



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 07:08 AM EDT

PDB ID : 1VVJ  
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 bound to Codon CCC-G on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-05-24  
Resolution : 3.44 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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

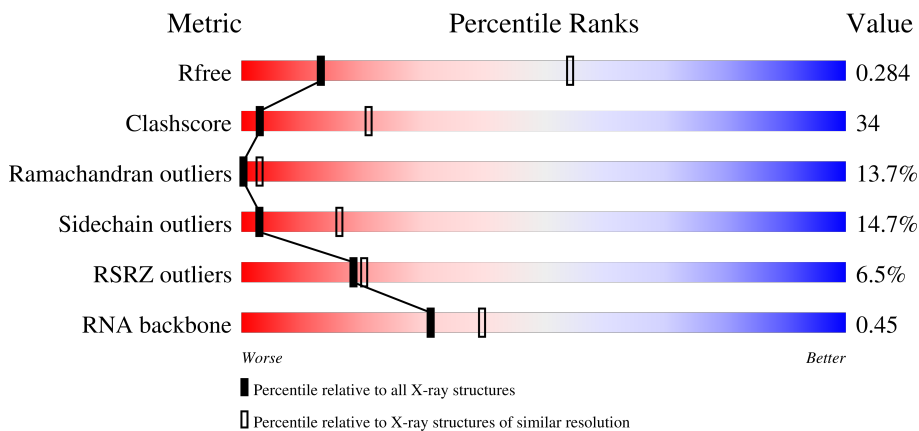
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	
1	XA	1522	
2	QB	256	
2	XB	256	

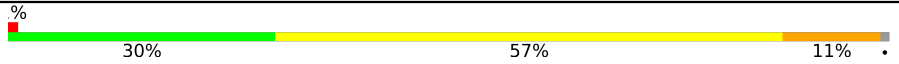
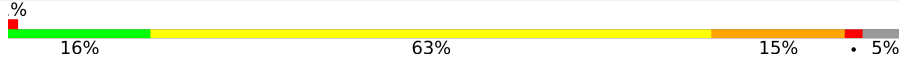
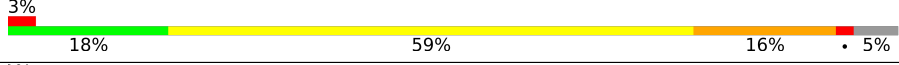
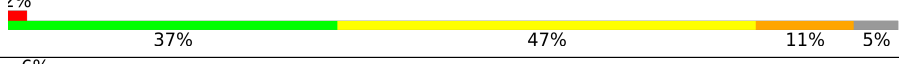
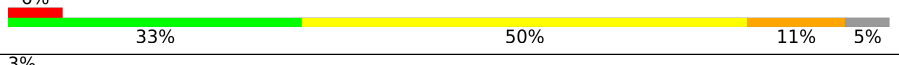
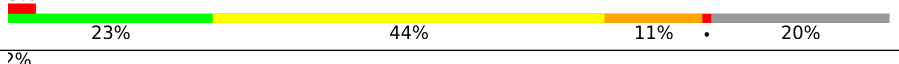
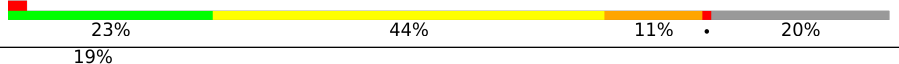
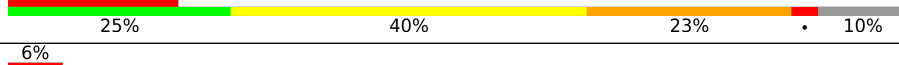
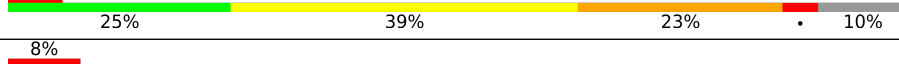
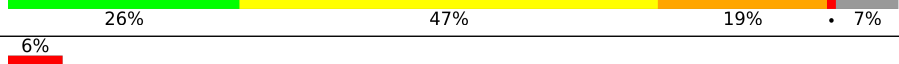
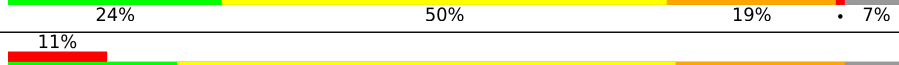
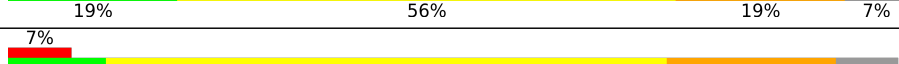
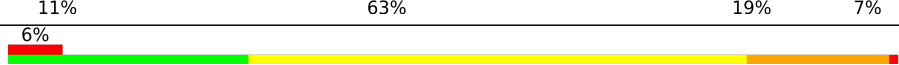
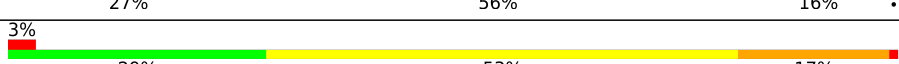
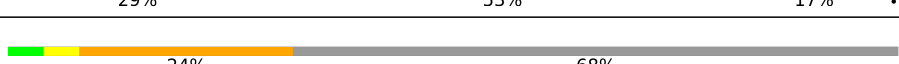

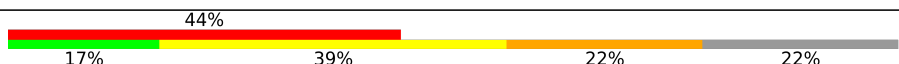
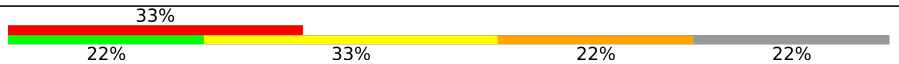
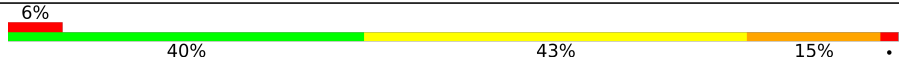


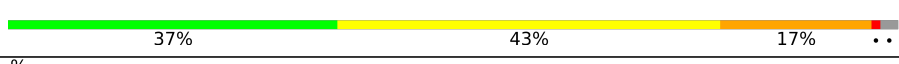
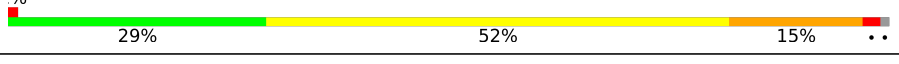
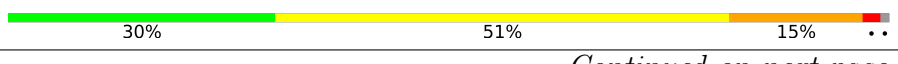

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain
28	RE	206	2% 22% 49% 24% 5%
28	YE	206	3% 24% 47% 24% 5%
29	RF	210	3% 37% 45% 13% . .
29	YF	210	2% 33% 49% 13% . .
30	RG	182	41% 23% 58% 16% . .
30	YG	182	14% 23% 58% 16% . .
31	RH	180	21% 23% 45% 19% 8% 6%
31	YH	180	6% 23% 44% 19% 8% 6%
32	RI	148	11% 22% 48% 26% . .
32	YI	148	2% 23% 46% 28% . .
33	RN	140	2% 17% 54% 26% . .
33	YN	140	% 19% 53% 26% . .
34	RO	122	2% 35% 54% 9% . .
34	YO	122	34% 55% 9% . .
35	RP	150	9% 19% 51% 23% 8%
35	YP	150	2% 21% 49% 23% 7%
36	RQ	141	5% 31% 50% 16% .
36	YQ	141	% 30% 50% 16% .
37	RR	118	33% 48% 16% .
37	YR	118	36% 47% 15% .
38	RS	112	4% 13% 62% 19% 5% .
38	YS	112	3% 12% 63% 20% . .
39	RT	146	7% 23% 49% 19% . 6%
39	YT	146	3% 23% 49% 19% . 6%
40	RU	118	4% 33% 53% 12% . .




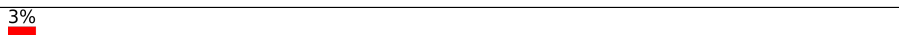
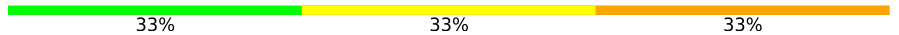
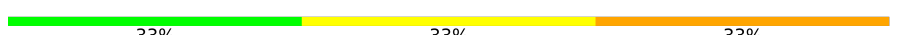
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Mol	Chain	Length	Quality of chain
40	YU	118	2% 28% 56% 14% ..
41	RV	101	11% 28% 51% 21%
41	YV	101	4% 28% 51% 21%
42	RW	113	4% 27% 51% 19% .
42	YW	113	27% 53% 18% .
43	RX	96	% 38% 44% 15% .
43	YX	96	2% 33% 48% 15% .
44	RY	110	18% 15% 45% 28% . 7%
44	YY	110	6% 18% 43% 28% . 7%
45	RZ	206	20% 17% 43% 18% 6% 17%
45	YZ	206	12% 17% 42% 19% 5% 17%
46	R0	85	% 39% 47% 9% ..
46	Y0	85	35% 48% 12% ..
47	R1	98	3% 29% 50% 17% ..
47	Y1	98	5% 27% 51% 18% ..
48	R2	72	4% 22% 54% 18% ..
48	Y2	72	3% 22% 54% 18% ..
49	R3	60	2% 33% 50% 15% .
49	Y3	60	3% 33% 50% 13% ..
50	R4	71	59% 6% 44% 39% 11%
50	Y4	71	32% 6% 44% 39% 11%
51	R5	60	12% 23% 47% 22% 7% .
51	Y5	60	5% 23% 47% 22% 7% .
52	R6	54	61% 7% 46% 31% 6% 9%
52	Y6	54	69% 9% 44% 31% 6% 9%

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	Z6	3	
55	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	QA	1615	-	-	-	X
56	MG	RA	3176	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	XA	1605	-	-	-	X
56	MG	YA	3012	-	-	-	X

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 291123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	Total 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1501	Total 32269	C 14363	N 5986	O 10420	P 1500	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	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	XB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			170	76	31	55	8			

- Molecule 24 is a RNA chain called messenger RNA.

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

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

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

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

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

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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	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- 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	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- 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	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- 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	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- 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	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

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

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

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

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

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

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

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

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

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

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

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

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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	172	1378	879	248	248	3	0	0	0
45	YZ	172	1378	879	248	248	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
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called tRNA acceptor end mimic.

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

- Molecule 55 is a RNA chain called RNA (5'-R(\*CP\*CP\*(PPU))-3').

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

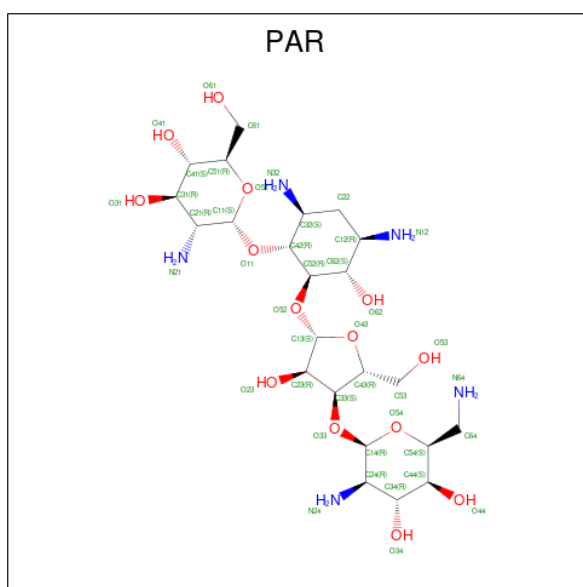
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	60	Total	Mg	0	0
			60	60		
56	QF	1	Total	Mg	0	0
			1	1		
56	QH	1	Total	Mg	0	0
			1	1		
56	QM	1	Total	Mg	0	0
			1	1		
56	QV	2	Total	Mg	0	0
			2	2		
56	QX	2	Total	Mg	0	0
			2	2		
56	RA	212	Total	Mg	0	0
			212	212		
56	RB	2	Total	Mg	0	0
			2	2		
56	RE	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RF	1	Total Mg 1 1	0	0
56	RP	1	Total Mg 1 1	0	0
56	R5	1	Total Mg 1 1	0	0
56	XA	63	Total Mg 63 63	0	0
56	XM	2	Total Mg 2 2	0	0
56	XV	2	Total Mg 2 2	0	0
56	YA	242	Total Mg 242 242	0	0
56	YB	2	Total Mg 2 2	0	0
56	YE	2	Total Mg 2 2	0	0
56	YX	1	Total Mg 1 1	0	0
56	Y5	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



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

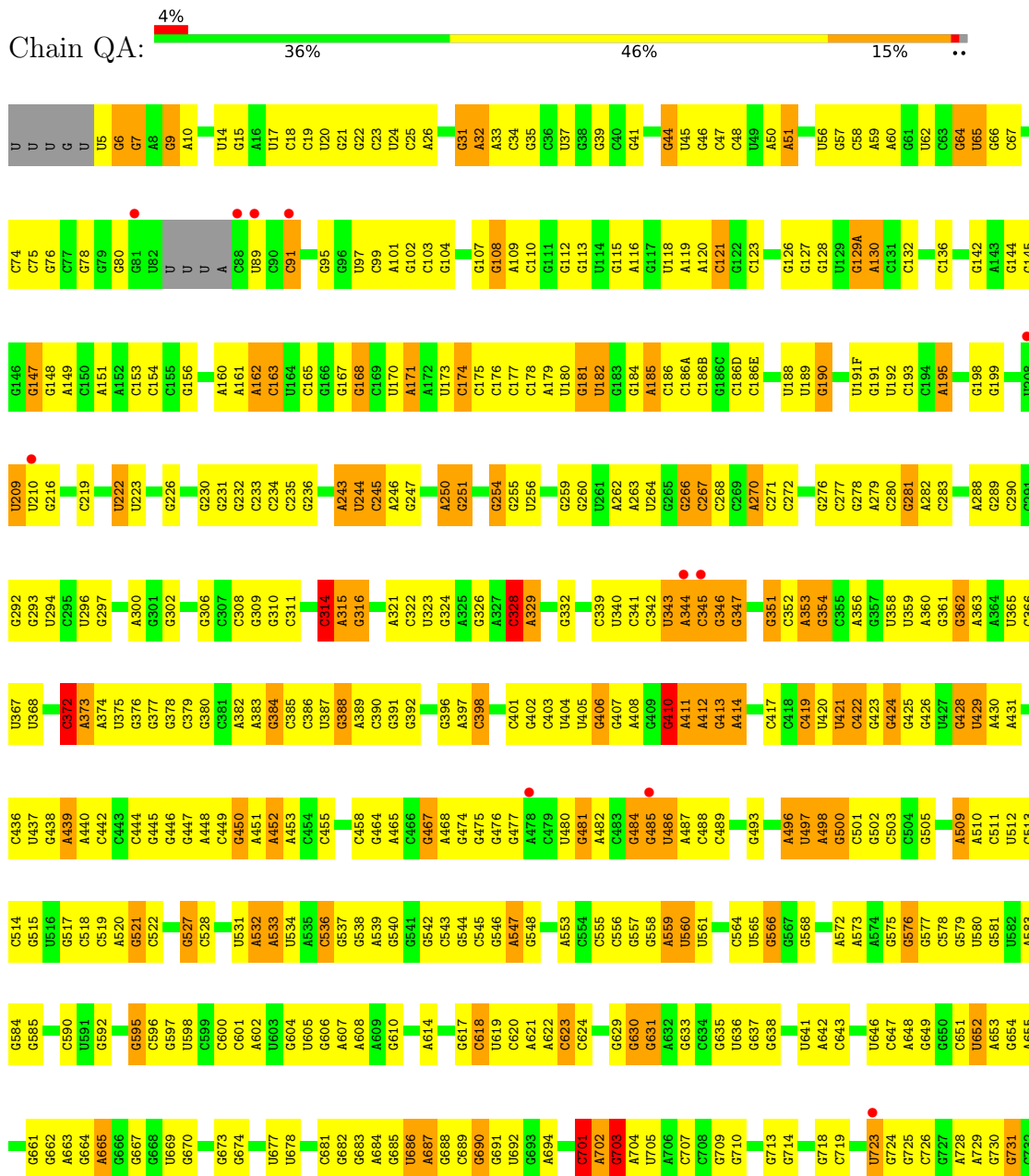
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

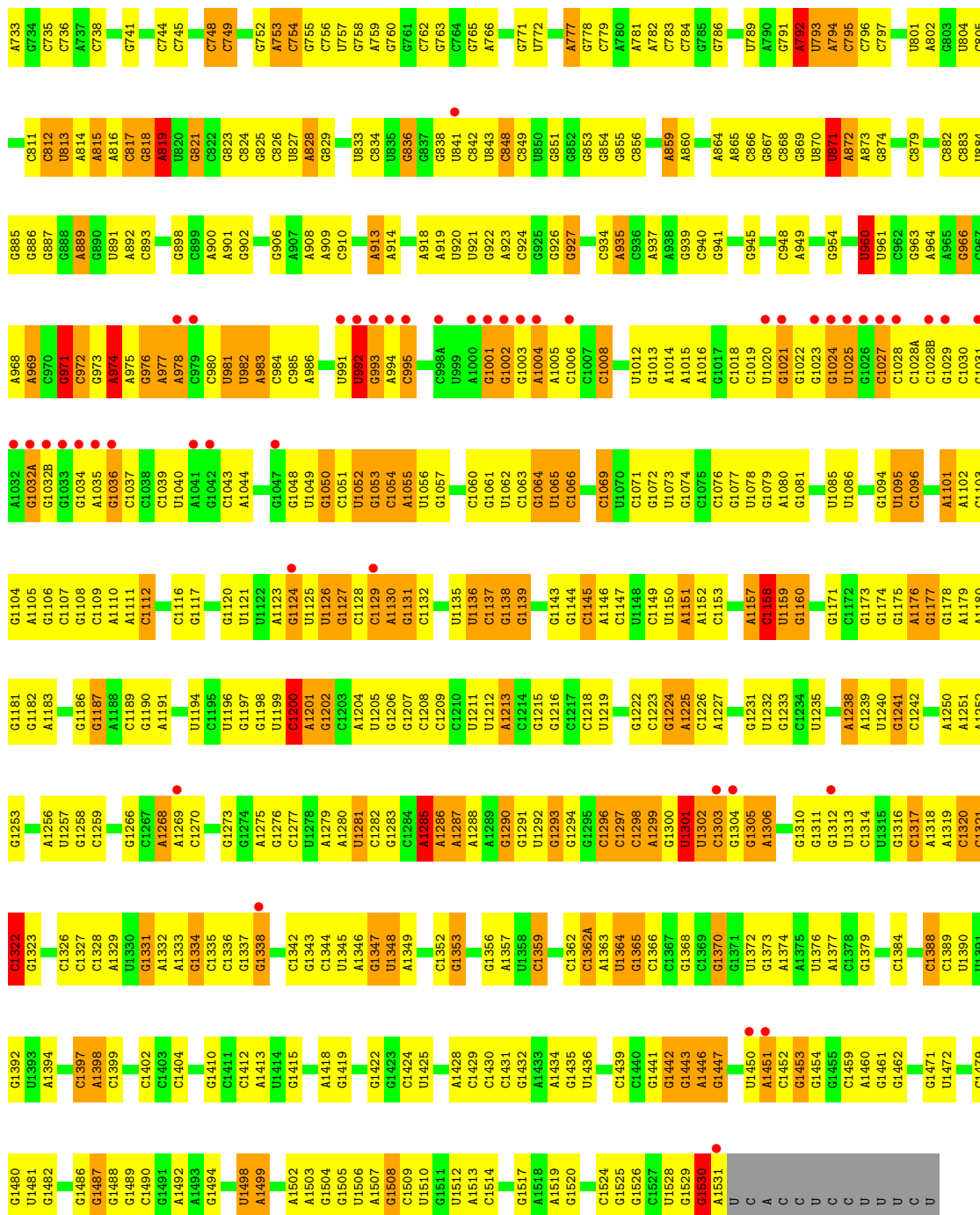
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QD	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XD	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots i

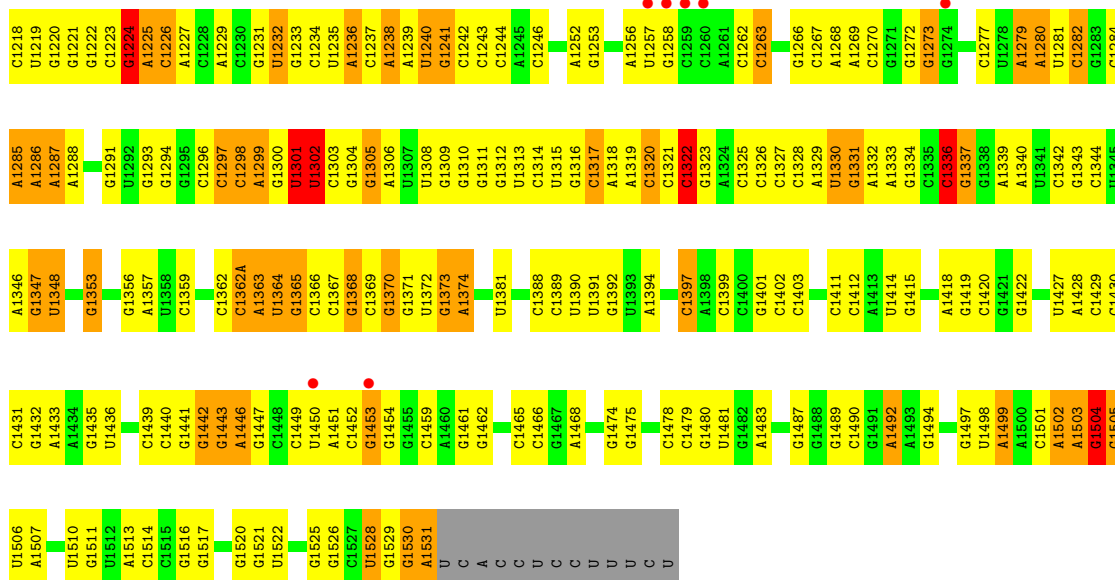
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

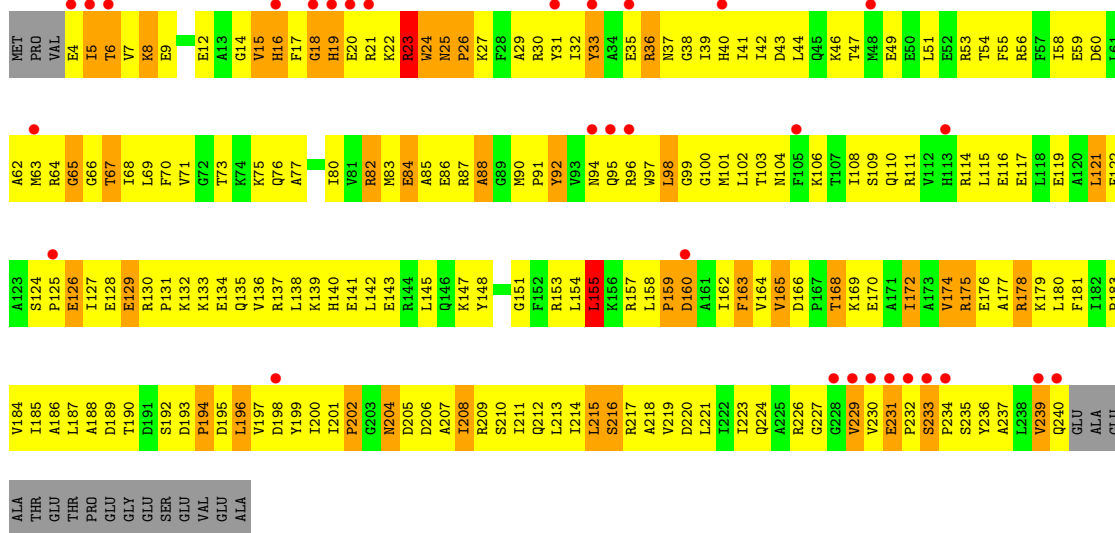
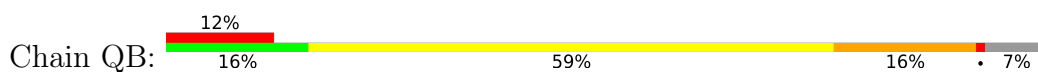




