



wwPDB EM Map/Model Validation Report ⓘ

Sep 29, 2016 – 03:52 PM EDT

PDB ID : 5JUS
EMDB ID: : EMD-6645
Title : Saccharomyces cerevisiae 80S ribosome bound with elongation factor eEF2-GDP-sordarin and Taura Syndrome Virus IRES, Structure III (mid-rotated 40S subunit)
Authors : Abeyrathne, P.; Koh, C.S.; Grant, T.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2016-05-10
Resolution : 4.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

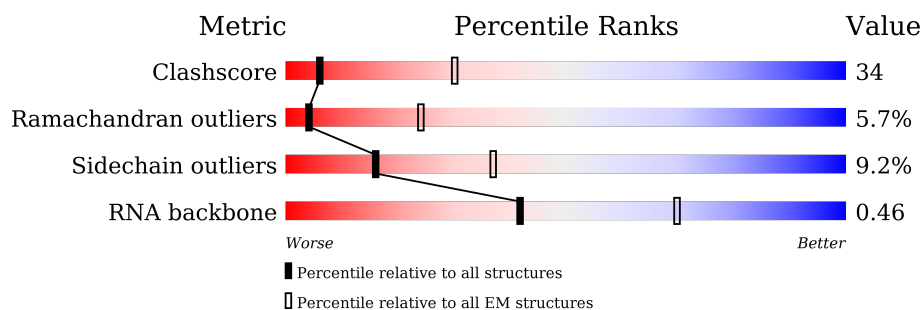
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



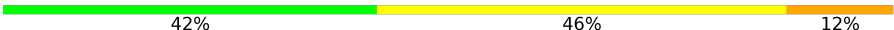


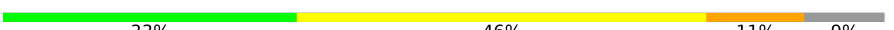
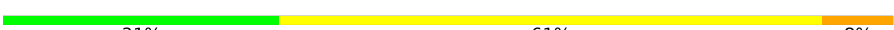
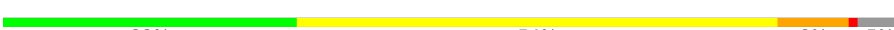




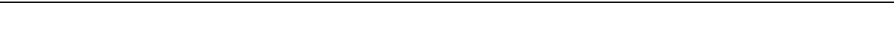

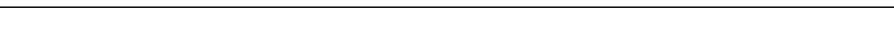
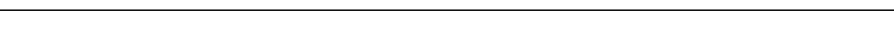










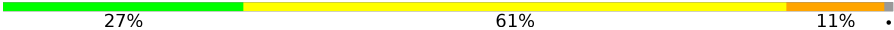
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1798	30% 57% 12% .
2	B	3396	21% 56% 19% . .
3	C	158	20% 62% 18% .
4	D	121	26% 63% 11% .
5	E	217	30% 40% 8% 21%
6	F	254	26% 62% 10% . .
7	G	387	29% 61% 9%
8	H	362	34% 56% 9% .




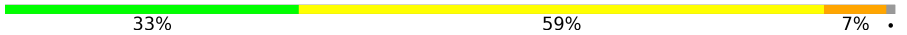
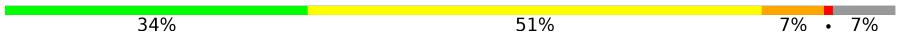
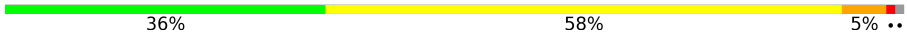
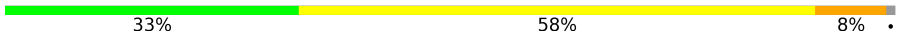
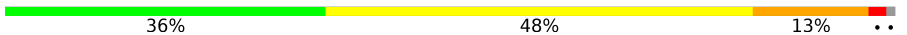

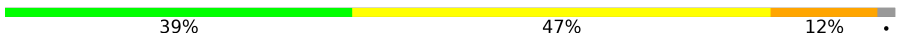


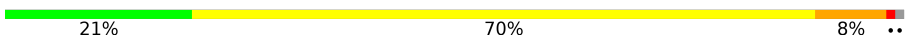
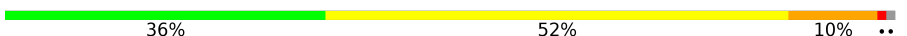


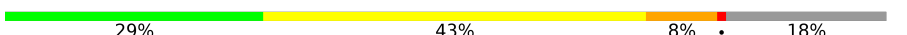








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Mol	Chain	Length	Quality of chain
9	I	297	
10	J	176	
11	K	244	
12	L	256	
13	M	191	
14	N	221	
15	O	174	
16	P	165	
17	Q	199	
18	R	138	
19	S	204	
20	T	199	
21	U	184	
22	V	186	
23	W	189	
24	X	172	
25	Y	160	
26	Z	121	
27	AA	137	
28	BA	155	
29	CA	142	
30	DA	127	
31	EA	136	
32	FA	149	
33	GA	59	


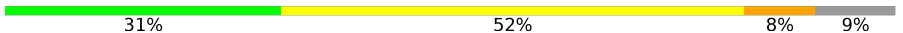
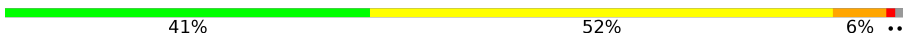



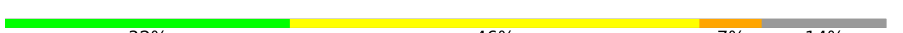




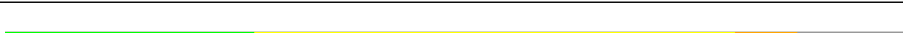













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Mol	Chain	Length	Quality of chain
34	HA	105	
35	IA	113	
36	JA	130	
37	KA	107	
38	LA	121	
39	MA	120	
40	NA	100	
41	OA	88	
42	PA	78	
43	QA	51	
44	RA	128	
45	SA	25	
46	TA	106	
47	UA	92	
48	VA	312	
49	WA	319	
50	XA	252	
51	YA	255	
52	ZA	254	
53	AB	240	
54	BB	261	
55	CB	225	
56	DB	236	
57	EB	190	
58	FB	200	

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

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 212680 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
1	A	1781	Total	C	N	O	P	0	0
			36760	16335	6359	12285	1781		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	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
21	U	183	Total	C	N	O	0	0
			1443	896	287	260		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

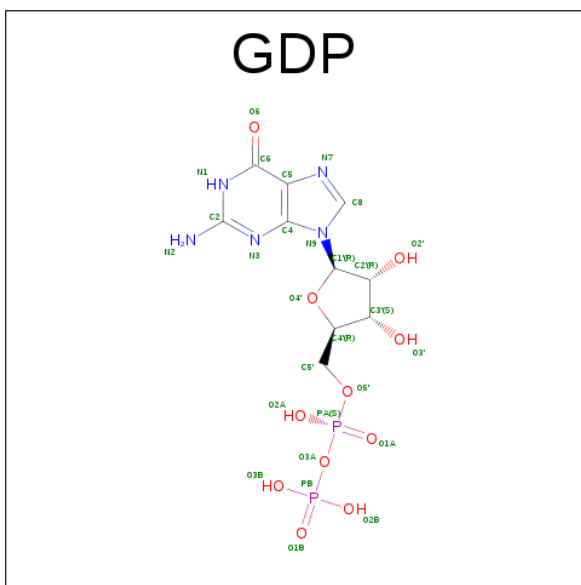
- Molecule 82 is a protein called yeast eEF2.

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

- Molecule 83 is a RNA chain called IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	EC	198	Total	C	N	O	P	0	0
			4129	1839	725	1367	198		

- Molecule 84 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

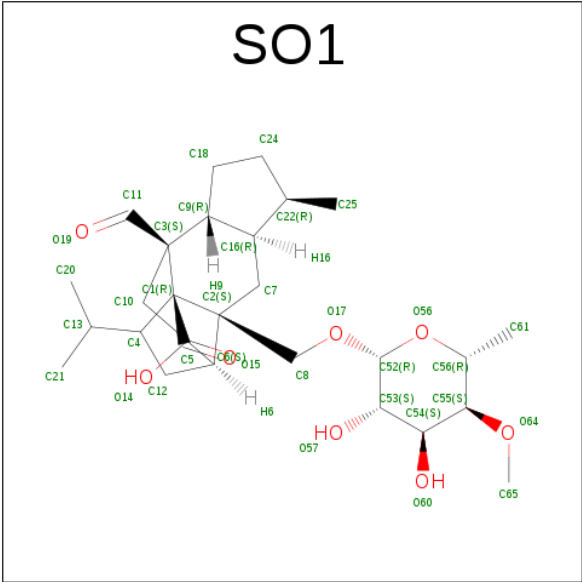


Mol	Chain	Residues	Atoms					AltConf
84	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

Mol	Chain	Residues	Atoms	AltConf
85	DC	1	Total Mg 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).

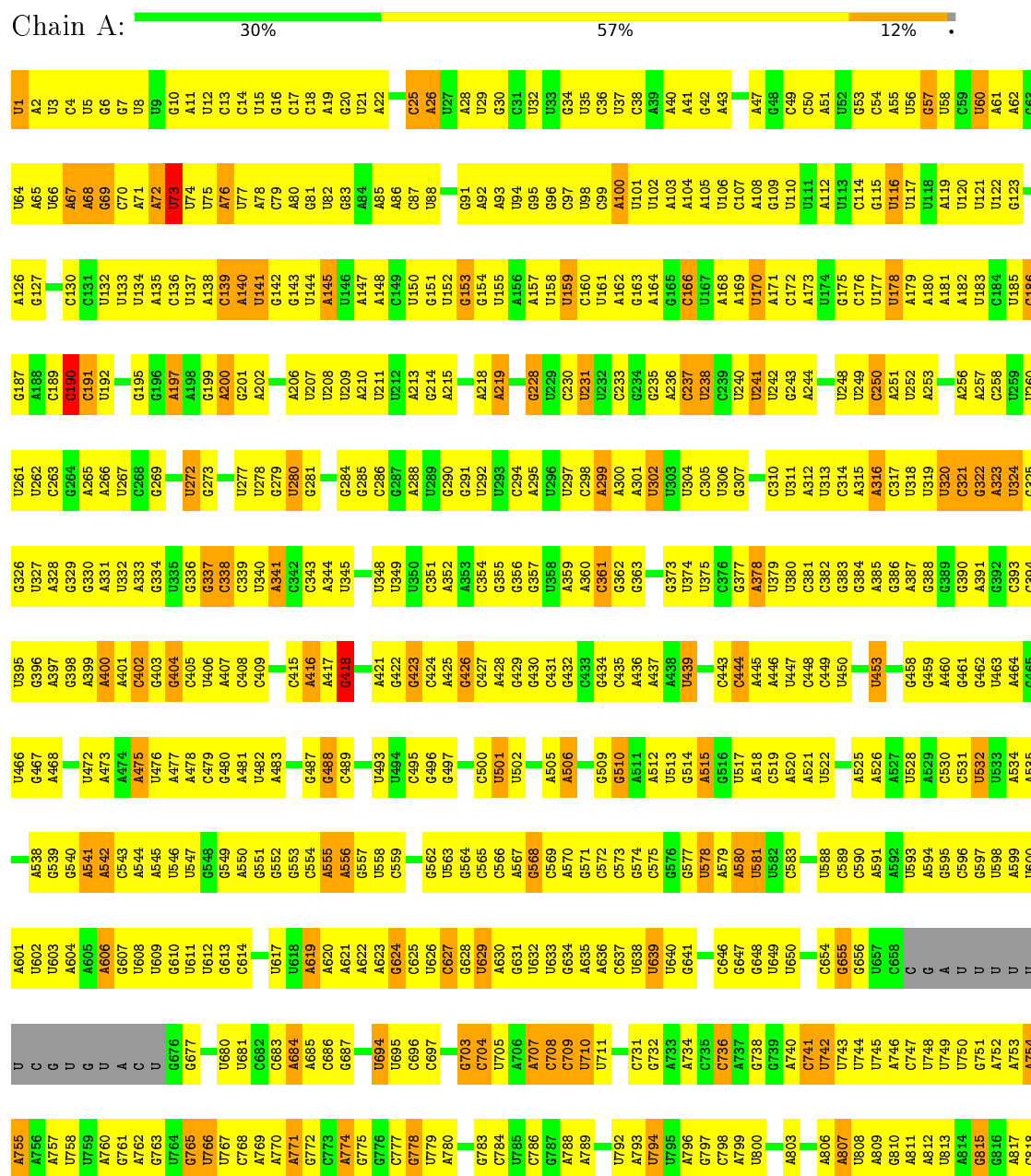


Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

3 Residue-property plots

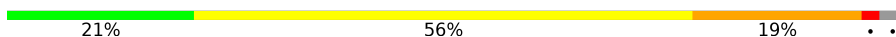
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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

Chain B:

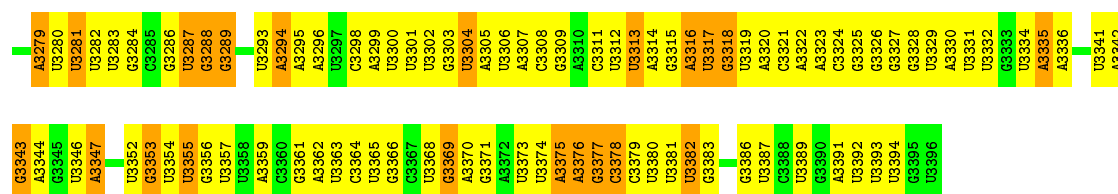


G	U	U	U	U	A6	C7	C8	C9	C10	A11	A12	A13	U14		G18	U19	A20	G21	G22	A23	A24	U25	A26	C27	C28	C29	G30	C31	U32	A33	A34	A35	A36		A39	A40	G41	C42	A43	U44	A45	U46	C47	A48	A49	U50	A51	A52	G53	C54	G55		G58	G59	A60	A61	A62	A63	A64
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U1109	C1045	A973	A913	G853	C788	G727	U654	G600	U536	G	A396	A327	C259	U194	C125	A65
U1110	A1046	G974	A914	G854	A789	G728	A665	A603	A537	U	A397	U328	U259	U195	U126	A66
U1111	A1047	C975	A915	U855	U790	C729	A666	A604	G538	U	A398	U329	U262	G196	G127	A67
A1112	A1048	U976	G916	G856	A791	C730	C667	G603	U	G	A399	U	C263	G197	G128	C68
G1113	G1049	C977	A917	G857	G792	U731	U669	U605	G542	U	G400	G335	A268	A198	U129	C69
U1114	U1050	G978	C918	A858	C793	C732	U669	C606	U	U	U401	A336	U269	A199	A130	A70
G1115	U1051	U979	U919	G859	U794	G733	C670	A607	C546	A	A402	G337	G269	C200	C131	A71
U1116	U1052	A980	A920	G860	G795	C734	U671	A608	G547	A	C403	A338	U270	A201	C132	C72
U1117	A1053	U981	A921	G861	U796	U735	U672	G609	G548	G	G404	C339	C271	G202	U133	C73
C1118	A1054	C982	U922	U862	U797	A736	U673	G610	G549	G	U405	C340	G272	G203	U134	G74
A1119	A1055	A983	C923	G863	U798	G737	G674	A611	U550	G	G406	C341	A273	G204	C135	G75
C1120	U1056	G984	G924	G864	G799	A738	C675	U612	A551	A	A407	A342	G274	G136	G136	G76
U1121	U1057	U985	A925	U865	G800	G739	G676	G613	G552	A	A408	U343	U275	C208	G137	A77
U1122	U1058	U986	A926	A866	A801	G740	A677	G614	U553	U	A409	A344	U276	A209	U138	U78
U1123	G1059	U987	C927	G867	C802	U741	U678	U615	A554	C	U410	G345	G277	U210	G139	U79
U1124	U	U988	C928	C868	C803	G742	U679	U616	U555	U	U411	G346	U278	A211	C140	G80
U1125	A1062	A989	A929	G869	C804	C743	U680	U617	U556	U	G412	G347	U279	G212	C141	C81
G1126	G1063	U990	U930	G870	G805	A744	U681	U625	U557	U	U413	G348	U280	A213	C142	C82
U1127	A1064	G991	C931	U871	A806	C745	U682	U626	U558	U	U414	G349	G281	G214	G143	U83
U1128	A1065	A992	U932	U872	A807	A746	U683	A621	U559	U	U415	C350	G282	G215	A144	U84
A1129	G1066	G993	A933	C873	A808	C747	U684	A622	U560	U	U416	C351	G283	G216	G145	A85
A1130	U1067	G994	G934	U874	G809	U748	G685	U623	C561	G	A417	G352	A284	U217	C146	G86
G1131	C1068	U995	U935	G875	A810	C749	U686	G624	C562	G	U418	G353	A285	G218	U147	U87
C1132	C1069	A996	A936	A876	U811	G750	U689	G625	U563	U	G421	U354	U286	G219	G148	A87
A1133	U1070	A997	G937	C877	G812	U	A690	U626	G564	U	A422	U355	G287	A219	U149	A88
G1134	U1071	A998	C938	G878	G813	C753	A691	U627	U565	U	A423	C356	C288	G220	U150	A89
A1135	G1072	U	U939	U879	U814	G754	A692	A628	G566	U	A424	U359	A289	A221	A151	C90
A1136	U1073	G1001	G940	G880	G815	A755	A693	G629	G567	U	G425	U359	G290	U223	U152	G91
C1137	U1074	A1002	G941	C881	A816	U756	C694	A630	G568	U	G426	A361	C291	C224	U153	G92
U1138	A1075	A1003	U942	A882	A817	C757	C695	U631	A569	U	G427	U362	U292	C225	G155	G93
G1139	C1076	U1004	U943	A883	C818	G758	C696	G632	A570	U	C427	U363	C293	G226	G156	G94
G1140	U1077	G1005	C944	A884	U819	U759	A697	C633	U571	U	A428	G363	U294	G227	A157	G95
A1143	U1078	A1006	C945	U885	A820	G760	U698	C634	A572	U	U429	G364	A295	U228	G158	U97
U1144	U	U1007	U946	C886	U821	A761	A699	G635	C573	U	U430	G365	A296	G229	A159	G98
G1145	U1082	U1008	G947	G887	G822	U762	C700	C636	U574	U	U431	A366	G297	U230	G160	A99
C1146	G1083	A1009	C948	A888	C823	G763	G701	C637	G575	U	G432	A367	U298	G231	G161	A100
G1147	A1084	G1010	C949	U889	C824	U764	C702	C638	C576	U	A433	G368	G299	G232	G162	G101
U1148	U	C1016	A951	G890	U825	C765	G703	G639	C577	U	A438	A369	G300	C233	C163	G102
G1149	U	C1017	A952	G891	U829	U766	U704	U640	A578	U	A439	U370	G301	G237	A164	G103
A1150	U1088	G1018	G953	C893	A830	C768	A706	U642	C580	U	U440	A372	U305	A238	C105	G104
U1089	G1089	G1019	U954	G894	A830	G769	U707	U643	U581	U	U441	A373	U306	A239	C106	A105
A1153	U	U1022	U956	A896	G833	G770	A708	G644	G582	U	U442	A374	A307	G240	U169	A107
U1154	C1092	A1154	C1023	A896	U834	A771	A709	A645	G583	U	G443	A375	A308	G241	G170	A108
C1155	A1093	C1023	C957	U897	G835	U772	A710	A646	G584	U	U444	G376	U311	C242	A109	A109
U1094	U1094	G1024	C958	U898	A836	G773	A711	A647	A585	U	G445	A377	U311	G243	G175	G110
G1157	U1095	A1025	C959	U899	A837	G774	G712	C648	G586	U	U446	A378	U312	G244	C176	C111
A1158	U1096	U1096	U960	G900	G838	A775	U713	C649	U587	U	U447	A379	U313	G245	G176	C112
A1159	G1097	G1029	C961	G901	C839	U776	G714	C650	G588	U	C453	C379	U314	U246	U181	G113
C1160	A1098	A1030	A962	G902	C840	U777	A715	G651	A589	U	C	U380	C315	U246	U182	A114
A1161	A1099	U	G963	U903	A841	U778	A716	G652	G590	U	C	U381	U316	U247	U183	A115
U1162	U1100	U1033	G964	A904	G842	G779	G717	A653	G591	U	U	U382	A317	U248	C185	A116
A1163	G1101	U1034	A965	U905	A843	A780	G718	C654	A592	U	U	G383	A318	U250	U186	A117
G1164	A1102	U966	U966	A906	G781	G781	U719	C655	C593	U	G	U384	A319	U251	U187	U118
A1165	A1103	U1039	A967	G907	A846	U782	A720	A656	U594	U	U	G388	A320	A252	U188	U119
G1166	G1104	A1040	C968	G908	A847	A783	G721	U657	G595	U	U	U389	A321	A253	G189	G120
U1167	A1105	U1041	C969	G909	A848	A784	U722	U658	C596	U	U	G389	A322	A254	U190	A121
U1168	G1106	U1042	A970	G910	U850	A785	U723	U660	U598	U	C	G390	A323	A255	U191	A122
A1169	C1107	C1043	G971	C911	U851	A786	U724	U662	U599	U	C	G394	A324	A256	G256	A123
A1170	U1108	U1044	A972	G912	U852	G787	G726	C663	C599	U	U	U395	A325	A257	U192	A124

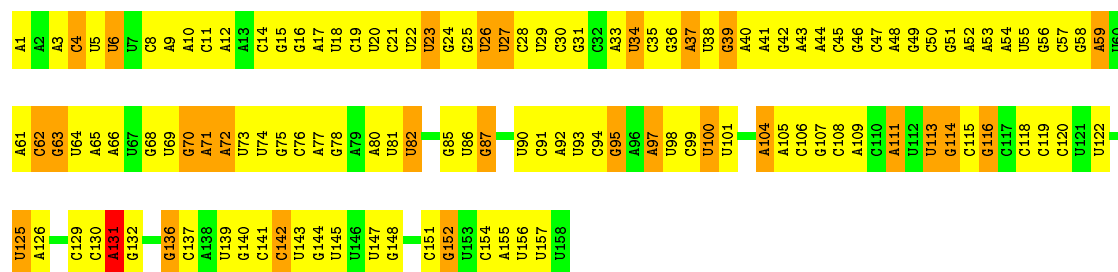
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A2182	C2118	U1880	U1819	A1752	U1616	A1546	G1483	C1359	C1238	G1172
A2183	A2119	A1881	U1820	G1753	U1629	G1547	U1494	C1360	C1239	U1173
A2184	A2120	G1882	U1821	G1754	U1630	C1548	C1423	U1361	G1174	G1174
G2185	G2121	A1883	A1822	C1755	C1631	U1549	U1425	G1362	U1241	C1175
U2186	G2122	A1884	A1823	C1756	G1631	C1550	G1487	A1363	U1242	C1176
U2187	G2123	U1885	U1824	A1757	A1632	C1551	U1427	C1364	G1177	G1177
A2188	G2124	A1886	G1825	C1758	C1633	G1552	A1428	G1365	A1245	G1178
U2189	U2127	A1887	C1826	C1759	G1634	U1553	G1429	A1366	G1246	A1179
C2192	C2128	U1888	C1827	U1765	G1635	U1554	A1491	G1367	U1247	U1180
U2193	U2129	G1889	A1828	G1766	U1636	U1555	G1492	C1368	C1248	U1181
G2194	G2130	U1890	G1829	C1767	A1637	G1556	G1493	A1369	G1249	A1182
C2195	A2131	U1891	U1830	U1768	A1638	A1557	U1494	G1370	G1250	C1183
C2196	U2132	U1892	U1831	U1769	C1639	A1558	U1495	C1371	A1251	A1184
C2197	U2133	A1893	C1832	U1770	G1640	C1562	C1496	C1372	A1252	C1185
C2198	G2134	A1894	G1833	G1771	A1641	U1563	C1437	G1313	U1253	C1186
G2199	U2135	G1895	U1834	A1772	A1642	C1563	U1438	C1314	G1254	C1187
C2200	C2136	G1896	A1835	C1773	G1644	U1564	U1439	U1315	C1255	U1188
G2201	U2137	G1897	C1836	C1774	U1645	G1565	G1440	C1316	G1256	C1189
G2202	U2138	A1900	U1837	G1775	G1646	A1566	G1441	C1317	C1257	A1190
C2203	A2139	G1901	U1838	C1779	G1647	U1567	U1442	A1318	U1258	U1191
U2204	U2140	G1902	A1839	G1780	A1648	U1568	G1443	G1319	A1259	C1192
C2205	G2141	G1903	U1840	G1781	G1649	U1569	G1444	C1320	A1260	A1193
U2206	A2142	U1904	A1841	A1782	G1650	U1570	U1445	G1321	G1261	G1194
G2207	A2143	G1905	A1842	G1783	U1651	A1571	A1446	G1322	G1262	A1195
A2208	A2144	G1906	C1843	U1784	G1652	U1572	G1447	C1323	A1263	C1198
C2209	U2145	C1907	G1844	U1785	G1653	U1573	U1448	U1324	G1264	C1199
C2210	C2146	G1908	G1845	G1786	A1654	U1574	A1449	U1325	A1265	G1200
G2211	A2147	A1909	C1846	G1787	G1655	G1575	G1450	A1326	G1266	A1201
C2212	U2148	U1910	A1847	U1788	G1656	C1576	U1451	C1327	U1267	C1202
G2213	A2149	U1911	G1848	G1789	A1657	C1577	U1452	G1328	G1268	A1203
C2214	G2150	U1912	C1849	U1790	C1658	U1578	A1453	U1329	U1269	A1204
A2215	C2151	G1913	A1850	A1723	U1659	A1579	A1454	A1330	A1270	U1208
C2216	A2152	G1914	G1851	U1724	C1660	C1581	U1455	G1331	C1271	G1209
U2217	U2153	U1915	C1852	C1725	G1661	C1582	A1456	A1332	A1272	U1210
G2218	U2154	C1916	U1853	C1726	G1662	A1583	U1457	C1333	A1273	U1211
C2219	G2155	C1917	C1854	G1727	C1663	U1584	U1458	G1334	C1274	G1212
U2220	C2156	U1918	U1855	G1728	U1664	C1585	C1459	C1335	C1275	U1213
A2221	A2157	G1919	C1856	A1729	G1665	G1586	A1460	U1336	U1276	A1214
C2222	U2158	U1920	C1857	G1730	C1666	A1587	A1461	A1337	C1277	G1215
A2223	U2159	A1921	A1858	U1731	G1667	U1588	U1462	C1338	A1278	U1216
C2224	G2160	U1922	A1859	U1732	C1668	A1589	G1463	C1339	C1279	U1217
U2225	C2161	C1923	G1860	G1733	U1669	G1590	G1464	A1401	C1280	U1218
U2226	G2162	U1924	G1861	G1734	C1670	G1591	U1465	C1402	G1281	C1219
C2227	U2163	U1925	U1862	G1735	C1671	G1592	G1466	C1403	C1282	A1220
A2228	A2164	C1926	G1863	G1736	U1672	A1593	G1467	G1404	C1283	A1221
C2229	G2165	G1927	A1864	U1737	U1673	A1594	A1468	A1405	G1284	G1222
U2230	A2166	G1928	C1865	C1738	U1674	U1595	C1469	A1406	G1285	A1223
C2231	A2167	U1929	A1866	U1739	G1675	C1596	U1470	A1407	A1286	A1224
A2232	U2168	A1930	A1867	U1740	U1676	C1597	U1471	G1408	U1287	G1225
C2233	A2169	U1931	G1868	U1741	G1678	U1532	U1472	U1347	U1288	U1226
G2234	U2170	A1932	C1869	U1742	U1680	A1533	U1473	U1348	G1289	G1230
C2235	G2171	U1933	U1870	G1743	U1681	A1534	G1474	A1349	A1290	A1231
G2236	G2172	C1934	U1871	G1744	A1682	A1535	A1475	A1350	A1291	A1232
U2173	U2173	G1935	A1872	C1745	G1683	A1536	G1476	U1351	U1292	G1233
G2174	G2173	A1936	U1873	U1746	C1684	A1537	A1477	A1352	U1293	A1294
U2175	U2174	U1937	A1874	G1747	U1685	U1538	C1478	A1353	G1295	G1234
A2242	U2176	G1938	U1875	G1748	U1686	U1539	U1479	G1354	U1296	U1235
C2243	U2177	U1939	U1876	A1749	U1687	U1540	U1480	A1355	G1297	A1236
A2244	G2177	G1940	G1877	U1750	U1688	A1541	G1481	U1356	C1298	
			G1878			A1612				

