



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2020 – 03:01 AM EDT

PDB ID : 6O3M
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-26
Resolution : 3.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

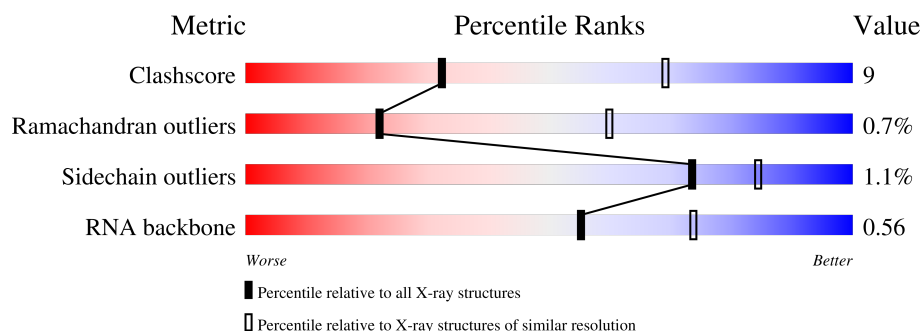
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RNA backbone	3102	1041 (4.84-3.00)













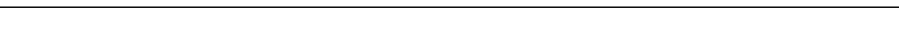

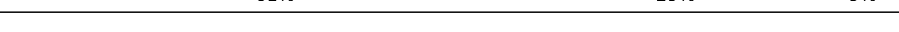

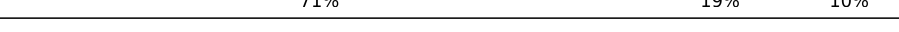








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	XA	1521	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	














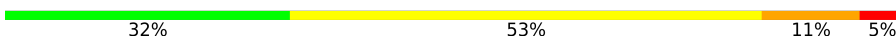











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Mol	Chain	Length	Quality of chain
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN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


























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Mol	Chain	Length	Quality of chain
16	XP	88	
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	XV	77	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	
28	RF	210	
28	YF	210	


























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Mol	Chain	Length	Quality of chain
29	RG	182	 74% 24% ...
29	YG	182	 68% 29% ..
30	RH	180	 69% 26% ..
30	YH	180	 78% 17% ..
31	RI	148	 82% 16% ..
31	YI	148	 85% 12% ..
32	RN	140	 80% 19% .
32	YN	140	 80% 18% ..
33	RO	122	 74% 26%
33	YO	122	 80% 20%
34	RP	150	 70% 30%
34	YP	150	 75% 23% .
35	RQ	141	 73% 26% .
35	YQ	141	 72% 26% .
36	RR	118	 75% 24% ..
36	YR	118	 84% 15% .
37	RS	112	 71% 29% .
37	YS	112	 76% 23% .
38	RT	146	 70% 22% . 6%
38	YT	146	 69% 23% . 6%
39	RU	118	 85% 13% ..
39	YU	118	 81% 17% ..
40	RV	101	 74% 24% .
40	YV	101	 74% 25% .
41	RW	113	 79% 21%



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Mol	Chain	Length	Quality of chain
41	YW	113	 85% 14% .
42	RX	96	 82% 14% .
42	YX	96	 81% 15% .
43	RY	110	 75% 22% .
43	YY	110	 70% 27% .
44	RZ	206	 67% 21% 11%
44	YZ	206	 69% 18% . 11%
45	R0	85	 75% 20% 5%
45	Y0	85	 65% 22% 13%
46	R1	98	 81% 18% .
46	Y1	98	 78% 17% 5%
47	R2	72	 72% 24% .
47	Y2	72	 74% 22% .
48	R3	60	 83% 15% .
48	Y3	60	 73% 20% 5% .
49	R4	71	 72% 25% .
49	Y4	71	 58% 37% . .
50	R5	60	 72% 27% .
50	Y5	60	 75% 22% . .
51	R6	54	 80% 19% .
51	Y6	54	 67% 31% .
52	R7	49	 86% 10% .
52	Y7	49	 82% 16% .
53	R8	65	 68% 28% . .
53	Y8	65	 72% 23% . .

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Mol	Chain	Length	Quality of chain
54	R9	37	 70%30%
54	Y9	37	 84%16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291782 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	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

- 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	125	Total	C	N	O		0	0	0
			989	627	191	171				
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 ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	733	295	542	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	733	295	542	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			
23	XX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
24	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	74	Total	C	N	O	S	0	0	0
			593	367	126	99	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

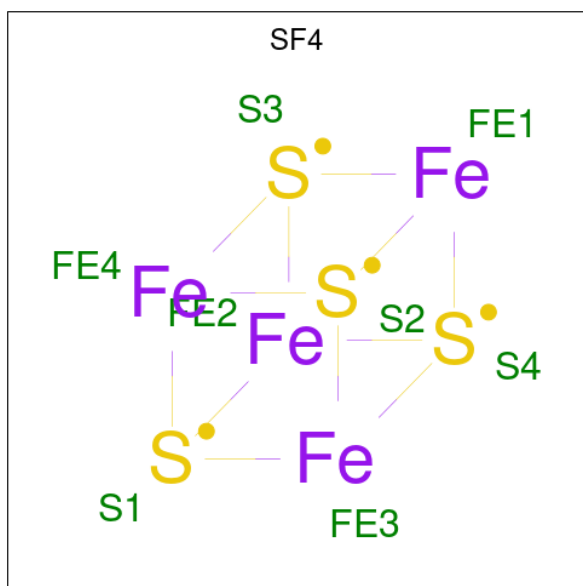
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	69	Total	Mg	0	0
			69	69		
55	YA	454	Total	Mg	0	0
			454	454		
55	Y5	1	Total	Mg	0	0
			1	1		
55	YR	2	Total	Mg	0	0
			2	2		
55	XE	1	Total	Mg	0	0
			1	1		
55	YD	2	Total	Mg	0	0
			2	2		
55	QV	1	Total	Mg	0	0
			1	1		
55	XA	67	Total	Mg	0	0
			67	67		
55	RQ	1	Total	Mg	0	0
			1	1		
55	Y0	1	Total	Mg	0	0
			1	1		
55	YQ	2	Total	Mg	0	0
			2	2		
55	RD	1	Total	Mg	0	0
			1	1		
55	R1	1	Total	Mg	0	0
			1	1		
55	Y7	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QH	1	Total 1	Mg 1	0	0
55	RA	381	Total 381	Mg 381	0	0
55	YP	1	Total 1	Mg 1	0	0
55	RE	1	Total 1	Mg 1	0	0
55	YB	8	Total 8	Mg 8	0	0
55	RB	9	Total 9	Mg 9	0	0
55	QE	1	Total 1	Mg 1	0	0
55	YE	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

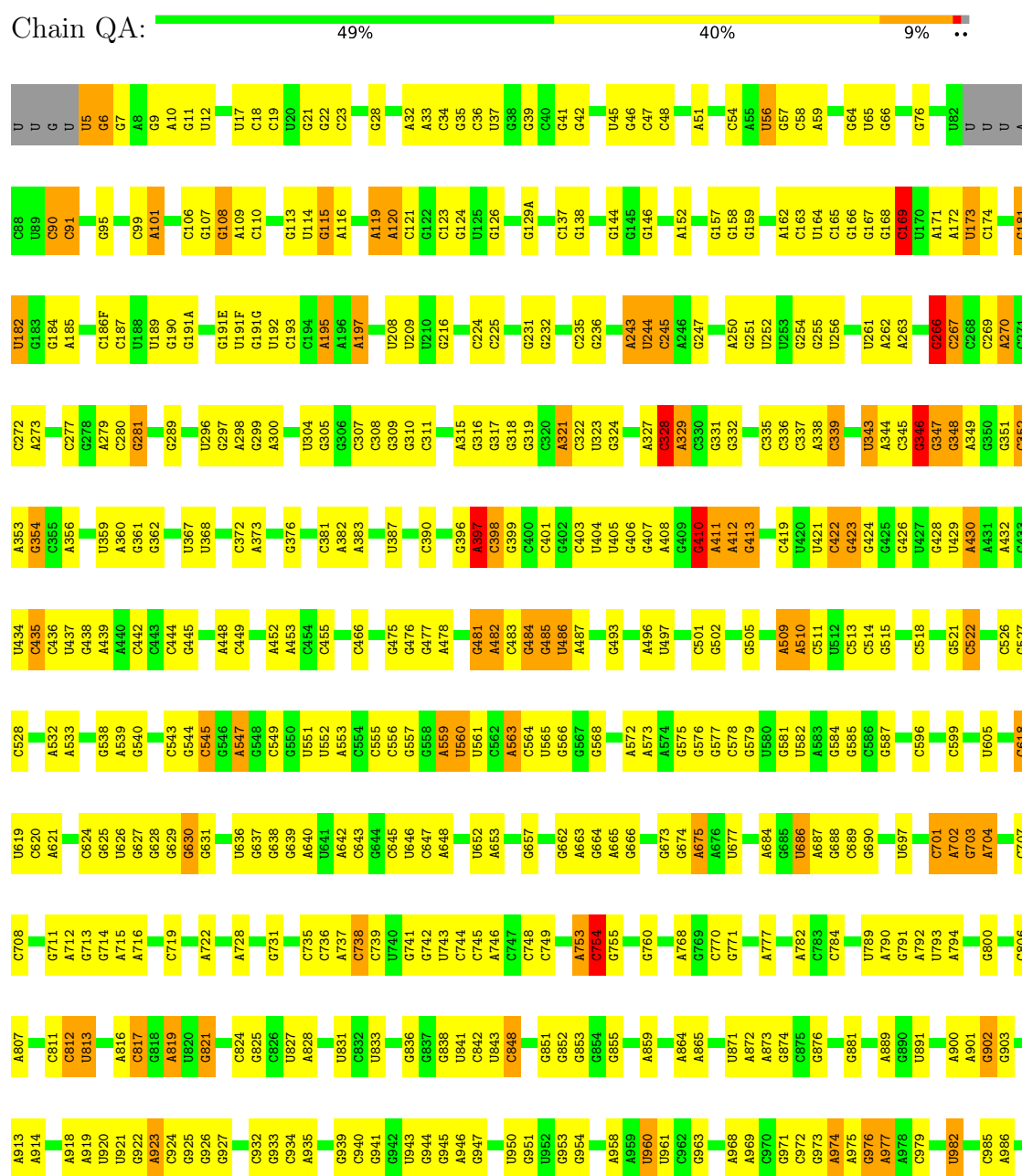
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total 1	Zn 1	0	0
57	YY	1	Total 1	Zn 1	0	0
57	Y6	1	Total 1	Zn 1	0	0
57	QN	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0
57	RY	1	Total 1	Zn 1	0	0
57	Y4	1	Total 1	Zn 1	0	0
57	R6	1	Total 1	Zn 1	0	0
57	Y5	1	Total 1	Zn 1	0	0
57	R5	1	Total 1	Zn 1	0	0
57	R4	1	Total 1	Zn 1	0	0
57	R9	1	Total 1	Zn 1	0	0

