



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 02:02 AM UTC

PDB ID : 5JUT / pdb_00005jut
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:

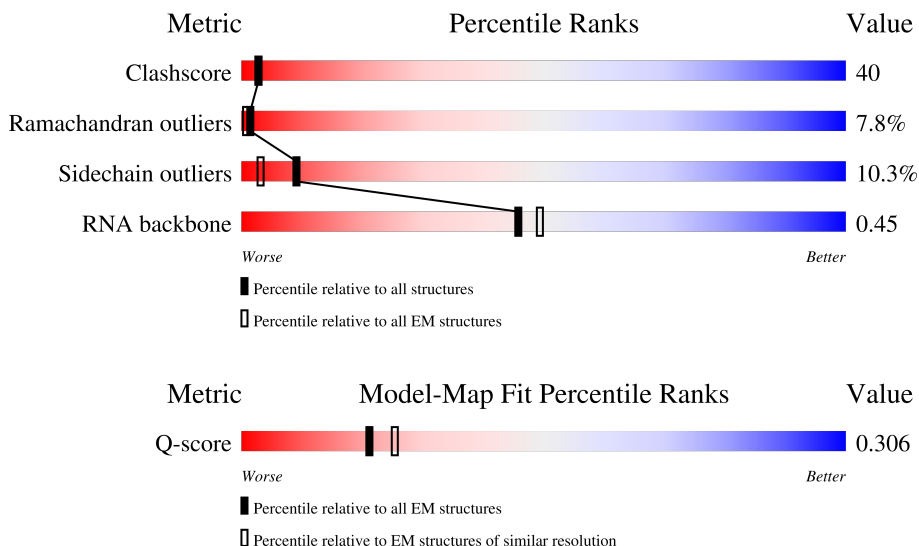
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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.



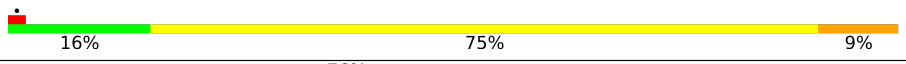

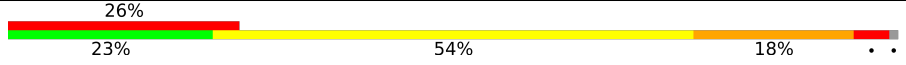
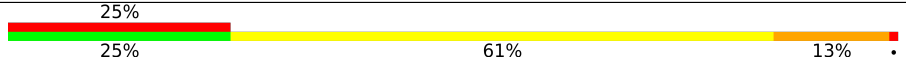
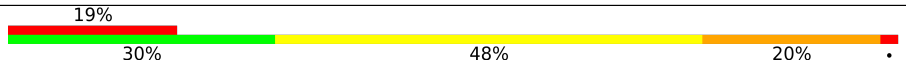
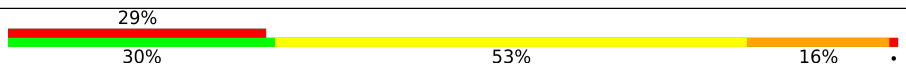
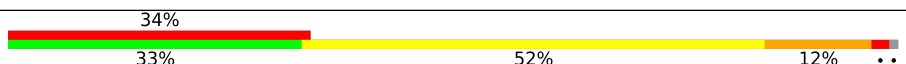
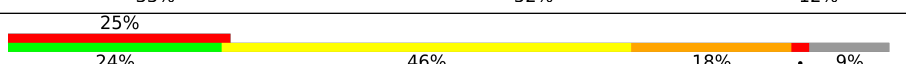
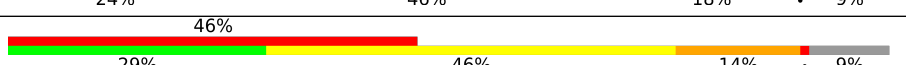
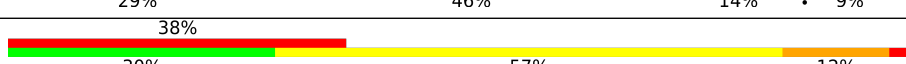
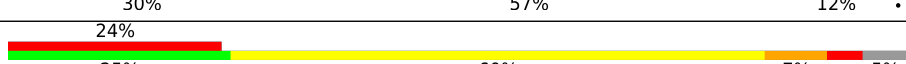
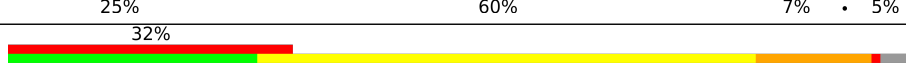

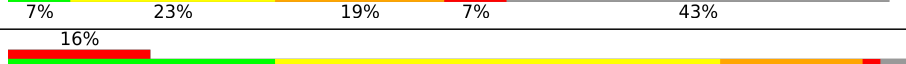
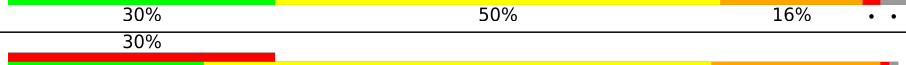
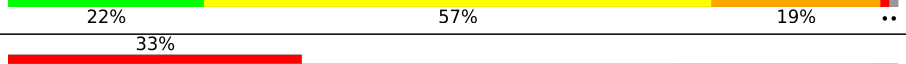
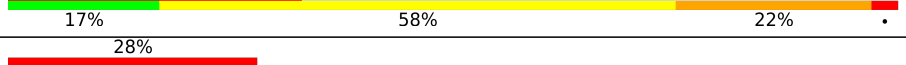
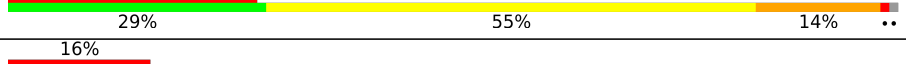
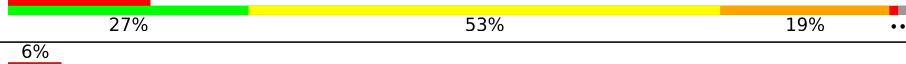
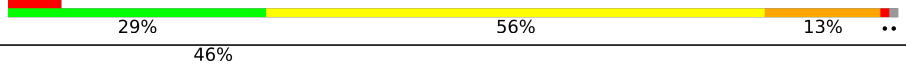
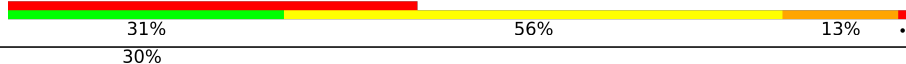
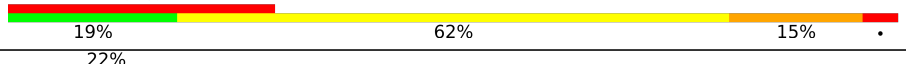
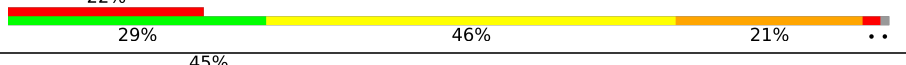

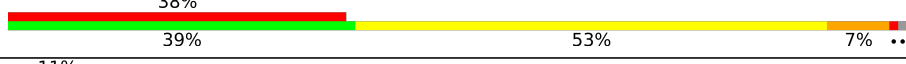
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	

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Mol	Chain	Length	Quality of chain
4	D	121	
5	E	217	
6	F	254	
7	G	387	
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	

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Mol	Chain	Length	Quality of chain
29	CA	142	54% 20% 49% 14% 15%
30	DA	127	17% 28% 57% 11%
31	EA	136	51% 28% 57% 12%
32	FA	149	15% 28% 54% 16%
33	GA	59	29% 42% 37% 17%
34	HA	105	14% 18% 64% 10% 8%
35	IA	113	17% 35% 48% 12%
36	JA	130	12% 37% 49% 11%
37	KA	107	43% 23% 64% 11%
38	LA	121	31% 29% 45% 15% 7%
39	MA	120	43% 27% 57% 15%
40	NA	100	27% 29% 53% 15%
41	OA	88	28% 33% 55% 9%
42	PA	78	87% 38% 51% 9%
43	QA	51	18% 24% 55% 18%
44	RA	128	20% 16% 59%
45	SA	25	76% 24% 52% 24%
46	TA	106	31% 28% 48% 19%
47	UA	92	27% 27% 60% 11%
48	VA	312	42% 13% 23% 21% 39%
49	WA	319	96% 33% 60% 7%
50	XA	252	60% 23% 46% 12% 18%
51	YA	255	48% 25% 49% 10% 16%
52	ZA	254	37% 29% 46% 10% 15%
53	AB	240	71% 41% 42% 10% 7%

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Mol	Chain	Length	Quality of chain
54	BB	261	
55	CB	225	
56	DB	236	
57	EB	190	
58	FB	200	
59	GB	197	
60	HB	105	
61	IB	156	
62	JB	143	
63	KB	151	
64	LB	137	
65	MB	142	
66	NB	143	
67	OB	136	
68	PB	146	
69	QB	144	
70	RB	121	
71	SB	87	
72	TB	130	
73	UB	145	
74	VB	135	
75	WB	108	
76	XB	119	
77	YB	82	
78	ZB	67	

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Mol	Chain	Length	Quality of chain
79	AC	56	
80	BC	63	
81	CC	152	
82	DC	842	
83	EC	201	

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
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	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		

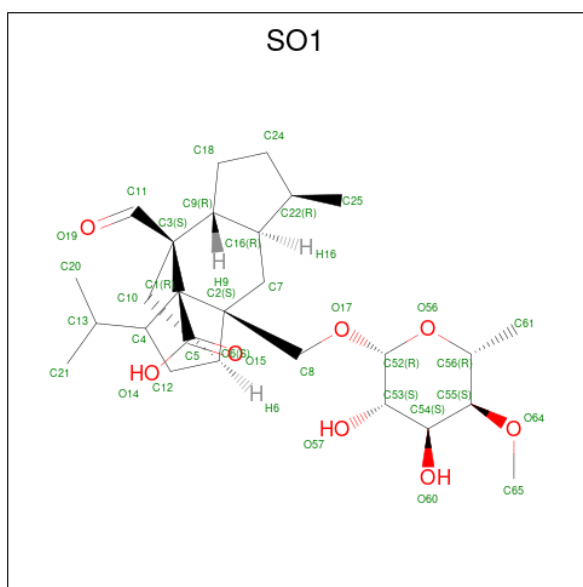
- Molecule 82 is a protein called yeast eEF2.

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 (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



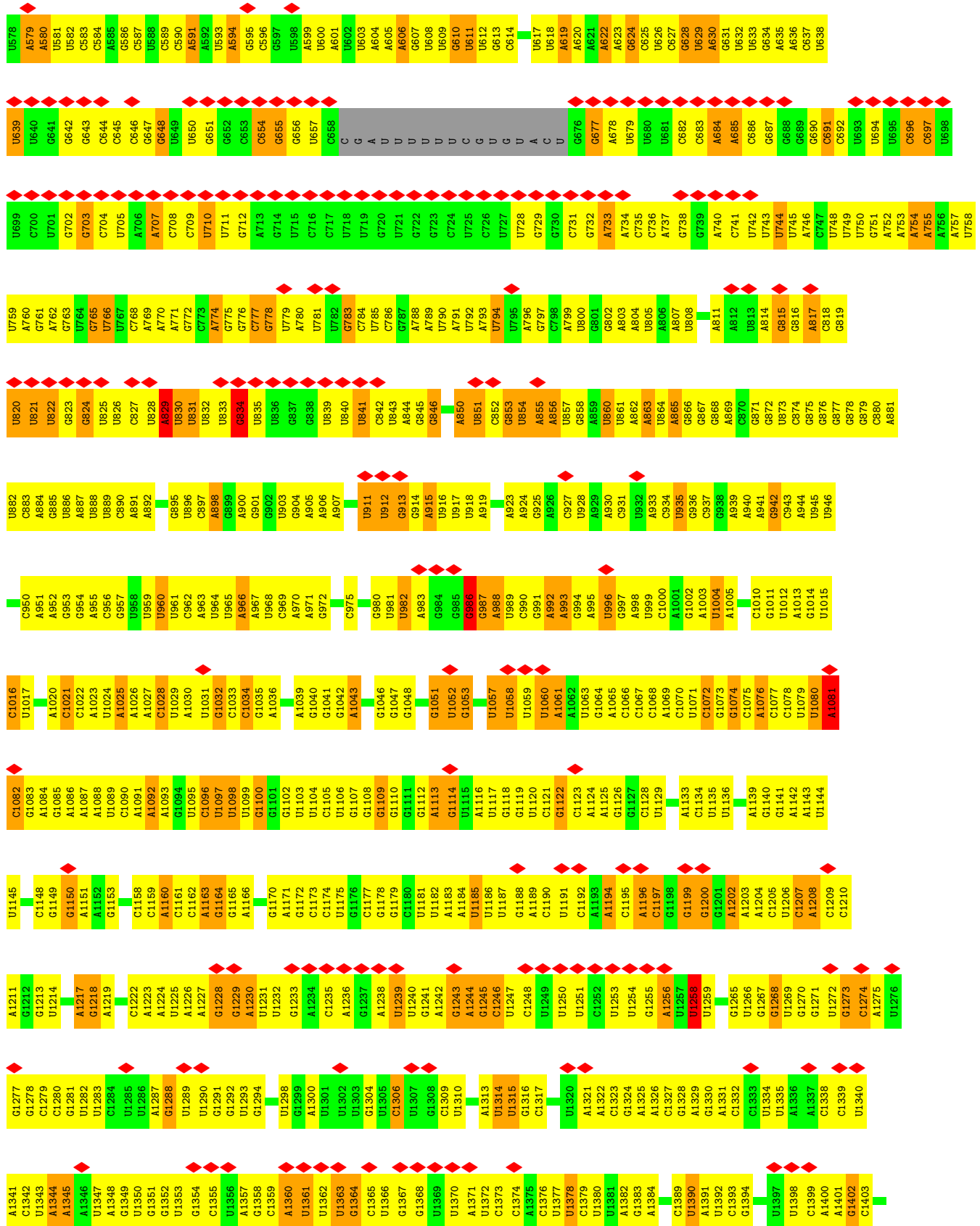
Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

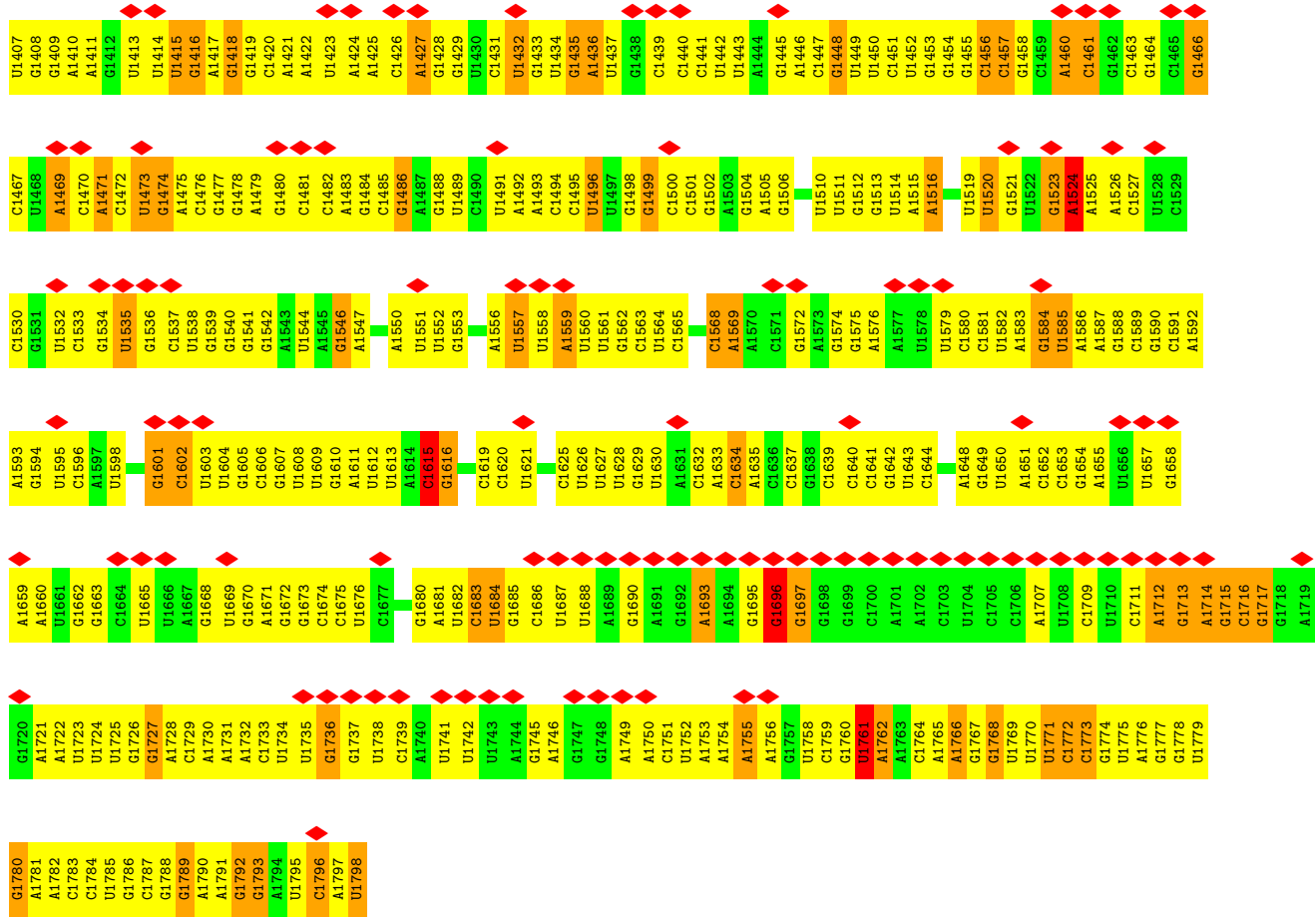
3 Residue-property plots

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.