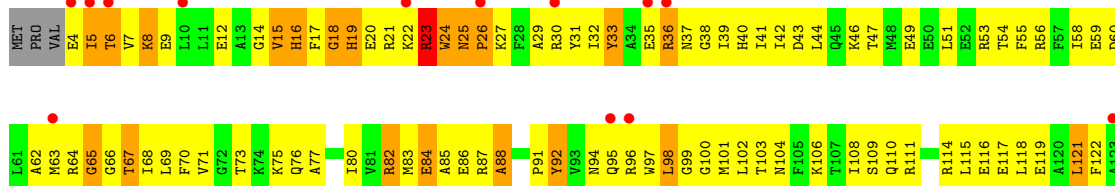




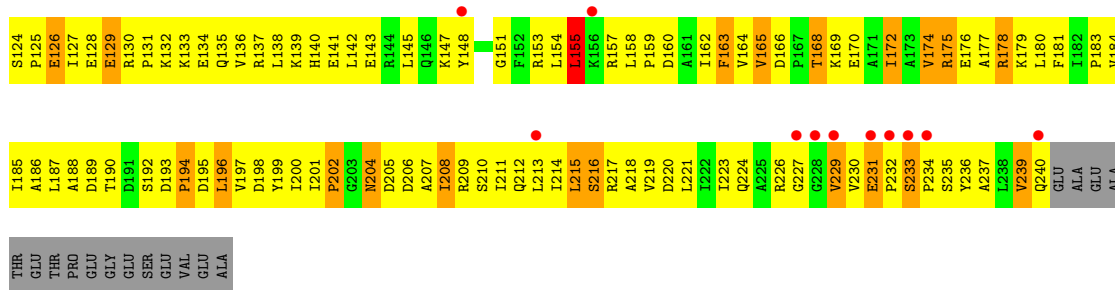
● Molecule 2: 30S ribosomal protein S2



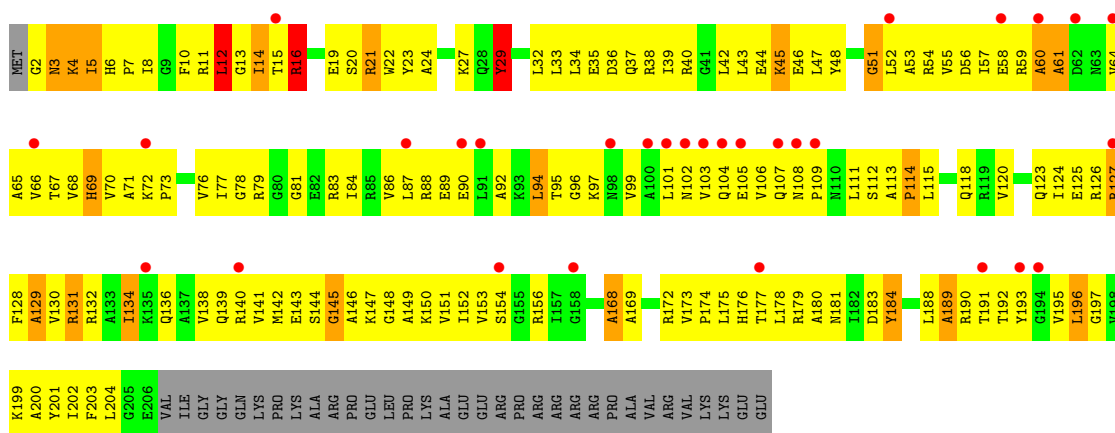
● Molecule 2: 30S ribosomal protein S2



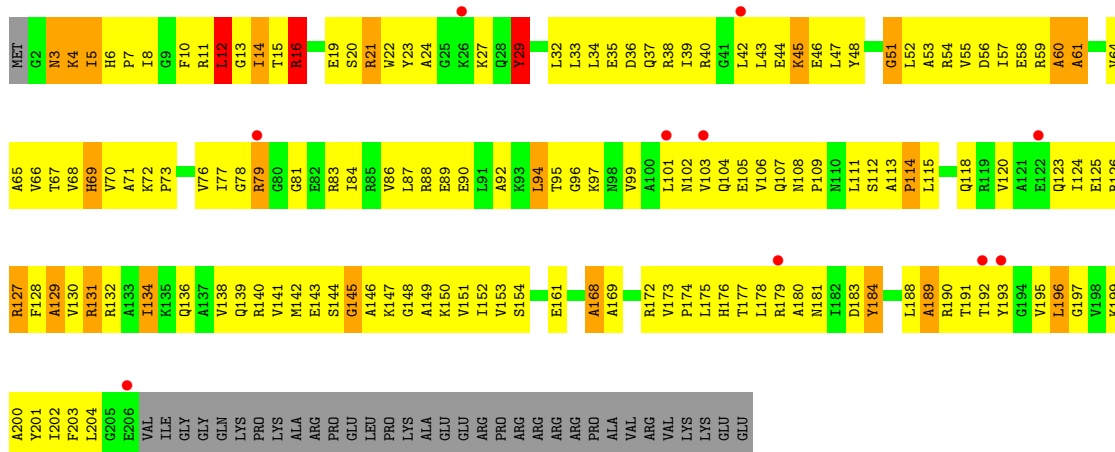




• Molecule 3: 30S ribosomal protein S3

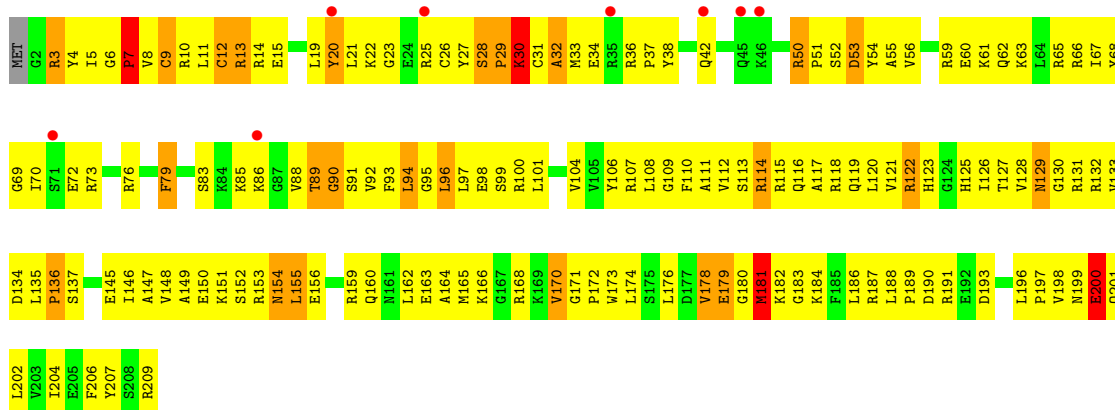


• Molecule 3: 30S ribosomal protein S3

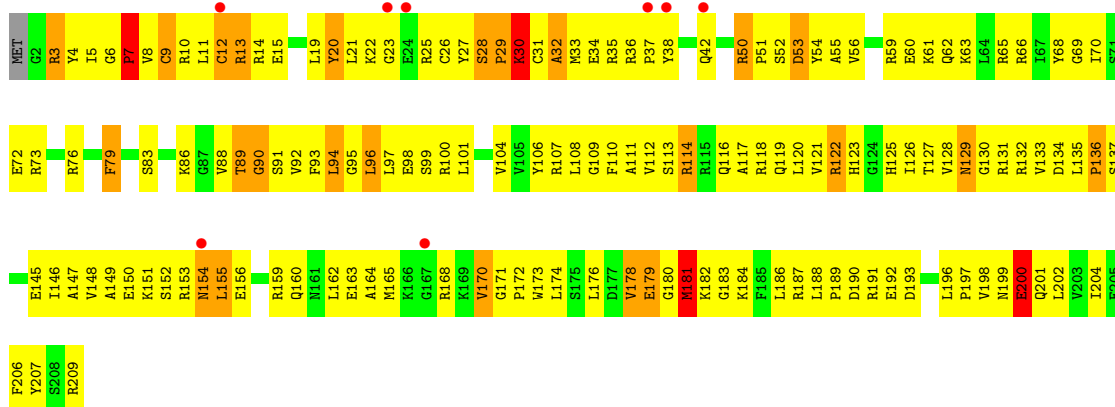


• Molecule 4: 30S ribosomal protein S4

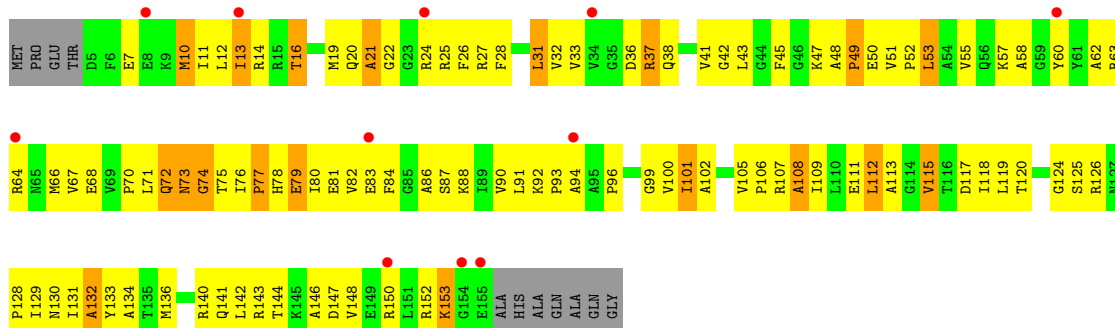




• Molecule 4: 30S ribosomal protein S4

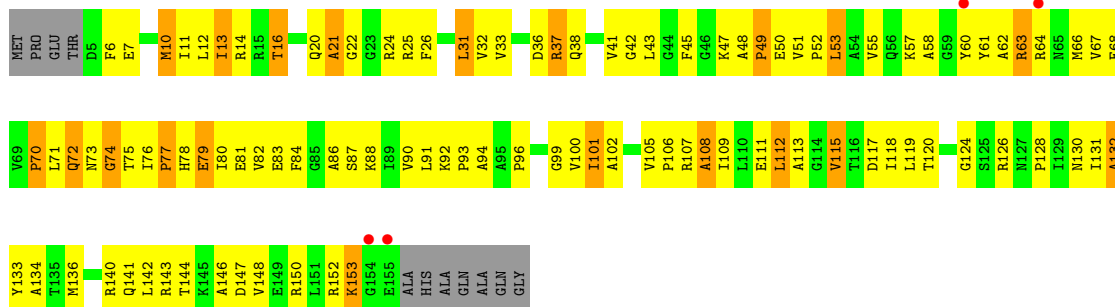


• Molecule 5: 30S ribosomal protein S5

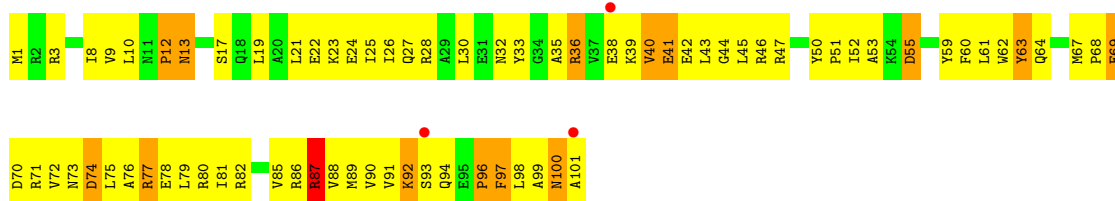


• Molecule 5: 30S ribosomal protein S5

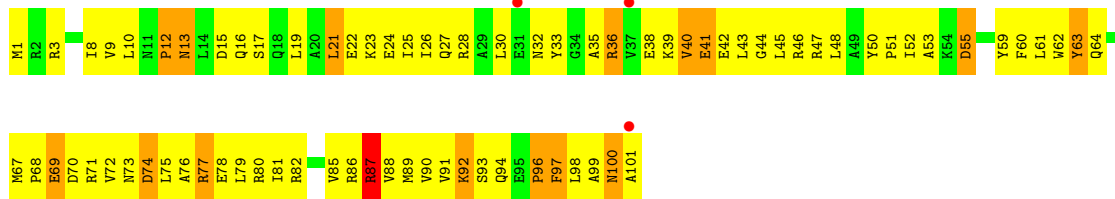




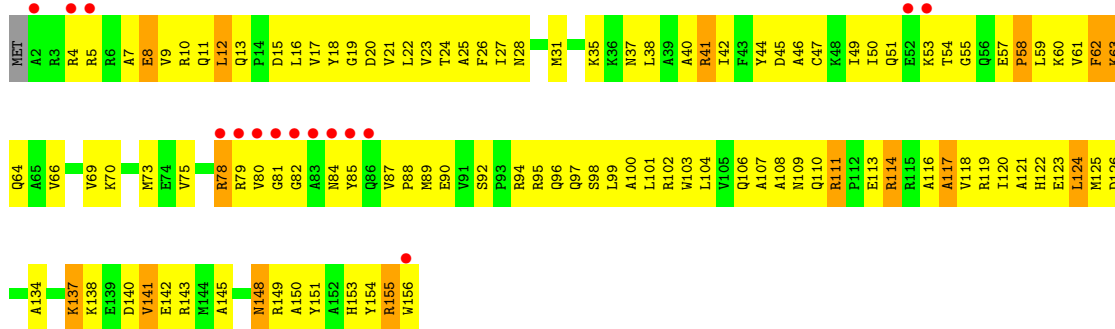
• Molecule 6: 30S ribosomal protein S6



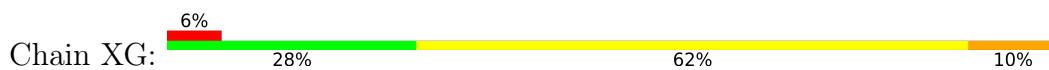
• Molecule 6: 30S ribosomal protein S6

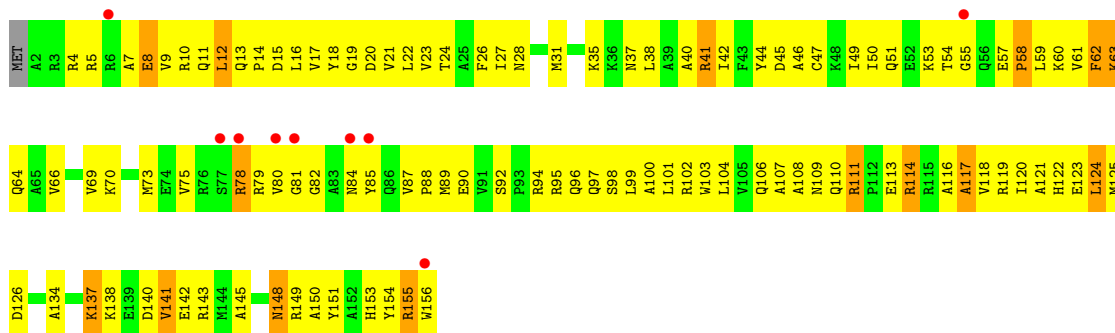


• Molecule 7: 30S ribosomal protein S7

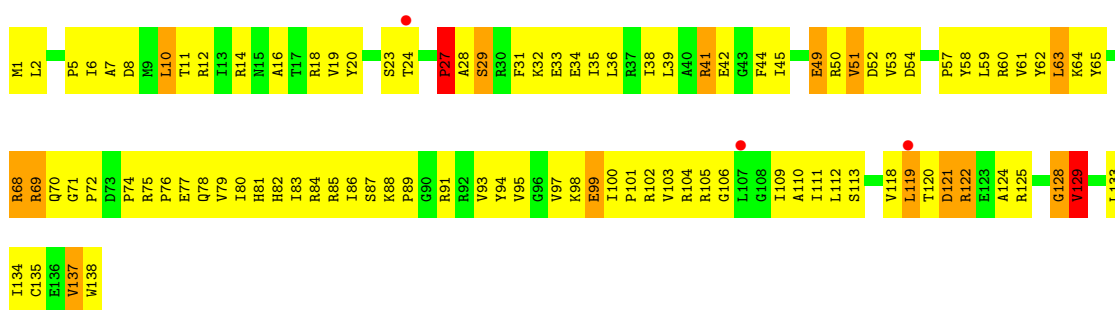
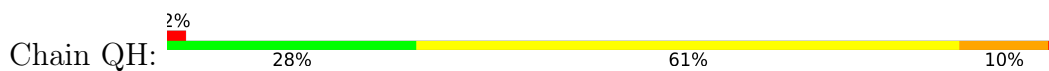


• Molecule 7: 30S ribosomal protein S7

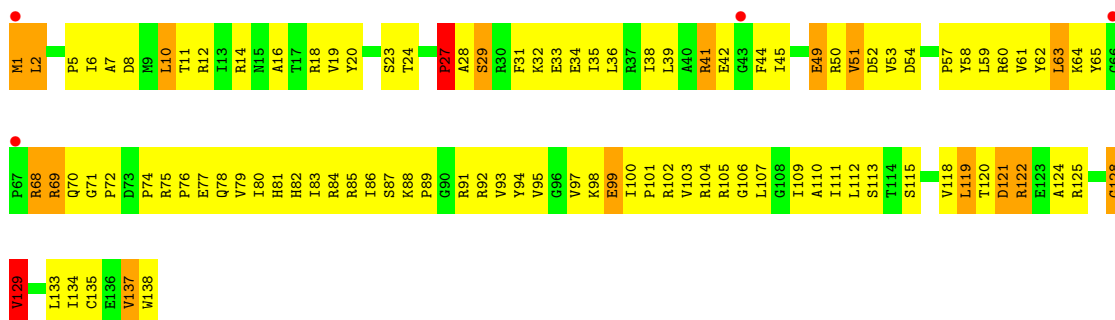




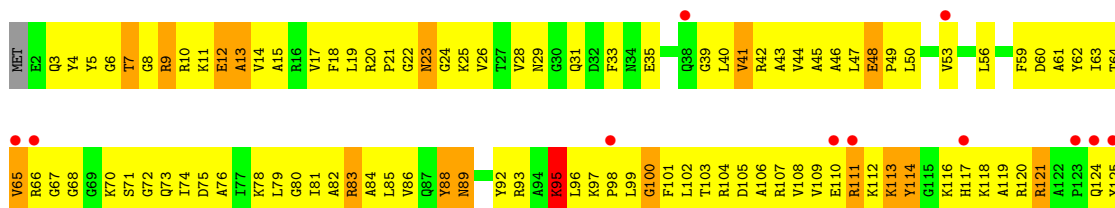
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



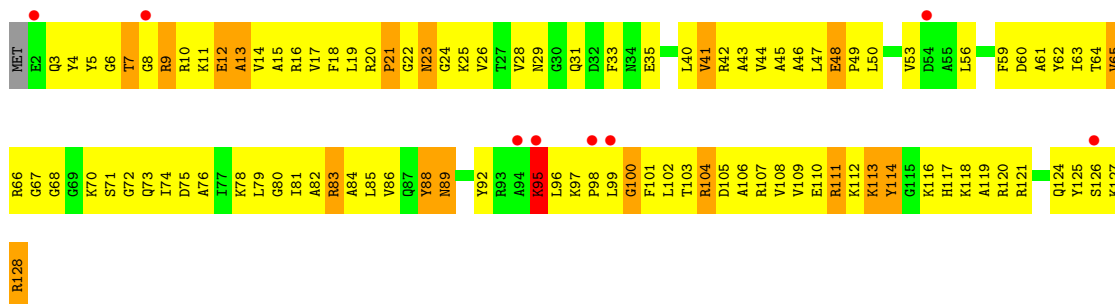
- Molecule 9: 30S ribosomal protein S9



S126  
K127  
R128

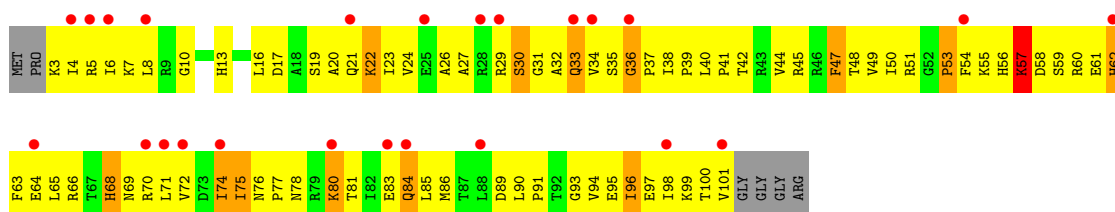
• Molecule 9: 30S ribosomal protein S9

Chain XI: 6% 20% 65% 14% ..



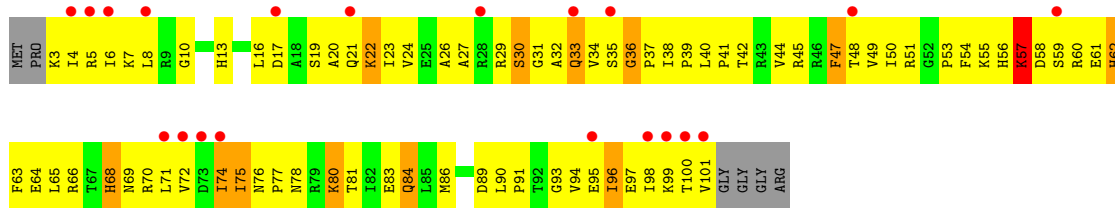
• Molecule 10: 30S ribosomal protein S10

Chain QJ: 23% 17% 64% 12% 6%



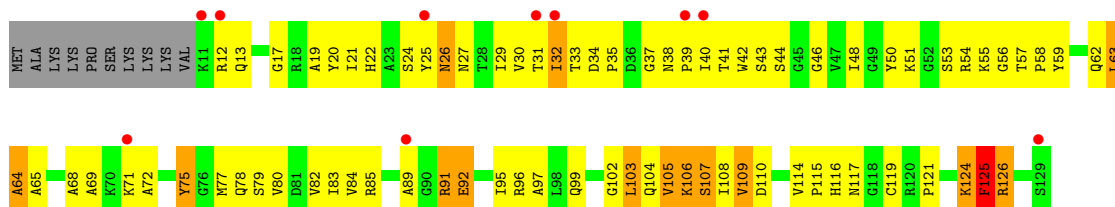
• Molecule 10: 30S ribosomal protein S10

Chain XJ: 19% 18% 64% 11% 6%



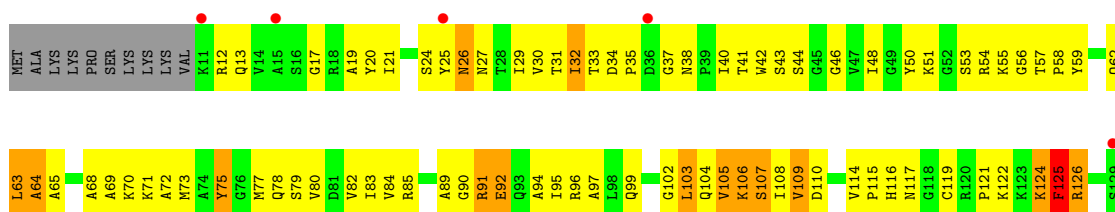
• Molecule 11: 30S ribosomal protein S11

Chain QK: 8% 31% 50% 11% 8%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 4% 29% 52% 11% 8%



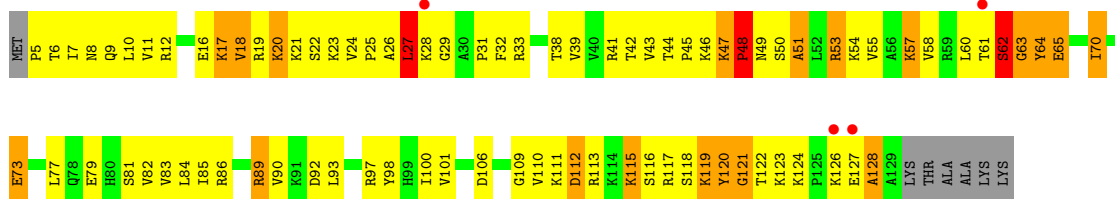
- Molecule 12: 30S ribosomal protein S12

Chain QL: 5% 30% 48% 15% 5%



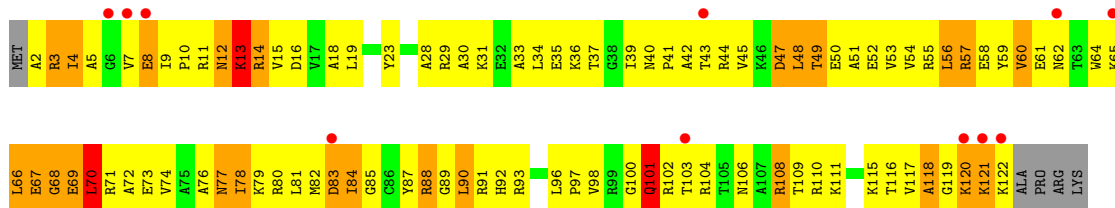
- Molecule 12: 30S ribosomal protein S12

Chain XL: 3% 30% 48% 14% 5%



- Molecule 13: 30S ribosomal protein S13

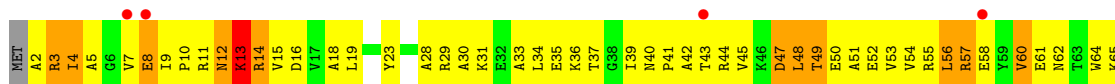
Chain QM: 9% 18% 56% 20% 5%



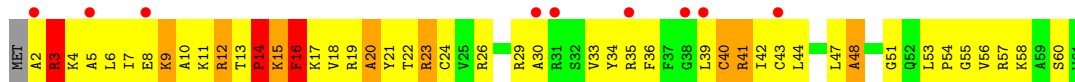
- Molecule 13: 30S ribosomal protein S13

Chain XM: 4% 19% 55% 19% 5%

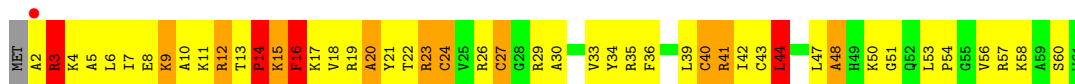




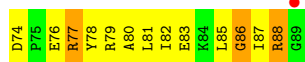
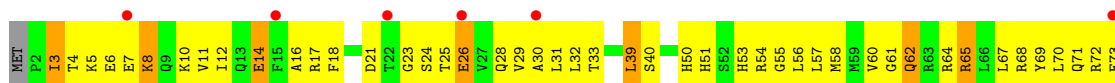
- Molecule 14: 30S ribosomal protein S14



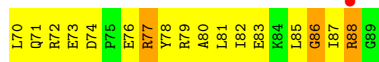
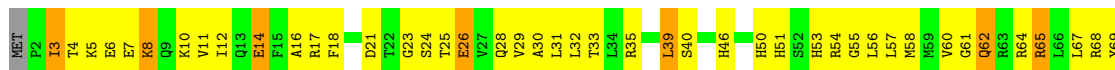
- Molecule 14: 30S ribosomal protein S14



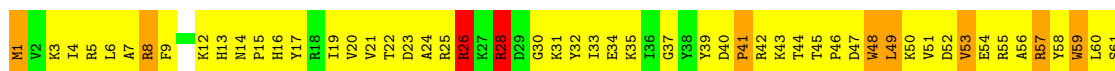
- Molecule 15: 30S ribosomal protein S15

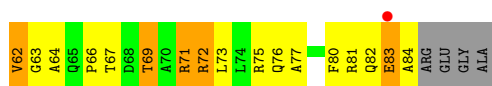


- Molecule 15: 30S ribosomal protein S15

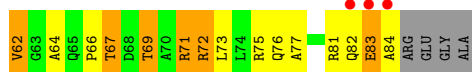
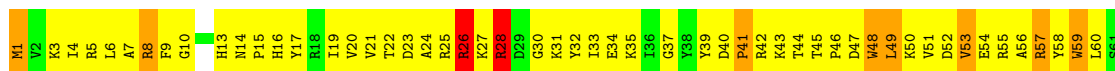


- Molecule 16: 30S ribosomal protein S16

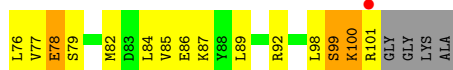
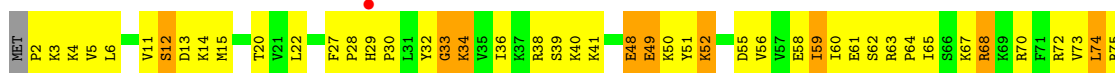




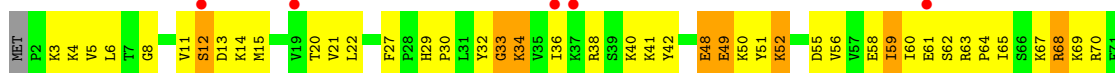
- Molecule 16: 30S ribosomal protein S16



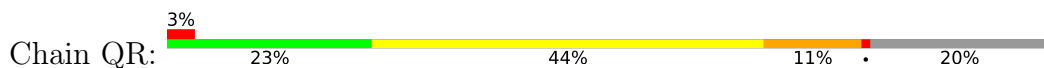
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

