



wwPDB EM Validation Summary Report ⓘ

Nov 26, 2022 – 11:36 PM EST

PDB ID : 5JUT
EMDB ID : EMD-6646
Title : Saccharomyces cerevisiae 80S ribosome bound with elongation factor eEF2-GDP-sordarin and Taura Syndrome Virus IRES, Structure IV (almost non-rotated 40S subunit)
Authors : Abeyrathne, P.; Koh, C.S.; Grant, T.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2016-05-10
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

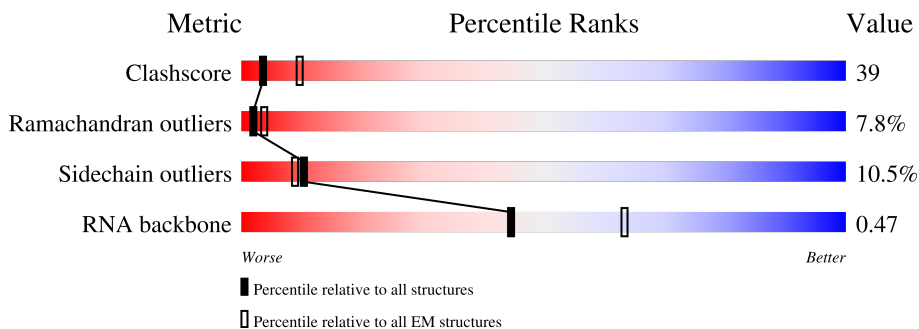
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

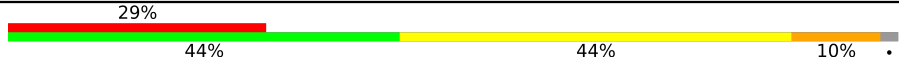
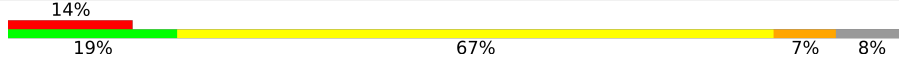
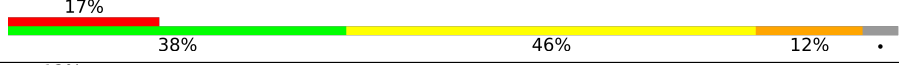
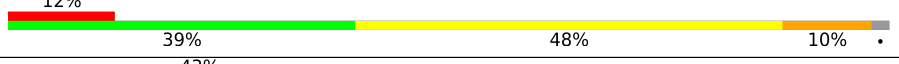
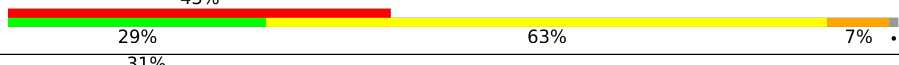
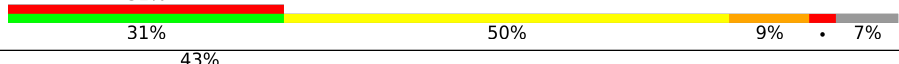
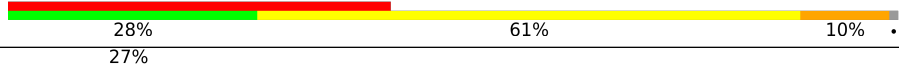
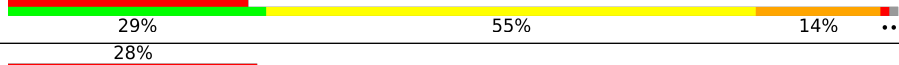

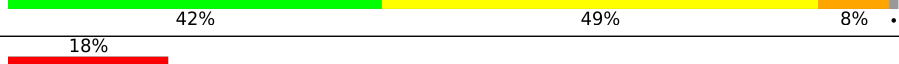


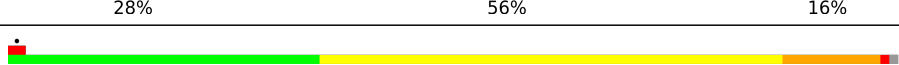
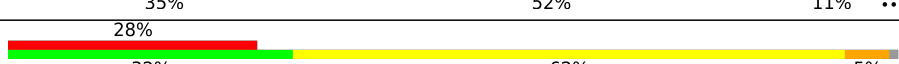

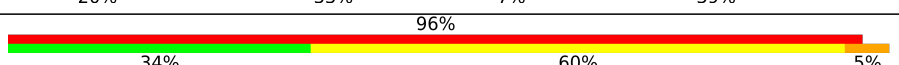
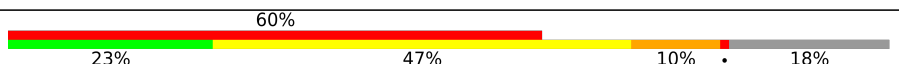
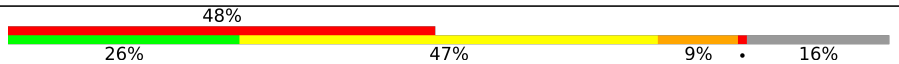
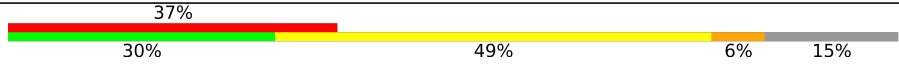


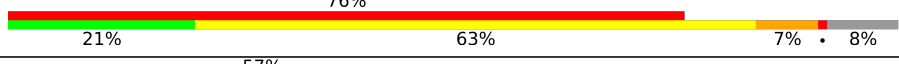



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Mol	Chain	Length	Quality of chain
8	H	362	19% 32% 51% 16% .
9	I	297	29% 32% 54% 13% .
10	J	176	34% 36% 52% 10% ..
11	K	244	25% 27% 49% 14% . 9%
12	L	256	46% 32% 49% 10% 9%
13	M	191	38% 31% 58% 10%
14	N	221	24% 30% 56% 10% 5%
15	O	174	32% 31% 53% 11% ..
16	P	165	41% 19% 27% 8% . 43%
17	Q	199	16% 35% 49% 13% ..
18	R	138	30% 25% 62% 11% ..
19	S	204	33% 20% 64% 15% .
20	T	199	28% 31% 59% 9% .
21	U	184	16% 32% 57% 11% ..
22	V	186	6% 30% 60% 9% ..
23	W	189	46% 35% 57% 6% ..
24	X	172	30% 22% 65% 12% .
25	Y	160	22% 32% 48% 19% ..
26	Z	121	45% 40% 41% . 17%
27	AA	137	38% 40% 52% 7% .
28	BA	155	11% 13% 20% 6% . 61%
29	CA	142	54% 25% 48% 12% . 15%
30	DA	127	17% 32% 52% 12% ..
31	EA	136	51% 29% 58% 10% ..
32	FA	149	15% 34% 55% 10% ..

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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	50% 30% 56% 8% 6%
59	GB	197	27% 29% 52% 13% 6%
60	HB	105	27% 22% 60% 10% 9%
61	IB	156	55% 26% 62% 12%
62	JB	143	81% 72% 14% 13%
63	KB	151	52% 33% 55% 11%
64	LB	137	38% 36% 48% 8% 7%
65	MB	142	71% 30% 44% 11% 14%
66	NB	143	80% 23% 64% 10%
67	OB	136	66% 39% 35% 10% 14%
68	PB	146	86% 31% 58% 10%
69	QB	144	81% 30% 54% 15%
70	RB	121	77% 25% 56% 7% 12%
71	SB	87	56% 31% 48% 18%
72	TB	130	56% 31% 61% 8%
73	UB	145	72% 33% 57% 8%
74	VB	135	64% 33% 59% 8%
75	WB	108	59% 20% 31% 12% 35%
76	XB	119	29% 24% 45% 10% 18%
77	YB	82	40% 24% 61% 12%
78	ZB	67	49% 33% 52% 9% 6%
79	AC	56	62% 36% 50% 7% 5%
80	BC	63	67% 40% 40% 14% 5%
81	CC	152	46% 39% 8% 53%
82	DC	842	45% 26% 58% 13%

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Mol	Chain	Length	Quality of chain
83	EC	201	 <p>72% 25% 38% 32% ..</p>

2 Entry composition i

There are 86 unique types of molecules in this entry. The entry contains 215222 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	37658	16811	6630	12436	1781	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
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	S	0	0
			1709	1084	310	311	4		

- 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	942	578	186	175	3	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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	S	0	0
			769	475	160	129	5		

- 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		

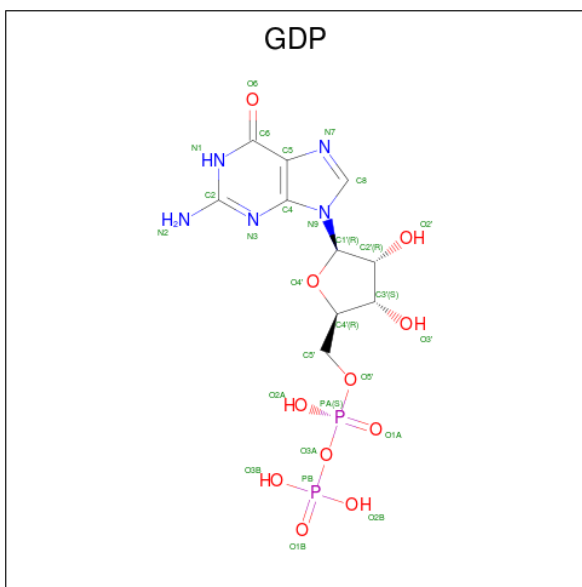
- Molecule 82 is a protein called yeast eEF2.

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: C₁₀H₁₅N₅O₁₁P₂).

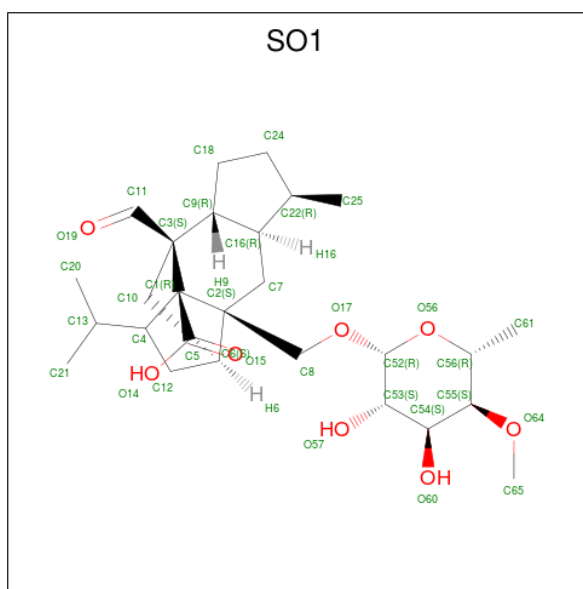


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
84	DC	1	28	10	5	11	2	0

- 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: C₂₇H₄₂O₈).

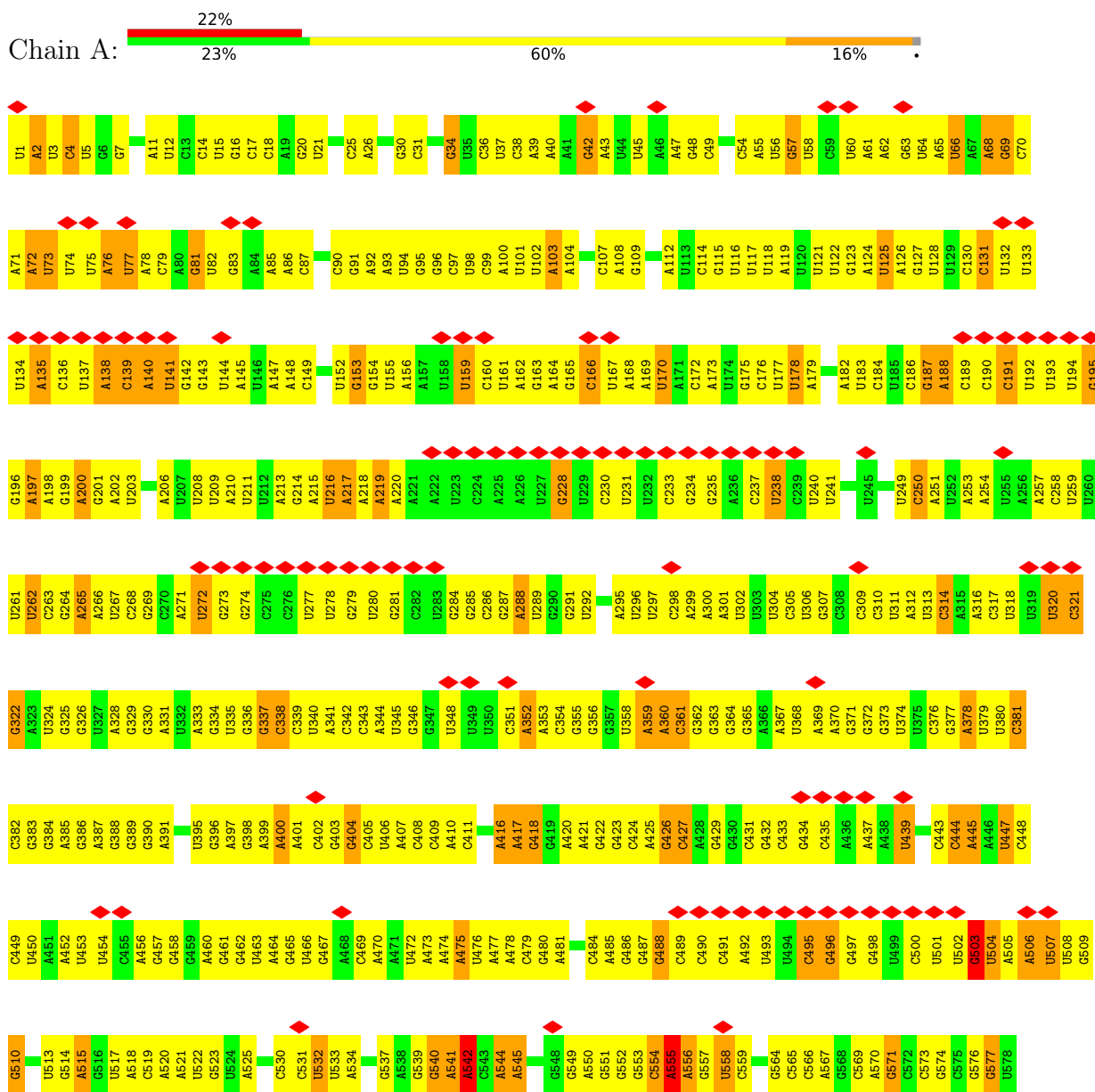


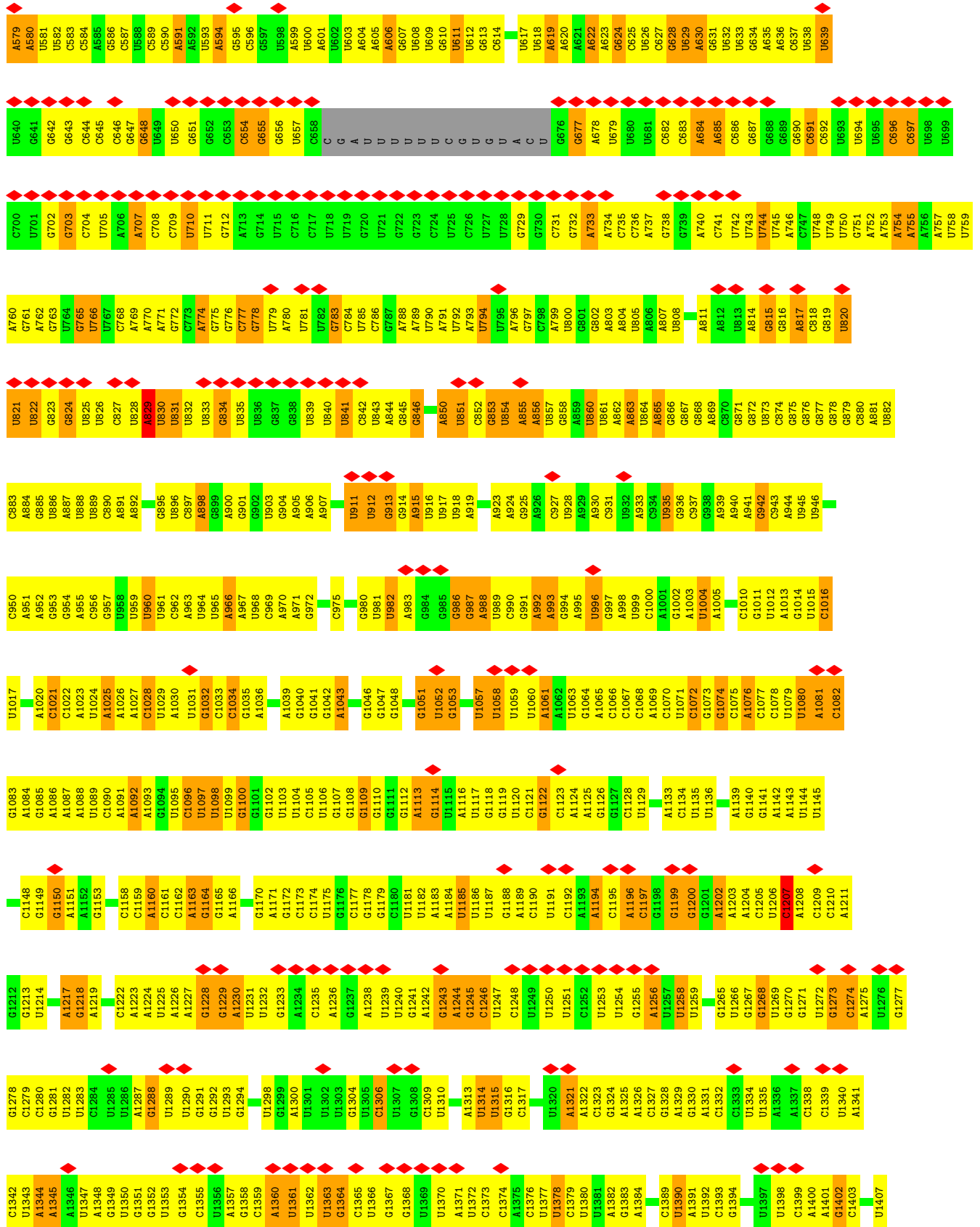
Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

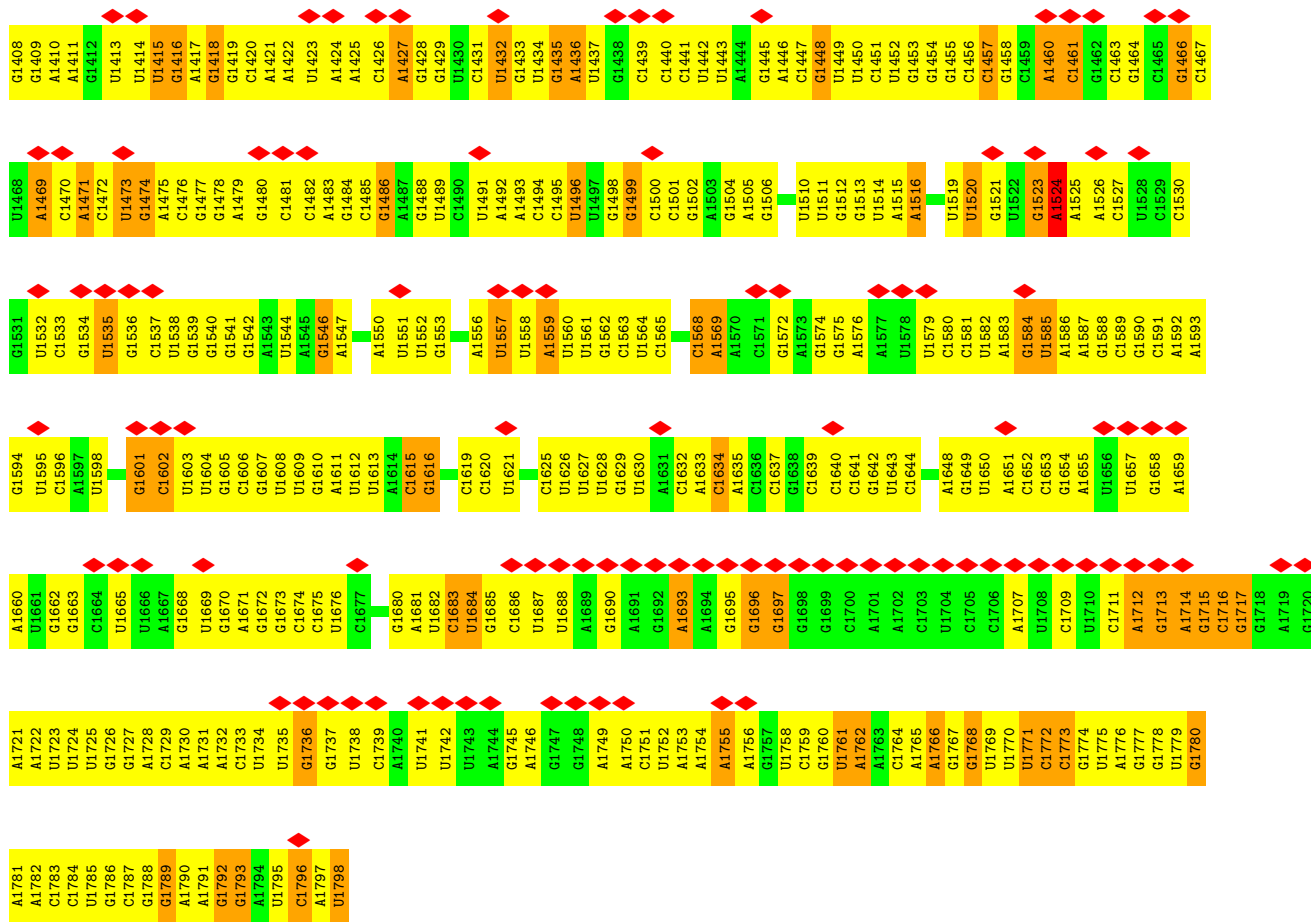
3 Residue-property plots

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.