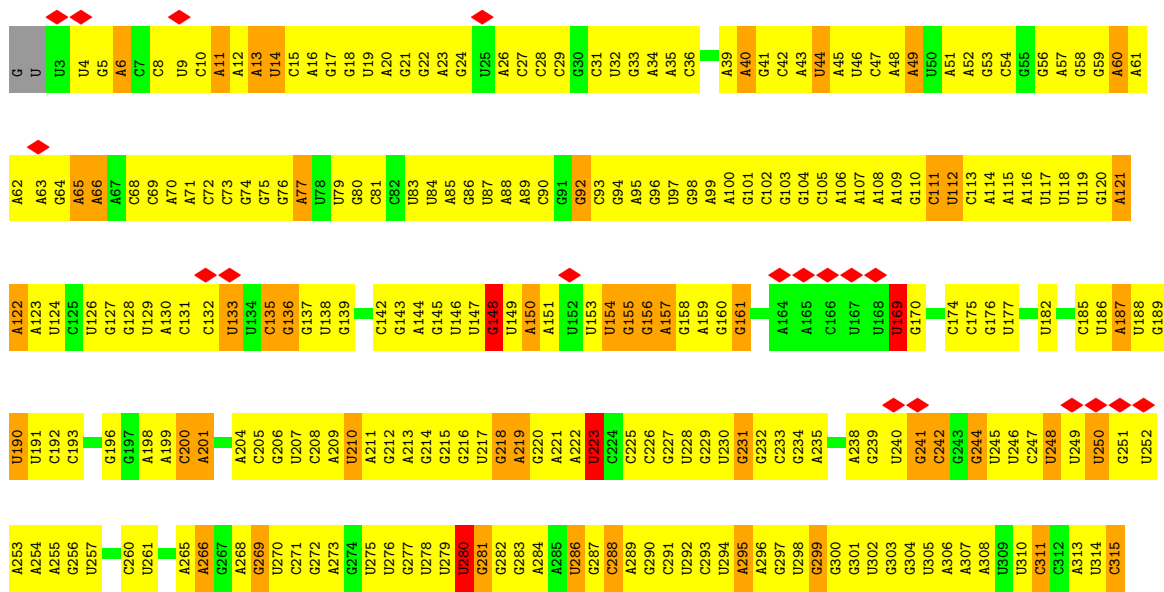
- Molecule 1: 18S ribosomal RNA

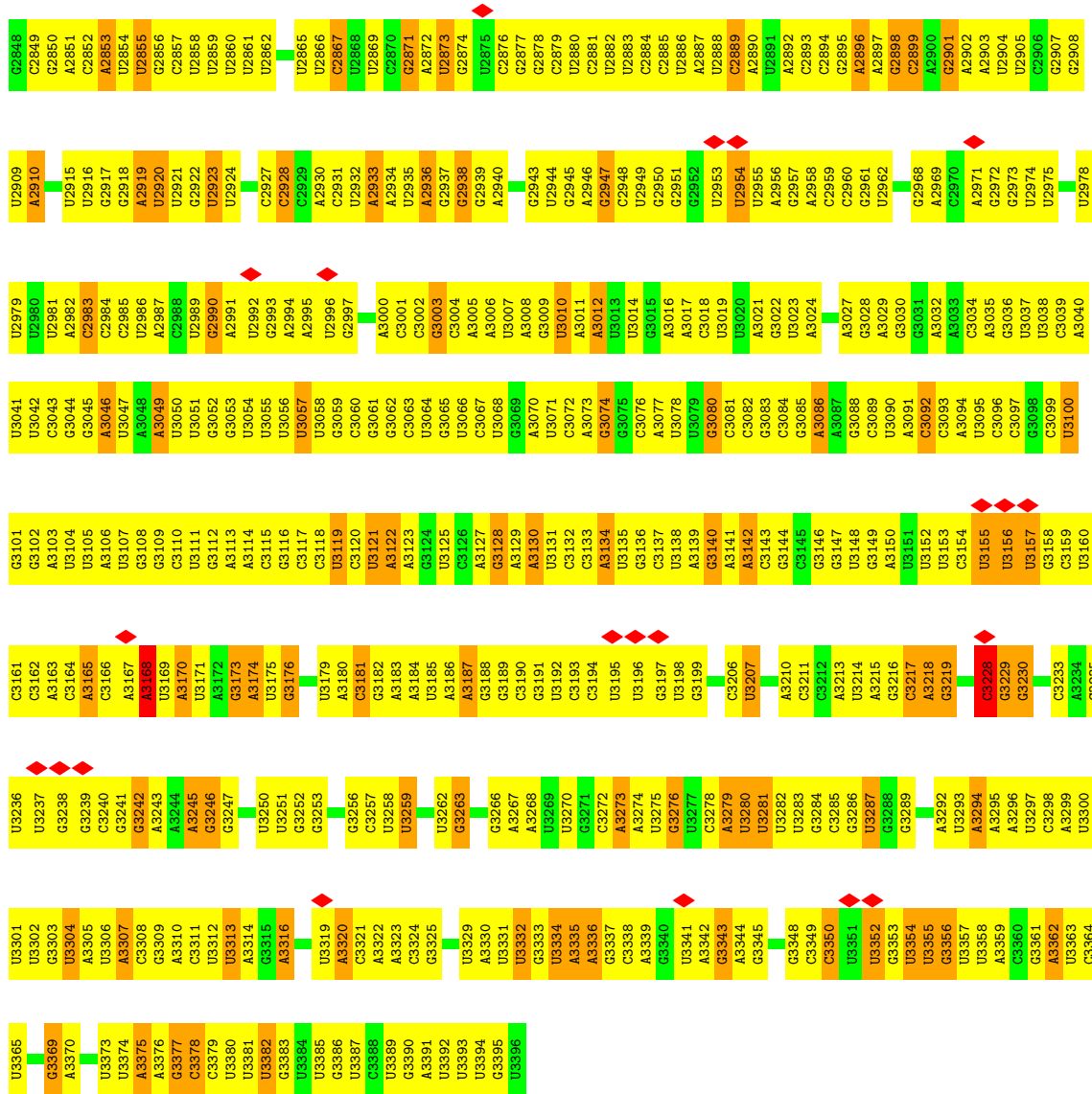




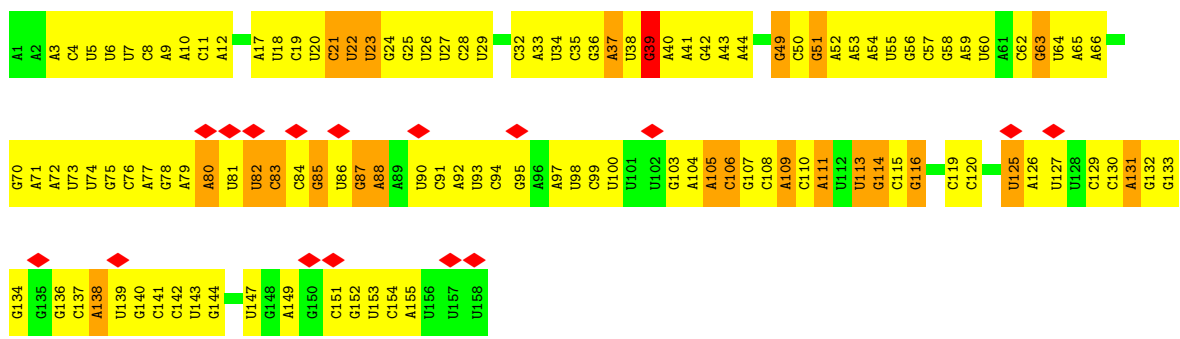


• Molecule 2: 25S ribosomal RNA



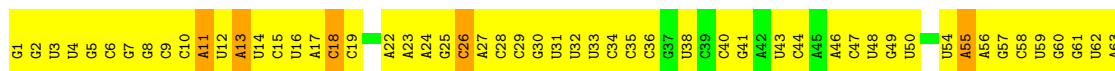


• Molecule 3: 5.8S ribosomal RNA

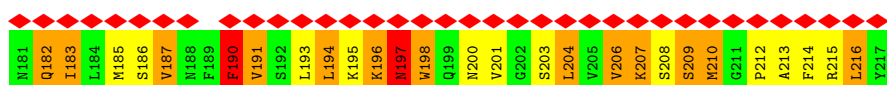
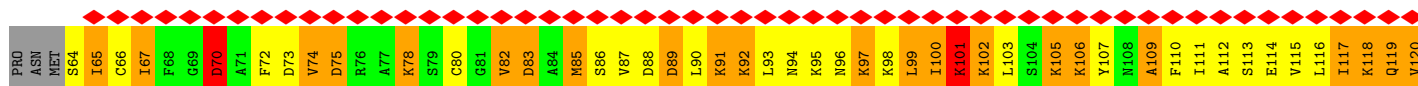
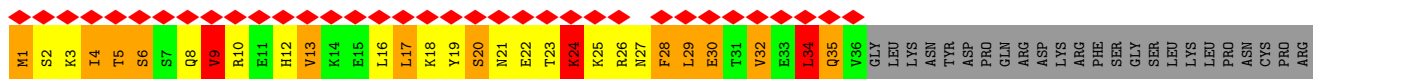
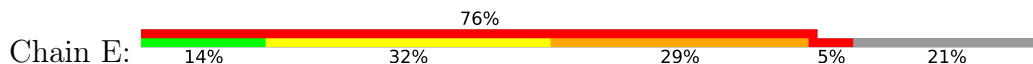


• Molecule 4: 5S ribosomal RNA

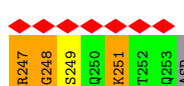
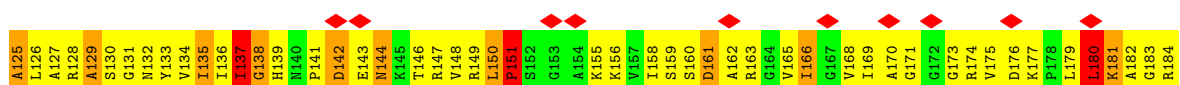
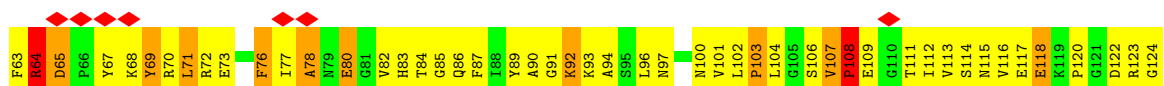




• Molecule 5: uL1 (yeast L1)

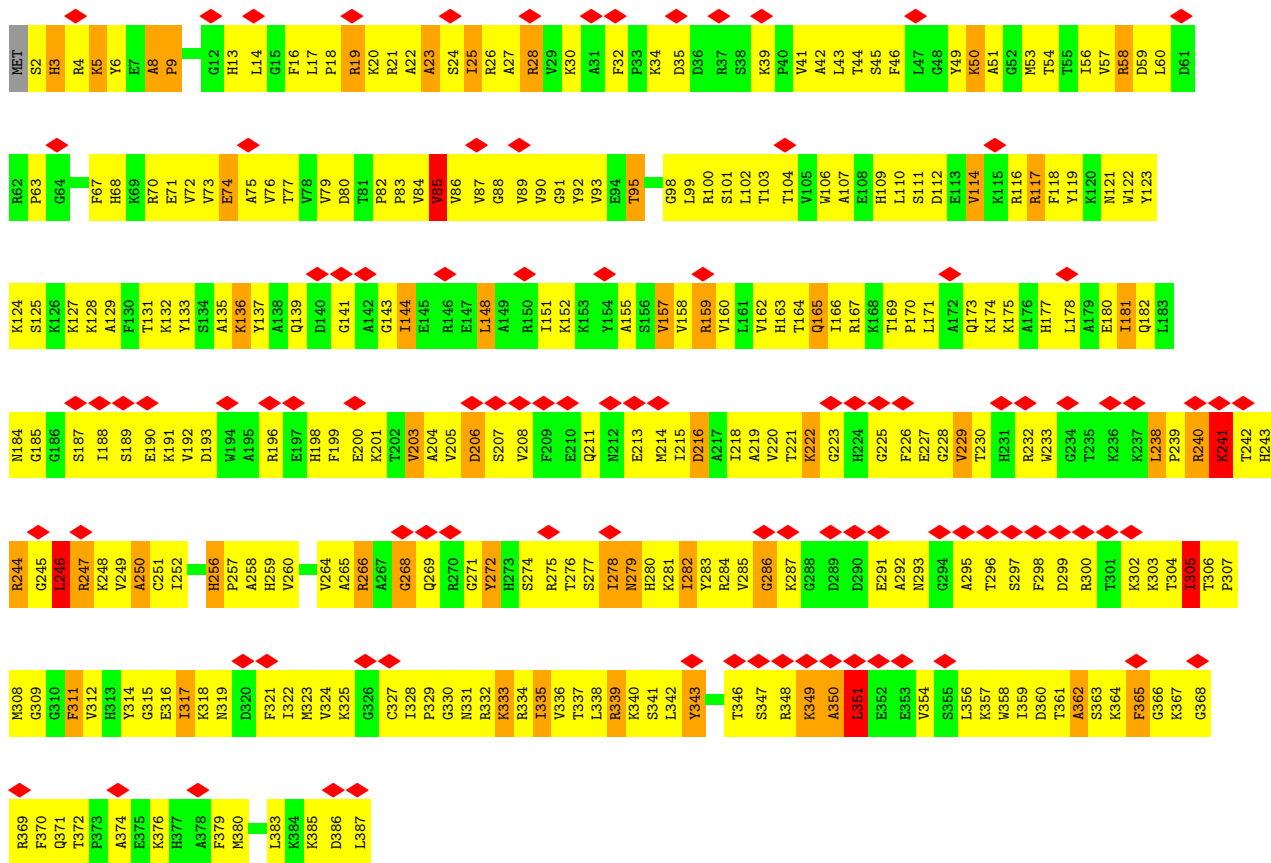


• Molecule 6: uL2 (yeast L2)

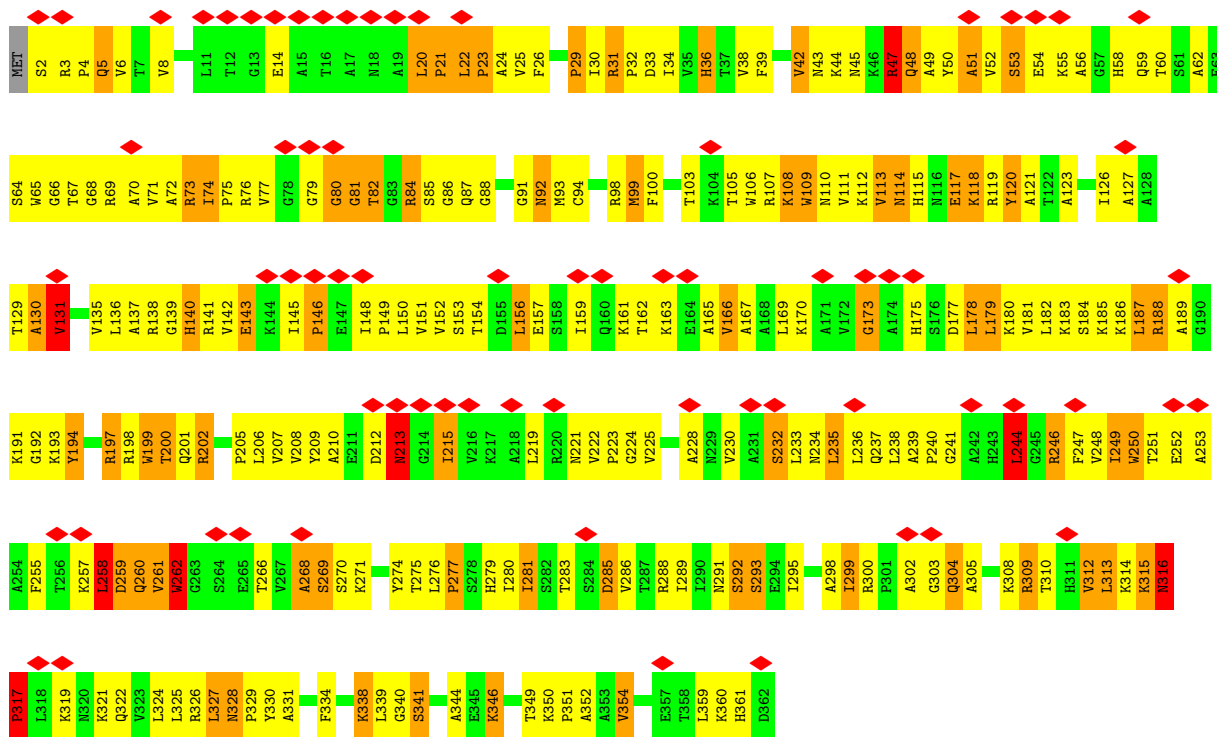


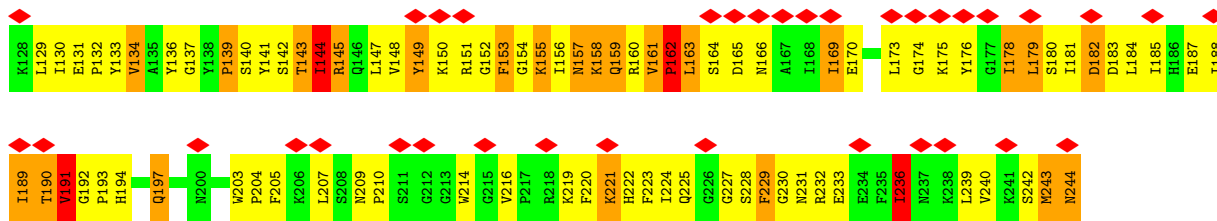
• Molecule 7: uL3 (yeast L3)



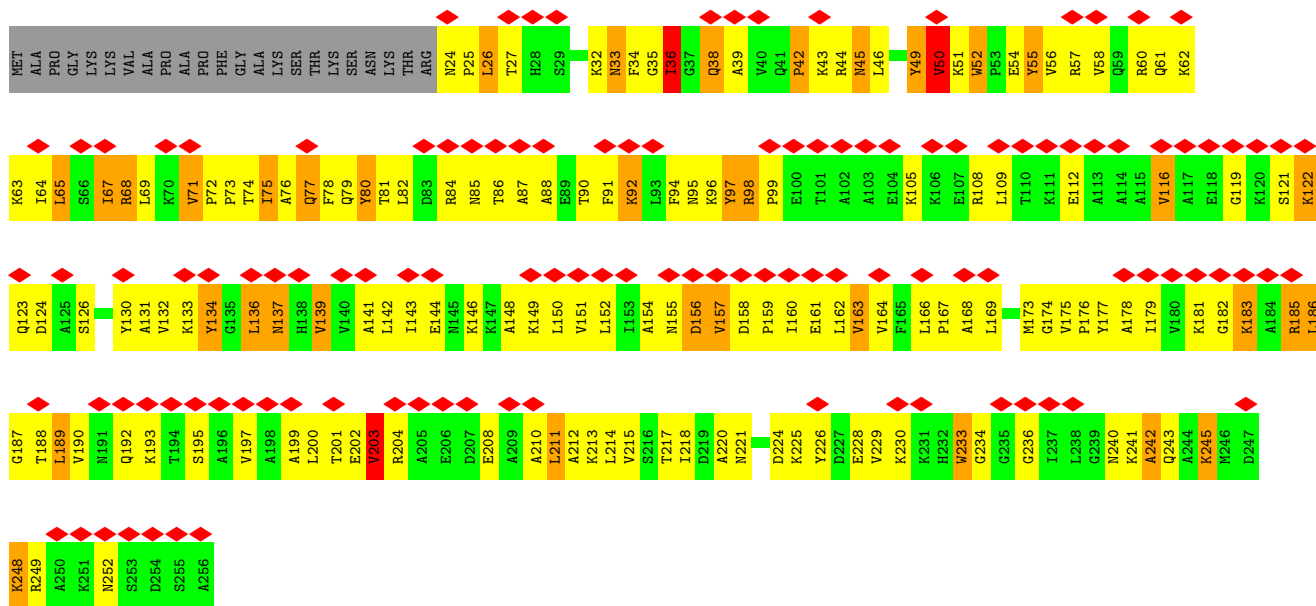


• Molecule 8: uL4 (yeast L4)

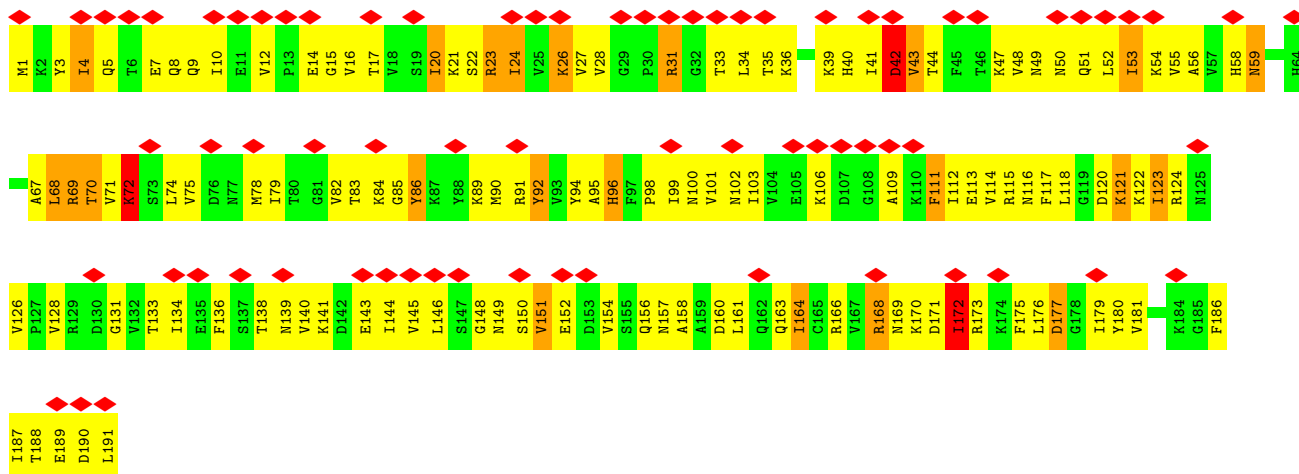




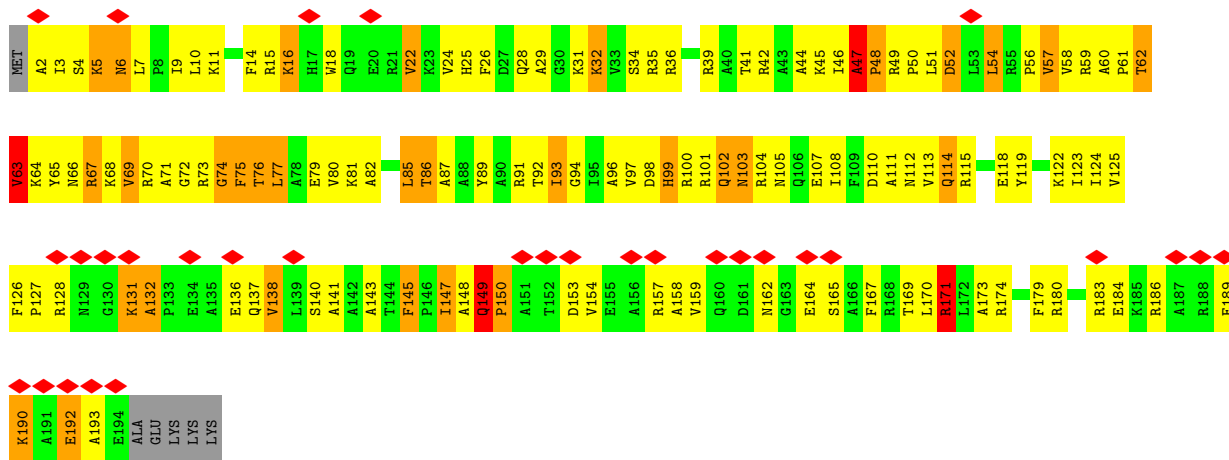
• Molecule 12: eL8 (yeast L8)



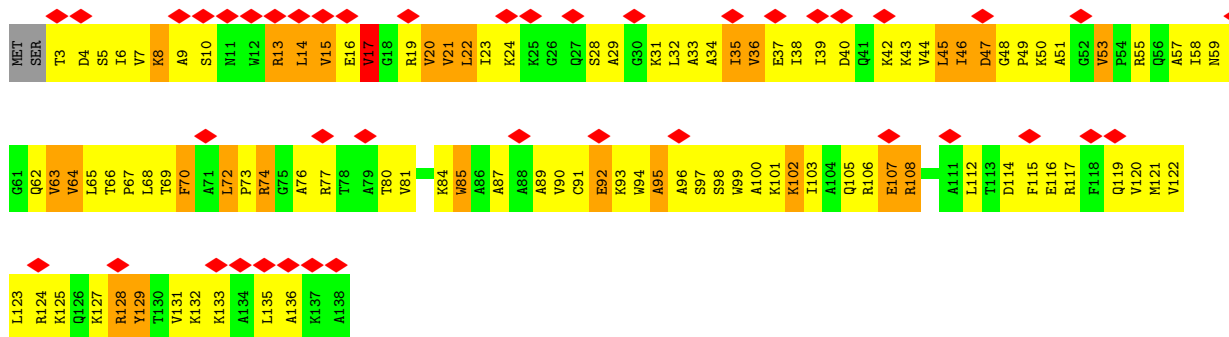
• Molecule 13: uL6 (yeast L9)



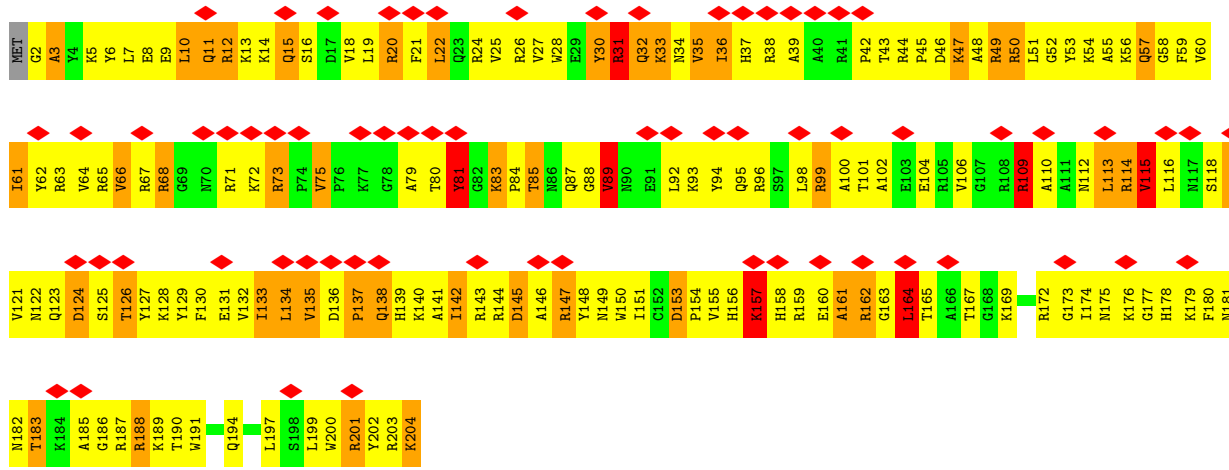
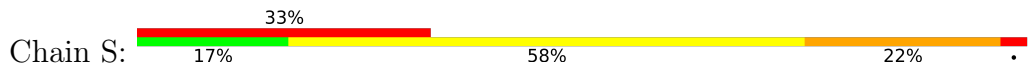
• Molecule 14: uL16 (yeast L10)



• Molecule 18: eL14 (yeast L14)

