wwPDB EM Validation Summary Report (i)

Nov 26, 2022 – 06:51 PM EST

PDB ID	:	5JUP
EMDB ID	:	EMD-6644
Title	:	Saccharomyces cerevisiae 80S ribosome bound with elongation factor eEF2-GDP-sordarin and Taura Syndrome Virus IRES, Structure II (mid-rotated 40S subunit)
Authors	:	Abeyrathne, P.; Koh, C.S.; Grant, T.; Grigorieff, N.; Korostelev, A.A.
Deposited on	:	2016-05-10
Resolution	:	3.50 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

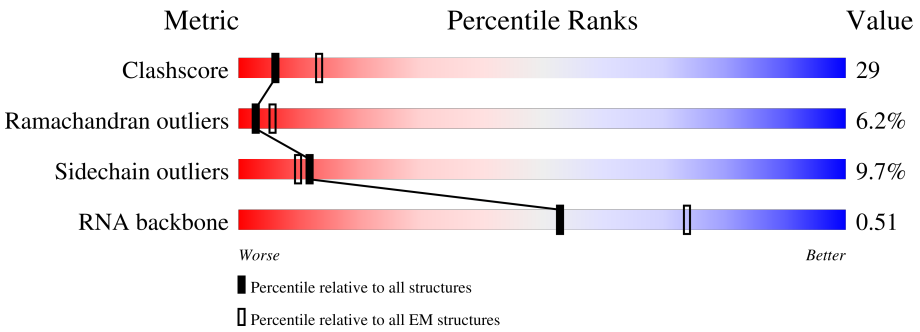
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1798	25%; 28%; 58%; 12%; ••
2	B	3396	6%; 31%; 54%; 11%; • •
3	C	158	•; 34%; 52%; 15%
4	D	121	23%; 69%; 7%
5	E	217	77%; 33%; 35%; 11%; 21%
6	F	254	12%; 34%; 57%; 7%; ••
7	G	387	7%; 47%; 46%; 7%

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Mol	Chain	Length	Quality of chain
8	H	362	40% 47% 12%
9	I	297	12% 39% 51% 10%
10	J	176	14% 51% 39% 8%
11	K	244	5% 37% 46% 7% 9%
12	L	256	17% 33% 46% 12% 9%
13	M	191	12% 43% 49% 6%
14	N	221	18% 40% 45% 10% 5%
15	O	174	11% 40% 47% 9%
16	P	165	52% 12% 35% 10% 43%
17	Q	199	12% 40% 47% 10%
18	R	138	9% 43% 43% 12%
19	S	204	7% 36% 56% 6%
20	T	199	7% 52% 43%
21	U	184	9% 53% 38% 9%
22	V	186	43% 53%
23	W	189	30% 43% 48% 8%
24	X	172	11% 37% 47% 16%
25	Y	160	9% 40% 48% 11%
26	Z	121	17% 39% 42% 17%
27	AA	137	17% 45% 47% 7%
28	BA	155	6% 15% 19% 5% 61%
29	CA	142	19% 29% 44% 12% 15%
30	DA	127	6% 33% 57% 8%
31	EA	136	16% 30% 54% 14%
32	FA	149	40% 49% 10%

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Mol	Chain	Length	Quality of chain
33	GA	59	20% 58% 37%
34	HA	105	10% 29% 51% 10% 8%
35	IA	113	11% 52% 41%
36	JA	130	7% 48% 45% 5%
37	KA	107	12% 45% 50% 5%
38	LA	121	17% 29% 53% 11% 7%
39	MA	120	10% 30% 55% 14%
40	NA	100	9% 49% 41% 9%
41	OA	88	8% 49% 41% 8%
42	PA	78	83% 50% 45%
43	QA	51	8% 27% 65% 6%
44	RA	128	16% 19% 5% 59%
45	SA	25	100% 40% 48% 12%
46	TA	106	10% 56% 42%
47	UA	92	17% 51% 38% 10%
48	VA	312	55% 17% 33% 10% 39%
49	WA	319	91% 33% 62% 5%
50	XA	252	52% 27% 47% 6% 18%
51	YA	255	84% 78% 6% 16%
52	ZA	254	21% 33% 49% 15%
53	AB	240	72% 39% 46% 8% 7%
54	BB	261	35% 30% 61% 8%
55	CB	225	80% 35% 48% 9% 8%
56	DB	236	48% 39% 53%
57	EB	190	84% 36% 50% 11%

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Mol	Chain	Length	Quality of chain
58	FB	200	52% 27% 59% 8% 6%
59	GB	197	25% 34% 53% 6% 6%
60	HB	105	61% 28% 51% 10% 9%
61	IB	156	65% 39% 49% 10%
62	JB	143	87% 79% 8% 13%
63	KB	151	50% 42% 50% 8%
64	LB	137	93% 83% 9% 7%
65	MB	142	68% 34% 43% 9% 14%
66	NB	143	85% 33% 57% 8%
67	OB	136	74% 42% 39% 5% 14%
68	PB	146	78% 38% 51% 9%
69	QB	144	78% 38% 52% 9%
70	RB	121	79% 27% 53% 8% 12%
71	SB	87	40% 36% 56% 7%
72	TB	130	45% 30% 60% 8%
73	UB	145	57% 39% 52% 8%
74	VB	135	42% 36% 56% 8%
75	WB	108	57% 15% 40% 10% 35%
76	XB	119	82% 67% 13% 18%
77	YB	82	57% 45% 50%
78	ZB	67	72% 34% 52% 7% 6%
79	AC	56	59% 48% 39% 7% 5%
80	BC	63	51% 38% 48% 10% 5%
81	CC	152	47% 39% 7% 53%
82	DC	842	43% 32% 56% 9%

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Mol	Chain	Length	Quality of chain
83	EC	201	92% (19% / 32% / 32% / 15%)

2 Entry composition (i)

There are 86 unique types of molecules in this entry. The entry contains 212656 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1781	36760	16335	6359	12285	1781	0	0

- Molecule 2 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	3309	70288	31354	12595	23030	3309	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	158	3354	1500	586	1110	158	0	0

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	121	2580	1152	461	846	121	0	0

- Molecule 5 is a protein called uL1 (yeast L1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	171	1359	869	232	251	7	0	0

- Molecule 6 is a protein called uL2 (yeast L2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	252	1918	1193	389	335	1	0	0

- Molecule 7 is a protein called uL3 (yeast L3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	386	3082	1956	584	534	8	0	0

- Molecule 8 is a protein called uL4 (yeast L4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	361	2750	1730	522	495	3	0	0

- Molecule 9 is a protein called uL18 (yeast L5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	296	2376	1501	414	459	2	0	0

- Molecule 10 is a protein called eL6 (yeast L6).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	175	1401	902	251	247	1	0	0

- Molecule 11 is a protein called uL30 (yeast L7).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	222	1785	1151	324	309	1	0	0

- Molecule 12 is a protein called eL8 (yeast L8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	233	1818	1159	326	330	3	0	0

- Molecule 13 is a protein called uL6 (yeast L9).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	191	1519	963	274	278	4	0	0

- Molecule 14 is a protein called uL16 (yeast L10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	211	1718	1089	325	298	6	0	0

- Molecule 15 is a protein called uL5 (yeast L11).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	169	1354	847	253	250	4	0	0

- Molecule 16 is a protein called uL11 (yeast L12).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	94	723	448	138	135	2	0	0

- Molecule 17 is a protein called eL13 (yeast L13).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	193	1543	962	315	266	0	0

- Molecule 18 is a protein called eL14 (yeast L14).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	136	1054	675	199	178	2	0	0

- Molecule 19 is a protein called eL15 (yeast L15).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	203	1721	1077	361	282	1	0	0

- Molecule 20 is a protein called uL13 (yeast L16).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	197	1556	1003	289	263	1	0	0

- Molecule 21 is a protein called uL22 (yeast L17).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	183	1443	896	287	260	0	0

- Molecule 22 is a protein called eL18 (yeast L18).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	185	1442	908	290	242	2	0	0

- Molecule 23 is a protein called eL19 (yeast L19).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	188	1522	935	326	261	0	0

- Molecule 24 is a protein called eL20 (yeast L20).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	172	1446	930	267	245	4	0	0

- Molecule 25 is a protein called eL21 (yeast L21).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	159	1277	805	246	222	4	0	0

- Molecule 26 is a protein called eL22 (yeast L22).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Z	100	796	516	131	149	0	0

- Molecule 27 is a protein called uL14 (yeast L23).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	AA	136	1004	628	189	180	7	0	0

- Molecule 28 is a protein called eL24 (yeast L24).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BA	61	509	328	100	80	1	0	0

- Molecule 29 is a protein called uL23 (yeast L25).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CA	121	969	623	170	174	2	0	0

- Molecule 30 is a protein called uL24 (yeast L26).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	DA	126	994	625	192	177	0	0

- Molecule 31 is a protein called eL27 (yeast L27).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	EA	135	1093	710	202	181	0	0

- Molecule 32 is a protein called uL15 (yeast L28).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	FA	148	1174	749	231	191	3	0	0

- Molecule 33 is a protein called eL29 (yeast L29).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	GA	58	463	289	100	74	0	0

- Molecule 34 is a protein called eL30 (yeast L30).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	HA	97	743	479	124	139	1	0	0

- Molecule 35 is a protein called eL31 (yeast L31).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	IA	109	890	565	168	156	1	0	0

- Molecule 36 is a protein called eL32 (yeast L32).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	JA	127	1020	647	205	167	1	0	0

- Molecule 37 is a protein called eL33 (yeast L33).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	KA	106	851	540	165	145	1	0	0

- Molecule 38 is a protein called eL34 (yeast L34).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LA	112	881	546	179	152	4	0	0

- Molecule 39 is a protein called uL29 (yeast L35).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	MA	119	970	615	186	168	1	0	0

- Molecule 40 is a protein called eL36 (yeast L36).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	NA	99	772	481	156	133	2	0	0

- Molecule 41 is a protein called eL37 (yeast L37).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	OA	87	682	414	148	115	5	0	0

- Molecule 42 is a protein called eL38 (yeast L38).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	PA	77	613	391	115	107	0	0

- Molecule 43 is a protein called eL39 (yeast L39).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	QA	50	437	272	97	66	2	0	0

- Molecule 44 is a protein called eL40 (yeast L40).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	RA	52	418	259	86	68	5	0	0

- Molecule 45 is a protein called eL41 (yeast L41).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	SA	25	234	142	63	28	1	0	0

- Molecule 46 is a protein called eL42 (yeast L42).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	TA	105	848	534	170	139	5	0	0

- Molecule 47 is a protein called eL43 (yeast L43).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	UA	91	695	429	138	122	6	0	0

- Molecule 48 is a protein called uL10 (yeast P0).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	VA	189	1473	942	257	270	4	0	0

- Molecule 49 is a protein called RACK1 (yeast Asc1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	WA	318	2445	1546	419	472	8	0	0

- Molecule 50 is a protein called uS2 (yeast S0).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	XA	206	1612	1034	285	291	2	0	0

- Molecule 51 is a protein called eS1 (yeast S1).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	YA	214	856	428	214	214	0	0

- Molecule 52 is a protein called uS5 (yeast S2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	ZA	217	1635	1047	289	297	2	0	0

- Molecule 53 is a protein called uS3 (yeast S3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	AB	223	1734	1101	313	314	6	0	0

- Molecule 54 is a protein called eS4 (yeast S4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BB	260	2069	1316	389	361	3	0	0

- Molecule 55 is a protein called uS7 (yeast S5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	CB	206	1610	1007	300	300	3	0	0

- Molecule 56 is a protein called eS6 (yeast S6).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	DB	226	1820	1142	350	325	3	0	0

- Molecule 57 is a protein called eS7 (yeast S7).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	EB	184	1481	951	265	265	0	0

- Molecule 58 is a protein called eS8 (yeast S8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	FB	188	1490	925	298	265	2	0	0

- Molecule 59 is a protein called uS4 (yeast S9).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	GB	185	1494	943	289	261	1	0	0

- Molecule 60 is a protein called eS10 (yeast S10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	HB	96	817	529	133	153	2	0	0

- Molecule 61 is a protein called uS17 (yeast S11).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	IB	155	1245	798	235	209	3	0	0

- Molecule 62 is a protein called eS12 (yeast S12).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	JB	124	496	248	124	124	0	0

- Molecule 63 is a protein called uS15 (yeast S13).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	KB	150	1193	759	224	208	2	0	0

- Molecule 64 is a protein called uS11 (yeast S14).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	LB	127	508	254	127	127	0	0

- Molecule 65 is a protein called uS19 (yeast S15).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	MB	122	975	622	182	164	7	0	0

- Molecule 66 is a protein called uS9 (yeast S16).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
66	NB	141	1106	708	203	195	0	0

- Molecule 67 is a protein called eS17 (yeast S17).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	OB	117	836	515	166	153	2	0	0

- Molecule 68 is a protein called uS13 (yeast S18).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	PB	145	1193	743	237	211	2	0	0

- Molecule 69 is a protein called eS19 (yeast S19).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	QB	143	1113	694	208	209	2	0	0

- Molecule 70 is a protein called uS10 (yeast S20).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	RB	107	856	539	156	160	1	0	0

- Molecule 71 is a protein called eS21 (yeast S21).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SB	87	685	420	125	138	2	0	0

- Molecule 72 is a protein called uS8 (yeast S22).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	TB	129	1022	650	188	181	3	0	0

- Molecule 73 is a protein called uS12 (yeast S23).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	UB	144	1122	708	220	192	2	0	0

- Molecule 74 is a protein called eS24 (yeast S24).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
74	VB	134	1074	676	208	190	0	0

- Molecule 75 is a protein called eS25 (yeast S25).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
75	WB	70	563	360	104	99	0	0

- Molecule 76 is a protein called eS26 (yeast S26).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	XB	97	388	194	97	97	0	0

- Molecule 77 is a protein called eS27 (yeast S27).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	YB	81	611	382	110	114	5	0	0

- Molecule 78 is a protein called eS28 (yeast S28).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	ZB	63	498	306	99	92	1	0	0

- Molecule 79 is a protein called uS14 (yeast S29).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	AC	53	444	275	92	73	4	0	0

- Molecule 80 is a protein called eS30 (yeast S30).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	BC	60	475	299	98	77	1	0	0

- Molecule 81 is a protein called eS31 (yeast S31).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
81	CC	71	284	142	71	71	0	0

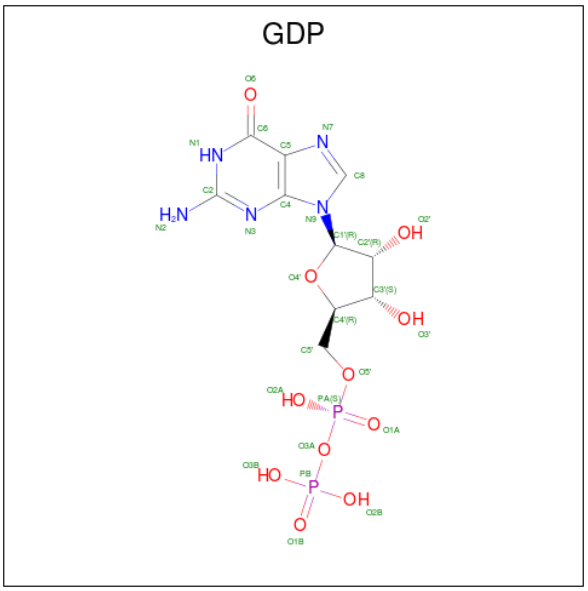
- Molecule 82 is a protein called yeast eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	DC	824	6419	4085	1096	1208	30	0	0

- Molecule 83 is a RNA chain called IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
83	EC	198	4105	1826	718	1363	198	0	0

- Molecule 84 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

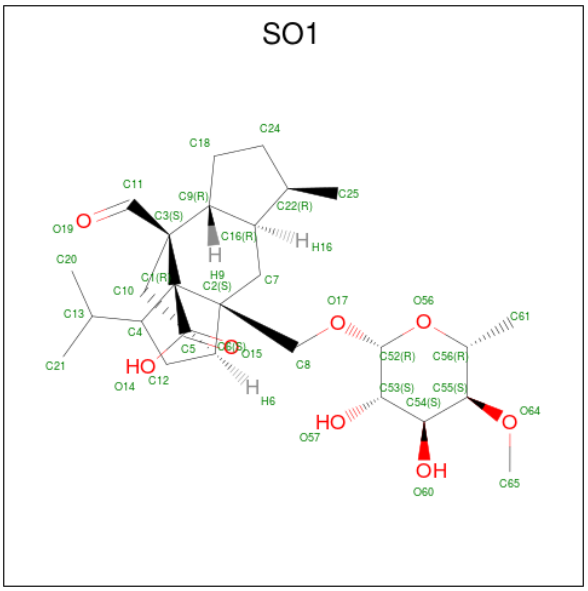


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
84	DC	1	28	10	5	11	2	0

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	DC	1	1	1	0

- Molecule 86 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: $C_{27}H_{42}O_8$).



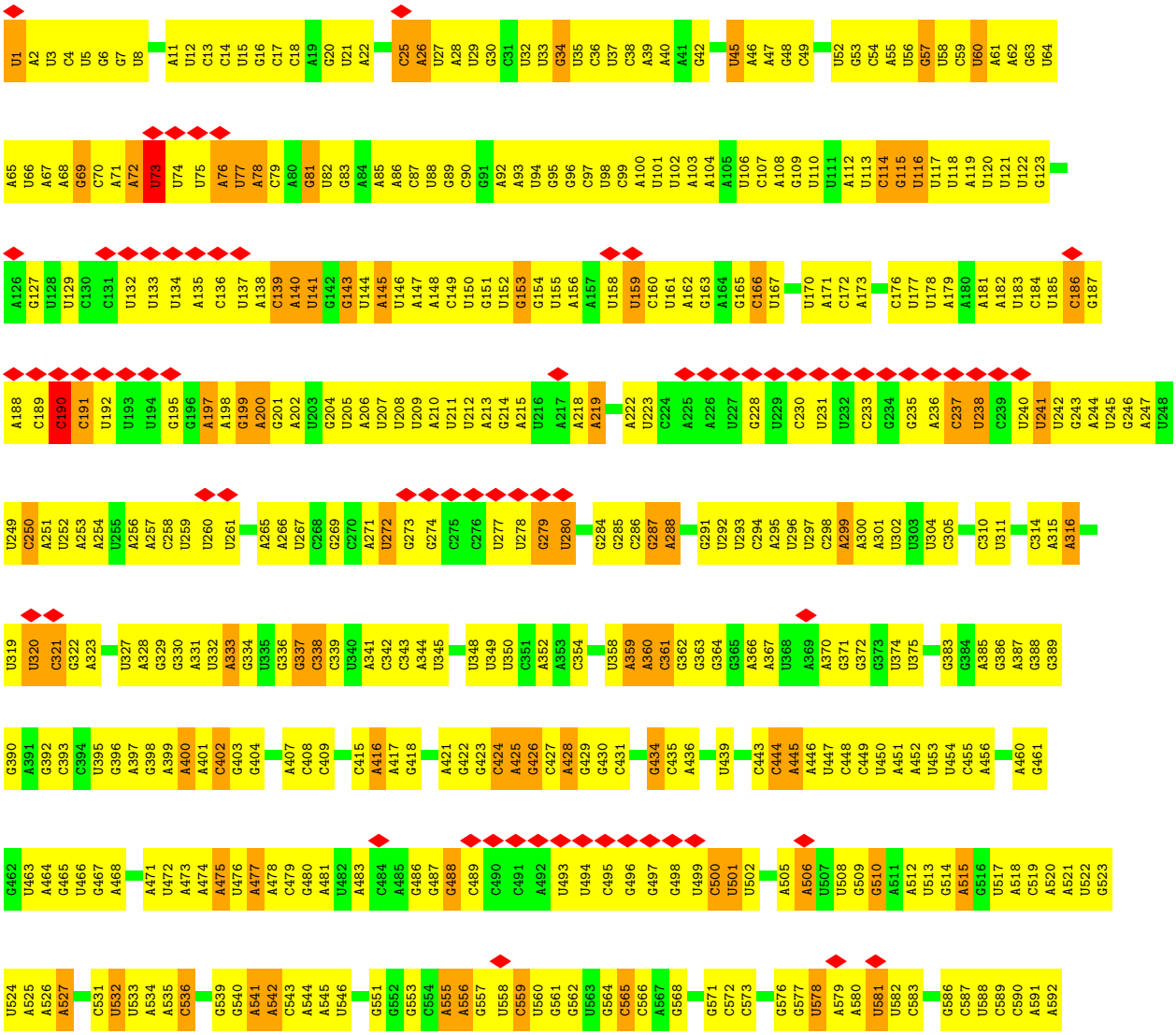
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
86	DC	1	35	27	8	0

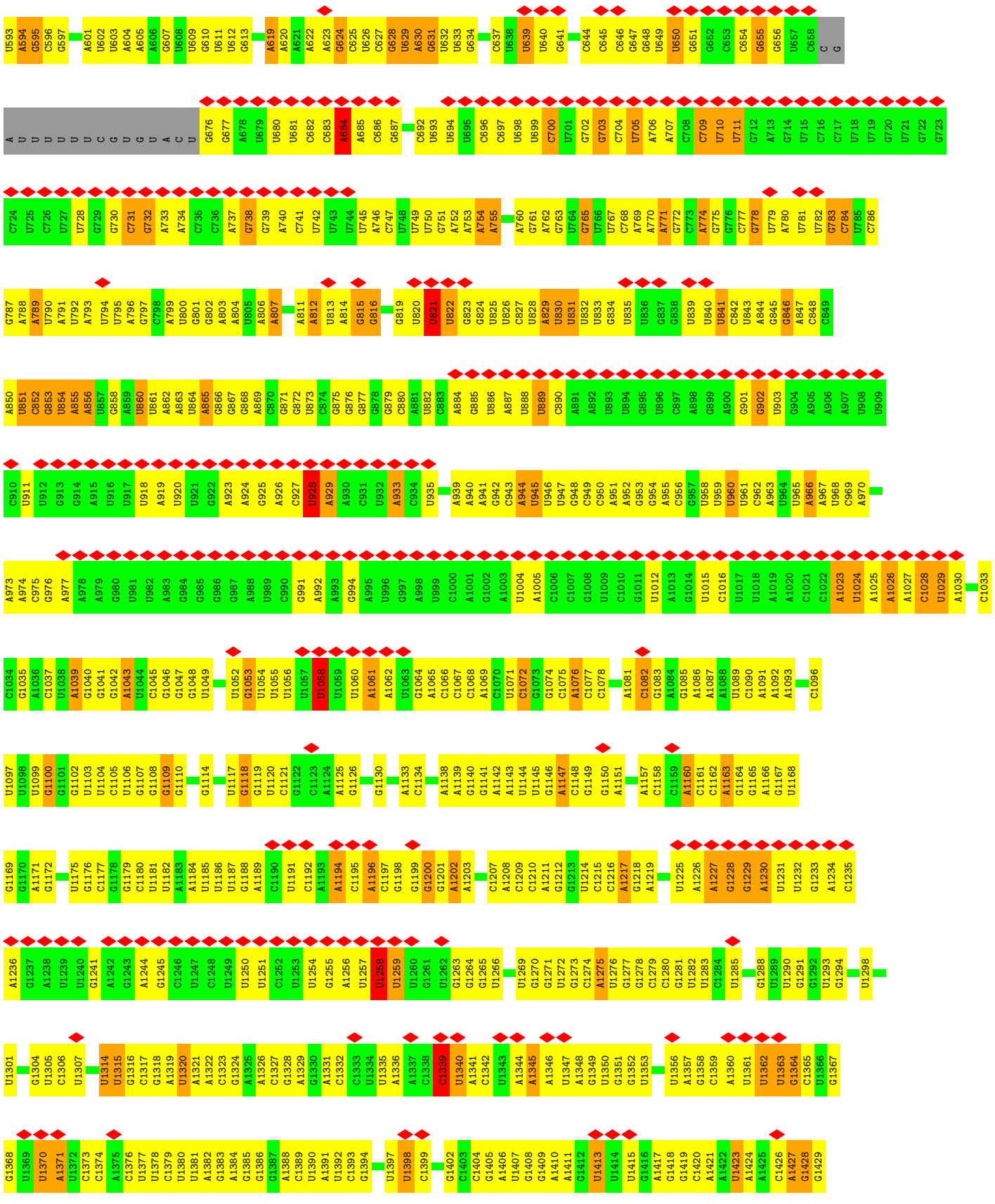
3 Residue-property plots (i)