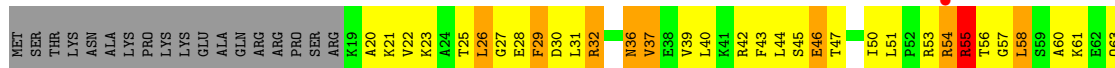
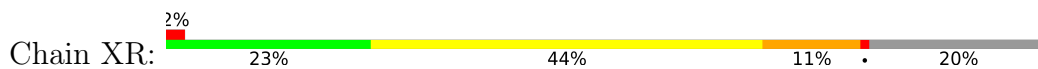


- Molecule 18: 30S ribosomal protein S18

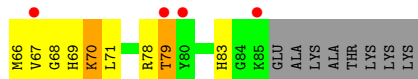
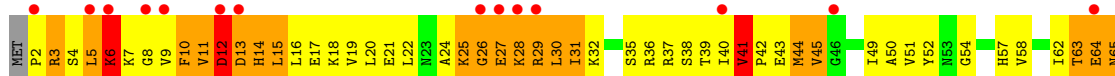
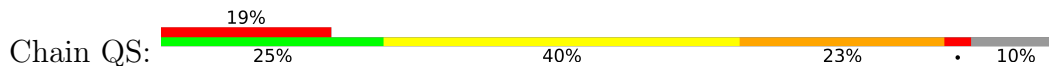


- Molecule 18: 30S ribosomal protein S18

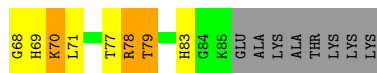
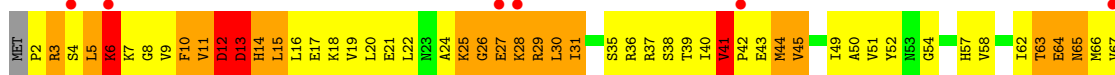
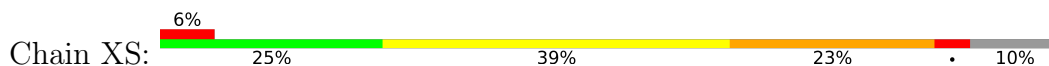




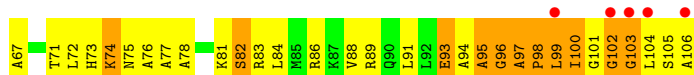
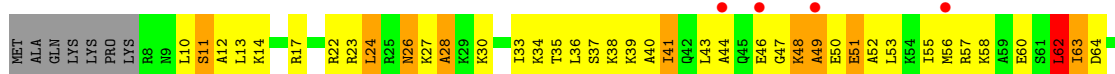
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

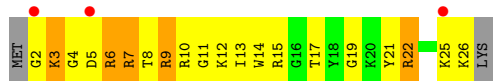


• Molecule 20: 30S ribosomal protein S20

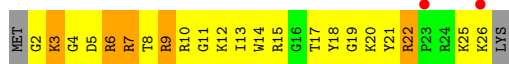
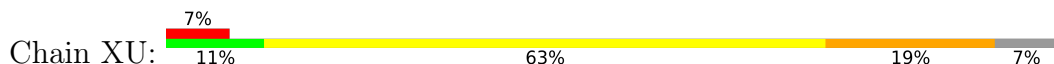




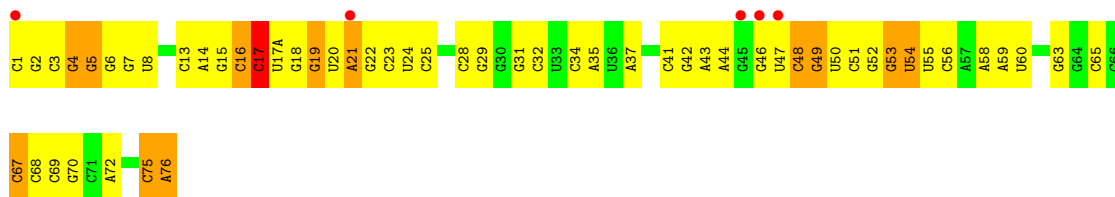
• Molecule 21: 30S ribosomal protein S21



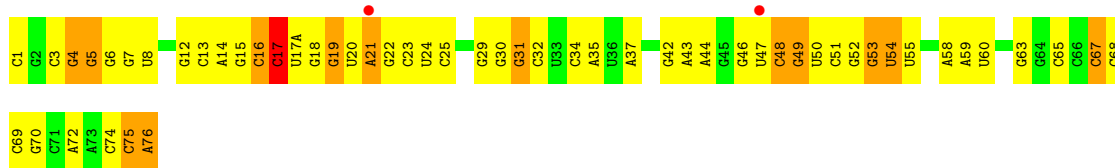
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: P-site tRNA fMet



• Molecule 22: P-site tRNA fMet



• Molecule 23: A-site ASL SufA6

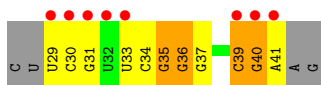
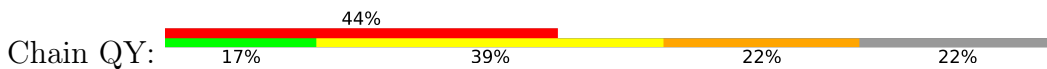


• Molecule 23: A-site ASL SufA6

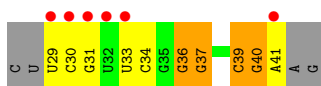
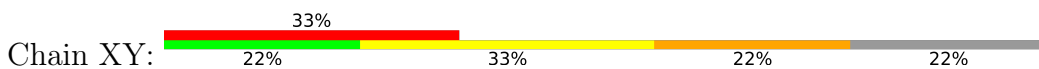




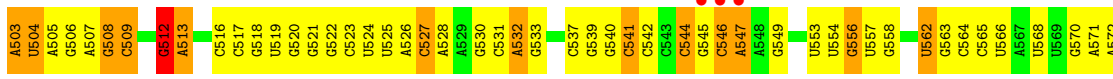
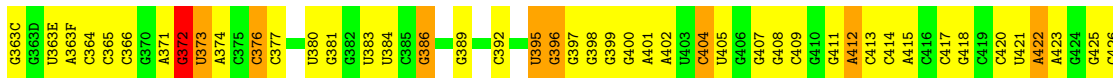
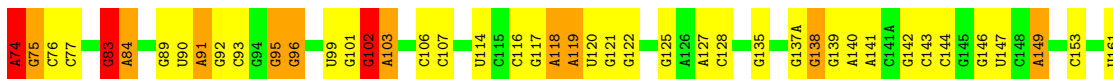
● Molecule 24: messenger RNA

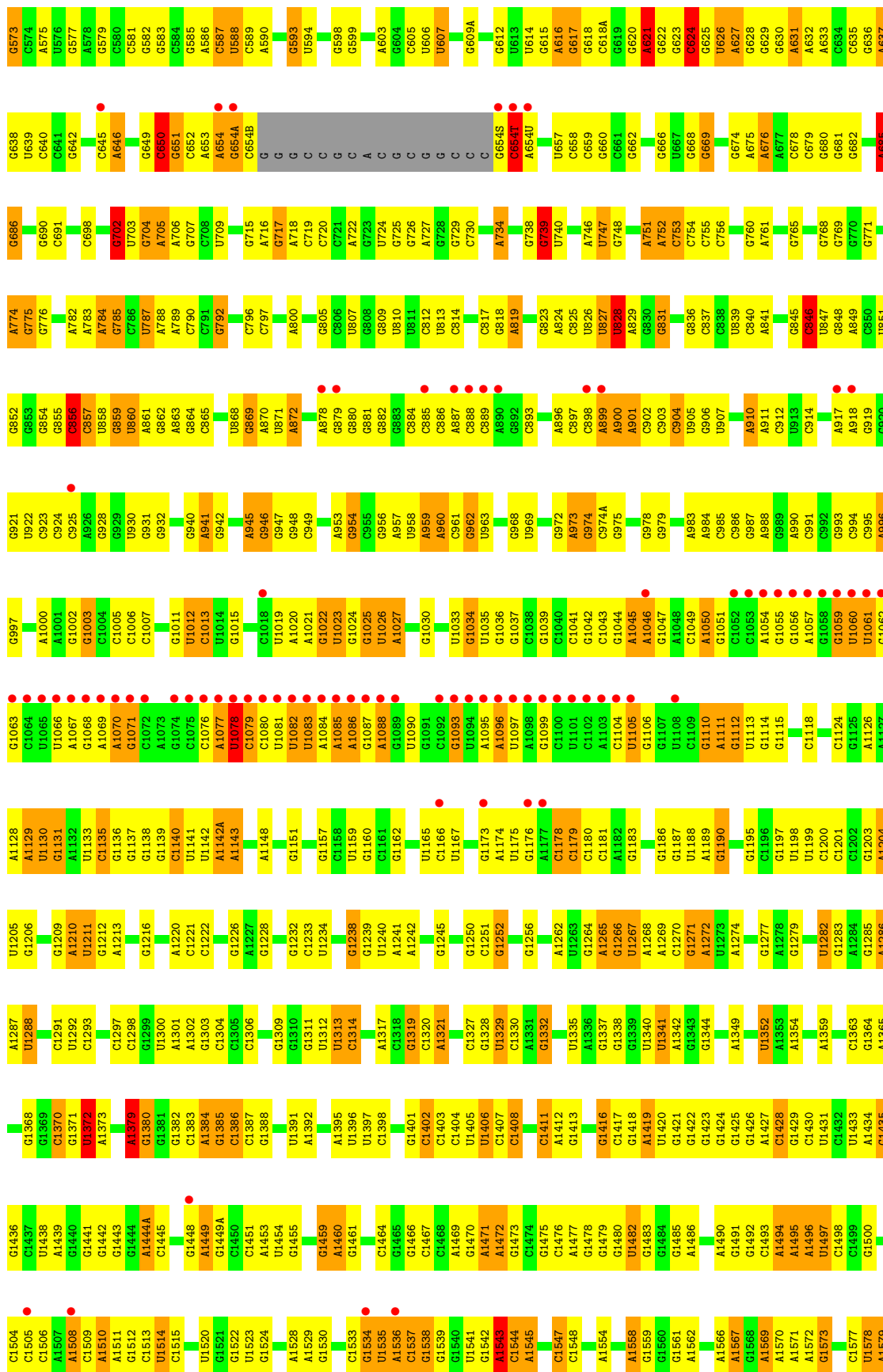


● Molecule 24: messenger RNA

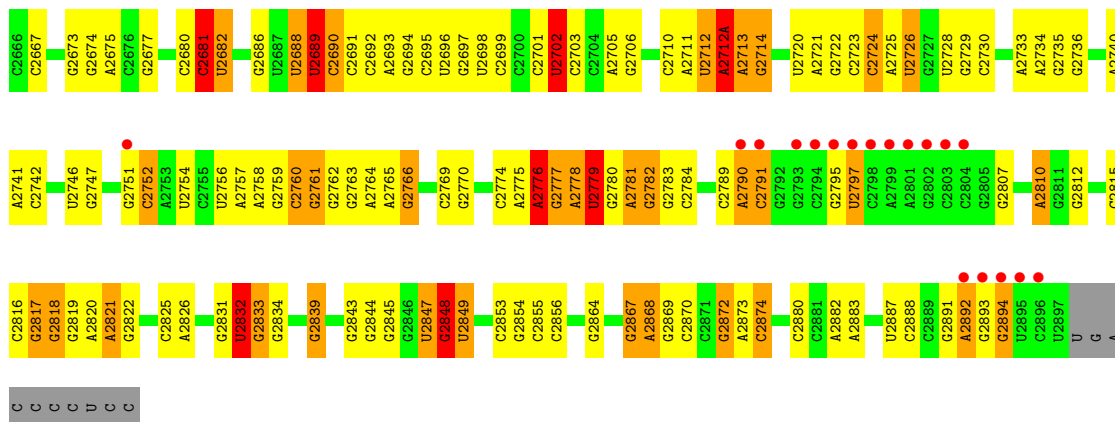


● Molecule 25: 23S rRNA

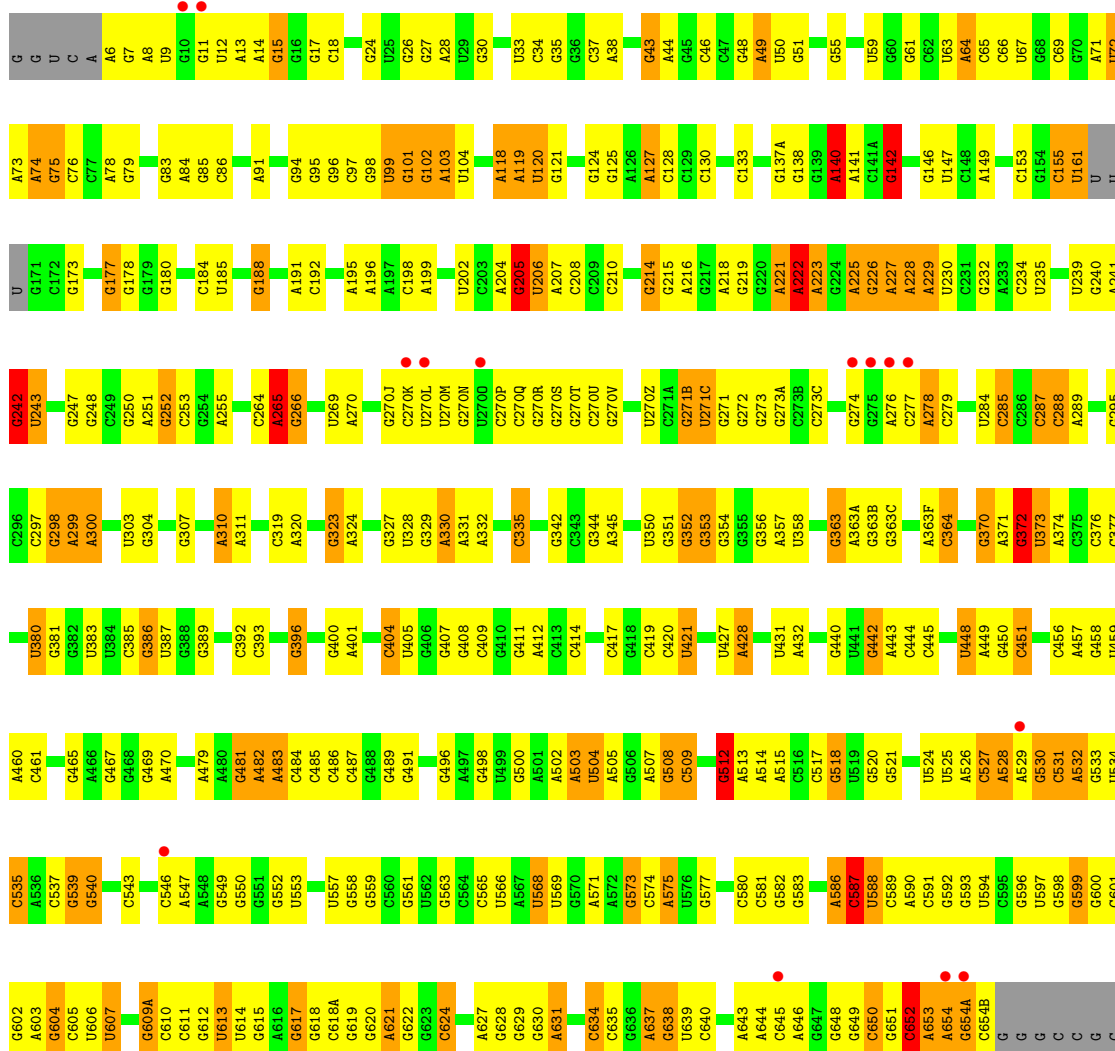
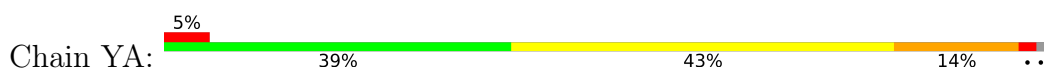


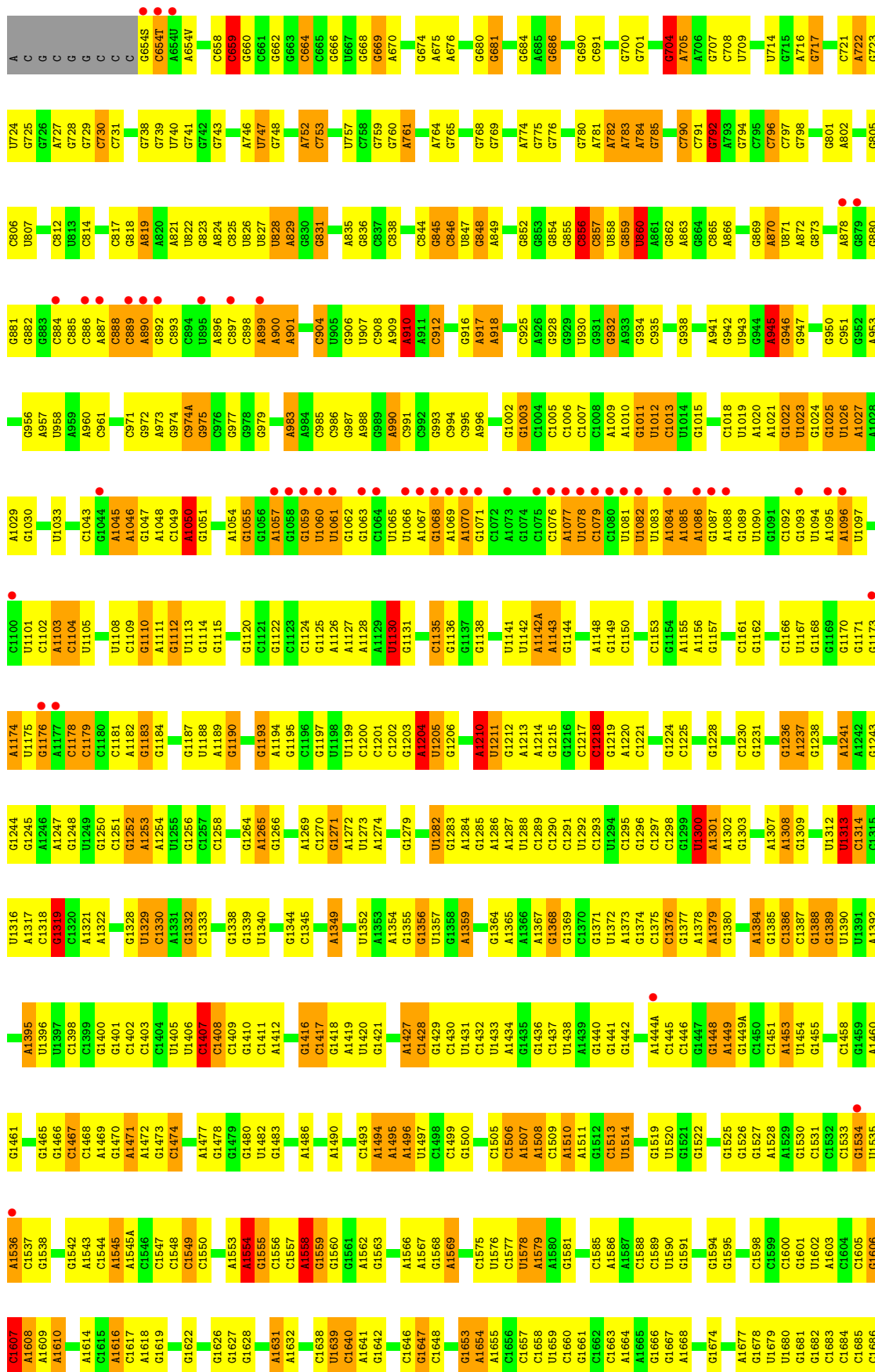






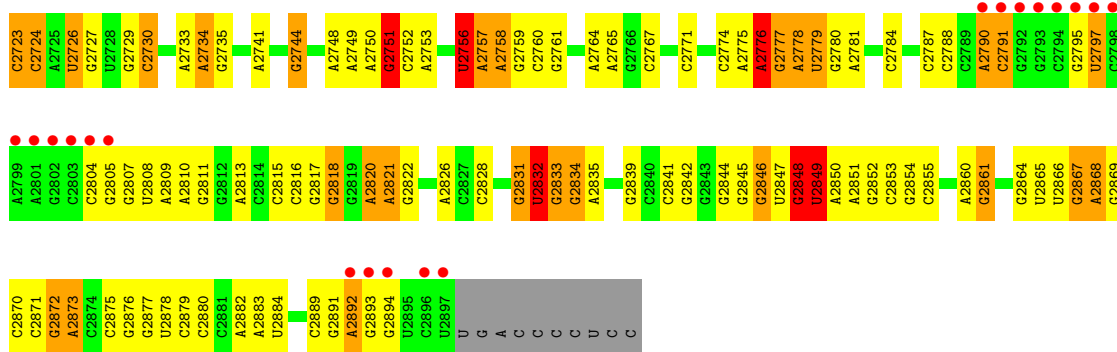
• Molecule 25: 23S rRNA



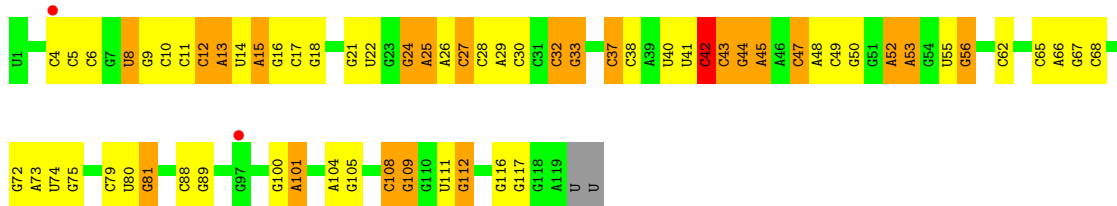


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U2649	G2577	A2426	U2357	G2211	U2144	G2070	U1993	A1917	A1844	G1776	A1690
A2653	U2504	C2427	G2358	A2212	C2145	A2071	C1994	A1918	A1845	A1779	C1691
G2505	C2359	G2428	C2359	U2213	C2146	U2074	U1995	A1919	A1846	U1780	U1692
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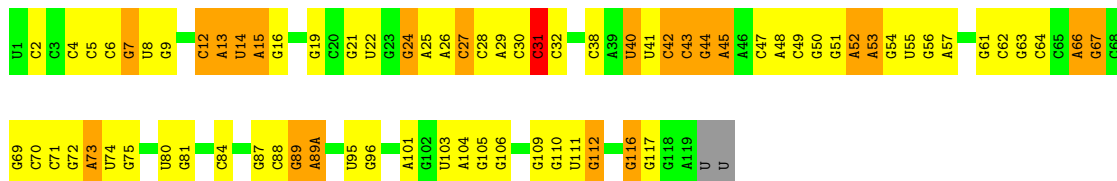
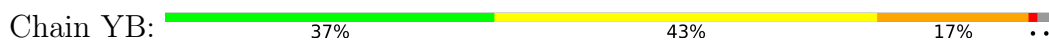




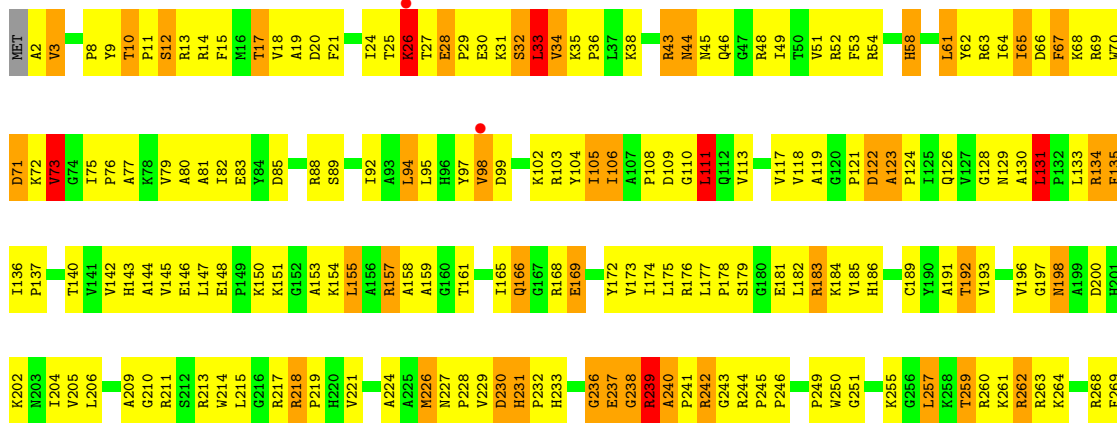
● Molecule 26: 5S rRNA



● Molecule 26: 5S rRNA



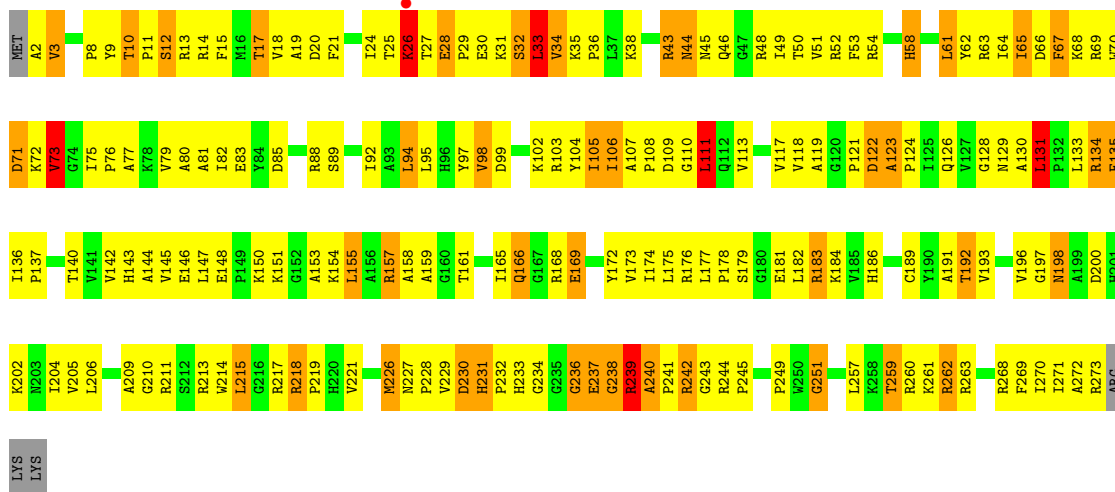
● Molecule 27: 50S ribosomal protein L2



I270  
I271  
A272  
R273  
ARG  
LYS  
LYS

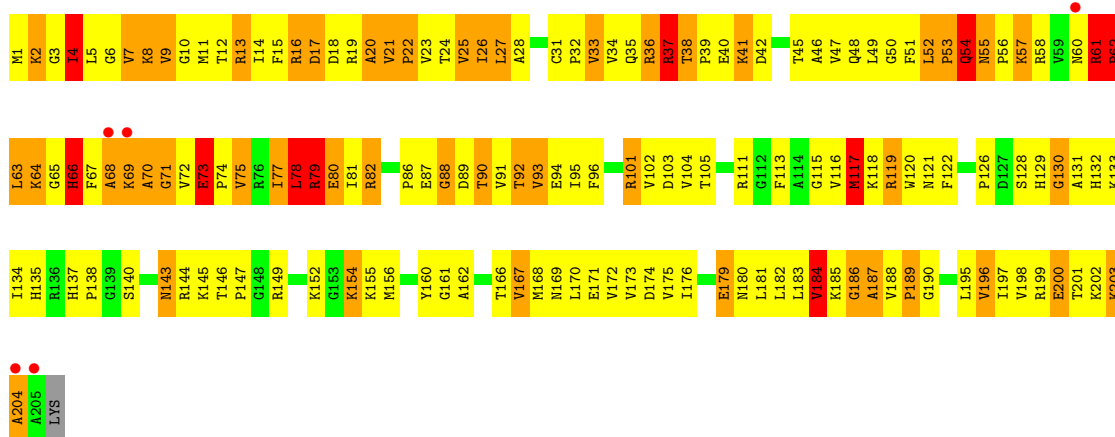
• Molecule 27: 50S ribosomal protein L2

Chain YD: 30% 51% 15% ..



