wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 08:25 AM EDT

PDB ID	:	6NTA
Title	:	Modified ASL proline bound to Thermus thermophilus 70S (cognate)
Authors	:	Hoffer, E.D.; Maehigashi, T.; Subaramanian, S.; Hong, S.; Dunham, C.M.
Deposited on	:	2019-01-28
Resolution	:	3.10 Å(reported)

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

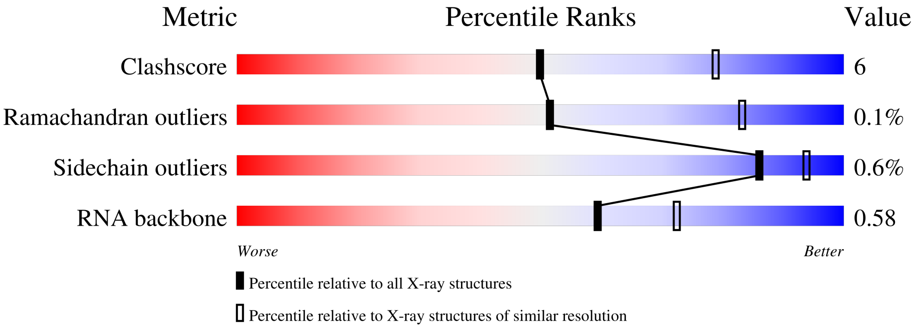
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	76% 18% • 5%
17	QQ	105	86% 8% • 5%
17	XQ	105	70% 23% • 5%
18	QR	88	59% 19% • 20%
18	XR	88	67% 13% 20%
19	QS	93	59% 26% • 11%
19	XS	93	56% 33% • 10%
20	QT	106	64% 25% • 7%
20	XT	106	73% 17% • 7%
21	QU	27	52% 41% 7%
21	XU	27	74% 19% 7%
22	QV	17	53% 47%
22	XV	17	35% 47% 6% 12%
23	QX	19	16% 26% 11% 47%
23	XX	19	26% 32% 5% 37%
24	RA	2915	61% 31% 7% •
24	YA	2915	62% 29% 7% ••
25	RB	122	66% 25% 6% • •
25	YB	122	69% 24% 6% •
26	RD	276	79% 18% • •
26	YD	276	74% 24% ••
27	RE	206	71% 26% •
27	YE	206	83% 15% •
28	RF	210	78% 18% • •
28	YF	210	76% 19% • •

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Mol	Chain	Length	Quality of chain
29	RG	182	 66% 31% • •
29	YG	182	 77% 20% • ••
30	RH	180	 75% 19% • •
30	YH	180	 85% 11% • •
31	RI	148	 78% 19% ••
31	YI	148	 79% 15% 5% •
32	RN	140	 76% 22% •
32	YN	140	 78% 19% ••
33	RO	122	 72% 27% •
33	YO	122	 82% 18%
34	RP	150	 73% 26% •
34	YP	150	 80% 18% •
35	RQ	141	 67% 30% •
35	YQ	141	 77% 23% •
36	RR	118	 81% 17% ••
36	YR	118	 78% 18% • ••
37	RS	112	 70% 28% • •
37	YS	112	 79% 18% • •
38	RT	146	 71% 20% • • 6%
38	YT	146	 70% 23% •• 6%
39	RU	118	 81% 15% • •
39	YU	118	 88% 11% •
40	RV	101	 84% 16%
40	YV	101	 89% 11%
41	RW	113	 84% 16%

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Mol	Chain	Length	Quality of chain
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	
53	R8	65	
53	Y8	65	

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Mol	Chain	Length	Quality of chain
54	R9	37	 78% 22%
54	Y9	37	 78% 22%

2 Entry composition ⓘ

There are 57 unique types of molecules in this entry. The entry contains 289311 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 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1500	Total 32249	C 14354	N 5984	O 10412	P 1499	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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
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 1155	C 729	N 218	O 204	S 4	0	0	0
5	XE	151	Total 1155	C 729	N 218	O 204	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total 843	C 531	N 155	O 154	S 3	0	0	0
6	XF	101	Total 843	C 531	N 155	O 154	S 3	0	0	0

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

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

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

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

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

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

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

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

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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
			Total	C	N	O	S			
16	QP	84	705	446	140	118	1	0	0	0
16	XP	84	705	446	140	118	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	QS	83	665	424	124	115	2	0	0	0
19	XS	84	674	430	126	116	2	0	0	0

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

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

- 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	17	Total	C	N	O	P	0	0	0
			365	163	65	120	17			
22	XV	15	Total	C	N	O	P	0	0	0
			322	144	57	106	15			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	10	Total	C	N	O	P	0	0	0
			217	97	43	67	10			
23	XX	12	Total	C	N	O	P	0	0	0
			262	117	53	80	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
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 2115	C 1335	N 420	O 357	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 882	C 556	N 176	O 150	0	0	0
37	YS	111	Total 882	C 556	N 176	O 150	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total 581	C 358	N 118	O 104	S 1	0	0	0
47	Y2	68	Total 575	C 355	N 117	O 102	S 1	0	0	0

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

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

- 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 565 356 103 101 5	0	0	0
49	Y4	69	Total C N O S 565 356 103 101 5	0	0	0

- 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 459 288 90 76 5	0	0	0
50	Y5	59	Total C N O S 459 288 90 76 5	0	0	0

- 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 453 281 91 77 4	0	0	0
51	Y6	53	Total C N O S 453 281 91 77 4	0	0	0

- 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 409 251 102 54 2	0	0	0
52	Y7	48	Total C N O S 418 257 104 55 2	0	0	0

- 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 517 331 102 82 2	0	0	0
53	Y8	64	Total C N O S 517 331 102 82 2	0	0	0

- 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 307 188 68 47 4	0	0	0
54	Y9	37	Total C N O S 307 188 68 47 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	QA	74	Total Mg 74 74	0	0
55	QC	1	Total Mg 1 1	0	0
55	QF	1	Total Mg 1 1	0	0
55	QH	1	Total Mg 1 1	0	0
55	QM	1	Total Mg 1 1	0	0
55	RA	487	Total Mg 487 487	0	0
55	RB	6	Total Mg 6 6	0	0
55	RE	4	Total Mg 4 4	0	0
55	RF	2	Total Mg 2 2	0	0
55	RI	1	Total Mg 1 1	0	0
55	RN	1	Total Mg 1 1	0	0
55	RO	1	Total Mg 1 1	0	0
55	RP	1	Total Mg 1 1	0	0
55	RQ	2	Total Mg 2 2	0	0

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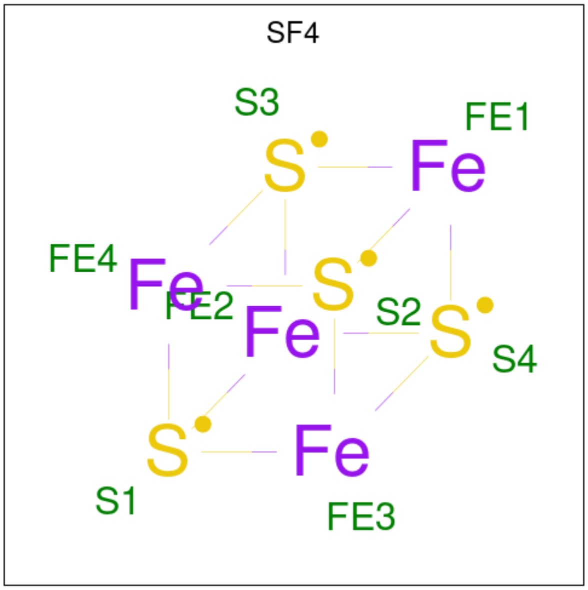
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	RR	2	Total Mg 2 2	0	0
55	RT	1	Total Mg 1 1	0	0
55	RX	1	Total Mg 1 1	0	0
55	RY	1	Total Mg 1 1	0	0
55	R0	1	Total Mg 1 1	0	0
55	R1	2	Total Mg 2 2	0	0
55	R8	1	Total Mg 1 1	0	0
55	XA	92	Total Mg 92 92	0	0
55	XE	1	Total Mg 1 1	0	0
55	XK	1	Total Mg 1 1	0	0
55	XL	2	Total Mg 2 2	0	0
55	XM	2	Total Mg 2 2	0	0
55	XN	1	Total Mg 1 1	0	0
55	XQ	1	Total Mg 1 1	0	0
55	XS	1	Total Mg 1 1	0	0
55	YA	542	Total Mg 542 542	0	0
55	YB	15	Total Mg 15 15	0	0
55	YD	3	Total Mg 3 3	0	0
55	YE	3	Total Mg 3 3	0	0
55	YO	1	Total Mg 1 1	0	0
55	YQ	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	YR	2	Total Mg 2 2	0	0
55	YX	2	Total Mg 2 2	0	0
55	Y0	2	Total Mg 2 2	0	0
55	Y1	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	1	Total Mg 1 1	0	0
55	Y8	2	Total Mg 2 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

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

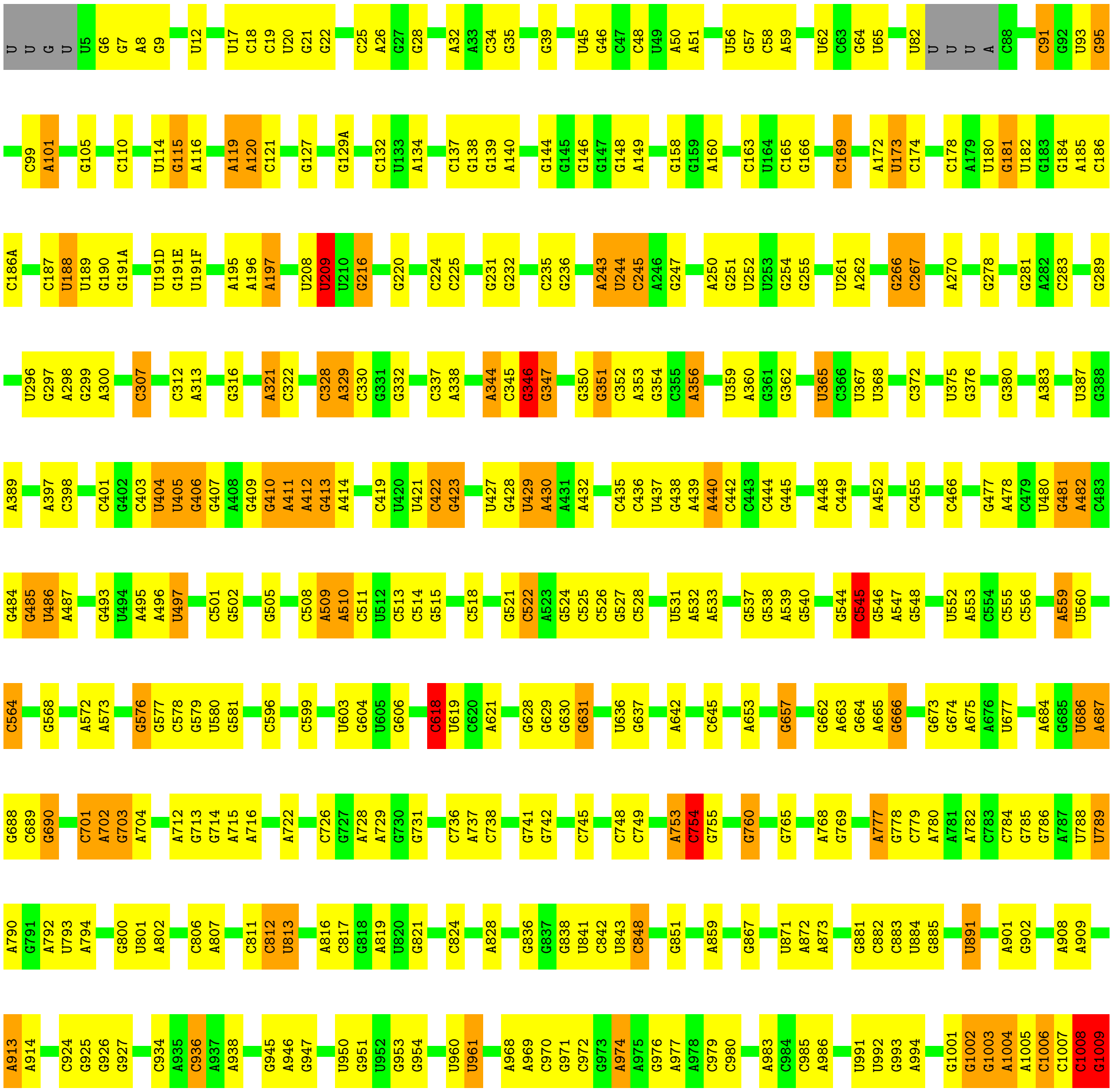
3 Residue-property plots ⓘ

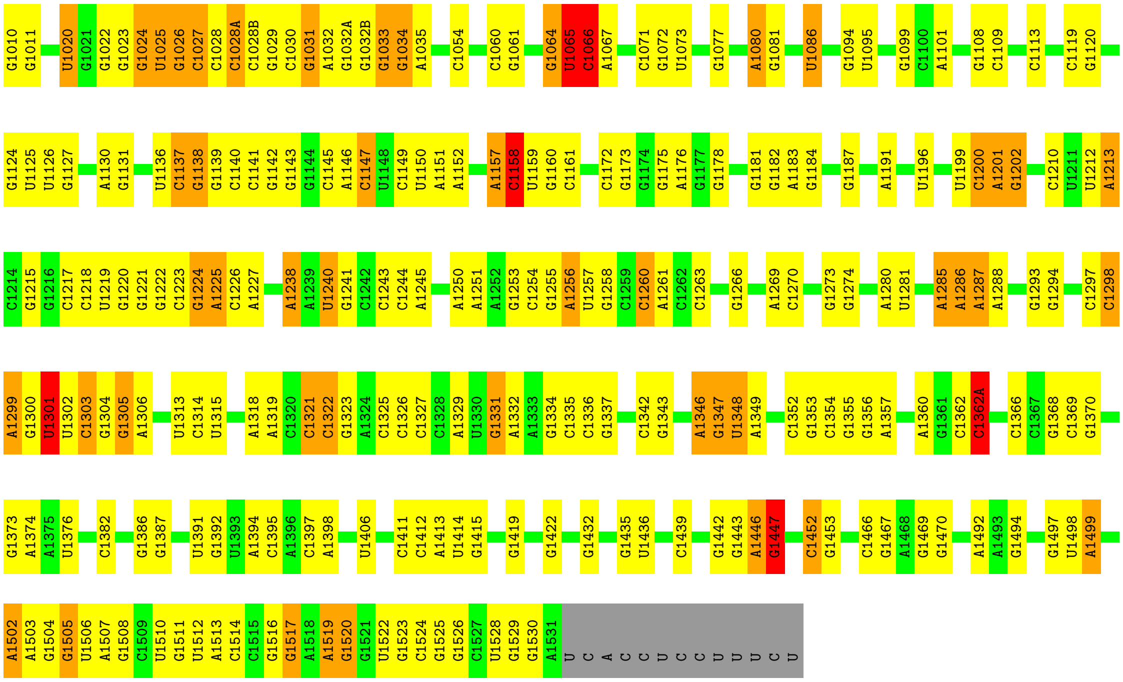
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