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: 18S ribosomal RNA

Chain A: 25% 28% 58% 12%

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A U U U U U C G U G U A C U G676 G677 A678 U679 U680 U681 C682 C683 A684 A685 C686 G687 C692 U693 U694 U695 C696 C697 U698 U699 C700 U701 G702 G703 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714 U715 C716 C717 U718 U719 G720 U721 G722 G723
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A973 A974 C975 G976 A977 A978 A979 G980 U981 U982 A983 G984 G985 G986 G987 A988 U989 C990 G991 A992 A993 G994 A995 U996 G997 A998 U999 C1000 A1001 G1002 A1003 U1004 A1005 C1006 C1007 G1008 U1009 C1010 G1011 U1012 A1013 G1014 U1015 C1016 U1017 U1018 A1019 A1020 C1021 C1022 A1023 U1024 A1025 A1026 A1027 C1028 U1029 A1030 C1033
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G1169 G1170 A1171 G1172 U1175 G1176 C1177 G1178 G1179 C1180 U1181 U1182 A1183 A1184 U1185 A1186 U1187 G1188 A1189 C1190 U1191 C1192 A1193 A1194 C1195 A1196 C1197 G1198 G1199 G1200 G1201 A1202 A1203 C1207 A1208 C1209 C1210 A1211 G1212 G1213 U1214 C1215 C1216 A1217 G1218 A1219 U1225 A1226 A1227 G1228 G1229 A1230 U1231 U1232 G1233 A1234 C1235
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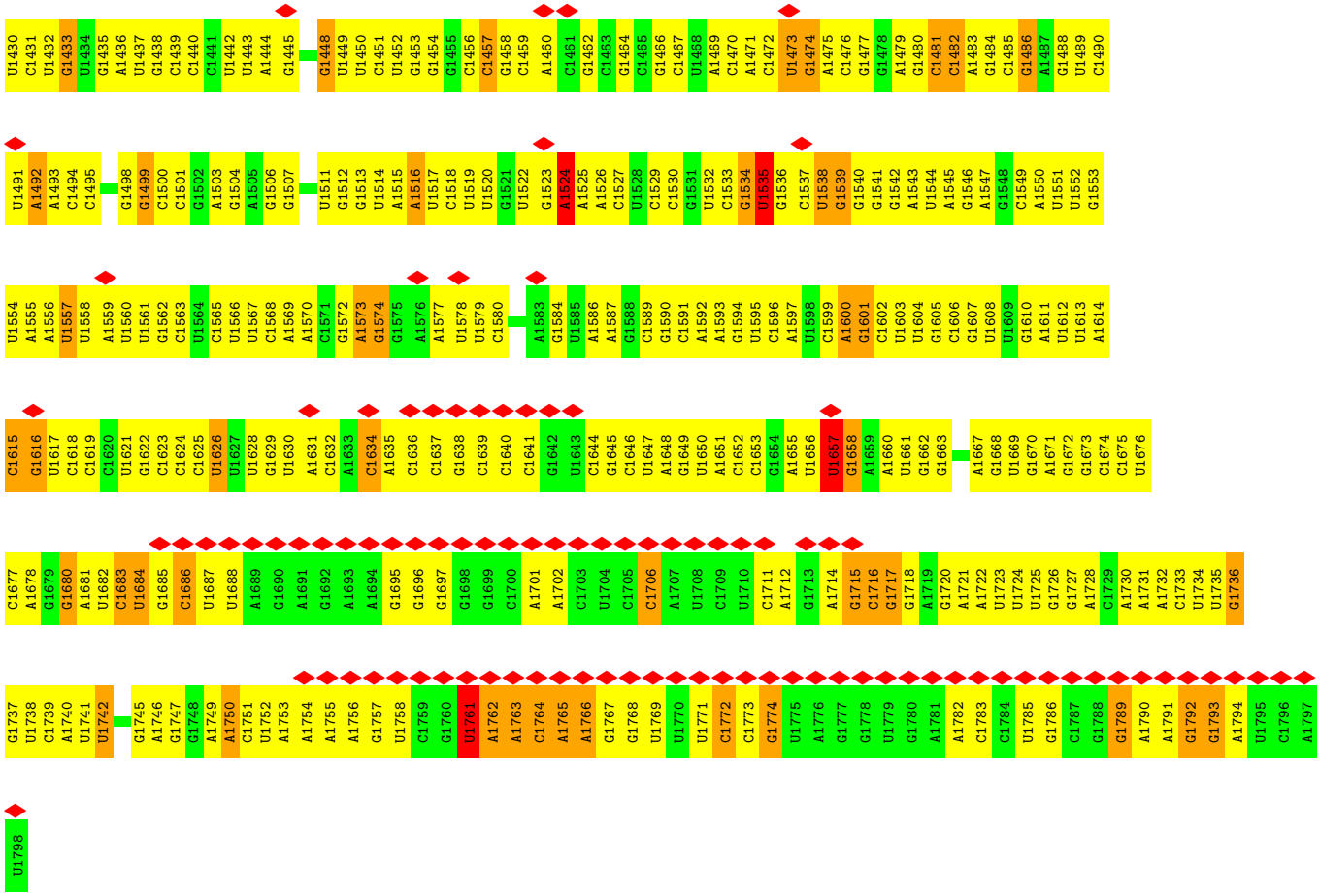
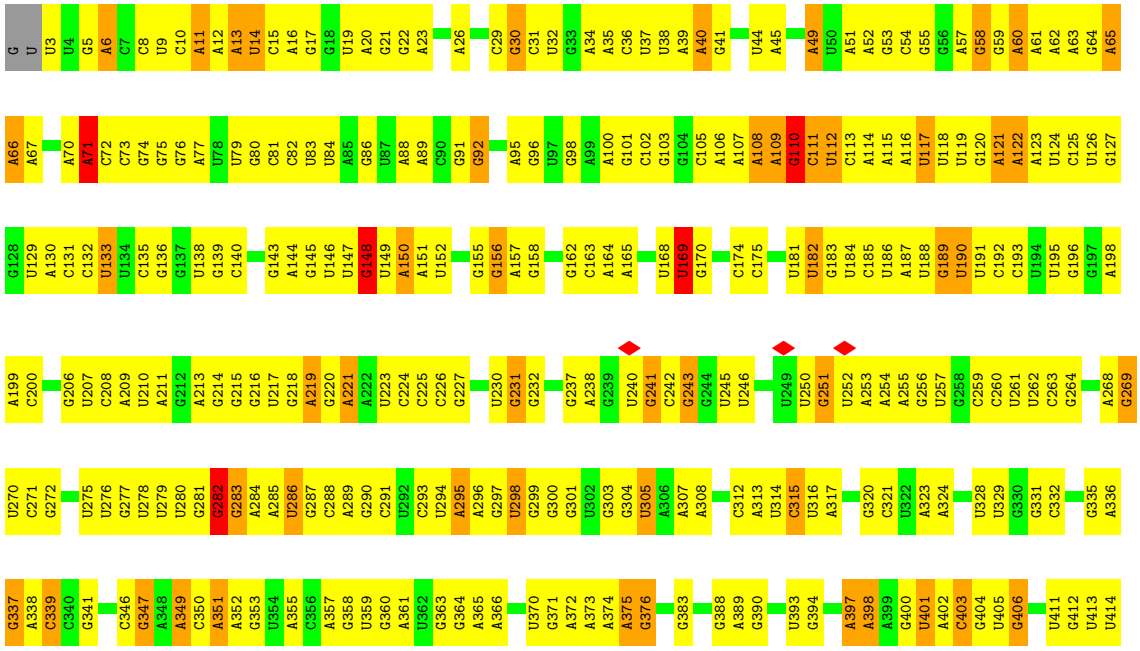
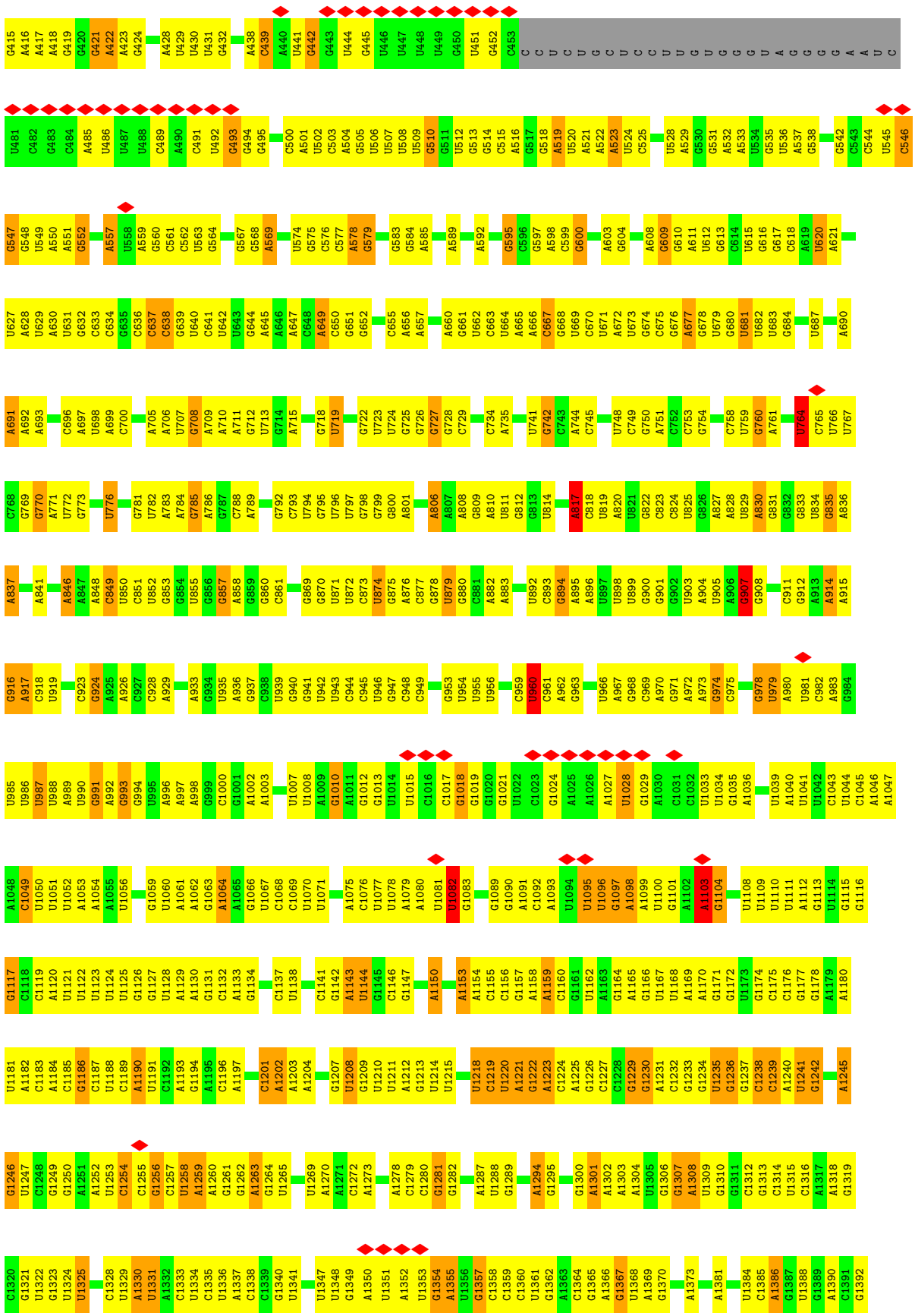


• Molecule 2: 25S ribosomal RNA

Chain B:

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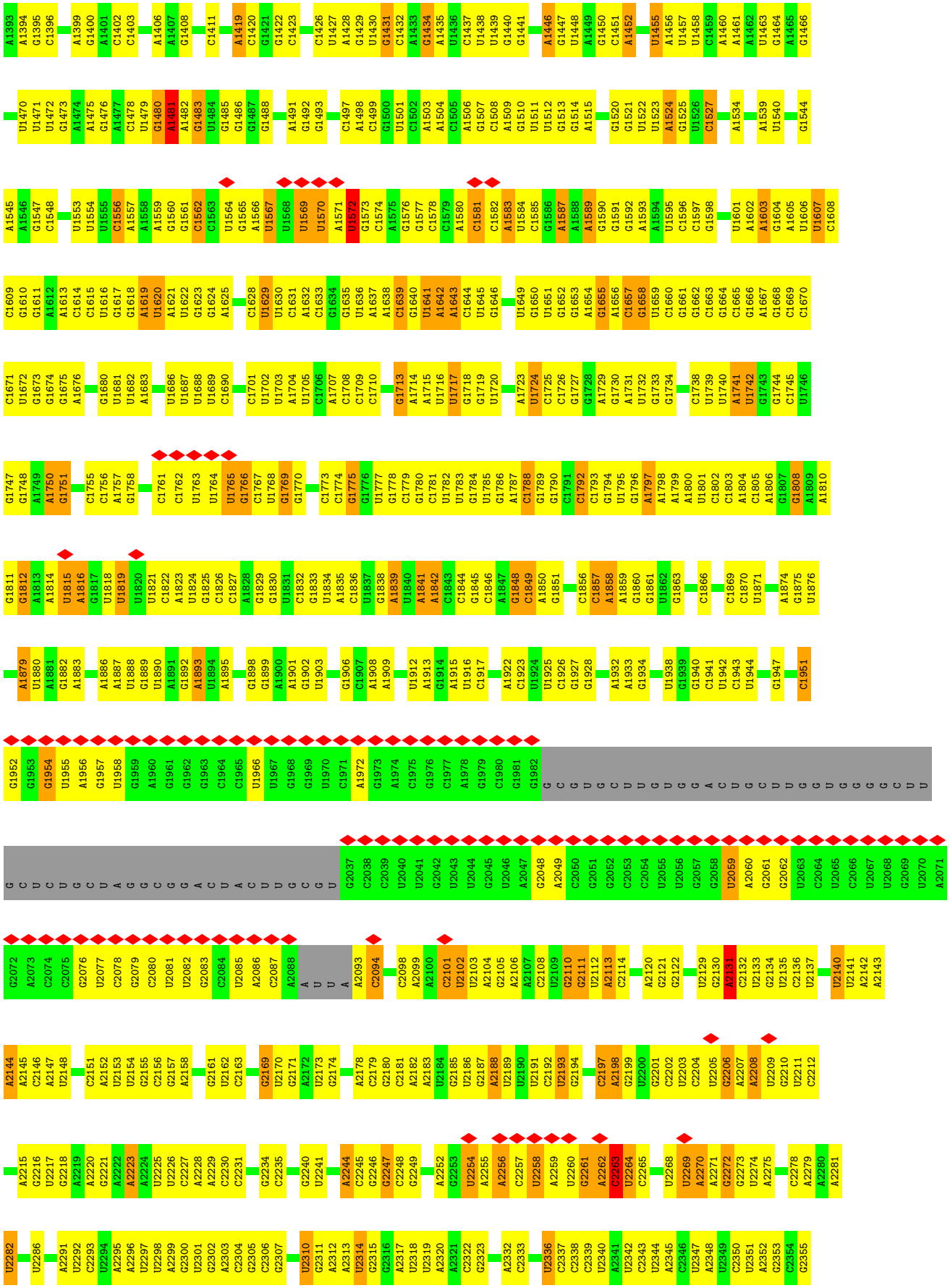
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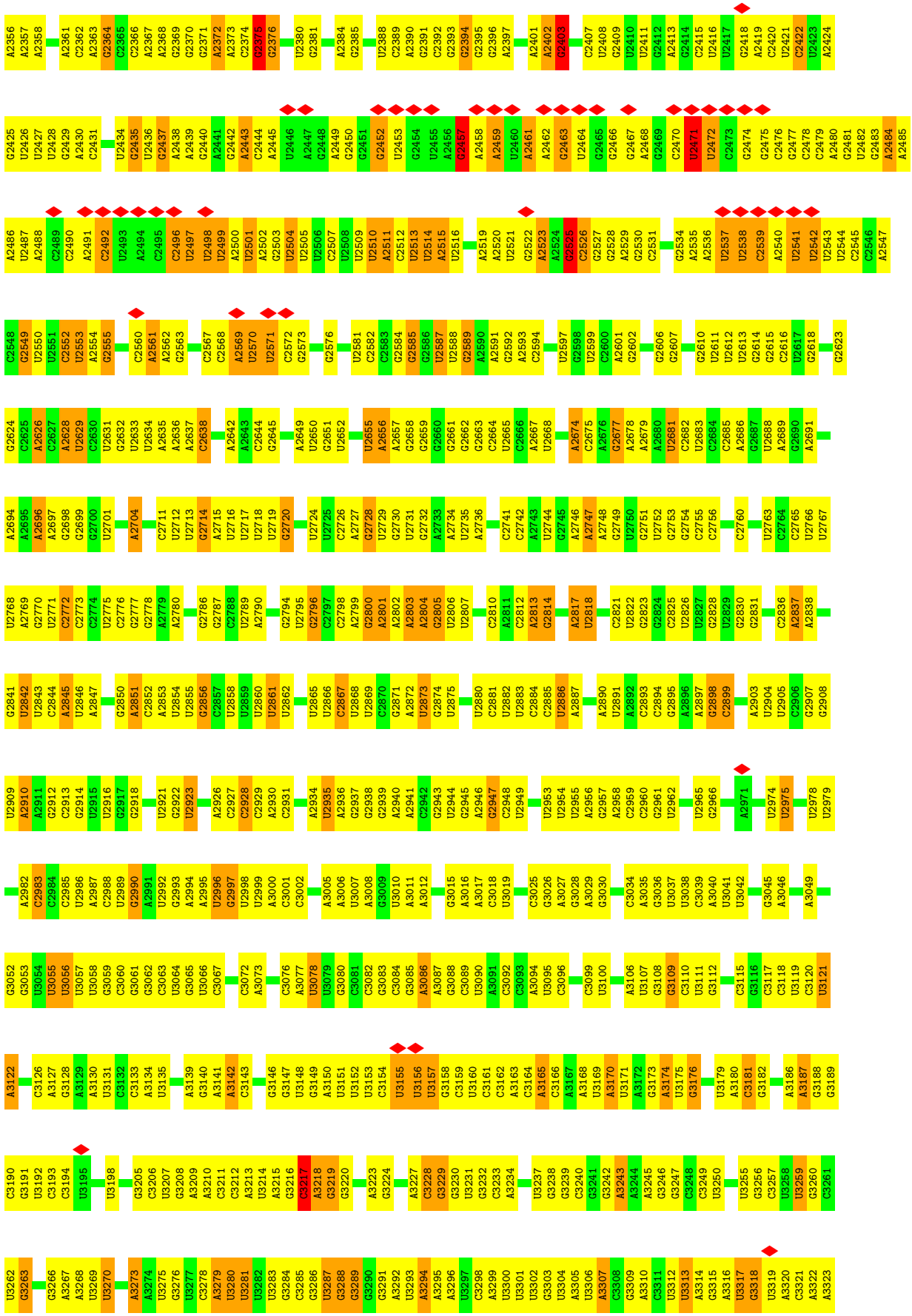
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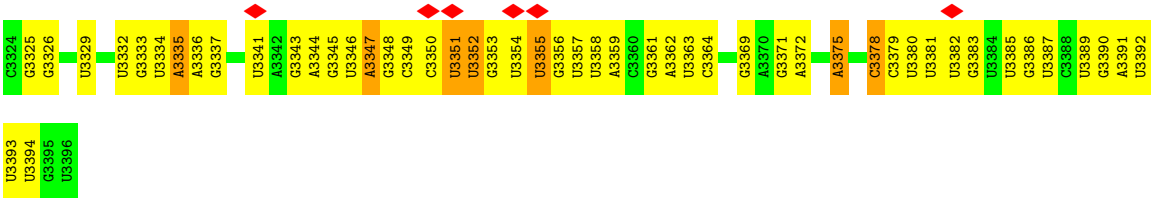

- Molecule 3: 5.8S ribosomal RNA

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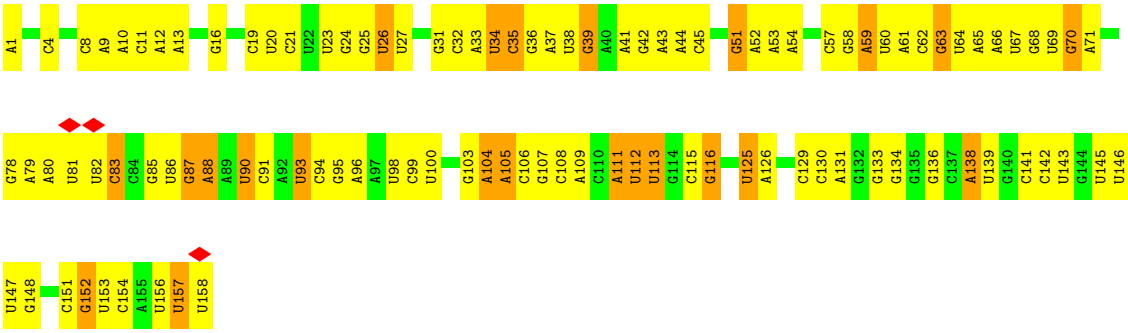
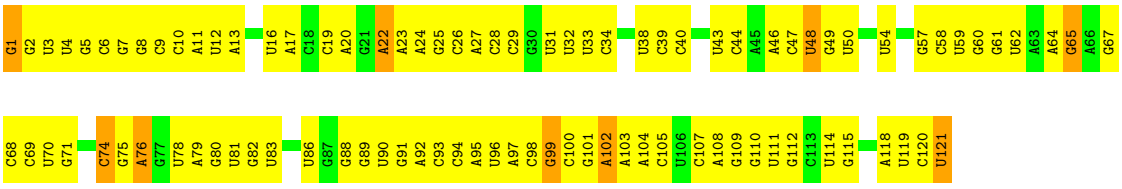


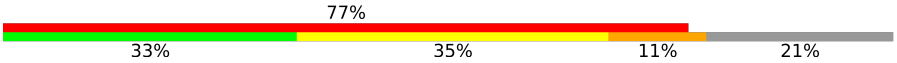
- Molecule 4: 5S ribosomal RNA

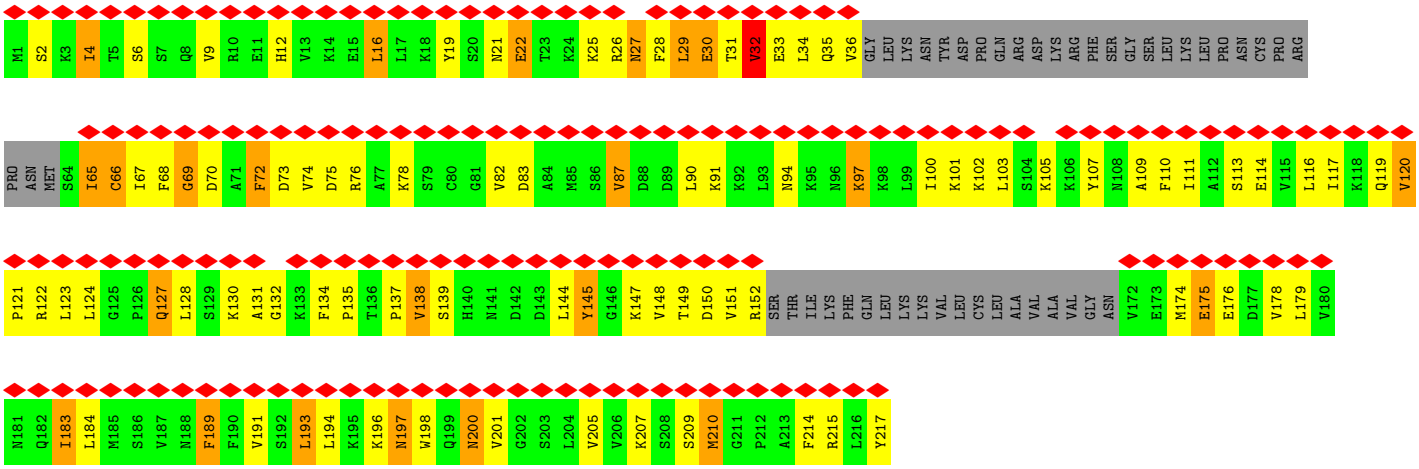
Chain D:



- Molecule 5: uL1 (yeast L1)

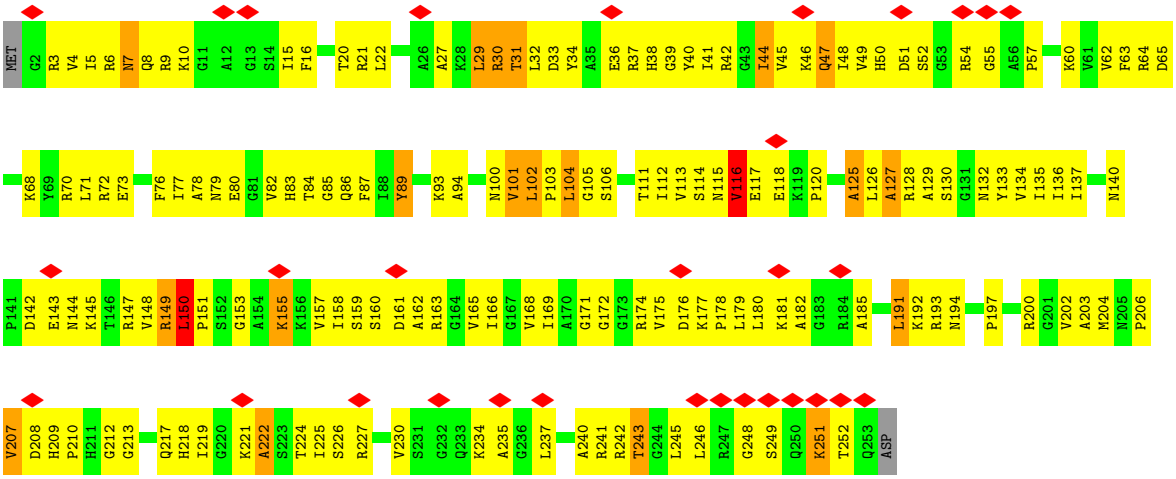
Chain E:





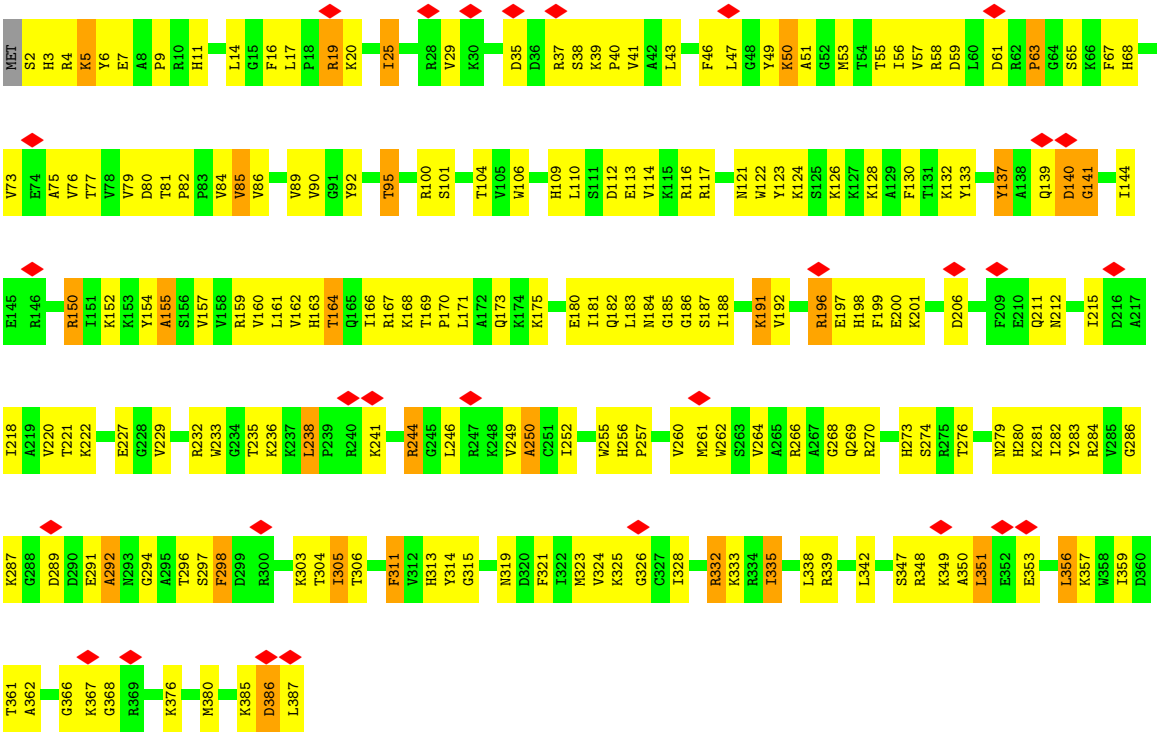
- Molecule 6: uL2 (yeast L2)

Chain F:



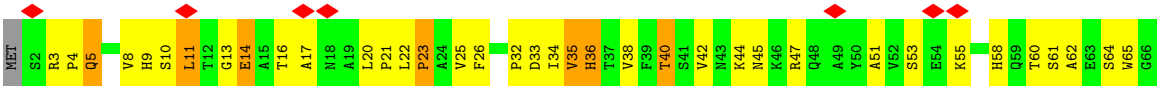
- Molecule 7: uL3 (yeast L3)

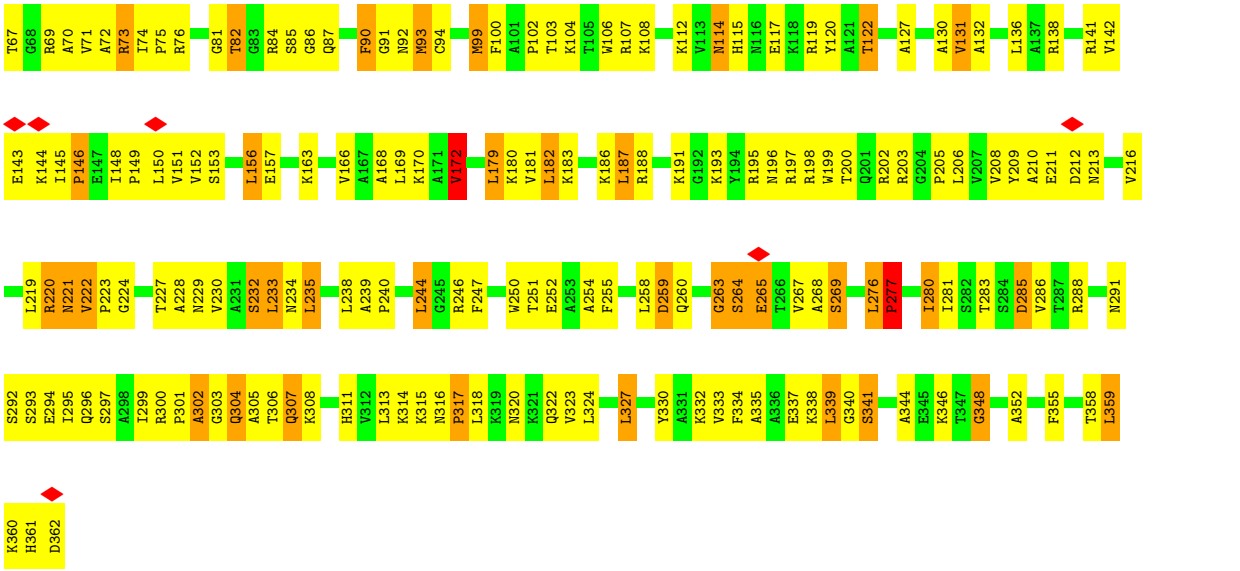
Chain G:



