



## wwPDB EM Map/Model Validation Report ⓘ

Sep 29, 2016 – 09:22 PM EDT

PDB ID : 5JUO  
EMDB ID: : EMD-6643  
Title : Saccharomyces cerevisiae 80S ribosome bound with elongation factor eEF2-GDP-sordarin and Taura Syndrome Virus IRES, Structure I (fully 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

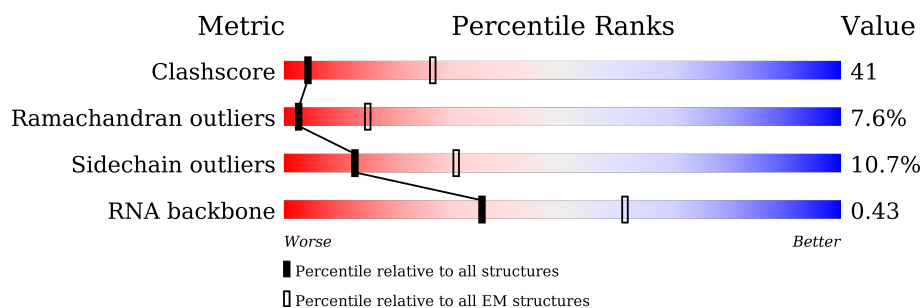
# 1 Overall quality at a glance

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.




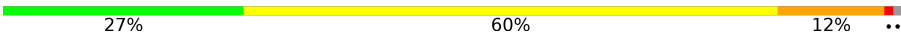
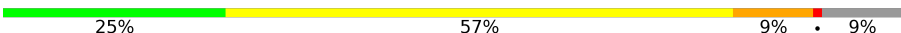


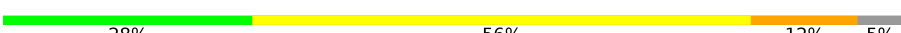
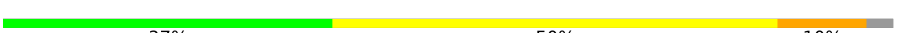




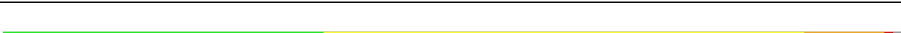






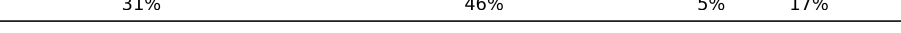


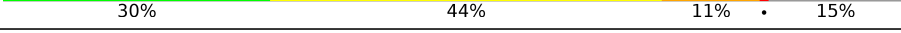



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	25% 60% 14% ..
2	B	3396	20% 59% 18% ..
3	C	158	18% 62% 18% .
4	D	121	16% 70% 14%
5	E	217	39% 31% 9% 21%
6	F	254	15% 66% 17% ..
7	G	387	25% 62% 11% .
8	H	362	27% 59% 13% .


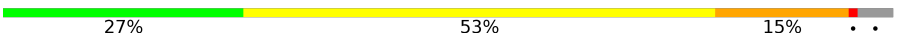


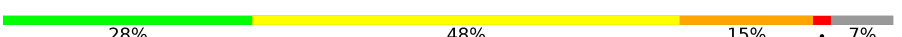
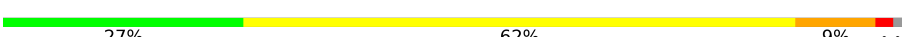
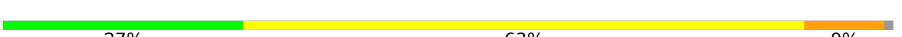




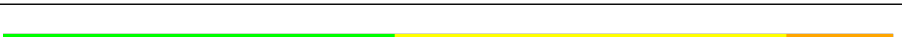

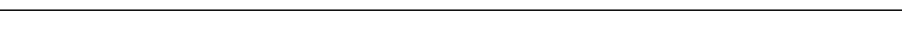
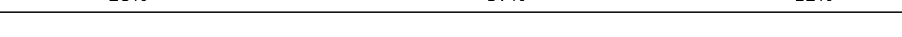
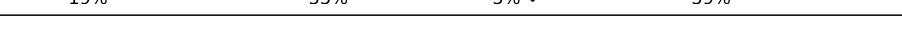

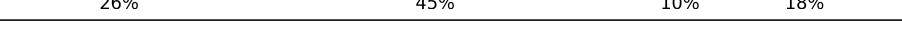
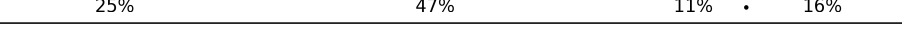
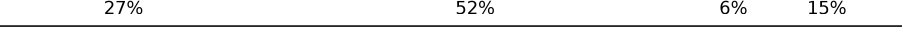


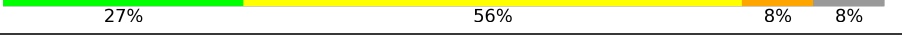


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Mol	Chain	Length	Quality of chain
9	I	297	
10	J	176	
11	K	244	
12	L	256	
13	M	191	
14	N	221	
15	O	174	
16	P	165	
17	Q	199	
18	R	138	
19	S	204	
20	T	199	
21	U	184	
22	V	186	
23	W	189	
24	X	172	
25	Y	160	
26	Z	121	
27	AA	137	
28	BA	155	
29	CA	142	
30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

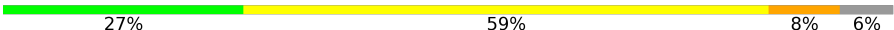



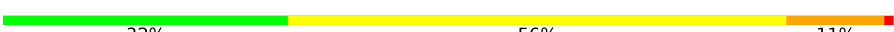
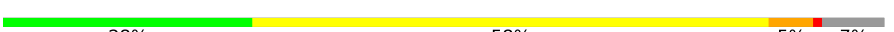
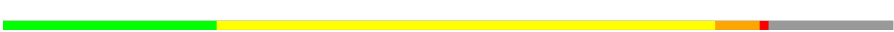





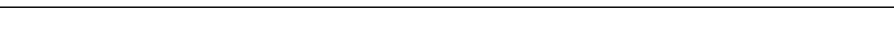

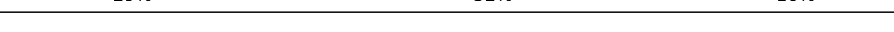

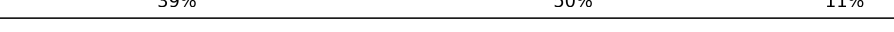







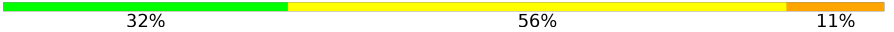
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Mol	Chain	Length	Quality of chain
34	HA	105	
35	IA	113	
36	JA	130	
37	KA	107	
38	LA	121	
39	MA	120	
40	NA	100	
41	OA	88	
42	PA	78	
43	QA	51	
44	RA	128	
45	SA	25	
46	TA	106	
47	UA	92	
48	VA	312	
49	WA	319	
50	XA	252	
51	YA	255	
52	ZA	254	
53	AB	240	
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 215363 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
			1611	1033	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		

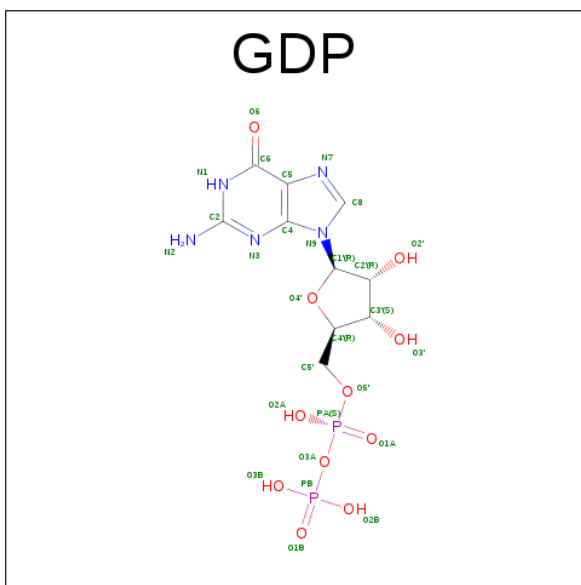
- Molecule 82 is a protein called yeast eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	DC	841	Total	C	N	O	S	0	0
			6561	4168	1125	1238	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>).

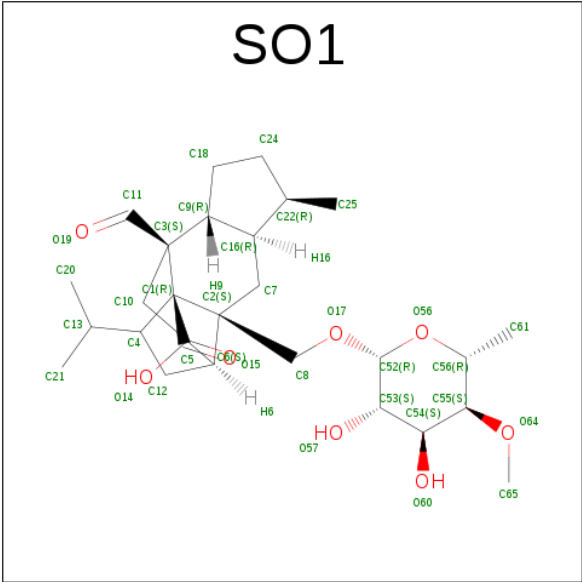


Mol	Chain	Residues	Atoms					AltConf
84	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

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



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



U1741	U1663	U1595	C1533	C1465	A1401	U1334	U1269	A1193	U1129	U1063	C1000	U935	U873	U805
U1742	G1668	C1596	G1534	C1468	G1402	U1335	U1270	A1194	G1130	G1064	U1004	G936	C874	A806
A1746	G1669	U1597	G1535	U1468	C1403	A1336	G1271	C1195	A1131	C1065	A1005	C937	G875	A807
	G1670	U1598	G1536	A1469	C1404	A1337	G1271	A1196	A1132	C1066	A1006	G938	G876	U808
	A1671	C1599	C1537	C1470	G1405	C1338	U1272	G1199	C1134	C1067	C1007	A939	G877	A809
A1749	G1672	A1600	U1538	A1471	A1406	C1339	G1273	G1200	C1134	C1068	C1007	A940	G878	G810
A1750	G1673	G1601	G1539	C1472	U1407	U1340	C1274	G1201	U1135	A1069	U1008	A941	G879	A811
C1751	G1674	C1602	U1540	U1473	G1408	A1341	C1275	G1202	U1136	C1071	U1009	G942	C880	A812
U1752	C1675	U1603	G1541	G1474	G1409	C1342	U1276	A1202	A1137	U1071	C1010	C943	C881	U813
A1753	U1676	G1605	A1542	C1475	A1410	U1343	U1277	A1203	A1138	C1072	U1011	U946	A884	A814
	C1677	C1606	U1544	G1477	G1412	A1344	U1278	A1204	A1139	G1073	U1012	U947	G885	G815
A1756	G1678	G1607	U1545	G1478	U1413	A1345	C1279	C1205	G1140	G1074	A1013	U948	G886	G816
U1758	G1679	U1608	G1546	A1479	U1414	A1346	U1280	U1206	G1141	G1075	G1014	U951	U887	
C1759	U1680	U1609	A1547	G1480	U1415	U1347	G1281	G1207	A1142	A1076	U1015	U952	U888	
G1760	A1681	G1548	G1481	C1416	G1349	A1348	U1282	A1208	A1143	C1077	U1016	G954	U889	U821
U1761	U1682	C1549	C1482	A1483	U1350	U1351	C1284	C1210	U1145	U1080	A1018	G955	C890	G823
A1762	C1683	A1611	U1550	G1484	G1418	G1351	U1285	A1211	G1146	A1081	A1019	G957	C891	G824
A1763	U1684	U1613	U1551	G1484	G1419	G1352	U1286	G1212	A1147	C1082	U1019	U958	A891	U825
C1764	G1685	A1614	U1552	C1485	C1420		U1287	G1213	C1148	G1083	C1022	U959	A892	U826
U1765	C1686	C1615	G1553	G1486	A1421	A1357	G1288	U1214	G1149	A1084	A1023	U960	U893	C827
A1766	U1687	U1616	A1487	A1487	A1422	C1358	U1289	C1215	G1150	G1085	U1024	U961	U894	U828
G1767	U1688	U1617	U1554	G1488	A1423	C1359	U1290	C1216	G1151	A1086	A1025	U962	U896	A829
U1768	A1689	C1618	A1556	U1489	A1424	A1360	G1291	A1217	U1151	A1087	A1026	A963	C897	U830
A1769	G1690	C1619	U1557	C1490	A1425	U1361	G1292	G1218	C1156	A1088	A1027	U964	A898	U831
U1770	A1691		U1558	U1491	C1426	U1362	U1293	A1219	A1157	U1089	C1028	U965	C899	U832
U1771		C1625	U1559	A1492	A1427	U1363	G1294		C1158	C1091	U1029	U966	A900	U833
C1772	A1694	U1626	A1493	A1493	G1428	A1364			C1159	A1091	A1030	A967	G901	G834
G1773			U1560		G1429	C1365		U1225	C1158	A1092	U1031	U968	G902	U835
U1774	A1631	A1631	G1562	G1498	U1430	C1366	U1297	U1226	A1160	G1093	G1032	C969	U903	U836
U1775	C1632	G1499	G1563	G1499	C1431	U1366	U1298	A1226	C1161	A1094	G1033	A970	G904	G837
A1776	U1633	C1500	U1564	C1500	U1432		A1300	G1228	A1163	U1095	C1034	A971	A905	
G1777	C1634	C1501	U1565	G1502	G1433	A1371	U1301	G1164	G1164	C1096	G1035	G972	A906	C842
U1778	A1635	U1567	U1566	C1503	U1434	U1372	U1302	G1229	A1165	U1097	A1036	A973	A907	U843
A1779			U1567	A1436	G1435	C1373	U1303	U1231	A1166	U1098	C1037	G974	U908	U844
G1780	G1638	G1504	C1568	G1504	A1436	C1374	G1304		G1167	U1099	U1038	C975	U909	G845
A1781	C1639	U1505	G1569	U1505	U1437	C1375	U1305	C1235	U1168	G1100	A1039	G976	C910	G846
C1782	U1570	G1506	A1570	G1506	G1438	C1376	C1306		G1169		G1040	A977	U911	A847
G1783			C1571	G1507		U1377	U1307	G1241	G1170	U1103	G1041	A978	U912	
C1784	A1719	G1642	G1572	U1508	U1443	U1378	G1308	A1242	A1171	U1104	G1042	A979	G913	A850
	U1720			G1513	A1444	C1379		G1243	G1172	C1105	A1043	G980	G914	U851
U1785	A1721	C1644	G1574	G1514	G1445	U1380	A1313	A1244	C1173	U1106	U1044	U981	A915	C852
	A1722	G1645	U1575	A1514		U1381	U1314	G1245	C1174	G1107	G1045	U982	U918	A856
U1724	U1724	C1646	A1576	A1515	G1448	A1382	U1315	G1246	U1175	G1108	G1046	G983	A919	U857
U1725	U1725	U1647		A1516	U1449	G1383	G1316	U1247	G1176	G1109	G1047	G984	A920	G858
			U1579	U1517	U1450	A1384	C1317		C1177		G1048	G985	U921	A859
A1726	G1727	G1648	C1580	C1518	C1451	G1387	A1321	U1250	G1180	G1112	G1049	G986	G923	U860
A1728	U1650	U1519	U1581	U1519	G1452	A1388	A1322	U1251	U1181	G1118	U1050	G987	A924	U861
C1729	A1651	U1582	U1582	U1582	G1453	C1389	A1323	G1254	U1182	G1119	G1051	U988	G925	A862
A1730	C1652	A1583	U1583	U1520	G1454	U1390	G1324	U1255	A1183	G1120	U1052	C990	G926	A863
A1731		G1653	U1584	G1623	G1455	U1391		G1256	U1184	G1121	G1053	G991	A926	U864
A1732	U1654	A1524	U1585	A1524	G1456	U1392	U1257	A1256	A1185	G1122	U1054	A992	G927	A865
C1733	A1655	A1525	A1586	A1525	G1457	U1393	C1327	U1258	U1186	G1123	U1055	A993	U928	G866
U1734	U1656	A1526	G1458	A1526	G1458	C1394	U1328	U1259	U1187	C1123	U1056	A994	G929	G867
U1735	U1657	C1527	C1459	C1527	G1459	G1395	A1329	U1260	G1188	A1124	U1057	U995	A930	G868
		U1528	A1460	U1528	A1460		G1330	G1261	G1189	A1125	U1058	U996	C931	A869
A1736	G1658	U1529	C1461	C1529	C1461		U1331	U1262	C1190	G1126	U1059	G997	U932	C870
G1737	A1659	C1530	C1462	C1530	C1462	U1398	A1331		U191	G1127	U1060	A998	A933	G871
U1738	U1660	G1531	C1463	G1531	C1463	C1399	C1332		C1192		A1061	G999	C934	G872
A1740		U1532	A1464	U1532	A1464	A1400	C1333				A1062	U999		