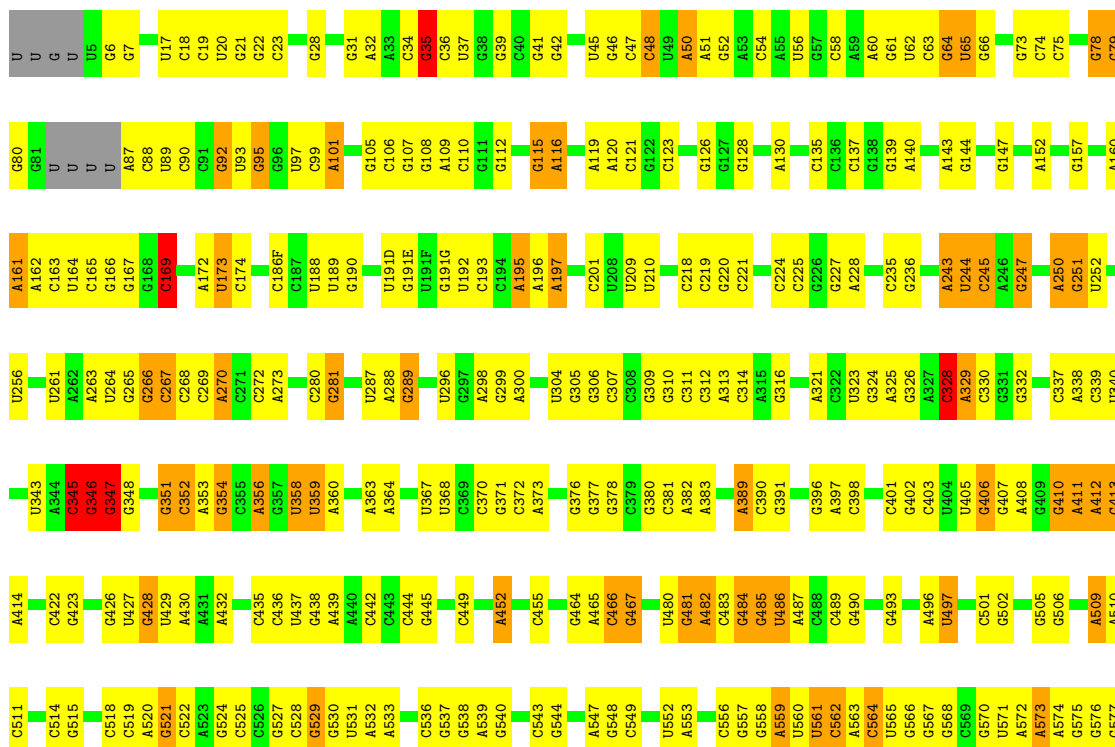
3 Residue-property plots

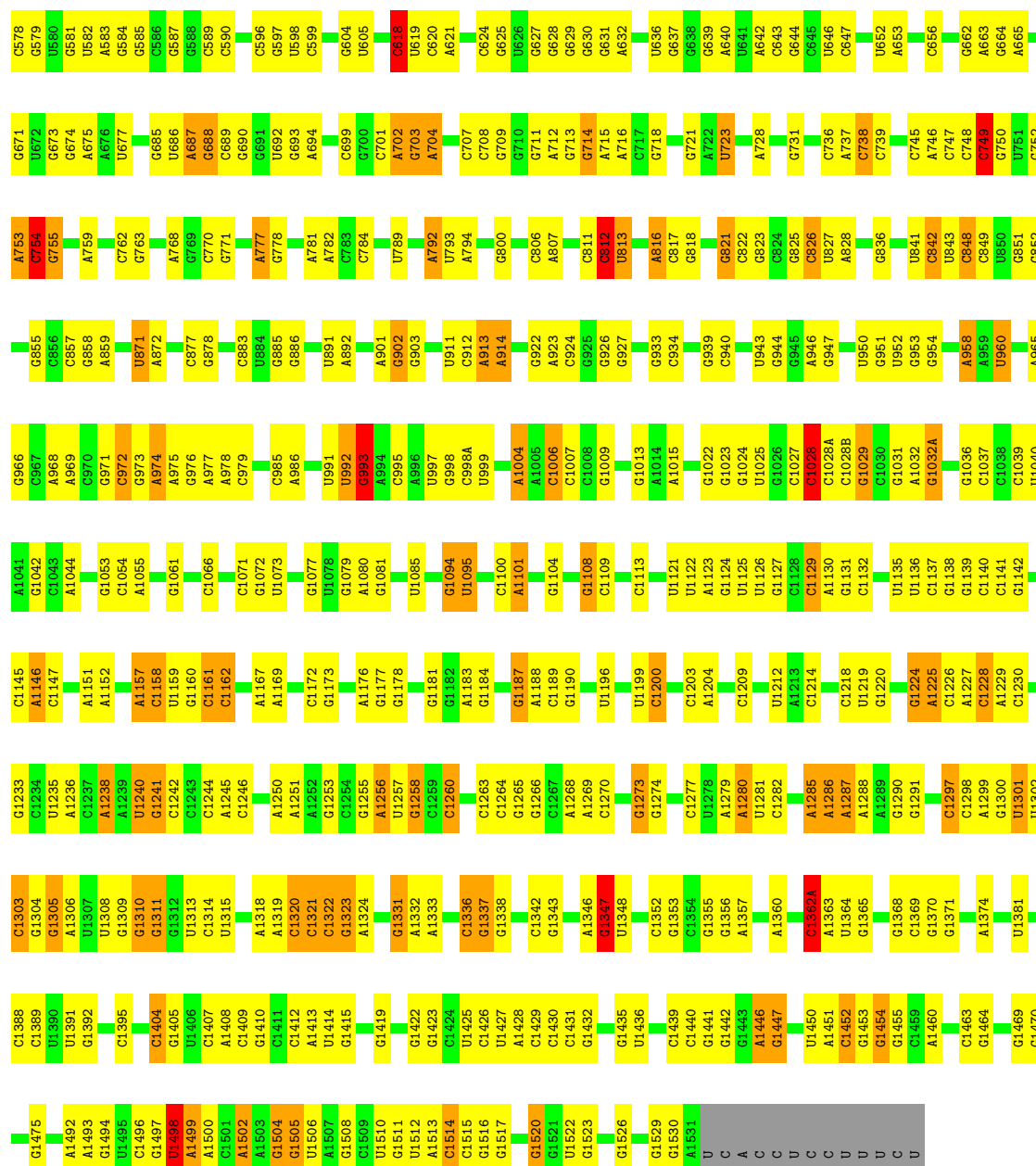
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

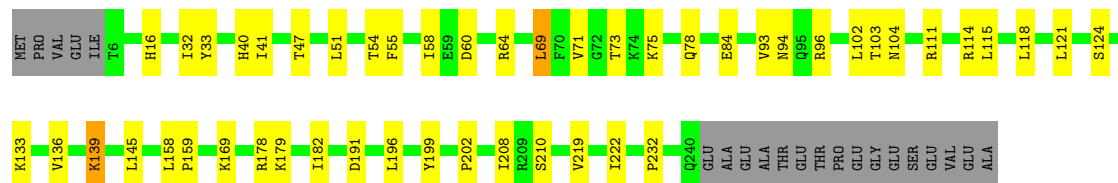






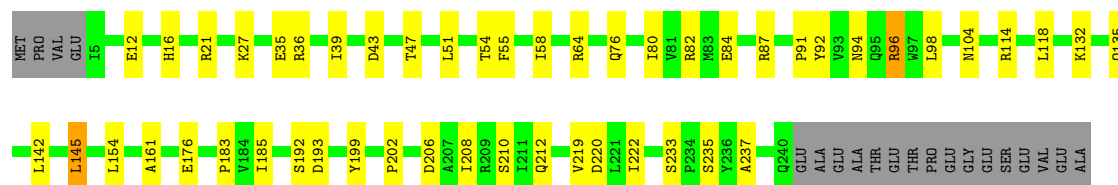
• Molecule 2: 30S ribosomal protein S2

Chain QB: 73% 18% 8%



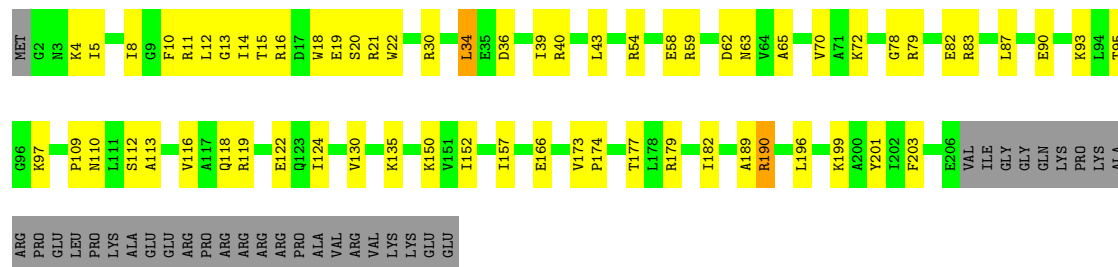
• Molecule 2: 30S ribosomal protein S2

Chain XB: 73% 19% 8%



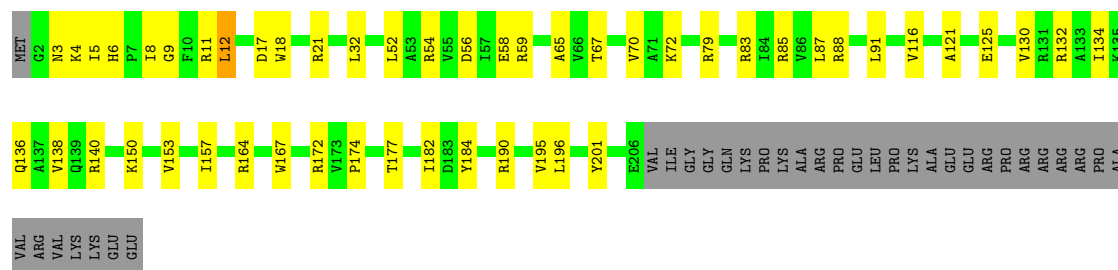
• Molecule 3: 30S ribosomal protein S3

Chain QC: 59% 26% 14%



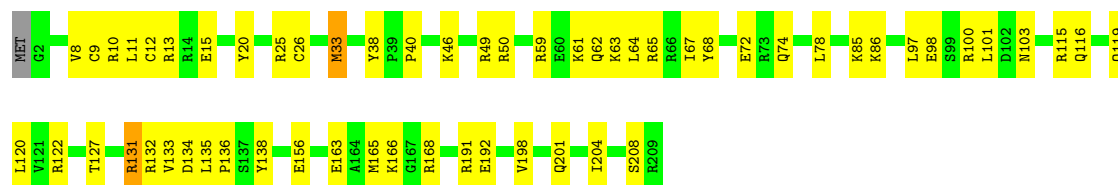
• Molecule 3: 30S ribosomal protein S3

Chain XC: 65% 21% 14%



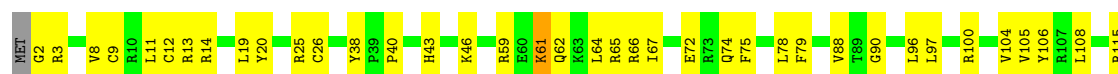
• Molecule 4: 30S ribosomal protein S4

Chain QD: 72% 27% 1%



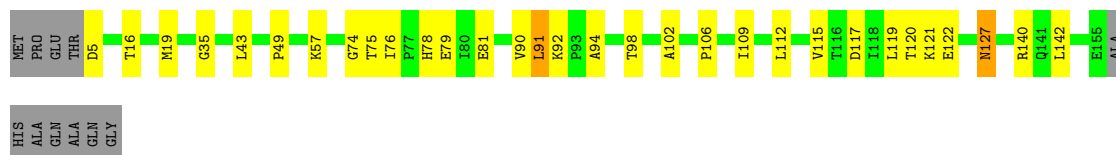
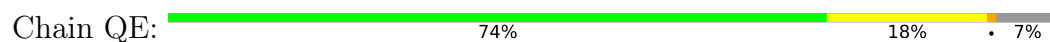
• Molecule 4: 30S ribosomal protein S4