- Molecule 8: uL4 (yeast L4)

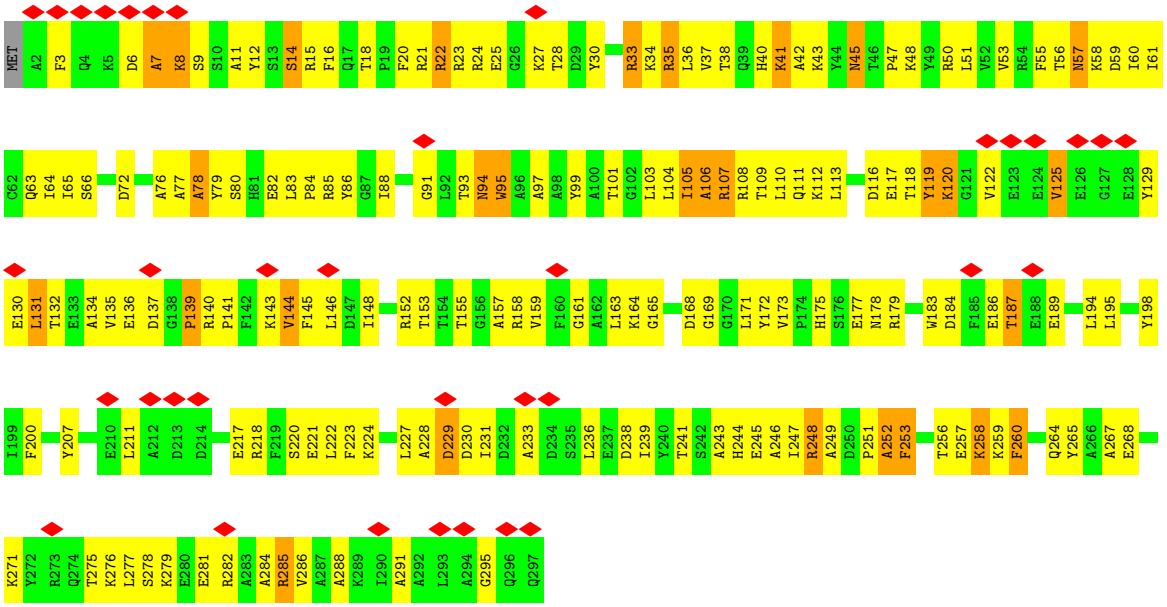
Chain H:





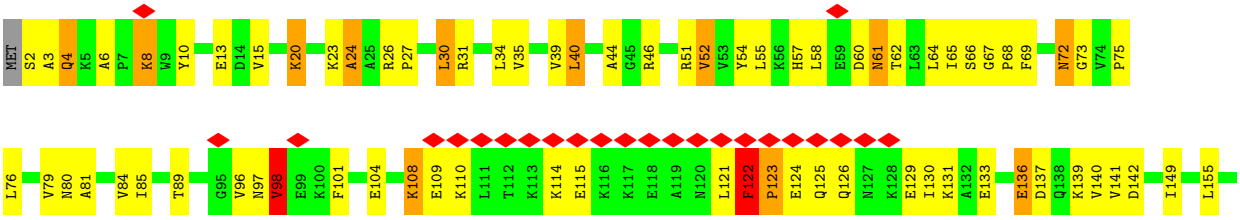
- Molecule 9: uL18 (yeast L5)

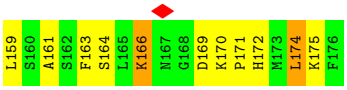
Chain I:



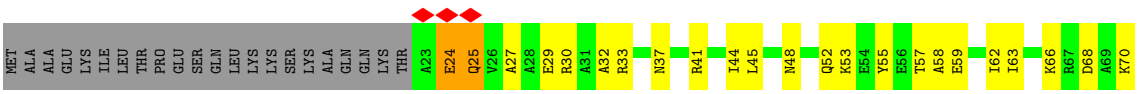
- Molecule 10: eL6 (yeast L6)

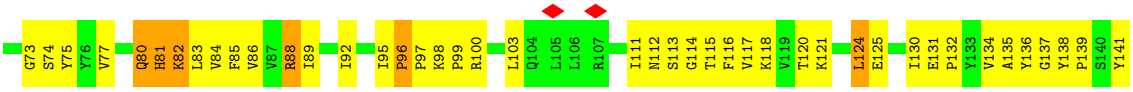
Chain J:

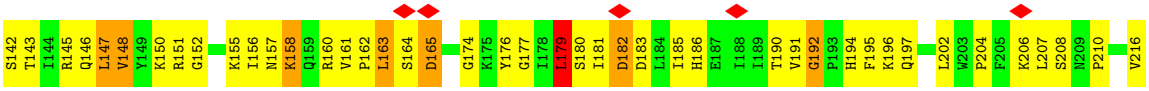


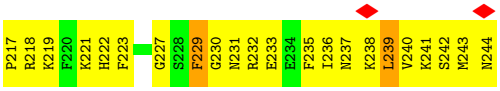


• Molecule 11: uL30 (yeast L7)

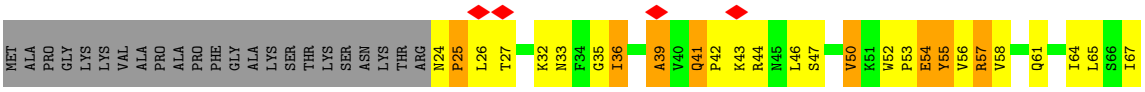


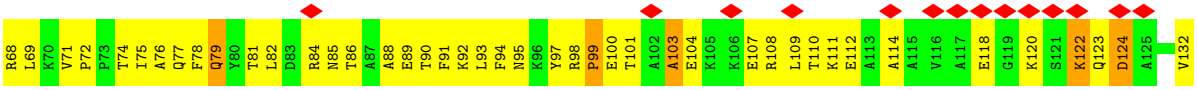


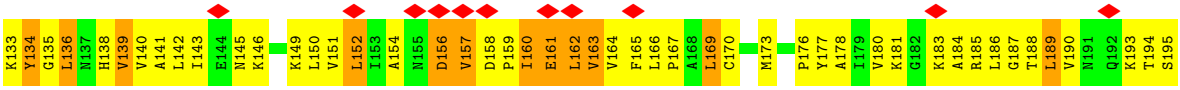


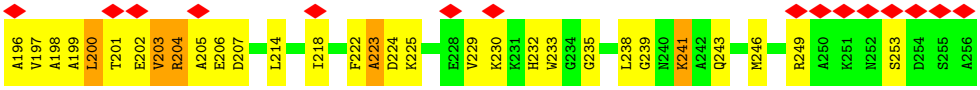


• Molecule 12: eL8 (yeast L8)

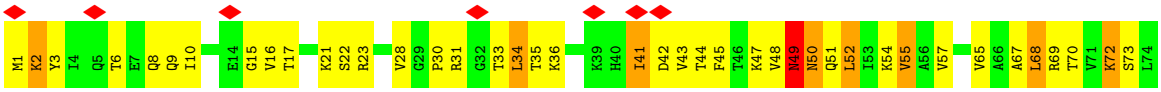


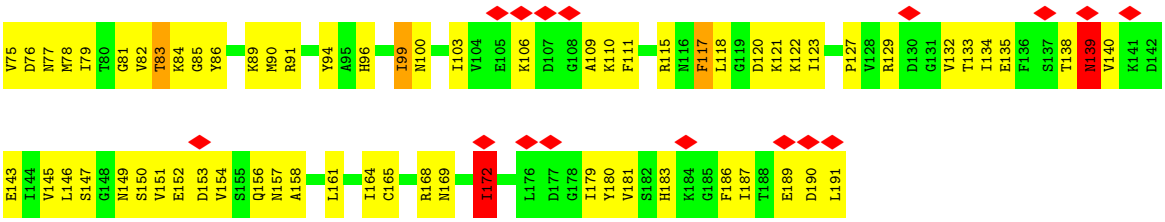






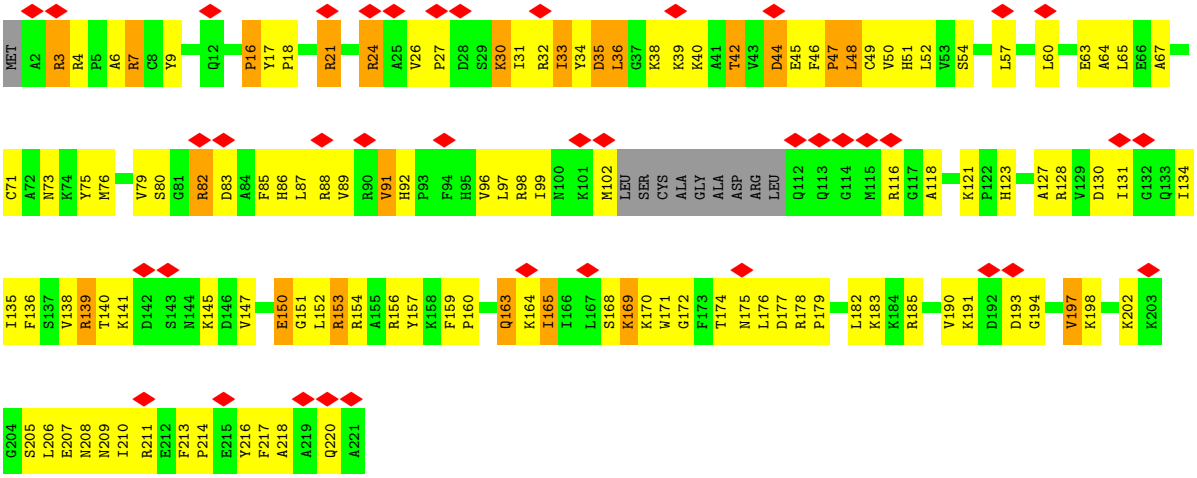
• Molecule 13: uL6 (yeast L9)





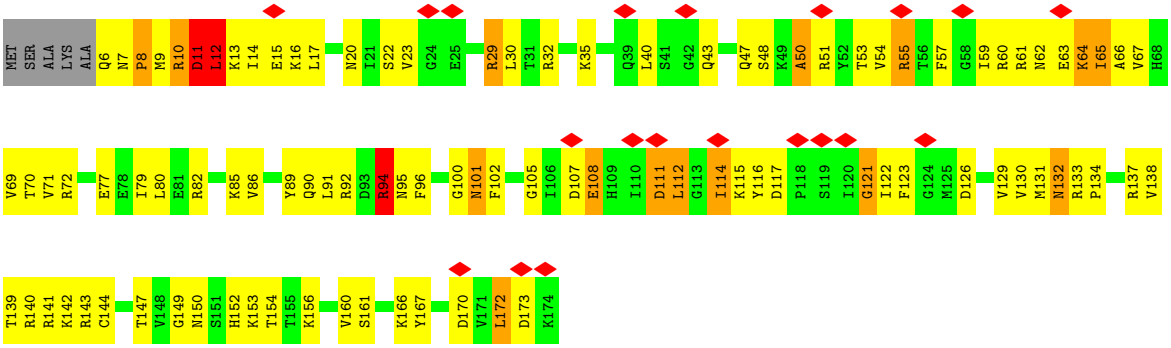
- Molecule 14: uL16 (yeast L10)

Chain N:



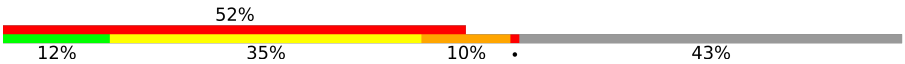
- Molecule 15: uL5 (yeast L11)

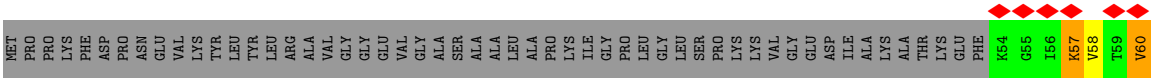
Chain O:

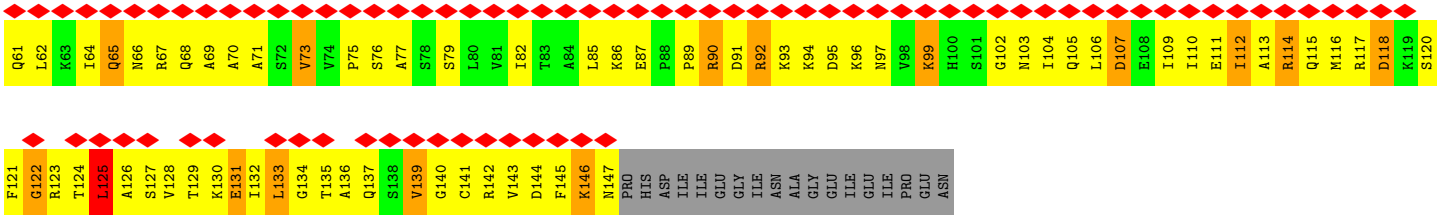


- Molecule 16: uL11 (yeast L12)

Chain P:

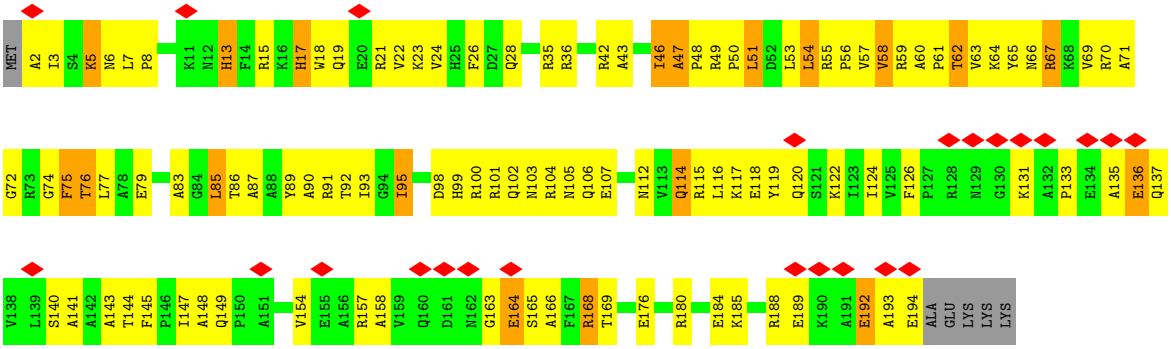






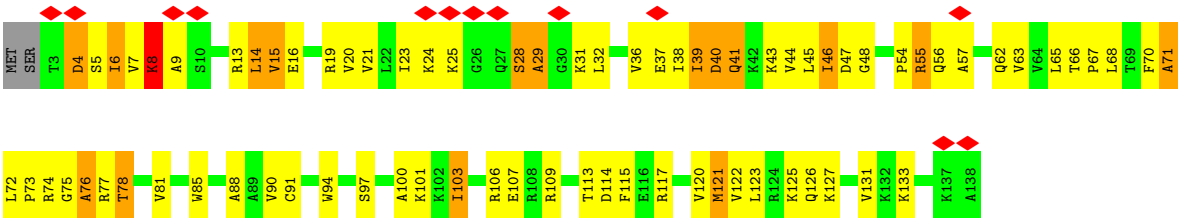
- Molecule 17: eL13 (yeast L13)

Chain Q:



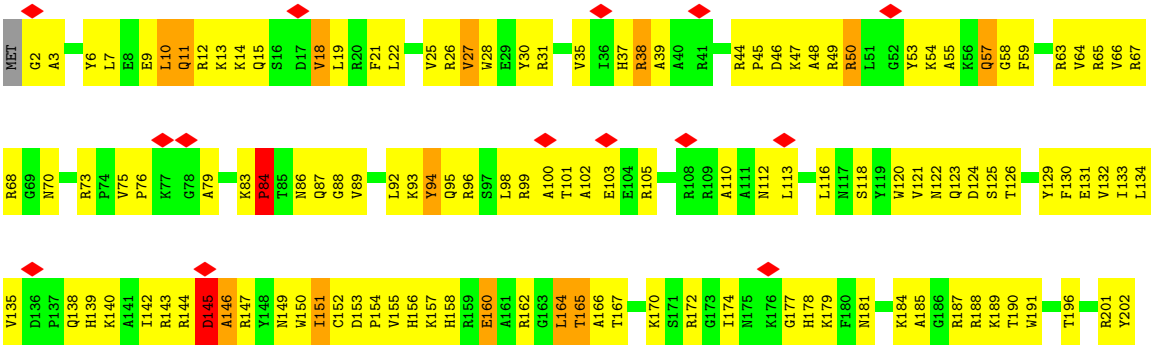
- Molecule 18: eL14 (yeast L14)

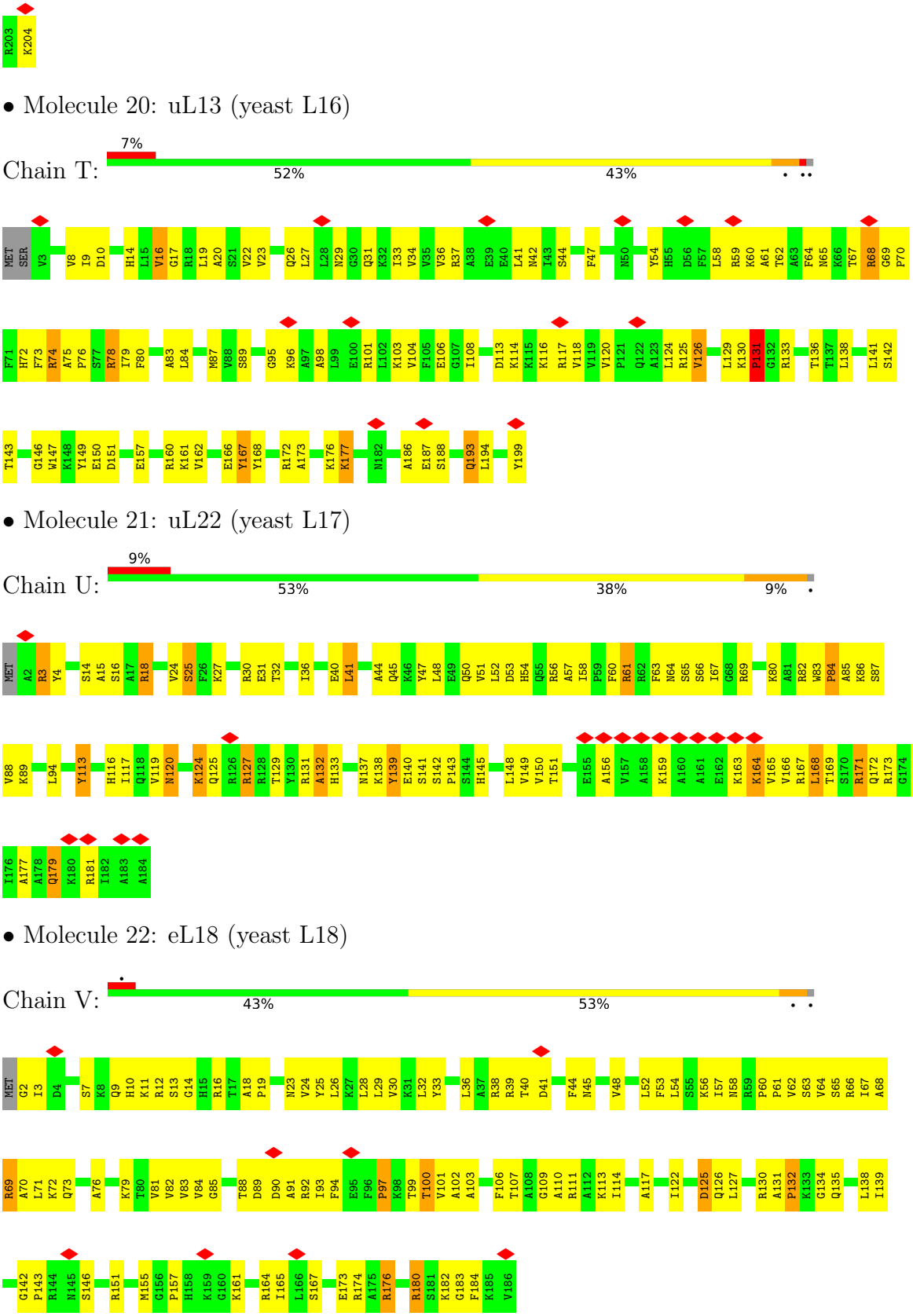
Chain R:



- Molecule 19: eL15 (yeast L15)

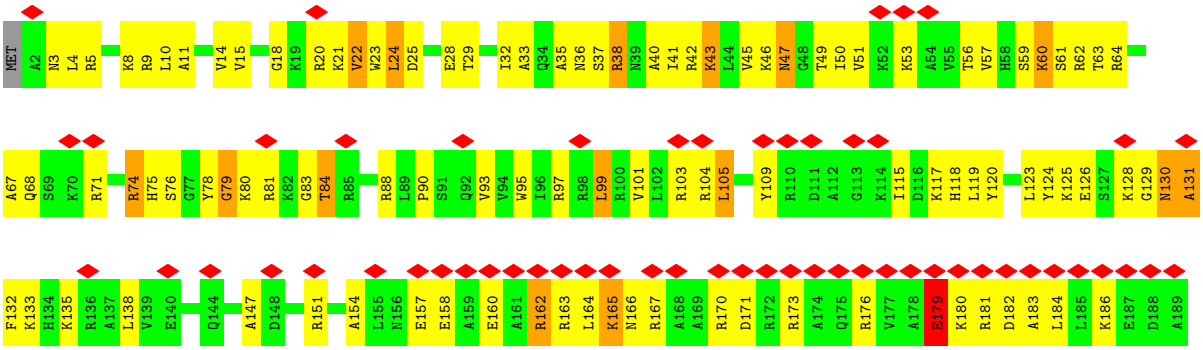
Chain S:





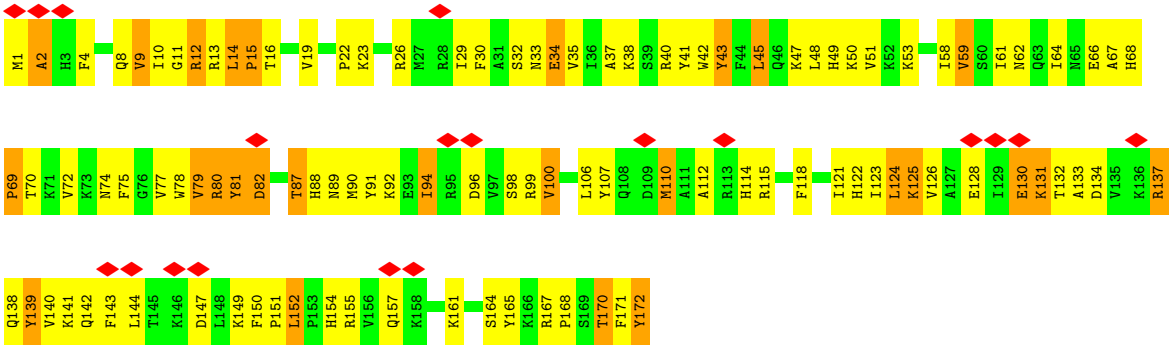
• Molecule 23: eL19 (yeast L19)

Chain W:



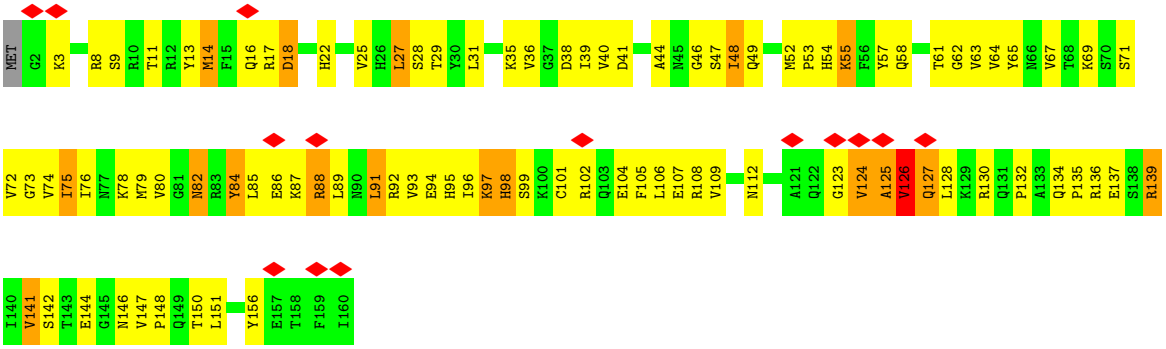
- Molecule 24: eL20 (yeast L20)

Chain X:



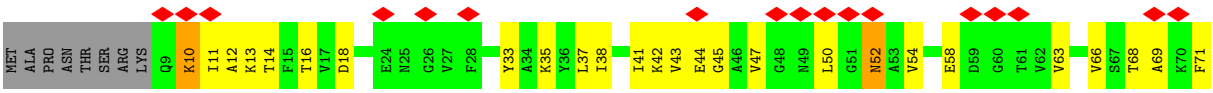
- Molecule 25: eL21 (yeast L21)

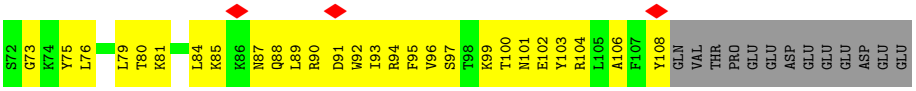
Chain Y:



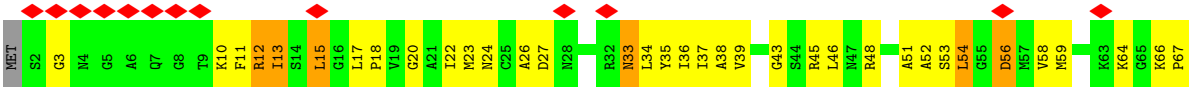
- Molecule 26: eL22 (yeast L22)

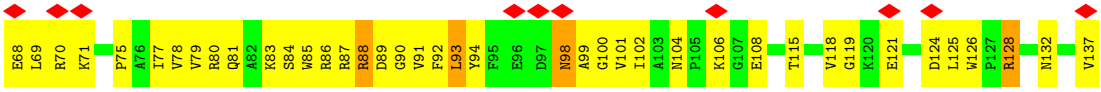
Chain Z:



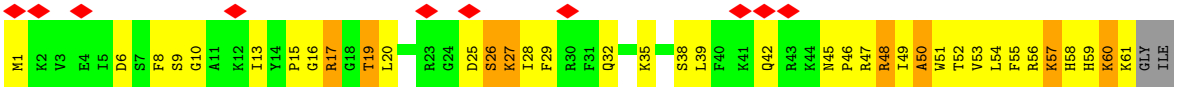


• Molecule 27: uL14 (yeast L23)

