



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2020 – 05:54 am BST

PDB ID : 6OXA
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S pre-cleavage (AAU)
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-13
Resolution : 3.25 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 : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

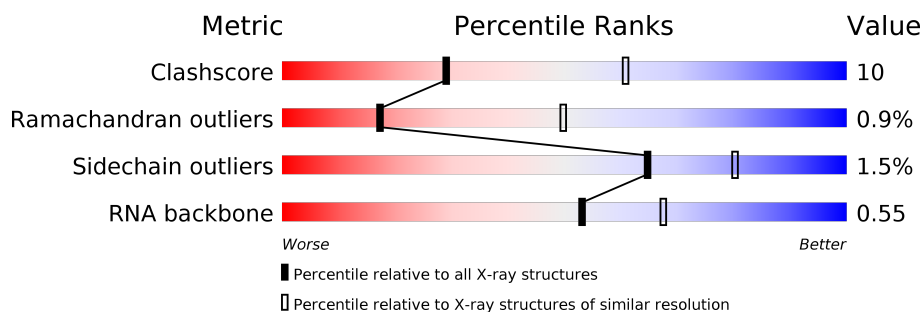
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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))
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

















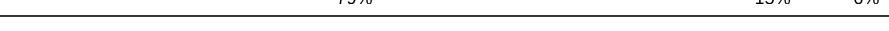

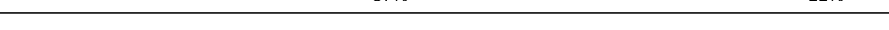
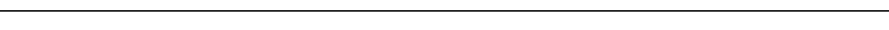
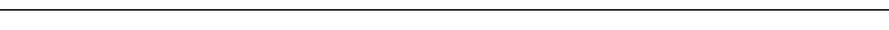
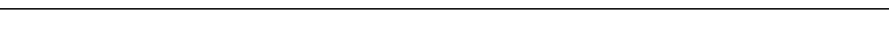
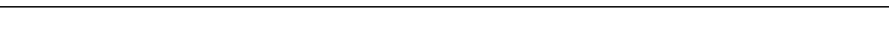
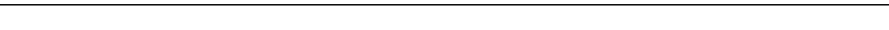

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	56% 33% 9% ..
1	XA	1521	58% 30% 10% ..
2	QB	256	33% 51% 7% • 8%
2	XB	256	79% 13% 8%
3	QC	239	70% 16% 14%
3	XC	239	77% 9% 14%
4	QD	209	81% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QM	126	
12	XM	126	
13	QN	61	
13	XN	61	
14	QO	89	
14	XO	89	
15	QP	88	
15	XP	88	
16	QQ	105	
16	XQ	105	















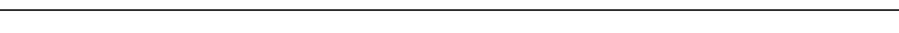




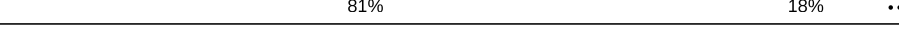

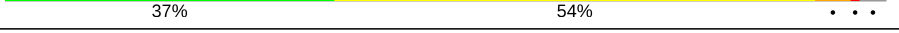



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	QR	88	
17	XR	88	
18	QS	93	
18	XS	93	
19	QT	106	
19	XT	106	
20	QU	27	
20	XU	27	
21	QV	77	
21	QW	77	
21	XV	77	
21	XW	77	
22	QX	22	
22	XX	22	
23	QY	84	
23	QZ	84	
23	XY	84	
23	XZ	84	
24	R0	85	
24	Y0	85	
25	R2	72	
25	Y2	72	
26	R3	60	
26	Y3	60	
27	R4	71	




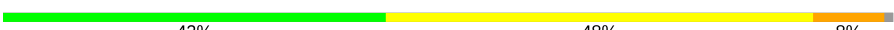

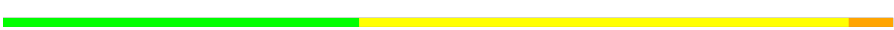



















Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	Y4	71	
28	R5	60	
28	Y5	60	
29	R6	54	
29	Y6	54	
30	R7	49	
30	Y7	49	
31	R9	37	
31	Y9	37	
32	RA	2915	
32	YA	2915	
33	RB	124	
33	YB	124	
34	RD	276	
34	YD	276	
35	RE	206	
35	YE	206	
36	RG	182	
36	YG	182	
37	RH	180	
37	YH	180	
38	RI	148	
38	YI	148	
39	RN	140	
39	YN	140	






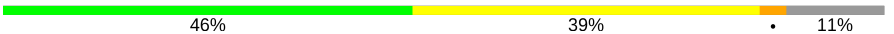

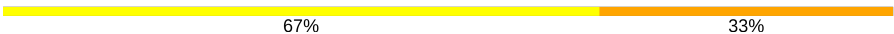
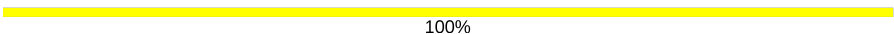
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	RO	122	 85% 15%
40	YO	122	 83% 17%
41	RP	150	 76% 20% .
41	YP	150	 43% 48% 8% .
42	RQ	141	 80% 19% .
42	YQ	141	 40% 55% 5%
43	RR	118	 87% 11% ..
43	YR	118	 90% 9% .
44	RS	112	 84% 15% .
44	YS	112	 76% 21% ...
45	RT	146	 71% 22% . 6%
45	YT	146	 70% 23% . 6%
46	RU	118	 83% 15% ..
46	YU	118	 86% 12% ..
47	RV	101	 86% 13% .
47	YV	101	 49% 50% .
48	RW	113	 80% 20%
48	YW	113	 86% 14%
49	RX	96	 82% 14% .
49	YX	96	 83% 13% .
50	RY	110	 83% 15% .
50	YY	110	 78% 18% ..
51	QL	132	 67% 25% .. 5%
51	XL	132	 78% 13% . 8%
52	R1	98	 57% 38% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	Y1	98	 82% 12% • 5%
53	R8	65	 57% 42% •
53	Y8	65	 77% 15% 5% • •
54	RF	210	 61% 33% • •
54	YF	210	 81% 14% •
55	RZ	206	 46% 39% • 11%
55	YZ	206	 58% 30% • 11%
56	ZA	3	 67% 33%
56	ZB	3	 100%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 298432 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	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	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	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	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
12	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
15	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
16	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QR	70	Total	C	N	O		0	0	0
			574	367	112	95				
17	XR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
18	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
19	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
20	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 21 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			
22	XX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			

- Molecule 23 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R3	59	Total	C	N	O		0	0	0
			469	298	90	81				
26	Y3	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
27	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
28	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
29	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
30	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
32	YA	2875	Total	C	N	O	P	0	0	0
			61921	27560	11583	19904	2874			

- Molecule 33 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
33	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 34 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
34	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 35 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
35	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
36	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
37	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
38	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
39	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 40 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
40	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
42	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RR	117	Total	C	N	O		0	0	0
			960	599	202	159				
43	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RS	111	Total	C	N	O		0	0	0
			882	556	176	150				
44	YS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
45	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
46	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 47 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
47	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
48	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 49 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
49	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
50	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 51 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
51	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			
52	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
53	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 54 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
54	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	94	Total	Mg	0	0
			94	94		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YV	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	QX	1	Total 1	Mg 1	0	0
57	YA	326	Total 326	Mg 326	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	QD	2	Total 2	Mg 2	0	0
57	RN	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	YD	5	Total 5	Mg 5	0	0
57	QV	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	116	Total 116	Mg 116	0	0
57	RQ	2	Total 2	Mg 2	0	0
57	R0	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YQ	3	Total 3	Mg 3	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RD	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	RA	302	Total 302	Mg 302	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	YF	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	YB	5	Total 5	Mg 5	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	3	Total 3	Mg 3	0	0
57	QE	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	5	Total 5	Mg 5	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

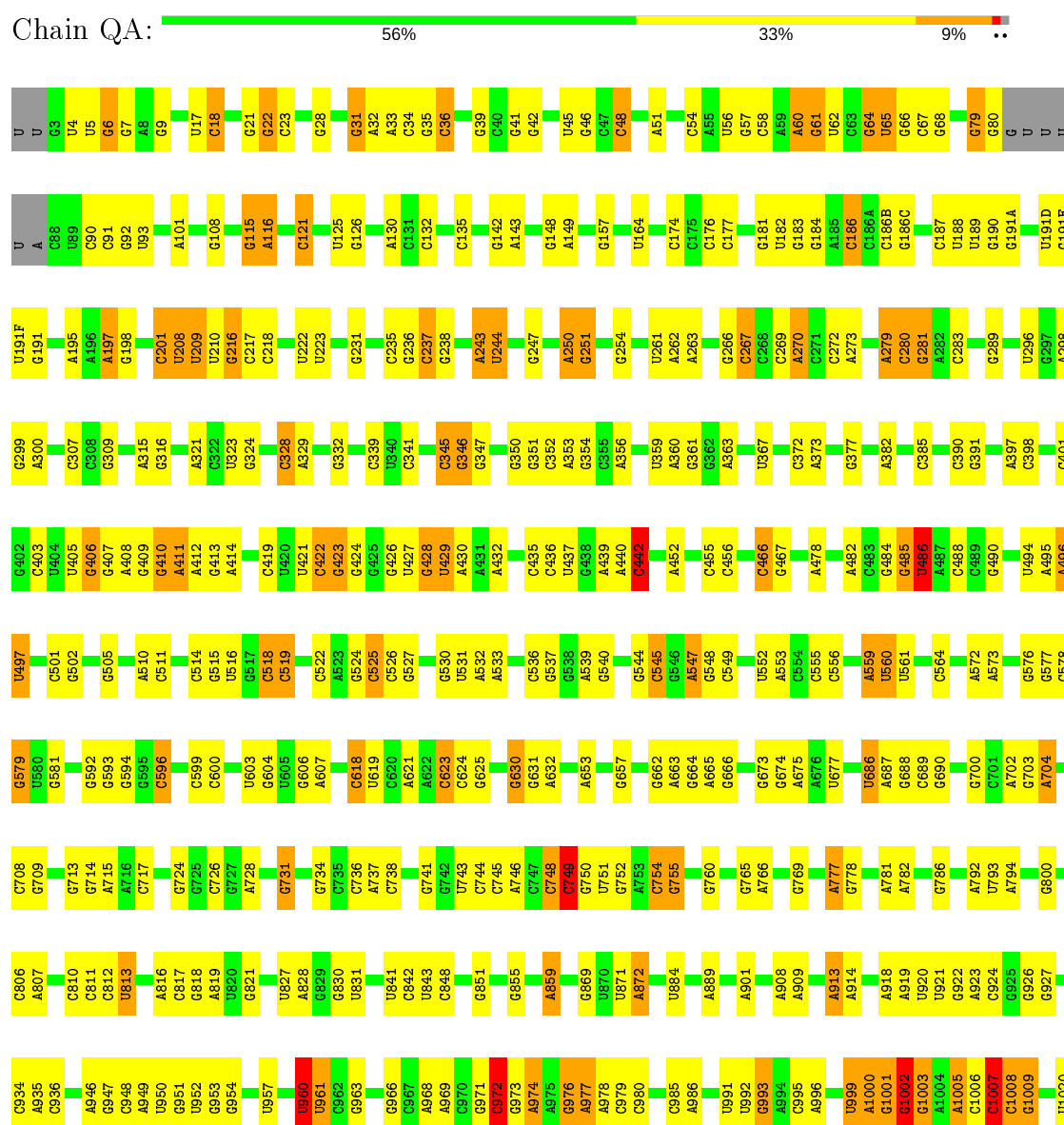
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

