



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2023 – 10:46 AM EDT

PDB ID : 8FON
Title : Crystal structure of tRNA^{Lys}(SUU) bound to AUA codon in the ribosomal P site
Authors : Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2023-01-02
Resolution : 3.64 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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) : 2.32.1

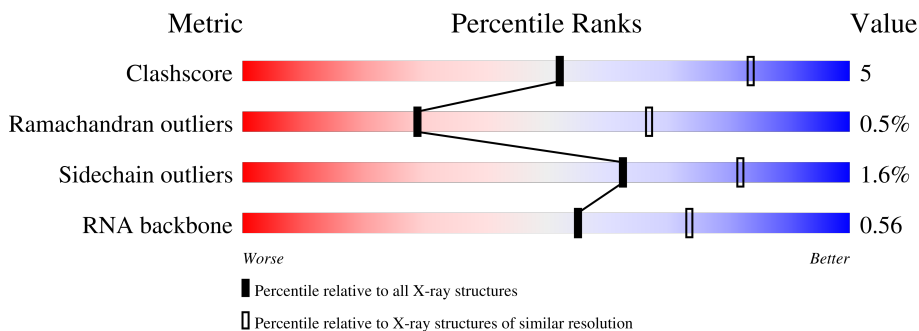
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

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 of 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	1522	61% 31% 6% ..
1	XA	1522	59% 34% 6% ..
2	QB	256	77% 14% 8%
2	XB	256	82% 10% 8%
3	QC	239	69% 16% 14%
3	XC	239	72% 13% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	82% 18%
4	XD	209	77% 22%
5	QE	162	83% 10% 7%
5	XE	162	81% 12% 7%
6	QF	101	91% 9%
6	XF	101	86% 14%
7	QG	156	91% 7% ..
7	XG	156	85% 15% .
8	QH	138	88% 11% ..
8	XH	138	87% 12% .
9	QI	128	62% 35% ..
9	XI	128	79% 20% .
10	QJ	105	73% 21% 6%
10	XJ	105	72% 19% 9%
11	QK	129	77% 16% 8%
11	XK	129	71% 19% 10%
12	QL	131	79% 16% . 5%
12	XL	131	78% 15% . 7%
13	QM	126	69% 25% . 5%
13	XM	126	81% 13% 6%
14	QN	61	79% 18% ..
14	XN	61	80% 16% ..
15	QO	89	90% 9% .
15	XO	89	90% 8% .
16	QP	88	83% 13% 5%

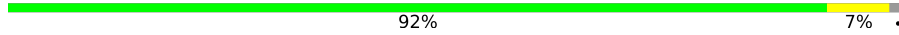
























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Mol	Chain	Length	Quality of chain
16	XP	88	84% 10% 5%
17	QQ	105	85% 10% 5%
17	XQ	105	86% 10% 5%
18	QR	88	68% 11% 20%
18	XR	88	66% 14% 20%
19	QS	93	73% 16% 11%
19	XS	93	70% 19% 10%
20	QT	106	79% 14% 7%
20	XT	106	81% 12% 7%
21	QU	27	89% 7%
21	XU	27	74% 19% 7%
22	QV	76	58% 29% 8% . .
22	XV	76	61% 26% 7% . .
23	QX	23	9% . 87%
23	XX	23	61% 26% 13%
24	R0	85	71% 19% 11%
24	Y0	85	71% 18% 12%
25	R1	98	80% 19% .
25	Y1	98	74% 20% 5%
26	R2	72	75% 21% .
26	Y2	72	83% 10% 6%
27	R3	60	85% 13% .
27	Y3	60	67% 22% 10% .
28	R4	71	82% 15% .
28	Y4	71	82% 13% . .


























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Mol	Chain	Length	Quality of chain
29	R5	60	 92% 7% .
29	Y5	60	 90% 8% .
30	R6	54	 81% 17% .
30	Y6	54	 81% 17% .
31	R7	49	 84% 12% .
31	Y7	49	 90% 8% .
32	R8	65	 57% 29% 12% .
32	Y8	65	 78% 20% .
33	R9	37	 81% 19%
33	Y9	37	 73% 27%
34	RA	2915	 63% 29% 6% ..
34	YA	2915	 63% 29% 6% .
35	RB	122	 70% 23% 5% .
35	YB	122	 70% 23% 5% .
36	RD	276	 80% 19% .
36	YD	276	 83% 15% .
37	RE	206	 79% 19% .
37	YE	206	 88% 10% .
38	RF	210	 79% 17% .
38	YF	210	 86% 10% .
39	RG	182	 70% 26% ...
39	YG	182	 70% 26% ...
40	RH	180	 66% 28% . .
40	YH	180	 81% 14% . .
41	RI	148	 70% 24% 5% .


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Mol	Chain	Length	Quality of chain
41	YI	148	 77% 16% 5% ..
42	RN	140	 82% 14% ..
42	YN	140	 84% 15% .
43	RO	122	 80% 20% .
43	YO	122	 80% 20%
44	RP	150	 83% 15% .
44	YP	150	 83% 13% ..
45	RQ	141	 77% 23%
45	YQ	141	 76% 23% .
46	RR	118	 86% 14% .
46	YR	118	 82% 17% .
47	RS	112	 75% 23% ..
47	YS	112	 79% 20% .
48	RT	146	 76% 16% . 6%
48	YT	146	 69% 24% . 6%
49	RU	118	 85% 13% ..
49	YU	118	 77% 19% ...
50	RV	101	 72% 25% ..
50	YV	101	 87% 11% ..
51	RW	113	 88% 12%
51	YW	113	 84% 15% .
52	RX	96	 85% 10% .
52	YX	96	 82% 14% .
53	RY	110	 86% 11% .
53	YY	110	 83% 15% .

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Mol	Chain	Length	Quality of chain
54	RZ	206	 76% 22% ..
54	YZ	206	 80% 17% ..
55	XY	17	 59% 35% 6%
56	Z6	3	 67% 33%
56	Z8	3	 67% 33%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292577 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
			Total	C	N	O	P			
1	QA	1500	Total 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1511	Total 32471	C 14454	N 6014	O 10493	P 1510	0	0	0

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

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

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

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

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

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

- 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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 P-site tRNA^{Lys}(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			
22	XV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
23	XX	23	Total	C	N	O	P	0	0	0
			499	223	96	157	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
24	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Y2	68	575	355	117	102	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	RA	2881	Total 62051	C 27618	N 11609	O 19944	P 2880	0	0	0
34	YA	2883	Total 62091	C 27636	N 11613	O 19960	P 2882	0	0	0

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	RB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0
35	YB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	RD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
36	YD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L3.

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

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
54	YZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			

- Molecule 55 is a RNA chain called A-site ASL^Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	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	73	Total	Mg	0	0
			73	73		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QJ	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

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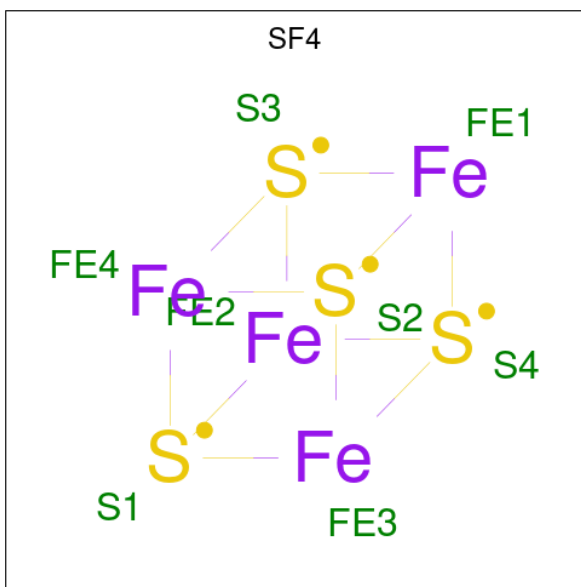
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R0	1	Total 1	Mg 1	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	483	Total 483	Mg 483	0	0
57	RB	7	Total 7	Mg 7	0	0
57	RE	4	Total 4	Mg 4	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	3	Total 3	Mg 3	0	0
57	RQ	3	Total 3	Mg 3	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RT	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	73	Total 73	Mg 73	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XK	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XQ	1	Total 1	Mg 1	0	0
57	XS	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y1	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	YA	538	Total 538	Mg 538	0	0
57	YB	13	Total 13	Mg 13	0	0
57	YD	3	Total 3	Mg 3	0	0
57	YE	4	Total 4	Mg 4	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	3	Total 3	Mg 3	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YX	2	Total 2	Mg 2	0	0
57	YY	1	Total 1	Mg 1	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	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	RY	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	Y5	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total 1	Zn 1	0	0
59	YY	1	Total 1	Zn 1	0	0

