



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:35 AM UTC

PDB ID : 4LNT / pdb_00004lnt
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-12
Resolution : 2.94 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

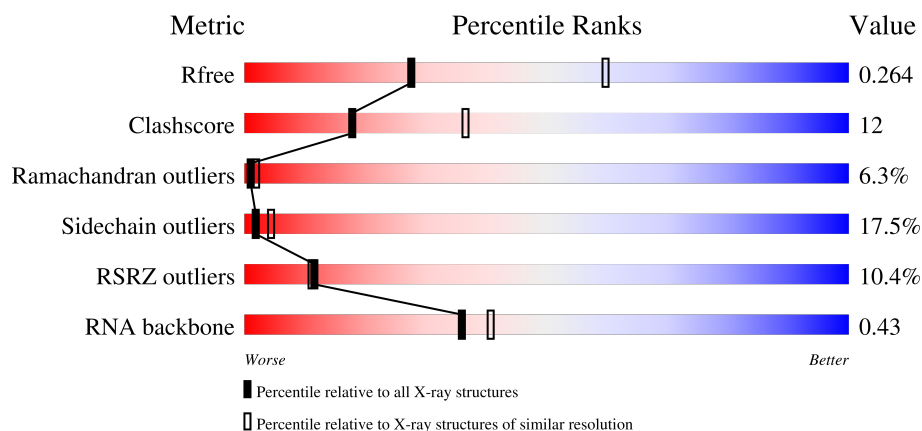
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)
RNA backbone	3983	1018 (3.14-2.74)

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	3% 51% 37% 10% .
1	XA	1522	2% 51% 37% 11% .
2	QB	256	23% 46% 38% 8% . 7%
2	XB	256	16% 44% 39% 9% . 7%

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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	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
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	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

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Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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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	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291993 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	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 messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 24 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
24	XX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

- 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
26	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 (CCD ID: 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	QH	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		

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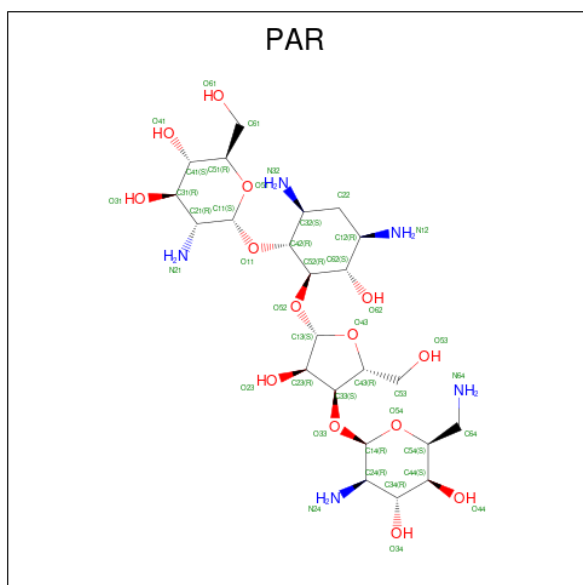
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	RA	242	Total 242	Mg 242	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	YA	268	Total 268	Mg 268	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YE	1	Total 1	Mg 1	0	0
57	YP	2	Total 2	Mg 2	0	0
57	YQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	YX	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $\text{C}_{23}\text{H}_{45}\text{N}_5\text{O}_{14}$).



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

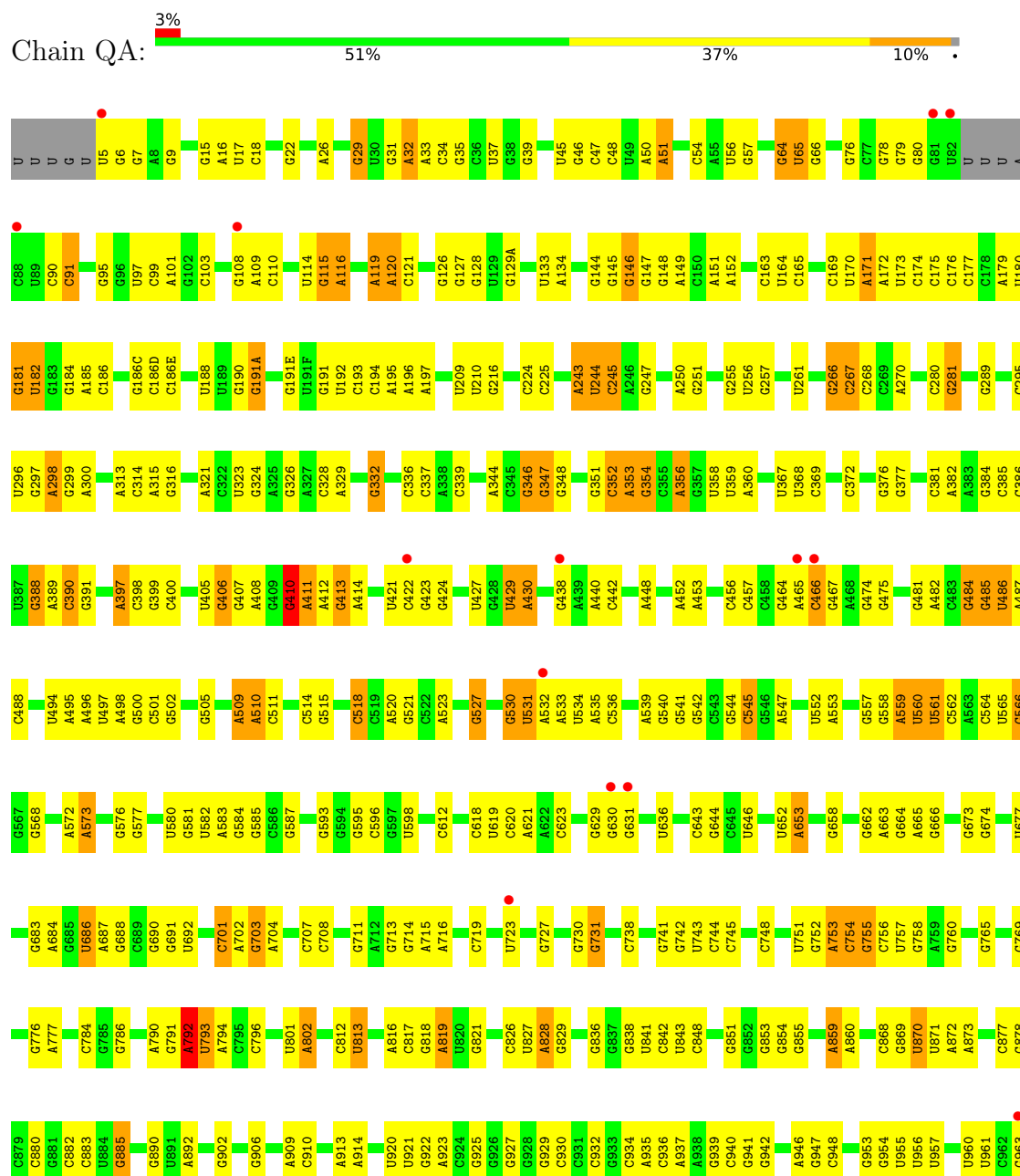
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

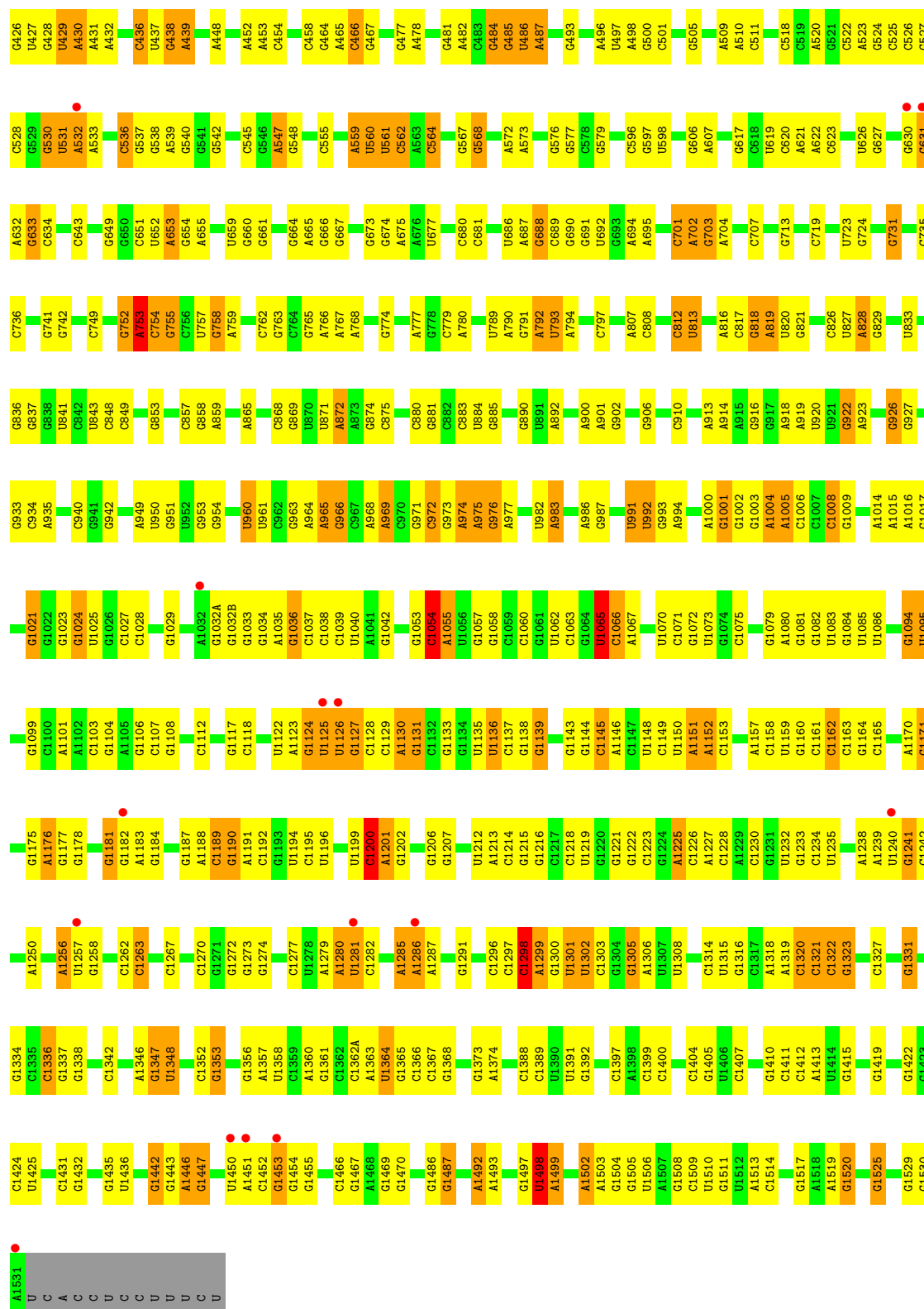
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	XD	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0

3 Residue-property plots

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

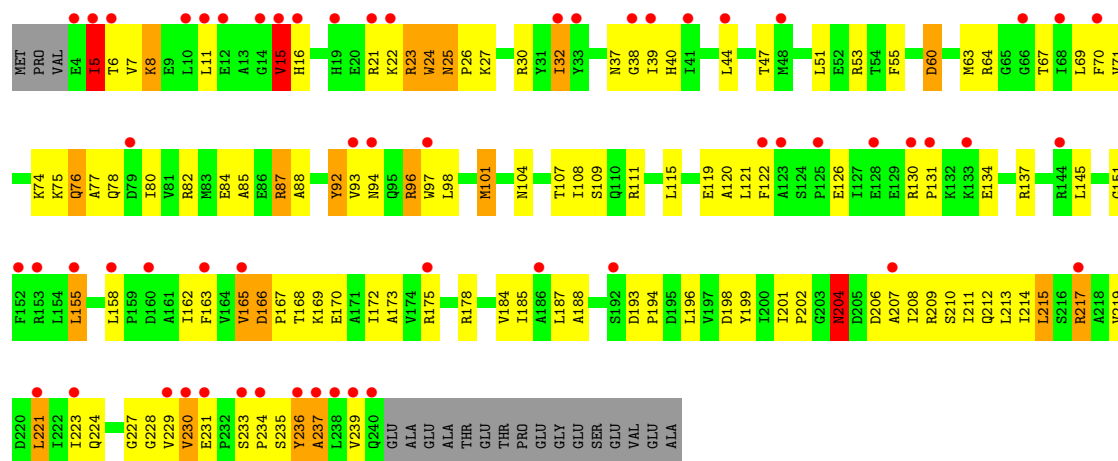
• Molecule 1: 16S rRNA



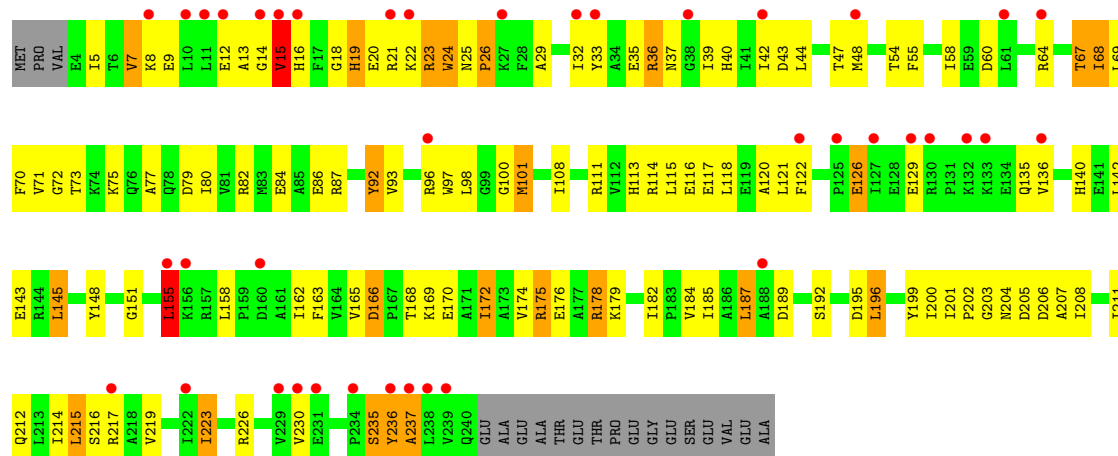


• Molecule 2: 30S ribosomal protein S2

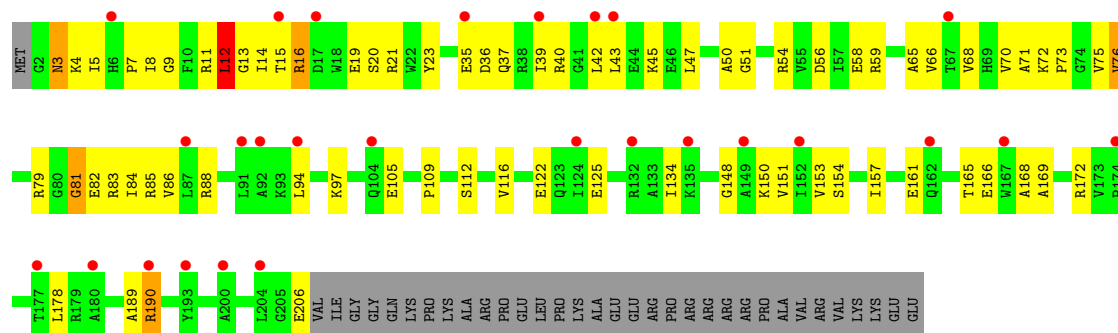




• Molecule 2: 30S ribosomal protein S2

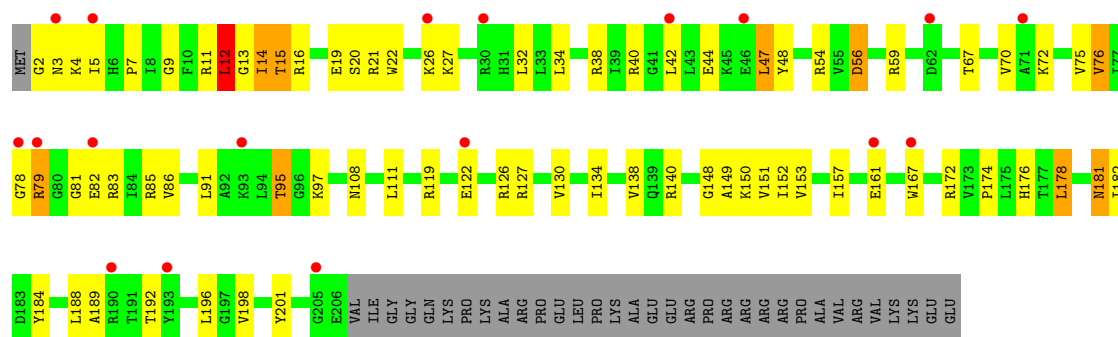


• Molecule 3: 30S ribosomal protein S3

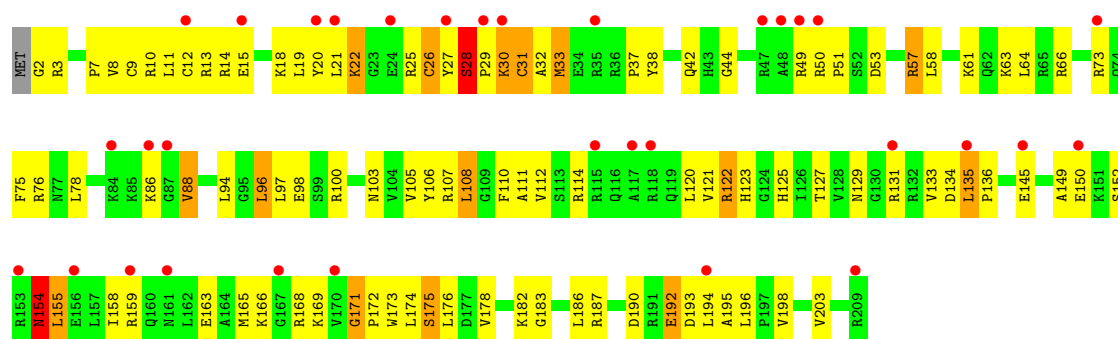


• Molecule 3: 30S ribosomal protein S3

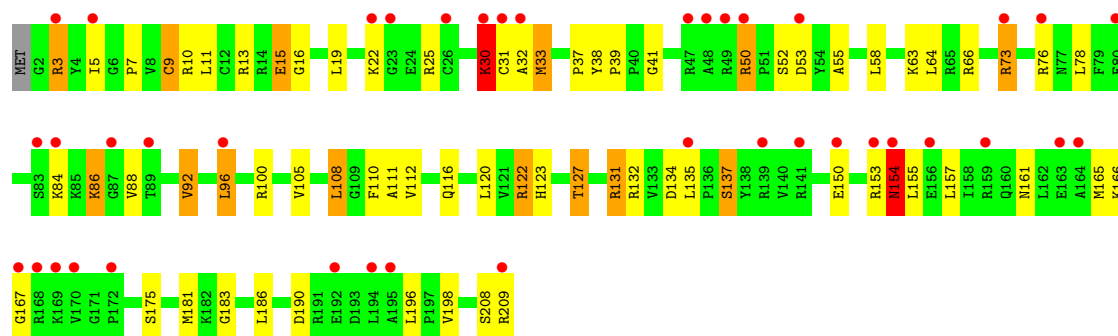




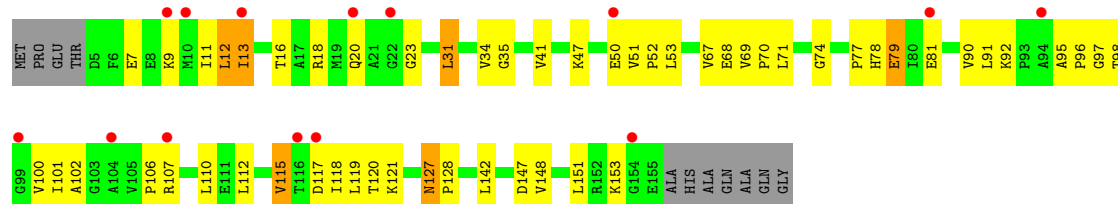
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

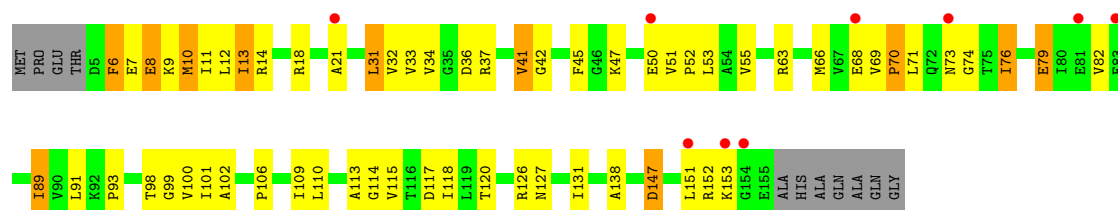


• Molecule 5: 30S ribosomal protein S5



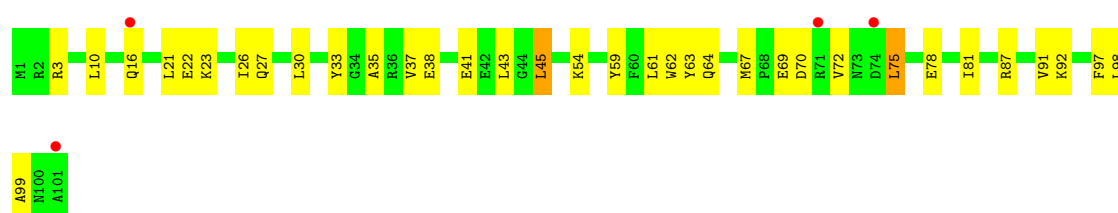
- Molecule 5: 30S ribosomal protein S5

Chain XE: 



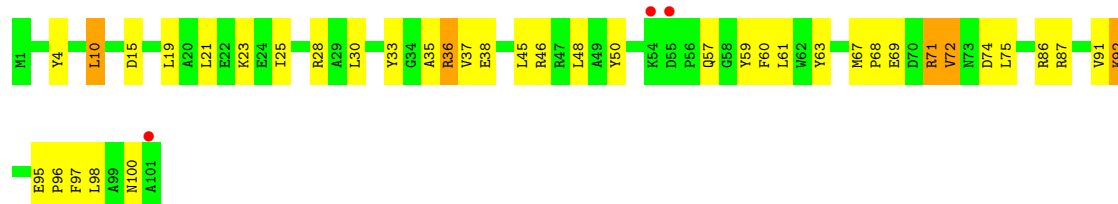
- Molecule 6: 30S ribosomal protein S6

Chain QF: 



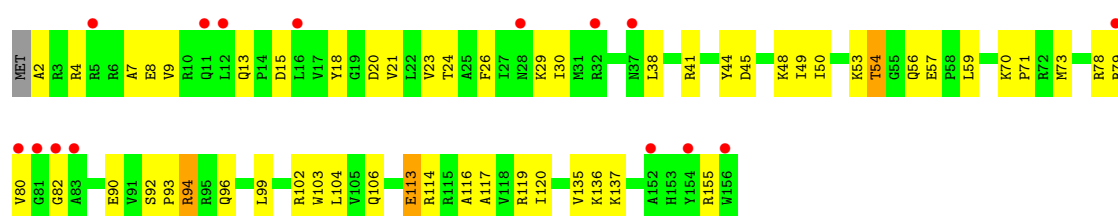
- Molecule 6: 30S ribosomal protein S6

Chain XF: 



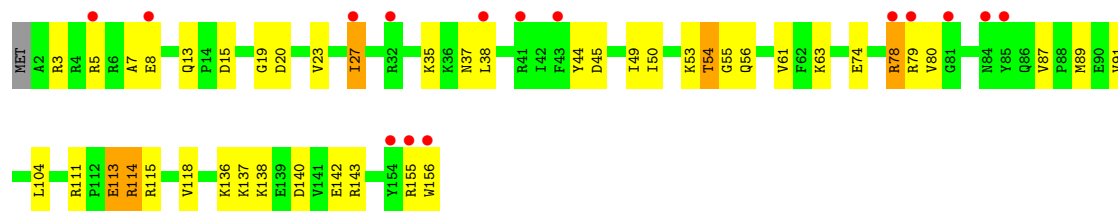
- Molecule 7: 30S ribosomal protein S7

Chain QG: 

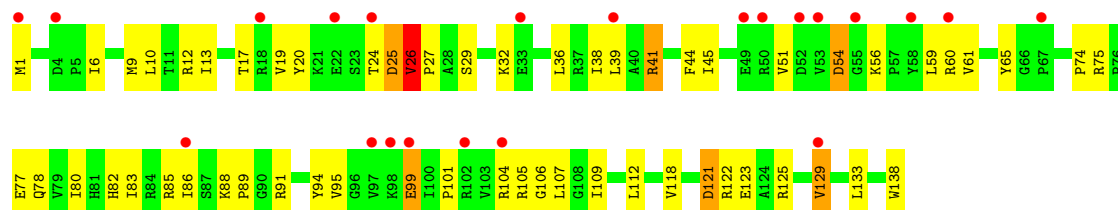


- Molecule 7: 30S ribosomal protein S7

Chain XG: 