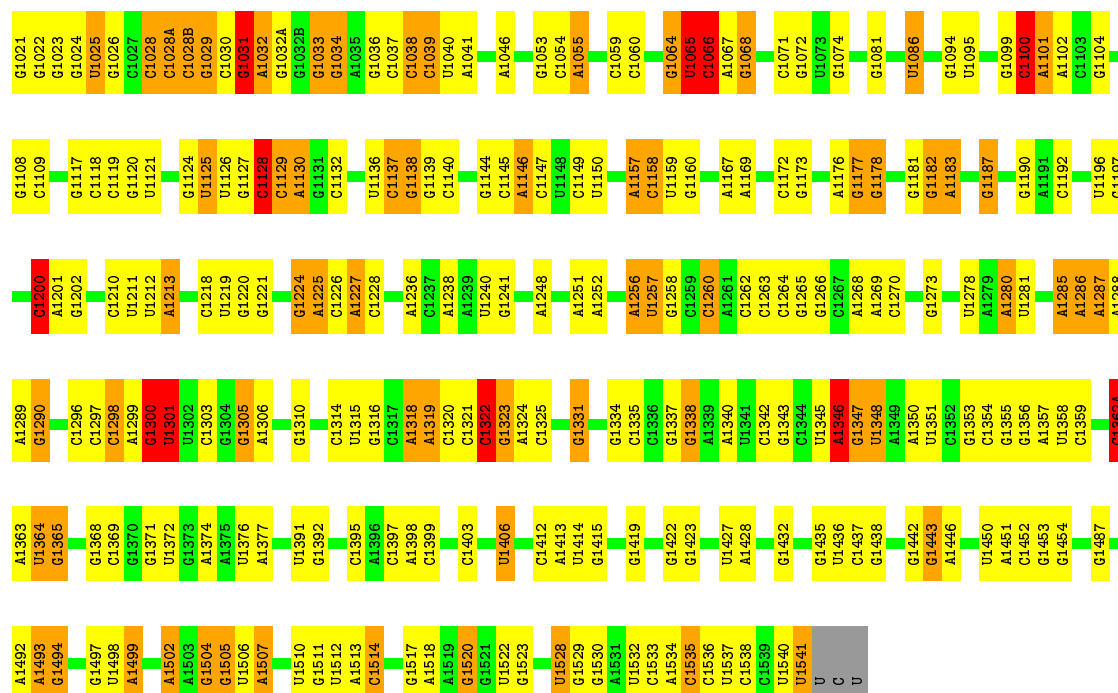
3 Residue-property plots

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.

Note EDS failed to run properly.

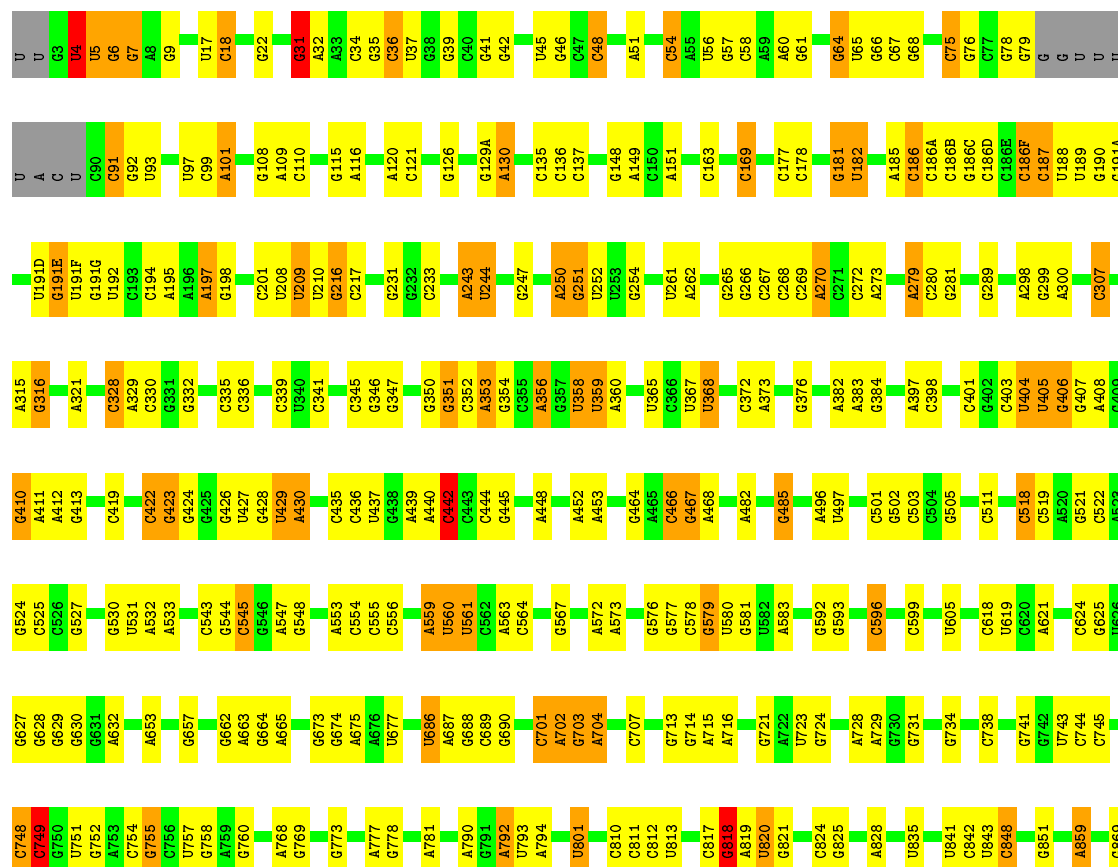
• Molecule 1: 16S rRNA



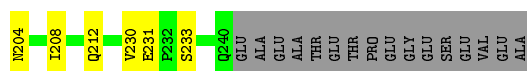


• Molecule 1: 16S rRNA

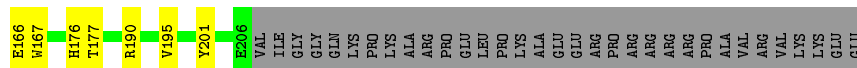
Chain XA: 58% 30% 10% 2%



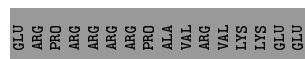
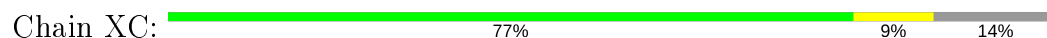




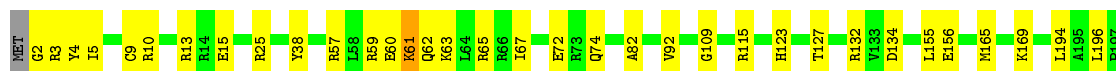
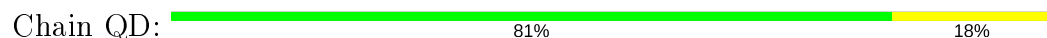
- Molecule 3: 30S ribosomal protein S3



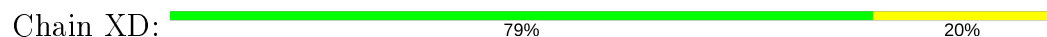
- Molecule 3: 30S ribosomal protein S3



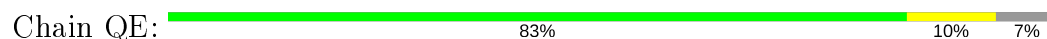
- Molecule 4: 30S ribosomal protein S4




- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



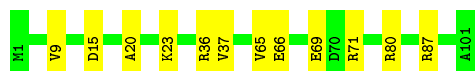
- Molecule 5: 30S ribosomal protein S5

Chain XE:  81% 12% 7%




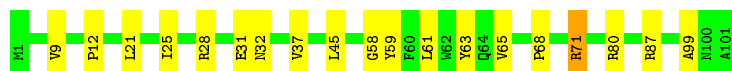
- Molecule 6: 30S ribosomal protein S6

Chain QF:  88% 12%



- Molecule 6: 30S ribosomal protein S6

Chain XF:  81% 18% .




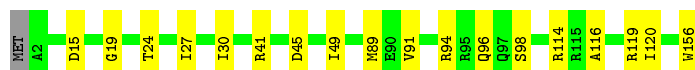
- Molecule 7: 30S ribosomal protein S7

Chain QG:  90% 10% .




- Molecule 7: 30S ribosomal protein S7

Chain XG:  88% 12% .



- Molecule 8: 30S ribosomal protein S8

Chain QH:  81% 17% ..




- Molecule 8: 30S ribosomal protein S8

Chain XH:  80% 20% .




- Molecule 9: 30S ribosomal protein S9

Chain QI:  74% 25%




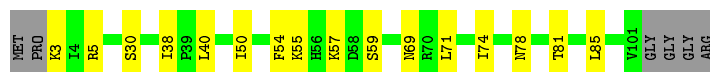
- Molecule 9: 30S ribosomal protein S9

Chain XI:  78% 20%



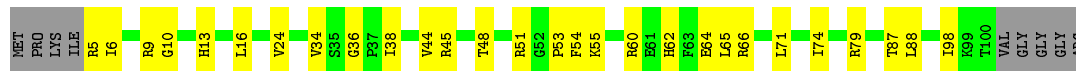
- Molecule 10: 30S ribosomal protein S10

Chain QJ:  79% 15% 6%




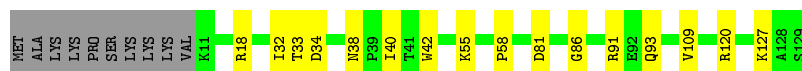
- Molecule 10: 30S ribosomal protein S10

Chain XJ:  65% 27% 9%




- Molecule 11: 30S ribosomal protein S11

Chain QK:  80% 12% 8%




- Molecule 11: 30S ribosomal protein S11

Chain XK:  77% 13% 10%




- Molecule 12: 30S ribosomal protein S13

Chain QM:  71% 21% 5%




- Molecule 12: 30S ribosomal protein S13

Chain XM:  79% 15% 6%



- Molecule 13: 30S ribosomal protein S14 type Z

Chain QN:  74% 25% .



- Molecule 13: 30S ribosomal protein S14 type Z

Chain XN:  87% 11% .




- Molecule 14: 30S ribosomal protein S15

Chain QO:  89% 10% .



- Molecule 14: 30S ribosomal protein S15

Chain XO:  84% 13% .



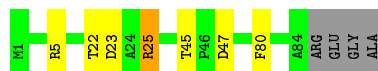
- Molecule 15: 30S ribosomal protein S16

Chain QP:  88% 8% 5%




- Molecule 15: 30S ribosomal protein S16

Chain XP:  88% 7% 5%




- Molecule 16: 30S ribosomal protein S17

Chain QQ:  83% 12% 5%



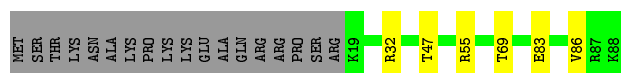
- Molecule 16: 30S ribosomal protein S17

Chain XQ:  84% 11% 5%




- Molecule 17: 30S ribosomal protein S18

Chain QR:  73% 7% 20%



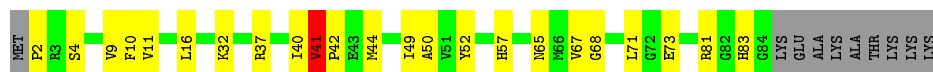
- Molecule 17: 30S ribosomal protein S18

Chain XR:  74% 6% 20%



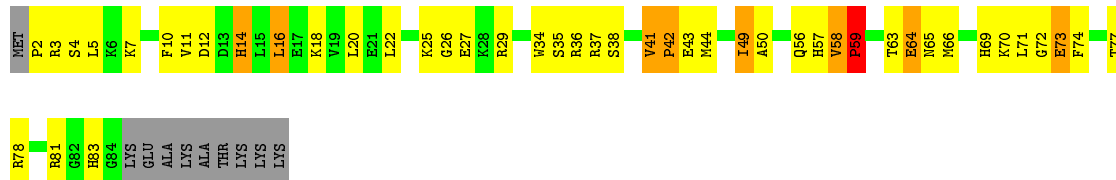
- Molecule 18: 30S ribosomal protein S19

