



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 01:10 AM EDT

PDB ID : 7LBM / pdb_00007lbm
EMDB ID : EMD-23255
Title : Structure of the human Mediator-bound transcription pre-initiation complex
Authors : Abdella, R.; Talyzina, A.; He, Y.
Deposited on : 2021-01-08
Resolution : 4.80 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:

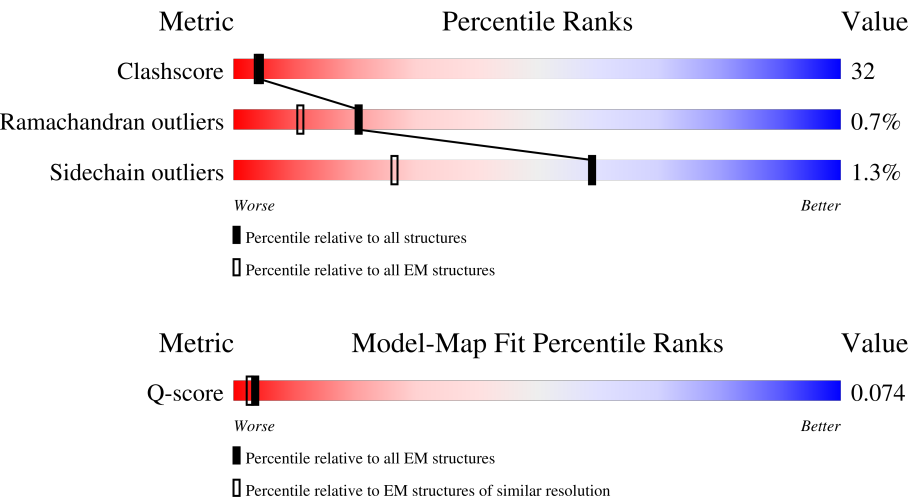
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.80 Å.

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



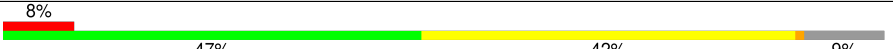
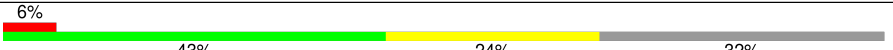
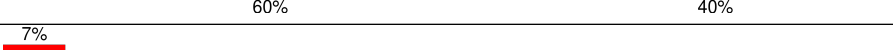
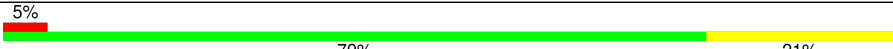
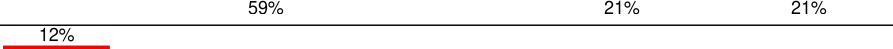
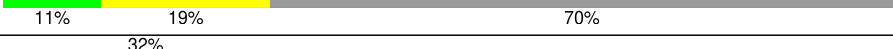
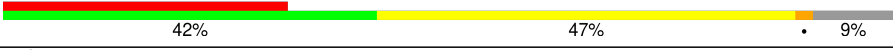
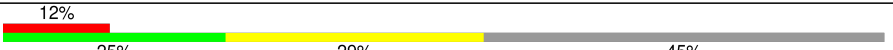
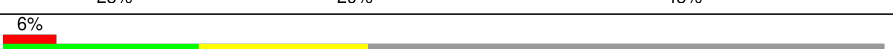
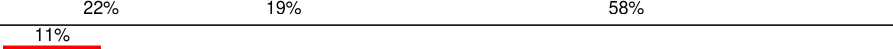
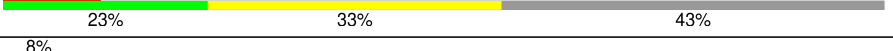
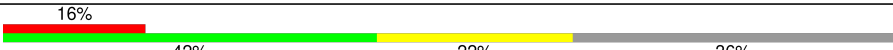
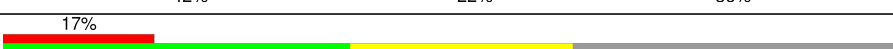
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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

Mol	Chain	Length	Quality of chain
1	0	841	
2	1	1368	
3	2	989	
4	3	747	

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Mol	Chain	Length	Quality of chain
5	A	1970	
6	B	1174	
7	C	275	
8	D	142	
9	E	210	
10	F	127	
11	G	172	
12	H	150	
13	I	125	
14	J	67	
15	K	117	
16	L	58	
17	M	376	
18	N	109	
19	O	316	
20	P	339	
21	Q	439	
22	R	291	
23	S	517	
24	T	249	
25	U	100	
26	V	100	
27	W	782	
28	X	760	
29	Y	548	

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Mol	Chain	Length	Quality of chain
30	Z	462	
31	a	395	
32	b	308	
33	c	71	
34	d	309	
35	e	346	
36	f	323	
37	g	246	
38	h	268	
39	i	117	
40	j	651	
41	k	208	
42	l	212	
43	m	200	
44	n	311	
45	o	178	
46	p	200	
47	q	178	
48	r	1454	
49	s	270	
50	t	233	
51	u	146	
52	v	135	
53	w	244	
54	x	144	

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Mol	Chain	Length	Quality of chain
55	y	131	18%5%70%14%11%
56	z	788	8%8%81%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 129277 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 Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			5864	3744	1005	1068	47		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	1317	Total	C	N	O	S	0	0
			10636	6878	1809	1880	69		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	897	Total	C	N	O	S	0	0
			7007	4487	1180	1284	56		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	195	Total	C	N	O	S	0	0
			1504	969	249	277	9		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1455	Total	C	N	O	S	0	0
			11519	7241	2052	2154	72		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1142	Total	C	N	O	S	0	0
			9129	5769	1604	1692	64		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	267	Total	C	N	O	S	0	0
			2147	1344	370	426	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			928	599	153	174	2		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 18 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 19 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 20 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 21 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 23 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	127	Total	C	N	O	S	0	0
			1059	671	196	189	3		

- Molecule 24 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 25 is a DNA chain called super core promoter sense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	64	Total	C	N	O	P	0	0
			1321	623	256	379	63		

- Molecule 26 is a DNA chain called super core promoter antisense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	64	Total	C	N	O	P	0	0
			1300	616	233	387	64		

- Molecule 27 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	574	Total	C	N	O	S	0	0
			4645	2973	807	835	30		

- Molecule 28 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	760	Total	C	N	O	S	0	0
			6109	3899	1066	1115	29		

- Molecule 29 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	218	Total	C	N	O	S	0	0
			1631	1028	290	305	8		

- Molecule 30 is a protein called General transcription factor IIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	436	Total	C	N	O	S	0	0
			3473	2239	609	611	14		

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	331	Total	C	N	O	S	0	0
			2580	1628	443	482	27		

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

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

- Molecule 34 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	275	Total	C	N	O	S	0	0
			2104	1315	368	410	11		

- Molecule 35 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	298	Total	C	N	O	S	0	0
			2376	1537	404	423	12		

- Molecule 36 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	281	Total	C	N	O	S	0	0
			2293	1465	394	416	18		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	130	Total	C	N	O	S	0	0
			1035	664	174	192	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	158	Total	C	N	O	S	0	0
			1230	767	214	246	3		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	110	Total	C	N	O	S	0	0
			863	527	160	172	4		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	504	Total	C	N	O	S	0	0
			4005	2530	719	739	17		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	185	Total	C	N	O	S	0	0
			1484	942	259	268	15		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	184	Total	C	N	O	S	0	0
			1425	907	235	267	16		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	125	Total	C	N	O	S	0	0
			1024	632	175	213	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	283	Total	C	N	O	S	0	0
			2279	1445	406	417	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	108	Total	C	N	O	S	0	0
			887	553	155	176	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	114	Total	C	N	O	S	0	0
			893	559	154	171	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	122	Total	C	N	O	S	0	0
			1007	628	188	182	9		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	1034	Total	C	N	O	S	0	0
			8174	5239	1427	1461	47		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	135	Total	C	N	O	S	0	0
			1084	676	191	212	5		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	116	Total	C	N	O	S	0	0
			975	621	175	173	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	60	Total	C	N	O	S	0	0
			501	314	93	90	4		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	131	Total	C	N	O	S	0	0
			1067	676	182	204	5		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	39	Total	C	N	O	S	0	0
			309	198	52	57	2		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	111	Total	C	N	O	S	0	0
			852	528	142	178	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	116	Total	C	N	O	S	0	0
			1003	649	177	172	5		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	149	Total	C	N	O	S	0	0
			1168	747	204	210	7		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	2	Total	Mg	0
			2	2	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	A	2	Total	Zn	0
			2	2	
58	B	1	Total	Zn	0
			1	1	
58	C	1	Total	Zn	0
			1	1	
58	I	2	Total	Zn	0
			2	2	
58	J	1	Total	Zn	0
			1	1	
58	L	1	Total	Zn	0
			1	1	
58	O	1	Total	Zn	0
			1	1	
58	Q	1	Total	Zn	0
			1	1	
58	a	3	Total	Zn	0
			3	3	
58	b	1	Total	Zn	0
			1	1	
58	d	2	Total	Zn	0
			2	2	

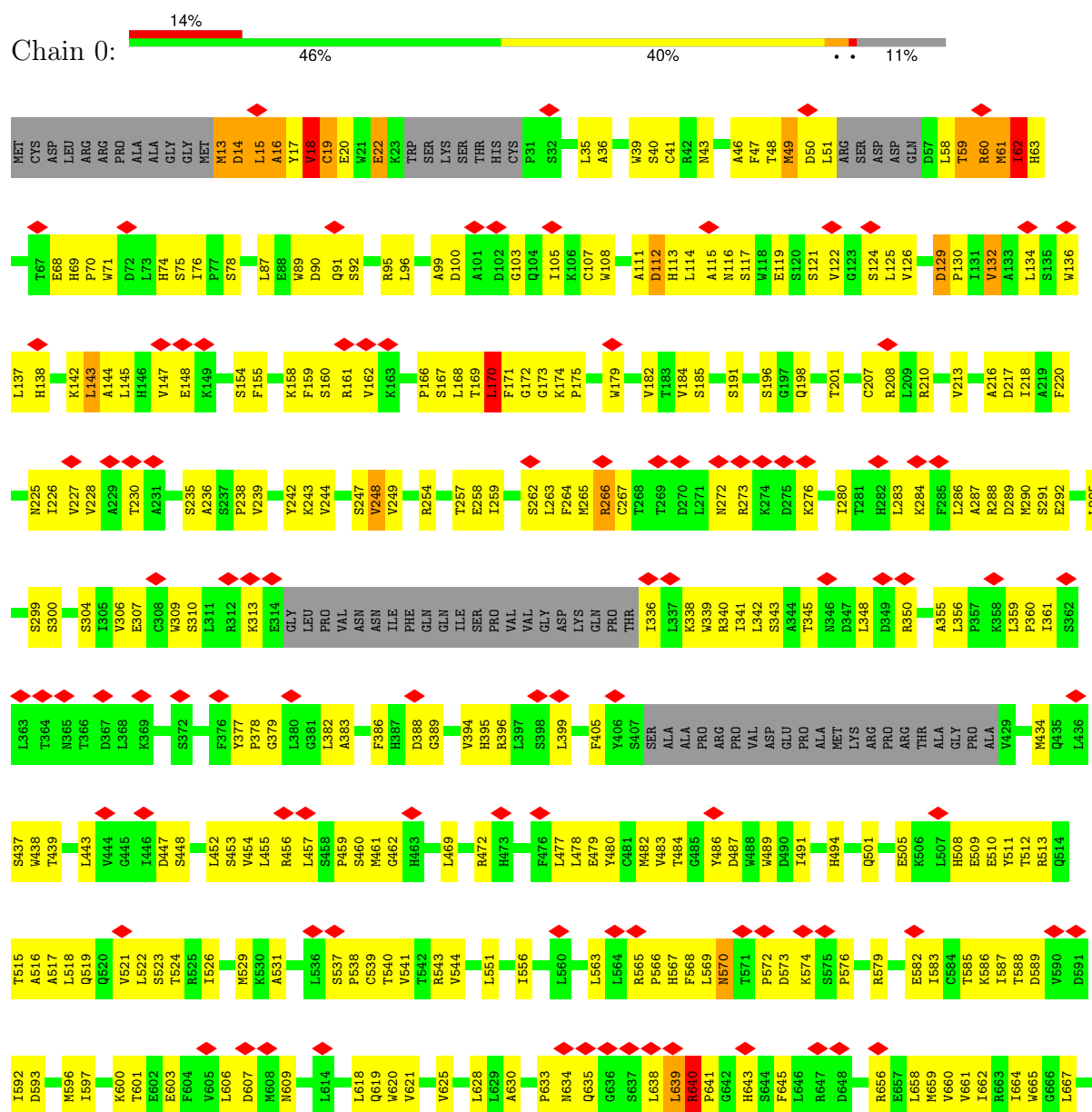
- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

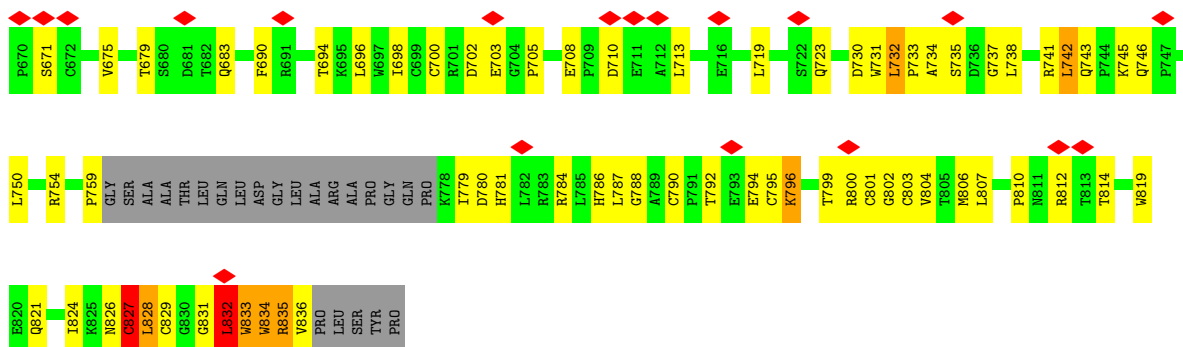
ltConf
0

3 Residue-property plots

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.

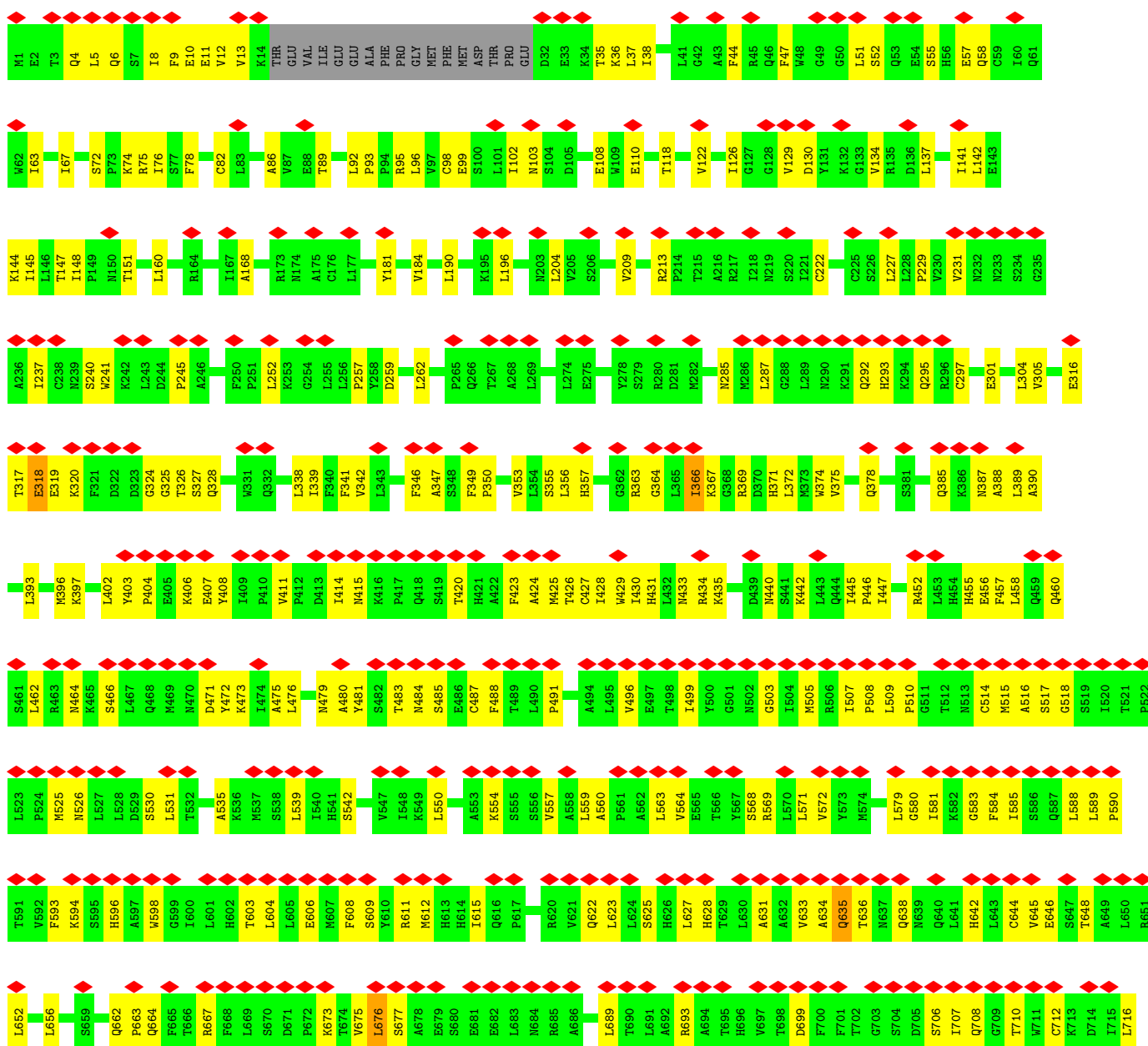
- Molecule 1: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

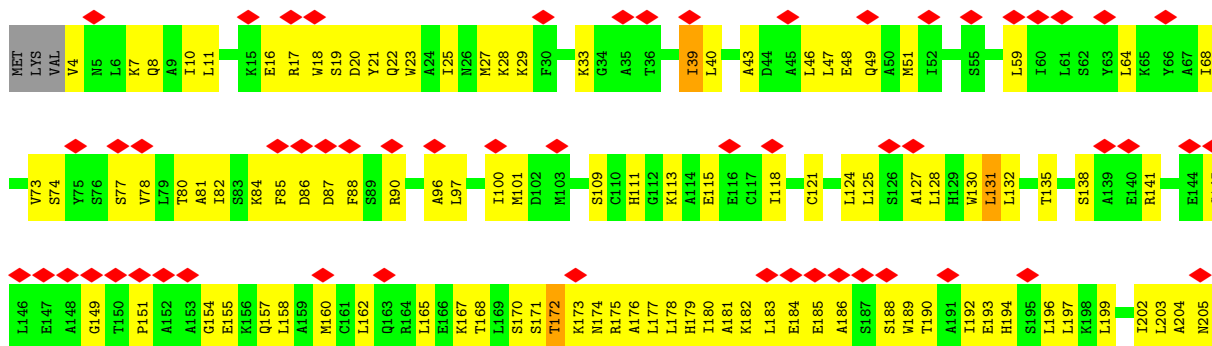
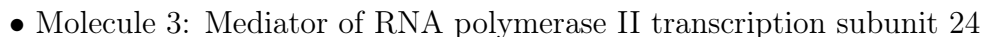