• Molecule 2: 25S ribosomal RNA

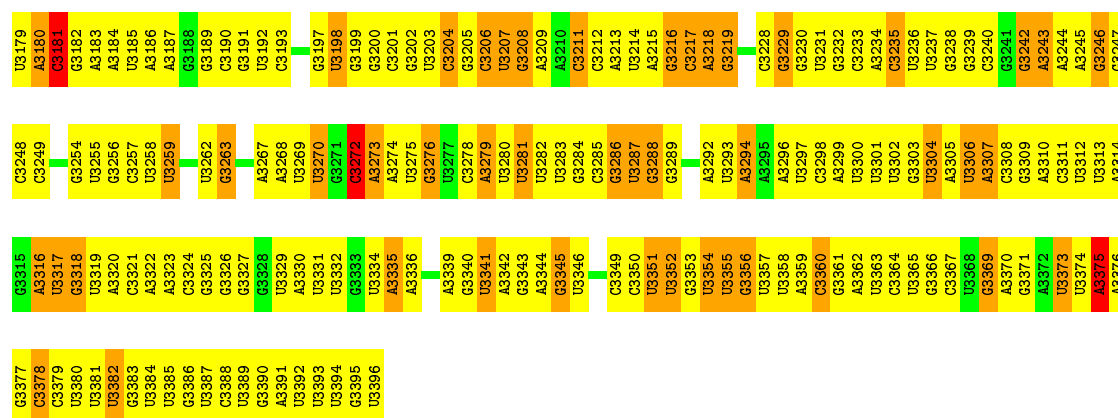
Chain B:  20% 59% 18%

C1038	A965	A904	G842	A775	U704	U642	G577	U508	U446	U381	A319	G258	C193	G127	A66	G
U1039	U966	U905	A843	U776	A705	U643	A578	U509	U447	U382	G320	C259	U194	G128	A67	U
A1040	A967	A906	G844	U777	A706	G844	G579	G510	U448	G383	C321	C260		U129	C68	U3
U1041	G968	G907	G845	U778	U707	G845	G580	G511	U449		A198	U261		A130	C69	U4
C1042	C969	G908	A846	G779	G708	A846	U581	U512	U450	A387	A323	U262		A131	A70	G5
C1043	A970	G909	A847	A780	A709	G847	G582	G513	U451	G388	A324	C263		C132	A71	A6
	G971	G910	A848	G781	A710	C848	G583	G514	G452	A389	A325	G264		U133	C72	C7
A1047	A972	C911	C849	U782	A711	C849	G584	C515	G453		U326	G265		U134	C73	C8
A1048	A973	G912		U783	G712	C850	A585	A516	C	G392	A327	A266		C135	G74	U9
C1049	G974	A913	G853	A784	U713	G851	G586	G517	C	U393	U328	G267		G136	G75	C10
U1050	C975	A914	G854	G785	G714	G852	U587	G518	U	U394	U329	A268		G137	G76	A11
U1051	U976	A915	U855	A786	A715	A653	A588	A519	C	A395	G330	G269		U138	A77	A12
U1052	C977	G916	G856	G787	A716	C654	G589	U520	U	A396	G331	U270		U139	A78	A13
A1053	G978	A917	G857	C788	C717	C855	G590	A521	G	A397	G332	C271			U79	U14
A1054	U979	C918	A858	A789	G718	A656	G591	A522	C	A398		A272		C142	G80	C15
A1055	U980	A919	G859	U790	U719	A657	A592	A523	U	A399	G335	G273		C143	C81	A16
U1056	U981	A920	G860	A791	A720	G658	A593	U524	C	G400		G274		A144	C82	G17
	C982	A921	C861	G792	G721		G595	C525	C	U401	A338	U275		G212	U83	G18
G1059	A983	U922	U862	C793		A660	C596	C526	U	A402	C339	U276		A213	U84	U19
U1060	G984	C923	C863	U794	G725	G661	G597	A527	U	C403	C340	G277		G214	A85	
A1061	U985	G924	G864	G795	G726	U662	A598	U528	G	G404	G341	U278		G215	G86	
A1062	U986	A925	U865	U796	G727	C663	C599	A529	U	U405	A342	U279		U149	U87	A23
G1063	U987	A926	A866	U797	G728	U664	G600	G530	G	G406	U343	U280		U150	A88	G24
A1064			G867	G798	C729	A665	G531	G531	G	A407	A344	G281		A151	A89	U25
A1065	U990	A929	C868	C799	C730	A666	A603	A408	U	A408	G345	G282		U152	C90	A26
G1066	G991	U930	G869	G800	U731	C667	G604	A409	U	A409	C346	G283		U153	G91	C27
U1067	A992	C931	G870		C732	U668	A607	G535	A	U410	G347	A284		U154	G92	C28
C1068	G993	U932	U871	G805		U669	A608	U536	G	U411	A348	A285		G155	C93	C29
	G994	G933	U872	A806	G739	C670	G609	A537	G	G412	A349	U286		G156	G94	G30
G1072	U995	A934	C873	A807	G740	U671	G610	G538	U	U413	C350	G287		A157	A95	C31
U1073	A996	U935	U874	A808		A672	A611		C	U414	A351	C288		G158	G96	U32
U1074	A997	A936	G875	A808	C743	U673		C543	A	G415	A352	A289		A159	U97	G33
A1075	G998	G937	A876	G809	A744	G674	U615	C544	U	A416	G353	G290		G160	G98	A34
C1076	U999	C938	C877	A810	C745	G675	G616	U545	U	A417	U354	C291		G161	A99	A35
U1077	G1000	U939	G878	U811	A746	C676	G617	C546	C	G418	A355	U292		A100	C36	
U1078	G1001	G940	U879	G812	A747	A677	G617	G547	U	G419	C356	C293		G101		U37
A1079	A1002	G941	G880	G813	U748	G678	C618	G548		G420	A357	U294		C163	G102	
A1080	A1003	U942	C881	U814	C749	U679	A619	U549	C484	G421	G358	A295		A165	G103	A40
U1081		U943	A882	G815	G750	G680	U620	A550	A485	A422	U359	A296		G104		G41
U1082	A1006	C944	A883	A816	A751	U681	A621	A551	U486	G423	G360	G297		C105	C42	G42
G1083	U1007	U945	A884	A817		U682	A622		U487	G424	A361			A106		A43
A1084	U1008	U946	U885	C752	C753	U683	U623		U488		U362			A107		U44
A1085	A1009	G947	C886	G754	A755	G684	G624	A554			C427			A108		A45
	G1010	C948	G887	G756			G625		C489		G363	U302		A109		U46
A1091	A1011	C949	A888	U821	U756	U687	G626	A557	A490		A364	G303		G110		C47
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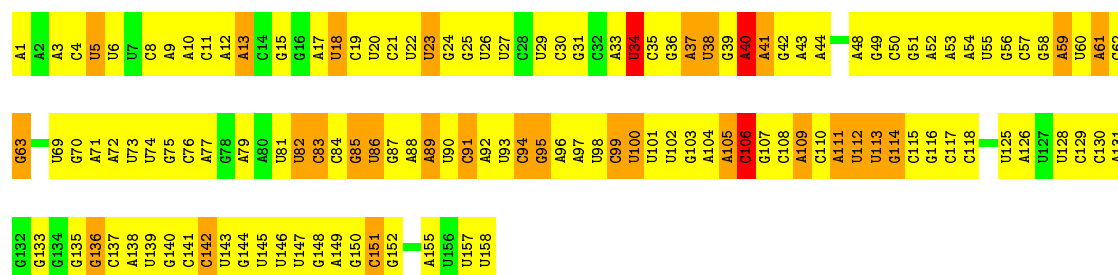
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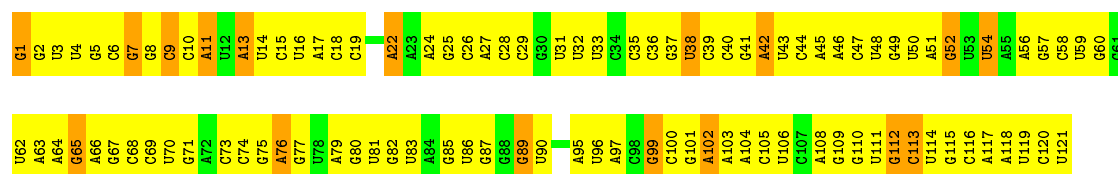
• Molecule 3: 5.8S ribosomal RNA

Chain C: 18% 62% 18%



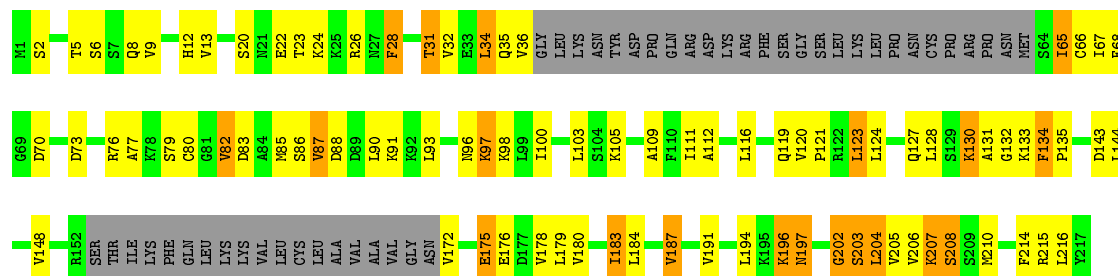
• Molecule 4: 5S ribosomal RNA

Chain D: 16% 70% 14%



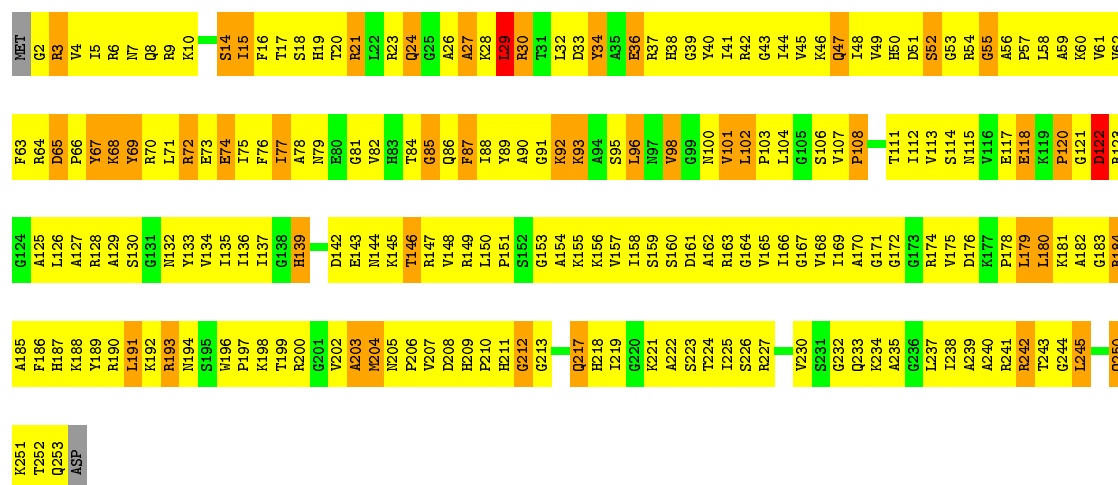
• Molecule 5: uL1 (yeast L1)