Chain QS:  65% 24% 11%




- Molecule 18: 30S ribosomal protein S19

Chain XS:  40% 40% 9% 11%

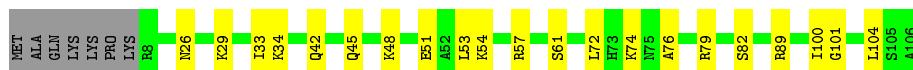


- Molecule 19: 30S ribosomal protein S20

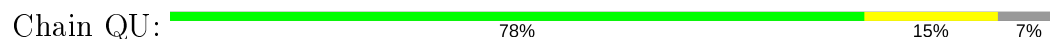
Chain QT:  85% 8% 7%



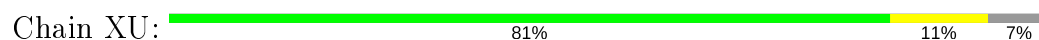
- Molecule 19: 30S ribosomal protein S20



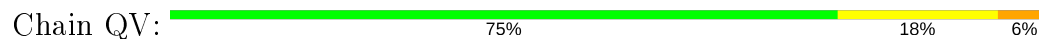
- Molecule 20: 30S ribosomal protein Thx



- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: P-site tRNA-fMet



- Molecule 21: P-site tRNA-fMet



- Molecule 21: P-site tRNA-fMet

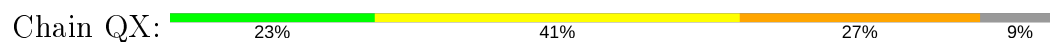


- Molecule 21: P-site tRNA-fMet

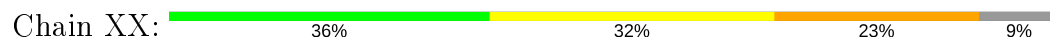




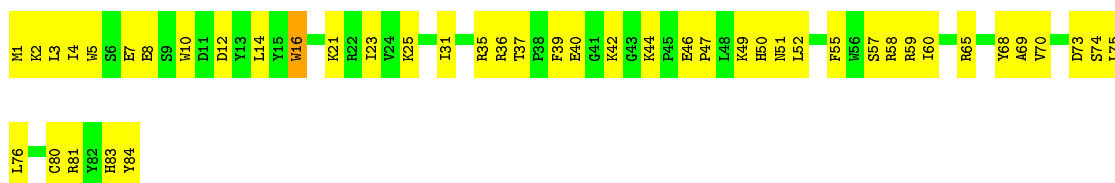
- Molecule 22: mRNA



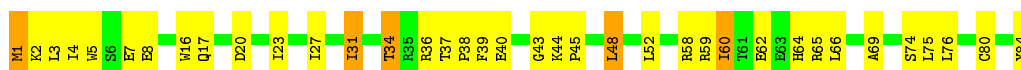
- Molecule 22: mRNA



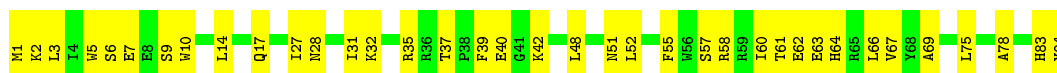
- Molecule 23: Addiction module toxin, Txe/YoeB family



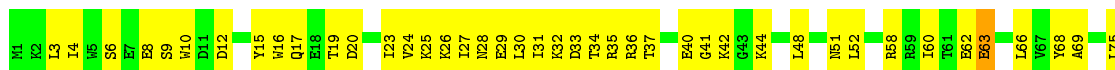
- Molecule 23: Addiction module toxin, Txe/YoeB family



- Molecule 23: Addiction module toxin, Txe/YoeB family



- Molecule 23: Addiction module toxin, Txe/YoeB family





- Molecule 24: 50S ribosomal protein L27

Chain R0: 76% 16% 5%



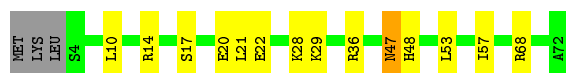
- Molecule 24: 50S ribosomal protein L27

Chain Y0: 84% 12% 2%



- Molecule 25: 50S ribosomal protein L29

Chain R2: 76% 18% 2%



- Molecule 25: 50S ribosomal protein L29

Chain Y2: 83% 13% 2%



- Molecule 26: 50S ribosomal protein L30

Chain R3: 92% 7% 1%



- Molecule 26: 50S ribosomal protein L30

Chain Y3: 88% 10% 2%

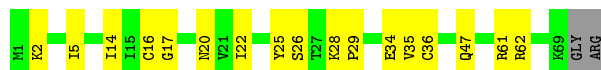


- Molecule 27: 50S ribosomal protein L31

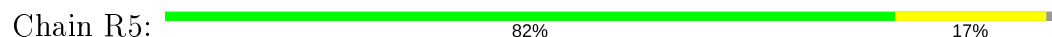
Chain R4: 66% 24% 6% 2%



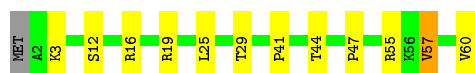
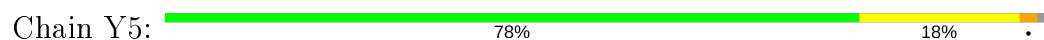
- Molecule 27: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L32



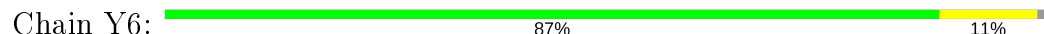
- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33



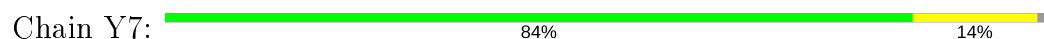
- Molecule 29: 50S ribosomal protein L33



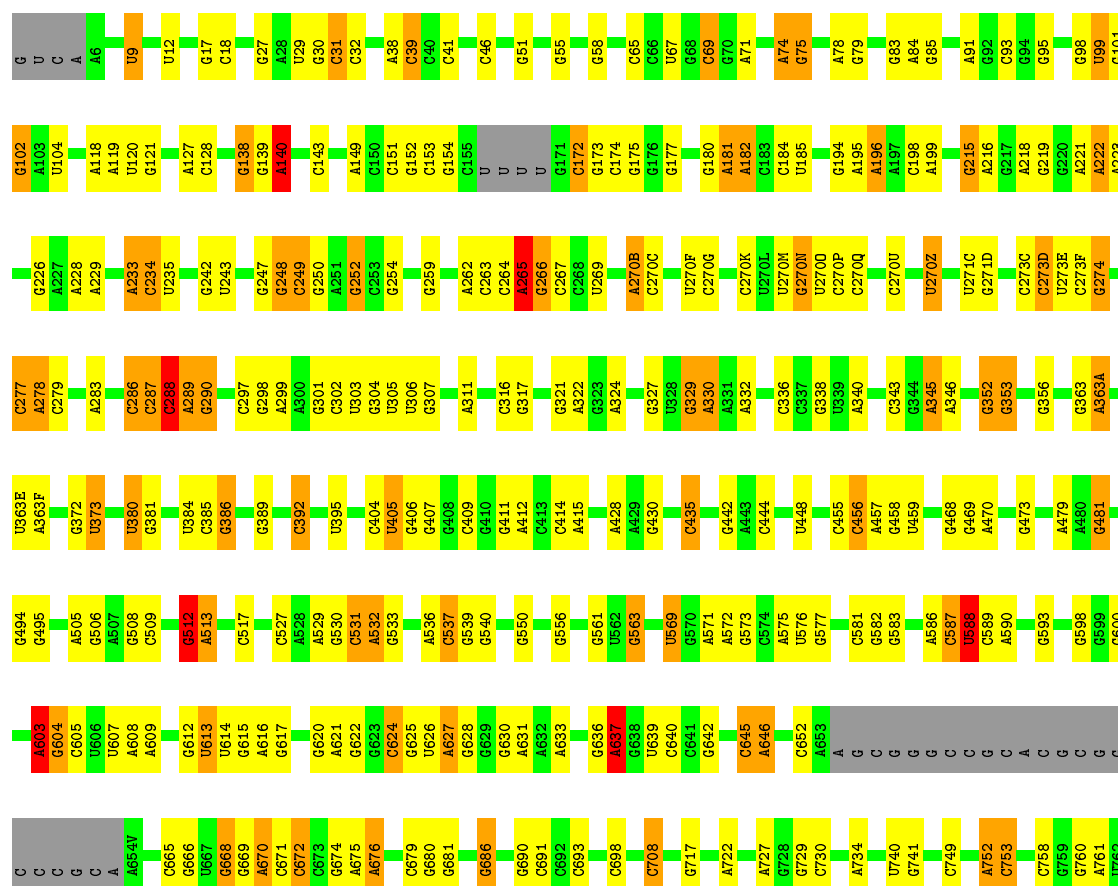
- Molecule 30: 50S ribosomal protein L34



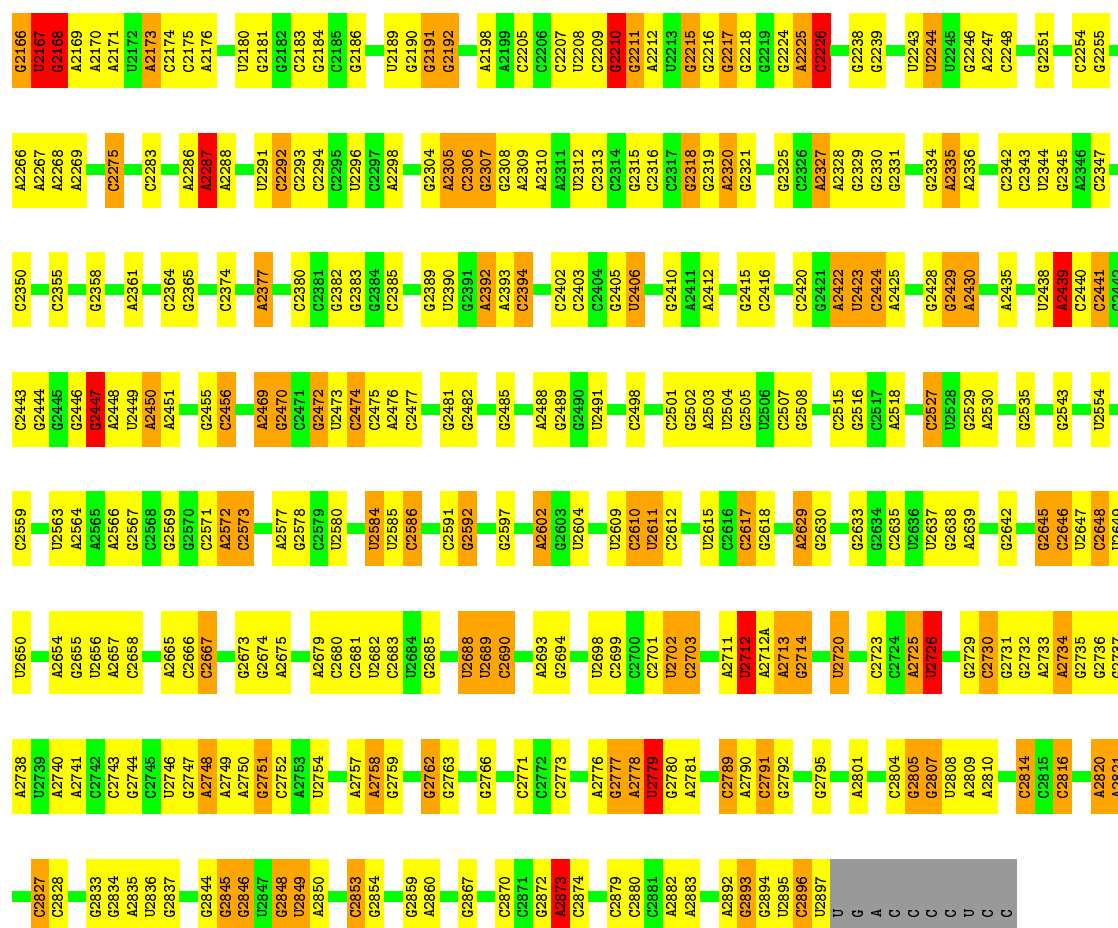
- Molecule 30: 50S ribosomal protein L34



