



## wwPDB EM Map/Model Validation Report ⓘ

Sep 29, 2016 – 07:22 PM EDT

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

This is a wwPDB EM 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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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

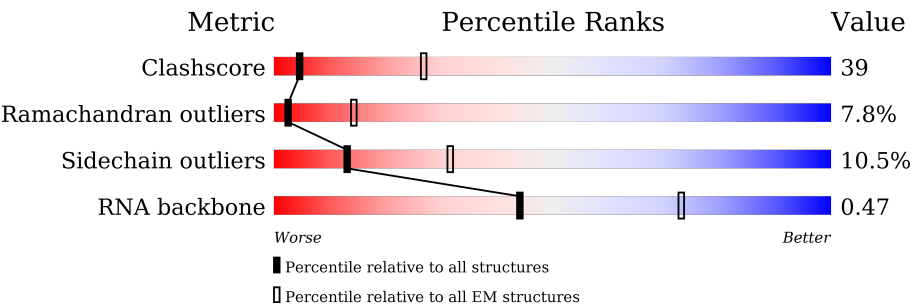


# 1 Overall quality at a glance i

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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244


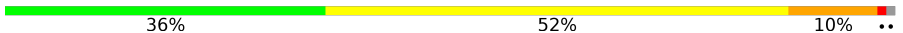
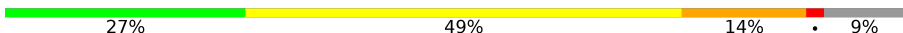


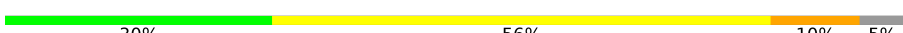
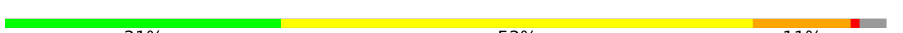




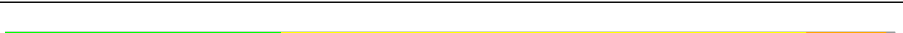









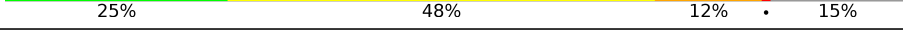



The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of 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	<div><div>23%</div><div>60%</div><div>16%</div><div>.</div></div>
2	B	3396	<div><div>19%</div><div>63%</div><div>15%</div><div>..</div></div>
3	C	158	<div><div>22%</div><div>63%</div><div>13%</div><div>.</div></div>
4	D	121	<div><div>18%</div><div>72%</div><div>10%</div><div></div></div>
5	E	217	<div><div>29%</div><div>43%</div><div>21%</div><div>..</div></div>
6	F	254	<div><div>24%</div><div>59%</div><div>14%</div><div>..</div></div>
7	G	387	<div><div>27%</div><div>62%</div><div>10%</div><div>.</div></div>
8	H	362	<div><div>32%</div><div>51%</div><div>16%</div><div>.</div></div>

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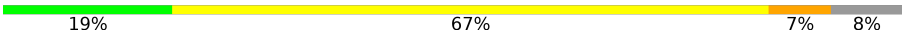
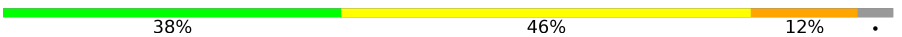



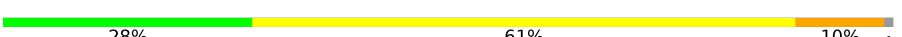
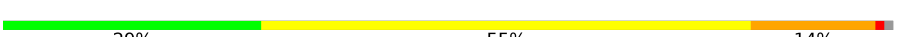
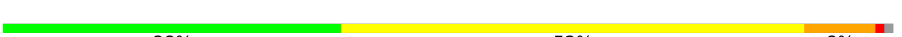
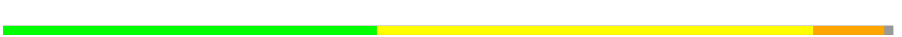


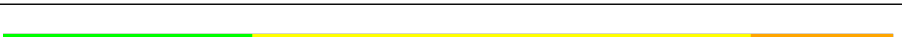

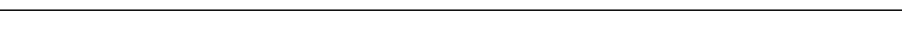
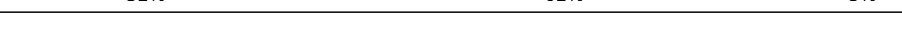
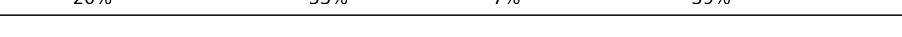

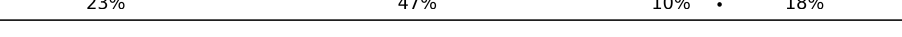
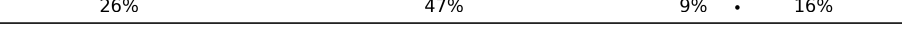
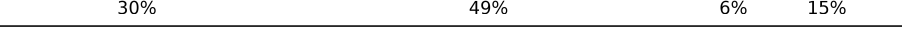


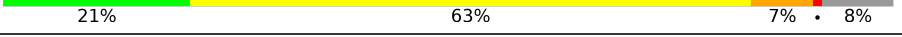


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Mol	Chain	Length	Quality of chain
9	I	297	
10	J	176	
11	K	244	
12	L	256	
13	M	191	
14	N	221	
15	O	174	
16	P	165	
17	Q	199	
18	R	138	
19	S	204	
20	T	199	
21	U	184	
22	V	186	
23	W	189	
24	X	172	
25	Y	160	
26	Z	121	
27	AA	137	
28	BA	155	
29	CA	142	
30	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 [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
1	A	1781	Total	C	N	O	P	0	0
			37658	16811	6630	12436	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	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	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
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	S	0	0
			942	578	186	175	3		

- 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	S	0	0
			769	475	160	129	5		

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



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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called yeast eEF2.

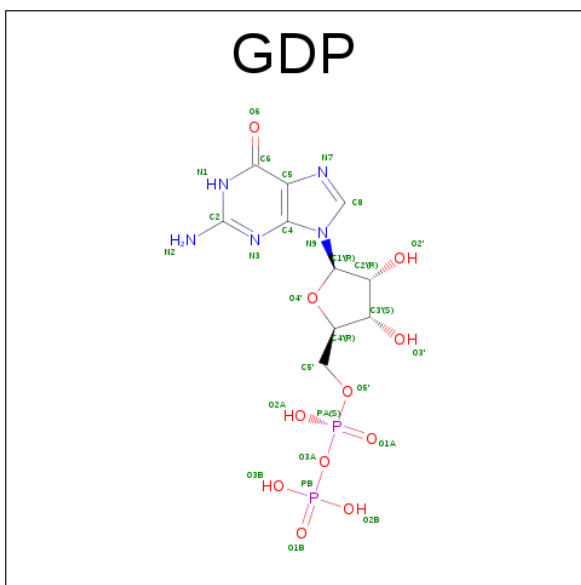
Mol	Chain	Residues	Atoms					AltConf	Trace
82	DC	824	Total	C	N	O	S	0	0
			6419	4085	1096	1208	30		

- Molecule 83 is a RNA chain called IRES.

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

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





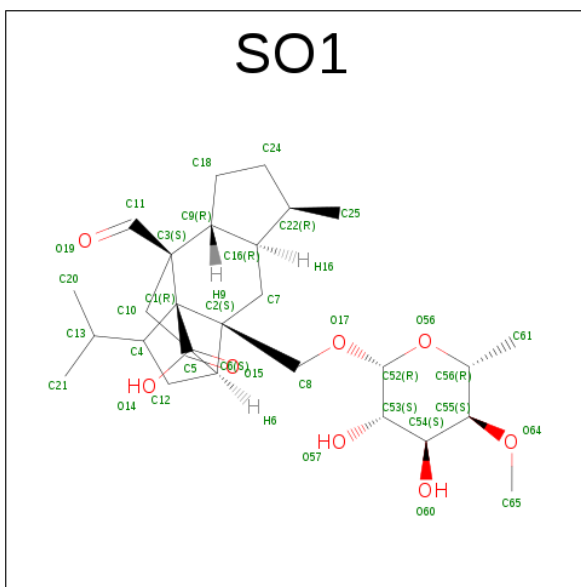
Mol	Chain	Residues	Atoms					AltConf
84	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

- 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:  $C_{27}H_{42}O_8$ ).





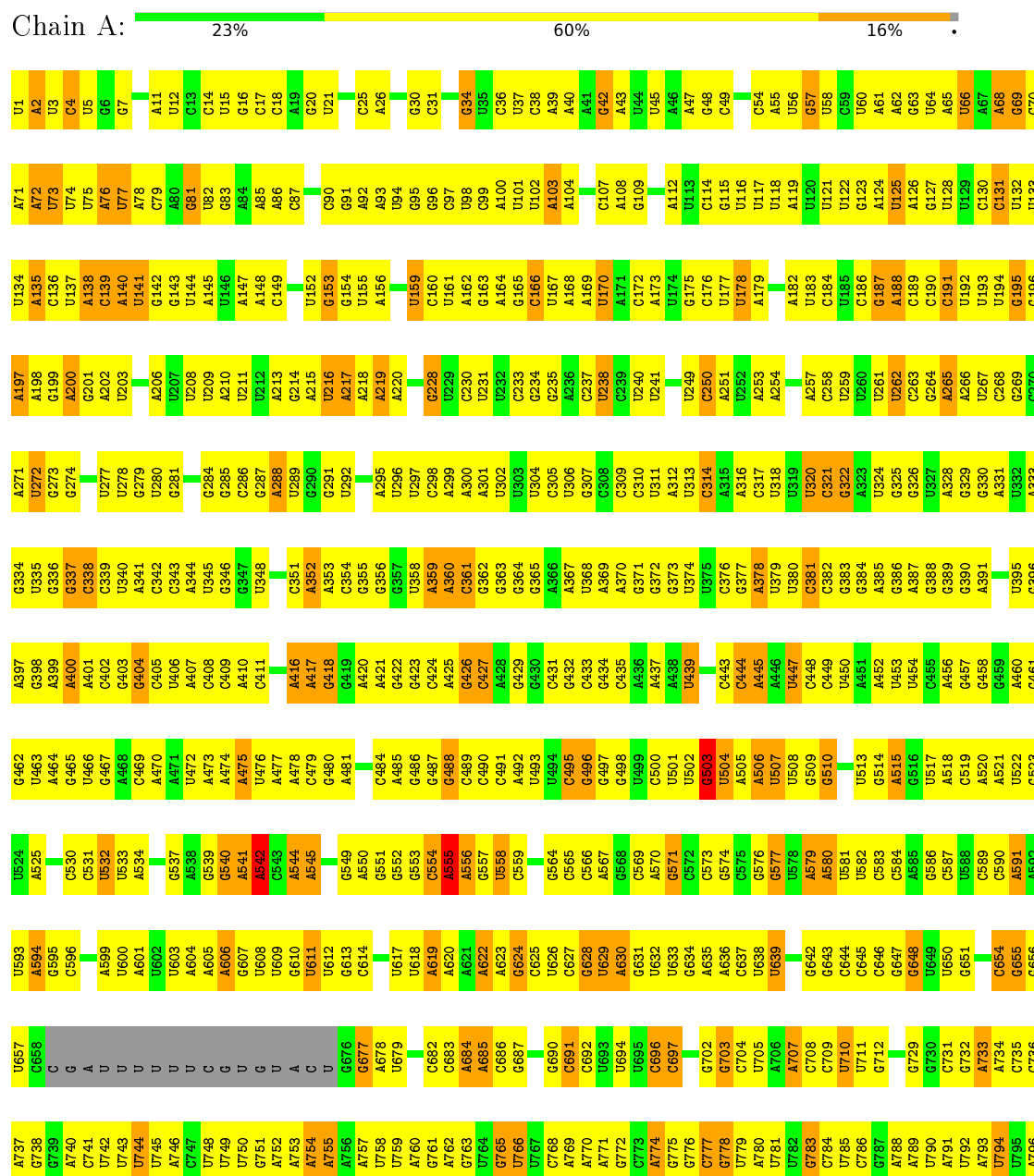
Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	