C3212	G3147	G3083	U3020	U2954	U2891	G2831	G2770	A2704	U2641	G2576	U2510	A2439	G2376	U2314	C2245
A3213	U3146	C3084	A3021	U2955	A2892	C2832	U2771	A2705	A2642	C2577	A2511	A2440	G2377	G2315	G2246
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A3215	A3150	A3086	G3026	G2957	C2894	G2834	C2773	C2707	C2644		U2513	G2442	U2379	A2317	C2248
G3216	U3151	G3087	A3027	A2958	G2895	U2835	C2774	G2714	C2645	U2581	U2514	A2443	U2380	U2318	G2249
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A3218	U3153	C3089	G3029	C2960	G2898	A2837	C2776	A2716	A2647	G2585	U2516			A2320	G2251
G3219	C3154	U3090	A3030	G2961	G2899	G2838	G2777	U2717	G2648	U2586	U2517	G2450	A2384	A2321	A2252
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G3230	C3166	G3102	C3039		A2910	G2848	G2787	A2727		U2596	G2528	A2462	G2395	C2332	U2269
G3231	A3167	A3103	A3040	U2975	A2911	G2849	C2788	G2728	G2660		A2529		G2396	U2334	A2270
A3232	U3168	U3104	U3041	A2976	G2912	G2850	U2789	G2729	G2661	C2600	G2530	G2466	A2397	U2335	A2271
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G3241	U3175	U3111	A3048	U2985	A2919	C2857	A2736	A2736	U2668	G2607	U2538	C2473	A2404	A2342	C2278
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A3243		A3106	C3043	U2987	G2914	U2859	A2738	A2738	G2670	A2609	A2540	G2475	C2406	U2344	A2280
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G3246	G3181	C3116	G3053	G2990	U2923	G2862	C2741	C2741	A2673	U2612	U2543	C2478	G2409	U2347	
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	A3187	A3122	G3059	U2996	C2931	U2868	U2747	U2747	U2682	G2618	G2549	A2484	C2415	G2353	A2291
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G3256	G3189		G3061	U2998	A2933	G2870	G2749	G2749	U2683	G2620	U2551	A2486	U2417	G2355	U2293
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C3261		U3131	U3066	G3003	G2938	U2875	G2754	G2754	U2688	C2625		C2492	C2422	C2360	U2298
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G3263	U3198	C3133	U3068	A3005	A2940	G2877	C2756	C2756	G2690	C2627		C2495	A2424	C2362	A2300
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A3267	G3202	C3137	A3073	G3009	U2944	C2881	A2820	C2760	A2694	U2631		U2499	U2428	C2366	C2304
A3268	U3203	U3138	G3074	U3010	G2945	U2882	G2761	G2761	A2695	G2632	C2567	A2500	G2429	A2367	C2305
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G3271	C3206	A3141	A3077	G3013	G2948	G2885	G2764	G2764	G2698	A2635	U2570	G2503		G2370	C2308
U3272	U3207	A3142	U3078	U3014	U2949	U2886	C2825	C2765	G2699	A2636	U2571	U2504		G2371	A2309
G3273	G3208	C3143	U3079	G3015	G2950	A2887	C2826	U2766	G2700	A2637	C2572	U2505	U2432	A2372	U2310
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U3275	C3210	C3145	C3081		G2952	U2889	U2768	U2768	A2702	C2639	G2574		U2437	C2374	A2312
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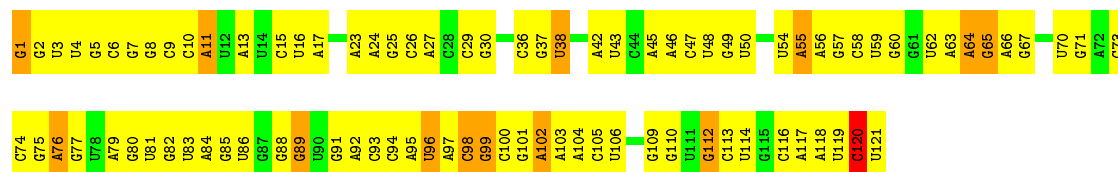
• Molecule 3: 5.8S ribosomal RNA

Chain C: 20% 62% 18%



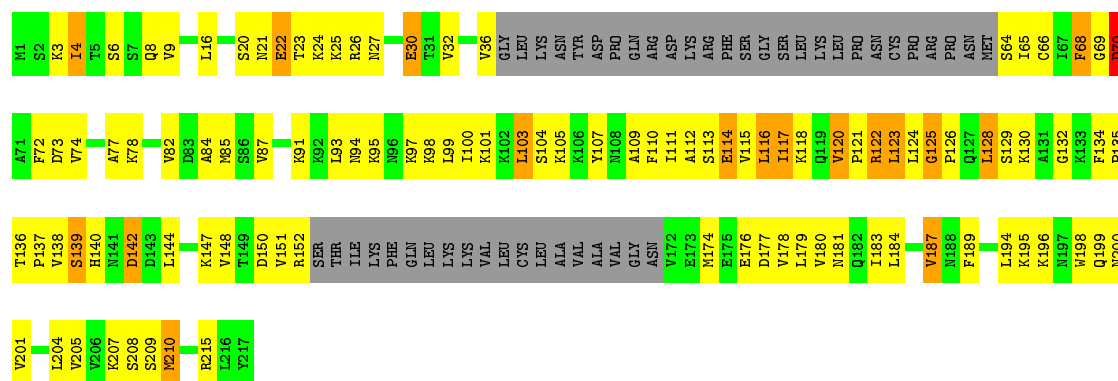
• Molecule 4: 5S ribosomal RNA

Chain D: 26% 63% 11%



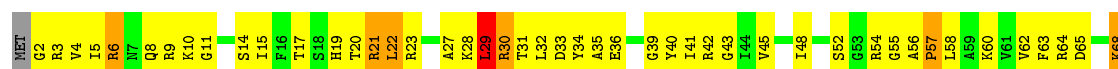
• Molecule 5: uL1 (yeast L1)

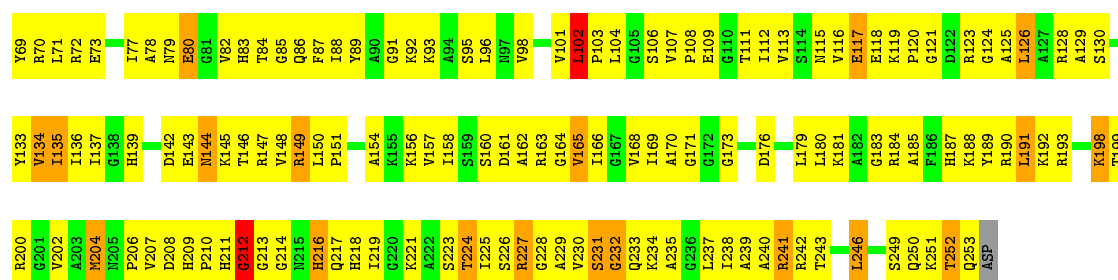
Chain E: 30% 40% 8% 21%



• Molecule 6: uL2 (yeast L2)

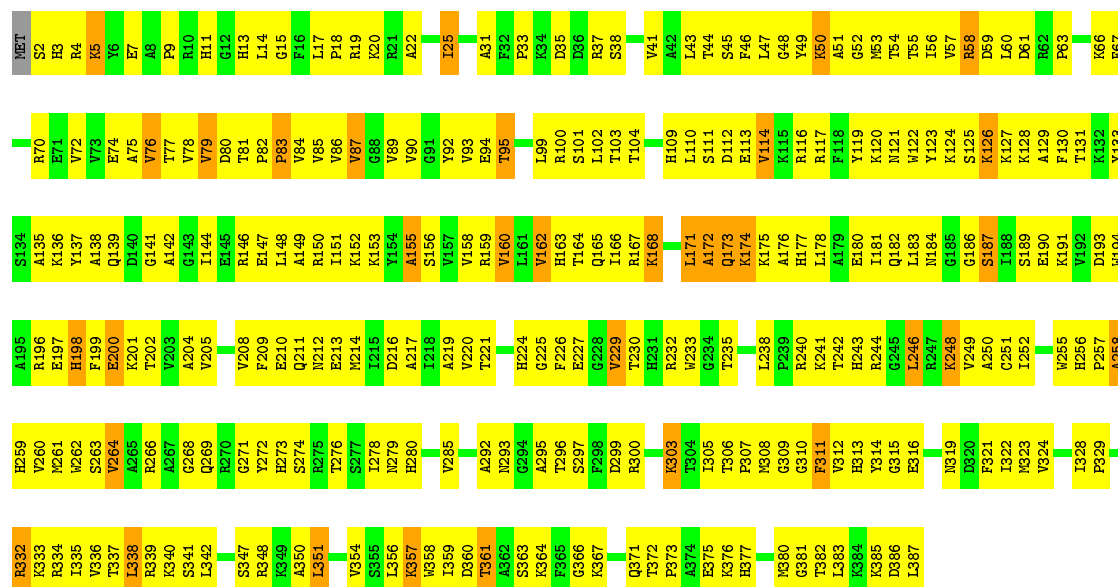
Chain F: 26% 62% 10%





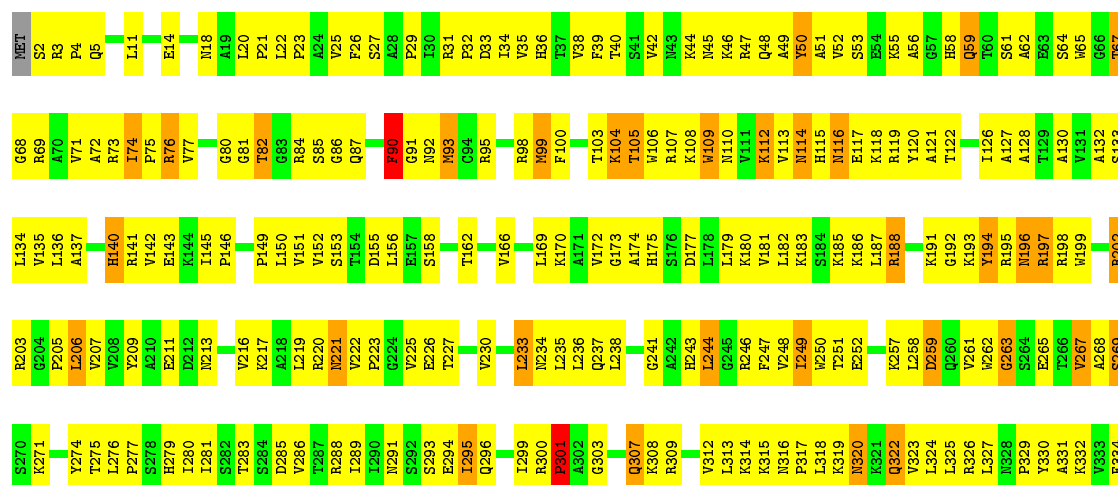
• Molecule 7: uL3 (yeast L3)

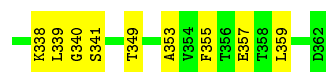
Chain G: 29% 61% 9%



• Molecule 8: uL4 (yeast L4)

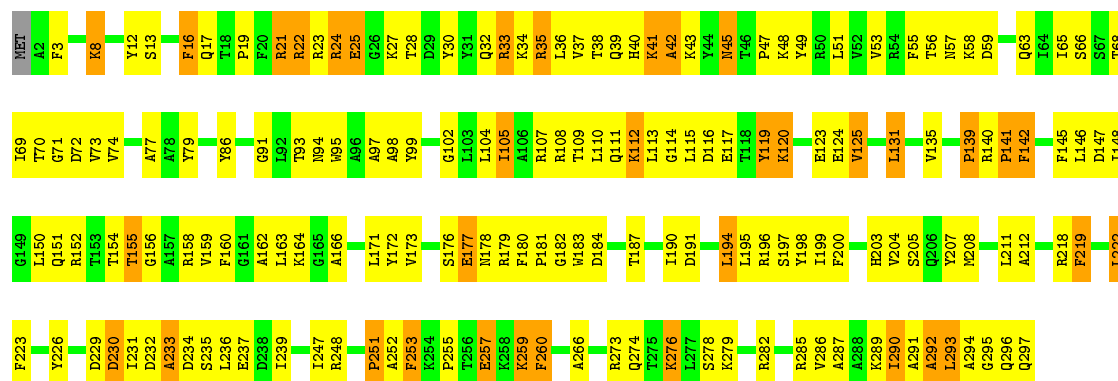
Chain H: 34% 56% 9%





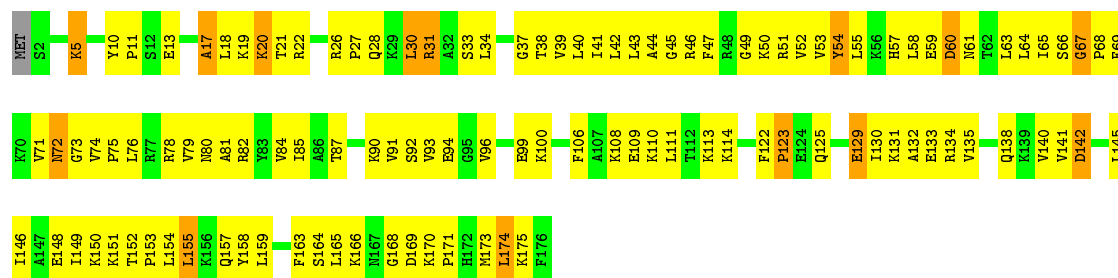
• Molecule 9: uL18 (yeast L5)

Chain I: 42% 46% 12%



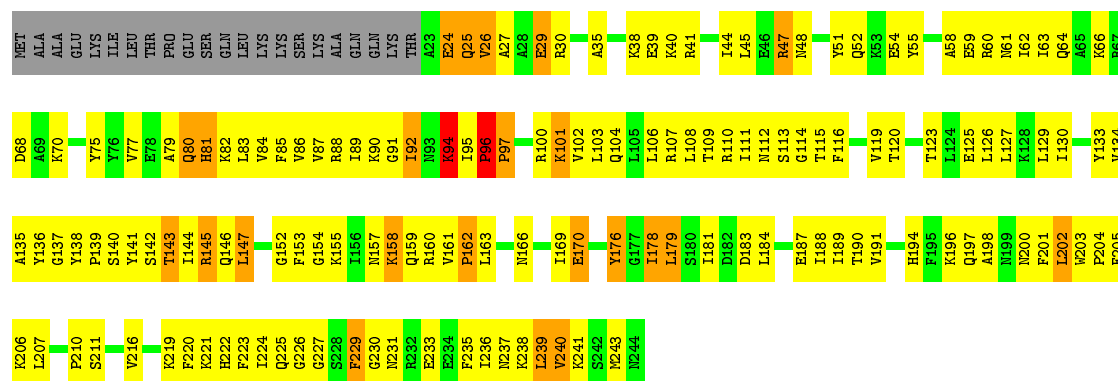
• Molecule 10: eL6 (yeast L6)