Chain XD: 67% 30% 3%





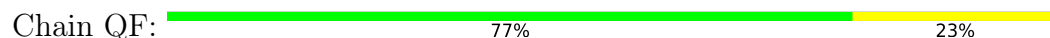
- Molecule 5: 30S ribosomal protein S5



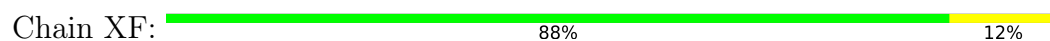
- Molecule 5: 30S ribosomal protein S5



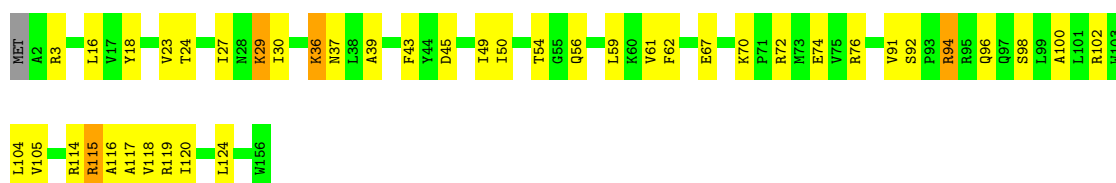
- Molecule 6: 30S ribosomal protein S6




- Molecule 6: 30S ribosomal protein S6

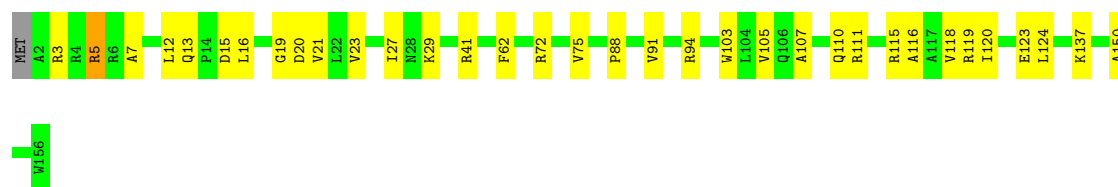


- Molecule 7: 30S ribosomal protein S7



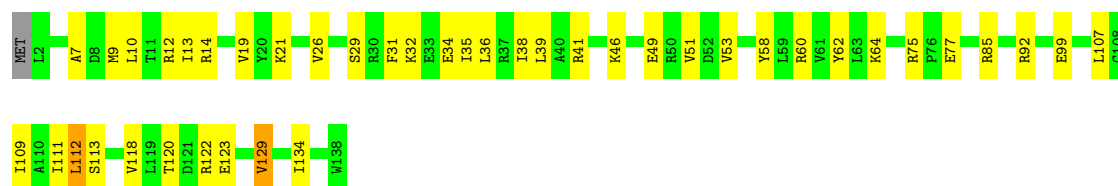
- Molecule 7: 30S ribosomal protein S7

Chain XG:  78% 21% ..



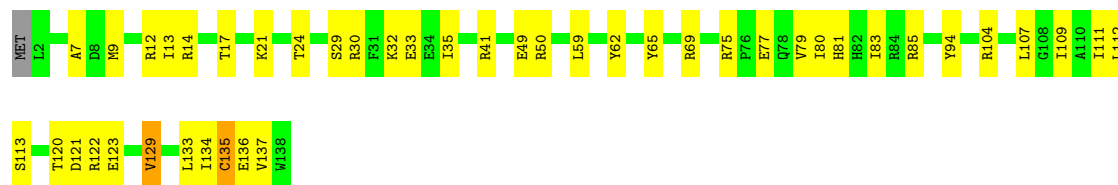
- Molecule 8: 30S ribosomal protein S8

Chain QH:  69% 29% ..



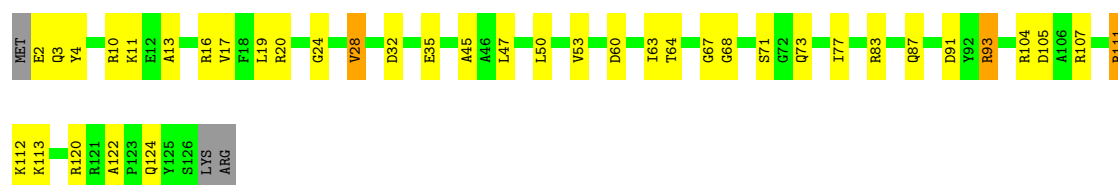
- Molecule 8: 30S ribosomal protein S8

Chain XH:  67% 30% ..



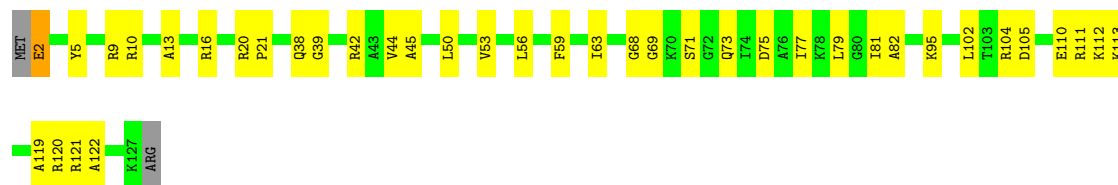
- Molecule 9: 30S ribosomal protein S9

Chain QI:  67% 28% ..



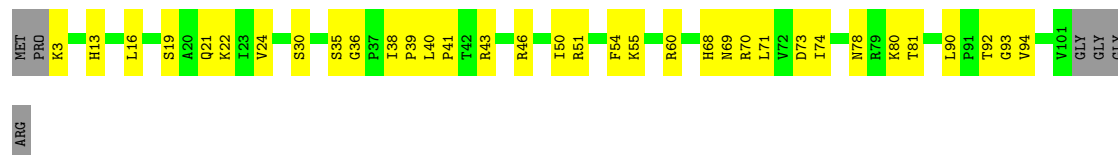
- Molecule 9: 30S ribosomal protein S9

Chain XI:  68% 30% ..



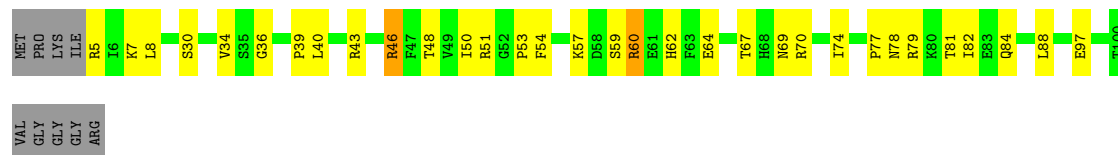
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 



- Molecule 10: 30S ribosomal protein S10

Chain XJ: 



- Molecule 11: 30S ribosomal protein S11

Chain QK: 



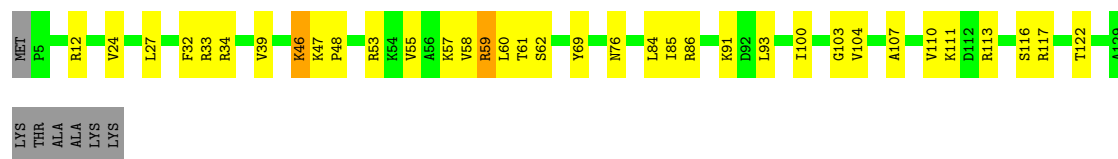
- Molecule 11: 30S ribosomal protein S11

Chain XK: 



- Molecule 12: 30S ribosomal protein S12

Chain QL: 



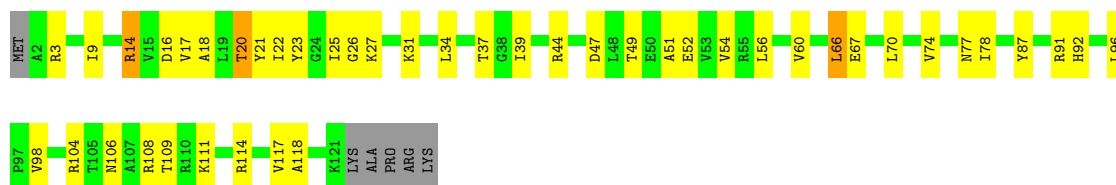
- Molecule 12: 30S ribosomal protein S12

Chain XL: 



- Molecule 13: 30S ribosomal protein S13

Chain QM:  60% 33% 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  67% 25% 6%



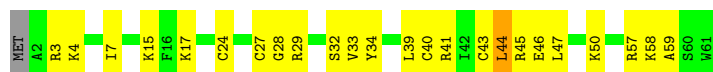
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  70% 25% 2%




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  59% 38% 2%




- Molecule 15: 30S ribosomal protein S15

Chain QO:  75% 24% 1%




- Molecule 15: 30S ribosomal protein S15

Chain XO:  80% 18% 2%




- Molecule 16: 30S ribosomal protein S16

Chain QP:  78% 17% 5%




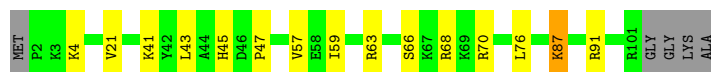
- Molecule 16: 30S ribosomal protein S16

Chain XP:  84% 11% 5%




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  81% 13% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  74% 20% 5%



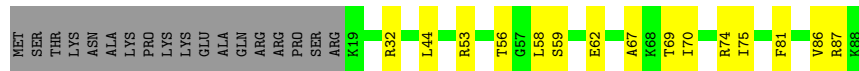
- Molecule 18: 30S ribosomal protein S18

Chain QR:  63% 17% 20%



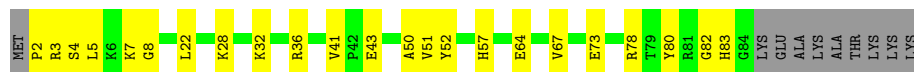
- Molecule 18: 30S ribosomal protein S18

Chain XR:  63% 17% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  65% 25% 11%




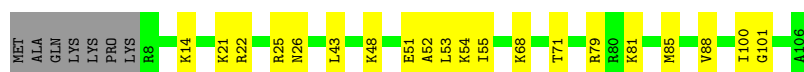
- Molecule 19: 30S ribosomal protein S19

Chain XS:  73% 17% 10%



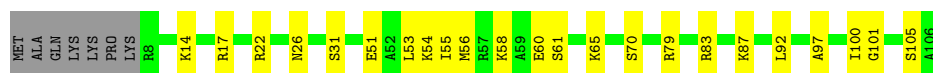
- Molecule 20: 30S ribosomal protein S20

Chain QT:  75% 19% 7%




- Molecule 20: 30S ribosomal protein S20

Chain XT:  72% 22% 7%



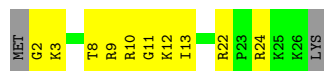
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  74% 19% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain XU:  56% 37% 7%