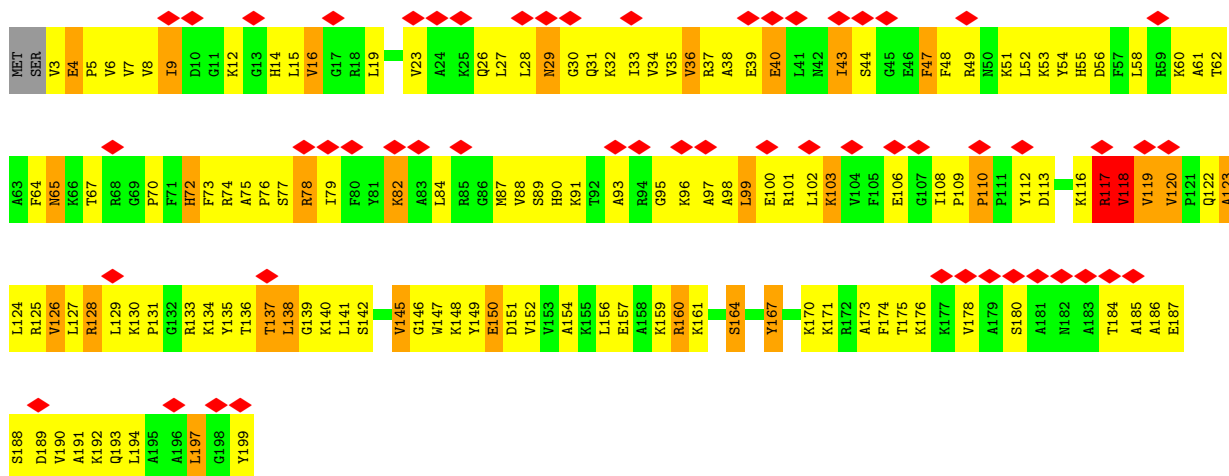


• Molecule 19: eL15 (yeast L15)

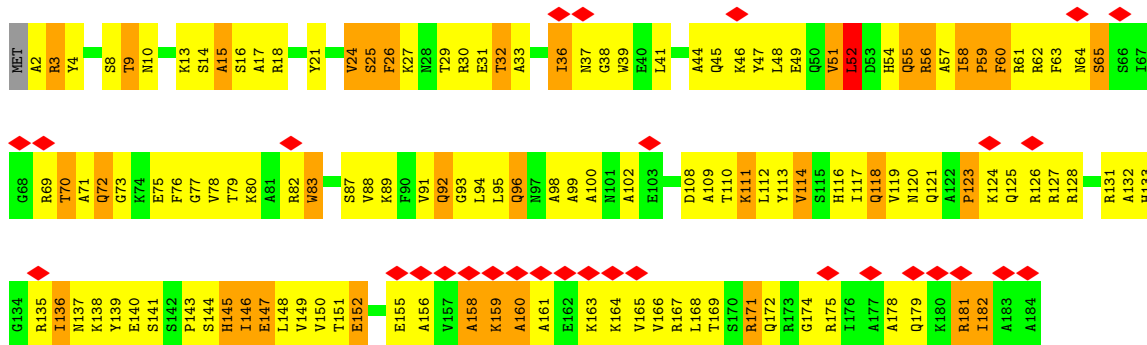


• Molecule 20: uL13 (yeast L16)

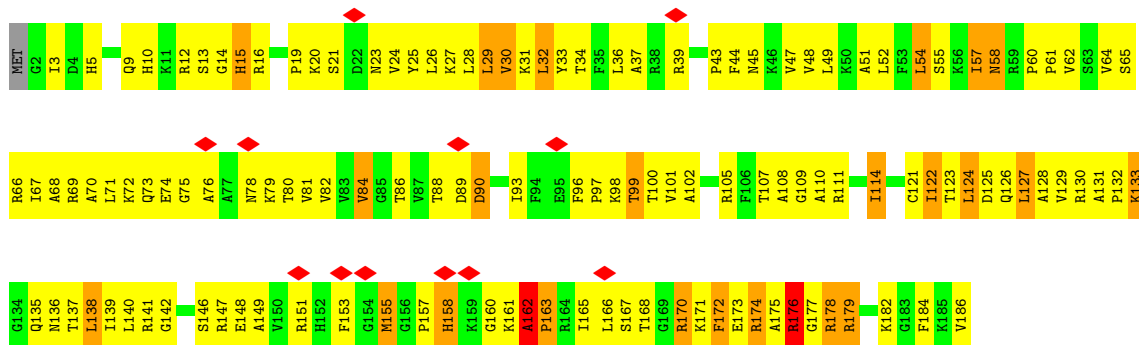




• Molecule 21: uL22 (yeast L17)

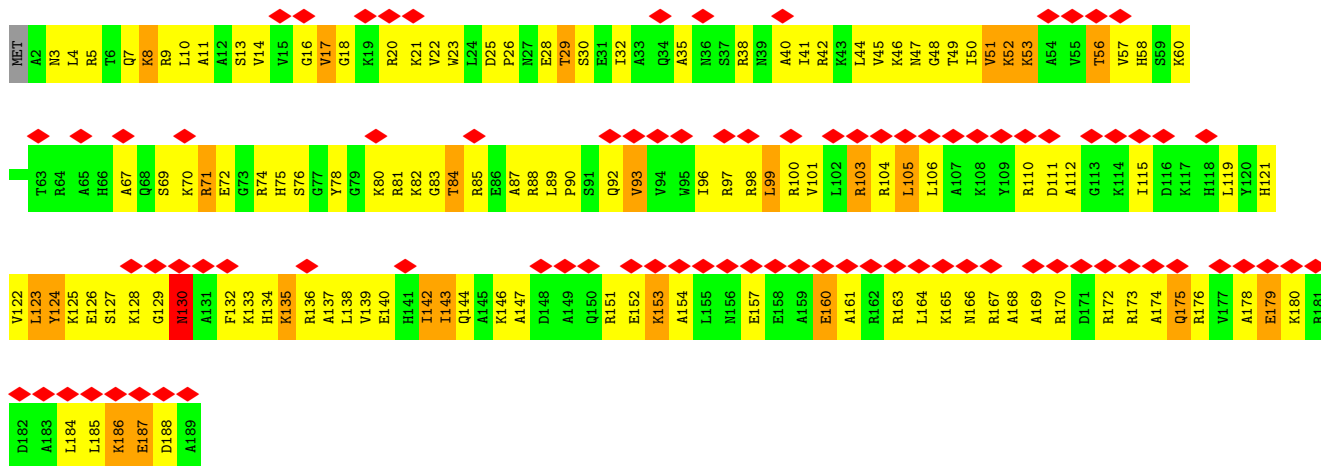


• Molecule 22: eL18 (yeast L18)

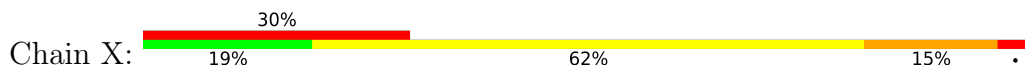


• Molecule 23: eL19 (yeast L19)

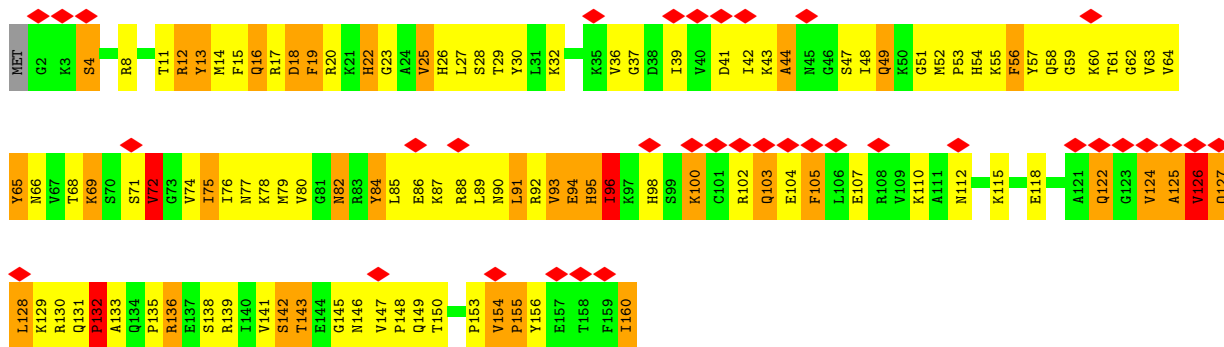




• Molecule 24: eL20 (yeast L20)

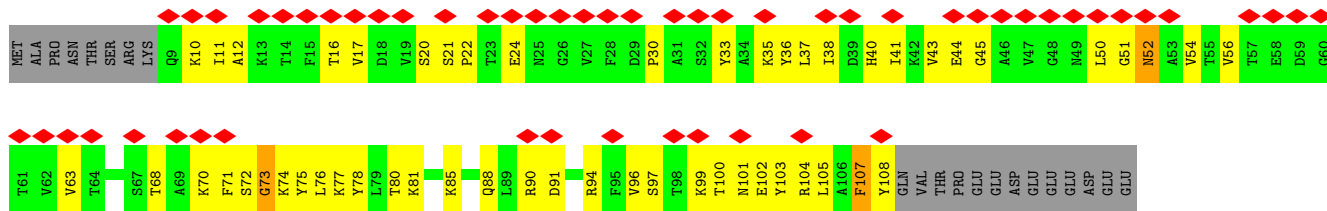


• Molecule 25: eL21 (yeast L21)

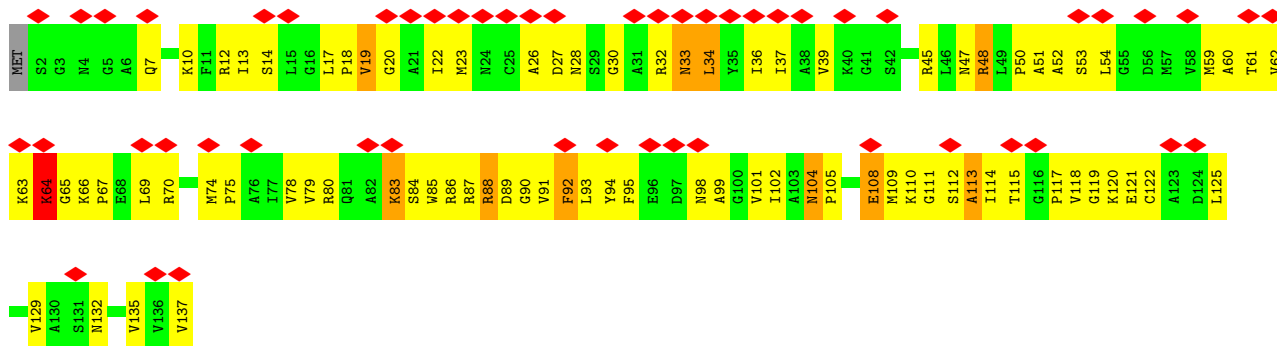
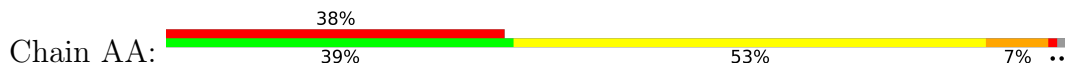


• Molecule 26: eL22 (yeast L22)

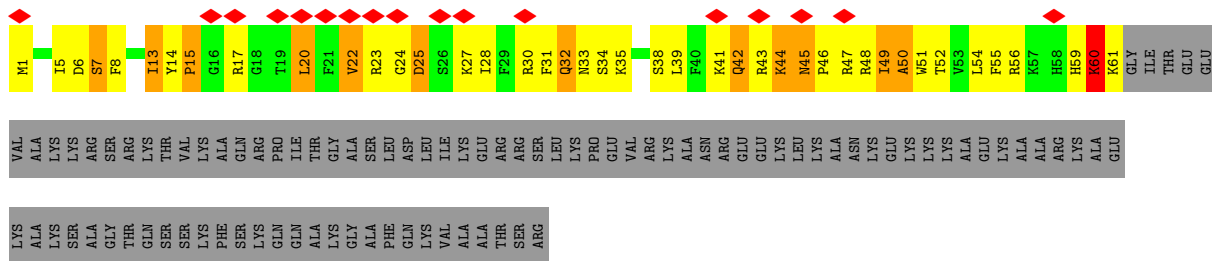




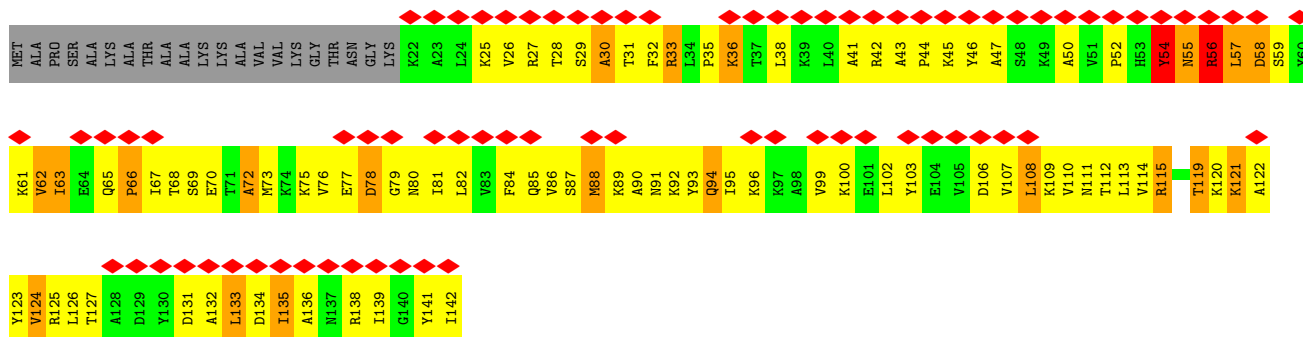
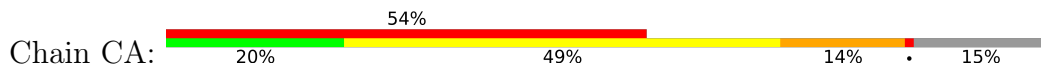
• Molecule 27: uL14 (yeast L23)



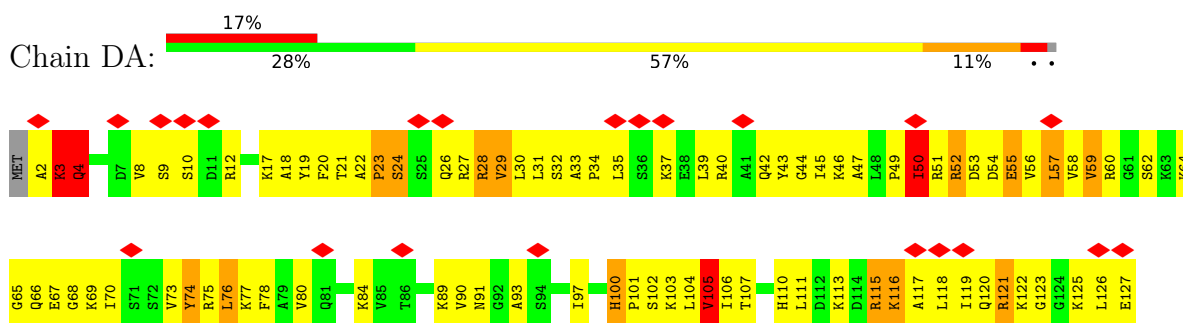
• Molecule 28: eL24 (yeast L24)



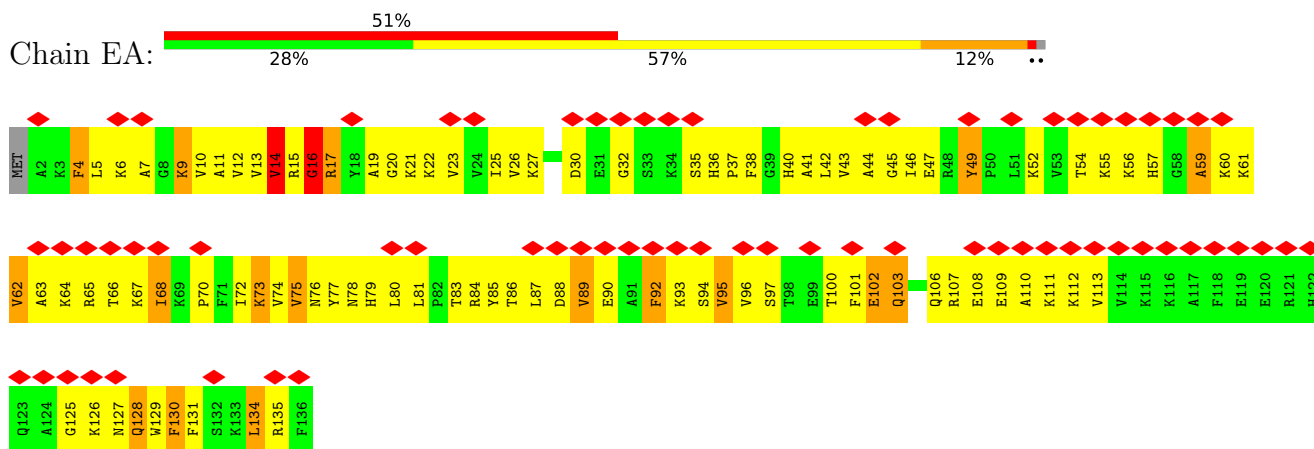
• Molecule 29: uL23 (yeast L25)



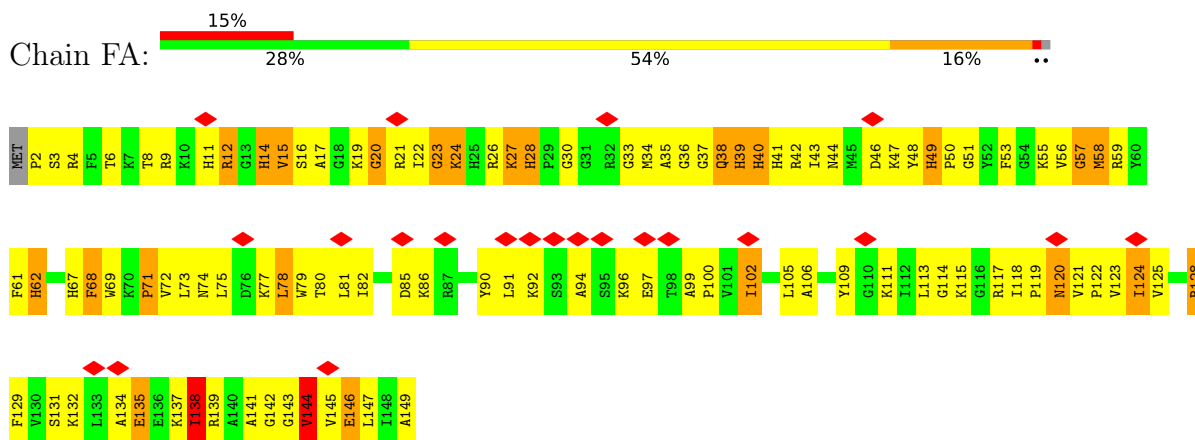
• Molecule 30: uL24 (yeast L26)



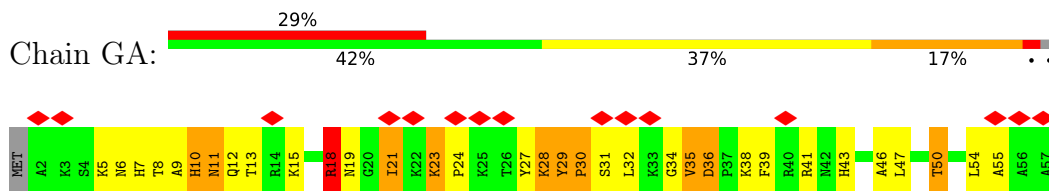
- Molecule 31: eL27 (yeast L27)



- Molecule 32: uL15 (yeast L28)

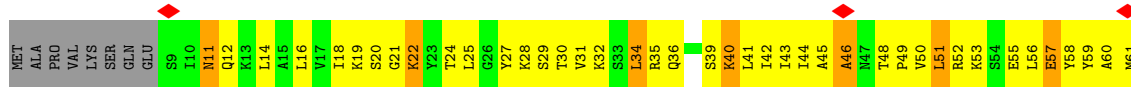


- Molecule 33: eL29 (yeast L29)

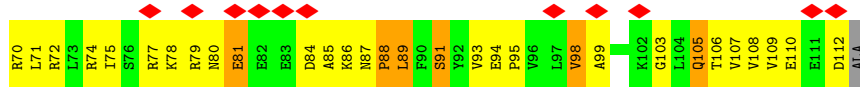
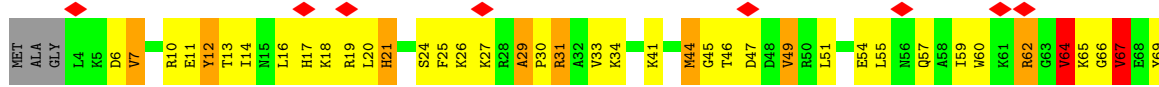


- Molecule 34: eL30 (yeast L30)

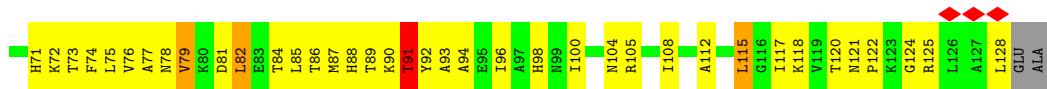
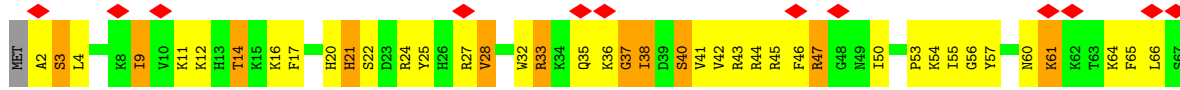




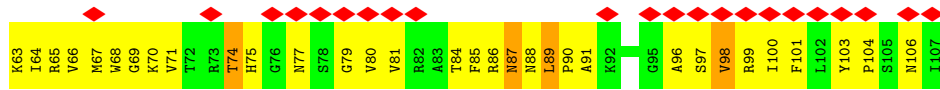
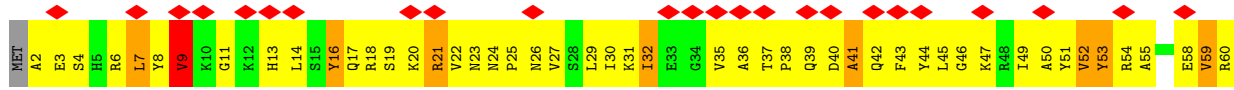
• Molecule 35: eL31 (yeast L31)



• Molecule 36: eL32 (yeast L32)



• Molecule 37: eL33 (yeast L33)

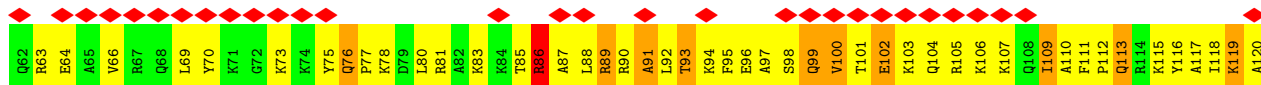


• Molecule 38: eL34 (yeast L34)

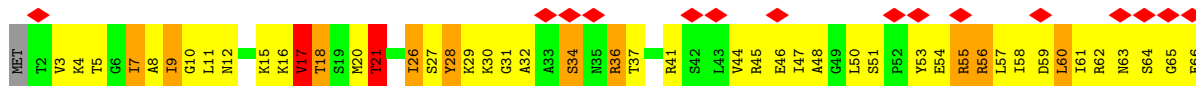
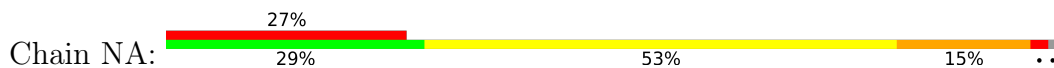




