wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 07:22 PM EDT

PDB ID	:	4LEL
Title	:	Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCG-G on the Ribosome
Authors	:	Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on	:	2013-06-25
Resolution	:	3.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

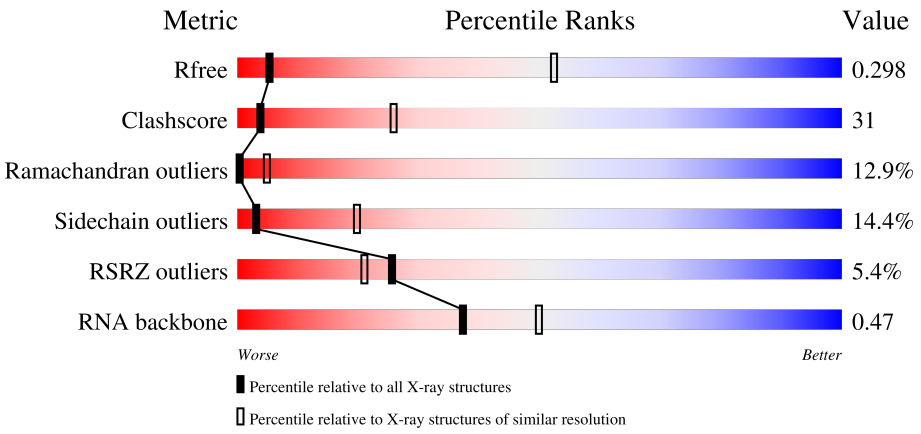
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	2%, 44%, 43%, 11%
1	XA	1522	%, 42%, 44%, 12%
2	QB	256	10%, 17%, 58%, 16%, 7%
2	XB	256	4%, 17%, 59%, 16%, 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	6% 23% 52% 10% 14%
3	XC	239	2% 23% 52% 10% 14%
4	QD	209	5% 25% 59% 13%
4	XD	209	2% 24% 62% 12%
5	QE	162	6% 28% 52% 12% 7%
5	XE	162	4% 30% 51% 12% 7%
6	QF	101	3% 26% 58% 15%
6	XF	101	4% 21% 62% 16%
7	QG	156	14% 28% 62% 10%
7	XG	156	8% 29% 60% 10%
8	QH	138	9% 28% 59% 12%
8	XH	138	4% 26% 61% 12%
9	QI	128	14% 22% 64% 12%
9	XI	128	4% 23% 62% 14%
10	QJ	105	21% 18% 63% 12% 6%
10	XJ	105	15% 17% 64% 12% 6%
11	QK	129	11% 34% 47% 11% 8%
11	XK	129	7% 32% 48% 12% 8%
12	QL	132	11% 31% 47% 14% 5%
12	XL	132	5% 29% 49% 14% 5%
13	QM	126	10% 20% 53% 21%
13	XM	126	4% 20% 53% 21%
14	QN	61	15% 16% 57% 16% 8%
14	XN	61	5% 13% 62% 18% 5%
15	QO	89	4% 34% 54% 11%

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Mol	Chain	Length	Quality of chain
15	XO	89	%, 31%, 56%, 11%
16	QP	88	13%, 16%, 63%, 15%, 5%
16	XP	88	11%, 19%, 58%, 16%, 5%
17	QQ	105	4%, 36%, 48%, 11%, 5%
17	XQ	105	8%, 33%, 50%, 11%, 5%
18	QR	88	9%, 24%, 43%, 11%, 20%
18	XR	88	6%, 23%, 44%, 11%, 20%
19	QS	93	15%, 25%, 39%, 24%, 10%
19	XS	93	5%, 26%, 39%, 22%, 10%
20	QT	106	2%, 25%, 49%, 19%, 7%
20	XT	106	7%, 25%, 49%, 19%, 7%
21	QU	27	56%, 26%, 48%, 19%, 7%
21	XU	27	22%, 22%, 52%, 19%, 7%
22	QV	77	%, 32%, 49%, 17%
22	XV	77	%, 32%, 51%, 16%
23	QX	25	8%, 8%, 12%, 12%, 68%
23	XX	25	8%, 12%, 8%, 12%, 68%
24	QY	18	11%, 33%, 28%, 17%, 22%
24	XY	18	33%, 28%, 17%, 22%
25	RA	2916	3%, 44%, 43%, 11%
25	YA	2916	3%, 44%, 42%, 12%
26	RB	122	2%, 52%, 35%, 11%
26	YB	122	51%, 37%, 11%
27	RD	276	%, 30%, 52%, 15%
27	YD	276	%, 29%, 53%, 15%

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Mol	Chain	Length	Quality of chain
28	RE	206	4% 24% 48% 23% 5%
28	YE	206	3% 23% 48% 23% 5%
29	RF	210	2% 34% 48% 13%
29	YF	210	2% 34% 49% 12%
30	RG	182	11% 23% 58% 16%
30	YG	182	4% 23% 58% 16%
31	RH	180	19% 23% 44% 19% 8% 6%
31	YH	180	8% 23% 44% 20% 8% 6%
32	RI	148	10% 36% 47% 14%
32	YI	148	5% 48% 36% 14%
33	RN	140	7% 18% 54% 26%
33	YN	140	2% 17% 54% 26%
34	RO	122	% 34% 56% 9%
34	YO	122	35% 54% 9%
35	RP	150	15% 19% 50% 23% 8%
35	YP	150	4% 20% 50% 23% 7%
36	RQ	141	6% 32% 50% 16%
36	YQ	141	% 33% 48% 16%
37	RR	118	33% 48% 16%
37	YR	118	% 32% 50% 15%
38	RS	112	9% 14% 61% 19% 5%
38	YS	112	2% 12% 62% 20%
39	RT	146	3% 22% 50% 19% 6%
39	YT	146	5% 21% 50% 20% 6%
40	RU	118	4% 33% 53% 12%

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Mol	Chain	Length	Quality of chain
40	YU	118	2%, 31%, 53%, 13%
41	RV	101	2%, 28%, 51%, 21%
41	YV	101	5%, 27%, 52%, 21%
42	RW	113	4%, 28%, 50%, 19%
42	YW	113	3%, 29%, 50%, 19%
43	RX	96	%, 39%, 43%, 15%
43	YX	96	2%, 36%, 45%, 15%
44	RY	110	30%, 16%, 45%, 28%, 7%
44	YY	110	10%, 18%, 43%, 28%, 7%
45	RZ	206	5%, 41%, 39%, 8%, 11%
45	YZ	206	%, 45%, 33%, 11%, 11%
46	R0	85	9%, 68%, 25%
46	Y0	85	64%, 31%
47	R1	98	8%, 31%, 47%, 18%
47	Y1	98	7%, 30%, 49%, 17%
48	R2	72	3%, 22%, 54%, 18%
48	Y2	72	3%, 22%, 54%, 18%
49	R3	60	30%, 33%, 50%, 15%
49	Y3	60	18%, 33%, 50%, 13%
50	R4	71	27%, 6%, 44%, 39%, 11%
50	Y4	71	3%, 7%, 42%, 39%, 11%
51	R5	60	7%, 22%, 47%, 23%, 7%
51	Y5	60	12%, 22%, 48%, 22%, 7%
52	R6	54	61%, 9%, 44%, 31%, 6%, 9%
52	Y6	54	69%, 11%, 43%, 31%, 6%, 9%

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Mol	Chain	Length	Quality of chain
53	R7	49	2% 37% 55% 8%
53	Y7	49	8% 33% 59% 8%
54	R8	65	6% 26% 40% 26% 6%
54	Y8	65	5% 22% 43% 28% 6%
55	R9	37	81% 49% 49%
55	Y9	37	97% 57% 38% 5%
56	Z6	3	67% 33%
56	Z8	3	33% 67%

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
57	MG	QA	1618	-	-	-	X
57	MG	QA	1623	-	-	-	X
57	MG	QA	1630	-	-	-	X
57	MG	QA	1661	-	-	-	X
57	MG	R0	101	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3124	-	-	-	X
57	MG	RA	3134	-	-	-	X
57	MG	RA	3163	-	-	-	X
57	MG	RA	3180	-	-	-	X
57	MG	RA	3189	-	-	-	X
57	MG	RA	3216	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RP	202	-	-	-	X
57	MG	XA	1605	-	-	-	X
57	MG	XA	1606	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1633	-	-	-	X
57	MG	XA	1643	-	-	-	X
57	MG	XA	1648	-	-	-	X
57	MG	XA	1654	-	-	-	X
57	MG	XA	1655	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3054	-	-	-	X
57	MG	YA	3089	-	-	-	X
57	MG	YA	3124	-	-	-	X
57	MG	YA	3128	-	-	-	X
57	MG	YA	3160	-	-	-	X
57	MG	YA	3174	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3229	-	-	-	X
57	MG	YA	3248	-	-	-	X
57	MG	YA	3258	-	-	-	X
57	MG	YB	202	-	-	-	X
57	MG	YD	302	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 291958 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	32247	14353	5981	10414	1499	0	0	0
1	XA	1500	32249	14354	5984	10412	1499	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	237	1924	1228	344	347	5	0	0	0
2	XB	237	1924	1228	344	347	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	QH	138	1116	705	215	193	3	0	0	0
8	XH	138	1116	705	215	193	3	0	0	0

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

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

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

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

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

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

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	121	964	597	199	166	2	0	0	0
13	XM	121	964	597	199	166	2	0	0	0

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

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

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

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

- 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	84	674	430	126	116	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 S21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	QV	77	1644	732	297	538	77	0	0	0
22	XV	77	1644	732	297	538	77	0	0	0

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	8	173	77	33	55	8	0	0	0
23	XX	8	173	77	33	55	8	0	0	0

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	QY	14	303	135	55	99	14	0	0	0
24	XY	14	303	135	55	99	14	0	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	RH	170	1307	829	245	232	1	0	0	0
31	YH	170	1307	829	245	232	1	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	RR	118	968	604	203	160	1	0	0	0
37	YR	118	968	604	203	160	1	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RY	102	785	505	150	125	5	0	0	0
44	YY	102	785	505	150	125	5	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	R0	82	648	401	138	108	1	0	0	0
46	Y0	82	648	401	138	108	1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	R4	71	581	364	108	104	5	0	0	0
50	Y4	71	581	364	108	104	5	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	R6	49	424	264	87	69	4	0	0	0
52	Y6	49	424	264	87	69	4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	R7	49	430	263	108	57	2	0	0	0
53	Y7	49	430	263	108	57	2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	Z6	3	74	40	13	19	2	0	0	0
56	Z8	3	74	40	13	19	2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	QA	65	65	65	0	0
57	QF	1	1	1	0	0
57	QM	1	1	1	0	0
57	QV	1	1	1	0	0
57	RA	242	242	242	0	0

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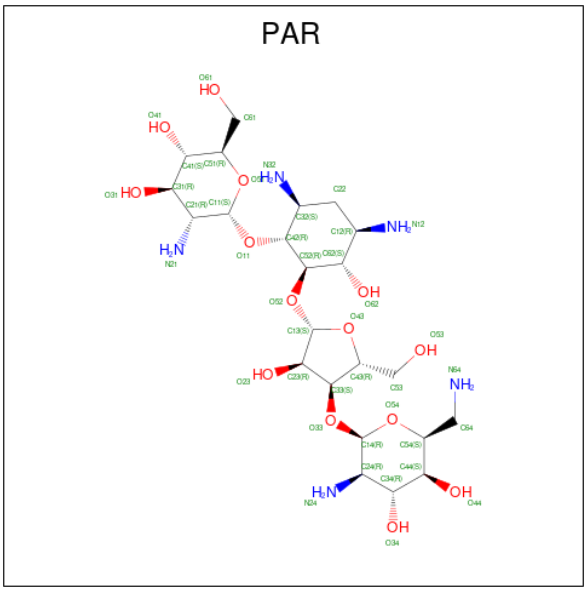
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	RB	2	2	2	0	0
57	RD	1	1	1	0	0
57	RE	2	2	2	0	0
57	RF	1	1	1	0	0
57	RP	2	2	2	0	0
57	R0	1	1	1	0	0
57	R5	1	1	1	0	0
57	R8	1	1	1	0	0
57	XA	70	70	70	0	0
57	XB	1	1	1	0	0
57	XM	1	1	1	0	0
57	XV	1	1	1	0	0
57	XX	1	1	1	0	0
57	YA	267	267	267	0	0
57	YB	3	3	3	0	0
57	YD	2	2	2	0	0
57	YE	1	1	1	0	0
57	YP	1	1	1	0	0
57	Y0	1	1	1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
58	QA	1	42	23	5	14	0	0
			Total	C	N	O		
58	XA	1	42	23	5	14	0	0

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

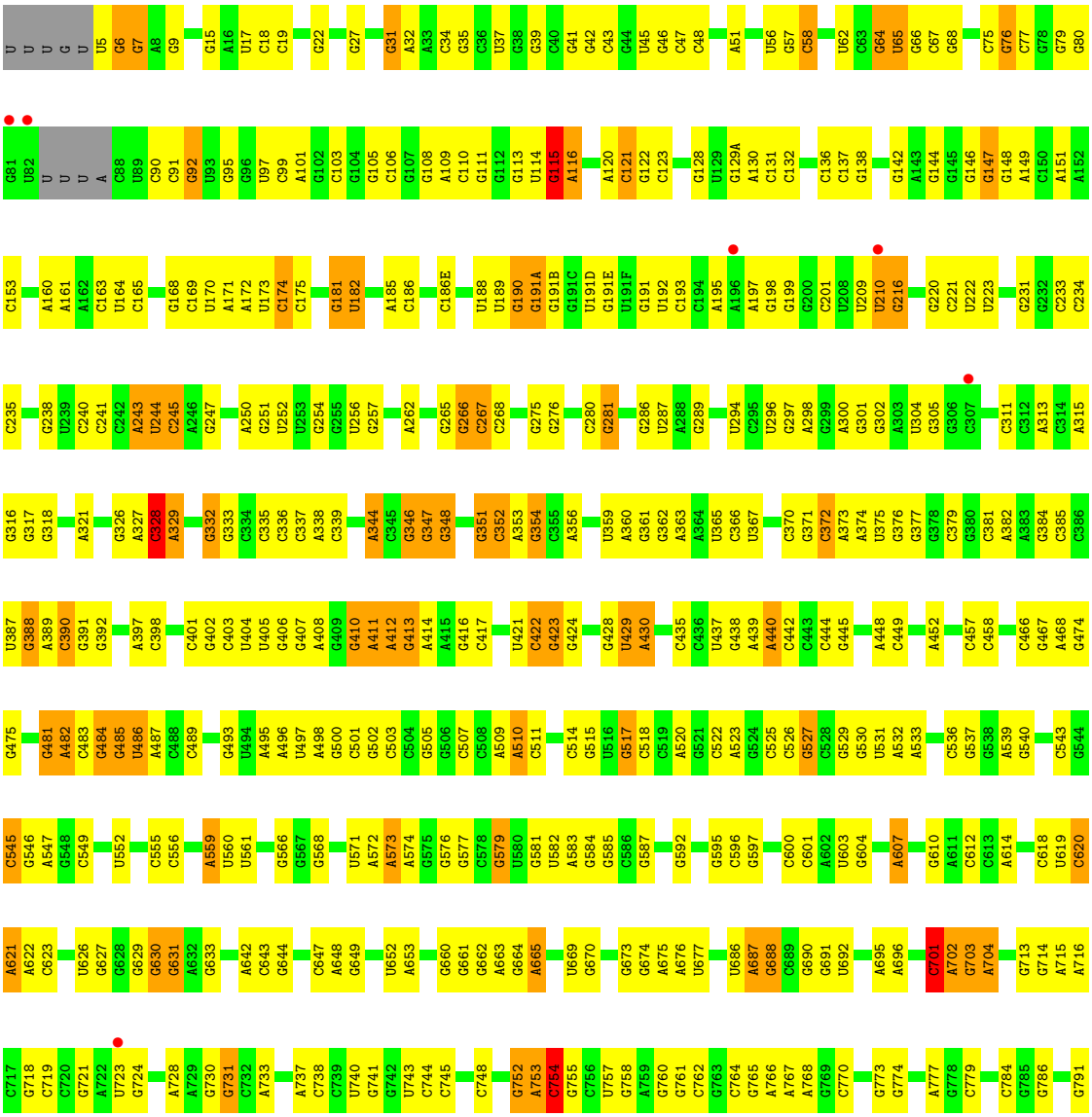
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QD	1	1	1	0	0
			Total	Zn		
59	QN	1	1	1	0	0
			Total	Zn		
59	XD	1	1	1	0	0
			Total	Zn		
59	XN	1	1	1	0	0

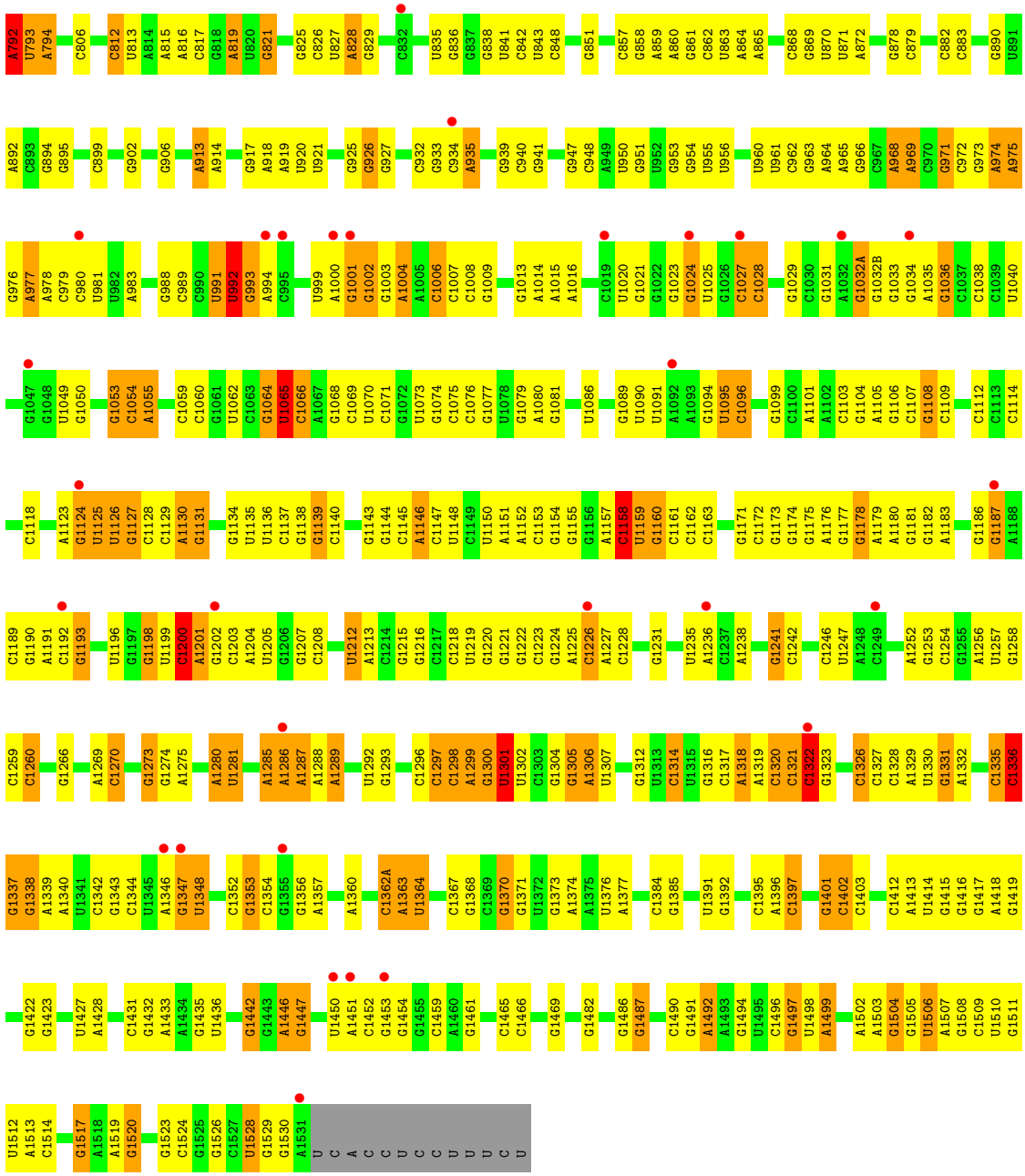
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: 16S rRNA

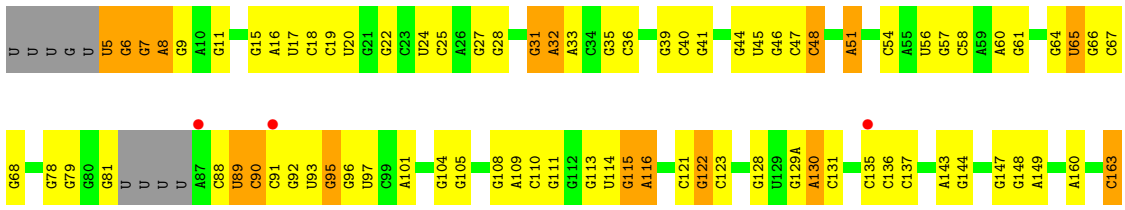
Chain QA: 2% 44% 43% 11%

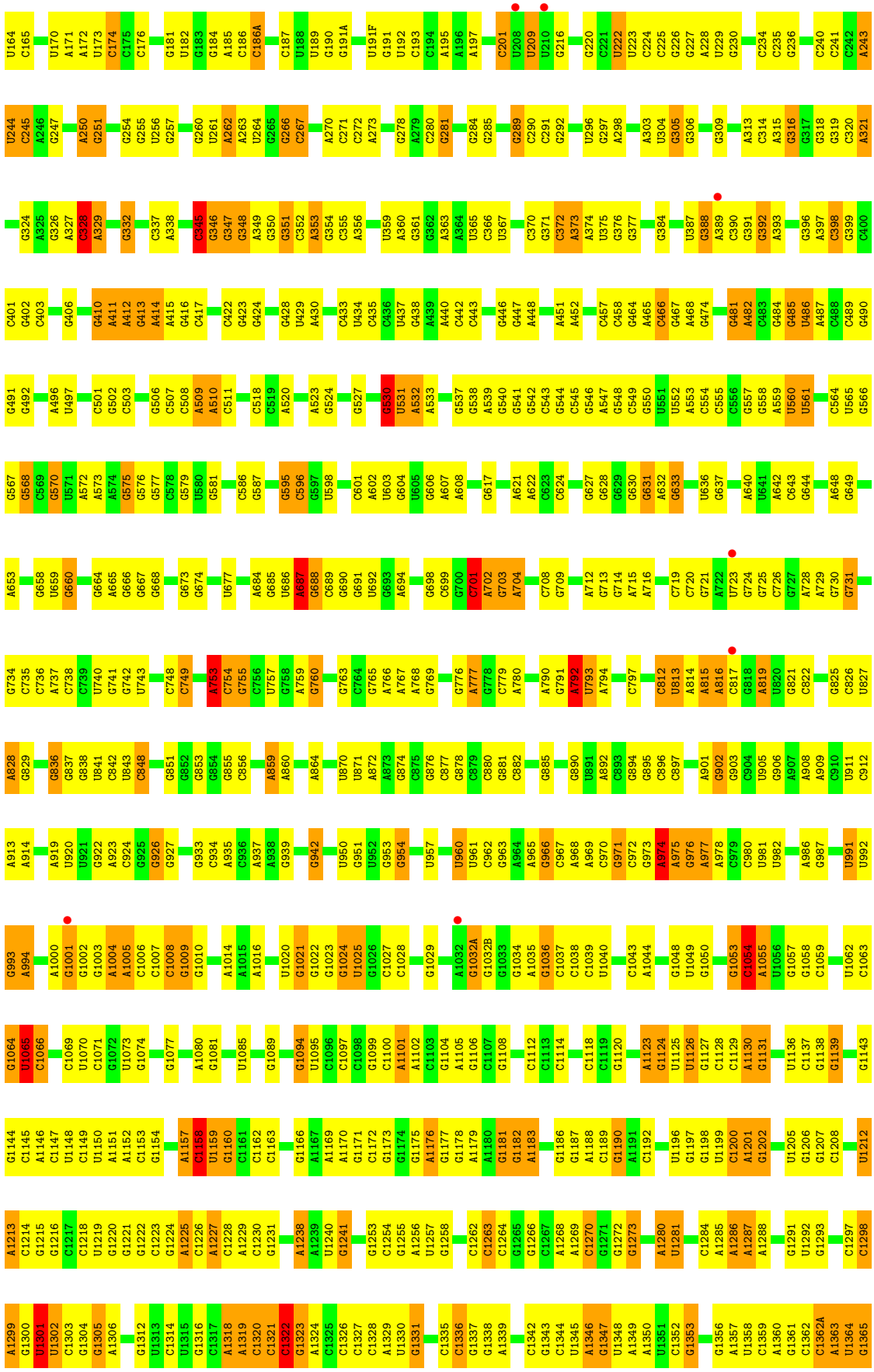


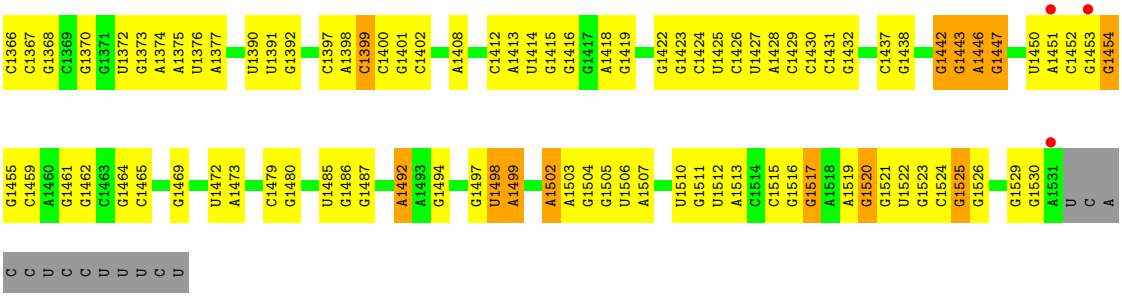


• Molecule 1: 16S rRNA

Chain XA:

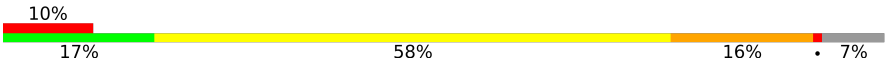


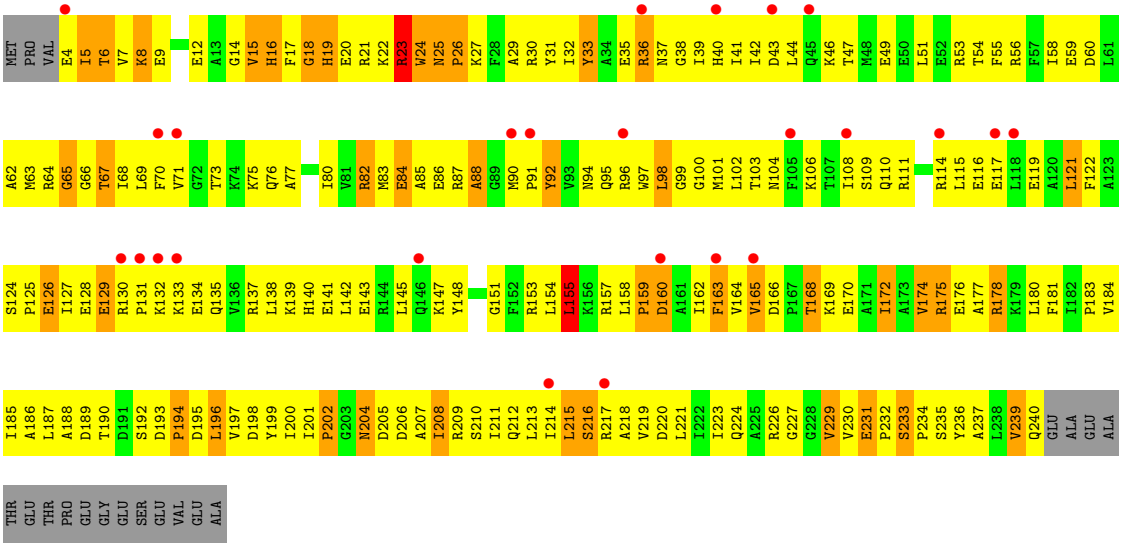

A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 C1335 C1336 G1337 G1338 A1339 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1362A A1363 U1364 G1365
A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 A1238 A1239 C1240 G1241 G1253 C1254 G1255 A1256 U1257 G1258 C1262 C1263 C1264 G1265 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 A1280 U1281 C1284 A1285 A1286 A1287 A1288 G1291 U1292 G1293 C1297 C1298
G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1166 A1167 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1186 G1187 A1188 C1189 G1190 A1191 C1192 U1196 G1197 G1198 U1199 C1200 A1201 G1202 U1205 G1206 G1207 C1208 U1212
G1064 U1065 C1066 C1069 U1070 C1071 G1072 U1073 G1074 G1077 A1080 G1081 U1085 G1089 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1112 C1113 C1114 C1118 C1119 G1120 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 U1136 C1137 G1138 G1139 G1143
G993 A994 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 A1014 A1015 A1016 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 G1029 A1032 G1032A G1032B G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 C1043 A1044 G1048 U1049 G1050 G1053 C1054 A1055 U1056 G1057 G1058 C1059 U1062 C1063
A913 A914 A919 U920 U921 G922 A923 C924 G925 G926 G927 G933 C934 A935 C936 A937 A938 G939 G942 U950 G951 U952 G953 G954 U957 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A986 G987 U991 U992
A828 G829 G836 G837 G838 U841 C842 U843 C848 G851 G852 G853 G854 G855 C856 A859 A860 A864 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 G885 G890 U891 A892 C893 G894 G895 C896 C897 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912
G734 C735 C736 A737 C738 C739 U740 G741 G742 U743 C748 C749 A753 C754 G755 C756 U757 G758 A759 G760 G763 C764 G765 A766 A767 A768 G769 G776 A777 G778 C779 A780 A790 G791 A792 U793 A794 C797 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G825 C826 U827
A653 G658 U659 G660 G664 A665 G666 G667 G668 G673 G674 U677 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 G698 C699 G700 C701 A702 G703 A704 C708 G709 A712 G713 G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731
G567 G568 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 C586 G587 G595 C596 G597 U598 C601 A602 U603 G604 U605 G606 A607 A608 G617 A621 A622 C623 C624 G627 G628 G629 G630 G631 A632 G633 U636 G637 A640 U641 A642 C643 G644 A648 G649
G491 G492 A496 U497 C501 G502 C503 G506 C507 C508 A509 A510 C511 C518 C519 A520 A523 G524 G527 G530 U531 A532 A533 G537 G538 A539 G540 G541 G542 G543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 C555 C556 G557 G558 A559 U560 U561 C564 U565 G566
C401 G402 C403 G406 G410 A411 A412 G413 A414 A415 G416 C417 C422 G423 G424 G428 U429 A430 C433 U434 C435 C436 U437 G438 A439 A440 C442 C443 G446 G447 A448 A451 A452 C457 C458 G464 A465 C466 G467 A468 G474 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490
G324 A325 G326 A327 C328 A329 G332 C337 A338 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 U359 A360 G361 C362 A363 A364 U365 C366 U367 C370 G371 C372 A373 A374 U375 G376 G377 G384 U387 G388 A389 C390 G391 G392 A393 G396 A397 C398 G399 C400
U244 C245 A246 G247 A250 G251 G254 G255 U256 G257 G260 U261 A262 A263 U264 G265 G266 C267 A270 C271 C272 A273 G278 A279 C280 G281 G284 G285 G289 C290 G291 G292 U296 G297 A298 A303 U304 G305 G306 G309 A313 C314 A315 G316 G317 G318 G319 C320 A321
U164 C165 U170 A171 A172 U173 C174 C175 C176 G181 U182 G183 G184 A185 C186 C186A C187 U188 U189 G190 G191A U191F G191 U192 C193 C194 A195 A196 A197 C201 U208 U209 U210 G216 G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 C234 C235 G236 C240 C241 C242 A243



