



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2020 – 06:20 am BST

PDB ID : 6OTR
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (AAU)
Authors : Pavelich, I.P.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-03
Resolution : 3.12 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
buster-report	:	1.1.7 (2018)
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

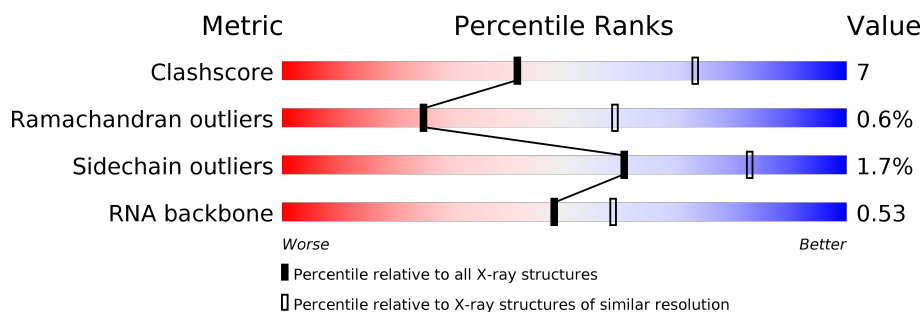
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)












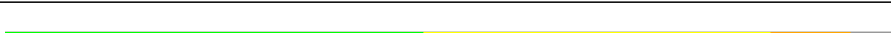


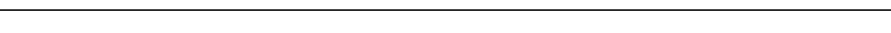




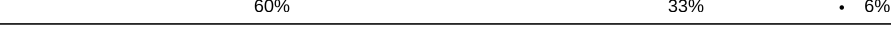





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	57% 29% 11% ..
1	XA	1521	56% 31% 10% ..
2	QB	256	62% 27% • 8%
2	XB	256	57% 30% • 8%
3	QC	239	56% 27% •• 14%
3	XC	239	64% 21% • 14%
4	QD	209	77% 22% •












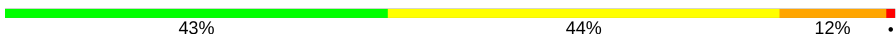


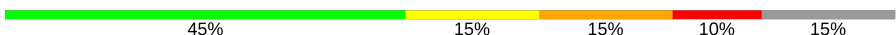
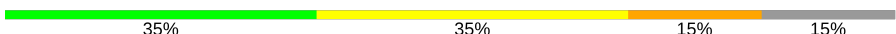









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Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	


























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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	















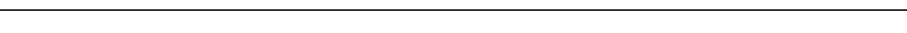




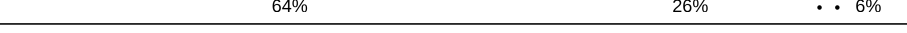





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Mol	Chain	Length	Quality of chain
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	124	
36	YB	124	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	








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Mol	Chain	Length	Quality of chain
40	RG	182	
40	YG	182	
41	RH	180	
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	

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Mol	Chain	Length	Quality of chain
52	YW	113	 89% 11%
53	RX	96	 79% 16% • •
53	YX	96	 88% 8% •
54	RY	110	 75% 21% • • •
54	YY	110	 78% 18% • •
55	RZ	206	 59% 25% • 11%
55	YZ	206	 55% 28% 5% 11%
56	ZA	3	 100%
56	ZB	3	 67% 33%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298517 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			

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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 S12.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

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

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

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

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

- Molecule 22 is a RNA chain called tRNA-fMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			
23	XX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
36	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- 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	87	Total	Mg	0	0
			87	87		

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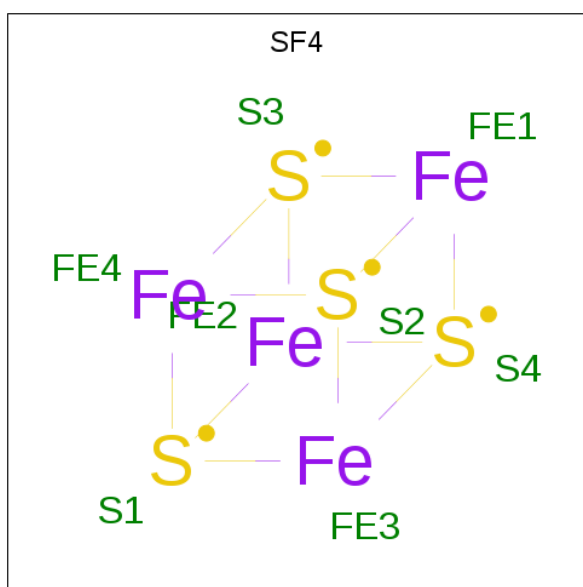
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YV	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	YA	329	Total 329	Mg 329	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	YR	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	YD	2	Total 2	Mg 2	0	0
57	QV	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	106	Total 106	Mg 106	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	305	Total 305	Mg 305	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	XL	1	Total 1	Mg 1	0	0
57	YB	6	Total 6	Mg 6	0	0
57	XV	4	Total 4	Mg 4	0	0
57	RB	3	Total 3	Mg 3	0	0
57	YS	1	Total 1	Mg 1	0	0
57	QE	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	YE	4	Total 4	Mg 4	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

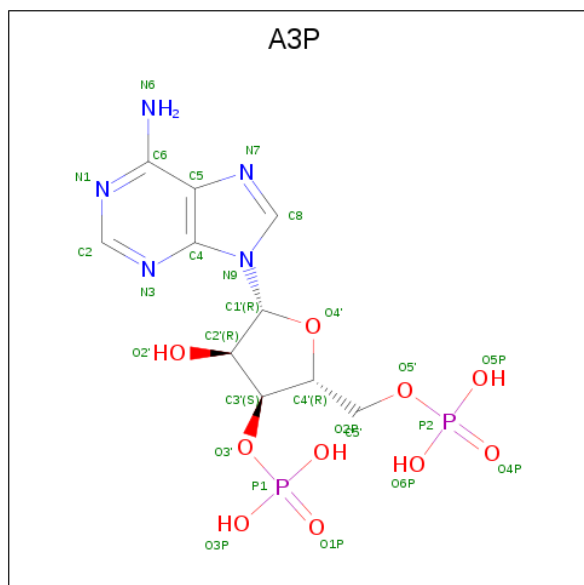


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- 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	R9	1	Total	Zn	0	0
			1	1		
59	R6	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		

- Molecule 60 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



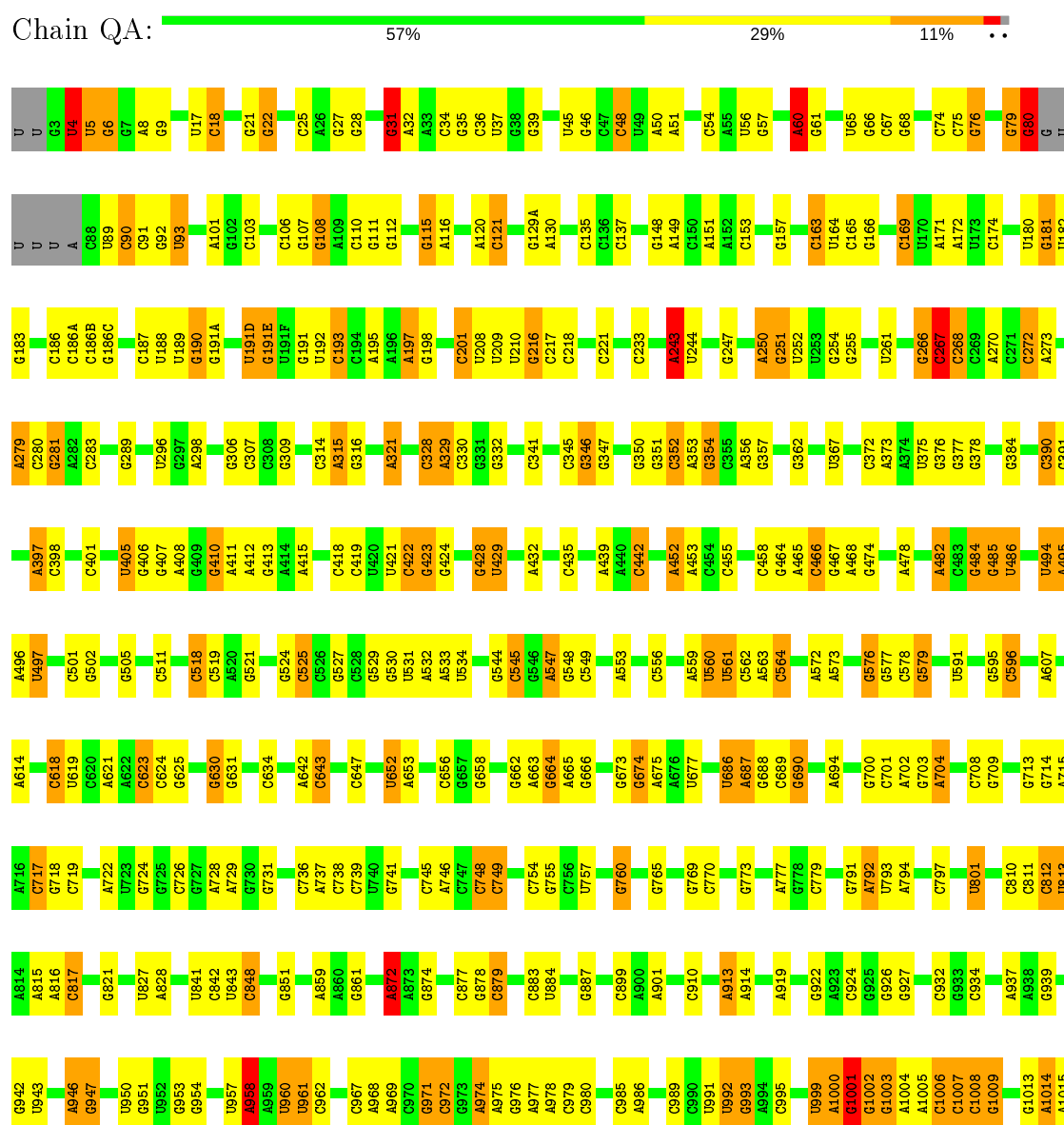
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	QX	1	Total	C	N	O P	0	0
			26	10	5 9	2		
60	XX	1	Total	C	N	O P	0	0
			26	10	5 9	2		

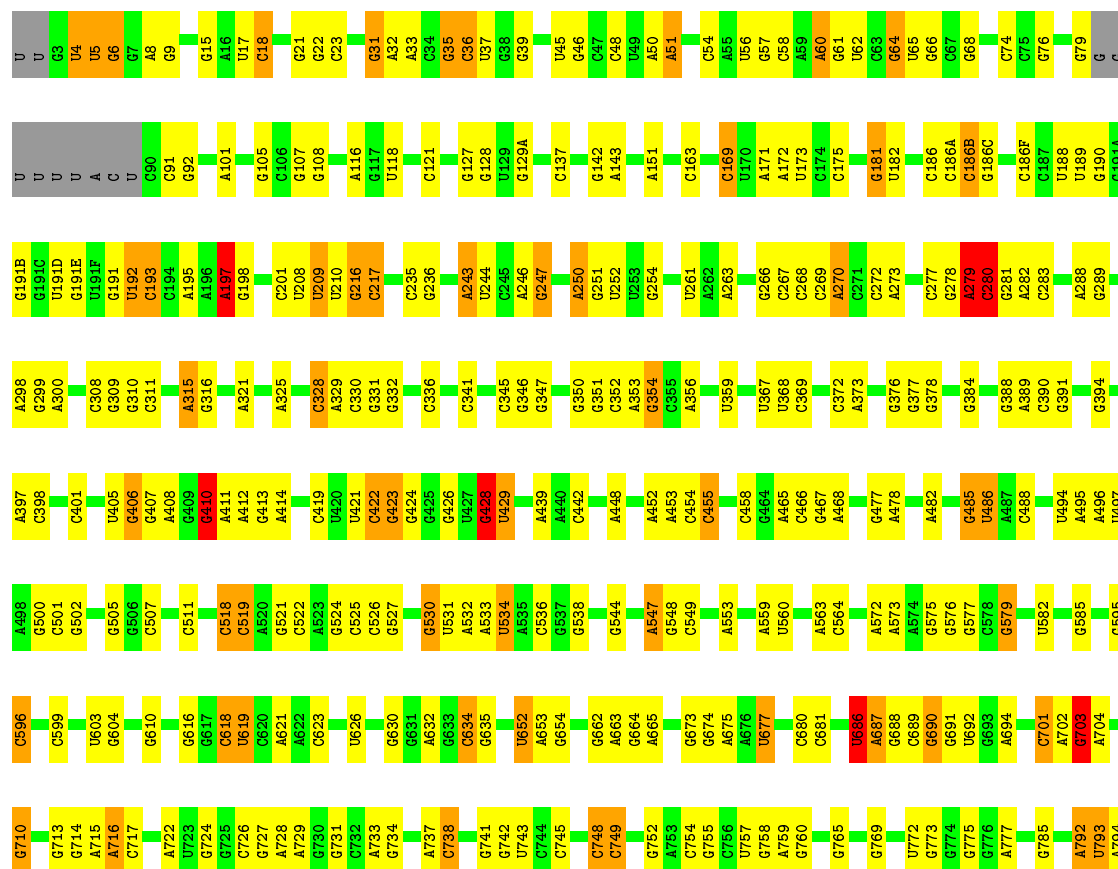
3 Residue-property plots [i](#)

