wwPDB EM Validation Summary Report

Nov 4, 2024 – 07:22 AM JST

PDB ID	:	7ENA
EMDB ID	:	EMD-31204
Title	:	TFIID-based PIC-Mediator holo-complex in pre-assembled state (pre-hPIC-MED)
Authors	:	Chen, X.; Qi, Y.; Wang, X.; Wu, Z.; Yin, X.; Li, J.; Liu, W.; Xu, Y.
Deposited on	:	2021-04-16
Resolution	:	4.07 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

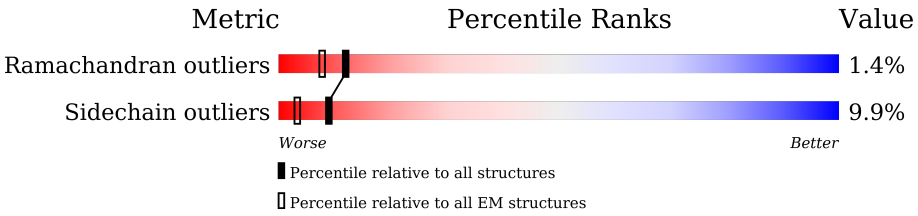
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.07 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	0	309	17% 83% 16%
2	8	346	8% 64% 23% 14%
3	9	323	33% 65% 24% 11%
4	DO	109	75% 14% 11%
5	DP	339	49% 48%
6	DQ	307	6% 34% 6% 60%
7	BA	316	75% 5% 19%
8	FA	517	25% 74%
9	FB	249	5% 74% 15% 11%

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Mol	Chain	Length	Quality of chain
10	PA	1970	61% 13% 25%
11	PB	1174	79% 17%
12	PC	275	76% 17% 7%
13	PD	142	75% 16% 9%
14	PE	210	83% 17%
15	PF	127	48% 14% 38%
16	PG	172	77% 21%
17	PH	150	83% 15%
18	PI	125	72% 18% 9%
19	PJ	67	81% 13%
20	PK	117	81% 19%
21	PL	58	55% 19% 24%
22	DA	1872	5% 29% 68%
23	DB	1199	8% 79% 20%
24	DD	1085	13% 85%
24	Dd	1085	15% 15% 85%
25	DE	800	10% 66% 32%
25	De	800	67% 67% 33%
26	DF	677	14% 50% 10% 40%
26	Df	677	34% 56% 40%
27	DG	349	5% 39% 58%
28	DH	310	10% 59% 8% 33%
29	DI	264	7% 39% 7% 55%
29	Di	264	46% 46% 54%
30	DJ	218	36% 5% 59%

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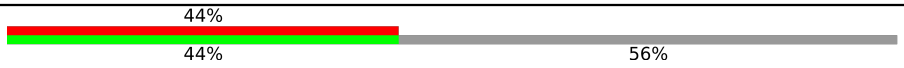
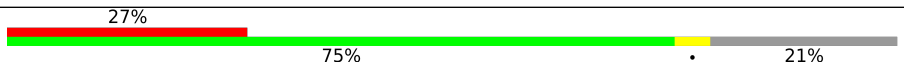
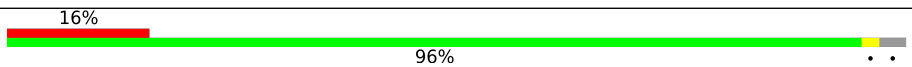
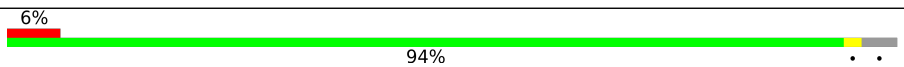
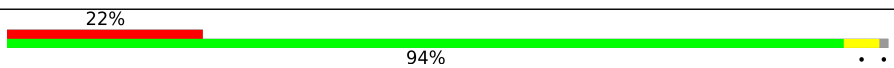
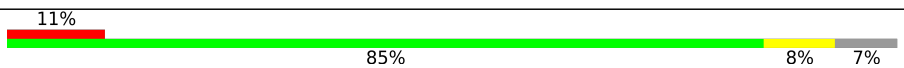
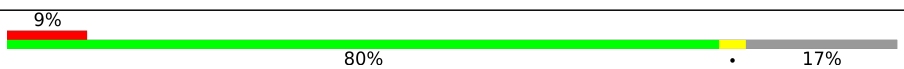
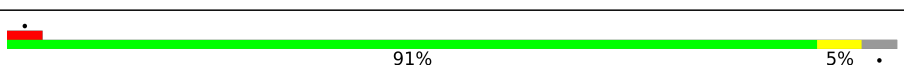
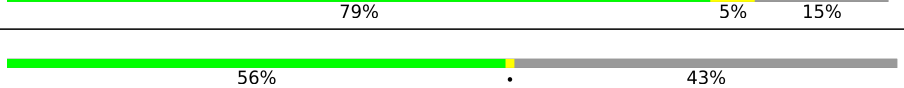
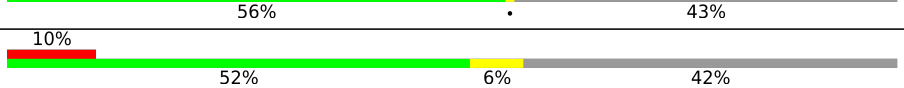
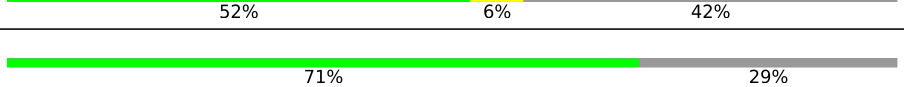
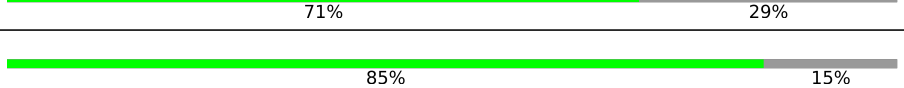
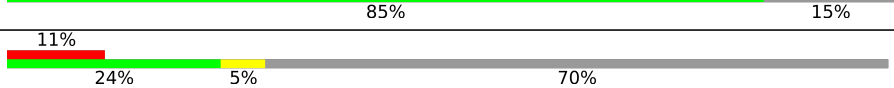
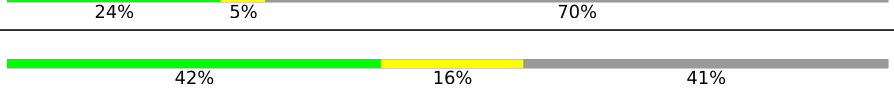
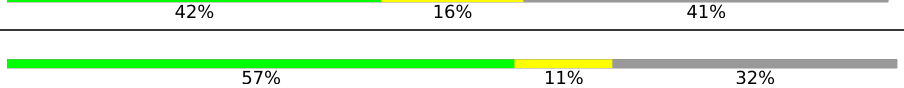
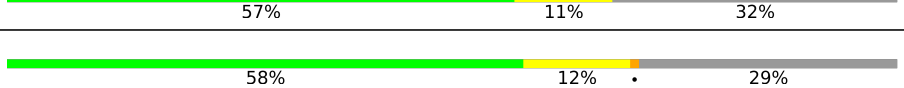
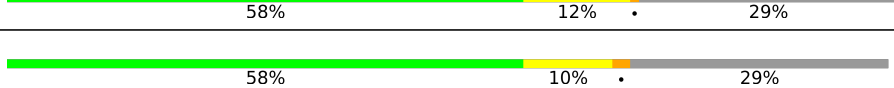
Mol	Chain	Length	Quality of chain
30	Dj	218	
31	DL	161	
31	Dl	161	
32	Dc	929	
33	Dk	211	
34	Dm	124	
35	EA	439	
36	EB	291	
37	1	548	
38	2	395	
39	3	308	
40	4	462	
41	5	71	
42	6	782	
43	7	760	
44	c	311	
45	e	178	
46	b	200	
47	l	178	
48	m	131	
49	a	1581	
50	d	270	
51	f	246	
52	g	233	
53	h	268	

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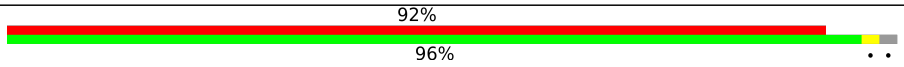
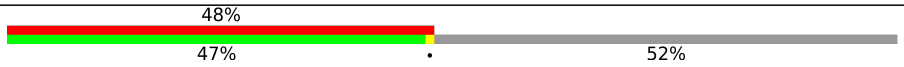
Mol	Chain	Length	Quality of chain
54	i	146	
55	j	135	
56	k	117	
57	n	1454	
58	o	788	
59	q	651	
60	r	208	
61	s	244	
62	t	212	
63	u	144	
64	v	200	
65	z	600	
66	x	989	
67	w	1368	
68	p	841	
69	X	69	
70	Y	69	

2 Entry composition (i)

There are 73 unique types of molecules in this entry. The entry contains 173965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	306	2255	1404	399	441	11	0	0

- Molecule 2 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	8	299	2378	1535	406	426	11	0	0

- Molecule 3 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	9	287	2307	1477	398	417	15	0	0

- Molecule 4 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	DO	97	771	491	133	145	2	0	0

- Molecule 5 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	DP	177	1412	918	249	238	7	0	0

- Molecule 6 is a protein called TFIIA-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	DQ	122	996	623	162	207	4	0	0

- Molecule 7 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	255	Total	C	N	O	S	0	0
			1959	1226	348	368	17		

- Molecule 8 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	FA	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 9 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	FB	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 10 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	PA	1475	Total	C	N	O	S	0	0
			11662	7336	2071	2183	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	PB	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	PC	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	PD	129	Total	C	N	O	S	0	0
			1021	643	174	200	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	PE	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	PF	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	PG	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	PH	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	PI	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 19 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	PJ	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 20 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	PK	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 21 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	PL	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DA	600	Total	C	N	O	S	0	0
			4918	3135	858	897	28		

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DB	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 24 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DD	159	Total	C	N	O	S	0	0
			1330	830	248	249	3		
24	Dd	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 25 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DE	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
25	De	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 26 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
26	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 27 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DG	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 28 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	DH	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 29 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	DI	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
29	Di	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 30 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DJ	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
30	Dj	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	DL	75	Total	C	N	O	S	0	0
			614	384	107	120	3		
31	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Dc	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Dk	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 34 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Dm	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 35 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	EA	179	Total	C	N	O	S	0	0
			1476	932	261	272	11		

- Molecule 36 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	EB	172	Total	C	N	O	S	0	0
			1404	893	243	264	4		

- Molecule 37 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	433	Total	C	N	O	S	0	0
			3436	2153	602	664	17		

- Molecule 38 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	385	Total	C	N	O	S	0	0
			3024	1909	524	564	27		

- Molecule 39 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	295	Total	C	N	O	S	0	0
			2306	1477	384	426	19		

- Molecule 40 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	457	Total	C	N	O	S	0	0
			3644	2341	641	648	14		

- Molecule 41 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 42 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	652	Total	C	N	O	S	0	0
			5255	3345	898	980	32		

- Molecule 43 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	732	Total	C	N	O	S	0	0
			5861	3742	1023	1068	28		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	263	Total	C	N	O	S	0	0
			2108	1337	378	382	11		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	e	102	Total	C	N	O	S	0	0
			832	520	146	163	3		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	b	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	l	126	Total	C	N	O	S	0	0
			1040	649	191	193	7		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	112	Total	C	N	O	S	0	0
			983	641	172	165	5		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	469	Total	C	N	O	S	0	0
			3585	2283	615	663	24		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	d	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	f	167	Total	C	N	O	S	0	0
			1329	851	231	242	5		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	g	166	Total	C	N	O	S	0	0
			1382	880	244	248	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	11	LEU	PRO	conflict	UNP O43513

- Molecule 53 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	h	190	Total	C	N	O	S	0	0
			1465	913	259	289	4		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	i	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	j	122	Total	C	N	O	S	0	0
			1001	636	174	187	4		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	k	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	n	994	Total	C	N	O	S	0	0
			7241	4576	1293	1334	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	133	LEU	ALA	conflict	UNP O60244

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	o	156	Total	C	N	O	S	0	0
			1221	780	212	222	7		

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	q	555	Total	C	N	O	S	0	0
			4276	2700	767	792	17		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	r	206	Total	C	N	O	S	0	0
			1630	1033	285	294	18		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	s	81	Total	C	N	O	S	0	0
			505	312	91	100	2		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	t	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	u	107	Total	C	N	O	S	0	0
			792	492	132	165	3		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	v	134	Total	C	N	O	S	0	0
			1083	668	185	226	4		

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	x	896	Total	C	N	O	S	0	0
			7050	4516	1188	1292	54		

- Molecule 67 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	w	1334	Total	C	N	O	S	0	0
			10772	6965	1827	1909	71		

- Molecule 68 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	p	406	Total	C	N	O	S	0	0
			3124	1982	536	585	21		

- Molecule 69 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	X	69	Total	C	N	O	P	0	0
			1429	672	279	409	69		

- Molecule 70 is a DNA chain called DNA(69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Y	69	Total	C	N	O	P	0	0
			1400	664	248	419	69		

- Molecule 71 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
71	0	2	Total	Zn	0
			2	2	
71	BA	1	Total	Zn	0
			1	1	
71	PA	2	Total	Zn	0
			2	2	
71	PB	1	Total	Zn	0
			1	1	
71	PC	1	Total	Zn	0
			1	1	
71	PI	2	Total	Zn	0
			2	2	

Continued on next page...

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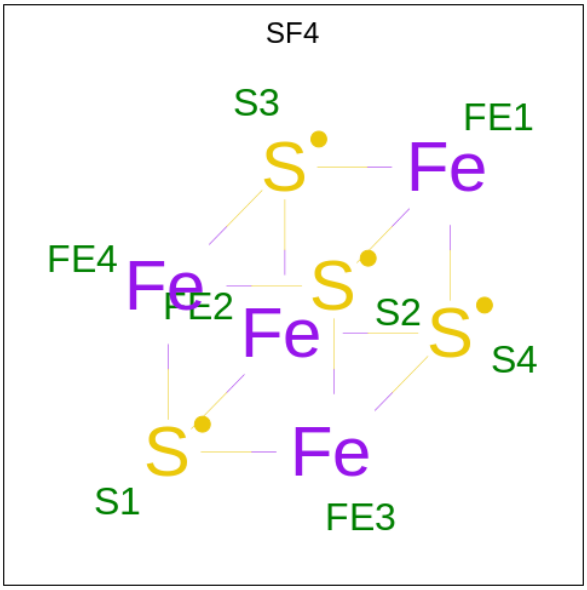
Mol	Chain	Residues	Atoms	AltConf
71	PJ	1	Total Zn 1 1	0
71	PL	1	Total Zn 1 1	0
71	EA	1	Total Zn 1 1	0
71	2	3	Total Zn 3 3	0
71	3	1	Total Zn 1 1	0

- Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
72	PA	1	Total Mg 1 1	0

- Molecule 73 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



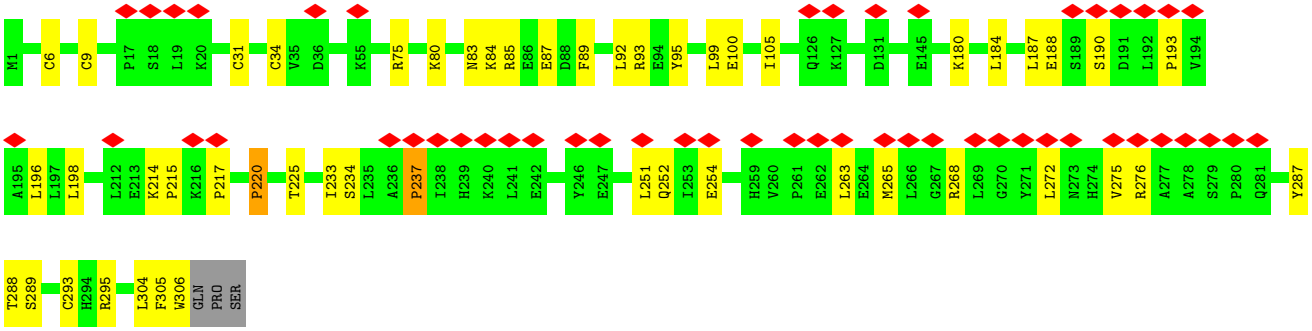
Mol	Chain	Residues	Atoms	AltConf
73	7	1	Total Fe S 8 4 4	0

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.

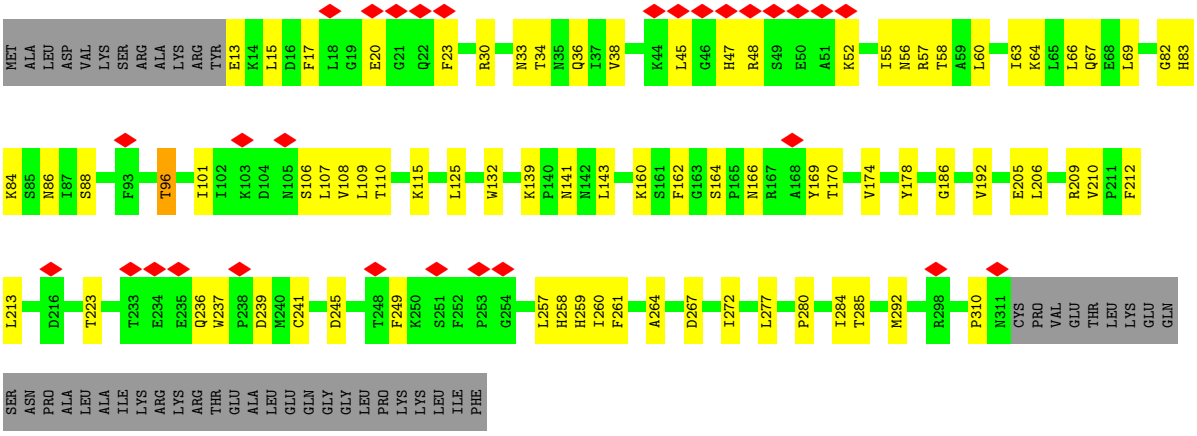
• Molecule 1: CDK-activating kinase assembly factor MAT1

Chain 0:



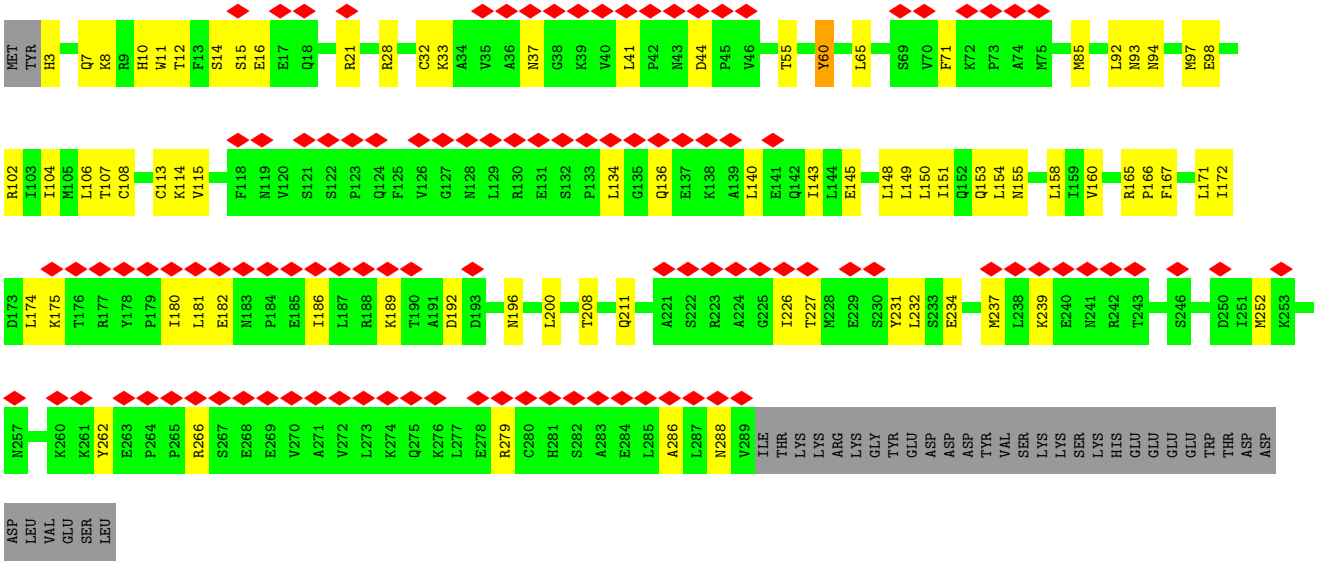
• Molecule 2: Cyclin-dependent kinase 7

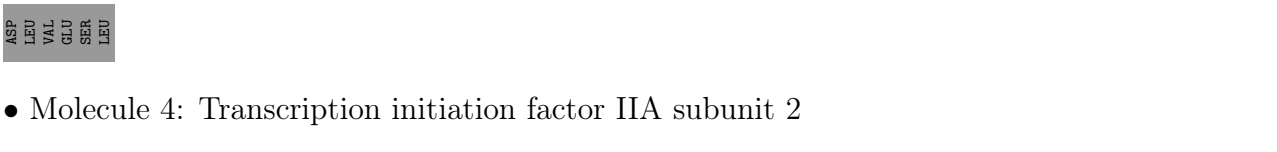
Chain 8:



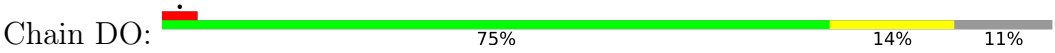
• Molecule 3: Cyclin-H

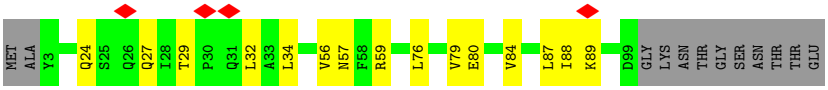
Chain 9:



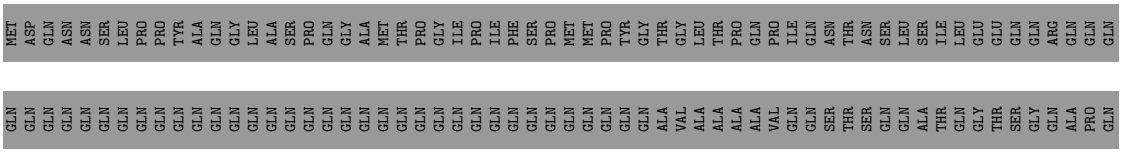


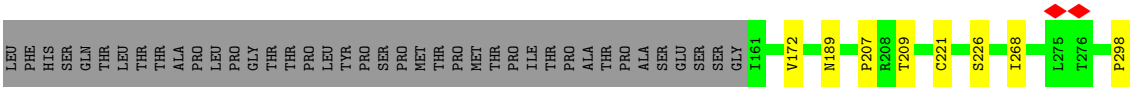
• Molecule 4: Transcription initiation factor IIA subunit 2



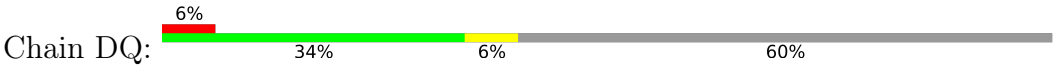


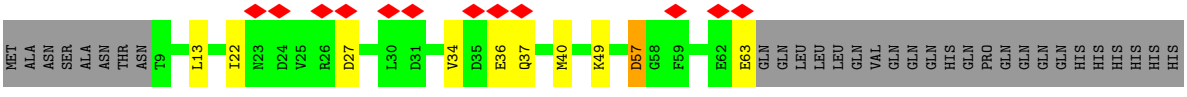
• Molecule 5: TATA-box-binding protein

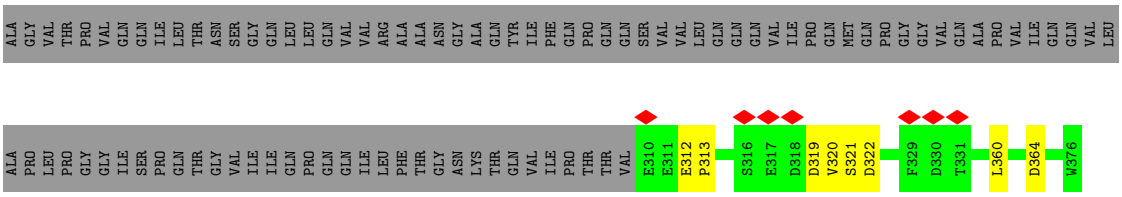




• Molecule 6: TFIIA-a

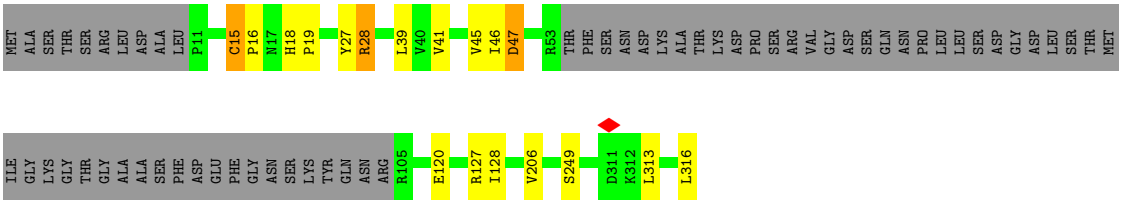






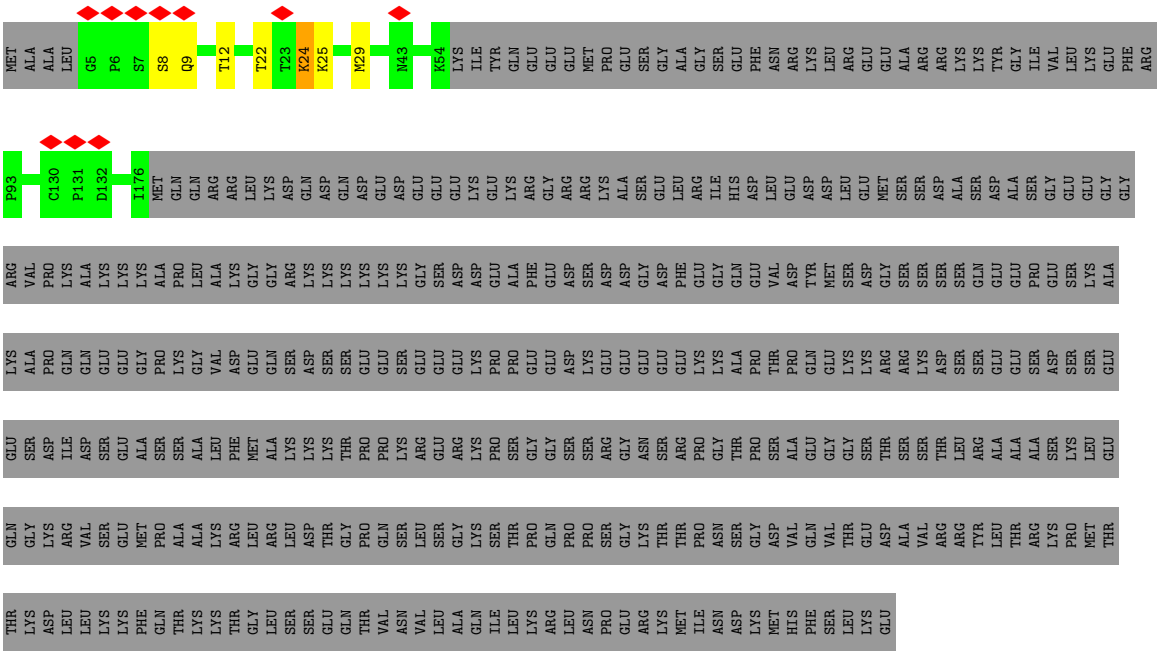
• Molecule 7: Transcription initiation factor IIB

Chain BA:



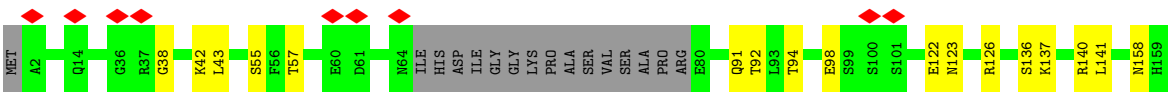
• Molecule 8: General transcription factor IIF subunit 1

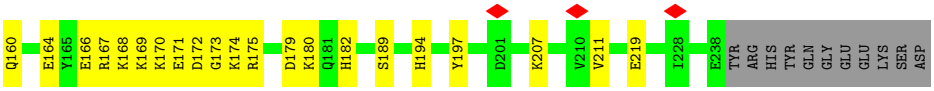
Chain FA:



• Molecule 9: General transcription factor IIF subunit 2

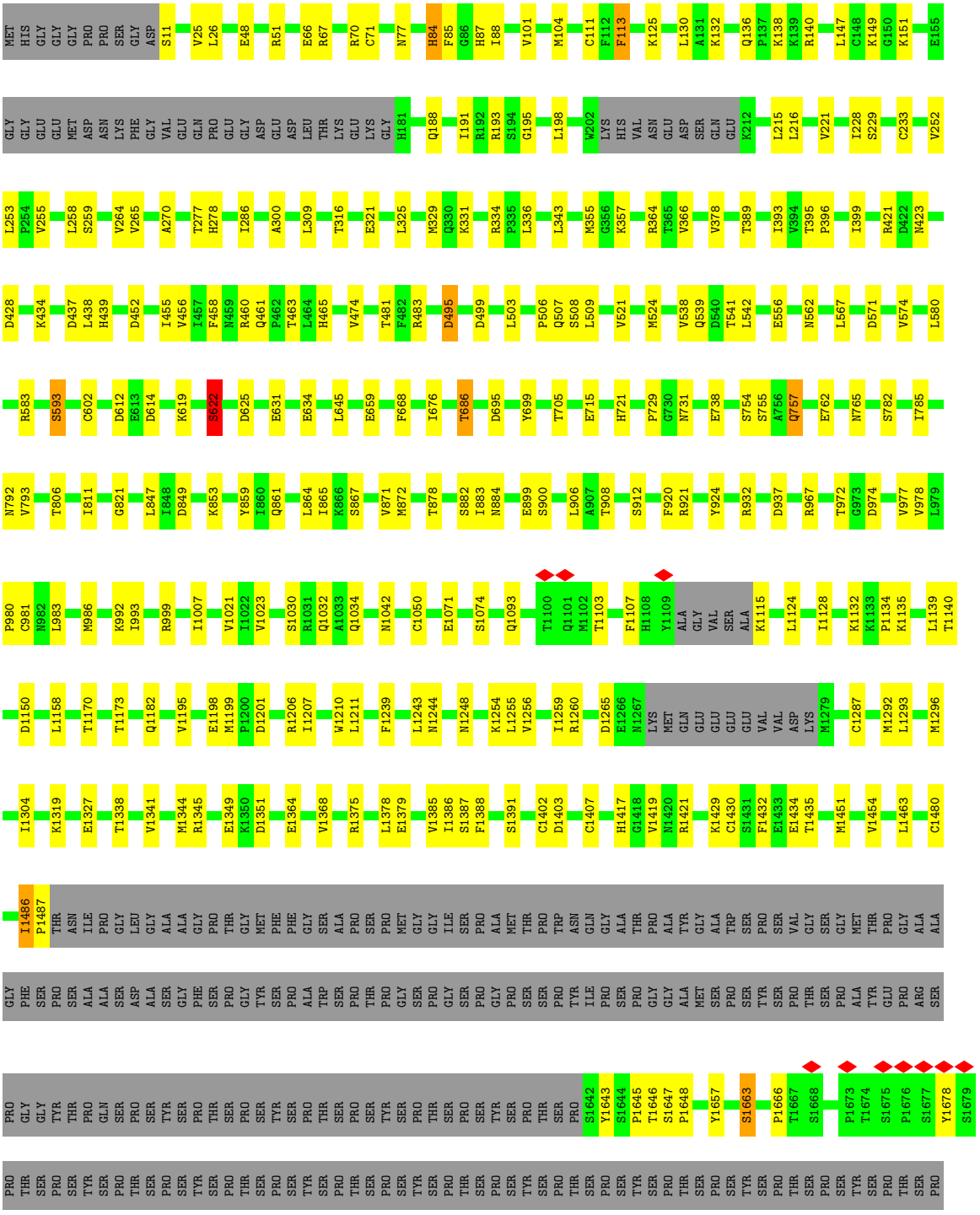
Chain FB:

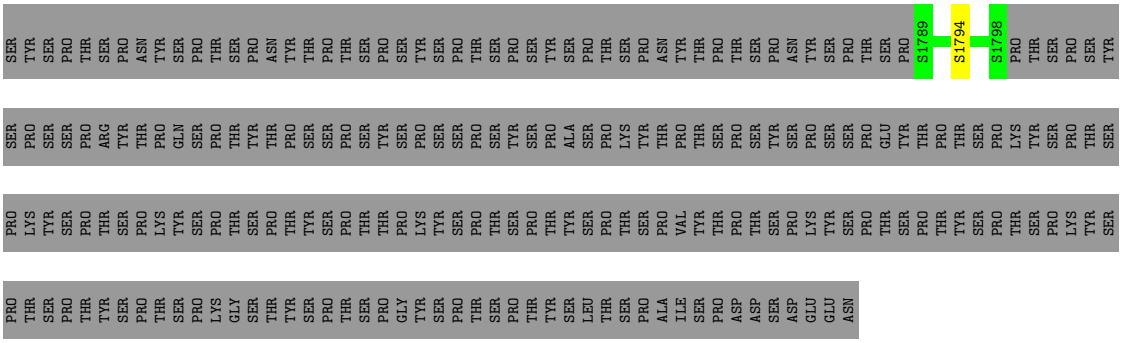




• Molecule 10: RPB1

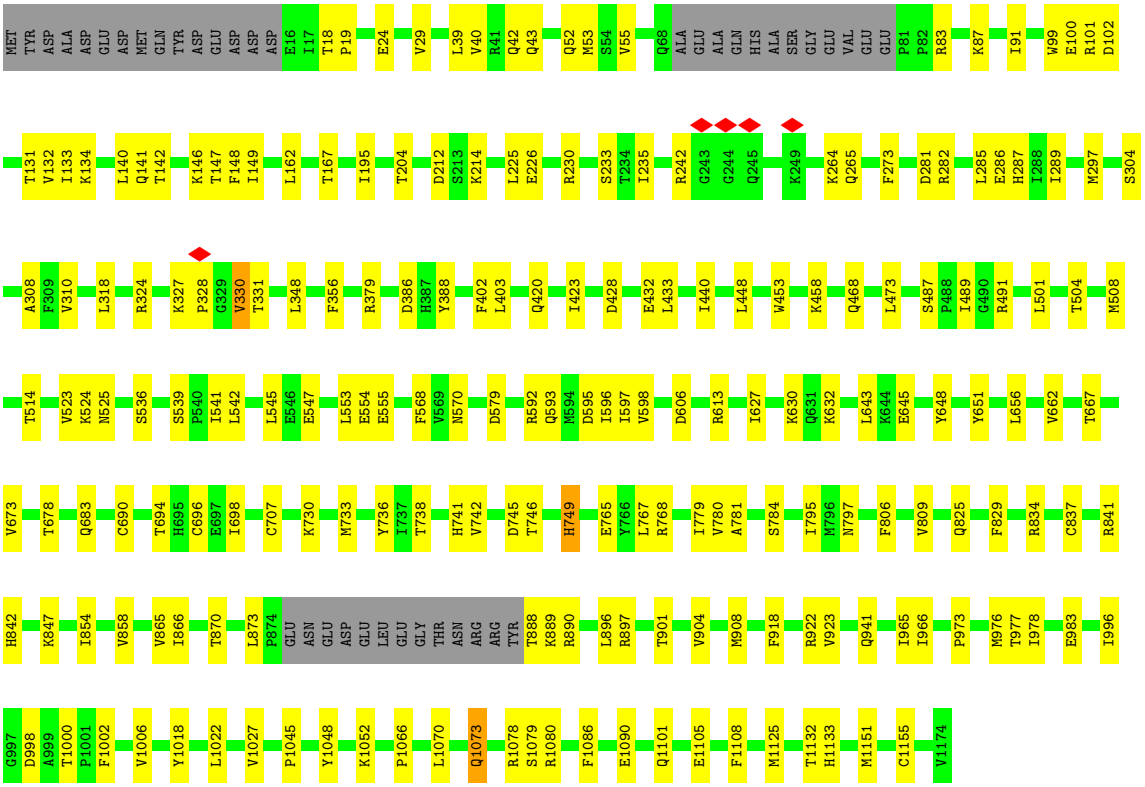
Chain PA:





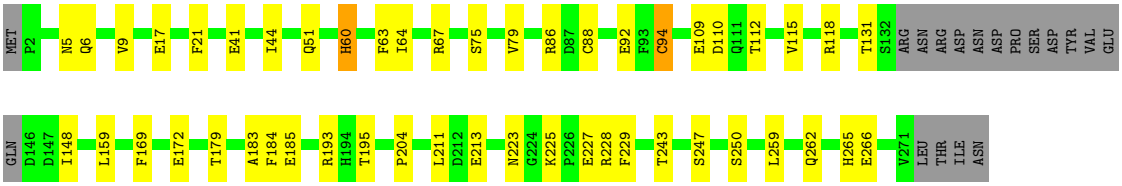
• Molecule 11: DNA-directed RNA polymerase subunit beta

Chain PB:



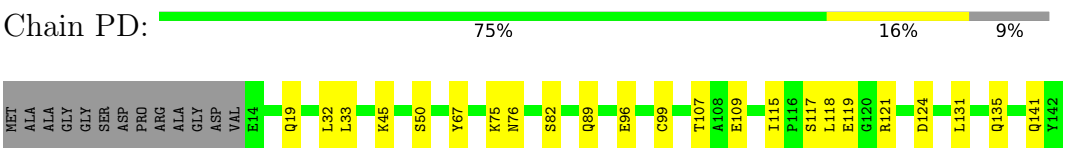
• Molecule 12: DNA-directed RNA polymerase II subunit RPB3

Chain PC:



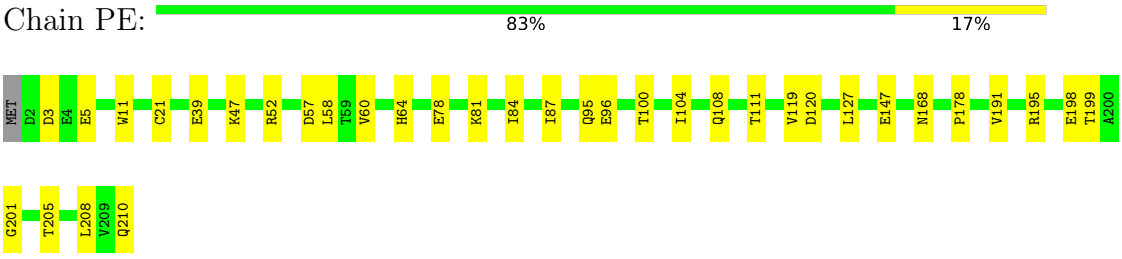
• Molecule 13: DNA-directed RNA polymerase II subunit RPB4

Chain PD:



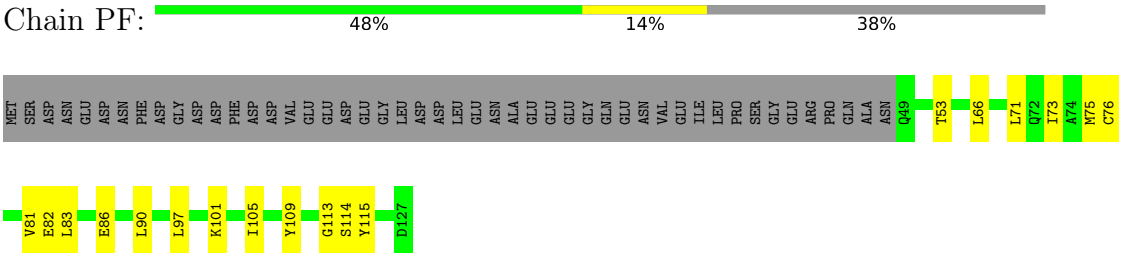
• Molecule 14: DNA-directed RNA polymerase II subunit E

Chain PE:



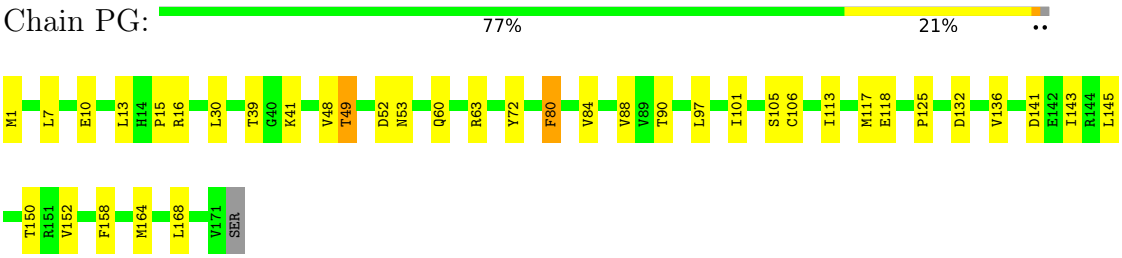
• Molecule 15: DNA-directed RNA polymerase II subunit F

Chain PF:



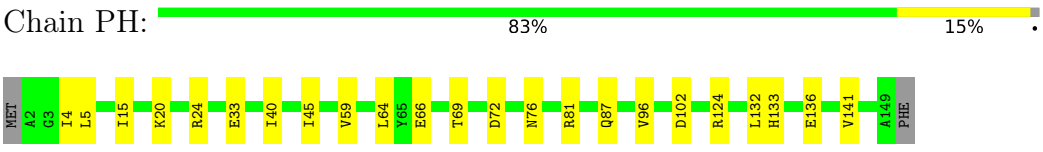
• Molecule 16: DNA-directed RNA polymerase II subunit RPB7

Chain PG:



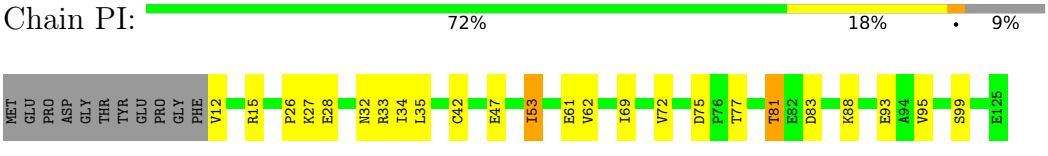
• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain PH:



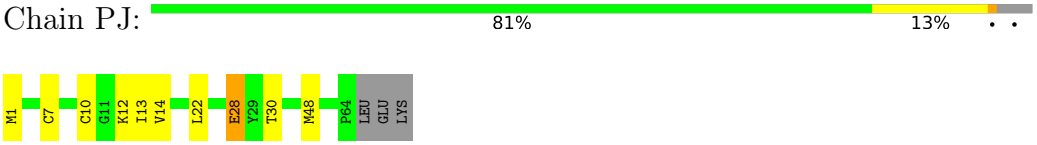
• Molecule 18: DNA-directed RNA polymerase II subunit RPB9

Chain PI:



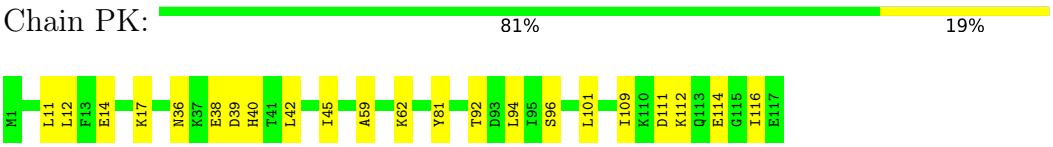
• Molecule 19: RPB10

Chain PJ:



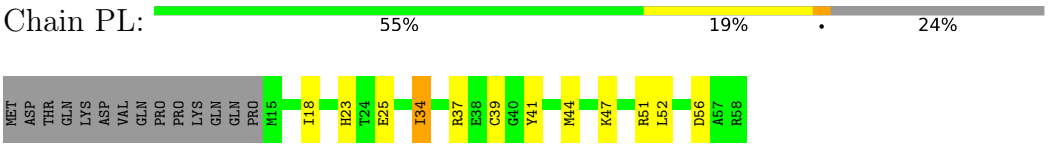
• Molecule 20: RNA_pol_L_2 domain-containing protein

Chain PK:



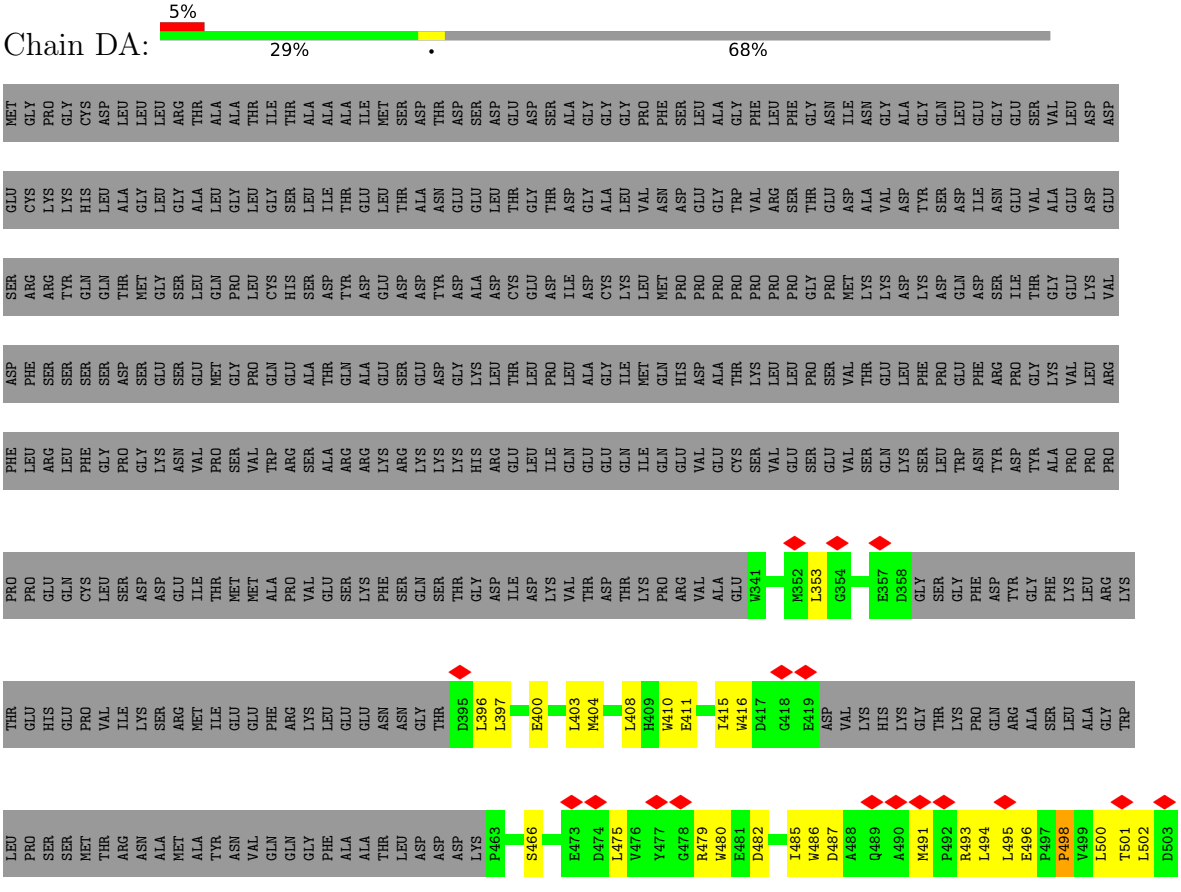
• Molecule 21: RPB12

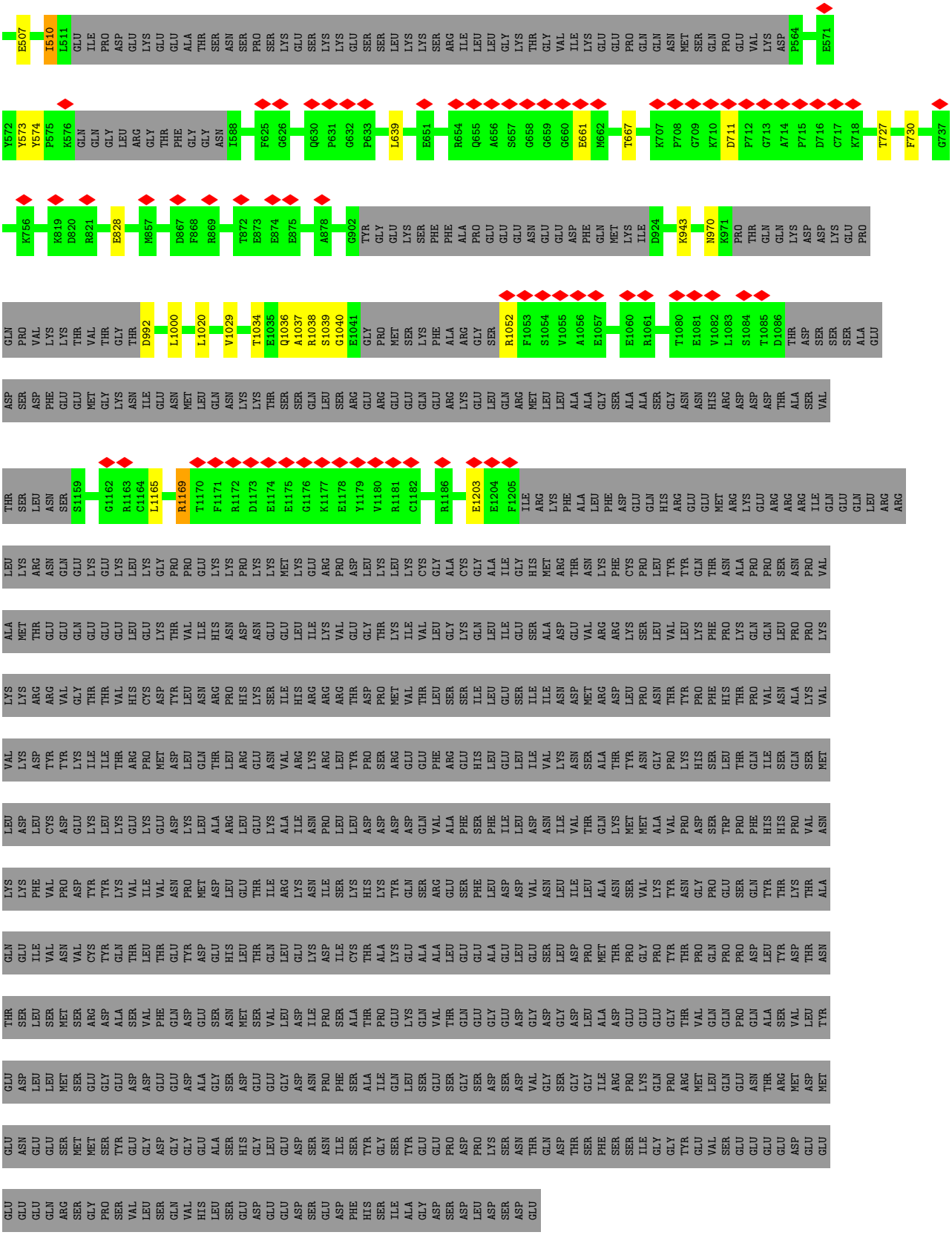
Chain PL:



• Molecule 22: Transcription initiation factor TFIID subunit 1

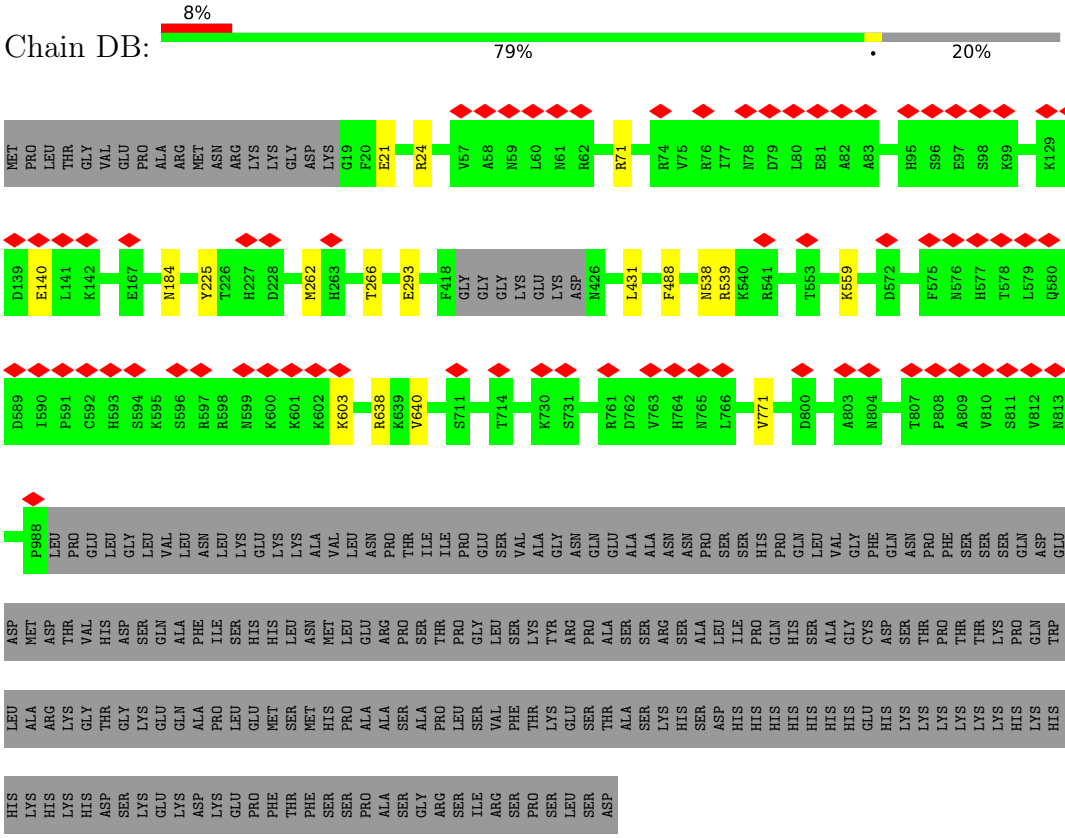
Chain DA:





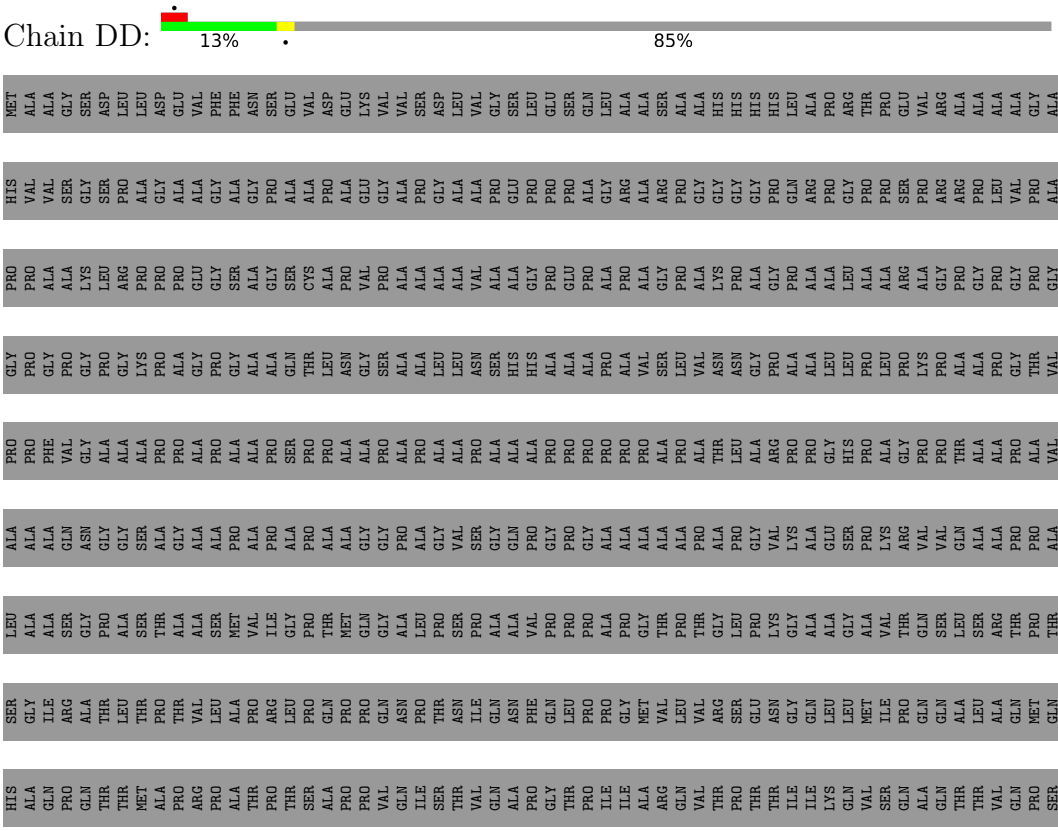
• Molecule 23: Transcription initiation factor TFIID subunit 2