• Molecule 2: Mediator of RNA polymerase II transcription subunit 23

Chain 1: 48% 60% 36%

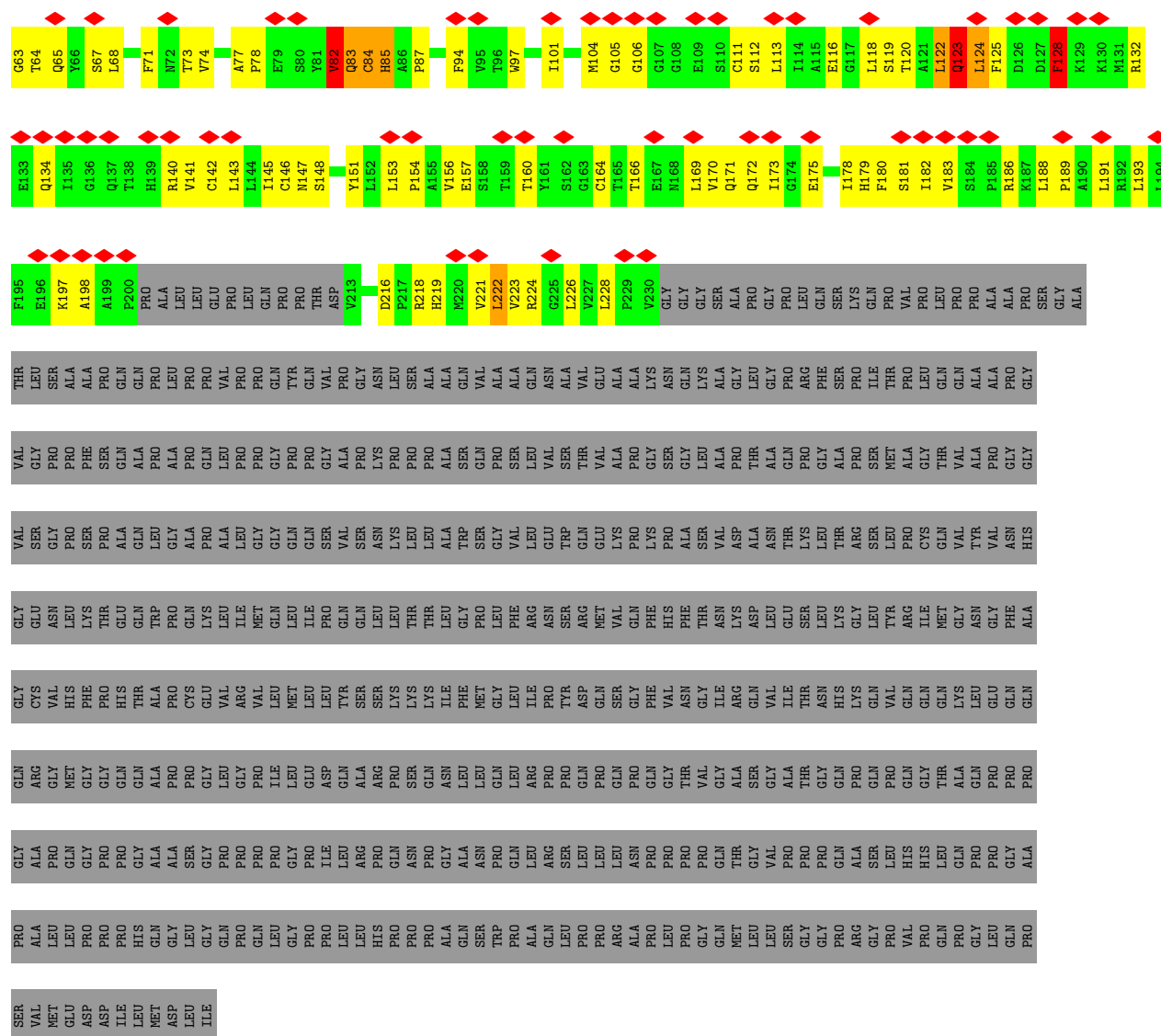






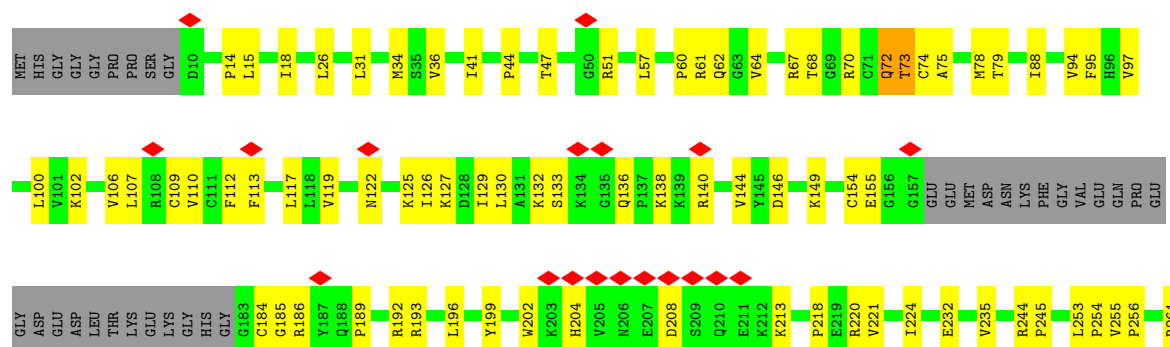
• Molecule 4: Mediator of RNA polymerase II transcription subunit 25



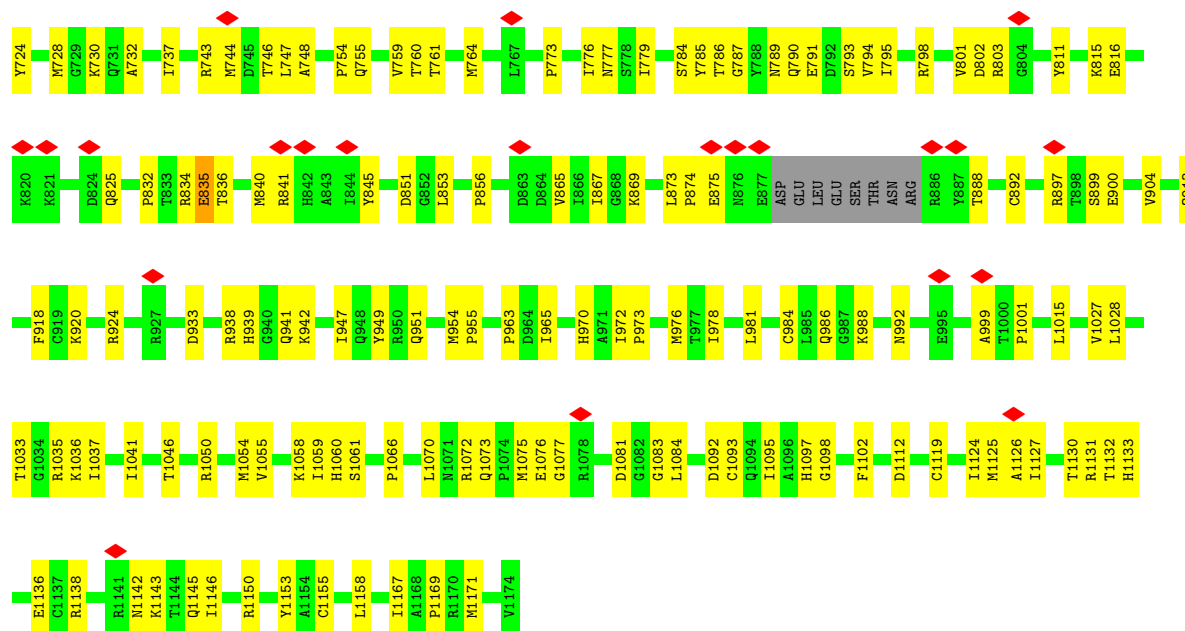


• Molecule 5: DNA-directed RNA polymerase II subunit RPB1

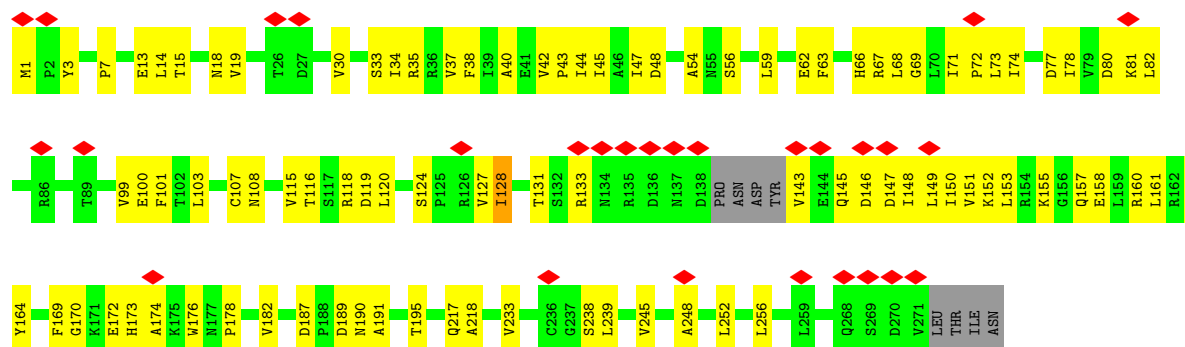
Chain A: 47% 26% 26%



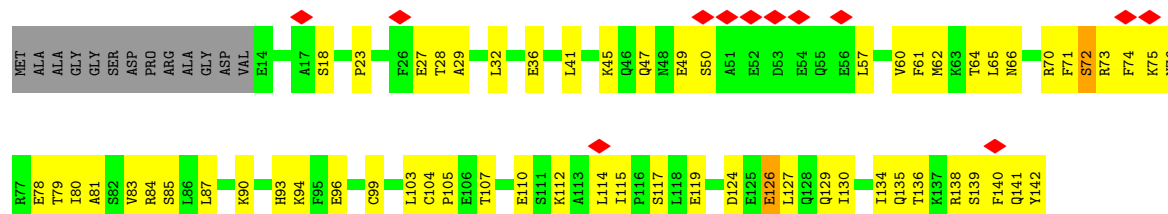
THR	V1436	R1345	N1263	G1120	R890	N780	C641	V538	K445	P262
PRO	V1346	V1346	S1264	V1121	V891	I781	L645	V538	K445	A263
TRP	L1347	L1347	D1265	R1122	E892	S782	L645	V538	V446	V264
ASN	S1348	S1348	V1195	R1123	E893	A786	V652	V538	V446	V265
GLN	E1349	E1349	Y1196	K1124	Q904	A787	V653	V538	V446	M266
ALA	K1350	K1350	E1198	K1125	N905	Q790	V654	V538	V446	Q267
THR	D1351	D1351	M1199	L1128	L906	E794	V655	V538	V446	G268
PRO	V1352	V1352	GLN	R1129	A907	R797	H654	V538	V446	S269
TRP	L1353	L1353	D1201	I1130	L909	E659	H655	V538	V446	A270
ALA	R1356	R1356	F1202	S1131	L909	M660	V656	V538	V446	R271
GLY	S1359	S1359	E1274	K1132	E917	F663	D663	V538	V446	N272
ALA	M1360	M1360	V1275	R1133	F920	I664	I664	V538	V446	D275
TRP	D1361	D1361	V1276	P1134	R921	R666	T665	V538	V446	K279
SER	I1362	I1362	I1207	L1044	R921	R666	L667	V538	V446	L280
PRO	V1363	V1363	S1208	H1045	Y924	F668	Y669	V538	V446	V284
VAL	E1364	E1364	P1137	R1046	E927	Y669	Y669	V538	V446	L290
GLY	V1368	V1368	F1142	L1049	R931	F810	V675	V538	V446	Q295
GLY	L1369	L1369	L1143	C1050	R928	R812	I676	V538	V446	N296
MET	E1372	E1372	G1145	S1051	R931	K812	N677	V538	V446	H301
THR	K1479	K1479	Q1146	R1052	R931	D814	L680	V538	V446	V302
PRO	K1481	K1481	S1147	R1053	R932	P817	L680	V538	V446	D306
GLY	V1482	V1482	R1148	M1054	T933	R820	I687	V538	V446	Q311
ALA	L1382	L1382	R1149	A1055	T933	V823	G688	V538	V446	H312
ALA	V1385	V1385	D1150	E1056	V939	E824	I689	V538	V446	H313
GLY	I1386	I1386	D1156	R1059	V942	V824	I689	V538	V446	V314
PHE	Y1392	Y1392	I1157	L1060	V948	E824	S692	V538	V446	A315
PRO	H1397	H1397	R1160	A1079	L952	L828	T698	V538	V446	T316
ALA	L1398	L1398	L1161	M1086	L952	E835	T698	V538	V446	D319
GLY	V1399	V1399	E1162	V1087	F956	E835	I702	V538	V446	N320
SER	L1401	L1401	H1163	T1164	F956	M841	I702	V538	V446	E321
ASP	L1411	L1411	T1165	Q1093	M959	E845	K710	V538	V446	L322
ALA	M1412	M1412	L1166	S1094	M959	E845	H721	V538	V446	L325
GLY	A1413	A1413	R1167	L1095	D962	E845	N722	V538	V446	P326
PRO	I1414	I1414	K1168	P1098	R963	D849	N723	V538	V446	R327
THR	H1417	H1417	T1170	A1099	R964	V852	E724	V538	V446	M329
MET	G1418	G1418	A1171	T1100	V965	K853	P727	V538	V446	Q330
SER	V1419	V1419	L1172	GLN	L966	E856	T605	V538	V446	A328
ALA	N1420	N1420	L1173	MET	R967	E856	T605	V538	V446	M423
TRP	R1421	R1421	L1175	THR	V968	Y859	L733	V538	V446	G424
SER	Q1422	Q1422	Y1176	ASN	R969	I860	R734	V538	V446	D425
PRO	D1423	D1423	D1177	THR	V977	I860	T752	V538	V446	R426
THR	P1426	P1426	F1178	PHE	V978	T665	G753	V538	V446	S332
GLY	L1427	L1427	P1179	HIS	L979	T665	G753	V538	V446	G333
PRO	M1428	M1428	Q1182	THR	N982	M668	Q757	V538	V446	R334
ILE	K1429	K1429	S1183	ALA	N982	M668	Q757	V538	V446	P335
SER	C1430	C1430	T1184	VAL	R985	V871	K767	V538	V446	L336
PRO	S1431	S1431	V1185	SER	R985	V871	S768	V538	V446	K337
GLY	F1432	F1432	V1186	ALA	R987	N881	V770	V538	V446	S338
PRO	E1433	E1433	K1115	ALA	N988	S882	V770	V538	V446	L339
MET	L1434	L1434	T1118	ALA	N989	K778	K778	V538	V446	K340
	M1435	M1435	L1119	ALA	K992	I779	I779	V538	V446	Q341
								V538	V446	R342
								V538	V446	L343



• Molecule 7: DNA-directed RNA polymerase II subunit RPB3

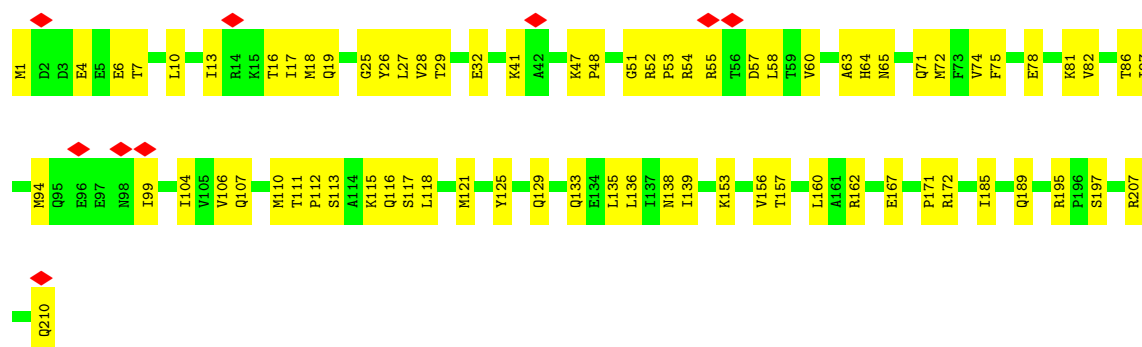


• Molecule 8: DNA-directed RNA polymerase II subunit RPB4

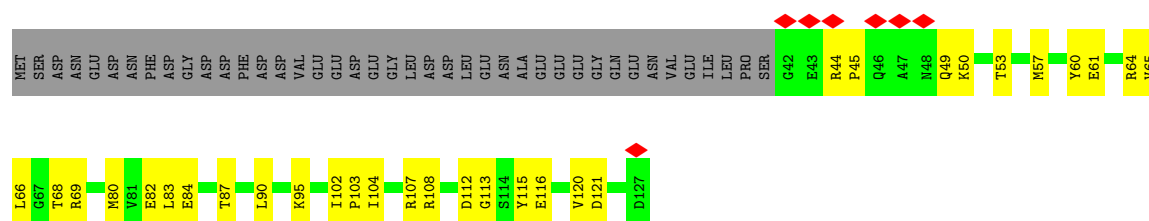


• Molecule 9: DNA-directed RNA polymerase II subunit RPB5

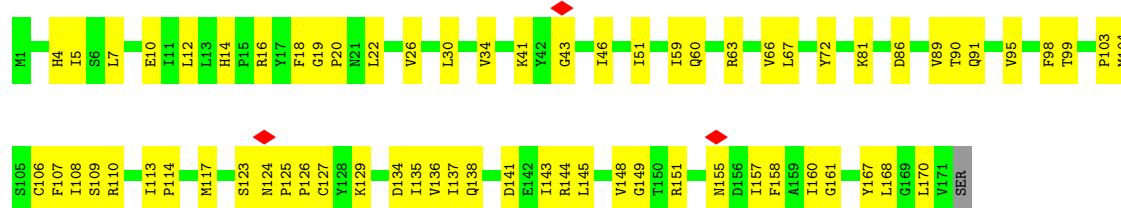




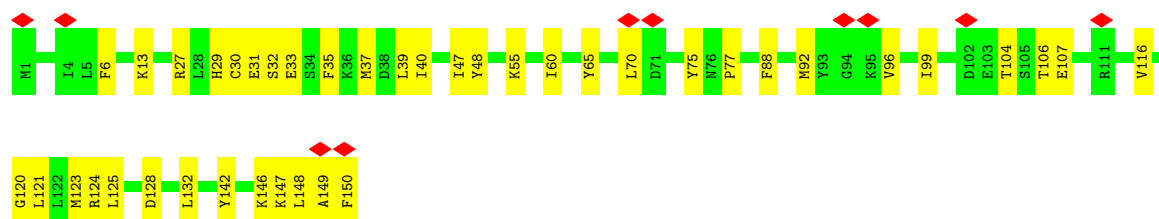
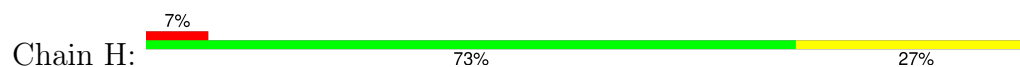
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 11: DNA-directed RNA polymerase II subunit RPB7