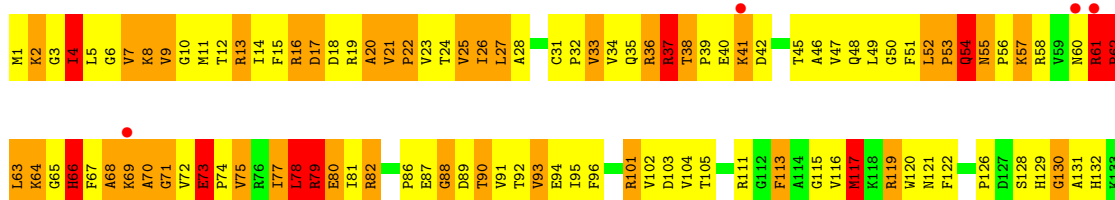
• Molecule 28: 50S ribosomal protein L3

Chain RE: 22% 49% 24% 5%



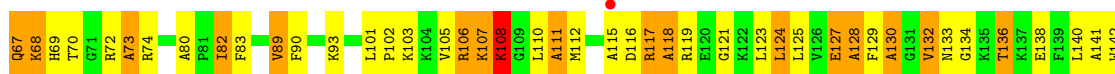
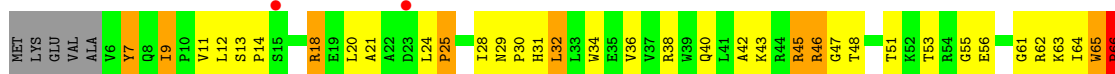
• Molecule 28: 50S ribosomal protein L3

Chain YE: 24% 47% 24% 5%

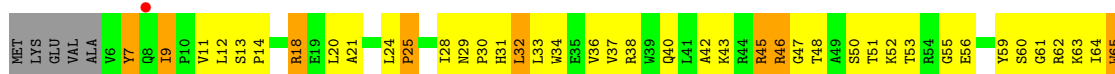




• Molecule 29: 50S ribosomal protein L4

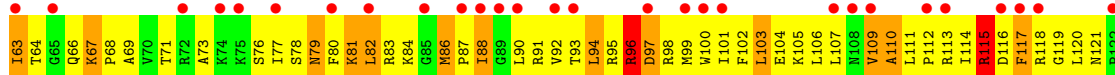


• Molecule 29: 50S ribosomal protein L4

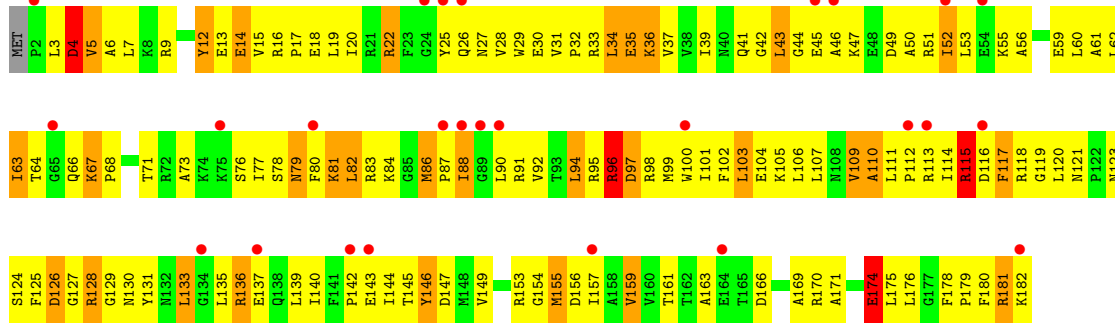


GLU  
ALA

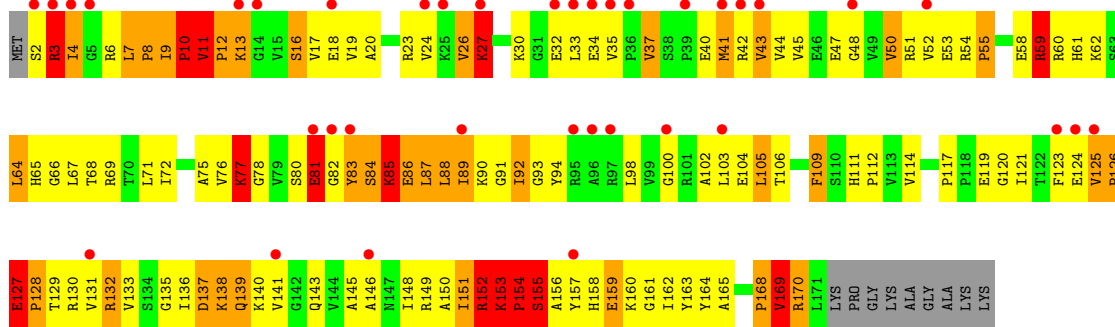
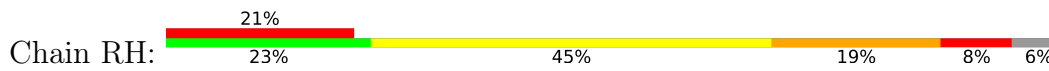
• Molecule 30: 50S ribosomal protein L5



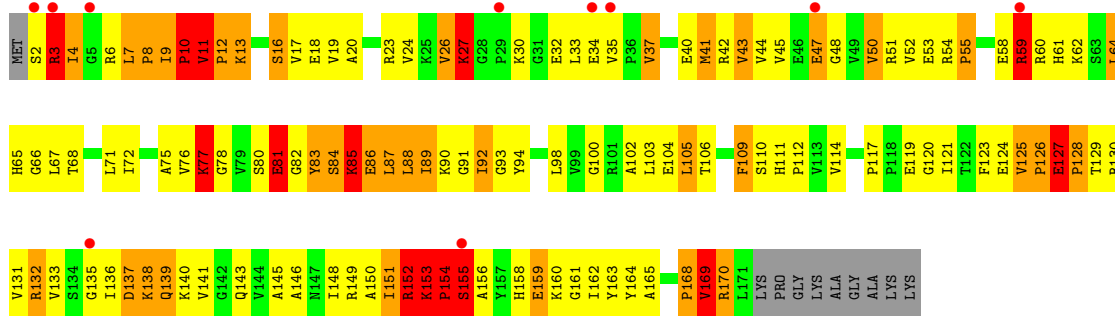
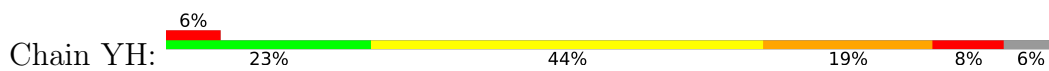
• Molecule 30: 50S ribosomal protein L5



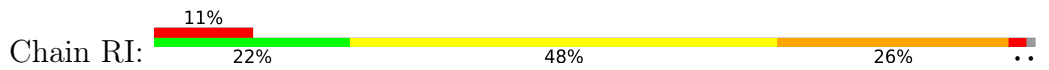
• Molecule 31: 50S ribosomal protein L6

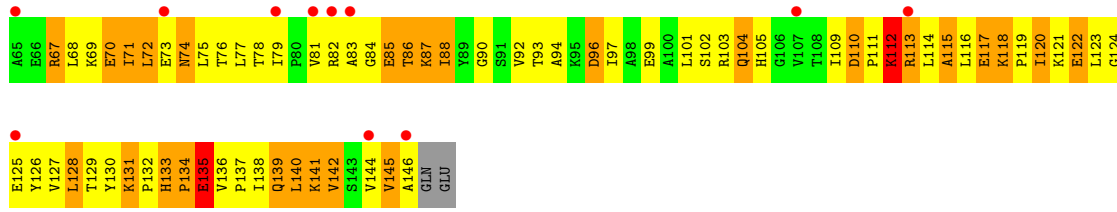


• Molecule 31: 50S ribosomal protein L6

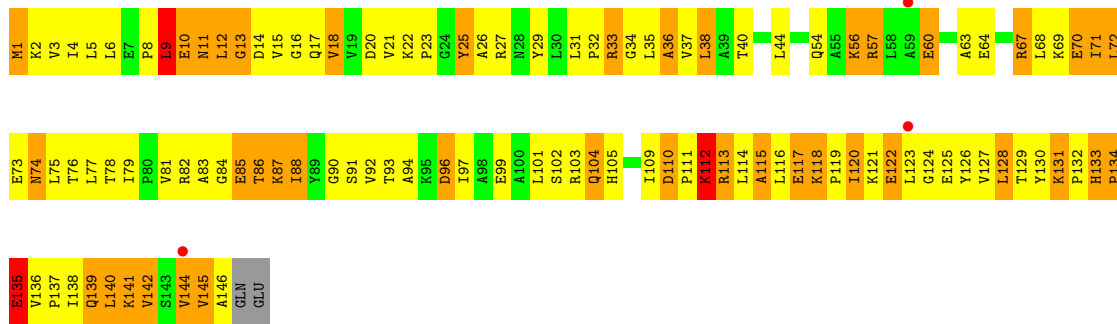
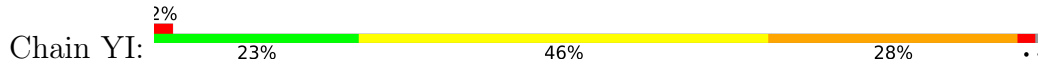


• Molecule 32: 50S ribosomal protein L9

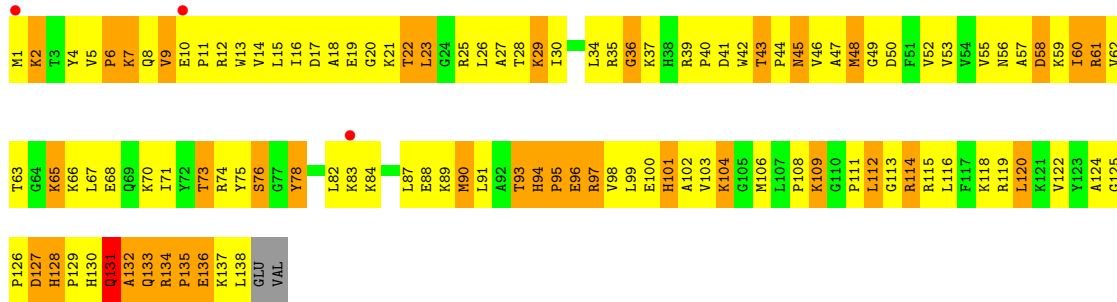
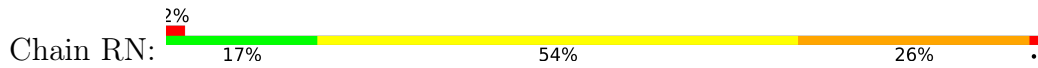




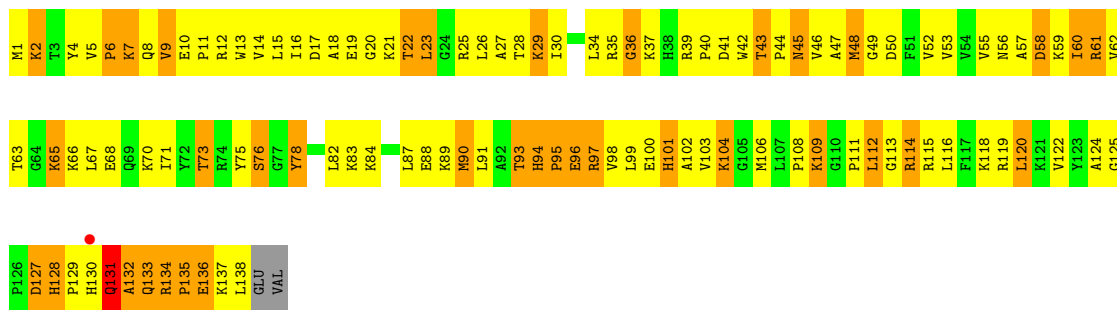
• Molecule 32: 50S ribosomal protein L9



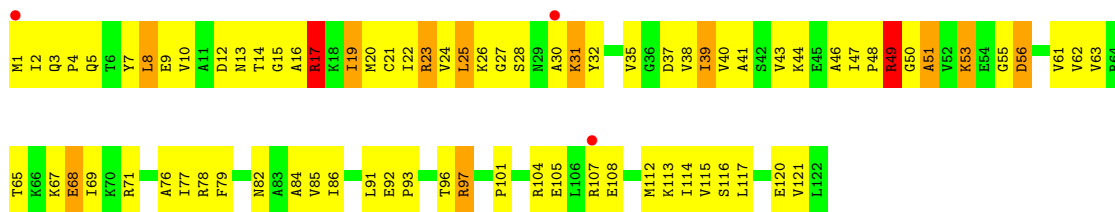
• Molecule 33: 50S ribosomal protein L13



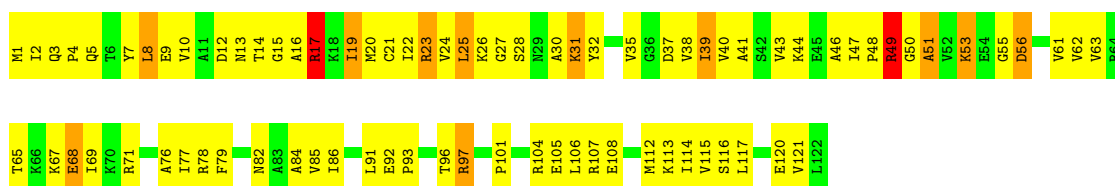
• Molecule 33: 50S ribosomal protein L13



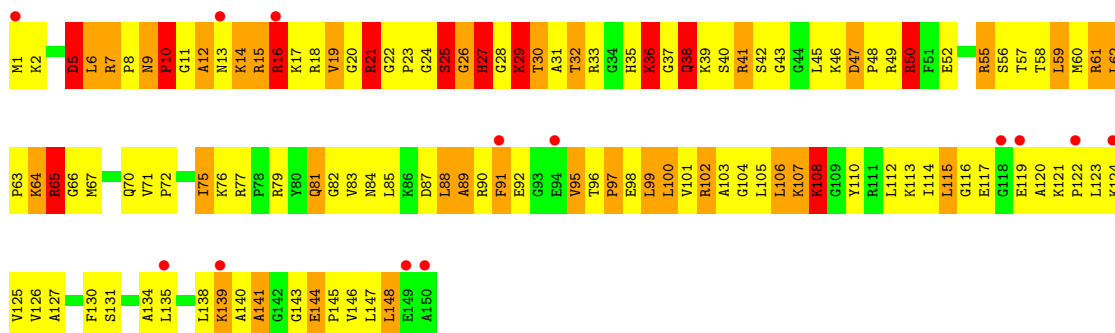
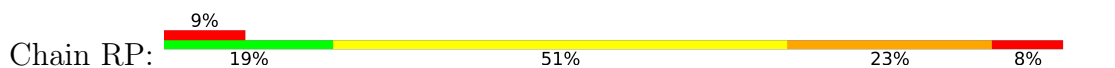
• Molecule 34: 50S ribosomal protein L14



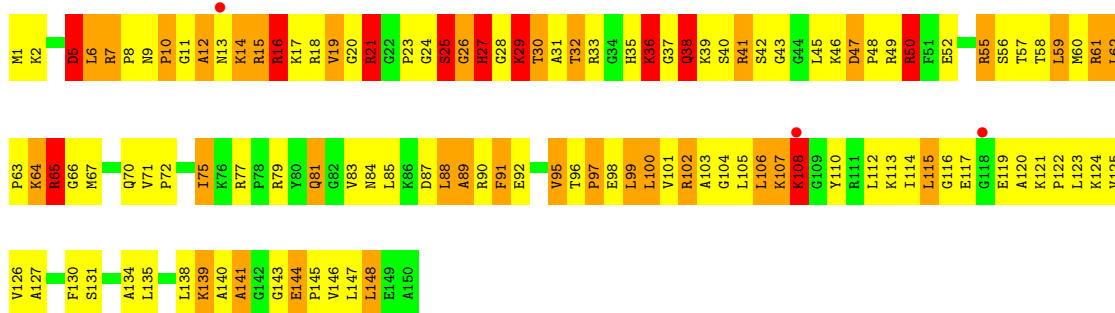
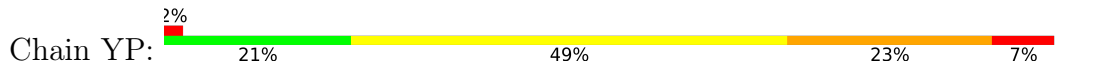
• Molecule 34: 50S ribosomal protein L14



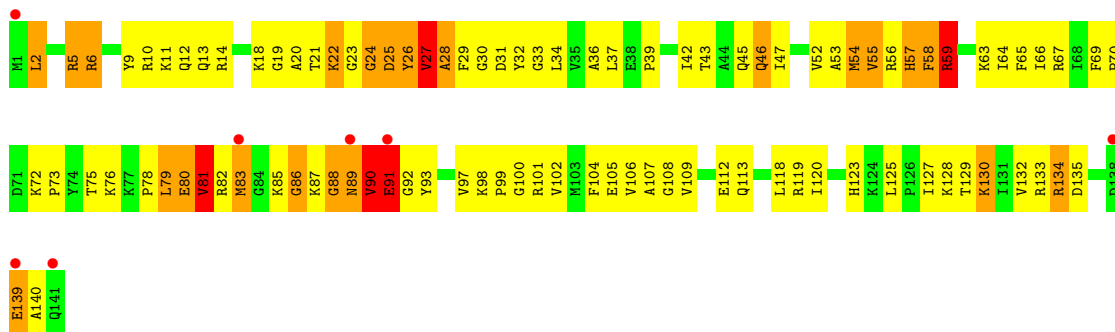
• Molecule 35: 50S ribosomal protein L15



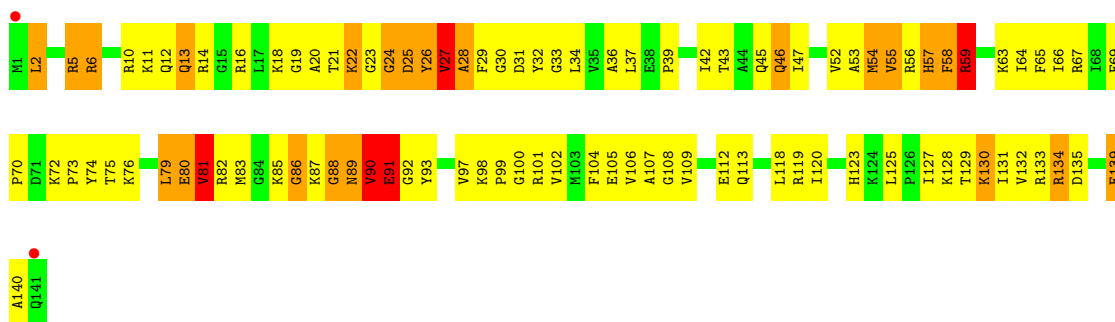
• Molecule 35: 50S ribosomal protein L15



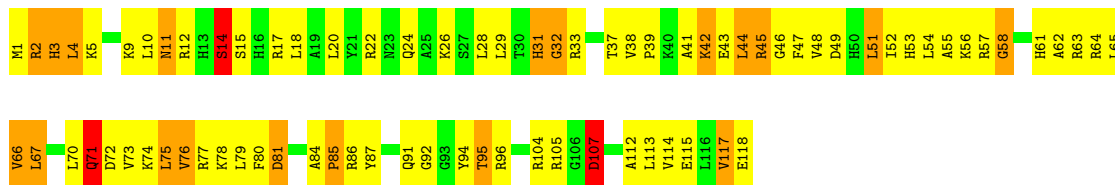
• Molecule 36: 50S ribosomal protein L16



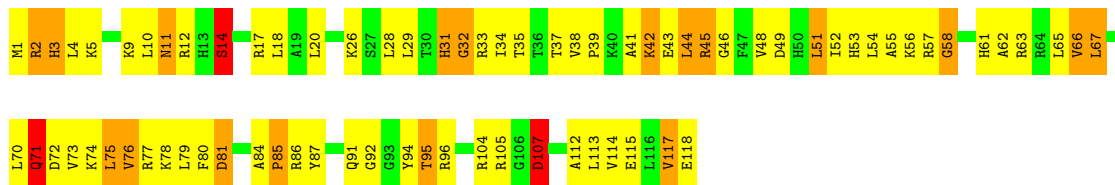
• Molecule 36: 50S ribosomal protein L16



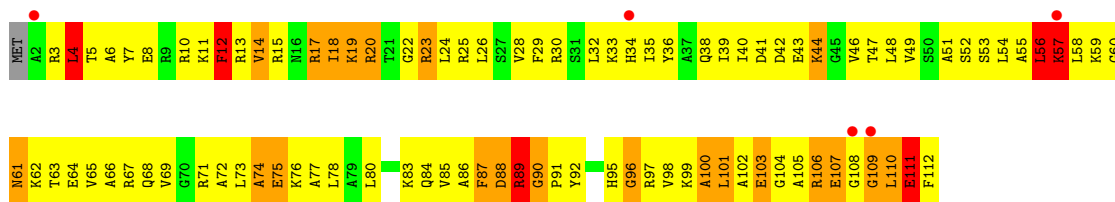
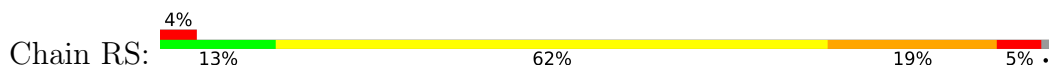
• Molecule 37: 50S ribosomal protein L17



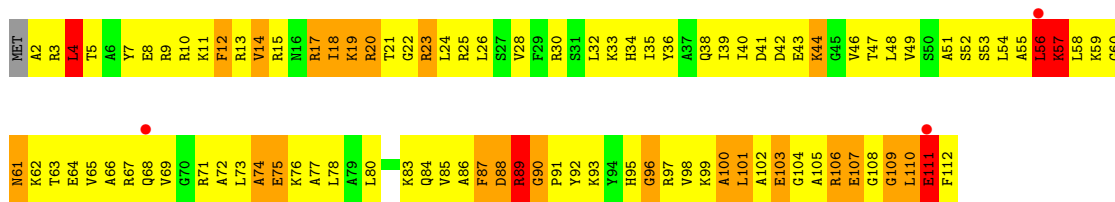
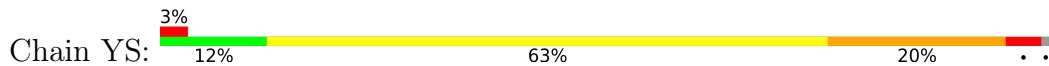
• Molecule 37: 50S ribosomal protein L17



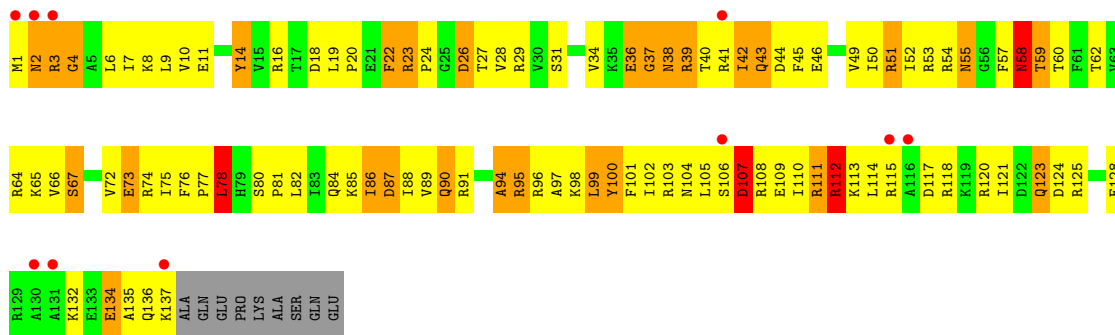
• Molecule 38: 50S ribosomal protein L18



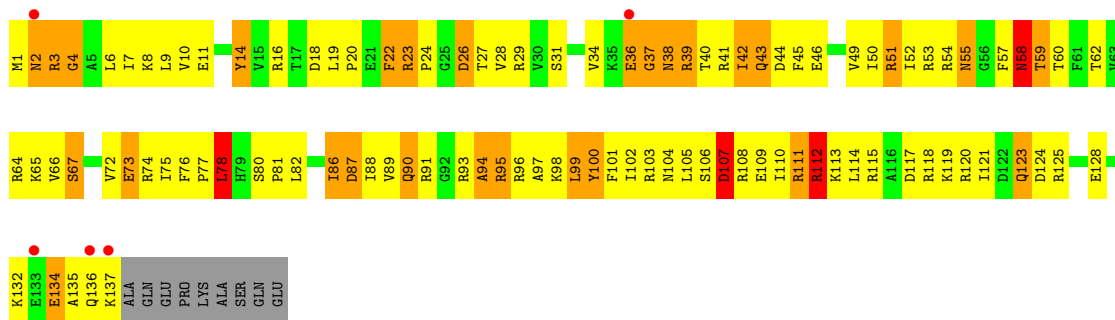
• Molecule 38: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L19

