



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 07:22 PM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

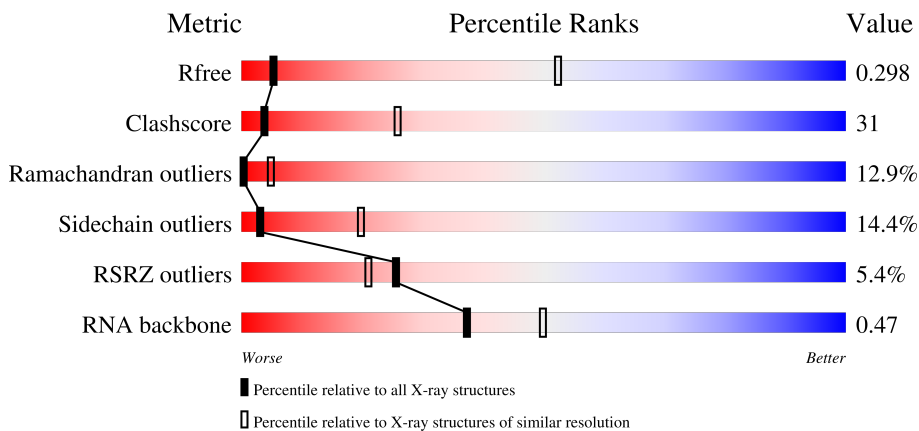
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



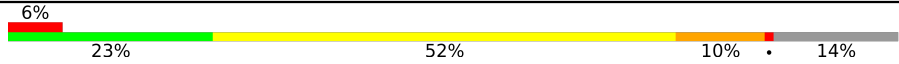
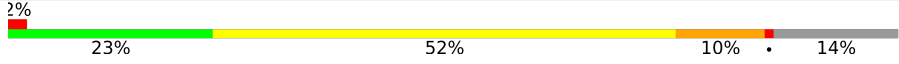
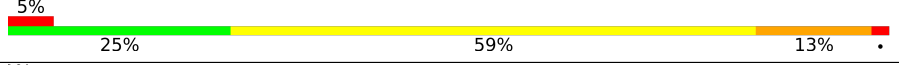
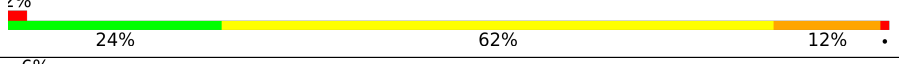
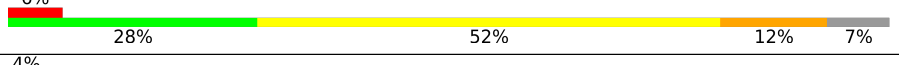
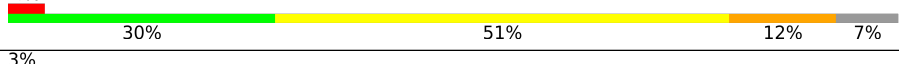
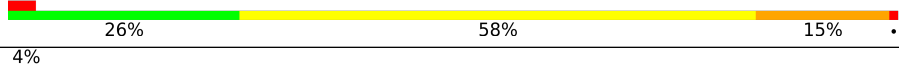
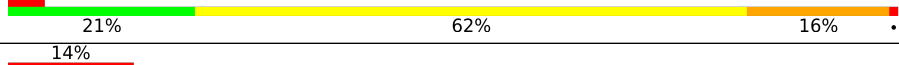
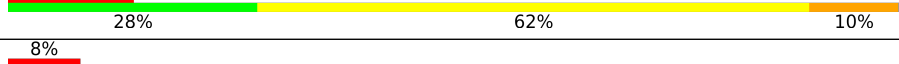
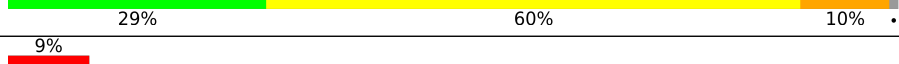

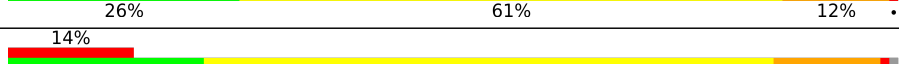
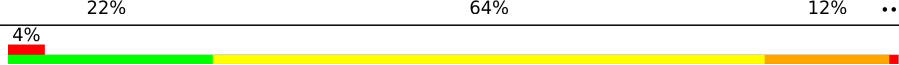
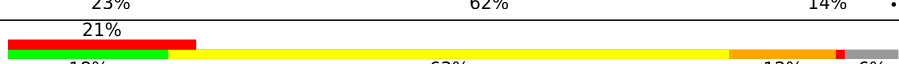
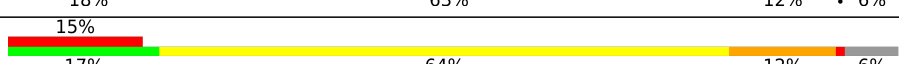
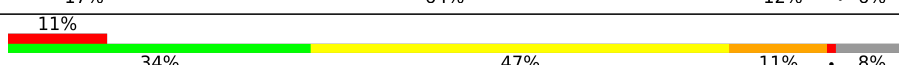
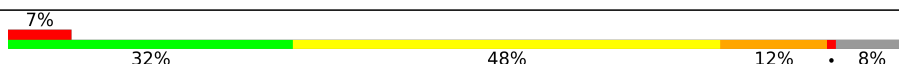
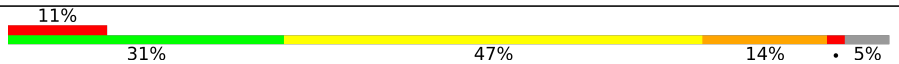
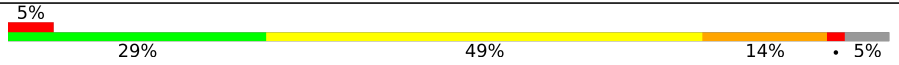
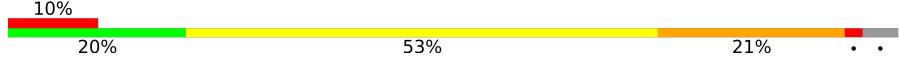
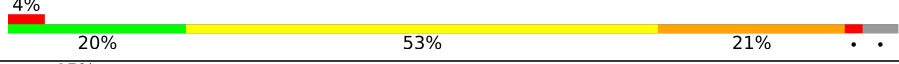
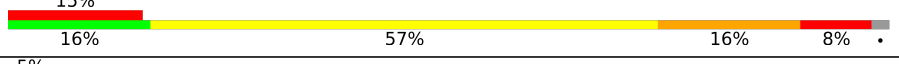

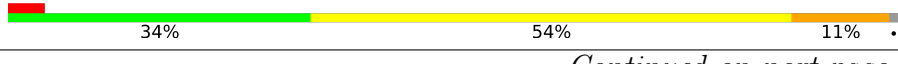

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

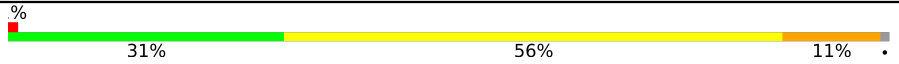
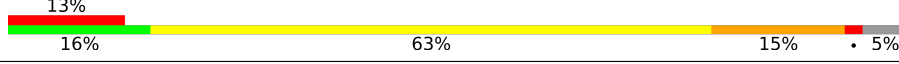
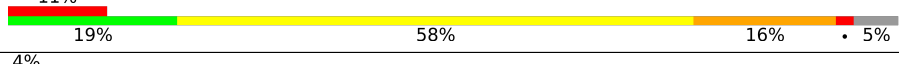
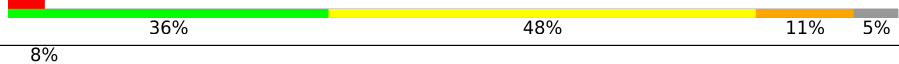
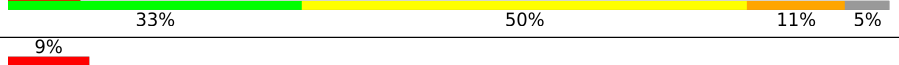
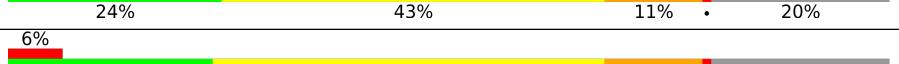
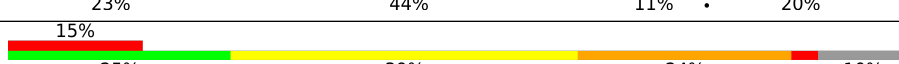
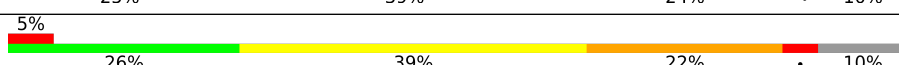
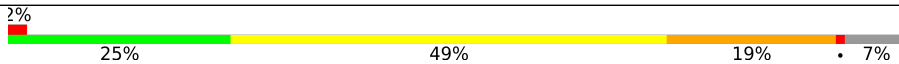
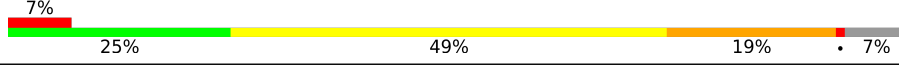
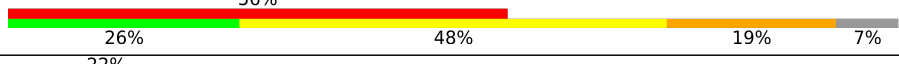
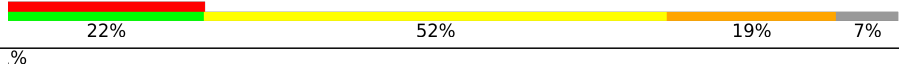
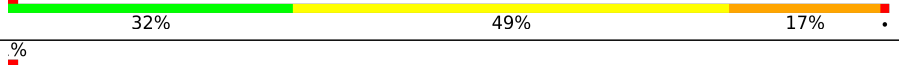


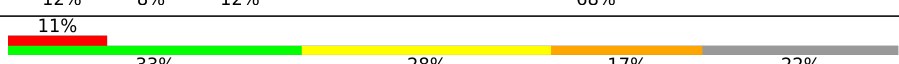
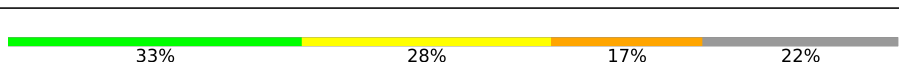
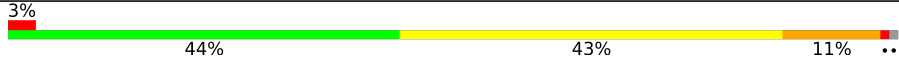
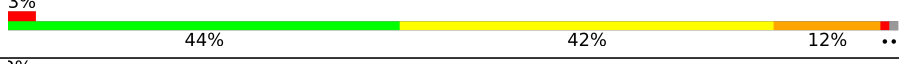
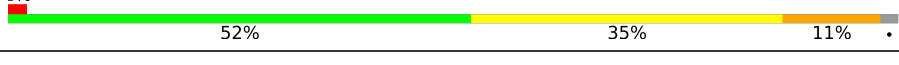





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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
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	4% 24% 48% 23% 5%
28	YE	206	3% 23% 48% 23% 5%
29	RF	210	2% 34% 48% 13% ..
29	YF	210	2% 34% 49% 12% ..
30	RG	182	11% 23% 58% 16% ..
30	YG	182	4% 23% 58% 16% ..
31	RH	180	19% 23% 44% 19% 8% 6%
31	YH	180	8% 23% 44% 20% 8% 6%
32	RI	148	10% 36% 47% 14% ..
32	YI	148	5% 48% 36% 14% ..
33	RN	140	7% 18% 54% 26% ..
33	YN	140	2% 17% 54% 26% ..
34	RO	122	% 34% 56% 9% .
34	YO	122	% 35% 54% 9% .
35	RP	150	15% 19% 50% 23% 8%
35	YP	150	4% 20% 50% 23% 7%
36	RQ	141	6% 32% 50% 16% .
36	YQ	141	% 33% 48% 16% .
37	RR	118	% 33% 48% 16% .
37	YR	118	% 32% 50% 15% .
38	RS	112	9% 14% 61% 19% 5% .
38	YS	112	2% 12% 62% 20% ..
39	RT	146	3% 22% 50% 19% . 6%
39	YT	146	5% 21% 50% 20% . 6%
40	RU	118	4% 33% 53% 12% ..

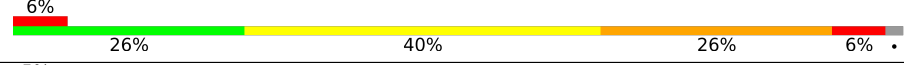
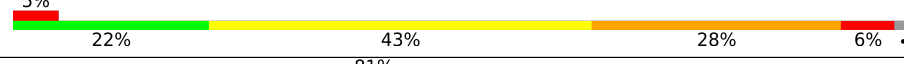
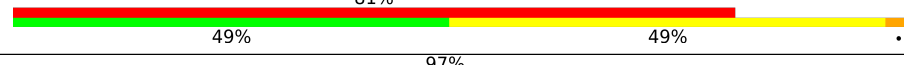
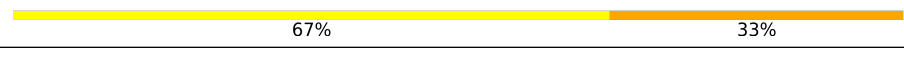

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Mol	Chain	Length	Quality of chain
40	YU	118	2% 31% 53% 13% ..
41	RV	101	2% 28% 51% 21%
41	YV	101	5% 27% 52% 21%
42	RW	113	4% 28% 50% 19% .
42	YW	113	3% 29% 50% 19% .
43	RX	96	% 39% 43% 15% .
43	YX	96	2% 36% 45% 15% .
44	RY	110	30% 16% 45% 28% . 7%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

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	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
57	MG	QA	1618	-	-	-	X
57	MG	QA	1623	-	-	-	X
57	MG	QA	1630	-	-	-	X
57	MG	QA	1661	-	-	-	X
57	MG	R0	101	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3124	-	-	-	X
57	MG	RA	3134	-	-	-	X
57	MG	RA	3163	-	-	-	X
57	MG	RA	3180	-	-	-	X
57	MG	RA	3189	-	-	-	X
57	MG	RA	3216	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RP	202	-	-	-	X
57	MG	XA	1605	-	-	-	X
57	MG	XA	1606	-	-	-	X

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

2 Entry composition [i](#)

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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
			173	77	33	55	8			
23	XX	8	Total	C	N	O	P	0	0	0
			173	77	33	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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
25	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

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

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

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

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

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

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

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

- 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	S			
43	RX	92	725	471	131	123		0	0	0
43	YX	92	725	471	131	123		0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 L31.

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 L32.

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 L33.

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 L34.

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 50S ribosomal protein L35.

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 protein called 50S ribosomal protein L36.

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

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

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

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

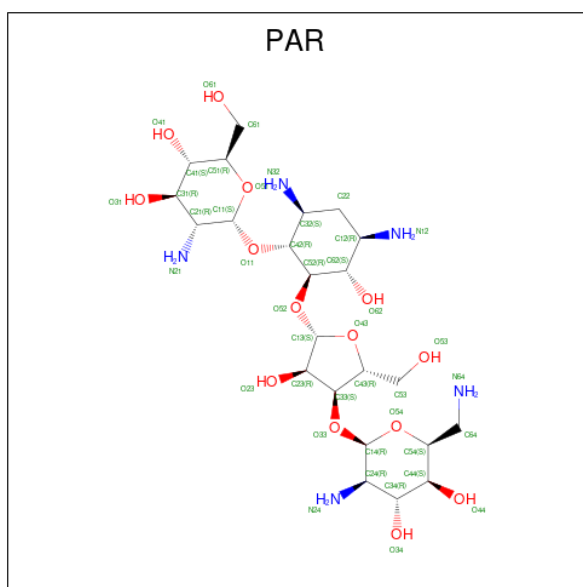
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	65	Total	Mg	0	0
			65	65		
57	QF	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		
57	RA	242	Total	Mg	0	0
			242	242		

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

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

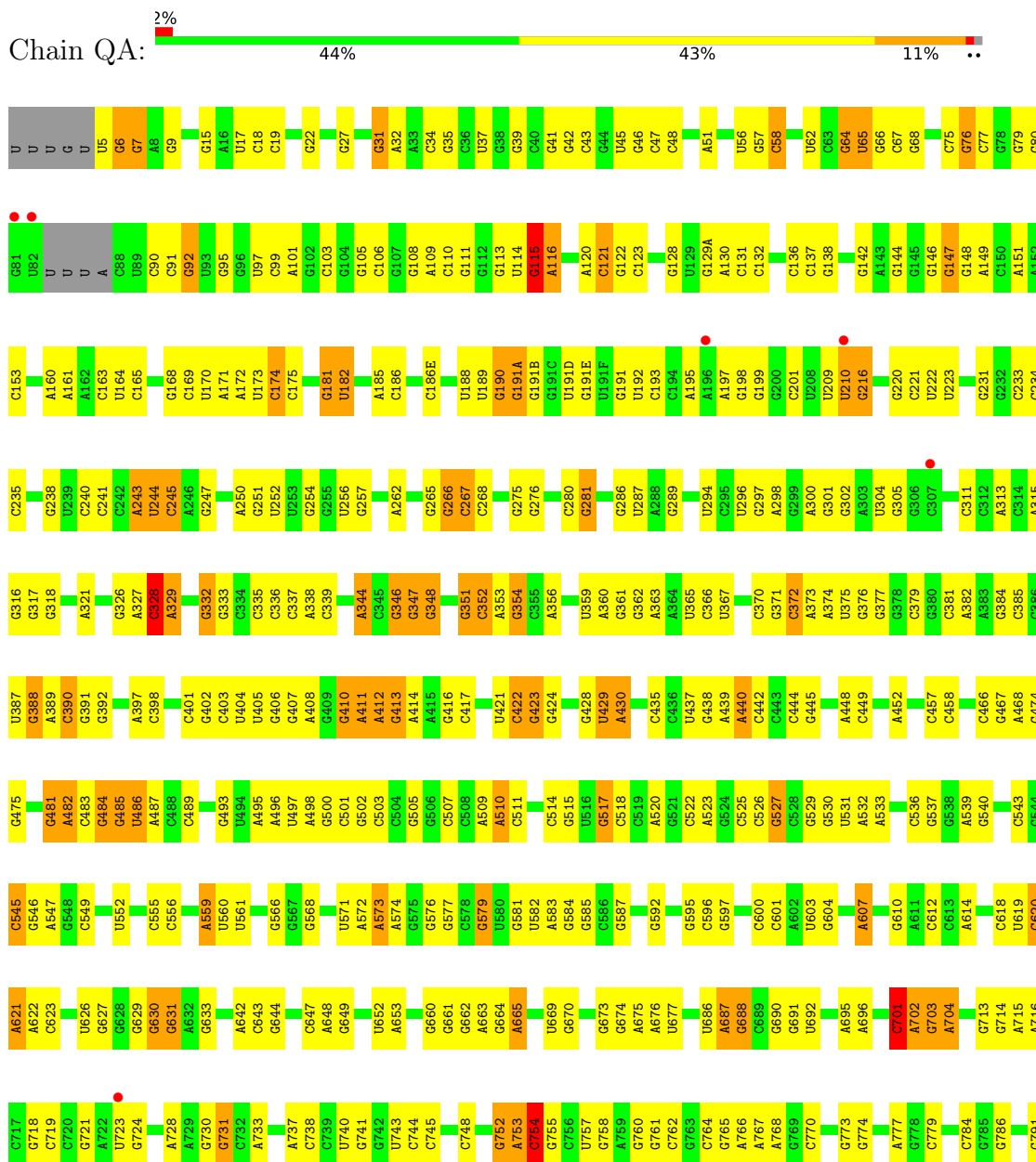
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