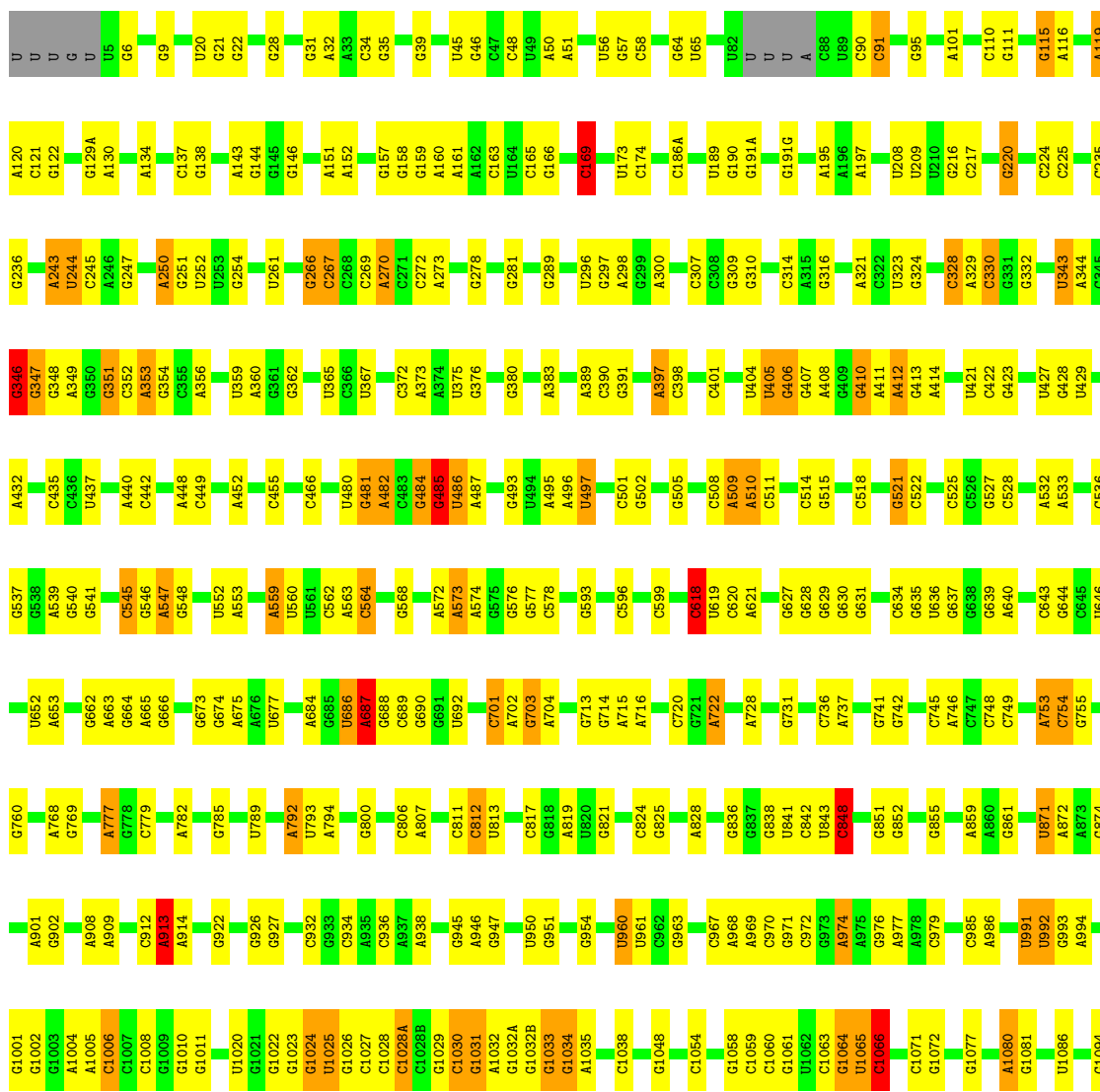
3 Residue-property plots i

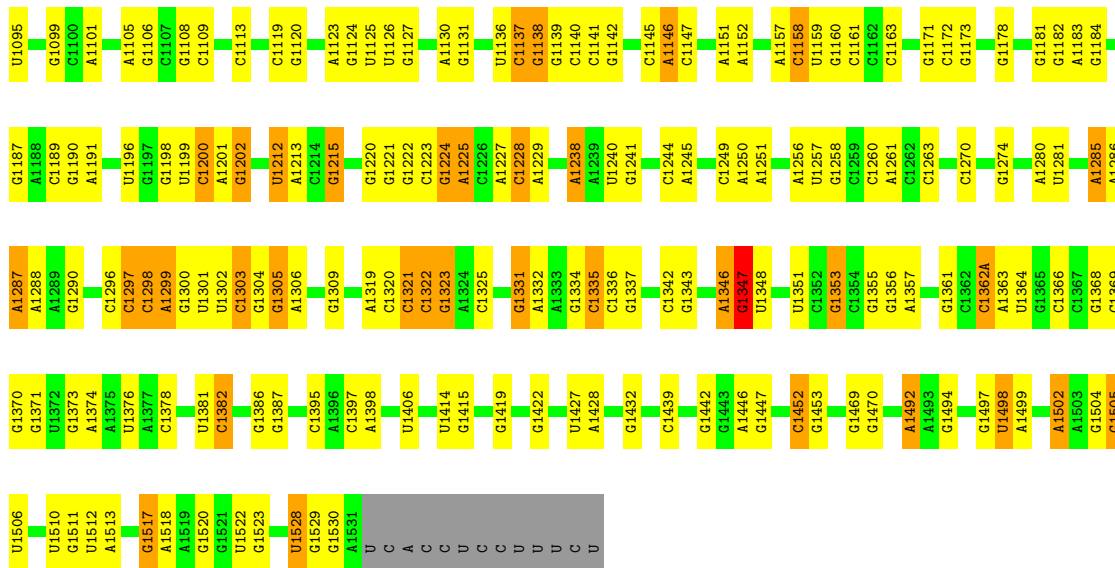
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

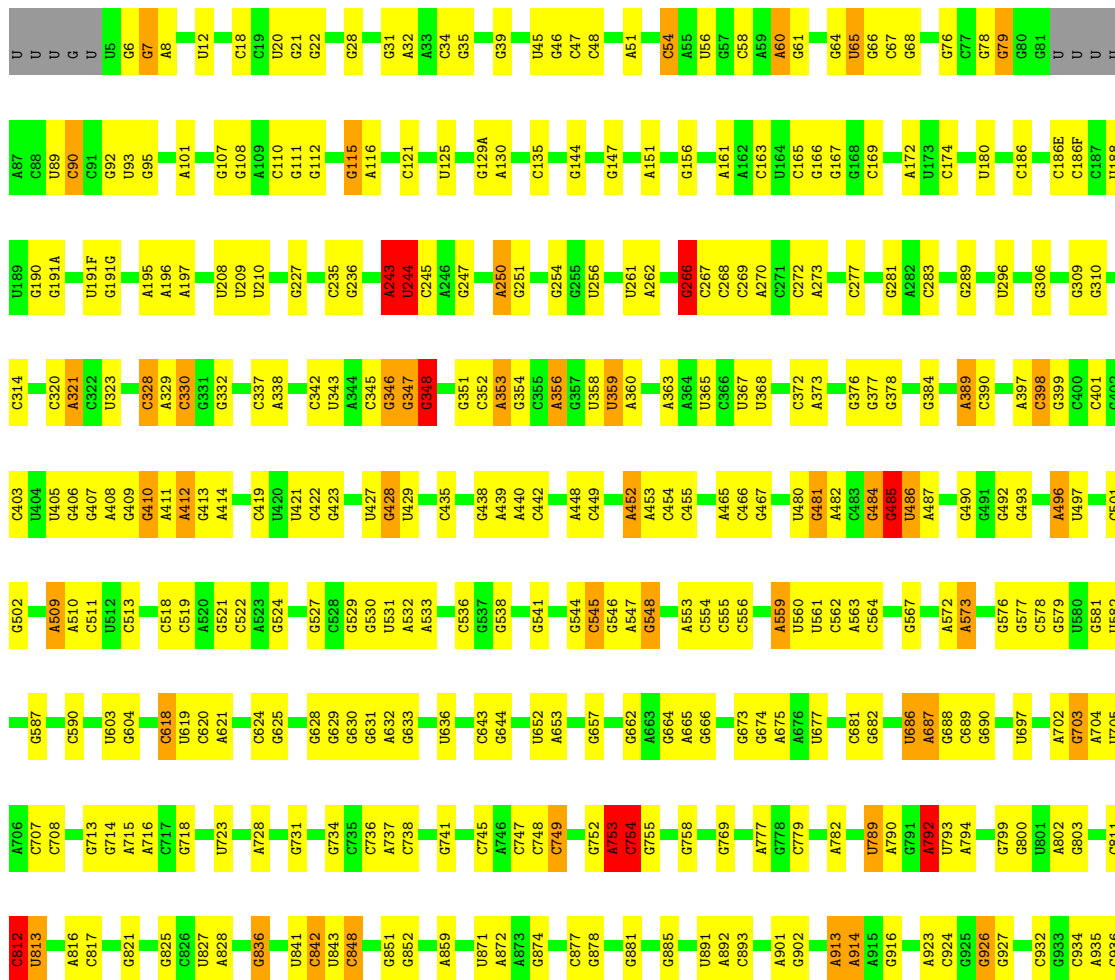
- Molecule 1: 16S rRNA

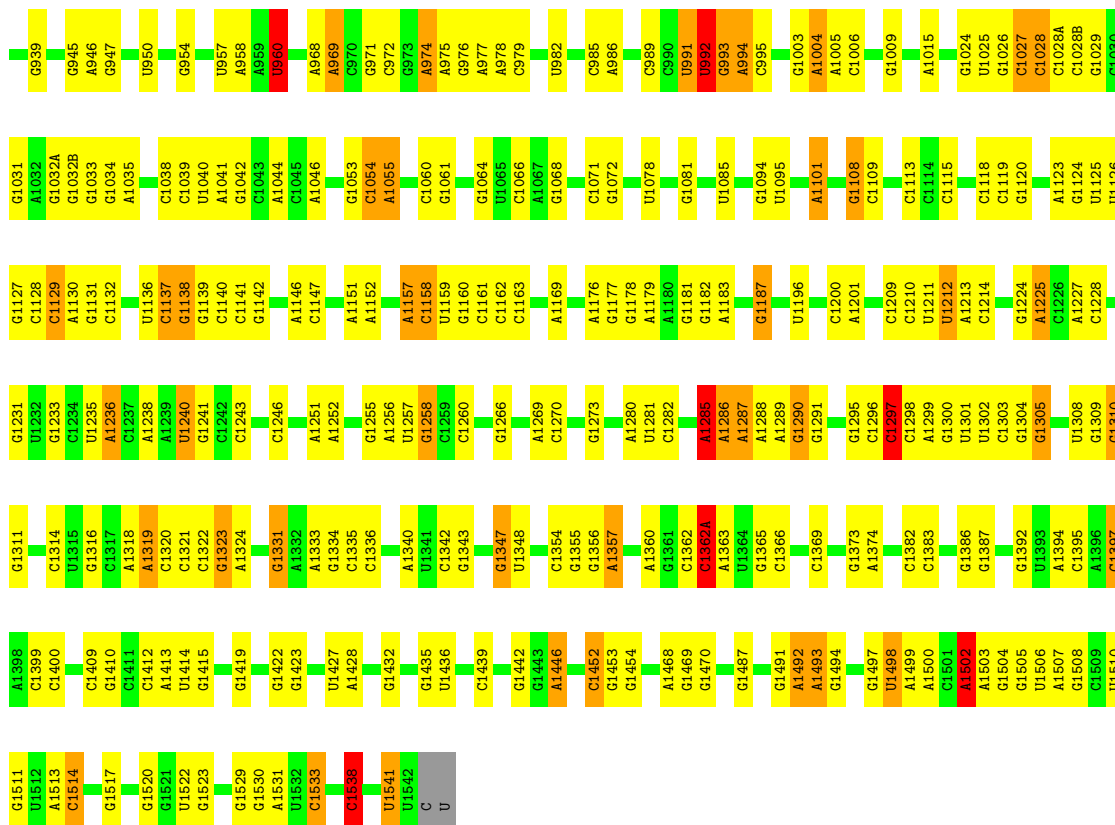
Chain QA:  61% 31% 6% ..