- Molecule 2: 30S ribosomal protein S2

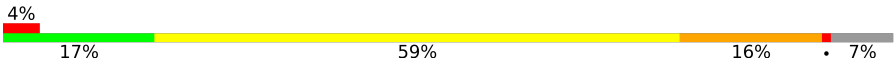
Chain QB:

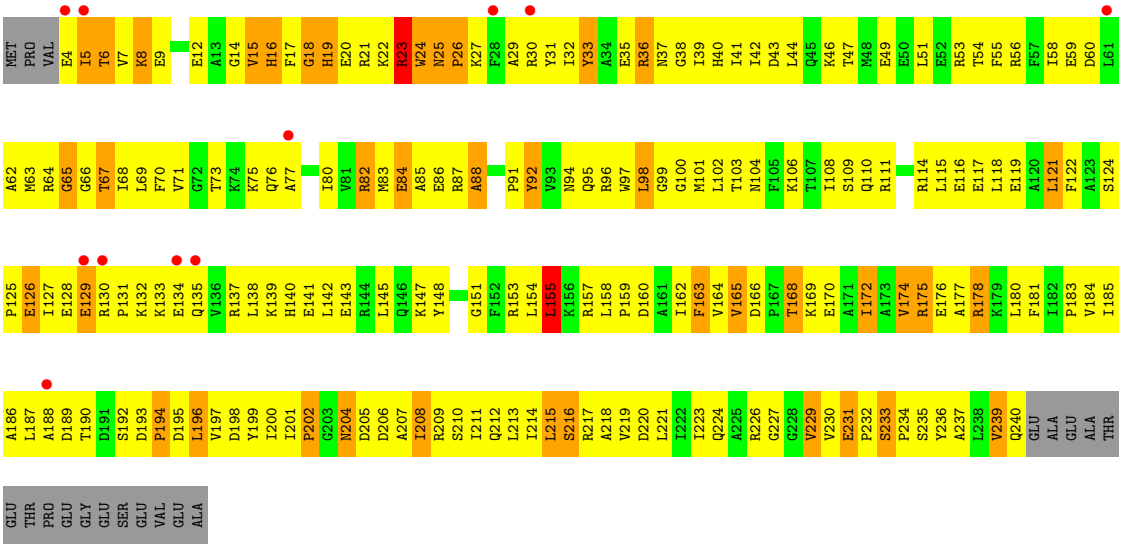




- Molecule 2: 30S ribosomal protein S2

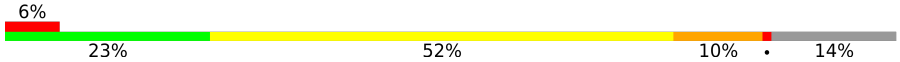
Chain XB:

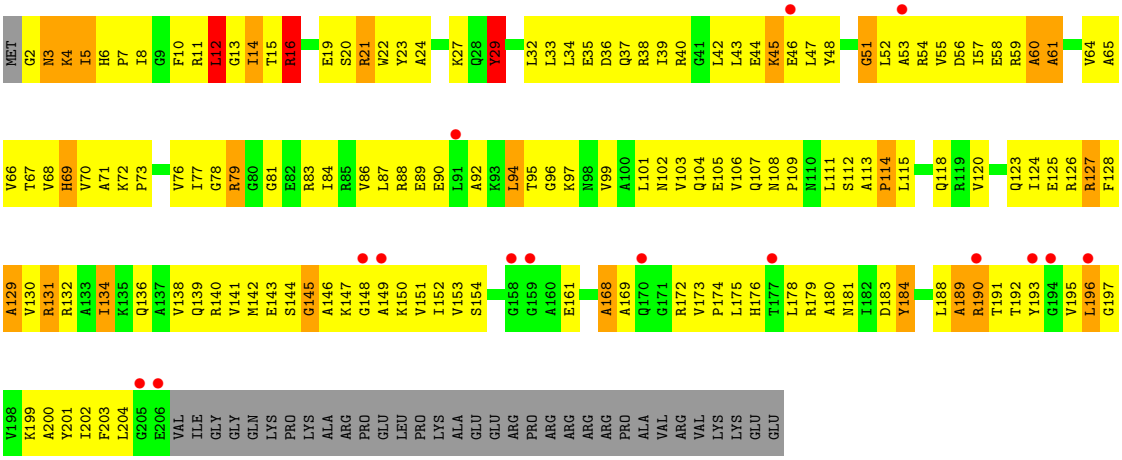




- Molecule 3: 30S ribosomal protein S3

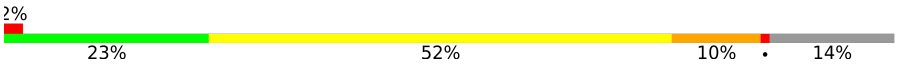
Chain QC:

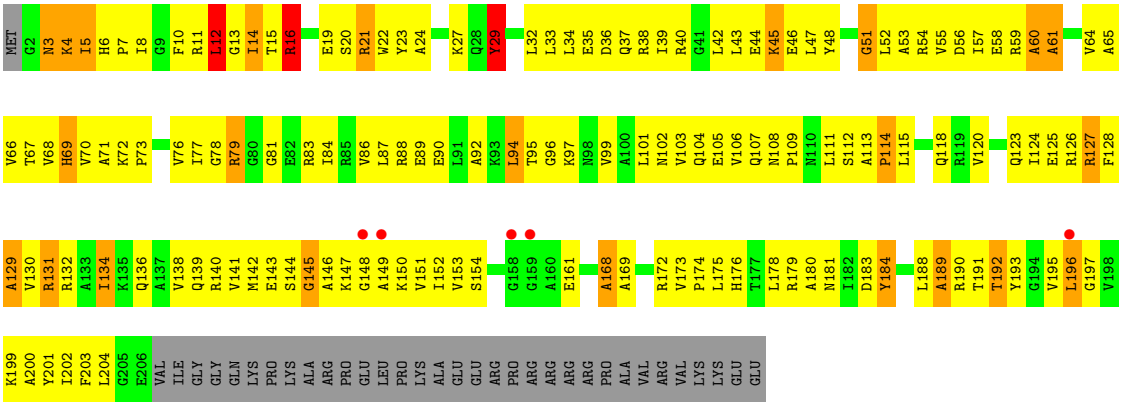




- Molecule 3: 30S ribosomal protein S3

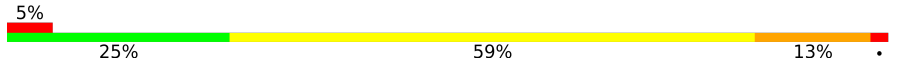
Chain XC:

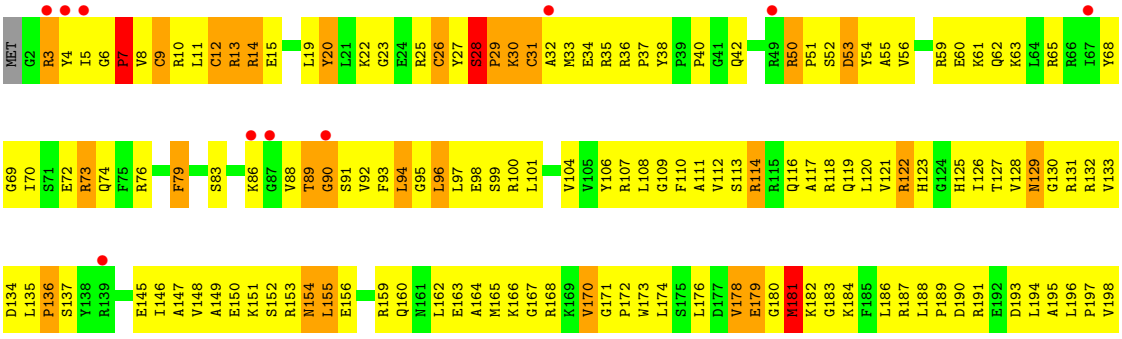


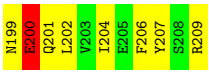


- Molecule 4: 30S ribosomal protein S4

Chain QD:

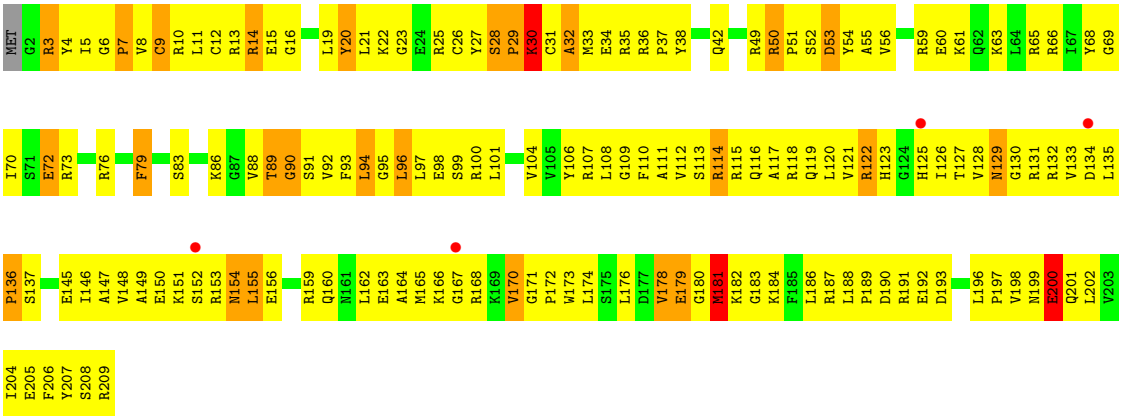






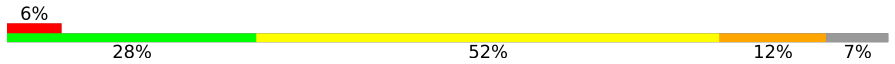
• Molecule 4: 30S ribosomal protein S4

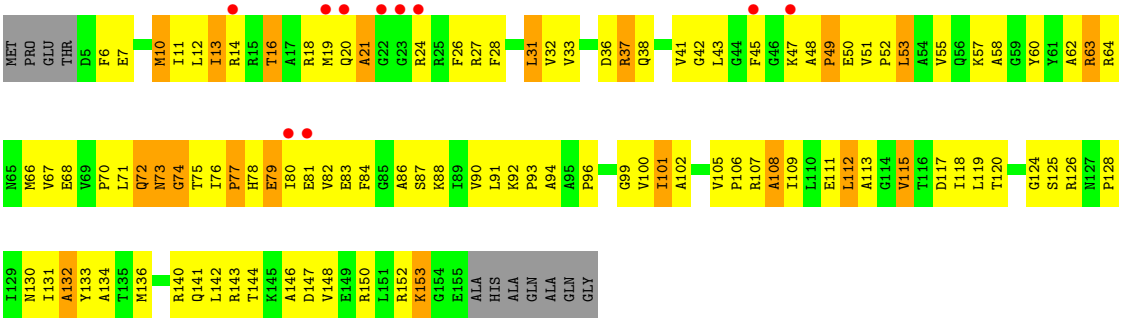
Chain XD:



• Molecule 5: 30S ribosomal protein S5

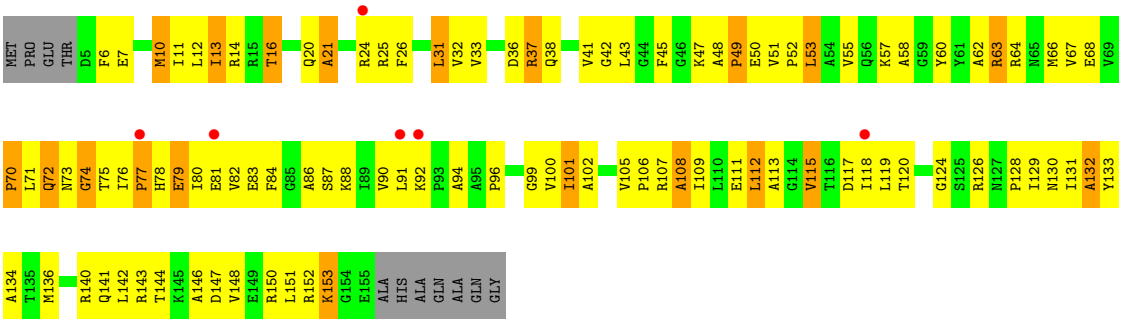
Chain QE:





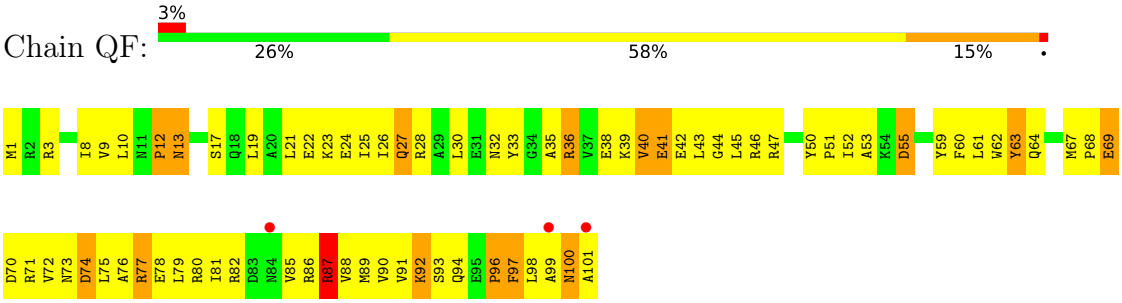
• Molecule 5: 30S ribosomal protein S5

Chain XE:



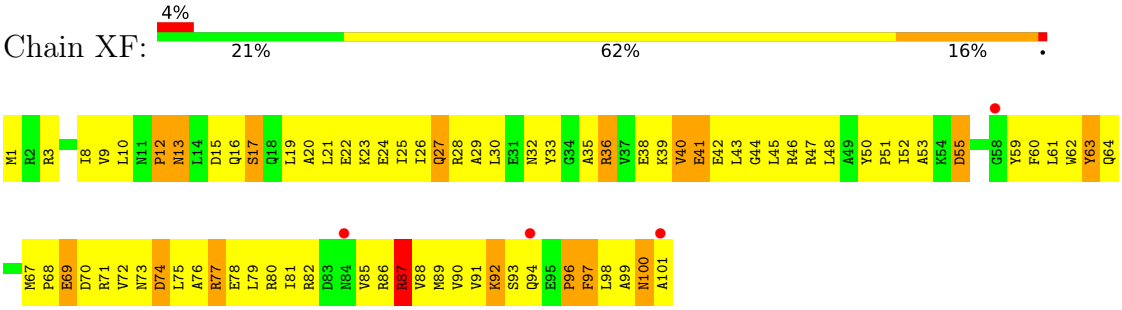
• Molecule 6: 30S ribosomal protein S6

Chain QF:



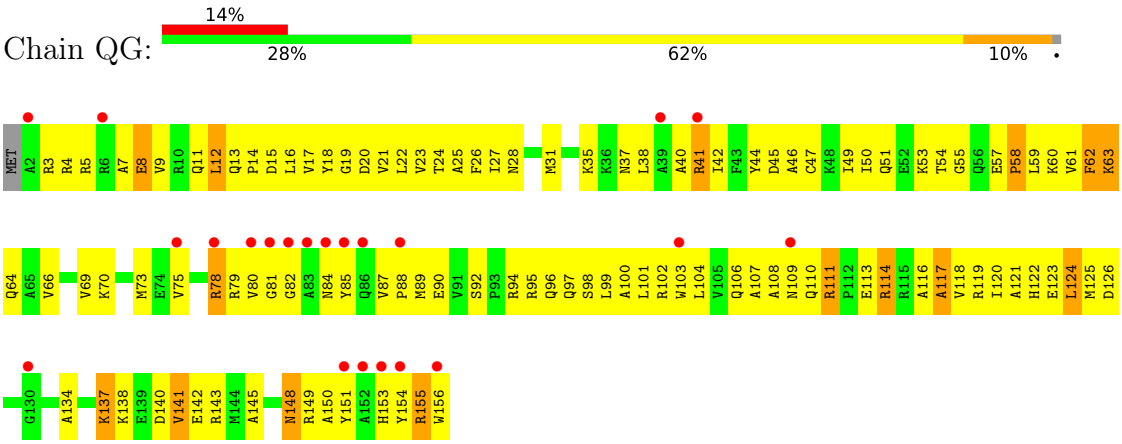
• Molecule 6: 30S ribosomal protein S6

Chain XF:



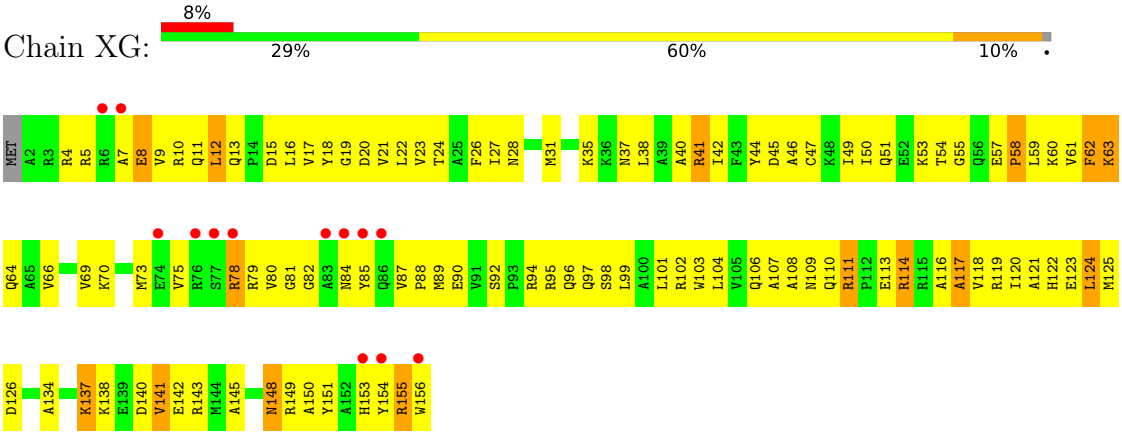
• Molecule 7: 30S ribosomal protein S7

Chain QG:



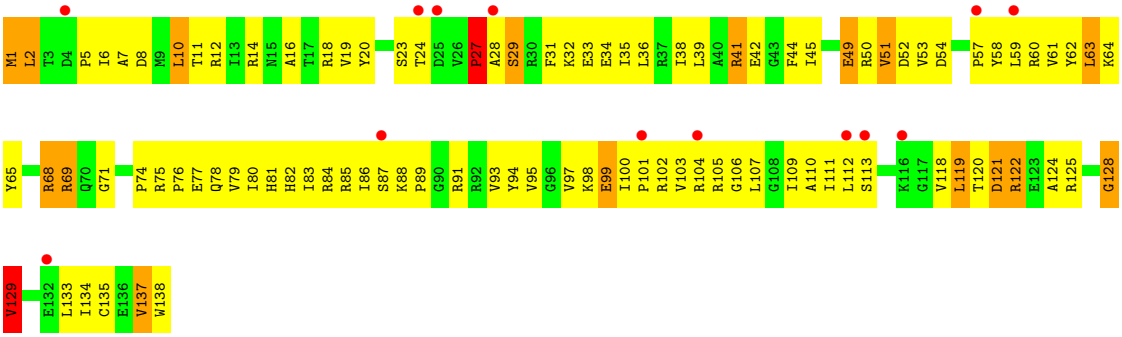
• Molecule 7: 30S ribosomal protein S7

Chain XG:



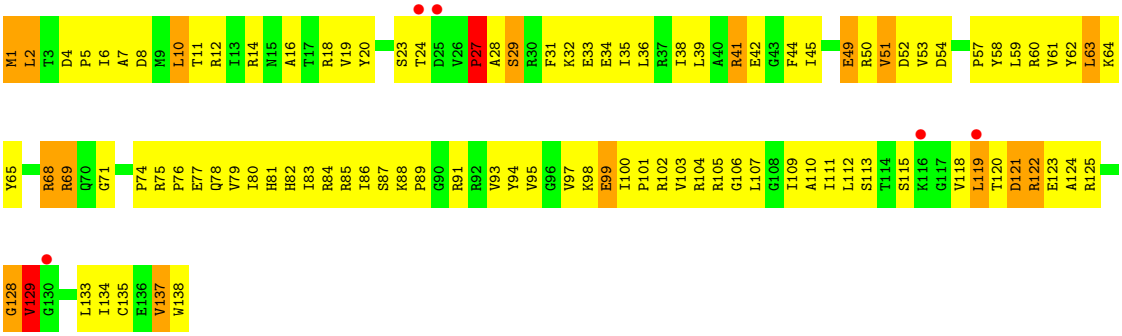
• Molecule 8: 30S ribosomal protein S8

Chain QH:



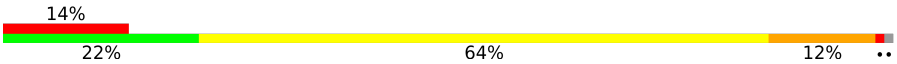
- Molecule 8: 30S ribosomal protein S8

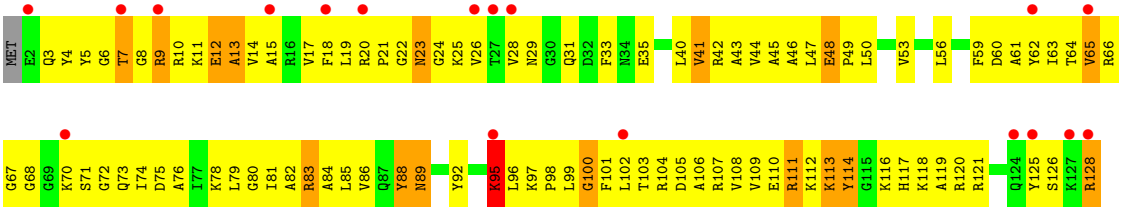
Chain XH:



- Molecule 9: 30S ribosomal protein S9

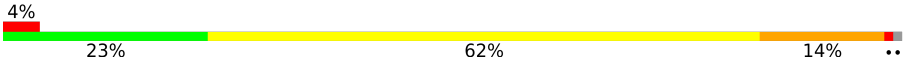
Chain QI:

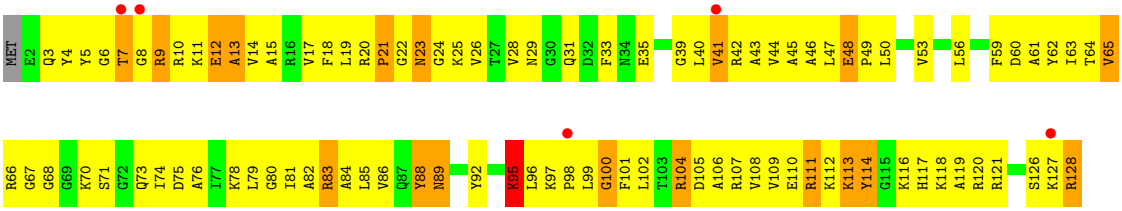




- Molecule 9: 30S ribosomal protein S9

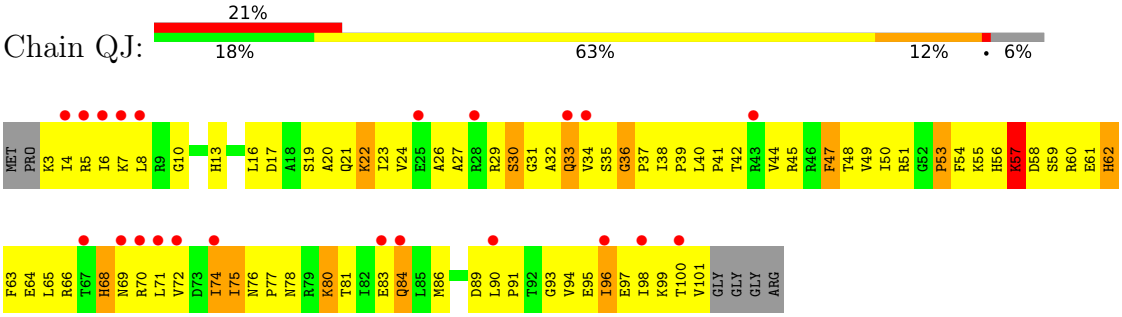
Chain XI:





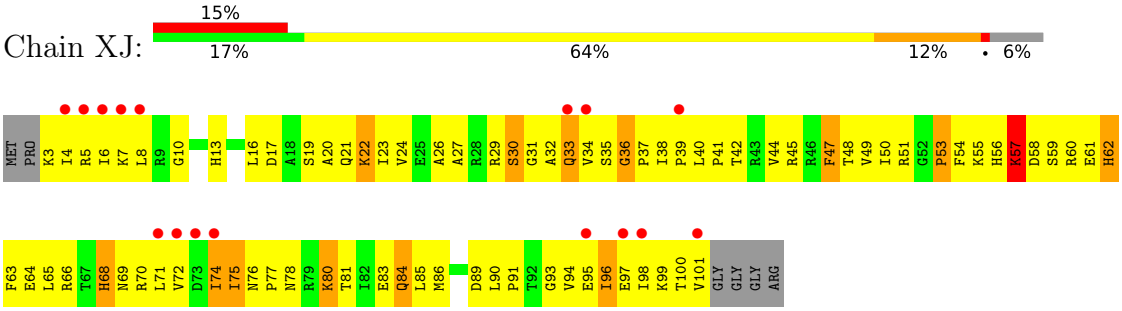
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



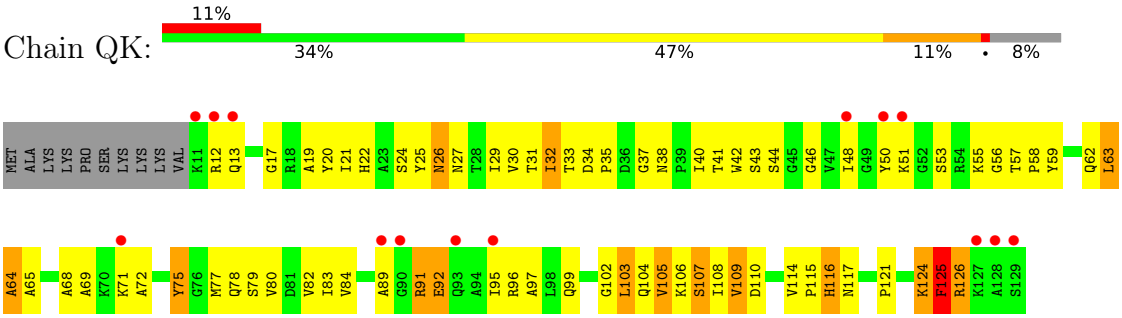
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



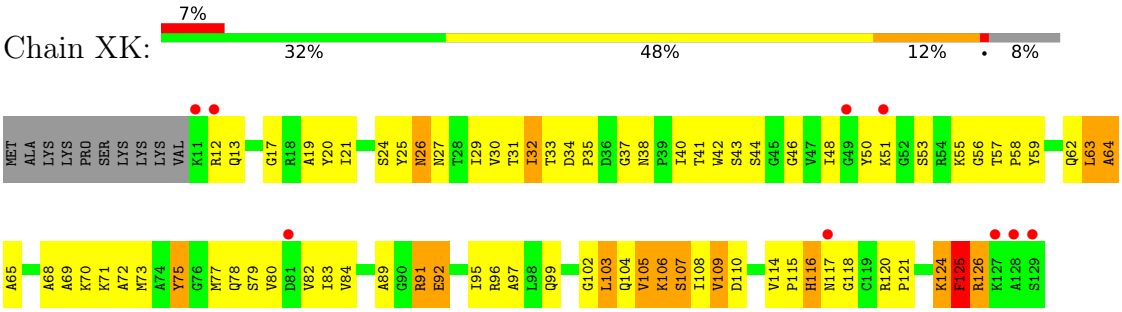
- Molecule 11: 30S ribosomal protein S11

Chain QK:



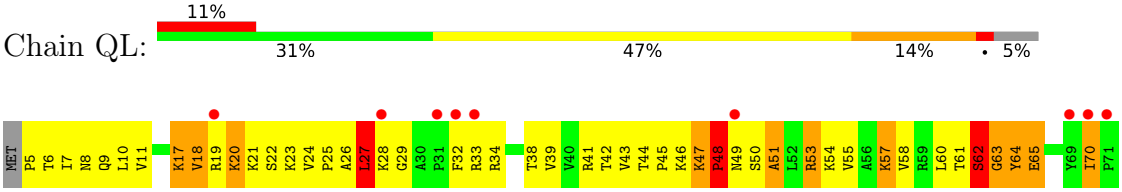
- Molecule 11: 30S ribosomal protein S11

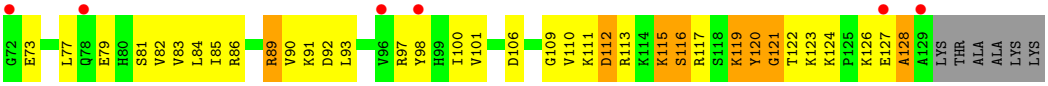
Chain XK:



- Molecule 12: 30S ribosomal protein S12

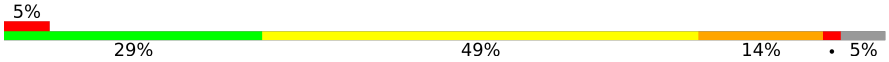
Chain QL:

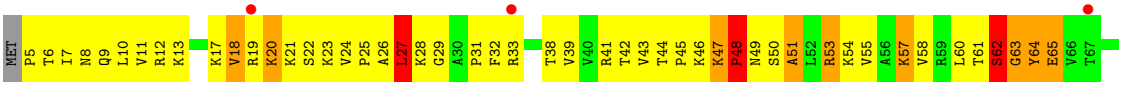


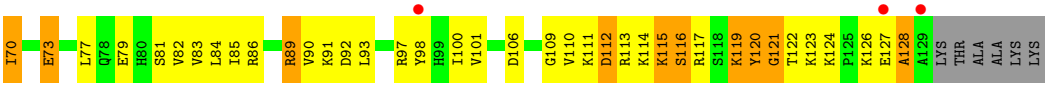


• Molecule 12: 30S ribosomal protein S12

Chain XL:

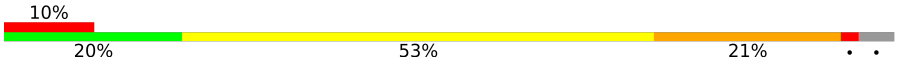


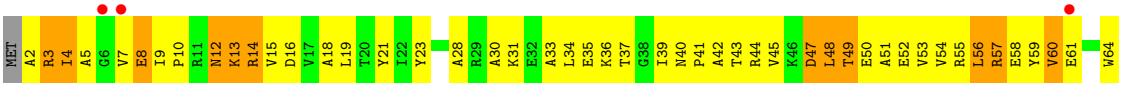


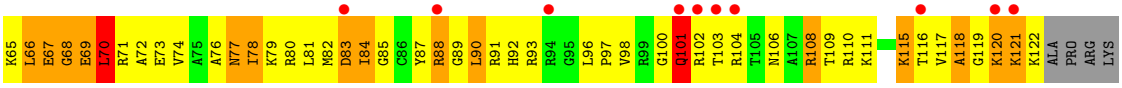


• Molecule 13: 30S ribosomal protein S13

Chain QM:

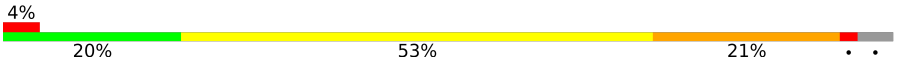


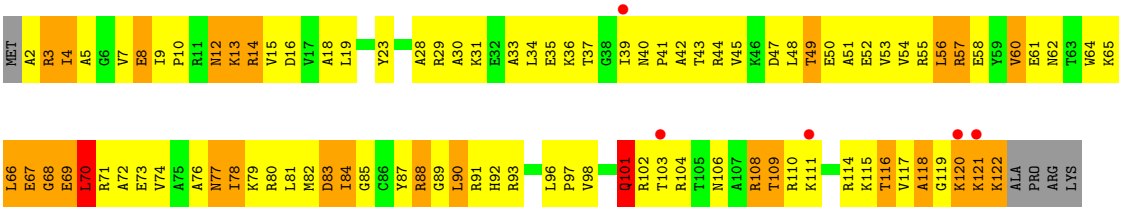




• Molecule 13: 30S ribosomal protein S13

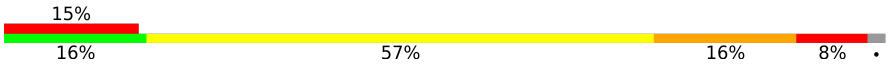
Chain XM:

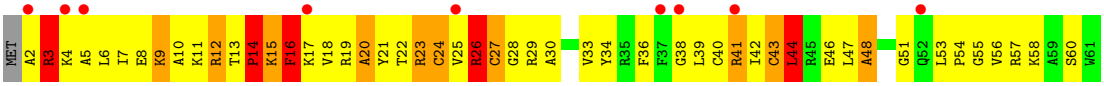




• Molecule 14: 30S ribosomal protein S14

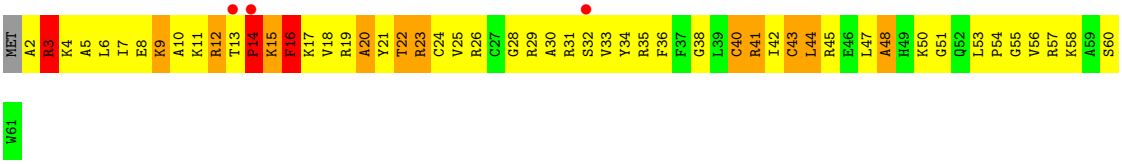
Chain QN:





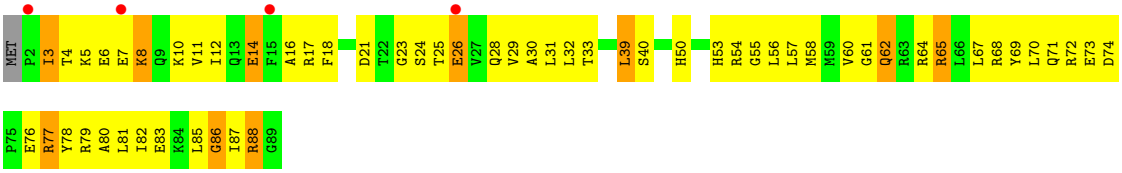
• Molecule 14: 30S ribosomal protein S14

Chain XN:



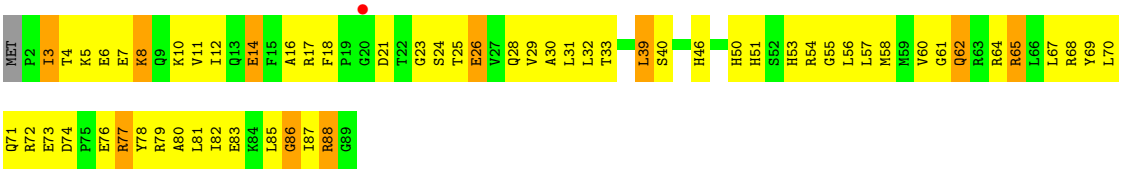
• Molecule 15: 30S ribosomal protein S15

Chain QO:



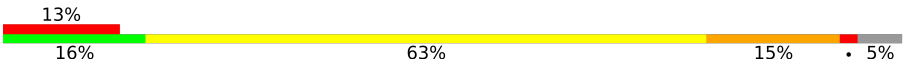
• Molecule 15: 30S ribosomal protein S15

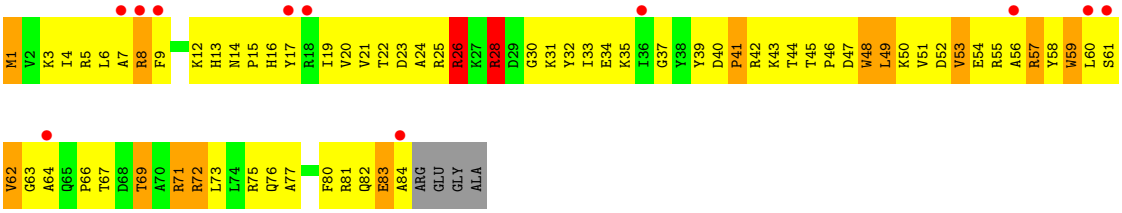
Chain XO:



• Molecule 16: 30S ribosomal protein S16

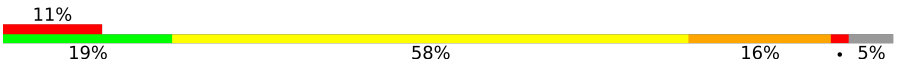
Chain QP:

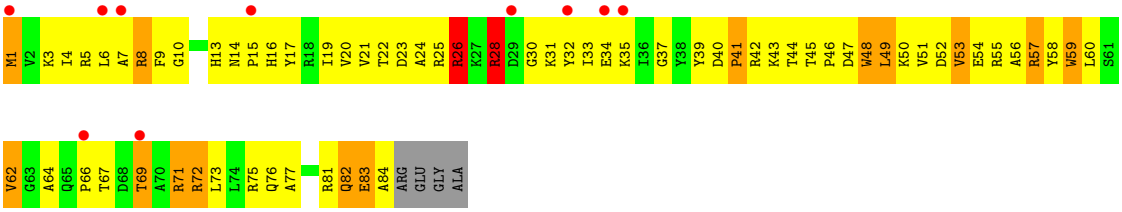




• Molecule 16: 30S ribosomal protein S16

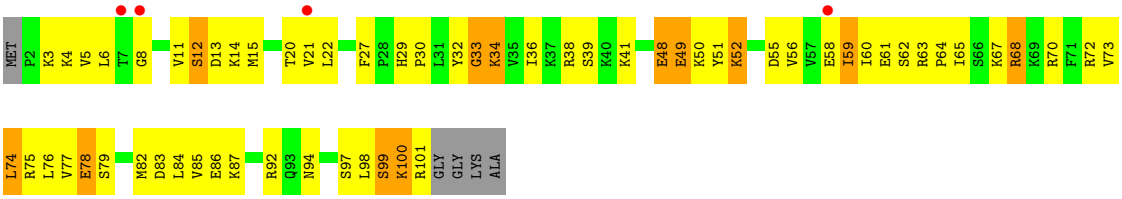
Chain XP:





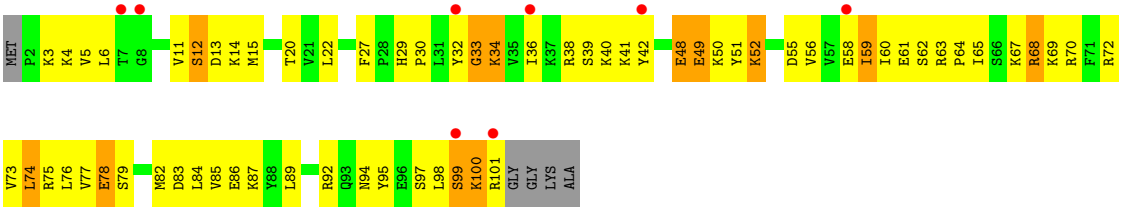
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



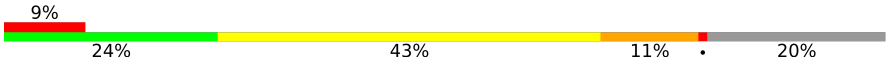
- Molecule 17: 30S ribosomal protein S17

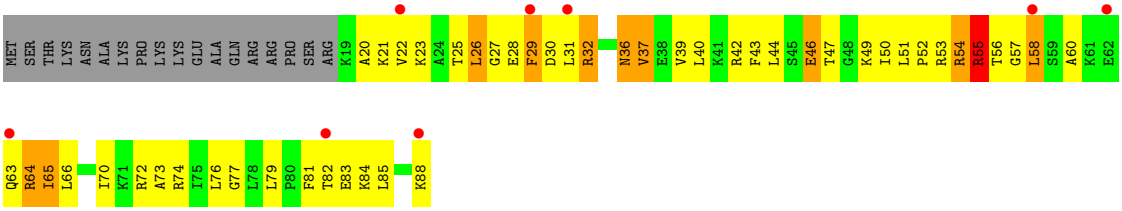
Chain XQ:



- Molecule 18: 30S ribosomal protein S18

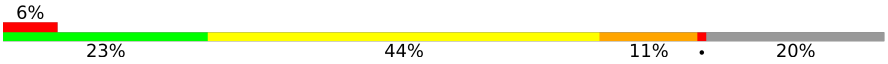
Chain QR:

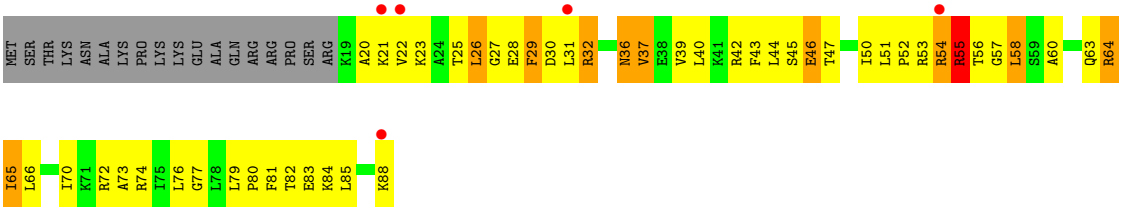




- Molecule 18: 30S ribosomal protein S18

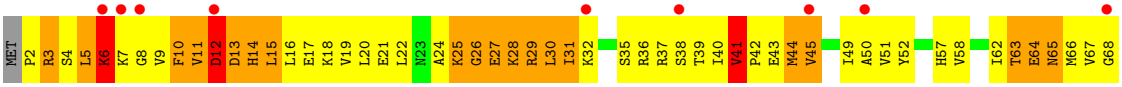
Chain XR:

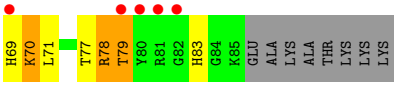




- Molecule 19: 30S ribosomal protein S19

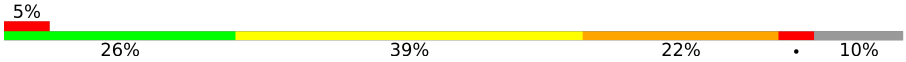
Chain QS:

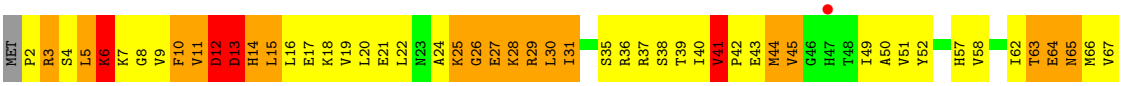


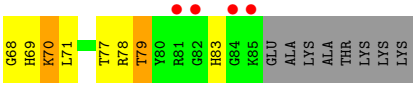


• Molecule 19: 30S ribosomal protein S19

Chain XS:

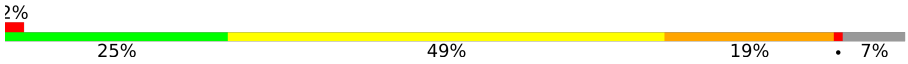


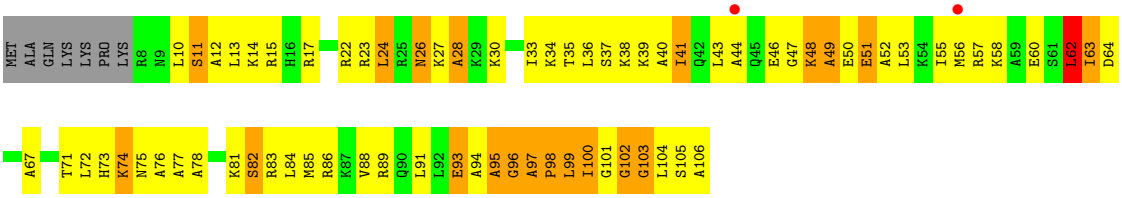




• Molecule 20: 30S ribosomal protein S20

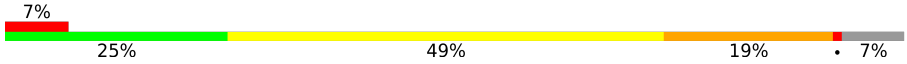
Chain QT:

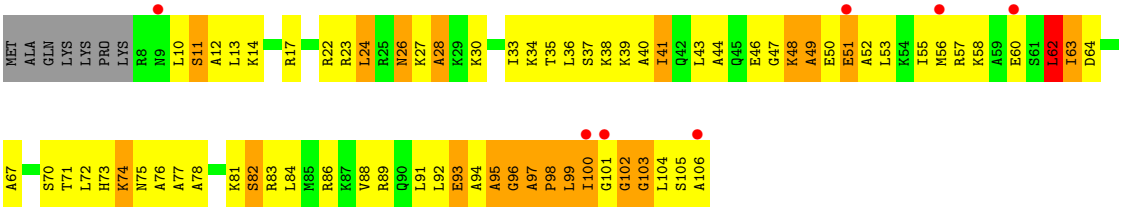




• Molecule 20: 30S ribosomal protein S20

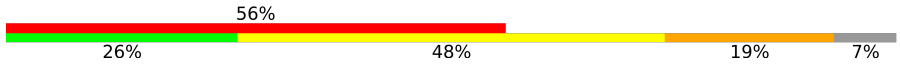
Chain XT:

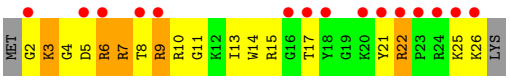




• Molecule 21: 30S ribosomal protein S21

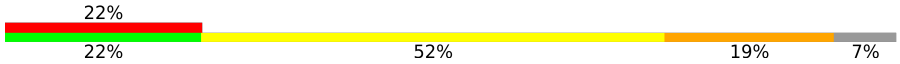
Chain QU:

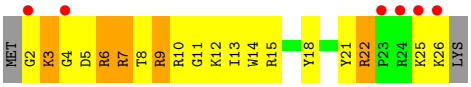




• Molecule 21: 30S ribosomal protein S21

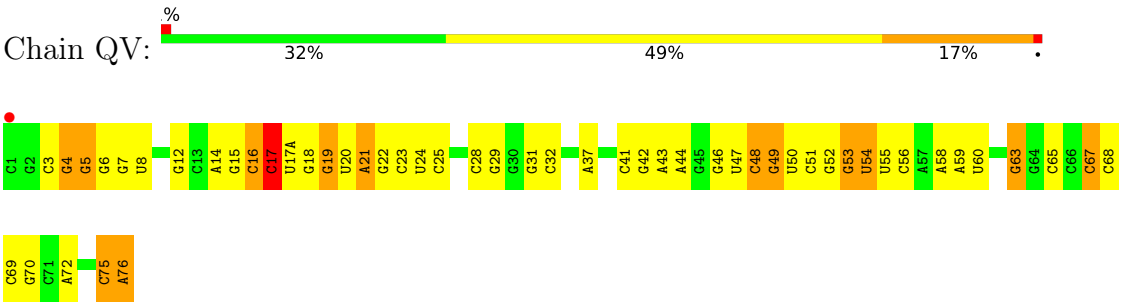
Chain XU:





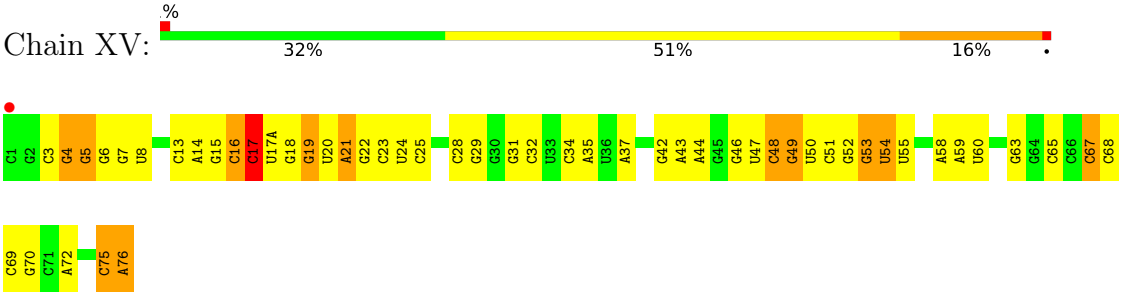
• Molecule 22: P-site tRNA fMet

Chain QV:



• Molecule 22: P-site tRNA fMet

Chain XV:



• Molecule 23: A-site ASL SufA6

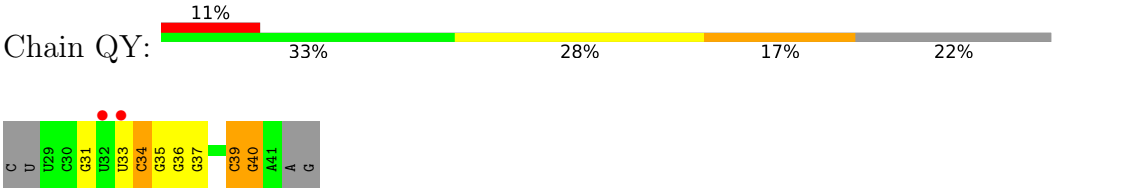
Chain QX:

• Molecule 23: A-site ASL SufA6

Chain XX:

• Molecule 24: messenger RNA

Chain QY:



• Molecule 24: messenger RNA

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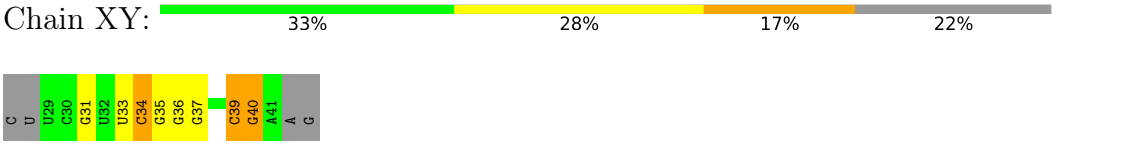

• Molecule 25: 23S rRNA

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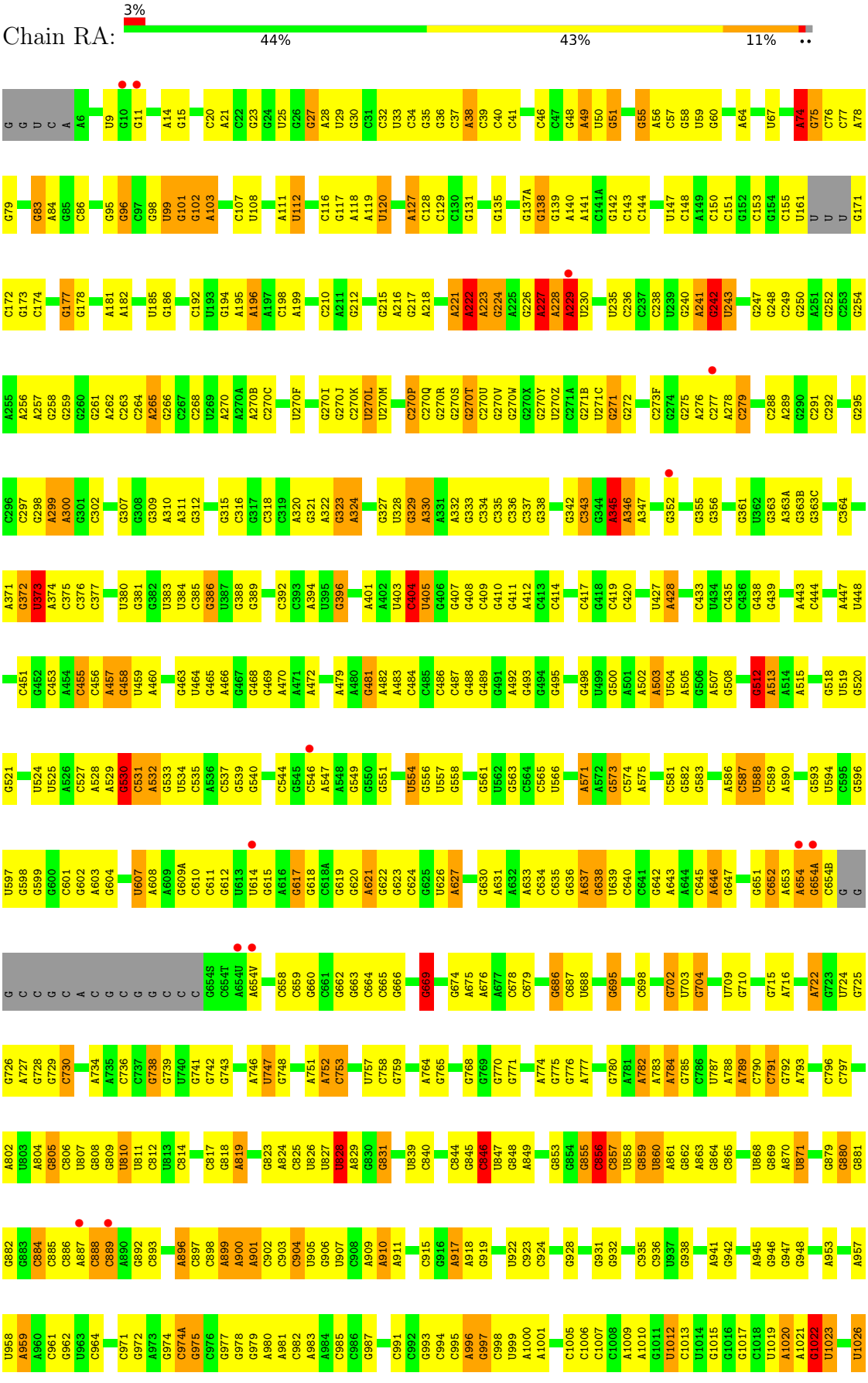

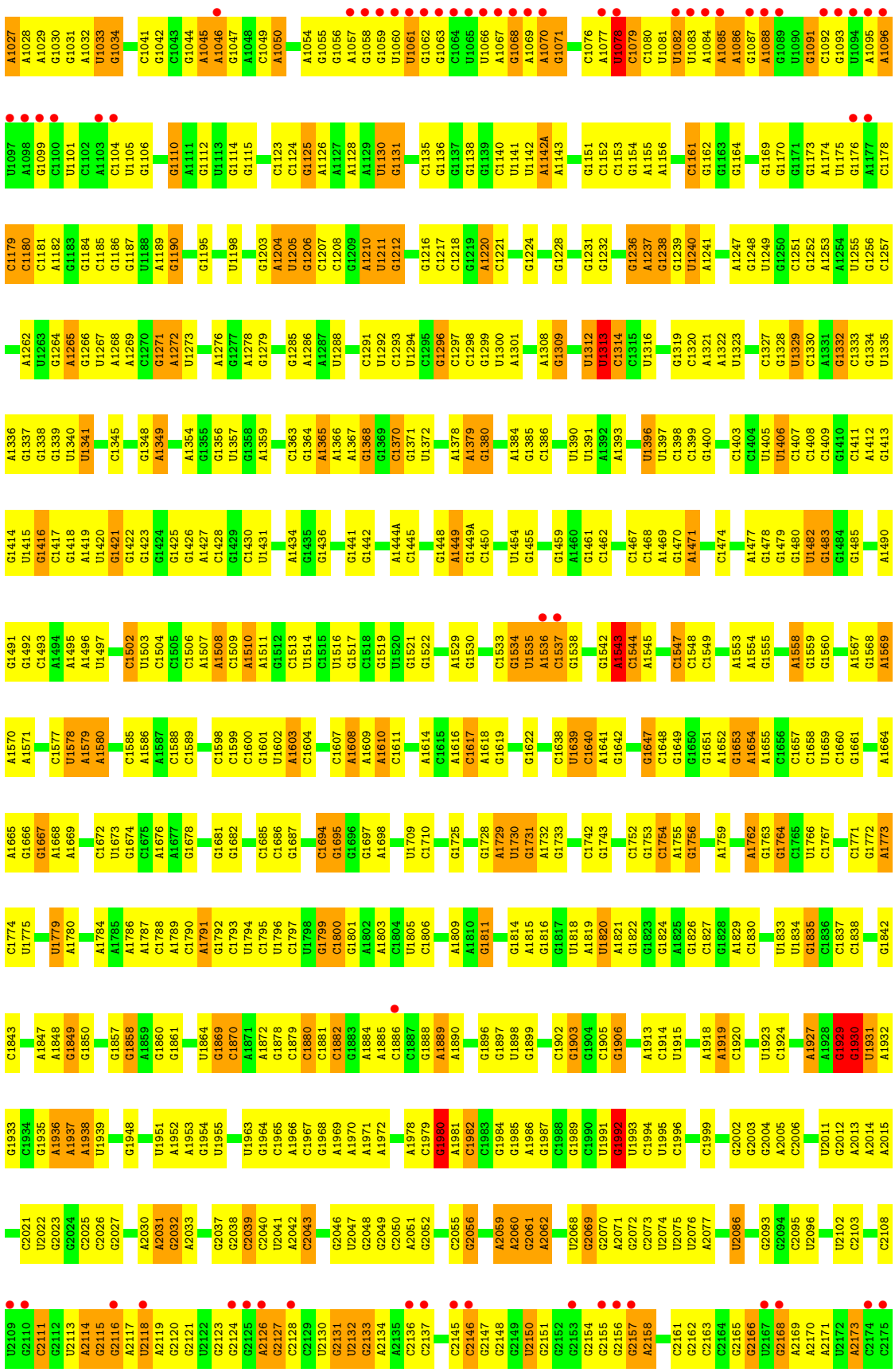
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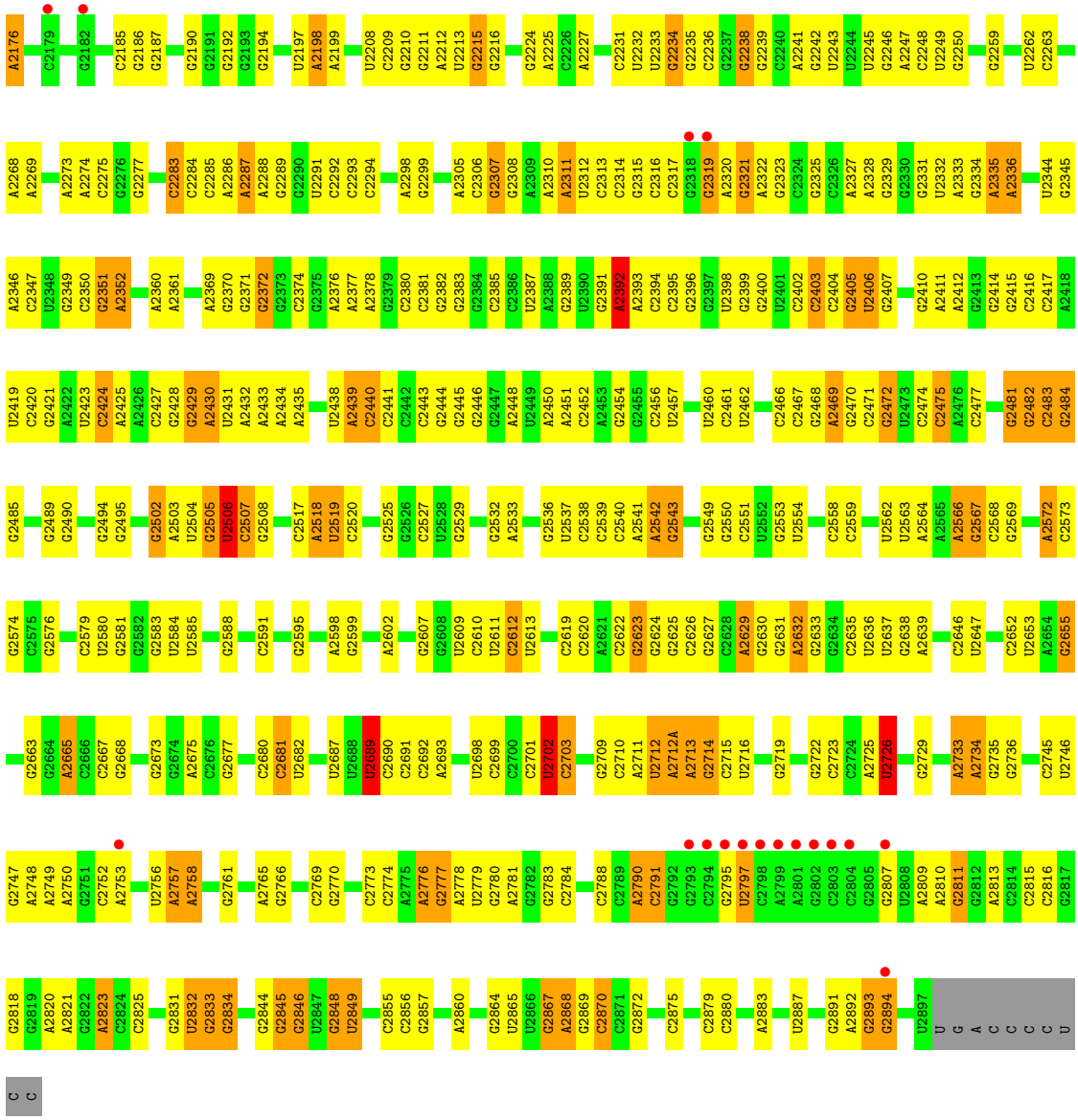
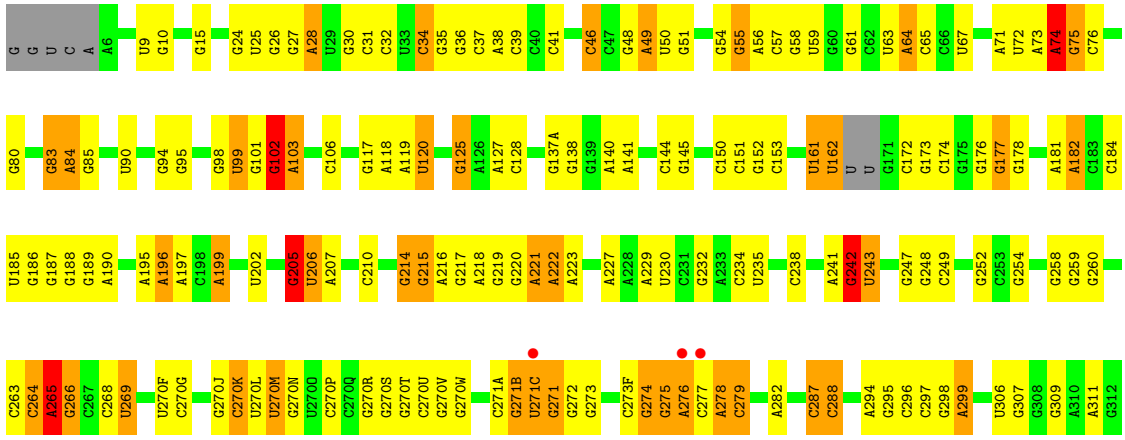
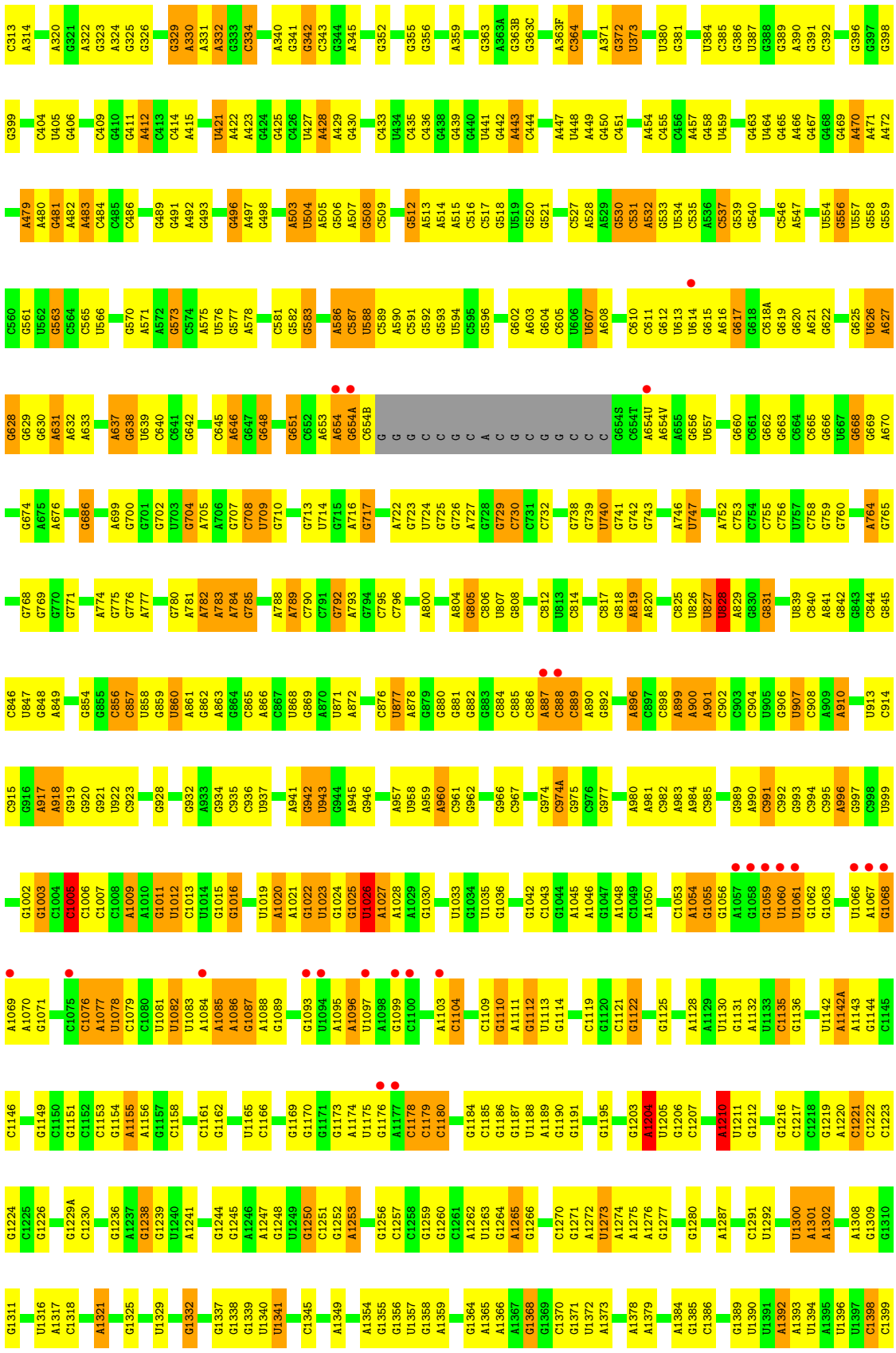