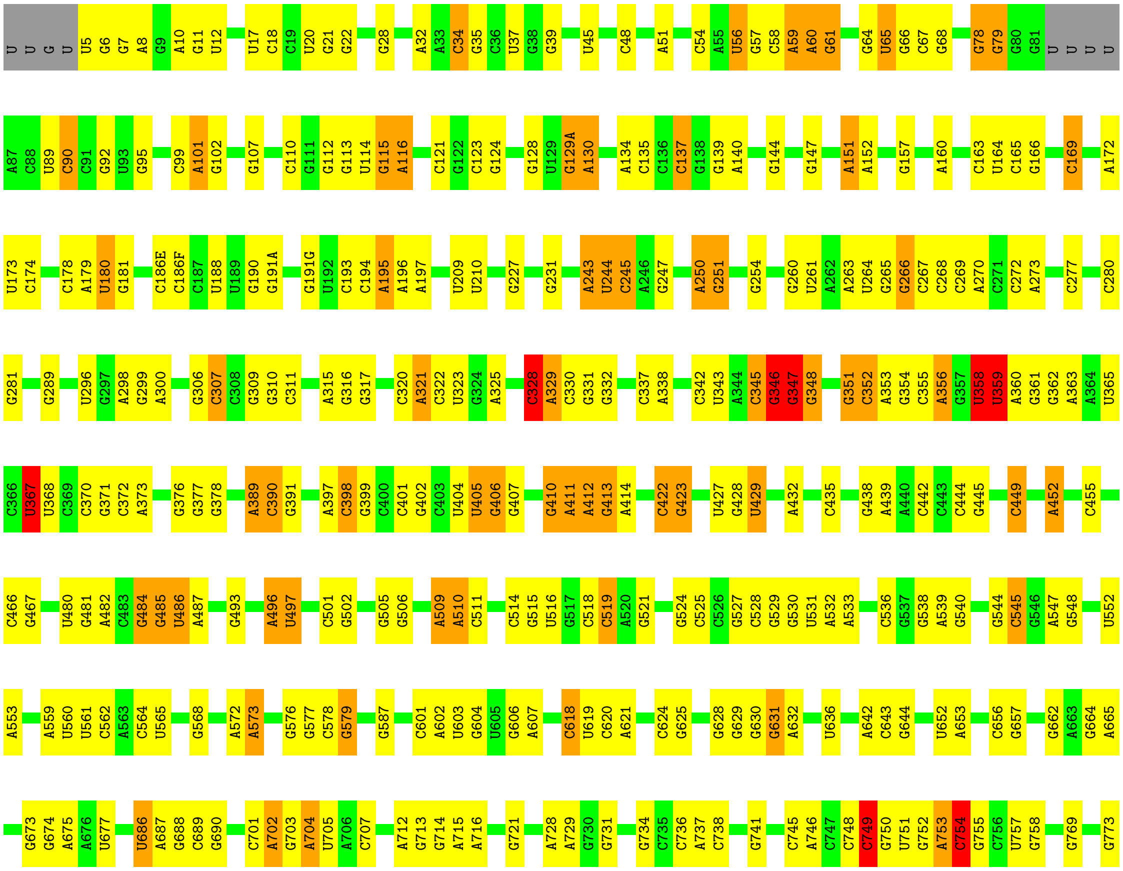
Chain QA:

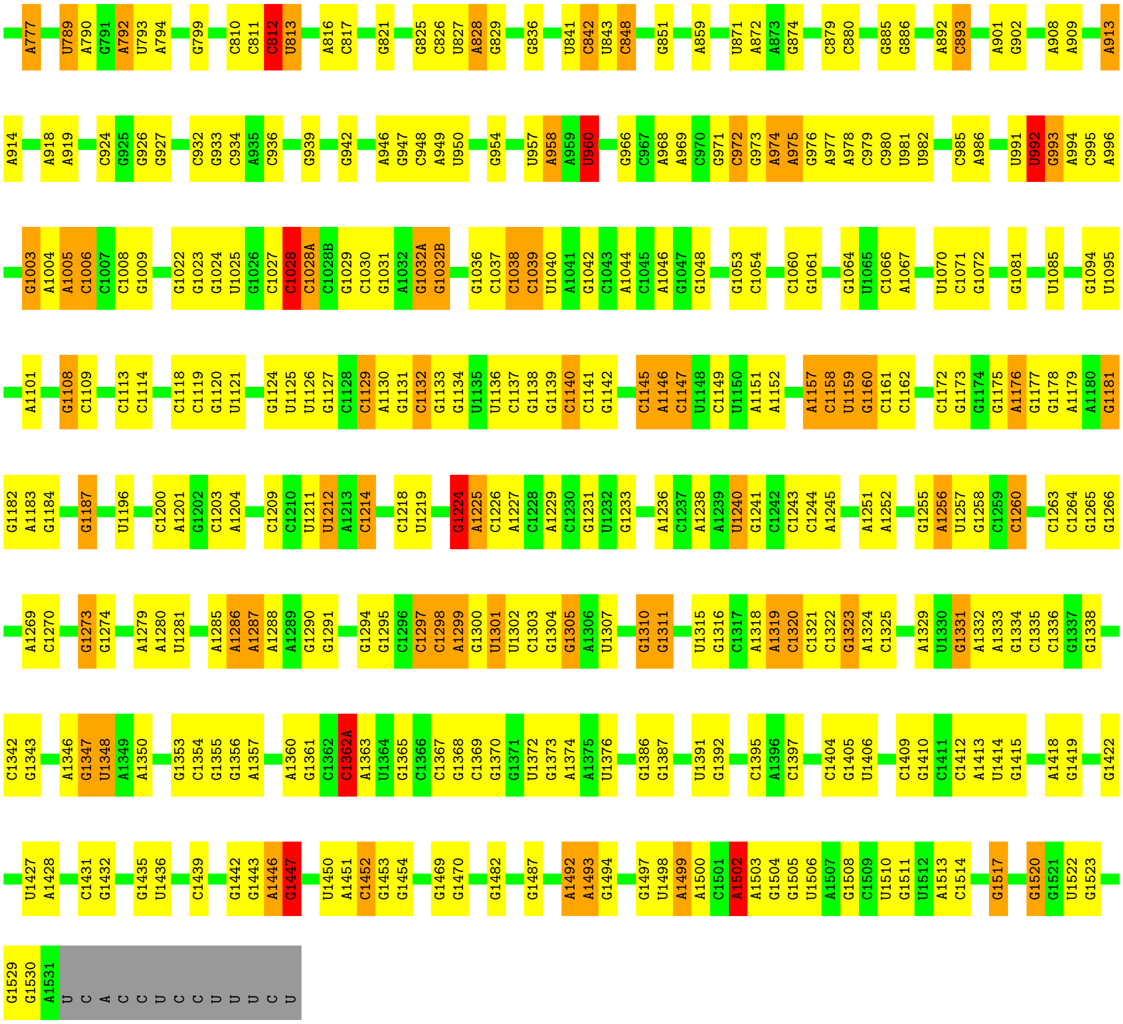





- Molecule 1: 16S rRNA

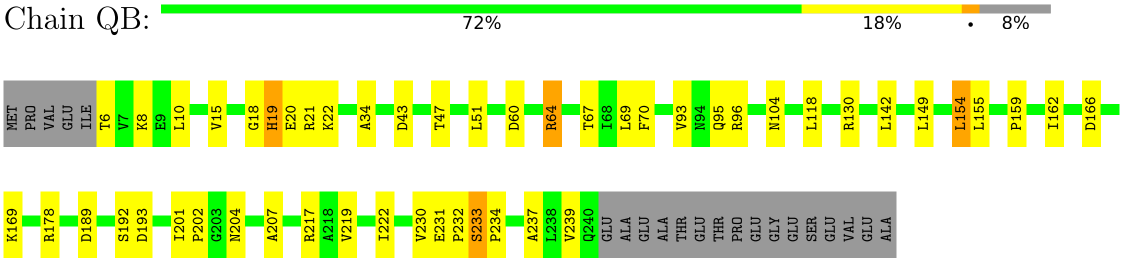
Chain XA:





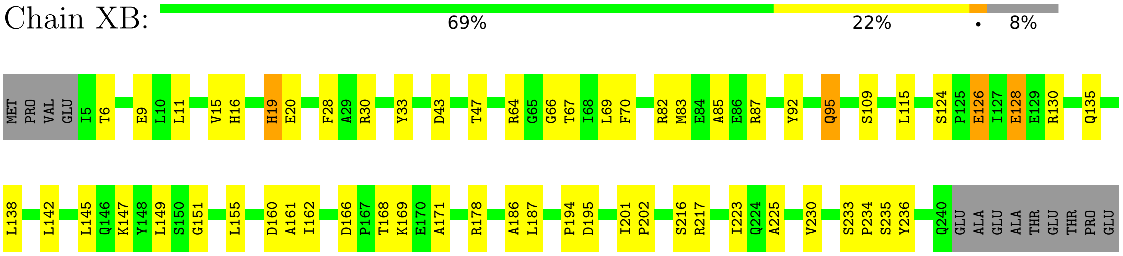
- Molecule 2: 30S ribosomal protein S2

Chain QB:

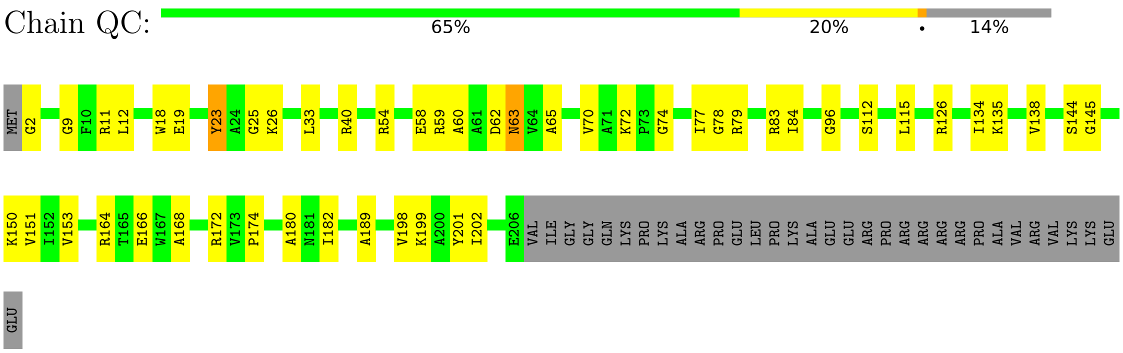


- Molecule 2: 30S ribosomal protein S2

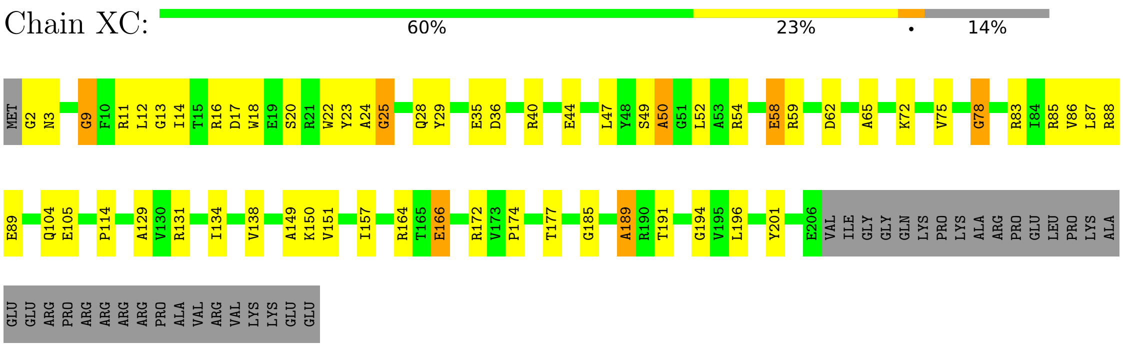
Chain XB:



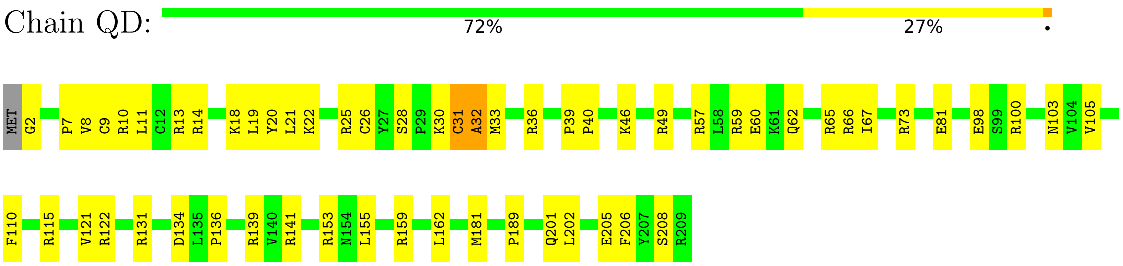
- Molecule 3: 30S ribosomal protein S3



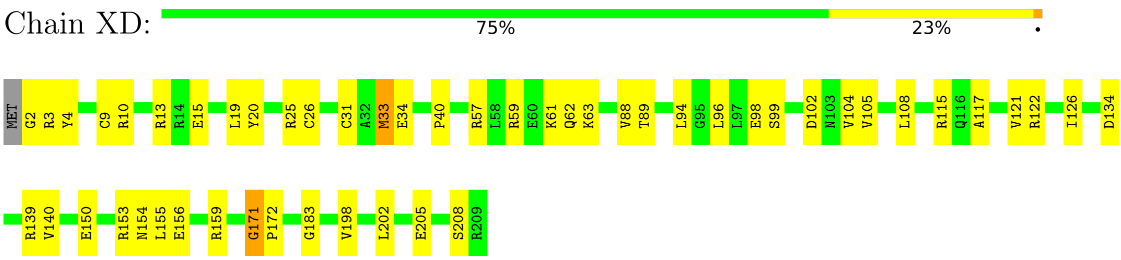
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

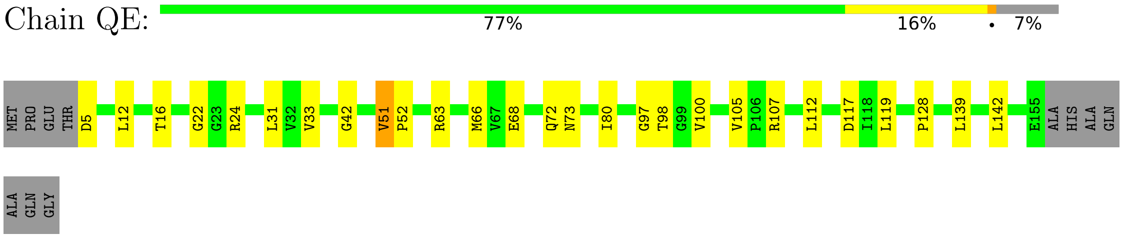


- Molecule 4: 30S ribosomal protein S4



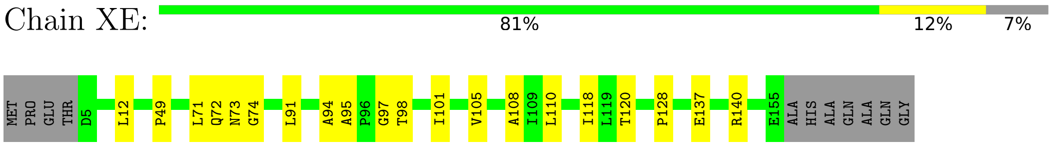
- Molecule 5: 30S ribosomal protein S5

Chain QE:



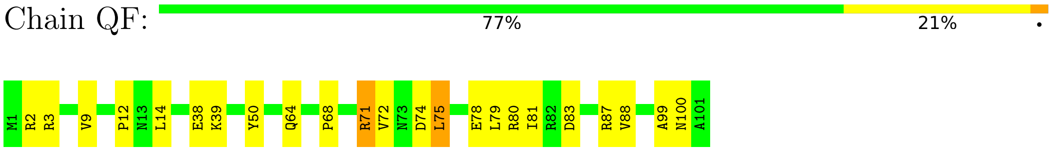
- Molecule 5: 30S ribosomal protein S5

Chain XE:



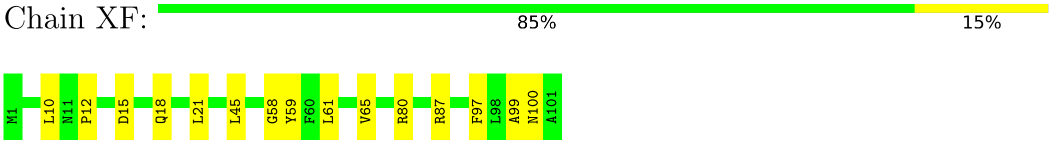
- Molecule 6: 30S ribosomal protein S6

Chain QF:



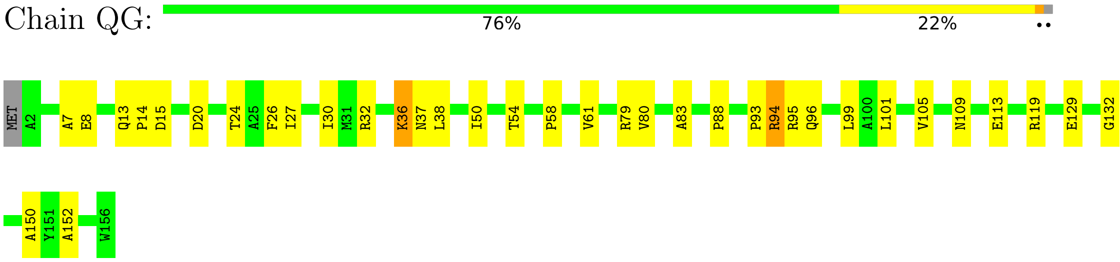
- Molecule 6: 30S ribosomal protein S6

Chain XF:



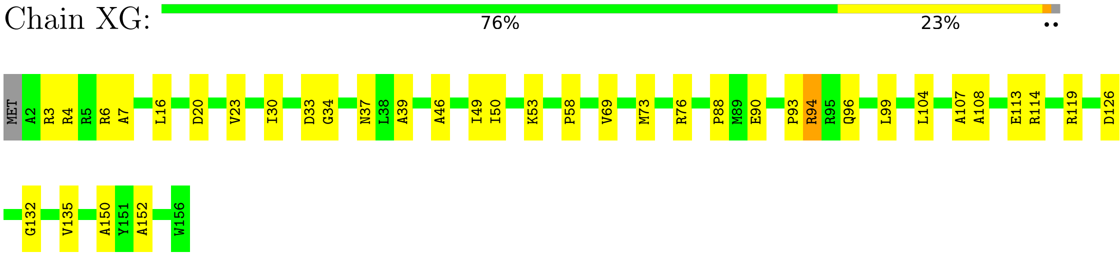
- Molecule 7: 30S ribosomal protein S7

Chain QG:



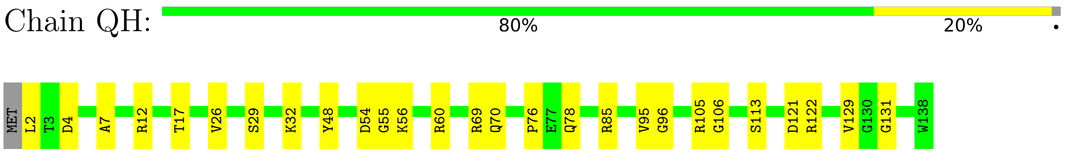
- Molecule 7: 30S ribosomal protein S7

Chain XG:



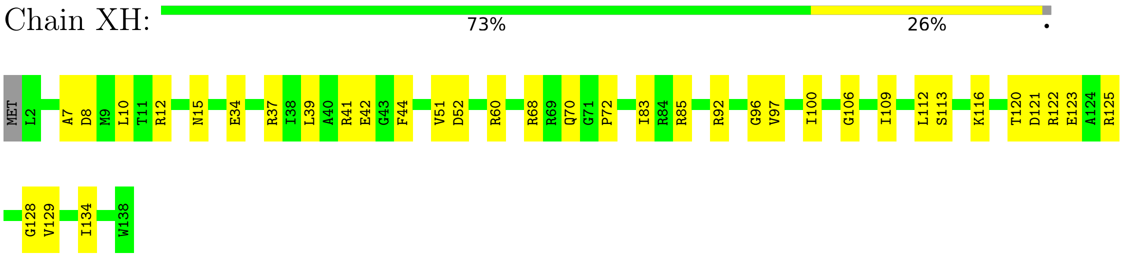
- Molecule 8: 30S ribosomal protein S8

Chain QH:



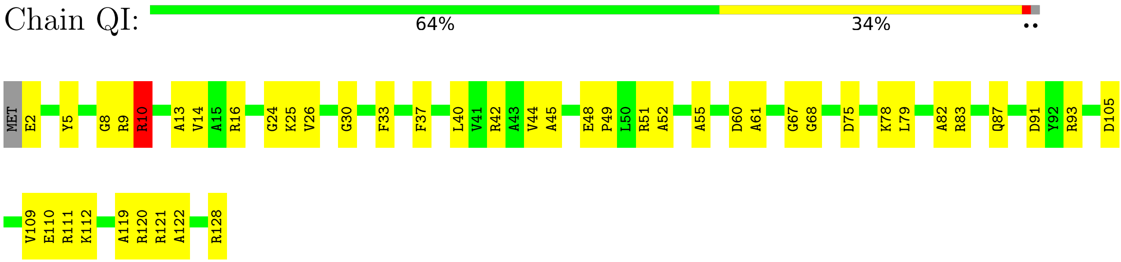
- Molecule 8: 30S ribosomal protein S8

Chain XH:



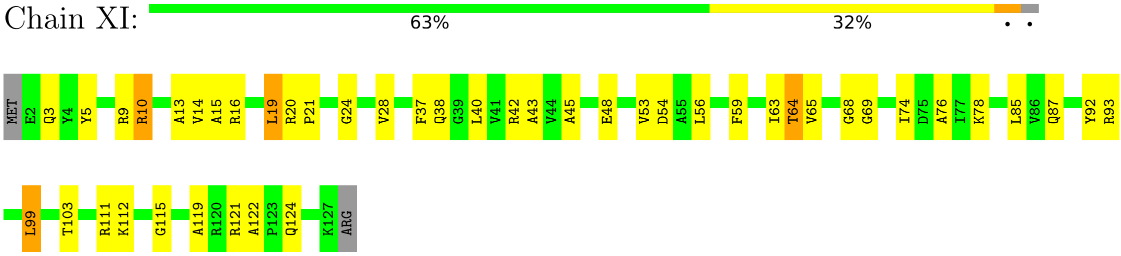
- Molecule 9: 30S ribosomal protein S9

Chain QI:



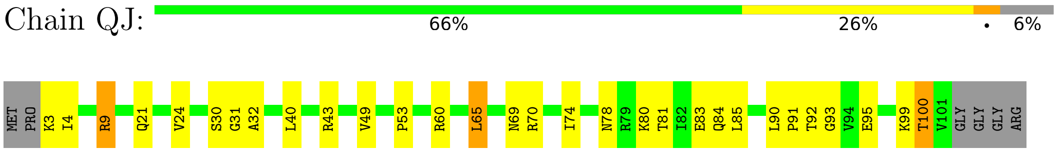
- Molecule 9: 30S ribosomal protein S9

Chain XI:



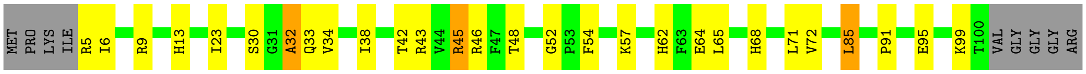
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



- Molecule 10: 30S ribosomal protein S10

Chain XJ:

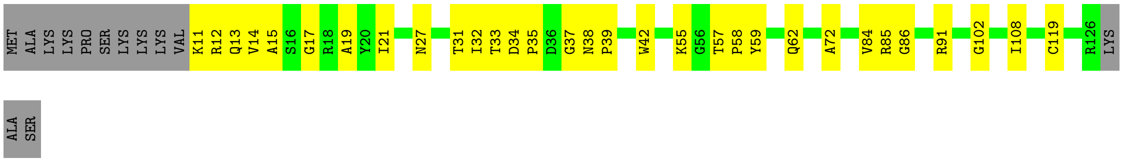


- Molecule 11: 30S ribosomal protein S11

Chain QK:

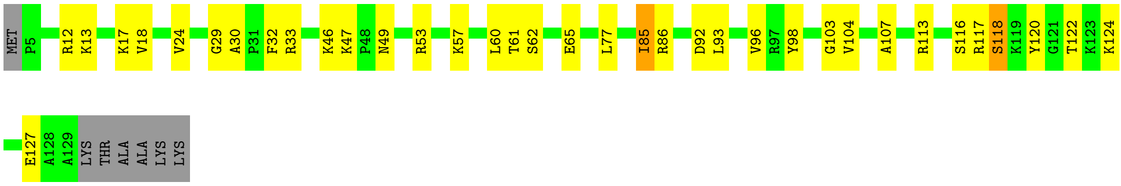
- Molecule 11: 30S ribosomal protein S11

Chain XK:



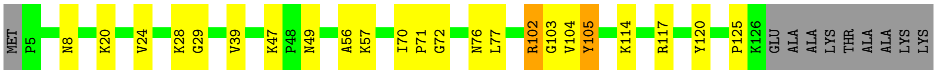
- Molecule 12: 30S ribosomal protein S12

Chain QL:



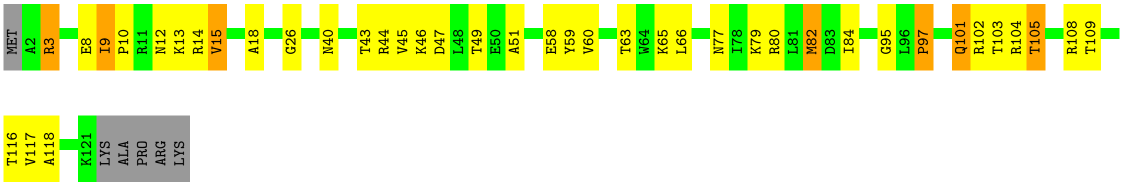
- Molecule 12: 30S ribosomal protein S12

Chain XL:

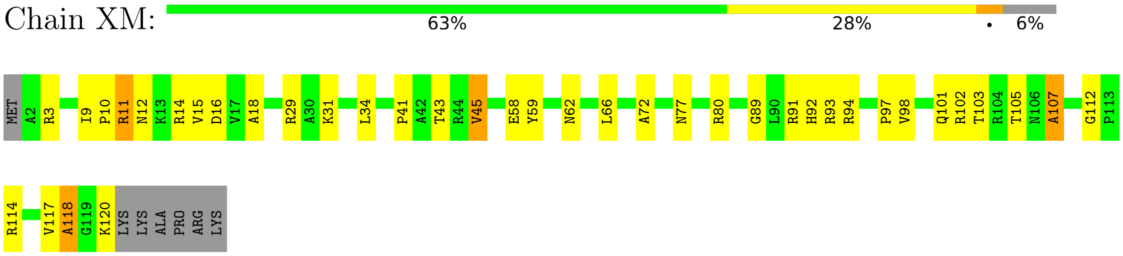


- Molecule 13: 30S ribosomal protein S13

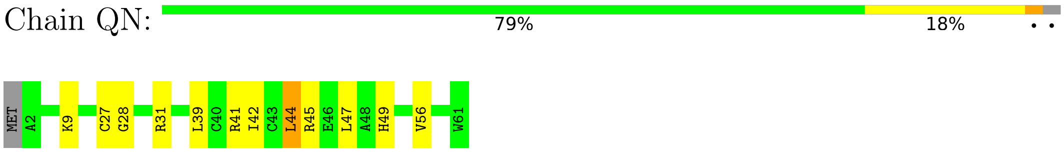
Chain QM:



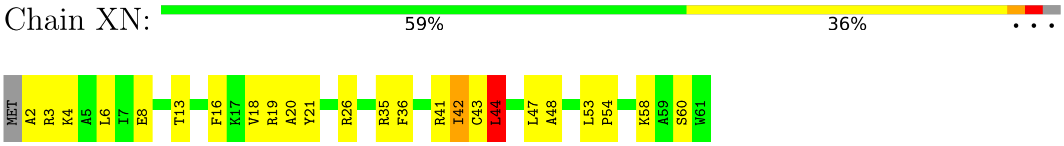
- Molecule 13: 30S ribosomal protein S13



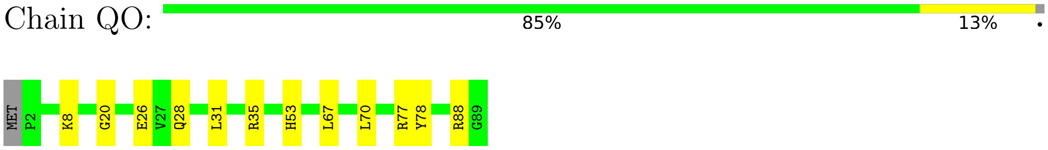
- Molecule 14: 30S ribosomal protein S14 type Z



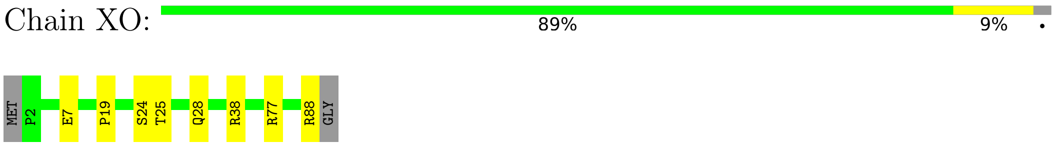
- Molecule 14: 30S ribosomal protein S14 type Z



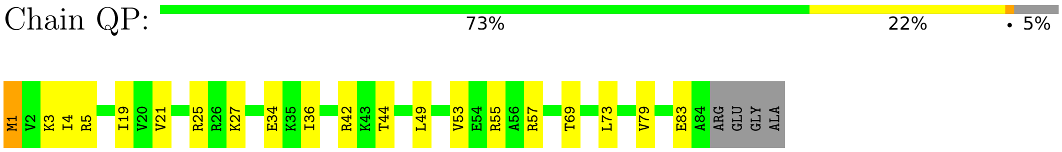
- Molecule 15: 30S ribosomal protein S15



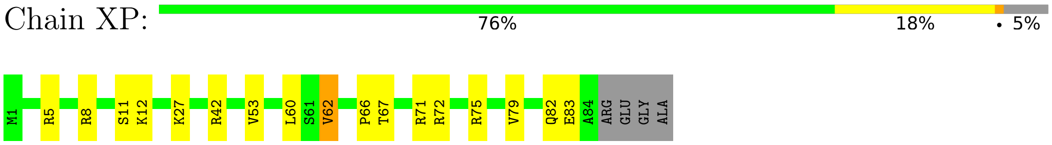
- Molecule 15: 30S ribosomal protein S15



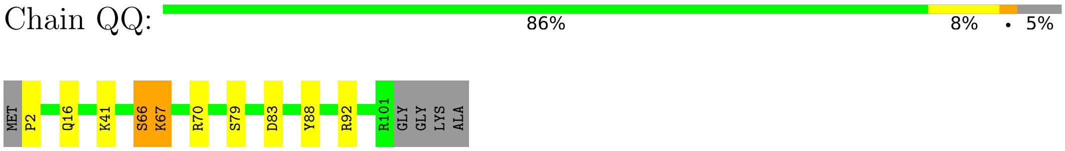
- Molecule 16: 30S ribosomal protein S16