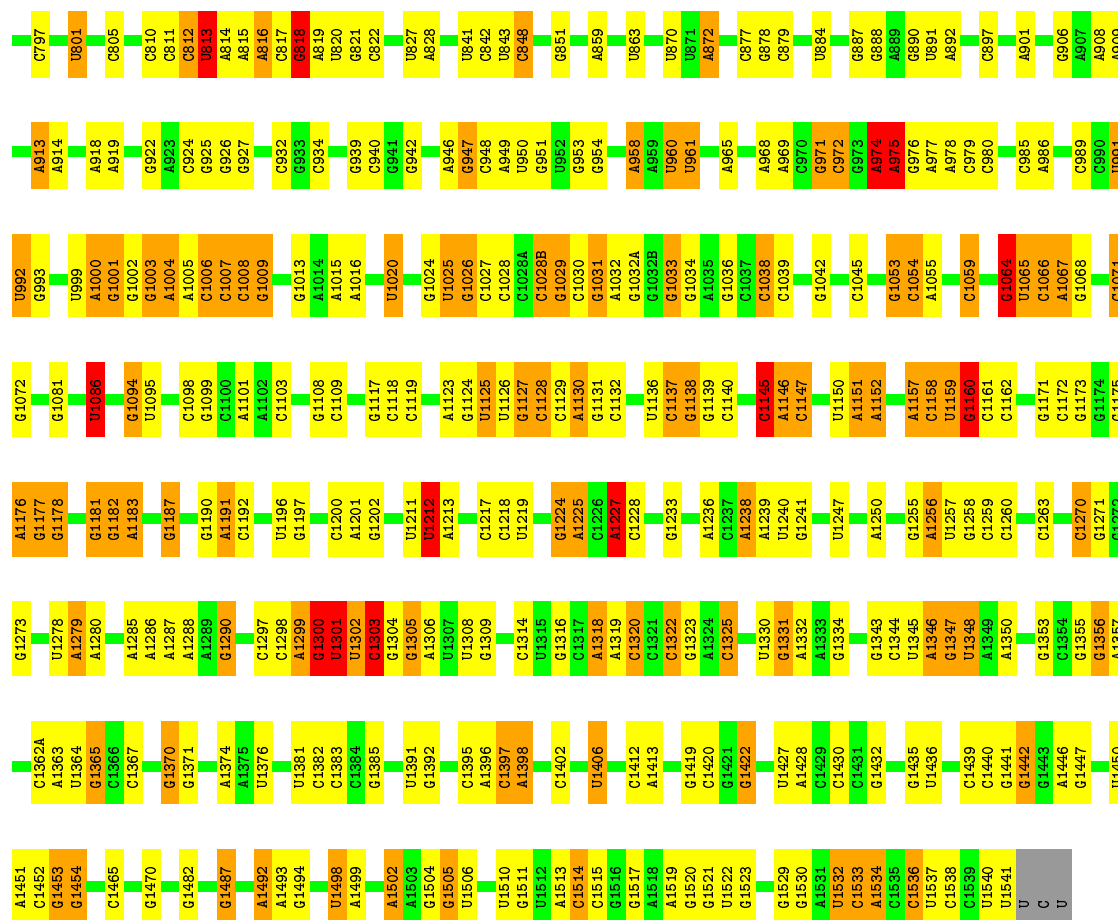
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

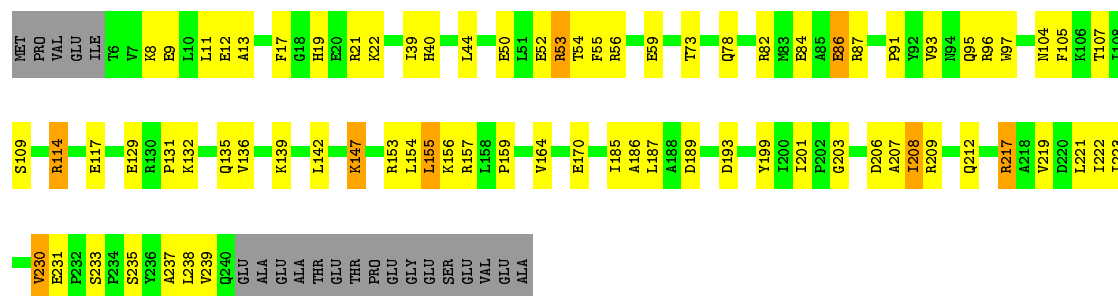






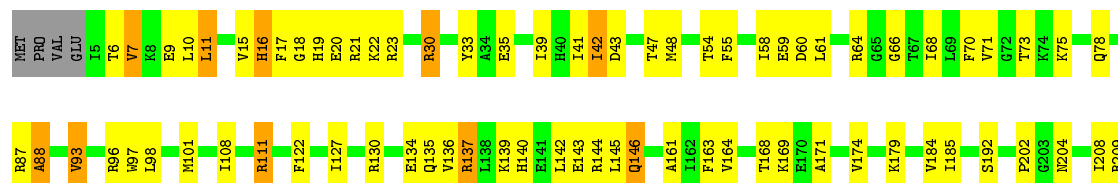
• Molecule 2: 30S ribosomal protein S2

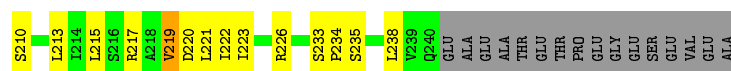
Chain QB: 62% 27% 8%



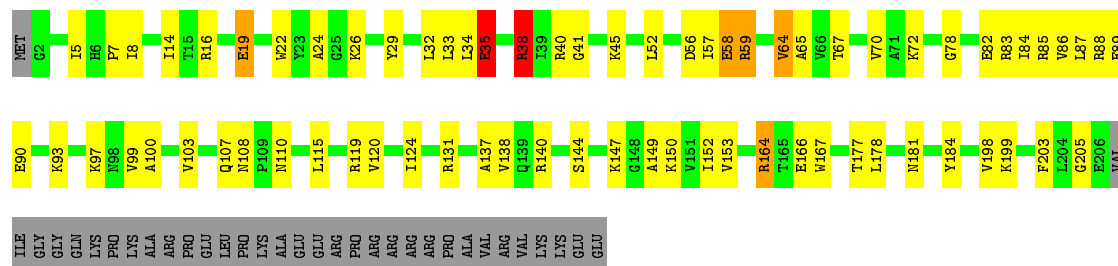
• Molecule 2: 30S ribosomal protein S2

Chain XB: 57% 30% 8%

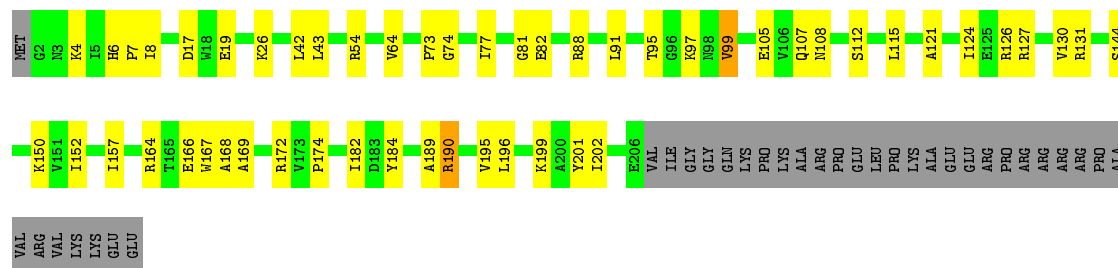




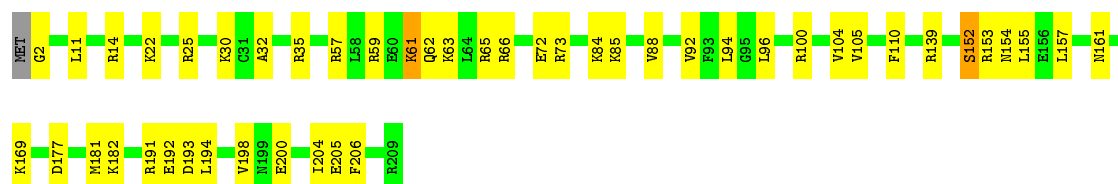
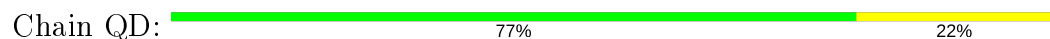
- Molecule 3: 30S ribosomal protein S3



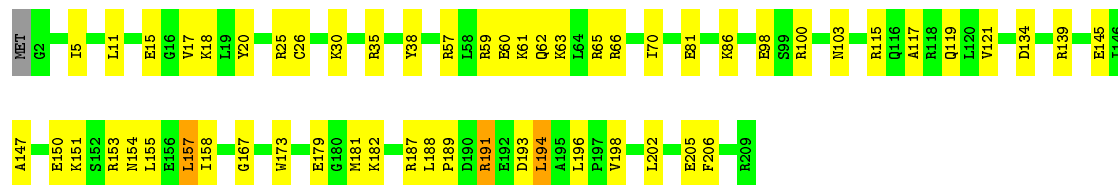
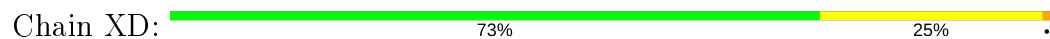
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

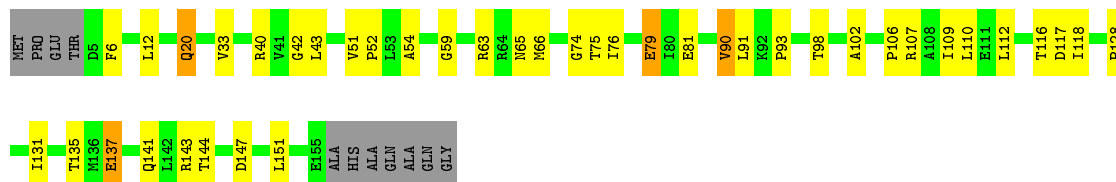


- Molecule 4: 30S ribosomal protein S4




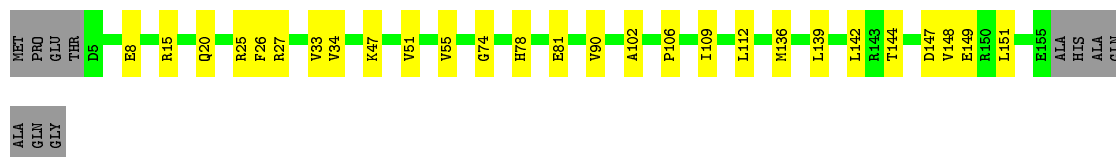
- Molecule 5: 30S ribosomal protein S5

Chain QE:  68% 23% 7%




- Molecule 5: 30S ribosomal protein S5

Chain XE:  77% 17% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  87% 12%



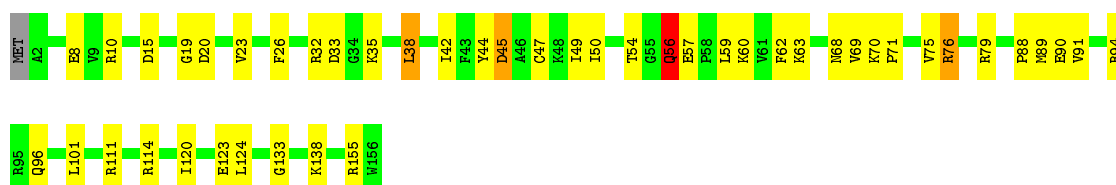
- Molecule 6: 30S ribosomal protein S6

Chain XF:  79% 21%




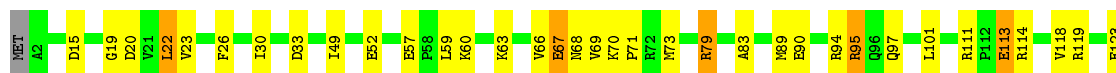
- Molecule 7: 30S ribosomal protein S7

Chain QG:  70% 27%



- Molecule 7: 30S ribosomal protein S7

Chain XG:  74% 22%





- Molecule 8: 30S ribosomal protein S8

Chain QH: 68% 29% ..



- Molecule 8: 30S ribosomal protein S8

Chain XH: 80% 20% .



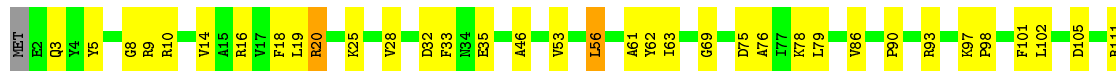
- Molecule 9: 30S ribosomal protein S9

Chain QI: 61% 33% 5% .



- Molecule 9: 30S ribosomal protein S9

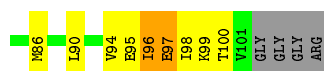
Chain XI: 69% 27% ..