• Molecule 25: 23S rRNA

Chain YA:

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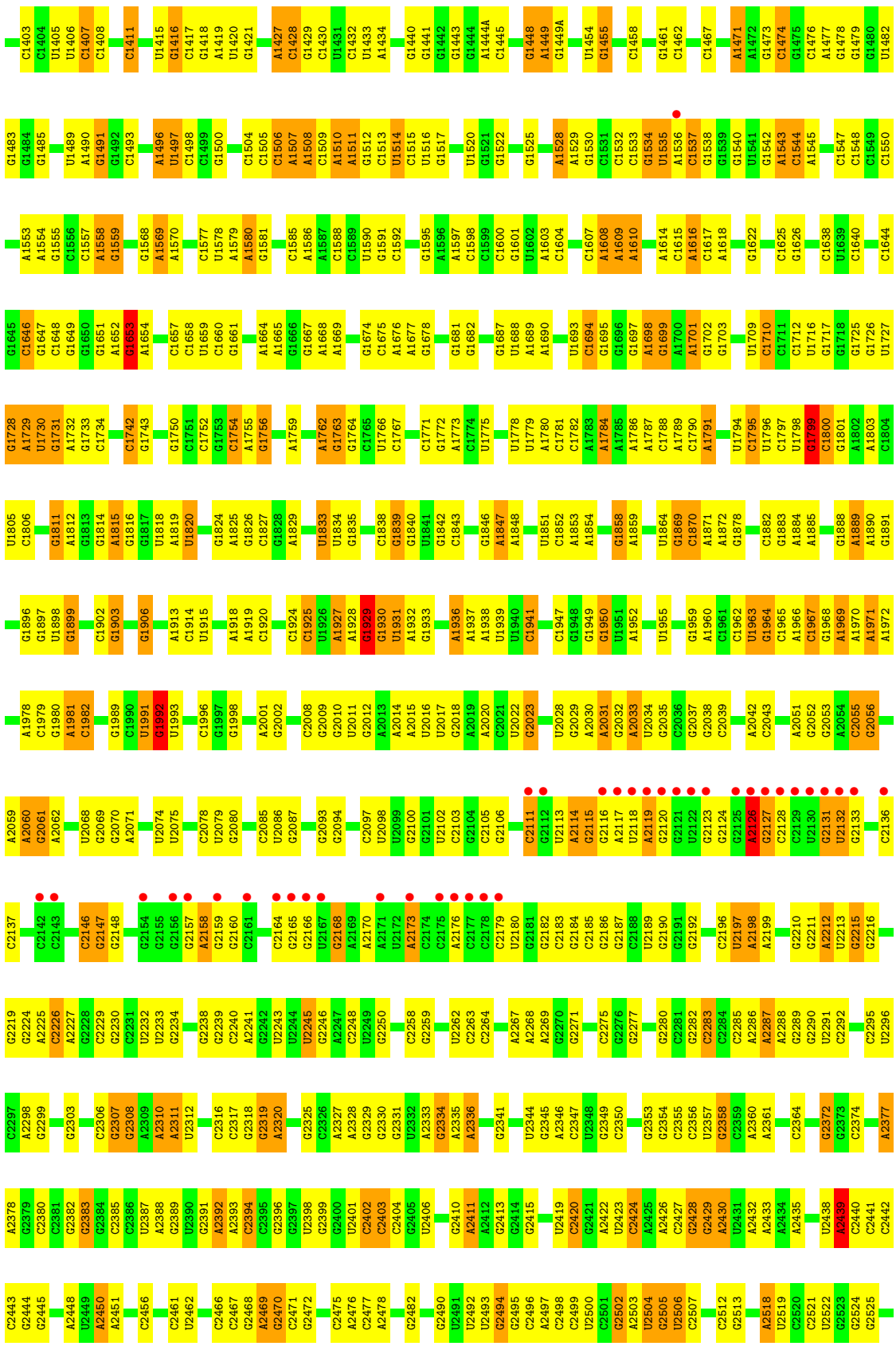
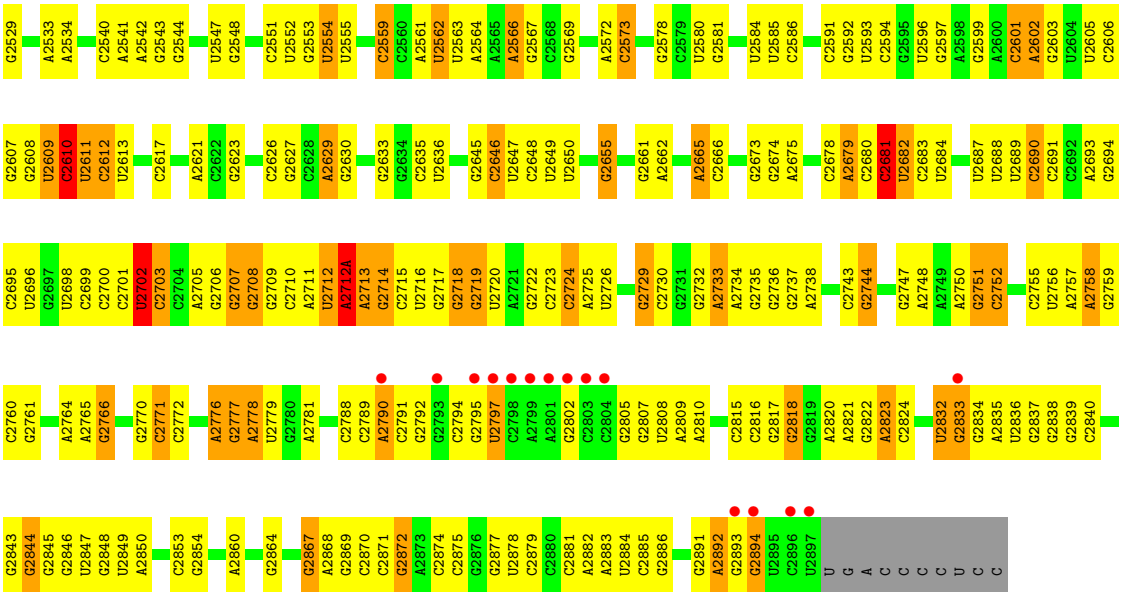
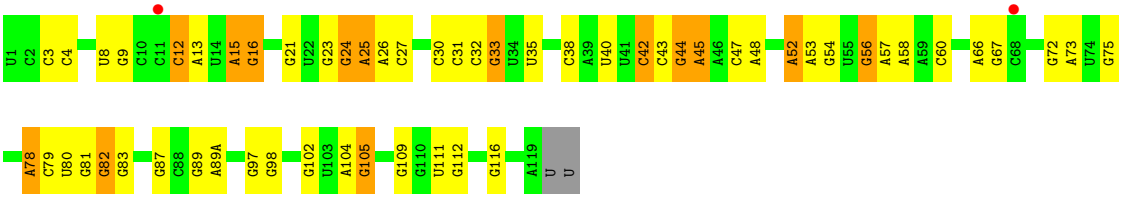




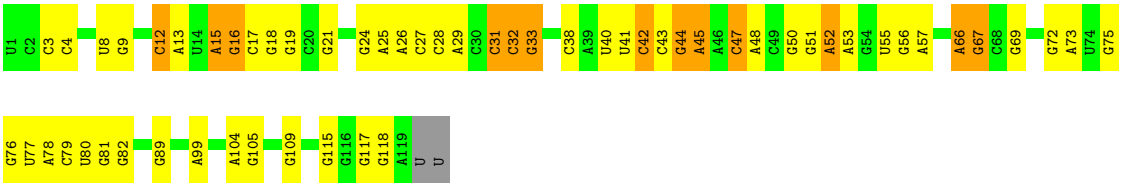
- Molecule 26: 5S rRNA

Chain RB:



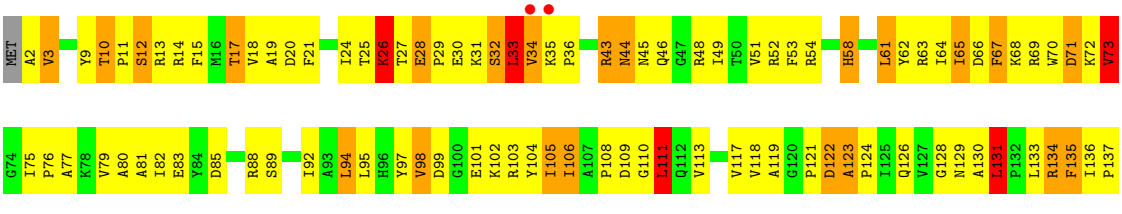
- Molecule 26: 5S rRNA

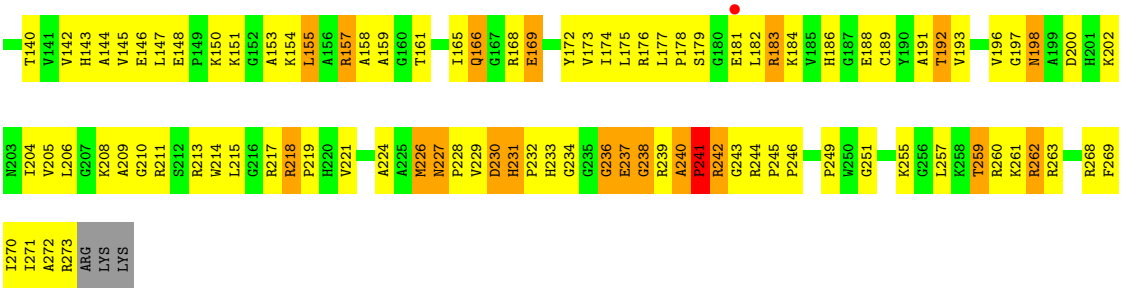
Chain YB:



- Molecule 27: 50S ribosomal protein L2

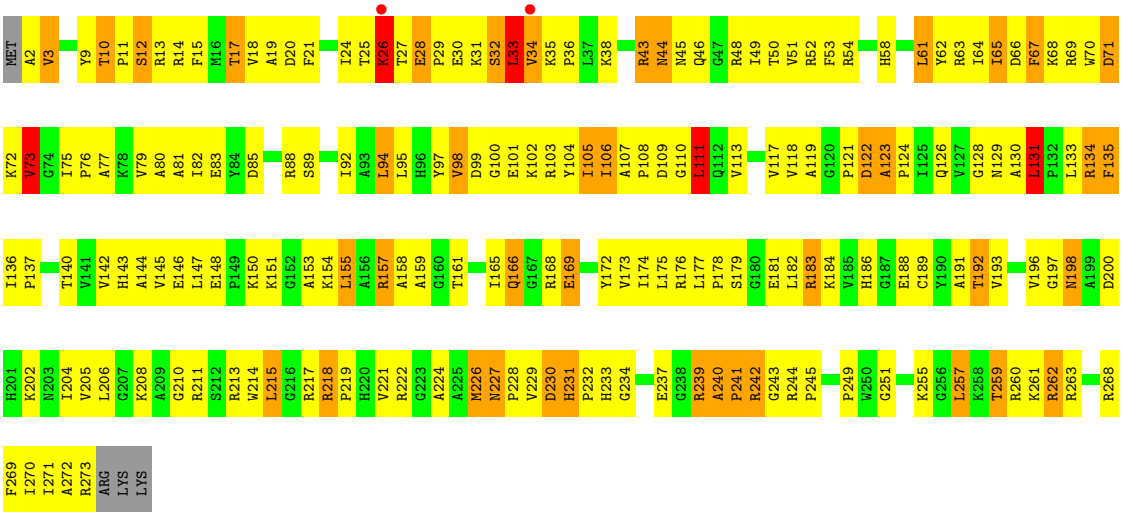
Chain RD:





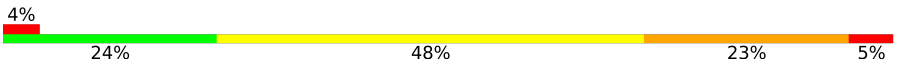
- Molecule 27: 50S ribosomal protein L2

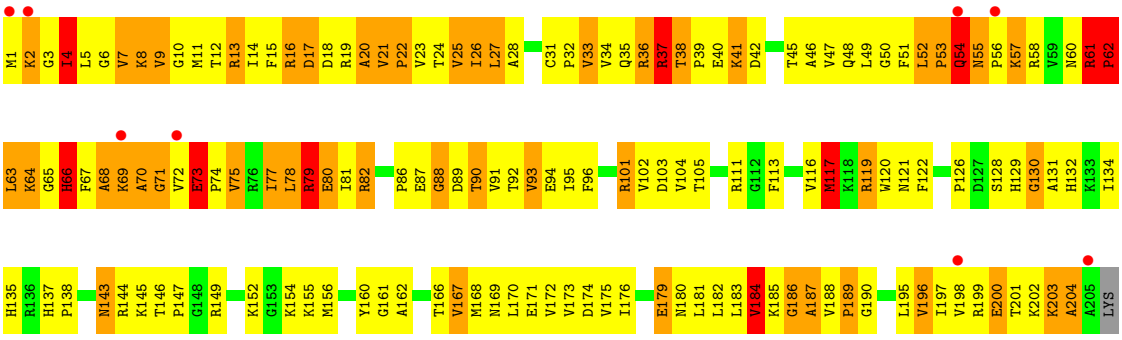
Chain YD:



- Molecule 28: 50S ribosomal protein L3

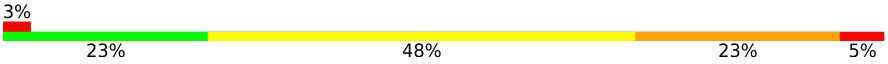
Chain RE:

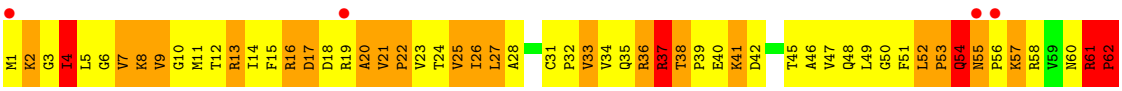


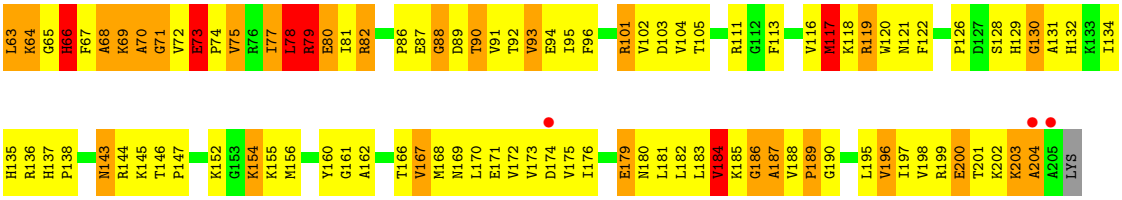


- Molecule 28: 50S ribosomal protein L3

Chain YE:

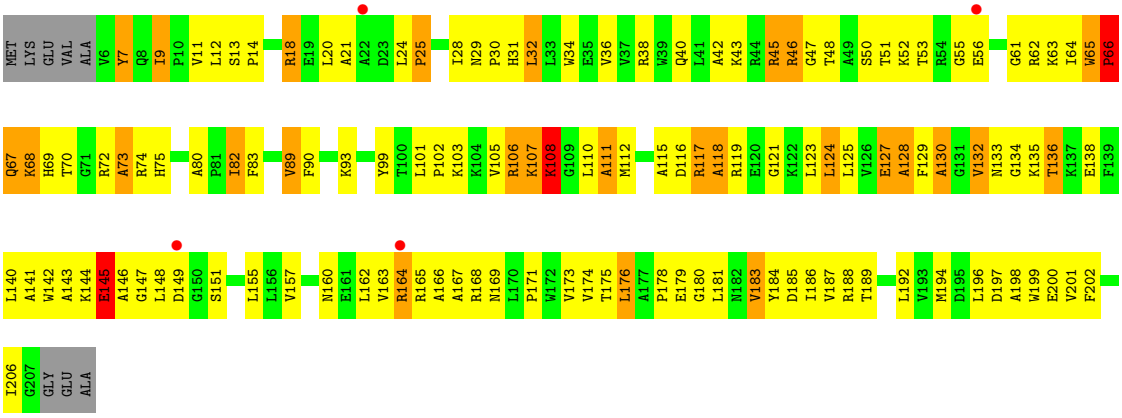






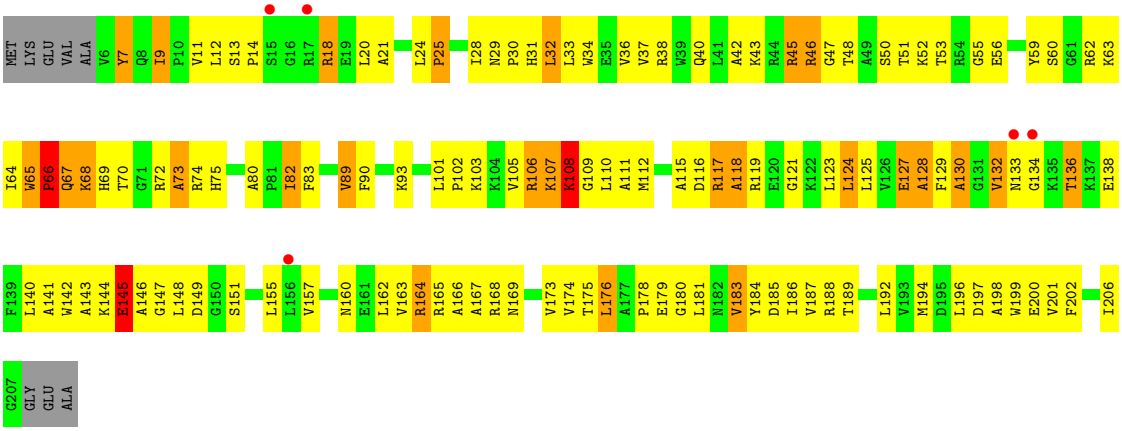
• Molecule 29: 50S ribosomal protein L4

Chain RF:



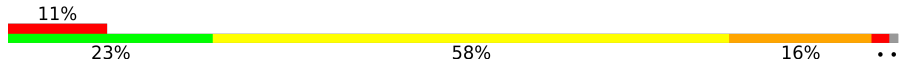
• Molecule 29: 50S ribosomal protein L4

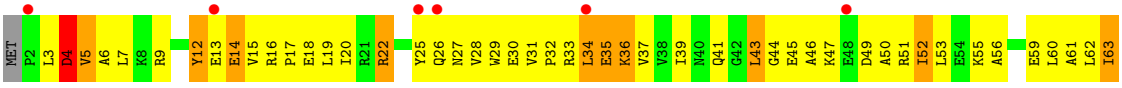
Chain YF:

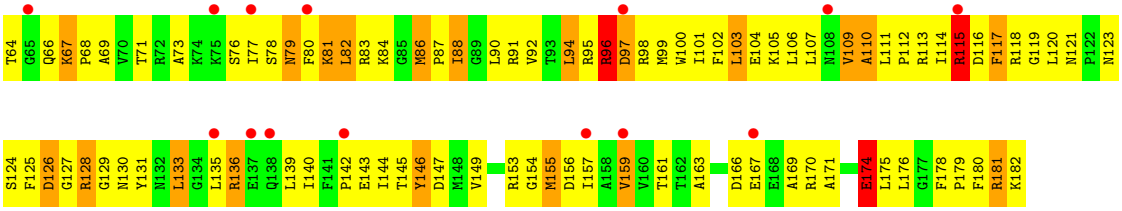


• Molecule 30: 50S ribosomal protein L5

Chain RG:

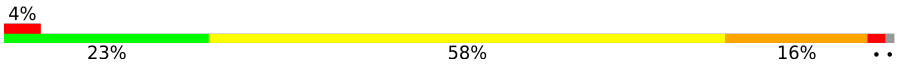


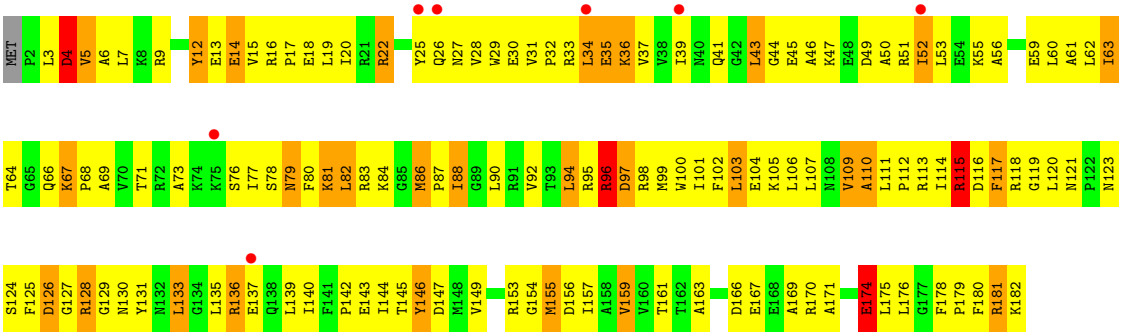




- Molecule 30: 50S ribosomal protein L5

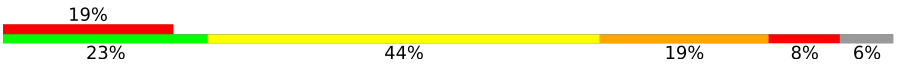
Chain YG:

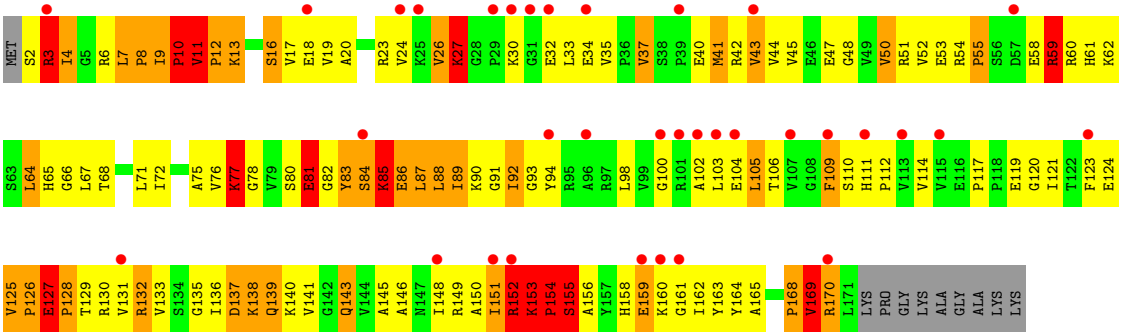




- Molecule 31: 50S ribosomal protein L6

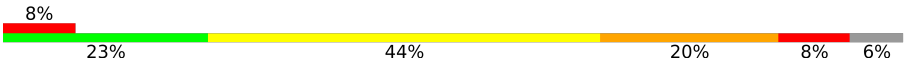
Chain RH:

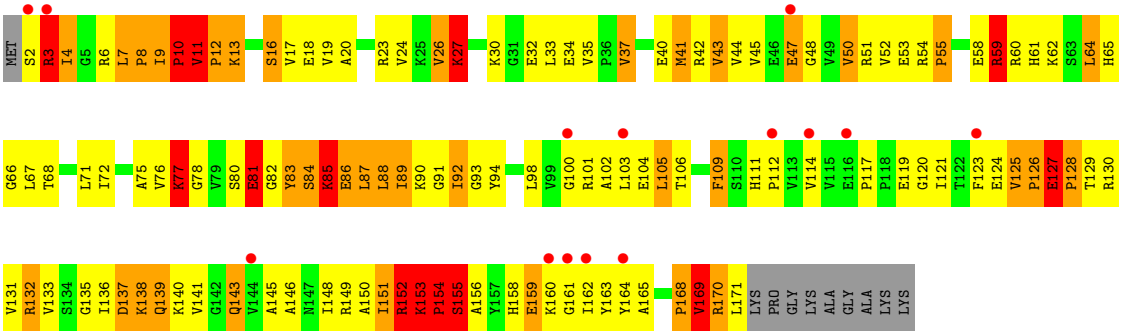




- Molecule 31: 50S ribosomal protein L6

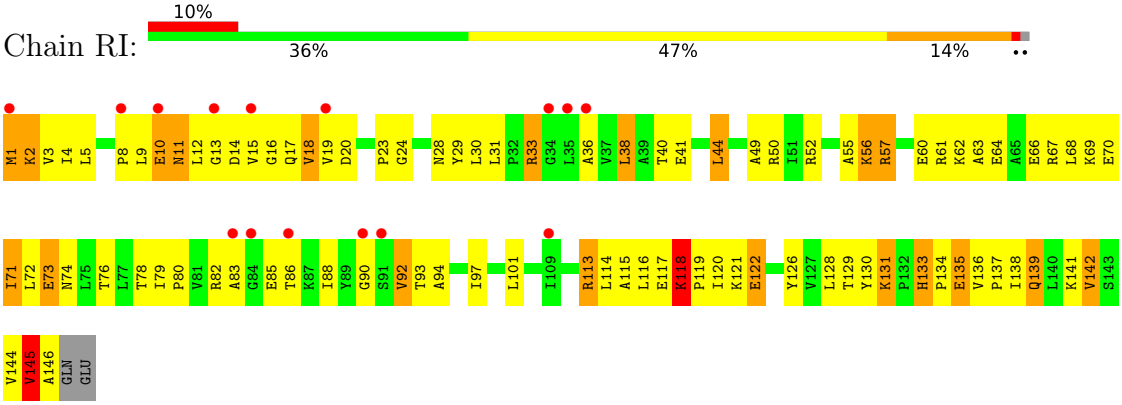
Chain YH:





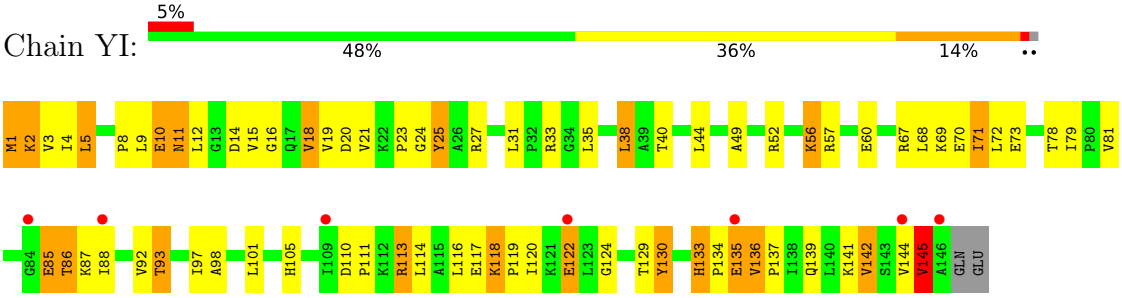
- Molecule 32: 50S ribosomal protein L9

Chain RI:



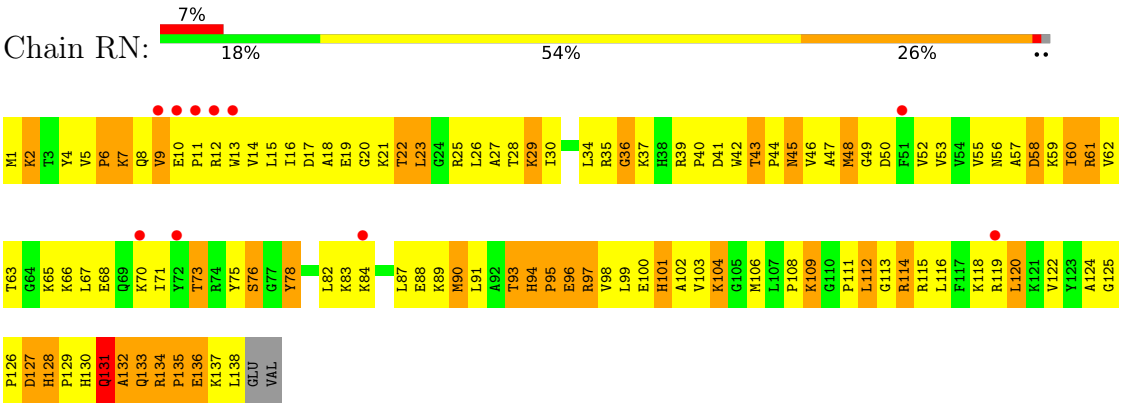
- Molecule 32: 50S ribosomal protein L9

Chain YI:



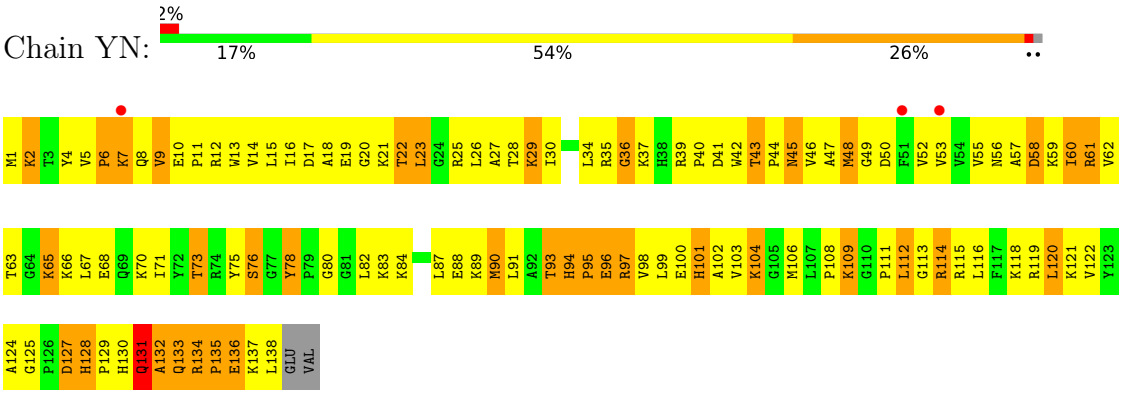
- Molecule 33: 50S ribosomal protein L13