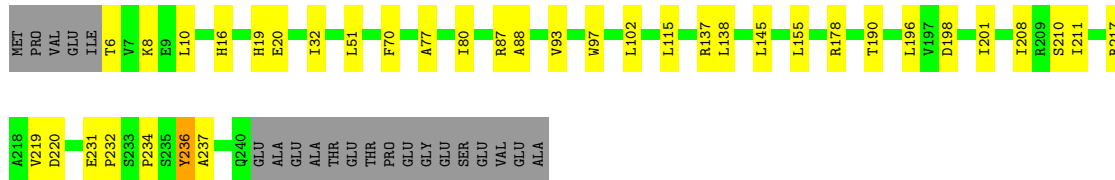
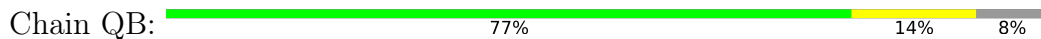


● Molecule 1: 16S rRNA

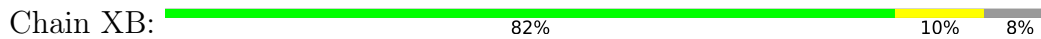




● Molecule 2: 30S ribosomal protein S2

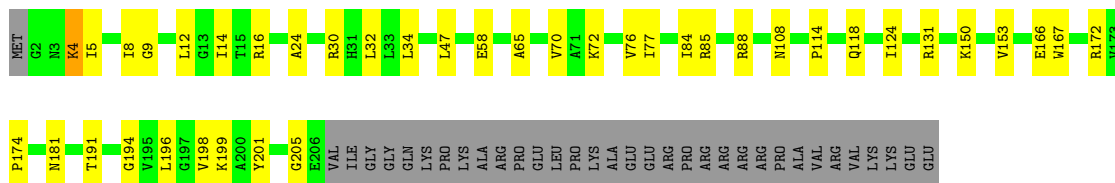


● Molecule 2: 30S ribosomal protein S2



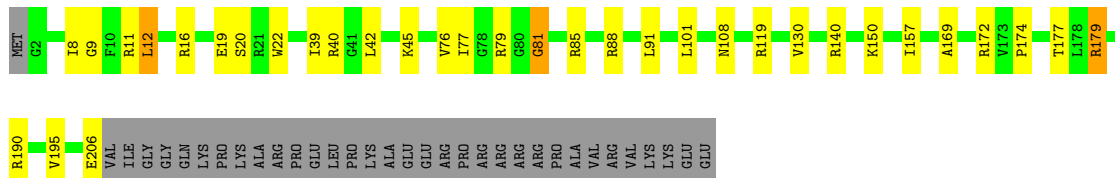
● Molecule 3: 30S ribosomal protein S3





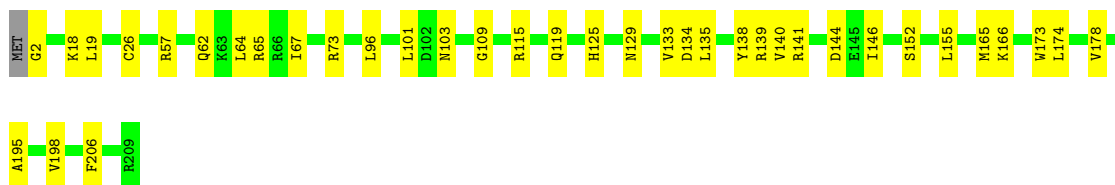
- Molecule 3: 30S ribosomal protein S3

Chain XC: 72% 13% 14%



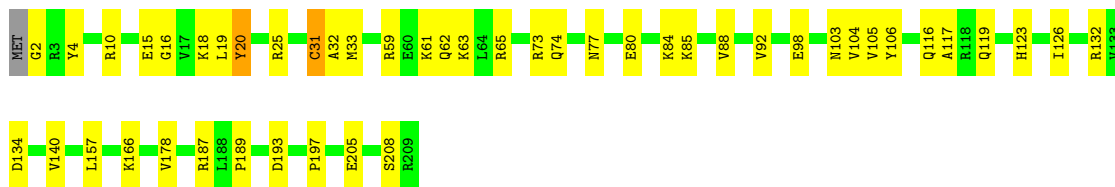
- Molecule 4: 30S ribosomal protein S4

Chain QD: 82% 18%



- Molecule 4: 30S ribosomal protein S4

Chain XD: 77% 22%



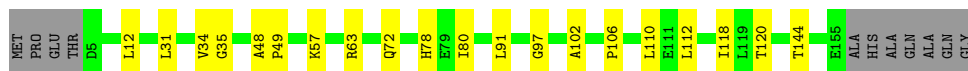
- Molecule 5: 30S ribosomal protein S5

Chain QE: 83% 10% 7%



- Molecule 5: 30S ribosomal protein S5

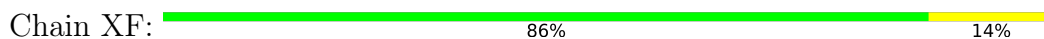
Chain XE: 81% 12% 7%



- Molecule 6: 30S ribosomal protein S6



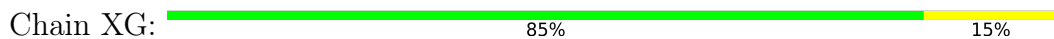
- Molecule 6: 30S ribosomal protein S6



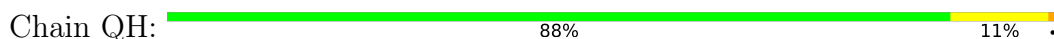
- Molecule 7: 30S ribosomal protein S7



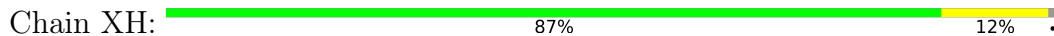
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

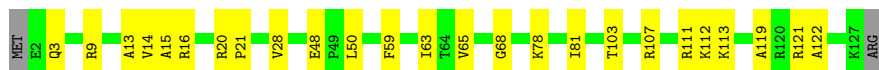
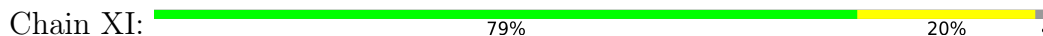


- Molecule 9: 30S ribosomal protein S9





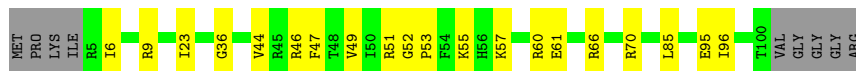
- Molecule 9: 30S ribosomal protein S9



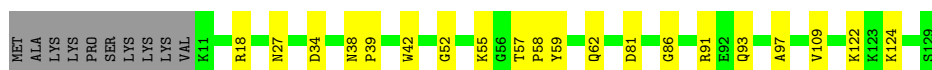
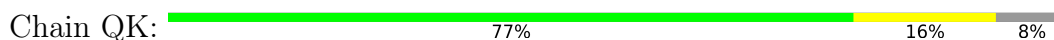
- Molecule 10: 30S ribosomal protein S10



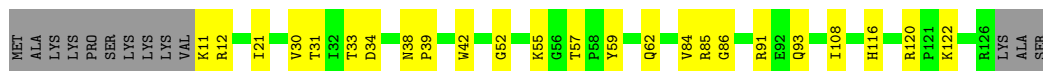
- Molecule 10: 30S ribosomal protein S10



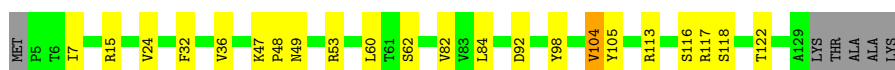
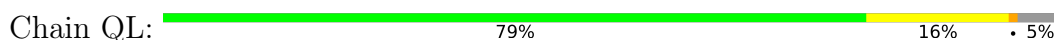
- Molecule 11: 30S ribosomal protein S11




- Molecule 11: 30S ribosomal protein S11

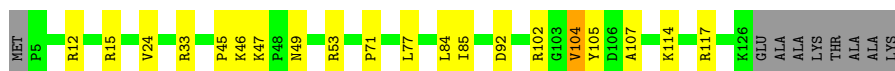


- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

Chain XL:  78% 15% 7%




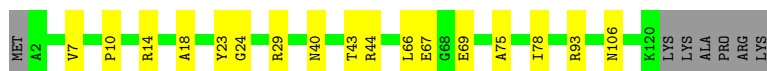
- Molecule 13: 30S ribosomal protein S13

Chain QM:  69% 25% 5%




- Molecule 13: 30S ribosomal protein S13

Chain XM:  81% 13% 6%




- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  79% 18% 2%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  80% 16% 2%



- Molecule 15: 30S ribosomal protein S15

Chain QO:  90% 9% 1%




- Molecule 15: 30S ribosomal protein S15

Chain XO:  90% 8% 2%




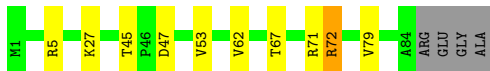
- Molecule 16: 30S ribosomal protein S16

Chain QP:  83% 13% 5%




- Molecule 16: 30S ribosomal protein S16

Chain XP:  84% 10% 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ:  85% 10% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  86% 10% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  68% 11% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  66% 14% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  73% 16% 11%



- Molecule 23: mRNA

Chain QX:  9% . 87%

G G C A A G G G U U A A U2 G3 A U U A U U C A A

- Molecule 23: mRNA

Chain XX:  61% 26% 13%

G-14 G-13 C-12 A-11 G-5 U-4 A-3 A-2 U4 A8

- Molecule 24: 50S ribosomal protein L27

Chain R0:  71% 19% 11%


MET ALA HIS LYS GLY LEU G9 R11 L21 G22 V23 E27 N35 V38 R39 Q40 R41 F45 G48 V51 R55 L59 V67 E68 V81 R82 P83 LEU ALA

- Molecule 24: 50S ribosomal protein L27

Chain Y0:  71% 18% 12%


MET ALA HIS LYS GLY LEU GLY S9 R14 K19 V23 E27 N35 R39 K46 P47 G48 K49 V51 E68 P69 Q70 R77 V78 V79 H80 P83 LEU ALA

- Molecule 25: 50S ribosomal protein L28

Chain R1:  80% 19% .

MET S2 S17 I18 Q19 I37 R40 N45 R52 V53 E57 V74 K78 G79 L80 L81 L85 S86 P87 I90 L97 L98

- Molecule 25: 50S ribosomal protein L28

Chain Y1:  74% 20% 5%


MET S2 E6 S17 I18 Q19 G28 I37 R40 V51 R52 E57 F60 R61 V62 V74 L80 K81 L85 G84 S86 P87 I90 K91 L94 LEU LYS LEU LEU

- Molecule 26: 50S ribosomal protein L29

Chain R2:  75% 21% .