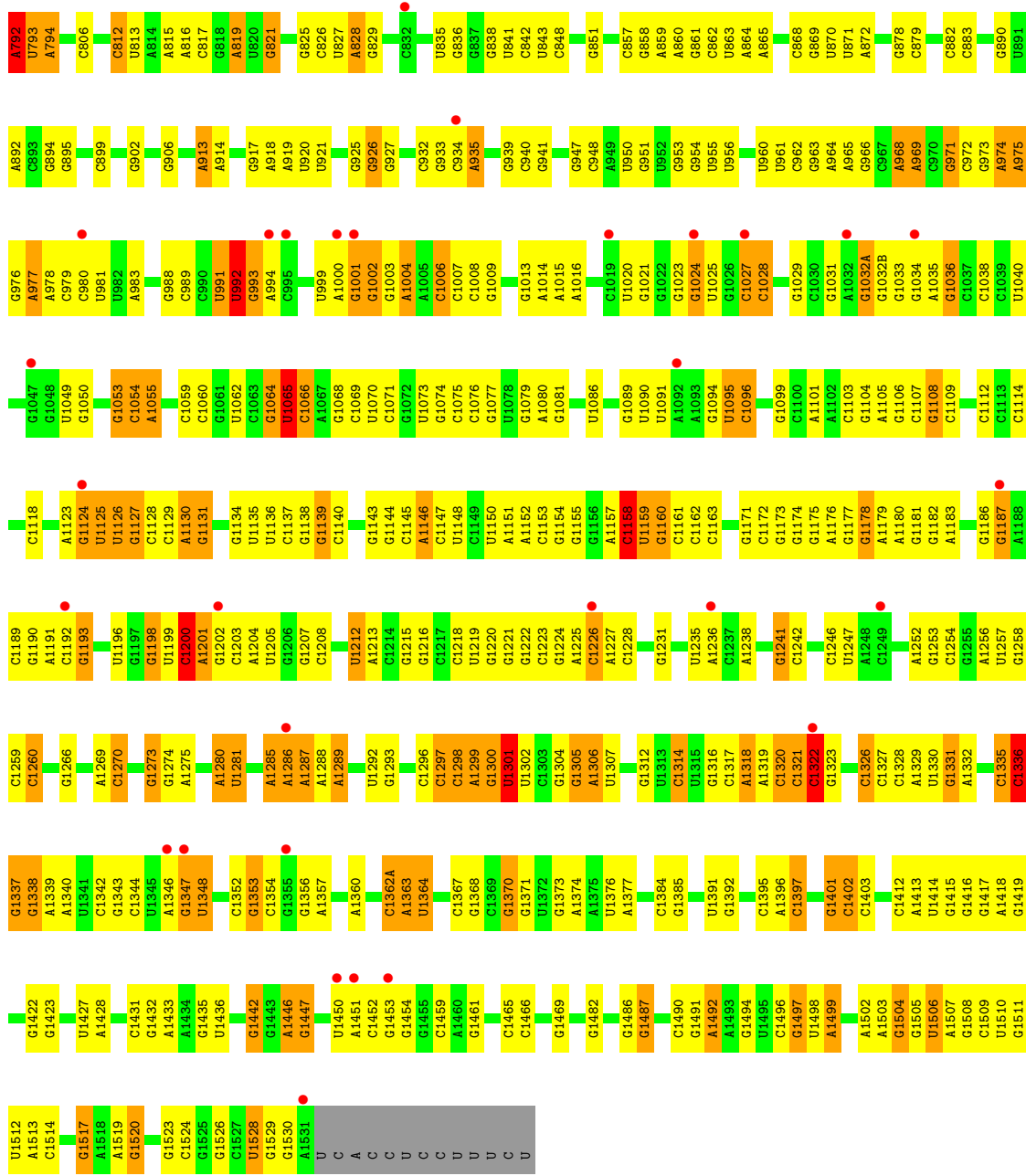
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QD	1	1	1	0	0
59	QN	1	1	1	0	0
59	XD	1	1	1	0	0
59	XN	1	1	1	0	0

3 Residue-property plots [i](#)

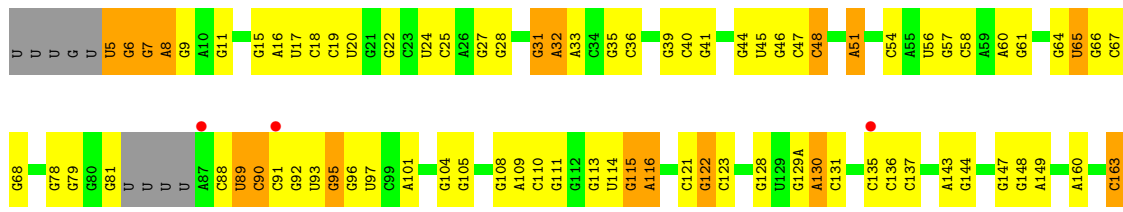
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

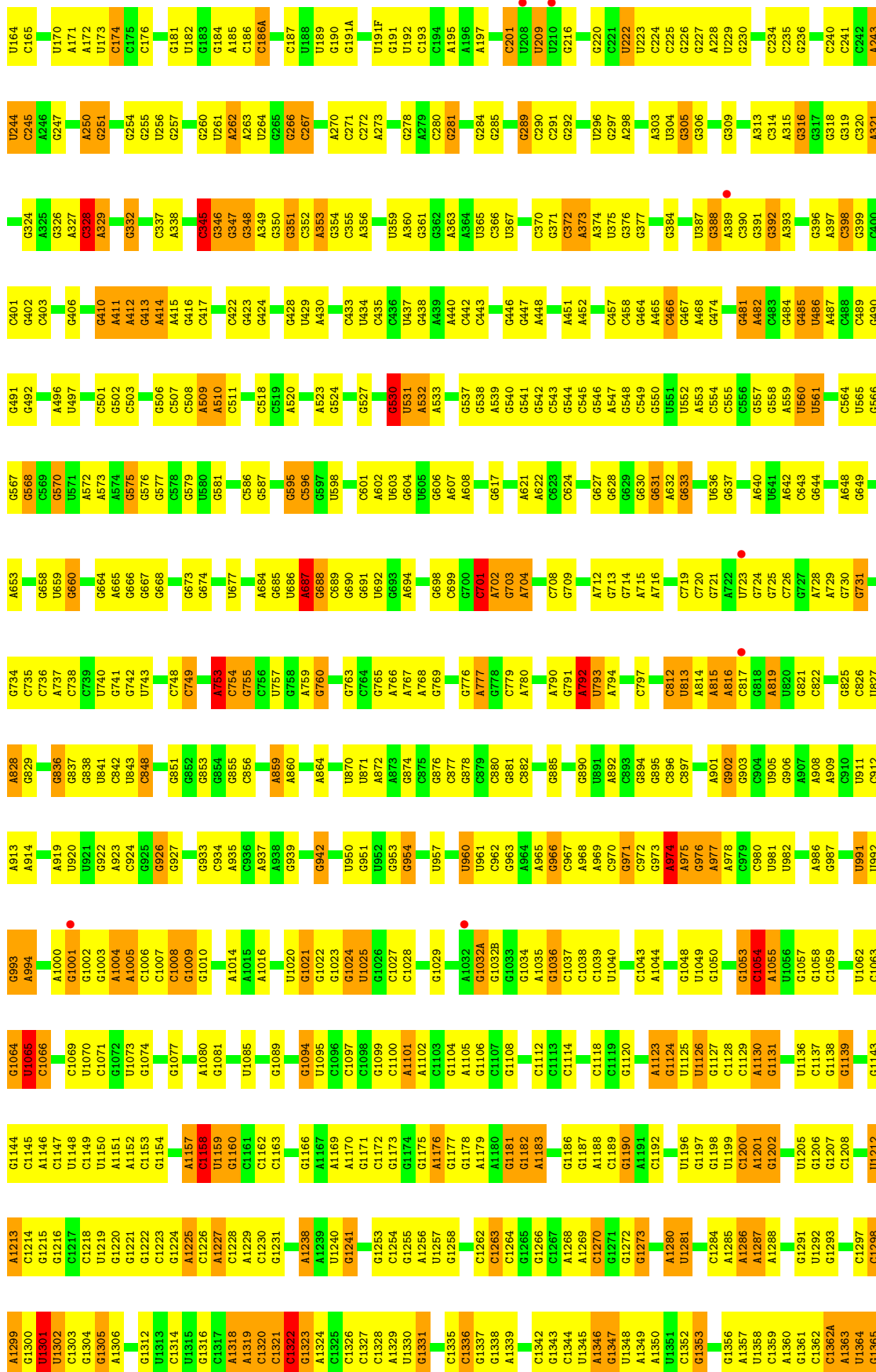
- Molecule 1: 16S rRNA

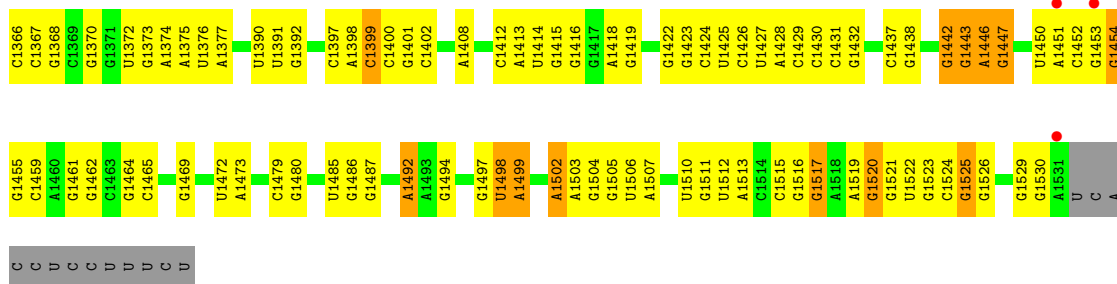




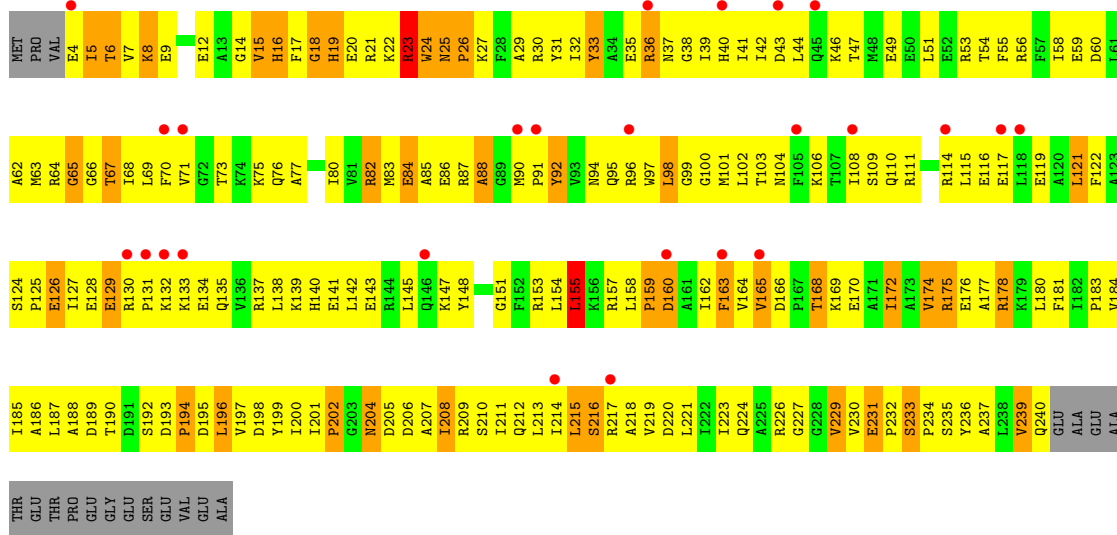
● Molecule 1: 16S rRNA



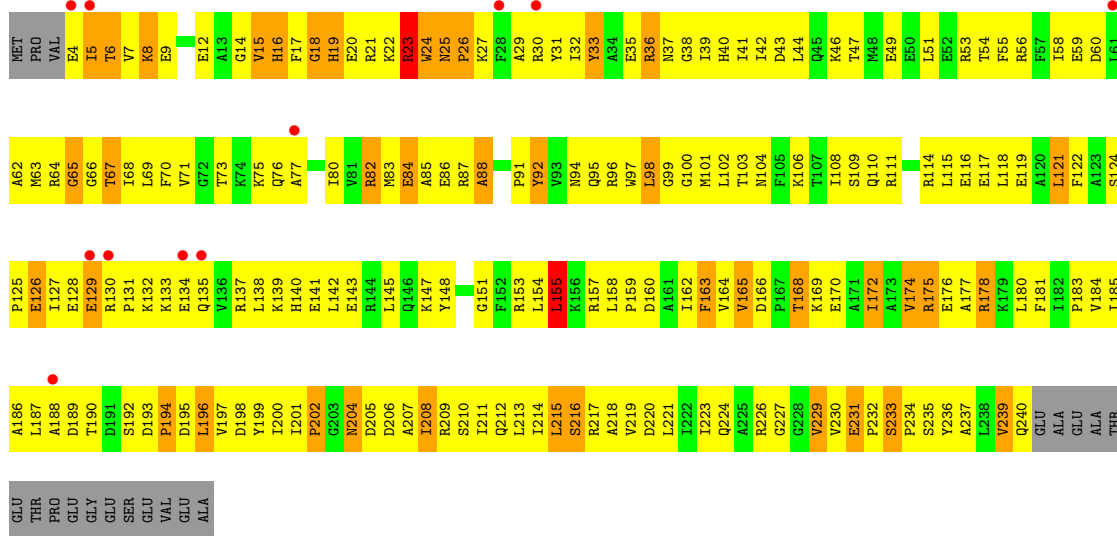




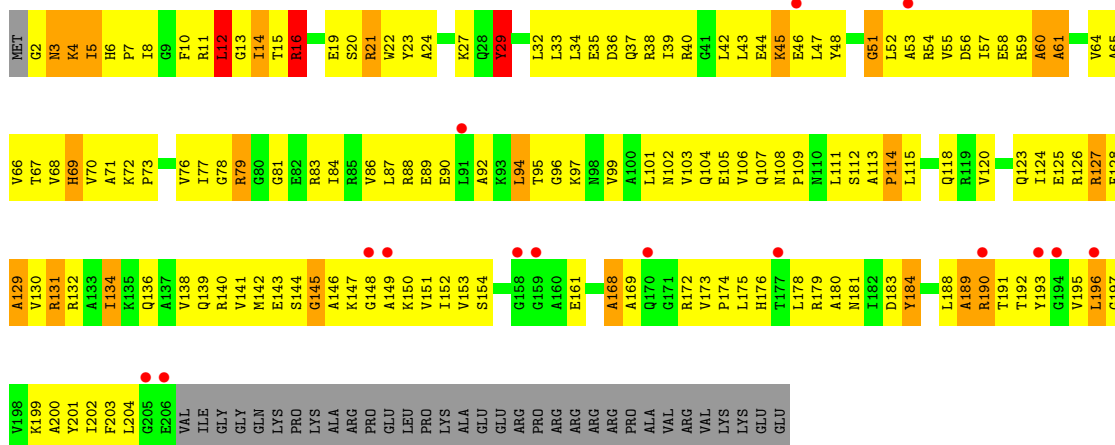
• Molecule 2: 30S ribosomal protein S2



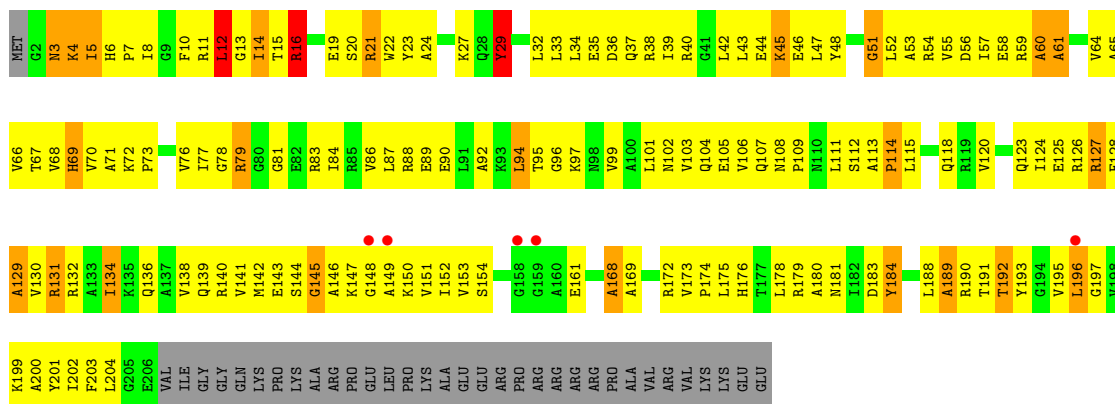
• Molecule 2: 30S ribosomal protein S2



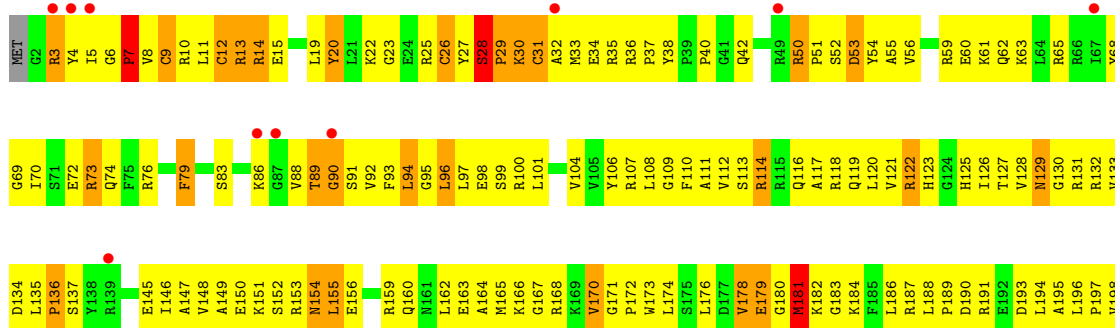
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4