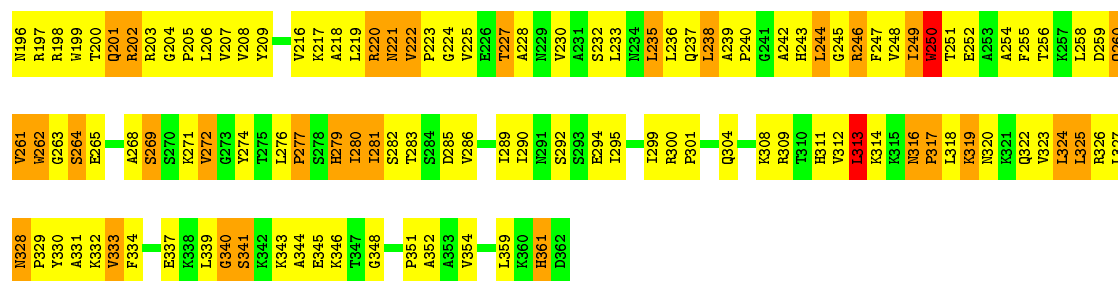
Chain E: 39% 31% 9% 21%



• Molecule 6: uL2 (yeast L2)

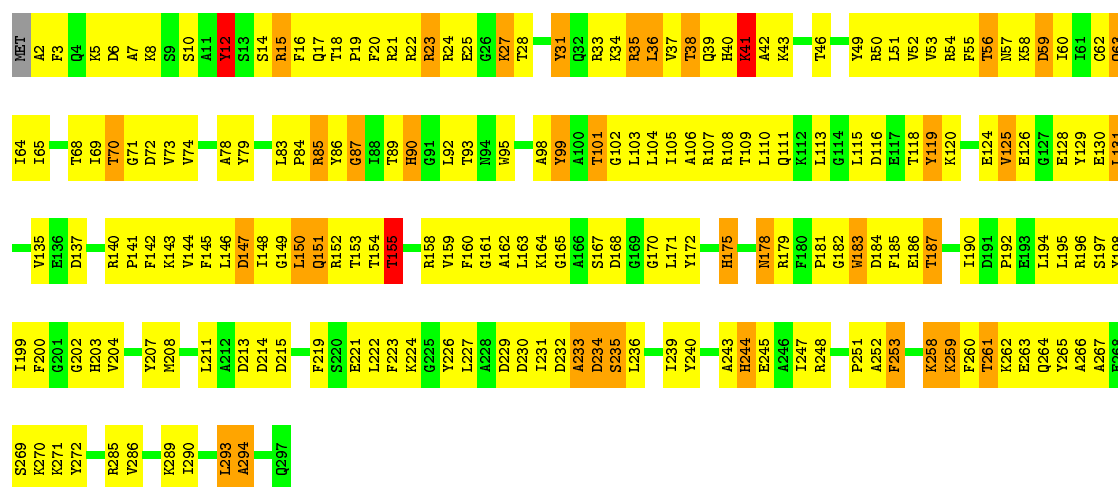
Chain F: 15% 66% 17%





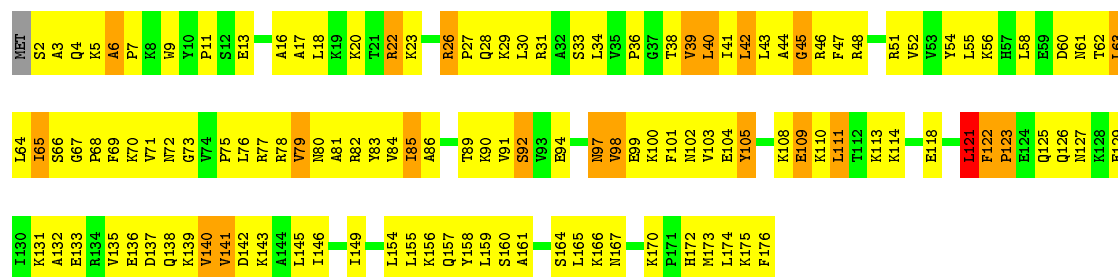
• Molecule 9: uL18 (yeast L5)

Chain I: 32% 54% 12% .



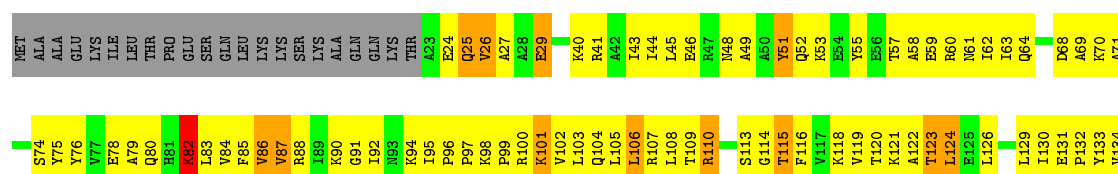
• Molecule 10: eL6 (yeast L6)

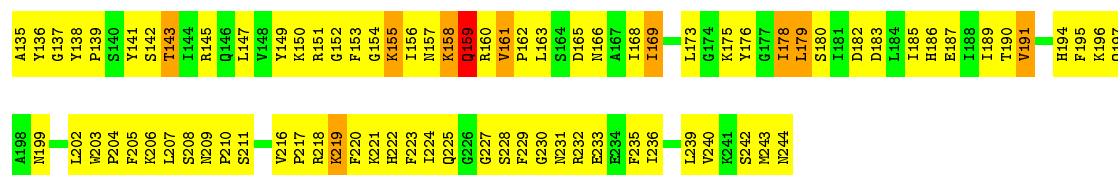
Chain J: 27% 60% 12% ..



• Molecule 11: uL30 (yeast L7)

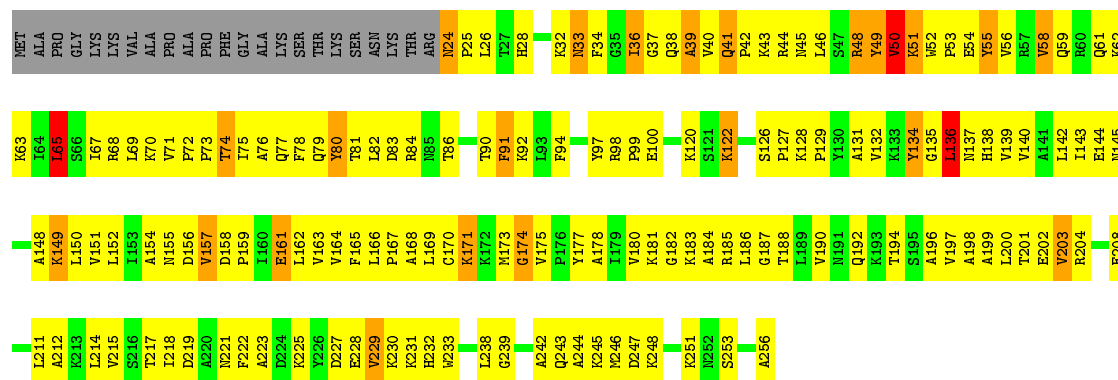
Chain K: 25% 57% 9% . 9%





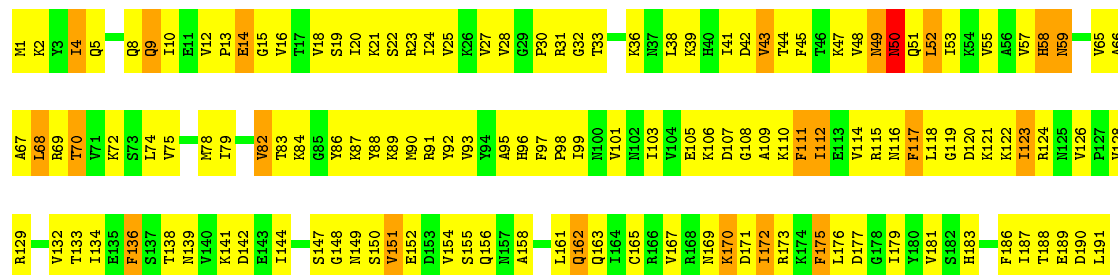
• Molecule 12: eL8 (yeast L8)

Chain L: 29% 52% 9% 9%



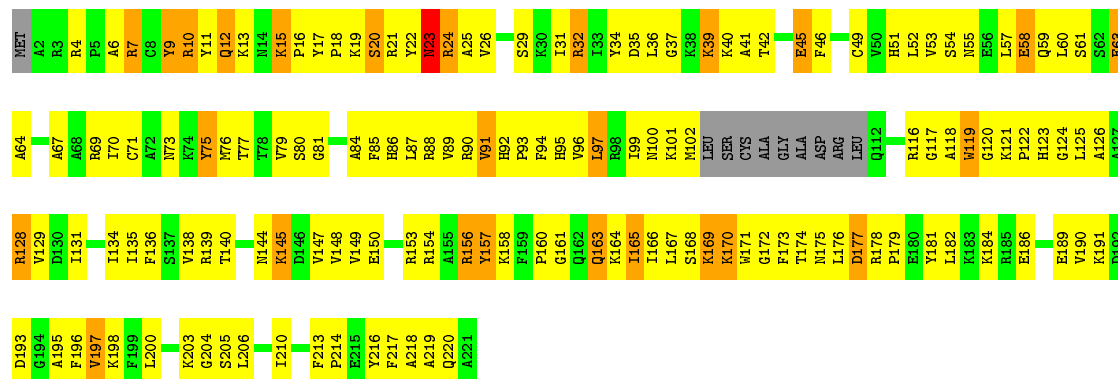
• Molecule 13: uL6 (yeast L9)

Chain M: 28% 60% 11%



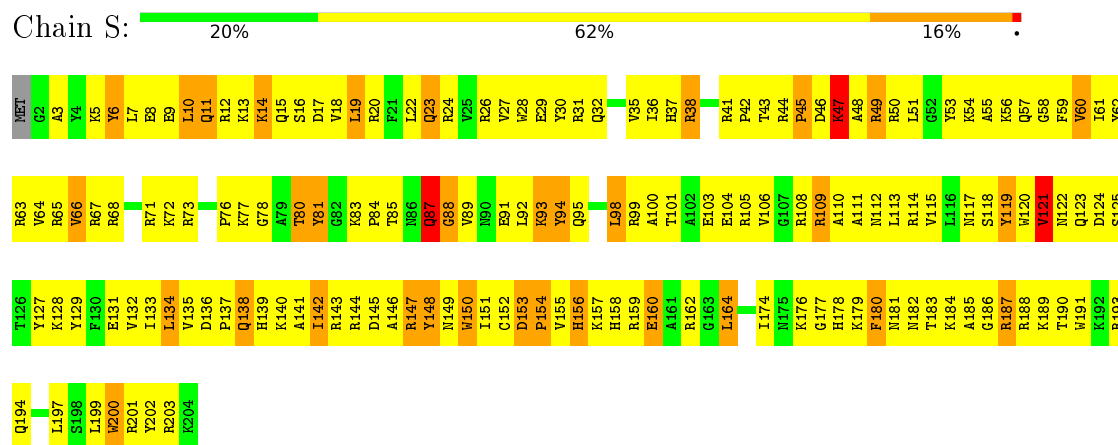
• Molecule 14: uL16 (yeast L10)

Chain N: 28% 56% 12% 5%

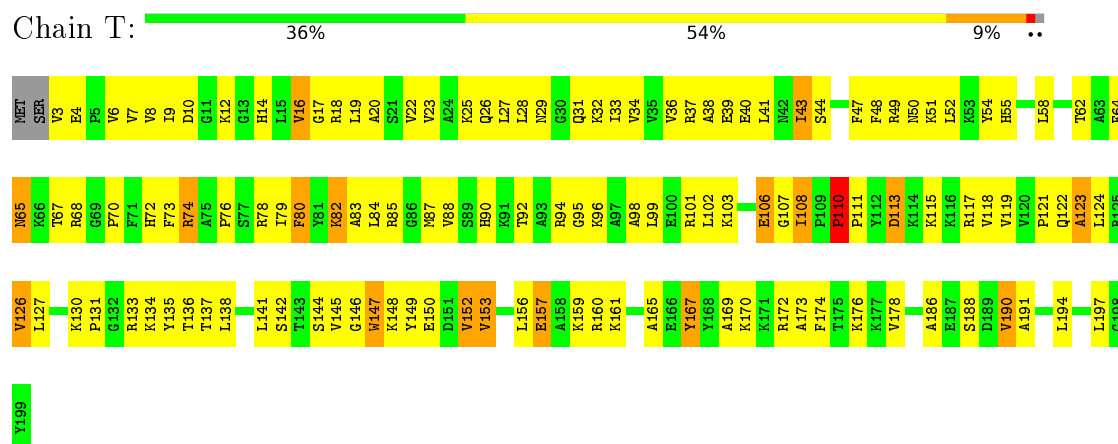


• Molecule 15: uL5 (yeast L11)

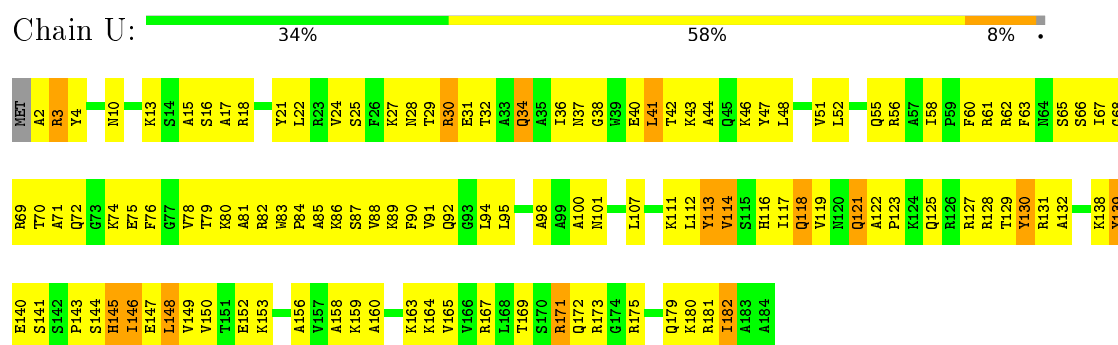




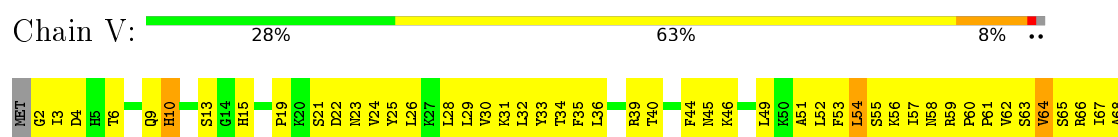
- Molecule 20: uL13 (yeast L16)