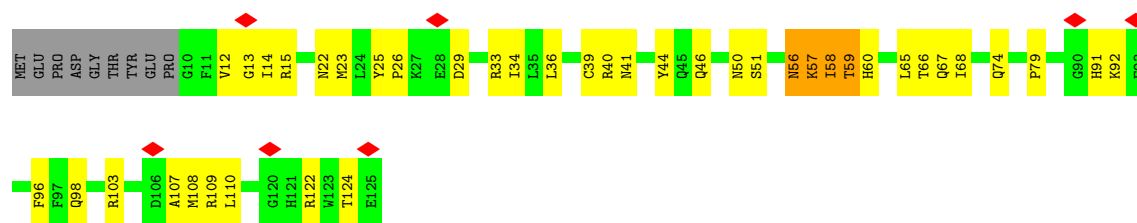


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3

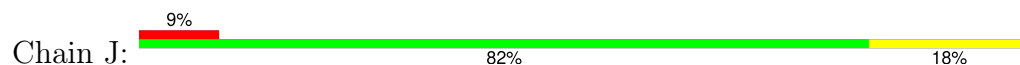


- Molecule 13: DNA-directed RNA polymerase II subunit RPB9

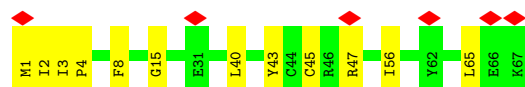




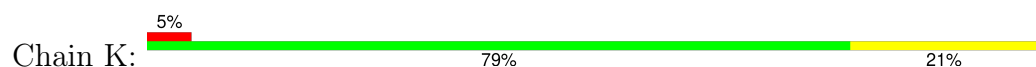
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



Chain J: 9% 82% 18%



- Molecule 15: DNA-directed RNA polymerase II subunit RPB11-a



Chain K: 5% 79% 21%



- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4



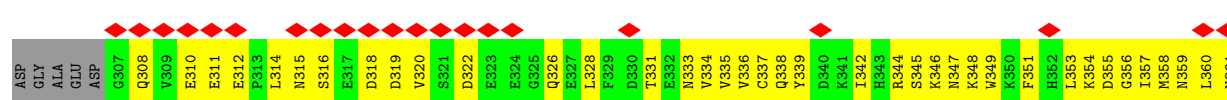
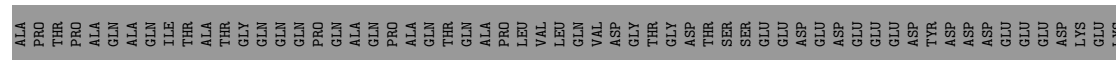
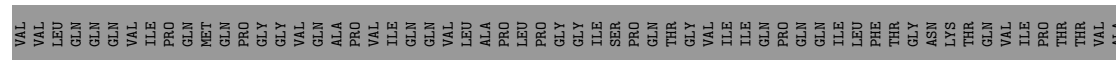
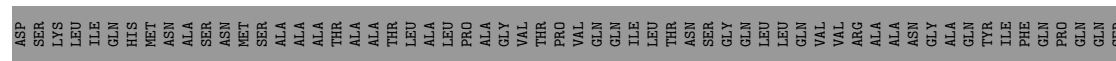
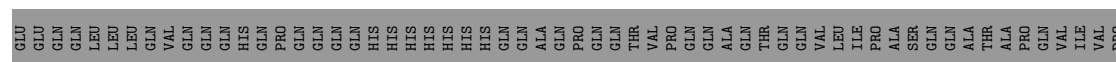
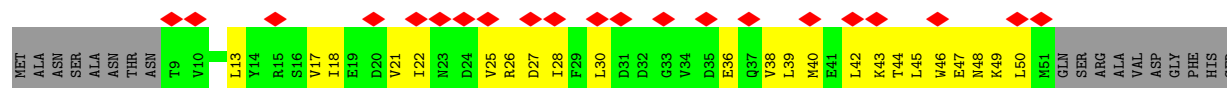
Chain L: 59% 21% 21%

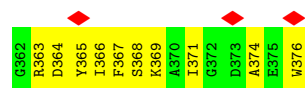


- Molecule 17: Transcription initiation factor IIA subunit 1

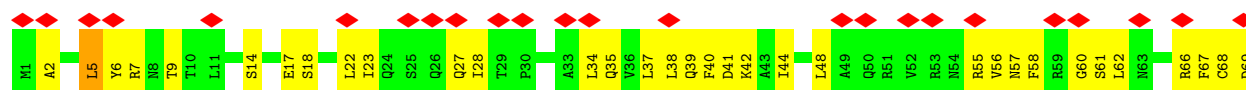
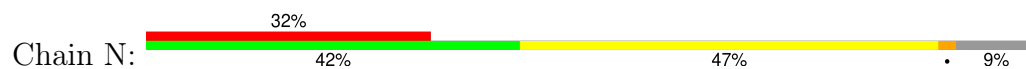


Chain M: 12% 11% 19% 70%

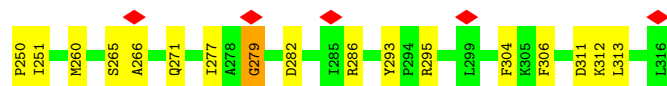
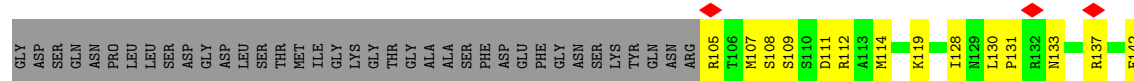
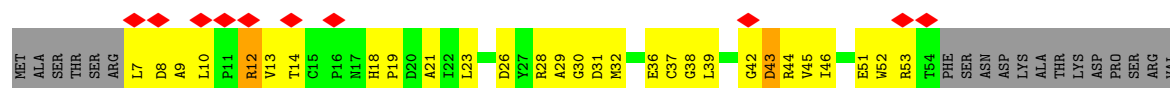




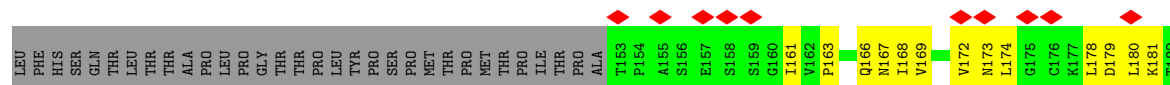
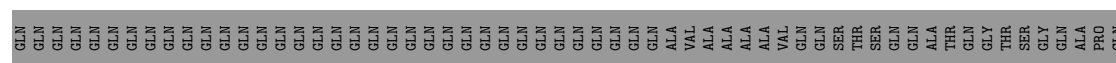
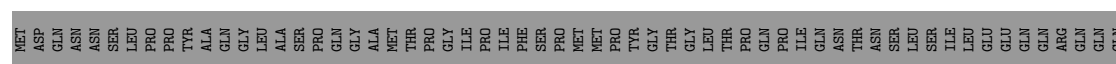
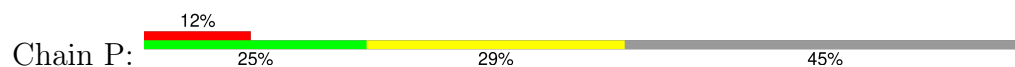
• Molecule 18: Transcription initiation factor IIA subunit 2

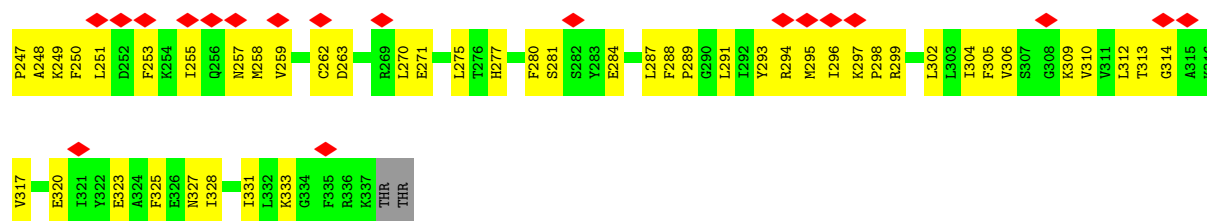


• Molecule 19: Transcription initiation factor IIB

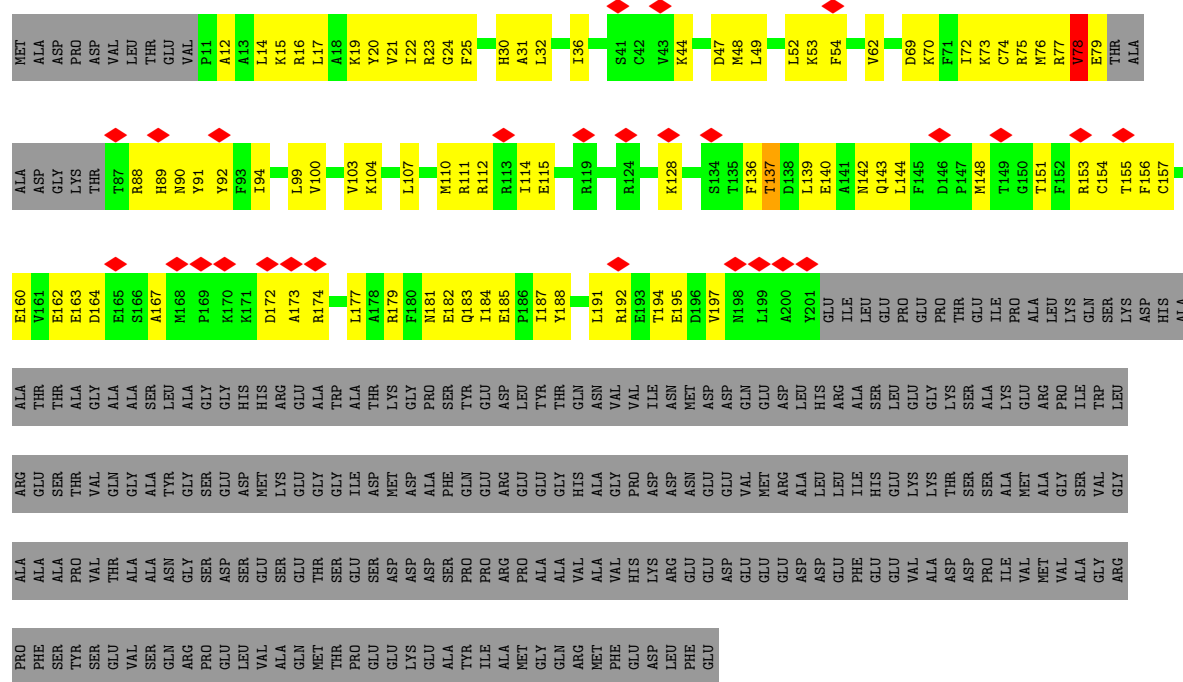


• Molecule 20: TATA-box-binding protein

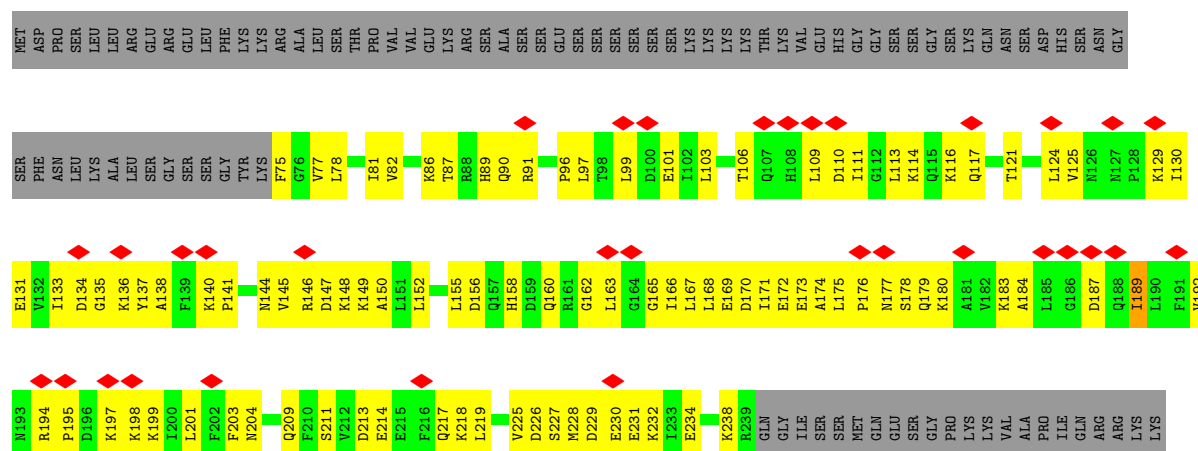
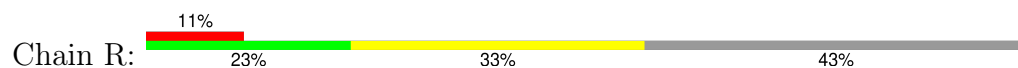




• Molecule 21: General transcription factor IIE subunit 1



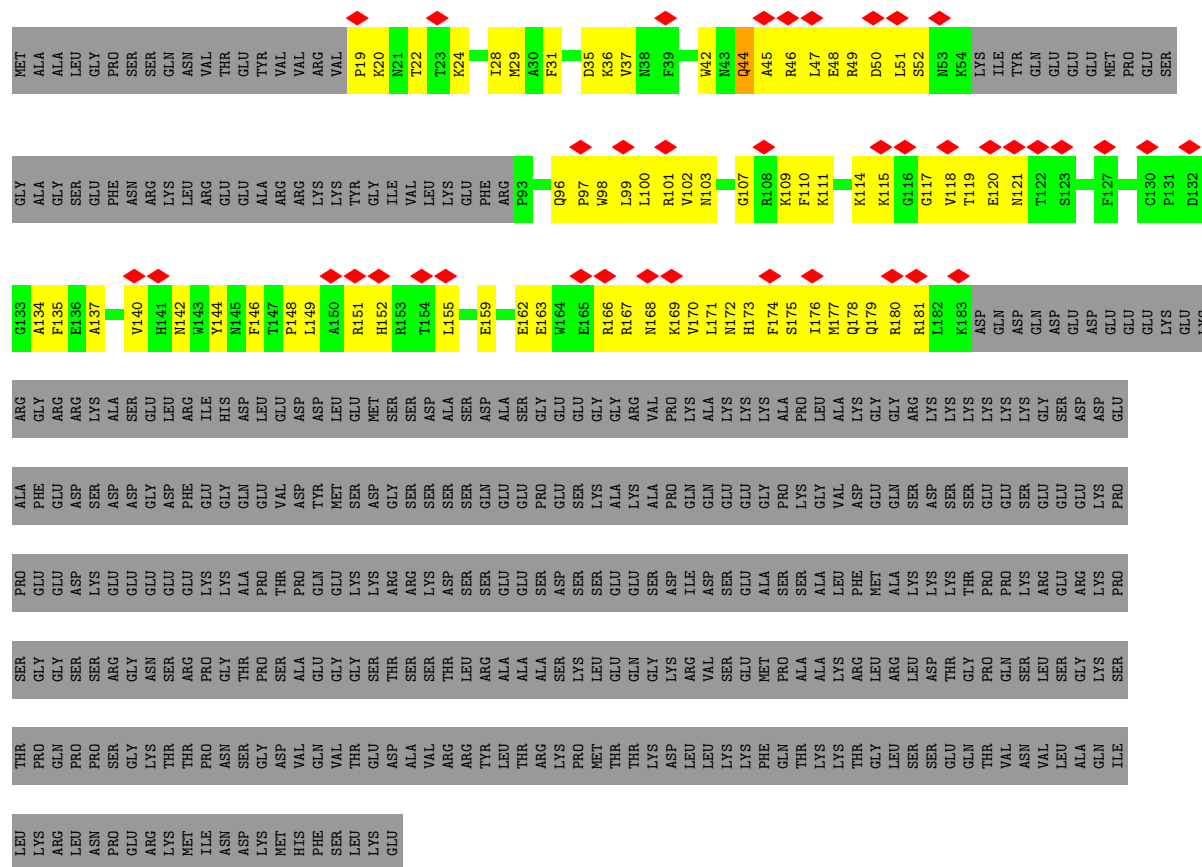
• Molecule 22: Transcription initiation factor IIE subunit beta



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

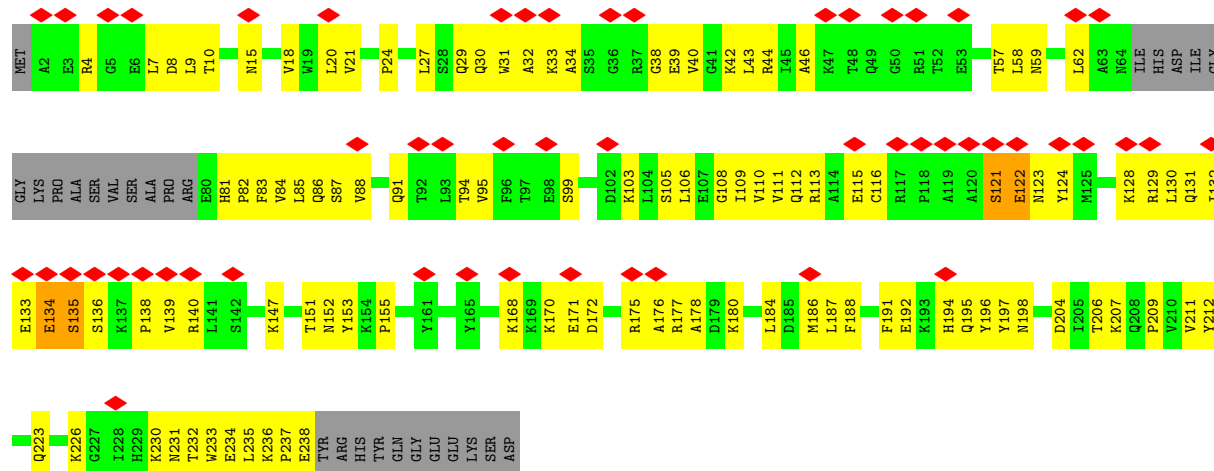
• Molecule 23: General transcription factor IIF subunit 1

