



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:25 AM UTC

PDB ID : 6O3M / pdb_00006o3m
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-26
Resolution : 3.97 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
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

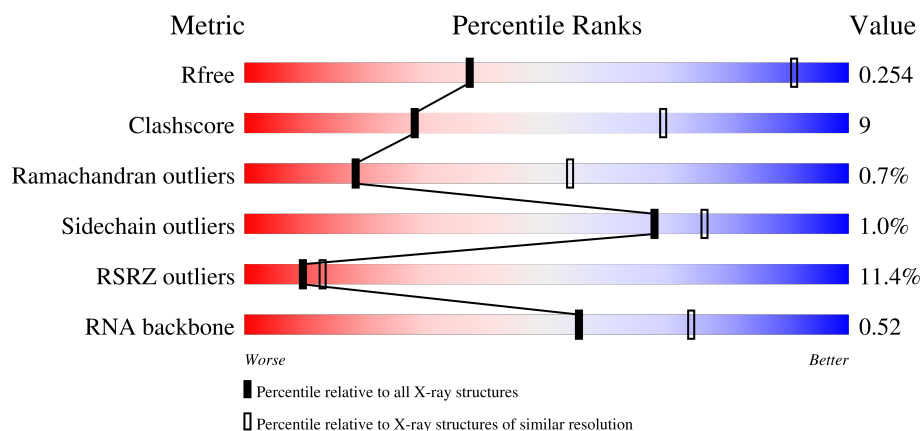
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)
RNA backbone	3983	1017 (4.84-3.10)

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	1521	9% 51% 39% 9%
1	XA	1521	10% 50% 40% 9%
2	QB	256	9% 73% 18% 8%
2	XB	256	11% 71% 21% 8%

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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	

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Mol	Chain	Length	Quality of chain
28	RF	210	
28	YF	210	
29	RG	182	
29	YG	182	
30	RH	180	
30	YH	180	
31	RI	148	
31	YI	148	
32	RN	140	
32	YN	140	
33	RO	122	
33	YO	122	
34	RP	150	
34	YP	150	
35	RQ	141	
35	YQ	141	
36	RR	118	
36	YR	118	
37	RS	112	
37	YS	112	
38	RT	146	
38	YT	146	
39	RU	118	
39	YU	118	
40	RV	101	

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Mol	Chain	Length	Quality of chain
40	YV	101	
41	RW	113	
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	

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Mol	Chain	Length	Quality of chain
53	R8	65	
53	Y8	65	
54	R9	37	
54	Y9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	QA	1635	-	-	-	X
55	MG	RA	3006	-	-	-	X
55	MG	RA	3025	-	-	-	X
55	MG	RA	3151	-	-	-	X
55	MG	RA	3186	-	-	-	X
55	MG	RA	3222	-	-	-	X
55	MG	RA	3249	-	-	-	X
55	MG	RA	3251	-	-	-	X
55	MG	RA	3252	-	-	-	X
55	MG	RA	3270	-	-	-	X
55	MG	RA	3297	-	-	-	X
55	MG	RA	3311	-	-	-	X
55	MG	RA	3341	-	-	-	X
55	MG	RA	3347	-	-	-	X
55	MG	RA	3349	-	-	-	X
55	MG	RA	3359	-	-	-	X
55	MG	XA	1607	-	-	-	X
55	MG	YA	3011	-	-	-	X
55	MG	YA	3045	-	-	-	X
55	MG	YA	3062	-	-	-	X
55	MG	YA	3100	-	-	-	X
55	MG	YA	3113	-	-	-	X
55	MG	YA	3135	-	-	-	X
55	MG	YA	3158	-	-	-	X
55	MG	YA	3181	-	-	-	X
55	MG	YA	3200	-	-	-	X
55	MG	YA	3211	-	-	-	X
55	MG	YA	3238	-	-	-	X
55	MG	YA	3254	-	-	-	X
55	MG	YA	3257	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3264	-	-	-	X
55	MG	YA	3266	-	-	-	X
55	MG	YA	3270	-	-	-	X
55	MG	YA	3280	-	-	-	X
55	MG	YA	3281	-	-	-	X
55	MG	YA	3285	-	-	-	X
55	MG	YA	3297	-	-	-	X
55	MG	YA	3311	-	-	-	X
55	MG	YA	3312	-	-	-	X
55	MG	YA	3319	-	-	-	X
55	MG	YA	3326	-	-	-	X
55	MG	YA	3339	-	-	-	X
55	MG	YA	3388	-	-	-	X
55	MG	YA	3402	-	-	-	X
55	MG	YA	3409	-	-	-	X
55	MG	YA	3422	-	-	-	X
55	MG	YA	3424	-	-	-	X
55	MG	YA	3440	-	-	-	X
55	MG	YD	302	-	-	-	X
56	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291782 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	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	125	Total	C	N	O		0	0	0
			989	627	191	171				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

- 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	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	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 Thx.

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

- Molecule 22 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	733	295	542	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	733	295	542	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			
23	XX	19	Total	C	N	O	P	0	0	0
			418	186	86	127	19			

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

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	74	Total	C	N	O	S	0	0	0
			593	367	126	99	1			

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

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

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

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

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

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
49	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
51	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

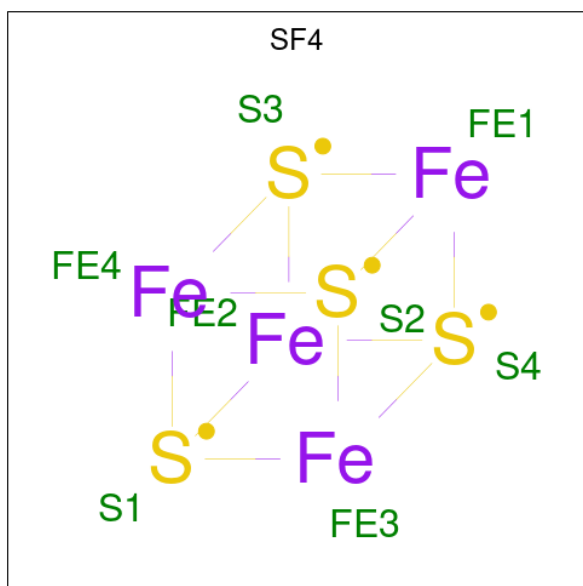
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	69	Total	Mg	0	0
			69	69		
55	QE	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	QV	1	Total	Mg	0	0
			1	1		
55	RA	381	Total	Mg	0	0
			381	381		
55	RB	9	Total	Mg	0	0
			9	9		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	1	Total	Mg	0	0
			1	1		
55	RQ	1	Total	Mg	0	0
			1	1		
55	R1	1	Total	Mg	0	0
			1	1		
55	XA	67	Total	Mg	0	0
			67	67		
55	XE	1	Total	Mg	0	0
			1	1		
55	YA	454	Total	Mg	0	0
			454	454		
55	YB	8	Total	Mg	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YD	2	Total	Mg	0	0
			2	2		
55	YE	1	Total	Mg	0	0
			1	1		
55	YP	1	Total	Mg	0	0
			1	1		
55	YQ	2	Total	Mg	0	0
			2	2		
55	YR	2	Total	Mg	0	0
			2	2		
55	Y0	1	Total	Mg	0	0
			1	1		
55	Y5	1	Total	Mg	0	0
			1	1		
55	Y7	2	Total	Mg	0	0
			2	2		

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

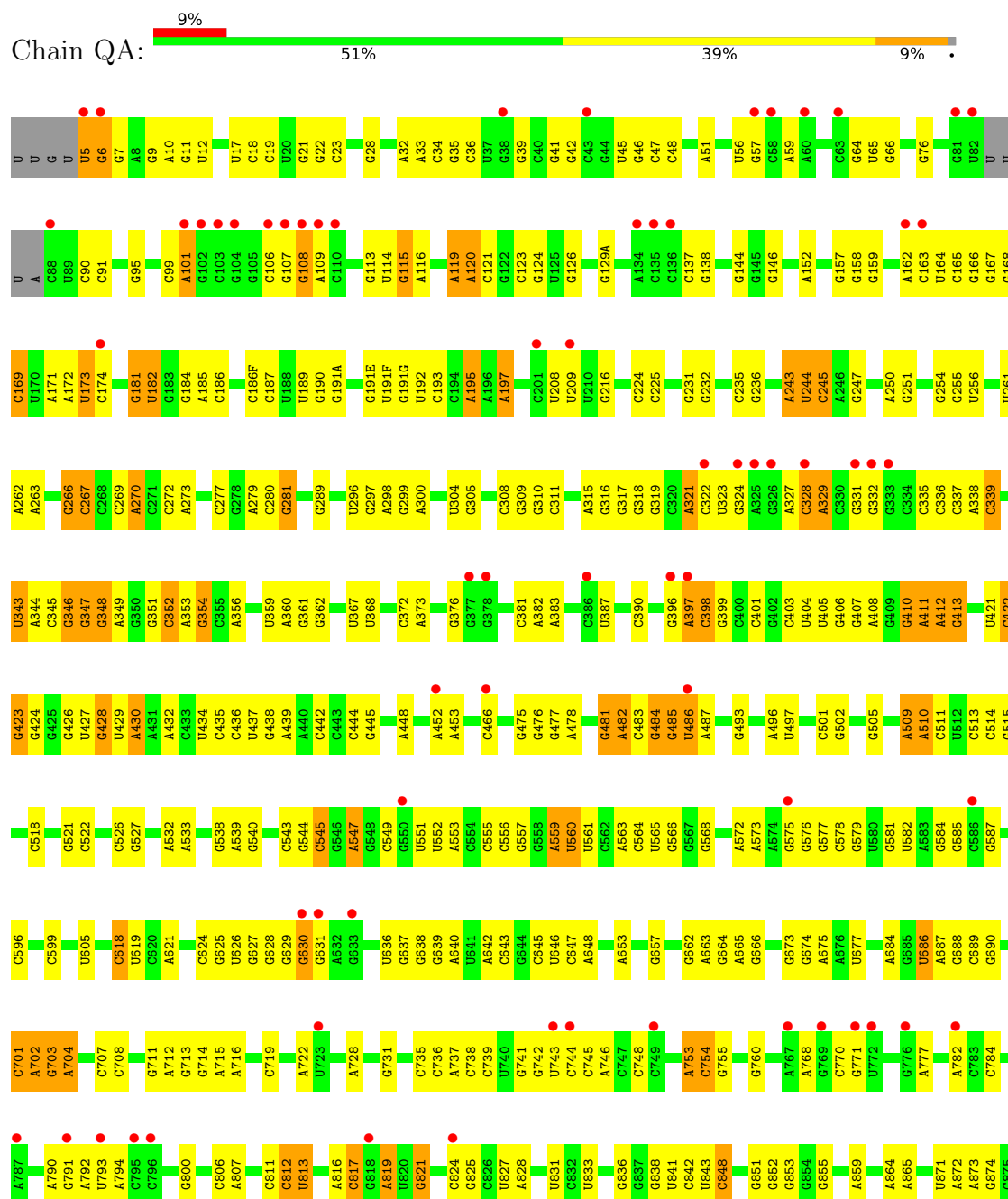
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

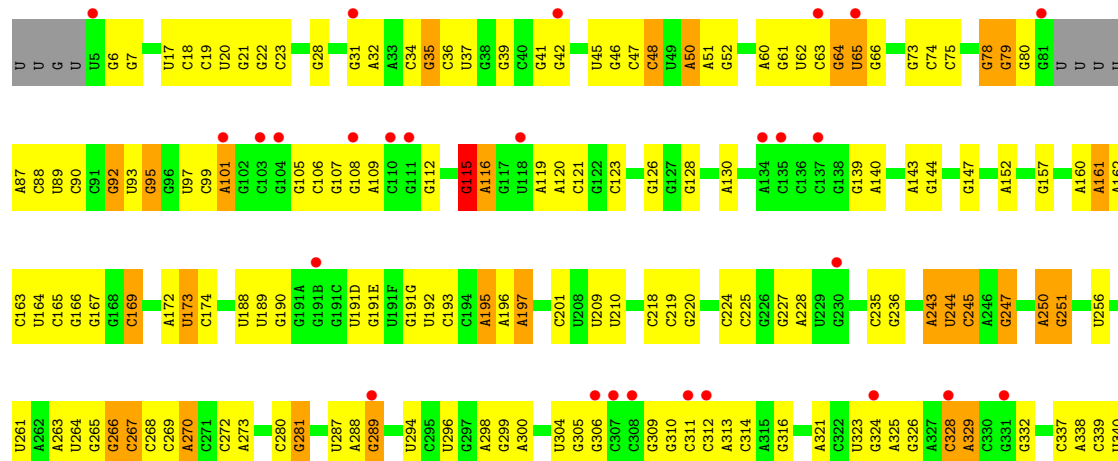
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total 1	Zn 1	0	0
57	RY	1	Total 1	Zn 1	0	0
57	R4	1	Total 1	Zn 1	0	0
57	R5	1	Total 1	Zn 1	0	0
57	R6	1	Total 1	Zn 1	0	0
57	R9	1	Total 1	Zn 1	0	0
57	XN	1	Total 1	Zn 1	0	0
57	YY	1	Total 1	Zn 1	0	0
57	Y4	1	Total 1	Zn 1	0	0
57	Y5	1	Total 1	Zn 1	0	0
57	Y6	1	Total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

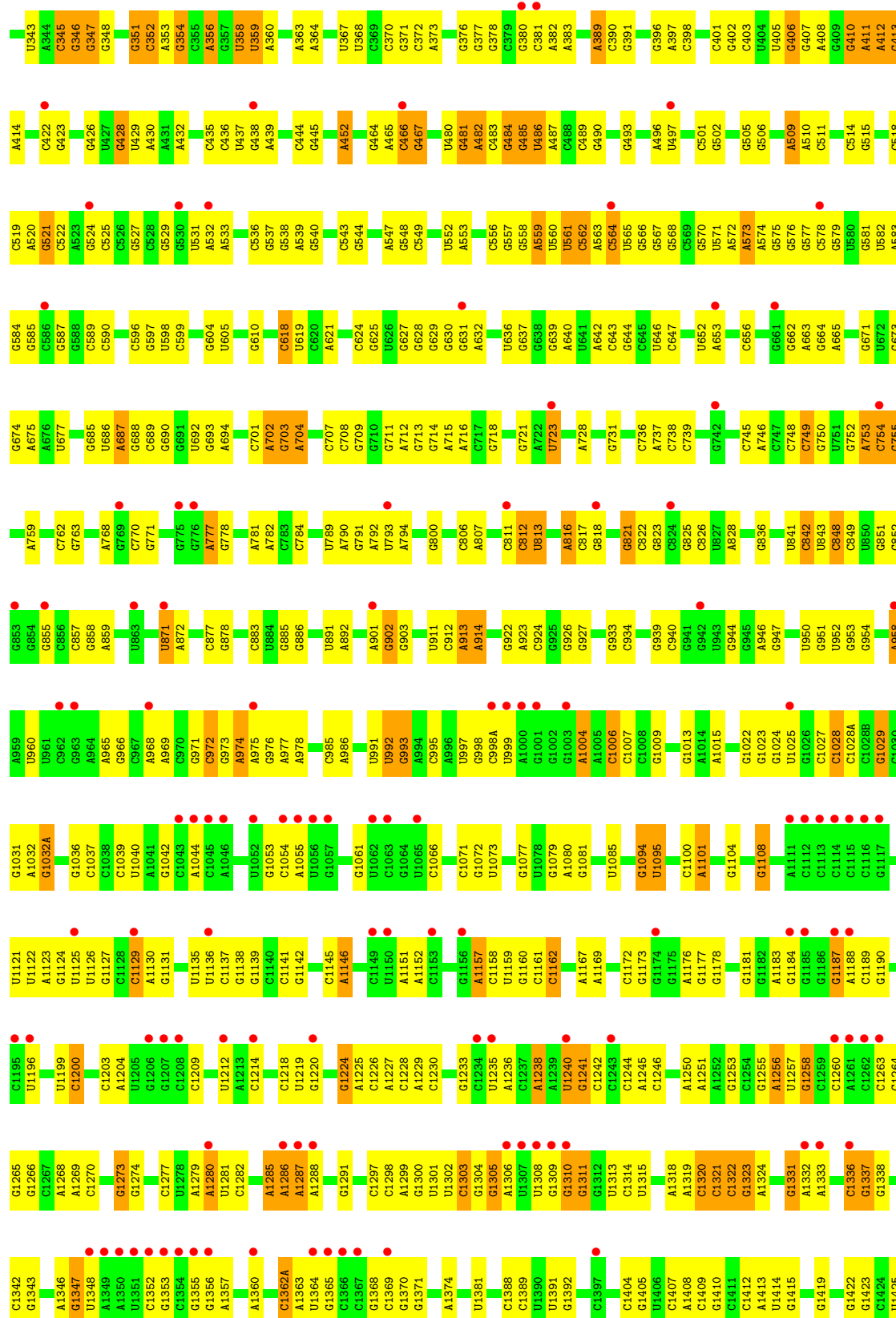
3 Residue-property plots

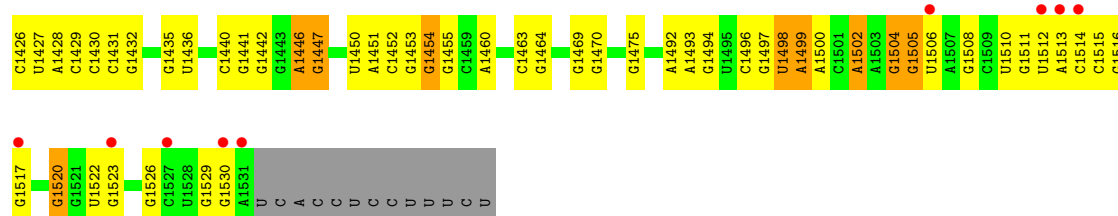
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

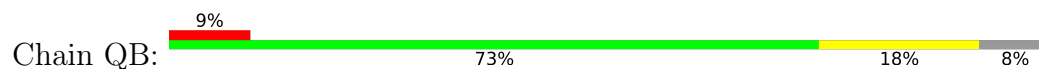




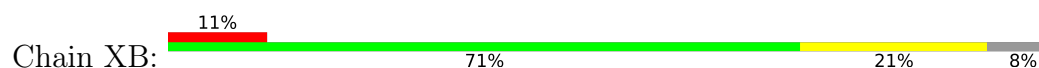




• Molecule 2: 30S ribosomal protein S2



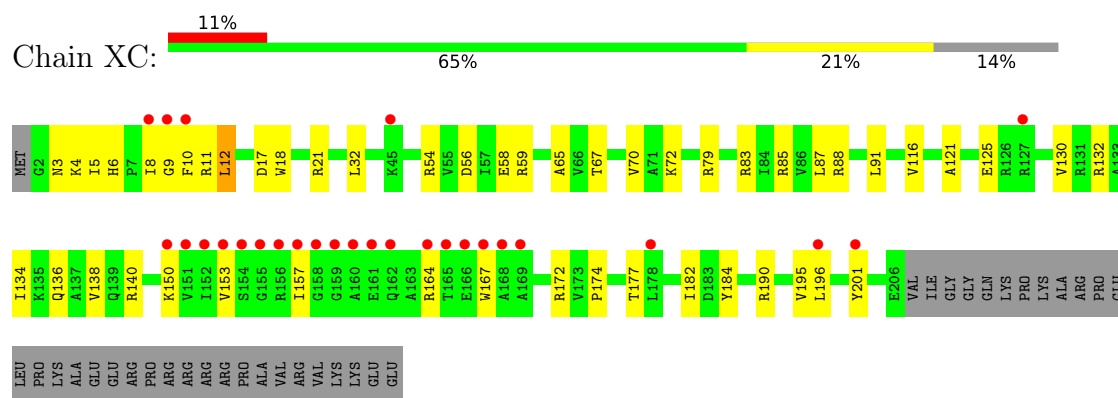
• Molecule 2: 30S ribosomal protein S2



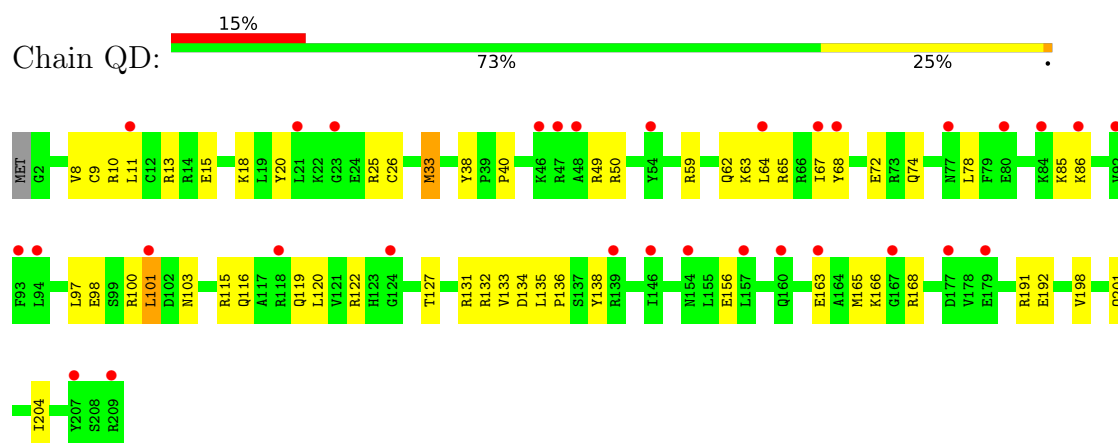
• Molecule 3: 30S ribosomal protein S3



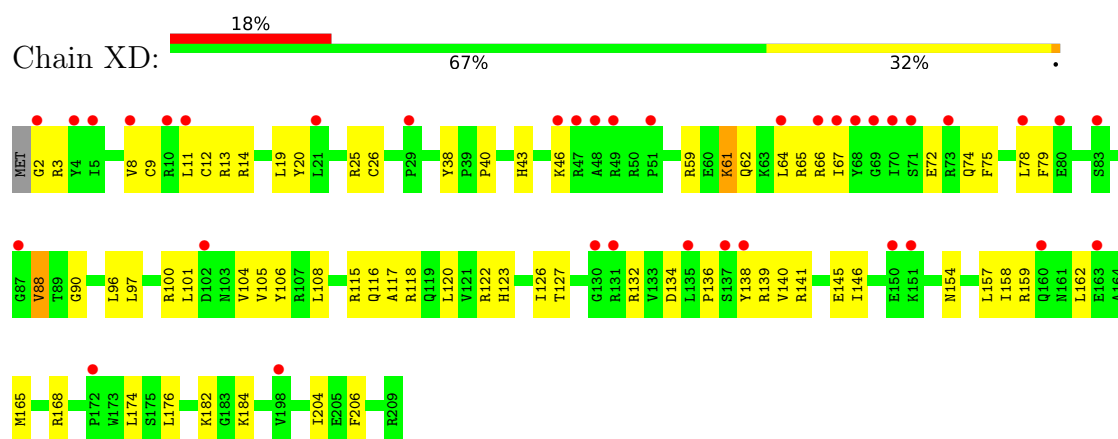
- Molecule 3: 30S ribosomal protein S3



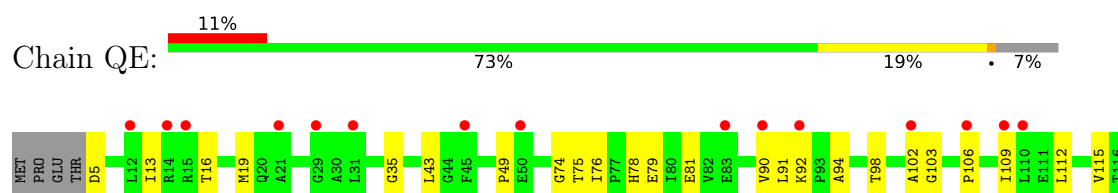
- Molecule 4: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