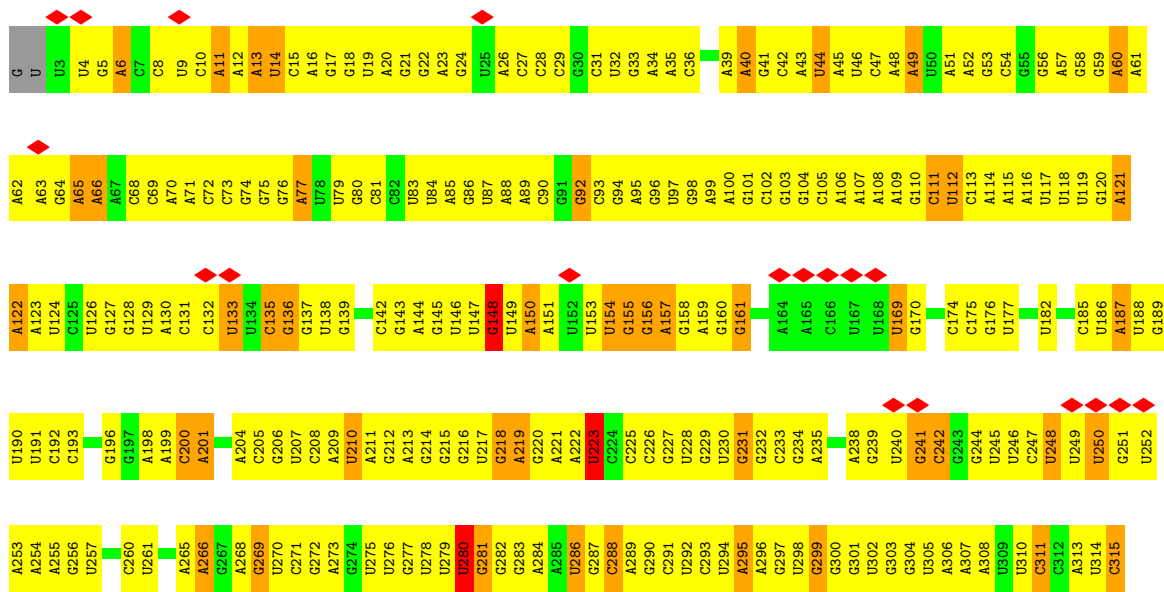
• Molecule 1: 18S ribosomal RNA

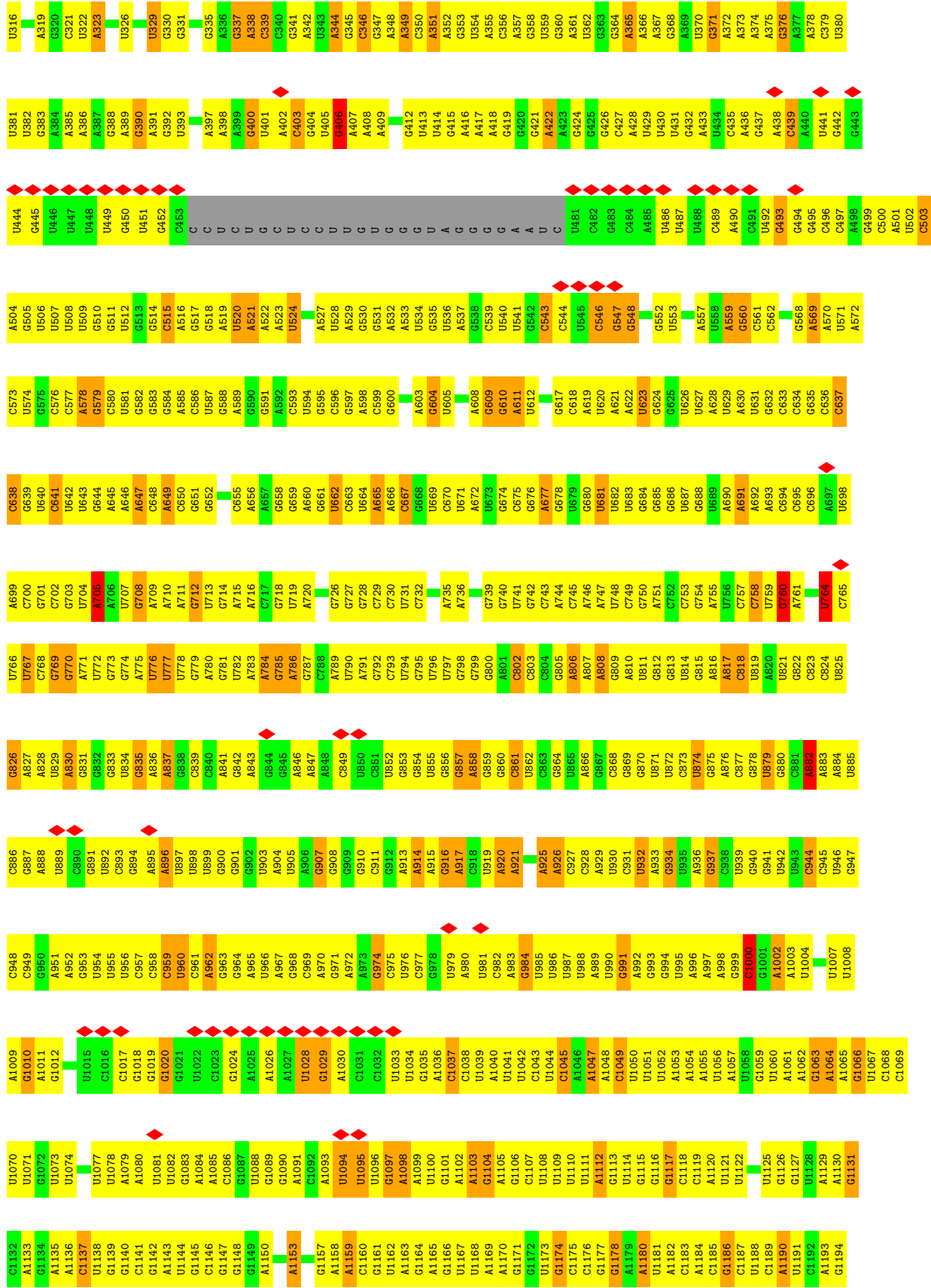




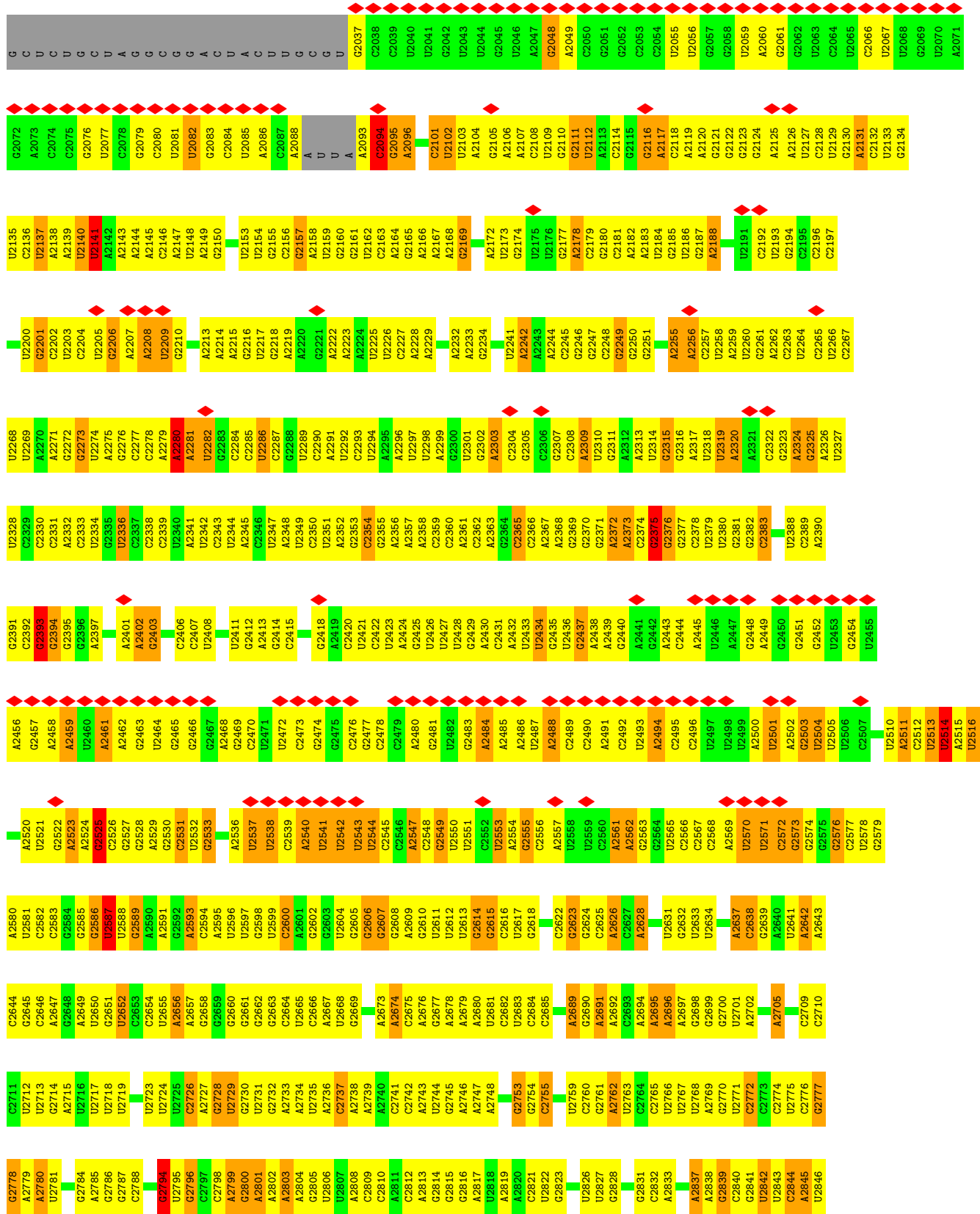


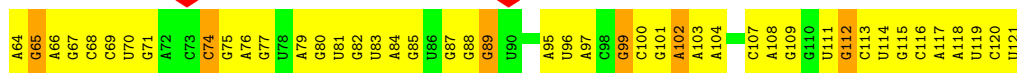
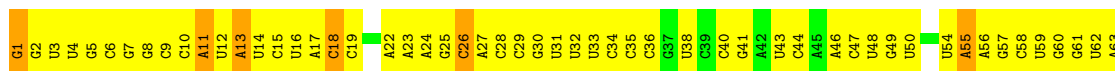
• Molecule 2: 25S ribosomal RNA



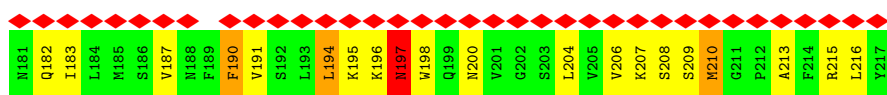
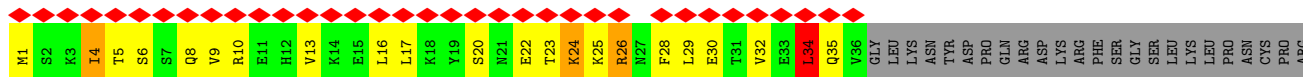
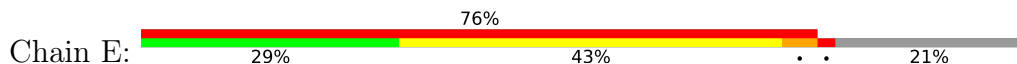


A1195	C1196	G1262	A1263	G1323	G1383	A1446	G1510	C1574	U1636	A1699	C1762	C1827	G1889	G1952
C1199	G1264	A1265	U1265	U1324	U1384	G1447	U1511	A1575	A1637	U1702	U1763	A1826	U1890	G1953
A1200	G1268	G1269	G1270	U1326	C1385	A1448	U1512	G1576	A1638	U1703	U1764	G1829	G1891	G1954
A1202	U1269	U1270	U1271	A1326	C1386	A1449	G1513	G1577	C1639	U1704	U1765	U1831	A1893	U1955
A1203	U1272	U1273	U1274	C1327	C1387	A1452	G1514	C1578	U1640	U1705	U1766	C1832	A1894	G1956
A1204	U1275	U1276	U1277	C1328	U1388	U1455	C1516	A1580	U1642	U1706	C1767	C1833	A1895	G1957
G1209	U1278	U1279	U1280	U1329	U1389	U1456	U1517	A1581	A1643	A1707	U1768	U1834	A1896	U1958
U1210	A1272	A1273	A1274	U1330	A1390	U1457	U1518	C1581	C1644	C1708	C1773	U1835	G1897	G1959
U1211	A1275	A1276	A1277	A1331	A1391	U1458	G1519	A1582	U1645	U1709	U1774	U1836	G1898	G1960
U1212	U1278	U1279	U1280	A1332	A1392	U1459	G1520	A1583	G1646	C1710	G1775	U1837	A1899	G1961
U1213	U1278	U1279	U1280	U1333	A1393	U1460	G1521	U1584	A1647	C1711	C1776	U1838	A1900	G1962
A1217	U1281	U1282	U1283	U1334	A1394	A1460	U1522	U1585	U1648	U1712	G1777	U1839	A1901	G1963
U1218	U1284	U1285	U1286	U1335	A1395	A1461	U1523	C1586	U1649	U1713	U1778	U1840	A1902	G1964
U1219	U1287	U1288	U1289	U1336	A1396	A1462	U1524	U1587	U1650	U1714	U1779	U1841	A1903	G1965
U1220	U1288	U1289	U1290	U1337	U1397	U1463	G1525	A1588	U1651	U1715	U1780	A1842	C1843	G1966
A1221	U1288	U1289	U1290	U1338	A1399	U1464	U1526	A1589	G1652	U1716	U1781	C1843	G1904	G1967
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A1225	U1288	U1289	U1290	U1340	A1401	U1466	U1528	U1591	U1654	U1718	U1783	G1845	G1906	G1969
G1226	U1288	U1289	U1290	U1341	U1405	C1469	U1532	A1592	A1655	U1719	U1784	C1846	G1907	G1970
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G1228	U1288	U1289	U1290	U1343	A1407	U1471	U1534	A1594	C1657	U1721	U1786	U1848	A1909	G1972
G1229	U1288	U1289	U1290	U1344	A1408	U1472	A1535	C1597	U1658	U1722	U1787	C1849	A1910	G1973
G1230	U1288	U1289	U1290	U1345	A1409	U1473	G1536	C1598	U1659	U1723	U1788	G1850	A1911	G1974
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G1237	U1288	U1289	U1290	U1352	G1415	U1480	U1543	U1605	U1666	U1730	U1795	U1857	U1918	G1981
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A1301	U1288	U1289	U1290	U1354	A1418	U1483	U1546	U1608	C1669	U1733	U1798	U1860	U1921	G
A1302	U1288	U1289	U1290	U1355	A1419	U1484	U1547	U1609	C1670	U1734	U1799	U1861	U1922	G
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G1242	U1288	U1289	U1290	U1358	G1422	U1487	U1550	U1612	U1673	U1737	C1802	U1864	U1925	G
G1243	U1288	U1289	U1290	U1359	G1423	U1488	U1551	U1613	U1674	U1738	C1803	U1865	U1926	G
A1244	U1288	U1289	U1290	C1359	C1426	A1489	U1552	U1614	G1675	U1739	A1804	U1866	U1927	G
A1245	U1288	U1289	U1290	C1360	C1427	A1490	U1553	U1615	G1676	U1740	C1805	U1867	U1928	G
G1246	U1288	U1289	U1290	U1361	U1428	A1491	U1554	U1616	G1677	A1741	C1806	U1868	U1929	G
U1247	U1288	U1289	U1290	U1362	A1429	A1492	U1555	U1617	G1678	U1742	C1807	U1869	U1930	G
C1248	U1288	U1289	U1290	C1363	G1430	U1493	U1556	U1618	U1679	U1743	C1808	U1870	U1931	G
U1249	U1288	U1289	U1290	U1364	U1431	U1494	A1557	U1619	G1680	U1744	C1809	U1871	U1932	G
G1250	U1288	U1289	U1290	A1366	U1432	U1495	U1558	U1620	U1681	U1745	A1812	U1872	U1933	G
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G1320	U1288	U1289	U1290	U1374	U1440	A1503	U1566	U1628	U1689	U1753	U1820	U1880	U1941	A
U1322	U1288	U1289	U1290	U1375	U1441	A1504	U1567	U1629	U1690	U1754	U1821	U1881	U1942	C
G1261	U1288	U1289	U1290	U1376	U1442	C1505	U1568	U1630	U1691	U1755	U1822	U1882	U1943	U
				U1377	U1443	U1506	U1569	U1631	U1692	U1756	U1823	U1883	U1944	C
				U1378	U1444	C1507	U1570	U1632	U1693	U1757	U1824	U1884	U1945	C
				U1379	U1445	U1508	U1571	U1633	U1694	U1758	U1825	U1885	U1946	U
				U1380	U1446	U1509	U1572	U1634	U1695	U1759	U1826	U1886	U1947	U
				U1381	U1447	U1510	U1573	U1635	U1696	U1760	U1827	U1887	U1948	U
				U1382	U1448	U1511	U1574	U1636	U1697	U1761	U1828	U1888	U1949	U
				G1382	U1449	U1512	U1575	U1637	U1698	U1762	U1829	U1889	U1950	U
					U1450	U1513	U1576	U1638	U1699	U1763	U1830	U1890	U1951	U

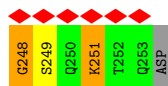
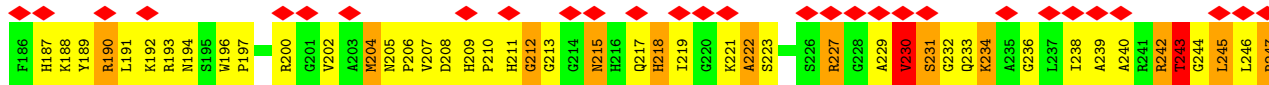
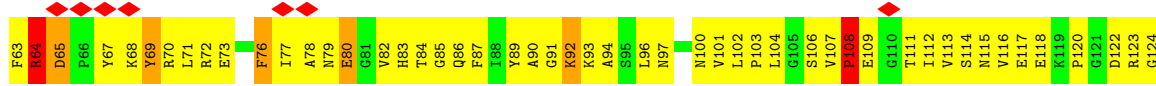
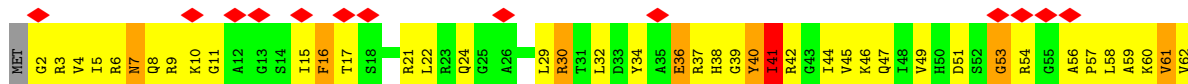




• Molecule 5: uL1 (yeast L1)

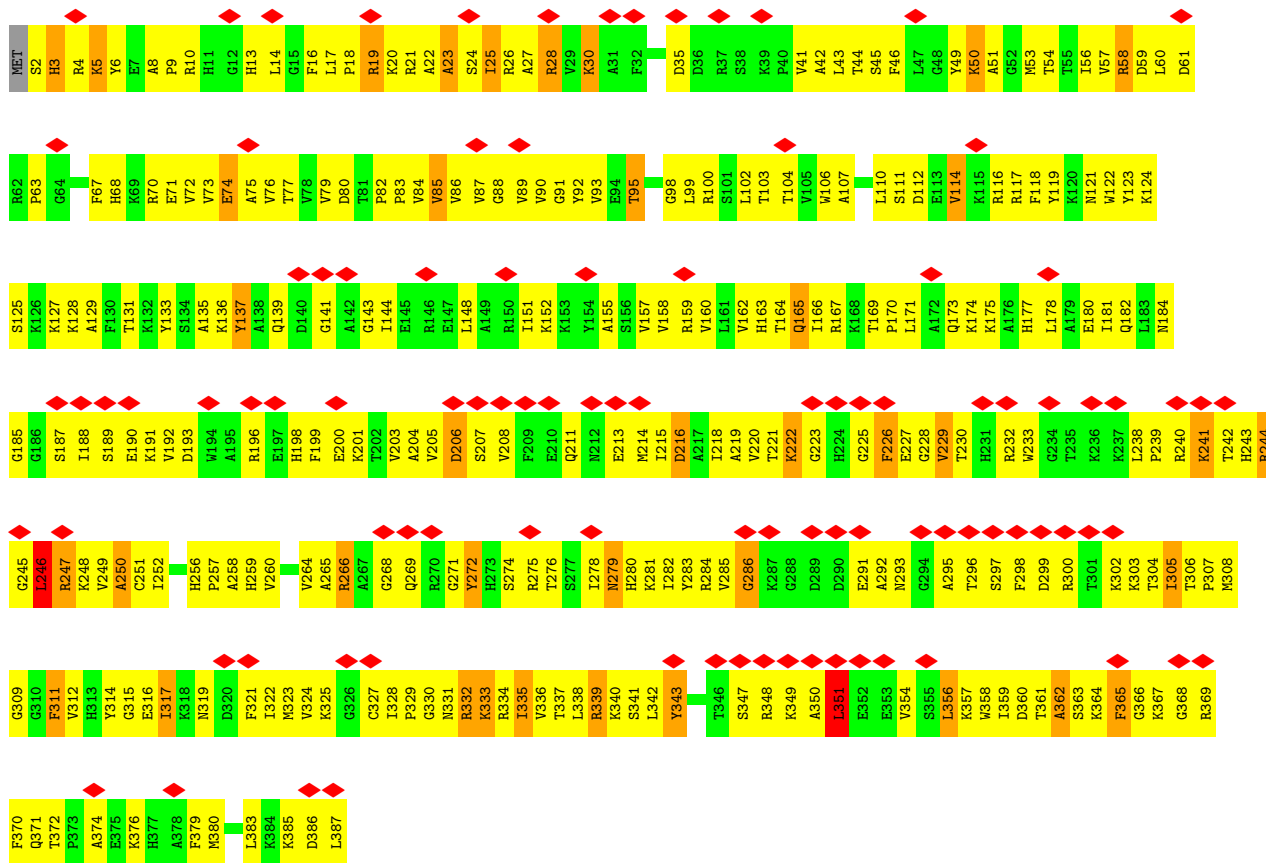


• Molecule 6: uL2 (yeast L2)

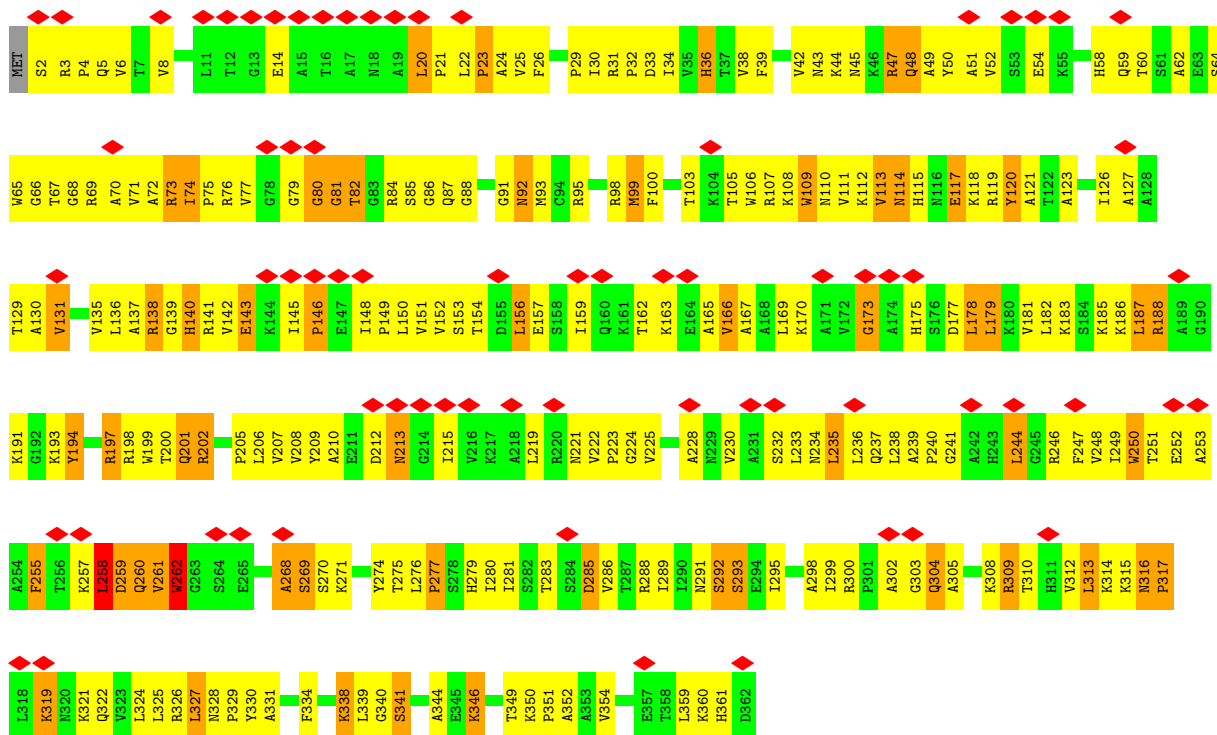


• Molecule 7: uL3 (yeast L3)

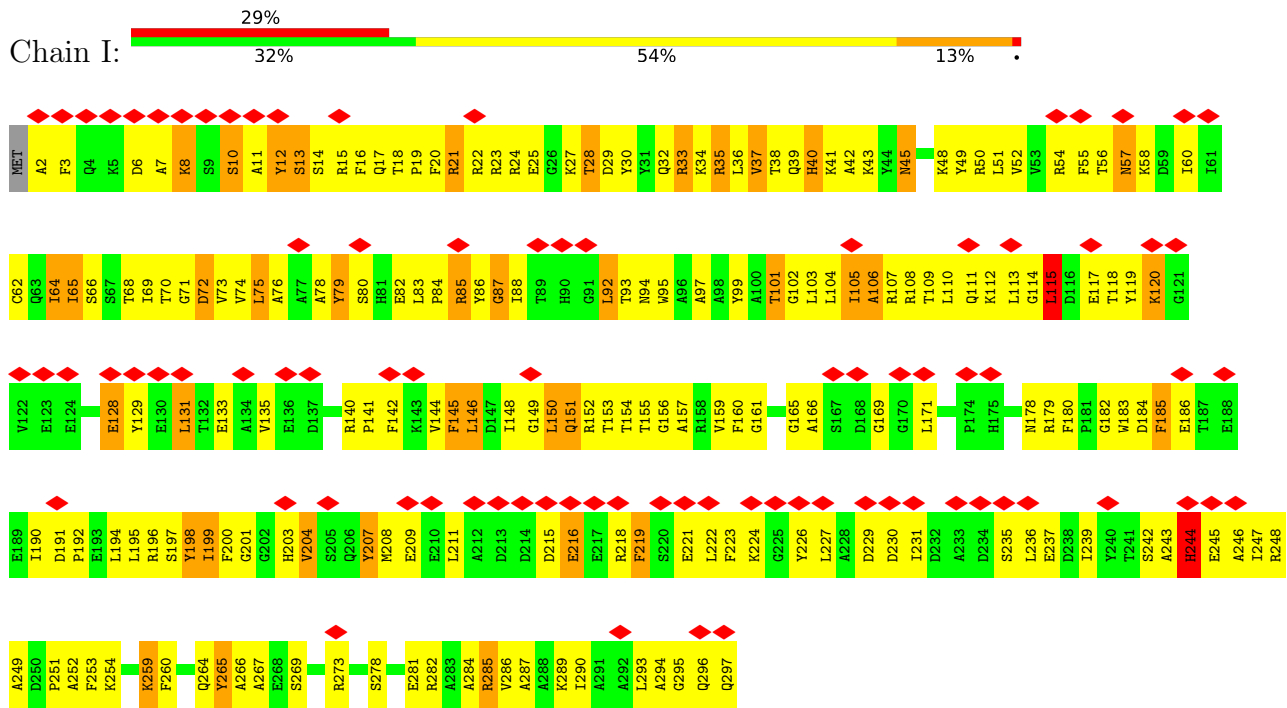




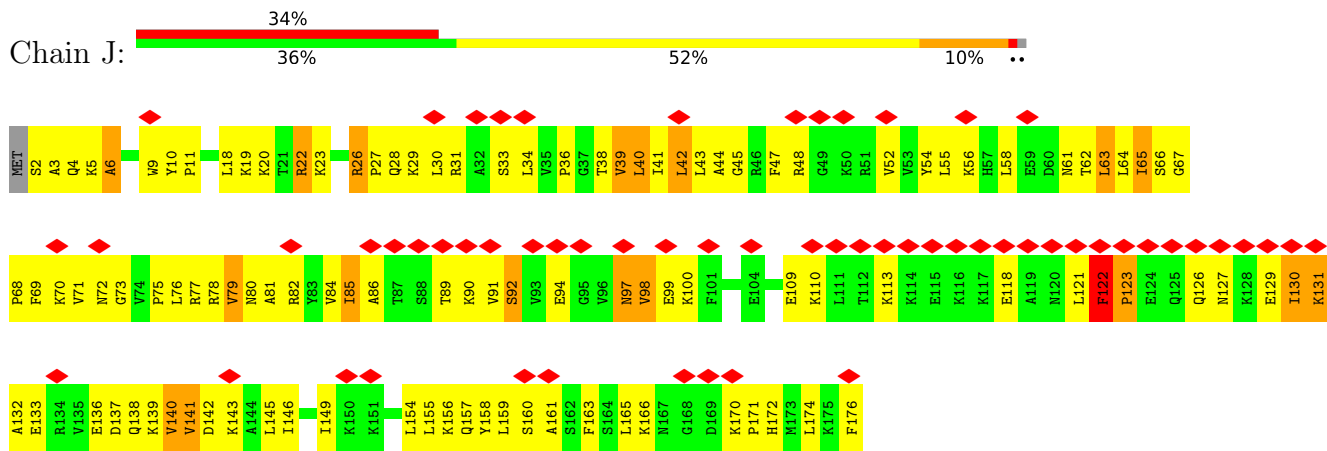
• Molecule 8: uL4 (yeast L4)