M199
E200
Q201
L202
V203
I204
F206
F207
Y206
S208
R209

• Molecule 4: 30S ribosomal protein S4

Chain XD: 2% 24% 62% 12%

MET G2 R3 Y4 I5 G6 P7 V8 C9 R10 L11 L12 C12 R13 R14 E15 G16 L19 Y20 L21 K22 G23 E24 R25 C26 Y27 S28 P29 R30 C31 A32 R33 E34 R35 R36 P37 Y38 Q42 R49 R50 P51 S52 D53 Y54 A55 V56 R59 E60 K61 Q62 K63 L64 R65 R66 Y67 G69

I70 S71 E72 R73 R76 F79 S83 L84 G86 G87 V88 T89 S91 Y92 F93 L94 G95 L96 L97 R98 S99 R100 L101 V104 V105 Y106 R107 L108 F110 A111 V112 S113 R114 Q116 A117 R118 Q119 L120 V121 R122 D123 G124 I125 T126 T127 V128 N129 G130 R131 R132 Y133 L135

P136 S137 E145 I146 A147 V148 A149 E150 L151 S152 R153 N154 L155 R159 Q160 F161 L162 E163 A164 M165 R166 G167 R168 K169 V170 G171 P172 W173 L174 S175 D177 F178 E179 G180 M181 G183 K184 F185 L186 R187 L188 P189 D190 R191 E192 D193 L196 P197 V198 N199 E200 Q201 L202 V203

I204
E205
F206
Y207
S208
R209

• Molecule 5: 30S ribosomal protein S5

Chain QE: 6% 28% 52% 12% 7%

MET PRD THR D5 F6 E7 M10 L11 L12 I13 R14 R15 T16 A17 R18 M19 Q20 A21 G22 G23 R24 R25 F26 R27 F28 L31 V32 V33 D36 R37 Q38 V41 G42 L43 G44 F45 G46 K47 A48 P49 E50 V51 P52 L53 A54 V55 Q56 K57 T105 P106 L107 A108 I109 L110 E111 L112 A113 G114 V115 T116 V56 Q56 K57 T120 G124 S125 A62 R63 G69 Y61 A62 R64

R65 M66 V67 E68 V69 L71 Q72 M73 G74 T75 I76 P77 H78 E79 R80 E81 V82 E83 F84 G85 A86 A87 K88 R89 V90 L91 K92 P93 A94 A95 P96 G99 I101 A102 V105 P106 L107 A108 I109 L110 E111 L112 A113 G114 V115 T116 L117 I118 L119 T120 G124 S125 A62 R63 G69 Y61 A62 R64

I129 M130 I131 A132 D133 A134 T135 M136 R140 Q141 L142 L143 R144 T144 F145 D146 V148 F149 R150 L151 R152 K153 G154 E155 ALA HIS ALA GLN ALA GLN GLY

• Molecule 5: 30S ribosomal protein S5

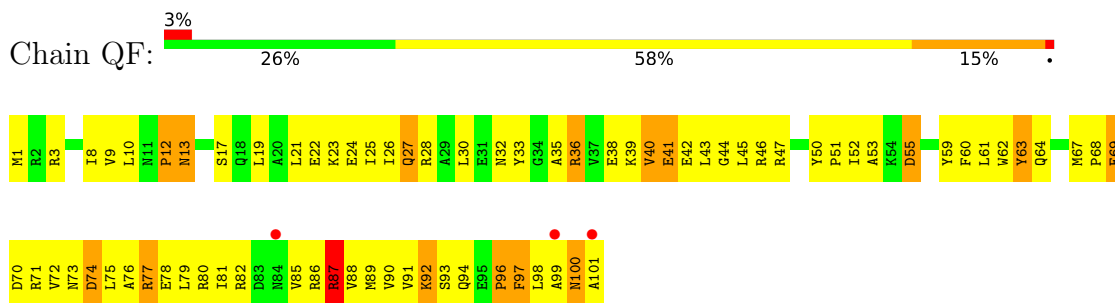
Chain XE: 4% 30% 51% 12% 7%

MET PRD GLU THR D5 F6 E7 M10 L11 L12 I13 R14 R15 T16 A17 Q20 A21 R24 R25 F26 L31 V32 V33 D36 R37 Q38 V41 G42 L43 G44 F45 G46 K47 A48 P49 E50 V51 P52 L53 A54 V55 Q56 K57 T105 P106 L107 A108 I109 L110 E111 L112 A113 G114 V115 T116 V56 Q56 K57 T120 G124 S125 A62 R63 G69 Y61 A62 R64

P70 L71 Q72 M73 T75 I76 P77 H78 E79 I80 E81 V82 E83 F84 G85 A86 A87 K88 R89 V90 L91 K92 P93 A94 A95 P96 G99 I101 A102 V105 P106 L107 A108 I109 L110 E111 L112 A113 G114 V115 T116 L117 I118 L119 T120 G124 S125 A62 R63 G69 Y61 A62 R64

A134 I135 M136 R140 Q141 L142 L143 R144 T144 K145 D146 V148 E149 R150 L151 R152 K153 G154 E155 ALA HIS ALA GLN ALA GLN GLY

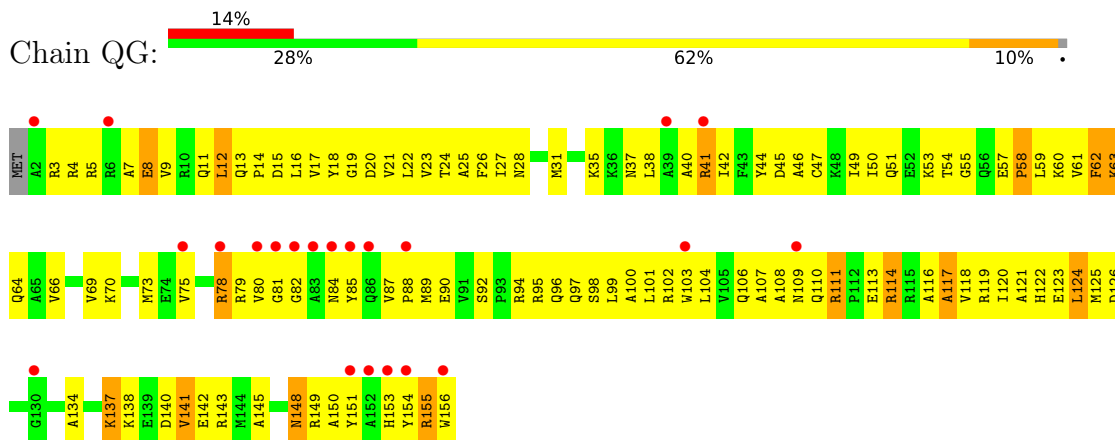
• Molecule 6: 30S ribosomal protein S6



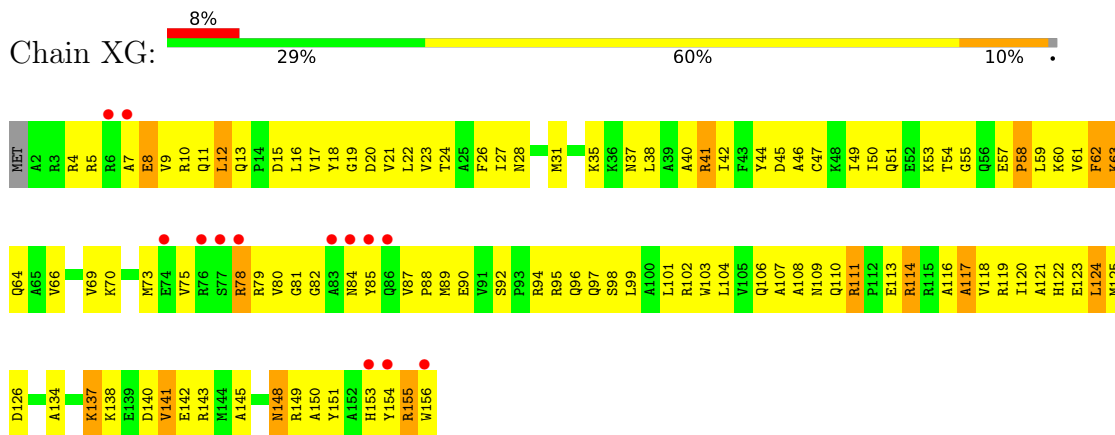
• Molecule 6: 30S ribosomal protein S6



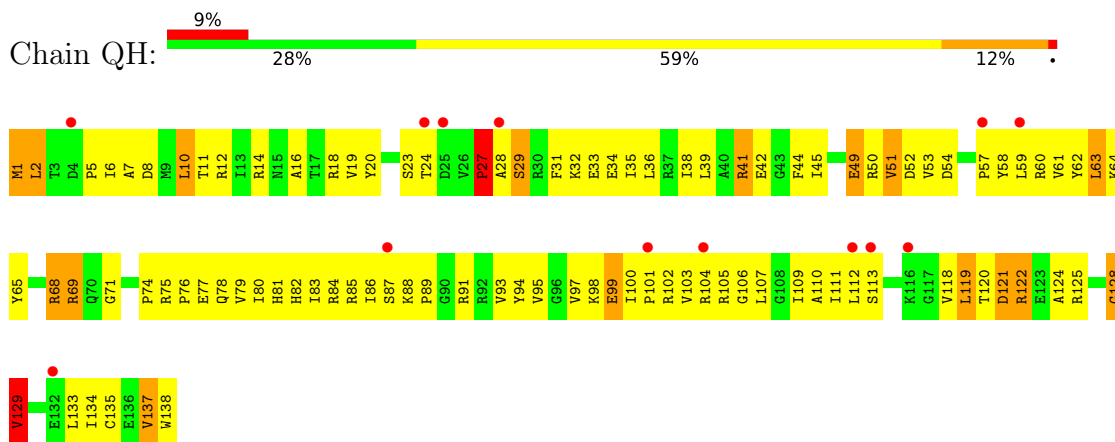
• Molecule 7: 30S ribosomal protein S7



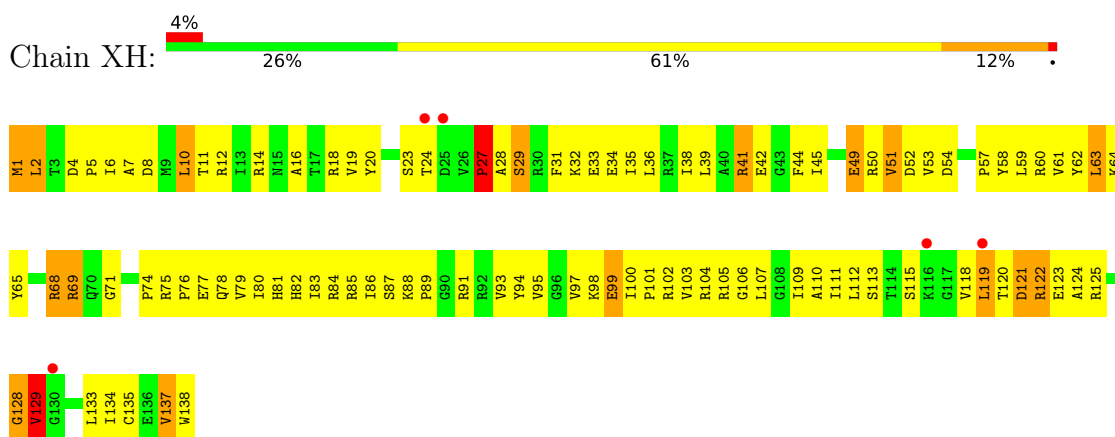
• Molecule 7: 30S ribosomal protein S7



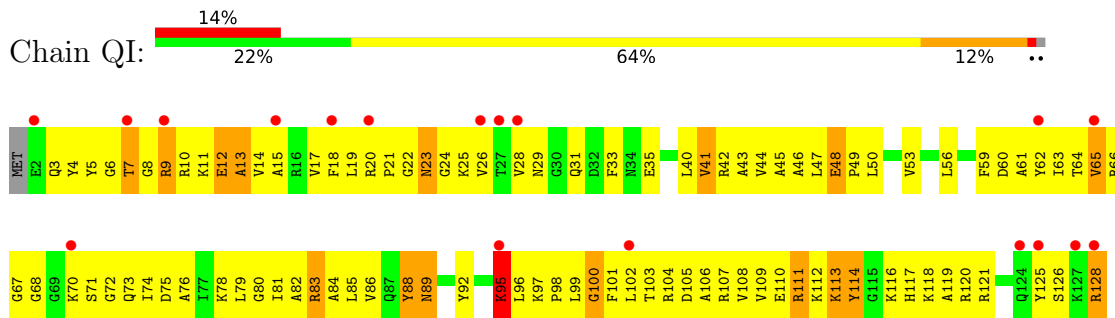
• Molecule 8: 30S ribosomal protein S8



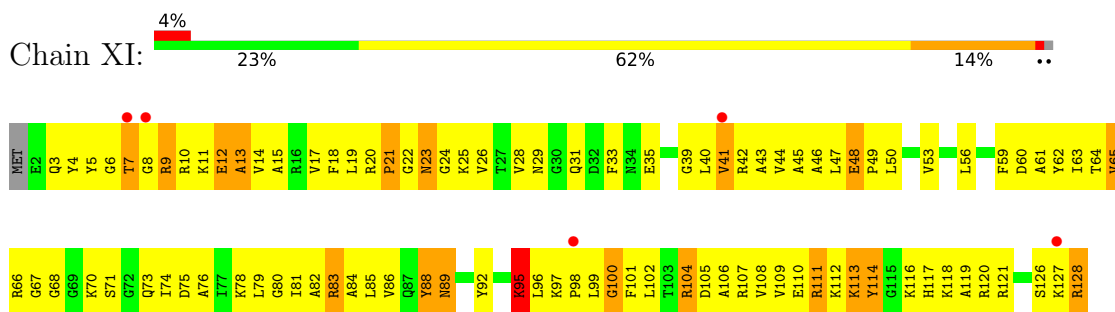
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

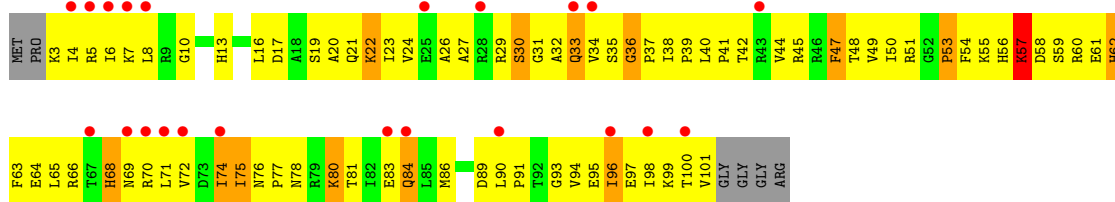


- Molecule 9: 30S ribosomal protein S9



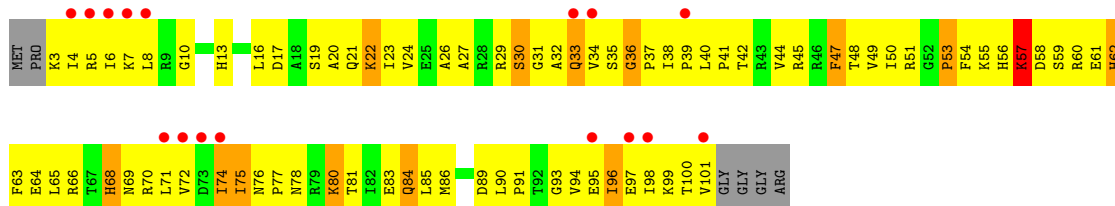
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 21%
18% 63% 12% 6%



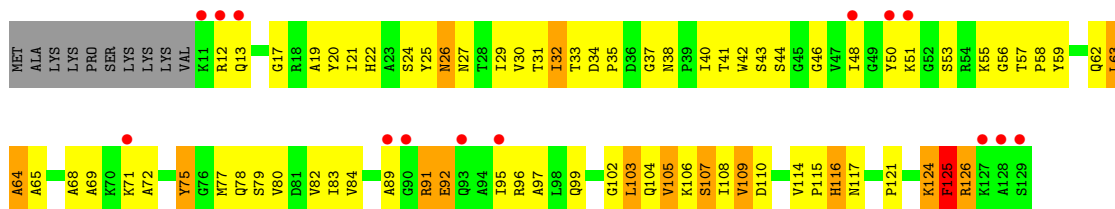
• Molecule 10: 30S ribosomal protein S10

Chain XJ: 15%
17% 64% 12% 6%



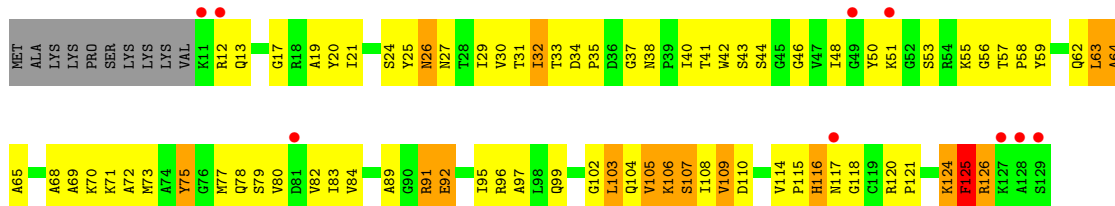
• Molecule 11: 30S ribosomal protein S11

Chain QK: 11%
34% 47% 11% 8%



• Molecule 11: 30S ribosomal protein S11

Chain XK: 7%
32% 48% 12% 8%



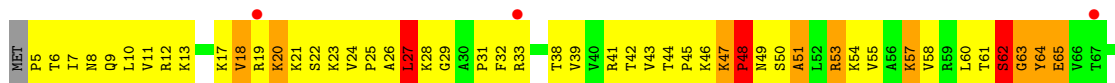
• Molecule 12: 30S ribosomal protein S12