Chain RN:



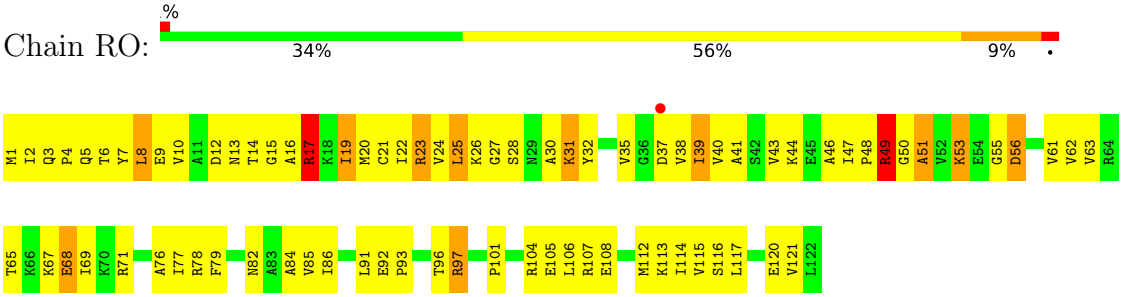
- Molecule 33: 50S ribosomal protein L13

Chain YN:



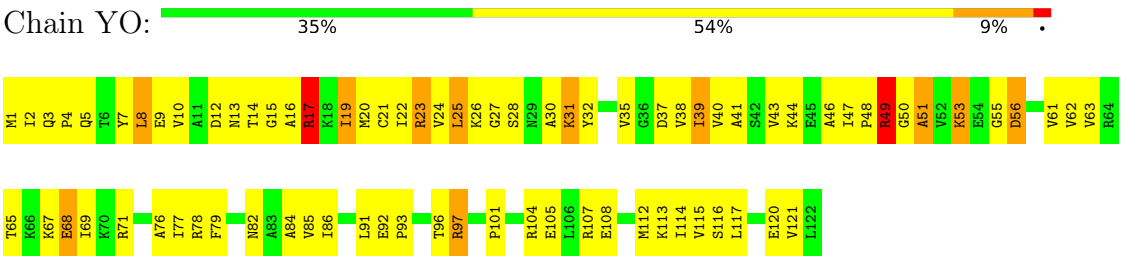
- Molecule 34: 50S ribosomal protein L14

Chain RO:



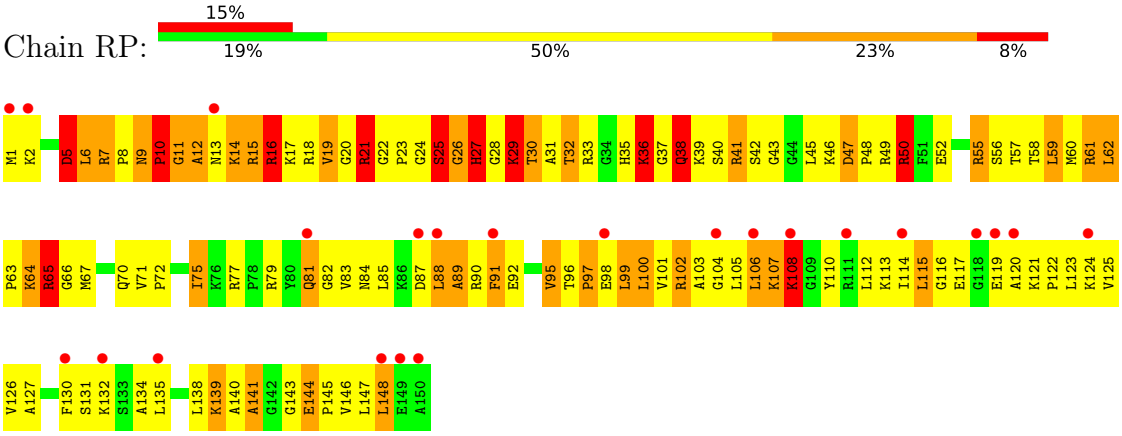
- Molecule 34: 50S ribosomal protein L14

Chain YO:



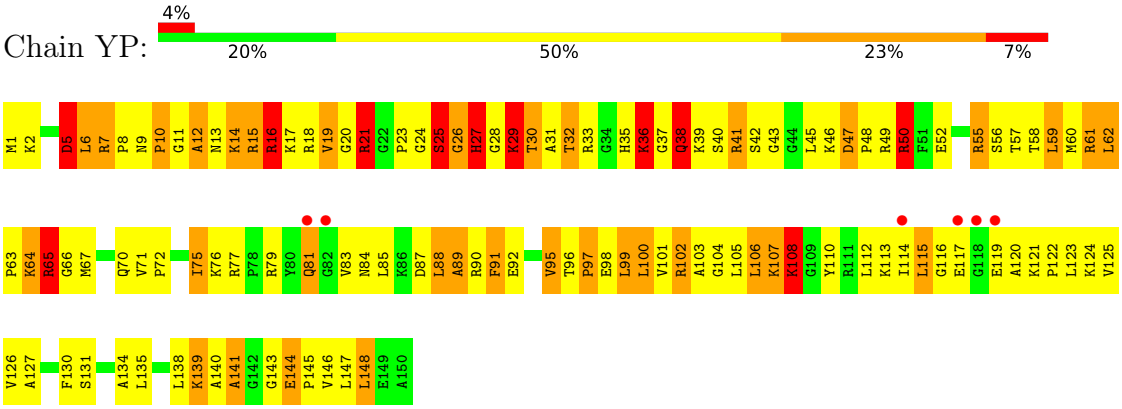
- Molecule 35: 50S ribosomal protein L15

Chain RP:



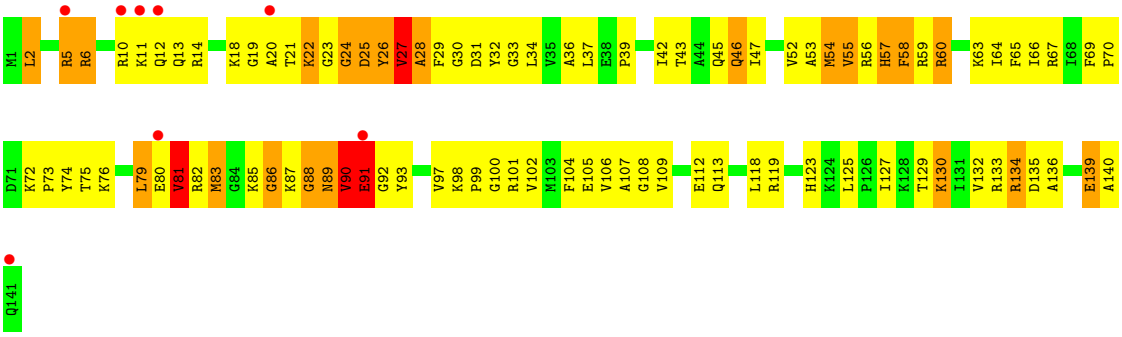
- Molecule 35: 50S ribosomal protein L15

Chain YP:



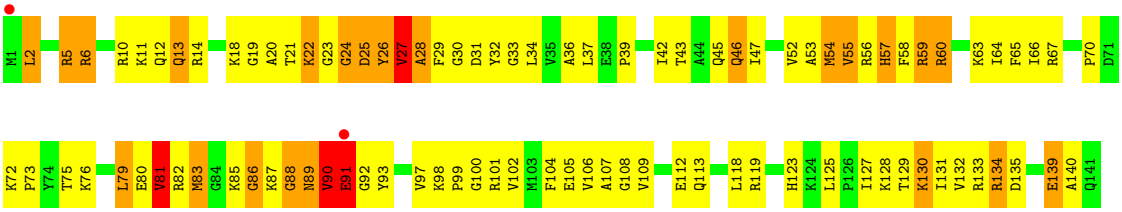
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



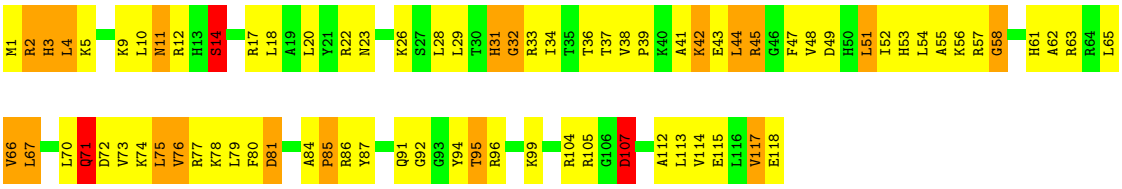
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



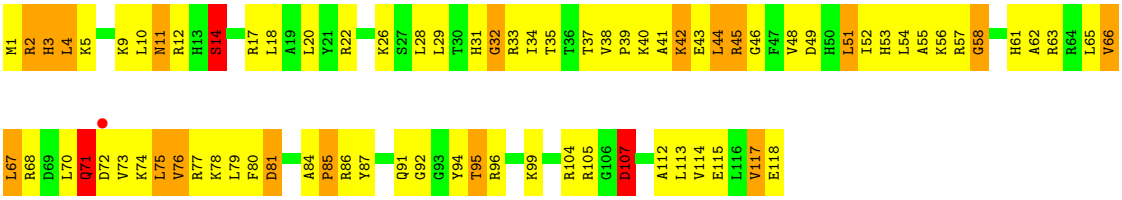
- Molecule 37: 50S ribosomal protein L17

Chain RR:



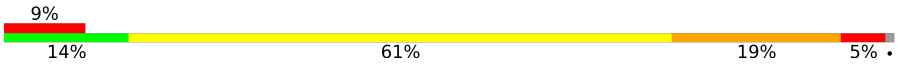
- Molecule 37: 50S ribosomal protein L17

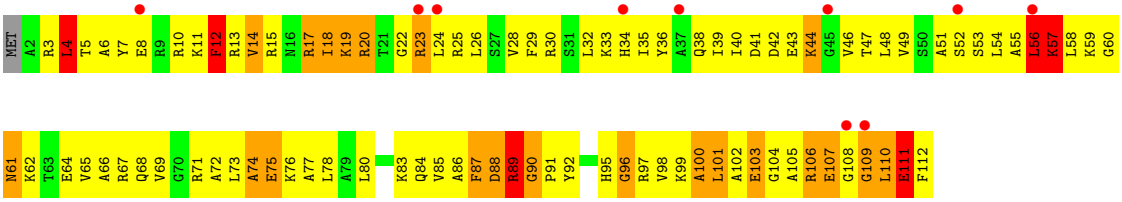
Chain YR:



- Molecule 38: 50S ribosomal protein L18

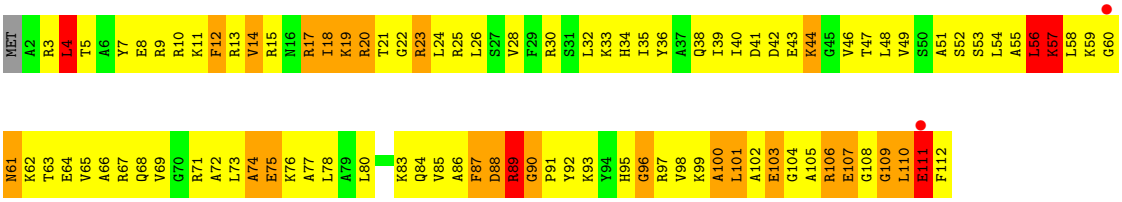
Chain RS:





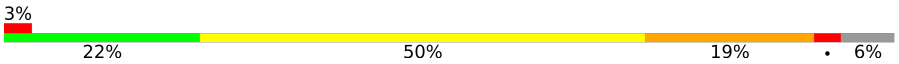
• Molecule 38: 50S ribosomal protein L18

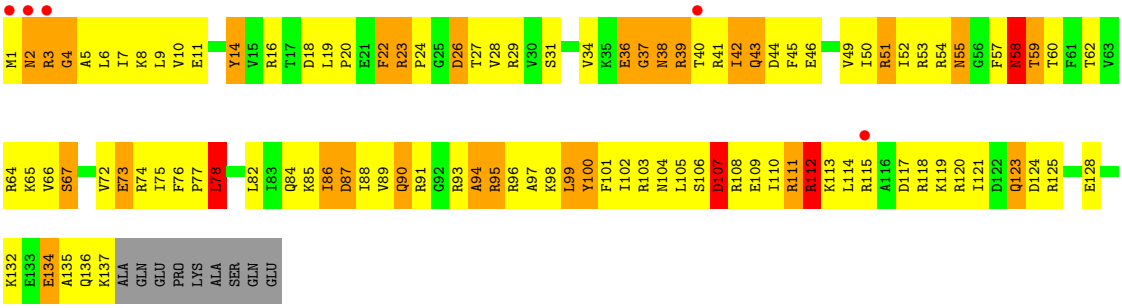
Chain YS:



• Molecule 39: 50S ribosomal protein L19

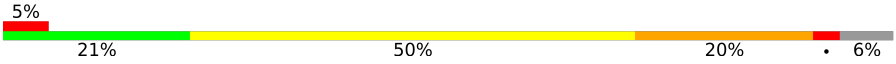
Chain RT:

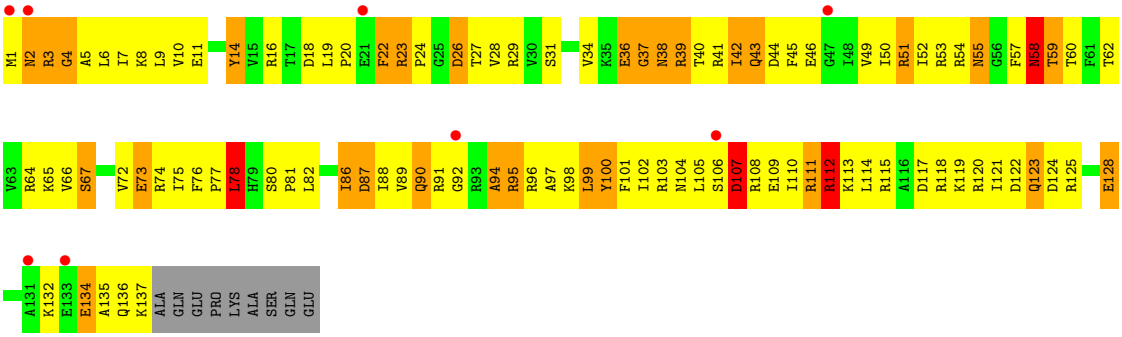




• Molecule 39: 50S ribosomal protein L19

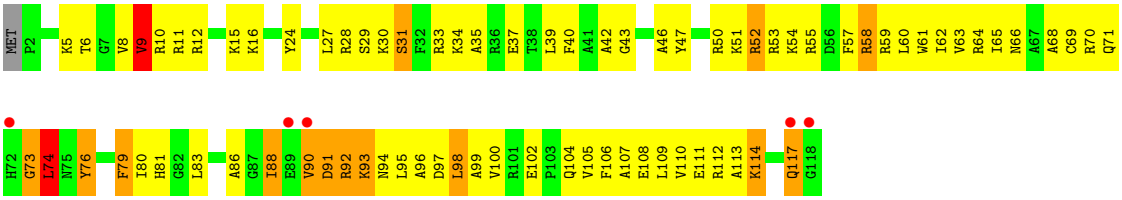
Chain YT:





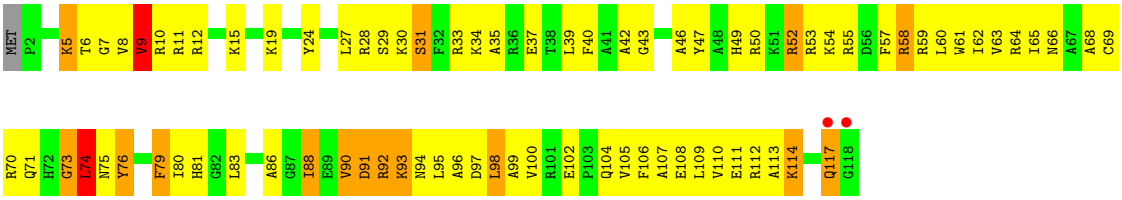
• Molecule 40: 50S ribosomal protein L20

Chain RU:



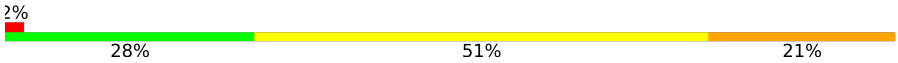
• Molecule 40: 50S ribosomal protein L20

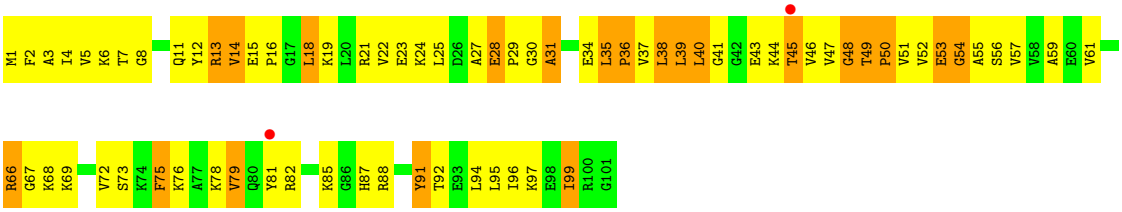
Chain YU:



• Molecule 41: 50S ribosomal protein L21

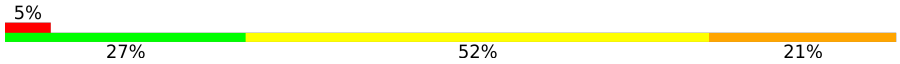
Chain RV:

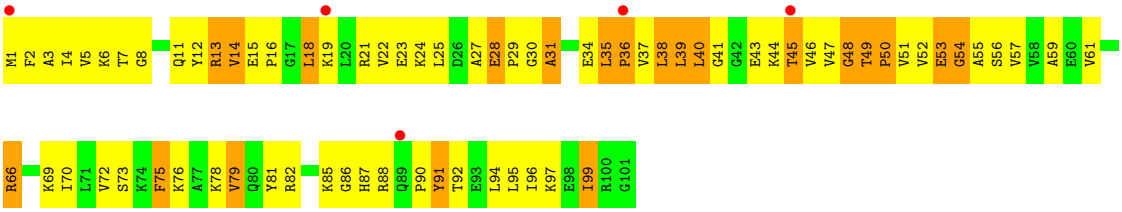




• Molecule 41: 50S ribosomal protein L21

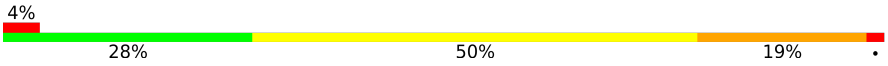
Chain YV:

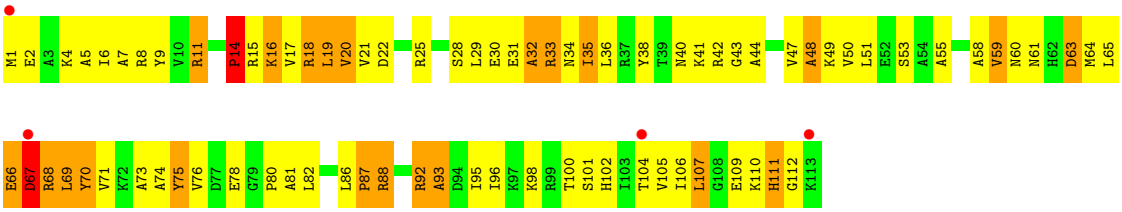




• Molecule 42: 50S ribosomal protein L22

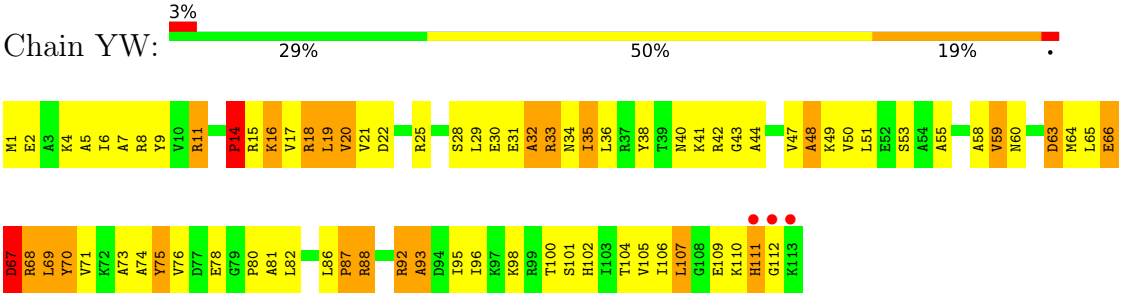
Chain RW:





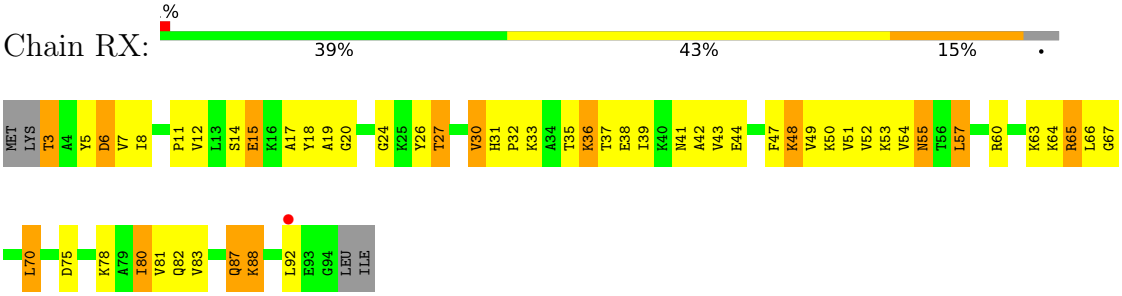
• Molecule 42: 50S ribosomal protein L22

Chain YW:



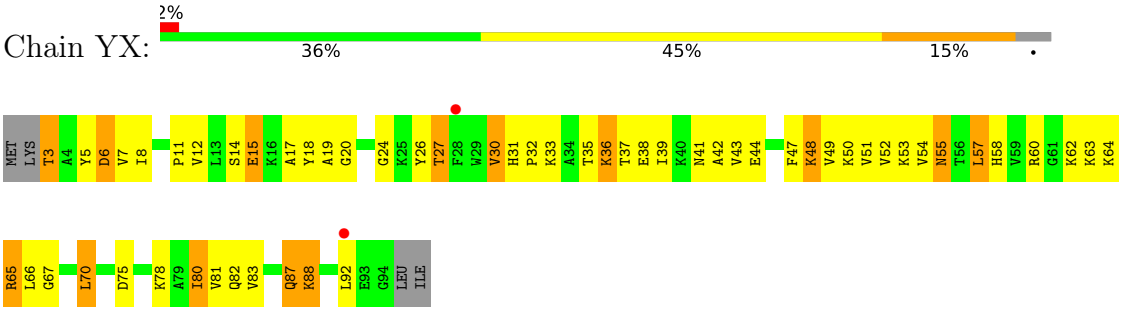
• Molecule 43: 50S ribosomal protein L23

Chain RX:



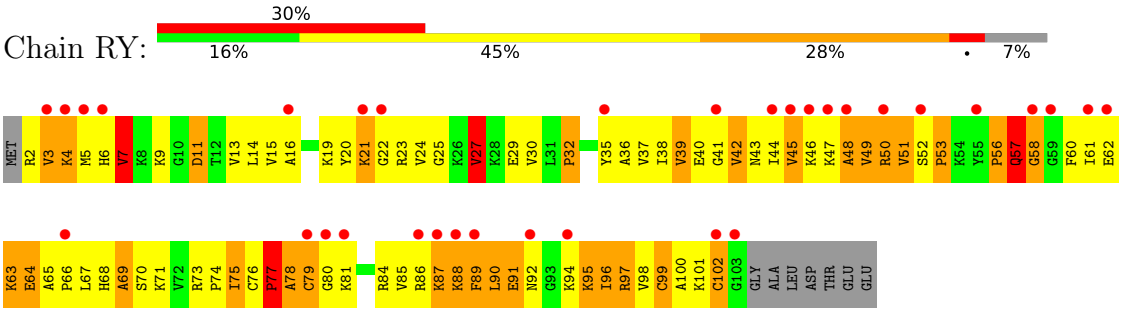
• Molecule 43: 50S ribosomal protein L23

Chain YX:



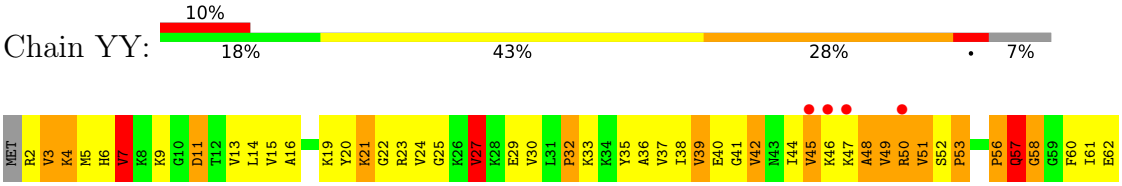
• Molecule 44: 50S ribosomal protein L24

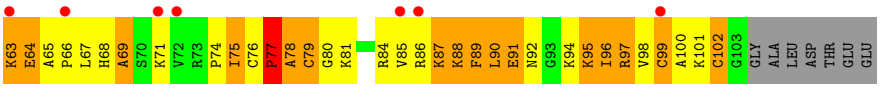
Chain RY:



• Molecule 44: 50S ribosomal protein L24

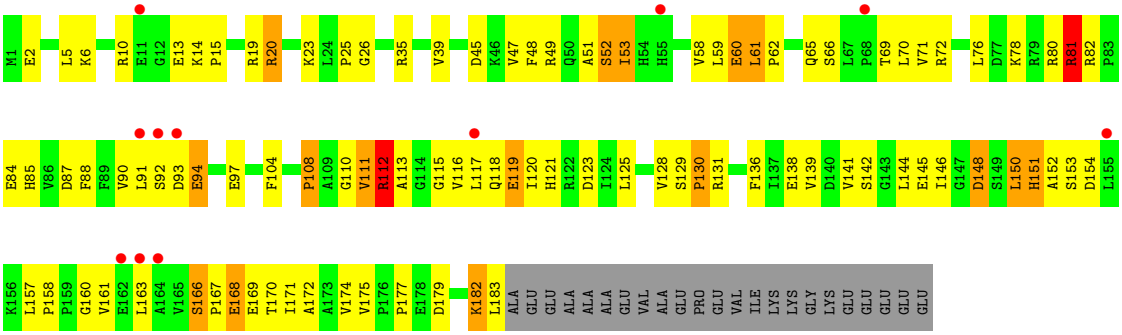
Chain YY:





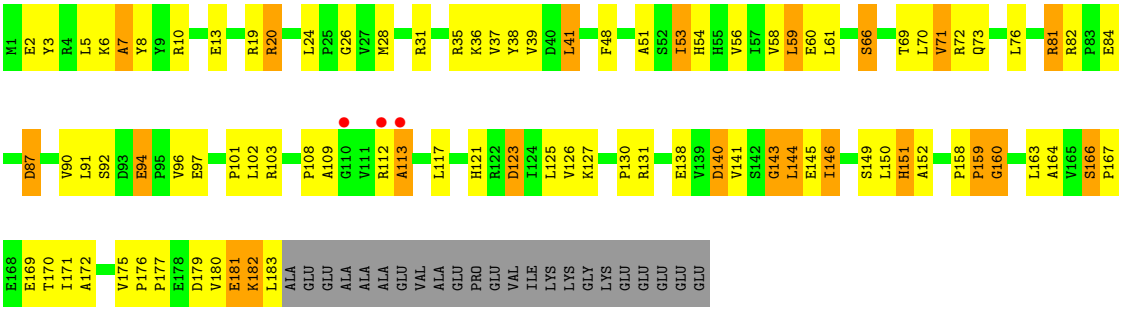
• Molecule 45: 50S ribosomal protein L25

Chain RZ:



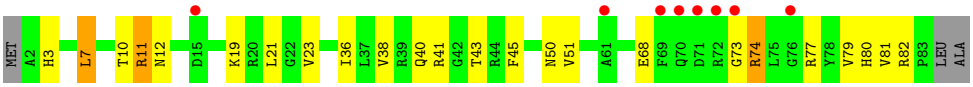
• Molecule 45: 50S ribosomal protein L25

Chain YZ:



• Molecule 46: 50S ribosomal protein L27

Chain R0:

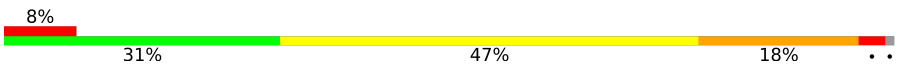


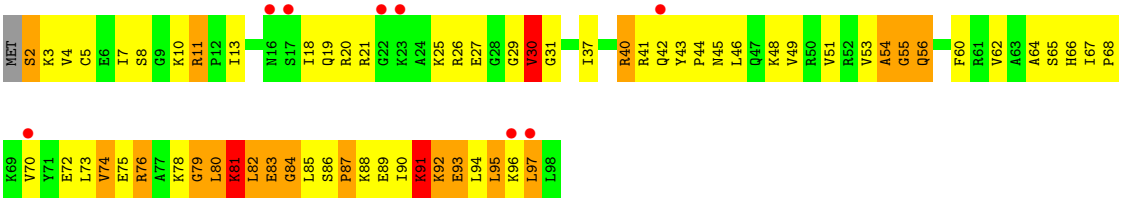
• Molecule 46: 50S ribosomal protein L27

Chain Y0:

• Molecule 47: 50S ribosomal protein L28

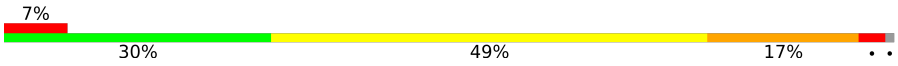
Chain R1:

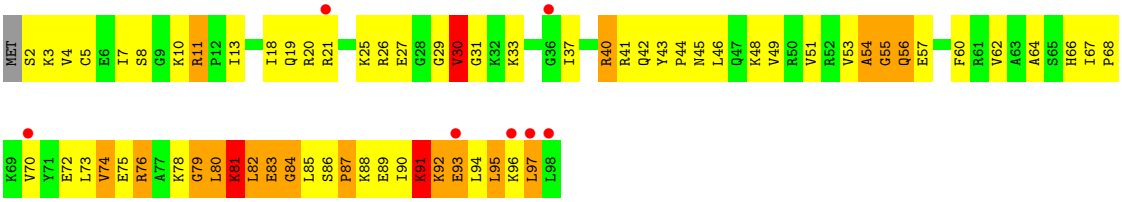




- Molecule 47: 50S ribosomal protein L28

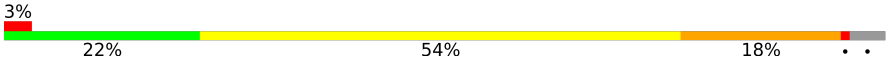
Chain Y1:





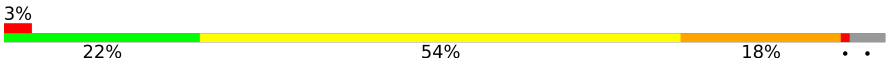
- Molecule 48: 50S ribosomal protein L29

Chain R2:



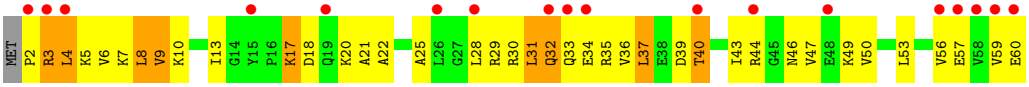
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