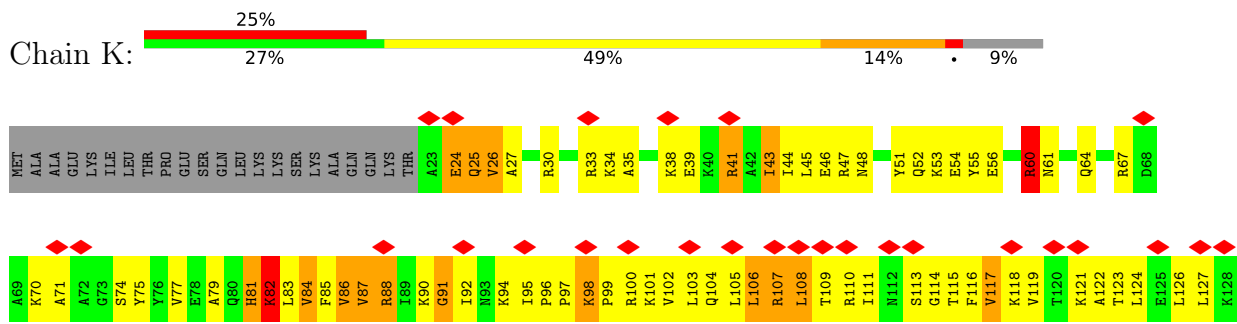
• Molecule 9: uL18 (yeast L5)

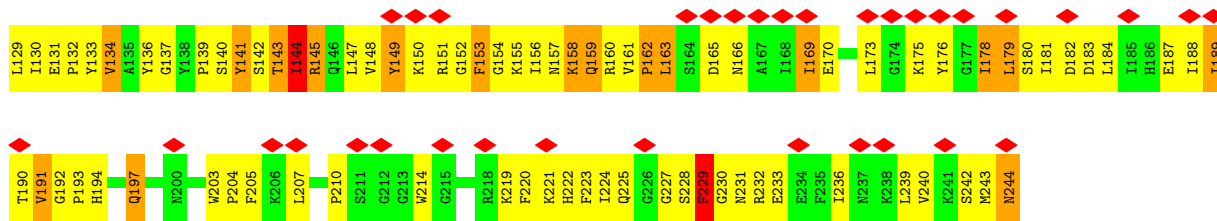


• Molecule 10: eL6 (yeast L6)

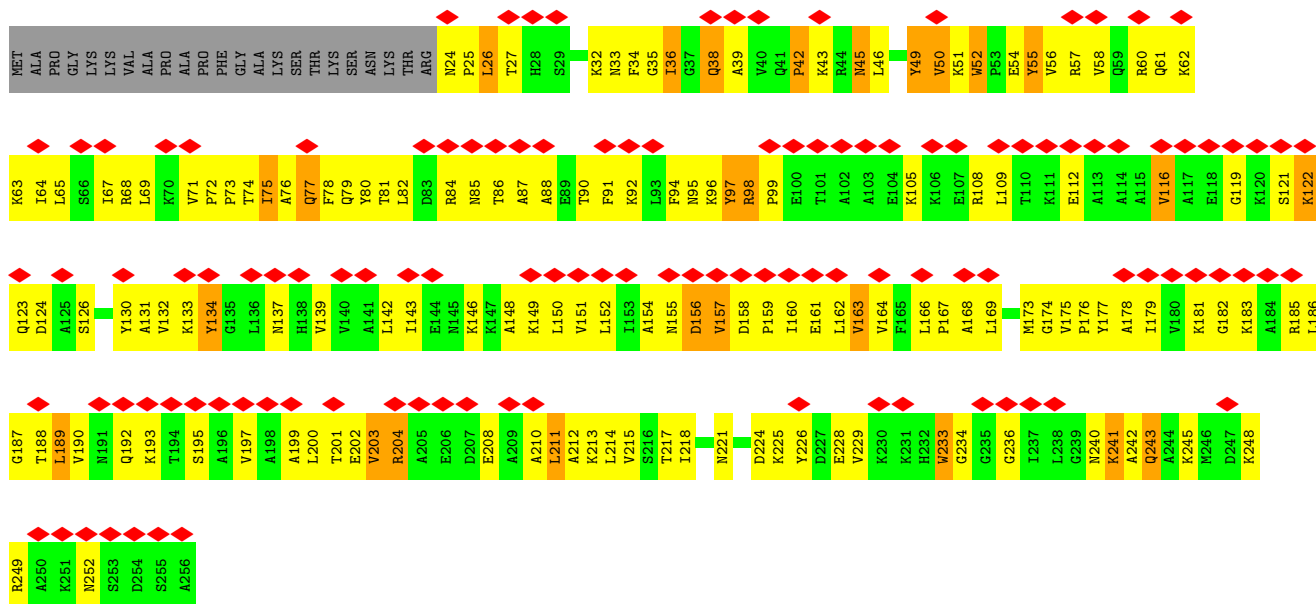


• Molecule 11: uL30 (yeast L7)

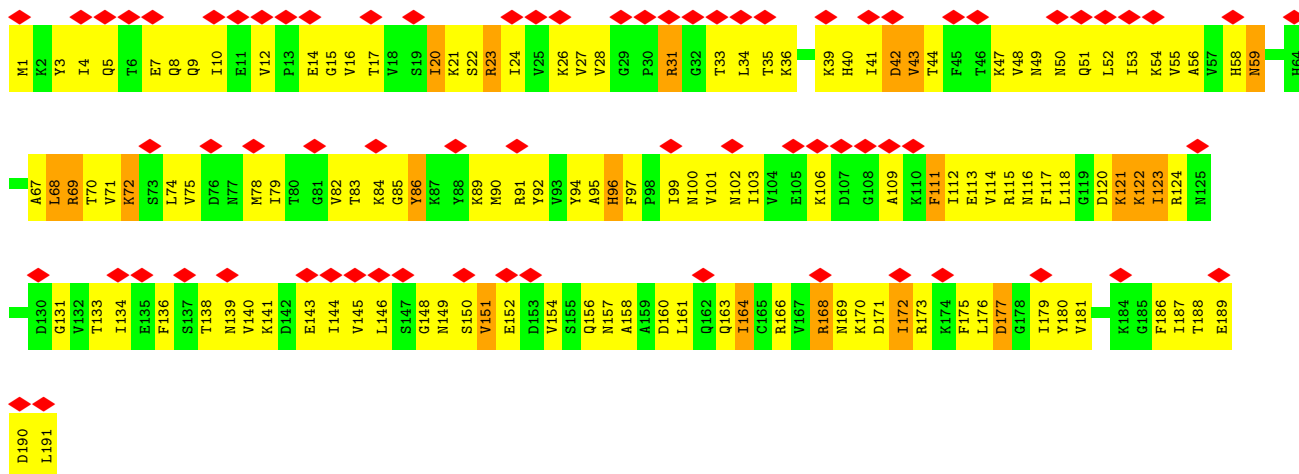




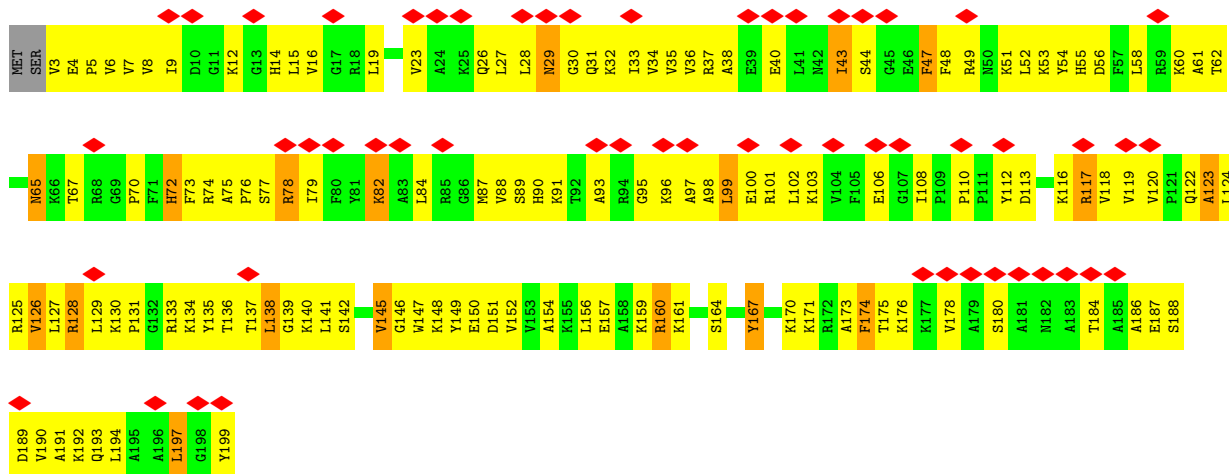
• Molecule 12: eL8 (yeast L8)



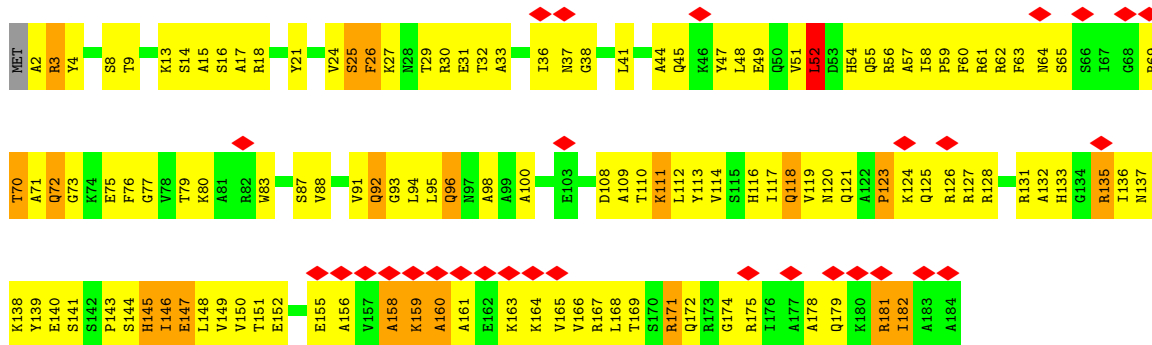
• Molecule 13: uL6 (yeast L9)



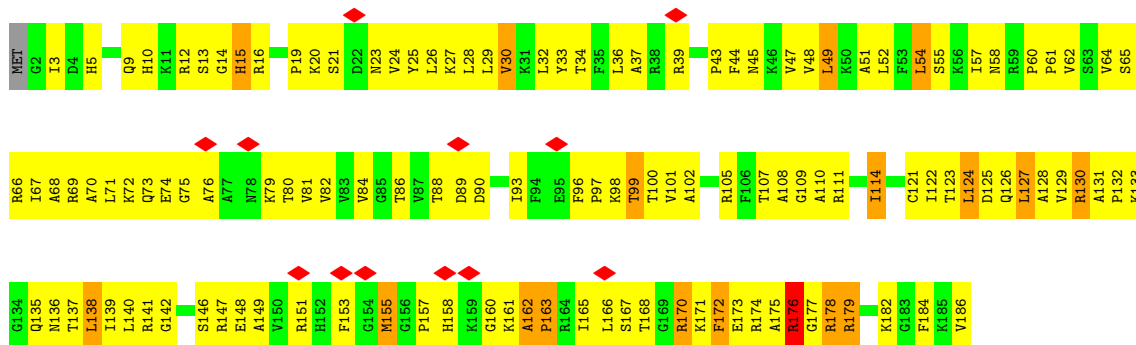
• Molecule 14: uL16 (yeast L10)



• Molecule 21: uL22 (yeast L17)

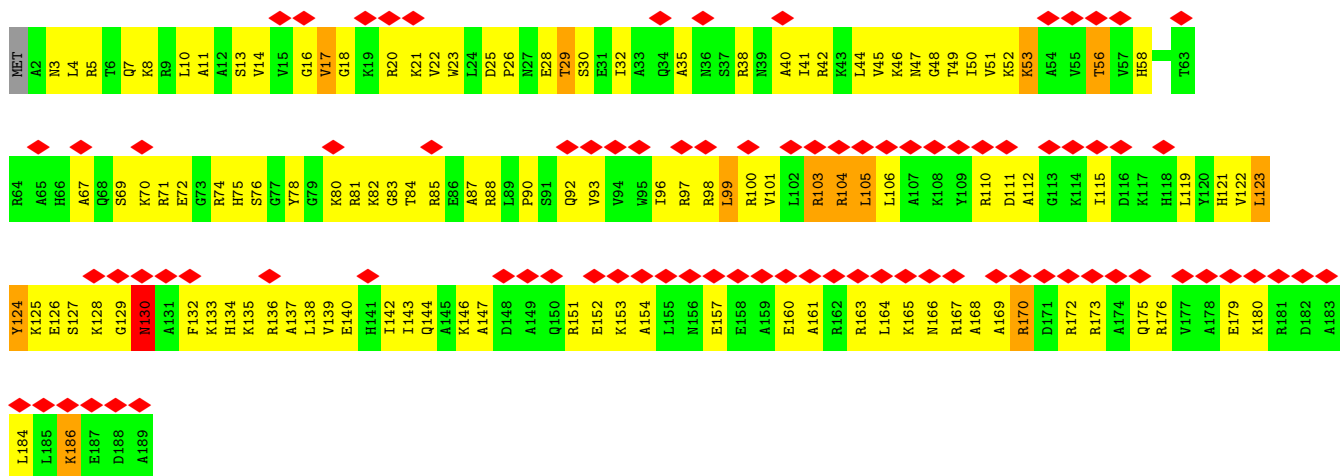


• Molecule 22: eL18 (yeast L18)

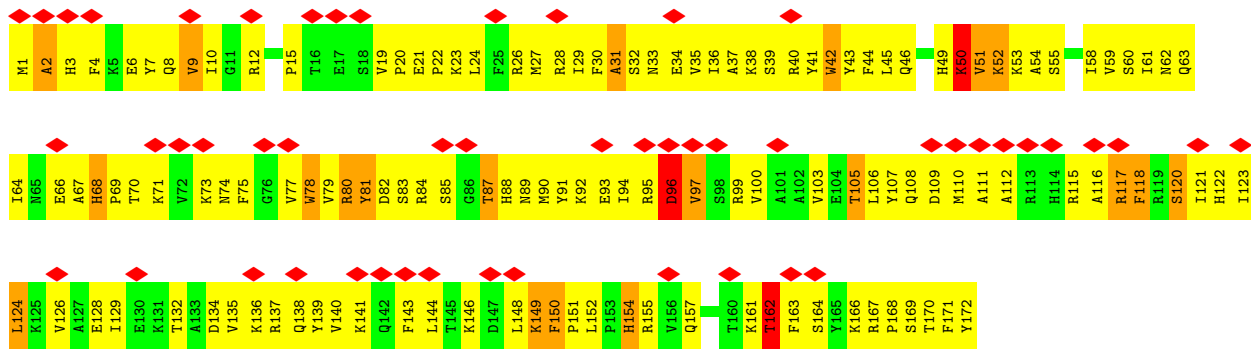


• Molecule 23: eL19 (yeast L19)

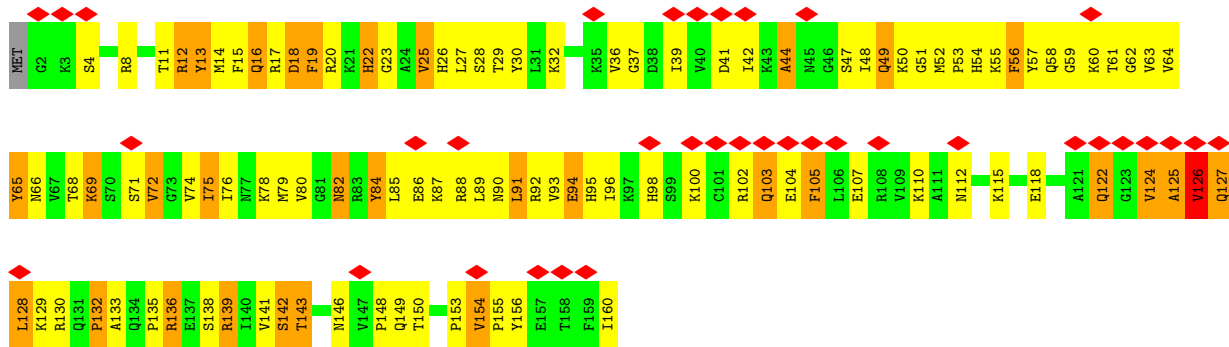




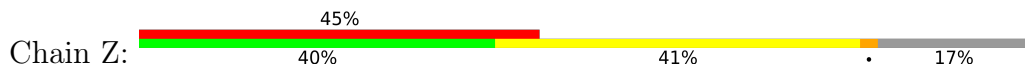
• Molecule 24: eL20 (yeast L20)

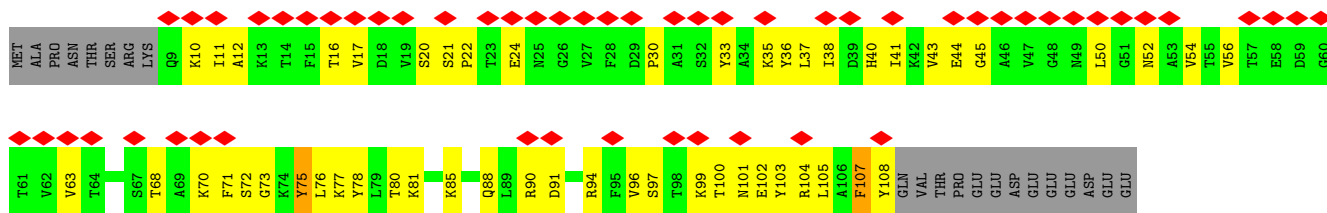


• Molecule 25: eL21 (yeast L21)

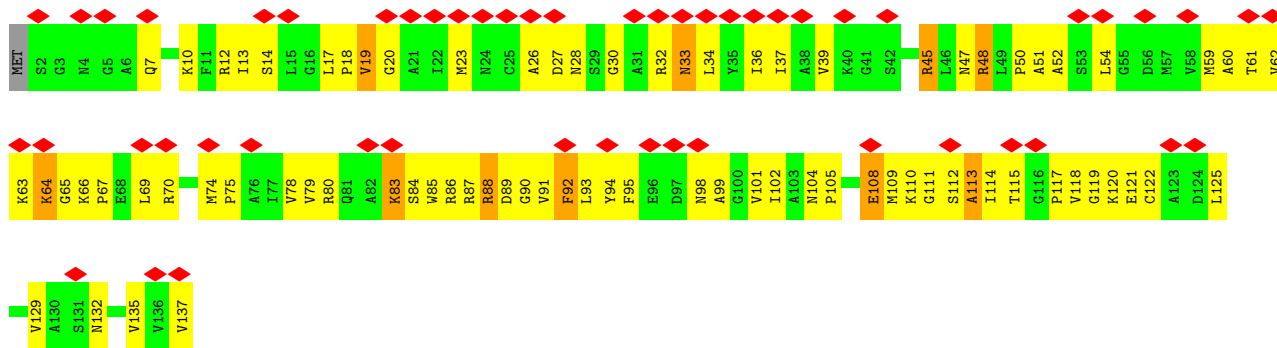
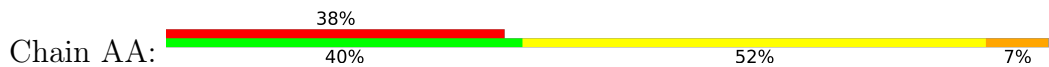


• Molecule 26: eL22 (yeast L22)

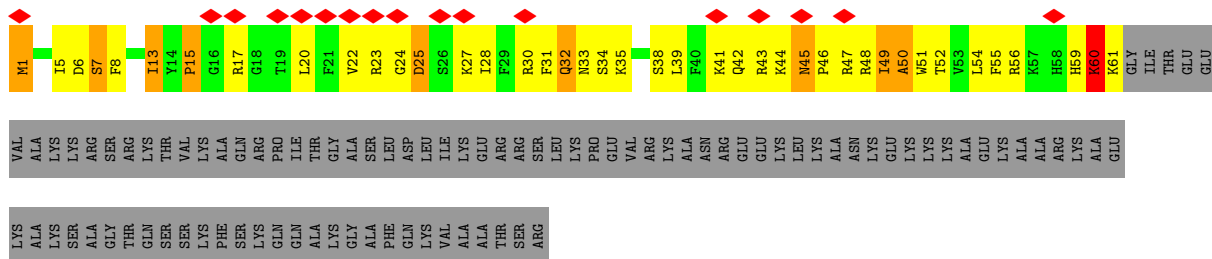
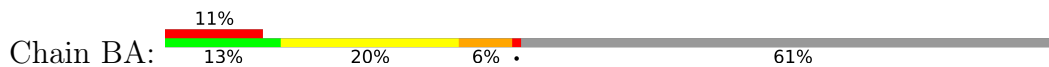




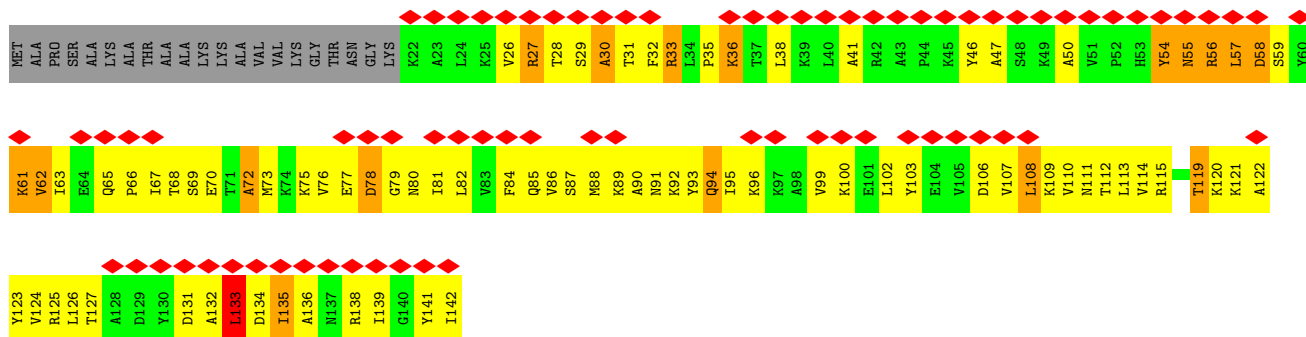
• Molecule 27: uL14 (yeast L23)