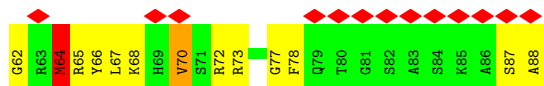
• Molecule 39: uL29 (yeast L35)



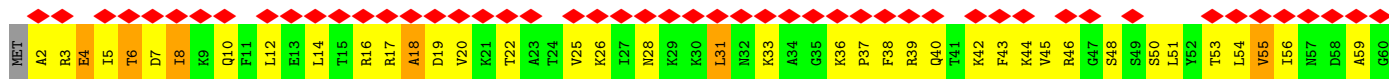
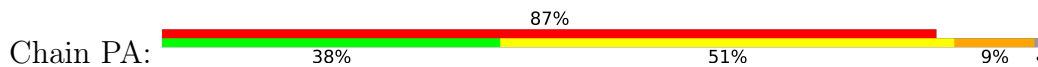
• Molecule 40: eL36 (yeast L36)



• Molecule 41: eL37 (yeast L37)



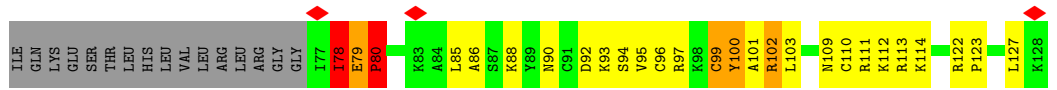
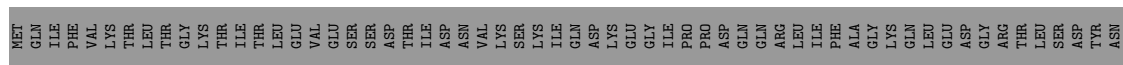
• Molecule 42: eL38 (yeast L38)



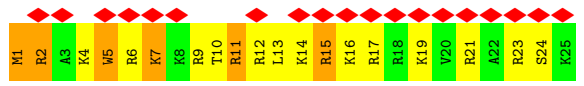
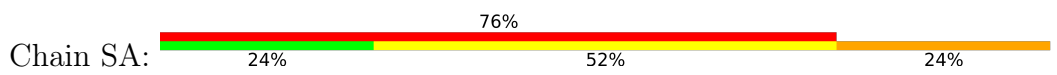
• Molecule 43: eL39 (yeast L39)



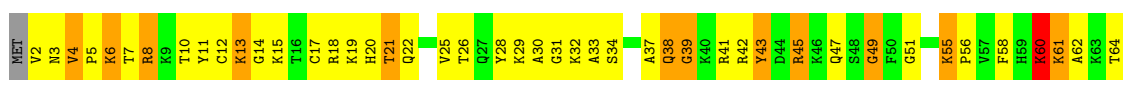
• Molecule 44: eL40 (yeast L40)



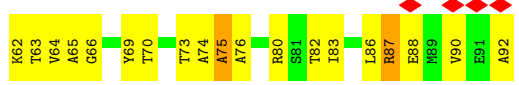
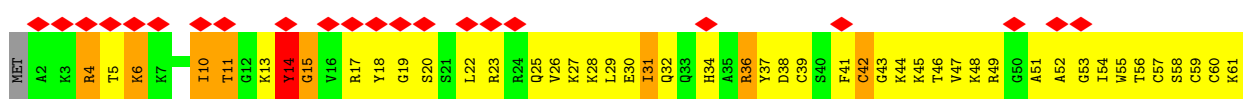
• Molecule 45: eL41 (yeast L41)



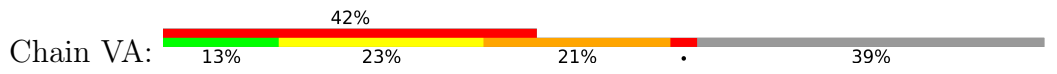
• Molecule 46: eL42 (yeast L42)

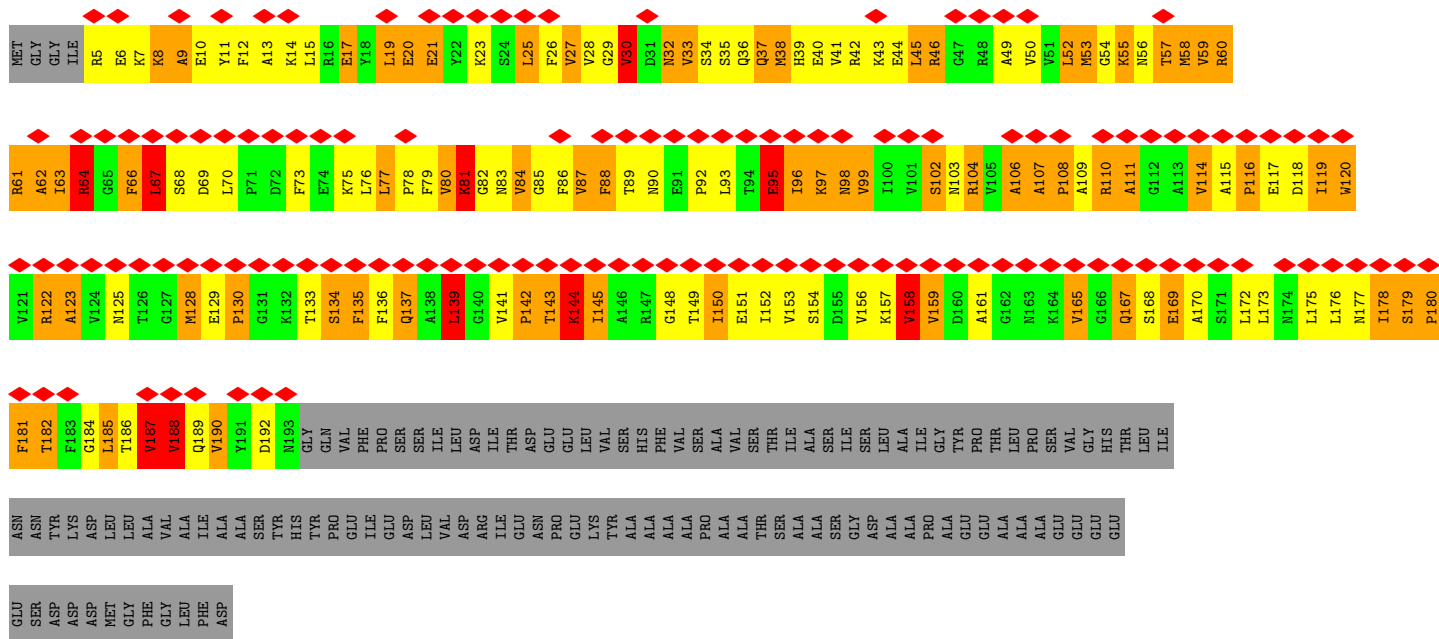


• Molecule 47: eL43 (yeast L43)

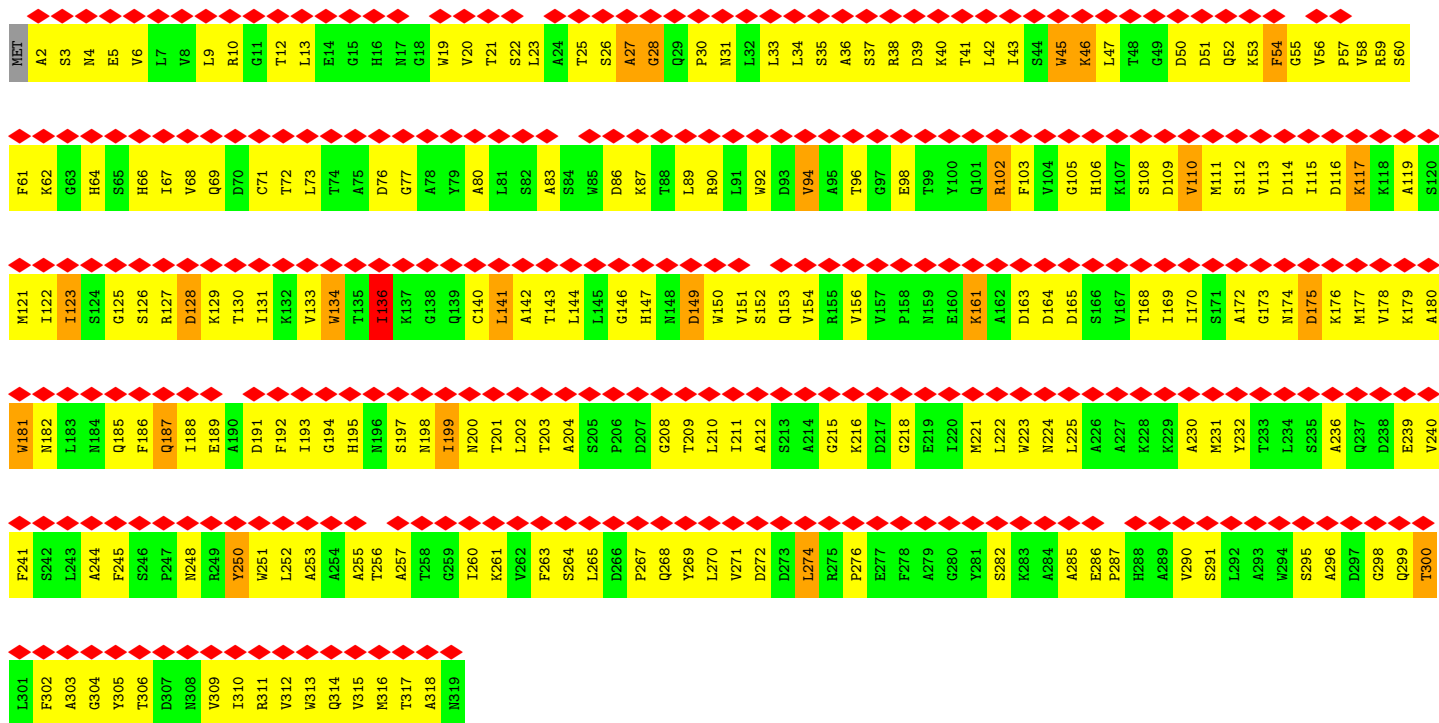


• Molecule 48: uL10 (yeast P0)

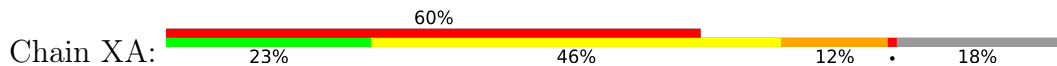


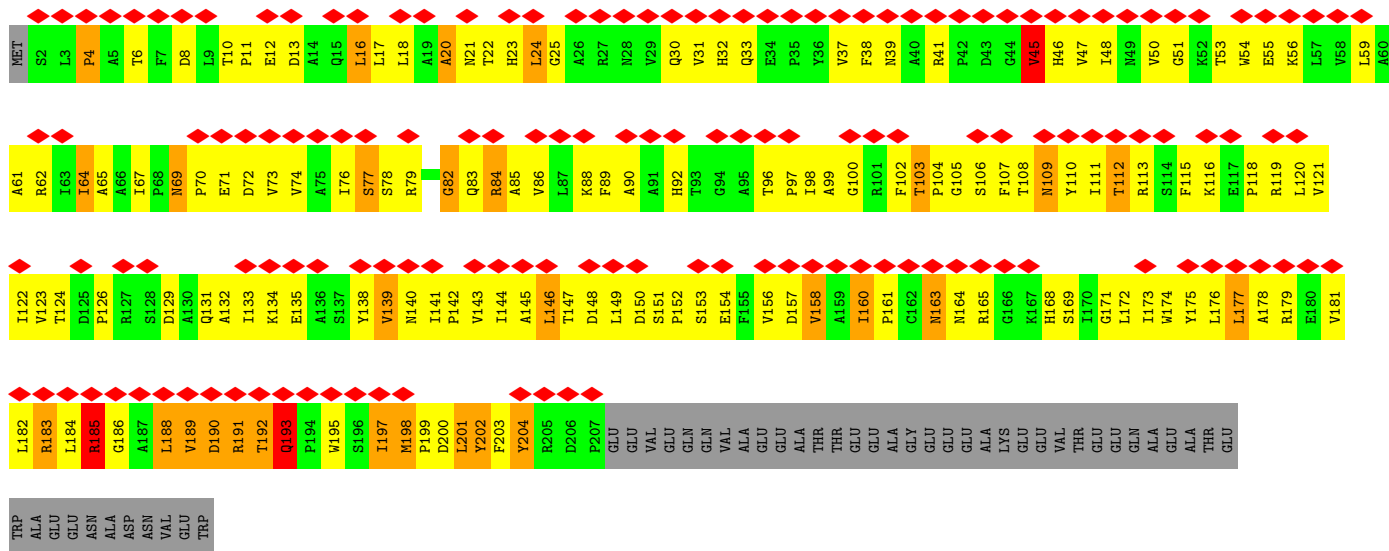


• Molecule 49: RACK1 (yeast Asc1)

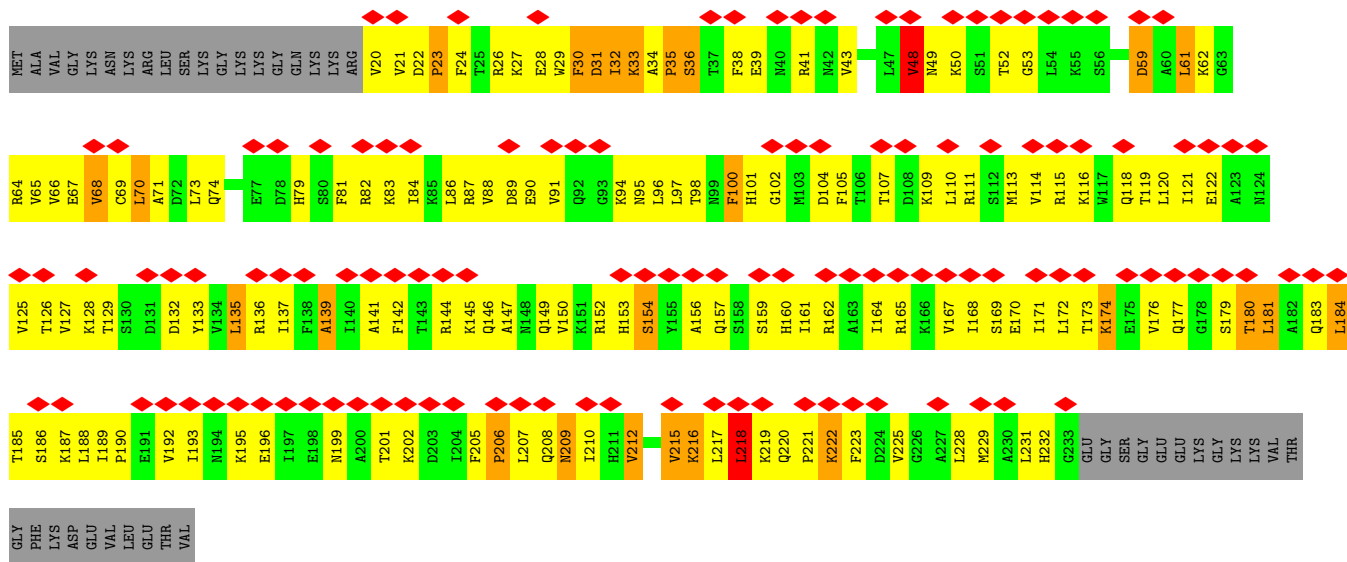


• Molecule 50: uS2 (yeast S0)

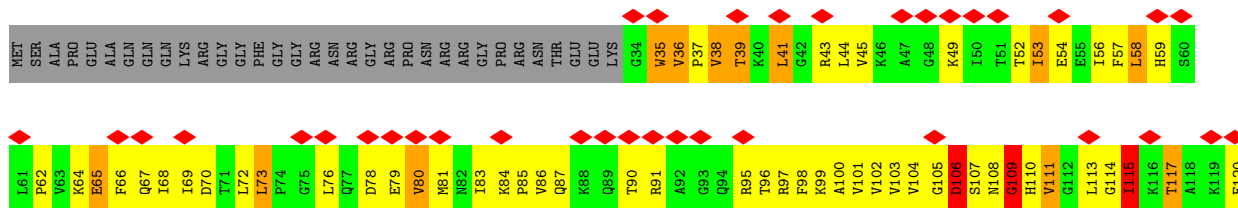




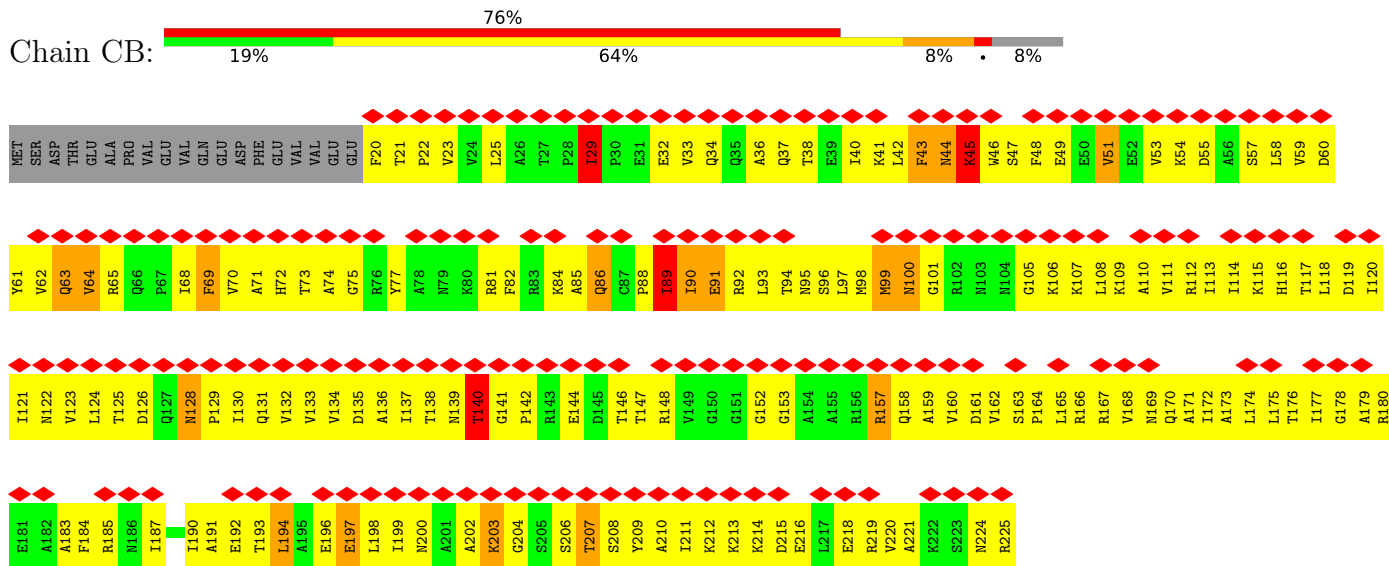
• Molecule 51: eS1 (yeast S1)



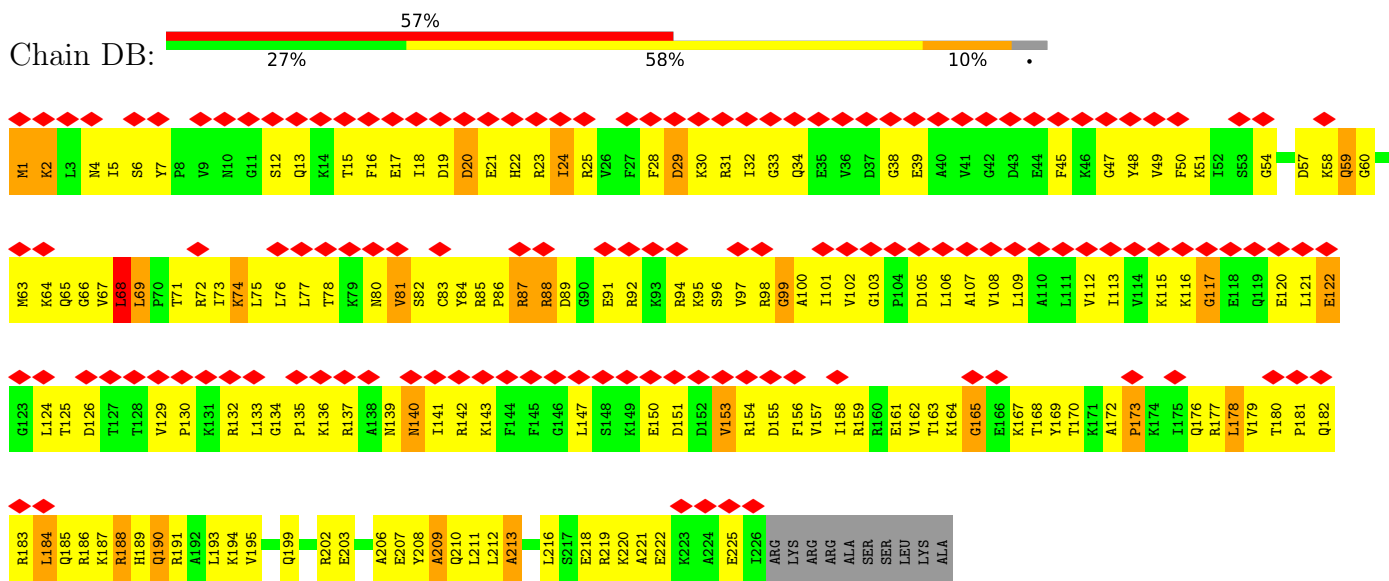
• Molecule 52: uS5 (yeast S2)



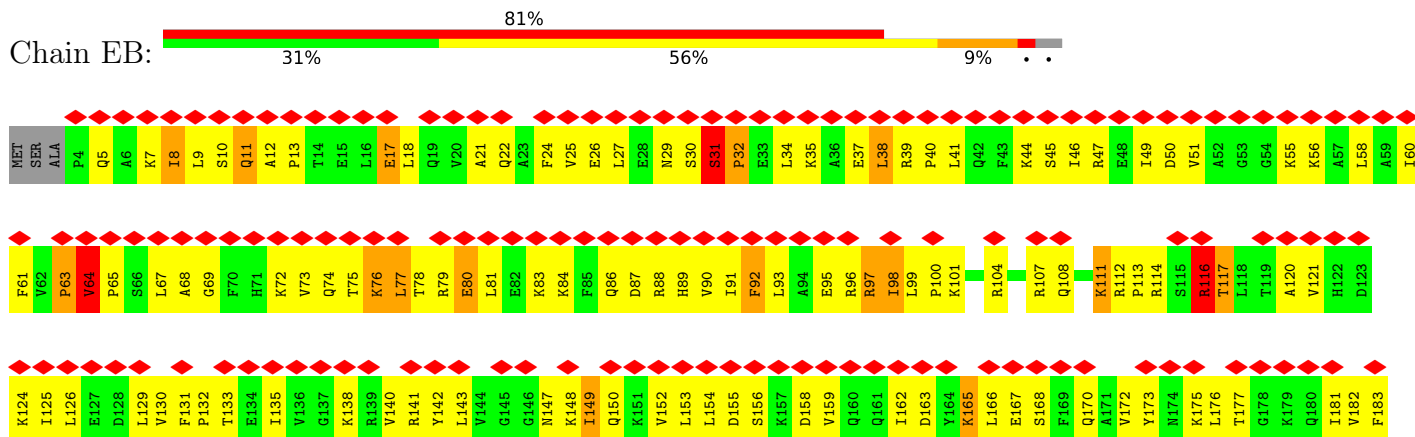
• Molecule 55: uS7 (yeast S5)

