



## wwPDB EM Validation Summary Report ⓘ

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

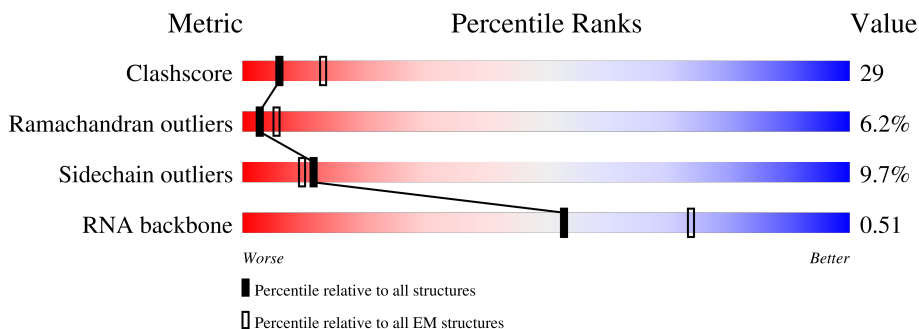
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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.






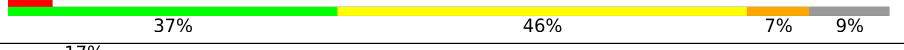
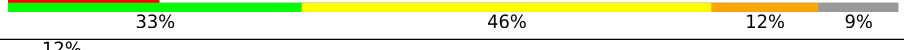
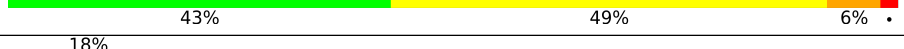


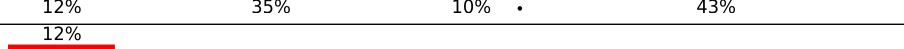
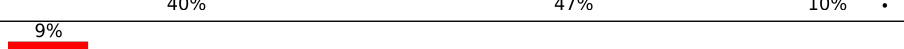
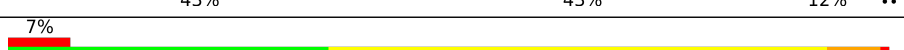

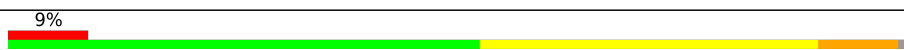
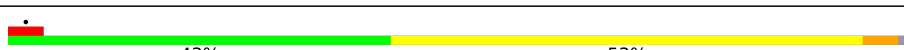
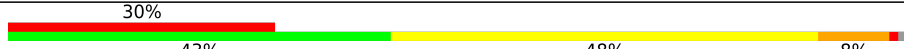
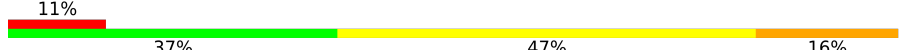
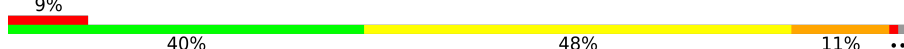



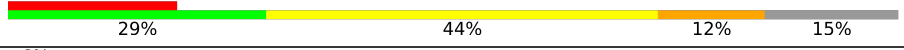

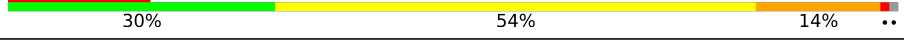


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1798	
2	B	3396	
3	C	158	
4	D	121	
5	E	217	
6	F	254	
7	G	387	

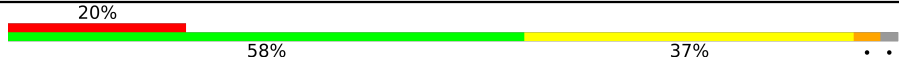
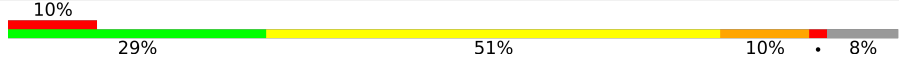

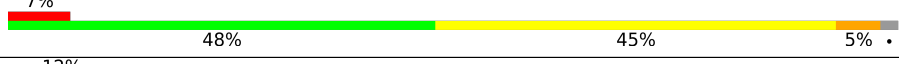
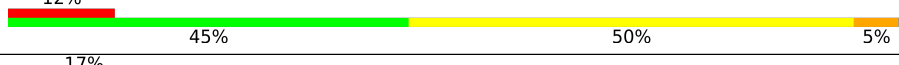
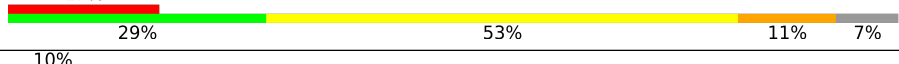
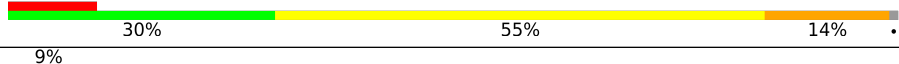
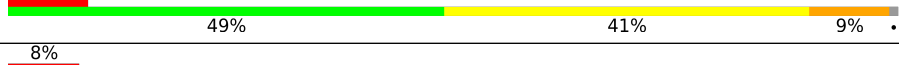



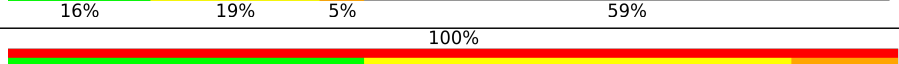
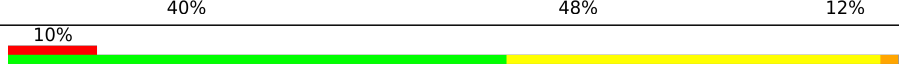

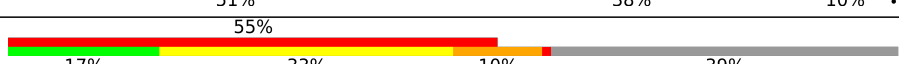
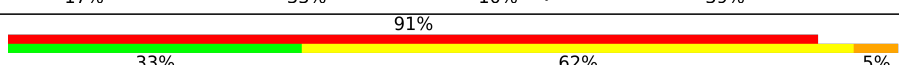
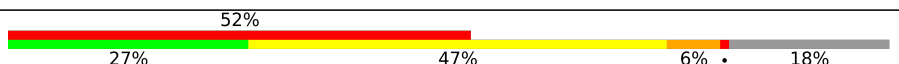

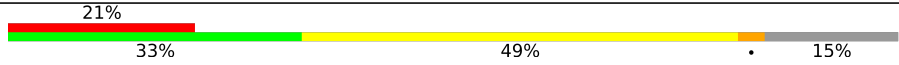



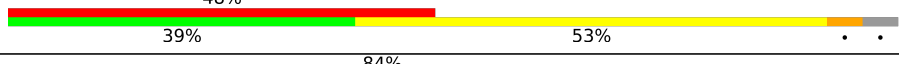


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Mol	Chain	Length	Quality of chain
8	H	362	
9	I	297	
10	J	176	
11	K	244	
12	L	256	
13	M	191	
14	N	221	
15	O	174	
16	P	165	
17	Q	199	
18	R	138	
19	S	204	
20	T	199	
21	U	184	
22	V	186	
23	W	189	
24	X	172	
25	Y	160	
26	Z	121	
27	AA	137	
28	BA	155	
29	CA	142	
30	DA	127	
31	EA	136	
32	FA	149	

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Mol	Chain	Length	Quality of chain
33	GA	59	
34	HA	105	
35	IA	113	
36	JA	130	
37	KA	107	
38	LA	121	
39	MA	120	
40	NA	100	
41	OA	88	
42	PA	78	
43	QA	51	
44	RA	128	
45	SA	25	
46	TA	106	
47	UA	92	
48	VA	312	
49	WA	319	
50	XA	252	
51	YA	255	
52	ZA	254	
53	AB	240	
54	BB	261	
55	CB	225	
56	DB	236	
57	EB	190	

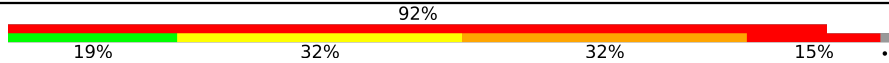
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Mol	Chain	Length	Quality of chain
58	FB	200	52% 27% 59% 8% 6%
59	GB	197	25% 34% 53% 6% 6%
60	HB	105	61% 28% 51% 10% 9%
61	IB	156	65% 39% 49% 10% ..
62	JB	143	87% 79% 8% 13%
63	KB	151	50% 42% 50% 8%
64	LB	137	93% 83% 9% 7%
65	MB	142	68% 34% 43% 9% 14%
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	 <p>92%</p> <p>19% 32% 32% 15%</p>

## 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
14	N	211	Total	C	N	O	S	0	0
			1718	1089	325	298	6		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
42	PA	77	Total	C	N	O	0	0
			613	391	115	107		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S		
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	S		
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	S		
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	S		
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
70	RB	107	Total	C	N	O	S	0	0
			856	539	156	160	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

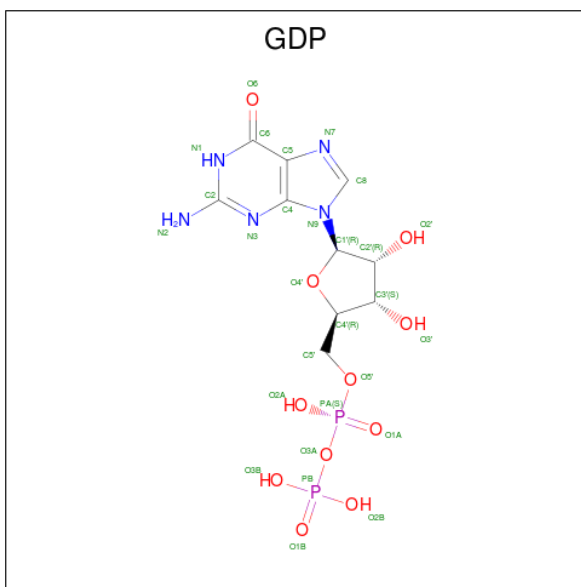
- Molecule 82 is a protein called yeast eEF2.

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

- Molecule 83 is a RNA chain called IRES.

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

- Molecule 84 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

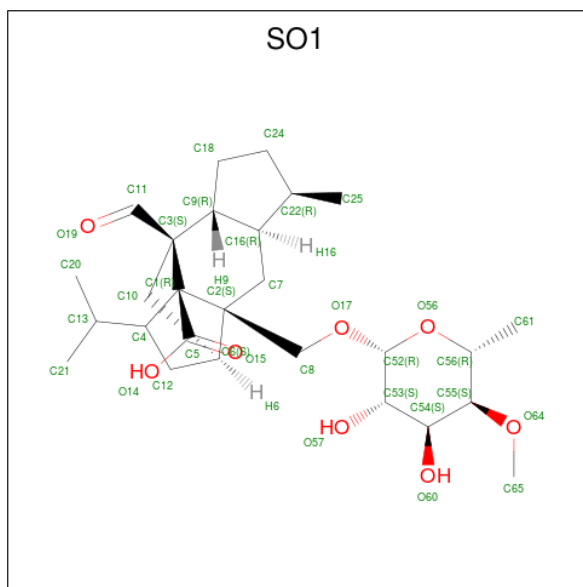


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
84	DC	1	28	10	5	11	2	0

- 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<sub>27</sub>H<sub>42</sub>O<sub>8</sub>).

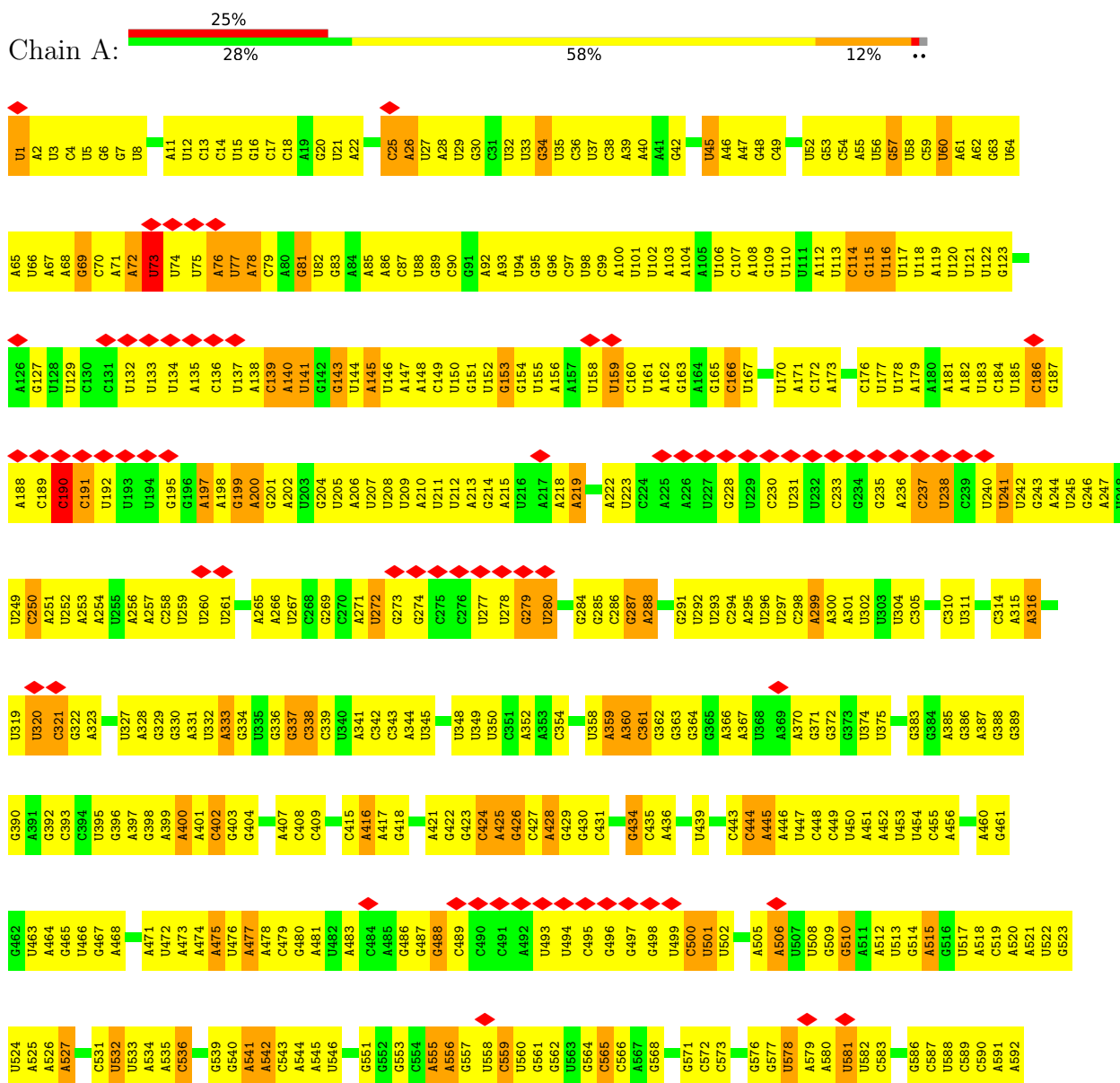


Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

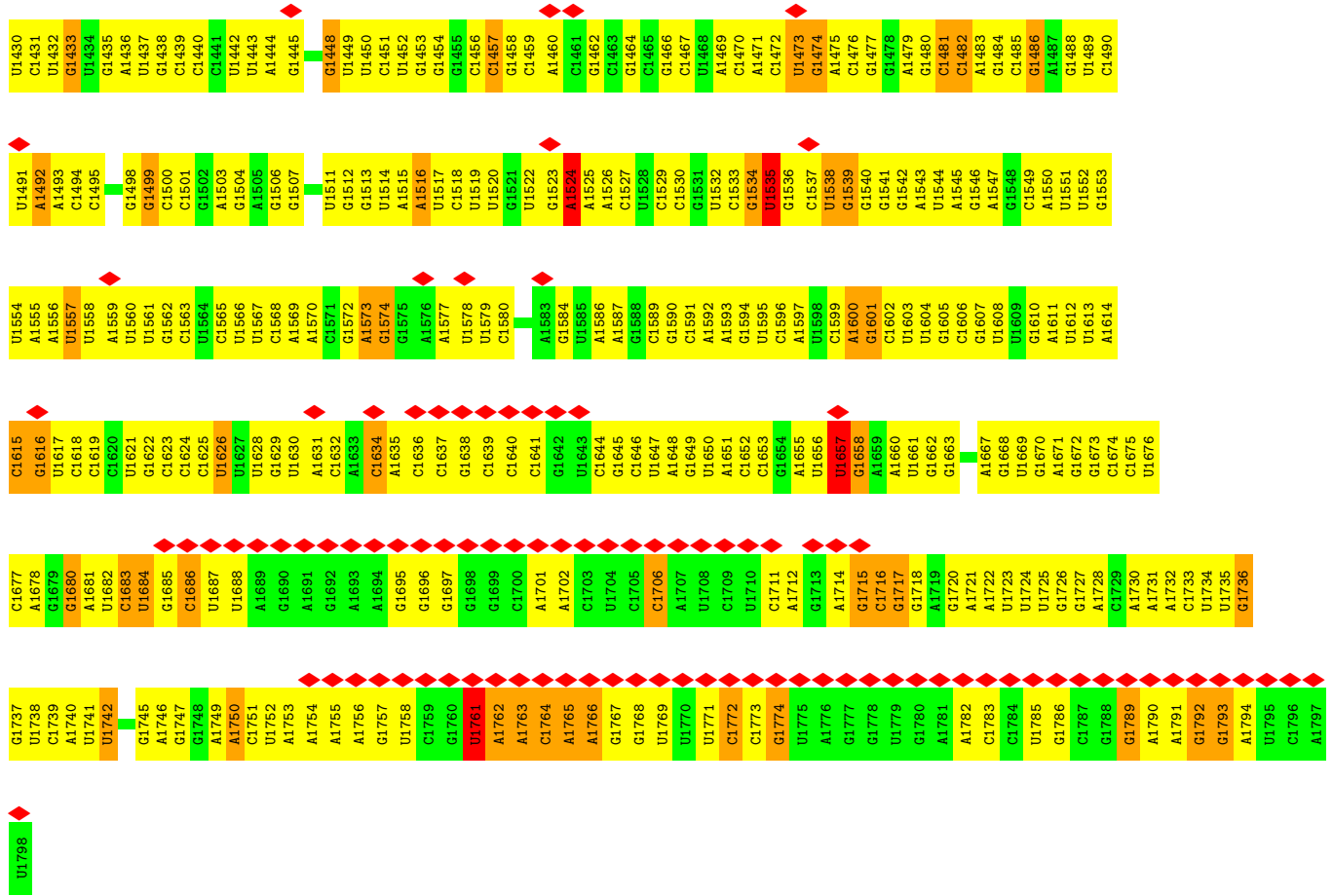
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