- Molecule 10: 30S ribosomal protein S10

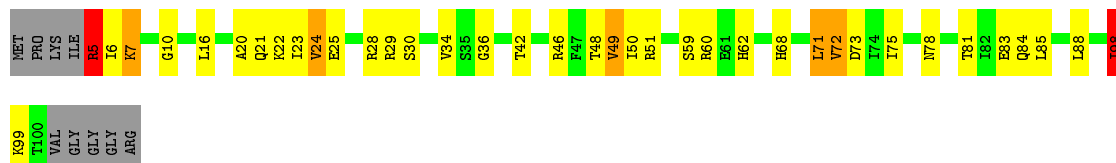
Chain QJ: 47% 39% 9% 6%





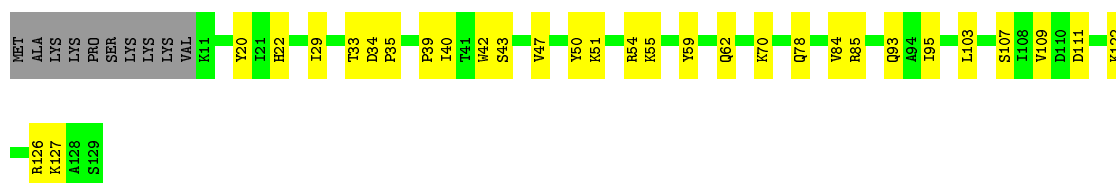
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 55% 30% 5% 9%



- Molecule 11: 30S ribosomal protein S11

Chain QK: 69% 23% 8%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 71% 19% 10%



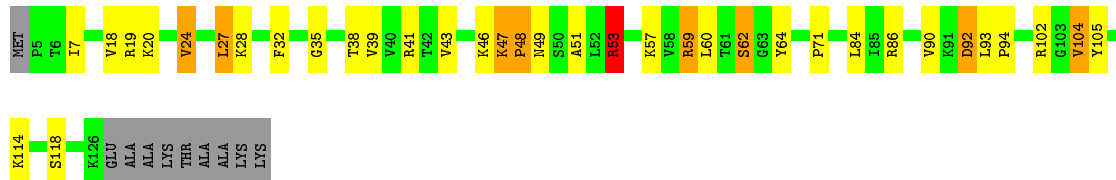
- Molecule 12: 30S ribosomal protein S12

Chain QL: 75% 18% 5%



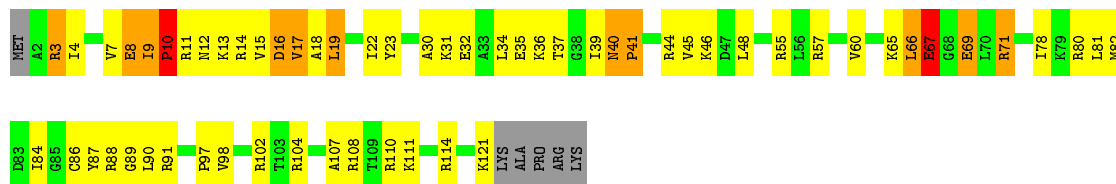
- Molecule 12: 30S ribosomal protein S12

Chain XL: 65% 20% 6% 8%



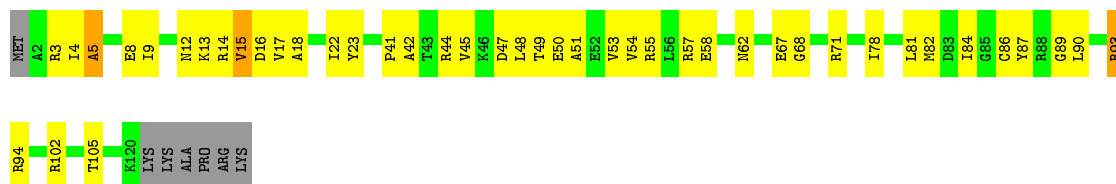
- Molecule 13: 30S ribosomal protein S13

Chain QM:  48% 37% 9% 5%




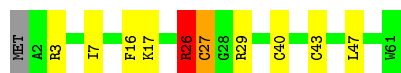
- Molecule 13: 30S ribosomal protein S13

Chain XM:  60% 33% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  82% 13% . . .




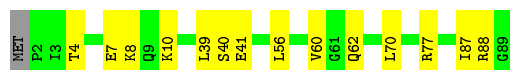
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  72% 26% .



- Molecule 15: 30S ribosomal protein S15

Chain QO:  83% 16% .




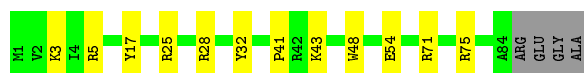
- Molecule 15: 30S ribosomal protein S15

Chain XO:  74% 19% . .



- Molecule 16: 30S ribosomal protein S16

Chain QP:  82% 14% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP: 75% 20% 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ: 78% 17% 5%



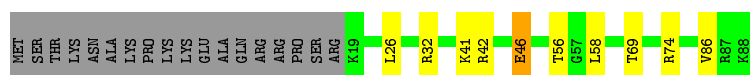
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 73% 22% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR: 68% 10% 20%



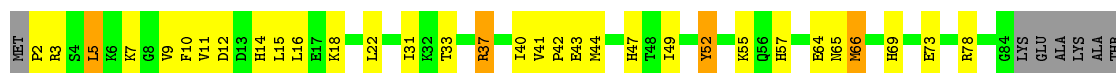
- Molecule 18: 30S ribosomal protein S18

Chain XR: 60% 18% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS: 55% 30% 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  70% 18% 11%



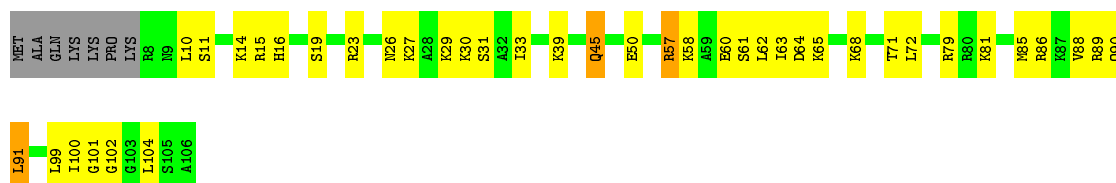
- Molecule 20: 30S ribosomal protein S20

Chain QT:  83% 9% 7%



- Molecule 20: 30S ribosomal protein S20

Chain XT:  56% 35% 7%




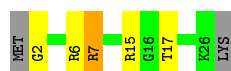
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  63% 30% 7%



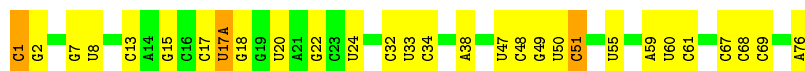
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  74% 15% 7%



- Molecule 22: tRNA-fMet

Chain QV:  62% 34% 1%



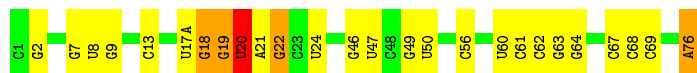
- Molecule 22: tRNA-fMet

Chain QW:  43% 44% 12%



- Molecule 22: tRNA-fMet

Chain XV:  66% 27% 5% .



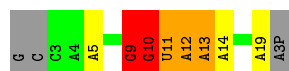
- Molecule 22: tRNA-fMet

Chain XW:  45% 43% 9% .



- Molecule 23: mRNA

Chain QX:  45% 15% 15% 10% 15%




- Molecule 23: mRNA

Chain XX:  35% 35% 15% 15%



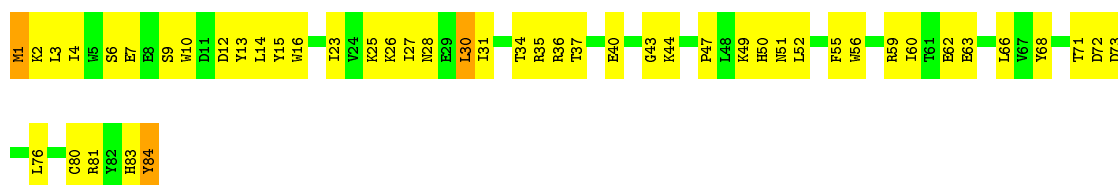
- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QY:  73% 26% .



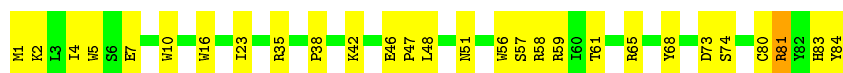
- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QZ:  43% 54% .

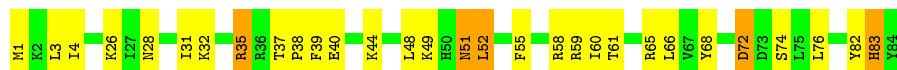


- Molecule 24: Addiction module toxin, Txe/YoeB family

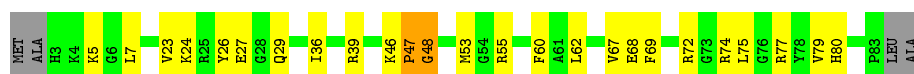
Chain XY:  67% 32% .



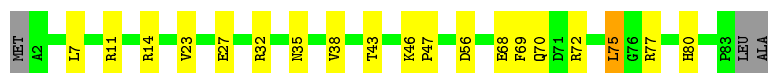
- Molecule 24: Addiction module toxin, Txe/YoeB family



- Molecule 25: 50S ribosomal protein L27



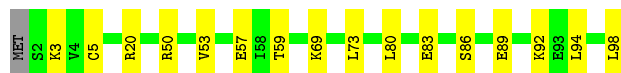
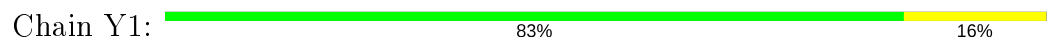
- Molecule 25: 50S ribosomal protein L27



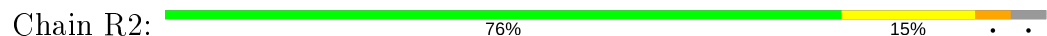
- Molecule 26: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L29

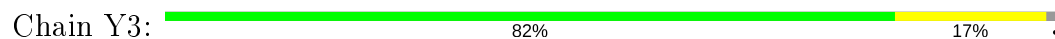




- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L31



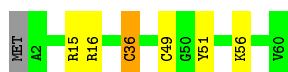
- Molecule 29: 50S ribosomal protein L31



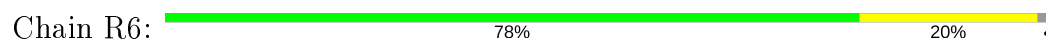
- Molecule 30: 50S ribosomal protein L32

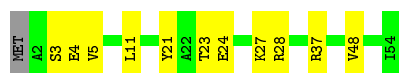


- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33





- Molecule 31: 50S ribosomal protein L33

Chain Y6: 83% 15% .



- Molecule 32: 50S ribosomal protein L34

Chain R7: 90% 6% .



- Molecule 32: 50S ribosomal protein L34

Chain Y7: 86% 12% .



- Molecule 33: 50S ribosomal protein L35

Chain R8: 72% 25% . .



- Molecule 33: 50S ribosomal protein L35

Chain Y8: 68% 26% 5% .



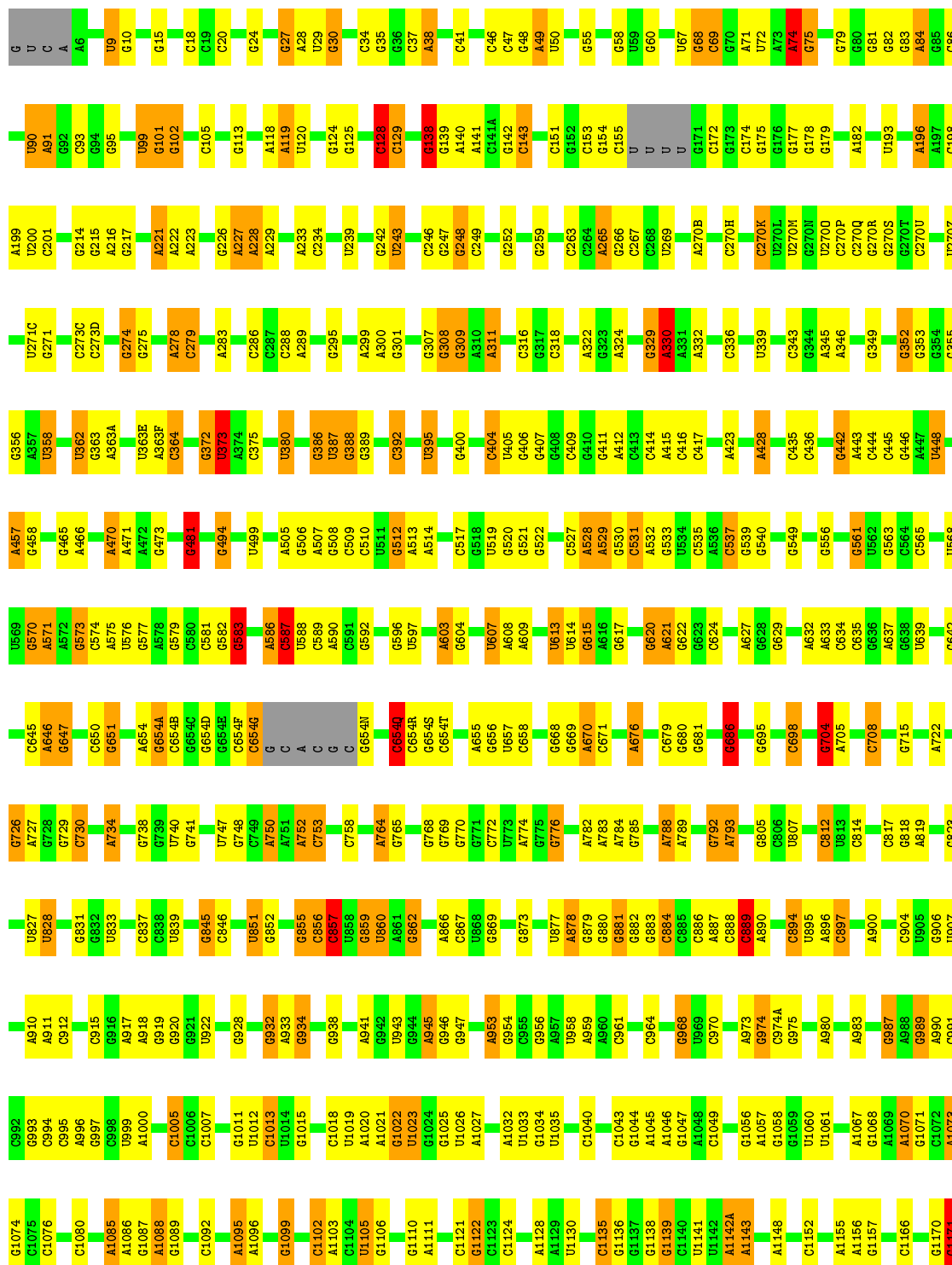
- Molecule 34: 50S ribosomal protein L36

Chain R9: 51% 35% 11% .