Chain J: 35% 57% 8%



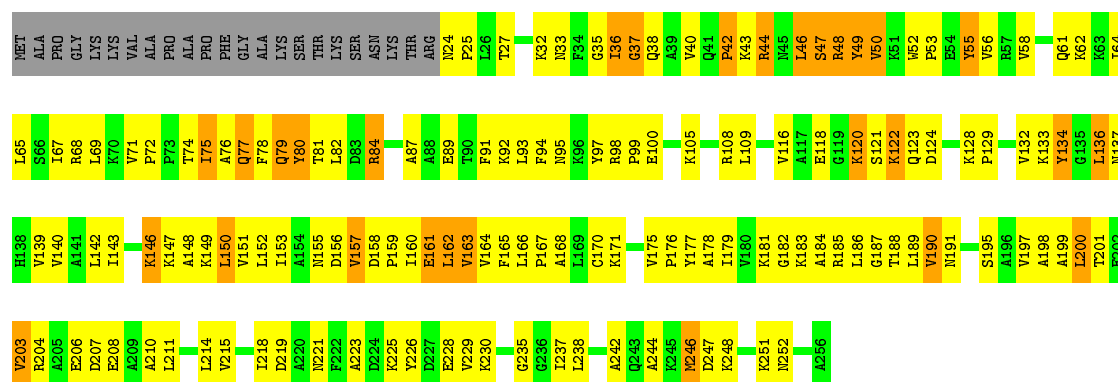
• Molecule 11: uL30 (yeast L7)

Chain K: 30% 51% 9% 9%



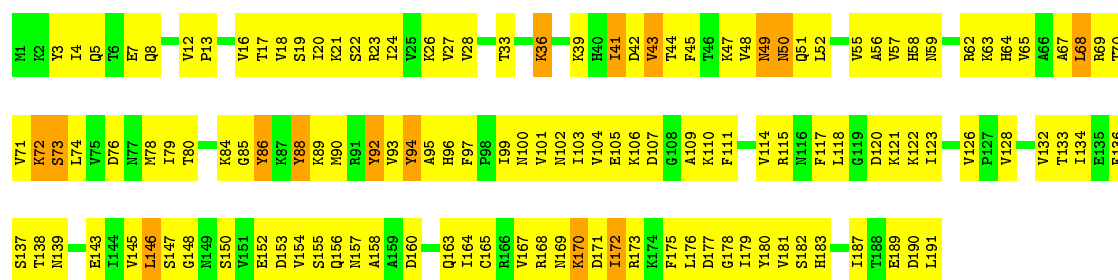
• Molecule 12: eL8 (yeast L8)

Chain L: 33% 46% 11% 9%



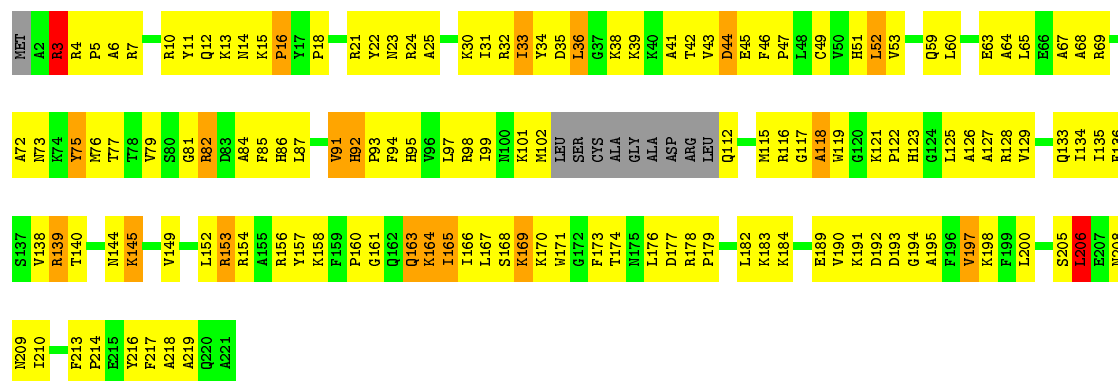
• Molecule 13: uL6 (yeast L9)

Chain M: 31% 61% 8%



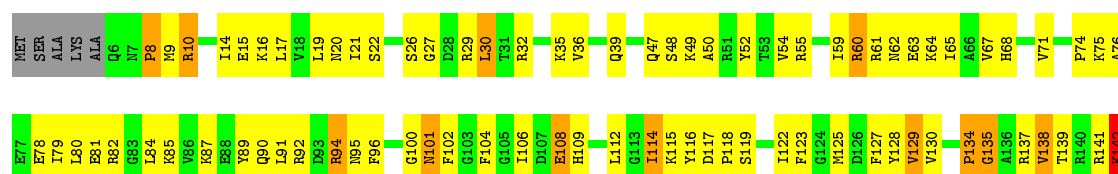
• Molecule 14: uL16 (yeast L10)

Chain N: 33% 54% 8% 5%



• Molecule 15: uL5 (yeast L11)

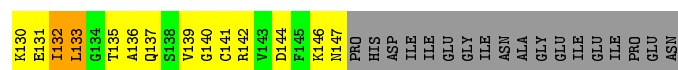
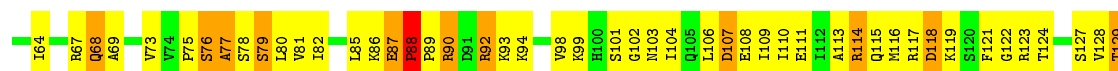
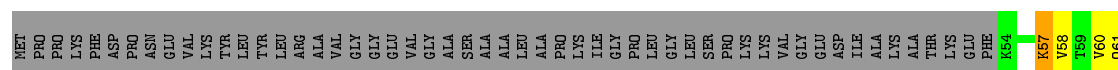
Chain O: 41% 48% 7%





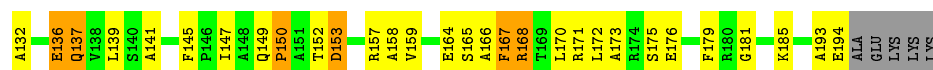
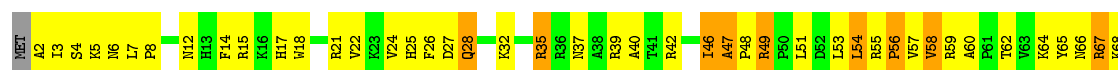
• Molecule 16: uL11 (yeast L12)

Chain P: 17% 31% 8% 43%



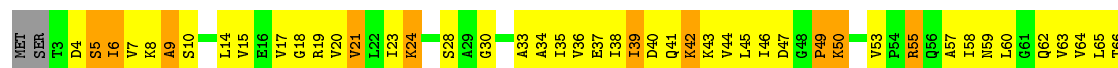
• Molecule 17: eL13 (yeast L13)

Chain Q: 36% 50% 11%



• Molecule 18: eL14 (yeast L14)

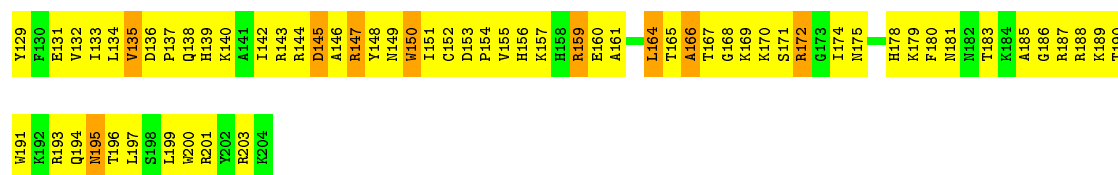
Chain R: 29% 58% 12%



• Molecule 19: eL15 (yeast L15)

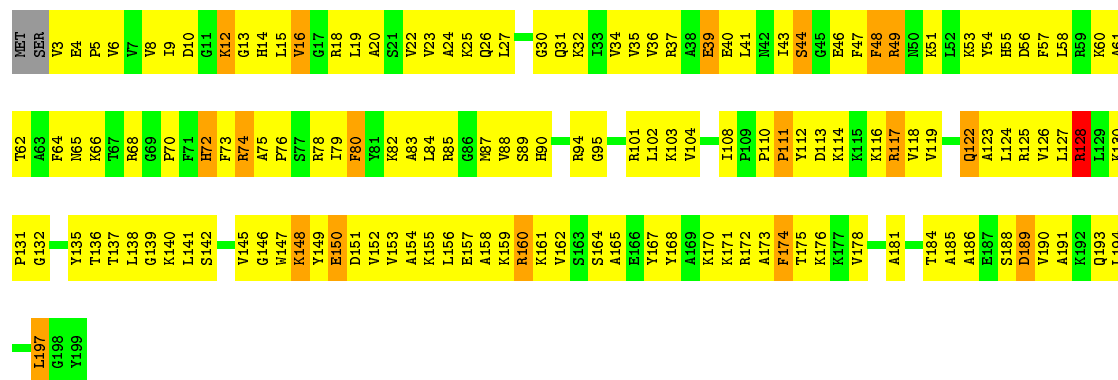
Chain S: 23% 65% 12%





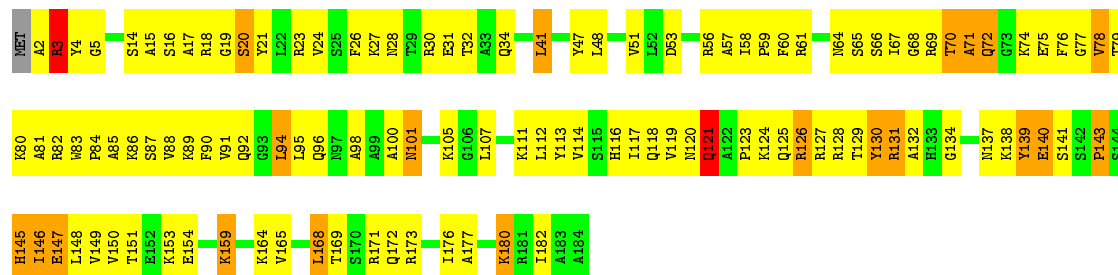
• Molecule 20: uL13 (yeast L16)

Chain T: 27% 62% 9% ..



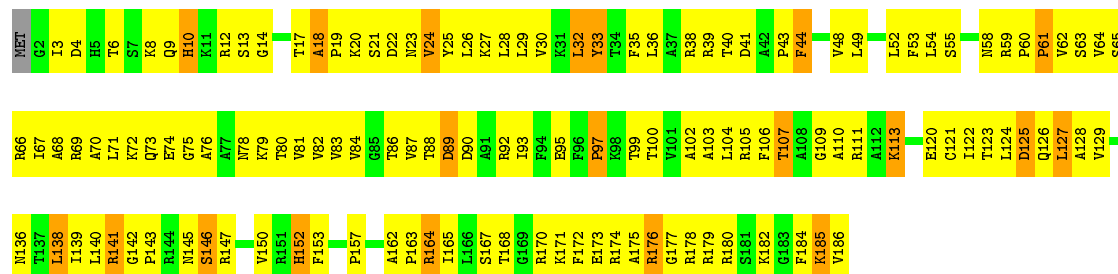
• Molecule 21: uL22 (yeast L17)

Chain U: 36% 51% 11% ..



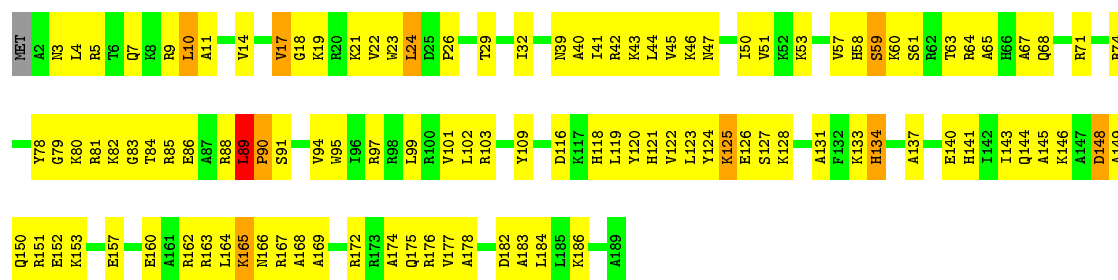
• Molecule 22: eL18 (yeast L18)

Chain V: 29% 60% 11% .

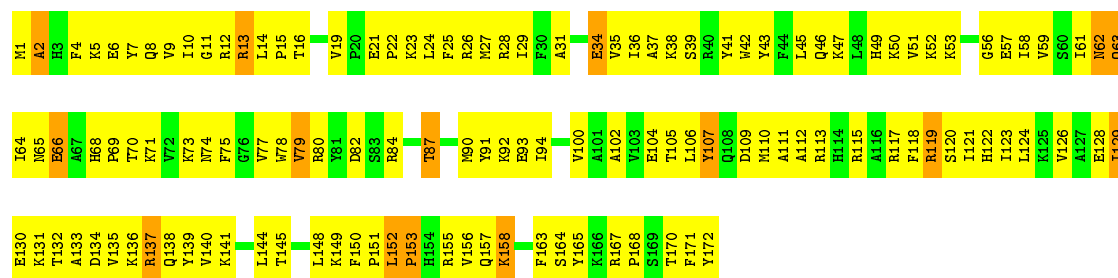
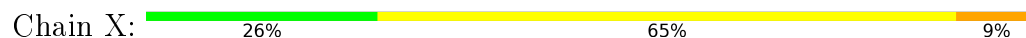


• Molecule 23: eL19 (yeast L19)

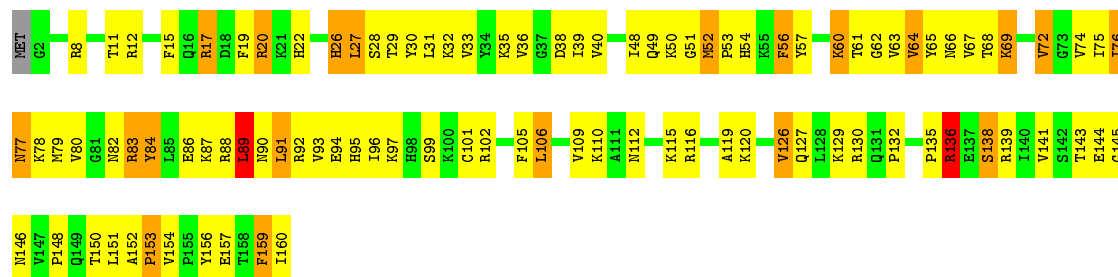
Chain W: 41% 53% 5% ..