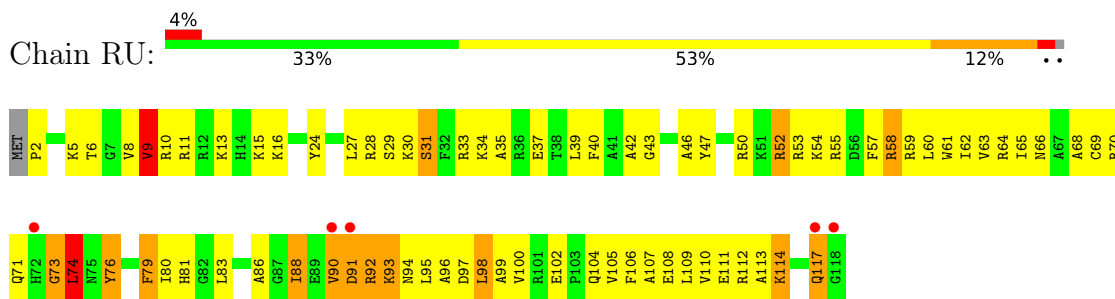


• Molecule 39: 50S ribosomal protein L19

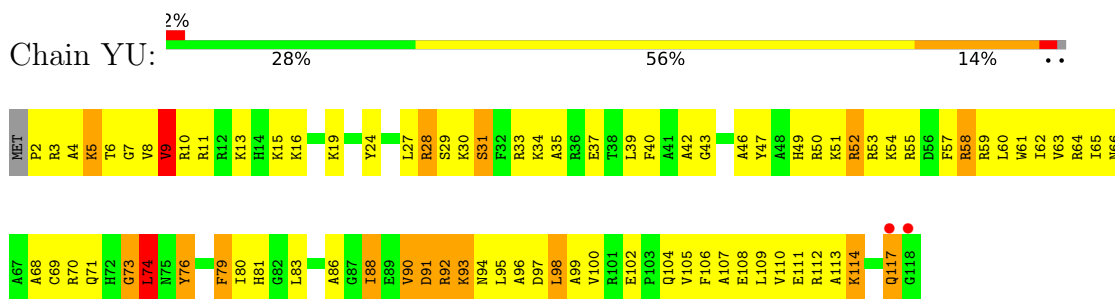


• Molecule 40: 50S ribosomal protein L20

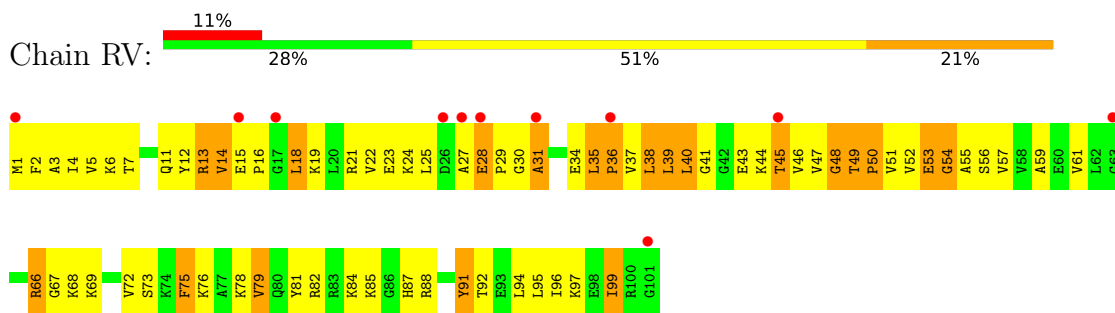




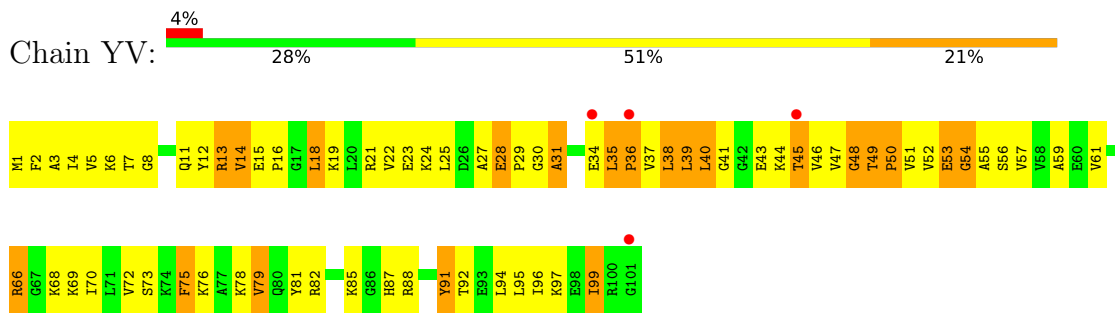
• Molecule 40: 50S ribosomal protein L20



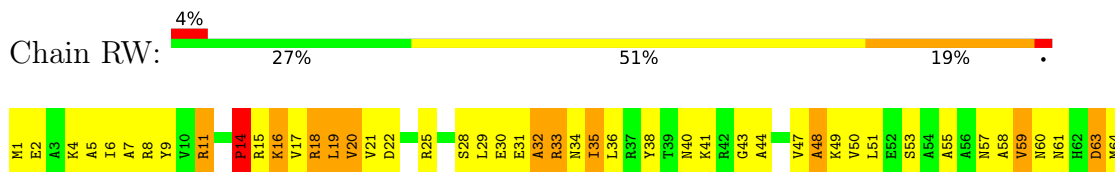
• Molecule 41: 50S ribosomal protein L21

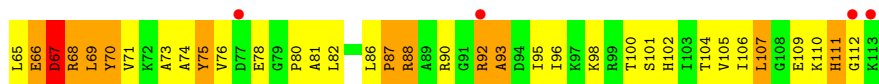


• Molecule 41: 50S ribosomal protein L21

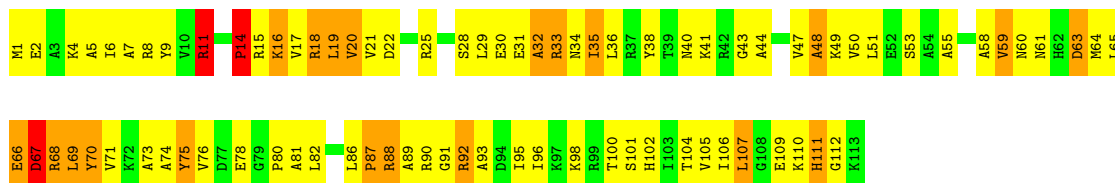


• Molecule 42: 50S ribosomal protein L22

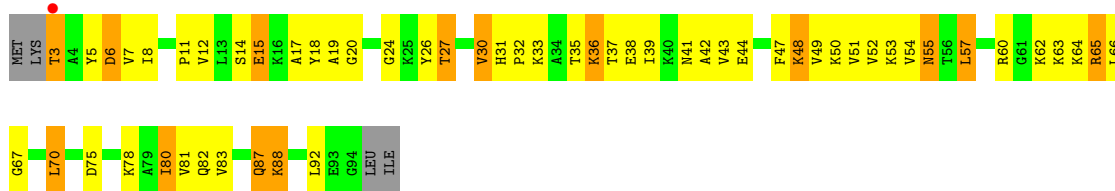




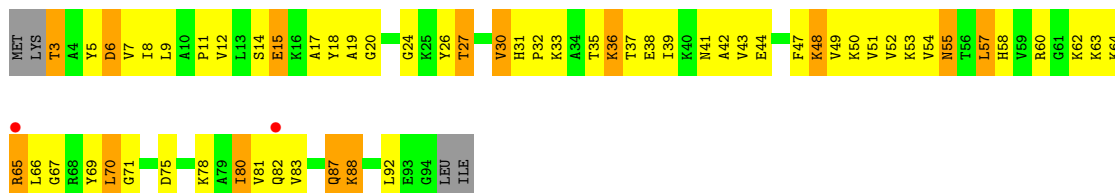
• Molecule 42: 50S ribosomal protein L22



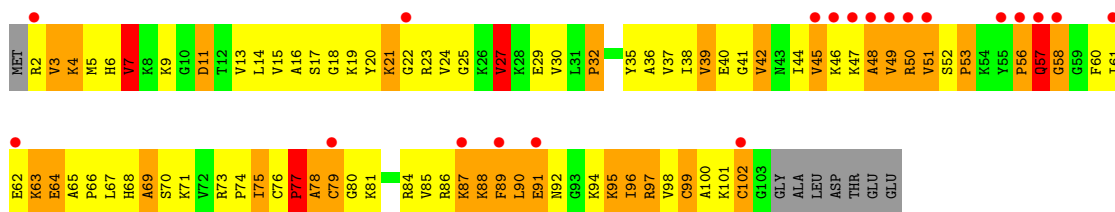
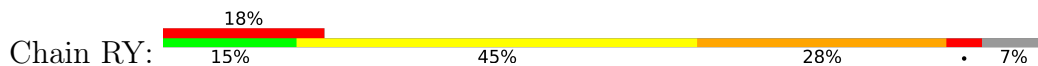
• Molecule 43: 50S ribosomal protein L23



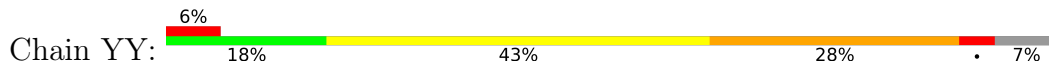
• Molecule 43: 50S ribosomal protein L23

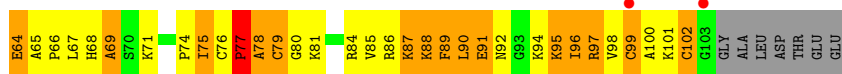


• Molecule 44: 50S ribosomal protein L24

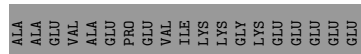
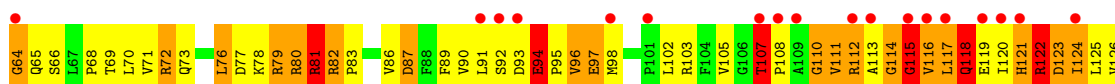
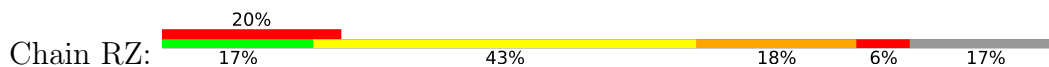


• Molecule 44: 50S ribosomal protein L24

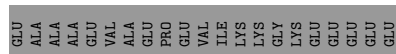
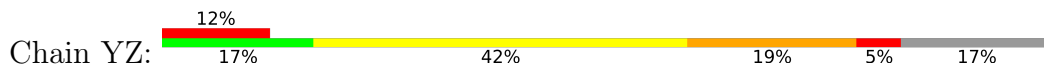




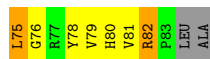
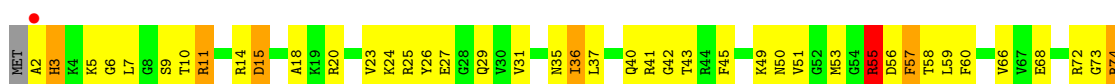
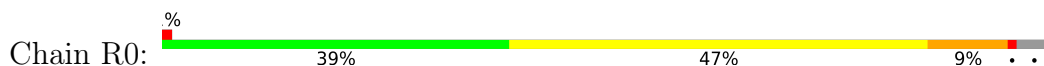
• Molecule 45: 50S ribosomal protein L25



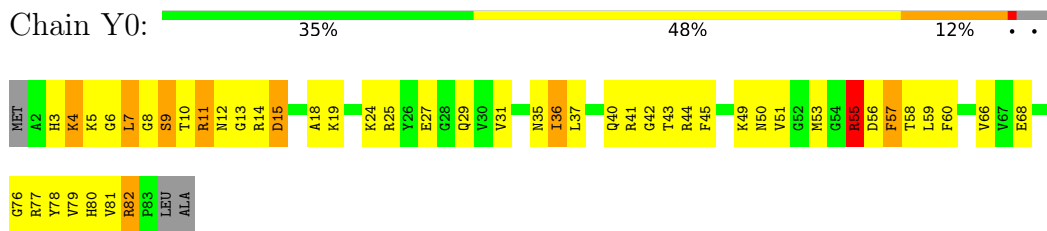
• Molecule 45: 50S ribosomal protein L25



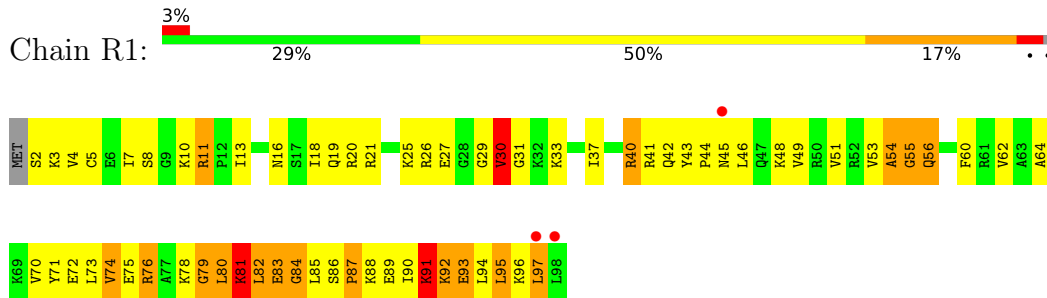
• Molecule 46: 50S ribosomal protein L27



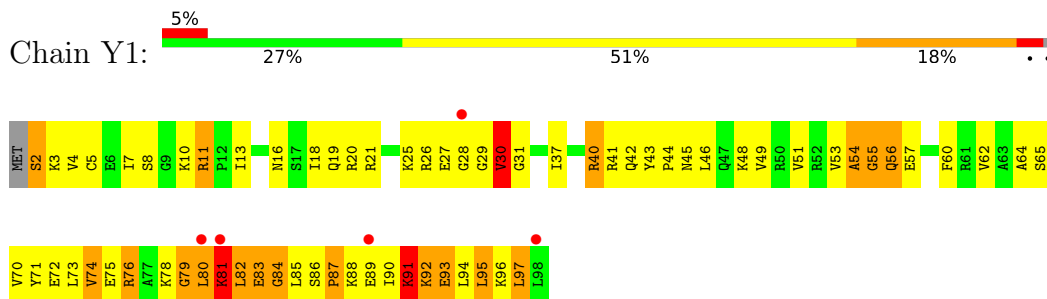
- Molecule 46: 50S ribosomal protein L27



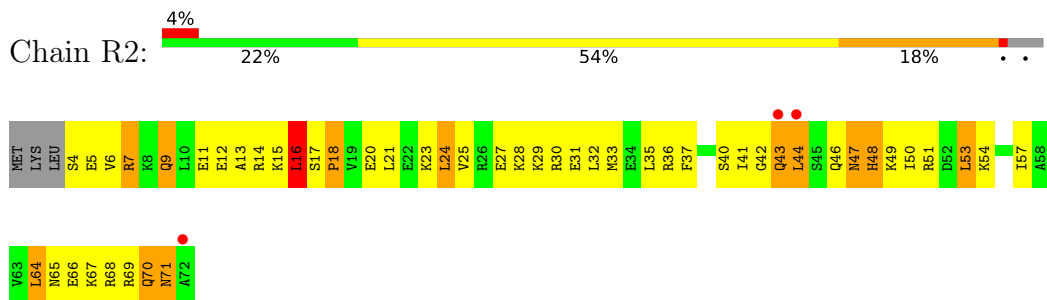
- Molecule 47: 50S ribosomal protein L28



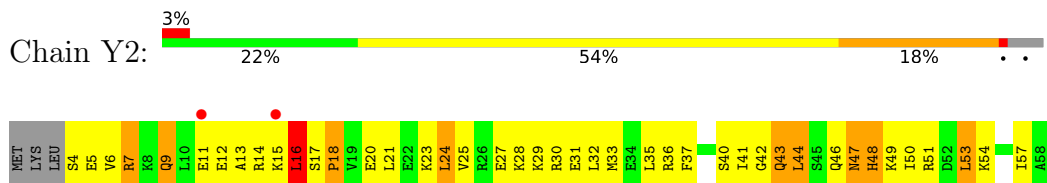
- Molecule 47: 50S ribosomal protein L28

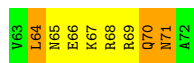


- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

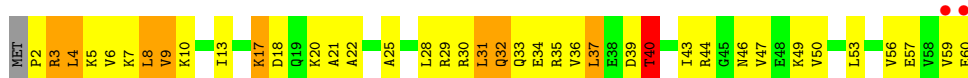




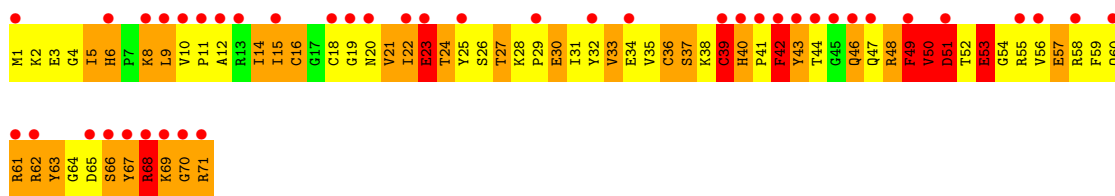
• Molecule 49: 50S ribosomal protein L30



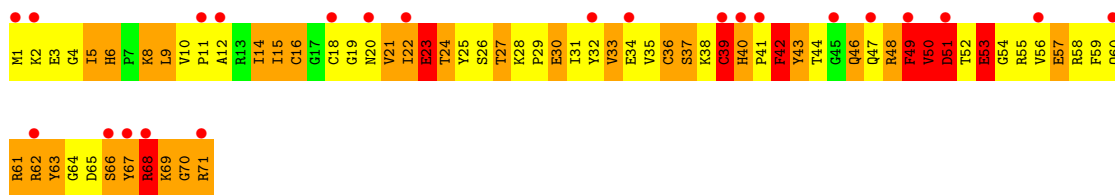
• Molecule 49: 50S ribosomal protein L30



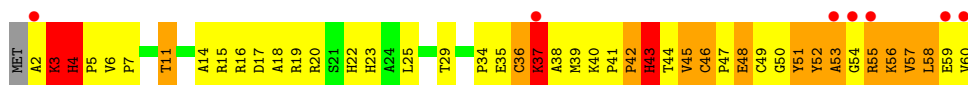
• Molecule 50: 50S ribosomal protein L32



• Molecule 50: 50S ribosomal protein L32

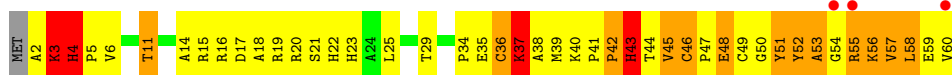


• Molecule 51: 50S ribosomal protein L33

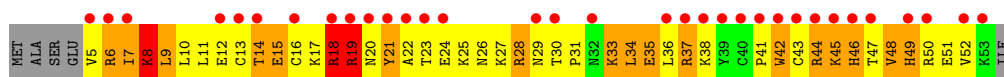


• Molecule 51: 50S ribosomal protein L33

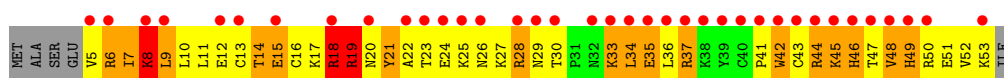




- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34



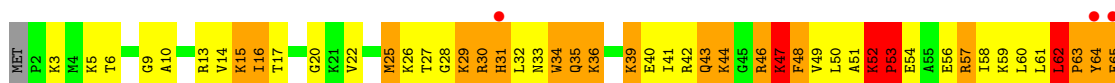
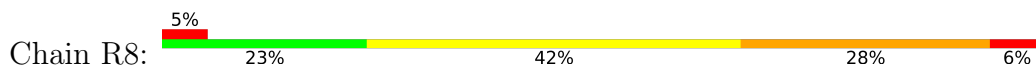
- Molecule 53: 50S ribosomal protein L35



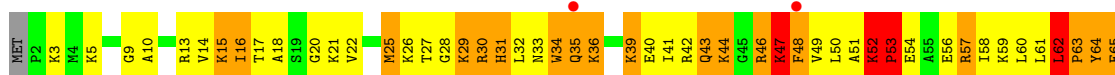
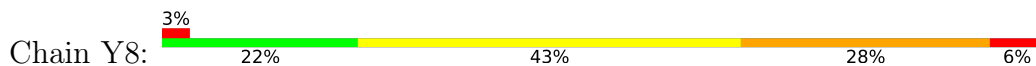
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: tRNA acceptor end mimic



- Molecule 54: tRNA acceptor end mimic



- Molecule 55: RNA (5'-R(\*CP\*CP\*(PPU))-3')





- Molecule 55: RNA (5'-R(\*CP\*CP\*(PPU))-3')

Chain Z8:  33% 33% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.55Å 449.21Å 619.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.81 – 3.44 34.81 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.81-3.44) 98.2 (34.81-3.26)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.243 , 0.285 0.243 , 0.284	Depositor DCC
$R_{free}$ test set	40944 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	291123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, 1MG, PPU, MG, 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	0.42	0/36098	0.97	58/56341 (0.1%)
1	XA	0.45	0/36123	1.00	71/56380 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.42	0/1733	0.69	1/2318 (0.0%)
4	XD	0.42	0/1733	0.70	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	0.60	0/1709
7	XG	0.37	0/1276	0.61	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	0.35	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	0.45	0/991	1.00	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.43	0/501	0.70	1/664 (0.2%)
14	XN	0.43	0/501	0.70	1/664 (0.2%)
15	QO	0.39	0/745	0.66	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.37	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	0.38	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	0.73	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	0.34	0/765	0.69	0/1007
20	XT	0.33	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.62	0/288
22	QV	0.52	0/1836	0.99	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.40	0/189	0.75	0/292
23	XX	0.66	0/189	1.09	2/292 (0.7%)
24	QY	0.51	0/311	0.88	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	0.52	2/69543 (0.0%)	1.06	149/108563 (0.1%)
25	YA	0.59	2/69521 (0.0%)	1.10	200/108529 (0.2%)
26	RB	0.44	0/2878	1.04	7/4490 (0.2%)
26	YB	0.46	0/2878	1.03	2/4490 (0.0%)
27	RD	0.62	2/2165 (0.1%)	0.90	3/2919 (0.1%)
27	YD	0.62	2/2165 (0.1%)	0.90	3/2919 (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	4/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.40	0/1151	0.80	1/1558 (0.1%)
32	YI	0.40	0/1151	0.79	1/1558 (0.1%)
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	0.53	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	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.53	0/1143	0.89	3/1527 (0.2%)
36	YQ	0.53	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	0.78	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.47	0/1408	0.77	1/1908 (0.1%)
45	YZ	0.47	0/1408	0.77	1/1908 (0.1%)
46	R0	0.57	0/657	0.80	0/874
46	Y0	0.60	0/657	0.85	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	0.50	0/583	0.84	1/771 (0.1%)
49	R3	0.43	0/474	0.71	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	0.51	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	Z6	0.82	0/40	1.81	1/60 (1.7%)
55	Z8	0.80	0/40	1.80	1/60 (1.7%)
All	All	0.50	8/315563 (0.0%)	0.98	571/471909 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	236	GLY	C-N	8.59	1.53	1.34
27	RD	236	GLY	C-N	8.55	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	YD	239	ARG	CA-C	-6.77	1.35	1.52
27	RD	239	ARG	CA-C	-6.76	1.35	1.52
25	YA	783	A	N7-C5	-5.95	1.35	1.39

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	47	LYS	C-N-CD	-20.50	75.51	120.60
12	XL	47	LYS	C-N-CD	-20.46	75.58	120.60
25	YA	761	A	N1-C6-N6	12.76	126.25	118.60
25	YA	945	A	N9-C1'-C2'	12.75	130.58	114.00
22	QV	17	C	C2-N1-C1'	11.85	131.84	118.80

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	16275	828	0
1	XA	32269	0	16289	816	0
2	QB	1924	0	1975	291	0
2	XB	1924	0	1975	301	0
3	QC	1605	0	1668	208	0
3	XC	1605	0	1668	209	1
4	QD	1703	0	1762	240	0
4	XD	1703	0	1763	215	0
5	QE	1155	0	1213	147	0
5	XE	1155	0	1213	142	0
6	QF	843	0	857	93	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	149	0
7	XG	1257	0	1296	147	0
8	QH	1116	0	1176	155	0
8	XH	1116	0	1177	164	0
9	QI	1010	0	1037	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	XI	1010	0	1037	160	0
10	QJ	801	0	849	138	0
10	XJ	801	0	849	136	0
11	QK	885	0	904	108	1
11	XK	885	0	904	118	0
12	QL	975	0	1062	109	0
12	XL	975	0	1062	113	0
13	QM	964	0	1034	171	0
13	XM	964	0	1034	180	0
14	QN	492	0	531	89	0
14	XN	492	0	529	87	0
15	QO	734	0	771	75	0
15	XO	734	0	771	74	0
16	QP	705	0	725	114	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	82	0
18	QR	574	0	644	68	0
18	XR	574	0	644	67	0
19	QS	674	0	699	104	0
19	XS	674	0	699	143	0
20	QT	763	0	860	108	0
20	XT	763	0	861	102	0
21	QU	217	0	234	30	0
21	XU	217	0	234	29	0
22	QV	1644	0	836	41	0
22	XV	1644	0	836	40	0
23	QX	170	0	87	16	0
23	XX	170	0	88	10	0
24	QY	303	0	154	13	0
24	XY	303	0	154	17	0
25	RA	62091	0	31301	1401	0
25	YA	62071	0	31286	1351	0
26	RB	2573	0	1306	70	0
26	YB	2573	0	1306	61	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	350	0
28	RE	1568	0	1634	277	0
28	YE	1568	0	1634	266	0
29	RF	1585	0	1632	174	0
29	YF	1585	0	1632	182	0
30	RG	1474	0	1535	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	YG	1474	0	1535	206	0
31	RH	1307	0	1382	217	0
31	YH	1307	0	1382	219	1
32	RI	1136	0	1223	179	0
32	YI	1136	0	1223	176	0
33	RN	1104	0	1180	194	0
33	YN	1104	0	1180	186	0
34	RO	933	0	996	123	0
34	YO	933	0	996	124	0
35	RP	1145	0	1228	248	0
35	YP	1145	0	1228	247	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	168	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	112	0
38	RS	882	0	943	158	0
38	YS	882	0	943	163	0
39	RT	1141	0	1202	152	0
39	YT	1141	0	1202	156	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	138	0
41	RV	779	0	852	132	0
41	YV	779	0	852	130	1
42	RW	900	0	964	101	0
42	YW	900	0	964	108	0
43	RX	725	0	778	68	0
43	YX	725	0	778	82	0
44	RY	785	0	878	163	0
44	YY	785	0	878	154	1
45	RZ	1378	0	1407	227	0
45	YZ	1378	0	1407	227	0
46	R0	648	0	672	88	0
46	Y0	648	0	672	85	0
47	R1	763	0	848	141	0
47	Y1	763	0	848	145	0
48	R2	581	0	629	80	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	40	0
49	Y3	469	0	518	41	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	180	0
51	R5	459	0	480	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Y5	459	0	480	75	1
52	R6	424	0	450	93	0
52	Y6	424	0	450	90	0
53	R7	430	0	480	47	0
53	Y7	430	0	480	42	0
54	R8	517	0	582	106	0
54	Y8	517	0	582	100	0
55	Z6	74	0	51	10	0
55	Z8	74	0	51	4	0
56	QA	60	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	2	0	0	0	0
56	QX	2	0	0	0	0
56	R5	1	0	0	0	0
56	RA	212	0	0	0	0
56	RB	2	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RP	1	0	0	0	0
56	XA	63	0	0	0	0
56	XM	2	0	0	0	0
56	XV	2	0	0	0	0
56	Y5	1	0	0	0	0
56	YA	242	0	0	0	0
56	YB	2	0	0	0	0
56	YE	2	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	4	0
57	XA	42	0	45	1	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
All	All	291123	0	197505	16608	3

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 34.