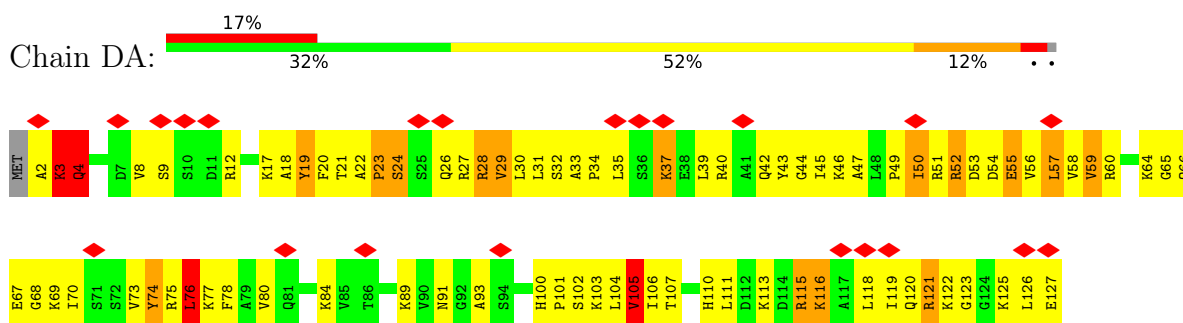
• Molecule 28: eL24 (yeast L24)



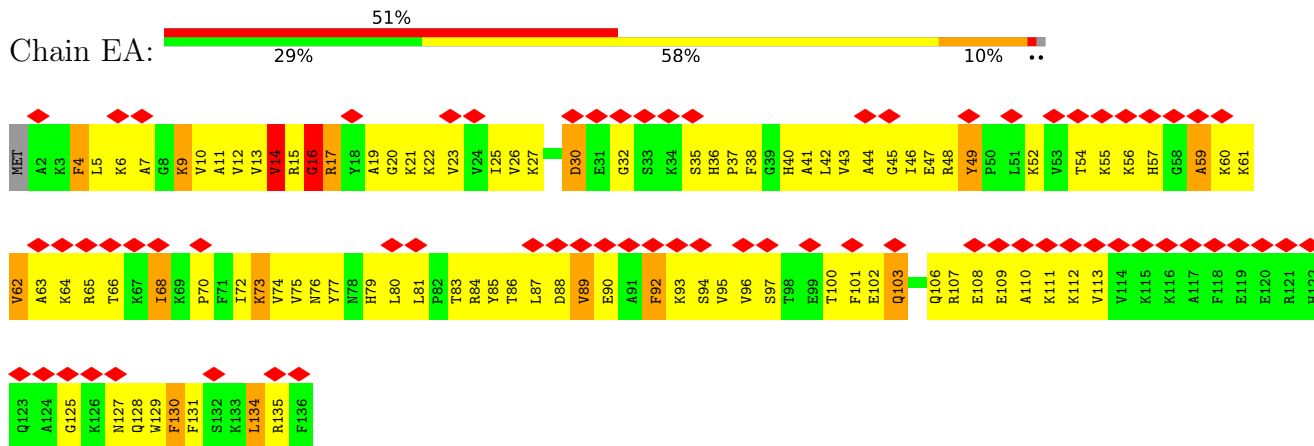
• Molecule 29: uL23 (yeast L25)



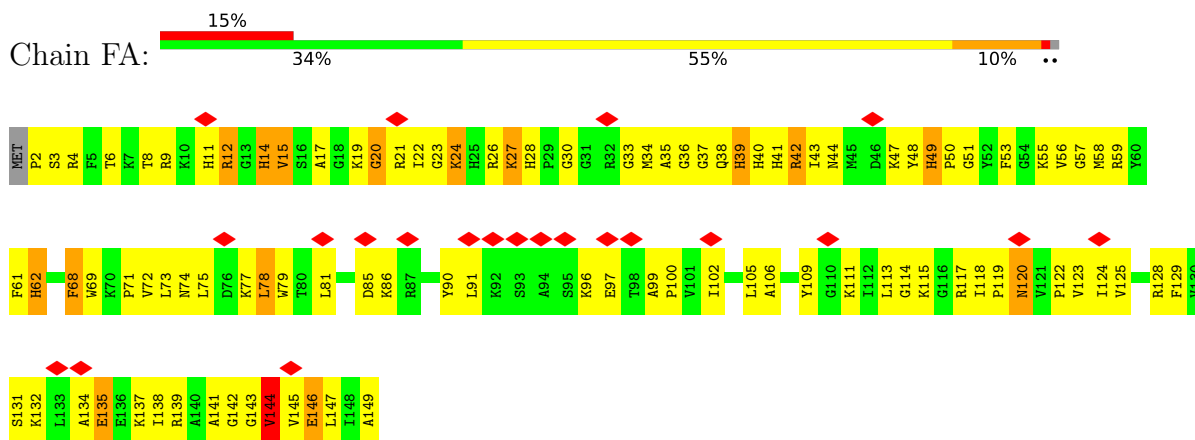
• Molecule 30: uL24 (yeast L26)



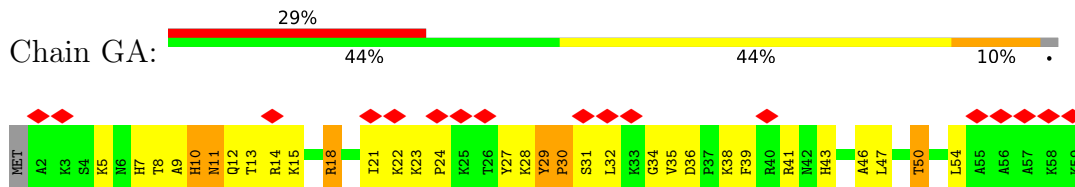
- Molecule 31: eL27 (yeast L27)



- Molecule 32: uL15 (yeast L28)

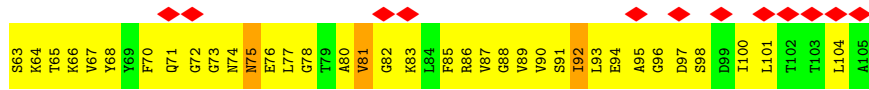
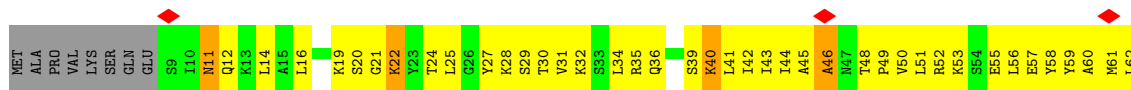


- Molecule 33: eL29 (yeast L29)



- Molecule 34: eL30 (yeast L30)

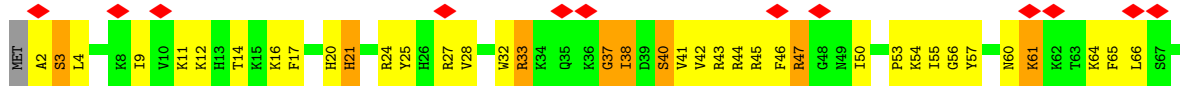




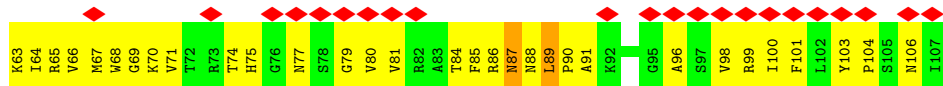
• Molecule 35: eL31 (yeast L31)



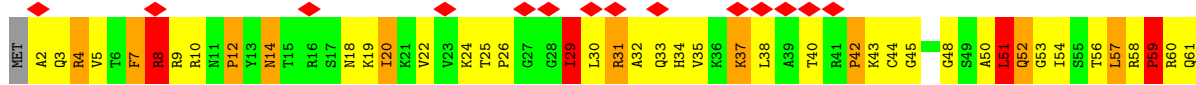
• Molecule 36: eL32 (yeast L32)

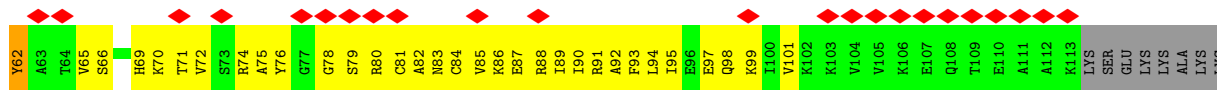


• Molecule 37: eL33 (yeast L33)

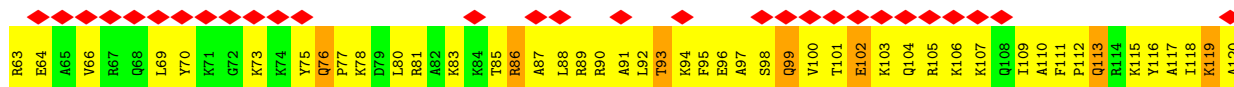
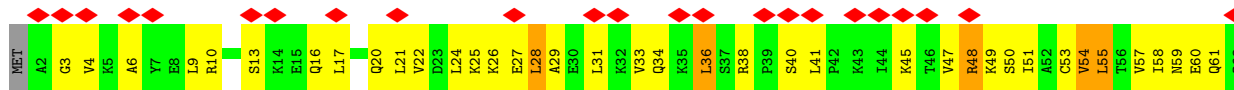
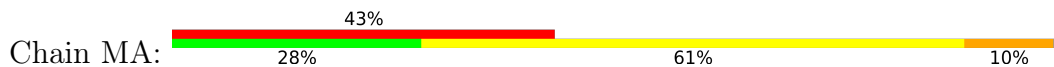


• Molecule 38: eL34 (yeast L34)

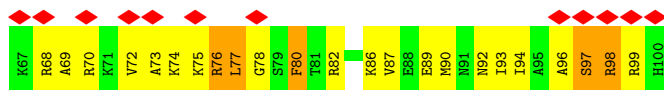
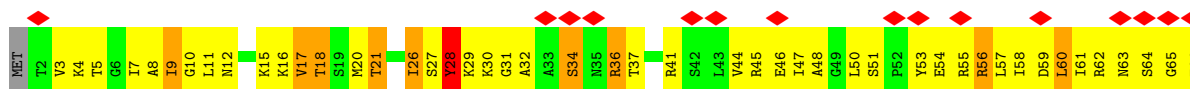




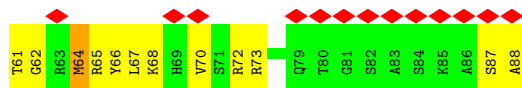
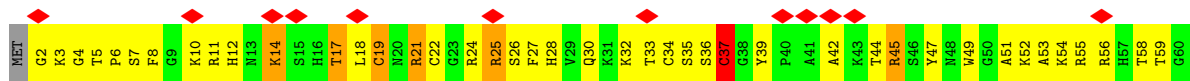
• Molecule 39: uL29 (yeast L35)



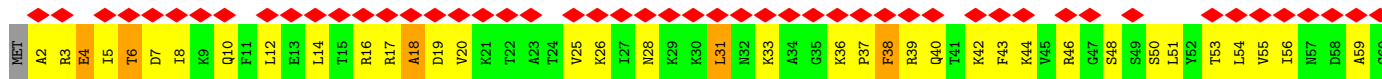
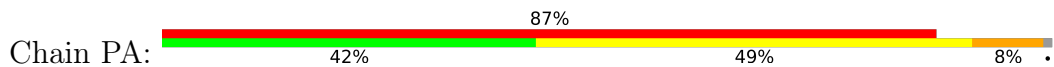
• Molecule 40: eL36 (yeast L36)



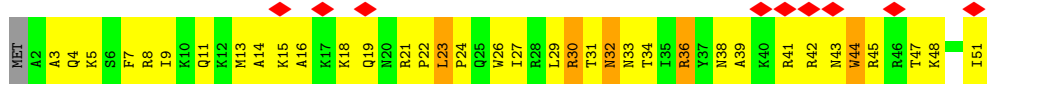
• Molecule 41: eL37 (yeast L37)



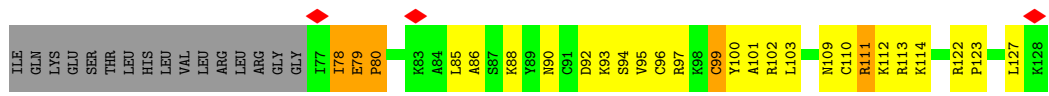
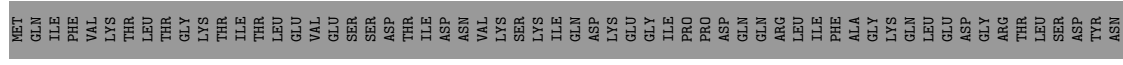
• Molecule 42: eL38 (yeast L38)



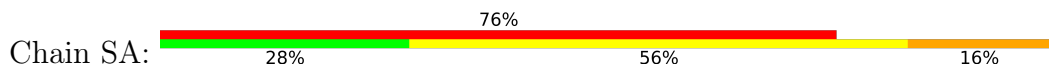
• Molecule 43: eL39 (yeast L39)



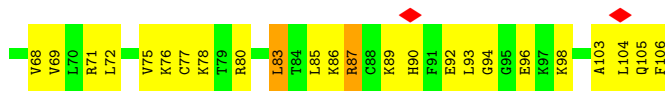
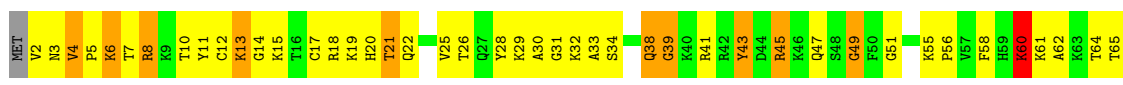
• Molecule 44: eL40 (yeast L40)



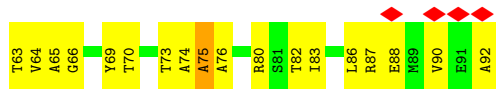
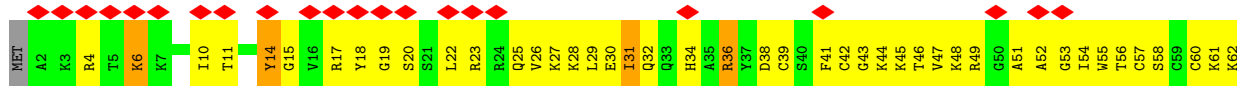
• Molecule 45: eL41 (yeast L41)



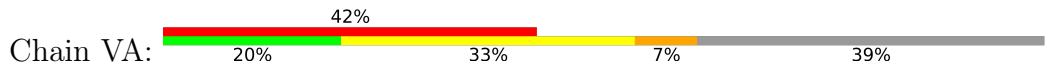
• Molecule 46: eL42 (yeast L42)

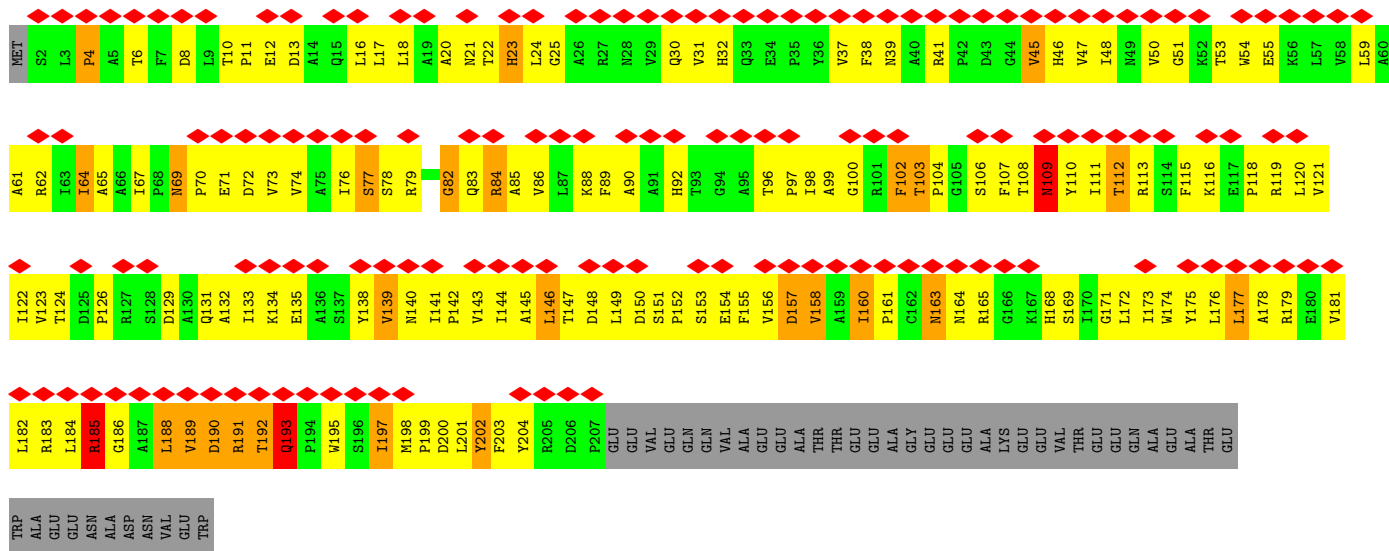


• Molecule 47: eL43 (yeast L43)

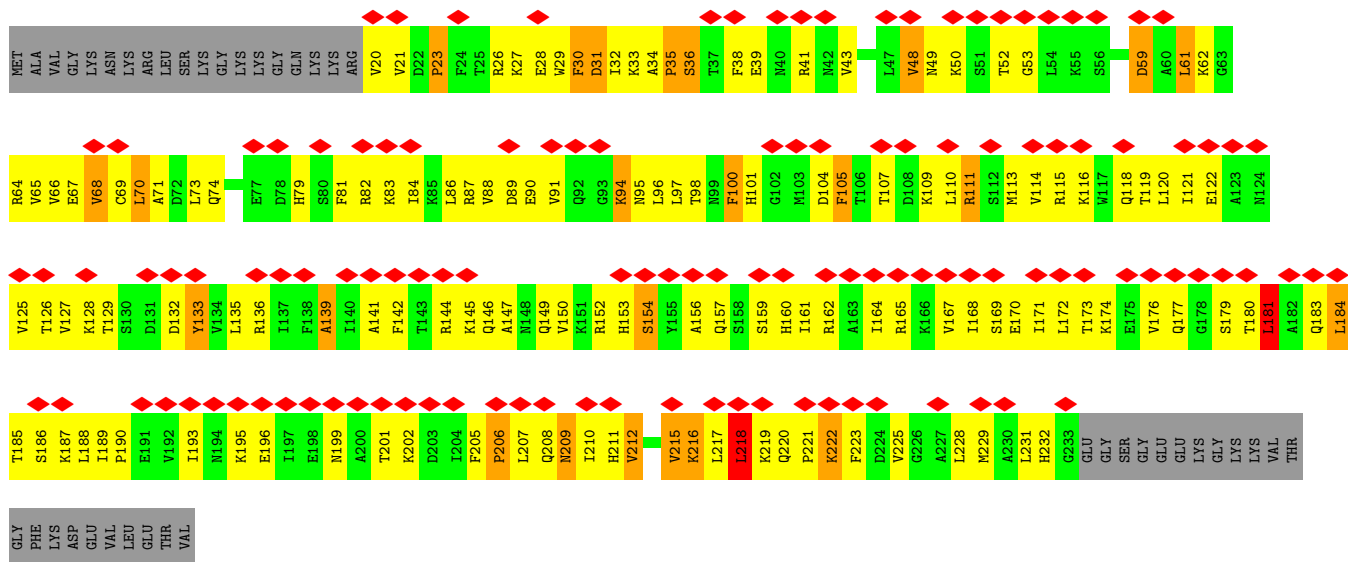


• Molecule 48: uL10 (yeast P0)

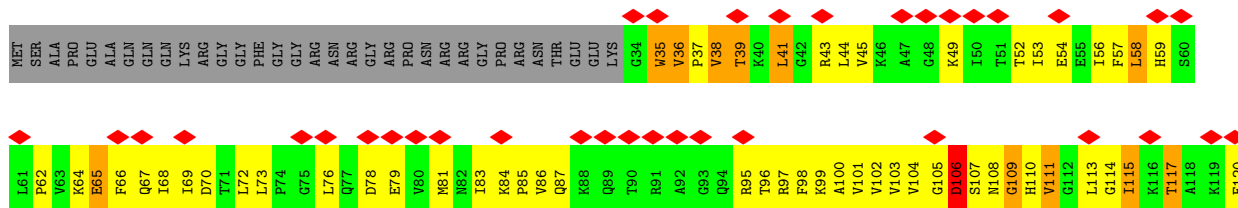


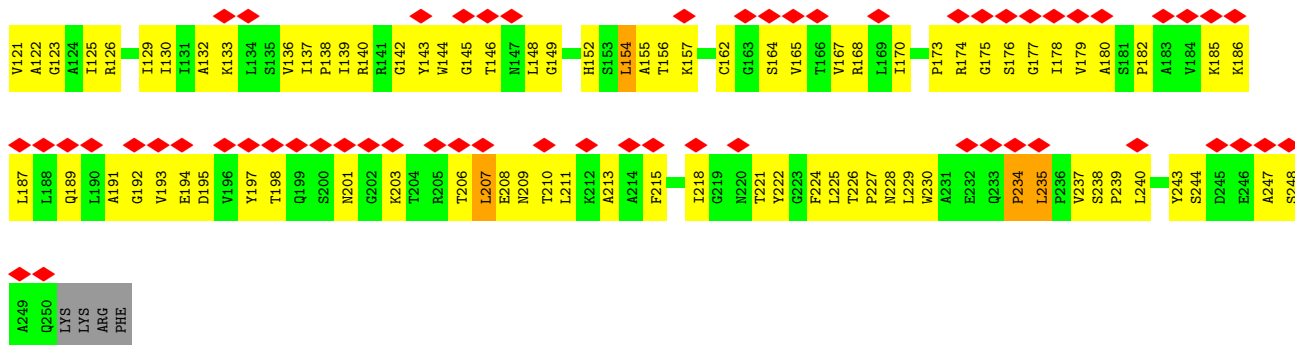


• Molecule 51: eS1 (yeast S1)

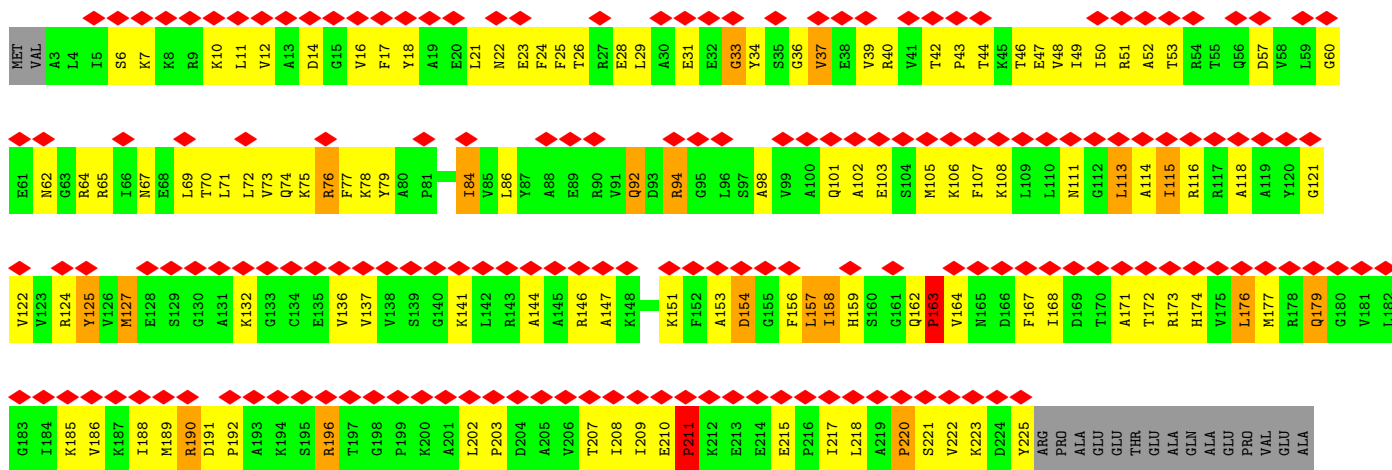
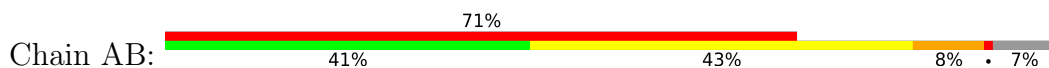


• Molecule 52: uS5 (yeast S2)

