



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 05:23 PM EDT

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

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

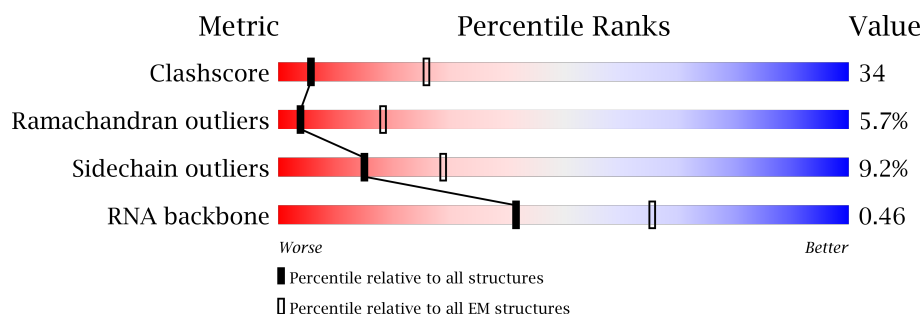
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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






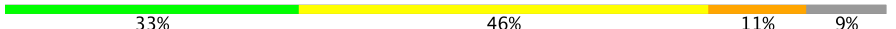
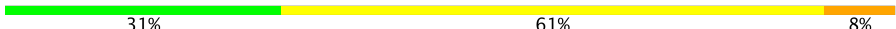
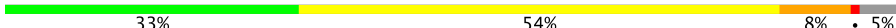
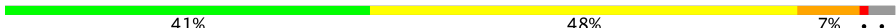


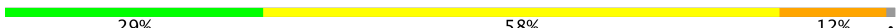
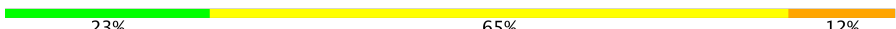
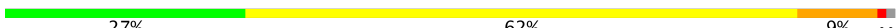




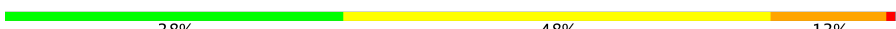
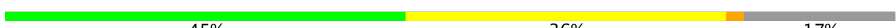


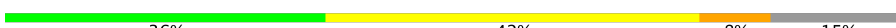

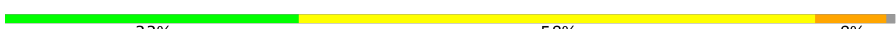


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

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


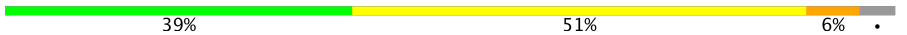
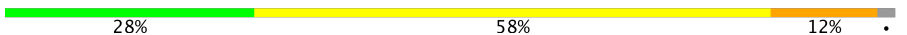



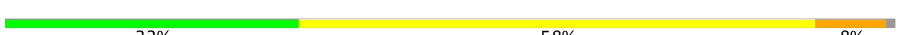
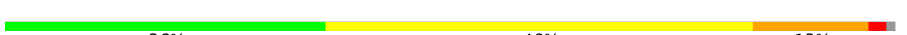



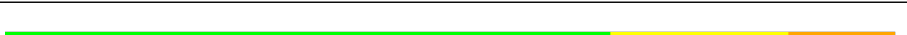

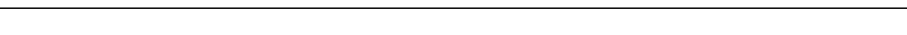
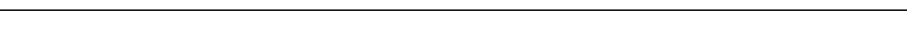
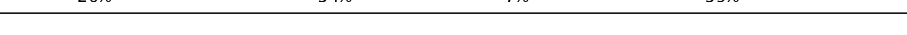

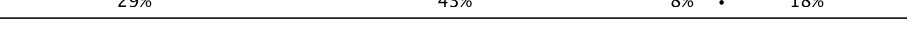







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Mol	Chain	Length	Quality of chain
9	I	297	
10	J	176	
11	K	244	
12	L	256	
13	M	191	
14	N	221	
15	O	174	
16	P	165	
17	Q	199	
18	R	138	
19	S	204	
20	T	199	
21	U	184	
22	V	186	
23	W	189	
24	X	172	
25	Y	160	
26	Z	121	
27	AA	137	
28	BA	155	
29	CA	142	
30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


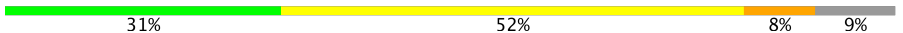
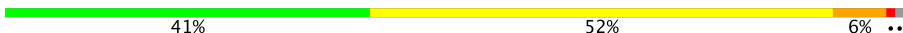



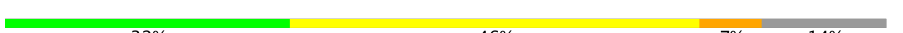




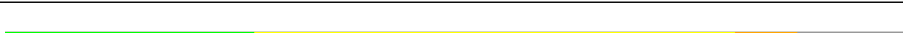













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Mol	Chain	Length	Quality of chain
34	HA	105	
35	IA	113	
36	JA	130	
37	KA	107	
38	LA	121	
39	MA	120	
40	NA	100	
41	OA	88	
42	PA	78	
43	QA	51	
44	RA	128	
45	SA	25	
46	TA	106	
47	UA	92	
48	VA	312	
49	WA	319	
50	XA	252	
51	YA	255	
52	ZA	254	
53	AB	240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

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Mol	Chain	Length	Quality of chain
59	GB	197	
60	HB	105	
61	IB	156	
62	JB	143	
63	KB	151	
64	LB	137	
65	MB	142	
66	NB	143	
67	OB	136	
68	PB	146	
69	QB	144	
70	RB	121	
71	SB	87	
72	TB	130	
73	UB	145	
74	VB	135	
75	WB	108	
76	XB	119	
77	YB	82	
78	ZB	67	
79	AC	56	
80	BC	63	
81	CC	152	
82	DC	842	
83	EC	201	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 212680 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1781	Total	C	N	O	P	0	0
			36760	16335	6359	12285	1781		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

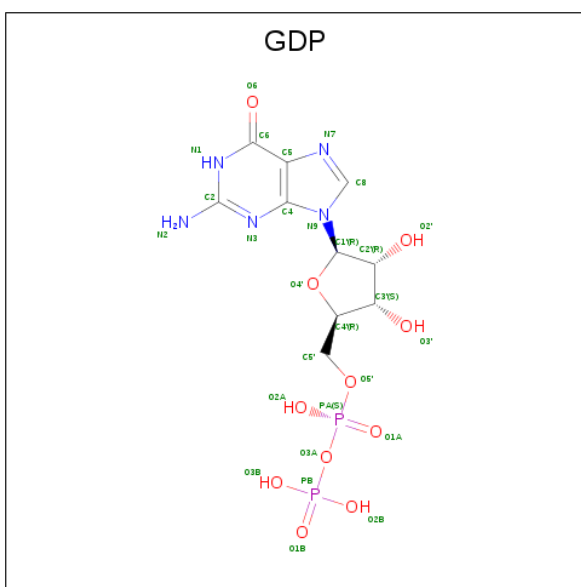
- Molecule 82 is a protein called yeast eEF2.

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

- Molecule 83 is a RNA chain called IRES.

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

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

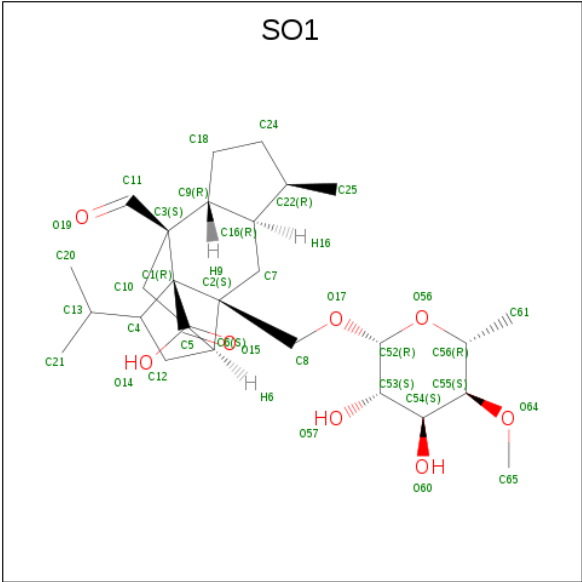


Mol	Chain	Residues	Atoms					AltConf
84	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

Mol	Chain	Residues	Atoms		AltConf
85	DC	1	Total	Mg	0
			1	1	

- Molecule 86 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: C₂₇H₄₂O₈).