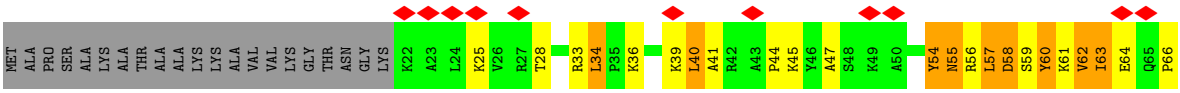


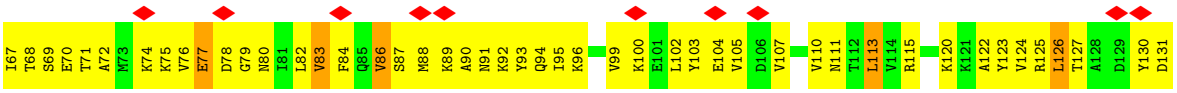


• Molecule 28: eL24 (yeast L24)

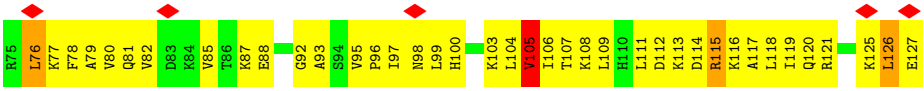


• Molecule 29: uL23 (yeast L25)



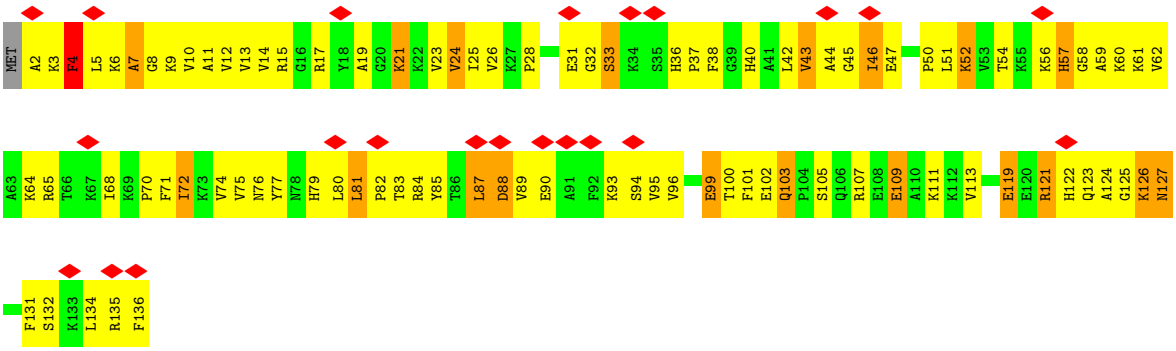


• Molecule 30: uL24 (yeast L26)



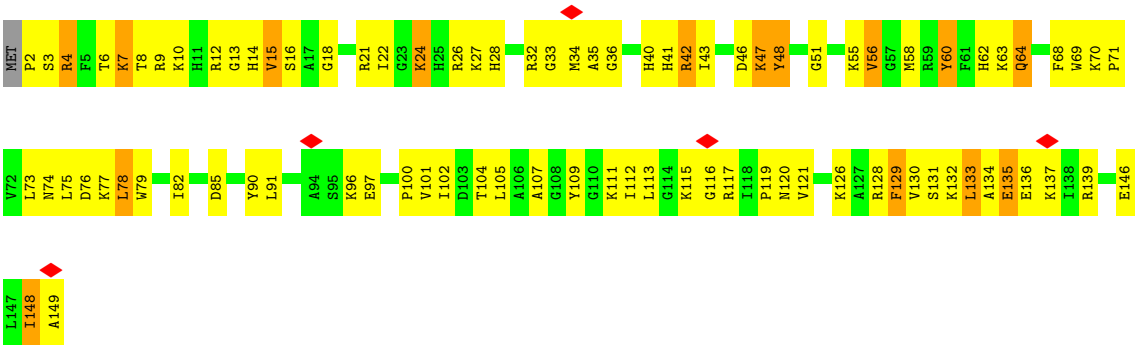
- Molecule 31: eL27 (yeast L27)

Chain EA:



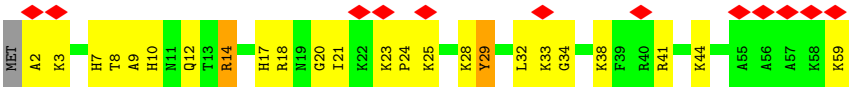
- Molecule 32: uL15 (yeast L28)

Chain FA:



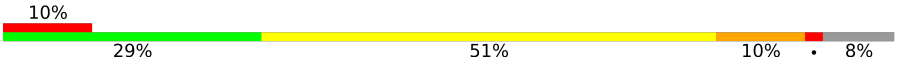
- Molecule 33: eL29 (yeast L29)

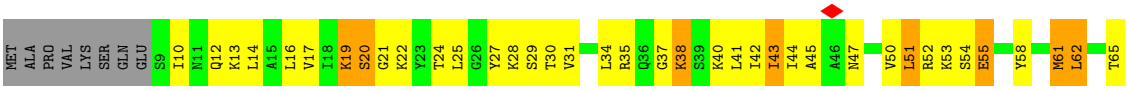
Chain GA:

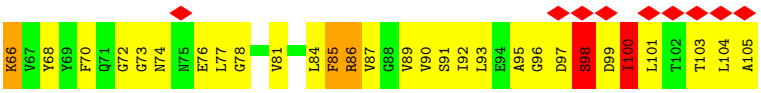


- Molecule 34: eL30 (yeast L30)

Chain HA:

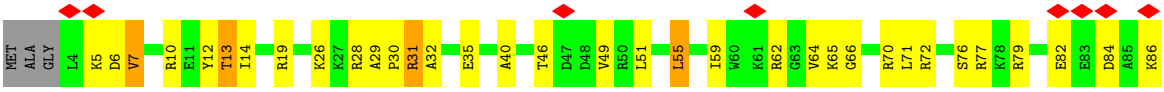


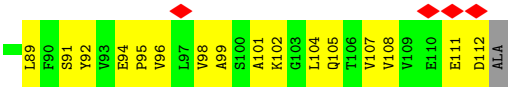




- Molecule 35: eL31 (yeast L31)

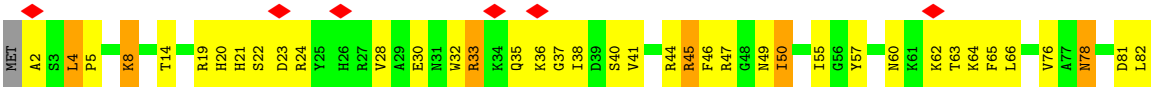
Chain IA:

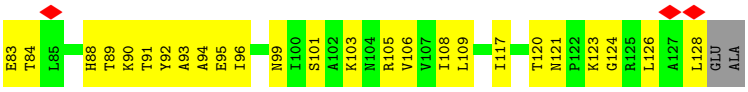




- Molecule 36: eL32 (yeast L32)

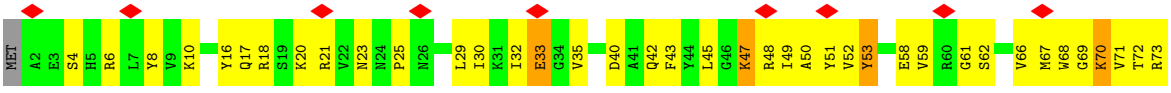
Chain JA:

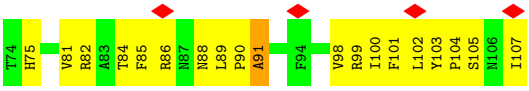




- Molecule 37: eL33 (yeast L33)

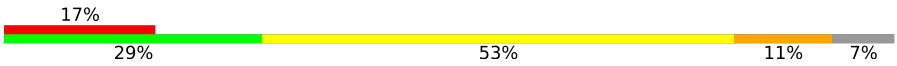
Chain KA:

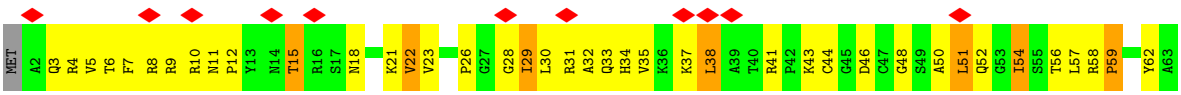


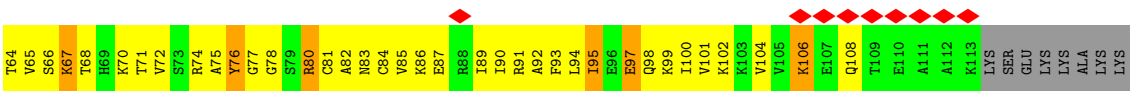


- Molecule 38: eL34 (yeast L34)

Chain LA:

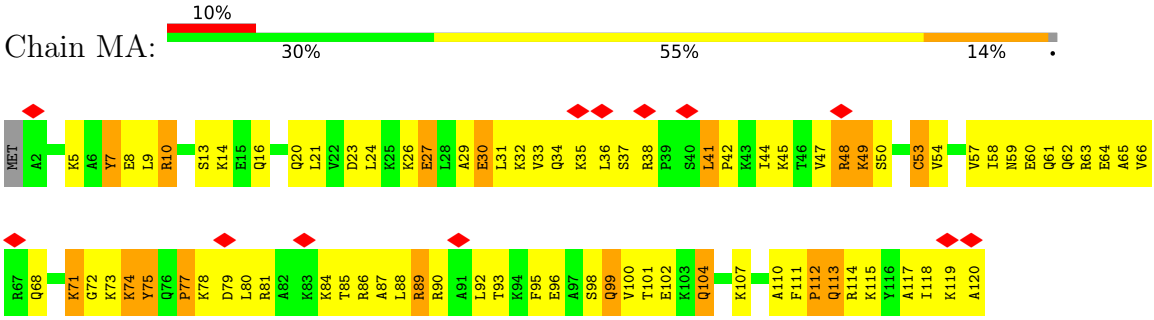






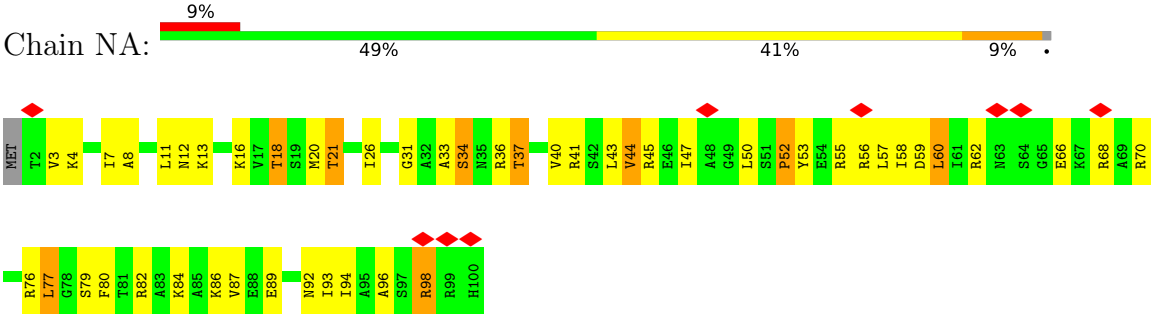
- Molecule 39: uL29 (yeast L35)

Chain MA:



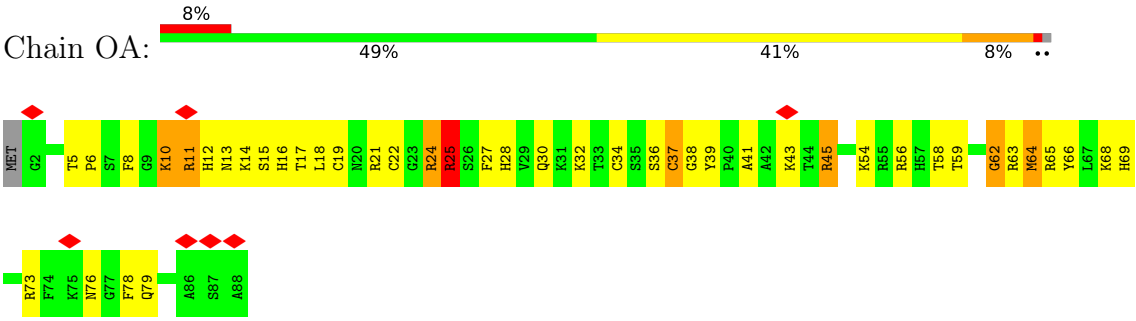
- Molecule 40: eL36 (yeast L36)

Chain NA:



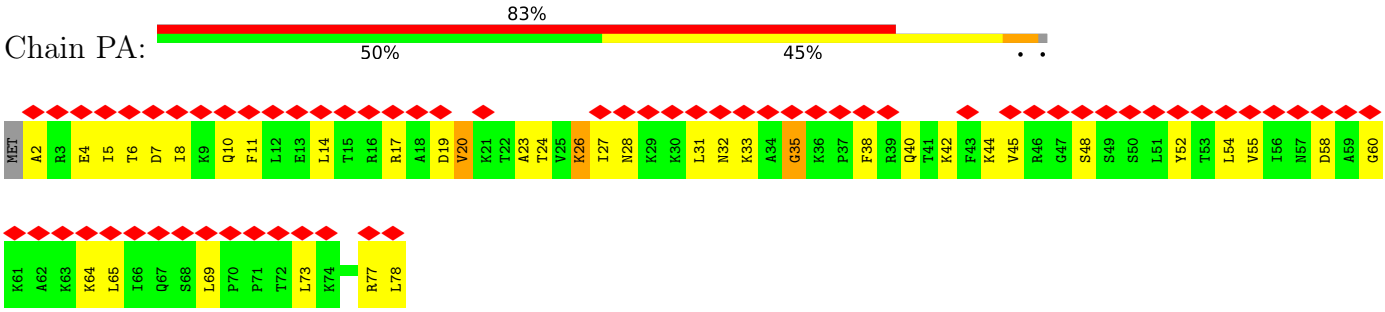
- Molecule 41: eL37 (yeast L37)

Chain OA:



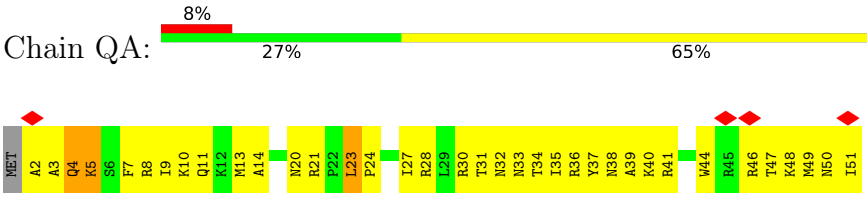
- Molecule 42: eL38 (yeast L38)

Chain PA:



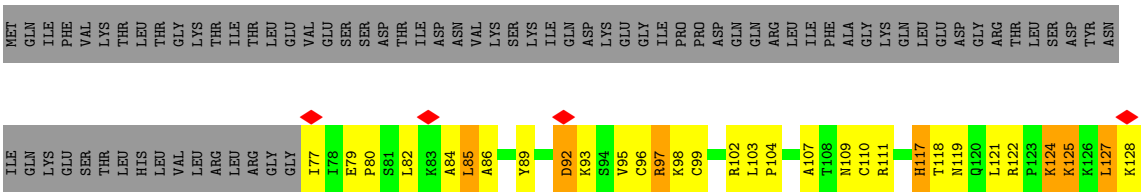
- Molecule 43: eL39 (yeast L39)

Chain QA:



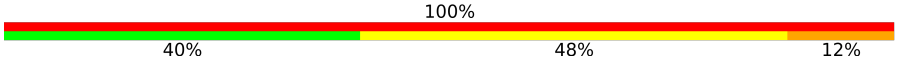
- Molecule 44: eL40 (yeast L40)

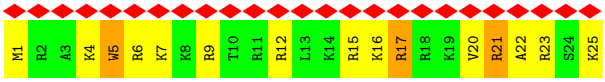
Chain RA:



- Molecule 45: eL41 (yeast L41)

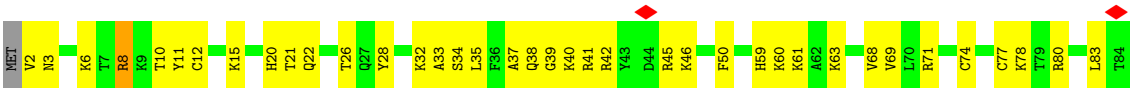
Chain SA:

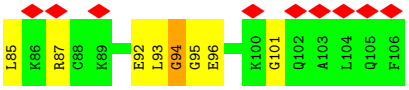




- Molecule 46: eL42 (yeast L42)

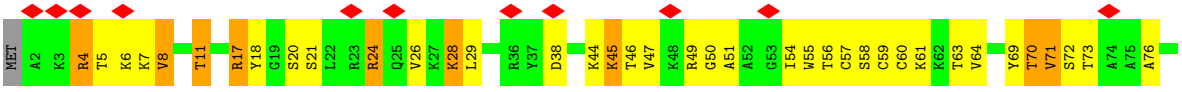
Chain TA:

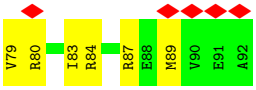




- Molecule 47: eL43 (yeast L43)

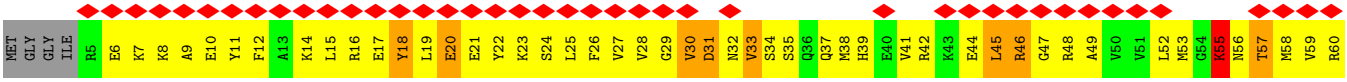
Chain UA:

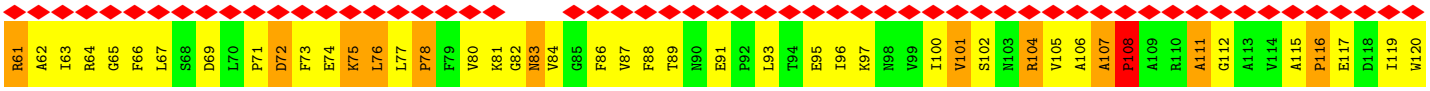


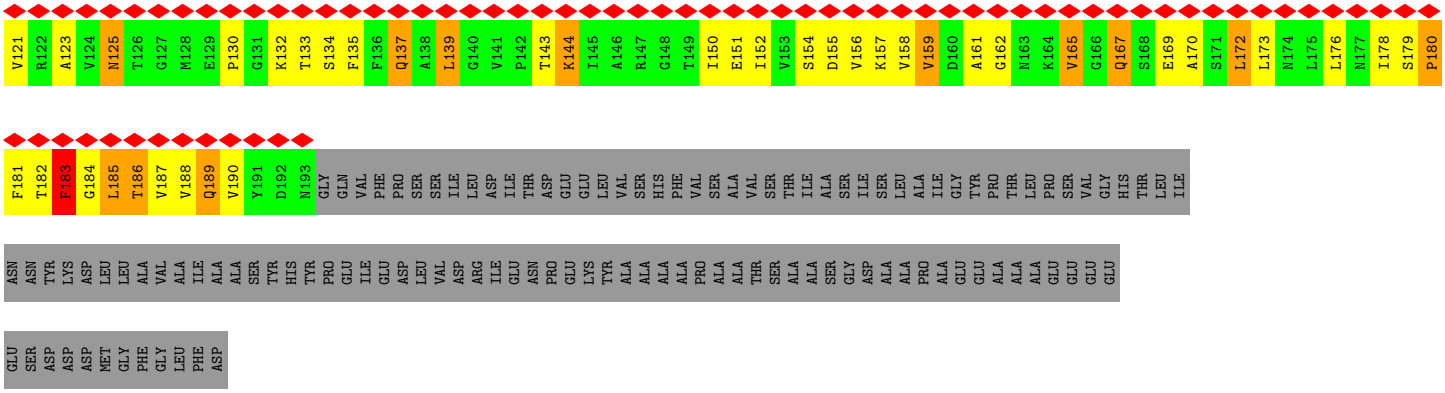


- Molecule 48: uL10 (yeast P0)

Chain VA:

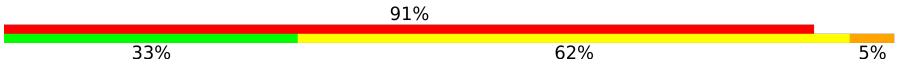






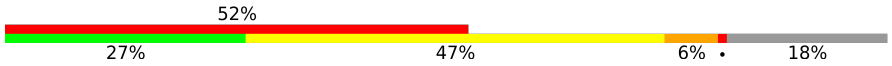
- Molecule 49: RACK1 (yeast Asc1)

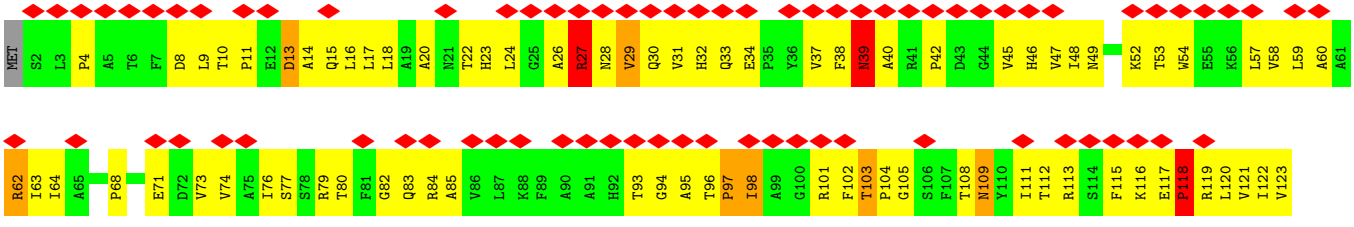
Chain WA:

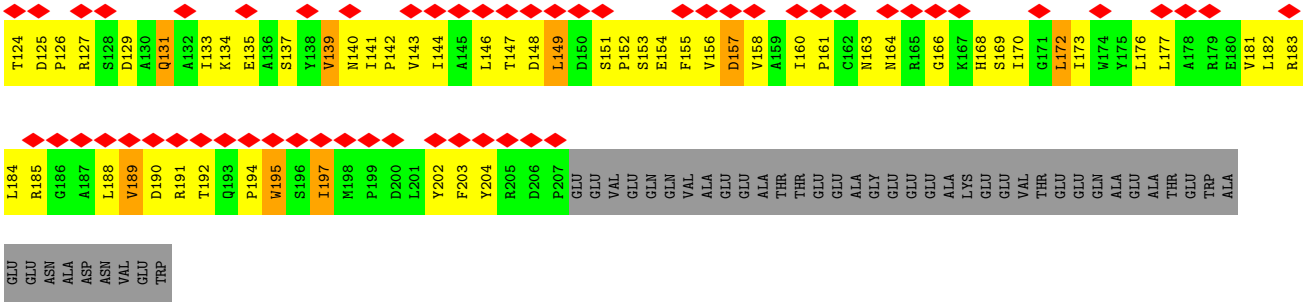


- Molecule 50: uS2 (yeast S0)

Chain XA:

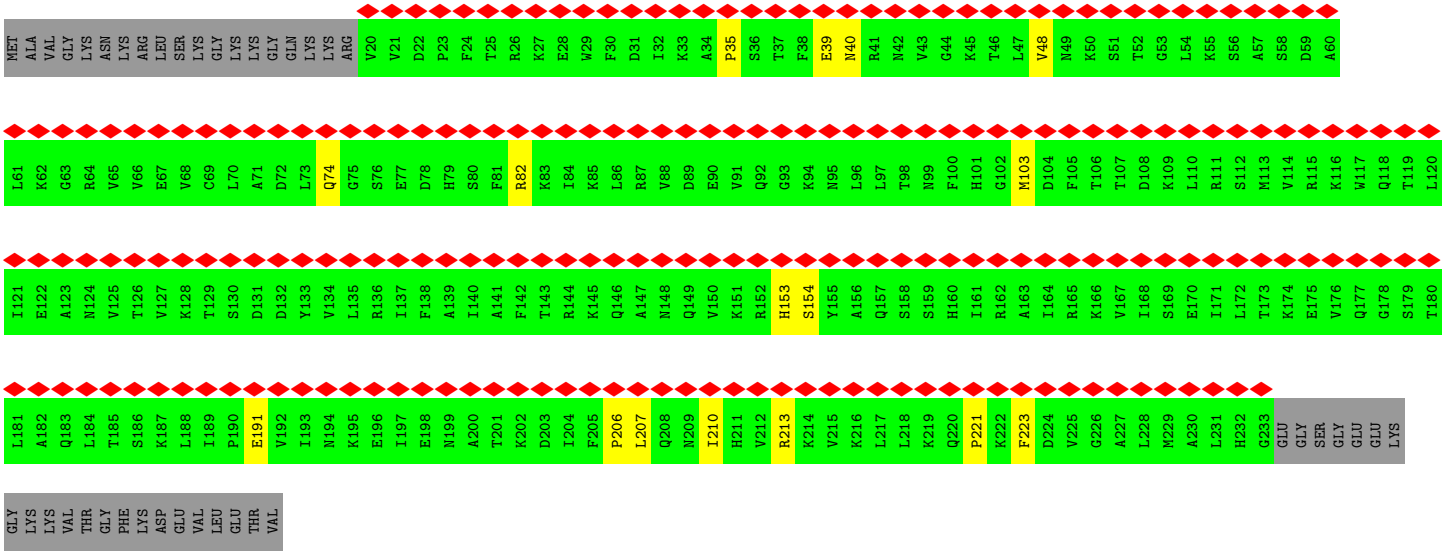






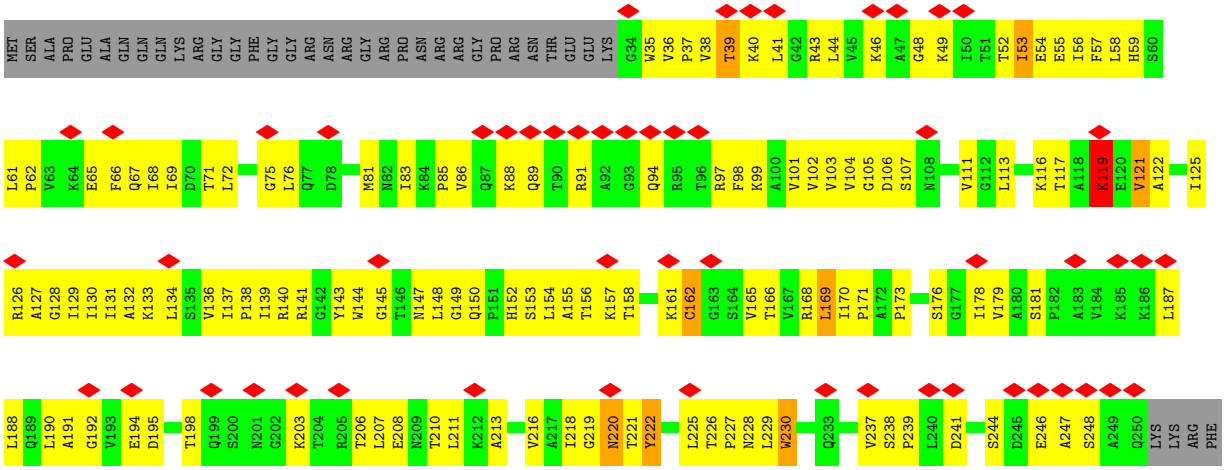
- Molecule 51: eS1 (yeast S1)

Chain YA:



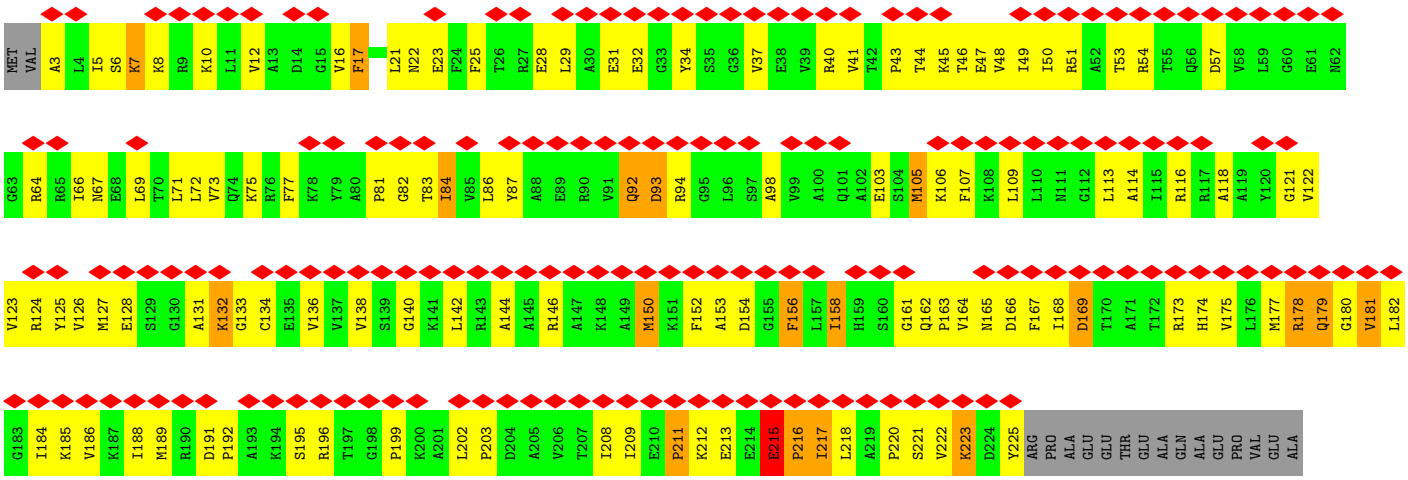
- Molecule 52: uS5 (yeast S2)

Chain ZA:



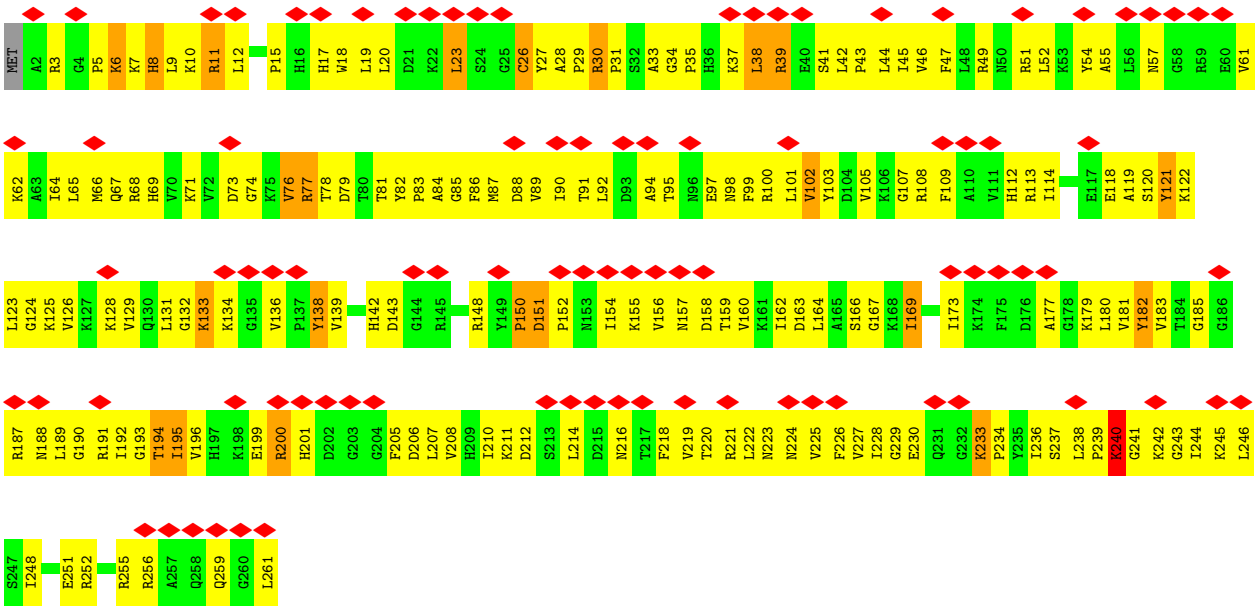
- Molecule 53: uS3 (yeast S3)

Chain AB: 72% (39% / 46% / 8% / 7%)



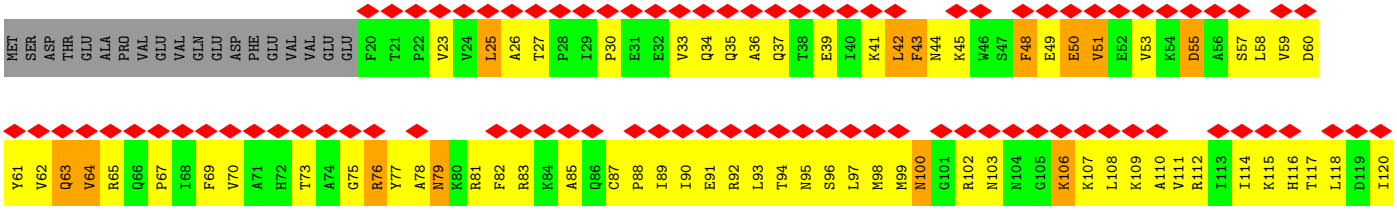
- Molecule 54: eS4 (yeast S4)

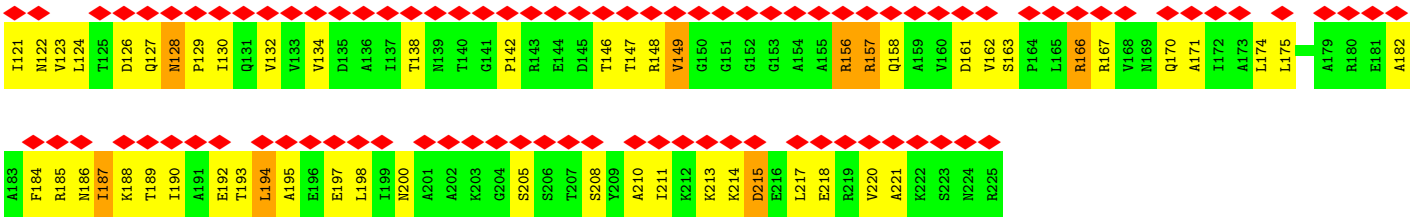
Chain BB: 35% (30% / 61% / 8%)



- Molecule 55: uS7 (yeast S5)

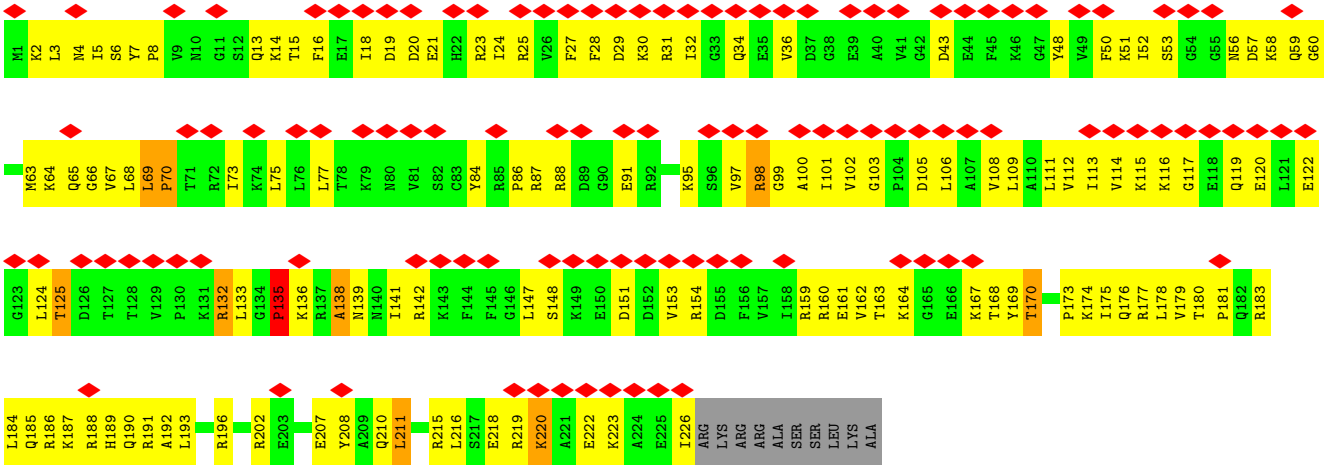
Chain CB: 80% (35% / 48% / 9% / 8%)





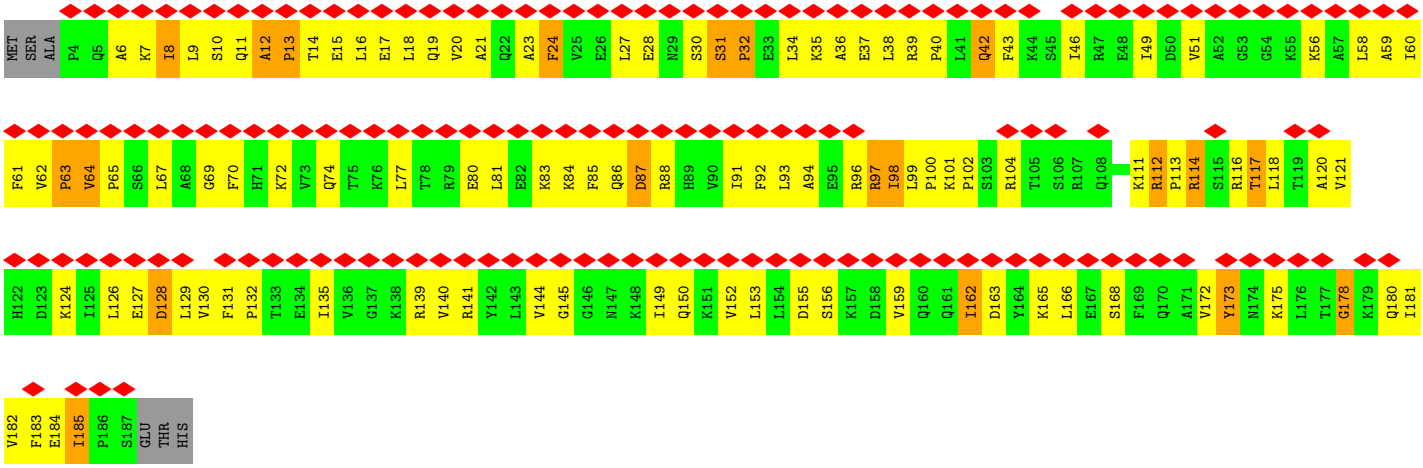
- Molecule 56: eS6 (yeast S6)

Chain DB:



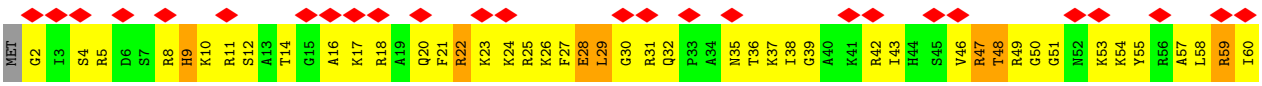
- Molecule 57: eS7 (yeast S7)

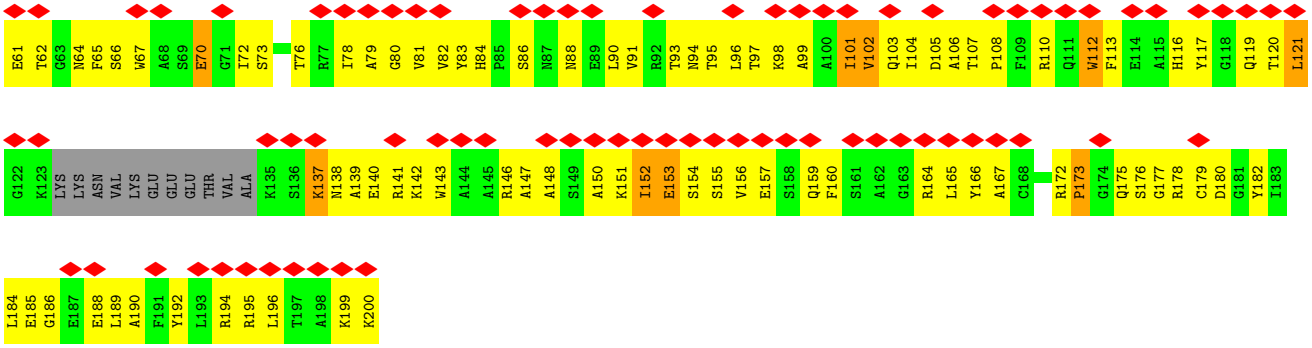
Chain EB:



- Molecule 58: eS8 (yeast S8)

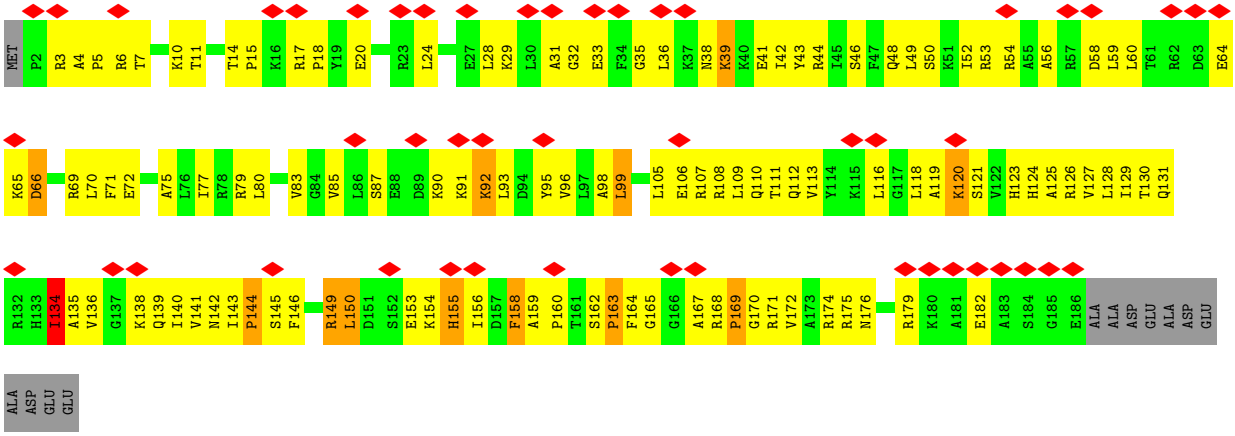
Chain FB:





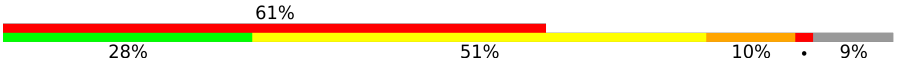
- Molecule 59: uS4 (yeast S9)

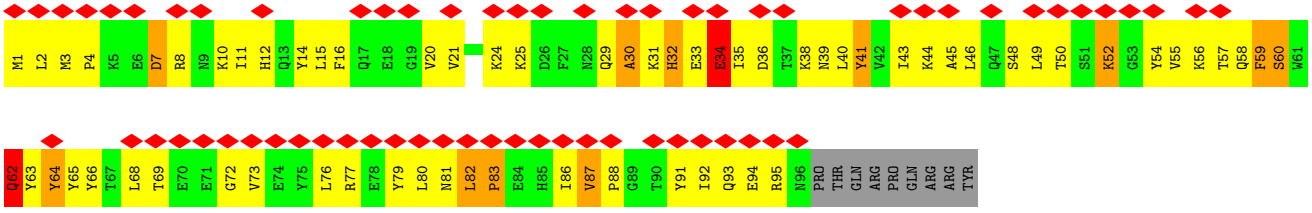
Chain GB:



- Molecule 60: eS10 (yeast S10)

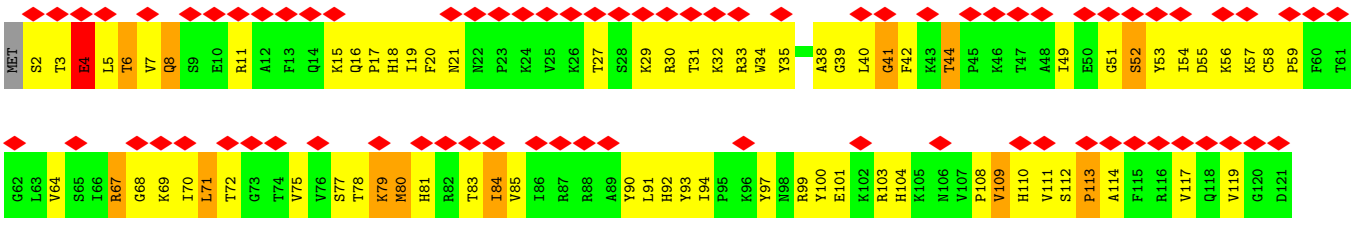
Chain HB:

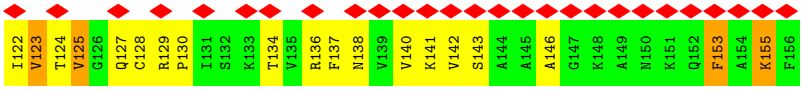




- Molecule 61: uS17 (yeast S11)

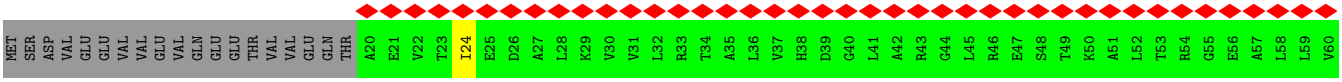
Chain IB:

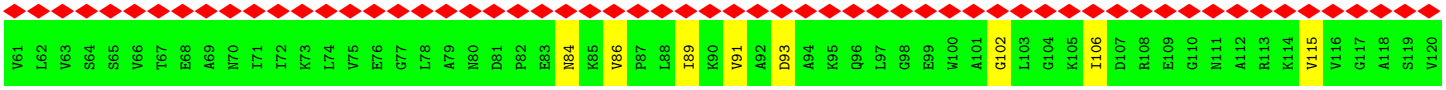


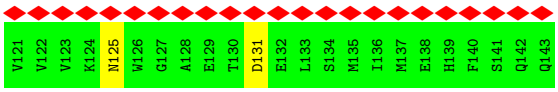


• Molecule 62: eS12 (yeast S12)

Chain JB:

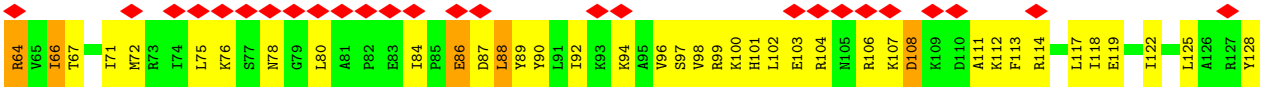


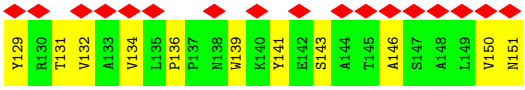




• Molecule 63: uS15 (yeast S13)

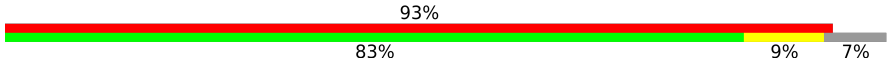
Chain KB:

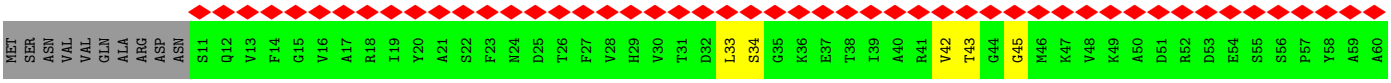


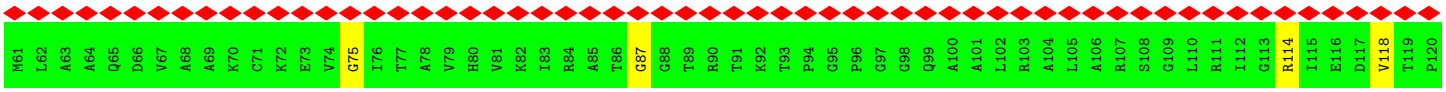


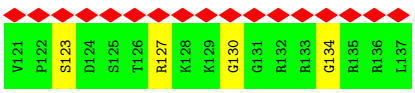
• Molecule 64: uS11 (yeast S14)

Chain LB:







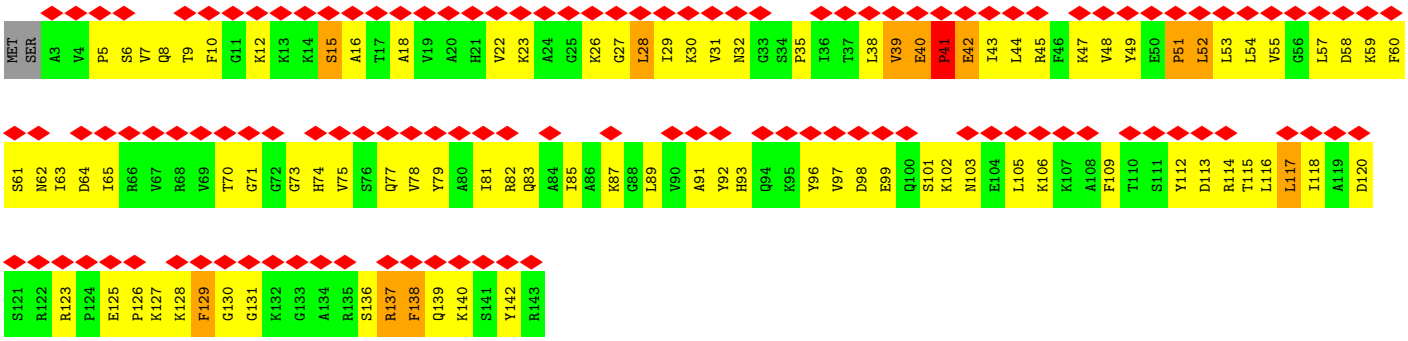


• Molecule 65: uS19 (yeast S15)

Chain MB:

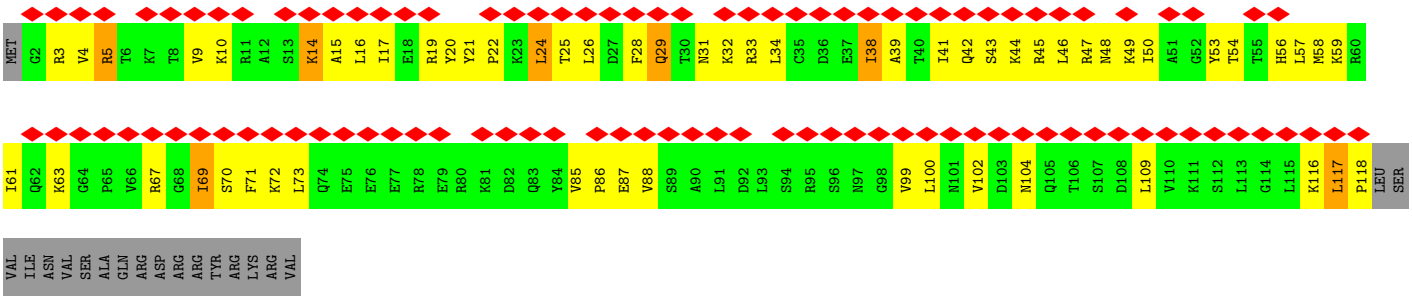
- Molecule 66: uS9 (yeast S16)

Chain NB:



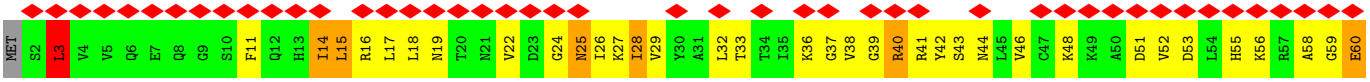
- Molecule 67: eS17 (yeast S17)

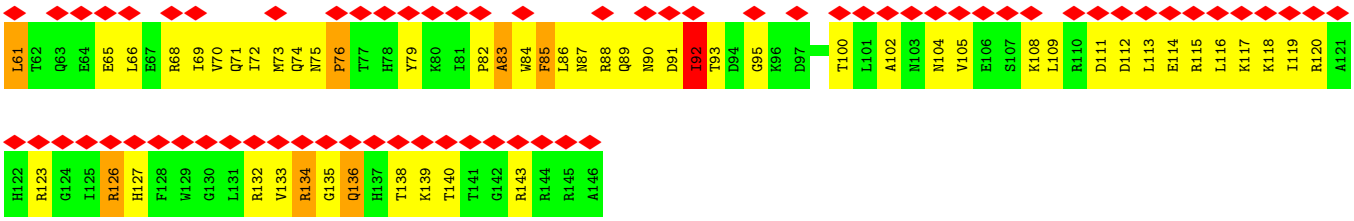
Chain OB:



- Molecule 68: uS13 (yeast S18)

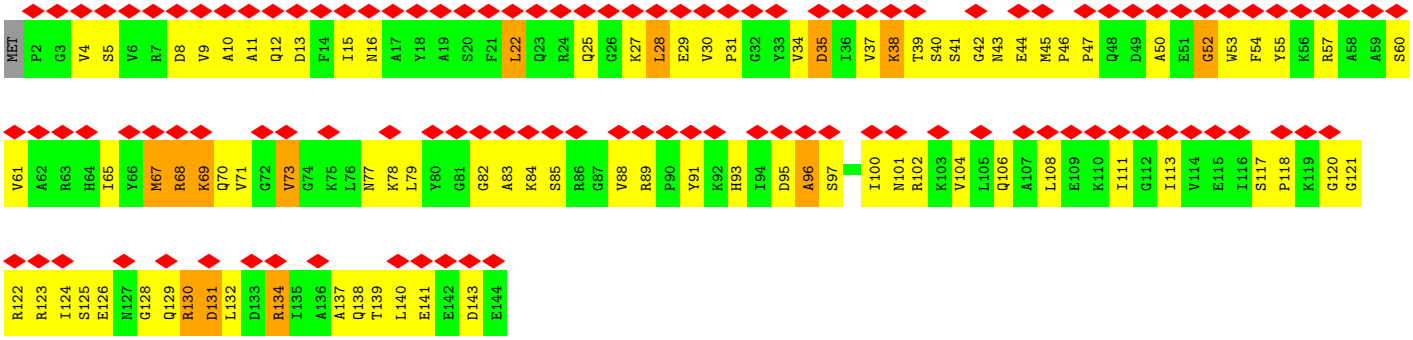
Chain PB:





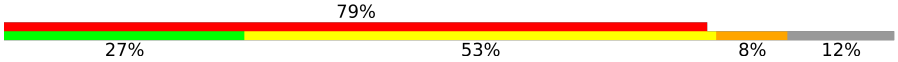
- Molecule 69: eS19 (yeast S19)

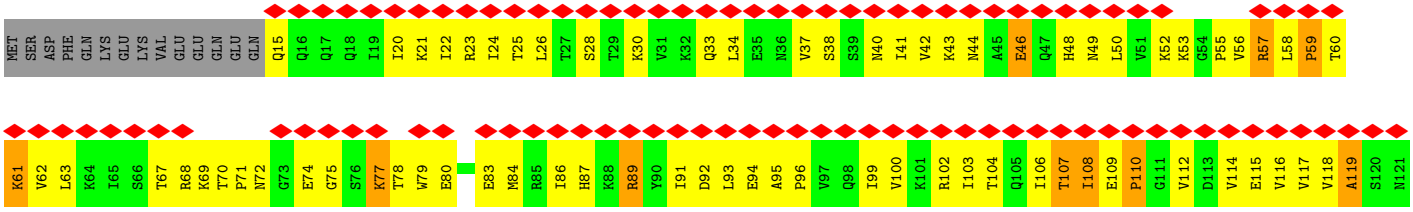
Chain QB:



- Molecule 70: uS10 (yeast S20)

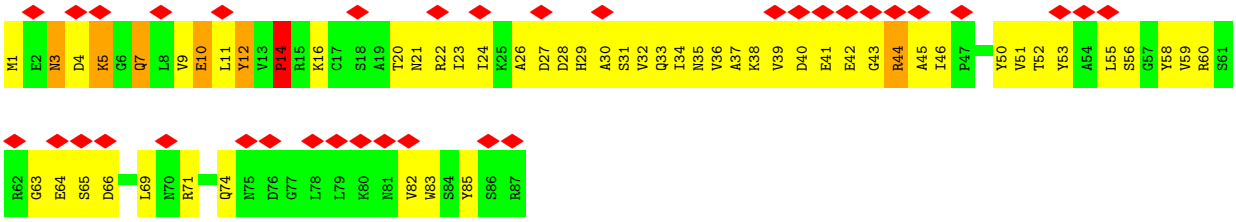
Chain RB:





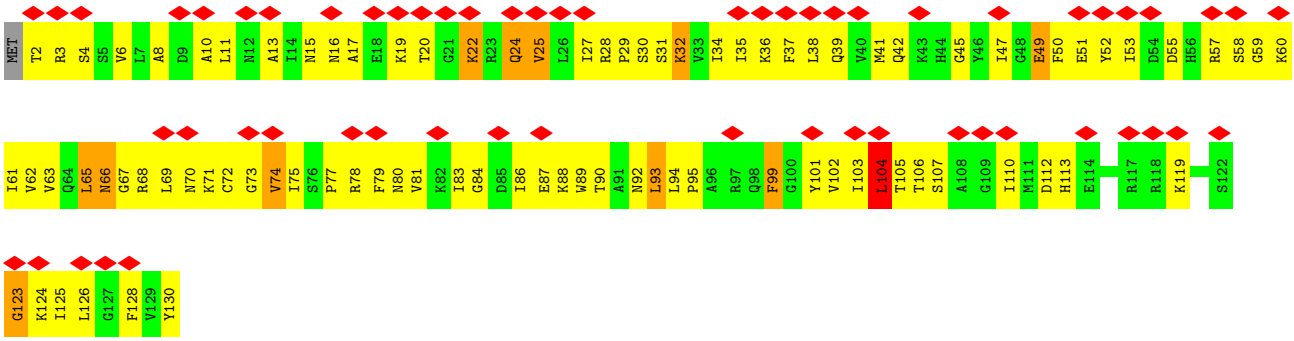
- Molecule 71: eS21 (yeast S21)

Chain SB:



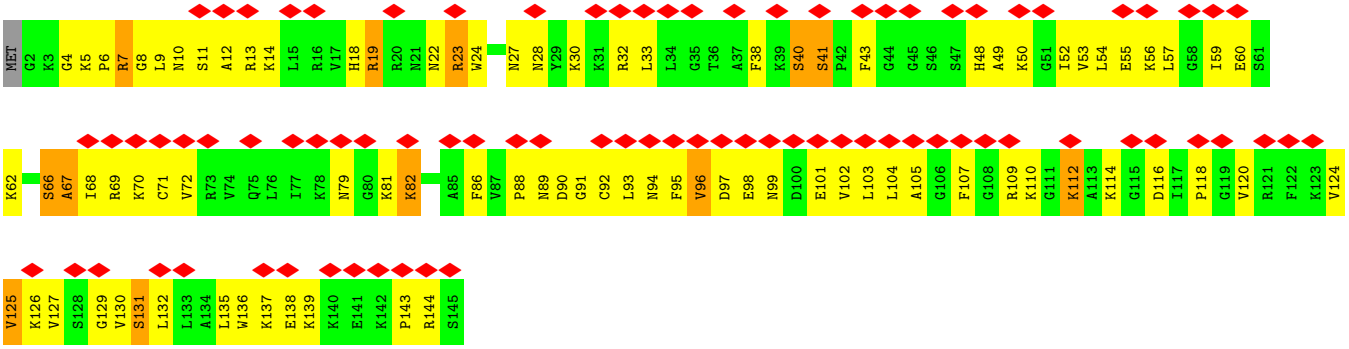
- Molecule 72: uS8 (yeast S22)

Chain TB:



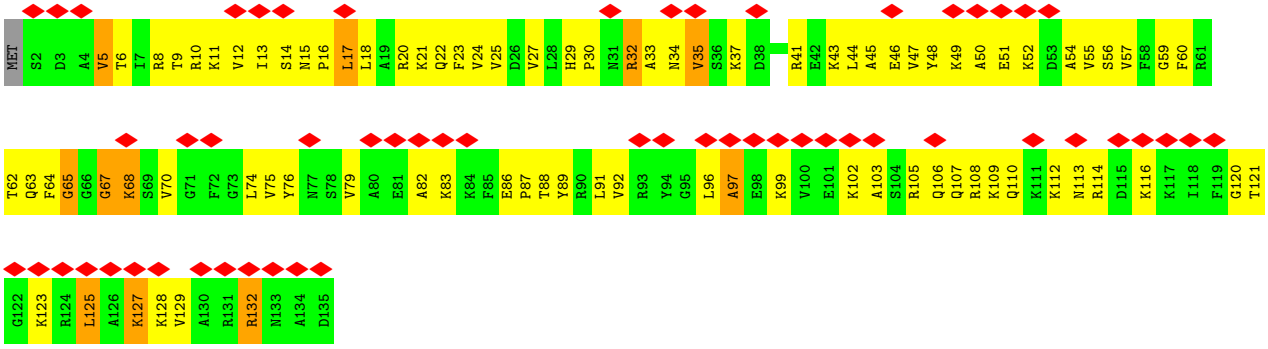
- Molecule 73: uS12 (yeast S23)

Chain UB:



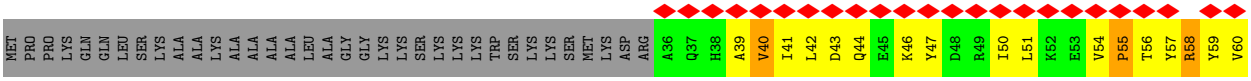
- Molecule 74: eS24 (yeast S24)

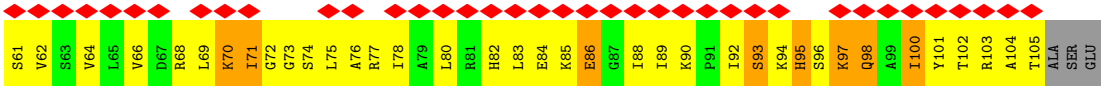
Chain VB:



- Molecule 75: eS25 (yeast S25)

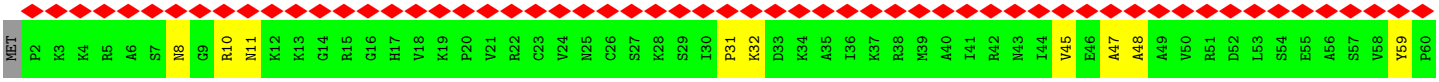
Chain WB:

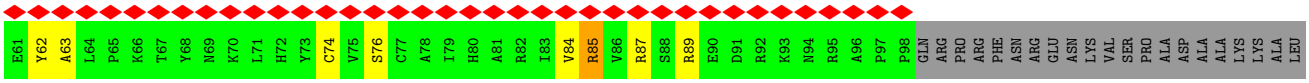




• Molecule 76: eS26 (yeast S26)

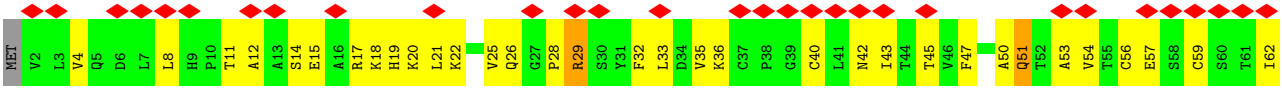
Chain XB:

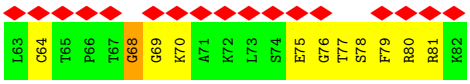




• Molecule 77: eS27 (yeast S27)

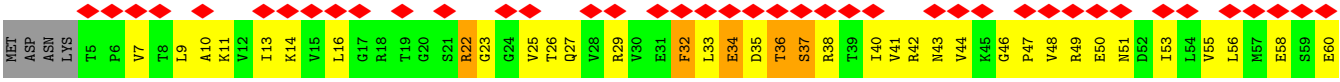
Chain YB:

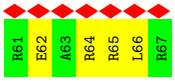




• Molecule 78: eS28 (yeast S28)

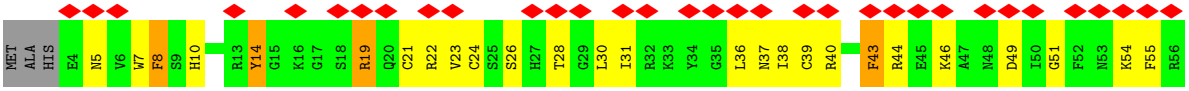
Chain ZB:





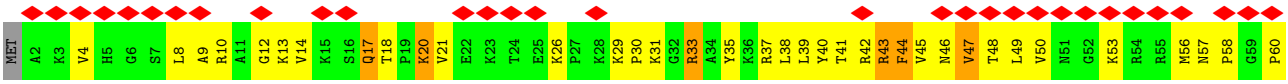
• Molecule 79: uS14 (yeast S29)

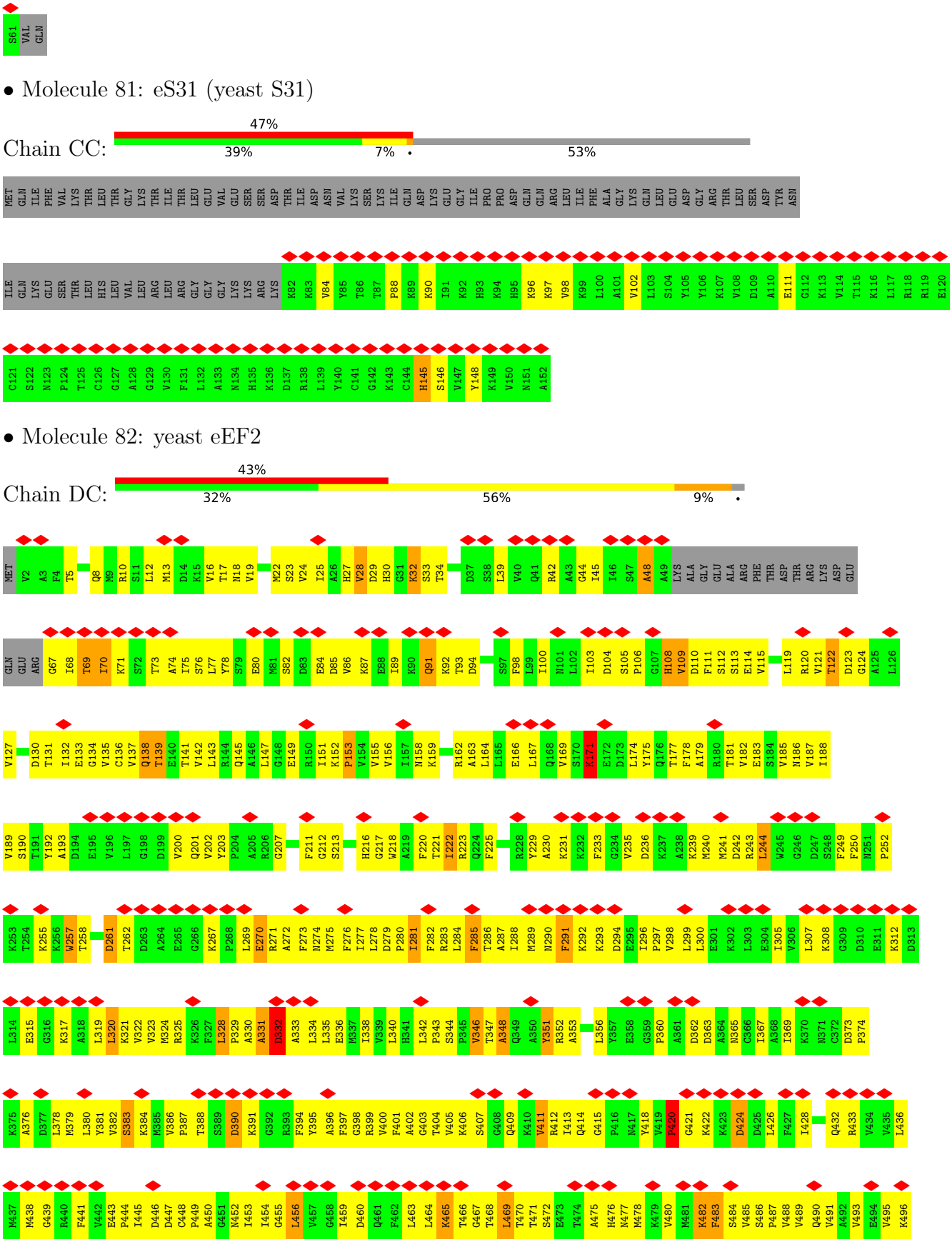
Chain AC:

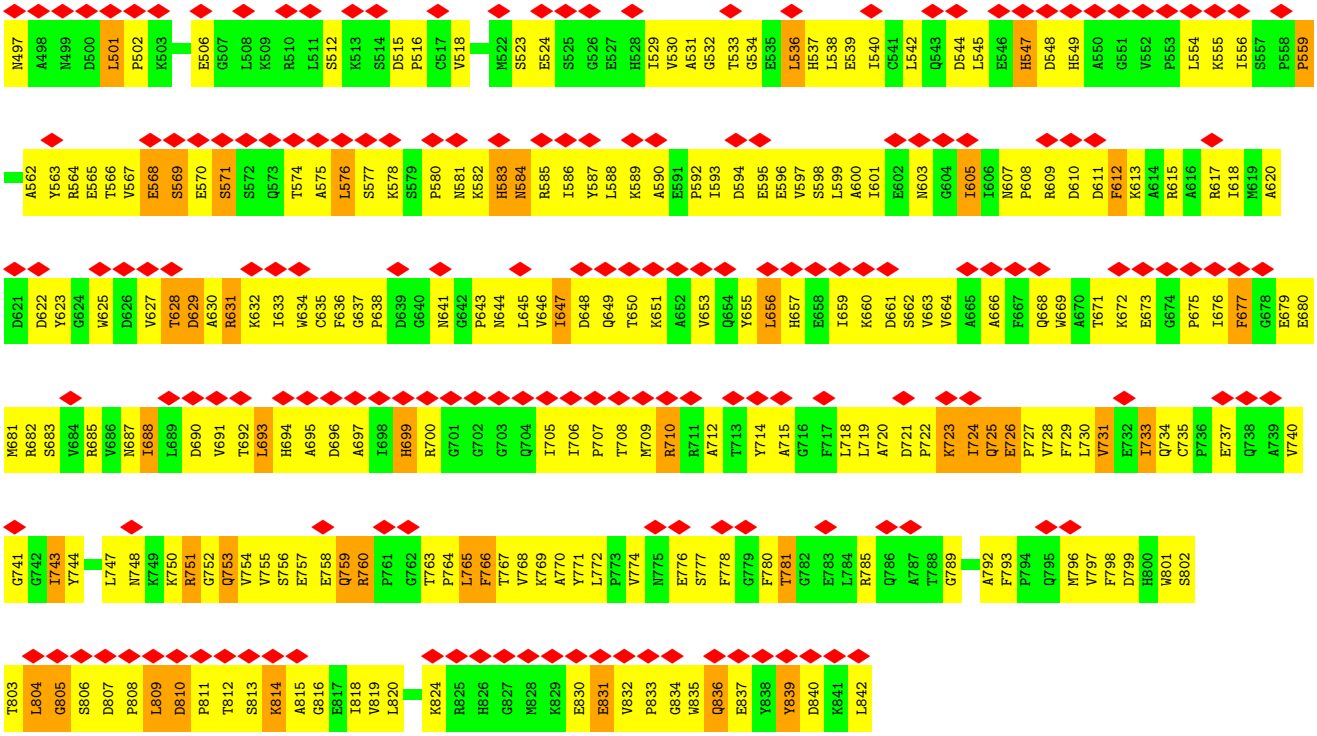


• Molecule 80: eS30 (yeast S30)

Chain BC:

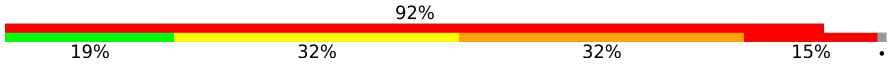


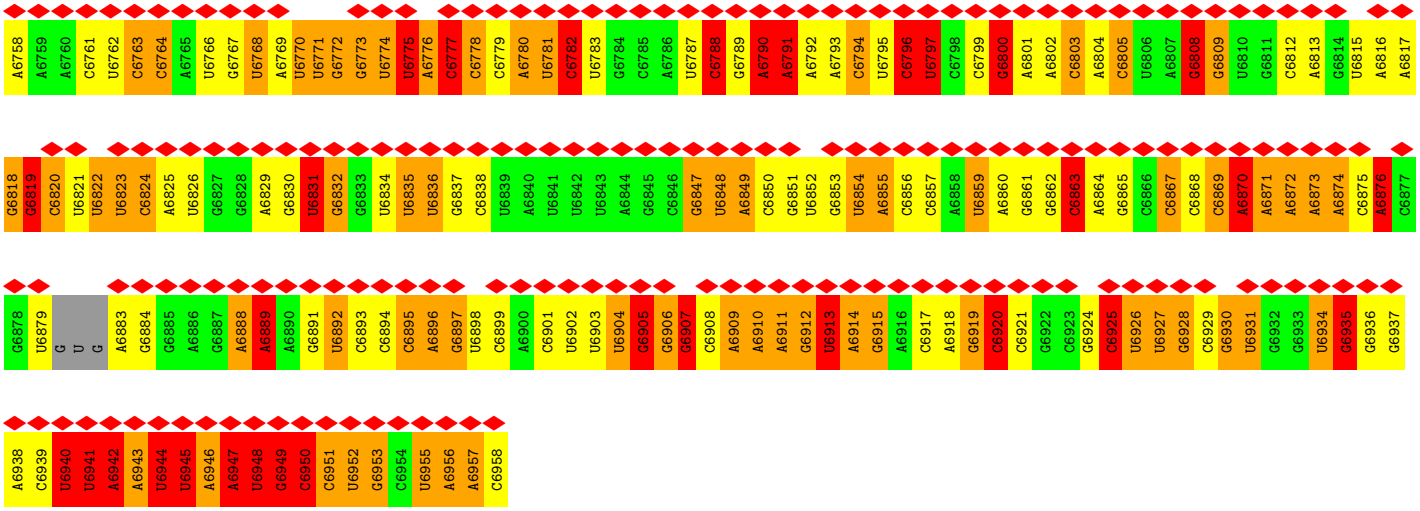

S61 VAL GLN
• Molecule 81: eS31 (yeast S31)
Chain CC:
47%
39%
7%
53%
MET GLN ILE PHE VAL LYS THR LEU THR GLY LYS THR ILE THR LEU GLU VAL GLU SER SER ASP THR ILE ASP ASN VAL LYS SER LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN
ILE GLN LYS GLU SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY GLY GLY LYS LYS ARG LYS K82 K83 V84 Y85 T86 T87 P88 K89 K90 I91 K92 H93 K94 H95 K96 K97 V98 K99 L100 A101 V102 L103 S104 Y105 Y106 K107 V108 D109 A110 E111 G112 K113 V114 T115 K116 L117 R118 R119 E120
C121 S122 N123 P124 T125 C126 G127 A128 G129 V130 F131 L132 A133 N134 H135 K136 D137 R138 L139 Y140 C141 G142 K143 C144 H145 S146 V147 Y148 K149 V150 N151 A152
• Molecule 82: yeast eEF2
Chain DC:
43%
32%
56%
9%
MET V2 A3 F4 T5 Q8 M9 R10 S11 L12 M13 D14 K15 V16 T17 N18 V19 M22 S23 V24 I25 A26 H27 V28 D29 H30 G31 K32 S33 T34 D37 S38 L39 V40 Q41 R42 A43 G44 I45 I46 S47 A48 A49 LYS ALA GLY GLU ALA ARG PHE THR ASP THR ARG LYS ASP GLU
GLN GLU ARG G67 I68 T69 I70 K71 S72 T73 A74 T75 S76 L77 Y78 S79 E80 M81 S82 D83 E84 D85 V86 K87 E88 I89 K90 Q91 K92 T93 D94 S97 F98 L99 I100 N101 L102 I103 D104 S105 P106 G107 H108 V109 D110 F111 S112 S113 E114 V115 L119 R120 V121 T122 D123 G124 A125 L126
V127 D130 T131 I132 E133 G134 V135 C136 V137 Q138 T139 E140 T141 V142 L143 R144 Q145 A146 L147 G148 E149 R150 I151 K152 P153 V154 V155 V156 I157 N158 K159 R162 A163 L164 L165 E166 L167 Q168 V169 S170 K171 E172 D173 L174 Y175 Q176 T177 F178 A179 R180 T181 V182 E183 S184 V185 N186 V187 I188
V189 S190 T191 Y192 A193 D194 E195 V196 L197 G198 D199 V200 Q201 V202 Y203 P204 A205 R206 G207 F211 G212 S213 H216 G217 W218 A219 F220 T221 I222 R223 Q224 F225 R228 Y229 A230 K231 K232 F233 G234 V235 D236 K237 A238 K239 M240 M241 D242 R243 L244 W245 G246 D247 S248 F249 F250 N251 P252
K253 T254 K255 K256 W257 T258 D261 T262 D263 A264 E265 G266 K267 P268 L269 E270 R271 A272 F273 N274 M275 F276 I277 L278 D279 P280 I281 F282 R283 L284 F285 T286 A287 I288 M289 N290 F291 K292 K293 D294 E295 I296 P297 V298 L299 L300 E301 K302 L303 E304 I305 V306 L307 K308 G309 D310 E311 K312 D313
L314 E315 G316 K317 A318 L319 L320 K321 V322 V323 M324 R325 K326 F327 L328 P329 A330 A331 D332 A333 L334 L335 E336 M337 I338 V339 L340 H341 L342 P343 S344 P345 V346 T347 A348 Q349 A350 Y351 R352 A353 L356 Y357 E358 G359 P360 A361 D362 D363 A364 N365 C366 I367 A368 I369 K370 N371 C372 D373 P374
K375 A376 D377 L378 M379 L380 Y381 V382 S383 K384 M385 V386 P387 T388 S389 D390 K391 G392 R393 F394 Y395 A396 F397 G398 R399 V400 F401 A402 G403 T404 V405 K406 S407 G408 Q409 K410 V411 R412 I413 Q414 G415 P416 N417 Y418 V419 P420 G421 K422 K423 D424 D425 L426 F427 I428 Q432 R433 V434 V435 L436
M437 M438 G439 R440 F441 V442 E443 P444 I445 D446 D447 C448 P449 A450 G451 N452 I453 I454 G455 L456 V457 G458 I459 D460 Q461 F462 L463 L464 K465 T466 G467 T468 L469 T470 T471 S472 E473 T474 A475 H476 N477 M478 K479 V480 M481 K482 F483 S484 V485 S486 P487 V488 V489 Q490 V491 A492 V493 E494 V495 K496



- Molecule 83: IRES

Chain EC:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.4	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	0.073	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DDE, MG, SO1, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	3/41014 (0.0%)	0.75	14/63809 (0.0%)
2	B	0.81	5/78631 (0.0%)	0.73	14/122552 (0.0%)
3	C	0.81	1/3747 (0.0%)	0.72	1/5832 (0.0%)
4	D	0.78	1/2884 (0.0%)	0.68	0/4491
5	E	2.02	2/1377 (0.1%)	0.83	1/1844 (0.1%)
6	F	0.80	0/1952	0.68	1/2622 (0.0%)
7	G	0.75	0/3153	0.62	0/4239
8	H	0.83	0/2802	0.67	0/3792
9	I	0.83	0/2426	0.62	0/3271
10	J	0.96	0/1425	0.68	0/1912
11	K	0.90	0/1822	0.66	1/2451 (0.0%)
12	L	0.79	0/1850	0.65	0/2495
13	M	0.82	0/1540	0.66	0/2073
14	N	0.93	0/1754	0.62	0/2350
15	O	0.77	0/1375	0.60	0/1842
16	P	1.93	0/728	0.86	2/975 (0.2%)
17	Q	0.82	0/1568	0.62	0/2106
18	R	0.91	0/1069	0.65	0/1438
19	S	0.84	0/1758	0.65	0/2354
20	T	0.81	0/1586	0.62	0/2128
21	U	0.83	0/1466	0.60	0/1968
22	V	0.84	0/1466	0.68	0/1965
23	W	0.76	0/1539	0.63	0/2050
24	X	0.93	0/1482	0.70	0/1990
25	Y	0.92	0/1301	0.62	0/1743
26	Z	0.71	0/812	0.54	0/1099
27	AA	0.80	0/1019	0.61	0/1369
28	BA	0.98	0/521	0.58	0/691
29	CA	0.88	0/984	0.71	1/1325 (0.1%)
30	DA	0.87	0/1005	0.67	1/1341 (0.1%)
31	EA	0.77	0/1119	0.59	0/1497
32	FA	0.79	0/1205	0.66	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	GA	0.79	0/474	0.59	0/629
34	HA	0.69	0/751	0.64	1/1008 (0.1%)
35	IA	0.72	0/904	0.61	0/1213
36	JA	0.85	0/1041	0.62	0/1394
37	KA	0.80	0/869	0.68	0/1168
38	LA	0.79	0/891	0.69	0/1191
39	MA	0.82	0/979	0.64	0/1301
40	NA	0.81	0/779	0.63	0/1034
41	OA	0.90	0/697	0.70	0/923
42	PA	0.83	0/619	0.61	0/826
43	QA	0.85	0/444	0.69	0/588
44	RA	0.88	0/424	0.66	0/562
45	SA	1.55	0/235	0.81	0/300
46	TA	0.86	0/861	0.65	0/1136
47	UA	0.78	0/702	0.65	0/934
48	VA	1.80	0/1498	1.03	9/2025 (0.4%)
49	WA	0.90	0/2498	0.60	0/3398
50	XA	0.66	0/1653	0.57	0/2261
51	YA	1.17	0/855	0.56	0/1067
52	ZA	0.66	0/1665	0.58	0/2263
53	AB	0.86	0/1759	0.59	0/2368
54	BB	0.81	0/2110	0.63	0/2839
55	CB	0.83	0/1630	0.58	0/2202
56	DB	0.83	0/1844	0.59	0/2464
57	EB	0.87	0/1506	0.60	0/2028
58	FB	0.93	0/1515	0.63	0/2021
59	GB	0.70	0/1519	0.59	0/2035
60	HB	0.98	0/837	0.59	0/1131
61	IB	0.95	0/1273	0.62	0/1712
62	JB	1.12	0/495	0.58	0/617
63	KB	0.88	0/1216	0.59	0/1638
64	LB	1.10	0/507	0.60	0/632
65	MB	0.97	0/996	0.63	0/1335
66	NB	0.90	0/1126	0.63	0/1510
67	OB	0.76	0/844	0.84	4/1120 (0.4%)
68	PB	0.88	0/1212	0.60	1/1628 (0.1%)
69	QB	0.86	0/1131	0.59	0/1517
70	RB	0.91	0/866	0.60	0/1169
71	SB	0.67	0/694	0.57	0/935
72	TB	0.74	0/1039	0.64	1/1395 (0.1%)
73	UB	0.82	0/1140	0.62	0/1518
74	VB	0.80	0/1088	0.57	0/1449
75	WB	0.87	0/571	0.59	0/768