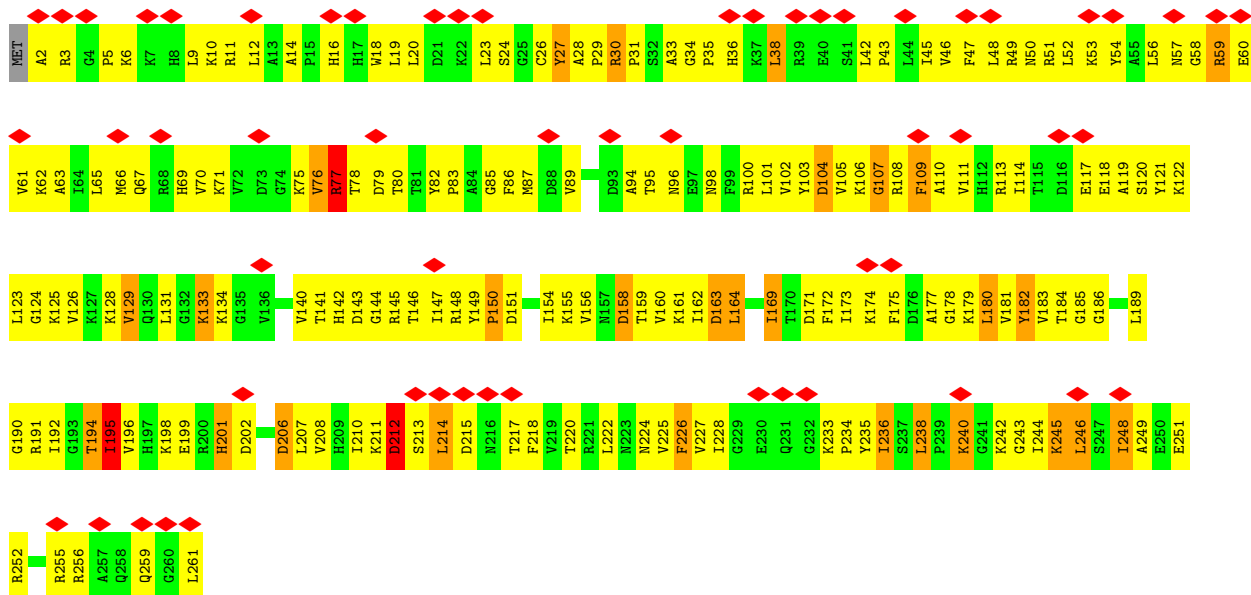




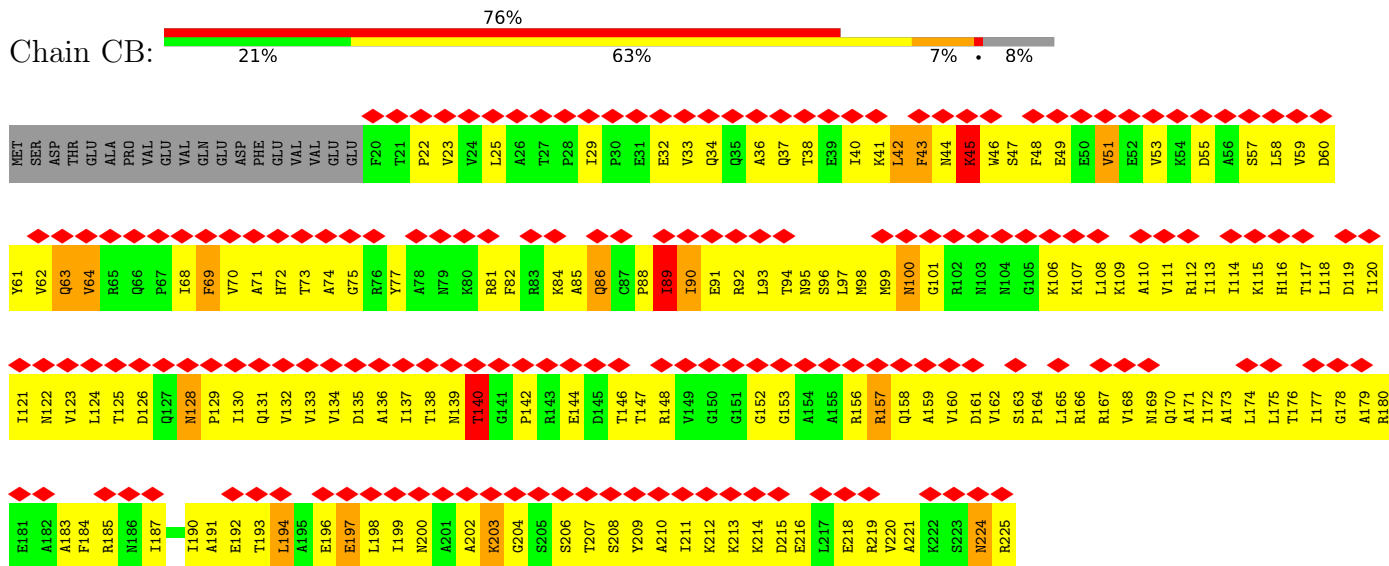
• Molecule 53: uS3 (yeast S3)



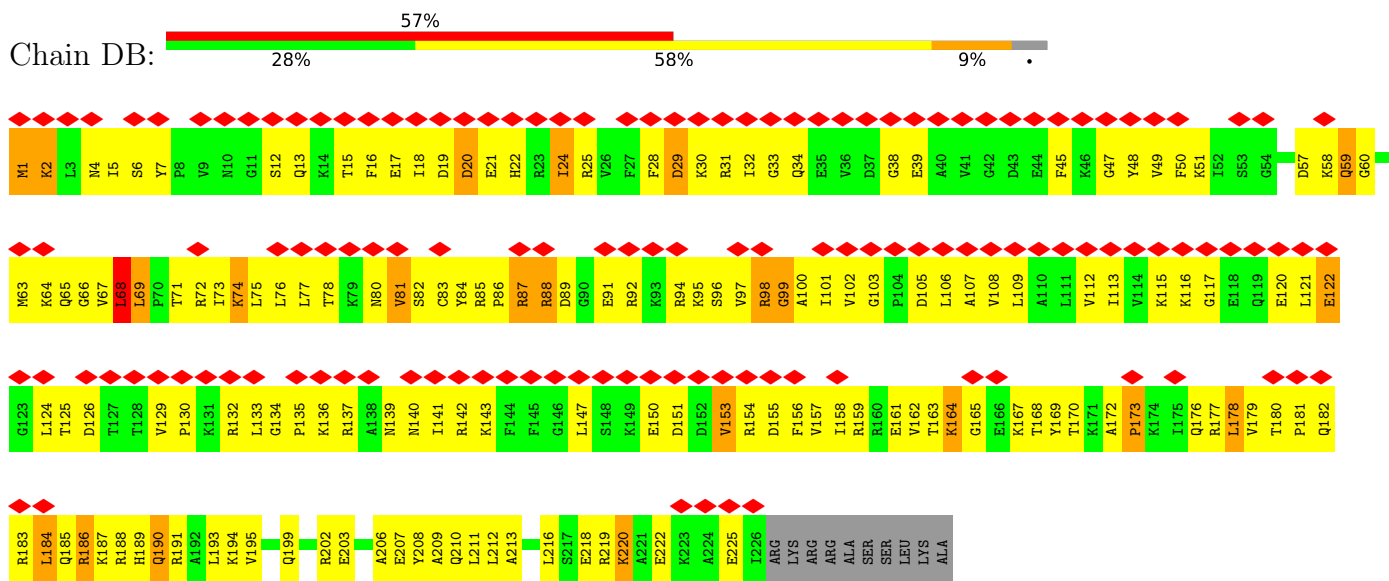
• Molecule 54: eS4 (yeast S4)



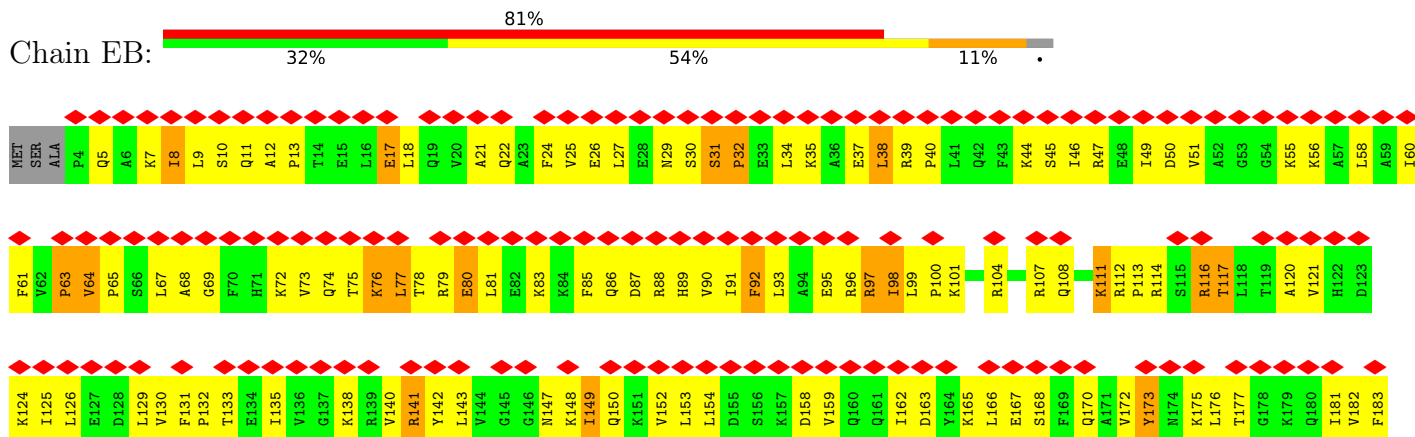
• Molecule 55: uS7 (yeast S5)



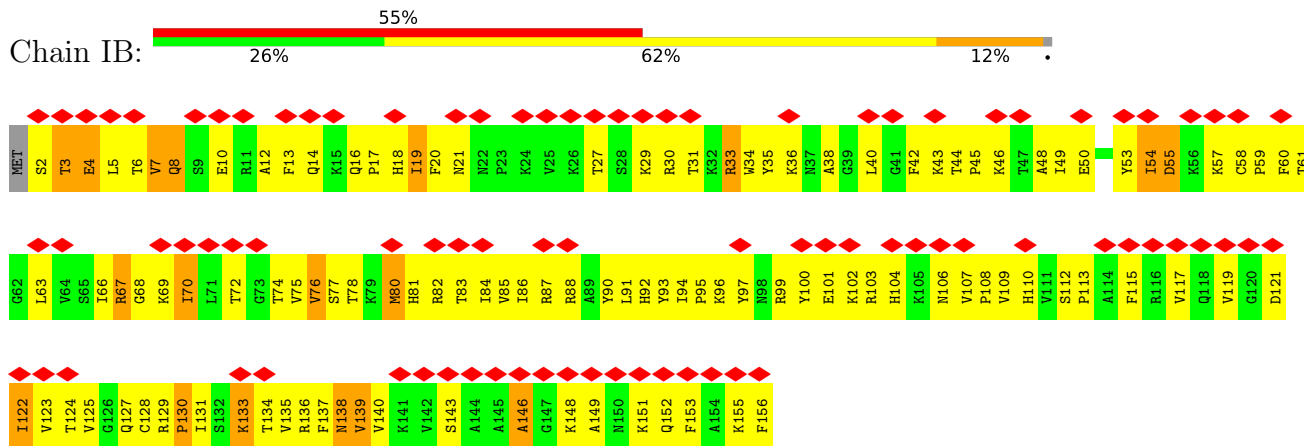
• Molecule 56: eS6 (yeast S6)



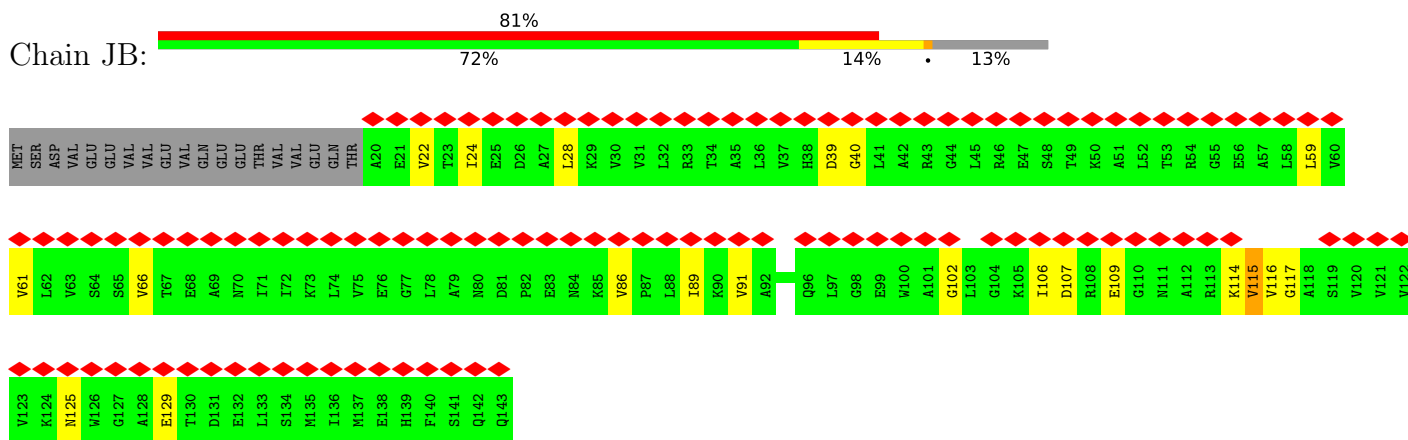
• Molecule 57: eS7 (yeast S7)



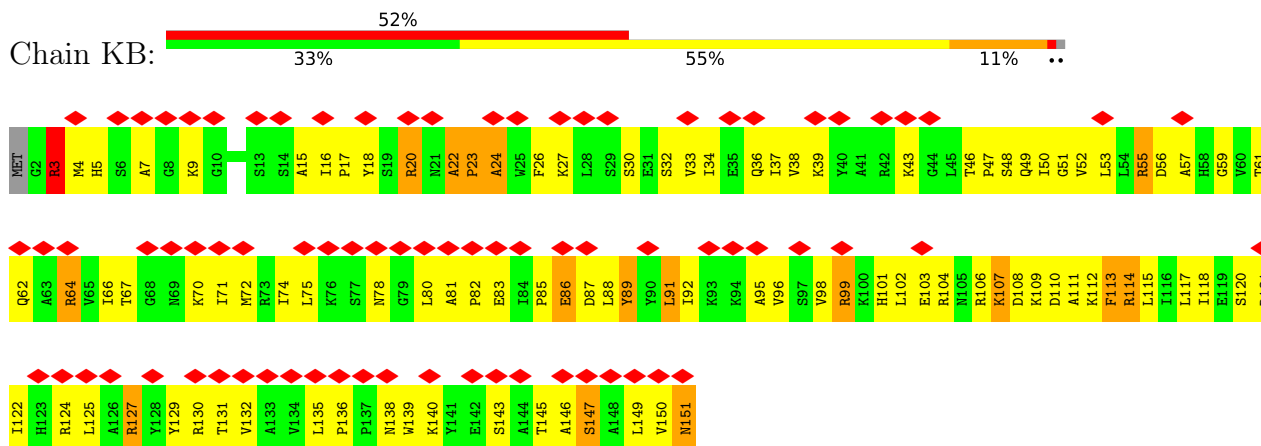
• Molecule 61: uS17 (yeast S11)



• Molecule 62: eS12 (yeast S12)

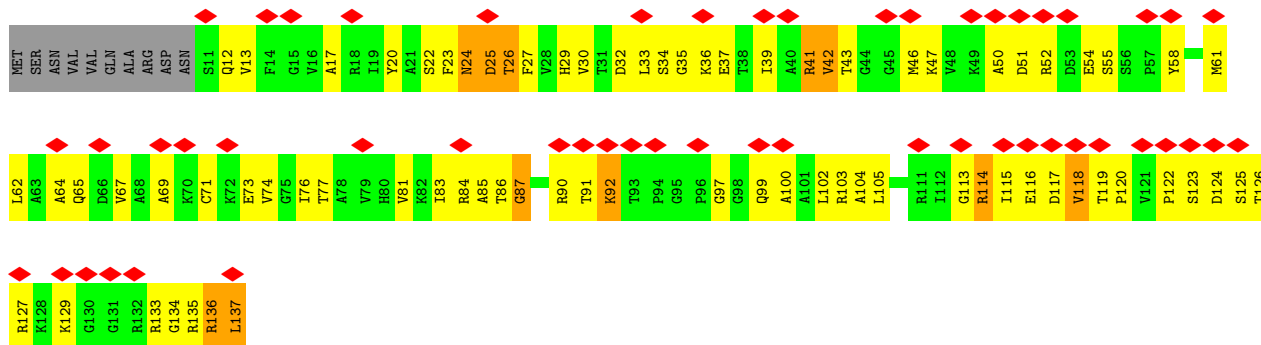


• Molecule 63: uS15 (yeast S13)

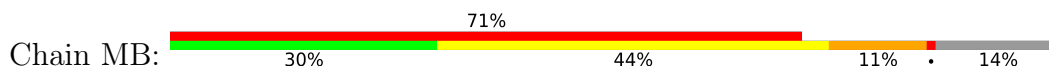


• Molecule 64: uS11 (yeast S14)

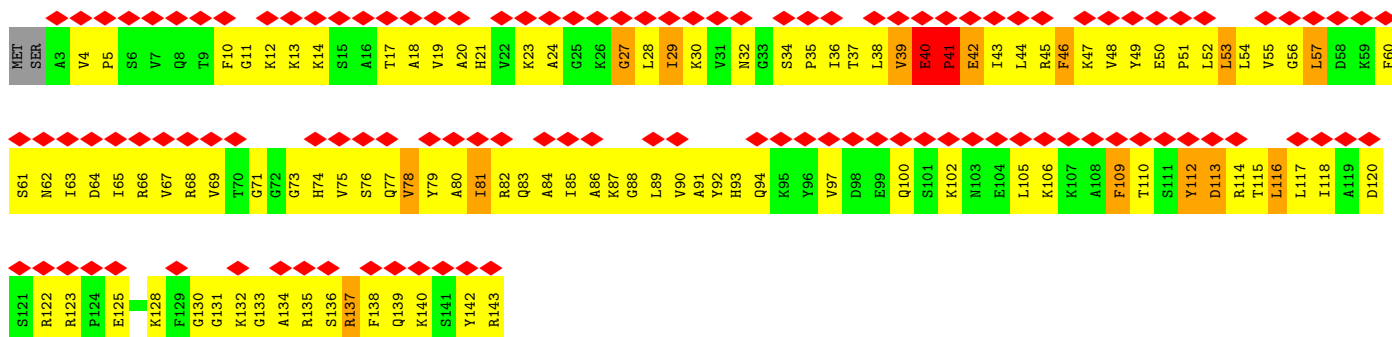
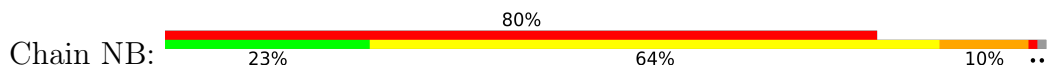




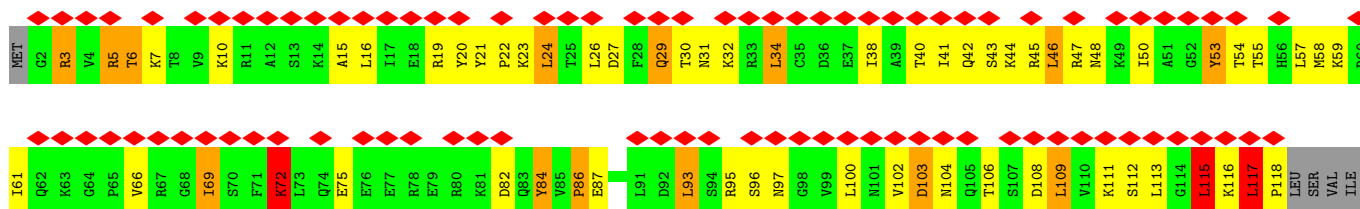
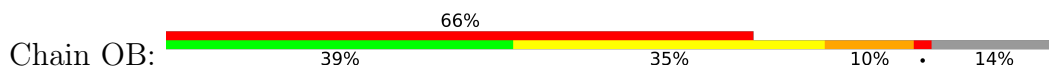
• Molecule 65: uS19 (yeast S15)



• Molecule 66: uS9 (yeast S16)

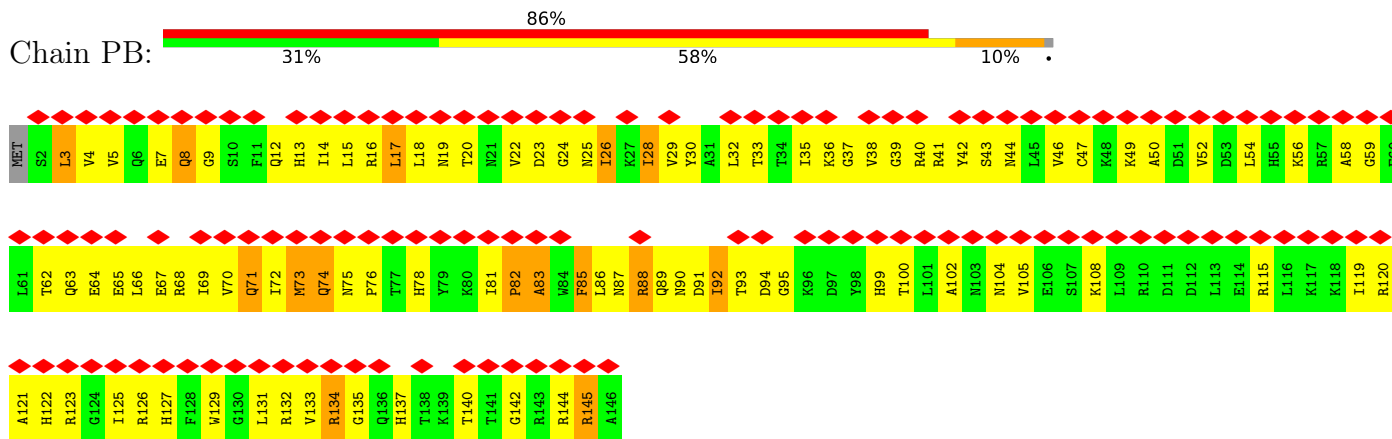


• Molecule 67: eS17 (yeast S17)

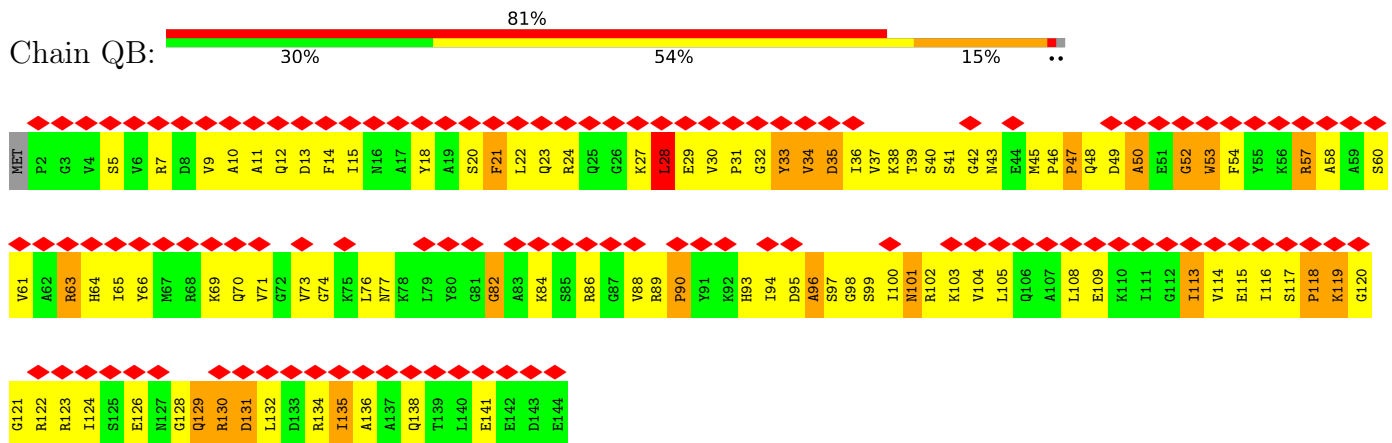


ASN	VAL	SER	ALA	GLN	ARG	ASP	ARG	ARG	ARG	LYS	ARG	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

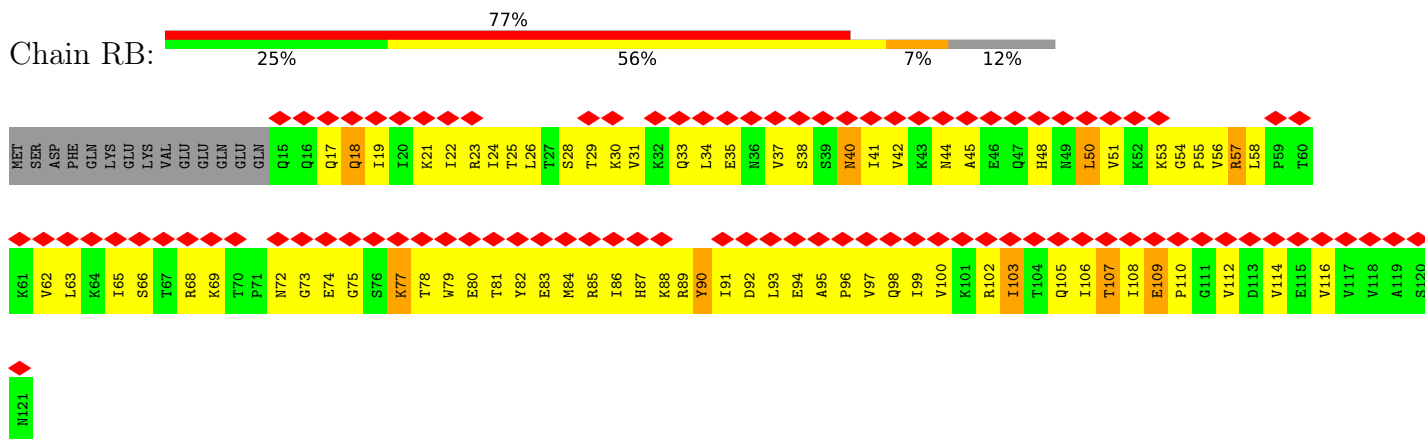
• Molecule 68: uS13 (yeast S18)