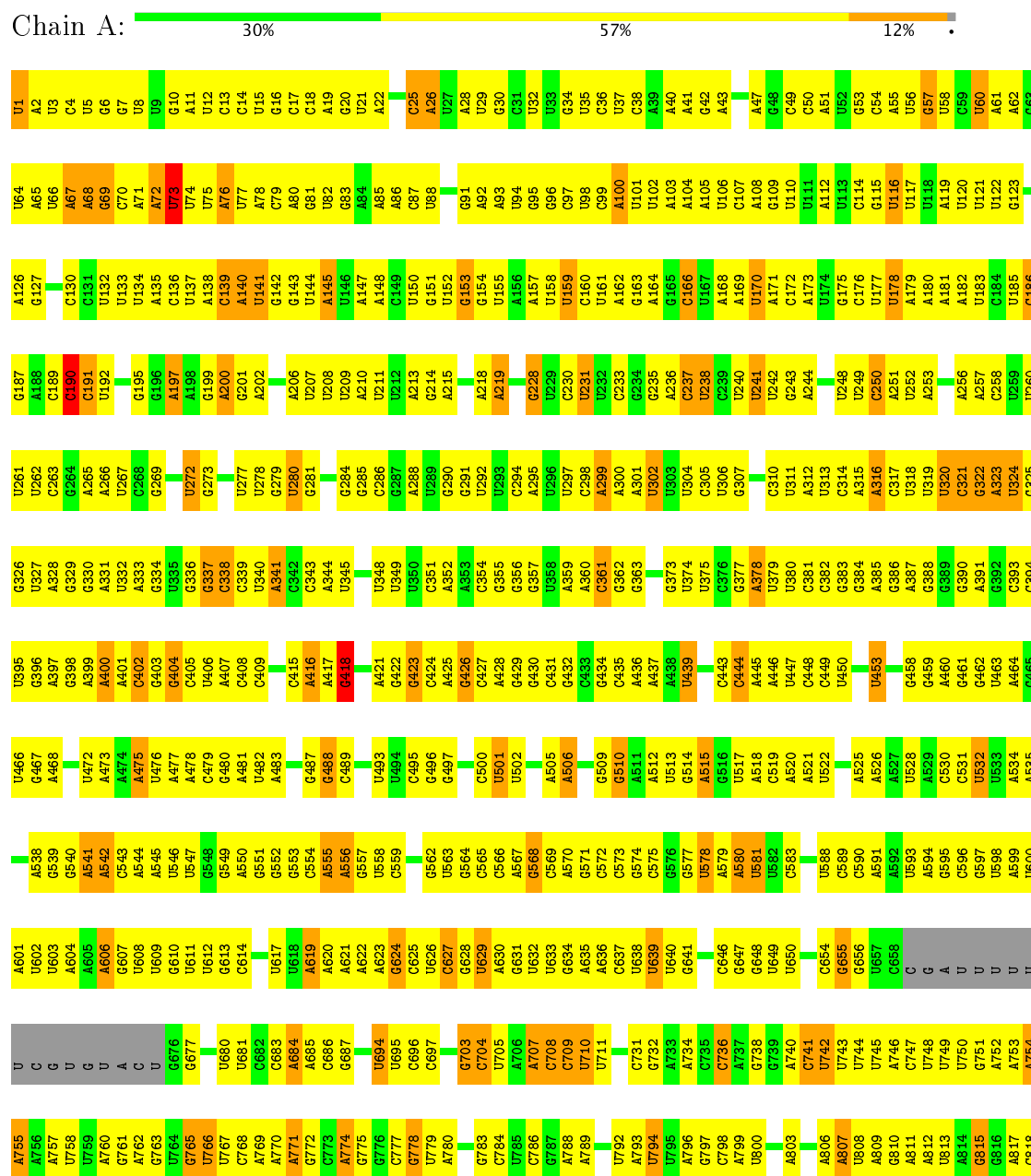


Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

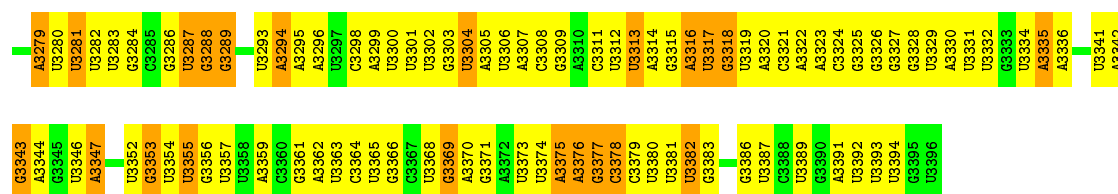
• Molecule 1: 18S ribosomal RNA



U1109	G1045	A973	A913	G853	G727	U654	G600	U536	G	A396	A327	C259	U194	C125	A65
U1110	A1046	G974	A914	G854	G728	A655	A603	A537	U	A397	U328	U259	U195	U126	A66
U1111	A1047	G975	A915	G855	G729	A656	A604	G538	G	A398	U329	U262	U196	G127	A67
U1112	A1048	U976	G916	G856	C730	C667	G603	U	G	A399	U329	C263	G197	G128	C68
U1113	G1049	C977	G917	G857	U731	G668	U605	G542	U	G400	G335	A268	A198	U129	C69
U1114	U1050	G978	C918	G858	C732	U669	C606	C546	A	U401	A336	G289	A199	A130	A70
U1115	U1051	U979	U919	G859	C733	C670	A607	C547	A	A402	G337	U270	C200	C131	A71
U1116	U1052	A980	A920	G860	C734	U671	A608	G548	G	C403	A338	G271	A201	C132	C72
U1117	A1053	U981	A921	G861	U735	U672	G609	G549	G	C404	C339	C271	G202	U133	C73
U1118	A1054	C982	U922	U862	G736	U673	G610	U549	G	C405	C340	G272	U134	U134	G74
U1119	A1055	A983	C923	G863	U737	G674	A611	U550	G	G406	G341	A273	C203	C135	G75
U1120	U1056	G984	G924	G864	A738	C675	U612	A551	A	A407	A342	G274	A204	G136	G76
U1121	A1057	U985	A925	U865	C739	G676	G613	G552	A	A408	U343	G275	C208	G137	A77
U1122	U1058	U986	A926	A866	G740	A677	G614	U553	U	A409	A344	U276	A209	U138	U78
U1123	G1059	U987	C927	G867	U741	G678	U615	A554	C	U410	G345	U277	U210	U139	U79
U1124	U1124	U988	C928	C868	G742	U679	U616	U555	U	U411	G346	G278	A211	C140	G80
U1125	G1063	A989	A929	G869	C743	U680	U617	U556	G	G412	G347	U279	G212	C141	C81
U1126	G1064	U990	G930	G870	A744	U681	U618	U557	U	U413	A348	U280	A213	C142	C82
U1127	A1064	G991	C931	U871	C745	U682	U620	U558	U	U414	A349	G281	G214	G143	U83
U1128	A1065	A992	U932	U872	A746	U683	A621	A559	U	G415	C350	G282	G215	A144	U84
U1129	G1066	G993	A933	C873	U747	U684	A622	U560	U	U416	A351	G283	G216	G145	A85
A1130	U1067	G994	G934	U874	U748	G685	U623	C561	G	G417	G352	A284	U217	C146	G86
G1131	C1068	U995	U935	G875	C749	U686	G624	C562	G	U418	G353	A285	G218	U147	U87
C1132	C1069	A996	A936	A876	G750	U689	G625	U563	U	G421	U354	U286	A219	U149	A88
A1133	U1070	A997	U937	C877	U751	U690	U626	G564	U	A422	U355	G287	G220	A150	A89
G1134	U1071	A998	C938	G878	C753	A691	U627	U565	U	G423	C356	G288	A221	A151	C90
A1135	G1072	U1001	U939	U879	G754	A692	A628	U566	U	G424	U359	A289	A222	U152	G91
A1136	U1073	A1002	G940	G880	U755	A693	U629	G567	U	G425	G360	A290	U223	U153	G92
C1137	U1074	U1003	C941	C881	U756	C694	U630	G568	U	G426	A361	C291	C224	U154	G93
A1138	A1075	U1004	U942	A882	C757	C695	A631	A569	U	G427	U362	U292	C225	G155	G94
G1139	C1076	U1005	U943	C883	U758	C696	G632	A570	U	A428	G363	C293	C226	G156	A95
G1140	U1077	A1006	C944	A884	U759	A697	C633	U571	U	U429	G364	U294	G227	A157	G96
A1143	U1078	U1007	C945	U885	G760	U698	C634	A572	U	U430	U370	A295	U228	G158	G97
U1144	U1081	U1008	U946	C886	A761	A699	G635	C573	U	U431	A365	A296	G229	A159	G98
G1145	U1082	U1009	G947	G887	U762	C700	C636	U574	U	G432	A366	G297	U230	G160	A99
C1146	G1083	C1009	C948	A888	C763	G701	C637	G575	U	G433	A367	U298	G231	G161	A100
G1147	A1084	G1010	C949	C824	U764	C702	C638	G576	U	U434	G368	G299	G232	G162	G101
G1148	A1085	U1011	G950	C825	C765	G703	G639	C577	U	U435	A369	G300	C233	C163	C102
U1149	U1088	C1016	A951	G891	U766	U704	U640	A578	U	U438	U370	G301	G237	A164	G103
A1150	U1089	C1017	A952	U829	U767	A705	C641	G579	U	U439	G371	U305	A238	A165	G104
A1153	U1092	G1018	G953	C830	C768	U706	U642	C580	U	U440	A372	A306	G239	U169	C105
C1155	A1093	G1019	U954	G834	U769	U707	U643	U581	U	U441	A373	A307	U240	G170	A106
G1156	U1094	U1022	U955	G833	A770	A708	G644	G582	U	U442	A374	A308	G241	G171	A107
G1157	U1095	C1023	U956	U834	A771	A709	A645	G583	U	U443	A375	U311	C242	A108	A108
G1158	U1096	G1024	C957	G835	U772	A710	A646	G584	U	U444	G376	U312	G243	G175	G110
A1159	U1097	A1025	C958	A836	C773	A711	A647	A585	U	U445	A377	U313	G244	C176	C111
C1160	G1097	U1029	U960	G838	U774	U713	C648	G586	U	U446	A378	U314	G245	U181	C113
A1161	A1098	G1030	C961	C839	U775	G714	C650	U587	U	U447	A379	U315	U246	U182	A114
G1162	U1099	A1030	A962	C840	U776	A715	G651	A589	U	U448	U380	U316	U249	C185	A115
A1163	A1100	U1033	G963	A841	U777	A716	G652	G590	U	U449	U381	A317	U250	U186	A116
G1164	G1101	U1034	U965	G842	C779	C717	A653	G591	U	U450	U382	A318	G251	U187	U117
A1165	A1102	U1035	A966	A843	U780	G718	C654	A592	U	U451	A383	A319	G252	U188	U118
G1166	A1103	U1036	U967	G844	C781	U719	C655	C593	U	U452	A384	G320	U253	U189	U119
A1167	G1104	U1037	G967	A845	U782	U720	A656	U594	U	U453	A385	G321	A254	G189	G120
U1168	A1105	U1040	C968	A846	C783	G721	U657	G595	U	U454	A386	U322	A255	U190	A121
A1169	G1106	U1041	C969	A847	A784	U722	U658	C596	U	U455	A387	A323	G256	U191	A122
C1170	C1107	U1042	G970	U850	U785	U723	U659	G597	U	U456	A388	A324	U257	C192	A123
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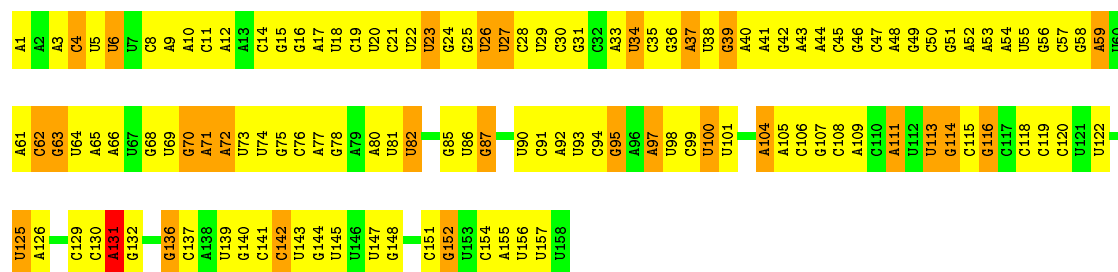
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A2182	C2118	U1880	U1819	A1752	U1691	U1616	A1546	G1483	G1422	C1359	U1299	C1238	G1172
A2183	A2119	A1881	U1820	G1753	C1692	U1629	G1547	U1494	C1423	C1360	G1300	C1239	U1173
G2184	A2120	G1882	U1821	G1754	C1693	U1633	C1548	U1495	C1424	U1361	A1301	C1240	G1174
G2185	G2122	A1883	C1822	C1755	U1694	C1630	U1549	G1486	U1425	G1362	A1302	U1241	C1175
U2186	G2123	A1884	A1823	C1756	U1695	C1631	C1550	G1487	C1426	A1363	A1303	U1242	C1176
G2187	G2124	U1885	U1824	A1757	U1696	A1632	C1551	G1488	U1427	C1364	A1304	G1177	G1177
A2188	U2127	A1886	G1825	C1758	C1698	C1633	G1552	A1489	A1428	G1365	U1305	A1245	G1178
U2189	C2128	A1887	C1826	C1759	C1699	G1634	G1553	A1490	G1429	A1366	G1306	G1246	A1179
C2192	U2129	U1888	C1827	U1765	G1700	G1635	U1554	A1491	U1430	G1367	G1307	U1247	U1180
U2193	U2130	G1889	A1828	G1766	C1701	U1636	U1555	A1492	U1431	U1368	A1308	C1248	U1181
G2194	A2131	U1890	G1829	C1767	U1702	A1637	G1556	G1493	G1433	A1369	U1309	G1249	A1182
C2195	U2132	U1891	U1830	G1768	U1703	A1638	A1557	U1494	G1434	G1370	G1310	G1250	C1183
C2196	U2133	U1892	U1831	U1769	A1704	C1639	A1558	U1495	A1435	G1371	G1311	A1251	A1184
C2197	G2037	U1893	C1832	G1770	U1705	G1640	C1562	C1496	U1436	C1372	G1312	A1252	C1185
U2198	G2048	U1894	G1833	G1771	U1706	A1641	C1563	C1497	U1438	C1373	G1313	U1253	C1186
C2199	G2057	G1897	U1834	C1773	A1707	A1642	U1564	G1500	U1439	C1376	U1315	C1255	U1188
G2200	G2058	G1898	A1835	C1774	C1708	U1644	G1565	U1501	G1440	G1377	C1316	G1256	C1189
G2201	U2137	G1899	C1836	G1775	C1709	U1645	A1566	C1502	G1441	U1378	C1317	C1257	A1190
C2202	G2059	A1900	U1837	U1776	C1710	G1646	U1567	C1503	U1442	G1379	A1318	U1258	U1191
U2203	U2138	G1901	U1838	C1779	G1712	G1647	U1568	A1504	G1443	G1380	A1319	A1259	C1192
C2204	A2141	G1902	A1839	G1780	G1713	A1648	U1569	C1505	G1444	A1381	C1320	A1260	A1193
U2205	G2062	U1903	U1840	C1781	G1714	U1649	U1570	A1506	G1445	G1382	G1321	G1261	G1194
G2206	G2076	G1904	A1841	U1782	A1715	G1650	A1571	G1507	U1446	G1383	U1322	G1262	A1195
A2207	U2077	G1905	A1842	U1783	U1716	U1651	U1572	C1508	G1447	U1384	G1323	A1263	C1198
A2208	C2078	U1906	C1844	G1784	U1717	G1652	U1573	A1509	U1448	C1385	U1324	G1264	C1199
U2209	G2079	A1907	G1845	U1785	G1718	G1653	U1574	A1510	A1449	A1386	U1325	A1265	G1200
G2210	C2080	G1908	C1846	G1786	U1719	A1654	U1511	C1506	G1450	G1387	A1326	G1266	A1201
U2211	U2081	A1911	A1847	A1787	U1720	G1655	G1512	U1518	A1457	U1388	C1327	U1267	C1202
C2212	U2082	U1912	G1848	C1788	U1721	A1656	C1513	G1519	U1458	G1389	C1328	G1268	A1203
G2213	U2083	G1913	C1849	G1789	U1722	C1657	C1514	C1520	C1459	A1390	U1329	U1269	A1204
A2214	C2084	G1914	A1850	G1790	A1723	G1658	A1515	G1521	A1460	C1391	A1330	A1270	U1208
C2215	U2085	G1915	G1851	C1791	U1724	C1659	U1516	U1522	U1461	G1392	A1331	C1271	G1209
G2216	A2086	U1916	C1852	C1792	C1725	C1660	C1517	C1523	U1462	A1393	A1332	C1272	U1210
U2217	C2087	U1917	U1853	C1793	G1726	G1661	A1583	A1524	G1463	A1394	C1333	A1273	U1211
G2218	A2088	C1918	C1854	G1794	G1727	G1662	U1584	G1525	G1464	A1401	U1341	G1280	G1212
U2219	A	U1919	U1855	U1795	G1728	C1663	C1585	G1526	G1465	C1402	C1342	C1281	U1213
A2220	C2157	G1920	C1856	G1796	A1729	G1664	G1586	U1527	U1466	C1403	U1343	G1282	C1219
A2221	U2157	U1921	C1857	A1797	G1730	C1665	A1587	U1528	A1467	G1404	G1344	C1283	U1220
A2222	U2158	A1922	A1858	U1798	U1731	C1666	A1588	U1529	U1468	A1406	G1345	G1284	A1221
A2223	G2160	C1923	G1859	A1799	U1732	A1667	A1590	U1526	G1465	C1407	G1346	A1285	G1222
U2224	C2093	C1924	G1860	A1800	G1733	C1668	G1591	C1527	G1466	C1408	U1347	A1286	A1223
C2225	C2094	U1925	G1861	U1801	G1734	C1669	G1592	G1528	U1467	C1409	U1348	U1287	C1224
U2226	G2095	U1926	U1862	C1802	G1735	C1670	U1593	U1529	U1470	G1407	U1349	A1288	A1225
C2227	A2096	C1927	G1863	C1803	G1736	U1672	C1596	C1597	U1471	G1408	U1347	U1289	G1226
A2228	C2164	G1928	A1864	A1804	U1737	U1673	G1597	U1533	U1472	G1409	U1348	G1290	G1230
A2229	C2165	U1929	C1865	C1805	U1738	C1671	A1602	A1534	U1473	U1410	U1349	A1291	A1231
C2230	U2102	U1930	A1867	A1806	C1738	U1672	G1603	A1535	A1474	U1411	A1350	C1292	A1232
C2231	U2103	A1931	G1868	G1807	U1740	G1678	G1604	A1537	G1475	U1415	A1351	U1293	G1233
A2232	A2107	G1932	C1869	A1808	U1741	U1680	A1605	U1538	G1476	U1416	A1352	A1294	G1234
G2233	U2108	C1933	U1870	A1810	G1742	U1681	U1606	U1540	C1477	G1417	A1353	G1295	U1235
C2234	G2110	G1934	U1871	G1811	G1743	A1683	U1607	G1541	U1478	A1418	U1354	U1296	G1236
G2235	G2111	A1935	C1872	A1812	C1745	C1685	U1608	U1542	U1479	A1419	U1355	C1297	
G2236	G2112	U1936	U1872	A1813	U1746	U1686	U1609	G1543	U1480				
U2241	G2113	U1937	U1873	A1814	G1747	U1687	A1612	G1544					
A2242	U2174	U1938	U1874	A1815	U1748	U1688							
A2243	U2175	G1939	U1877	A1816	A1749	U1689							
A2244	G2177	G1940	G1878	G1817	A1750	U1699							