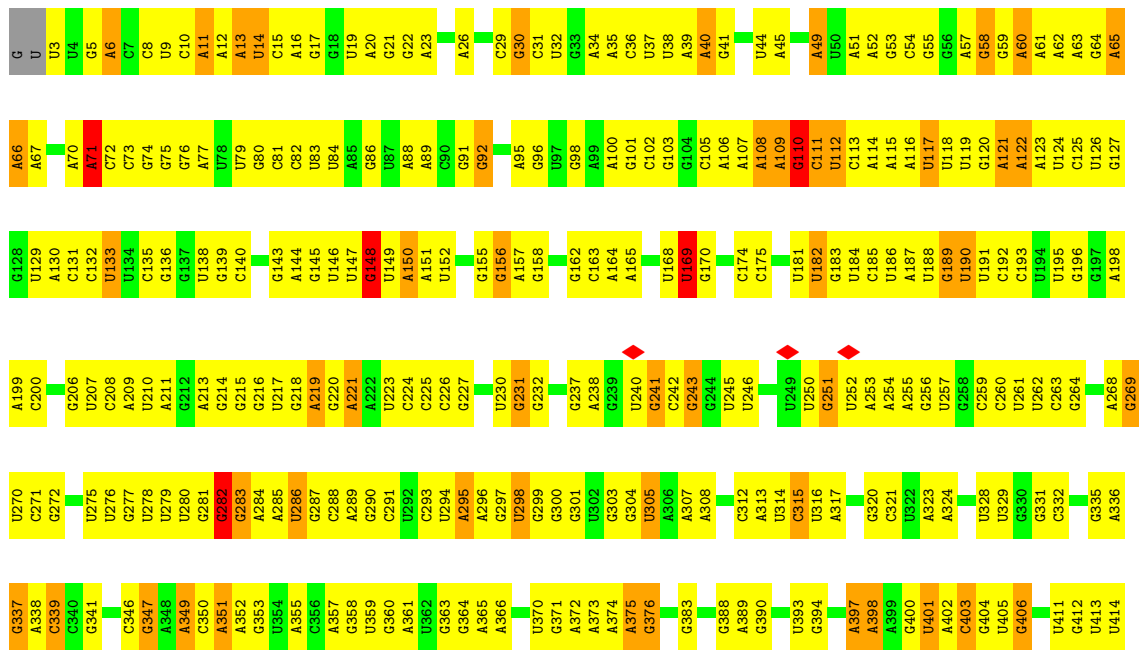
#### • Molecule 1: 18S ribosomal RNA

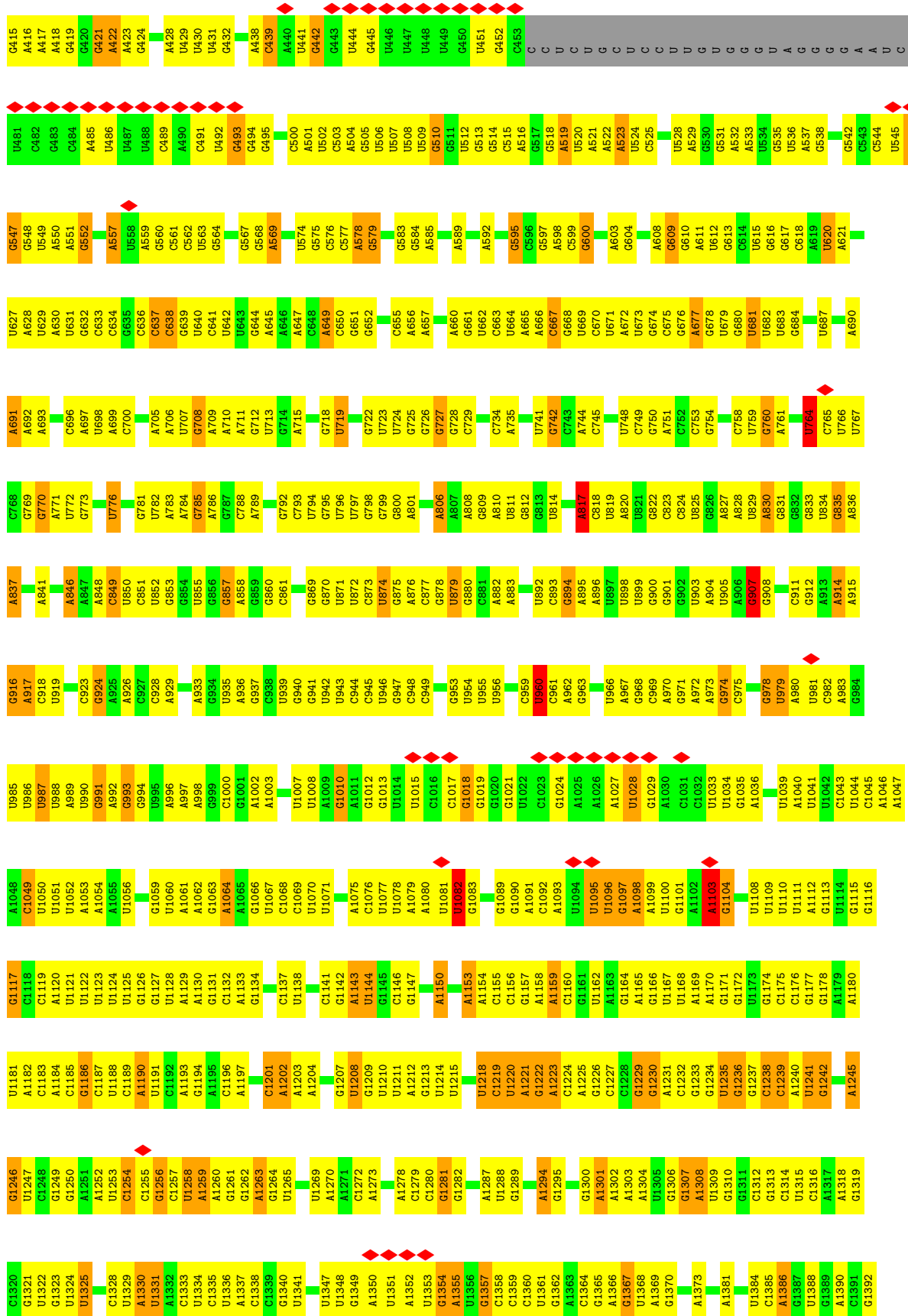




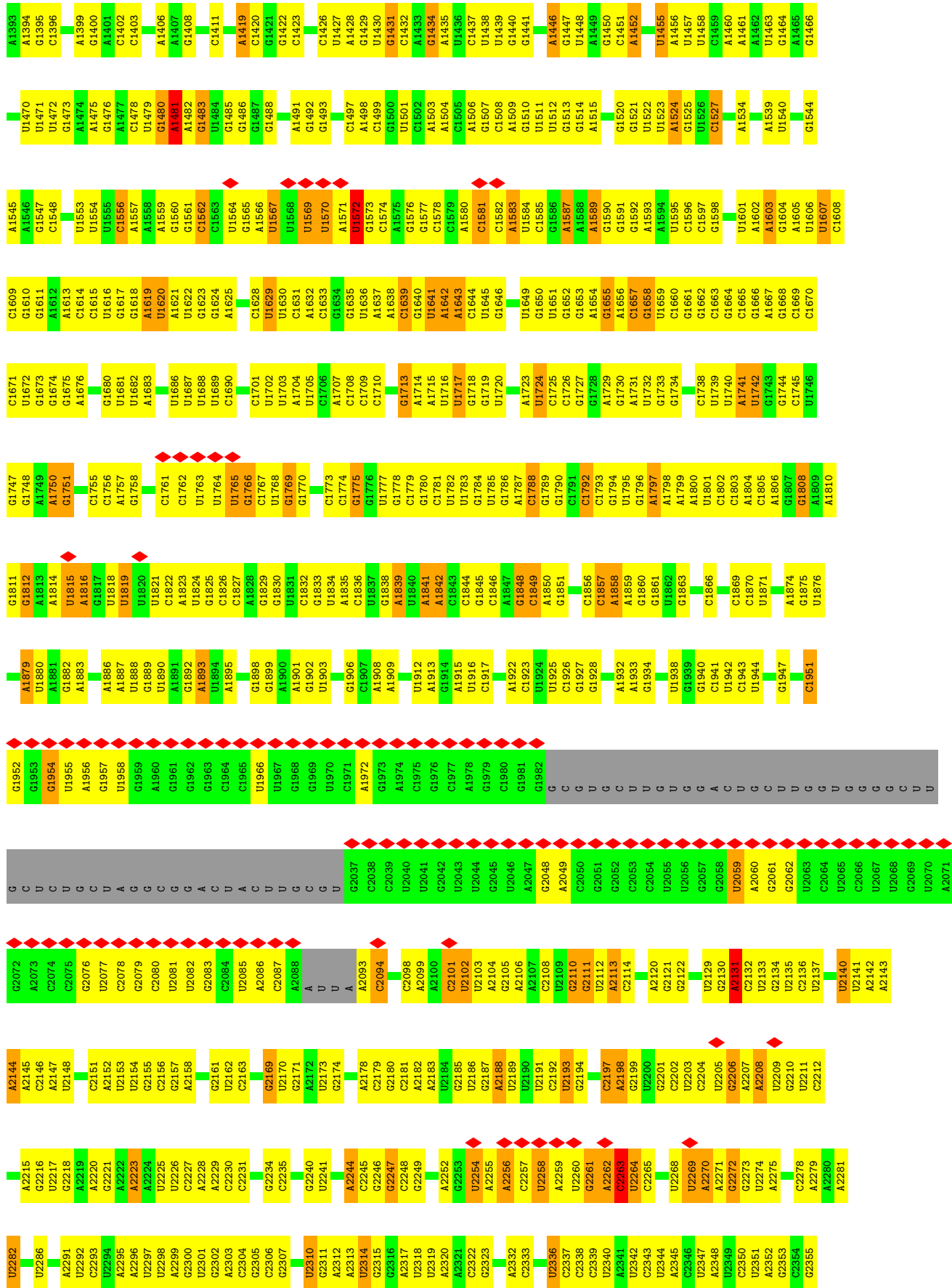


• Molecule 2: 25S ribosomal RNA

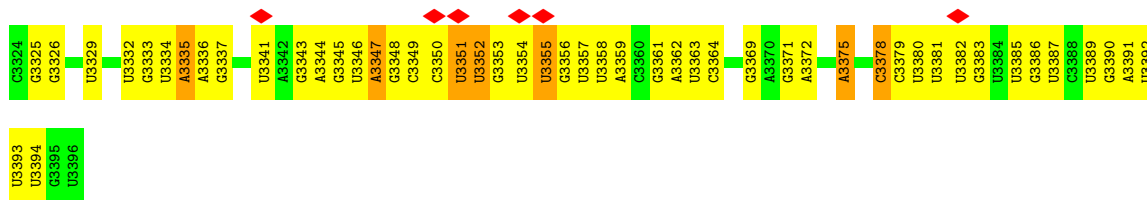








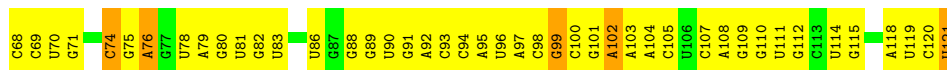
A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2380	A2381	A2384	A2385	A2388	A2389	A2390	A2391	A2392	A2393	A2401	A2402	A2403	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424								
G2425	U2426	U2427	U2428	U2429	A2430	C2431	U2434	U2435	U2436	G2437	A2438	A2439	G2440	A2441	A2442	A2443	C2444	A2445	U2446	A2447	A2448	A2449	G2450	G2451	U2452	U2453	U2454	U2455	A2456	A2457	A2458	A2459	U2460	A2461	A2462	G2463	U2464	G2465	G2466	G2467	A2468	G2469	C2470	U2471	U2472	G2473	G2474	G2475	G2476	G2477	G2478	C2479	A2480	U2481	U2482	G2483	A2484	A2485	
A2486	U2487	A2488	C2489	A2490	A2491	C2492	U2493	A2494	C2495	U2496	U2497	U2498	U2499	A2500	U2501	A2502	U2503	U2504	U2505	U2506	C2507	U2508	U2509	U2510	A2511	C2512	U2513	U2514	A2515	U2516	A2519	A2520	U2521	C2522	A2523	G2524	C2525	C2526	G2527	C2528	A2529	C2530	C2531	G2534	A2535	A2536	U2537	U2538	C2539	A2540	U2541	U2542	U2543	U2544	C2545	A2547			
C2548	G2549	U2550	U2551	U2552	U2553	U2554	G2555	C2556	A2557	A2558	A2559	A2560	A2561	A2562	G2563	C2564	C2565	C2566	A2567	A2568	A2569	A2570	U2571	C2572	G2573	G2576	U2581	C2582	C2583	A2584	C2585	U2586	A2587	U2588	U2589	A2590	A2591	C2592	A2593	C2594	U2597	G2598	U2599	C2600	G2601	G2602	G2606	G2607	G2610	U2611	U2612	U2613	U2614	G2615	G2616	U2617	U2618	G2623	
G2624	C2625	A2626	C2627	A2628	U2629	C2630	U2631	G2632	U2633	U2634	U2635	A2636	A2637	C2638	A2639	A2640	A2641	A2642	A2643	U2644	G2645	A2649	U2650	G2651	U2652	U2655	A2656	A2657	G2658	G2659	G2660	A2661	U2662	G2663	A2664	A2665	C2666	A2667	U2668	A2674	C2675	A2676	A2677	C2678	A2679	U2680	U2681	U2682	U2683	A2684	U2685	U2686	A2687	A2688	U2689	A2691			
A2694	A2695	A2696	C2697	G2698	U2699	C2700	U2701	A2704	U2705	U2706	C2711	U2712	U2713	G2714	A2715	U2716	U2717	U2718	U2719	G2720	U2724	C2725	C2726	A2727	G2728	A2729	G2730	A2731	G2732	A2733	A2734	U2735	U2736	A2737	C2741	C2742	A2743	U2744	G2745	A2746	A2747	A2748	G2749	U2750	G2751	G2752	G2753	G2754	C2755	C2756	C2757	C2758	C2759	C2760	U2763	C2764	C2765	U2766	U2767
U2768	A2769	G2770	U2771	C2772	U2773	C2774	U2775	C2776	G2777	G2778	A2779	A2780	G2786	G2787	C2788	U2789	A2790	G2794	U2795	G2796	C2797	C2798	A2799	G2800	A2801	A2802	A2803	A2804	G2805	A2806	U2807	C2810	U2811	C2812	A2813	G2814	A2817	U2818	C2821	U2822	G2823	G2824	U2825	U2826	U2827	G2828	U2829	G2830	G2831	C2836	A2837	A2838	A2839						
G2841	U2842	C2843	C2844	U2845	A2846	A2847	G2850	C2851	C2852	U2853	A2854	U2855	C2856	C2857	U2858	U2859	U2860	U2861	U2862	U2865	C2866	U2868	G2869	C2870	G2871	A2872	U2873	U2874	C2875	U2880	C2881	U2882	U2883	C2884	U2885	U2886	A2887	A2889	U2891	A2892	C2893	C2894	G2895	A2896	A2897	U2898	C2899	U2903	U2904	U2905	C2906	G2907	G2908						
U2909	A2910	A2911	G2912	C2913	U2914	U2915	U2916	U2917	G2918	U2919	U2921	U2922	U2923	A2926	C2927	C2928	C2929	A2930	C3001	C3002	A3005	A3006	U3007	G3008	G3009	U3010	A3011	A3012	G3015	A3016	U3017	U3018	U3019	C3025	G3026	A3027	G3028	A3029	G3030	C3034	U3037	G3036	G3037	U3038	C3039	A3040	U3041	U3042	U3043	G3045	A3046	A3049							
G3052	G3053	U3054	U3055	U3056	U3057	U3058	G3059	C3060	G3061	G3062	C3063	U3064	G3065	U3066	C3067	C3072	A3073	C3076	A3077	U3078	U3079	G3080	C3081	G3082	C3083	C3084	G3085	A3086	A3087	G3088	C3089	U3090	A3091	C3092	C3093	A3094	U3095	C3096	C3099	U3100	A3106	U3107	G3108	G3109	C3110	U3111	G3112	C3115	G3116	C3117	C3118	U3119	C3120	U3121					
A3122	C3126	A3127	C3128	A3129	A3130	U3131	C3132	C3133	A3134	U3135	A3139	G3140	A3141	A3142	C3143	G3146	U3148	G3149	A3150	U3151	U3152	U3153	C3154	U3155	U3156	U3157	G3158	C3159	U3160	C3161	C3162	A3163	A3165	C3166	A3167	U3168	U3169	A3170	U3171	A3172	G3173	A3174	U3175	G3176	U3179	A3180	C3181	G3182	A3186	C3187	G3188	G3189							
C3190	G3191	U3192	C3193	C3194	U3195	U3198	G3205	C3206	U3207	G3208	A3209	C3210	C3211	C3212	A3213	A3214	A3215	C3217	A3218	G3219	G3220	A3223	C3224	A3227	C3228	G3229	G3230	U3231	G3232	C3233	A3234	U3237	G3238	C3239	C3240	G3241	A3243	A3244	A3245	G3246	G3247	C3248	C3249	U3250	U3255	G3256	C3257	U3258	C3259	G3260	C3261								
U3262	G3263	G3266	A3267	A3268	U3269	U3270	A3273	A3274	U3275	G3276	U3277	C3278	A3279	U3280	U3281	U3282	U3283	C3284	C3285	G3286	U3287	G3288	G3289	G3290	C3291	A3292	U3293	A3294	A3295	C3296	C3298	A3299	U3300	U3301	U3302	G3303	U3304	A3305	U3306	A3307	C3308	G3309	A3310	C3311	U3312	U3313	A3314	G3315	A3316	U3317	G3318	U3319	A3320	C3321	U3322	A3323			



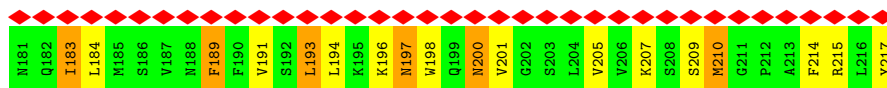
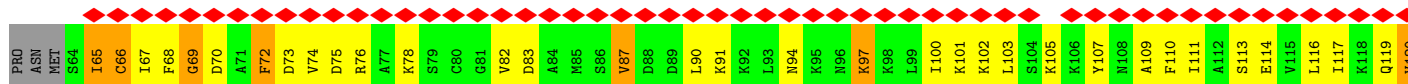
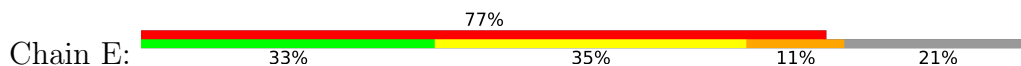
• Molecule 3: 5.8S ribosomal RNA



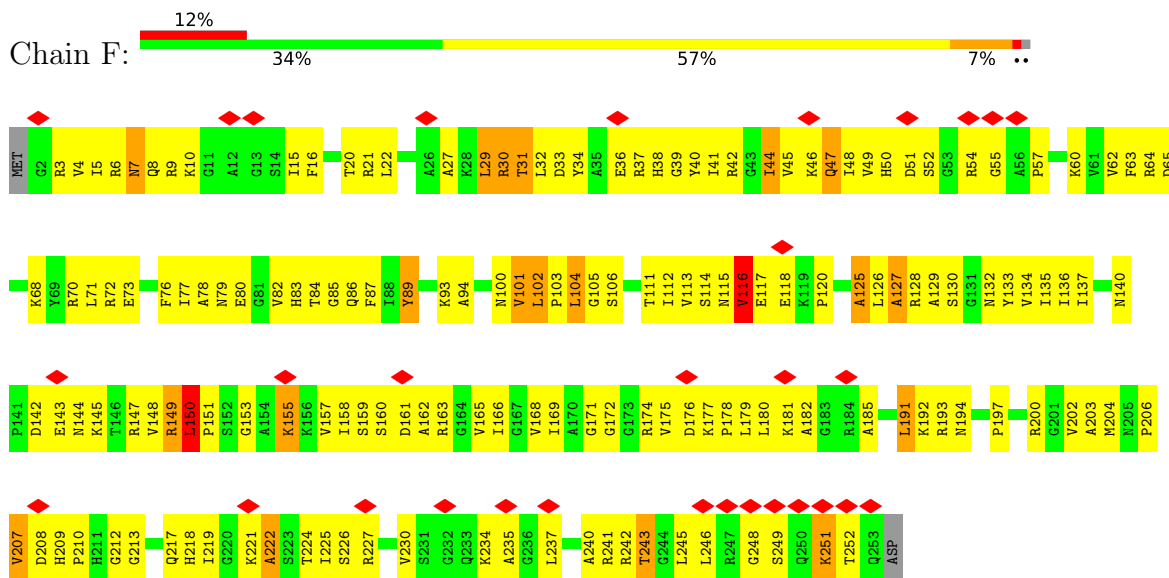
• Molecule 4: 5S ribosomal RNA



• Molecule 5: uL1 (yeast L1)



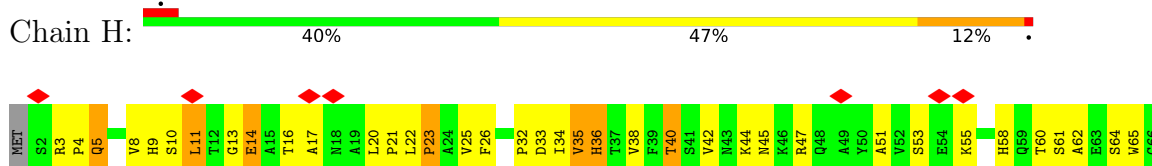
• Molecule 6: uL2 (yeast L2)

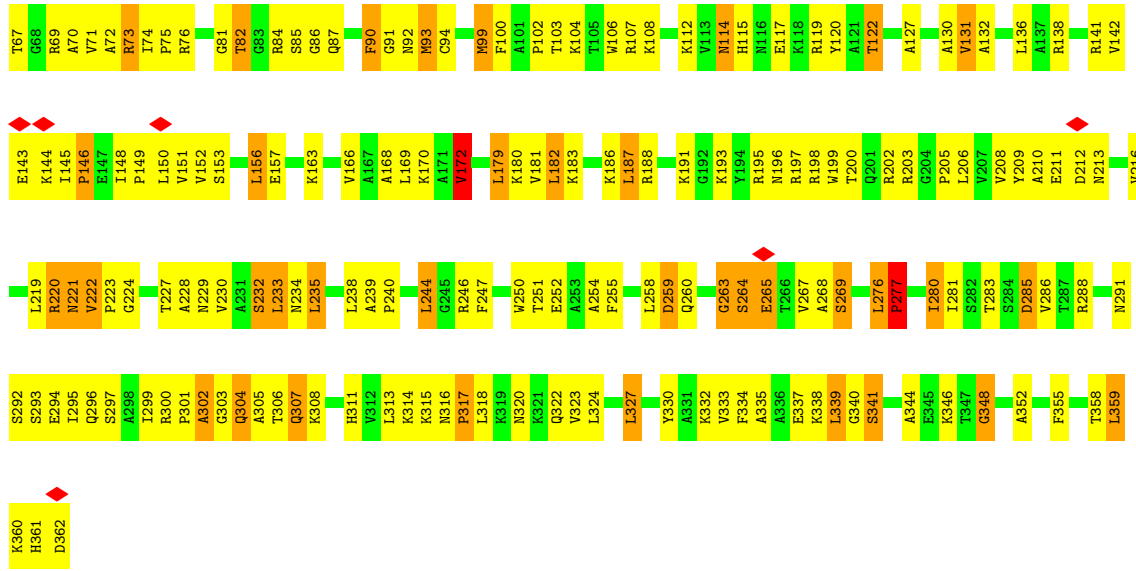


• Molecule 7: uL3 (yeast L3)