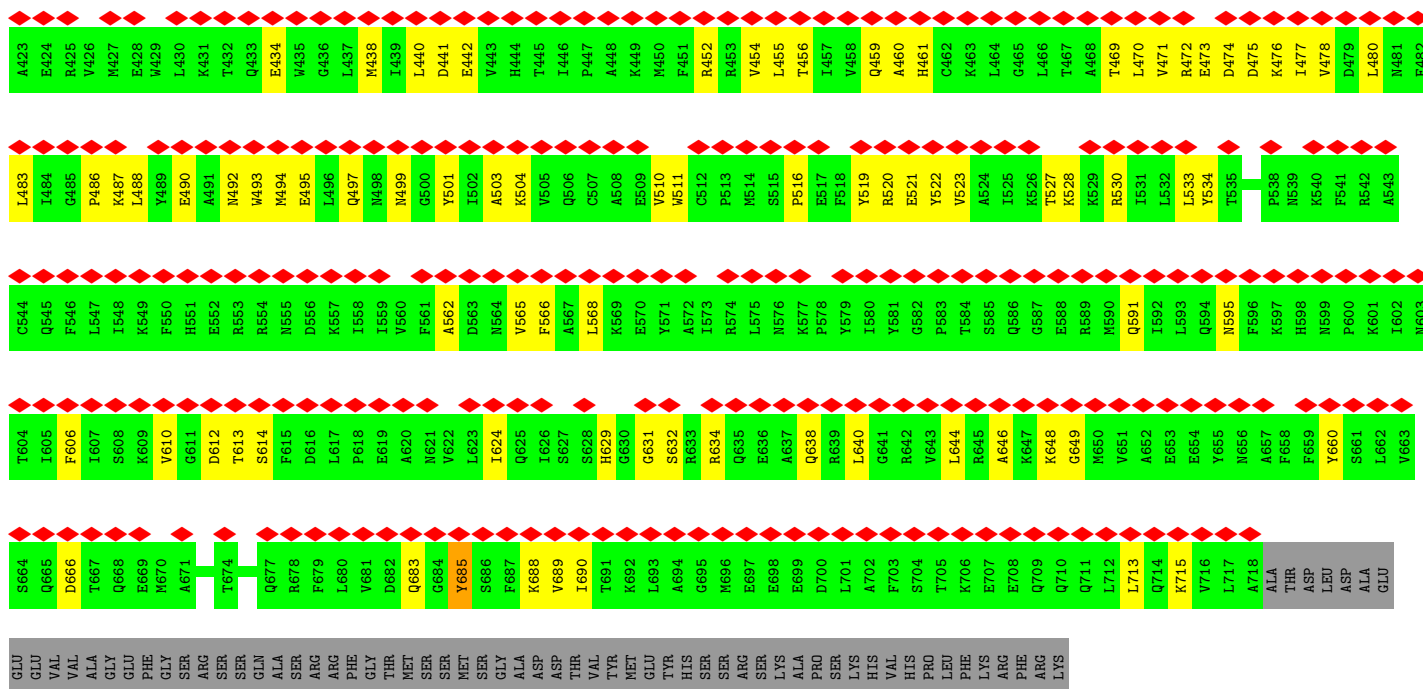
Chain S: 



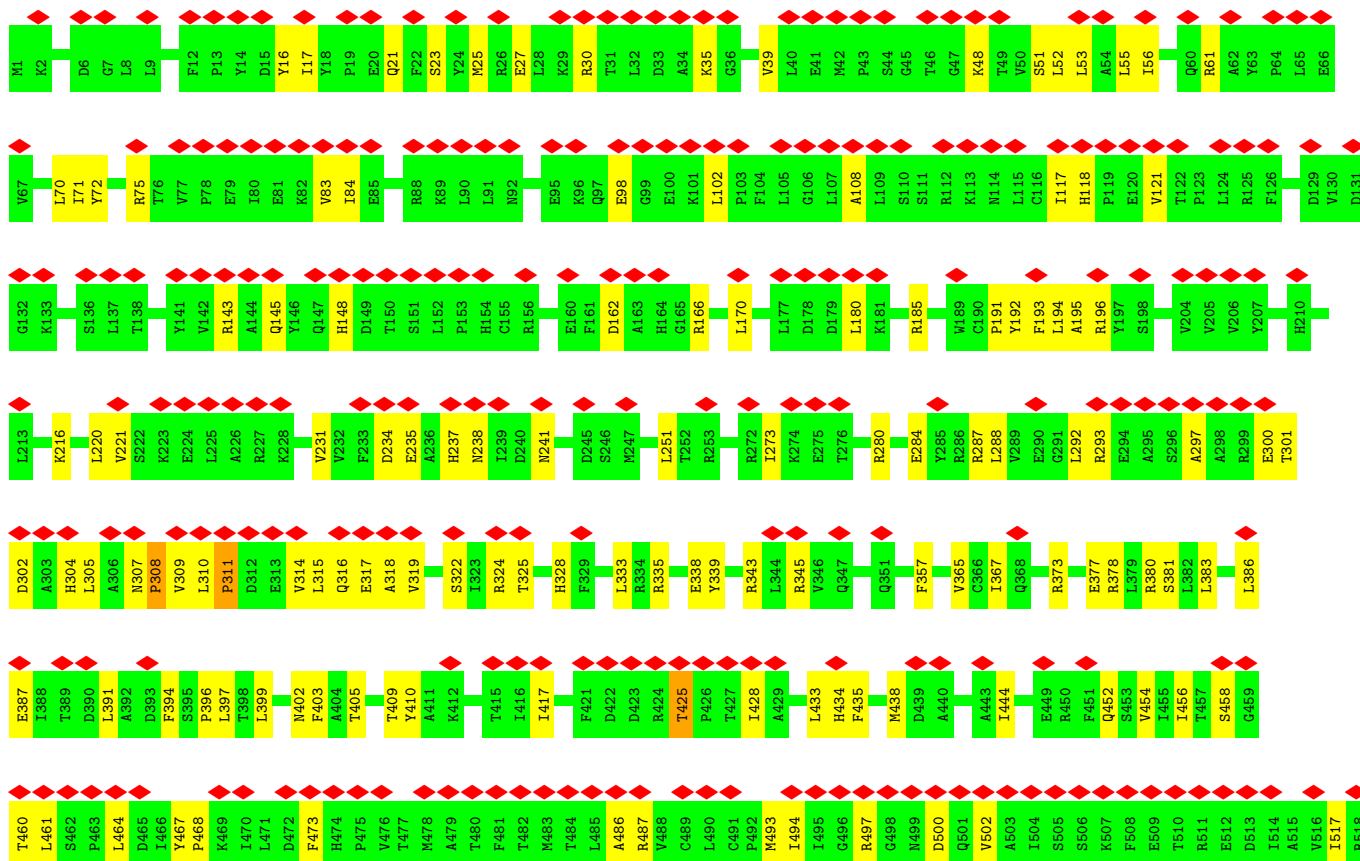
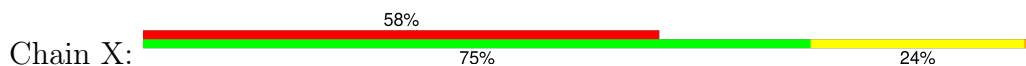
• Molecule 24: General transcription factor IIF subunit 2

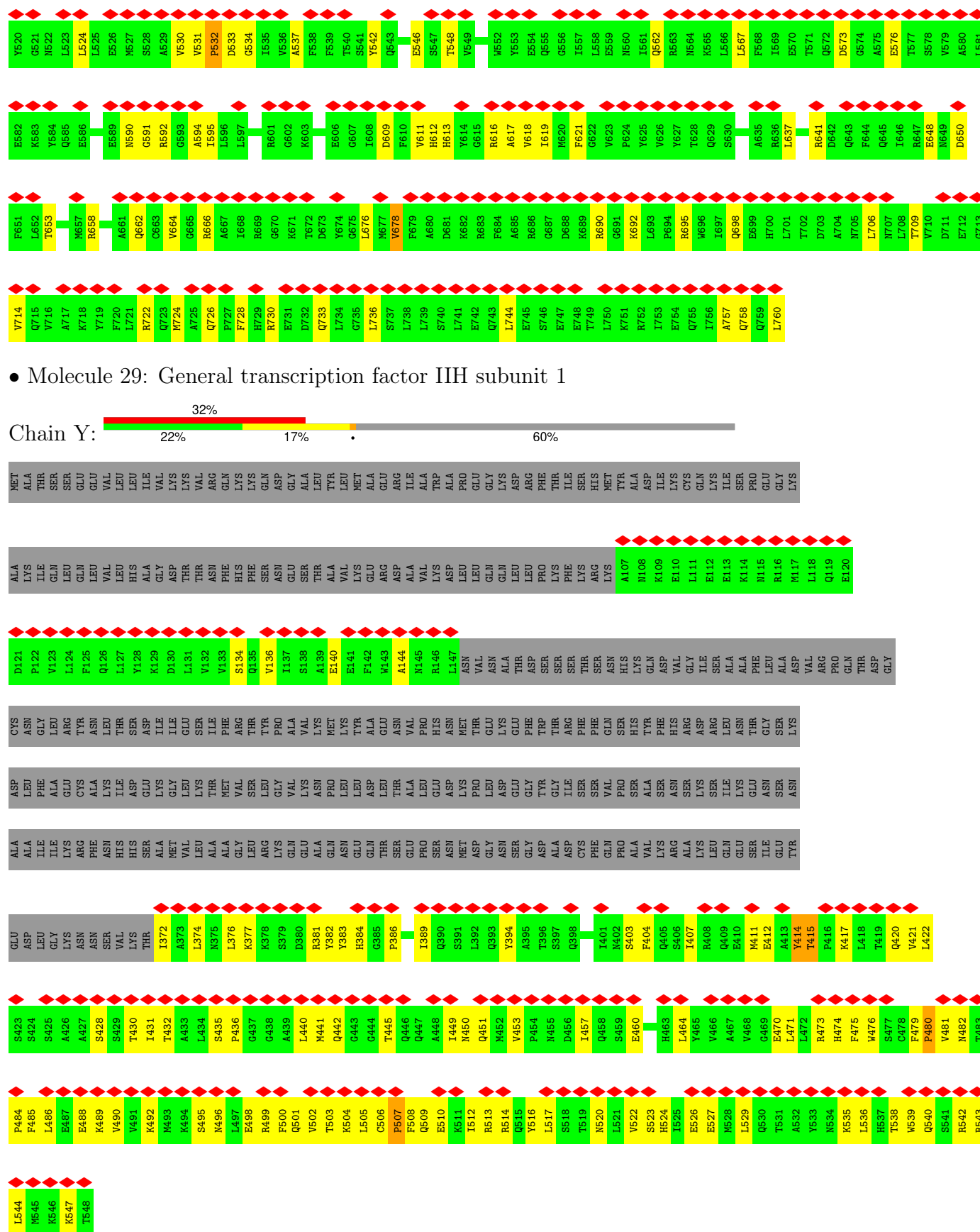
Chain T: 





• Molecule 28: TFIID basal transcription factor complex helicase XPD subunit

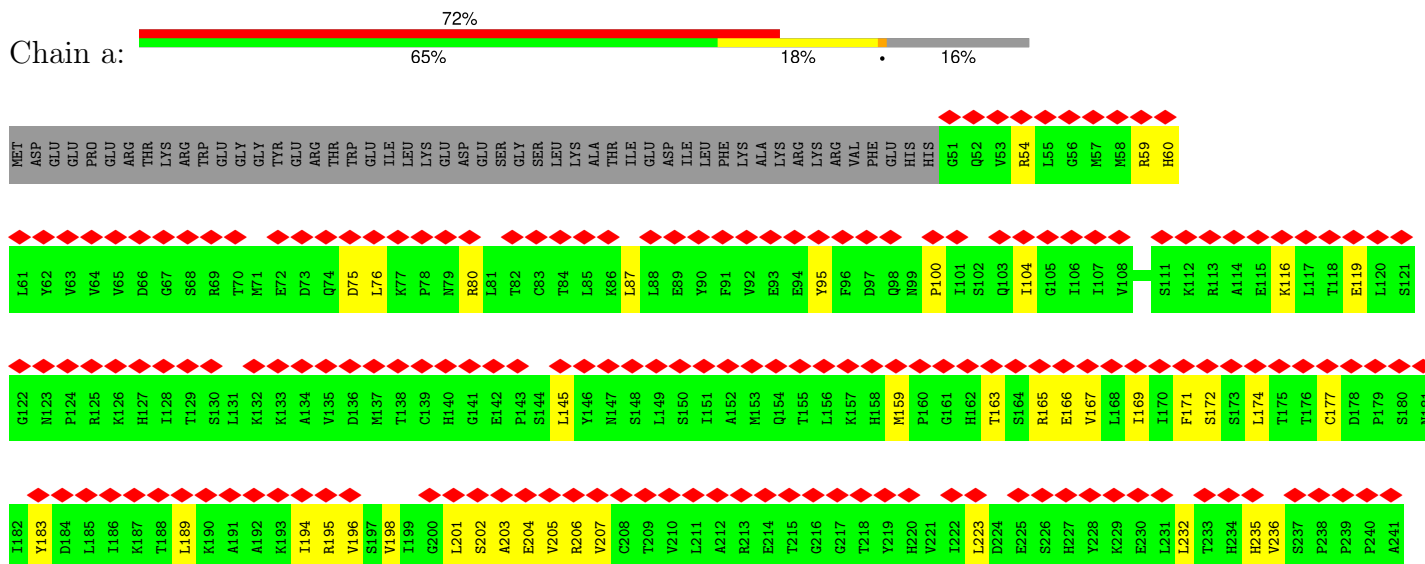


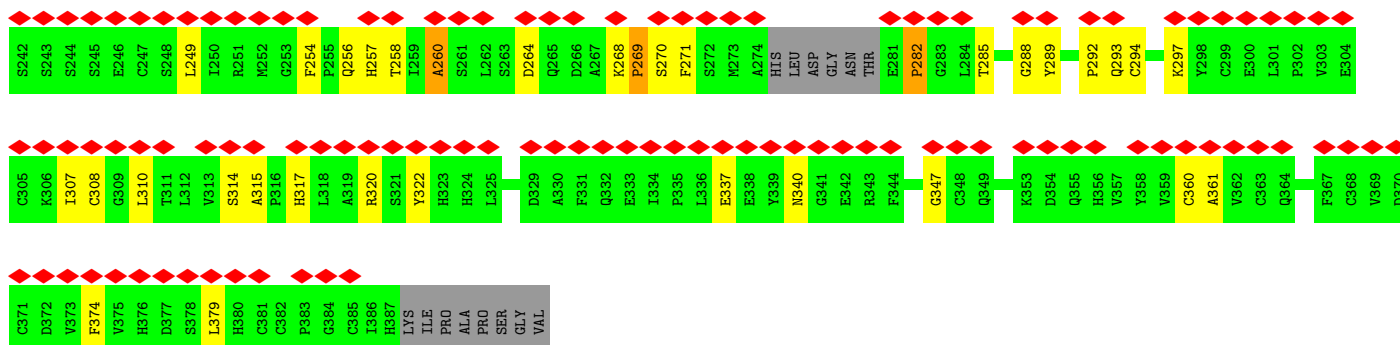


Chain Z:

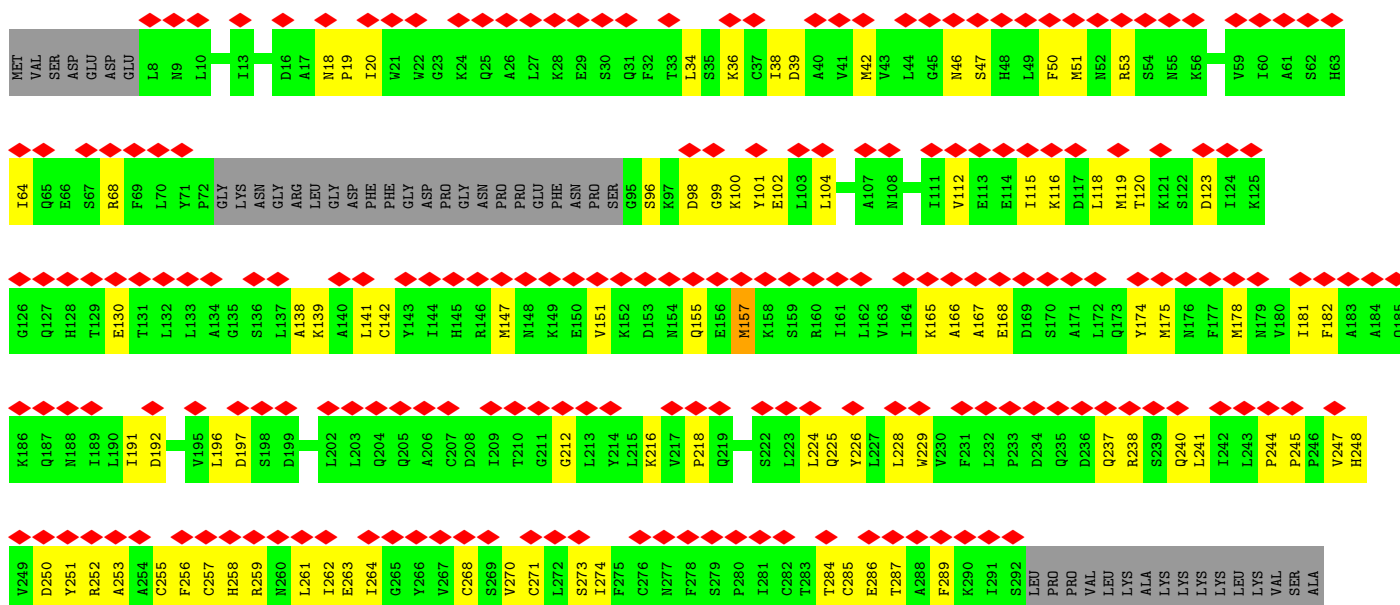


Chain a:

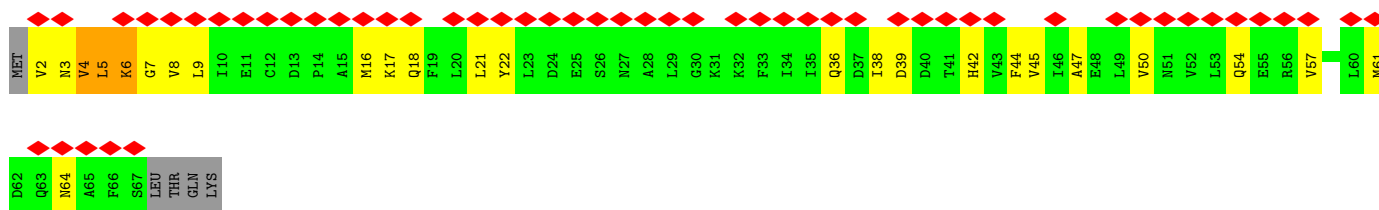
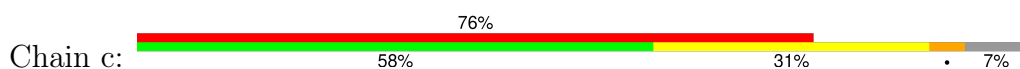




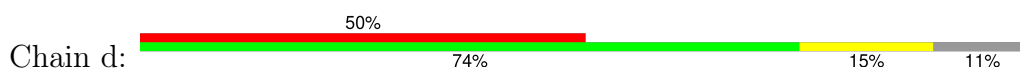
• Molecule 32: General transcription factor IIH subunit 3