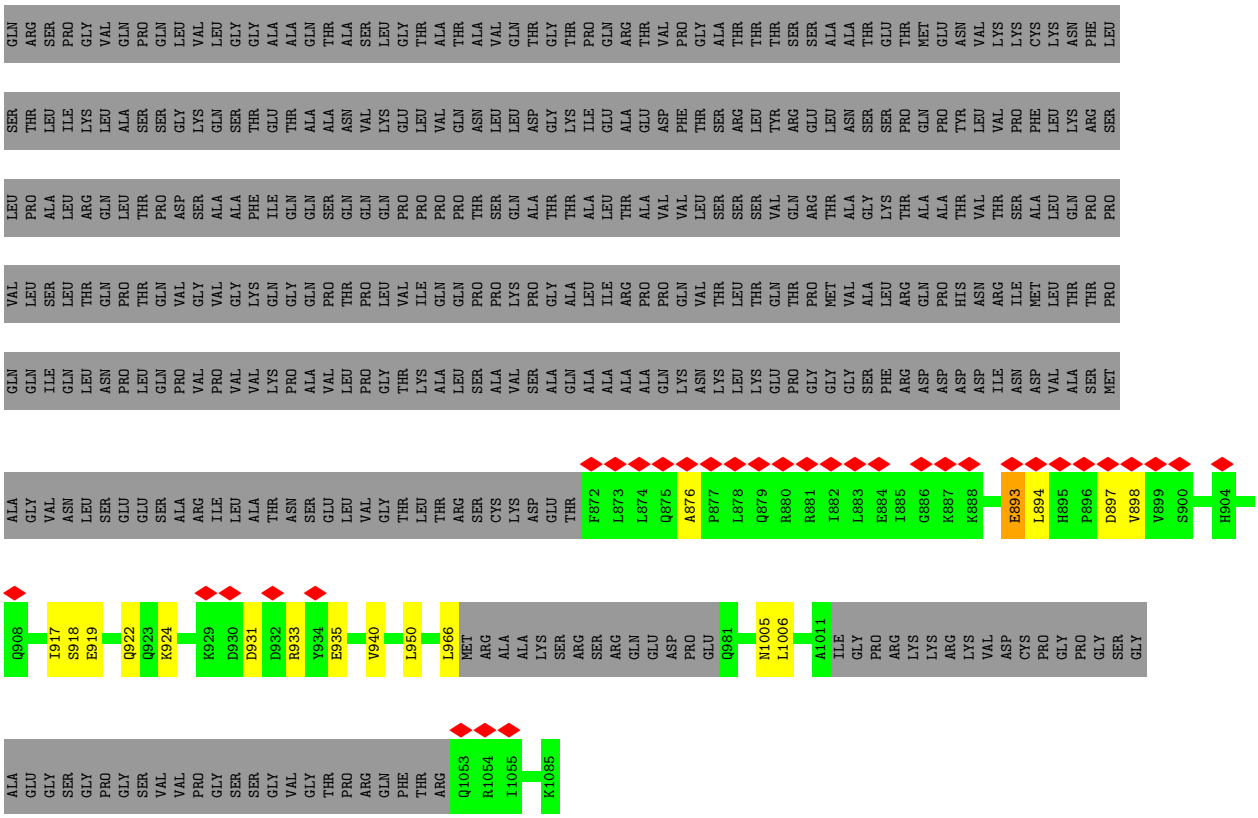
Chain DB:



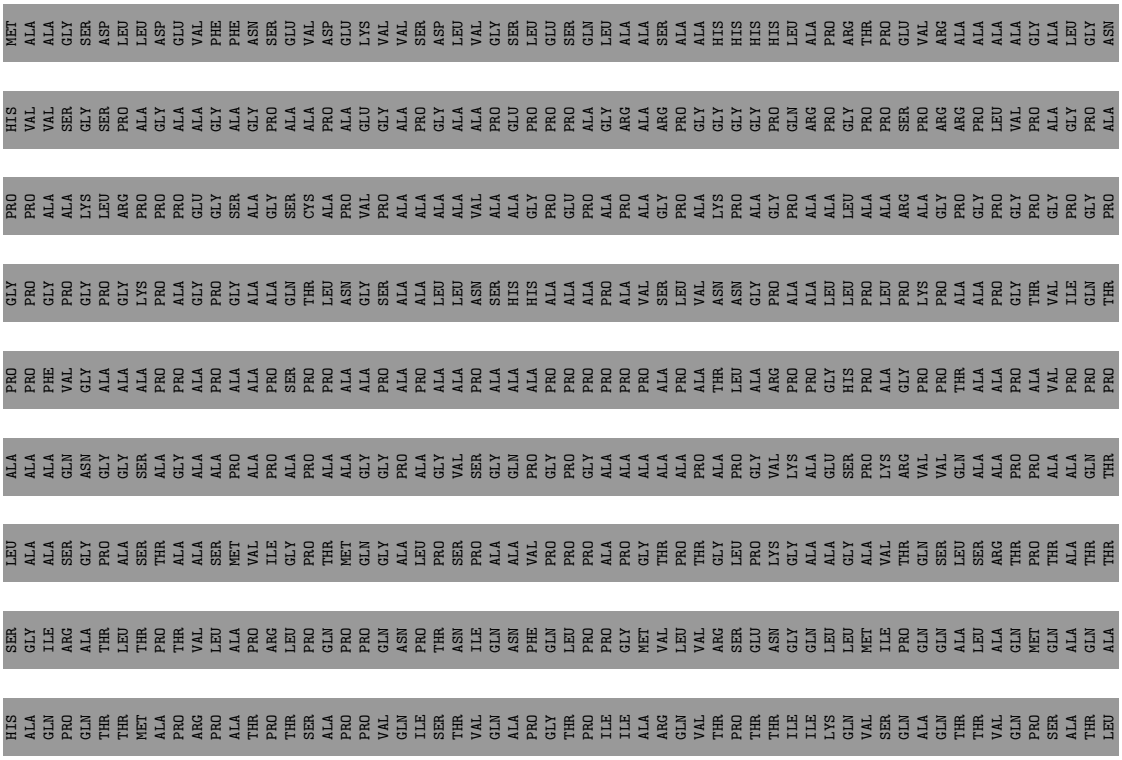
• Molecule 24: Transcription initiation factor TFIID subunit 4

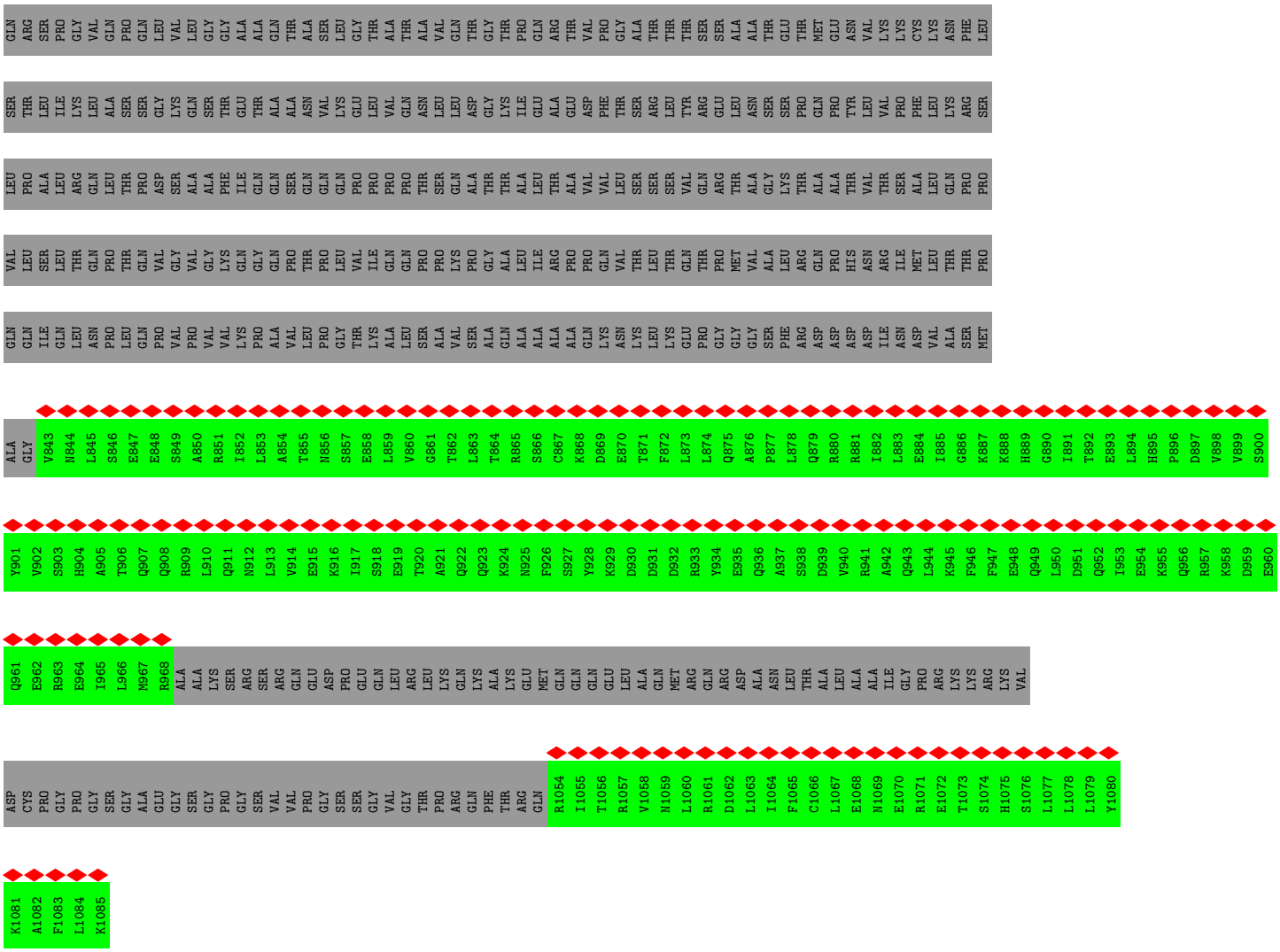
Chain DD:





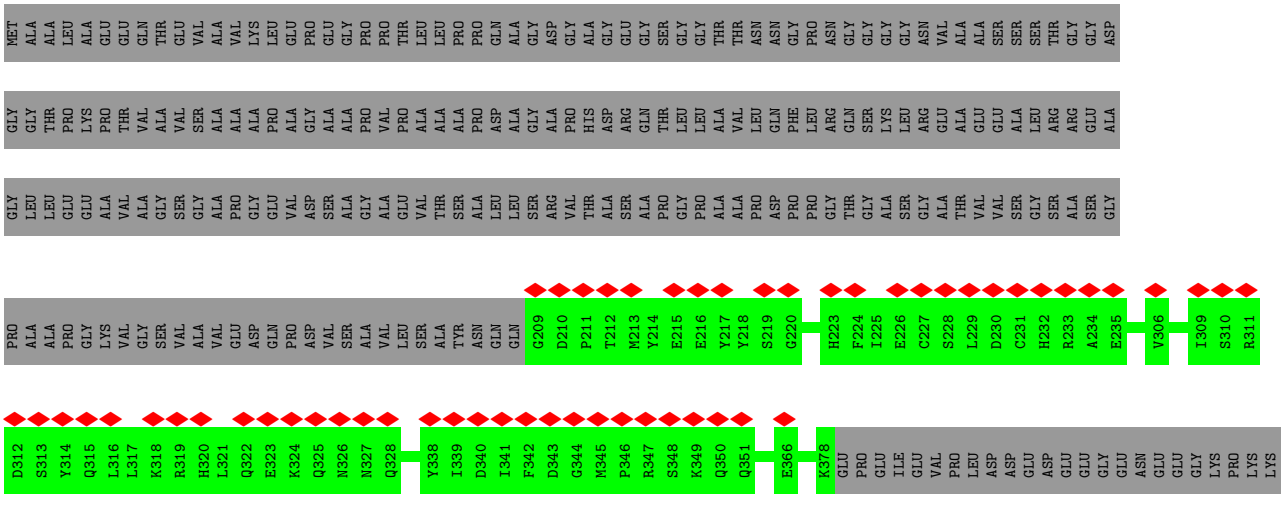
• Molecule 24: Transcription initiation factor TFIID subunit 4

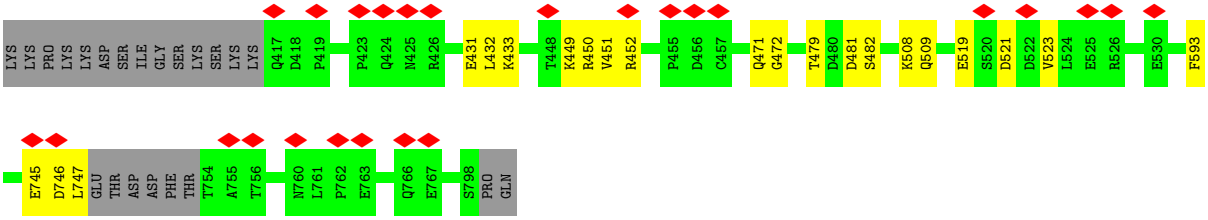




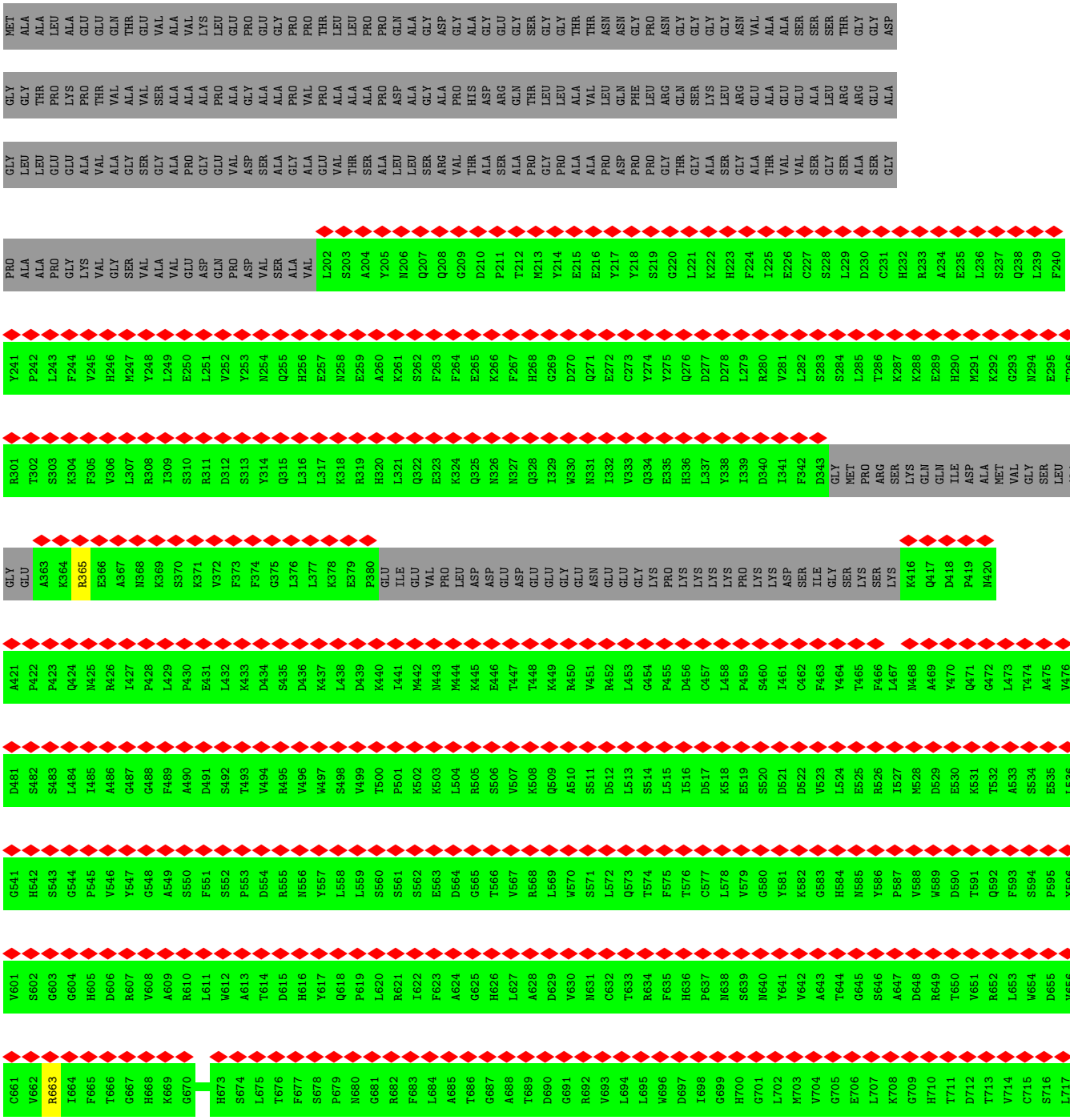
• Molecule 25: Transcription initiation factor TFIID subunit 5

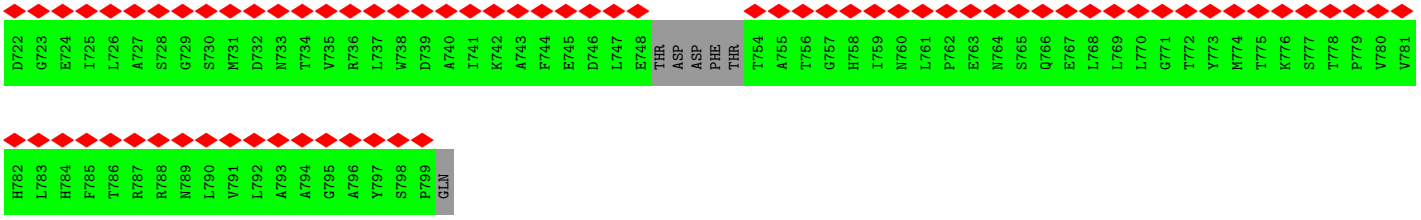
Chain DE:



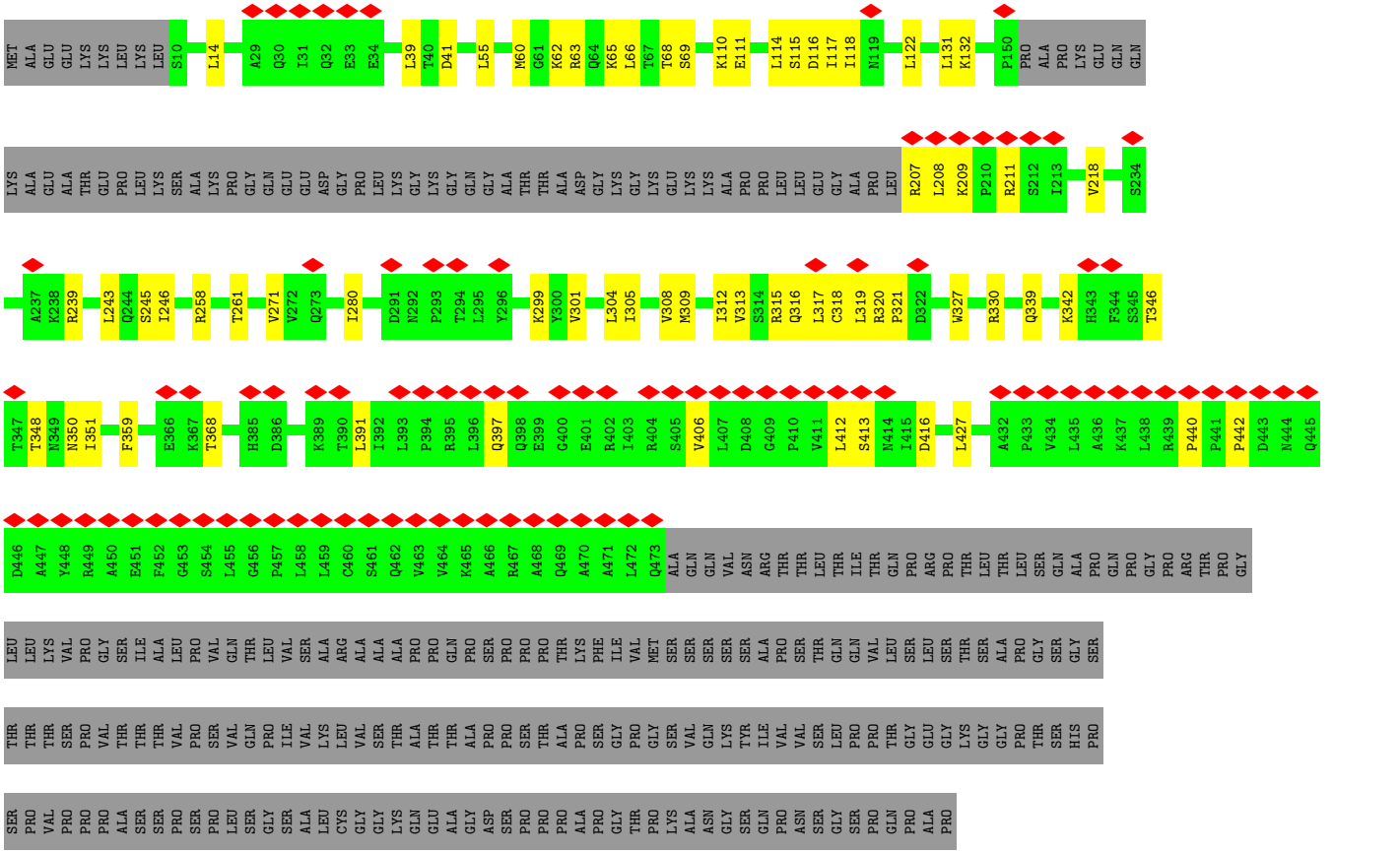


• Molecule 25: Transcription initiation factor TFIID subunit 5

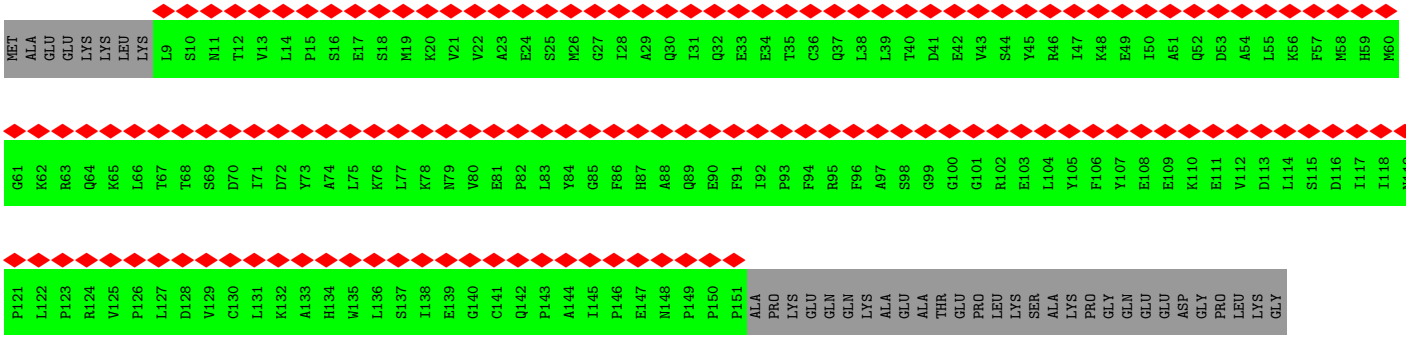


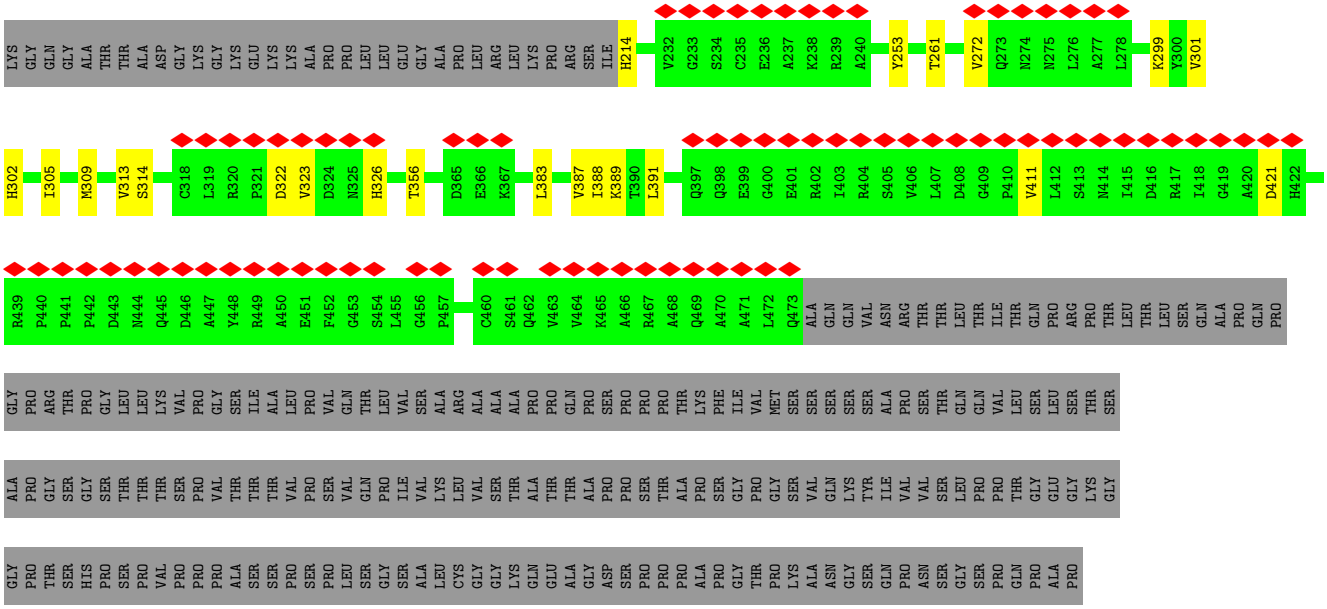


• Molecule 26: Transcription initiation factor TFIID subunit 6



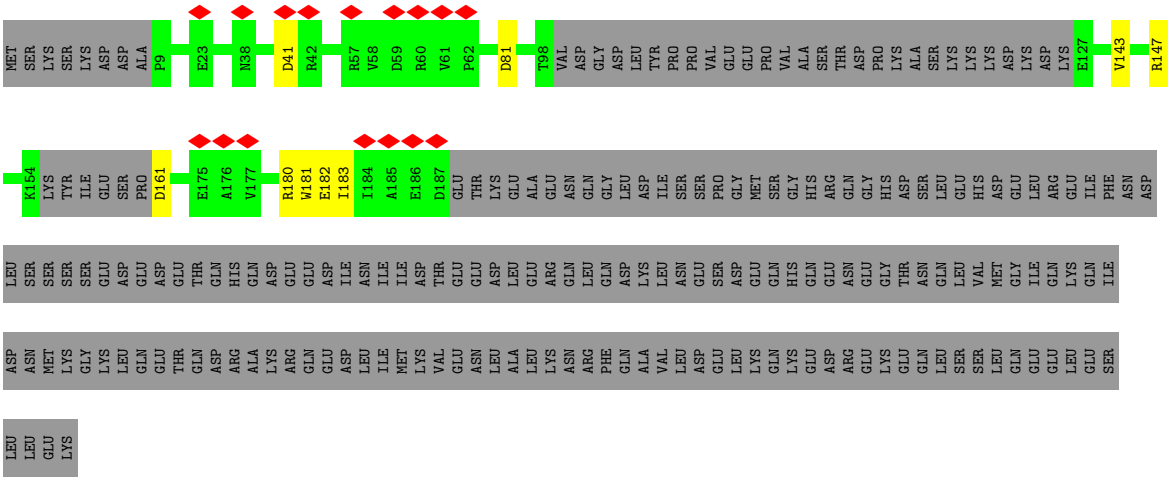
• Molecule 26: Transcription initiation factor TFIID subunit 6





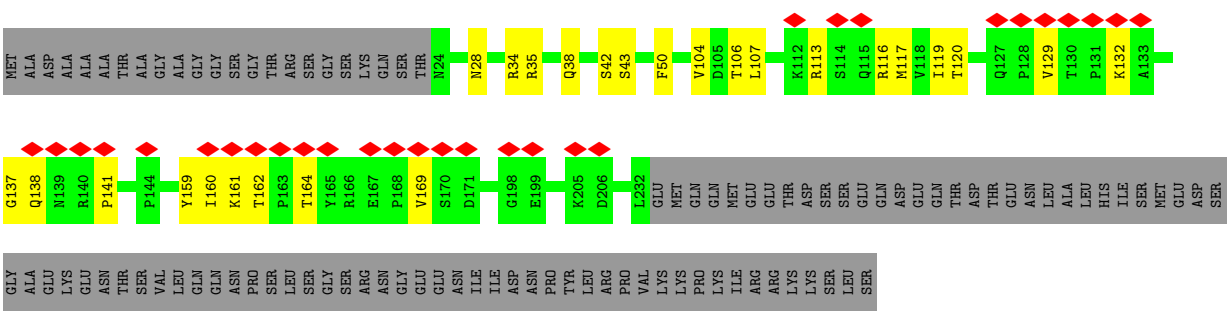
• Molecule 27: Transcription initiation factor TFIID subunit 7

