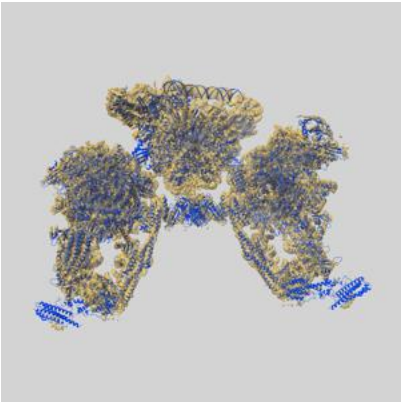
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

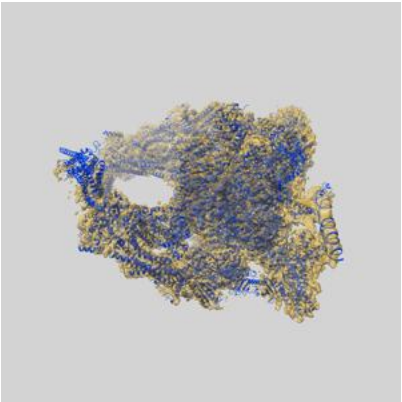
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26551 and PDB model 7UIO. Per-residue inclusion information can be found in section 3 on page 17.

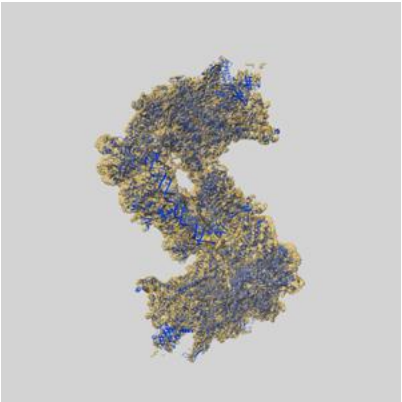
9.1 Map-model overlay (i)



X



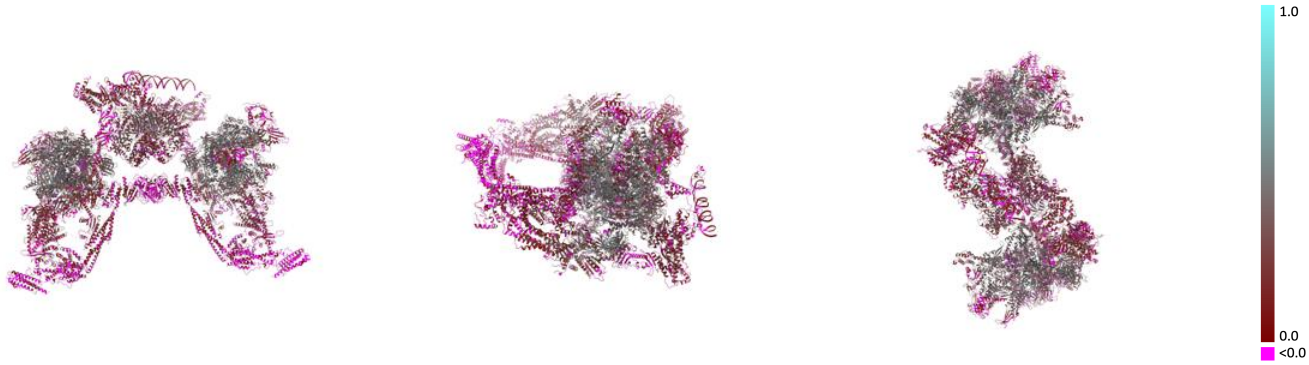
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