MET LYS LEU S4 E5 V6 R14 S17 P18 V19 E20 L21 E22 I41 L44 M47 L53 Q56 R59 E66 K67 R68 M72

- Molecule 26: 50S ribosomal protein L29

Chain Y2:  83% 10% 6%



- Molecule 27: 50S ribosomal protein L30

Chain R3:  85% 13%




- Molecule 27: 50S ribosomal protein L30

Chain Y3:  67% 22% 10%




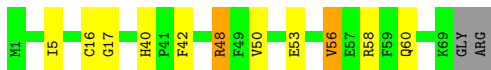
- Molecule 28: 50S ribosomal protein L31

Chain R4:  82% 15%



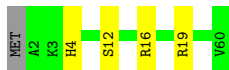
- Molecule 28: 50S ribosomal protein L31

Chain Y4:  82% 13%



- Molecule 29: 50S ribosomal protein L32

Chain R5:  92% 7%




- Molecule 29: 50S ribosomal protein L32

Chain Y5:  90% 8%




- Molecule 30: 50S ribosomal protein L33

Chain R6:  81% 17%




- Molecule 30: 50S ribosomal protein L33

Chain Y6:  81% 17%



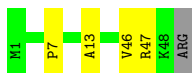
- Molecule 31: 50S ribosomal protein L34

Chain R7:  84% 12%



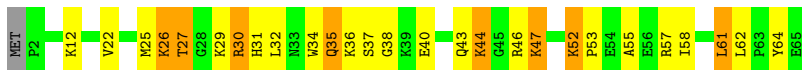
- Molecule 31: 50S ribosomal protein L34

Chain Y7:  90% 8%




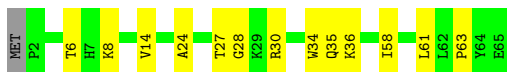
- Molecule 32: 50S ribosomal protein L35

