



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:46 am BST

PDB ID : 6GSL
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Arg} in the A-site
Authors : Rozov, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2018-06-14
Resolution : 3.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

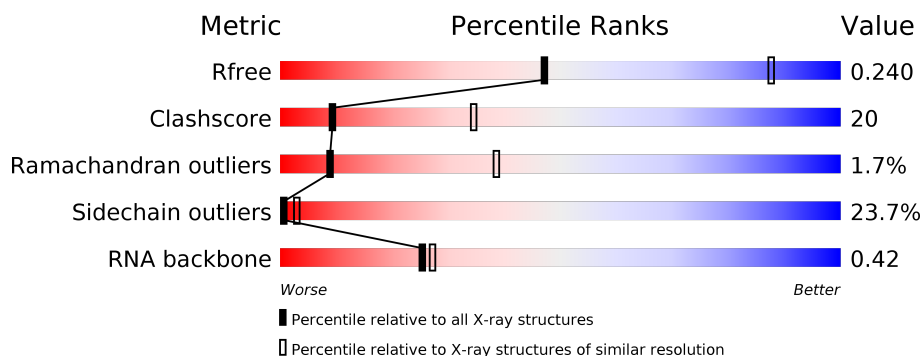
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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.





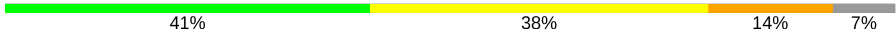



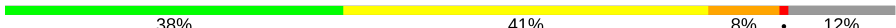


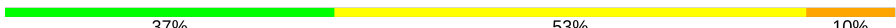
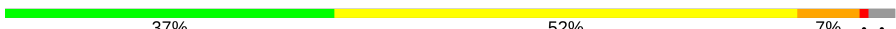
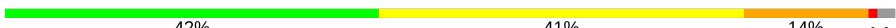
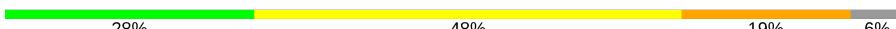





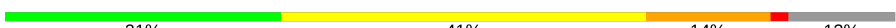
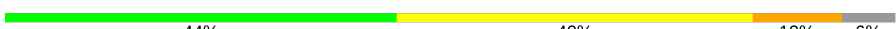
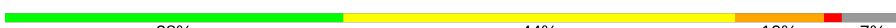




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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

Mol	Chain	Length	Quality of chain
1	13	1522	28% (green) 45% (yellow) 22% (orange) . . (red)
1	1G	1522	33% (green) 45% (yellow) 19% (orange) . . (red)
2	12	256	30% (green) 46% (yellow) 14% (orange) . 7% (grey)
2	1E	256	28% (green) 48% (yellow) 13% (orange) . 10% (grey)
3	22	239	38% (green) 34% (yellow) 9% (orange) 18% (grey)
3	2E	239	48% (green) 32% (yellow) 6% (orange) 14% (grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	
15	6I	89	
16	7A	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	77	
22	1L	77	
23	2K	77	
23	2L	77	
24	3K	77	
24	3L	77	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	71	229	
28	79	229	

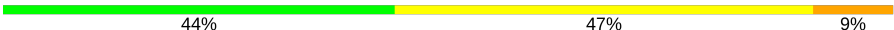
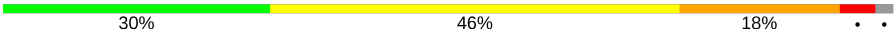
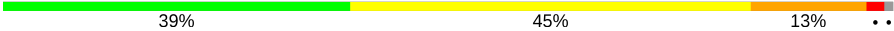













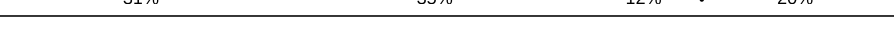

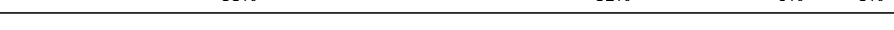
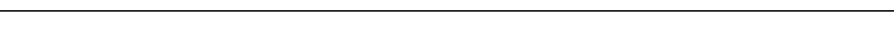
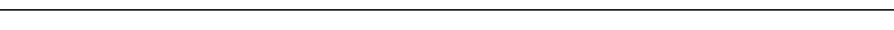
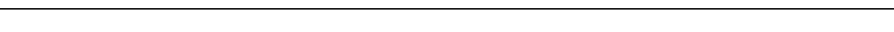
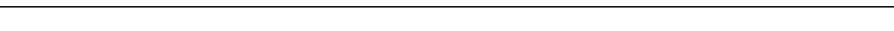
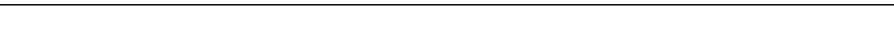

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	18	125	
34	28	125	
35	61	148	
35	69	148	
36	38	173	
37	48	147	
38	15	140	
38	58	140	
39	25	122	
39	68	122	
40	35	150	
40	78	150	
41	45	141	
41	88	141	
42	55	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	98	118	
43	65	112	
43	A8	112	
44	75	146	
44	B8	146	
45	85	118	
45	C8	118	
46	95	101	
46	D8	101	
47	A5	113	
47	E8	113	
48	B5	96	
48	F8	96	
49	C5	110	
49	G8	110	
50	D5	206	
50	H8	206	
51	E5	85	
51	I8	85	
52	F5	98	
52	J8	98	
53	G5	72	
53	K8	72	
54	H5	60	
54	L8	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	M8	71	
56	J5	60	
56	N8	60	
57	O8	54	
58	L5	49	
58	P8	49	
59	M5	65	
59	Q8	65	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	SF4	32	303	-	-	X	-
61	SF4	3E	303	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1512	Total	C	N	O	P	0	0	0
			32497	14464	6017	10504	1512			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1533	969	297	266	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1690	1058	336	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				
9	82	124	Total	C	N	O		0	0	0
			983	624	190	169				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			936	579	191	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			887	549	180	156	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			499	317	105	72	5			
14	5A	57	Total	C	N	O	S	0	0	0
			466	297	97	68	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	67	Total	C	N	O	0	0	0
			544	349	104	91			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	80	Total	C	N	O	S	0	0	0
			643	411	118	112	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	98	Total	C	N	O	S	0	0	0
			751	464	158	127	2			
20	BA	98	Total	C	N	O	S	0	0	0
			757	467	161	127	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	1B	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called tRNAArg.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1544	690	282	498	72	2			
22	1L	74	Total	C	N	O	P	S	0	0	0
			1584	708	287	513	74	2			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNAArg.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	73	Total	C	N	O	P	0	0	0
			1561	696	285	507	73			
24	3L	74	Total	C	N	O	P	0	0	0
			1581	705	287	515	74			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3K	6	U	C	conflict	GB 1387059712
3L	6	U	C	conflict	GB 1387059712

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			462	207	97	137	21			
25	4L	17	Total	C	N	O	P	0	0	0
			374	167	77	113	17			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2895	Total	C	N	O	P	0	0	0
			62351	27751	11658	20047	2895			
26	14	2895	Total	C	N	O	P	0	0	0
			62347	27751	11660	20042	2894			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	134	Total	C	N	O	S	0	0	0
			1043	659	196	187	1			
28	79	130	Total	C	N	O	S	0	0	0
			1010	637	188	184	1			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	206	Total	C	N	O	S	0	0	0
			1610	1026	301	281	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			

- Molecule 34 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	18	30	Total	C	N	O	S	0	0	0
			237	150	38	48	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	28	30	Total	C	N	O	S	0	0	0
			237	150	38	48	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
35	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 36 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	38	143	Total	C	N	O	S	0	0	0
			1089	694	191	202	2			

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	48	142	Total	C	N	O	S	0	0	0
			1047	665	184	193	5			

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
38	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
39	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
40	35	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	187	7			
41	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
42	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
43	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B8	136	Total	C	N	O	S	0	0	0
			1132	704	232	195	1			
44	75	134	Total	C	N	O		0	0	0
			1115	694	229	192				

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
46	95	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
47	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
48	B5	94	Total	C	N	O	S	0	0	0
			738	479	133	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	G8	105	Total	C	N	O	S	0	0	0
			784	504	147	128	5			
49	C5	106	Total	C	N	O	S	0	0	0
			785	504	147	129	5			

- Molecule 50 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	H8	165	Total	C	N	O	S	0	0	0
			1330	851	241	236	2			
50	D5	200	Total	C	N	O	S	0	0	0
			1582	1008	279	292	3			

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	I8	81	Total	C	N	O	S	0	0	0
			630	389	133	107	1			
51	E5	78	Total	C	N	O	S	0	0	0
			616	381	130	104	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	J8	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			
52	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	K8	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			
53	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 54 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			
54	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M8	48	Total	C	N	O	S	0	0	0
			371	237	62	67	5			

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N8	50	Total	C	N	O	S	0	0	0
			386	241	77	63	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 57 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 58 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
58	L5	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 59 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
59	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	98	2	Total	Mg	0	0
			2	2		
60	45	2	Total	Mg	0	0
			2	2		
60	P8	1	Total	Mg	0	0
			1	1		
60	6I	1	Total	Mg	0	0
			1	1		
60	C5	1	Total	Mg	0	0
			1	1		
60	13	227	Total	Mg	0	0
			227	227		
60	1J	8	Total	Mg	0	0
			8	8		

Continued on next page...

Continued from previous page...

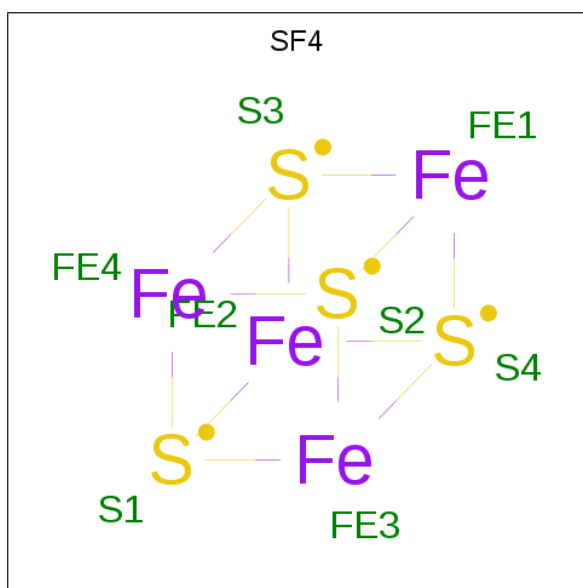
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	35	1	Total 1	Mg 1	0	0
60	4L	2	Total 2	Mg 2	0	0
60	16	20	Total 20	Mg 20	0	0
60	25	2	Total 2	Mg 2	0	0
60	M5	1	Total 1	Mg 1	0	0
60	21	2	Total 2	Mg 2	0	0
60	31	2	Total 2	Mg 2	0	0
60	Q8	1	Total 1	Mg 1	0	0
60	75	1	Total 1	Mg 1	0	0
60	I8	2	Total 2	Mg 2	0	0
60	32	2	Total 2	Mg 2	0	0
60	52	1	Total 1	Mg 1	0	0
60	2A	1	Total 1	Mg 1	0	0
60	5E	2	Total 2	Mg 2	0	0
60	29	5	Total 5	Mg 5	0	0
60	2K	7	Total 7	Mg 7	0	0
60	1L	1	Total 1	Mg 1	0	0
60	39	2	Total 2	Mg 2	0	0
60	1G	167	Total 167	Mg 167	0	0
60	11	6	Total 6	Mg 6	0	0
60	1H	669	Total 669	Mg 669	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	F5	1	Total 1	Mg 1	0	0
60	E5	1	Total 1	Mg 1	0	0
60	88	4	Total 4	Mg 4	0	0
60	N8	1	Total 1	Mg 1	0	0
60	14	607	Total 607	Mg 607	0	0
60	78	1	Total 1	Mg 1	0	0
60	3E	2	Total 2	Mg 2	0	0
60	55	2	Total 2	Mg 2	0	0
60	4K	1	Total 1	Mg 1	0	0
60	1K	2	Total 2	Mg 2	0	0
60	41	1	Total 1	Mg 1	0	0
60	2L	2	Total 2	Mg 2	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	3E	1	Total	Fe	S	0	0
			8	4	4		
61	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	5A	1	Total	Zn	0	0
			1	1		
62	5I	1	Total	Zn	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	13	544	Total	O	0	0
			544	544		
63	1E	1	Total	O	0	0
			1	1		
63	3E	1	Total	O	0	0
			1	1		
63	4E	2	Total	O	0	0
			2	2		
63	8E	1	Total	O	0	0
			1	1		
63	1I	1	Total	O	0	0
			1	1		
63	3I	5	Total	O	0	0
			5	5		
63	5I	3	Total	O	0	0
			3	3		
63	6I	4	Total	O	0	0
			4	4		
63	BI	1	Total	O	0	0
			1	1		
63	1F	1	Total	O	0	0
			1	1		
63	1K	1	Total	O	0	0
			1	1		
63	2K	16	Total	O	0	0
			16	16		
63	4K	13	Total	O	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1H	1966	Total 1966	O 1966	0	0
63	16	42	Total 42	O 42	0	0
63	11	12	Total 12	O 12	0	0
63	21	9	Total 9	O 9	0	0
63	31	8	Total 8	O 8	0	0
63	58	3	Total 3	O 3	0	0
63	78	10	Total 10	O 10	0	0
63	88	7	Total 7	O 7	0	0
63	98	1	Total 1	O 1	0	0
63	A8	2	Total 2	O 2	0	0
63	B8	3	Total 3	O 3	0	0
63	C8	7	Total 7	O 7	0	0
63	D8	1	Total 1	O 1	0	0
63	F8	1	Total 1	O 1	0	0
63	G8	3	Total 3	O 3	0	0
63	I8	5	Total 5	O 5	0	0
63	J8	10	Total 10	O 10	0	0
63	L8	4	Total 4	O 4	0	0
63	P8	1	Total 1	O 1	0	0
63	Q8	7	Total 7	O 7	0	0
63	1G	397	Total 397	O 397	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	32	5	Total 5	O 5	0	0
63	42	1	Total 1	O 1	0	0
63	52	4	Total 4	O 4	0	0
63	3A	2	Total 2	O 2	0	0
63	5A	1	Total 1	O 1	0	0
63	6A	1	Total 1	O 1	0	0
63	7A	2	Total 2	O 2	0	0
63	9A	2	Total 2	O 2	0	0
63	BA	2	Total 2	O 2	0	0
63	2L	7	Total 7	O 7	0	0
63	4L	8	Total 8	O 8	0	0
63	14	1520	Total 1520	O 1520	0	0
63	1J	23	Total 23	O 23	0	0
63	19	12	Total 12	O 12	0	0
63	29	9	Total 9	O 9	0	0
63	39	8	Total 8	O 8	0	0
63	15	1	Total 1	O 1	0	0
63	25	13	Total 13	O 13	0	0
63	35	5	Total 5	O 5	0	0
63	45	4	Total 4	O 4	0	0
63	85	4	Total 4	O 4	0	0

Continued on next page...

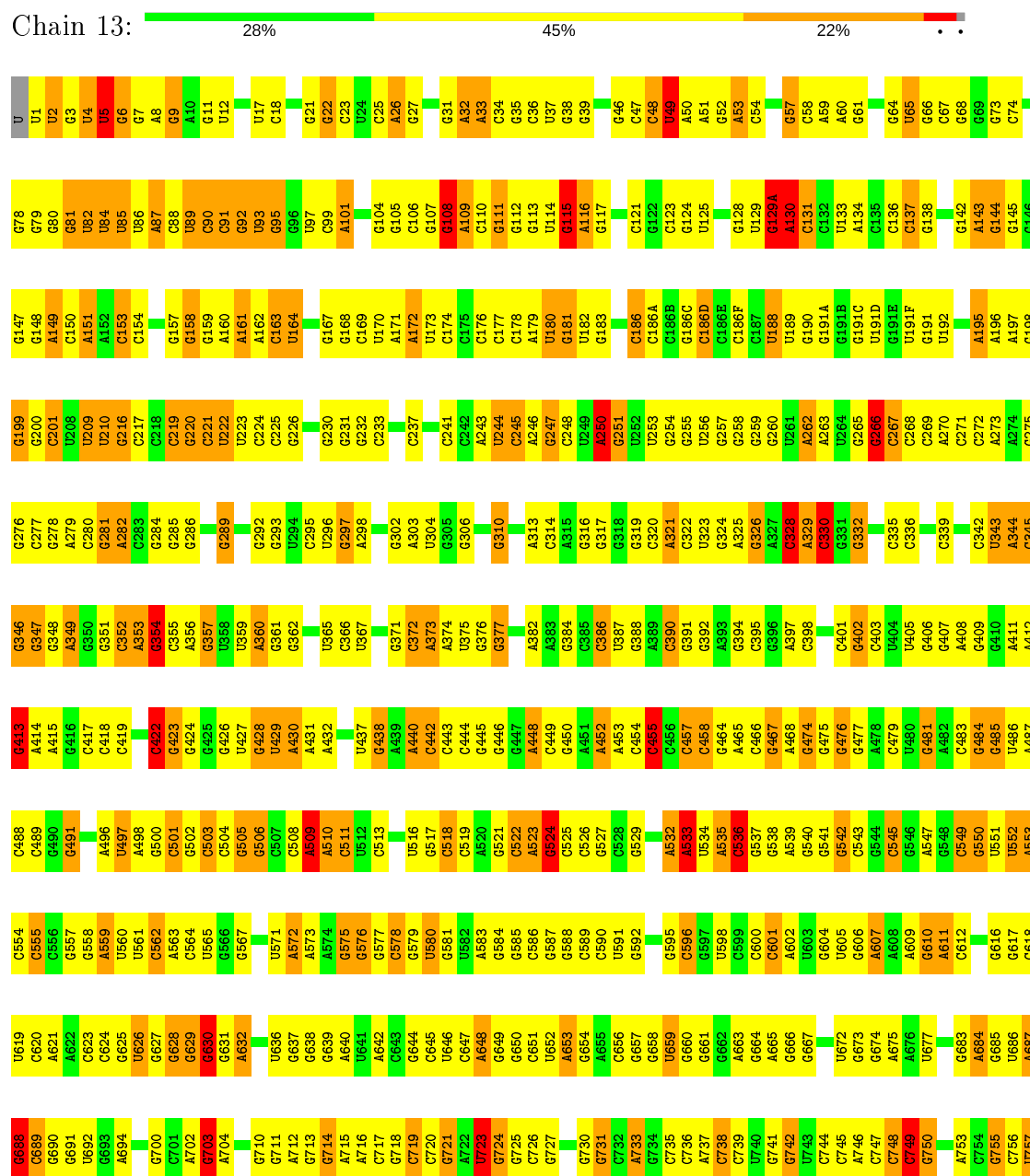
Continued from previous page...