- Molecule 21: uL22 (yeast L17)



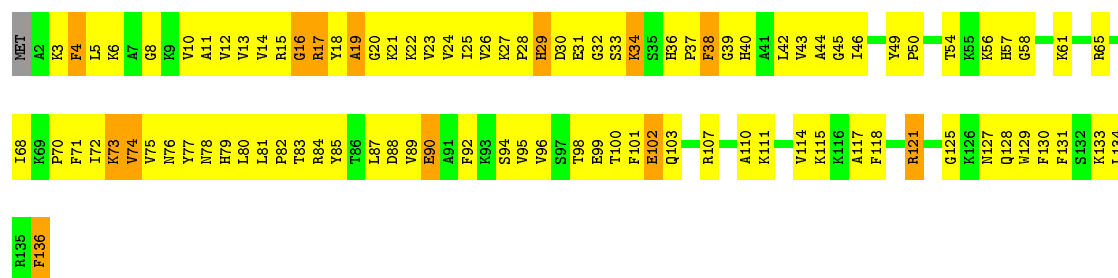
- Molecule 22: eL18 (yeast L18)





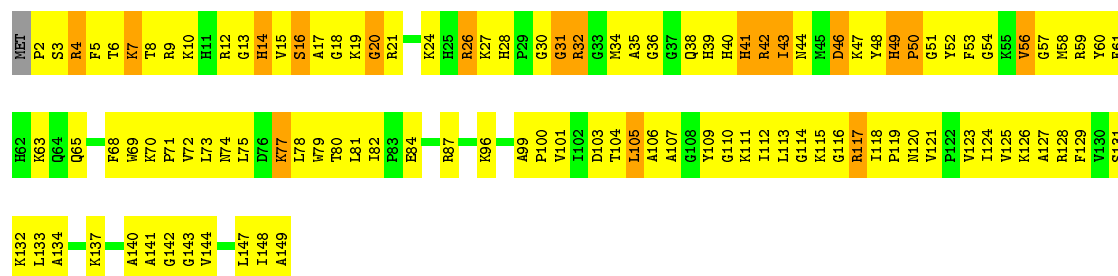






- Molecule 32: uL15 (yeast L28)

Chain FA: 25% 62% 12%



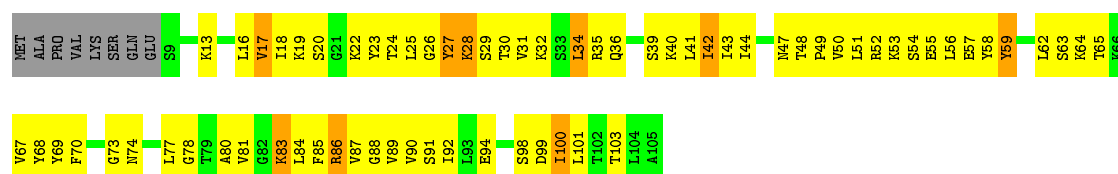
- Molecule 33: eL29 (yeast L29)

Chain GA: 47% 44% 7%



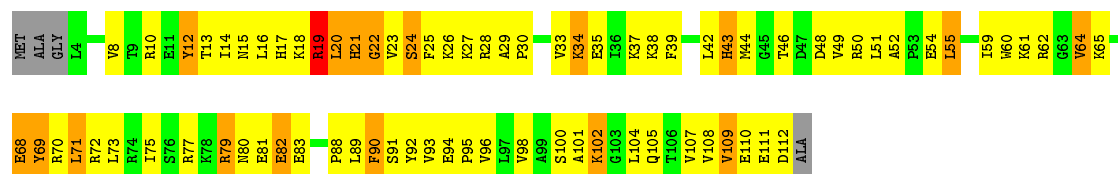
- Molecule 34: eL30 (yeast L30)

Chain HA: 27% 57% 9% 8%

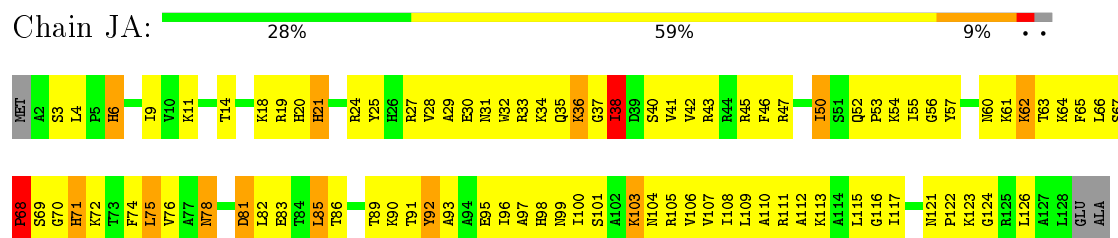


- Molecule 35: eL31 (yeast L31)

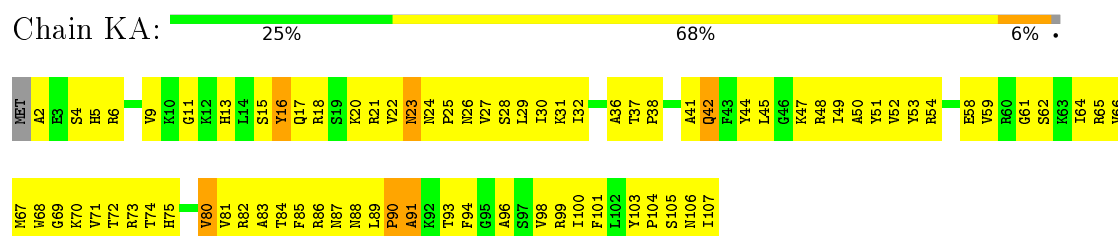
Chain IA: 27% 53% 15%



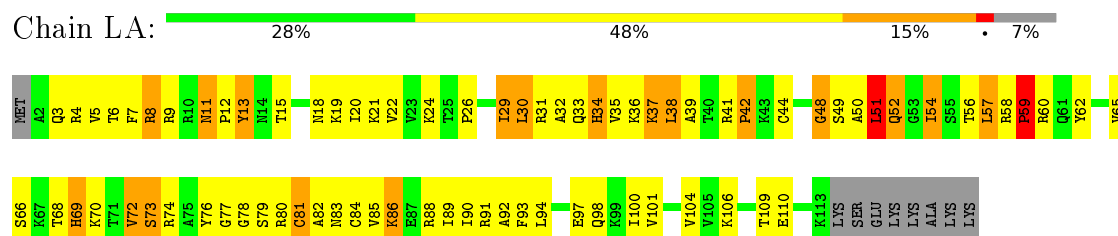
- Molecule 36: eL32 (yeast L32)



- Molecule 37: eL33 (yeast L33)



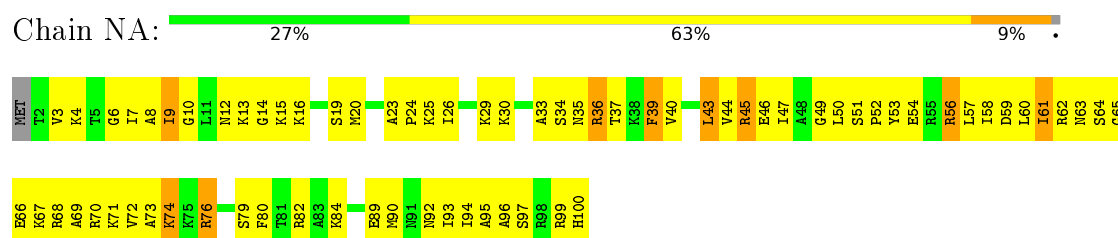
- Molecule 38: eL34 (yeast L34)



- Molecule 39: uL29 (yeast L35)

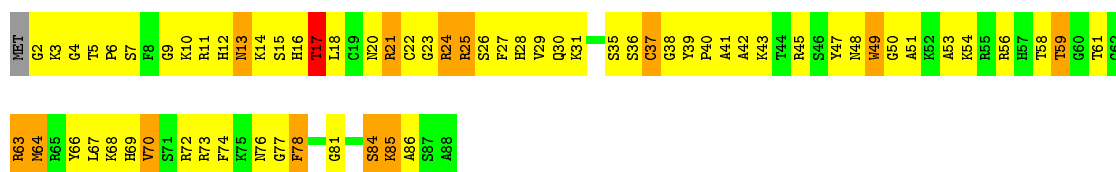


- Molecule 40: eL36 (yeast L36)



- Molecule 41: eL37 (yeast L37)





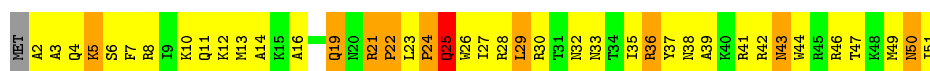
- Molecule 42: eL38 (yeast L38)

Chain PA: 49% 46% ..



- Molecule 43: eL39 (yeast L39)

Chain QA: 20% 59% 18% ..



- Molecule 44: eL40 (yeast L40)

Chain RA: 13% 23% 59% ..



- Molecule 45: eL41 (yeast L41)

Chain SA: 44% 44% 12%



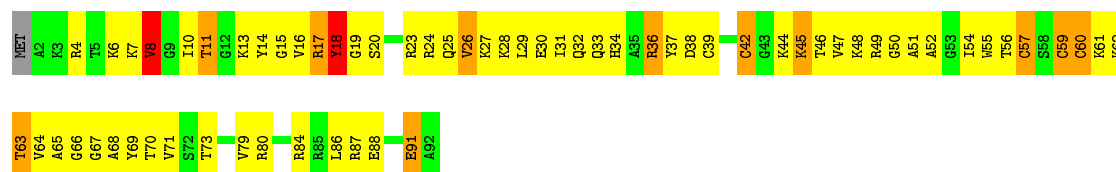
- Molecule 46: eL42 (yeast L42)

Chain TA: 27% 57% 13% ..

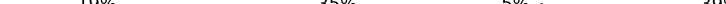


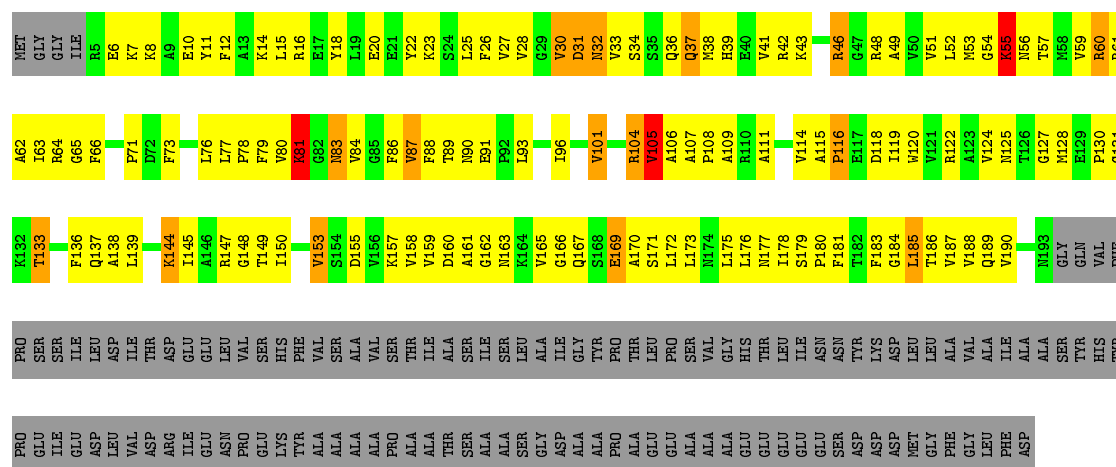
- Molecule 47: eL43 (yeast L43)

Chain UA:  28% 57% 12% 3%



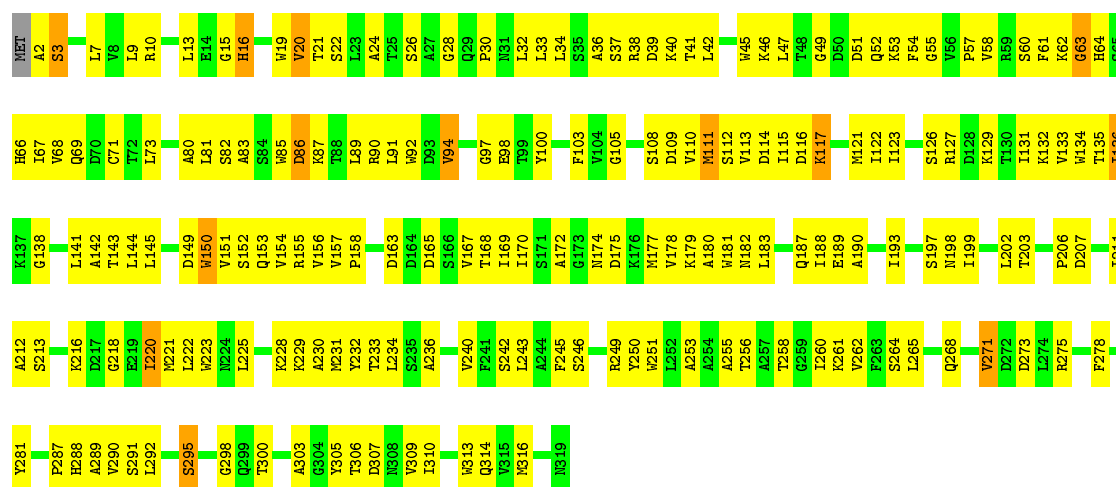
- Molecule 48: uL10 (yeast P0)

Chain VA:  19% 35% 5% 39%



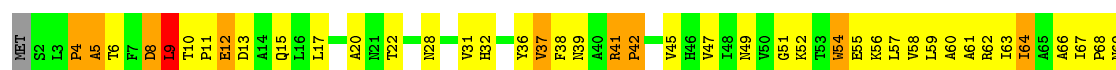
- Molecule 49: RACK1 (yeast Asc1)

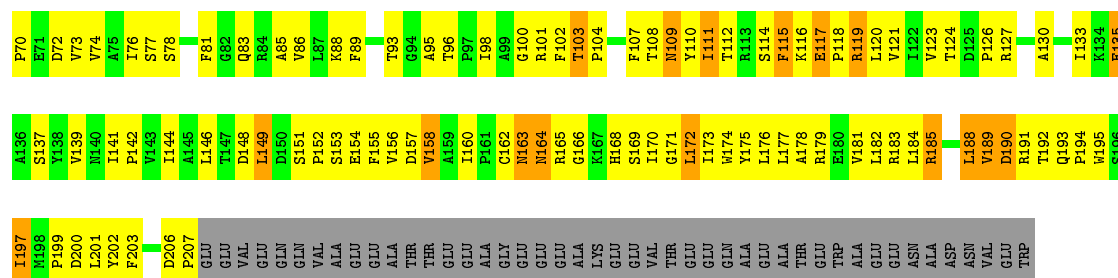
Chain WA:  40% 55% .