Chain QL: 11%
31% 47% 14% 5%

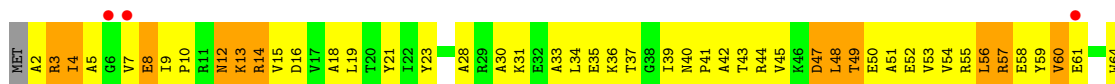




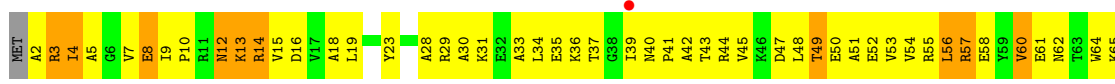
- Molecule 12: 30S ribosomal protein S12



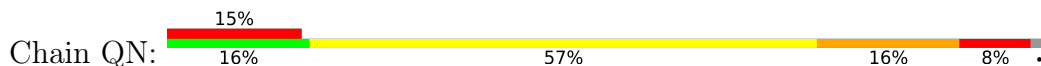
- Molecule 13: 30S ribosomal protein S13



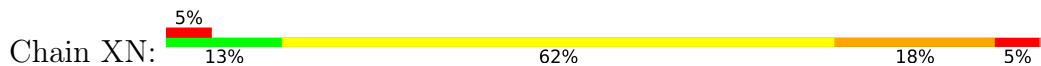
- Molecule 13: 30S ribosomal protein S13

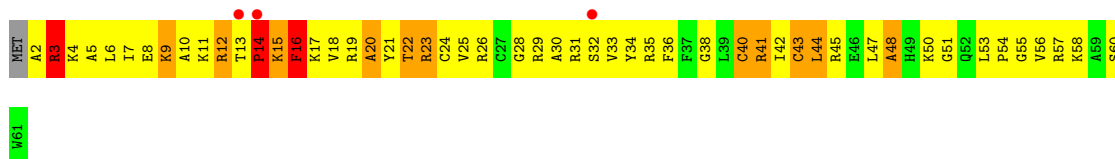


- Molecule 14: 30S ribosomal protein S14

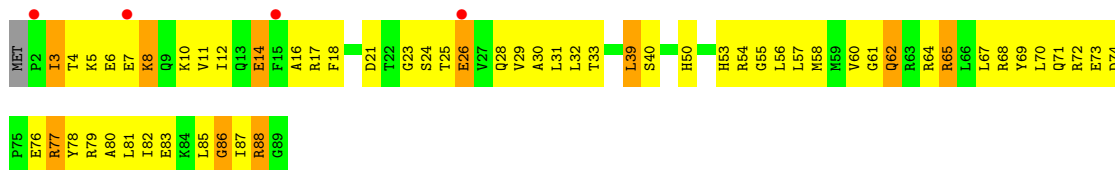


- Molecule 14: 30S ribosomal protein S14

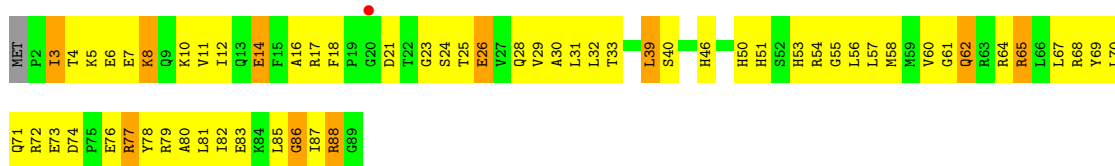




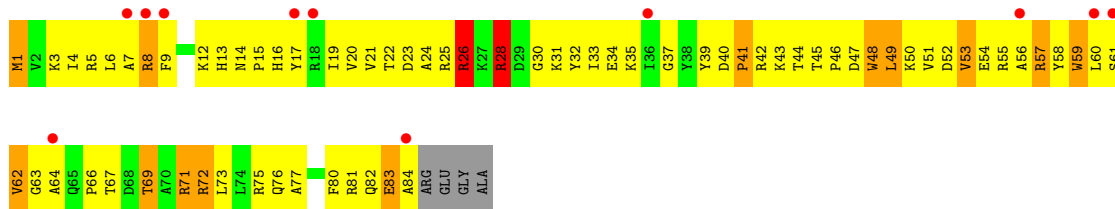
• Molecule 15: 30S ribosomal protein S15



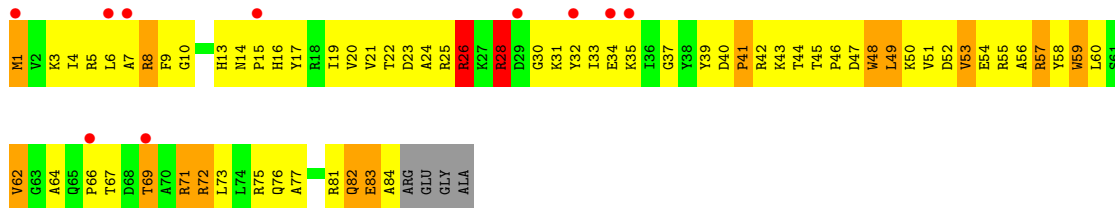
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16

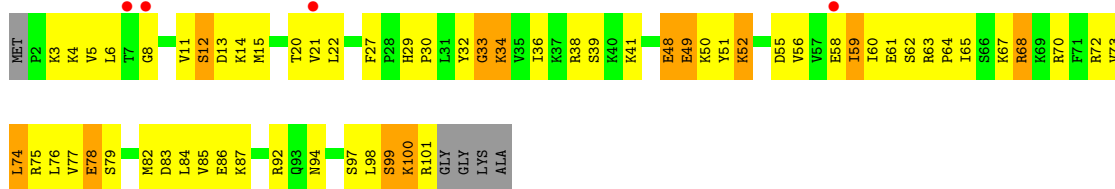


• Molecule 16: 30S ribosomal protein S16



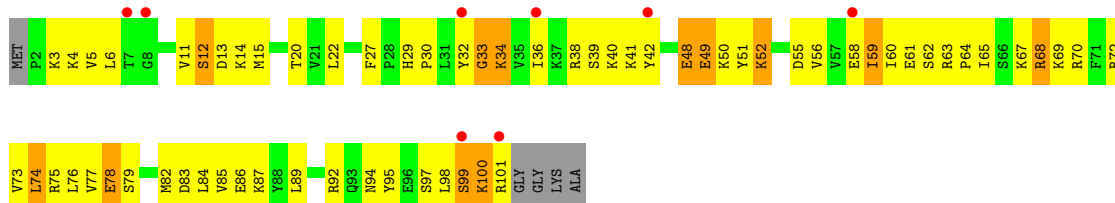
• Molecule 17: 30S ribosomal protein S17

Chain QQ: 4% 36% 48% 11% 5%



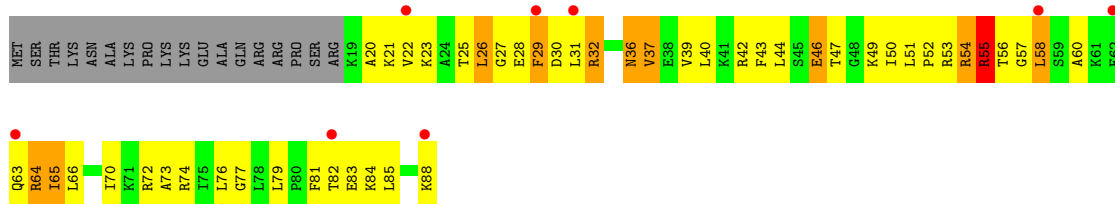
• Molecule 17: 30S ribosomal protein S17

Chain XQ: 8% 33% 50% 11% 5%



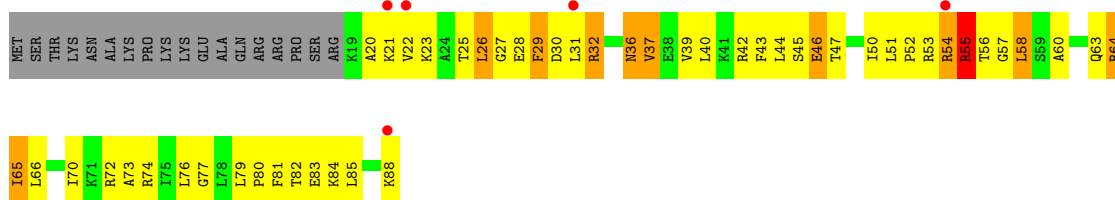
• Molecule 18: 30S ribosomal protein S18

Chain QR: 9% 24% 43% 11% 20%



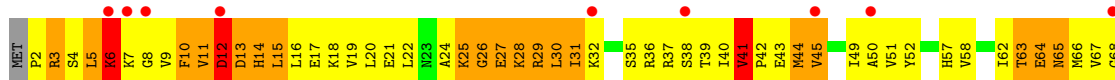
• Molecule 18: 30S ribosomal protein S18

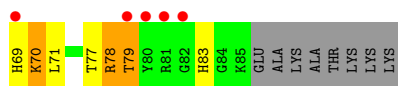
Chain XR: 6% 23% 44% 11% 20%



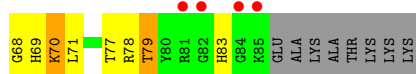
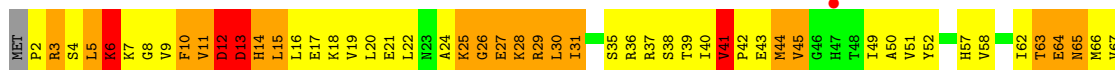
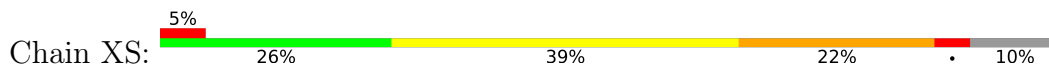
• Molecule 19: 30S ribosomal protein S19

Chain QS: 15% 25% 39% 24% 10%

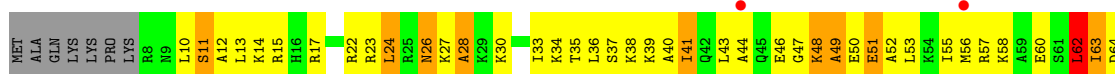




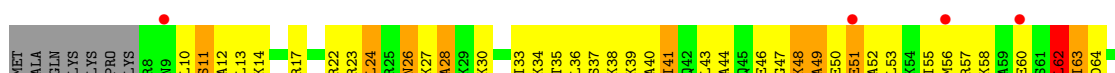
- Molecule 19: 30S ribosomal protein S19



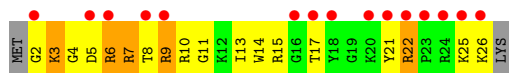
- Molecule 20: 30S ribosomal protein S20



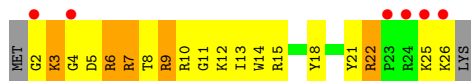
- Molecule 20: 30S ribosomal protein S20



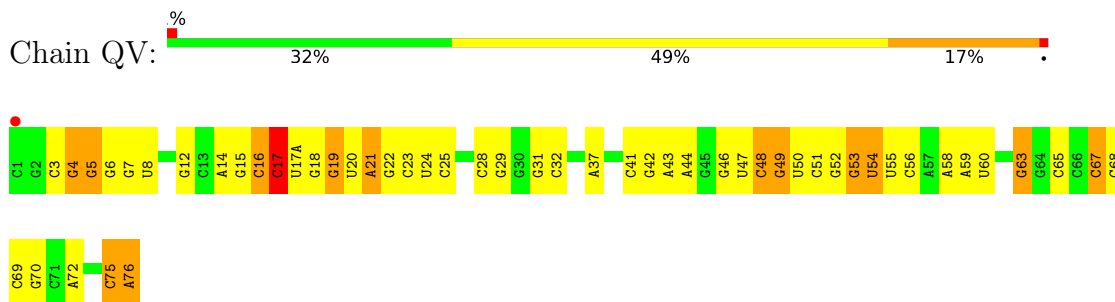
- Molecule 21: 30S ribosomal protein S21



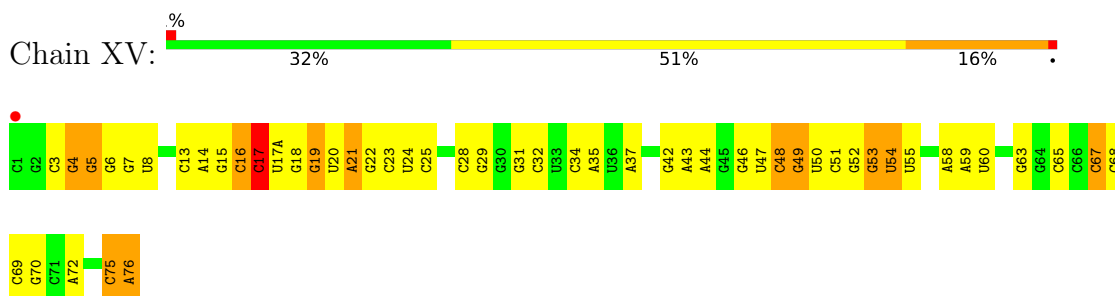
- Molecule 21: 30S ribosomal protein S21