- Molecule 22: P-site ASLPro

Chain QV:  52% 35% 13%



- Molecule 22: P-site ASLPro

Chain XV:  58% 26% 16%



- Molecule 23: mRNA

Chain QX:  32% 53% 11% 5%



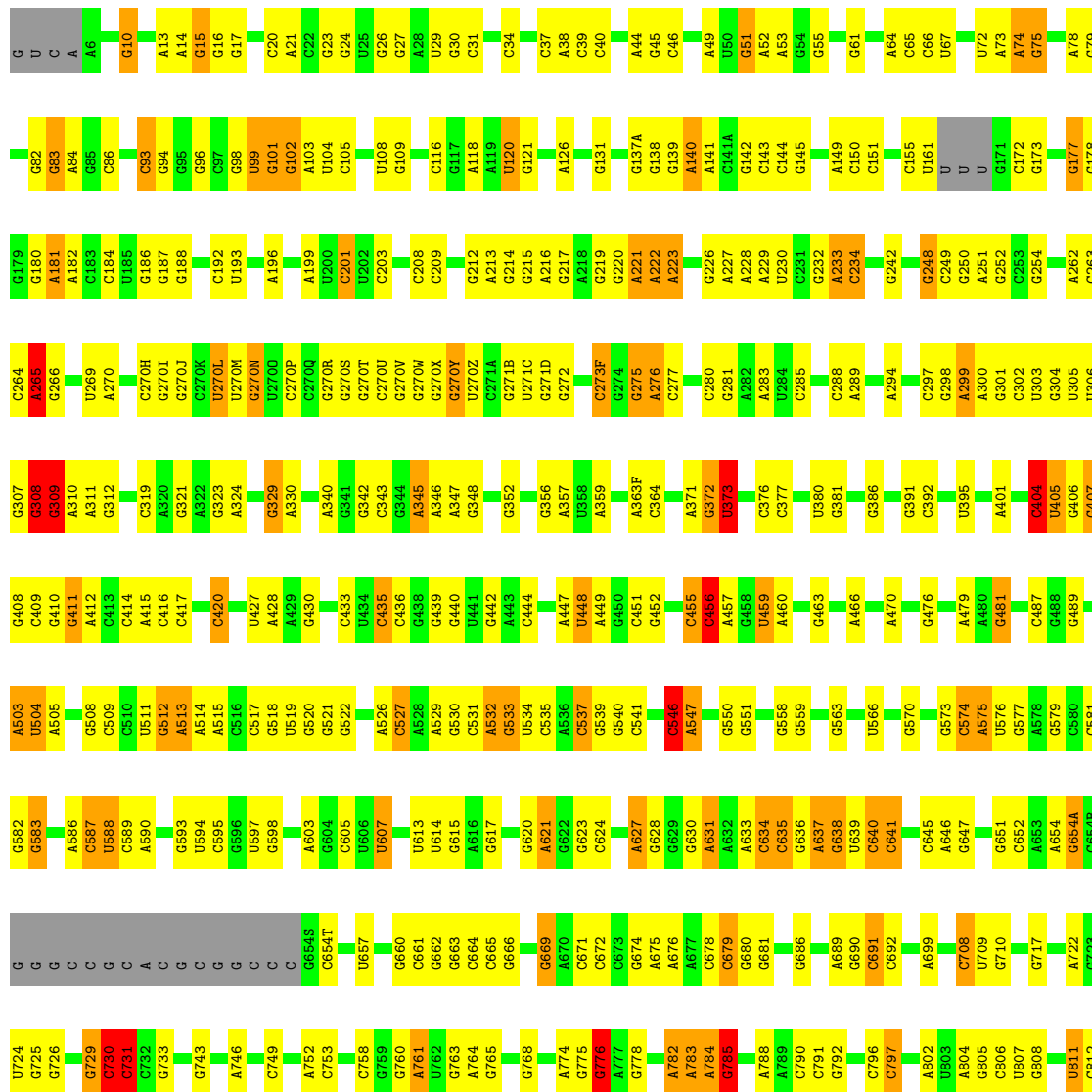
• Molecule 23: mRNA

Chain XX:  37% 58% 5%



• Molecule 24: 23S rRNA

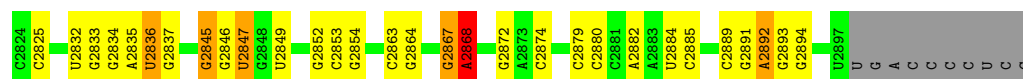
Chain RA:  49% 39% 10% ..



A2019	A1923	G1822	A1732	G1539	C1467	U1391	C1297	U1211	A1054	G975	C977	C815
A2020	C1924	G1823	G1733	G1540	C1468	A1392	C1298	G1212	A1055	C976	C976	C816
C2021	A1927	G1824	C1742	U1541	A1469	A1393	G1299	G1216	G1056	A980	A899	C817
U2022	A1928	G1825	G1743	G1542	G1470	A1394	U1300	G1217	A1057	A981	A900	C818
G2023	G1929	G1826	G1744	A1543	A1471	A1395	A1301	A1220	G1058	A982	C902	G819
C2025	G1930	C1827	G1745	C1544	A1472	A1396	A1302	C1221	G1059	A983	C903	A819
C2026	U1931	G1830	G1750	A1545	G1473	U1397	G1309	A1222	U1060	G987	C904	U822
A2030	A1938	G1831	C1751	A1546	C1474	C1398	G1310	G1224	U1061	A988	G905	G823
G2032	G1939	C1832	C1752	C1547	G1475	C1399	G1311	C1225	G1062	G989	G906	A824
A2033	U1940	G1833	G1753	C1548	G1476	G1400	G1312	G1226	G1063	G990	U907	
A2034	C1941	U1834	A1755	C1549	G1477	C1401	U1313	A1227	C1064	G991		
G2035	G1942	G1835	G1756	C1550	G1478	C1402	C1314		U1065	G992		U827
U2036	C1947	C1836	U1757	C1551	U1482	C1403	C1315		U1066	C993		U828
G2037	U1948	G1837	G1758	G1552	G1483	C1404	C1316	C1230	U1067	C994		U829
G2038	U1949	C1838			G1484	U1405	A1317	G1231	A1070	C995		G830
G2039	U1950	U1841	A1762	C1557	G1485	C1406	U1318	G1232	A1071	C996		G831
G2040	U1951	G1842	G1763	G1558	G1486	C1407	G1319	G1233	C1072	C997		G832
G2041	A1952	G1843	G1764	G1559	G1487	A1408	A1321	G1235	A1073	C998		G833
G2042	U1953	C1844			G1488	C1409	U1326	G1236	C1074	C999		U834
G2043	U1954	U1845			G1489	G1410	U1327	A1237	G1075	A1000		C835
G2044	U1955	A1846	C1771	G1561	A1490	C1411	U1328	G1238	A1076	A1001		A836
G2045	U1956	A1847	G1772	G1562	C1493	G1412	U1329	A1246	U1077	A1002		U839
G2046	U1957	G1848	G1773	G1563	C1494	G1413	G1332	A1247	U1078	G1002		C840
G2047	U1958	U1849	A1774	A1564	A1495	G1414	A1333	A1248	C1080	G1003		A841
G2048	U1959	G1850	U1775	A1565	A1496	G1415	G1334	A1253	U1081	C1004		C846
A2051	U1960	G1851			A1497	A1416	G1335	A1254	U1082	C1005		U847
G2052	U1961	A1852			G1498	A1417	U1336	U1255	U1083	C1006		G848
G2053	U1962	G1853	A1780	G1566	U1499	A1418	G1337	G1256	A1084	A1009		A849
G2054	U1963	C1854	C1781	G1567	C1499	A1419	U1338	G1257	A1085	G1011		
G2055	U1964	U1855	G1782	G1568	G1499	G1420	G1339	C1258	A1086	U1012		C856
G2056	U1965	G1856	U1783	G1569	G1499	A1421	U1340	G1259	G1087	C1013		C857
G2057	U1966	C1857	A1784	A1571	C1501	G1422	U1341	G1260	A1088	U1019		U858
G2058	U1967	U1858		A1572	G1502	G1423	A1342	G1261	C1091	A941		U859
G2059	U1968	G1859			U1503	A1424	A1343	G1262	C1092	U922		U860
G2060	U1969	C1860	G1792	U1576	C1504	G1425	A1344	U1263	G1093	C923		A861
G2061	U1970	G1861	C1793	U1577	C1505	G1426	A1345	U1264	A1094	C924		C862
G2062	U1971	A1862	G1794	U1578	C1506	A1427	G1346	G1265	A1095	C925		U863
G2063	U1972	G1863	U1795	A1579	C1507	A1428	U1347	A1266	U1097	G945		G864
G2064	U1973	C1864	G1796	A1580	A1507	G1429	G1348	U1267	G1106	G946		A865
G2065	U1974	U1865	U1797	G1581	A1508	A1430	U1349	U1268	G1107	G947		C866
G2066	U1975	G1866	C1798	G1582	C1509	U1431	G1350	C1270	G1108	U1026		C867
G2067	U1976	C1867	G1799	U1583	A1510	A1432	U1351	C1271	U1109	A1027		U868
G2068	U1977	U1868	U1799	G1584	C1511	G1433	G1352	G1272	C1110	G1030		G869
G2069	U1978	G1869	C1800	A1586	U1514	U1434	A1363	A1273	G1111	U1033		A872
G2070	U1979	A1870	G1801	U1590	G1519	A1444	G1364	U1274	A1112	U1034		G873
G2071	U1980	G1871	A1802	G1591	U1520	A1445	A1365	A1275	A1113	G1035		G874
G2072	U1981	C1872	A1803	C1592	G1521	G1446	U1366	A1276	U1114	G1036		C875
G2073	U1982	G1873	C1804	G1593	G1522	A1447	A1367	U1277	G1115	G1042		G876
G2074	U1983	U1874	A1805	G1594	G1523	G1448	G1368	G1278	G1116	C1043		C877
G2075	U1984	C1875	A1806	G1595	G1524	G1449	U1369	G1279	G1117	C1044		C878
C2081	G2004	G1906	G1811	C1596	G1525	U1454	U1370	A1286	G1118	G1045		A877
A2082	A2005	C1907	A1812	C1597	G1526	G1455	U1371	U1287	G1119	A1046		C879
C2083	C2007	C1908	G1813	C1598	G1527	G1456	U1372	A1288	C970	U969		C880
U2086	G2008	A1913	G1814	C1599	A1528	C1457	A1378	C1289	C971	U969		C881
G2087	G2009	U1914	A1815	G1600	G1529	G1458	A1379	C1290	G972	C972		C882
G2088	G2010	U1915	G1816	G1601	C1533	G1459	G1380	G1291	G973	C1049		C883
G2089	U2011	G1916	G1817	G1602	G1534	A1460	U1381	U1292	C1120	A1050		C884
G2090	G2012	U1917	U1818	U1603	U1535	G1461	G1382	C1293	G1121	C1051		C885
U2096	U2013	G1918	A1819	A1604	A1536	C1462	G1383	U1294	C1122	G1052		C886
G2097	G2014	U1919	U1820	A1605	A1537	C1463	G1384	C1295	C1123	C1053		A896
			A1821	C1611	G1538	C1464	U1390	G1296	G1125			