- Molecule 49: 50S ribosomal protein L30

Chain R3:

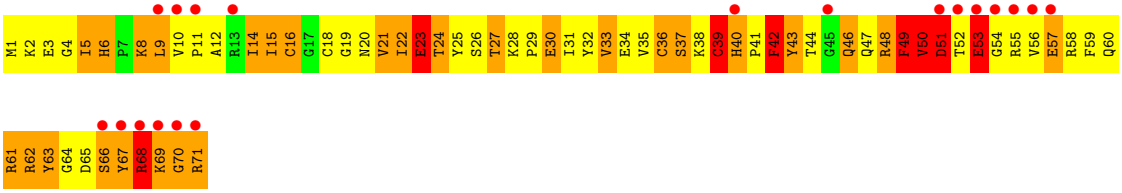


- Molecule 49: 50S ribosomal protein L30

Chain Y3:

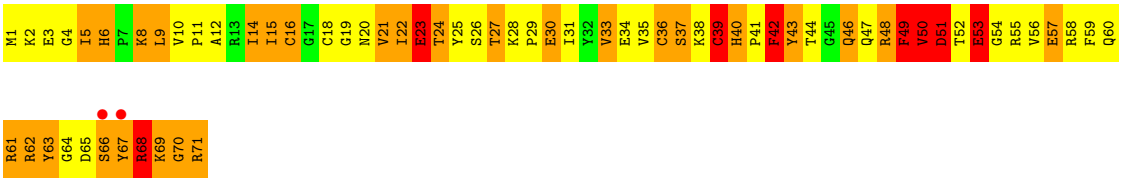
- Molecule 50: 50S ribosomal protein L31

Chain R4:



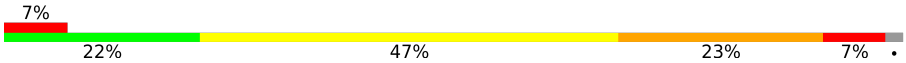
- Molecule 50: 50S ribosomal protein L31

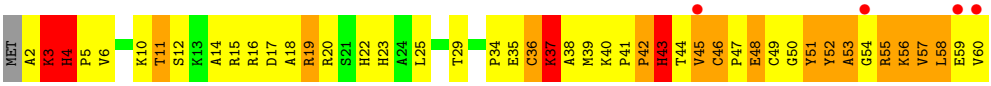
Chain Y4:



- Molecule 51: 50S ribosomal protein L32

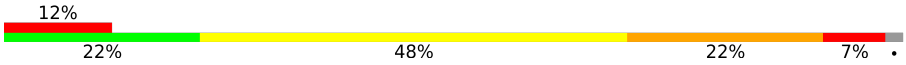
Chain R5:

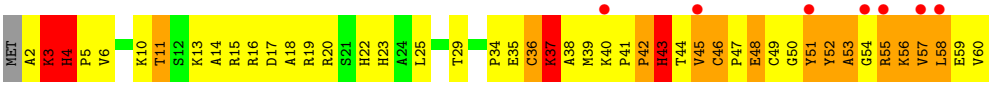




- Molecule 51: 50S ribosomal protein L32

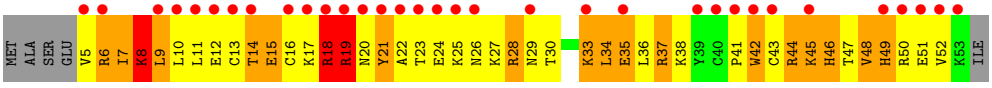
Chain Y5:





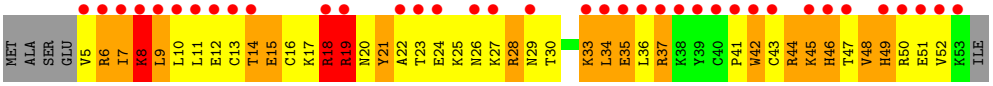
- Molecule 52: 50S ribosomal protein L33

Chain R6:



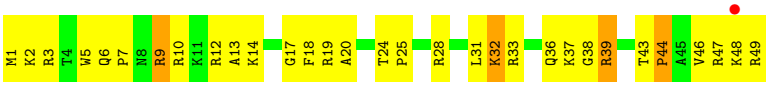
- Molecule 52: 50S ribosomal protein L33

Chain Y6:



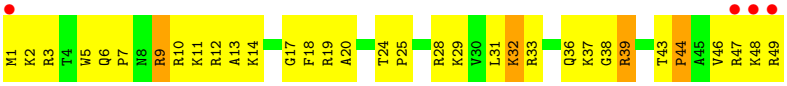
• Molecule 53: 50S ribosomal protein L34

Chain R7:



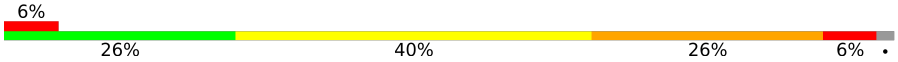
• Molecule 53: 50S ribosomal protein L34

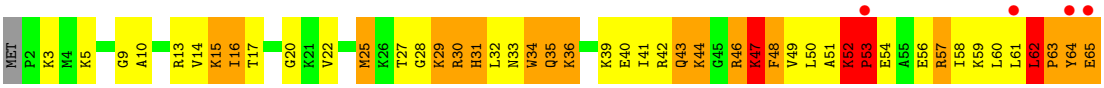
Chain Y7:



• Molecule 54: 50S ribosomal protein L35

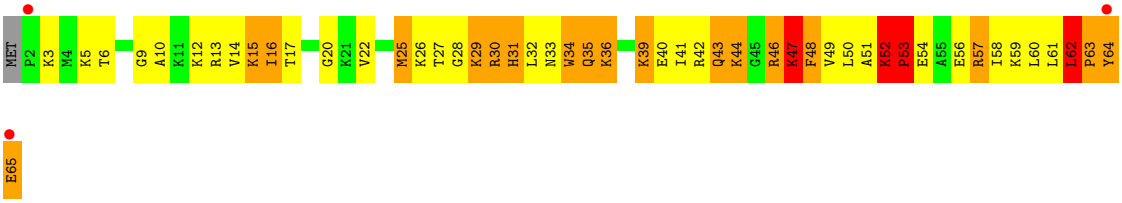
Chain R8:





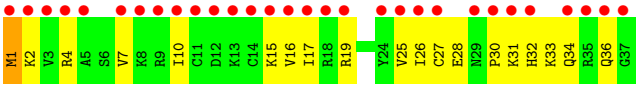
• Molecule 54: 50S ribosomal protein L35

Chain Y8:



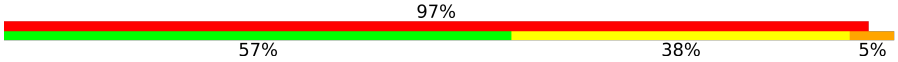
• Molecule 55: 50S ribosomal protein L36

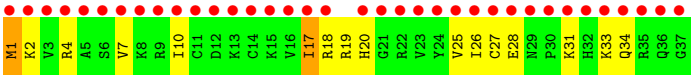
Chain R9:



• Molecule 55: 50S ribosomal protein L36

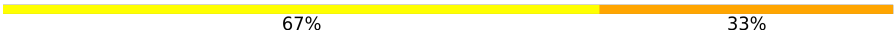
Chain Y9:





- Molecule 56: tRNA acceptor end mimic

Chain Z6:



- Molecule 56: tRNA acceptor end mimic

Chain Z8:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.03Å 447.05Å 619.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.90 49.88 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.88-3.90) 97.9 (49.88-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.252 , 0.298 0.252 , 0.298	Depositor DCC
R_{free} test set	29573 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	291958	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PPU, MG, PAR, 1MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	QA	0.31	0/36098	0.87	34/56341 (0.1%)
1	XA	0.33	0/36101	0.89	31/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.61	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.36	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.45	0/991	1.00	4/1327 (0.3%)
12	XL	0.46	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.52	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	1.00	6/2859 (0.2%)
23	QX	0.32	0/193	0.83	0/299
23	XX	0.30	0/193	0.83	0/299
24	QY	0.66	2/311 (0.6%)	0.86	0/483
24	XY	0.66	2/311 (0.6%)	0.86	0/483
25	RA	0.37	0/69521	0.92	63/108529 (0.1%)
25	YA	0.39	0/69543	0.94	68/108563 (0.1%)
26	RB	0.31	0/2878	0.86	0/4490
26	YB	0.36	0/2878	0.91	1/4490 (0.0%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.29	0/1151	0.55	0/1558
32	YI	0.27	0/1151	0.55	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.94	3/1544 (0.2%)
35	YP	0.50	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.78	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.27	0/1493	0.51	0/2026
45	YZ	0.29	0/1493	0.53	0/2026
46	R0	0.28	0/657	0.51	0/874
46	Y0	0.31	0/657	0.53	0/874
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.50	0/583	0.83	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.72	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.50	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.60	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.80	1/60 (1.7%)
All	All	0.39	6/316339 (0.0%)	0.87	274/472939 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	RD	236	GLY	C-N	8.58	1.53	1.34
24	XY	34	C	C2-N3	7.54	1.41	1.35
24	QY	34	C	C2-N3	7.34	1.41	1.35
24	XY	34	C	C2-O2	6.60	1.30	1.24
24	QY	34	C	C2-O2	6.51	1.30	1.24

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	XL	47	LYS	C-N-CD	-20.47	75.57	120.60
12	QL	47	LYS	C-N-CD	-20.46	75.59	120.60
22	XV	17	C	C2-N1-C1'	11.76	131.74	118.80
22	QV	17	C	C2-N1-C1'	11.76	131.73	118.80
28	YE	21	VAL	C-N-CD	-10.09	98.41	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	630	0
1	XA	32249	0	16279	668	0
2	QB	1924	0	1975	286	0
2	XB	1924	0	1975	288	0
3	QC	1605	0	1668	225	0
3	XC	1605	0	1668	208	1
4	QD	1703	0	1765	276	0
4	XD	1703	0	1765	212	3
5	QE	1155	0	1213	144	0
5	XE	1155	0	1213	136	0
6	QF	843	0	857	93	0
6	XF	843	0	857	123	0
7	QG	1257	0	1296	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	138	0
8	QH	1116	0	1177	148	0
8	XH	1116	0	1177	154	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	149	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	105	1
11	XK	885	0	904	123	0
12	QL	975	0	1062	103	0
12	XL	975	0	1062	103	0
13	QM	964	0	1034	157	0
13	XM	964	0	1034	161	0
14	QN	492	0	529	100	0
14	XN	492	0	529	96	0
15	QO	734	0	771	74	0
15	XO	734	0	771	73	0
16	QP	705	0	725	110	0
16	XP	705	0	725	110	0
17	QQ	834	0	904	80	0
17	XQ	834	0	904	80	0
18	QR	574	0	644	67	0
18	XR	574	0	644	68	0
19	QS	674	0	699	106	0
19	XS	674	0	699	129	0
20	QT	763	0	860	106	0
20	XT	763	0	861	101	0
21	QU	217	0	234	26	0
21	XU	217	0	234	27	0
22	QV	1644	0	836	29	0
22	XV	1644	0	836	28	0
23	QX	173	0	88	5	0
23	XX	173	0	88	2	0
24	QY	303	0	154	4	0
24	XY	303	0	154	5	0
25	RA	62071	0	31290	1129	0
25	YA	62091	0	31295	1166	0
26	RB	2573	0	1306	46	0
26	YB	2573	0	1306	41	0
27	RD	2115	0	2195	317	3
27	YD	2115	0	2195	336	0
28	RE	1568	0	1634	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	175	0
30	RG	1474	0	1535	194	0
30	YG	1474	0	1535	193	0
31	RH	1307	0	1382	224	0
31	YH	1307	0	1382	220	3
32	RI	1136	0	1223	57	0
32	YI	1136	0	1223	40	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	124	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	243	0
35	YP	1145	0	1227	235	0
36	RQ	1122	0	1179	148	0
36	YQ	1122	0	1179	143	0
37	RR	968	0	1033	109	0
37	YR	968	0	1033	114	0
38	RS	882	0	943	153	0
38	YS	882	0	943	157	0
39	RT	1141	0	1202	156	0
39	YT	1141	0	1202	164	0
40	RU	964	0	1022	131	0
40	YU	964	0	1022	134	0
41	RV	779	0	852	130	0
41	YV	779	0	852	135	3
42	RW	900	0	964	95	0
42	YW	900	0	964	105	0
43	RX	725	0	778	68	0
43	YX	725	0	778	70	0
44	RY	785	0	878	160	0
44	YY	785	0	878	149	3
45	RZ	1461	0	1493	60	0
45	YZ	1461	0	1493	61	0
46	R0	648	0	671	19	0
46	Y0	648	0	672	23	0
47	R1	763	0	848	139	0
47	Y1	763	0	848	133	0
48	R2	581	0	629	81	0
48	Y2	581	0	629	71	0
49	R3	469	0	518	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	42	0
50	R4	581	0	574	154	0
50	Y4	581	0	574	169	0
51	R5	459	0	480	74	0
51	Y5	459	0	480	78	3
52	R6	424	0	450	88	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	40	0
53	Y7	430	0	480	43	0
54	R8	517	0	582	97	0
54	Y8	517	0	582	105	0
55	R9	307	0	338	20	0
55	Y9	307	0	338	19	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	242	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	XA	70	0	0	0	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	1	0	0	0	0
57	YA	267	0	0	0	0
57	YB	3	0	0	0	0
57	YD	2	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
58	QA	42	0	45	3	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291958	0	198347	15046	10

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 31.

The worst 5 of 15046 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:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.52
4:QD:167:GLY:HA2	27:YD:135:PHE:CZ	1.42	1.52
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52

The worst 5 of 10 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)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.69	0.51
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	1.99	0.21
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.03	0.17
41:YV:51:VAL:CB	51:Y5:60:VAL:OXT[4_445]	2.07	0.13
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.08	0.12

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	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	12
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	12
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	11
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	0	7
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	10
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	10
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	12
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	9
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
11	XK	117/129 (91%)	86 (74%)	22 (19%)	9 (8%)	1	16
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	7
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	7
13	QM	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	3
13	XM	119/126 (94%)	72 (60%)	26 (22%)	21 (18%)	0	3
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	17
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	17
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	17
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	10
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	6
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	105 (73%)	25 (17%)	14 (10%)	0	11
32	YI	144/148 (97%)	101 (70%)	29 (20%)	14 (10%)	0	11
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	10
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	10
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
40	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	131 (72%)	32 (18%)	18 (10%)	0	10
45	YZ	181/206 (88%)	129 (71%)	33 (18%)	19 (10%)	0	9
46	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	12	48
46	Y0	80/85 (94%)	70 (88%)	9 (11%)	1 (1%)	12	48
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0 2
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0 2
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
All	All	11470/12128 (95%)	7661 (67%)	2332 (20%)	1477 (13%)	0 5

5 of 1477 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	QB	205/220 (93%)	181 (88%)	24 (12%)	5 26
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5 26
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7 30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7 30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6 27
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11 39
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12 41
5	XE	116/123 (94%)	108 (93%)	8 (7%)	15 45
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2 17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2 17
7	QG	126/127 (99%)	115 (91%)	11 (9%)	10 37
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	28
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	28
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	22
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	22
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	15
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	15
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	26
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	18
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	68 (90%)	8 (10%)	7	29
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	53
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	53
27	RD	214/218 (98%)	176 (82%)	38 (18%)	2	12
27	YD	214/218 (98%)	176 (82%)	38 (18%)	2	12
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	23
29	YF	161/166 (97%)	140 (87%)	21 (13%)	4	23
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	16
30	YG	155/156 (99%)	130 (84%)	25 (16%)	2	16
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	9
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	9
32	RI	122/124 (98%)	100 (82%)	22 (18%)	1	12
32	YI	122/124 (98%)	98 (80%)	24 (20%)	1	9
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	16
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	16
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	15
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	15
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	18
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	18
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	10
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	10
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	21
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	21
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	22
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	22
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	16
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	16
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	18
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	13
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
45	RZ	162/179 (90%)	140 (86%)	22 (14%)	3	22
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	6	27
46	R0	65/67 (97%)	61 (94%)	4 (6%)	18	48
46	Y0	65/67 (97%)	61 (94%)	4 (6%)	18	48
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	11
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	11
48	R2	64/67 (96%)	57 (89%)	7 (11%)	6	28
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	28
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	7
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	7
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	5
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	44
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	44
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49
All	All	9702/10066 (96%)	8303 (86%)	1399 (14%)	3	20

5 of 1399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	YD	71	ASP
35	YP	146	VAL
27	YD	262	ARG
27	YD	67	PHE
31	YH	4	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
6	XF	64	GLN
19	XS	65	ASN
7	XG	28	ASN
11	XK	99	GLN
27	YD	166	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	313 (20%)	45 (3%)
1	XA	1499/1522 (98%)	315 (21%)	47 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	3 (42%)	2 (28%)
23	XX	7/25 (28%)	3 (42%)	2 (28%)
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	667 (23%)	61 (2%)
25	YA	2880/2916 (98%)	675 (23%)	58 (2%)
26	RB	119/122 (97%)	24 (20%)	1 (0%)
26	YB	119/122 (97%)	26 (21%)	1 (0%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2096 (22%)	221 (2%)

5 of 2096 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A

5 of 221 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	89	U
1	XA	992	U
25	YA	2832	U

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Mol	Chain	Res	Type
25	YA	1275	A
1	XA	244	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	1MG	QY	37	24	18,26,27	2.20	2 (11%)	19,39,42	1.56	4 (21%)
24	1MG	XY	37	24	18,26,27	2.21	2 (11%)	19,39,42	1.54	4 (21%)
56	PPU	Z8	76	25,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
56	PPU	Z6	76	25,56	32,40,41	2.56	6 (18%)	33,57,60	2.16	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3
56	PPU	Z8	76	25,56	-	2/21/43/44	0/4/4/4
56	PPU	Z6	76	25,56	-	2/21/43/44	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.25	1.41	1.23
56	Z6	76	PPU	O-C	9.24	1.41	1.23
24	XY	37	1MG	C2-N2	7.47	1.47	1.34
24	QY	37	1MG	C2-N2	7.41	1.47	1.34
56	Z6	76	PPU	C9-N6	-5.94	1.32	1.45

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z6	76	PPU	C3'-N3'-C	-8.67	110.13	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.62	110.21	123.21
56	Z8	76	PPU	N3-C2-N1	-4.67	121.38	128.68
56	Z6	76	PPU	N3-C2-N1	-4.67	121.38	128.68
56	Z8	76	PPU	CA-C-N3'	4.01	121.71	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	8	0
56	Z6	76	PPU	9	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 676 ligands modelled in this entry, 674 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PAR	QA	1666	-	45,45,45	1.62	9 (20%)	64,67,67	1.46	11 (17%)
58	PAR	XA	1671	-	45,45,45	1.69	10 (22%)	64,67,67	1.80	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	6/18/94/94	0/4/4/4
58	PAR	XA	1671	-	-	4/18/94/94	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C64-C54	6.03	1.60	1.52
58	XA	1671	PAR	C31-C21	4.76	1.59	1.53
58	XA	1671	PAR	C64-C54	4.55	1.58	1.52
58	XA	1671	PAR	C11-C21	3.79	1.59	1.52
58	QA	1666	PAR	C52-C42	2.94	1.58	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	XA	1671	PAR	O33-C14-C24	4.85	116.57	108.22
58	QA	1666	PAR	O54-C54-C64	4.62	114.61	106.01
58	XA	1671	PAR	C32-C22-C12	-3.96	103.05	111.18
58	XA	1671	PAR	O54-C54-C64	3.62	112.75	106.01
58	QA	1666	PAR	C14-O54-C54	3.48	120.52	113.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1671	PAR	C44-C54-C64-N64
58	XA	1671	PAR	O54-C54-C64-N64
58	XA	1671	PAR	O51-C51-C61-O61

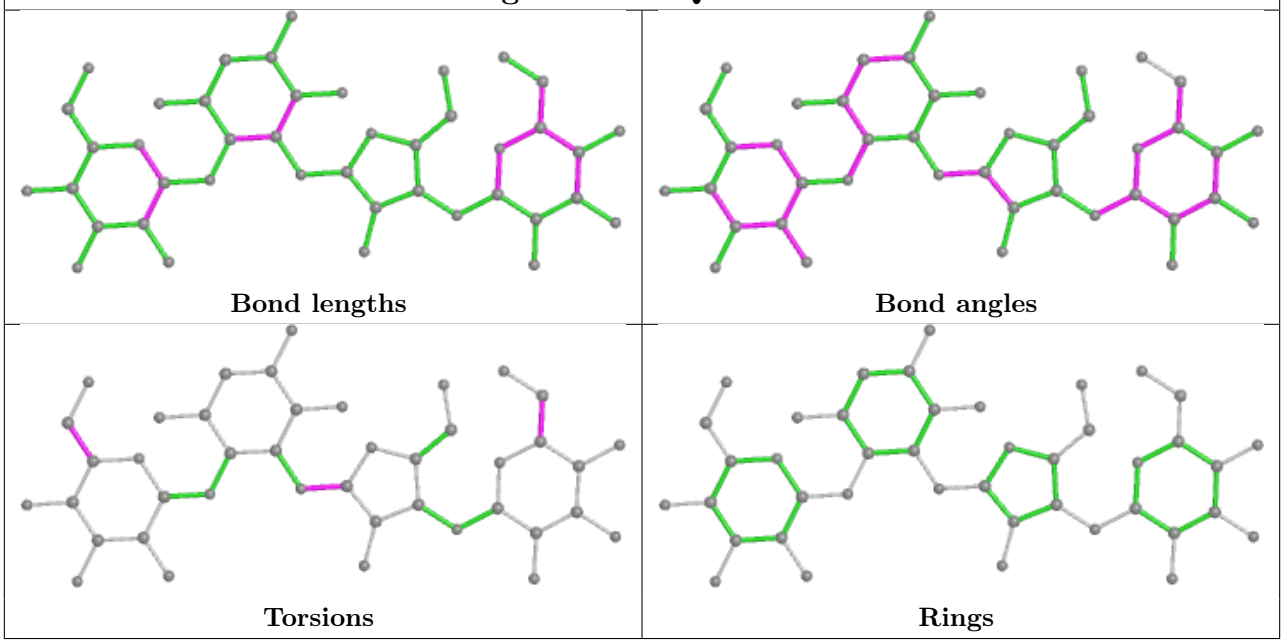
There are no ring outliers.

2 monomers are involved in 5 short contacts:

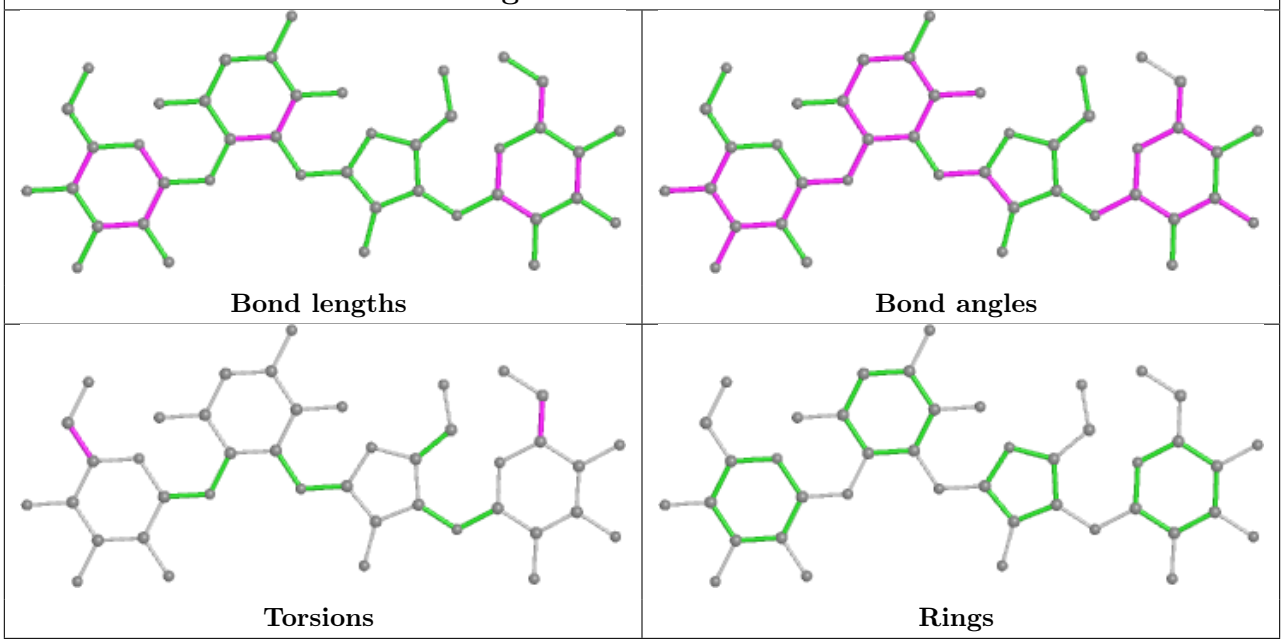
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1666	PAR	3	0
58	XA	1671	PAR	2	0

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

Ligand PAR QA 1666



Ligand PAR XA 1671



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	QA	1500/1522 (98%)	0.07	36 (2%)	59	48	35, 87, 182, 299	0
1	XA	1500/1522 (98%)	-0.09	13 (0%)	84	77	21, 74, 169, 271	0
2	QB	237/256 (92%)	0.66	25 (10%)	6	5	84, 154, 204, 236	0
2	XB	237/256 (92%)	0.27	11 (4%)	32	26	51, 121, 182, 226	0
3	QC	205/239 (85%)	0.26	15 (7%)	15	11	57, 135, 182, 201	0
3	XC	205/239 (85%)	0.01	5 (2%)	59	48	32, 89, 145, 177	0
4	QD	208/209 (99%)	0.35	10 (4%)	30	25	38, 99, 165, 221	0
4	XD	208/209 (99%)	0.26	4 (1%)	66	57	27, 106, 160, 186	0
5	QE	151/162 (93%)	0.43	10 (6%)	18	13	36, 111, 158, 185	0
5	XE	151/162 (93%)	0.21	6 (3%)	38	30	3, 85, 142, 170	0
6	QF	101/101 (100%)	0.28	3 (2%)	50	38	33, 99, 158, 181	0
6	XF	101/101 (100%)	0.17	4 (3%)	38	30	25, 95, 145, 243	0
7	QG	155/156 (99%)	0.68	22 (14%)	2	3	55, 123, 179, 210	0
7	XG	155/156 (99%)	0.34	13 (8%)	11	9	42, 99, 156, 197	0
8	QH	138/138 (100%)	0.56	13 (9%)	8	7	61, 120, 167, 193	0
8	XH	138/138 (100%)	0.37	5 (3%)	42	33	20, 94, 147, 198	0
9	QI	127/128 (99%)	0.89	18 (14%)	2	3	67, 134, 193, 224	0
9	XI	127/128 (99%)	0.34	5 (3%)	39	30	29, 107, 165, 195	0
10	QJ	99/105 (94%)	1.38	22 (22%)	0	0	46, 149, 202, 222	0
10	XJ	99/105 (94%)	0.75	16 (16%)	1	2	35, 115, 175, 201	0
11	QK	119/129 (92%)	0.60	14 (11%)	4	4	42, 104, 158, 202	0
11	XK	119/129 (92%)	0.47	9 (7%)	13	10	27, 87, 148, 170	0
12	QL	125/132 (94%)	0.56	15 (12%)	4	4	21, 93, 142, 192	0
12	XL	125/132 (94%)	0.20	6 (4%)	30	25	20, 66, 131, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.45	13 (10%) 6 5	58, 122, 175, 214	0
13	XM	121/126 (96%)	0.19	5 (4%) 37 29	28, 92, 144, 180	0
14	QN	60/61 (98%)	0.87	9 (15%) 2 2	55, 129, 181, 204	0
14	XN	60/61 (98%)	0.26	3 (5%) 28 24	33, 82, 135, 170	0
15	QO	88/89 (98%)	0.25	4 (4%) 33 27	54, 105, 154, 178	0
15	XO	88/89 (98%)	0.15	1 (1%) 80 73	25, 91, 141, 171	0
16	QP	84/88 (95%)	0.76	11 (13%) 3 3	42, 86, 157, 171	0
16	XP	84/88 (95%)	0.75	10 (11%) 4 4	51, 101, 152, 235	0
17	QQ	100/105 (95%)	0.45	4 (4%) 38 30	33, 91, 144, 165	0
17	XQ	100/105 (95%)	0.56	8 (8%) 12 10	37, 95, 147, 200	0
18	QR	70/88 (79%)	0.80	8 (11%) 5 4	42, 110, 160, 212	0
18	XR	70/88 (79%)	0.47	5 (7%) 16 11	34, 86, 147, 168	0
19	QS	84/93 (90%)	0.93	14 (16%) 1 2	60, 131, 184, 190	0
19	XS	84/93 (90%)	0.44	5 (5%) 21 16	45, 97, 141, 220	0
20	QT	99/106 (93%)	0.32	2 (2%) 65 55	34, 91, 154, 181	0
20	XT	99/106 (93%)	0.58	7 (7%) 16 11	50, 112, 158, 181	0
21	QU	25/27 (92%)	2.69	15 (60%) 0 0	62, 132, 185, 206	0
21	XU	25/27 (92%)	1.47	6 (24%) 0 0	45, 89, 136, 166	0
22	QV	77/77 (100%)	0.03	1 (1%) 77 68	26, 99, 158, 205	0
22	XV	77/77 (100%)	-0.12	1 (1%) 77 68	28, 70, 121, 185	0
23	QX	8/25 (32%)	1.29	2 (25%) 0 0	70, 95, 129, 169	0
23	XX	8/25 (32%)	1.19	2 (25%) 0 0	36, 51, 102, 163	0
24	QY	13/18 (72%)	1.12	2 (15%) 2 2	104, 150, 249, 294	0
24	XY	13/18 (72%)	0.89	0 100 100	70, 106, 221, 249	0
25	RA	2882/2916 (98%)	-0.02	90 (3%) 49 38	14, 60, 203, 320	0
25	YA	2883/2916 (98%)	-0.13	82 (2%) 53 41	14, 50, 194, 329	0
26	RB	120/122 (98%)	0.13	2 (1%) 70 60	64, 113, 177, 203	0
26	YB	120/122 (98%)	-0.39	0 100 100	37, 69, 95, 158	0
27	RD	272/276 (98%)	0.09	3 (1%) 80 73	7, 56, 113, 177	0
27	YD	272/276 (98%)	0.11	2 (0%) 87 82	3, 49, 98, 152	0
28	RE	205/206 (99%)	0.35	8 (3%) 39 30	23, 73, 150, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	YE	205/206 (99%)	0.38	7 (3%) 45 35	15, 77, 151, 200	0
29	RF	202/210 (96%)	0.18	4 (1%) 65 55	4, 85, 151, 184	0
29	YF	202/210 (96%)	0.04	5 (2%) 57 47	8, 65, 124, 184	0
30	RG	181/182 (99%)	0.59	20 (11%) 5 5	52, 137, 205, 232	0
30	YG	181/182 (99%)	0.28	7 (3%) 39 30	25, 98, 166, 203	0
31	RH	170/180 (94%)	1.04	34 (20%) 1 1	69, 150, 202, 250	0
31	YH	170/180 (94%)	0.53	14 (8%) 11 9	32, 94, 152, 204	0
32	RI	146/148 (98%)	0.50	15 (10%) 6 5	29, 108, 161, 182	0
32	YI	146/148 (98%)	0.16	7 (4%) 30 25	18, 95, 158, 203	0
33	RN	138/140 (98%)	0.52	10 (7%) 15 11	33, 94, 152, 192	0
33	YN	138/140 (98%)	0.07	3 (2%) 62 51	19, 75, 132, 162	0
34	RO	122/122 (100%)	0.18	1 (0%) 86 79	6, 64, 120, 163	0
34	YO	122/122 (100%)	0.14	0 100 100	18, 60, 114, 144	0
35	RP	150/150 (100%)	0.71	23 (15%) 2 2	5, 87, 160, 191	0
35	YP	150/150 (100%)	0.37	6 (4%) 38 30	17, 75, 166, 203	0
36	RQ	141/141 (100%)	0.51	8 (5%) 23 19	25, 94, 140, 212	0
36	YQ	141/141 (100%)	0.16	2 (1%) 75 66	11, 61, 126, 169	0
37	RR	118/118 (100%)	0.03	0 100 100	12, 58, 116, 154	0
37	YR	118/118 (100%)	0.26	1 (0%) 86 79	24, 68, 127, 155	0
38	RS	111/112 (99%)	0.67	10 (9%) 9 7	40, 116, 169, 194	0
38	YS	111/112 (99%)	0.23	2 (1%) 68 59	9, 79, 133, 232	0
39	RT	137/146 (93%)	0.22	5 (3%) 42 33	19, 77, 171, 214	0
39	YT	137/146 (93%)	0.16	8 (5%) 23 18	30, 84, 164, 206	0
40	RU	117/118 (99%)	0.10	5 (4%) 35 28	17, 78, 154, 194	0
40	YU	117/118 (99%)	-0.06	2 (1%) 70 60	15, 65, 152, 189	0
41	RV	101/101 (100%)	0.28	2 (1%) 65 55	36, 105, 157, 216	0
41	YV	101/101 (100%)	0.34	5 (4%) 28 24	23, 84, 144, 243	0
42	RW	113/113 (100%)	0.39	4 (3%) 44 34	20, 65, 137, 216	0
42	YW	113/113 (100%)	0.14	3 (2%) 54 43	12, 56, 114, 193	0
43	RX	92/96 (95%)	0.15	1 (1%) 80 73	14, 69, 125, 158	0
43	YX	92/96 (95%)	0.27	2 (2%) 62 51	12, 56, 113, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	RY	102/110 (92%)	1.48	33 (32%)	0	0	36, 115, 175, 230	0
44	YY	102/110 (92%)	0.63	11 (10%)	5	5	24, 83, 156, 204	0
45	RZ	183/206 (88%)	0.39	11 (6%)	21	16	42, 122, 174, 213	0
45	YZ	183/206 (88%)	0.10	3 (1%)	72	62	23, 98, 153, 211	0
46	R0	82/85 (96%)	0.70	8 (9%)	7	6	13, 74, 111, 143	0
46	Y0	82/85 (96%)	0.46	0	100	100	11, 54, 85, 133	0
47	R1	97/98 (98%)	0.71	8 (8%)	11	9	11, 74, 170, 241	0
47	Y1	97/98 (98%)	0.48	7 (7%)	15	11	11, 64, 144, 205	0
48	R2	69/72 (95%)	0.16	2 (2%)	51	40	26, 101, 176, 197	0
48	Y2	69/72 (95%)	0.18	2 (2%)	51	40	26, 69, 141, 177	0
49	R3	59/60 (98%)	1.56	18 (30%)	0	0	19, 95, 150, 200	0
49	Y3	59/60 (98%)	0.79	11 (18%)	1	1	9, 70, 131, 166	0
50	R4	71/71 (100%)	1.04	19 (26%)	0	0	89, 171, 218, 267	0
50	Y4	71/71 (100%)	0.28	2 (2%)	53	41	69, 145, 208, 248	0
51	R5	59/60 (98%)	0.39	4 (6%)	17	12	13, 74, 179, 222	0
51	Y5	59/60 (98%)	0.45	7 (11%)	4	4	17, 78, 189, 225	0
52	R6	49/54 (90%)	3.36	33 (67%)	0	0	101, 150, 215, 233	0
52	Y6	49/54 (90%)	2.89	37 (75%)	0	0	73, 147, 211, 217	0
53	R7	49/49 (100%)	0.22	1 (2%)	65	55	17, 47, 108, 188	0
53	Y7	49/49 (100%)	0.33	4 (8%)	11	9	6, 40, 118, 133	0
54	R8	64/65 (98%)	0.51	4 (6%)	20	14	24, 80, 155, 197	0
54	Y8	64/65 (98%)	0.28	3 (4%)	31	25	6, 54, 120, 197	0
55	R9	37/37 (100%)	4.05	30 (81%)	0	0	94, 143, 197, 202	0
55	Y9	37/37 (100%)	4.82	36 (97%)	0	0	62, 123, 202, 228	0
56	Z6	2/3 (66%)	0.55	0	100	100	30, 30, 30, 75	0
56	Z8	2/3 (66%)	0.03	0	100	100	30, 30, 30, 47	0
All	All	20871/21494 (97%)	0.23	1135 (5%)	25	21	3, 80, 177, 329	0