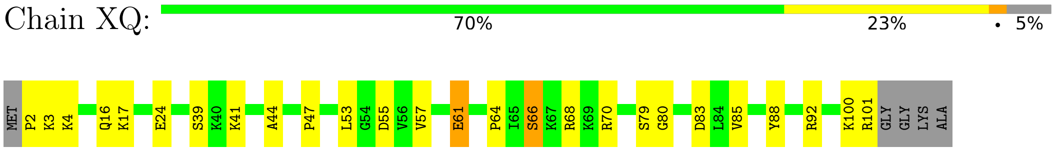
- Molecule 16: 30S ribosomal protein S16



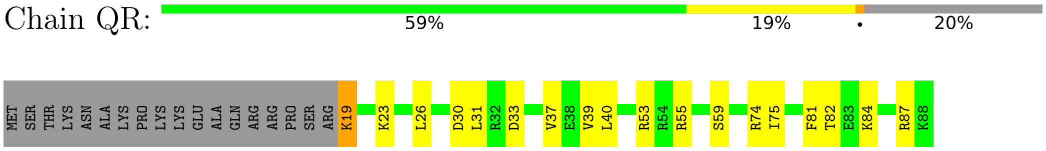
- Molecule 17: 30S ribosomal protein S17



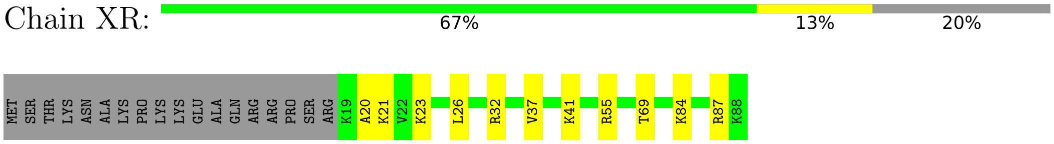
- Molecule 17: 30S ribosomal protein S17



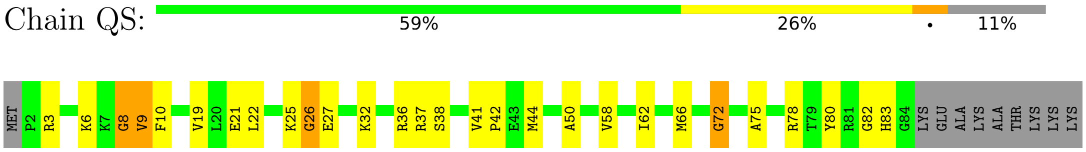
- Molecule 18: 30S ribosomal protein S18



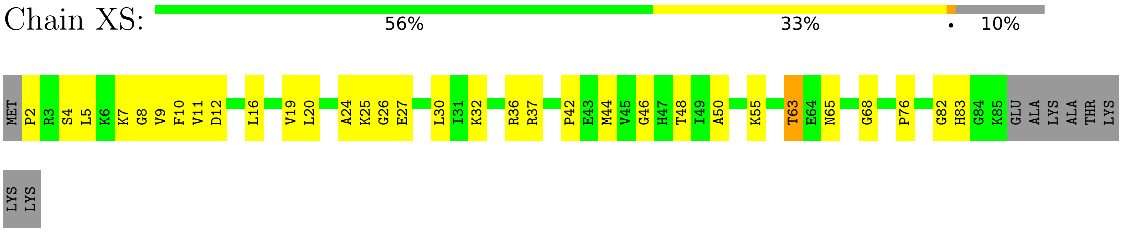
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



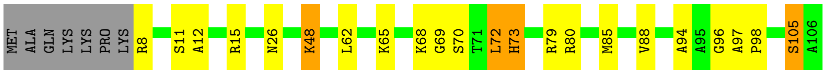
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

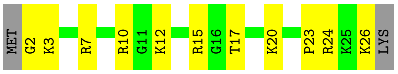
- Molecule 20: 30S ribosomal protein S20

Chain XT:



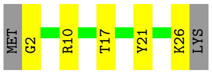
- Molecule 21: 30S ribosomal protein Thx

Chain QU:



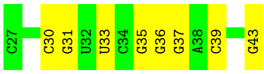
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



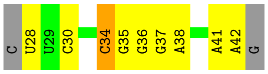
- Molecule 22: P-site ASLPro

Chain QV:



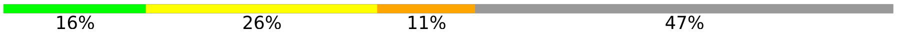
- Molecule 22: P-site ASLPro

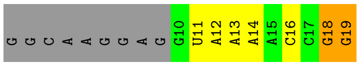
Chain XV:



- Molecule 23: mRNA

Chain QX:



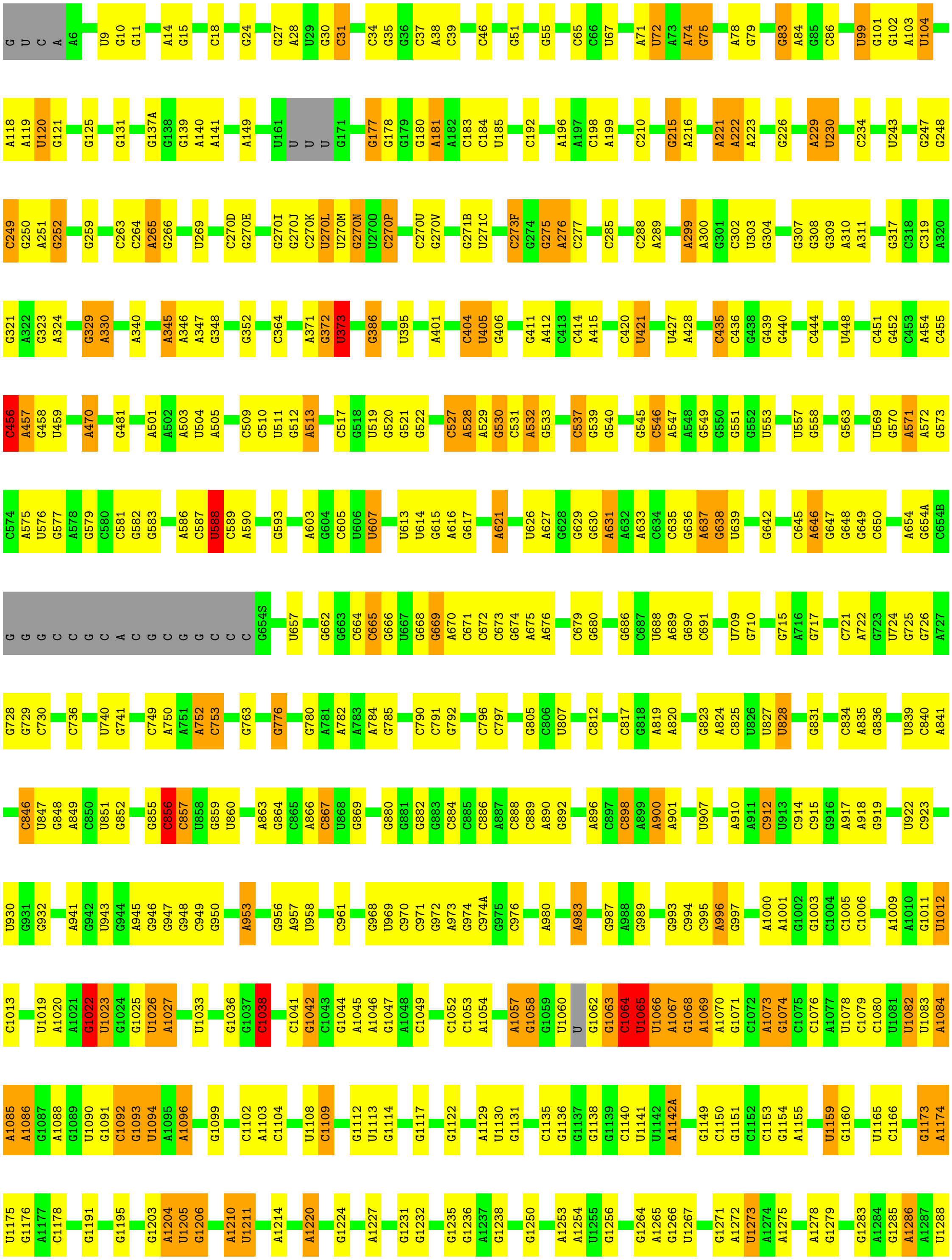


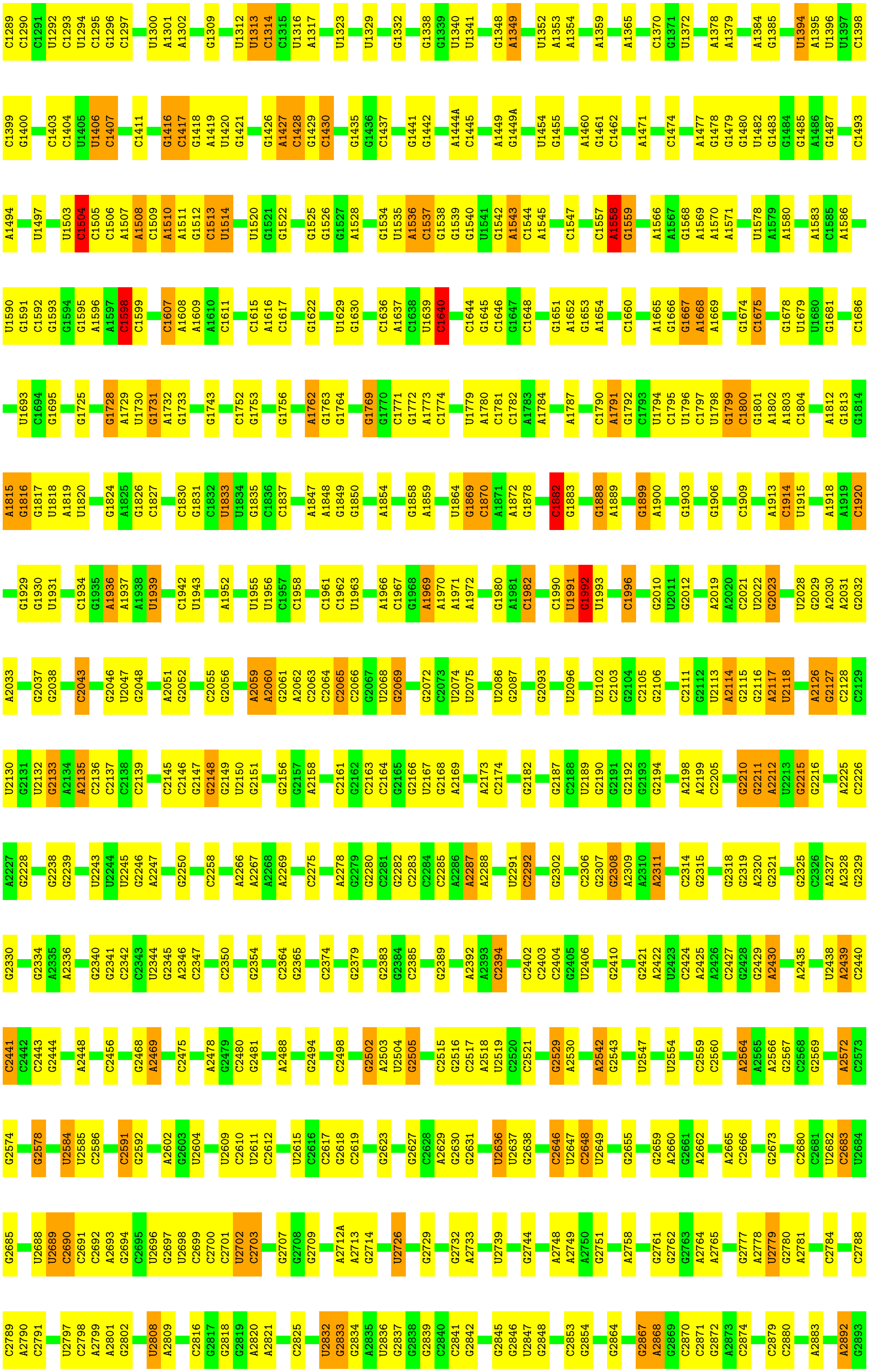
- Molecule 23: mRNA

Chain XX:

- Molecule 24: 23S rRNA

Chain RA:




C1289 C1290 C1291 U1292 C1293 U1294 C1295 G1296 C1297 U1300 A1301 A1302 G1309 U1312 U1313 C1314 C1315 U1316 A1317 U1323 U1329 G1332 G1338 G1339 U1340 U1341 G1348 A1349 U1352 A1353 A1354 A1359 A1365 C1370 G1371 U1372 A1378 A1379 A1384 G1385 U1394 A1395 U1396 U1397 C1398
C1399 G1400 C1403 C1404 U1405 U1406 C1407 C1411 G1416 C1417 G1418 A1419 U1420 G1421 G1426 A1427 C1428 G1429 C1430 G1435 G1436 C1437 G1441 G1442 A1444A C1445 A1449 G1449A U1454 G1455 A1460 G1461 C1462 A1471 C1474 A1477 G1478 G1479 G1480 U1482 G1483 G1484 G1485 A1486 G1487 C1493
A1494 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 U1520 G1521 G1522 G1525 G1526 G1527 A1528 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1547 C1557 A1558 G1559 A1566 A1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 A1583 C1585 A1586
U1590 G1591 C1592 G1593 G1594 G1595 A1596 A1597 C1598 C1599 C1607 A1608 A1609 A1610 C1611 C1615 A1616 C1617 G1622 U1629 G1630 C1636 A1637 C1638 U1639 C1640 C1644 G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 C1660 A1665 G1666 G1667 A1668 A1669 G1674 C1675 G1678 U1679 U1680 G1681 C1686
U1693 C1694 G1695 G1725 G1728 A1729 U1730 G1731 A1732 G1733 G1743 C1752 G1753 G1756 A1762 G1763 G1764 G1769 G1770 C1771 G1772 A1773 C1774 U1779 A1780 C1781 C1782 A1783 A1784 A1787 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 A1812 G1813 G1814
A1815 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 A1847 A1848 G1849 G1850 A1854 G1858 A1859 U1864 G1869 C1870 A1871 A1872 G1878 C1882 G1883 G1888 A1889 G1899 A1900 G1903 G1906 C1909 A1913 C1914 U1915 A1918 A1919 C1920
G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 C1942 U1943 A1952 U1955 U1956 C1957 C1958 C1961 C1962 U1963 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 C1982 C1990 U1991 G1992 U1993 C1996 G2010 U2011 G2012 A2019 A2020 C2021 U2022 G2023 U2028 G2029 A2030 A2031 G2032
A2033 G2037 G2038 C2043 G2046 U2047 G2048 A2051 G2052 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2072 C2073 U2074 U2075 U2086 G2087 G2093 U2096 U2102 C2103 G2104 C2105 G2106 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2126 G2127 C2128 C2129
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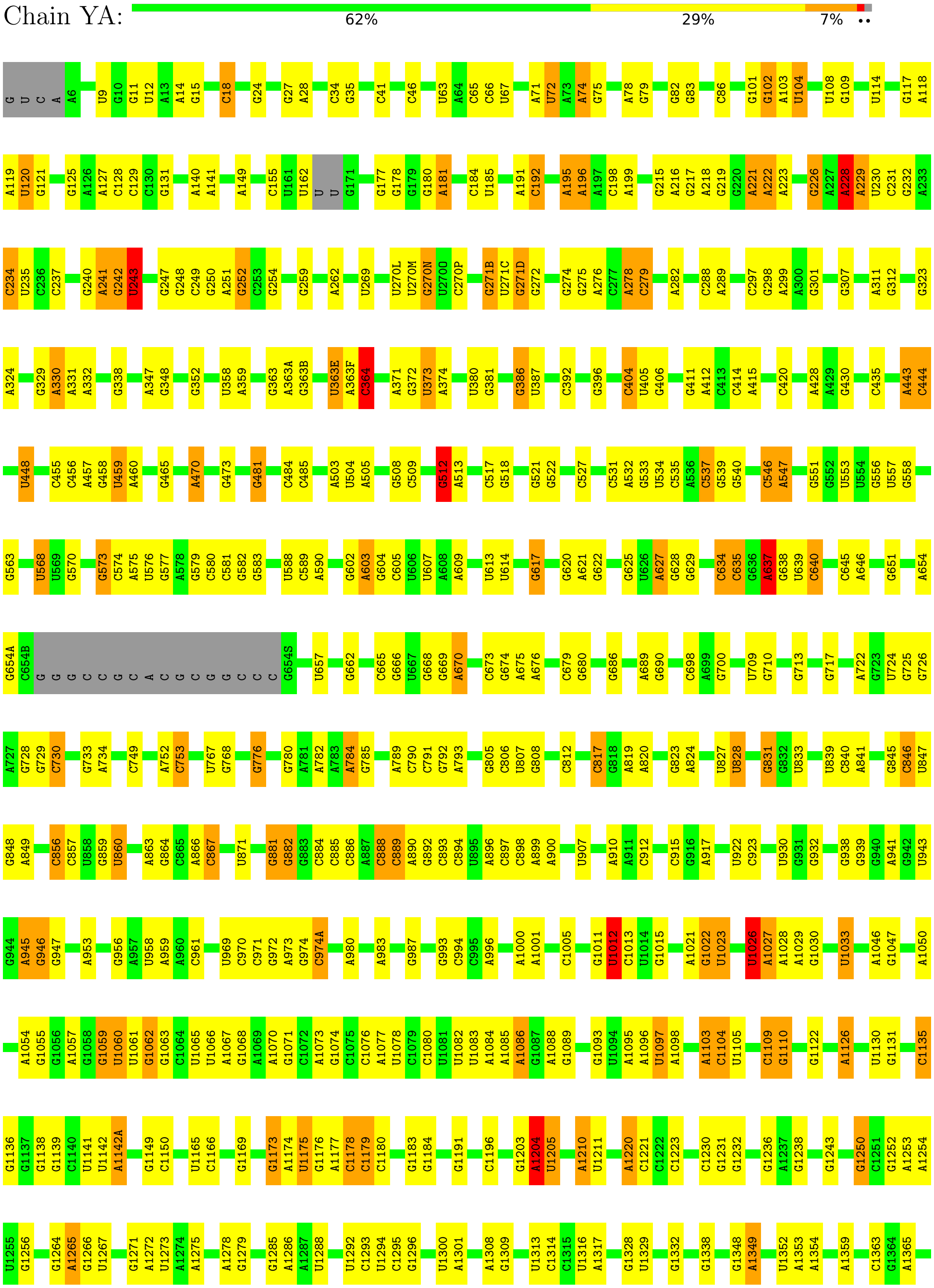
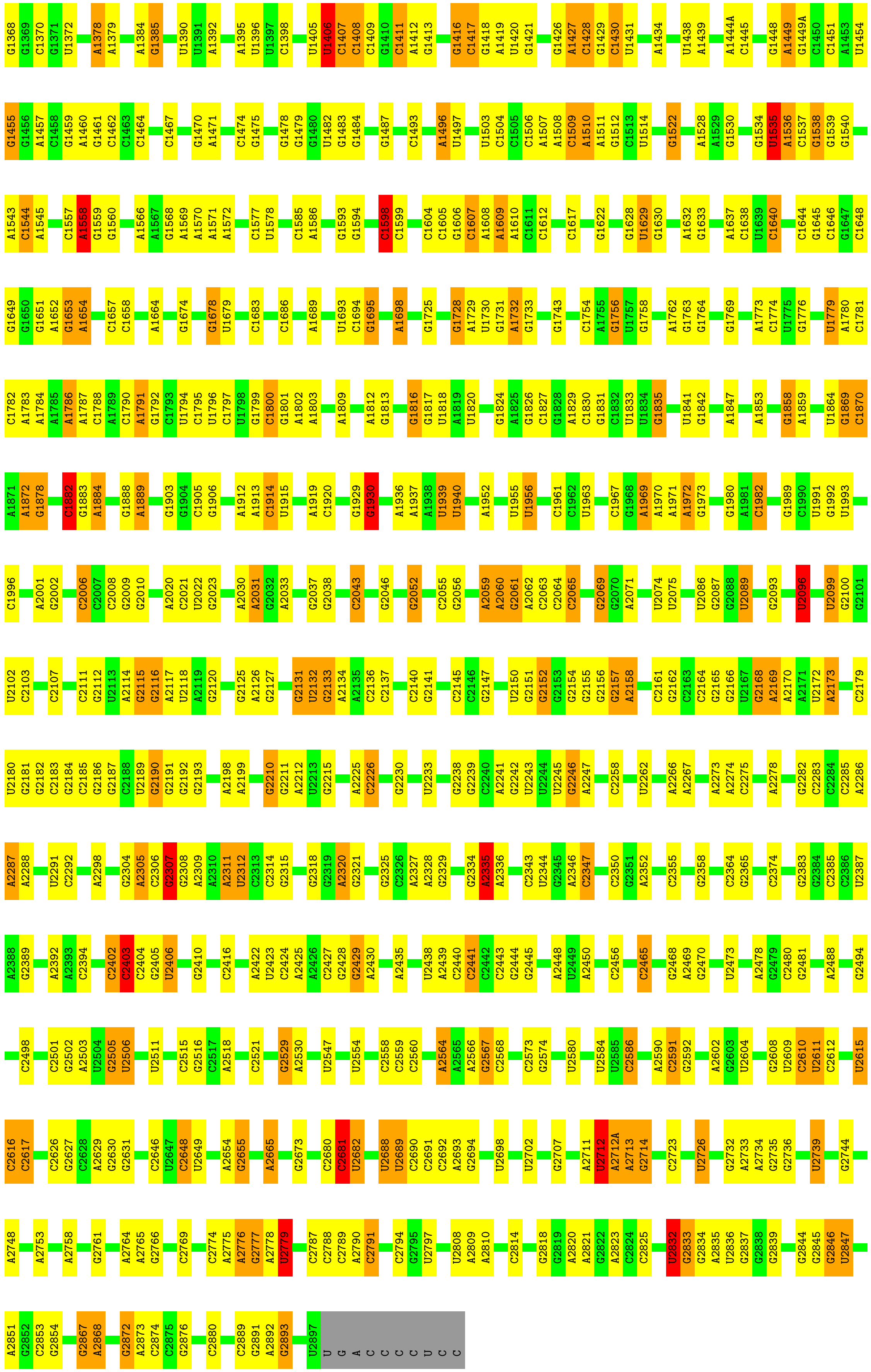
- Molecule 24: 23S rRNA

Chain YA:

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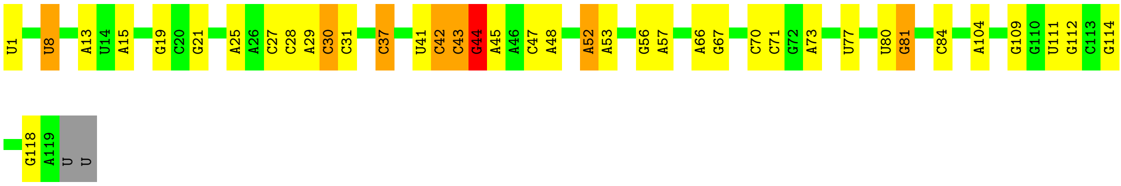
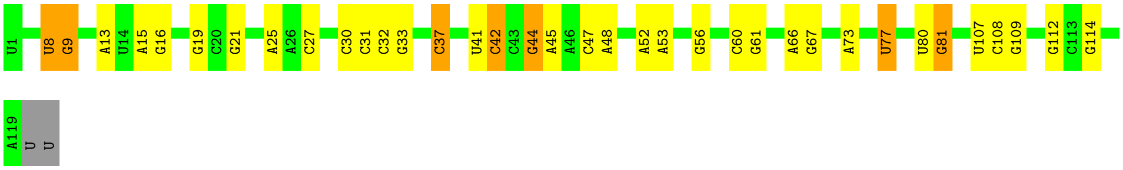
- Molecule 25: 5S rRNA

Chain RB:



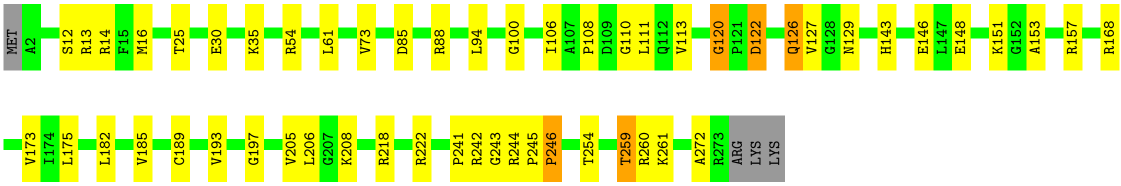
- Molecule 25: 5S rRNA

Chain YB:



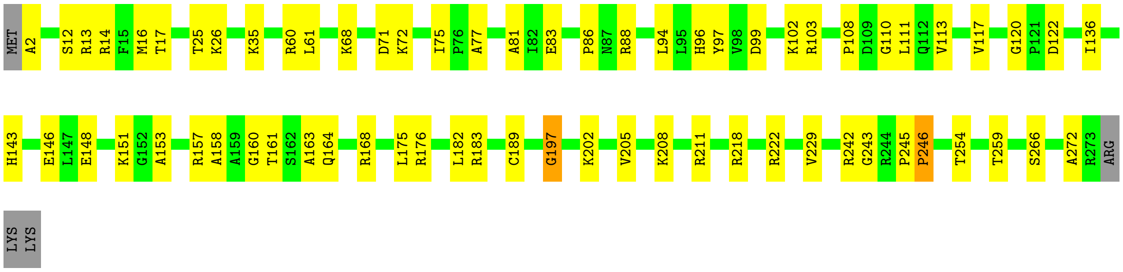
- Molecule 26: 50S ribosomal protein L2

Chain RD:



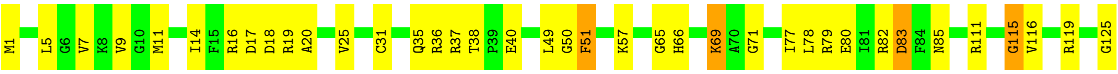
- Molecule 26: 50S ribosomal protein L2

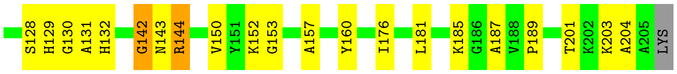
Chain YD:



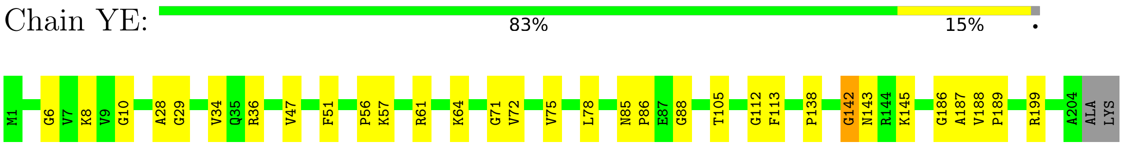
- Molecule 27: 50S ribosomal protein L3

Chain RE:

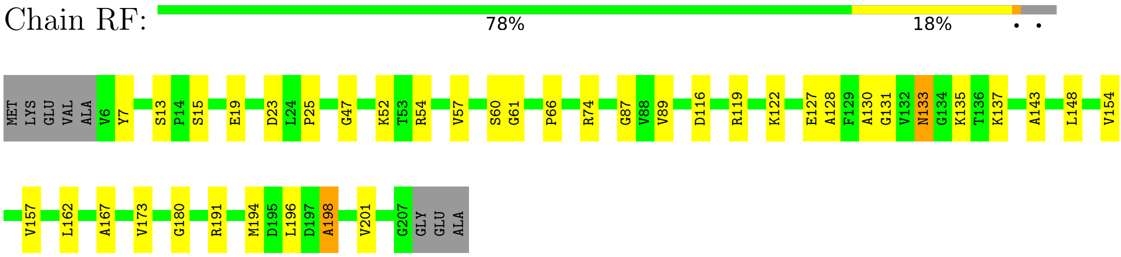




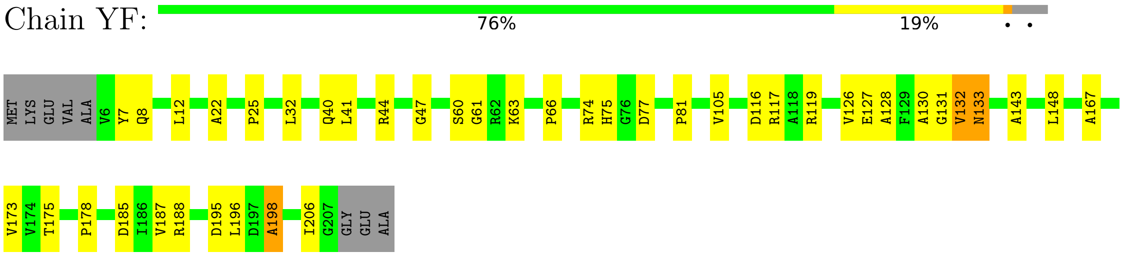
- Molecule 27: 50S ribosomal protein L3



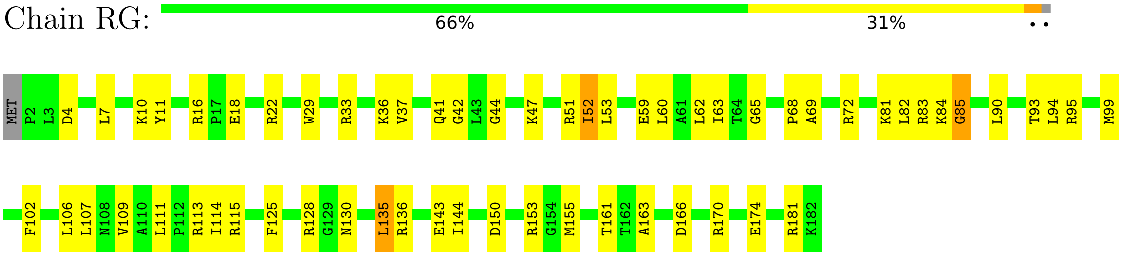
- Molecule 28: 50S ribosomal protein L4



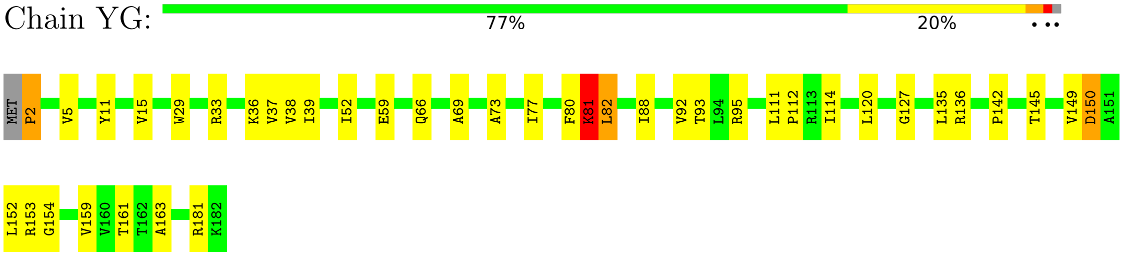
- Molecule 28: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L5