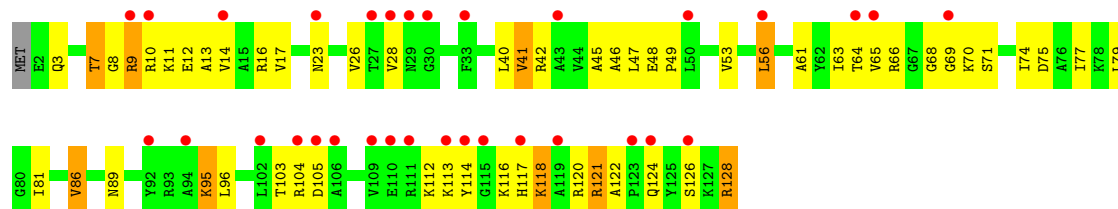
• Molecule 8: 30S ribosomal protein S8



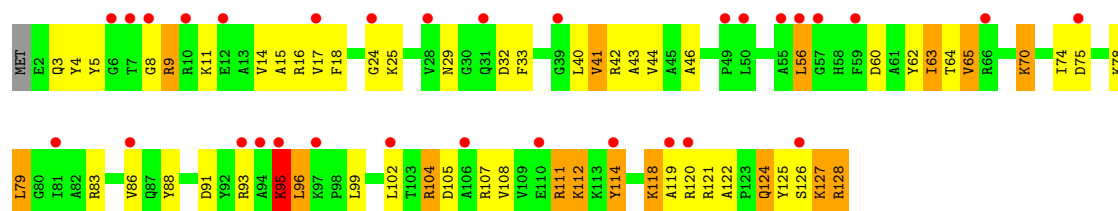
• Molecule 8: 30S ribosomal protein S8



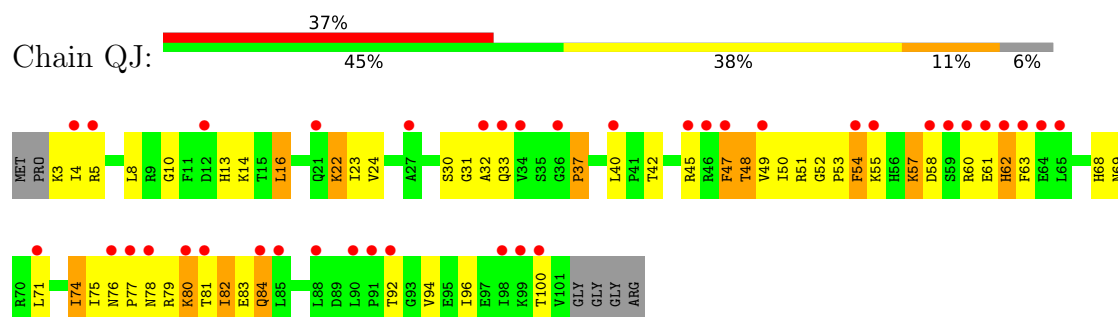
• Molecule 9: 30S ribosomal protein S9



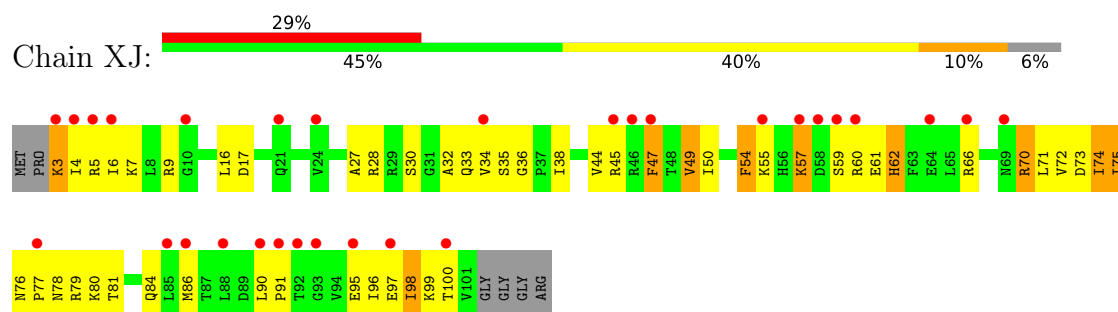
• Molecule 9: 30S ribosomal protein S9



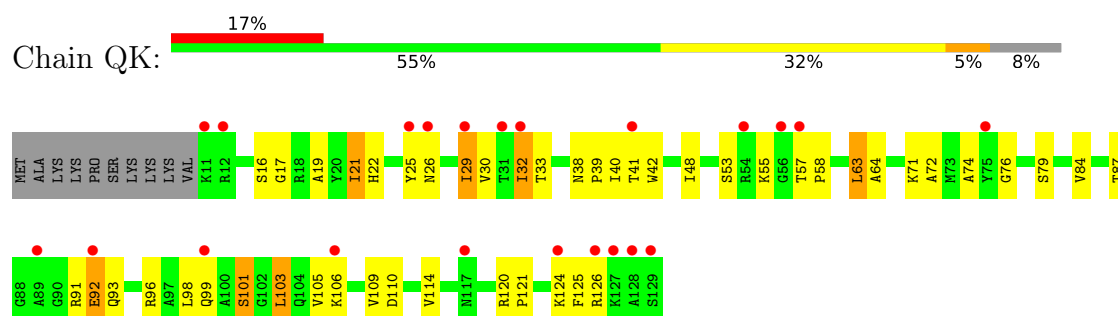
- Molecule 10: 30S ribosomal protein S10



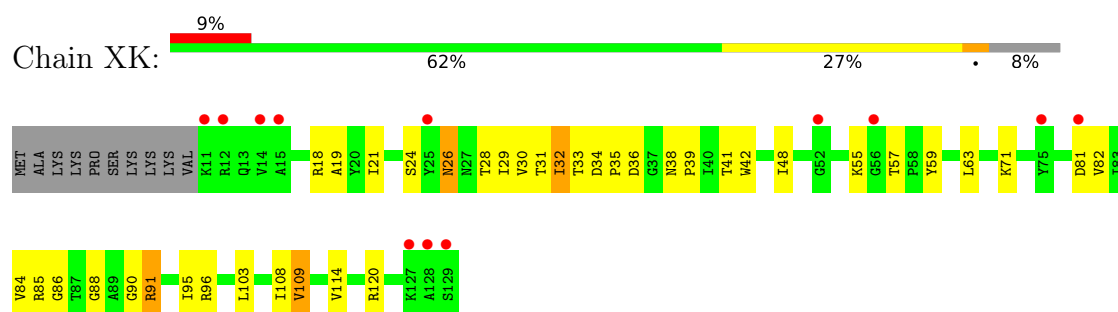
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

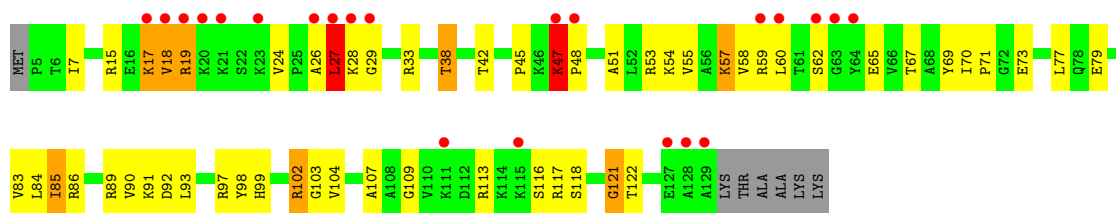


- Molecule 11: 30S ribosomal protein S11

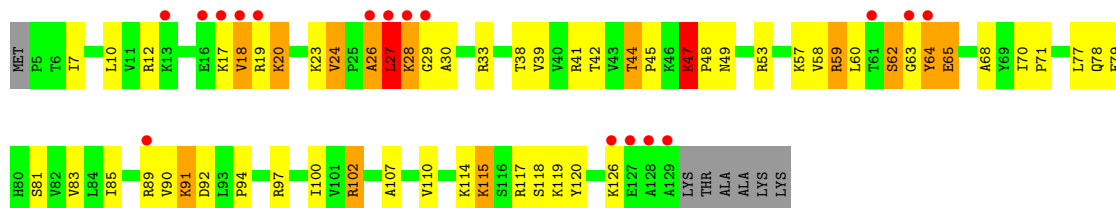


- Molecule 12: 30S ribosomal protein S12

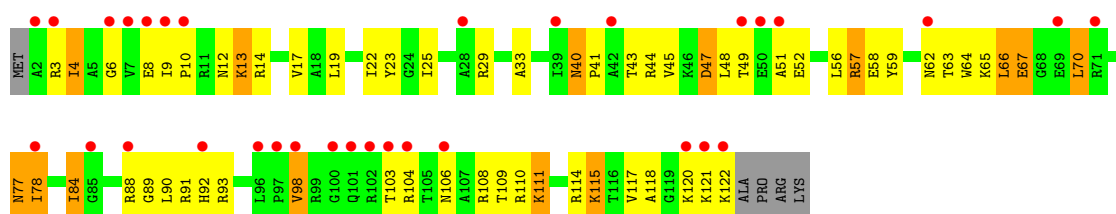




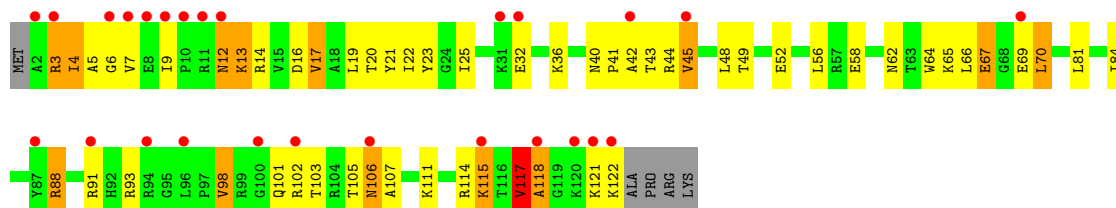
• Molecule 12: 30S ribosomal protein S12



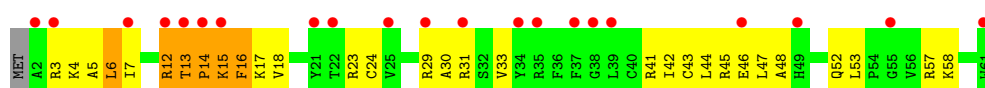
• Molecule 13: 30S ribosomal protein S13



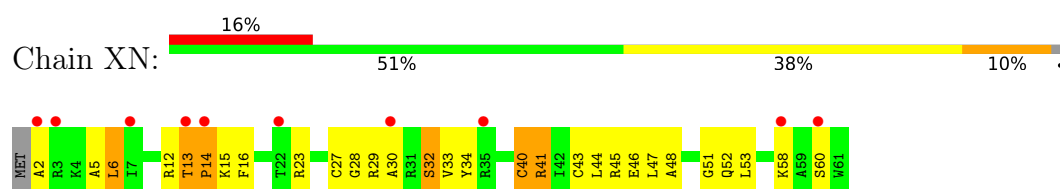
• Molecule 13: 30S ribosomal protein S13



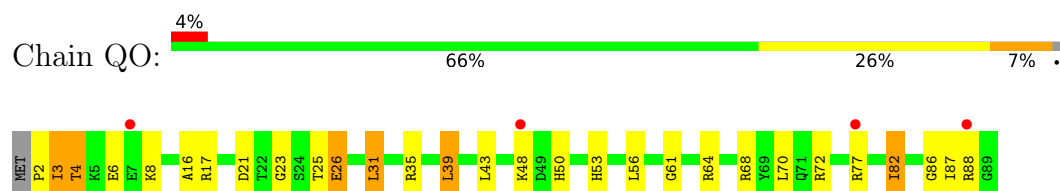
• Molecule 14: 30S ribosomal protein S14



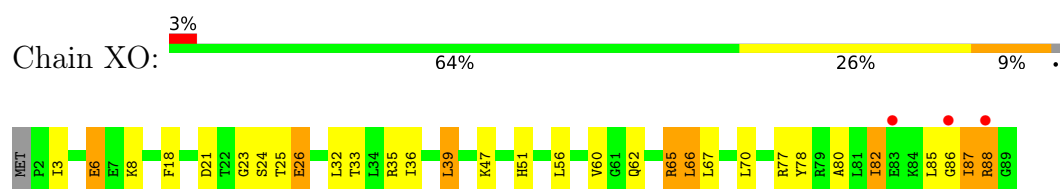
• Molecule 14: 30S ribosomal protein S14



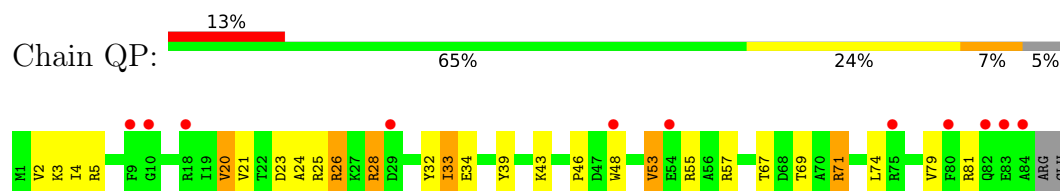
- Molecule 15: 30S ribosomal protein S15



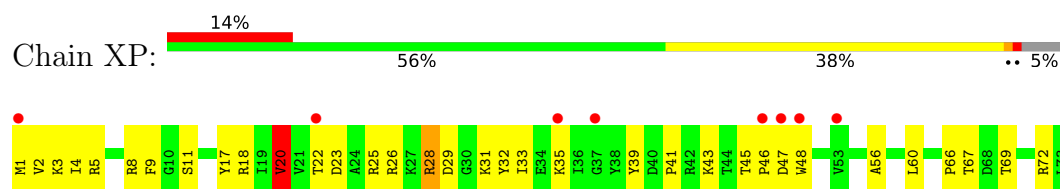
- Molecule 15: 30S ribosomal protein S15



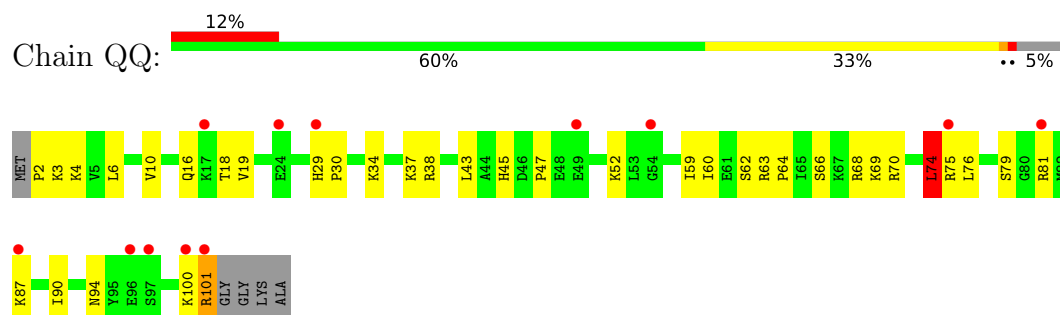
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

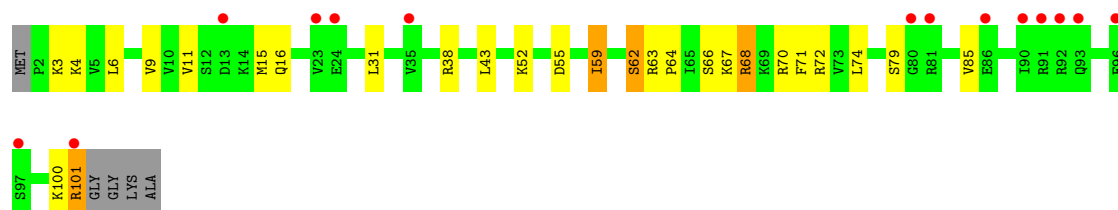


- Molecule 17: 30S ribosomal protein S17



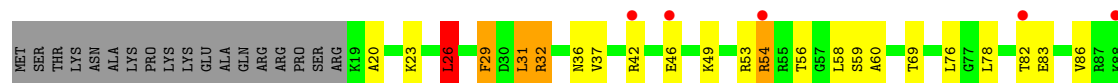
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 

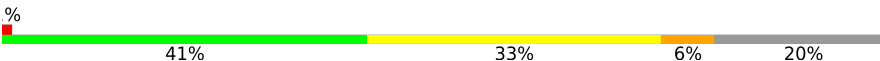


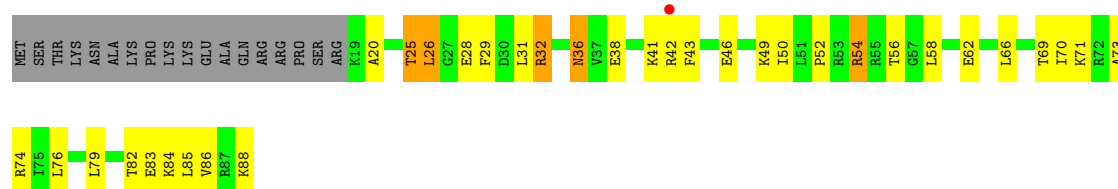
- Molecule 18: 30S ribosomal protein S18

Chain QR: 



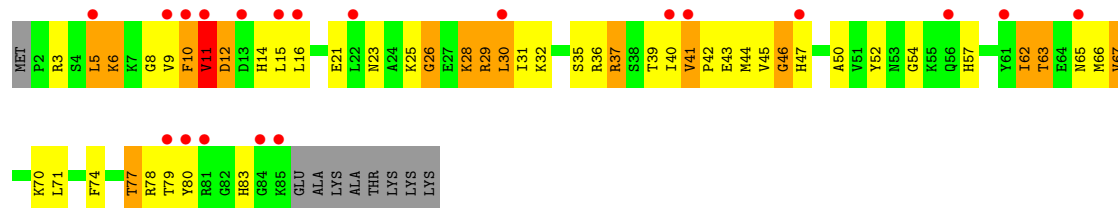
- Molecule 18: 30S ribosomal protein S18

Chain XR: 

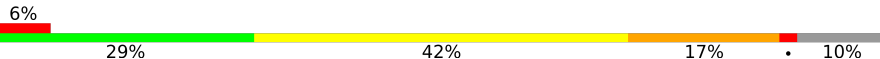


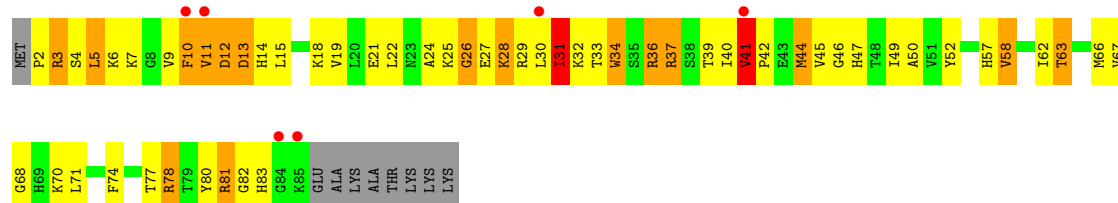
- Molecule 19: 30S ribosomal protein S19

Chain QS: 



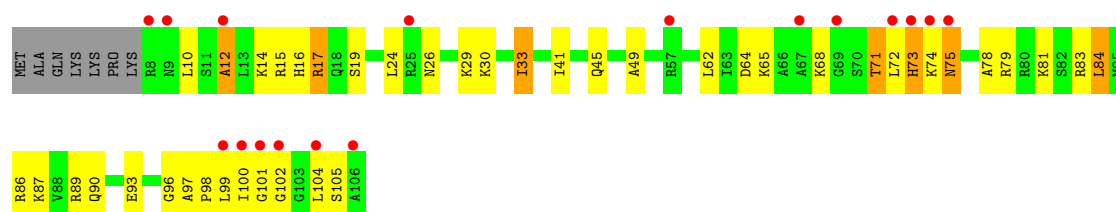
- Molecule 19: 30S ribosomal protein S19

Chain XS: 



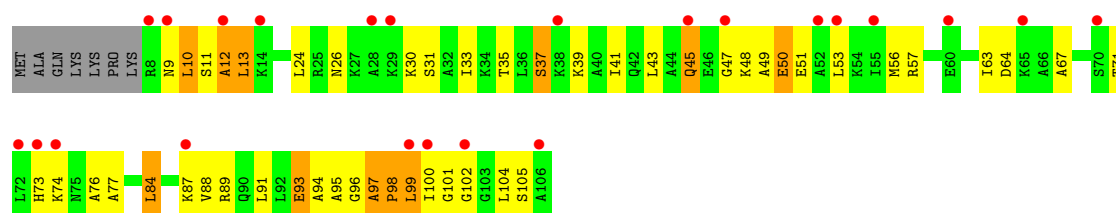
- Molecule 20: 30S ribosomal protein S20

Chain QT: 



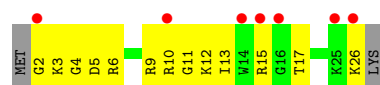
- Molecule 20: 30S ribosomal protein S20

Chain XT: 



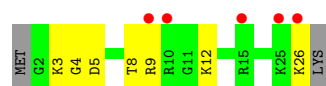
- Molecule 21: 30S ribosomal protein S21

Chain QU: 



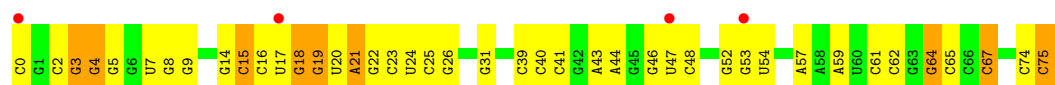
- Molecule 21: 30S ribosomal protein S21

Chain XU: 



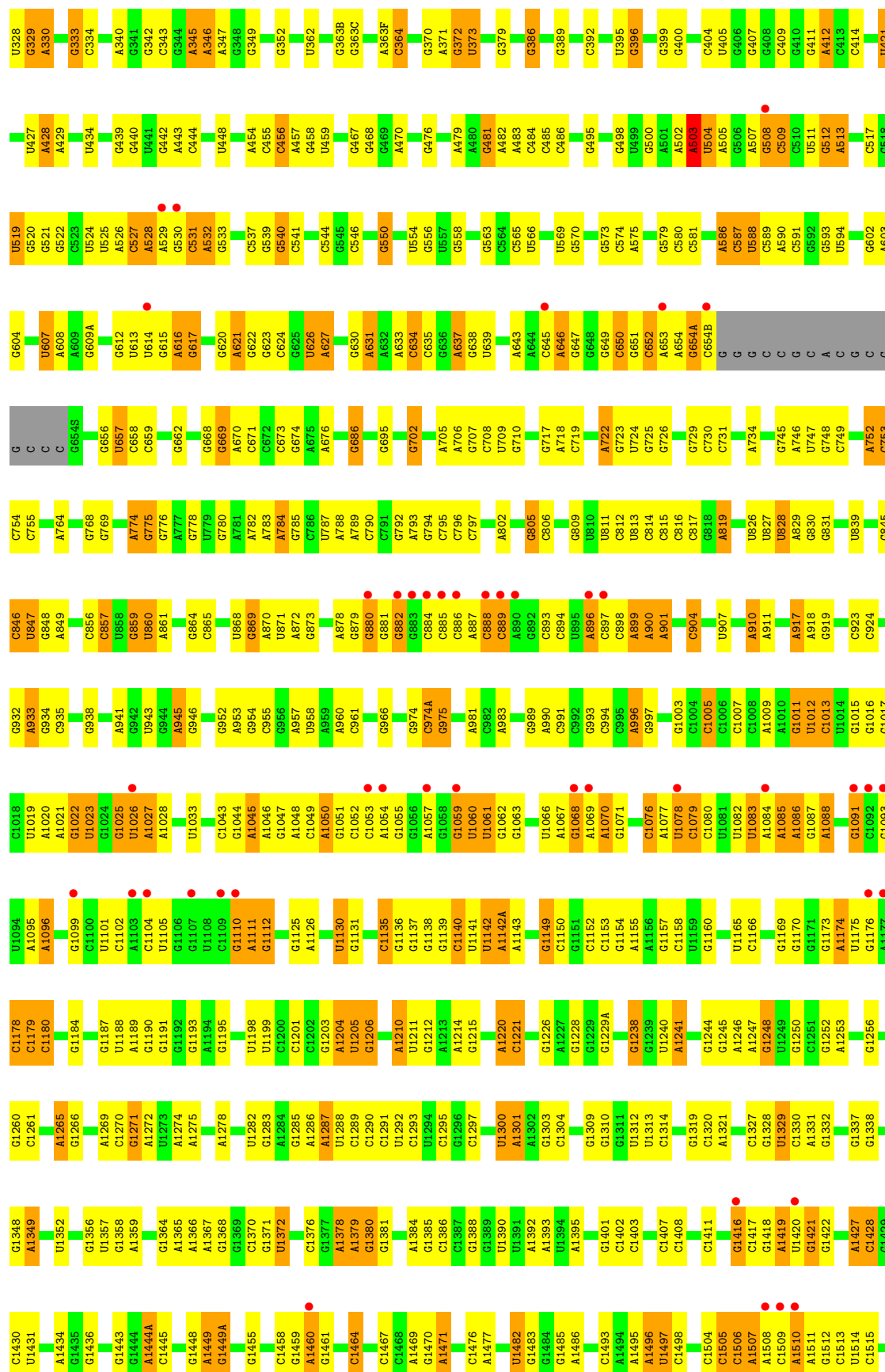
- Molecule 22: P-site tRNA fMet

Chain QV: 