C2283	C2284	C2285	C2286	A2287	U2291	C2292	C2293	C2294	C2295	U2296	C2297	A2298	C2304	A2305	C2306	G2307	G2308	C2309	A2310	C2311	U2312	C2313	C2316	C2317	G2318	G2319	A2320	G2325	A2328	C2329	G2334	A2335	A2336	C2343	U2344	G2345	A2346	C2347	G2349	C2350	G2351	A2352	C2362	C2363	C2364	G2365	G2373																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2181	G2182	C2183	G2184	C2185	G2186	G2187	C2188	U2189	C2190	G2191	C2192	U2197	A2198	A2199	C2200	C2201	U2208	C2209	G2210	G2211	G2212	C2213	C2215	G2219	G2224	A2225	C2226	U2233	G2234	C2235	G2236	G2237	G2238	G2239	U2243	U2244	U2245	G2246	C2247	C2248	C2254	C2259	C2260	A2266	A2267	A2268	A2269	G2270	C2364	G2365	C2275																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U2109	G2110	G2111	G2112	C2113	G2114	C2115	G2116	A2117	U2118	A2119	G2120	G2124	G2125	G2126	G2127	C2128	G2129	U2130	G2131	U2132	G2133	A2134	C2140	G2141	G2142	U2143	U2144	C2145	G2146	G2147	G2148	G2149	U2150	G2154	G2155	G2156	G2157	A2158	G2161	G2162	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2269	C2364	G2365	C2275																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G2023	G2024	C2025	C2026	G2027	A2030	A2031	G2032	A2033	G2037	G2038	C2039	C2040	U2041	A2042	C2043	G2044	G2046	U2047	G2048	G2049	G2051	G2052	G2053	A2054	C2055	G2056	A2059	A2060	C2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	C2069	U2074	U2075	C2081	A2082	U2086	U2092	G2093	A2098	U2099	U2102	C2103	G2104	C2108																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U1911	A1912	A1913	C1914	C1920	G1929	G1930	U1931	G1935	A1936	A1937	A1938	U1939	U1940	C1941	C1942	C1947	G1948	G1949	G1950	U1955	U1956	C1957	C1958	U1963	G1964	C1967	A1970	A1971	A1972	C1979	G1980	A1981	G1982	U1991	G1992	U1993	C1996	G2002	C2006	C1902	G2010	A2019	A2020	C2021	U2022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C1800	G1801	A1802	A1803	A1812	G1813	G1816	U1817	U1818	A1819	U1820	G1824	G1827	G1828	A1829	C1830	G1835	G1838	G1839	A1847	U1851	G1852	A1853	G1858	G1869	C1870	A1871	A1872	C1878	C1879	C1880	C1881	G1883	A1884	G1888	A1889	A1890	G1899	A1900	A1901	C1902	G1903	G1906	A2019	C2021	C1909	G1910																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1682	C1686	G1687	C1688	A1689	C1694	G1695	U1696	A1698	G1699	A1700	U1701	G1725	G1728	U1729	A1731	G1732	G1733	G1734	C1735	U1743	C1754	A1755	G1756	A1762	G1764	G1765	U1766	G1769	A1773	C1774	U1775	U1779	A1780	C1781	C1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	C1790	A1791	G1792																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C1585	A1586	G1587	C1588	C1592	G1593	G1594	G1595	C1598	C1599	U1602	A1603	C1604	G1605	C1606	C1607	U1608	A1609	A1610	U1629	G1630	G1635	C1636	A1637	C1638	C1640	G1643	C1644	C1648	G1649	G1650	G1651	A1652	G1653	A1654	A1655	C1656	G1657	G1666	G1667	A1668	G1669	A1674	U1679	U1680	G1681																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A1486	G1487	G1488	U1489	A1490	C1493	C1499	C1499	C1499	C1502	C1505	C1509	A1510	U1514	C1515	U1520	G1521	G1522	U1523	G1524	G1525	G1526	G1527	A1528	C1533	G1534	U1535	A1536	C1537	G1542	A1543	C1544	A1545	C1547	C1550	A1554	A1558	G1559	G1560	A1566	A1567	G1568	A1569	A1570	A1571	A1572	U1578																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1388	A1392	A1393	U1394	A1395	U1396	C1403	C1404	U1405	U1406	U1407	C1408	U1415	C1416	C1417	G1418	U1419	U1420	G1421	A1427	C1428	G1429	U1431	C1437	A1444A	A1449	G1449A	A1453	U1454	G1455	A1460	G1461	C1464	C1467	A1471	C1474	G1475	A1476	A1477	G1478	A1479	G1480	U1482	G1483																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
C1270	G1271	U1272	U1273	G1281	A1286	A1287	U1288	U1294	U1300	A1301	A1302	C1303	C1304	A1309	G1309	G1310	G1311	U1312	U1313	C1314	C1315	U1316	A1317	C1318	G1319	U1329	G1332	G1339	U1340	U1341	A1342	G1343	U1352	A1353	A1354	A1359	G1364	A1365	G1368	A1379	G1380	A1384	G1385	C1387																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U1175	G1176	A1177	C1178	C1180	C1181	A1182	G1183	C1185	G1186	G1187	G1191	A1085	A1086	U1087	A1088	G1089	C1095	A1096	U1101	C1102	A1103	U1205	G1206	A1210	U1211	G1212	A1220	C1221	C1224	C1235	C1236	U1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	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	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	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	C1403	C1404	C1405	C1406	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	C1470	C1471	C1472	C1473	C1474	C1475	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	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	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	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	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000

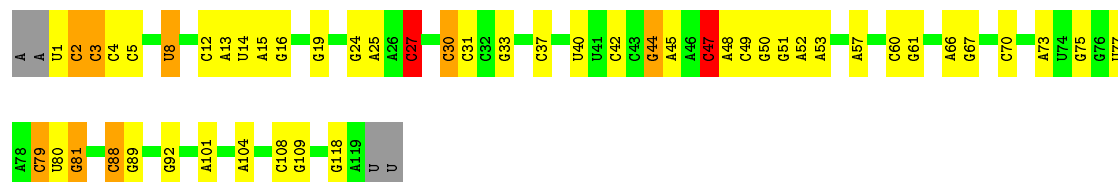


G2095	G1997	C1902	C1795	U1679	G1581	C1499	U1415	G1309	C1202	C1102	U1019	G932	C856	G763
U2096	A2001	C1905	U1796	U1680	C1585	G1500	G1416	G1310	G1203	A1103	G1022	A933	C857	A764
U2099	G2002	G1906	C1797	G1681	A1586	G1501	G1417	U1312	U1204	U1104	G1023	G938	U858	G765
G2100	C2006	C1909	G1799	G1694	A1587	C1505	G1418	U1313	U1205	U1105	G1024	G939	G859	A774
U2102	G2010	G1912	G1800	G1696	C1588	A1508	A1419	C1314	G1210	U1106	G1025	G940	A861	G775
C2103	U2011	A1913	G1801	G1697	C1592	C1509	U1420	C1315	U1211	U1113	U1026	A941	G862	G776
G2104	G2012	C1914	A1802	G1698	G1593	A1510	G1421	U1316	G1212	G1114	A1027	A945	A863	U779
C2111	C1915	U1915	C1804	G1699	C1598	U1514	G1422	G1317	U1213	U1114	A1032	G946	C864	G780
G2112	A2020	U1916	A1809	A1700	C1599	C1515	G1423	G1318	A1220	G1122	U1033	A949	C865	A781
U2113	C2021	U1917	A1812	G1703	C1600	C1518	G1424	G1319	A1226	A1126	G1034	G950	C866	A782
A2114	U2022	A1918	G1813	G1725	G1601	U1519	G1425	G1324	G1226	A1127	U1035	G953	U868	A783
G2115	G2023	C1919	G1814	G1726	U1602	U1520	A1427	G1325	C1230	A1128	G1042	A953	G867	A784
G2116	C1920	A1920	G1815	G1727	C1607	G1521	G1428	U1329	G1231	G1131	G1043	G954	C868	G785
A2117	C2026	G1927	A1816	A1728	C1608	G1522	A1430	C1330	C1232	G1132	A1045	G955	U877	A789
G2120	G2027	A1928	G1817	U1730	C1612	G1526	U1431	G1332	G1233	U1133	A1046	G956	A878	C791
G2121	G2028	G1928	G1817	G1731	C1616	U1527	A1434	A1342	G1236	G1135	G1047	U957	C879	G792
G2122	G2029	G1929	U1816	G1732	A1616	A1528	G1435	U1352	A1237	G1136	A1048	U959	G880	A793
G2123	A2030	U1930	G1819	C1734	C1617	U1528	G1436	U1352	G1243	G1139	C1049	A960	G881	C797
G2124	G2032	A1932	G1820	G1735	A1618	G1534	C1437	A1353	G1247	C1140	A1050	C961	G882	
G2125	G2033	C1933	U1820	G1741	C1622	U1535	A1444	A1354	U1248	U1141	G1051	G968	G883	G805
A2126	A2034	G1934	G1826	G1742	G1622	A1536	A1444	A1354	G1248	U1142	C1052	U969	C884	C806
G2127	G2035	G1935	A1829	G1743	G1628	C1537	A1449	G1355	U1249	A1143	C1053	U969	C885	U807
C2128	C2036	A1936	G1830	C1754	U1629	G1538	G1449A	U1358	G1250	G1143	A1054	C970	C886	
C2129	G2037	A1937	G1831	A1755	G1630	G1539	G1450	G1359	U1251	G1144	G1055	C971	C887	
U2130	G2038	A1938	G1835	G1756	G1630	U1541	U1454	A1360	A1253	C1153	A1056	G972	C889	U811
G2131	U2041	C1947	G1836	U1757	G1635	U1542	G1455	G1363	U1254	G1154	A1057	G973	A890	C812
U2132	G2042	G1948	C1837	G1758	C1636	G1543	C1458	C1368	U1255	U1159	G1058	C974A	C894	G818
G2133	C2043	C2043	G1842	A1762	A1637	C1544	G1459	G1368	G1256	G1162	G1059	G975	U895	A819
A2134	G2046	U1955	G1845	G1763	C1638	A1545	A1460	U1378	A1262	C1162	U1061	A980	A896	A820
C2137	A2051	U1956	G1846	G1764	U1639	G1547	G1461	A1379	G1263	U1165	C1064	A983	C897	U826
G2139	C2055	C1957	A1847	G1765	C1640	G1548	G1462	G1380	U1264	U1166	A1070	A900	U827	U828
G2140	C2056	C1958	U1851	U1766	A1641	C1549	C1463	U1384	A1265	U1167	G1071	G987	G830	
C2142	G2056	U1963	U1851	G1769	G1642	U1554	C1464	A1384	U1267	G1168	C1072	G987	G831	G830
C2143	A2059	G1964	G1858	A1773	C1644	A1554	C1467	C1386	C1270	G1169	G1073	G989	G906	G831
U2144	A2060	C1965	U1864	C1774	C1648	A1558	A1471	U1391	G1271	G1170	G1074	G990	U907	G832
C2145	C2061	A1966	G1869	U1779	A1652	G1559	G1475	A1392	A1275	U1175	C1075	G991	C908	G836
G2147	A2062	C1967	C1870	C1781	A1653	A1566	G1478	U1396	G1281	U1176	C1076	G992	A910	
G2148	C2063	A1970	A1871	C1782	A1654	A1567	U1482	U1399	U1286	A1177	C1079	G993	C914	U839
U2150	C2065	A1971	A1872	A1783	A1655	G1568	G1483	C1402	A1287	G1178	A1085	G997	C915	C840
G2151	U2068	A1972	G1878	A1784	C1657	A1569	G1484	C1403	U1288	C1179	A1086	C998	A917	G842
C2155	G2069	C1979	C1881	A1785	C1658	A1570	G1485	U1404	A1288	C1180	G1087	U999	A918	G845
G2156	C2073	G1980	C1882	A1786	G1667	A1571	G1486	C1405	U1294	G1184	A1088	A1000	G919	C846
G2157	U2074	C1981	G1883	A1787	A1668	A1572	G1488	U1406	U1294	G1187	G1089	A1001	U922	U847
A2158	U2075	C1982	G1888	A1788	A1669	A1575	U1489	U1407	C1295	U1188	C1092	C1005	C923	G848
G2159	U2075	C1990	A1889	A1789	A1669	U1576	A1490	C1408	U1300	G1187	C1092	C1006	G928	C850
G2160	U2086	U1991	G1899	A1791	G1674	U1577	A1490	C1408	A1301	U1188	A1095	C1006	G929	U851
C2161	G2087	U1992	A1900	C1792	C1675	U1578	C1493	C1408	U1301	G1191	A1096	U1012	G931	G852
G2162	G2094	U1993	A1901	U1794	G1678	A1580	A1496	A1411	A1308	G1195	G1099			G853



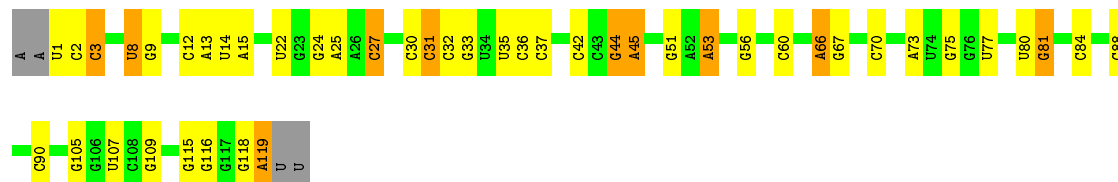
• Molecule 33: 5S rRNA

Chain RB: 56% 32% 6% . .