The worst 5 of 16608 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:QN:39:LEU:HD22	14:QN:43:CYS:SG	1.33	1.63
36:YQ:81:VAL:HG23	46:Y0:7:LEU:CD2	1.21	1.60
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.54
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.35	1.52
19:QS:5:LEU:HD22	50:R4:67:TYR:CE2	1.45	1.51

All (3) 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]	1.98	0.22
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.04	0.16
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.06	0.14

## 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	4
2	XB	235/256 (92%)	152 (65%)	53 (23%)	30 (13%)	0	4
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
3	XC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	7
4	QD	206/209 (99%)	133 (65%)	51 (25%)	22 (11%)	0	6
4	XD	206/209 (99%)	133 (65%)	50 (24%)	23 (11%)	0	5
5	QE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	6
5	XE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	6
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	7
7	QG	153/156 (98%)	102 (67%)	37 (24%)	14 (9%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	0	6
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	5
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	4
10	QJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	6
10	XJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	7
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
11	XK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	9
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	5
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	5
13	QM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	1
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	1
14	QN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
14	XN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	11
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	11
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	3
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	9
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	9
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	5
19	QS	82/93 (88%)	46 (56%)	18 (22%)	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	1
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	1
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
27	RD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	10
27	YD	270/276 (98%)	204 (76%)	46 (17%)	20 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	1
29	RF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	6
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	0	6
30	RG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	5
30	YG	179/182 (98%)	120 (67%)	38 (21%)	21 (12%)	0	5
31	RH	168/180 (93%)	94 (56%)	35 (21%)	39 (23%)	0	1
31	YH	168/180 (93%)	95 (56%)	35 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	83 (58%)	33 (23%)	28 (19%)	0	1
32	YI	144/148 (97%)	85 (59%)	32 (22%)	27 (19%)	0	1
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	2
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	10
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	10
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%)	94 (68%)	30 (22%)	15 (11%)	0	5
36	YQ	139/141 (99%)	94 (68%)	30 (22%)	15 (11%)	0	5
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	4
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	2
38	YS	109/112 (97%)	63 (58%)	27 (25%)	19 (17%)	0	2
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	9
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	9
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	6
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	4
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	16
44	RY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
44	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
45	RZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
45	YZ	170/206 (82%)	91 (54%)	40 (24%)	39 (23%)	0	1
46	R0	80/85 (94%)	61 (76%)	14 (18%)	5 (6%)	1	13
46	Y0	80/85 (94%)	62 (78%)	12 (15%)	6 (8%)	1	10
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	5
48	R2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	3
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	16
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	0
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
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	13
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	13
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
All	All	11378/12054 (94%)	7461 (66%)	2359 (21%)	1558 (14%)	0	3

5 of 1558 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	24
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	24
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	31
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	31
4	QD	180/181 (99%)	164 (91%)	16 (9%)	9	36
4	XD	180/181 (99%)	164 (91%)	16 (9%)	9	36
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	42
5	XE	116/123 (94%)	108 (93%)	8 (7%)	15	47
6	QF	90/90 (100%)	77 (86%)	13 (14%)	3	17
6	XF	90/90 (100%)	77 (86%)	13 (14%)	3	17
7	QG	126/127 (99%)	115 (91%)	11 (9%)	10	37
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
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	26
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	26
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	31
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	31
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	19
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	19
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	11
13	XM	97/101 (96%)	80 (82%)	17 (18%)	2	9
14	QN	49/50 (98%)	45 (92%)	4 (8%)	11	40
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	43
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	43
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	21
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	21
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	50
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	25
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	25
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	15
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	15
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	57
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	10
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	10
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	3
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	3
29	RF	161/166 (97%)	140 (87%)	21 (13%)	4	20
29	YF	161/166 (97%)	139 (86%)	22 (14%)	3	18
30	RG	155/156 (99%)	130 (84%)	25 (16%)	2	13
30	YG	155/156 (99%)	131 (84%)	24 (16%)	2	14
31	RH	142/148 (96%)	115 (81%)	27 (19%)	1	6
31	YH	142/148 (96%)	115 (81%)	27 (19%)	1	6
32	RI	122/124 (98%)	98 (80%)	24 (20%)	1	5
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	5
33	RN	117/119 (98%)	98 (84%)	19 (16%)	2	12
33	YN	117/119 (98%)	98 (84%)	19 (16%)	2	12
34	RO	100/100 (100%)	90 (90%)	10 (10%)	7	31
34	YO	100/100 (100%)	90 (90%)	10 (10%)	7	31
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	3
36	RQ	111/111 (100%)	92 (83%)	19 (17%)	2	10
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	10
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	11
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	11
38	RS	87/88 (99%)	74 (85%)	13 (15%)	3	16
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	16
39	RT	120/127 (94%)	97 (81%)	23 (19%)	1	6
39	YT	120/127 (94%)	97 (81%)	23 (19%)	1	6
40	RU	93/94 (99%)	80 (86%)	13 (14%)	3	17
40	YU	93/94 (99%)	80 (86%)	13 (14%)	3	17
41	RV	82/82 (100%)	71 (87%)	11 (13%)	4	19
41	YV	82/82 (100%)	71 (87%)	11 (13%)	4	19
42	RW	92/92 (100%)	77 (84%)	15 (16%)	2	12
42	YW	92/92 (100%)	77 (84%)	15 (16%)	2	12
43	RX	74/78 (95%)	63 (85%)	11 (15%)	3	16
43	YX	74/78 (95%)	63 (85%)	11 (15%)	3	16
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	9
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	9
45	RZ	152/179 (85%)	124 (82%)	28 (18%)	1	7
45	YZ	152/179 (85%)	124 (82%)	28 (18%)	1	7
46	R0	65/67 (97%)	55 (85%)	10 (15%)	2	14
46	Y0	65/67 (97%)	56 (86%)	9 (14%)	3	18
47	R1	82/83 (99%)	67 (82%)	15 (18%)	1	7
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	7
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	4
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	4
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	3
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	5
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	R7	42/42 (100%)	39 (93%)	3 (7%)	14	46
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	46
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	2
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	2
All	All	9614/9998 (96%)	8197 (85%)	1417 (15%)	3	16

5 of 1417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	YD	43	ARG
35	YP	99	LEU
27	YD	237	GLU
27	YD	33	LEU
30	YG	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
5	XE	72	GLN
27	YD	44	ASN
46	Y0	3	HIS
6	XF	64	GLN
11	XK	117	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	343 (22%)	51 (3%)
1	XA	1499/1522 (98%)	333 (22%)	55 (3%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	6 (85%)	1 (14%)
23	XX	7/25 (28%)	2 (28%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	QY	13/18 (72%)	6 (46%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2880/2916 (98%)	734 (25%)	76 (2%)
25	YA	2879/2916 (98%)	747 (25%)	75 (2%)
26	RB	119/122 (97%)	30 (25%)	2 (1%)
26	YB	119/122 (97%)	38 (31%)	1 (0%)
55	Z6	1/3 (33%)	0	0
55	Z8	1/3 (33%)	0	0
All	All	9189/9366 (98%)	2304 (25%)	265 (2%)

5 of 2304 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	9	G
1	QA	32	A
1	QA	39	G

5 of 265 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	1653	G
25	YA	1929	G
25	YA	2832	U
25	RA	1379	A
25	RA	1266	G

## 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
55	PPU	Z6	76	55,25	32,40,41	2.55	6 (18%)	33,57,60	2.14	5 (15%)
55	PPU	Z8	76	55,25	32,40,41	2.54	6 (18%)	33,57,60	2.14	5 (15%)
24	1MG	XY	37	24	18,26,27	2.28	2 (11%)	19,39,42	1.58	2 (10%)
24	1MG	QY	37	24	18,26,27	2.31	2 (11%)	19,39,42	1.53	3 (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
55	PPU	Z6	76	55,25	-	2/21/43/44	0/4/4/4
55	PPU	Z8	76	55,25	-	2/21/43/44	0/4/4/4
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Z6	76	PPU	O-C	9.21	1.41	1.23
55	Z8	76	PPU	O-C	9.21	1.41	1.23
24	QY	37	1MG	C2-N2	7.88	1.48	1.34
24	XY	37	1MG	C2-N2	7.84	1.48	1.34
55	Z6	76	PPU	C9-N6	-5.95	1.32	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Z8	76	PPU	C3'-N3'-C	-8.58	110.27	123.21
55	Z6	76	PPU	C3'-N3'-C	-8.58	110.28	123.21
55	Z6	76	PPU	N3-C2-N1	-4.69	121.35	128.68
55	Z8	76	PPU	N3-C2-N1	-4.67	121.38	128.68
24	XY	37	1MG	C8-N7-C5	4.22	111.03	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Z6	76	PPU	10	0
55	Z8	76	PPU	4	0
24	XY	37	IMG	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 607 ligands modelled in this entry, 605 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
57	PAR	QA	1661	-	45,45,45	1.43	7 (15%)	64,67,67	1.36	8 (12%)
57	PAR	XA	1664	-	45,45,45	1.46	7 (15%)	64,67,67	1.33	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	QA	1661	-	-	7/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	XA	1664	-	-	4/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1661	PAR	C64-C54	4.85	1.58	1.52
57	XA	1664	PAR	C64-C54	4.83	1.58	1.52
57	XA	1664	PAR	C52-C42	3.02	1.58	1.52
57	XA	1664	PAR	C11-C21	2.98	1.58	1.52
57	QA	1661	PAR	C52-C42	2.97	1.58	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	XA	1664	PAR	O33-C14-C24	4.33	115.67	108.22
57	QA	1661	PAR	C14-O54-C54	4.20	121.94	113.69
57	XA	1664	PAR	C14-O54-C54	4.06	121.65	113.69
57	QA	1661	PAR	O33-C14-C24	3.79	114.74	108.22
57	QA	1661	PAR	O52-C13-C23	3.79	115.81	107.96

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1661	PAR	C44-C54-C64-N64
57	QA	1661	PAR	O54-C54-C64-N64
57	XA	1664	PAR	O51-C51-C61-O61
57	XA	1664	PAR	C41-C51-C61-O61
57	QA	1661	PAR	O51-C51-C61-O61

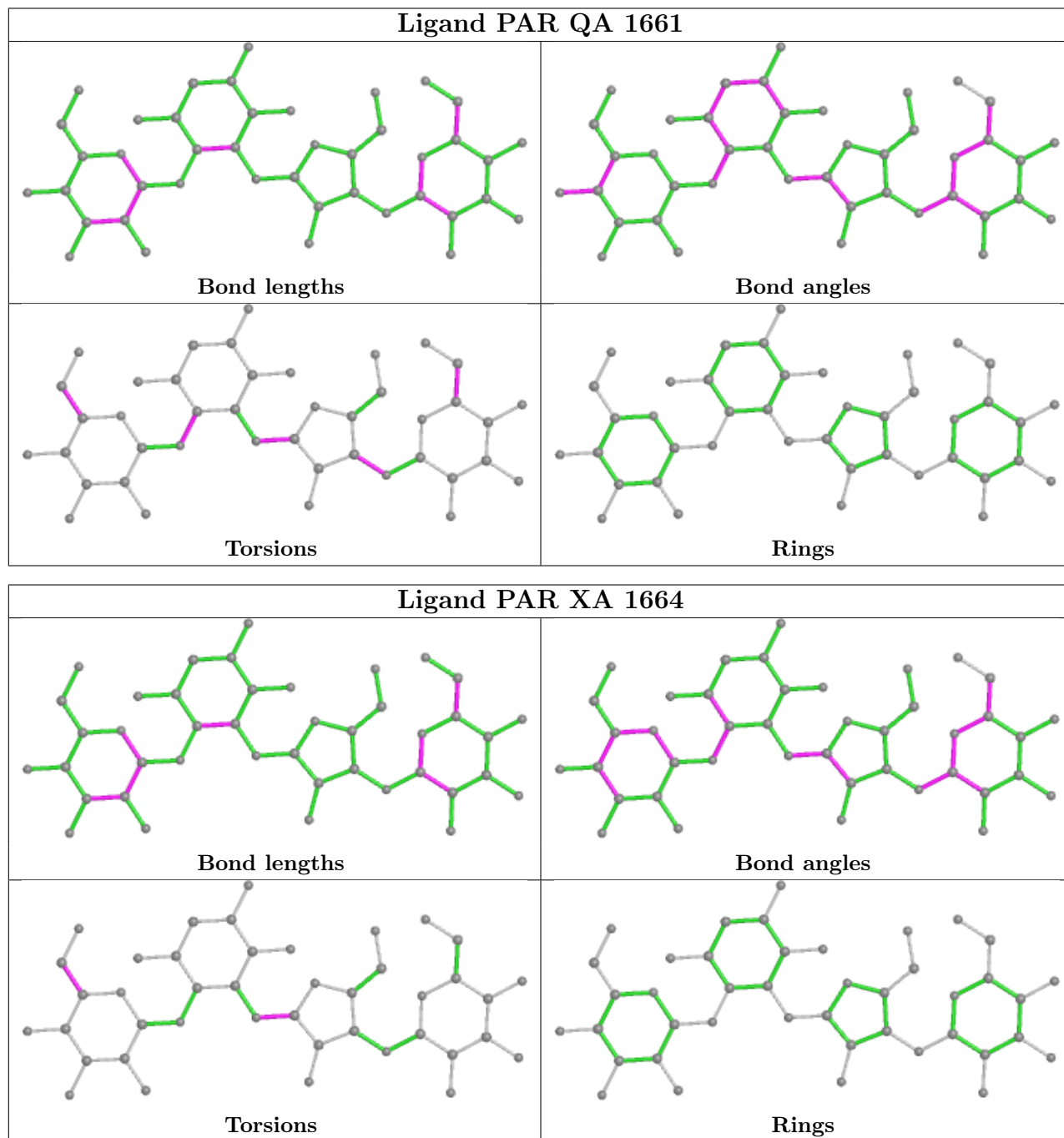
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1661	PAR	4	0
57	XA	1664	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.19	57 (3%) 40 39	30, 83, 175, 356	0
1	XA	1501/1522 (98%)	0.06	50 (3%) 46 45	30, 76, 171, 324	0
2	QB	237/256 (92%)	0.84	31 (13%) 3 5	56, 138, 222, 266	0
2	XB	237/256 (92%)	0.50	24 (10%) 7 9	55, 126, 194, 238	0
3	QC	205/239 (85%)	0.69	30 (14%) 2 3	54, 122, 199, 216	0
3	XC	205/239 (85%)	0.25	10 (4%) 29 30	39, 95, 158, 217	0
4	QD	208/209 (99%)	0.17	8 (3%) 40 39	44, 92, 154, 184	0
4	XD	208/209 (99%)	0.30	8 (3%) 40 39	39, 95, 161, 234	0
5	QE	151/162 (93%)	0.57	11 (7%) 15 17	29, 104, 175, 237	0
5	XE	151/162 (93%)	0.12	4 (2%) 56 54	34, 79, 149, 229	0
6	QF	101/101 (100%)	0.11	3 (2%) 50 48	44, 86, 125, 222	0
6	XF	101/101 (100%)	0.10	3 (2%) 50 48	36, 86, 144, 209	0
7	QG	155/156 (99%)	0.50	15 (9%) 7 10	51, 106, 181, 215	0
7	XG	155/156 (99%)	0.28	9 (5%) 23 24	46, 103, 177, 230	0
8	QH	138/138 (100%)	0.25	3 (2%) 62 60	48, 108, 167, 204	0
8	XH	138/138 (100%)	0.18	4 (2%) 51 50	48, 96, 158, 208	0
9	QI	127/128 (99%)	0.69	14 (11%) 5 8	53, 124, 188, 214	0
9	XI	127/128 (99%)	0.55	8 (6%) 20 21	43, 116, 194, 219	0
10	QJ	99/105 (94%)	1.30	24 (24%) 0 1	67, 145, 212, 246	0
10	XJ	99/105 (94%)	0.90	20 (20%) 1 1	37, 119, 193, 210	0
11	QK	119/129 (92%)	0.52	10 (8%) 11 14	42, 92, 152, 199	0
11	XK	119/129 (92%)	0.31	5 (4%) 36 35	39, 89, 165, 204	0
12	QL	125/132 (94%)	0.39	6 (4%) 30 31	42, 84, 176, 269	0
12	XL	125/132 (94%)	0.08	4 (3%) 47 46	30, 66, 131, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.53	11 (9%) 9 11	43, 124, 197, 254	0
13	XM	121/126 (96%)	0.24	5 (4%) 37 36	44, 98, 183, 264	0
14	QN	60/61 (98%)	1.05	9 (15%) 2 3	61, 128, 195, 227	0
14	XN	60/61 (98%)	0.09	1 (1%) 70 68	47, 87, 134, 161	0
15	QO	88/89 (98%)	0.44	7 (7%) 12 15	42, 97, 165, 235	0
15	XO	88/89 (98%)	-0.07	1 (1%) 80 77	39, 79, 130, 178	0
16	QP	84/88 (95%)	0.28	1 (1%) 79 76	41, 79, 136, 206	0
16	XP	84/88 (95%)	0.38	3 (3%) 42 42	54, 92, 151, 203	0
17	QQ	100/105 (95%)	0.27	2 (2%) 65 63	53, 102, 165, 210	0
17	XQ	100/105 (95%)	0.42	6 (6%) 21 23	38, 101, 159, 213	0
18	QR	70/88 (79%)	0.12	3 (4%) 35 34	34, 90, 156, 213	0
18	XR	70/88 (79%)	0.10	2 (2%) 51 50	30, 88, 138, 206	0
19	QS	84/93 (90%)	1.23	18 (21%) 0 1	87, 149, 204, 237	0
19	XS	84/93 (90%)	0.56	6 (7%) 16 18	55, 105, 176, 244	0
20	QT	99/106 (93%)	0.53	9 (9%) 9 11	48, 101, 192, 233	0
20	XT	99/106 (93%)	0.25	6 (6%) 21 23	50, 107, 163, 197	0
21	QU	25/27 (92%)	1.03	3 (12%) 4 6	41, 100, 139, 189	0
21	XU	25/27 (92%)	0.72	2 (8%) 12 15	52, 96, 135, 165	0
22	QV	77/77 (100%)	0.46	5 (6%) 18 20	40, 91, 151, 170	0
22	XV	77/77 (100%)	0.18	2 (2%) 56 54	34, 77, 126, 180	0
23	QX	8/25 (32%)	0.64	0 100 100	61, 82, 137, 169	0
23	XX	8/25 (32%)	0.65	1 (12%) 3 6	39, 67, 104, 175	0
24	QY	13/18 (72%)	4.04	8 (61%) 0 0	93, 213, 294, 312	0
24	XY	13/18 (72%)	2.83	6 (46%) 0 0	69, 188, 276, 278	0
25	RA	2883/2916 (98%)	0.12	174 (6%) 21 23	24, 57, 221, 389	0
25	YA	2882/2916 (98%)	-0.00	158 (5%) 25 26	17, 48, 215, 377	0
26	RB	120/122 (98%)	0.11	2 (1%) 70 68	52, 91, 141, 150	0
26	YB	120/122 (98%)	-0.12	0 100 100	44, 74, 109, 158	0
27	RD	272/276 (98%)	0.06	2 (0%) 87 85	19, 60, 98, 243	0
27	YD	272/276 (98%)	-0.12	1 (0%) 92 91	13, 50, 85, 221	0
28	RE	205/206 (99%)	0.16	5 (2%) 59 57	24, 78, 165, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	0.19	6 (2%) 51 50	22, 76, 161, 238	0
29	RF	202/210 (96%)	0.21	7 (3%) 44 43	21, 82, 158, 250	0
29	YF	202/210 (96%)	0.04	4 (1%) 65 63	13, 64, 130, 197	0
30	RG	181/182 (99%)	1.89	74 (40%) 0 0	58, 164, 258, 303	0
30	YG	181/182 (99%)	0.90	26 (14%) 2 4	59, 108, 186, 248	0
31	RH	170/180 (94%)	1.29	37 (21%) 0 1	78, 171, 239, 267	0
31	YH	170/180 (94%)	0.46	10 (5%) 22 24	39, 100, 156, 260	0
32	RI	146/148 (98%)	0.66	16 (10%) 5 8	56, 118, 204, 240	0
32	YI	146/148 (98%)	0.24	3 (2%) 63 62	40, 104, 169, 214	0
33	RN	138/140 (98%)	0.08	3 (2%) 62 60	32, 84, 153, 194	0
33	YN	138/140 (98%)	-0.06	1 (0%) 87 85	31, 78, 128, 166	0
34	RO	122/122 (100%)	0.04	3 (2%) 57 55	24, 71, 133, 170	0
34	YO	122/122 (100%)	0.08	0 100 100	23, 66, 114, 153	0
35	RP	150/150 (100%)	0.35	13 (8%) 10 13	15, 79, 185, 232	0
35	YP	150/150 (100%)	0.12	3 (2%) 65 63	5, 68, 135, 230	0
36	RQ	141/141 (100%)	0.31	7 (4%) 28 29	38, 85, 149, 219	0
36	YQ	141/141 (100%)	0.02	2 (1%) 75 72	27, 66, 118, 196	0
37	RR	118/118 (100%)	-0.09	0 100 100	28, 68, 107, 171	0
37	YR	118/118 (100%)	-0.08	0 100 100	20, 64, 114, 153	0
38	RS	111/112 (99%)	0.26	5 (4%) 33 32	40, 90, 146, 203	0
38	YS	111/112 (99%)	0.07	3 (2%) 54 52	36, 77, 134, 207	0
39	RT	137/146 (93%)	0.31	10 (7%) 15 17	39, 90, 189, 221	0
39	YT	137/146 (93%)	0.27	5 (3%) 42 42	41, 78, 176, 220	0
40	RU	117/118 (99%)	0.14	5 (4%) 35 34	27, 73, 155, 249	0
40	YU	117/118 (99%)	-0.05	2 (1%) 70 68	20, 59, 129, 212	0
41	RV	101/101 (100%)	0.46	11 (10%) 5 8	28, 88, 167, 278	0
41	YV	101/101 (100%)	0.16	4 (3%) 38 37	25, 82, 143, 255	0
42	RW	113/113 (100%)	0.09	4 (3%) 44 43	28, 63, 127, 241	0
42	YW	113/113 (100%)	-0.10	0 100 100	22, 60, 109, 204	0
43	RX	92/96 (95%)	0.00	1 (1%) 80 77	31, 65, 108, 137	0
43	YX	92/96 (95%)	0.12	2 (2%) 62 60	21, 50, 92, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.94	20 (19%) 1 1	46, 106, 214, 270	0
44	YY	102/110 (92%)	0.34	7 (6%) 16 19	25, 85, 144, 243	0
45	RZ	172/206 (83%)	1.50	42 (24%) 0 1	62, 130, 264, 332	0
45	YZ	172/206 (83%)	0.89	25 (14%) 2 4	33, 111, 243, 361	0
46	R0	82/85 (96%)	0.25	1 (1%) 79 76	35, 72, 104, 143	0
46	Y0	82/85 (96%)	0.03	0 100 100	28, 63, 99, 116	0
47	R1	97/98 (98%)	0.40	3 (3%) 49 48	24, 67, 167, 259	0
47	Y1	97/98 (98%)	0.27	5 (5%) 27 28	20, 65, 161, 211	0
48	R2	69/72 (95%)	0.07	3 (4%) 35 34	34, 82, 149, 217	0
48	Y2	69/72 (95%)	0.11	2 (2%) 51 50	22, 72, 138, 203	0
49	R3	59/60 (98%)	0.24	1 (1%) 70 68	35, 81, 147, 173	0
49	Y3	59/60 (98%)	0.05	2 (3%) 45 44	33, 67, 108, 178	0
50	R4	71/71 (100%)	3.14	42 (59%) 0 0	102, 207, 282, 352	0
50	Y4	71/71 (100%)	1.83	23 (32%) 0 0	88, 160, 251, 277	0
51	R5	59/60 (98%)	0.49	7 (11%) 4 6	12, 64, 224, 264	0
51	Y5	59/60 (98%)	-0.07	3 (5%) 28 28	20, 71, 220, 229	0
52	R6	49/54 (90%)	4.18	33 (67%) 0 0	119, 196, 290, 297	0
52	Y6	49/54 (90%)	3.70	37 (75%) 0 0	120, 182, 235, 265	0
53	R7	49/49 (100%)	-0.25	0 100 100	19, 44, 100, 216	0
53	Y7	49/49 (100%)	-0.06	3 (6%) 21 23	15, 37, 100, 216	0
54	R8	64/65 (98%)	0.22	3 (4%) 31 31	18, 62, 156, 228	0
54	Y8	64/65 (98%)	0.23	2 (3%) 49 48	20, 61, 116, 173	0
55	Z6	2/3 (66%)	0.38	0 100 100	49, 49, 49, 51	0
55	Z8	2/3 (66%)	0.22	0 100 100	36, 36, 36, 37	0
All	All	20776/21420 (96%)	0.27	1351 (6%) 18 20	5, 78, 194, 389	0

The worst 5 of 1351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	YA	2173	A	16.7
25	RA	2116	G	15.6
52	R6	43	CYS	15.1
25	YA	2175	C	15.0
24	QY	32	U	14.9