C3212	G3147	G3083	U3020	U2954	U2891	G2831	G2770	A2704	U2641	G2576	U2510	A2439	G2376	U2314	C2245
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A3218	U3153	C3089	G3028	C2960	G2897	A2837	C2776	A2715	A2647	G2586	U2516	G2450	A2384	A2320	G2251
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		C3092	G3031	G2964	A2900	C2840	A2779	U2718	G2651	G2589				G2323	
A3223	U3159	C3093	A3032	U2965	G2901	G2841	A2780	U2719						A2324	
G3224	U3160	A3094	C3033	G2966	G2905	U2842	U2781		C2852	A2590	G2522	U2455	C2389		A2261
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G3242	U3175	U3111	A3048	C2985	A2919	U2857	G2796	A2736	U2668	G2608	U2539	C2474	U2410	U2342	C2278
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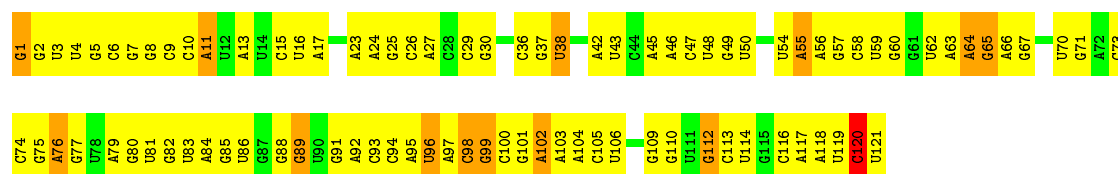
• Molecule 3: 5.8S ribosomal RNA

Chain C: 20% 62% 18%



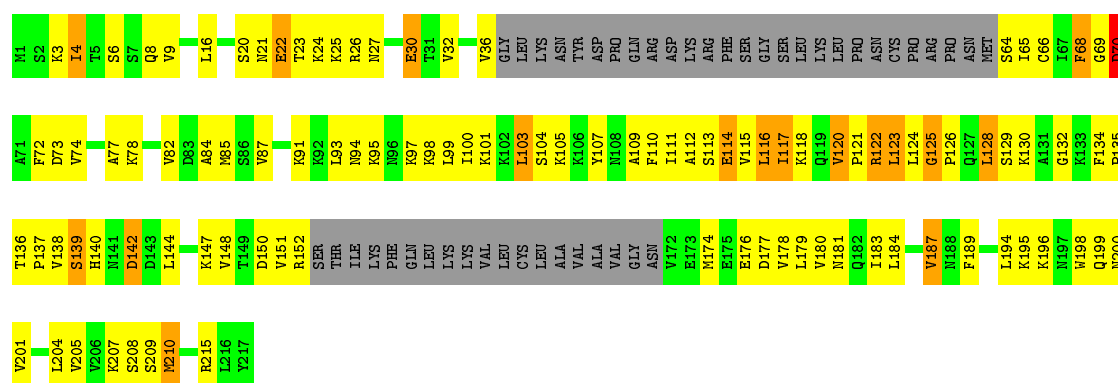
• Molecule 4: 5S ribosomal RNA

Chain D: 26% 63% 11%



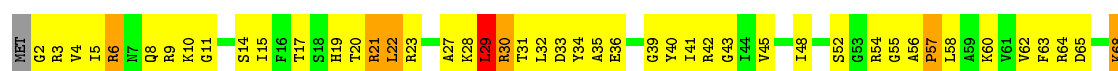
• Molecule 5: uL1 (yeast L1)

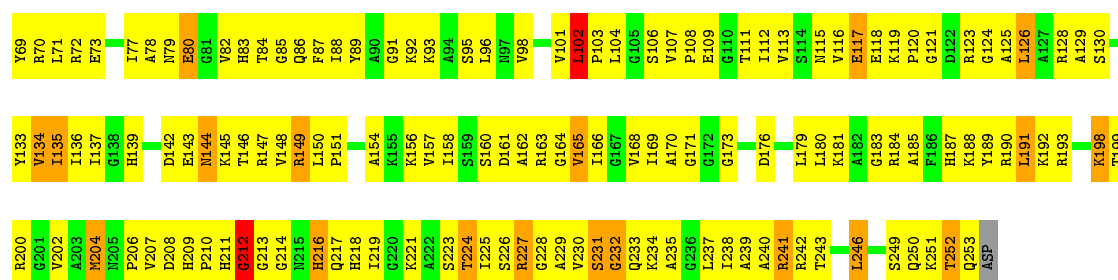
Chain E: 30% 40% 8% 21%



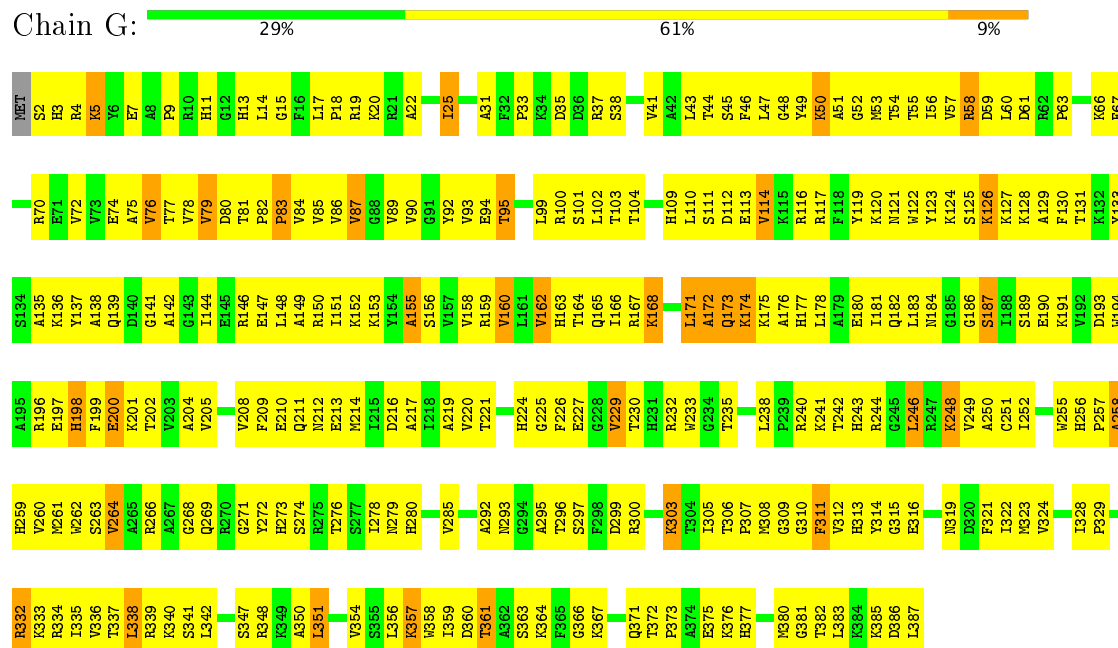
• Molecule 6: uL2 (yeast L2)

Chain F: 26% 62% 10%

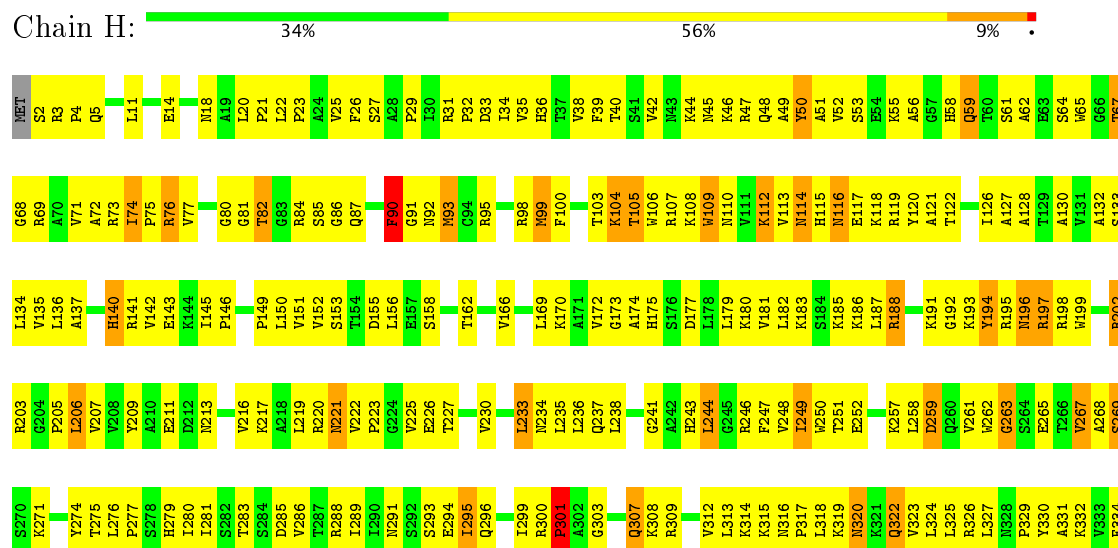


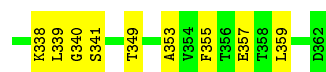


• Molecule 7: uL3 (yeast L3)

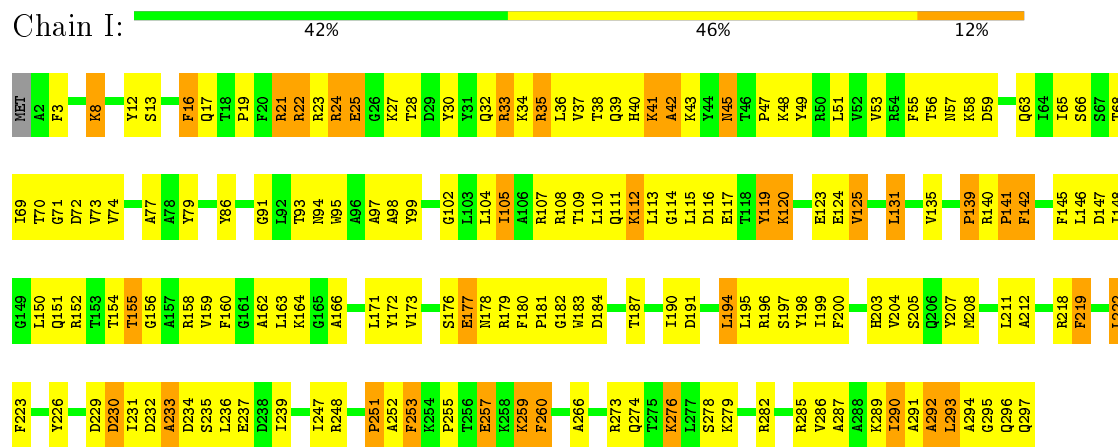


• Molecule 8: uL4 (yeast L4)

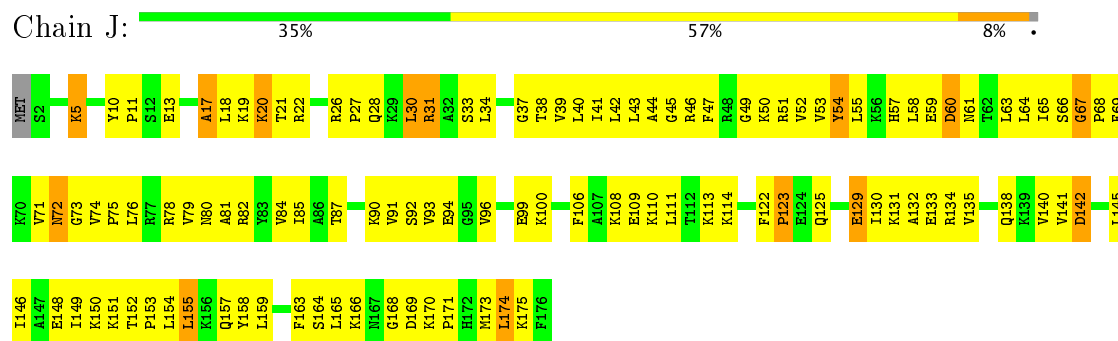




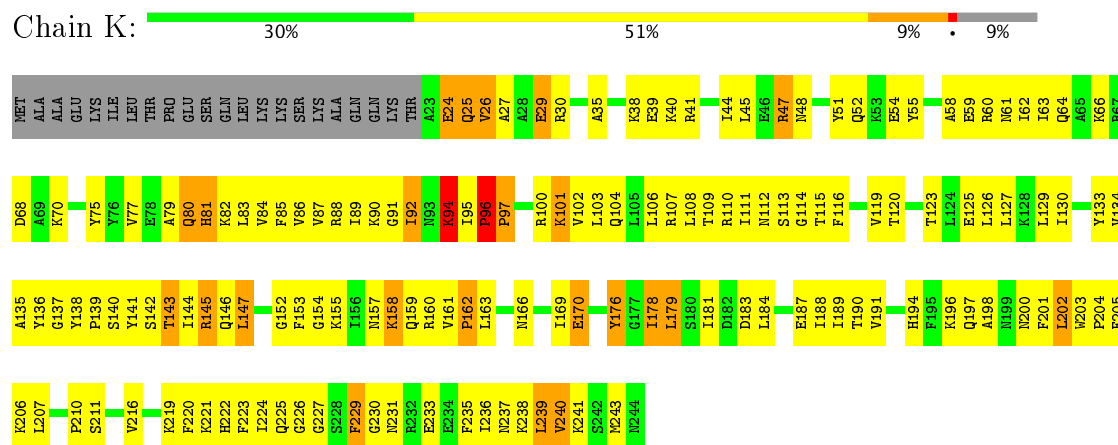
- Molecule 9: uL18 (yeast L5)