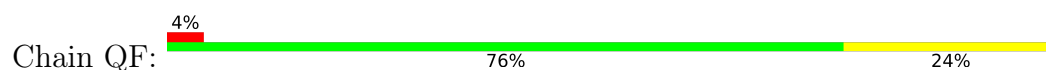




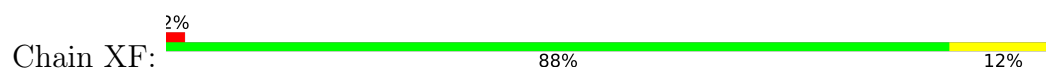
- Molecule 5: 30S ribosomal protein S5



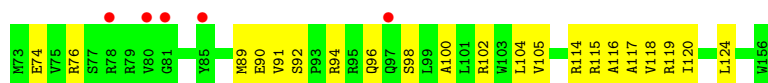
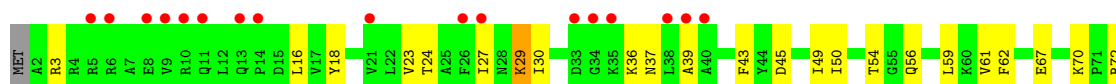
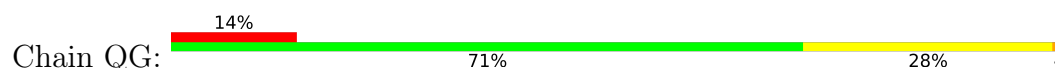
- Molecule 6: 30S ribosomal protein S6



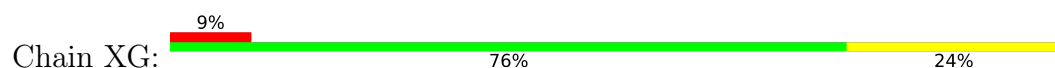
- Molecule 6: 30S ribosomal protein S6

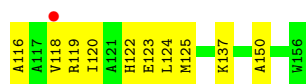


- Molecule 7: 30S ribosomal protein S7

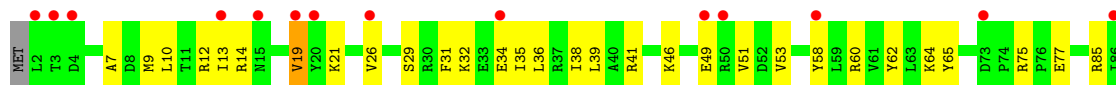
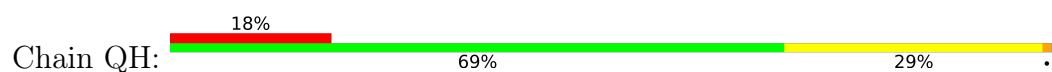


- Molecule 7: 30S ribosomal protein S7

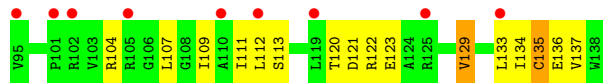




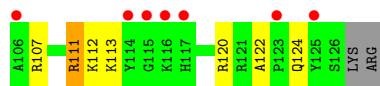
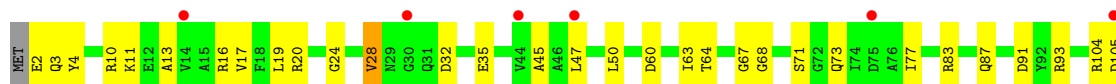
- Molecule 8: 30S ribosomal protein S8



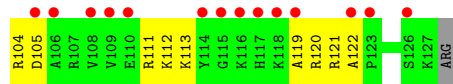
- Molecule 8: 30S ribosomal protein S8



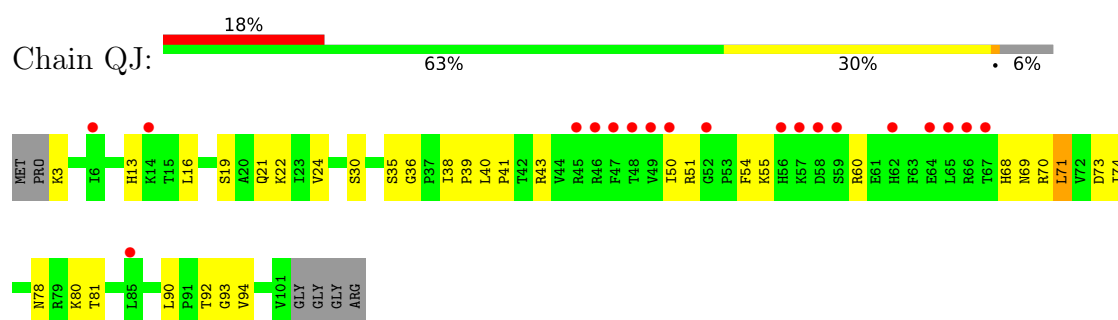
- Molecule 9: 30S ribosomal protein S9



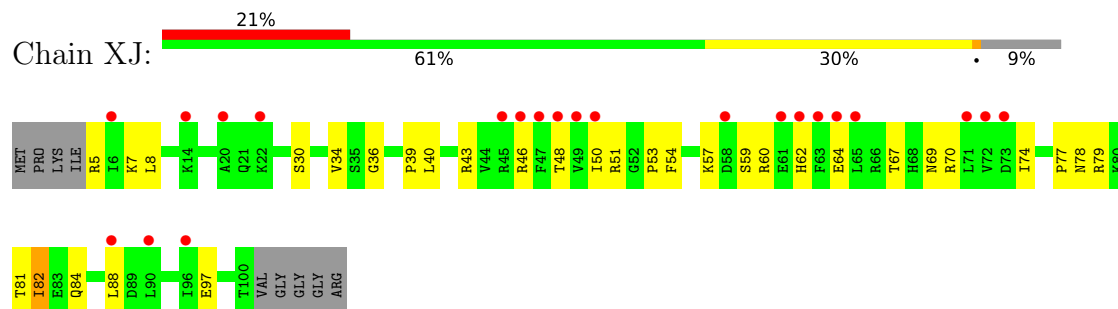
- Molecule 9: 30S ribosomal protein S9



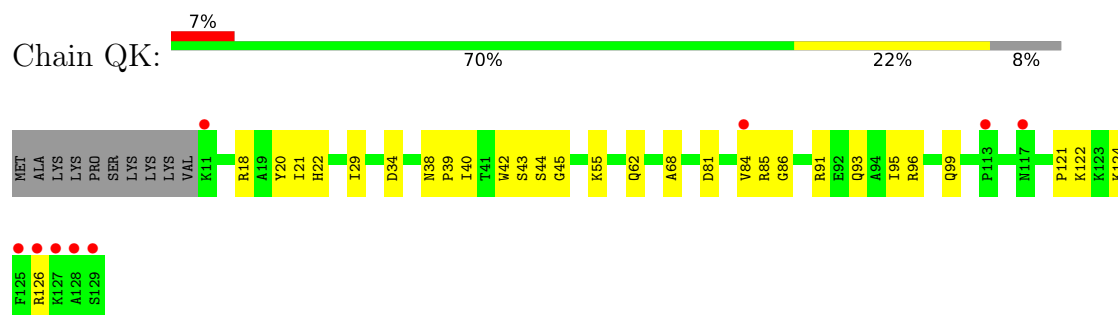
- Molecule 10: 30S ribosomal protein S10



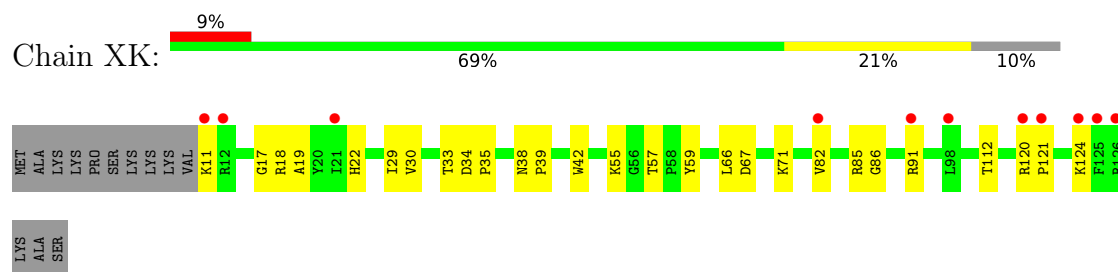
- Molecule 10: 30S ribosomal protein S10



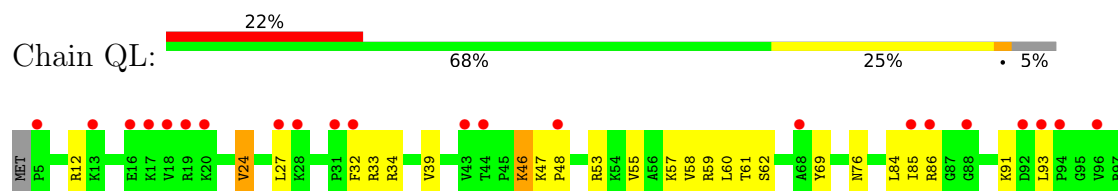
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

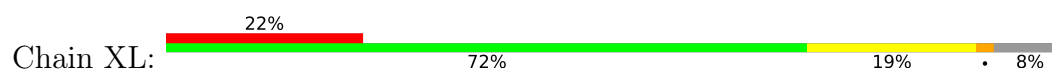


- Molecule 12: 30S ribosomal protein S12

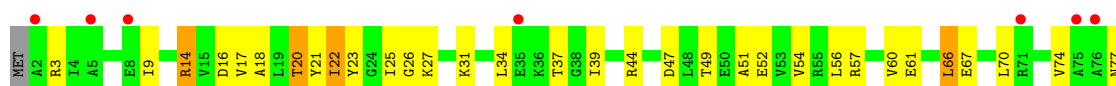




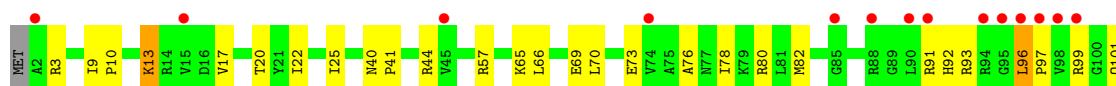
- Molecule 12: 30S ribosomal protein S12



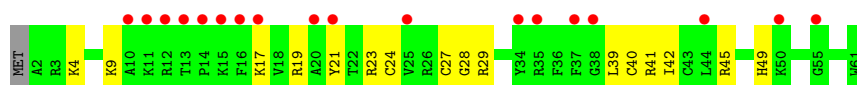
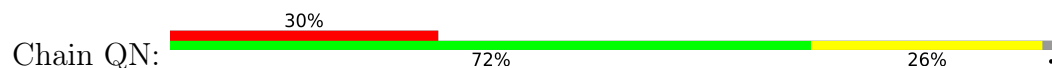
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

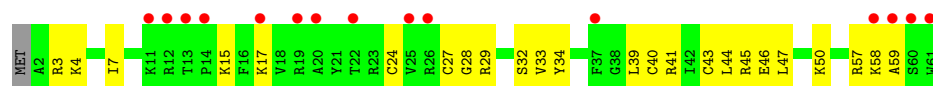


- Molecule 14: 30S ribosomal protein S14 type Z

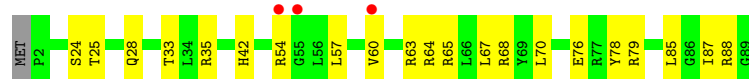
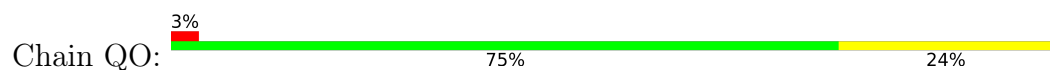


- Molecule 14: 30S ribosomal protein S14 type Z

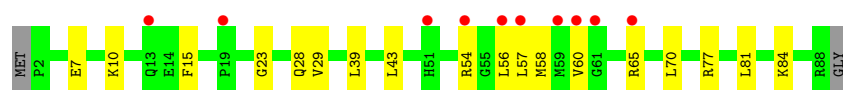
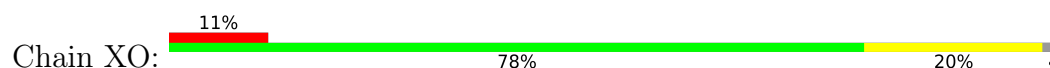




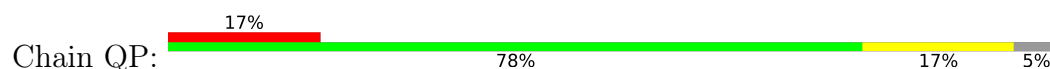
- Molecule 15: 30S ribosomal protein S15



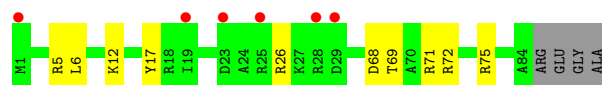
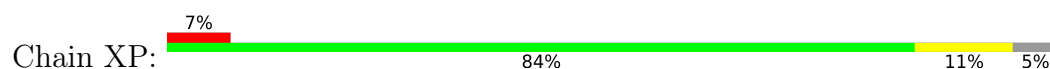
- Molecule 15: 30S ribosomal protein S15



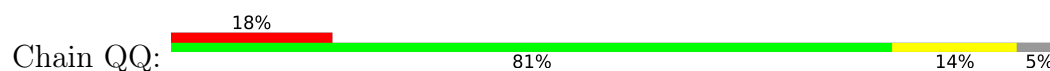
- Molecule 16: 30S ribosomal protein S16



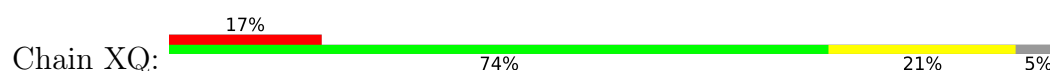
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



LYS
ALA

- Molecule 18: 30S ribosomal protein S18



MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG K19 K23 R32 V37 K49 L58 K61 E62 T69 I70 K71 R72 A73 R74 I75 L76 G77 L78 F81 K88

- Molecule 18: 30S ribosomal protein S18



MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG K19 L31 R32 L44 R53 T56 G57 L58 S59 E62 A67 K68 T69 I70 R74 I75 L76 F81 V86 R87 K88

- Molecule 19: 30S ribosomal protein S19



MET P2 R3 S4 L5 K6 K7 G8 V9 L22 K28 R32 R36 I40 V41 P42 E43 M44 A50 V51 Y52 H57 V58 P59 T63 E64 N65 M66 V67 G68 H69 E73 F76 T77 R78 Y80 R81 G82 H83 G84 LYS GLU ALA LYS THR LYS LYS

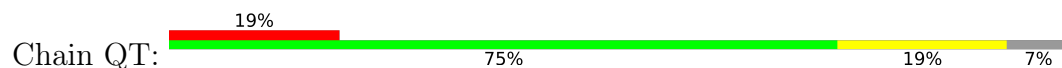
- Molecule 19: 30S ribosomal protein S19



MET P2 R3 S4 L5 K6 K7 G8 V9 F10 D12 D13 L16 E17 K18 V19 L20 N23 L30 I31 K32 R36 R37 S38 T39 V41 P42 E43 M44 T49 A50 G54 K55 Q56 H57 V58 T63 E64 N65 M66 V67 G68 H69 K70 L71 G72 P76 Y80 R81

G84 K85 GLU LYS LYS ALA THR LYS

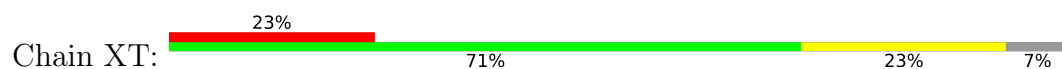
- Molecule 20: 30S ribosomal protein S20

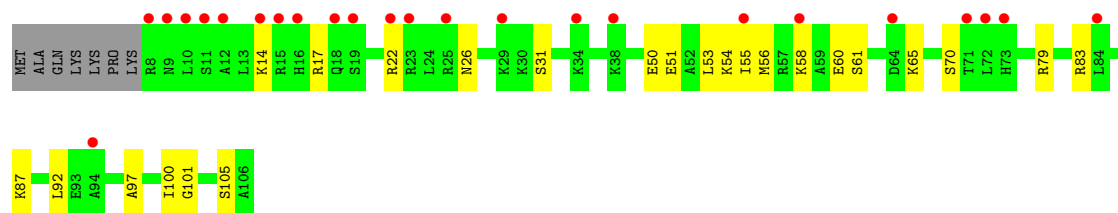


MET ALA GLN LYS PRO LYS R8 R9 L10 S11 A12 L13 K14 Q18 S19 L20 K21 R22 R23 L24 R25 N26 K29 K30 L43 K48 E51 A52 L53 K54 I55 K56 E60 A66 A67 K68 T71 L72 H73 K74 N75 R79 R80 K81 M85 V88 I100

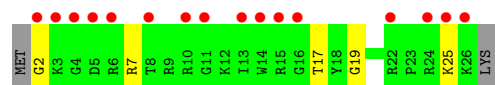
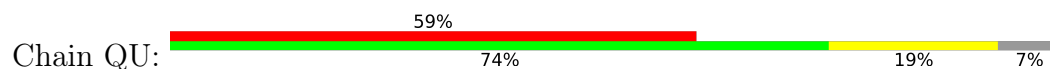
G101 A106

- Molecule 20: 30S ribosomal protein S20

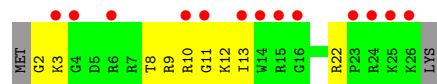




- Molecule 21: 30S ribosomal protein Thx



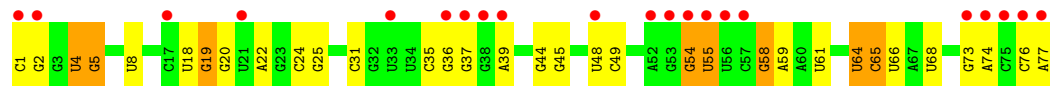
- Molecule 21: 30S ribosomal protein Thx



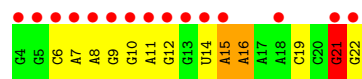
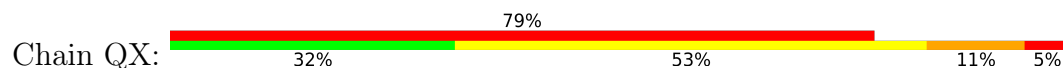
- Molecule 22: P-site ASLPro



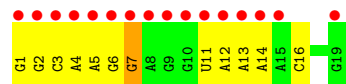
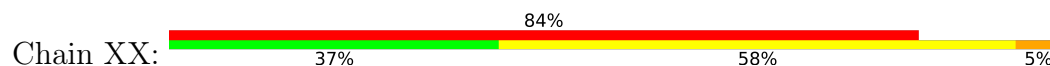
- Molecule 22: P-site ASLPro