### 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

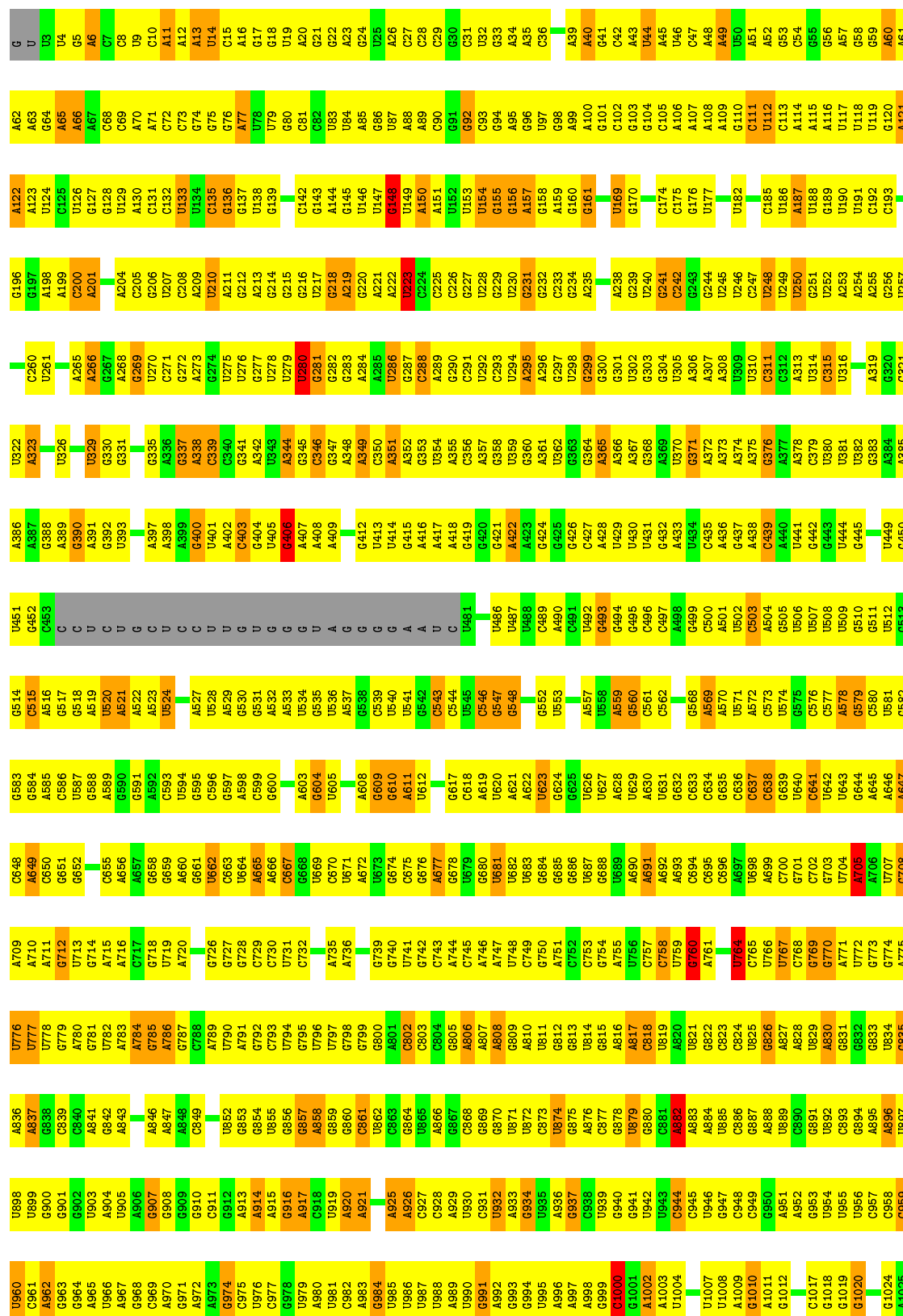




G1788	G1726	G1652	A1586	U1520	C1457	C1393	A1329	G1255	A1193	A1124	G1064	A995	U928	A863	G797
G1789	G1727	C1653	A1587	G1521	G1468	G1394	G1330	A1286	A1194	A1125	A1065	U996	A929	U864	C798
A1790	A1728	G1654	C1469	U1522	C1469	U1398	C1331	U1287	A1196	G1126	C1066	G997	A930	A865	A799
A1791	C1729	A1655	G1588	G1523	A1460	C1332	C1332	U1259	U1197	G1127	C1067	U998	C931	G866	U800
G1792	A1730	U1656	G1590	A1524	C1462	C1399	U1334	U1259	C1197	C1068	C1068	U999	U932	G801	G802
G1793	A1731	U1657	C1591	A1525	G1463	A1400	U1335	U1259	G1198	U1128	A1069	C1000	A933	G868	G803
A1794	A1732	G1658	A1592	A1526	C1463	A1401	U1335	U1259	G1199	U1129	C1070	A1001	C934	A869	A803
U1795	C1733	A1659	A1593	C1527	G1464	G1402	C1338	U1266	G1200	A1133	U1072	G1002	U935	C870	A804
C1796	U1734	A1660	A1594	U1527	C1465	C1403	C1338	U1267	G1201	C1134	C1071	A1003	U936	C871	U805
A1797	G1735	U1661	U1595	G1530	G1466	U1407	C1339	U1268	A1202	U1135	G1073	A1004	C937	G872	A806
U1798	G1736	G1662	C1596	G1531	C1467	G1408	U1340	U1269	A1203	U1136	G1074	A1005	U938	U873	A807
C1799	G1737	G1663	U1597	U1532	U1468	G1409	A1341	G1270	A1204	A1139	C1075	U1076	A939	C874	U808
U1799	U1738	C1664	A1598	C1533	A1469	G1409	C1342	G1271	C1205	G1140	C1076	A1077	A940	C875	U809
	C1739	U1685	U1598	G1534	C1470	A1410	U1343	U1272	U1206	G1141	C1077	G1011	A941	C876	U810
	A1740	G1601	U1601	U1535	A1471	A1411	A1344	U1273	C1207	G1142	C1078	U1012	G942	C877	A811
U1741	U1741	C1602	C1472	G1536	C1472	G1412	A1345	C1274	A1208	G1143	C1079	U1013	G943	C878	A814
U1742	U1742	U1603	U1473	C1537	U1473	U1413	A1346	A1275	C1209	G1144	C1080	G1014	A944	C879	G815
		G1604	G1474	U1538	G1474	U1414	U1347	U1276	C1210	A1143	U1080	G1015	U945	C880	G816
	G1745	G1605	A1475	G1539	A1475	U1415	A1348	G1277	A1211	U1144	A1081	U1016	U946	C881	A817
A1746	A1746	G1606	C1476	G1540	C1476	G1416	G1349	G1278	G1212	U1145	C1082	U1017	U947	C882	C818
		G1607	G1477	U1541	G1477	A1417	U1350	C1279	G1213	C1148	A1083	U1018	C950	C883	C819
A1749	A1749	U1608	G1478	G1542	G1478	G1418	G1351	C1280	U1214	G1149	G1085	A1020	A951	C884	G818
A1750	A1750	A1543	A1479	G1543	A1479	G1419	G1352	G1281	U1215	G1150	A1086	A1021	A952	C885	U821
C1751	C1751	U1544	G1480	U1545	C1480	C1420	U1353	U1282	A1217	A1151	A1087	C1022	G953	U886	U822
U1752	U1752	A1545	A1481	U1546	C1481	A1421	G1354	U1283	G1218	A1152	A1088	A1023	G954	A887	G823
A1753	A1753	G1546	C1482	G1547	C1482	A1422	C1355	U1284	A1219	G1153	U1089	U1024	A955	U888	G824
		U1547	A1483	A1547	U1483	U1423	U1356	A1287	C1222	C1158	C1090	A1025	C956	U889	U825
		A1548	G1484	U1548	G1484	U1424	A1357	G1288	U1223	C1159	A1091	A1026	C957	U890	U826
		U1549	C1485	U1550	G1485	C1425	G1358	U1289	A1223	G1160	A1092	A1027	U958	C891	C827
		A1551	G1486	U1551	C1486	C1426	C1359	U1290	A1224	A1161	A1093	C1028	U959	A892	U828
		U1552	A1487	U1552	G1487	A1427	A1360	G1291	U1225	C1162	G1094	U1029	U960	A893	A838
		G1553	G1488	G1553	U1488	G1428	U1361	G1292	A1226	C1163	U1095	A1030	U961	U830	U830
		U1554	U1489	U1554	U1489	G1429	U1362	G1293	A1227	A1164	C1096	A1031	C962	U831	U831
		A1556	C1490	A1556	C1490	U1430	U1363	G1294	G1228	G1165	U1098	C1033	U964	U832	U833
		U1557	U1491	U1557	U1491	C1431	G1364	U1294	G1229	A1166	U1099	C1034	U965	G899	G834
		A1558	A1492	U1558	A1492	U1432	C1365	U1298	U1231	G1170	G1100	G1035	A966	A900	U835
		A1559	A1493	U1559	A1493	U1433	U1366	U1299	U1232	G1171	G1101	A1036	A967	G901	U836
		U1560	C1494	U1560	C1494	U1434	G1367	A1300	U1233	A1172	G1102	A1039	U968	U839	U839
		U1561	C1495	U1561	C1495	U1435	G1368	G1304	G1233	G1173	U1103	A1039	C969	U903	U840
		G1562	U1496	G1562	U1496	A1436	U1369	U1305	A1234	U1104	C1103	G1040	A970	G904	U841
		C1563	U1497	U1563	U1497	U1437	U1370	C1306	C1235	C1174	C1105	G1041	A971	A905	C842
		U1564	G1498	U1564	G1498	G1438	A1371	C1307	A1236	U1175	U1106	G1042	G972	U943	U843
		C1565	G1499	C1565	G1499	C1439	U1372	C1309	G1237	G1176	G1107	A1043	U973	A906	U844
		G1568	C1500	G1568	C1500	C1440	C1373	U1310	A1238	C1177	G1108	U1044	C975	A844	G845
		A1569	G1501	A1569	G1501	U1441	C1374	U1311	U1239	G1178	G1109	G1046	U911	U911	G846
		U1570	G1502	U1570	G1502	U1442	A1375	U1312	U1240	G1179	G1110	G1047	G980	U912	A850
		G1572	A1503	G1572	A1503	U1443	C1376	A1313	G1241	G1180	G1111	G1048	U981	G913	U851
		A1573	G1504	A1573	G1504	A1444	U1377	U1314	G1242	G1181	G1112	U1051	U982	G914	C852
		G1574	A1505	G1574	A1505	G1445	U1378	U1315	G1243	U1182	G1113	G1052	A983	U916	G853
		U1575	G1506	U1575	G1506	A1446	C1379	G1316	G1244	U1183	G1114	U1053	G986	U917	U854
		A1576	U1510	A1576	U1510	C1447	U1381	C1317	G1245	A1184	U1115	G1053	U987	U918	A855
		U1579	G1511	U1579	G1511	U1449	A1382	U1321	U1247	U1185	A1116	U1057	A988	A919	A856
		C1580	G1513	C1580	G1513	U1450	G1383	A1322	C1248	U1186	G1117	U1058	U989	U857	G858
		C1581	U1514	C1581	U1514	U1451	A1384	G1324	U1249	U1187	G1118	U1059	C990	A924	A859
		U1582	A1515	U1582	A1515	U1452	U1389	U1325	U1250	G1188	G1119	U1060	G991	A925	U860
		A1583	A1516	A1583	A1516	G1453	U1390	A1326	U1251	A1189	U1120	A1061	A992	U861	U861
		U1584	U1517	U1584	U1517	G1454	U1391	C1327	C1252	C1190	G1121	A1062	A993	A926	U862
		U1585	U1519	U1585	U1519	C1456	U1392	G1328	U1254	C1192	C1123	U1063	G994	C927	A862



Chain B:  19% 63% 15% . .