Chain DG:



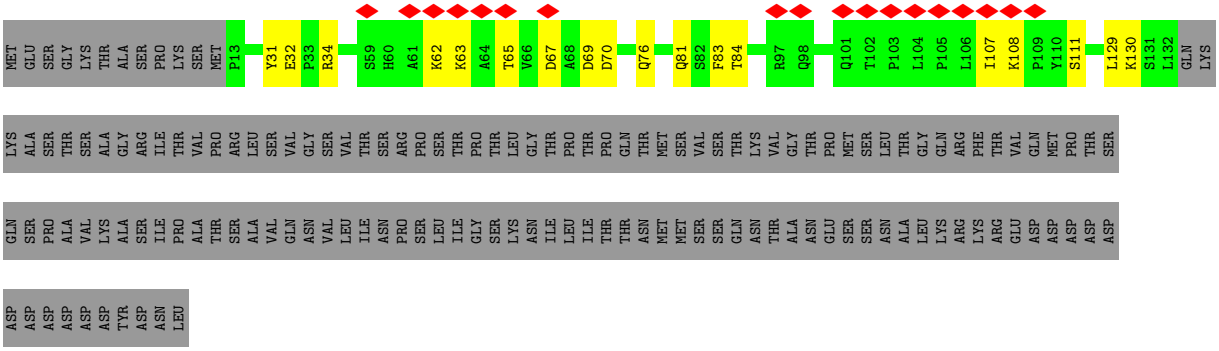
• Molecule 28: Transcription initiation factor TFIID subunit 8

Chain DH:



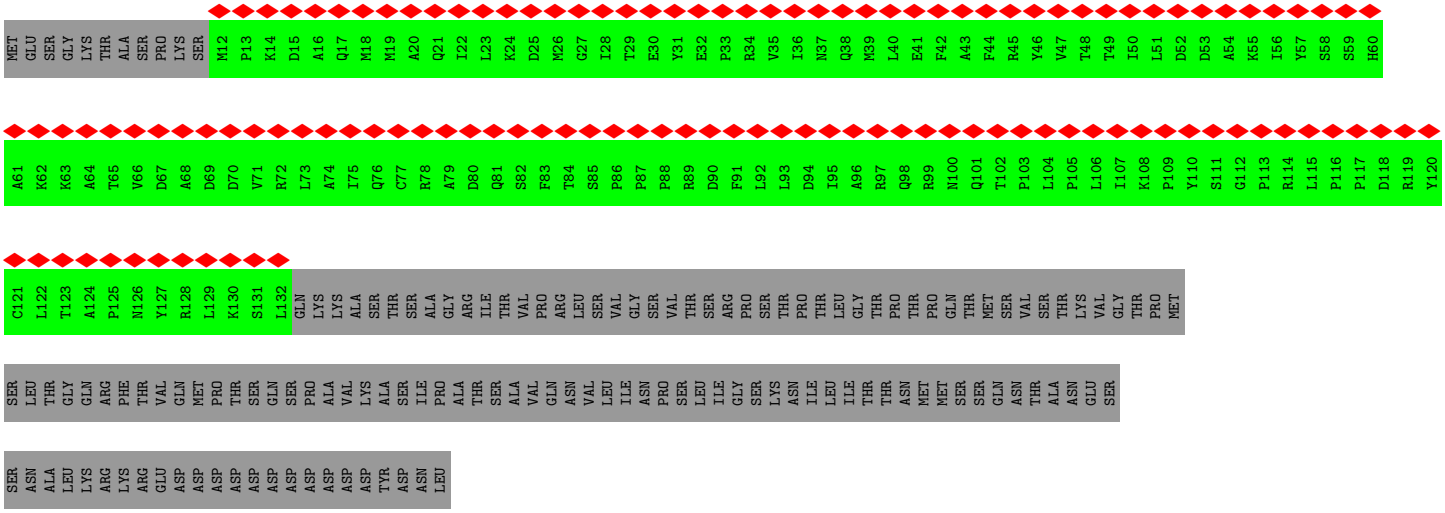
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain DI:



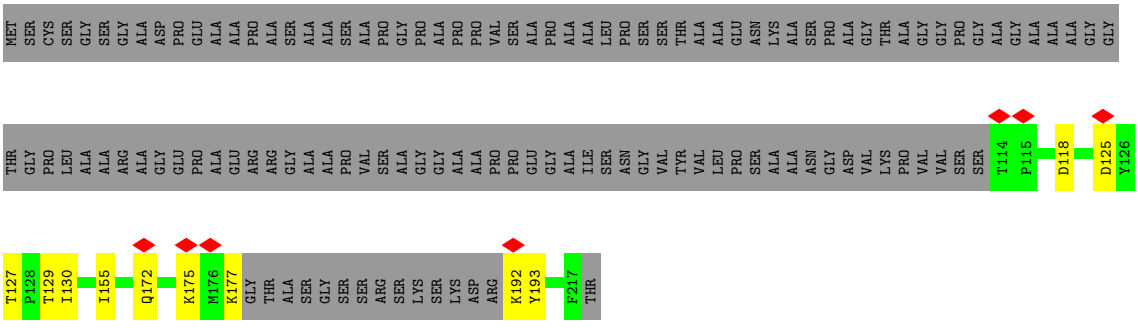
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain Di:



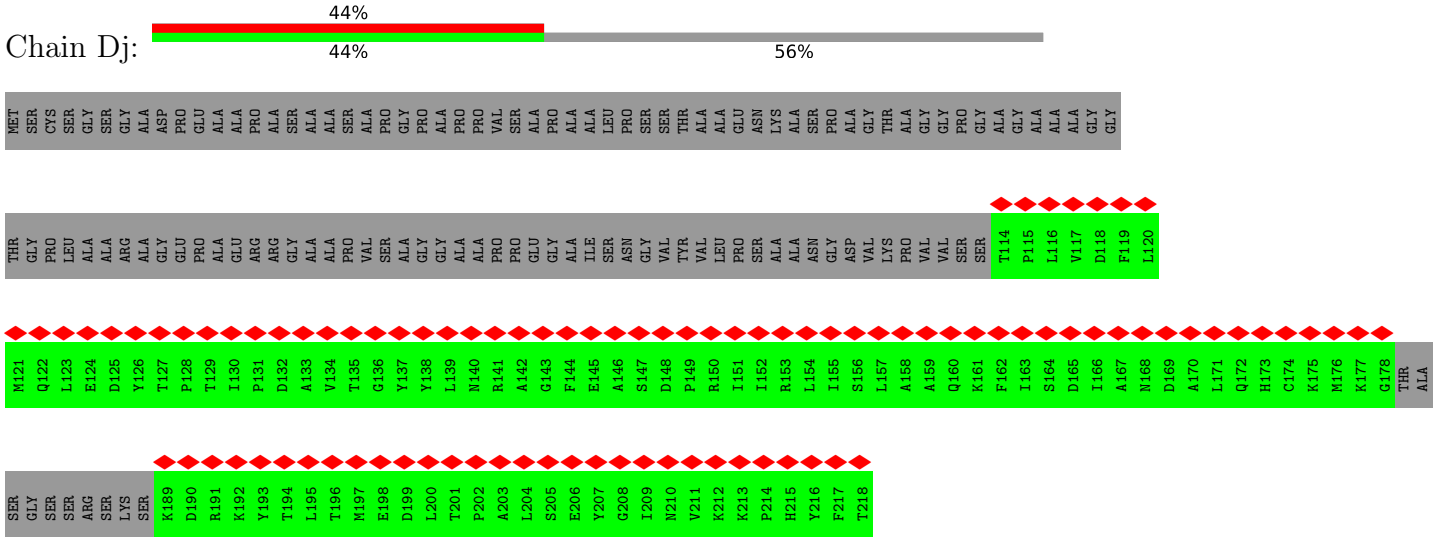
• Molecule 30: Transcription initiation factor TFIID subunit 10

Chain DJ:



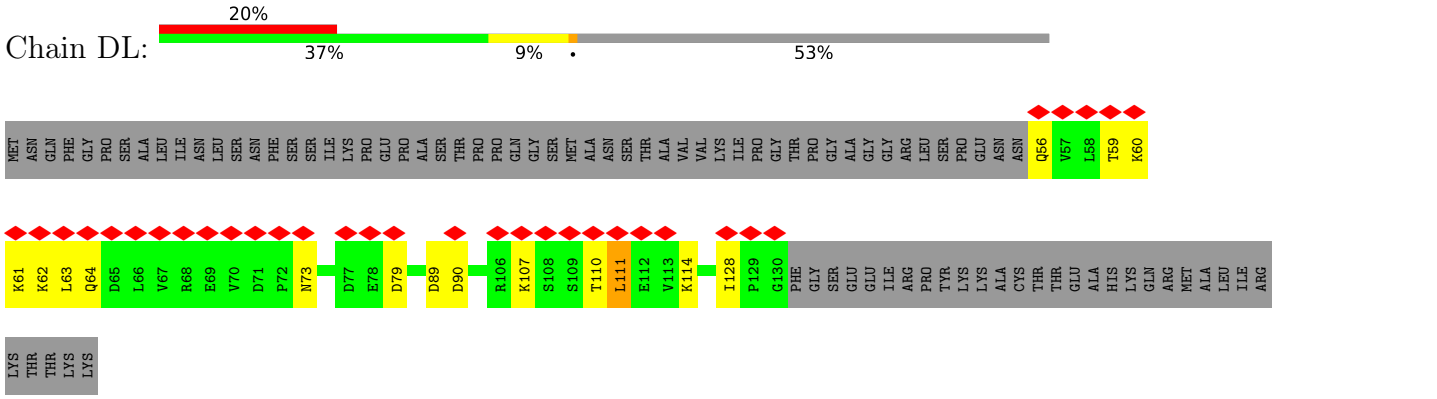
• Molecule 30: Transcription initiation factor TFIID subunit 10

Chain Dj:



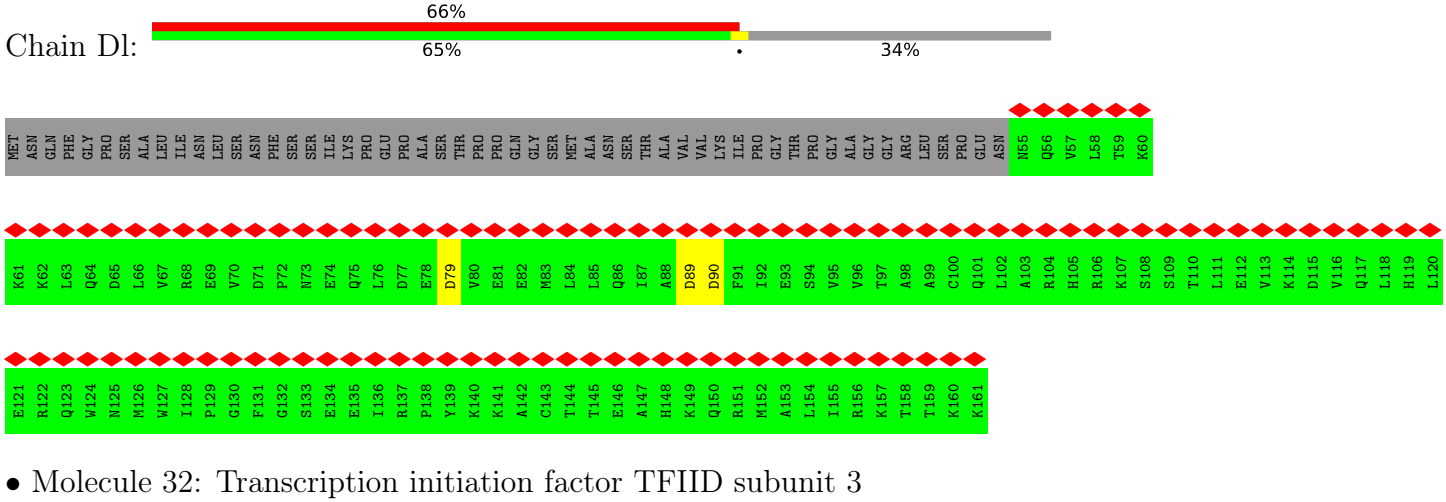
• Molecule 31: Transcription initiation factor TFIID subunit 12

Chain DL:



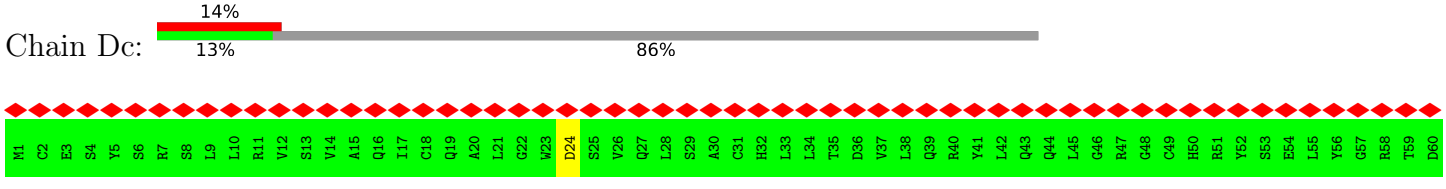
• Molecule 31: Transcription initiation factor TFIID subunit 12

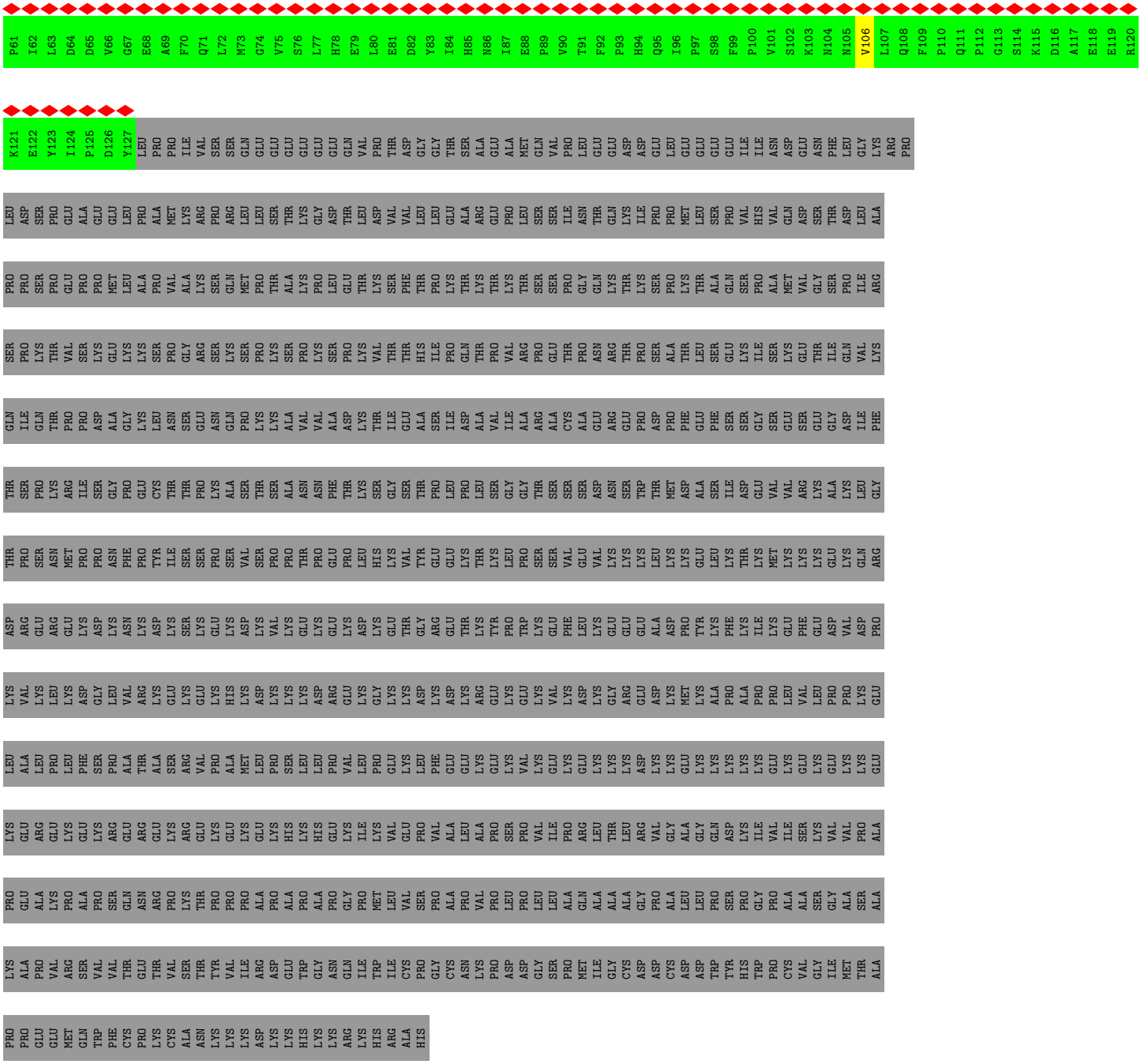
Chain Dl:



• Molecule 32: Transcription initiation factor TFIID subunit 3

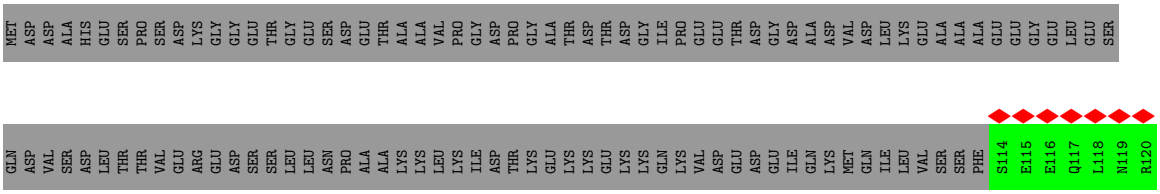
Chain Dc:

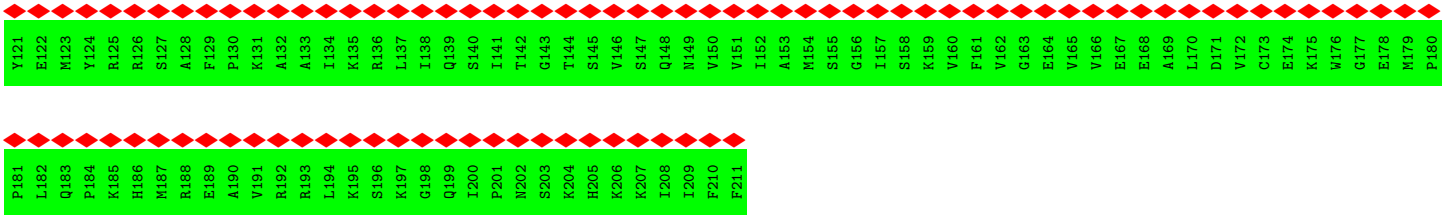




- Molecule 33: Transcription initiation factor TFIID subunit 11

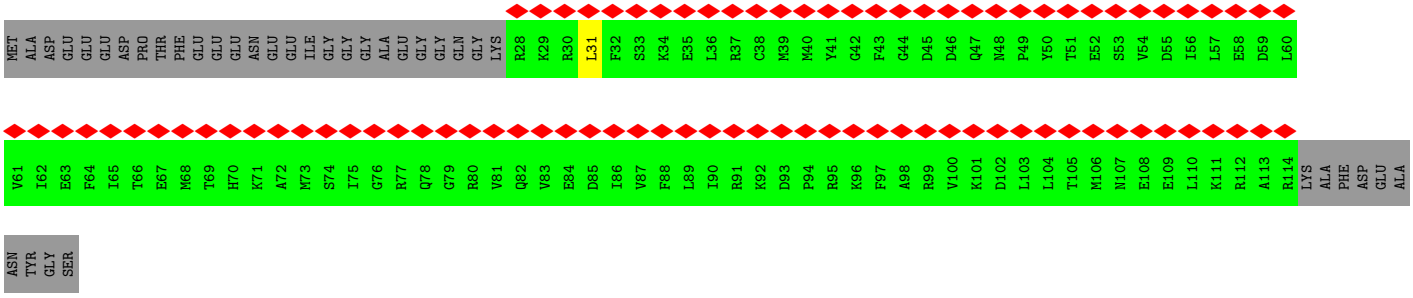
Chain Dk:





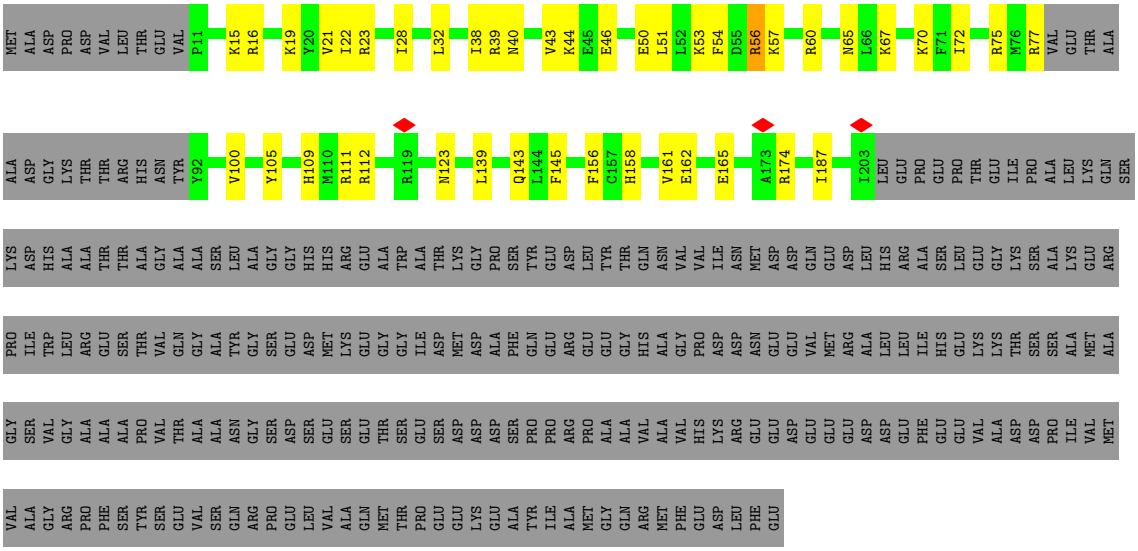
• Molecule 34: Transcription initiation factor TFIID subunit 13

Chain Dm:



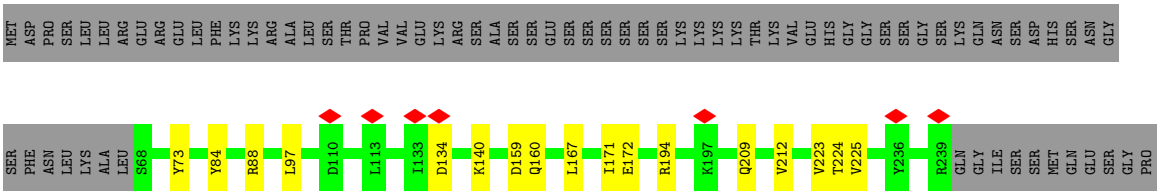
• Molecule 35: General transcription factor IIE subunit 1

Chain EA:



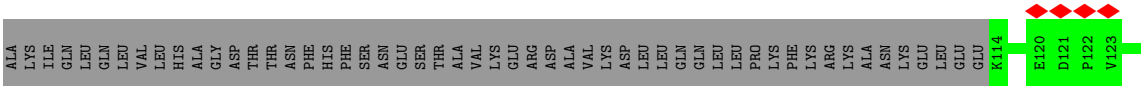
• Molecule 36: Transcription initiation factor IIE subunit beta

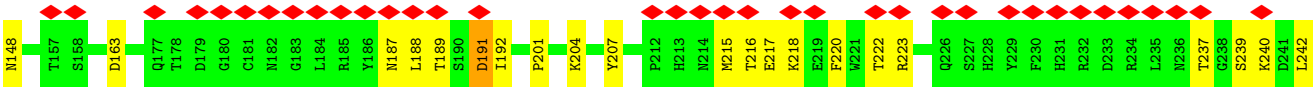
Chain EB:

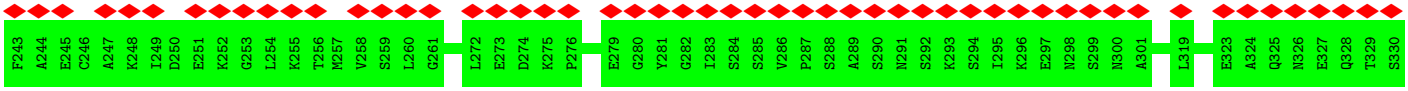


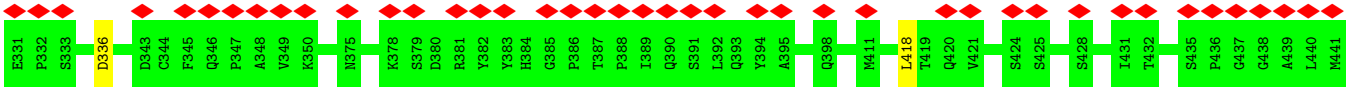
• Molecule 37: General transcription factor IIH subunit 1

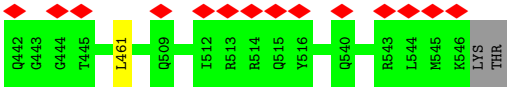
Chain 1:





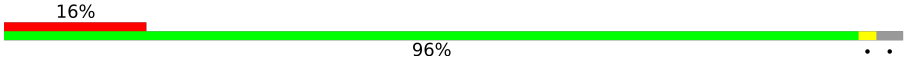


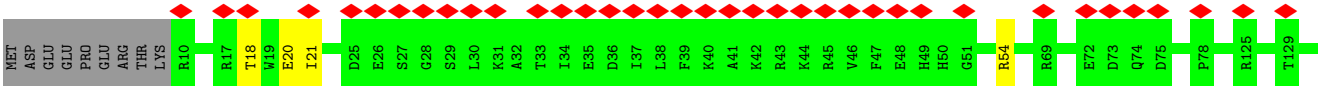


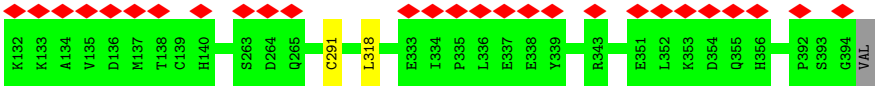


• Molecule 38: General transcription factor IIH subunit 2

Chain 2:

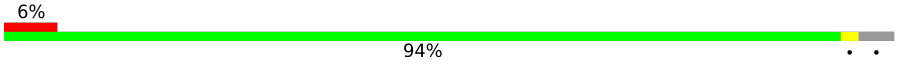


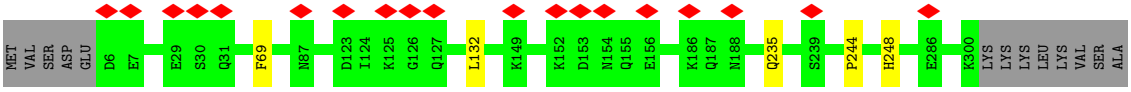




• Molecule 39: General transcription factor IIH subunit 3

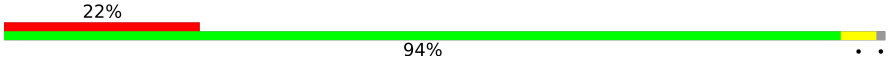
Chain 3:

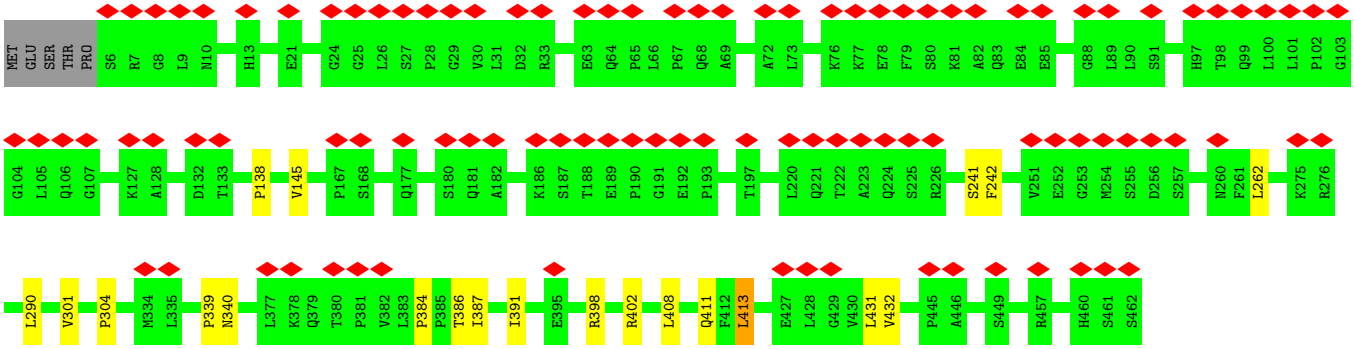




• Molecule 40: General transcription factor IIH subunit 4

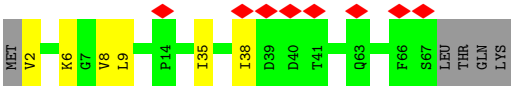
Chain 4:





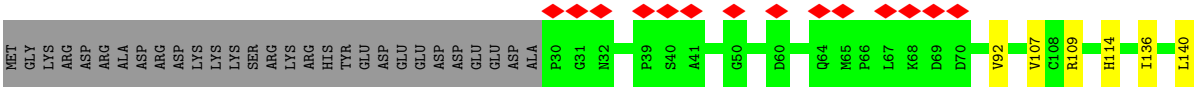
• Molecule 41: General transcription factor IIH subunit 5

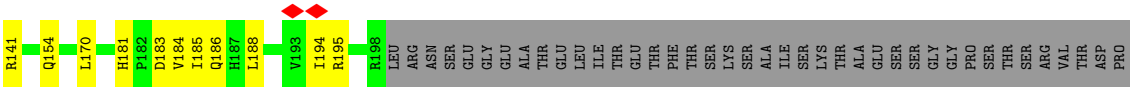
Chain 5:

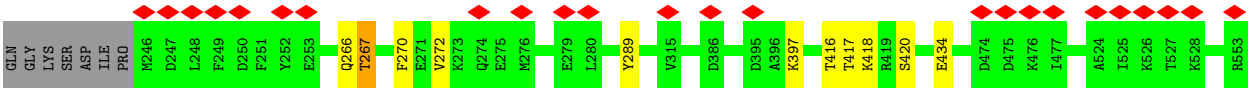


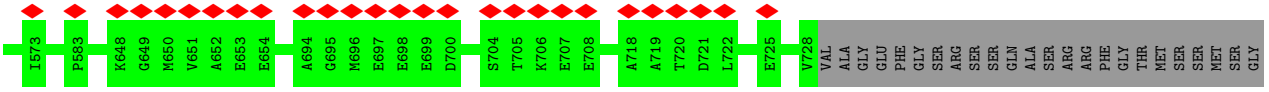
• Molecule 42: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 6:



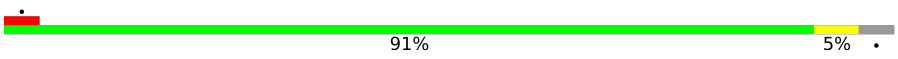


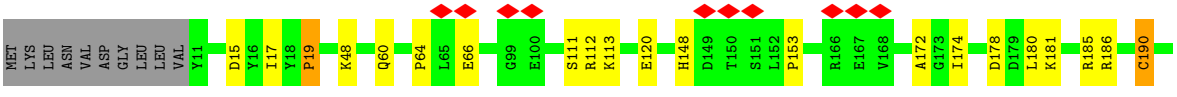


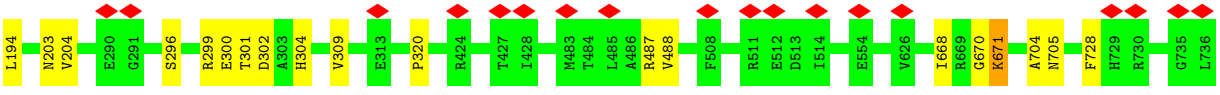


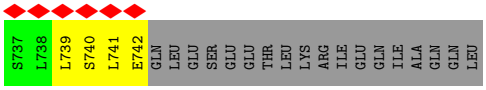
• Molecule 43: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 7:

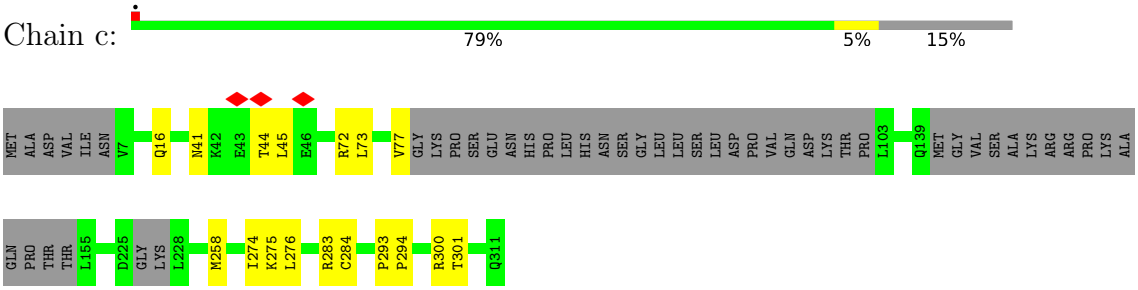




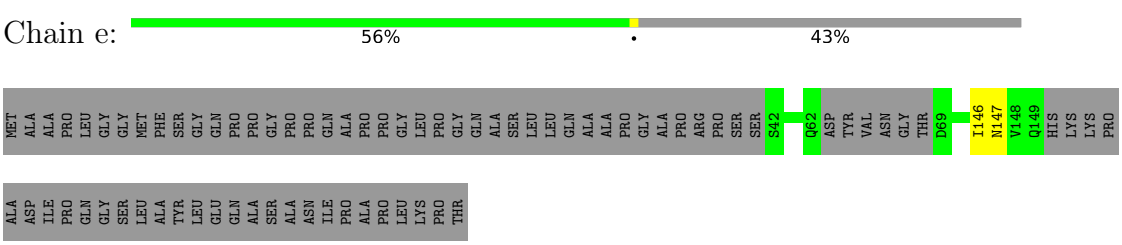




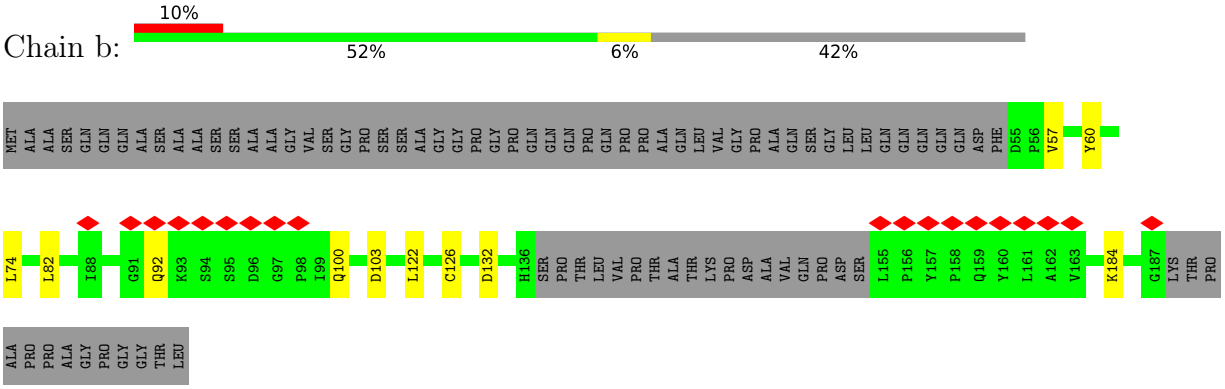
• Molecule 44: Mediator of RNA polymerase II transcription subunit 27



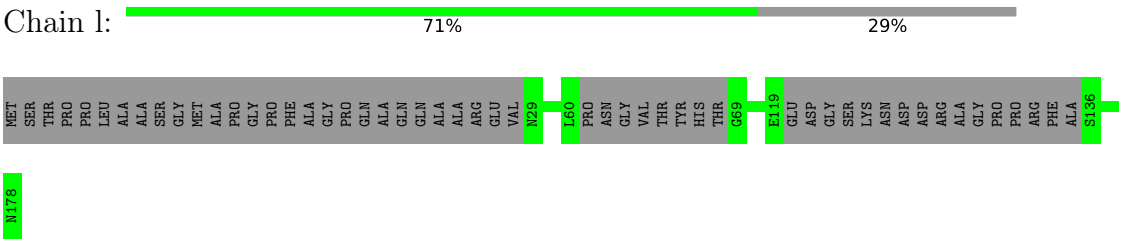
• Molecule 45: Mediator of RNA polymerase II transcription subunit 28



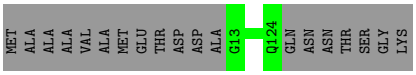
• Molecule 46: Mediator of RNA polymerase II transcription subunit 29



• Molecule 47: Mediator of RNA polymerase II transcription subunit 30

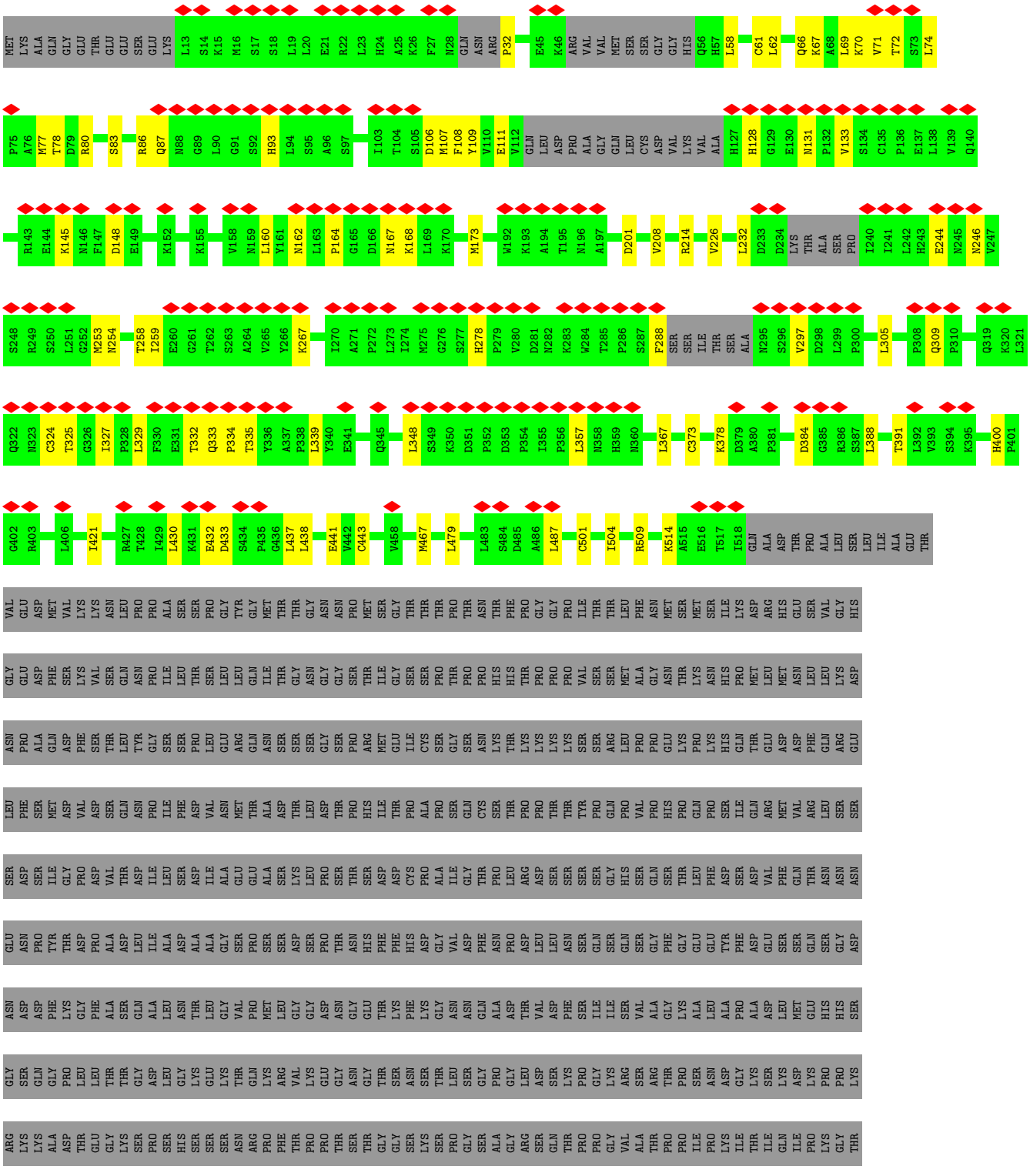


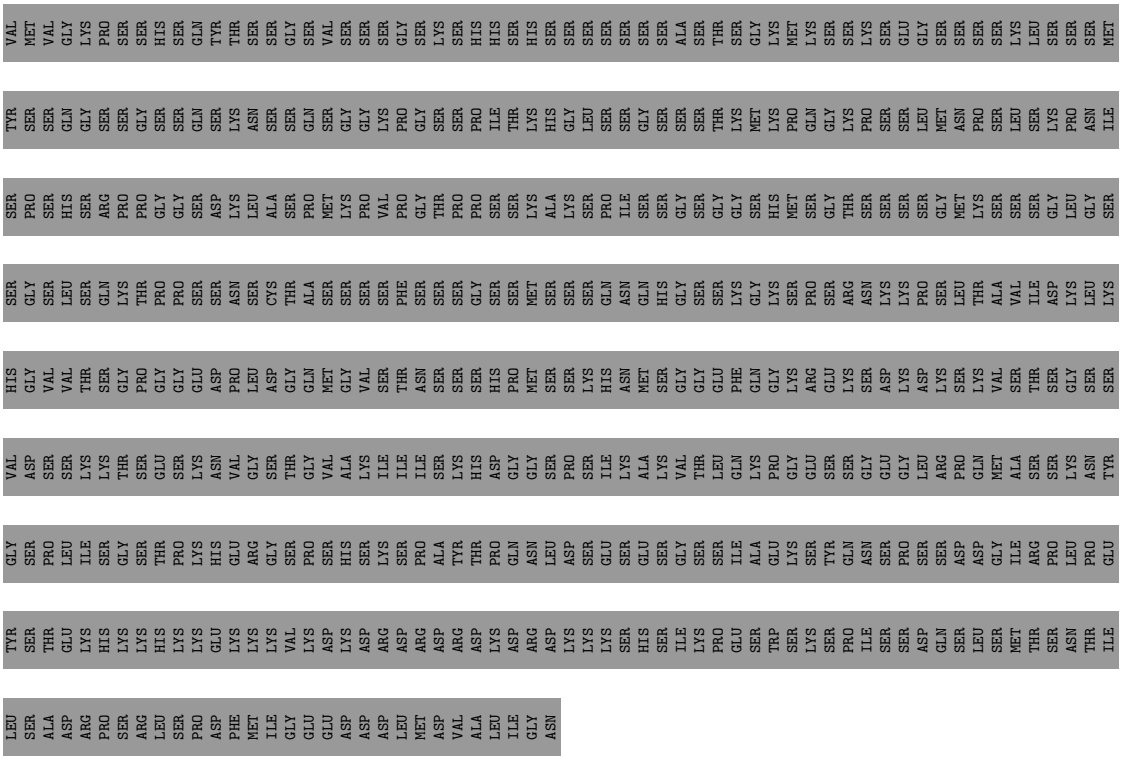
• Molecule 48: Mediator of RNA polymerase II transcription subunit 31



• Molecule 49: Mediator of RNA polymerase II transcription subunit 1

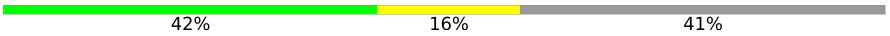
Chain a:

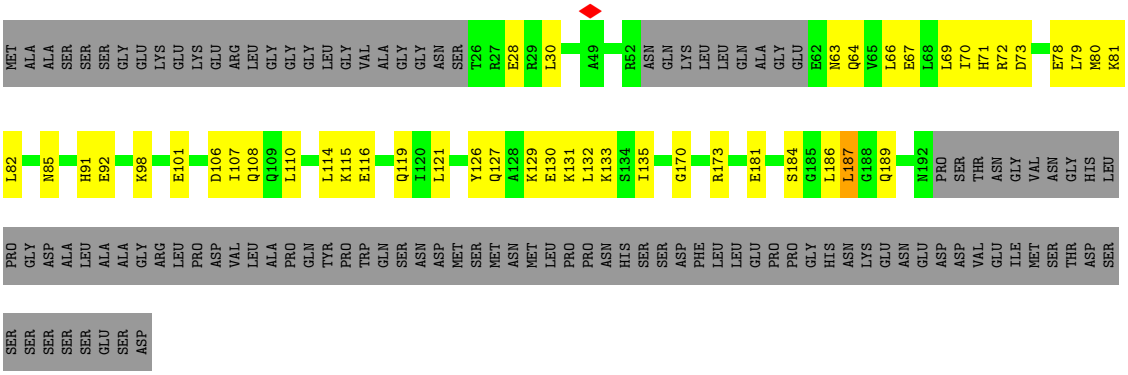




• Molecule 50: Mediator of RNA polymerase II transcription subunit 4

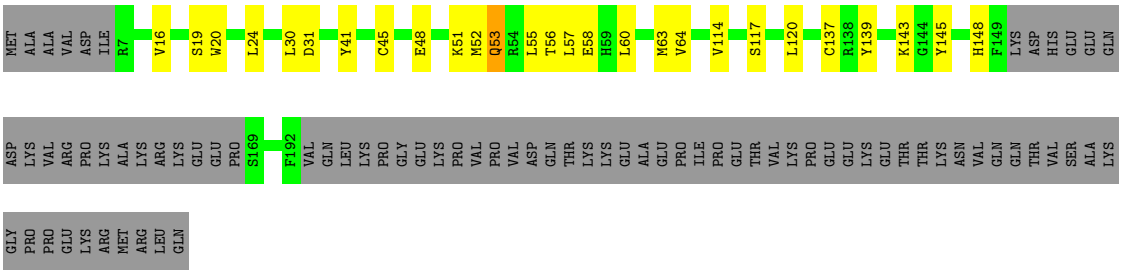
Chain d:





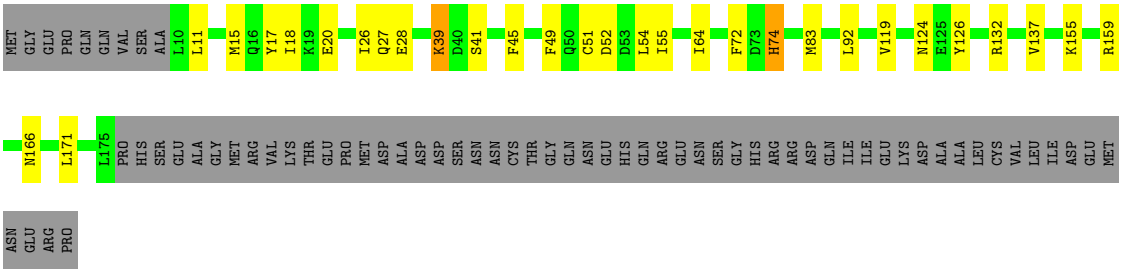
• Molecule 51: Mediator of RNA polymerase II transcription subunit 6

Chain f:



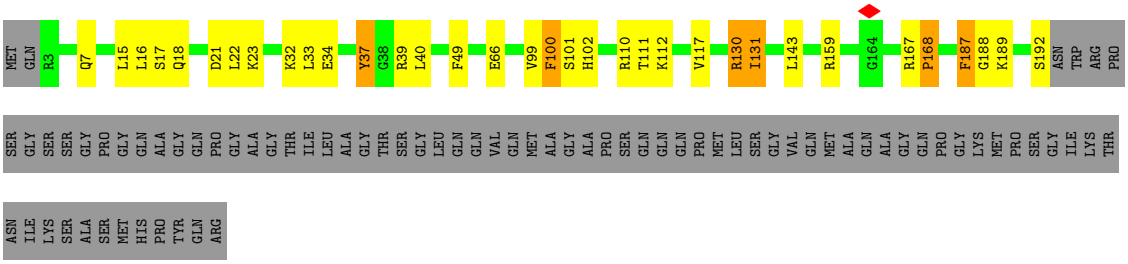
• Molecule 52: Mediator of RNA polymerase II transcription subunit 7

Chain g:



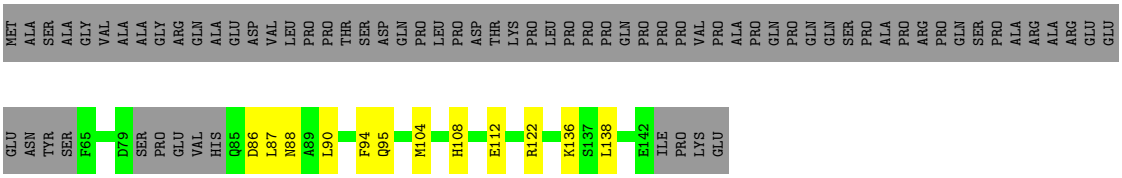
• Molecule 53: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

Chain h:



• Molecule 54: Mediator of RNA polymerase II transcription subunit 9

Chain i:

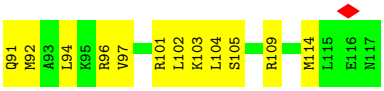


• Molecule 55: Mediator of RNA polymerase II transcription subunit 10

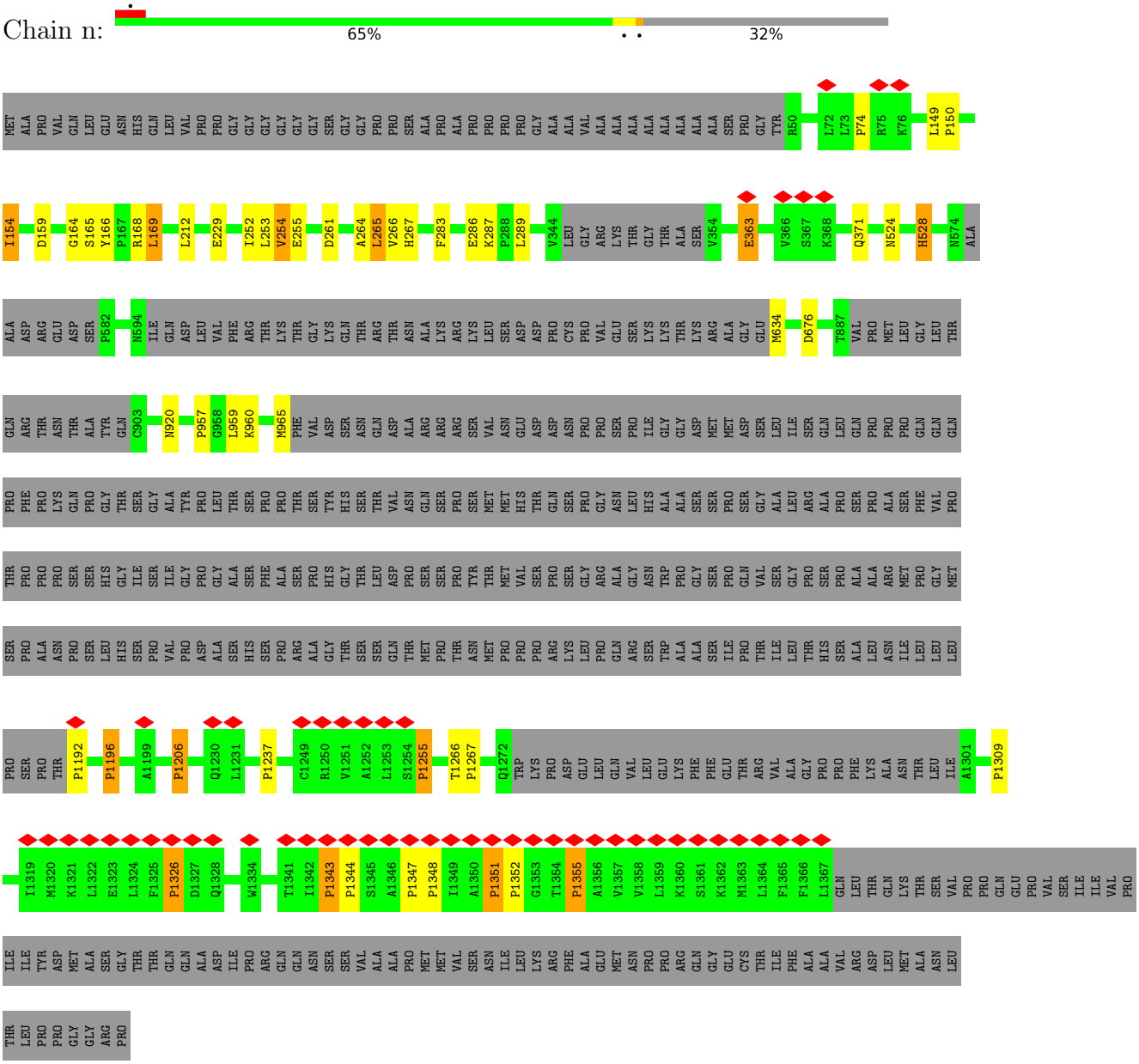
Chain j:

• Molecule 56: Mediator of RNA polymerase II transcription subunit 11

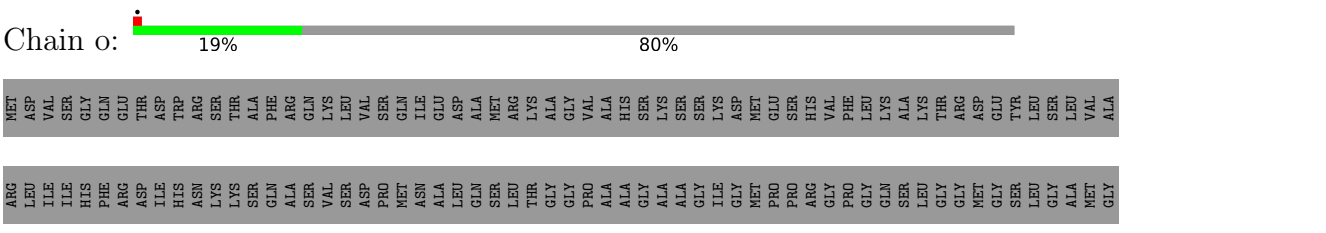
Chain k:

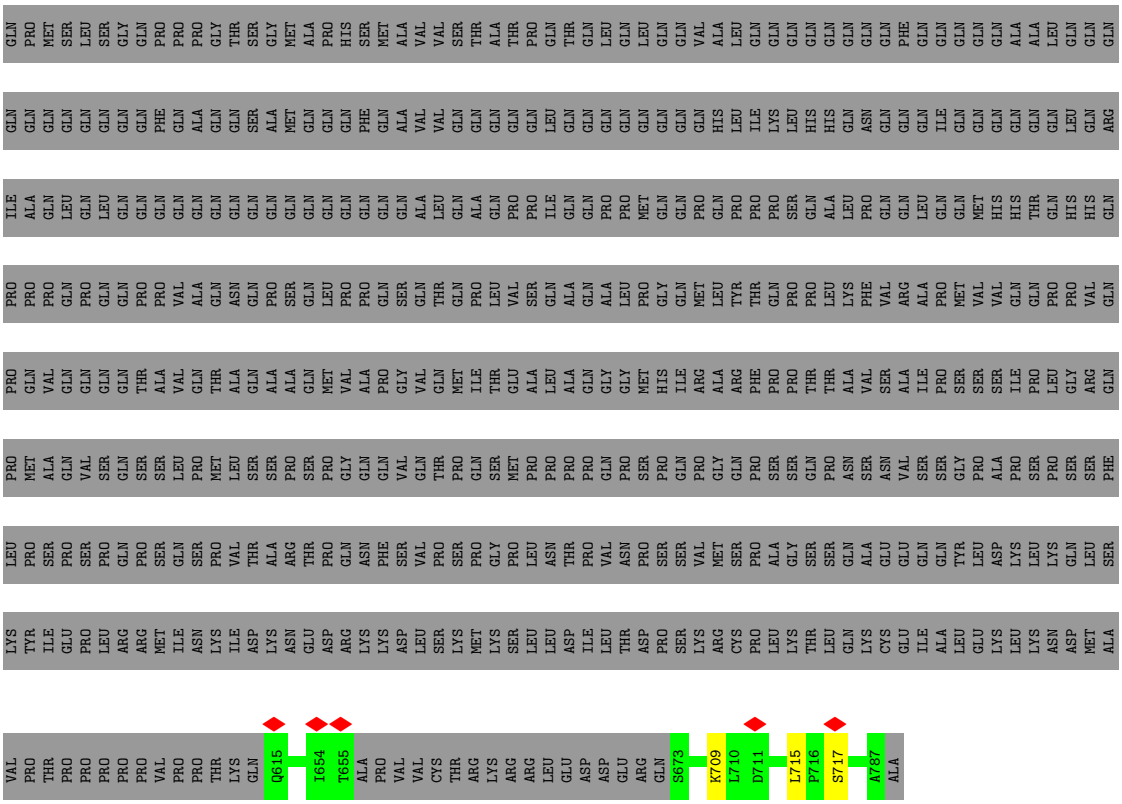


• Molecule 57: Mediator of RNA polymerase II transcription subunit 14



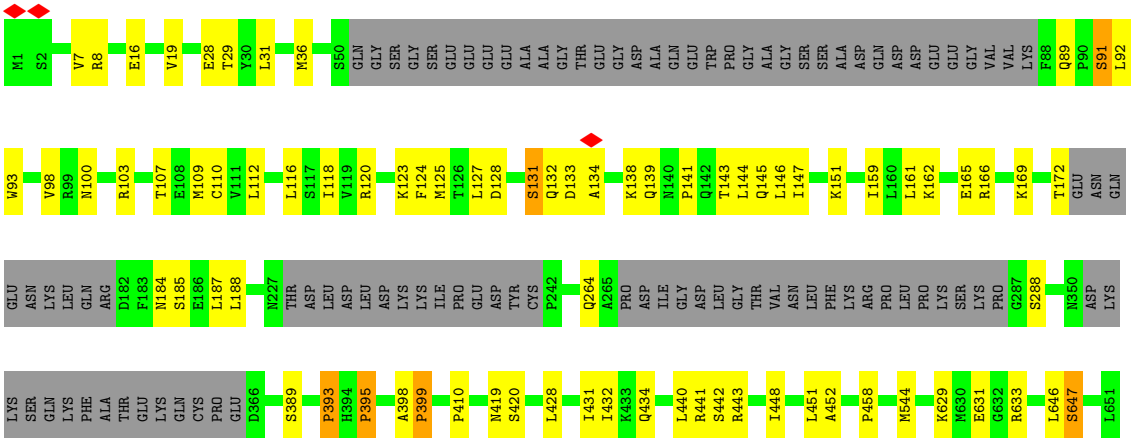
• Molecule 58: Mediator of RNA polymerase II transcription subunit 15