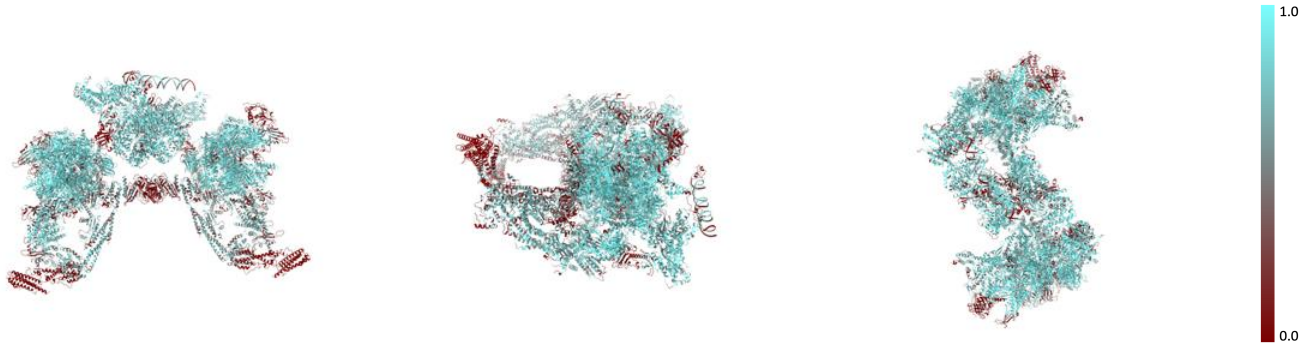
9.2 Q-score mapped to coordinate model (i)



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.

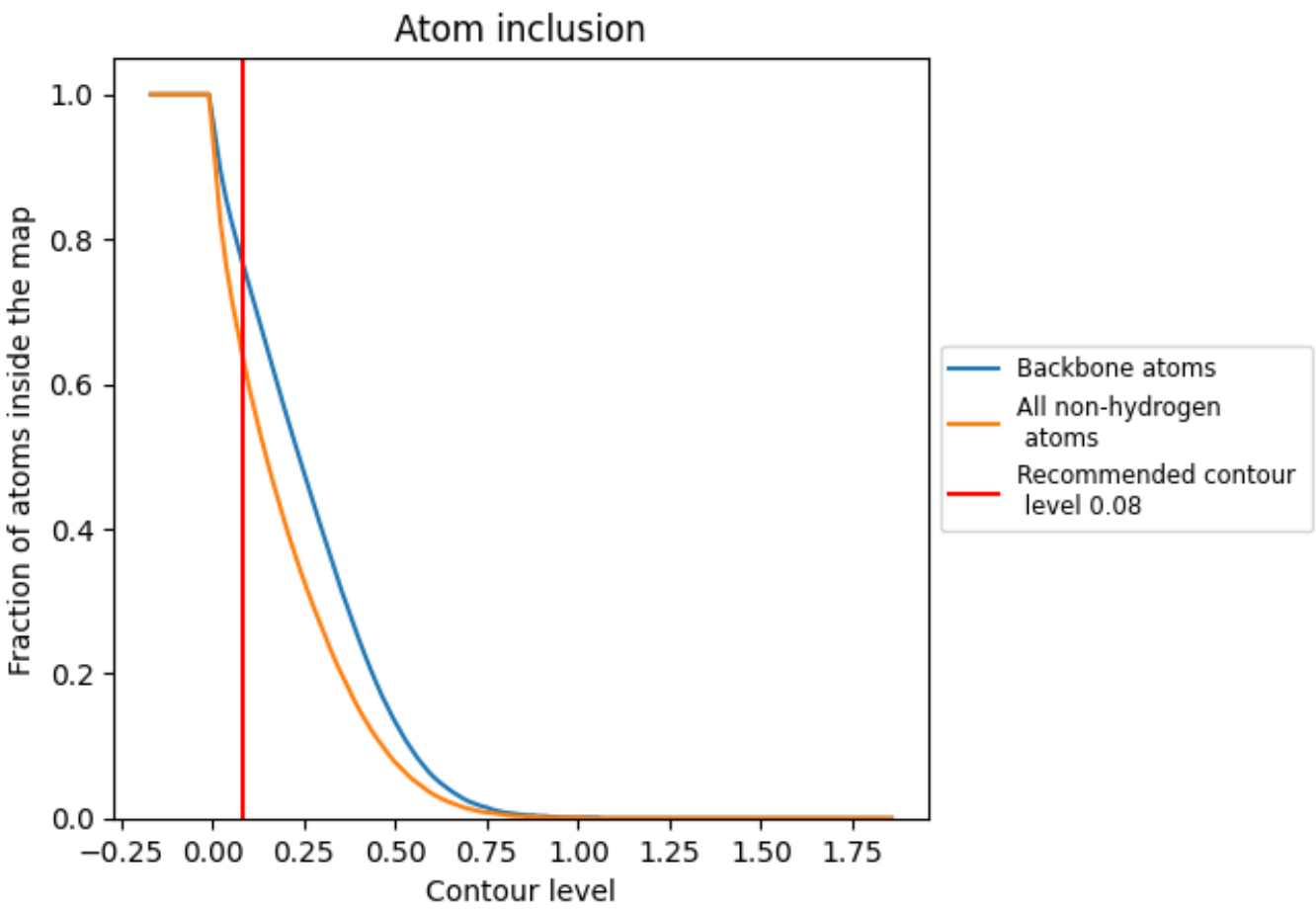
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.2390
A	0.4750	0.0510
AA	0.8380	0.3950
AB	0.8000	0.3830
AC	0.8530	0.4170
AD	0.3120	0.0760
AE	0.8330	0.3800
AF	0.8510	0.4290
AG	0.4900	0.2330
AH	0.8330	0.4180
AI	0.7700	0.3470
AJ	0.7950	0.3470
AK	0.8480	0.4140
AL	0.6490	0.2930
AM	0.8690	0.4370
AP	0.1720	0.1230
AQ	0.1000	0.0740
AS	0.4470	0.1410
Aa	0.1940	0.0130
Ab	0.8230	0.1860
Ac	0.7420	0.1550
Ad	0.5100	0.0600
Ae	0.7560	0.2180
Af	0.4840	0.0830
Ag	0.4270	0.0400
Ah	0.5970	0.1310
Ai	0.5050	0.0870
Aj	0.0380	-0.0370
Ak	0.6460	0.1780
An	0.4210	0.1050
Ao	0.7240	0.1500
Ap	0.7370	0.2470
Aq	0.5930	0.1740
Ar	0.8470	0.4070
As	0.0190	-0.0400