- Molecule 50: uS2 (yeast S0)

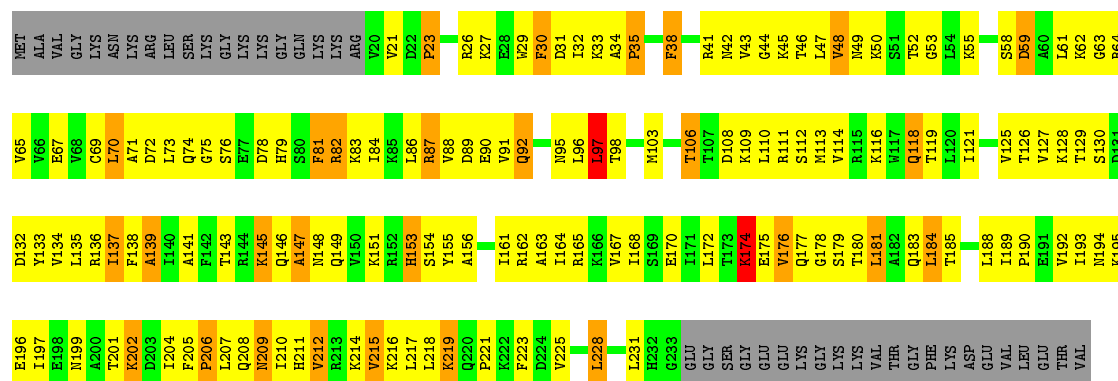
Chain XA: 





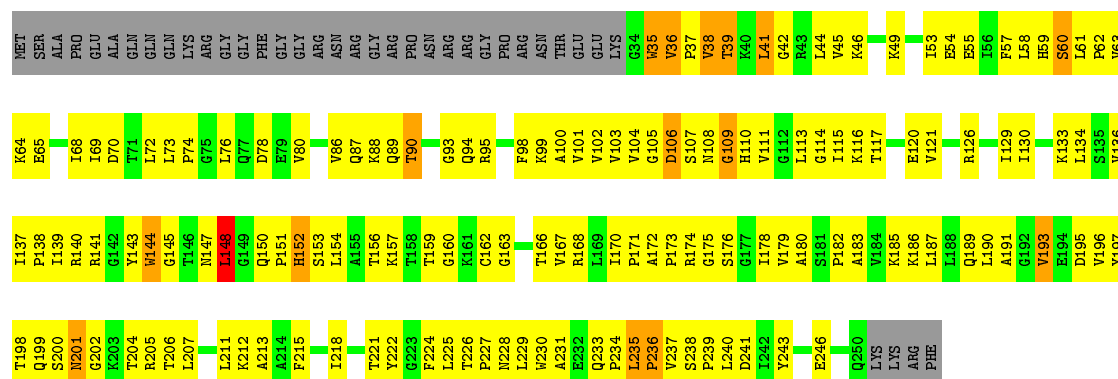
• Molecule 51: eS1 (yeast S1)

Chain YA: 25% 47% 11% 16%



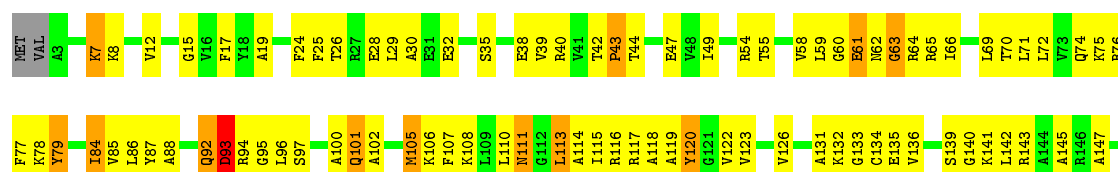
• Molecule 52: uS5 (yeast S2)

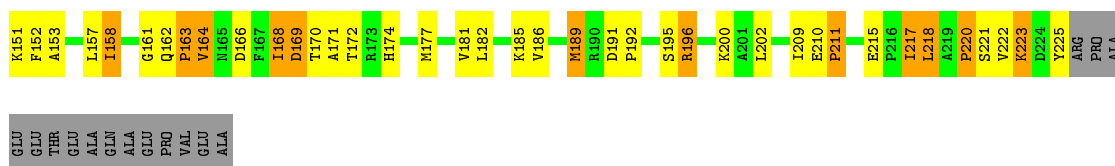
Chain ZA: 27% 52% 6% 15%



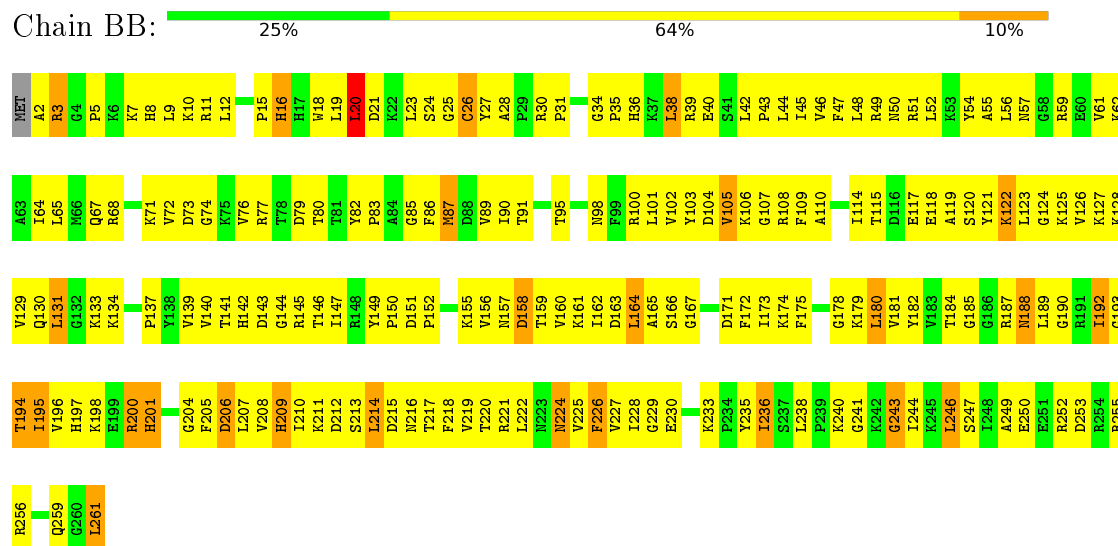
• Molecule 53: uS3 (yeast S3)

Chain AB: 40% 42% 10% 7%

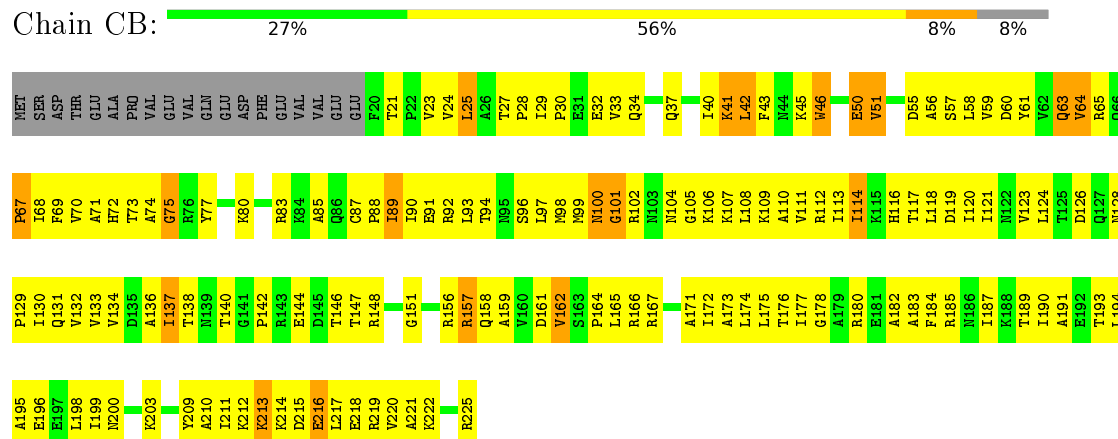




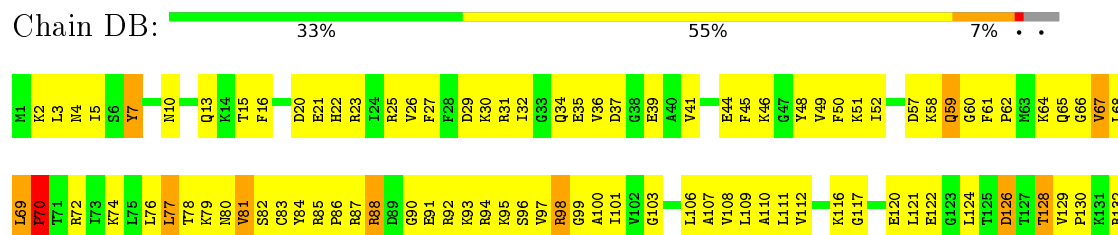
• Molecule 54: eS4 (yeast S4)

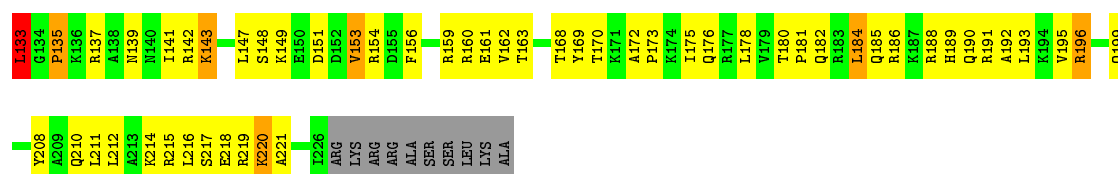


• Molecule 55: uS7 (yeast S5)

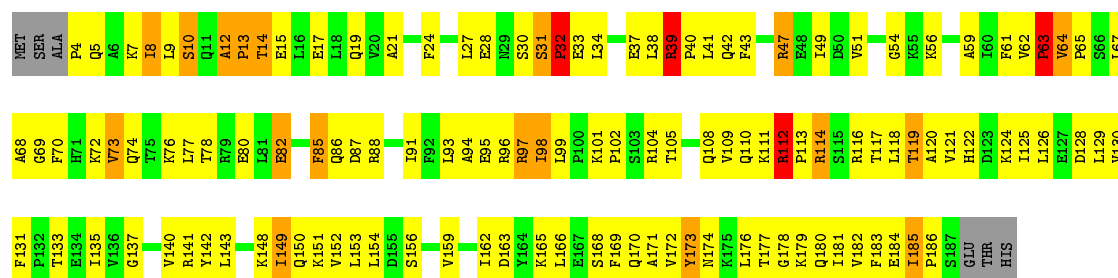


• Molecule 56: eS6 (yeast S6)

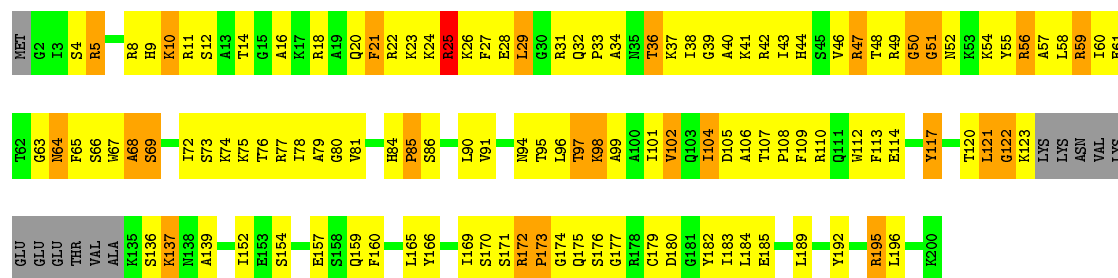




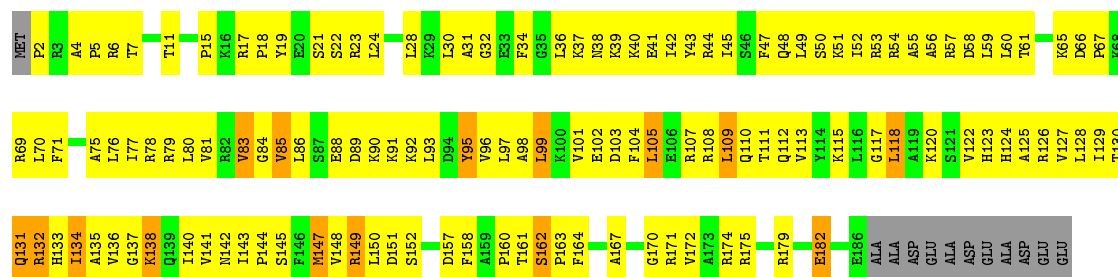
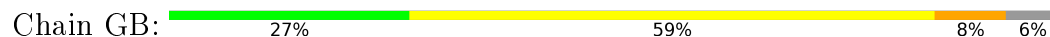
- Molecule 57: eS7 (yeast S7)



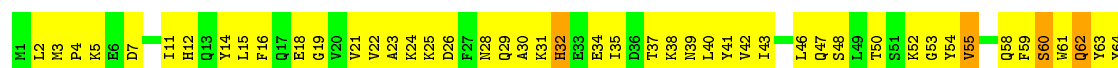
- Molecule 58: eS8 (yeast S8)



- Molecule 59: uS4 (yeast S9)

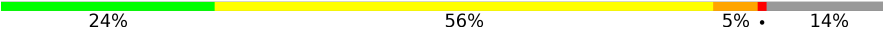


- Molecule 60: eS10 (yeast S10)