The worst 5 of 1135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	13.9
28	YE	205	ALA	12.2

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Mol	Chain	Res	Type	RSRZ
25	RA	2799	A	11.1
55	R9	11	CYS	9.8
55	Y9	34	GLN	9.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	1MG	QY	37	24/25	0.90	0.24	99,99,99,99	0
56	PPU	Z8	76	37/38	0.92	0.29	38,38,38,38	0
56	PPU	Z6	76	37/38	0.93	0.27	41,41,41,41	0
24	1MG	XY	37	24/25	0.93	0.16	59,59,59,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	R0	101	1/1	0.03	0.76	29,29,29,29	0
57	MG	RA	3194	1/1	0.21	0.28	54,54,54,54	0
57	MG	RA	3216	1/1	0.43	0.81	39,39,39,39	0
57	MG	RP	202	1/1	0.44	0.52	65,65,65,65	0
57	MG	YA	3072	1/1	0.46	0.17	7,7,7,7	0
57	MG	RA	3232	1/1	0.48	1.04	80,80,80,80	0
57	MG	YA	3185	1/1	0.49	0.37	14,14,14,14	0
57	MG	YA	3128	1/1	0.53	0.68	25,25,25,25	0
57	MG	YA	3241	1/1	0.54	0.29	34,34,34,34	0
57	MG	YD	302	1/1	0.55	0.56	49,49,49,49	0
57	MG	QA	1623	1/1	0.56	0.86	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3229	1/1	0.56	0.61	30,30,30,30	0
57	MG	YA	3234	1/1	0.58	0.32	1,1,1,1	0
57	MG	XA	1605	1/1	0.59	0.66	18,18,18,18	0
57	MG	YA	3174	1/1	0.61	0.41	47,47,47,47	0
57	MG	RA	3220	1/1	0.61	0.52	1,1,1,1	0
57	MG	RA	3242	1/1	0.62	0.36	7,7,7,7	0
57	MG	QA	1658	1/1	0.63	0.25	90,90,90,90	0
57	MG	XA	1648	1/1	0.63	0.42	28,28,28,28	0
57	MG	YA	3124	1/1	0.64	0.64	19,19,19,19	0
57	MG	RA	3134	1/1	0.65	0.46	24,24,24,24	0
57	MG	RA	3222	1/1	0.65	0.37	45,45,45,45	0
57	MG	YA	3012	1/1	0.65	1.31	80,80,80,80	0
57	MG	YB	202	1/1	0.66	0.54	21,21,21,21	0
57	MG	YA	3054	1/1	0.66	0.82	80,80,80,80	0
57	MG	RA	3189	1/1	0.67	0.43	55,55,55,55	0
57	MG	YA	3258	1/1	0.68	1.75	80,80,80,80	0
57	MG	YA	3236	1/1	0.68	0.16	24,24,24,24	0
57	MG	YA	3207	1/1	0.68	0.30	20,20,20,20	0
57	MG	XA	1655	1/1	0.69	0.70	40,40,40,40	0
57	MG	RA	3124	1/1	0.69	0.58	35,35,35,35	0
57	MG	RA	3221	1/1	0.70	0.77	15,15,15,15	0
57	MG	YA	3201	1/1	0.70	0.39	2,2,2,2	0
57	MG	YA	3167	1/1	0.71	0.33	49,49,49,49	0
57	MG	QA	1618	1/1	0.71	0.42	49,49,49,49	0
57	MG	RA	3154	1/1	0.71	0.15	17,17,17,17	0
57	MG	YA	3161	1/1	0.71	0.35	6,6,6,6	0
57	MG	RA	3101	1/1	0.72	0.21	32,32,32,32	0
57	MG	XA	1664	1/1	0.72	0.25	8,8,8,8	0
57	MG	YA	3246	1/1	0.72	0.21	7,7,7,7	0
57	MG	XA	1606	1/1	0.72	0.53	29,29,29,29	0
57	MG	QA	1626	1/1	0.72	0.21	10,10,10,10	0
57	MG	XA	1654	1/1	0.72	0.43	23,23,23,23	0
57	MG	QA	1665	1/1	0.73	0.36	27,27,27,27	0
57	MG	YA	3163	1/1	0.73	0.24	41,41,41,41	0
57	MG	YA	3248	1/1	0.73	0.56	17,17,17,17	0
57	MG	RA	3217	1/1	0.73	0.22	18,18,18,18	0
57	MG	RA	3192	1/1	0.73	0.18	0,0,0,0	0
57	MG	RA	3026	1/1	0.73	1.19	80,80,80,80	0
57	MG	RA	3065	1/1	0.74	0.55	80,80,80,80	0
57	MG	XA	1614	1/1	0.74	0.23	2,2,2,2	0
57	MG	QA	1632	1/1	0.74	0.28	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3218	1/1	0.75	0.14	4,4,4,4	0
57	MG	RA	3225	1/1	0.75	0.33	18,18,18,18	0
57	MG	YA	3076	1/1	0.75	0.38	2,2,2,2	0
57	MG	RA	3230	1/1	0.75	0.35	2,2,2,2	0
57	MG	RA	3009	1/1	0.75	0.49	84,84,84,84	0
57	MG	QA	1630	1/1	0.75	0.45	54,54,54,54	0
57	MG	YA	3043	1/1	0.75	0.46	6,6,6,6	0
57	MG	XA	1670	1/1	0.76	0.33	17,17,17,17	0
57	MG	YA	3075	1/1	0.76	0.22	3,3,3,3	0
57	MG	YA	3208	1/1	0.76	0.17	43,43,43,43	0
57	MG	XA	1626	1/1	0.76	0.33	11,11,11,11	0
57	MG	XA	1643	1/1	0.76	0.49	34,34,34,34	0
57	MG	RA	3180	1/1	0.76	0.52	21,21,21,21	0
57	MG	XA	1635	1/1	0.77	0.29	42,42,42,42	0
57	MG	YA	3122	1/1	0.77	0.36	8,8,8,8	0
57	MG	RA	3186	1/1	0.77	0.23	71,71,71,71	0
57	MG	QA	1627	1/1	0.77	0.26	22,22,22,22	0
57	MG	RA	3163	1/1	0.77	0.91	13,13,13,13	0
57	MG	RA	3138	1/1	0.77	0.40	51,51,51,51	0
57	MG	XA	1628	1/1	0.77	0.10	28,28,28,28	0
57	MG	RA	3234	1/1	0.78	0.51	7,7,7,7	0
57	MG	RA	3006	1/1	0.78	1.47	80,80,80,80	0
57	MG	YA	3238	1/1	0.78	0.19	11,11,11,11	0
57	MG	YA	3160	1/1	0.78	0.74	51,51,51,51	0
57	MG	YA	3205	1/1	0.78	0.37	38,38,38,38	0
57	MG	RF	301	1/1	0.78	0.20	49,49,49,49	0
57	MG	YA	3085	1/1	0.78	0.36	37,37,37,37	0
57	MG	YA	3223	1/1	0.78	0.41	27,27,27,27	0
57	MG	QA	1641	1/1	0.78	0.21	6,6,6,6	0
59	ZN	QN	101	1/1	0.78	0.12	102,102,102,102	0
57	MG	YA	3045	1/1	0.79	0.36	20,20,20,20	0
57	MG	YA	3089	1/1	0.79	0.54	4,4,4,4	0
57	MG	RA	3208	1/1	0.79	0.39	29,29,29,29	0
57	MG	RA	3097	1/1	0.79	1.10	80,80,80,80	0
57	MG	YA	3264	1/1	0.79	0.38	35,35,35,35	0
57	MG	XA	1633	1/1	0.79	0.48	33,33,33,33	0
57	MG	YA	3145	1/1	0.79	0.28	16,16,16,16	0
57	MG	QA	1661	1/1	0.79	0.62	9,9,9,9	0
57	MG	RA	3184	1/1	0.80	0.37	13,13,13,13	0
57	MG	YA	3155	1/1	0.80	0.58	38,38,38,38	0
57	MG	YA	3064	1/1	0.80	0.26	4,4,4,4	0
57	MG	XA	1656	1/1	0.80	0.21	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1662	1/1	0.80	0.36	51,51,51,51	0
57	MG	RA	3182	1/1	0.80	0.45	23,23,23,23	0
57	MG	YA	3243	1/1	0.80	0.29	0,0,0,0	0
57	MG	RA	3085	1/1	0.81	0.27	4,4,4,4	0
57	MG	QA	1603	1/1	0.81	1.09	27,27,27,27	0
57	MG	XA	1660	1/1	0.81	0.57	21,21,21,21	0
57	MG	RA	3002	1/1	0.81	0.52	4,4,4,4	0
57	MG	RA	3067	1/1	0.81	0.24	57,57,57,57	0
57	MG	RA	3190	1/1	0.82	0.38	8,8,8,8	0
57	MG	YA	3156	1/1	0.82	0.22	6,6,6,6	0
57	MG	XA	1659	1/1	0.82	0.17	54,54,54,54	0
57	MG	RD	301	1/1	0.82	0.68	11,11,11,11	0
57	MG	RA	3177	1/1	0.82	0.22	3,3,3,3	0
57	MG	XA	1634	1/1	0.82	0.73	23,23,23,23	0
57	MG	RA	3129	1/1	0.82	0.25	21,21,21,21	0
57	MG	YA	3115	1/1	0.82	0.25	31,31,31,31	0
57	MG	YA	3187	1/1	0.82	0.13	55,55,55,55	0
57	MG	YA	3190	1/1	0.82	0.13	22,22,22,22	0
57	MG	YA	3261	1/1	0.82	0.99	8,8,8,8	0
57	MG	QA	1601	1/1	0.82	0.32	12,12,12,12	0
57	MG	YB	201	1/1	0.82	0.43	48,48,48,48	0
57	MG	RA	3048	1/1	0.82	0.24	20,20,20,20	0
57	MG	QA	1631	1/1	0.82	0.35	15,15,15,15	0
57	MG	QA	1647	1/1	0.82	0.56	29,29,29,29	0
57	MG	YA	3182	1/1	0.83	0.66	30,30,30,30	0
57	MG	RA	3229	1/1	0.83	0.35	9,9,9,9	0
57	MG	YA	3058	1/1	0.83	0.66	4,4,4,4	0
57	MG	QA	1634	1/1	0.83	0.45	6,6,6,6	0
57	MG	RA	3153	1/1	0.83	0.19	24,24,24,24	0
57	MG	RA	3179	1/1	0.83	0.33	12,12,12,12	0
57	MG	QA	1657	1/1	0.83	0.13	65,65,65,65	0
57	MG	RA	3181	1/1	0.83	0.59	28,28,28,28	0
57	MG	YA	3026	1/1	0.83	0.49	32,32,32,32	0
57	MG	YA	3164	1/1	0.83	0.26	8,8,8,8	0
57	MG	XA	1627	1/1	0.83	0.27	9,9,9,9	0
57	MG	RA	3226	1/1	0.83	0.24	26,26,26,26	0
57	MG	RB	201	1/1	0.84	0.19	30,30,30,30	0
57	MG	RA	3113	1/1	0.84	0.40	3,3,3,3	0
57	MG	RA	3199	1/1	0.84	0.45	60,60,60,60	0
57	MG	XB	301	1/1	0.84	0.21	26,26,26,26	0
57	MG	RA	3204	1/1	0.84	0.19	33,33,33,33	0
57	MG	RA	3205	1/1	0.84	0.28	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1646	1/1	0.84	0.24	6,6,6,6	0
57	MG	YA	3199	1/1	0.84	0.51	60,60,60,60	0
57	MG	R5	101	1/1	0.84	0.22	33,33,33,33	0
57	MG	QA	1625	1/1	0.84	0.14	25,25,25,25	0
57	MG	YA	3267	1/1	0.84	0.47	19,19,19,19	0
57	MG	QA	1612	1/1	0.84	0.24	5,5,5,5	0
57	MG	QA	1645	1/1	0.84	0.11	5,5,5,5	0
57	MG	RA	3191	1/1	0.84	0.16	26,26,26,26	0
57	MG	RA	3168	1/1	0.84	0.80	55,55,55,55	0
57	MG	YA	3052	1/1	0.85	0.33	3,3,3,3	0
57	MG	RA	3169	1/1	0.85	0.27	3,3,3,3	0
57	MG	XA	1661	1/1	0.85	0.52	32,32,32,32	0
57	MG	R8	101	1/1	0.85	0.29	19,19,19,19	0
57	MG	RA	3170	1/1	0.85	0.47	23,23,23,23	0
57	MG	XA	1665	1/1	0.85	0.51	38,38,38,38	0
57	MG	RA	3203	1/1	0.85	0.40	30,30,30,30	0
57	MG	RA	3125	1/1	0.85	0.25	37,37,37,37	0
57	MG	RA	3178	1/1	0.85	0.86	4,4,4,4	0
57	MG	YA	3175	1/1	0.85	0.28	43,43,43,43	0
57	MG	YA	3106	1/1	0.85	0.22	84,84,84,84	0
57	MG	YA	3183	1/1	0.85	0.32	10,10,10,10	0
57	MG	YA	3107	1/1	0.85	0.32	22,22,22,22	0
57	MG	YA	3015	1/1	0.85	0.11	4,4,4,4	0
57	MG	YA	3119	1/1	0.85	0.21	2,2,2,2	0
57	MG	QA	1628	1/1	0.85	0.53	62,62,62,62	0
57	MG	RA	3062	1/1	0.85	0.74	1,1,1,1	0
57	MG	YA	3203	1/1	0.85	0.33	21,21,21,21	0
57	MG	QA	1611	1/1	0.85	0.23	2,2,2,2	0
57	MG	XA	1639	1/1	0.86	0.25	13,13,13,13	0
57	MG	XA	1607	1/1	0.86	0.39	15,15,15,15	0
57	MG	XA	1609	1/1	0.86	0.35	12,12,12,12	0
57	MG	RA	3008	1/1	0.86	0.43	3,3,3,3	0
57	MG	QA	1624	1/1	0.86	0.46	49,49,49,49	0
57	MG	XX	101	1/1	0.86	0.23	11,11,11,11	0
57	MG	YA	3251	1/1	0.86	0.52	6,6,6,6	0
57	MG	QA	1656	1/1	0.86	0.35	25,25,25,25	0
57	MG	RA	3237	1/1	0.86	0.28	5,5,5,5	0
57	MG	RA	3031	1/1	0.86	0.33	13,13,13,13	0
57	MG	YA	3097	1/1	0.86	0.34	11,11,11,11	0
57	MG	YA	3030	1/1	0.86	0.37	6,6,6,6	0
57	MG	RA	3227	1/1	0.86	0.26	16,16,16,16	0
57	MG	YA	3109	1/1	0.86	1.52	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3007	1/1	0.86	0.64	26,26,26,26	0
57	MG	YA	3237	1/1	0.87	0.27	38,38,38,38	0
57	MG	RA	3149	1/1	0.87	0.15	15,15,15,15	0
57	MG	YA	3240	1/1	0.87	0.38	23,23,23,23	0
57	MG	RA	3058	1/1	0.87	0.37	9,9,9,9	0
57	MG	YA	3147	1/1	0.87	0.60	27,27,27,27	0
57	MG	YA	3150	1/1	0.87	0.22	11,11,11,11	0
57	MG	YA	3041	1/1	0.87	0.38	10,10,10,10	0
57	MG	XA	1640	1/1	0.87	0.32	25,25,25,25	0
57	MG	QA	1664	1/1	0.87	0.15	24,24,24,24	0
57	MG	RA	3117	1/1	0.87	0.26	58,58,58,58	0
57	MG	QA	1602	1/1	0.87	0.51	9,9,9,9	0
57	MG	RA	3209	1/1	0.87	0.25	35,35,35,35	0
57	MG	RA	3235	1/1	0.87	0.17	11,11,11,11	0
57	MG	RA	3212	1/1	0.87	0.52	10,10,10,10	0
57	MG	RA	3240	1/1	0.87	0.32	2,2,2,2	0
57	MG	YA	3125	1/1	0.87	0.21	10,10,10,10	0
57	MG	QA	1622	1/1	0.88	0.41	44,44,44,44	0
57	MG	RA	3236	1/1	0.88	0.59	4,4,4,4	0
57	MG	YA	3081	1/1	0.88	0.57	0,0,0,0	0
57	MG	YA	3138	1/1	0.88	0.18	1,1,1,1	0
57	MG	YA	3082	1/1	0.88	0.51	0,0,0,0	0
57	MG	RA	3201	1/1	0.88	0.41	1,1,1,1	0
57	MG	YA	3149	1/1	0.88	0.22	17,17,17,17	0
57	MG	RA	3156	1/1	0.88	0.40	19,19,19,19	0
57	MG	RA	3228	1/1	0.88	0.23	43,43,43,43	0
57	MG	YA	3202	1/1	0.88	0.30	4,4,4,4	0
57	MG	YA	3256	1/1	0.88	0.55	8,8,8,8	0
57	MG	RA	3160	1/1	0.88	0.15	10,10,10,10	0
57	MG	RA	3120	1/1	0.88	0.56	4,4,4,4	0
57	MG	QA	1648	1/1	0.88	0.34	30,30,30,30	0
57	MG	XA	1653	1/1	0.88	0.39	13,13,13,13	0
57	MG	YA	3217	1/1	0.88	0.22	14,14,14,14	0
57	MG	YA	3222	1/1	0.88	0.29	3,3,3,3	0
57	MG	RA	3233	1/1	0.88	0.17	17,17,17,17	0
57	MG	YE	301	1/1	0.88	0.30	55,55,55,55	0
57	MG	RA	3195	1/1	0.88	0.27	8,8,8,8	0
57	MG	YA	3099	1/1	0.89	0.28	2,2,2,2	0
57	MG	YA	3218	1/1	0.89	0.19	2,2,2,2	0
57	MG	YA	3104	1/1	0.89	0.10	3,3,3,3	0
57	MG	RA	3109	1/1	0.89	0.43	26,26,26,26	0
57	MG	RA	3110	1/1	0.89	0.64	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3230	1/1	0.89	0.20	10,10,10,10	0
57	MG	RA	3017	1/1	0.89	0.25	11,11,11,11	0
57	MG	YA	3171	1/1	0.89	0.23	24,24,24,24	0
57	MG	YA	3172	1/1	0.89	0.20	41,41,41,41	0
57	MG	XA	1637	1/1	0.89	0.10	28,28,28,28	0
57	MG	RA	3172	1/1	0.89	0.15	4,4,4,4	0
57	MG	RA	3239	1/1	0.89	0.19	3,3,3,3	0
57	MG	YA	3067	1/1	0.89	0.60	5,5,5,5	0
57	MG	QA	1638	1/1	0.89	0.62	27,27,27,27	0
57	MG	YA	3186	1/1	0.89	0.27	4,4,4,4	0
57	MG	QA	1662	1/1	0.89	0.14	30,30,30,30	0
57	MG	YA	3253	1/1	0.89	0.50	5,5,5,5	0
57	MG	YA	3134	1/1	0.89	0.21	11,11,11,11	0
57	MG	YA	3191	1/1	0.89	0.13	23,23,23,23	0
57	MG	YA	3193	1/1	0.89	0.25	2,2,2,2	0
57	MG	XA	1647	1/1	0.89	0.12	44,44,44,44	0
57	MG	RA	3032	1/1	0.89	1.58	80,80,80,80	0
57	MG	XA	1617	1/1	0.89	0.28	2,2,2,2	0
57	MG	QA	1617	1/1	0.89	0.46	8,8,8,8	0
57	MG	YA	3088	1/1	0.89	1.32	80,80,80,80	0
57	MG	RA	3010	1/1	0.89	0.51	4,4,4,4	0
57	MG	RA	3166	1/1	0.89	0.23	20,20,20,20	0
57	MG	QA	1639	1/1	0.90	0.16	18,18,18,18	0
57	MG	QA	1614	1/1	0.90	0.22	26,26,26,26	0
57	MG	XA	1603	1/1	0.90	0.49	5,5,5,5	0
57	MG	QA	1649	1/1	0.90	0.14	2,2,2,2	0
57	MG	RA	3070	1/1	0.90	0.33	6,6,6,6	0
57	MG	YA	3035	1/1	0.90	0.85	80,80,80,80	0
57	MG	RA	3188	1/1	0.90	0.16	11,11,11,11	0
57	MG	RA	3213	1/1	0.90	0.21	42,42,42,42	0
57	MG	YA	3252	1/1	0.90	0.47	16,16,16,16	0
57	MG	RA	3079	1/1	0.90	0.26	11,11,11,11	0
57	MG	QA	1644	1/1	0.90	0.07	34,34,34,34	0
57	MG	QA	1619	1/1	0.90	0.21	40,40,40,40	0
57	MG	RA	3130	1/1	0.90	0.38	30,30,30,30	0
57	MG	RA	3193	1/1	0.90	0.18	17,17,17,17	0
57	MG	RA	3132	1/1	0.90	0.16	4,4,4,4	0
57	MG	RA	3099	1/1	0.90	0.24	6,6,6,6	0
57	MG	QF	201	1/1	0.90	0.39	1,1,1,1	0
57	MG	YD	301	1/1	0.90	0.76	80,80,80,80	0
57	MG	YA	3131	1/1	0.90	0.17	7,7,7,7	0
57	MG	RA	3108	1/1	0.90	0.31	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3061	1/1	0.90	0.16	32,32,32,32	0
57	MG	YA	3116	1/1	0.91	0.52	80,80,80,80	0
57	MG	YA	3197	1/1	0.91	0.36	1,1,1,1	0
57	MG	RA	3013	1/1	0.91	0.49	5,5,5,5	0
57	MG	YA	3031	1/1	0.91	1.20	80,80,80,80	0
57	MG	YA	3034	1/1	0.91	0.36	4,4,4,4	0
57	MG	RA	3219	1/1	0.91	0.11	4,4,4,4	0
57	MG	XA	1641	1/1	0.91	0.27	2,2,2,2	0
57	MG	RA	3162	1/1	0.91	0.19	22,22,22,22	0
57	MG	RA	3016	1/1	0.91	0.11	1,1,1,1	0
57	MG	YA	3209	1/1	0.91	0.43	69,69,69,69	0
57	MG	RA	3003	1/1	0.91	0.37	4,4,4,4	0
57	MG	YA	3143	1/1	0.91	0.26	10,10,10,10	0
57	MG	RA	3018	1/1	0.91	0.72	8,8,8,8	0
57	MG	YA	3146	1/1	0.91	0.32	4,4,4,4	0
57	MG	YA	3225	1/1	0.91	0.39	34,34,34,34	0
57	MG	QA	1640	1/1	0.91	0.16	46,46,46,46	0
57	MG	RA	3074	1/1	0.91	0.16	10,10,10,10	0
57	MG	YA	3233	1/1	0.91	0.39	68,68,68,68	0
57	MG	RA	3197	1/1	0.91	0.06	12,12,12,12	0
57	MG	YA	3235	1/1	0.91	0.31	8,8,8,8	0
57	MG	YA	3153	1/1	0.91	0.52	21,21,21,21	0
57	MG	RA	3078	1/1	0.91	0.12	5,5,5,5	0
57	MG	RA	3174	1/1	0.91	0.46	17,17,17,17	0
57	MG	YA	3157	1/1	0.91	0.46	18,18,18,18	0
57	MG	RA	3231	1/1	0.91	0.48	7,7,7,7	0
57	MG	YA	3079	1/1	0.91	0.27	22,22,22,22	0
57	MG	YA	3245	1/1	0.91	0.34	3,3,3,3	0
57	MG	QA	1637	1/1	0.91	0.20	46,46,46,46	0
57	MG	QA	1633	1/1	0.91	0.28	35,35,35,35	0
57	MG	YA	3083	1/1	0.91	0.14	7,7,7,7	0
57	MG	RA	3133	1/1	0.91	0.19	33,33,33,33	0
57	MG	RA	3034	1/1	0.91	0.44	2,2,2,2	0
57	MG	RA	3036	1/1	0.91	0.47	2,2,2,2	0
57	MG	YA	3095	1/1	0.91	0.47	1,1,1,1	0
57	MG	YA	3259	1/1	0.91	0.32	0,0,0,0	0
57	MG	YA	3176	1/1	0.91	0.18	28,28,28,28	0
57	MG	RA	3001	1/1	0.91	0.73	8,8,8,8	0
57	MG	RA	3104	1/1	0.91	0.19	5,5,5,5	0
57	MG	RA	3049	1/1	0.91	0.40	4,4,4,4	0
57	MG	QA	1615	1/1	0.91	0.19	74,74,74,74	0
57	MG	YA	3018	1/1	0.91	0.75	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3025	1/1	0.91	1.66	80,80,80,80	0
57	MG	XA	1638	1/1	0.91	0.18	37,37,37,37	0
57	MG	Y0	101	1/1	0.91	0.27	3,3,3,3	0
58	PAR	XA	1671	42/42	0.91	0.26	40,40,40,40	0
57	MG	YA	3192	1/1	0.91	0.10	6,6,6,6	0
57	MG	YA	3118	1/1	0.92	0.37	63,63,63,63	0
57	MG	RA	3175	1/1	0.92	0.28	20,20,20,20	0
57	MG	QV	101	1/1	0.92	0.69	80,80,80,80	0
57	MG	YA	3123	1/1	0.92	0.24	24,24,24,24	0
57	MG	RA	3196	1/1	0.92	0.29	8,8,8,8	0
57	MG	YA	3032	1/1	0.92	0.50	8,8,8,8	0
57	MG	RA	3155	1/1	0.92	0.27	24,24,24,24	0
57	MG	YA	3210	1/1	0.92	0.26	39,39,39,39	0
57	MG	RE	301	1/1	0.92	0.21	18,18,18,18	0
57	MG	YA	3133	1/1	0.92	0.12	8,8,8,8	0
57	MG	RA	3223	1/1	0.92	0.17	11,11,11,11	0
57	MG	RP	201	1/1	0.92	0.50	10,10,10,10	0
57	MG	YA	3224	1/1	0.92	0.39	5,5,5,5	0
57	MG	RA	3224	1/1	0.92	0.23	19,19,19,19	0
57	MG	QA	1663	1/1	0.92	0.07	33,33,33,33	0
57	MG	RA	3158	1/1	0.92	0.13	12,12,12,12	0
57	MG	YA	3055	1/1	0.92	0.39	4,4,4,4	0
57	MG	XA	1651	1/1	0.92	0.30	22,22,22,22	0
57	MG	YA	3063	1/1	0.92	0.27	11,11,11,11	0
57	MG	RA	3202	1/1	0.92	0.21	9,9,9,9	0
57	MG	YA	3154	1/1	0.92	0.14	8,8,8,8	0
57	MG	XA	1601	1/1	0.92	1.43	80,80,80,80	0
57	MG	YA	3239	1/1	0.92	0.21	19,19,19,19	0
57	MG	RA	3095	1/1	0.92	0.47	2,2,2,2	0
57	MG	XA	1604	1/1	0.92	0.86	13,13,13,13	0
57	MG	QA	1660	1/1	0.92	0.24	26,26,26,26	0
57	MG	RA	3098	1/1	0.92	0.94	80,80,80,80	0
57	MG	YA	3080	1/1	0.92	0.26	9,9,9,9	0
57	MG	QA	1651	1/1	0.92	0.28	6,6,6,6	0
57	MG	YA	3249	1/1	0.92	0.37	3,3,3,3	0
57	MG	RA	3141	1/1	0.92	0.14	3,3,3,3	0
57	MG	RA	3210	1/1	0.92	0.20	27,27,27,27	0
57	MG	RA	3145	1/1	0.92	0.23	5,5,5,5	0
57	MG	YA	3086	1/1	0.92	0.29	6,6,6,6	0
57	MG	XA	1668	1/1	0.92	0.14	31,31,31,31	0
57	MG	XA	1669	1/1	0.92	0.34	13,13,13,13	0
57	MG	YA	3091	1/1	0.92	0.33	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3146	1/1	0.92	0.15	3,3,3,3	0
57	MG	RA	3171	1/1	0.92	0.21	15,15,15,15	0
57	MG	QA	1620	1/1	0.92	0.16	22,22,22,22	0
57	MG	YA	3002	1/1	0.92	0.97	80,80,80,80	0
57	MG	YB	203	1/1	0.92	0.14	33,33,33,33	0
57	MG	XA	1629	1/1	0.92	0.19	3,3,3,3	0
57	MG	XA	1630	1/1	0.92	0.15	4,4,4,4	0
57	MG	RA	3238	1/1	0.92	0.48	7,7,7,7	0
57	MG	YP	201	1/1	0.92	0.14	8,8,8,8	0
57	MG	YA	3114	1/1	0.92	0.16	29,29,29,29	0
58	PAR	QA	1666	42/42	0.92	0.23	58,58,58,58	0
57	MG	YA	3019	1/1	0.92	0.69	10,10,10,10	0
57	MG	RA	3014	1/1	0.92	0.15	2,2,2,2	0
57	MG	RA	3140	1/1	0.93	0.28	17,17,17,17	0
57	MG	RA	3122	1/1	0.93	0.09	5,5,5,5	0
57	MG	RA	3165	1/1	0.93	0.16	25,25,25,25	0
57	MG	XA	1658	1/1	0.93	0.21	0,0,0,0	0
57	MG	YA	3132	1/1	0.93	0.09	31,31,31,31	0
57	MG	RA	3144	1/1	0.93	0.30	2,2,2,2	0
57	MG	QA	1654	1/1	0.93	0.10	55,55,55,55	0
57	MG	YA	3135	1/1	0.93	0.22	1,1,1,1	0
57	MG	RA	3039	1/1	0.93	0.21	2,2,2,2	0
57	MG	YA	3141	1/1	0.93	0.57	7,7,7,7	0
57	MG	YA	3142	1/1	0.93	0.18	28,28,28,28	0
57	MG	RA	3044	1/1	0.93	0.37	2,2,2,2	0
57	MG	YA	3144	1/1	0.93	0.14	25,25,25,25	0
57	MG	RA	3150	1/1	0.93	0.17	25,25,25,25	0
57	MG	YA	3250	1/1	0.93	0.51	6,6,6,6	0
57	MG	YA	3200	1/1	0.93	0.42	10,10,10,10	0
57	MG	YA	3092	1/1	0.93	0.28	13,13,13,13	0
57	MG	RA	3152	1/1	0.93	0.17	3,3,3,3	0
57	MG	YA	3254	1/1	0.93	0.53	1,1,1,1	0
57	MG	YA	3048	1/1	0.93	0.24	21,21,21,21	0
57	MG	RA	3173	1/1	0.93	0.33	54,54,54,54	0
57	MG	RA	3087	1/1	0.93	0.22	1,1,1,1	0
57	MG	RA	3131	1/1	0.93	0.21	0,0,0,0	0
57	MG	YA	3056	1/1	0.93	0.23	0,0,0,0	0
57	MG	RA	3019	1/1	0.93	0.35	14,14,14,14	0
57	MG	YA	3112	1/1	0.93	0.22	11,11,11,11	0
57	MG	QA	1605	1/1	0.93	0.48	5,5,5,5	0
57	MG	YA	3219	1/1	0.93	0.14	17,17,17,17	0
57	MG	RA	3050	1/1	0.93	0.29	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3159	1/1	0.93	0.18	0,0,0,0	0
57	MG	XA	1616	1/1	0.93	0.23	10,10,10,10	0
57	MG	YA	3017	1/1	0.93	0.45	8,8,8,8	0
57	MG	YA	3226	1/1	0.93	0.48	4,4,4,4	0
57	MG	YA	3228	1/1	0.93	0.26	9,9,9,9	0
57	MG	RA	3057	1/1	0.93	0.28	8,8,8,8	0
57	MG	XA	1623	1/1	0.93	0.33	4,4,4,4	0
57	MG	RA	3084	1/1	0.94	0.19	1,1,1,1	0
57	MG	XA	1619	1/1	0.94	0.29	13,13,13,13	0
57	MG	YA	3098	1/1	0.94	0.17	2,2,2,2	0
57	MG	XA	1620	1/1	0.94	0.31	5,5,5,5	0
57	MG	YA	3102	1/1	0.94	0.49	3,3,3,3	0
57	MG	RA	3200	1/1	0.94	0.38	4,4,4,4	0
57	MG	RA	3116	1/1	0.94	0.08	2,2,2,2	0
57	MG	RA	3161	1/1	0.94	0.57	75,75,75,75	0
57	MG	RA	3022	1/1	0.94	0.28	1,1,1,1	0
57	MG	YA	3165	1/1	0.94	0.31	7,7,7,7	0
57	MG	RA	3143	1/1	0.94	0.29	14,14,14,14	0
57	MG	YA	3169	1/1	0.94	0.11	3,3,3,3	0
57	MG	RA	3118	1/1	0.94	0.33	13,13,13,13	0
57	MG	XA	1663	1/1	0.94	0.11	29,29,29,29	0
57	MG	YA	3173	1/1	0.94	0.45	0,0,0,0	0
57	MG	XA	1631	1/1	0.94	0.33	0,0,0,0	0
57	MG	YA	3117	1/1	0.94	0.30	11,11,11,11	0
57	MG	RA	3206	1/1	0.94	0.26	40,40,40,40	0
57	MG	XA	1666	1/1	0.94	0.15	16,16,16,16	0
57	MG	YA	3121	1/1	0.94	0.38	9,9,9,9	0
57	MG	YA	3060	1/1	0.94	0.29	3,3,3,3	0
57	MG	QA	1610	1/1	0.94	0.21	3,3,3,3	0
57	MG	RA	3045	1/1	0.94	0.18	23,23,23,23	0
57	MG	RA	3046	1/1	0.94	0.41	1,1,1,1	0
57	MG	QA	1643	1/1	0.94	0.10	1,1,1,1	0
57	MG	YA	3129	1/1	0.94	0.27	0,0,0,0	0
57	MG	RA	3068	1/1	0.94	0.23	68,68,68,68	0
57	MG	YA	3196	1/1	0.94	0.68	6,6,6,6	0
57	MG	RA	3069	1/1	0.94	0.56	2,2,2,2	0
57	MG	YA	3260	1/1	0.94	0.30	2,2,2,2	0
57	MG	YA	3077	1/1	0.94	0.44	3,3,3,3	0
57	MG	YA	3263	1/1	0.94	0.24	7,7,7,7	0
57	MG	YA	3078	1/1	0.94	0.43	0,0,0,0	0
57	MG	YA	3265	1/1	0.94	0.46	1,1,1,1	0
57	MG	YA	3008	1/1	0.94	0.14	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3009	1/1	0.94	0.43	0,0,0,0	0
57	MG	RA	3004	1/1	0.94	0.51	13,13,13,13	0
57	MG	YA	3014	1/1	0.94	0.42	2,2,2,2	0
57	MG	RA	3005	1/1	0.94	0.34	6,6,6,6	0
57	MG	XA	1645	1/1	0.94	0.32	2,2,2,2	0
57	MG	RA	3051	1/1	0.94	0.45	3,3,3,3	0
57	MG	RA	3176	1/1	0.94	0.36	14,14,14,14	0
57	MG	XA	1615	1/1	0.94	0.41	2,2,2,2	0
57	MG	YA	3148	1/1	0.94	0.15	42,42,42,42	0
57	MG	XA	1649	1/1	0.94	0.13	33,33,33,33	0
57	MG	QA	1659	1/1	0.94	0.24	11,11,11,11	0
59	ZN	XD	301	1/1	0.94	0.22	5,5,5,5	0
57	MG	QA	1629	1/1	0.95	0.18	29,29,29,29	0
57	MG	RA	3081	1/1	0.95	0.32	3,3,3,3	0
57	MG	YA	3220	1/1	0.95	0.29	2,2,2,2	0
57	MG	YA	3005	1/1	0.95	0.24	68,68,68,68	0
57	MG	YA	3006	1/1	0.95	0.30	2,2,2,2	0
57	MG	YA	3111	1/1	0.95	0.22	19,19,19,19	0
57	MG	YA	3158	1/1	0.95	0.25	23,23,23,23	0
57	MG	RA	3135	1/1	0.95	0.17	7,7,7,7	0
57	MG	YA	3062	1/1	0.95	0.19	5,5,5,5	0
57	MG	XA	1652	1/1	0.95	0.13	1,1,1,1	0
57	MG	YA	3010	1/1	0.95	0.36	0,0,0,0	0
57	MG	YA	3231	1/1	0.95	0.15	2,2,2,2	0
57	MG	RA	3136	1/1	0.95	0.22	7,7,7,7	0
57	MG	YA	3069	1/1	0.95	0.37	10,10,10,10	0
57	MG	YA	3071	1/1	0.95	0.13	40,40,40,40	0
57	MG	YA	3170	1/1	0.95	0.25	26,26,26,26	0
57	MG	RA	3137	1/1	0.95	0.34	2,2,2,2	0
57	MG	RA	3083	1/1	0.95	0.27	12,12,12,12	0
57	MG	QA	1604	1/1	0.95	0.16	17,17,17,17	0
57	MG	RA	3207	1/1	0.95	0.19	96,96,96,96	0
57	MG	QA	1650	1/1	0.95	0.11	13,13,13,13	0
57	MG	YA	3127	1/1	0.95	0.20	11,11,11,11	0
57	MG	YA	3244	1/1	0.95	0.11	0,0,0,0	0
57	MG	YA	3024	1/1	0.95	0.29	17,17,17,17	0
57	MG	RA	3066	1/1	0.95	0.53	8,8,8,8	0
57	MG	YA	3247	1/1	0.95	0.54	32,32,32,32	0
57	MG	RA	3167	1/1	0.95	0.23	6,6,6,6	0
57	MG	QA	1607	1/1	0.95	0.16	5,5,5,5	0
57	MG	QA	1652	1/1	0.95	0.17	0,0,0,0	0
57	MG	YA	3188	1/1	0.95	0.13	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3189	1/1	0.95	0.36	0,0,0,0	0
57	MG	RA	3123	1/1	0.95	0.22	24,24,24,24	0
57	MG	RA	3038	1/1	0.95	0.30	9,9,9,9	0
57	MG	YA	3136	1/1	0.95	0.10	14,14,14,14	0
57	MG	YA	3137	1/1	0.95	0.14	2,2,2,2	0
57	MG	YA	3195	1/1	0.95	0.10	0,0,0,0	0
57	MG	RA	3056	1/1	0.95	0.35	21,21,21,21	0
57	MG	XA	1667	1/1	0.95	0.14	32,32,32,32	0
57	MG	YA	3198	1/1	0.95	0.15	16,16,16,16	0
57	MG	RA	3100	1/1	0.95	0.55	36,36,36,36	0
57	MG	YA	3044	1/1	0.95	0.16	75,75,75,75	0
57	MG	RA	3071	1/1	0.95	0.57	23,23,23,23	0
57	MG	YA	3046	1/1	0.95	0.45	0,0,0,0	0
57	MG	YA	3047	1/1	0.95	0.47	14,14,14,14	0
57	MG	YA	3204	1/1	0.95	0.15	23,23,23,23	0
57	MG	RA	3024	1/1	0.95	0.44	28,28,28,28	0
57	MG	YA	3206	1/1	0.95	0.25	25,25,25,25	0
57	MG	YA	3100	1/1	0.95	0.44	3,3,3,3	0
57	MG	RA	3025	1/1	0.95	0.17	66,66,66,66	0
57	MG	YA	3103	1/1	0.95	1.27	80,80,80,80	0
57	MG	YA	3151	1/1	0.95	0.08	26,26,26,26	0
57	MG	YA	3212	1/1	0.95	0.14	17,17,17,17	0
57	MG	YA	3216	1/1	0.95	0.16	38,38,38,38	0
57	MG	YA	3152	1/1	0.95	0.71	3,3,3,3	0
59	ZN	XN	101	1/1	0.95	0.20	82,82,82,82	0
57	MG	YA	3159	1/1	0.96	0.34	12,12,12,12	0
57	MG	RA	3075	1/1	0.96	0.22	3,3,3,3	0
57	MG	XA	1618	1/1	0.96	0.24	26,26,26,26	0
57	MG	YA	3162	1/1	0.96	0.22	49,49,49,49	0
57	MG	RA	3076	1/1	0.96	0.38	13,13,13,13	0
57	MG	RA	3105	1/1	0.96	0.18	6,6,6,6	0
57	MG	RA	3043	1/1	0.96	0.22	6,6,6,6	0
57	MG	RA	3139	1/1	0.96	0.25	12,12,12,12	0
57	MG	YA	3168	1/1	0.96	0.23	18,18,18,18	0
57	MG	RA	3027	1/1	0.96	0.25	4,4,4,4	0
57	MG	YA	3057	1/1	0.96	0.27	27,27,27,27	0
57	MG	RA	3028	1/1	0.96	0.20	2,2,2,2	0
57	MG	RA	3111	1/1	0.96	0.12	1,1,1,1	0
57	MG	YA	3120	1/1	0.96	0.37	0,0,0,0	0
57	MG	QA	1646	1/1	0.96	0.20	36,36,36,36	0
57	MG	RA	3114	1/1	0.96	0.23	2,2,2,2	0
57	MG	XM	201	1/1	0.96	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3065	1/1	0.96	0.31	38,38,38,38	0
57	MG	XA	1632	1/1	0.96	0.18	36,36,36,36	0
57	MG	YA	3184	1/1	0.96	0.16	51,51,51,51	0
57	MG	QA	1616	1/1	0.96	0.18	10,10,10,10	0
57	MG	RA	3148	1/1	0.96	0.17	39,39,39,39	0
57	MG	QA	1606	1/1	0.96	0.12	5,5,5,5	0
57	MG	YA	3073	1/1	0.96	0.35	23,23,23,23	0
57	MG	RB	202	1/1	0.96	0.19	2,2,2,2	0
57	MG	RA	3086	1/1	0.96	0.25	19,19,19,19	0
57	MG	RA	3119	1/1	0.96	0.24	18,18,18,18	0
57	MG	RA	3214	1/1	0.96	0.22	12,12,12,12	0
57	MG	RA	3215	1/1	0.96	0.18	1,1,1,1	0
57	MG	YA	3194	1/1	0.96	0.25	13,13,13,13	0
57	MG	QA	1655	1/1	0.96	0.17	6,6,6,6	0
57	MG	XA	1644	1/1	0.96	0.17	3,3,3,3	0
57	MG	YA	3139	1/1	0.96	0.16	19,19,19,19	0
57	MG	YA	3140	1/1	0.96	0.22	8,8,8,8	0
57	MG	RA	3121	1/1	0.96	0.24	2,2,2,2	0
57	MG	RA	3185	1/1	0.96	0.19	16,16,16,16	0
57	MG	YA	3021	1/1	0.96	0.46	15,15,15,15	0
57	MG	RA	3088	1/1	0.96	0.46	5,5,5,5	0
57	MG	YA	3266	1/1	0.96	0.36	1,1,1,1	0
57	MG	RA	3187	1/1	0.96	0.14	10,10,10,10	0
57	MG	RA	3089	1/1	0.96	0.48	2,2,2,2	0
57	MG	RA	3090	1/1	0.96	0.45	3,3,3,3	0
57	MG	RA	3092	1/1	0.96	0.34	1,1,1,1	0
57	MG	YA	3094	1/1	0.96	0.29	0,0,0,0	0
57	MG	QA	1613	1/1	0.96	0.25	36,36,36,36	0
57	MG	RA	3096	1/1	0.96	0.45	2,2,2,2	0
57	MG	XA	1608	1/1	0.96	0.18	81,81,81,81	0
57	MG	YA	3036	1/1	0.96	0.24	7,7,7,7	0
57	MG	YA	3040	1/1	0.96	0.61	0,0,0,0	0
57	MG	RA	3052	1/1	0.96	0.30	3,3,3,3	0
57	MG	RA	3054	1/1	0.96	0.25	41,41,41,41	0
57	MG	RA	3055	1/1	0.96	0.48	1,1,1,1	0
57	MG	QA	1635	1/1	0.96	0.17	8,8,8,8	0
57	MG	RA	3211	1/1	0.97	0.09	6,6,6,6	0
57	MG	YA	3038	1/1	0.97	0.22	5,5,5,5	0
57	MG	RA	3157	1/1	0.97	0.27	1,1,1,1	0
57	MG	XA	1621	1/1	0.97	0.12	23,23,23,23	0
57	MG	YA	3042	1/1	0.97	0.23	2,2,2,2	0
57	MG	QA	1621	1/1	0.97	0.22	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1624	1/1	0.97	0.18	23,23,23,23	0
57	MG	XA	1625	1/1	0.97	0.24	6,6,6,6	0
57	MG	RA	3241	1/1	0.97	0.33	29,29,29,29	0
57	MG	YA	3110	1/1	0.97	0.41	18,18,18,18	0
57	MG	RA	3029	1/1	0.97	0.31	1,1,1,1	0
57	MG	RA	3023	1/1	0.97	0.13	0,0,0,0	0
57	MG	YA	3049	1/1	0.97	0.47	6,6,6,6	0
57	MG	YA	3051	1/1	0.97	0.26	3,3,3,3	0
57	MG	QM	201	1/1	0.97	0.10	25,25,25,25	0
57	MG	QA	1642	1/1	0.97	0.14	20,20,20,20	0
57	MG	RA	3073	1/1	0.97	0.28	37,37,37,37	0
57	MG	RE	302	1/1	0.97	0.27	10,10,10,10	0
57	MG	RA	3164	1/1	0.97	0.15	34,34,34,34	0
57	MG	XV	101	1/1	0.97	0.21	3,3,3,3	0
57	MG	RA	3112	1/1	0.97	0.27	5,5,5,5	0
57	MG	YA	3178	1/1	0.97	0.37	2,2,2,2	0
57	MG	YA	3242	1/1	0.97	0.14	7,7,7,7	0
57	MG	YA	3180	1/1	0.97	0.13	7,7,7,7	0
57	MG	YA	3181	1/1	0.97	0.19	4,4,4,4	0
57	MG	RA	3047	1/1	0.97	0.33	1,1,1,1	0
57	MG	YA	3003	1/1	0.97	0.19	9,9,9,9	0
57	MG	RA	3091	1/1	0.97	0.30	1,1,1,1	0
57	MG	YA	3126	1/1	0.97	0.38	5,5,5,5	0
57	MG	RA	3115	1/1	0.97	0.10	11,11,11,11	0
57	MG	YA	3066	1/1	0.97	0.21	6,6,6,6	0
57	MG	RA	3059	1/1	0.97	0.25	4,4,4,4	0
57	MG	RA	3093	1/1	0.97	0.21	1,1,1,1	0
57	MG	YA	3070	1/1	0.97	0.25	5,5,5,5	0
57	MG	XA	1602	1/1	0.97	0.30	2,2,2,2	0
57	MG	YA	3011	1/1	0.97	0.28	2,2,2,2	0
57	MG	YA	3257	1/1	0.97	0.50	5,5,5,5	0
57	MG	RA	3094	1/1	0.97	0.62	3,3,3,3	0
57	MG	RA	3035	1/1	0.97	0.38	1,1,1,1	0
57	MG	RA	3077	1/1	0.97	0.41	19,19,19,19	0
57	MG	RA	3015	1/1	0.97	0.31	0,0,0,0	0
57	MG	YA	3262	1/1	0.97	0.14	5,5,5,5	0
57	MG	RA	3063	1/1	0.97	0.61	0,0,0,0	0
57	MG	RA	3037	1/1	0.97	0.15	15,15,15,15	0
57	MG	YA	3020	1/1	0.97	0.28	12,12,12,12	0
57	MG	RA	3082	1/1	0.97	0.40	18,18,18,18	0
57	MG	YA	3023	1/1	0.97	0.38	6,6,6,6	0
57	MG	XA	1611	1/1	0.97	0.37	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1612	1/1	0.97	0.13	7,7,7,7	0
57	MG	RA	3021	1/1	0.97	0.25	5,5,5,5	0
57	MG	YA	3028	1/1	0.97	0.28	1,1,1,1	0
57	MG	RA	3126	1/1	0.97	0.12	8,8,8,8	0
57	MG	RA	3127	1/1	0.97	0.20	10,10,10,10	0
57	MG	RA	3128	1/1	0.97	0.11	2,2,2,2	0
57	MG	YA	3033	1/1	0.97	0.62	5,5,5,5	0
57	MG	XA	1657	1/1	0.97	0.16	27,27,27,27	0
57	MG	YA	3211	1/1	0.97	0.18	1,1,1,1	0
59	ZN	QD	301	1/1	0.97	0.20	21,21,21,21	0
57	MG	YA	3096	1/1	0.97	0.55	2,2,2,2	0
57	MG	YA	3214	1/1	0.97	0.12	7,7,7,7	0
57	MG	RA	3102	1/1	0.97	0.09	4,4,4,4	0
57	MG	YA	3177	1/1	0.98	0.29	5,5,5,5	0
57	MG	YA	3084	1/1	0.98	0.46	17,17,17,17	0
57	MG	RA	3041	1/1	0.98	0.36	13,13,13,13	0
57	MG	YA	3232	1/1	0.98	0.32	5,5,5,5	0
57	MG	RA	3053	1/1	0.98	0.32	4,4,4,4	0
57	MG	YA	3087	1/1	0.98	0.38	8,8,8,8	0
57	MG	RA	3042	1/1	0.98	0.19	14,14,14,14	0
57	MG	RA	3151	1/1	0.98	0.28	10,10,10,10	0
57	MG	YA	3013	1/1	0.98	0.41	1,1,1,1	0
57	MG	QA	1609	1/1	0.98	0.06	9,9,9,9	0
57	MG	YA	3093	1/1	0.98	0.14	8,8,8,8	0
57	MG	YA	3050	1/1	0.98	0.47	10,10,10,10	0
57	MG	RA	3011	1/1	0.98	0.18	5,5,5,5	0
57	MG	YA	3016	1/1	0.98	0.27	2,2,2,2	0
57	MG	RA	3012	1/1	0.98	0.49	7,7,7,7	0
57	MG	RA	3072	1/1	0.98	0.18	3,3,3,3	0
57	MG	XA	1610	1/1	0.98	0.10	6,6,6,6	0
57	MG	XA	1636	1/1	0.98	0.19	5,5,5,5	0
57	MG	YA	3101	1/1	0.98	0.38	1,1,1,1	0
57	MG	QA	1636	1/1	0.98	0.12	13,13,13,13	0
57	MG	YA	3022	1/1	0.98	0.24	2,2,2,2	0
57	MG	YA	3061	1/1	0.98	0.31	2,2,2,2	0
57	MG	YA	3105	1/1	0.98	0.49	1,1,1,1	0
57	MG	RA	3198	1/1	0.98	0.20	7,7,7,7	0
57	MG	RA	3103	1/1	0.98	0.19	1,1,1,1	0
57	MG	YA	3108	1/1	0.98	0.70	15,15,15,15	0
57	MG	RA	3020	1/1	0.98	0.18	5,5,5,5	0
57	MG	RA	3060	1/1	0.98	0.41	65,65,65,65	0
57	MG	RA	3106	1/1	0.98	0.23	3,3,3,3	0