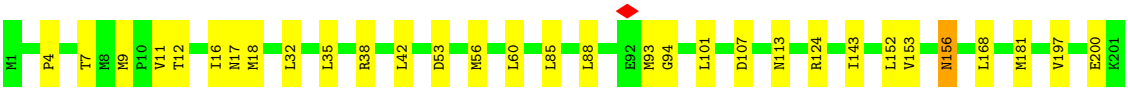
• Molecule 59: Mediator of RNA polymerase II transcription subunit 17

Chain q:



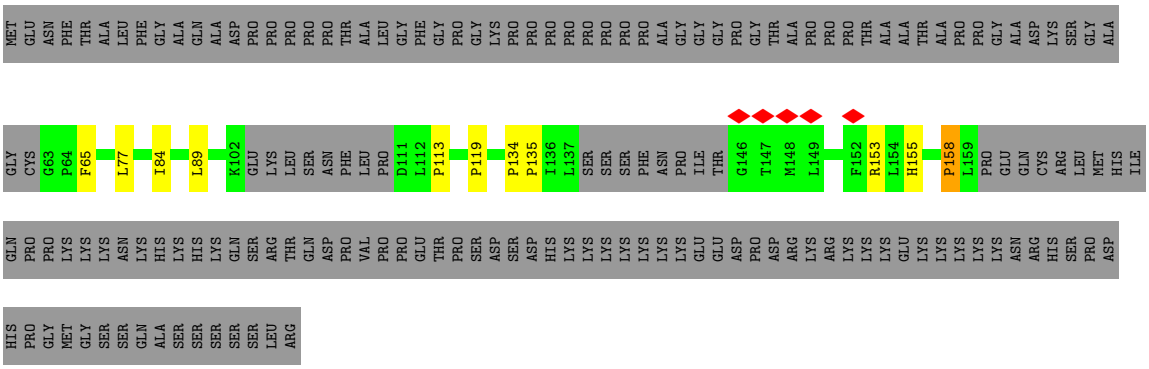
• Molecule 60: Mediator of RNA polymerase II transcription subunit 18

Chain r:



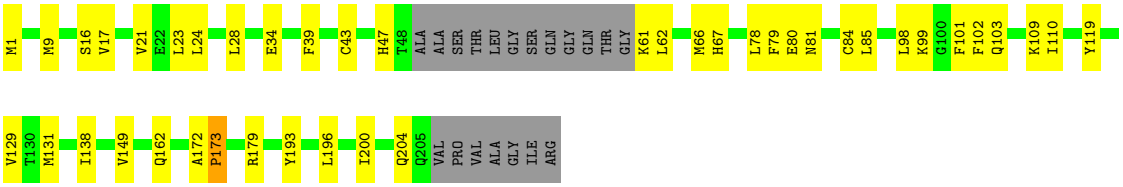
• Molecule 61: Mediator of RNA polymerase II transcription subunit 19

Chain s:



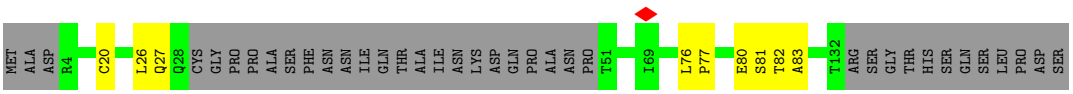
• Molecule 62: Mediator of RNA polymerase II transcription subunit 20

Chain t:



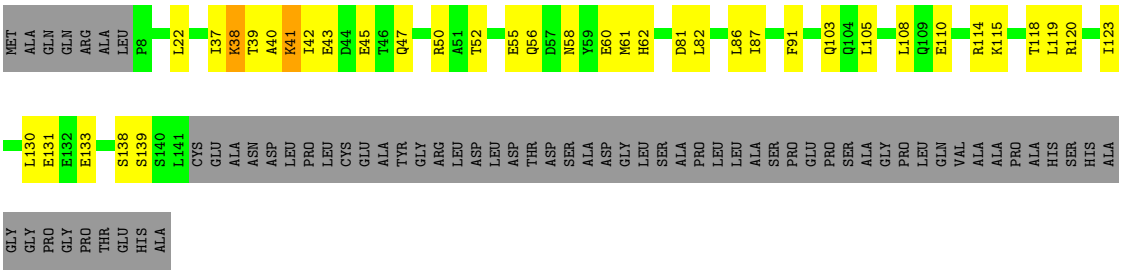
• Molecule 63: Mediator of RNA polymerase II transcription subunit 21

Chain u:



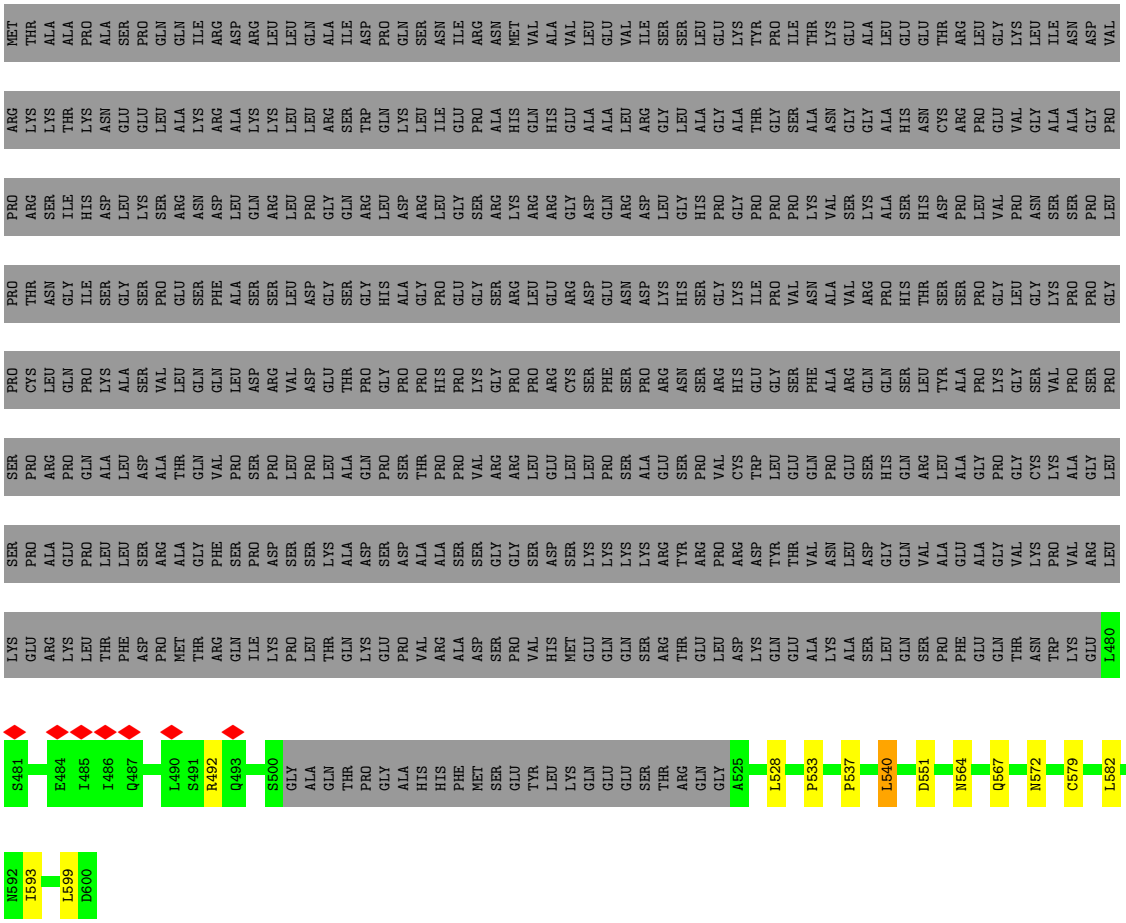
• Molecule 64: Mediator of RNA polymerase II transcription subunit 22

Chain v:



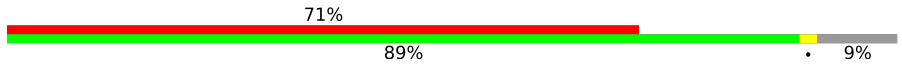
• Molecule 65: Mediator of RNA polymerase II transcription subunit 26

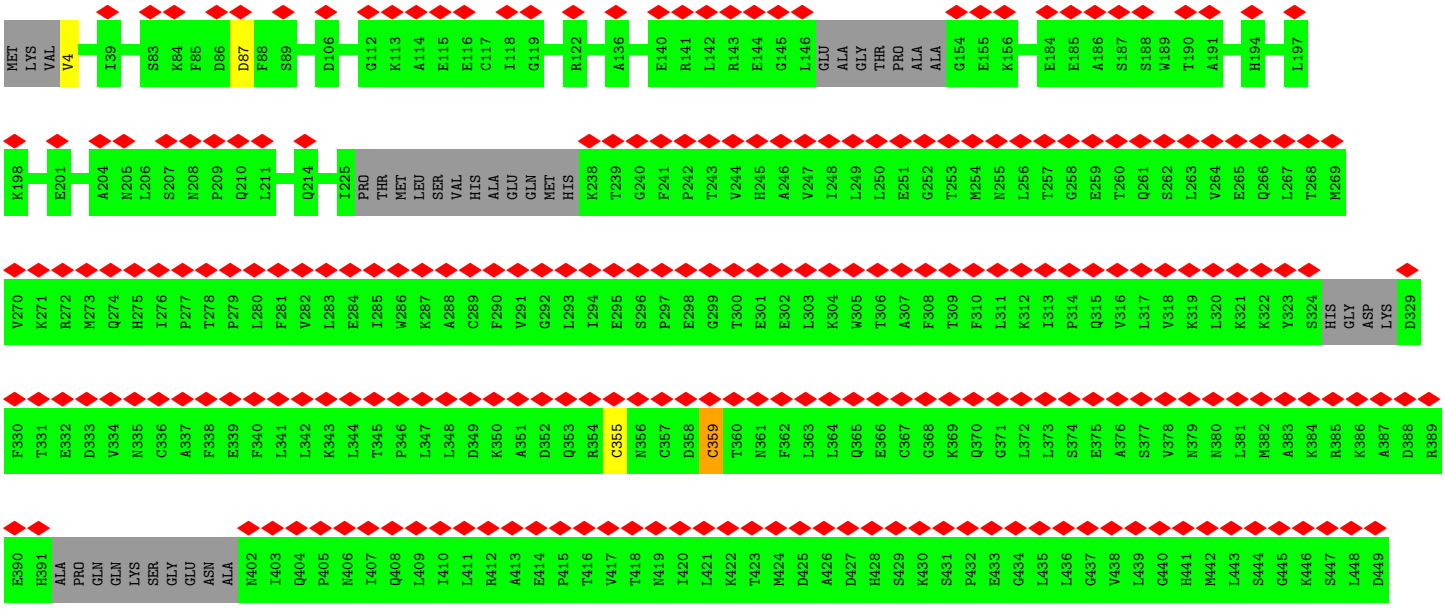
Chain z:

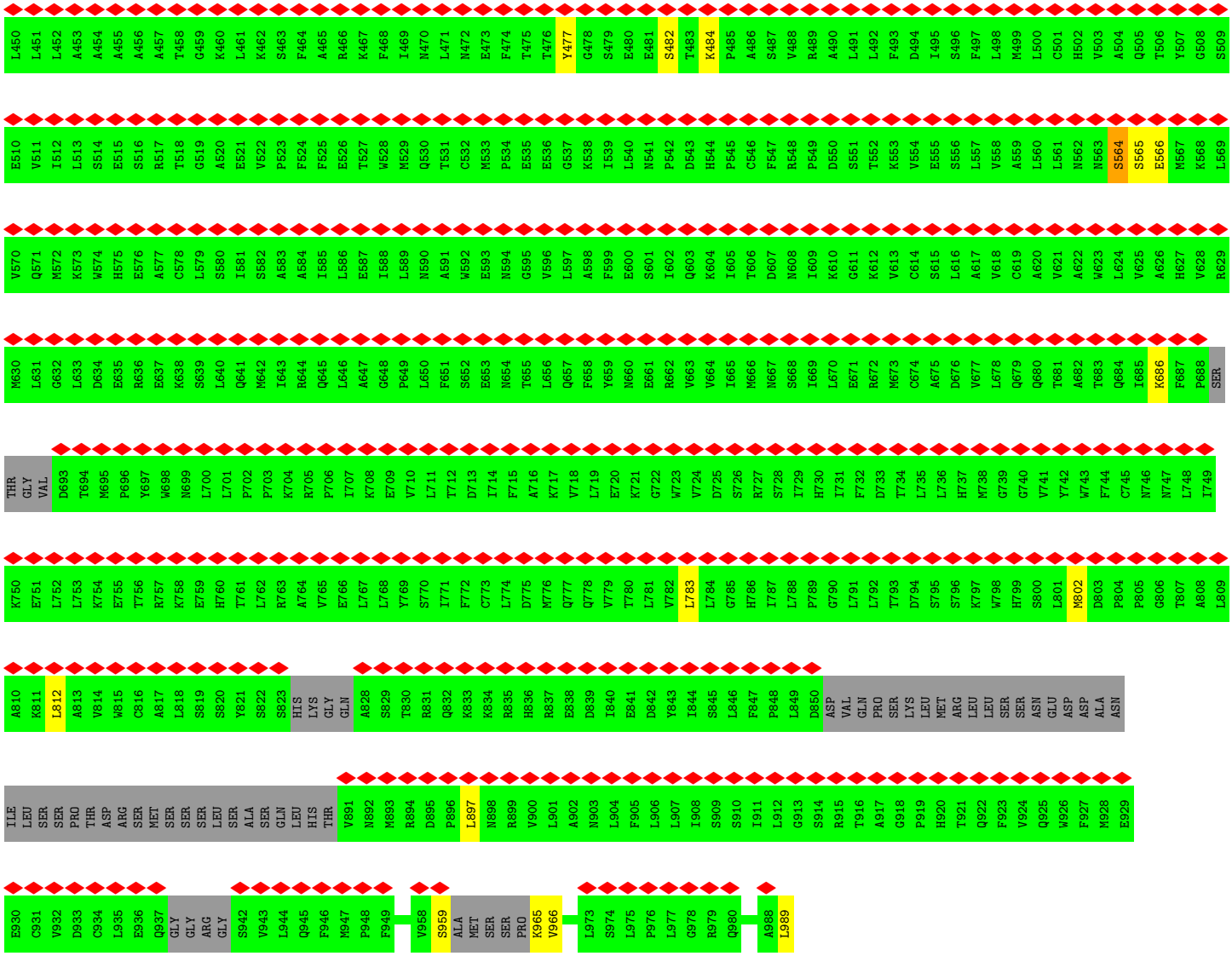


• Molecule 66: Mediator of RNA polymerase II transcription subunit 24

Chain x:

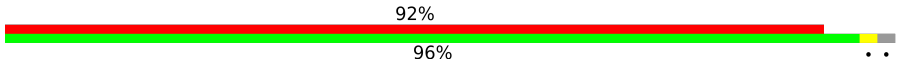


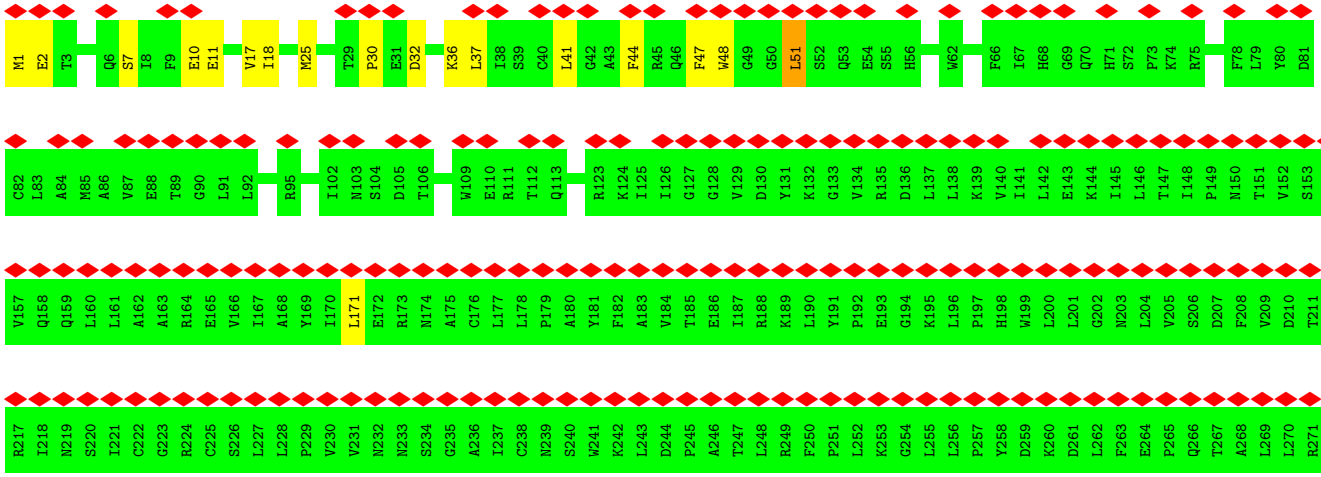


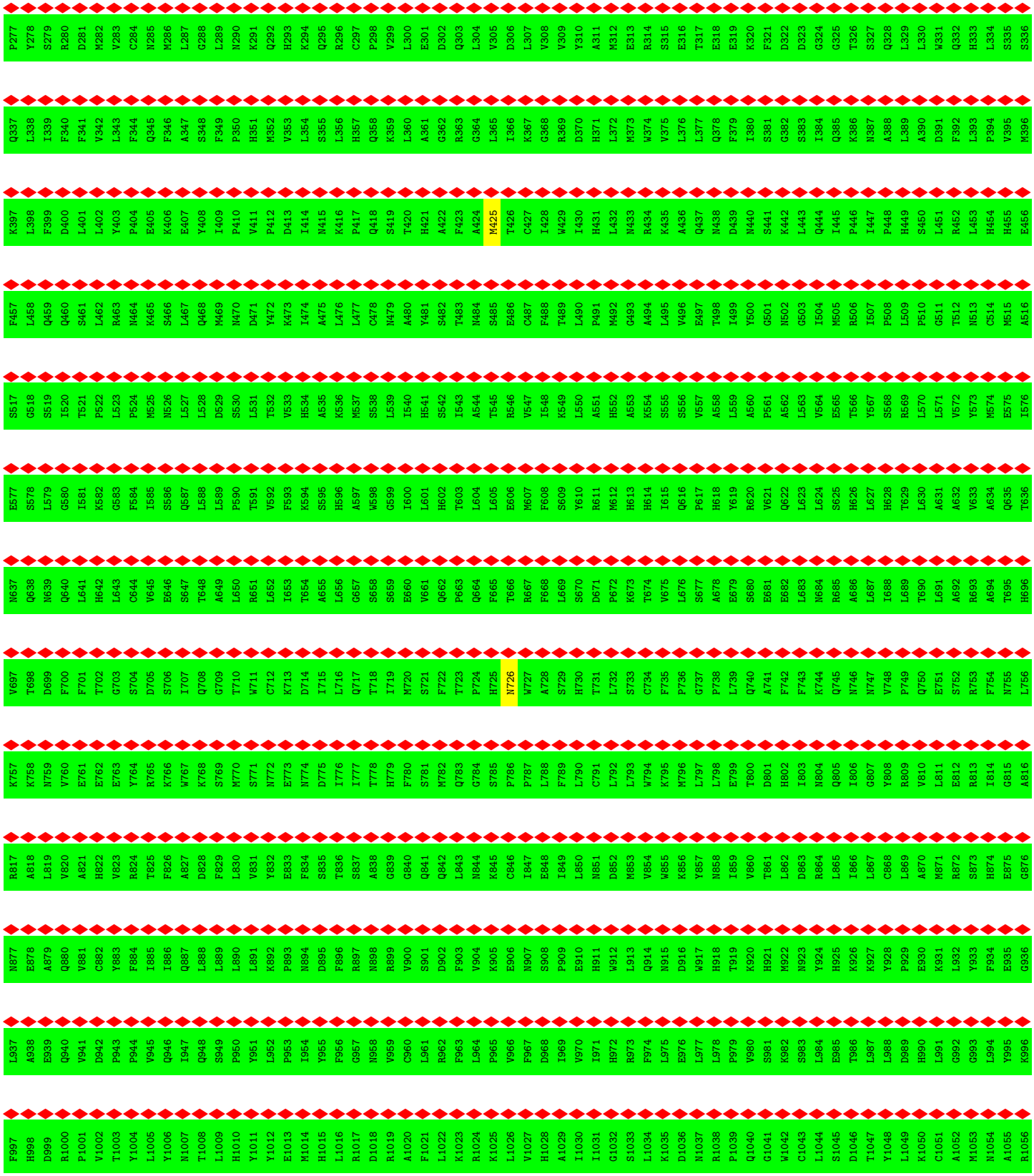


• Molecule 67: Mediator of RNA polymerase II transcription subunit 23

Chain w:



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Q337 L338 I339 F340 F341 V342 L343 F344 Q345 F346 A347 S348 F349 P350 H351 M352 V353 L354 S355 L356 H357 Q358 K359 L360 A361 G362 R363 G364 L365 I366 K367 G368 R369 D370 H371 L372 M373 W374 V375 L376 L377 Q378 F379 I380 S381 G382 S383 I384 Q385 K386 N387 A388 L389 A390 D391 F392 L393 P394 V395 M396
K397 L398 F399 D400 L401 L402 Y403 P404 E405 K406 E407 Y408 I409 P410 V411 P412 D413 I414 N415 K416 P417 Q418 S419 T420 H421 A422 F423 A424 M425 T426 C427 I428 W429 I430 H431 L432 N433 R434 K435 A436 Q437 N438 D439 N440 S441 K442 L443 Q444 I445 P446 I447 P448 H449 S450 L451 R452 L453 H454 H455 E456
F457 L458 Q459 Q460 S461 L462 R463 N464 K465 S466 L467 Q468 M469 N470 D471 Y472 K473 I474 A475 L476 L477 C478 N479 A480 Y481 S482 T483 N484 S485 E486 C487 F488 T489 L490 P491 M492 G493 A494 L495 V496 E497 T498 I499 Y500 G501 N502 G503 I504 M505 R506 I507 P508 S509 L510 G511 T512 N513 C514 M515 A516
S517 G518 S519 I520 T521 P522 L523 P524 M525 N526 L527 L528 D529 S530 L531 T532 V533 H534 A535 K536 M537 S538 L539 I540 H541 S542 I543 A544 T545 R546 V547 I548 K549 L550 A551 H552 A553 K554 S555 S556 V557 A558 L559 A560 P561 A562 L563 V564 E565 T566 Y567 S568 R569 L570 L571 V572 Y573 M574 E575 I576
E577 S578 L579 G580 I581 K582 G583 F584 I585 S586 Q587 L588 L589 P590 T591 V592 F593 K594 S595 H596 A597 W598 G599 I600 L601 H602 T603 L604 L605 E606 M607 F608 S609 Y610 R611 M612 H613 H614 I615 Q616 P617 H618 Y619 R620 V621 Q622 L623 L624 S625 H626 L627 H628 T629 L630 A631 A632 V633 A634 Q635 T636
N637 Q638 N639 Q640 L641 H642 L643 C644 V645 E646 S647 T648 A649 L650 R651 L652 I653 T654 A655 L656 G657 S658 S659 E660 V661 Q662 P663 Q664 F665 T666 R667 F668 L669 S670 D671 P672 K673 T674 V675 L676 S677 A678 E679 S680 E681 E682 L683 N684 R685 A686 L687 I688 L689 T690 L691 A692 R693 A694 T695 H696
V697 T698 D699 F700 F701 T702 G703 S704 D705 S706 I707 Q708 G709 T710 W711 C712 K713 D714 I715 L716 Q717 T718 I719 M720 S721 F722 T723 P724 H725 N726 W727 A728 S729 H730 T731 L732 S733 C734 F735 P736 G737 P738 L739 Q740 A741 F742 F743 K744 Q745 N746 N747 V748 P749 Q750 E751 S752 R753 F754 N755 L756
K757 K758 N759 V760 E761 E762 E763 Y764 R765 K766 W767 K768 S769 M770 S771 N772 E773 N774 D775 I776 I777 T778 H779 F780 S781 M782 Q783 G784 S785 P786 P787 L788 F789 L790 C791 L792 L793 W794 K795 M796 L797 L798 E799 T800 D801 H802 I803 N804 Q805 I806 G807 Y808 R809 V810 L811 E812 R813 I814 G815 A816
R817 A818 L819 V820 A821 H822 V823 R824 T825 F826 A827 D828 F829 L830 V831 Y832 E833 F834 S835 T836 S837 A838 G839 G840 Q841 Q842 L843 N844 K845 C846 I847 E848 I849 L850 N851 D852 M853 V854 W855 K856 Y857 N858 I859 V860 T861 L862 D863 R864 L865 I866 L867 C868 L869 A870 M871 R872 S873 H874 E875 G876
N877 E878 A879 Q880 V881 C882 Y883 F884 I885 I886 Q887 L888 L889 L890 L891 K892 P893 N894 D895 F896 R897 N898 R899 V900 S901 D902 F903 V904 K905 E906 N907 S908 P909 E910 H911 W912 L913 Q914 N915 D916 W917 H918 T919 K920 H921 M922 N923 Y924 H925 K926 K927 Y928 P929 E930 K931 L932 Y933 F934 E935 G936
L937 A938 E939 Q940 V941 D942 P943 P944 V945 Q946 I947 Q948 S949 P950 Y951 L952 P953 I954 Y955 F956 G957 N958 V959 C960 L961 R962 F963 L964 P965 V966 F967 D968 I969 V970 I971 H972 R973 F974 L975 E976 L977 L978 P979 V980 S981 K982 S983 L984 E985 T986 L987 I988 D989 H990 L991 G992 G993 L994 Y995 K996
F997 H998 D999 R1000 P1001 V1002 T1003 Y1004 L1005 Y1006 N1007 T1008 L1009 H1010 Y1011 Y1012 E1013 M1014 H1015 L1016 R1017 D1018 R1019 A1020 F1021 L1022 K1023 R1024 K1025 L1026 V1027 H1028 A1029 I1030 I1031 G1032 S1033 L1034 K1035 D1036 N1037 R1038 P1039 Q1040 G1041 W1042 C1043 L1044 S1045 D1046 T1047 Y1048 L1049 K1050 C1051 A1052 M1053 N1054 A1055 R1056