G1375	U1454	C1376	U1292	A1210	U1130	G1056	U963	C884	C814	C731	G	G600	G520	U427	G326
C1376	U1455	G1377	C1293	U1211	G1131	A1057	C964	C885	C815	C731	G	G600	G521	U428	G327
A1378	G1455	G1378	U1294	U1212	C1135	G1058	U969	C886	C816	U740	G	A603	G522	A429	U328
A1379	G1459	C1297	C1298	C1221	G1136	U1060	C970	A887	C817	G741	C	G604	C523	G430	G329
A1384	A1460	G1298	G1299	G1224	G1137	U1061	C971	C888	G818	G742	C	U607	U524	U431	A330
G1385	C1461	U1300	G1299	G1225	G1138	G1062	G972	C889	G819	G743	G654S	A608	U525	A432	A331
C1463	C1462	A1301	G1300	G1226	G1139	G1063	A973	C890	A820		C654T	A609	A526	C433	A332
C1464	C1464	C1306	U1302	G1226	U1141	U1066	G974	C893	A821	A746	C658	A608	C527	C434	
C1467	C1467	G1309	G1310	G1230	U1142	U1066	G975	A896	U822		C659	A609	A529	C435	G338
A1471	A1471	G1309	G1310	G1231	A1142A	G1067	C976	A900	G823		C660	A610	G530	C436	U339
C1474	C1474	G1313	G1314	U1234	A1143	A1068	A980	U907	U827	A752	C661	U614	C531	C439	A340
G1478	G1478	U1313	C1314	G1235	G1150	A1070	A983	U907	U828	C753	G662	U614	A532	C440	G352
U1482	U1482	C1315	U1316	G1236	G1151	G1071	A983	U907	U829	C754	G663	U614	A533	C441	U358
G1483	G1483	G1325	G1325	G1237	G1155	C1072	A987	U907	U830	C755	G664	U614	A534	C442	A359
G1487	G1487	U1329	U1330	G1238	A1155	G1074	G997	A910	C834	U757	G665	U614	A535	C443	
A1490	A1490	U1341	U1342	G1245	A1156	C1075	G993	A911	C835	U758	U667	A621	A536	C444	G363
G1491	G1491	G1342	G1343	A1247	A1157	C1076	C994	A912	C836	U759	G668	A621	A537	C445	A363A
G1492	G1492	C1344	C1345	G1248	C1158	C1077	C995	A913	C837	A761	G669	A621	A538	C446	G363B
G1493	G1493	U1346	U1347	U1249	C1159	A1078	A996	A914	C838	A762	G670	A621	A539	C447	G363C
A1494	A1494	G1347	G1348	G1250	U1159	C1079	A997	A915	C839	A763	G671	A621	A540	C448	G363D
A1495	A1495	U1348	U1349	G1251	C1160	C1080	A1000	A916	C840	U764	G672	A621	A541	C449	U363E
U1496	U1496	G1349	G1350	G1252	G1161	C1081	A1001	A917	C841	U765	A675	A621	A542	C450	A363F
U1497	U1497	U1351	U1352	G1253	A1162	U1081	A1001	A918	C842	U766	A676	A621	A543	C451	C364
C1498	C1498	G1353	G1354	A1249	G1163	U1082	C1005	A919	C843	U767	C679	A621	A544	C452	A371
C1499	C1499	U1355	U1356	G1254	C1164	U1083	C1006	A920	C844	U768	C679	A621	A545	C453	U373
G1500	G1500	G1357	G1358	G1255	U1165	C1084	C1006	C925	C845	U769	C680	A621	A546	C454	U373
C1504	C1504	U1359	U1360	G1256	A1166	A1085	C1006	C926	C846	U770	C681	A621	A547	C455	
C1505	C1505	G1361	G1362	G1257	G1167	C1086	A1009	C927	C847	U771	C682	A621	A548	C456	U380
C1506	C1506	U1363	U1364	G1258	U1168	C1087	A1010	C928	C848	U772	C683	A621	A549	C457	G381
A1507	A1507	G1365	G1366	G1259	G1169	U1088	A1011	C929	C849	U773	C684	A621	A550	C458	U382
C1508	C1508	U1367	U1368	G1260	G1170	C1089	A1012	C930	C850	U774	C685	A621	A551	C459	U383
C1509	C1509	G1369	G1370	G1261	U1171	U1090	C1013	C931	C851	U775	C686	A621	A552	C460	G384
A1510	A1510	U1371	U1372	G1262	C1172	U1091	C1013	C932	C852	U776	C687	A621	A553	C461	U385
G1512	G1512	G1373	G1374	G1263	U1173	U1092	C1013	C933	C853	U777	C688	A621	A554	C462	U386
C1513	C1513	U1375	U1376	G1264	G1174	U1093	C1013	C934	C854	U778	C689	A621	A555	C463	G387
C1515	C1515	G1377	G1378	G1265	U1175	U1094	C1013	C935	C855	U779	C690	A621	A556	C464	U388
U1516	U1516	U1379	U1380	G1266	G1176	U1095	C1013	C936	C856	U780	C691	A621	A557	C465	U389
G1517	G1517	G1381	G1382	G1267	U1177	U1096	C1013	C937	C857	U781	C692	A621	A558	C466	U390
U1520	U1520	U1383	U1384	G1268	C1178	U1097	C1013	C938	C858	U782	C693	A621	A559	C467	U391
G1521	G1521	G1385	G1386	G1269	U1179	U1098	C1013	C939	C859	U783	C694	A621	A560	C468	U392
G1522	G1522	U1387	U1388	G1270	G1180	U1099	C1013	C940	C860	U784	C695	A621	A561	C469	U393
G1526	G1526	G1389	G1390	G1271	U1181	U1100	C1013	C941	C861	U785	C696	A621	A562	C470	U394
G1527	G1527	U1391	U1392	G1272	G1182	U1101	C1013	C942	C862	U786	C697	A621	A563	C471	U395
A1528	A1528	G1393	G1394	G1273	U1183	U1102	C1013	C943	C863	U787	C698	A621	A564	C472	U396
U1529	U1529	C1370	C1371	G1274	G1184	U1103	C1013	C944	C864	U788	C699	A621	A565	C473	U397
G1530	G1530	U1372	U1373	G1275	U1185	U1104	C1013	C945	C865	U789	C700	A621	A566	C474	U398
		G1444	G1445	G1276	G1186	U1105	C1013	C946	C866	U790	C701	A621	A567	C475	U399
		C1445	C1446	G1277	G1187	U1106	C1013	C947	C867	U791	C702	A621	A568	C476	U400
		A1449	A1450	G1278	G1188	U1107	C1013	C948	C868	U792	C703	A621	A569	C477	U401
		G1449A	G1449A	G1279	U1189	U1108	C1013	C949	C869	U793	C704	A621	A570	C478	U402
				G1280	G1190	U1109	C1013	C950	C870	U794	C705	A621	A571	C479	U403
				G1281	U1191	U1110	C1013	C951	C871	U795	C706	A621	A572	C480	U404
				G1282	G1192	U1111	C1013	C952	C872	U796	C707	A621	A573	C481	U405
				G1283	U1193	U1112	C1013	C953	C873	U797	C708	A621	A574	C482	U406
				G1284	G1194	U1113	C1013	C954	C874	U798	C709	A621	A575	C483	U407
				G1285	U1195	U1114	C1013	C955	C875	U799	C710	A621	A576	C484	U408
				G1286	G1196	U1115	C1013	C956	C876	U800	C711	A621	A577	C485	U409
				G1287	U1197	U1116	C1013	C957	C877	U801	C712	A621	A578	C486	U410
				G1288	G1198	U1117	C1013	C958	C878	U802	C713	A621	A579	C487	U411
				G1289	U1199	U1118	C1013	C959	C879	U803	C714	A621	A580	C488	U412
				G1290	G1200	U1119	C1013	C960	C880	U804	C715	A621	A581	C489	U413
				G1291	G1201	U1120	C1013	C961	C881	U805	C716	A621	A582	C490	U414
				G1292	G1202	U1121	C1013	C962	C882	U806	C717	A621	A583	C491	U415
				G1293	G1203	U1122	C1013	C963	C883	U807	C718	A621	A584	C492	U416
				G1294	G1204	U1123	C1013	C964	C884	U808	C719	A621	A585	C493	U417
				G1295	G1205	U1124	C1013	C965	C885	U809	C720	A621	A586	C494	U418
				G1296	U1206	U1125	C1013	C966	C886	U810	C721	A621	A587	C495	U419
				G1297	G1207	U1126	C1013	C967	C887	U811	C722	A621	A588	C496	U420
				G1298	U1208	U1127	C1013	C968	C888	U812	C723	A621	A589	C497	U421
				G1299	G1209	U1128	C1013	C969	C889	U813	C724	A621	A590	C498	U422
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				G1301	G1211	U1130	C1013	C971	C891	U815	C726	A621	A592	C500	U424
				G1302	U1212	U1131	C1013	C972	C892	U816	C727	A621	A593	C501	U425
				G1303	G1213	U1132	C1013	C973	C893	U817	C728	A621	A594	C502	U426
				G1304	U1214	U1133	C1013	C974	C894	U818	C729	A621	A595	C503	U427
				G1305	G1215	U1134	C1013	C975	C895	U819	C730	A621	A596	C504	U428
				G1306	U1216	U1135	C1013	C976	C896	U820	C731	A621	A597	C505	U429
				G1307	G1217	U1136	C1013	C977	C897	U821	C732	A621	A598	C506	U430
				G1308	U1218	U1137	C1013	C978	C898	U822	C733	A621	A599	C507	U431
				G1309	G1219	U1138	C1013	C979	C899	U823	C734	A621	A600	C508	U432
				G1310	U1220	U1139	C1013	C980	C900	U824	C735	A621	A601	C509	U433
				G1311	G1221	U1140	C1013	C981	A900	U825	C736	A621	A602	C510	U434
				G1312	U1222	U1141	C1013	C982	U907	U826	C737	A621	A603	C511	U435
				G1313	G1223	U1142	C1013	C983	U907	U827	C738	A621	A604	C512	U436
				G1314	U1224	U1143	C1013	C984	U907	U828	C739	A621	A605	C513	U437
				G1315	G1225	U1144	C1013	C985	U907	U829	C740	A621	A606	C514	U438
				G1316	U1226	U1145	C1013	C986	U907	U830	C741	A621	A607	C515	U439
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				G1318	U1228	U1147	C1013	C988	U907	U832	C743	A621	A609	C517	U441
				G1319	G1229	U1148	C1013	C989	U907	U833	C744	A621	A610	C518	U442
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				G1321	G1231	U1150	C1013	C991	U907	U835	C746	A6			

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C2798	G2727	A2654	C2374	A2469	C2374	U2296	G2192	G2120	U2041	U1955	G1858	U1779	A1669	C1588
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G2816	G2745	C2674	C2395	G2482	C2395	G2316	G2224	C2136	G2062	A1972	C1884	C1795	C1684	C1605
G2817	G2746	G2675	G2396	G2483	G2396	G2317	A2225	C2137	A2063	C1979	G1885	U1796	G1685	G1606
G2818	G2747	C2676	G2397	G2484	G2397	C2138	G2228	C2138	C2064	C1980	A1889	U1797	C1686	C1607
A2820	A2748	G2677	U2401	G2485	U2401	C2139	G2229	C2139	C2065	U1798	A1890	U1798	C1686	A1608
A2821	G2749	C2678	C2402	G2486	C2402	C2140	G2230	C2140	C2066	A1981	G1891	C1799	C1686	
G2822	A2750	U2583	C2403	G2487	C2403	G2321	G2230	C2140	C2066					
A2823	G2751	U2585	G2494	G2494	G2494	G2323	G2230	G2141	C2066					



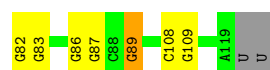
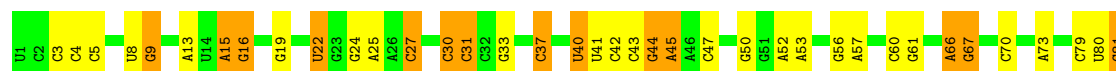
• Molecule 25: 5S rRNA

Chain RB: 60% 27% 10% . .



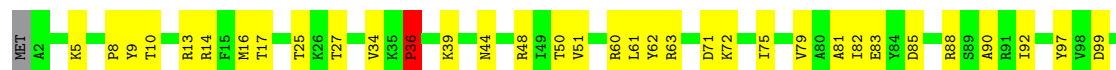
• Molecule 25: 5S rRNA

Chain YB: 61% 25% 12% .



• Molecule 26: 50S ribosomal protein L2

Chain RD: 72% 26% .



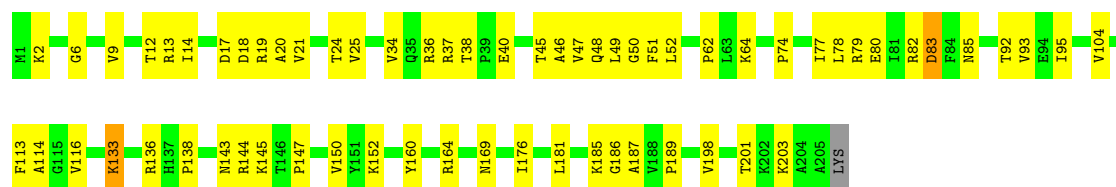
• Molecule 26: 50S ribosomal protein L2

Chain YD: 74% 24% .



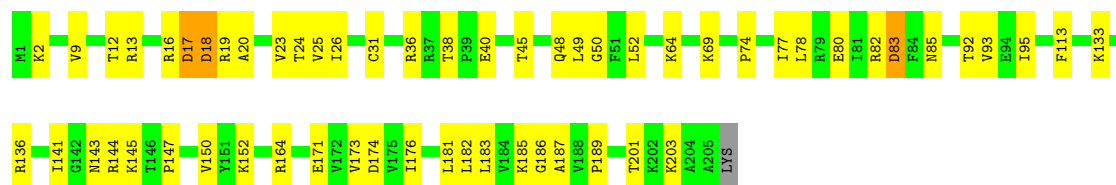
• Molecule 27: 50S ribosomal protein L3

Chain RE:  68% 30% .




- Molecule 27: 50S ribosomal protein L3

Chain YE:  71% 27% .




- Molecule 28: 50S ribosomal protein L4

Chain RF:  81% 15% .




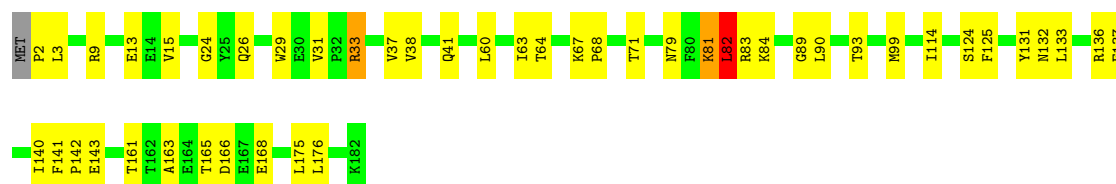
- Molecule 28: 50S ribosomal protein L4

Chain YF:  82% 14% .