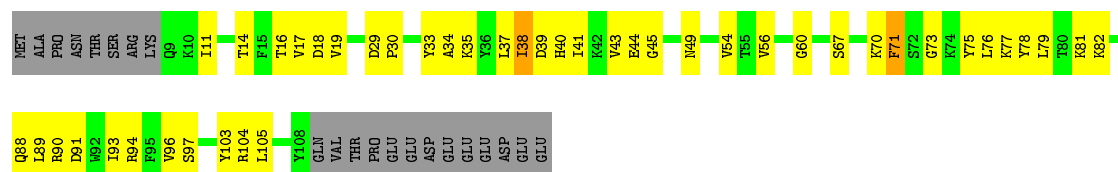
• Molecule 24: eL20 (yeast L20)



• Molecule 25: eL21 (yeast L21)

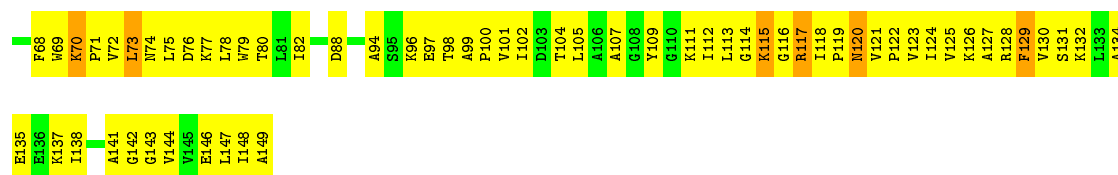


• Molecule 26: eL22 (yeast L22)



• Molecule 27: uL14 (yeast L23)





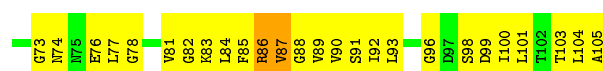
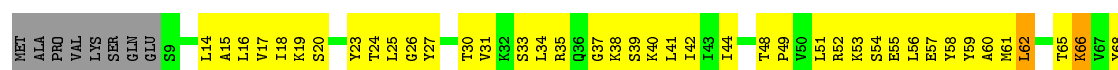
- Molecule 33: eL29 (yeast L29)

Chain GA: 49% 46%



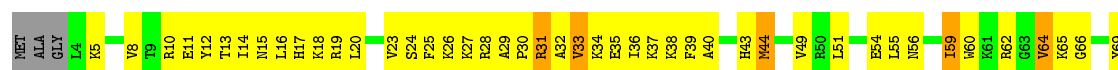
- Molecule 34: eL30 (yeast L30)

Chain HA: 29% 60% 8%



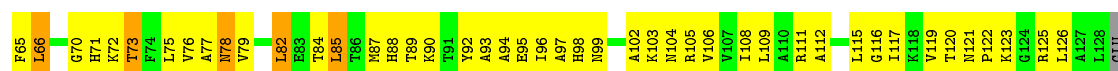
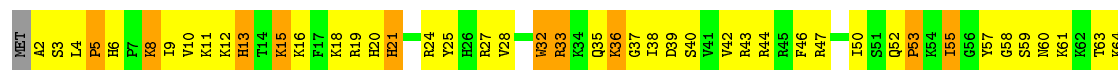
- Molecule 35: eL31 (yeast L31)

Chain IA: 39% 51% 6%



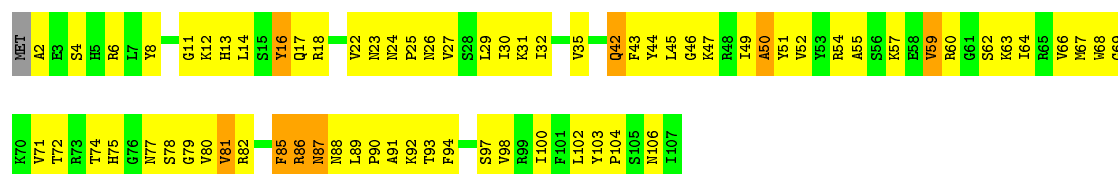
- Molecule 36: eL32 (yeast L32)

Chain JA: 28% 58% 12%



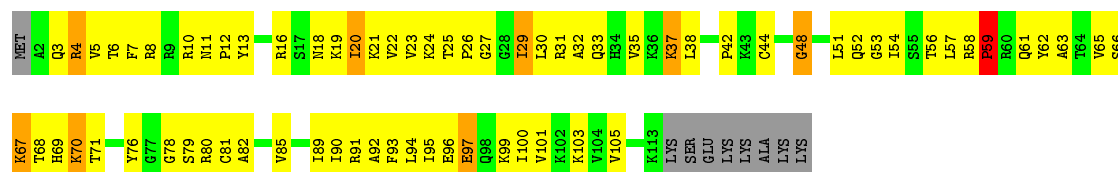
- Molecule 37: eL33 (yeast L33)

Chain KA: 33% 59% 7%



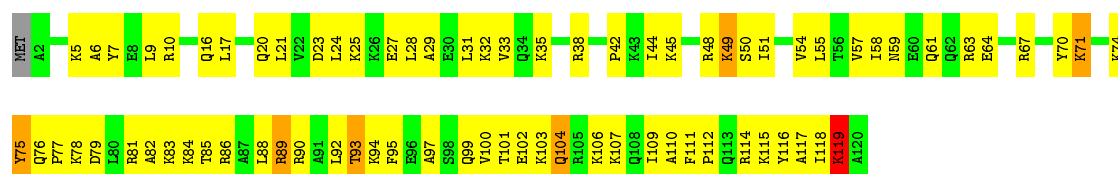
• Molecule 38: eL34 (yeast L34)

Chain LA: 34% 51% 7% • 7%



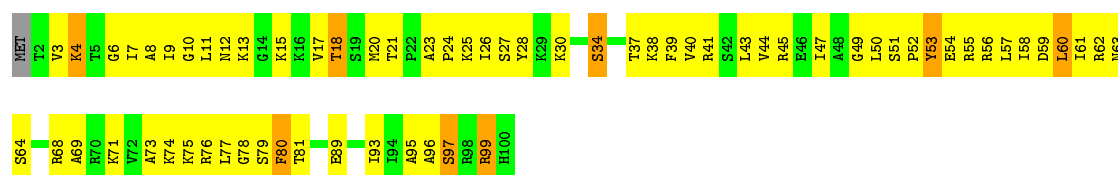
• Molecule 39: uL29 (yeast L35)

Chain MA: 36% 58% 5% ••



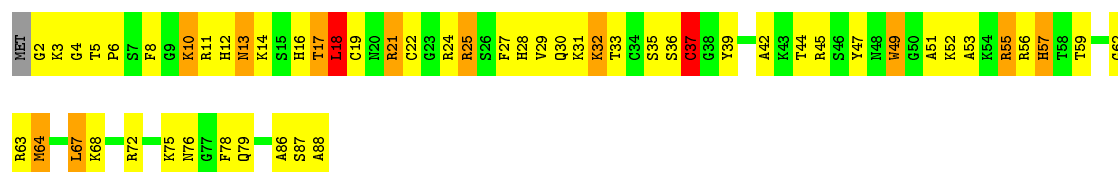
• Molecule 40: eL36 (yeast L36)

Chain NA: 33% 58% 8% •



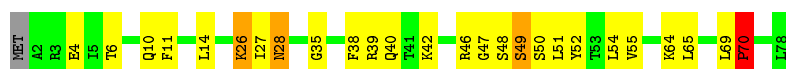
• Molecule 41: eL37 (yeast L37)

Chain OA: 36% 48% 13% ••



• Molecule 42: eL38 (yeast L38)

Chain PA: 65% 28% •••



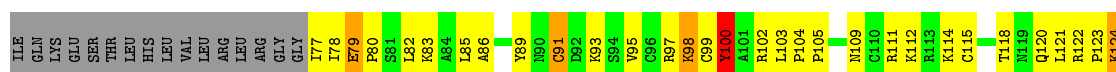
- Molecule 43: eL39 (yeast L39)

Chain QA: 39% 47% 12%



- Molecule 44: eL40 (yeast L40)

Chain RA: 15% 21% 59%



- Molecule 45: eL41 (yeast L41)

Chain SA: 68% 20% 12%



- Molecule 46: eL42 (yeast L42)

Chain TA: 21% 70% 8%

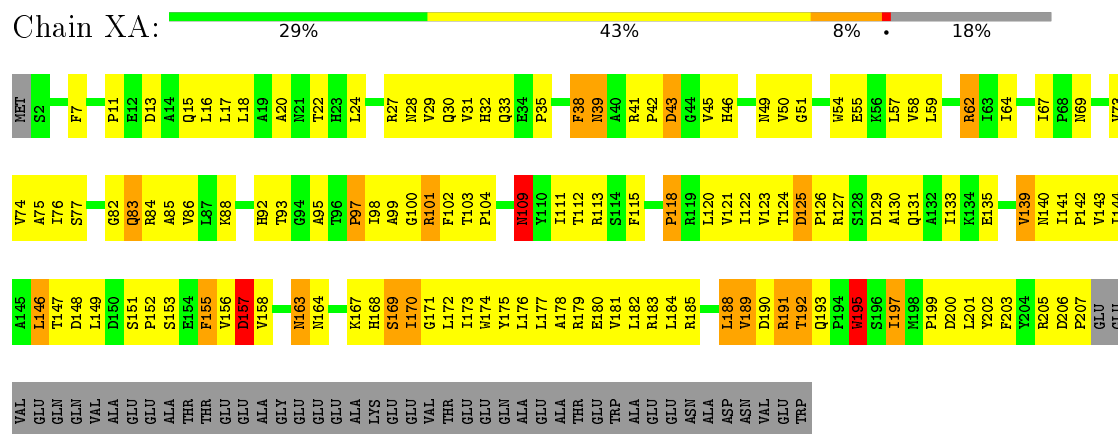


- Molecule 47: eL43 (yeast L43)

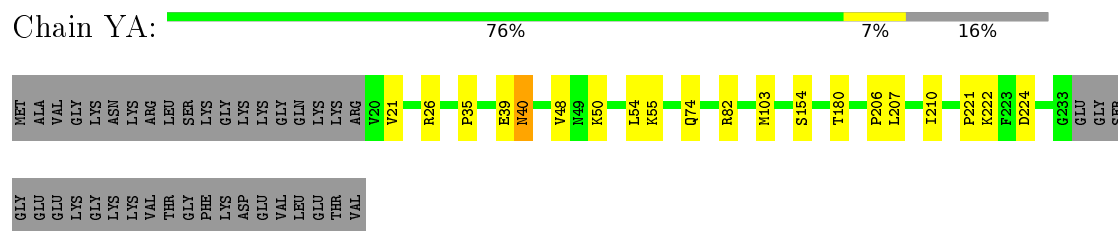
Chain UA: 36% 52% 10%



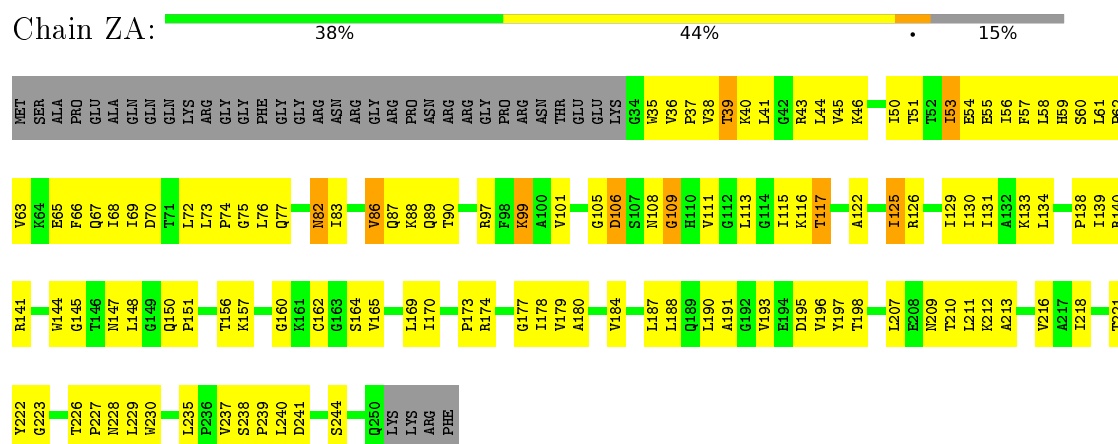
- Molecule 48: uL10 (yeast P0)



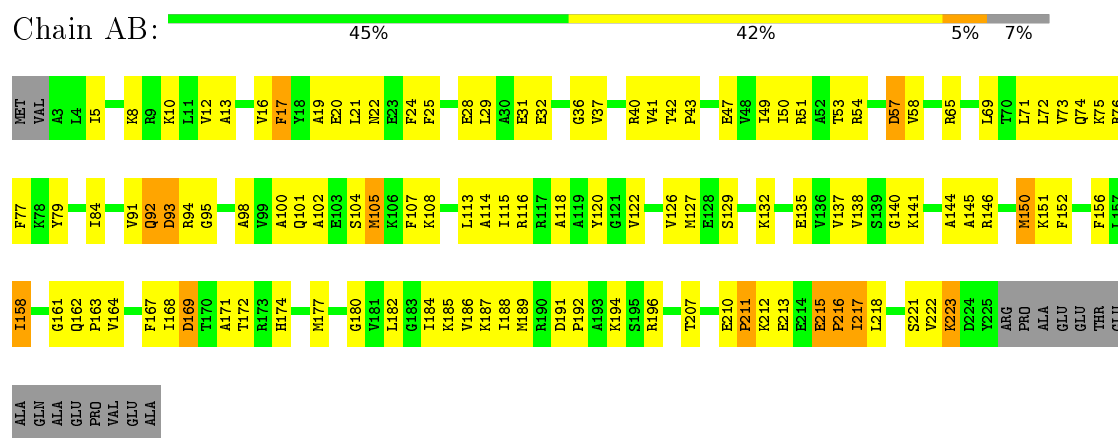
- Molecule 51: eS1 (yeast S1)