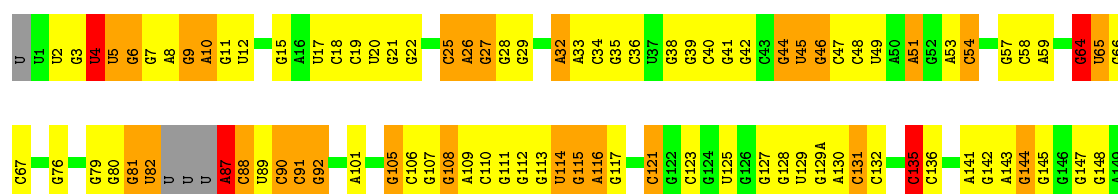
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	A5	1	Total	O	0	0
			1	1		
63	B5	1	Total	O	0	0
			1	1		
63	C5	1	Total	O	0	0
			1	1		
63	E5	3	Total	O	0	0
			3	3		
63	F5	6	Total	O	0	0
			6	6		
63	L5	2	Total	O	0	0
			2	2		
63	M5	9	Total	O	0	0
			9	9		

3 Residue-property plots

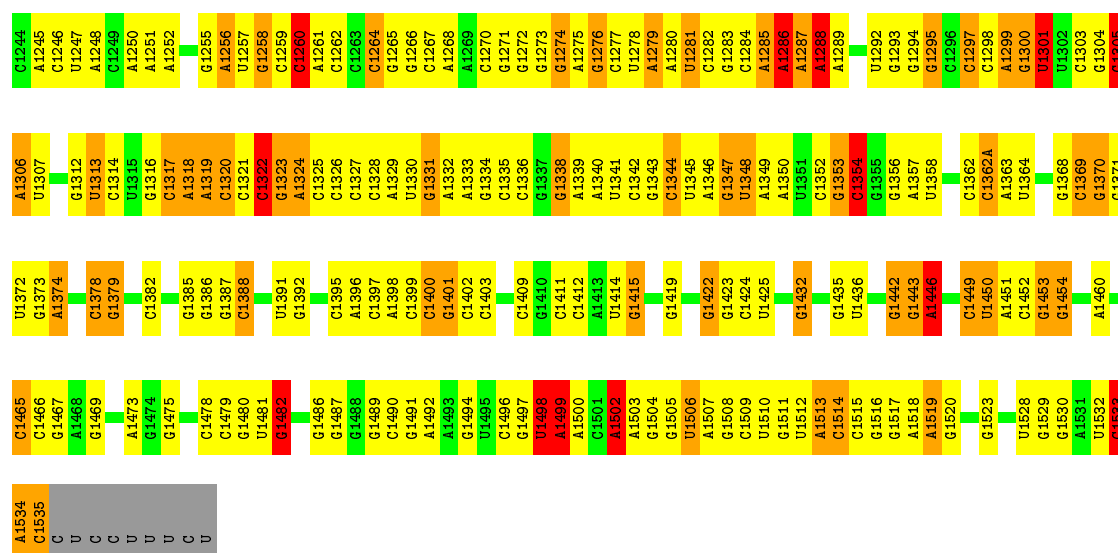
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 16S ribosomal RNA

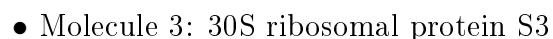




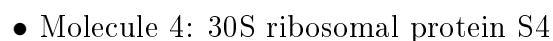
A1180	A1181	A1182	A1183	A1184	A1185	C1112	C1113	C1114	C1117	C1118	C1119	A1188	A1189	A1190	A1191	A1192	C1195	U1196	U1197	U1198	U1199	U1200	U1201	A1202	A1203	A1204	U1205	U1206	U1207	C1208	C1209	C1210	C1211	U1211	U1212	A1213	A1214	G1215	G1216	G1217	U1218	U1219	G1220	G1221	G1222	G1223	G1224	A1225	A1226	C1227	U1232	G1233	C1234	U1235	A1236	C1237	G1238	A1239	U1240	G1241	C1242	C1243																																																																																																																																																																																																							
G1042	C1043	A1044	C1045	A1046	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	C1059	C1060	G1061	U1062	G1063	G1064	C1071	G1072	U1073	G1077	U1078	A1079	G1080	A1081	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	G1092	A1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111																																																																																																																																																																																																														
C984	C985	A986	G987	C990	U991	U992	C993	A994	C995	U996	U997	G998	C998A	U999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	C1007	C1008	G1011	A1014	A1015	A1016	G1017	U1018	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111																																																																																																																																																																																																													
A918	A919	U920	U921	G922	A923	G926	G927	G928	G929	C932	G933	C934	A935	C936	G939	C940	G941	A942	U943	G944	G947	C948	A949	U950	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	G966	C967	A968	C969	A970	C970	G971	G972	A973	C974	G975	A976	G977	C978	A979	C980	A981	C982	A983	C984	A985	C986	A987	C988	A989	C990	A991	C992	A993	C994	A995	C996	A997	C998	A999	C1000	A1001	C1002	A1003	C1004	A1005	C1006	A1007	C1008	A1009	C1010	A1011	C1012	A1013	C1014	A1015	C1016	A1017	C1018	A1019	C1020	A1021	C1022	A1023	C1024	A1025	C1026	A1027	C1028	A1029	C1030	A1031	C1032	A1033	C1034	A1035	C1036	A1037	C1038	A1039	C1040	A1041	C1042	A1043	C1044	A1045	C1046	A1047	C1048	A1049	C1050	A1051	C1052	A1053	C1054	A1055	C1056	A1057	C1058	A1059	C1060	A1061	C1062	A1063	C1064	A1065	C1066	A1067	C1068	A1069	C1070	A1071	C1072	A1073	C1074	A1075	C1076	A1077	C1078	A1079	C1080	A1081	C1082	A1083	C1084	A1085	C1086	A1087	C1088	A1089	C1090	A1091	C1092	A1093	C1094	A1095	C1096	C1097	C1098	A1099	C1100	A1101	C1102	A1103	C1104	A1105	C1106	A1107	C1108	A1109	C1110	A1111																																																																															
C848	C849	U850	G851	G852	G853	G854	G855	C856	C857	G858	A859	A860	G861	U862	A863	A864	A865	C866	G867	C868	G869	U870	U871	A872	A873	C874	C875	G878	C879	C880	G881	C882	G883	A884	A885	C886	C887	A888	C889	A890	C891	C892	C893	A894	A895	C896	C897	G898	A899	C900	C901	C902	A903	C904	U905	G906	A907	C908	A909	C910	C911	C912	A913	A914	C915	A916	C917	C918	A919	C920	A921	C922	A923	C924	A925	C926	A927	C928	A929	C930	A931	C932	A933	C934	A935	C936	A937	C938	A939	C940	A941	C942	A943	C944	A945	C946	A947	C948	A949	C950	A951	C952	A953	C954	A955	C956	A957	C958	A959	C960	A961	C962	A963	C964	A965	C966	A967	C968	A969	C970	A971	C972	A973	C974	A975	C976	A977	C978	A979	C980	A981	C982	A983	C984	A985	C986	A987	C988	A989	C990	A991	C992	A993	C994	A995	C996	A997	C998	A999	C1000	A1001	C1002	A1003	C1004	A1005	C1006	A1007	C1008	A1009	C1010	A1011	C1012	A1013	C1014	A1015	C1016	A1017	C1018	A1019	C1020	A1021	C1022	A1023	C1024	A1025	C1026	A1027	C1028	A1029	C1030	A1031	C1032	A1033	C1034	A1035	C1036	A1037	C1038	A1039	C1040	A1041	C1042	A1043	C1044	A1045	C1046	A1047	C1048	A1049	C1050	A1051	C1052	A1053	C1054	A1055	C1056	A1057	C1058	A1059	C1060	A1061	C1062	A1063	C1064	A1065	C1066	A1067	C1068	A1069	C1070	A1071	C1072	A1073	C1074	A1075	C1076	A1077	C1078	A1079	C1080	A1081	C1082	A1083	C1084	A1085	C1086	A1087	C1088	A1089	C1090	A1091	C1092	A1093	C1094	A1095	C1096	C1097	C1098	A1099	C1100	A1101	C1102	A1103	C1104	A1105	C1106	A1107	C1108	A1109	C1110	A1111
C894	C895	A896	G897	C899	U891	U892	C893	A894	C895	U896	U897	G898	C898A	U899	A900	G901	G902	G903	A904	A905	C906	C907	C908	G909	C910	C911	C912	A913	A914	C915	A916	C917	G918	C919	C920	A921	C922	A923	C924	A925	C926	A927	C928	A929	C930	A931	C932	A933	C934	A935	C936	A937	C938	A939	C940	A941	C942	A943	C944	A945	C946	A947	C948	A949	C950	A951	C952	A953	C954	A955	C956	A957	C958	A959	C960	A961	C962	A963	C964	A965	C966	A967	C968	A969	C970	A971	C972	A973	C974	A975	C976	A977	C978	A979	C980	A981	C982	A983	C984	A985	C986	A987	C988	A989	C990	A991	C992	A993	C994	A995	C996	A997	C998	A999	C1000	A1001	C1002	A1003	C1004	A1005	C1006	A1007	C1008	A1009	C1010	A1011	C1012	A1013	C1014	A1015	C1016	A1017	C1018	A1019	C1020	A1021	C1022	A1023	C1024	A1025	C1026	A1027	C1028	A1029	C1030	A1031	C1032	A1033	C1034	A1035	C1036	A1037	C1038	A1039	C1040	A1041	C1042	A1043	C1044	A1045	C1046	A1047	C1048	A1049	C1050	A1051	C1052	A1053	C1054	A1055	C1056	A1057	C1058	A1059	C1060	A1061	C1062	A1063	C1064	A1065	C1066	A1067	C1068	A1069	C1070	A1071	C1072	A1073	C1074	A1075	C1076	A1077	C1078	A1079	C1080	A1081	C1082	A1083	C1084	A1085	C1086	A1087	C1088	A1089	C1090	A1091	C1092	A1093	C1094	A1095	C1096	C1097	C1098	A1099	C1100	A1101	C1102	A1103	C1104	A1105	C1106	A1107	C1108	A1109	C1110	A1111																																			
C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243																																																																																																																																																																																																							
G299	A300	A315	C320	A321	C322	U323	C324	A325	G326	A327	C328	A329	C330	G331	C332	G333	C337	U340	C341	A344	C345	U352	G252	G254	G257	G258	G259	G260	C187	U188	G266	C267	C272	A273	G275	G276	C277	G278	C280	A195	A196	A197	G198	G199	G200	C201	U208	U209	U210	G216	C217	A298																																																																																																																																																																																																																	
C221	U222	U223	C224	C225	G226	G227	G232	C233	C234	U164	C235	G236	C237	U238	C240	A243	U244	A246	G247	A250	G251	U252	G254	G257	G258	G259	G260	C187	U188	G266	C267	C272	A273	G275	G276	C277	G278	C280	A195	A196	A197	G198	G199	G200	C201	U208	U209	U210	G216	C217	A298																																																																																																																																																																																																																		
C299	A300	A315	C320	A321	C322	U323	C324	A325	G326	A327	C328	A329	C330	G331	C332	G333	C337	U340	C341	A344	C345	U352	G252	G254	G257	G258	G259	G260	C187	U188	G266	C267	C272	A273	G275	G276	C277	G278	C280	A195	A196	A197	G198	G199	G200	C201	U208	U209	U210	G216	C217	A298																																																																																																																																																																																																																	
C390	C394	C395	A396	C397	C398	G402	U403	G404	A405	G406	A407	A408	G409	C410	A411	A412	G413	A414	A415	G416	C419	A420	U421	C422	G423	G424	A425	G426	U427	G428	A429	A430	A431	U434	C435	G436	U437	G438	A439	A440	C442	C443	G447	A448	C449	G450	A451	A452	A453	C458	G464	A465	C466	G467																																																																																																																																																																																																															
A468	G474	G475	G481	A482	C483	G484	U485	A486	C488	G493	U494	A495	A496	U497	A498	G500	C501	U502	A503	A504	G505	G506	C507	G508	A509	A510	G511	U512	C513	A514	G515	U516	G517	C518	C519	A520	G521	C522	A523	C526	G527	C528	G529	G530	A531	A532	A533	A535	A536	C537	G538	C539	A540	C541	G542																																																																																																																																																																																																														
G542	A547	G550	C555	C556	G557	G558	A559	U560	U561	C562	A563	U565	G566	G567	G570	U571	A572	A573	A574	G575	C576	G577	C578	A579	A580	G581	U582	A583	G584	G588	C589	C590	U591	G592	C596	G597	C600	G601	C602	U603	G604	U605	G606	A607	A608	U609	C612	C613	A614	G615	G616																																																																																																																																																																																																																		
G617	C618	U619	G620	A621	G622	C623	C624	U625	A626	G627	U628	G629	G630	G637	G638	C645	U646	C647	G650	C651	G652	A653	G654	C655	G656	G660	A663	G664	A665	G666	U669	G670	C673	G674	A675	U677	U678	C679	G683	A684	G685	U686	A687	G688	C689	G690	U691	U692	G693																																																																																																																																																																																																																				
A694	A695	A696	C699	G700	G701	A702	G703	U704	U705	A706	C707	C708	G711	A712	G713	G714	A715	C717	G718	C719	C720	G721	A722	U723	G724	G725	C726	G727	A728	A729	G730	G731	C735	C736	A737	C738	C739	U740	G741	G742	C745	A746	C747	C748	C749	U750	U751	G752	A753	C754	G755	C756	U757	U758																																																																																																																																																																																																															
A759	G760	C764	G765	A766	A767	G768	A769	G774	G775	A776	A777	G778	A780	C784	G785	G786	G787	U788	A789	U790	C791	A792	C793	A794	G800	U804	C805	G806	G807	C811	C812	A815	A816	C817	G818	A819	U820	G821	G825	C826	U827	A828	G829	U833	C834	G837	G838	U841	C842	U843																																																																																																																																																																																																																			
C848	C849	U850	G851	G852	G853	G854	G855	C856	C857	G858	A859	A860	G861	U862	A863	A864	A865	C866	G867	C868	G869	U870	U871	A872	A873	C874	C875	G878	C879	C880	G881	C882	G883	A884	A885	C886	C887	A888	C889	A890	C891	C892	C893	A894	A895	C896																																																																																																																																																																																																																							



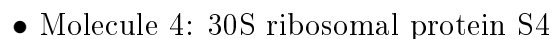
Device Type	Percentage
Smartphone	48%
Tablet	32%
Smartwatch	6%
Other	14%



Response	Percentage
Yes, the current government is responsible	38%
No, the crisis is the result of the economic situation	34%
Yes, but the crisis is also the result of the economic situation	9%
Don't know	18%

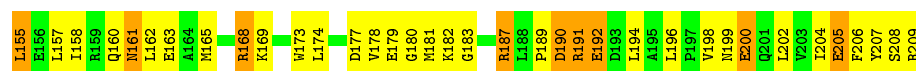


Response	Percentage
Used	50%
Not used	41%
Don't know	9%



Response	Percentage
Yes, the U.S. should take action to address climate change	42%
No, the U.S. should focus on other issues	44%
Don't know	14%





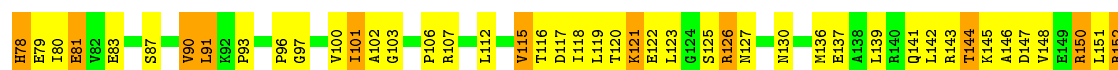
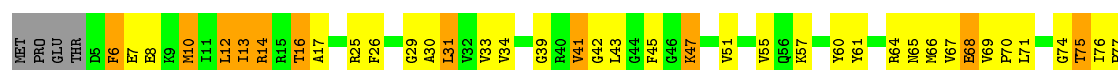
- Molecule 5: 30S ribosomal protein S5

Chain 4E: 49% 34% 9% 8%



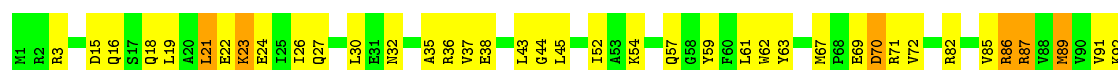
- Molecule 5: 30S ribosomal protein S5

Chain 42: 41% 38% 14% 7%



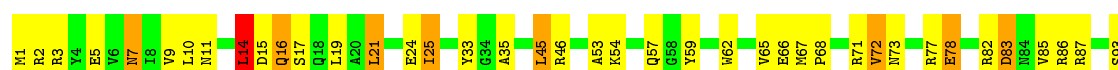
- Molecule 6: 30S ribosomal protein S6

Chain 5E: 57% 37% 6%



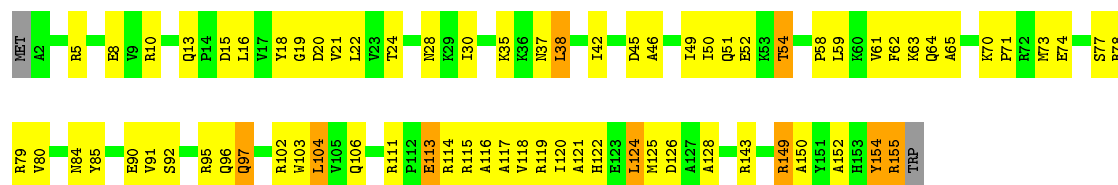
- Molecule 6: 30S ribosomal protein S6

Chain 52: 58% 33% 8%



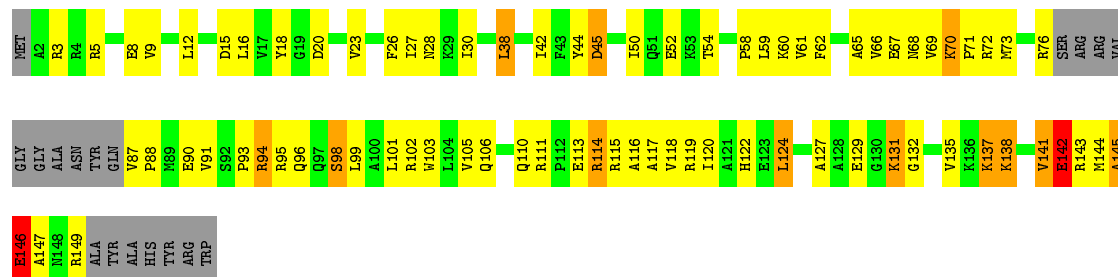
- Molecule 7: 30S ribosomal protein S7

Chain 6E: 52% 41% 6%



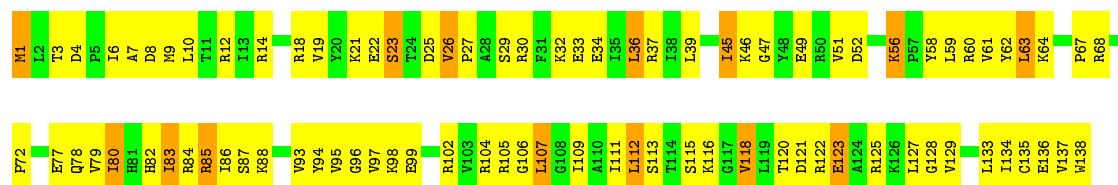
• Molecule 7: 30S ribosomal protein S7

Chain 62: 38% 41% 8% 12%



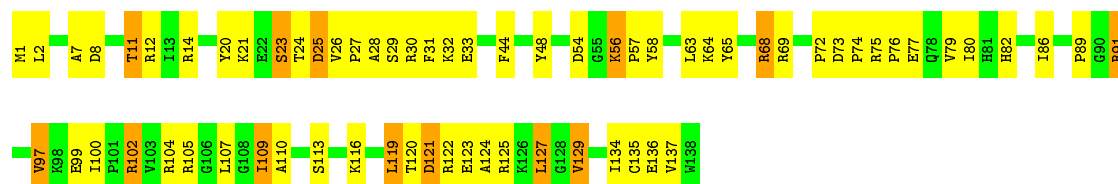
• Molecule 8: 30S ribosomal protein S8

Chain 7E: 37% 53% 10%



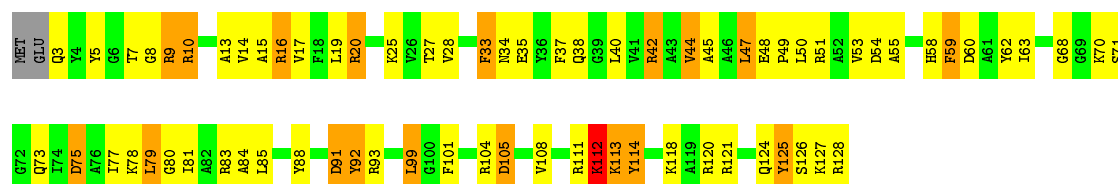
• Molecule 8: 30S ribosomal protein S8

Chain 72: 51% 39% 9%



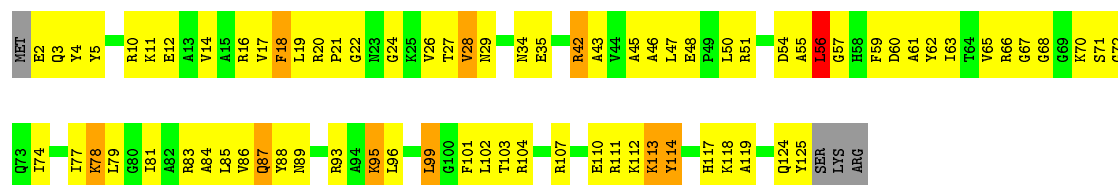
• Molecule 9: 30S ribosomal protein S9

Chain 8E: 42% 41% 14%

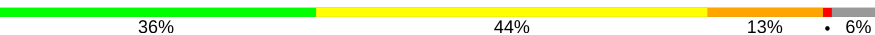


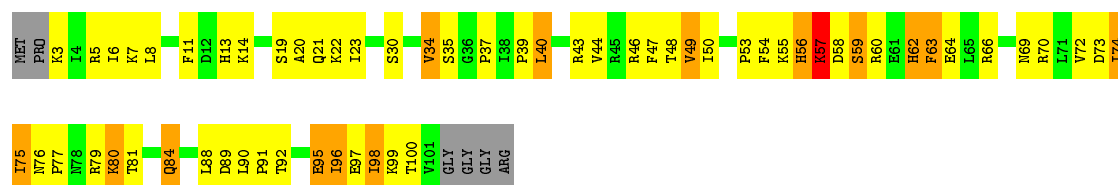
- Molecule 9: 30S ribosomal protein S9

Chain 82:  37% 52% 7% ..