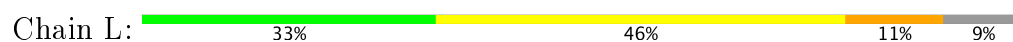
- Molecule 10: eL6 (yeast L6)

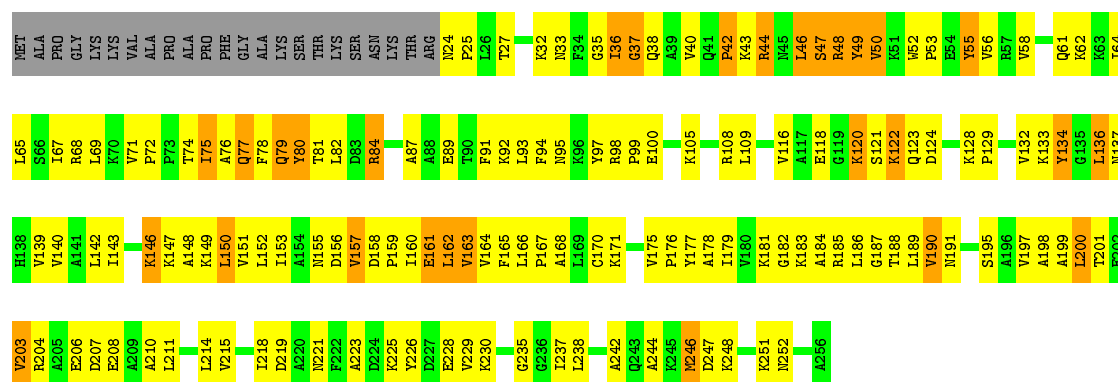


- Molecule 11: uL30 (yeast L7)



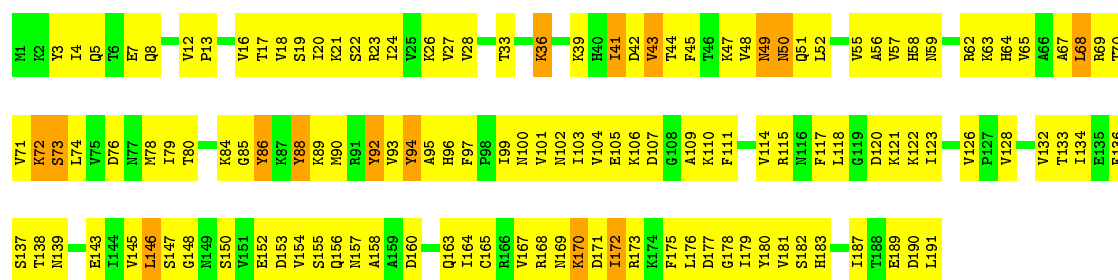
- Molecule 12: eL8 (yeast L8)





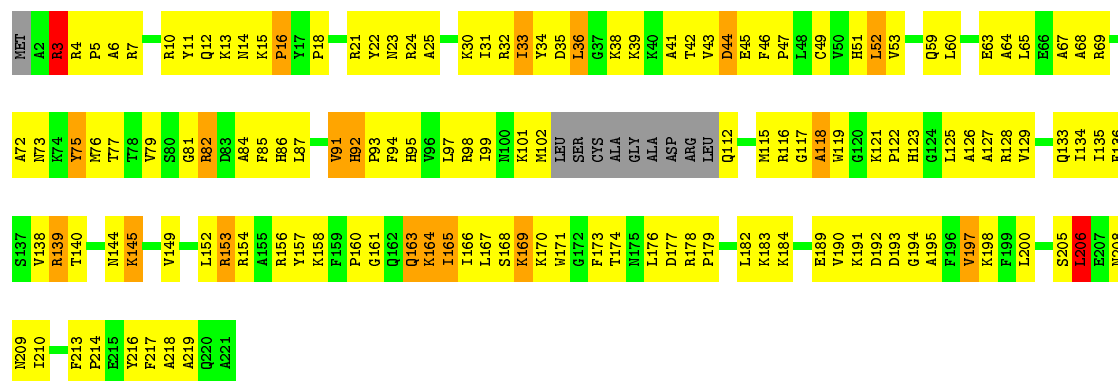
• Molecule 13: uL6 (yeast L9)

Chain M: 31% 61% 8%



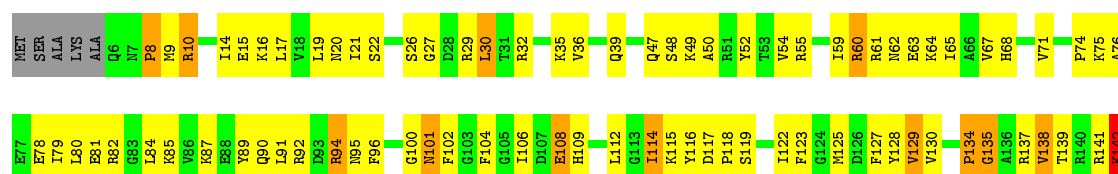
• Molecule 14: uL16 (yeast L10)

Chain N: 33% 54% 8% 5%



• Molecule 15: uL5 (yeast L11)

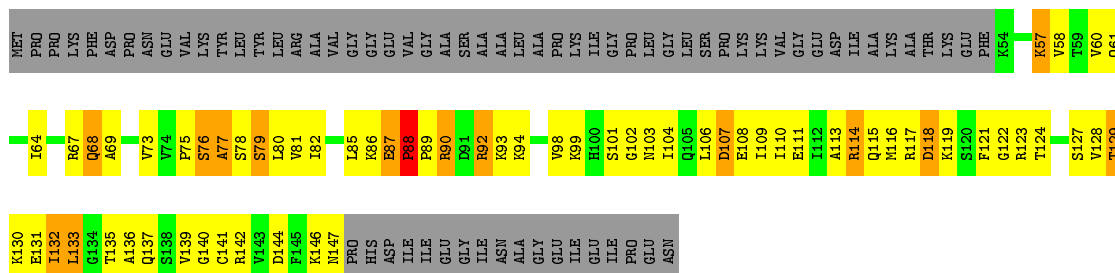
Chain O: 41% 48% 7%





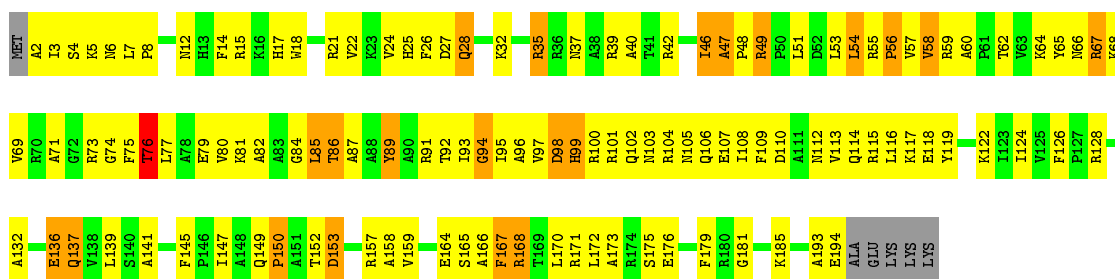
• Molecule 16: uL11 (yeast L12)

Chain P: 17% 31% 8% 43%



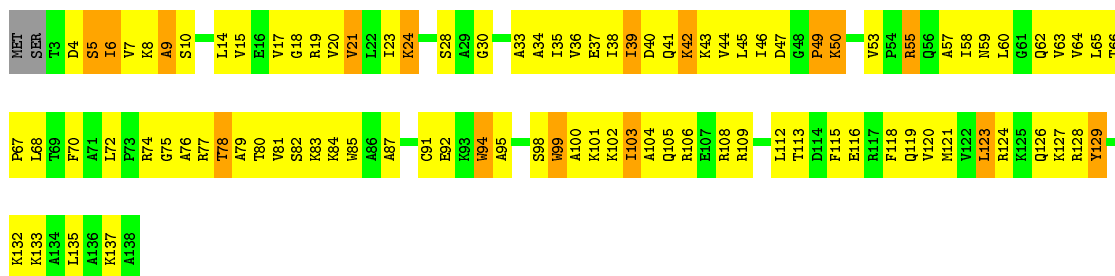
• Molecule 17: eL13 (yeast L13)

Chain Q: 36% 50% 11%



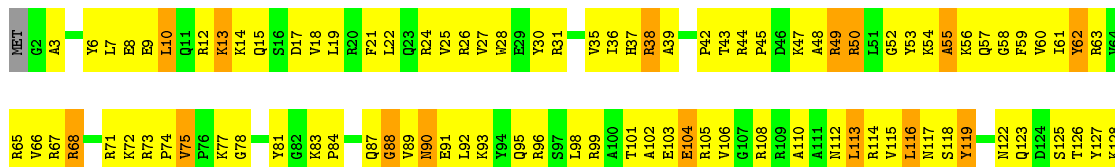
• Molecule 18: eL14 (yeast L14)

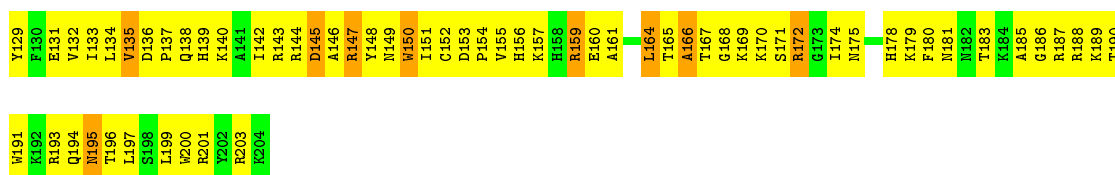
Chain R: 29% 58% 12%



• Molecule 19: eL15 (yeast L15)

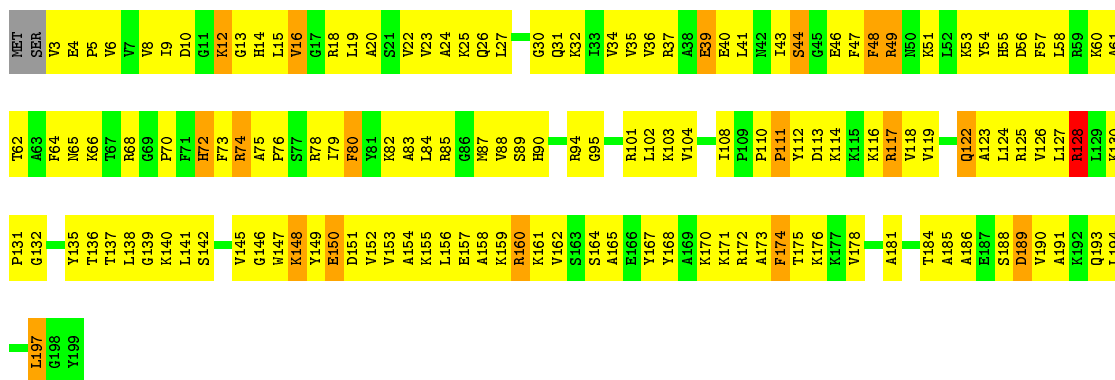
Chain S: 23% 65% 12%





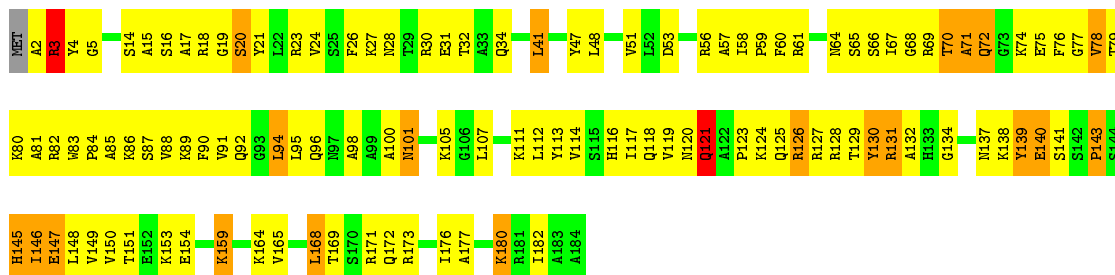
• Molecule 20: uL13 (yeast L16)

Chain T: 27% 62% 9% ..