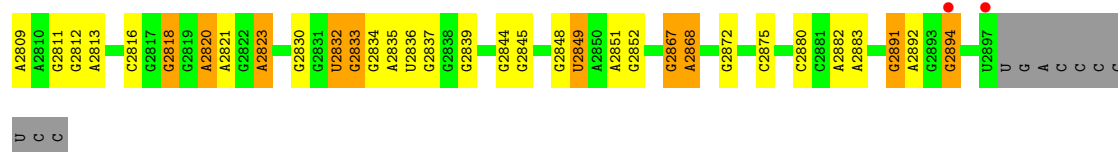


- Molecule 22: P-site tRNA fMet

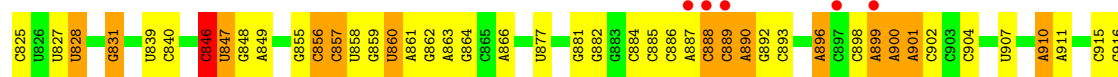
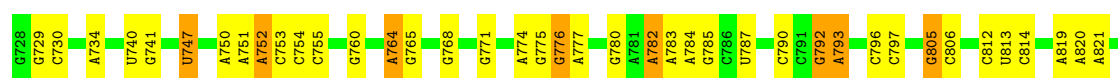
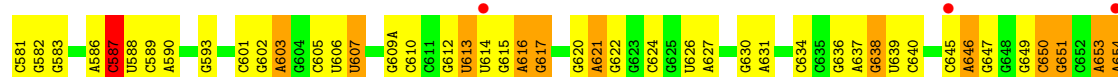
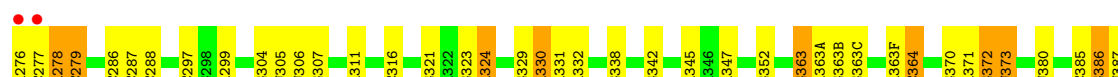
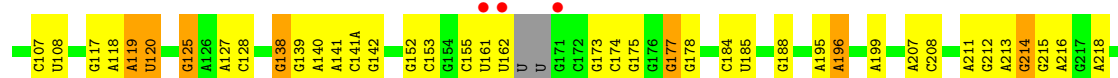
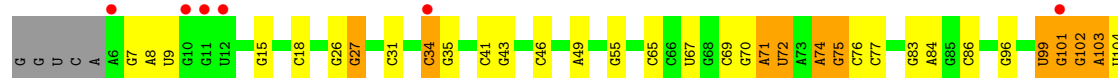
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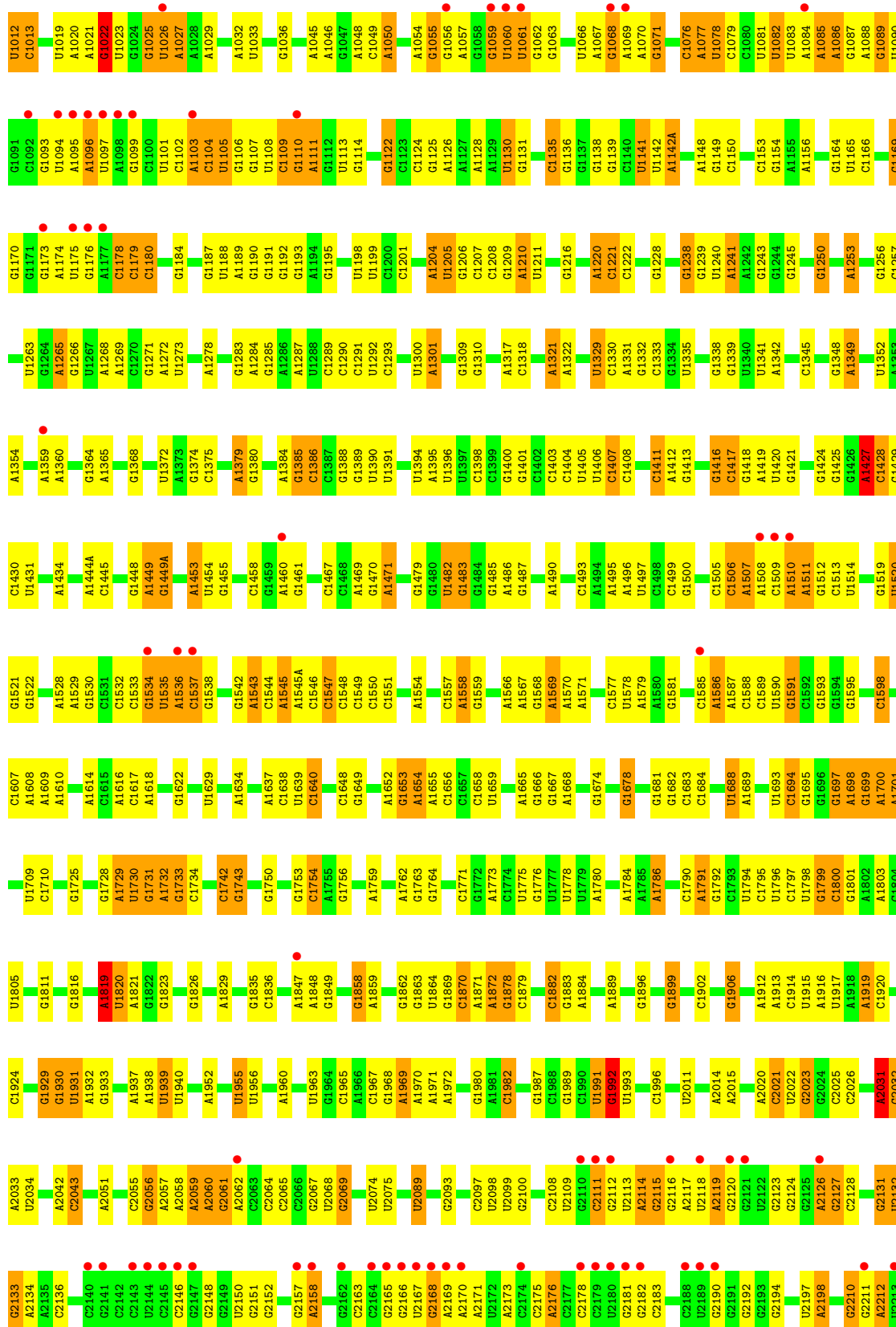


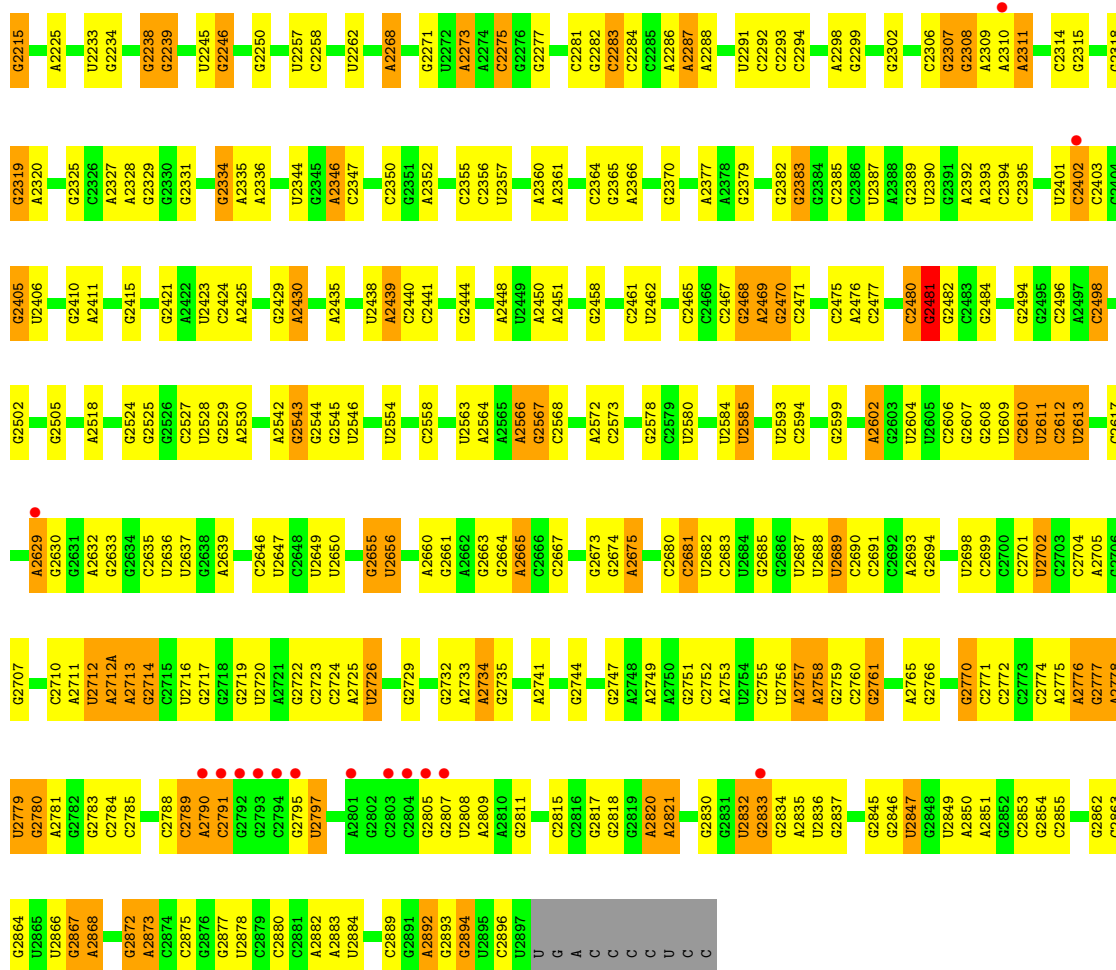
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G2735	U2563	C2297	G2471	G2385	U2296	U2189	U2118	U2028	G1929	C1827	A1614	G1521
C2648	A2564	C2298	C2474	G2389	C2299	G2190	U2119	A2031	G1930	A1829	G1617	G1522
U2739	U2650	A2565	A2476	U2390	G2300	G2191	U2120	G2032	U1931	G1828	G1526	G1526
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G2747	G2659	G2569	G2482	C2393	G2303	A2199	G2124	G2037	A1936	U1834	G1635	G1528
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G2751	G2663	A2571	G2484	U2401	A2305	G2210	G2126	C2039	A1938	C1837	A1637	U1535
C2752	G2664	C2573	G2487	C2402	G2306	G2211	U2127	G2042	U1939	G1838	A1536	U1536
A2753	A2665	U2580	G2491	C2403	G2307	G2212	G2128	A2042	G1945	G1839	G1758	C1537
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A2757	G2673	C2586	U2494	U2406	U2312	A2225	G2133	C2052	A1952	G1845	G1649	A1543
A2758	G2674	U2593	G2494	G2410	G2318	U2233	A2135	G2053	U1955	G1846	G1650	C1544
C2759	A2675	C2594	C2496	A2411	G2319	G2234	G2136	A2054	U1956	A1847	A1652	A1545
C2760	G2677	A2497	A2497	G2415	A2320	G2235	G2137	G2055	C1957	G1848	G1653	C1548
G2761	G2679	C2498	U2498	C2416	G2321	G2238	G2138	G2056	C1958	G1850	A1655	C1548
A2764	C2683	G2599	G2499	C2417	A2322	G2239	G2139	A2059	C1962	U1851	G1656	A1554
A2765	U2688	A2602	G2502	A2418	G2323	U2243	G2141	A2060	U1963	G1852	G1657	A1558
C2766	U2689	U2603	A2503	U2419	C2324	U2244	G2142	G2061	G1964	G1857	C1658	G1559
C2767	C2690	G2604	G2505	C2420	G2325	U2245	U2143	A2062	C1967	G1858	C1660	A1566
C2768	C2696	U2605	G2506	U2423	C2326	G2246	G2144	C2063	U1968	G1862	G1661	A1569
C2769	U2698	C2606	C2507	C2424	A2327	A2247	G2145	C2064	A1969	G1863	A1665	A1570
C2770	C2699	U2609	G2508	A2425	G2328	C2248	G2146	C2065	A1970	U1864	G1666	A1570
C2771	C2700	C2610	A2518	G2429	G2329	U2249	G2147	U2068	A1971	G1865	C1667	C1575
C2772	C2701	U2611	U2519	A2430	G2330	G2250	U2150	G2069	A1972	G1866	A1668	U1576
C2773	C2702	C2612	C2519	U2431	G2331	U2251	G2151	G2070	A1973	C1871	A1669	C1577
A2774	C2703	U2613	G2527	U2434	G2334	U2252	G2154	A2071	C1974	A1872	C1670	C1577
A2775	A2614	A2614	U2528	A2435	A2335	C2262	G2155	U2074	G1980	G1878	G1674	U1578
A2776	C2617	C2617	G2529	A2436	A2336	C2264	G2156	U2075	A1981	C1882	C1675	A1579
A2777	G2708	G2618	U2530	A2437	C2342	A2267	G2157	G2086	C1982	G1883	G1678	A1580
C2778	C2709	A2531	G2531	U2438	C2343	G2271	A2158	U2087	G1989	A1884	G1681	G1581
A2779	C2619	G2532	A2533	A2439	U2344	U2272	G2159	G2087	C1990	A1885	G1682	C1582
A2780	C2620	A2533	A2533	C2440	G2345	G2273	G2160	G2093	U1991	C1886	U1688	A1583
A2781	U2712	G2623	U2537	C2441	A2346	A2274	G2161	G2099	G1992	G1887	U1689	A1586
C2782	A2712A	A2713	C2538	G2442	C2347	C2275	G2162	U2099	C1993	G1888	A1689	A1587
C2783	C2626	C2626	C2539	C2443	C2348	G2276	G2163	G2100	U1993	A1890	U1693	C1588
C2784	C2627	C2628	C2540	G2444	C2350	G2277	G2164	G2101	C2006	G1891	C1693	C1589
C2785	U2716	A2541	A2541	G2445	C2351	G2278	G2165	U2102	G2006	C1892	G1694	G1593
C2788	G2717	G2630	G2542	A2448	C2359	G2280	U2167	C2103	G2010	G1799	G1695	G1594
C2789	U2720	G2631	G2543	A2449	A2360	G2281	G2168	C2107	U2011	C1800	A1698	G1595
C2791	G2632	G2632	G2544	A2451	C2364	G2282	A2170	C2108	G2012	G1801	A1701	C1598
G2795	G2633	G2633	A2547	G2455	A2369	C2283	U2172	U2109	A2013	A1803	G1725	C1599
C2796	C2634	G2634	U2552	C2456	A2374	A2286	G2173	G2110	A2014	C1804	G1726	C1607
C2797	C2635	C2635	G2553	A2459	G2375	A2287	G2174	G2112	A2015	U1805	U1727	A1608
C2798	U2636	U2636	U2554	U2460	A2376	U2291	G2175	U2113	A2019	C1806	G1817	A1609
A2799	U2637	U2637	U2554	U2460	A2377	C2292	A2176	C2114	A2020	G1816	A1729	A1610
C2807	G2638	G2638	G2557	U2466	A2378	C2293	G2182	G2115	U2022	U1915		
U2808	G2641	G2641		G2466								



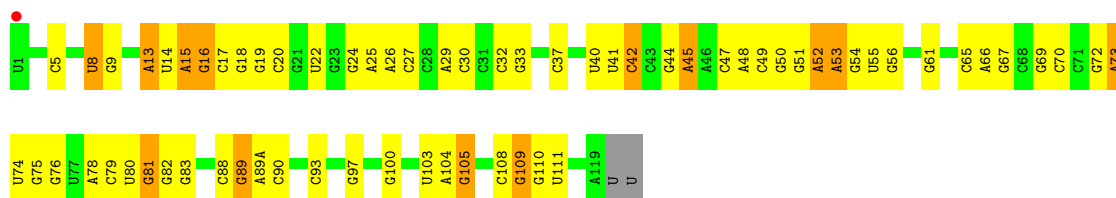
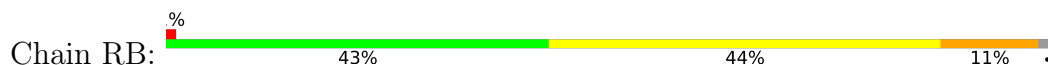
Molecule 25: 23S rRNA



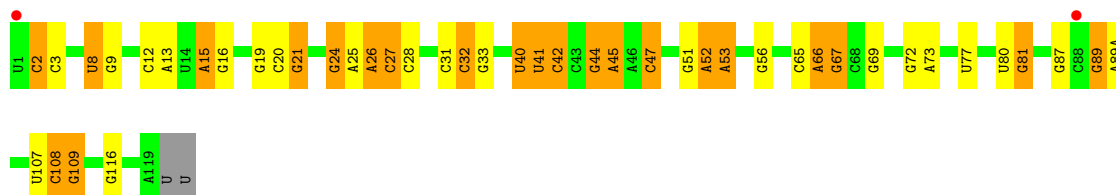




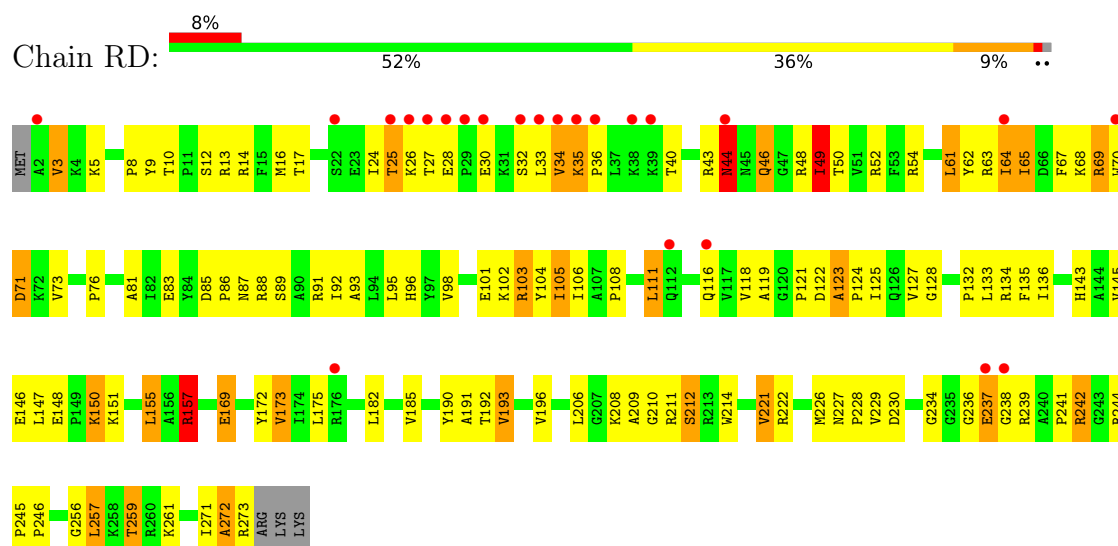
• Molecule 26: 5S rRNA



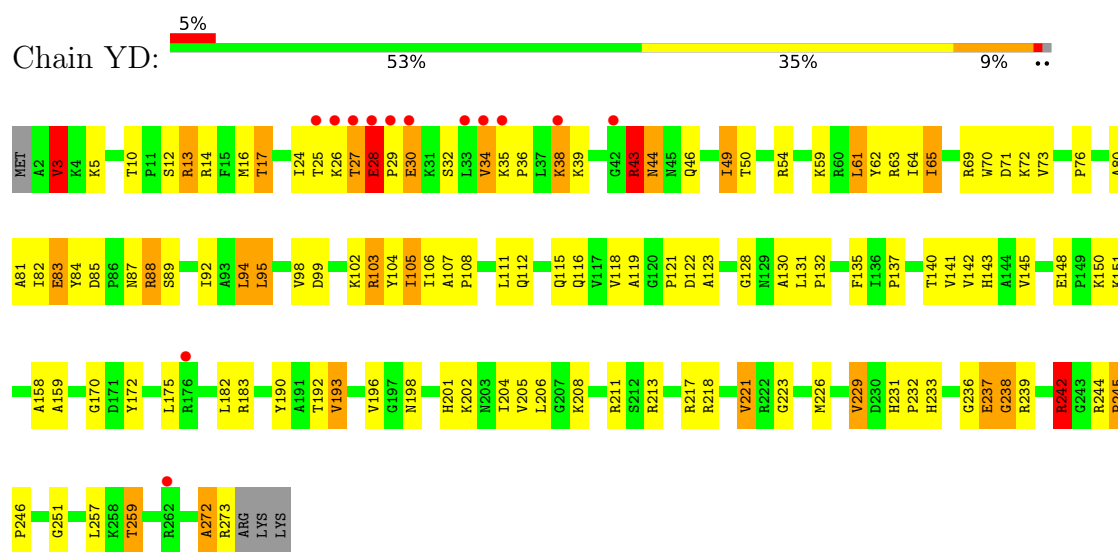
• Molecule 26: 5S rRNA



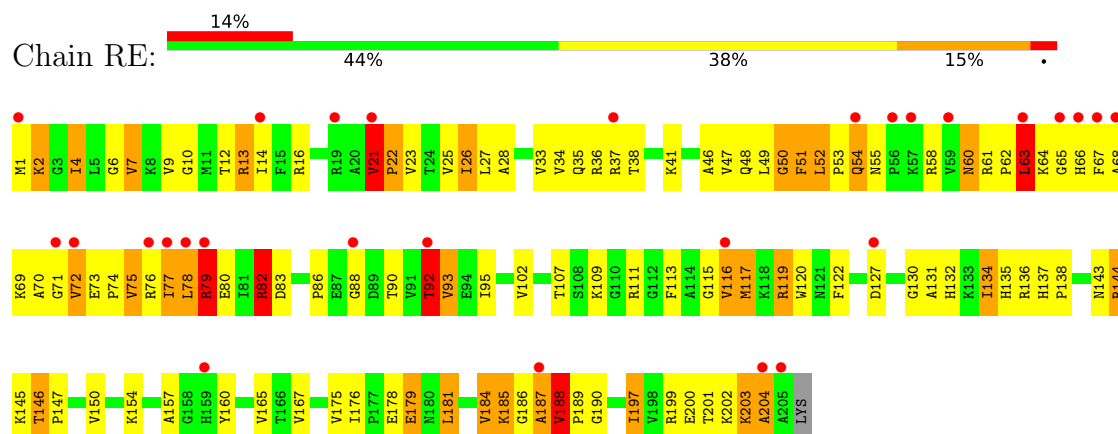
• Molecule 27: 50S ribosomal protein L2



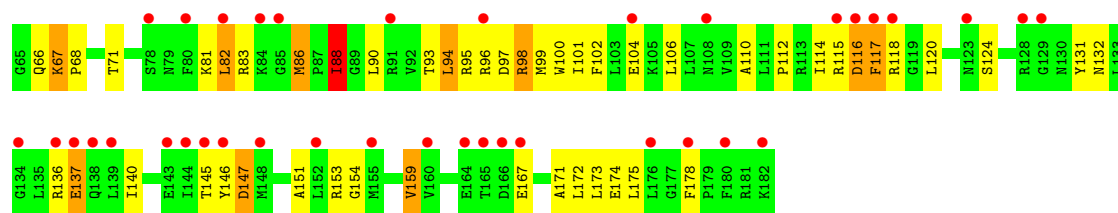
• Molecule 27: 50S ribosomal protein L2



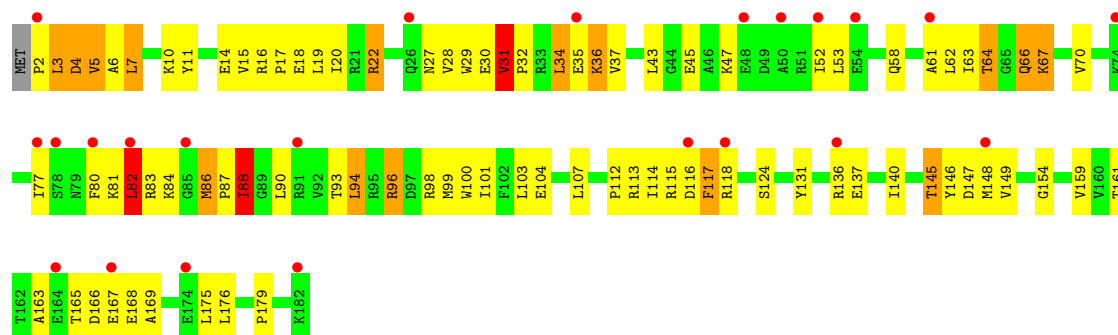
• Molecule 28: 50S ribosomal protein L3



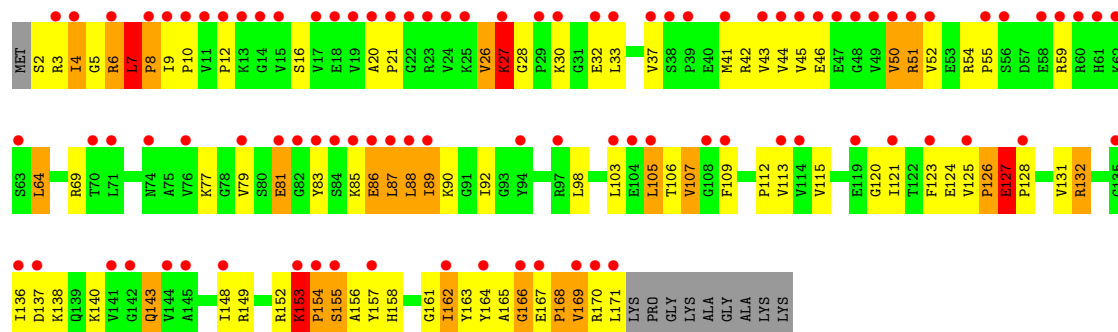
• Molecule 28: 50S ribosomal protein L3



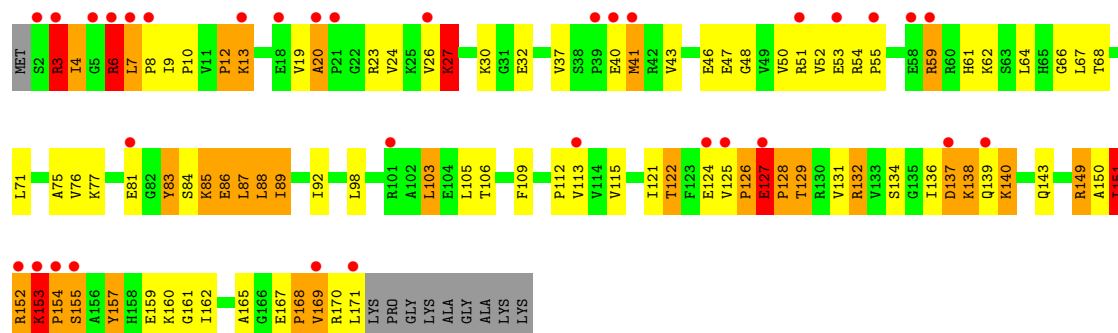
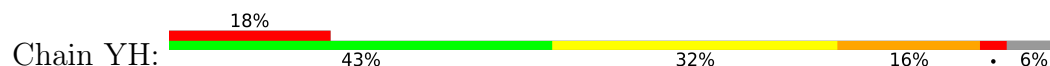
• Molecule 30: 50S ribosomal protein L5