Chain R8:  57% 29% 12%




- Molecule 32: 50S ribosomal protein L35

Chain Y8:  78% 20%



- Molecule 33: 50S ribosomal protein L36

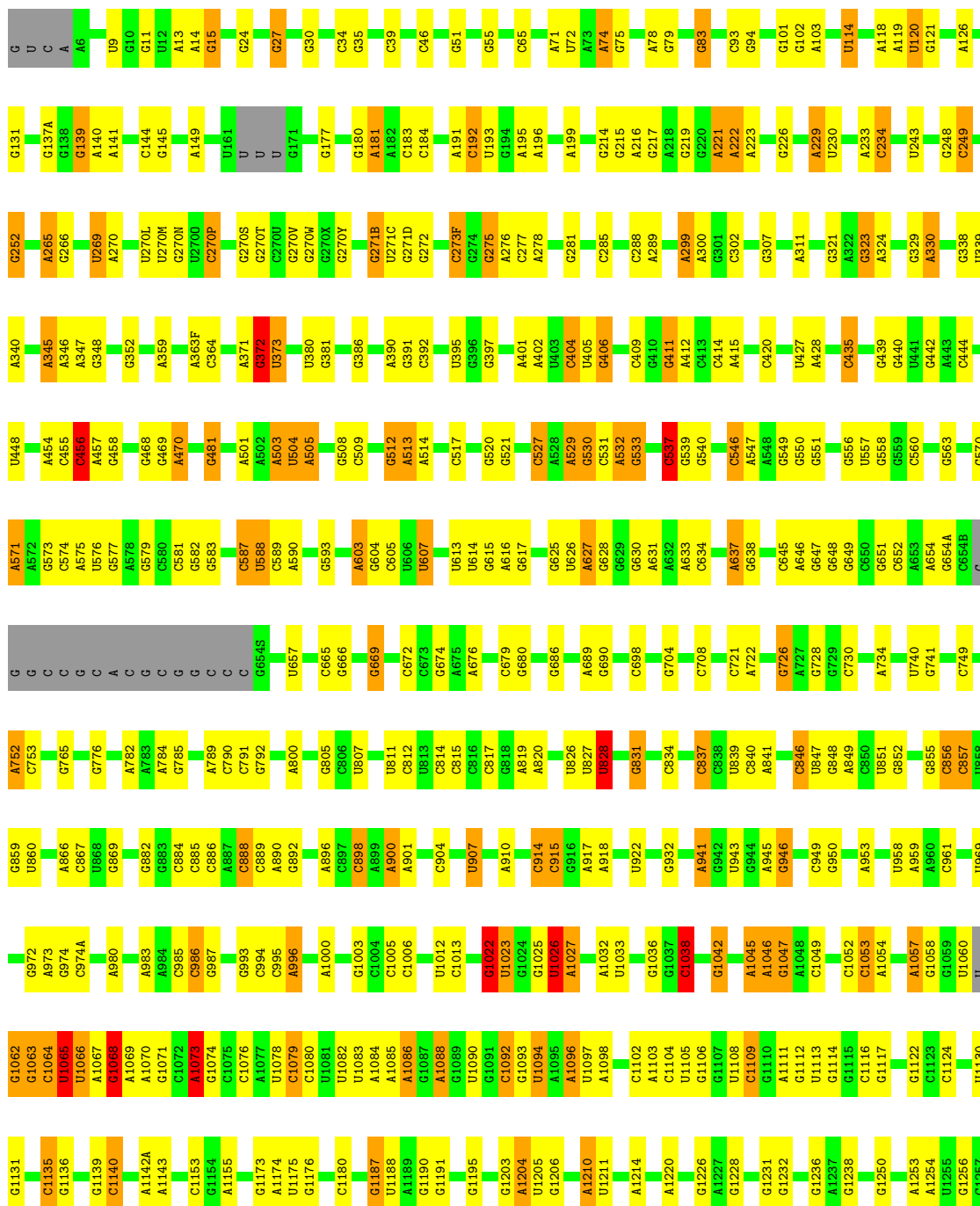
Chain R9:  81% 19%



- Molecule 33: 50S ribosomal protein L36



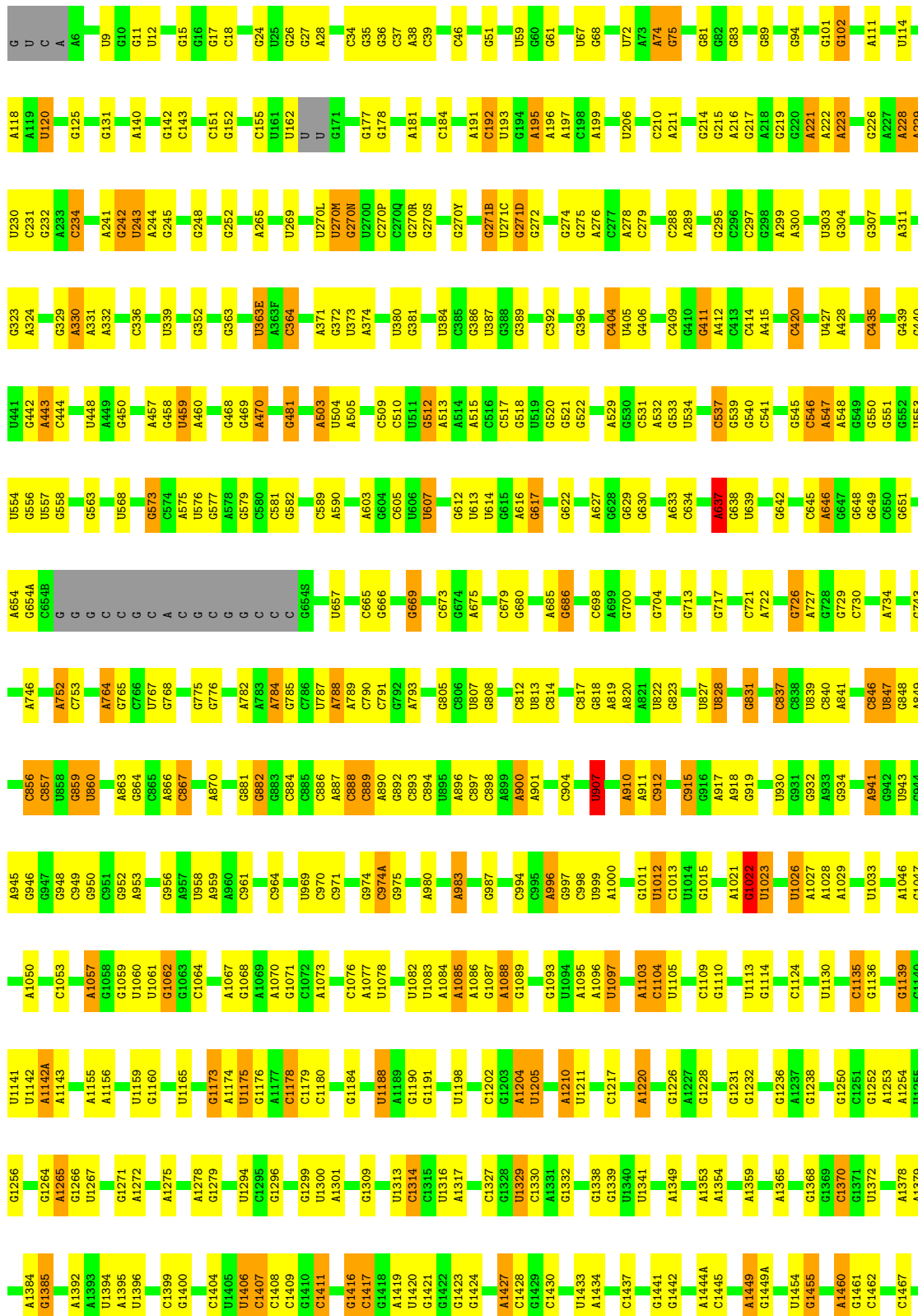
● Molecule 34: 23S rRNA

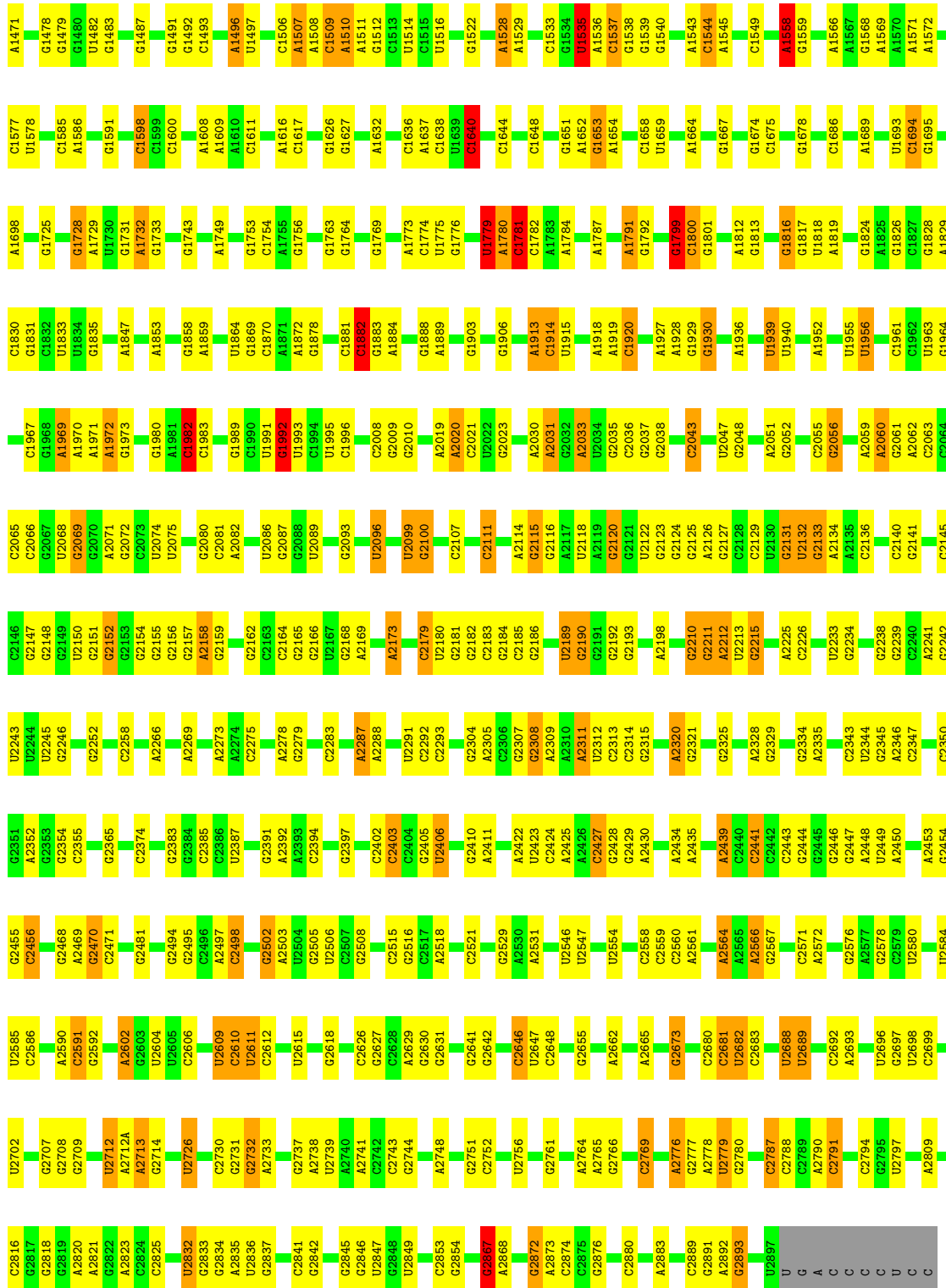


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A2825	U2720	C2612	A2486	G2375	C2188	A2060	U1963	U1834	C1882	G1484	G1259
A2826	G2726	A2614	G2494	A2378	C2162	G2061	G1984	G1835	A1583	A1384	G1264
U2832	U2726	U2615	G2495	G2379	C2164	C2063	A1965	C1844	C1586	U1330	A1265
C2833	G2729	G2618	C2498	G2383	G2185	U2068	G1967	G1845	A1587	U1395	G1266
A2834	C2730	G2623	G2502	G2389	U2186	G2069	A1968	G1846	U1267	U1396	U1267
U2835	G2731	G2623	A2503	G2394	G2187	G2070	A1970	A1847	G1595	C1403	G1271
U2836	C2732	G2627	A2503	C2395	U2187	U2074	A1971	A1848	C1404	U1272	U1273
G2837	A2733	G2628	G2505	A2189	A2169	U2075	A1972	A1859	U1406	U1406	U1278
C2841	U2739	A2629	G2508	A2173	A2173	G2080	G1980	G1869	C1407	A1504	A1278
G2842	A2740	G2630	G2508	G2182	G2182	G2081	A1981	C1870	C1506	G1506	G1279
G2843	A2741	G2631	C2515	G2182	A2182	A2082	C1982	A1871	A1507	U1288	U1288
A2844	G2745	A2639	G2517	G2187	G2187	G2086	G1989	G1872	A1508	G1416	U1300
G2845	C2745	C2403	G2517	G2188	G2188	U2087	G1990	G1878	C1417	U1416	U1300
U2846	G2745	G2404	A2518	U2189	U2189	G2087	C1991	C1878	A1509	C1417	U1300
G2848	U2748	G2405	U2519	G2190	G2190	U2093	U1991	C1881	A1510	G1418	A1301
C2853	A2749	U2406	G2529	G2194	G2194	G2093	G1992	C1882	A1511	U1419	C1304
G2854	A2750	A2311	A2311	G2194	G2194	U2096	C1993	G1883	C1512	U1420	C1304
G2855	G2751	C2313	U2312	A2198	A2198	U2096	C1994	C1888	C1513	G1421	C1309
C2859	C2752	C2314	C2314	A2199	A2199	C2103	C1995	A1889	U1514	G1422	G1309
A2860	G2759	G2315	G2315	A2199	A2199	C2107	C1996	A1889	G1522	G1424	U1312
G2867	C2760	G2318	G2318	G2210	G2210	G2004	G2004	C1902	U1523	U1523	U1313
A2868	G2761	A2320	A2320	G2211	G2211	C2008	C2008	G1903	G1524	A1427	U1313
A2868	A2762	G2320	G2320	U2112	U2112	G2009	G2009	G1903	A1428	C1428	C1314
G2872	A2765	G2321	G2321	U2113	U2113	G2010	G2010	G1906	G1526	G1429	C1314
A2873	G2766	G2321	A2114	U2113	U2113	G2010	G2010	U1907	G1527	C1430	A1317
C2874	G2777	G2325	G2116	U2114	U2114	A2013	A2013	C1908	A1528	A1434	C1327
C2879	A2778	A2328	A2117	U2118	U2118	A2014	A2014	A1913	A1529	G1435	G1327
C2880	U2779	G2329	A2117	U2118	U2118	A2019	A2019	A1914	G1436	U1329	U1329
C2881	G2780	G2330	U2118	U2118	U2118	A2020	A2020	U1915	A1535	A1331	A1331
A2882	G2780	G2330	U2118	U2118	U2118	C2021	C2021	U1915	A1536	G1332	G1332
A2883	G2784	G2334	U2233	U2233	U2233	G2022	G2022	C1920	C1537	C1333	C1333
G2886	C2787	A2335	G2234	U2234	U2234	G2023	G2023	G1929	G1538	U1341	G1334
C2889	C2788	A2336	G2234	U2244	U2244	G2023	G2023	G1930	A1542	U1449	U1341
C2891	C2789	A2336	G2234	U2244	U2244	G2030	G2030	G1931	A1543	G1449A	U1341
A2892	A2790	C2342	G2342	U2244	U2244	A2031	A2031	U1931	C1544	U1454	A1349
G2893	C2791	G2342	G2342	U2244	U2244	G2032	G2032	C1934	A1545	G1455	A1349
G2894	G2792	A2346	A2346	U2244	U2244	A2033	A2033	G1935	A1546	U1459	U1352
U2895	U2797	C2347	C2347	U2244	U2244	C2036	C2036	A1936	G1816	G1459	A1353
C2896	C2798	C2350	C2350	U2246	U2246	G2037	G2037	U1939	G1817	A1460	A1354
U2897	G2803	G2354	G2354	A2247	A2247	G2038	G2038	U1940	U1818	G1461	G1355
U	G	U2702	U2584	U2459	U2459	U2132	U2132	C1947	A1819	C1462	A1359
G	A	C2703	U2585	U2460	U2460	C2133	C2133	G1681	G1470	A1588	U1378
C	A2809	G2707	C2586	A2469	A2469	A2134	A2134	U1824	A1471	G1559	A1379
C	C	G2707	A2602	G2252	G2252	C2136	C2136	A1825	C1474	C1662	C1370
C	C	C2710	G2603	A2361	A2361	G2048	G2048	G1826	A1566	C1667	G1371
C	C	A2711	U2604	A2364	A2364	G2052	G2052	C1827	A1477	A1668	U1372
U	U	U2712	U2609	G2365	G2365	G2148	G2148	U1955	G1478	A1689	A1378
C	A2820	A2713	G2372	G2372	G2372	G2156	G2156	C1957	A1579	A1698	A1379
C			G2373	G2373	G2373	G2157	G2157	C1958	U1482	A1580	G1380