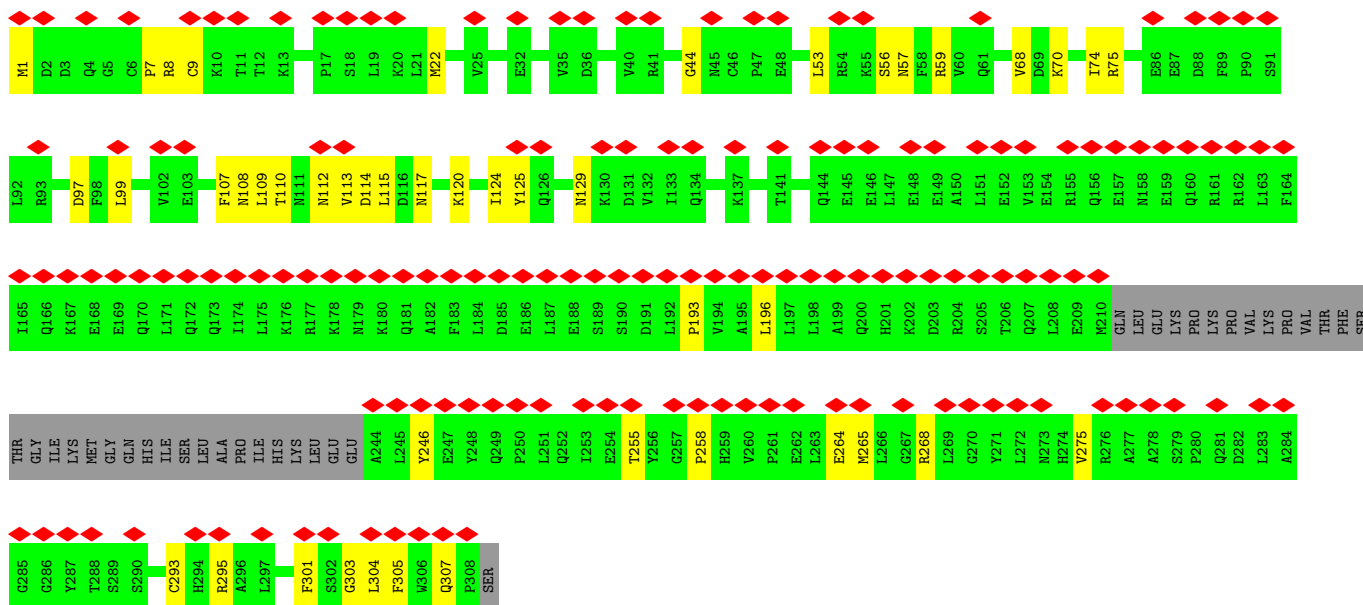


• Molecule 33: General transcription factor IIH subunit 5



• Molecule 34: CDK-activating kinase assembly factor MAT1

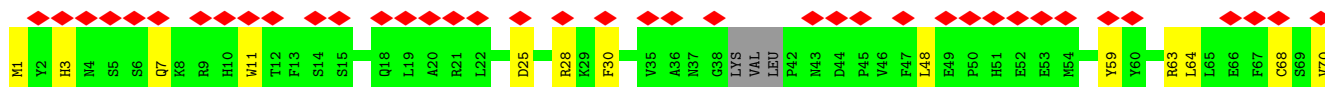


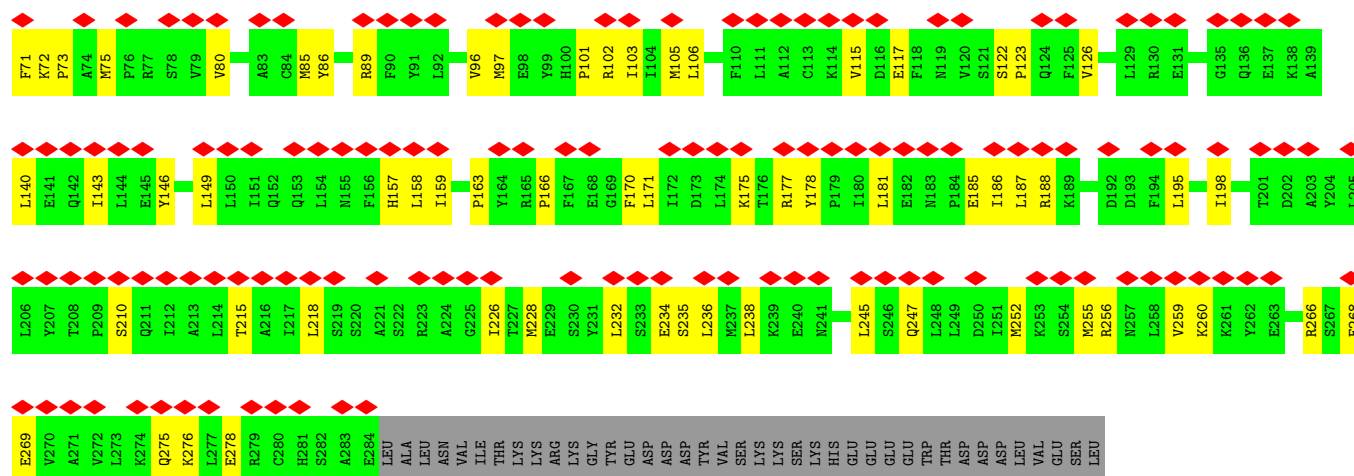


- Molecule 35: Cyclin-dependent kinase 7



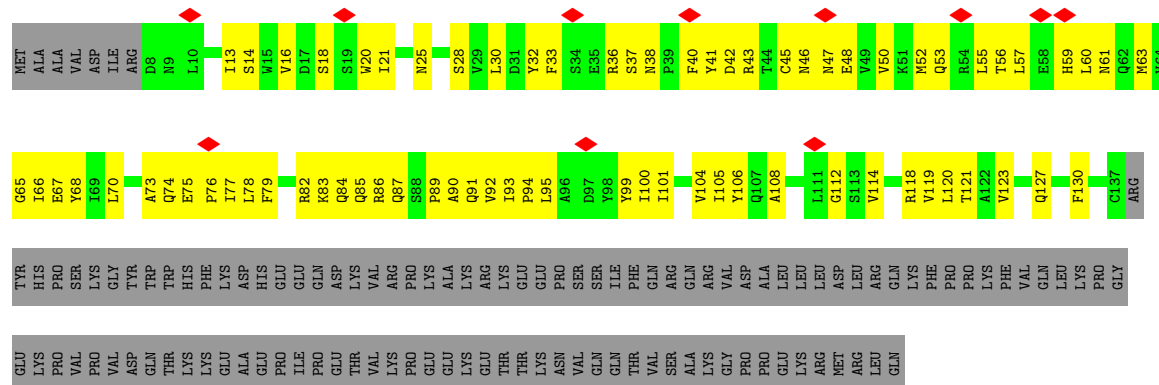
- Molecule 36: Cyclin-H





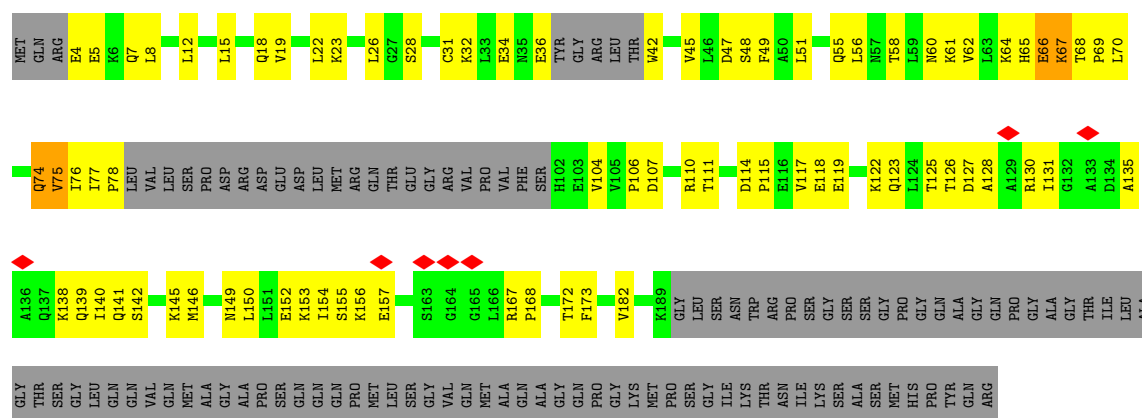
• Molecule 37: Mediator of RNA polymerase II transcription subunit 6

Chain g: 23% 30% 47%

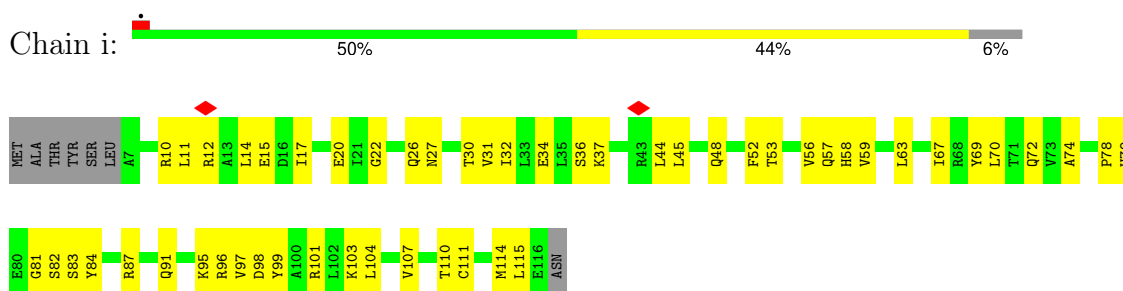


• Molecule 38: Mediator of RNA polymerase II transcription subunit 8

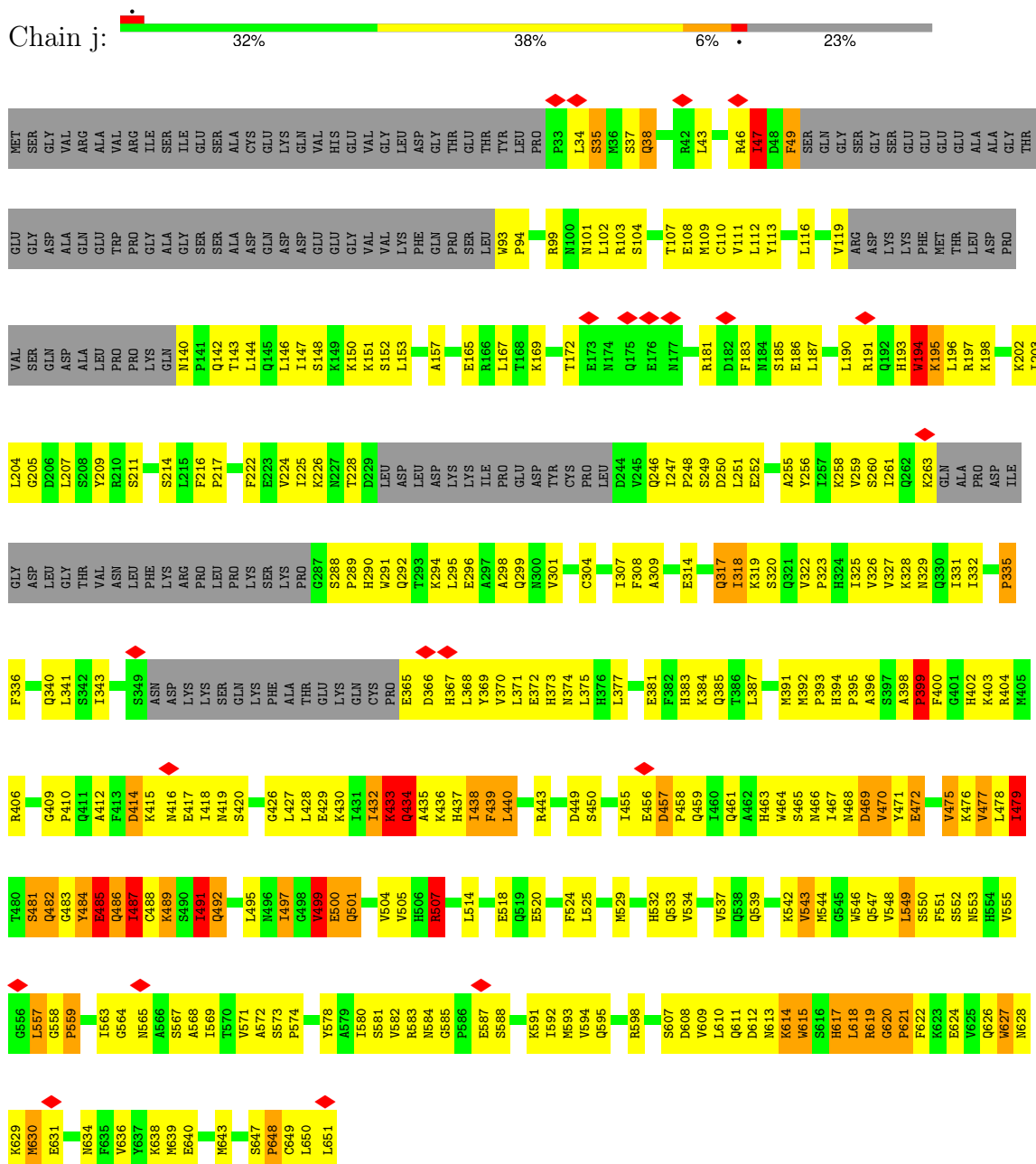
Chain h: 29% 28% 41%



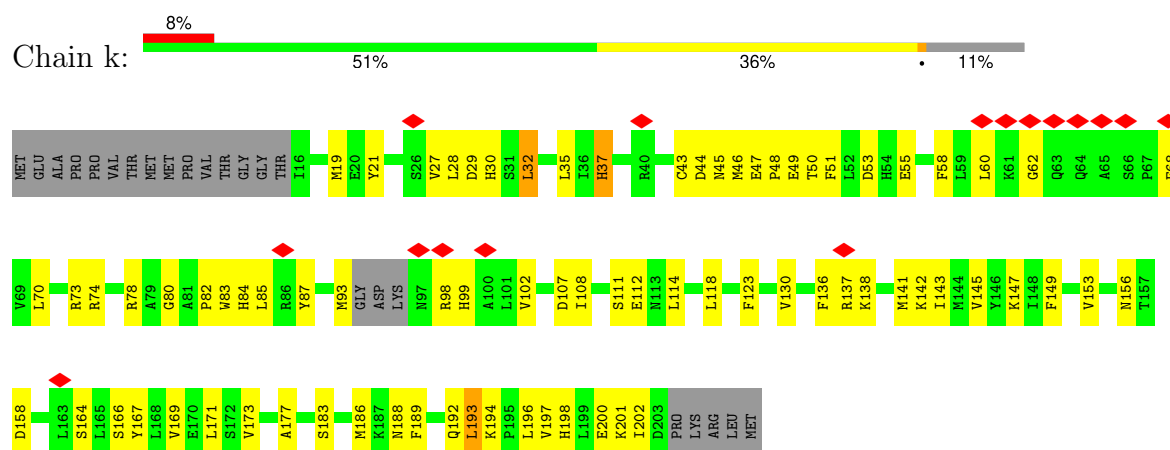
• Molecule 39: Mediator of RNA polymerase II transcription subunit 11



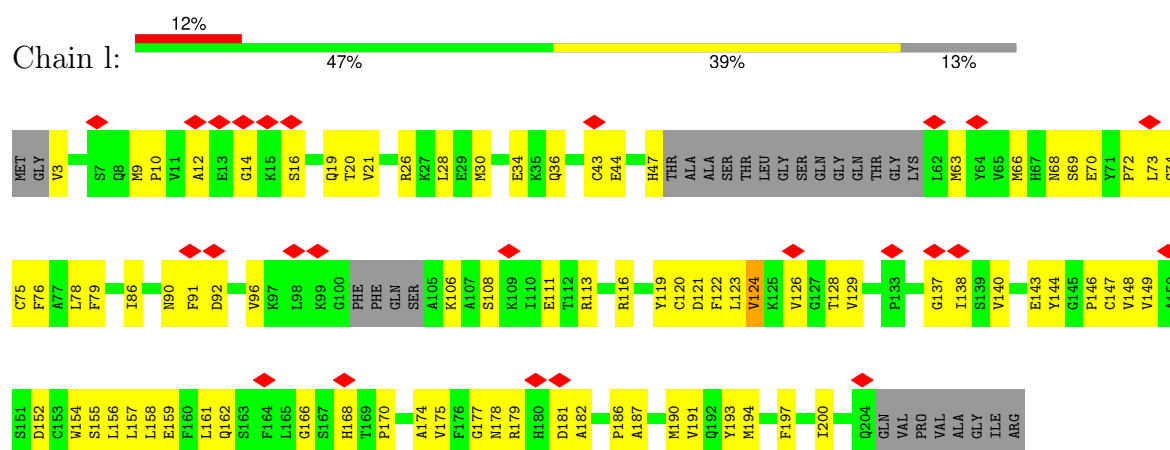
- Molecule 40: Mediator of RNA polymerase II transcription subunit 17



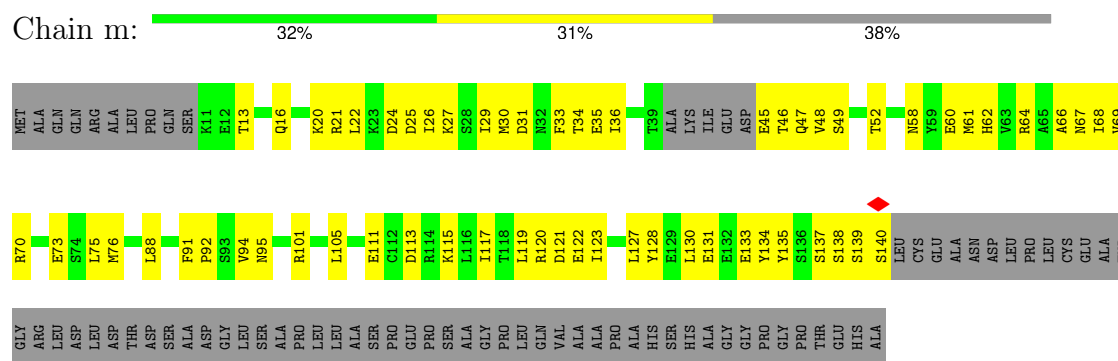
- Molecule 41: Mediator of RNA polymerase II transcription subunit 18



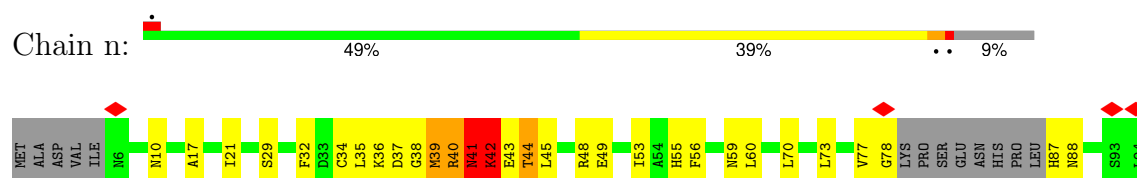
- Molecule 42: Mediator of RNA polymerase II transcription subunit 20