G	A1910	G1786	G1718	G1655	A1593	C1527	A1465	G1400	G1340	G1280	A1217	G1149	U1088	A1026
A	C1849	A1787	G1719	A1656	A1594	C1532	G1466	A1401	U1341	G1281	U1218	A1150	G1089	A1027
C	A1850	G1788	U1720	C1657	C1597	U1533	C1469	U1405	A1343	C1282	C1219	A1153	G1090	U1028
U	G1851	G1789	U1721	G1658	C1597	A1534	U1470	A1406	A1343	C1283	U1220	A1153	A1091	G1029
C	G1852	G1790	U1722	U1659	G1598	A1535	U1471	A1407	G1344	C1284	C1221	G1157	C1092	A1030
G	U1853	C1791	A1723	C1660	G1599	A1536	U1472	G1408	G1345	C1285	G1222	U1158	A1094	U1033
U	C1854	G1792	U1724	G1661	U1600	A1537	U1473	G1409	G1346	A1286	A1225	A1158	U1095	U1034
U	U1855	C1793	C1725	G1662	U1601	G1538	G1473	U1410	U1347	U1287	A1225	A1159	U1096	G1035
G	C1856	G1794	C1726	C1663	A1602	G1541	G1476	U1411	U1348	U1288	G1226	A1158	U1095	U1033
U	C1857	A1797	G1727	G1664	A1603	G1541	A1477	C1412	G1349	G1289	C1227	A1160	U1096	G1035
G	G1919	G1728	U1728	G1665	G1604	A1545	C1478	C1411	U1349	G1290	G1227	G1161	G1097	A1036
G	A1859	A1729	G1730	G1666	A1605	A1546	U1479	G1413	A1350	A1291	C1228	A1162	A1098	C1037
G	G1860	G1730	A1731	A1667	U1607	A1546	G1480	G1414	A1351	A1291	G1229	A1163	A1099	C1038
G	G1861	A1731	G1731	G1668	U1607	A1546	G1480	U1415	U1353	U1293	A1231	A1165	U1100	U1039
U	U1862	G1732	G1732	C1669	C1608	G1547	A1481	C1416	G1354	A1294	C1232	G1166	A1102	U1041
C	C1863	G1733	G1733	C1670	C1609	C1548	A1482	U1417	U1355	G1295	C1233	U1167	A1103	U1042
U	A1864	G1734	G1734	U1671	G1610	U1549	G1483	A1418	U1356	G1234	U1235	A1168	G1104	C1043
U	A1865	U1672	U1672	C1671	G1611	U1550	U1484	A1419	G1357	C1297	U1235	A1169	A105	U1044
C	C1866	G1673	G1673	G1673	C1614	C1551	G1485	C1420	C1358	C1298	G1236	A1170	G1106	C1045
C	A1867	G1674	G1674	G1675	C1615	G1552	G1486	G1421	C1359	U1299	G1237	G1171	C1107	U1046
U	G1868	G1675	U1737	G1676	C1616	U1553	G1487	C1422	C1360	G1300	C1238	G1172	C1108	A1047
C	C1869	G1677	G1738	A1676	U1616	U1554	A1488	C1423	U1361	A1301	C1239	U1173	U1109	A1048
U	C1870	G1678	G1678	G1678	G1617	U1555	A1489	C1423	G1362	A1302	A1240	U1174	U1110	C1049
C	U1871	A1741	U1742	A1679	A1619	C1556	A1490	U1426	A1363	A1303	U1241	C1175	U1111	U1050
C	C1872	G1743	G1743	A1679	U1620	A1557	A1491	U1427	C1364	A1304	G1242	C1176	A1112	U1051
U	U1873	G1744	G1744	G1680	U1621	A1558	G1492	A1428	G1365	U1305	G1243	G1177	G1113	U1052
A	A1874	C1745	C1745	U1681	A1622	A1559	G1493	G1429	A1366	G1306	A1244	A1178	U1114	A1053
G	G1875	U1746	U1746	U1682	U1622	A1560	U1494	U1430	G1367	A1245	A1245	A1179	G1115	A1054
C	U1876	G1747	G1747	A1683	G1623	G1561	U1495	G1431	U1368	A1308	G1246	A1180	G1116	U1055
C	C1941	G1817	G1748	U1684	G1624	C1562	G1496	C1432	A1369	U1309	U1247	U1181	G1117	A1056
U	U1942	G1818	A1749	C1685	A1625	C1563	C1497	A1433	G1370	G1310	G1248	A1182	C1118	U1057
G	A1879	U1819	U1760	U1686	U1626	U1564	A1498	G1434	G1371	G1311	G1249	C1183	C1119	U1058
A	U1880	U1820	G1751	U1687	U1627	C1565	C1499	U1435	C1372	G1312	G1250	A1184	A1120	G1059
C	A1881	U1821	C1756	U1688	C1628	A1566	G1500	U1436	C1373	G1313	G1251	C1185	U1121	U1060
U	G1882	C1822	C1761	U1689	U1629	U1567	U1501	C1437	G1374	G1314	U1253	G1186	U1122	A1061
A	A1886	A1823	G1758	C1690	U1630	U1568	C1502	U1438	G1375	C1315	C1255	C1187	U1125	G1063
U	A1887	G1825	C1759	U1691	C1631	U1569	A1503	U1439	C1376	C1316	G1256	C1188	G1126	A1064
U	U1888	C1826	A1760	U1692	A1632	U1570	A1504	G1440	G1377	A1317	G1257	A1190	U1127	A1065
G	G1889	U1827	U1761	U1695	C1633	A1571	C1505	G1441	U1378	A1318	C1257	A1191	U1128	G1066
C	U1890	G1828	C1762	A1696	G1634	U1572	A1506	U1442	G1379	G1319	U1258	C1192	A1129	U1067
G	A1891	G1829	U1763	G1696	G1635	C1573	C1507	G1443	G1380	C1320	A1259	A1193	A1130	C1068
U	G1892	G1830	U1764	A1699	U1636	A1574	C1508	G1444	A1381	G1321	G1261	G1194	G1131	C1069
C	A1893	U1831	U1765	A1699	A1637	A1575	A1509	U1445	G1382	U1322	G1262	A1195	C1132	U1070
G	U1894	C1832	G1766	U1702	A1638	G1576	G1510	A1446	G1383	G1323	A1263	C1196	A1133	U1071
C	A1895	U1833	C1767	U1703	U1639	G1577	U1511	G1447	U1384	U1324	G1264	C1199	G1134	G1072
U	G1896	A1704	G1768	A1704	U1641	C1578	G1512	U1448	C1385	U1325	U1265	A1200	A1135	U1073
C	C1897	U1834	G1769	U1705	A1642	C1579	G1513	A1449	G1387	C1327	U1265	A1201	A1136	U1074
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U	A1899	U1837	C1773	C1706	U1644	C1581	C1516	A1452	G1389	U1329	U1269	A1202	U1138	U1078
C	A1900	G1838	C1774	C1708	U1645	A1582	C1517	U1455	A1390	U1330	A1270	A1203	G1139	U1079
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U	G1902	U1840	C1776	C1710	G1647	C1585	U1518	U1457	G1392	A1332	C1272	C1209	C1141	U1081
U	U1903	A1841	C1779	C1711	A1648	G1586	G1519	U1458	A1393	C1333	A1273	G1209	G1142	U1082
C	C1904	A1842	G1780	G1712	U1649	A1587	G1520	C1459	A1394	C1334	A1274	A1210	A1143	G1083
U	G1905	G1713	C1781	G1713	G1650	A1588	U1522	A1460	G1395	C1335	C1275	U1211	U1144	G1084
U	U1906	A1714	U1782	A1714	U1651	A1589	U1523	A1461	C1396	U1336	U1276	A1212	G1145	A1085
U	C1907	G1845	U1783	A1715	G1652	G1590	A1524	A1462	C1397	A1337	C1277	G1213	G1146	C1086
C	U1908	G1784	U1785	U1716	G1653	G1591	U1525	U1463	U1398	C1338	A1278	U1214	G1147	C1087
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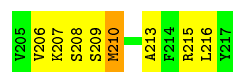


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G3061	G2997	C2931	C2867	A2802	G2732	G2663	G2599		C2469		C2339	A2209	A2209	A2143	U2080
G3062		U2932	U2868	A2803	A2733	G2664	C2600		C2470	C2406	U2340	A2210	G2210	A2144	U2081
C3063	A3000	C2933	U2869	A2804	A2734	G2665	A2601		U2471	C2407	C2341	A2213		C2145	U2082
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C3067	C3004	U2937	U2873	A2808	A2738	G2669	G2605		C2475	G2412	C2346	U2286	U2217	A2149	A2086
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G3105	A3045			G2850	C2774	G2715	A2648		U2454			C2323			
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G3108	A3048		G2918	U2854	U2718	U2718	G2651		A2457			U2326			
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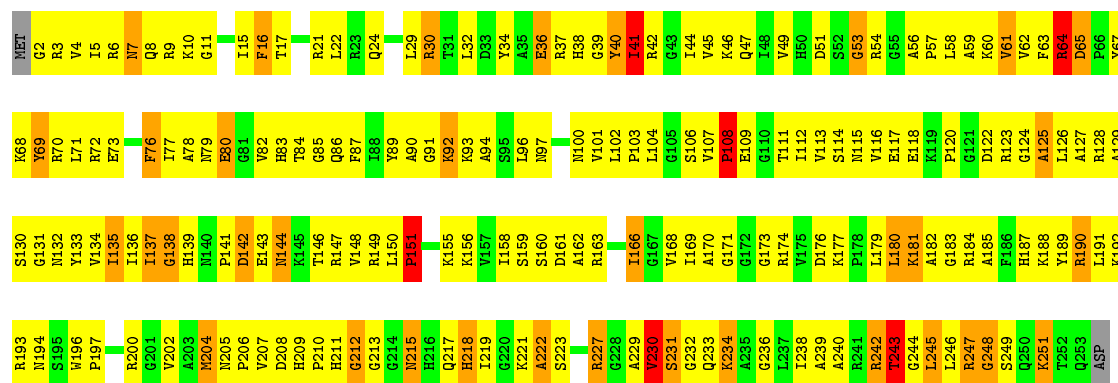




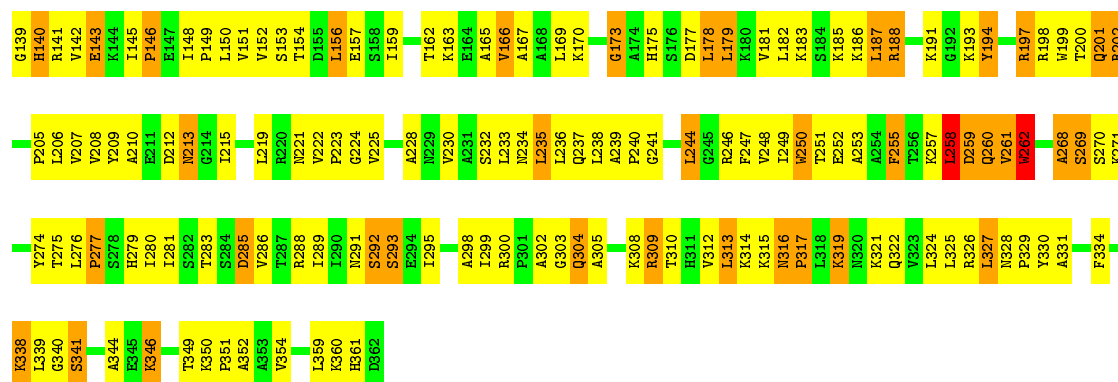


• Molecule 6: uL2 (yeast L2)

Chain F: 24% 59% 14% ..

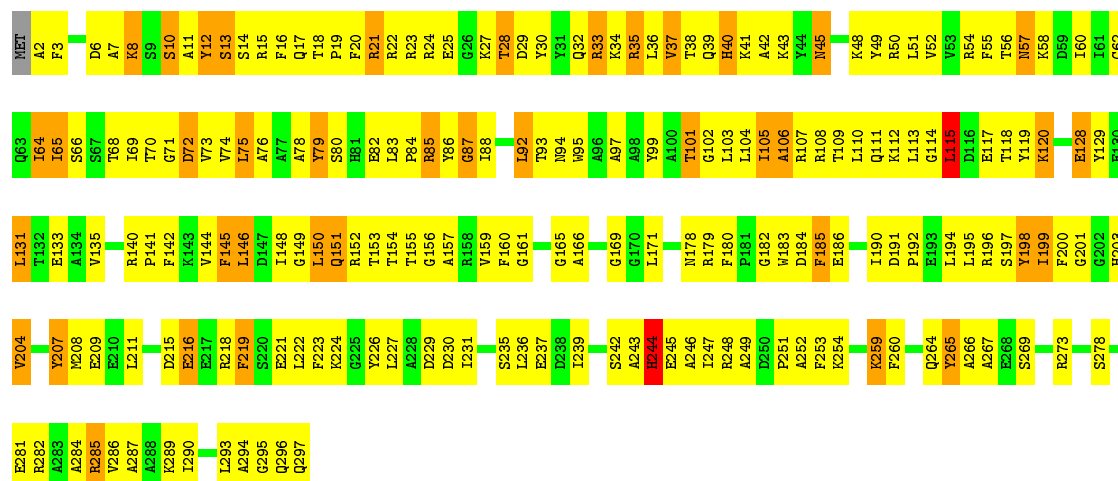






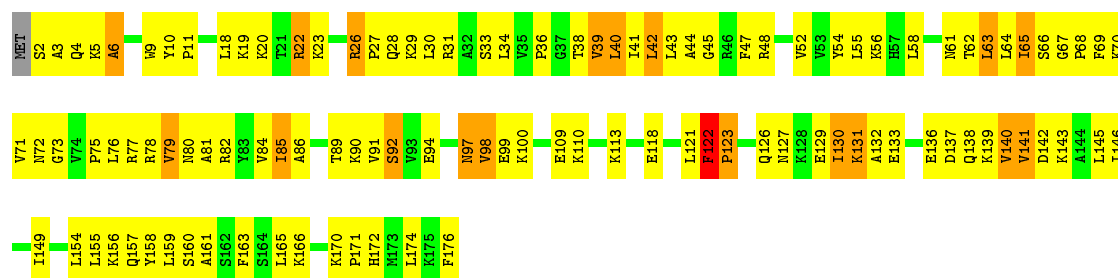
• Molecule 9: uL18 (yeast L5)

Chain I: 32% 54% 13%



• Molecule 10: eL6 (yeast L6)

Chain J: 36% 52% 10%



• Molecule 11: uL30 (yeast L7)

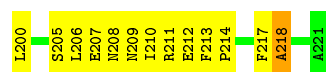
Chain K: 27% 49% 14% 9%





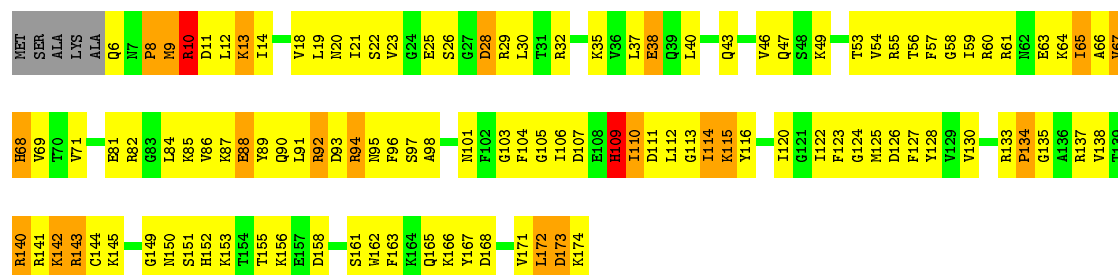






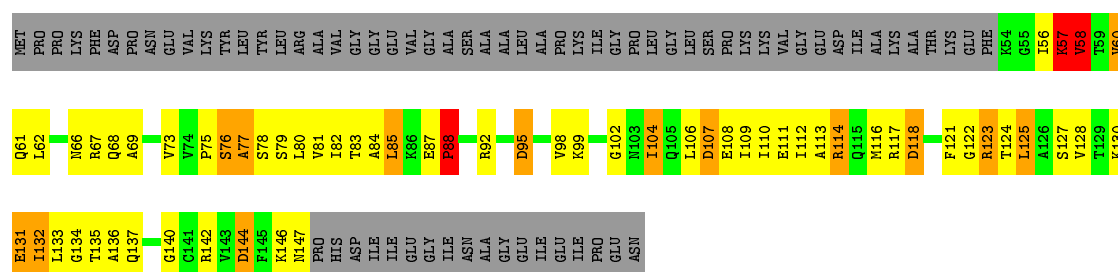
### • Molecule 15: uL5 (yeast L11)

Chain O: 31% 53% 11% ..