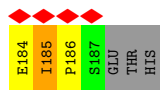


• Molecule 56: eS6 (yeast S6)



• Molecule 57: eS7 (yeast S7)

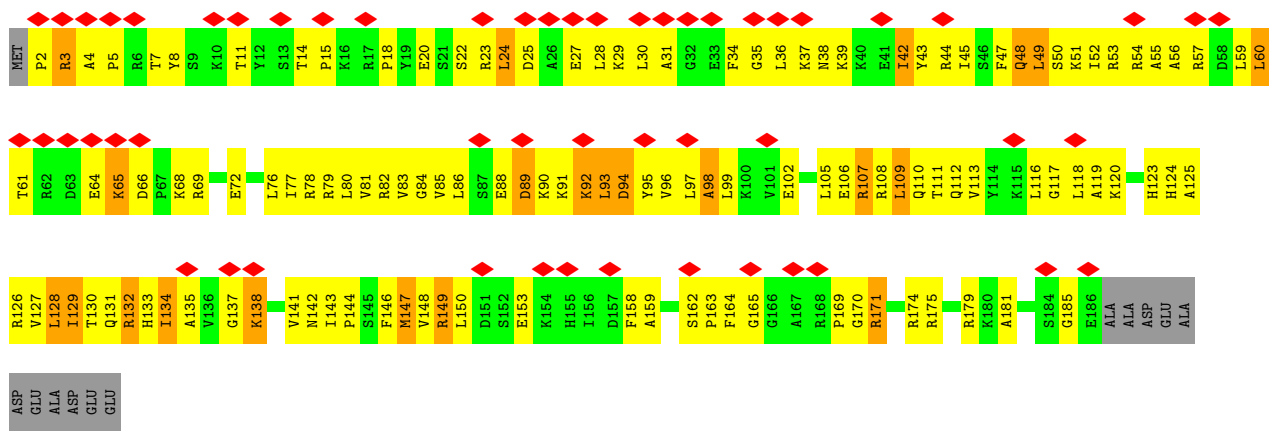
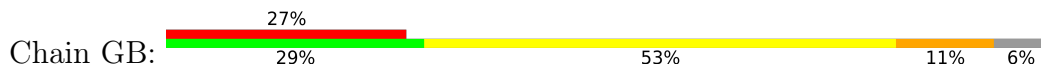




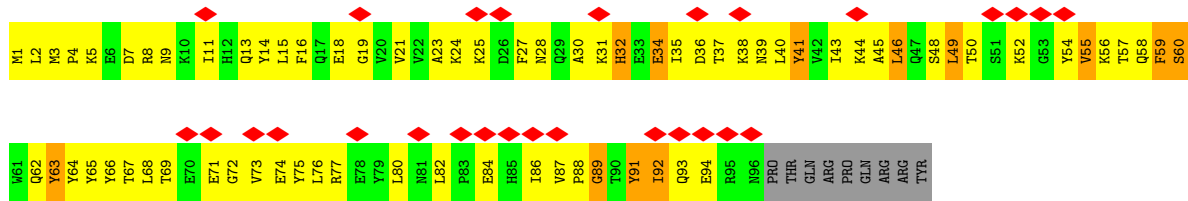
• Molecule 58: eS8 (yeast S8)

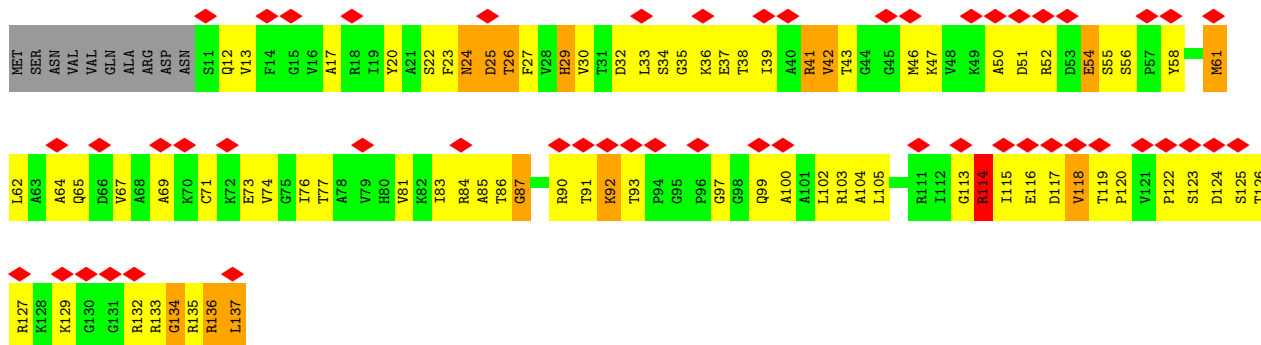


• Molecule 59: uS4 (yeast S9)

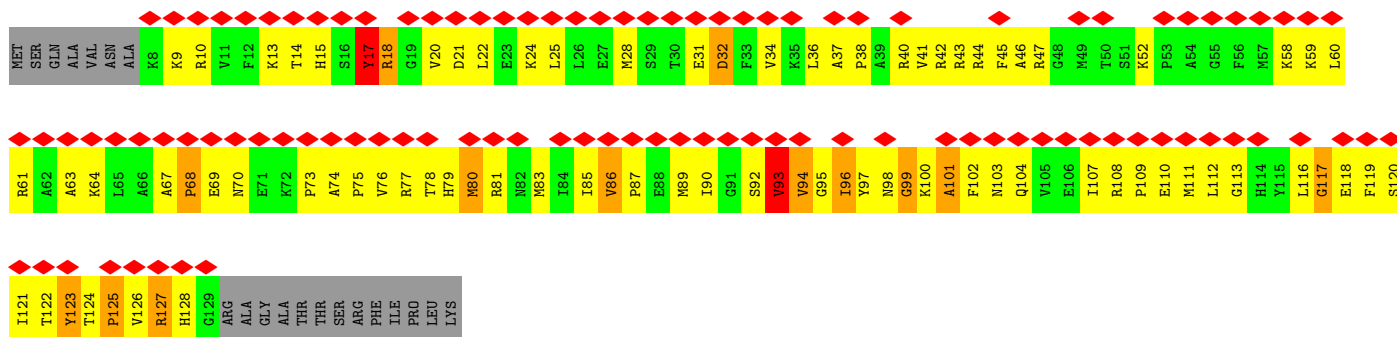
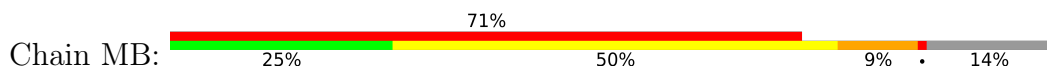


• Molecule 60: eS10 (yeast S10)

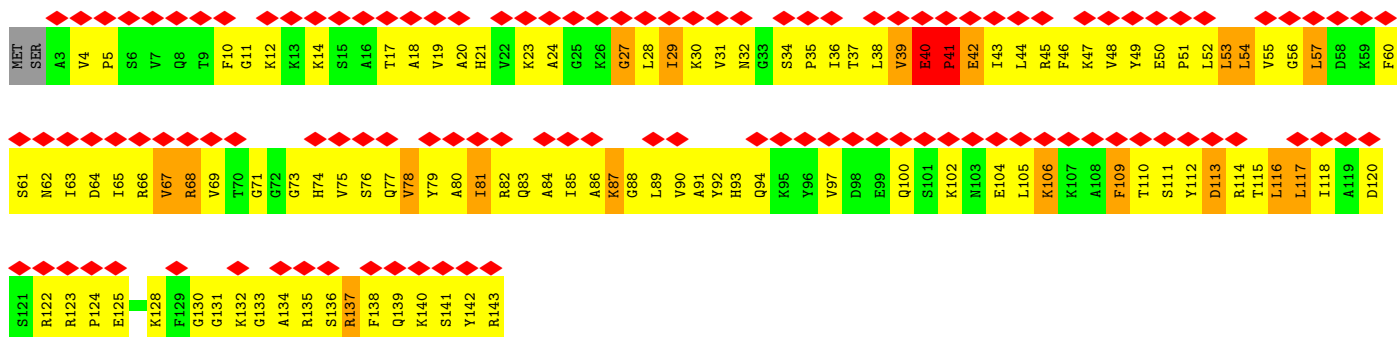
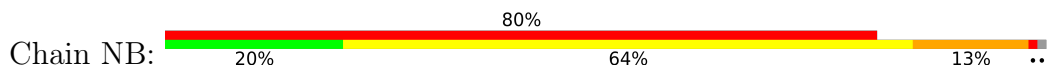




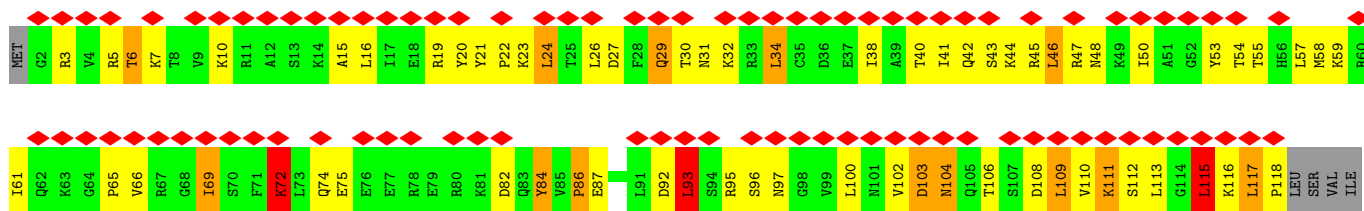
• Molecule 65: uS19 (yeast S15)



• Molecule 66: uS9 (yeast S16)

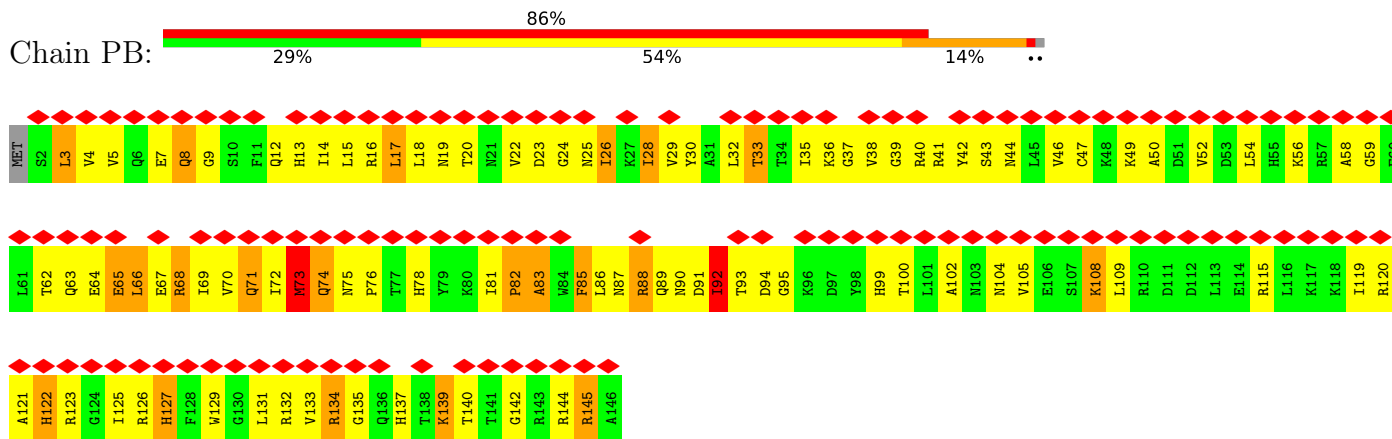


• Molecule 67: eS17 (yeast S17)

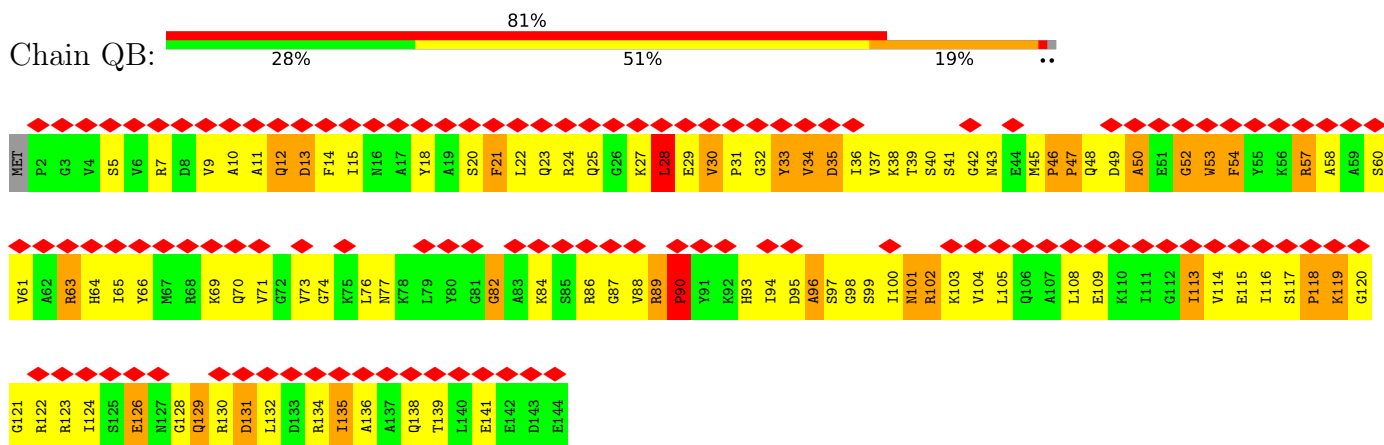


ASN	VAL
SER	SER
ALA	ALA
GLN	GLN
ARG	ARG
ASP	ASP
ARG	ARG
ARG	ARG
LYS	LYS
ARG	VAL

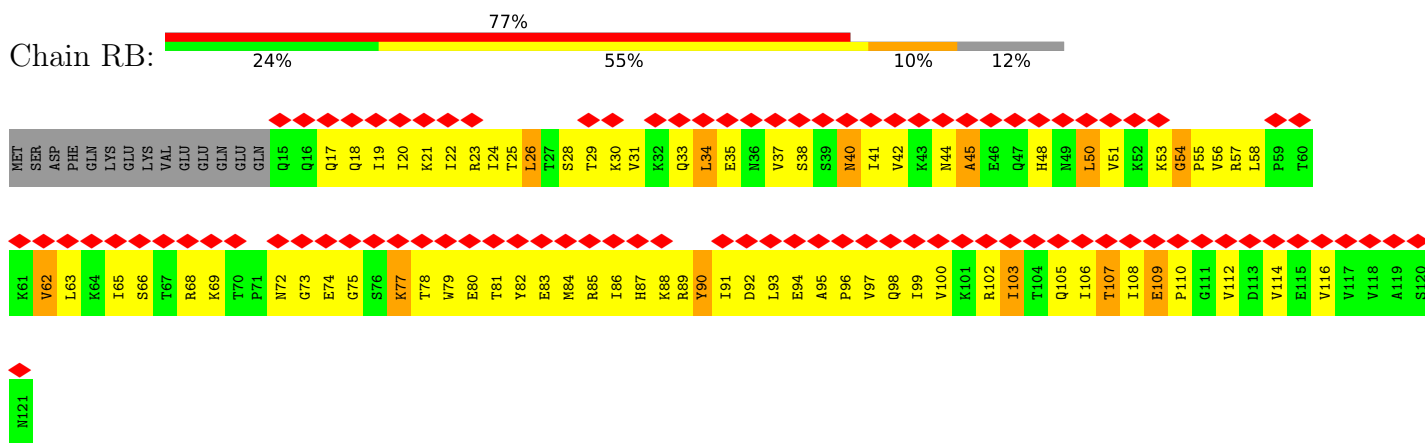
• Molecule 68: uS13 (yeast S18)



• Molecule 69: eS19 (yeast S19)

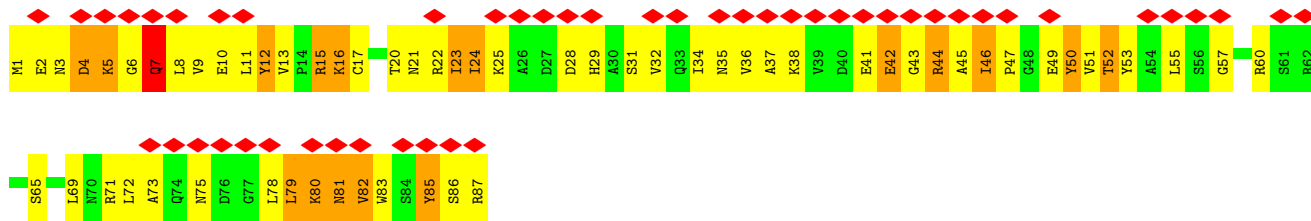


• Molecule 70: uS10 (yeast S20)

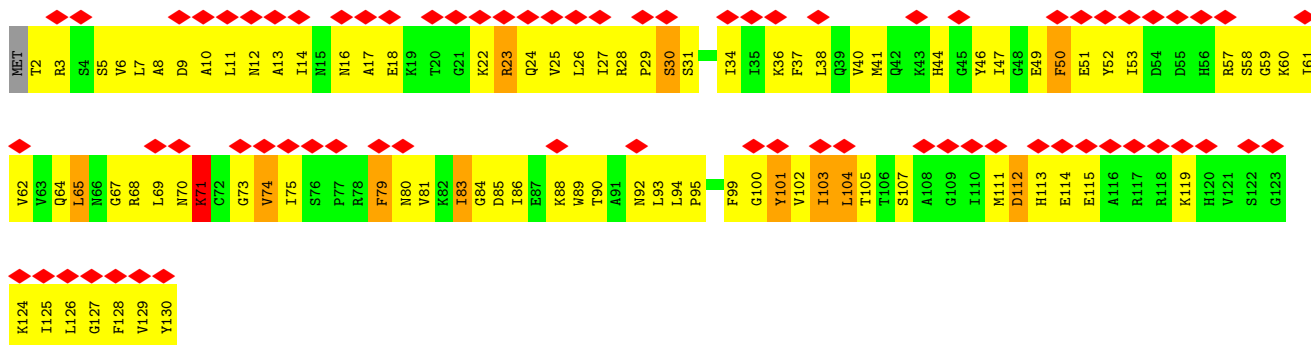


• Molecule 71: eS21 (yeast S21)

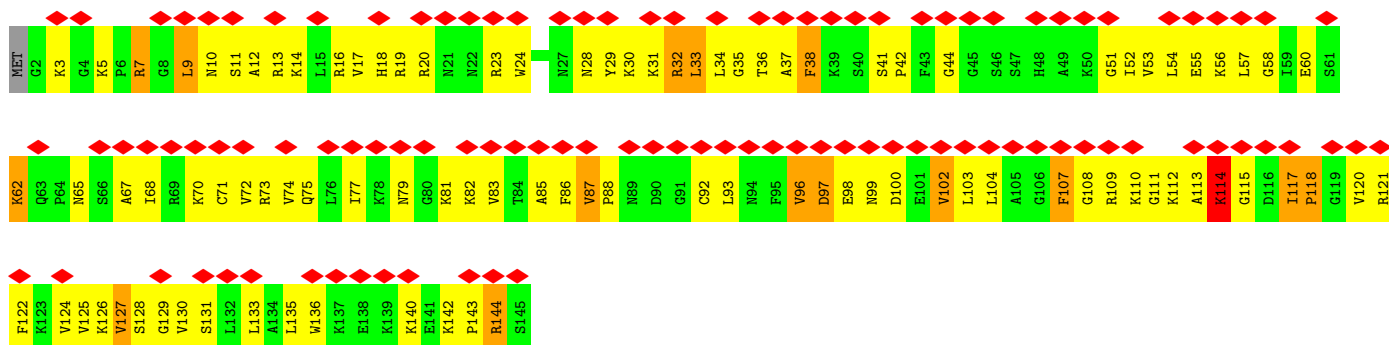
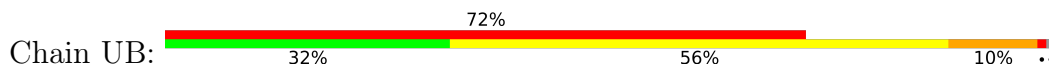




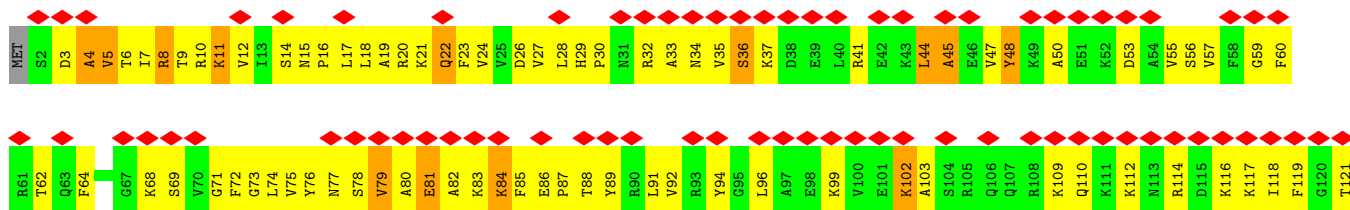
• Molecule 72: uS8 (yeast S22)

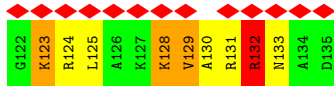


• Molecule 73: uS12 (yeast S23)

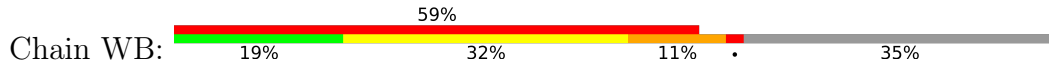


• Molecule 74: eS24 (yeast S24)

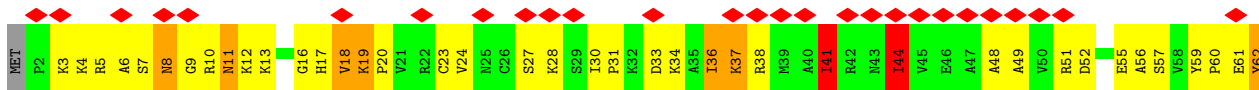




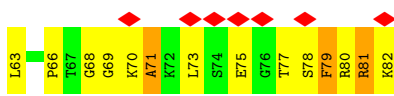
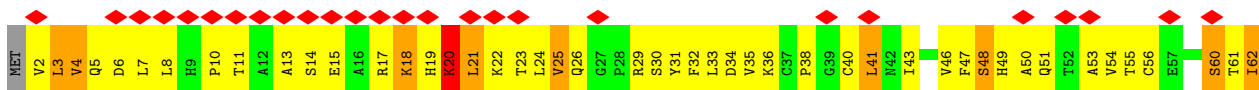
• Molecule 75: eS25 (yeast S25)