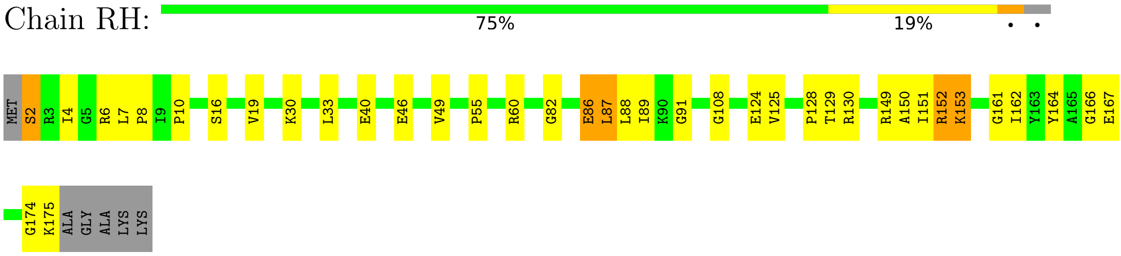


- Molecule 29: 50S ribosomal protein L5



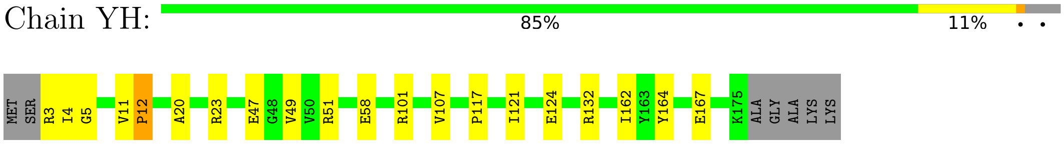
- Molecule 30: 50S ribosomal protein L6

Chain RH:



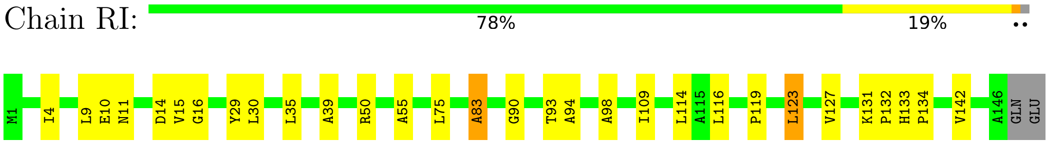
- Molecule 30: 50S ribosomal protein L6

Chain YH:



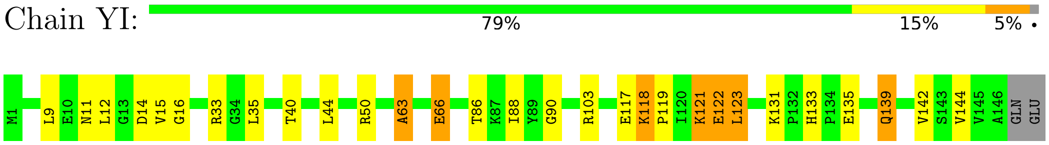
- Molecule 31: 50S ribosomal protein L9

Chain RI:



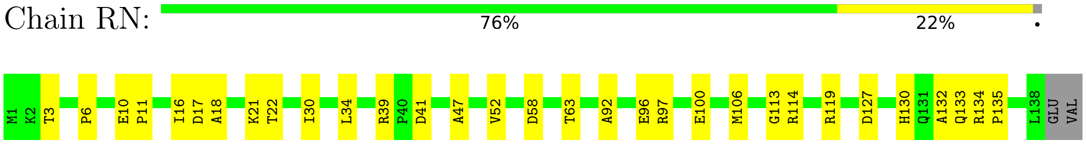
- Molecule 31: 50S ribosomal protein L9

Chain YI:



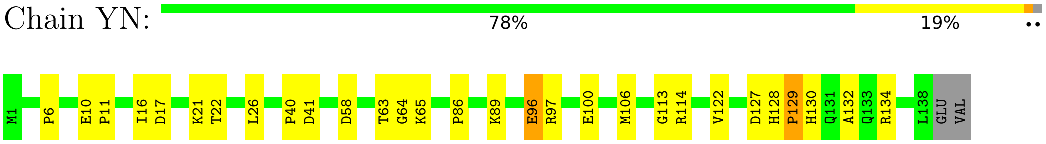
- Molecule 32: 50S ribosomal protein L13

Chain RN:



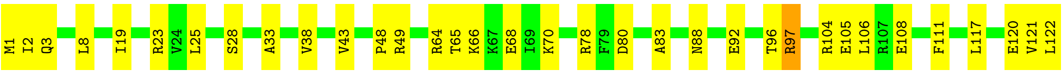
- Molecule 32: 50S ribosomal protein L13

Chain YN:



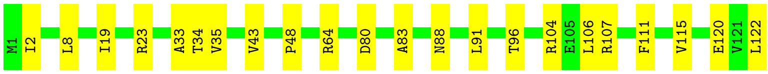
- Molecule 33: 50S ribosomal protein L14

Chain RO:



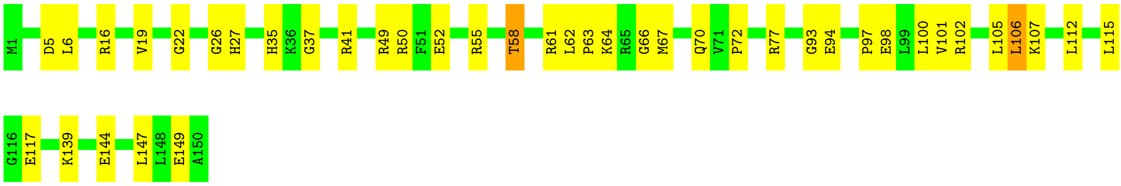
- Molecule 33: 50S ribosomal protein L14

Chain YO:



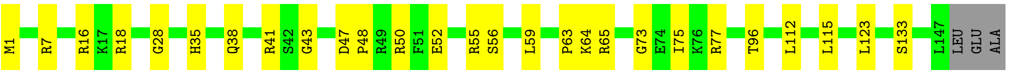
- Molecule 34: 50S ribosomal protein L15

Chain RP:



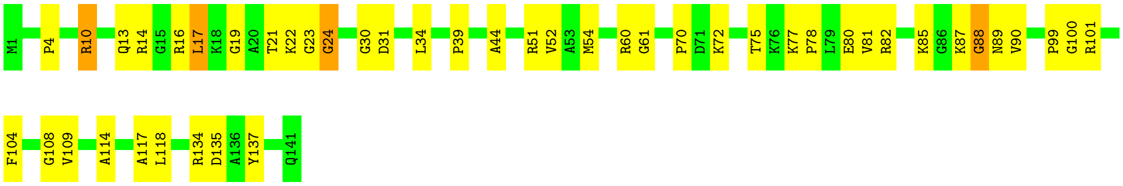
- Molecule 34: 50S ribosomal protein L15

Chain YP:



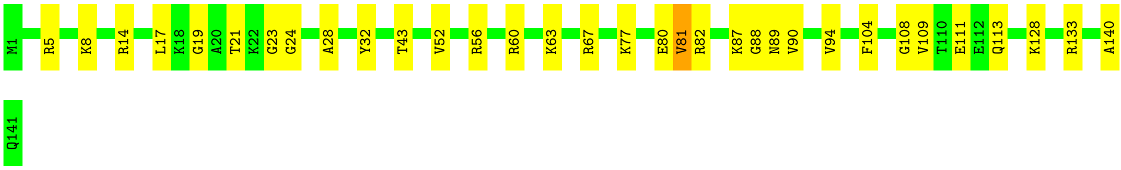
- Molecule 35: 50S ribosomal protein L16

Chain RQ:



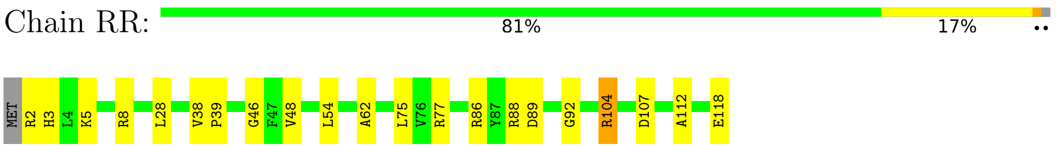
- Molecule 35: 50S ribosomal protein L16

Chain YQ:



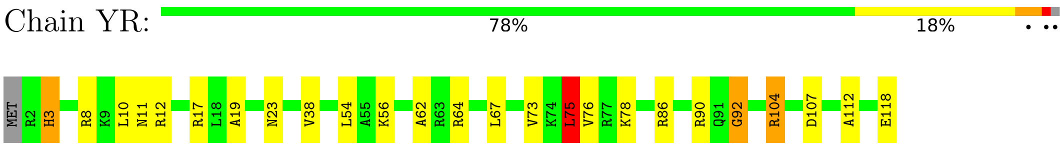
- Molecule 36: 50S ribosomal protein L17

Chain RR:



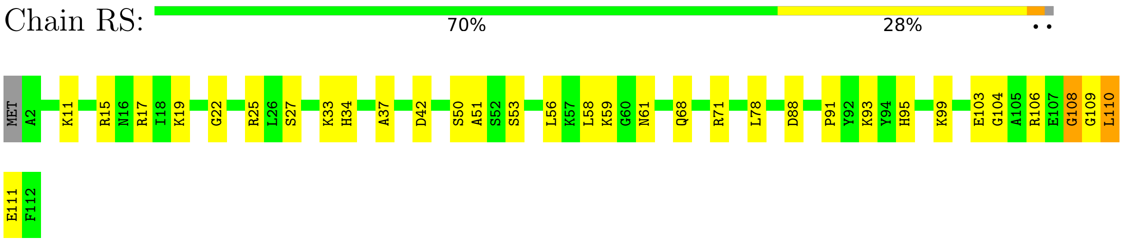
- Molecule 36: 50S ribosomal protein L17

Chain YR:



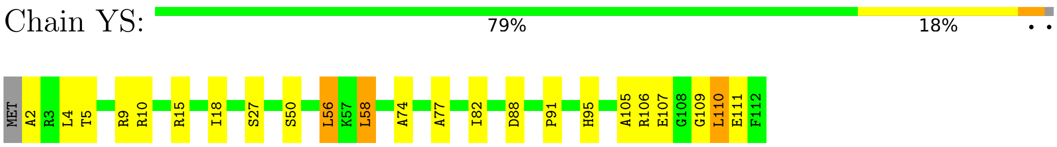
- Molecule 37: 50S ribosomal protein L18

Chain RS:



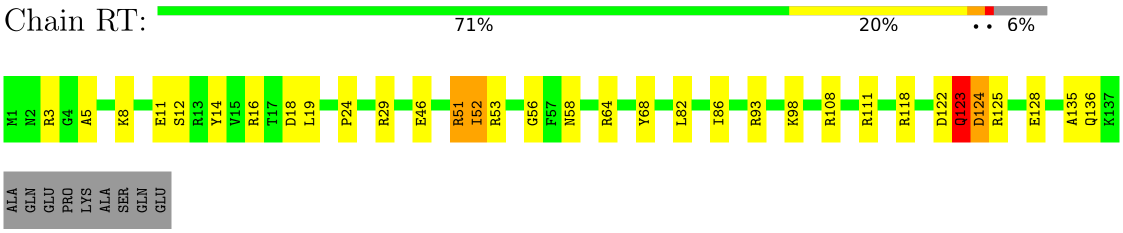
- Molecule 37: 50S ribosomal protein L18

Chain YS:



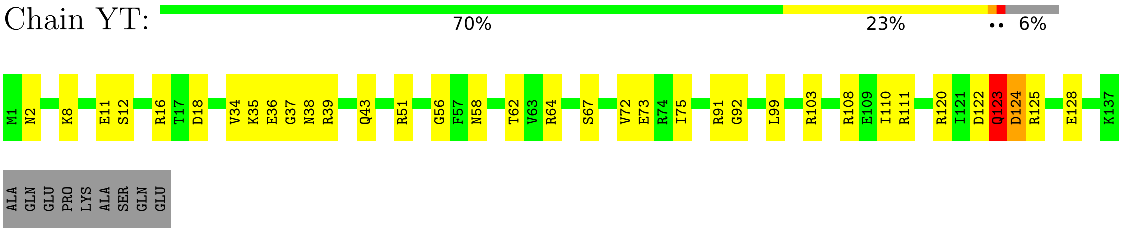
- Molecule 38: 50S ribosomal protein L19

Chain RT:



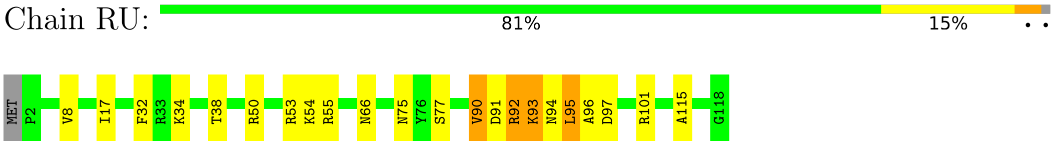
- Molecule 38: 50S ribosomal protein L19

Chain YT:



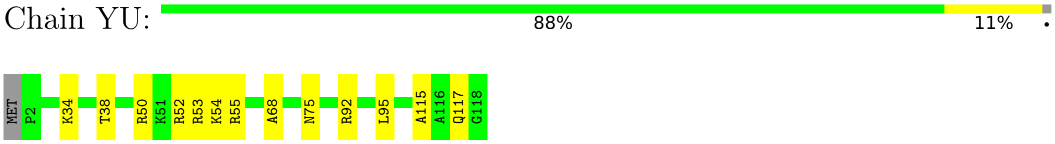
- Molecule 39: 50S ribosomal protein L20

Chain RU:



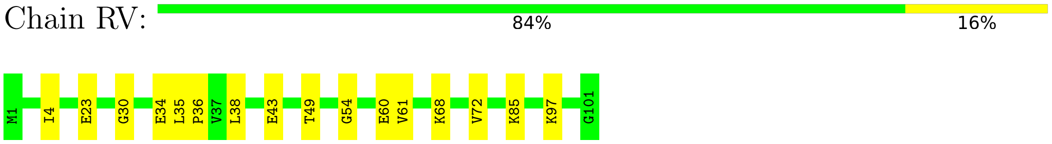
• Molecule 39: 50S ribosomal protein L20

Chain YU:



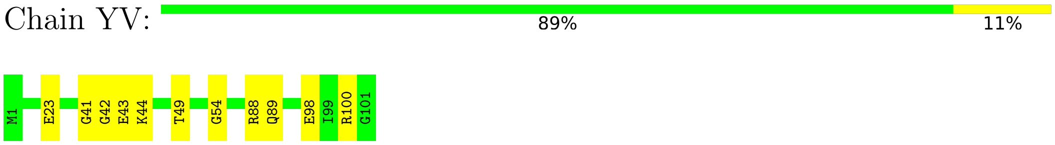
• Molecule 40: 50S ribosomal protein L21

Chain RV:



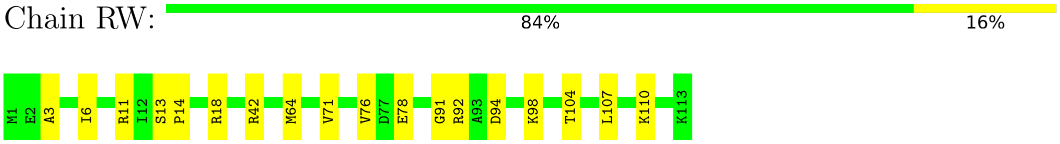
• Molecule 40: 50S ribosomal protein L21

Chain YV:



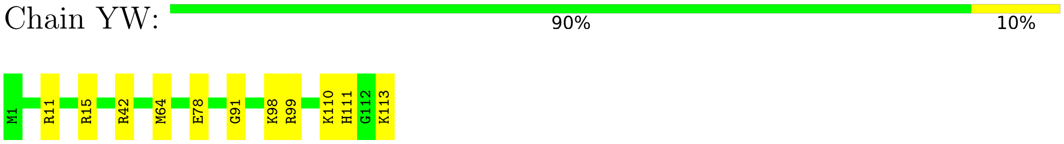
• Molecule 41: 50S ribosomal protein L22

Chain RW:



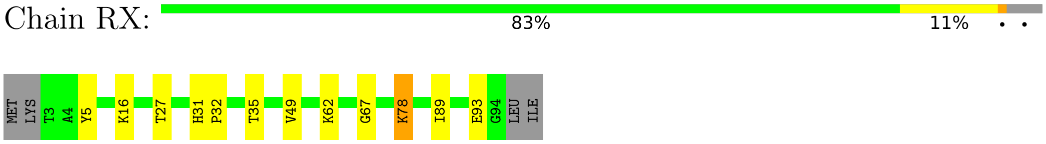
• Molecule 41: 50S ribosomal protein L22

Chain YW:

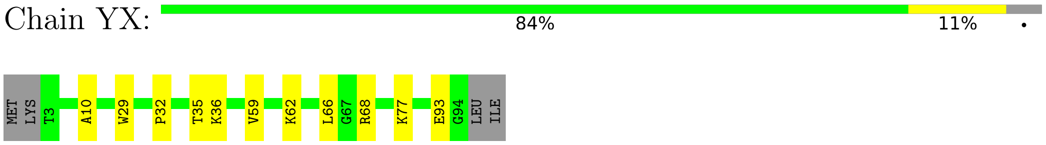


• Molecule 42: 50S ribosomal protein L23

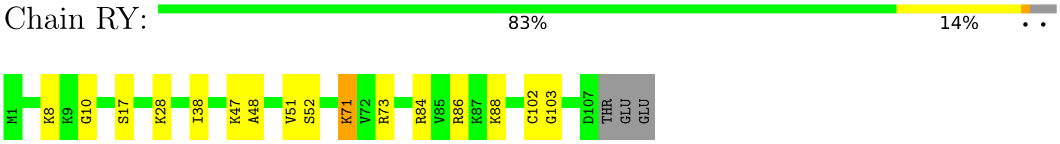
Chain RX:



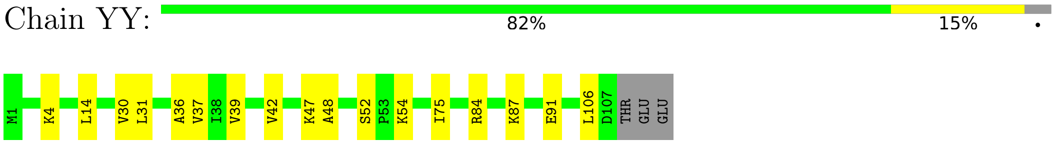
• Molecule 42: 50S ribosomal protein L23



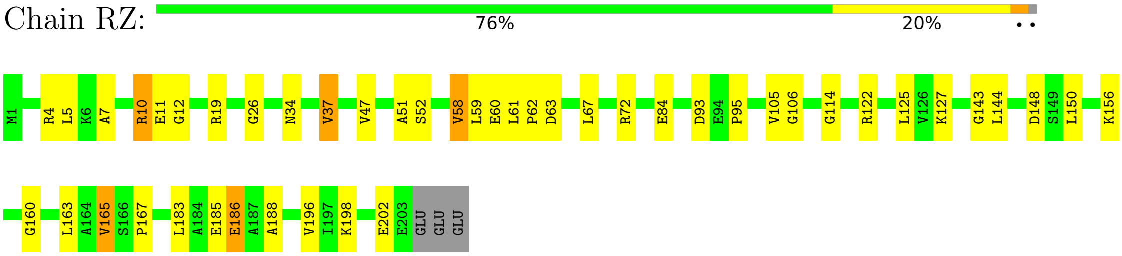
- Molecule 43: 50S ribosomal protein L24



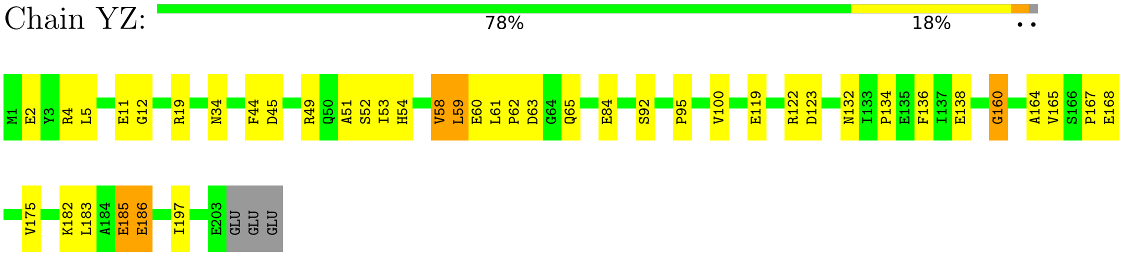
- Molecule 43: 50S ribosomal protein L24



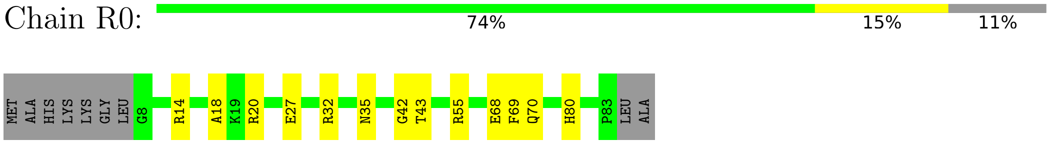
- Molecule 44: 50S ribosomal protein L25



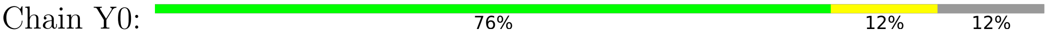
- Molecule 44: 50S ribosomal protein L25

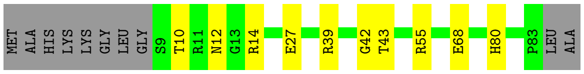


- Molecule 45: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L27





- Molecule 46: 50S ribosomal protein L28

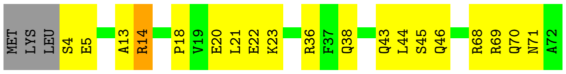
Chain R1:

- Molecule 46: 50S ribosomal protein L28

Chain Y1:

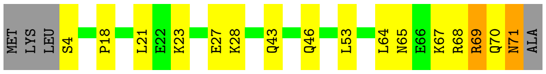
- Molecule 47: 50S ribosomal protein L29

Chain R2:



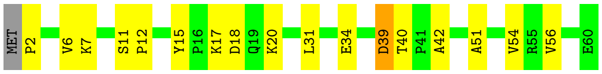
- Molecule 47: 50S ribosomal protein L29

Chain Y2:



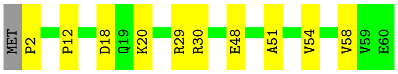
- Molecule 48: 50S ribosomal protein L30

Chain R3:



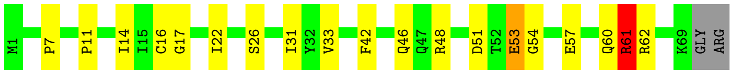
- Molecule 48: 50S ribosomal protein L30

Chain Y3:



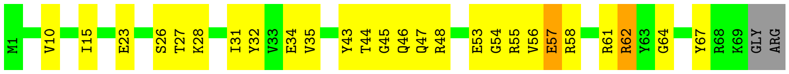
- Molecule 49: 50S ribosomal protein L31

Chain R4:



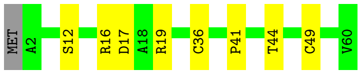
- Molecule 49: 50S ribosomal protein L31

Chain Y4:



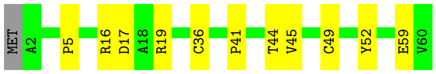
- Molecule 50: 50S ribosomal protein L32

Chain R5:



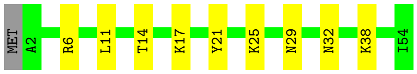
- Molecule 50: 50S ribosomal protein L32

Chain Y5:



- Molecule 51: 50S ribosomal protein L33

Chain R6:

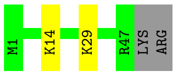


- Molecule 51: 50S ribosomal protein L33

Chain Y6:

- Molecule 52: 50S ribosomal protein L34

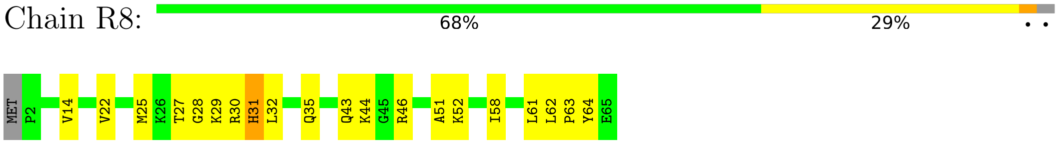
Chain R7:



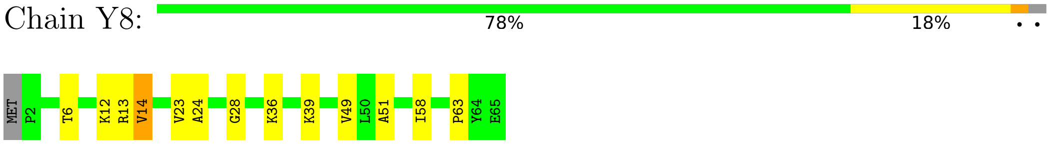
- Molecule 52: 50S ribosomal protein L34

Chain Y7:

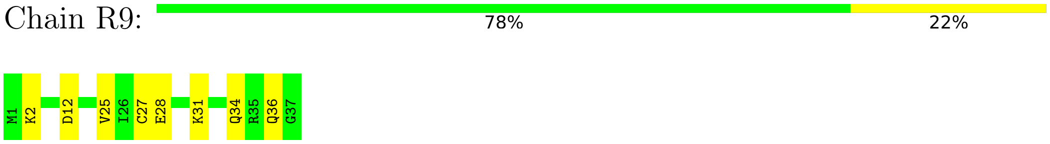
- Molecule 53: 50S ribosomal protein L35



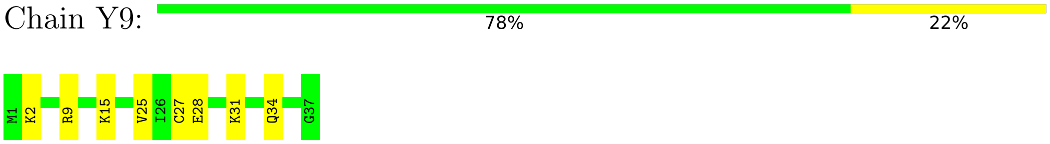
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



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	209.79Å 451.91Å 621.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.71 – 3.10	Depositor
% Data completeness (in resolution range)	98.0 (152.71-3.10)	Depositor
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.244 , 0.274	Depositor
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.231	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	289311	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 1MG, ZN, MG, 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	0.36	0/36098	1.03	113/56341 (0.2%)
1	XA	0.37	2/36101 (0.0%)	1.04	128/56346 (0.2%)
2	QB	0.27	0/1942	0.54	0/2619
2	XB	0.27	0/1950	0.51	0/2630
3	QC	0.27	0/1629	0.53	0/2195
3	XC	0.26	0/1629	0.57	1/2195 (0.0%)
4	QD	0.44	0/1733	0.77	2/2318 (0.1%)
4	XD	0.35	0/1733	0.78	3/2318 (0.1%)
5	QE	0.27	0/1171	0.51	0/1576
5	XE	0.28	0/1171	0.51	0/1576
6	QF	0.26	0/856	0.46	0/1154
6	XF	0.25	0/856	0.47	0/1154
7	QG	0.27	0/1276	0.51	0/1709
7	XG	0.25	0/1276	0.48	0/1709
8	QH	0.27	0/1128	0.49	0/1517
8	XH	0.27	0/1128	0.49	0/1517
9	QI	0.27	0/1029	0.58	1/1379 (0.1%)
9	XI	0.28	0/1017	0.66	2/1365 (0.1%)
10	QJ	0.27	0/814	0.56	0/1095
10	XJ	0.27	0/790	0.51	0/1063
11	QK	0.27	0/900	0.51	0/1213
11	XK	0.26	0/879	0.49	0/1187
12	QL	0.29	0/991	0.52	0/1327
12	XL	0.28	0/972	0.52	0/1301
13	QM	0.27	0/965	0.57	0/1292
13	XM	0.26	0/956	0.55	0/1281
14	QN	0.30	0/501	0.58	1/664 (0.2%)
14	XN	0.29	0/501	0.55	1/664 (0.2%)
15	QO	0.26	0/745	0.48	0/992
15	XO	0.23	0/740	0.42	0/987
16	QP	0.27	0/721	0.50	0/970
16	XP	0.26	0/721	0.46	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.26	0/847	0.49	0/1131
17	XQ	0.27	0/847	0.47	0/1131
18	QR	0.27	0/579	0.56	0/768
18	XR	0.25	0/579	0.51	0/768
19	QS	0.27	0/680	0.60	0/915
19	XS	0.25	0/689	0.54	0/926
20	QT	0.28	0/765	0.52	0/1007
20	XT	0.24	0/765	0.54	1/1007 (0.1%)
21	QU	0.26	0/221	0.52	0/288
21	XU	0.25	0/221	0.53	0/288
22	QV	0.31	0/380	1.06	2/590 (0.3%)
22	XV	0.29	0/332	1.00	0/515
23	QX	0.53	0/243	1.05	0/377
23	XX	0.58	0/294	1.15	1/457 (0.2%)
24	RA	0.43	0/69498	1.05	263/108491 (0.2%)
24	YA	0.49	0/69543	1.05	237/108563 (0.2%)
25	RB	0.37	0/2878	1.11	19/4490 (0.4%)
25	YB	0.44	0/2878	1.10	17/4490 (0.4%)
26	RD	0.31	0/2165	0.49	0/2919
26	YD	0.33	0/2165	0.50	0/2919
27	RE	0.31	0/1601	0.58	0/2160
27	YE	0.32	0/1596	0.53	0/2153
28	RF	0.30	0/1620	0.50	0/2194
28	YF	0.32	0/1620	0.48	0/2194
29	RG	0.27	0/1499	0.57	0/2016
29	YG	0.27	0/1499	0.59	2/2016 (0.1%)
30	RH	0.28	0/1362	0.56	0/1841
30	YH	0.31	0/1356	0.52	0/1833
31	RI	0.27	0/1151	0.62	0/1558
31	YI	0.27	0/1151	0.57	0/1558
32	RN	0.28	0/1131	0.50	0/1525
32	YN	0.32	0/1131	0.51	0/1525
33	RO	0.31	0/943	0.50	0/1269
33	YO	0.32	0/943	0.52	0/1269
34	RP	0.30	0/1162	0.62	0/1544
34	YP	0.31	0/1139	0.54	0/1514
35	RQ	0.29	0/1143	0.56	0/1527
35	YQ	0.32	0/1143	0.57	0/1527
36	RR	0.28	0/974	0.53	0/1302
36	YR	0.30	0/974	0.55	1/1302 (0.1%)
37	RS	0.27	0/892	0.61	1/1187 (0.1%)
37	YS	0.29	0/892	0.61	1/1187 (0.1%)
38	RT	0.27	0/1155	0.56	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YT	0.30	0/1155	0.55	1/1542 (0.1%)
39	RU	0.28	0/982	0.49	0/1306
39	YU	0.31	0/982	0.44	0/1306
40	RV	0.29	0/790	0.54	0/1057
40	YV	0.33	0/790	0.54	0/1057
41	RW	0.28	0/911	0.48	0/1220
41	YW	0.31	0/911	0.50	0/1220
42	RX	0.29	0/739	0.50	0/993
42	YX	0.31	0/739	0.52	0/993
43	RY	0.28	0/831	0.48	0/1108
43	YY	0.30	0/831	0.47	0/1108
44	RZ	0.32	0/1634	0.61	1/2216 (0.0%)
44	YZ	0.31	0/1634	0.56	0/2216
45	R0	0.29	0/611	0.49	0/814
45	Y0	0.32	0/607	0.50	0/809
46	R1	0.30	0/770	0.54	0/1022
46	Y1	0.31	0/736	0.54	0/978
47	R2	0.24	0/583	0.42	0/771
47	Y2	0.30	0/577	0.45	0/764
48	R3	0.26	0/474	0.51	0/635
48	Y3	0.27	0/474	0.52	0/635
49	R4	0.29	0/578	0.59	0/776
49	Y4	0.28	0/578	0.56	0/776
50	R5	0.30	0/473	0.48	0/639
50	Y5	0.32	0/473	0.49	0/639
51	R6	0.28	0/460	0.47	0/613
51	Y6	0.31	0/460	0.47	0/613
52	R7	0.27	0/417	0.42	0/550
52	Y7	0.30	0/426	0.45	0/561
53	R8	0.31	0/525	0.54	0/691
53	Y8	0.33	0/525	0.50	0/691
54	R9	0.27	0/310	0.44	0/407
54	Y9	0.31	0/310	0.45	0/407
All	All	0.39	2/312861 (0.0%)	0.94	799/467540 (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
1	XA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	17
2	XB	0	22
3	QC	0	16
3	XC	0	19
5	QE	0	5
5	XE	0	8
6	QF	0	5
7	QG	0	8
7	XG	0	8
8	QH	0	4
8	XH	0	5
9	QI	0	12
9	XI	0	11
10	QJ	0	12
10	XJ	0	9
11	QK	0	1
11	XK	0	4
12	QL	0	10
12	XL	0	10
13	QM	0	19
13	XM	0	15
14	QN	0	1
14	XN	0	7
15	QO	0	2
15	XO	0	2
16	QP	0	3
16	XP	0	4
17	QQ	0	3
17	XQ	0	4
18	QR	0	5
18	XR	0	3
19	QS	0	12
19	XS	0	21
20	QT	0	16
20	XT	0	12
21	QU	0	2
21	XU	0	2
26	RD	0	11
26	YD	0	8
27	RE	0	20
27	YE	0	7
28	RF	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	YF	0	14
29	RG	0	16
29	YG	0	13
30	RH	0	24
30	YH	0	2
31	RI	0	21
31	YI	0	22
32	RN	0	12
32	YN	0	10
33	RO	0	1
33	YO	0	1
34	RP	0	25
34	YP	0	8
35	RQ	0	14
35	YQ	0	13
36	RR	0	3
36	YR	0	5
37	RS	0	13
37	YS	0	9
38	RT	0	13
38	YT	0	11
39	RU	0	7
39	YU	0	2
40	RV	0	6
40	YV	0	6
41	RW	0	4
41	YW	0	3
42	RX	0	4
42	YX	0	2
43	RY	0	4
43	YY	0	4
44	RZ	0	20
44	YZ	0	16
45	R0	0	2
45	Y0	0	2
46	R1	0	7
46	Y1	0	8
47	R2	0	8
47	Y2	0	3
48	R3	0	1
48	Y3	0	2
49	R4	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	Y4	0	12
50	Y5	0	1
53	R8	0	12
53	Y8	0	1
54	R9	0	1
All	All	0	775