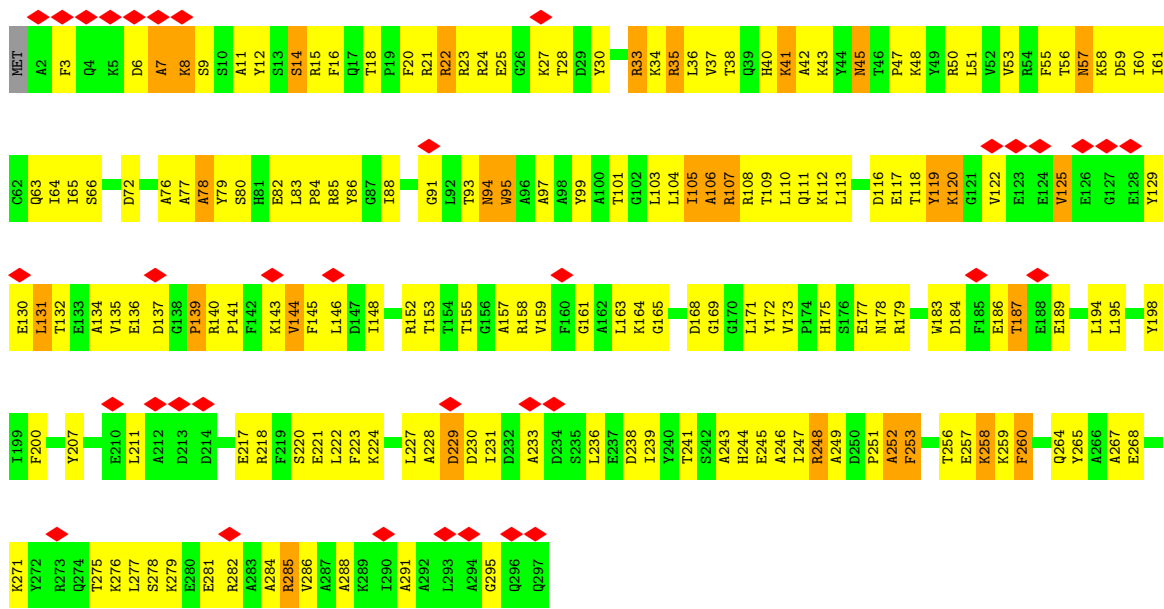


• Molecule 8: uL4 (yeast L4)

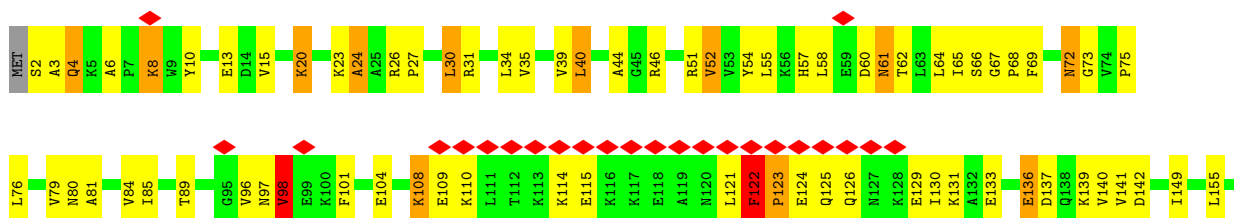


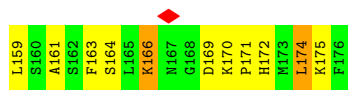


• Molecule 9: uL18 (yeast L5)

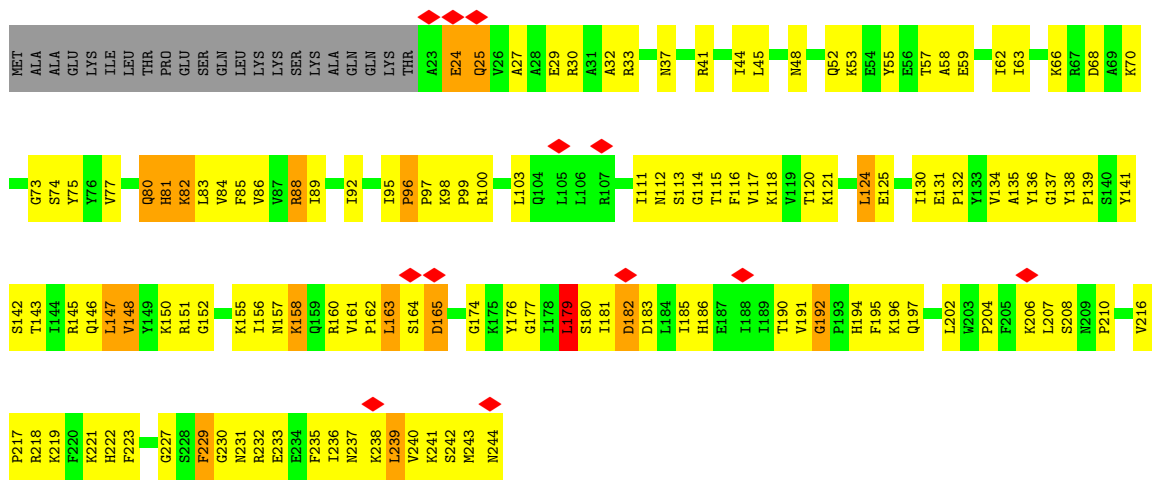


• Molecule 10: eL6 (yeast L6)

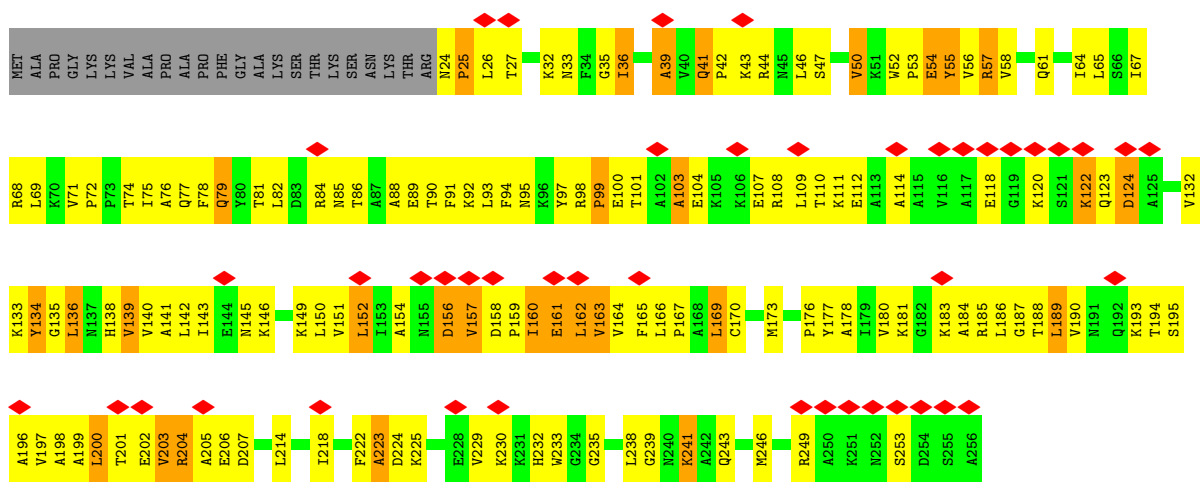




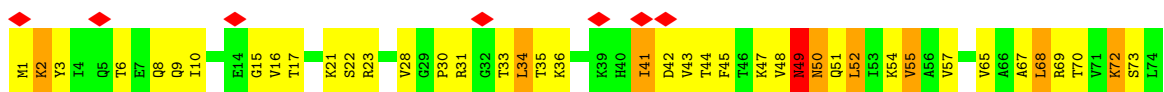
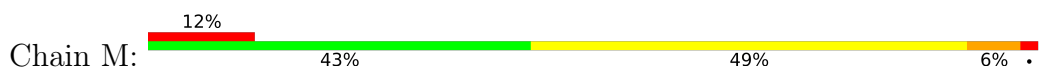
• Molecule 11: uL30 (yeast L7)

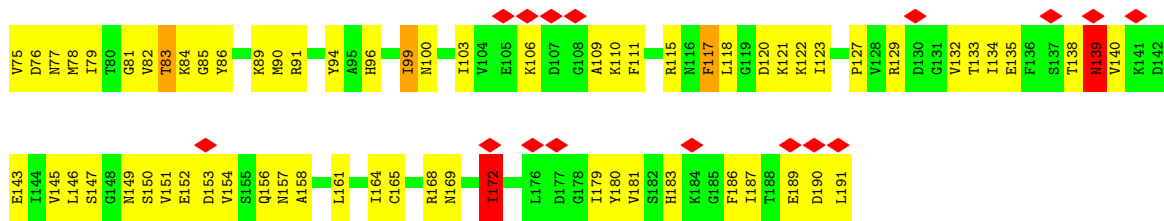


• Molecule 12: eL8 (yeast L8)

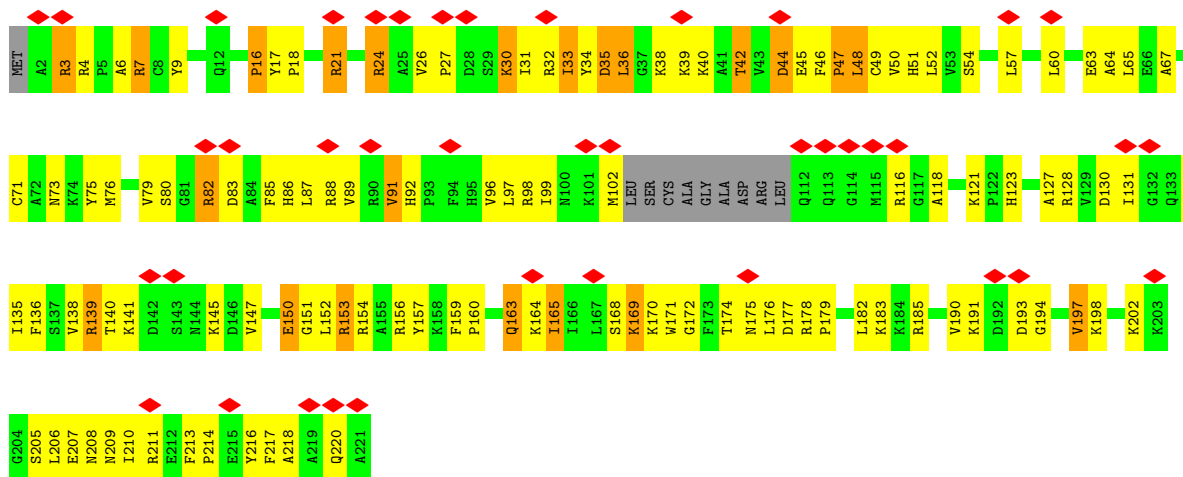


• Molecule 13: uL6 (yeast L9)

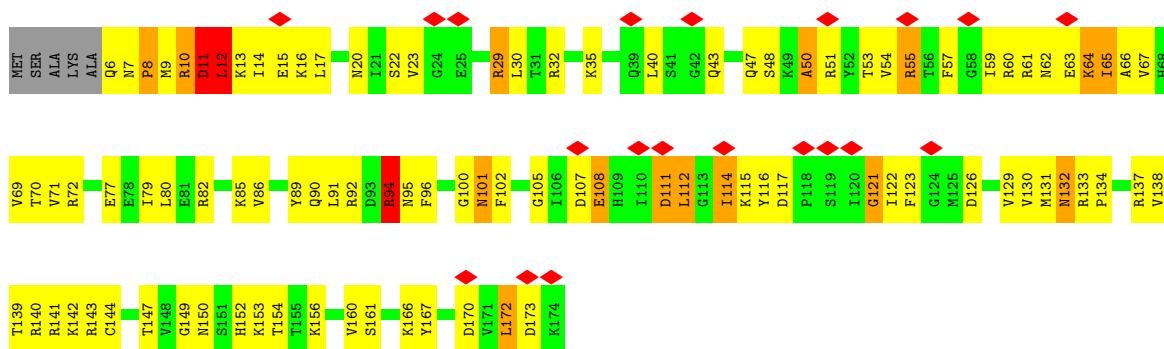




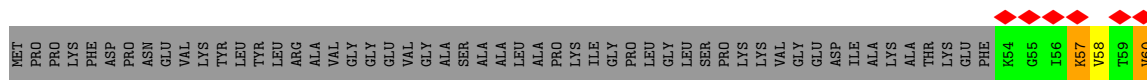
• Molecule 14: uL16 (yeast L10)

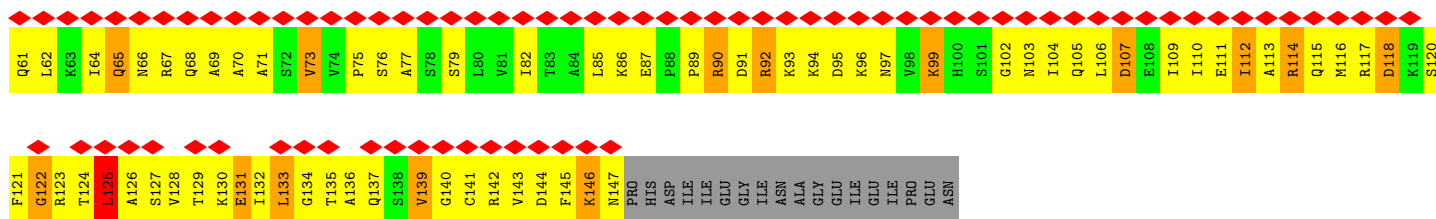


• Molecule 15: uL5 (yeast L11)

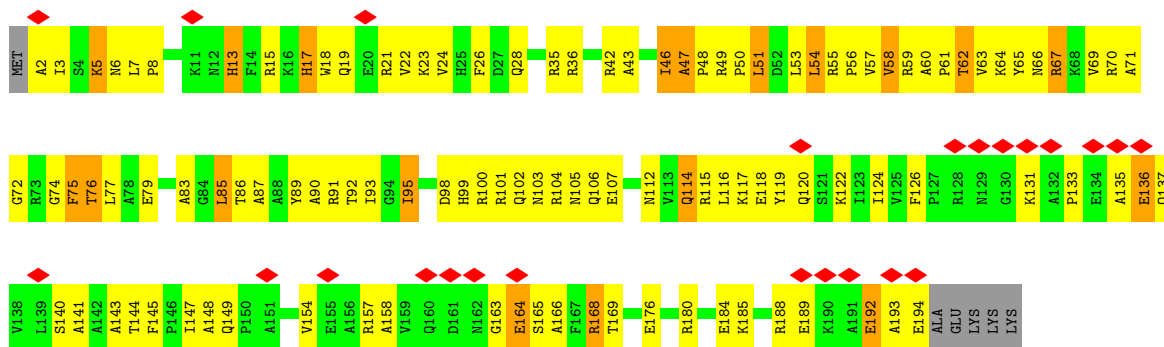


• Molecule 16: uL11 (yeast L12)

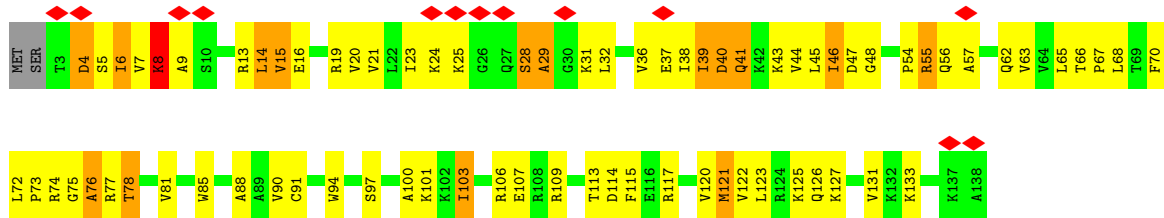




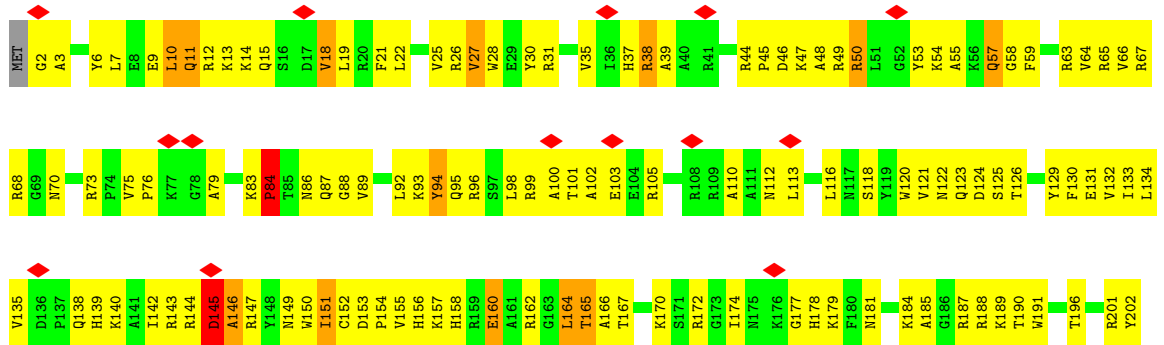
• Molecule 17: eL13 (yeast L13)



• Molecule 18: eL14 (yeast L14)



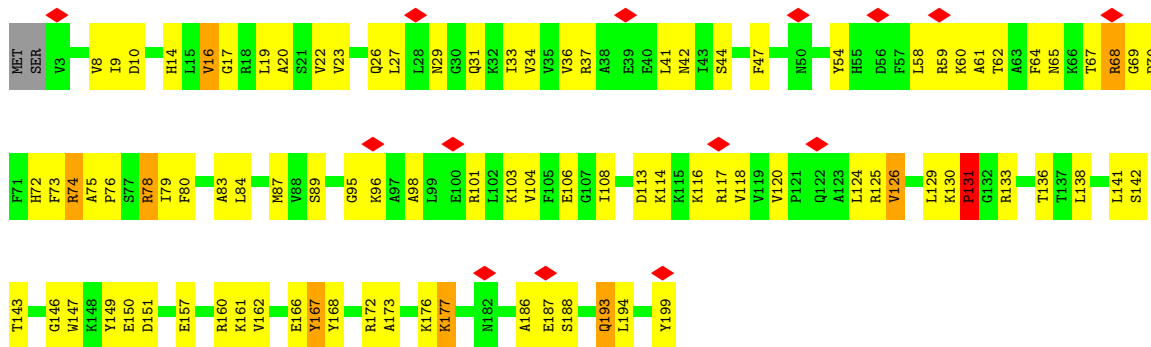
• Molecule 19: eL15 (yeast L15)



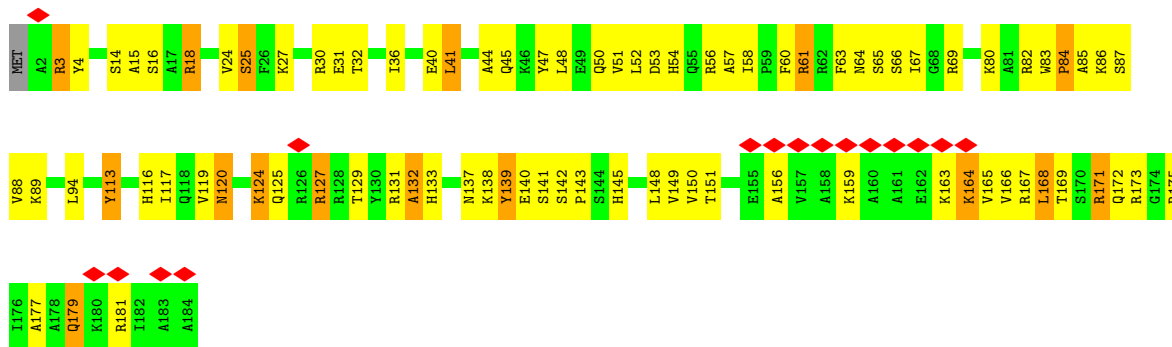




- Molecule 20: uL13 (yeast L16)



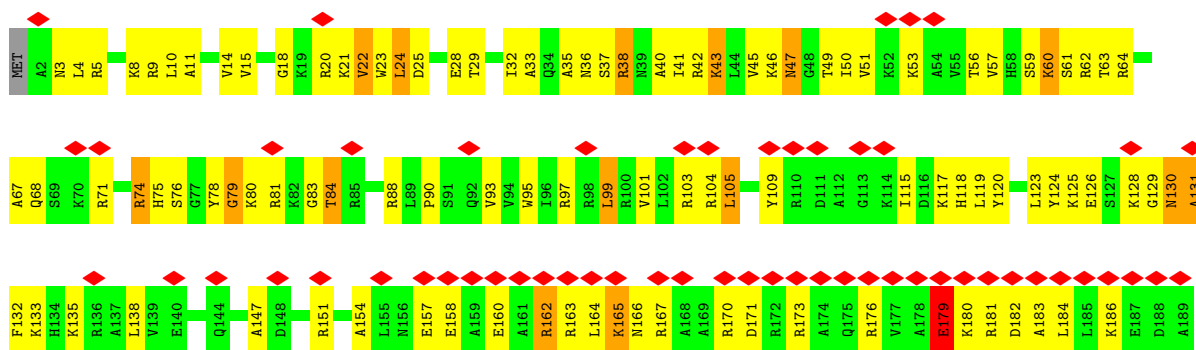
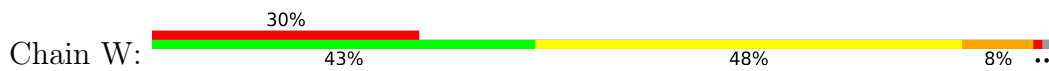
- Molecule 21: uL22 (yeast L17)