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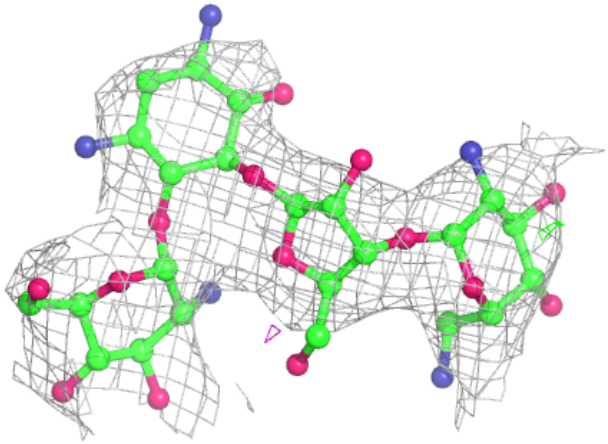
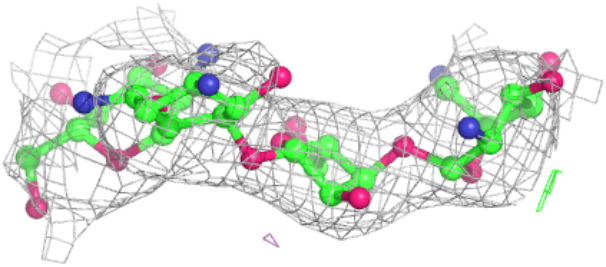
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3029	1/1	0.98	0.19	0,0,0,0	0
57	MG	YA	3113	1/1	0.98	0.19	2,2,2,2	0
57	MG	YA	3068	1/1	0.98	0.23	3,3,3,3	0
57	MG	RA	3107	1/1	0.98	0.08	3,3,3,3	0
57	MG	RA	3142	1/1	0.98	0.10	28,28,28,28	0
57	MG	RA	3183	1/1	0.98	0.13	12,12,12,12	0
57	MG	QA	1608	1/1	0.98	0.08	11,11,11,11	0
57	MG	YA	3213	1/1	0.98	0.28	17,17,17,17	0
57	MG	XA	1622	1/1	0.98	0.21	9,9,9,9	0
57	MG	YA	3215	1/1	0.98	0.15	25,25,25,25	0
57	MG	YA	3166	1/1	0.98	0.13	45,45,45,45	0
57	MG	YA	3074	1/1	0.98	0.29	0,0,0,0	0
57	MG	YA	3001	1/1	0.98	0.53	0,0,0,0	0
57	MG	QA	1653	1/1	0.98	0.25	16,16,16,16	0
57	MG	YA	3037	1/1	0.98	0.38	7,7,7,7	0
57	MG	YA	3221	1/1	0.98	0.30	42,42,42,42	0
57	MG	XA	1650	1/1	0.98	0.09	27,27,27,27	0
57	MG	YA	3039	1/1	0.98	0.18	0,0,0,0	0
57	MG	RA	3030	1/1	0.98	0.40	2,2,2,2	0
57	MG	RA	3040	1/1	0.98	0.31	11,11,11,11	0
57	MG	YA	3007	1/1	0.98	0.18	4,4,4,4	0
57	MG	YA	3227	1/1	0.98	0.24	0,0,0,0	0
57	MG	RA	3147	1/1	0.98	0.24	0,0,0,0	0
57	MG	RA	3080	1/1	0.99	0.25	2,2,2,2	0
57	MG	RA	3064	1/1	0.99	0.20	12,12,12,12	0
57	MG	YA	3053	1/1	0.99	0.30	1,1,1,1	0
57	MG	YA	3130	1/1	0.99	0.08	7,7,7,7	0
57	MG	YA	3090	1/1	0.99	0.22	14,14,14,14	0
57	MG	RA	3033	1/1	0.99	0.52	5,5,5,5	0
57	MG	XA	1613	1/1	0.99	0.08	0,0,0,0	0
57	MG	YA	3027	1/1	0.99	0.25	3,3,3,3	0
57	MG	YA	3179	1/1	0.99	0.05	4,4,4,4	0
57	MG	XA	1642	1/1	0.99	0.30	7,7,7,7	0
57	MG	YA	3004	1/1	0.99	0.34	18,18,18,18	0
57	MG	YA	3059	1/1	0.99	0.25	3,3,3,3	0
57	MG	YA	3255	1/1	0.99	0.13	19,19,19,19	0

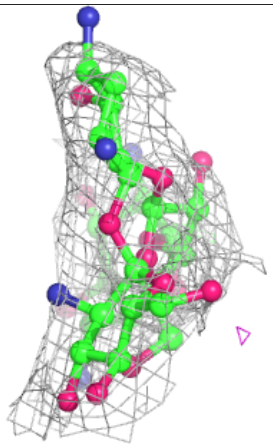
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR XA 1671:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

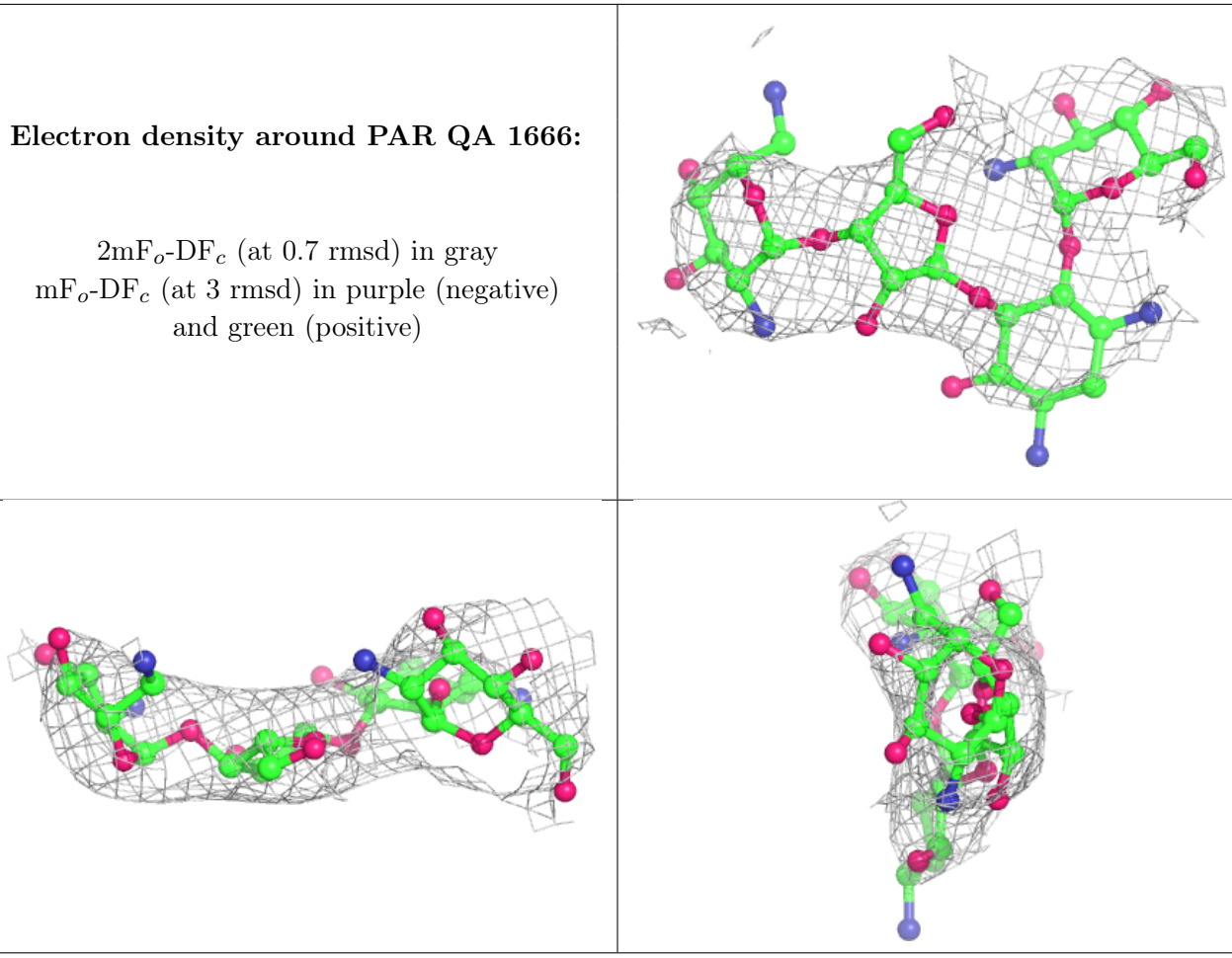






Electron density around PAR QA 1666:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.