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	1MG	QY	37	24/25	0.83	0.24	124,124,124,124	0
24	1MG	XY	37	24/25	0.93	0.15	89,89,89,89	0
55	PPU	Z6	76	37/38	0.94	0.28	53,53,53,53	0
55	PPU	Z8	76	37/38	0.95	0.25	40,40,40,40	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	RA	3203	1/1	0.57	0.27	73,73,73,73	0
56	MG	QH	201	1/1	0.63	0.31	124,124,124,124	0
56	MG	QA	1639	1/1	0.64	0.13	44,44,44,44	0
56	MG	XA	1605	1/1	0.65	0.41	126,126,126,126	0
56	MG	QA	1615	1/1	0.67	0.76	46,46,46,46	0
56	MG	YA	3173	1/1	0.67	0.20	43,43,43,43	0
56	MG	XA	1648	1/1	0.68	0.32	25,25,25,25	0
56	MG	YA	3012	1/1	0.70	1.51	80,80,80,80	0
56	MG	RA	3176	1/1	0.71	0.53	71,71,71,71	0
56	MG	RA	3201	1/1	0.72	0.34	22,22,22,22	0
56	MG	YA	3171	1/1	0.72	0.30	72,72,72,72	0
56	MG	XM	202	1/1	0.72	0.32	43,43,43,43	0
56	MG	RA	3141	1/1	0.73	0.37	43,43,43,43	0
56	MG	YA	3236	1/1	0.74	0.24	57,57,57,57	0
56	MG	YA	3172	1/1	0.75	0.17	55,55,55,55	0
56	MG	XA	1619	1/1	0.76	0.15	46,46,46,46	0
56	MG	YA	3177	1/1	0.76	0.17	35,35,35,35	0
56	MG	RA	3173	1/1	0.76	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	ZN	QN	101	1/1	0.76	0.13	155,155,155,155	0
56	MG	RA	3202	1/1	0.77	0.41	84,84,84,84	0
56	MG	YA	3169	1/1	0.78	0.21	84,84,84,84	0
56	MG	YE	302	1/1	0.79	0.19	13,13,13,13	0
56	MG	YA	3156	1/1	0.80	0.15	33,33,33,33	0
56	MG	YA	3239	1/1	0.81	0.44	48,48,48,48	0
56	MG	YA	3120	1/1	0.81	0.23	36,36,36,36	0
56	MG	YA	3176	1/1	0.81	0.17	54,54,54,54	0
56	MG	YA	3084	1/1	0.83	0.19	23,23,23,23	0
56	MG	YA	3158	1/1	0.83	0.12	20,20,20,20	0
56	MG	YA	3105	1/1	0.83	0.22	16,16,16,16	0
56	MG	RA	3187	1/1	0.83	0.49	68,68,68,68	0
56	MG	YA	3165	1/1	0.84	0.24	42,42,42,42	0
56	MG	XA	1644	1/1	0.84	0.28	59,59,59,59	0
56	MG	XA	1647	1/1	0.84	0.52	58,58,58,58	0
56	MG	QA	1620	1/1	0.84	0.50	40,40,40,40	0
56	MG	RA	3192	1/1	0.84	0.29	56,56,56,56	0
56	MG	RA	3200	1/1	0.84	0.23	58,58,58,58	0
56	MG	RA	3096	1/1	0.84	0.16	8,8,8,8	0
56	MG	YA	3181	1/1	0.84	0.28	51,51,51,51	0
56	MG	QA	1627	1/1	0.84	0.36	57,57,57,57	0
56	MG	QA	1613	1/1	0.84	0.33	56,56,56,56	0
56	MG	YA	3240	1/1	0.84	0.14	45,45,45,45	0
56	MG	RA	3175	1/1	0.84	0.25	99,99,99,99	0
56	MG	QA	1643	1/1	0.84	0.20	24,24,24,24	0
56	MG	RA	3167	1/1	0.85	0.19	35,35,35,35	0
56	MG	YA	3116	1/1	0.85	0.20	28,28,28,28	0
56	MG	XA	1638	1/1	0.86	0.21	55,55,55,55	0
56	MG	XA	1642	1/1	0.86	0.27	49,49,49,49	0
56	MG	QA	1614	1/1	0.86	0.25	38,38,38,38	0
56	MG	YA	3133	1/1	0.86	0.73	43,43,43,43	0
56	MG	RA	3162	1/1	0.86	0.28	56,56,56,56	0
56	MG	YA	3183	1/1	0.86	0.12	36,36,36,36	0
56	MG	RA	3208	1/1	0.86	0.14	47,47,47,47	0
56	MG	YA	3164	1/1	0.86	0.30	25,25,25,25	0
56	MG	QF	201	1/1	0.86	0.17	56,56,56,56	0
56	MG	XA	1618	1/1	0.86	0.14	24,24,24,24	0
56	MG	RA	3186	1/1	0.86	0.22	90,90,90,90	0
56	MG	RA	3210	1/1	0.87	0.34	38,38,38,38	0
56	MG	YA	3207	1/1	0.87	0.30	66,66,66,66	0
56	MG	YA	3228	1/1	0.87	0.17	45,45,45,45	0
56	MG	RA	3122	1/1	0.87	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3083	1/1	0.87	0.20	26,26,26,26	0
56	MG	RA	3117	1/1	0.87	0.24	42,42,42,42	0
56	MG	RA	3163	1/1	0.87	0.18	38,38,38,38	0
56	MG	YA	3122	1/1	0.87	0.17	35,35,35,35	0
56	MG	RA	3207	1/1	0.88	0.12	51,51,51,51	0
56	MG	RA	3196	1/1	0.88	0.23	53,53,53,53	0
56	MG	RA	3209	1/1	0.88	0.25	49,49,49,49	0
56	MG	RA	3197	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3186	1/1	0.88	0.28	50,50,50,50	0
56	MG	YA	3190	1/1	0.88	0.24	51,51,51,51	0
56	MG	YA	3162	1/1	0.88	0.27	34,34,34,34	0
56	MG	YA	3227	1/1	0.88	0.14	22,22,22,22	0
56	MG	RA	3144	1/1	0.88	0.18	36,36,36,36	0
56	MG	YA	3039	1/1	0.88	0.20	30,30,30,30	0
56	MG	RA	3190	1/1	0.88	0.18	50,50,50,50	0
56	MG	QA	1657	1/1	0.88	0.10	76,76,76,76	0
56	MG	RA	3195	1/1	0.88	0.25	28,28,28,28	0
56	MG	RA	3205	1/1	0.88	0.23	54,54,54,54	0
56	MG	RA	3056	1/1	0.89	0.15	26,26,26,26	0
56	MG	RA	3169	1/1	0.89	0.14	23,23,23,23	0
56	MG	YA	3016	1/1	0.89	0.14	19,19,19,19	0
56	MG	RA	3080	1/1	0.89	0.27	44,44,44,44	0
56	MG	RA	3133	1/1	0.89	0.13	32,32,32,32	0
56	MG	QA	1625	1/1	0.89	0.14	66,66,66,66	0
56	MG	YA	3107	1/1	0.89	0.22	25,25,25,25	0
56	MG	XA	1621	1/1	0.89	0.15	22,22,22,22	0
56	MG	YA	3188	1/1	0.89	0.20	38,38,38,38	0
56	MG	XA	1626	1/1	0.89	0.32	27,27,27,27	0
56	MG	RA	3180	1/1	0.89	0.21	28,28,28,28	0
56	MG	XA	1641	1/1	0.89	0.13	24,24,24,24	0
56	MG	QA	1640	1/1	0.89	0.18	54,54,54,54	0
56	MG	YA	3234	1/1	0.89	0.22	34,34,34,34	0
56	MG	RA	3147	1/1	0.89	0.41	49,49,49,49	0
56	MG	XA	1645	1/1	0.89	0.19	31,31,31,31	0
56	MG	RA	3106	1/1	0.89	0.50	24,24,24,24	0
56	MG	RA	3108	1/1	0.89	0.17	26,26,26,26	0
56	MG	XA	1654	1/1	0.89	0.12	50,50,50,50	0
56	MG	RA	3185	1/1	0.90	0.37	44,44,44,44	0
56	MG	XA	1652	1/1	0.90	0.16	64,64,64,64	0
56	MG	RA	3097	1/1	0.90	0.21	24,24,24,24	0
56	MG	XA	1656	1/1	0.90	0.18	37,37,37,37	0
56	MG	XA	1658	1/1	0.90	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3152	1/1	0.90	0.18	26,26,26,26	0
56	MG	QA	1622	1/1	0.90	0.27	60,60,60,60	0
56	MG	RF	301	1/1	0.90	0.24	45,45,45,45	0
56	MG	RA	3191	1/1	0.90	0.17	62,62,62,62	0
56	MG	YA	3056	1/1	0.90	0.19	9,9,9,9	0
56	MG	QA	1632	1/1	0.90	0.24	41,41,41,41	0
56	MG	QA	1644	1/1	0.90	0.19	23,23,23,23	0
56	MG	RA	3072	1/1	0.90	0.27	24,24,24,24	0
56	MG	YA	3192	1/1	0.90	0.28	40,40,40,40	0
56	MG	RA	3130	1/1	0.90	0.31	44,44,44,44	0
56	MG	RA	3174	1/1	0.90	0.39	68,68,68,68	0
56	MG	QA	1652	1/1	0.90	0.16	36,36,36,36	0
56	MG	YA	3130	1/1	0.90	0.19	16,16,16,16	0
56	MG	QA	1618	1/1	0.90	0.16	41,41,41,41	0
56	MG	YA	3139	1/1	0.90	0.22	32,32,32,32	0
56	MG	QA	1660	1/1	0.90	0.19	45,45,45,45	0
56	MG	RA	3183	1/1	0.90	0.33	49,49,49,49	0
57	PAR	QA	1661	42/42	0.90	0.23	75,75,75,75	0
56	MG	RA	3206	1/1	0.90	0.28	38,38,38,38	0
56	MG	RA	3181	1/1	0.91	0.28	34,34,34,34	0
56	MG	QA	1601	1/1	0.91	0.23	27,27,27,27	0
56	MG	YA	3117	1/1	0.91	0.34	60,60,60,60	0
56	MG	YA	3182	1/1	0.91	0.24	30,30,30,30	0
56	MG	XA	1653	1/1	0.91	0.22	44,44,44,44	0
56	MG	QA	1637	1/1	0.91	0.17	49,49,49,49	0
56	MG	RA	3098	1/1	0.91	0.13	11,11,11,11	0
56	MG	RA	3101	1/1	0.91	0.11	50,50,50,50	0
56	MG	XA	1663	1/1	0.91	0.29	85,85,85,85	0
56	MG	YA	3194	1/1	0.91	0.30	42,42,42,42	0
56	MG	YA	3200	1/1	0.91	0.12	15,15,15,15	0
56	MG	YA	3201	1/1	0.91	0.10	122,122,122,122	0
56	MG	YA	3151	1/1	0.91	0.51	26,26,26,26	0
56	MG	XA	1631	1/1	0.91	0.32	45,45,45,45	0
56	MG	YA	3003	1/1	0.91	0.13	13,13,13,13	0
56	MG	RA	3171	1/1	0.91	0.33	49,49,49,49	0
56	MG	RA	3103	1/1	0.91	0.61	48,48,48,48	0
56	MG	QA	1638	1/1	0.91	0.31	53,53,53,53	0
56	MG	RA	3027	1/1	0.91	0.74	80,80,80,80	0
56	MG	YA	3065	1/1	0.91	0.13	12,12,12,12	0
56	MG	YX	101	1/1	0.91	0.09	28,28,28,28	0
56	MG	RA	3111	1/1	0.91	0.30	52,52,52,52	0
57	PAR	XA	1664	42/42	0.91	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3159	1/1	0.91	0.42	26,26,26,26	0
56	MG	QA	1659	1/1	0.92	0.26	79,79,79,79	0
56	MG	XA	1614	1/1	0.92	0.11	14,14,14,14	0
56	MG	RA	3033	1/1	0.92	0.21	62,62,62,62	0
56	MG	RA	3188	1/1	0.92	0.28	58,58,58,58	0
56	MG	RA	3153	1/1	0.92	0.16	36,36,36,36	0
56	MG	YA	3061	1/1	0.92	0.12	35,35,35,35	0
56	MG	YA	3063	1/1	0.92	0.12	6,6,6,6	0
56	MG	QA	1634	1/1	0.92	0.10	48,48,48,48	0
56	MG	YA	3071	1/1	0.92	0.14	18,18,18,18	0
56	MG	RA	3066	1/1	0.92	0.24	12,12,12,12	0
56	MG	YA	3098	1/1	0.92	0.18	49,49,49,49	0
56	MG	QA	1611	1/1	0.92	0.08	32,32,32,32	0
56	MG	RA	3164	1/1	0.92	0.15	52,52,52,52	0
56	MG	RA	3073	1/1	0.92	0.38	5,5,5,5	0
56	MG	RA	3075	1/1	0.92	0.35	4,4,4,4	0
56	MG	RA	3115	1/1	0.92	0.26	59,59,59,59	0
56	MG	QA	1610	1/1	0.92	0.21	33,33,33,33	0
56	MG	QV	102	1/1	0.92	0.19	8,8,8,8	0
56	MG	XA	1651	1/1	0.92	0.14	18,18,18,18	0
56	MG	YA	3230	1/1	0.92	0.39	43,43,43,43	0
56	MG	RA	3123	1/1	0.92	0.14	32,32,32,32	0
56	MG	YA	3150	1/1	0.92	0.19	54,54,54,54	0
56	MG	RA	3091	1/1	0.92	0.17	21,21,21,21	0
56	MG	YA	3152	1/1	0.92	0.39	38,38,38,38	0
56	MG	YB	202	1/1	0.92	0.16	42,42,42,42	0
56	MG	RA	3178	1/1	0.92	0.25	62,62,62,62	0
56	MG	RA	3092	1/1	0.92	0.10	18,18,18,18	0
56	MG	RA	3095	1/1	0.92	0.14	31,31,31,31	0
56	MG	RA	3015	1/1	0.92	0.15	15,15,15,15	0
56	MG	RA	3146	1/1	0.92	0.30	44,44,44,44	0
56	MG	QA	1633	1/1	0.93	0.36	50,50,50,50	0
56	MG	YA	3082	1/1	0.93	0.15	13,13,13,13	0
56	MG	XA	1646	1/1	0.93	0.18	23,23,23,23	0
56	MG	RA	3120	1/1	0.93	0.11	10,10,10,10	0
56	MG	YA	3178	1/1	0.93	0.22	68,68,68,68	0
56	MG	RA	3157	1/1	0.93	0.38	20,20,20,20	0
56	MG	RA	3158	1/1	0.93	0.16	14,14,14,14	0
56	MG	QA	1645	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3102	1/1	0.93	0.25	32,32,32,32	0
56	MG	QA	1631	1/1	0.93	0.15	55,55,55,55	0
56	MG	XA	1655	1/1	0.93	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3124	1/1	0.93	0.22	22,22,22,22	0
56	MG	QA	1635	1/1	0.93	0.18	31,31,31,31	0
56	MG	YA	3198	1/1	0.93	0.26	32,32,32,32	0
56	MG	RA	3134	1/1	0.93	0.21	18,18,18,18	0
56	MG	RA	3168	1/1	0.93	0.10	31,31,31,31	0
56	MG	YA	3141	1/1	0.93	0.48	43,43,43,43	0
56	MG	YA	3208	1/1	0.93	0.21	53,53,53,53	0
56	MG	YA	3226	1/1	0.93	0.15	14,14,14,14	0
56	MG	YA	3142	1/1	0.93	0.16	30,30,30,30	0
56	MG	RA	3193	1/1	0.93	0.15	49,49,49,49	0
56	MG	XV	102	1/1	0.93	0.12	22,22,22,22	0
56	MG	RA	3139	1/1	0.93	0.13	31,31,31,31	0
56	MG	RA	3007	1/1	0.93	0.13	8,8,8,8	0
56	MG	RA	3143	1/1	0.93	0.47	16,16,16,16	0
56	MG	YA	3160	1/1	0.93	0.19	37,37,37,37	0
56	MG	YA	3242	1/1	0.93	0.32	34,34,34,34	0
56	MG	XA	1632	1/1	0.93	0.19	11,11,11,11	0
56	MG	YE	301	1/1	0.93	0.11	1,1,1,1	0
56	MG	RA	3012	1/1	0.93	0.37	26,26,26,26	0
56	MG	RA	3114	1/1	0.93	0.11	30,30,30,30	0
56	MG	YA	3168	1/1	0.93	0.29	65,65,65,65	0
56	MG	QA	1619	1/1	0.93	0.29	48,48,48,48	0
56	MG	RA	3150	1/1	0.93	0.25	26,26,26,26	0
56	MG	YA	3018	1/1	0.94	0.32	24,24,24,24	0
56	MG	YA	3033	1/1	0.94	0.24	6,6,6,6	0
56	MG	RA	3137	1/1	0.94	0.17	36,36,36,36	0
56	MG	QA	1623	1/1	0.94	0.15	28,28,28,28	0
56	MG	YA	3170	1/1	0.94	0.35	10,10,10,10	0
56	MG	XA	1636	1/1	0.94	0.15	58,58,58,58	0
56	MG	RA	3009	1/1	0.94	0.17	21,21,21,21	0
56	MG	RA	3040	1/1	0.94	0.13	9,9,9,9	0
56	MG	YA	3174	1/1	0.94	0.19	29,29,29,29	0
56	MG	YA	3175	1/1	0.94	0.12	12,12,12,12	0
56	MG	YA	3066	1/1	0.94	0.48	18,18,18,18	0
56	MG	YA	3067	1/1	0.94	0.14	15,15,15,15	0
56	MG	RA	3199	1/1	0.94	0.18	47,47,47,47	0
56	MG	RA	3078	1/1	0.94	0.19	15,15,15,15	0
56	MG	QA	1656	1/1	0.94	0.22	53,53,53,53	0
56	MG	YA	3088	1/1	0.94	0.26	20,20,20,20	0
56	MG	YA	3184	1/1	0.94	0.17	33,33,33,33	0
56	MG	RA	3121	1/1	0.94	0.65	35,35,35,35	0
56	MG	RA	3149	1/1	0.94	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3082	1/1	0.94	0.14	13,13,13,13	0
56	MG	YA	3191	1/1	0.94	0.13	24,24,24,24	0
56	MG	XA	1650	1/1	0.94	0.26	39,39,39,39	0
56	MG	RA	3179	1/1	0.94	0.21	22,22,22,22	0
56	MG	YA	3196	1/1	0.94	0.13	33,33,33,33	0
56	MG	YA	3197	1/1	0.94	0.16	33,33,33,33	0
56	MG	RA	3057	1/1	0.94	0.06	22,22,22,22	0
56	MG	YA	3199	1/1	0.94	0.21	42,42,42,42	0
56	MG	YA	3121	1/1	0.94	0.16	23,23,23,23	0
56	MG	RA	3127	1/1	0.94	0.18	47,47,47,47	0
56	MG	YA	3205	1/1	0.94	0.15	28,28,28,28	0
56	MG	RA	3128	1/1	0.94	0.20	27,27,27,27	0
56	MG	YA	3126	1/1	0.94	0.18	27,27,27,27	0
56	MG	YA	3211	1/1	0.94	0.18	42,42,42,42	0
56	MG	YA	3212	1/1	0.94	0.10	21,21,21,21	0
56	MG	YA	3214	1/1	0.94	0.15	42,42,42,42	0
56	MG	YA	3215	1/1	0.94	0.15	51,51,51,51	0
56	MG	YA	3223	1/1	0.94	0.09	30,30,30,30	0
56	MG	YA	3127	1/1	0.94	0.53	44,44,44,44	0
56	MG	RA	3104	1/1	0.94	0.24	44,44,44,44	0
56	MG	YA	3131	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3131	1/1	0.94	0.20	77,77,77,77	0
56	MG	YA	3231	1/1	0.94	0.29	32,32,32,32	0
56	MG	RA	3160	1/1	0.94	0.17	25,25,25,25	0
56	MG	XA	1662	1/1	0.94	0.24	27,27,27,27	0
56	MG	RA	3161	1/1	0.94	0.16	32,32,32,32	0
56	MG	YA	3149	1/1	0.94	0.30	26,26,26,26	0
56	MG	YA	3241	1/1	0.94	0.28	33,33,33,33	0
56	MG	XM	201	1/1	0.94	0.12	28,28,28,28	0
56	MG	RA	3189	1/1	0.94	0.23	34,34,34,34	0
56	MG	QX	102	1/1	0.94	0.09	42,42,42,42	0
56	MG	RA	3069	1/1	0.94	0.30	43,43,43,43	0
56	MG	YA	3005	1/1	0.94	0.12	19,19,19,19	0
56	MG	YA	3159	1/1	0.94	0.30	43,43,43,43	0
56	MG	XA	1625	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3135	1/1	0.94	0.27	32,32,32,32	0
56	MG	YA	3004	1/1	0.95	0.23	13,13,13,13	0
56	MG	QA	1617	1/1	0.95	0.22	41,41,41,41	0
56	MG	XA	1637	1/1	0.95	0.11	39,39,39,39	0
56	MG	YA	3134	1/1	0.95	0.10	29,29,29,29	0
56	MG	RA	3047	1/1	0.95	0.23	7,7,7,7	0
56	MG	XA	1639	1/1	0.95	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	RA	3048	1/1	0.95	0.22	13,13,13,13	0
56	MG	YA	3145	1/1	0.95	0.15	42,42,42,42	0
56	MG	YA	3148	1/1	0.95	0.11	25,25,25,25	0
56	MG	QA	1655	1/1	0.95	0.36	50,50,50,50	0
56	MG	YA	3045	1/1	0.95	0.37	22,22,22,22	0
56	MG	QA	1629	1/1	0.95	0.17	68,68,68,68	0
56	MG	RA	3065	1/1	0.95	0.28	21,21,21,21	0
56	MG	YA	3154	1/1	0.95	0.16	15,15,15,15	0
56	MG	YA	3155	1/1	0.95	0.24	22,22,22,22	0
56	MG	RA	3094	1/1	0.95	0.12	19,19,19,19	0
56	MG	RA	3136	1/1	0.95	0.24	49,49,49,49	0
56	MG	QA	1649	1/1	0.95	0.34	45,45,45,45	0
56	MG	RB	202	1/1	0.95	0.07	31,31,31,31	0
56	MG	YA	3220	1/1	0.95	0.14	18,18,18,18	0
56	MG	YA	3221	1/1	0.95	0.21	26,26,26,26	0
56	MG	YA	3070	1/1	0.95	0.13	22,22,22,22	0
56	MG	YA	3224	1/1	0.95	0.18	18,18,18,18	0
56	MG	RA	3116	1/1	0.95	0.22	69,69,69,69	0
56	MG	RP	201	1/1	0.95	0.34	37,37,37,37	0
56	MG	RA	3166	1/1	0.95	0.23	56,56,56,56	0
56	MG	YA	3085	1/1	0.95	0.10	41,41,41,41	0
56	MG	XA	1609	1/1	0.95	0.24	15,15,15,15	0
56	MG	YA	3232	1/1	0.95	0.29	43,43,43,43	0
56	MG	RA	3018	1/1	0.95	0.22	6,6,6,6	0
56	MG	RA	3119	1/1	0.95	0.39	34,34,34,34	0
56	MG	RA	3023	1/1	0.95	0.29	24,24,24,24	0
56	MG	XA	1660	1/1	0.95	0.08	61,61,61,61	0
56	MG	XA	1661	1/1	0.95	0.20	38,38,38,38	0
56	MG	QA	1650	1/1	0.95	0.14	36,36,36,36	0
56	MG	RA	3099	1/1	0.95	0.13	21,21,21,21	0
56	MG	RA	3148	1/1	0.95	0.20	21,21,21,21	0
56	MG	XA	1627	1/1	0.95	0.29	31,31,31,31	0
56	MG	RA	3005	1/1	0.95	0.26	8,8,8,8	0
56	MG	RA	3125	1/1	0.95	0.32	24,24,24,24	0
56	MG	YA	3128	1/1	0.95	0.21	23,23,23,23	0
56	MG	YA	3185	1/1	0.95	0.09	10,10,10,10	0
56	MG	RA	3001	1/1	0.96	0.19	36,36,36,36	0
56	MG	YA	3100	1/1	0.96	0.32	1,1,1,1	0
56	MG	YA	3102	1/1	0.96	0.25	5,5,5,5	0
56	MG	YA	3179	1/1	0.96	0.41	31,31,31,31	0
56	MG	RE	302	1/1	0.96	0.38	22,22,22,22	0
56	MG	RA	3003	1/1	0.96	0.23	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3115	1/1	0.96	0.14	21,21,21,21	0
56	MG	RA	3034	1/1	0.96	0.28	16,16,16,16	0
56	MG	XA	1657	1/1	0.96	0.13	28,28,28,28	0
56	MG	YA	3119	1/1	0.96	0.37	35,35,35,35	0
56	MG	YA	3187	1/1	0.96	0.36	58,58,58,58	0
56	MG	RA	3184	1/1	0.96	0.30	33,33,33,33	0
56	MG	XA	1659	1/1	0.96	0.10	60,60,60,60	0
56	MG	RA	3038	1/1	0.96	0.15	14,14,14,14	0
56	MG	YA	3123	1/1	0.96	0.12	15,15,15,15	0
56	MG	XA	1612	1/1	0.96	0.31	21,21,21,21	0
56	MG	YA	3125	1/1	0.96	0.13	18,18,18,18	0
56	MG	RA	3087	1/1	0.96	0.11	9,9,9,9	0
56	MG	XA	1615	1/1	0.96	0.24	19,19,19,19	0
56	MG	XA	1617	1/1	0.96	0.14	26,26,26,26	0
56	MG	RA	3088	1/1	0.96	0.17	24,24,24,24	0
56	MG	RA	3090	1/1	0.96	0.11	14,14,14,14	0
56	MG	YA	3202	1/1	0.96	0.07	21,21,21,21	0
56	MG	YA	3203	1/1	0.96	0.13	24,24,24,24	0
56	MG	XA	1620	1/1	0.96	0.10	55,55,55,55	0
56	MG	RA	3004	1/1	0.96	0.11	5,5,5,5	0
56	MG	RA	3124	1/1	0.96	0.33	21,21,21,21	0
56	MG	YA	3210	1/1	0.96	0.11	35,35,35,35	0
56	MG	YA	3008	1/1	0.96	0.27	17,17,17,17	0
56	MG	YA	3009	1/1	0.96	0.45	27,27,27,27	0
56	MG	YA	3144	1/1	0.96	0.16	13,13,13,13	0
56	MG	RA	3041	1/1	0.96	0.17	5,5,5,5	0
56	MG	YA	3219	1/1	0.96	0.26	29,29,29,29	0
56	MG	RA	3044	1/1	0.96	0.29	21,21,21,21	0
56	MG	QA	1602	1/1	0.96	0.34	19,19,19,19	0
56	MG	QA	1604	1/1	0.96	0.10	33,33,33,33	0
56	MG	YA	3034	1/1	0.96	0.19	3,3,3,3	0
56	MG	YA	3225	1/1	0.96	0.16	32,32,32,32	0
56	MG	RA	3051	1/1	0.96	0.40	1,1,1,1	0
56	MG	RA	3052	1/1	0.96	0.42	24,24,24,24	0
56	MG	RA	3008	1/1	0.96	0.20	13,13,13,13	0
56	MG	YA	3060	1/1	0.96	0.23	13,13,13,13	0
56	MG	QA	1624	1/1	0.96	0.34	24,24,24,24	0
56	MG	RA	3063	1/1	0.96	0.20	27,27,27,27	0
56	MG	QA	1612	1/1	0.96	0.07	37,37,37,37	0
56	MG	QA	1653	1/1	0.96	0.26	39,39,39,39	0
56	MG	YA	3163	1/1	0.96	0.20	40,40,40,40	0
56	MG	RA	3140	1/1	0.96	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3016	1/1	0.96	0.26	2,2,2,2	0
56	MG	QA	1626	1/1	0.96	0.34	77,77,77,77	0
56	MG	YA	3074	1/1	0.96	0.17	28,28,28,28	0
56	MG	RA	3177	1/1	0.96	0.15	59,59,59,59	0
56	MG	YA	3083	1/1	0.96	0.42	21,21,21,21	0
56	MG	RA	3020	1/1	0.96	0.27	29,29,29,29	0
56	MG	QA	1616	1/1	0.96	0.09	42,42,42,42	0
56	MG	RA	3212	1/1	0.96	0.28	18,18,18,18	0
58	ZN	QD	301	1/1	0.96	0.19	59,59,59,59	0
56	MG	YA	3097	1/1	0.96	0.24	19,19,19,19	0
56	MG	RA	3002	1/1	0.97	0.24	8,8,8,8	0
56	MG	YA	3143	1/1	0.97	0.13	33,33,33,33	0
56	MG	XA	1610	1/1	0.97	0.17	37,37,37,37	0
56	MG	RA	3068	1/1	0.97	0.13	16,16,16,16	0
56	MG	YA	3146	1/1	0.97	0.11	50,50,50,50	0
56	MG	RA	3100	1/1	0.97	0.16	44,44,44,44	0
56	MG	RA	3138	1/1	0.97	0.17	21,21,21,21	0
56	MG	YA	3014	1/1	0.97	0.39	12,12,12,12	0
56	MG	QA	1608	1/1	0.97	0.18	27,27,27,27	0
56	MG	RA	3071	1/1	0.97	0.19	32,32,32,32	0
56	MG	YA	3019	1/1	0.97	0.39	21,21,21,21	0
56	MG	YA	3020	1/1	0.97	0.34	8,8,8,8	0
56	MG	YA	3026	1/1	0.97	0.40	9,9,9,9	0
56	MG	YA	3157	1/1	0.97	0.16	29,29,29,29	0
56	MG	YA	3029	1/1	0.97	0.35	17,17,17,17	0
56	MG	YA	3030	1/1	0.97	0.27	24,24,24,24	0
56	MG	QA	1642	1/1	0.97	0.09	49,49,49,49	0
56	MG	RA	3037	1/1	0.97	0.26	10,10,10,10	0
56	MG	YA	3035	1/1	0.97	0.20	10,10,10,10	0
56	MG	RA	3105	1/1	0.97	0.12	50,50,50,50	0
56	MG	YA	3040	1/1	0.97	0.12	1,1,1,1	0
56	MG	YA	3167	1/1	0.97	0.06	12,12,12,12	0
56	MG	YA	3041	1/1	0.97	0.28	6,6,6,6	0
56	MG	XA	1623	1/1	0.97	0.39	31,31,31,31	0
56	MG	YA	3047	1/1	0.97	0.26	6,6,6,6	0
56	MG	YA	3051	1/1	0.97	0.22	4,4,4,4	0
56	MG	YA	3054	1/1	0.97	0.14	14,14,14,14	0
56	MG	YA	3055	1/1	0.97	0.22	16,16,16,16	0
56	MG	RA	3145	1/1	0.97	0.22	37,37,37,37	0
56	MG	YA	3057	1/1	0.97	0.49	22,22,22,22	0
56	MG	YA	3059	1/1	0.97	0.15	74,74,74,74	0
56	MG	RA	3074	1/1	0.97	0.32	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	QA	1609	1/1	0.97	0.28	34,34,34,34	0
56	MG	XA	1629	1/1	0.97	0.13	49,49,49,49	0
56	MG	YA	3180	1/1	0.97	0.11	53,53,53,53	0
56	MG	RA	3076	1/1	0.97	0.40	22,22,22,22	0
56	MG	RA	3077	1/1	0.97	0.32	14,14,14,14	0
56	MG	XA	1633	1/1	0.97	0.23	32,32,32,32	0
56	MG	YA	3069	1/1	0.97	0.16	16,16,16,16	0
56	MG	XA	1634	1/1	0.97	0.29	28,28,28,28	0
56	MG	QA	1605	1/1	0.97	0.17	51,51,51,51	0
56	MG	YA	3072	1/1	0.97	0.14	10,10,10,10	0
56	MG	RA	3151	1/1	0.97	0.23	23,23,23,23	0
56	MG	YA	3189	1/1	0.97	0.11	31,31,31,31	0
56	MG	YA	3077	1/1	0.97	0.15	8,8,8,8	0
56	MG	YA	3080	1/1	0.97	0.30	3,3,3,3	0
56	MG	YA	3081	1/1	0.97	0.30	18,18,18,18	0
56	MG	YA	3193	1/1	0.97	0.14	39,39,39,39	0
56	MG	QA	1621	1/1	0.97	0.18	48,48,48,48	0
56	MG	RA	3081	1/1	0.97	0.47	28,28,28,28	0
56	MG	XA	1640	1/1	0.97	0.19	47,47,47,47	0
56	MG	RA	3155	1/1	0.97	0.21	12,12,12,12	0
56	MG	RA	3118	1/1	0.97	0.14	14,14,14,14	0
56	MG	YA	3090	1/1	0.97	0.39	11,11,11,11	0
56	MG	YA	3092	1/1	0.97	0.16	11,11,11,11	0
56	MG	XA	1643	1/1	0.97	0.17	47,47,47,47	0
56	MG	RA	3198	1/1	0.97	0.09	53,53,53,53	0
56	MG	RA	3042	1/1	0.97	0.20	11,11,11,11	0
56	MG	YA	3101	1/1	0.97	0.27	5,5,5,5	0
56	MG	QA	1647	1/1	0.97	0.10	41,41,41,41	0
56	MG	RA	3085	1/1	0.97	0.11	15,15,15,15	0
56	MG	YA	3106	1/1	0.97	0.29	32,32,32,32	0
56	MG	QA	1636	1/1	0.97	0.08	15,15,15,15	0
56	MG	YA	3213	1/1	0.97	0.13	41,41,41,41	0
56	MG	YA	3110	1/1	0.97	0.08	10,10,10,10	0
56	MG	YA	3112	1/1	0.97	0.11	41,41,41,41	0
56	MG	YA	3216	1/1	0.97	0.09	42,42,42,42	0
56	MG	YA	3218	1/1	0.97	0.11	19,19,19,19	0
56	MG	YA	3113	1/1	0.97	0.27	21,21,21,21	0
56	MG	XA	1649	1/1	0.97	0.36	28,28,28,28	0
56	MG	QV	101	1/1	0.97	0.19	17,17,17,17	0
56	MG	RA	3204	1/1	0.97	0.12	30,30,30,30	0
56	MG	YA	3118	1/1	0.97	0.17	12,12,12,12	0
56	MG	QA	1606	1/1	0.97	0.16	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	QX	101	1/1	0.97	0.10	24,24,24,24	0
56	MG	QA	1630	1/1	0.97	0.12	66,66,66,66	0
56	MG	RA	3093	1/1	0.97	0.08	24,24,24,24	0
56	MG	RA	3129	1/1	0.97	0.20	26,26,26,26	0
56	MG	RA	3021	1/1	0.97	0.42	27,27,27,27	0
56	MG	RA	3211	1/1	0.97	0.27	13,13,13,13	0
56	MG	YA	3233	1/1	0.97	0.38	44,44,44,44	0
56	MG	RA	3170	1/1	0.97	0.09	41,41,41,41	0
56	MG	RA	3060	1/1	0.97	0.22	25,25,25,25	0
56	MG	RE	301	1/1	0.97	0.12	22,22,22,22	0
56	MG	YA	3129	1/1	0.97	0.07	22,22,22,22	0
56	MG	RA	3172	1/1	0.97	0.21	29,29,29,29	0
56	MG	RA	3132	1/1	0.97	0.21	12,12,12,12	0
56	MG	YA	3132	1/1	0.97	0.11	13,13,13,13	0
56	MG	QA	1607	1/1	0.97	0.14	22,22,22,22	0
56	MG	R5	101	1/1	0.97	0.14	27,27,27,27	0
56	MG	YA	3136	1/1	0.97	0.15	4,4,4,4	0
56	MG	YA	3138	1/1	0.97	0.16	15,15,15,15	0
56	MG	XA	1602	1/1	0.97	0.15	15,15,15,15	0
56	MG	YA	3140	1/1	0.97	0.29	2,2,2,2	0
56	MG	RA	3026	1/1	0.97	0.22	6,6,6,6	0
56	MG	RA	3045	1/1	0.98	0.29	12,12,12,12	0
56	MG	YA	3064	1/1	0.98	0.18	23,23,23,23	0
56	MG	RA	3046	1/1	0.98	0.35	31,31,31,31	0
56	MG	RA	3142	1/1	0.98	0.11	15,15,15,15	0
56	MG	RA	3010	1/1	0.98	0.36	4,4,4,4	0
56	MG	YA	3161	1/1	0.98	0.09	30,30,30,30	0
56	MG	YA	3068	1/1	0.98	0.31	12,12,12,12	0
56	MG	XA	1601	1/1	0.98	0.12	15,15,15,15	0
56	MG	RA	3110	1/1	0.98	0.12	51,51,51,51	0
56	MG	XA	1603	1/1	0.98	0.07	23,23,23,23	0
56	MG	YA	3166	1/1	0.98	0.19	51,51,51,51	0
56	MG	RA	3182	1/1	0.98	0.34	25,25,25,25	0
56	MG	YA	3073	1/1	0.98	0.25	24,24,24,24	0
56	MG	XA	1606	1/1	0.98	0.25	17,17,17,17	0
56	MG	YA	3075	1/1	0.98	0.10	14,14,14,14	0
56	MG	YA	3076	1/1	0.98	0.37	7,7,7,7	0
56	MG	XA	1608	1/1	0.98	0.16	7,7,7,7	0
56	MG	YA	3078	1/1	0.98	0.39	25,25,25,25	0
56	MG	YA	3079	1/1	0.98	0.26	18,18,18,18	0
56	MG	RA	3079	1/1	0.98	0.20	32,32,32,32	0
56	MG	RA	3112	1/1	0.98	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	XA	1611	1/1	0.98	0.17	29,29,29,29	0
56	MG	RA	3113	1/1	0.98	0.27	24,24,24,24	0
56	MG	QA	1651	1/1	0.98	0.21	70,70,70,70	0
56	MG	RA	3028	1/1	0.98	0.19	12,12,12,12	0
56	MG	YA	3086	1/1	0.98	0.14	3,3,3,3	0
56	MG	YA	3087	1/1	0.98	0.24	7,7,7,7	0
56	MG	XV	101	1/1	0.98	0.21	14,14,14,14	0
56	MG	RA	3029	1/1	0.98	0.15	2,2,2,2	0
56	MG	YA	3091	1/1	0.98	0.13	23,23,23,23	0
56	MG	YA	3001	1/1	0.98	0.43	13,13,13,13	0
56	MG	YA	3094	1/1	0.98	0.29	10,10,10,10	0
56	MG	RA	3030	1/1	0.98	0.28	15,15,15,15	0
56	MG	RA	3084	1/1	0.98	0.30	17,17,17,17	0
56	MG	YA	3099	1/1	0.98	0.34	11,11,11,11	0
56	MG	RA	3031	1/1	0.98	0.29	26,26,26,26	0
56	MG	YA	3006	1/1	0.98	0.24	0,0,0,0	0
56	MG	RA	3154	1/1	0.98	0.13	12,12,12,12	0
56	MG	YA	3103	1/1	0.98	0.08	12,12,12,12	0
56	MG	YA	3195	1/1	0.98	0.09	55,55,55,55	0
56	MG	XA	1622	1/1	0.98	0.07	40,40,40,40	0
56	MG	YA	3010	1/1	0.98	0.15	3,3,3,3	0
56	MG	RA	3086	1/1	0.98	0.22	33,33,33,33	0
56	MG	YA	3109	1/1	0.98	0.25	25,25,25,25	0
56	MG	RA	3194	1/1	0.98	0.14	14,14,14,14	0
56	MG	YA	3015	1/1	0.98	0.43	10,10,10,10	0
56	MG	RA	3058	1/1	0.98	0.20	13,13,13,13	0
56	MG	YA	3017	1/1	0.98	0.11	16,16,16,16	0
56	MG	QM	201	1/1	0.98	0.15	34,34,34,34	0
56	MG	YA	3206	1/1	0.98	0.10	24,24,24,24	0
56	MG	XA	1628	1/1	0.98	0.17	24,24,24,24	0
56	MG	RA	3089	1/1	0.98	0.28	26,26,26,26	0
56	MG	YA	3209	1/1	0.98	0.18	41,41,41,41	0
56	MG	YA	3021	1/1	0.98	0.32	12,12,12,12	0
56	MG	YA	3022	1/1	0.98	0.21	6,6,6,6	0
56	MG	YA	3024	1/1	0.98	0.19	10,10,10,10	0
56	MG	YA	3025	1/1	0.98	0.18	6,6,6,6	0
56	MG	XA	1630	1/1	0.98	0.14	39,39,39,39	0
56	MG	YA	3027	1/1	0.98	0.11	5,5,5,5	0
56	MG	RA	3061	1/1	0.98	0.21	28,28,28,28	0
56	MG	YA	3217	1/1	0.98	0.09	35,35,35,35	0
56	MG	RA	3062	1/1	0.98	0.38	21,21,21,21	0
56	MG	YA	3032	1/1	0.98	0.21	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3126	1/1	0.98	0.24	27,27,27,27	0
56	MG	QA	1628	1/1	0.98	0.28	14,14,14,14	0
56	MG	YA	3222	1/1	0.98	0.05	9,9,9,9	0
56	MG	RA	3064	1/1	0.98	0.40	25,25,25,25	0
56	MG	YA	3036	1/1	0.98	0.23	3,3,3,3	0
56	MG	YA	3038	1/1	0.98	0.13	12,12,12,12	0
56	MG	RA	3165	1/1	0.98	0.09	5,5,5,5	0
56	MG	RA	3035	1/1	0.98	0.12	21,21,21,21	0
56	MG	QA	1658	1/1	0.98	0.08	68,68,68,68	0
56	MG	YA	3229	1/1	0.98	0.10	52,52,52,52	0
56	MG	YA	3137	1/1	0.98	0.08	15,15,15,15	0
56	MG	YA	3043	1/1	0.98	0.39	9,9,9,9	0
56	MG	YA	3044	1/1	0.98	0.22	9,9,9,9	0
56	MG	RA	3067	1/1	0.98	0.06	7,7,7,7	0
56	MG	RA	3019	1/1	0.98	0.16	10,10,10,10	0
56	MG	YA	3048	1/1	0.98	0.16	4,4,4,4	0
56	MG	YA	3237	1/1	0.98	0.08	15,15,15,15	0
56	MG	YA	3238	1/1	0.98	0.26	34,34,34,34	0
56	MG	YA	3049	1/1	0.98	0.27	15,15,15,15	0
56	MG	YA	3050	1/1	0.98	0.18	2,2,2,2	0
56	MG	RA	3039	1/1	0.98	0.26	18,18,18,18	0
56	MG	YA	3052	1/1	0.98	0.23	17,17,17,17	0
56	MG	YB	201	1/1	0.98	0.15	21,21,21,21	0
56	MG	RA	3070	1/1	0.98	0.31	37,37,37,37	0
56	MG	QA	1641	1/1	0.98	0.17	25,25,25,25	0
56	MG	QA	1654	1/1	0.98	0.15	14,14,14,14	0
56	MG	RA	3022	1/1	0.98	0.33	3,3,3,3	0
56	MG	Y5	101	1/1	0.98	0.15	25,25,25,25	0
56	MG	RB	201	1/1	0.98	0.05	13,13,13,13	0
56	MG	YA	3153	1/1	0.98	0.22	26,26,26,26	0
56	MG	RA	3043	1/1	0.98	0.11	30,30,30,30	0
56	MG	QA	1646	1/1	0.98	0.25	14,14,14,14	0
58	ZN	XD	301	1/1	0.98	0.23	49,49,49,49	0
58	ZN	XN	101	1/1	0.98	0.12	107,107,107,107	0
56	MG	YA	3108	1/1	0.99	0.11	5,5,5,5	0
56	MG	RA	3014	1/1	0.99	0.24	10,10,10,10	0
56	MG	YA	3028	1/1	0.99	0.18	23,23,23,23	0
56	MG	YA	3111	1/1	0.99	0.23	30,30,30,30	0
56	MG	RA	3006	1/1	0.99	0.17	3,3,3,3	0
56	MG	XA	1613	1/1	0.99	0.13	45,45,45,45	0
56	MG	YA	3114	1/1	0.99	0.24	6,6,6,6	0
56	MG	YA	3031	1/1	0.99	0.35	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	RA	3059	1/1	0.99	0.27	21,21,21,21	0
56	MG	RA	3032	1/1	0.99	0.16	17,17,17,17	0
56	MG	XA	1616	1/1	0.99	0.11	20,20,20,20	0
56	MG	QA	1603	1/1	0.99	0.05	28,28,28,28	0
56	MG	RA	3024	1/1	0.99	0.45	4,4,4,4	0
56	MG	YA	3037	1/1	0.99	0.20	3,3,3,3	0
56	MG	RA	3025	1/1	0.99	0.14	9,9,9,9	0
56	MG	RA	3036	1/1	0.99	0.33	10,10,10,10	0
56	MG	YA	3007	1/1	0.99	0.17	6,6,6,6	0
56	MG	RA	3156	1/1	0.99	0.16	22,22,22,22	0
56	MG	YA	3042	1/1	0.99	0.31	28,28,28,28	0
56	MG	RA	3017	1/1	0.99	0.12	13,13,13,13	0
56	MG	RA	3049	1/1	0.99	0.15	10,10,10,10	0
56	MG	YA	3011	1/1	0.99	0.26	13,13,13,13	0
56	MG	YA	3046	1/1	0.99	0.13	4,4,4,4	0
56	MG	XA	1624	1/1	0.99	0.13	35,35,35,35	0
56	MG	YA	3013	1/1	0.99	0.31	3,3,3,3	0
56	MG	RA	3050	1/1	0.99	0.14	0,0,0,0	0
56	MG	RA	3011	1/1	0.99	0.17	30,30,30,30	0
56	MG	YA	3135	1/1	0.99	0.10	33,33,33,33	0
56	MG	YA	3089	1/1	0.99	0.23	2,2,2,2	0
56	MG	QA	1648	1/1	0.99	0.03	100,100,100,100	0
56	MG	YA	3235	1/1	0.99	0.13	26,26,26,26	0
56	MG	RA	3053	1/1	0.99	0.17	5,5,5,5	0
56	MG	YA	3053	1/1	0.99	0.15	4,4,4,4	0
56	MG	YA	3093	1/1	0.99	0.14	18,18,18,18	0
56	MG	XA	1604	1/1	0.99	0.07	31,31,31,31	0
56	MG	YA	3095	1/1	0.99	0.29	5,5,5,5	0
56	MG	YA	3096	1/1	0.99	0.22	15,15,15,15	0
56	MG	RA	3054	1/1	0.99	0.23	5,5,5,5	0
56	MG	RA	3055	1/1	0.99	0.15	12,12,12,12	0
56	MG	XA	1607	1/1	0.99	0.07	5,5,5,5	0
56	MG	YA	3147	1/1	0.99	0.11	11,11,11,11	0
56	MG	YA	3058	1/1	0.99	0.30	16,16,16,16	0
56	MG	RA	3107	1/1	0.99	0.28	21,21,21,21	0
56	MG	YA	3023	1/1	0.99	0.26	4,4,4,4	0
56	MG	RA	3013	1/1	0.99	0.22	10,10,10,10	0
56	MG	YA	3104	1/1	0.99	0.24	6,6,6,6	0
56	MG	YA	3062	1/1	0.99	0.11	6,6,6,6	0
56	MG	XA	1635	1/1	0.99	0.07	36,36,36,36	0
56	MG	RA	3109	1/1	0.99	0.07	26,26,26,26	0
56	MG	YA	3204	1/1	0.99	0.16	43,43,43,43	0