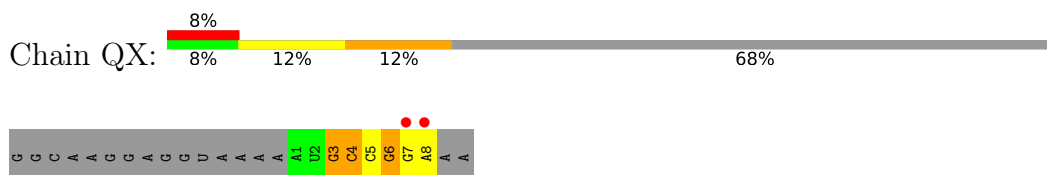
- Molecule 22: P-site tRNA fMet



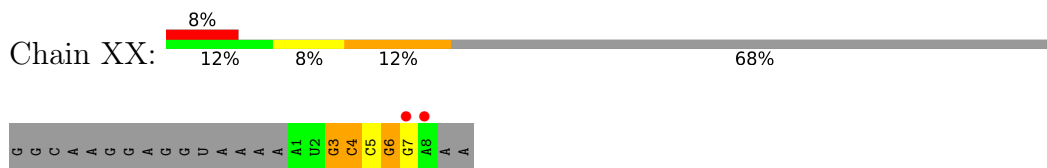
- Molecule 22: P-site tRNA fMet



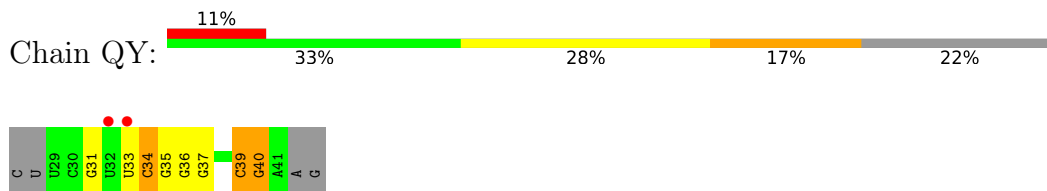
- Molecule 23: A-site ASL SufA6



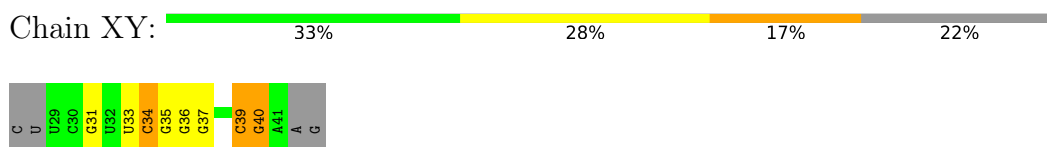
- Molecule 23: A-site ASL SufA6



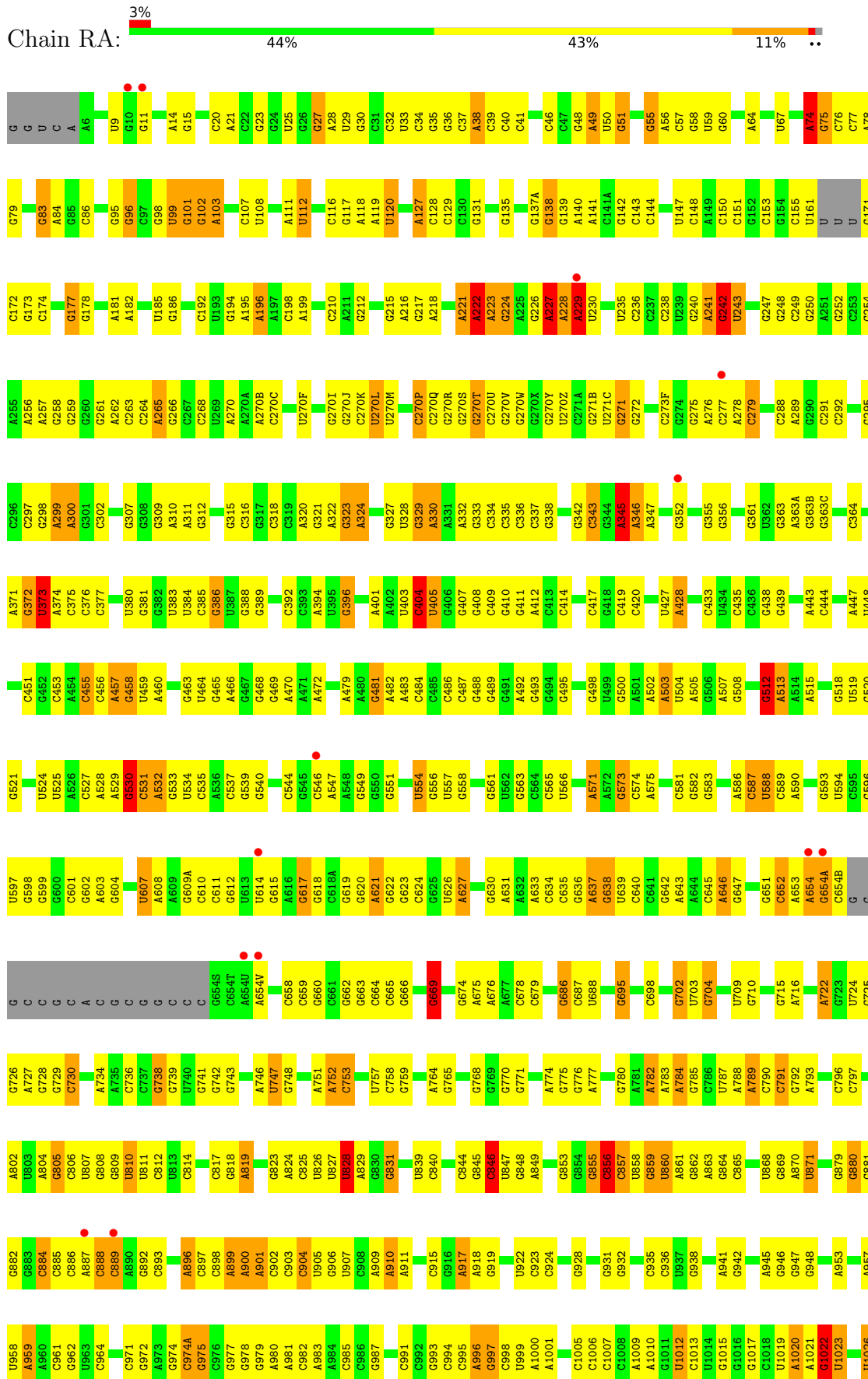
- Molecule 24: messenger RNA

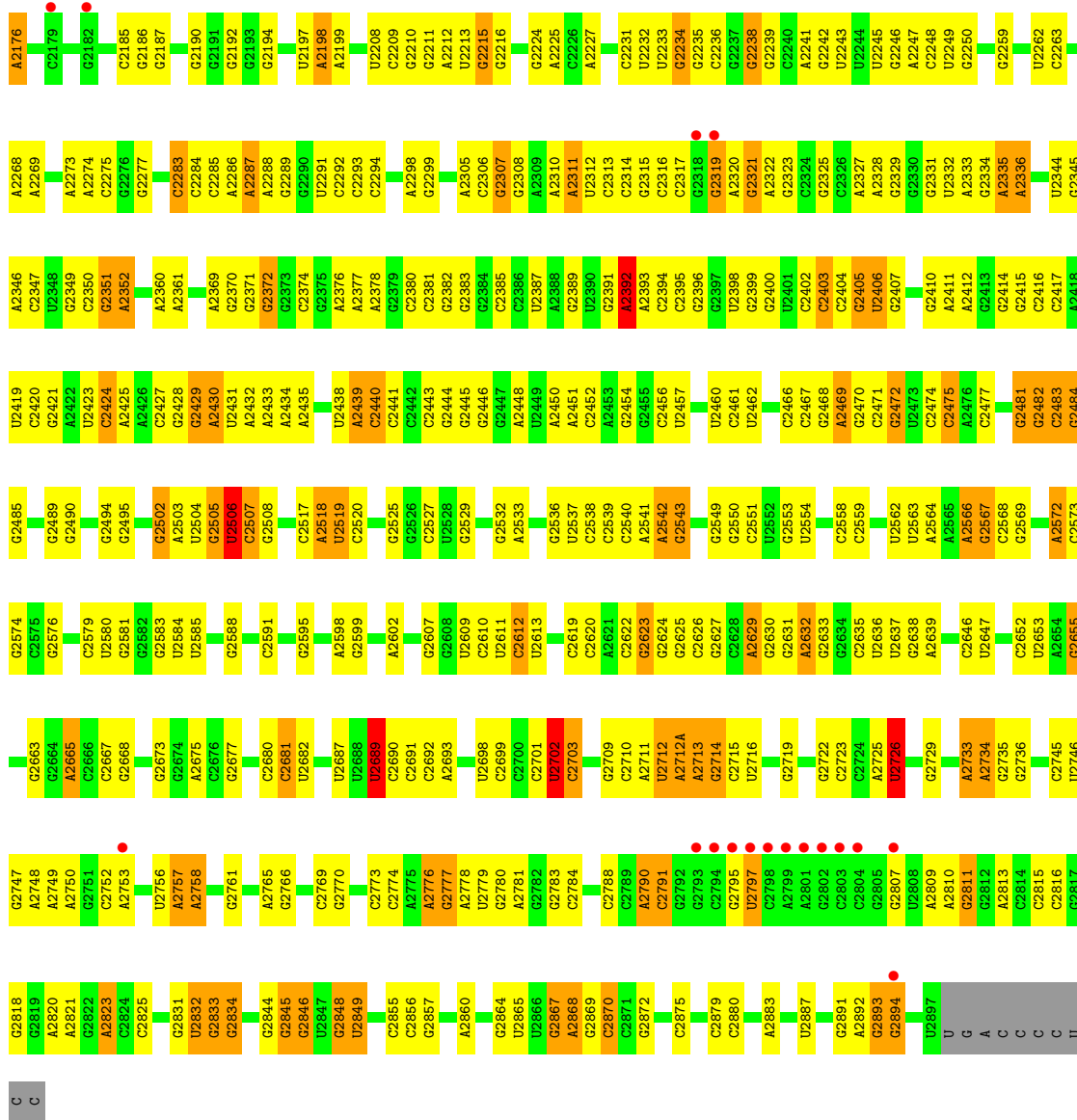


- Molecule 24: messenger RNA

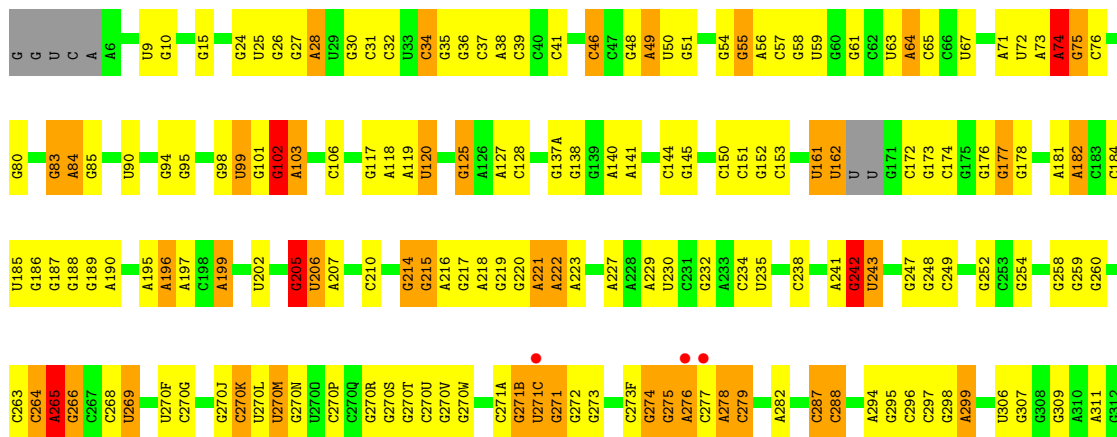
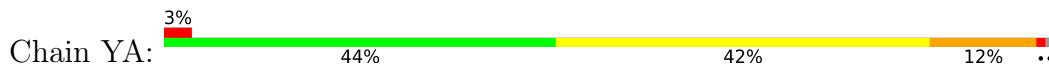