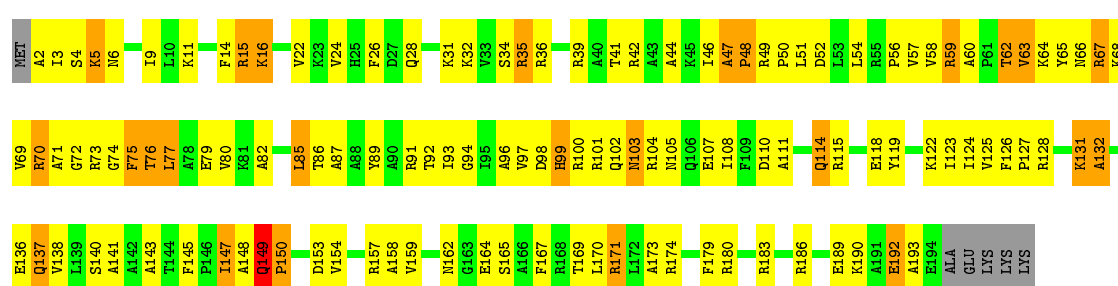
### • Molecule 16: uL11 (yeast L12)

Chain P: 19% 27% 8% 43%



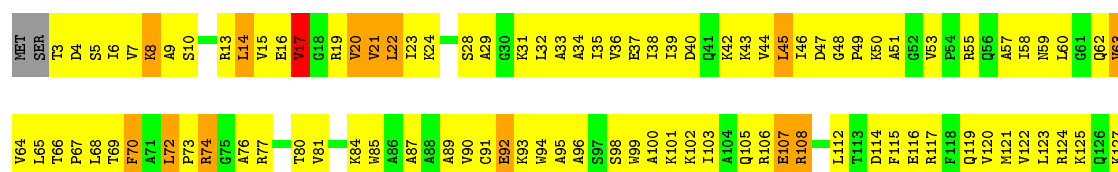
### • Molecule 17: eL13 (yeast L13)

Chain Q: 35% 49% 13% ..



### • Molecule 18: eL14 (yeast L14)

Chain R: 25% 62% 11% ..

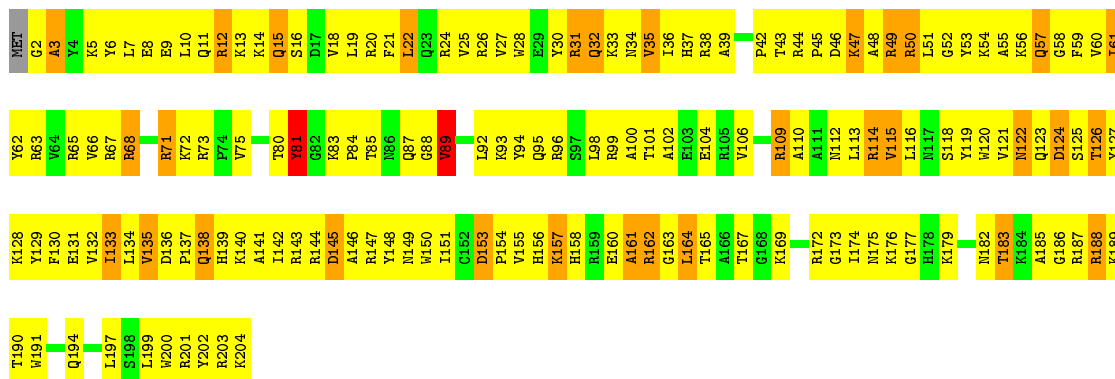






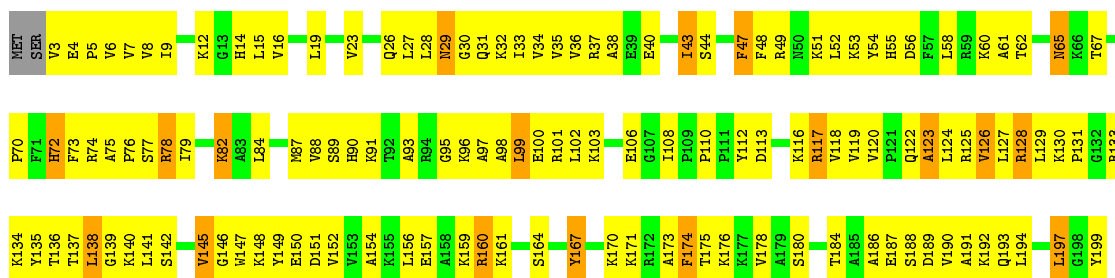
• Molecule 19: eL15 (yeast L15)

Chain S: 20% 64% 15%



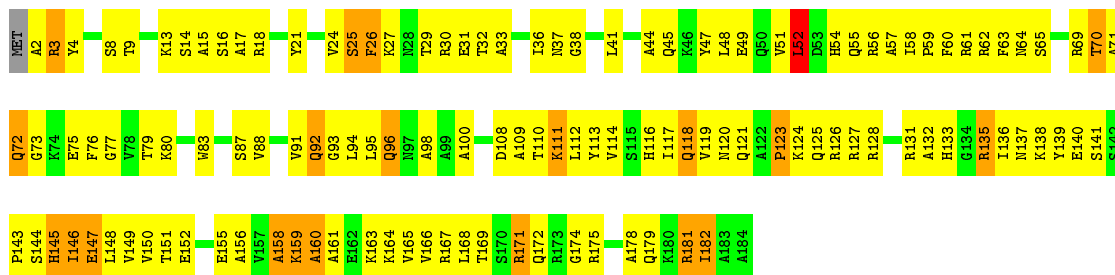
• Molecule 20: uL13 (yeast L16)

Chain T: 31% 59% 9%



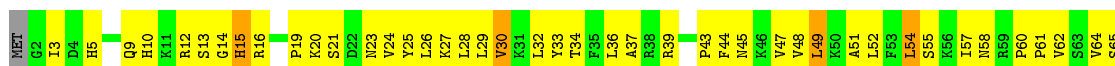
• Molecule 21: uL22 (yeast L17)

Chain U: 32% 57% 11%

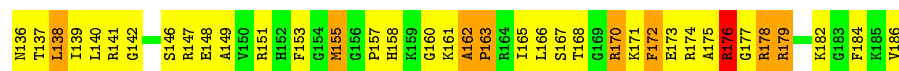
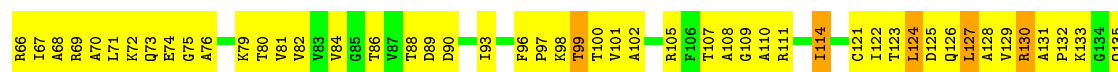


• Molecule 22: eL18 (yeast L18)

Chain V: 30% 60% 9%

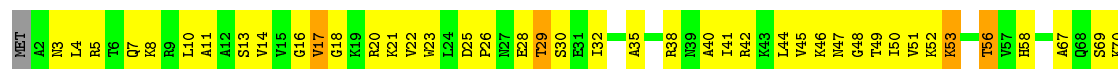






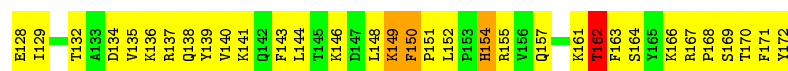
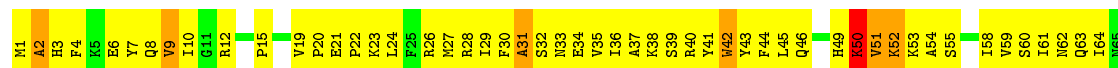
• Molecule 23: eL19 (yeast L19)

Chain W: 35% 57% 6% ..



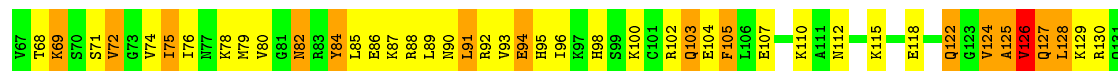
• Molecule 24: eL20 (yeast L20)

Chain X: 22% 65% 12% .



• Molecule 25: eL21 (yeast L21)

Chain Y: 32% 48% 19% ..



• Molecule 26: eL22 (yeast L22)

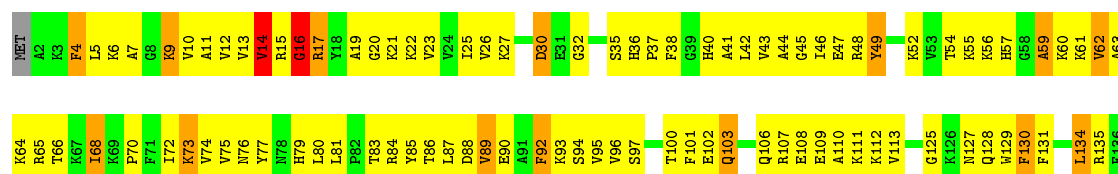
Chain Z: 40% 41% 17% .





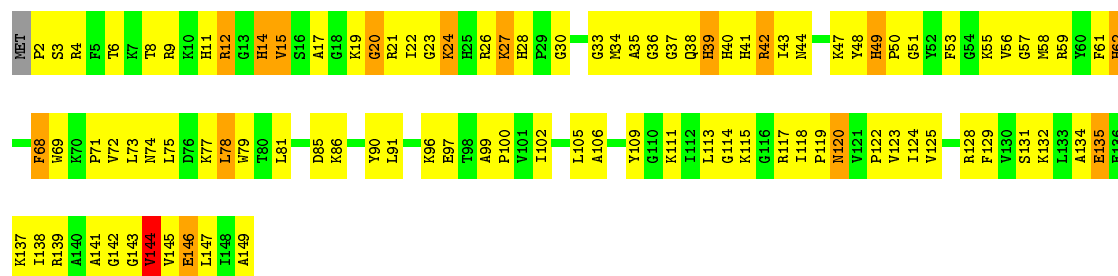






• Molecule 32: uL15 (yeast L28)

Chain FA: 34% 55% 10% ..



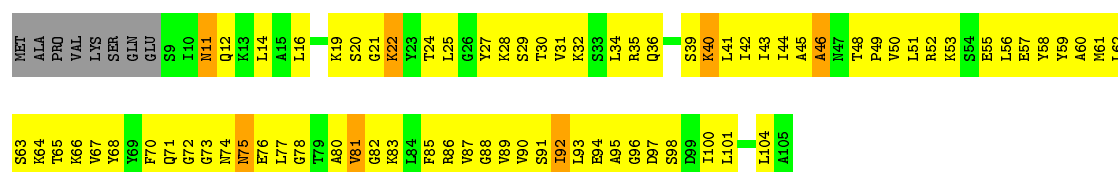
• Molecule 33: eL29 (yeast L29)

Chain GA: 44% 44% 10% .



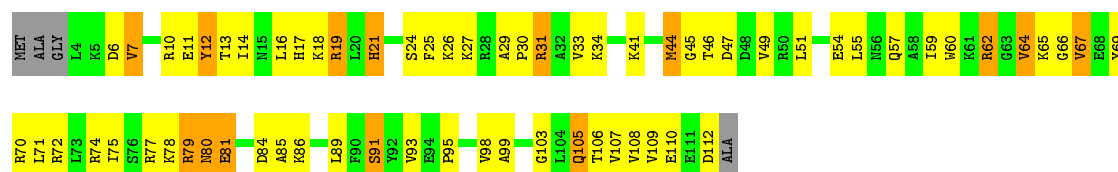
• Molecule 34: eL30 (yeast L30)

Chain HA: 19% 67% 7% 8%



• Molecule 35: eL31 (yeast L31)

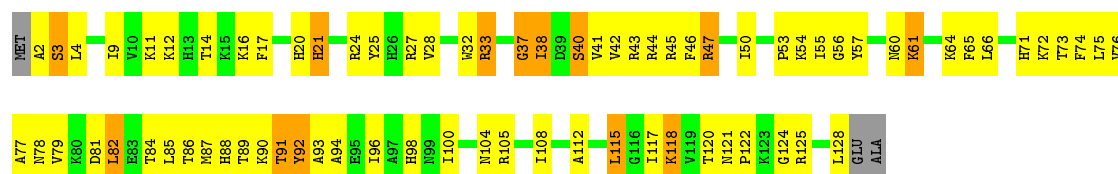
Chain IA: 38% 46% 12% .



• Molecule 36: eL32 (yeast L32)

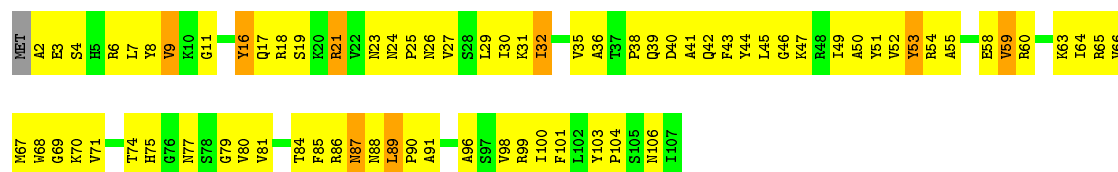
Chain JA: 39% 48% 10% .