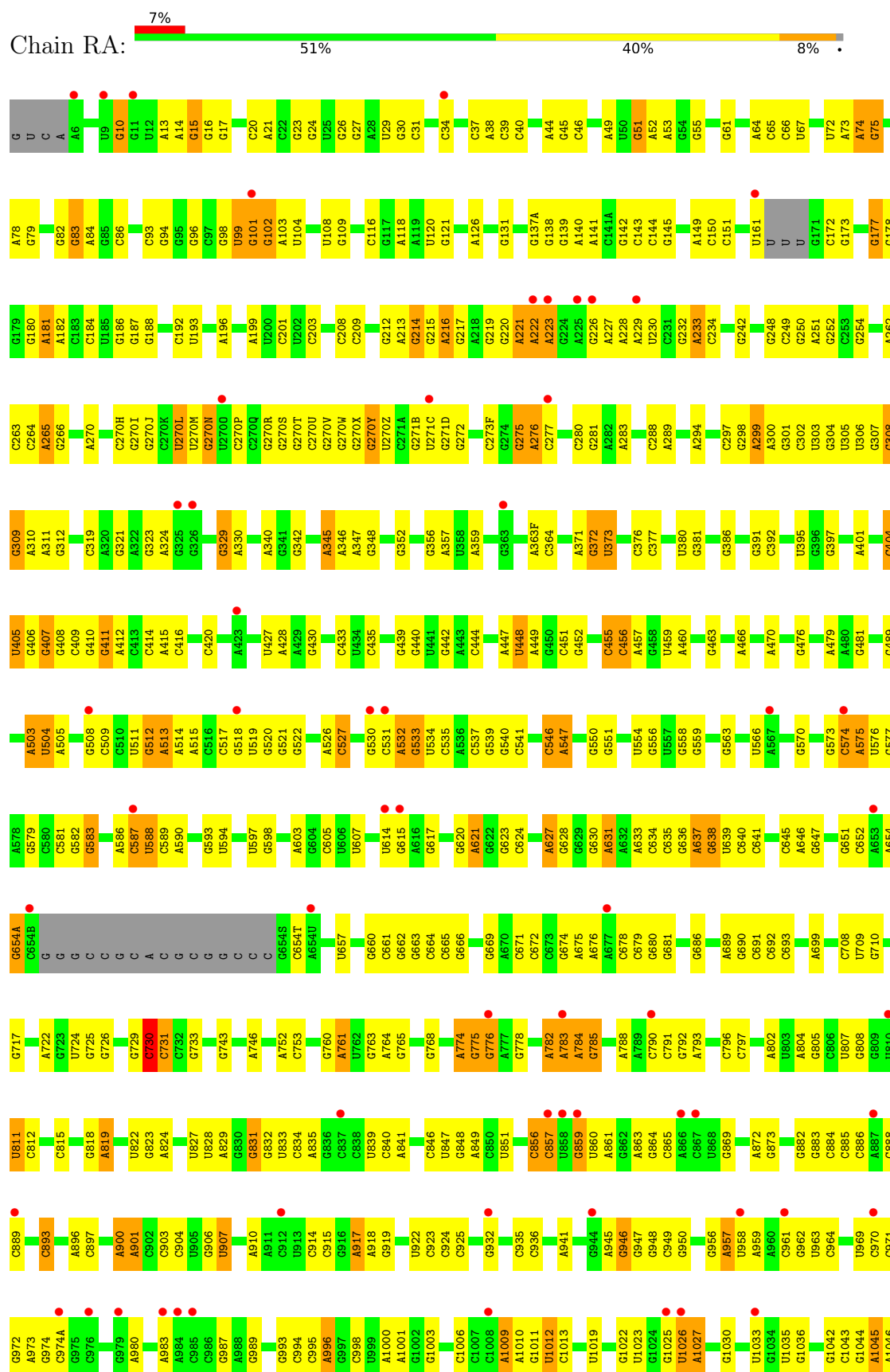
- Molecule 23: mRNA



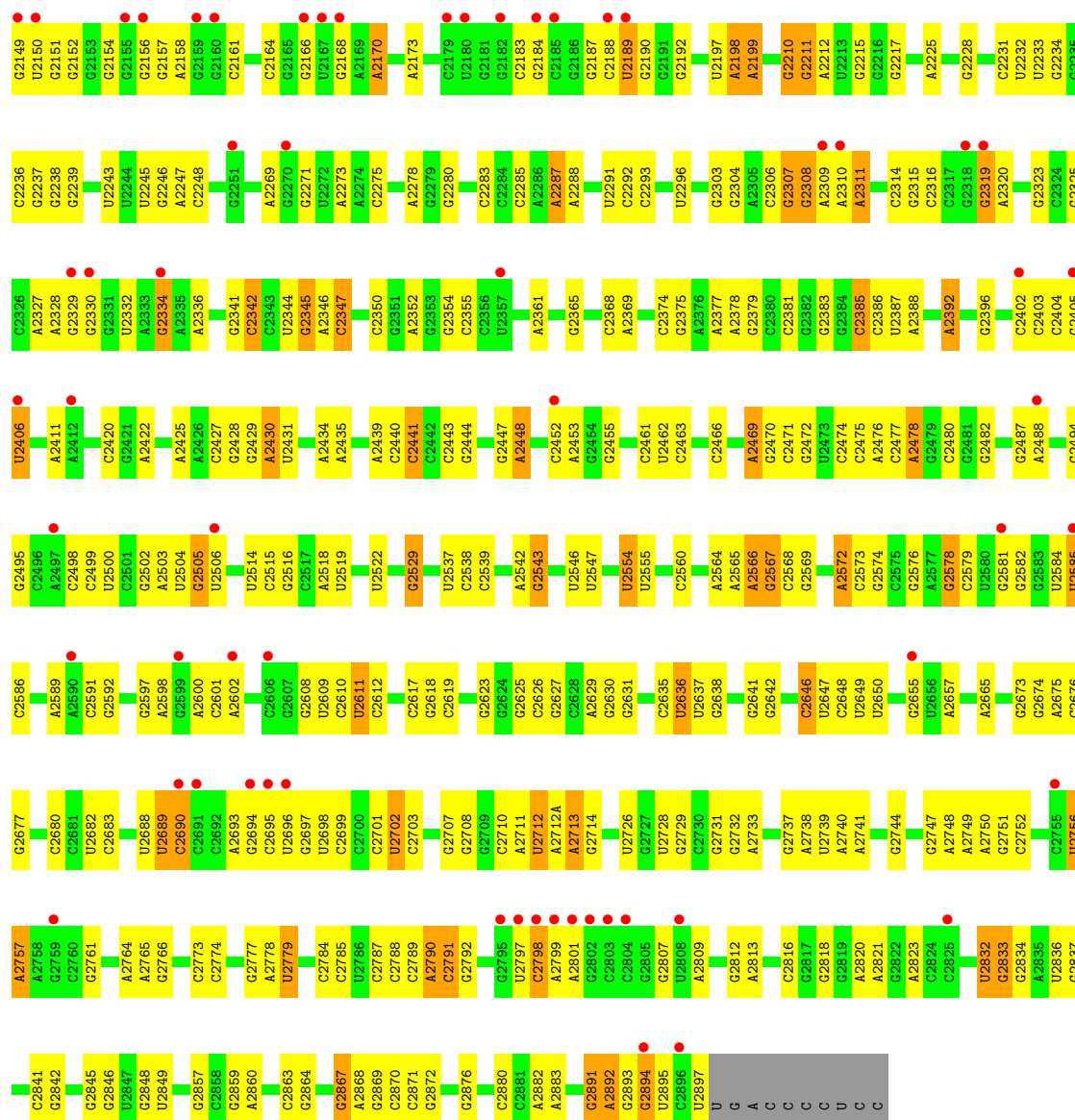
- Molecule 23: mRNA



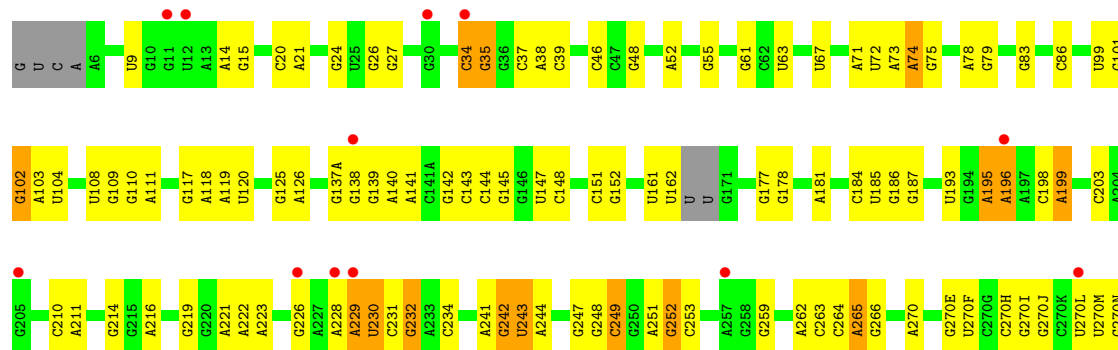
● Molecule 24: 23S rRNA

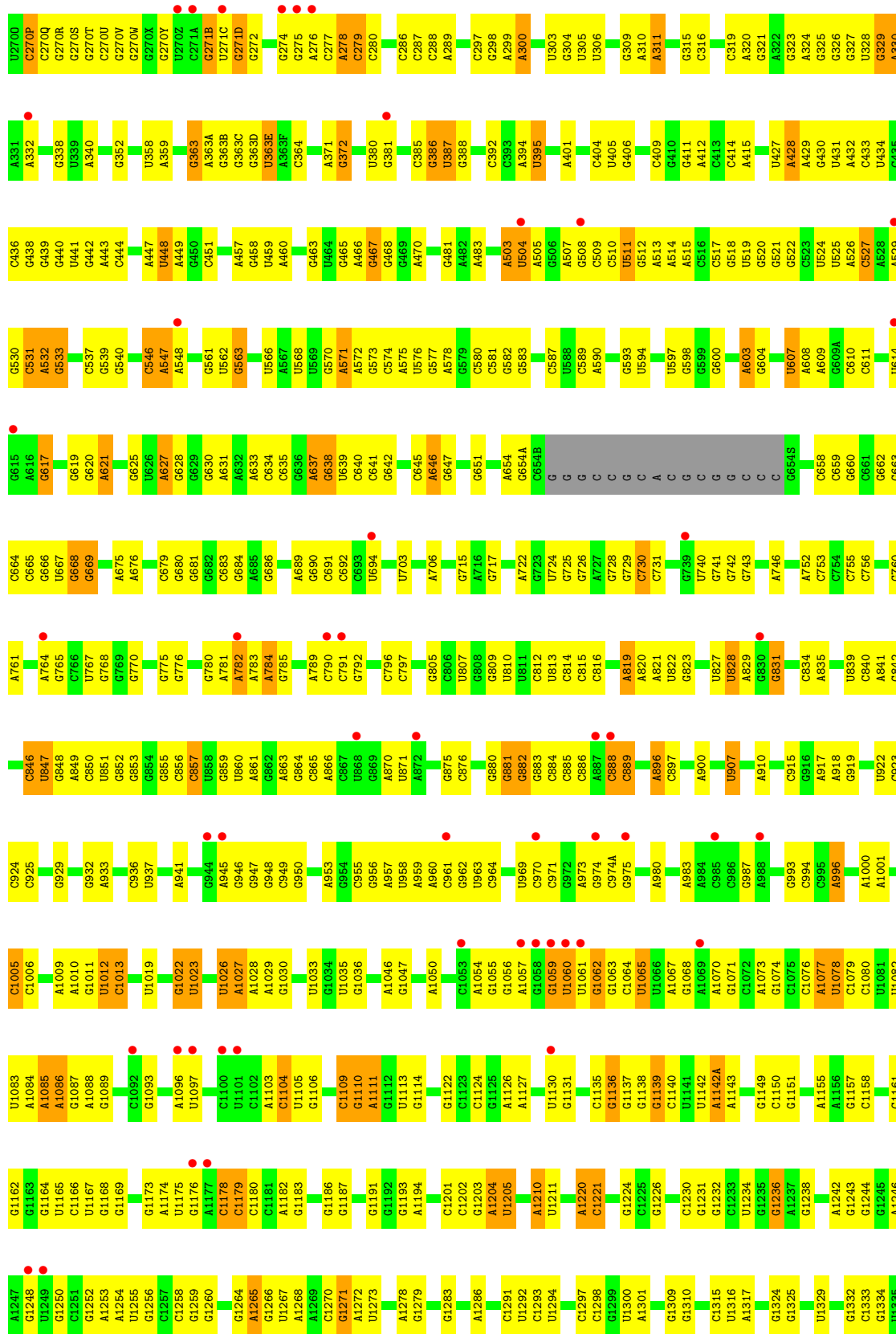




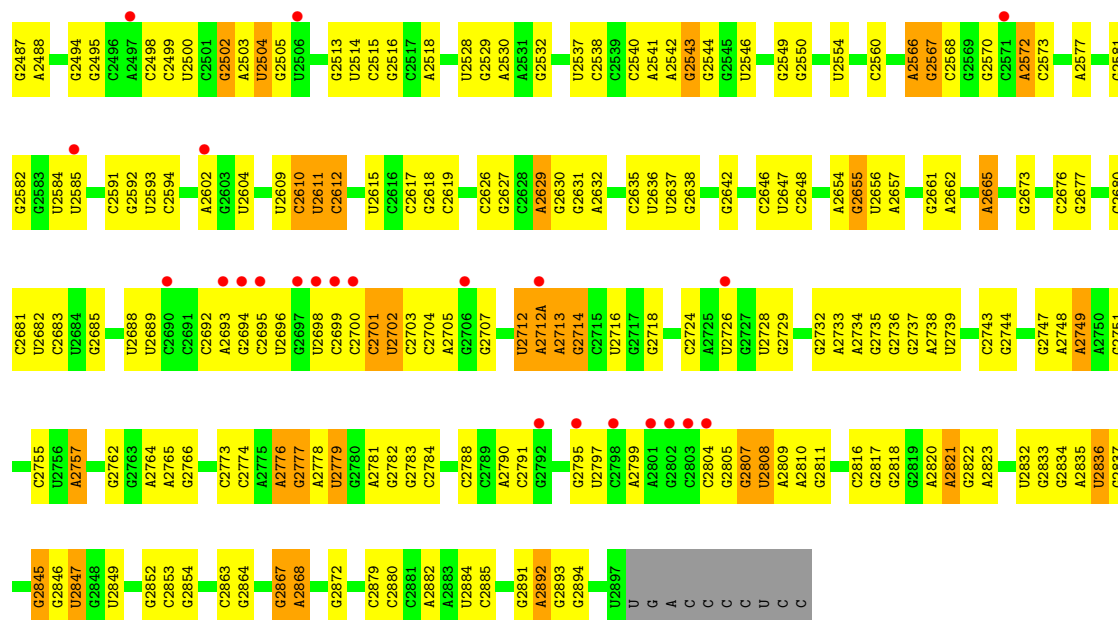


• Molecule 24: 23S rRNA

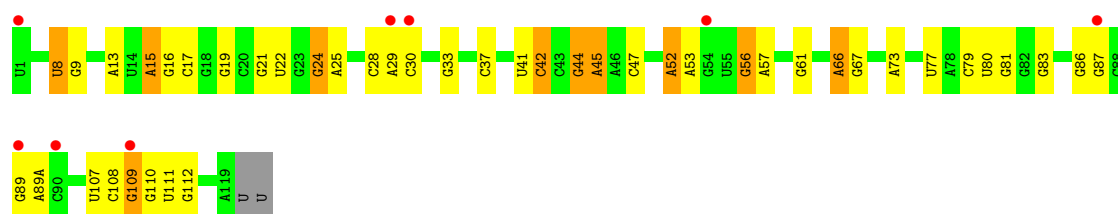




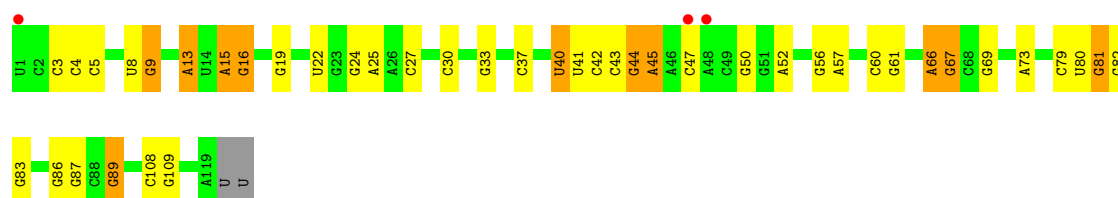
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C2394	G2318	G2224	G2142	C2064	G1869	A1785	G1674	C1592	A1507	G1418	G1337
G2395	G2319	A2225	G2143	C2065	C1870	A1786	C1675	G1593	A1508	G1419	G1338
G2396	G2320			C2066	A1871	A1787		G1594	C1509	U1420	
U2401	A2321	G2228	C2146	G2067	G1872	C1790	G1678	G1595	A1510	G1421	U1341
C2402	A2322	G2229	G2147	G2068	G1878	A1791	U1680	G1596	A1511	G1422	C1345
C2403	G2323	G2230	G2148	G2069	C1882	G1792	G1681	A1597	G1512	G1423	G1346
U2406	G2324			A2071	G1883	G1793	G1682	C1604	C1515	G1425	G1347
G2410	G2325	U2233	G2151	G2070	G1888	U1794	G1683	C1605	G1517	G1426	A1349
G2411	G2326	G2234	G2152	G2072	A1889	C1795	C1684	G1606	U1520	A1427	G1348
G2420	A2327	G2238	G2154	C2081	A1890	U1796	U1693	G1607	G1429	G1428	U1352
U2423	G2328	G2239	G2155	A2082	U1798	C1797	C1694	A1608	C1430	C1427	A1353
C2424	G2329		G2156		G1799	U1798	G1695	A1609	G1522	A1427	A1354
C2425	G2330	U2243	G2157	U2086	G1999	C1800	G1699	C1611	G1530	G1435	G1355
A2426	G2331	U2244	A2158	G2087	C1902	G1801		G1612	G1436	G1435	G1356
A2427	A2332	U2245	G2159	C2007	G1903	A1802	U1709	G1613	U1534	C1437	A1359
G2428	A2333	U2246	G2160	C2008	C1904	A1803	C1710	A1614	U1535	U1438	A1365
G2429	G2334	G2247	C2161	G2009	G1906		C1711	C1615	A1536	U1439	
A2430	A2335		G2162	G2010	G1907	A1812		A1616	G1538	G1444	G1368
G2435	A2336	G2250	G2163	G2011	C1914	G1813	G1725	C1617	G1539	G1444	G1369
A2439	G2337	U2257	C2164	G2012	A1919	A1815	U1727	A1618	G1540	C1445	G1370
C2440	G2340	U2258	G2165	A2020	C1919	G1816	G1728	G1622	U1541		G1371
C2441	G2341		G2166	C2021	U1923	G1817		G1625	G1542	A1449	U1372
C2442	C2342	A2266	G2167	U2022	C1924	U1818	U1729	C1626	A1543	G1449A	
C2443	U2343	A2269	A2170	G2023	G1924	A1819	U1730	G1627	C1544	U1454	C1376
G2444	G2344		A2171	G2024	G1929	U1820	G1731	G1628	A1545	G1455	G1377
A2445	A2345	G2273	U2172	C2025	G1930	A1821	A1732	U1629	A1546A		A1378
G2447	C2346	A2274	G2173	G2026	U1931	G1822		G1630	C1547	G1459	
A2448	G2347	G2275	G2174	A2030		G1823	G1743	C1631	C1550	A1460	A1384
U2449	G2351	G2279	G2175	A2031	A1936	G1824	G1748	G1636	C1551	G1461	G1385
G2450	A2352	G2280	A2176	G2032	A1937	A1825	A1749	A1637	A1558	A1471	A1392
A2451	G2353		C2177	A2033	A1938	G1826		C1638	G1559		A1393
C2452	G2354	G2283	C2178	U2034	U1939	C1827	G1754	U1639		A1478	U1394
A2453	C2355	A2287	C2179	G2035	U1940	G1828	G1755	C1640	A1566	G1478	A1395
G2454	G2356	A2288	U2180	G2036	C1941	A1829	U1757	G1645	U1567	U1482	U1396
U2461	U2357	G2289	G2181	G2037	G1942	G1830	G1758	G1646	G1568	G1483	C1398
C2462	A2361	G2290	G2182	G2038	U1943	C1832		G1647	A1569		C1399
C2466	G2365	U2291	C2183	G2039	G1948	U1833		C1648	A1570	G1487	G1400
A2467	G2366	C2292	G2184	C2040		G1834	A1762	A1562	U1576	A1490	C1402
G2470	G2367	C2293	G2185	U2041	A1952	C1835	G1763	G1553	G1491	G1490	C1403
C2471	G2371	C2294	G2186	A2042	U1955	G1836	G1764	A1654	G1492	C1404	C1404
G2472	G2372	U2296	A2126	C2043	U1956	C1844		A1655	A1578	U1405	U1406
A2476	G2373		G2127	G2046	U1963	G1845	U1772	C1656	A1580	C1407	C1407
C2477	C2374	G2303	G2131	U2047	U1963	A1847	A1773	C1657	A1496	C1408	C1408
G2478	A2377	C2306	U2132	A2051	G1967		U1777	U1659	C1585	U1497	G1410
A2479	G2378	G2307	G2133	G2052	C1968	A1853	U1778	A1586	A1587	C1498	
C2481	A2379	A2308	A2134	C2055	A1969		U1779	A1669	C1588	C1499	C1411
	G2383	A2309	G2135	G2056	A1970	G1858	C1781	U1670	C1589	G1500	A1412
	C2384	A2310	C2136	A2059	A1971			C1672			G1416
	C2385	A2311	G2137	A2060	A1972						
	A2392	C2314	C2140	A2062							



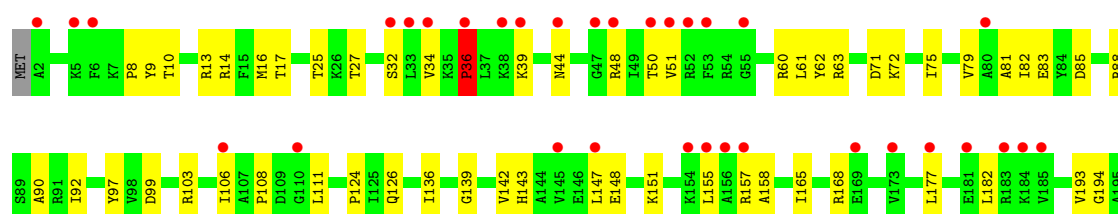
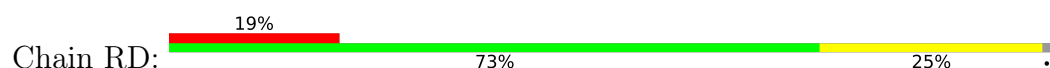
• Molecule 25: 5S rRNA



• Molecule 25: 5S rRNA

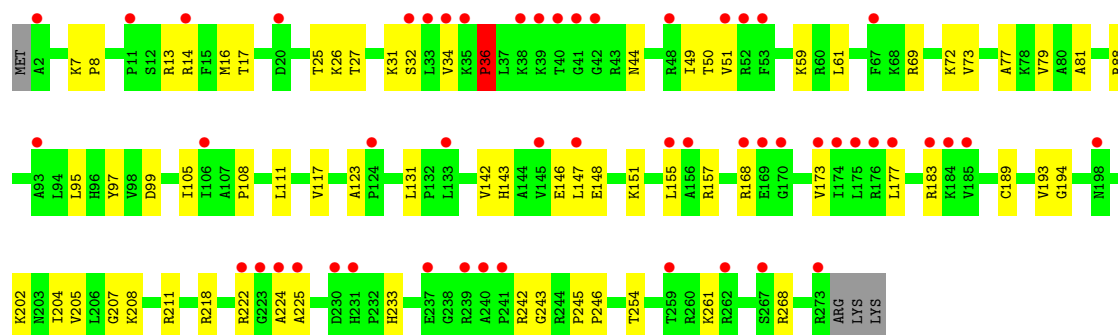
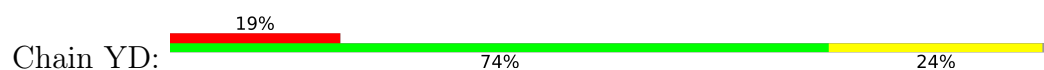


• Molecule 26: 50S ribosomal protein L2

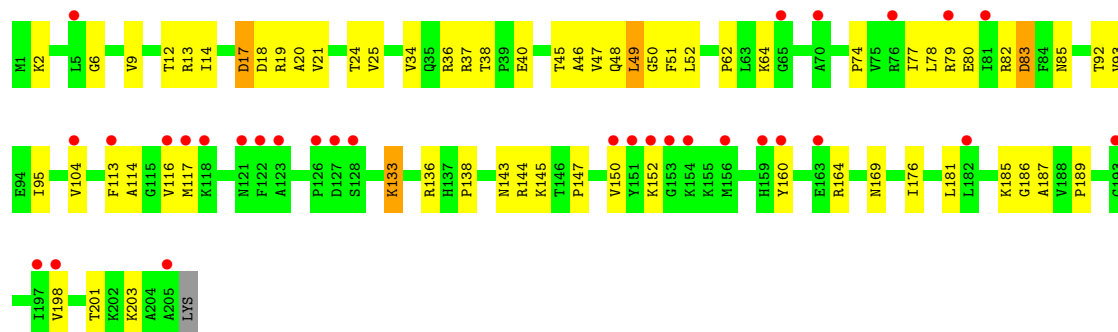




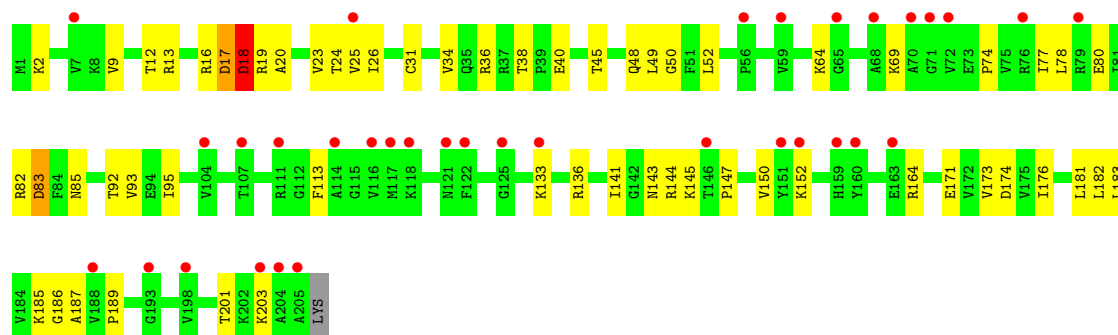
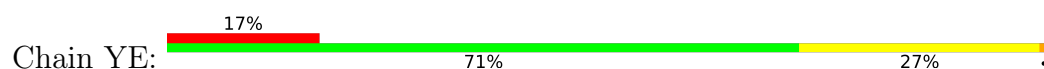
• Molecule 26: 50S ribosomal protein L2



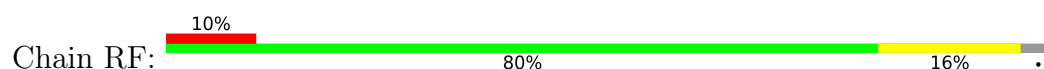
• Molecule 27: 50S ribosomal protein L3

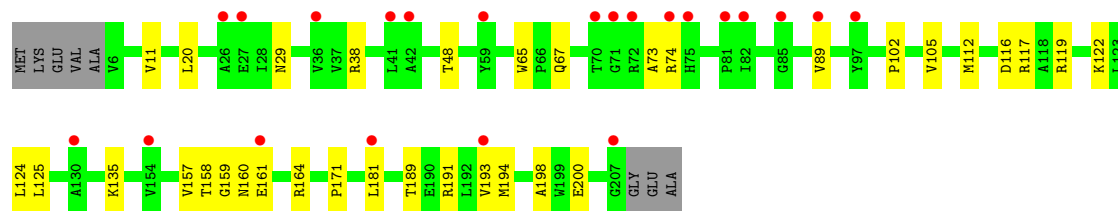


• Molecule 27: 50S ribosomal protein L3

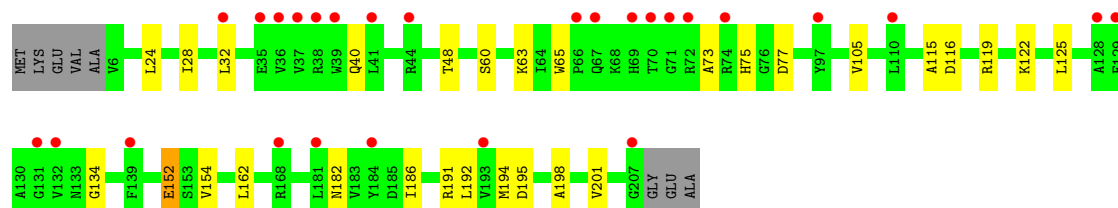
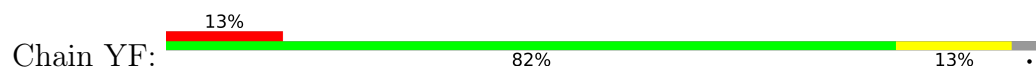


• Molecule 28: 50S ribosomal protein L4

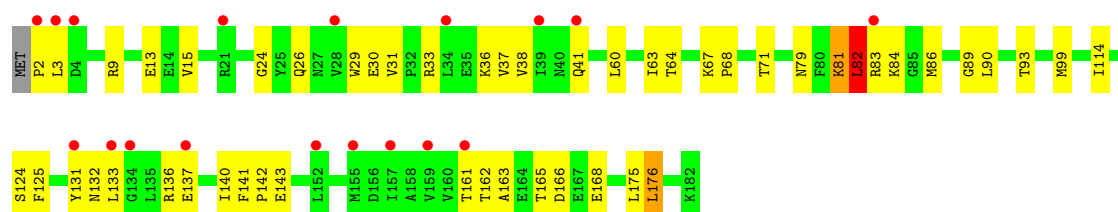
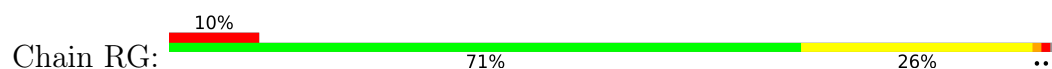