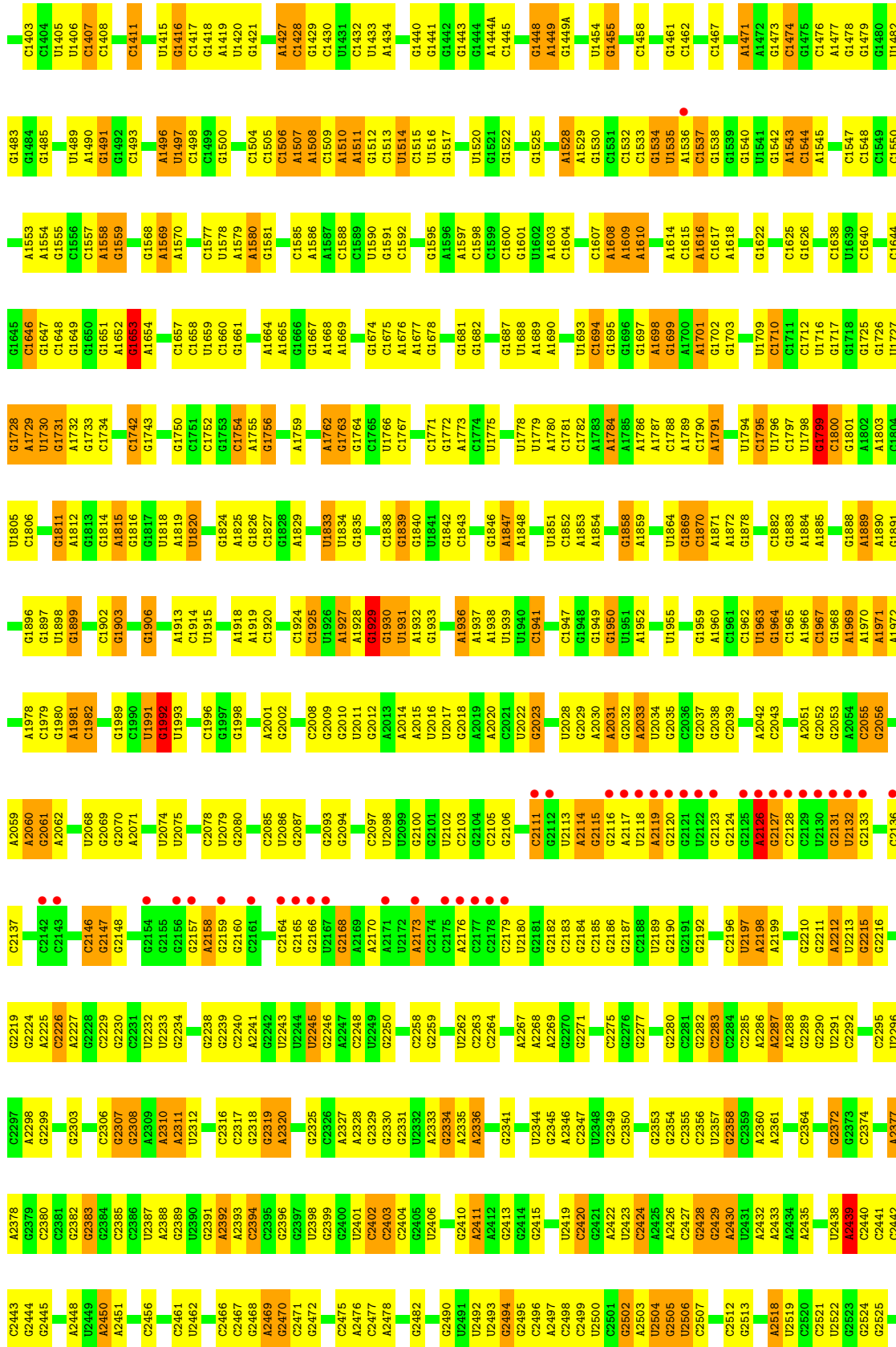
- Molecule 25: 23S rRNA

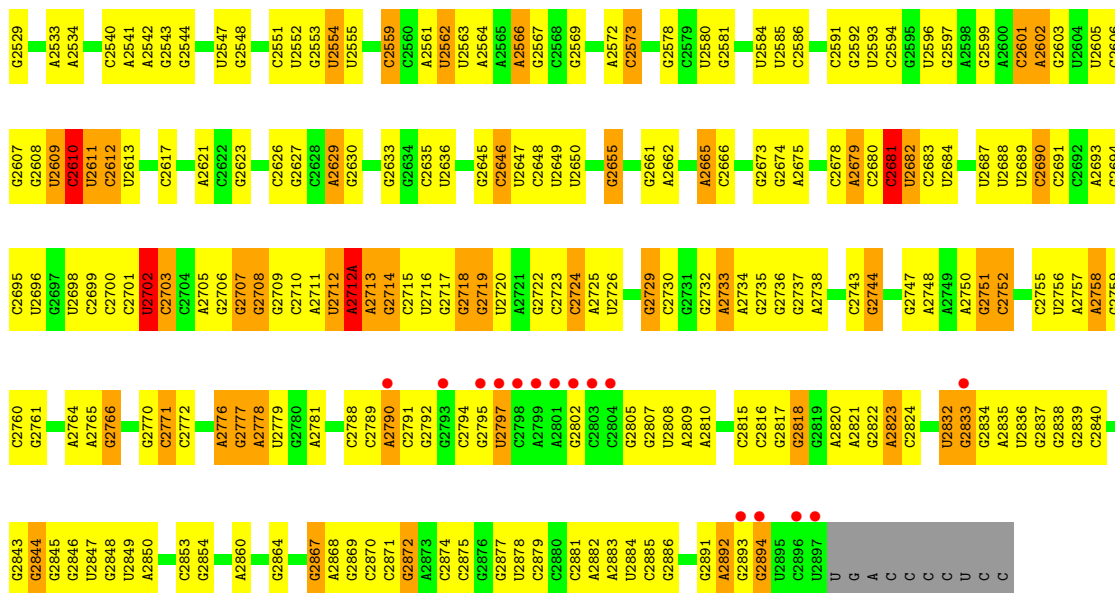




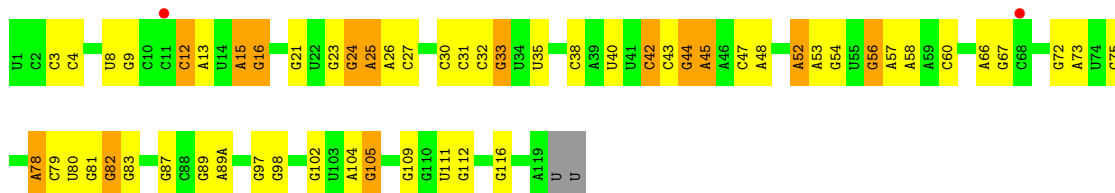
• Molecule 25: 23S rRNA



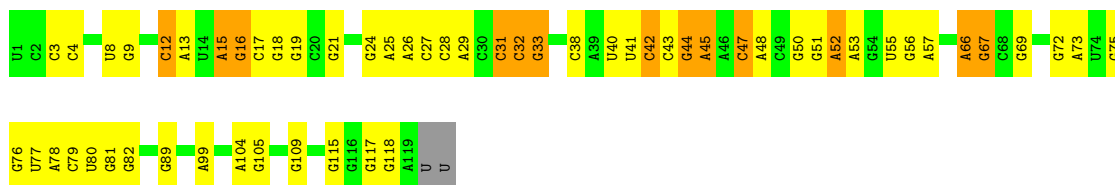




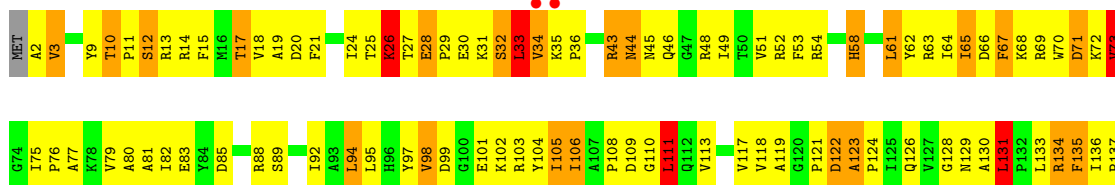
• Molecule 26: 5S rRNA

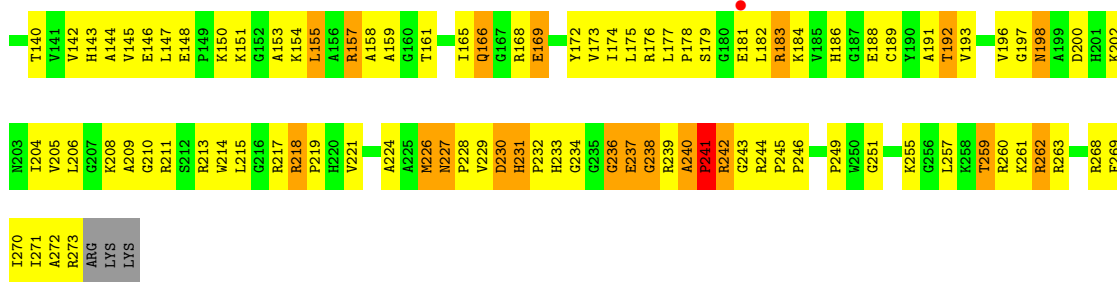


• Molecule 26: 5S rRNA

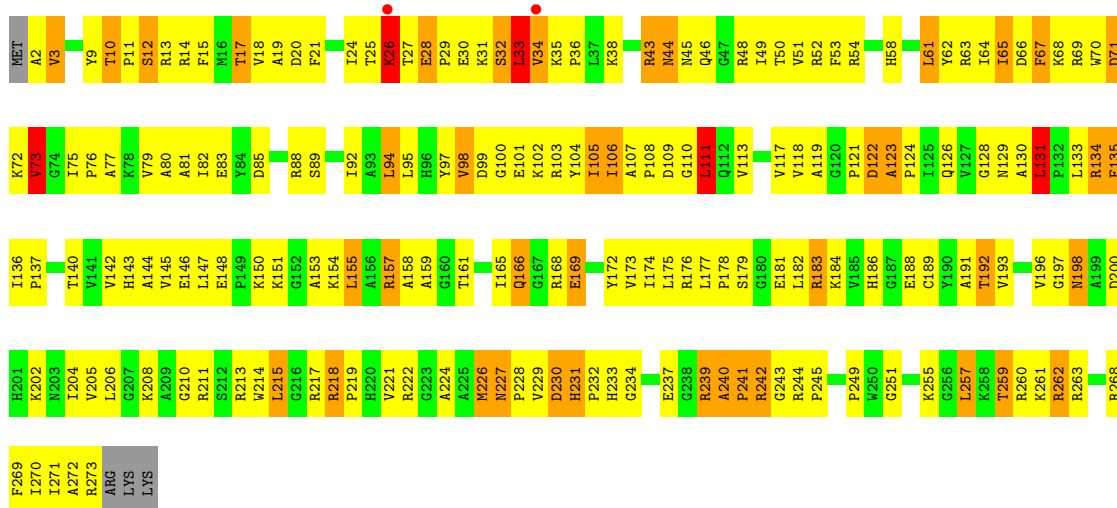


• Molecule 27: 50S ribosomal protein L2

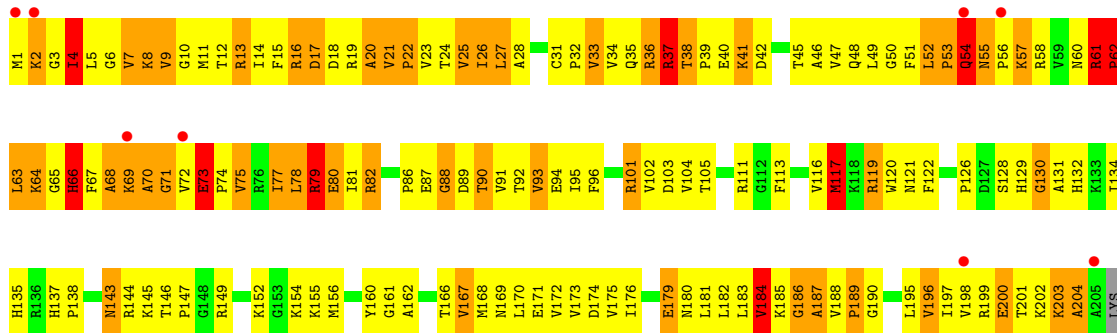




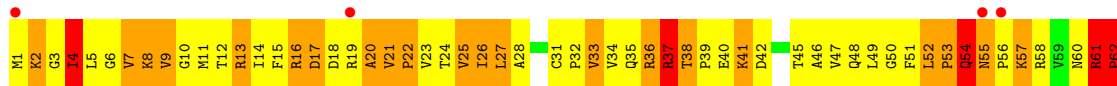
• Molecule 27: 50S ribosomal protein L2

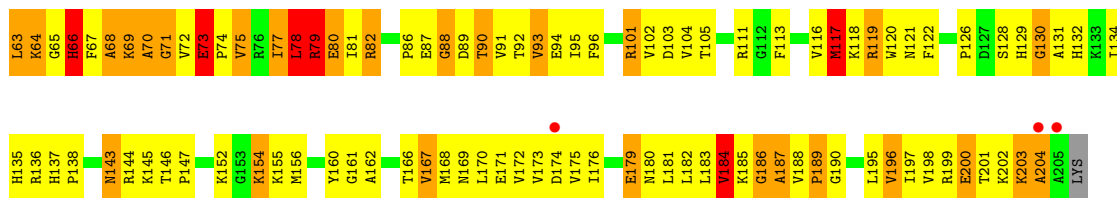


• Molecule 28: 50S ribosomal protein L3

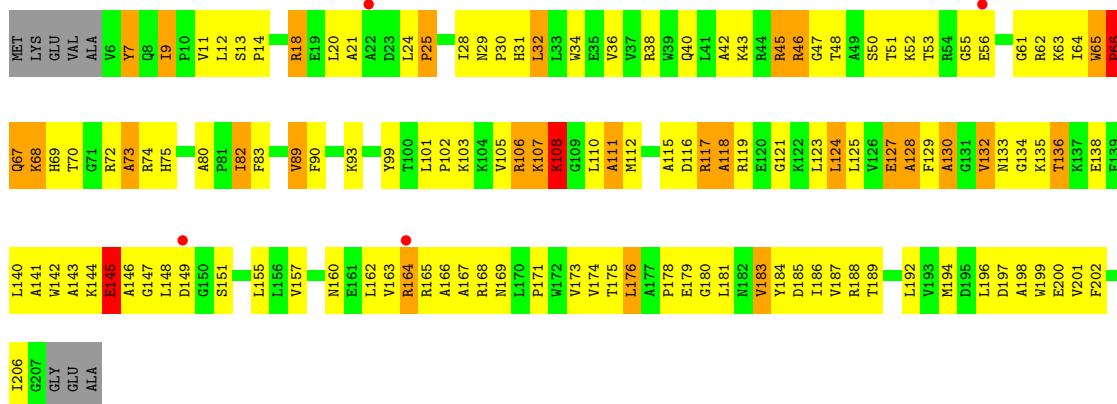


• Molecule 28: 50S ribosomal protein L3

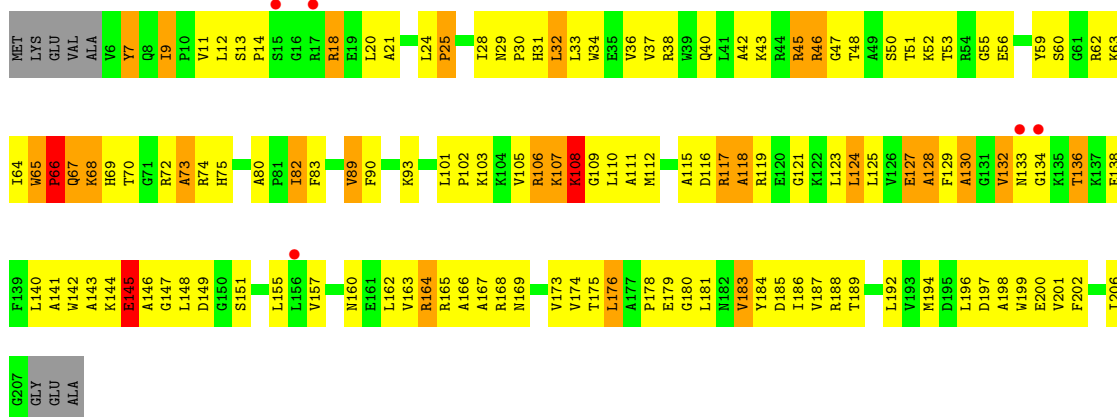




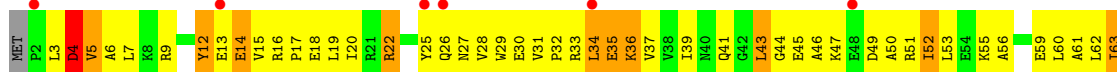
• Molecule 29: 50S ribosomal protein L4

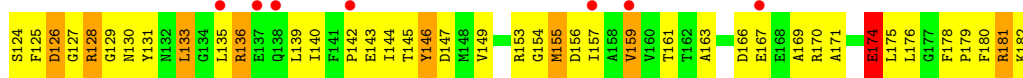


• Molecule 29: 50S ribosomal protein L4

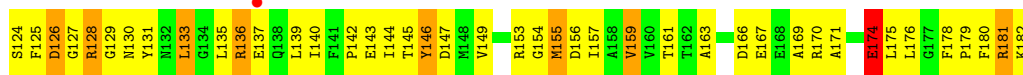


• Molecule 30: 50S ribosomal protein L5

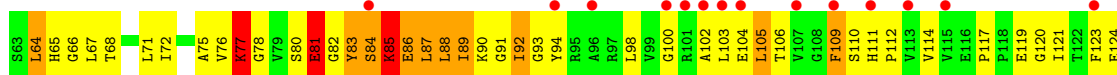
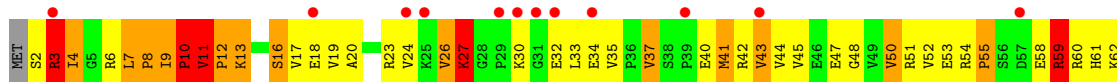
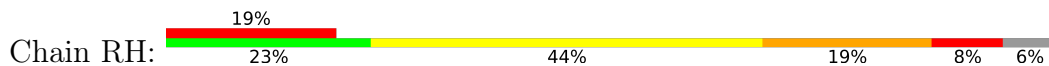




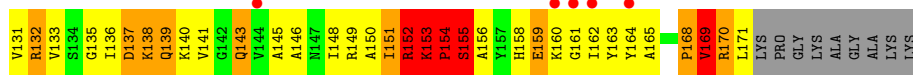
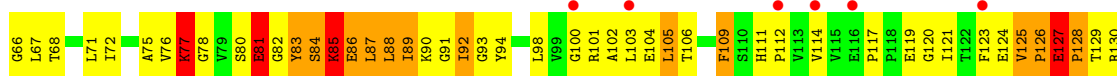
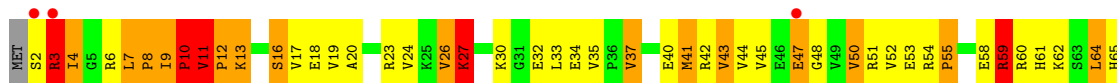
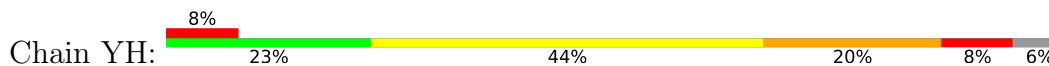
• Molecule 30: 50S ribosomal protein L5



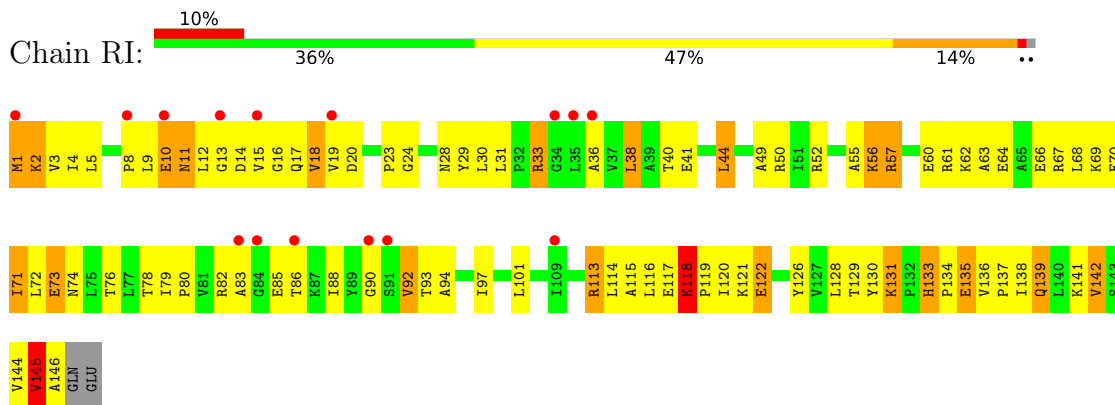
• Molecule 31: 50S ribosomal protein L6



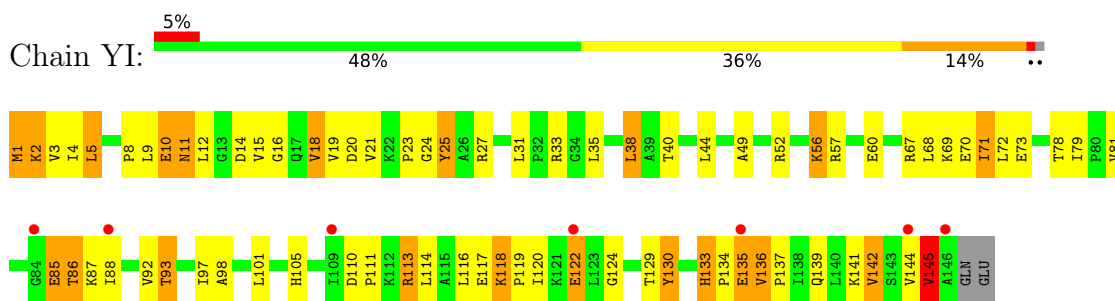
• Molecule 31: 50S ribosomal protein L6



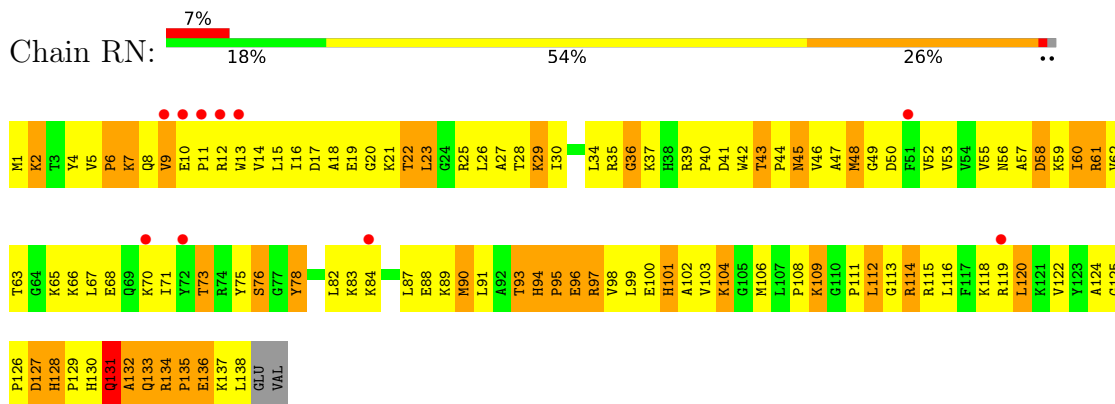
• Molecule 32: 50S ribosomal protein L9



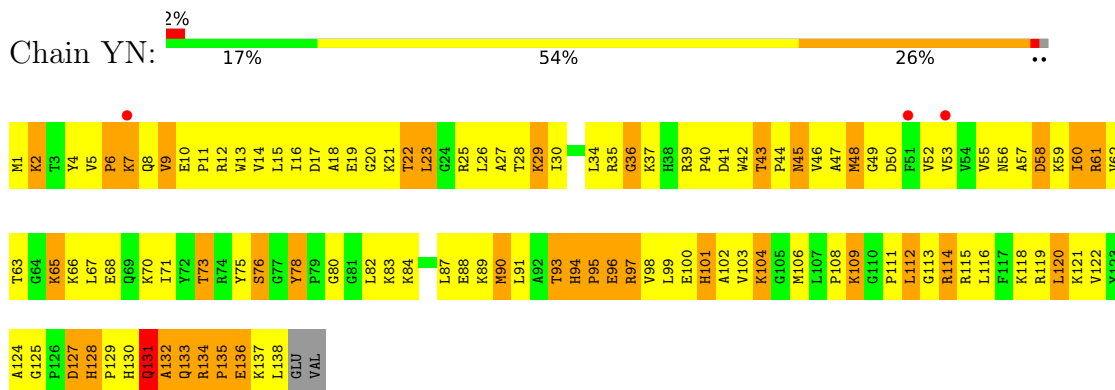
• Molecule 32: 50S ribosomal protein L9



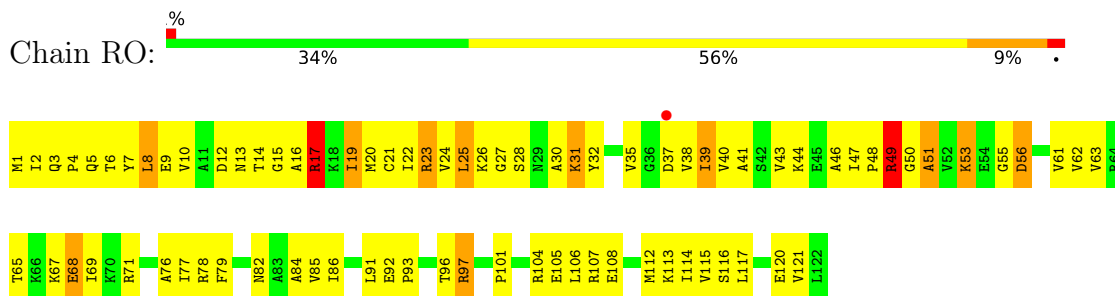
• Molecule 33: 50S ribosomal protein L13



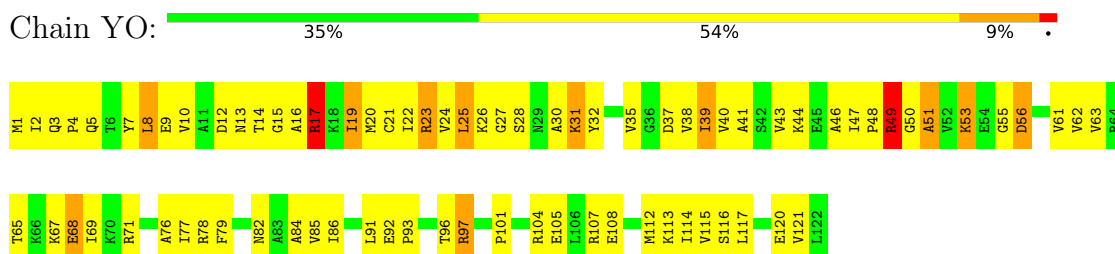
• Molecule 33: 50S ribosomal protein L13



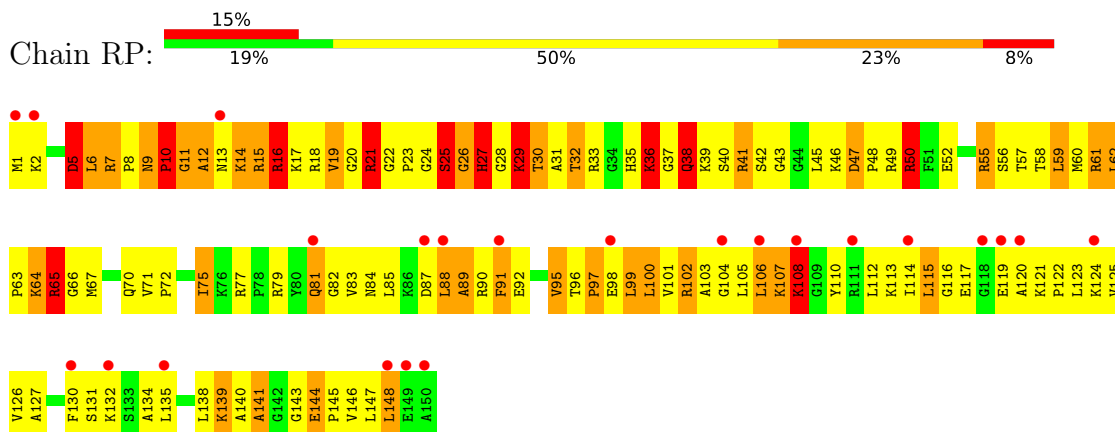
- Molecule 34: 50S ribosomal protein L14



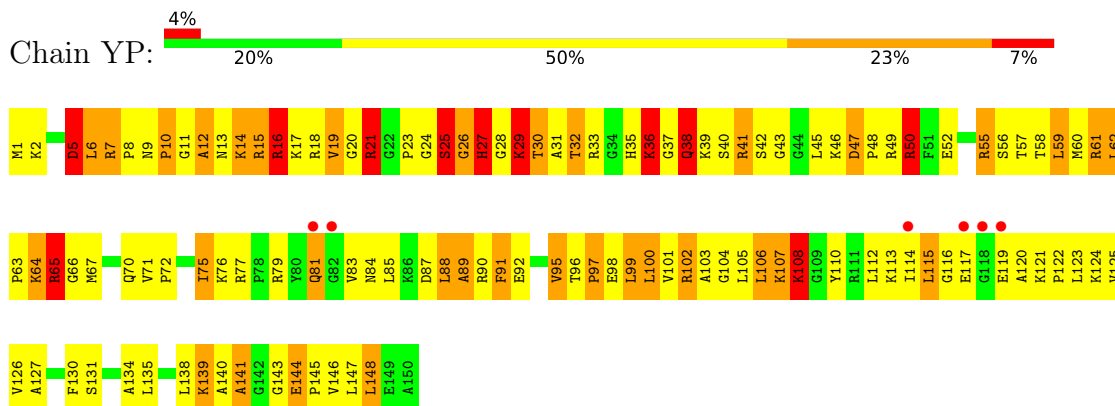
- Molecule 34: 50S ribosomal protein L14