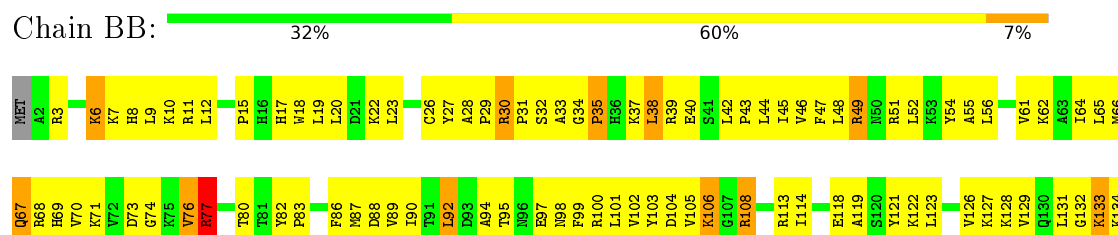
- Molecule 52: uS5 (yeast S2)

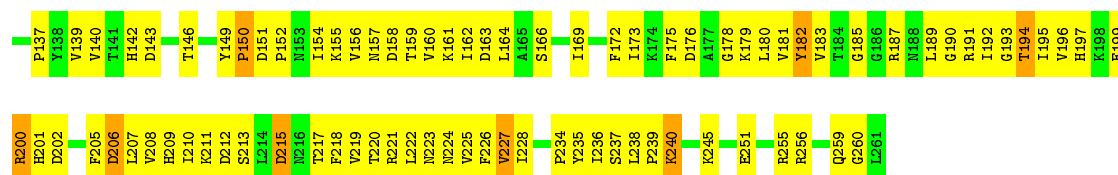


- Molecule 53: uS3 (yeast S3)

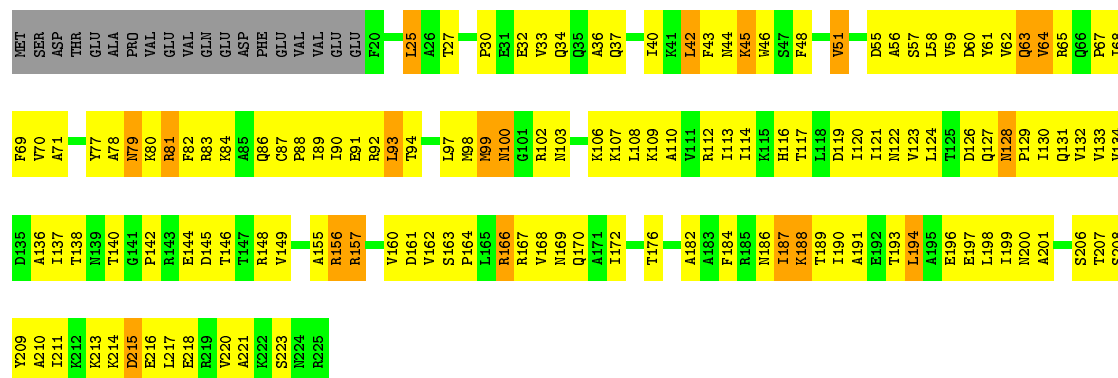


- Molecule 54: eS4 (yeast S4)





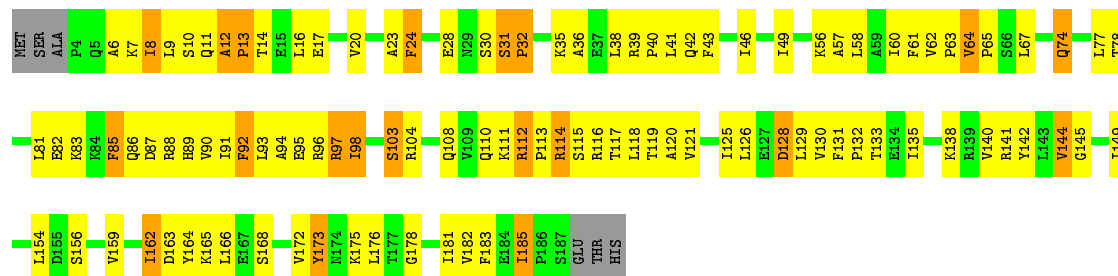
• Molecule 55: uS7 (yeast S5)



• Molecule 56: eS6 (yeast S6)

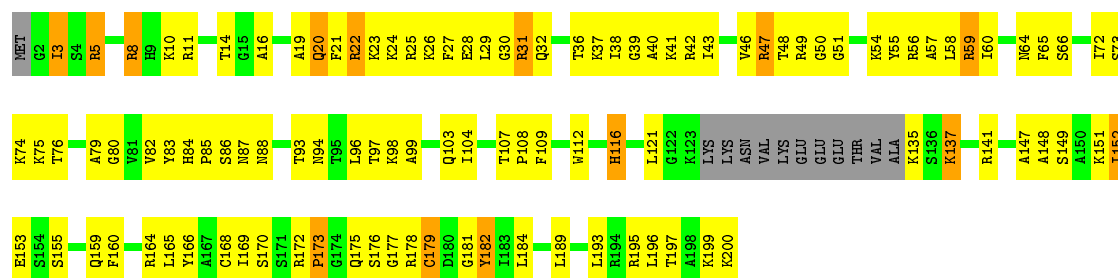


• Molecule 57: eS7 (yeast S7)



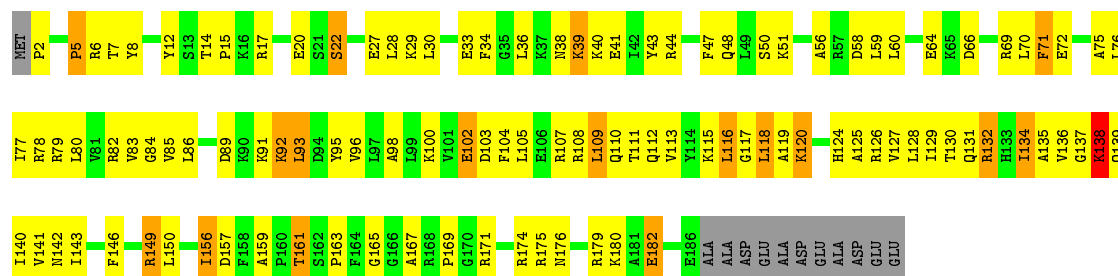
• Molecule 58: eS8 (yeast S8)





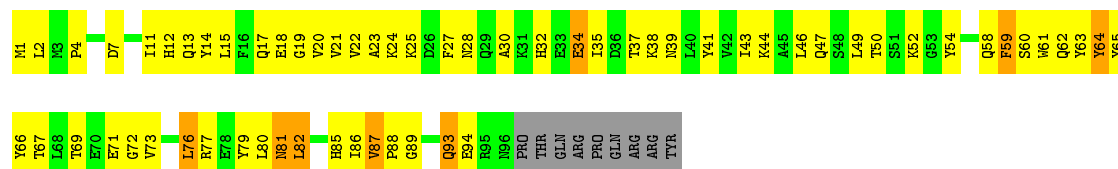
• Molecule 59: uS4 (yeast S9)

Chain GB: 38% 47% 9% 6%



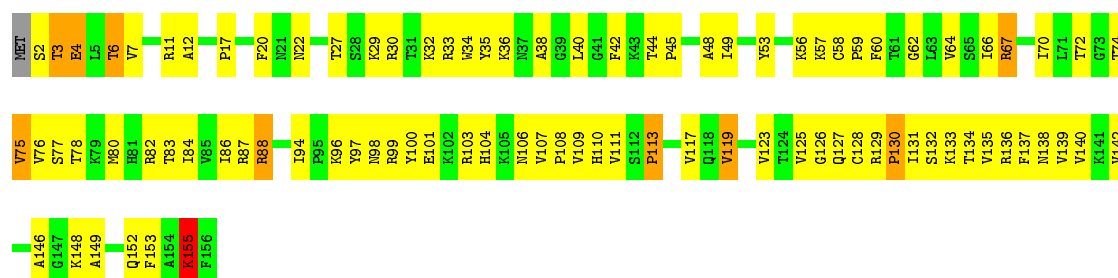
• Molecule 60: eS10 (yeast S10)

Chain HB: 31% 52% 8% 9%



• Molecule 61: uS17 (yeast S11)

Chain IB: 41% 52% 6% 2%



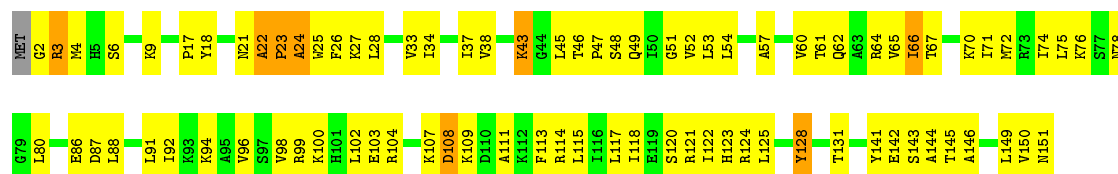
• Molecule 62: eS12 (yeast S12)

Chain JB: 79% 8% 13%




- Molecule 63: uS15 (yeast S13)

Chain KB: 



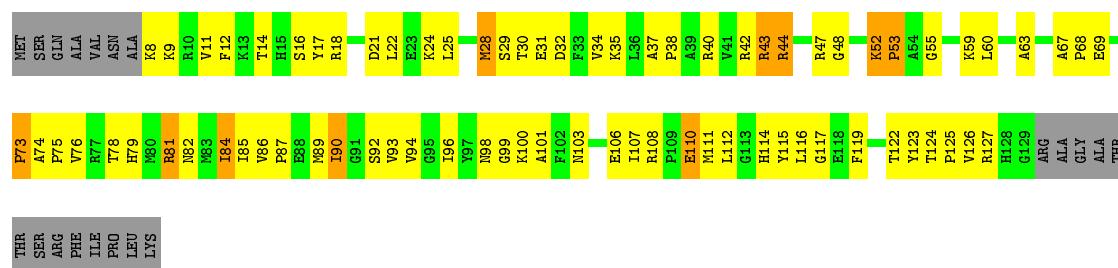
- Molecule 64: uS11 (yeast S14)

Chain LB: 



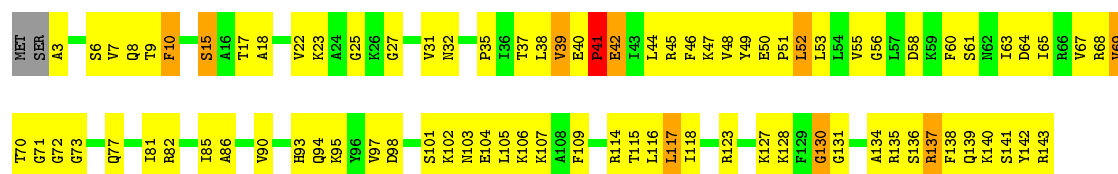
- Molecule 65: uS19 (yeast S15)

Chain MB: 



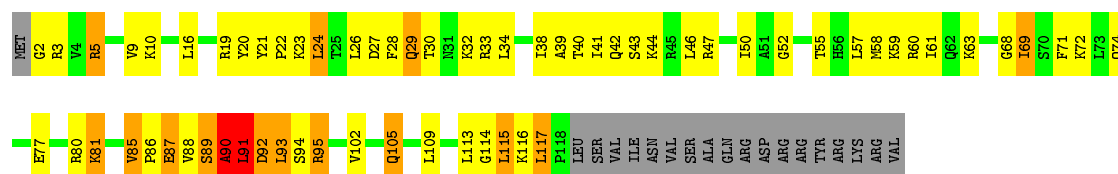
- Molecule 66: uS9 (yeast S16)

Chain NB: 

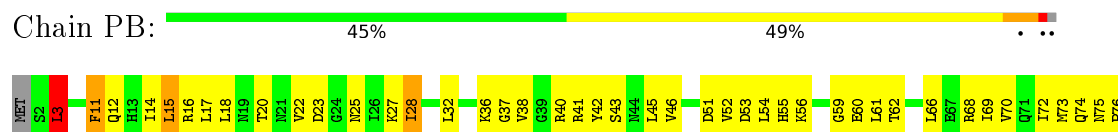


- Molecule 67: eS17 (yeast S17)

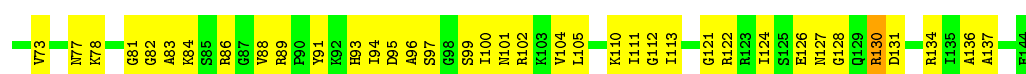
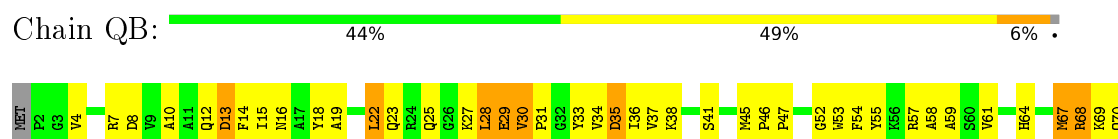
Chain OB: 



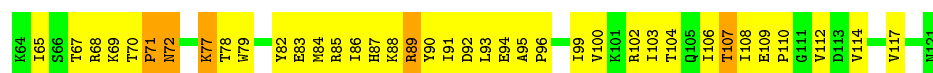
- Molecule 68: uS13 (yeast S18)



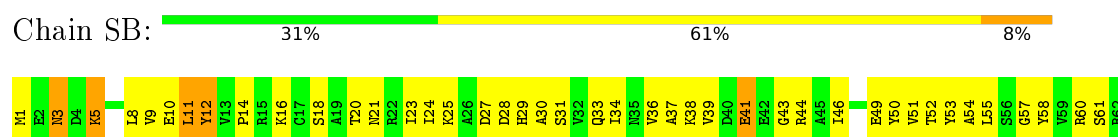
• Molecule 69: eS19 (yeast S19)



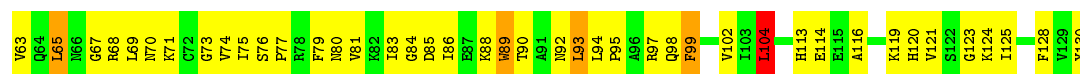
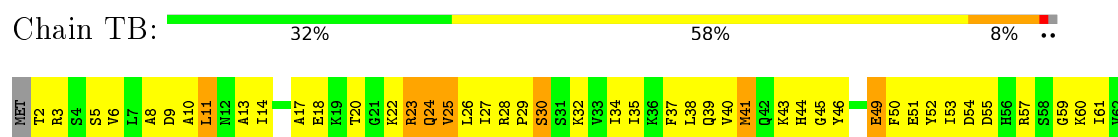
• Molecule 70: uS10 (yeast S20)



• Molecule 71: eS21 (yeast S21)