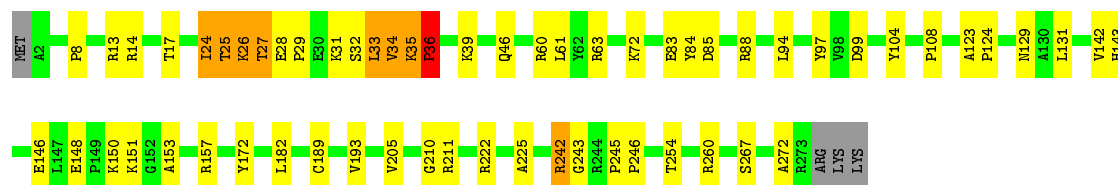
• Molecule 33: 5S rRNA

Chain YB: 60% 28% 8% .



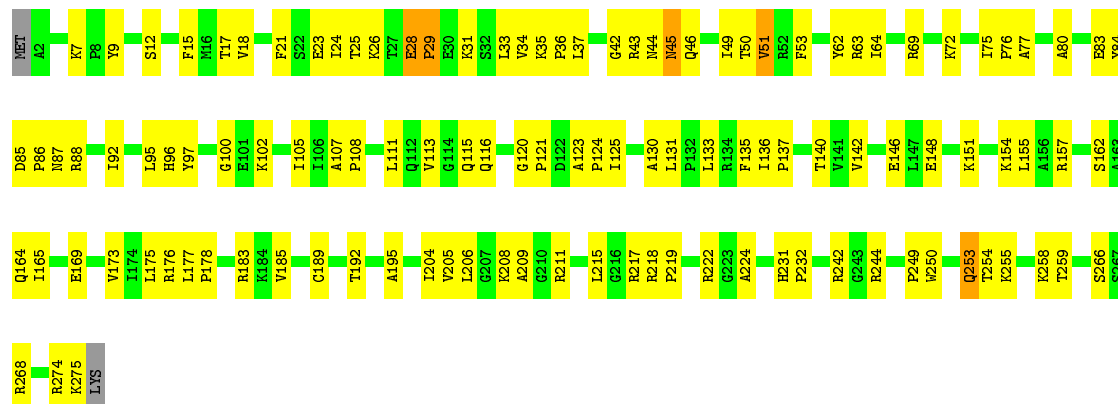
• Molecule 34: 50S ribosomal protein L2

Chain RD: 77% 18% . .



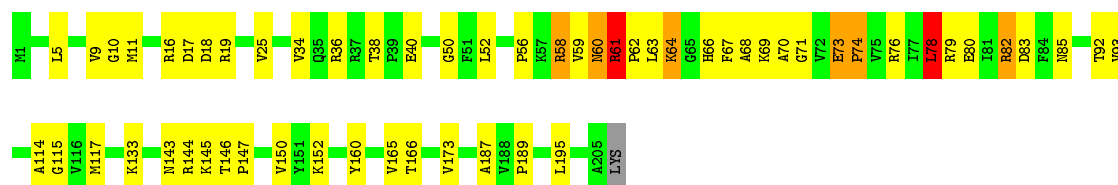
• Molecule 34: 50S ribosomal protein L2

Chain YD: 57% 40% ..



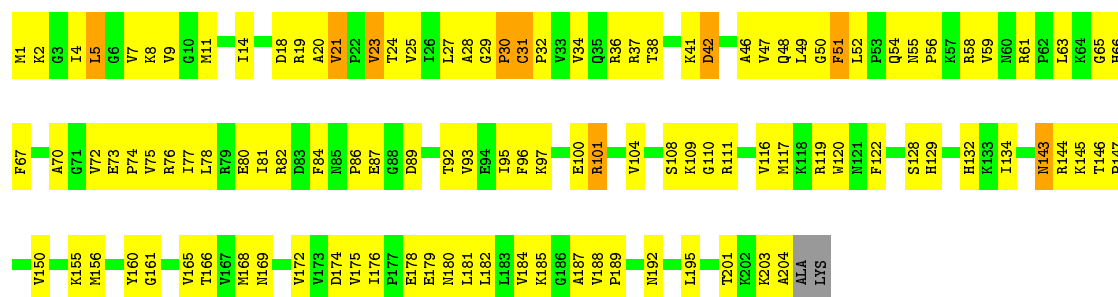
• Molecule 35: 50S ribosomal protein L3

Chain RE: 71% 24% ..



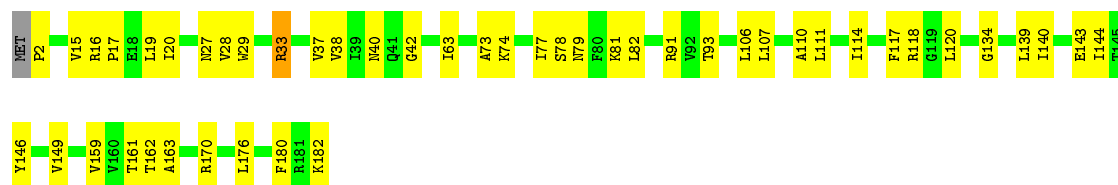
• Molecule 35: 50S ribosomal protein L3

Chain YE: 44% 51% ..



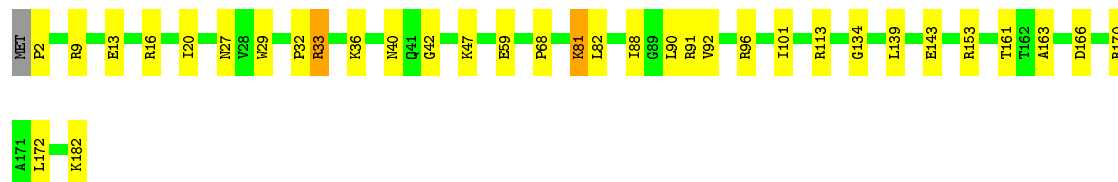
• Molecule 36: 50S ribosomal protein L5

Chain RG: 74% 25% ..



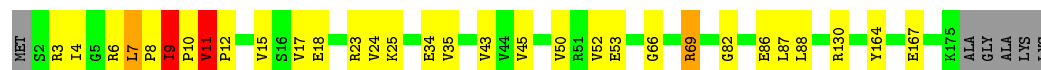
- Molecule 36: 50S ribosomal protein L5

Chain YG: 81% 18% ..



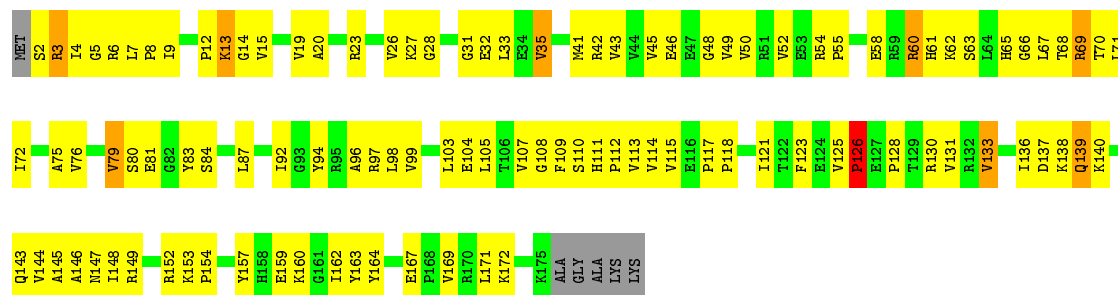
- Molecule 37: 50S ribosomal protein L6

Chain RH: 79% 15% ..



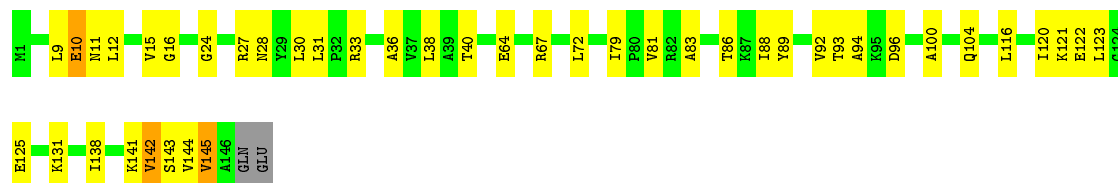
- Molecule 37: 50S ribosomal protein L6

Chain YH: 37% 54% ..



- Molecule 38: 50S ribosomal protein L9

Chain RI: 70% 27% ..



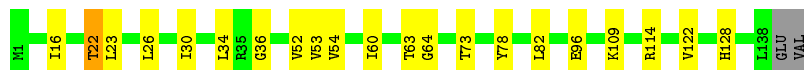
- Molecule 38: 50S ribosomal protein L9

Chain YI: 89% 9% ..



- Molecule 39: 50S ribosomal protein L13

Chain RN: 84% 14% ..



- Molecule 39: 50S ribosomal protein L13

Chain YN: 86% 12% ..



- Molecule 40: 50S ribosomal protein L14

Chain RO: 85% 15%



- Molecule 40: 50S ribosomal protein L14

Chain YO: 83% 17%



- Molecule 41: 50S ribosomal protein L15

Chain RP: 76% 20% .




- Molecule 41: 50S ribosomal protein L15

Chain YP: 43% 48% 8% .



- Molecule 42: 50S ribosomal protein L16

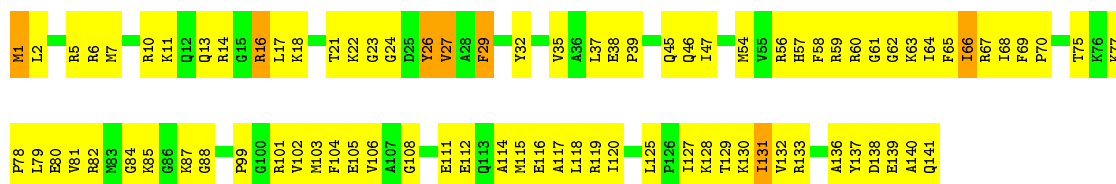


Chain RQ:  80% 19%




- Molecule 42: 50S ribosomal protein L16

Chain YQ:  40% 55% 5%



- Molecule 43: 50S ribosomal protein L17

Chain RR:  87% 11%




- Molecule 43: 50S ribosomal protein L17

Chain YR:  90% 9%




- Molecule 44: 50S ribosomal protein L18

Chain RS:  84% 15%



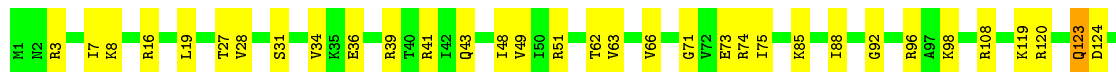
- Molecule 44: 50S ribosomal protein L18

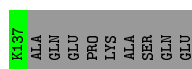
Chain YS:  76% 21%



- Molecule 45: 50S ribosomal protein L19

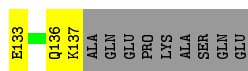
Chain RT:  71% 22% 6%





- Molecule 45: 50S ribosomal protein L19

Chain YT: 70% 23% 6%



- Molecule 46: 50S ribosomal protein L20

Chain RU: 83% 15% ..