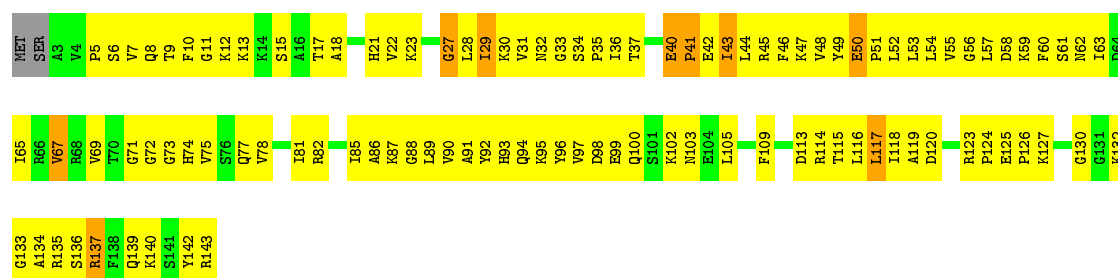


Chain MB: 



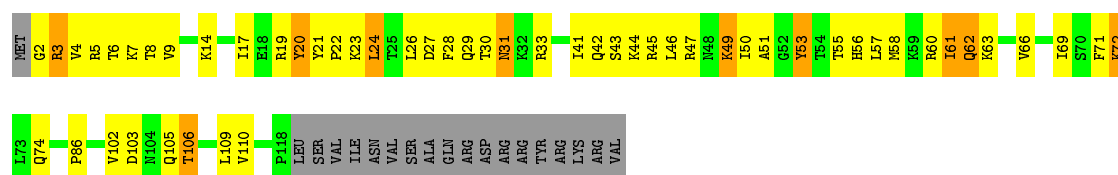
- Molecule 66: uS9 (yeast S16)

Chain NB: 




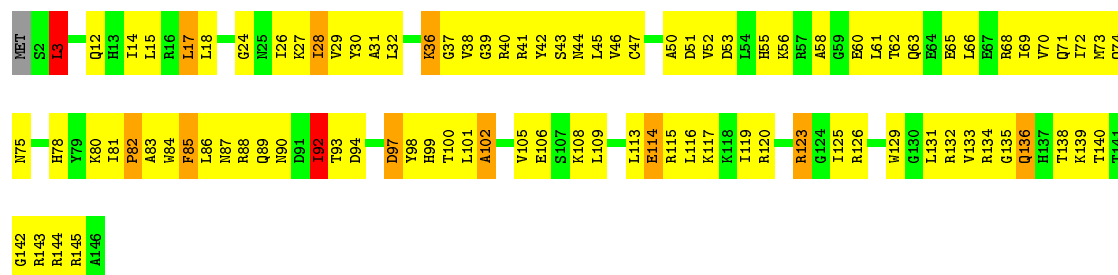
- Molecule 67: eS17 (yeast S17)

Chain OB: 



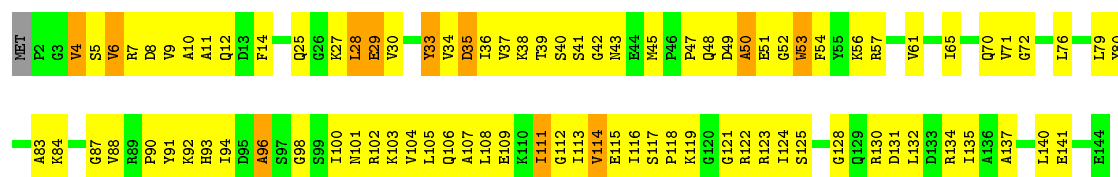
- Molecule 68: uS13 (yeast S18)

Chain PB: 

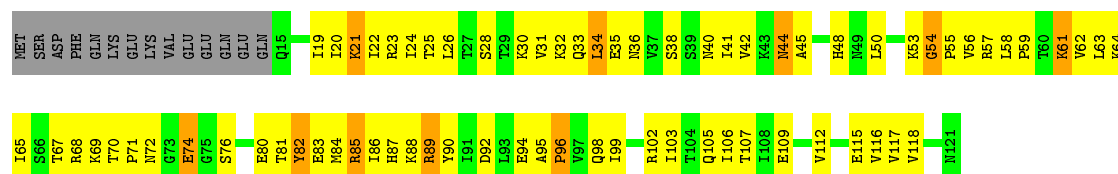


- Molecule 69: eS19 (yeast S19)

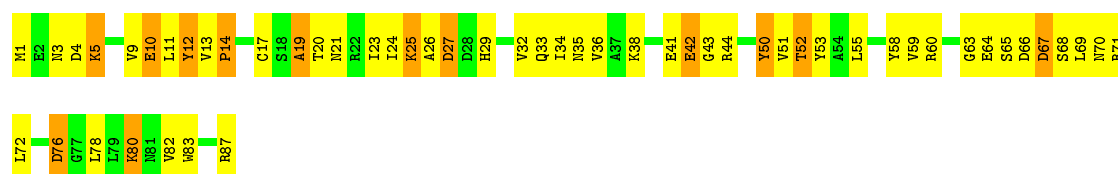
Chain QB: 



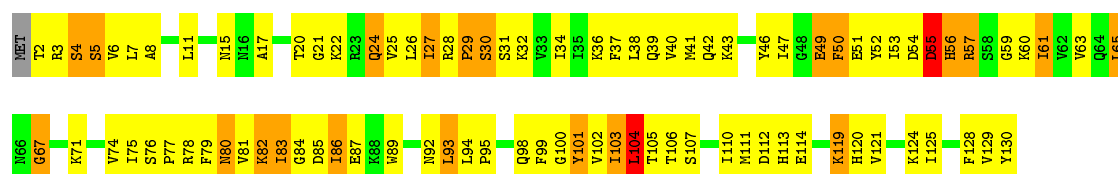
• Molecule 70: uS10 (yeast S20)



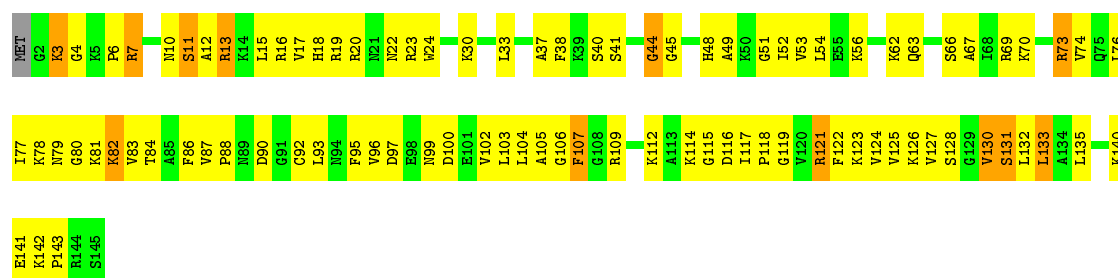
• Molecule 71: eS21 (yeast S21)



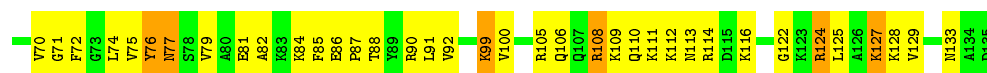
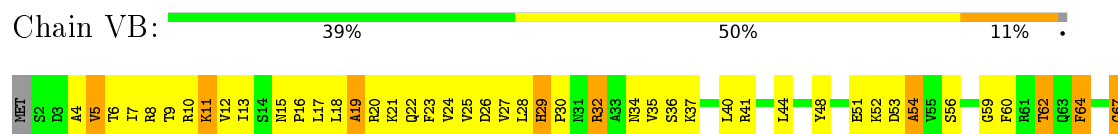
• Molecule 72: uS8 (yeast S22)



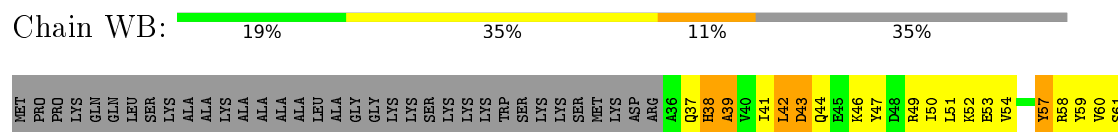
• Molecule 73: uS12 (yeast S23)



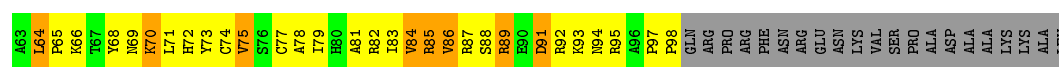
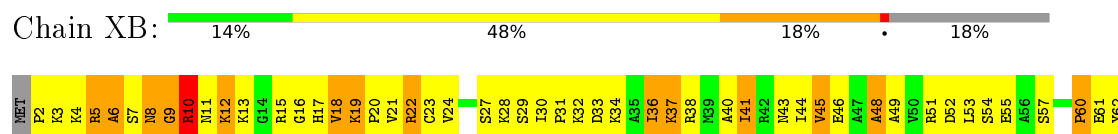
• Molecule 74: eS24 (yeast S24)



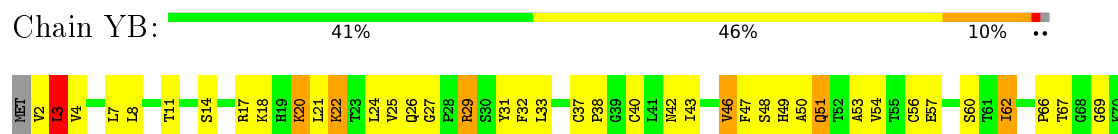
• Molecule 75: eS25 (yeast S25)



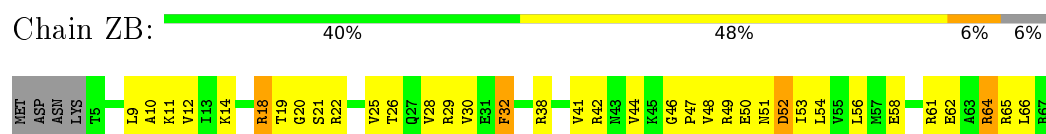
• Molecule 76: eS26 (yeast S26)



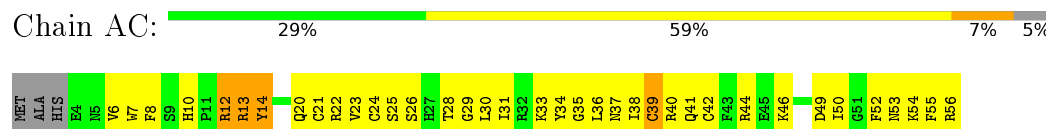
• Molecule 77: eS27 (yeast S27)



• Molecule 78: eS28 (yeast S28)



• Molecule 79: uS14 (yeast S29)

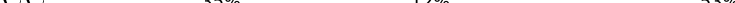


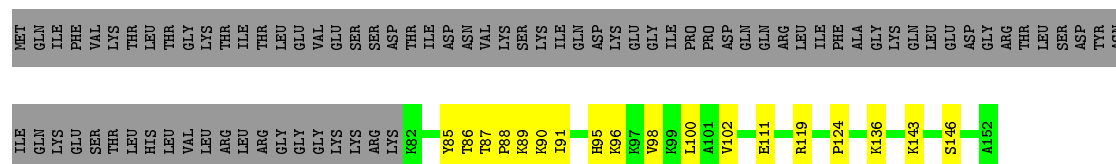
- Molecule 80: eS30 (yeast S30)

Chain BC: 



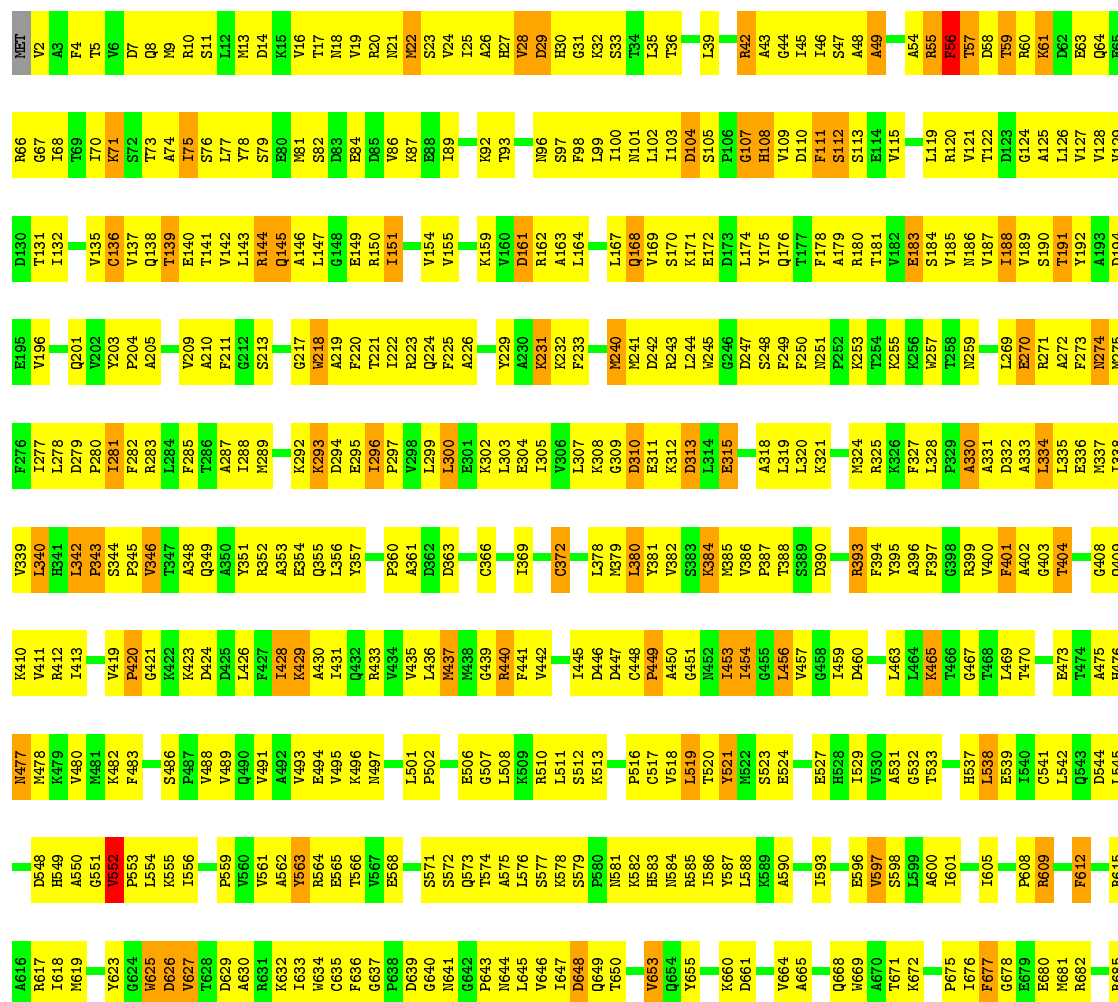
- Molecule 81: eS31 (yeast S31)