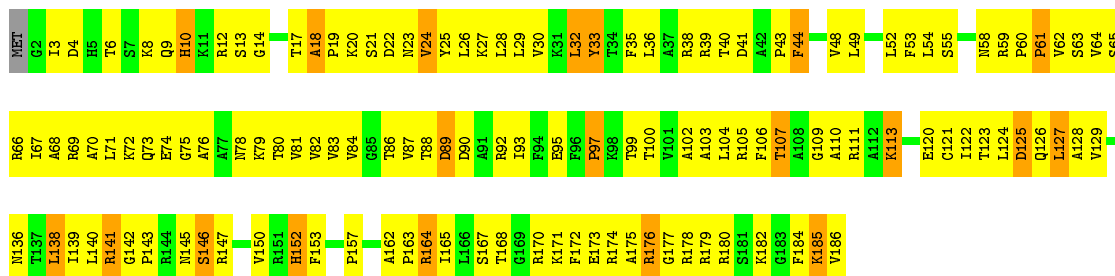
• Molecule 21: uL22 (yeast L17)

Chain U: 36% 51% 11% ..



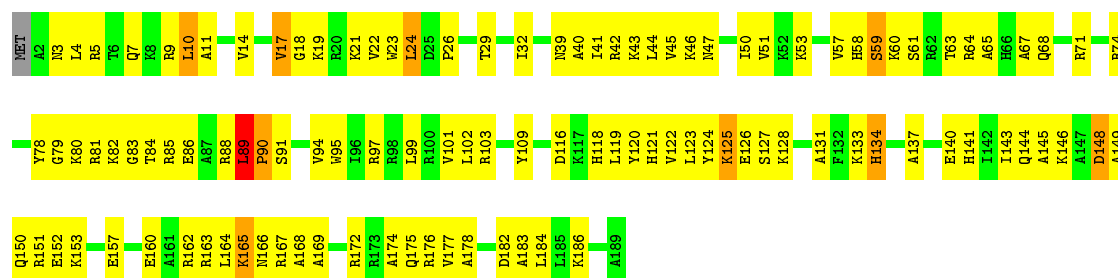
• Molecule 22: eL18 (yeast L18)

Chain V: 29% 60% 11% .

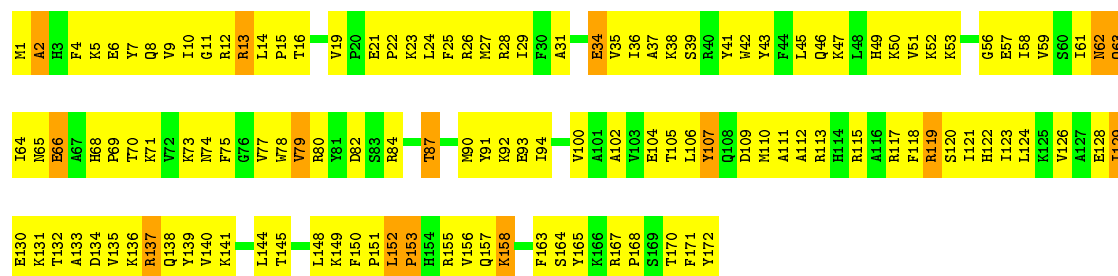
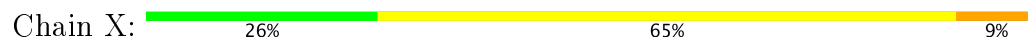


• Molecule 23: eL19 (yeast L19)

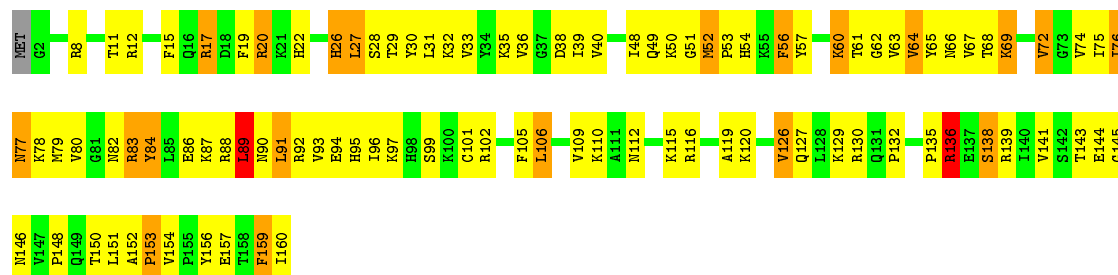
Chain W: 41% 53% 5% ..



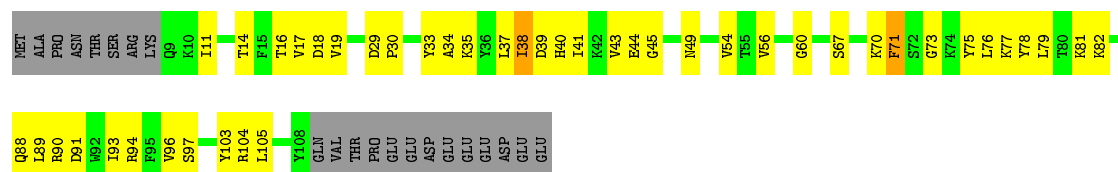
• Molecule 24: eL20 (yeast L20)



• Molecule 25: eL21 (yeast L21)



• Molecule 26: eL22 (yeast L22)



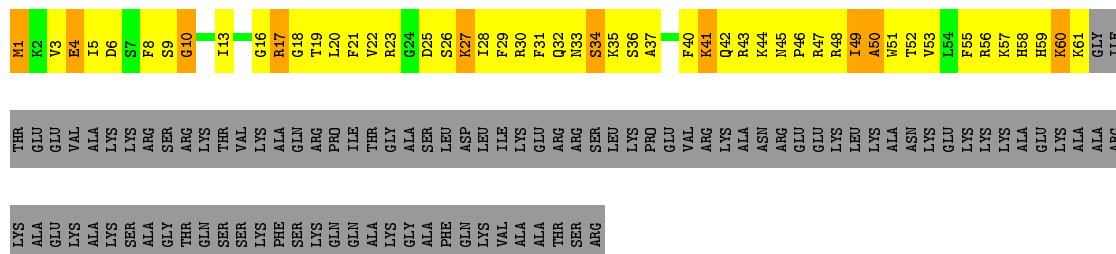
• Molecule 27: uL14 (yeast L23)

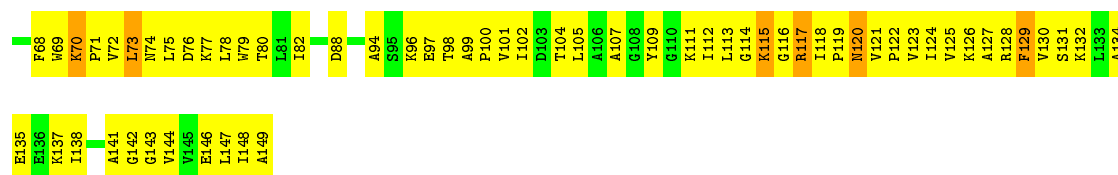




• Molecule 28: eL24 (yeast L24)

Chain BA: 6% 26% 6% 61%





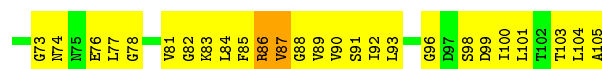
- Molecule 33: eL29 (yeast L29)

Chain GA: 49% 46%



- Molecule 34: eL30 (yeast L30)

Chain HA: 29% 60% 8%



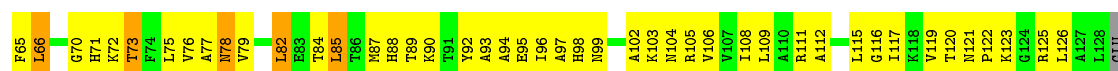
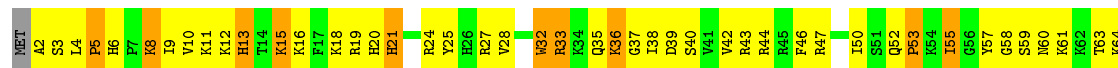
- Molecule 35: eL31 (yeast L31)

Chain IA: 39% 51% 6%



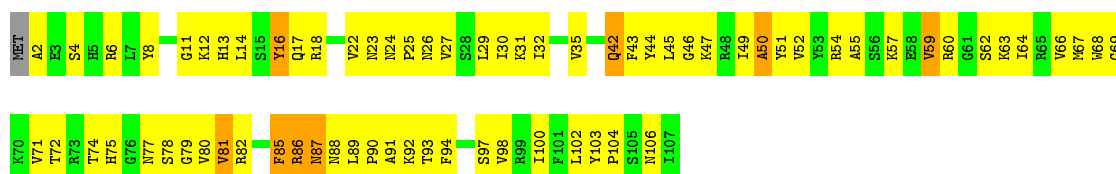
- Molecule 36: eL32 (yeast L32)

Chain JA: 28% 58% 12%

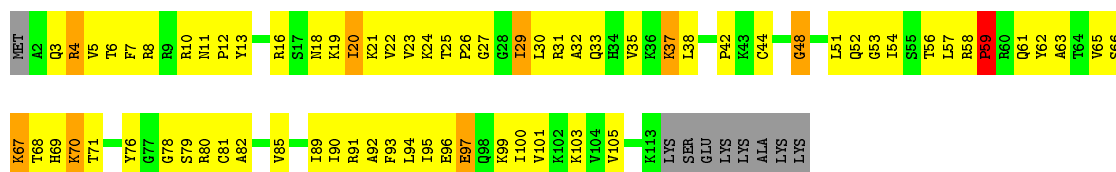


- Molecule 37: eL33 (yeast L33)

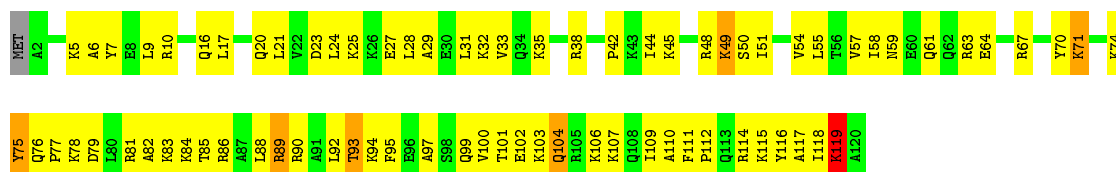
Chain KA: 33% 59% 7%



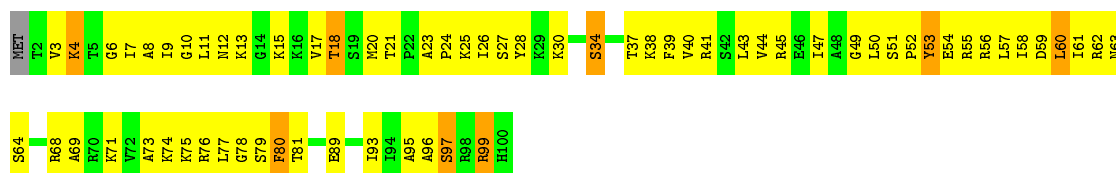
- Molecule 38: eL34 (yeast L34)



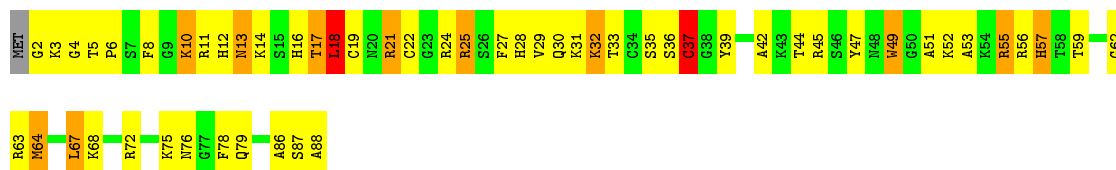
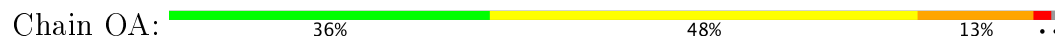
- Molecule 39: uL29 (yeast L35)



- Molecule 40: eL36 (yeast L36)

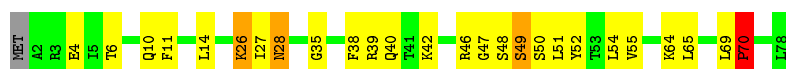


- Molecule 41: eL37 (yeast L37)



- Molecule 42: eL38 (yeast L38)

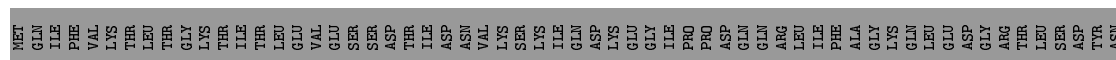




- Molecule 43: eL39 (yeast L39)



- Molecule 44: eL40 (yeast L40)



- Molecule 45: eL41 (yeast L41)



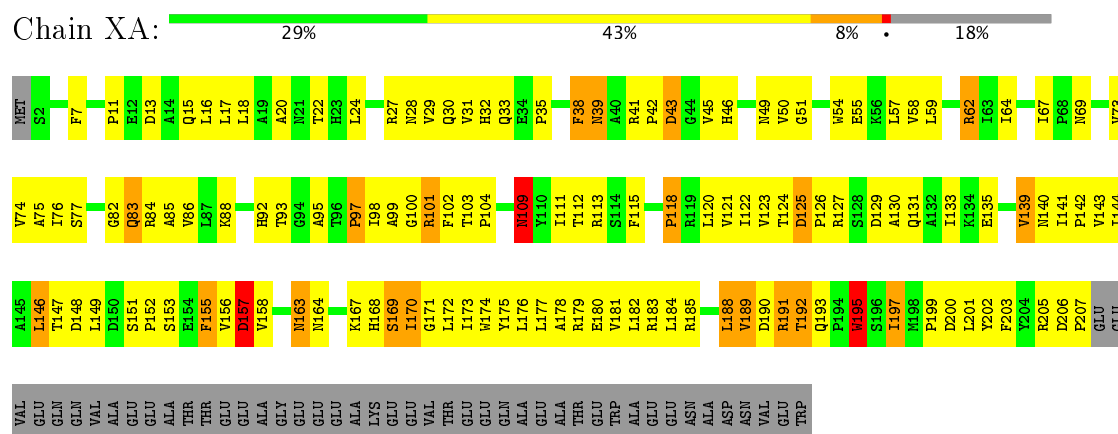
- Molecule 46: eL42 (yeast L42)