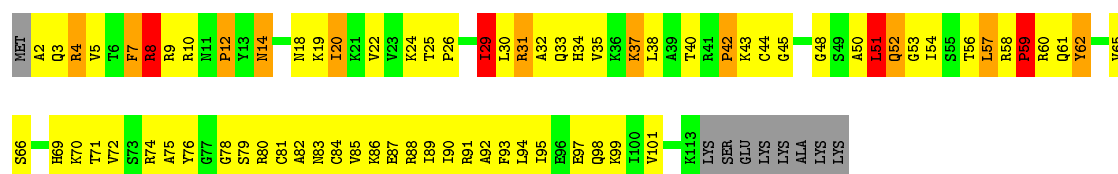
- Molecule 37: eL33 (yeast L33)

Chain KA: 29% 63% 7%



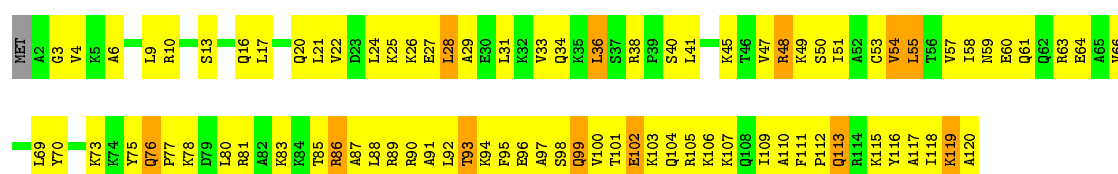
- Molecule 38: eL34 (yeast L34)

Chain LA: 31% 50% 9% 7%



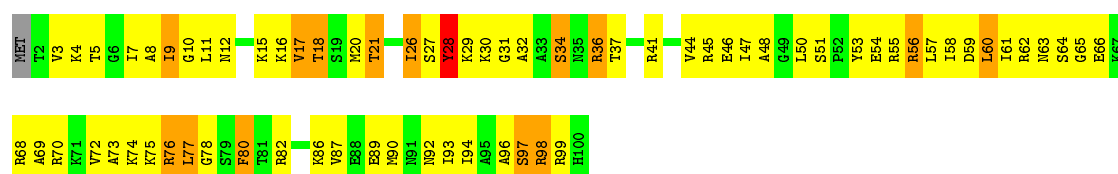
- Molecule 39: uL29 (yeast L35)

Chain MA: 28% 61% 10%



- Molecule 40: eL36 (yeast L36)

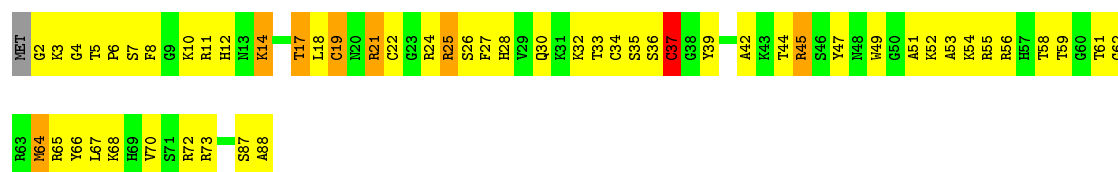
Chain NA: 29% 55% 14%



- Molecule 41: eL37 (yeast L37)

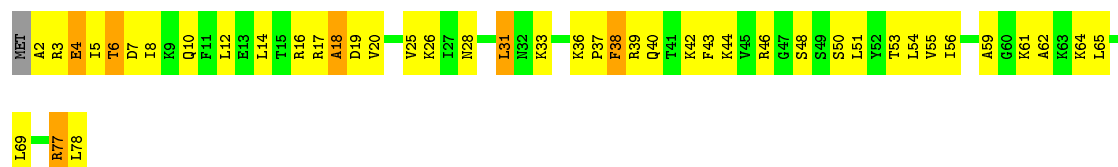
Chain OA: 38% 52% 8%





- Molecule 42: eL38 (yeast L38)

Chain PA: 42% 49% 8%



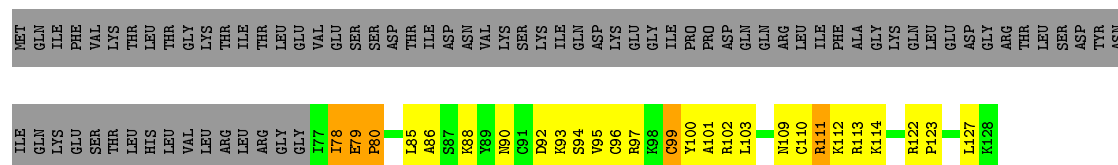
- Molecule 43: eL39 (yeast L39)

Chain QA: 27% 61% 10%



- Molecule 44: eL40 (yeast L40)

Chain RA: 20% 17% 59%



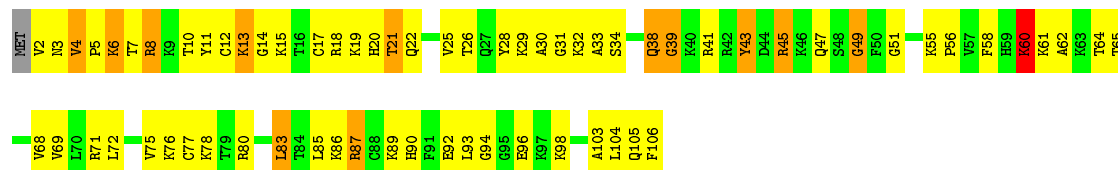
- Molecule 45: eL41 (yeast L41)

Chain SA: 28% 56% 16%



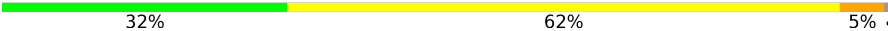
- Molecule 46: eL42 (yeast L42)

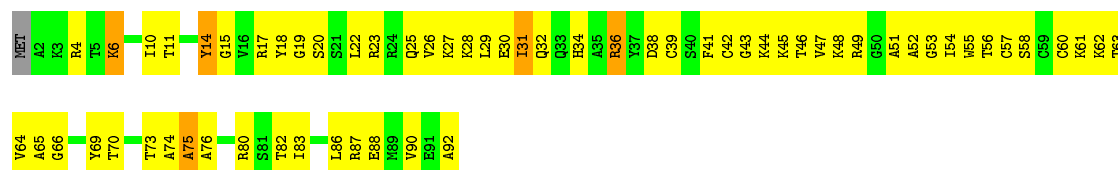
Chain TA: 35% 52% 11%



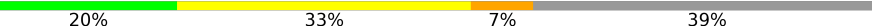
- Molecule 47: eL43 (yeast L43)

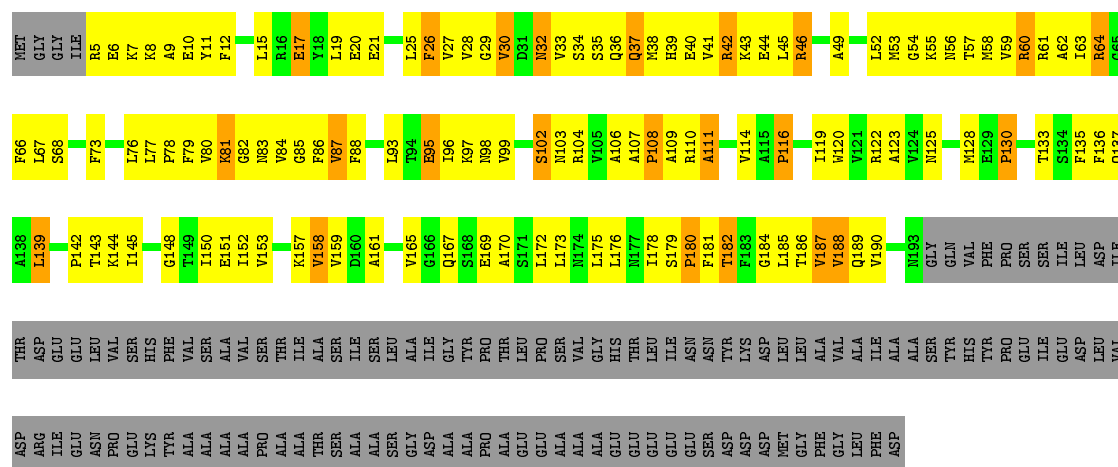


Chain UA: 

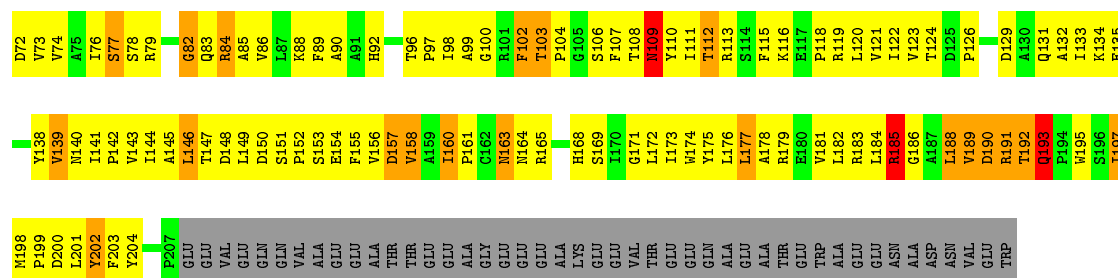


• Molecule 48: uL10 (yeast P0)

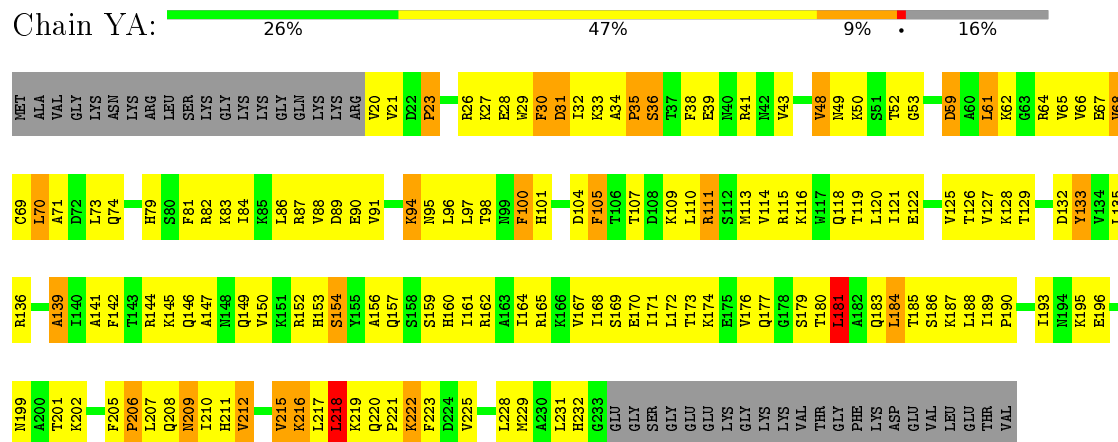
Chain VA: 



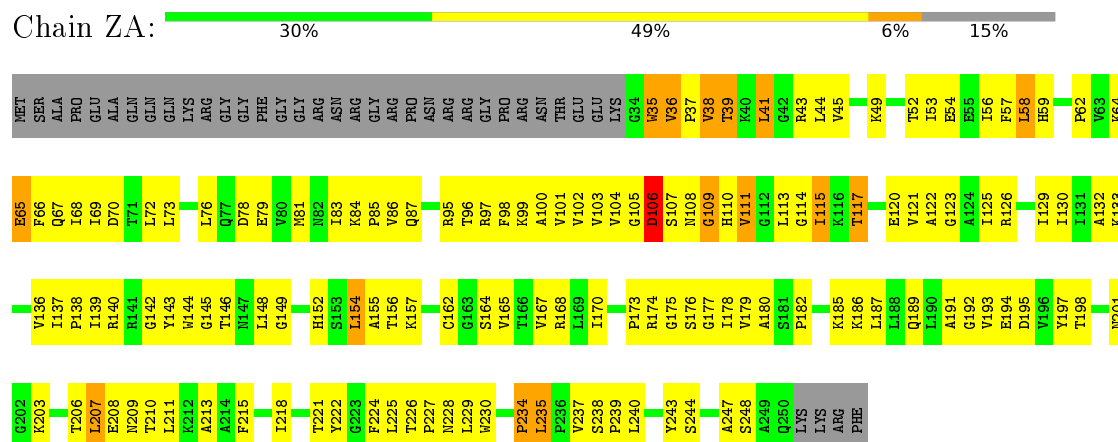




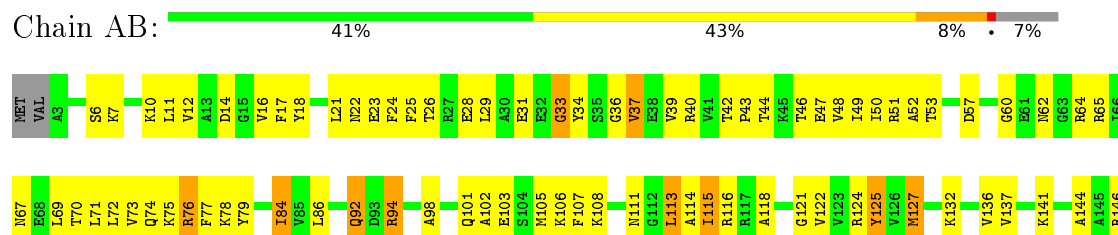
• Molecule 51: eS1 (yeast S1)



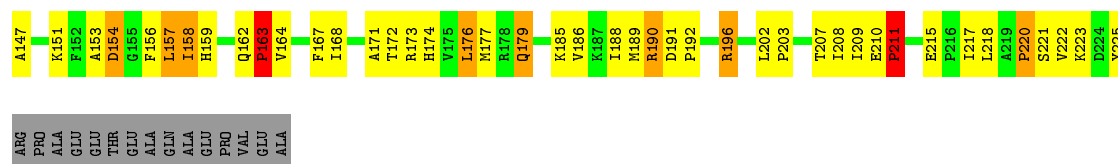
• Molecule 52: uS5 (yeast S2)