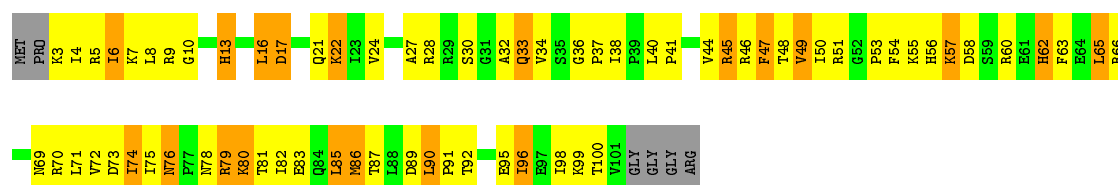
- Molecule 10: 30S ribosomal protein S10

Chain 1I:  36% 44% 13% • 6%



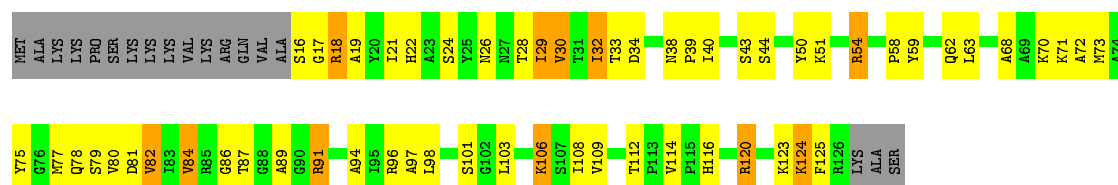
- Molecule 10: 30S ribosomal protein S10

Chain 1A:  28% 48% 19% 6%



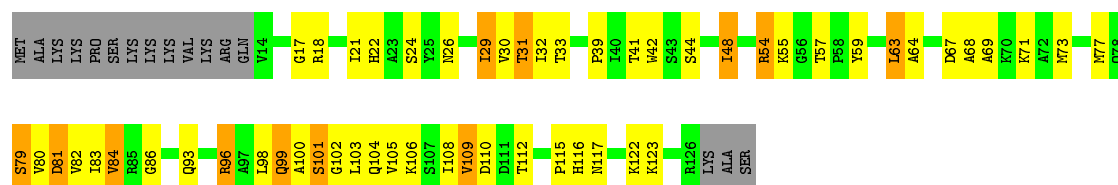
- Molecule 11: 30S ribosomal protein S11

Chain 2I:  40% 37% 9% 14%

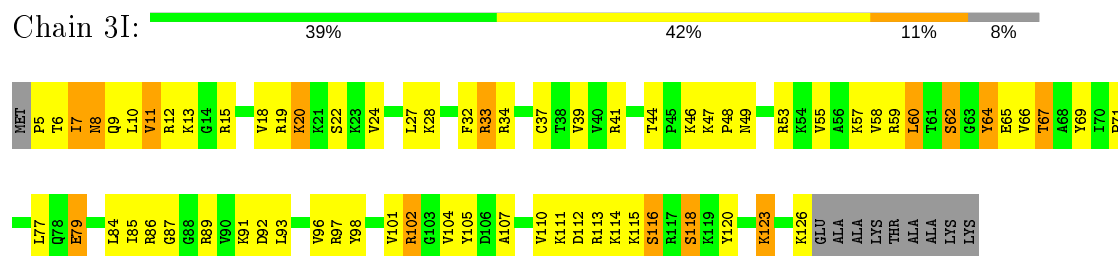


- Molecule 11: 30S ribosomal protein S11

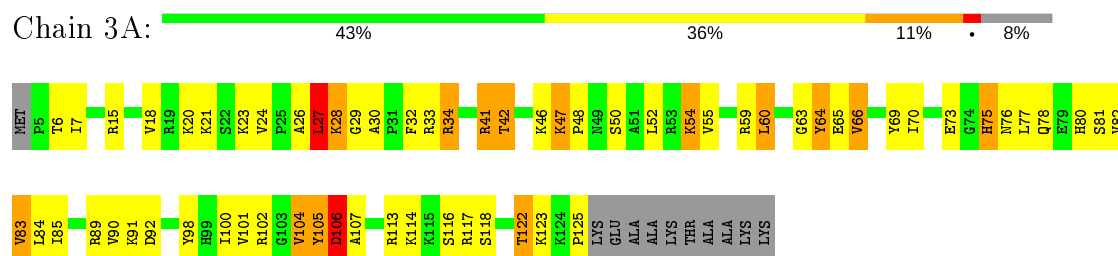
Chain 2A:  45% 33% 9% 12%



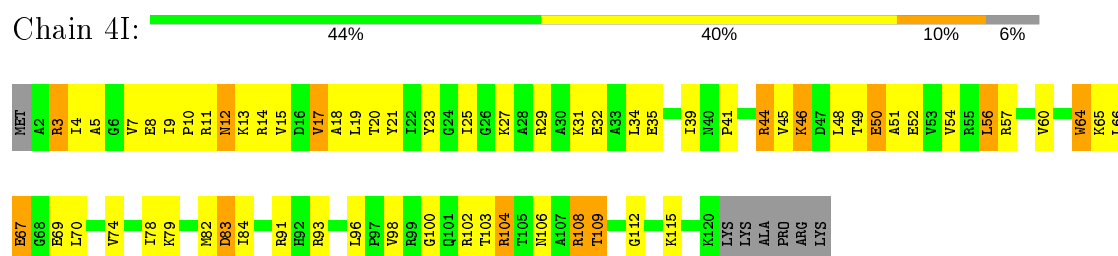
- Molecule 12: 30S ribosomal protein S12



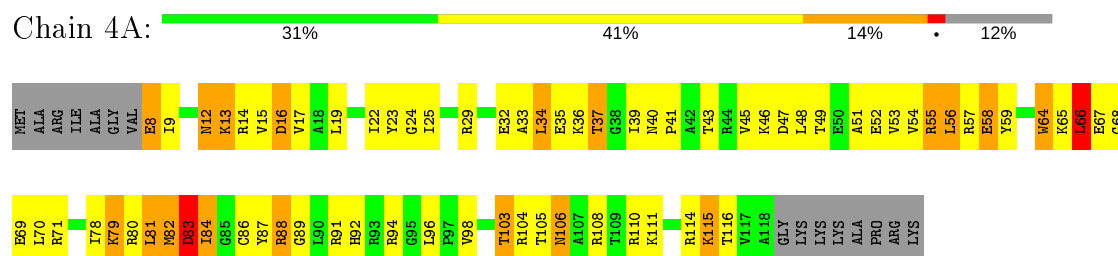
- Molecule 12: 30S ribosomal protein S12



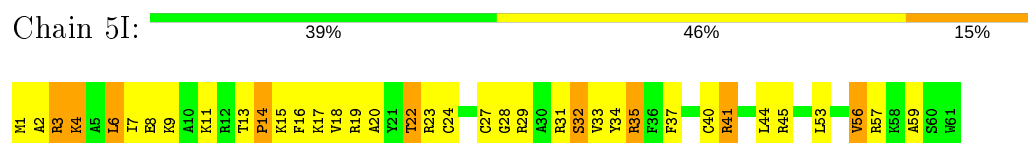
- Molecule 13: 30S ribosomal protein S13



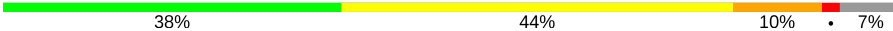
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



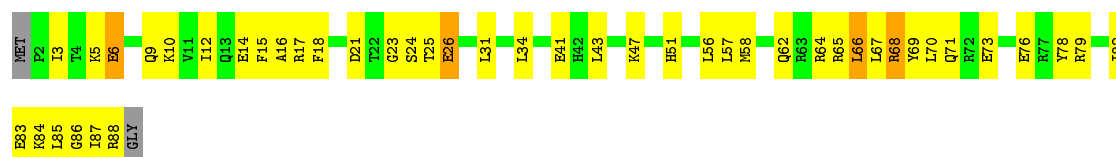
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A: 



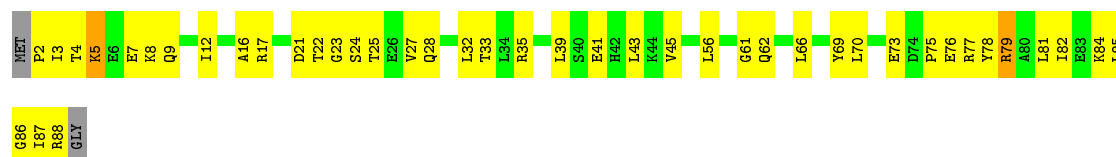
- Molecule 15: 30S ribosomal protein S15

Chain 6I: 



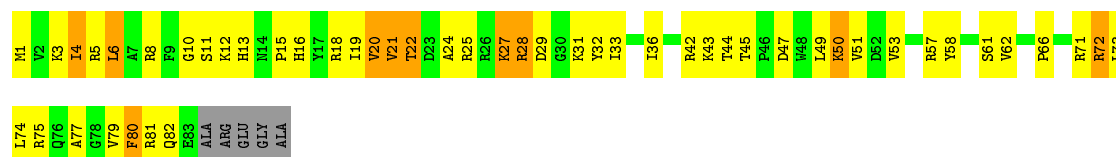
- Molecule 15: 30S ribosomal protein S15

Chain 6A: 



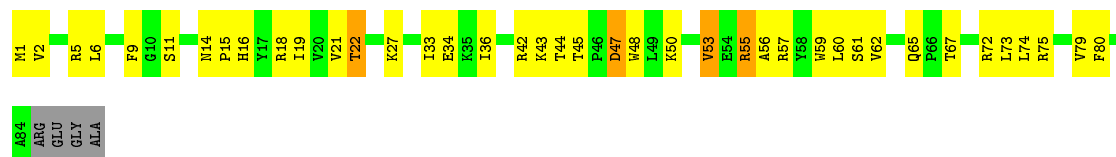
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 



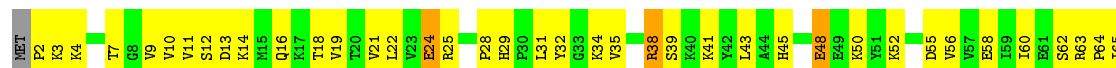
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 



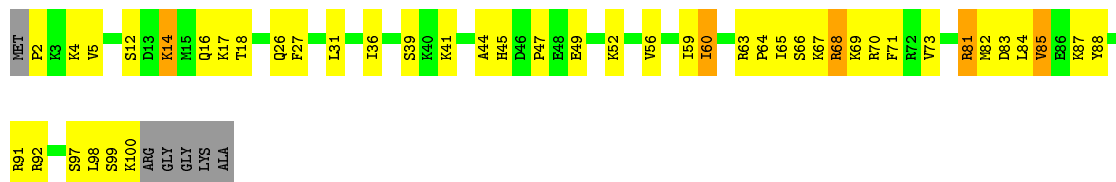
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 

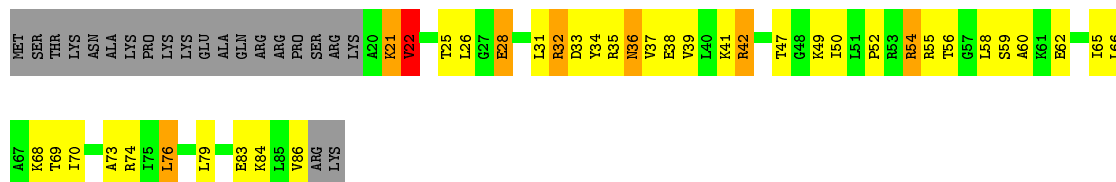




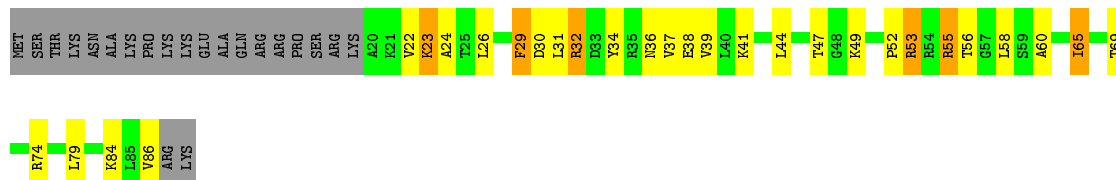
- Molecule 17: 30S ribosomal protein S17



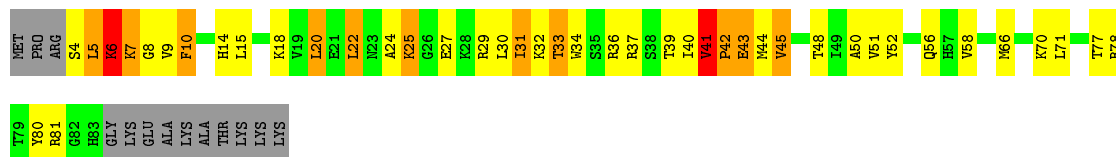
- Molecule 18: 30S ribosomal protein S18



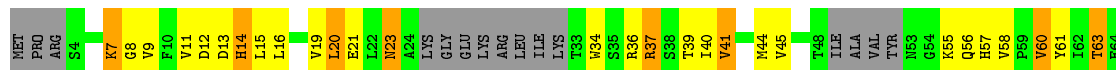
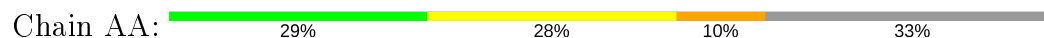
- Molecule 18: 30S ribosomal protein S18

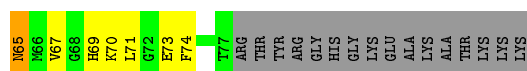


- Molecule 19: 30S ribosomal protein S19

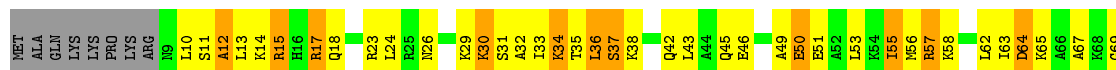


- Molecule 19: 30S ribosomal protein S19

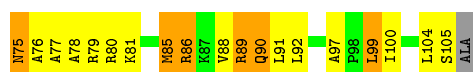
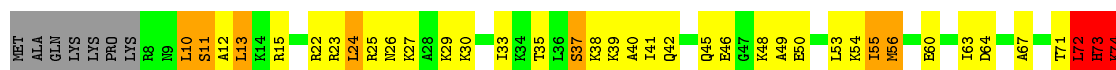




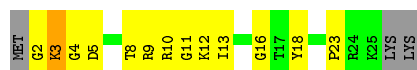
- Molecule 20: 30S ribosomal protein S20



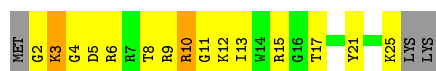
- Molecule 20: 30S ribosomal protein S20



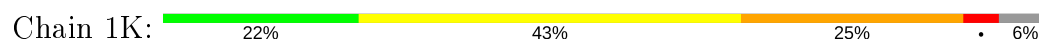
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

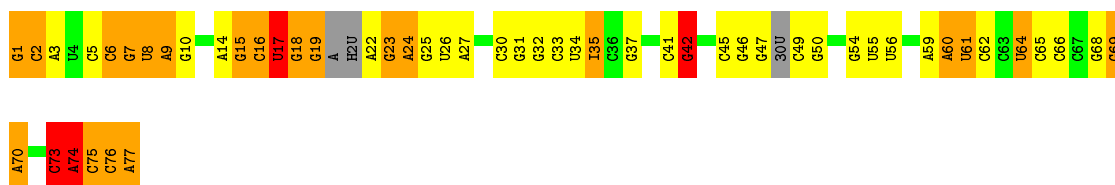


- Molecule 22: tRNAArg

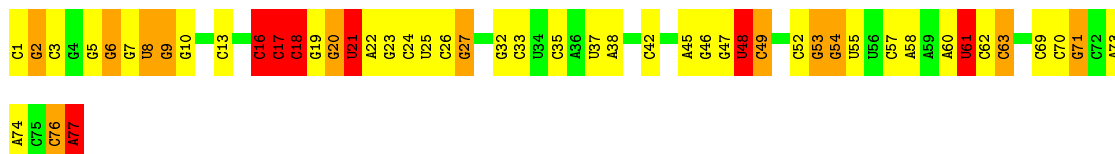


- Molecule 22: tRNAArg

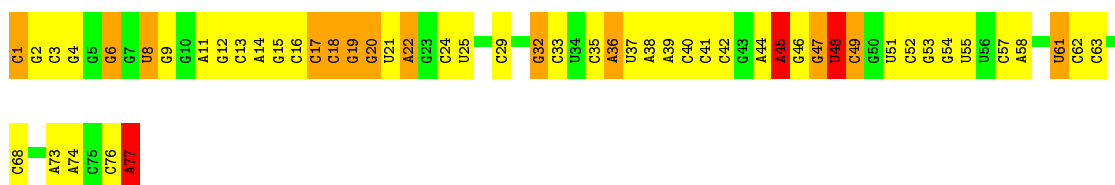
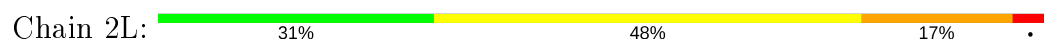