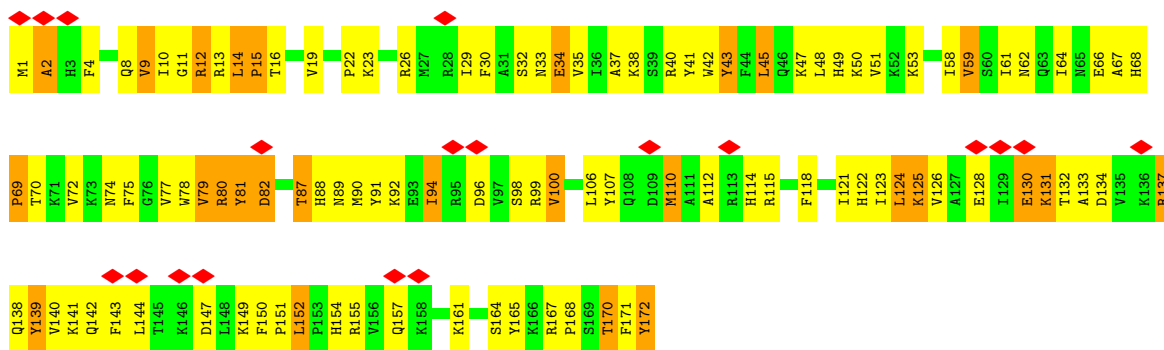
- Molecule 22: eL18 (yeast L18)



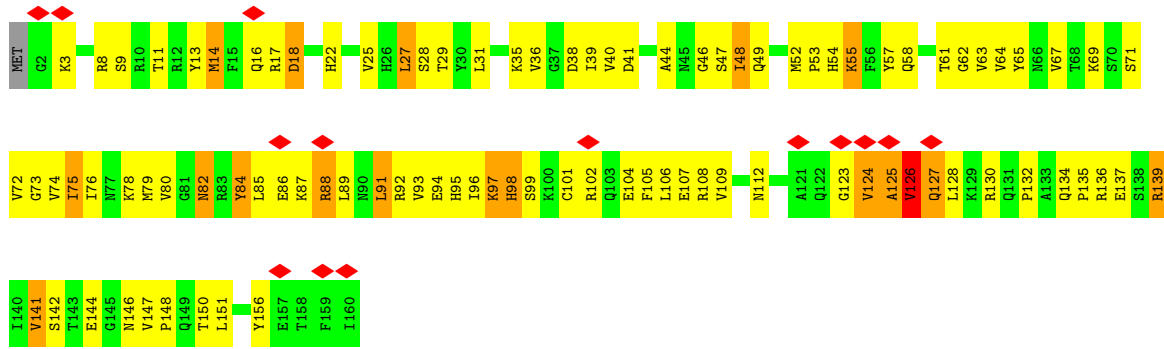
- Molecule 23: eL19 (yeast L19)



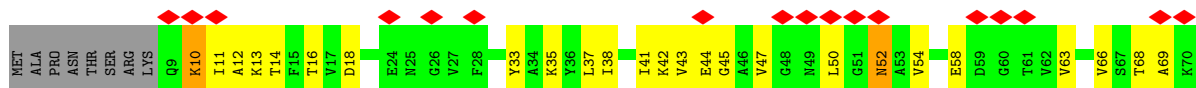
• Molecule 24: eL20 (yeast L20)

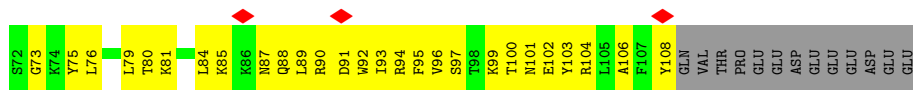


• Molecule 25: eL21 (yeast L21)

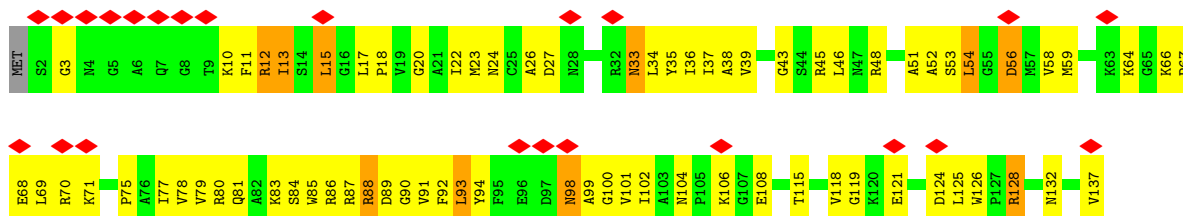


• Molecule 26: eL22 (yeast L22)

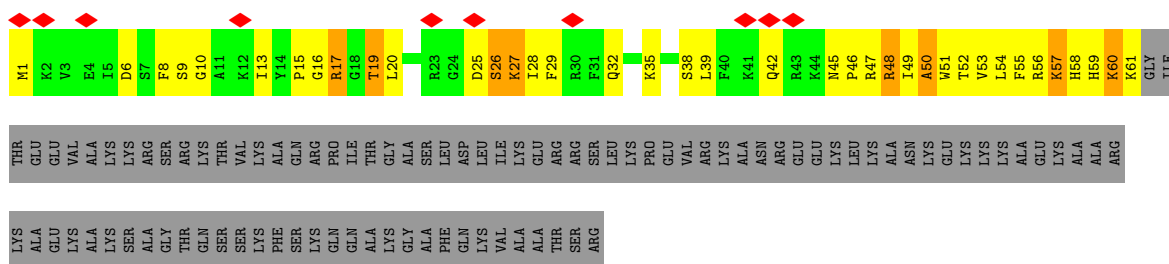
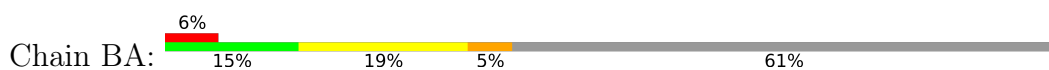




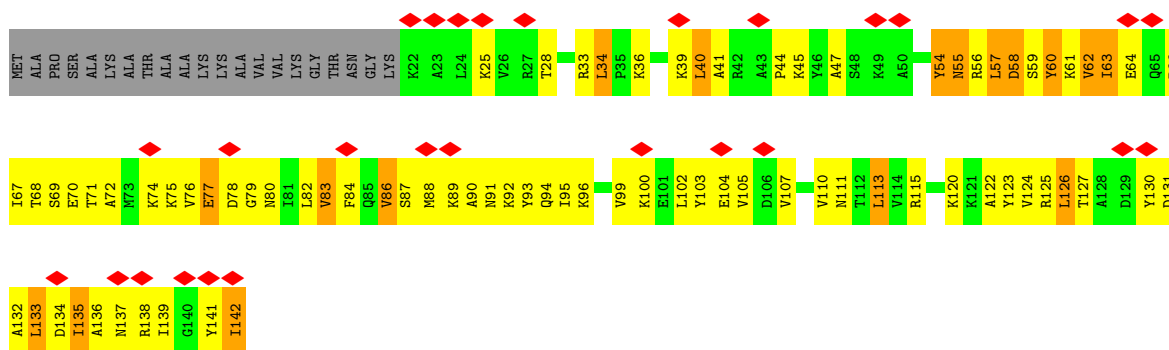
• Molecule 27: uL14 (yeast L23)



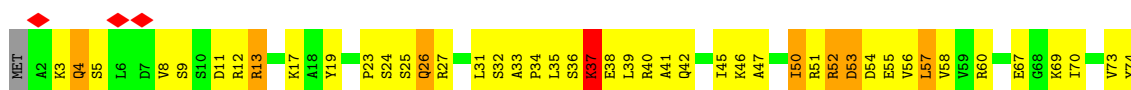
• Molecule 28: eL24 (yeast L24)

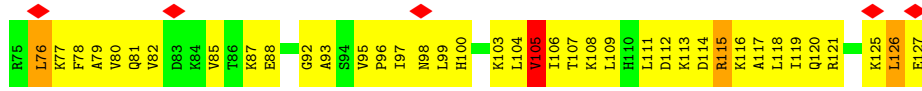


• Molecule 29: uL23 (yeast L25)

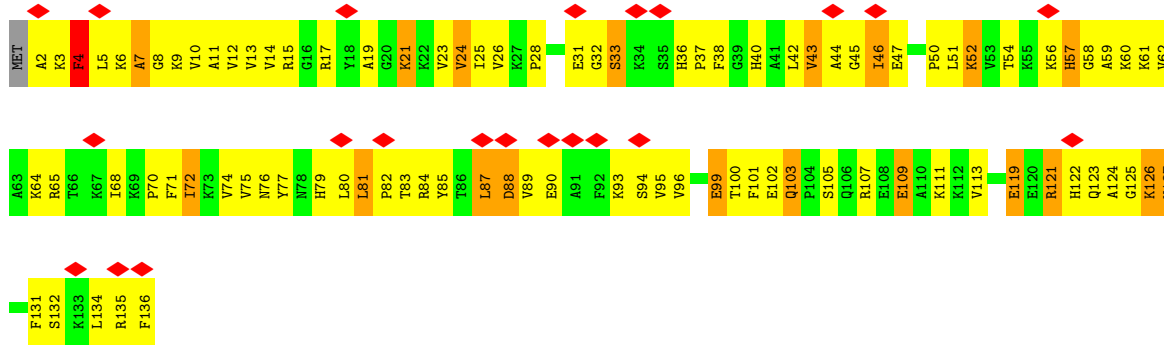


• Molecule 30: uL24 (yeast L26)

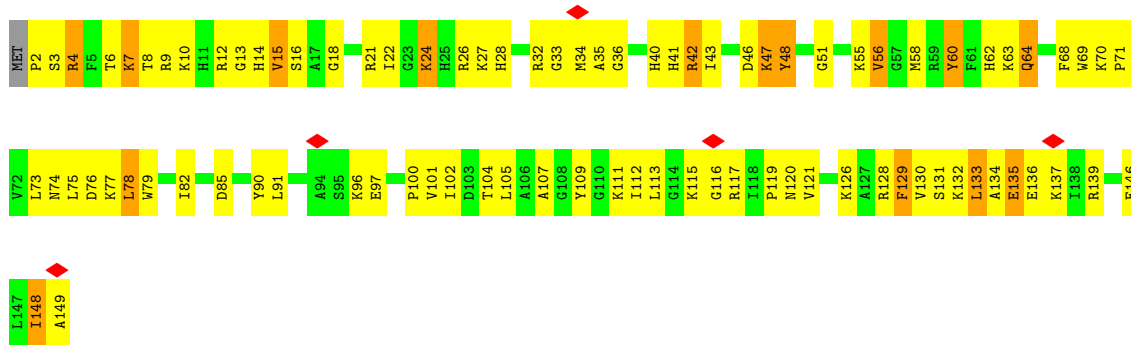




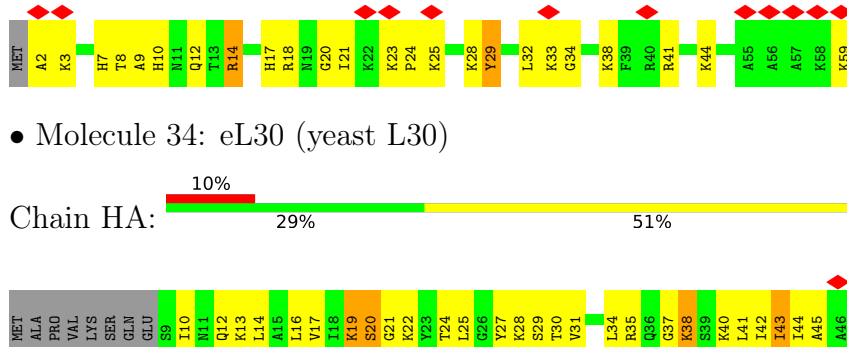
• Molecule 31: eL27 (yeast L27)



• Molecule 32: uL15 (yeast L28)



• Molecule 33: eL29 (yeast L29)

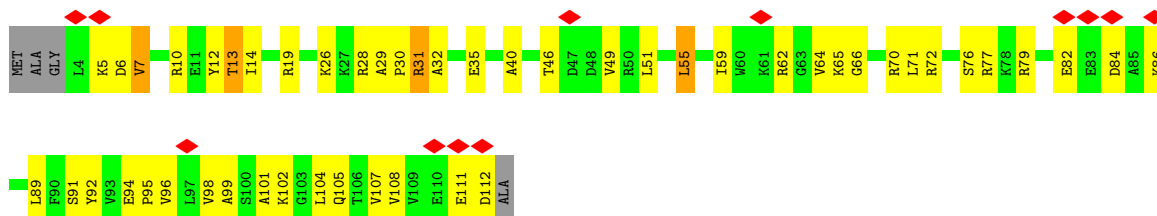


• Molecule 34: eL30 (yeast L30)

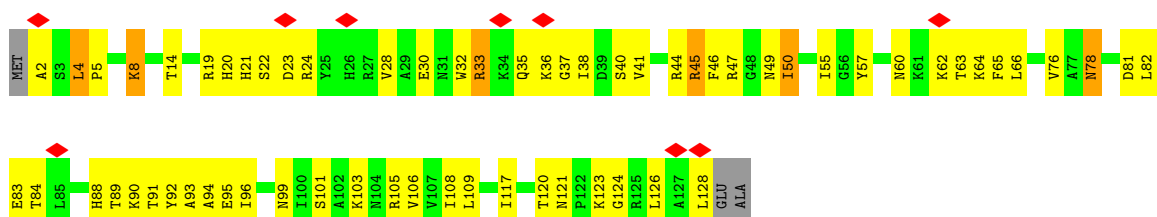




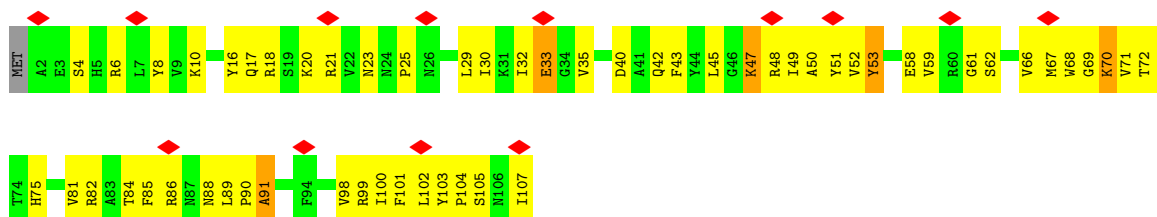
• Molecule 35: eL31 (yeast L31)



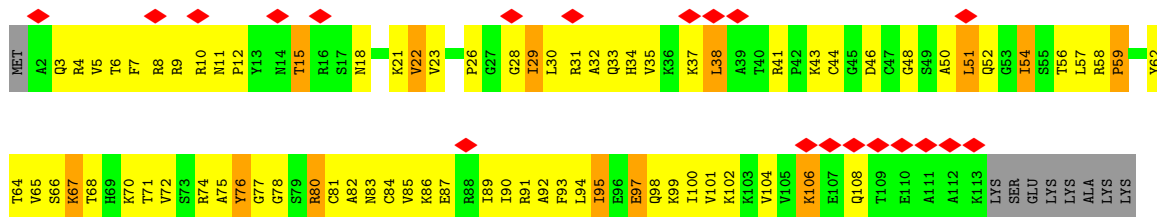
• Molecule 36: eL32 (yeast L32)



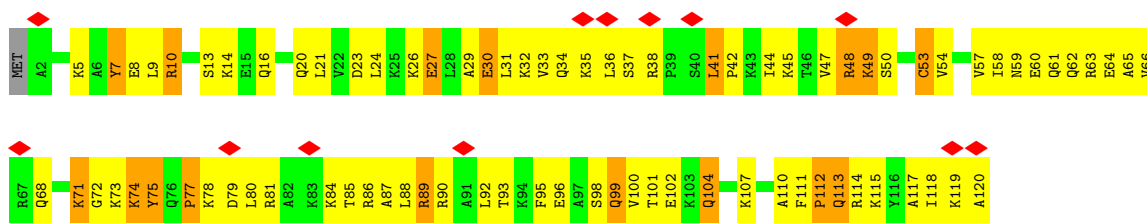
• Molecule 37: eL33 (yeast L33)



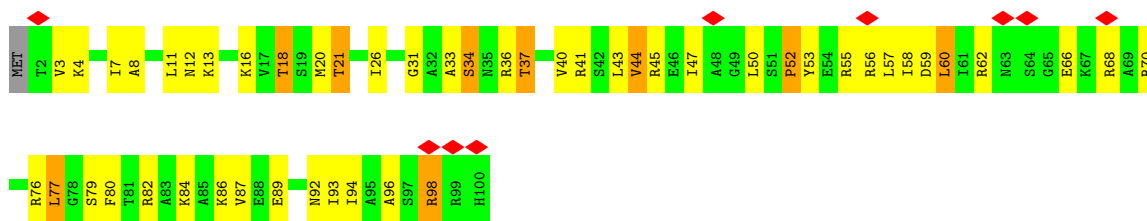
• Molecule 38: eL34 (yeast L34)



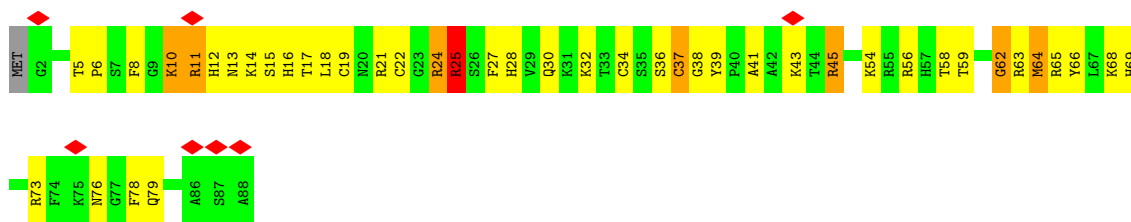
• Molecule 39: uL29 (yeast L35)



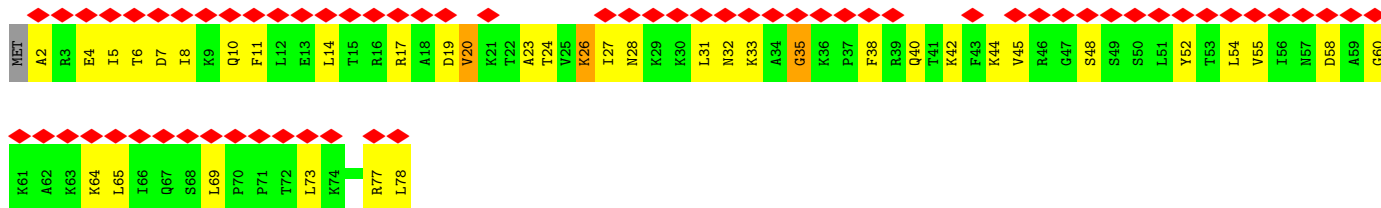
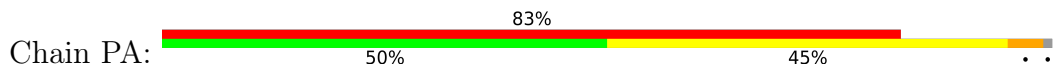
• Molecule 40: eL36 (yeast L36)



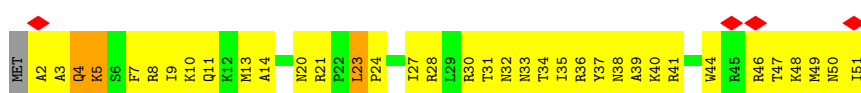
• Molecule 41: eL37 (yeast L37)



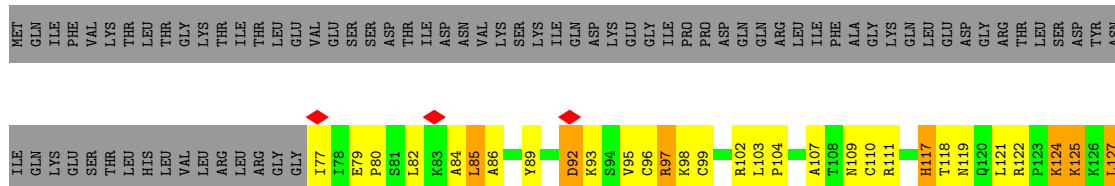
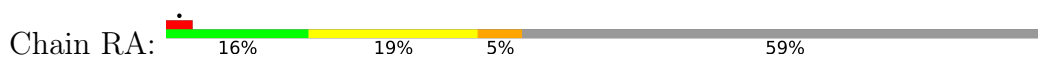
• Molecule 42: eL38 (yeast L38)



• Molecule 43: eL39 (yeast L39)



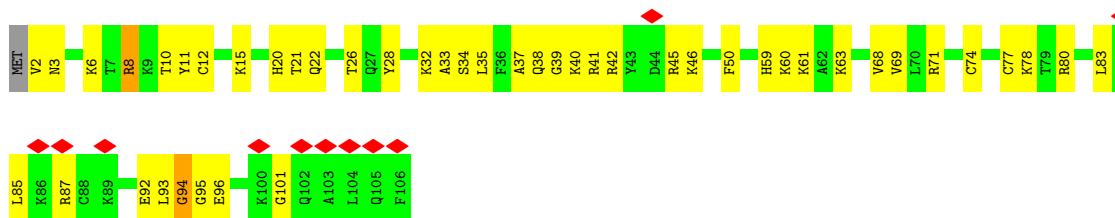
• Molecule 44: eL40 (yeast L40)



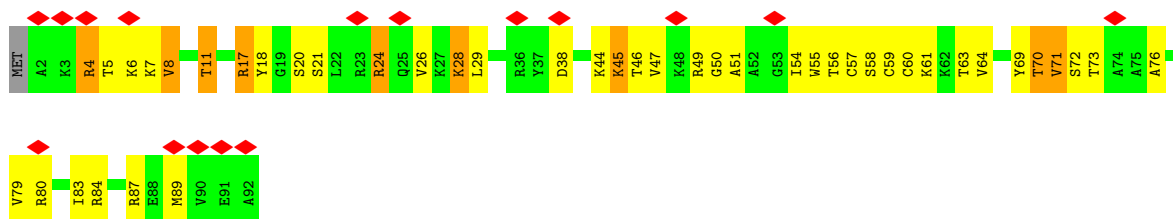
• Molecule 45: eL41 (yeast L41)