• Molecule 69: eS19 (yeast S19)

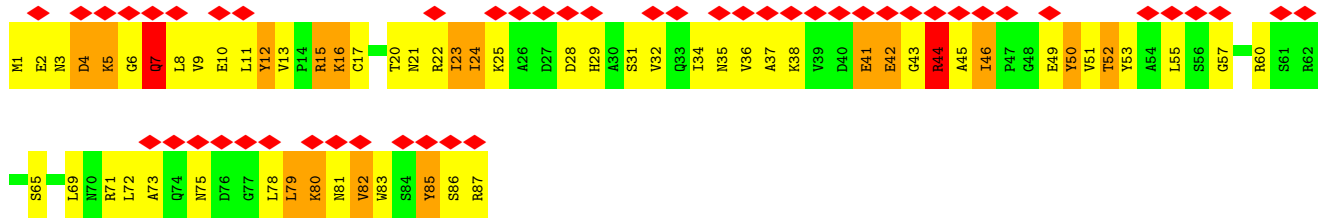


• Molecule 70: uS10 (yeast S20)

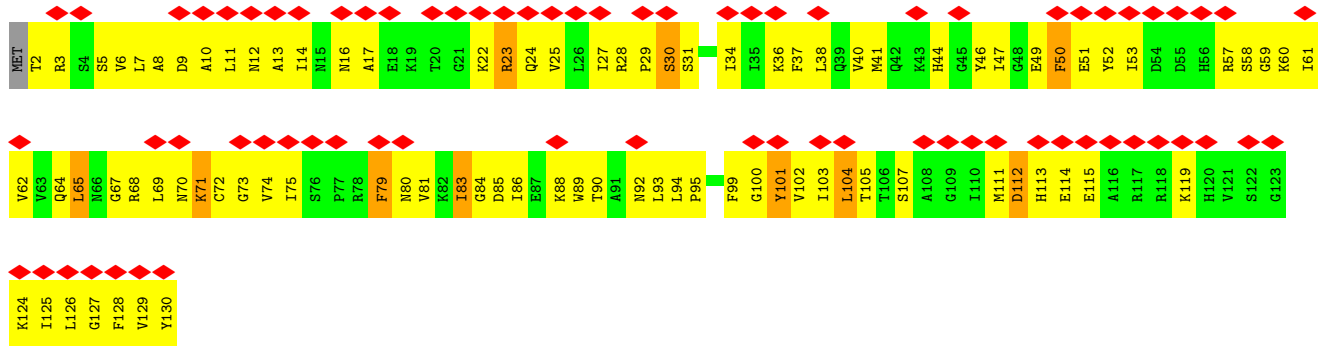


• Molecule 71: eS21 (yeast S21)

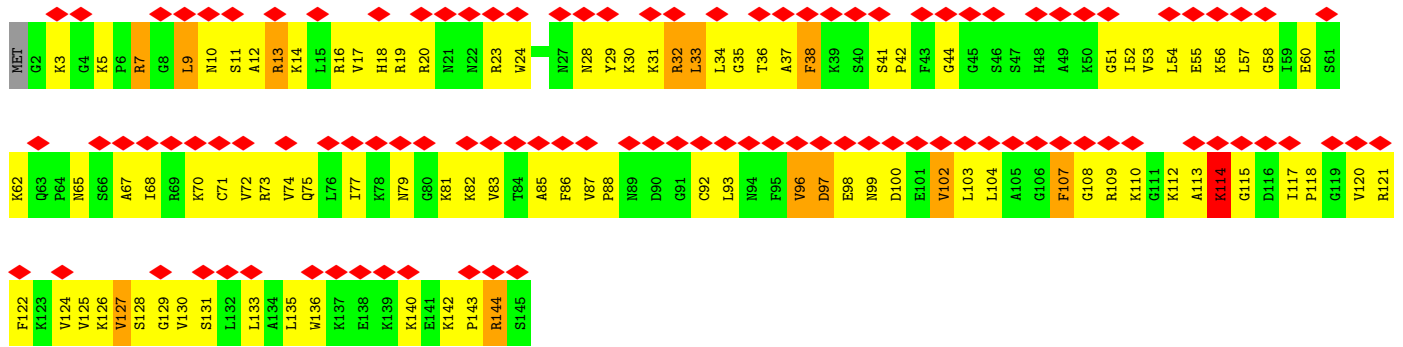
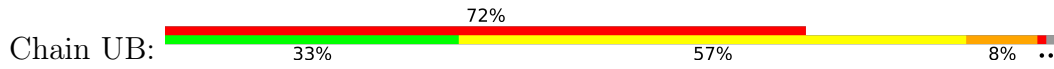




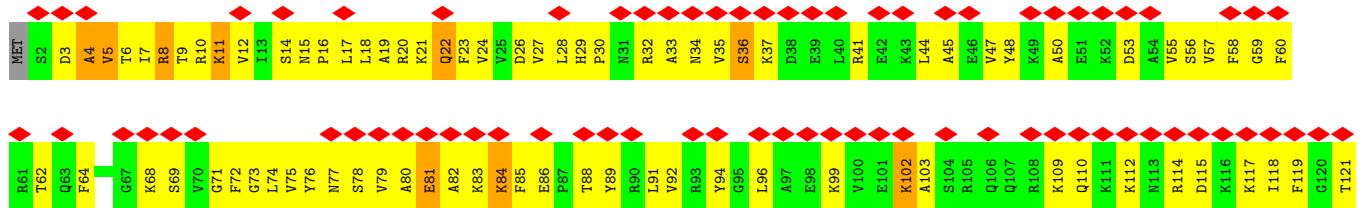
• Molecule 72: uS8 (yeast S22)

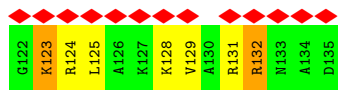


• Molecule 73: uS12 (yeast S23)

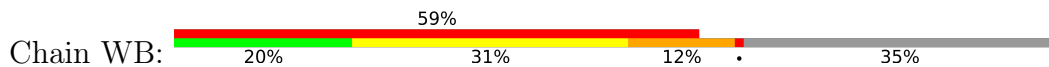


• Molecule 74: eS24 (yeast S24)

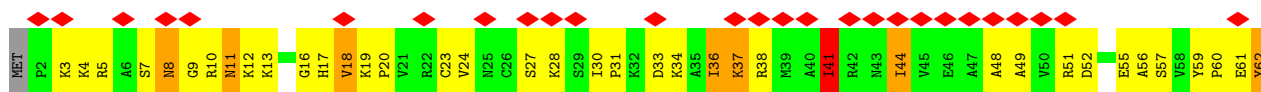




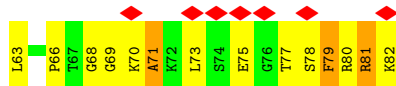
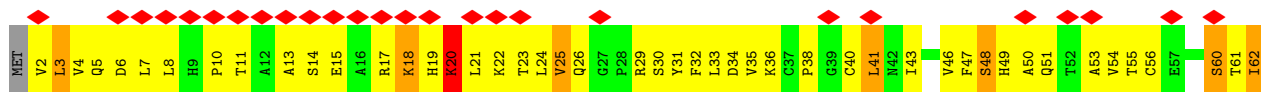
• Molecule 75: eS25 (yeast S25)



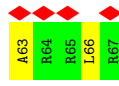
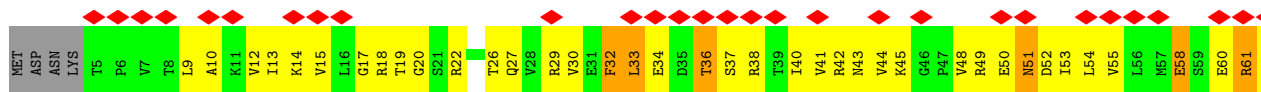
• Molecule 76: eS26 (yeast S26)



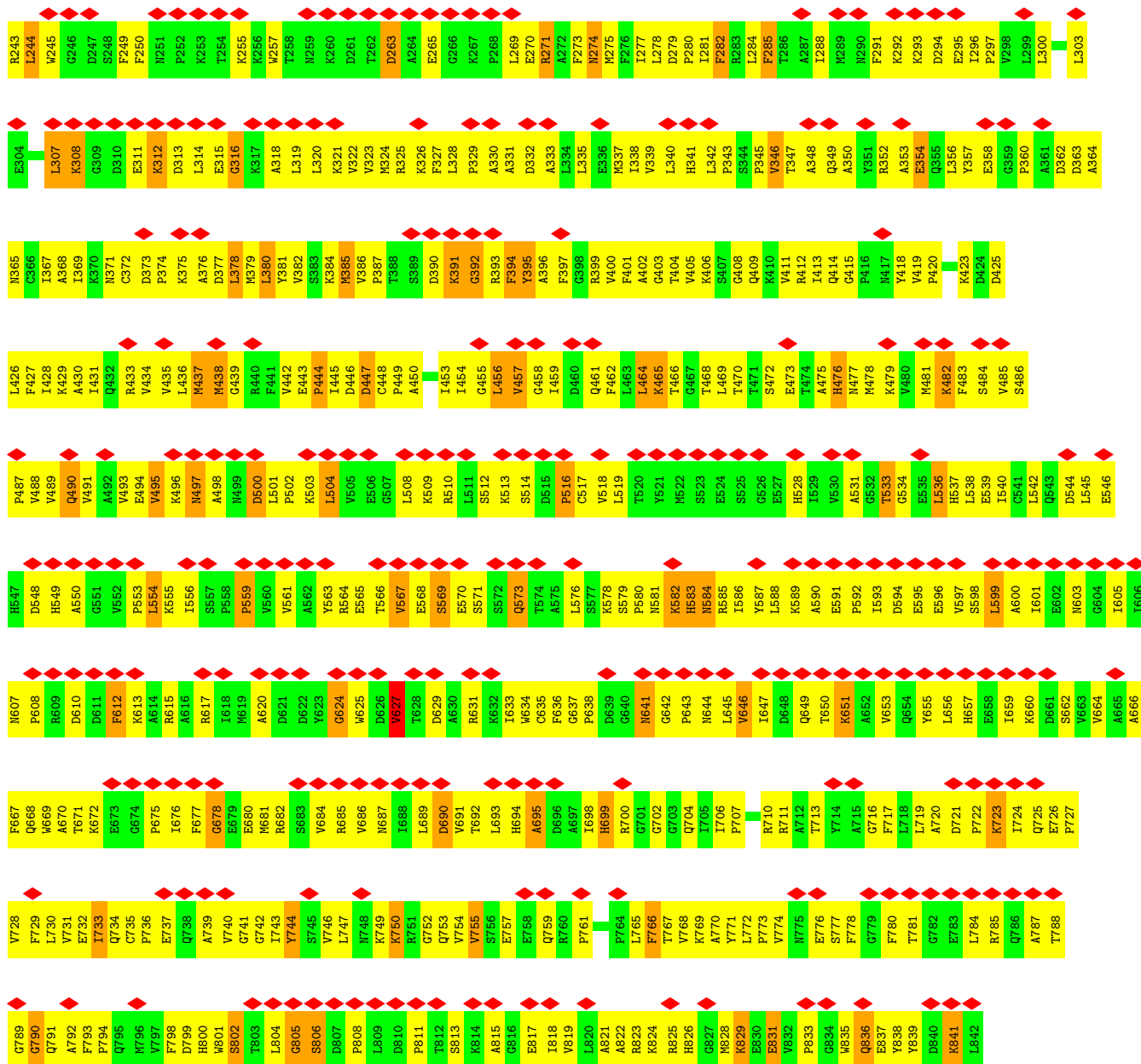
• Molecule 77: eS27 (yeast S27)



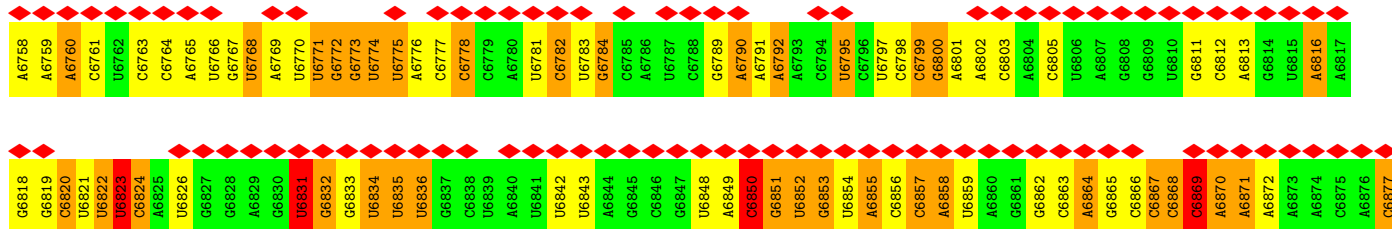
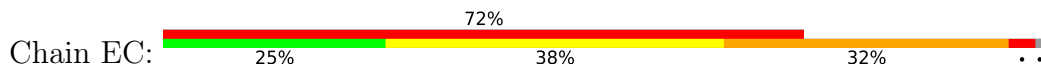
• Molecule 78: eS28 (yeast S28)



• Molecule 79: uS14 (yeast S29)



• Molecule 83: IRES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31871	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	0.064	Depositor
Minimum map value	-0.026	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO1, MG, DDE, 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	0.86	1/42096 (0.0%)	0.75	11/65570 (0.0%)
2	B	1.13	16/78631 (0.0%)	0.77	25/122552 (0.0%)
3	C	1.18	1/3747 (0.0%)	0.76	2/5832 (0.0%)
4	D	1.08	1/2884 (0.0%)	0.76	0/4491
5	E	1.77	0/1377	0.79	2/1844 (0.1%)
6	F	1.01	0/1952	0.72	1/2622 (0.0%)
7	G	0.98	0/3153	0.66	1/4239 (0.0%)
8	H	1.09	0/2802	0.67	0/3792
9	I	0.91	0/2426	0.63	0/3271
10	J	1.05	0/1425	0.68	2/1912 (0.1%)
11	K	1.14	0/1822	0.66	0/2451
12	L	0.95	0/1850	0.63	0/2495
13	M	1.00	0/1540	0.64	0/2073
14	N	1.07	0/1754	0.65	0/2350
15	O	0.84	0/1375	0.60	0/1842
16	P	1.71	0/728	0.75	0/975
17	Q	1.03	0/1568	0.65	0/2106
18	R	1.13	0/1069	0.64	0/1438
19	S	1.13	0/1758	0.69	0/2354
20	T	1.08	0/1586	0.65	0/2128
21	U	1.06	0/1466	0.66	1/1968 (0.1%)
22	V	1.04	0/1466	0.69	1/1965 (0.1%)
23	W	0.87	0/1539	0.61	0/2050
24	X	1.19	0/1482	0.66	0/1990
25	Y	1.13	0/1301	0.68	0/1743
26	Z	0.78	0/812	0.58	0/1099
27	AA	1.06	0/1019	0.63	0/1369
28	BA	1.10	0/521	0.62	0/691
29	CA	1.09	0/984	0.68	1/1325 (0.1%)
30	DA	1.05	0/1005	0.71	1/1341 (0.1%)
31	EA	0.85	0/1119	0.61	1/1497 (0.1%)
32	FA	1.07	0/1205	0.65	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	GA	0.97	0/474	0.68	0/629
34	HA	0.79	0/751	0.63	0/1008
35	IA	0.93	0/904	0.61	0/1213
36	JA	1.10	0/1041	0.62	0/1394
37	KA	1.15	0/869	0.68	0/1168
38	LA	0.99	0/891	0.66	0/1191
39	MA	0.95	0/979	0.66	0/1301
40	NA	0.92	0/779	0.64	0/1034
41	OA	1.19	0/697	0.66	0/923
42	PA	0.88	0/619	0.60	0/826
43	QA	1.01	0/444	0.68	0/588
44	RA	1.05	0/424	0.60	0/562
45	SA	0.89	0/235	0.67	0/300
46	TA	1.03	0/861	0.67	0/1136
47	UA	1.02	0/702	0.61	0/934
48	VA	1.58	0/1498	0.79	0/2025
49	WA	0.83	0/2498	0.56	0/3398
50	XA	0.71	0/1653	0.65	3/2261 (0.1%)
51	YA	0.75	0/1735	0.59	1/2335 (0.0%)
52	ZA	0.74	0/1665	0.59	0/2263
53	AB	0.86	0/1759	0.57	0/2368
54	BB	0.72	0/2110	0.59	0/2839
55	CB	0.79	0/1630	0.58	0/2202
56	DB	0.74	0/1844	0.58	0/2464
57	EB	0.78	0/1506	0.58	0/2028
58	FB	0.88	0/1515	0.58	0/2021
59	GB	0.70	0/1519	0.59	0/2035
60	HB	0.93	0/837	0.56	0/1131
61	IB	0.91	0/1273	0.62	0/1712
62	JB	1.02	0/495	0.61	0/617
63	KB	0.83	0/1216	0.61	0/1638
64	LB	0.67	0/953	0.57	0/1279
65	MB	0.97	0/996	0.64	0/1335
66	NB	0.83	0/1126	0.61	0/1510
67	OB	0.80	1/844 (0.1%)	0.82	4/1120 (0.4%)
68	PB	0.87	0/1212	0.59	0/1628
69	QB	0.84	0/1131	0.62	0/1517
70	RB	0.86	0/866	0.59	0/1169
71	SB	0.71	0/694	0.57	0/935
72	TB	0.77	0/1039	0.59	0/1395
73	UB	0.90	0/1140	0.60	0/1518
74	VB	0.76	0/1088	0.58	0/1449
75	WB	0.83	0/571	0.65	0/768

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	XB	0.71	0/782	0.57	0/1047
77	YB	0.76	0/621	0.57	0/838
78	ZB	0.75	0/500	0.60	0/670
79	AC	0.98	0/454	0.61	1/602 (0.2%)
80	BC	0.85	0/483	0.62	0/643
81	CC	0.99	0/283	0.66	0/352
82	DC	1.39	5/6521 (0.1%)	0.71	4/8830 (0.0%)
83	EC	1.96	34/4579 (0.7%)	0.94	10/7119 (0.1%)
All	All	1.06	59/230768 (0.0%)	0.72	72/338255 (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	11
2	B	0	64
3	C	0	2
4	D	0	1
50	XA	0	1
83	EC	0	10
All	All	0	89

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	3	ALA	N-CA	12.70	1.71	1.46
82	DC	4	PHE	CD1-CE1	12.26	1.63	1.39
82	DC	4	PHE	CB-CG	11.48	1.70	1.51
83	EC	6763	C	N1-C2	7.78	1.48	1.40
4	D	1	G	OP3-P	-6.91	1.52	1.61

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	XA	192	THR	O-C-N	-10.45	105.98	122.70
83	EC	6878	G	N9-C1'-C2'	9.91	126.89	114.00
67	OB	97	ASN	N-CA-C	-9.28	85.94	111.00
1	A	103	A	C2'-C3'-O3'	8.12	127.36	109.50
2	B	764	U	N1-C1'-C2'	7.82	124.16	114.00

There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	U	Sidechain
1	A	287	G	Sidechain
1	A	322	G	Sidechain
1	A	447	U	Sidechain
1	A	834	G	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	37658	0	18908	1719	0
2	B	70288	0	35262	3754	0
3	C	3354	0	1695	185	0
4	D	2580	0	1304	138	0
5	E	1359	0	1425	118	0
6	F	1918	0	1987	283	0
7	G	3082	0	3165	394	0
8	H	2750	0	2863	334	0
9	I	2376	0	2325	261	0
10	J	1401	0	1501	141	0
11	K	1785	0	1862	238	0
12	L	1818	0	1908	210	0
13	M	1519	0	1587	173	0
14	N	1718	0	1754	182	0
15	O	1354	0	1383	144	0
16	P	723	0	774	109	0
17	Q	1543	0	1608	181	0
18	R	1054	0	1149	157	0
19	S	1721	0	1779	281	0
20	T	1556	0	1659	184	0
21	U	1443	0	1485	158	0
22	V	1442	0	1543	181	0
23	W	1522	0	1617	171	0
24	X	1446	0	1487	248	0
25	Y	1277	0	1323	195	0
26	Z	796	0	812	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	1004	0	1048	113	0
28	BA	509	0	537	46	0
29	CA	969	0	1036	132	0
30	DA	994	0	1081	115	0
31	EA	1093	0	1155	135	0
32	FA	1174	0	1215	156	0
33	GA	463	0	491	49	0
34	HA	743	0	797	100	0
35	IA	890	0	938	84	0
36	JA	1020	0	1090	92	0
37	KA	851	0	880	115	0
38	LA	881	0	949	133	0
39	MA	970	0	1078	125	0
40	NA	772	0	849	101	0
41	OA	682	0	687	81	0
42	PA	613	0	682	44	0
43	QA	437	0	475	56	0
44	RA	418	0	459	32	0
45	SA	234	0	284	29	0
46	TA	848	0	918	83	0
47	UA	695	0	738	75	0
48	VA	1473	0	1514	198	0
49	WA	2445	0	2401	191	0
50	XA	1612	0	1623	188	0
51	YA	1709	0	1784	191	0
52	ZA	1635	0	1723	159	0
53	AB	1734	0	1817	120	0
54	BB	2069	0	2154	231	0
55	CB	1610	0	1675	198	0
56	DB	1820	0	1918	177	0
57	EB	1481	0	1572	152	0
58	FB	1490	0	1525	166	0
59	GB	1494	0	1573	165	0
60	HB	817	0	804	78	0
61	IB	1245	0	1314	136	0
62	JB	496	0	141	2	0
63	KB	1193	0	1255	135	0
64	LB	942	0	979	100	0
65	MB	975	0	1017	103	0
66	NB	1106	0	1166	147	0
67	OB	836	0	826	74	0
68	PB	1193	0	1222	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	QB	1113	0	1124	135	0
70	RB	856	0	917	93	0
71	SB	685	0	672	92	0
72	TB	1022	0	1060	108	0
73	UB	1122	0	1196	109	0
74	VB	1074	0	1132	95	0
75	WB	563	0	603	66	0
76	XB	769	0	818	112	0
77	YB	611	0	633	73	0
78	ZB	498	0	535	51	0
79	AC	444	0	436	50	0
80	BC	475	0	525	41	0
81	CC	284	0	76	0	0
82	DC	6419	0	6493	729	0
83	EC	4105	0	2063	138	0
84	DC	28	0	12	4	0
85	DC	1	0	0	0	0
86	DC	35	0	41	3	0
All	All	215222	0	159891	14740	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 39.