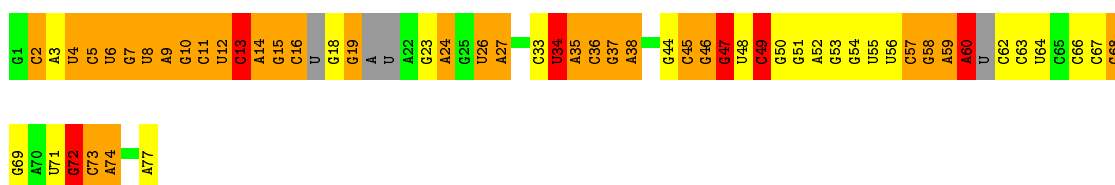
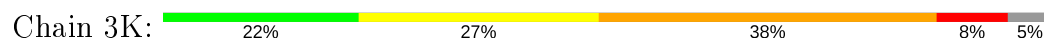
- Molecule 23: tRNA^{fMet}



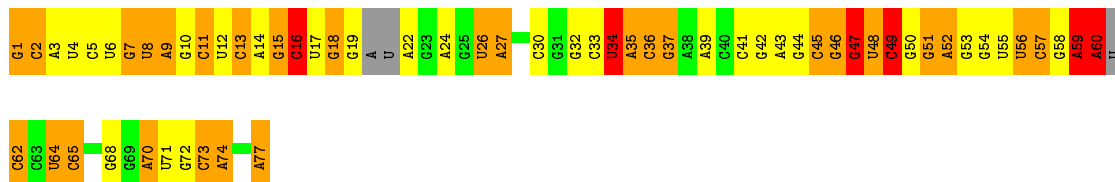
- Molecule 23: tRNA^{fMet}



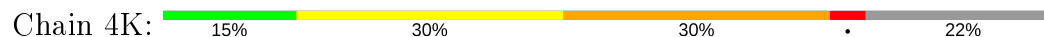
- Molecule 24: tRNA^{Arg}



- Molecule 24: tRNA^{Arg}

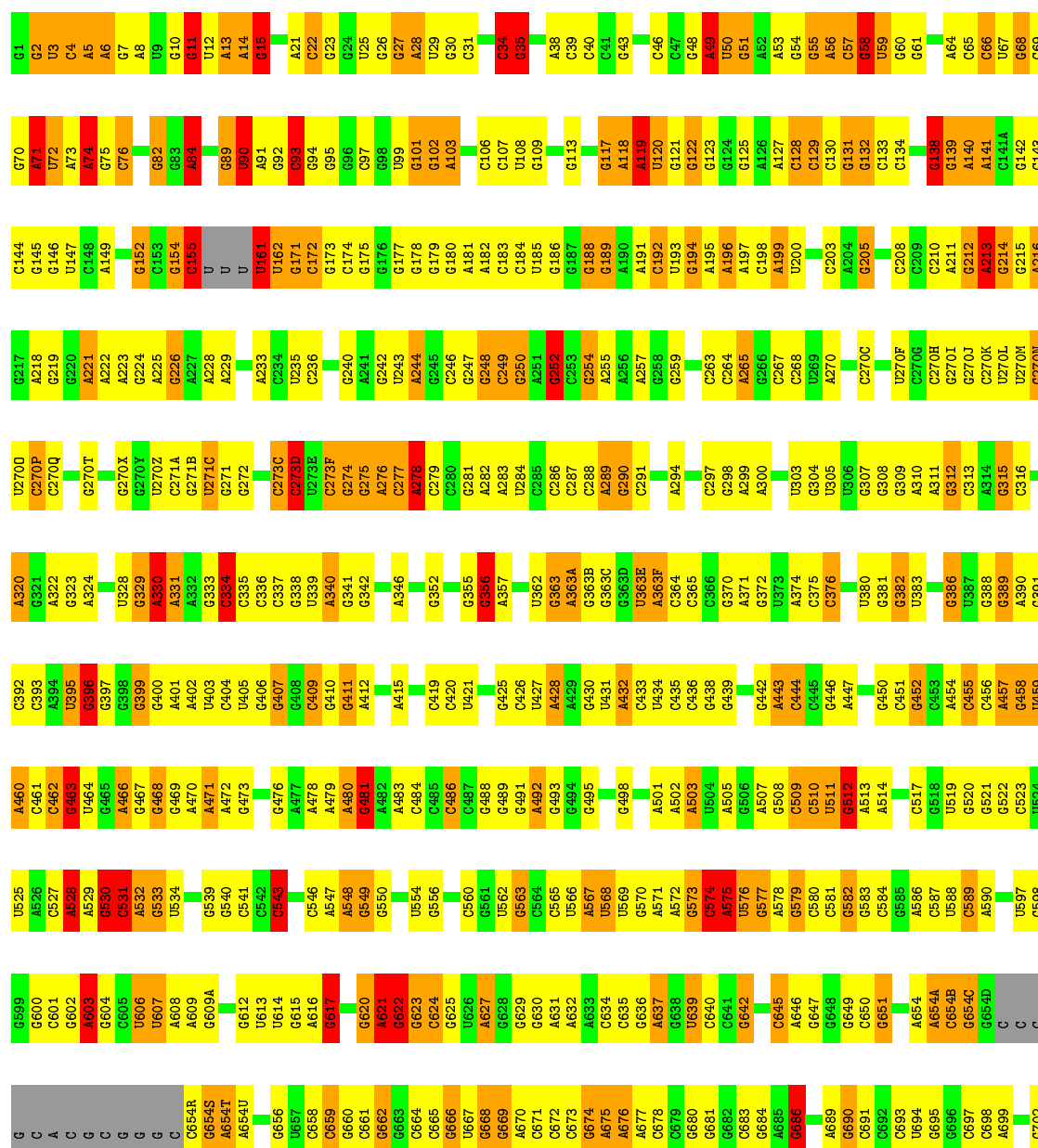


- Molecule 25: mRNA



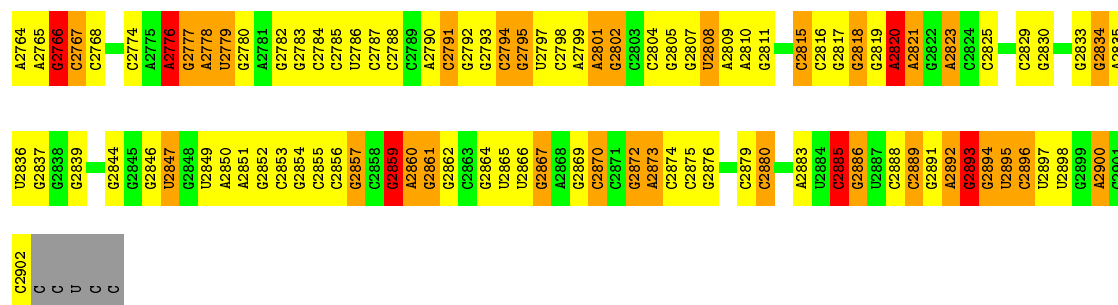
C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1630A	C1631	C1632	C1633	C1634																																																																																																																																																																																																																																																																																																																																																																										
G1539	G1540	A1543	A1544	A1545	C1547	C1548	C1549	C1550	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	C1564	C1565	C1566	C1567	C1568	A1569	A1570	A1571	A1572	G1573	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604																																																																																																																																																																																																																																																																																																																																																	
G1470	A1471	A1472	G1473	C1474	G1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540																																																																																																																																																																																																																																																																																																																																		
C1403	C1404	U1405	U1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469																																																																																																																																																																																																																																																																																																																																						
A1342	G1343	C1344	C1345	G1346	G1347	G1348	G1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402																																																																																																																																																																																																																																																																																																																																												
A1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341																																																																																																																																																																																																																																																																																																																																									
U1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341																																																																																																																																																																																																																																																																						
G1144	C1145	C1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341																																																																																																																																																																																																			
C949	G950	C951	C952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341
C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184																																																																																												



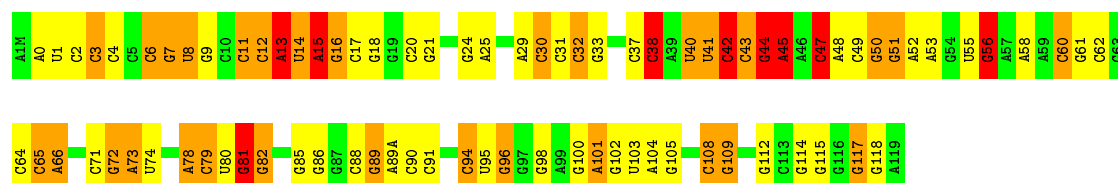


C1643	C1644	C1645	C1646	C1647	C1648	A1579	A1580	G1504	U1433	G1369	A1301	G1238	G1163	A1095	G1030	C837	A774	U703
C1644	C1645	C1646	C1647	C1648	A1579	A1580	G1504	U1433	G1369	C1370	A1302	G1239	G1164	A1096	U1033	C838	G775	A704
C1645	C1646	C1647	C1648	A1579	A1580	G1504	U1433	G1369	G1440	G1371	A1303	U1240	U1165	G1097	U1034	U839	G776	A705
C1646	C1647	C1648	A1579	A1580	G1504	U1433	G1369	G1441	G1442	U1372	A1304	U1241	C1166	A1098	U1035	C840	A777	A706
C1647	C1648	A1579	A1580	G1504	U1433	G1369	G1442	G1373	G1374	U1373	C1306	A1242	U1167	G1099	G1036	C841	G707	A707
C1648	A1579	A1580	G1504	U1433	G1369	G1442	G1374	U1374	U1375	G1380	A1307	G1243	G1168		G971	C842	G780	C708
A1579	A1580	G1504	U1433	G1369	G1442	G1374	U1375	U1376	C1375	C1381	C1308		G1169	A1103	G1037	G843	A781	U709
A1580	G1504	U1433	G1369	G1442	G1374	U1376	C1375	C1376	C1376	C1382	G1309	A1246	G1170	G1109	G1038	G844	A782	
G1504	U1433	G1369	G1442	G1374	U1376	C1376	C1376	C1377	C1377	C1383	G1310	A1247	G1171	A1105	G1039	G845	A783	G712
U1433	G1369	G1442	G1374	U1376	C1376	C1377	C1377	C1378	C1378	C1384	G1311	G1248	G1173	G1106	C1040	C846	A784	G713
C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	U1312	U1249	A1174	G1107	C1041	U847	G785	
C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	U1313	G1250	U1175	U1108	G1042	C848	C786	G717
C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1314	G1251	U1176	C1109	G1043	U912	U787	
C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1315	G1252	U1177	G1110	C1044	C849	A788	A722
C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1316	A1253	A1177	A1111	C1045	C850	A789	A723
C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	A1317	U1249	G1174	G1112	A1046	C851	C790	U724
C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1320	U1255	C1180	U1113	C1047	G853	C791	G725
C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	A1321	U1256	C1181	G1114	A1048	C854	G792	
C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	A1322	C1257	A1182	G1115	C1049	C855	A793	G729
C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	A1323	C1258	A1183	G1116	C1050	C856		G730
C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	U1324	G1260	A1184	G1117	C1051	C857	C796	C731
C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	G1324	G1261	C1185		U922	U858	C797	C732
C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	G1325	C1262	U1198		C932	C859	G798	G733
C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	U1326	C1263	U1187		C933	C860	G799	A734
C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	A1327	C1264	U1188		C934	C861	A800	A735
C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1327	C1265	G1191		C935	C862	A801	
C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	G1328	A1266	G1190	G1063	C936	C863	A802	C736
C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	U1329	G1267	G1192		C937	C864	U803	C737
C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	A1330	U1267	U1058		C938	C865	A804	G738
C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	G1331	U1268	U1059		C939	C866	G805	G739
C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	G1332	U1269	U1099		C940	C867	C806	U740
C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	U1333	C1270	C1201		U1061	C868	U807	G741
C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	U1334	G1271	C1202		C935	U868	G742	G744
C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	G1335	G1272	C1203		C936	C869	U809	G745
C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	G1336	U1273	U1205		C937	C870	U810	
C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	U1337	U1274	U1206		C938	C871	U811	A746
C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	G1338	G1275	G1207		C939	C872	C812	U747
C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	U1340	A1276	G1208		C940	C873	U813	G748
C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	U1341	G1277	G1209		C941	C874	C814	A749
C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	U1342	G1278	G1210		C942	C875	C815	C750
C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	U1343	A1278	U1141		C943	C876	C816	A751
C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1344	U1279	U1211		C944	U877	C817	A752
C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1345	G1280	G1212		C945	C878	C818	C753
C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	G1346	U1281	G1213		C946	C879	A819	
C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	G1347	U1282	G1214		C947	C880	A820	C754
C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	U1348	U1283	G1215		C948	C881	A821	C755
C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1349	G1284	G1216		C949	C882	A822	C756
C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1350	A1284	C1217		C950	C883	G823	
C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1351	G1285			C951	C884	A824	G759
C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	U1352	A1286	A1220		C952	C885	C825	G760
C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	U1353	A1287			C953	C886	U826	A761
C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1357	U1288	G1224		C954	C887	U827	
C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	U1358	U1289	G1225		C955	C888	A828	A764
C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	G1358	U1290	G1226		C956	C889	A829	C766
C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	U1359	U1291	G1227		C957	C890	A830	G767
C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1360	C1292	G1228		C958	C891	G831	G768
C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1361	C1293	G1229		C959	C892	A832	
C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1362				C960	C893	G833	G769
C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1363	G1296	G1232		C961	C894	U834	G770
C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	G1364	C1297	G1233		C962	C895	U835	C771
C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	A1365	C1298	G1234		C963	C896	A836	C772
C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	A1366	C1299	G1235		C964	C897	U837	U772
C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	A1367	U1300	G1236		C965	C898	A837	
C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	A1368	U1301	G1237		C966	C899	U838	
C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1369	U1302	G1238		C967	C900	A838	
C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1370	U1303	G1239		C968	C901	A839	
C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1371	U1304	G1240		C969	C902	A840	
C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1372	U1305	G1241		C970	C903	G842	
C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1373	U1306	G1242		C971	C904	A781	
C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1374	U1307	G1243		C972	C905	A782	
C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1375	U1308	G1244		C973	C906	A783	
C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1376	U1309	G1245		C974	C907	A784	
C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1377	U1310	G1246		C975	C908	A785	
C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1378	U1311	G1247		C976			

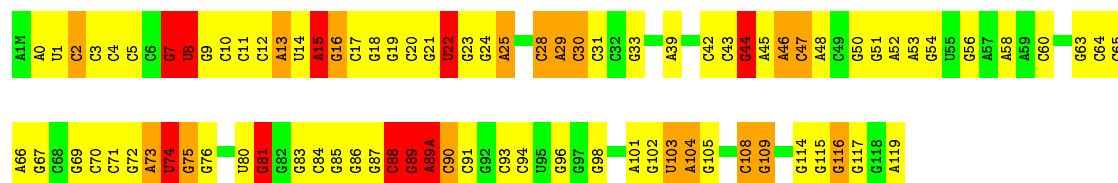
U2698	C2699	C2700	C2701	U2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	U2712	A2713	C2714	C2715	C2718	C2719	U2720	A2721	C2724	A2725	U2726	C2727	C2731	C2732	A2733	A2734	C2735	C2736	U2739	A2740	A2741	C2742	C2743	C2744	C2745	C2680	C2681	U2746	U2682	C2683	C2684	U2685	C2686	C2687	U2688	C2689	C2690	A2693	C2694	C2695	U2696	C2697										
G2624	G2625	A2629	A2630	A2631	A2632	C2635	C2636	C2637	C2638	A2639	C2640	C2645	C2646	C2647	C2648	C2649	C2652	U2653	A2654	C2655	U2656	C2659	A2662	A2665	C2666	C2667	C2668	A2671	G2672	C2673	C2674	A2675	C2680	C2681	C2682	C2683	U2684	C2685	C2686	U2687	U2688	C2689	A2693	C2694	C2695	U2696	C2697																		
C2556	G2557	C2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	U2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	U2613	A2614	U2615	C2616	C2617	C2618	C2619	C2620	A2621
G2489	G2490	U2491	U2492	U2493	G2494	G2495	C2498	C2499	U2500	C2501	C2502	A2503	U2504	G2505	U2506	C2507	C2508	C2509	C2510	U2511	C2512	C2513	C2516	C2517	C2518	U2519	C2520	C2521	C2522	C2523	C2524	C2525	U2528	C2529	A2530	C2531	C2532	C2533	A2534	U2535	C2536	U2537	U2637	C2538	C2542	C2543	C2544	U2547	U2548	C2549	U2552	C2553	U2554	U2555	C2556	C2557	C2558	C2559	C2560	A2561					
A2422	U2423	C2424	A2425	C2426	C2427	G2428	C2429	A2430	U2431	A2432	U2433	A2434	C2435	C2436	U2437	U2438	U2439	C2440	C2441	C2442	C2443	C2444	C2447	C2448	A2451	C2452	U2453	C2454	C2455	C2456	U2457	C2458	A2459	U2460	C2461	U2462	C2463	C2464	C2467	C2468	A2469	C2470	C2471	C2472	U2473	C2474	C2475	C2476	C2477	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2498							
G2353	G2354	C2355	C2356	U2357	C2358	C2359	A2360	C2361	C2362	C2363	C2364	C2365	A2366	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2383	C2384	C2385	C2386	U2387	C2388	C2389	C2392	C2393	C2394	C2395	C2396	C2399	C2400	U2401	C2402	C2403	C2404	U2405	U2406	C2411	A2412	C2413	C2414	C2415	C2416	C2417	C2418	U2419													
C2292	C2293	C2294	C2295	U2296	C2297	A2298	C2299	C2300	C2301	C2302	C2303	C2304	A2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	A2328	C2329	C2330	C2331	U2332	C2333	C2334	A2335	A2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	U2344	C2345	A2346	C2347	C2350	A2352								
G2228	C2229	C2230	C2231	U2232	U2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	A2241	U2242	U2243	U2244	U2245	C2246	A2247	G2250	C2251	C2252	C2253	C2254	C2255	C2256	U2257	C2258	C2261	U2262	C2263	C2264	C2267	A2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	U2291									
U2150	G2151	C2152	G2153	U2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	A2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2198	C2199	C2200	C2201	C2202	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2215	C2216	C2217	C2224	C2225	C2226	A2227								
G2087	C2088	U2089	C2090	U2091	U2092	C2093	C2094	C2097	U2098	C2099	U2099	C2100	C2101	U2102	C2103	U2104	C2105	C2106	C2107	C2108	U2109	C2110	C2111	G	U2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	U2122	C2123	C2124	C2125	A2126	C2127	C2128	C2129	U2130	C2131	U2132	C2133	A2134	C2135	C2136	C2137	C2138	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149							
C2021	U2022	C2023	G2024	C2025	C2026	C2027	U2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	U2041	C2042	C2043	C2044	C2049	C2050	A2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	U2068	C2069	C2072	C2073	U2074	U2075	U2076	U2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086										
U1796	C1797	U1798	C1799	A1885	C1886	C1887	A1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	A1900	C1901	C1902	C1903	C1904	C1905	C1906	C1909	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	U1943	C1944	C1945	C1946								
C1741	C1742	C1743	C1746	C1747	C1748	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1822	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1842	C1847	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1869	C1870	C1878																							
U1796	C1797	U1798	C1799	A1885	C1886	C1887	A1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	A1900	C1901	C1902	C1903	C1904	C1905	C1906	C1909	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	U1943	C1944	C1945	C1946								