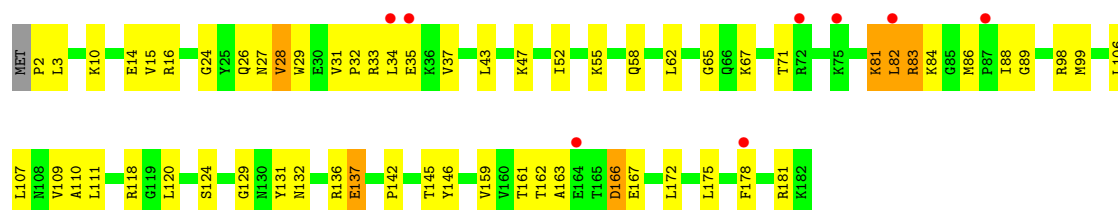
• Molecule 28: 50S ribosomal protein L4



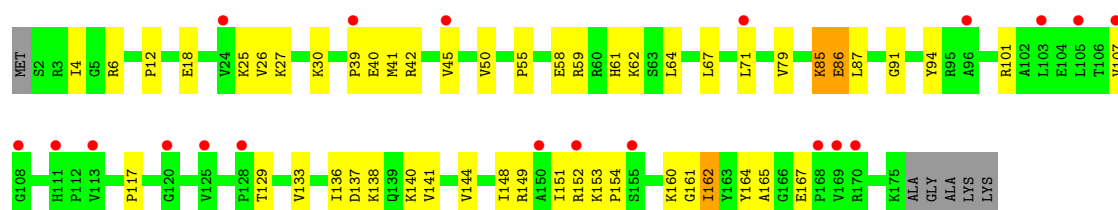
• Molecule 29: 50S ribosomal protein L5



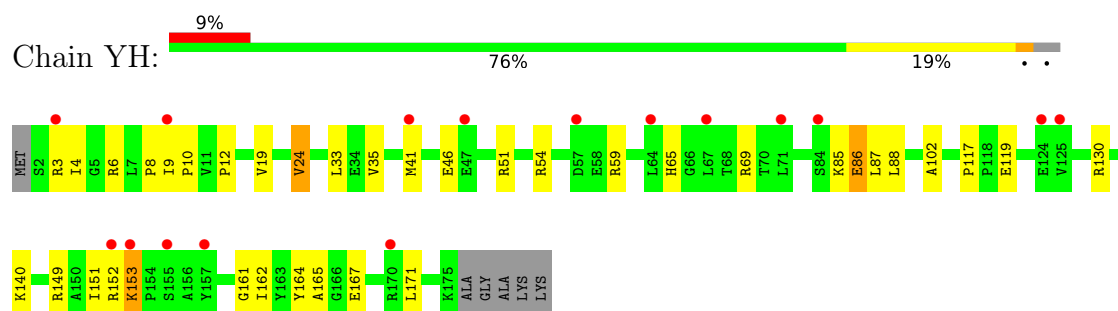
• Molecule 29: 50S ribosomal protein L5



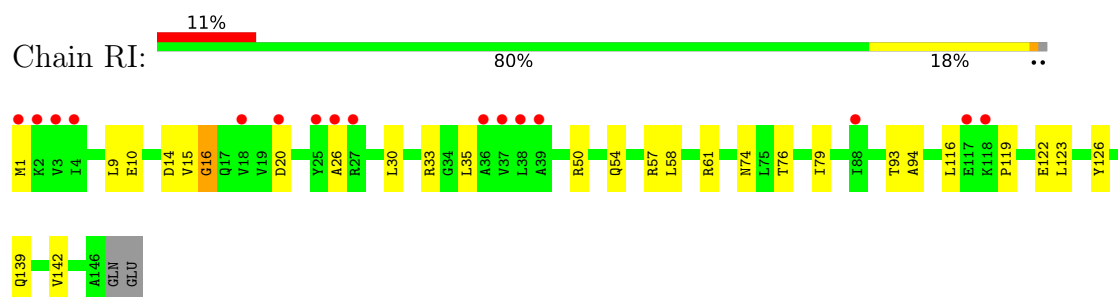
• Molecule 30: 50S ribosomal protein L6



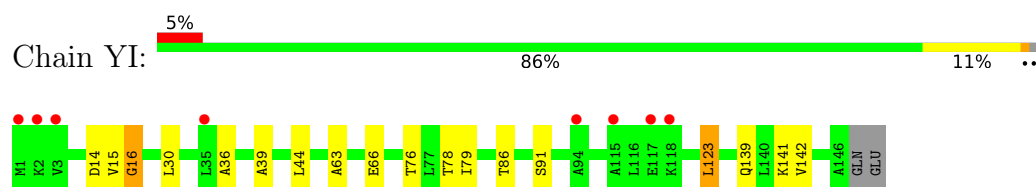
- Molecule 30: 50S ribosomal protein L6



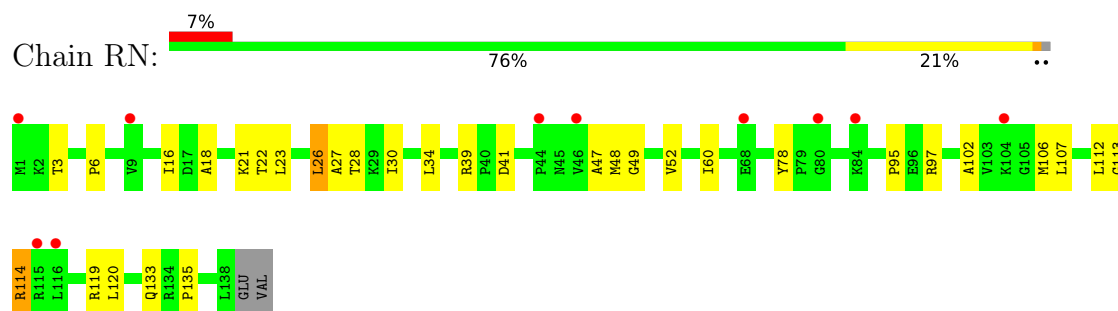
- Molecule 31: 50S ribosomal protein L9



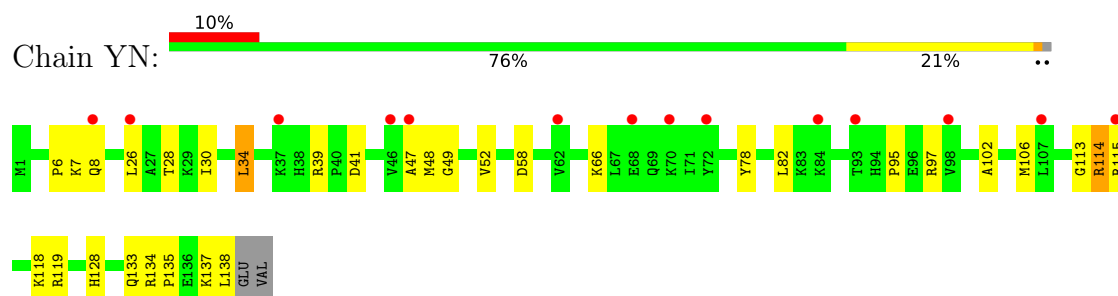
- Molecule 31: 50S ribosomal protein L9



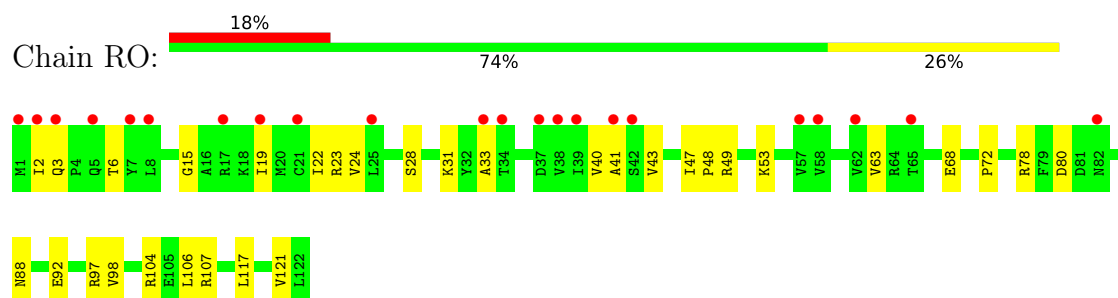
- Molecule 32: 50S ribosomal protein L13



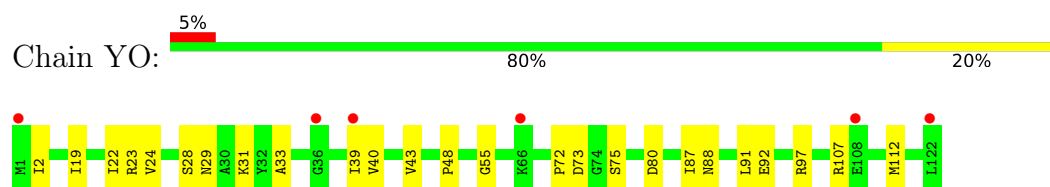
- Molecule 32: 50S ribosomal protein L13



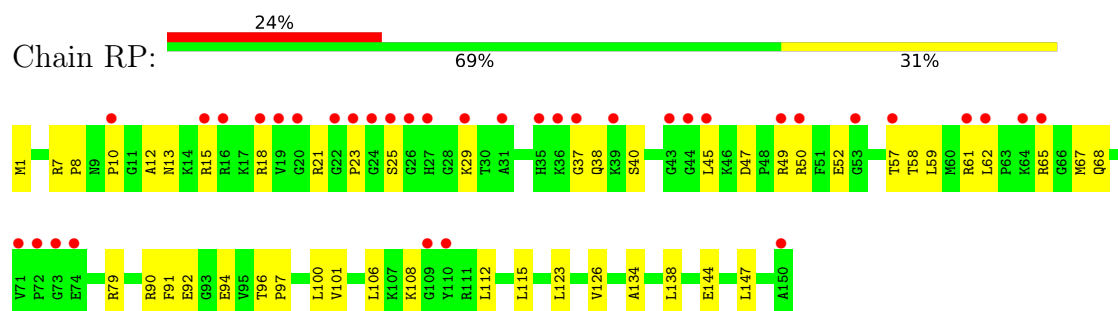
- Molecule 33: 50S ribosomal protein L14



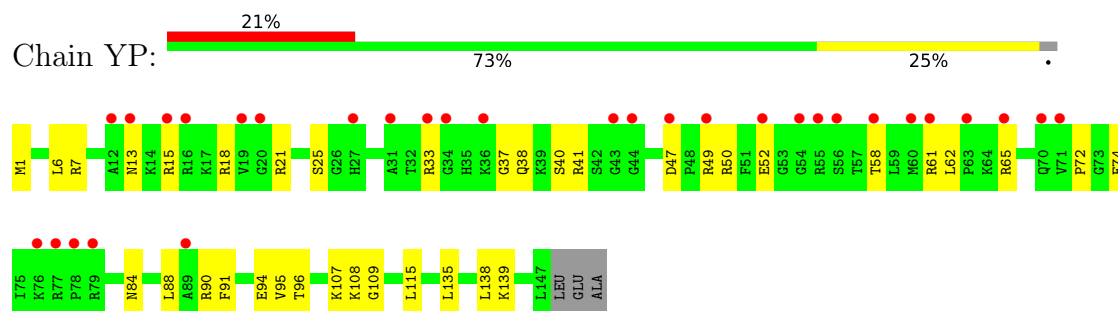
- Molecule 33: 50S ribosomal protein L14



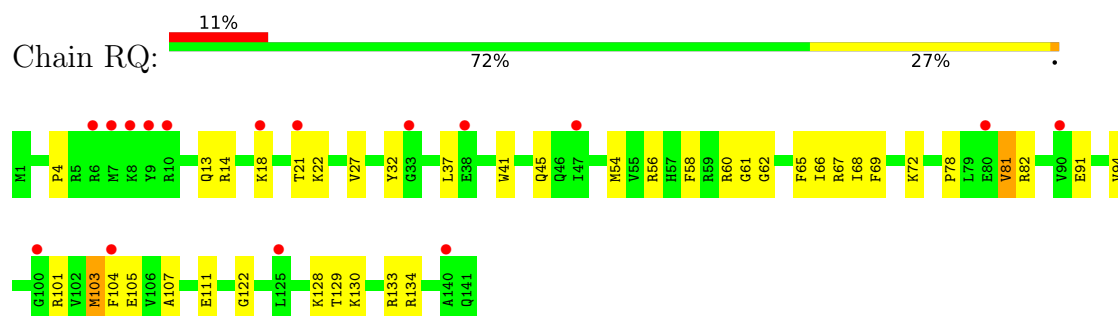
- Molecule 34: 50S ribosomal protein L15



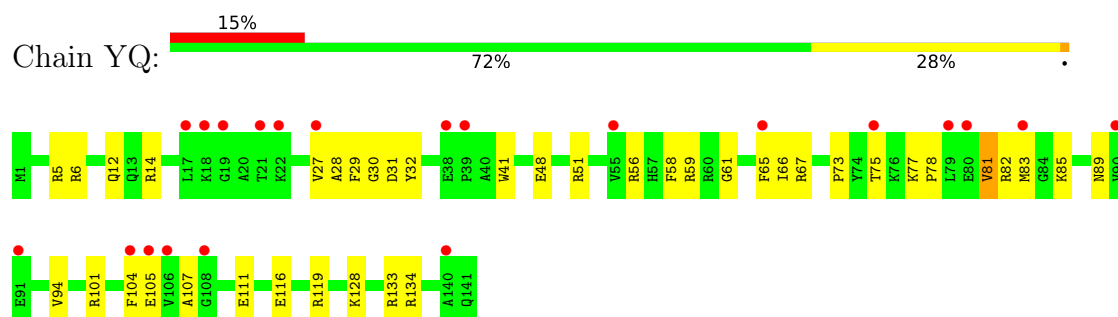
- Molecule 34: 50S ribosomal protein L15



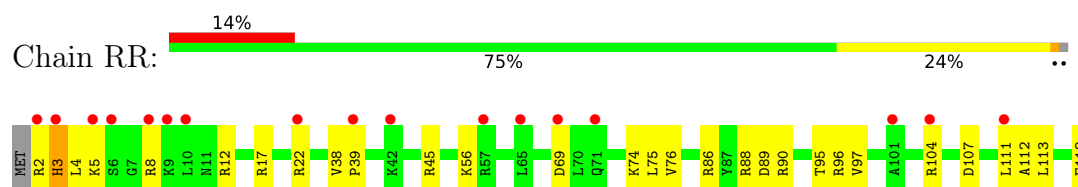
- Molecule 35: 50S ribosomal protein L16



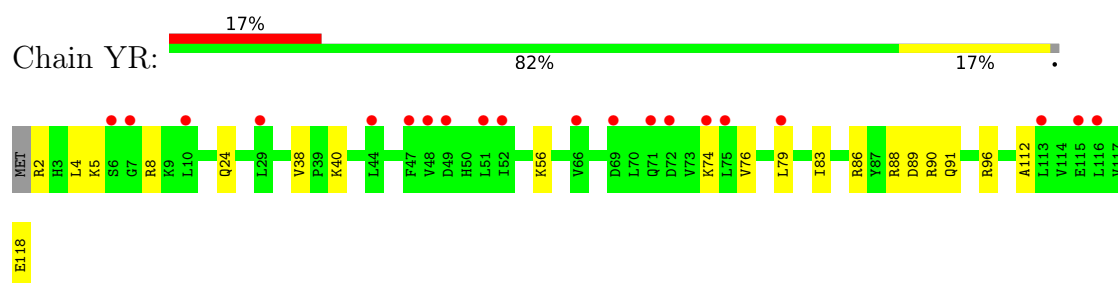
- Molecule 35: 50S ribosomal protein L16



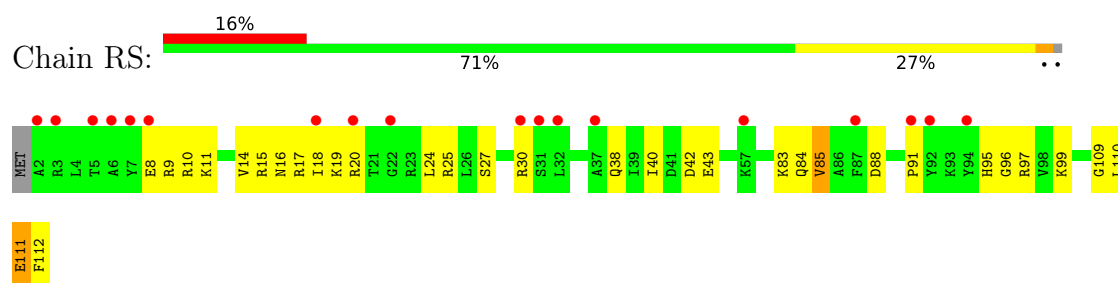
- Molecule 36: 50S ribosomal protein L17



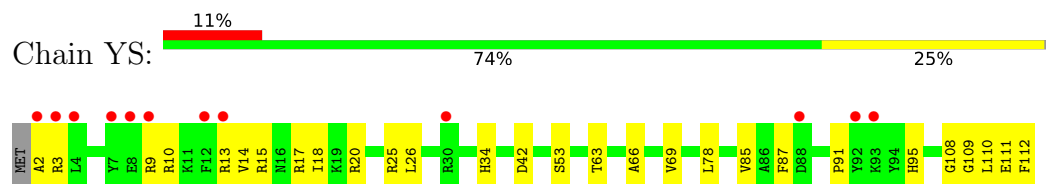
- Molecule 36: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L18

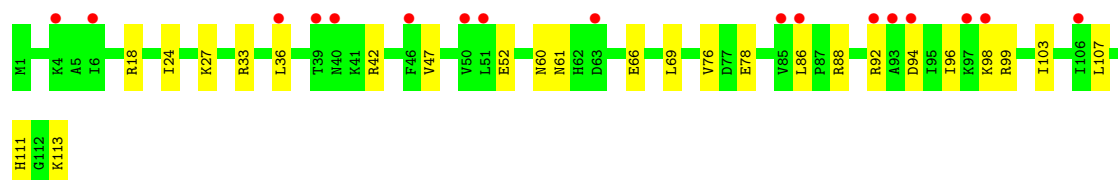


- Molecule 37: 50S ribosomal protein L18

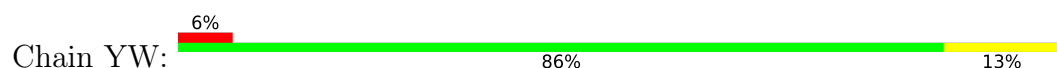


- Molecule 38: 50S ribosomal protein L19

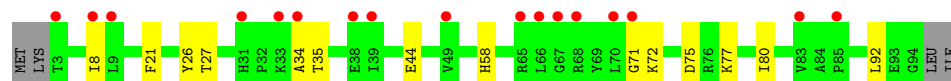
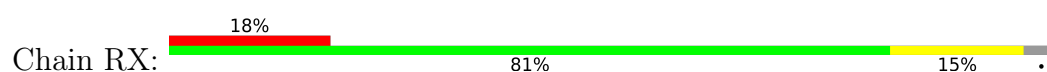




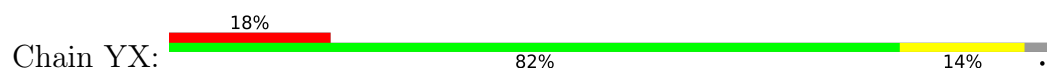
- Molecule 41: 50S ribosomal protein L22



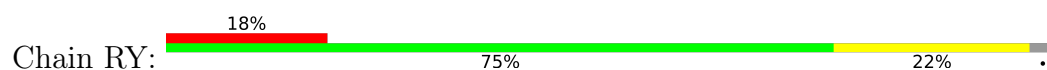
- Molecule 42: 50S ribosomal protein L23



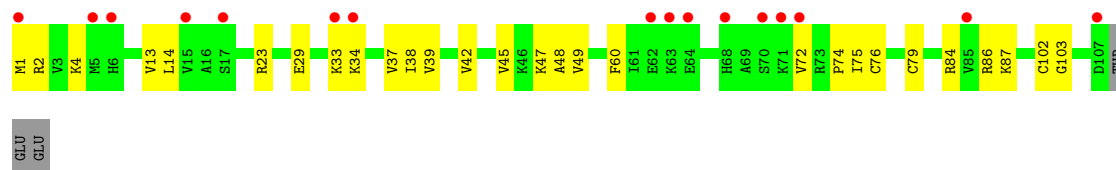
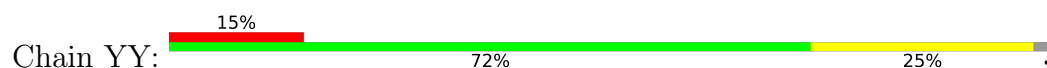
- Molecule 42: 50S ribosomal protein L23



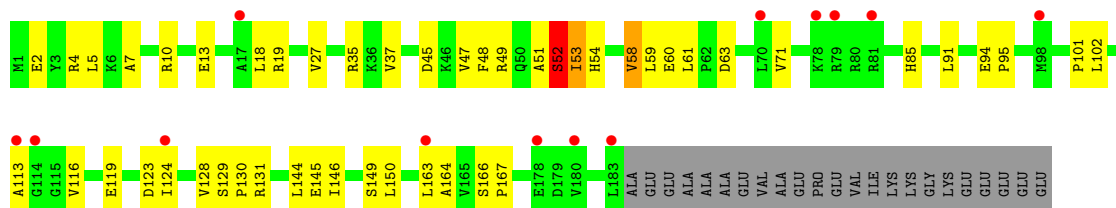
- Molecule 43: 50S ribosomal protein L24



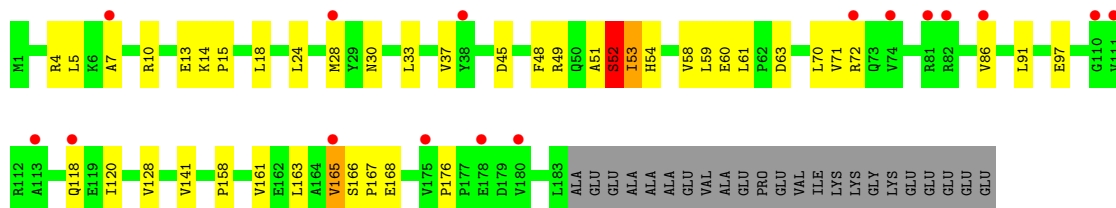
- Molecule 43: 50S ribosomal protein L24



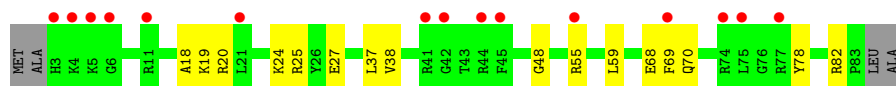
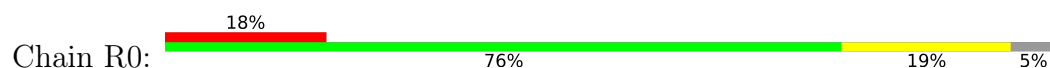
- Molecule 44: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L25



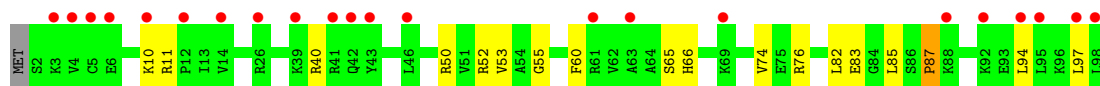
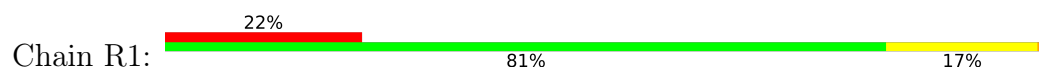
- Molecule 45: 50S ribosomal protein L27



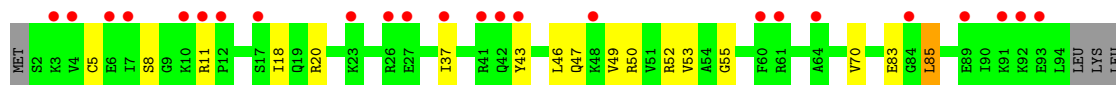
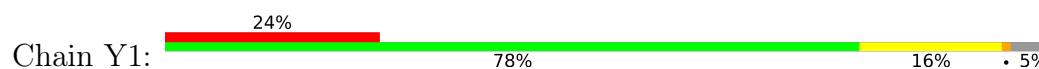
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28



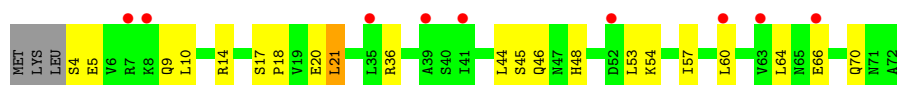
- Molecule 46: 50S ribosomal protein L28



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- Molecule 47: 50S ribosomal protein L29

Chain R2: 