The worst 5 of 14740 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)
82:DC:3:ALA:CA	82:DC:3:ALA:N	1.71	1.50
2:B:1719:G:H4'	2:B:1732:U:H4'	1.22	1.18
1:A:754:A:H3'	1:A:755:A:H5'	1.25	1.14
22:V:54:LEU:HB3	22:V:58:ASN:HB2	1.26	1.14
55:CB:29:ILE:HG21	66:NB:57:LEU:HD11	1.27	1.14

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%)	124 (75%)	28 (17%)	13 (8%)	1	14
6	F	250/254 (98%)	159 (64%)	61 (24%)	30 (12%)	0	5
7	G	384/387 (99%)	280 (73%)	84 (22%)	20 (5%)	2	21
8	H	359/362 (99%)	241 (67%)	77 (21%)	41 (11%)	0	6
9	I	294/297 (99%)	210 (71%)	64 (22%)	20 (7%)	1	17
10	J	173/176 (98%)	124 (72%)	35 (20%)	14 (8%)	1	13
11	K	220/244 (90%)	160 (73%)	37 (17%)	23 (10%)	0	8
12	L	231/256 (90%)	162 (70%)	50 (22%)	19 (8%)	1	13
13	M	189/191 (99%)	143 (76%)	32 (17%)	14 (7%)	1	15
14	N	207/221 (94%)	157 (76%)	35 (17%)	15 (7%)	1	16
15	O	167/174 (96%)	121 (72%)	30 (18%)	16 (10%)	0	10
16	P	92/165 (56%)	64 (70%)	14 (15%)	14 (15%)	0	3
17	Q	191/199 (96%)	141 (74%)	33 (17%)	17 (9%)	1	12
18	R	134/138 (97%)	103 (77%)	24 (18%)	7 (5%)	2	21
19	S	201/204 (98%)	148 (74%)	39 (19%)	14 (7%)	1	16
20	T	195/199 (98%)	152 (78%)	37 (19%)	6 (3%)	4	31
21	U	181/184 (98%)	127 (70%)	39 (22%)	15 (8%)	1	13
22	V	183/186 (98%)	120 (66%)	47 (26%)	16 (9%)	1	12
23	W	186/189 (98%)	142 (76%)	35 (19%)	9 (5%)	2	23
24	X	170/172 (99%)	119 (70%)	41 (24%)	10 (6%)	1	19
25	Y	157/160 (98%)	105 (67%)	31 (20%)	21 (13%)	0	4
26	Z	98/121 (81%)	64 (65%)	28 (29%)	6 (6%)	1	19
27	AA	134/137 (98%)	97 (72%)	32 (24%)	5 (4%)	3	28
28	BA	59/155 (38%)	41 (70%)	10 (17%)	8 (14%)	0	4
29	CA	119/142 (84%)	79 (66%)	24 (20%)	16 (13%)	0	4
30	DA	124/127 (98%)	96 (77%)	19 (15%)	9 (7%)	1	15
31	EA	133/136 (98%)	95 (71%)	21 (16%)	17 (13%)	0	5
32	FA	146/149 (98%)	95 (65%)	39 (27%)	12 (8%)	1	13
33	GA	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	1	12
34	HA	95/105 (90%)	70 (74%)	19 (20%)	6 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	IA	107/113 (95%)	79 (74%)	24 (22%)	4 (4%)	3	28
36	JA	125/130 (96%)	87 (70%)	30 (24%)	8 (6%)	1	18
37	KA	104/107 (97%)	77 (74%)	24 (23%)	3 (3%)	4	32
38	LA	110/121 (91%)	69 (63%)	30 (27%)	11 (10%)	0	9
39	MA	117/120 (98%)	87 (74%)	23 (20%)	7 (6%)	1	19
40	NA	97/100 (97%)	69 (71%)	18 (19%)	10 (10%)	0	8
41	OA	85/88 (97%)	58 (68%)	23 (27%)	4 (5%)	2	23
42	PA	75/78 (96%)	58 (77%)	14 (19%)	3 (4%)	3	26
43	QA	48/51 (94%)	35 (73%)	9 (19%)	4 (8%)	1	13
44	RA	50/128 (39%)	36 (72%)	10 (20%)	4 (8%)	1	14
45	SA	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
46	TA	103/106 (97%)	66 (64%)	25 (24%)	12 (12%)	0	6
47	UA	89/92 (97%)	68 (76%)	17 (19%)	4 (4%)	2	24
48	VA	187/312 (60%)	138 (74%)	37 (20%)	12 (6%)	1	18
49	WA	316/319 (99%)	243 (77%)	60 (19%)	13 (4%)	3	25
50	XA	204/252 (81%)	147 (72%)	41 (20%)	16 (8%)	1	14
51	YA	212/255 (83%)	154 (73%)	41 (19%)	17 (8%)	1	14
52	ZA	215/254 (85%)	155 (72%)	45 (21%)	15 (7%)	1	16
53	AB	221/240 (92%)	170 (77%)	37 (17%)	14 (6%)	1	18
54	BB	258/261 (99%)	173 (67%)	64 (25%)	21 (8%)	1	13
55	CB	204/225 (91%)	152 (74%)	35 (17%)	17 (8%)	1	13
56	DB	224/236 (95%)	174 (78%)	36 (16%)	14 (6%)	1	18
57	EB	182/190 (96%)	128 (70%)	43 (24%)	11 (6%)	1	19
58	FB	184/200 (92%)	136 (74%)	36 (20%)	12 (6%)	1	18
59	GB	183/197 (93%)	143 (78%)	26 (14%)	14 (8%)	1	14
60	HB	94/105 (90%)	66 (70%)	20 (21%)	8 (8%)	1	12
61	IB	153/156 (98%)	109 (71%)	31 (20%)	13 (8%)	1	12
62	JB	122/143 (85%)	74 (61%)	29 (24%)	19 (16%)	0	3
63	KB	148/151 (98%)	113 (76%)	28 (19%)	7 (5%)	2	23
64	LB	125/137 (91%)	87 (70%)	29 (23%)	9 (7%)	1	16
65	MB	120/142 (84%)	83 (69%)	27 (22%)	10 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	102 (73%)	27 (19%)	10 (7%)	1	16
67	OB	115/136 (85%)	79 (69%)	29 (25%)	7 (6%)	1	19
68	PB	143/146 (98%)	101 (71%)	27 (19%)	15 (10%)	0	8
69	QB	141/144 (98%)	99 (70%)	28 (20%)	14 (10%)	0	9
70	RB	105/121 (87%)	81 (77%)	22 (21%)	2 (2%)	8	40
71	SB	85/87 (98%)	55 (65%)	19 (22%)	11 (13%)	0	4
72	TB	127/130 (98%)	95 (75%)	25 (20%)	7 (6%)	2	21
73	UB	142/145 (98%)	94 (66%)	41 (29%)	7 (5%)	2	22
74	VB	132/135 (98%)	93 (70%)	32 (24%)	7 (5%)	2	21
75	WB	68/108 (63%)	42 (62%)	14 (21%)	12 (18%)	0	2
76	XB	95/119 (80%)	57 (60%)	24 (25%)	14 (15%)	0	3
77	YB	79/82 (96%)	41 (52%)	27 (34%)	11 (14%)	0	4
78	ZB	61/67 (91%)	44 (72%)	12 (20%)	5 (8%)	1	13
79	AC	51/56 (91%)	37 (72%)	10 (20%)	4 (8%)	1	14
80	BC	58/63 (92%)	40 (69%)	14 (24%)	4 (7%)	1	16
81	CC	69/152 (45%)	37 (54%)	20 (29%)	12 (17%)	0	2
82	DC	819/842 (97%)	592 (72%)	171 (21%)	56 (7%)	1	17
All	All	12207/13416 (91%)	8728 (72%)	2527 (21%)	952 (8%)	2	14

5 of 952 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	35	GLN
5	E	127	GLN
5	E	140	HIS
5	E	174	MET
6	F	65	ASP

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%)	137 (87%)	20 (13%)	4	22
6	F	194/196 (99%)	171 (88%)	23 (12%)	5	24
7	G	322/323 (100%)	288 (89%)	34 (11%)	6	27
8	H	288/289 (100%)	255 (88%)	33 (12%)	5	25
9	I	244/245 (100%)	211 (86%)	33 (14%)	4	21
10	J	152/153 (99%)	143 (94%)	9 (6%)	19	48
11	K	186/205 (91%)	163 (88%)	23 (12%)	4	22
12	L	191/208 (92%)	174 (91%)	17 (9%)	9	34
13	M	171/171 (100%)	155 (91%)	16 (9%)	8	31
14	N	180/187 (96%)	162 (90%)	18 (10%)	7	29
15	O	147/150 (98%)	134 (91%)	13 (9%)	10	35
16	P	81/136 (60%)	69 (85%)	12 (15%)	3	17
17	Q	154/159 (97%)	134 (87%)	20 (13%)	4	22
18	R	107/109 (98%)	91 (85%)	16 (15%)	3	17
19	S	175/176 (99%)	150 (86%)	25 (14%)	3	19
20	T	160/162 (99%)	142 (89%)	18 (11%)	6	25
21	U	145/146 (99%)	130 (90%)	15 (10%)	7	28
22	V	150/151 (99%)	141 (94%)	9 (6%)	19	47
23	W	153/154 (99%)	139 (91%)	14 (9%)	9	32
24	X	156/156 (100%)	137 (88%)	19 (12%)	5	23
25	Y	136/137 (99%)	117 (86%)	19 (14%)	3	20
26	Z	87/107 (81%)	85 (98%)	2 (2%)	50	70
27	AA	104/105 (99%)	95 (91%)	9 (9%)	10	35
28	BA	54/129 (42%)	47 (87%)	7 (13%)	4	22
29	CA	105/118 (89%)	94 (90%)	11 (10%)	7	27
30	DA	109/110 (99%)	94 (86%)	15 (14%)	3	20
31	EA	115/116 (99%)	107 (93%)	8 (7%)	15	43
32	FA	118/119 (99%)	112 (95%)	6 (5%)	24	52
33	GA	46/47 (98%)	41 (89%)	5 (11%)	6	26
34	HA	81/88 (92%)	74 (91%)	7 (9%)	10	37
35	IA	96/97 (99%)	83 (86%)	13 (14%)	4	21
36	JA	109/111 (98%)	97 (89%)	12 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	83 (92%)	7 (8%)	12	39
38	LA	95/103 (92%)	84 (88%)	11 (12%)	5	24
39	MA	104/105 (99%)	96 (92%)	8 (8%)	13	40
40	NA	81/82 (99%)	69 (85%)	12 (15%)	3	17
41	OA	70/71 (99%)	62 (89%)	8 (11%)	5	25
42	PA	68/69 (99%)	63 (93%)	5 (7%)	13	41
43	QA	45/46 (98%)	42 (93%)	3 (7%)	16	44
44	RA	47/116 (40%)	43 (92%)	4 (8%)	10	37
45	SA	23/23 (100%)	19 (83%)	4 (17%)	2	12
46	TA	90/91 (99%)	82 (91%)	8 (9%)	9	34
47	UA	71/72 (99%)	66 (93%)	5 (7%)	15	43
48	VA	160/254 (63%)	143 (89%)	17 (11%)	6	27
49	WA	261/262 (100%)	237 (91%)	24 (9%)	9	32
50	XA	173/210 (82%)	151 (87%)	22 (13%)	4	22
51	YA	191/224 (85%)	173 (91%)	18 (9%)	8	31
52	ZA	176/205 (86%)	168 (96%)	8 (4%)	27	55
53	AB	182/195 (93%)	164 (90%)	18 (10%)	8	29
54	BB	221/222 (100%)	199 (90%)	22 (10%)	7	29
55	CB	173/191 (91%)	160 (92%)	13 (8%)	13	41
56	DB	193/201 (96%)	174 (90%)	19 (10%)	8	29
57	EB	165/170 (97%)	146 (88%)	19 (12%)	5	25
58	FB	150/161 (93%)	137 (91%)	13 (9%)	10	35
59	GB	158/166 (95%)	141 (89%)	17 (11%)	6	27
60	HB	89/98 (91%)	82 (92%)	7 (8%)	12	39
61	IB	136/137 (99%)	124 (91%)	12 (9%)	10	35
63	KB	127/128 (99%)	110 (87%)	17 (13%)	4	21
64	LB	96/105 (91%)	89 (93%)	7 (7%)	14	42
65	MB	103/118 (87%)	90 (87%)	13 (13%)	4	22
66	NB	117/119 (98%)	102 (87%)	15 (13%)	4	22
67	OB	82/124 (66%)	70 (85%)	12 (15%)	3	18
68	PB	128/129 (99%)	120 (94%)	8 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	QB	115/116 (99%)	104 (90%)	11 (10%)	8	30
70	RB	100/114 (88%)	91 (91%)	9 (9%)	9	34
71	SB	74/74 (100%)	64 (86%)	10 (14%)	4	21
72	TB	110/111 (99%)	102 (93%)	8 (7%)	14	42
73	UB	119/120 (99%)	107 (90%)	12 (10%)	7	29
74	VB	112/113 (99%)	101 (90%)	11 (10%)	8	29
75	WB	61/89 (68%)	53 (87%)	8 (13%)	4	21
76	XB	83/101 (82%)	76 (92%)	7 (8%)	11	37
77	YB	70/71 (99%)	66 (94%)	4 (6%)	20	49
78	ZB	56/60 (93%)	53 (95%)	3 (5%)	22	50
79	AC	47/49 (96%)	42 (89%)	5 (11%)	6	27
80	BC	51/54 (94%)	40 (78%)	11 (22%)	1	6
82	DC	699/714 (98%)	605 (87%)	94 (13%)	4	21
All	All	10235/11032 (93%)	9165 (90%)	1070 (10%)	10	27

5 of 1070 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
73	UB	144	ARG
77	YB	3	LEU
73	UB	127	VAL
82	DC	495	VAL
25	Y	19	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 287 such sidechains are listed below:

Mol	Chain	Res	Type
69	QB	138	GLN
82	DC	836	GLN
71	SB	21	ASN
79	AC	20	GLN
28	BA	32	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1755/1798 (97%)	378 (21%)	18 (1%)
2	B	3267/3396 (96%)	613 (18%)	27 (0%)
3	C	157/158 (99%)	31 (19%)	2 (1%)
4	D	120/121 (99%)	14 (11%)	0
83	EC	187/201 (93%)	77 (41%)	3 (1%)
All	All	5486/5674 (96%)	1113 (20%)	50 (0%)

5 of 1113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	C
1	A	25	C
1	A	26	A
1	A	34	G

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1307	G
2	B	2501	U
83	EC	6935	G
2	B	1329	U
2	B	1556	C

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	1.98	3 (21%)	14,28,30	2.17	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	CBW-CBI	4.96	1.61	1.53
82	DC	699	DDE	CAT-CE1	3.69	1.55	1.50
82	DC	699	DDE	OAG-CBI	2.03	1.27	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	DC	699	DDE	CAU-CBW-CBI	-5.47	100.34	111.20
82	DC	699	DDE	OAG-CBI-CBW	-3.66	115.85	120.49
82	DC	699	DDE	OAG-CBI-NAD	2.48	127.32	123.00
82	DC	699	DDE	CG-ND1-CE1	2.35	110.00	103.05
82	DC	699	DDE	CG-CD2-NE2	-2.22	104.67	109.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	DC	699	DDE	CAU-CAT-CE1-NE2
82	DC	699	DDE	OAG-CBI-CBW-CAU
82	DC	699	DDE	NAD-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

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
84	GDP	DC	901	85	24,30,30	1.67	4 (16%)	30,47,47	1.82	7 (23%)
86	SO1	DC	903	-	35,39,39	2.44	15 (42%)	39,64,64	1.94	8 (20%)

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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O56-C52	-4.48	1.30	1.41
86	DC	903	SO1	C12-C6	4.16	1.63	1.53
86	DC	903	SO1	C1-C5	4.15	1.60	1.50
86	DC	903	SO1	O17-C52	3.97	1.47	1.40
86	DC	903	SO1	C55-C56	3.84	1.59	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	DC	903	SO1	C12-C6-C10	-5.90	103.23	107.91
84	DC	901	GDP	PA-O3A-PB	-5.47	114.04	132.83
86	DC	903	SO1	C25-C22-C24	4.70	128.70	113.56
84	DC	901	GDP	C8-N7-C5	3.58	109.81	102.99
86	DC	903	SO1	C10-C6-C2	3.44	108.29	104.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

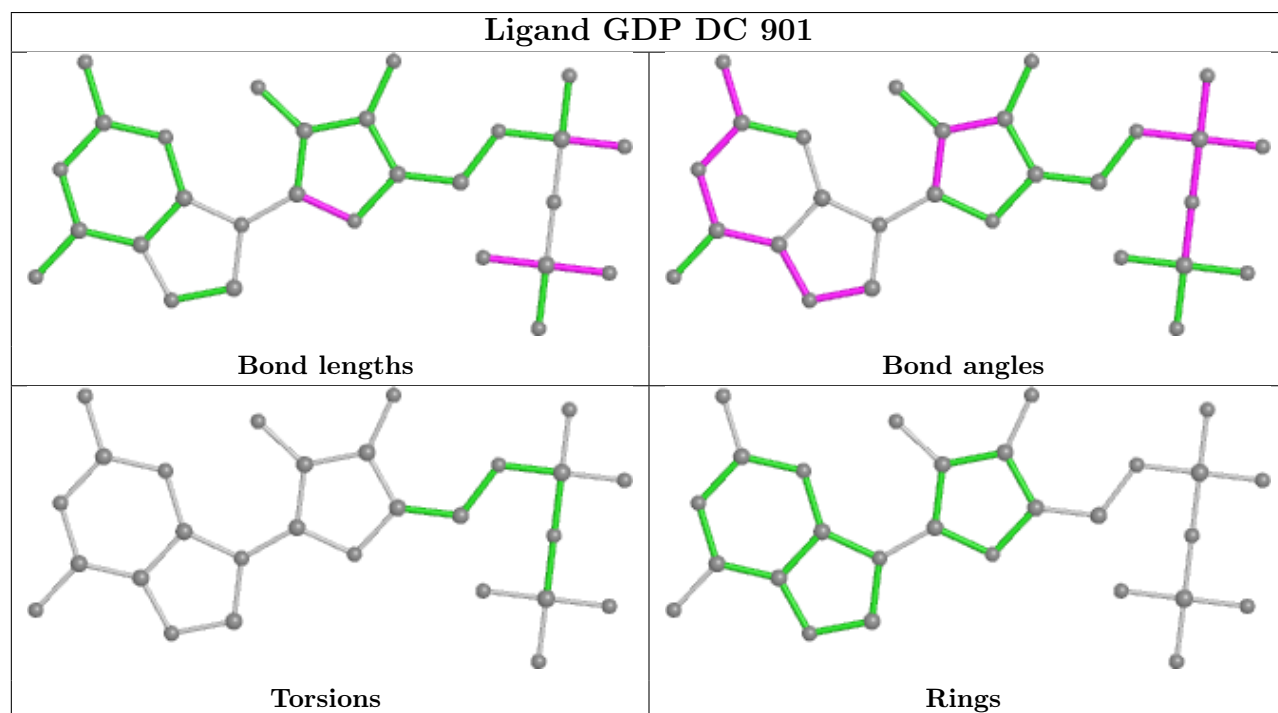
Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15

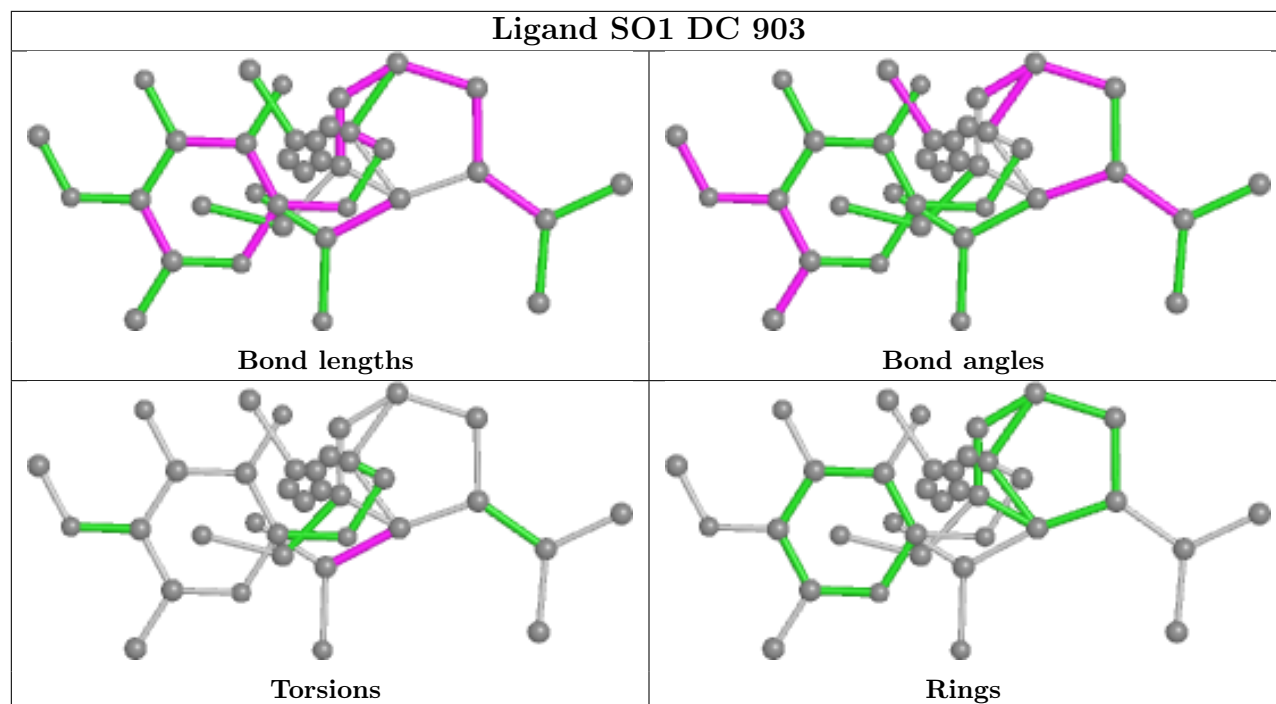
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	DC	901	GDP	4	0
86	DC	903	SO1	3	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.

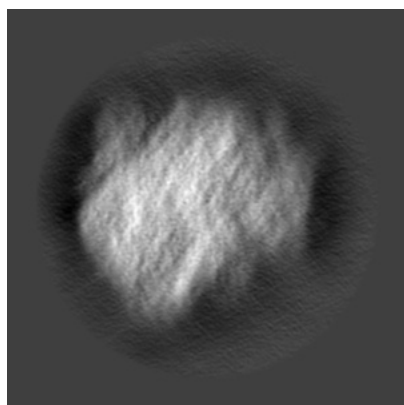
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6646. These allow visual inspection of the internal detail of the map and identification of artifacts.

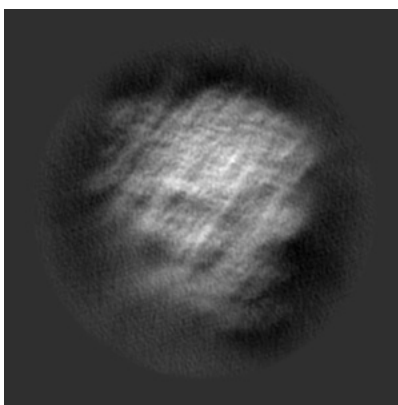
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

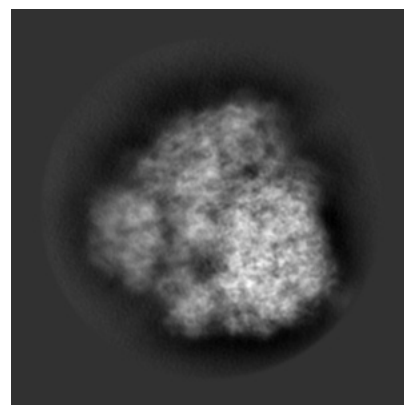
6.1.1 Primary map



X



Y

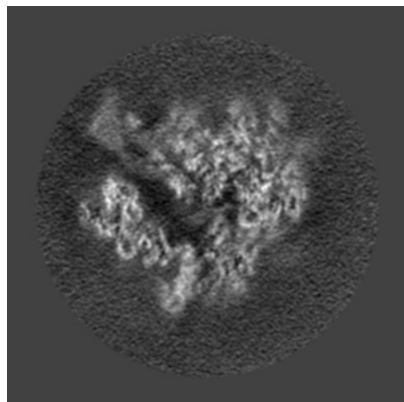


Z

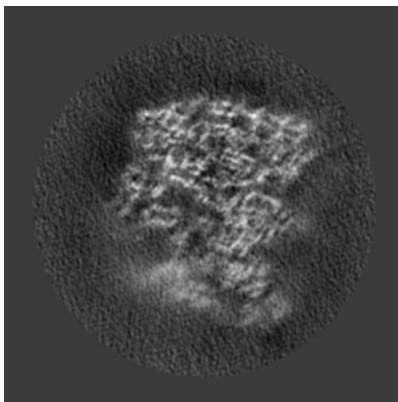
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

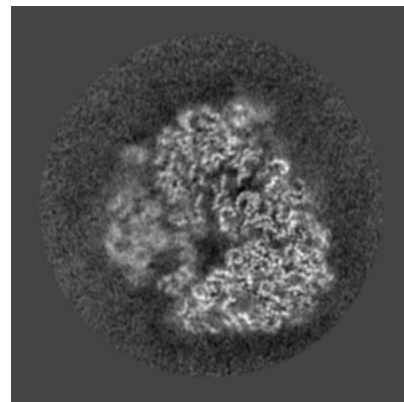
6.2.1 Primary map



X Index: 256



Y Index: 256

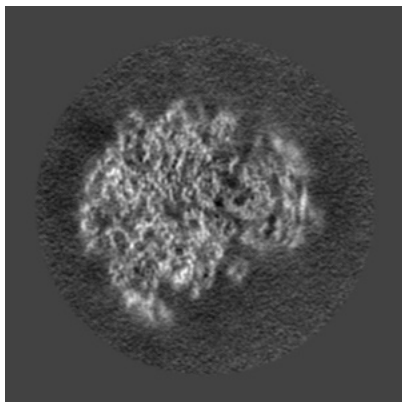


Z Index: 256

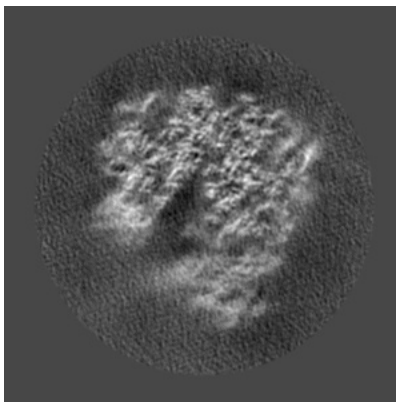
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