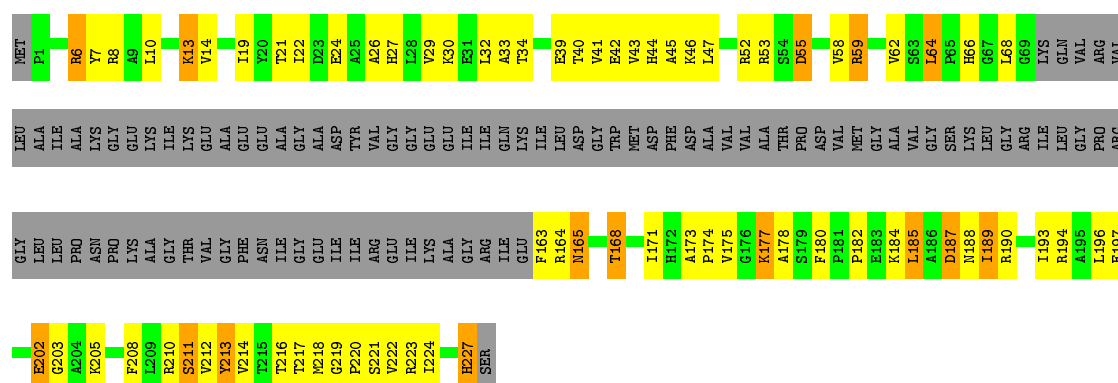
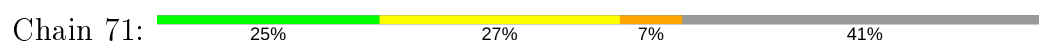
• Molecule 27: 5S ribosomal RNA



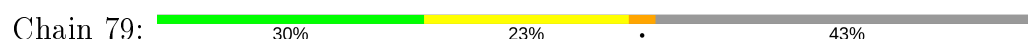
• Molecule 27: 5S ribosomal RNA

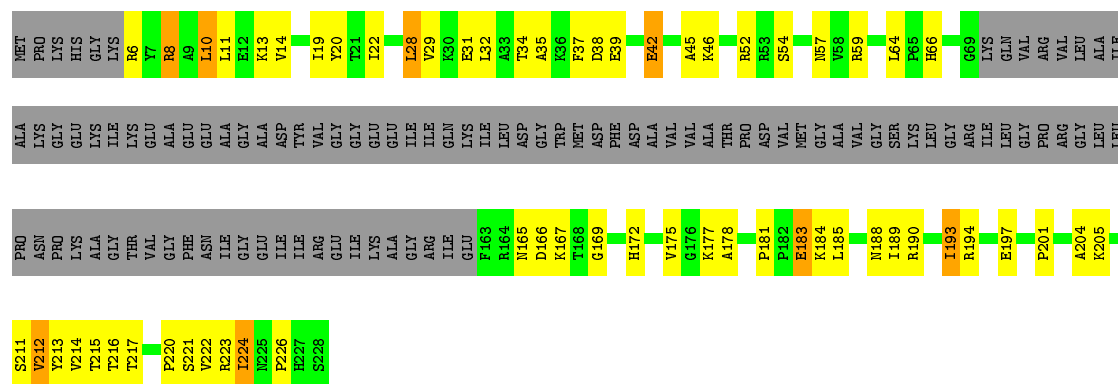


• Molecule 28: 50S ribosomal protein L1



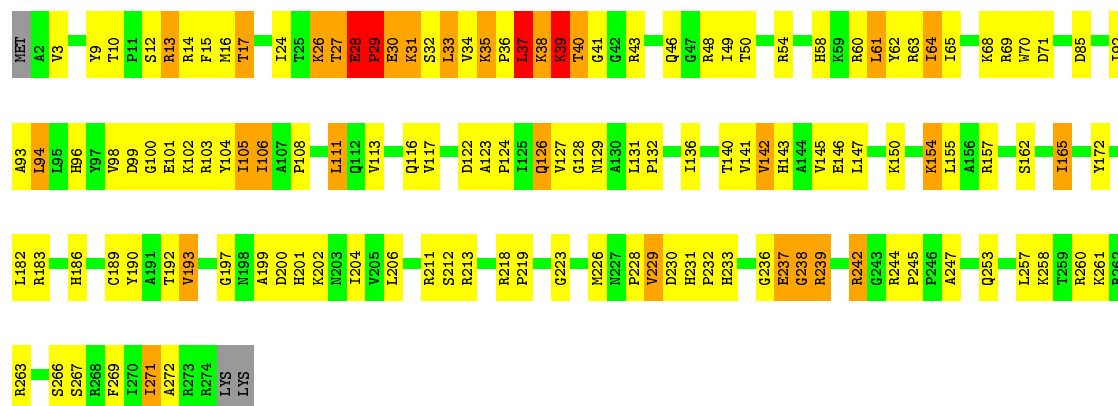
• Molecule 28: 50S ribosomal protein L1





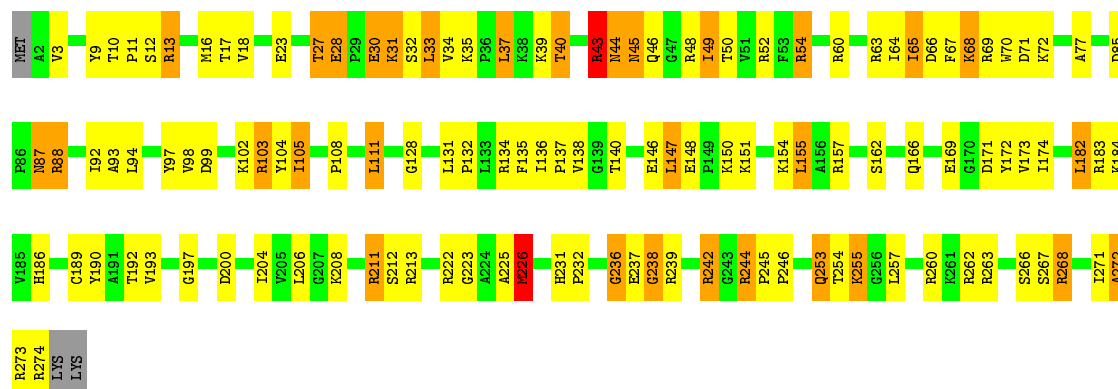
• Molecule 29: 50S ribosomal protein L2

Chain 11: 51% 37% 10% ..



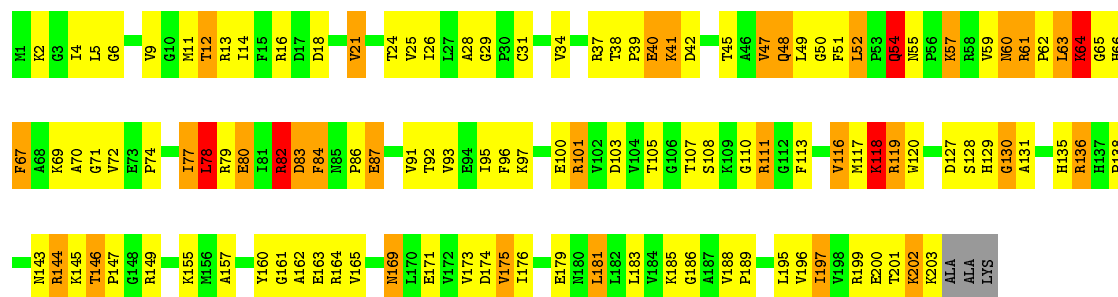
• Molecule 29: 50S ribosomal protein L2

Chain 19: 54% 33% 11% ..



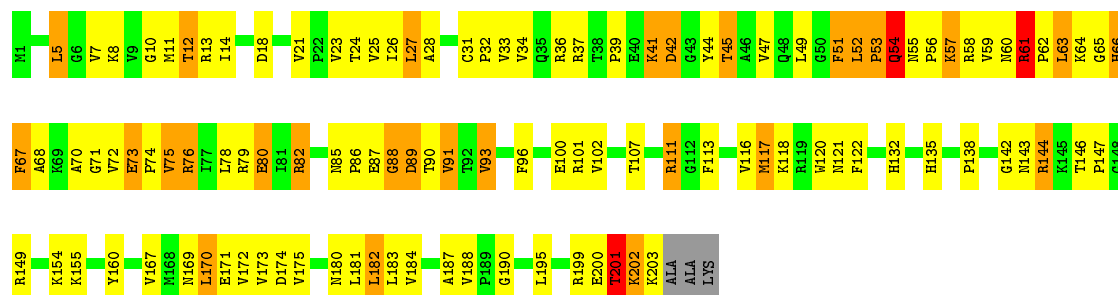
• Molecule 30: 50S ribosomal protein L3

Chain 21: 40% 42% 15% ..



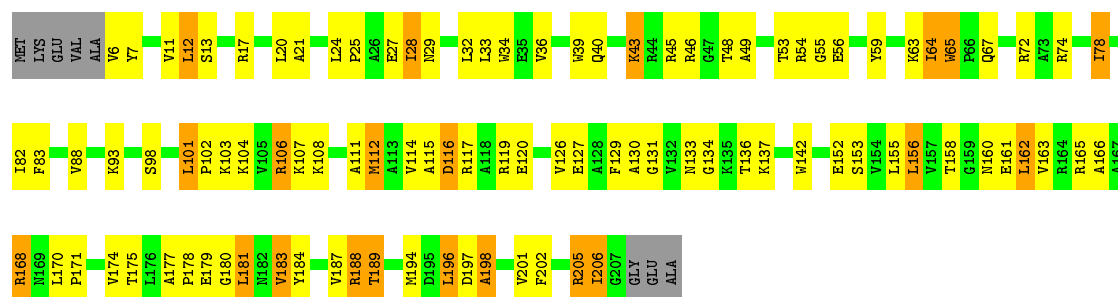
- Molecule 30: 50S ribosomal protein L3

Chain 29: 44% 40% 14% ..



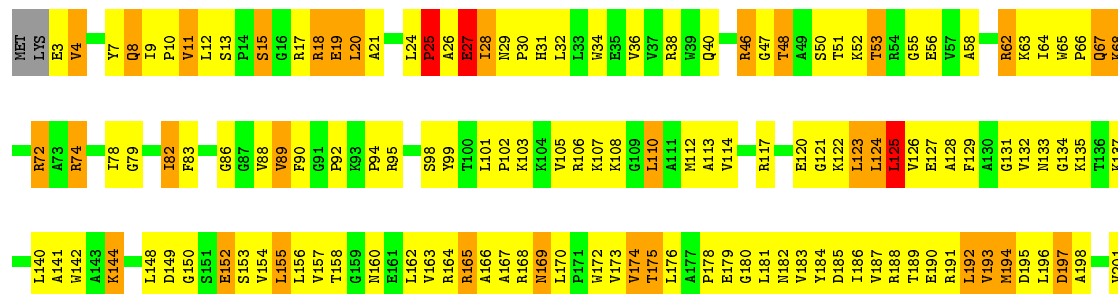
- Molecule 31: 50S ribosomal protein L4

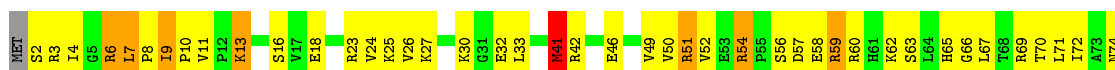
Chain 31: 49% 38% 10% .

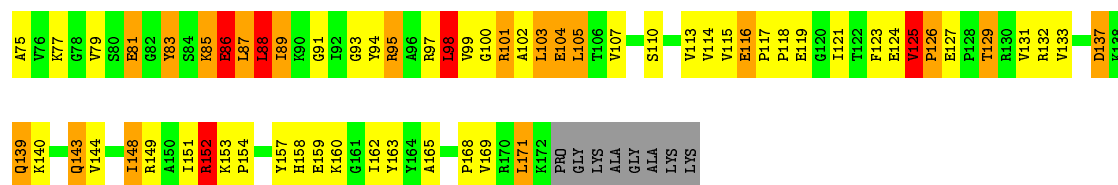


- Molecule 31: 50S ribosomal protein L4

Chain 39: 30% 50% 16% ..

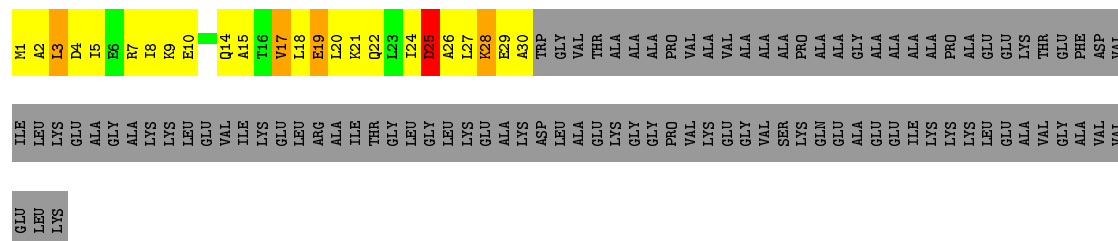






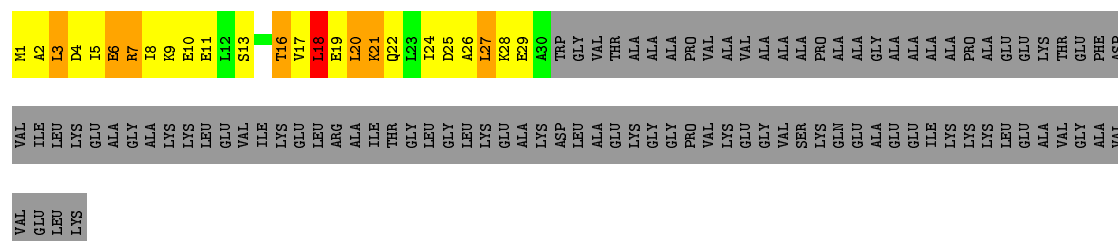
• Molecule 34: 50S ribosomal protein L7/L12

Chain 18: 5% 15% 76%



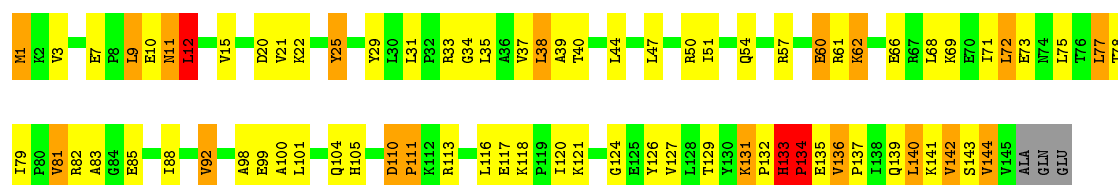
• Molecule 34: 50S ribosomal protein L7/L12

Chain 28: 14% 6% 76%



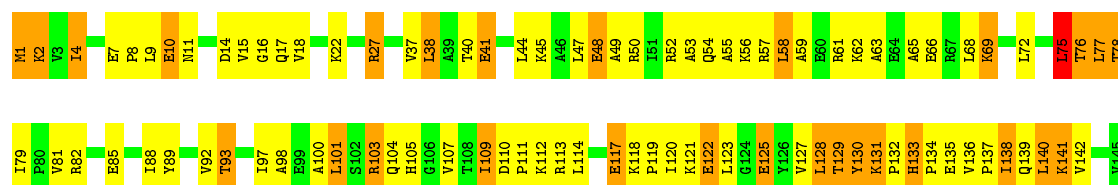
• Molecule 35: 50S ribosomal protein L9

Chain 61: 46% 38% 12%



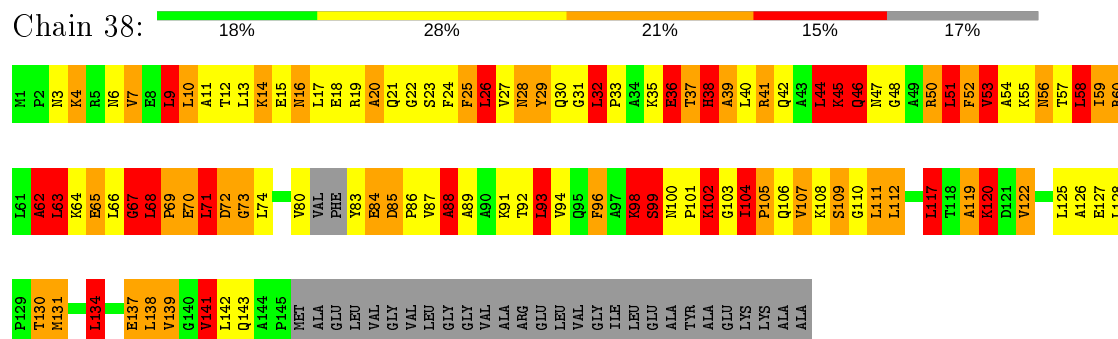
• Molecule 35: 50S ribosomal protein L9

Chain 69: 36% 42% 19%

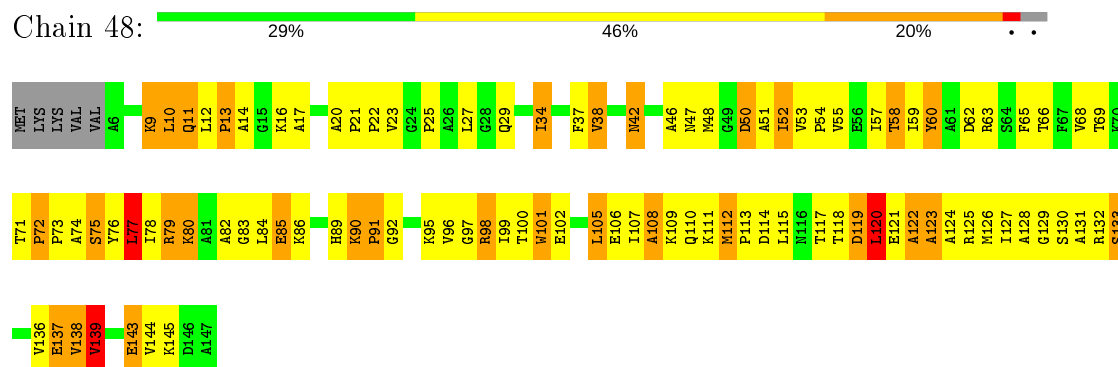


ALA
GLN
GLU

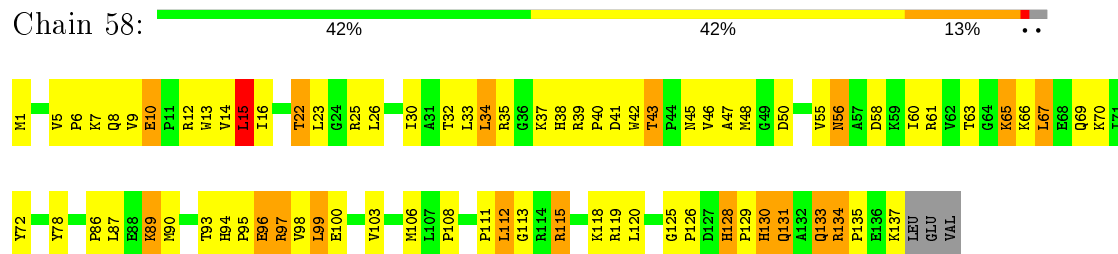
• Molecule 36: 50S ribosomal protein L10