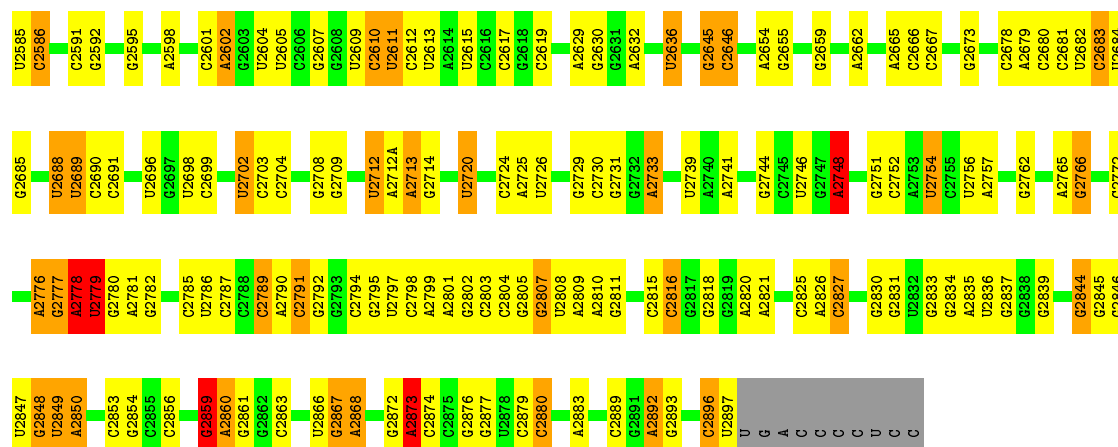


- Molecule 34: 50S ribosomal protein L36

Chain Y9: 70% 30%

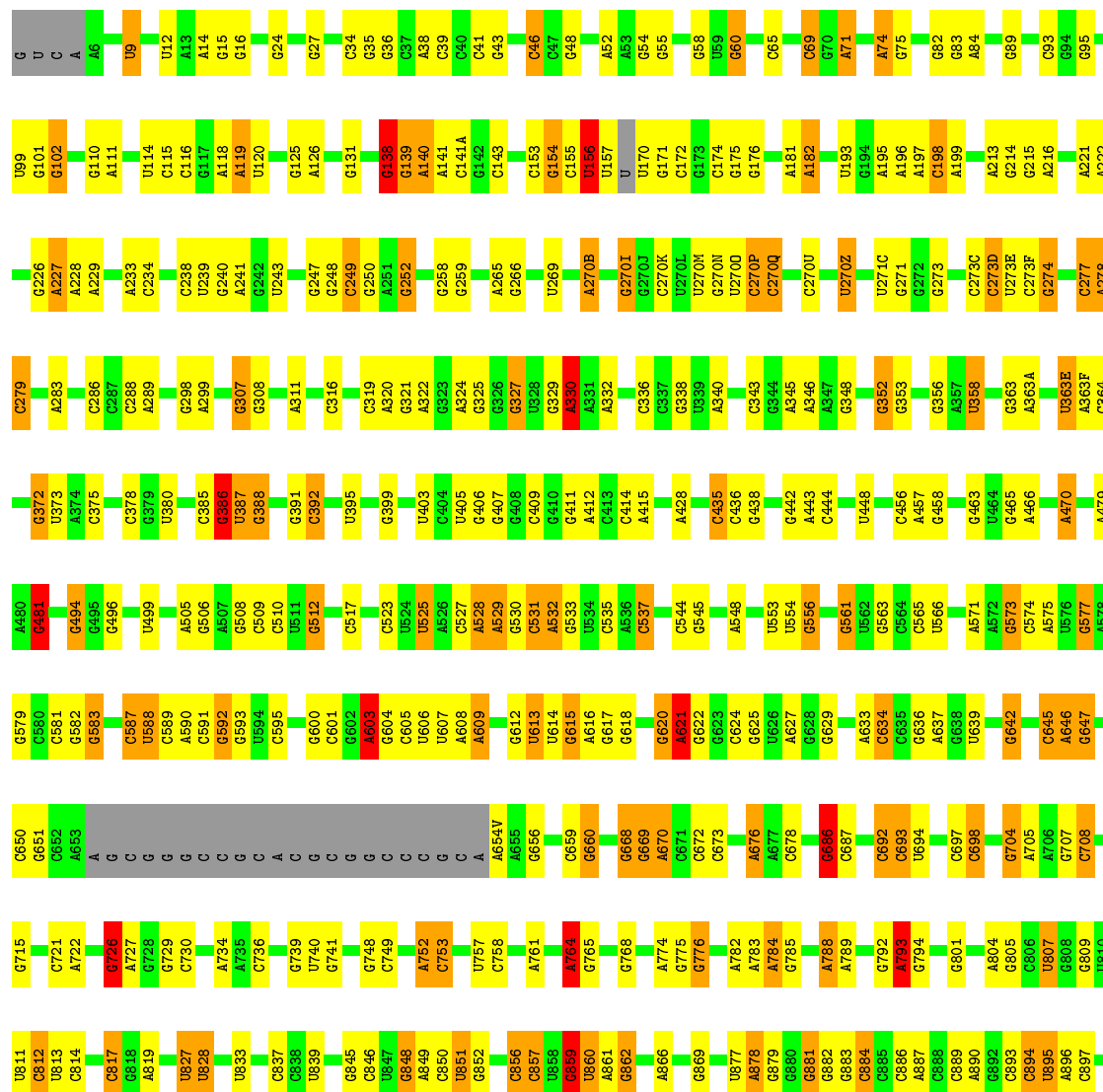


G2494	A2422	C2321	G2131	C2043	G1947	U1834	U1730	C1615	A1528	G1443	A1342	G1271	G1173
A2423	G2325	G2325	U2132	G2046	G1948	G1835	G1731	A1616	A1529	G1444	G1345	A1272	A1174
C2424	C2326	G2238	A2134	G2052	G1950	C1836	A1732	C1617	C1533	G1444A	C1346	U1273	U1175
A2425	A2327	G2239	A2135	G2055	U1955	G1838	G1734	G1619	U1535	G1445	U1352	A1275	G1176
A2426	A2328	G2242	G2141	C2056	U1956	G1839	C1735	A1631	A1536	C1446	A1353	C1278	A1177
C2427	G2243	U2244	U2144	G2059	C1961	G1846	G1743	C1636	A1537	A1449	A1354	C1279	C1179
G2428	A2334	U2245	C2145	A2060	U1962	A1847	G1750	A1637	G1538	G1449A	G1359	G1280	C1180
A2430	A2335	G2246	G2146	G2061	U1963	U1851	C1751	C1638	G1539	C1450	A1360	G1281	U1188
U2431	A2336	G2247	G2147	A2062	U1964	A1854	C1754	U1639	G1541	A1453	G1364	G1282	G1191
A2432	G2248	G2250	G2148	C2063	C1965	G1857	A1755	A1641	G1542	U1454	A1365	G1285	G1196
A2435	C2243	G2253	G2149	C2065	A1966	G1858	G1756	G1642	A1543	G1455	A1366	A1286	C1196
U2438	U2344	G2259	U2150	C2066	C1967	G1859	A1762	C1644	A1545	C1458	A1367	A1287	U1197
A2439	G2260	G2260	G2156	G2069	A1970	U1864	G1763	C1648	G1547	G1459	G1368	U1288	U1198
C2440	C2261	G2266	G2157	G2080	A1971	G1869	G1764	G1649	C1550	A1460	C1370	C1290	U1199
C2441	A2266	U2272	C2161	U2086	A1972	A1872	C1771	A1652	C1551	C1467	A1378	C1293	C1202
G2442	U2272	G2273	G2162	G2087	C1979	G1878	G1772	G1653	A1554	A1471	A1379	G1294	G1203
G2443	A2273	G2274	C2163	G2088	G1980	C1879	A1773	G1654	A1558	C1474	G1380	C1295	A1204
G2444	G2275	G2276	G2164	U2089	C1981	G1880	C1774	A1657	G1559	G1475	G1385	U1300	U1205
G2445	C2275	G2276	G2165	G2090	C1982	C1881	U1775	C1657	G1560	C1387	G1388	G1303	A1214
G2446	C2276	G2277	U2167	G2091	U1989	G1882	G1776	C1658	A1562	U1391	U1391	C1304	A1220
A2448	C2277	G2279	U2168	U2092	G1992	A1885	U1779	G1667	A1566	U1394	U1394	C1306	G1228
U2449	A2286	G2283	A2169	G2093	G1993	G1888	A1780	A1668	A1567	A1395	A1395	A1307	G1233
C2450	A2287	C2284	G2170	G2094	C1994	A1889	C1781	A1669	A1570	U1396	U1396	G1309	U1234
A2451	C2285	G2285	U2172	C2095	U1995	A1890	A1786	C1670	A1571	U1397	U1397	G1310	G1235
G2452	A2286	G2286	A2173	U2098	G2006	G1891	U1786	G1678	A1572	A1489	G1400	U1312	G1236
G2453	A2287	G2287	C2178	U2099	G2010	A1900	C1790	G1674	G1573	A1490	G1400	U1313	A1241
G2454	A2287	G2287	G2178	U2100	G2011	A1901	A1791	G1678	C1574	C1493	C1404	G1314	A1242
U2457	U2291	U2291	C2183	C2103	U2011	G1906	G1792	G1681	U1578	C1499	U1406	U1316	G1243
G2458	C2292	C2292	G2184	G2104	G2012	U1907	C1797	C1686	U1585	C1502	C1407	G1317	G1244
A2459	C2293	C2293	U2189	C2108	A2019	G1909	C1800	C1686	A1586	G1505	U1415	G1319	G1248
U2460	C2294	C2294	G2190	G2109	A2020	C1909	G1801	C1686	A1587	C1506	G1416	C1320	C1251
C2461	C2295	C2295	G2191	C2110	G2021	U1914	A1802	A1689	C1588	A1507	G1417	U1326	G1252
G2468	C2296	C2296	G2192	C2111	G2022	C1914	A1803	U1693	C1588	A1508	G1418	C1327	A1253
A2469	A2297	A2297	C2196	U2112	G2023	U1914	C1804	C1694	C1588	A1509	U1420	A1254	U1255
C2470	C2298	C2298	U2197	U2113	C2026	C1920	U1805	G1695	C1588	A1510	G1421	U1329	G1256
G2471	G2304	G2304	G2198	A2114	G2027	U1924	G1816	G1696	C1588	C1513	A1427	G1332	A1262
U2473	A2305	A2305	A2199	G2115	U2028	C1924	G1817	G1696	C1588	U1514	C1428	C1333	U1263
C2474	C2306	C2306	G2205	G2116	G2029	U1927	U1818	A1697	C1588	U1523	G1429	G1334	G1264
G2475	G2307	G2307	C2205	A2117	G2030	A1927	A1819	G1697	C1588	G1524	A1430	A1265	A1265
A2476	C2308	C2308	C2209	U2118	A2031	A1928	A1820	A1698	C1588	G1525	A1434	G1266	U1267
C2477	A2309	A2309	G2210	A2119	G2032	U1929	U1820	A1698	C1588	G1526	A1437	U1341	
G2481	A2310	A2310	G2211	G2120	G2033	G1930	G1824	G1703	A1603	U1514	A1427	G1332	
A2482	U2311	U2311	G2212	G2123	A2033	U1931	G1827	C1708	A1603	U1523	C1428	G1333	
C2483	C2312	C2312	U2213	G2124	G2036	C1934	A1828	G1725	A1608	G1524	G1429	G1334	
G2484	G2314	G2314	G2215	A2125	G2037	G1935	A1829	G1728	A1608	G1525	A1430	G1338	
U2489	C2315	C2315	A2225	G2127	G2038	G1936	A1830	G1728	A1608	G1526	A1437	G1339	
G2490	G2318	G2318	C2226	G2127	U2041	A1937	C1830	G1728	A1608	G1527	A1437	U1341	
U2491	A2320	A2320	C2229	C2128	U2042	A1938	U1833	A1729	A1614				
U2584	A2320	A2320	C2229	U2130	A2042	A1938	U1833	A1729	A1614				