• Molecule 53: uS3 (yeast S3)

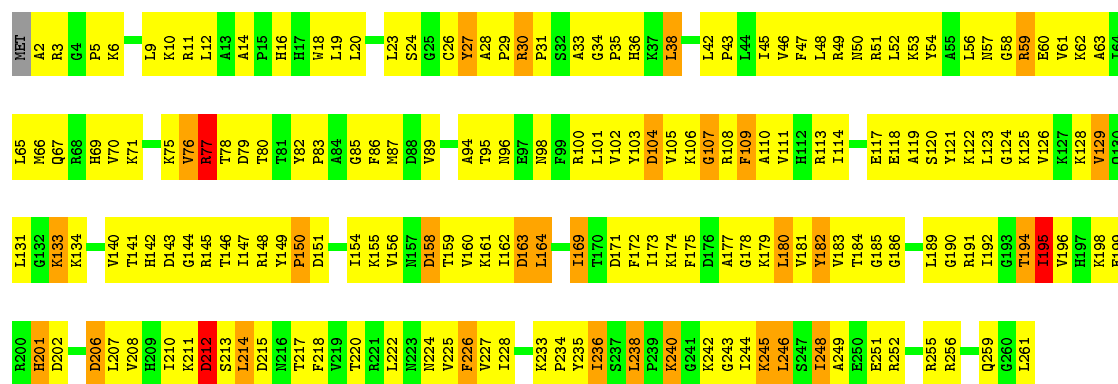




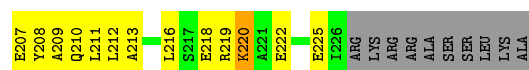


• Molecule 54: eS4 (yeast S4)

Chain BB: 30% 58% 11%

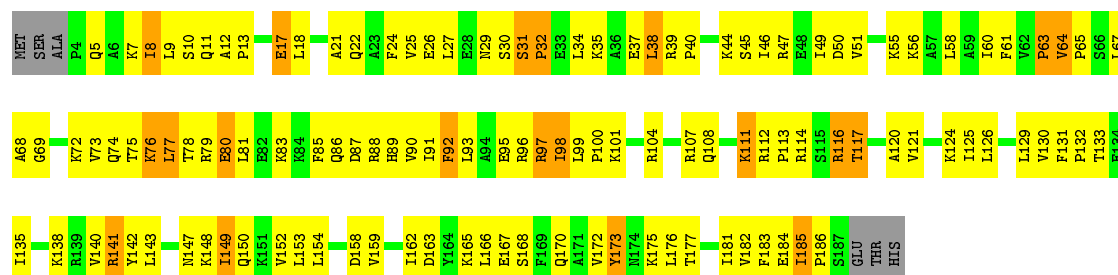






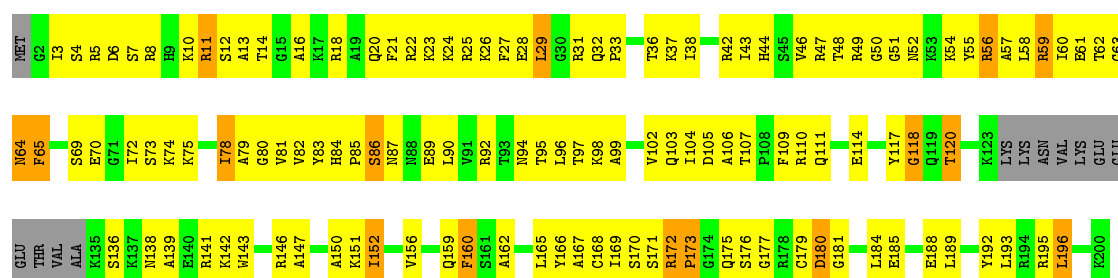
• Molecule 57: eS7 (yeast S7)

Chain EB: 32% 54% 11%



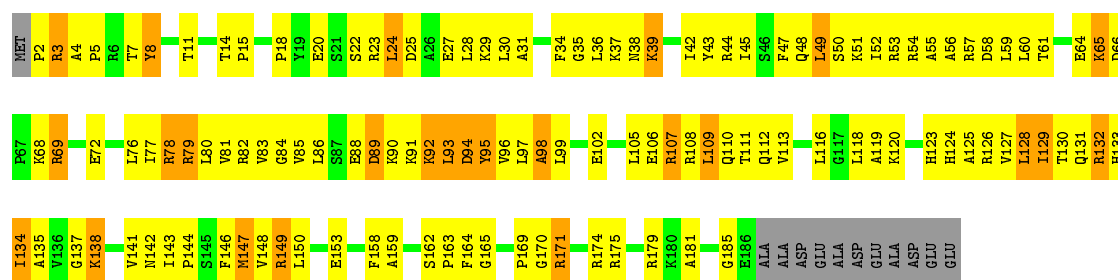
• Molecule 58: eS8 (yeast S8)

Chain FB: 31% 56% 8% 6%



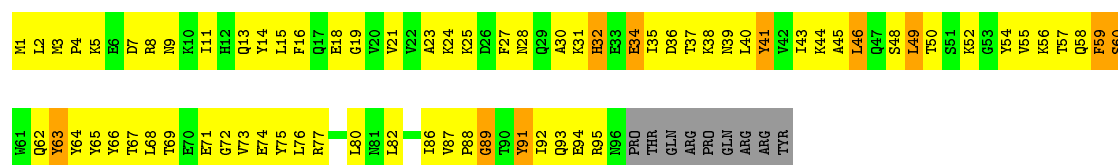
• Molecule 59: uS4 (yeast S9)

Chain GB: 29% 52% 13% 6%



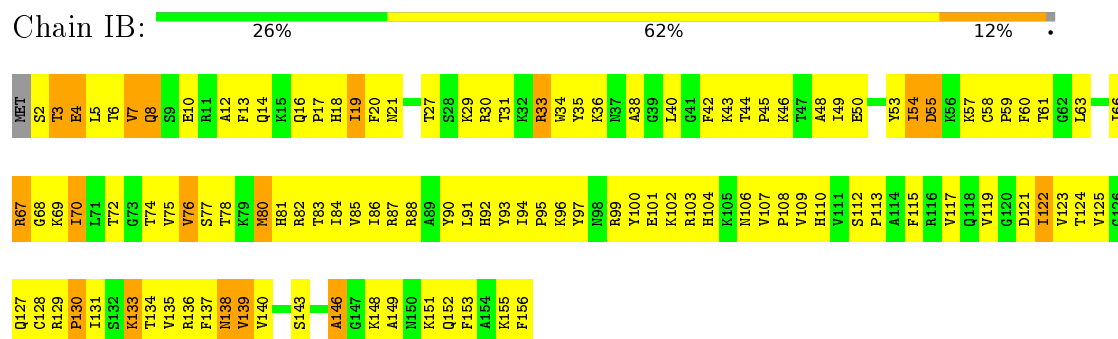
• Molecule 60: eS10 (yeast S10)

Chain HB: 22% 60% 10% 9%

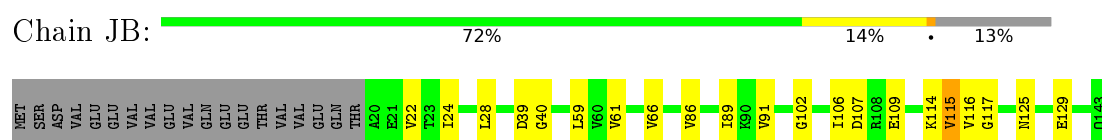




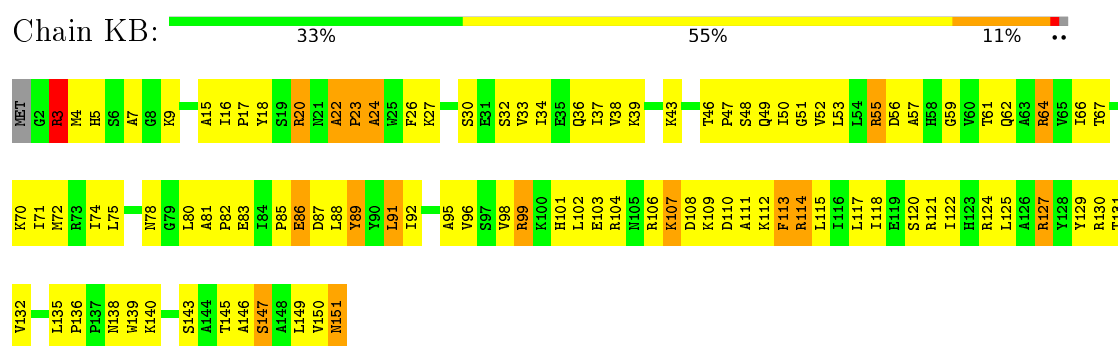
- Molecule 61: uS17 (yeast S11)



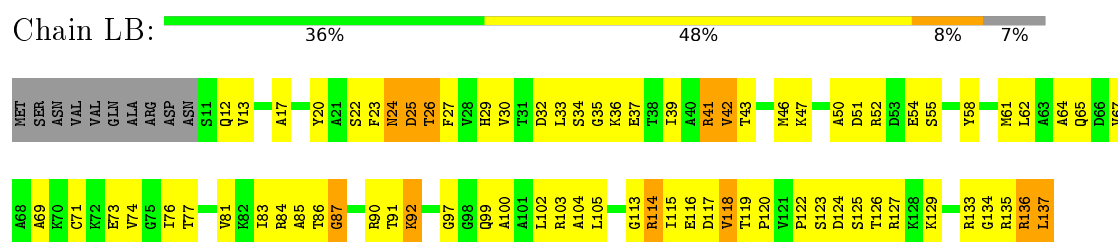
- Molecule 62: eS12 (yeast S12)



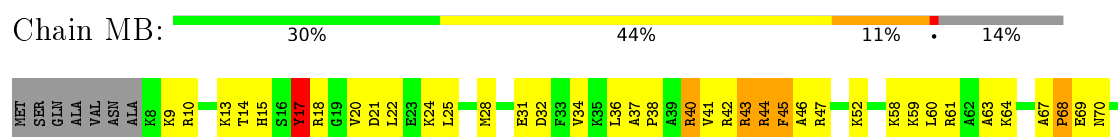
- Molecule 63: uS15 (yeast S13)



- Molecule 64: uS11 (yeast S14)



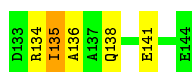
- Molecule 65: uS19 (yeast S15)





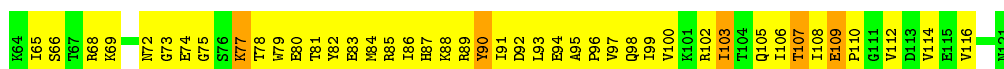
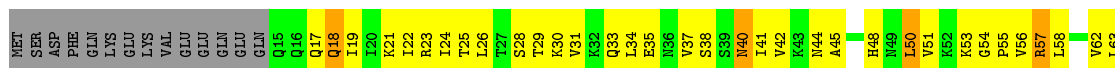






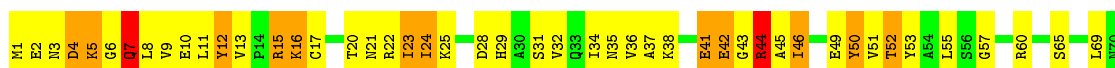
• Molecule 70: uS10 (yeast S20)

Chain RB:



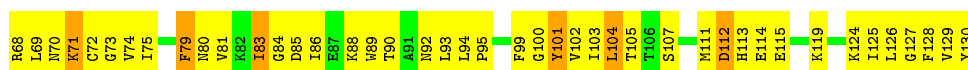
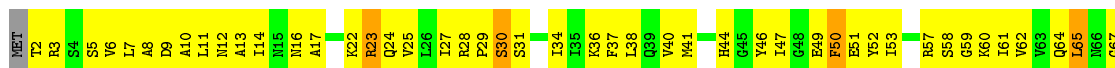
• Molecule 71: eS21 (yeast S21)

Chain SB:



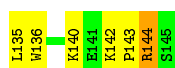
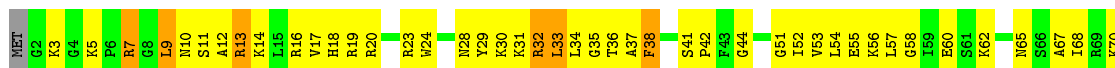
• Molecule 72: uS8 (yeast S22)

Chain TB:



• Molecule 73: uS12 (yeast S23)

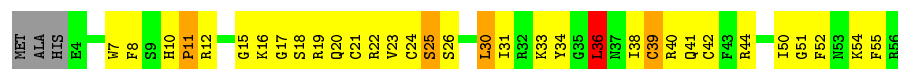
Chain UB:



• Molecule 74: eS24 (yeast S24)

Chain VB:







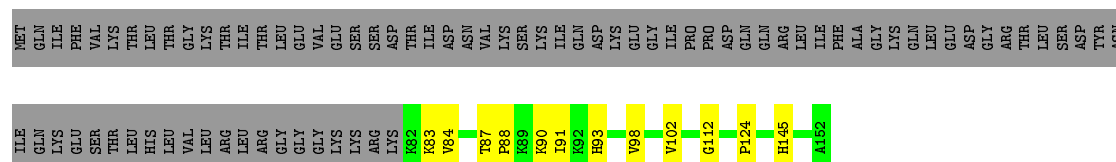
- Molecule 80: eS30 (yeast S30)

Chain BC: 