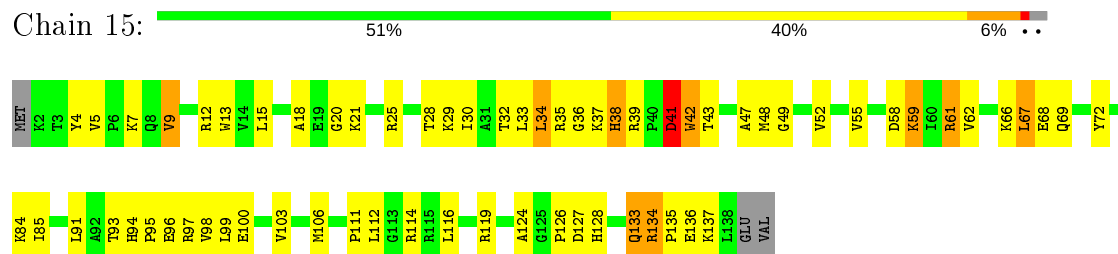
• Molecule 37: 50S ribosomal protein L11



• Molecule 38: 50S ribosomal protein L13

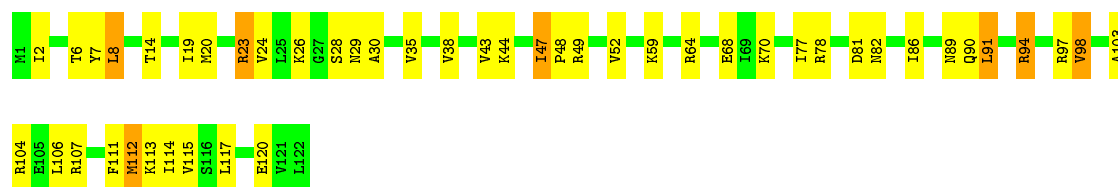


• Molecule 38: 50S ribosomal protein L13



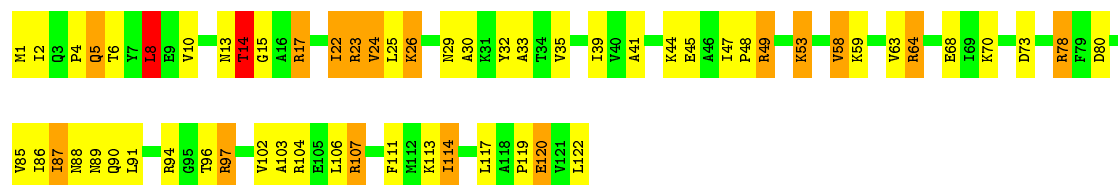
• Molecule 39: 50S ribosomal protein L14

Chain 68: 



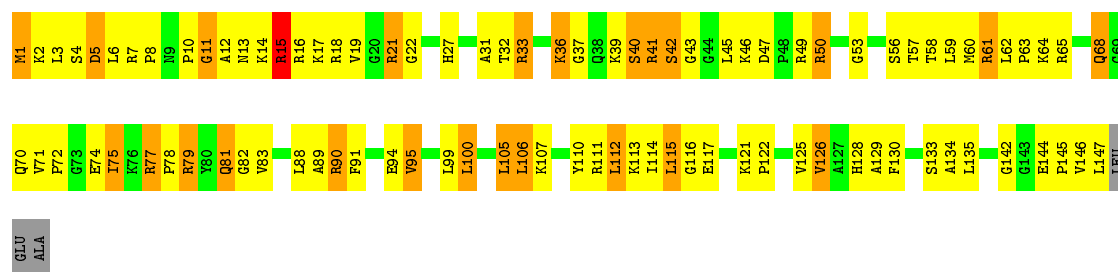
- Molecule 39: 50S ribosomal protein L14

Chain 25: 



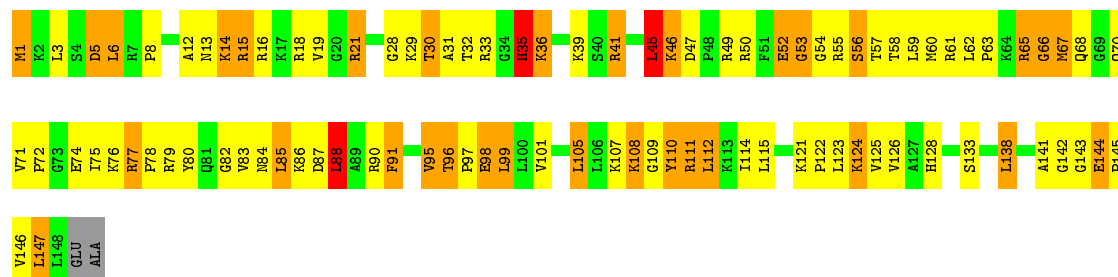
- Molecule 40: 50S ribosomal protein L15

Chain 78: 



- Molecule 40: 50S ribosomal protein L15

Chain 35: 



- Molecule 41: 50S ribosomal protein L16

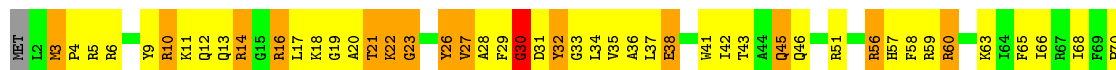
Chain 88: 





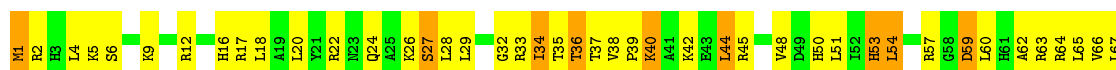
- Molecule 41: 50S ribosomal protein L16

Chain 45: 35% 40% 21% ..



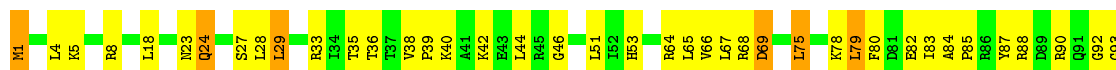
- Molecule 42: 50S ribosomal protein L17

Chain 98: 44% 47% 9%



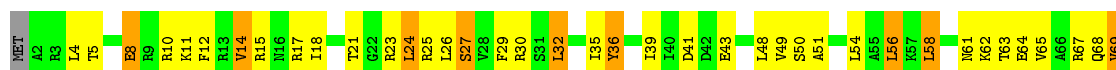
- Molecule 42: 50S ribosomal protein L17

Chain 55: 55% 39% 6%



- Molecule 43: 50S ribosomal protein L18

Chain A8: 39% 45% 13% ..



- Molecule 43: 50S ribosomal protein L18

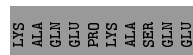
Chain 65: 30% 46% 18% ..





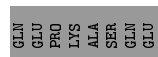
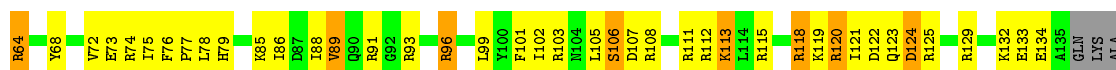
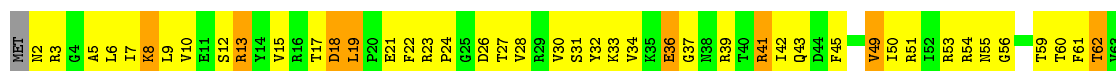
- Molecule 44: 50S ribosomal protein L19

Chain B8:



- Molecule 44: 50S ribosomal protein L19

Chain 75:



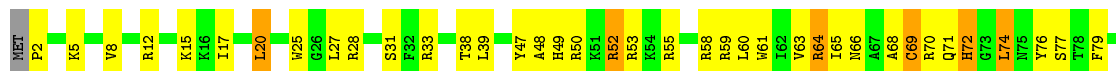
- Molecule 45: 50S ribosomal protein L20

Chain C8:

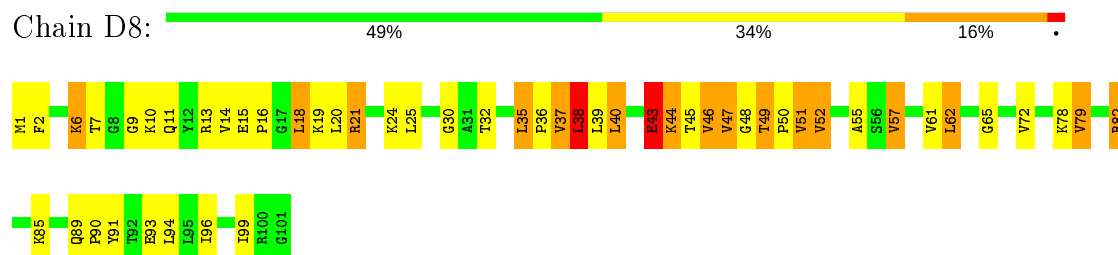


- Molecule 45: 50S ribosomal protein L20

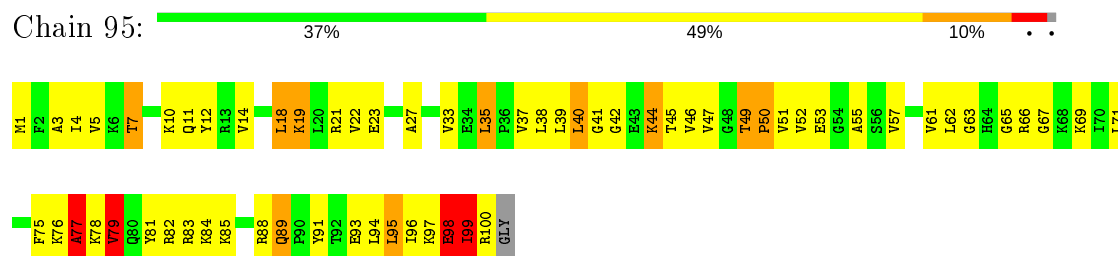
Chain 85:



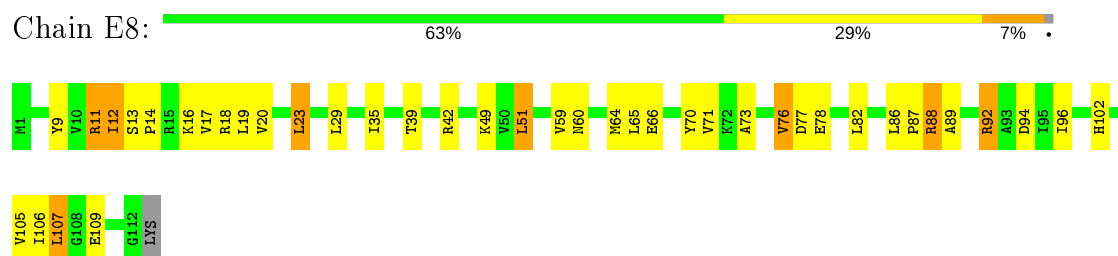
- Molecule 46: 50S ribosomal protein L21



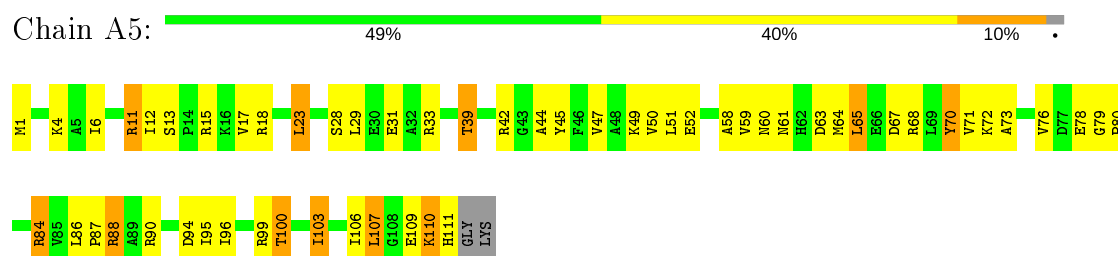
- Molecule 46: 50S ribosomal protein L21



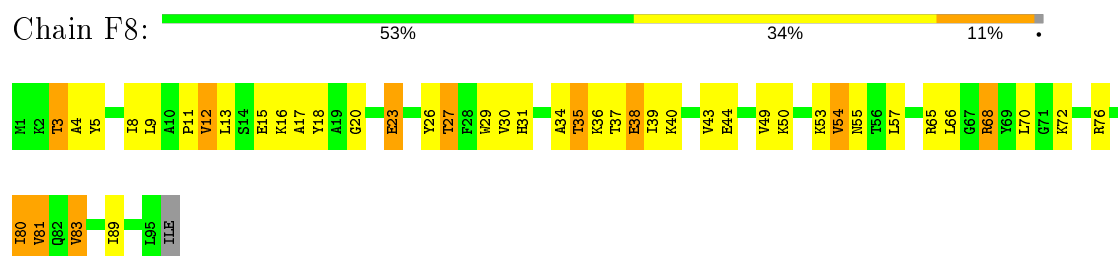
- Molecule 47: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L22

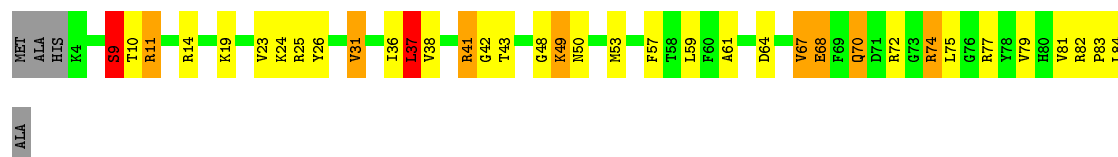


- Molecule 48: 50S ribosomal protein L23

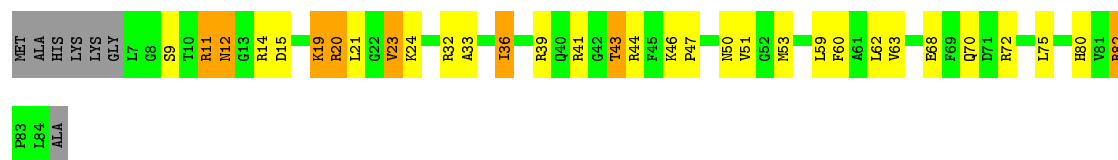


- Molecule 48: 50S ribosomal protein L23

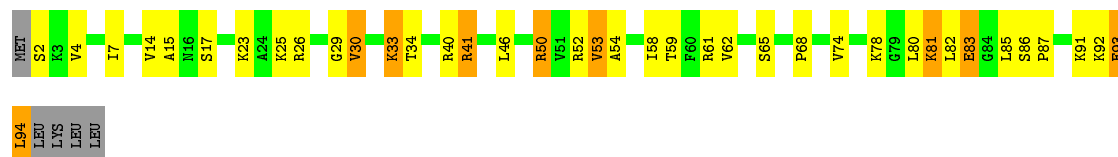
- Molecule 51: 50S ribosomal protein L27



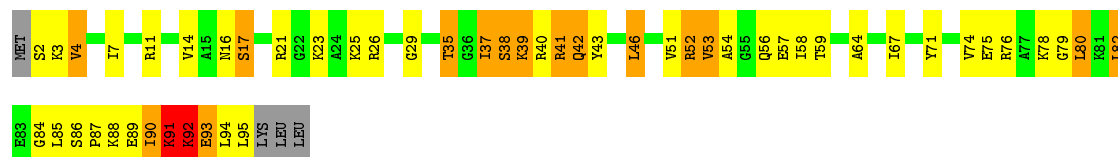
- Molecule 51: 50S ribosomal protein L27



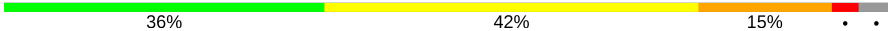
- Molecule 52: 50S ribosomal protein L28

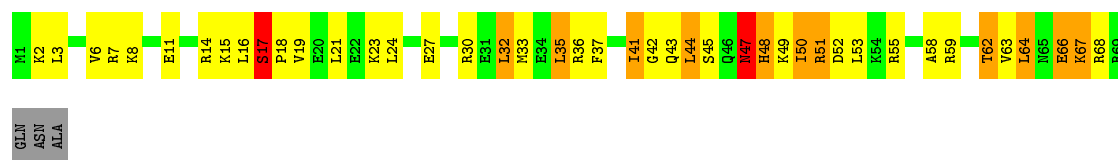


- Molecule 52: 50S ribosomal protein L28



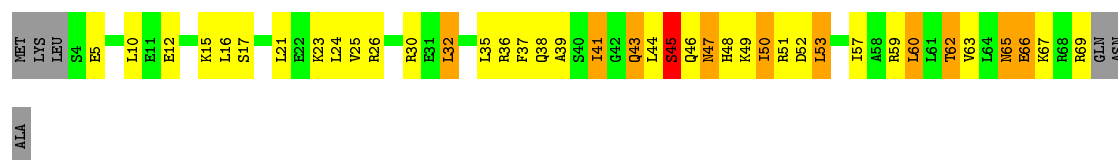
- Molecule 53: 50S ribosomal protein L29

Chain K8: 



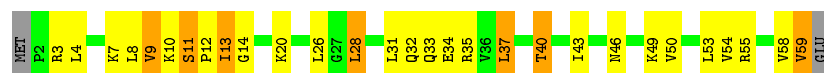
- Molecule 53: 50S ribosomal protein L29

Chain G5: 



- Molecule 54: 50S ribosomal protein L30

Chain L8: 



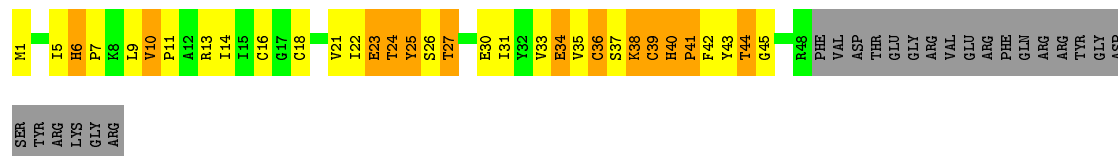
- Molecule 54: 50S ribosomal protein L30

Chain H5: 



- Molecule 55: 50S ribosomal protein L31

Chain M8: 



- Molecule 56: 50S ribosomal protein L32

Chain N8: 

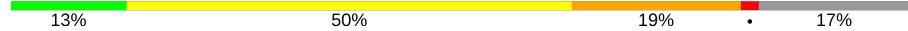


- Molecule 56: 50S ribosomal protein L32

Chain J5: 



- Molecule 57: 50S ribosomal protein L33

Chain O8: 



- Molecule 58: 50S ribosomal protein L34

Chain P8: 



- Molecule 58: 50S ribosomal protein L34

Chain L5: 



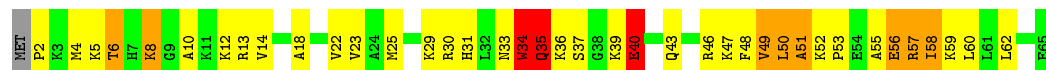
- Molecule 59: 50S ribosomal protein L35

Chain Q8: 