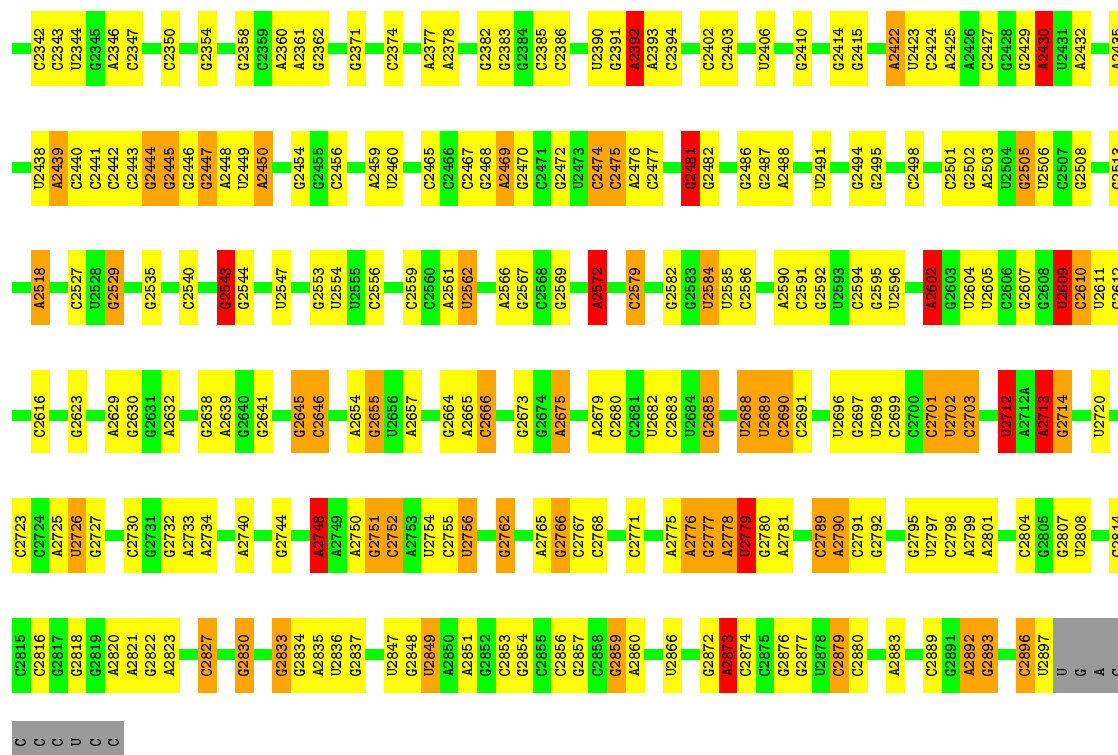


• Molecule 35: 23S rRNA

Chain YA: 57% 30% 10% ..

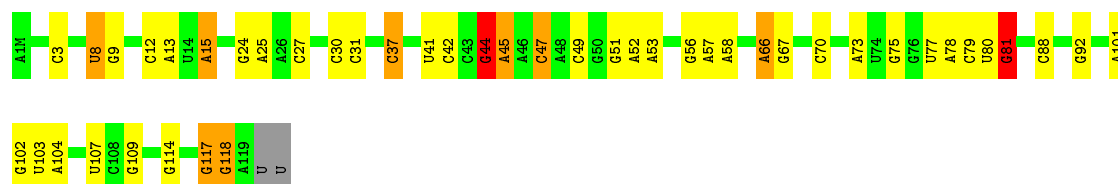






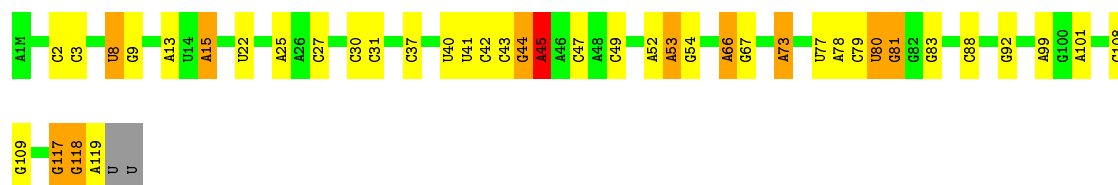
• Molecule 36: 5S rRNA

Chain RB: 



• Molecule 36: 5S rRNA

Chain YB: 



• Molecule 37: 50S ribosomal protein L2

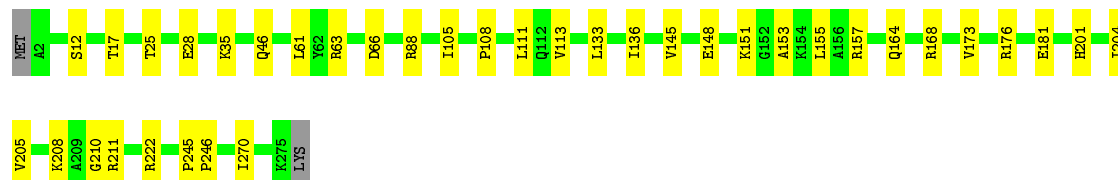
Chain RD: 





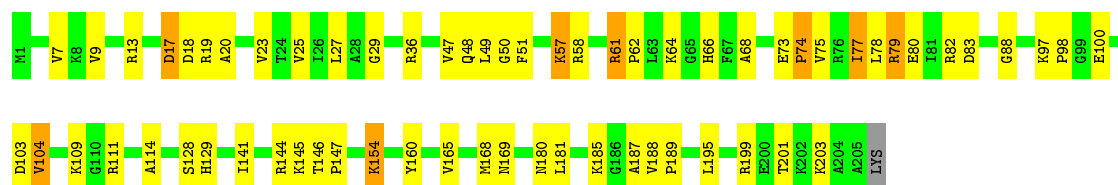
- Molecule 37: 50S ribosomal protein L2

Chain YD: 86% 13% .



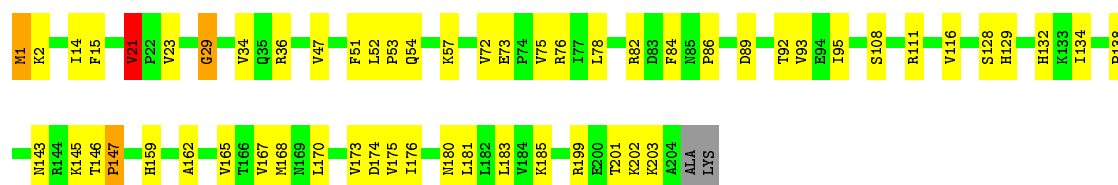
- Molecule 38: 50S ribosomal protein L3

Chain RE: 68% 27% .



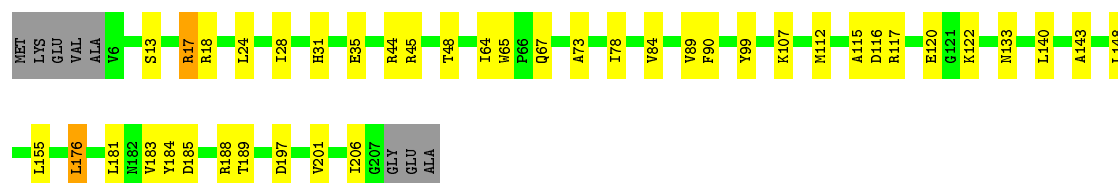
- Molecule 38: 50S ribosomal protein L3

Chain YE: 71% 26% ..



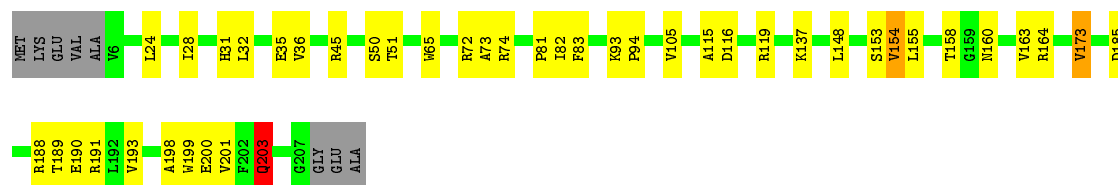
- Molecule 39: 50S ribosomal protein L4

Chain RF: 77% 19% ..



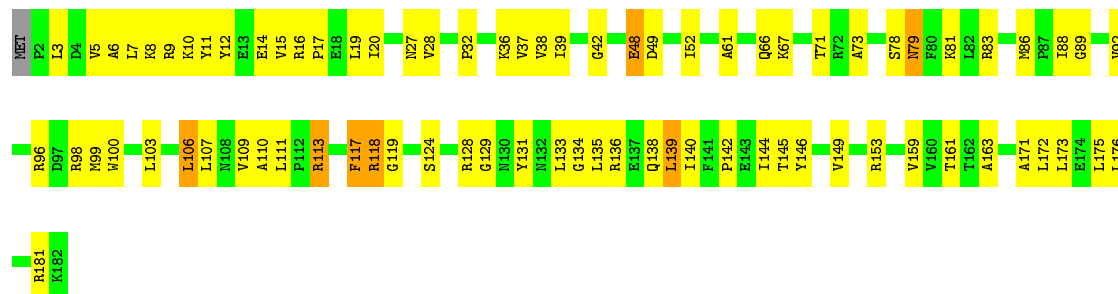
- Molecule 39: 50S ribosomal protein L4

Chain YF: 76% 19% ..



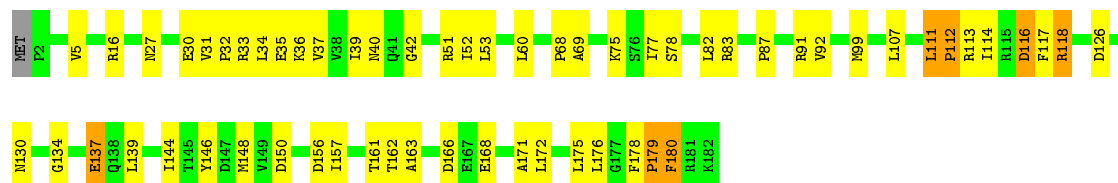
- Molecule 40: 50S ribosomal protein L5

Chain RG: 56% 40% . .



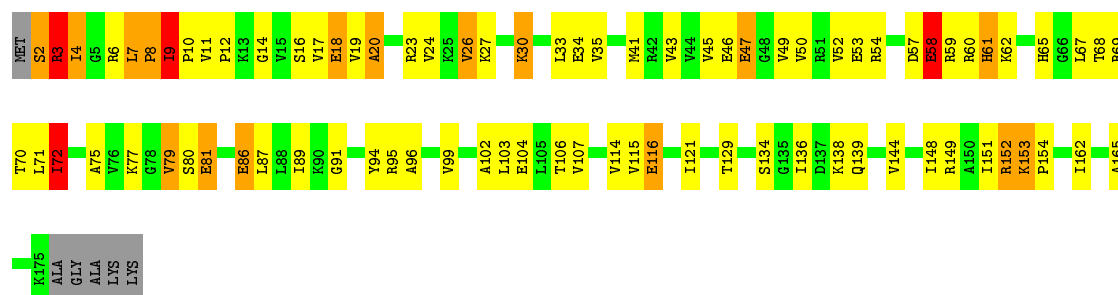
- Molecule 40: 50S ribosomal protein L5

Chain YG: 66% 29% . .



- Molecule 41: 50S ribosomal protein L6

Chain RH: 51% 35% 9% . .



- Molecule 41: 50S ribosomal protein L6

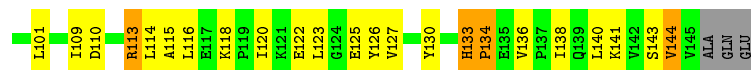
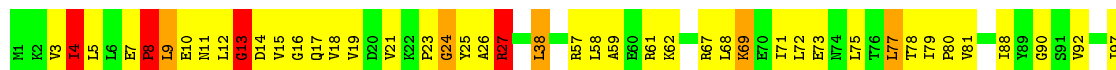
Chain YH: 73% 20% . . .





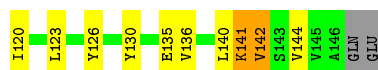
- Molecule 42: 50S ribosomal protein L9

Chain RI: 53% 36% 6% . .



- Molecule 42: 50S ribosomal protein L9

Chain YI: 68% 25% 5% . .



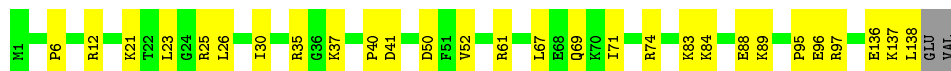
- Molecule 43: 50S ribosomal protein L13

Chain RN: 73% 24% . .



- Molecule 43: 50S ribosomal protein L13

Chain YN: 79% 20% .



- Molecule 44: 50S ribosomal protein L14

Chain RO: 79% 20% .