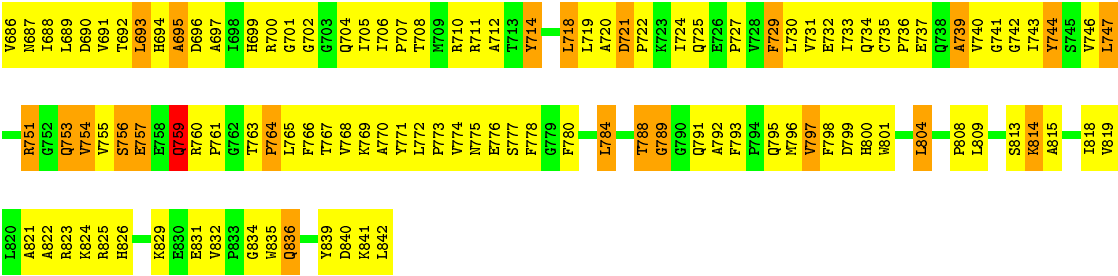
Chain CC:  35% 12% 53%



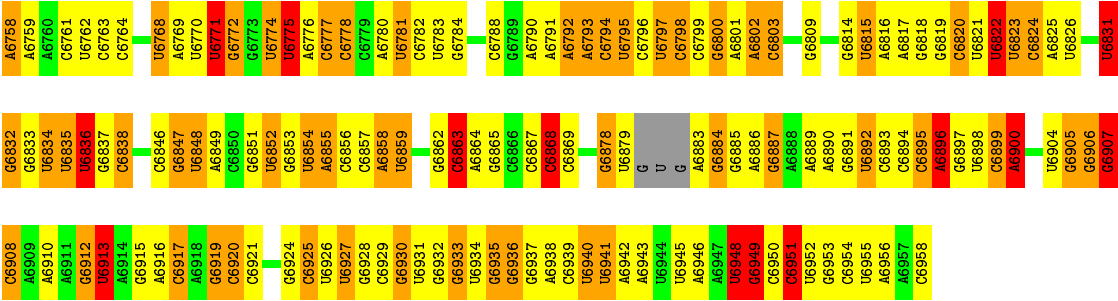
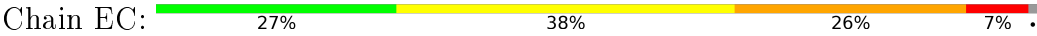
- Molecule 82: yeast eEF2

Chain DC:  32% 56% 11%





● Molecule 83: IRES



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	38047	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	0.98	2/42096 (0.0%)	0.78	11/65570 (0.0%)
10	J	1.09	0/1425	0.72	3/1912 (0.2%)
11	K	1.27	0/1822	0.68	0/2451
12	L	1.04	0/1850	0.66	1/2495 (0.0%)
13	M	1.10	0/1540	0.66	0/2073
14	N	1.17	0/1754	0.68	1/2350 (0.0%)
15	O	0.91	0/1375	0.60	0/1842
16	P	1.70	0/728	0.77	1/975 (0.1%)
17	Q	1.10	0/1568	0.67	0/2106
18	R	1.21	0/1069	0.67	0/1438
19	S	1.27	0/1758	0.75	0/2354
2	B	1.34	49/78631 (0.1%)	0.82	47/122552 (0.0%)
20	T	1.19	0/1586	0.67	0/2128
21	U	1.27	0/1466	0.70	0/1968
22	V	1.19	0/1466	0.71	1/1965 (0.1%)
23	W	1.00	1/1539 (0.1%)	0.66	1/2050 (0.0%)
24	X	1.26	0/1482	0.63	0/1990
25	Y	1.28	0/1301	0.68	0/1743
26	Z	0.87	0/812	0.57	0/1099
27	AA	1.17	0/1019	0.70	0/1369
28	BA	1.31	0/521	0.67	0/691
29	CA	1.22	0/984	0.68	0/1325
3	C	1.42	7/3747 (0.2%)	0.81	3/5832 (0.1%)
30	DA	1.22	0/1005	0.71	0/1341
31	EA	0.99	0/1119	0.57	0/1497
32	FA	1.19	0/1205	0.71	0/1612
33	GA	1.03	0/474	0.64	0/629
34	HA	0.90	0/751	0.72	0/1008
35	IA	1.09	0/904	0.70	2/1213 (0.2%)
36	JA	1.26	0/1041	0.64	0/1394
37	KA	1.24	0/869	0.65	0/1168
38	LA	1.08	0/891	0.70	2/1191 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	MA	1.12	0/979	0.69	1/1301 (0.1%)
4	D	1.20	2/2884 (0.1%)	0.76	1/4491 (0.0%)
40	NA	1.02	0/779	0.66	0/1034
41	OA	1.37	0/697	0.70	0/923
42	PA	0.97	0/619	0.58	0/826
43	QA	1.22	0/444	0.73	0/588
44	RA	1.16	0/424	0.65	0/562
45	SA	1.07	0/235	0.62	0/300
46	TA	1.14	0/861	0.68	0/1136
47	UA	1.12	0/702	0.65	0/934
48	VA	1.64	0/1498	0.79	0/2025
49	WA	0.86	0/2498	0.57	0/3398
5	E	1.78	0/1377	0.74	1/1844 (0.1%)
50	XA	0.74	0/1651	0.59	0/2257
51	YA	0.80	0/1735	0.60	0/2335
52	ZA	0.79	0/1665	0.60	0/2263
53	AB	0.91	0/1759	0.58	0/2368
54	BB	0.79	0/2110	0.60	0/2839
55	CB	0.80	0/1630	0.58	0/2202
56	DB	0.78	0/1844	0.58	0/2464
57	EB	0.87	0/1506	0.60	0/2028
58	FB	0.94	0/1515	0.59	0/2021
59	GB	0.74	0/1519	0.57	0/2035
6	F	1.16	0/1952	0.73	2/2622 (0.1%)
60	HB	0.99	0/837	0.56	0/1131
61	IB	1.05	0/1273	0.60	0/1712
62	JB	1.01	0/495	0.52	0/617
63	KB	0.92	0/1216	0.63	1/1638 (0.1%)
64	LB	0.72	0/953	0.60	0/1279
65	MB	1.01	0/996	0.62	0/1335
66	NB	0.87	0/1126	0.55	0/1510
67	OB	0.82	0/844	0.60	0/1120
68	PB	0.91	0/1212	0.62	1/1628 (0.1%)
69	QB	0.87	0/1131	0.60	0/1517
7	G	1.11	0/3153	0.69	1/4239 (0.0%)
70	RB	0.92	0/866	0.62	0/1169
71	SB	0.78	0/694	0.58	0/935
72	TB	0.90	0/1039	0.63	1/1395 (0.1%)
73	UB	0.94	0/1140	0.61	0/1518
74	VB	0.76	0/1088	0.57	0/1449
75	WB	0.84	0/571	0.59	0/768
76	XB	0.80	0/782	0.58	0/1047
77	YB	0.86	0/621	0.61	0/838



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
78	ZB	0.75	0/500	0.59	0/670
79	AC	1.03	0/454	0.66	0/602
8	H	1.20	1/2802 (0.0%)	0.69	0/3792
80	BC	0.84	0/483	0.57	0/643
81	CC	1.00	0/283	0.63	0/352
82	DC	1.44	0/6665	0.70	3/9022 (0.0%)
83	EC	2.03	50/4579 (1.1%)	0.97	14/7119 (0.2%)
9	I	1.03	0/2426	0.63	0/3271
All	All	1.20	112/230910 (0.0%)	0.75	99/338443 (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	21
2	B	0	92
3	C	0	4
4	D	0	3
6	F	0	1
83	EC	0	8
All	All	0	129

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	C	O3'-P	10.15	1.73	1.61
83	EC	6796	C	N1-C2	7.38	1.47	1.40
83	EC	6775	U	N1-C2	6.90	1.44	1.38
4	D	1	G	OP3-P	-6.88	1.52	1.61
1	A	1	U	OP3-P	-6.77	1.53	1.61

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	C	P-O3'-C3'	10.74	132.58	119.70
83	EC	6949	G	N9-C1'-C2'	8.39	124.91	114.00
2	B	961	C	C5'-C4'-O4'	7.63	118.26	109.10
2	B	705	A	N9-C1'-C2'	7.58	123.86	114.00
83	EC	6900	A	N9-C1'-C2'	7.42	123.65	114.00

There are no chirality outliers.

5 of 129 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	U	Sidechain
1	A	309	C	Sidechain
1	A	322	G	Sidechain
1	A	324	U	Sidechain
1	A	98	U	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	1685	0
2	B	70288	0	35262	4094	0
3	C	3354	0	1695	203	0
4	D	2580	0	1304	168	0
5	E	1359	0	1425	90	0
6	F	1918	0	1987	409	0
7	G	3082	0	3165	404	0
8	H	2750	0	2863	430	0
9	I	2376	0	2325	304	0
10	J	1401	0	1500	271	0
11	K	1785	0	1862	248	0
12	L	1818	0	1908	230	0
13	M	1519	0	1587	187	0
14	N	1718	0	1754	196	0
15	O	1354	0	1383	135	0
16	P	723	0	774	103	0
17	Q	1543	0	1608	194	0
18	R	1054	0	1149	188	0
19	S	1721	0	1779	299	0
20	T	1556	0	1659	182	0
21	U	1443	0	1485	177	0
22	V	1442	0	1543	231	0
23	W	1522	0	1617	208	0
24	X	1446	0	1487	210	0
25	Y	1277	0	1323	146	0
26	Z	796	0	812	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	1004	0	1048	109	0
28	BA	509	0	537	69	0
29	CA	969	0	1036	100	0
30	DA	994	0	1081	150	0
31	EA	1093	0	1155	128	0
32	FA	1174	0	1215	159	0
33	GA	463	0	491	39	0
34	HA	743	0	797	133	0
35	IA	890	0	938	116	0
36	JA	1020	0	1090	165	0
37	KA	851	0	880	172	0
38	LA	881	0	949	135	0
39	MA	970	0	1078	96	0
40	NA	772	0	849	97	0
41	OA	682	0	687	86	0
42	PA	613	0	682	39	0
43	QA	437	0	475	73	0
44	RA	418	0	459	60	0
45	SA	234	0	284	28	0
46	TA	848	0	918	96	0
47	UA	695	0	738	112	0
48	VA	1473	0	1514	145	0
49	WA	2445	0	2401	194	0
50	XA	1611	0	1618	165	0
51	YA	1709	0	1784	201	0
52	ZA	1635	0	1723	197	0
53	AB	1734	0	1817	130	0
54	BB	2069	0	2154	268	0
55	CB	1610	0	1675	190	0
56	DB	1820	0	1918	171	0
57	EB	1481	0	1572	150	0
58	FB	1490	0	1525	182	0
59	GB	1494	0	1573	161	0
60	HB	817	0	804	67	0
61	IB	1245	0	1314	155	0
62	JB	496	0	141	3	0
63	KB	1193	0	1255	155	0
64	LB	942	0	979	116	0
65	MB	975	0	1017	86	0
66	NB	1106	0	1166	132	0
67	OB	836	0	827	51	0
68	PB	1193	0	1222	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	QB	1113	0	1124	103	0
70	RB	856	0	917	107	0
71	SB	685	0	672	83	0
72	TB	1022	0	1060	149	0
73	UB	1122	0	1196	115	0
74	VB	1074	0	1132	86	0
75	WB	563	0	603	68	0
76	XB	769	0	818	121	0
77	YB	611	0	633	57	0
78	ZB	498	0	535	52	0
79	AC	444	0	436	54	0
80	BC	475	0	525	34	0
81	CC	284	0	76	0	0
82	DC	6561	0	6629	663	0
83	EC	4105	0	2063	82	0
84	DC	28	0	12	3	0
85	DC	1	0	0	0	0
86	DC	35	0	40	6	0
All	All	215363	0	160021	15325	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 41.