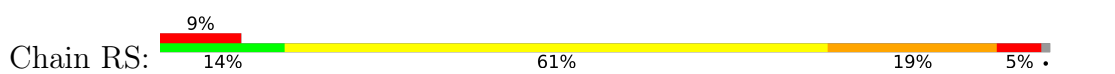
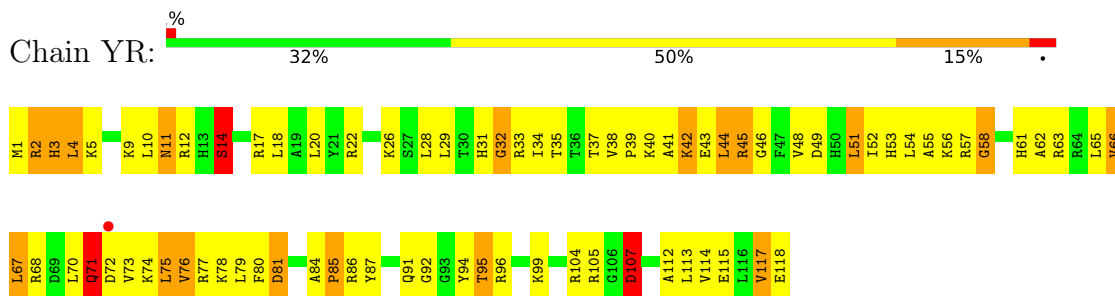
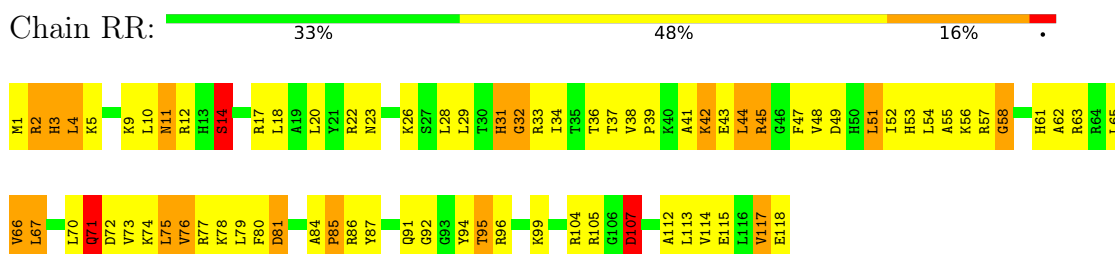
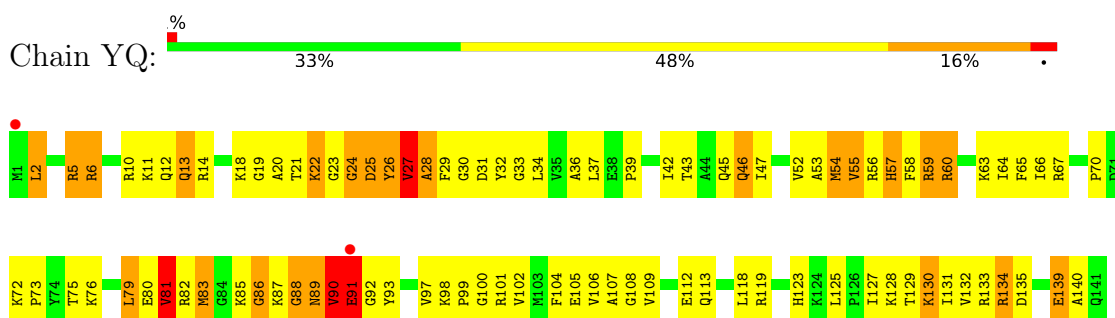
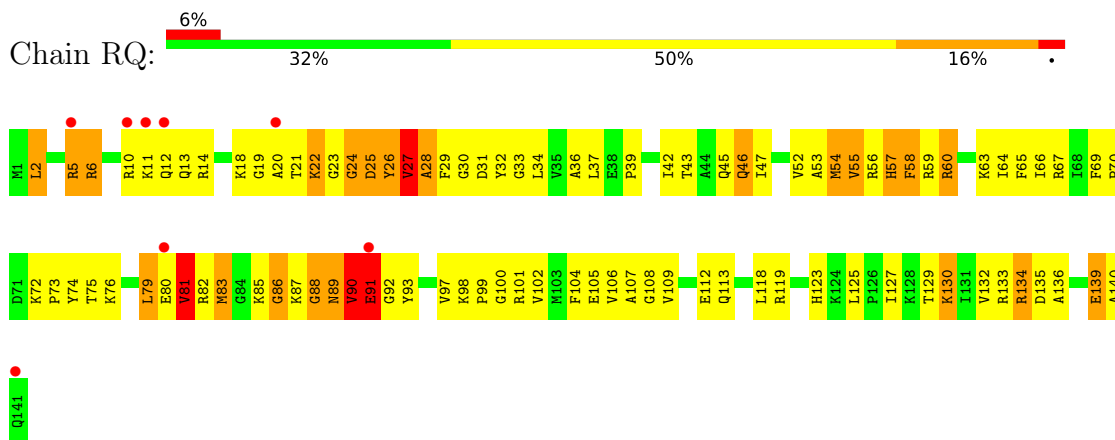
- Molecule 35: 50S ribosomal protein L15

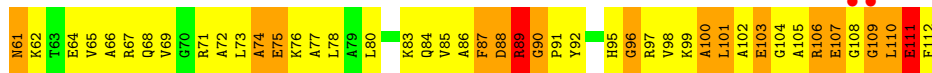
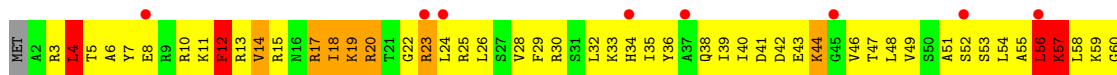


- Molecule 35: 50S ribosomal protein L15

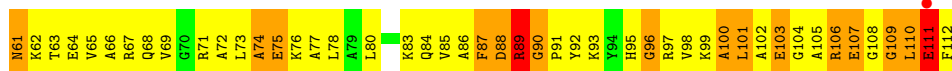
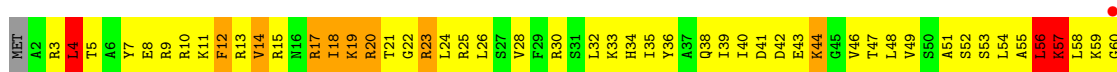
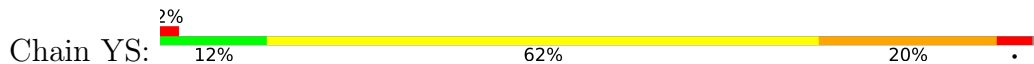


- Molecule 36: 50S ribosomal protein L16

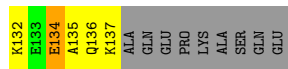




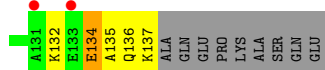
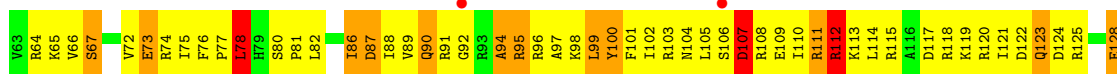
• Molecule 38: 50S ribosomal protein L18



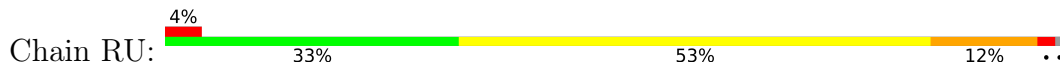
• Molecule 39: 50S ribosomal protein L19

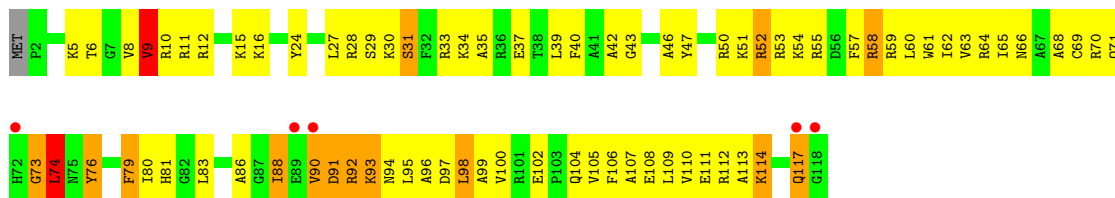


• Molecule 39: 50S ribosomal protein L19

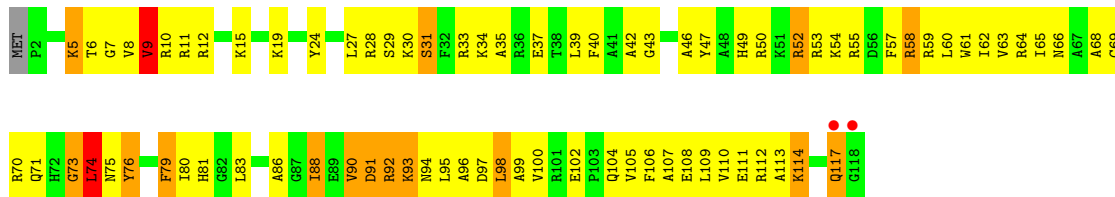


• Molecule 40: 50S ribosomal protein L20

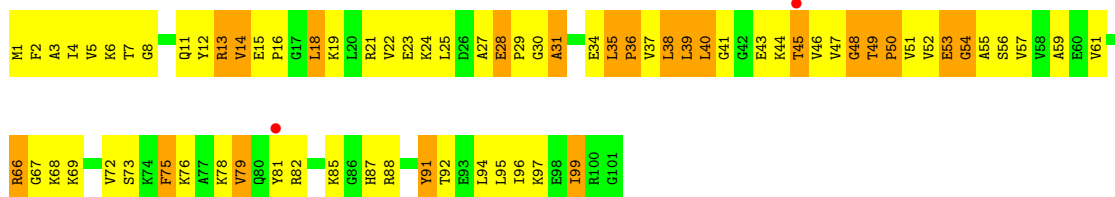




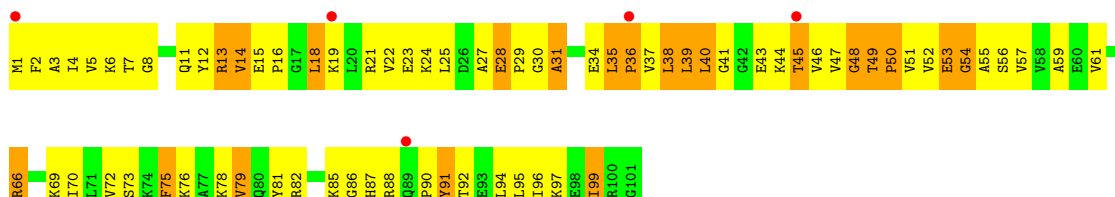
• Molecule 40: 50S ribosomal protein L20



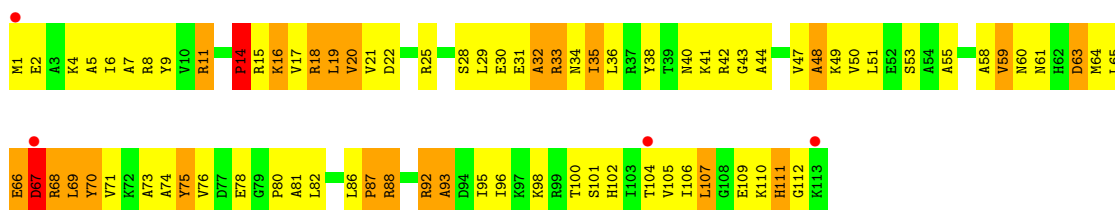
• Molecule 41: 50S ribosomal protein L21



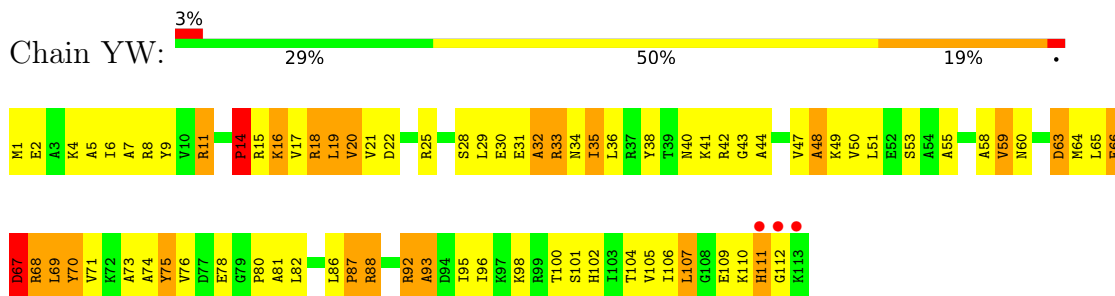
• Molecule 41: 50S ribosomal protein L21



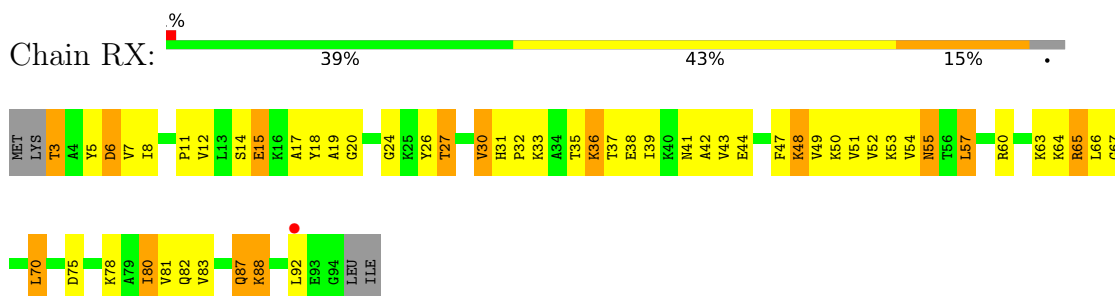
• Molecule 42: 50S ribosomal protein L22



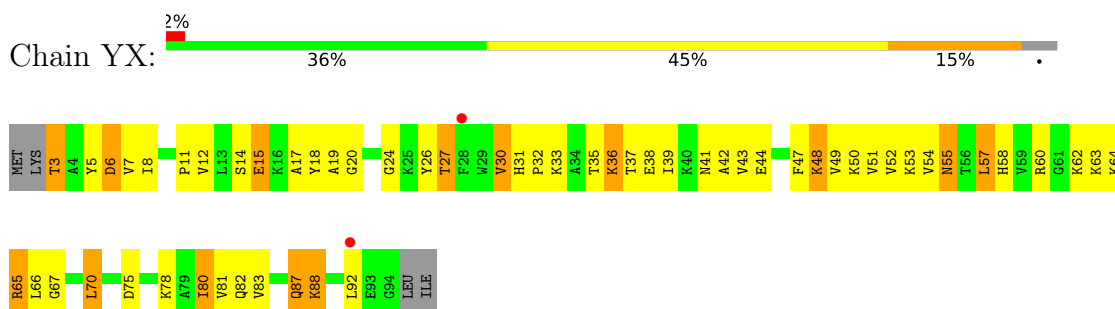
- Molecule 42: 50S ribosomal protein L22



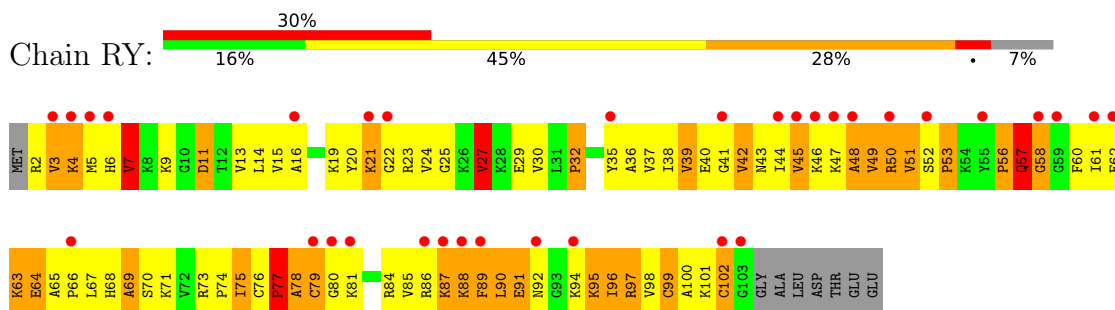
- Molecule 43: 50S ribosomal protein L23



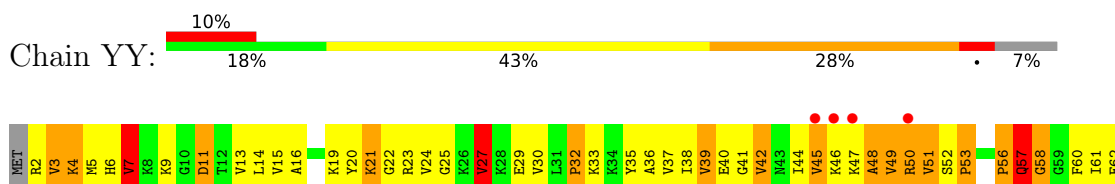
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24

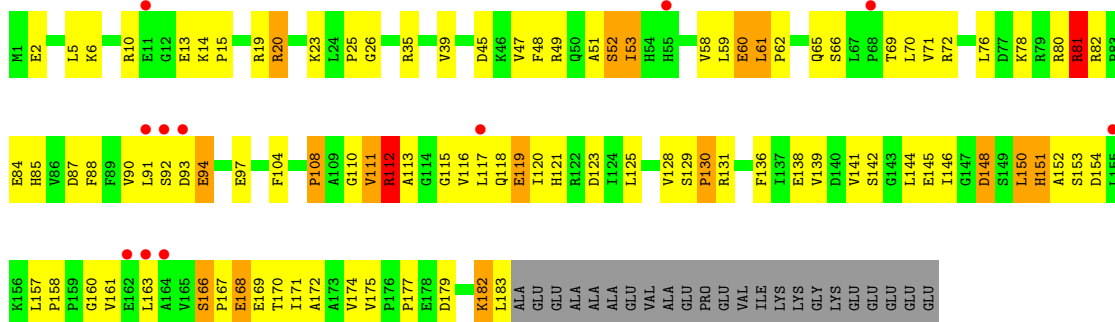


- Molecule 44: 50S ribosomal protein L24

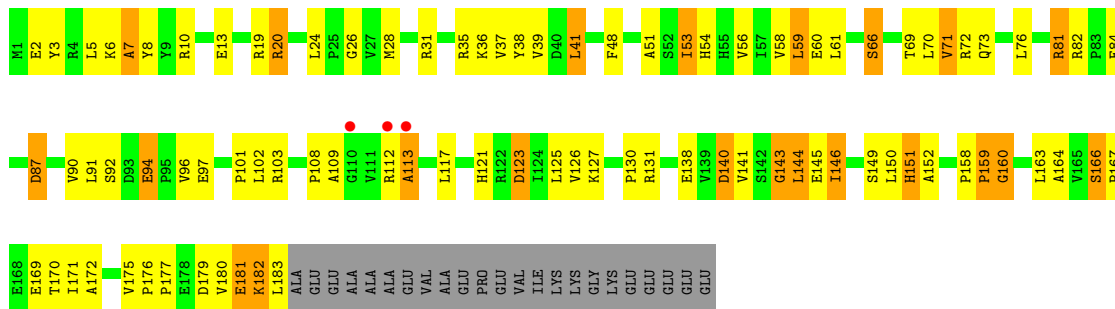




• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27

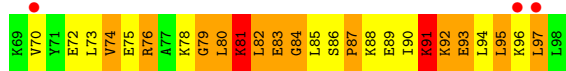


• Molecule 46: 50S ribosomal protein L27

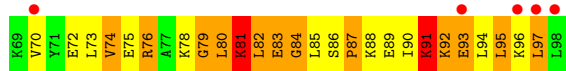


• Molecule 47: 50S ribosomal protein L28

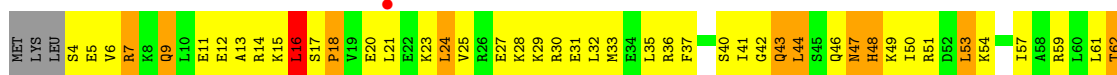




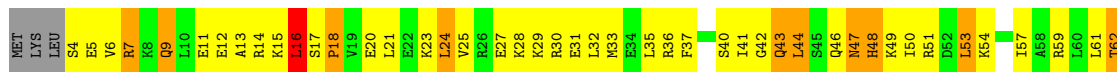
• Molecule 47: 50S ribosomal protein L28