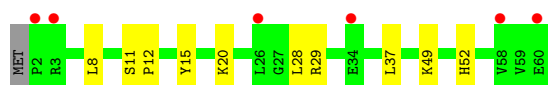
- Molecule 47: 50S ribosomal protein L29

Chain Y2: 



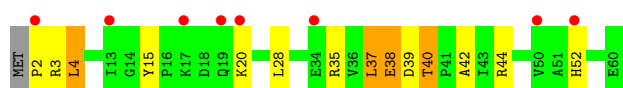
- Molecule 48: 50S ribosomal protein L30

Chain R3: 



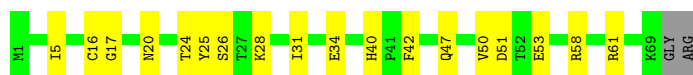
- Molecule 48: 50S ribosomal protein L30

Chain Y3: 



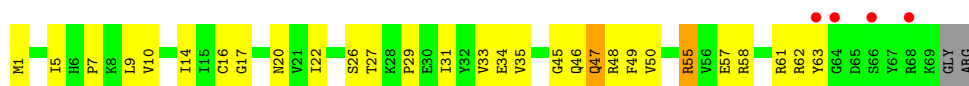
- Molecule 49: 50S ribosomal protein L31

Chain R4: 



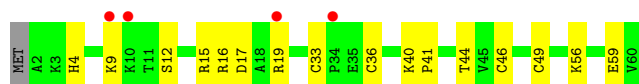
- Molecule 49: 50S ribosomal protein L31

Chain Y4: 

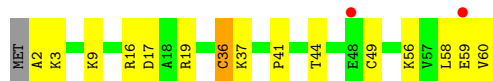
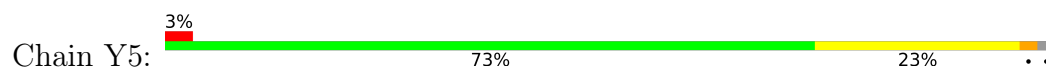


- Molecule 50: 50S ribosomal protein L32

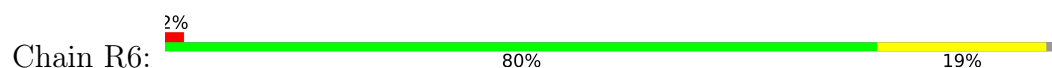
Chain R5: 



- Molecule 50: 50S ribosomal protein L32



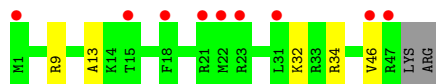
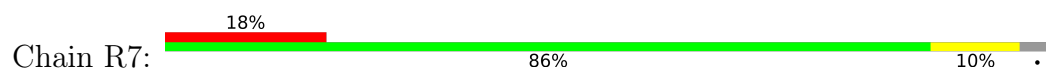
- Molecule 51: 50S ribosomal protein L33



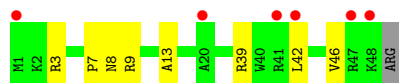
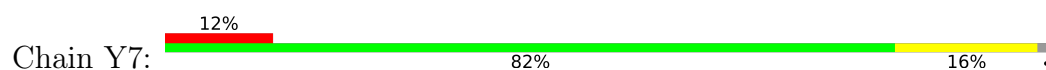
- Molecule 51: 50S ribosomal protein L33



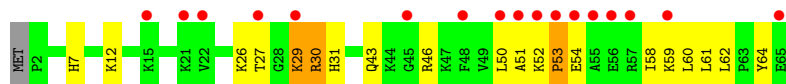
- Molecule 52: 50S ribosomal protein L34



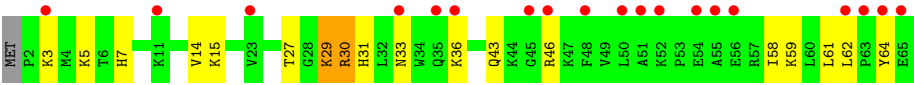
- Molecule 52: 50S ribosomal protein L34



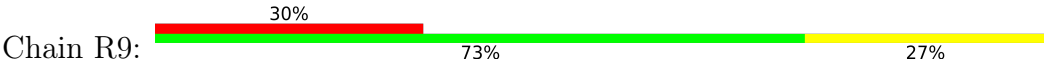
- Molecule 53: 50S ribosomal protein L35



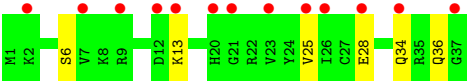
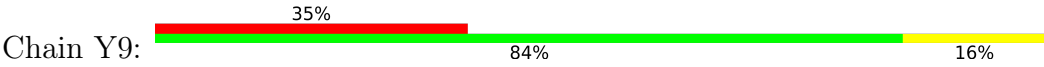
- Molecule 53: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L36



• Molecule 54: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.97Å 450.71Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 3.97 49.82 – 3.97	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.82-3.97) 98.6 (49.82-3.97)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.228 , 0.255 0.228 , 0.254	Depositor DCC
R_{free} test set	21855 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	146.0	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	291782	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: ZN, SF4, MG

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	0.24	0/36098	0.34	0/56341
1	XA	0.24	0/36101	0.34	4/56346 (0.0%)
2	QB	0.46	0/1942	0.78	0/2619
2	XB	0.49	0/1950	0.82	2/2630 (0.1%)
3	QC	0.46	0/1629	0.80	0/2195
3	XC	0.46	0/1629	0.83	0/2195
4	QD	0.43	1/1733 (0.1%)	0.73	0/2318
4	XD	0.49	1/1733 (0.1%)	0.74	0/2318
5	QE	0.43	0/1171	0.74	0/1576
5	XE	0.45	0/1171	0.81	0/1576
6	QF	0.48	0/856	0.77	2/1154 (0.2%)
6	XF	0.41	0/856	0.73	0/1154
7	QG	0.48	0/1276	0.72	0/1709
7	XG	0.48	0/1276	0.81	1/1709 (0.1%)
8	QH	0.41	0/1128	0.66	1/1517 (0.1%)
8	XH	0.38	0/1128	0.66	0/1517
9	QI	0.48	0/1008	0.83	1/1354 (0.1%)
9	XI	0.46	0/1017	0.87	1/1365 (0.1%)
10	QJ	0.43	0/814	0.73	0/1095
10	XJ	0.43	0/790	0.74	0/1063
11	QK	0.35	0/900	0.55	0/1213
11	XK	0.42	0/879	0.70	0/1187
12	QL	0.43	0/991	0.79	0/1327
12	XL	0.39	0/972	0.78	0/1301
13	QM	0.50	0/965	0.85	0/1292
13	XM	0.51	0/956	1.00	2/1281 (0.2%)
14	QN	0.42	0/501	0.70	0/664
14	XN	0.51	0/501	0.81	0/664
15	QO	0.38	0/745	0.60	0/992
15	XO	0.43	0/740	0.71	0/987
16	QP	0.41	0/721	0.64	0/970
16	XP	0.43	0/721	0.75	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.32	0/847	0.59	0/1131
17	XQ	0.36	0/847	0.65	0/1131
18	QR	0.36	0/579	0.59	0/768
18	XR	0.41	0/579	0.66	0/768
19	QS	0.39	0/680	0.83	1/915 (0.1%)
19	XS	0.46	0/689	0.86	0/926
20	QT	0.38	0/765	0.63	0/1007
20	XT	0.58	0/765	0.87	0/1007
21	QU	0.39	0/221	0.68	0/288
21	XU	0.37	0/221	0.64	0/288
22	QV	0.20	0/1840	0.35	0/2866
22	XV	0.18	0/1840	0.33	0/2866
23	QX	0.19	0/470	0.48	1/733 (0.1%)
23	XX	0.17	0/470	0.32	0/733
24	RA	0.30	0/69521	0.37	5/108529 (0.0%)
24	YA	0.35	0/69543	0.38	2/108563 (0.0%)
25	RB	0.22	0/2878	0.32	0/4490
25	YB	0.30	0/2878	0.34	0/4490
26	RD	0.46	0/2165	0.75	6/2919 (0.2%)
26	YD	0.48	0/2165	0.74	5/2919 (0.2%)
27	RE	0.42	0/1601	0.85	2/2160 (0.1%)
27	YE	0.45	0/1601	0.79	1/2160 (0.0%)
28	RF	0.45	0/1620	0.72	0/2194
28	YF	0.51	0/1620	0.77	1/2194 (0.0%)
29	RG	0.45	0/1499	0.85	0/2016
29	YG	0.51	0/1499	0.88	3/2016 (0.1%)
30	RH	0.44	0/1362	0.89	2/1841 (0.1%)
30	YH	0.49	0/1362	0.88	5/1841 (0.3%)
31	RI	0.44	0/1151	0.89	0/1558
31	YI	0.48	0/1151	0.87	0/1558
32	RN	0.41	0/1131	0.75	3/1525 (0.2%)
32	YN	0.49	0/1131	0.82	3/1525 (0.2%)
33	RO	0.46	0/943	0.70	0/1269
33	YO	0.48	0/943	0.68	0/1269
34	RP	0.47	0/1162	0.86	0/1544
34	YP	0.46	0/1139	0.82	0/1514
35	RQ	0.42	0/1143	0.81	2/1527 (0.1%)
35	YQ	0.47	0/1143	0.87	2/1527 (0.1%)
36	RR	0.47	0/974	0.74	0/1302
36	YR	0.48	0/974	0.76	0/1302
37	RS	0.43	0/892	0.86	0/1187
37	YS	0.43	0/892	0.84	0/1187
38	RT	0.45	0/1155	0.82	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.49	0/1155	0.81	0/1542
39	RU	0.47	0/982	0.77	2/1306 (0.2%)
39	YU	0.55	0/982	0.79	0/1306
40	RV	0.44	0/790	0.80	1/1057 (0.1%)
40	YV	0.48	1/790 (0.1%)	0.78	0/1057
41	RW	0.51	0/911	0.78	0/1220
41	YW	0.49	0/911	0.74	0/1220
42	RX	0.37	0/739	0.66	0/993
42	YX	0.45	0/739	0.74	0/993
43	RY	0.37	0/831	0.62	0/1108
43	YY	0.38	0/831	0.63	0/1108
44	RZ	0.48	0/1493	0.93	4/2026 (0.2%)
44	YZ	0.44	0/1493	0.86	1/2026 (0.0%)
45	R0	0.35	0/652	0.56	0/867
45	Y0	0.39	0/601	0.58	0/801
46	R1	0.43	0/770	0.73	0/1022
46	Y1	0.47	0/736	0.83	2/978 (0.2%)
47	R2	0.52	0/583	0.79	0/771
47	Y2	0.49	0/583	0.81	0/771
48	R3	0.49	0/474	0.77	0/635
48	Y3	0.52	0/474	0.80	0/635
49	R4	0.39	0/578	0.91	0/776
49	Y4	0.50	0/578	0.92	0/776
50	R5	0.45	0/473	0.61	0/639
50	Y5	0.54	0/473	0.78	1/639 (0.2%)
51	R6	0.35	0/460	0.67	0/613
51	Y6	0.41	0/460	0.71	0/613
52	R7	0.47	0/417	0.73	0/550
52	Y7	0.51	0/426	0.78	0/561
53	R8	0.53	0/525	0.94	2/691 (0.3%)
53	Y8	0.59	0/525	0.91	0/691
54	R9	0.37	0/310	0.65	0/407
54	Y9	0.40	0/310	0.62	0/407
All	All	0.35	3/316004 (0.0%)	0.51	71/472499 (0.0%)

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
4	QD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	XL	0	1
27	YE	0	1
29	RG	0	1
29	YG	0	1
44	RZ	0	1
44	YZ	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	XD	61	LYS	CE-NZ	9.21	1.76	1.49
4	QD	13	ARG	CZ-NH1	7.05	1.42	1.32
40	YV	53	GLU	CA-CB	5.02	1.60	1.53

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	846	C	C2'-C3'-O3'	9.47	123.71	109.50
13	XM	66	LEU	CA-C-N	9.03	135.54	121.19
13	XM	66	LEU	C-N-CA	9.03	135.54	121.19
23	QX	21	G	C2'-C3'-O3'	8.53	126.49	113.70
50	Y5	60	VAL	CA-C-O	-8.47	95.59	121.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	33	MET	Peptide
29	RG	82	LEU	Peptide
44	RZ	52	SER	Peptide
12	XL	104	VAL	Peptide
27	YE	17	ASP	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	16276	509	0
1	XA	32249	0	16279	515	1
2	QB	1907	0	1958	29	0
2	XB	1915	0	1969	35	0
3	QC	1605	0	1668	40	0
3	XC	1605	0	1668	28	1
4	QD	1703	0	1763	38	0
4	XD	1703	0	1763	53	1
5	QE	1155	0	1213	22	0
5	XE	1155	0	1213	26	0
6	QF	843	0	857	17	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	28	0
7	XG	1257	0	1296	24	0
8	QH	1108	0	1165	30	0
8	XH	1108	0	1165	30	0
9	QI	989	0	1011	29	0
9	XI	998	0	1024	25	0
10	QJ	801	0	849	26	0
10	XJ	777	0	816	27	0
11	QK	885	0	904	23	1
11	XK	864	0	881	17	0
12	QL	975	0	1062	30	0
12	XL	956	0	1046	17	0
13	QM	955	0	1021	40	0
13	XM	946	0	1008	20	0
14	QN	492	0	528	16	0
14	XN	492	0	531	37	0
15	QO	734	0	771	14	0
15	XO	729	0	768	12	0
16	QP	705	0	725	10	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	18	0
18	QR	574	0	644	14	0
18	XR	574	0	644	12	0
19	QS	665	0	686	20	0
19	XS	674	0	699	16	0
20	QT	763	0	861	17	0
20	XT	763	0	861	21	0
21	QU	217	0	234	6	0
21	XU	217	0	234	8	0
22	QV	1647	0	832	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	XV	1647	0	832	19	0
23	QX	418	0	209	10	0
23	XX	418	0	209	9	0
24	RA	62071	0	31291	835	4
24	YA	62091	0	31297	822	0
25	RB	2573	0	1306	27	0
25	YB	2573	0	1306	26	0
26	RD	2115	0	2195	51	0
26	YD	2115	0	2195	52	0
27	RE	1568	0	1634	53	0
27	YE	1568	0	1634	41	0
28	RF	1585	0	1632	27	0
28	YF	1585	0	1632	22	0
29	RG	1474	0	1535	36	0
29	YG	1474	0	1535	45	0
30	RH	1336	0	1418	35	0
30	YH	1336	0	1418	22	1
31	RI	1136	0	1223	17	0
31	YI	1136	0	1223	11	0
32	RN	1104	0	1180	27	0
32	YN	1104	0	1180	24	0
33	RO	933	0	996	23	0
33	YO	933	0	996	18	0
34	RP	1145	0	1228	37	0
34	YP	1122	0	1206	31	0
35	RQ	1122	0	1179	30	0
35	YQ	1122	0	1179	30	0
36	RR	960	0	1021	20	0
36	YR	960	0	1021	12	0
37	RS	882	0	942	21	0
37	YS	882	0	943	20	0
38	RT	1141	0	1202	26	0
38	YT	1141	0	1202	25	0
39	RU	964	0	1022	22	0
39	YU	964	0	1022	26	0
40	RV	779	0	852	18	0
40	YV	779	0	852	15	1
41	RW	900	0	964	17	0
41	YW	900	0	964	9	0
42	RX	725	0	778	11	0
42	YX	725	0	778	10	0
43	RY	818	0	909	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	YY	818	0	909	18	1
44	RZ	1461	0	1493	32	0
44	YZ	1461	0	1493	25	0
45	R0	643	0	667	12	0
45	Y0	593	0	612	15	0
46	R1	763	0	848	13	0
46	Y1	729	0	802	11	0
47	R2	581	0	629	12	0
47	Y2	581	0	629	10	2
48	R3	469	0	518	7	0
48	Y3	469	0	518	10	0
49	R4	565	0	557	13	0
49	Y4	565	0	557	22	0
50	R5	459	0	476	14	0
50	Y5	459	0	477	13	1
51	R6	453	0	473	9	0
51	Y6	453	0	473	11	0
52	R7	409	0	454	4	0
52	Y7	418	0	467	7	0
53	R8	517	0	582	18	0
53	Y8	517	0	582	19	0
54	R9	307	0	335	8	0
54	Y9	307	0	335	5	0
55	QA	69	0	0	0	0
55	QE	1	0	0	0	0
55	QH	1	0	0	0	0
55	QV	1	0	0	0	0
55	R1	1	0	0	0	0
55	RA	381	0	0	0	0
55	RB	9	0	0	0	0
55	RD	1	0	0	0	0
55	RE	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	67	0	0	0	0
55	XE	1	0	0	0	0
55	Y0	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	2	0	0	0	0
55	YA	454	0	0	0	0
55	YB	8	0	0	0	0
55	YD	2	0	0	0	0
55	YE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	YP	1	0	0	0	0
55	YQ	2	0	0	0	0
55	YR	2	0	0	0	0
56	QD	8	0	0	1	0
56	XD	8	0	0	3	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291782	0	197805	4256	7

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 9.

The worst 5 of 4256 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:YN:24:CYS:SG	14:YN:40:CYS:HB2	1.54	1.47
4:XD:61:LYS:NZ	4:XD:61:LYS:CE	1.77	1.47
14:YN:29:ARG:HD2	14:YN:40:CYS:SG	1.67	1.33
14:YN:24:CYS:SG	14:YN:40:CYS:CB	2.36	1.14
14:YN:29:ARG:CD	14:YN:40:CYS:SG	2.36	1.13

The worst 5 of 7 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)
40:YV:53:GLU:CB	50:Y5:59:GLU:OE1[4_445]	1.95	0.25
11:QK:99:GLN:OE1	3:XC:79:ARG:CD[4_555]	2.01	0.19
24:RA:2137:C:OP1	1:XA:999:U:O2'[4_555]	2.05	0.15
30:YH:46:GLU:OE2	43:YY:23:ARG:NH1[4_445]	2.08	0.12
24:RA:306:U:O3'	47:Y2:17:SER:OG[3_555]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	204 (88%)	27 (12%)	2 (1%)	14	48
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	189 (93%)	13 (6%)	1 (0%)	24	60
3	XC	203/239 (85%)	184 (91%)	18 (9%)	1 (0%)	24	60
4	QD	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
4	XD	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	QE	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	18	54
5	XE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	123/128 (96%)	113 (92%)	9 (7%)	1 (1%)	16	51
9	XI	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
10	QJ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	110 (96%)	4 (4%)	0	100	100
12	QL	123/132 (93%)	111 (90%)	11 (9%)	1 (1%)	16	51
12	XL	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	16	51
13	QM	118/126 (94%)	102 (86%)	15 (13%)	1 (1%)	16	51
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	14	48
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	36
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	82/93 (88%)	68 (83%)	14 (17%)	0	100	100
20	QT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	6 (6%)	1 (1%)	12	45
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	245 (91%)	23 (8%)	2 (1%)	18	54
26	YD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	18	54
27	RE	203/206 (98%)	170 (84%)	31 (15%)	2 (1%)	12	45
27	YE	203/206 (98%)	166 (82%)	35 (17%)	2 (1%)	12	45
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	11	44
29	YG	179/182 (98%)	150 (84%)	27 (15%)	2 (1%)	11	44
30	RH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	3	27
30	YH	172/180 (96%)	150 (87%)	18 (10%)	4 (2%)	5	31
31	RI	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	5	32
31	YI	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	5	32
32	RN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	18	54
32	YN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
33	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	RP	148/150 (99%)	120 (81%)	26 (18%)	2 (1%)	9	39
34	YP	145/150 (97%)	119 (82%)	25 (17%)	1 (1%)	18	54
35	RQ	139/141 (99%)	119 (86%)	19 (14%)	1 (1%)	18	54
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	18	54
36	RR	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	7	36
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	48
37	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	14	48
37	YS	109/112 (97%)	92 (84%)	17 (16%)	0	100	100
38	RT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	8	38
38	YT	135/146 (92%)	114 (84%)	19 (14%)	2 (2%)	8	38
39	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	48
39	YU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	48
40	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	45
40	YV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	12	45
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	48
41	YW	111/113 (98%)	101 (91%)	9 (8%)	1 (1%)	14	48
42	RX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
42	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
43	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	RZ	181/206 (88%)	146 (81%)	32 (18%)	3 (2%)	7	36
44	YZ	181/206 (88%)	149 (82%)	29 (16%)	3 (2%)	7	36
45	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
45	Y0	72/85 (85%)	69 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
47	R2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	8	38
47	Y2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	8	38
48	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	38
50	R5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	Y5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	48 (77%)	11 (18%)	3 (5%)	2	19
53	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	25
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11449/12128 (94%)	10319 (90%)	1055 (9%)	75 (1%)	18	54

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
53	R8	30	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	81	82
2	XB	204/220 (93%)	202 (99%)	2 (1%)	68	76
3	QC	159/188 (85%)	156 (98%)	3 (2%)	50	67
3	XC	159/188 (85%)	158 (99%)	1 (1%)	78	81
4	QD	180/181 (99%)	178 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	176 (98%)	4 (2%)	45	64
5	QE	116/123 (94%)	114 (98%)	2 (2%)	53	68
5	XE	116/123 (94%)	114 (98%)	2 (2%)	53	68
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	125 (99%)	1 (1%)	73	77
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	73	77
8	XH	118/119 (99%)	116 (98%)	2 (2%)	53	68
9	QI	96/99 (97%)	95 (99%)	1 (1%)	68	76
9	XI	97/99 (98%)	96 (99%)	1 (1%)	68	76
10	QJ	89/92 (97%)	87 (98%)	2 (2%)	45	64
10	XJ	86/92 (94%)	84 (98%)	2 (2%)	44	64
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	86 (98%)	2 (2%)	44	64
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	76
12	XL	103/109 (94%)	101 (98%)	2 (2%)	50	67
13	QM	96/101 (95%)	91 (95%)	5 (5%)	21	44
13	XM	95/101 (94%)	93 (98%)	2 (2%)	47	65
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	59	71
19	XS	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	75 (99%)	1 (1%)	61	72
20	XT	76/82 (93%)	75 (99%)	1 (1%)	61	72
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	213 (100%)	1 (0%)	81	82
26	YD	214/218 (98%)	212 (99%)	2 (1%)	70	76
27	RE	165/166 (99%)	162 (98%)	3 (2%)	51	67
27	YE	165/166 (99%)	164 (99%)	1 (1%)	78	81
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	153 (99%)	2 (1%)	61	72
29	YG	155/156 (99%)	153 (99%)	2 (1%)	61	72
30	RH	145/148 (98%)	144 (99%)	1 (1%)	76	79
30	YH	145/148 (98%)	143 (99%)	2 (1%)	59	71
31	RI	122/124 (98%)	121 (99%)	1 (1%)	73	77
31	YI	122/124 (98%)	122 (100%)	0	100	100
32	RN	117/119 (98%)	116 (99%)	1 (1%)	70	76
32	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	115 (99%)	1 (1%)	70	76
34	YP	114/116 (98%)	113 (99%)	1 (1%)	70	76
35	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	76
35	YQ	111/111 (100%)	110 (99%)	1 (1%)	70	76
36	RR	100/101 (99%)	100 (100%)	0	100	100
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	86 (99%)	1 (1%)	65	74
37	YS	87/88 (99%)	86 (99%)	1 (1%)	65	74
38	RT	120/127 (94%)	120 (100%)	0	100	100
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	YU	93/94 (99%)	92 (99%)	1 (1%)	65	74
40	RV	82/82 (100%)	79 (96%)	3 (4%)	30	52
40	YV	82/82 (100%)	79 (96%)	3 (4%)	30	52
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	90 (98%)	2 (2%)	45	64
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	74 (100%)	0	100	100
43	RY	88/91 (97%)	87 (99%)	1 (1%)	65	74
43	YY	88/91 (97%)	87 (99%)	1 (1%)	65	74
44	RZ	162/179 (90%)	160 (99%)	2 (1%)	63	73
44	YZ	162/179 (90%)	159 (98%)	3 (2%)	50	67
45	R0	65/67 (97%)	65 (100%)	0	100	100
45	Y0	60/67 (90%)	60 (100%)	0	100	100
46	R1	82/83 (99%)	81 (99%)	1 (1%)	63	73
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	61 (95%)	3 (5%)	23	46
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	48	66
48	Y3	51/52 (98%)	45 (88%)	6 (12%)	5	21
49	R4	62/63 (98%)	61 (98%)	1 (2%)	55	70
49	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	70
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	49 (96%)	2 (4%)	28	50
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	53 (98%)	1 (2%)	50	67
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	50	67
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9684/10066 (96%)	9585 (99%)	99 (1%)	68 76