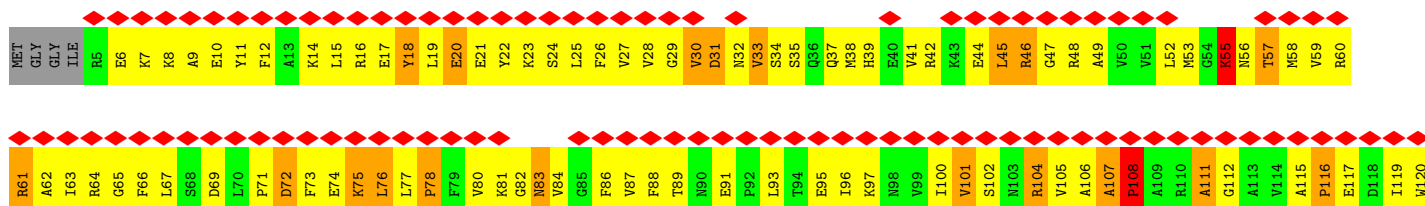
• Molecule 46: eL42 (yeast L42)



• Molecule 47: eL43 (yeast L43)

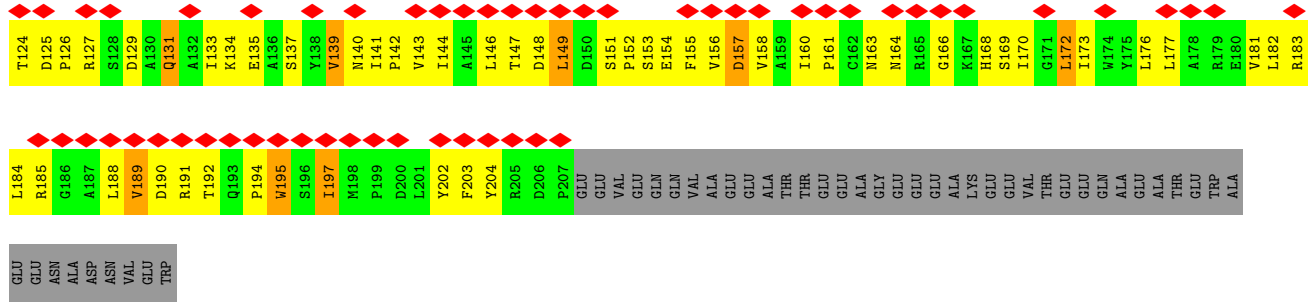


• Molecule 48: uL10 (yeast P0)



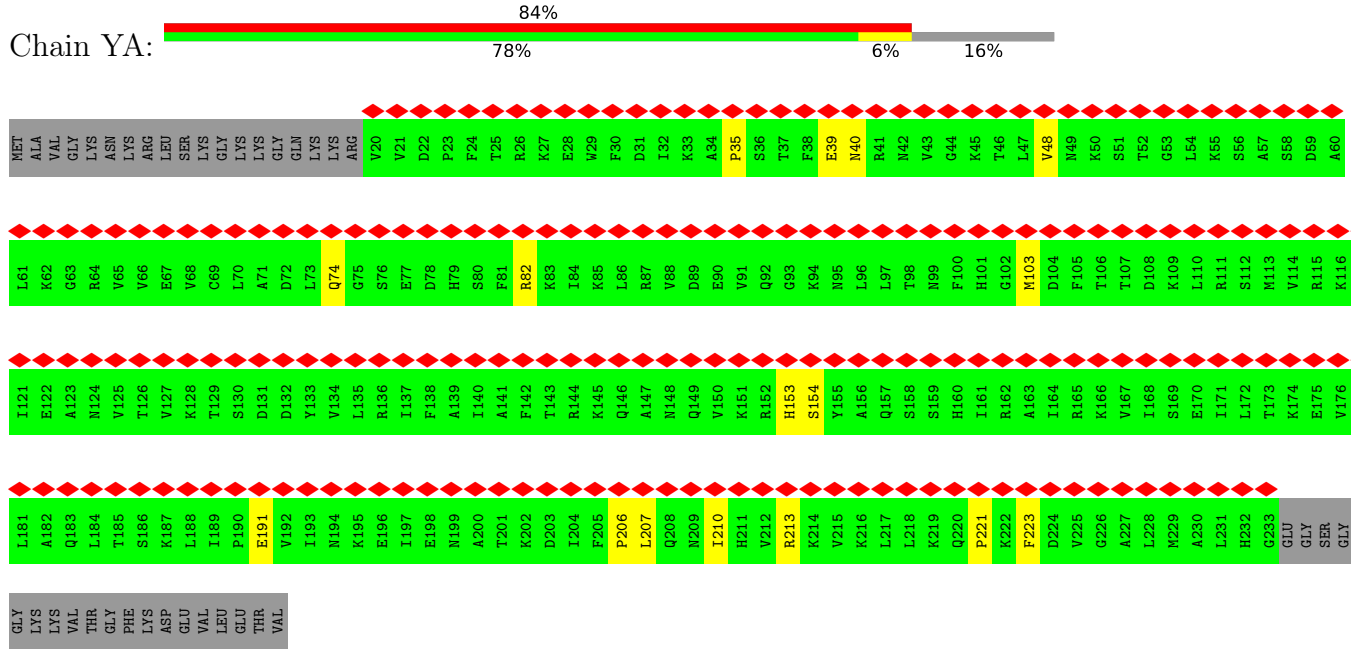






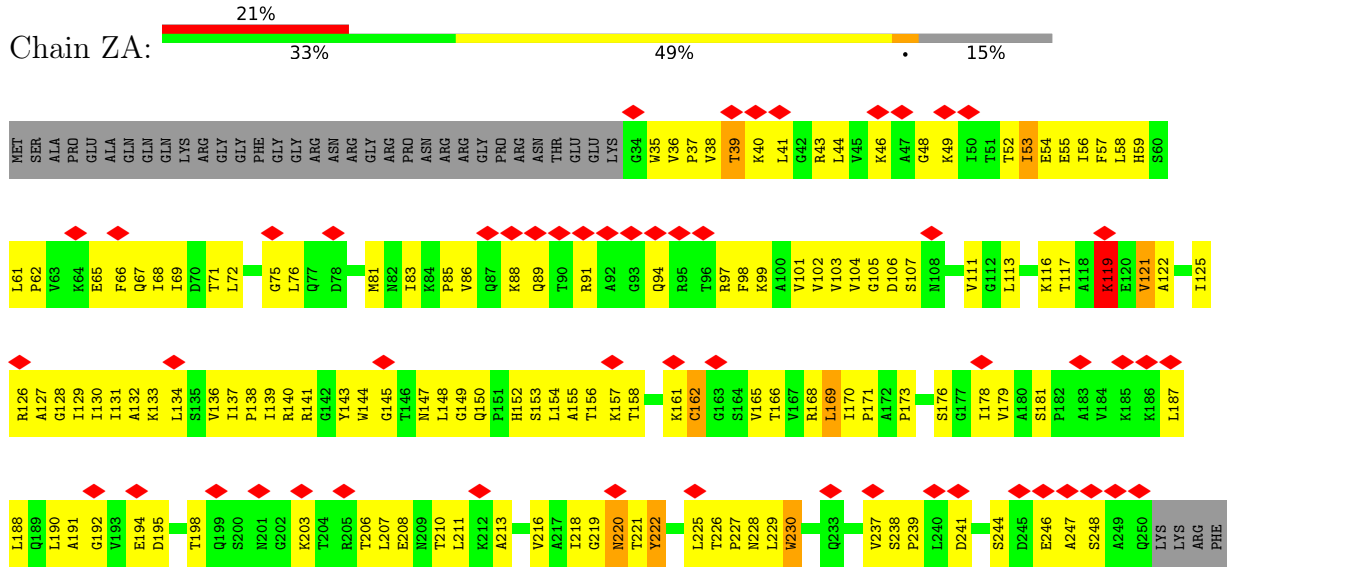
• Molecule 51: eS1 (yeast S1)

Chain YA:



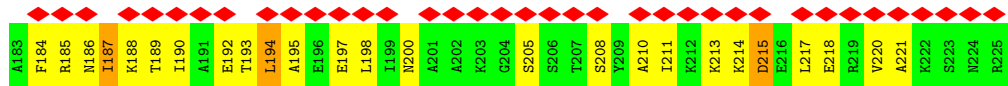
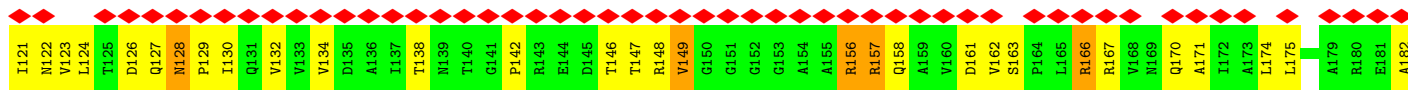
• Molecule 52: uS5 (yeast S2)

Chain ZA:

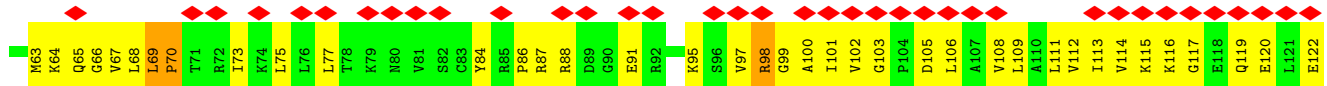


• Molecule 53: uS3 (yeast S3)

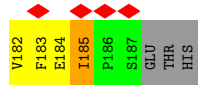
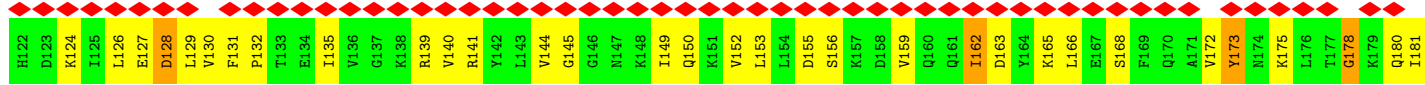
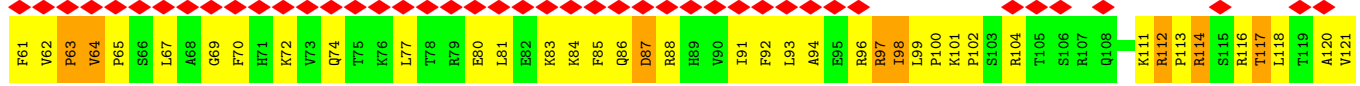
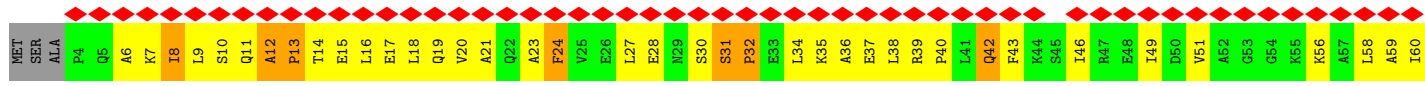
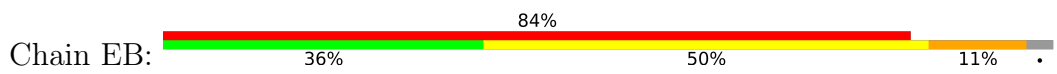




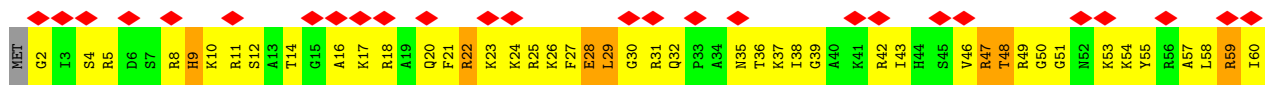
• Molecule 56: eS6 (yeast S6)

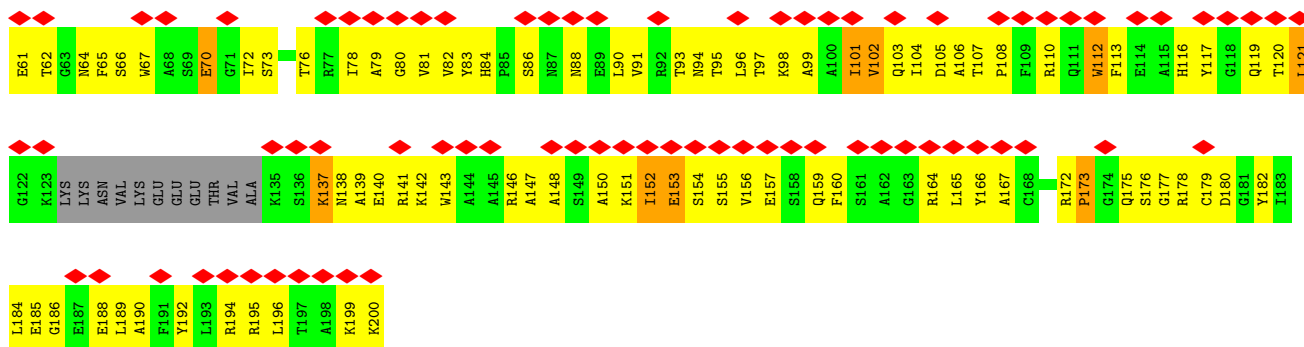


• Molecule 57: eS7 (yeast S7)

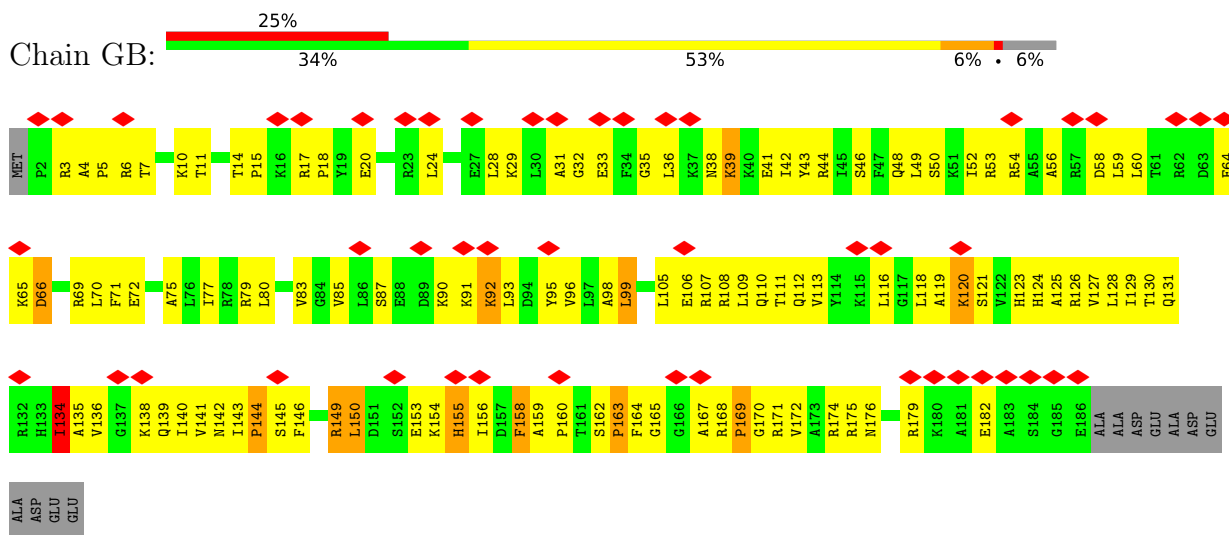


• Molecule 58: eS8 (yeast S8)

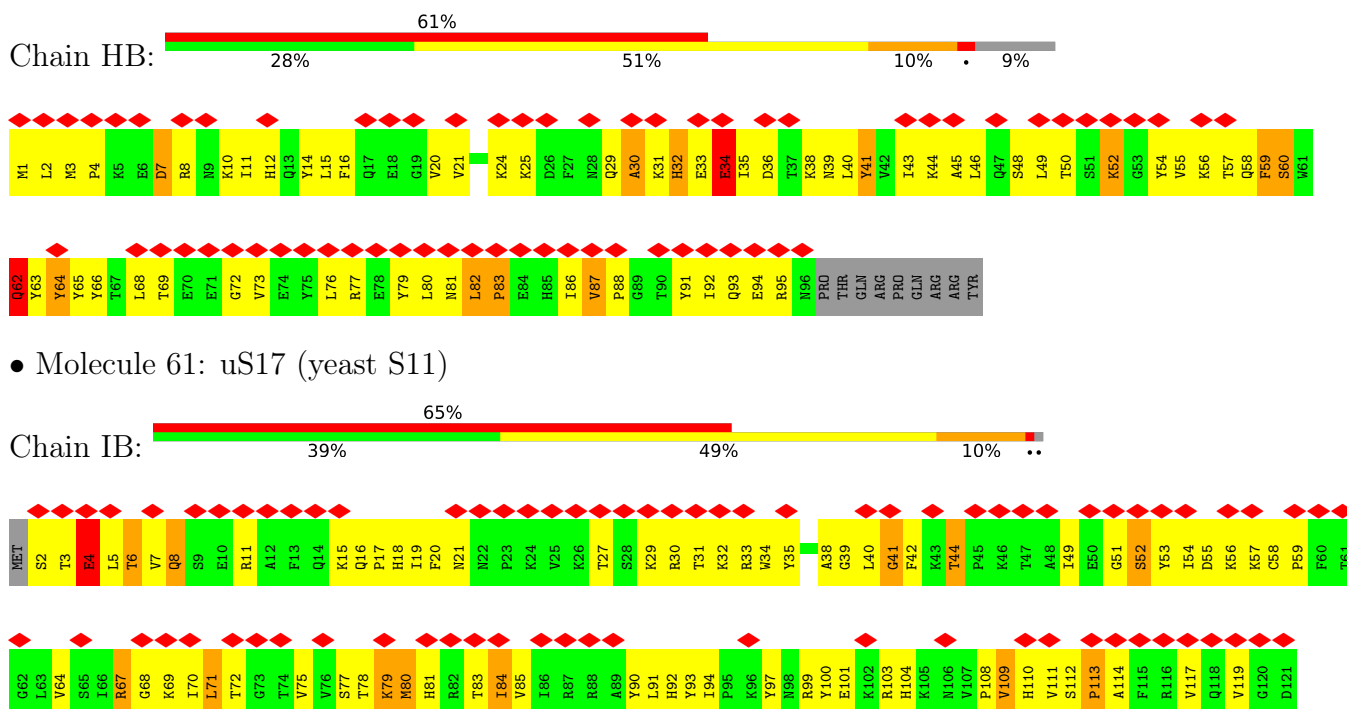


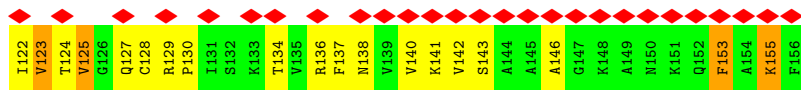


• Molecule 59: uS4 (yeast S9)

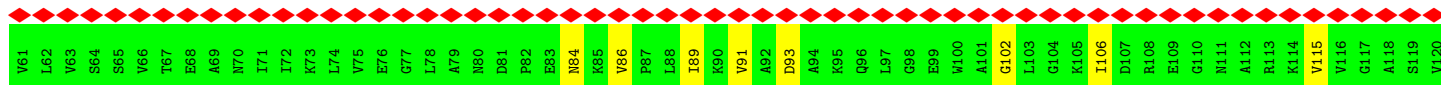
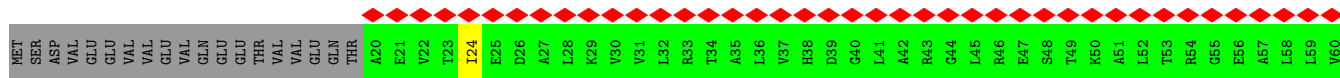
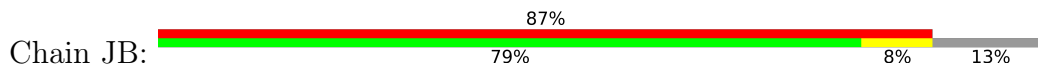


• Molecule 61: uS17 (yeast S11)

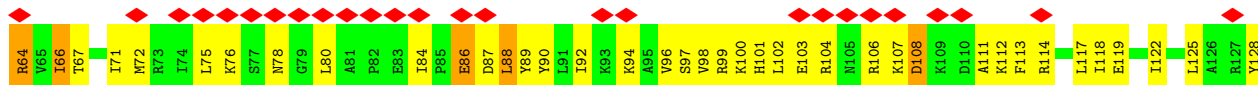
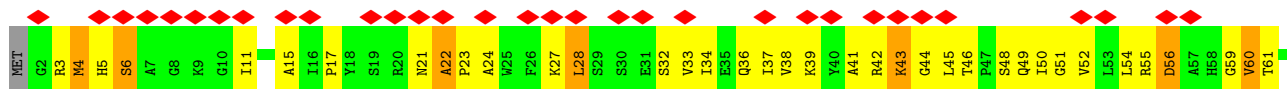
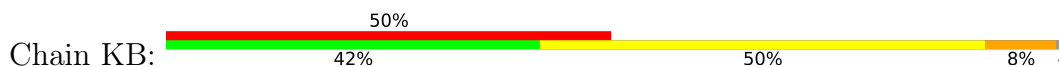