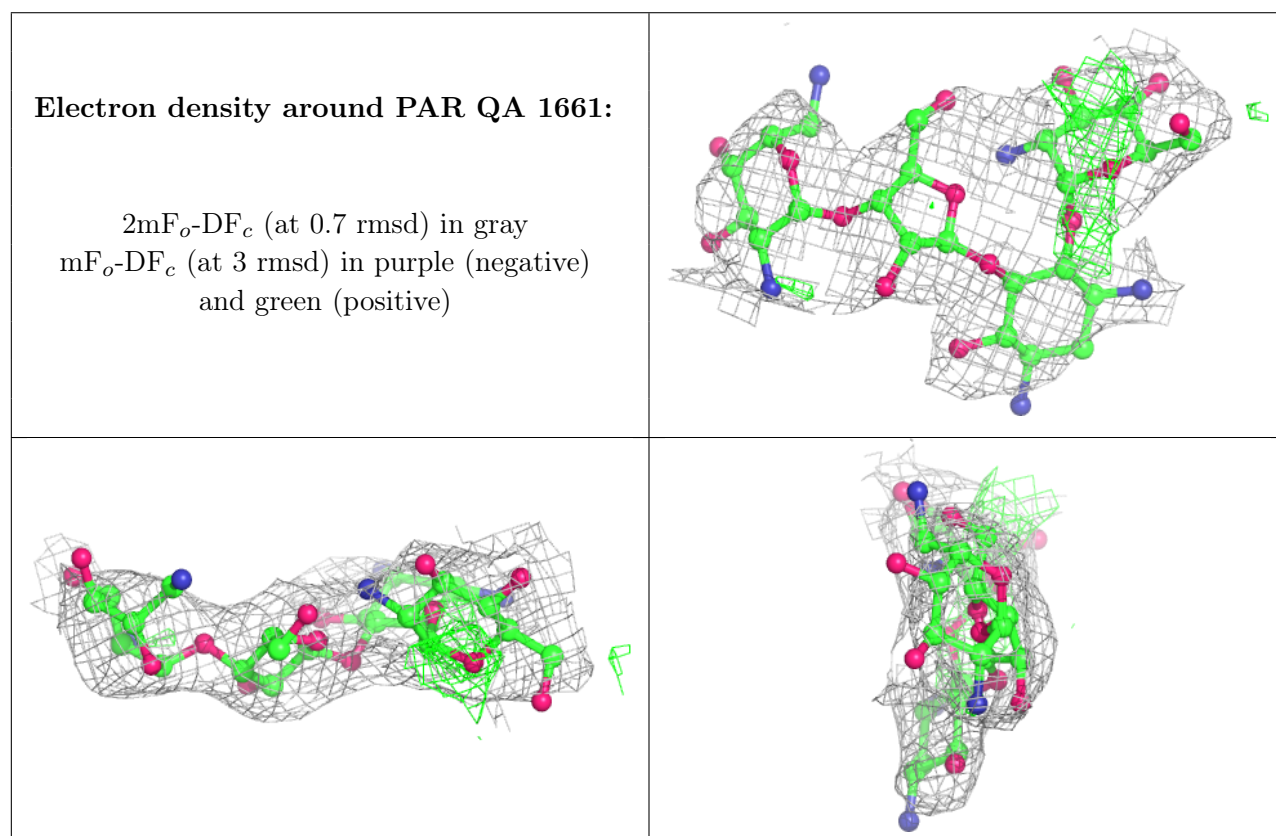
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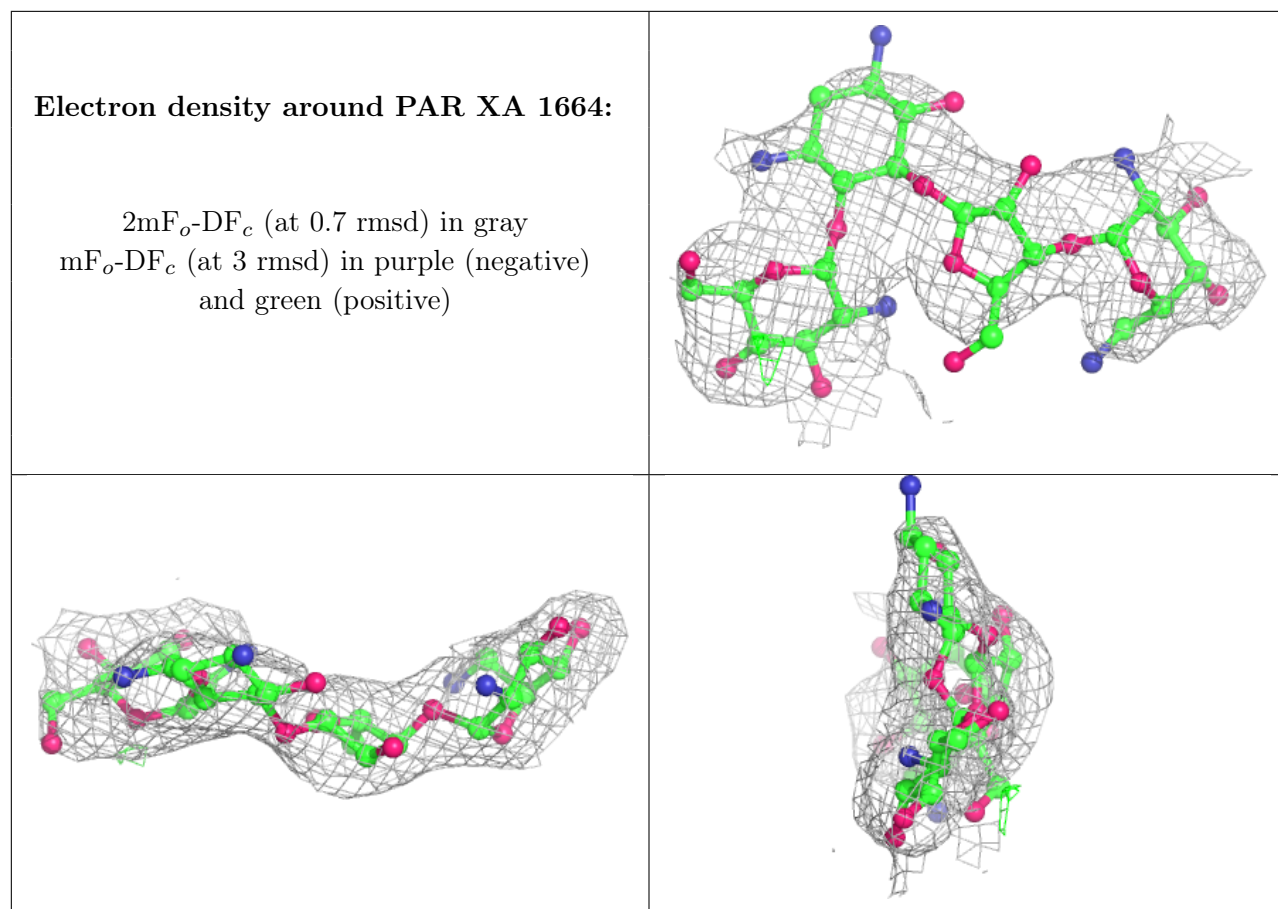


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	YA	3002	1/1	1.00	0.38	15,15,15,15	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.