E1057 E1058 N1059 P1060 W1061 V1062 P1063 D1064 D1065 T1066 Y1067 Y1068 C1069 R1070 L1071 I1072 G1073 R1074 L1075 V1076 D1077 T1078 M1079 A1080 G1081 K1082 S1083 P1084 G1085 P1086 F1087 P1088 N1089 C1090 D1091 W1092 R1093 F1094 N1095 E1096 F1097 P1098 N1099 P1100 A1101 A1102 H1103 A1104 L1105 H1106 V1107 T1108 C1109 V1110 E1111 L1112 M1113 A1114 L1115 A1116

V1117 S1118 G1119 K1120 E1121 V1122 G1123 N1124 A1125 L1126 L1127 N1128 V1129 V1130 L1131 K1132 S1133 Q1134 P1135 L1136 V1137 P1138 R1139 E1140 N1141 I1142 T1143 A1144 W1145 M1146 N1147 A1148 I1149 G1150 L1151 I1152 I1153 T1154 A1155 L1156 P1157 E1158 P1159 Y1160 W1161 I1162 V1163 L1164 H1165 D1166 R1167 I1168 V1169 S1170 V1171 I1172 S1173 S1174 P1175 S1176

L1177 T1178 S1179 E1180 T1181 E1182 W1183 V1184 G1185 Y1186 P1187 F1188 R1189 L1190 F1191 D1192 F1193 T1194 A1195 C1196 H1197 Q1198 S1199 Y1200 S1201 E1202 M1203 S1204 C1205 S1206 Y1207 T1208 L1209 A1210 L1211 A1212 H1213 A1214 V1215 W1216 H1217 H1218 S1219 S1220 I1221 G1222 Q1223 L1224 S1225 L1226 I1227 P1228 K1229 F1230 L1231 T1232 E1233 V1234 L1235 L1236

P1237 I1238 V1239 K1240 T1241 E1242 F1243 Q1244 L1245 L1246 Y1247 V1248 Y1249 H1250 L1251 V1252 G1253 P1254 F1255 L1256 Q1257 R1258 F1259 Q1260 Q1261 E1262 R1263 T1264 R1265 C1266 M1267 I1268 E1269 I1270 G1271 V1272 A1273 F1274 Y1275 D1276 M1277 L1278 L1279 N1280 V1281 D1282 Q1283 C1284 S1285 T1286 H1287 L1288 N1289 Y1290 M1291 D1292 P1293 I1294 C1295 D1296

F1297 L1298 Y1299 H1300 M1301 K1302 Y1303 M1304 F1305 T1306 G1307 D1308 S1309 V1310 K1311 E1312 Q1313 V1314 E1315 K1316 I1317 I1318 C1319 N1320 L1321 K1322 P1323 A1324 L1325 K1326 L1327 R1328 L1329 R1330 F1331 I1332 T1333 H1334 ILE SER LYS MET GLU PRO ALA ALA VAL PRO PRO GLN ALA MET ASN SER GLY SER PRO ALA PRO GLN

SER ASN GLN VAL PRO VAL SER LEU PRO VAL THR GLN

- Molecule 68: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p:

MET CYS ASP LEU ARG ARG PRO ALA ALA GLY GLY MET M13 D14 L15 A16 Y17 V18 C19 E20 W21 E22 K23 W24 S25 K26 S27 T28 H29 C30 P31 S32 V33 P34 L35 A36 C37 A38 W39 S40 C41 R42 N43 L44 I45 A46 F47 T48 M49 D50 L51 R52 S53 D54 D55 Q56 D57 L58 T59 R60

M61 I62 H63 I64 L65 D66 T67 E68 H69 P70 W71 D72 L73 H74 S75 I76 P77 S78 E79 H80 H81 E82 A83 I84 T85 C86 L87 E88 W89 D90 Q91 S92 G93 S94 R95 L96 L97 S98 A99 D100 A101 D102 G103 Q104 I105 K106 C107 W108 S109 M110 A111 D112 H113 L114 A115 N116 S117 W118 E119 S120

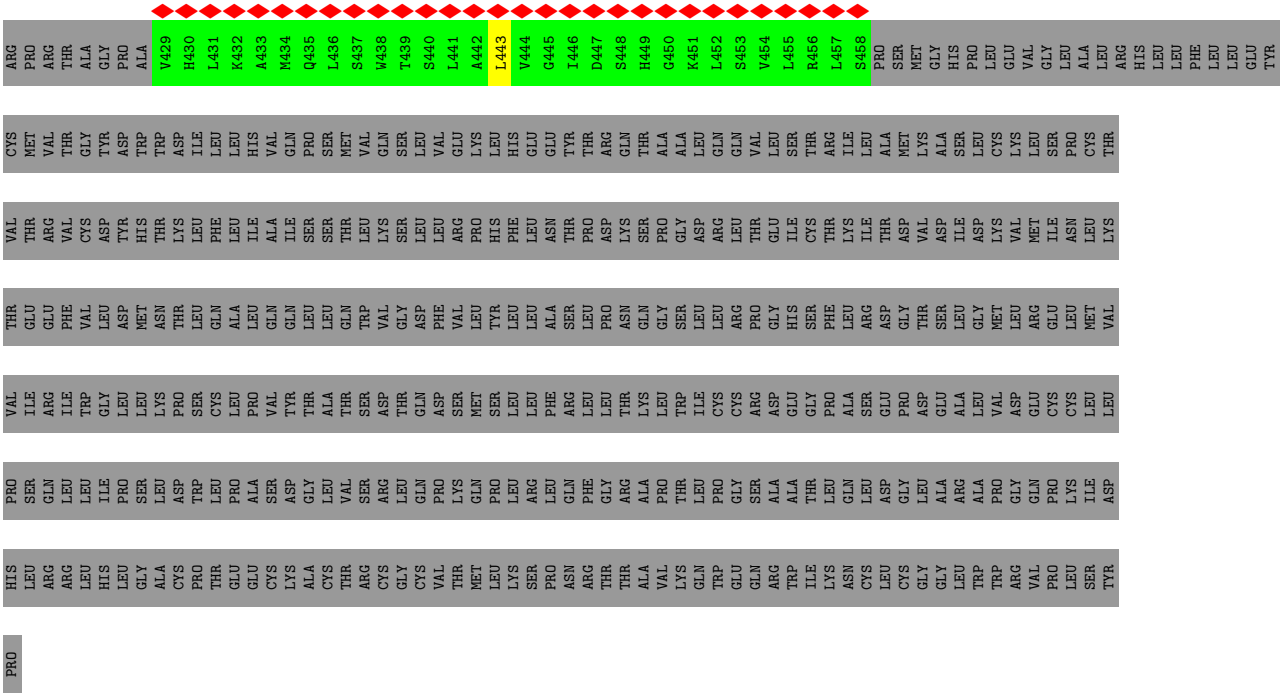
S121 V122 G123 S124 L125 V126 E127 G128 D129 P130 I131 V132 A133 L134 S135 W136 L137 H138 N139 G140 V141 K142 L143 A144 L145 H146 V147 E148 K149 S150 G151 A152 S153 S154 F155 G156 E157 K158 F159 S160 R161 V162 K163 F164 S165 P166 S167 L168 T169 L170 F171 G172 G173 K174 P175 M176 E177 G178 W179 I180

A181 V182 T183 V184 S185 G186 L187 V188 T189 V190 S191 L192 L193 K194 P195 S196 G197 Q198 V199 L200 T201 S202 T203 E204 S205 L206 C207 R208 L209 R210 G211 R212 V213 A214 L215 A216 D217 I218 A219 P220 T221 G222 G223 G224 N225 I226 V227 V228 A229 T230 A231 D232 G233 S234 S235 A236 S237 P238 V239 Q240

F241 Y242 K243 V244 C245 V246 S247 V248 V249 S250 E251 K252 C253 R254 I255 D256 T257 E258 I259 L260 P261 S262 L263 F264 M265 R266 C267 T268 T269 D270 L271 N272 R273 K274 D275 K276 F277 P278 A279 I280 T281 H282 L283 K284 F285 L286 A287 R288 D289 M290 S291 E292 Q293 V294 L295 L296 C297 A298 S299 S300

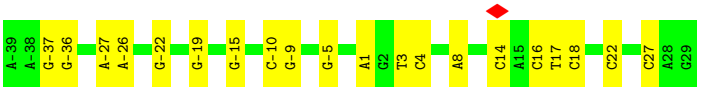
Q301 T302 S303 S304 I305 V306 E307 C308 W309 S310 L311 R312 K313 E314 GLY LEU PRO VAL ASN ASN ILE PHE GLN GLN ILE SER PRO VAL VAL GLY ASP LYS GLN PRO T335 I336 L337 K338 W339 R340 I341 L342 S343 A344 T345 N346 D347 L348 D349 R350 V351 S352 A353 V354 A355 L356 P357 K358 L359 P360

I361 S362 L363 T364 N365 T366 D367 L368 K369 V370 A371 S372 D373 T374 Q375 F376 Y377 P378 G379 L380 G381 L382 A383 L384 A385 F386 H387 D388 G389 S390 V391 H392 I393 V394 H395 R396 L397 S398 L399 Q400 T401 M402 A403 V404 F405 Y406 S407 S408 ALA ALA PRO ARG PRO VAL ASP GLU PRO ALA MET LYS



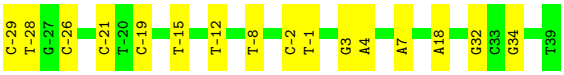
- Molecule 69: DNA (69-MER)

Chain X:



- Molecule 70: DNA(69-MER)

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.884	Depositor
Minimum map value	-4.573	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	674.56, 674.56, 674.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3175, 1.3175, 1.3175	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0	0.61	0/2288	0.81	4/3101 (0.1%)
2	8	0.66	0/2437	0.97	0/3306
3	9	0.73	0/2356	0.97	1/3185 (0.0%)
4	DO	0.56	0/781	0.75	0/1061
5	DP	0.62	0/1438	0.73	0/1935
6	DQ	0.54	0/1013	0.64	0/1366
7	BA	0.46	0/1987	0.75	2/2684 (0.1%)
8	FA	0.47	0/1130	0.57	0/1528
9	FB	0.55	0/1817	0.66	0/2445
10	PA	0.73	6/11888 (0.1%)	1.00	13/16066 (0.1%)
11	PB	0.77	1/9243 (0.0%)	1.01	15/12475 (0.1%)
12	PC	0.86	0/2102	1.19	7/2857 (0.2%)
13	PD	0.63	0/1036	0.97	0/1397
14	PE	0.58	0/1751	0.90	0/2366
15	PF	0.83	1/645 (0.2%)	1.07	1/871 (0.1%)
16	PG	0.65	0/1365	1.06	4/1853 (0.2%)
17	PH	0.67	0/1207	1.05	1/1628 (0.1%)
18	PI	0.62	0/948	1.06	1/1284 (0.1%)
19	PJ	0.86	0/516	1.19	0/696
20	PK	0.81	0/956	1.07	3/1294 (0.2%)
21	PL	0.70	0/377	0.95	0/500
22	DA	0.50	0/5037	0.65	2/6794 (0.0%)
23	DB	0.47	0/7993	0.61	0/10836
24	DD	0.58	0/1343	0.70	0/1795
24	Dd	0.29	0/1321	0.49	0/1772
25	DE	0.43	0/4469	0.58	0/6050
25	De	0.34	0/4433	0.55	0/6004
26	DF	0.55	0/3167	0.71	0/4303
26	Df	0.44	0/3140	0.64	0/4268
27	DG	0.53	0/1199	0.63	0/1612
28	DH	0.46	0/1673	0.60	0/2285
29	DI	0.46	0/981	0.57	0/1332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	Di	0.31	0/989	0.46	0/1343
30	DJ	0.48	0/736	0.60	1/998 (0.1%)
30	Dj	0.31	0/775	0.52	0/1049
31	DL	0.43	0/622	0.69	3/841 (0.4%)
31	Dl	0.30	0/888	0.56	3/1194 (0.3%)
32	Dc	0.40	0/1035	0.54	0/1406
33	Dk	0.31	0/799	0.48	0/1070
34	Dm	0.32	0/733	0.52	0/977
35	EA	0.61	0/1499	0.74	0/2012
36	EB	0.64	0/1428	0.64	0/1917
37	1	0.36	0/3502	0.65	0/4731
38	2	0.42	0/3094	0.67	0/4188
39	3	0.44	0/2353	0.74	0/3187
40	4	0.49	0/3729	0.73	0/5053
41	5	0.50	0/528	0.70	0/713
42	6	0.42	0/5365	0.68	0/7247
43	7	0.46	0/5984	0.69	0/8104
44	c	0.46	0/2146	0.62	0/2899
45	e	0.26	0/840	0.36	0/1128
46	b	0.51	0/911	0.62	0/1229
47	l	0.26	0/1048	0.41	0/1405
48	m	0.26	0/1010	0.37	0/1359
49	a	0.62	0/3660	0.75	1/4971 (0.0%)
50	d	0.62	0/1281	0.65	0/1718
51	f	0.57	0/1359	0.69	1/1845 (0.1%)
52	g	0.58	0/1411	0.81	0/1901
53	h	0.62	0/1485	0.72	1/2008 (0.0%)
54	i	0.67	0/612	0.71	0/815
55	j	0.41	0/1016	0.64	5/1363 (0.4%)
56	k	0.66	0/885	0.60	0/1190
57	n	0.34	0/7371	0.55	17/10037 (0.2%)
58	o	0.36	0/1256	0.62	0/1724
59	q	0.48	2/4351 (0.0%)	0.55	4/5886 (0.1%)
60	r	0.60	0/1663	0.79	1/2241 (0.0%)
61	s	0.59	0/510	0.77	5/694 (0.7%)
62	t	0.71	1/1530 (0.1%)	0.89	0/2066
63	u	0.38	0/797	0.52	0/1082
64	v	0.66	0/1092	0.73	0/1468
65	z	0.64	0/781	0.81	0/1067
66	x	0.59	0/7179	0.63	3/9712 (0.0%)
67	w	0.57	0/11053	0.62	2/15018 (0.0%)
68	p	0.71	0/3191	0.73	4/4333 (0.1%)
69	X	1.00	16/1607 (1.0%)	1.16	8/2481 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
70	Y	1.00	15/1565 (1.0%)	1.10	2/2410 (0.1%)
All	All	0.57	42/177706 (0.0%)	0.75	115/241029 (0.0%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	q	264	GLN	C-N	7.96	1.52	1.34
69	X	-26	DA	C1'-N9	-7.92	1.36	1.47
69	X	-27	DA	C1'-N9	-7.66	1.36	1.47
69	X	-19	DG	C1'-N9	-7.58	1.36	1.47
69	X	-36	DG	C1'-N9	-7.06	1.37	1.47

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	X	3	DT	P-O3'-C3'	-13.62	103.35	119.70
69	X	-10	DC	O5'-P-OP2	-9.57	97.08	105.70
70	Y	-2	DC	P-O3'-C3'	8.34	129.71	119.70
57	n	1355	PRO	N-CA-CB	6.88	111.55	103.30
67	w	47	PHE	CB-CA-C	6.87	124.14	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	304/309 (98%)	242 (80%)	51 (17%)	11 (4%)	3 24
2	8	297/346 (86%)	266 (90%)	20 (7%)	11 (4%)	2 23
3	9	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	12 46
4	DO	95/109 (87%)	83 (87%)	11 (12%)	1 (1%)	12 46
5	DP	175/339 (52%)	166 (95%)	7 (4%)	2 (1%)	12 46
6	DQ	118/307 (38%)	105 (89%)	8 (7%)	5 (4%)	2 21
7	BA	251/316 (79%)	237 (94%)	10 (4%)	4 (2%)	8 39
8	FA	130/517 (25%)	117 (90%)	12 (9%)	1 (1%)	16 53
9	FB	218/249 (88%)	200 (92%)	13 (6%)	5 (2%)	5 32
10	PA	1461/1970 (74%)	1363 (93%)	81 (6%)	17 (1%)	11 44
11	PB	1128/1174 (96%)	1029 (91%)	83 (7%)	16 (1%)	9 41
12	PC	253/275 (92%)	229 (90%)	18 (7%)	6 (2%)	5 31
13	PD	127/142 (89%)	123 (97%)	3 (2%)	1 (1%)	16 53
14	PE	207/210 (99%)	201 (97%)	5 (2%)	1 (0%)	25 62
15	PF	77/127 (61%)	72 (94%)	3 (4%)	2 (3%)	4 29
16	PG	169/172 (98%)	159 (94%)	8 (5%)	2 (1%)	11 44
17	PH	146/150 (97%)	129 (88%)	16 (11%)	1 (1%)	19 56
18	PI	112/125 (90%)	102 (91%)	8 (7%)	2 (2%)	7 36
19	PJ	62/67 (92%)	59 (95%)	2 (3%)	1 (2%)	8 39
20	PK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14 50
21	PL	42/58 (72%)	38 (90%)	3 (7%)	1 (2%)	5 31
22	DA	582/1872 (31%)	539 (93%)	33 (6%)	10 (2%)	7 37
23	DB	959/1199 (80%)	912 (95%)	47 (5%)	0	100 100
24	DD	153/1085 (14%)	144 (94%)	6 (4%)	3 (2%)	6 34
24	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
25	DE	540/800 (68%)	500 (93%)	36 (7%)	4 (1%)	19 56
25	De	531/800 (66%)	484 (91%)	47 (9%)	0	100 100
26	DF	404/677 (60%)	369 (91%)	29 (7%)	6 (2%)	8 40
26	Df	399/677 (59%)	371 (93%)	27 (7%)	1 (0%)	37 71
27	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100 100
28	DH	207/310 (67%)	183 (88%)	20 (10%)	4 (2%)	6 35
29	DI	118/264 (45%)	103 (87%)	14 (12%)	1 (1%)	16 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
30	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
30	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
31	DL	73/161 (45%)	65 (89%)	5 (7%)	3 (4%)	2	21
31	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
32	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
33	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
34	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
35	EA	175/439 (40%)	160 (91%)	12 (7%)	3 (2%)	7	37
36	EB	170/291 (58%)	160 (94%)	6 (4%)	4 (2%)	5	31
37	1	431/548 (79%)	350 (81%)	73 (17%)	8 (2%)	6	35
38	2	383/395 (97%)	311 (81%)	72 (19%)	0	100	100
39	3	293/308 (95%)	238 (81%)	51 (17%)	4 (1%)	9	41
40	4	455/462 (98%)	374 (82%)	70 (15%)	11 (2%)	5	31
41	5	64/71 (90%)	57 (89%)	6 (9%)	1 (2%)	8	39
42	6	648/782 (83%)	514 (79%)	123 (19%)	11 (2%)	7	37
43	7	730/760 (96%)	600 (82%)	112 (15%)	18 (2%)	4	30
44	c	255/311 (82%)	235 (92%)	17 (7%)	3 (1%)	11	44
45	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	34
46	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	50
47	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
48	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
49	a	457/1581 (29%)	421 (92%)	31 (7%)	5 (1%)	12	46
50	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	10	43
51	f	163/246 (66%)	145 (89%)	13 (8%)	5 (3%)	3	26
52	g	164/233 (70%)	150 (92%)	11 (7%)	3 (2%)	7	36
53	h	188/268 (70%)	163 (87%)	15 (8%)	10 (5%)	1	18
54	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	27
55	j	120/135 (89%)	107 (89%)	9 (8%)	4 (3%)	3	25
56	k	110/117 (94%)	98 (89%)	10 (9%)	2 (2%)	7	36
57	n	980/1454 (67%)	876 (89%)	83 (8%)	21 (2%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
58	o	152/788 (19%)	138 (91%)	13 (9%)	1 (1%)	19 56
59	q	543/651 (83%)	476 (88%)	53 (10%)	14 (3%)	4 29
60	r	204/208 (98%)	190 (93%)	10 (5%)	4 (2%)	6 34
61	s	75/244 (31%)	64 (85%)	7 (9%)	4 (5%)	1 18
62	t	189/212 (89%)	168 (89%)	17 (9%)	4 (2%)	5 33
63	u	103/144 (72%)	99 (96%)	0	4 (4%)	2 22
64	v	132/200 (66%)	117 (89%)	9 (7%)	6 (4%)	2 20
65	z	93/600 (16%)	84 (90%)	6 (6%)	3 (3%)	3 26
66	x	876/989 (89%)	824 (94%)	50 (6%)	2 (0%)	44 76
67	w	1332/1368 (97%)	1266 (95%)	62 (5%)	4 (0%)	37 71
68	p	400/841 (48%)	366 (92%)	33 (8%)	1 (0%)	37 71
All	All	21285/34555 (62%)	19303 (91%)	1689 (8%)	293 (1%)	12 41

5 of 293 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	214	LYS
1	0	220	PRO
1	0	237	PRO
10	PA	539	GLN
10	PA	980	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	209/283 (74%)	172 (82%)	37 (18%)	1 10
2	8	259/299 (87%)	190 (73%)	69 (27%)	0 3
3	9	252/296 (85%)	177 (70%)	75 (30%)	0 2
4	DO	84/98 (86%)	70 (83%)	14 (17%)	2 11
5	DP	153/293 (52%)	145 (95%)	8 (5%)	19 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	DQ	111/269 (41%)	97 (87%)	14 (13%)	3 18
7	BA	214/268 (80%)	199 (93%)	15 (7%)	12 35
8	FA	117/448 (26%)	110 (94%)	7 (6%)	16 39
9	FB	196/218 (90%)	163 (83%)	33 (17%)	1 11
10	PA	1305/1748 (75%)	1060 (81%)	245 (19%)	1 8
11	PB	993/1027 (97%)	817 (82%)	176 (18%)	1 10
12	PC	234/252 (93%)	196 (84%)	38 (16%)	2 12
13	PD	108/126 (86%)	86 (80%)	22 (20%)	1 6
14	PE	191/192 (100%)	157 (82%)	34 (18%)	1 10
15	PF	69/111 (62%)	55 (80%)	14 (20%)	1 6
16	PG	147/153 (96%)	113 (77%)	34 (23%)	0 4
17	PH	129/131 (98%)	108 (84%)	21 (16%)	2 12
18	PI	103/112 (92%)	80 (78%)	23 (22%)	1 5
19	PJ	53/56 (95%)	43 (81%)	10 (19%)	1 8
20	PK	106/106 (100%)	88 (83%)	18 (17%)	1 11
21	PL	41/55 (74%)	29 (71%)	12 (29%)	0 2
22	DA	532/1665 (32%)	486 (91%)	46 (9%)	8 29
23	DB	876/1083 (81%)	855 (98%)	21 (2%)	44 63
24	DD	144/815 (18%)	128 (89%)	16 (11%)	5 20
24	Dd	146/815 (18%)	146 (100%)	0	100 100
25	DE	478/657 (73%)	461 (96%)	17 (4%)	30 53
25	De	475/657 (72%)	473 (100%)	2 (0%)	89 91
26	DF	324/574 (56%)	262 (81%)	62 (19%)	1 8
26	Df	322/574 (56%)	301 (94%)	21 (6%)	14 37
27	DG	133/322 (41%)	124 (93%)	9 (7%)	13 36
28	DH	181/270 (67%)	159 (88%)	22 (12%)	4 18
29	DI	106/235 (45%)	89 (84%)	17 (16%)	2 13
29	Di	107/235 (46%)	107 (100%)	0	100 100
30	DJ	79/154 (51%)	69 (87%)	10 (13%)	3 17
30	Dj	83/154 (54%)	83 (100%)	0	100 100
31	DL	70/141 (50%)	59 (84%)	11 (16%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	Dl	98/141 (70%)	98 (100%)	0	100 100
32	Dc	113/833 (14%)	111 (98%)	2 (2%)	54 72
33	Dk	87/182 (48%)	87 (100%)	0	100 100
34	Dm	80/106 (76%)	79 (99%)	1 (1%)	65 77
35	EA	163/373 (44%)	122 (75%)	41 (25%)	0 3
36	EB	155/261 (59%)	142 (92%)	13 (8%)	9 30
37	1	384/484 (79%)	367 (96%)	17 (4%)	24 47
38	2	342/352 (97%)	336 (98%)	6 (2%)	54 72
39	3	259/272 (95%)	258 (100%)	1 (0%)	89 91
40	4	394/399 (99%)	383 (97%)	11 (3%)	38 60
41	5	59/64 (92%)	54 (92%)	5 (8%)	8 30
42	6	576/688 (84%)	558 (97%)	18 (3%)	35 56
43	7	630/664 (95%)	601 (95%)	29 (5%)	23 46
44	c	231/280 (82%)	217 (94%)	14 (6%)	15 39
45	e	94/152 (62%)	94 (100%)	0	100 100
46	b	102/163 (63%)	92 (90%)	10 (10%)	6 23
47	l	116/155 (75%)	116 (100%)	0	100 100
48	m	102/115 (89%)	102 (100%)	0	100 100
49	a	393/1391 (28%)	315 (80%)	78 (20%)	1 7
50	d	139/230 (60%)	95 (68%)	44 (32%)	0 2
51	f	144/223 (65%)	122 (85%)	22 (15%)	2 13
52	g	157/216 (73%)	128 (82%)	29 (18%)	1 9
53	h	161/225 (72%)	132 (82%)	29 (18%)	1 9
54	i	71/133 (53%)	61 (86%)	10 (14%)	3 16
55	j	113/124 (91%)	110 (97%)	3 (3%)	40 61
56	k	94/98 (96%)	48 (51%)	46 (49%)	0 0
57	n	689/1272 (54%)	662 (96%)	27 (4%)	27 50
58	o	141/697 (20%)	139 (99%)	2 (1%)	62 76
59	q	461/577 (80%)	396 (86%)	65 (14%)	3 16
60	r	180/183 (98%)	151 (84%)	29 (16%)	2 12
61	s	31/208 (15%)	28 (90%)	3 (10%)	6 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	t	166/178 (93%)	128 (77%)	38 (23%)	0 4
63	u	78/119 (66%)	73 (94%)	5 (6%)	14 37
64	v	122/173 (70%)	88 (72%)	34 (28%)	0 3
65	z	89/512 (17%)	77 (86%)	12 (14%)	3 16
66	x	787/864 (91%)	771 (98%)	16 (2%)	50 68
67	w	1202/1232 (98%)	1185 (99%)	17 (1%)	62 76
68	p	353/736 (48%)	346 (98%)	7 (2%)	50 68
All	All	18686/29967 (62%)	16829 (90%)	1857 (10%)	9 23

5 of 1857 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	DA	410	TRP
64	v	38	LYS
31	DL	107	LYS
62	t	109	LYS
56	k	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 381 such sidechains are listed below:

Mol	Chain	Res	Type
46	b	129	GLN
57	n	267	HIS
48	m	80	GLN
50	d	127	GLN
58	o	705	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
73	SF4	7	801	43	0,12,12	-	-	-		

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
73	SF4	7	801	43	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

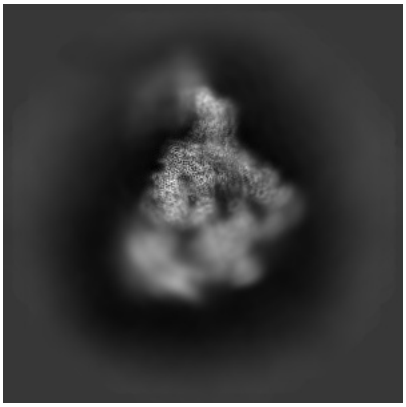
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31204. These allow visual inspection of the internal detail of the map and identification of artifacts.

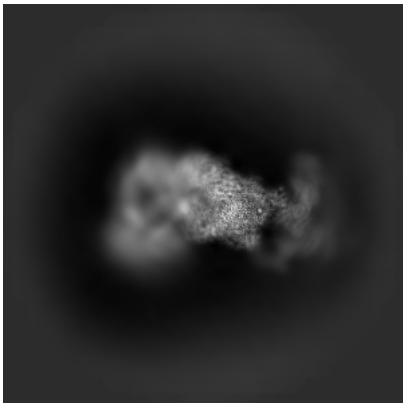
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

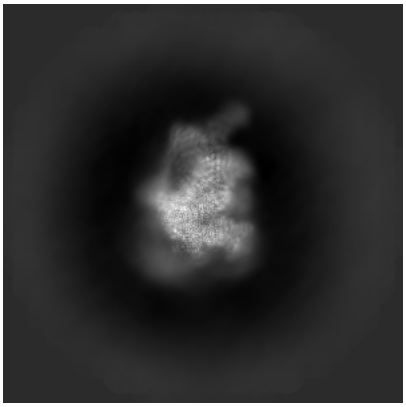
6.1.1 Primary map



X



Y

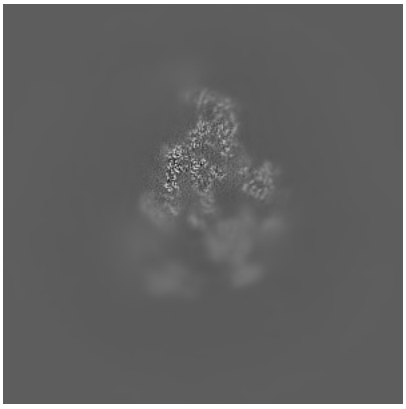


Z

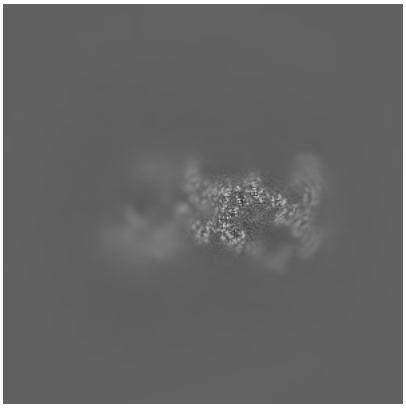
The images above show the map projected in three orthogonal directions.