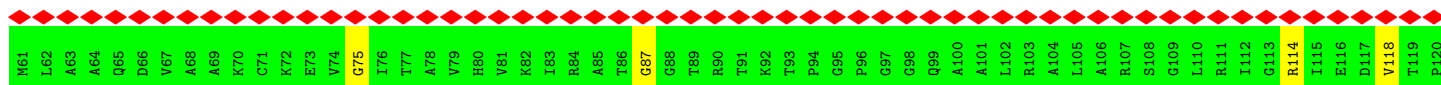
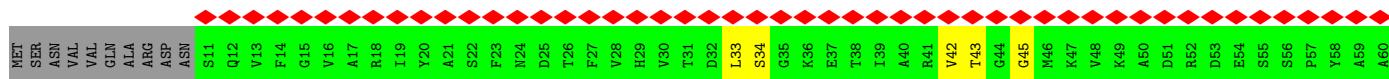
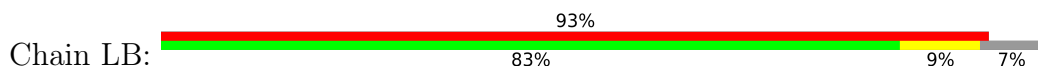
• Molecule 62: eS12 (yeast S12)



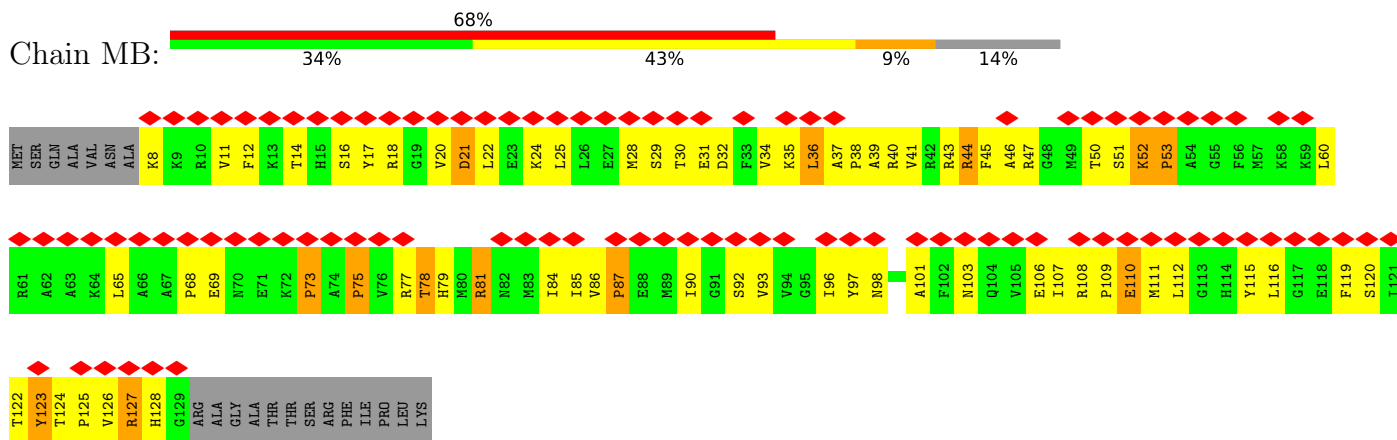
• Molecule 63: uS15 (yeast S13)



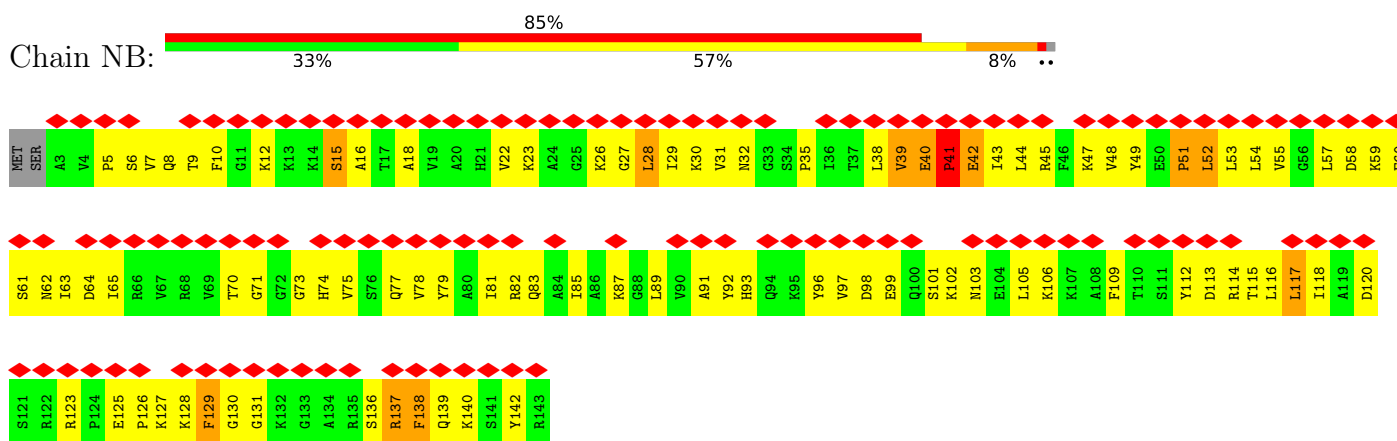
• Molecule 64: uS11 (yeast S14)



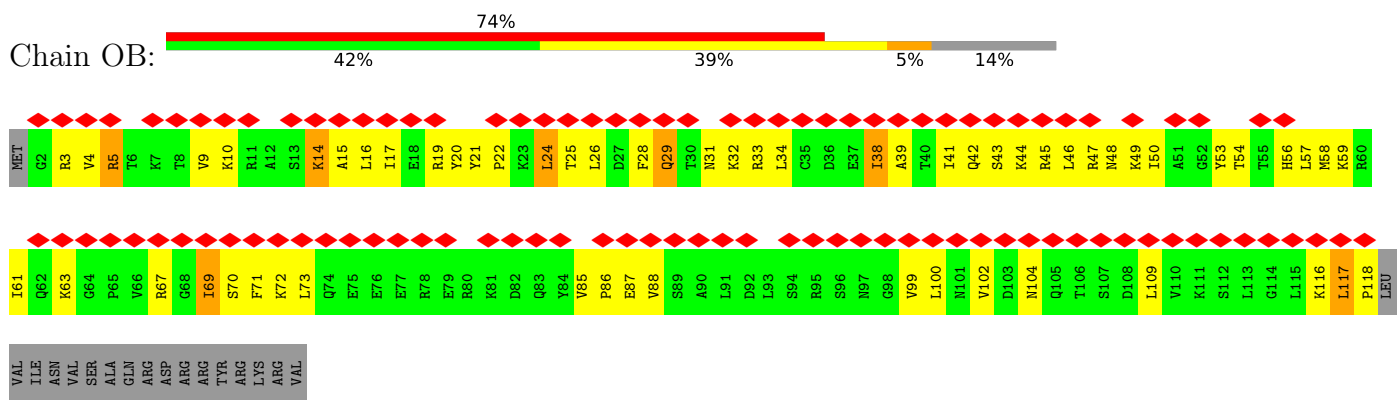
• Molecule 65: uS19 (yeast S15)



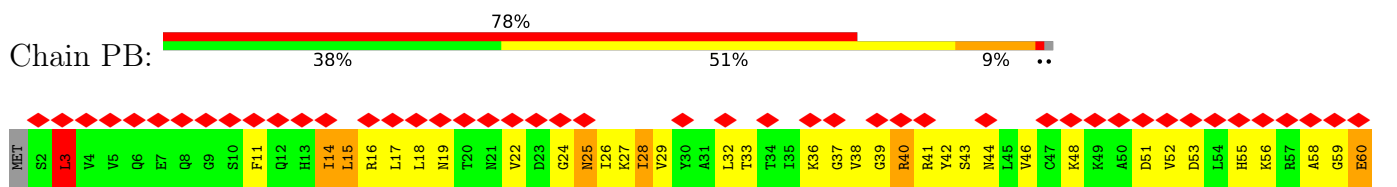
• Molecule 66: uS9 (yeast S16)

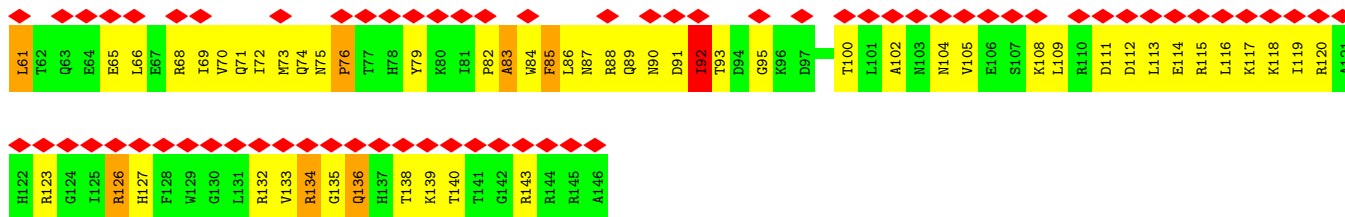


• Molecule 67: eS17 (yeast S17)

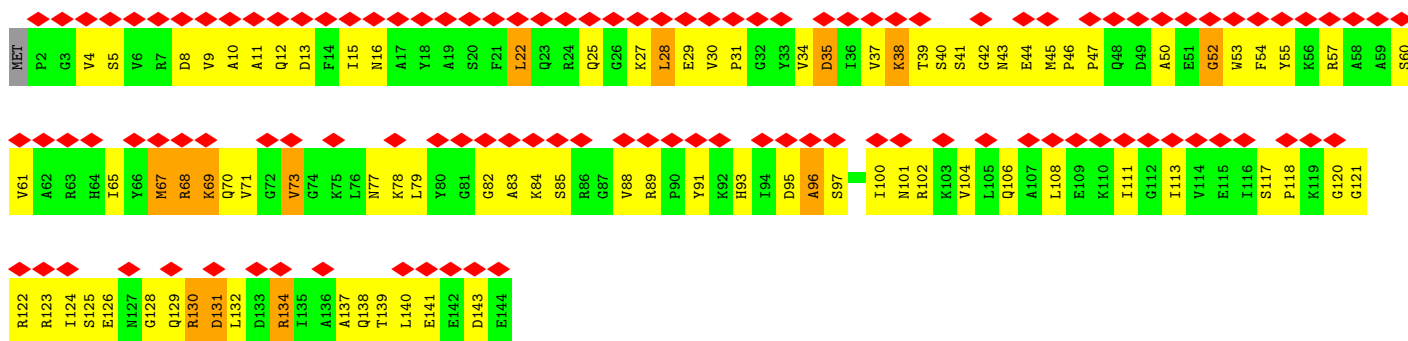
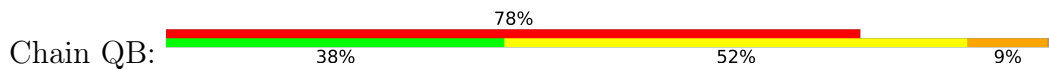


• Molecule 68: uS13 (yeast S18)

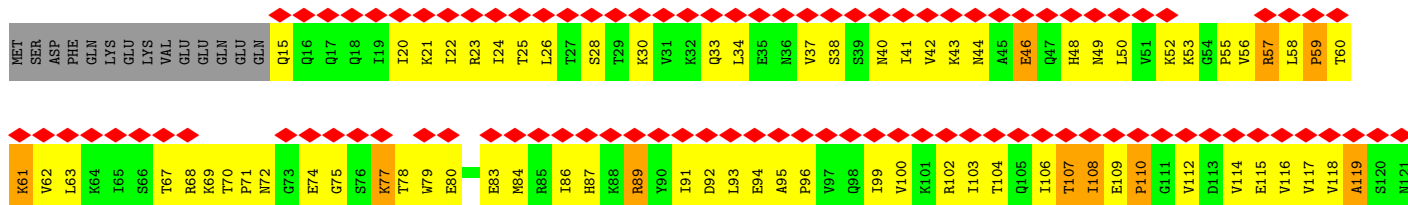
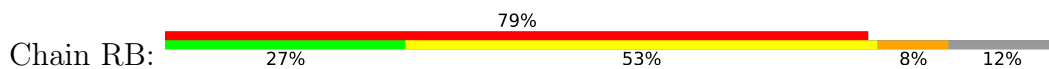




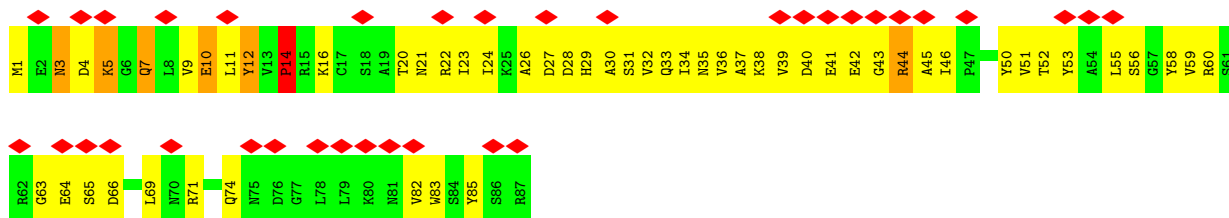
• Molecule 69: eS19 (yeast S19)



• Molecule 70: uS10 (yeast S20)

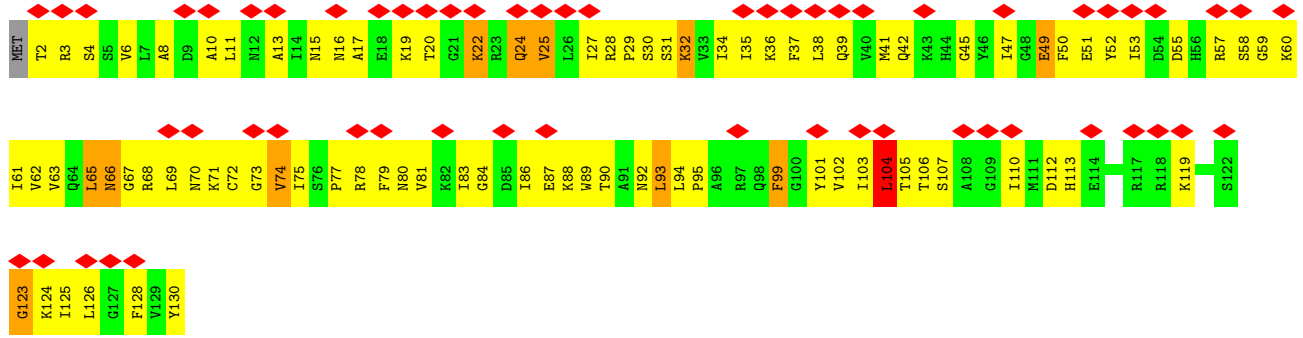


• Molecule 71: eS21 (yeast S21)

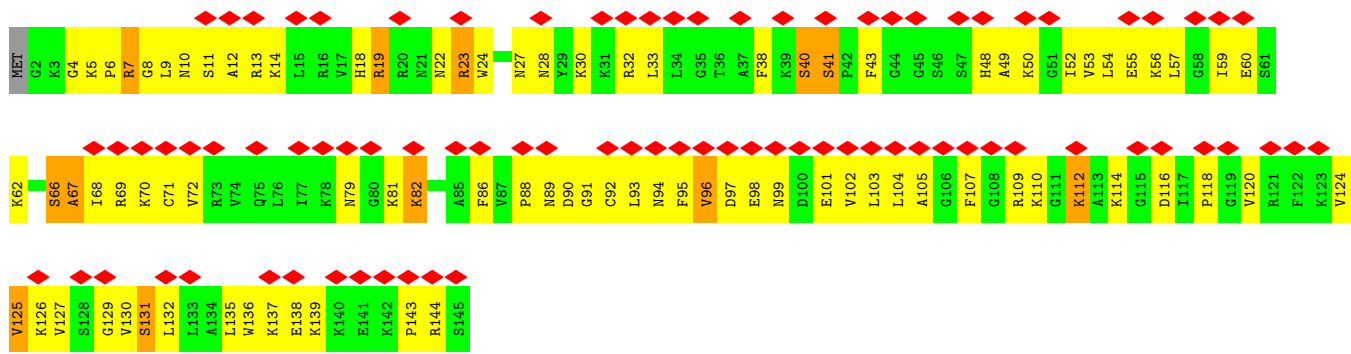


• Molecule 72: uS8 (yeast S22)

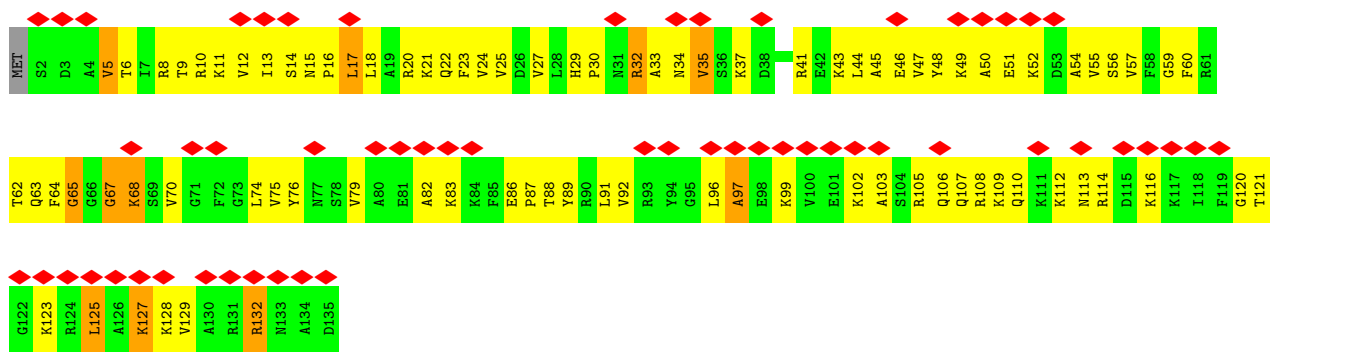




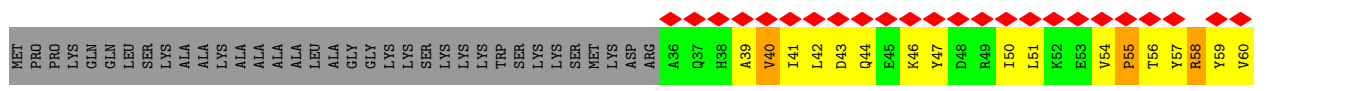
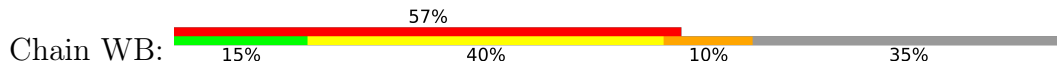
• Molecule 73: uS12 (yeast S23)



• Molecule 74: eS24 (yeast S24)



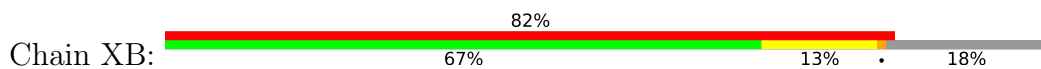
• Molecule 75: eS25 (yeast S25)



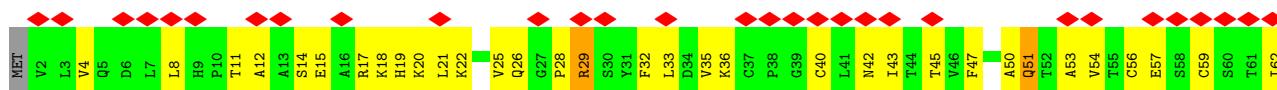




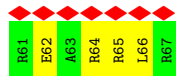
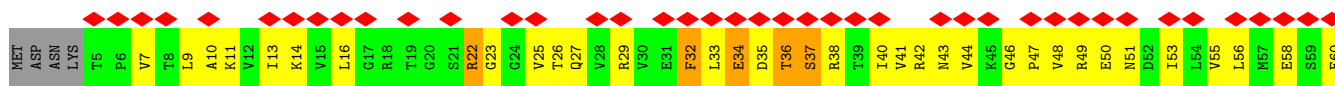
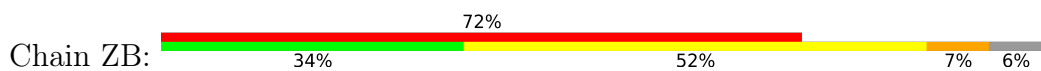
• Molecule 76: eS26 (yeast S26)



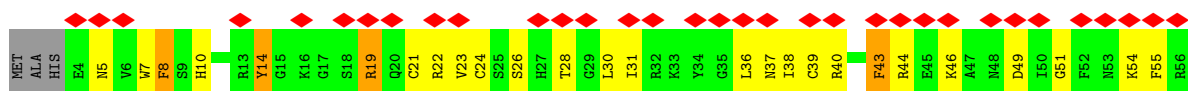
• Molecule 77: eS27 (yeast S27)



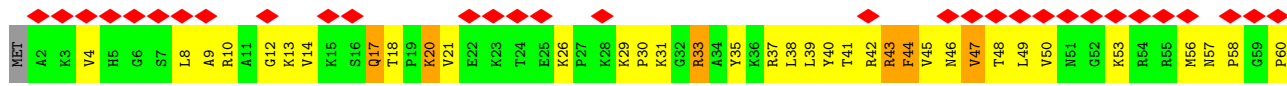
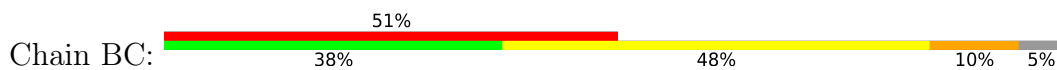
• Molecule 78: eS28 (yeast S28)



• Molecule 79: uS14 (yeast S29)