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	XH	135	CYS
29	YG	28	VAL
10	XJ	5	ARG
13	XM	25	ILE
32	YN	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
48	R3	46	ASN
44	YZ	55	HIS
11	XK	104	GLN
43	YY	6	HIS
36	YR	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	271 (18%)	37 (2%)
1	XA	1498/1521 (98%)	254 (16%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	2 (11%)
23	XX	18/19 (94%)	5 (27%)	1 (5%)
24	RA	2879/2915 (98%)	571 (19%)	41 (1%)
24	YA	2880/2915 (98%)	576 (20%)	42 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9182/9308 (98%)	1753 (19%)	157 (1%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G

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

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	221	A
24	YA	1786	A
24	YA	278	A
24	YA	1022	G
24	YA	2681	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1022 ligands modelled in this entry, 1020 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	SF4	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	XD	301	4	-	-	0/6/5/5
56	SF4	QD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	XD	301	SF4	3	0
56	QD	301	SF4	1	0

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	1500/1521 (98%)	0.54	136 (9%)	15 16	137, 186, 345, 447	0
1	XA	1500/1521 (98%)	0.60	153 (10%)	12 14	117, 197, 361, 445	0
2	QB	235/256 (91%)	0.49	22 (9%)	14 16	188, 240, 277, 304	0
2	XB	236/256 (92%)	0.72	29 (12%)	8 11	172, 220, 264, 298	0
3	QC	205/239 (85%)	0.50	21 (10%)	12 14	194, 242, 289, 326	0
3	XC	205/239 (85%)	0.62	27 (13%)	7 10	193, 236, 276, 320	0
4	QD	208/209 (99%)	0.81	31 (14%)	5 9	153, 198, 243, 285	0
4	XD	208/209 (99%)	0.97	37 (17%)	4 6	154, 210, 252, 301	0
5	QE	151/162 (93%)	0.53	18 (11%)	9 12	148, 189, 227, 263	0
5	XE	151/162 (93%)	0.57	16 (10%)	11 13	138, 185, 222, 236	0
6	QF	101/101 (100%)	0.34	4 (3%)	42 32	154, 207, 240, 273	0
6	XF	101/101 (100%)	0.18	2 (1%)	65 47	135, 182, 221, 259	0
7	QG	155/156 (99%)	0.68	22 (14%)	6 10	221, 278, 318, 347	0
7	XG	155/156 (99%)	0.60	14 (9%)	15 17	224, 287, 321, 327	0
8	QH	137/138 (99%)	0.98	25 (18%)	3 6	140, 202, 237, 277	0
8	XH	137/138 (99%)	0.84	21 (15%)	5 9	138, 188, 215, 237	0
9	QI	125/128 (97%)	0.87	13 (10%)	11 14	195, 286, 320, 335	0
9	XI	126/128 (98%)	1.09	22 (17%)	4 7	178, 278, 313, 331	0
10	QJ	99/105 (94%)	1.15	19 (19%)	3 6	245, 289, 331, 345	0
10	XJ	96/105 (91%)	1.20	22 (22%)	2 4	232, 305, 333, 366	0
11	QK	119/129 (92%)	0.33	9 (7%)	20 19	154, 194, 237, 273	0
11	XK	116/129 (89%)	0.32	11 (9%)	14 16	136, 181, 225, 263	0
12	QL	125/132 (94%)	1.22	29 (23%)	2 4	127, 164, 202, 247	0
12	XL	122/132 (92%)	1.26	29 (23%)	2 4	128, 163, 193, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.88	19 (15%)	5 8	201, 278, 316, 331	0
13	XM	119/126 (94%)	0.92	21 (17%)	4 7	240, 283, 320, 334	0
14	QN	60/61 (98%)	1.42	18 (30%)	1 3	220, 278, 326, 416	0
14	XN	60/61 (98%)	1.42	15 (25%)	2 4	209, 257, 285, 312	0
15	QO	88/89 (98%)	0.44	3 (3%)	48 35	138, 176, 219, 244	0
15	XO	87/89 (97%)	0.57	10 (11%)	9 12	121, 153, 189, 199	0
16	QP	84/88 (95%)	1.06	15 (17%)	3 6	145, 181, 219, 253	0
16	XP	84/88 (95%)	0.66	6 (7%)	22 20	158, 210, 249, 274	0
17	QQ	100/105 (95%)	0.99	19 (19%)	3 6	150, 182, 211, 227	0
17	XQ	100/105 (95%)	0.88	18 (18%)	3 6	131, 172, 202, 217	0
18	QR	70/88 (79%)	0.26	1 (1%)	73 54	153, 194, 228, 256	0
18	XR	70/88 (79%)	0.17	2 (2%)	53 39	127, 174, 210, 219	0
19	QS	83/93 (89%)	0.75	11 (13%)	7 10	243, 277, 311, 325	0
19	XS	84/93 (90%)	1.69	27 (32%)	1 2	254, 296, 317, 341	0
20	QT	99/106 (93%)	1.05	20 (20%)	3 5	126, 172, 215, 233	0
20	XT	99/106 (93%)	1.30	24 (24%)	2 4	127, 187, 233, 247	0
21	QU	25/27 (92%)	2.64	16 (64%)	0 1	199, 233, 270, 291	0
21	XU	25/27 (92%)	2.43	13 (52%)	0 1	209, 260, 273, 282	0
22	QV	77/77 (100%)	0.68	9 (11%)	9 12	262, 300, 338, 374	0
22	XV	77/77 (100%)	1.49	21 (27%)	1 3	409, 455, 519, 559	0
23	QX	19/19 (100%)	3.49	15 (78%)	0 0	235, 378, 498, 513	0
23	XX	19/19 (100%)	3.93	16 (84%)	0 0	230, 374, 393, 395	0
24	RA	2882/2915 (98%)	0.46	218 (7%)	20 19	89, 142, 314, 708	0
24	YA	2883/2915 (98%)	0.36	161 (5%)	30 25	74, 113, 236, 618	0
25	RB	120/122 (98%)	0.59	8 (6%)	24 21	154, 216, 251, 291	0
25	YB	120/122 (98%)	0.03	3 (2%)	58 43	104, 144, 169, 199	0
26	RD	272/276 (98%)	1.01	52 (19%)	3 6	98, 133, 165, 247	0
26	YD	272/276 (98%)	1.07	52 (19%)	3 6	91, 116, 153, 250	0
27	RE	205/206 (99%)	0.91	31 (15%)	5 9	108, 140, 187, 247	0
27	YE	205/206 (99%)	0.89	34 (16%)	4 7	84, 121, 175, 255	0
28	RF	202/210 (96%)	0.73	22 (10%)	10 13	102, 153, 211, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YF	202/210 (96%)	0.79	27 (13%) 7 10	81, 116, 177, 234	0
29	RG	181/182 (99%)	0.41	18 (9%) 13 15	196, 238, 298, 344	0
29	YG	181/182 (99%)	0.31	8 (4%) 39 30	119, 184, 248, 289	0
30	RH	174/180 (96%)	0.74	20 (11%) 9 12	135, 199, 259, 279	0
30	YH	174/180 (96%)	0.70	16 (9%) 14 16	96, 134, 170, 242	0
31	RI	146/148 (98%)	0.56	16 (10%) 10 13	134, 185, 237, 288	0
31	YI	146/148 (98%)	0.34	8 (5%) 30 25	118, 166, 209, 237	0
32	RN	138/140 (98%)	0.70	10 (7%) 21 20	116, 150, 203, 229	0
32	YN	138/140 (98%)	0.78	14 (10%) 12 14	75, 114, 168, 237	0
33	RO	122/122 (100%)	0.97	22 (18%) 3 6	94, 131, 169, 188	0
33	YO	122/122 (100%)	0.52	6 (4%) 35 28	87, 120, 153, 174	0
34	RP	150/150 (100%)	1.12	36 (24%) 2 4	121, 167, 211, 286	0
34	YP	147/150 (98%)	1.04	31 (21%) 2 4	96, 127, 174, 210	0
35	RQ	141/141 (100%)	0.83	16 (11%) 10 13	130, 169, 211, 249	0
35	YQ	141/141 (100%)	0.96	21 (14%) 5 9	85, 123, 166, 223	0
36	RR	117/118 (99%)	1.03	17 (14%) 6 9	98, 129, 161, 235	0
36	YR	117/118 (99%)	1.09	20 (17%) 4 7	87, 118, 148, 228	0
37	RS	111/112 (99%)	0.82	18 (16%) 4 8	150, 193, 242, 278	0
37	YS	111/112 (99%)	0.56	12 (10%) 11 13	112, 140, 190, 256	0
38	RT	137/146 (93%)	0.70	13 (9%) 14 16	99, 149, 254, 273	0
38	YT	137/146 (93%)	0.87	20 (14%) 6 9	102, 138, 218, 266	0
39	RU	117/118 (99%)	0.97	18 (15%) 5 9	116, 168, 234, 258	0
39	YU	117/118 (99%)	0.79	12 (10%) 12 14	79, 111, 154, 215	0
40	RV	101/101 (100%)	0.46	10 (9%) 13 15	98, 168, 212, 271	0
40	YV	101/101 (100%)	0.58	13 (12%) 7 11	87, 124, 184, 238	0
41	RW	113/113 (100%)	0.86	17 (15%) 5 9	85, 118, 180, 289	0
41	YW	113/113 (100%)	0.62	7 (6%) 26 23	77, 104, 152, 234	0
42	RX	92/96 (95%)	1.21	17 (18%) 3 6	100, 135, 177, 192	0
42	YX	92/96 (95%)	0.99	17 (18%) 3 6	82, 113, 152, 191	0
43	RY	107/110 (97%)	0.84	20 (18%) 3 6	119, 171, 209, 244	0
43	YY	107/110 (97%)	0.87	16 (14%) 5 9	101, 137, 174, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RZ	183/206 (88%)	0.42	13 (7%) 22 20	161, 212, 259, 303	0
44	YZ	183/206 (88%)	0.52	16 (8%) 16 17	108, 159, 204, 245	0
45	R0	81/85 (95%)	1.04	15 (18%) 3 6	129, 163, 226, 282	0
45	Y0	74/85 (87%)	0.89	14 (18%) 3 6	99, 127, 151, 160	0
46	R1	97/98 (98%)	1.42	22 (22%) 2 4	110, 146, 196, 237	0
46	Y1	93/98 (94%)	1.34	24 (25%) 1 4	92, 125, 173, 197	0
47	R2	69/72 (95%)	0.77	9 (13%) 7 11	110, 165, 216, 285	0
47	Y2	69/72 (95%)	1.06	9 (13%) 7 11	86, 117, 158, 186	0
48	R3	59/60 (98%)	0.82	6 (10%) 12 14	115, 165, 223, 268	0
48	Y3	59/60 (98%)	0.96	8 (13%) 7 10	81, 117, 176, 229	0
49	R4	69/71 (97%)	0.29	0 100 100	206, 267, 328, 379	0
49	Y4	69/71 (97%)	0.17	4 (5%) 29 25	166, 262, 333, 360	0
50	R5	59/60 (98%)	0.43	4 (6%) 23 21	100, 131, 216, 233	0
50	Y5	59/60 (98%)	0.42	2 (3%) 48 35	84, 110, 198, 255	0
51	R6	53/54 (98%)	0.25	1 (1%) 66 48	142, 172, 214, 247	0
51	Y6	53/54 (98%)	0.54	5 (9%) 14 16	111, 144, 183, 190	0
52	R7	47/49 (95%)	0.96	9 (19%) 3 6	98, 122, 145, 169	0
52	Y7	48/49 (97%)	0.83	6 (12%) 8 11	76, 100, 150, 179	0
53	R8	64/65 (98%)	1.49	17 (26%) 1 4	115, 151, 201, 266	0
53	Y8	64/65 (98%)	1.48	19 (29%) 1 3	90, 117, 147, 238	0
54	R9	37/37 (100%)	1.62	11 (29%) 1 3	161, 200, 292, 294	0
54	Y9	37/37 (100%)	1.54	13 (35%) 1 2	132, 153, 189, 210	0
All	All	20842/21436 (97%)	0.66	2375 (11%) 10 13	74, 162, 306, 708	0