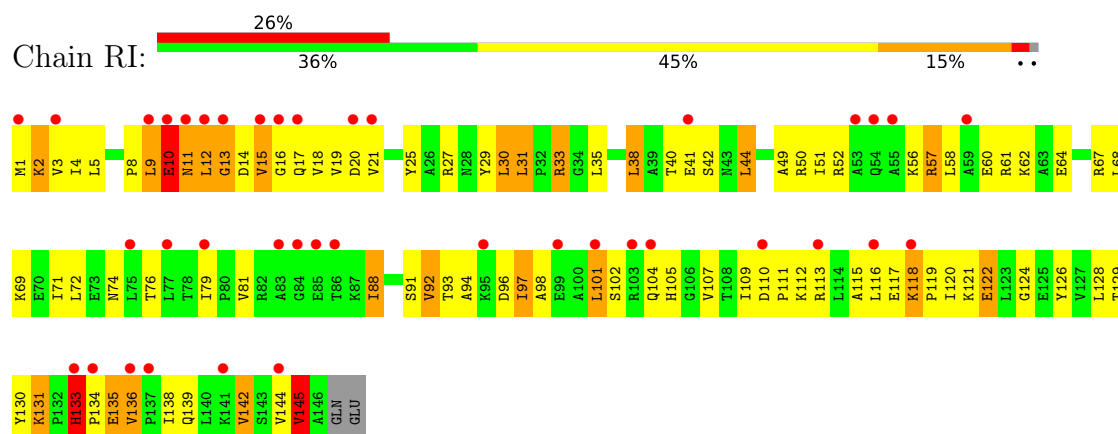
• Molecule 31: 50S ribosomal protein L6



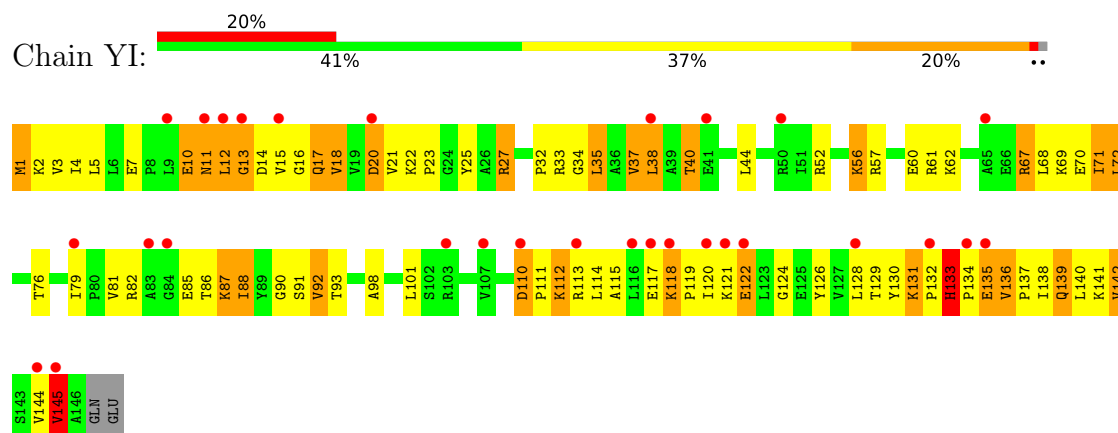
• Molecule 31: 50S ribosomal protein L6



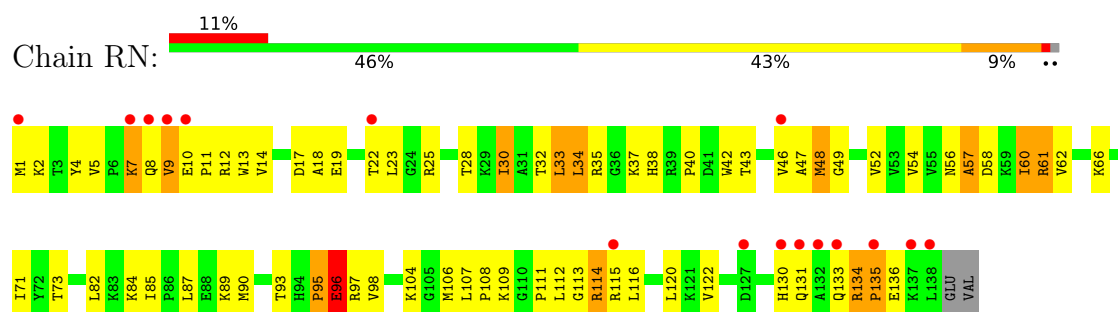
- Molecule 32: 50S ribosomal protein L9



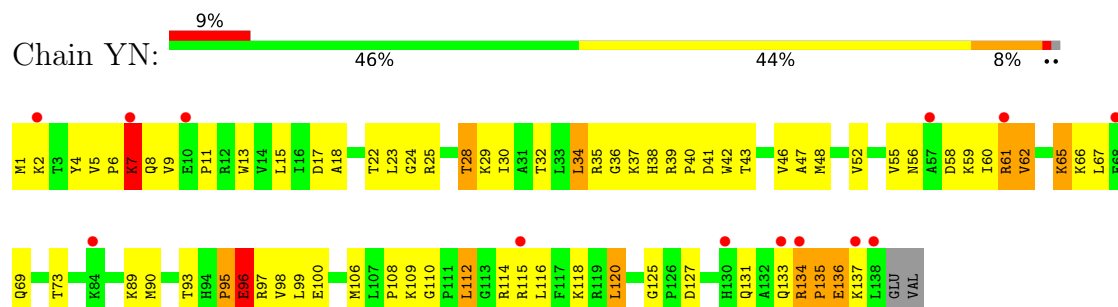
- Molecule 32: 50S ribosomal protein L9



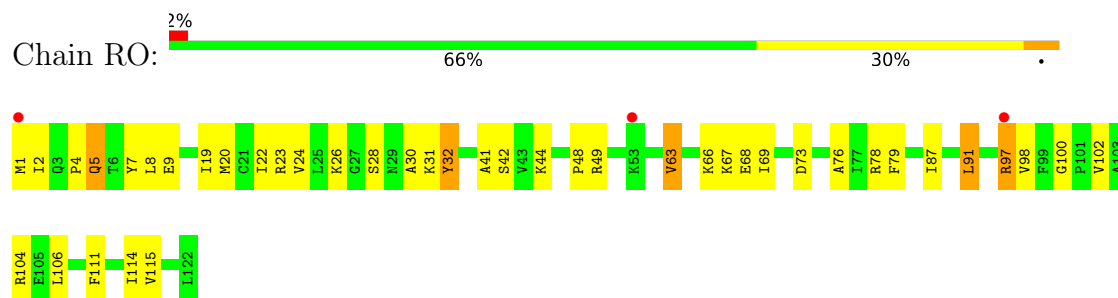
- Molecule 33: 50S ribosomal protein L13



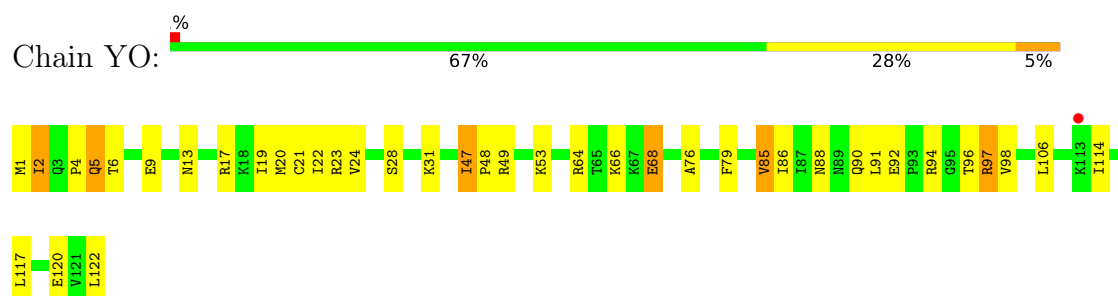
- Molecule 33: 50S ribosomal protein L13



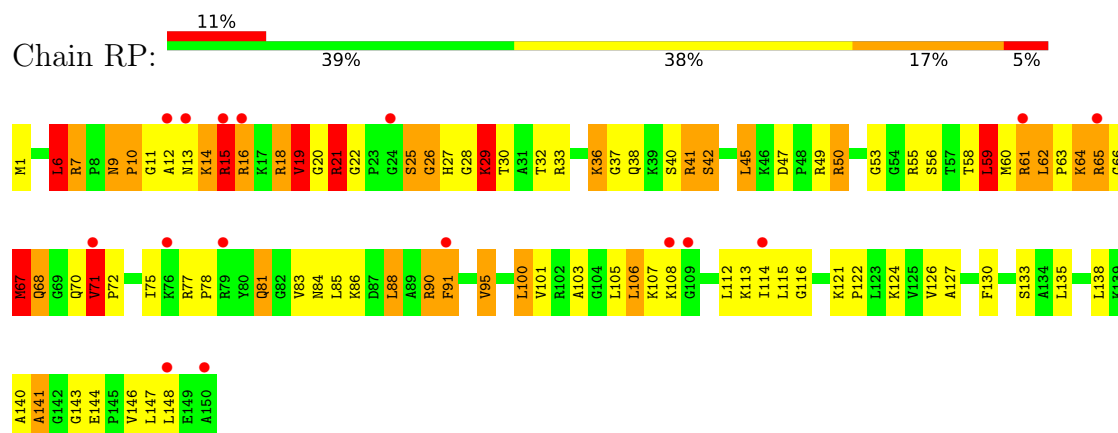
- Molecule 34: 50S ribosomal protein L14



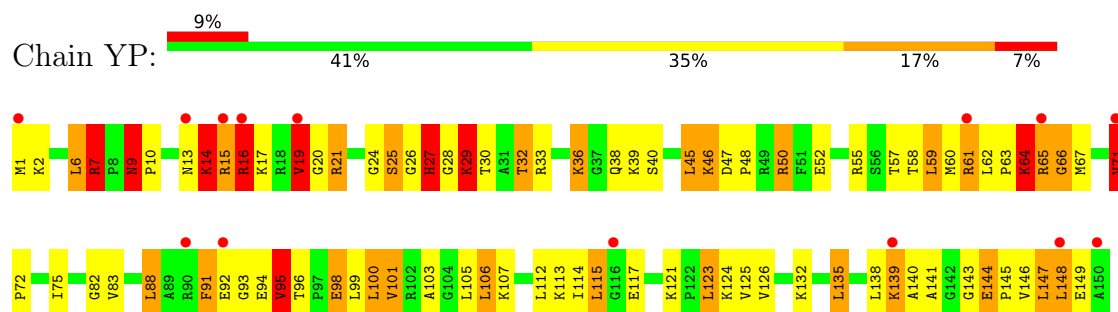
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

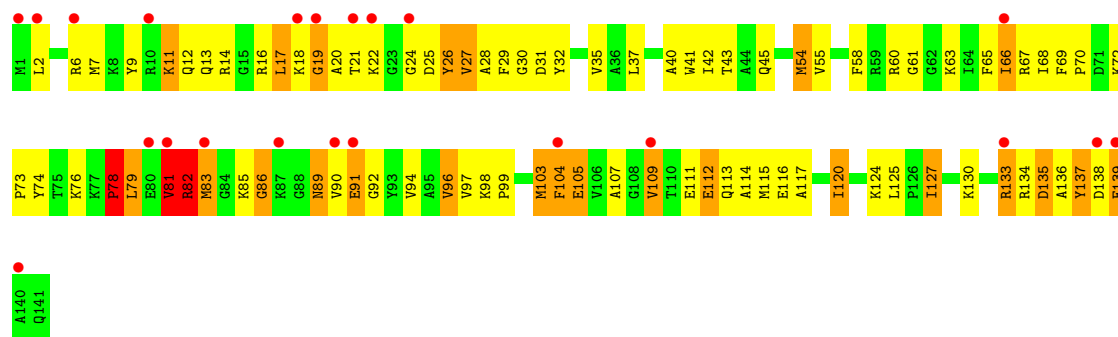


- Molecule 35: 50S ribosomal protein L15

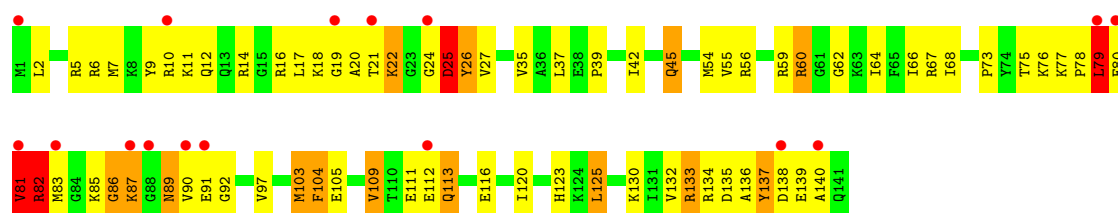


- Molecule 36: 50S ribosomal protein L16

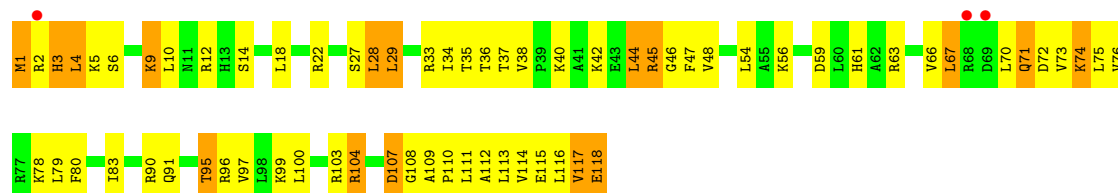
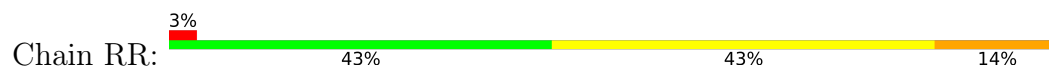




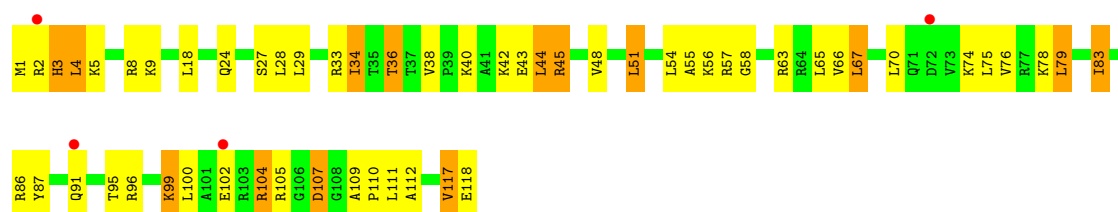
• Molecule 36: 50S ribosomal protein L16



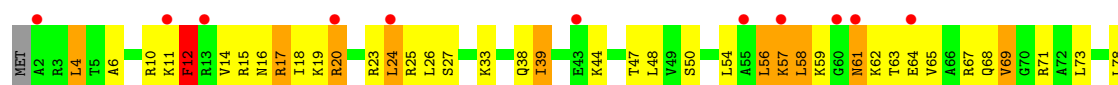
• Molecule 37: 50S ribosomal protein L17

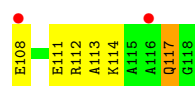


• Molecule 37: 50S ribosomal protein L17



• Molecule 38: 50S ribosomal protein L18

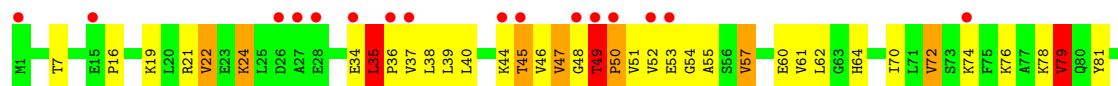




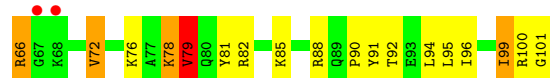
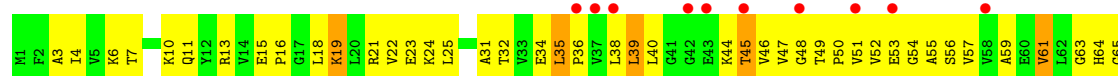
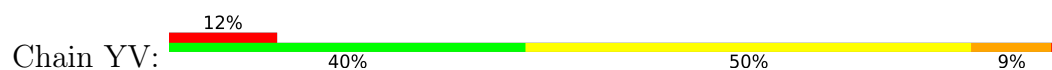
- Molecule 40: 50S ribosomal protein L20



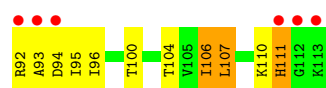
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

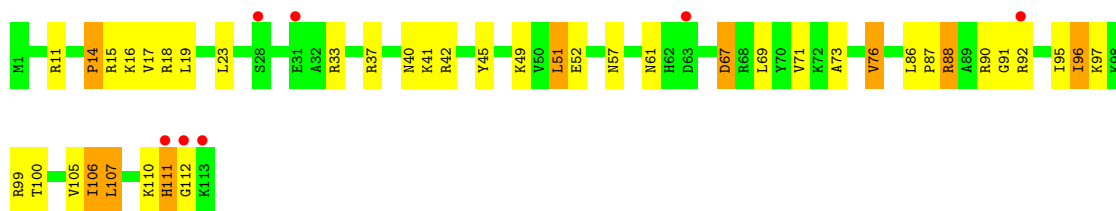


- Molecule 42: 50S ribosomal protein L22

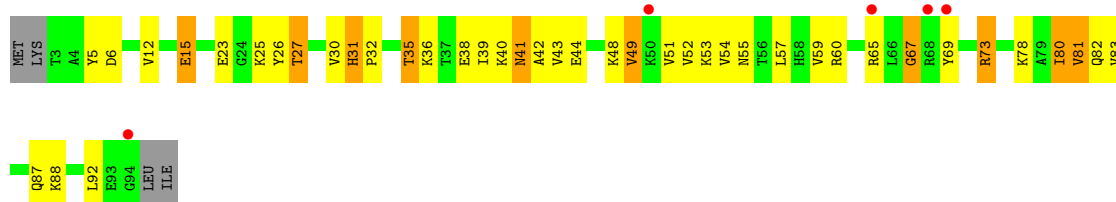


- Molecule 42: 50S ribosomal protein L22

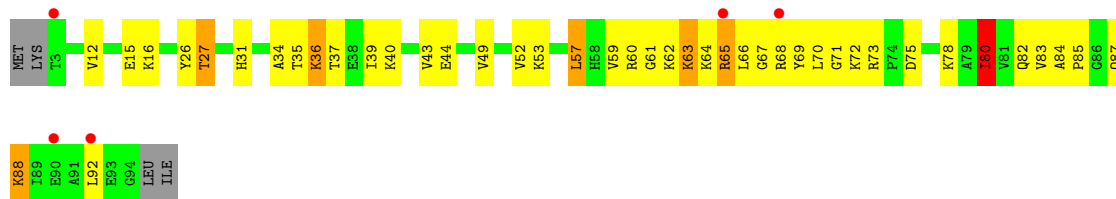




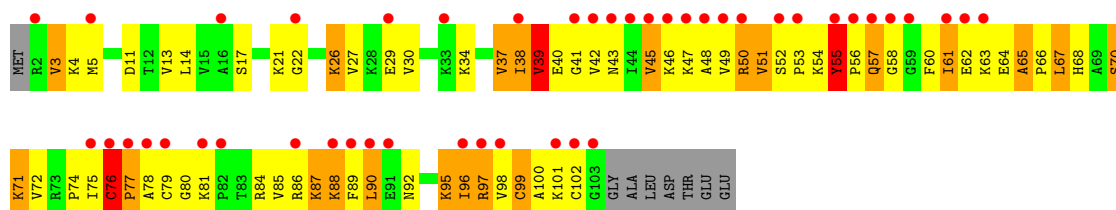
• Molecule 43: 50S ribosomal protein L23



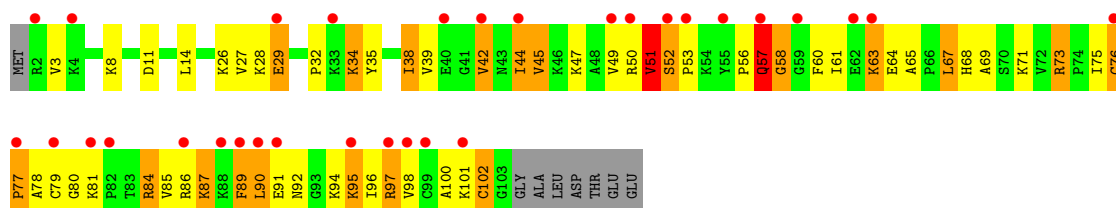
• Molecule 43: 50S ribosomal protein L23



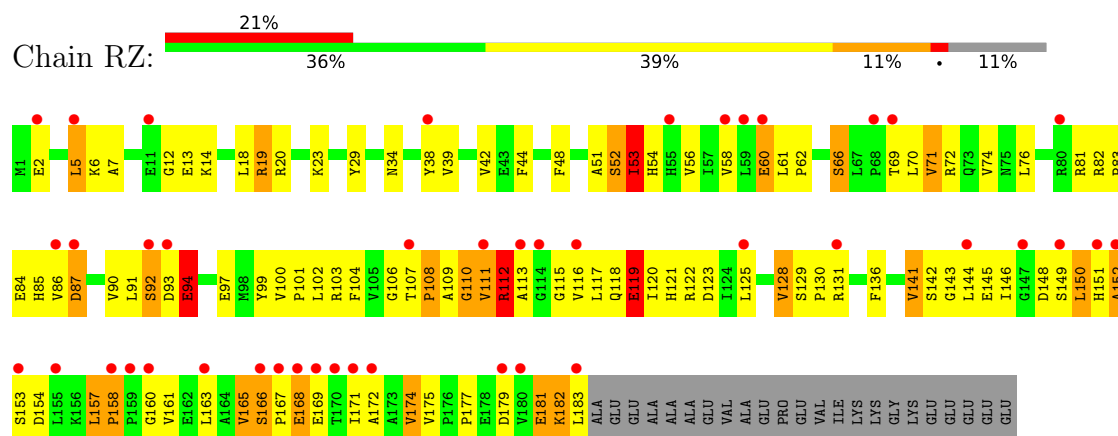
• Molecule 44: 50S ribosomal protein L24



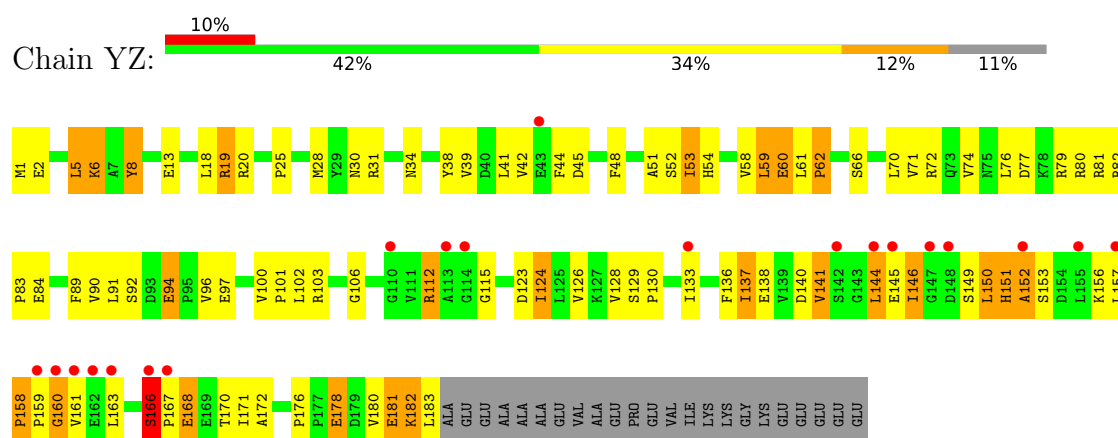
• Molecule 44: 50S ribosomal protein L24



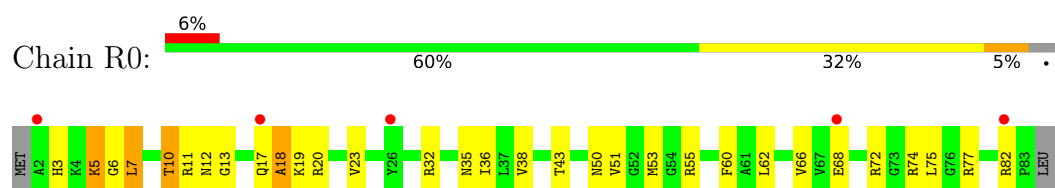
- Molecule 45: 50S ribosomal protein L25



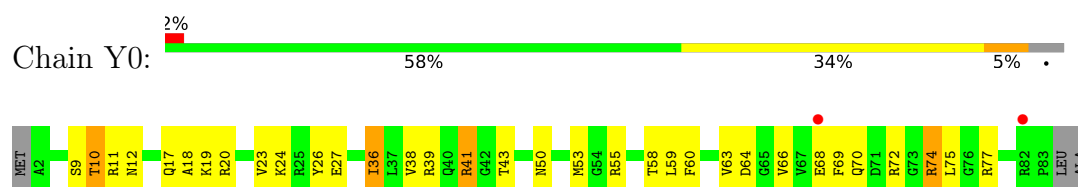
- Molecule 45: 50S ribosomal protein L25



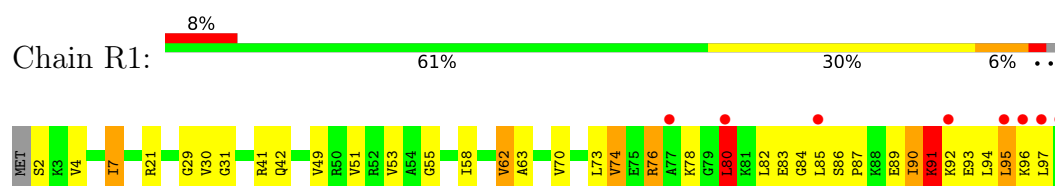
- Molecule 46: 50S ribosomal protein L27



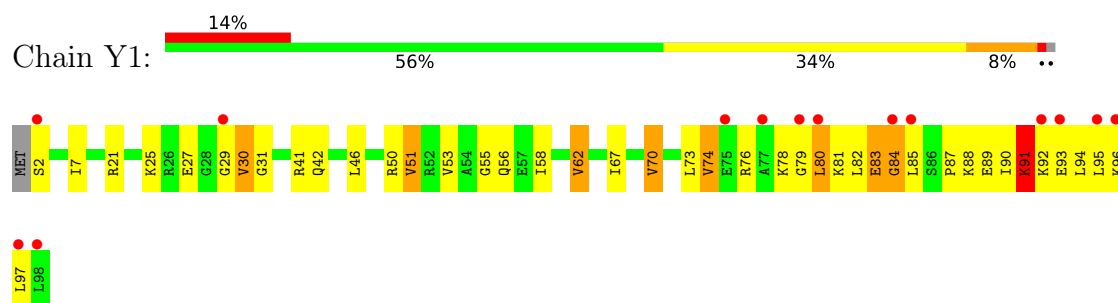
- Molecule 46: 50S ribosomal protein L27