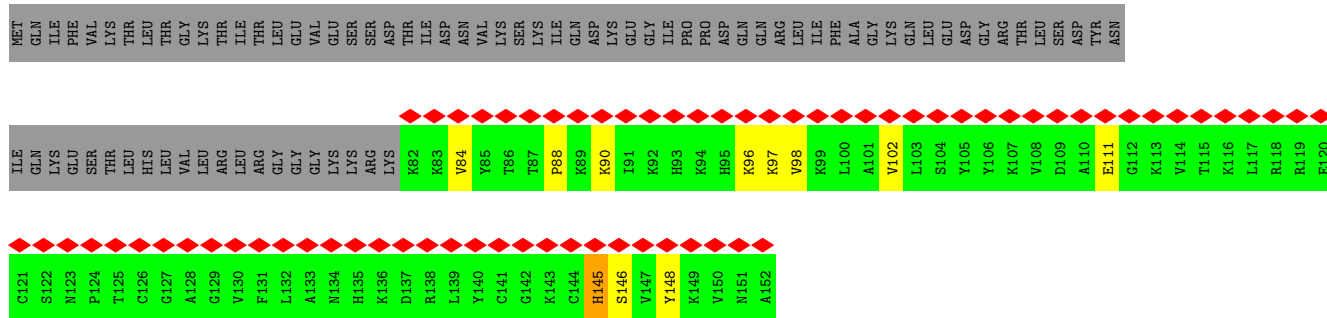
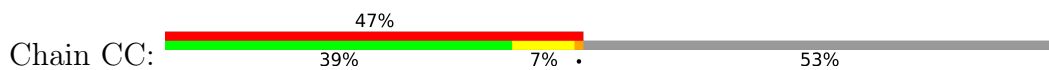


• Molecule 80: eS30 (yeast S30)

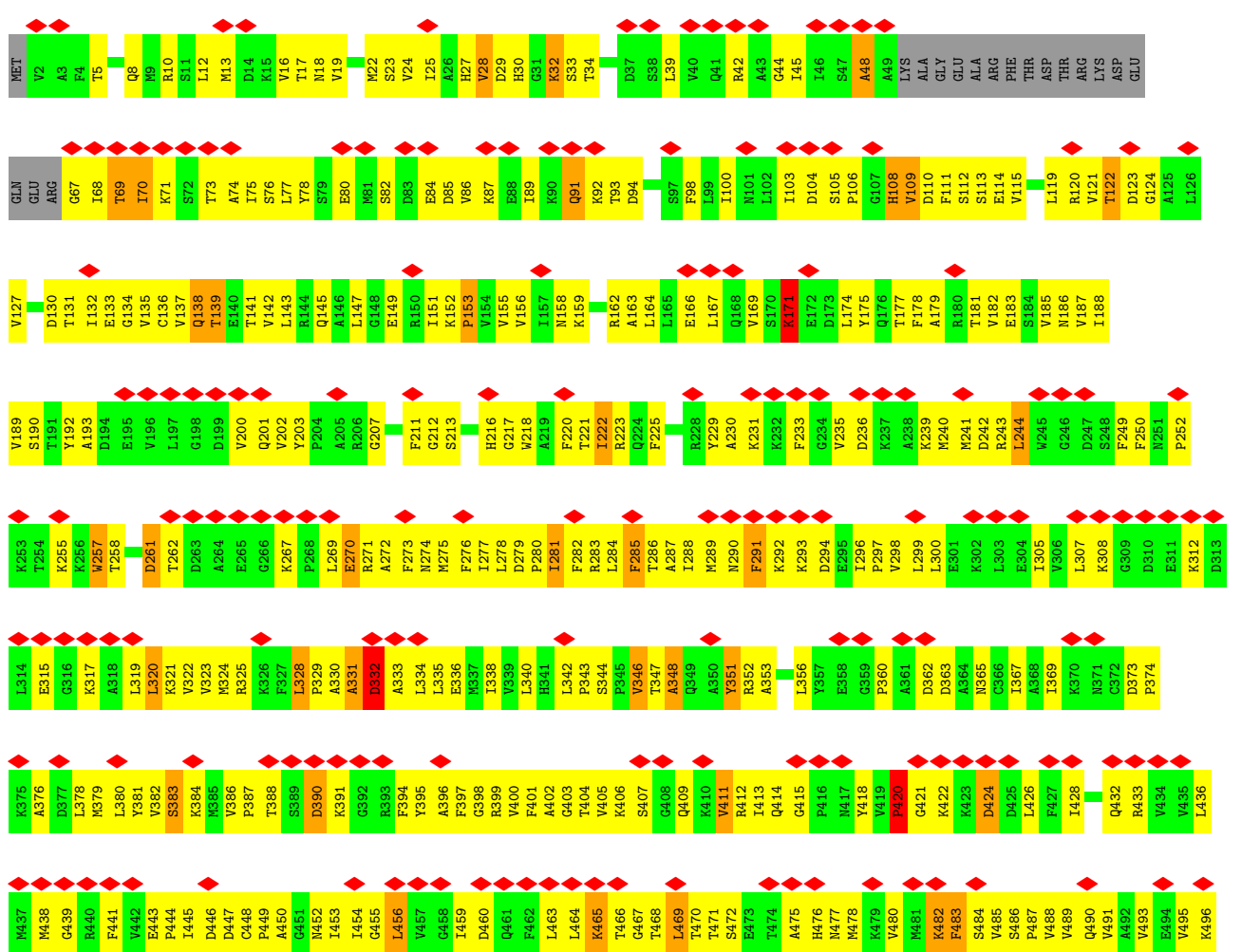


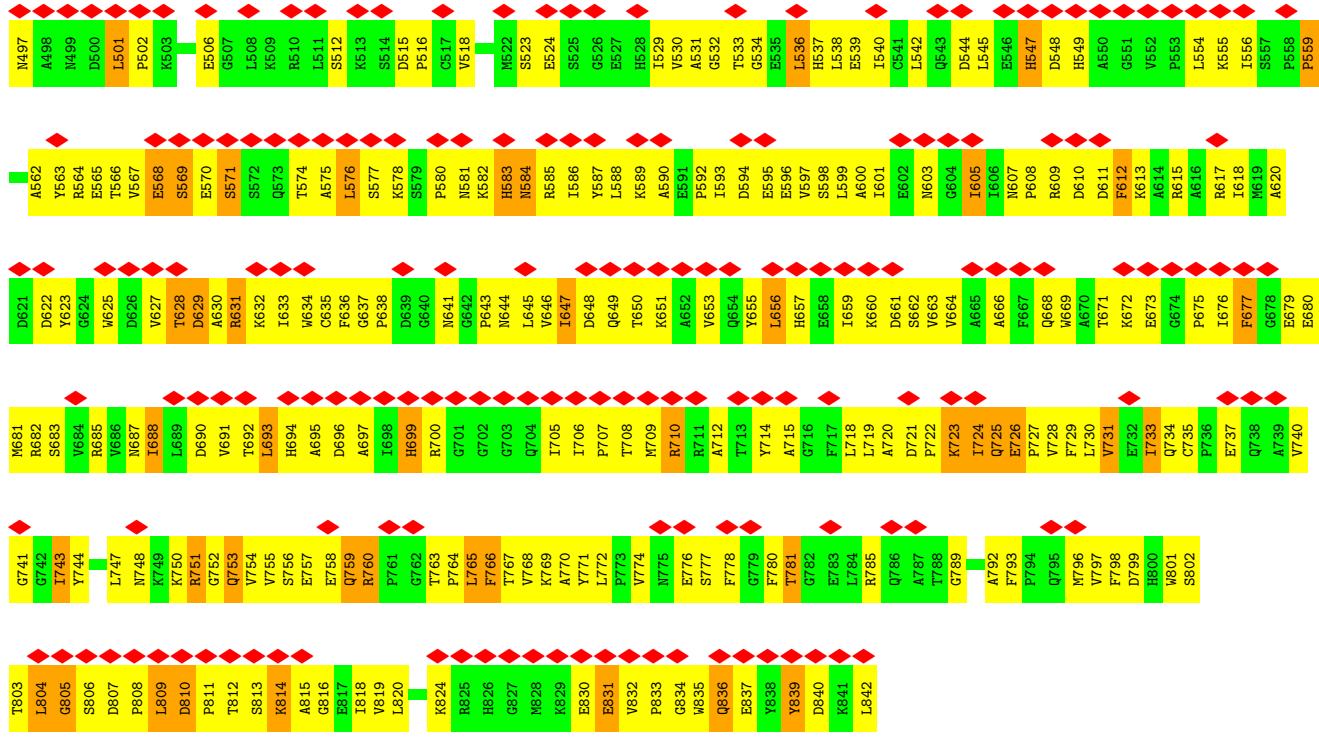
661  
VAL  
GLN

• Molecule 81: eS31 (yeast S31)

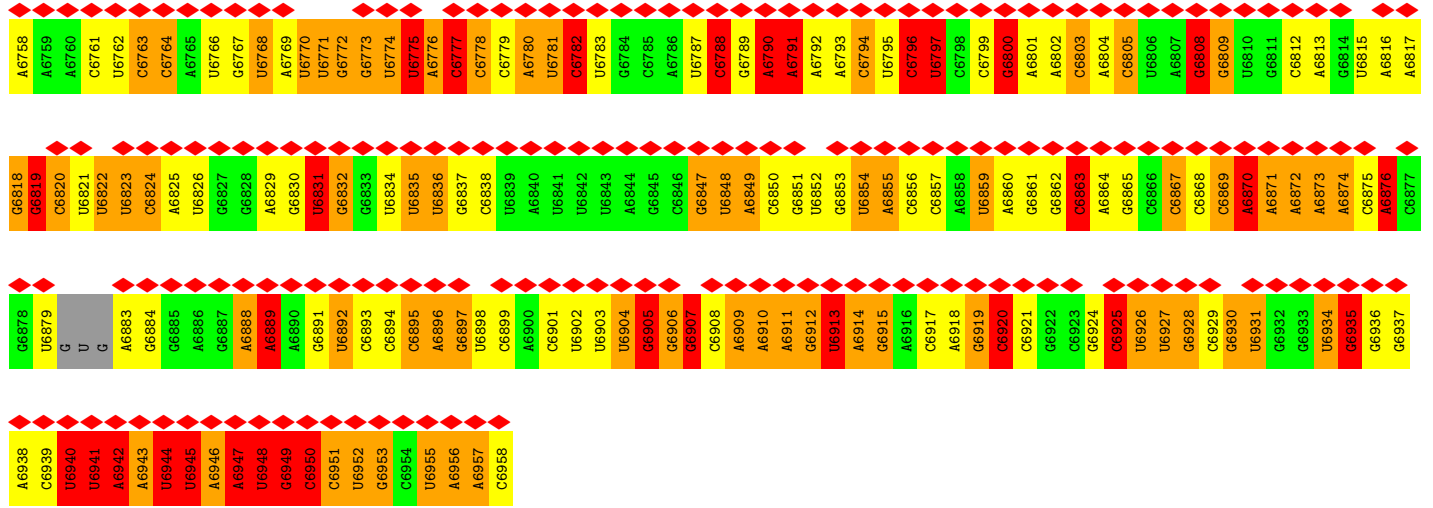
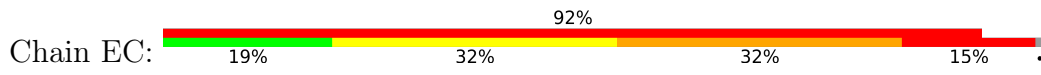


• Molecule 82: yeast eEF2





• Molecule 83: IRES



## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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:

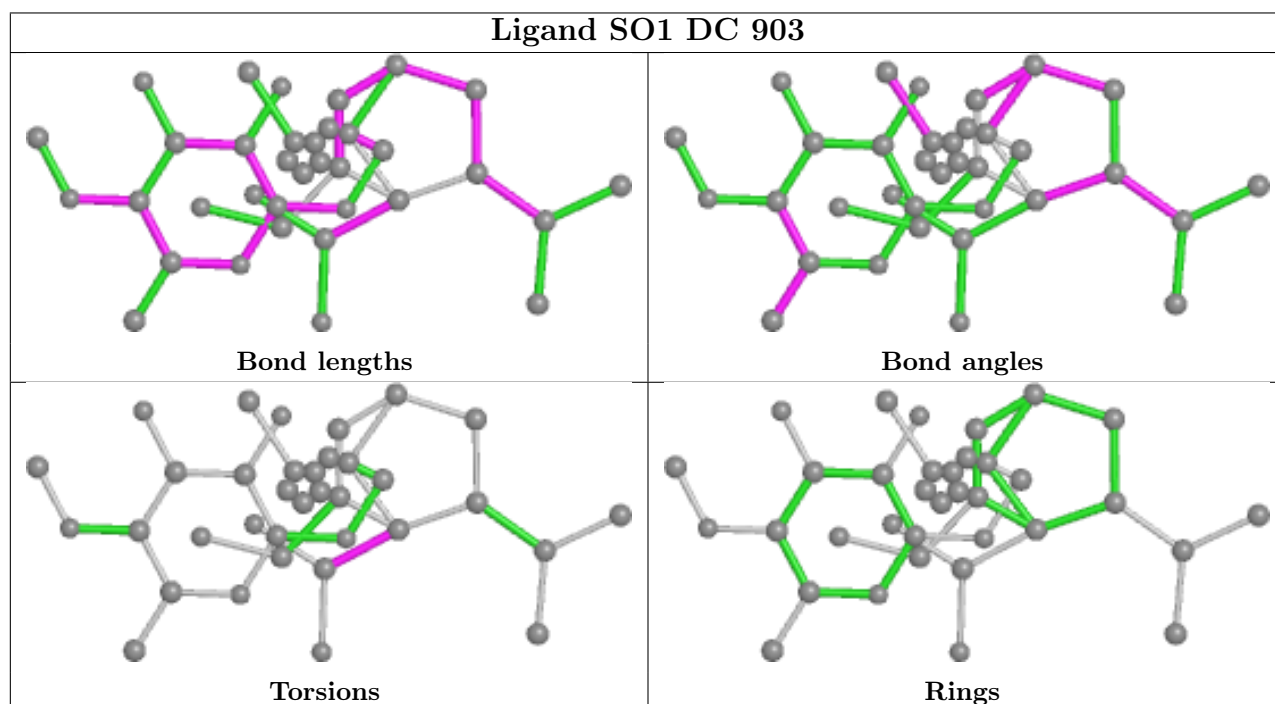
Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15

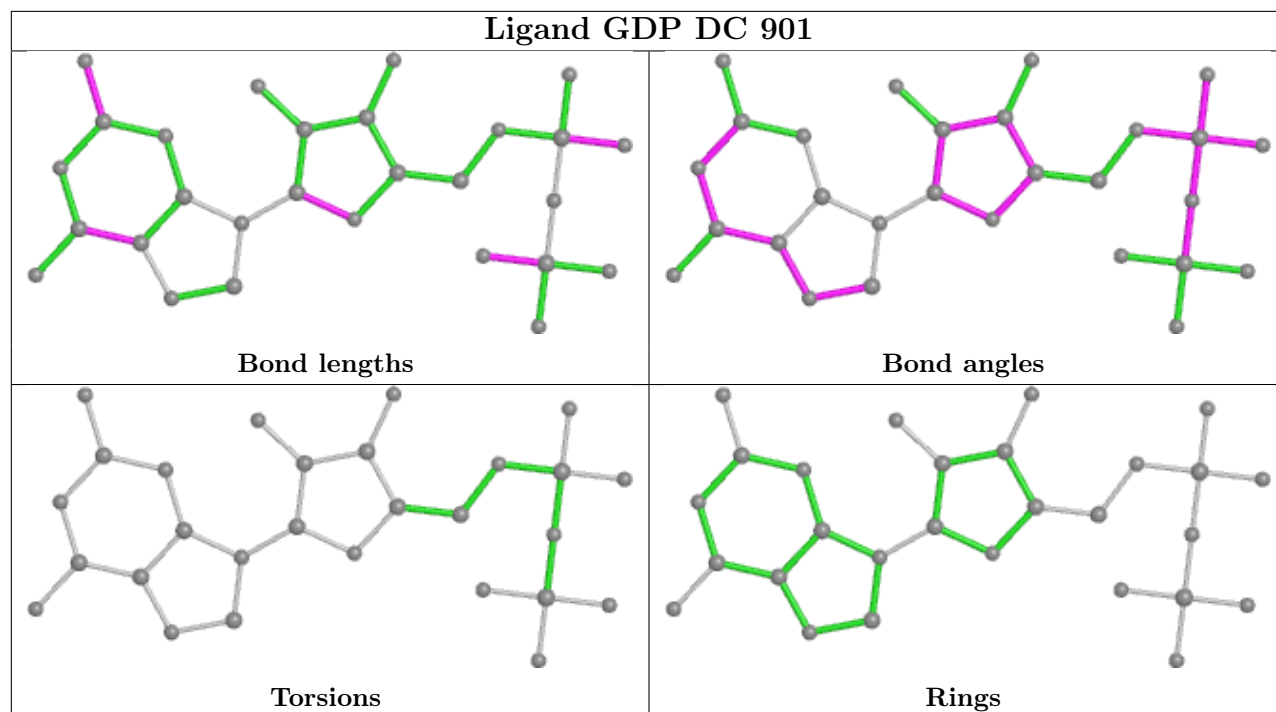
There are no ring outliers.

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 than 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.





## 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.

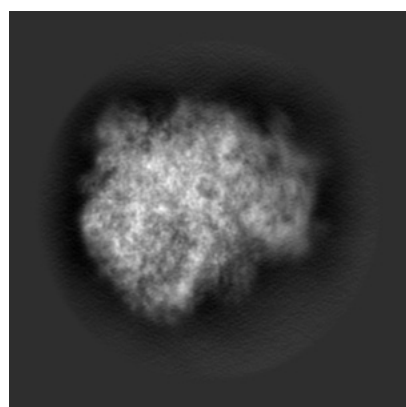
## 6 Map visualisation [i](#)

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.

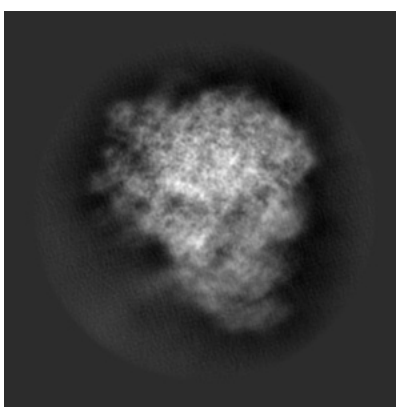
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

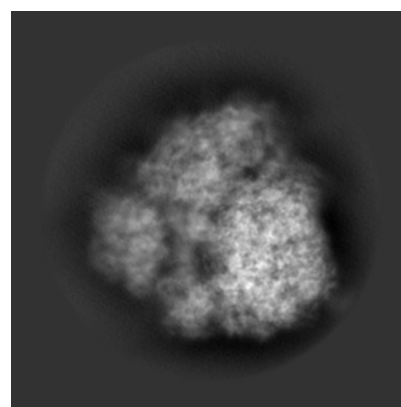
#### 6.1.1 Primary map



X



Y

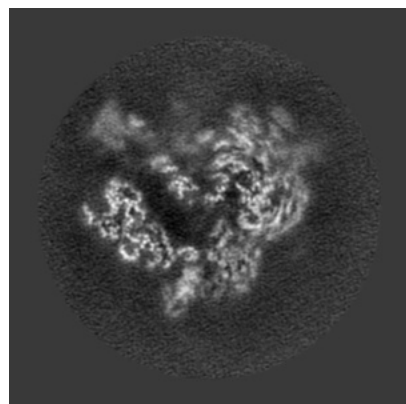


Z

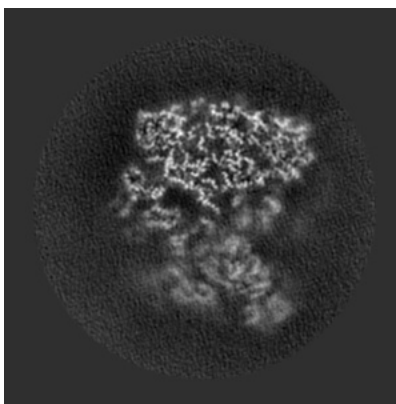
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

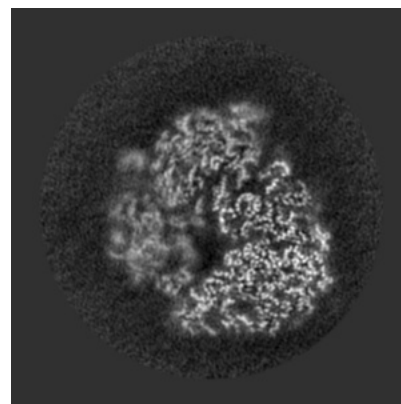
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

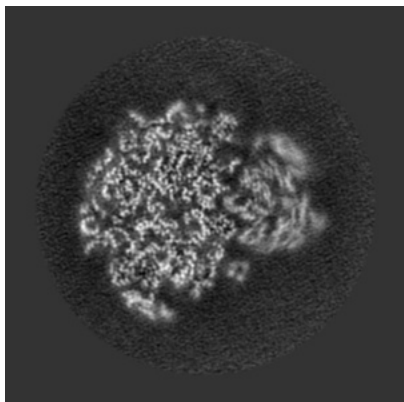


Z Index: 256

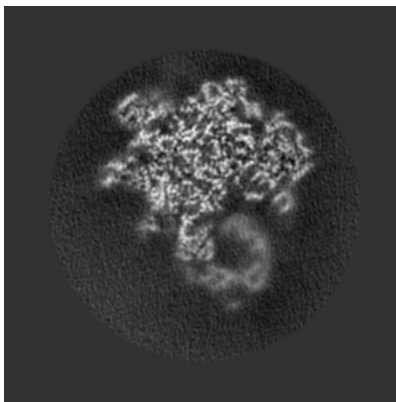
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