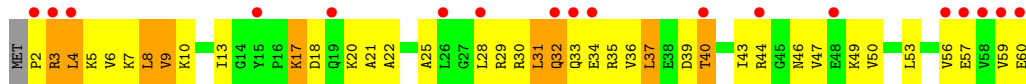
• Molecule 48: 50S ribosomal protein L29



• Molecule 48: 50S ribosomal protein L29

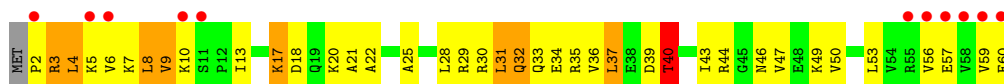


• Molecule 49: 50S ribosomal protein L30

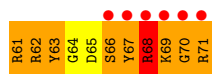
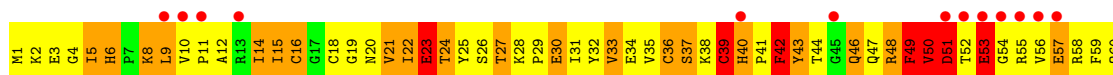


• Molecule 49: 50S ribosomal protein L30

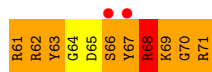




- Molecule 50: 50S ribosomal protein L31



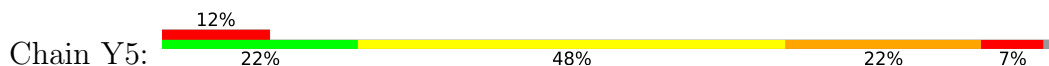
- Molecule 50: 50S ribosomal protein L31



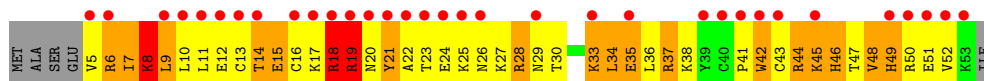
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32

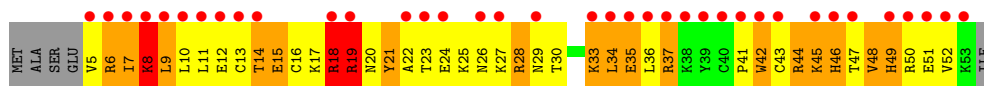


- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33





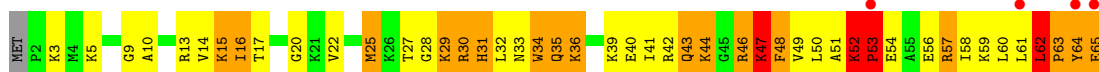
• Molecule 53: 50S ribosomal protein L34



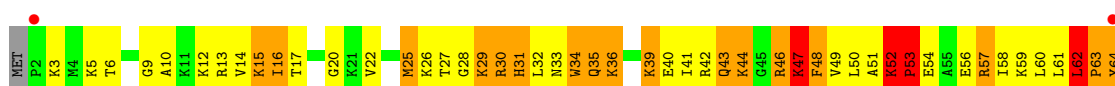
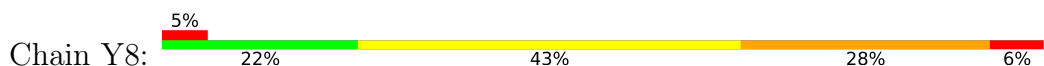
• Molecule 53: 50S ribosomal protein L34



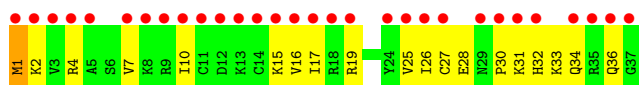
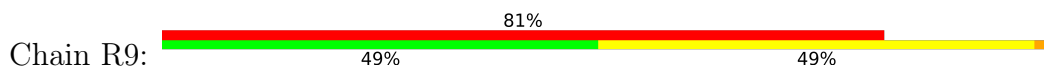
• Molecule 54: 50S ribosomal protein L35



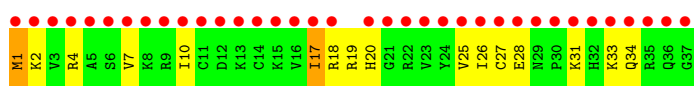
• Molecule 54: 50S ribosomal protein L35



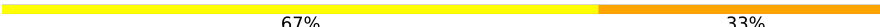
• Molecule 55: 50S ribosomal protein L36



• Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic

Chain Z6:  67% 33%

C74
C75
A76

- Molecule 56: tRNA acceptor end mimic

Chain Z8:  33% 67%

C74
C75
A76

4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 15046 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:YN:32:SER:CB	14:YN:41:ARG:HB3	1.23	1.55
14:YN:32:SER:HB3	14:YN:41:ARG:CB	1.28	1.54
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.36	1.52
4:QD:167:GLY:HA2	27:YD:135:PHE:CZ	1.42	1.52
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YV:51:VAL:N	51:Y5:60:VAL:O[4_445]	1.69	0.51
41:YV:50:PRO:CG	51:Y5:60:VAL:O[4_445]	1.99	0.21
31:YH:47:GLU:OE2	44:YY:79:CYS:CB[4_445]	2.03	0.17
41:YV:51:VAL:CB	51:Y5:60:VAL:OXT[4_445]	2.07	0.13
11:QK:99:GLN:NE2	3:XC:79:ARG:NH2[4_555]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

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

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

5 of 1477 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

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

5 of 2096 RNA backbone outliers are listed below:

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

5 of 221 RNA pucker outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 17 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

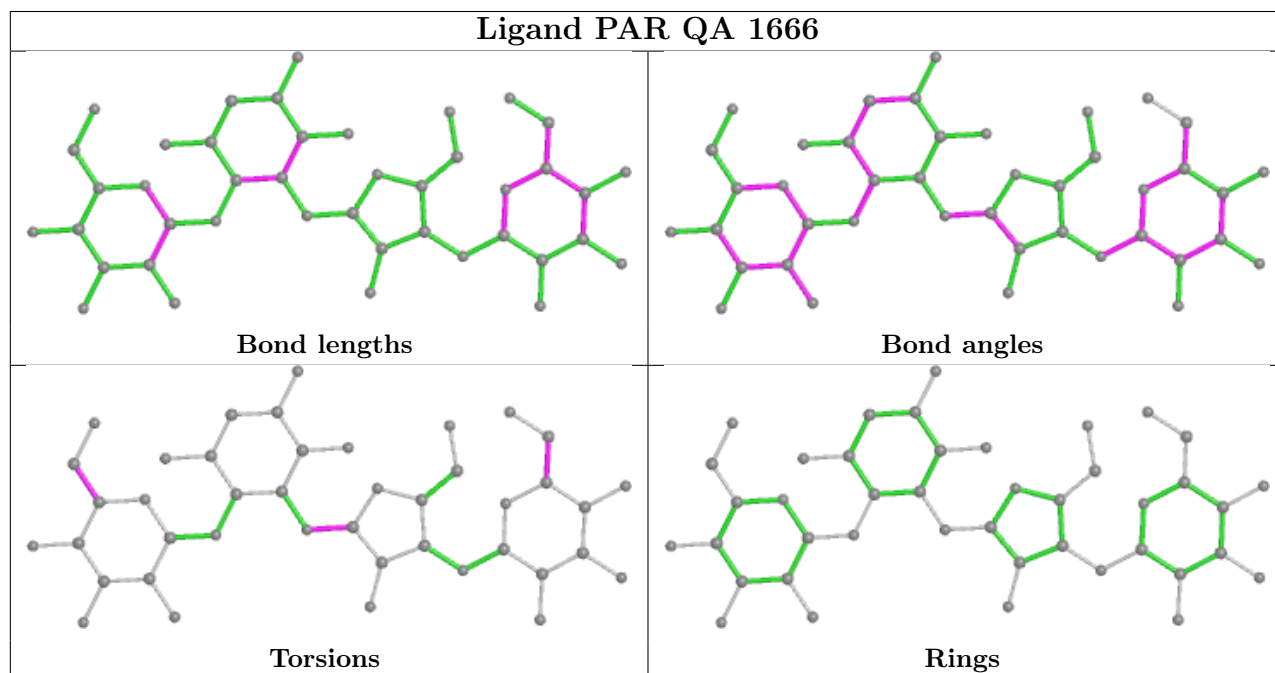
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1671	PAR	C44-C54-C64-N64
58	XA	1671	PAR	O54-C54-C64-N64
58	XA	1671	PAR	O51-C51-C61-O61

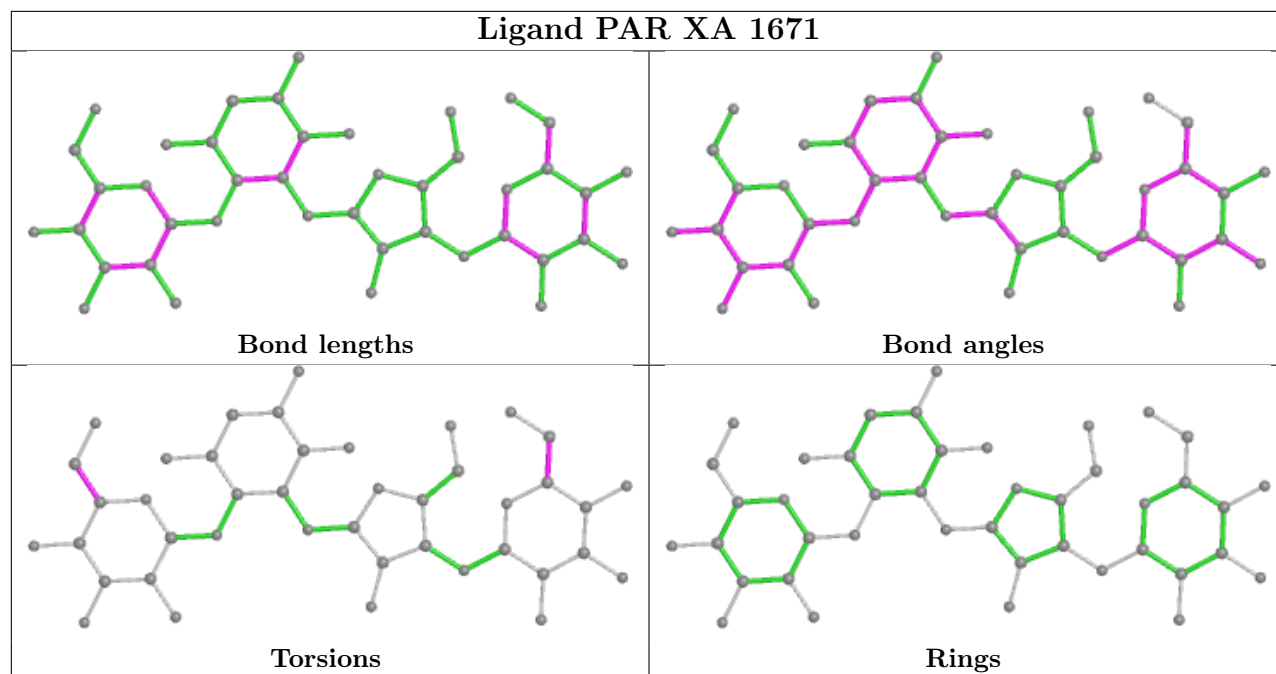
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

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

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

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

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

The worst 5 of 1135 RSRZ outliers are listed below:

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

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

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

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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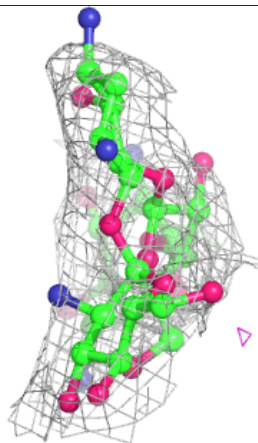
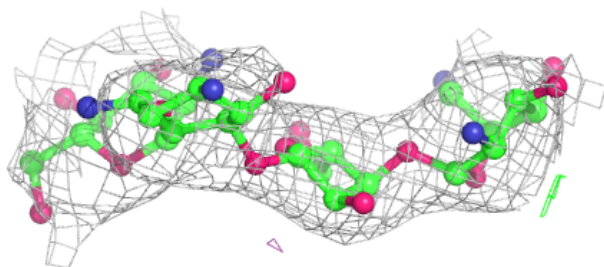
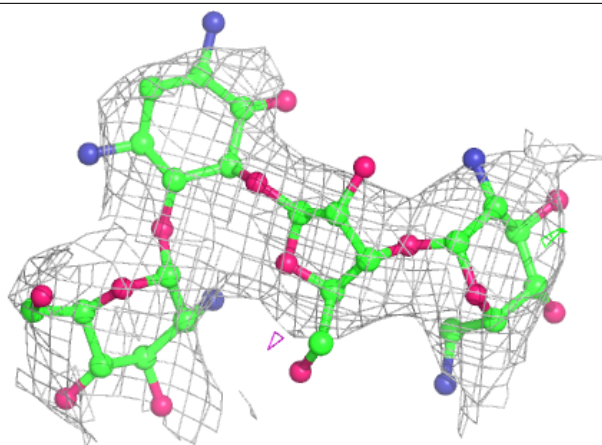
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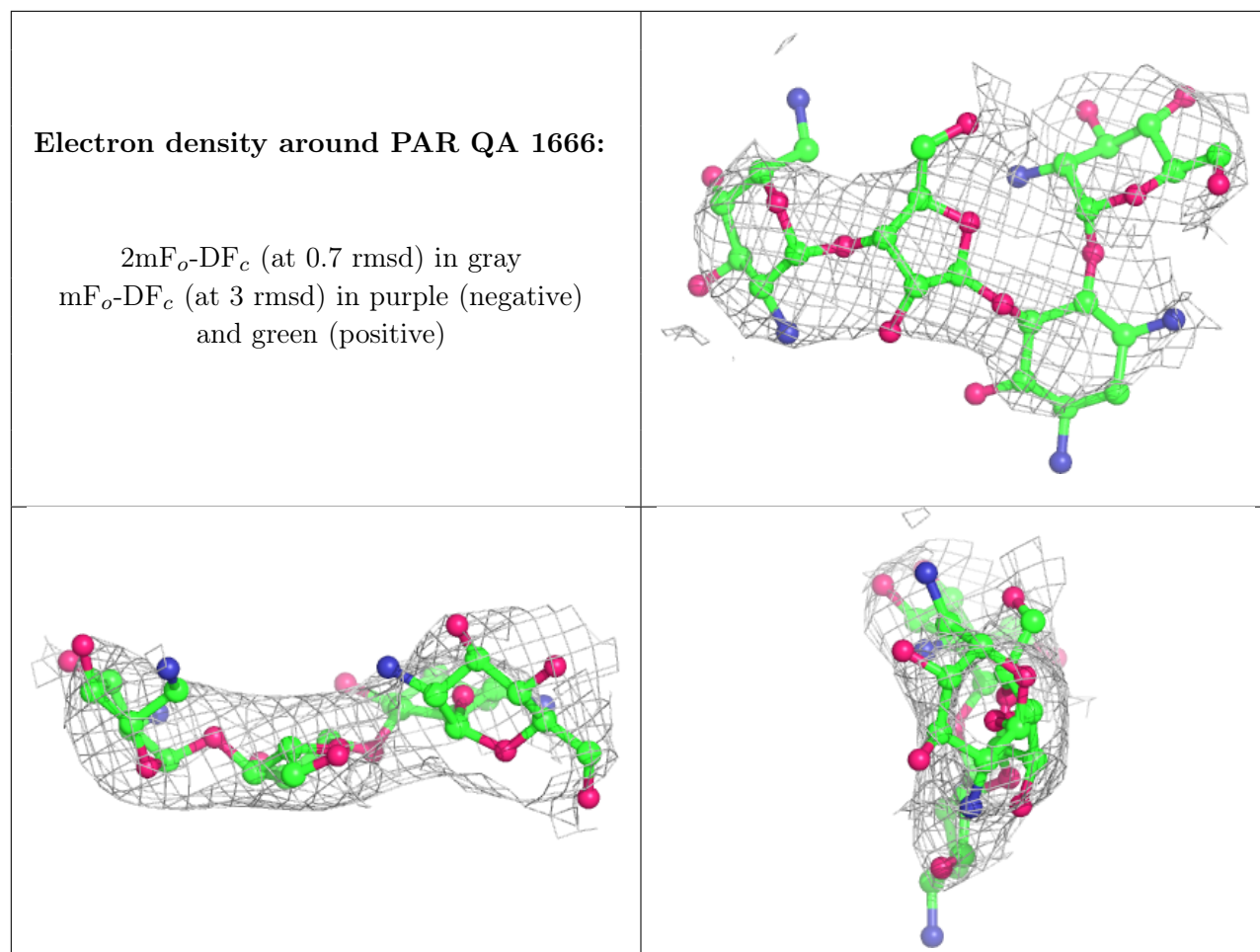
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	YA	3029	1/1	0.98	0.19	0,0,0,0	0
57	MG	YA	3113	1/1	0.98	0.19	2,2,2,2	0
57	MG	YA	3068	1/1	0.98	0.23	3,3,3,3	0
57	MG	RA	3107	1/1	0.98	0.08	3,3,3,3	0
57	MG	RA	3142	1/1	0.98	0.10	28,28,28,28	0
57	MG	RA	3183	1/1	0.98	0.13	12,12,12,12	0
57	MG	QA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

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

Electron density around PAR XA 1671:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.