- Molecule 43: Mediator of RNA polymerase II transcription subunit 22

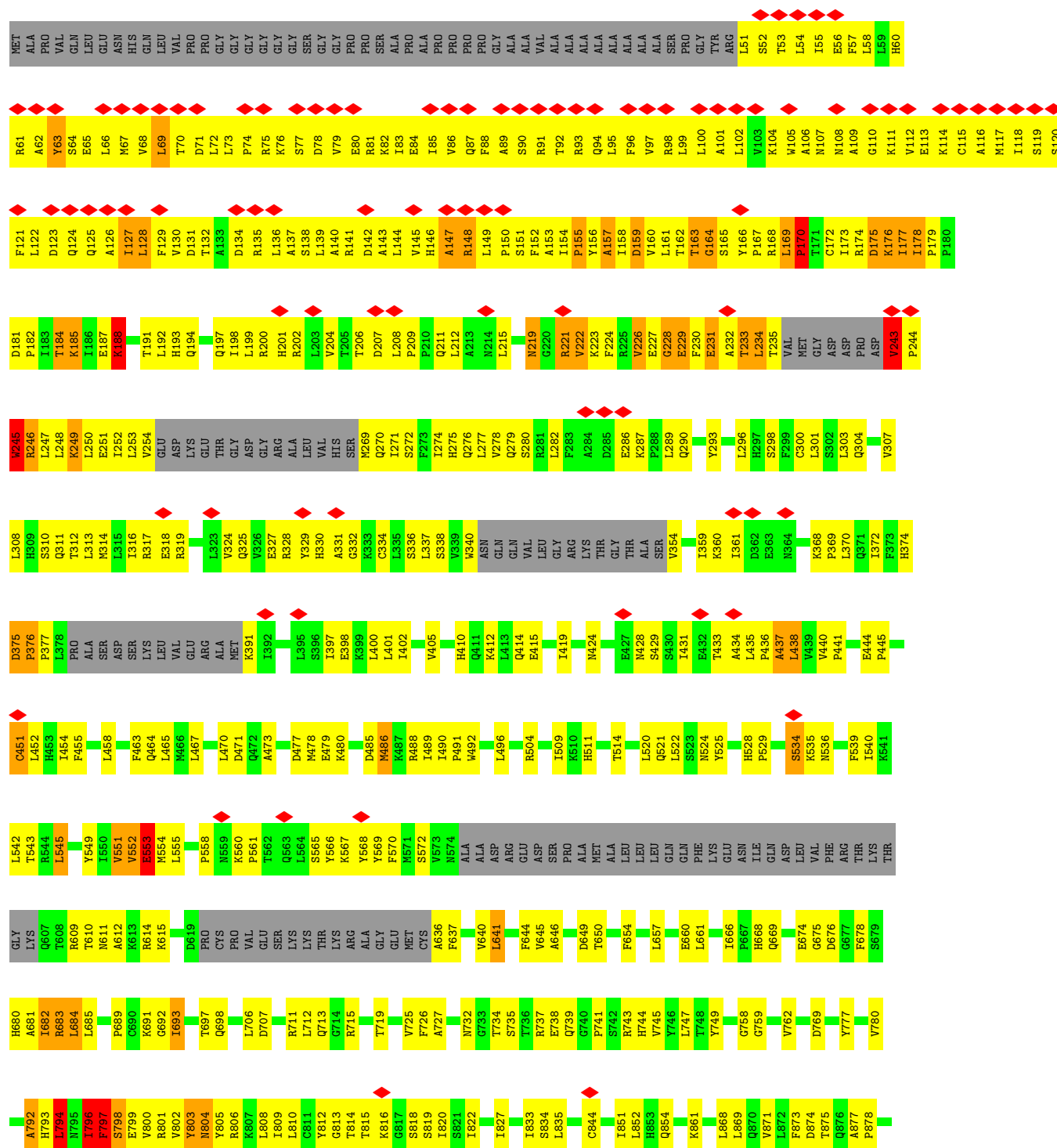


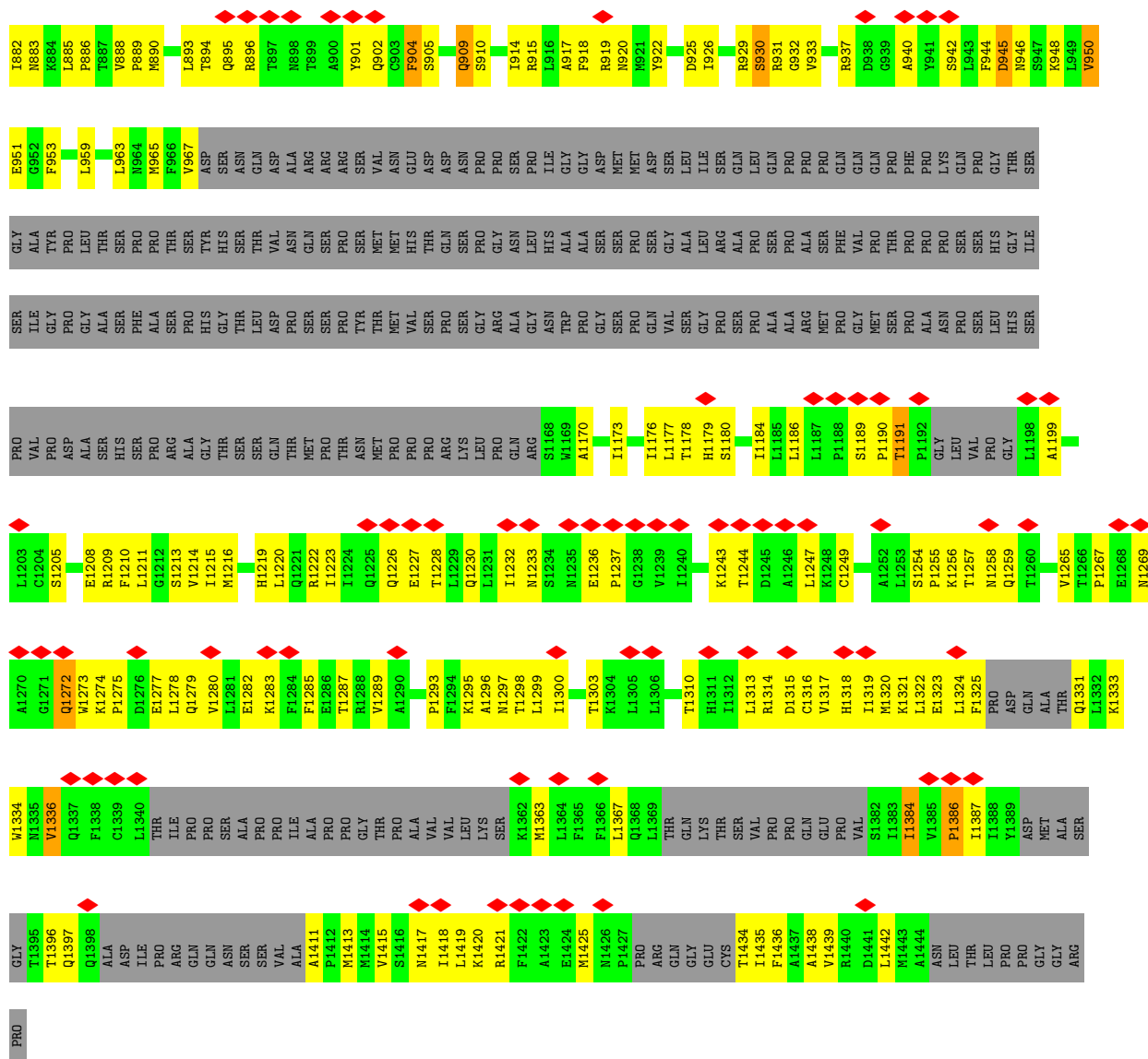
- Molecule 44: Mediator of RNA polymerase II transcription subunit 27



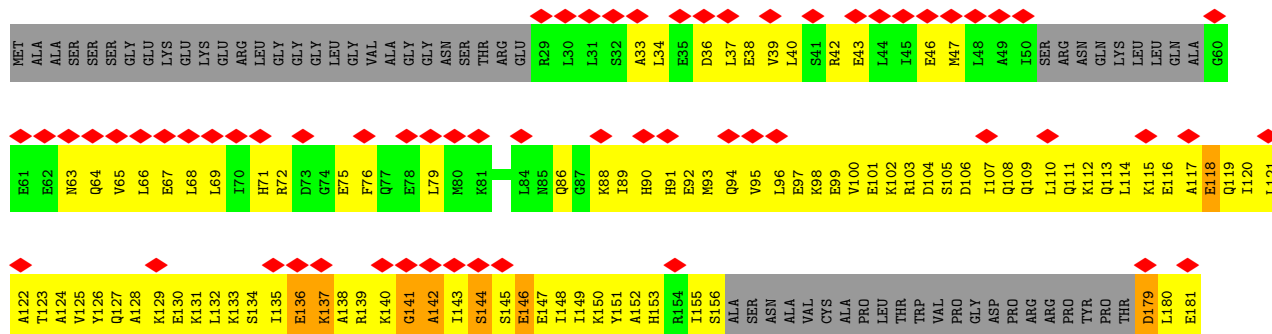


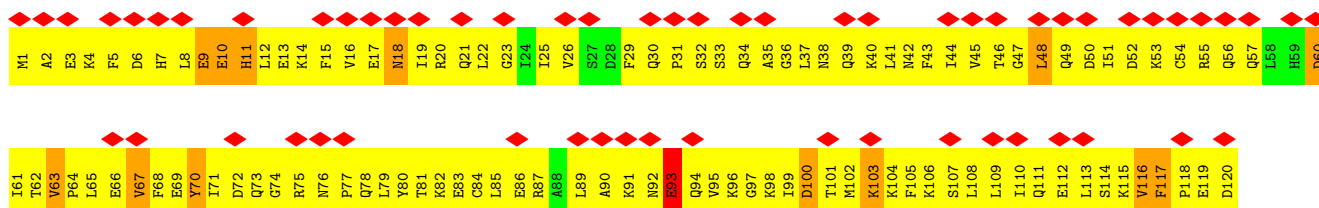
• Molecule 48: Mediator of RNA polymerase II transcription subunit 14

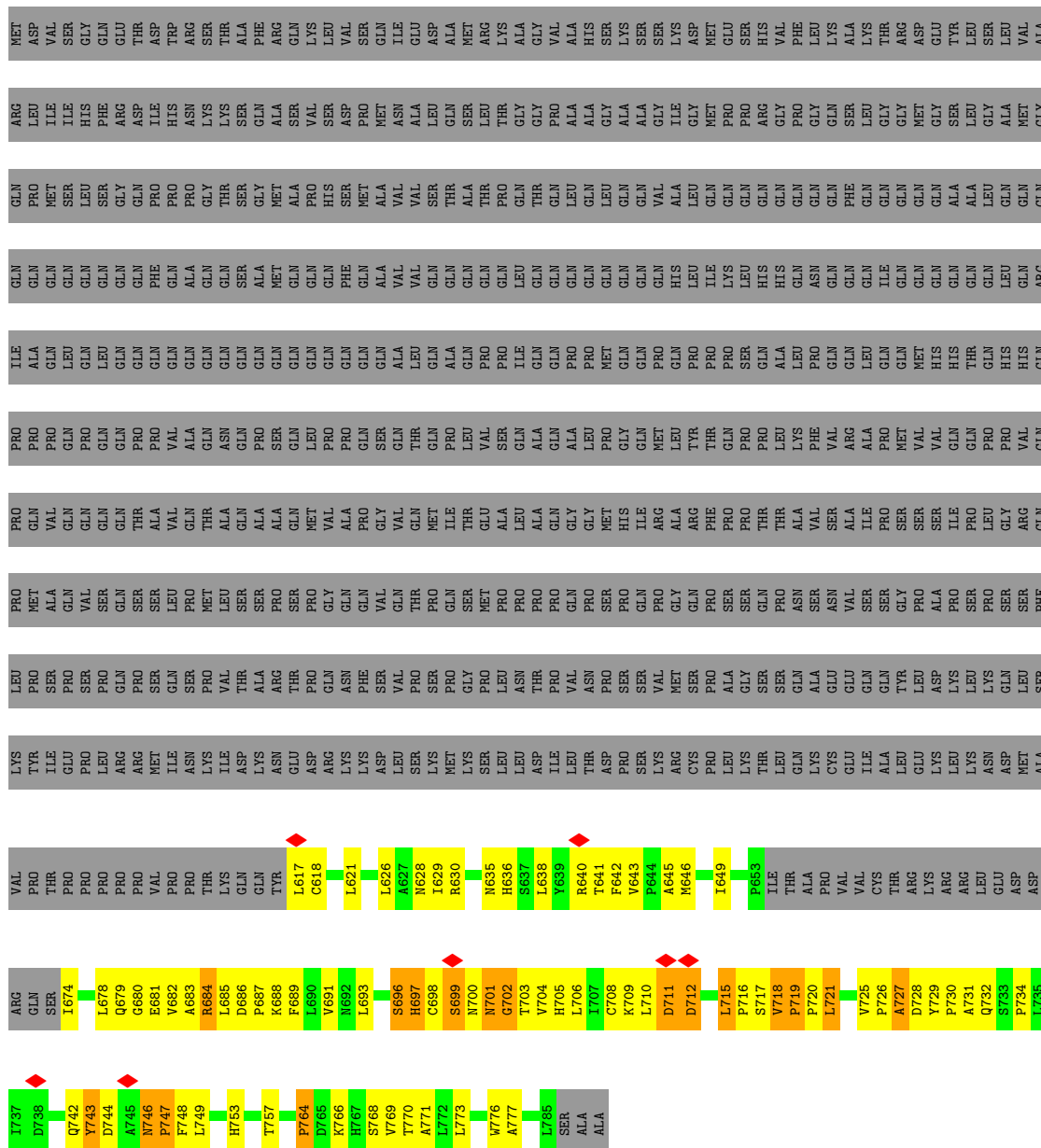




• Molecule 49: Mediator of RNA polymerase II transcription subunit 4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156383	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31.5	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	2.116	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, 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	0.70	18/5990 (0.3%)	0.75	13/8137 (0.2%)
2	1	0.35	0/10913	0.51	0/14828
3	2	0.48	9/7141 (0.1%)	0.59	2/9672 (0.0%)
4	3	0.74	4/1540 (0.3%)	0.73	2/2093 (0.1%)
5	A	0.33	0/11733	0.63	15/15844 (0.1%)
6	B	0.33	0/9310	0.50	2/12567 (0.0%)
7	C	0.34	0/2190	0.52	0/2975
8	D	0.22	0/1077	0.54	1/1446 (0.1%)
9	E	0.28	0/1753	0.50	0/2368
10	F	0.31	0/700	0.48	0/946
11	G	0.27	0/1382	0.53	0/1874
12	H	0.31	0/1227	0.53	0/1654
13	I	0.27	0/964	0.62	2/1305 (0.2%)
14	J	0.36	0/542	0.50	0/730
15	K	0.31	0/947	0.48	0/1282
16	L	0.28	0/394	0.61	0/524
17	M	0.21	0/945	0.60	1/1274 (0.1%)
18	N	0.22	0/816	0.52	0/1105
19	O	0.27	0/2049	0.54	0/2769
20	P	0.22	0/1489	0.47	0/2005
21	Q	0.23	0/1545	0.58	0/2075
22	R	0.22	0/1380	0.57	0/1854
23	S	0.23	0/1086	0.65	1/1461 (0.1%)
24	T	0.23	0/1817	0.61	1/2445 (0.0%)
25	U	0.25	0/1485	0.32	0/2293
26	V	0.26	0/1454	0.35	0/2239
27	W	0.35	0/4744	0.65	1/6402 (0.0%)
28	X	0.40	0/6236	0.73	2/8444 (0.0%)
29	Y	0.35	0/1660	0.79	5/2253 (0.2%)
30	Z	0.38	1/3552 (0.0%)	0.71	5/4814 (0.1%)
31	a	0.38	0/2637	0.67	2/3572 (0.1%)
32	b	0.35	0/2102	0.57	0/2844

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.33	0/528	0.71	0/713
34	d	0.30	0/2137	0.59	0/2890
35	e	0.34	0/2434	0.56	2/3300 (0.1%)
36	f	0.34	0/2342	0.45	0/3159
37	g	0.26	0/1058	0.53	0/1441
38	h	0.32	0/1245	0.60	0/1679
39	i	0.35	0/869	0.53	0/1168
40	j	0.94	32/4079 (0.8%)	0.92	17/5504 (0.3%)
41	k	0.37	0/1512	0.61	0/2034
42	l	0.35	0/1453	0.58	0/1963
43	m	0.41	0/1032	0.57	0/1385
44	n	0.58	2/2324 (0.1%)	0.73	5/3143 (0.2%)
45	o	0.39	0/897	0.59	0/1208
46	p	0.42	0/906	0.48	0/1222
47	q	0.41	0/1015	0.59	0/1360
48	r	0.72	11/8336 (0.1%)	0.89	32/11299 (0.3%)
49	s	0.99	1/1089 (0.1%)	1.05	2/1450 (0.1%)
50	t	1.22	1/991 (0.1%)	1.25	6/1331 (0.5%)
51	u	0.50	0/504	0.71	1/668 (0.1%)
52	v	1.04	3/1082 (0.3%)	1.09	5/1450 (0.3%)
53	w	0.89	0/311	1.02	0/412
54	x	1.22	0/858	1.28	8/1161 (0.7%)
55	y	1.23	3/1027 (0.3%)	1.16	6/1379 (0.4%)
56	z	1.14	8/1202 (0.7%)	1.29	11/1650 (0.7%)
All	All	0.50	93/132031 (0.1%)	0.67	150/179063 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	4
3	2	0	5
4	3	0	2
5	A	0	1
6	B	0	3
7	C	0	1
8	D	0	2
13	I	0	2
17	M	0	1
19	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
23	S	0	1
27	W	0	3
28	X	0	3
29	Y	0	1
30	Z	0	2
31	a	0	2
34	d	0	1
37	g	0	1
38	h	0	1
39	i	0	1
40	j	0	9
44	n	0	4
45	o	0	2
48	r	0	13
49	s	0	5
50	t	0	3
52	v	0	1
53	w	0	4
54	x	0	5
55	y	0	1
56	z	0	1
All	All	0	88

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	z	719	PRO	CA-C	-15.14	1.42	1.52
48	r	245	TRP	C-N	14.21	1.53	1.33
40	j	440	LEU	CA-C	-10.54	1.39	1.52
56	z	721	LEU	CA-C	-9.09	1.42	1.52
40	j	497	ILE	CA-C	-8.21	1.43	1.52

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	z	715	LEU	CA-C-N	23.33	149.00	119.84
56	z	715	LEU	C-N-CA	23.33	149.00	119.84
5	A	1623	SER	CA-C-N	19.00	139.04	119.85
5	A	1623	SER	C-N-CA	19.00	139.04	119.85
48	r	245	TRP	CA-C-N	-13.47	102.58	122.65

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	112	ASP	Peptide
1	0	170	LEU	Peptide
1	0	569	LEU	Peptide
1	0	732	LEU	Peptide
3	2	597	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5864	0	5967	384	0
2	1	10636	0	10706	350	0
3	2	7007	0	7171	331	0
4	3	1504	0	1492	119	0
5	A	11519	0	11611	513	0
6	B	9129	0	9143	291	0
7	C	2147	0	2091	78	0
8	D	1062	0	1042	125	0
9	E	1723	0	1744	58	0
10	F	689	0	715	29	0
11	G	1351	0	1358	63	0
12	H	1205	0	1168	35	0
13	I	942	0	871	43	0
14	J	533	0	554	12	0
15	K	928	0	953	23	0
16	L	388	0	394	10	0
17	M	930	0	888	76	0
18	N	806	0	818	60	0
19	O	2018	0	2061	80	0
20	P	1462	0	1549	118	0
21	Q	1520	0	1520	110	0
22	R	1357	0	1381	86	0
23	S	1059	0	1036	65	0
24	T	1788	0	1819	119	0
25	U	1321	0	716	44	0
26	V	1300	0	718	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	W	4645	0	4692	485	0
28	X	6109	0	6137	223	0
29	Y	1631	0	1532	267	0
30	Z	3473	0	3511	450	0
31	a	2580	0	2550	147	0
32	b	2065	0	2096	302	0
33	c	522	0	526	173	0
34	d	2104	0	1946	37	0
35	e	2376	0	2402	109	0
36	f	2293	0	2315	65	0
37	g	1035	0	1023	84	0
38	h	1230	0	1236	106	0
39	i	863	0	869	116	0
40	j	4005	0	4053	659	0
41	k	1484	0	1488	142	0
42	l	1425	0	1409	159	0
43	m	1024	0	1000	260	0
44	n	2279	0	2285	206	0
45	o	887	0	880	103	0
46	p	893	0	900	99	0
47	q	1007	0	1044	172	0
48	r	8174	0	8275	803	0
49	s	1084	0	1118	231	0
50	t	975	0	1005	284	0
51	u	501	0	530	56	0
52	v	1067	0	1080	307	0
53	w	309	0	309	82	0
54	x	852	0	842	255	0
55	y	1003	0	991	311	0
56	z	1168	0	1162	233	0
57	A	2	0	0	0	0
58	A	2	0	0	0	0
58	B	1	0	0	0	0
58	C	1	0	0	0	0
58	I	2	0	0	0	0
58	J	1	0	0	0	0
58	L	1	0	0	0	0
58	O	1	0	0	0	0
58	Q	1	0	0	0	0
58	a	3	0	0	0	0
58	b	1	0	0	0	0
58	d	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	X	8	0	0	0	0
All	All	129277	0	128692	8213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