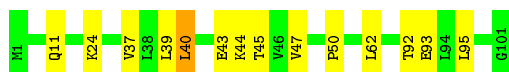
- Molecule 46: 50S ribosomal protein L20

Chain YU: 86% 12% ..



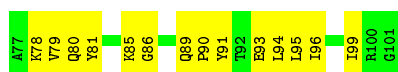
- Molecule 47: 50S ribosomal protein L21

Chain RV: 86% 13% .



- Molecule 47: 50S ribosomal protein L21

Chain YV: 49% 50% .



- Molecule 48: 50S ribosomal protein L22

Chain RW: 80% 20%



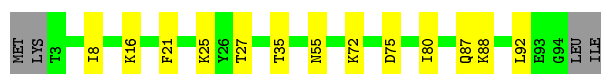
- Molecule 48: 50S ribosomal protein L22

Chain YW: 86% 14%



- Molecule 49: 50S ribosomal protein L23

Chain RX: 82% 14% .



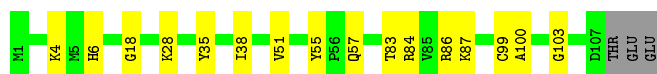
- Molecule 49: 50S ribosomal protein L23

Chain YX: 83% 13% .



- Molecule 50: 50S ribosomal protein L24

Chain RY: 83% 15% .



- Molecule 50: 50S ribosomal protein L24

Chain YY: 78% 18% ..



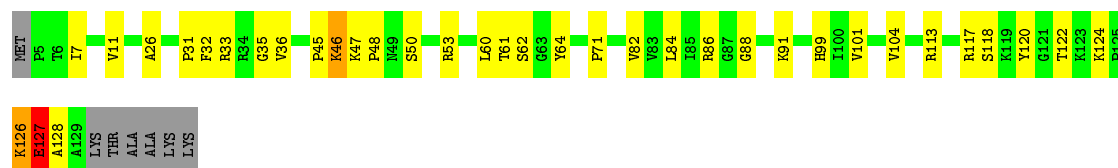
- Molecule 51: 30S ribosomal protein S12

Chain XL: 78% 13% . 8%



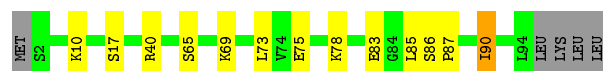
- Molecule 51: 30S ribosomal protein S12

Chain QL: 67% 25% .. 5%



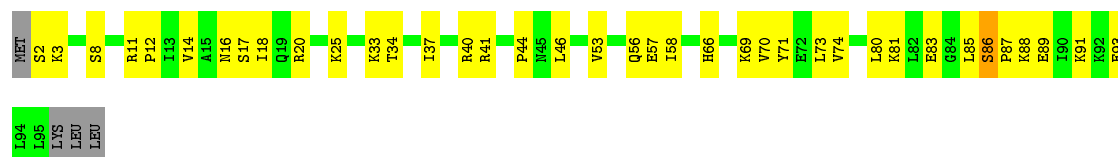
- Molecule 52: 50S ribosomal protein L28

Chain Y1: 82% 12% • 5%



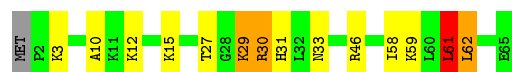
- Molecule 52: 50S ribosomal protein L28

Chain R1: 57% 38% • •



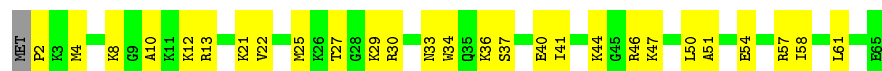
- Molecule 53: 50S ribosomal protein L35

Chain Y8: 77% 15% 5% • •



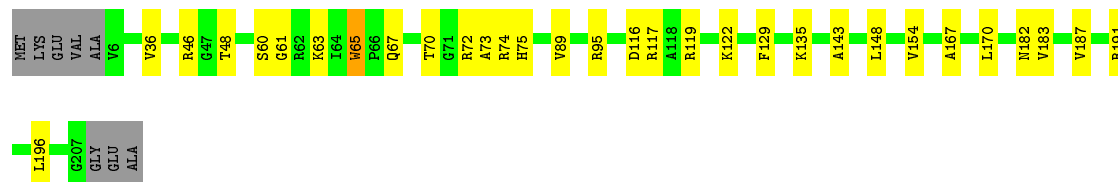
- Molecule 53: 50S ribosomal protein L35

Chain R8: 57% 42% •



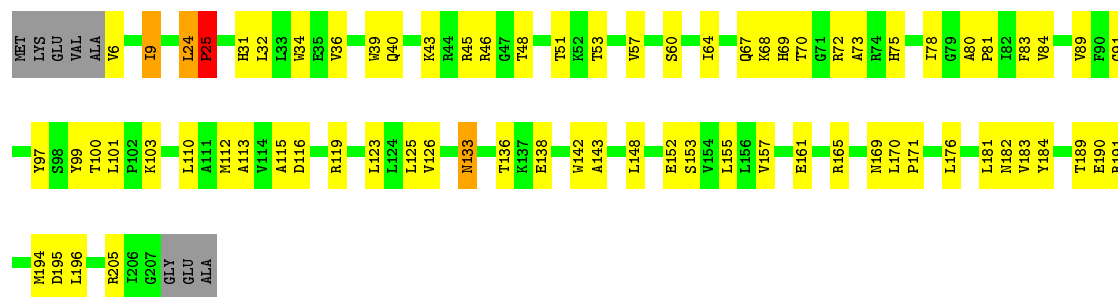
- Molecule 54: 50S ribosomal protein L4

Chain YF: 81% 14% •

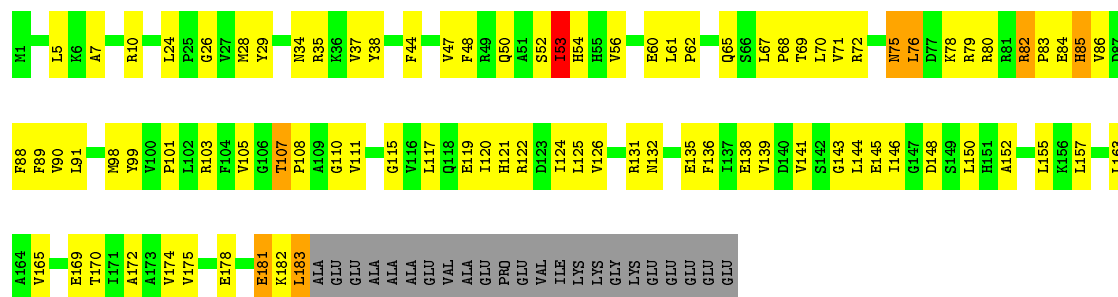


- Molecule 54: 50S ribosomal protein L4

Chain RF: 61% 33% • •



- Molecule 55: 50S ribosomal protein L25



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.79Å 453.08Å 608.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.59 – 3.25	Depositor
% Data completeness (in resolution range)	93.4 (146.59-3.25)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.256	Depositor
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.347	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298432	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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: ZN, PPU, SF4, MG, OMU, A2M

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	QA	0.44	0/36324	1.10	168/56690 (0.3%)
1	XA	0.46	2/36254 (0.0%)	1.08	154/56581 (0.3%)
2	QB	0.72	3/1942 (0.2%)	0.75	1/2619 (0.0%)
2	XB	0.37	0/1950	0.61	0/2630
3	QC	0.32	0/1629	0.56	0/2195
3	XC	0.31	0/1629	0.55	0/2195
4	QD	0.34	0/1733	0.57	0/2318
4	XD	0.35	0/1733	0.56	0/2318
5	QE	0.30	0/1171	0.55	0/1576
5	XE	0.33	0/1171	0.58	0/1576
6	QF	0.34	0/856	0.56	0/1154
6	XF	0.30	0/856	0.56	0/1154
7	QG	0.31	0/1276	0.52	0/1709
7	XG	0.34	0/1276	0.52	0/1709
8	QH	0.54	2/1128 (0.2%)	0.62	1/1517 (0.1%)
8	XH	0.34	0/1128	0.54	0/1517
9	QI	0.37	0/1029	0.68	0/1379
9	XI	0.36	0/1017	0.64	0/1365
10	QJ	0.33	0/814	0.59	0/1095
10	XJ	0.36	0/790	0.64	0/1063
11	QK	0.31	0/900	0.55	0/1213
11	XK	0.32	0/879	0.56	0/1187
12	QM	0.39	0/965	0.69	0/1292
12	XM	0.34	0/956	0.68	0/1281
13	QN	0.38	0/501	0.64	0/664
13	XN	0.35	0/501	0.61	0/664
14	QO	0.29	0/745	0.52	0/992
14	XO	0.30	0/740	0.50	0/987
15	QP	0.31	0/721	0.57	0/970
15	XP	0.32	0/721	0.58	0/970
16	QQ	0.30	0/847	0.53	0/1131
16	XQ	0.32	0/847	0.57	1/1131 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QR	0.29	0/579	0.58	0/768
17	XR	0.31	0/579	0.56	0/768
18	QS	0.37	0/680	0.65	0/915
18	XS	1.02	4/671 (0.6%)	0.84	2/904 (0.2%)
19	QT	0.30	0/765	0.58	0/1007
19	XT	0.31	0/765	0.59	0/1007
20	QU	0.25	0/221	0.56	0/288
20	XU	0.28	0/221	0.66	0/288
21	QV	0.38	0/1832	1.02	2/2855 (0.1%)
21	QW	0.31	0/1832	1.07	8/2855 (0.3%)
21	XV	0.40	0/1832	1.05	5/2855 (0.2%)
21	XW	0.33	0/1832	1.10	6/2855 (0.2%)
22	QX	0.41	0/414	0.89	0/645
22	XX	0.35	0/414	0.91	0/645
23	QY	0.60	0/743	0.67	0/1002
23	QZ	0.60	0/743	0.69	0/1002
23	XY	0.59	0/743	0.72	0/1002
23	XZ	0.60	0/743	0.60	0/1002
24	R0	0.36	0/652	0.68	1/867 (0.1%)
24	Y0	0.40	0/657	0.66	2/874 (0.2%)
25	R2	0.31	0/583	0.61	0/771
25	Y2	0.36	0/583	0.64	0/771
26	R3	0.31	0/474	0.54	0/635
26	Y3	0.33	0/474	0.56	0/635
27	R4	0.54	1/578 (0.2%)	1.01	5/776 (0.6%)
27	Y4	0.36	0/578	0.71	0/776
28	R5	0.34	0/473	0.55	0/639
28	Y5	0.38	0/473	0.56	0/639
29	R6	0.30	0/460	0.55	0/613
29	Y6	0.30	0/460	0.53	0/613
30	R7	0.30	0/417	0.53	0/550
30	Y7	0.30	0/426	0.53	0/561
31	R9	0.32	0/310	0.55	0/407
31	Y9	0.27	0/310	0.54	0/407
32	RA	0.51	2/69739 (0.0%)	1.15	477/108870 (0.4%)
32	YA	0.52	1/69353 (0.0%)	1.13	428/108267 (0.4%)
33	RB	0.46	0/2881	1.16	18/4494 (0.4%)
33	YB	0.51	1/2881 (0.0%)	1.16	23/4494 (0.5%)
34	RD	0.40	1/2165 (0.0%)	0.74	6/2919 (0.2%)
34	YD	0.67	2/2185 (0.1%)	0.81	2/2944 (0.1%)
35	RE	0.40	0/1601	0.78	3/2160 (0.1%)
35	YE	0.64	1/1592 (0.1%)	0.83	1/2149 (0.0%)
36	RG	0.37	0/1499	0.66	0/2016