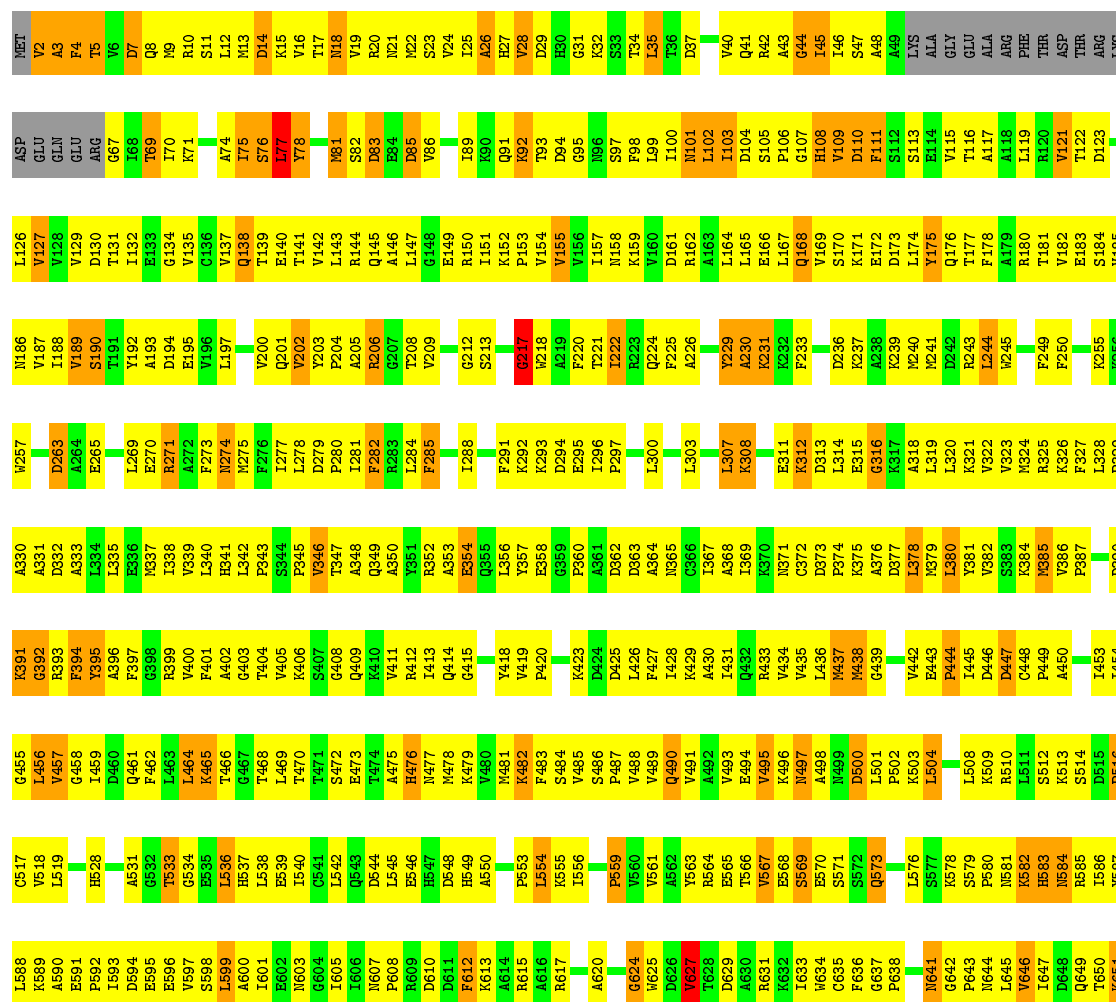
- Molecule 81: eS31 (yeast S31)

Chain CC: 

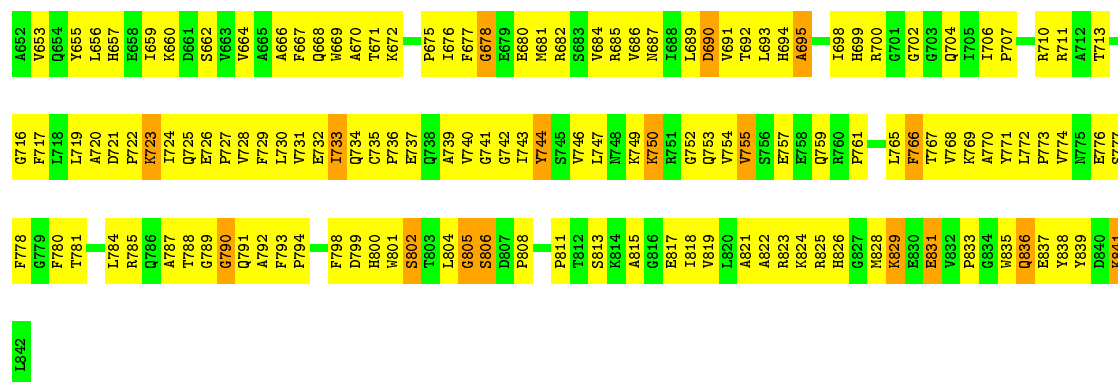


- Molecule 82: yeast eEF2

Chain DC: 

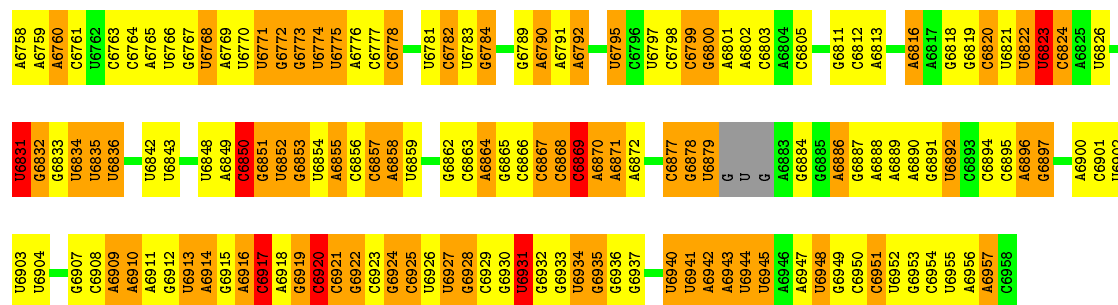






• Molecule 83: IRES

Chain EC: 25% 38% 32% . .





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	31871	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	0.86	1/42096 (0.0%)	0.75	11/65570 (0.0%)
10	J	1.05	0/1425	0.68	2/1912 (0.1%)
11	K	1.14	0/1822	0.66	0/2451
12	L	0.95	0/1850	0.63	0/2495
13	M	1.00	0/1540	0.64	0/2073
14	N	1.07	0/1754	0.65	0/2350
15	O	0.84	0/1375	0.60	0/1842
16	P	1.71	0/728	0.75	0/975
17	Q	1.03	0/1568	0.65	0/2106
18	R	1.13	0/1069	0.64	0/1438
19	S	1.13	0/1758	0.69	0/2354
2	B	1.13	16/78631 (0.0%)	0.77	25/122552 (0.0%)
20	T	1.08	0/1586	0.65	0/2128
21	U	1.06	0/1466	0.66	1/1968 (0.1%)
22	V	1.04	0/1466	0.69	1/1965 (0.1%)
23	W	0.87	0/1539	0.61	0/2050
24	X	1.19	0/1482	0.66	0/1990
25	Y	1.13	0/1301	0.68	0/1743
26	Z	0.78	0/812	0.58	0/1099
27	AA	1.06	0/1019	0.63	0/1369
28	BA	1.10	0/521	0.62	0/691
29	CA	1.09	0/984	0.68	1/1325 (0.1%)
3	C	1.18	1/3747 (0.0%)	0.76	2/5832 (0.0%)
30	DA	1.05	0/1005	0.71	1/1341 (0.1%)
31	EA	0.85	0/1119	0.61	1/1497 (0.1%)
32	FA	1.07	0/1205	0.65	0/1612
33	GA	0.97	0/474	0.68	0/629
34	HA	0.79	0/751	0.63	0/1008
35	IA	0.93	0/904	0.61	0/1213
36	JA	1.10	0/1041	0.62	0/1394
37	KA	1.15	0/869	0.68	0/1168
38	LA	0.99	0/891	0.66	0/1191



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	MA	0.95	0/979	0.66	0/1301
4	D	1.08	1/2884 (0.0%)	0.76	0/4491
40	NA	0.92	0/779	0.64	0/1034
41	OA	1.19	0/697	0.66	0/923
42	PA	0.88	0/619	0.60	0/826
43	QA	1.01	0/444	0.68	0/588
44	RA	1.05	0/424	0.60	0/562
45	SA	0.89	0/235	0.67	0/300
46	TA	1.03	0/861	0.67	0/1136
47	UA	1.02	0/702	0.61	0/934
48	VA	1.58	0/1498	0.79	0/2025
49	WA	0.83	0/2498	0.56	0/3398
5	E	1.77	0/1377	0.79	2/1844 (0.1%)
50	XA	0.71	0/1653	0.65	3/2261 (0.1%)
51	YA	0.75	0/1735	0.59	1/2335 (0.0%)
52	ZA	0.74	0/1665	0.59	0/2263
53	AB	0.86	0/1759	0.57	0/2368
54	BB	0.72	0/2110	0.59	0/2839
55	CB	0.79	0/1630	0.58	0/2202
56	DB	0.74	0/1844	0.58	0/2464
57	EB	0.78	0/1506	0.58	0/2028
58	FB	0.88	0/1515	0.58	0/2021
59	GB	0.70	0/1519	0.59	0/2035
6	F	1.01	0/1952	0.72	1/2622 (0.0%)
60	HB	0.93	0/837	0.56	0/1131
61	IB	0.91	0/1273	0.62	0/1712
62	JB	1.02	0/495	0.61	0/617
63	KB	0.83	0/1216	0.61	0/1638
64	LB	0.67	0/953	0.57	0/1279
65	MB	0.97	0/996	0.64	0/1335
66	NB	0.83	0/1126	0.61	0/1510
67	OB	0.80	1/844 (0.1%)	0.82	4/1120 (0.4%)
68	PB	0.87	0/1212	0.59	0/1628
69	QB	0.84	0/1131	0.62	0/1517
7	G	0.98	0/3153	0.66	1/4239 (0.0%)
70	RB	0.86	0/866	0.59	0/1169
71	SB	0.71	0/694	0.57	0/935
72	TB	0.77	0/1039	0.59	0/1395
73	UB	0.90	0/1140	0.60	0/1518
74	VB	0.76	0/1088	0.58	0/1449
75	WB	0.83	0/571	0.65	0/768
76	XB	0.71	0/782	0.57	0/1047
77	YB	0.76	0/621	0.57	0/838



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	ZB	0.75	0/500	0.60	0/670
79	AC	0.98	0/454	0.61	1/602 (0.2%)
8	H	1.09	0/2802	0.67	0/3792
80	BC	0.85	0/483	0.62	0/643
81	CC	0.99	0/283	0.66	0/352
82	DC	1.39	5/6521 (0.1%)	0.71	4/8830 (0.0%)
83	EC	1.96	34/4579 (0.7%)	0.94	10/7119 (0.1%)
9	I	0.91	0/2426	0.63	0/3271
All	All	1.06	59/230768 (0.0%)	0.72	72/338255 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
2	B	0	64
3	C	0	2
4	D	0	1
50	XA	0	1
83	EC	0	10
All	All	0	89

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

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

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

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



There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	U	Sidechain
1	A	287	G	Sidechain
1	A	322	G	Sidechain
1	A	447	U	Sidechain
1	A	834	G	Sidechain

## 5.2 Too-close contacts

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 14740 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:DC:3:ALA:CA	82:DC:3:ALA:N	1.71	1.50
2:B:1719:G:H4'	2:B:1732:U:H4'	1.22	1.18
1:A:754:A:H3'	1:A:755:A:H5'	1.25	1.14
22:V:54:LEU:HB3	22:V:58:ASN:HB2	1.26	1.14
55:CB:29:ILE:HG21	66:NB:57:LEU:HD11	1.27	1.14