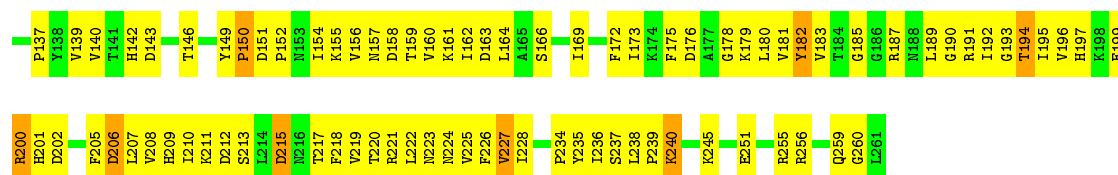
- Molecule 47: eL43 (yeast L43)



- Molecule 48: uL10 (yeast P0)

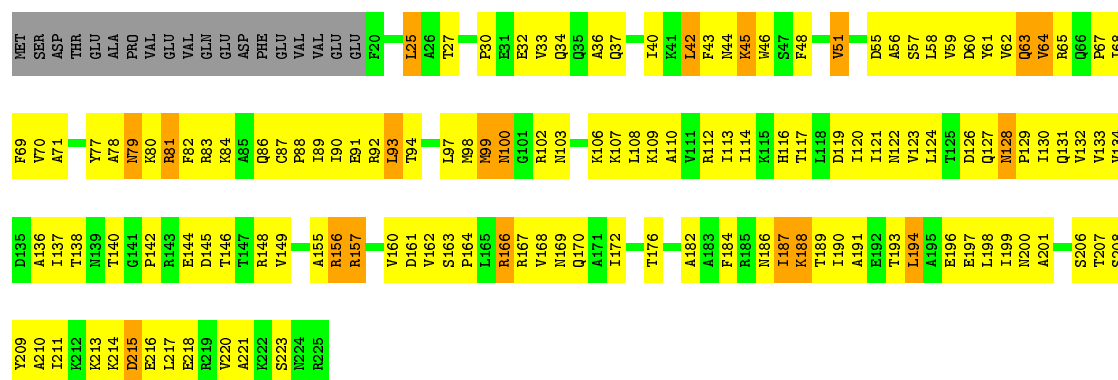


- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Q67 | R68 | H69 | V70 | V72 | D73 | G74 | G75 | V76 | K77 | T80 | T81 | T82 | D93 | A94 | T95 | N96 | E97 | N98 | F99 | R100 | L101 | V102 | I103 | D104 | V105 | K106 | G107 | R108 | R113 | I114 | E118 | A119 | S120 | I121 | K122 | L123 | L126 | V127 | K128 | V129 | Q130 | L131 | G132 | K133 | K134 | | | | | | | | | |
| MET | A3 | R3 | K6 | K7 | H8 | L9 | K10 | R11 | L12 | P15 | H16 | H17 | M18 | L19 | L20 | D21 | K22 | L23 | C26 | Z27 | A28 | P29 | P31 | S32 | A33 | G34 | P35 | H36 | L38 | R39 | E40 | S41 | L42 | P43 | L44 | I46 | V46 | F47 | L48 | R49 | N50 | R51 | L52 | K53 | Y54 | A55 | L56 | V61 | K62 | A63 | I64 | L65 | L66 | L66 |



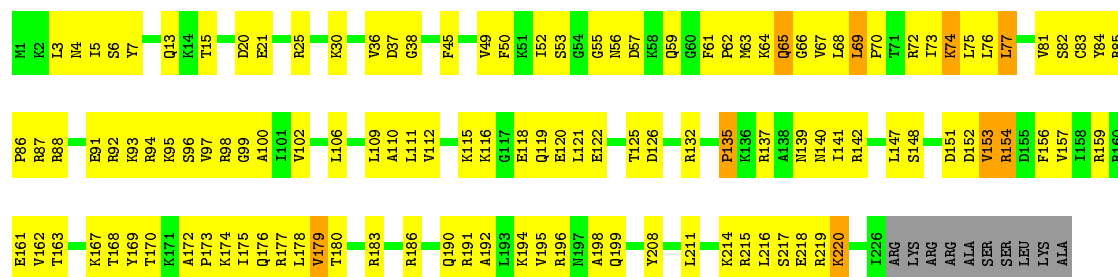
• Molecule 55: uS7 (yeast S5)

Chain CB:



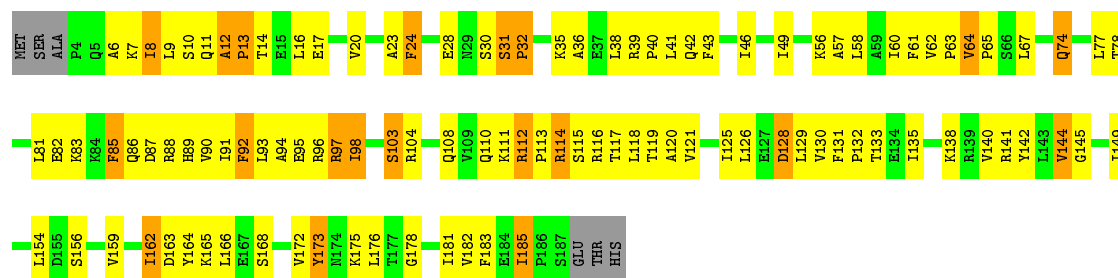
• Molecule 56: eS6 (yeast S6)

Chain DB:



• Molecule 57: eS7 (yeast S7)

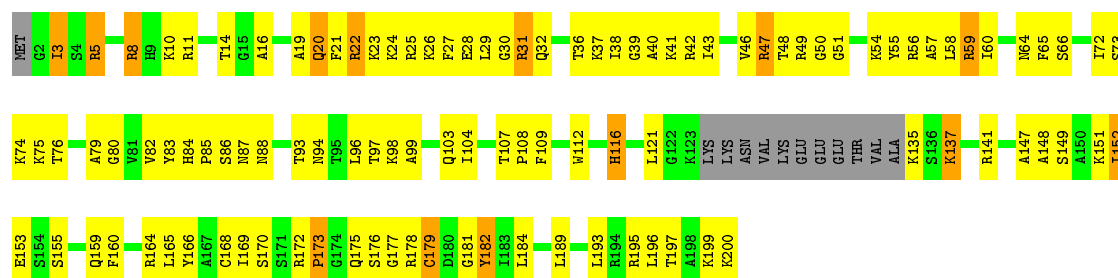
Chain EB:



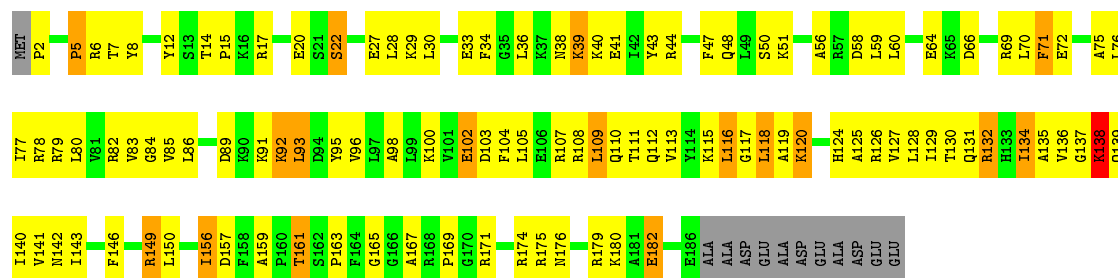
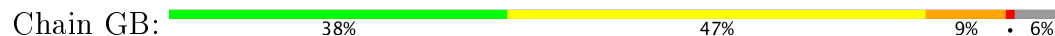
• Molecule 58: eS8 (yeast S8)

Chain FB:

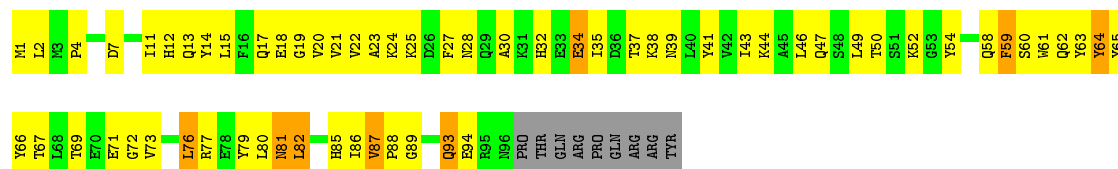




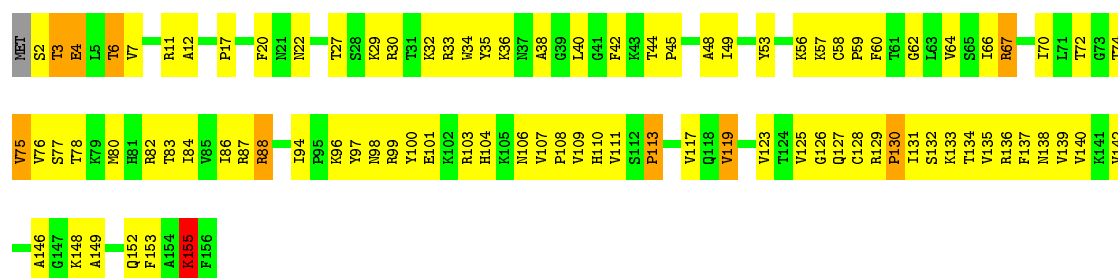
- Molecule 59: uS4 (yeast S9)



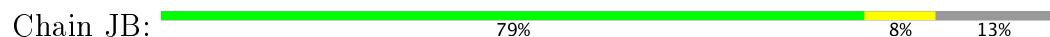
- Molecule 60: eS10 (yeast S10)



- Molecule 61: uS17 (yeast S11)

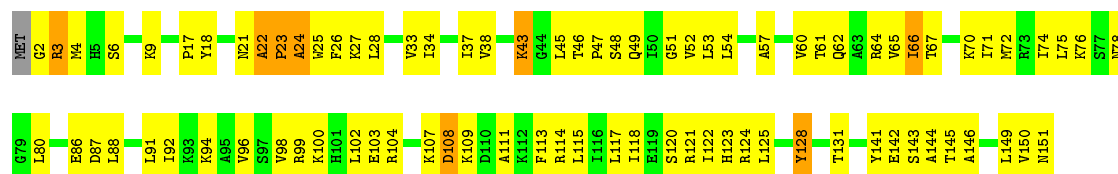


- Molecule 62: eS12 (yeast S12)




- Molecule 63: uS15 (yeast S13)

Chain KB: 



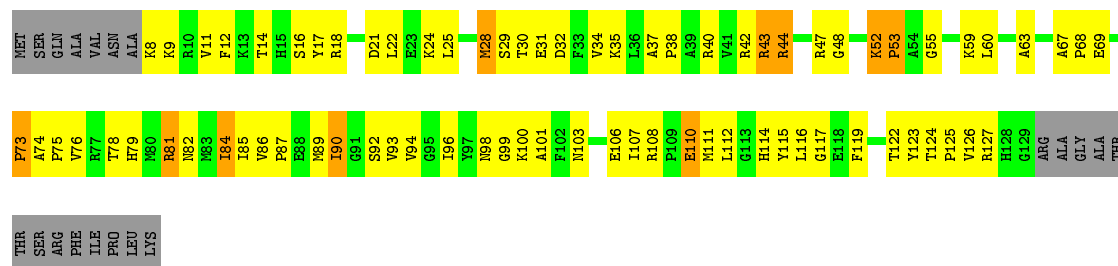
- Molecule 64: uS11 (yeast S14)

Chain LB: 



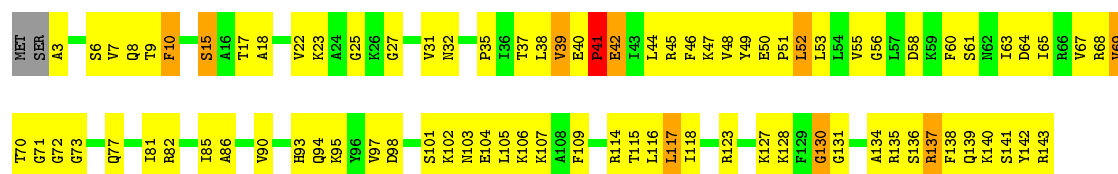
- Molecule 65: uS19 (yeast S15)

Chain MB: 



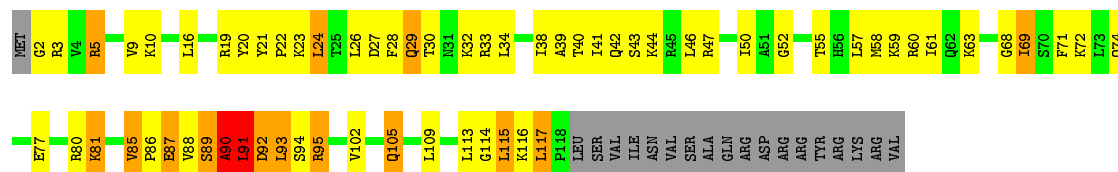
- Molecule 66: uS9 (yeast S16)

Chain NB: 