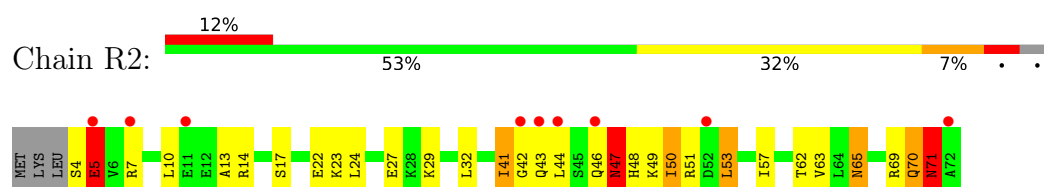
- Molecule 47: 50S ribosomal protein L28



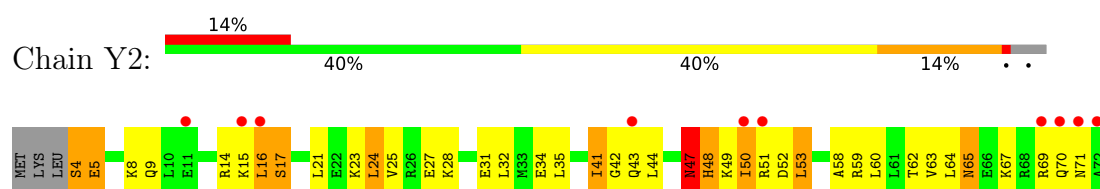
- Molecule 47: 50S ribosomal protein L28



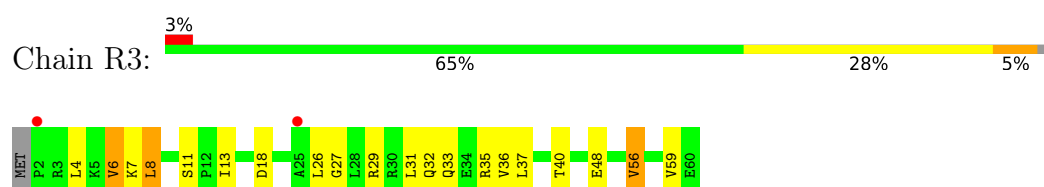
- Molecule 48: 50S ribosomal protein L29



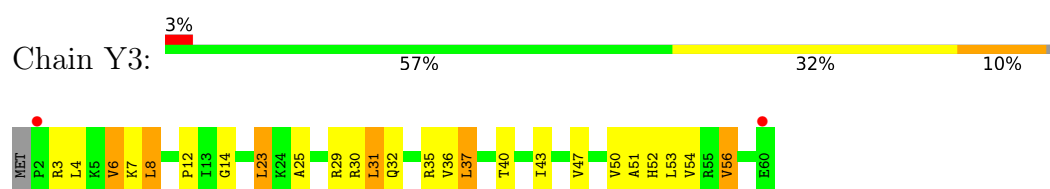
- Molecule 48: 50S ribosomal protein L29



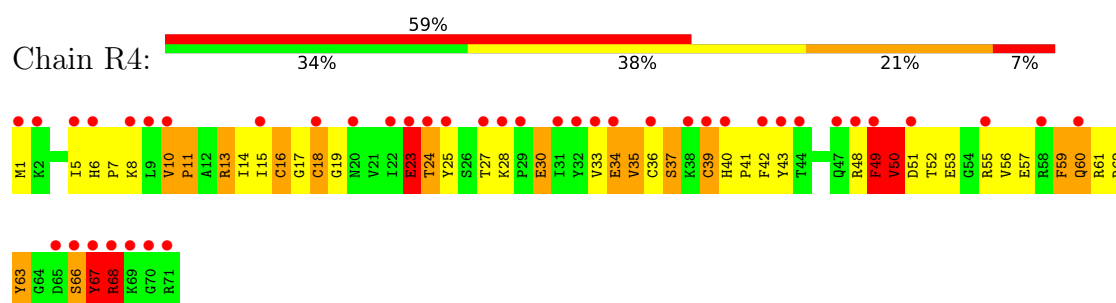
- Molecule 49: 50S ribosomal protein L30



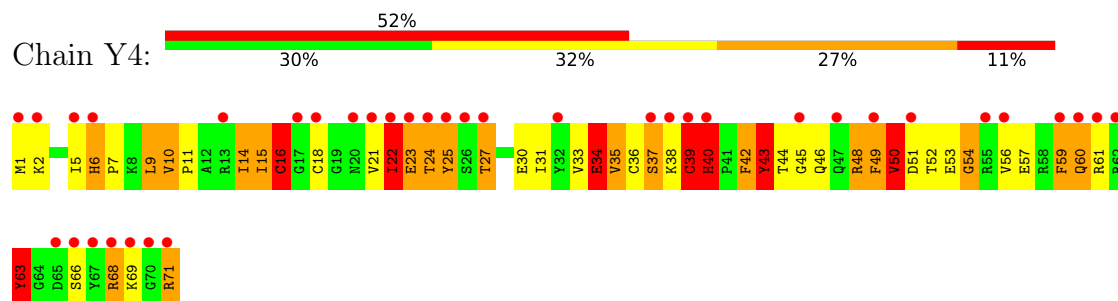
- Molecule 49: 50S ribosomal protein L30



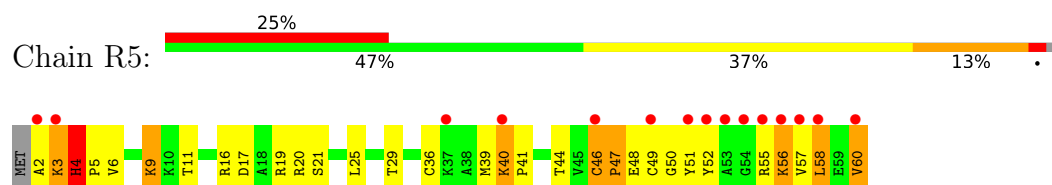
- Molecule 50: 50S ribosomal protein L31



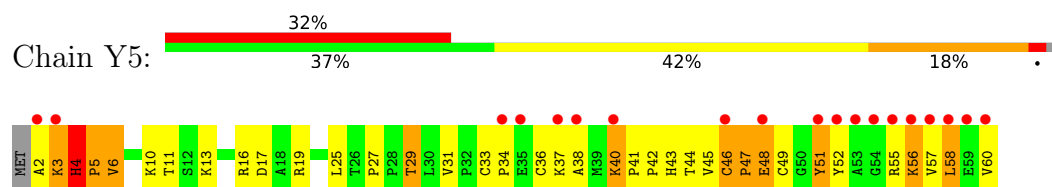
- Molecule 50: 50S ribosomal protein L31



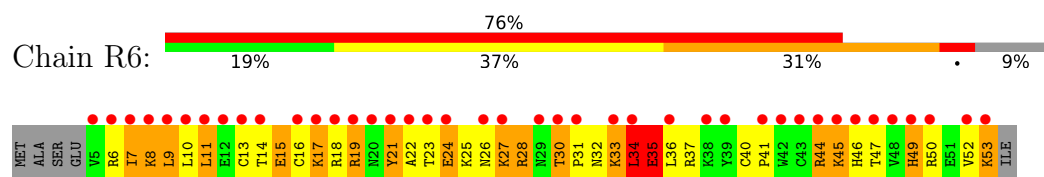
- Molecule 51: 50S ribosomal protein L32



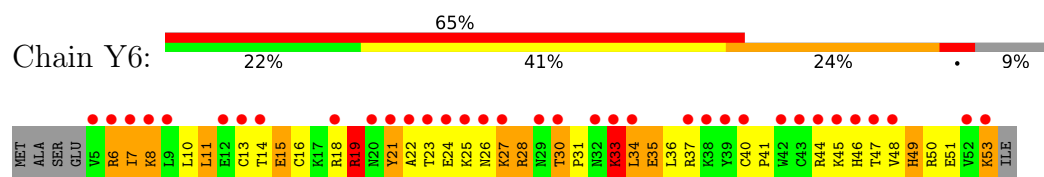
- Molecule 51: 50S ribosomal protein L32



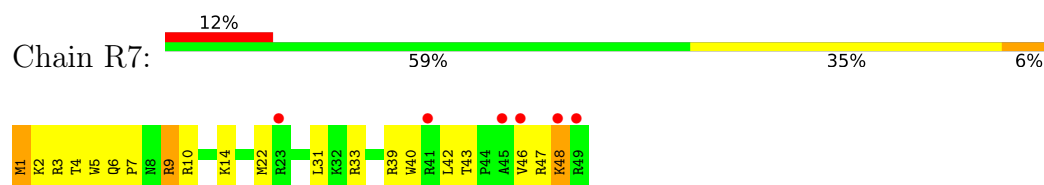
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33

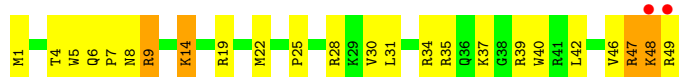


- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34





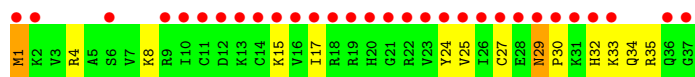
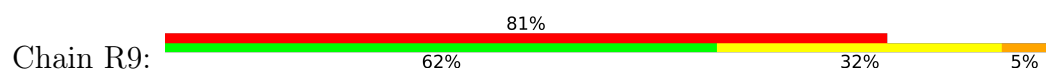
- Molecule 54: 50S ribosomal protein L35



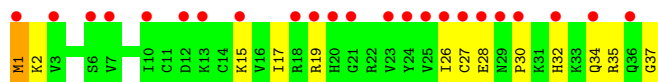
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94 155.22 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.6 (155.22-2.94) 98.6 (155.22-2.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.265 0.220 , 0.264	Depositor DCC
R_{free} test set	64589 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	291993	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.27	0/36098	0.50	6/56341 (0.0%)
1	XA	0.31	0/36101	0.54	12/56346 (0.0%)
2	QB	0.39	0/1959	0.86	4/2642 (0.2%)
2	XB	0.39	0/1959	0.89	4/2642 (0.2%)
3	QC	0.43	0/1629	0.86	0/2195
3	XC	0.48	0/1629	0.85	0/2195
4	QD	0.47	0/1733	0.97	3/2318 (0.1%)
4	XD	0.51	0/1733	0.96	5/2318 (0.2%)
5	QE	0.45	0/1171	0.95	6/1576 (0.4%)
5	XE	0.52	0/1171	0.94	2/1576 (0.1%)
6	QF	0.45	0/856	0.80	0/1154
6	XF	0.51	0/856	0.88	0/1154
7	QG	0.42	0/1276	0.84	0/1709
7	XG	0.46	0/1276	0.85	1/1709 (0.1%)
8	QH	0.43	0/1136	0.93	2/1527 (0.1%)
8	XH	0.47	0/1136	0.92	4/1527 (0.3%)
9	QI	0.40	0/1029	0.90	1/1379 (0.1%)
9	XI	0.42	0/1029	0.89	1/1379 (0.1%)
10	QJ	0.43	0/814	0.92	2/1095 (0.2%)
10	XJ	0.48	0/814	1.00	3/1095 (0.3%)
11	QK	0.48	0/900	0.91	1/1213 (0.1%)
11	XK	0.51	0/900	0.93	0/1213
12	QL	0.47	0/991	0.96	3/1327 (0.2%)
12	XL	0.58	0/991	1.14	9/1327 (0.7%)
13	QM	0.42	0/974	0.98	2/1303 (0.2%)
13	XM	0.47	0/974	0.98	1/1303 (0.1%)
14	QN	0.48	0/501	0.90	0/664
14	XN	0.57	0/501	1.04	3/664 (0.5%)
15	QO	0.45	0/745	0.80	0/992
15	XO	0.49	0/745	0.89	0/992
16	QP	0.47	0/721	0.93	2/970 (0.2%)
16	XP	0.47	0/721	0.88	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.42	0/847	0.85	0/1131
17	XQ	0.42	0/847	0.83	0/1131
18	QR	0.44	0/579	0.89	0/768
18	XR	0.47	0/579	0.85	1/768 (0.1%)
19	QS	0.44	0/689	0.99	3/926 (0.3%)
19	XS	0.47	0/689	1.01	6/926 (0.6%)
20	QT	0.46	0/765	0.96	2/1007 (0.2%)
20	XT	0.42	0/765	0.97	2/1007 (0.2%)
21	QU	0.36	0/221	0.79	0/288
21	XU	0.37	0/221	0.82	0/288
22	QV	0.26	0/1836	0.46	0/2859
22	XV	0.31	0/1836	0.53	0/2859
23	QY	0.35	1/333 (0.3%)	0.42	0/517
23	XY	0.37	1/333 (0.3%)	0.49	0/517
24	QX	0.26	0/185	0.69	0/285
24	XX	0.38	0/185	0.49	0/285
25	RA	0.34	0/69521	0.56	14/108529 (0.0%)
25	YA	0.39	0/69543	0.61	24/108563 (0.0%)
26	RB	0.28	0/2878	0.50	0/4490
26	YB	0.33	0/2878	0.58	0/4490
27	RD	0.63	0/2165	1.07	9/2919 (0.3%)
27	YD	0.73	0/2165	1.13	13/2919 (0.4%)
28	RE	0.56	0/1601	1.07	6/2160 (0.3%)
28	YE	0.60	0/1601	1.11	10/2160 (0.5%)
29	RF	0.53	0/1620	0.95	4/2194 (0.2%)
29	YF	0.60	0/1620	1.08	9/2194 (0.4%)
30	RG	0.40	0/1499	0.91	0/2016
30	YG	0.50	0/1499	0.91	2/2016 (0.1%)
31	RH	0.41	0/1332	1.02	9/1802 (0.5%)
31	YH	0.59	0/1332	1.10	7/1802 (0.4%)
32	RI	0.50	0/1151	1.03	4/1558 (0.3%)
32	YI	0.52	0/1151	0.97	5/1558 (0.3%)
33	RN	0.52	0/1131	1.01	2/1525 (0.1%)
33	YN	0.56	0/1131	0.94	1/1525 (0.1%)
34	RO	0.55	0/943	0.98	3/1269 (0.2%)
34	YO	0.60	0/943	0.97	0/1269
35	RP	0.60	0/1162	1.20	11/1544 (0.7%)
35	YP	0.67	0/1162	1.27	9/1544 (0.6%)
36	RQ	0.63	0/1143	1.09	4/1527 (0.3%)
36	YQ	0.73	1/1143 (0.1%)	1.13	7/1527 (0.5%)
37	RR	0.54	0/982	0.99	1/1312 (0.1%)
37	YR	0.56	0/982	1.04	3/1312 (0.2%)
38	RS	0.42	0/892	0.88	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.51	0/892	0.99	1/1187 (0.1%)
39	RT	0.53	0/1155	0.98	3/1542 (0.2%)
39	YT	0.58	0/1155	1.05	7/1542 (0.5%)
40	RU	0.53	0/982	1.04	6/1306 (0.5%)
40	YU	0.62	0/982	1.05	3/1306 (0.2%)
41	RV	0.47	0/790	0.97	5/1057 (0.5%)
41	YV	0.58	0/790	1.01	2/1057 (0.2%)
42	RW	0.64	0/911	0.98	0/1220
42	YW	0.60	0/911	1.00	0/1220
43	RX	0.59	0/739	0.96	4/993 (0.4%)
43	YX	0.60	0/739	1.00	1/993 (0.1%)
44	RY	0.54	0/798	1.07	6/1064 (0.6%)
44	YY	0.59	0/798	1.09	5/1064 (0.5%)
45	RZ	0.45	0/1493	1.00	10/2026 (0.5%)
45	YZ	0.49	0/1493	1.01	6/2026 (0.3%)
46	R0	0.55	0/657	0.98	3/874 (0.3%)
46	Y0	0.60	0/657	0.98	1/874 (0.1%)
47	R1	0.55	0/770	0.97	0/1022
47	Y1	0.58	0/770	0.96	1/1022 (0.1%)
48	R2	0.46	0/583	1.01	1/771 (0.1%)
48	Y2	0.60	0/583	1.05	1/771 (0.1%)
49	R3	0.46	0/474	0.91	0/635
49	Y3	0.53	0/474	0.86	0/635
50	R4	0.45	0/594	1.18	8/795 (1.0%)
50	Y4	0.48	0/594	1.16	6/795 (0.8%)
51	R5	0.62	0/473	1.22	4/639 (0.6%)
51	Y5	0.64	0/473	1.32	7/639 (1.1%)
52	R6	0.53	0/431	1.01	2/575 (0.3%)
52	Y6	0.56	0/431	1.00	2/575 (0.3%)
53	R7	0.63	0/438	1.04	2/575 (0.3%)
53	Y7	0.70	0/438	1.02	3/575 (0.5%)
54	R8	0.69	0/525	1.17	4/691 (0.6%)
54	Y8	0.75	0/525	1.15	5/691 (0.7%)
55	R9	0.34	0/310	0.81	0/407
55	Y9	0.45	0/310	0.80	0/407
56	Z6	0.46	0/40	0.62	0/60
56	Z8	0.45	0/40	0.62	0/60
All	All	0.40	3/316367 (0.0%)	0.70	358/472979 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	QL	0	1
12	XL	0	1
28	RE	0	1
28	YE	0	1
29	YF	0	1
31	RH	0	2
31	YH	0	2
38	YS	0	1
45	YZ	0	1
48	Y2	0	1
54	R8	0	2
54	Y8	0	2
All	All	0	16

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	YQ	82	ARG	N-CA	5.50	1.51	1.46
23	XY	37	1MG	O3'-P	5.17	1.61	1.56
23	QY	37	1MG	O3'-P	5.07	1.61	1.56

The worst 5 of 358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RQ	82	ARG	N-CA-C	11.98	124.55	110.41
51	Y5	4	HIS	CA-C-N	-11.21	108.55	119.76
51	Y5	4	HIS	C-N-CA	-11.21	108.55	119.76
35	YP	59	LEU	N-CA-C	-10.56	99.93	112.92
4	QD	28	SER	CA-C-N	-10.43	108.87	120.45

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
54	R8	30	ARG	Peptide
28	RE	21	VAL	Peptide
31	RH	127	GLU	Peptide
31	RH	153	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	494	0
1	XA	32249	0	16279	527	1
2	QB	1924	0	1975	68	0
2	XB	1924	0	1975	87	0
3	QC	1605	0	1668	42	0
3	XC	1605	0	1668	62	0
4	QD	1703	0	1763	66	0
4	XD	1703	0	1764	51	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	42	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	37	0
7	XG	1257	0	1296	22	0
8	QH	1116	0	1175	38	0
8	XH	1116	0	1177	26	0
9	QI	1010	0	1037	34	0
9	XI	1010	0	1037	50	0
10	QJ	801	0	849	50	0
10	XJ	801	0	849	42	0
11	QK	885	0	904	28	0
11	XK	885	0	904	27	0
12	QL	975	0	1062	37	0
12	XL	975	0	1062	47	0
13	QM	964	0	1034	41	0
13	XM	964	0	1034	40	0
14	QN	492	0	529	24	0
14	XN	492	0	529	17	0
15	QO	734	0	771	21	0
15	XO	734	0	771	19	0
16	QP	705	0	725	17	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	19	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	11	0
18	XR	574	0	644	21	0
19	QS	674	0	699	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	44	0
20	QT	763	0	860	26	0
20	XT	763	0	861	37	0
21	QU	217	0	234	11	0
21	XU	217	0	234	5	0
22	QV	1644	0	836	25	0
22	XV	1644	0	836	17	0
23	QY	323	0	165	3	0
23	XY	323	0	165	6	0
24	QX	167	0	87	0	0
24	XX	167	0	87	0	0
25	RA	62071	0	31288	927	1
25	YA	62091	0	31295	883	0
26	RB	2573	0	1306	44	1
26	YB	2573	0	1306	32	0
27	RD	2115	0	2195	99	0
27	YD	2115	0	2195	102	0
28	RE	1568	0	1634	74	0
28	YE	1568	0	1634	67	0
29	RF	1585	0	1632	84	0
29	YF	1585	0	1632	67	0
30	RG	1474	0	1535	56	0
30	YG	1474	0	1535	61	0
31	RH	1307	0	1382	61	0
31	YH	1307	0	1382	69	0
32	RI	1136	0	1223	59	1
32	YI	1136	0	1223	51	0
33	RN	1104	0	1180	46	0
33	YN	1104	0	1180	52	0
34	RO	933	0	996	30	0
34	YO	933	0	996	27	0
35	RP	1145	0	1227	90	0
35	YP	1145	0	1227	97	0
36	RQ	1122	0	1179	66	0
36	YQ	1122	0	1178	52	0
37	RR	968	0	1033	49	0
37	YR	968	0	1033	38	0
38	RS	882	0	943	47	0
38	YS	882	0	943	41	0
39	RT	1141	0	1202	55	0
39	YT	1141	0	1202	50	0
40	RU	964	0	1022	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YU	964	0	1022	60	0
41	RV	779	0	852	20	0
41	YV	779	0	852	44	0
42	RW	900	0	964	28	0
42	YW	900	0	964	29	0
43	RX	725	0	778	30	0
43	YX	725	0	778	27	0
44	RY	785	0	878	52	0
44	YY	785	0	878	41	0
45	RZ	1461	0	1493	64	0
45	YZ	1461	0	1493	56	0
46	R0	648	0	672	21	0
46	Y0	648	0	672	28	0
47	R1	763	0	848	26	0
47	Y1	763	0	848	29	0
48	R2	581	0	629	19	0
48	Y2	581	0	629	26	0
49	R3	469	0	518	8	0
49	Y3	469	0	518	17	0
50	R4	581	0	574	26	0
50	Y4	581	0	574	48	0
51	R5	459	0	480	26	0
51	Y5	459	0	480	35	0
52	R6	424	0	450	27	0
52	Y6	424	0	450	30	0
53	R7	430	0	480	16	0
53	Y7	430	0	480	19	0
54	R8	517	0	582	31	0
54	Y8	517	0	582	44	0
55	R9	307	0	338	9	0
55	Y9	307	0	338	9	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	5	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	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	Y5	1	0	0	0	0
57	YA	268	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291993	0	198359	5966	2

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 12.