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	358	U	O4'-C1'	-6.29	1.33	1.41
1	XA	358	U	C5'-C4'	5.05	1.57	1.51

The worst 5 of 799 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	359	U	C2-N1-C1'	-18.46	95.55	117.70
1	XA	359	U	O5'-P-OP1	-17.99	89.11	110.70
1	XA	359	U	C6-N1-C1'	16.75	144.64	121.20
1	XA	328	C	N1-C2-O2	13.70	127.12	118.90
24	RA	1092	C	N1-C2-O2	13.63	127.08	118.90

There are no chirality outliers.

5 of 775 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
2	QB	19	HIS	Peptide
2	QB	21	ARG	Peptide
2	QB	22	LYS	Peptide
2	QB	34	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	362	0
1	XA	32249	0	16278	389	0
2	QB	1907	0	1958	22	0
2	XB	1915	0	1969	24	0
3	QC	1605	0	1668	22	0
3	XC	1605	0	1668	28	0
4	QD	1703	0	1763	47	0
4	XD	1703	0	1763	36	0
5	QE	1155	0	1213	13	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	13	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	20	0
8	QH	1108	0	1165	15	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	26	0
9	XI	998	0	1024	23	0
10	QJ	801	0	849	16	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	14	0
11	XK	864	0	881	20	0
12	QL	975	0	1062	21	0
12	XL	956	0	1046	11	0
13	QM	955	0	1021	18	0
13	XM	946	0	1008	22	0
14	QN	492	0	529	10	0
14	XN	492	0	529	14	0
15	QO	734	0	771	7	0
15	XO	729	0	768	5	0
16	QP	705	0	725	13	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	8	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	8	0
18	XR	574	0	644	7	0
19	QS	665	0	686	15	0
19	XS	674	0	699	9	0
20	QT	763	0	861	16	0
20	XT	763	0	861	10	0
21	QU	217	0	234	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	XU	217	0	234	3	0
22	QV	365	0	186	4	0
22	XV	322	0	164	6	0
23	QX	217	0	110	5	0
23	XX	262	0	132	3	0
24	RA	62051	0	31280	482	0
24	YA	62091	0	31294	478	0
25	RB	2573	0	1306	20	0
25	YB	2573	0	1306	15	0
26	RD	2115	0	2195	37	0
26	YD	2115	0	2195	42	0
27	RE	1568	0	1634	32	0
27	YE	1563	0	1629	19	0
28	RF	1585	0	1632	19	0
28	YF	1585	0	1632	20	0
29	RG	1474	0	1535	31	0
29	YG	1474	0	1535	21	0
30	RH	1336	0	1418	12	0
30	YH	1330	0	1413	11	0
31	RI	1136	0	1223	6	0
31	YI	1136	0	1223	8	0
32	RN	1104	0	1180	13	0
32	YN	1104	0	1180	12	0
33	RO	933	0	996	22	0
33	YO	933	0	996	15	0
34	RP	1145	0	1227	14	0
34	YP	1122	0	1205	17	0
35	RQ	1122	0	1178	24	0
35	YQ	1122	0	1179	20	0
36	RR	960	0	1021	11	0
36	YR	960	0	1021	17	0
37	RS	882	0	943	17	0
37	YS	882	0	943	11	0
38	RT	1141	0	1202	19	0
38	YT	1141	0	1202	18	0
39	RU	964	0	1021	14	0
39	YU	964	0	1021	10	0
40	RV	779	0	852	6	0
40	YV	779	0	852	3	0
41	RW	900	0	964	9	0
41	YW	900	0	964	6	0
42	RX	725	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	YX	725	0	778	6	0
43	RY	818	0	909	11	0
43	YY	818	0	909	8	0
44	RZ	1601	0	1630	22	0
44	YZ	1601	0	1630	24	0
45	R0	603	0	620	7	0
45	Y0	599	0	617	5	0
46	R1	763	0	848	9	0
46	Y1	729	0	802	7	0
47	R2	581	0	629	7	0
47	Y2	575	0	624	9	0
48	R3	469	0	518	10	0
48	Y3	469	0	518	5	0
49	R4	565	0	557	9	0
49	Y4	565	0	557	12	0
50	R5	459	0	476	7	0
50	Y5	459	0	476	8	0
51	R6	453	0	473	6	0
51	Y6	453	0	473	7	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	4	0
53	R8	517	0	582	10	0
53	Y8	517	0	582	8	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	6	0
55	QA	74	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QM	1	0	0	0	0
55	R0	1	0	0	0	0
55	R1	2	0	0	0	0
55	R8	1	0	0	0	0
55	RA	487	0	0	0	0
55	RB	6	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RI	1	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	RX	1	0	0	0	0
55	RY	1	0	0	0	0
55	XA	92	0	0	0	0
55	XE	1	0	0	0	0
55	XK	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XN	1	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	542	0	0	0	0
55	YB	15	0	0	0	0
55	YD	3	0	0	0	0
55	YE	3	0	0	0	0
55	YO	1	0	0	0	0
55	YQ	3	0	0	0	0
55	YR	2	0	0	0	0
55	YX	2	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	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	289311	0	196538	2694	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 6.

The worst 5 of 2694 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)
35:RQ:51:ARG:NH2	44:RZ:186:GLU:OE1	1.59	1.34
24:RA:2135:A:N6	24:RA:2156:G:H21	1.54	1.05
47:Y2:65:ASN:O	47:Y2:69:ARG:HG3	1.55	1.05
35:YQ:52:VAL:HG13	44:YZ:183:LEU:CD1	1.88	1.03
24:RA:2135:A:H62	24:RA:2156:G:N2	1.57	1.02

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%)	211 (91%)	22 (9%)	0	100	100
2	XB	234/256 (91%)	213 (91%)	21 (9%)	0	100	100
3	QC	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	QD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	10	39
4	XD	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	15	49
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	QI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
10	XJ	94/105 (90%)	90 (96%)	4 (4%)	0	100	100
11	QK	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	113 (92%)	10 (8%)	0	100	100
12	XL	120/132 (91%)	107 (89%)	13 (11%)	0	100	100
13	QM	118/126 (94%)	105 (89%)	12 (10%)	1 (1%)	19	54
13	XM	117/126 (93%)	103 (88%)	14 (12%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
14	XN	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	11 (13%)	0	100	100
20	QT	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	QU	23/27 (85%)	23 (100%)	0	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	258 (96%)	12 (4%)	0	100	100
26	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
27	RE	203/206 (98%)	171 (84%)	32 (16%)	0	100	100
27	YE	202/206 (98%)	193 (96%)	9 (4%)	0	100	100
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
29	YG	179/182 (98%)	161 (90%)	17 (10%)	1 (1%)	25	59
30	RH	172/180 (96%)	153 (89%)	18 (10%)	1 (1%)	25	59
30	YH	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
31	RI	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
31	YI	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
32	RN	136/140 (97%)	124 (91%)	12 (9%)	0	100	100
32	YN	136/140 (97%)	125 (92%)	11 (8%)	0	100	100
33	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
33	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	RP	148/150 (99%)	133 (90%)	15 (10%)	0	100	100
34	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	22	57
35	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	57
35	YQ	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
36	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
36	YR	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
37	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
37	YS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
38	RT	135/146 (92%)	123 (91%)	10 (7%)	2 (2%)	10	39
38	YT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	10	39
39	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	52
39	YU	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
40	RV	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
40	YV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
41	RW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
41	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
42	RX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
43	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	RZ	201/206 (98%)	182 (90%)	19 (10%)	0	100	100
44	YZ	201/206 (98%)	181 (90%)	20 (10%)	0	100	100
45	R0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
47	R2	67/72 (93%)	66 (98%)	1 (2%)	0	100	100
47	Y2	66/72 (92%)	63 (96%)	2 (3%)	1 (2%)	10	39
48	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	57 (85%)	10 (15%)	0	100	100
49	Y4	67/71 (94%)	54 (81%)	13 (19%)	0	100	100
50	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	51 (100%)	0	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	46 (100%)	0	0	100	100
53	R8	62/65 (95%)	49 (79%)	13 (21%)	0	100	100
53	Y8	62/65 (95%)	62 (100%)	0	0	100	100
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11484/12128 (95%)	10666 (93%)	802 (7%)	16 (0%)	51	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	155	LEU
38	RT	124	ASP
4	XD	155	LEU
4	XD	171	GLY
34	YP	63	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	203 (100%)	0	100	100
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	94
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	87
4	QD	180/181 (99%)	174 (97%)	6 (3%)	38	69
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	89
5	QE	116/123 (94%)	113 (97%)	3 (3%)	46	74
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	78
6	XF	90/90 (100%)	88 (98%)	2 (2%)	52	78
7	QG	126/127 (99%)	124 (98%)	2 (2%)	62	84
7	XG	126/127 (99%)	125 (99%)	1 (1%)	81	92
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	97 (99%)	1 (1%)	76	90
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	79
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	102 (99%)	1 (1%)	76	90
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76	90
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	71 (99%)	1 (1%)	67	86
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	60 (98%)	1 (2%)	62	84
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%)	72 (99%)	1 (1%)	67	86
20	QT	76/82 (93%)	76 (100%)	0	100	100
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
26	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
26	YD	214/218 (98%)	214 (100%)	0	100	100
27	RE	165/166 (99%)	165 (100%)	0	100	100
27	YE	165/166 (99%)	164 (99%)	1 (1%)	86	94
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%)	155 (100%)	0	100	100
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
30	RH	145/148 (98%)	144 (99%)	1 (1%)	84	93
30	YH	144/148 (97%)	143 (99%)	1 (1%)	84	93
31	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
31	YI	122/124 (98%)	121 (99%)	1 (1%)	81	92
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
33	RO	100/100 (100%)	99 (99%)	1 (1%)	76	90
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
35	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	90
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	120 (100%)	0	100	100
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	73 (99%)	1 (1%)	67	86
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	174/179 (97%)	172 (99%)	2 (1%)	73	89
44	YZ	174/179 (97%)	171 (98%)	3 (2%)	60	83
45	R0	61/67 (91%)	60 (98%)	1 (2%)	62	84
45	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
46	R1	82/83 (99%)	82 (100%)	0	100	100
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%)	62 (97%)	2 (3%)	40	70
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	80
49	R4	62/63 (98%)	61 (98%)	1 (2%)	62	84
49	Y4	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	57	81
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9706/10066 (96%)	9649 (99%)	57 (1%)	86	94

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R4	61	ARG
48	Y3	30	ARG
7	XG	94	ARG
47	Y2	71	ASN
44	YZ	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
7	XG	28	ASN
16	XP	14	ASN
29	RG	132	ASN
35	RQ	123	HIS
39	RU	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1521 (98%)	276 (18%)	34 (2%)
1	XA	1499/1521 (98%)	278 (18%)	35 (2%)
22	QV	16/17 (94%)	1 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	14/17 (82%)	2 (14%)	0
23	QX	9/19 (47%)	4 (44%)	1 (11%)
23	XX	11/19 (57%)	5 (45%)	0
24	RA	2877/2915 (98%)	547 (19%)	37 (1%)
24	YA	2880/2915 (98%)	529 (18%)	41 (1%)
25	RB	119/122 (97%)	17 (14%)	1 (0%)
25	YB	119/122 (97%)	16 (13%)	1 (0%)
All	All	9042/9188 (98%)	1675 (18%)	150 (1%)

5 of 1675 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	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	404	C
24	YA	2610	C
24	YA	827	U
24	YA	1210	A
24	RA	846	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
22	1MG	XV	37	22	18,26,27	0.75	0	19,39,42	0.98	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
22	1MG	QV	37	22	18,26,27	0.74	0	19,39,42	1.00	2 (10%)

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	1MG	XV	37	22	-	0/3/25/26	0/3/3/3
22	1MG	QV	37	22	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	XV	37	1MG	C5-C6-N1	2.31	117.37	113.90
22	QV	37	1MG	C5-C6-N1	2.29	117.34	113.90
22	XV	37	1MG	C8-N7-C5	2.24	107.25	102.99
22	QV	37	1MG	C8-N7-C5	2.22	107.22	102.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1285 ligands modelled in this entry, 1283 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	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	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
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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