• Molecule 34: 23S rRNA

Chain YA:  63% 29% 6%

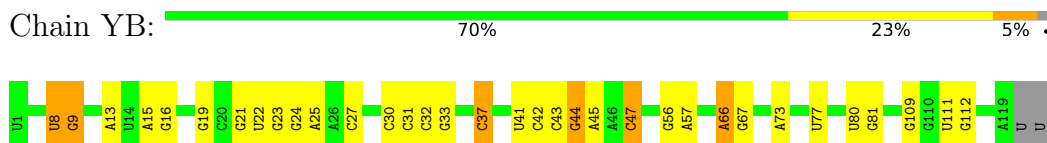




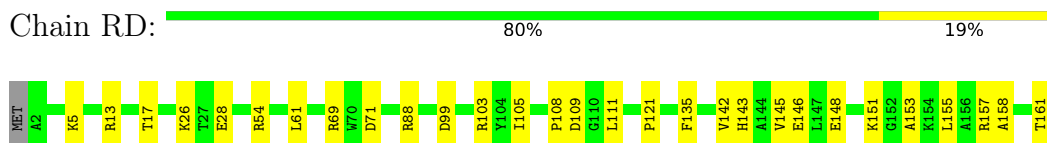
• Molecule 35: 5S rRNA



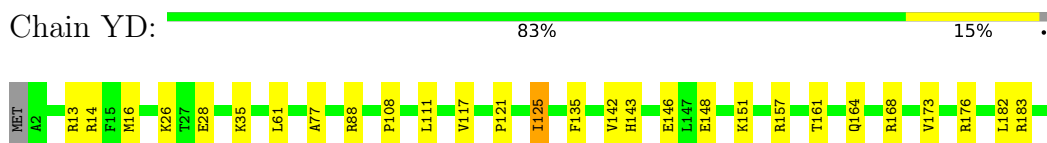
- Molecule 35: 5S rRNA



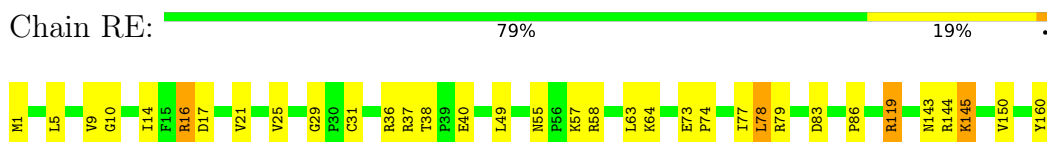
- Molecule 36: 50S ribosomal protein L2



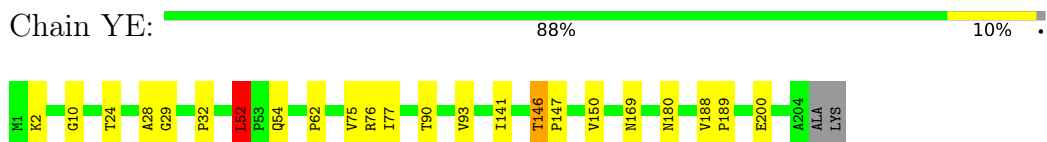
- Molecule 36: 50S ribosomal protein L2



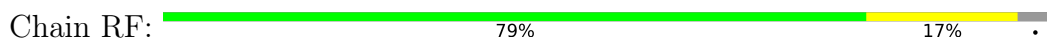
- Molecule 37: 50S ribosomal protein L3

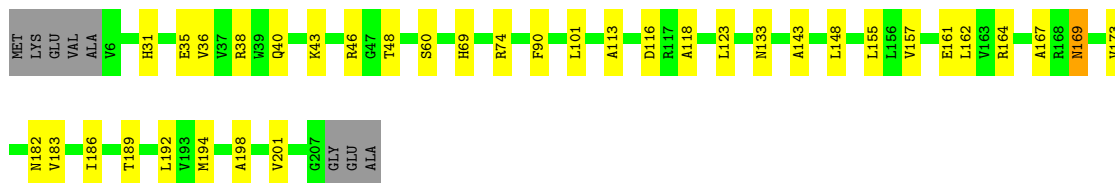


- Molecule 37: 50S ribosomal protein L3



- Molecule 38: 50S ribosomal protein L4





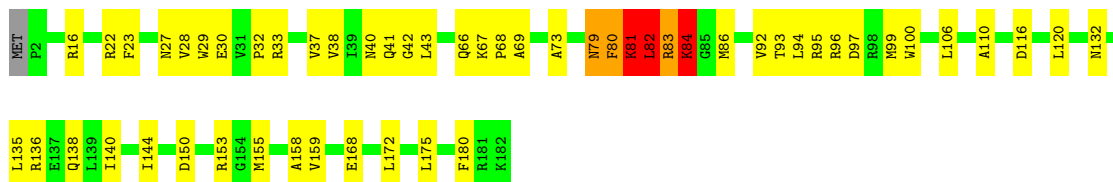
- Molecule 38: 50S ribosomal protein L4

Chain YF: 86% 10%



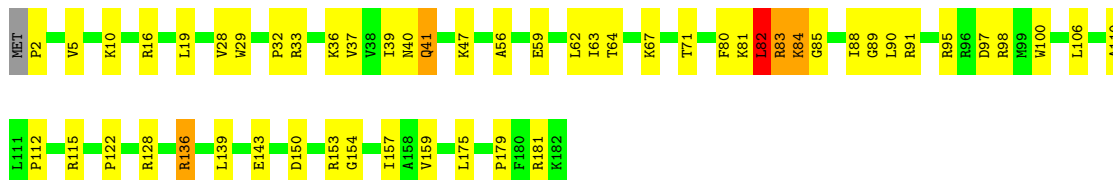
- Molecule 39: 50S ribosomal protein L5

Chain RG: 70% 26%



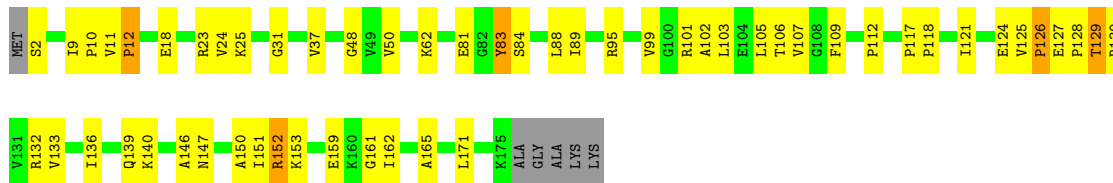
- Molecule 39: 50S ribosomal protein L5

Chain YG: 70% 26%



- Molecule 40: 50S ribosomal protein L6

Chain RH: 66% 28%



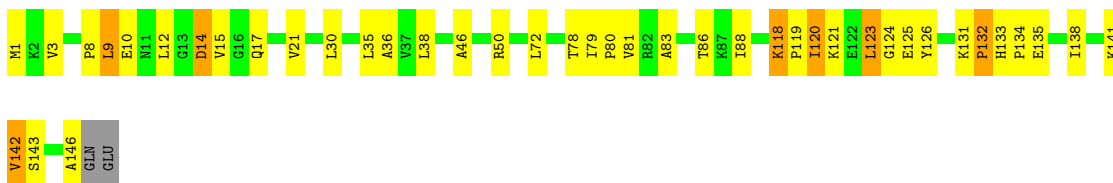
- Molecule 40: 50S ribosomal protein L6

Chain YH: 81% 14%




LYS


- Molecule 41: 50S ribosomal protein L9

Chain RI:  70% 24% 5%


- Molecule 41: 50S ribosomal protein L9

Chain YI:  77% 16% 5%


- Molecule 42: 50S ribosomal protein L13

Chain RN:  82% 14% 5%


- Molecule 42: 50S ribosomal protein L13

Chain YN:  84% 15% 5%


- Molecule 43: 50S ribosomal protein L14

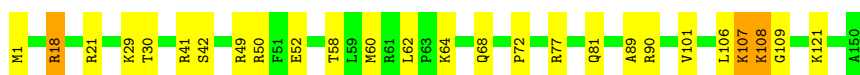
Chain RO:  80% 20% 5%

- Molecule 43: 50S ribosomal protein L14


Chain YO:  80% 20% 5%

- Molecule 44: 50S ribosomal protein L15

Chain RP:  83% 15%




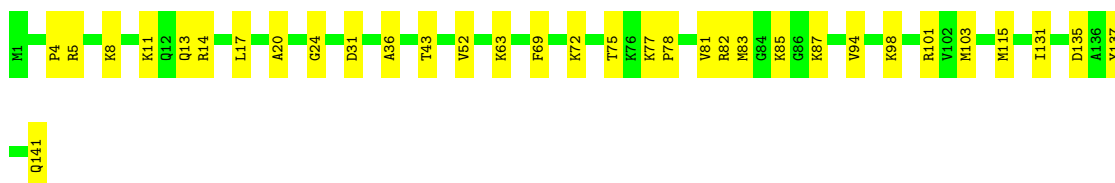
- Molecule 44: 50S ribosomal protein L15

Chain YP:  83% 13%




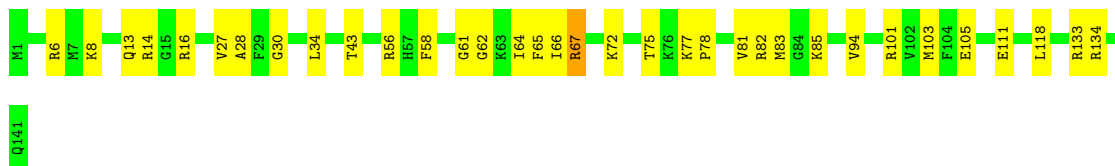
- Molecule 45: 50S ribosomal protein L16

Chain RQ:  77% 23%




- Molecule 45: 50S ribosomal protein L16

Chain YQ:  76% 23%




- Molecule 46: 50S ribosomal protein L17

Chain RR:  86% 14%




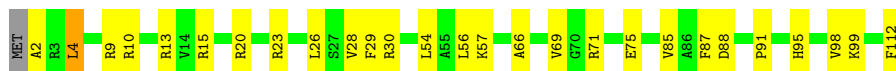
- Molecule 46: 50S ribosomal protein L17

Chain YR:  82% 17%

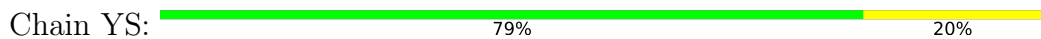


- Molecule 47: 50S ribosomal protein L18

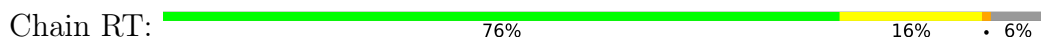
Chain RS:  75% 23%



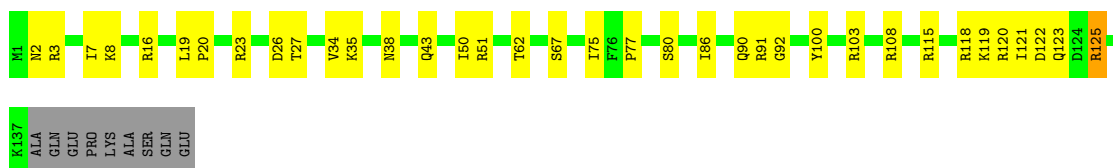
- Molecule 47: 50S ribosomal protein L18



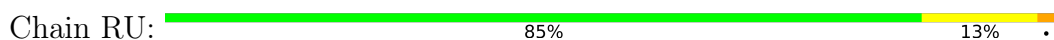
- Molecule 48: 50S ribosomal protein L19



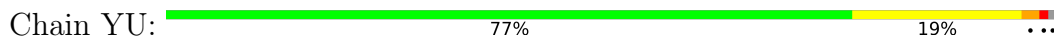
- Molecule 48: 50S ribosomal protein L19



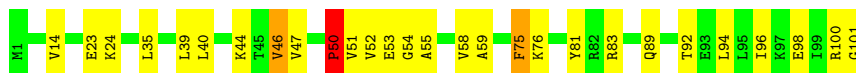
- Molecule 49: 50S ribosomal protein L20




- Molecule 49: 50S ribosomal protein L20

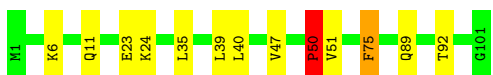


- Molecule 50: 50S ribosomal protein L21



- Molecule 50: 50S ribosomal protein L21

Chain YV:  87% 11% ..




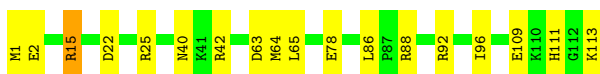
- Molecule 51: 50S ribosomal protein L22

Chain RW:  88% 12%




- Molecule 51: 50S ribosomal protein L22

Chain YW:  84% 15%




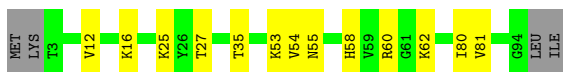
- Molecule 52: 50S ribosomal protein L23

Chain RX:  85% 10%




- Molecule 52: 50S ribosomal protein L23

Chain YX:  82% 14%




- Molecule 53: 50S ribosomal protein L24

Chain RY:  86% 11%




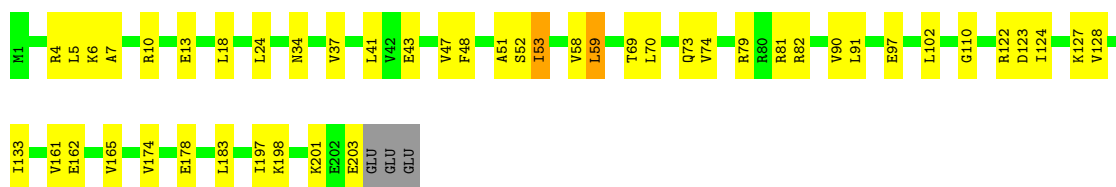
- Molecule 53: 50S ribosomal protein L24

Chain YY:  83% 15%




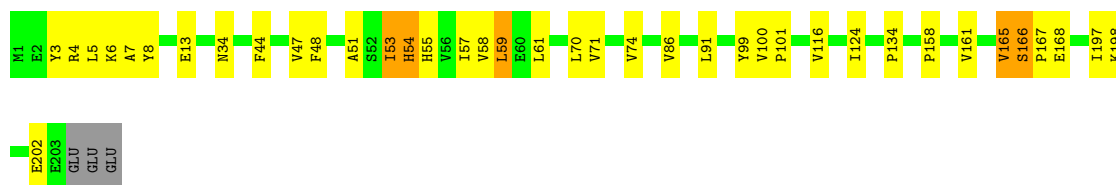
- Molecule 54: 50S ribosomal protein L25

Chain RZ:  76% 22% ..



- Molecule 54: 50S ribosomal protein L25

Chain YZ:  80% 17% ..