The worst 5 of 5966 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)
4:QD:22:LYS:HG3	4:QD:26:CYS:SG	1.85	1.16
25:RA:2701:C:H3'	25:RA:2702:U:H5''	1.30	1.13
25:YA:2701:C:H3'	25:YA:2702:U:H5''	1.32	1.07
25:RA:1359:A:N6	25:RA:1372:U:O4	1.87	1.07
27:YD:43:ARG:NH1	27:YD:44:ASN:OD1	1.86	1.06

All (2) 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)
25:RA:1593:G:O2'	26:RB:54:G:OP1[1_655]	2.12	0.08
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.15	0.05

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%)	175 (74%)	43 (18%)	17 (7%)	1	1
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	2
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	3	9
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	8	23
4	QD	206/209 (99%)	175 (85%)	25 (12%)	6 (3%)	3	9
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	4	13
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	7
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	6	17
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	25
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	25
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	18	40
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	9
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	2	5
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	3	8
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	3	8
10	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	1	3
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	4	12
11	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	7	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	2
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	1
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	1
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	1
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	1
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	1
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	27
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	14
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	10	27
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	10	27
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	6	17
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	4
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	23
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	0
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	0
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	2
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	2
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	4
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	4
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	4
27	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	3	7
28	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	1
28	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	1
29	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	2
29	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	2	5
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	1
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	1
31	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	0
31	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	0
32	RI	144/148 (97%)	101 (70%)	30 (21%)	13 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	YI	144/148 (97%)	104 (72%)	23 (16%)	17 (12%)	0	0
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	0	1
33	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	1
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	20
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	7	20
35	RP	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	0	1
35	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	0
36	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	0
36	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	0
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	4
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	1	3
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	1
38	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	0
39	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	0	1
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	1
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	7
40	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	7
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	2
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	1
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	2	6
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	6	19
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	5	15
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	5	15
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	0
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	0
45	RZ	181/206 (88%)	124 (68%)	32 (18%)	25 (14%)	0	0
45	YZ	181/206 (88%)	124 (68%)	40 (22%)	17 (9%)	0	1
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	9	25
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	1
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	1
48	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	0	1
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	7
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	19
50	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	7
51	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	7
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	15
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	15
54	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	1
54	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	2
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9215 (80%)	1533 (13%)	722 (6%)	1	2

5 of 722 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
13	QM	67	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	169 (82%)	36 (18%)	2	4
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	15
3	QC	159/188 (85%)	147 (92%)	12 (8%)	12	29
3	XC	159/188 (85%)	145 (91%)	14 (9%)	9	23
4	QD	180/181 (99%)	155 (86%)	25 (14%)	3	9
4	XD	180/181 (99%)	155 (86%)	25 (14%)	3	9
5	QE	116/123 (94%)	102 (88%)	14 (12%)	5	13
5	XE	116/123 (94%)	100 (86%)	16 (14%)	3	10
6	QF	90/90 (100%)	79 (88%)	11 (12%)	5	13
6	XF	90/90 (100%)	78 (87%)	12 (13%)	4	11
7	QG	126/127 (99%)	115 (91%)	11 (9%)	9	24
7	XG	126/127 (99%)	112 (89%)	14 (11%)	6	16
8	QH	119/119 (100%)	105 (88%)	14 (12%)	5	14
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	17
9	QI	98/99 (99%)	80 (82%)	18 (18%)	1	4
9	XI	98/99 (99%)	77 (79%)	21 (21%)	1	2
10	QJ	89/92 (97%)	75 (84%)	14 (16%)	2	8
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	5
11	QK	90/99 (91%)	79 (88%)	11 (12%)	5	13
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	19
12	QL	104/109 (95%)	91 (88%)	13 (12%)	4	12
12	XL	104/109 (95%)	90 (86%)	14 (14%)	4	10
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	1
13	XM	97/101 (96%)	79 (81%)	18 (19%)	1	3
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	4
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	9
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	23
15	XO	79/80 (99%)	68 (86%)	11 (14%)	3	9
16	QP	72/74 (97%)	62 (86%)	10 (14%)	3	9
16	XP	72/74 (97%)	66 (92%)	6 (8%)	10	26
17	QQ	95/97 (98%)	86 (90%)	9 (10%)	8	21
17	XQ	95/97 (98%)	88 (93%)	7 (7%)	13	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	4
18	XR	61/77 (79%)	50 (82%)	11 (18%)	2	4
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	3
19	XS	73/80 (91%)	56 (77%)	17 (23%)	1	1
20	QT	76/82 (93%)	66 (87%)	10 (13%)	4	11
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	11
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	170 (79%)	44 (21%)	1	3
27	YD	214/218 (98%)	176 (82%)	38 (18%)	2	4
28	RE	165/166 (99%)	122 (74%)	43 (26%)	0	1
28	YE	165/166 (99%)	134 (81%)	31 (19%)	1	3
29	RF	161/166 (97%)	127 (79%)	34 (21%)	1	2
29	YF	161/166 (97%)	134 (83%)	27 (17%)	2	6
30	RG	155/156 (99%)	135 (87%)	20 (13%)	4	12
30	YG	155/156 (99%)	131 (84%)	24 (16%)	2	8
31	RH	142/148 (96%)	116 (82%)	26 (18%)	2	4
31	YH	142/148 (96%)	111 (78%)	31 (22%)	1	2
32	RI	122/124 (98%)	95 (78%)	27 (22%)	1	2
32	YI	122/124 (98%)	90 (74%)	32 (26%)	0	0
33	RN	117/119 (98%)	94 (80%)	23 (20%)	1	3
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	3
34	RO	100/100 (100%)	91 (91%)	9 (9%)	9	23
34	YO	100/100 (100%)	85 (85%)	15 (15%)	3	8
35	RP	116/116 (100%)	83 (72%)	33 (28%)	0	0
35	YP	116/116 (100%)	81 (70%)	35 (30%)	0	0
36	RQ	111/111 (100%)	90 (81%)	21 (19%)	1	3
36	YQ	111/111 (100%)	94 (85%)	17 (15%)	3	8
37	RR	101/101 (100%)	81 (80%)	20 (20%)	1	3
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	2
38	RS	87/88 (99%)	67 (77%)	20 (23%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	65 (75%)	22 (25%)	0	1
39	RT	120/127 (94%)	101 (84%)	19 (16%)	2	8
39	YT	120/127 (94%)	93 (78%)	27 (22%)	1	2
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	8
40	YU	93/94 (99%)	79 (85%)	14 (15%)	3	8
41	RV	82/82 (100%)	63 (77%)	19 (23%)	1	1
41	YV	82/82 (100%)	66 (80%)	16 (20%)	1	3
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	2
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	5
43	RX	74/78 (95%)	61 (82%)	13 (18%)	2	4
43	YX	74/78 (95%)	59 (80%)	15 (20%)	1	2
44	RY	85/91 (93%)	56 (66%)	29 (34%)	0	0
44	YY	85/91 (93%)	62 (73%)	23 (27%)	0	0
45	RZ	162/179 (90%)	129 (80%)	33 (20%)	1	2
45	YZ	162/179 (90%)	130 (80%)	32 (20%)	1	3
46	R0	65/67 (97%)	58 (89%)	7 (11%)	6	17
46	Y0	65/67 (97%)	57 (88%)	8 (12%)	4	13
47	R1	82/83 (99%)	74 (90%)	8 (10%)	7	20
47	Y1	82/83 (99%)	69 (84%)	13 (16%)	2	7
48	R2	64/67 (96%)	49 (77%)	15 (23%)	1	1
48	Y2	64/67 (96%)	48 (75%)	16 (25%)	0	1
49	R3	51/52 (98%)	43 (84%)	8 (16%)	2	8
49	Y3	51/52 (98%)	44 (86%)	7 (14%)	3	10
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	0
50	Y4	63/63 (100%)	42 (67%)	21 (33%)	0	0
51	R5	51/52 (98%)	35 (69%)	16 (31%)	0	0
51	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	0
52	R6	48/52 (92%)	32 (67%)	16 (33%)	0	0
52	Y6	48/52 (92%)	34 (71%)	14 (29%)	0	0
53	R7	42/42 (100%)	35 (83%)	7 (17%)	2	6
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	43 (80%)	11 (20%)	1	2
54	Y8	54/55 (98%)	37 (68%)	17 (32%)	0	0
55	R9	34/34 (100%)	30 (88%)	4 (12%)	5	14
55	Y9	34/34 (100%)	31 (91%)	3 (9%)	9	23
All	All	9702/10066 (96%)	8009 (82%)	1693 (18%)	2	4

5 of 1693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	XE	101	ILE
27	YD	229	VAL
48	Y2	27	GLU
7	XG	136	LYS
5	XE	89	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
27	YD	164	GLN
33	YN	133	GLN
44	YY	57	GLN
36	RQ	45	GLN
36	RQ	13	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	306 (20%)	48 (3%)
1	XA	1498/1522 (98%)	314 (20%)	50 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QY	14/17 (82%)	5 (35%)	1 (7%)
23	XY	14/17 (82%)	6 (42%)	1 (7%)
24	QX	7/25 (28%)	3 (42%)	2 (28%)
24	XX	7/25 (28%)	1 (14%)	0
25	RA	2879/2916 (98%)	664 (23%)	74 (2%)
25	YA	2880/2916 (98%)	628 (21%)	75 (2%)
26	RB	119/122 (97%)	29 (24%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	YB	119/122 (97%)	29 (24%)	3 (2%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	2023 (22%)	258 (2%)

5 of 2023 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	29	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	1819	A
25	YA	2126	A
25	RA	1608	A
25	RA	1312	U
25	YA	2439	A

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	$\# Z > 2$
56	PPU	Z6	76	25,56	37,40,41	2.58	8 (21%)	47,57,60	2.57	15 (31%)
23	1MG	XY	37	23	23,26,27	2.46	4 (17%)	33,39,42	1.96	6 (18%)
56	PPU	Z8	76	25,56	37,40,41	2.57	8 (21%)	47,57,60	2.56	15 (31%)
23	1MG	QY	37	23	23,26,27	2.49	4 (17%)	33,39,42	2.03	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	76	25,56	-	2/25/43/44	0/4/4/4
23	1MG	XY	37	23	-	0/7/25/26	0/3/3/3
56	PPU	Z8	76	25,56	-	2/25/43/44	0/4/4/4
23	1MG	QY	37	23	-	0/7/25/26	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.65	1.41	1.23
56	Z8	76	PPU	O-C	9.58	1.41	1.23
23	XY	37	1MG	C2-N2	7.98	1.48	1.34
23	QY	37	1MG	C2-N2	7.76	1.47	1.34
23	QY	37	1MG	C4-N3	6.54	1.49	1.34

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z6	76	PPU	C3'-N3'-C	-8.55	110.19	123.20
56	Z8	76	PPU	C3'-N3'-C	-8.53	110.22	123.20
23	QY	37	1MG	N2-C2-N1	6.47	123.99	118.79
56	Z8	76	PPU	C2'-C1'-N9	-5.96	98.49	113.30
56	Z6	76	PPU	C2'-C1'-N9	-5.95	98.53	113.30

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.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	XY	37	1MG	1	0
56	Z8	76	PPU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 683 ligands modelled in this entry, 681 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	XA	1673	-	44,45,45	1.33	6 (13%)	63,67,67	1.30	4 (6%)
58	PAR	QA	1666	-	44,45,45	1.28	6 (13%)	63,67,67	1.33	9 (14%)

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	XA	1673	-	-	6/18/94/94	0/4/4/4
58	PAR	QA	1666	-	-	8/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C52-C42	3.13	1.58	1.52
58	XA	1673	PAR	C52-C42	3.00	1.58	1.52
58	XA	1673	PAR	O54-C14	2.86	1.49	1.41
58	XA	1673	PAR	C11-C21	2.86	1.57	1.52
58	QA	1666	PAR	O54-C14	2.85	1.49	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1673	PAR	O33-C14-C24	5.04	116.32	108.08
58	XA	1673	PAR	C14-O54-C54	4.32	122.16	113.72
58	QA	1666	PAR	O33-C14-C24	4.04	114.69	108.08
58	QA	1666	PAR	C14-O54-C54	3.84	121.21	113.72
58	QA	1666	PAR	O11-C42-C52	3.16	115.44	107.42

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

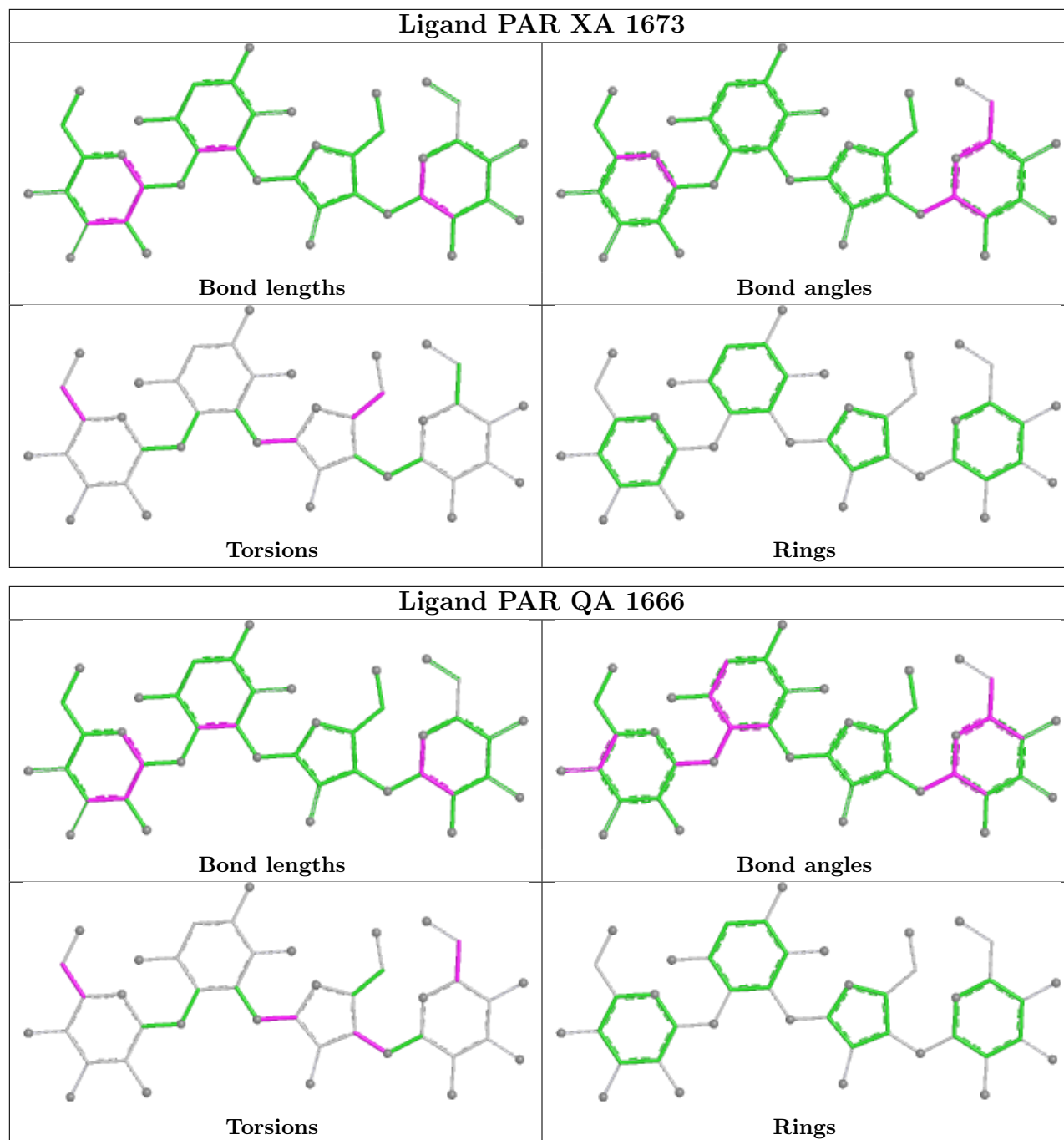
Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	XA	1673	PAR	O51-C51-C61-O61
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1673	PAR	C41-C51-C61-O61

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1673	PAR	1	0
58	QA	1666	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.19	51 (3%)	48	40	14, 55, 134, 294	0
1	XA	1500/1522 (98%)	-0.06	25 (1%)	69	61	7, 42, 133, 270	0
2	QB	237/256 (92%)	1.46	58 (24%)	2	2	42, 98, 171, 216	0
2	XB	237/256 (92%)	1.11	40 (16%)	4	4	27, 78, 141, 206	0
3	QC	205/239 (85%)	1.15	27 (13%)	7	7	37, 91, 139, 192	0
3	XC	205/239 (85%)	0.70	18 (8%)	15	14	11, 53, 103, 148	0
4	QD	208/209 (99%)	0.92	32 (15%)	5	5	23, 54, 106, 136	0
4	XD	208/209 (99%)	0.99	40 (19%)	3	3	17, 51, 103, 175	0
5	QE	151/162 (93%)	0.72	14 (9%)	14	13	29, 65, 114, 172	0
5	XE	151/162 (93%)	0.42	9 (5%)	27	23	15, 43, 86, 138	0
6	QF	101/101 (100%)	0.31	4 (3%)	42	34	13, 48, 78, 119	0
6	XF	101/101 (100%)	0.25	3 (2%)	52	44	12, 46, 76, 153	0
7	QG	155/156 (99%)	0.82	15 (9%)	13	12	23, 73, 121, 172	0
7	XG	155/156 (99%)	0.60	15 (9%)	13	12	18, 62, 109, 143	0
8	QH	138/138 (100%)	1.12	22 (15%)	5	5	30, 67, 99, 116	0
8	XH	138/138 (100%)	0.66	9 (6%)	25	21	13, 48, 84, 127	0
9	QI	127/128 (99%)	1.43	32 (25%)	1	1	33, 89, 129, 180	0
9	XI	127/128 (99%)	1.48	31 (24%)	2	2	19, 69, 124, 167	0
10	QJ	99/105 (94%)	1.76	39 (39%)	1	0	27, 98, 176, 200	0
10	XJ	99/105 (94%)	1.40	30 (30%)	1	1	5, 72, 131, 162	0
11	QK	119/129 (92%)	1.13	22 (18%)	3	3	22, 55, 110, 180	0
11	XK	119/129 (92%)	0.37	12 (10%)	12	11	16, 43, 106, 177	0
12	QL	125/132 (94%)	1.05	22 (17%)	4	3	14, 47, 100, 195	0
12	XL	125/132 (94%)	0.53	17 (13%)	7	7	7, 30, 103, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	QM	121/126 (96%)	1.61	32 (26%)	1	1	27, 84, 121, 226	0
13	XM	121/126 (96%)	1.24	26 (21%)	2	2	24, 57, 113, 211	0
14	QN	60/61 (98%)	1.51	21 (35%)	1	1	38, 80, 105, 122	0
14	XN	60/61 (98%)	0.95	10 (16%)	4	4	22, 43, 76, 100	0
15	QO	88/89 (98%)	0.49	4 (4%)	38	30	15, 52, 101, 137	0
15	XO	88/89 (98%)	0.31	3 (3%)	48	40	10, 42, 80, 97	0
16	QP	84/88 (95%)	0.91	11 (13%)	7	7	26, 50, 96, 135	0
16	XP	84/88 (95%)	0.97	12 (14%)	6	6	25, 57, 102, 179	0
17	QQ	100/105 (95%)	0.89	13 (13%)	7	7	27, 56, 100, 119	0
17	XQ	100/105 (95%)	0.75	14 (14%)	6	6	23, 55, 94, 109	0
18	QR	70/88 (79%)	0.47	5 (7%)	22	19	18, 55, 97, 111	0
18	XR	70/88 (79%)	0.27	1 (1%)	73	66	16, 50, 102, 113	0
19	QS	84/93 (90%)	1.38	20 (23%)	2	2	50, 96, 144, 180	0
19	XS	84/93 (90%)	0.58	6 (7%)	22	19	20, 65, 113, 176	0
20	QT	99/106 (93%)	0.99	17 (17%)	4	4	20, 59, 117, 189	0
20	XT	99/106 (93%)	1.16	23 (23%)	2	2	30, 68, 122, 151	0
21	QU	25/27 (92%)	1.24	7 (28%)	1	1	30, 73, 126, 140	0
21	XU	25/27 (92%)	0.87	5 (20%)	3	3	31, 45, 98, 136	0
22	QV	77/77 (100%)	0.44	4 (5%)	33	27	13, 59, 116, 149	0
22	XV	77/77 (100%)	-0.05	4 (5%)	33	27	3, 42, 86, 154	0
23	QY	14/17 (82%)	1.44	3 (21%)	2	2	60, 101, 150, 155	0
23	XY	14/17 (82%)	0.50	2 (14%)	6	6	24, 79, 120, 138	0
24	QX	8/25 (32%)	0.68	1 (12%)	8	8	30, 49, 70, 98	0
24	XX	8/25 (32%)	-0.49	0	100	100	15, 25, 40, 55	0
25	RA	2882/2916 (98%)	-0.30	106 (3%)	45	36	1, 31, 175, 318	0
25	YA	2883/2916 (98%)	-0.44	112 (3%)	43	35	0, 21, 170, 311	0
26	RB	120/122 (98%)	0.19	1 (0%)	82	77	29, 55, 88, 110	0
26	YB	120/122 (98%)	-0.32	2 (1%)	69	61	14, 37, 58, 106	0
27	RD	272/276 (98%)	0.27	23 (8%)	16	15	0, 24, 63, 135	0
27	YD	272/276 (98%)	-0.09	13 (4%)	35	29	0, 14, 46, 168	0
28	RE	205/206 (99%)	0.52	28 (13%)	6	6	1, 36, 109, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.73	32 (15%)	5 5	0, 32, 113, 183	0
29	RF	202/210 (96%)	0.49	19 (9%)	14 13	2, 41, 94, 154	0
29	YF	202/210 (96%)	0.12	9 (4%)	38 30	0, 27, 83, 144	0
30	RG	181/182 (99%)	1.73	66 (36%)	1 1	26, 79, 130, 185	0
30	YG	181/182 (99%)	0.63	23 (12%)	8 7	14, 43, 93, 158	0
31	RH	170/180 (94%)	2.18	94 (55%)	0 0	42, 117, 172, 219	0
31	YH	170/180 (94%)	1.10	33 (19%)	3 3	12, 50, 96, 160	0
32	RI	146/148 (98%)	1.44	39 (26%)	1 1	22, 74, 128, 179	0
32	YI	146/148 (98%)	1.17	29 (19%)	3 3	16, 74, 128, 161	0
33	RN	138/140 (98%)	0.65	16 (11%)	9 9	16, 43, 86, 150	0
33	YN	138/140 (98%)	0.55	13 (9%)	14 13	10, 35, 87, 139	0
34	RO	122/122 (100%)	-0.05	3 (2%)	58 49	10, 34, 75, 103	0
34	YO	122/122 (100%)	-0.14	1 (0%)	82 77	1, 25, 48, 76	0
35	RP	150/150 (100%)	0.74	16 (10%)	11 10	3, 48, 112, 222	0
35	YP	150/150 (100%)	0.43	14 (9%)	14 13	2, 32, 95, 190	0
36	RQ	141/141 (100%)	0.82	22 (15%)	5 5	4, 47, 104, 139	0
36	YQ	141/141 (100%)	0.20	16 (11%)	10 10	1, 27, 82, 153	0
37	RR	118/118 (100%)	-0.01	3 (2%)	58 49	3, 30, 55, 88	0
37	YR	118/118 (100%)	0.09	4 (3%)	48 40	6, 31, 58, 113	0
38	RS	111/112 (99%)	0.82	15 (13%)	7 7	23, 58, 109, 127	0
38	YS	111/112 (99%)	0.58	13 (11%)	9 9	13, 40, 93, 150	0
39	RT	137/146 (93%)	0.54	14 (10%)	12 11	16, 42, 124, 206	0
39	YT	137/146 (93%)	0.78	21 (15%)	5 5	9, 35, 131, 196	0
40	RU	117/118 (99%)	0.47	8 (6%)	23 20	6, 34, 96, 165	0
40	YU	117/118 (99%)	0.09	9 (7%)	19 17	2, 21, 85, 144	0
41	RV	101/101 (100%)	0.84	17 (16%)	4 4	7, 53, 108, 198	0
41	YV	101/101 (100%)	0.58	12 (11%)	9 8	0, 46, 93, 208	0
42	RW	113/113 (100%)	0.10	7 (6%)	26 22	3, 25, 69, 172	0
42	YW	113/113 (100%)	0.08	7 (6%)	26 22	1, 25, 79, 174	0
43	RX	92/96 (95%)	0.22	5 (5%)	31 25	0, 33, 64, 106	0
43	YX	92/96 (95%)	-0.01	5 (5%)	31 25	0, 22, 59, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	2.06	45 (44%)	0 0	10, 65, 132, 205	0
44	YY	102/110 (92%)	1.59	31 (30%)	1 1	8, 46, 109, 201	0
45	RZ	183/206 (88%)	1.32	43 (23%)	2 2	28, 81, 152, 203	0
45	YZ	183/206 (88%)	0.72	20 (10%)	10 10	16, 59, 135, 195	0
46	R0	82/85 (96%)	0.27	5 (6%)	27 22	13, 36, 60, 83	0
46	Y0	82/85 (96%)	-0.24	2 (2%)	59 50	2, 22, 41, 74	0
47	R1	97/98 (98%)	0.61	8 (8%)	17 15	5, 33, 134, 196	0
47	Y1	97/98 (98%)	0.65	14 (14%)	6 6	1, 29, 123, 178	0
48	R2	69/72 (95%)	0.49	9 (13%)	7 7	15, 51, 121, 133	0
48	Y2	69/72 (95%)	0.58	10 (14%)	6 6	8, 32, 85, 167	0
49	R3	59/60 (98%)	0.33	2 (3%)	48 40	15, 41, 78, 134	0
49	Y3	59/60 (98%)	0.12	2 (3%)	48 40	10, 30, 81, 142	0
50	R4	71/71 (100%)	2.61	42 (59%)	0 0	59, 140, 202, 292	0
50	Y4	71/71 (100%)	2.40	37 (52%)	0 0	39, 97, 174, 227	0
51	R5	59/60 (98%)	1.00	15 (25%)	1 1	2, 33, 145, 188	0
51	Y5	59/60 (98%)	1.08	19 (32%)	1 1	1, 39, 172, 198	0
52	R6	49/54 (90%)	3.67	41 (83%)	0 0	68, 125, 194, 221	0
52	Y6	49/54 (90%)	3.08	35 (71%)	0 0	70, 113, 183, 206	0
53	R7	49/49 (100%)	0.03	6 (12%)	8 8	2, 12, 67, 170	0
53	Y7	49/49 (100%)	-0.06	2 (4%)	41 33	0, 7, 50, 140	0
54	R8	64/65 (98%)	0.59	9 (14%)	6 6	8, 31, 93, 151	0
54	Y8	64/65 (98%)	0.71	13 (20%)	3 3	0, 25, 81, 172	0
55	R9	37/37 (100%)	3.35	30 (81%)	0 0	55, 105, 158, 176	0
55	Y9	37/37 (100%)	2.91	23 (62%)	0 0	47, 87, 153, 202	0
56	Z6	2/3 (66%)	0.28	0	100 100	21, 21, 21, 24	0
56	Z8	2/3 (66%)	-0.02	0	100 100	5, 5, 5, 14	0
All	All	20873/21492 (97%)	0.36	2164 (10%)	11 11	0, 43, 135, 318	0

The worst 5 of 2164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	11.6
11	QK	128	ALA	10.7

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Mol	Chain	Res	Type	RSRZ
11	QK	127	LYS	10.5
30	YG	80	PHE	9.8
11	XK	129	SER	9.8