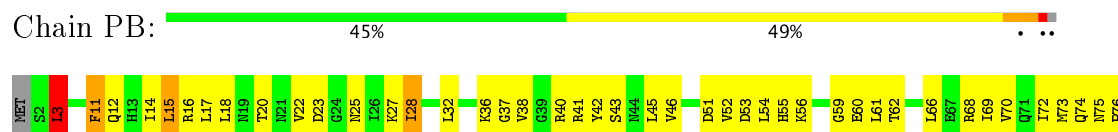


- Molecule 67: eS17 (yeast S17)

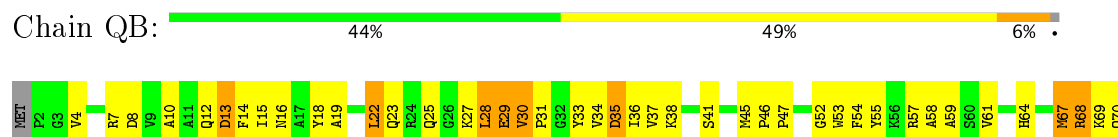
Chain OB: 



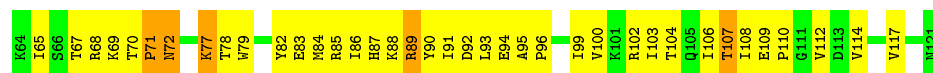
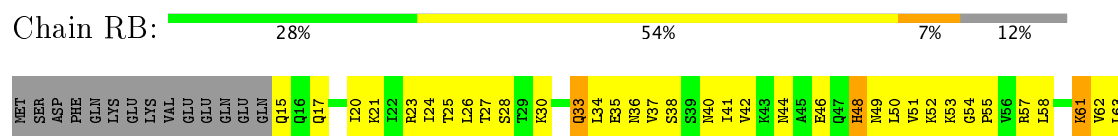
- Molecule 68: uS13 (yeast S18)



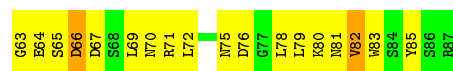
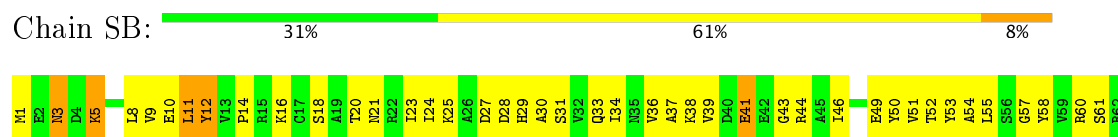
• Molecule 69: eS19 (yeast S19)



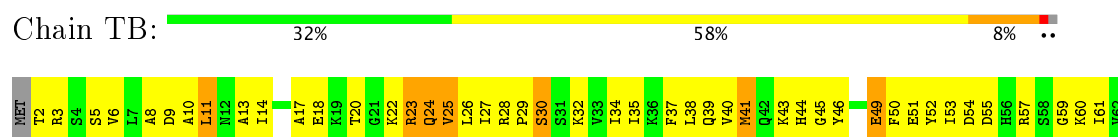
• Molecule 70: uS10 (yeast S20)



• Molecule 71: eS21 (yeast S21)

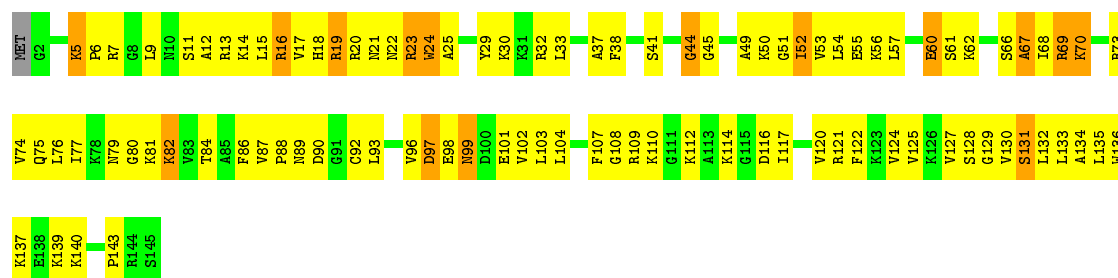


• Molecule 72: uS8 (yeast S22)



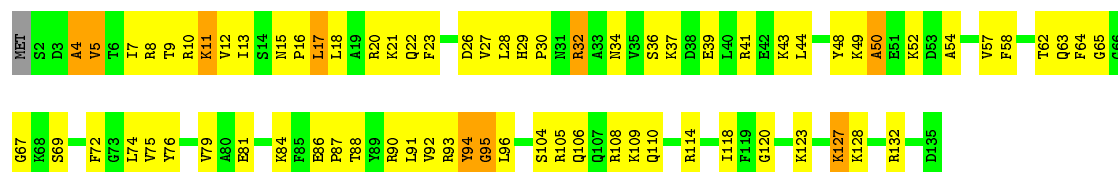
• Molecule 73: uS12 (yeast S23)





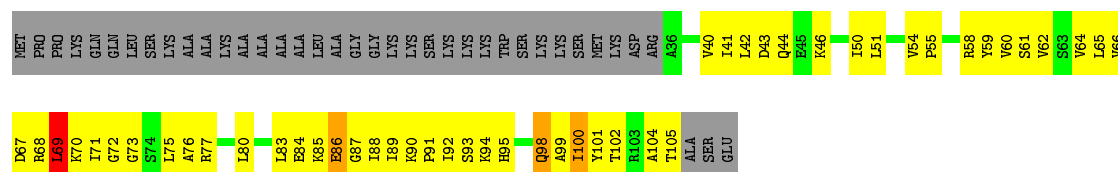
- Molecule 74: eS24 (yeast S24)

Chain VB: 45% 47% 7% .



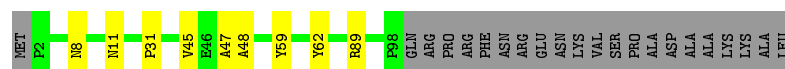
- Molecule 75: eS25 (yeast S25)

Chain WB: 19% 42% 35% . .



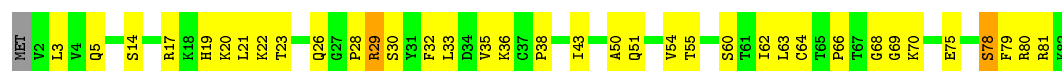
- Molecule 76: eS26 (yeast S26)

Chain XB: 74% 8% 18%



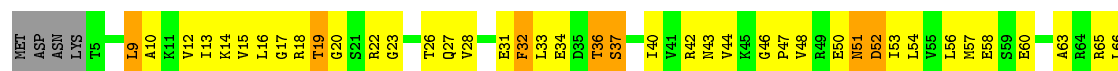
- Molecule 77: eS27 (yeast S27)

Chain YB: 55% 41% . .



- Molecule 78: eS28 (yeast S28)

Chain ZB: 33% 51% 10% 6%



R67

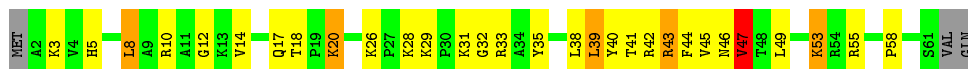
- Molecule 79: uS14 (yeast S29)

Chain AC:  48% 45% 5%



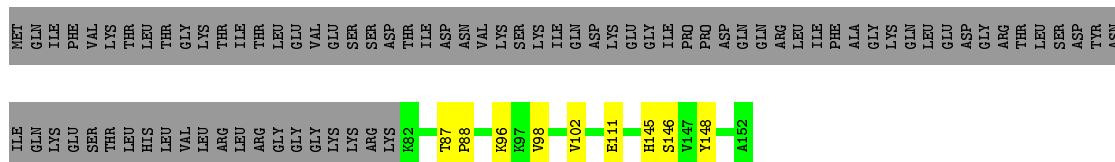
- Molecule 80: eS30 (yeast S30)

Chain BC:  48% 38% 8% 5%

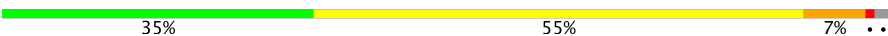


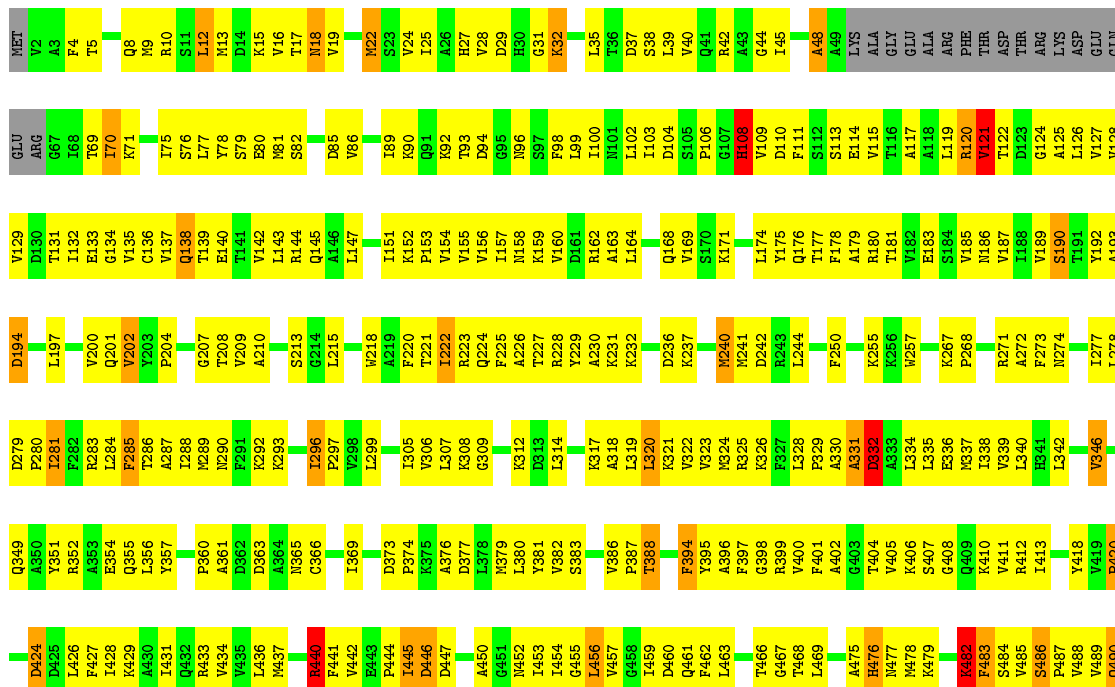
- Molecule 81: eS31 (yeast S31)

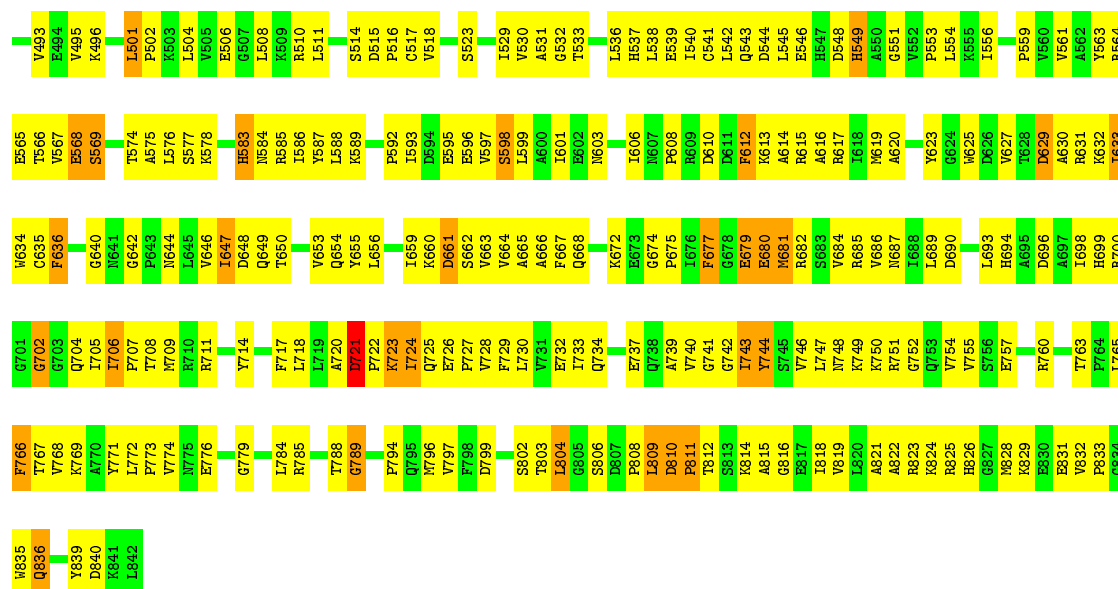
Chain CC:  41% 6% 53%



- Molecule 82: yeast eEF2

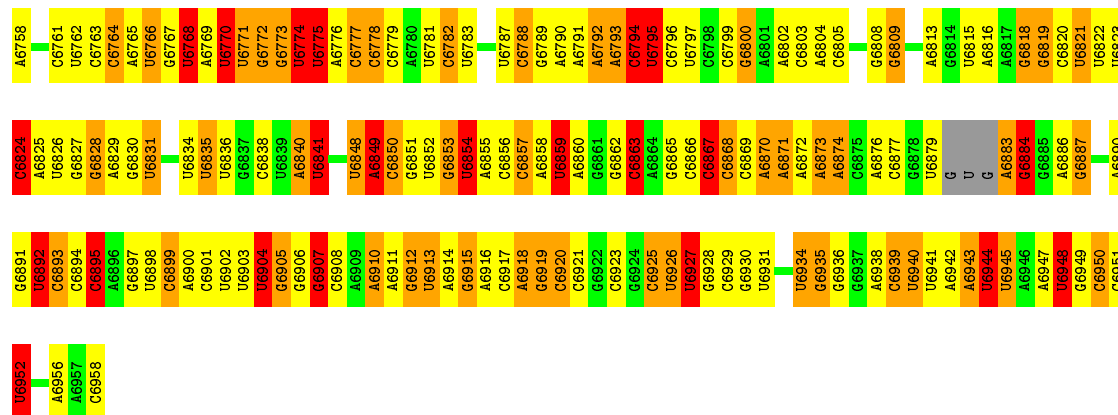
Chain DC:  35% 55% 7% ..