The worst 5 of 2375 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	QJ	58	ASP	12.8
26	YD	34	VAL	12.0
11	QK	127	LYS	10.4
24	RA	1093	G	10.1
24	RA	1092	C	9.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
55	MG	YA	3419	1/1	-0.04	0.27	90,90,90,90	0
55	MG	RD	301	1/1	0.01	0.31	89,89,89,89	0
55	MG	QA	1607	1/1	0.01	0.16	116,116,116,116	0
55	MG	YA	3236	1/1	0.07	0.30	73,73,73,73	0
55	MG	RA	3284	1/1	0.09	0.35	73,73,73,73	0
55	MG	QA	1626	1/1	0.13	0.18	88,88,88,88	0
55	MG	RA	3057	1/1	0.13	0.33	54,54,54,54	0
55	MG	RA	3316	1/1	0.15	0.29	69,69,69,69	0
55	MG	RA	3182	1/1	0.15	0.26	80,80,80,80	0
55	MG	YA	3014	1/1	0.17	0.24	82,82,82,82	0
55	MG	RA	3229	1/1	0.17	0.18	114,114,114,114	0
55	MG	RA	3228	1/1	0.17	0.26	81,81,81,81	0
55	MG	RA	3141	1/1	0.18	0.21	111,111,111,111	0
55	MG	YA	3438	1/1	0.19	0.38	95,95,95,95	0
55	MG	RA	3254	1/1	0.20	0.20	94,94,94,94	0
55	MG	RA	3211	1/1	0.21	0.34	83,83,83,83	0
55	MG	RA	3227	1/1	0.21	0.19	101,101,101,101	0
55	MG	YA	3290	1/1	0.21	0.35	91,91,91,91	0
55	MG	YA	3408	1/1	0.21	0.29	75,75,75,75	0
55	MG	XA	1653	1/1	0.21	0.16	86,86,86,86	0
55	MG	XA	1654	1/1	0.21	0.28	114,114,114,114	0
55	MG	YA	3410	1/1	0.22	0.20	82,82,82,82	0
55	MG	YA	3257	1/1	0.23	0.55	94,94,94,94	0
55	MG	YA	3183	1/1	0.23	0.37	95,95,95,95	0
55	MG	RA	3234	1/1	0.24	0.32	74,74,74,74	0
55	MG	YA	3233	1/1	0.27	0.27	85,85,85,85	0
55	MG	QA	1645	1/1	0.27	0.22	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3182	1/1	0.28	0.25	76,76,76,76	0
55	MG	XA	1643	1/1	0.28	0.19	102,102,102,102	0
55	MG	YA	3205	1/1	0.29	0.25	70,70,70,70	0
55	MG	YA	3360	1/1	0.29	0.10	78,78,78,78	0
55	MG	RA	3285	1/1	0.29	0.23	79,79,79,79	0
55	MG	RA	3380	1/1	0.30	0.21	57,57,57,57	0
55	MG	YA	3309	1/1	0.31	0.36	87,87,87,87	0
55	MG	RA	3349	1/1	0.31	0.45	93,93,93,93	0
55	MG	RA	3344	1/1	0.31	0.28	86,86,86,86	0
55	MG	YA	3341	1/1	0.32	0.25	90,90,90,90	0
55	MG	YA	3301	1/1	0.32	0.27	70,70,70,70	0
55	MG	RA	3268	1/1	0.33	0.19	93,93,93,93	0
55	MG	RA	3222	1/1	0.33	0.41	68,68,68,68	0
55	MG	RA	3264	1/1	0.33	0.21	79,79,79,79	0
55	MG	YD	302	1/1	0.33	0.40	99,99,99,99	0
55	MG	RA	3363	1/1	0.34	0.33	87,87,87,87	0
55	MG	YA	3170	1/1	0.34	0.20	104,104,104,104	0
55	MG	RA	3001	1/1	0.34	0.16	82,82,82,82	0
55	MG	YA	3367	1/1	0.35	0.17	72,72,72,72	0
55	MG	YA	3449	1/1	0.35	0.28	47,47,47,47	0
55	MG	RA	3249	1/1	0.35	0.49	102,102,102,102	0
55	MG	XA	1659	1/1	0.36	0.16	70,70,70,70	0
55	MG	YA	3424	1/1	0.37	0.47	88,88,88,88	0
55	MG	RA	3356	1/1	0.37	0.13	62,62,62,62	0
55	MG	RA	3325	1/1	0.38	0.31	105,105,105,105	0
55	MG	QA	1661	1/1	0.39	0.29	74,74,74,74	0
55	MG	RA	3327	1/1	0.39	0.40	87,87,87,87	0
55	MG	RA	3251	1/1	0.39	0.57	84,84,84,84	0
55	MG	XA	1646	1/1	0.39	0.33	82,82,82,82	0
55	MG	RA	3330	1/1	0.40	0.18	70,70,70,70	0
55	MG	YA	3218	1/1	0.40	0.30	82,82,82,82	0
55	MG	YA	3169	1/1	0.40	0.19	79,79,79,79	0
55	MG	RA	3006	1/1	0.40	0.54	103,103,103,103	0
55	MG	RA	3062	1/1	0.40	0.38	72,72,72,72	0
55	MG	YA	3001	1/1	0.40	0.29	82,82,82,82	0
55	MG	RA	3308	1/1	0.41	0.33	73,73,73,73	0
55	MG	QA	1635	1/1	0.41	0.49	93,93,93,93	0
55	MG	YA	3409	1/1	0.41	0.54	88,88,88,88	0
55	MG	YA	3011	1/1	0.42	0.50	71,71,71,71	0
55	MG	YA	3407	1/1	0.42	0.18	62,62,62,62	0
55	MG	RB	207	1/1	0.42	0.23	80,80,80,80	0
55	MG	RA	3292	1/1	0.42	0.28	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3297	1/1	0.42	0.58	88,88,88,88	0
55	MG	RA	3245	1/1	0.43	0.24	82,82,82,82	0
55	MG	XA	1603	1/1	0.43	0.18	70,70,70,70	0
55	MG	RA	3376	1/1	0.43	0.24	47,47,47,47	0
55	MG	RA	3248	1/1	0.43	0.15	91,91,91,91	0
55	MG	QE	201	1/1	0.43	0.31	85,85,85,85	0
55	MG	YB	207	1/1	0.44	0.21	76,76,76,76	0
55	MG	YA	3357	1/1	0.44	0.33	76,76,76,76	0
55	MG	RA	3331	1/1	0.45	0.15	101,101,101,101	0
55	MG	YA	3368	1/1	0.45	0.24	53,53,53,53	0
55	MG	RA	3279	1/1	0.45	0.23	85,85,85,85	0
55	MG	RE	301	1/1	0.46	0.37	84,84,84,84	0
55	MG	RA	3203	1/1	0.46	0.33	105,105,105,105	0
55	MG	YA	3335	1/1	0.46	0.30	82,82,82,82	0
55	MG	RA	3193	1/1	0.46	0.15	84,84,84,84	0
55	MG	YA	3405	1/1	0.46	0.23	86,86,86,86	0
55	MG	RA	3109	1/1	0.47	0.15	85,85,85,85	0
55	MG	RA	3213	1/1	0.47	0.27	94,94,94,94	0
55	MG	RA	3204	1/1	0.47	0.34	113,113,113,113	0
55	MG	RA	3209	1/1	0.47	0.38	83,83,83,83	0
55	MG	QA	1621	1/1	0.48	0.13	87,87,87,87	0
55	MG	YA	3002	1/1	0.49	0.17	87,87,87,87	0
55	MG	YA	3416	1/1	0.49	0.27	80,80,80,80	0
55	MG	RA	3165	1/1	0.49	0.37	74,74,74,74	0
55	MG	YA	3324	1/1	0.49	0.20	90,90,90,90	0
55	MG	RA	3225	1/1	0.49	0.39	59,59,59,59	0
55	MG	YA	3057	1/1	0.49	0.28	51,51,51,51	0
55	MG	YA	3344	1/1	0.49	0.22	88,88,88,88	0
55	MG	RA	3240	1/1	0.49	0.36	58,58,58,58	0
55	MG	RA	3206	1/1	0.50	0.34	93,93,93,93	0
55	MG	RB	209	1/1	0.50	0.22	105,105,105,105	0
55	MG	YA	3039	1/1	0.50	0.34	15,15,15,15	0
55	MG	RA	3256	1/1	0.50	0.14	69,69,69,69	0
55	MG	YA	3440	1/1	0.50	0.43	68,68,68,68	0
55	MG	YA	3211	1/1	0.50	0.44	78,78,78,78	0
55	MG	RA	3295	1/1	0.50	0.29	97,97,97,97	0
55	MG	YA	3307	1/1	0.50	0.25	87,87,87,87	0
55	MG	QA	1659	1/1	0.51	0.30	72,72,72,72	0
55	MG	YA	3187	1/1	0.51	0.34	94,94,94,94	0
55	MG	RA	3134	1/1	0.51	0.29	62,62,62,62	0
55	MG	QH	201	1/1	0.51	0.30	84,84,84,84	0
55	MG	RA	3210	1/1	0.51	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3255	1/1	0.51	0.36	90,90,90,90	0
55	MG	RA	3197	1/1	0.51	0.26	59,59,59,59	0
55	MG	YA	3253	1/1	0.51	0.29	59,59,59,59	0
55	MG	RA	3199	1/1	0.51	0.31	89,89,89,89	0
55	MG	YA	3263	1/1	0.51	0.28	79,79,79,79	0
55	MG	RA	3265	1/1	0.51	0.25	93,93,93,93	0
55	MG	RA	3150	1/1	0.51	0.14	106,106,106,106	0
55	MG	YA	3282	1/1	0.52	0.29	75,75,75,75	0
55	MG	YA	3164	1/1	0.52	0.22	52,52,52,52	0
55	MG	YA	3397	1/1	0.52	0.30	78,78,78,78	0
55	MG	RA	3381	1/1	0.52	0.22	80,80,80,80	0
55	MG	RA	3370	1/1	0.53	0.13	69,69,69,69	0
55	MG	QA	1640	1/1	0.53	0.23	92,92,92,92	0
55	MG	YA	3189	1/1	0.53	0.23	81,81,81,81	0
55	MG	RA	3171	1/1	0.53	0.17	79,79,79,79	0
55	MG	RA	3063	1/1	0.53	0.18	71,71,71,71	0
55	MG	YA	3215	1/1	0.53	0.25	67,67,67,67	0
55	MG	YA	3264	1/1	0.53	0.69	82,82,82,82	0
55	MG	YA	3426	1/1	0.54	0.23	85,85,85,85	0
55	MG	YA	3198	1/1	0.54	0.23	64,64,64,64	0
55	MG	RA	3030	1/1	0.54	0.17	72,72,72,72	0
55	MG	RA	3198	1/1	0.54	0.22	69,69,69,69	0
55	MG	YA	3361	1/1	0.54	0.20	84,84,84,84	0
55	MG	RA	3246	1/1	0.54	0.19	98,98,98,98	0
55	MG	YA	3199	1/1	0.55	0.24	78,78,78,78	0
55	MG	RA	3205	1/1	0.55	0.27	66,66,66,66	0
55	MG	RA	3366	1/1	0.55	0.26	90,90,90,90	0
55	MG	YA	3238	1/1	0.55	0.43	83,83,83,83	0
55	MG	YA	3412	1/1	0.55	0.11	91,91,91,91	0
55	MG	RA	3252	1/1	0.55	0.50	85,85,85,85	0
55	MG	YA	3406	1/1	0.55	0.39	78,78,78,78	0
55	MG	YA	3062	1/1	0.56	0.49	72,72,72,72	0
55	MG	YA	3421	1/1	0.56	0.23	89,89,89,89	0
55	MG	YA	3259	1/1	0.56	0.21	61,61,61,61	0
55	MG	RA	3247	1/1	0.57	0.32	78,78,78,78	0
55	MG	RA	3191	1/1	0.57	0.31	39,39,39,39	0
55	MG	RA	3081	1/1	0.57	0.23	95,95,95,95	0
55	MG	XA	1605	1/1	0.57	0.26	74,74,74,74	0
55	MG	YA	3214	1/1	0.57	0.14	60,60,60,60	0
55	MG	XA	1608	1/1	0.57	0.21	93,93,93,93	0
55	MG	YA	3272	1/1	0.57	0.14	91,91,91,91	0
55	MG	YA	3443	1/1	0.57	0.22	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3201	1/1	0.57	0.32	60,60,60,60	0
55	MG	RA	3289	1/1	0.57	0.20	114,114,114,114	0
55	MG	QA	1612	1/1	0.57	0.23	113,113,113,113	0
55	MG	RA	3111	1/1	0.58	0.12	82,82,82,82	0
55	MG	YA	3273	1/1	0.58	0.23	56,56,56,56	0
55	MG	RB	201	1/1	0.58	0.40	86,86,86,86	0
55	MG	YA	3347	1/1	0.58	0.25	74,74,74,74	0
55	MG	XA	1607	1/1	0.58	0.40	67,67,67,67	0
55	MG	RA	3219	1/1	0.58	0.18	83,83,83,83	0
55	MG	YA	3009	1/1	0.58	0.32	73,73,73,73	0
55	MG	RA	3324	1/1	0.58	0.26	82,82,82,82	0
55	MG	RA	3119	1/1	0.58	0.18	73,73,73,73	0
55	MG	YA	3384	1/1	0.58	0.18	69,69,69,69	0
55	MG	YA	3310	1/1	0.58	0.20	63,63,63,63	0
55	MG	YA	3401	1/1	0.58	0.22	72,72,72,72	0
55	MG	YA	3315	1/1	0.58	0.23	100,100,100,100	0
55	MG	YA	3318	1/1	0.58	0.30	51,51,51,51	0
55	MG	QA	1660	1/1	0.58	0.29	84,84,84,84	0
55	MG	RB	205	1/1	0.59	0.34	83,83,83,83	0
55	MG	RA	3359	1/1	0.59	0.57	97,97,97,97	0
55	MG	YA	3291	1/1	0.59	0.30	50,50,50,50	0
55	MG	RA	3215	1/1	0.59	0.12	66,66,66,66	0
55	MG	RA	3351	1/1	0.59	0.21	68,68,68,68	0
55	MG	YA	3442	1/1	0.59	0.25	101,101,101,101	0
55	MG	YA	3305	1/1	0.59	0.28	74,74,74,74	0
55	MG	YA	3389	1/1	0.59	0.34	77,77,77,77	0
55	MG	YB	206	1/1	0.59	0.17	105,105,105,105	0
55	MG	XA	1633	1/1	0.59	0.24	65,65,65,65	0
55	MG	RA	3008	1/1	0.59	0.21	34,34,34,34	0
55	MG	YA	3147	1/1	0.60	0.13	89,89,89,89	0
55	MG	RA	3117	1/1	0.60	0.31	70,70,70,70	0
55	MG	RA	3297	1/1	0.60	0.50	100,100,100,100	0
55	MG	XA	1606	1/1	0.60	0.15	103,103,103,103	0
55	MG	RB	204	1/1	0.60	0.20	90,90,90,90	0
55	MG	RA	3026	1/1	0.60	0.35	58,58,58,58	0
55	MG	XA	1609	1/1	0.60	0.15	89,89,89,89	0
55	MG	YA	3239	1/1	0.60	0.29	62,62,62,62	0
55	MG	RA	3216	1/1	0.60	0.25	75,75,75,75	0
55	MG	RA	3003	1/1	0.60	0.34	69,69,69,69	0
55	MG	RA	3350	1/1	0.60	0.13	59,59,59,59	0
55	MG	RA	3269	1/1	0.60	0.12	83,83,83,83	0
55	MG	RA	3343	1/1	0.61	0.21	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3194	1/1	0.61	0.21	80,80,80,80	0
55	MG	YA	3319	1/1	0.61	0.41	64,64,64,64	0
55	MG	YA	3274	1/1	0.61	0.37	81,81,81,81	0
55	MG	YA	3326	1/1	0.61	0.41	64,64,64,64	0
55	MG	YA	3363	1/1	0.61	0.26	85,85,85,85	0
55	MG	YA	3136	1/1	0.61	0.36	73,73,73,73	0
55	MG	YA	3313	1/1	0.61	0.23	97,97,97,97	0
55	MG	RA	3212	1/1	0.62	0.23	36,36,36,36	0
55	MG	RA	3195	1/1	0.62	0.19	68,68,68,68	0
55	MG	RA	3273	1/1	0.62	0.22	85,85,85,85	0
55	MG	YA	3381	1/1	0.62	0.14	69,69,69,69	0
55	MG	QA	1613	1/1	0.62	0.20	104,104,104,104	0
55	MG	YA	3311	1/1	0.62	0.43	54,54,54,54	0
55	MG	YA	3260	1/1	0.62	0.22	76,76,76,76	0
55	MG	RA	3089	1/1	0.63	0.18	102,102,102,102	0
55	MG	RA	3333	1/1	0.63	0.24	51,51,51,51	0
55	MG	YA	3329	1/1	0.63	0.13	87,87,87,87	0
55	MG	YA	3331	1/1	0.63	0.29	58,58,58,58	0
55	MG	RA	3335	1/1	0.63	0.16	86,86,86,86	0
55	MG	RA	3367	1/1	0.63	0.32	91,91,91,91	0
55	MG	YA	3100	1/1	0.63	0.43	50,50,50,50	0
55	MG	YA	3188	1/1	0.63	0.26	71,71,71,71	0
55	MG	YA	3117	1/1	0.63	0.19	61,61,61,61	0
55	MG	YA	3280	1/1	0.63	0.47	82,82,82,82	0
55	MG	RA	3341	1/1	0.63	0.58	66,66,66,66	0
55	MG	RA	3007	1/1	0.63	0.34	86,86,86,86	0
55	MG	XA	1652	1/1	0.63	0.33	96,96,96,96	0
55	MG	XA	1660	1/1	0.64	0.24	71,71,71,71	0
55	MG	YA	3064	1/1	0.64	0.26	45,45,45,45	0
55	MG	YA	3222	1/1	0.64	0.34	47,47,47,47	0
55	MG	RA	3282	1/1	0.64	0.30	57,57,57,57	0
55	MG	RA	3339	1/1	0.64	0.34	84,84,84,84	0
55	MG	RA	3214	1/1	0.64	0.32	87,87,87,87	0
55	MG	YA	3144	1/1	0.64	0.14	66,66,66,66	0
55	MG	RA	3183	1/1	0.64	0.33	84,84,84,84	0
55	MG	RA	3278	1/1	0.64	0.24	89,89,89,89	0
55	MG	RA	3162	1/1	0.64	0.12	89,89,89,89	0
55	MG	XA	1610	1/1	0.64	0.21	56,56,56,56	0
55	MG	YA	3302	1/1	0.64	0.11	80,80,80,80	0
55	MG	YA	3079	1/1	0.65	0.31	51,51,51,51	0
55	MG	RA	3267	1/1	0.65	0.27	111,111,111,111	0
55	MG	XA	1630	1/1	0.65	0.10	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3225	1/1	0.65	0.37	25,25,25,25	0
55	MG	YA	3372	1/1	0.65	0.36	77,77,77,77	0
55	MG	YA	3262	1/1	0.65	0.15	74,74,74,74	0
55	MG	YA	3181	1/1	0.65	0.77	78,78,78,78	0
55	MG	YA	3453	1/1	0.65	0.22	59,59,59,59	0
55	MG	YB	204	1/1	0.65	0.18	26,26,26,26	0
55	MG	XA	1632	1/1	0.65	0.14	93,93,93,93	0
55	MG	QA	1647	1/1	0.65	0.24	107,107,107,107	0
55	MG	RA	3132	1/1	0.65	0.17	72,72,72,72	0
55	MG	RA	3352	1/1	0.66	0.28	24,24,24,24	0
55	MG	QA	1628	1/1	0.66	0.10	88,88,88,88	0
55	MG	RA	3085	1/1	0.66	0.23	49,49,49,49	0
55	MG	YA	3308	1/1	0.66	0.34	68,68,68,68	0
55	MG	RA	3345	1/1	0.66	0.22	88,88,88,88	0
55	MG	YA	3387	1/1	0.66	0.35	67,67,67,67	0
55	MG	RA	3326	1/1	0.66	0.14	72,72,72,72	0
55	MG	YA	3392	1/1	0.66	0.32	94,94,94,94	0
55	MG	YA	3342	1/1	0.66	0.23	73,73,73,73	0
55	MG	YA	3083	1/1	0.66	0.17	49,49,49,49	0
55	MG	YA	3312	1/1	0.66	0.58	92,92,92,92	0
55	MG	YA	3351	1/1	0.66	0.38	72,72,72,72	0
55	MG	RA	3224	1/1	0.66	0.18	89,89,89,89	0
55	MG	YA	3104	1/1	0.66	0.24	52,52,52,52	0
55	MG	QA	1664	1/1	0.66	0.26	102,102,102,102	0
55	MG	RA	3375	1/1	0.66	0.34	74,74,74,74	0
55	MG	XA	1656	1/1	0.67	0.17	89,89,89,89	0
55	MG	YA	3194	1/1	0.67	0.22	85,85,85,85	0
55	MG	RA	3113	1/1	0.67	0.19	67,67,67,67	0
55	MG	YA	3173	1/1	0.67	0.23	71,71,71,71	0
55	MG	RA	3192	1/1	0.67	0.31	48,48,48,48	0
55	MG	RA	3275	1/1	0.67	0.20	58,58,58,58	0
55	MG	YA	3242	1/1	0.67	0.34	86,86,86,86	0
55	MG	YA	3251	1/1	0.67	0.30	75,75,75,75	0
55	MG	RA	3077	1/1	0.67	0.24	64,64,64,64	0
55	MG	YA	3285	1/1	0.67	0.41	74,74,74,74	0
55	MG	RA	3319	1/1	0.67	0.24	82,82,82,82	0
55	MG	RA	3187	1/1	0.67	0.38	94,94,94,94	0
55	MG	YA	3417	1/1	0.68	0.12	71,71,71,71	0
55	MG	YA	3339	1/1	0.68	0.41	78,78,78,78	0
55	MG	YA	3254	1/1	0.68	0.44	60,60,60,60	0
55	MG	YA	3423	1/1	0.68	0.19	78,78,78,78	0
55	MG	RA	3239	1/1	0.68	0.22	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3197	1/1	0.68	0.16	59,59,59,59	0
55	MG	YA	3022	1/1	0.68	0.28	42,42,42,42	0
55	MG	RA	3270	1/1	0.68	0.55	87,87,87,87	0
55	MG	RA	3056	1/1	0.68	0.24	29,29,29,29	0
55	MG	XA	1647	1/1	0.68	0.20	101,101,101,101	0
55	MG	YA	3323	1/1	0.68	0.34	55,55,55,55	0
55	MG	RA	3163	1/1	0.68	0.11	59,59,59,59	0
55	MG	YA	3306	1/1	0.68	0.22	87,87,87,87	0
55	MG	RA	3223	1/1	0.68	0.28	80,80,80,80	0
55	MG	YA	3252	1/1	0.68	0.25	66,66,66,66	0
55	MG	RA	3362	1/1	0.68	0.21	64,64,64,64	0
55	MG	YQ	202	1/1	0.68	0.17	79,79,79,79	0
55	MG	YA	3015	1/1	0.69	0.20	73,73,73,73	0
55	MG	YA	3266	1/1	0.69	0.61	87,87,87,87	0
55	MG	YA	3348	1/1	0.69	0.21	72,72,72,72	0
55	MG	YA	3267	1/1	0.69	0.28	77,77,77,77	0
55	MG	YA	3268	1/1	0.69	0.17	78,78,78,78	0
55	MG	YA	3358	1/1	0.69	0.26	66,66,66,66	0
55	MG	QA	1663	1/1	0.69	0.10	104,104,104,104	0
55	MG	QA	1652	1/1	0.69	0.10	96,96,96,96	0
55	MG	YA	3045	1/1	0.69	0.58	63,63,63,63	0
55	MG	YA	3317	1/1	0.69	0.21	59,59,59,59	0
55	MG	RA	3230	1/1	0.69	0.18	75,75,75,75	0
55	MG	YA	3246	1/1	0.69	0.33	76,76,76,76	0
55	MG	RA	3368	1/1	0.69	0.27	65,65,65,65	0
55	MG	QA	1666	1/1	0.69	0.25	78,78,78,78	0
55	MG	YA	3003	1/1	0.69	0.24	77,77,77,77	0
55	MG	RQ	201	1/1	0.69	0.32	97,97,97,97	0
55	MG	YA	3330	1/1	0.69	0.13	65,65,65,65	0
55	MG	YA	3010	1/1	0.69	0.23	52,52,52,52	0
55	MG	XA	1613	1/1	0.69	0.10	72,72,72,72	0
55	MG	YA	3224	1/1	0.69	0.19	51,51,51,51	0
55	MG	RA	3372	1/1	0.69	0.11	64,64,64,64	0
55	MG	YA	3226	1/1	0.69	0.16	21,21,21,21	0
55	MG	YA	3084	1/1	0.70	0.27	61,61,61,61	0
55	MG	RA	3260	1/1	0.70	0.36	89,89,89,89	0
55	MG	YA	3303	1/1	0.70	0.12	80,80,80,80	0
55	MG	RA	3342	1/1	0.70	0.14	49,49,49,49	0
55	MG	QA	1602	1/1	0.70	0.34	79,79,79,79	0
55	MG	RA	3166	1/1	0.70	0.11	88,88,88,88	0
55	MG	QA	1653	1/1	0.70	0.08	89,89,89,89	0
55	MG	RA	3346	1/1	0.70	0.29	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3160	1/1	0.70	0.17	73,73,73,73	0
55	MG	RA	3177	1/1	0.70	0.22	89,89,89,89	0
55	MG	XA	1629	1/1	0.70	0.21	90,90,90,90	0
55	MG	YA	3234	1/1	0.70	0.16	79,79,79,79	0
55	MG	YA	3235	1/1	0.70	0.14	72,72,72,72	0
55	MG	QA	1603	1/1	0.70	0.27	64,64,64,64	0
55	MG	YA	3227	1/1	0.71	0.12	66,66,66,66	0
55	MG	RA	3099	1/1	0.71	0.40	70,70,70,70	0
55	MG	YA	3163	1/1	0.71	0.10	76,76,76,76	0
55	MG	RA	3208	1/1	0.71	0.28	74,74,74,74	0
55	MG	YA	3167	1/1	0.71	0.19	64,64,64,64	0
55	MG	YA	3322	1/1	0.71	0.37	78,78,78,78	0
55	MG	RA	3306	1/1	0.71	0.11	76,76,76,76	0
55	MG	RA	3015	1/1	0.71	0.28	77,77,77,77	0
55	MG	YA	3444	1/1	0.71	0.40	80,80,80,80	0
55	MG	YA	3016	1/1	0.71	0.18	78,78,78,78	0
55	MG	RA	3138	1/1	0.71	0.30	88,88,88,88	0
55	MG	YA	3024	1/1	0.71	0.36	38,38,38,38	0
55	MG	YA	3032	1/1	0.71	0.34	40,40,40,40	0
55	MG	RA	3172	1/1	0.71	0.36	76,76,76,76	0
55	MG	RA	3321	1/1	0.71	0.12	80,80,80,80	0
55	MG	RA	3139	1/1	0.71	0.09	83,83,83,83	0
55	MG	YA	3129	1/1	0.72	0.14	65,65,65,65	0
55	MG	YA	3281	1/1	0.72	0.45	83,83,83,83	0
55	MG	YA	3398	1/1	0.72	0.26	75,75,75,75	0
55	MG	RA	3004	1/1	0.72	0.12	52,52,52,52	0
55	MG	YA	3143	1/1	0.72	0.24	59,59,59,59	0
55	MG	RA	3112	1/1	0.72	0.25	82,82,82,82	0
55	MG	YA	3300	1/1	0.73	0.36	71,71,71,71	0
55	MG	RA	3184	1/1	0.73	0.10	79,79,79,79	0
55	MG	YA	3232	1/1	0.73	0.32	67,67,67,67	0
55	MG	YA	3156	1/1	0.73	0.27	57,57,57,57	0
55	MG	RA	3253	1/1	0.73	0.28	81,81,81,81	0
55	MG	YA	3076	1/1	0.73	0.10	69,69,69,69	0
55	MG	RA	3153	1/1	0.73	0.28	78,78,78,78	0
55	MG	XA	1655	1/1	0.73	0.14	84,84,84,84	0
55	MG	YA	3391	1/1	0.73	0.09	75,75,75,75	0
55	MG	RA	3051	1/1	0.73	0.17	70,70,70,70	0
55	MG	YA	3395	1/1	0.73	0.17	56,56,56,56	0
55	MG	RA	3313	1/1	0.73	0.26	76,76,76,76	0
55	MG	RA	3136	1/1	0.73	0.19	78,78,78,78	0
55	MG	YA	3248	1/1	0.73	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3028	1/1	0.73	0.24	56,56,56,56	0
55	MG	YA	3220	1/1	0.73	0.26	41,41,41,41	0
55	MG	XA	1635	1/1	0.73	0.18	83,83,83,83	0
55	MG	RA	3286	1/1	0.73	0.08	106,106,106,106	0
55	MG	RA	3095	1/1	0.73	0.22	79,79,79,79	0
55	MG	RA	3151	1/1	0.73	0.87	75,75,75,75	0
55	MG	XA	1611	1/1	0.74	0.21	40,40,40,40	0
55	MG	QA	1636	1/1	0.74	0.10	71,71,71,71	0
55	MG	RA	3173	1/1	0.74	0.25	52,52,52,52	0
55	MG	YA	3213	1/1	0.74	0.11	60,60,60,60	0
55	MG	RA	3312	1/1	0.74	0.27	78,78,78,78	0
55	MG	RA	3035	1/1	0.74	0.18	62,62,62,62	0
55	MG	YA	3294	1/1	0.74	0.15	59,59,59,59	0
55	MG	QA	1656	1/1	0.74	0.15	86,86,86,86	0
55	MG	RA	3250	1/1	0.74	0.13	82,82,82,82	0
55	MG	YB	202	1/1	0.74	0.24	47,47,47,47	0
55	MG	QA	1637	1/1	0.74	0.16	88,88,88,88	0
55	MG	RA	3156	1/1	0.74	0.14	89,89,89,89	0
55	MG	YA	3093	1/1	0.74	0.25	48,48,48,48	0
55	MG	YA	3097	1/1	0.74	0.18	60,60,60,60	0
55	MG	RA	3266	1/1	0.74	0.19	83,83,83,83	0