The worst 5 of 15325 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)
10:J:31:ARG:CD	37:KA:107:ILE:HA	1.38	1.53
10:J:158:TYR:CE1	18:R:115:PHE:HA	1.45	1.50
10:J:165:LEU:HG	37:KA:6:ARG:O	1.26	1.33
10:J:31:ARG:HD3	37:KA:107:ILE:CA	1.57	1.33
10:J:165:LEU:O	37:KA:6:ARG:CB	1.80	1.28

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%)	125 (76%)	32 (19%)	8 (5%)	3	32
6	F	250/254 (98%)	152 (61%)	66 (26%)	32 (13%)	0	7
7	G	384/387 (99%)	268 (70%)	80 (21%)	36 (9%)	1	16
8	H	359/362 (99%)	239 (67%)	79 (22%)	41 (11%)	0	9
9	I	294/297 (99%)	213 (72%)	57 (19%)	24 (8%)	1	18
10	J	173/176 (98%)	124 (72%)	33 (19%)	16 (9%)	1	16
11	K	220/244 (90%)	165 (75%)	46 (21%)	9 (4%)	3	37
12	L	231/256 (90%)	165 (71%)	52 (22%)	14 (6%)	2	27
13	M	189/191 (99%)	134 (71%)	41 (22%)	14 (7%)	1	21
14	N	207/221 (94%)	150 (72%)	42 (20%)	15 (7%)	1	23
15	O	167/174 (96%)	118 (71%)	32 (19%)	17 (10%)	1	13
16	P	92/165 (56%)	61 (66%)	23 (25%)	8 (9%)	1	17
17	Q	191/199 (96%)	138 (72%)	36 (19%)	17 (9%)	1	17
18	R	134/138 (97%)	102 (76%)	23 (17%)	9 (7%)	1	25
19	S	201/204 (98%)	130 (65%)	58 (29%)	13 (6%)	1	26
20	T	195/199 (98%)	164 (84%)	23 (12%)	8 (4%)	3	37
21	U	181/184 (98%)	137 (76%)	36 (20%)	8 (4%)	3	35
22	V	183/186 (98%)	130 (71%)	42 (23%)	11 (6%)	2	27
23	W	186/189 (98%)	140 (75%)	35 (19%)	11 (6%)	2	28
24	X	170/172 (99%)	116 (68%)	42 (25%)	12 (7%)	1	23
25	Y	157/160 (98%)	107 (68%)	34 (22%)	16 (10%)	1	13
26	Z	98/121 (81%)	70 (71%)	24 (24%)	4 (4%)	3	37
27	AA	134/137 (98%)	103 (77%)	27 (20%)	4 (3%)	5	45
28	BA	59/155 (38%)	38 (64%)	14 (24%)	7 (12%)	0	8
29	CA	119/142 (84%)	83 (70%)	23 (19%)	13 (11%)	0	11
30	DA	124/127 (98%)	95 (77%)	19 (15%)	10 (8%)	1	19
31	EA	133/136 (98%)	92 (69%)	32 (24%)	9 (7%)	1	24
32	FA	146/149 (98%)	89 (61%)	40 (27%)	17 (12%)	0	9
33	GA	56/59 (95%)	46 (82%)	9 (16%)	1 (2%)	11	55
34	HA	95/105 (90%)	70 (74%)	21 (22%)	4 (4%)	3	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	IA	107/113 (95%)	78 (73%)	19 (18%)	10 (9%)	1	16
36	JA	125/130 (96%)	88 (70%)	34 (27%)	3 (2%)	7	50
37	KA	104/107 (97%)	72 (69%)	27 (26%)	5 (5%)	3	32
38	LA	110/121 (91%)	70 (64%)	28 (26%)	12 (11%)	0	11
39	MA	117/120 (98%)	93 (80%)	16 (14%)	8 (7%)	1	24
40	NA	97/100 (97%)	72 (74%)	21 (22%)	4 (4%)	3	37
41	OA	85/88 (97%)	45 (53%)	27 (32%)	13 (15%)	0	5
42	PA	75/78 (96%)	64 (85%)	11 (15%)	0	100	100
43	QA	48/51 (94%)	29 (60%)	12 (25%)	7 (15%)	0	5
44	RA	50/128 (39%)	30 (60%)	15 (30%)	5 (10%)	1	13
45	SA	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
46	TA	103/106 (97%)	67 (65%)	29 (28%)	7 (7%)	1	24
47	UA	89/92 (97%)	55 (62%)	25 (28%)	9 (10%)	1	13
48	VA	187/312 (60%)	137 (73%)	34 (18%)	16 (9%)	1	17
49	WA	316/319 (99%)	236 (75%)	67 (21%)	13 (4%)	3	37
50	XA	204/252 (81%)	141 (69%)	45 (22%)	18 (9%)	1	17
51	YA	212/255 (83%)	142 (67%)	51 (24%)	19 (9%)	1	17
52	ZA	215/254 (85%)	160 (74%)	41 (19%)	14 (6%)	1	26
53	AB	221/240 (92%)	169 (76%)	35 (16%)	17 (8%)	1	20
54	BB	258/261 (99%)	188 (73%)	53 (20%)	17 (7%)	1	25
55	CB	204/225 (91%)	156 (76%)	32 (16%)	16 (8%)	1	20
56	DB	224/236 (95%)	169 (75%)	42 (19%)	13 (6%)	2	28
57	EB	182/190 (96%)	118 (65%)	44 (24%)	20 (11%)	0	10
58	FB	184/200 (92%)	130 (71%)	36 (20%)	18 (10%)	1	14
59	GB	183/197 (93%)	132 (72%)	35 (19%)	16 (9%)	1	17
60	HB	94/105 (90%)	63 (67%)	22 (23%)	9 (10%)	1	14
61	IB	153/156 (98%)	102 (67%)	41 (27%)	10 (6%)	1	26
62	JB	122/143 (85%)	87 (71%)	20 (16%)	15 (12%)	0	8
63	KB	148/151 (98%)	114 (77%)	25 (17%)	9 (6%)	2	27
64	LB	125/137 (91%)	90 (72%)	28 (22%)	7 (6%)	2	29
65	MB	120/142 (84%)	81 (68%)	30 (25%)	9 (8%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	106 (76%)	24 (17%)	9 (6%)	1	26
67	OB	115/136 (85%)	90 (78%)	19 (16%)	6 (5%)	2	31
68	PB	143/146 (98%)	99 (69%)	34 (24%)	10 (7%)	1	23
69	QB	141/144 (98%)	108 (77%)	23 (16%)	10 (7%)	1	23
70	RB	105/121 (87%)	77 (73%)	25 (24%)	3 (3%)	6	46
71	SB	85/87 (98%)	64 (75%)	13 (15%)	8 (9%)	1	16
72	TB	127/130 (98%)	89 (70%)	28 (22%)	10 (8%)	1	19
73	UB	142/145 (98%)	102 (72%)	31 (22%)	9 (6%)	2	27
74	VB	132/135 (98%)	94 (71%)	31 (24%)	7 (5%)	2	31
75	WB	68/108 (63%)	48 (71%)	11 (16%)	9 (13%)	0	6
76	XB	95/119 (80%)	60 (63%)	19 (20%)	16 (17%)	0	4
77	YB	79/82 (96%)	50 (63%)	24 (30%)	5 (6%)	2	27
78	ZB	61/67 (91%)	42 (69%)	19 (31%)	0	100	100
79	AC	51/56 (91%)	41 (80%)	7 (14%)	3 (6%)	2	28
80	BC	58/63 (92%)	41 (71%)	13 (22%)	4 (7%)	1	24
81	CC	69/152 (45%)	37 (54%)	14 (20%)	18 (26%)	0	1
82	DC	838/842 (100%)	629 (75%)	153 (18%)	56 (7%)	1	25
All	All	12226/13416 (91%)	8741 (72%)	2555 (21%)	930 (8%)	2	20

5 of 930 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	21	ARG
6	F	77	ILE
6	F	93	LYS
6	F	120	PRO
6	F	203	ALA

### 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%)	135 (86%)	22 (14%)	4	29
6	F	194/196 (99%)	173 (89%)	21 (11%)	8	39
7	G	322/323 (100%)	284 (88%)	38 (12%)	6	35
8	H	288/289 (100%)	251 (87%)	37 (13%)	5	31
9	I	244/245 (100%)	215 (88%)	29 (12%)	6	34
10	J	152/153 (99%)	142 (93%)	10 (7%)	21	60
11	K	186/205 (91%)	165 (89%)	21 (11%)	7	37
12	L	191/208 (92%)	171 (90%)	20 (10%)	8	40
13	M	171/171 (100%)	152 (89%)	19 (11%)	8	38
14	N	180/187 (96%)	159 (88%)	21 (12%)	7	35
15	O	147/150 (98%)	136 (92%)	11 (8%)	17	56
16	P	81/136 (60%)	62 (76%)	19 (24%)	1	8
17	Q	154/159 (97%)	135 (88%)	19 (12%)	6	33
18	R	107/109 (98%)	95 (89%)	12 (11%)	7	37
19	S	175/176 (99%)	140 (80%)	35 (20%)	1	13
20	T	160/162 (99%)	147 (92%)	13 (8%)	15	52
21	U	145/146 (99%)	129 (89%)	16 (11%)	8	38
22	V	150/151 (99%)	139 (93%)	11 (7%)	17	57
23	W	153/154 (99%)	139 (91%)	14 (9%)	11	46
24	X	156/156 (100%)	129 (83%)	27 (17%)	2	19
25	Y	136/137 (99%)	111 (82%)	25 (18%)	2	15
26	Z	87/107 (81%)	80 (92%)	7 (8%)	15	53
27	AA	104/105 (99%)	92 (88%)	12 (12%)	7	36
28	BA	54/129 (42%)	44 (82%)	10 (18%)	2	15
29	CA	105/118 (89%)	91 (87%)	14 (13%)	5	30
30	DA	109/110 (99%)	94 (86%)	15 (14%)	4	29
31	EA	115/116 (99%)	103 (90%)	12 (10%)	9	40
32	FA	118/119 (99%)	107 (91%)	11 (9%)	11	46
33	GA	46/47 (98%)	40 (87%)	6 (13%)	5	31
34	HA	81/88 (92%)	72 (89%)	9 (11%)	8	38
35	IA	96/97 (99%)	82 (85%)	14 (15%)	4	26
36	JA	109/111 (98%)	95 (87%)	14 (13%)	5	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	87 (97%)	3 (3%)	45	77
38	LA	95/103 (92%)	83 (87%)	12 (13%)	5	31
39	MA	104/105 (99%)	88 (85%)	16 (15%)	3	24
40	NA	81/82 (99%)	70 (86%)	11 (14%)	5	30
41	OA	70/71 (99%)	63 (90%)	7 (10%)	9	42
42	PA	68/69 (99%)	64 (94%)	4 (6%)	24	64
43	QA	45/46 (98%)	38 (84%)	7 (16%)	3	24
44	RA	47/116 (40%)	44 (94%)	3 (6%)	22	61
45	SA	23/23 (100%)	19 (83%)	4 (17%)	2	18
46	TA	90/91 (99%)	72 (80%)	18 (20%)	1	13
47	UA	71/72 (99%)	60 (84%)	11 (16%)	3	24
48	VA	160/254 (63%)	139 (87%)	21 (13%)	5	30
49	WA	261/262 (100%)	248 (95%)	13 (5%)	30	68
50	XA	172/210 (82%)	155 (90%)	17 (10%)	10	43
51	YA	191/224 (85%)	170 (89%)	21 (11%)	8	38
52	ZA	176/205 (86%)	166 (94%)	10 (6%)	25	65
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%)	162 (94%)	11 (6%)	22	61
56	DB	193/201 (96%)	180 (93%)	13 (7%)	20	60
57	EB	165/170 (97%)	149 (90%)	16 (10%)	10	43
58	FB	150/161 (93%)	135 (90%)	15 (10%)	9	42
59	GB	158/166 (95%)	150 (95%)	8 (5%)	29	68
60	HB	89/98 (91%)	83 (93%)	6 (7%)	20	60
61	IB	136/137 (99%)	125 (92%)	11 (8%)	15	52
63	KB	127/128 (99%)	112 (88%)	15 (12%)	6	35
64	LB	96/105 (91%)	92 (96%)	4 (4%)	36	72
65	MB	103/118 (87%)	95 (92%)	8 (8%)	16	54
66	NB	117/119 (98%)	109 (93%)	8 (7%)	20	59
67	OB	82/124 (66%)	74 (90%)	8 (10%)	10	43
68	PB	128/129 (99%)	113 (88%)	15 (12%)	7	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
69	QB	115/116 (99%)	110 (96%)	5 (4%)	35 72
70	RB	100/114 (88%)	92 (92%)	8 (8%)	15 53
71	SB	74/74 (100%)	67 (90%)	7 (10%)	11 45
72	TB	110/111 (99%)	93 (84%)	17 (16%)	3 24
73	UB	119/120 (99%)	110 (92%)	9 (8%)	16 55
74	VB	112/113 (99%)	101 (90%)	11 (10%)	10 43
75	WB	61/89 (68%)	56 (92%)	5 (8%)	14 51
76	XB	83/101 (82%)	71 (86%)	12 (14%)	4 27
77	YB	70/71 (99%)	65 (93%)	5 (7%)	18 58
78	ZB	56/60 (93%)	52 (93%)	4 (7%)	18 58
79	AC	47/49 (96%)	40 (85%)	7 (15%)	4 26
80	BC	51/54 (94%)	44 (86%)	7 (14%)	4 29
82	DC	713/714 (100%)	630 (88%)	83 (12%)	7 36
All	All	10248/11032 (93%)	9148 (89%)	1100 (11%)	13 39

5 of 1100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	DA	115	ARG
42	PA	49	SER
80	BC	55	ARG
32	FA	14	HIS
36	JA	78	ASN

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

Mol	Chain	Res	Type
27	AA	132	ASN
39	MA	68	GLN
77	YB	19	HIS
29	CA	55	ASN
33	GA	45	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1755/1798 (97%)	369 (21%)	14 (0%)
2	B	3267/3396 (96%)	679 (20%)	26 (0%)
3	C	157/158 (99%)	36 (22%)	2 (1%)
4	D	120/121 (99%)	17 (14%)	0
83	EC	187/201 (93%)	74 (39%)	3 (1%)
All	All	5486/5674 (96%)	1175 (21%)	45 (0%)

5 of 1175 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	42	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	961	C
2	B	1329	U
3	C	85	G
2	B	1103	A
2	B	1352	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	1.97	3 (23%)	12,28,30	2.11	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	OAG-CBI	2.01	1.27	1.23
82	DC	699	DDE	CB-CA	2.38	1.58	1.53
82	DC	699	DDE	CBW-CBI	4.71	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	-2.46	105.77	110.72
82	DC	699	DDE	CAC-NCB-CBW	2.20	115.55	110.57
82	DC	699	DDE	OAG-CBI-NAD	2.23	126.76	123.06
82	DC	699	DDE	CAU-CAT-CE1	5.32	141.28	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	DC	699	DDE	2	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	2.12	8 (33%)	26,47,47	1.79	5 (19%)
86	SO1	DC	903	-	36,39,39	2.85	18 (50%)	36,64,64	1.71	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 26 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	C54-C55	2.00	1.58	1.52
86	DC	903	SO1	C52-C53	2.19	1.59	1.52
86	DC	903	SO1	C24-C18	2.27	1.60	1.54
84	DC	901	GDP	PB-O3B	2.28	1.62	1.54

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	DC	901	GDP	N3-C2-N1	-4.90	120.89	127.56
84	DC	901	GDP	C5-C6-N1	-3.91	118.41	123.52
86	DC	903	SO1	C7-C2-C8	-2.90	104.93	110.16
86	DC	903	SO1	C18-C9-C16	-2.88	99.38	103.42
86	DC	903	SO1	C65-O64-C55	-2.58	107.36	114.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	DC	901	GDP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	DC	903	SO1	6	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.