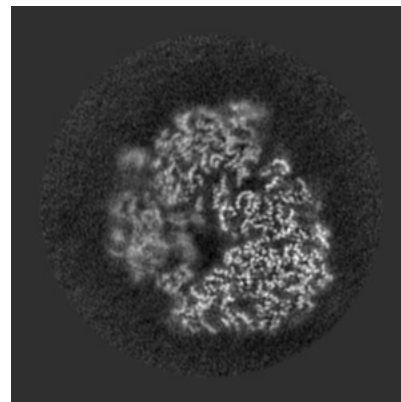
### 6.3.1 Primary map



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](#)

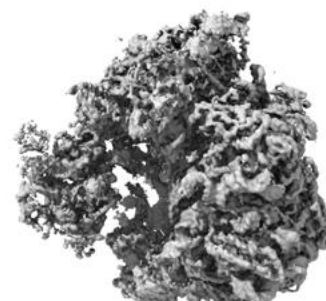
### 6.4.1 Primary map



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

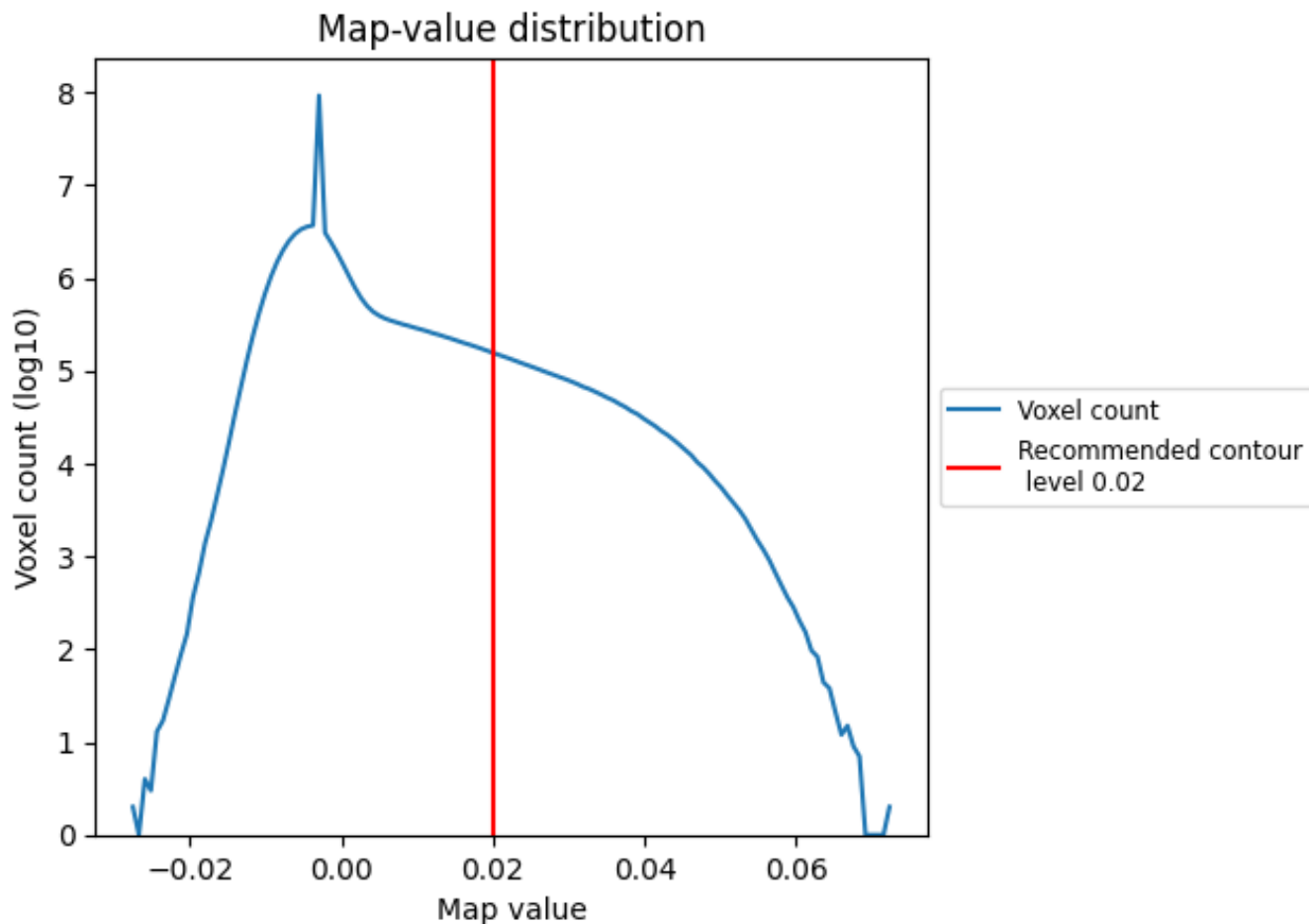
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

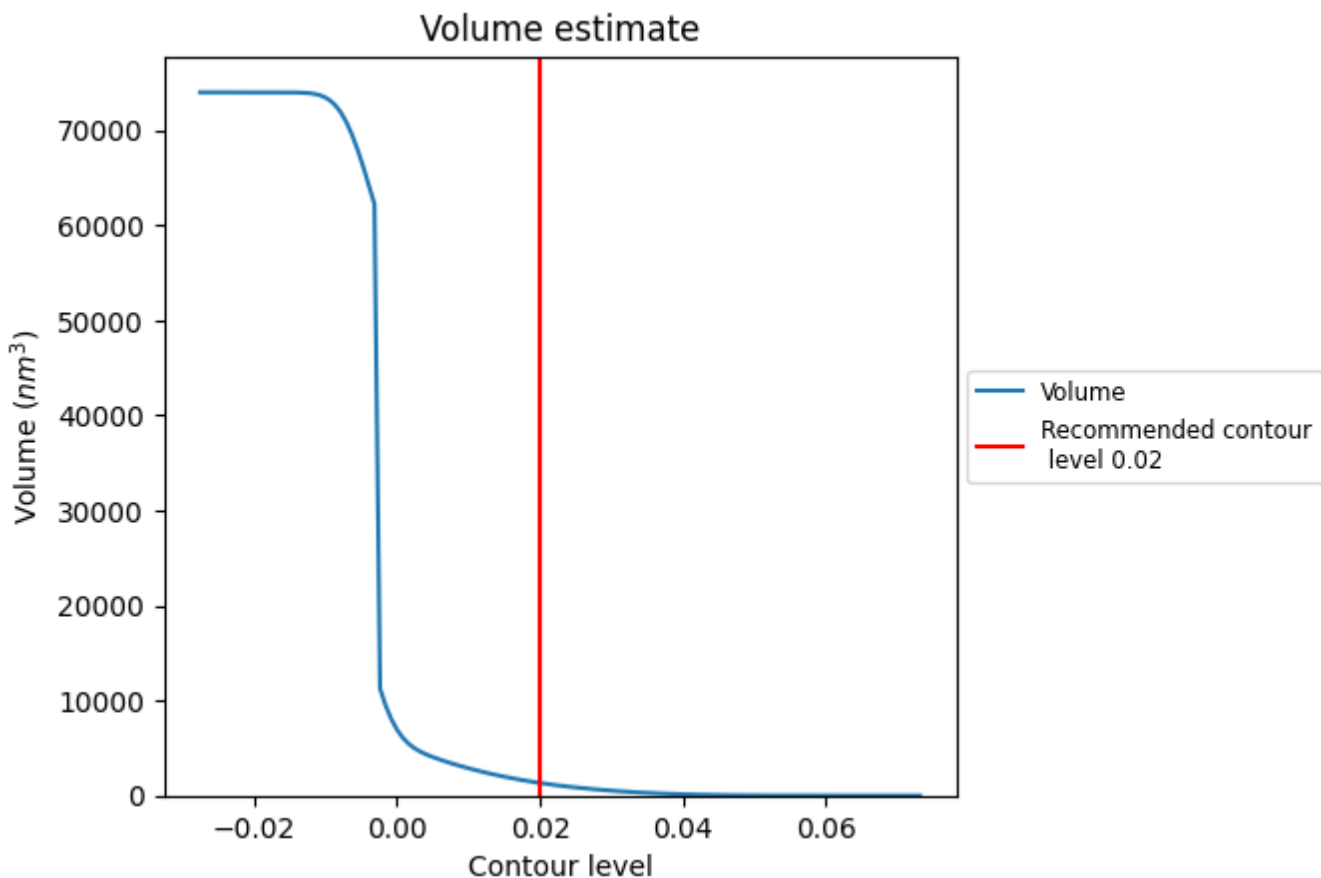
This section contains the results of statistical analysis of the map.

### 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.

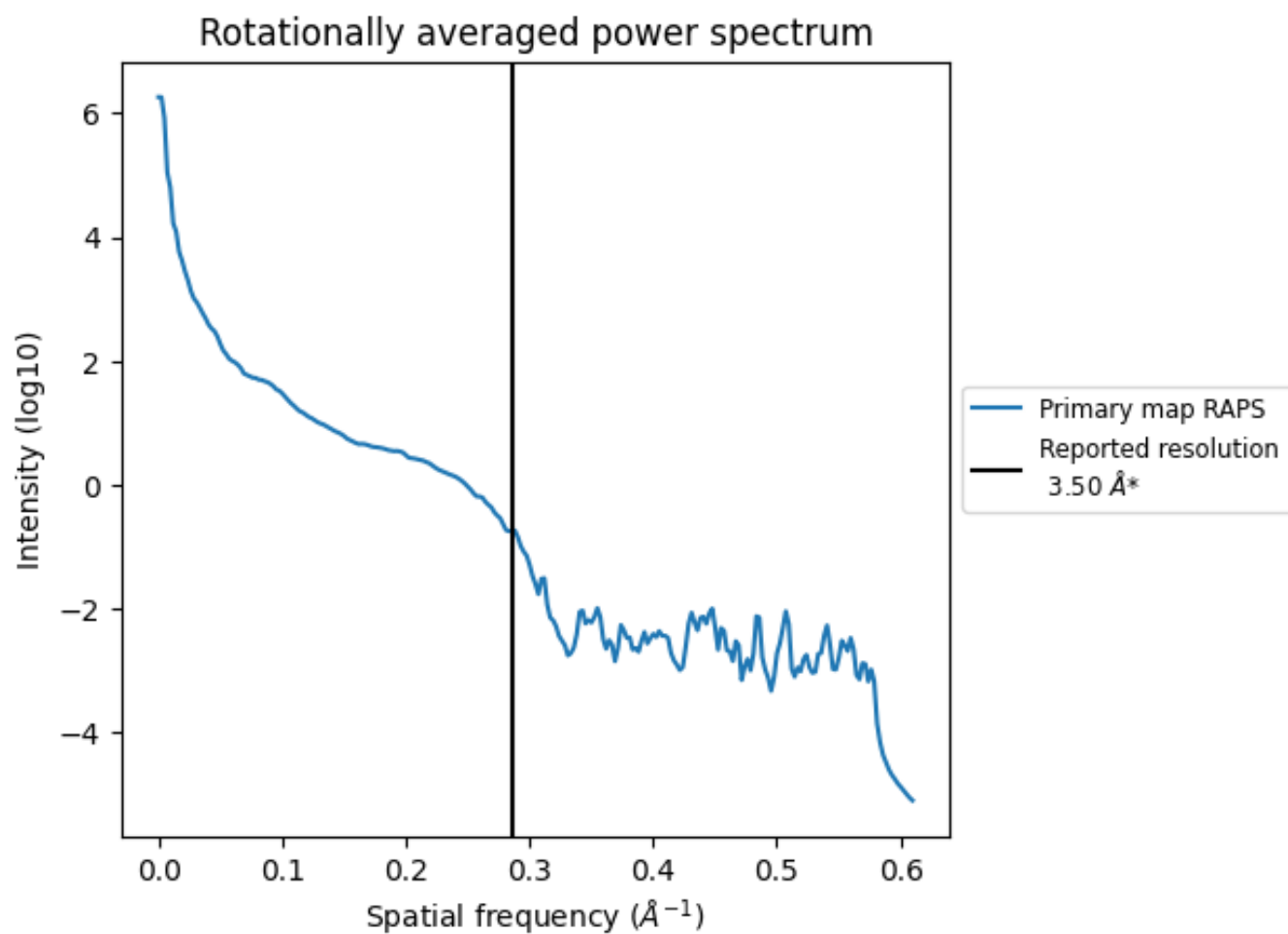
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1328  $\text{nm}^3$ ; 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  $0.286 \text{\AA}^{-1}$

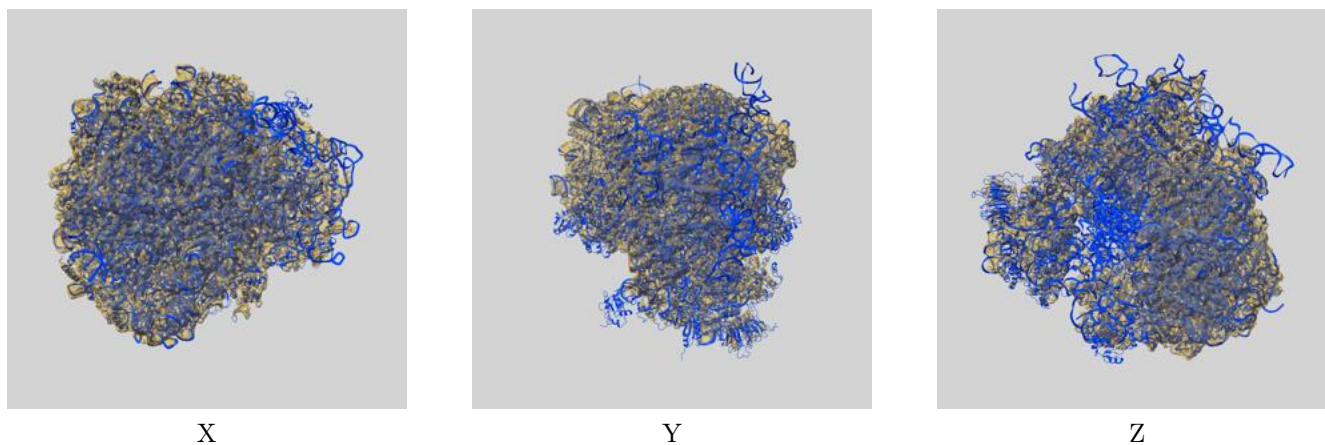
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

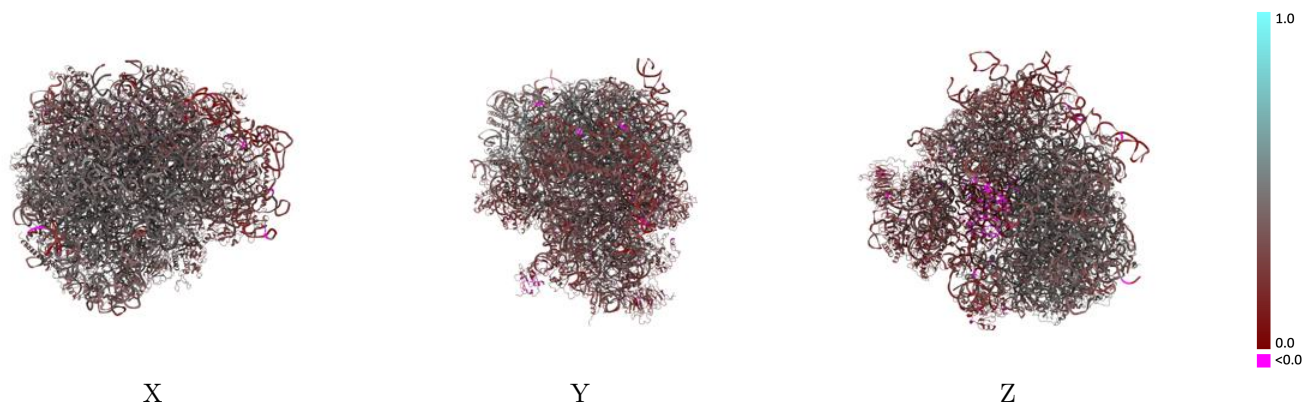
This section contains information regarding the fit between EMDB map EMD-6644 and PDB model 5JUP. Per-residue inclusion information can be found in section 3 on page 21.

### 9.1 Map-model overlay [i](#)



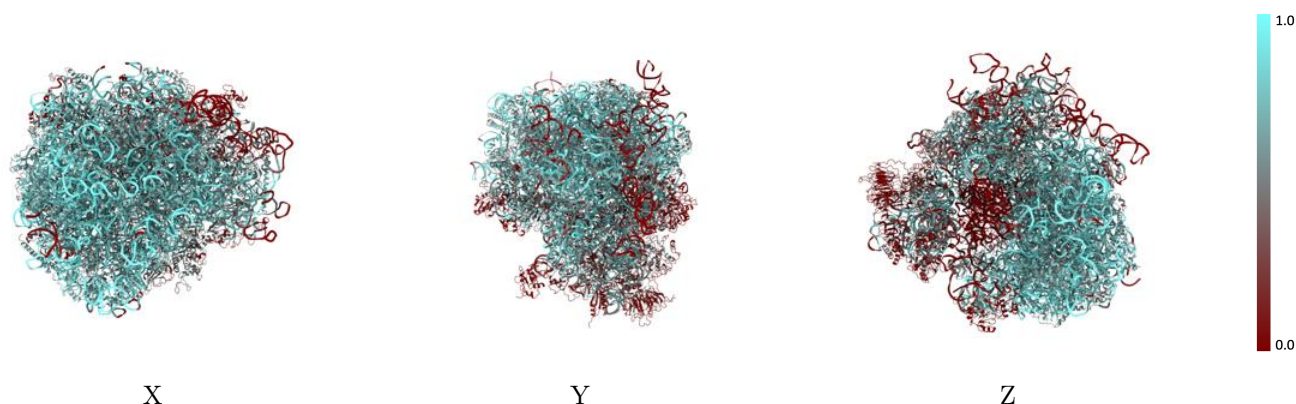
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



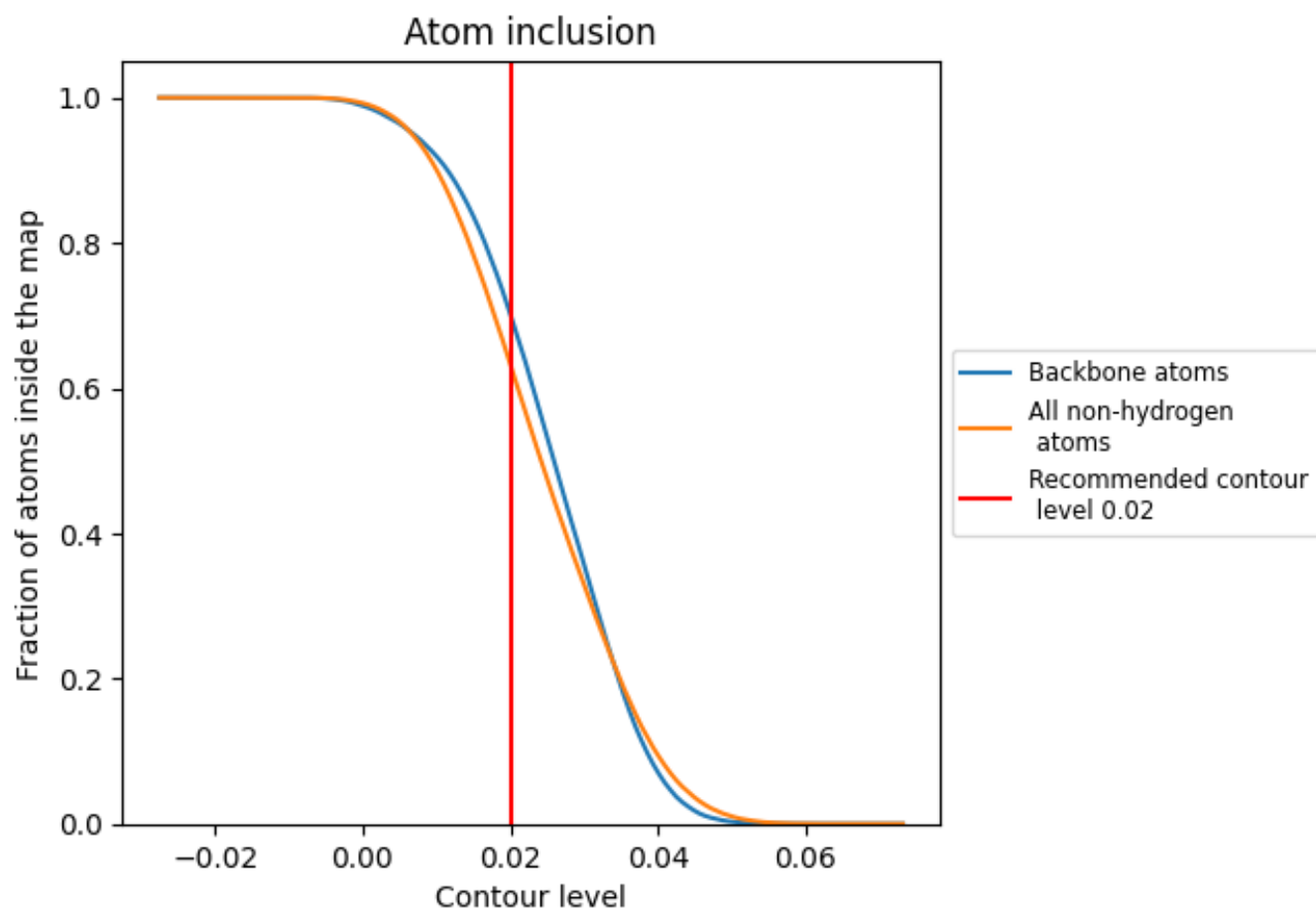
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 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

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