6.2 Central slices

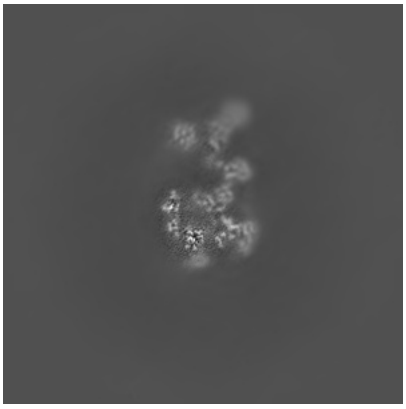
6.2.1 Primary map



X Index: 256



Y Index: 256

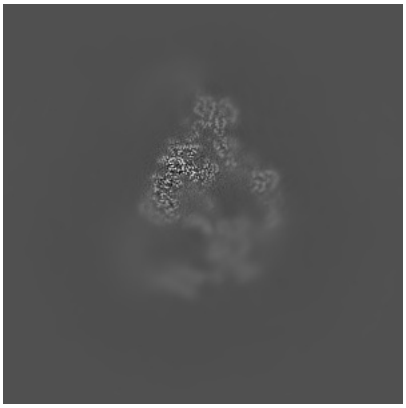


Z Index: 256

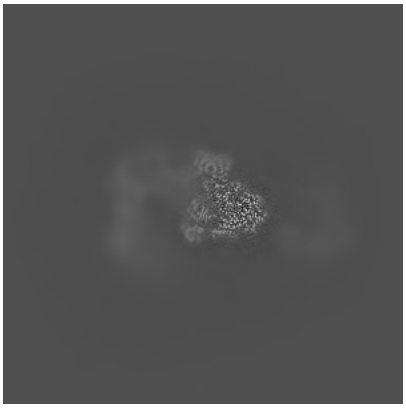
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

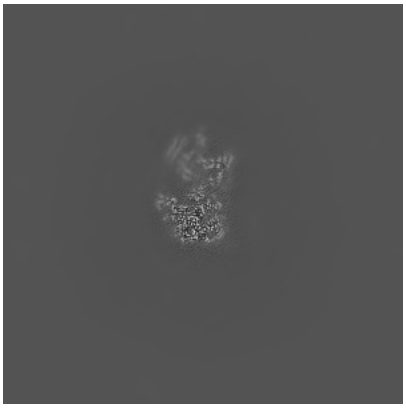
6.3.1 Primary map



X Index: 245



Y Index: 219

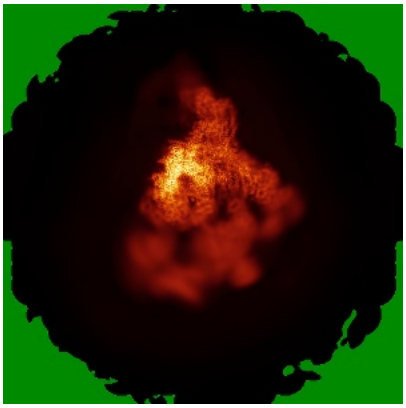


Z Index: 301

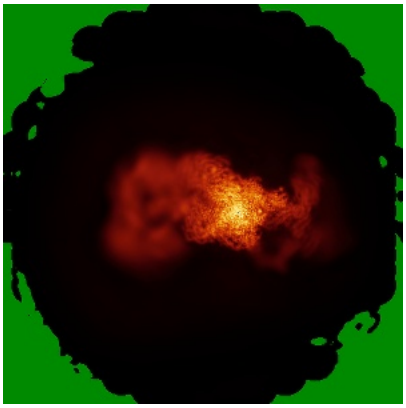
The images above show the largest variance slices of the map in three orthogonal directions.

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

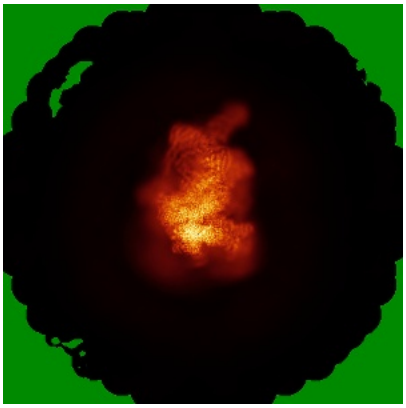
6.4.1 Primary map



X



Y

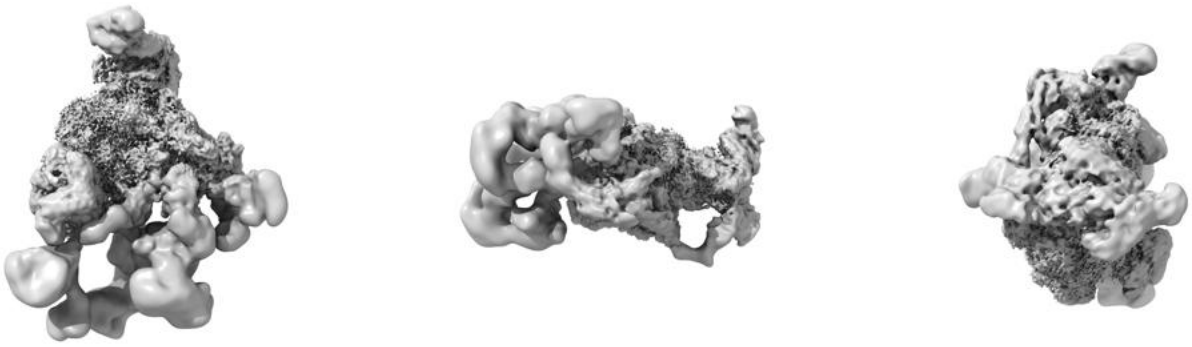


Z

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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

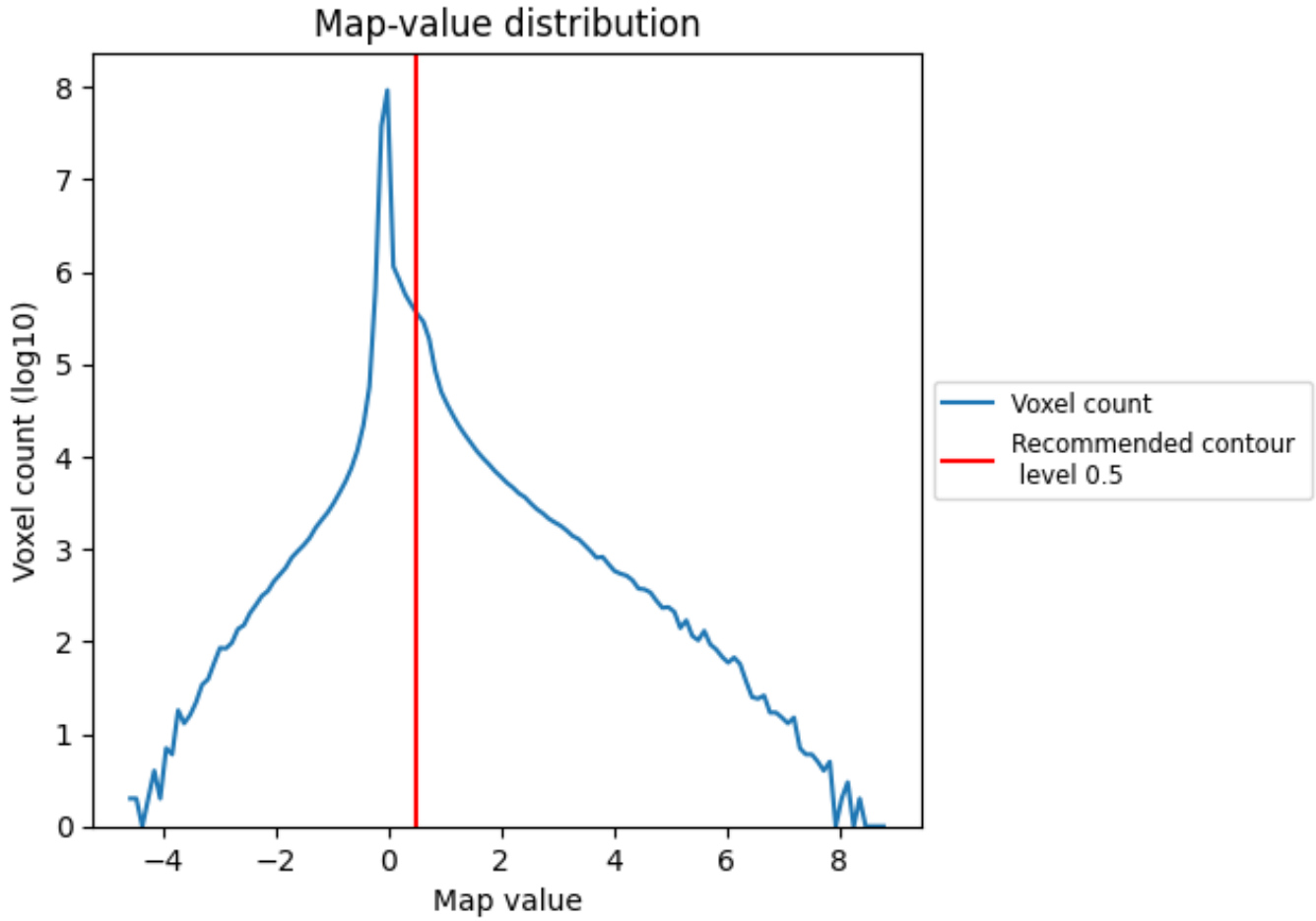
6.6 Mask visualisation (i)

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

7 Map analysis

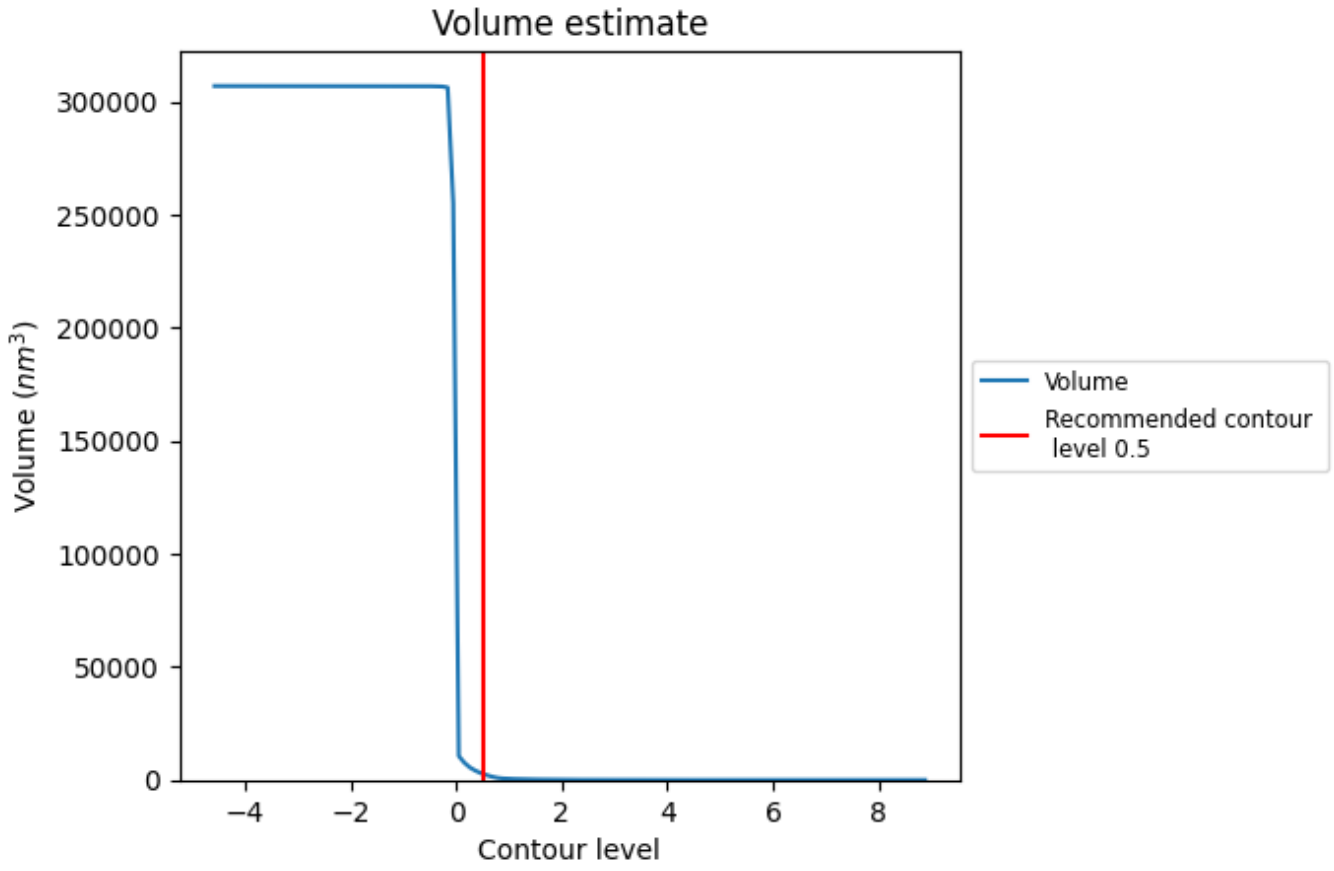
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

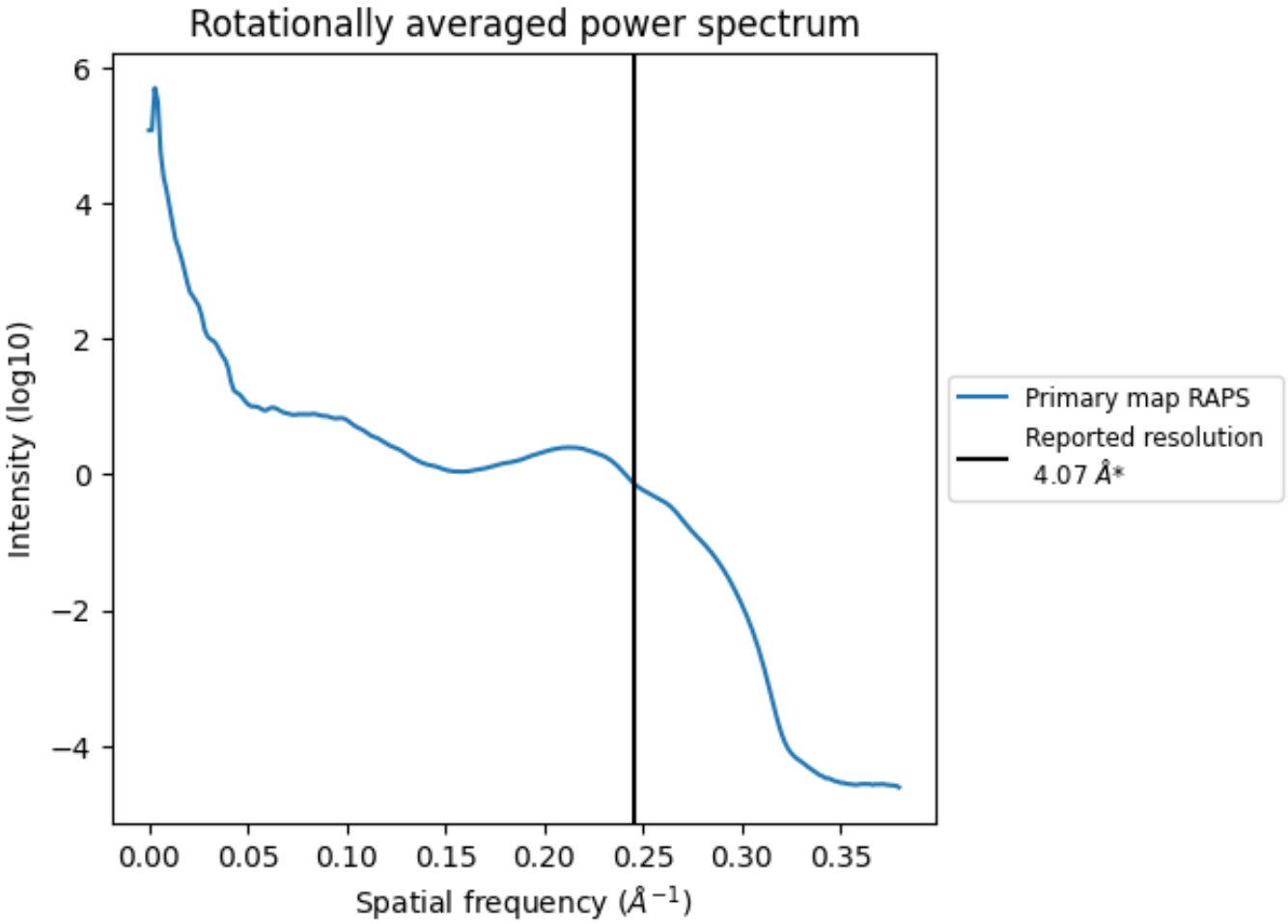
7.2 Volume estimate



The volume at the recommended contour level is 2784 nm^3; this corresponds to an approximate mass of 2515 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

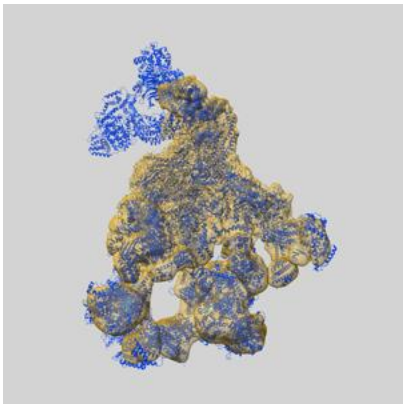
8 Fourier-Shell correlation (i)

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

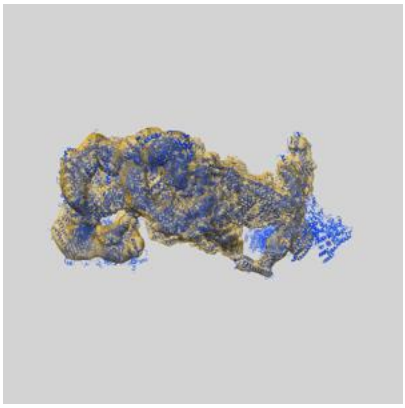
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31204 and PDB model 7ENA. Per-residue inclusion information can be found in section 3 on page 18.

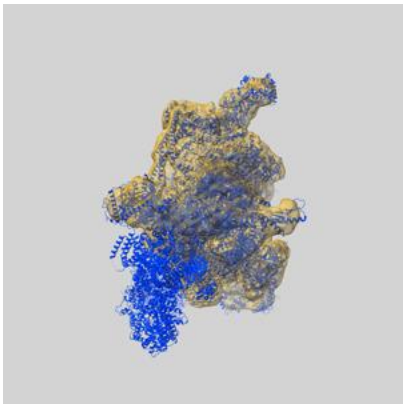
9.1 Map-model overlay



X



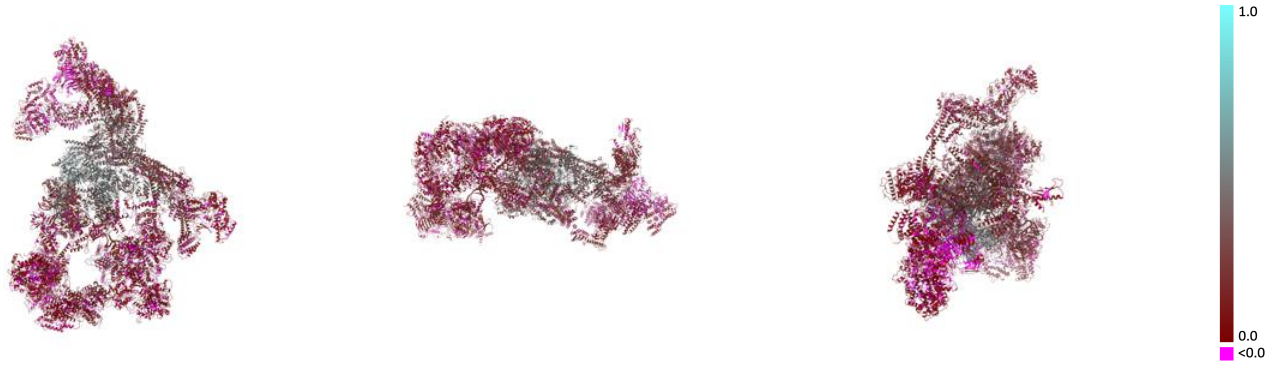
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

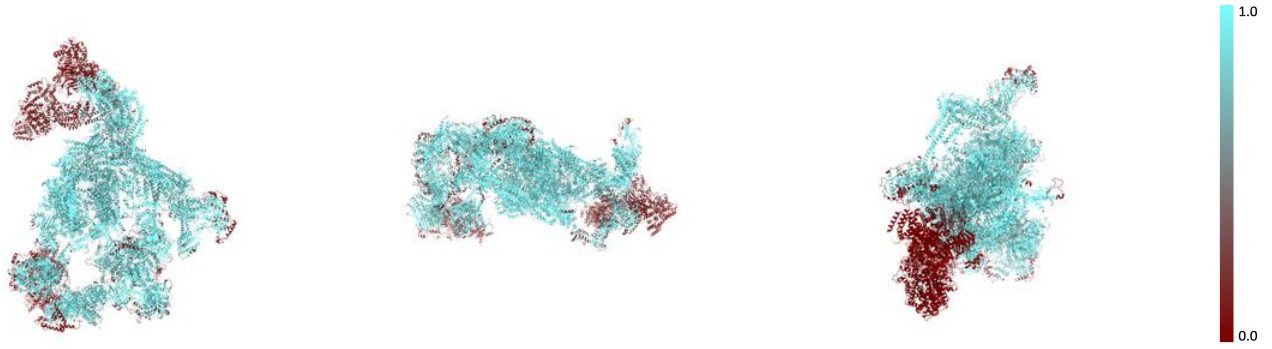
9.2 Q-score mapped to coordinate model



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.

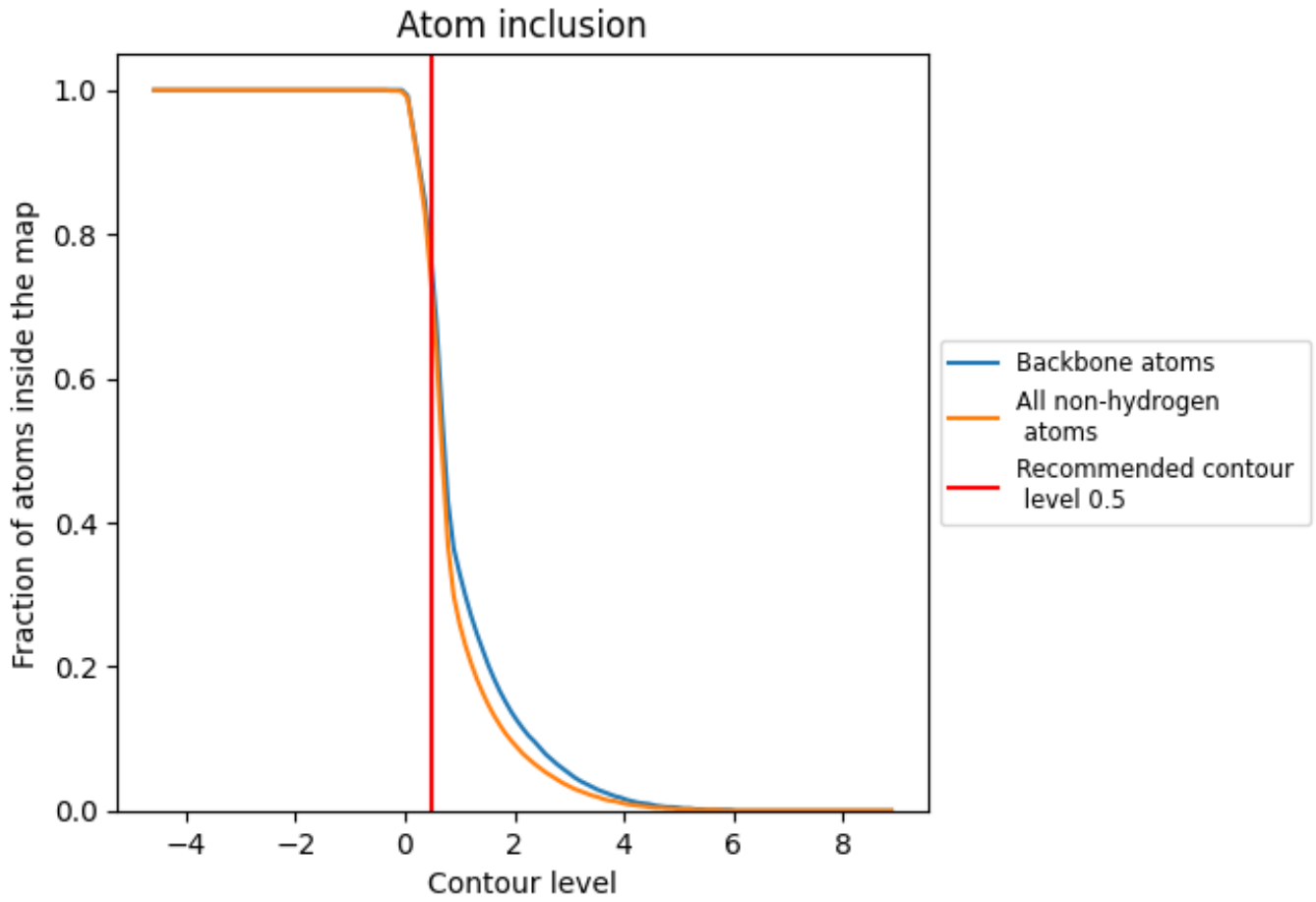
9.3 Atom inclusion mapped to coordinate model



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.1680
0	0.7760	0.1210
1	0.6320	0.0350
2	0.8070	0.0600
3	0.9160	0.0610
4	0.7590	0.0700
5	0.8320	0.0600
6	0.8640	0.0830
7	0.9110	0.1070
8	0.8330	0.1070
9	0.6160	0.0680
BA	0.9210	0.2770
DA	0.8310	0.0650
DB	0.8880	0.0600
DD	0.7420	0.0830
DE	0.8120	0.0650
DF	0.7670	0.0520
DG	0.8530	0.0550
DH	0.8340	0.0500
DI	0.8170	0.0540
DJ	0.8740	0.0580
DL	0.5260	0.0640
DO	0.9130	0.1060
DP	0.9510	0.1750
DQ	0.7990	0.1050
Dc	0.0000	0.0350
Dd	0.0000	0.0350
De	0.0040	0.0330
Df	0.4390	0.0530
Di	0.0000	0.0290
Dj	0.0000	0.0260
Dk	0.0000	0.0420
Dl	0.0000	0.0460
Dm	0.0000	0.0440
EA	0.9470	0.1860

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Chain	Atom inclusion	Q-score
EB	0.9150	0.1040
FA	0.8960	0.0700
FB	0.8840	0.1080
PA	0.9540	0.4180
PB	0.9500	0.4520
PC	0.9630	0.4890
PD	0.9350	0.4060
PE	0.9720	0.3600
PF	0.9770	0.5210
PG	0.9610	0.4380
PH	0.9610	0.4530
PI	0.9710	0.3540
PJ	0.9740	0.5150
PK	0.9360	0.4430
PL	0.9580	0.4470
X	0.9510	0.1560
Y	0.9660	0.1760
a	0.5990	0.0940
b	0.7900	0.1460
c	0.8980	0.2830
d	0.9100	0.1440
e	0.8860	0.1890
f	0.9330	0.2460
g	0.9520	0.1380
h	0.8910	0.2730
i	0.9110	0.1540
j	0.9320	0.1050
k	0.9320	0.2870
l	0.9220	0.1950
m	0.9190	0.1730
n	0.8870	0.1890
o	0.9030	0.1670
p	0.0000	-0.0140
q	0.9170	0.3040
r	0.9260	0.3830
s	0.9400	0.1130
t	0.8860	0.3610
u	0.9390	0.1550
v	0.9140	0.3410
w	0.0420	0.0510
x	0.1950	0.0640
z	0.8980	0.1220