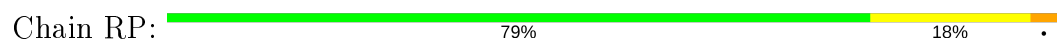


- Molecule 44: 50S ribosomal protein L14

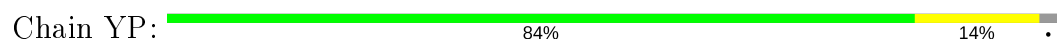
Chain YO: 82% 18%



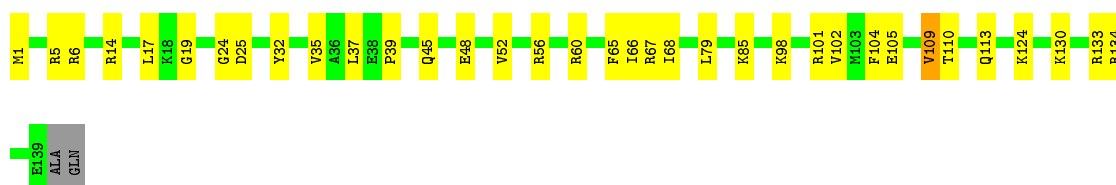
- Molecule 45: 50S ribosomal protein L15



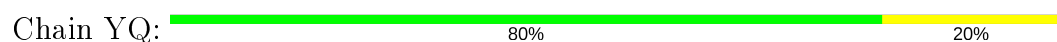
- Molecule 45: 50S ribosomal protein L15



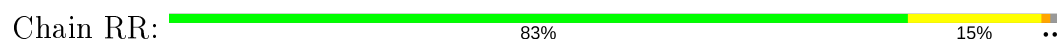
- Molecule 46: 50S ribosomal protein L16



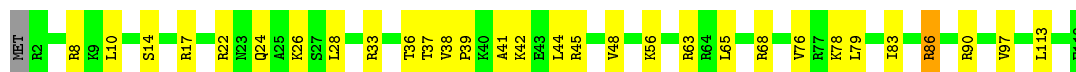
- Molecule 46: 50S ribosomal protein L16



- Molecule 47: 50S ribosomal protein L17

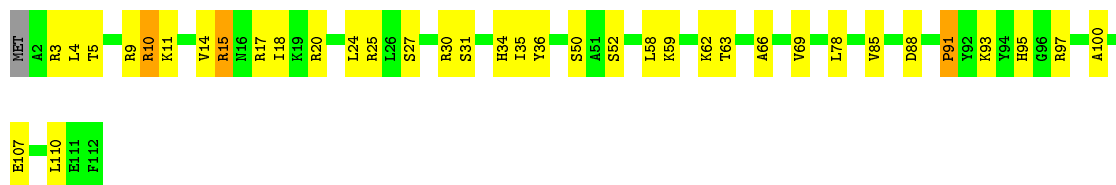


- Molecule 47: 50S ribosomal protein L17



- Molecule 48: 50S ribosomal protein L18

Chain RS:  66% 30% ..



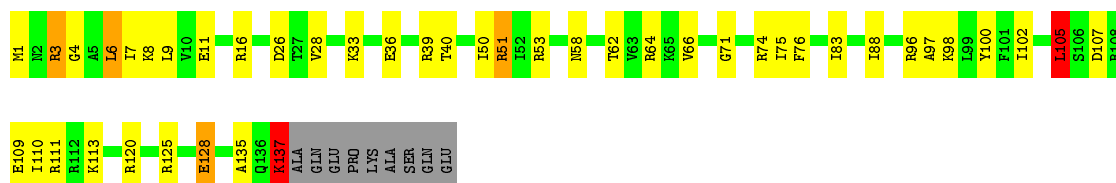
- Molecule 48: 50S ribosomal protein L18

Chain YS:  74% 25% .



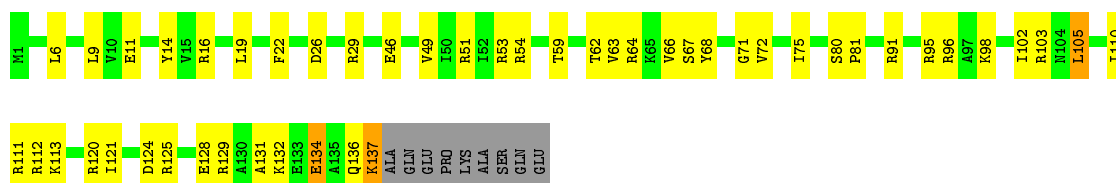
- Molecule 49: 50S ribosomal protein L19

Chain RT:  64% 26% .. 6%



- Molecule 49: 50S ribosomal protein L19

Chain YT:  61% 31% . 6%



- Molecule 50: 50S ribosomal protein L20

Chain RU:  89% 9% ..




- Molecule 50: 50S ribosomal protein L20

Chain YU:  72% 25% ..

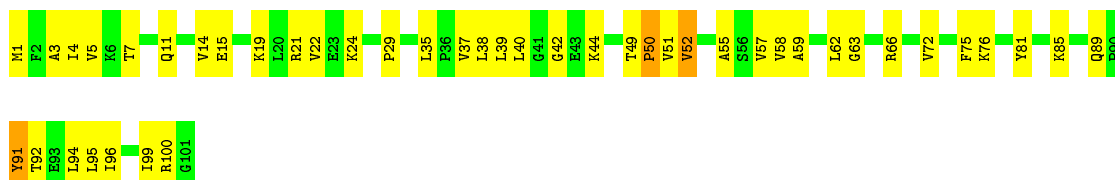


G118


- Molecule 51: 50S ribosomal protein L21

Chain RV:  73% 26%


- Molecule 51: 50S ribosomal protein L21

Chain YV:  56% 41%



- Molecule 52: 50S ribosomal protein L22

Chain RW:  88% 12%


- Molecule 52: 50S ribosomal protein L22

Chain YW:  89% 11%



- Molecule 53: 50S ribosomal protein L23

Chain RX:  79% 16%


- Molecule 53: 50S ribosomal protein L23


Chain YX:  88% 8%

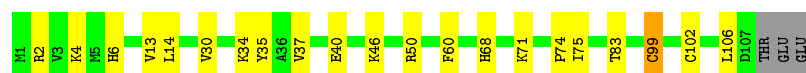

- Molecule 54: 50S ribosomal protein L24

Chain RY:  75% 21% ..



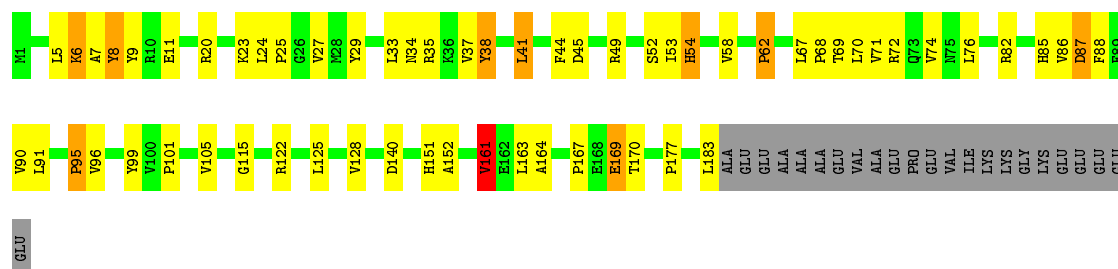
- Molecule 54: 50S ribosomal protein L24

Chain YY:  78% 18% ..



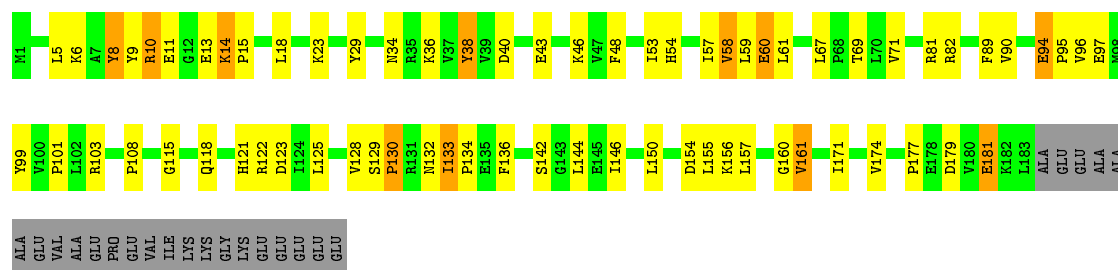
- Molecule 55: 50S ribosomal protein L25

Chain RZ:  59% 25% • 11%



- Molecule 55: 50S ribosomal protein L25

Chain YZ:  55% 28% 5% 11%



- Molecule 56: CCPuro

Chain ZA:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: CCPuro

Chain ZB:  67% 33%



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	213.36Å 451.70Å 607.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.15 – 3.12	Depositor
% Data completeness (in resolution range)	98.6 (146.15-3.12)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.232 , 0.257	Depositor
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.211	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298517	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: MG, A3P, ZN, PPU, SF4

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	0.52	1/36324 (0.0%)	1.39	420/56690 (0.7%)
1	XA	0.52	1/36254 (0.0%)	1.39	416/56581 (0.7%)
2	QB	0.68	1/1942 (0.1%)	1.02	9/2619 (0.3%)
2	XB	0.75	4/1950 (0.2%)	1.01	10/2630 (0.4%)
3	QC	1.04	8/1629 (0.5%)	1.01	9/2195 (0.4%)
3	XC	0.60	1/1629 (0.1%)	0.87	6/2195 (0.3%)
4	QD	0.58	1/1733 (0.1%)	0.81	5/2318 (0.2%)
4	XD	0.62	1/1733 (0.1%)	0.84	4/2318 (0.2%)
5	QE	0.66	3/1171 (0.3%)	0.80	3/1576 (0.2%)
5	XE	0.51	0/1171	0.78	1/1576 (0.1%)
6	QF	0.52	0/856	0.73	1/1154 (0.1%)
6	XF	0.57	0/856	0.76	1/1154 (0.1%)
7	QG	0.62	1/1276 (0.1%)	0.93	4/1709 (0.2%)
7	XG	0.55	0/1276	0.88	6/1709 (0.4%)
8	QH	0.61	1/1128 (0.1%)	0.79	3/1517 (0.2%)
8	XH	0.55	0/1128	0.74	0/1517
9	QI	0.88	5/1029 (0.5%)	1.05	3/1379 (0.2%)
9	XI	0.73	2/1017 (0.2%)	1.01	6/1365 (0.4%)
10	QJ	0.82	0/814	1.24	11/1095 (1.0%)
10	XJ	0.82	5/790 (0.6%)	1.01	5/1063 (0.5%)
11	QK	0.83	4/900 (0.4%)	0.88	3/1213 (0.2%)
11	XK	0.51	1/879 (0.1%)	0.76	2/1187 (0.2%)
12	QL	0.59	1/991 (0.1%)	0.83	1/1327 (0.1%)
12	XL	0.65	1/972 (0.1%)	0.93	5/1301 (0.4%)
13	QM	1.62	19/965 (2.0%)	1.53	18/1292 (1.4%)
13	XM	0.55	0/956	0.93	2/1281 (0.2%)
14	QN	0.71	2/501 (0.4%)	0.95	1/664 (0.2%)
14	XN	0.65	0/501	0.93	1/664 (0.2%)
15	QO	0.58	0/745	0.78	1/992 (0.1%)
15	XO	0.71	1/740 (0.1%)	1.06	6/987 (0.6%)
16	QP	0.45	0/721	0.80	3/970 (0.3%)
16	XP	0.58	1/721 (0.1%)	0.74	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.48	0/847	0.75	0/1131
17	XQ	0.52	0/847	0.73	1/1131 (0.1%)
18	QR	0.62	1/579 (0.2%)	0.88	2/768 (0.3%)
18	XR	0.55	0/579	0.93	1/768 (0.1%)
19	QS	0.86	3/680 (0.4%)	1.02	1/915 (0.1%)
19	XS	0.54	0/680	0.91	1/915 (0.1%)
20	QT	0.58	1/765 (0.1%)	0.86	1/1007 (0.1%)
20	XT	0.80	3/765 (0.4%)	1.14	4/1007 (0.4%)
21	QU	0.61	0/221	0.89	0/288
21	XU	0.66	0/221	1.01	1/288 (0.3%)
22	QV	0.55	0/1832	1.43	23/2855 (0.8%)
22	QW	0.45	0/1832	1.41	26/2855 (0.9%)
22	XV	0.54	0/1832	1.36	10/2855 (0.4%)
22	XW	0.48	0/1832	1.38	24/2855 (0.8%)
23	QX	0.51	0/417	1.27	4/650 (0.6%)
23	XX	0.51	0/417	1.31	2/650 (0.3%)
24	QY	0.60	1/743 (0.1%)	0.86	1/1002 (0.1%)
24	QZ	0.64	0/743	1.02	2/1002 (0.2%)
24	XY	0.64	0/743	0.84	0/1002
24	XZ	0.36	0/743	0.57	0/1002
25	R0	0.51	0/652	0.82	1/867 (0.1%)
25	Y0	0.45	0/657	0.67	1/874 (0.1%)
26	R1	0.66	1/770 (0.1%)	1.01	4/1022 (0.4%)
26	Y1	0.60	0/770	0.84	1/1022 (0.1%)
27	R2	0.63	1/583 (0.2%)	0.84	3/771 (0.4%)
27	Y2	0.74	2/583 (0.3%)	1.09	4/771 (0.5%)
28	R3	0.56	0/474	0.78	1/635 (0.2%)
28	Y3	0.53	0/474	0.96	3/635 (0.5%)
29	R4	1.46	6/578 (1.0%)	1.20	7/776 (0.9%)
29	Y4	0.74	1/578 (0.2%)	1.19	5/776 (0.6%)
30	R5	0.59	2/473 (0.4%)	0.67	1/639 (0.2%)
30	Y5	0.67	1/473 (0.2%)	0.73	0/639
31	R6	0.62	0/460	0.67	0/613
31	Y6	0.96	1/460 (0.2%)	1.05	3/613 (0.5%)
32	R7	0.49	0/417	0.75	0/550
32	Y7	0.45	0/426	0.65	0/561
33	R8	0.63	1/525 (0.2%)	1.01	5/691 (0.7%)
33	Y8	0.92	3/525 (0.6%)	0.87	0/691
34	R9	0.95	3/310 (1.0%)	1.56	6/407 (1.5%)
34	Y9	0.47	0/310	0.75	0/407
35	RA	0.58	10/69739 (0.0%)	1.49	1148/108870 (1.1%)
35	YA	0.60	18/69419 (0.0%)	1.50	1151/108369 (1.1%)
36	RB	0.55	0/2928	1.50	43/4568 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	YB	0.54	0/2928	1.49	44/4568 (1.0%)
37	RD	0.71	7/2165 (0.3%)	0.84	5/2919 (0.2%)
37	YD	0.56	2/2185 (0.1%)	0.73	0/2944
38	RE	0.66	5/1601 (0.3%)	0.88	3/2160 (0.1%)
38	YE	0.63	1/1596 (0.1%)	0.78	1/2153 (0.0%)
39	RF	0.60	1/1620 (0.1%)	0.80	6/2194 (0.3%)
39	YF	0.61	3/1620 (0.2%)	0.79	1/2194 (0.0%)
40	RG	0.75	5/1499 (0.3%)	1.05	6/2016 (0.3%)
40	YG	0.94	7/1499 (0.5%)	1.02	8/2016 (0.4%)
41	RH	1.16	10/1362 (0.7%)	1.23	17/1841 (0.9%)
41	YH	0.88	4/1362 (0.3%)	1.00	4/1841 (0.2%)
42	RI	1.21	14/1146 (1.2%)	1.13	8/1551 (0.5%)
42	YI	0.75	2/1151 (0.2%)	1.01	5/1558 (0.3%)
43	RN	0.59	0/1131	0.88	3/1525 (0.2%)
43	YN	0.57	0/1131	0.78	0/1525
44	RO	0.70	3/943 (0.3%)	0.88	4/1269 (0.3%)
44	YO	0.62	1/943 (0.1%)	0.80	1/1269 (0.1%)
45	RP	0.73	2/1162 (0.2%)	1.02	5/1544 (0.3%)
45	YP	0.53	0/1139	0.78	1/1514 (0.1%)
46	RQ	0.69	3/1128 (0.3%)	0.89	1/1508 (0.1%)
46	YQ	0.54	0/1143	0.78	1/1527 (0.1%)
47	RR	0.59	1/974 (0.1%)	0.76	0/1302
47	YR	0.53	0/974	0.81	1/1302 (0.1%)
48	RS	0.77	1/892 (0.1%)	1.10	7/1187 (0.6%)
48	YS	0.56	1/892 (0.1%)	0.86	2/1187 (0.2%)
49	RT	0.94	5/1155 (0.4%)	1.17	9/1542 (0.6%)
49	YT	0.71	3/1155 (0.3%)	0.89	1/1542 (0.1%)
50	RU	0.58	0/982	0.68	2/1306 (0.2%)
50	YU	0.66	2/982 (0.2%)	0.84	2/1306 (0.2%)
51	RV	0.63	0/790	0.83	1/1057 (0.1%)
51	YV	0.61	0/790	0.88	4/1057 (0.4%)
52	RW	0.55	1/911 (0.1%)	0.73	0/1220
52	YW	0.54	0/911	0.70	0/1220
53	RX	0.61	1/739 (0.1%)	0.70	1/993 (0.1%)
53	YX	0.59	0/739	0.70	1/993 (0.1%)
54	RY	0.71	3/831 (0.4%)	0.74	1/1108 (0.1%)
54	YY	0.61	1/831 (0.1%)	0.89	4/1108 (0.4%)
55	RZ	0.78	7/1493 (0.5%)	0.99	6/2026 (0.3%)
55	YZ	0.99	10/1493 (0.7%)	0.99	8/2026 (0.4%)
56	ZA	0.41	0/40	1.24	0/60
56	ZB	0.45	0/40	1.35	0/60
All	All	0.61	230/323268 (0.1%)	1.33	3631/483159 (0.8%)