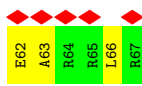
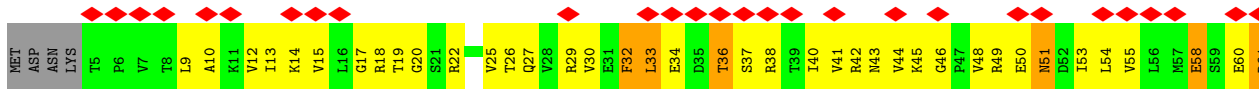
• Molecule 76: eS26 (yeast S26)



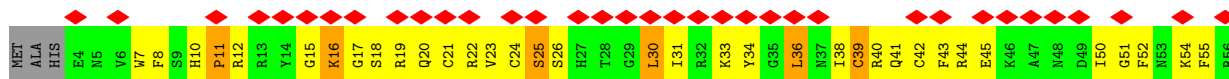
• Molecule 77: eS27 (yeast S27)



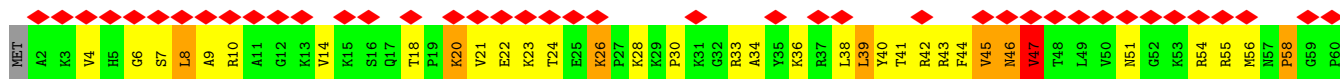
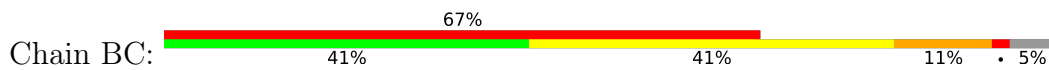
• Molecule 78: eS28 (yeast S28)



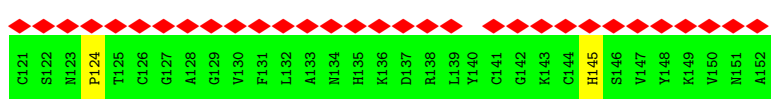
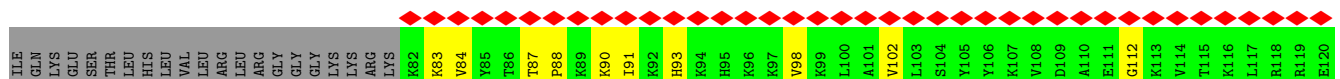
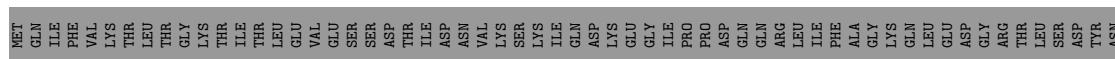
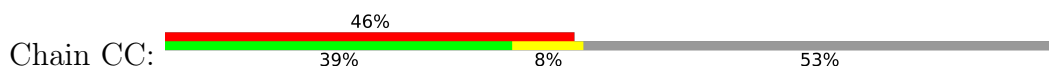
• Molecule 79: uS14 (yeast S29)



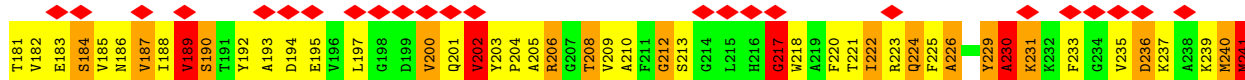
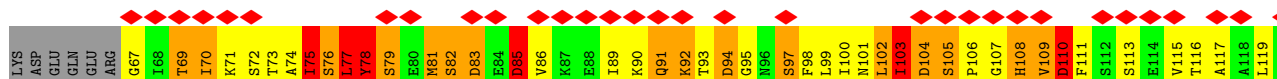
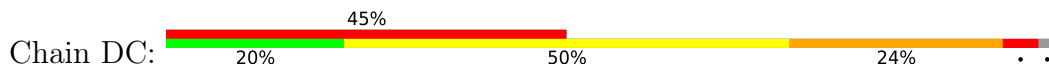
• Molecule 80: eS30 (yeast S30)

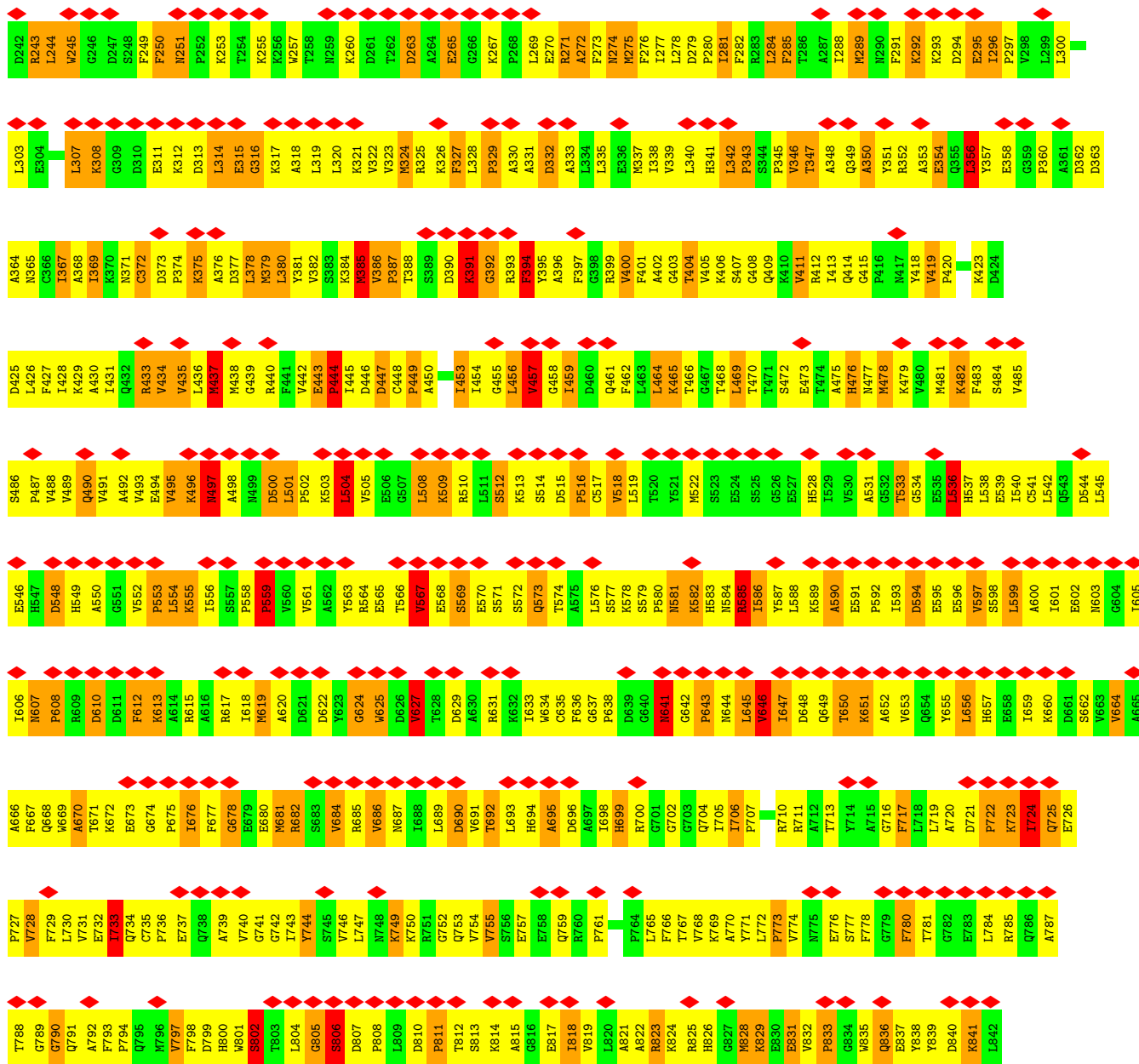


• Molecule 81: eS31 (yeast S31)

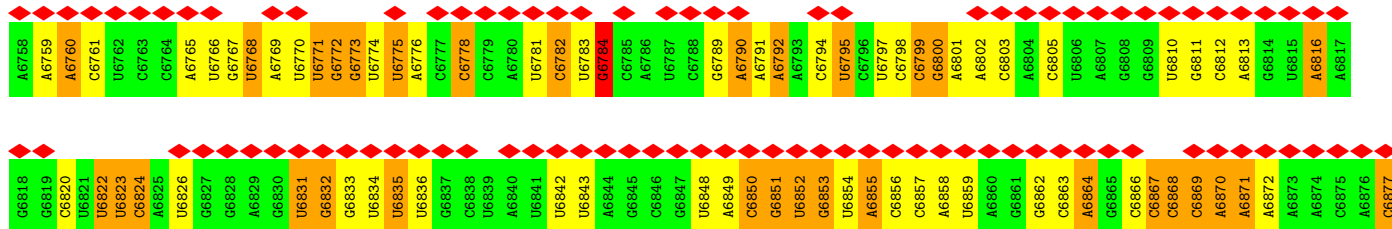
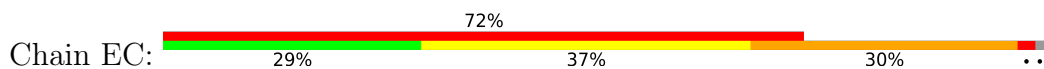


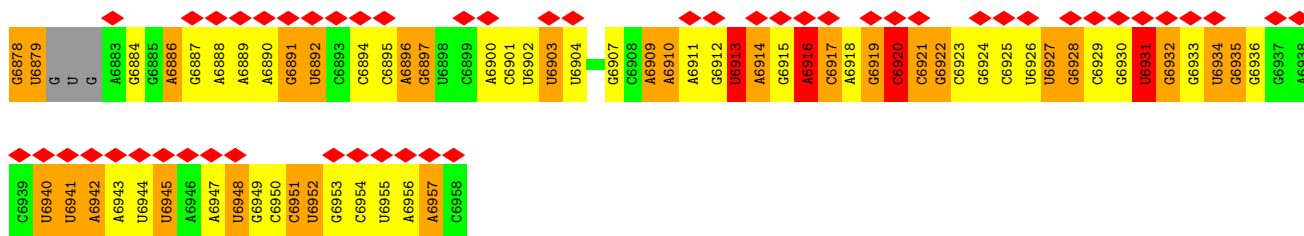
• Molecule 82: yeast eEF2





● Molecule 83: IRES





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	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 i

5.1 Standard geometry i

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

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	0.70	0/42096	0.65	31/65570 (0.0%)
2	B	0.84	0/78631	0.69	56/122552 (0.0%)
3	C	0.88	0/3747	0.69	2/5832 (0.0%)
4	D	0.82	0/2884	0.67	3/4491 (0.1%)
5	E	2.60	118/1377 (8.6%)	1.15	2/1844 (0.1%)
6	F	1.53	16/1952 (0.8%)	1.06	9/2622 (0.3%)
7	G	1.42	14/3153 (0.4%)	0.97	14/4239 (0.3%)
8	H	1.60	21/2802 (0.7%)	1.04	8/3792 (0.2%)
9	I	1.32	7/2426 (0.3%)	1.00	11/3271 (0.3%)
10	J	1.52	10/1425 (0.7%)	0.98	2/1912 (0.1%)
11	K	1.60	12/1822 (0.7%)	1.07	14/2451 (0.6%)
12	L	1.43	5/1850 (0.3%)	1.02	10/2495 (0.4%)
13	M	1.55	9/1540 (0.6%)	0.93	1/2073 (0.0%)
14	N	1.51	11/1754 (0.6%)	0.96	3/2350 (0.1%)
15	O	1.27	1/1375 (0.1%)	0.95	6/1842 (0.3%)
16	P	2.73	72/728 (9.9%)	1.27	8/975 (0.8%)
17	Q	1.52	13/1568 (0.8%)	1.08	11/2106 (0.5%)
18	R	1.67	7/1069 (0.7%)	1.06	5/1438 (0.3%)
19	S	1.58	17/1758 (1.0%)	1.09	11/2354 (0.5%)
20	T	1.56	13/1586 (0.8%)	1.06	5/2128 (0.2%)
21	U	1.56	16/1466 (1.1%)	1.05	10/1968 (0.5%)
22	V	1.52	5/1466 (0.3%)	1.05	4/1965 (0.2%)
23	W	1.30	2/1539 (0.1%)	1.11	16/2050 (0.8%)
24	X	1.69	21/1482 (1.4%)	1.02	5/1990 (0.3%)
25	Y	1.61	8/1301 (0.6%)	1.04	5/1743 (0.3%)
26	Z	1.16	0/812	0.87	2/1099 (0.2%)
27	AA	1.59	6/1019 (0.6%)	0.87	0/1369
28	BA	1.47	3/521 (0.6%)	1.01	3/691 (0.4%)
29	CA	1.65	10/984 (1.0%)	1.00	5/1325 (0.4%)
30	DA	1.56	5/1005 (0.5%)	1.01	1/1341 (0.1%)
31	EA	1.28	0/1119	0.93	3/1497 (0.2%)
32	FA	1.53	9/1205 (0.7%)	1.05	8/1612 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	GA	1.46	5/474 (1.1%)	1.22	5/629 (0.8%)
34	HA	1.19	0/751	0.93	4/1008 (0.4%)
35	IA	1.39	6/904 (0.7%)	0.92	2/1213 (0.2%)
36	JA	1.59	4/1041 (0.4%)	0.92	1/1394 (0.1%)
37	KA	1.58	9/869 (1.0%)	0.99	4/1168 (0.3%)
38	LA	1.52	6/891 (0.7%)	1.00	7/1191 (0.6%)
39	MA	1.42	2/979 (0.2%)	1.04	7/1301 (0.5%)
40	NA	1.38	3/779 (0.4%)	1.02	3/1034 (0.3%)
41	OA	1.68	5/697 (0.7%)	0.95	1/923 (0.1%)
42	PA	1.45	3/619 (0.5%)	0.91	0/826
43	QA	1.47	4/444 (0.9%)	1.06	3/588 (0.5%)
44	RA	1.53	1/424 (0.2%)	0.83	0/562
45	SA	1.28	0/235	1.18	3/300 (1.0%)
46	TA	1.48	5/861 (0.6%)	0.97	5/1136 (0.4%)
47	UA	1.46	3/702 (0.4%)	1.08	5/934 (0.5%)
48	VA	2.29	87/1498 (5.8%)	1.30	17/2025 (0.8%)
49	WA	1.34	4/2498 (0.2%)	0.81	7/3398 (0.2%)
50	XA	1.12	0/1653	1.03	11/2261 (0.5%)
51	YA	1.20	0/1735	0.88	6/2335 (0.3%)
52	ZA	1.25	5/1665 (0.3%)	0.92	6/2263 (0.3%)
53	AB	1.37	0/1759	0.92	7/2368 (0.3%)
54	BB	1.13	1/2110 (0.0%)	0.89	4/2839 (0.1%)
55	CB	1.27	2/1630 (0.1%)	0.96	5/2202 (0.2%)
56	DB	1.17	0/1844	0.92	6/2464 (0.2%)
57	EB	1.26	1/1506 (0.1%)	0.90	3/2028 (0.1%)
58	FB	1.30	2/1515 (0.1%)	0.90	5/2021 (0.2%)
59	GB	1.05	0/1519	0.96	2/2035 (0.1%)
60	HB	1.40	1/837 (0.1%)	0.90	0/1131
61	IB	1.36	1/1273 (0.1%)	0.93	6/1712 (0.4%)
62	JB	1.93	4/495 (0.8%)	1.28	3/617 (0.5%)
63	KB	1.28	1/1216 (0.1%)	1.05	5/1638 (0.3%)
64	LB	1.09	0/953	0.87	3/1279 (0.2%)
65	MB	1.53	7/996 (0.7%)	0.97	4/1335 (0.3%)
66	NB	1.33	3/1126 (0.3%)	0.95	4/1510 (0.3%)
67	OB	1.29	2/844 (0.2%)	1.28	10/1120 (0.9%)
68	PB	1.37	0/1212	0.95	8/1628 (0.5%)
69	QB	1.32	5/1131 (0.4%)	1.05	6/1517 (0.4%)
70	RB	1.43	2/866 (0.2%)	0.87	2/1169 (0.2%)
71	SB	1.14	1/694 (0.1%)	0.88	1/935 (0.1%)
72	TB	1.18	1/1039 (0.1%)	0.92	0/1395
73	UB	1.34	3/1140 (0.3%)	0.89	4/1518 (0.3%)
74	VB	1.15	0/1088	0.98	9/1449 (0.6%)
75	WB	1.37	1/571 (0.2%)	1.04	2/768 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	XB	1.19	1/782 (0.1%)	0.86	1/1047 (0.1%)
77	YB	1.22	0/621	0.76	1/838 (0.1%)
78	ZB	1.26	0/500	0.86	2/670 (0.3%)
79	AC	1.41	0/454	0.87	1/602 (0.2%)
80	BC	1.35	0/483	0.98	0/643
81	CC	1.86	0/283	1.01	0/352
82	DC	2.04	185/6521 (2.8%)	1.11	35/8830 (0.4%)
83	EC	1.34	0/4579	0.89	21/7119 (0.3%)
All	All	1.17	807/230768 (0.3%)	0.82	531/338255 (0.2%)

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 807 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	3	ALA	N-CA	19.36	1.71	1.45
11	K	96	PRO	CA-C	12.97	1.59	1.51
16	P	106	LEU	CA-C	12.70	1.61	1.52
82	DC	296	ILE	CA-CB	10.71	1.59	1.54
46	TA	65	THR	CA-C	10.64	1.59	1.53

The worst 5 of 531 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	118	GLU	N-CA-C	-12.55	100.31	114.62
50	XA	192	THR	O-C-N	-12.49	105.98	122.59
67	OB	96	SER	N-CA-C	12.46	129.21	108.90
1	A	103	A	C2'-C3'-O3'	11.91	127.36	109.50
82	DC	3	ALA	CA-C-O	-11.88	108.09	121.87

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

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	1718	0
2	B	70288	0	35262	3752	0
3	C	3354	0	1695	185	0
4	D	2580	0	1304	138	0
5	E	1359	0	1425	123	0
6	F	1918	0	1987	289	0
7	G	3082	0	3165	411	0
8	H	2750	0	2863	355	0
9	I	2376	0	2325	267	0
10	J	1401	0	1501	145	0
11	K	1785	0	1862	245	0
12	L	1818	0	1908	218	0
13	M	1519	0	1587	177	0
14	N	1718	0	1754	192	0
15	O	1354	0	1383	150	0
16	P	723	0	774	112	0
17	Q	1543	0	1608	187	0
18	R	1054	0	1149	160	0
19	S	1721	0	1779	290	0
20	T	1556	0	1659	188	0
21	U	1443	0	1485	161	0
22	V	1442	0	1543	187	0
23	W	1522	0	1617	177	0
24	X	1446	0	1487	253	0
25	Y	1277	0	1323	201	0
26	Z	796	0	812	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	1004	0	1048	117	0
28	BA	509	0	537	50	0
29	CA	969	0	1036	134	0
30	DA	994	0	1081	116	0
31	EA	1093	0	1155	140	0
32	FA	1174	0	1215	164	0
33	GA	463	0	491	50	0
34	HA	743	0	797	103	0
35	IA	890	0	938	86	0
36	JA	1020	0	1090	94	0
37	KA	851	0	880	116	0
38	LA	881	0	949	134	0
39	MA	970	0	1078	130	0
40	NA	772	0	849	103	0
41	OA	682	0	687	86	0
42	PA	613	0	682	44	0
43	QA	437	0	475	64	0
44	RA	418	0	459	33	0
45	SA	234	0	284	30	0
46	TA	848	0	918	88	0
47	UA	695	0	738	80	0
48	VA	1473	0	1514	205	0
49	WA	2445	0	2401	200	0
50	XA	1612	0	1623	191	0
51	YA	1709	0	1784	196	0
52	ZA	1635	0	1723	161	0
53	AB	1734	0	1817	122	0
54	BB	2069	0	2154	237	0
55	CB	1610	0	1675	200	0
56	DB	1820	0	1918	181	0
57	EB	1481	0	1572	155	0
58	FB	1490	0	1525	174	0
59	GB	1494	0	1573	168	0
60	HB	817	0	804	78	0
61	IB	1245	0	1314	142	0
62	JB	496	0	141	3	0
63	KB	1193	0	1255	137	0
64	LB	942	0	979	106	0
65	MB	975	0	1017	109	0
66	NB	1106	0	1166	150	0
67	OB	836	0	827	76	0
68	PB	1193	0	1222	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	QB	1113	0	1124	139	0
70	RB	856	0	917	93	0
71	SB	685	0	672	93	0
72	TB	1022	0	1060	108	0
73	UB	1122	0	1196	109	0
74	VB	1074	0	1132	98	0
75	WB	563	0	603	68	0
76	XB	769	0	818	117	0
77	YB	611	0	633	75	0
78	ZB	498	0	535	52	0
79	AC	444	0	436	52	0
80	BC	475	0	525	43	0
81	CC	284	0	76	0	0
82	DC	6419	0	6493	752	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	159892	15068	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 40.