The worst 5 of 8213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:57:MET:HG2	32:b:51:MET:SD	1.28	1.71
27:W:85:PHE:HZ	30:Z:336:TYR:CD2	1.07	1.67
27:W:520:ARG:HA	33:c:22:TYR:CE1	1.19	1.64
27:W:85:PHE:CZ	30:Z:336:TYR:CD2	1.77	1.63
43:m:130:LEU:CB	47:q:160:MET:HE2	1.23	1.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	740/841 (88%)	619 (84%)	114 (15%)	7 (1%)	14	49
2	1	1313/1368 (96%)	1201 (92%)	108 (8%)	4 (0%)	36	71
3	2	885/989 (90%)	774 (88%)	105 (12%)	6 (1%)	18	55
4	3	189/747 (25%)	167 (88%)	22 (12%)	0	100	100
5	A	1443/1970 (73%)	1316 (91%)	119 (8%)	8 (1%)	21	58
6	B	1134/1174 (97%)	1028 (91%)	103 (9%)	3 (0%)	36	71
7	C	263/275 (96%)	240 (91%)	23 (9%)	0	100	100
8	D	127/142 (89%)	114 (90%)	12 (9%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	208/210 (99%)	190 (91%)	18 (9%)	0	100	100
10	F	84/127 (66%)	80 (95%)	4 (5%)	0	100	100
11	G	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
12	H	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	18	55
13	I	114/125 (91%)	95 (83%)	18 (16%)	1 (1%)	14	49
14	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
15	K	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
16	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
17	M	109/376 (29%)	91 (84%)	18 (16%)	0	100	100
18	N	97/109 (89%)	83 (86%)	14 (14%)	0	100	100
19	O	256/316 (81%)	232 (91%)	21 (8%)	3 (1%)	10	42
20	P	183/339 (54%)	178 (97%)	5 (3%)	0	100	100
21	Q	180/439 (41%)	153 (85%)	25 (14%)	2 (1%)	11	45
22	R	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
23	S	123/517 (24%)	97 (79%)	25 (20%)	1 (1%)	16	52
24	T	218/249 (88%)	182 (84%)	33 (15%)	3 (1%)	9	39
27	W	568/782 (73%)	518 (91%)	49 (9%)	1 (0%)	43	78
28	X	758/760 (100%)	666 (88%)	92 (12%)	0	100	100
29	Y	214/548 (39%)	179 (84%)	35 (16%)	0	100	100
30	Z	432/462 (94%)	391 (90%)	39 (9%)	2 (0%)	24	63
31	a	327/395 (83%)	287 (88%)	40 (12%)	0	100	100
32	b	259/308 (84%)	244 (94%)	15 (6%)	0	100	100
33	c	64/71 (90%)	60 (94%)	4 (6%)	0	100	100
34	d	271/309 (88%)	236 (87%)	33 (12%)	2 (1%)	18	55
35	e	294/346 (85%)	277 (94%)	17 (6%)	0	100	100
36	f	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
37	g	128/246 (52%)	111 (87%)	17 (13%)	0	100	100
38	h	152/268 (57%)	133 (88%)	16 (10%)	3 (2%)	6	31
39	i	108/117 (92%)	103 (95%)	5 (5%)	0	100	100
40	j	492/651 (76%)	409 (83%)	72 (15%)	11 (2%)	5	28
41	k	181/208 (87%)	159 (88%)	22 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l	178/212 (84%)	150 (84%)	27 (15%)	1 (1%)	21	58
43	m	121/200 (60%)	118 (98%)	3 (2%)	0	100	100
44	n	277/311 (89%)	225 (81%)	46 (17%)	6 (2%)	5	28
45	o	106/178 (60%)	95 (90%)	9 (8%)	2 (2%)	6	32
46	p	110/200 (55%)	106 (96%)	4 (4%)	0	100	100
47	q	116/178 (65%)	107 (92%)	9 (8%)	0	100	100
48	r	1004/1454 (69%)	819 (82%)	165 (16%)	20 (2%)	6	31
49	s	129/270 (48%)	98 (76%)	27 (21%)	4 (3%)	3	21
50	t	110/233 (47%)	76 (69%)	32 (29%)	2 (2%)	6	33
51	u	54/146 (37%)	49 (91%)	5 (9%)	0	100	100
52	v	129/135 (96%)	92 (71%)	35 (27%)	2 (2%)	7	37
53	w	31/244 (13%)	21 (68%)	9 (29%)	1 (3%)	3	21
54	x	107/144 (74%)	81 (76%)	26 (24%)	0	100	100
55	y	112/131 (86%)	71 (63%)	36 (32%)	5 (4%)	2	17
56	z	145/788 (18%)	126 (87%)	14 (10%)	5 (3%)	3	20
All	All	15623/21786 (72%)	13748 (88%)	1768 (11%)	107 (1%)	20	55

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	170	LEU
1	0	570	ASN
3	2	687	PHE
5	A	1617	PRO
5	A	1620	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	666/736 (90%)	644 (97%)	22 (3%)	33	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	1187/1232 (96%)	1183 (100%)	4 (0%)	86	84
3	2	780/864 (90%)	775 (99%)	5 (1%)	78	81
4	3	165/601 (28%)	155 (94%)	10 (6%)	17	39
5	A	1285/1748 (74%)	1278 (100%)	7 (0%)	81	82
6	B	999/1028 (97%)	999 (100%)	0	100	100
7	C	244/252 (97%)	244 (100%)	0	100	100
8	D	119/126 (94%)	119 (100%)	0	100	100
9	E	192/192 (100%)	192 (100%)	0	100	100
10	F	74/111 (67%)	74 (100%)	0	100	100
11	G	152/153 (99%)	152 (100%)	0	100	100
12	H	131/131 (100%)	131 (100%)	0	100	100
13	I	104/112 (93%)	104 (100%)	0	100	100
14	J	56/56 (100%)	56 (100%)	0	100	100
15	K	105/106 (99%)	105 (100%)	0	100	100
16	L	43/55 (78%)	43 (100%)	0	100	100
17	M	105/324 (32%)	105 (100%)	0	100	100
18	N	90/98 (92%)	88 (98%)	2 (2%)	45	64
19	O	222/268 (83%)	222 (100%)	0	100	100
20	P	159/293 (54%)	159 (100%)	0	100	100
21	Q	167/373 (45%)	167 (100%)	0	100	100
22	R	150/261 (58%)	149 (99%)	1 (1%)	76	79
23	S	111/448 (25%)	111 (100%)	0	100	100
24	T	196/218 (90%)	196 (100%)	0	100	100
27	W	508/688 (74%)	497 (98%)	11 (2%)	45	64
28	X	661/664 (100%)	659 (100%)	2 (0%)	86	84
29	Y	162/484 (34%)	162 (100%)	0	100	100
30	Z	372/399 (93%)	365 (98%)	7 (2%)	50	66
31	a	296/352 (84%)	296 (100%)	0	100	100
32	b	234/272 (86%)	233 (100%)	1 (0%)	84	83
33	c	59/64 (92%)	54 (92%)	5 (8%)	10	29
34	d	210/283 (74%)	210 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	e	259/299 (87%)	259 (100%)	0	100	100
36	f	256/296 (86%)	256 (100%)	0	100	100
37	g	115/223 (52%)	115 (100%)	0	100	100
38	h	139/225 (62%)	139 (100%)	0	100	100
39	i	92/98 (94%)	92 (100%)	0	100	100
40	j	452/577 (78%)	426 (94%)	26 (6%)	18	40
41	k	164/183 (90%)	161 (98%)	3 (2%)	51	67
42	l	158/178 (89%)	157 (99%)	1 (1%)	78	81
43	m	118/173 (68%)	118 (100%)	0	100	100
44	n	256/280 (91%)	254 (99%)	2 (1%)	73	78
45	o	102/152 (67%)	102 (100%)	0	100	100
46	p	102/163 (63%)	102 (100%)	0	100	100
47	q	114/155 (74%)	114 (100%)	0	100	100
48	r	905/1271 (71%)	875 (97%)	30 (3%)	33	55
49	s	119/230 (52%)	118 (99%)	1 (1%)	73	78
50	t	110/216 (51%)	109 (99%)	1 (1%)	70	77
51	u	59/133 (44%)	58 (98%)	1 (2%)	53	68
52	v	119/124 (96%)	113 (95%)	6 (5%)	22	43
53	w	34/208 (16%)	33 (97%)	1 (3%)	37	58
54	x	92/119 (77%)	82 (89%)	10 (11%)	6	21
55	y	105/115 (91%)	93 (89%)	12 (11%)	5	19
56	z	135/697 (19%)	129 (96%)	6 (4%)	25	47
All	All	14009/19107 (73%)	13832 (99%)	177 (1%)	59	72

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	r	188	LYS
52	v	48	LEU
48	r	227	GLU
48	r	693	ILE
54	x	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 316 such sidechains are listed below:

Mol	Chain	Res	Type
40	j	517	GLN
49	s	64	GLN
40	j	617	HIS
45	o	105	GLN
54	x	27	GLN

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 19 ligands modelled in this entry, 18 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	$\# Z > 2$
59	SF4	X	1000	28	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
59	SF4	X	1000	28	-	-	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.

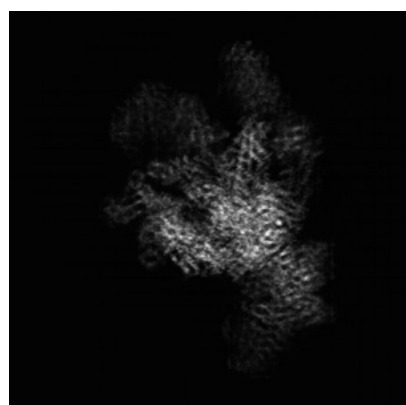
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23255. These allow visual inspection of the internal detail of the map and identification of artifacts.

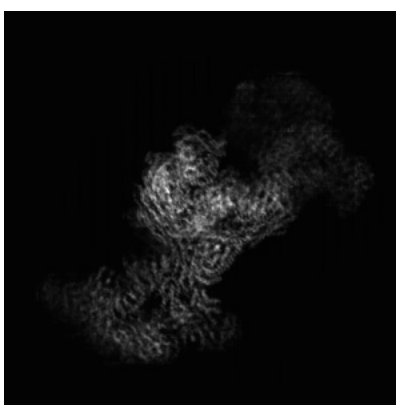
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

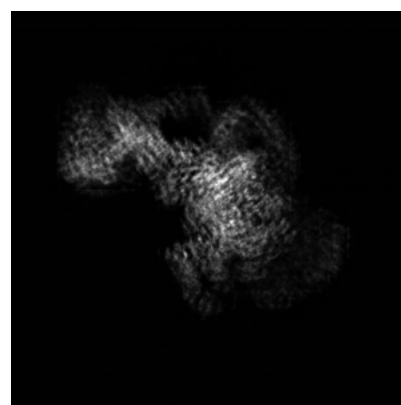
6.1.1 Primary map



X



Y

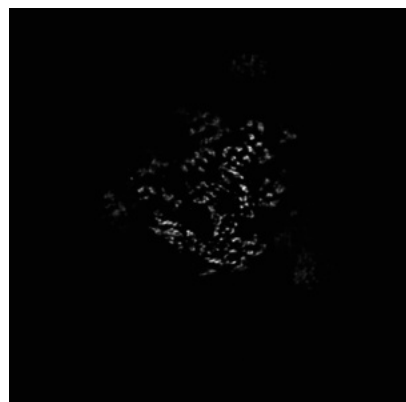


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210



Z Index: 210

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: 221



Y Index: 254

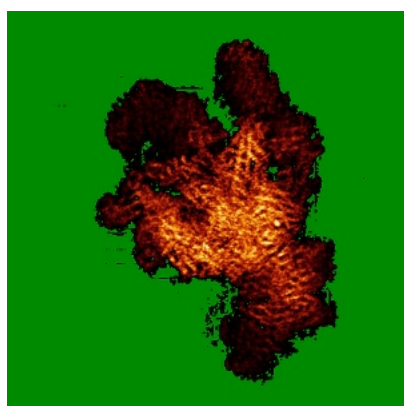


Z Index: 182

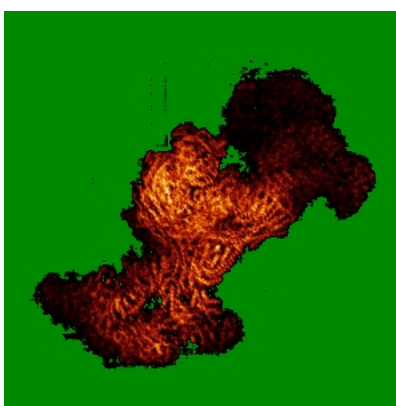
The images above show the largest variance slices of the map in three orthogonal directions.

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

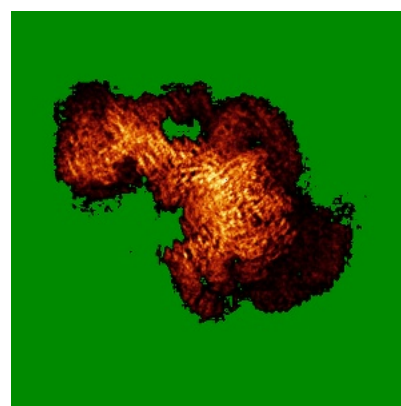
6.4.1 Primary map



X



Y

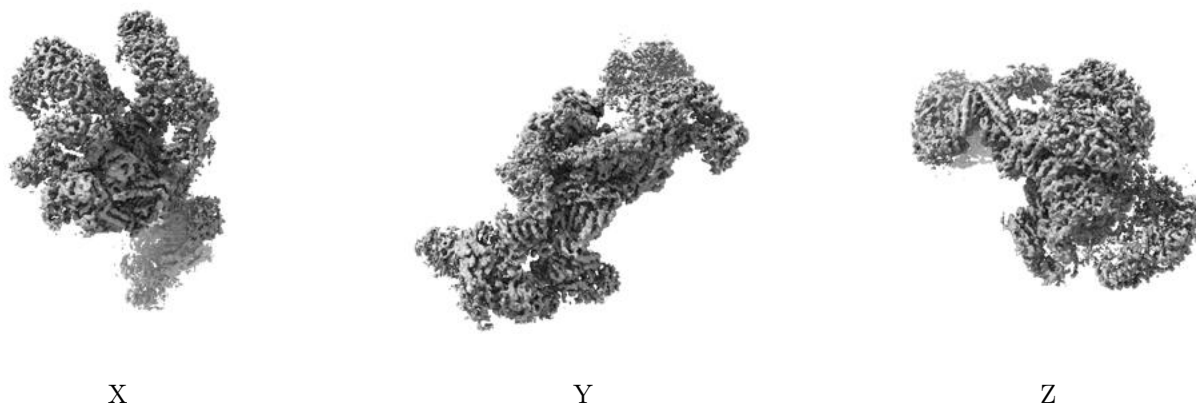


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

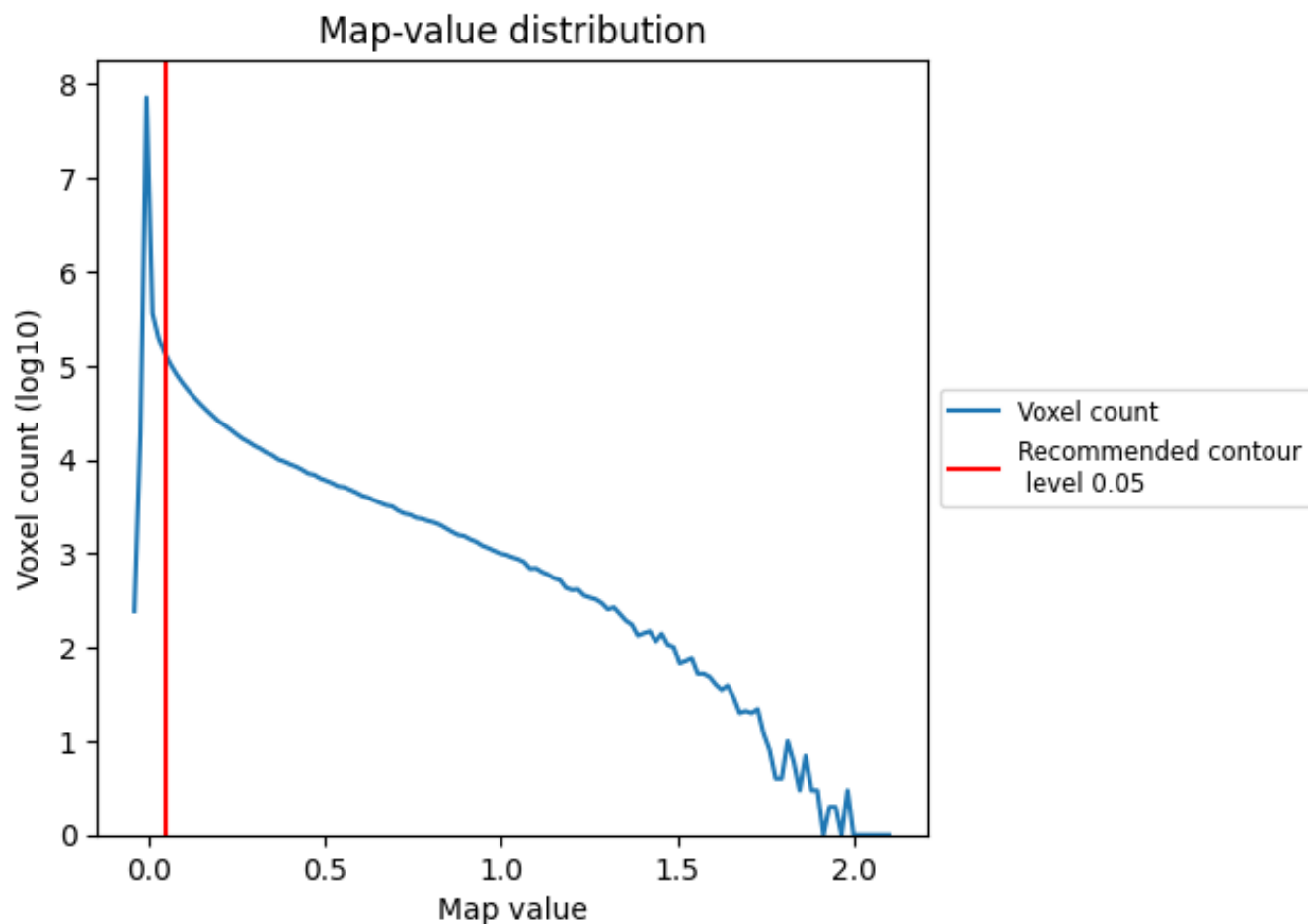
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