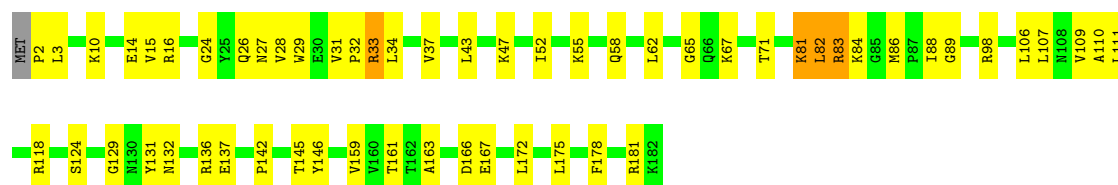
- Molecule 29: 50S ribosomal protein L5

Chain RG:  74% 24% ...



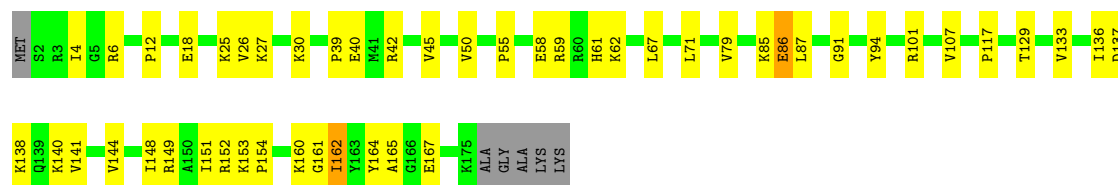
- Molecule 29: 50S ribosomal protein L5

Chain YG:  68% 29% ..




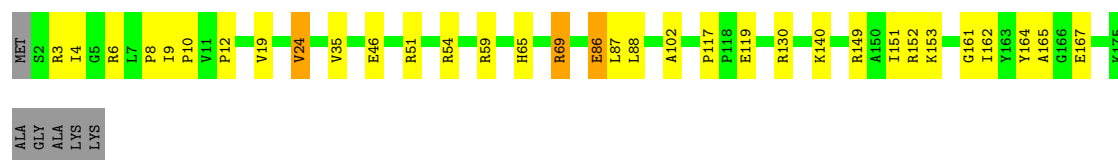
- Molecule 30: 50S ribosomal protein L6

Chain RH:  69% 26% ..




- Molecule 30: 50S ribosomal protein L6

Chain YH:  78% 17% ..




- Molecule 31: 50S ribosomal protein L9

Chain RI:  82% 16% ..




- Molecule 31: 50S ribosomal protein L9

Chain YI:  85% 12% ..




- Molecule 32: 50S ribosomal protein L13

Chain RN:  80% 19% .




- Molecule 32: 50S ribosomal protein L13

Chain YN:  80% 18% ..




- Molecule 33: 50S ribosomal protein L14

Chain RO:  74% 26%



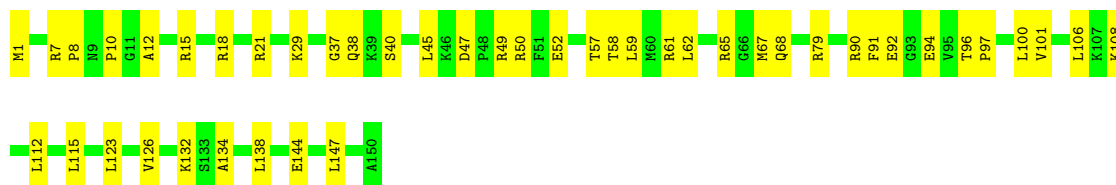
- Molecule 33: 50S ribosomal protein L14

Chain YO:  80% 20%




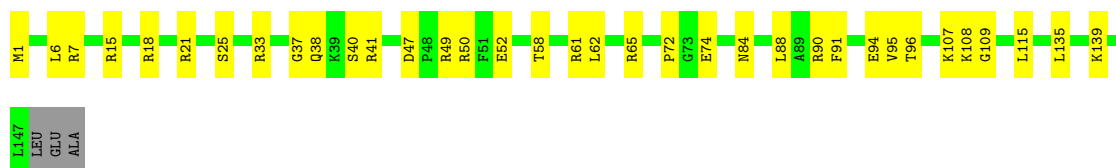
- Molecule 34: 50S ribosomal protein L15

Chain RP:  70% 30%




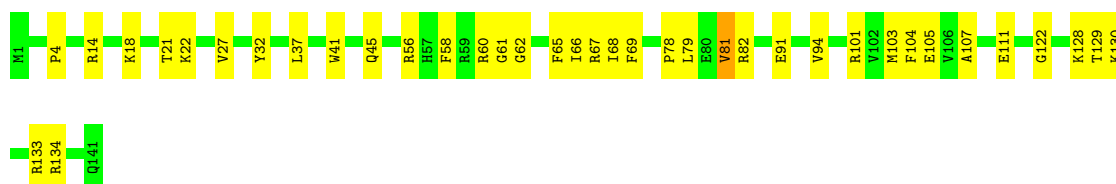
- Molecule 34: 50S ribosomal protein L15

Chain YP:  75% 23% .

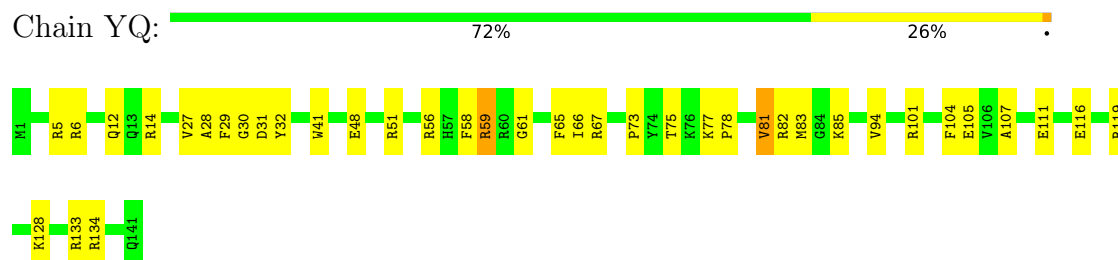


- Molecule 35: 50S ribosomal protein L16

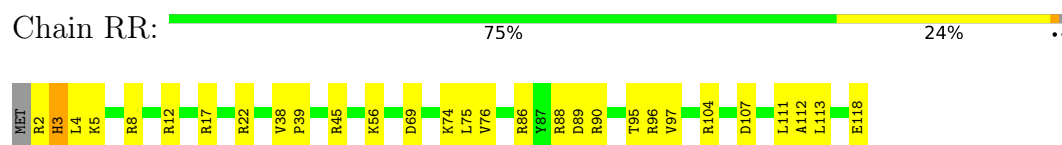
Chain RQ:  73% 26% .



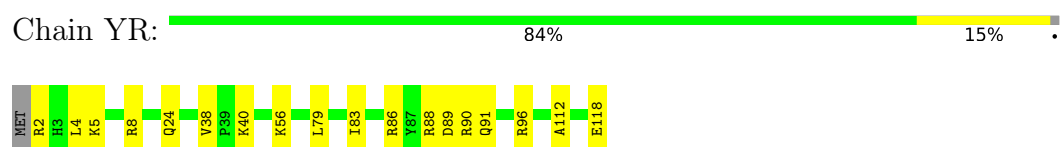
• Molecule 35: 50S ribosomal protein L16



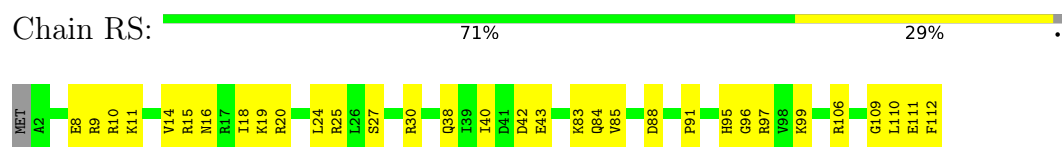
• Molecule 36: 50S ribosomal protein L17



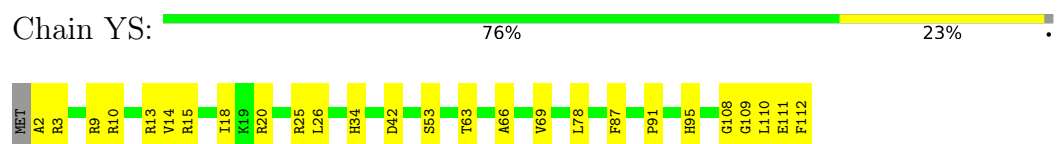
• Molecule 36: 50S ribosomal protein L17



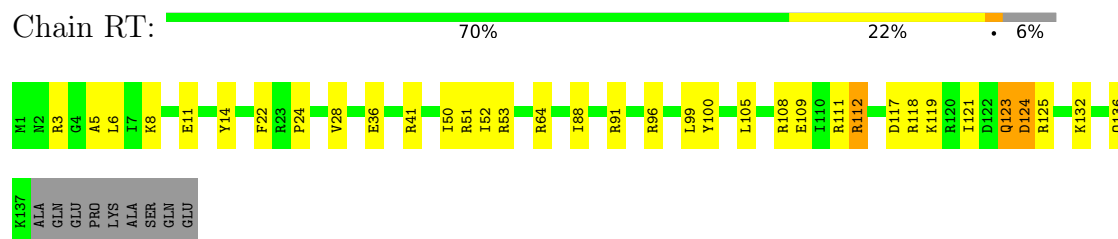
• Molecule 37: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L18

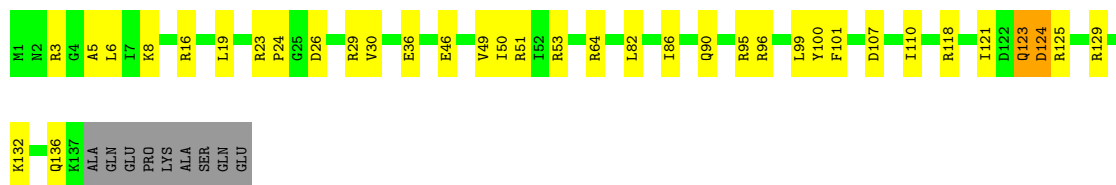


• Molecule 38: 50S ribosomal protein L19




• Molecule 38: 50S ribosomal protein L19

Chain YT:  69% 23% 6%




- Molecule 39: 50S ribosomal protein L20

Chain RU:  85% 13% ..




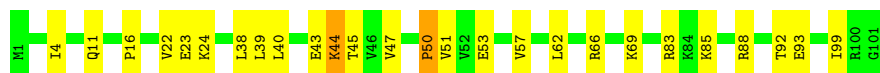
- Molecule 39: 50S ribosomal protein L20

Chain YU:  81% 17% ..




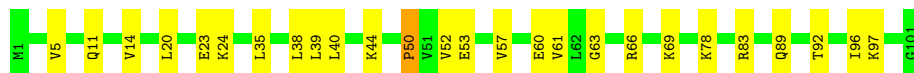
- Molecule 40: 50S ribosomal protein L21

Chain RV:  74% 24% .




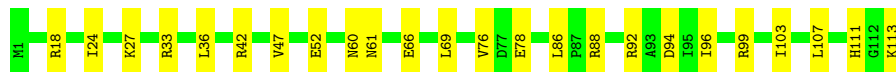
- Molecule 40: 50S ribosomal protein L21

Chain YV:  74% 25% .




- Molecule 41: 50S ribosomal protein L22

Chain RW:  79% 21%




- Molecule 41: 50S ribosomal protein L22

Chain YW:  85% 14% .




- Molecule 42: 50S ribosomal protein L23

Chain RX:  82% 14% .




- Molecule 42: 50S ribosomal protein L23

Chain YX:  81% 15% .



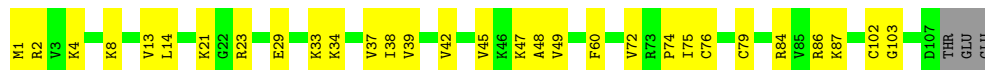
- Molecule 43: 50S ribosomal protein L24

Chain RY:  75% 22% .