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
56	PPU	Z6	76	37/38	0.92	0.15	27,27,27,27	0
56	PPU	Z8	76	37/38	0.93	0.13	14,14,14,14	0
23	1MG	QY	37	24/25	0.95	0.09	53,53,53,53	0
23	1MG	XY	37	24/25	0.96	0.08	30,30,30,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	YA	3139	1/1	0.03	0.34	55,55,55,55	0
57	MG	QH	201	1/1	0.05	0.23	74,74,74,74	0
57	MG	RA	3192	1/1	0.26	0.22	68,68,68,68	0
57	MG	QA	1625	1/1	0.32	0.19	70,70,70,70	0
57	MG	RA	3091	1/1	0.36	0.20	23,23,23,23	0
57	MG	RA	3193	1/1	0.42	0.23	63,63,63,63	0
57	MG	RA	3120	1/1	0.43	0.34	80,80,80,80	0
57	MG	RA	3139	1/1	0.47	0.33	59,59,59,59	0
57	MG	QA	1661	1/1	0.48	0.17	138,138,138,138	0
57	MG	RA	3223	1/1	0.51	0.25	59,59,59,59	0
57	MG	YA	3104	1/1	0.54	0.16	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1628	1/1	0.57	0.18	37,37,37,37	0
57	MG	YA	3120	1/1	0.58	0.20	21,21,21,21	0
57	MG	XA	1629	1/1	0.60	0.25	32,32,32,32	0
57	MG	RA	3227	1/1	0.60	0.13	32,32,32,32	0
57	MG	QA	1656	1/1	0.61	0.20	89,89,89,89	0
57	MG	RA	3130	1/1	0.65	0.16	43,43,43,43	0
57	MG	XA	1670	1/1	0.66	0.12	35,35,35,35	0
57	MG	XA	1665	1/1	0.66	0.22	56,56,56,56	0
57	MG	YA	3140	1/1	0.67	0.14	2,2,2,2	0
57	MG	YA	3165	1/1	0.68	0.29	40,40,40,40	0
57	MG	YA	3204	1/1	0.68	0.11	17,17,17,17	0
57	MG	RA	3135	1/1	0.69	0.21	31,31,31,31	0
57	MG	XA	1653	1/1	0.70	0.27	70,70,70,70	0
57	MG	YA	3130	1/1	0.73	0.18	20,20,20,20	0
57	MG	YA	3266	1/1	0.74	0.33	51,51,51,51	0
57	MG	RA	3155	1/1	0.75	0.11	10,10,10,10	0
57	MG	RA	3194	1/1	0.75	0.15	13,13,13,13	0
57	MG	RB	202	1/1	0.75	0.20	46,46,46,46	0
57	MG	RP	202	1/1	0.75	0.25	85,85,85,85	0
57	MG	YA	3084	1/1	0.76	0.17	2,2,2,2	0
57	MG	QA	1636	1/1	0.76	0.27	39,39,39,39	0
57	MG	QA	1637	1/1	0.76	0.17	16,16,16,16	0
57	MG	YA	3160	1/1	0.77	0.10	18,18,18,18	0
57	MG	YA	3240	1/1	0.77	0.13	32,32,32,32	0
57	MG	YA	3249	1/1	0.77	0.29	42,42,42,42	0
57	MG	YA	3016	1/1	0.77	0.14	0,0,0,0	0
57	MG	XA	1669	1/1	0.78	0.14	49,49,49,49	0
57	MG	XA	1639	1/1	0.79	0.23	58,58,58,58	0
57	MG	RA	3228	1/1	0.79	0.18	43,43,43,43	0
57	MG	XA	1631	1/1	0.79	0.20	33,33,33,33	0
57	MG	QA	1608	1/1	0.80	0.10	22,22,22,22	0
57	MG	RA	3026	1/1	0.81	0.16	3,3,3,3	0
57	MG	RA	3206	1/1	0.81	0.23	44,44,44,44	0
57	MG	RA	3138	1/1	0.81	0.16	6,6,6,6	0
57	MG	RD	301	1/1	0.81	0.16	35,35,35,35	0
57	MG	YA	3164	1/1	0.81	0.23	45,45,45,45	0
57	MG	YP	201	1/1	0.81	0.15	96,96,96,96	0
57	MG	QA	1629	1/1	0.82	0.17	30,30,30,30	0
57	MG	YA	3207	1/1	0.82	0.34	46,46,46,46	0
57	MG	QA	1632	1/1	0.82	0.12	88,88,88,88	0
57	MG	YA	3197	1/1	0.83	0.16	42,42,42,42	0
57	MG	XA	1672	1/1	0.83	0.19	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1663	1/1	0.83	0.14	38,38,38,38	0
57	MG	RA	3187	1/1	0.83	0.31	66,66,66,66	0
57	MG	QF	201	1/1	0.83	0.30	54,54,54,54	0
57	MG	QA	1630	1/1	0.83	0.18	48,48,48,48	0
57	MG	YB	201	1/1	0.83	0.11	39,39,39,39	0
57	MG	YA	3127	1/1	0.83	0.15	26,26,26,26	0
57	MG	RA	3238	1/1	0.84	0.18	14,14,14,14	0
57	MG	YA	3235	1/1	0.84	0.23	30,30,30,30	0
57	MG	XM	201	1/1	0.84	0.09	58,58,58,58	0
57	MG	RA	3196	1/1	0.84	0.19	42,42,42,42	0
57	MG	QA	1631	1/1	0.84	0.09	39,39,39,39	0
57	MG	YA	3198	1/1	0.84	0.31	69,69,69,69	0
57	MG	RA	3220	1/1	0.84	0.10	31,31,31,31	0
57	MG	YA	3150	1/1	0.85	0.28	62,62,62,62	0
57	MG	YA	3221	1/1	0.85	0.17	29,29,29,29	0
57	MG	QA	1663	1/1	0.85	0.14	67,67,67,67	0
57	MG	YA	3129	1/1	0.85	0.17	28,28,28,28	0
57	MG	YA	3242	1/1	0.85	0.18	33,33,33,33	0
57	MG	XA	1652	1/1	0.85	0.12	47,47,47,47	0
57	MG	RA	3209	1/1	0.85	0.26	47,47,47,47	0
57	MG	XX	101	1/1	0.85	0.14	45,45,45,45	0
57	MG	YA	3142	1/1	0.85	0.04	8,8,8,8	0
58	PAR	QA	1666	42/42	0.85	0.19	43,43,43,43	0
57	MG	QA	1622	1/1	0.86	0.18	40,40,40,40	0
57	MG	RA	3171	1/1	0.86	0.26	33,33,33,33	0
57	MG	RB	201	1/1	0.86	0.12	41,41,41,41	0
57	MG	R0	101	1/1	0.87	0.19	15,15,15,15	0
57	MG	YA	3220	1/1	0.87	0.18	32,32,32,32	0
57	MG	YA	3102	1/1	0.87	0.22	44,44,44,44	0
57	MG	QA	1657	1/1	0.87	0.12	37,37,37,37	0
57	MG	RA	3175	1/1	0.87	0.13	19,19,19,19	0
57	MG	RA	3118	1/1	0.87	0.11	22,22,22,22	0
57	MG	QA	1647	1/1	0.87	0.08	32,32,32,32	0
57	MG	YA	3178	1/1	0.87	0.17	29,29,29,29	0
57	MG	RA	3142	1/1	0.87	0.15	32,32,32,32	0
57	MG	YA	3131	1/1	0.87	0.27	34,34,34,34	0
57	MG	YQ	201	1/1	0.87	0.24	142,142,142,142	0
57	MG	YX	101	1/1	0.87	0.15	46,46,46,46	0
57	MG	RA	3058	1/1	0.87	0.18	34,34,34,34	0
57	MG	RA	3189	1/1	0.88	0.18	46,46,46,46	0
57	MG	YA	3173	1/1	0.88	0.10	49,49,49,49	0
57	MG	RA	3145	1/1	0.88	0.26	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1627	1/1	0.88	0.16	22,22,22,22	0
57	MG	RA	3068	1/1	0.88	0.14	16,16,16,16	0
57	MG	RA	3124	1/1	0.88	0.23	24,24,24,24	0
57	MG	YA	3152	1/1	0.88	0.17	31,31,31,31	0
57	MG	QA	1633	1/1	0.88	0.36	35,35,35,35	0
57	MG	YA	3071	1/1	0.88	0.08	0,0,0,0	0
57	MG	YA	3232	1/1	0.88	0.27	47,47,47,47	0
57	MG	RA	3084	1/1	0.89	0.10	7,7,7,7	0
57	MG	QX	101	1/1	0.89	0.22	26,26,26,26	0
57	MG	YA	3182	1/1	0.89	0.16	18,18,18,18	0
57	MG	YA	3193	1/1	0.89	0.21	18,18,18,18	0
57	MG	XA	1651	1/1	0.89	0.08	95,95,95,95	0
57	MG	YA	3117	1/1	0.89	0.36	24,24,24,24	0
57	MG	RA	3115	1/1	0.89	0.11	5,5,5,5	0
57	MG	RA	3010	1/1	0.89	0.27	38,38,38,38	0
57	MG	QA	1665	1/1	0.89	0.21	31,31,31,31	0
57	MG	RA	3156	1/1	0.89	0.12	31,31,31,31	0
57	MG	QA	1655	1/1	0.89	0.20	38,38,38,38	0
57	MG	RU	201	1/1	0.89	0.26	117,117,117,117	0
57	MG	QA	1660	1/1	0.89	0.20	38,38,38,38	0
57	MG	R5	101	1/1	0.89	0.10	21,21,21,21	0
57	MG	XA	1622	1/1	0.89	0.18	33,33,33,33	0
57	MG	XA	1624	1/1	0.89	0.21	16,16,16,16	0
57	MG	YA	3054	1/1	0.89	0.19	48,48,48,48	0
57	MG	YA	3161	1/1	0.89	0.34	34,34,34,34	0
57	MG	YA	3061	1/1	0.89	0.13	17,17,17,17	0
57	MG	RA	3078	1/1	0.89	0.23	23,23,23,23	0
57	MG	YA	3172	1/1	0.89	0.12	25,25,25,25	0
58	PAR	XA	1673	42/42	0.89	0.14	31,31,31,31	0
57	MG	RA	3121	1/1	0.90	0.21	36,36,36,36	0
57	MG	YA	3122	1/1	0.90	0.15	3,3,3,3	0
57	MG	YA	3039	1/1	0.90	0.17	10,10,10,10	0
57	MG	YA	3045	1/1	0.90	0.18	1,1,1,1	0
57	MG	RA	3242	1/1	0.90	0.32	31,31,31,31	0
57	MG	RA	3101	1/1	0.90	0.09	2,2,2,2	0
57	MG	YA	3245	1/1	0.90	0.28	28,28,28,28	0
57	MG	YA	3180	1/1	0.90	0.24	41,41,41,41	0
57	MG	YA	3251	1/1	0.90	0.27	38,38,38,38	0
57	MG	YA	3265	1/1	0.90	0.16	17,17,17,17	0
57	MG	RA	3174	1/1	0.90	0.13	25,25,25,25	0
57	MG	RA	3221	1/1	0.90	0.14	39,39,39,39	0
57	MG	YA	3196	1/1	0.90	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YP	202	1/1	0.90	0.10	5,5,5,5	0
57	MG	RA	3146	1/1	0.90	0.17	27,27,27,27	0
57	MG	QA	1603	1/1	0.90	0.23	22,22,22,22	0
57	MG	YA	3106	1/1	0.90	0.19	12,12,12,12	0
57	MG	RA	3203	1/1	0.90	0.09	47,47,47,47	0
57	MG	RA	3050	1/1	0.91	0.29	30,30,30,30	0
57	MG	RA	3222	1/1	0.91	0.14	36,36,36,36	0
57	MG	YA	3208	1/1	0.91	0.09	29,29,29,29	0
57	MG	YA	3154	1/1	0.91	0.07	3,3,3,3	0
57	MG	YA	3155	1/1	0.91	0.40	50,50,50,50	0
57	MG	YA	3158	1/1	0.91	0.16	14,14,14,14	0
57	MG	YA	3234	1/1	0.91	0.18	25,25,25,25	0
57	MG	RA	3176	1/1	0.91	0.14	10,10,10,10	0
57	MG	RA	3168	1/1	0.91	0.11	19,19,19,19	0
57	MG	YA	3241	1/1	0.91	0.20	37,37,37,37	0
57	MG	RA	3134	1/1	0.91	0.18	23,23,23,23	0
57	MG	YA	3033	1/1	0.91	0.28	9,9,9,9	0
57	MG	YA	3166	1/1	0.91	0.32	156,156,156,156	0
57	MG	RA	3172	1/1	0.91	0.08	15,15,15,15	0
57	MG	XA	1658	1/1	0.91	0.23	12,12,12,12	0
57	MG	YA	3174	1/1	0.91	0.07	7,7,7,7	0
57	MG	XA	1621	1/1	0.91	0.28	23,23,23,23	0
57	MG	XA	1664	1/1	0.91	0.17	44,44,44,44	0
57	MG	YA	3070	1/1	0.91	0.21	18,18,18,18	0
57	MG	RA	3213	1/1	0.91	0.14	17,17,17,17	0
57	MG	QA	1652	1/1	0.91	0.16	32,32,32,32	0
57	MG	YA	3146	1/1	0.91	0.28	37,37,37,37	0
57	MG	YA	3148	1/1	0.91	0.13	21,21,21,21	0
57	MG	YA	3195	1/1	0.92	0.17	26,26,26,26	0
57	MG	XA	1608	1/1	0.92	0.07	34,34,34,34	0
57	MG	XA	1614	1/1	0.92	0.08	7,7,7,7	0
57	MG	XA	1620	1/1	0.92	0.16	10,10,10,10	0
57	MG	YA	3011	1/1	0.92	0.23	14,14,14,14	0
57	MG	YA	3015	1/1	0.92	0.27	15,15,15,15	0
57	MG	QA	1662	1/1	0.92	0.12	58,58,58,58	0
57	MG	YA	3216	1/1	0.92	0.22	30,30,30,30	0
57	MG	RA	3119	1/1	0.92	0.13	30,30,30,30	0
57	MG	RA	3141	1/1	0.92	0.17	15,15,15,15	0
57	MG	RA	3181	1/1	0.92	0.17	29,29,29,29	0
57	MG	YA	3153	1/1	0.92	0.11	13,13,13,13	0
57	MG	YA	3046	1/1	0.92	0.25	20,20,20,20	0
57	MG	YA	3238	1/1	0.92	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3239	1/1	0.92	0.15	38,38,38,38	0
57	MG	QA	1653	1/1	0.92	0.10	88,88,88,88	0
57	MG	RA	3044	1/1	0.92	0.17	18,18,18,18	0
57	MG	XA	1646	1/1	0.92	0.21	30,30,30,30	0
57	MG	RA	3045	1/1	0.92	0.14	6,6,6,6	0
57	MG	YA	3075	1/1	0.92	0.27	24,24,24,24	0
57	MG	RA	3147	1/1	0.92	0.09	14,14,14,14	0
57	MG	RA	3126	1/1	0.92	0.34	33,33,33,33	0
57	MG	XA	1654	1/1	0.92	0.12	37,37,37,37	0
57	MG	YA	3267	1/1	0.92	0.30	24,24,24,24	0
57	MG	RA	3092	1/1	0.92	0.19	17,17,17,17	0
57	MG	RA	3132	1/1	0.92	0.23	24,24,24,24	0
57	MG	RA	3204	1/1	0.92	0.24	33,33,33,33	0
57	MG	RA	3170	1/1	0.92	0.15	33,33,33,33	0
57	MG	QM	201	1/1	0.92	0.15	58,58,58,58	0
57	MG	YA	3186	1/1	0.92	0.09	15,15,15,15	0
57	MG	QA	1649	1/1	0.92	0.13	31,31,31,31	0
57	MG	YA	3163	1/1	0.93	0.20	25,25,25,25	0
57	MG	QA	1621	1/1	0.93	0.09	30,30,30,30	0
57	MG	QA	1615	1/1	0.93	0.12	28,28,28,28	0
57	MG	YA	3018	1/1	0.93	0.25	16,16,16,16	0
57	MG	YA	3171	1/1	0.93	0.26	29,29,29,29	0
57	MG	XA	1607	1/1	0.93	0.14	22,22,22,22	0
57	MG	RA	3070	1/1	0.93	0.27	13,13,13,13	0
57	MG	RA	3149	1/1	0.93	0.16	22,22,22,22	0
57	MG	RA	3153	1/1	0.93	0.18	29,29,29,29	0
57	MG	YA	3179	1/1	0.93	0.27	35,35,35,35	0
57	MG	RA	3154	1/1	0.93	0.25	26,26,26,26	0
57	MG	QA	1640	1/1	0.93	0.20	24,24,24,24	0
57	MG	YA	3185	1/1	0.93	0.08	8,8,8,8	0
57	MG	RA	3041	1/1	0.93	0.28	22,22,22,22	0
57	MG	RA	3212	1/1	0.93	0.05	13,13,13,13	0
57	MG	XA	1630	1/1	0.93	0.14	13,13,13,13	0
57	MG	RA	3161	1/1	0.93	0.06	17,17,17,17	0
57	MG	YA	3089	1/1	0.93	0.21	16,16,16,16	0
57	MG	XA	1634	1/1	0.93	0.09	6,6,6,6	0
57	MG	YA	3201	1/1	0.93	0.05	2,2,2,2	0
57	MG	YA	3103	1/1	0.93	0.17	8,8,8,8	0
57	MG	XA	1636	1/1	0.93	0.19	24,24,24,24	0
57	MG	YA	3105	1/1	0.93	0.14	24,24,24,24	0
57	MG	RA	3127	1/1	0.93	0.16	12,12,12,12	0
57	MG	RA	3086	1/1	0.93	0.27	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3088	1/1	0.93	0.27	25,25,25,25	0
57	MG	YA	3226	1/1	0.93	0.23	4,4,4,4	0
57	MG	QA	1616	1/1	0.93	0.18	28,28,28,28	0
57	MG	RA	3224	1/1	0.93	0.09	18,18,18,18	0
57	MG	QA	1617	1/1	0.93	0.28	31,31,31,31	0
57	MG	XA	1655	1/1	0.93	0.27	39,39,39,39	0
57	MG	XA	1657	1/1	0.93	0.14	21,21,21,21	0
57	MG	QA	1620	1/1	0.93	0.13	16,16,16,16	0
57	MG	XA	1659	1/1	0.93	0.14	43,43,43,43	0
57	MG	XA	1661	1/1	0.93	0.12	23,23,23,23	0
57	MG	YA	3243	1/1	0.93	0.17	21,21,21,21	0
57	MG	YA	3145	1/1	0.93	0.14	18,18,18,18	0
57	MG	XA	1662	1/1	0.93	0.37	40,40,40,40	0
57	MG	YA	3147	1/1	0.93	0.08	2,2,2,2	0
57	MG	RA	3236	1/1	0.93	0.22	28,28,28,28	0
57	MG	RA	3112	1/1	0.93	0.23	21,21,21,21	0
57	MG	RA	3052	1/1	0.93	0.19	7,7,7,7	0
57	MG	RA	3182	1/1	0.93	0.09	6,6,6,6	0
57	MG	YB	202	1/1	0.93	0.19	16,16,16,16	0
57	MG	YB	203	1/1	0.93	0.15	18,18,18,18	0
57	MG	RA	3053	1/1	0.93	0.20	12,12,12,12	0
57	MG	RA	3188	1/1	0.93	0.17	29,29,29,29	0
57	MG	YA	3157	1/1	0.93	0.18	23,23,23,23	0
57	MG	RA	3143	1/1	0.93	0.12	35,35,35,35	0
57	MG	RR	201	1/1	0.93	0.15	20,20,20,20	0
57	MG	RA	3190	1/1	0.93	0.22	27,27,27,27	0
57	MG	RA	3018	1/1	0.94	0.13	17,17,17,17	0
57	MG	YA	3068	1/1	0.94	0.25	12,12,12,12	0
57	MG	XA	1632	1/1	0.94	0.17	21,21,21,21	0
57	MG	XA	1633	1/1	0.94	0.16	16,16,16,16	0
57	MG	YA	3073	1/1	0.94	0.17	8,8,8,8	0
57	MG	RA	3059	1/1	0.94	0.15	4,4,4,4	0
57	MG	YA	3184	1/1	0.94	0.17	26,26,26,26	0
57	MG	QA	1618	1/1	0.94	0.15	13,13,13,13	0
57	MG	RA	3184	1/1	0.94	0.06	26,26,26,26	0
57	MG	XA	1641	1/1	0.94	0.17	33,33,33,33	0
57	MG	RA	3029	1/1	0.94	0.20	3,3,3,3	0
57	MG	XA	1650	1/1	0.94	0.13	27,27,27,27	0
57	MG	RA	3032	1/1	0.94	0.25	27,27,27,27	0
57	MG	RA	3150	1/1	0.94	0.11	25,25,25,25	0
57	MG	RA	3082	1/1	0.94	0.20	35,35,35,35	0
57	MG	RA	3241	1/1	0.94	0.20	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3191	1/1	0.94	0.07	16,16,16,16	0
57	MG	QA	1658	1/1	0.94	0.18	39,39,39,39	0
57	MG	RA	3085	1/1	0.94	0.13	6,6,6,6	0
57	MG	YA	3217	1/1	0.94	0.05	9,9,9,9	0
57	MG	RA	3043	1/1	0.94	0.18	7,7,7,7	0
57	MG	RP	201	1/1	0.94	0.34	144,144,144,144	0
57	MG	YA	3133	1/1	0.94	0.14	26,26,26,26	0
57	MG	YA	3229	1/1	0.94	0.13	19,19,19,19	0
57	MG	YA	3231	1/1	0.94	0.19	20,20,20,20	0
57	MG	YA	3134	1/1	0.94	0.16	19,19,19,19	0
57	MG	QA	1602	1/1	0.94	0.27	22,22,22,22	0
57	MG	RA	3197	1/1	0.94	0.10	9,9,9,9	0
57	MG	RA	3201	1/1	0.94	0.04	17,17,17,17	0
57	MG	YA	3143	1/1	0.94	0.23	33,33,33,33	0
57	MG	RA	3162	1/1	0.94	0.06	2,2,2,2	0
57	MG	QA	1610	1/1	0.94	0.21	14,14,14,14	0
57	MG	QA	1646	1/1	0.94	0.18	38,38,38,38	0
57	MG	RA	3099	1/1	0.94	0.25	12,12,12,12	0
57	MG	XA	1610	1/1	0.94	0.12	7,7,7,7	0
57	MG	RA	3210	1/1	0.94	0.14	18,18,18,18	0
57	MG	XA	1618	1/1	0.94	0.21	11,11,11,11	0
57	MG	YA	3260	1/1	0.94	0.19	13,13,13,13	0
57	MG	YA	3262	1/1	0.94	0.12	4,4,4,4	0
57	MG	YA	3263	1/1	0.94	0.23	16,16,16,16	0
57	MG	YA	3013	1/1	0.94	0.19	7,7,7,7	0
57	MG	RA	3211	1/1	0.94	0.17	30,30,30,30	0
57	MG	QA	1612	1/1	0.94	0.24	9,9,9,9	0
57	MG	RA	3111	1/1	0.94	0.24	14,14,14,14	0
57	MG	YA	3024	1/1	0.94	0.21	1,1,1,1	0
57	MG	YA	3032	1/1	0.94	0.21	4,4,4,4	0
57	MG	XA	1623	1/1	0.94	0.17	13,13,13,13	0
57	MG	RA	3216	1/1	0.94	0.18	33,33,33,33	0
57	MG	XA	1627	1/1	0.94	0.24	28,28,28,28	0
57	MG	RA	3219	1/1	0.94	0.25	159,159,159,159	0
57	MG	RA	3011	1/1	0.94	0.35	36,36,36,36	0
57	MG	YA	3059	1/1	0.94	0.18	19,19,19,19	0
57	MG	YA	3162	1/1	0.95	0.06	16,16,16,16	0
57	MG	YA	3023	1/1	0.95	0.21	6,6,6,6	0
57	MG	RA	3102	1/1	0.95	0.18	28,28,28,28	0
57	MG	RA	3109	1/1	0.95	0.08	3,3,3,3	0
57	MG	RA	3198	1/1	0.95	0.06	27,27,27,27	0
57	MG	YA	3170	1/1	0.95	0.05	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1624	1/1	0.95	0.19	30,30,30,30	0
57	MG	QA	1664	1/1	0.95	0.14	17,17,17,17	0
57	MG	RA	3113	1/1	0.95	0.19	29,29,29,29	0
57	MG	YA	3049	1/1	0.95	0.22	8,8,8,8	0
57	MG	RA	3023	1/1	0.95	0.18	5,5,5,5	0
57	MG	YA	3055	1/1	0.95	0.17	11,11,11,11	0
57	MG	RA	3062	1/1	0.95	0.10	29,29,29,29	0
57	MG	RA	3157	1/1	0.95	0.20	25,25,25,25	0
57	MG	RA	3158	1/1	0.95	0.25	40,40,40,40	0
57	MG	RA	3159	1/1	0.95	0.15	24,24,24,24	0
57	MG	RA	3025	1/1	0.95	0.18	12,12,12,12	0
57	MG	YA	3187	1/1	0.95	0.12	25,25,25,25	0
57	MG	YA	3188	1/1	0.95	0.29	33,33,33,33	0
57	MG	YA	3189	1/1	0.95	0.07	1,1,1,1	0
57	MG	RA	3215	1/1	0.95	0.07	24,24,24,24	0
57	MG	YA	3194	1/1	0.95	0.07	17,17,17,17	0
57	MG	QA	1638	1/1	0.95	0.17	27,27,27,27	0
57	MG	RA	3163	1/1	0.95	0.14	19,19,19,19	0
57	MG	RA	3166	1/1	0.95	0.18	28,28,28,28	0
57	MG	RA	3071	1/1	0.95	0.22	22,22,22,22	0
57	MG	YA	3200	1/1	0.95	0.17	12,12,12,12	0
57	MG	RA	3122	1/1	0.95	0.23	32,32,32,32	0
57	MG	XA	1645	1/1	0.95	0.13	15,15,15,15	0
57	MG	YA	3205	1/1	0.95	0.16	27,27,27,27	0
57	MG	RA	3073	1/1	0.95	0.10	10,10,10,10	0
57	MG	RA	3028	1/1	0.95	0.19	2,2,2,2	0
57	MG	YA	3214	1/1	0.95	0.12	25,25,25,25	0
57	MG	YA	3110	1/1	0.95	0.17	14,14,14,14	0