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	XB	1.15	0/387	0.60	0/482
77	YB	0.81	0/621	0.59	0/838
78	ZB	0.84	0/500	0.60	0/670
79	AC	0.94	0/454	0.56	0/602
80	BC	0.82	0/483	0.62	0/643
81	CC	1.03	0/283	0.64	0/352
82	DC	1.42	0/6521	0.70	1/8830 (0.0%)
83	EC	2.32	82/4579 (1.8%)	0.94	15/7119 (0.2%)
All	All	0.94	94/227965 (0.0%)	0.71	68/334014 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
2	B	0	70
3	C	0	4
48	VA	0	2
82	DC	0	1
83	EC	0	9
All	All	0	104

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	EC	6831	U	N1-C2	7.29	1.45	1.38
83	EC	6908	C	N1-C2	7.27	1.47	1.40
83	EC	6867	C	N1-C2	7.03	1.47	1.40
2	B	2263	C	N1-C2	6.96	1.47	1.40
4	D	1	G	OP3-P	-6.96	1.52	1.61

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	VA	108	PRO	CB-CA-C	-16.97	69.58	112.00
67	OB	73	LEU	N-CA-C	9.72	137.25	111.00
48	VA	108	PRO	CA-C-N	-8.74	97.97	117.20
83	EC	6788	C	N1-C1'-C2'	8.43	124.96	114.00
1	A	1339	C	N1-C1'-C2'	8.29	124.78	114.00

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	G	Sidechain
1	A	199	G	Sidechain
1	A	207	U	Sidechain
1	A	287	G	Sidechain
1	A	60	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36760	0	18348	1440	0
2	B	70288	0	35262	2381	0
3	C	3354	0	1695	114	0
4	D	2580	0	1304	103	0
5	E	1359	0	1425	110	0
6	F	1918	0	1987	209	0
7	G	3082	0	3165	226	0
8	H	2750	0	2863	225	0
9	I	2376	0	2325	197	0
10	J	1401	0	1501	88	0
11	K	1785	0	1862	134	0
12	L	1818	0	1908	178	0
13	M	1519	0	1587	116	0
14	N	1718	0	1754	136	0
15	O	1354	0	1383	102	0
16	P	723	0	774	128	0
17	Q	1543	0	1608	145	0
18	R	1054	0	1149	87	0
19	S	1721	0	1779	155	0
20	T	1556	0	1659	98	0
21	U	1443	0	1485	99	0
22	V	1442	0	1543	117	0
23	W	1522	0	1617	104	0
24	X	1446	0	1487	145	0
25	Y	1277	0	1323	107	0
26	Z	796	0	812	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	1004	0	1048	71	0
28	BA	509	0	537	35	0
29	CA	969	0	1036	80	0
30	DA	994	0	1081	100	0
31	EA	1093	0	1155	102	0
32	FA	1174	0	1215	119	0
33	GA	463	0	491	20	0
34	HA	743	0	797	91	0
35	IA	890	0	938	44	0
36	JA	1020	0	1090	60	0
37	KA	851	0	880	59	0
38	LA	881	0	949	101	0
39	MA	970	0	1078	108	0
40	NA	772	0	849	43	0
41	OA	682	0	687	55	0
42	PA	613	0	682	36	0
43	QA	437	0	475	43	0
44	RA	418	0	459	33	0
45	SA	234	0	284	12	0
46	TA	848	0	918	36	0
47	UA	695	0	738	52	0
48	VA	1473	0	1514	186	0
49	WA	2445	0	2401	213	0
50	XA	1612	0	1623	134	0
51	YA	856	0	226	0	0
52	ZA	1635	0	1723	131	0
53	AB	1734	0	1817	132	0
54	BB	2069	0	2154	263	0
55	CB	1610	0	1675	140	0
56	DB	1820	0	1918	153	0
57	EB	1481	0	1572	131	0
58	FB	1490	0	1525	146	0
59	GB	1494	0	1573	154	0
60	HB	817	0	804	76	0
61	IB	1245	0	1314	106	0
62	JB	496	0	141	0	0
63	KB	1193	0	1255	87	0
64	LB	508	0	151	2	0
65	MB	975	0	1017	88	0
66	NB	1106	0	1166	101	0
67	OB	836	0	827	61	0
68	PB	1193	0	1222	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	QB	1113	0	1124	89	0
70	RB	856	0	917	91	0
71	SB	685	0	672	66	0
72	TB	1022	0	1060	84	0
73	UB	1122	0	1196	103	0
74	VB	1074	0	1132	112	0
75	WB	563	0	603	59	0
76	XB	388	0	96	3	0
77	YB	611	0	633	41	0
78	ZB	498	0	535	48	0
79	AC	444	0	436	34	0
80	BC	475	0	525	48	0
81	CC	284	0	76	1	0
82	DC	6419	0	6493	651	0
83	EC	4105	0	2063	133	0
84	DC	28	0	12	5	0
85	DC	1	0	0	0	0
86	DC	35	0	42	3	0
All	All	212656	0	156225	10781	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 29.

The worst 5 of 10781 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)
83:EC:6927:U:H3'	83:EC:6928:G:H5'	1.22	1.17
2:B:1235:U:H4'	2:B:1236:G:H5'	1.17	1.14
48:VA:108:PRO:HA	48:VA:179:SER:HA	1.14	1.13
1:A:230:C:H3'	1:A:231:U:H5"	1.31	1.12
58:FB:12:SER:HA	58:FB:18:ARG:HH21	1.10	1.11

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	
5	E	165/217 (76%)	128 (78%)	27 (16%)	10 (6%)	1	15
6	F	250/254 (98%)	175 (70%)	61 (24%)	14 (6%)	2	17
7	G	384/387 (99%)	305 (79%)	64 (17%)	15 (4%)	3	25
8	H	359/362 (99%)	255 (71%)	70 (20%)	34 (10%)	0	8
9	I	294/297 (99%)	217 (74%)	58 (20%)	19 (6%)	1	14
10	J	173/176 (98%)	131 (76%)	34 (20%)	8 (5%)	2	21
11	K	220/244 (90%)	171 (78%)	40 (18%)	9 (4%)	3	23
12	L	231/256 (90%)	168 (73%)	44 (19%)	19 (8%)	1	9
13	M	189/191 (99%)	140 (74%)	39 (21%)	10 (5%)	2	17
14	N	207/221 (94%)	161 (78%)	36 (17%)	10 (5%)	2	20
15	O	167/174 (96%)	126 (75%)	26 (16%)	15 (9%)	1	8
16	P	92/165 (56%)	65 (71%)	20 (22%)	7 (8%)	1	10
17	Q	191/199 (96%)	142 (74%)	40 (21%)	9 (5%)	2	20
18	R	134/138 (97%)	107 (80%)	16 (12%)	11 (8%)	1	9
19	S	201/204 (98%)	150 (75%)	45 (22%)	6 (3%)	4	30
20	T	195/199 (98%)	158 (81%)	33 (17%)	4 (2%)	7	38
21	U	181/184 (98%)	150 (83%)	24 (13%)	7 (4%)	3	25
22	V	183/186 (98%)	133 (73%)	43 (24%)	7 (4%)	3	25
23	W	186/189 (98%)	153 (82%)	26 (14%)	7 (4%)	3	25
24	X	170/172 (99%)	131 (77%)	28 (16%)	11 (6%)	1	14
25	Y	157/160 (98%)	124 (79%)	21 (13%)	12 (8%)	1	10
26	Z	98/121 (81%)	72 (74%)	21 (21%)	5 (5%)	2	19
27	AA	134/137 (98%)	114 (85%)	19 (14%)	1 (1%)	22	61
28	BA	59/155 (38%)	47 (80%)	7 (12%)	5 (8%)	1	9
29	CA	119/142 (84%)	92 (77%)	19 (16%)	8 (7%)	1	13
30	DA	124/127 (98%)	88 (71%)	30 (24%)	6 (5%)	2	20
31	EA	133/136 (98%)	95 (71%)	27 (20%)	11 (8%)	1	9
32	FA	146/149 (98%)	105 (72%)	30 (20%)	11 (8%)	1	11
33	GA	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	2	17
34	HA	95/105 (90%)	71 (75%)	19 (20%)	5 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	IA	107/113 (95%)	89 (83%)	14 (13%)	4 (4%)	3	26
36	JA	125/130 (96%)	102 (82%)	20 (16%)	3 (2%)	6	35
37	KA	104/107 (97%)	89 (86%)	10 (10%)	5 (5%)	2	20
38	LA	110/121 (91%)	87 (79%)	18 (16%)	5 (4%)	2	21
39	MA	117/120 (98%)	91 (78%)	19 (16%)	7 (6%)	1	15
40	NA	97/100 (97%)	70 (72%)	18 (19%)	9 (9%)	0	8
41	OA	85/88 (97%)	59 (69%)	20 (24%)	6 (7%)	1	12
42	PA	75/78 (96%)	61 (81%)	11 (15%)	3 (4%)	3	24
43	QA	48/51 (94%)	37 (77%)	8 (17%)	3 (6%)	1	14
44	RA	50/128 (39%)	39 (78%)	5 (10%)	6 (12%)	0	5
45	SA	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	22
46	TA	103/106 (97%)	78 (76%)	19 (18%)	6 (6%)	1	16
47	UA	89/92 (97%)	74 (83%)	13 (15%)	2 (2%)	6	37
48	VA	187/312 (60%)	138 (74%)	32 (17%)	17 (9%)	1	8
49	WA	316/319 (99%)	230 (73%)	73 (23%)	13 (4%)	3	23
50	XA	204/252 (81%)	147 (72%)	42 (21%)	15 (7%)	1	11
51	YA	212/255 (83%)	150 (71%)	46 (22%)	16 (8%)	1	11
52	ZA	215/254 (85%)	160 (74%)	47 (22%)	8 (4%)	3	26
53	AB	221/240 (92%)	168 (76%)	40 (18%)	13 (6%)	1	15
54	BB	258/261 (99%)	183 (71%)	61 (24%)	14 (5%)	2	17
55	CB	204/225 (91%)	155 (76%)	39 (19%)	10 (5%)	2	19
56	DB	224/236 (95%)	172 (77%)	42 (19%)	10 (4%)	2	21
57	EB	182/190 (96%)	124 (68%)	39 (21%)	19 (10%)	0	7
58	FB	184/200 (92%)	136 (74%)	33 (18%)	15 (8%)	1	9
59	GB	183/197 (93%)	142 (78%)	28 (15%)	13 (7%)	1	12
60	HB	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	0	8
61	IB	153/156 (98%)	97 (63%)	42 (28%)	14 (9%)	1	8
62	JB	122/143 (85%)	80 (66%)	31 (25%)	11 (9%)	1	8
63	KB	148/151 (98%)	118 (80%)	23 (16%)	7 (5%)	2	20
64	LB	125/137 (91%)	85 (68%)	30 (24%)	10 (8%)	1	10
65	MB	120/142 (84%)	82 (68%)	21 (18%)	17 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	109 (78%)	21 (15%)	9 (6%)	1	14
67	OB	115/136 (85%)	85 (74%)	23 (20%)	7 (6%)	1	15
68	PB	143/146 (98%)	111 (78%)	22 (15%)	10 (7%)	1	12
69	QB	141/144 (98%)	120 (85%)	15 (11%)	6 (4%)	2	22
70	RB	105/121 (87%)	79 (75%)	21 (20%)	5 (5%)	2	20
71	SB	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	1	9
72	TB	127/130 (98%)	92 (72%)	29 (23%)	6 (5%)	2	20
73	UB	142/145 (98%)	98 (69%)	29 (20%)	15 (11%)	0	7
74	VB	132/135 (98%)	100 (76%)	26 (20%)	6 (4%)	2	21
75	WB	68/108 (63%)	51 (75%)	7 (10%)	10 (15%)	0	3
76	XB	95/119 (80%)	56 (59%)	26 (27%)	13 (14%)	0	4
77	YB	79/82 (96%)	53 (67%)	22 (28%)	4 (5%)	2	19
78	ZB	61/67 (91%)	44 (72%)	15 (25%)	2 (3%)	4	28
79	AC	51/56 (91%)	44 (86%)	6 (12%)	1 (2%)	7	39
80	BC	58/63 (92%)	34 (59%)	18 (31%)	6 (10%)	0	7
81	CC	69/152 (45%)	44 (64%)	14 (20%)	11 (16%)	0	2
82	DC	819/842 (97%)	628 (77%)	144 (18%)	47 (6%)	1	16
All	All	12207/13416 (91%)	9156 (75%)	2296 (19%)	755 (6%)	3	15

5 of 755 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	2	SER
5	E	120	VAL
5	E	135	PRO
5	E	175	GLU
6	F	222	ALA

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	
5	E	157/198 (79%)	129 (82%)	28 (18%)	2	10
6	F	194/196 (99%)	175 (90%)	19 (10%)	8	33
7	G	322/323 (100%)	297 (92%)	25 (8%)	12	42
8	H	288/289 (100%)	255 (88%)	33 (12%)	5	26
9	I	244/245 (100%)	220 (90%)	24 (10%)	8	33
10	J	152/153 (99%)	139 (91%)	13 (9%)	10	38
11	K	186/205 (91%)	170 (91%)	16 (9%)	10	38
12	L	191/208 (92%)	171 (90%)	20 (10%)	7	31
13	M	171/171 (100%)	157 (92%)	14 (8%)	11	40
14	N	180/187 (96%)	157 (87%)	23 (13%)	4	22
15	O	147/150 (98%)	134 (91%)	13 (9%)	10	38
16	P	81/136 (60%)	64 (79%)	17 (21%)	1	5
17	Q	154/159 (97%)	132 (86%)	22 (14%)	3	19
18	R	107/109 (98%)	96 (90%)	11 (10%)	7	32
19	S	175/176 (99%)	154 (88%)	21 (12%)	5	24
20	T	160/162 (99%)	152 (95%)	8 (5%)	24	58
21	U	145/146 (99%)	129 (89%)	16 (11%)	6	29
22	V	150/151 (99%)	142 (95%)	8 (5%)	22	55
23	W	153/154 (99%)	133 (87%)	20 (13%)	4	21
24	X	156/156 (100%)	133 (85%)	23 (15%)	3	18
25	Y	136/137 (99%)	120 (88%)	16 (12%)	5	25
26	Z	87/107 (81%)	82 (94%)	5 (6%)	20	53
27	AA	104/105 (99%)	90 (86%)	14 (14%)	4	21
28	BA	54/129 (42%)	49 (91%)	5 (9%)	9	35
29	CA	105/118 (89%)	90 (86%)	15 (14%)	3	19
30	DA	109/110 (99%)	97 (89%)	12 (11%)	6	29
31	EA	115/116 (99%)	97 (84%)	18 (16%)	2	15
32	FA	118/119 (99%)	106 (90%)	12 (10%)	7	32
33	GA	46/47 (98%)	44 (96%)	2 (4%)	29	62
34	HA	81/88 (92%)	70 (86%)	11 (14%)	3	20
35	IA	96/97 (99%)	88 (92%)	8 (8%)	11	40
36	JA	109/111 (98%)	99 (91%)	10 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	87 (97%)	3 (3%)	38	68
38	LA	95/103 (92%)	82 (86%)	13 (14%)	3	20
39	MA	104/105 (99%)	90 (86%)	14 (14%)	4	21
40	NA	81/82 (99%)	75 (93%)	6 (7%)	13	44
41	OA	70/71 (99%)	64 (91%)	6 (9%)	10	38
42	PA	68/69 (99%)	65 (96%)	3 (4%)	28	62
43	QA	45/46 (98%)	42 (93%)	3 (7%)	16	48
44	RA	47/116 (40%)	44 (94%)	3 (6%)	17	50
45	SA	23/23 (100%)	18 (78%)	5 (22%)	1	5
46	TA	90/91 (99%)	88 (98%)	2 (2%)	52	78
47	UA	71/72 (99%)	63 (89%)	8 (11%)	6	27
48	VA	160/254 (63%)	133 (83%)	27 (17%)	2	12
49	WA	261/262 (100%)	243 (93%)	18 (7%)	15	47
50	XA	173/210 (82%)	153 (88%)	20 (12%)	5	26
52	ZA	176/205 (86%)	165 (94%)	11 (6%)	18	51
53	AB	182/195 (93%)	162 (89%)	20 (11%)	6	29
54	BB	221/222 (100%)	202 (91%)	19 (9%)	10	38
55	CB	173/191 (91%)	155 (90%)	18 (10%)	7	31
56	DB	193/201 (96%)	185 (96%)	8 (4%)	30	63
57	EB	165/170 (97%)	154 (93%)	11 (7%)	16	48
58	FB	150/161 (93%)	141 (94%)	9 (6%)	19	52
59	GB	158/166 (95%)	148 (94%)	10 (6%)	18	51
60	HB	89/98 (91%)	79 (89%)	10 (11%)	6	27
61	IB	136/137 (99%)	127 (93%)	9 (7%)	16	49
63	KB	127/128 (99%)	114 (90%)	13 (10%)	7	32
65	MB	103/118 (87%)	97 (94%)	6 (6%)	20	53
66	NB	117/119 (98%)	106 (91%)	11 (9%)	8	35
67	OB	82/124 (66%)	75 (92%)	7 (8%)	10	39
68	PB	128/129 (99%)	117 (91%)	11 (9%)	10	38
69	QB	115/116 (99%)	106 (92%)	9 (8%)	12	42
70	RB	100/114 (88%)	92 (92%)	8 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	SB	74/74 (100%)	68 (92%)	6 (8%)	11	41
72	TB	110/111 (99%)	98 (89%)	12 (11%)	6	29
73	UB	119/120 (99%)	112 (94%)	7 (6%)	19	53
74	VB	112/113 (99%)	106 (95%)	6 (5%)	22	55
75	WB	61/89 (68%)	54 (88%)	7 (12%)	5	26
77	YB	70/71 (99%)	69 (99%)	1 (1%)	67	85
78	ZB	56/60 (93%)	52 (93%)	4 (7%)	14	46
79	AC	47/49 (96%)	42 (89%)	5 (11%)	6	30
80	BC	51/54 (94%)	45 (88%)	6 (12%)	5	25
82	DC	699/714 (98%)	621 (89%)	78 (11%)	6	27
All	All	9865/10602 (93%)	8910 (90%)	955 (10%)	12	33

5 of 955 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	FA	42	ARG
82	DC	149	GLU
48	VA	45	LEU
82	DC	32	LYS
82	DC	753	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 251 such sidechains are listed below:

Mol	Chain	Res	Type
37	KA	106	ASN
73	UB	22	ASN
50	XA	164	ASN
72	TB	64	GLN
82	DC	341	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1682/1798 (93%)	330 (19%)	11 (0%)
2	B	3267/3396 (96%)	533 (16%)	31 (0%)
3	C	157/158 (99%)	26 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	120/121 (99%)	11 (9%)	0
83	EC	187/201 (93%)	79 (42%)	5 (2%)
All	All	5413/5674 (95%)	979 (18%)	47 (0%)

5 of 979 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	25	C
1	A	26	A
1	A	34	G
1	A	45	U

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2248	C
2	B	2818	U
2	B	2263	C
2	B	2513	U
2	B	3218	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
82	DDE	DC	699	82	14,20,21	1.95	4 (28%)	14,28,30	1.76	5 (35%)

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
82	DDE	DC	699	82	-	3/20/21/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	CBW-CBI	5.08	1.61	1.53
82	DC	699	DDE	CAT-CE1	2.30	1.53	1.50
82	DC	699	DDE	OAG-CBI	2.07	1.27	1.23
82	DC	699	DDE	CD2-NE2	2.04	1.39	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	DC	699	DDE	OAG-CBI-CBW	-3.55	115.99	120.49
82	DC	699	DDE	CAU-CBW-CBI	-2.62	106.01	111.20
82	DC	699	DDE	CG-ND1-CE1	2.52	110.50	103.05
82	DC	699	DDE	OAG-CBI-NAD	2.20	126.82	123.00
82	DC	699	DDE	CG-CD2-NE2	-2.13	104.86	109.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	DC	699	DDE	O-C-CA-CB
82	DC	699	DDE	CA-CB-CG-ND1
82	DC	699	DDE	OAG-CBI-CBW-CAU

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	DC	699	DDE	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
86	SO1	DC	903	-	35,39,39	2.30	16 (45%)	39,64,64	2.01	8 (20%)
84	GDP	DC	901	85	24,30,30	1.54	5 (20%)	30,47,47	2.01	9 (30%)

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
86	SO1	DC	903	-	-	2/21/104/104	0/7/5/5
84	GDP	DC	901	85	-	0/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O17-C52	3.82	1.46	1.40
84	DC	901	GDP	PB-O1B	3.80	1.62	1.50
86	DC	903	SO1	O56-C52	-3.78	1.32	1.41
86	DC	903	SO1	C1-C5	3.74	1.59	1.50
86	DC	903	SO1	C10-C6	3.58	1.60	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	DC	901	GDP	PA-O3A-PB	-6.43	110.75	132.83
86	DC	903	SO1	C12-C6-C10	-6.12	103.05	107.91
86	DC	903	SO1	C25-C22-C24	4.95	129.50	113.56
86	DC	903	SO1	C10-C6-C2	3.52	108.39	104.16
86	DC	903	SO1	C1-C4-C13	3.35	122.04	118.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15

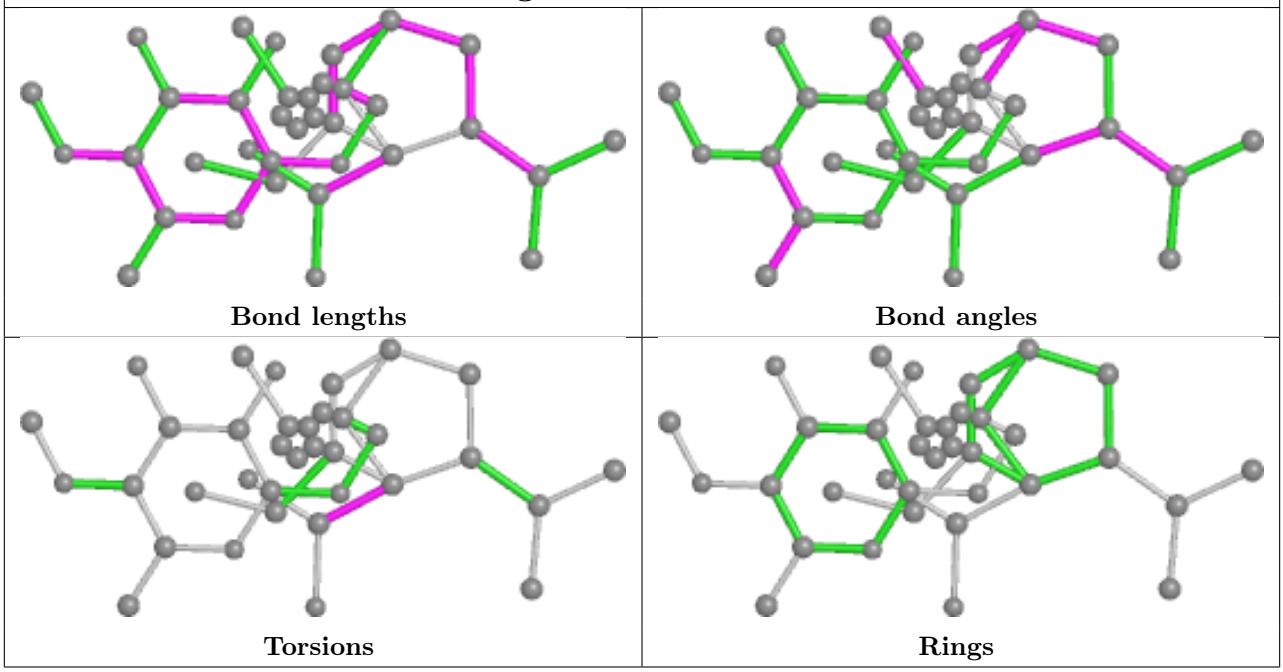
There are no ring outliers.

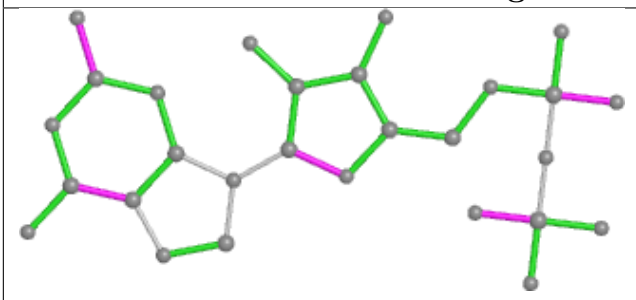
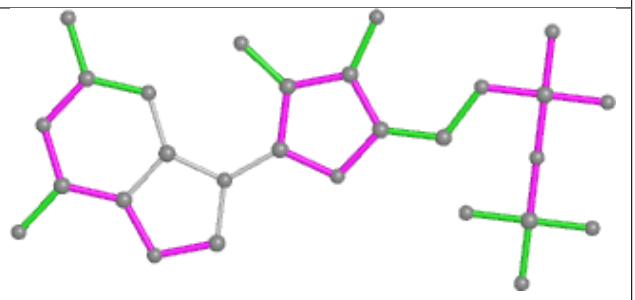
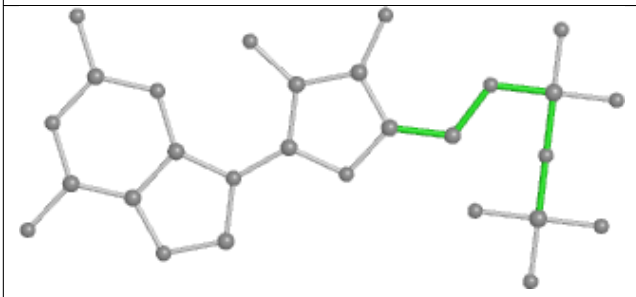
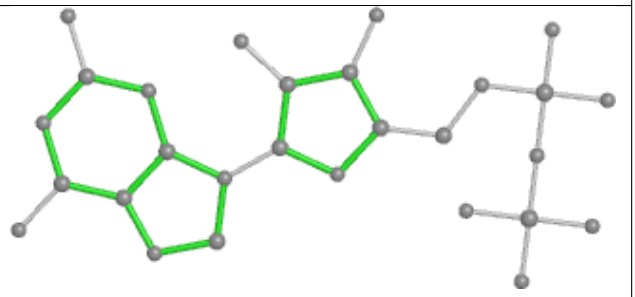
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	DC	903	SO1	3	0
84	DC	901	GDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SO1 DC 903



Ligand GDP DC 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

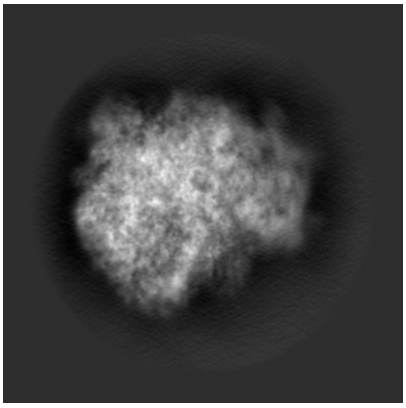
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6644. These allow visual inspection of the internal detail of the map and identification of artifacts.