• Molecule 83: IRES

Chain EC: 22% 41% 25% 11% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	38054	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
2	B	0	72
3	C	0	6
4	D	0	2
50	XA	0	1
83	EC	0	5
All	All	0	100

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

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

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

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

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	U	Sidechain
1	A	324	U	Sidechain
1	A	447	U	Sidechain
1	A	53	G	Sidechain
1	A	568	G	Sidechain

5.2 Too-close contacts

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 12389 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:KA:67:MET:CE	37:KA:67:MET:SD	2.03	1.47
66:NB:93:HIS:HA	66:NB:97:VAL:HB	1.20	1.19
2:B:1494:U:H4'	2:B:1495:U:H5'	1.24	1.14
2:B:2954:U:H4'	2:B:2955:U:H5'	1.26	1.13
2:B:1719:G:H4'	2:B:1732:U:H4'	1.30	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	165/217 (76%)	129 (78%)	26 (16%)	10 (6%)	2	24
6	F	250/254 (98%)	177 (71%)	56 (22%)	17 (7%)	1	21
7	G	384/387 (99%)	293 (76%)	70 (18%)	21 (6%)	2	26
8	H	359/362 (99%)	259 (72%)	77 (21%)	23 (6%)	1	23
9	I	294/297 (99%)	226 (77%)	49 (17%)	19 (6%)	1	23
10	J	173/176 (98%)	125 (72%)	33 (19%)	15 (9%)	1	16
11	K	220/244 (90%)	165 (75%)	39 (18%)	16 (7%)	1	19
12	L	231/256 (90%)	180 (78%)	38 (16%)	13 (6%)	2	26
13	M	189/191 (99%)	150 (79%)	36 (19%)	3 (2%)	11	52
14	N	207/221 (94%)	169 (82%)	28 (14%)	10 (5%)	2	29
15	O	167/174 (96%)	128 (77%)	31 (19%)	8 (5%)	2	29
16	P	92/165 (56%)	62 (67%)	20 (22%)	10 (11%)	0	10
17	Q	191/199 (96%)	144 (75%)	35 (18%)	12 (6%)	1	23
18	R	134/138 (97%)	103 (77%)	23 (17%)	8 (6%)	2	24
19	S	201/204 (98%)	144 (72%)	46 (23%)	11 (6%)	2	26
20	T	195/199 (98%)	160 (82%)	27 (14%)	8 (4%)	3	32
21	U	181/184 (98%)	133 (74%)	35 (19%)	13 (7%)	1	20
22	V	183/186 (98%)	131 (72%)	39 (21%)	13 (7%)	1	20
23	W	186/189 (98%)	162 (87%)	19 (10%)	5 (3%)	6	42
24	X	170/172 (99%)	130 (76%)	31 (18%)	9 (5%)	2	27
25	Y	157/160 (98%)	124 (79%)	25 (16%)	8 (5%)	2	27
26	Z	98/121 (81%)	69 (70%)	23 (24%)	6 (6%)	2	24
27	AA	134/137 (98%)	107 (80%)	24 (18%)	3 (2%)	8	46
28	BA	59/155 (38%)	43 (73%)	11 (19%)	5 (8%)	1	16
29	CA	119/142 (84%)	84 (71%)	29 (24%)	6 (5%)	2	28
30	DA	124/127 (98%)	89 (72%)	28 (23%)	7 (6%)	2	26
31	EA	133/136 (98%)	108 (81%)	19 (14%)	6 (4%)	3	30
32	FA	146/149 (98%)	106 (73%)	31 (21%)	9 (6%)	2	24
33	GA	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
34	HA	95/105 (90%)	80 (84%)	13 (14%)	2 (2%)	8	47

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	NB	139/143 (97%)	108 (78%)	24 (17%)	7 (5%)	2	28
67	OB	115/136 (85%)	79 (69%)	24 (21%)	12 (10%)	0	11
68	PB	143/146 (98%)	111 (78%)	24 (17%)	8 (6%)	2	26
69	QB	141/144 (98%)	122 (86%)	16 (11%)	3 (2%)	8	47
70	RB	105/121 (87%)	85 (81%)	15 (14%)	5 (5%)	2	29
71	SB	85/87 (98%)	63 (74%)	17 (20%)	5 (6%)	2	24
72	TB	127/130 (98%)	99 (78%)	24 (19%)	4 (3%)	5	39
73	UB	142/145 (98%)	108 (76%)	22 (16%)	12 (8%)	1	16
74	VB	132/135 (98%)	105 (80%)	20 (15%)	7 (5%)	2	27
75	WB	68/108 (63%)	47 (69%)	17 (25%)	4 (6%)	2	24
76	XB	95/119 (80%)	54 (57%)	32 (34%)	9 (10%)	1	14
77	YB	79/82 (96%)	59 (75%)	17 (22%)	3 (4%)	4	34
78	ZB	61/67 (91%)	43 (70%)	15 (25%)	3 (5%)	2	28
79	AC	51/56 (91%)	39 (76%)	11 (22%)	1 (2%)	9	48
80	BC	58/63 (92%)	38 (66%)	16 (28%)	4 (7%)	1	20
81	CC	69/152 (45%)	42 (61%)	18 (26%)	9 (13%)	0	6
82	DC	819/842 (97%)	646 (79%)	137 (17%)	36 (4%)	3	31
All	All	12207/13416 (91%)	9316 (76%)	2192 (18%)	699 (6%)	4	25

5 of 699 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	157/198 (79%)	136 (87%)	21 (13%)	4	27
6	F	194/196 (99%)	172 (89%)	22 (11%)	7	32
7	G	322/323 (100%)	295 (92%)	27 (8%)	13	46
8	H	288/289 (100%)	249 (86%)	39 (14%)	4	26
9	I	244/245 (100%)	220 (90%)	24 (10%)	9	38
10	J	152/153 (99%)	141 (93%)	11 (7%)	17	52
11	K	186/205 (91%)	165 (89%)	21 (11%)	7	32
12	L	191/208 (92%)	169 (88%)	22 (12%)	6	31
13	M	171/171 (100%)	154 (90%)	17 (10%)	9	37
14	N	180/187 (96%)	161 (89%)	19 (11%)	8	35
15	O	147/150 (98%)	134 (91%)	13 (9%)	12	43
16	P	81/136 (60%)	70 (86%)	11 (14%)	4	26
17	Q	154/159 (97%)	136 (88%)	18 (12%)	6	31
18	R	107/109 (98%)	96 (90%)	11 (10%)	8	36
19	S	175/176 (99%)	150 (86%)	25 (14%)	4	25
20	T	160/162 (99%)	141 (88%)	19 (12%)	6	30
21	U	145/146 (99%)	122 (84%)	23 (16%)	3	20
22	V	150/151 (99%)	134 (89%)	16 (11%)	8	35
23	W	153/154 (99%)	138 (90%)	15 (10%)	9	38
24	X	156/156 (100%)	141 (90%)	15 (10%)	10	39
25	Y	136/137 (99%)	114 (84%)	22 (16%)	3	20
26	Z	87/107 (81%)	85 (98%)	2 (2%)	56	79
27	AA	104/105 (99%)	93 (89%)	11 (11%)	8	35
28	BA	54/129 (42%)	45 (83%)	9 (17%)	2	18
29	CA	105/118 (89%)	97 (92%)	8 (8%)	15	50
30	DA	109/110 (99%)	94 (86%)	15 (14%)	4	26
31	EA	115/116 (99%)	105 (91%)	10 (9%)	12	43
32	FA	118/119 (99%)	105 (89%)	13 (11%)	7	33
33	GA	46/47 (98%)	42 (91%)	4 (9%)	12	43
34	HA	81/88 (92%)	75 (93%)	6 (7%)	16	51
35	IA	96/97 (99%)	89 (93%)	7 (7%)	16	51
36	JA	109/111 (98%)	100 (92%)	9 (8%)	13	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	KA	90/91 (99%)	80 (89%)	10 (11%)	7	33
38	LA	95/103 (92%)	90 (95%)	5 (5%)	26	61
39	MA	104/105 (99%)	96 (92%)	8 (8%)	15	50
40	NA	81/82 (99%)	75 (93%)	6 (7%)	16	51
41	OA	70/71 (99%)	60 (86%)	10 (14%)	4	25
42	PA	68/69 (99%)	63 (93%)	5 (7%)	16	51
43	QA	45/46 (98%)	39 (87%)	6 (13%)	4	27
44	RA	47/116 (40%)	44 (94%)	3 (6%)	20	55
45	SA	23/23 (100%)	20 (87%)	3 (13%)	5	28
46	TA	90/91 (99%)	80 (89%)	10 (11%)	7	33
47	UA	71/72 (99%)	65 (92%)	6 (8%)	12	46
48	VA	160/254 (63%)	147 (92%)	13 (8%)	14	47
49	WA	261/262 (100%)	246 (94%)	15 (6%)	24	59
50	XA	173/210 (82%)	155 (90%)	18 (10%)	8	35
52	ZA	176/205 (86%)	170 (97%)	6 (3%)	42	72
53	AB	182/195 (93%)	167 (92%)	15 (8%)	13	47
54	BB	221/222 (100%)	202 (91%)	19 (9%)	12	45
55	CB	173/191 (91%)	162 (94%)	11 (6%)	20	55
56	DB	193/201 (96%)	187 (97%)	6 (3%)	45	73
57	EB	165/170 (97%)	157 (95%)	8 (5%)	30	64
58	FB	150/161 (93%)	141 (94%)	9 (6%)	22	58
59	GB	158/166 (95%)	143 (90%)	15 (10%)	10	39
60	HB	89/98 (91%)	83 (93%)	6 (7%)	19	54
61	IB	136/137 (99%)	127 (93%)	9 (7%)	19	54
63	KB	127/128 (99%)	119 (94%)	8 (6%)	21	56
65	MB	103/118 (87%)	98 (95%)	5 (5%)	29	63
66	NB	117/119 (98%)	108 (92%)	9 (8%)	15	50
67	OB	82/124 (66%)	77 (94%)	5 (6%)	22	57
68	PB	128/129 (99%)	116 (91%)	12 (9%)	10	40
69	QB	115/116 (99%)	105 (91%)	10 (9%)	12	43
70	RB	100/114 (88%)	90 (90%)	10 (10%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	SB	74/74 (100%)	66 (89%)	8 (11%)	7	34
72	TB	110/111 (99%)	99 (90%)	11 (10%)	9	37
73	UB	119/120 (99%)	110 (92%)	9 (8%)	15	50
74	VB	112/113 (99%)	103 (92%)	9 (8%)	14	48
75	WB	61/89 (68%)	56 (92%)	5 (8%)	13	47
77	YB	70/71 (99%)	69 (99%)	1 (1%)	71	87
78	ZB	56/60 (93%)	49 (88%)	7 (12%)	5	29
79	AC	47/49 (96%)	44 (94%)	3 (6%)	20	55
80	BC	51/54 (94%)	45 (88%)	6 (12%)	6	31
82	DC	699/714 (98%)	641 (92%)	58 (8%)	13	46
All	All	9865/10602 (93%)	8962 (91%)	903 (9%)	15	41

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

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

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

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

5.3.3 RNA ⓘ

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

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

5 of 1062 RNA backbone outliers are listed below:

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

5 of 40 RNA pucker outliers are listed below:

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

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	DDE	DC	699	82	15,20,21	2.73	7 (46%)	15,28,30	1.82	5 (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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	DC	699	DDE	CB-CA	2.08	1.58	1.53
82	DC	699	DDE	CD2-NE2	2.11	1.39	1.36
82	DC	699	DDE	OAG-CBI	2.25	1.28	1.23
82	DC	699	DDE	CB-CG	2.28	1.59	1.51
82	DC	699	DDE	CAT-CE1	4.33	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	DC	699	DDE	OAG-CBI-CBW	-4.00	115.72	120.64
82	DC	699	DDE	CAU-CBW-CBI	-2.78	105.65	111.12
82	DC	699	DDE	CG-CD2-NE2	-2.13	104.86	109.25
82	DC	699	DDE	CB-CA-C	2.20	115.65	111.41
82	DC	699	DDE	OAG-CBI-NAD	2.44	126.80	123.06

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	25,30,30	2.31	9 (36%)	26,47,47	2.03	6 (23%)
86	SO1	DC	903	-	34,39,39	2.94	21 (61%)	35,64,64	2.00	7 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	GDP	DC	901	85	-	0/12/32/32	0/3/3/3
86	SO1	DC	903	-	-	0/15/104/104	0/2/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	903	SO1	O56-C52	-3.79	1.32	1.41
86	DC	903	SO1	C61-C56	2.02	1.56	1.51
86	DC	903	SO1	C24-C18	2.05	1.59	1.54
86	DC	903	SO1	C7-C16	2.11	1.56	1.53
86	DC	903	SO1	C54-C55	2.13	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	DC	903	SO1	C12-C6-C10	-6.82	102.42	107.70
84	DC	901	GDP	N3-C2-N1	-4.58	120.76	127.46
84	DC	901	GDP	C5-C6-N1	-3.50	118.50	123.48
86	DC	903	SO1	C18-C9-C16	-3.36	98.83	103.64
86	DC	903	SO1	C7-C2-C8	-3.35	103.97	110.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.