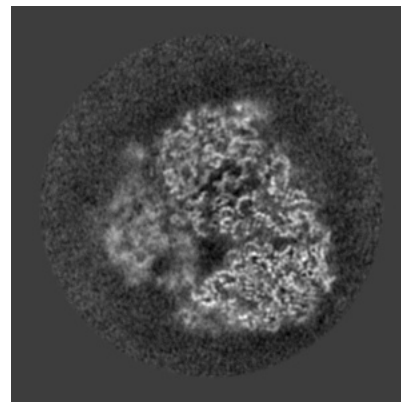
6.3.1 Primary map



X Index: 290



Y Index: 222

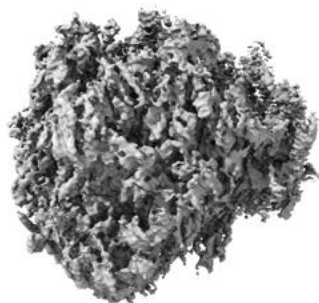


Z Index: 261

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

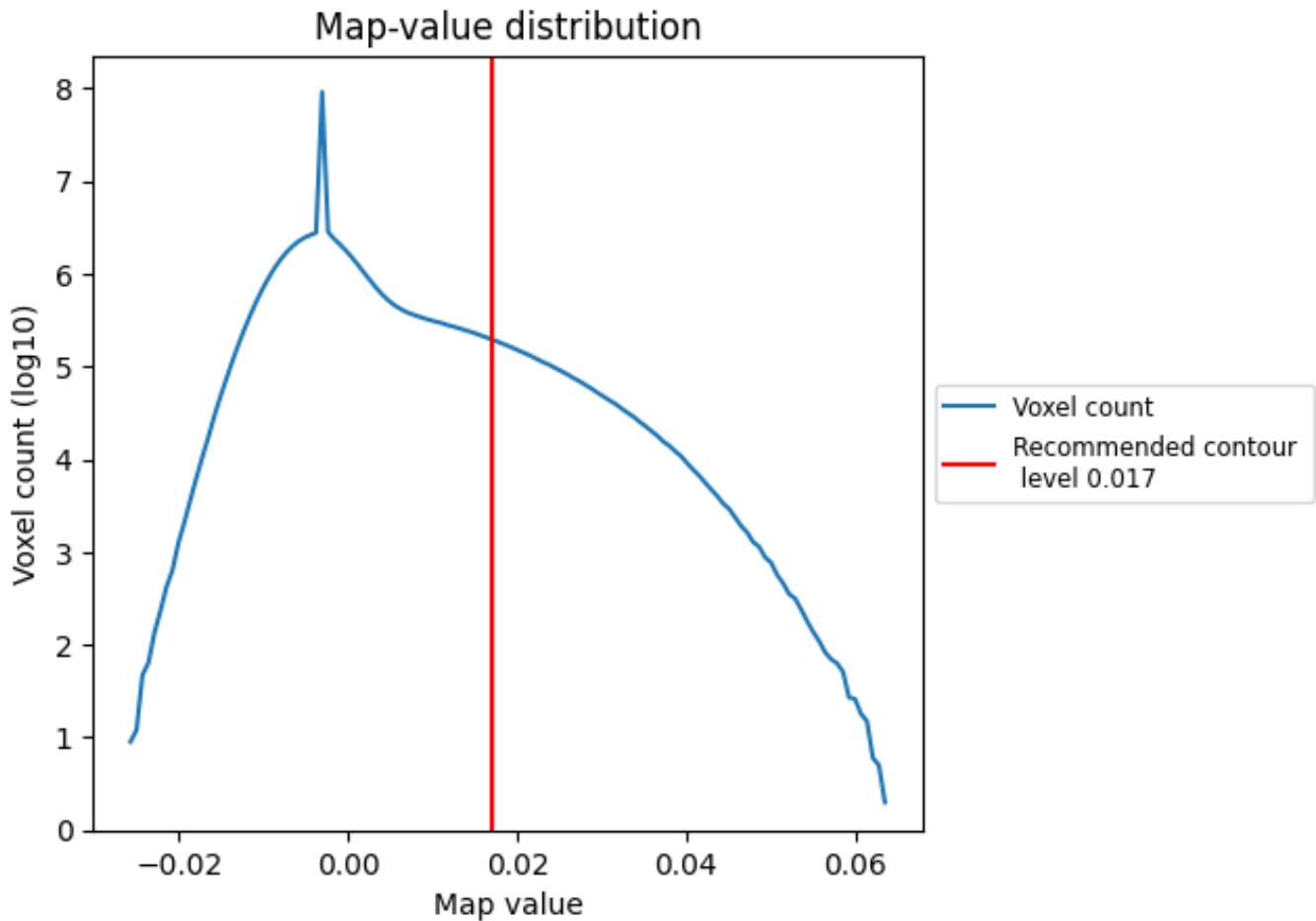
6.5 Mask visualisation

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

7 Map analysis [i](#)

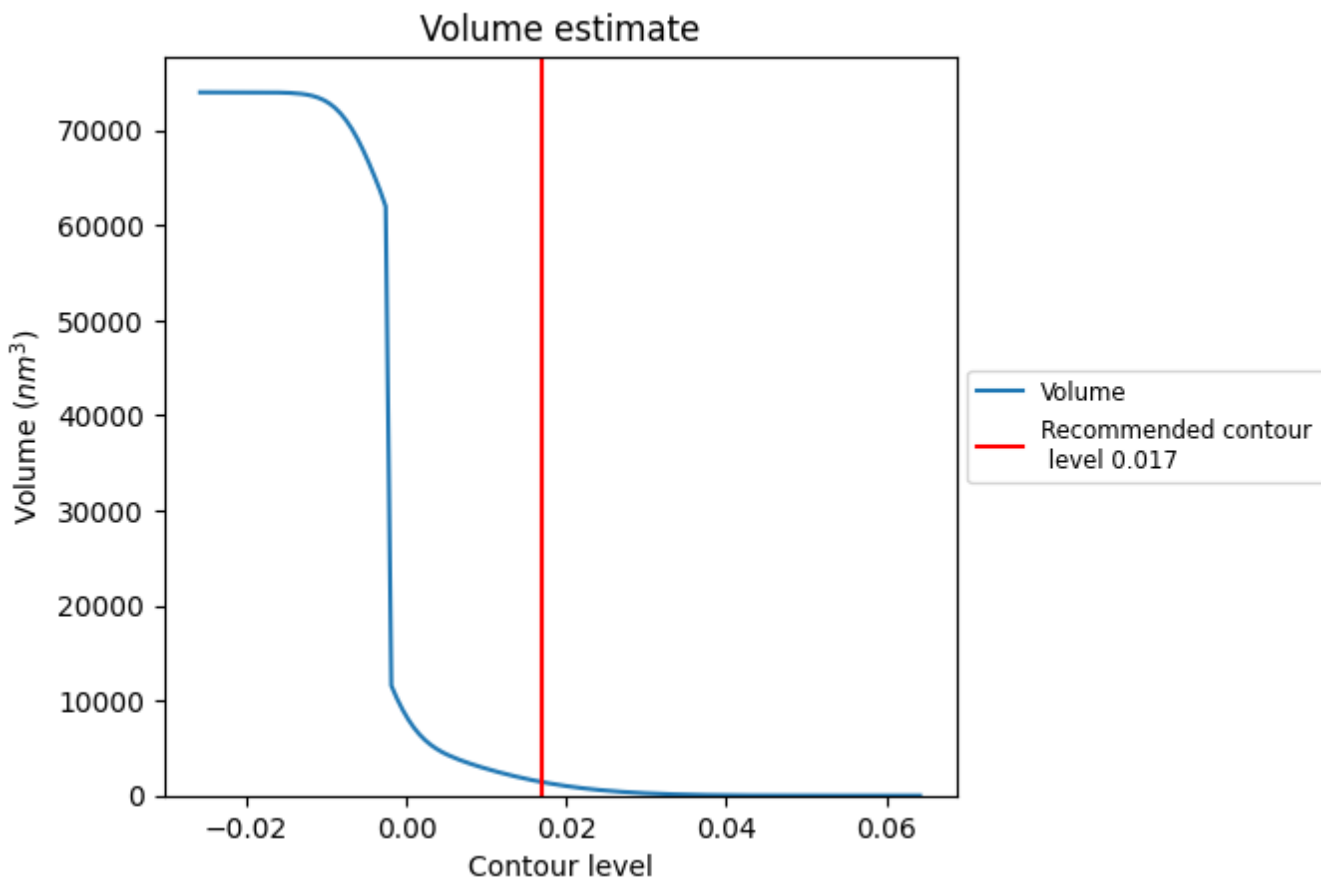
This section contains the results of statistical analysis of the map.

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.

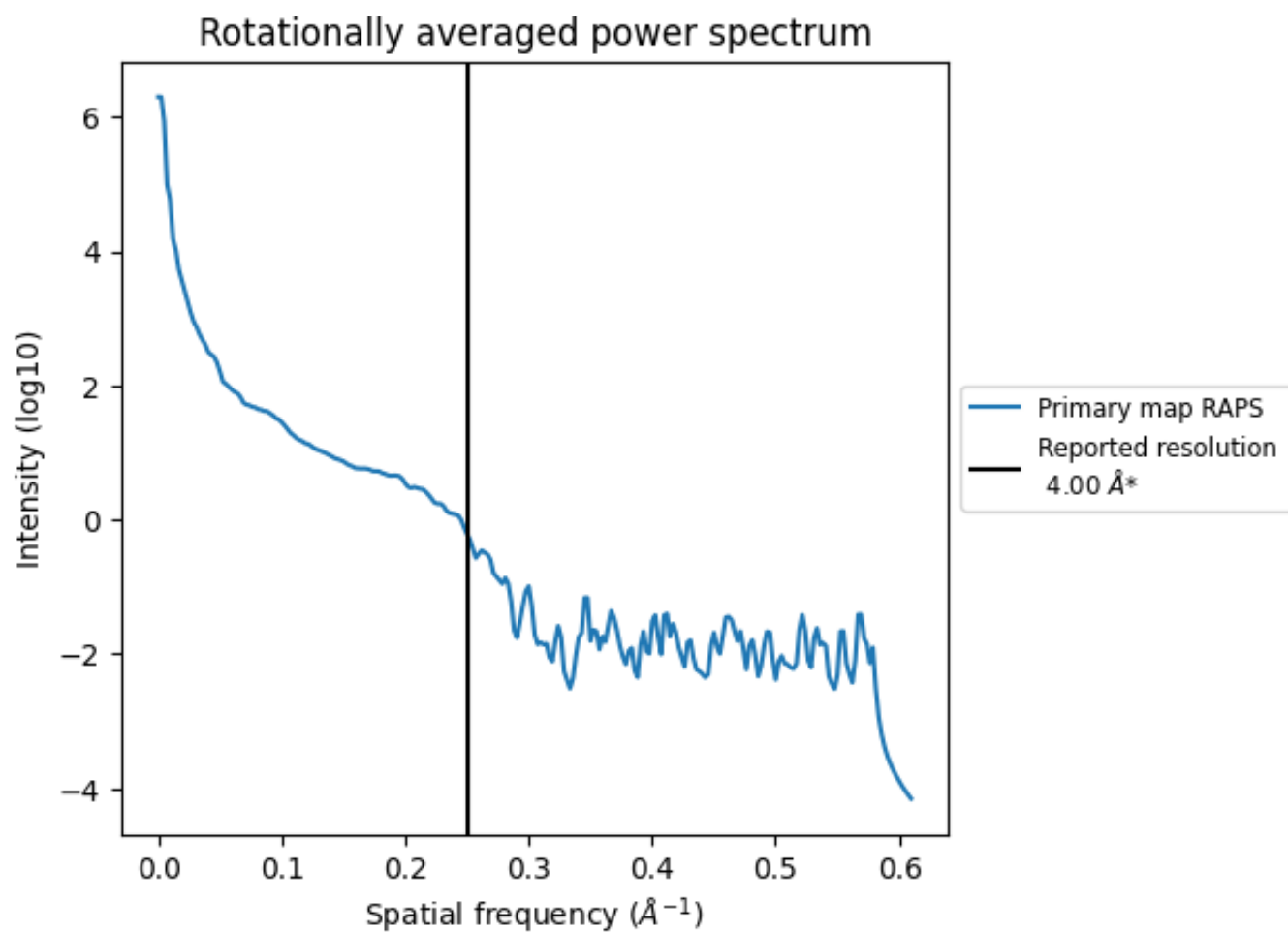
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1421 nm³; this corresponds to an approximate mass of 1283 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 0.250\AA^{-1}

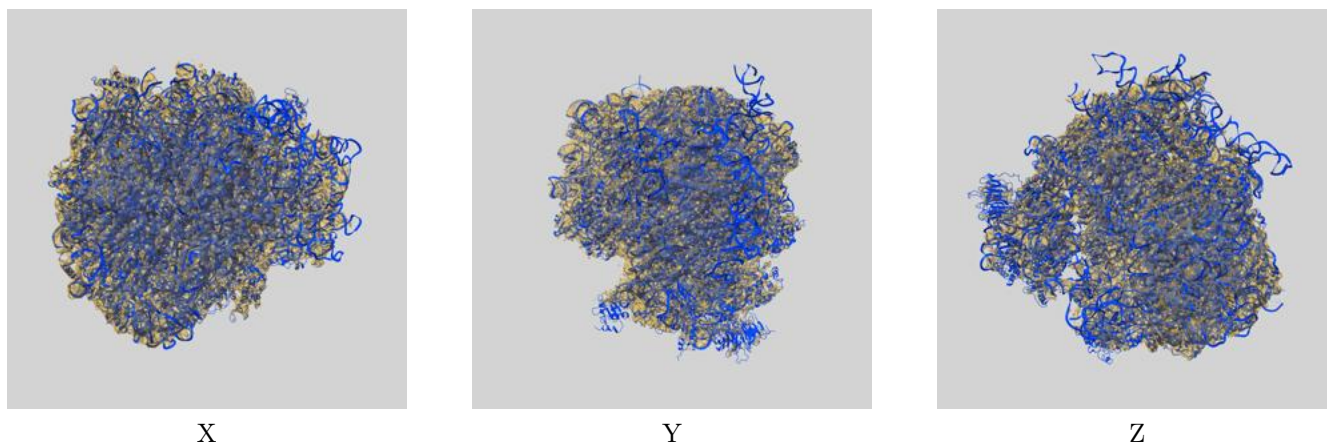
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

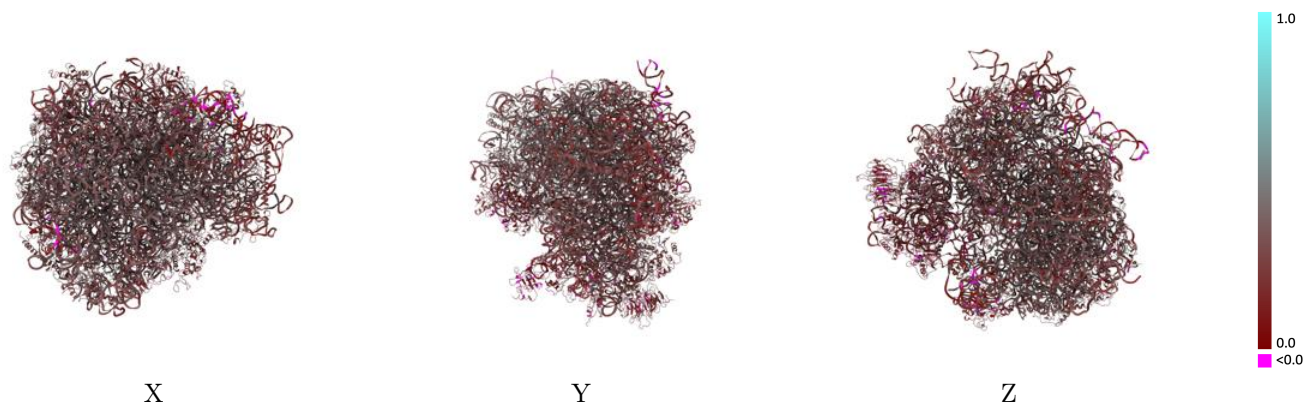
This section contains information regarding the fit between EMDB map EMD-6646 and PDB model 5JUT. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



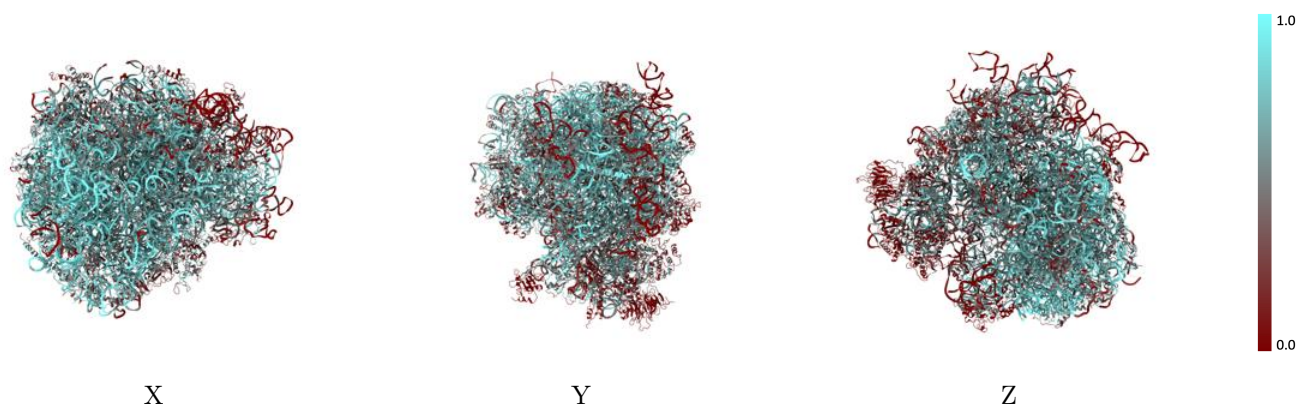
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



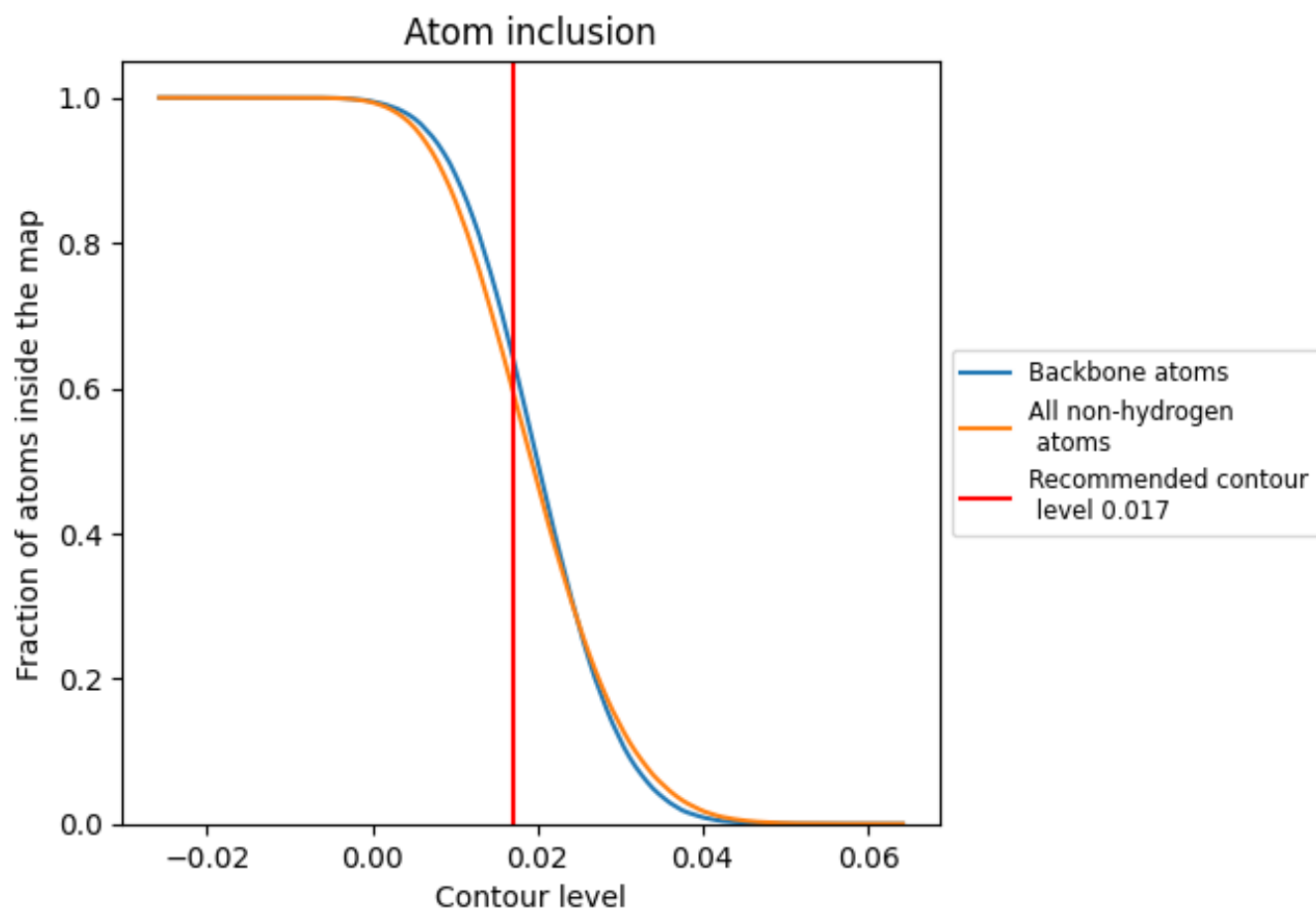
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 60% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5970	 0.3060
A	 0.6388	 0.2830
AA	 0.4571	 0.3800
AB	 0.2161	 0.2380
AC	 0.3012	 0.2220
B	 0.7888	 0.3290
BA	 0.5578	 0.3690
BB	 0.6074	 0.3230
BC	 0.2658	 0.2870
C	 0.7865	 0.3270
CA	 0.3041	 0.3340
CB	 0.1838	 0.2300
CC	 0.0106	 0.1740
D	 0.8686	 0.3200
DA	 0.6319	 0.3180
DB	 0.3501	 0.3030
DC	 0.4275	 0.2750
E	 0.0596	 0.2200
EA	 0.3993	 0.2820
EB	 0.1921	 0.2860
EC	 0.2650	 0.2170
F	 0.6076	 0.3450
FA	 0.6973	 0.3680
FB	 0.4161	 0.3150
G	 0.5716	 0.3680
GA	 0.6203	 0.3490
GB	 0.5430	 0.2960
H	 0.6328	 0.3620
HA	 0.6881	 0.3020
HB	 0.5650	 0.2080
I	 0.5664	 0.2980
IA	 0.6169	 0.3560
IB	 0.3690	 0.3360
J	 0.4764	 0.3230
JA	 0.7223	 0.3790

















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Chain	Atom inclusion	Q-score
JB	 0.0484	 0.1360
K	 0.5433	 0.3350
KA	 0.4623	 0.3680
KB	 0.4230	 0.2980
L	 0.4149	 0.2850
LA	 0.5176	 0.3080
LB	 0.4518	 0.3190
M	 0.4755	 0.3330
MA	 0.4322	 0.3040
MB	 0.1595	 0.1660
N	 0.5544	 0.3310
NA	 0.5965	 0.3350
NB	 0.1694	 0.2170
O	 0.5251	 0.2950
OA	 0.6006	 0.3360
OB	 0.1890	 0.2680
P	 0.2370	 0.1390
PA	 0.1267	 0.2740
PB	 0.1264	 0.1960
Q	 0.6960	 0.3410
QA	 0.6635	 0.3540
QB	 0.1728	 0.2100
R	 0.5385	 0.3130
RA	 0.6856	 0.3510
RB	 0.1605	 0.2210
S	 0.5324	 0.3200
SA	 0.2911	 0.3570
SB	 0.3880	 0.3130
T	 0.5452	 0.3480
TA	 0.7756	 0.3710
TB	 0.3714	 0.3170
U	 0.6521	 0.3510
UA	 0.5537	 0.3260
UB	 0.2886	 0.3150
V	 0.7264	 0.3680
VA	 0.2860	 0.2080
VB	 0.3225	 0.2910
W	 0.4568	 0.3020
WA	 0.0523	 0.2330
WB	 0.1005	 0.1970
X	 0.5502	 0.3390
XA	 0.2594	 0.2870

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Chain	Atom inclusion	Q-score
XB	 0.5156	 0.3390
Y	 0.5907	 0.3590
YA	 0.3955	 0.2850
YB	 0.4850	 0.3020
Z	 0.3696	 0.3140
ZA	 0.4353	 0.3260
ZB	 0.3808	 0.2640