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	4
2	XB	0	2
3	QC	0	2
3	XC	0	1
4	XD	0	1
7	XG	0	1
10	QJ	0	1
10	XJ	0	2
12	XL	0	3
13	QM	0	2
14	QN	0	1
18	QR	0	1
18	XR	0	2
19	XS	0	1
27	Y2	0	3
28	R3	0	1
29	R4	0	1
29	Y4	0	3
34	R9	0	1
37	RD	0	1
38	RE	0	2
38	YE	0	1
40	YG	0	1
41	RH	0	3
41	YH	0	2
42	RI	0	3
42	YI	0	2
43	RN	0	1
45	RP	0	2
46	RQ	0	1
48	RS	0	1
49	RT	0	1
50	YU	0	1
55	RZ	0	1
All	All	0	56

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R4	34	GLU	CB-CG	-22.72	1.08	1.52
13	QM	71	ARG	CZ-NH1	18.52	1.57	1.33
41	RH	18	GLU	CG-CD	-18.50	1.24	1.51
40	YG	112	PRO	N-CD	15.77	1.70	1.47
49	RT	3	ARG	CA-CB	15.24	1.87	1.53

The worst 5 of 3631 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1913	A	C5-C6-N6	-21.10	106.82	123.70
13	QM	90	LEU	CB-CG-CD2	-20.03	76.94	111.00
35	RA	309	G	O5'-P-OP1	-19.70	87.06	110.70
49	RT	3	ARG	CA-CB-CG	17.17	151.18	113.40
3	QC	38	ARG	NE-CZ-NH2	-15.93	112.34	120.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	114	ARG	Peptide
2	QB	131	PRO	Peptide
2	QB	153	ARG	Peptide
2	QB	217	ARG	Sidechain
3	QC	35	GLU	Sidechain

5.2 Too-close contacts [i](#)

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	16383	225	0
1	XA	32389	0	16350	231	0
2	QB	1907	0	1958	58	0
2	XB	1915	0	1969	82	0
3	QC	1605	0	1668	46	0
3	XC	1605	0	1668	30	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	43	0
5	QE	1155	0	1213	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	XE	1155	0	1213	18	0
6	QF	843	0	857	7	0
6	XF	843	0	857	16	0
7	QG	1257	0	1296	42	0
7	XG	1257	0	1296	25	0
8	QH	1108	0	1165	31	0
8	XH	1108	0	1165	18	0
9	QI	1010	0	1037	49	0
9	XI	998	0	1024	29	0
10	QJ	801	0	849	72	0
10	XJ	777	0	816	29	0
11	QK	885	0	904	18	0
11	XK	864	0	881	14	0
12	QL	975	0	1062	24	0
12	XL	956	0	1046	32	0
13	QM	955	0	1021	78	0
13	XM	946	0	1007	43	0
14	QN	492	0	530	5	0
14	XN	492	0	529	16	0
15	QO	734	0	771	6	0
15	XO	729	0	768	16	0
16	QP	705	0	725	11	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	6	0
18	XR	574	0	644	7	0
19	QS	665	0	686	47	0
19	XS	665	0	686	18	0
20	QT	763	0	861	10	0
20	XT	763	0	861	30	0
21	QU	217	0	234	6	0
21	XU	217	0	234	7	0
22	QV	1640	0	837	2	0
22	QW	1640	0	837	19	0
22	XV	1640	0	837	7	0
22	XW	1640	0	837	8	0
23	QX	370	0	186	3	0
23	XX	370	0	186	5	0
24	QY	723	0	713	37	0
24	QZ	723	0	713	81	0
24	XY	723	0	713	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	XZ	723	0	713	55	0
25	R0	643	0	667	23	0
25	Y0	648	0	672	14	0
26	R1	763	0	848	23	0
26	Y1	763	0	848	10	0
27	R2	581	0	629	8	0
27	Y2	581	0	629	18	0
28	R3	469	0	518	8	0
28	Y3	469	0	518	6	0
29	R4	565	0	561	32	0
29	Y4	565	0	557	25	0
30	R5	459	0	480	8	0
30	Y5	459	0	480	3	0
31	R6	453	0	475	11	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	5	0
32	Y7	418	0	467	5	0
33	R8	517	0	582	12	0
33	Y8	517	0	582	20	0
34	R9	307	0	336	15	0
34	Y9	307	0	336	7	0
35	RA	62266	0	31389	339	0
35	YA	61981	0	31240	292	0
36	RB	2617	0	1328	15	0
36	YB	2617	0	1328	6	0
37	RD	2115	0	2195	69	0
37	YD	2135	0	2221	25	0
38	RE	1568	0	1634	50	0
38	YE	1563	0	1629	41	0
39	RF	1585	0	1632	25	0
39	YF	1585	0	1631	35	0
40	RG	1474	0	1535	82	0
40	YG	1474	0	1535	44	0
41	RH	1336	0	1418	121	0
41	YH	1336	0	1418	29	0
42	RI	1131	0	1218	76	0
42	YI	1136	0	1223	44	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	21	0
44	RO	933	0	996	18	0
44	YO	933	0	996	21	0
45	RP	1145	0	1228	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	YP	1122	0	1206	15	0
46	RQ	1107	0	1166	26	0
46	YQ	1122	0	1179	21	0
47	RR	960	0	1021	15	0
47	YR	960	0	1020	19	0
48	RS	882	0	943	38	0
48	YS	882	0	943	17	0
49	RT	1141	0	1202	34	0
49	YT	1141	0	1202	37	0
50	RU	964	0	1022	10	0
50	YU	964	0	1022	37	0
51	RV	779	0	852	20	0
51	YV	779	0	852	50	0
52	RW	900	0	964	10	0
52	YW	900	0	964	17	0
53	RX	725	0	778	13	0
53	YX	725	0	778	7	0
54	RY	818	0	913	14	0
54	YY	818	0	913	12	0
55	RZ	1461	0	1493	44	0
55	YZ	1461	0	1493	58	0
56	ZA	74	0	51	0	0
56	ZB	74	0	51	1	0
57	QA	87	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	2	0	0	0	0
57	R5	1	0	0	0	0
57	RA	305	0	0	0	0
57	RB	3	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	106	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XV	4	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	329	0	0	0	0
57	YB	6	0	0	0	0
57	YD	2	0	0	0	0
57	YE	4	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	1	0	0	0	0
57	YS	1	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	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y6	1	0	0	0	0
60	QX	26	0	11	5	0
60	XX	26	0	11	2	0
All	All	298517	0	202833	3434	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 7.

The worst 5 of 3434 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)
5:QE:90:VAL:CG1	5:QE:90:VAL:CB	1.74	1.63
2:XB:137:ARG:CD	2:XB:137:ARG:CG	1.77	1.62
49:RT:3:ARG:CD	49:RT:3:ARG:CG	1.76	1.62
13:QM:67:GLU:CG	13:QM:67:GLU:CB	1.74	1.62
55:YZ:14:LYS:CA	55:YZ:14:LYS:CB	1.75	1.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	205 (88%)	27 (12%)	1 (0%)	34	68
2	XB	234/256 (91%)	204 (87%)	29 (12%)	1 (0%)	34	68
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	QD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
4	XD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	63
5	QE	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	22	56
5	XE	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	22	56
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	56
7	XG	153/156 (98%)	148 (97%)	5 (3%)	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%)	108 (86%)	17 (14%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	48
10	XJ	94/105 (90%)	88 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	12 (10%)	1 (1%)	19	53
12	XL	120/132 (91%)	108 (90%)	10 (8%)	2 (2%)	9	35
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	9	35
13	XM	117/126 (93%)	100 (86%)	16 (14%)	1 (1%)	17	51
14	QN	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	3 (4%)	1 (1%)	13	43
20	QT	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	QU	23/27 (85%)	23 (100%)	0	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
24	QY	82/84 (98%)	71 (87%)	11 (13%)	0	100	100
24	QZ	82/84 (98%)	74 (90%)	7 (8%)	1 (1%)	13	43
24	XY	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
24	XZ	82/84 (98%)	71 (87%)	10 (12%)	1 (1%)	13	43
25	R0	79/85 (93%)	71 (90%)	7 (9%)	1 (1%)	12	41
25	Y0	80/85 (94%)	77 (96%)	3 (4%)	0	100	100
26	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
26	Y1	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	14	45
27	R2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
27	Y2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
28	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	18 (27%)	3 (4%)	2	14
29	Y4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	5
30	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	Y6	51/54 (94%)	51 (100%)	0	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	4	21
33	Y8	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	21
34	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
34	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
37	RD	270/276 (98%)	256 (95%)	14 (5%)	0	100	100
37	YD	272/276 (99%)	262 (96%)	10 (4%)	0	100	100
38	RE	203/206 (98%)	177 (87%)	22 (11%)	4 (2%)	7	30
38	YE	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	10	38
39	RF	200/210 (95%)	194 (97%)	6 (3%)	0	100	100
39	YF	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
40	RG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	45
40	YG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	25	59
41	RH	172/180 (96%)	137 (80%)	30 (17%)	5 (3%)	4	23
41	YH	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	9	35
42	RI	143/148 (97%)	121 (85%)	17 (12%)	5 (4%)	3	19
42	YI	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	7	29
43	RN	136/140 (97%)	123 (90%)	11 (8%)	2 (2%)	10	38
43	YN	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	22	56
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
45	RP	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	24
45	YP	145/150 (97%)	138 (95%)	7 (5%)	0	100	100
46	RQ	137/141 (97%)	122 (89%)	14 (10%)	1 (1%)	22	56
46	YQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	22	56
47	RR	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	17	51
47	YR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
48	RS	109/112 (97%)	87 (80%)	21 (19%)	1 (1%)	17	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
49	RT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
49	YT	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
50	RU	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
50	YU	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	17	51
51	RV	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	48
51	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	48
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
54	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
55	RZ	181/206 (88%)	168 (93%)	12 (7%)	1 (1%)	25	59
55	YZ	181/206 (88%)	176 (97%)	5 (3%)	0	100	100
All	All	11788/12464 (95%)	10894 (92%)	822 (7%)	72 (1%)	25	59