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 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%)	124 (75%)	28 (17%)	13 (8%)	1	19
6	F	250/254 (98%)	159 (64%)	61 (24%)	30 (12%)	0	8
7	G	384/387 (99%)	280 (73%)	84 (22%)	20 (5%)	2	31
8	H	359/362 (99%)	241 (67%)	77 (21%)	41 (11%)	0	9
9	I	294/297 (99%)	210 (71%)	64 (22%)	20 (7%)	1	24
10	J	173/176 (98%)	124 (72%)	35 (20%)	14 (8%)	1	19
11	K	220/244 (90%)	160 (73%)	37 (17%)	23 (10%)	1	11
12	L	231/256 (90%)	162 (70%)	50 (22%)	19 (8%)	1	18
13	M	189/191 (99%)	143 (76%)	32 (17%)	14 (7%)	1	21
14	N	207/221 (94%)	157 (76%)	35 (17%)	15 (7%)	1	23
15	O	167/174 (96%)	121 (72%)	30 (18%)	16 (10%)	1	14
16	P	92/165 (56%)	64 (70%)	14 (15%)	14 (15%)	0	5
17	Q	191/199 (96%)	141 (74%)	33 (17%)	17 (9%)	1	17
18	R	134/138 (97%)	103 (77%)	24 (18%)	7 (5%)	2	31
19	S	201/204 (98%)	148 (74%)	39 (19%)	14 (7%)	1	23
20	T	195/199 (98%)	152 (78%)	37 (19%)	6 (3%)	5	45
21	U	181/184 (98%)	127 (70%)	39 (22%)	15 (8%)	1	18
22	V	183/186 (98%)	120 (66%)	47 (26%)	16 (9%)	1	17
23	W	186/189 (98%)	142 (76%)	35 (19%)	9 (5%)	3	32
24	X	170/172 (99%)	119 (70%)	41 (24%)	10 (6%)	2	28
25	Y	157/160 (98%)	105 (67%)	31 (20%)	21 (13%)	0	6
26	Z	98/121 (81%)	64 (65%)	28 (29%)	6 (6%)	2	27
27	AA	134/137 (98%)	97 (72%)	32 (24%)	5 (4%)	4	40
28	BA	59/155 (38%)	41 (70%)	10 (17%)	8 (14%)	0	6
29	CA	119/142 (84%)	79 (66%)	24 (20%)	16 (13%)	0	6
30	DA	124/127 (98%)	96 (77%)	19 (15%)	9 (7%)	1	22
31	EA	133/136 (98%)	95 (71%)	21 (16%)	17 (13%)	0	7
32	FA	146/149 (98%)	95 (65%)	39 (27%)	12 (8%)	1	18
33	GA	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	1	17
34	HA	95/105 (90%)	70 (74%)	19 (20%)	6 (6%)	2	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	IA	107/113 (95%)	79 (74%)	24 (22%)	4 (4%)	4	40
36	JA	125/130 (96%)	87 (70%)	30 (24%)	8 (6%)	2	26
37	KA	104/107 (97%)	77 (74%)	24 (23%)	3 (3%)	6	46
38	LA	110/121 (91%)	69 (63%)	30 (27%)	11 (10%)	1	13
39	MA	117/120 (98%)	87 (74%)	23 (20%)	7 (6%)	2	27
40	NA	97/100 (97%)	69 (71%)	18 (19%)	10 (10%)	1	12
41	OA	85/88 (97%)	58 (68%)	23 (27%)	4 (5%)	3	33
42	PA	75/78 (96%)	58 (77%)	14 (19%)	3 (4%)	4	37
43	QA	48/51 (94%)	35 (73%)	9 (19%)	4 (8%)	1	18
44	RA	50/128 (39%)	36 (72%)	10 (20%)	4 (8%)	1	19
45	SA	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
46	TA	103/106 (97%)	66 (64%)	25 (24%)	12 (12%)	0	9
47	UA	89/92 (97%)	68 (76%)	17 (19%)	4 (4%)	3	34
48	VA	187/312 (60%)	138 (74%)	37 (20%)	12 (6%)	2	26
49	WA	316/319 (99%)	243 (77%)	60 (19%)	13 (4%)	3	37
50	XA	204/252 (81%)	147 (72%)	41 (20%)	16 (8%)	1	20
51	YA	212/255 (83%)	154 (73%)	41 (19%)	17 (8%)	1	19
52	ZA	215/254 (85%)	155 (72%)	45 (21%)	15 (7%)	1	23
53	AB	221/240 (92%)	170 (77%)	37 (17%)	14 (6%)	2	27
54	BB	258/261 (99%)	173 (67%)	64 (25%)	21 (8%)	1	19
55	CB	204/225 (91%)	152 (74%)	35 (17%)	17 (8%)	1	18
56	DB	224/236 (95%)	174 (78%)	36 (16%)	14 (6%)	2	27
57	EB	182/190 (96%)	128 (70%)	43 (24%)	11 (6%)	2	27
58	FB	184/200 (92%)	136 (74%)	36 (20%)	12 (6%)	1	26
59	GB	183/197 (93%)	143 (78%)	26 (14%)	14 (8%)	1	20
60	HB	94/105 (90%)	66 (70%)	20 (21%)	8 (8%)	1	17
61	IB	153/156 (98%)	109 (71%)	31 (20%)	13 (8%)	1	17
62	JB	122/143 (85%)	74 (61%)	29 (24%)	19 (16%)	0	5
63	KB	148/151 (98%)	113 (76%)	28 (19%)	7 (5%)	3	33
64	LB	125/137 (91%)	87 (70%)	29 (23%)	9 (7%)	1	23
65	MB	120/142 (84%)	83 (69%)	27 (22%)	10 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	102 (73%)	27 (19%)	10 (7%)	1	23
67	OB	115/136 (85%)	79 (69%)	29 (25%)	7 (6%)	2	27
68	PB	143/146 (98%)	101 (71%)	27 (19%)	15 (10%)	1	11
69	QB	141/144 (98%)	99 (70%)	28 (20%)	14 (10%)	1	13
70	RB	105/121 (87%)	81 (77%)	22 (21%)	2 (2%)	10	54
71	SB	85/87 (98%)	55 (65%)	19 (22%)	11 (13%)	0	7
72	TB	127/130 (98%)	95 (75%)	25 (20%)	7 (6%)	2	30
73	UB	142/145 (98%)	94 (66%)	41 (29%)	7 (5%)	3	32
74	VB	132/135 (98%)	93 (70%)	32 (24%)	7 (5%)	2	31
75	WB	68/108 (63%)	42 (62%)	14 (21%)	12 (18%)	0	3
76	XB	95/119 (80%)	57 (60%)	24 (25%)	14 (15%)	0	5
77	YB	79/82 (96%)	41 (52%)	27 (34%)	11 (14%)	0	6
78	ZB	61/67 (91%)	44 (72%)	12 (20%)	5 (8%)	1	18
79	AC	51/56 (91%)	37 (72%)	10 (20%)	4 (8%)	1	20
80	BC	58/63 (92%)	40 (69%)	14 (24%)	4 (7%)	1	24
81	CC	69/152 (45%)	37 (54%)	20 (29%)	12 (17%)	0	3
82	DC	819/842 (97%)	592 (72%)	171 (21%)	56 (7%)	1	24
All	All	12207/13416 (91%)	8728 (72%)	2527 (21%)	952 (8%)	2	20

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 ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	157/198 (79%)	137 (87%)	20 (13%)	5	31
6	F	194/196 (99%)	171 (88%)	23 (12%)	6	34
7	G	322/323 (100%)	288 (89%)	34 (11%)	8	39
8	H	288/289 (100%)	255 (88%)	33 (12%)	7	36
9	I	244/245 (100%)	211 (86%)	33 (14%)	5	30
10	J	152/153 (99%)	143 (94%)	9 (6%)	24	64
11	K	186/205 (91%)	163 (88%)	23 (12%)	6	32
12	L	191/208 (92%)	174 (91%)	17 (9%)	12	48
13	M	171/171 (100%)	155 (91%)	16 (9%)	11	45
14	N	180/187 (96%)	162 (90%)	18 (10%)	9	42
15	O	147/150 (98%)	134 (91%)	13 (9%)	12	48
16	P	81/136 (60%)	69 (85%)	12 (15%)	4	26
17	Q	154/159 (97%)	134 (87%)	20 (13%)	5	31
18	R	107/109 (98%)	91 (85%)	16 (15%)	3	25
19	S	175/176 (99%)	150 (86%)	25 (14%)	4	28
20	T	160/162 (99%)	142 (89%)	18 (11%)	7	37
21	U	145/146 (99%)	130 (90%)	15 (10%)	9	40
22	V	150/151 (99%)	141 (94%)	9 (6%)	24	63
23	W	153/154 (99%)	139 (91%)	14 (9%)	11	46
24	X	156/156 (100%)	137 (88%)	19 (12%)	6	33
25	Y	136/137 (99%)	117 (86%)	19 (14%)	4	29
26	Z	87/107 (81%)	85 (98%)	2 (2%)	58	83
27	AA	104/105 (99%)	95 (91%)	9 (9%)	13	48
28	BA	54/129 (42%)	47 (87%)	7 (13%)	5	31
29	CA	105/118 (89%)	94 (90%)	11 (10%)	8	40
30	DA	109/110 (99%)	94 (86%)	15 (14%)	4	29
31	EA	115/116 (99%)	107 (93%)	8 (7%)	19	58
32	FA	118/119 (99%)	112 (95%)	6 (5%)	29	68
33	GA	46/47 (98%)	41 (89%)	5 (11%)	8	38
34	HA	81/88 (92%)	74 (91%)	7 (9%)	13	50
35	IA	96/97 (99%)	83 (86%)	13 (14%)	5	30
36	JA	109/111 (98%)	97 (89%)	12 (11%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	83 (92%)	7 (8%)	16	54
38	LA	95/103 (92%)	84 (88%)	11 (12%)	7	36
39	MA	104/105 (99%)	96 (92%)	8 (8%)	16	55
40	NA	81/82 (99%)	69 (85%)	12 (15%)	4	26
41	OA	70/71 (99%)	62 (89%)	8 (11%)	7	36
42	PA	68/69 (99%)	63 (93%)	5 (7%)	17	56
43	QA	45/46 (98%)	42 (93%)	3 (7%)	20	60
44	RA	47/116 (40%)	43 (92%)	4 (8%)	13	51
45	SA	23/23 (100%)	19 (83%)	4 (17%)	2	18
46	TA	90/91 (99%)	82 (91%)	8 (9%)	12	48
47	UA	71/72 (99%)	66 (93%)	5 (7%)	19	58
48	VA	160/254 (63%)	143 (89%)	17 (11%)	8	39
49	WA	261/262 (100%)	237 (91%)	24 (9%)	11	46
50	XA	173/210 (82%)	151 (87%)	22 (13%)	5	31
51	YA	191/224 (85%)	173 (91%)	18 (9%)	11	45
52	ZA	176/205 (86%)	168 (96%)	8 (4%)	34	71
53	AB	182/195 (93%)	164 (90%)	18 (10%)	10	43
54	BB	221/222 (100%)	199 (90%)	22 (10%)	9	42
55	CB	173/191 (91%)	160 (92%)	13 (8%)	17	56
56	DB	193/201 (96%)	174 (90%)	19 (10%)	10	43
57	EB	165/170 (97%)	146 (88%)	19 (12%)	7	36
58	FB	150/161 (93%)	137 (91%)	13 (9%)	13	48
59	GB	158/166 (95%)	141 (89%)	17 (11%)	8	39
60	HB	89/98 (91%)	82 (92%)	7 (8%)	15	54
61	IB	136/137 (99%)	124 (91%)	12 (9%)	12	48
63	KB	127/128 (99%)	110 (87%)	17 (13%)	5	30
64	LB	96/105 (91%)	89 (93%)	7 (7%)	17	57
65	MB	103/118 (87%)	90 (87%)	13 (13%)	5	31
66	NB	117/119 (98%)	102 (87%)	15 (13%)	5	31
67	OB	82/124 (66%)	70 (85%)	12 (15%)	4	26
68	PB	128/129 (99%)	120 (94%)	8 (6%)	22	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	QB	115/116 (99%)	104 (90%)	11 (10%)	10	44
70	RB	100/114 (88%)	91 (91%)	9 (9%)	12	47
71	SB	74/74 (100%)	64 (86%)	10 (14%)	5	30
72	TB	110/111 (99%)	102 (93%)	8 (7%)	17	57
73	UB	119/120 (99%)	107 (90%)	12 (10%)	9	41
74	VB	112/113 (99%)	101 (90%)	11 (10%)	10	43
75	WB	61/89 (68%)	53 (87%)	8 (13%)	5	30
76	XB	83/101 (82%)	76 (92%)	7 (8%)	14	51
77	YB	70/71 (99%)	66 (94%)	4 (6%)	25	65
78	ZB	56/60 (93%)	53 (95%)	3 (5%)	27	67
79	AC	47/49 (96%)	42 (89%)	5 (11%)	8	39
80	BC	51/54 (94%)	40 (78%)	11 (22%)	1	10
82	DC	699/714 (98%)	605 (87%)	94 (13%)	5	30
All	All	10235/11032 (93%)	9165 (90%)	1070 (10%)	13	40

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

Mol	Chain	Res	Type
35	IA	81	GLU
49	WA	54	PHE
82	DC	81	MET
36	JA	115	LEU
41	OA	25	ARG

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

Mol	Chain	Res	Type
42	PA	40	GLN
51	YA	79	HIS
82	DC	101	ASN
43	QA	20	ASN
48	VA	39	HIS

### 5.3.3 RNA ⓘ



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

5 of 1113 RNA backbone outliers are listed below:

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

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	547	G
2	B	1287	A
3	C	131	A
2	B	637	C
2	B	1103	A

## 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	1.75	2 (15%)	12,28,30	2.44	4 (33%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	OAG-CBI	2.04	1.27	1.23
82	DC	699	DDE	CBW-CBI	4.80	1.61	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	DC	699	DDE	CAU-CBW-CBI	-5.15	100.34	110.72
82	DC	699	DDE	CG-CD2-NE2	-2.05	104.67	109.20
82	DC	699	DDE	OAG-CBI-NAD	2.58	127.32	123.06
82	DC	699	DDE	CAU-CAT-CE1	5.25	140.92	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	1.92	6 (25%)	26,47,47	2.12	7 (26%)
86	SO1	DC	903	-	36,39,39	2.80	18 (50%)	36,64,64	1.63	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 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O56-C52	-4.42	1.30	1.41
86	DC	903	SO1	C24-C18	2.06	1.59	1.54
86	DC	903	SO1	C53-C54	2.11	1.57	1.52
84	DC	901	GDP	PB-O3B	2.27	1.62	1.54
86	DC	903	SO1	C52-C53	2.49	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	DC	901	GDP	N3-C2-N1	-5.84	119.62	127.56
84	DC	901	GDP	C5-C6-N1	-4.22	118.01	123.52
86	DC	903	SO1	C7-C2-C8	-3.16	104.45	110.16
86	DC	903	SO1	C18-C9-C16	-3.08	99.09	103.42
86	DC	903	SO1	C12-C6-C10	-2.58	103.23	107.47

There are no chirality outliers.

There are no torsion outliers.

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	DC	903	SO1	3	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.