- Molecule 59: 50S ribosomal protein L35

Chain M5: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.05Å 449.39Å 618.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.44 – 3.16 153.44 – 3.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.44-3.16) 88.4 (153.44-3.16)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	(Not available) , (Not available) 0.196 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	306138	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, 7MG, SF4, MG, 2MA, 4SU, RSP, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.81	8/36375 (0.0%)	1.50	549/56770 (1.0%)
1	1G	0.71	1/36309 (0.0%)	1.36	301/56668 (0.5%)
2	12	0.49	0/1959	0.70	4/2642 (0.2%)
2	1E	0.46	0/1908	0.65	1/2573 (0.0%)
3	22	0.43	0/1556	0.63	1/2098 (0.0%)
3	2E	0.50	0/1629	0.66	0/2195
4	32	0.48	0/1732	0.67	1/2318 (0.0%)
4	3E	0.50	0/1720	0.68	0/2305
5	42	0.49	0/1171	0.66	1/1576 (0.1%)
5	4E	0.50	0/1158	0.67	0/1559
6	52	0.52	0/855	0.65	1/1154 (0.1%)
6	5E	0.55	0/855	0.67	0/1154
7	62	0.48	0/1122	0.65	2/1500 (0.1%)
7	6E	0.44	0/1259	0.59	0/1686
8	72	0.40	0/1135	0.61	0/1527
8	7E	0.47	0/1135	0.66	0/1527
9	82	0.39	0/1002	0.58	0/1346
9	8E	0.44	0/1019	0.65	0/1367
10	1A	0.44	0/814	0.71	1/1095 (0.1%)
10	1I	0.52	0/814	0.71	0/1095
11	2A	0.45	0/850	0.60	0/1150
11	2I	0.52	0/838	0.67	0/1133
12	3A	0.50	0/963	0.73	0/1290
12	3I	0.59	0/972	0.80	0/1301
13	4A	0.42	0/897	0.69	1/1204 (0.1%)
13	4I	0.48	0/946	0.66	0/1270
14	5A	0.47	0/475	0.75	0/632
14	5I	0.56	0/508	0.74	0/674
15	6A	0.44	0/740	0.61	0/987
15	6I	0.49	0/740	0.62	0/987
16	7A	0.45	0/721	0.64	0/970
16	7I	0.46	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.51	0/836	0.64	0/1117
17	8I	0.58	1/847 (0.1%)	0.67	0/1131
18	9A	0.53	0/549	0.77	0/732
18	9I	0.51	0/549	0.75	0/732
19	AA	0.44	0/490	0.70	0/662
19	AI	0.54	0/657	0.82	0/885
20	BA	0.46	0/759	0.67	0/1000
20	BI	0.44	0/753	0.67	0/993
21	1B	0.38	0/212	0.66	0/277
21	1F	0.48	0/212	0.71	0/277
22	1K	0.78	3/1578 (0.2%)	1.35	12/2445 (0.5%)
22	1L	0.81	3/1623 (0.2%)	1.27	16/2517 (0.6%)
23	2K	0.90	1/1721 (0.1%)	1.64	42/2682 (1.6%)
23	2L	0.75	1/1721 (0.1%)	1.38	22/2682 (0.8%)
24	3K	0.82	0/1741	1.38	22/2703 (0.8%)
24	3L	0.84	0/1764	1.44	26/2741 (0.9%)
25	4K	0.92	0/521	1.37	1/812 (0.1%)
25	4L	0.79	1/420 (0.2%)	1.34	2/652 (0.3%)
26	14	0.94	72/69830 (0.1%)	1.65	1642/109010 (1.5%)
26	1H	1.08	153/69835 (0.2%)	1.82	2345/109020 (2.2%)
27	16	0.82	0/2928	1.65	67/4568 (1.5%)
27	1J	0.78	2/2928 (0.1%)	1.52	50/4568 (1.1%)
28	71	0.38	0/1066	0.59	0/1439
28	79	0.34	0/1031	0.58	1/1394 (0.1%)
29	11	0.76	3/2170 (0.1%)	0.94	6/2926 (0.2%)
29	19	0.65	1/2170 (0.0%)	0.87	4/2926 (0.1%)
30	21	0.62	0/1591	0.82	1/2146 (0.0%)
30	29	0.57	0/1591	0.79	0/2146
31	31	0.67	1/1620 (0.1%)	0.80	1/2194 (0.0%)
31	39	0.56	0/1645	0.78	1/2228 (0.0%)
32	41	0.53	1/1481 (0.1%)	0.74	2/1994 (0.1%)
32	49	0.44	0/1481	0.66	1/1994 (0.1%)
33	51	0.57	0/1337	0.87	2/1809 (0.1%)
33	59	0.45	0/1337	0.79	5/1809 (0.3%)
34	18	0.53	0/236	0.81	0/315
34	28	0.51	0/236	0.86	1/315 (0.3%)
35	61	0.48	0/1146	0.74	1/1551 (0.1%)
35	69	0.49	0/1146	0.73	1/1551 (0.1%)
36	38	0.62	1/1104 (0.1%)	1.25	16/1494 (1.1%)
37	48	0.42	0/1067	0.82	1/1448 (0.1%)
38	15	0.43	0/1123	0.64	0/1515
38	58	0.54	0/1123	0.74	1/1514 (0.1%)
39	25	0.58	0/942	0.78	2/1269 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	68	0.60	0/942	0.76	0/1269
40	35	0.60	0/1147	0.96	3/1525 (0.2%)
40	78	0.61	0/1139	0.95	2/1514 (0.1%)
41	45	0.59	0/1120	0.85	2/1498 (0.1%)
41	88	0.67	0/1134	0.83	0/1519
42	55	0.55	0/981	0.80	0/1312
42	98	0.54	0/981	0.78	0/1312
43	65	0.51	0/886	0.77	1/1180 (0.1%)
43	A8	0.57	0/891	0.90	3/1187 (0.3%)
44	75	0.68	1/1129 (0.1%)	0.71	0/1509
44	B8	0.58	0/1146	0.76	1/1531 (0.1%)
45	85	0.54	0/981	0.75	1/1306 (0.1%)
45	C8	0.64	0/968	0.87	4/1289 (0.3%)
46	95	0.55	0/785	0.78	0/1052
46	D8	0.66	0/789	0.86	5/1057 (0.5%)
47	A5	0.57	0/897	0.75	0/1204
47	E8	0.63	0/901	0.78	1/1209 (0.1%)
48	B5	0.63	0/752	0.74	0/1010
48	F8	0.67	0/757	0.79	0/1017
49	C5	0.53	0/798	0.83	2/1071 (0.2%)
49	G8	0.68	1/797 (0.1%)	0.79	1/1068 (0.1%)
50	D5	0.47	0/1615	0.77	2/2191 (0.1%)
50	H8	0.47	0/1359	0.78	2/1841 (0.1%)
51	E5	0.52	0/624	0.71	0/832
51	I8	0.74	2/638 (0.3%)	0.89	1/851 (0.1%)
52	F5	0.59	0/744	0.79	1/989 (0.1%)
52	J8	0.62	0/736	0.82	0/978
53	G5	0.61	0/560	0.71	0/741
53	K8	0.63	0/578	0.85	1/766 (0.1%)
54	H5	0.52	0/464	0.66	0/623
54	L8	0.58	0/464	0.72	0/623
55	M8	0.53	0/380	0.81	0/514
56	J5	0.61	0/448	0.74	0/606
56	N8	0.68	0/399	0.78	0/541
57	O8	0.69	0/396	1.08	3/529 (0.6%)
58	L5	0.65	0/417	0.84	1/550 (0.2%)
58	P8	0.73	0/409	0.95	2/540 (0.4%)
59	M5	0.83	3/524 (0.6%)	0.93	1/691 (0.1%)
59	Q8	0.67	0/524	0.91	2/691 (0.3%)
All	All	0.83	260/325210 (0.1%)	1.45	5199/486635 (1.1%)

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
2	12	0	3
2	1E	0	5
3	22	0	1
3	2E	0	1
4	32	0	4
4	3E	0	1
5	4E	0	1
9	8E	0	1
10	1I	0	1
12	3A	0	2
12	3I	0	3
13	4A	0	4
14	5I	0	1
18	9I	0	2
19	AA	0	2
19	AI	0	4
20	BA	0	4
20	BI	0	2
29	11	0	7
29	19	0	6
30	21	0	6
30	29	0	7
31	31	0	2
31	39	0	5
32	41	0	2
32	49	0	3
33	51	0	5
33	59	0	5
34	18	0	2
34	28	0	2
35	61	0	3
35	69	0	1
36	38	0	21
37	48	0	11
38	15	0	2
38	58	0	1
40	35	0	7
40	78	0	4
41	45	0	9
43	A8	0	1
44	75	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
45	85	0	2
45	C8	0	4
46	95	0	4
46	D8	0	2
48	F8	0	1
49	C5	0	8
49	G8	0	3
50	D5	0	10
50	H8	0	2
52	F5	0	2
52	J8	0	1
53	G5	0	3
53	K8	0	1
55	M8	0	3
57	O8	0	2
59	M5	0	4
59	Q8	0	1
All	All	0	208

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	783	A	N9-C4	-12.97	1.30	1.37
26	1H	774	A	N9-C4	-12.58	1.30	1.37
44	75	106	SER	CA-CB	11.37	1.70	1.52
29	11	239	ARG	C-N	-10.85	1.09	1.34
26	1H	2476	A	N9-C4	9.90	1.43	1.37

The worst 5 of 5199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	945	A	N1-C6-N6	19.92	130.55	118.60
26	1H	676	A	C2-N3-C4	-19.33	100.94	110.60
26	1H	945	A	N1-C6-N6	17.89	129.34	118.60
26	14	783	A	C5-N7-C8	-17.43	95.19	103.90
26	14	783	A	C2-N3-C4	-17.33	101.93	110.60

There are no chirality outliers.

5 of 208 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide
2	1E	19	HIS	Peptide
2	1E	230	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide

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	13	32497	0	16403	888	0
1	1G	32437	0	16372	860	0
2	12	1924	0	1975	127	0
2	1E	1874	0	1926	113	0
3	22	1533	0	1595	77	0
3	2E	1605	0	1668	55	0
4	32	1702	0	1765	94	0
4	3E	1690	0	1737	83	0
5	42	1155	0	1213	57	0
5	4E	1142	0	1204	50	0
6	52	842	0	857	33	0
6	5E	842	0	857	30	0
7	62	1110	0	1163	67	0
7	6E	1242	0	1286	50	0
8	72	1115	0	1177	54	0
8	7E	1115	0	1177	66	0
9	82	983	0	1006	68	0
9	8E	1000	0	1031	65	0
10	1A	801	0	849	85	0
10	1I	801	0	848	56	0
11	2A	835	0	847	36	0
11	2I	823	0	833	41	0
12	3A	947	0	1033	63	0
12	3I	956	0	1046	58	0
13	4A	887	0	935	66	0
13	4I	936	0	986	52	0
14	5A	466	0	499	29	0
14	5I	499	0	542	36	0
15	6A	729	0	768	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	26	0
16	7A	705	0	725	26	0
16	7I	700	0	720	54	0
17	8A	823	0	891	34	0
17	8I	834	0	904	61	0
18	9A	544	0	605	21	0
18	9I	544	0	605	36	0
19	AA	481	0	468	28	0
19	AI	643	0	662	33	0
20	BA	757	0	856	47	0
20	BI	751	0	848	56	0
21	1B	208	0	221	21	0
21	1F	208	0	221	9	0
22	1K	1544	0	791	49	0
22	1L	1584	0	811	51	0
23	2K	1646	0	845	40	0
23	2L	1646	0	845	39	0
24	3K	1561	0	796	51	0
24	3L	1581	0	805	63	0
25	4K	462	0	229	11	0
25	4L	374	0	187	10	0
26	14	62347	0	31431	1547	0
26	1H	62351	0	31424	1621	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	89	0
28	71	1043	0	1066	44	0
28	79	1010	0	1025	51	0
29	11	2120	0	2196	112	0
29	19	2120	0	2197	103	0
30	21	1558	0	1624	92	0
30	29	1558	0	1624	93	0
31	31	1585	0	1632	85	0
31	39	1610	0	1655	122	0
32	41	1457	0	1514	87	0
32	49	1457	0	1514	83	0
33	51	1312	0	1384	77	0
33	59	1312	0	1384	102	0
34	18	237	0	257	22	0
34	28	237	0	257	21	0
35	61	1131	0	1218	45	0
35	69	1131	0	1218	69	0
36	38	1089	0	1149	108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	48	1047	0	1082	87	0
38	15	1096	0	1168	39	0
38	58	1096	0	1169	59	0
39	25	932	0	996	53	0
39	68	932	0	996	31	0
40	35	1130	0	1217	111	0
40	78	1122	0	1206	95	0
41	45	1099	0	1152	88	0
41	88	1113	0	1157	55	0
42	55	967	0	1033	37	0
42	98	967	0	1033	48	0
43	65	876	0	938	88	0
43	A8	881	0	943	45	0
44	75	1115	0	1169	66	0
44	B8	1132	0	1189	70	0
45	85	963	0	1022	68	0
45	C8	950	0	1011	49	0
46	95	774	0	849	63	0
46	D8	778	0	852	40	1
47	A5	886	0	948	34	0
47	E8	890	0	951	24	0
48	B5	738	0	792	44	0
48	F8	743	0	794	39	0
49	C5	785	0	844	62	0
49	G8	784	0	853	44	0
50	D5	1582	0	1613	79	0
50	H8	1330	0	1360	75	0
51	E5	616	0	633	38	0
51	I8	630	0	640	28	0
52	F5	737	0	813	48	0
52	J8	729	0	802	30	0
53	G5	558	0	610	27	0
53	K8	576	0	628	45	0
54	H5	459	0	512	12	0
54	L8	459	0	512	20	0
55	M8	371	0	372	35	0
56	J5	434	0	454	19	0
56	N8	386	0	402	31	0
57	O8	389	0	404	33	0
58	L5	409	0	454	17	0
58	P8	401	0	436	19	0
59	M5	516	0	582	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Q8	516	0	582	36	0
60	11	6	0	0	0	0
60	13	227	0	0	0	0
60	14	607	0	0	0	0
60	16	20	0	0	0	0
60	1G	167	0	0	0	0
60	1H	669	0	0	0	0
60	1J	8	0	0	0	0
60	1K	2	0	0	0	0
60	1L	1	0	0	0	0
60	21	2	0	0	0	0
60	25	2	0	0	0	0
60	29	5	0	0	0	0
60	2A	1	0	0	0	0
60	2K	7	0	0	0	0
60	2L	2	0	0	0	0
60	31	2	0	0	0	0
60	32	2	0	0	0	0
60	35	1	0	0	0	0
60	39	2	0	0	0	0
60	3E	2	0	0	0	0
60	41	1	0	0	0	0
60	45	2	0	0	0	0
60	4K	1	0	0	0	0
60	4L	2	0	0	0	0
60	52	1	0	0	0	0
60	55	2	0	0	0	0
60	5E	2	0	0	0	0
60	6I	1	0	0	0	0
60	75	1	0	0	0	0
60	78	1	0	0	0	0
60	88	4	0	0	0	0
60	98	2	0	0	0	0
60	C5	1	0	0	0	0
60	E5	1	0	0	0	0
60	F5	1	0	0	0	0
60	I8	2	0	0	0	0
60	M5	1	0	0	0	0
60	N8	1	0	0	0	0
60	P8	1	0	0	0	0
60	Q8	1	0	0	0	0
61	32	8	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	3E	8	0	0	2	0
62	5A	1	0	0	0	0
62	5I	1	0	0	0	0
63	11	12	0	0	2	0
63	13	544	0	0	91	0
63	14	1520	0	0	275	0
63	15	1	0	0	0	0
63	16	42	0	0	7	0
63	19	12	0	0	4	0
63	1E	1	0	0	0	0
63	1F	1	0	0	0	0
63	1G	397	0	0	60	0
63	1H	1966	0	0	358	2
63	1I	1	0	0	0	0
63	1J	23	0	0	3	0
63	1K	1	0	0	0	0
63	21	9	0	0	2	0
63	25	13	0	0	1	0
63	29	9	0	0	1	0
63	2K	16	0	0	5	0
63	2L	7	0	0	0	0
63	31	8	0	0	0	0
63	32	5	0	0	0	0
63	35	5	0	0	1	0
63	39	8	0	0	1	0
63	3A	2	0	0	0	0
63	3E	1	0	0	0	0
63	3I	5	0	0	0	0
63	42	1	0	0	0	0
63	45	4	0	0	0	0
63	4E	2	0	0	0	0
63	4K	13	0	0	0	0
63	4L	8	0	0	1	0
63	52	4	0	0	1	0
63	58	3	0	0	0	0
63	5A	1	0	0	0	0
63	5I	3	0	0	2	0
63	6A	1	0	0	0	0
63	6I	4	0	0	0	0
63	78	10	0	0	4	0
63	7A	2	0	0	0	0
63	85	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	88	7	0	0	0	0
63	8E	1	0	0	0	0
63	98	1	0	0	0	0
63	9A	2	0	0	0	0
63	A5	1	0	0	0	0
63	A8	2	0	0	0	0
63	B5	1	0	0	0	0
63	B8	3	0	0	0	0
63	BA	2	0	0	0	0
63	BI	1	0	0	0	0
63	C5	1	0	0	0	0
63	C8	7	0	0	0	1
63	D8	1	0	0	0	0
63	E5	3	0	0	0	0
63	F5	6	0	0	1	0
63	F8	1	0	0	0	0
63	G8	3	0	0	0	0
63	I8	5	0	0	1	0
63	J8	10	0	0	2	0
63	L5	2	0	0	0	0
63	L8	4	0	0	2	0
63	M5	9	0	0	0	0
63	P8	1	0	0	0	0
63	Q8	7	0	0	0	0
All	All	306138	0	202999	9699	2

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 20.