The worst 5 of 15068 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	12
6	F	250/254 (98%)	159 (64%)	61 (24%)	30 (12%)	0	5
7	G	384/387 (99%)	280 (73%)	84 (22%)	20 (5%)	1	18
8	H	359/362 (99%)	241 (67%)	77 (21%)	41 (11%)	0	5
9	I	294/297 (99%)	210 (71%)	64 (22%)	20 (7%)	1	14
10	J	173/176 (98%)	124 (72%)	35 (20%)	14 (8%)	1	11
11	K	220/244 (90%)	160 (73%)	37 (17%)	23 (10%)	0	7
12	L	231/256 (90%)	162 (70%)	50 (22%)	19 (8%)	0	11
13	M	189/191 (99%)	143 (76%)	32 (17%)	14 (7%)	1	13
14	N	207/221 (94%)	157 (76%)	35 (17%)	15 (7%)	1	13
15	O	167/174 (96%)	121 (72%)	30 (18%)	16 (10%)	0	9
16	P	92/165 (56%)	64 (70%)	14 (15%)	14 (15%)	0	3
17	Q	191/199 (96%)	141 (74%)	33 (17%)	17 (9%)	0	10
18	R	134/138 (97%)	103 (77%)	24 (18%)	7 (5%)	1	18
19	S	201/204 (98%)	148 (74%)	39 (19%)	14 (7%)	1	14
20	T	195/199 (98%)	152 (78%)	37 (19%)	6 (3%)	3	25
21	U	181/184 (98%)	127 (70%)	39 (22%)	15 (8%)	0	11
22	V	183/186 (98%)	120 (66%)	47 (26%)	16 (9%)	0	10
23	W	186/189 (98%)	142 (76%)	35 (19%)	9 (5%)	2	19
24	X	170/172 (99%)	119 (70%)	41 (24%)	10 (6%)	1	16
25	Y	157/160 (98%)	105 (67%)	31 (20%)	21 (13%)	0	3
26	Z	98/121 (81%)	64 (65%)	28 (29%)	6 (6%)	1	15
27	AA	134/137 (98%)	97 (72%)	32 (24%)	5 (4%)	2	22
28	BA	59/155 (38%)	41 (70%)	10 (17%)	8 (14%)	0	3
29	CA	119/142 (84%)	79 (66%)	24 (20%)	16 (13%)	0	3
30	DA	124/127 (98%)	96 (77%)	19 (15%)	9 (7%)	1	13
31	EA	133/136 (98%)	95 (71%)	21 (16%)	17 (13%)	0	4
32	FA	146/149 (98%)	95 (65%)	39 (27%)	12 (8%)	0	11
33	GA	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	0	10
34	HA	95/105 (90%)	70 (74%)	19 (20%)	6 (6%)	1	15

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

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

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%)	133 (85%)	24 (15%)	3	15
6	F	194/196 (99%)	171 (88%)	23 (12%)	5	21
7	G	322/323 (100%)	290 (90%)	32 (10%)	7	27
8	H	288/289 (100%)	252 (88%)	36 (12%)	4	20
9	I	244/245 (100%)	218 (89%)	26 (11%)	6	24
10	J	152/153 (99%)	141 (93%)	11 (7%)	13	37
11	K	186/205 (91%)	162 (87%)	24 (13%)	4	19
12	L	191/208 (92%)	170 (89%)	21 (11%)	6	23
13	M	171/171 (100%)	154 (90%)	17 (10%)	7	27
14	N	180/187 (96%)	163 (91%)	17 (9%)	8	29
15	O	147/150 (98%)	137 (93%)	10 (7%)	14	39
16	P	81/136 (60%)	69 (85%)	12 (15%)	3	16
17	Q	154/159 (97%)	137 (89%)	17 (11%)	6	23
18	R	107/109 (98%)	90 (84%)	17 (16%)	2	15
19	S	175/176 (99%)	149 (85%)	26 (15%)	3	16
20	T	160/162 (99%)	140 (88%)	20 (12%)	4	20
21	U	145/146 (99%)	129 (89%)	16 (11%)	6	23
22	V	150/151 (99%)	138 (92%)	12 (8%)	11	35
23	W	153/154 (99%)	138 (90%)	15 (10%)	7	27
24	X	156/156 (100%)	144 (92%)	12 (8%)	12	35
25	Y	136/137 (99%)	117 (86%)	19 (14%)	3	17
26	Z	87/107 (81%)	86 (99%)	1 (1%)	65	74
27	AA	104/105 (99%)	96 (92%)	8 (8%)	12	35
28	BA	54/129 (42%)	48 (89%)	6 (11%)	6	23
29	CA	105/118 (89%)	96 (91%)	9 (9%)	10	33
30	DA	109/110 (99%)	95 (87%)	14 (13%)	4	20
31	EA	115/116 (99%)	106 (92%)	9 (8%)	11	35
32	FA	118/119 (99%)	111 (94%)	7 (6%)	18	42
33	GA	46/47 (98%)	42 (91%)	4 (9%)	9	32
34	HA	81/88 (92%)	74 (91%)	7 (9%)	10	33
35	IA	96/97 (99%)	84 (88%)	12 (12%)	4	20
36	JA	109/111 (98%)	96 (88%)	13 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	83 (92%)	7 (8%)	11	35
38	LA	95/103 (92%)	86 (90%)	9 (10%)	8	28
39	MA	104/105 (99%)	96 (92%)	8 (8%)	12	35
40	NA	81/82 (99%)	71 (88%)	10 (12%)	4	20
41	OA	70/71 (99%)	64 (91%)	6 (9%)	10	33
42	PA	68/69 (99%)	62 (91%)	6 (9%)	9	32
43	QA	45/46 (98%)	42 (93%)	3 (7%)	15	39
44	RA	47/116 (40%)	41 (87%)	6 (13%)	4	20
45	SA	23/23 (100%)	19 (83%)	4 (17%)	2	13
46	TA	90/91 (99%)	80 (89%)	10 (11%)	6	23
47	UA	71/72 (99%)	67 (94%)	4 (6%)	19	43
48	VA	160/254 (63%)	142 (89%)	18 (11%)	5	22
49	WA	261/262 (100%)	240 (92%)	21 (8%)	11	35
50	XA	173/210 (82%)	152 (88%)	21 (12%)	5	21
51	YA	191/224 (85%)	171 (90%)	20 (10%)	6	24
52	ZA	176/205 (86%)	161 (92%)	15 (8%)	10	33
53	AB	182/195 (93%)	164 (90%)	18 (10%)	7	27
54	BB	221/222 (100%)	206 (93%)	15 (7%)	14	39
55	CB	173/191 (91%)	160 (92%)	13 (8%)	12	36
56	DB	193/201 (96%)	177 (92%)	16 (8%)	10	33
57	EB	165/170 (97%)	147 (89%)	18 (11%)	6	23
58	FB	150/161 (93%)	137 (91%)	13 (9%)	9	32
59	GB	158/166 (95%)	147 (93%)	11 (7%)	14	38
60	HB	89/98 (91%)	81 (91%)	8 (9%)	9	31
61	IB	136/137 (99%)	121 (89%)	15 (11%)	6	23
63	KB	127/128 (99%)	114 (90%)	13 (10%)	7	25
64	LB	96/105 (91%)	86 (90%)	10 (10%)	7	25
65	MB	103/118 (87%)	97 (94%)	6 (6%)	18	42
66	NB	117/119 (98%)	103 (88%)	14 (12%)	5	21
67	OB	82/124 (66%)	73 (89%)	9 (11%)	6	23
68	PB	128/129 (99%)	117 (91%)	11 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	QB	115/116 (99%)	103 (90%)	12 (10%)	7	25
70	RB	100/114 (88%)	90 (90%)	10 (10%)	7	26
71	SB	74/74 (100%)	66 (89%)	8 (11%)	6	24
72	TB	110/111 (99%)	99 (90%)	11 (10%)	7	26
73	UB	119/120 (99%)	108 (91%)	11 (9%)	8	30
74	VB	112/113 (99%)	101 (90%)	11 (10%)	7	27
75	WB	61/89 (68%)	54 (88%)	7 (12%)	5	22
76	XB	83/101 (82%)	76 (92%)	7 (8%)	10	33
77	YB	70/71 (99%)	65 (93%)	5 (7%)	13	38
78	ZB	56/60 (93%)	53 (95%)	3 (5%)	20	44
79	AC	47/49 (96%)	42 (89%)	5 (11%)	6	24
80	BC	51/54 (94%)	43 (84%)	8 (16%)	2	15
82	DC	699/714 (98%)	596 (85%)	103 (15%)	3	16
All	All	10235/11032 (93%)	9179 (90%)	1056 (10%)	9	25

5 of 1056 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
76	XB	36	ILE
82	DC	2	VAL
76	XB	19	LYS
82	DC	681	MET
25	Y	13	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 332 such sidechains are listed below:

Mol	Chain	Res	Type
58	FB	175	GLN
73	UB	99	ASN
60	HB	9	ASN
68	PB	6	GLN
77	YB	9	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1753/1798 (97%)	380 (21%)	18 (1%)
2	B	3265/3396 (96%)	612 (18%)	27 (0%)
3	C	157/158 (99%)	31 (19%)	2 (1%)
4	D	120/121 (99%)	14 (11%)	0
83	EC	185/201 (92%)	77 (41%)	3 (1%)
All	All	5480/5674 (96%)	1114 (20%)	50 (0%)

5 of 1114 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	18,20,21	2.56	5 (27%)	17,28,30	2.53	4 (23%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	CD2-CG	7.16	1.51	1.36
82	DC	699	DDE	CBW-CBI	4.66	1.61	1.53
82	DC	699	DDE	CBW-NCB	3.72	1.61	1.54
82	DC	699	DDE	CAT-CE1	3.39	1.55	1.49
82	DC	699	DDE	OAG-CBI	2.12	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	DC	699	DDE	CAU-CAT-CE1	7.12	140.92	114.38
82	DC	699	DDE	CAU-CBW-CBI	-5.56	100.34	111.22
82	DC	699	DDE	CD2-NE2-CE1	3.16	110.19	107.55
82	DC	699	DDE	OAG-CBI-NAD	2.43	127.32	123.04

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	DC	699	DDE	OAG-CBI-CBW-NCB
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 oligosaccharides 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	29,30,30	1.90	4 (13%)	45,47,47	1.82	10 (22%)
86	SO1	DC	903	-	34,39,39	2.44	14 (41%)	38,64,64	2.00	9 (23%)

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	-	0/16/32/32	0/3/3/3
86	SO1	DC	903	-	-	2/21/104/104	0/7/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	DC	901	GDP	PA-O3A	6.59	1.66	1.59
86	DC	903	SO1	O56-C52	-4.42	1.30	1.41
86	DC	903	SO1	C12-C6	4.29	1.63	1.53
86	DC	903	SO1	C1-C5	4.13	1.60	1.50
86	DC	903	SO1	O17-C52	4.06	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	DC	903	SO1	C12-C6-C10	-5.99	103.23	107.92
84	DC	901	GDP	C2-N3-C4	5.28	121.39	112.30
84	DC	901	GDP	C5-C4-N3	-4.76	120.82	128.39
86	DC	903	SO1	C25-C22-C24	4.74	128.70	113.64
84	DC	901	GDP	N9-C4-N3	3.66	133.27	125.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

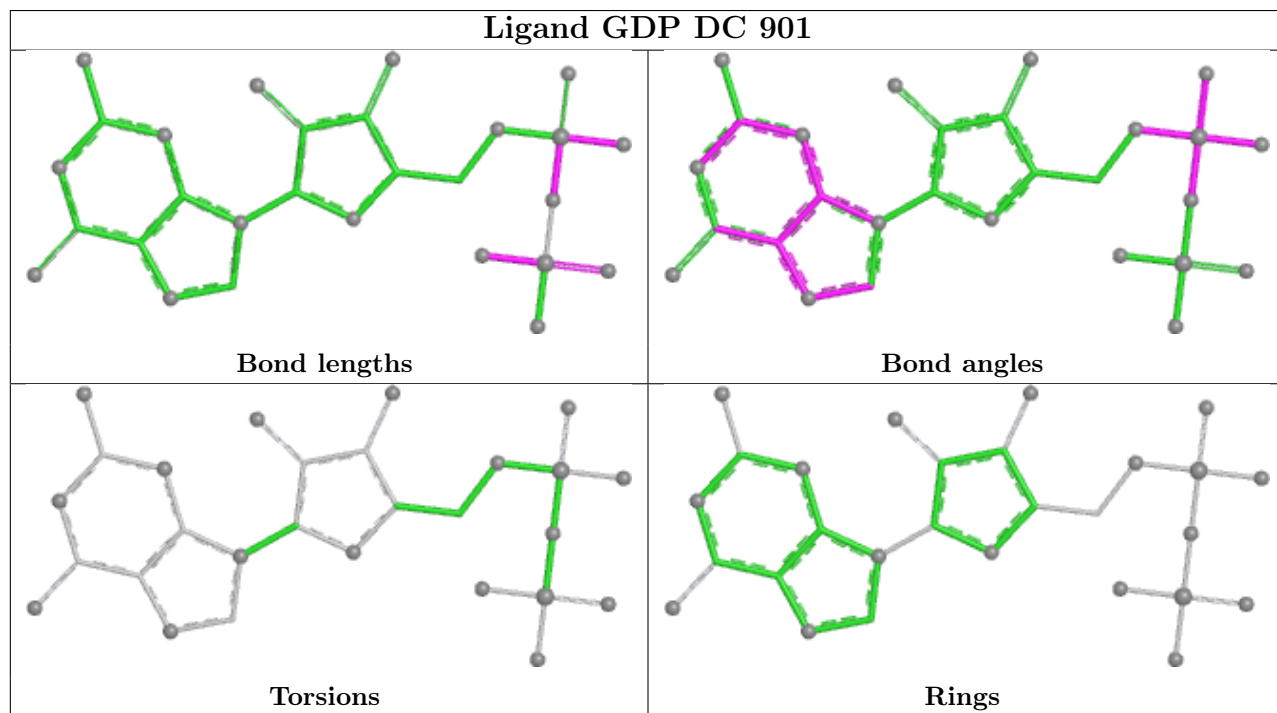
Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15

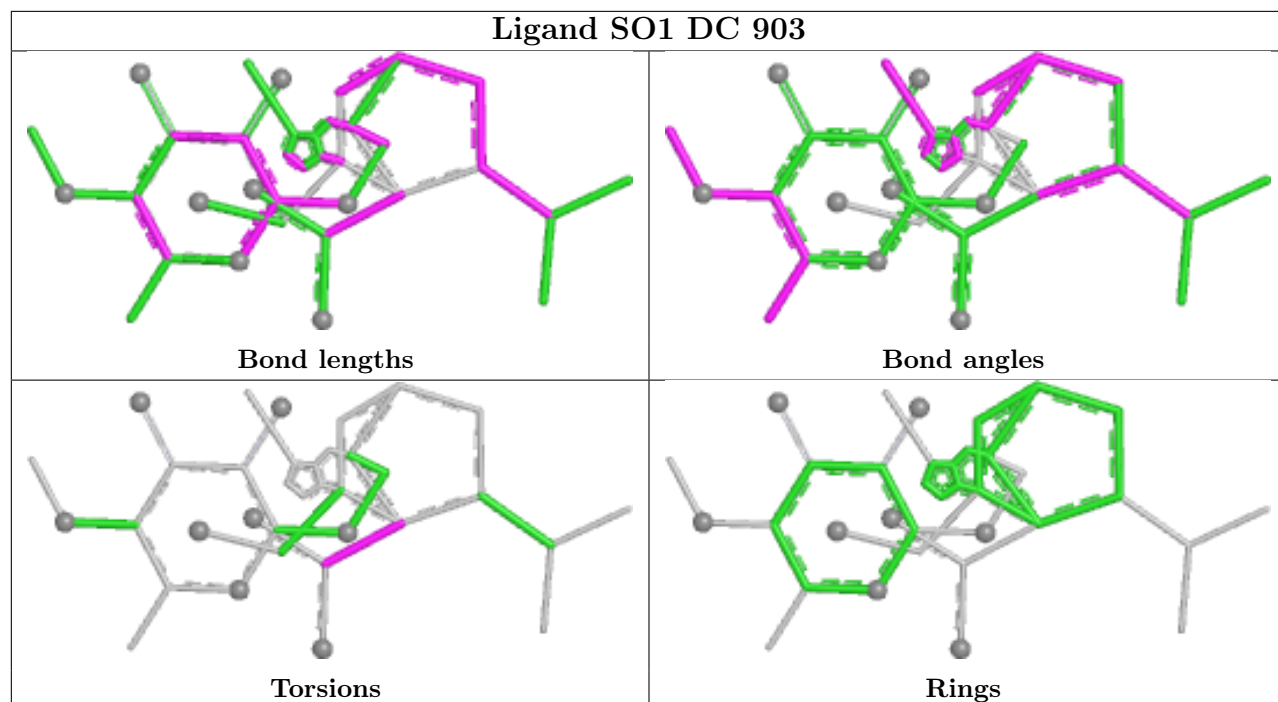
There are no ring outliers.

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.

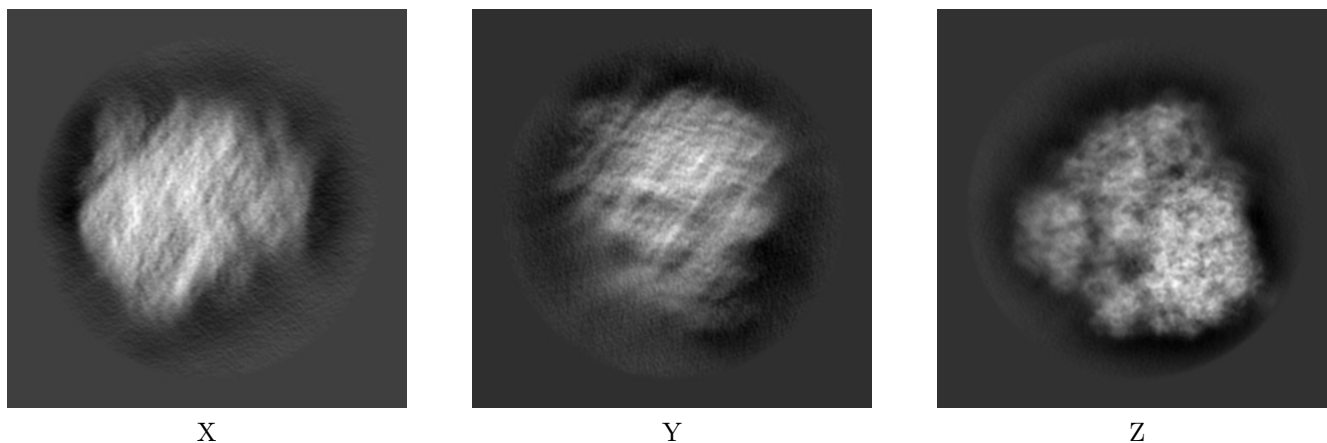
6 Map visualisation [i](#)

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](#)

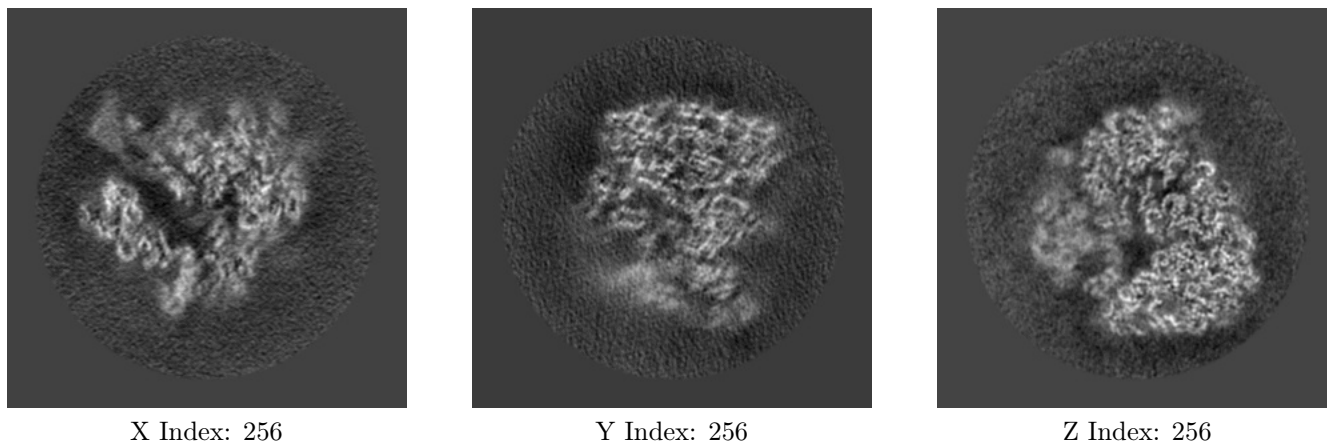
6.1.1 Primary map



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

6.2 Central slices [i](#)

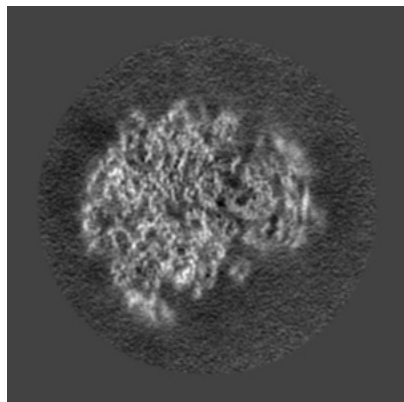
6.2.1 Primary map



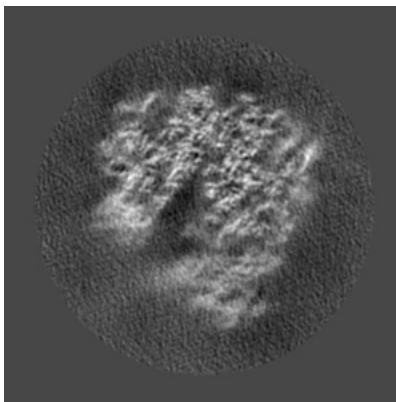
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

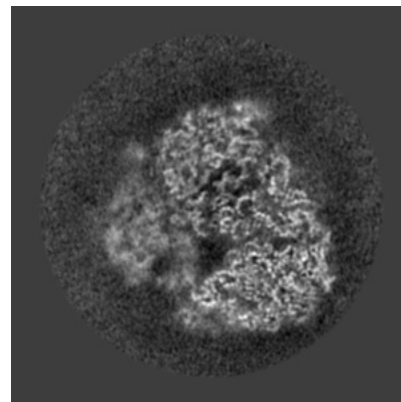
6.3.1 Primary map



X Index: 290



Y Index: 222

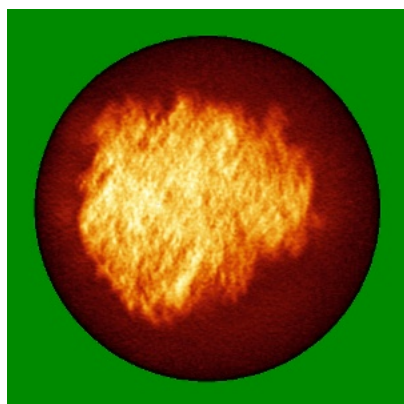


Z Index: 261

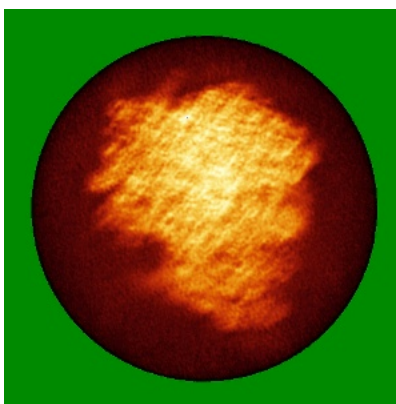
The images above show the largest variance slices of the map in three orthogonal directions.