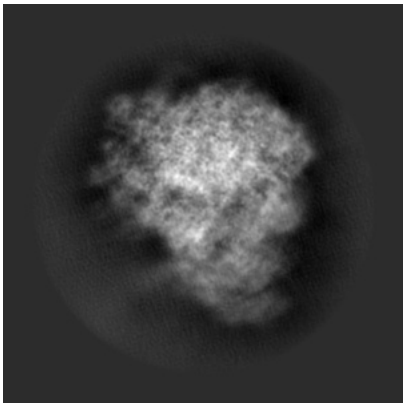
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

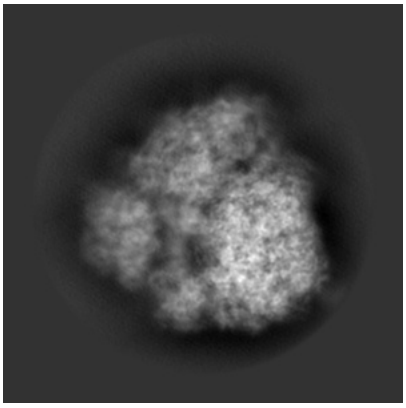
6.1.1 Primary map



X



Y

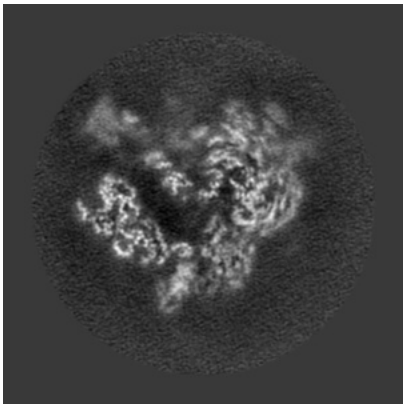


Z

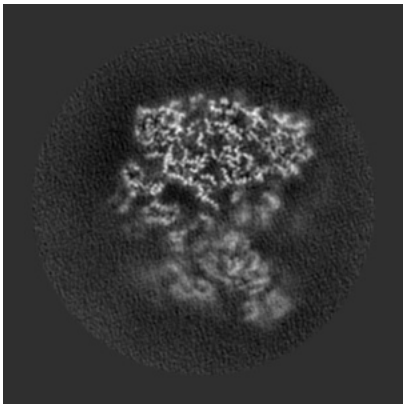
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

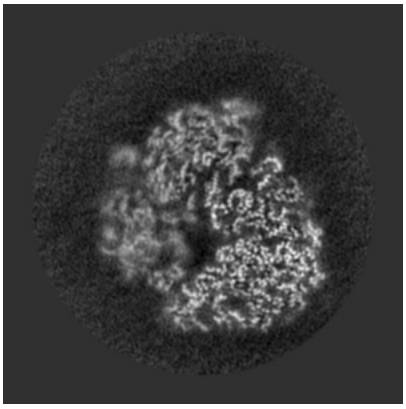
6.2.1 Primary map



X Index: 256



Y Index: 256

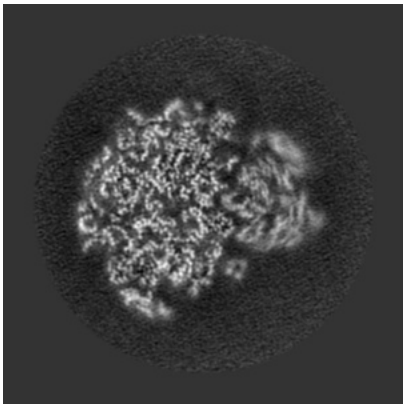


Z Index: 256

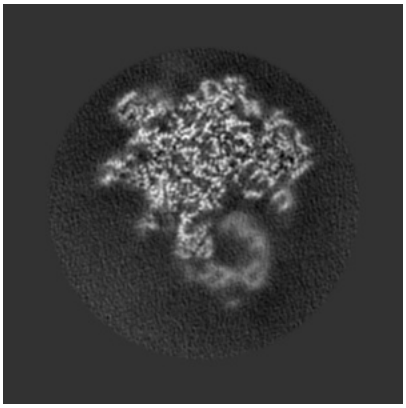
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

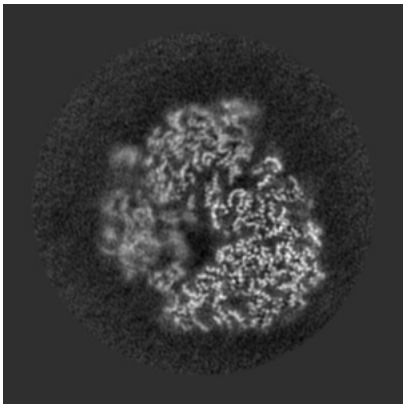
6.3.1 Primary map



X Index: 290



Y Index: 163

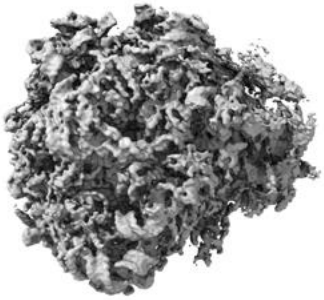


Z Index: 255

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

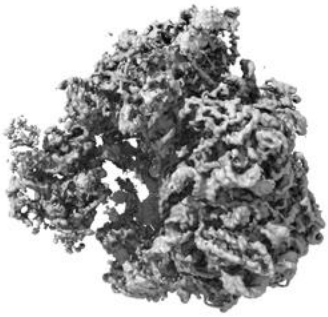
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

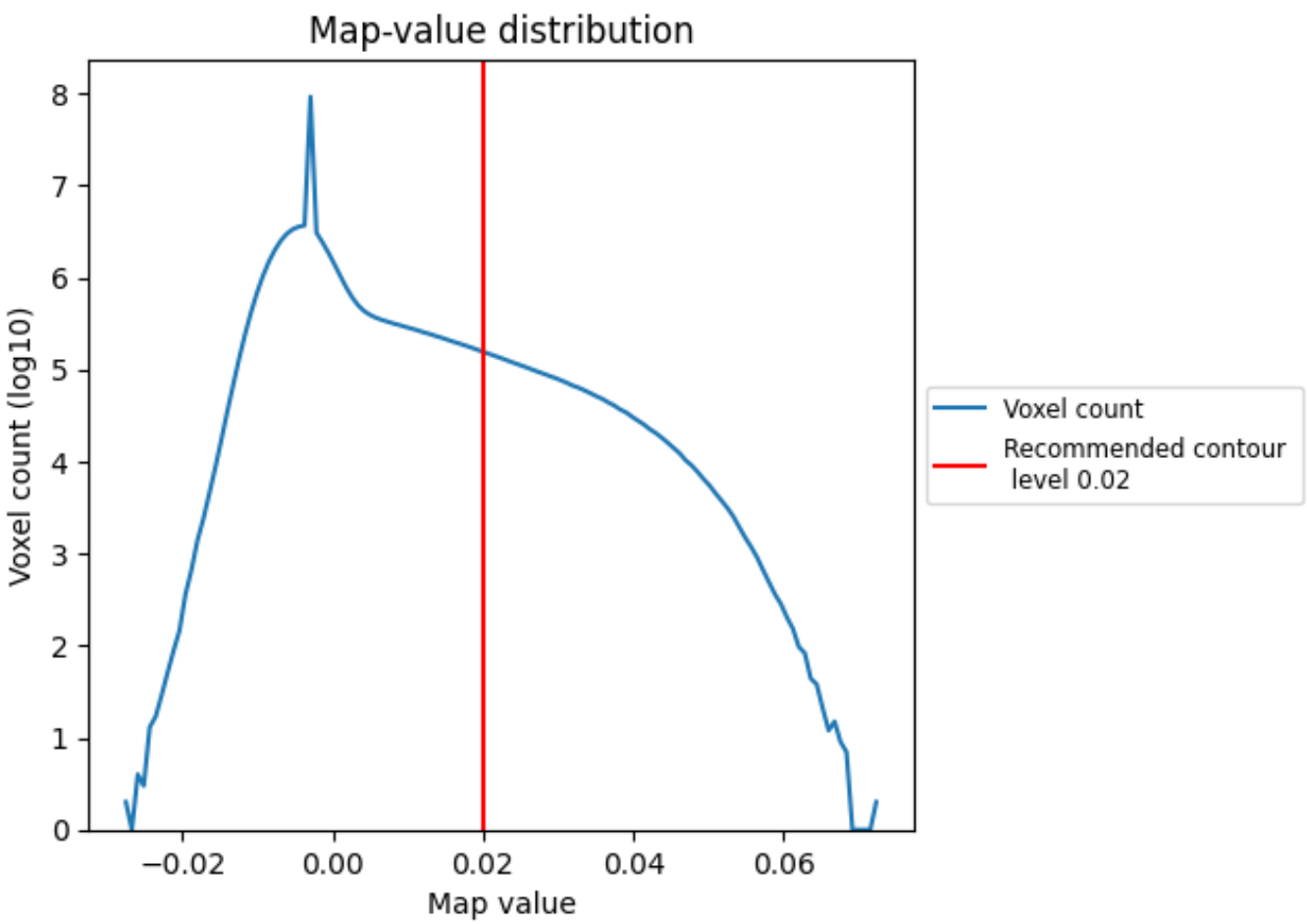
6.5 Mask visualisation (i)

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

7 Map analysis (i)

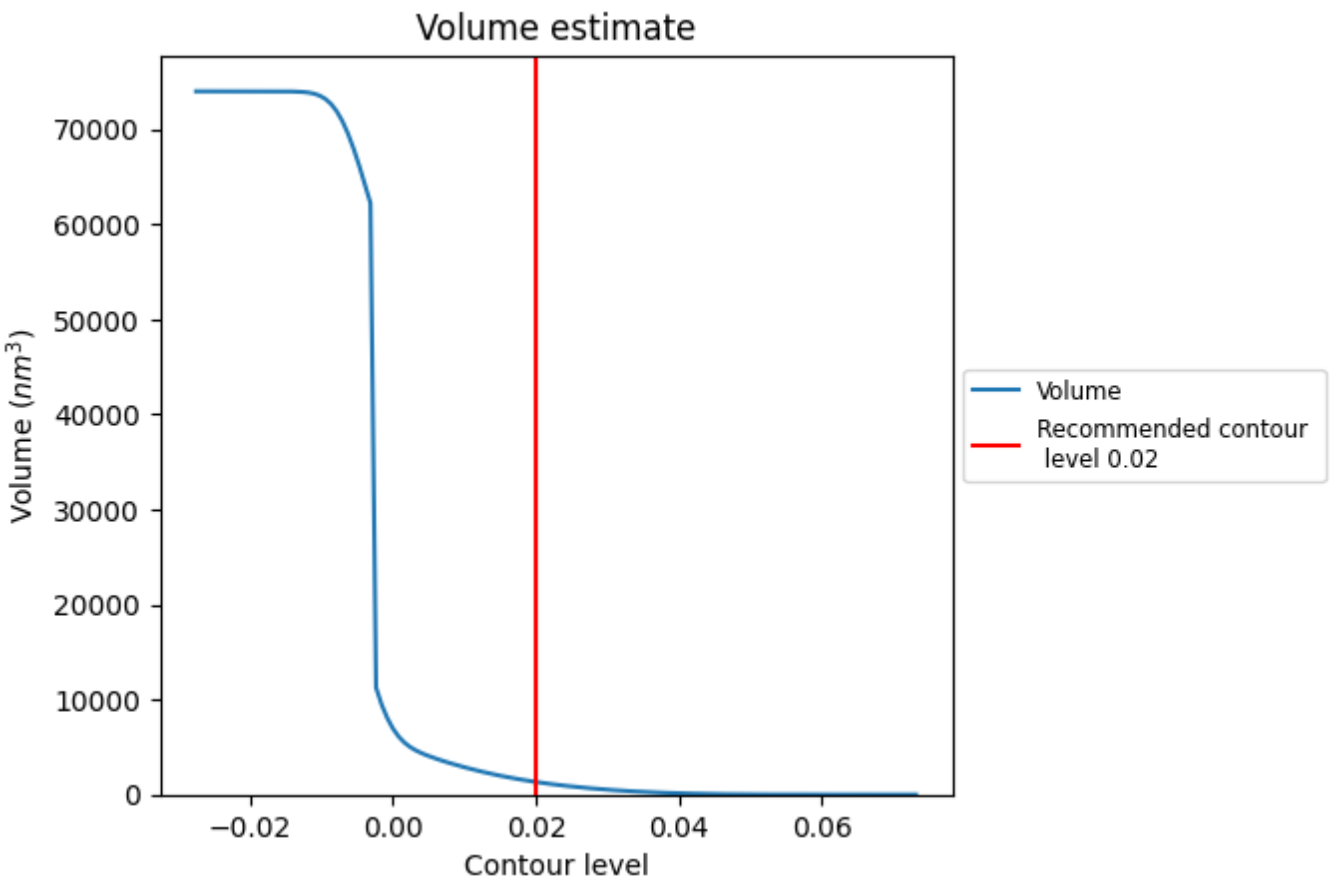
This section contains the results of statistical analysis of the map.

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.

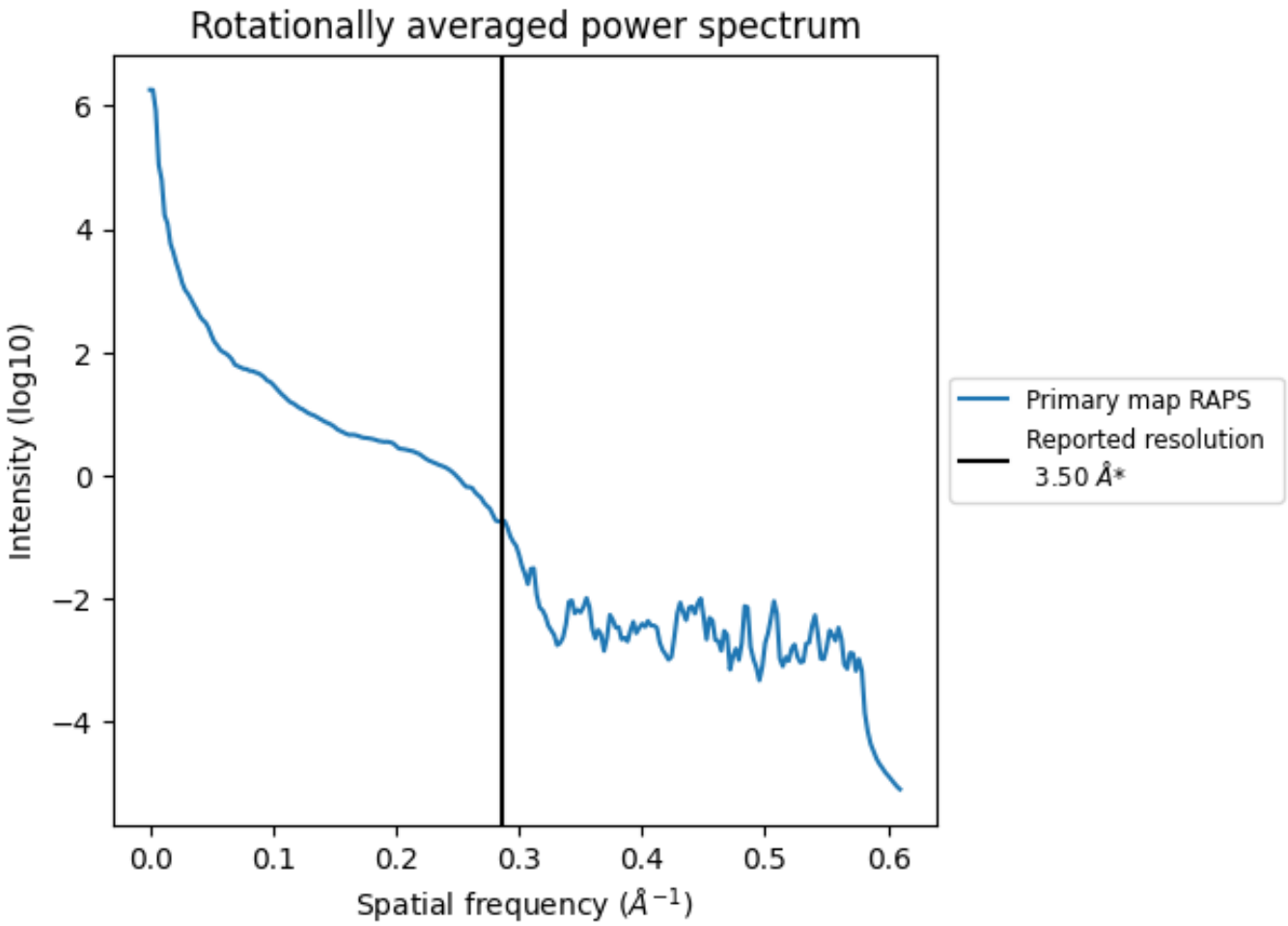
7.2 Volume estimate (i)



The volume at the recommended contour level is 1328 nm^3; this corresponds to an approximate mass of 1200 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 0.286 Å^{-1}

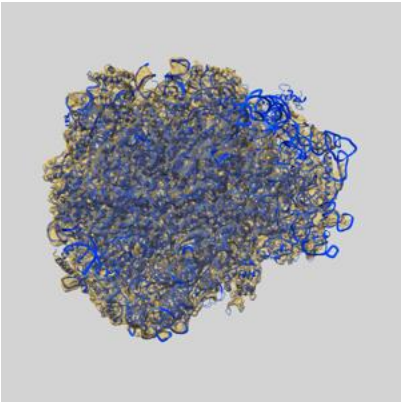
8 Fourier-Shell correlation (i)

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

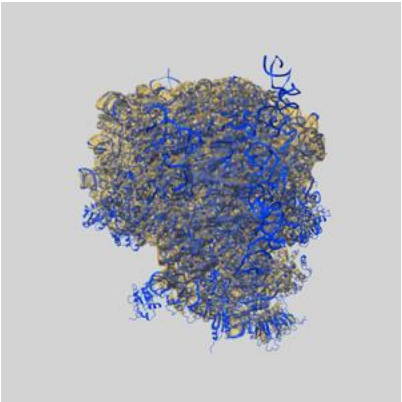
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6644 and PDB model 5JUP. Per-residue inclusion information can be found in section 3 on page 21.

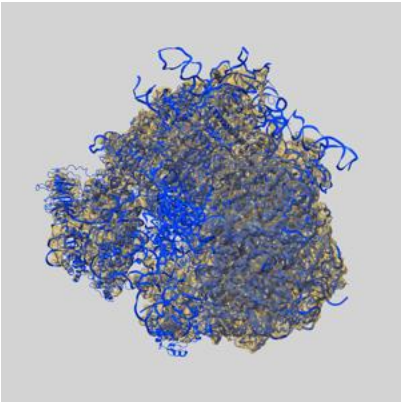
9.1 Map-model overlay (i)



X



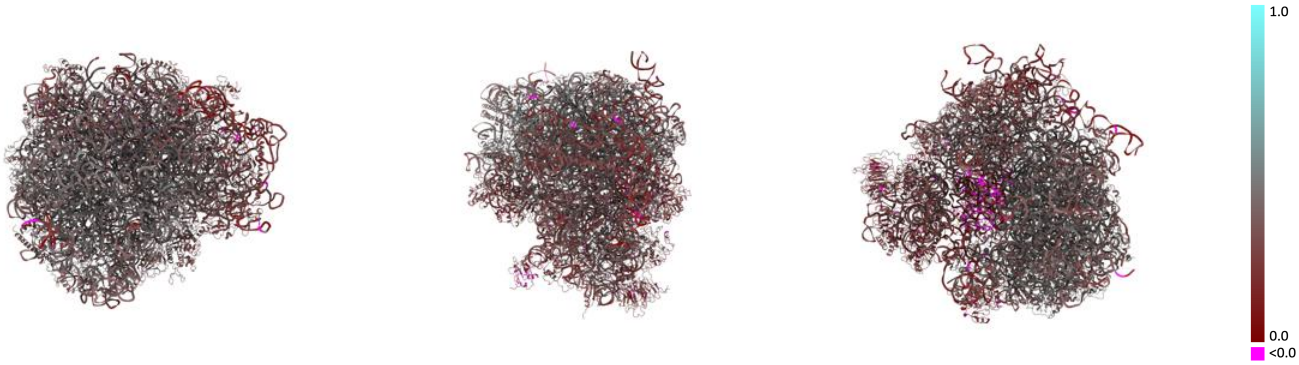
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

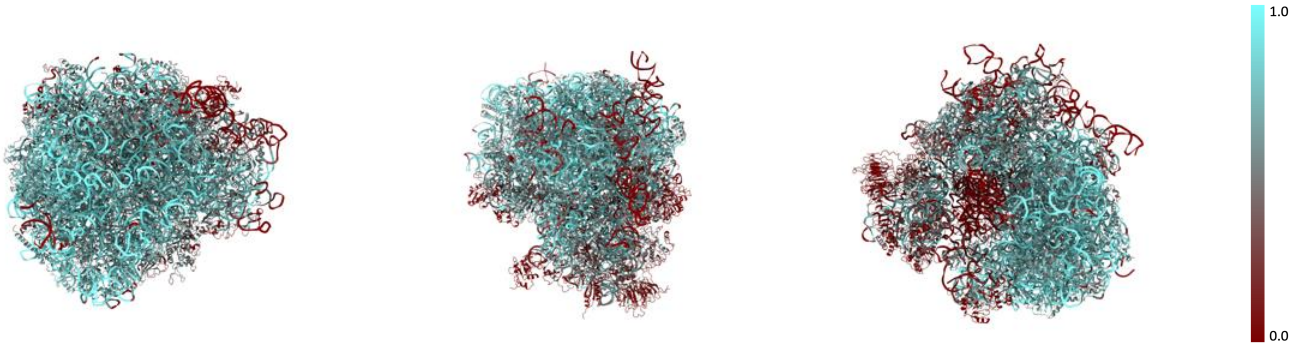
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

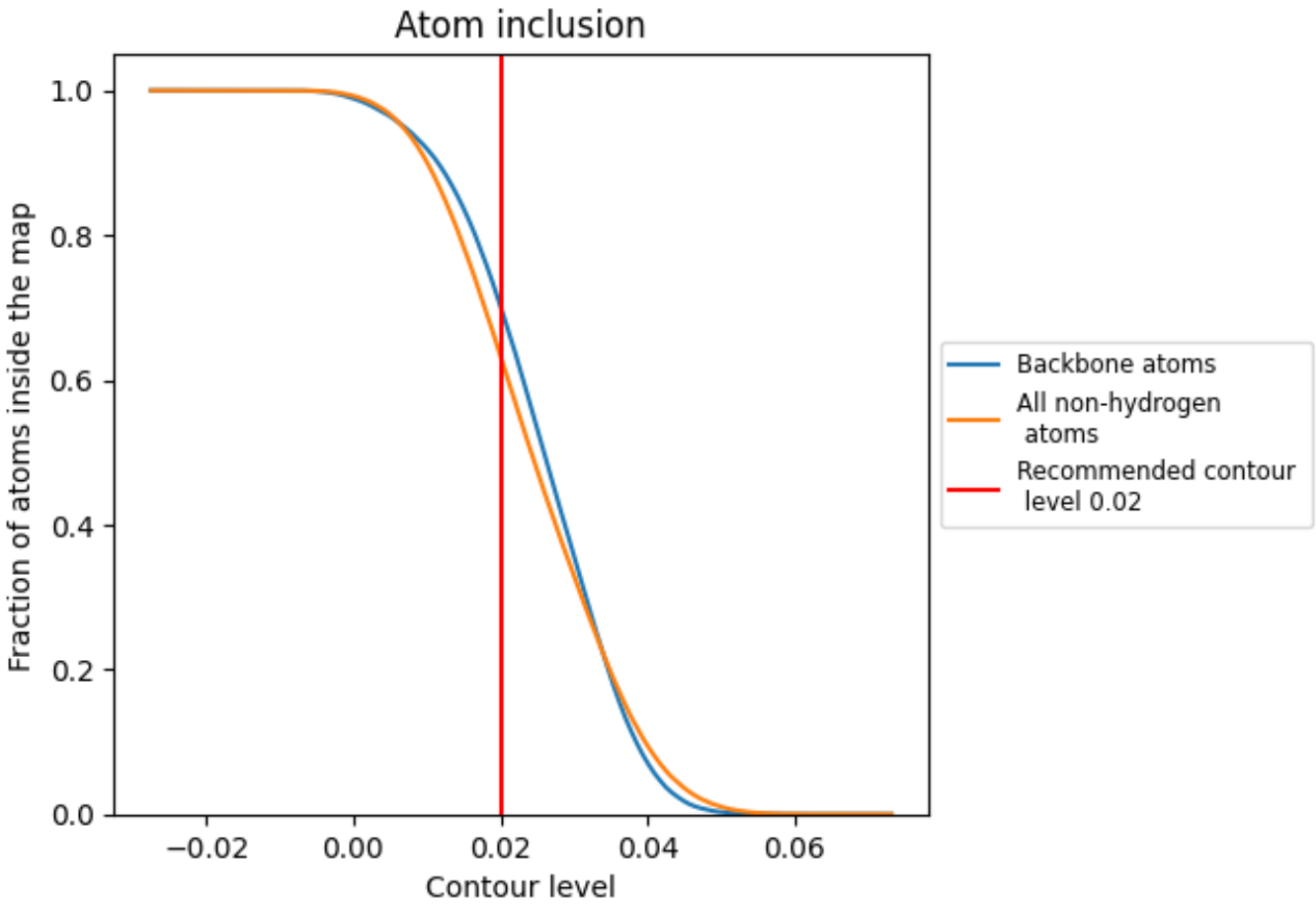
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6333	0.3620
A	0.6430	0.3080
AA	0.5449	0.4530
AB	0.2351	0.3110
AC	0.3694	0.3020
B	0.8559	0.4010
BA	0.6146	0.4350
BB	0.5186	0.3280
BC	0.3486	0.3350
C	0.8951	0.4130
CA	0.5565	0.4100
CB	0.1768	0.2580
CC	0.0000	0.1720
D	0.9469	0.3960
DA	0.6794	0.4090
DB	0.4000	0.2980
DC	0.4300	0.3220
E	0.0298	0.2420
EA	0.5746	0.3780
EB	0.1377	0.3160
EC	0.1213	0.2040
F	0.6114	0.4330
FA	0.6955	0.4450
FB	0.4057	0.3340
G	0.6587	0.4470
GA	0.6115	0.4240
GB	0.5333	0.3340
H	0.7054	0.4390
HA	0.6553	0.3880
HB	0.2925	0.2580
I	0.6567	0.3720
IA	0.6725	0.4330
IB	0.3188	0.3480
J	0.6007	0.3960
JA	0.6730	0.4560

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Chain	Atom inclusion	Q-score
JB	0.0000	0.1650
K	0.6730	0.4200
KA	0.6180	0.4520
KB	0.4074	0.3250
L	0.5952	0.3770
LA	0.5798	0.4110
LB	0.0000	0.1200
M	0.6184	0.4160
MA	0.6186	0.3790
MB	0.2059	0.2590
N	0.5790	0.4060
NA	0.6716	0.3970
NB	0.1639	0.2610
O	0.6147	0.3640
OA	0.6646	0.4450
OB	0.1730	0.2620
P	0.0931	0.1920
PA	0.1617	0.3450
PB	0.1870	0.2730
Q	0.6866	0.4160
QA	0.6803	0.4420
QB	0.2338	0.2730
R	0.6738	0.4040
RA	0.6733	0.4290
RB	0.1011	0.3020
S	0.6453	0.4320
SA	0.0000	0.1530
SB	0.4662	0.3660
T	0.6383	0.4300
TA	0.6381	0.4430
TB	0.4404	0.3670
U	0.6793	0.4440
UA	0.5776	0.4140
UB	0.3744	0.3860
V	0.7170	0.4420
VA	0.0970	0.2630
VB	0.4520	0.2820
W	0.5082	0.3770
WA	0.1039	0.2650
WB	0.1335	0.2470
X	0.6308	0.4300
XA	0.3140	0.3290

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Chain	Atom inclusion	Q-score
XB	0.0000	0.1230
Y	0.6535	0.4420
YA	0.0000	0.1290
YB	0.3322	0.3360
Z	0.5550	0.3800
ZA	0.5149	0.3800
ZB	0.2155	0.2810