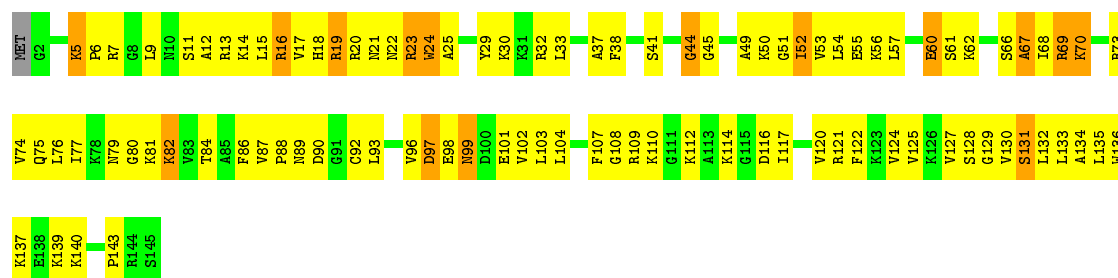


• Molecule 72: uS8 (yeast S22)



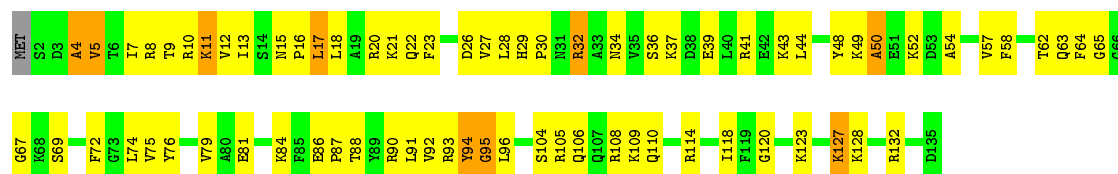
• Molecule 73: uS12 (yeast S23)





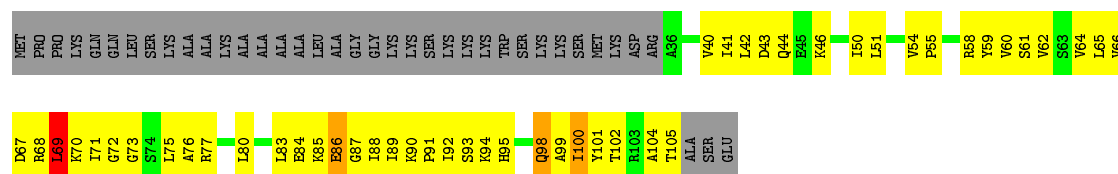
- Molecule 74: eS24 (yeast S24)

Chain VB: 45% 47% 7%



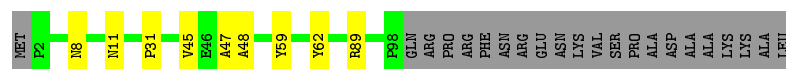
- Molecule 75: eS25 (yeast S25)

Chain WB: 19% 42% 35%



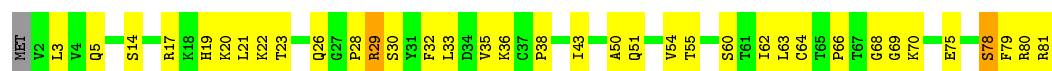
- Molecule 76: eS26 (yeast S26)

Chain XB: 74% 8% 18%



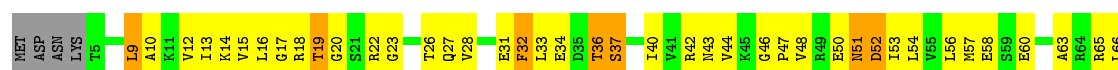
- Molecule 77: eS27 (yeast S27)

Chain YB: 55% 41% 4%



- Molecule 78: eS28 (yeast S28)

Chain ZB: 33% 51% 10% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	38054	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.15	8/41014 (0.0%)	0.77	15/63809 (0.0%)
10	J	1.34	0/1425	0.66	0/1912
11	K	1.49	1/1822 (0.1%)	0.68	0/2451
12	L	1.15	0/1850	0.65	0/2495
13	M	1.27	0/1540	0.65	0/2073
14	N	1.32	0/1754	0.65	1/2350 (0.0%)
15	O	1.03	0/1375	0.57	0/1842
16	P	1.82	0/728	0.73	0/975
17	Q	1.32	0/1568	0.68	0/2106
18	R	1.40	1/1069 (0.1%)	0.67	0/1438
19	S	1.43	0/1758	0.70	0/2354
2	B	1.62	229/78631 (0.3%)	0.82	50/122552 (0.0%)
20	T	1.45	0/1586	0.67	0/2128
21	U	1.46	0/1466	0.70	1/1968 (0.1%)
22	V	1.43	0/1466	0.70	0/1965
23	W	1.13	0/1539	0.65	0/2050
24	X	1.54	0/1482	0.67	0/1990
25	Y	1.47	0/1301	0.64	1/1743 (0.1%)
26	Z	0.99	0/812	0.54	0/1099
27	AA	1.37	0/1019	0.66	1/1369 (0.1%)
28	BA	1.50	0/521	0.66	0/691
29	CA	1.33	0/984	0.65	0/1325
3	C	1.60	10/3747 (0.3%)	0.79	0/5832
30	DA	1.34	0/1005	0.73	3/1341 (0.2%)
31	EA	1.06	0/1119	0.54	0/1497
32	FA	1.41	0/1205	0.67	0/1612
33	GA	1.28	0/474	0.68	0/629
34	HA	1.02	0/751	0.60	0/1008
35	IA	1.23	0/904	0.63	0/1213
36	JA	1.47	0/1041	0.67	1/1394 (0.1%)
37	KA	1.56	0/869	0.70	0/1168
38	LA	1.22	0/891	0.65	0/1191

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	MA	1.22	0/979	0.64	0/1301
4	D	1.44	6/2884 (0.2%)	0.77	2/4491 (0.0%)
40	NA	1.17	0/779	0.63	0/1034
41	OA	1.53	0/697	0.70	1/923 (0.1%)
42	PA	1.06	0/619	0.61	0/826
43	QA	1.38	0/444	0.77	0/588
44	RA	1.31	0/424	0.66	0/562
45	SA	1.57	0/235	0.71	0/300
46	TA	1.30	0/861	0.70	0/1136
47	UA	1.30	0/702	0.65	0/934
48	VA	1.78	0/1498	0.83	3/2025 (0.1%)
49	WA	0.92	0/2498	0.56	0/3398
5	E	1.93	0/1377	0.71	0/1844
50	XA	0.78	0/1653	0.58	0/2261
51	YA	1.13	0/855	0.51	0/1067
52	ZA	0.91	0/1665	0.59	0/2263
53	AB	0.97	0/1759	0.56	0/2368
54	BB	0.89	0/2110	0.59	0/2839
55	CB	0.85	0/1630	0.56	0/2202
56	DB	0.89	0/1844	0.57	0/2464
57	EB	0.92	0/1506	0.58	0/2028
58	FB	1.07	0/1515	0.61	0/2021
59	GB	0.84	0/1519	0.59	0/2035
6	F	1.35	0/1952	0.67	2/2622 (0.1%)
60	HB	1.03	0/837	0.57	0/1131
61	IB	1.16	0/1273	0.62	0/1712
62	JB	1.06	0/495	0.56	0/617
63	KB	1.01	0/1216	0.59	0/1638
64	LB	1.02	0/507	0.53	0/632
65	MB	1.03	0/996	0.60	0/1335
66	NB	0.94	0/1126	0.55	0/1510
67	OB	1.04	2/844 (0.2%)	0.90	4/1120 (0.4%)
68	PB	0.93	0/1212	0.59	2/1628 (0.1%)
69	QB	0.89	0/1131	0.58	0/1517
7	G	1.35	0/3153	0.65	0/4239
70	RB	0.97	0/866	0.56	0/1169
71	SB	0.85	0/694	0.55	0/935
72	TB	0.95	0/1039	0.62	2/1395 (0.1%)
73	UB	1.12	0/1140	0.62	0/1518
74	VB	0.89	0/1088	0.54	0/1449
75	WB	0.87	0/571	0.57	0/768
76	XB	1.09	0/387	0.62	0/482
77	YB	0.87	0/621	0.55	0/838

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	ZB	0.85	0/500	0.56	0/670
79	AC	1.09	0/454	0.57	0/602
8	H	1.45	0/2802	0.70	0/3792
80	BC	0.96	0/483	0.59	0/643
81	CC	0.97	0/283	0.59	0/352
82	DC	1.63	0/6521	0.69	1/8830 (0.0%)
83	EC	2.33	88/4608 (1.9%)	0.94	11/7166 (0.2%)
9	I	1.15	0/2426	0.60	0/3271
All	All	1.41	345/227994 (0.2%)	0.75	101/334061 (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	14
2	B	0	72
3	C	0	6
4	D	0	2
50	XA	0	1
83	EC	0	5
All	All	0	100

The worst 5 of 345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	C	O3'-P	-14.02	1.44	1.61
2	B	1285	G	O3'-P	-9.98	1.49	1.61
2	B	3318	G	O3'-P	8.71	1.71	1.61
2	B	493	G	P-OP2	-8.52	1.34	1.49
67	OB	91	LEU	C-O	8.41	1.39	1.23

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	493	G	O5'-P-OP1	-40.69	61.87	110.70
2	B	493	G	O5'-P-OP2	19.84	134.51	110.70
2	B	487	U	P-O3'-C3'	16.13	139.06	119.70
1	A	627	C	O3'-P-O5'	9.79	122.59	104.00
67	OB	93	LEU	C-N-CA	-8.61	100.19	121.70

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	U	Sidechain
1	A	324	U	Sidechain
1	A	447	U	Sidechain
1	A	53	G	Sidechain
1	A	568	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	36760	0	18348	1356	0
2	B	70288	0	35262	3569	0
3	C	3354	0	1695	188	0
4	D	2580	0	1304	125	0
5	E	1359	0	1425	98	0
6	F	1918	0	1987	258	0
7	G	3082	0	3165	358	0
8	H	2750	0	2863	326	0
9	I	2376	0	2325	219	0
10	J	1401	0	1501	144	0
11	K	1785	0	1862	193	0
12	L	1818	0	1908	192	0
13	M	1519	0	1587	156	0
14	N	1718	0	1754	166	0
15	O	1354	0	1383	86	0
16	P	723	0	774	98	0
17	Q	1543	0	1608	208	0
18	R	1054	0	1149	157	0
19	S	1721	0	1779	241	0
20	T	1556	0	1659	203	0
21	U	1443	0	1485	146	0
22	V	1442	0	1543	197	0
23	W	1522	0	1617	117	0
24	X	1446	0	1487	196	0
25	Y	1277	0	1323	148	0
26	Z	796	0	812	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	1004	0	1048	93	0
28	BA	509	0	537	68	0
29	CA	969	0	1036	71	0
30	DA	994	0	1081	114	0
31	EA	1093	0	1155	116	0
32	FA	1174	0	1215	163	0
33	GA	463	0	491	45	0
34	HA	743	0	797	88	0
35	IA	890	0	938	78	0
36	JA	1020	0	1090	117	0
37	KA	851	0	880	95	0
38	LA	881	0	949	103	0
39	MA	970	0	1078	112	0
40	NA	772	0	849	83	0
41	OA	682	0	687	96	0
42	PA	613	0	682	20	0
43	QA	437	0	475	46	0
44	RA	418	0	459	48	0
45	SA	234	0	284	16	0
46	TA	848	0	918	110	0
47	UA	695	0	738	72	0
48	VA	1473	0	1514	177	0
49	WA	2445	0	2401	155	0
50	XA	1612	0	1623	146	0
51	YA	856	0	226	2	0
52	ZA	1635	0	1723	137	0
53	AB	1734	0	1817	122	0
54	BB	2069	0	2154	223	0
55	CB	1610	0	1675	162	0
56	DB	1820	0	1918	118	0
57	EB	1481	0	1572	129	0
58	FB	1490	0	1525	152	0
59	GB	1494	0	1573	121	0
60	HB	817	0	804	61	0
61	IB	1245	0	1314	104	0
62	JB	496	0	141	0	0
63	KB	1193	0	1255	99	0
64	LB	508	0	151	4	0
65	MB	975	0	1017	68	0
66	NB	1106	0	1166	121	0
67	OB	836	0	827	84	0
68	PB	1193	0	1222	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	QB	1113	0	1124	90	0
70	RB	856	0	917	75	0
71	SB	685	0	672	74	0
72	TB	1022	0	1060	107	0
73	UB	1122	0	1196	123	0
74	VB	1074	0	1132	76	0
75	WB	563	0	603	55	0
76	XB	388	0	96	0	0
77	YB	611	0	633	38	0
78	ZB	498	0	535	48	0
79	AC	444	0	436	30	0
80	BC	475	0	525	27	0
81	CC	284	0	76	0	0
82	DC	6419	0	6493	587	0
83	EC	4129	0	2078	97	0
84	DC	28	0	12	2	0
85	DC	1	0	0	0	0
86	DC	35	0	41	2	0
All	All	212680	0	156239	12389	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 34.