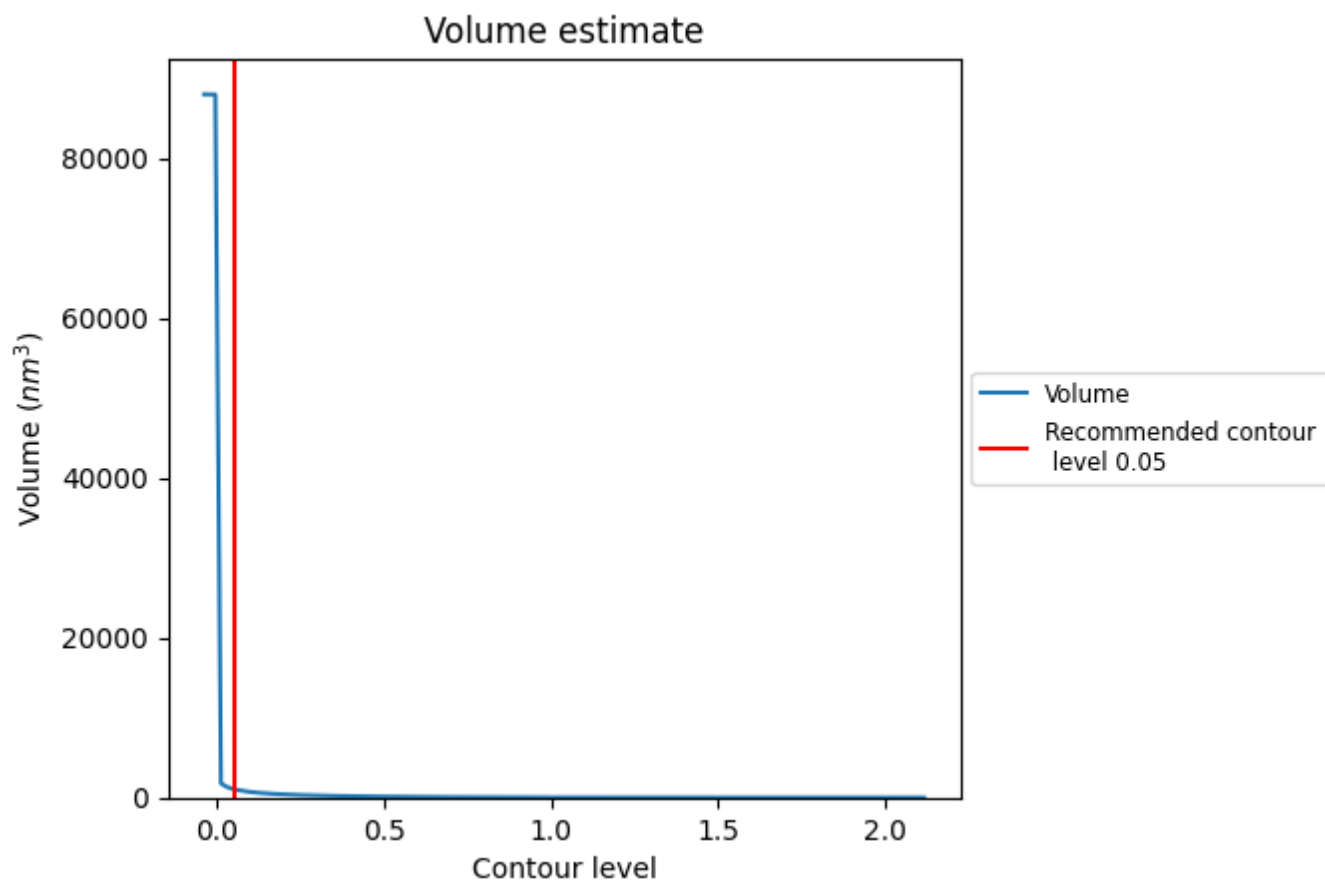
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

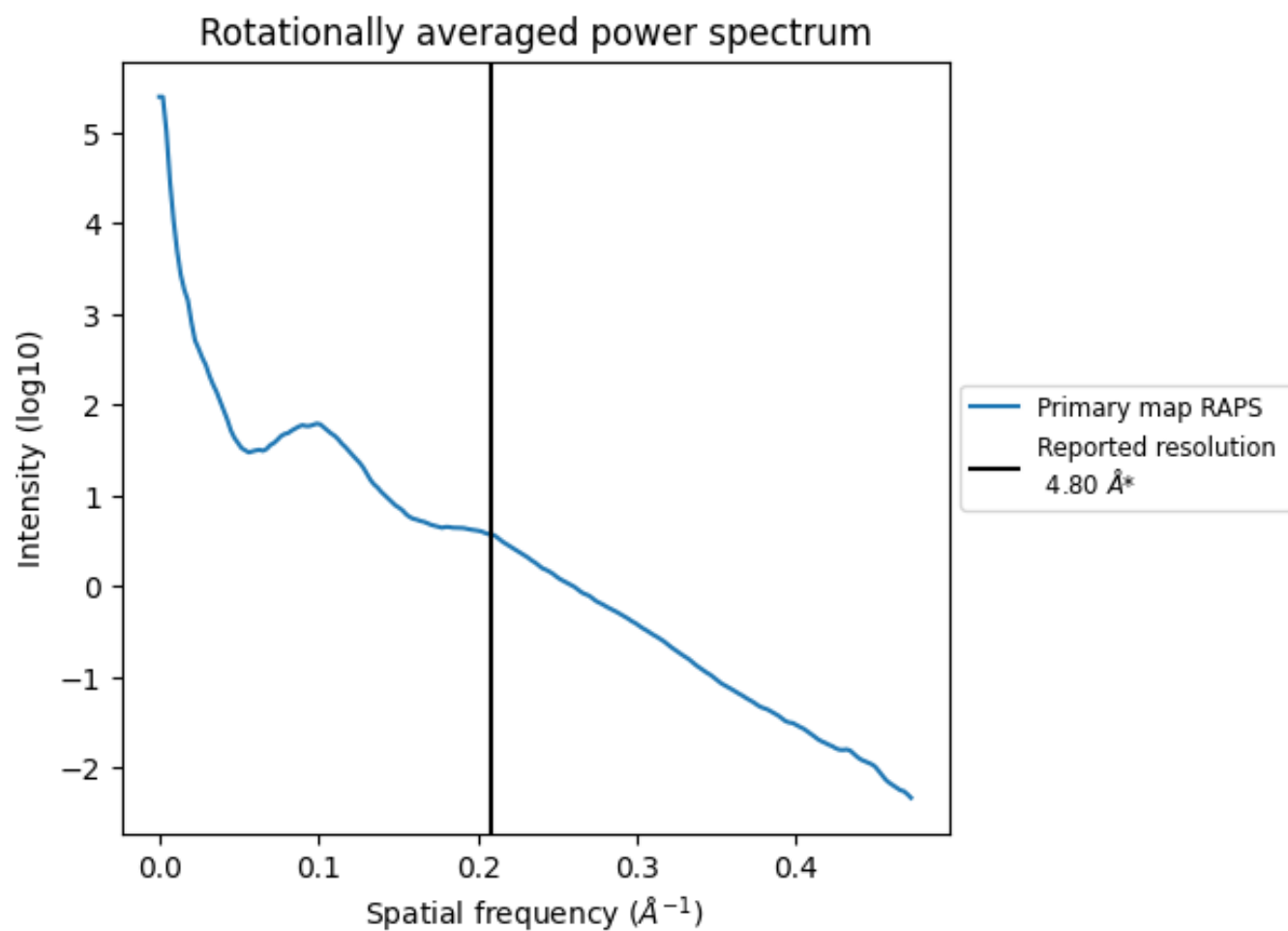
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1055 nm³; this corresponds to an approximate mass of 953 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

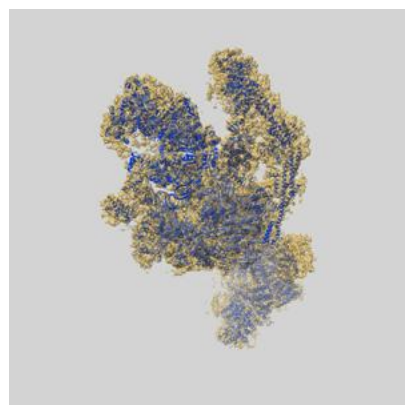
8 Fourier-Shell correlation ⓘ

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

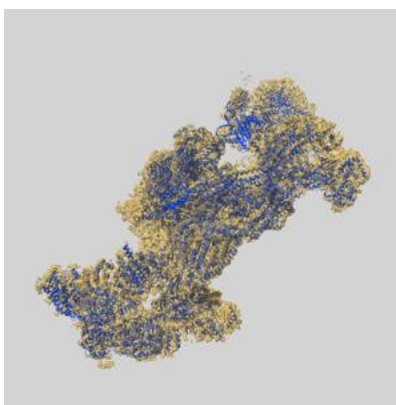
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23255 and PDB model 7LBM. Per-residue inclusion information can be found in section [3](#) on page [16](#).

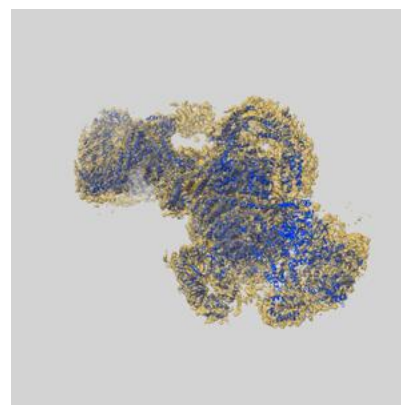
9.1 Map-model overlay [i](#)



X



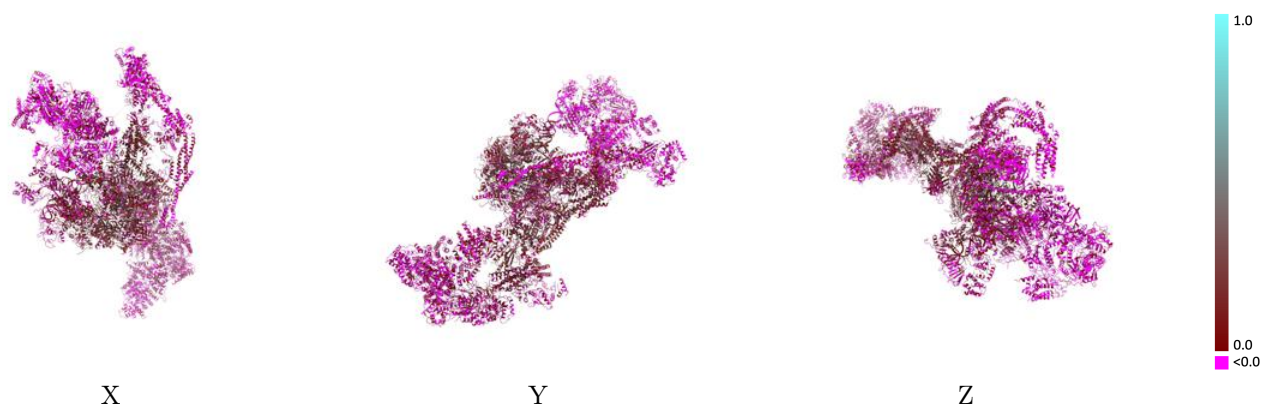
Y



Z

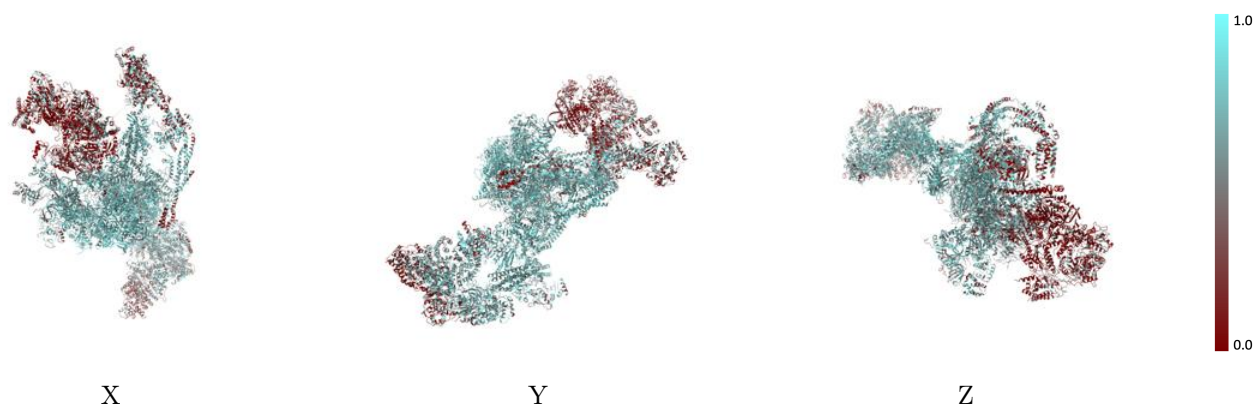
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



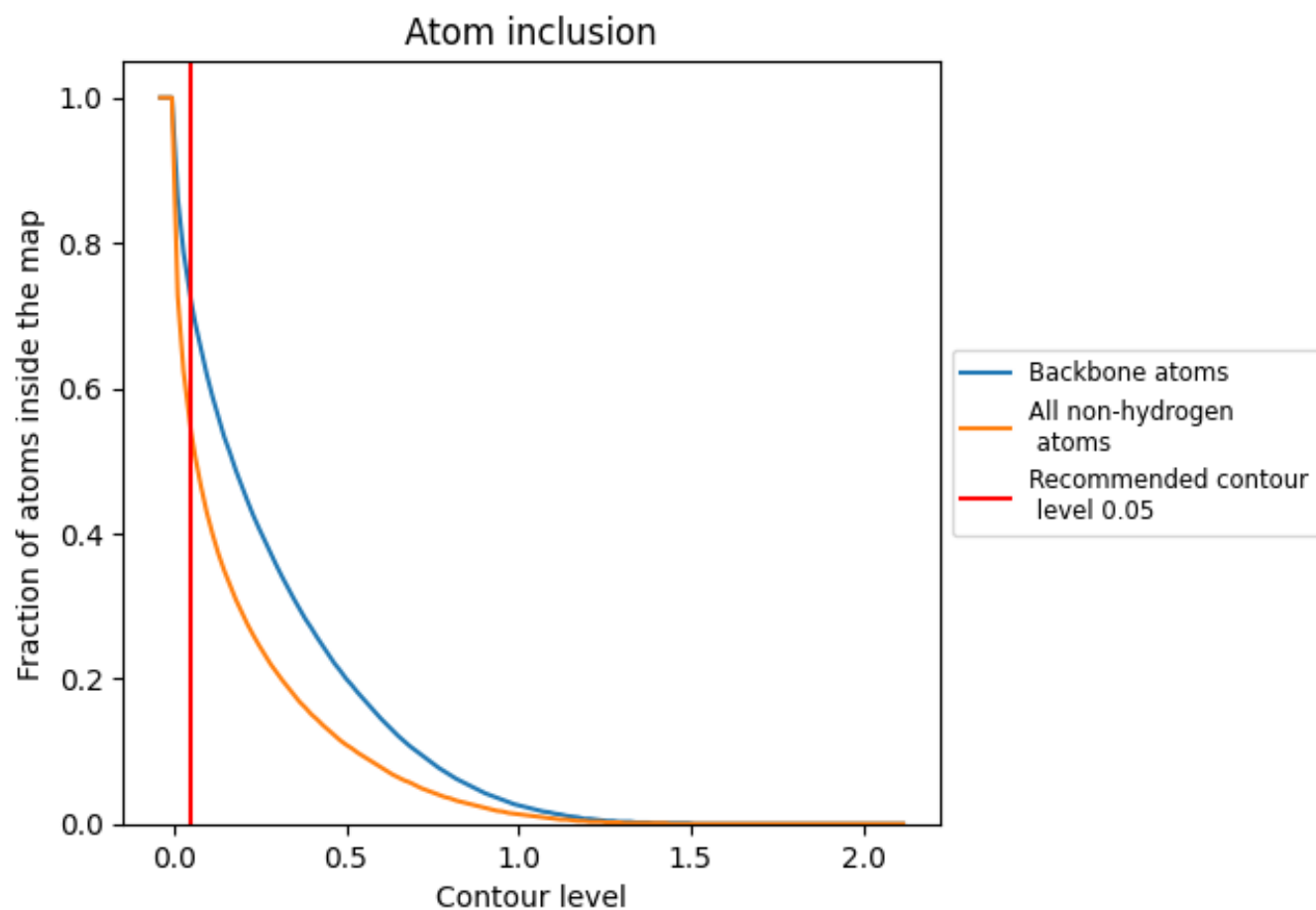
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 54% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5400	 0.0740
0	 0.6280	 0.0650
1	 0.4060	 -0.0060
2	 0.5140	 0.0300
3	 0.5240	 0.0330
A	 0.7150	 0.1930
B	 0.7240	 0.2010
C	 0.6720	 0.1450
D	 0.6640	 0.1400
E	 0.7060	 0.1630
F	 0.7070	 0.2010
G	 0.7280	 0.1730
H	 0.6740	 0.1380
I	 0.7120	 0.1510
J	 0.6810	 0.1180
K	 0.6870	 0.1510
L	 0.7020	 0.1860
M	 0.4900	 -0.0110
N	 0.4860	 0.0020
O	 0.6640	 0.1200
P	 0.6060	 0.0650
Q	 0.6220	 0.0780
R	 0.6070	 0.0470
S	 0.5410	 0.0520
T	 0.5720	 0.0580
U	 0.5970	 0.0640
V	 0.5890	 0.0520
W	 0.0960	 -0.0490
X	 0.3510	 -0.0060
Y	 0.2250	 -0.0660
Z	 0.1720	 -0.0670
a	 0.1290	 -0.0590
b	 0.2200	 -0.0550
c	 0.1850	 -0.0860
d	 0.3580	 -0.0120



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Chain	Atom inclusion	Q-score
e	 0.3920	 -0.0170
f	 0.3390	 -0.0590
g	 0.6910	 0.0790
h	 0.7060	 0.1450
i	 0.7250	 0.1740
j	 0.7350	 0.1960
k	 0.6540	 0.1170
l	 0.6410	 0.1080
m	 0.7310	 0.2080
n	 0.7070	 0.1790
o	 0.6650	 0.1300
p	 0.6440	 0.1040
q	 0.6880	 0.1560
r	 0.6350	 0.1010
s	 0.4180	 0.0040
t	 0.5380	 0.0180
u	 0.3480	 -0.0210
v	 0.4240	 -0.0400
w	 0.3930	 -0.0220
x	 0.5280	 0.0110
y	 0.6030	 0.0470
z	 0.7130	 0.1360