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	YG	0.33	0/1499	0.65	0/2016
37	RH	0.46	1/1362 (0.1%)	0.74	2/1841 (0.1%)
37	YH	0.64	0/1356	0.80	1/1834 (0.1%)
38	RI	0.55	1/1151 (0.1%)	0.91	6/1558 (0.4%)
38	YI	0.33	0/1151	0.69	1/1558 (0.1%)
39	RN	0.33	0/1131	0.67	2/1525 (0.1%)
39	YN	0.32	0/1131	0.66	2/1525 (0.1%)
40	RO	0.34	0/943	0.56	0/1269
40	YO	0.34	0/943	0.57	0/1269
41	RP	0.39	0/1162	0.80	1/1544 (0.1%)
41	YP	0.61	0/1152	0.71	0/1533
42	RQ	0.37	0/1143	0.67	0/1527
42	YQ	0.61	0/1143	0.75	0/1527
43	RR	0.32	0/974	0.62	1/1302 (0.1%)
43	YR	0.30	0/974	0.61	0/1302
44	RS	0.36	0/892	0.69	0/1187
44	YS	0.35	0/892	0.73	2/1187 (0.2%)
45	RT	0.32	0/1155	0.67	0/1542
45	YT	0.35	0/1155	0.71	2/1542 (0.1%)
46	RU	0.36	0/982	0.56	0/1306
46	YU	0.34	0/982	0.58	0/1306
47	RV	0.39	0/790	0.74	0/1057
47	YV	0.62	0/790	0.87	1/1057 (0.1%)
48	RW	0.31	0/911	0.56	0/1220
48	YW	0.33	0/911	0.56	0/1220
49	RX	0.34	0/739	0.54	0/993
49	YX	0.33	0/739	0.55	0/993
50	RY	0.38	0/831	0.62	1/1108 (0.1%)
50	YY	0.33	0/831	0.56	0/1108
51	QL	0.29	0/991	0.55	0/1327
51	XL	0.35	0/972	0.64	1/1301 (0.1%)
52	R1	0.39	0/744	0.55	0/989
52	Y1	0.42	0/736	0.59	0/978
53	R8	0.52	0/525	0.58	0/691
53	Y8	0.42	0/525	0.92	4/691 (0.6%)
54	RF	0.48	2/1620 (0.1%)	0.54	1/2194 (0.0%)
54	YF	0.39	0/1620	0.60	0/2194
55	RZ	0.53	2/1493 (0.1%)	0.65	0/2026
55	YZ	0.36	0/1493	0.52	0/2026
56	ZA	1.50	1/40 (2.5%)	0.89	0/60
56	ZB	0.27	0/40	0.53	0/60
All	All	0.47	27/323056 (0.0%)	1.01	1342/482845 (0.3%)

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	QB	0	1
24	Y0	0	1
32	YA	0	1
37	YH	0	1
41	RP	0	1
51	QL	0	1
53	R8	0	1
All	All	0	7

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	YD	29	PRO	N-CA	13.69	1.70	1.47
18	XS	42	PRO	N-CA	13.61	1.70	1.47
18	XS	59	PRO	N-CA	13.52	1.70	1.47
54	RF	25	PRO	N-CA	13.16	1.69	1.47
38	RI	142	VAL	N-CA	-13.01	1.20	1.46

The worst 5 of 1342 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	RA	309	G	O5'-P-OP2	-24.58	81.20	110.70
32	RA	2614	A	C6-N1-C2	-16.89	108.46	118.60
32	RA	2053	G	C5-N7-C8	-16.23	96.18	104.30
32	RA	308	G	OP2-P-O3'	-14.86	72.52	105.20
32	RA	2053	G	C4-C5-N7	14.51	116.61	110.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Mainchain
41	RP	11	GLY	Mainchain
24	Y0	8	GLY	Mainchain
32	YA	1162	G	Sidechain
37	YH	13	LYS	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	QA	32452	0	16381	373	0
1	XA	32389	0	16350	345	0
2	QB	1907	0	1958	287	0
2	XB	1915	0	1969	18	0
3	QC	1605	0	1668	24	0
3	XC	1605	0	1668	13	0
4	QD	1703	0	1763	29	0
4	XD	1703	0	1763	37	0
5	QE	1155	0	1213	8	0
5	XE	1155	0	1213	10	0
6	QF	843	0	857	6	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	9	0
7	XG	1257	0	1296	13	0
8	QH	1108	0	1165	16	0
8	XH	1108	0	1165	16	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	20	0
10	QJ	801	0	849	13	0
10	XJ	777	0	816	21	0
11	QK	885	0	904	11	0
11	XK	864	0	881	11	0
12	QM	955	0	1021	22	0
12	XM	946	0	1008	15	0
13	QN	492	0	529	11	0
13	XN	492	0	529	4	0
14	QO	734	0	771	8	0
14	XO	729	0	768	7	0
15	QP	705	0	725	4	0
15	XP	705	0	725	5	0
16	QQ	834	0	904	10	0
16	XQ	834	0	904	7	0
17	QR	574	0	644	4	0
17	XR	574	0	644	4	0
18	QS	665	0	686	44	0
18	XS	656	0	666	73	0
19	QT	763	0	861	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XT	763	0	861	18	0
20	QU	217	0	234	4	0
20	XU	217	0	234	1	0
21	QV	1640	0	837	11	0
21	QW	1640	0	837	28	0
21	XV	1640	0	837	15	0
21	XW	1640	0	837	22	0
22	QX	435	0	225	19	0
22	XX	435	0	225	12	0
23	QY	723	0	713	91	0
23	QZ	723	0	713	104	0
23	XY	723	0	713	59	0
23	XZ	723	0	713	81	0
24	R0	643	0	667	9	0
24	Y0	648	0	672	15	0
25	R2	581	0	629	11	0
25	Y2	581	0	629	5	0
26	R3	469	0	518	2	0
26	Y3	469	0	518	5	0
27	R4	565	0	559	15	0
27	Y4	565	0	557	10	0
28	R5	459	0	476	9	0
28	Y5	459	0	480	11	0
29	R6	453	0	473	17	0
29	Y6	453	0	473	4	0
30	R7	409	0	454	4	0
30	Y7	418	0	467	6	0
31	R9	307	0	335	5	0
31	Y9	307	0	335	8	0
32	RA	62266	0	31390	616	0
32	YA	61921	0	31212	693	0
33	RB	2576	0	1305	32	0
33	YB	2576	0	1305	22	0
34	RD	2115	0	2194	46	0
34	YD	2135	0	2220	165	0
35	RE	1568	0	1634	50	0
35	YE	1559	0	1618	225	0
36	RG	1474	0	1535	28	0
36	YG	1474	0	1535	22	0
37	RH	1336	0	1418	38	0
37	YH	1330	0	1407	191	0
38	RI	1136	0	1223	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	YI	1136	0	1223	7	0
39	RN	1104	0	1180	12	0
39	YN	1104	0	1180	10	0
40	RO	933	0	996	17	0
40	YO	933	0	996	14	0
41	RP	1145	0	1228	75	0
41	YP	1135	0	1212	193	0
42	RQ	1122	0	1179	29	0
42	YQ	1122	0	1179	172	0
43	RR	960	0	1021	12	0
43	YR	960	0	1021	8	0
44	RS	882	0	943	13	0
44	YS	882	0	943	17	0
45	RT	1141	0	1202	23	0
45	YT	1141	0	1202	41	0
46	RU	964	0	1022	22	0
46	YU	964	0	1021	30	0
47	RV	779	0	852	9	0
47	YV	779	0	852	88	0
48	RW	900	0	964	14	0
48	YW	900	0	964	11	0
49	RX	725	0	778	9	0
49	YX	725	0	778	8	0
50	RY	818	0	913	13	0
50	YY	818	0	913	16	0
51	QL	975	0	1062	40	0
51	XL	956	0	1046	15	0
52	R1	737	0	813	36	0
52	Y1	729	0	802	7	0
53	R8	517	0	582	65	0
53	Y8	517	0	582	31	0
54	RF	1585	0	1632	82	0
54	YF	1585	0	1632	24	0
55	RZ	1461	0	1493	107	0
55	YZ	1461	0	1493	106	0
56	ZA	74	0	51	15	0
56	ZB	74	0	51	14	0
57	QA	94	0	0	0	0
57	QD	2	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QV	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	2	0	0	0	0
57	RR	2	0	0	0	0
57	RY	1	0	0	0	0
57	XA	116	0	0	0	0
57	XD	1	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	Y0	2	0	0	0	0
57	Y3	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	326	0	0	0	0
57	YB	5	0	0	0	0
57	YD	5	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	298432	0	202696	4712	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4712 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)
42:YQ:64:ILE:CD1	55:YZ:178:GLU:HG3	1.19	1.65
37:YH:123:PHE:CE1	37:YH:133:VAL:HG12	1.26	1.62
37:YH:5:GLY:HA3	37:YH:65:HIS:CE1	1.22	1.59
41:YP:100:LEU:CD1	41:YP:112:LEU:HD11	1.37	1.55
54:RF:9:ILE:HD11	54:RF:125:LEU:CD1	1.39	1.51

There are no symmetry-related clashes.

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	QB	233/256 (91%)	212 (91%)	18 (8%)	3 (1%)	12	41
2	XB	234/256 (91%)	208 (89%)	25 (11%)	1 (0%)	34	67
3	QC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
3	XC	203/239 (85%)	193 (95%)	10 (5%)	0	100	100
4	QD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	47
4	XD	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	47
5	QE	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22	56
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	56
6	QF	99/101 (98%)	99 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
9	QI	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	52
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	14	46
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QM	118/126 (94%)	101 (86%)	13 (11%)	4 (3%)	3	22
12	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	17	50
13	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	36
13	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	36
14	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
14	XO	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
15	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
16	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
17	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	QS	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	43
18	XS	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	5	28
19	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
19	XT	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	QU	23/27 (85%)	23 (100%)	0	0	100	100
20	XU	23/27 (85%)	23 (100%)	0	0	100	100
23	QY	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
23	QZ	82/84 (98%)	76 (93%)	6 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	XY	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
23	XZ	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	R0	79/85 (93%)	73 (92%)	4 (5%)	2 (2%)	5	28
24	Y0	80/85 (94%)	77 (96%)	3 (4%)	0	100	100
25	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	39
25	Y2	67/72 (93%)	64 (96%)	3 (4%)	0	100	100
26	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	10
27	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	39
28	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	R7	45/49 (92%)	45 (100%)	0	0	100	100
30	Y7	46/49 (94%)	46 (100%)	0	0	100	100
31	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	Y9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	RD	270/276 (98%)	237 (88%)	26 (10%)	7 (3%)	5	27
34	YD	272/276 (99%)	261 (96%)	11 (4%)	0	100	100
35	RE	203/206 (98%)	159 (78%)	34 (17%)	10 (5%)	2	14
35	YE	202/206 (98%)	190 (94%)	9 (4%)	3 (2%)	10	39
36	RG	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	14	46
36	YG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	25	59
37	RH	172/180 (96%)	145 (84%)	20 (12%)	7 (4%)	3	17
37	YH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	13	43
38	RI	144/148 (97%)	115 (80%)	24 (17%)	5 (4%)	3	21
38	YI	144/148 (97%)	119 (83%)	21 (15%)	4 (3%)	5	25
39	RN	136/140 (97%)	115 (85%)	18 (13%)	3 (2%)	6	31
39	YN	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	10	39
40	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	YO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
41	RP	148/150 (99%)	112 (76%)	32 (22%)	4 (3%)	5	26
41	YP	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	11	40
42	RQ	139/141 (99%)	115 (83%)	22 (16%)	2 (1%)	11	40
42	YQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	56
43	RR	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	50
43	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	50
44	RS	109/112 (97%)	91 (84%)	18 (16%)	0	100	100
44	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	50
45	RT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	10	39
45	YT	135/146 (92%)	114 (84%)	19 (14%)	2 (2%)	10	39
46	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	50
46	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	50
47	RV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	47
47	YV	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
48	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	50
48	YW	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	17	50
49	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
49	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
50	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
50	YY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
51	QL	123/132 (93%)	109 (89%)	13 (11%)	1 (1%)	19	52
51	XL	120/132 (91%)	100 (83%)	19 (16%)	1 (1%)	19	52
52	R1	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	6	31
52	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
53	R8	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	Y8	62/65 (95%)	47 (76%)	12 (19%)	3 (5%)	2	14
54	RF	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	29	62
54	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	47
55	RZ	181/206 (88%)	171 (94%)	9 (5%)	1 (1%)	25	59
55	YZ	181/206 (88%)	175 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11786/12464 (95%)	10743 (91%)	935 (8%)	108 (1%)	17	50