- Molecule 55: A-site ASL^Phe

Chain XY:  59% 35% 6%



- Molecule 56: CC-puro

Chain Z6:  67% 33%



- Molecule 56: CC-puro

Chain Z8:  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	210.56Å 447.23Å 618.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.01 – 3.64	Depositor
% Data completeness (in resolution range)	95.7 (174.01-3.64)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.278	Depositor
Wilson B-factor (Å ²)	105.8	Xtrriage
Anisotropy	0.167	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	292577	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PPU, MG, MNU, T6A, SF4, ZN

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	0.33	0/36098	1.06	143/56341 (0.3%)
1	XA	0.33	0/36346	1.06	155/56725 (0.3%)
2	QB	0.29	0/1942	0.54	0/2619
2	XB	0.28	0/1950	0.55	0/2630
3	QC	0.28	0/1629	0.54	0/2195
3	XC	0.28	0/1629	0.57	0/2195
4	QD	0.28	0/1733	0.50	0/2318
4	XD	0.30	0/1733	0.52	0/2318
5	QE	0.27	0/1171	0.53	0/1576
5	XE	0.27	0/1171	0.55	0/1576
6	QF	0.25	0/856	0.51	0/1154
6	XF	0.25	0/856	0.50	0/1154
7	QG	0.26	0/1276	0.49	0/1709
7	XG	0.27	0/1276	0.54	0/1709
8	QH	0.25	0/1128	0.49	0/1517
8	XH	0.25	0/1128	0.51	0/1517
9	QI	0.53	3/1029 (0.3%)	0.73	2/1379 (0.1%)
9	XI	0.32	0/1017	0.61	0/1365
10	QJ	0.28	0/814	0.56	1/1095 (0.1%)
10	XJ	0.27	0/790	0.59	0/1063
11	QK	0.26	0/900	0.50	0/1213
11	XK	0.27	0/879	0.49	0/1187
12	QL	0.30	0/991	0.57	0/1327
12	XL	0.30	0/972	0.56	0/1301
13	QM	0.30	0/965	0.58	0/1292
13	XM	0.28	0/956	0.62	0/1281
14	QN	0.35	0/501	0.58	0/664
14	XN	0.31	0/501	0.62	0/664
15	QO	0.25	0/745	0.49	0/992
15	XO	0.25	0/740	0.45	0/987
16	QP	0.26	0/721	0.51	0/970
16	XP	0.26	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.25	0/847	0.49	0/1131
17	XQ	0.26	0/847	0.50	0/1131
18	QR	0.28	0/579	0.61	0/768
18	XR	0.27	0/579	0.56	0/768
19	QS	0.28	0/680	0.59	0/915
19	XS	0.27	0/689	0.62	1/926 (0.1%)
20	QT	0.29	0/765	0.56	0/1007
20	XT	0.29	0/765	0.55	0/1007
21	QU	0.25	0/221	0.44	0/288
21	XU	0.23	0/221	0.48	0/288
22	QV	0.43	1/1706 (0.1%)	1.22	13/2652 (0.5%)
22	XV	0.39	0/1706	1.20	13/2652 (0.5%)
23	QX	0.35	0/72	1.01	0/110
23	XX	0.32	0/560	1.09	2/872 (0.2%)
24	R0	0.25	0/611	0.49	0/814
24	Y0	0.26	0/607	0.47	0/809
25	R1	0.28	0/770	0.56	0/1022
25	Y1	0.28	0/736	0.55	0/978
26	R2	0.26	0/583	0.54	0/771
26	Y2	0.27	0/577	0.51	0/764
27	R3	0.26	0/474	0.52	0/635
27	Y3	0.35	0/474	0.61	0/635
28	R4	0.29	0/578	0.60	0/776
28	Y4	0.29	0/578	0.57	0/776
29	R5	0.26	0/473	0.50	0/639
29	Y5	0.25	0/473	0.49	0/639
30	R6	0.24	0/460	0.50	0/613
30	Y6	0.25	0/460	0.47	0/613
31	R7	0.25	0/417	0.44	0/550
31	Y7	0.24	0/426	0.44	0/561
32	R8	0.40	0/525	0.72	0/691
32	Y8	0.27	0/525	0.51	0/691
33	R9	0.23	0/310	0.48	0/407
33	Y9	0.23	0/310	0.46	0/407
34	RA	0.35	0/69498	1.08	333/108491 (0.3%)
34	YA	0.34	0/69543	1.07	307/108563 (0.3%)
35	RB	0.35	0/2878	1.13	18/4490 (0.4%)
35	YB	0.36	0/2878	1.13	17/4490 (0.4%)
36	RD	0.29	0/2165	0.54	0/2919
36	YD	0.30	0/2165	0.53	0/2919
37	RE	0.35	0/1601	0.64	1/2160 (0.0%)
37	YE	0.30	0/1596	0.55	0/2153
38	RF	0.30	0/1620	0.61	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.29	0/1620	0.60	0/2194
39	RG	0.31	0/1499	0.61	0/2016
39	YG	0.33	0/1499	0.61	0/2016
40	RH	0.36	0/1362	0.71	1/1841 (0.1%)
40	YH	0.28	0/1356	0.52	0/1833
41	RI	0.36	0/1151	0.66	0/1558
41	YI	0.41	1/1151 (0.1%)	0.65	0/1558
42	RN	0.29	0/1131	0.53	0/1525
42	YN	0.27	0/1131	0.53	0/1525
43	RO	0.28	0/943	0.52	0/1269
43	YO	0.27	0/943	0.52	0/1269
44	RP	0.31	0/1162	0.66	0/1544
44	YP	0.30	0/1139	0.59	0/1514
45	RQ	0.30	0/1143	0.60	0/1527
45	YQ	0.31	0/1143	0.60	0/1527
46	RR	0.26	0/974	0.57	0/1302
46	YR	0.27	0/974	0.57	0/1302
47	RS	0.31	0/892	0.68	1/1187 (0.1%)
47	YS	0.30	0/892	0.64	1/1187 (0.1%)
48	RT	0.30	0/1155	0.59	0/1542
48	YT	0.29	0/1155	0.58	0/1542
49	RU	0.30	0/982	0.59	1/1306 (0.1%)
49	YU	0.33	0/982	0.64	1/1306 (0.1%)
50	RV	0.34	0/790	0.70	2/1057 (0.2%)
50	YV	0.34	0/790	0.73	3/1057 (0.3%)
51	RW	0.26	0/911	0.51	0/1220
51	YW	0.29	0/911	0.54	0/1220
52	RX	0.27	0/739	0.53	1/993 (0.1%)
52	YX	0.27	0/739	0.52	0/993
53	RY	0.26	0/831	0.51	0/1108
53	YY	0.27	0/831	0.51	0/1108
54	RZ	0.32	0/1634	0.64	2/2216 (0.1%)
54	YZ	0.31	0/1634	0.56	0/2216
55	XY	0.34	0/405	1.11	0/630
56	Z6	0.44	0/40	1.44	0/60
56	Z8	0.40	0/40	1.28	0/60
All	All	0.33	5/316386 (0.0%)	0.96	1019/473016 (0.2%)

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
27	Y3	0	1
37	YE	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	YI	133	HIS	C-N	8.27	1.50	1.34
9	QI	10	ARG	CZ-NH1	6.74	1.41	1.33
9	QI	37	PHE	CA-CB	6.25	1.67	1.53
9	QI	10	ARG	CA-CB	5.60	1.66	1.53
22	QV	53	G	C2-N3	-5.05	1.28	1.32

The worst 5 of 1019 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	53	G	OP1-P-O3'	-14.20	73.97	105.20
1	QA	1158	C	N1-C2-O2	12.73	126.54	118.90
1	QA	1158	C	C2-N1-C1'	12.38	132.42	118.80
22	QV	53	G	C2-N3-C4	12.10	117.95	111.90
35	RB	31	C	C2-N1-C1'	10.59	130.45	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Y3	34	GLU	Mainchain
37	YE	146	THR	Peptide

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	32247	0	16278	248	0
1	XA	32471	0	16395	253	0
2	QB	1907	0	1958	20	0
2	XB	1915	0	1969	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	QC	1605	0	1668	30	0
3	XC	1605	0	1668	20	0
4	QD	1703	0	1767	21	0
4	XD	1703	0	1767	46	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	5	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	13	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	11	0
9	QI	1010	0	1037	31	0
9	XI	998	0	1024	16	0
10	QJ	801	0	849	15	0
10	XJ	777	0	816	14	0
11	QK	885	0	904	16	0
11	XK	864	0	881	16	0
12	QL	975	0	1062	20	0
12	XL	956	0	1046	24	0
13	QM	955	0	1021	29	0
13	XM	946	0	1008	13	0
14	QN	492	0	531	8	0
14	XN	492	0	529	8	0
15	QO	734	0	771	4	0
15	XO	729	0	768	5	0
16	QP	705	0	725	8	0
16	XP	705	0	725	8	0
17	QQ	834	0	904	7	0
17	XQ	834	0	904	7	0
18	QR	574	0	644	6	0
18	XR	574	0	644	11	0
19	QS	665	0	686	13	0
19	XS	674	0	699	11	0
20	QT	763	0	861	11	0
20	XT	763	0	861	8	0
21	QU	217	0	234	1	0
21	XU	217	0	234	5	0
22	QV	1584	0	808	12	0
22	XV	1584	0	808	14	0
23	QX	65	0	33	1	0
23	XX	499	0	249	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	R0	603	0	620	12	0
24	Y0	599	0	617	11	0
25	R1	763	0	848	12	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	8	0
26	Y2	575	0	624	7	0
27	R3	469	0	518	4	0
27	Y3	469	0	518	22	0
28	R4	565	0	557	6	0
28	Y4	565	0	559	7	0
29	R5	459	0	478	4	0
29	Y5	459	0	477	6	0
30	R6	453	0	477	5	0
30	Y6	453	0	476	5	0
31	R7	409	0	454	4	0
31	Y7	418	0	467	3	0
32	R8	517	0	582	45	0
32	Y8	517	0	582	9	0
33	R9	307	0	337	5	0
33	Y9	307	0	336	8	0
34	RA	62051	0	31279	371	0
34	YA	62091	0	31298	424	0
35	RB	2573	0	1306	16	0
35	YB	2573	0	1306	11	0
36	RD	2115	0	2195	43	0
36	YD	2115	0	2195	37	0
37	RE	1568	0	1634	29	0
37	YE	1563	0	1629	19	0
38	RF	1585	0	1632	23	0
38	YF	1585	0	1632	16	0
39	RG	1474	0	1535	51	0
39	YG	1474	0	1535	45	0
40	RH	1336	0	1418	47	0
40	YH	1330	0	1413	15	0
41	RI	1136	0	1223	32	0
41	YI	1136	0	1223	55	0
42	RN	1104	0	1180	29	0
42	YN	1104	0	1180	11	0
43	RO	933	0	996	17	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	35	0
44	YP	1122	0	1204	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	RQ	1122	0	1179	24	0
45	YQ	1122	0	1179	28	0
46	RR	960	0	1021	11	0
46	YR	960	0	1021	11	0
47	RS	882	0	943	19	0
47	YS	882	0	943	17	0
48	RT	1141	0	1202	29	0
48	YT	1141	0	1202	32	0
49	RU	964	0	1022	26	0
49	YU	964	0	1022	50	0
50	RV	779	0	852	31	0
50	YV	779	0	852	16	0
51	RW	900	0	964	9	0
51	YW	900	0	964	29	0
52	RX	725	0	778	6	0
52	YX	725	0	778	10	0
53	RY	818	0	910	8	0
53	YY	818	0	911	11	0
54	RZ	1601	0	1630	32	0
54	YZ	1601	0	1630	30	0
55	XY	362	0	186	4	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	2	0
57	QA	73	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QJ	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	RA	483	0	0	0	0
57	RB	7	0	0	0	0
57	RE	4	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	3	0	0	0	0
57	RQ	3	0	0	0	0
57	RR	1	0	0	0	0
57	RT	1	0	0	0	0
57	RY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XA	73	0	0	0	0
57	XE	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XQ	1	0	0	0	0
57	XS	1	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	YA	538	0	0	0	0
57	YB	13	0	0	0	0
57	YD	3	0	0	0	0
57	YE	4	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YR	2	0	0	0	0
57	YX	2	0	0	0	0
57	YY	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	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	292577	0	198284	2581	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 5.