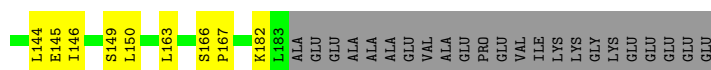
- Molecule 43: 50S ribosomal protein L24

Chain YY:  70% 27% .



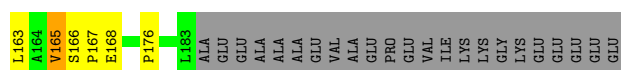
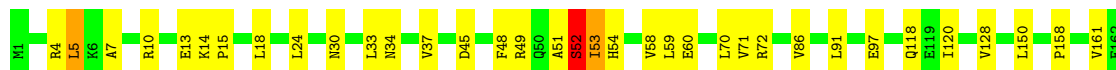
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  67% 21% 11%




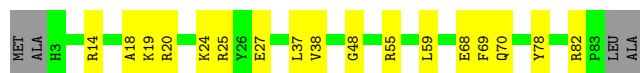
- Molecule 44: 50S ribosomal protein L25

Chain YZ:  69% 18% 11%



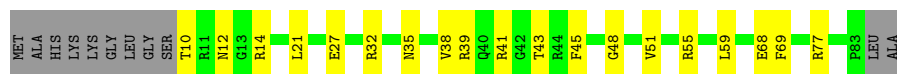
- Molecule 45: 50S ribosomal protein L27

Chain R0:  75% 20% 5%




- Molecule 45: 50S ribosomal protein L27

Chain Y0:  65% 22% 13%




- Molecule 46: 50S ribosomal protein L28

Chain R1:  81% 18% .



- Molecule 46: 50S ribosomal protein L28

Chain Y1:  78% 17% 5%




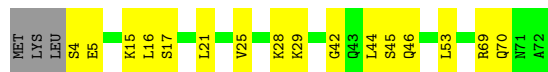
- Molecule 47: 50S ribosomal protein L29

Chain R2:  72% 24% .




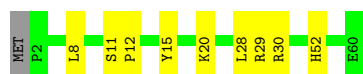
- Molecule 47: 50S ribosomal protein L29

Chain Y2:  74% 22% .




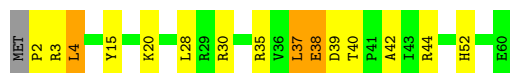
- Molecule 48: 50S ribosomal protein L30

Chain R3:  83% 15% .



- Molecule 48: 50S ribosomal protein L30

Chain Y3:  73% 20% 5% .



- Molecule 49: 50S ribosomal protein L31

Chain R4:  72% 25% .



- Molecule 49: 50S ribosomal protein L31

Chain Y4:  58% 37% . .




- Molecule 50: 50S ribosomal protein L32

Chain R5:  72% 27% .




- Molecule 50: 50S ribosomal protein L32

Chain Y5:  75% 22% . .



- Molecule 51: 50S ribosomal protein L33

Chain R6:  80% 19% .




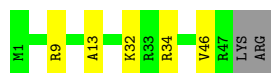
- Molecule 51: 50S ribosomal protein L33

Chain Y6:  67% 31% .




- Molecule 52: 50S ribosomal protein L34

Chain R7:  86% 10% .



- Molecule 52: 50S ribosomal protein L34

Chain Y7:  82% 16% .



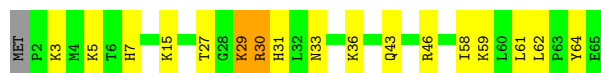
- Molecule 53: 50S ribosomal protein L35

Chain R8:  68% 28% . .



- Molecule 53: 50S ribosomal protein L35

Chain Y8:  72% 23% . .




- Molecule 54: 50S ribosomal protein L36

Chain R9:  70% 30%



- Molecule 54: 50S ribosomal protein L36

Chain Y9:  84% 16%



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	209.97Å 450.71Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 3.97	Depositor
% Data completeness (in resolution range)	98.7 (49.82-3.97)	Depositor
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.228 , 0.255	Depositor
Wilson B-factor (Å ²)	146.0	Xtriage
Anisotropy	0.246	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291782	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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, ZN, 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	0.59	0/36098	1.09	116/56341 (0.2%)
1	XA	0.59	0/36101	1.09	126/56346 (0.2%)
2	QB	0.44	0/1942	0.69	1/2619 (0.0%)
2	XB	0.46	0/1950	0.68	0/2630
3	QC	0.46	0/1629	0.72	0/2195
3	XC	0.44	0/1629	0.72	0/2195
4	QD	0.47	1/1733 (0.1%)	0.67	0/2318
4	XD	0.53	1/1733 (0.1%)	0.65	0/2318
5	QE	0.46	1/1171 (0.1%)	0.68	1/1576 (0.1%)
5	XE	0.45	0/1171	0.69	0/1576
6	QF	0.46	0/856	0.69	0/1154
6	XF	0.41	0/856	0.66	0/1154
7	QG	0.46	0/1276	0.67	0/1709
7	XG	0.45	0/1276	0.70	0/1709
8	QH	0.45	0/1128	0.64	1/1517 (0.1%)
8	XH	0.41	0/1128	0.63	0/1517
9	QI	0.46	0/1008	0.77	3/1354 (0.2%)
9	XI	0.45	0/1017	0.79	2/1365 (0.1%)
10	QJ	0.45	0/814	0.69	1/1095 (0.1%)
10	XJ	0.46	0/790	0.71	0/1063
11	QK	0.42	0/900	0.59	0/1213
11	XK	0.42	0/879	0.66	0/1187
12	QL	0.44	0/991	0.69	0/1327
12	XL	0.43	0/972	0.70	0/1301
13	QM	0.46	0/965	0.74	0/1292
13	XM	0.49	0/956	0.83	1/1281 (0.1%)
14	QN	0.42	0/501	0.70	1/664 (0.2%)
14	XN	0.51	0/501	0.76	1/664 (0.2%)
15	QO	0.40	0/745	0.56	0/992
15	XO	0.41	0/740	0.62	0/987
16	QP	0.46	0/721	0.63	0/970
16	XP	0.43	0/721	0.70	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.38	0/847	0.61	0/1131
17	XQ	0.39	0/847	0.63	0/1131
18	QR	0.40	0/579	0.61	0/768
18	XR	0.44	0/579	0.65	0/768
19	QS	0.39	0/680	0.74	1/915 (0.1%)
19	XS	0.46	0/689	0.75	0/926
20	QT	0.37	0/765	0.61	0/1007
20	XT	0.49	0/765	0.75	0/1007
21	QU	0.41	0/221	0.68	0/288
21	XU	0.40	0/221	0.71	0/288
22	QV	0.47	1/1840 (0.1%)	1.02	6/2866 (0.2%)
22	XV	0.42	1/1840 (0.1%)	1.02	9/2866 (0.3%)
23	QX	0.28	0/470	0.86	1/733 (0.1%)
23	XX	0.33	0/470	0.90	0/733
24	RA	0.76	1/69521 (0.0%)	1.14	353/108529 (0.3%)
24	YA	0.89	3/69543 (0.0%)	1.17	381/108563 (0.4%)
25	RB	0.56	0/2878	1.14	22/4490 (0.5%)
25	YB	0.78	0/2878	1.19	15/4490 (0.3%)
26	RD	0.51	0/2165	0.71	2/2919 (0.1%)
26	YD	0.53	0/2165	0.68	2/2919 (0.1%)
27	RE	0.45	0/1601	0.72	0/2160
27	YE	0.47	0/1601	0.68	0/2160
28	RF	0.49	0/1620	0.64	0/2194
28	YF	0.55	0/1620	0.66	0/2194
29	RG	0.44	0/1499	0.73	0/2016
29	YG	0.46	0/1499	0.73	0/2016
30	RH	0.48	0/1362	0.75	0/1841
30	YH	0.49	0/1362	0.74	0/1841
31	RI	0.43	0/1151	0.76	0/1558
31	YI	0.46	0/1151	0.76	1/1558 (0.1%)
32	RN	0.42	0/1131	0.67	0/1525
32	YN	0.50	0/1131	0.69	0/1525
33	RO	0.52	0/943	0.67	0/1269
33	YO	0.51	0/943	0.67	0/1269
34	RP	0.47	0/1162	0.78	0/1544
34	YP	0.47	0/1139	0.73	0/1514
35	RQ	0.45	0/1143	0.70	0/1527
35	YQ	0.51	0/1143	0.71	0/1527
36	RR	0.45	0/974	0.67	0/1302
36	YR	0.46	0/974	0.67	0/1302
37	RS	0.43	0/892	0.76	0/1187
37	YS	0.44	0/892	0.72	0/1187
38	RT	0.46	0/1155	0.75	2/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.48	0/1155	0.74	2/1542 (0.1%)
39	RU	0.46	0/982	0.65	0/1306
39	YU	0.55	0/982	0.64	0/1306
40	RV	0.48	0/790	0.72	0/1057
40	YV	0.49	0/790	0.70	0/1057
41	RW	0.50	0/911	0.67	0/1220
41	YW	0.50	0/911	0.64	0/1220
42	RX	0.43	0/739	0.64	1/993 (0.1%)
42	YX	0.50	0/739	0.67	1/993 (0.1%)
43	RY	0.44	0/831	0.60	0/1108
43	YY	0.46	0/831	0.58	0/1108
44	RZ	0.49	0/1493	0.79	0/2026
44	YZ	0.44	0/1493	0.74	2/2026 (0.1%)
45	R0	0.41	0/652	0.61	0/867
45	Y0	0.44	0/601	0.60	0/801
46	R1	0.46	0/770	0.66	0/1022
46	Y1	0.50	0/736	0.69	0/978
47	R2	0.49	0/583	0.68	0/771
47	Y2	0.46	0/583	0.68	0/771
48	R3	0.43	0/474	0.65	0/635
48	Y3	0.49	0/474	0.66	0/635
49	R4	0.44	0/578	0.73	0/776
49	Y4	0.48	0/578	0.76	0/776
50	R5	0.46	0/473	0.62	0/639
50	Y5	0.50	0/473	0.78	1/639 (0.2%)
51	R6	0.40	0/460	0.60	0/613
51	Y6	0.45	0/460	0.62	0/613
52	R7	0.44	0/417	0.65	0/550
52	Y7	0.49	0/426	0.64	0/561
53	R8	0.52	0/525	0.75	0/691
53	Y8	0.59	0/525	0.76	0/691
54	R9	0.37	0/310	0.62	0/407
54	Y9	0.42	0/310	0.59	0/407
All	All	0.68	9/316004 (0.0%)	1.03	1056/472499 (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
4	QD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	XL	0	1
27	YE	0	1
29	RG	0	1
29	YG	0	1
44	RZ	0	1
44	YZ	0	1
All	All	0	7

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	XD	61	LYS	CE-NZ	11.17	1.76	1.49
22	QV	1	C	OP3-P	-10.43	1.48	1.61
22	XV	1	C	OP3-P	-10.41	1.48	1.61
4	QD	13	ARG	CZ-NH1	7.36	1.42	1.33
5	QE	57	LYS	CD-CE	5.31	1.64	1.51