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

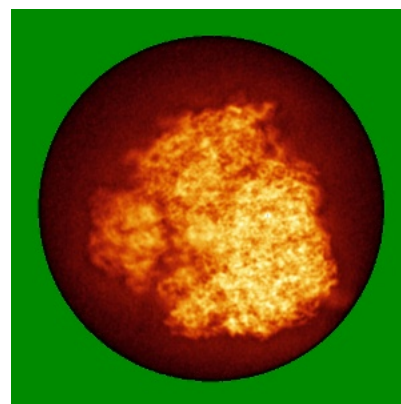
6.4.1 Primary map



X



Y

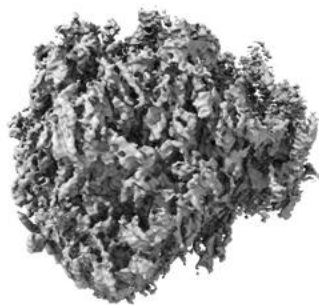


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

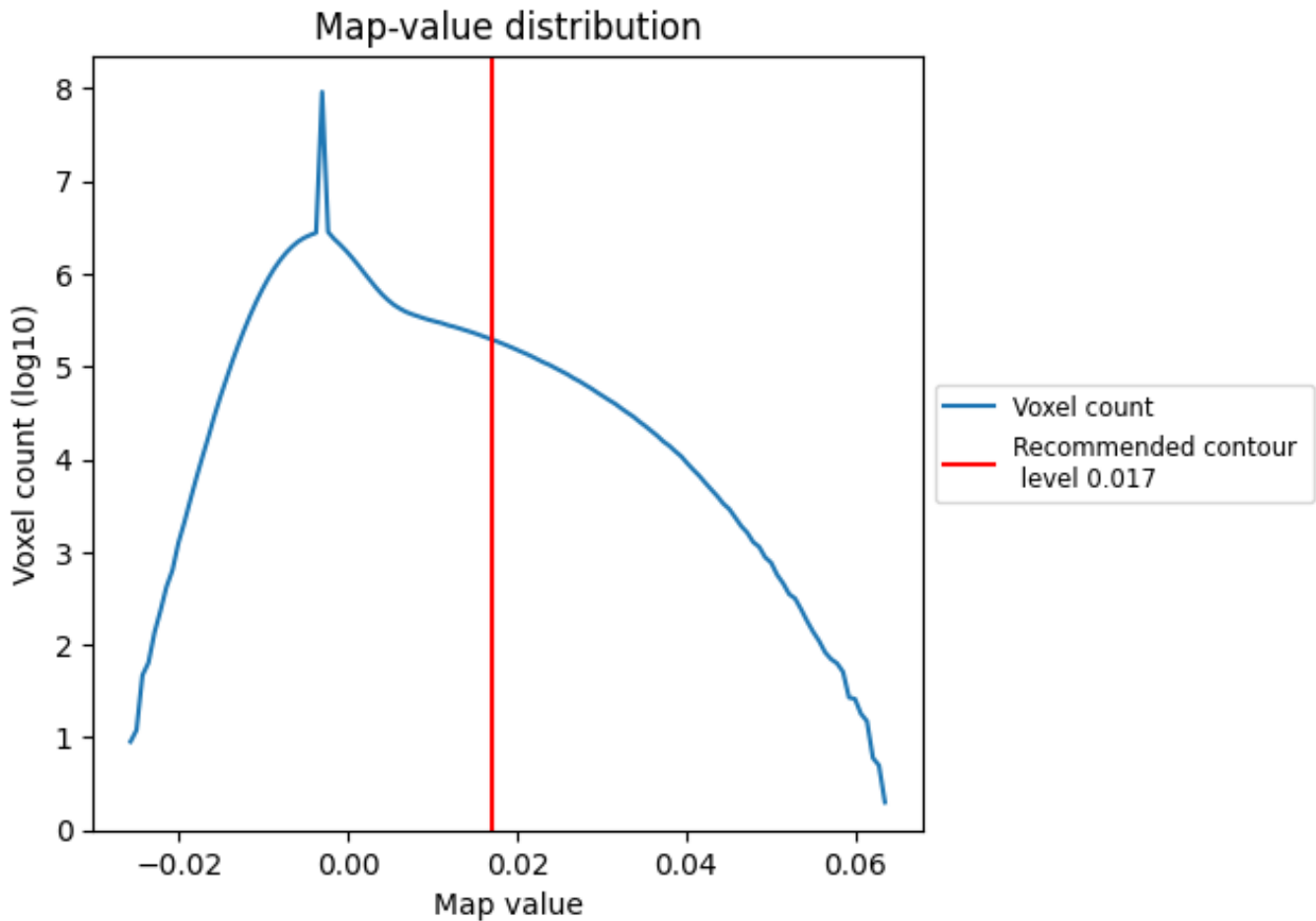
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

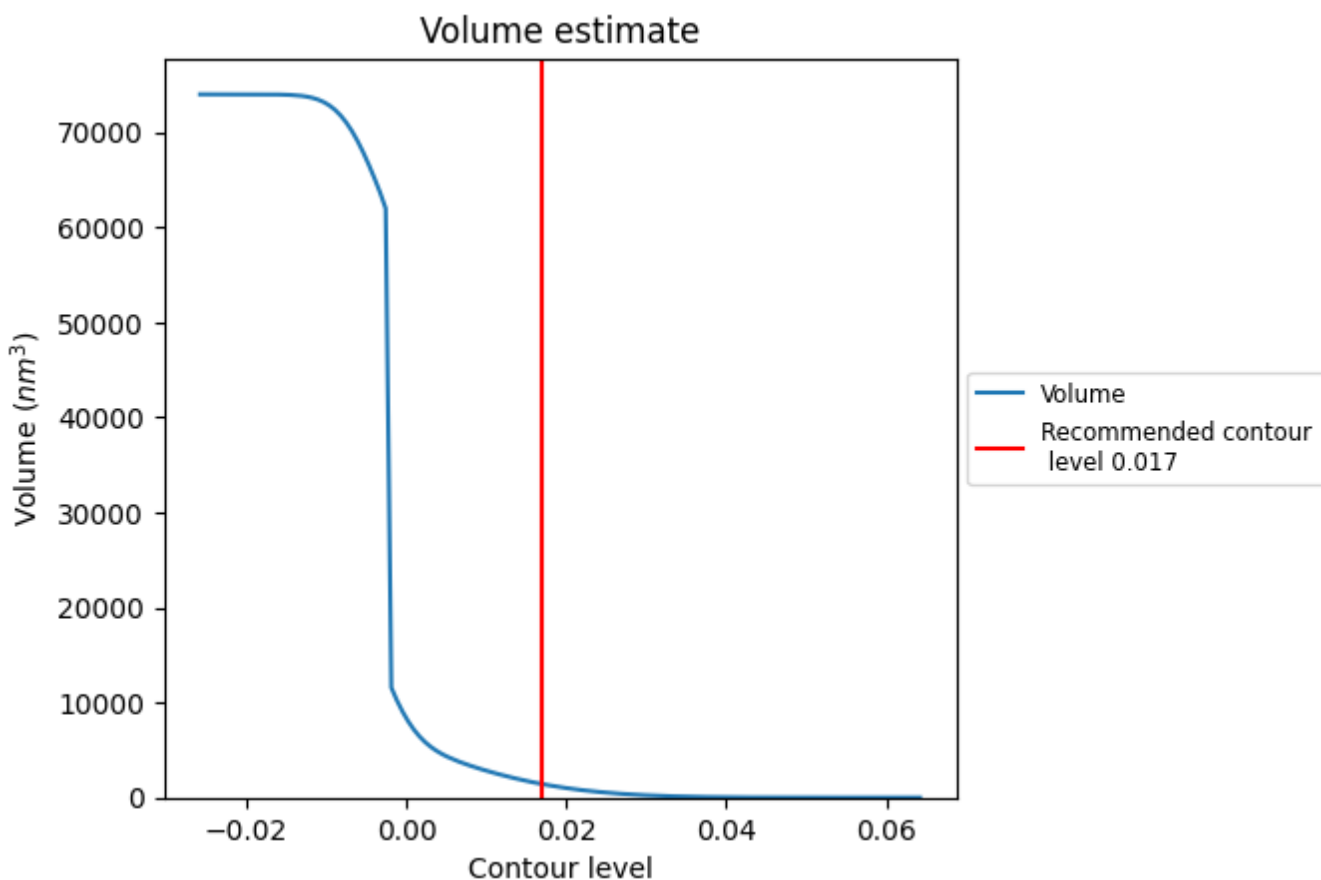
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

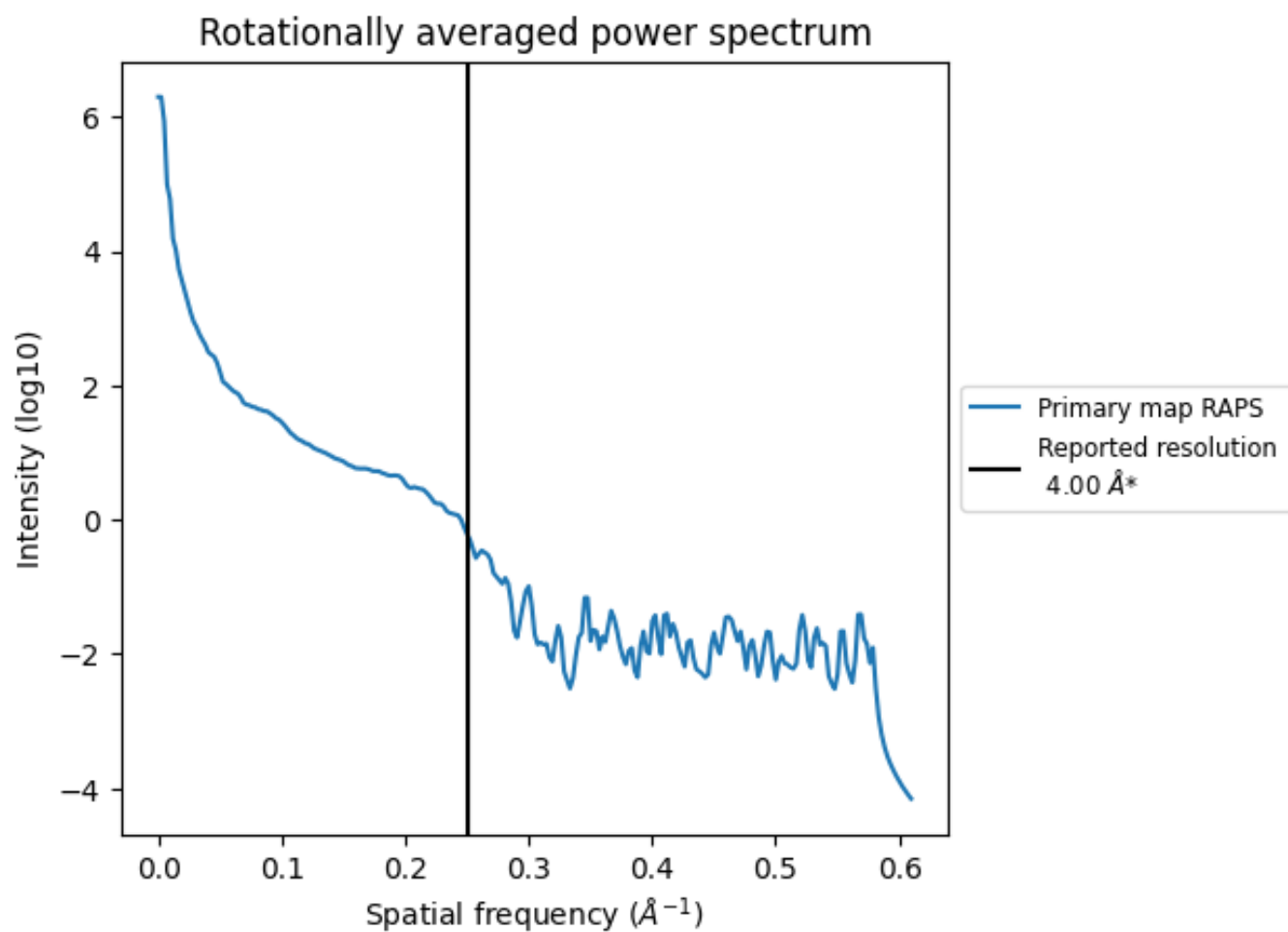
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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}

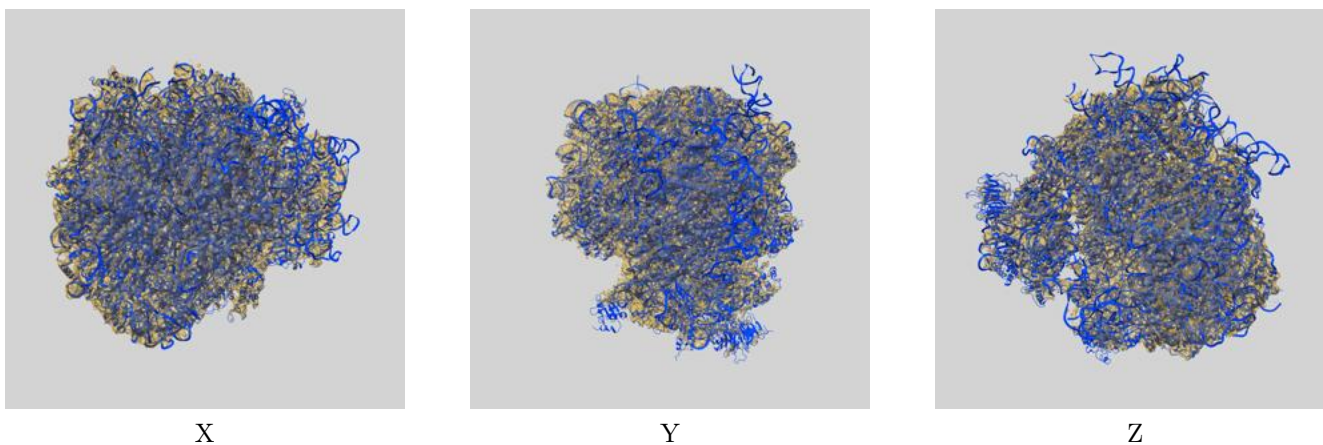
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

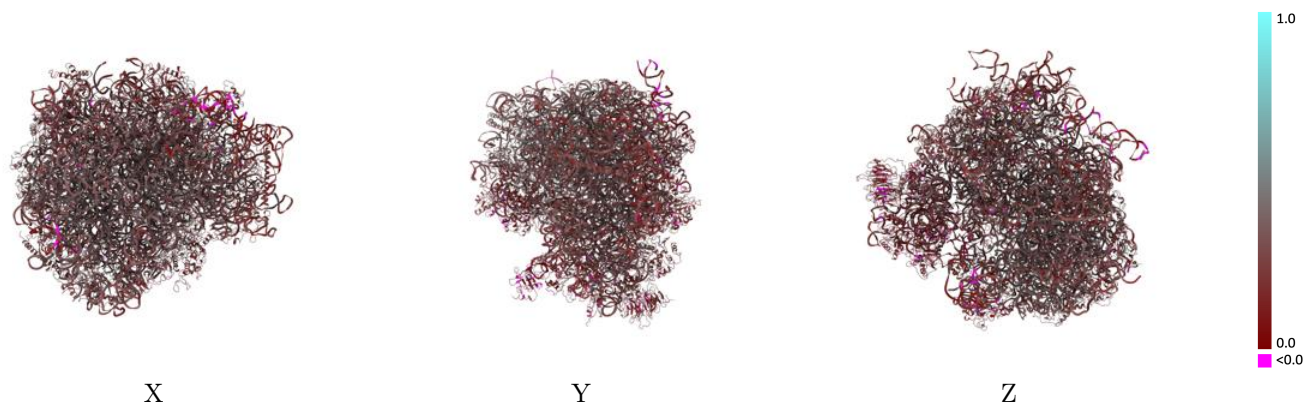
This section contains information regarding the fit between EMDB map EMD-6646 and PDB model 5JUT. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



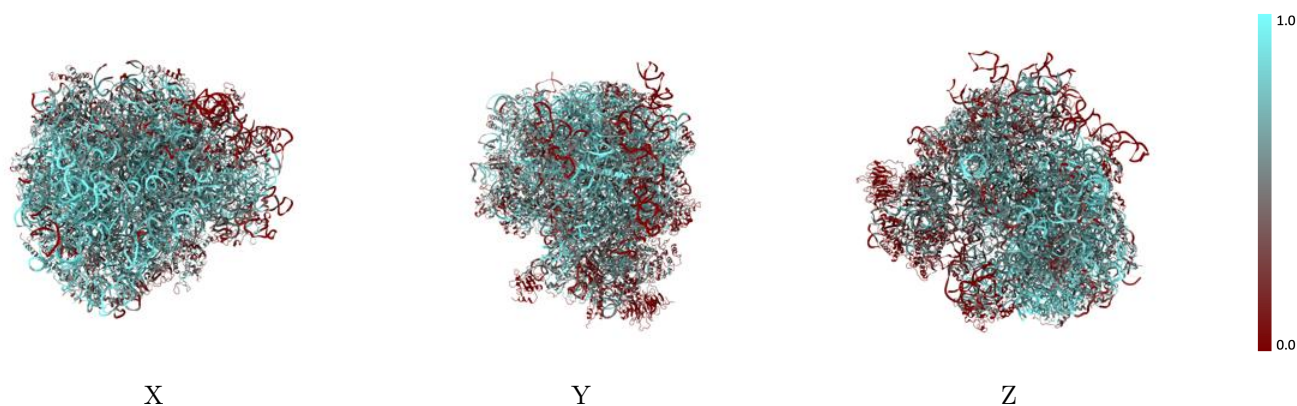
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



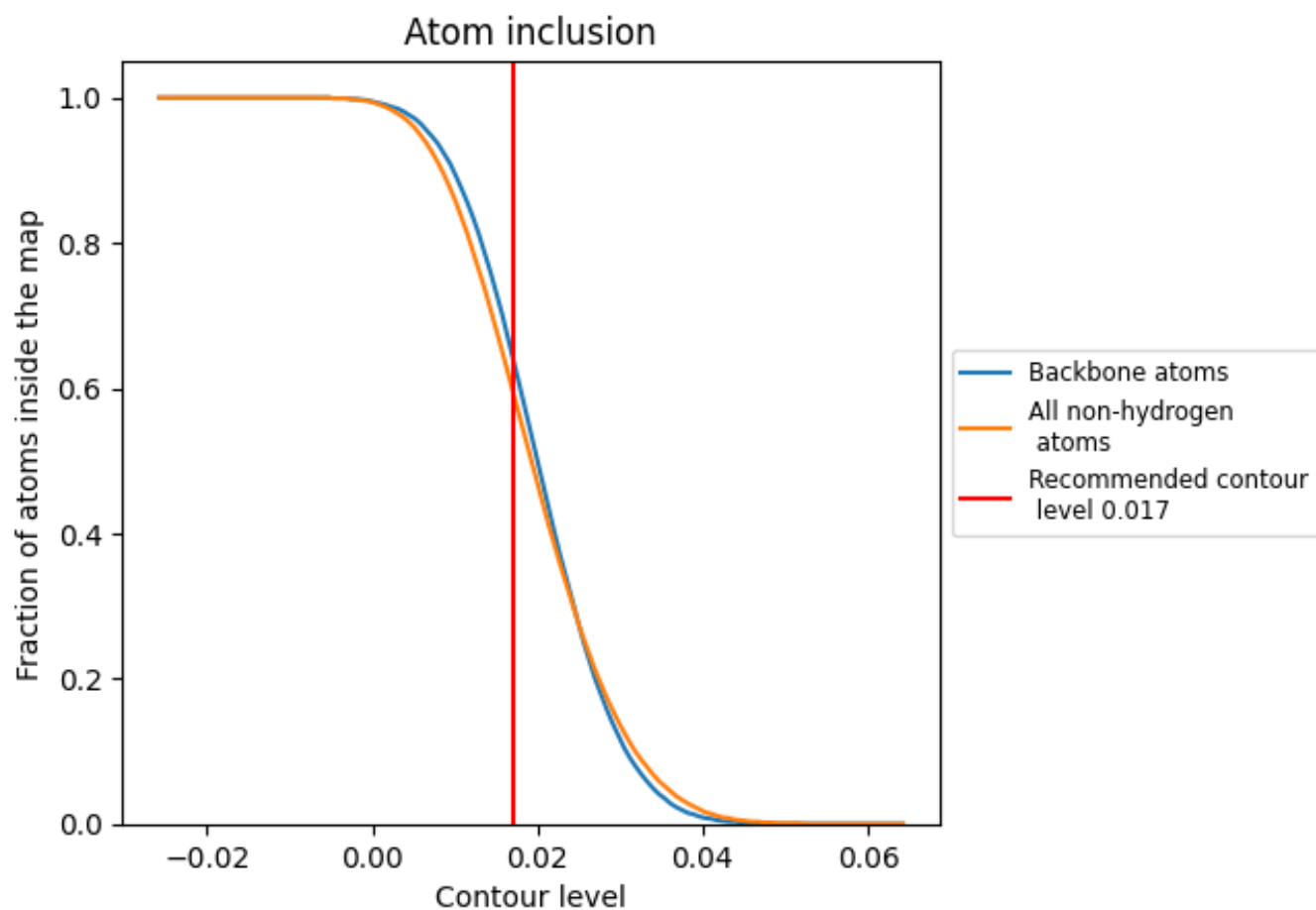
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6390	 0.2830
AA	 0.4570	 0.3800
AB	 0.2160	 0.2380
AC	 0.3010	 0.2220
B	 0.7890	 0.3290
BA	 0.5580	 0.3690
BB	 0.6070	 0.3230
BC	 0.2660	 0.2870
C	 0.7860	 0.3270
CA	 0.3040	 0.3340
CB	 0.1840	 0.2300
CC	 0.0110	 0.1740
D	 0.8690	 0.3200
DA	 0.6320	 0.3180
DB	 0.3500	 0.3030
DC	 0.4270	 0.2750
E	 0.0600	 0.2200
EA	 0.3990	 0.2820
EB	 0.1920	 0.2860
EC	 0.2650	 0.2170
F	 0.6080	 0.3450
FA	 0.6970	 0.3680
FB	 0.4160	 0.3150
G	 0.5720	 0.3680
GA	 0.6200	 0.3490
GB	 0.5430	 0.2960
H	 0.6330	 0.3620
HA	 0.6880	 0.3020
HB	 0.5650	 0.2080
I	 0.5660	 0.2980
IA	 0.6170	 0.3560
IB	 0.3690	 0.3360
J	 0.4760	 0.3230
JA	 0.7220	 0.3790

















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Chain	Atom inclusion	Q-score
JB	 0.0480	 0.1360
K	 0.5430	 0.3350
KA	 0.4620	 0.3680
KB	 0.4230	 0.2990
L	 0.4150	 0.2850
LA	 0.5180	 0.3080
LB	 0.4520	 0.3190
M	 0.4750	 0.3330
MA	 0.4320	 0.3040
MB	 0.1600	 0.1660
N	 0.5540	 0.3310
NA	 0.5970	 0.3350
NB	 0.1690	 0.2170
O	 0.5250	 0.2950
OA	 0.6010	 0.3360
OB	 0.1890	 0.2680
P	 0.2370	 0.1390
PA	 0.1270	 0.2740
PB	 0.1260	 0.1960
Q	 0.6960	 0.3410
QA	 0.6630	 0.3540
QB	 0.1730	 0.2100
R	 0.5380	 0.3130
RA	 0.6860	 0.3510
RB	 0.1610	 0.2210
S	 0.5320	 0.3200
SA	 0.2910	 0.3570
SB	 0.3880	 0.3130
T	 0.5450	 0.3480
TA	 0.7760	 0.3710
TB	 0.3710	 0.3170
U	 0.6520	 0.3510
UA	 0.5540	 0.3260
UB	 0.2890	 0.3150
V	 0.7260	 0.3680
VA	 0.2860	 0.2080
VB	 0.3230	 0.2910
W	 0.4570	 0.3020
WA	 0.0520	 0.2330
WB	 0.1010	 0.1970
X	 0.5500	 0.3390
XA	 0.2590	 0.2870

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Chain	Atom inclusion	Q-score
XB	 0.5160	 0.3390
Y	 0.5910	 0.3590
YA	 0.3960	 0.2850
YB	 0.4850	 0.3020
Z	 0.3700	 0.3140
ZA	 0.4350	 0.3260
ZB	 0.3810	 0.2640