The worst 5 of 2581 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)
51:YW:1:MET:HG3	51:YW:64:MET:CE	1.51	1.41
50:YV:40:LEU:CD2	50:YV:47:VAL:HG12	1.52	1.40
4:XD:19:LEU:CD2	4:XD:197:PRO:HG3	1.59	1.33
1:QA:1189:C:H5 ⁺	3:QC:5:ILE:CD1	1.56	1.33
41:YI:61:ARG:HB2	41:YI:133:HIS:CE1	1.73	1.23

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%)	210 (90%)	22 (9%)	1 (0%)	34	70
2	XB	234/256 (91%)	211 (90%)	22 (9%)	1 (0%)	34	70
3	QC	203/239 (85%)	195 (96%)	8 (4%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	10 (5%)	2 (1%)	15	54
4	QD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
4	XD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	15	54
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
12	QL	123/131 (94%)	115 (94%)	7 (6%)	1 (1%)	19	58
12	XL	120/131 (92%)	109 (91%)	11 (9%)	0	100	100
13	QM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	9	43
13	XM	117/126 (93%)	102 (87%)	14 (12%)	1 (1%)	17	56
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	43
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	43
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	85/89 (96%)	82 (96%)	3 (4%)	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%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	15	54
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
24	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
24	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
25	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
25	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
28	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	46
29	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	R6	51/54 (94%)	51 (100%)	0	0	100	100
30	Y6	51/54 (94%)	51 (100%)	0	0	100	100
31	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
31	Y7	46/49 (94%)	46 (100%)	0	0	100	100
32	R8	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	16
32	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	R9	35/37 (95%)	35 (100%)	0	0	100	100
33	Y9	35/37 (95%)	35 (100%)	0	0	100	100
36	RD	270/276 (98%)	254 (94%)	15 (6%)	1 (0%)	34	70
36	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
37	RE	203/206 (98%)	170 (84%)	33 (16%)	0	100	100
37	YE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15	54
38	RF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
38	YF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
39	RG	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	9	43
39	YG	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	25	63
40	RH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	9	43
40	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100	100
41	RI	144/148 (97%)	127 (88%)	14 (10%)	3 (2%)	7	39
41	YI	144/148 (97%)	127 (88%)	12 (8%)	5 (4%)	3	29
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	61
42	YN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22	61
43	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
43	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
44	RP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	11	47
44	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	61
45	YQ	139/141 (99%)	122 (88%)	15 (11%)	2 (1%)	11	47
46	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
46	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	56
47	RS	109/112 (97%)	90 (83%)	17 (16%)	2 (2%)	8	42
47	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
48	RT	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
48	YT	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
49	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	56
49	YU	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	9	43
50	RV	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	7	40
50	YV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	54
51	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
51	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	56
52	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
52	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
53	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
53	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
54	RZ	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	29	67
54	YZ	201/206 (98%)	186 (92%)	12 (6%)	3 (2%)	10	46
All	All	11484/12126 (95%)	10639 (93%)	787 (7%)	58 (0%)	29	67

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	R8	62	LEU
40	RH	12	PRO
41	RI	132	PRO
44	RP	108	LYS
50	RV	46	VAL

5.3.2 Protein sidechains [i](#)

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%)	201 (99%)	2 (1%)	76	88
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	156 (98%)	3 (2%)	57	79
3	XC	159/188 (85%)	156 (98%)	3 (2%)	57	79
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	87
4	XD	180/181 (99%)	179 (99%)	1 (1%)	86	94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	89
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	87
7	QG	126/127 (99%)	124 (98%)	2 (2%)	62	82
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	82
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	91
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	70
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	86
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	87
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76	88
12	XL	103/108 (95%)	102 (99%)	1 (1%)	76	88
13	QM	96/101 (95%)	94 (98%)	2 (2%)	53	77
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	63
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	78
15	QO	79/80 (99%)	78 (99%)	1 (1%)	69	85
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	84
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	87
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38	68
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	85
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	61/67 (91%)	61 (100%)	0	100	100
24	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	82
25	R1	82/83 (99%)	82 (100%)	0	100	100
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	82
27	R3	51/52 (98%)	50 (98%)	1 (2%)	55	78
27	Y3	51/52 (98%)	44 (86%)	7 (14%)	3	22
28	R4	62/63 (98%)	61 (98%)	1 (2%)	62	82
28	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	69
29	R5	51/52 (98%)	51 (100%)	0	100	100
29	Y5	51/52 (98%)	51 (100%)	0	100	100
30	R6	51/52 (98%)	51 (100%)	0	100	100
30	Y6	51/52 (98%)	51 (100%)	0	100	100
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	46 (85%)	8 (15%)	3	19
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	RD	214/218 (98%)	214 (100%)	0	100	100
36	YD	214/218 (98%)	213 (100%)	1 (0%)	88	95
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49	74
37	YE	165/166 (99%)	163 (99%)	2 (1%)	71	86
38	RF	161/166 (97%)	159 (99%)	2 (1%)	71	86
38	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	RG	155/156 (99%)	147 (95%)	8 (5%)	23	57
39	YG	155/156 (99%)	150 (97%)	5 (3%)	39	69
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21	55
40	YH	144/148 (97%)	142 (99%)	2 (1%)	67	84
41	RI	122/124 (98%)	113 (93%)	9 (7%)	13	45
41	YI	122/124 (98%)	114 (93%)	8 (7%)	16	50
42	RN	117/119 (98%)	113 (97%)	4 (3%)	37	68
42	YN	117/119 (98%)	117 (100%)	0	100	100
43	RO	100/100 (100%)	98 (98%)	2 (2%)	55	78
43	YO	100/100 (100%)	100 (100%)	0	100	100
44	RP	116/116 (100%)	113 (97%)	3 (3%)	46	73
44	YP	114/116 (98%)	112 (98%)	2 (2%)	59	80
45	RQ	111/111 (100%)	110 (99%)	1 (1%)	78	89
45	YQ	111/111 (100%)	108 (97%)	3 (3%)	44	72
46	RR	100/101 (99%)	100 (100%)	0	100	100
46	YR	100/101 (99%)	100 (100%)	0	100	100
47	RS	87/88 (99%)	86 (99%)	1 (1%)	73	87
47	YS	87/88 (99%)	86 (99%)	1 (1%)	73	87
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47	74
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60	81
49	RU	93/94 (99%)	91 (98%)	2 (2%)	52	76
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52	76
50	RV	82/82 (100%)	79 (96%)	3 (4%)	34	65
50	YV	82/82 (100%)	79 (96%)	3 (4%)	34	65
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	YW	92/92 (100%)	89 (97%)	3 (3%)	38	68
52	RX	74/78 (95%)	74 (100%)	0	100	100
52	YX	74/78 (95%)	74 (100%)	0	100	100
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	88 (100%)	0	100	100
54	RZ	174/179 (97%)	170 (98%)	4 (2%)	50	75
54	YZ	174/179 (97%)	169 (97%)	5 (3%)	42	71
All	All	9706/10064 (96%)	9554 (98%)	152 (2%)	62	82

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	YF	38	ARG
50	YV	75	PHE
39	YG	84	LYS
41	YI	133	HIS
54	YZ	59	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
51	RW	111	HIS
7	XG	28	ASN
39	YG	41	GLN
30	Y6	26	ASN
30	Y6	29	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	266 (17%)	30 (2%)
1	XA	1509/1522 (99%)	293 (19%)	25 (1%)
22	QV	71/76 (93%)	17 (23%)	0
22	XV	71/76 (93%)	17 (23%)	0
23	QX	2/23 (8%)	0	0
23	XX	22/23 (95%)	4 (18%)	2 (9%)
34	RA	2877/2915 (98%)	549 (19%)	37 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	YA	2880/2915 (98%)	511 (17%)	37 (1%)
35	RB	119/122 (97%)	16 (13%)	1 (0%)
35	YB	119/122 (97%)	18 (15%)	1 (0%)
55	XY	16/17 (94%)	3 (18%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9339 (98%)	1694 (18%)	133 (1%)

5 of 1694 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	31	G
1	QA	32	A
1	QA	39	G

5 of 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	YA	1204	A
34	YA	1558	A
34	YA	2832	U
34	RA	1065	U
34	RA	1057	A

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

6 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	T6A	QV	37	22	27,34,35	0.97	1 (3%)	29,49,52	1.72	6 (20%)
22	T6A	XV	37	22	27,34,35	0.95	2 (7%)	29,49,52	1.61	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	MNU	XV	34	22,23	20,24,25	1.32	3 (15%)	28,34,37	1.82	8 (28%)
56	PPU	Z6	76	34,56	32,40,41	0.87	1 (3%)	33,57,60	1.49	7 (21%)
22	MNU	QV	34	22,23	20,24,25	1.30	3 (15%)	28,34,37	1.63	8 (28%)
56	PPU	Z8	76	34,56	32,40,41	0.89	1 (3%)	33,57,60	1.56	7 (21%)

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	T6A	QV	37	22	-	13/19/41/42	0/3/3/3
22	T6A	XV	37	22	-	14/19/41/42	0/3/3/3
22	MNU	XV	34	22,23	-	0/9/28/29	0/2/2/2
56	PPU	Z6	76	34,56	-	4/21/43/44	0/4/4/4
22	MNU	QV	34	22,23	-	0/9/28/29	0/2/2/2
56	PPU	Z8	76	34,56	-	3/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	34	MNU	C2-N1	3.13	1.43	1.38
22	QV	34	MNU	C2-N1	2.92	1.43	1.38
22	QV	34	MNU	C4-N3	-2.85	1.33	1.38
22	XV	34	MNU	C4-N3	-2.83	1.33	1.38
56	Z8	76	PPU	C5-C4	2.68	1.48	1.40

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	37	T6A	C2-N1-C6	5.54	121.34	116.59
22	XV	37	T6A	C2-N1-C6	5.26	121.10	116.59
22	XV	34	MNU	N3-C2-N1	4.45	120.79	114.89
56	Z6	76	PPU	N1-C6-N6	4.30	121.58	117.06
22	QV	34	MNU	N3-C2-N1	4.27	120.55	114.89

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QV	37	T6A	O10-C10-N6-C6
22	QV	37	T6A	N11-C10-N6-C6
22	QV	37	T6A	N6-C10-N11-C12
22	QV	37	T6A	O10-C10-N11-C12
22	QV	37	T6A	N11-C12-C13-ODA

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	T6A	1	0
22	XV	37	T6A	1	0
22	QV	34	MNU	1	0
56	Z8	76	PPU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1253 ligands modelled in this entry, 1251 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	XD	301	-	0,12,12	-	-	-		
58	SF4	QD	301	4	0,12,12	-	-	-		

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	XD	301	-	-	-	0/6/5/5
58	SF4	QD	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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