The worst 5 of 9699 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)
26:1H:1268:A:OP1	63:1H:3723:HOH:O	1.66	1.12
26:14:1604:C:OP2	63:14:3715:HOH:O	1.65	1.11
26:1H:2032:G:H21	30:21:146:THR:HG23	1.17	1.07
26:1H:2711:A:OP2	63:1H:3724:HOH:O	1.71	1.06
26:14:1603:A:OP1	63:14:3715:HOH:O	1.74	1.05

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:D8:45:THR:CG2	63:1H:4620:HOH:O[4_465]	1.38	0.82
63:1H:4955:HOH:O	63:C8:206:HOH:O[4_565]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	12	235/256 (92%)	183 (78%)	47 (20%)	5 (2%)	7	33
2	1E	227/256 (89%)	171 (75%)	54 (24%)	2 (1%)	17	53
3	22	191/239 (80%)	149 (78%)	41 (22%)	1 (0%)	29	65
3	2E	203/239 (85%)	169 (83%)	33 (16%)	1 (0%)	29	65
4	32	206/209 (99%)	168 (82%)	34 (16%)	4 (2%)	8	36
4	3E	205/209 (98%)	172 (84%)	31 (15%)	2 (1%)	15	51
5	42	149/162 (92%)	132 (89%)	17 (11%)	0	100	100
5	4E	147/162 (91%)	128 (87%)	18 (12%)	1 (1%)	22	59
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
7	62	134/156 (86%)	108 (81%)	24 (18%)	2 (2%)	10	41
7	6E	152/156 (97%)	139 (91%)	13 (9%)	0	100	100
8	72	136/138 (99%)	120 (88%)	16 (12%)	0	100	100
8	7E	136/138 (99%)	116 (85%)	20 (15%)	0	100	100
9	82	122/128 (95%)	104 (85%)	17 (14%)	1 (1%)	19	55
9	8E	124/128 (97%)	100 (81%)	22 (18%)	2 (2%)	9	40
10	1A	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
10	1I	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	15	51
11	2A	111/129 (86%)	94 (85%)	16 (14%)	1 (1%)	17	53
11	2I	109/129 (84%)	94 (86%)	15 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3A	119/132 (90%)	91 (76%)	23 (19%)	5 (4%)	3	17
12	3I	120/132 (91%)	101 (84%)	19 (16%)	0	100	100
13	4A	109/126 (86%)	84 (77%)	24 (22%)	1 (1%)	17	53
13	4I	117/126 (93%)	91 (78%)	25 (21%)	1 (1%)	17	53
14	5A	55/61 (90%)	38 (69%)	15 (27%)	2 (4%)	3	20
14	5I	59/61 (97%)	48 (81%)	9 (15%)	2 (3%)	3	21
15	6A	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
15	6I	85/89 (96%)	72 (85%)	13 (15%)	0	100	100
16	7A	82/88 (93%)	71 (87%)	11 (13%)	0	100	100
16	7I	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	8A	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	8I	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	9A	65/88 (74%)	56 (86%)	9 (14%)	0	100	100
18	9I	65/88 (74%)	57 (88%)	6 (9%)	2 (3%)	4	23
19	AA	56/93 (60%)	44 (79%)	12 (21%)	0	100	100
19	AI	78/93 (84%)	57 (73%)	15 (19%)	6 (8%)	1	5
20	BA	96/106 (91%)	79 (82%)	14 (15%)	3 (3%)	4	23
20	BI	96/106 (91%)	75 (78%)	17 (18%)	4 (4%)	3	17
21	1B	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	16
21	1F	22/27 (82%)	19 (86%)	2 (9%)	1 (4%)	2	16
28	7I	130/229 (57%)	114 (88%)	16 (12%)	0	100	100
28	79	126/229 (55%)	107 (85%)	19 (15%)	0	100	100
29	11	271/276 (98%)	231 (85%)	37 (14%)	3 (1%)	14	48
29	19	271/276 (98%)	234 (86%)	37 (14%)	0	100	100
30	21	201/206 (98%)	149 (74%)	44 (22%)	8 (4%)	3	18
30	29	201/206 (98%)	145 (72%)	50 (25%)	6 (3%)	4	24
31	31	200/210 (95%)	169 (84%)	28 (14%)	3 (2%)	10	41
31	39	204/210 (97%)	152 (74%)	46 (22%)	6 (3%)	4	25
32	41	177/182 (97%)	150 (85%)	26 (15%)	1 (1%)	25	62
32	49	177/182 (97%)	142 (80%)	32 (18%)	3 (2%)	9	38
33	51	169/180 (94%)	125 (74%)	35 (21%)	9 (5%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	59	169/180 (94%)	108 (64%)	54 (32%)	7 (4%)	3	18
34	18	28/125 (22%)	20 (71%)	7 (25%)	1 (4%)	3	20
34	28	28/125 (22%)	23 (82%)	4 (14%)	1 (4%)	3	20
35	61	143/148 (97%)	104 (73%)	35 (24%)	4 (3%)	5	26
35	69	143/148 (97%)	109 (76%)	30 (21%)	4 (3%)	5	26
36	38	141/173 (82%)	65 (46%)	54 (38%)	22 (16%)	0	1
37	48	140/147 (95%)	75 (54%)	57 (41%)	8 (6%)	1	12
38	15	135/140 (96%)	115 (85%)	20 (15%)	0	100	100
38	58	135/140 (96%)	108 (80%)	25 (18%)	2 (2%)	10	41
39	25	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	19	55
39	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
40	35	146/150 (97%)	95 (65%)	43 (30%)	8 (6%)	2	12
40	78	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	22	59
41	45	136/141 (96%)	98 (72%)	33 (24%)	5 (4%)	3	19
41	88	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	11	43
42	55	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
42	98	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
43	65	108/112 (96%)	82 (76%)	22 (20%)	4 (4%)	3	19
43	A8	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
44	75	132/146 (90%)	110 (83%)	22 (17%)	0	100	100
44	B8	134/146 (92%)	105 (78%)	29 (22%)	0	100	100
45	85	115/118 (98%)	96 (84%)	19 (16%)	0	100	100
45	C8	113/118 (96%)	93 (82%)	18 (16%)	2 (2%)	8	37
46	95	98/101 (97%)	71 (72%)	21 (21%)	6 (6%)	1	10
46	D8	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
47	A5	109/113 (96%)	97 (89%)	12 (11%)	0	100	100
47	E8	110/113 (97%)	95 (86%)	15 (14%)	0	100	100
48	B5	92/96 (96%)	79 (86%)	13 (14%)	0	100	100
48	F8	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	14	48
49	C5	104/110 (94%)	66 (64%)	31 (30%)	7 (7%)	1	8
49	G8	103/110 (94%)	73 (71%)	30 (29%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D5	198/206 (96%)	136 (69%)	54 (27%)	8 (4%)	3	18
50	H8	161/206 (78%)	123 (76%)	32 (20%)	6 (4%)	3	19
51	E5	76/85 (89%)	65 (86%)	11 (14%)	0	100	100
51	I8	79/85 (93%)	63 (80%)	15 (19%)	1 (1%)	12	44
52	F5	92/98 (94%)	81 (88%)	9 (10%)	2 (2%)	6	32
52	J8	91/98 (93%)	79 (87%)	12 (13%)	0	100	100
53	G5	64/72 (89%)	58 (91%)	5 (8%)	1 (2%)	9	40
53	K8	67/72 (93%)	57 (85%)	8 (12%)	2 (3%)	4	24
54	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
54	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
55	M8	46/71 (65%)	24 (52%)	20 (44%)	2 (4%)	2	17
56	J5	54/60 (90%)	47 (87%)	7 (13%)	0	100	100
56	N8	48/60 (80%)	42 (88%)	6 (12%)	0	100	100
57	O8	43/54 (80%)	26 (60%)	16 (37%)	1 (2%)	6	31
58	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
58	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
59	M5	62/65 (95%)	49 (79%)	12 (19%)	1 (2%)	9	40
59	Q8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	22
All	All	11677/12957 (90%)	9408 (81%)	2067 (18%)	202 (2%)	9	38

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	4I	12	ASN
30	21	78	LEU
30	21	83	ASP
33	51	10	PRO
34	18	25	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	12	205/220 (93%)	155 (76%)	50 (24%)	0	2
2	1E	200/220 (91%)	146 (73%)	54 (27%)	0	1
3	22	153/188 (81%)	114 (74%)	39 (26%)	0	2
3	2E	159/188 (85%)	126 (79%)	33 (21%)	1	5
4	32	180/181 (99%)	143 (79%)	37 (21%)	1	5
4	3E	178/181 (98%)	145 (82%)	33 (18%)	1	8
5	42	116/123 (94%)	84 (72%)	32 (28%)	0	1
5	4E	115/123 (94%)	92 (80%)	23 (20%)	1	6
6	52	90/90 (100%)	77 (86%)	13 (14%)	3	14
6	5E	90/90 (100%)	74 (82%)	16 (18%)	2	8
7	62	114/127 (90%)	89 (78%)	25 (22%)	1	4
7	6E	125/127 (98%)	102 (82%)	23 (18%)	1	8
8	72	119/119 (100%)	101 (85%)	18 (15%)	3	13
8	7E	119/119 (100%)	94 (79%)	25 (21%)	1	5
9	82	95/99 (96%)	69 (73%)	26 (27%)	0	1
9	8E	97/99 (98%)	69 (71%)	28 (29%)	0	1
10	1A	89/92 (97%)	67 (75%)	22 (25%)	0	2
10	1I	89/92 (97%)	68 (76%)	21 (24%)	1	3
11	2A	85/99 (86%)	66 (78%)	19 (22%)	1	4
11	2I	84/99 (85%)	61 (73%)	23 (27%)	0	1
12	3A	102/109 (94%)	81 (79%)	21 (21%)	1	5
12	3I	103/109 (94%)	80 (78%)	23 (22%)	1	4
13	4A	90/101 (89%)	63 (70%)	27 (30%)	0	1
13	4I	93/101 (92%)	72 (77%)	21 (23%)	1	4
14	5A	47/50 (94%)	32 (68%)	15 (32%)	0	0
14	5I	50/50 (100%)	41 (82%)	9 (18%)	1	8
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	12
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	7A	72/74 (97%)	59 (82%)	13 (18%)	1	8
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	7
18	9I	58/77 (75%)	48 (83%)	10 (17%)	2	9
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	5
19	AI	70/80 (88%)	52 (74%)	18 (26%)	0	2
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	3
20	BI	75/82 (92%)	54 (72%)	21 (28%)	0	1
21	1B	19/22 (86%)	18 (95%)	1 (5%)	22	55
21	1F	19/22 (86%)	17 (90%)	2 (10%)	7	26
28	71	110/181 (61%)	82 (74%)	28 (26%)	0	2
28	79	107/181 (59%)	97 (91%)	10 (9%)	9	31
29	11	214/218 (98%)	170 (79%)	44 (21%)	1	5
29	19	214/218 (98%)	163 (76%)	51 (24%)	0	3
30	21	165/166 (99%)	119 (72%)	46 (28%)	0	1
30	29	165/166 (99%)	129 (78%)	36 (22%)	1	5
31	31	161/166 (97%)	122 (76%)	39 (24%)	0	2
31	39	163/166 (98%)	119 (73%)	44 (27%)	0	1
32	41	153/156 (98%)	117 (76%)	36 (24%)	1	3
32	49	153/156 (98%)	111 (72%)	42 (28%)	0	1
33	51	142/148 (96%)	100 (70%)	42 (30%)	0	1
33	59	142/148 (96%)	105 (74%)	37 (26%)	0	2
34	18	26/90 (29%)	18 (69%)	8 (31%)	0	1
34	28	26/90 (29%)	13 (50%)	13 (50%)	0	0
35	61	122/124 (98%)	90 (74%)	32 (26%)	0	2
35	69	122/124 (98%)	84 (69%)	38 (31%)	0	1
36	38	115/135 (85%)	64 (56%)	51 (44%)	0	0
37	48	106/111 (96%)	67 (63%)	39 (37%)	0	0
38	15	116/119 (98%)	89 (77%)	27 (23%)	1	3
38	58	116/119 (98%)	88 (76%)	28 (24%)	0	2
39	25	100/100 (100%)	78 (78%)	22 (22%)	1	4
39	68	100/100 (100%)	89 (89%)	11 (11%)	6	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	35	115/116 (99%)	82 (71%)	33 (29%)	0	1
40	78	114/116 (98%)	77 (68%)	37 (32%)	0	0
41	45	109/111 (98%)	79 (72%)	30 (28%)	0	1
41	88	109/111 (98%)	93 (85%)	16 (15%)	3	13
42	55	101/101 (100%)	82 (81%)	19 (19%)	1	7
42	98	101/101 (100%)	77 (76%)	24 (24%)	0	3
43	65	87/88 (99%)	59 (68%)	28 (32%)	0	0
43	A8	87/88 (99%)	57 (66%)	30 (34%)	0	0
44	75	117/127 (92%)	85 (73%)	32 (27%)	0	1
44	B8	119/127 (94%)	87 (73%)	32 (27%)	0	1
45	85	93/94 (99%)	77 (83%)	16 (17%)	2	9
45	C8	92/94 (98%)	73 (79%)	19 (21%)	1	5
46	95	82/82 (100%)	66 (80%)	16 (20%)	1	7
46	D8	82/82 (100%)	58 (71%)	24 (29%)	0	1
47	A5	91/92 (99%)	68 (75%)	23 (25%)	0	2
47	E8	91/92 (99%)	75 (82%)	16 (18%)	2	9
48	B5	75/78 (96%)	59 (79%)	16 (21%)	1	5
48	F8	75/78 (96%)	60 (80%)	15 (20%)	1	6
49	C5	81/91 (89%)	58 (72%)	23 (28%)	0	1
49	G8	82/91 (90%)	66 (80%)	16 (20%)	1	7
50	D5	173/179 (97%)	129 (75%)	44 (25%)	0	2
50	H8	147/179 (82%)	112 (76%)	35 (24%)	0	3
51	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
51	I8	62/67 (92%)	48 (77%)	14 (23%)	1	4
52	F5	79/83 (95%)	53 (67%)	26 (33%)	0	0
52	J8	78/83 (94%)	61 (78%)	17 (22%)	1	5
53	G5	62/67 (92%)	43 (69%)	19 (31%)	0	1
53	K8	63/67 (94%)	44 (70%)	19 (30%)	0	1
54	H5	50/52 (96%)	43 (86%)	7 (14%)	3	15
54	L8	50/52 (96%)	38 (76%)	12 (24%)	0	3
55	M8	42/63 (67%)	30 (71%)	12 (29%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	J5	48/52 (92%)	38 (79%)	10 (21%)	1	5
56	N8	44/52 (85%)	34 (77%)	10 (23%)	1	4
57	O8	44/52 (85%)	29 (66%)	15 (34%)	0	0
58	L5	40/42 (95%)	34 (85%)	6 (15%)	3	13
58	P8	38/42 (90%)	34 (90%)	4 (10%)	7	26
59	M5	54/55 (98%)	40 (74%)	14 (26%)	0	2
59	Q8	54/55 (98%)	41 (76%)	13 (24%)	0	2
All	All	9836/10671 (92%)	7504 (76%)	2332 (24%)	1	3

5 of 2332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	F8	68	ARG
3	22	141	VAL
47	A5	110	LYS
50	H8	46	LYS
55	M8	43	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
16	7A	16	HIS
29	19	44	ASN
43	65	95	HIS
28	79	44	HIS
30	29	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1511/1522 (99%)	381 (25%)	36 (2%)
1	1G	1508/1522 (99%)	380 (25%)	37 (2%)
22	1K	67/77 (87%)	31 (46%)	5 (7%)
22	1L	70/77 (90%)	28 (40%)	6 (8%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	68/77 (88%)	36 (52%)	4 (5%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	3L	70/77 (90%)	37 (52%)	3 (4%)
25	4K	20/27 (74%)	14 (70%)	1 (5%)
25	4L	15/27 (55%)	9 (60%)	0
26	14	2892/2917 (99%)	722 (24%)	51 (1%)
26	1H	2893/2917 (99%)	705 (24%)	67 (2%)
27	16	121/122 (99%)	28 (23%)	2 (1%)
27	1J	121/122 (99%)	32 (26%)	1 (0%)
All	All	9508/9638 (98%)	2440 (25%)	216 (2%)

5 of 2440 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

5 of 216 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	1757	U
1	1G	87	A
26	14	1819	A
26	1H	1899	G
26	1H	2439	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

22 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
23	5MU	2K	55	23	15,22,23	2.17	3 (20%)	16,32,35	1.78	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	5MU	2L	55	23	15,22,23	2.15	3 (20%)	16,32,35	1.77	2 (12%)
22	5MU	1K	55	22	15,22,23	2.23	3 (20%)	16,32,35	1.88	2 (12%)
22	4SU	1L	8	22	14,21,22	3.35	2 (14%)	15,30,33	1.41	2 (13%)
22	RSP	1L	33	22	15,21,22	3.32	6 (40%)	16,30,33	1.79	2 (12%)
23	4SU	2K	8	23	14,21,22	3.31	3 (21%)	15,30,33	1.20	2 (13%)
22	PSU	1K	56	22	17,21,22	1.04	1 (5%)	20,30,33	3.55	5 (25%)
23	OMC	2L	33	23	15,22,23	2.27	4 (26%)	17,31,34	1.57	2 (11%)
22	5MU	1L	55	22	15,22,23	2.16	3 (20%)	16,32,35	1.87	2 (12%)
23	PSU	2K	56	23	17,21,22	1.11	1 (5%)	20,30,33	2.97	7 (35%)
22	2MA	1L	38	22	17,25,26	3.55	6 (35%)	19,37,40	2.19	5 (26%)
23	PSU	2L	56	23	17,21,22	1.19	1 (5%)	20,30,33	3.44	5 (25%)
22	2MA	1K	38	22	17,25,26	3.10	6 (35%)	19,37,40	2.12	4 (21%)
22	PSU	1L	56	22,41	17,21,22	1.00	1 (5%)	20,30,33	3.20	6 (30%)
22	RSP	1K	33	22	15,21,22	3.42	6 (40%)	16,30,33	1.79	2 (12%)
23	OMC	2K	33	23	15,22,23	2.22	4 (26%)	17,31,34	1.36	2 (11%)
22	4SU	1K	8	22	14,21,22	3.08	3 (21%)	15,30,33	1.42	3 (20%)
23	7MG	2K	47	23	22,26,27	3.33	6 (27%)	28,39,42	2.49	11 (39%)
23	7MG	2L	47	23	22,26,27	3.48	7 (31%)	28,39,42	2.53	11 (39%)
22	7MG	1K	47	22	22,26,27	3.49	6 (27%)	28,39,42	2.48	11 (39%)
22	7MG	1L	47	22	22,26,27	3.40	6 (27%)	28,39,42	2.46	10 (35%)
23	4SU	2L	8	23	14,21,22	3.29	2 (14%)	15,30,33	1.01	1 (6%)

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
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
22	5MU	1K	55	22	-	0/5/25/26	0/2/2/2
22	4SU	1L	8	22	-	2/5/25/26	0/2/2/2
22	RSP	1L	33	22	-	3/5/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
22	PSU	1K	56	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/7/27/28	0/2/2/2
22	5MU	1L	55	22	-	0/5/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	2MA	1L	38	22	-	0/3/25/26	0/3/3/3
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	2MA	1K	38	22	-	0/3/25/26	0/3/3/3
22	PSU	1L	56	22,41	-	0/7/25/26	0/2/2/2
22	RSP	1K	33	22	-	3/5/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
22	4SU	1K	8	22	-	2/5/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3
22	7MG	1K	47	22	-	3/7/37/38	0/3/3/3
22	7MG	1L	47	22	-	2/7/37/38	0/3/3/3
23	4SU	2L	8	23	-	0/5/25/26	0/2/2/2

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	47	7MG	C4-N3	11.63	1.49	1.34
23	2L	47	7MG	C4-N3	11.11	1.48	1.34
23	2K	47	7MG	C4-N3	10.84	1.48	1.34
22	1L	47	7MG	C4-N3	10.69	1.47	1.34
23	2K	8	4SU	C5-C4	10.09	1.49	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	N1-C2-N3	-12.19	118.74	128.43
22	1K	56	PSU	N1-C2-N3	-11.16	119.56	128.43
22	1L	56	PSU	N1-C2-N3	-10.30	120.24	128.43
23	2K	56	PSU	N1-C2-N3	-9.39	120.97	128.43
22	1K	56	PSU	C4-N3-C2	7.61	121.57	115.14

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	8	4SU	C2'-C1'-N1-C6
22	1L	33	RSP	C2'-C1'-N1-C6
22	1K	33	RSP	C2'-C1'-N1-C6
22	1K	33	RSP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2K	33	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	55	5MU	3	0
23	2L	55	5MU	2	0
22	1L	8	4SU	1	0
22	1L	33	RSP	4	0
23	2K	8	4SU	1	0
22	1K	56	PSU	1	0
23	2L	33	OMC	1	0
22	1L	55	5MU	1	0
22	1K	38	2MA	2	0
22	1L	56	PSU	1	0
22	1K	33	RSP	3	0
23	2K	33	OMC	1	0
22	1K	8	4SU	4	0
23	2K	47	7MG	1	0
23	2L	47	7MG	4	0
22	1K	47	7MG	3	0
23	2L	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1768 ligands modelled in this entry, 1766 are 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
61	SF4	32	303	4	0,12,12	0.00	-	-		
61	SF4	3E	303	4	0,12,12	0.00	-	-		

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
61	SF4	32	303	4	-	-	0/6/5/5
61	SF4	3E	303	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

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
61	32	303	SF4	2	0
61	3E	303	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	11	1
24	3K	1
32	41	1
24	3L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	49:C	O3'	50:G	P	6.50
1	3K	49:C	O3'	50:G	P	5.32
1	41	140:ILE	C	141:PHE	N	1.19
1	11	239:ARG	C	240:ALA	N	1.09

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.