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Chain	Atom inclusion	Q-score
At	0.8400	0.4070
Au	0.4360	0.0360
Av	0.6160	0.1580
Aw	0.6330	0.0890
Az	0.5300	0.1110
B	0.4170	0.0490
BA	0.8440	0.3860
BB	0.8030	0.3730
BC	0.8610	0.4070
BD	0.3070	0.0790
BE	0.8400	0.3790
BF	0.8560	0.4160
BG	0.4820	0.2340
BH	0.8400	0.4090
BI	0.7620	0.3380
BJ	0.7980	0.3390
BK	0.8520	0.4050
BL	0.6560	0.2850
BM	0.8650	0.4190
BP	0.1460	0.1290
BQ	0.0810	0.0760
BS	0.4470	0.1310
Ba	0.1860	0.0240
Bb	0.8350	0.1850
Bc	0.7450	0.1540
Bd	0.5250	0.0780
Be	0.7560	0.2210
Bf	0.4930	0.0950
Bg	0.4280	0.0550
Bh	0.6160	0.1460
Bi	0.5170	0.1000
Bj	0.0300	-0.0290
Bk	0.6480	0.1830
Bn	0.4160	0.1090
Bo	0.7160	0.1420
Bp	0.7340	0.2480
Bq	0.6000	0.1750
Br	0.8520	0.3970
Bs	0.0160	-0.0300
Bt	0.8330	0.3960
Bu	0.4420	0.0530
Bv	0.6390	0.1600

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Chain	Atom inclusion	Q-score
Bw	0.6560	0.1100
Bz	0.5250	0.1340
GA	0.4130	0.0250
GB	0.4360	0.0070