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QM	12	ASN
18	QS	41	VAL
27	R4	24	THR
27	R4	25	TYR
34	RD	25	THR

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	QB	203/220 (92%)	180 (89%)	23 (11%)	6	22
2	XB	204/220 (93%)	202 (99%)	2 (1%)	76	85
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	91
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	87
5	XE	116/123 (94%)	114 (98%)	2 (2%)	60	78
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	74
6	XF	90/90 (100%)	88 (98%)	2 (2%)	52	74
7	QG	126/127 (99%)	125 (99%)	1 (1%)	81	89
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	79
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	89
8	XH	118/119 (99%)	116 (98%)	2 (2%)	60	78
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	83
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	84
12	QM	96/101 (95%)	96 (100%)	0	100	100
12	XM	95/101 (94%)	95 (100%)	0	100	100
13	QN	49/50 (98%)	49 (100%)	0	100	100
13	XN	49/50 (98%)	49 (100%)	0	100	100
14	QO	79/80 (99%)	79 (100%)	0	100	100
14	XO	79/80 (99%)	79 (100%)	0	100	100
15	QP	72/74 (97%)	72 (100%)	0	100	100
15	XP	72/74 (97%)	71 (99%)	1 (1%)	67	81
16	QQ	95/97 (98%)	95 (100%)	0	100	100
16	XQ	95/97 (98%)	95 (100%)	0	100	100
17	QR	61/77 (79%)	61 (100%)	0	100	100
17	XR	61/77 (79%)	61 (100%)	0	100	100
18	QS	72/80 (90%)	69 (96%)	3 (4%)	30	59
18	XS	69/80 (86%)	62 (90%)	7 (10%)	7	27
19	QT	76/82 (93%)	76 (100%)	0	100	100
19	XT	76/82 (93%)	75 (99%)	1 (1%)	69	82
20	QU	20/22 (91%)	20 (100%)	0	100	100
20	XU	20/22 (91%)	19 (95%)	1 (5%)	24	55
23	QY	78/78 (100%)	77 (99%)	1 (1%)	69	82
23	QZ	78/78 (100%)	72 (92%)	6 (8%)	13	38
23	XY	78/78 (100%)	78 (100%)	0	100	100
23	XZ	78/78 (100%)	77 (99%)	1 (1%)	69	82
24	R0	65/67 (97%)	63 (97%)	2 (3%)	40	67
24	Y0	65/67 (97%)	64 (98%)	1 (2%)	65	80
25	R2	64/67 (96%)	64 (100%)	0	100	100
25	Y2	64/67 (96%)	64 (100%)	0	100	100
26	R3	51/52 (98%)	50 (98%)	1 (2%)	55	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	76
27	R4	62/63 (98%)	59 (95%)	3 (5%)	25	56
27	Y4	62/63 (98%)	62 (100%)	0	100	100
28	R5	51/52 (98%)	51 (100%)	0	100	100
28	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	76
29	R6	51/52 (98%)	51 (100%)	0	100	100
29	Y6	51/52 (98%)	51 (100%)	0	100	100
30	R7	40/42 (95%)	40 (100%)	0	100	100
30	Y7	41/42 (98%)	41 (100%)	0	100	100
31	R9	34/34 (100%)	34 (100%)	0	100	100
31	Y9	34/34 (100%)	34 (100%)	0	100	100
34	RD	214/218 (98%)	213 (100%)	1 (0%)	88	93
34	YD	216/218 (99%)	212 (98%)	4 (2%)	57	76
35	RE	165/166 (99%)	161 (98%)	4 (2%)	49	72
35	YE	164/166 (99%)	158 (96%)	6 (4%)	34	62
36	RG	155/156 (99%)	153 (99%)	2 (1%)	69	82
36	YG	155/156 (99%)	154 (99%)	1 (1%)	86	91
37	RH	145/148 (98%)	140 (97%)	5 (3%)	37	64
37	YH	144/148 (97%)	136 (94%)	8 (6%)	21	52
38	RI	122/124 (98%)	122 (100%)	0	100	100
38	YI	122/124 (98%)	122 (100%)	0	100	100
39	RN	117/119 (98%)	117 (100%)	0	100	100
39	YN	117/119 (98%)	117 (100%)	0	100	100
40	RO	100/100 (100%)	100 (100%)	0	100	100
40	YO	100/100 (100%)	100 (100%)	0	100	100
41	RP	116/116 (100%)	115 (99%)	1 (1%)	78	87
41	YP	115/116 (99%)	104 (90%)	11 (10%)	8	29
42	RQ	111/111 (100%)	111 (100%)	0	100	100
42	YQ	111/111 (100%)	104 (94%)	7 (6%)	18	47
43	RR	100/101 (99%)	100 (100%)	0	100	100
43	YR	100/101 (99%)	100 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RS	87/88 (99%)	87 (100%)	0	100	100
44	YS	87/88 (99%)	87 (100%)	0	100	100
45	RT	120/127 (94%)	120 (100%)	0	100	100
45	YT	120/127 (94%)	118 (98%)	2 (2%)	60	78
46	RU	93/94 (99%)	93 (100%)	0	100	100
46	YU	93/94 (99%)	93 (100%)	0	100	100
47	RV	82/82 (100%)	80 (98%)	2 (2%)	49	72
47	YV	82/82 (100%)	81 (99%)	1 (1%)	71	83
48	RW	92/92 (100%)	91 (99%)	1 (1%)	73	84
48	YW	92/92 (100%)	92 (100%)	0	100	100
49	RX	74/78 (95%)	74 (100%)	0	100	100
49	YX	74/78 (95%)	74 (100%)	0	100	100
50	RY	88/91 (97%)	87 (99%)	1 (1%)	73	84
50	YY	88/91 (97%)	87 (99%)	1 (1%)	73	84
51	QL	104/109 (95%)	102 (98%)	2 (2%)	57	76
51	XL	103/109 (94%)	103 (100%)	0	100	100
52	R1	79/83 (95%)	79 (100%)	0	100	100
52	Y1	78/83 (94%)	75 (96%)	3 (4%)	33	62
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	RF	161/166 (97%)	159 (99%)	2 (1%)	71	83
54	YF	161/166 (97%)	160 (99%)	1 (1%)	86	91
55	RZ	162/179 (90%)	155 (96%)	7 (4%)	29	59
55	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	83
All	All	9997/10378 (96%)	9849 (98%)	148 (2%)	65	80

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	XF	71	ARG
52	Y1	78	LYS
54	RF	133	ASN
7	XG	89	MET
11	XK	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
34	YD	45	ASN
34	YD	115	GLN
55	YZ	34	ASN
34	YD	87	ASN
34	YD	116	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	308 (20%)	50 (3%)
1	XA	1505/1521 (98%)	301 (20%)	48 (3%)
21	QV	77/77 (100%)	7 (9%)	2 (2%)
21	QW	76/77 (98%)	14 (18%)	1 (1%)
21	XV	77/77 (100%)	7 (9%)	1 (1%)
21	XW	76/77 (98%)	15 (19%)	1 (1%)
22	QX	19/22 (86%)	9 (47%)	1 (5%)
22	XX	19/22 (86%)	7 (36%)	2 (10%)
32	RA	2888/2915 (99%)	598 (20%)	47 (1%)
32	YA	2872/2915 (98%)	580 (20%)	42 (1%)
33	RB	119/124 (95%)	26 (21%)	1 (0%)
33	YB	119/124 (95%)	21 (17%)	1 (0%)
56	ZA	1/3 (33%)	1 (100%)	0
56	ZB	1/3 (33%)	0	0
All	All	9357/9478 (98%)	1894 (20%)	197 (2%)

5 of 1894 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G

5 of 197 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	RA	2211	G
1	XA	243	A
32	YA	2166	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	RA	2422	A
32	RA	2859	G

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

8 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$
22	A2M	QX	19	22	18,25,26	1.04	1 (5%)	18,36,39	1.29	2 (11%)
22	A2M	QX	20	22	18,25,26	1.09	1 (5%)	18,36,39	1.17	2 (11%)
22	A2M	XX	19	22	18,25,26	0.96	1 (5%)	18,36,39	1.31	2 (11%)
22	A2M	XX	20	22	18,25,26	0.97	1 (5%)	18,36,39	1.23	2 (11%)
22	OMU	QX	21	1,22	14,22,23	1.66	2 (14%)	14,31,34	1.45	2 (14%)
22	OMU	XX	21	1,22	14,22,23	0.78	1 (7%)	14,31,34	0.79	0
56	PPU	ZA	76	32,56	32,40,41	1.30	5 (15%)	33,57,60	1.49	6 (18%)
56	PPU	ZB	76	32,56	32,40,41	0.82	1 (3%)	33,57,60	1.47	6 (18%)

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
22	A2M	QX	19	22	-	0/5/27/28	0/3/3/3
22	A2M	QX	20	22	-	2/5/27/28	0/3/3/3
22	A2M	XX	19	22	-	2/5/27/28	0/3/3/3
22	A2M	XX	20	22	-	2/5/27/28	0/3/3/3
22	OMU	QX	21	1,22	-	4/7/27/28	0/2/2/2
22	OMU	XX	21	1,22	-	2/7/27/28	0/2/2/2
56	PPU	ZA	76	32,56	-	5/21/43/44	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	ZB	76	32,56	-	6/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QX	21	OMU	C6-N1	-4.02	1.30	1.35
22	QX	21	OMU	C2-N3	-3.20	1.31	1.38
22	QX	20	A2M	C5-C4	2.58	1.47	1.40
22	QX	19	A2M	C5-C4	2.55	1.47	1.40
56	ZA	76	PPU	C2'-C1'	-2.40	1.50	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	ZA	76	PPU	N1-C6-N6	4.20	121.48	117.06
56	ZA	76	PPU	C10-N6-C6	-3.55	108.77	119.51
56	ZB	76	PPU	N1-C6-N6	3.50	120.74	117.06
22	XX	19	A2M	N3-C2-N1	-3.50	123.21	128.68
56	ZB	76	PPU	C10-N6-C6	-3.44	109.10	119.51

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QX	21	OMU	C2'-C1'-N1-C6
22	QX	21	OMU	O4'-C1'-N1-C6
22	XX	21	OMU	C3'-C4'-C5'-O5'
22	XX	21	OMU	O4'-C4'-C5'-O5'
56	ZA	76	PPU	C4'-C3'-N3'-C

There are no ring outliers.

8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QX	19	A2M	3	0
22	QX	20	A2M	2	0
22	XX	19	A2M	5	0
22	XX	20	A2M	3	0
22	QX	21	OMU	3	0
22	XX	21	OMU	2	0
56	ZA	76	PPU	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	ZB	76	PPU	12	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 906 ligands modelled in this entry, 904 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	$\# Z > 2$
58	SF4	QD	301	4	0,12,12	0.00	-	-		
58	SF4	XD	301	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
58	SF4	QD	301	4	-	-	0/6/5/5
58	SF4	XD	301	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.