The worst 5 of 1056 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1774	C	C2-N1-C1'	19.55	140.31	118.80
24	RA	1774	C	C6-N1-C1'	-15.44	102.27	120.80
1	XA	359	U	C2-N1-C1'	13.62	134.05	117.70
24	YA	1158	C	C2-N1-C1'	13.17	133.29	118.80
1	QA	1301	U	N1-C2-O2	12.01	131.21	122.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	33	MET	Peptide
29	RG	82	LEU	Peptide
44	RZ	52	SER	Peptide
12	XL	104	VAL	Peptide
27	YE	17	ASP	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	16276	508	0
1	XA	32249	0	16279	516	1
2	QB	1907	0	1958	28	0
2	XB	1915	0	1969	33	0
3	QC	1605	0	1668	40	0
3	XC	1605	0	1668	27	1
4	QD	1703	0	1763	39	0
4	XD	1703	0	1763	53	1
5	QE	1155	0	1213	21	0
5	XE	1155	0	1213	24	0
6	QF	843	0	857	17	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	27	0
7	XG	1257	0	1296	22	0
8	QH	1108	0	1165	29	0
8	XH	1108	0	1165	30	0
9	QI	989	0	1011	29	0
9	XI	998	0	1024	26	0
10	QJ	801	0	849	26	0
10	XJ	777	0	816	27	0
11	QK	885	0	904	24	1
11	XK	864	0	881	17	0
12	QL	975	0	1062	29	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	38	0
13	XM	946	0	1008	20	0
14	QN	492	0	528	16	0
14	XN	492	0	531	36	0
15	QO	734	0	771	14	0
15	XO	729	0	768	11	0
16	QP	705	0	725	10	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	18	0
18	QR	574	0	644	14	0
18	XR	574	0	644	12	0
19	QS	665	0	686	18	0
19	XS	674	0	699	14	0
20	QT	763	0	861	15	0
20	XT	763	0	861	21	0
21	QU	217	0	234	5	0
21	XU	217	0	234	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	QV	1647	0	832	20	0
22	XV	1647	0	832	18	0
23	QX	418	0	209	10	0
23	XX	418	0	209	9	0
24	RA	62071	0	31291	830	4
24	YA	62091	0	31297	821	0
25	RB	2573	0	1306	27	0
25	YB	2573	0	1306	26	0
26	RD	2115	0	2195	50	0
26	YD	2115	0	2195	52	0
27	RE	1568	0	1634	53	0
27	YE	1568	0	1634	41	0
28	RF	1585	0	1632	25	0
28	YF	1585	0	1632	21	0
29	RG	1474	0	1535	33	0
29	YG	1474	0	1535	42	0
30	RH	1336	0	1418	33	0
30	YH	1336	0	1418	20	1
31	RI	1136	0	1223	15	0
31	YI	1136	0	1223	10	0
32	RN	1104	0	1180	23	0
32	YN	1104	0	1180	21	0
33	RO	933	0	996	23	0
33	YO	933	0	996	17	0
34	RP	1145	0	1228	35	0
34	YP	1122	0	1206	29	0
35	RQ	1122	0	1179	27	0
35	YQ	1122	0	1179	29	0
36	RR	960	0	1021	20	0
36	YR	960	0	1021	11	0
37	RS	882	0	942	19	0
37	YS	882	0	943	19	0
38	RT	1141	0	1202	26	0
38	YT	1141	0	1202	24	0
39	RU	964	0	1022	19	0
39	YU	964	0	1022	22	0
40	RV	779	0	852	18	0
40	YV	779	0	852	16	1
41	RW	900	0	964	16	0
41	YW	900	0	964	10	0
42	RX	725	0	778	9	0
42	YX	725	0	778	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	RY	818	0	909	16	0
43	YY	818	0	909	18	1
44	RZ	1461	0	1493	32	0
44	YZ	1461	0	1493	24	0
45	R0	643	0	667	12	0
45	Y0	593	0	612	15	0
46	R1	763	0	848	11	0
46	Y1	729	0	802	11	0
47	R2	581	0	629	11	0
47	Y2	581	0	629	9	2
48	R3	469	0	518	6	0
48	Y3	469	0	518	9	0
49	R4	565	0	557	12	0
49	Y4	565	0	557	21	0
50	R5	459	0	476	16	0
50	Y5	459	0	477	13	1
51	R6	453	0	473	9	0
51	Y6	453	0	473	11	0
52	R7	409	0	454	4	0
52	Y7	418	0	467	7	0
53	R8	517	0	582	17	0
53	Y8	517	0	582	19	0
54	R9	307	0	335	9	0
54	Y9	307	0	335	5	0
55	QA	69	0	0	0	0
55	QE	1	0	0	0	0
55	QH	1	0	0	0	0
55	QV	1	0	0	0	0
55	R1	1	0	0	0	0
55	RA	381	0	0	0	0
55	RB	9	0	0	0	0
55	RD	1	0	0	0	0
55	RE	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	67	0	0	0	0
55	XE	1	0	0	0	0
55	Y0	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	2	0	0	0	0
55	YA	454	0	0	0	0
55	YB	8	0	0	0	0
55	YD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	YE	1	0	0	0	0
55	YP	1	0	0	0	0
55	YQ	2	0	0	0	0
55	YR	2	0	0	0	0
56	QD	8	0	0	1	0
56	XD	8	0	0	3	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291782	0	197805	4186	7

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 9.

The worst 5 of 4186 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)
14:XN:24:CYS:SG	14:XN:40:CYS:HB2	1.54	1.47
4:XD:61:LYS:CE	4:XD:61:LYS:NZ	1.77	1.47
14:XN:29:ARG:HD2	14:XN:40:CYS:SG	1.67	1.33
14:XN:24:CYS:SG	14:XN:40:CYS:CB	2.36	1.14
14:XN:29:ARG:CD	14:XN:40:CYS:SG	2.36	1.13

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YV:53:GLU:CB	50:Y5:59:GLU:OE1[4_445]	1.95	0.25
11:QK:99:GLN:OE1	3:XC:79:ARG:CD[4_555]	2.01	0.19
24:RA:2137:C:OP1	1:XA:999:U:O2'[4_555]	2.05	0.15
30:YH:46:GLU:OE2	43:YY:23:ARG:NH1[4_445]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:306:U:O3'	47:Y2:17:SER:OG[3_555]	2.12	0.08

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%)	204 (88%)	27 (12%)	2 (1%)	17	54
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	189 (93%)	13 (6%)	1 (0%)	29	66
3	XC	203/239 (85%)	184 (91%)	18 (9%)	1 (0%)	29	66
4	QD	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
4	XD	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	QE	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22	60
5	XE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	123/128 (96%)	113 (92%)	9 (7%)	1 (1%)	19	57
9	XI	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
10	QJ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	111 (90%)	11 (9%)	1 (1%)	19	57
12	XL	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	57
13	QM	118/126 (94%)	102 (86%)	15 (13%)	1 (1%)	19	57
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	17	54
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	42
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	42
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	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%)	62 (91%)	6 (9%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	82/93 (88%)	68 (83%)	14 (17%)	0	100	100
20	QT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	6 (6%)	1 (1%)	15	52
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	245 (91%)	23 (8%)	2 (1%)	22	60
26	YD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	22	60
27	RE	203/206 (98%)	170 (84%)	31 (15%)	2 (1%)	15	52
27	YE	203/206 (98%)	166 (82%)	35 (17%)	2 (1%)	15	52
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	14	50
29	YG	179/182 (98%)	150 (84%)	27 (15%)	2 (1%)	14	50
30	RH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	4	32
30	YH	172/180 (96%)	150 (87%)	18 (10%)	4 (2%)	6	37
31	RI	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YI	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	7	38
32	RN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22	60
32	YN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
33	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
34	RP	148/150 (99%)	120 (81%)	26 (18%)	2 (1%)	11	45
34	YP	145/150 (97%)	119 (82%)	25 (17%)	1 (1%)	22	60
35	RQ	139/141 (99%)	119 (86%)	19 (14%)	1 (1%)	22	60
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
36	RR	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	42
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
37	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	17	54
37	YS	109/112 (97%)	92 (84%)	17 (16%)	0	100	100
38	RT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	10	45
38	YT	135/146 (92%)	114 (84%)	19 (14%)	2 (2%)	10	45
39	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
39	YU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	54
40	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	52
40	YV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	52
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
41	YW	111/113 (98%)	101 (91%)	9 (8%)	1 (1%)	17	54
42	RX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
42	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
43	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	RZ	181/206 (88%)	146 (81%)	32 (18%)	3 (2%)	9	42
44	YZ	181/206 (88%)	149 (82%)	29 (16%)	3 (2%)	9	42
45	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
45	Y0	72/85 (85%)	69 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	10	45
47	Y2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	10	45
48	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	45
49	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	45
50	R5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	Y5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	48 (77%)	11 (18%)	3 (5%)	2	23
53	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	31
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11449/12128 (94%)	10319 (90%)	1055 (9%)	75 (1%)	22	60

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
53	R8	30	ARG

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%)	200 (98%)	3 (2%)	65	79
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	79
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	63
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	81
4	QD	180/181 (99%)	176 (98%)	4 (2%)	52	71
4	XD	180/181 (99%)	175 (97%)	5 (3%)	43	65
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	87
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	87
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	122 (97%)	4 (3%)	39	62
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	79
8	QH	118/119 (99%)	116 (98%)	2 (2%)	60	78
8	XH	118/119 (99%)	116 (98%)	2 (2%)	60	78
9	QI	96/99 (97%)	94 (98%)	2 (2%)	53	72
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	72
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	84
10	XJ	86/92 (94%)	83 (96%)	3 (4%)	36	61
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	84
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	76	85
12	XL	103/109 (94%)	102 (99%)	1 (1%)	76	85
13	QM	96/101 (95%)	93 (97%)	3 (3%)	40	63
13	XM	95/101 (94%)	92 (97%)	3 (3%)	39	62
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	57
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
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%)	94 (99%)	1 (1%)	73	84
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	84

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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%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	80
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	81
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	52
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	52
26	RD	214/218 (98%)	212 (99%)	2 (1%)	78	87
26	YD	214/218 (98%)	212 (99%)	2 (1%)	78	87
27	RE	165/166 (99%)	164 (99%)	1 (1%)	86	91
27	YE	165/166 (99%)	165 (100%)	0	100	100
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	154 (99%)	1 (1%)	86	91
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	91
30	RH	145/148 (98%)	144 (99%)	1 (1%)	84	90
30	YH	145/148 (98%)	143 (99%)	2 (1%)	67	80
31	RI	122/124 (98%)	122 (100%)	0	100	100
31	YI	122/124 (98%)	121 (99%)	1 (1%)	81	88
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	87
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	114 (98%)	2 (2%)	60	78
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	77
35	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	77
36	RR	100/101 (99%)	100 (100%)	0	100	100
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	86 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	119 (99%)	1 (1%)	81	88
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	84
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	81 (99%)	1 (1%)	71	83
40	YV	82/82 (100%)	80 (98%)	2 (2%)	49	69
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	90 (98%)	2 (2%)	52	71
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	74 (100%)	0	100	100
43	RY	88/91 (97%)	87 (99%)	1 (1%)	73	84
43	YY	88/91 (97%)	86 (98%)	2 (2%)	50	70
44	RZ	162/179 (90%)	162 (100%)	0	100	100
44	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	83
45	R0	65/67 (97%)	64 (98%)	1 (2%)	65	79
45	Y0	60/67 (90%)	59 (98%)	1 (2%)	60	78
46	R1	82/83 (99%)	81 (99%)	1 (1%)	71	83
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	55	73
48	Y3	51/52 (98%)	45 (88%)	6 (12%)	5	24
49	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
49	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	62
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	73
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	50 (98%)	1 (2%)	55	73
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	R8	54/55 (98%)	53 (98%)	1 (2%)	57	75
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9684/10066 (96%)	9578 (99%)	106 (1%)	73	84

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	R0	14	ARG
4	XD	139	ARG
48	Y3	4	LEU
48	R3	30	ARG
2	XB	96	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	95	GLN
6	XF	7	ASN
27	YE	66	HIS
47	R2	9	GLN
2	XB	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	271 (18%)	37 (2%)
1	XA	1498/1521 (98%)	254 (16%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	2 (11%)
23	XX	18/19 (94%)	5 (27%)	1 (5%)
24	RA	2879/2915 (98%)	571 (19%)	41 (1%)
24	YA	2880/2915 (98%)	576 (20%)	42 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9182/9308 (98%)	1753 (19%)	157 (1%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	RA	1992	G
1	XA	244	U
24	YA	1930	G
24	RA	2126	A
24	RA	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1022 ligands modelled in this entry, 1020 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	$\# Z > 2$
56	SF4	XD	301	4	0,12,12	0.00	-	-		
56	SF4	QD	301	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	XD	301	4	-	-	0/6/5/5
56	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	XD	301	SF4	3	0
56	QD	301	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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.