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	QM	15	VAL
29	R4	25	TYR
38	RE	18	ASP
42	RI	15	VAL
42	RI	133	HIS

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%)	203 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XB	204/220 (93%)	197 (97%)	7 (3%)	37	68
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	69
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	86
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	88
4	XD	180/181 (99%)	177 (98%)	3 (2%)	60	83
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	77
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	88
7	QG	126/127 (99%)	123 (98%)	3 (2%)	49	75
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	84
8	QH	118/119 (99%)	115 (98%)	3 (2%)	47	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	69
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	78
10	QJ	89/92 (97%)	85 (96%)	4 (4%)	27	59
10	XJ	86/92 (94%)	84 (98%)	2 (2%)	50	76
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	88/99 (89%)	86 (98%)	2 (2%)	50	76
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	100 (97%)	3 (3%)	42	71
13	QM	96/101 (95%)	94 (98%)	2 (2%)	53	78
13	XM	95/101 (94%)	93 (98%)	2 (2%)	53	78
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	76 (96%)	3 (4%)	33	65
15	XO	79/80 (99%)	77 (98%)	2 (2%)	47	75
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	92 (97%)	3 (3%)	39	69
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	58 (95%)	3 (5%)	25	57
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	85
19	XS	72/80 (90%)	72 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	86
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	56
24	QY	78/78 (100%)	78 (100%)	0	100	100
24	QZ	78/78 (100%)	75 (96%)	3 (4%)	33	65
24	XY	78/78 (100%)	76 (97%)	2 (3%)	46	74
24	XZ	78/78 (100%)	72 (92%)	6 (8%)	13	40
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	64 (98%)	1 (2%)	65	85
26	R1	82/83 (99%)	79 (96%)	3 (4%)	34	66
26	Y1	82/83 (99%)	81 (99%)	1 (1%)	71	87
27	R2	64/67 (96%)	63 (98%)	1 (2%)	62	84
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	84
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	62/63 (98%)	59 (95%)	3 (5%)	25	57
29	Y4	62/63 (98%)	62 (100%)	0	100	100
30	R5	51/52 (98%)	49 (96%)	2 (4%)	32	64
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	R6	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	Y6	51/52 (98%)	50 (98%)	1 (2%)	55	79
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	32 (94%)	2 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	71
37	RD	214/218 (98%)	209 (98%)	5 (2%)	50	76
37	YD	216/218 (99%)	216 (100%)	0	100	100
38	RE	165/166 (99%)	162 (98%)	3 (2%)	59	82
38	YE	165/166 (99%)	160 (97%)	5 (3%)	41	70
39	RF	161/166 (97%)	159 (99%)	2 (1%)	71	87
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	93
40	RG	155/156 (99%)	152 (98%)	3 (2%)	57	80
40	YG	155/156 (99%)	153 (99%)	2 (1%)	69	86
41	RH	145/148 (98%)	142 (98%)	3 (2%)	53	78
41	YH	145/148 (98%)	142 (98%)	3 (2%)	53	78
42	RI	122/124 (98%)	118 (97%)	4 (3%)	38	68
42	YI	122/124 (98%)	118 (97%)	4 (3%)	38	68
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	89
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	116/116 (100%)	116 (100%)	0	100	100
45	YP	114/116 (98%)	112 (98%)	2 (2%)	59	82
46	RQ	110/111 (99%)	110 (100%)	0	100	100
46	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
47	RR	100/101 (99%)	99 (99%)	1 (1%)	76	89
47	YR	100/101 (99%)	100 (100%)	0	100	100
48	RS	87/88 (99%)	86 (99%)	1 (1%)	73	88
48	YS	87/88 (99%)	87 (100%)	0	100	100
49	RT	120/127 (94%)	117 (98%)	3 (2%)	47	75
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	90 (97%)	3 (3%)	39	69
51	RV	82/82 (100%)	79 (96%)	3 (4%)	34	66
51	YV	82/82 (100%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
52	YW	92/92 (100%)	91 (99%)	1 (1%)	73	88
53	RX	74/78 (95%)	73 (99%)	1 (1%)	67	85
53	YX	74/78 (95%)	74 (100%)	0	100	100
54	RY	88/91 (97%)	86 (98%)	2 (2%)	50	76
54	YY	88/91 (97%)	86 (98%)	2 (2%)	50	76
55	RZ	162/179 (90%)	158 (98%)	4 (2%)	47	75
55	YZ	162/179 (90%)	156 (96%)	6 (4%)	34	66
All	All	10007/10378 (96%)	9836 (98%)	171 (2%)	60	83

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	RV	44	LYS
3	XC	88	ARG
49	YT	137	LYS
52	RW	113	LYS
55	RZ	87	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	QC	108	ASN
10	QJ	76	ASN
37	RD	96	HIS
27	Y2	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	311 (20%)	52 (3%)
1	XA	1505/1521 (98%)	303 (20%)	50 (3%)
22	QV	77/77 (100%)	12 (15%)	4 (5%)
22	QW	76/77 (98%)	18 (23%)	1 (1%)
22	XV	76/77 (98%)	13 (17%)	3 (3%)
22	XW	76/77 (98%)	21 (27%)	1 (1%)
23	QX	16/20 (80%)	8 (50%)	2 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	XX	16/20 (80%)	7 (43%)	1 (6%)
35	RA	2888/2915 (99%)	606 (20%)	49 (1%)
35	YA	2875/2915 (98%)	593 (20%)	46 (1%)
36	RB	121/124 (97%)	21 (17%)	1 (0%)
36	YB	121/124 (97%)	20 (16%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9357/9474 (98%)	1933 (20%)	211 (2%)

5 of 1933 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 211 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	RA	2211	G
1	XA	281	G
35	YA	2191	G
35	RA	2439	A
35	RA	2859	G

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

2 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	$\# Z > 2$
56	PPU	ZA	3	56,35	32,40,41	0.91	2 (6%)	33,57,60	1.51	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PPU	ZB	3	56,35	32,40,41	0.89	2 (6%)	33,57,60	1.44	5 (15%)

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
56	PPU	ZA	3	56,35	-	4/21/43/44	0/4/4/4
56	PPU	ZB	3	56,35	-	3/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ZA	3	PPU	C5-C4	2.76	1.48	1.40
56	ZB	3	PPU	C5-C4	2.73	1.48	1.40
56	ZA	3	PPU	C6-N1	2.18	1.36	1.33
56	ZB	3	PPU	C6-N1	2.02	1.36	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	ZB	3	PPU	C4-C5-N7	-3.49	105.76	109.40
56	ZA	3	PPU	C4-C5-N7	-3.46	105.79	109.40
56	ZA	3	PPU	C3'-N3'-C	-3.34	118.18	123.21
56	ZA	3	PPU	N3-C2-N1	-3.25	123.60	128.68
56	ZB	3	PPU	N3-C2-N1	-3.24	123.61	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZA	3	PPU	C5-C6-N6-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	ZB	3	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 883 ligands modelled in this entry, 879 are monoatomic - leaving 4 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
60	A3P	QX	101	23	23,28,29	5.17	7 (30%)	23,42,45	1.46	3 (13%)
58	SF4	XD	301	4	0,12,12	0.00	-	-		
58	SF4	QD	301	4	0,12,12	0.00	-	-		
60	A3P	XX	101	23	23,28,29	5.26	7 (30%)	23,42,45	1.59	4 (17%)

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
60	A3P	QX	101	23	-	2/8/30/31	0/3/3/3
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	301	4	-	-	0/6/5/5
60	A3P	XX	101	23	-	0/8/30/31	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	XX	101	A3P	O4'-C1'	18.58	1.67	1.41
60	QX	101	A3P	O4'-C1'	18.11	1.66	1.41
60	XX	101	A3P	C2'-C1'	-13.95	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	QX	101	A3P	C2'-C1'	-13.75	1.32	1.53
60	QX	101	A3P	O4'-C4'	-6.31	1.30	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	XX	101	A3P	N3-C2-N1	-4.92	120.99	128.68
60	QX	101	A3P	N3-C2-N1	-4.77	121.22	128.68
60	XX	101	A3P	C3'-C2'-C1'	3.31	107.22	99.89
60	QX	101	A3P	C4-C5-N7	-3.24	106.02	109.40
60	XX	101	A3P	C4-C5-N7	-2.87	106.40	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

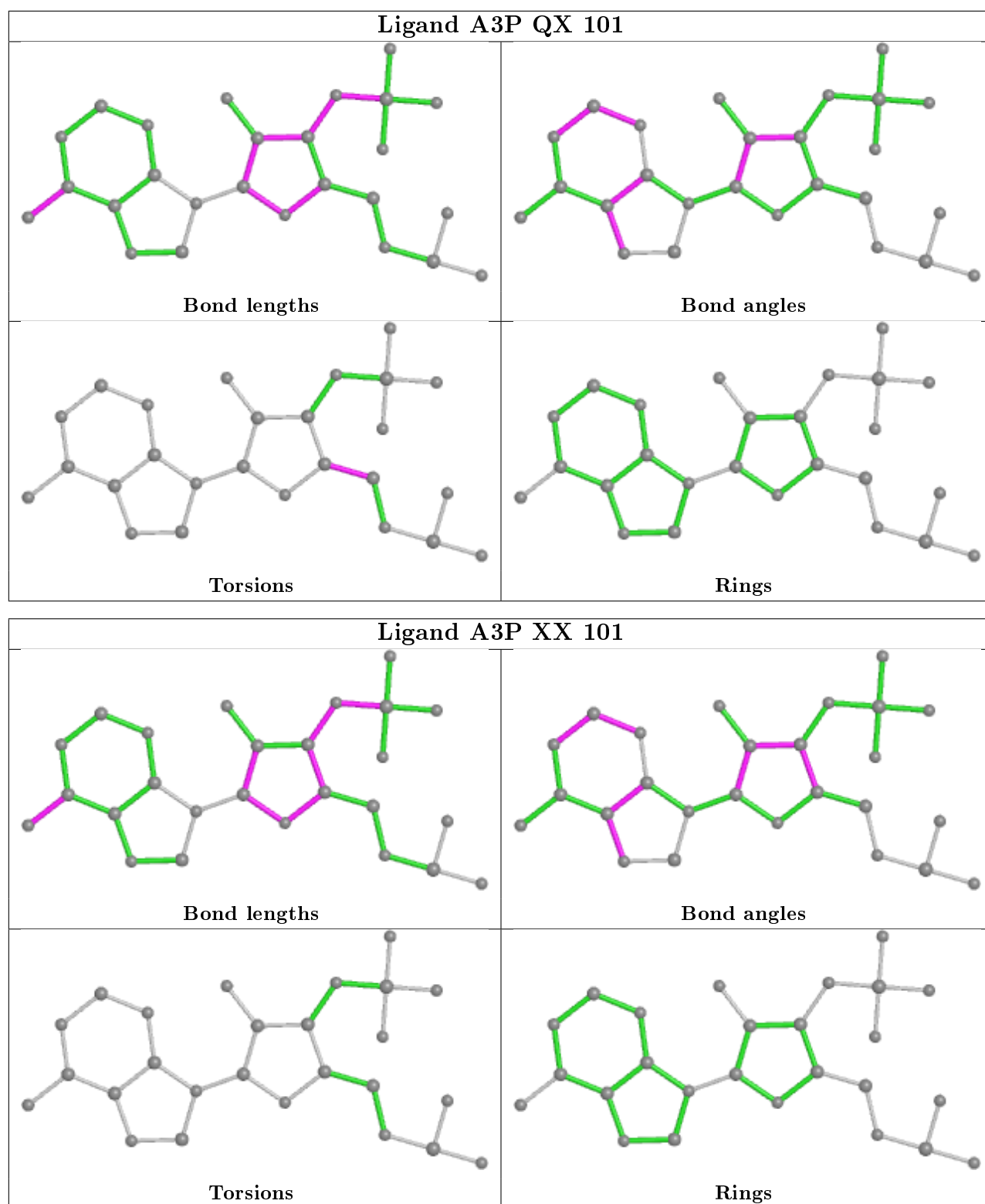
Mol	Chain	Res	Type	Atoms
60	QX	101	A3P	C3'-C4'-C5'-O5'
60	QX	101	A3P	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	QX	101	A3P	5	0
60	XX	101	A3P	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.