57	MG	YA	3112	1/1	0.95	0.16	11,11,11,11	0
57	MG	YA	3113	1/1	0.95	0.12	11,11,11,11	0
57	MG	RA	3226	1/1	0.95	0.13	15,15,15,15	0
57	MG	YA	3223	1/1	0.95	0.15	20,20,20,20	0
57	MG	YA	3224	1/1	0.95	0.09	14,14,14,14	0
57	MG	QA	1648	1/1	0.95	0.16	34,34,34,34	0
57	MG	YA	3228	1/1	0.95	0.05	11,11,11,11	0
57	MG	YA	3121	1/1	0.95	0.18	27,27,27,27	0
57	MG	YA	3230	1/1	0.95	0.17	18,18,18,18	0
57	MG	QA	1614	1/1	0.95	0.08	20,20,20,20	0
57	MG	YA	3124	1/1	0.95	0.20	9,9,9,9	0
57	MG	RA	3232	1/1	0.95	0.18	10,10,10,10	0
57	MG	YA	3128	1/1	0.95	0.20	3,3,3,3	0
57	MG	RA	3235	1/1	0.95	0.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3034	1/1	0.95	0.22	17,17,17,17	0
57	MG	RA	3177	1/1	0.95	0.18	24,24,24,24	0
57	MG	RA	3179	1/1	0.95	0.04	2,2,2,2	0
57	MG	RA	3180	1/1	0.95	0.14	18,18,18,18	0
57	MG	QA	1642	1/1	0.95	0.17	43,43,43,43	0
57	MG	QA	1644	1/1	0.95	0.09	21,21,21,21	0
57	MG	YA	3141	1/1	0.95	0.10	17,17,17,17	0
57	MG	RA	3136	1/1	0.95	0.04	14,14,14,14	0
57	MG	YA	3255	1/1	0.95	0.26	20,20,20,20	0
57	MG	RA	3137	1/1	0.95	0.22	7,7,7,7	0
57	MG	RA	3002	1/1	0.95	0.15	26,26,26,26	0
57	MG	RA	3007	1/1	0.95	0.24	5,5,5,5	0
57	MG	XA	1671	1/1	0.95	0.06	18,18,18,18	0
57	MG	RA	3095	1/1	0.95	0.21	6,6,6,6	0
57	MG	RA	3096	1/1	0.95	0.14	18,18,18,18	0
57	MG	YA	3268	1/1	0.95	0.17	17,17,17,17	0
57	MG	YA	3151	1/1	0.95	0.26	30,30,30,30	0
57	MG	RA	3098	1/1	0.95	0.22	7,7,7,7	0
57	MG	YA	3009	1/1	0.95	0.26	2,2,2,2	0
57	MG	YE	301	1/1	0.95	0.14	0,0,0,0	0
57	MG	XA	1602	1/1	0.95	0.19	18,18,18,18	0
57	MG	XA	1603	1/1	0.95	0.26	13,13,13,13	0
57	MG	XA	1604	1/1	0.95	0.33	19,19,19,19	0
57	MG	RA	3008	1/1	0.95	0.23	30,30,30,30	0
57	MG	Y5	101	1/1	0.95	0.11	12,12,12,12	0
57	MG	YA	3017	1/1	0.95	0.14	18,18,18,18	0
57	MG	QA	1654	1/1	0.95	0.10	36,36,36,36	0
57	MG	YA	3053	1/1	0.96	0.18	0,0,0,0	0
57	MG	RA	3039	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3080	1/1	0.96	0.19	17,17,17,17	0
57	MG	QA	1609	1/1	0.96	0.11	13,13,13,13	0
57	MG	RA	3239	1/1	0.96	0.30	28,28,28,28	0
57	MG	YA	3062	1/1	0.96	0.15	7,7,7,7	0
57	MG	YA	3065	1/1	0.96	0.14	0,0,0,0	0
57	MG	YA	3177	1/1	0.96	0.08	12,12,12,12	0
57	MG	RA	3083	1/1	0.96	0.18	17,17,17,17	0
57	MG	QA	1619	1/1	0.96	0.09	1,1,1,1	0
57	MG	QA	1639	1/1	0.96	0.09	25,25,25,25	0
57	MG	QA	1604	1/1	0.96	0.15	4,4,4,4	0
57	MG	YA	3074	1/1	0.96	0.12	2,2,2,2	0
57	MG	RA	3199	1/1	0.96	0.04	10,10,10,10	0
57	MG	YA	3077	1/1	0.96	0.19	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3078	1/1	0.96	0.21	14,14,14,14	0
57	MG	RA	3087	1/1	0.96	0.17	25,25,25,25	0
57	MG	YA	3085	1/1	0.96	0.16	9,9,9,9	0
57	MG	YA	3192	1/1	0.96	0.12	19,19,19,19	0
57	MG	RA	3202	1/1	0.96	0.14	15,15,15,15	0
57	MG	YA	3090	1/1	0.96	0.30	39,39,39,39	0
57	MG	YA	3091	1/1	0.96	0.16	29,29,29,29	0
57	MG	YA	3098	1/1	0.96	0.17	2,2,2,2	0
57	MG	YA	3101	1/1	0.96	0.15	3,3,3,3	0
57	MG	XA	1656	1/1	0.96	0.25	31,31,31,31	0
57	MG	RA	3164	1/1	0.96	0.18	20,20,20,20	0
57	MG	RA	3165	1/1	0.96	0.07	14,14,14,14	0
57	MG	YA	3203	1/1	0.96	0.05	25,25,25,25	0
57	MG	RA	3048	1/1	0.96	0.17	1,1,1,1	0
57	MG	RA	3207	1/1	0.96	0.07	60,60,60,60	0
57	MG	YA	3206	1/1	0.96	0.18	14,14,14,14	0
57	MG	RA	3208	1/1	0.96	0.11	7,7,7,7	0
57	MG	RA	3090	1/1	0.96	0.11	8,8,8,8	0
57	MG	QA	1641	1/1	0.96	0.12	22,22,22,22	0
57	MG	YA	3114	1/1	0.96	0.17	13,13,13,13	0
57	MG	YA	3115	1/1	0.96	0.23	18,18,18,18	0
57	MG	YA	3116	1/1	0.96	0.22	39,39,39,39	0
57	MG	XA	1605	1/1	0.96	0.24	17,17,17,17	0
57	MG	YA	3119	1/1	0.96	0.25	23,23,23,23	0
57	MG	XA	1668	1/1	0.96	0.18	15,15,15,15	0
57	MG	YA	3225	1/1	0.96	0.14	3,3,3,3	0
57	MG	XA	1606	1/1	0.96	0.26	12,12,12,12	0
57	MG	YA	3227	1/1	0.96	0.13	8,8,8,8	0
57	MG	RA	3021	1/1	0.96	0.19	2,2,2,2	0
57	MG	QA	1601	1/1	0.96	0.26	34,34,34,34	0
57	MG	YA	3125	1/1	0.96	0.13	9,9,9,9	0
57	MG	YA	3126	1/1	0.96	0.11	1,1,1,1	0
57	MG	XA	1609	1/1	0.96	0.23	14,14,14,14	0
57	MG	YA	3233	1/1	0.96	0.04	6,6,6,6	0
57	MG	RA	3054	1/1	0.96	0.13	2,2,2,2	0
57	MG	RA	3057	1/1	0.96	0.15	6,6,6,6	0
57	MG	YA	3236	1/1	0.96	0.04	24,24,24,24	0
57	MG	YA	3237	1/1	0.96	0.25	25,25,25,25	0
57	MG	YA	3002	1/1	0.96	0.19	1,1,1,1	0
57	MG	YA	3003	1/1	0.96	0.14	1,1,1,1	0
57	MG	YA	3006	1/1	0.96	0.24	0,0,0,0	0
57	MG	YA	3008	1/1	0.96	0.16	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3135	1/1	0.96	0.09	3,3,3,3	0
57	MG	YA	3136	1/1	0.96	0.17	14,14,14,14	0
57	MG	YA	3244	1/1	0.96	0.23	30,30,30,30	0
57	MG	QA	1634	1/1	0.96	0.10	35,35,35,35	0
57	MG	YA	3246	1/1	0.96	0.14	26,26,26,26	0
57	MG	RA	3217	1/1	0.96	0.08	14,14,14,14	0
57	MG	QA	1645	1/1	0.96	0.09	20,20,20,20	0
57	MG	YA	3253	1/1	0.96	0.23	2,2,2,2	0
57	MG	QA	1635	1/1	0.96	0.10	18,18,18,18	0
57	MG	RA	3065	1/1	0.96	0.14	9,9,9,9	0
57	MG	QA	1613	1/1	0.96	0.30	37,37,37,37	0
57	MG	RA	3069	1/1	0.96	0.04	1,1,1,1	0
57	MG	YA	3019	1/1	0.96	0.21	8,8,8,8	0
57	MG	YA	3022	1/1	0.96	0.14	1,1,1,1	0
57	MG	XA	1628	1/1	0.96	0.05	1,1,1,1	0
57	MG	RA	3148	1/1	0.96	0.20	15,15,15,15	0
57	MG	YA	3026	1/1	0.96	0.22	2,2,2,2	0
57	MG	YA	3027	1/1	0.96	0.15	9,9,9,9	0
57	MG	RA	3003	1/1	0.96	0.25	4,4,4,4	0
57	MG	RA	3114	1/1	0.96	0.16	19,19,19,19	0
57	MG	RA	3004	1/1	0.96	0.21	14,14,14,14	0
57	MG	YA	3040	1/1	0.96	0.19	0,0,0,0	0
57	MG	YA	3044	1/1	0.96	0.20	4,4,4,4	0
57	MG	RA	3230	1/1	0.96	0.21	7,7,7,7	0
57	MG	RA	3037	1/1	0.96	0.13	11,11,11,11	0
57	MG	YA	3047	1/1	0.96	0.20	4,4,4,4	0
57	MG	XA	1635	1/1	0.96	0.28	12,12,12,12	0
57	MG	QA	1607	1/1	0.97	0.05	10,10,10,10	0
57	MG	XA	1625	1/1	0.97	0.07	6,6,6,6	0
57	MG	YA	3034	1/1	0.97	0.21	13,13,13,13	0
57	MG	YA	3036	1/1	0.97	0.11	4,4,4,4	0
57	MG	YA	3037	1/1	0.97	0.15	0,0,0,0	0
57	MG	RA	3027	1/1	0.97	0.19	1,1,1,1	0
57	MG	RA	3013	1/1	0.97	0.19	11,11,11,11	0
57	MG	RA	3214	1/1	0.97	0.18	13,13,13,13	0
57	MG	RA	3123	1/1	0.97	0.17	28,28,28,28	0
57	MG	RA	3167	1/1	0.97	0.09	22,22,22,22	0
57	MG	RA	3014	1/1	0.97	0.17	3,3,3,3	0
57	MG	YA	3048	1/1	0.97	0.21	11,11,11,11	0
57	MG	YA	3167	1/1	0.97	0.07	1,1,1,1	0
57	MG	RA	3218	1/1	0.97	0.17	17,17,17,17	0
57	MG	YA	3051	1/1	0.97	0.27	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3169	1/1	0.97	0.22	30,30,30,30	0
57	MG	RA	3016	1/1	0.97	0.18	1,1,1,1	0
57	MG	RA	3056	1/1	0.97	0.19	1,1,1,1	0
57	MG	YA	3175	1/1	0.97	0.23	23,23,23,23	0
57	MG	YA	3176	1/1	0.97	0.09	2,2,2,2	0
57	MG	YA	3057	1/1	0.97	0.20	1,1,1,1	0
57	MG	XA	1637	1/1	0.97	0.13	20,20,20,20	0
57	MG	YA	3060	1/1	0.97	0.21	1,1,1,1	0
57	MG	XA	1638	1/1	0.97	0.05	20,20,20,20	0
57	MG	YA	3181	1/1	0.97	0.23	36,36,36,36	0
57	MG	RA	3128	1/1	0.97	0.12	4,4,4,4	0
57	MG	YA	3183	1/1	0.97	0.15	13,13,13,13	0
57	MG	YA	3064	1/1	0.97	0.13	6,6,6,6	0
57	MG	RA	3173	1/1	0.97	0.05	1,1,1,1	0
57	MG	RA	3033	1/1	0.97	0.24	3,3,3,3	0
57	MG	RA	3225	1/1	0.97	0.10	40,40,40,40	0
57	MG	XA	1649	1/1	0.97	0.13	8,8,8,8	0
57	MG	YA	3072	1/1	0.97	0.18	9,9,9,9	0
57	MG	RA	3089	1/1	0.97	0.13	2,2,2,2	0
57	MG	RA	3017	1/1	0.97	0.11	0,0,0,0	0
57	MG	RA	3035	1/1	0.97	0.17	0,0,0,0	0
57	MG	YA	3076	1/1	0.97	0.26	15,15,15,15	0
57	MG	RA	3178	1/1	0.97	0.09	26,26,26,26	0
57	MG	RA	3060	1/1	0.97	0.20	0,0,0,0	0
57	MG	YA	3080	1/1	0.97	0.18	1,1,1,1	0
57	MG	YA	3081	1/1	0.97	0.18	10,10,10,10	0
57	MG	YA	3082	1/1	0.97	0.08	0,0,0,0	0
57	MG	RA	3233	1/1	0.97	0.08	13,13,13,13	0
57	MG	RA	3094	1/1	0.97	0.15	8,8,8,8	0
57	MG	YA	3087	1/1	0.97	0.18	1,1,1,1	0
57	MG	YA	3088	1/1	0.97	0.19	5,5,5,5	0
57	MG	QA	1626	1/1	0.97	0.10	21,21,21,21	0
57	MG	RA	3064	1/1	0.97	0.23	13,13,13,13	0
57	MG	YA	3210	1/1	0.97	0.13	26,26,26,26	0
57	MG	YA	3212	1/1	0.97	0.05	20,20,20,20	0
57	MG	YA	3213	1/1	0.97	0.06	6,6,6,6	0
57	MG	RA	3140	1/1	0.97	0.18	17,17,17,17	0
57	MG	YA	3215	1/1	0.97	0.05	18,18,18,18	0
57	MG	YA	3096	1/1	0.97	0.14	5,5,5,5	0
57	MG	YA	3097	1/1	0.97	0.15	14,14,14,14	0
57	MG	XA	1660	1/1	0.97	0.05	6,6,6,6	0
57	MG	YA	3099	1/1	0.97	0.18	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3222	1/1	0.97	0.12	27,27,27,27	0
57	MG	RA	3185	1/1	0.97	0.04	16,16,16,16	0
57	MG	RA	3186	1/1	0.97	0.05	14,14,14,14	0
57	MG	RA	3097	1/1	0.97	0.17	4,4,4,4	0
57	MG	RA	3019	1/1	0.97	0.15	13,13,13,13	0
57	MG	RA	3066	1/1	0.97	0.27	17,17,17,17	0
57	MG	XA	1666	1/1	0.97	0.04	13,13,13,13	0
57	MG	YA	3108	1/1	0.97	0.23	12,12,12,12	0
57	MG	YA	3109	1/1	0.97	0.07	5,5,5,5	0
57	MG	XA	1667	1/1	0.97	0.26	29,29,29,29	0
57	MG	RA	3144	1/1	0.97	0.20	8,8,8,8	0
57	MG	RA	3100	1/1	0.97	0.10	6,6,6,6	0
57	MG	RA	3067	1/1	0.97	0.13	3,3,3,3	0
57	MG	QA	1650	1/1	0.97	0.16	20,20,20,20	0
57	MG	RA	3103	1/1	0.97	0.06	2,2,2,2	0
57	MG	RA	3195	1/1	0.97	0.08	1,1,1,1	0
57	MG	YA	3118	1/1	0.97	0.24	22,22,22,22	0
57	MG	XV	101	1/1	0.97	0.13	0,0,0,0	0
57	MG	RA	3108	1/1	0.97	0.12	8,8,8,8	0
57	MG	RA	3042	1/1	0.97	0.18	10,10,10,10	0
57	MG	RA	3152	1/1	0.97	0.15	11,11,11,11	0
57	MG	YA	3004	1/1	0.97	0.17	0,0,0,0	0
57	MG	RA	3110	1/1	0.97	0.16	2,2,2,2	0
57	MG	YA	3007	1/1	0.97	0.14	9,9,9,9	0
57	MG	RA	3200	1/1	0.97	0.30	23,23,23,23	0
57	MG	RA	3022	1/1	0.97	0.17	3,3,3,3	0
57	MG	YA	3250	1/1	0.97	0.25	22,22,22,22	0
57	MG	QA	1659	1/1	0.97	0.14	21,21,21,21	0
57	MG	YA	3012	1/1	0.97	0.25	2,2,2,2	0
57	MG	YA	3254	1/1	0.97	0.13	18,18,18,18	0
57	MG	QA	1651	1/1	0.97	0.12	18,18,18,18	0
57	MG	YA	3014	1/1	0.97	0.21	4,4,4,4	0
57	MG	YA	3261	1/1	0.97	0.21	19,19,19,19	0
57	MG	RA	3077	1/1	0.97	0.16	13,13,13,13	0
57	MG	RA	3205	1/1	0.97	0.18	5,5,5,5	0
57	MG	YA	3264	1/1	0.97	0.09	7,7,7,7	0
57	MG	XA	1615	1/1	0.97	0.18	2,2,2,2	0
57	MG	YA	3137	1/1	0.97	0.11	1,1,1,1	0
57	MG	YA	3138	1/1	0.97	0.13	0,0,0,0	0
57	MG	XA	1616	1/1	0.97	0.13	6,6,6,6	0
57	MG	RA	3046	1/1	0.97	0.14	8,8,8,8	0
57	MG	YA	3021	1/1	0.97	0.14	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1619	1/1	0.97	0.10	7,7,7,7	0
57	MG	RA	3117	1/1	0.97	0.12	2,2,2,2	0
57	MG	RA	3160	1/1	0.97	0.06	12,12,12,12	0
57	MG	YA	3025	1/1	0.97	0.12	6,6,6,6	0
57	MG	RA	3047	1/1	0.97	0.24	12,12,12,12	0
57	MG	RA	3081	1/1	0.97	0.08	10,10,10,10	0
57	MG	YA	3029	1/1	0.97	0.17	1,1,1,1	0
57	MG	YA	3030	1/1	0.97	0.25	6,6,6,6	0
57	MG	YA	3031	1/1	0.97	0.23	1,1,1,1	0
57	MG	RA	3151	1/1	0.98	0.05	0,0,0,0	0
57	MG	RA	3125	1/1	0.98	0.07	13,13,13,13	0
57	MG	RA	3240	1/1	0.98	0.20	14,14,14,14	0
57	MG	YA	3050	1/1	0.98	0.17	2,2,2,2	0
57	MG	RA	3015	1/1	0.98	0.11	5,5,5,5	0
57	MG	YA	3052	1/1	0.98	0.11	1,1,1,1	0
57	MG	RA	3061	1/1	0.98	0.16	2,2,2,2	0
57	MG	YA	3199	1/1	0.98	0.20	11,11,11,11	0
57	MG	YA	3123	1/1	0.98	0.18	4,4,4,4	0
57	MG	RA	3005	1/1	0.98	0.22	9,9,9,9	0
57	MG	YA	3202	1/1	0.98	0.09	13,13,13,13	0
57	MG	RA	3183	1/1	0.98	0.12	1,1,1,1	0
57	MG	YA	3056	1/1	0.98	0.14	1,1,1,1	0
57	MG	YA	3001	1/1	0.98	0.18	1,1,1,1	0
57	MG	YA	3058	1/1	0.98	0.15	0,0,0,0	0
57	MG	RA	3129	1/1	0.98	0.06	10,10,10,10	0
57	MG	RA	3063	1/1	0.98	0.22	1,1,1,1	0
57	MG	YA	3209	1/1	0.98	0.04	11,11,11,11	0
57	MG	RA	3131	1/1	0.98	0.11	13,13,13,13	0
57	MG	YA	3132	1/1	0.98	0.07	5,5,5,5	0
57	MG	RA	3104	1/1	0.98	0.08	9,9,9,9	0
57	MG	YA	3063	1/1	0.98	0.14	3,3,3,3	0
57	MG	RA	3133	1/1	0.98	0.07	6,6,6,6	0
57	MG	RA	3006	1/1	0.98	0.22	17,17,17,17	0
57	MG	YA	3066	1/1	0.98	0.26	12,12,12,12	0
57	MG	YA	3219	1/1	0.98	0.10	31,31,31,31	0
57	MG	RA	3030	1/1	0.98	0.18	0,0,0,0	0
57	MG	YA	3069	1/1	0.98	0.11	6,6,6,6	0
57	MG	YA	3010	1/1	0.98	0.15	1,1,1,1	0
57	MG	R8	101	1/1	0.98	0.15	25,25,25,25	0
57	MG	XA	1640	1/1	0.98	0.21	15,15,15,15	0
57	MG	XA	1601	1/1	0.98	0.17	7,7,7,7	0
57	MG	YA	3144	1/1	0.98	0.10	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1643	1/1	0.98	0.11	12,12,12,12	0
57	MG	XA	1644	1/1	0.98	0.22	23,23,23,23	0
57	MG	QV	101	1/1	0.98	0.15	9,9,9,9	0
57	MG	QA	1623	1/1	0.98	0.20	19,19,19,19	0
57	MG	YA	3149	1/1	0.98	0.10	9,9,9,9	0
57	MG	XA	1647	1/1	0.98	0.13	23,23,23,23	0
57	MG	XA	1648	1/1	0.98	0.03	14,14,14,14	0
57	MG	RA	3020	1/1	0.98	0.14	8,8,8,8	0
57	MG	RA	3001	1/1	0.98	0.12	4,4,4,4	0
57	MG	YA	3083	1/1	0.98	0.14	0,0,0,0	0
57	MG	QA	1606	1/1	0.98	0.11	11,11,11,11	0
57	MG	YA	3156	1/1	0.98	0.17	13,13,13,13	0
57	MG	RA	3012	1/1	0.98	0.12	7,7,7,7	0
57	MG	YA	3086	1/1	0.98	0.16	10,10,10,10	0
57	MG	YA	3159	1/1	0.98	0.21	16,16,16,16	0
57	MG	RA	3116	1/1	0.98	0.13	0,0,0,0	0
57	MG	RA	3072	1/1	0.98	0.15	3,3,3,3	0
57	MG	RA	3093	1/1	0.98	0.19	8,8,8,8	0
57	MG	YA	3028	1/1	0.98	0.14	2,2,2,2	0
57	MG	XA	1611	1/1	0.98	0.20	7,7,7,7	0
57	MG	YA	3247	1/1	0.98	0.24	16,16,16,16	0
57	MG	YA	3248	1/1	0.98	0.25	30,30,30,30	0
57	MG	YA	3093	1/1	0.98	0.15	9,9,9,9	0
57	MG	YA	3094	1/1	0.98	0.11	4,4,4,4	0
57	MG	YA	3095	1/1	0.98	0.13	5,5,5,5	0
57	MG	YA	3252	1/1	0.98	0.35	17,17,17,17	0
57	MG	YA	3169	1/1	0.98	0.20	12,12,12,12	0
57	MG	XA	1612	1/1	0.98	0.10	3,3,3,3	0
57	MG	XA	1613	1/1	0.98	0.04	6,6,6,6	0
57	MG	YA	3256	1/1	0.98	0.22	3,3,3,3	0
57	MG	YA	3259	1/1	0.98	0.22	13,13,13,13	0
57	MG	RA	3024	1/1	0.98	0.14	7,7,7,7	0
57	MG	RA	3229	1/1	0.98	0.08	26,26,26,26	0
57	MG	YA	3100	1/1	0.98	0.20	1,1,1,1	0
57	MG	RA	3074	1/1	0.98	0.14	0,0,0,0	0
57	MG	YA	3035	1/1	0.98	0.11	1,1,1,1	0
57	MG	XA	1617	1/1	0.98	0.11	8,8,8,8	0
57	MG	RA	3075	1/1	0.98	0.07	6,6,6,6	0
57	MG	YA	3038	1/1	0.98	0.10	4,4,4,4	0
57	MG	RA	3076	1/1	0.98	0.13	0,0,0,0	0
57	MG	YA	3107	1/1	0.98	0.17	2,2,2,2	0
57	MG	RA	3234	1/1	0.98	0.14	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3041	1/1	0.98	0.19	2,2,2,2	0
57	MG	YA	3042	1/1	0.98	0.14	4,4,4,4	0
57	MG	YA	3111	1/1	0.98	0.06	8,8,8,8	0
57	MG	YA	3043	1/1	0.98	0.18	1,1,1,1	0
57	MG	QA	1643	1/1	0.98	0.04	21,21,21,21	0
57	MG	QA	1605	1/1	0.98	0.30	23,23,23,23	0
57	MG	RA	3237	1/1	0.98	0.32	28,28,28,28	0
57	MG	YA	3190	1/1	0.98	0.08	0,0,0,0	0
57	MG	YA	3191	1/1	0.98	0.16	14,14,14,14	0
59	ZN	QD	301	1/1	0.98	0.11	58,58,58,58	0
59	ZN	QN	101	1/1	0.98	0.05	95,95,95,95	0
59	ZN	XD	301	1/1	0.98	0.16	39,39,39,39	0
57	MG	RA	3049	1/1	0.99	0.05	1,1,1,1	0
57	MG	QA	1611	1/1	0.99	0.21	12,12,12,12	0
57	MG	YA	3257	1/1	0.99	0.24	3,3,3,3	0
57	MG	YA	3258	1/1	0.99	0.14	2,2,2,2	0
57	MG	RA	3051	1/1	0.99	0.08	4,4,4,4	0
57	MG	RA	3079	1/1	0.99	0.15	11,11,11,11	0
57	MG	YA	3067	1/1	0.99	0.10	2,2,2,2	0
57	MG	RA	3038	1/1	0.99	0.10	1,1,1,1	0
57	MG	YA	3092	1/1	0.99	0.13	3,3,3,3	0
57	MG	YA	3005	1/1	0.99	0.12	6,6,6,6	0
57	MG	YA	3211	1/1	0.99	0.02	0,0,0,0	0
57	MG	XA	1642	1/1	0.99	0.11	7,7,7,7	0
57	MG	RA	3231	1/1	0.99	0.15	1,1,1,1	0
57	MG	RE	301	1/1	0.99	0.09	1,1,1,1	0
57	MG	XA	1626	1/1	0.99	0.12	9,9,9,9	0
57	MG	RE	302	1/1	0.99	0.14	5,5,5,5	0
57	MG	YA	3168	1/1	0.99	0.09	0,0,0,0	0
57	MG	YA	3218	1/1	0.99	0.05	1,1,1,1	0
57	MG	RF	301	1/1	0.99	0.15	24,24,24,24	0
57	MG	RA	3031	1/1	0.99	0.12	3,3,3,3	0
57	MG	RA	3040	1/1	0.99	0.19	15,15,15,15	0
57	MG	RA	3055	1/1	0.99	0.09	8,8,8,8	0
57	MG	RA	3009	1/1	0.99	0.04	0,0,0,0	0
57	MG	RA	3105	1/1	0.99	0.10	6,6,6,6	0
57	MG	RA	3106	1/1	0.99	0.10	4,4,4,4	0
57	MG	RA	3107	1/1	0.99	0.11	6,6,6,6	0
57	MG	RA	3036	1/1	0.99	0.14	2,2,2,2	0
57	MG	YA	3020	1/1	0.99	0.23	10,10,10,10	0
59	ZN	XN	101	1/1	0.99	0.02	42,42,42,42	0
57	MG	YA	3079	1/1	1.00	0.06	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.