The worst 5 of 12389 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)
37:KA:67:MET:CE	37:KA:67:MET:SD	2.03	1.47
66:NB:93:HIS:HA	66:NB:97:VAL:HB	1.20	1.19
2:B:1494:U:H4'	2:B:1495:U:H5'	1.24	1.14
2:B:2954:U:H4'	2:B:2955:U:H5'	1.26	1.13
2:B:1719:G:H4'	2:B:1732:U:H4'	1.30	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	129 (78%)	26 (16%)	10 (6%)	2	27
6	F	250/254 (98%)	177 (71%)	56 (22%)	17 (7%)	1	24
7	G	384/387 (99%)	293 (76%)	70 (18%)	21 (6%)	2	30
8	H	359/362 (99%)	259 (72%)	77 (21%)	23 (6%)	2	26
9	I	294/297 (99%)	226 (77%)	49 (17%)	19 (6%)	1	26
10	J	173/176 (98%)	125 (72%)	33 (19%)	15 (9%)	1	17
11	K	220/244 (90%)	165 (75%)	39 (18%)	16 (7%)	1	22
12	L	231/256 (90%)	180 (78%)	38 (16%)	13 (6%)	2	29
13	M	189/191 (99%)	150 (79%)	36 (19%)	3 (2%)	12	57
14	N	207/221 (94%)	169 (82%)	28 (14%)	10 (5%)	3	32
15	O	167/174 (96%)	128 (77%)	31 (19%)	8 (5%)	3	32
16	P	92/165 (56%)	62 (67%)	20 (22%)	10 (11%)	0	11
17	Q	191/199 (96%)	144 (75%)	35 (18%)	12 (6%)	2	27
18	R	134/138 (97%)	103 (77%)	23 (17%)	8 (6%)	2	27
19	S	201/204 (98%)	144 (72%)	46 (23%)	11 (6%)	2	30
20	T	195/199 (98%)	160 (82%)	27 (14%)	8 (4%)	3	36
21	U	181/184 (98%)	133 (74%)	35 (19%)	13 (7%)	1	22
22	V	183/186 (98%)	131 (72%)	39 (21%)	13 (7%)	1	23
23	W	186/189 (98%)	162 (87%)	19 (10%)	5 (3%)	6	47
24	X	170/172 (99%)	130 (76%)	31 (18%)	9 (5%)	2	30
25	Y	157/160 (98%)	124 (79%)	25 (16%)	8 (5%)	2	31
26	Z	98/121 (81%)	69 (70%)	23 (24%)	6 (6%)	2	27
27	AA	134/137 (98%)	107 (80%)	24 (18%)	3 (2%)	8	51
28	BA	59/155 (38%)	43 (73%)	11 (19%)	5 (8%)	1	17
29	CA	119/142 (84%)	84 (71%)	29 (24%)	6 (5%)	3	31
30	DA	124/127 (98%)	89 (72%)	28 (23%)	7 (6%)	2	29
31	EA	133/136 (98%)	108 (81%)	19 (14%)	6 (4%)	3	34
32	FA	146/149 (98%)	106 (73%)	31 (21%)	9 (6%)	2	27
33	GA	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
34	HA	95/105 (90%)	80 (84%)	13 (14%)	2 (2%)	9	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	IA	107/113 (95%)	87 (81%)	17 (16%)	3 (3%)	6	46
36	JA	125/130 (96%)	95 (76%)	23 (18%)	7 (6%)	2	29
37	KA	104/107 (97%)	81 (78%)	17 (16%)	6 (6%)	2	28
38	LA	110/121 (91%)	76 (69%)	26 (24%)	8 (7%)	1	22
39	MA	117/120 (98%)	93 (80%)	20 (17%)	4 (3%)	5	42
40	NA	97/100 (97%)	80 (82%)	10 (10%)	7 (7%)	1	22
41	OA	85/88 (97%)	62 (73%)	18 (21%)	5 (6%)	2	28
42	PA	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	4	37
43	QA	48/51 (94%)	35 (73%)	9 (19%)	4 (8%)	1	18
44	RA	50/128 (39%)	32 (64%)	10 (20%)	8 (16%)	0	5
45	SA	23/25 (92%)	23 (100%)	0	0	100	100
46	TA	103/106 (97%)	75 (73%)	22 (21%)	6 (6%)	2	28
47	UA	89/92 (97%)	63 (71%)	18 (20%)	8 (9%)	1	16
48	VA	187/312 (60%)	132 (71%)	39 (21%)	16 (9%)	1	17
49	WA	316/319 (99%)	247 (78%)	63 (20%)	6 (2%)	10	54
50	XA	204/252 (81%)	146 (72%)	40 (20%)	18 (9%)	1	17
51	YA	212/255 (83%)	159 (75%)	36 (17%)	17 (8%)	1	19
52	ZA	215/254 (85%)	169 (79%)	37 (17%)	9 (4%)	3	35
53	AB	221/240 (92%)	191 (86%)	24 (11%)	6 (3%)	6	47
54	BB	258/261 (99%)	185 (72%)	60 (23%)	13 (5%)	3	31
55	CB	204/225 (91%)	159 (78%)	33 (16%)	12 (6%)	2	28
56	DB	224/236 (95%)	192 (86%)	21 (9%)	11 (5%)	3	32
57	EB	182/190 (96%)	130 (71%)	34 (19%)	18 (10%)	1	13
58	FB	184/200 (92%)	141 (77%)	36 (20%)	7 (4%)	4	39
59	GB	183/197 (93%)	144 (79%)	27 (15%)	12 (7%)	1	25
60	HB	94/105 (90%)	73 (78%)	15 (16%)	6 (6%)	2	26
61	IB	153/156 (98%)	113 (74%)	30 (20%)	10 (6%)	1	26
62	JB	122/143 (85%)	90 (74%)	21 (17%)	11 (9%)	1	16
63	KB	148/151 (98%)	124 (84%)	19 (13%)	5 (3%)	5	42
64	LB	125/137 (91%)	88 (70%)	26 (21%)	11 (9%)	1	17
65	MB	120/142 (84%)	91 (76%)	15 (12%)	14 (12%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	108 (78%)	24 (17%)	7 (5%)	3	31
67	OB	115/136 (85%)	79 (69%)	24 (21%)	12 (10%)	1	12
68	PB	143/146 (98%)	111 (78%)	24 (17%)	8 (6%)	2	29
69	QB	141/144 (98%)	122 (86%)	16 (11%)	3 (2%)	9	52
70	RB	105/121 (87%)	85 (81%)	15 (14%)	5 (5%)	3	32
71	SB	85/87 (98%)	63 (74%)	17 (20%)	5 (6%)	2	28
72	TB	127/130 (98%)	99 (78%)	24 (19%)	4 (3%)	5	44
73	UB	142/145 (98%)	108 (76%)	22 (16%)	12 (8%)	1	17
74	VB	132/135 (98%)	105 (80%)	20 (15%)	7 (5%)	2	30
75	WB	68/108 (63%)	47 (69%)	17 (25%)	4 (6%)	2	28
76	XB	95/119 (80%)	54 (57%)	32 (34%)	9 (10%)	1	15
77	YB	79/82 (96%)	59 (75%)	17 (22%)	3 (4%)	4	39
78	ZB	61/67 (91%)	43 (70%)	15 (25%)	3 (5%)	3	32
79	AC	51/56 (91%)	39 (76%)	11 (22%)	1 (2%)	9	53
80	BC	58/63 (92%)	38 (66%)	16 (28%)	4 (7%)	1	24
81	CC	69/152 (45%)	42 (61%)	18 (26%)	9 (13%)	0	7
82	DC	819/842 (97%)	646 (79%)	137 (17%)	36 (4%)	3	34
All	All	12207/13416 (91%)	9316 (76%)	2192 (18%)	699 (6%)	4	28

5 of 699 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	70	ASP
6	F	29	LEU
6	F	34	TYR
6	F	68	LYS
7	G	187	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	157/198 (79%)	136 (87%)	21 (13%)	5	30
6	F	194/196 (99%)	172 (89%)	22 (11%)	7	37
7	G	322/323 (100%)	295 (92%)	27 (8%)	14	51
8	H	288/289 (100%)	249 (86%)	39 (14%)	5	30
9	I	244/245 (100%)	220 (90%)	24 (10%)	10	43
10	J	152/153 (99%)	141 (93%)	11 (7%)	18	58
11	K	186/205 (91%)	165 (89%)	21 (11%)	7	37
12	L	191/208 (92%)	169 (88%)	22 (12%)	7	36
13	M	171/171 (100%)	154 (90%)	17 (10%)	10	43
14	N	180/187 (96%)	161 (89%)	19 (11%)	8	39
15	O	147/150 (98%)	134 (91%)	13 (9%)	12	48
16	P	81/136 (60%)	70 (86%)	11 (14%)	5	29
17	Q	154/159 (97%)	136 (88%)	18 (12%)	7	35
18	R	107/109 (98%)	96 (90%)	11 (10%)	9	40
19	S	175/176 (99%)	150 (86%)	25 (14%)	4	28
20	T	160/162 (99%)	141 (88%)	19 (12%)	6	34
21	U	145/146 (99%)	122 (84%)	23 (16%)	3	23
22	V	150/151 (99%)	134 (89%)	16 (11%)	8	39
23	W	153/154 (99%)	138 (90%)	15 (10%)	10	43
24	X	156/156 (100%)	141 (90%)	15 (10%)	10	44
25	Y	136/137 (99%)	114 (84%)	22 (16%)	3	22
26	Z	87/107 (81%)	85 (98%)	2 (2%)	58	83
27	AA	104/105 (99%)	93 (89%)	11 (11%)	8	39
28	BA	54/129 (42%)	45 (83%)	9 (17%)	3	21
29	CA	105/118 (89%)	97 (92%)	8 (8%)	16	56
30	DA	109/110 (99%)	94 (86%)	15 (14%)	4	29
31	EA	115/116 (99%)	105 (91%)	10 (9%)	13	48
32	FA	118/119 (99%)	105 (89%)	13 (11%)	8	38
33	GA	46/47 (98%)	42 (91%)	4 (9%)	13	48
34	HA	81/88 (92%)	75 (93%)	6 (7%)	17	56
35	IA	96/97 (99%)	89 (93%)	7 (7%)	17	57
36	JA	109/111 (98%)	100 (92%)	9 (8%)	14	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	80 (89%)	10 (11%)	8	38
38	LA	95/103 (92%)	90 (95%)	5 (5%)	28	67
39	MA	104/105 (99%)	96 (92%)	8 (8%)	16	55
40	NA	81/82 (99%)	75 (93%)	6 (7%)	17	56
41	OA	70/71 (99%)	60 (86%)	10 (14%)	4	28
42	PA	68/69 (99%)	63 (93%)	5 (7%)	17	56
43	QA	45/46 (98%)	39 (87%)	6 (13%)	5	30
44	RA	47/116 (40%)	44 (94%)	3 (6%)	22	61
45	SA	23/23 (100%)	20 (87%)	3 (13%)	5	31
46	TA	90/91 (99%)	80 (89%)	10 (11%)	8	38
47	UA	71/72 (99%)	65 (92%)	6 (8%)	13	51
48	VA	160/254 (63%)	147 (92%)	13 (8%)	15	52
49	WA	261/262 (100%)	246 (94%)	15 (6%)	25	65
50	XA	173/210 (82%)	155 (90%)	18 (10%)	9	40
52	ZA	176/205 (86%)	170 (97%)	6 (3%)	44	77
53	AB	182/195 (93%)	167 (92%)	15 (8%)	14	52
54	BB	221/222 (100%)	202 (91%)	19 (9%)	13	50
55	CB	173/191 (91%)	162 (94%)	11 (6%)	22	61
56	DB	193/201 (96%)	187 (97%)	6 (3%)	47	78
57	EB	165/170 (97%)	157 (95%)	8 (5%)	31	69
58	FB	150/161 (93%)	141 (94%)	9 (6%)	24	63
59	GB	158/166 (95%)	143 (90%)	15 (10%)	11	44
60	HB	89/98 (91%)	83 (93%)	6 (7%)	20	60
61	IB	136/137 (99%)	127 (93%)	9 (7%)	21	60
63	KB	127/128 (99%)	119 (94%)	8 (6%)	22	61
65	MB	103/118 (87%)	98 (95%)	5 (5%)	31	69
66	NB	117/119 (98%)	108 (92%)	9 (8%)	16	55
67	OB	82/124 (66%)	77 (94%)	5 (6%)	23	63
68	PB	128/129 (99%)	116 (91%)	12 (9%)	11	45
69	QB	115/116 (99%)	105 (91%)	10 (9%)	13	48
70	RB	100/114 (88%)	90 (90%)	10 (10%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	SB	74/74 (100%)	66 (89%)	8 (11%)	8	39
72	TB	110/111 (99%)	99 (90%)	11 (10%)	9	42
73	UB	119/120 (99%)	110 (92%)	9 (8%)	16	56
74	VB	112/113 (99%)	103 (92%)	9 (8%)	15	53
75	WB	61/89 (68%)	56 (92%)	5 (8%)	14	52
77	YB	70/71 (99%)	69 (99%)	1 (1%)	74	89
78	ZB	56/60 (93%)	49 (88%)	7 (12%)	6	32
79	AC	47/49 (96%)	44 (94%)	3 (6%)	22	61
80	BC	51/54 (94%)	45 (88%)	6 (12%)	6	35
82	DC	699/714 (98%)	641 (92%)	58 (8%)	14	51
All	All	9865/10602 (93%)	8962 (91%)	903 (9%)	16	46

5 of 903 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Y	136	ARG
37	KA	42	GLN
78	ZB	58	GLU
27	AA	102	ILE
31	EA	38	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 283 such sidechains are listed below:

Mol	Chain	Res	Type
35	IA	56	ASN
41	OA	30	GLN
72	TB	98	GLN
36	JA	13	HIS
37	KA	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1682/1798 (93%)	312 (18%)	11 (0%)
2	B	3267/3396 (96%)	632 (19%)	27 (0%)
3	C	157/158 (99%)	32 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	120/121 (99%)	12 (10%)	0
83	EC	189/201 (94%)	74 (39%)	2 (1%)
All	All	5415/5674 (95%)	1062 (19%)	40 (0%)

5 of 1062 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	25	C
1	A	26	A
1	A	34	G
1	A	47	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1144	U
2	B	1456	A
2	B	3317	U
2	B	1307	G
2	B	1815	U

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

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	13,20,21	1.94	5 (38%)	12,28,30	2.05	3 (25%)

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	-	0/19/21/23	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-NE2	2.08	1.39	1.36
82	DC	699	DDE	CB-CA	2.15	1.58	1.53
82	DC	699	DDE	CB-CG	2.19	1.59	1.51
82	DC	699	DDE	OAG-CBI	2.24	1.28	1.23
82	DC	699	DDE	CBW-CBI	4.45	1.60	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	DC	699	DDE	CAU-CBW-CBI	-2.51	105.65	110.72
82	DC	699	DDE	OAG-CBI-NAD	2.26	126.80	123.06
82	DC	699	DDE	CAU-CAT-CE1	5.10	140.11	112.58

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	GDP	DC	901	85	24,30,30	2.21	8 (33%)	26,47,47	1.80	4 (15%)
86	SO1	DC	903	-	36,39,39	3.17	22 (61%)	36,64,64	1.68	8 (22%)

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	-	-	0/15/104/104	0/2/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O56-C52	-3.67	1.32	1.41
86	DC	903	SO1	C7-C16	2.01	1.56	1.53
86	DC	903	SO1	C24-C18	2.02	1.59	1.54
86	DC	903	SO1	C54-C55	2.05	1.58	1.52
86	DC	903	SO1	C53-C54	2.37	1.58	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	DC	901	GDP	N3-C2-N1	-4.99	120.76	127.56
84	DC	901	GDP	C5-C6-N1	-3.84	118.50	123.52
86	DC	903	SO1	C7-C2-C8	-3.43	103.97	110.16
86	DC	903	SO1	C18-C9-C16	-3.27	98.83	103.42
86	DC	903	SO1	C12-C6-C10	-3.07	102.42	107.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	DC	901	GDP	2	0
86	DC	903	SO1	2	0

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.