55	MG	Y0	101	1/1	0.74	0.27	68,68,68,68	0
55	MG	YA	3292	1/1	0.75	0.22	66,66,66,66	0
55	MG	YA	3212	1/1	0.75	0.09	57,57,57,57	0
55	MG	RA	3236	1/1	0.75	0.10	93,93,93,93	0
55	MG	YA	3299	1/1	0.75	0.25	77,77,77,77	0
55	MG	RA	3300	1/1	0.75	0.39	76,76,76,76	0
55	MG	RA	3037	1/1	0.75	0.12	40,40,40,40	0
55	MG	YA	3283	1/1	0.75	0.34	59,59,59,59	0
55	MG	YA	3270	1/1	0.75	0.66	92,92,92,92	0
55	MG	YA	3430	1/1	0.75	0.25	46,46,46,46	0
55	MG	YA	3193	1/1	0.75	0.12	84,84,84,84	0
55	MG	RA	3348	1/1	0.75	0.15	92,92,92,92	0
55	MG	YA	3441	1/1	0.75	0.20	53,53,53,53	0
55	MG	RA	3082	1/1	0.76	0.24	58,58,58,58	0
55	MG	RA	3311	1/1	0.76	0.51	74,74,74,74	0
55	MG	XA	1616	1/1	0.76	0.19	99,99,99,99	0
55	MG	RA	3025	1/1	0.76	0.44	63,63,63,63	0
55	MG	RA	3071	1/1	0.76	0.14	86,86,86,86	0
55	MG	QA	1625	1/1	0.76	0.32	101,101,101,101	0
55	MG	QA	1634	1/1	0.76	0.10	61,61,61,61	0
55	MG	RA	3196	1/1	0.76	0.31	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3415	1/1	0.76	0.38	74,74,74,74	0
55	MG	YA	3174	1/1	0.76	0.12	60,60,60,60	0
55	MG	YA	3128	1/1	0.76	0.22	42,42,42,42	0
55	MG	RA	3103	1/1	0.76	0.14	64,64,64,64	0
55	MG	RA	3146	1/1	0.76	0.16	77,77,77,77	0
55	MG	RA	3149	1/1	0.76	0.09	81,81,81,81	0
55	MG	YP	201	1/1	0.76	0.22	80,80,80,80	0
55	MG	RA	3190	1/1	0.76	0.39	81,81,81,81	0
55	MG	YA	3012	1/1	0.76	0.15	70,70,70,70	0
55	MG	YA	3375	1/1	0.77	0.33	66,66,66,66	0
55	MG	QA	1631	1/1	0.77	0.13	70,70,70,70	0
55	MG	YA	3105	1/1	0.77	0.24	54,54,54,54	0
55	MG	RA	3299	1/1	0.77	0.24	89,89,89,89	0
55	MG	YA	3153	1/1	0.77	0.28	60,60,60,60	0
55	MG	YA	3127	1/1	0.77	0.10	67,67,67,67	0
55	MG	YA	3177	1/1	0.77	0.27	55,55,55,55	0
55	MG	YA	3158	1/1	0.77	0.59	79,79,79,79	0
55	MG	YA	3362	1/1	0.77	0.10	75,75,75,75	0
55	MG	RA	3218	1/1	0.77	0.30	64,64,64,64	0
55	MG	YA	3399	1/1	0.77	0.22	35,35,35,35	0
55	MG	YA	3206	1/1	0.77	0.11	63,63,63,63	0
55	MG	YE	301	1/1	0.77	0.24	70,70,70,70	0
55	MG	YA	3402	1/1	0.77	0.55	77,77,77,77	0
55	MG	XA	1625	1/1	0.77	0.22	73,73,73,73	0
55	MG	RA	3301	1/1	0.77	0.21	71,71,71,71	0
55	MG	YA	3200	1/1	0.78	0.44	75,75,75,75	0
55	MG	YA	3172	1/1	0.78	0.08	66,66,66,66	0
55	MG	YA	3139	1/1	0.78	0.22	47,47,47,47	0
55	MG	YA	3353	1/1	0.78	0.21	75,75,75,75	0
55	MG	YA	3431	1/1	0.78	0.30	24,24,24,24	0
55	MG	YA	3433	1/1	0.78	0.25	44,44,44,44	0
55	MG	RA	3152	1/1	0.78	0.25	92,92,92,92	0
55	MG	YA	3058	1/1	0.78	0.32	51,51,51,51	0
55	MG	RA	3079	1/1	0.78	0.20	63,63,63,63	0
55	MG	RA	3176	1/1	0.78	0.13	72,72,72,72	0
55	MG	YA	3155	1/1	0.78	0.14	56,56,56,56	0
55	MG	YA	3110	1/1	0.78	0.17	63,63,63,63	0
55	MG	YA	3364	1/1	0.78	0.20	54,54,54,54	0
55	MG	YA	3115	1/1	0.78	0.20	39,39,39,39	0
55	MG	YA	3278	1/1	0.78	0.17	107,107,107,107	0
55	MG	RA	3332	1/1	0.78	0.37	92,92,92,92	0
55	MG	RA	3298	1/1	0.78	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1612	1/1	0.78	0.35	67,67,67,67	0
55	MG	YA	3382	1/1	0.78	0.10	69,69,69,69	0
55	MG	QA	1624	1/1	0.78	0.12	90,90,90,90	0
55	MG	YA	3418	1/1	0.78	0.15	74,74,74,74	0
55	MG	YA	3135	1/1	0.78	0.40	109,109,109,109	0
55	MG	RA	3055	1/1	0.78	0.07	97,97,97,97	0
55	MG	Y7	102	1/1	0.78	0.20	72,72,72,72	0
55	MG	RA	3046	1/1	0.79	0.25	33,33,33,33	0
55	MG	RA	3315	1/1	0.79	0.19	53,53,53,53	0
55	MG	YA	3204	1/1	0.79	0.25	63,63,63,63	0
55	MG	YA	3102	1/1	0.79	0.14	54,54,54,54	0
55	MG	RA	3161	1/1	0.79	0.22	74,74,74,74	0
55	MG	YA	3296	1/1	0.79	0.30	63,63,63,63	0
55	MG	RA	3186	1/1	0.79	0.50	80,80,80,80	0
55	MG	YA	3061	1/1	0.79	0.20	33,33,33,33	0
55	MG	YA	3113	1/1	0.79	0.51	72,72,72,72	0
55	MG	YA	3184	1/1	0.79	0.18	74,74,74,74	0
55	MG	QA	1604	1/1	0.79	0.27	58,58,58,58	0
55	MG	YA	3411	1/1	0.79	0.14	78,78,78,78	0
55	MG	RA	3355	1/1	0.79	0.21	46,46,46,46	0
55	MG	YA	3413	1/1	0.79	0.13	67,67,67,67	0
55	MG	RA	3235	1/1	0.79	0.16	64,64,64,64	0
55	MG	XA	1665	1/1	0.79	0.18	114,114,114,114	0
55	MG	YA	3279	1/1	0.79	0.23	90,90,90,90	0
55	MG	RA	3090	1/1	0.79	0.08	80,80,80,80	0
55	MG	RA	3347	1/1	0.79	0.66	88,88,88,88	0
55	MG	YA	3256	1/1	0.79	0.28	70,70,70,70	0
55	MG	R1	101	1/1	0.79	0.16	59,59,59,59	0
55	MG	YA	3284	1/1	0.79	0.32	100,100,100,100	0
55	MG	YA	3432	1/1	0.80	0.43	38,38,38,38	0
55	MG	YA	3287	1/1	0.80	0.17	58,58,58,58	0
55	MG	YA	3243	1/1	0.80	0.23	85,85,85,85	0
55	MG	RA	3124	1/1	0.80	0.12	85,85,85,85	0
55	MG	YA	3131	1/1	0.80	0.09	74,74,74,74	0
55	MG	YA	3293	1/1	0.80	0.38	86,86,86,86	0
55	MG	RA	3131	1/1	0.80	0.15	75,75,75,75	0
55	MG	YA	3388	1/1	0.80	0.41	87,87,87,87	0
55	MG	RA	3016	1/1	0.80	0.28	52,52,52,52	0
55	MG	YA	3230	1/1	0.80	0.32	29,29,29,29	0
55	MG	YB	201	1/1	0.80	0.09	56,56,56,56	0
55	MG	YA	3165	1/1	0.80	0.15	71,71,71,71	0
55	MG	RA	3244	1/1	0.80	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3373	1/1	0.80	0.27	93,93,93,93	0
55	MG	RA	3361	1/1	0.80	0.18	79,79,79,79	0
55	MG	YA	3422	1/1	0.80	0.42	77,77,77,77	0
55	MG	YA	3033	1/1	0.80	0.33	36,36,36,36	0
55	MG	QA	1633	1/1	0.80	0.27	96,96,96,96	0
55	MG	QA	1662	1/1	0.80	0.22	119,119,119,119	0
55	MG	RA	3123	1/1	0.80	0.17	66,66,66,66	0
55	MG	YA	3265	1/1	0.80	0.14	83,83,83,83	0
55	MG	YA	3258	1/1	0.81	0.23	53,53,53,53	0
55	MG	YA	3088	1/1	0.81	0.20	50,50,50,50	0
55	MG	RA	3042	1/1	0.81	0.30	56,56,56,56	0
55	MG	RA	3027	1/1	0.81	0.24	54,54,54,54	0
55	MG	YA	3099	1/1	0.81	0.36	37,37,37,37	0
55	MG	YA	3337	1/1	0.81	0.36	95,95,95,95	0
55	MG	XA	1663	1/1	0.81	0.35	72,72,72,72	0
55	MG	YA	3190	1/1	0.81	0.17	73,73,73,73	0
55	MG	RA	3047	1/1	0.81	0.18	47,47,47,47	0
55	MG	XA	1634	1/1	0.81	0.12	103,103,103,103	0
55	MG	QA	1606	1/1	0.81	0.23	88,88,88,88	0
55	MG	RA	3180	1/1	0.81	0.09	65,65,65,65	0
55	MG	QA	1658	1/1	0.81	0.14	79,79,79,79	0
55	MG	YA	3114	1/1	0.81	0.25	69,69,69,69	0
55	MG	RA	3101	1/1	0.81	0.10	56,56,56,56	0
55	MG	YA	3276	1/1	0.81	0.32	70,70,70,70	0
55	MG	XA	1650	1/1	0.81	0.19	71,71,71,71	0
55	MG	YA	3126	1/1	0.81	0.12	59,59,59,59	0
55	MG	YA	3207	1/1	0.81	0.09	66,66,66,66	0
55	MG	QA	1610	1/1	0.81	0.14	44,44,44,44	0
55	MG	YA	3250	1/1	0.81	0.28	78,78,78,78	0
55	MG	YA	3074	1/1	0.81	0.32	66,66,66,66	0
55	MG	RA	3041	1/1	0.81	0.15	46,46,46,46	0
55	MG	RA	3110	1/1	0.81	0.14	64,64,64,64	0
55	MG	YA	3132	1/1	0.81	0.11	62,62,62,62	0
55	MG	RA	3200	1/1	0.81	0.22	68,68,68,68	0
55	MG	RA	3357	1/1	0.81	0.23	107,107,107,107	0
55	MG	RB	203	1/1	0.82	0.06	84,84,84,84	0
55	MG	RA	3039	1/1	0.82	0.23	72,72,72,72	0
55	MG	YA	3325	1/1	0.82	0.25	62,62,62,62	0
55	MG	YA	3098	1/1	0.82	0.11	53,53,53,53	0
55	MG	RA	3014	1/1	0.82	0.14	61,61,61,61	0
55	MG	YA	3385	1/1	0.82	0.23	68,68,68,68	0
55	MG	YA	3425	1/1	0.82	0.28	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1668	1/1	0.82	0.14	79,79,79,79	0
55	MG	YA	3148	1/1	0.82	0.17	75,75,75,75	0
55	MG	YA	3334	1/1	0.82	0.26	75,75,75,75	0
55	MG	XA	1614	1/1	0.82	0.15	71,71,71,71	0
55	MG	YA	3191	1/1	0.82	0.12	68,68,68,68	0
55	MG	RA	3328	1/1	0.82	0.11	81,81,81,81	0
55	MG	QA	1646	1/1	0.82	0.12	118,118,118,118	0
55	MG	RA	3133	1/1	0.82	0.13	80,80,80,80	0
55	MG	RA	3115	1/1	0.82	0.46	60,60,60,60	0
55	MG	YA	3400	1/1	0.82	0.19	49,49,49,49	0
55	MG	XA	1631	1/1	0.82	0.08	86,86,86,86	0
55	MG	YA	3445	1/1	0.82	0.34	63,63,63,63	0
55	MG	RA	3257	1/1	0.82	0.36	56,56,56,56	0
55	MG	YA	3451	1/1	0.82	0.15	47,47,47,47	0
55	MG	YA	3116	1/1	0.82	0.30	51,51,51,51	0
55	MG	RA	3274	1/1	0.82	0.19	55,55,55,55	0
55	MG	YA	3354	1/1	0.82	0.23	82,82,82,82	0
55	MG	RA	3353	1/1	0.82	0.32	53,53,53,53	0
55	MG	RA	3018	1/1	0.82	0.09	33,33,33,33	0
55	MG	YA	3209	1/1	0.82	0.17	72,72,72,72	0
55	MG	XA	1638	1/1	0.82	0.21	63,63,63,63	0
55	MG	XA	1639	1/1	0.82	0.23	71,71,71,71	0
55	MG	RA	3263	1/1	0.82	0.28	70,70,70,70	0
55	MG	YA	3176	1/1	0.82	0.16	58,58,58,58	0
55	MG	RA	3322	1/1	0.82	0.34	84,84,84,84	0
55	MG	RA	3005	1/1	0.82	0.21	46,46,46,46	0
57	ZN	R5	101	1/1	0.82	0.09	205,205,205,205	0
55	MG	RA	3140	1/1	0.83	0.19	61,61,61,61	0
55	MG	RA	3033	1/1	0.83	0.18	64,64,64,64	0
55	MG	YA	3437	1/1	0.83	0.26	61,61,61,61	0
55	MG	QA	1650	1/1	0.83	0.21	80,80,80,80	0
55	MG	YA	3439	1/1	0.83	0.29	70,70,70,70	0
55	MG	RA	3120	1/1	0.83	0.27	53,53,53,53	0
55	MG	XA	1641	1/1	0.83	0.12	104,104,104,104	0
55	MG	YA	3369	1/1	0.83	0.35	56,56,56,56	0
55	MG	RA	3074	1/1	0.83	0.10	43,43,43,43	0
55	MG	YA	3373	1/1	0.83	0.19	82,82,82,82	0
55	MG	RB	206	1/1	0.83	0.23	67,67,67,67	0
55	MG	YA	3380	1/1	0.83	0.21	60,60,60,60	0
55	MG	YA	3286	1/1	0.83	0.19	74,74,74,74	0
55	MG	YA	3192	1/1	0.83	0.13	70,70,70,70	0
55	MG	RA	3338	1/1	0.83	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3026	1/1	0.83	0.19	35,35,35,35	0
55	MG	YA	3145	1/1	0.83	0.29	71,71,71,71	0
55	MG	RA	3314	1/1	0.83	0.16	81,81,81,81	0
55	MG	YA	3350	1/1	0.83	0.12	45,45,45,45	0
55	MG	RA	3040	1/1	0.83	0.23	100,100,100,100	0
55	MG	YA	3008	1/1	0.83	0.10	75,75,75,75	0
55	MG	YA	3321	1/1	0.83	0.27	56,56,56,56	0
55	MG	YQ	201	1/1	0.83	0.08	66,66,66,66	0
55	MG	RA	3116	1/1	0.83	0.30	64,64,64,64	0
55	MG	YR	201	1/1	0.83	0.22	39,39,39,39	0
55	MG	YA	3042	1/1	0.83	0.14	43,43,43,43	0
55	MG	YA	3277	1/1	0.83	0.43	81,81,81,81	0
55	MG	YA	3231	1/1	0.83	0.18	53,53,53,53	0
55	MG	YA	3133	1/1	0.84	0.37	53,53,53,53	0
55	MG	RA	3029	1/1	0.84	0.15	41,41,41,41	0
55	MG	YA	3179	1/1	0.84	0.18	34,34,34,34	0
55	MG	RA	3083	1/1	0.84	0.33	57,57,57,57	0
55	MG	RA	3017	1/1	0.84	0.20	56,56,56,56	0
55	MG	RA	3309	1/1	0.84	0.10	79,79,79,79	0
55	MG	QA	1620	1/1	0.84	0.12	85,85,85,85	0
55	MG	YA	3314	1/1	0.84	0.19	76,76,76,76	0
55	MG	RA	3022	1/1	0.84	0.16	24,24,24,24	0
55	MG	YA	3316	1/1	0.84	0.36	68,68,68,68	0
55	MG	RA	3358	1/1	0.84	0.21	52,52,52,52	0
55	MG	YA	3359	1/1	0.84	0.24	56,56,56,56	0
55	MG	RA	3154	1/1	0.84	0.23	79,79,79,79	0
55	MG	RA	3258	1/1	0.84	0.32	79,79,79,79	0
55	MG	RA	3217	1/1	0.84	0.30	100,100,100,100	0
55	MG	RA	3050	1/1	0.84	0.37	57,57,57,57	0
55	MG	XA	1666	1/1	0.84	0.43	86,86,86,86	0
55	MG	YA	3366	1/1	0.84	0.17	56,56,56,56	0
55	MG	RA	3317	1/1	0.84	0.20	72,72,72,72	0
55	MG	RA	3097	1/1	0.84	0.19	64,64,64,64	0
55	MG	YA	3414	1/1	0.84	0.23	68,68,68,68	0
55	MG	QA	1644	1/1	0.84	0.10	73,73,73,73	0
55	MG	YA	3328	1/1	0.84	0.36	70,70,70,70	0
55	MG	YA	3004	1/1	0.84	0.09	61,61,61,61	0
55	MG	QA	1667	1/1	0.84	0.13	101,101,101,101	0
55	MG	QA	1639	1/1	0.84	0.09	65,65,65,65	0
55	MG	YA	3332	1/1	0.84	0.17	87,87,87,87	0
55	MG	RA	3142	1/1	0.84	0.28	85,85,85,85	0
55	MG	RA	3143	1/1	0.84	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3082	1/1	0.84	0.29	45,45,45,45	0
55	MG	RA	3105	1/1	0.84	0.14	64,64,64,64	0
57	ZN	YY	201	1/1	0.84	0.11	211,211,211,211	0
55	MG	XA	1649	1/1	0.85	0.09	67,67,67,67	0
55	MG	YA	3396	1/1	0.85	0.15	59,59,59,59	0
55	MG	RA	3241	1/1	0.85	0.20	78,78,78,78	0
55	MG	YA	3289	1/1	0.85	0.28	51,51,51,51	0
55	MG	YA	3196	1/1	0.85	0.13	74,74,74,74	0
55	MG	RA	3243	1/1	0.85	0.11	59,59,59,59	0
55	MG	RA	3067	1/1	0.85	0.28	82,82,82,82	0
55	MG	RA	3159	1/1	0.85	0.21	84,84,84,84	0
55	MG	RA	3068	1/1	0.85	0.18	57,57,57,57	0
55	MG	RA	3069	1/1	0.85	0.20	53,53,53,53	0
55	MG	RA	3034	1/1	0.85	0.10	58,58,58,58	0
55	MG	RA	3293	1/1	0.85	0.17	69,69,69,69	0
55	MG	RA	3294	1/1	0.85	0.08	54,54,54,54	0
55	MG	RA	3320	1/1	0.85	0.15	85,85,85,85	0
55	MG	RA	3061	1/1	0.85	0.11	71,71,71,71	0
55	MG	YA	3370	1/1	0.85	0.26	65,65,65,65	0
55	MG	RA	3106	1/1	0.85	0.17	66,66,66,66	0
55	MG	YA	3275	1/1	0.85	0.30	66,66,66,66	0
55	MG	RA	3168	1/1	0.85	0.08	74,74,74,74	0
55	MG	YA	3249	1/1	0.85	0.27	79,79,79,79	0
55	MG	RA	3170	1/1	0.85	0.15	66,66,66,66	0
55	MG	RA	3049	1/1	0.85	0.10	58,58,58,58	0
55	MG	YA	3383	1/1	0.85	0.53	56,56,56,56	0
55	MG	RA	3094	1/1	0.85	0.13	32,32,32,32	0
55	MG	YA	3343	1/1	0.85	0.27	77,77,77,77	0
55	MG	RA	3002	1/1	0.85	0.37	68,68,68,68	0
55	MG	RA	3379	1/1	0.85	0.10	65,65,65,65	0
55	MG	YA	3255	1/1	0.85	0.20	68,68,68,68	0
55	MG	YA	3162	1/1	0.85	0.31	72,72,72,72	0
55	MG	RA	3221	1/1	0.85	0.18	72,72,72,72	0
55	MG	RA	3114	1/1	0.86	0.10	39,39,39,39	0
55	MG	YA	3356	1/1	0.86	0.08	44,44,44,44	0
55	MG	YA	3229	1/1	0.86	0.41	60,60,60,60	0
55	MG	YA	3320	1/1	0.86	0.13	59,59,59,59	0
55	MG	RA	3181	1/1	0.86	0.25	81,81,81,81	0
55	MG	YA	3027	1/1	0.86	0.23	44,44,44,44	0
55	MG	RA	3276	1/1	0.86	0.19	54,54,54,54	0
55	MG	RA	3329	1/1	0.86	0.12	62,62,62,62	0
55	MG	YA	3096	1/1	0.86	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3011	1/1	0.86	0.23	55,55,55,55	0
55	MG	YA	3203	1/1	0.86	0.22	80,80,80,80	0
55	MG	RA	3122	1/1	0.86	0.12	61,61,61,61	0
55	MG	RA	3155	1/1	0.86	0.29	82,82,82,82	0
55	MG	YA	3138	1/1	0.86	0.28	56,56,56,56	0
55	MG	RA	3175	1/1	0.86	0.12	89,89,89,89	0
55	MG	YA	3142	1/1	0.86	0.43	51,51,51,51	0
55	MG	YA	3247	1/1	0.86	0.26	63,63,63,63	0
55	MG	YA	3055	1/1	0.86	0.14	41,41,41,41	0
55	MG	YA	3376	1/1	0.86	0.19	83,83,83,83	0
55	MG	QA	1643	1/1	0.86	0.09	96,96,96,96	0
55	MG	YA	3340	1/1	0.86	0.20	42,42,42,42	0
55	MG	RA	3088	1/1	0.86	0.28	52,52,52,52	0
55	MG	YA	3106	1/1	0.86	0.13	42,42,42,42	0
55	MG	RA	3226	1/1	0.86	0.15	67,67,67,67	0
55	MG	RA	3340	1/1	0.86	0.20	86,86,86,86	0
55	MG	RA	3290	1/1	0.86	0.15	60,60,60,60	0
55	MG	RA	3291	1/1	0.86	0.19	69,69,69,69	0
55	MG	Y5	102	1/1	0.86	0.12	54,54,54,54	0
55	MG	Y7	101	1/1	0.86	0.33	44,44,44,44	0
55	MG	RA	3310	1/1	0.86	0.14	81,81,81,81	0
55	MG	XA	1662	1/1	0.86	0.08	79,79,79,79	0
55	MG	YA	3161	1/1	0.86	0.08	59,59,59,59	0
55	MG	RA	3137	1/1	0.87	0.11	81,81,81,81	0
55	MG	YA	3031	1/1	0.87	0.26	36,36,36,36	0
55	MG	YA	3345	1/1	0.87	0.16	54,54,54,54	0
55	MG	RA	3064	1/1	0.87	0.12	64,64,64,64	0
55	MG	RA	3271	1/1	0.87	0.12	74,74,74,74	0
55	MG	YA	3295	1/1	0.87	0.10	30,30,30,30	0
55	MG	YA	3037	1/1	0.87	0.13	32,32,32,32	0
55	MG	YA	3450	1/1	0.87	0.21	33,33,33,33	0
55	MG	YA	3089	1/1	0.87	0.17	23,23,23,23	0
55	MG	YA	3091	1/1	0.87	0.22	51,51,51,51	0
55	MG	RA	3288	1/1	0.87	0.11	76,76,76,76	0
55	MG	RA	3262	1/1	0.87	0.14	101,101,101,101	0
55	MG	RA	3144	1/1	0.87	0.12	61,61,61,61	0
55	MG	YB	205	1/1	0.87	0.25	52,52,52,52	0
55	MG	RA	3307	1/1	0.87	0.10	77,77,77,77	0
55	MG	RA	3020	1/1	0.87	0.11	51,51,51,51	0
55	MG	RA	3147	1/1	0.87	0.17	83,83,83,83	0
55	MG	RA	3238	1/1	0.87	0.11	67,67,67,67	0
55	MG	RA	3072	1/1	0.87	0.25	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1648	1/1	0.87	0.33	80,80,80,80	0
55	MG	YA	3429	1/1	0.87	0.18	41,41,41,41	0
55	MG	YA	3201	1/1	0.87	0.09	65,65,65,65	0
55	MG	YA	3175	1/1	0.87	0.09	59,59,59,59	0
55	MG	YA	3072	1/1	0.87	0.27	33,33,33,33	0
55	MG	XA	1622	1/1	0.87	0.21	58,58,58,58	0
55	MG	RA	3296	1/1	0.87	0.19	71,71,71,71	0
55	MG	YA	3371	1/1	0.87	0.07	56,56,56,56	0
55	MG	YA	3078	1/1	0.87	0.09	59,59,59,59	0
55	MG	RA	3129	1/1	0.88	0.09	59,59,59,59	0
55	MG	XA	1664	1/1	0.88	0.16	66,66,66,66	0
55	MG	RA	3130	1/1	0.88	0.15	55,55,55,55	0
55	MG	YA	3403	1/1	0.88	0.19	74,74,74,74	0
55	MG	YA	3304	1/1	0.88	0.35	86,86,86,86	0
55	MG	RA	3102	1/1	0.88	0.16	76,76,76,76	0
55	MG	RA	3233	1/1	0.88	0.09	87,87,87,87	0
55	MG	RA	3365	1/1	0.88	0.43	53,53,53,53	0
55	MG	YA	3338	1/1	0.88	0.33	87,87,87,87	0
55	MG	YA	3077	1/1	0.88	0.13	35,35,35,35	0
55	MG	RA	3070	1/1	0.88	0.21	61,61,61,61	0
55	MG	QA	1615	1/1	0.88	0.11	83,83,83,83	0
55	MG	YA	3006	1/1	0.88	0.10	92,92,92,92	0
55	MG	YA	3454	1/1	0.88	0.18	140,140,140,140	0
55	MG	YA	3157	1/1	0.88	0.17	79,79,79,79	0
55	MG	RA	3080	1/1	0.88	0.18	46,46,46,46	0
55	MG	RA	3369	1/1	0.88	0.15	74,74,74,74	0
55	MG	YA	3086	1/1	0.88	0.18	34,34,34,34	0
55	MG	RA	3237	1/1	0.88	0.31	75,75,75,75	0
55	MG	YA	3228	1/1	0.88	0.26	25,25,25,25	0
55	MG	XA	1657	1/1	0.88	0.10	91,91,91,91	0
55	MG	YA	3049	1/1	0.88	0.19	40,40,40,40	0
55	MG	YA	3053	1/1	0.88	0.09	41,41,41,41	0
55	MG	YA	3390	1/1	0.88	0.11	86,86,86,86	0
55	MG	YA	3054	1/1	0.88	0.20	42,42,42,42	0
55	MG	YA	3168	1/1	0.88	0.20	54,54,54,54	0
55	MG	YA	3427	1/1	0.88	0.12	48,48,48,48	0
55	MG	YA	3134	1/1	0.88	0.11	61,61,61,61	0
55	MG	RA	3054	1/1	0.88	0.13	57,57,57,57	0
55	MG	RA	3028	1/1	0.88	0.44	40,40,40,40	0
55	MG	YA	3137	1/1	0.88	0.16	50,50,50,50	0
55	MG	RA	3126	1/1	0.88	0.15	65,65,65,65	0
55	MG	RA	3281	1/1	0.89	0.06	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3355	1/1	0.89	0.18	57,57,57,57	0
55	MG	QA	1616	1/1	0.89	0.18	109,109,109,109	0
55	MG	RA	3091	1/1	0.89	0.08	62,62,62,62	0
55	MG	RA	3354	1/1	0.89	0.22	15,15,15,15	0
55	MG	XA	1604	1/1	0.89	0.21	73,73,73,73	0
55	MG	YA	3159	1/1	0.89	0.15	60,60,60,60	0
55	MG	RA	3038	1/1	0.89	0.21	51,51,51,51	0
55	MG	YA	3298	1/1	0.89	0.26	47,47,47,47	0
55	MG	YA	3436	1/1	0.89	0.14	39,39,39,39	0
55	MG	YA	3216	1/1	0.89	0.14	56,56,56,56	0
55	MG	RA	3160	1/1	0.89	0.12	55,55,55,55	0
55	MG	YA	3219	1/1	0.89	0.26	48,48,48,48	0
55	MG	YA	3240	1/1	0.89	0.48	41,41,41,41	0
55	MG	RA	3287	1/1	0.89	0.32	60,60,60,60	0
55	MG	RA	3084	1/1	0.89	0.24	96,96,96,96	0
55	MG	RA	3179	1/1	0.89	0.08	112,112,112,112	0
55	MG	RA	3259	1/1	0.89	0.10	48,48,48,48	0
55	MG	YA	3021	1/1	0.89	0.23	32,32,32,32	0
57	ZN	R4	101	1/1	0.89	0.12	301,301,301,301	0
55	MG	RA	3096	1/1	0.89	0.07	55,55,55,55	0
55	MG	YA	3081	1/1	0.89	0.23	33,33,33,33	0
57	ZN	Y4	101	1/1	0.89	0.11	321,321,321,321	0
55	MG	RA	3378	1/1	0.90	0.06	79,79,79,79	0
55	MG	RA	3178	1/1	0.90	0.21	57,57,57,57	0
55	MG	QA	1638	1/1	0.90	0.19	93,93,93,93	0
55	MG	YA	3017	1/1	0.90	0.22	40,40,40,40	0
55	MG	YA	3217	1/1	0.90	0.42	46,46,46,46	0
55	MG	RA	3052	1/1	0.90	0.08	87,87,87,87	0
55	MG	QA	1609	1/1	0.90	0.10	62,62,62,62	0
55	MG	RA	3231	1/1	0.90	0.29	77,77,77,77	0
55	MG	YA	3025	1/1	0.90	0.15	43,43,43,43	0
55	MG	YA	3186	1/1	0.90	0.22	72,72,72,72	0
55	MG	YA	3067	1/1	0.90	0.16	73,73,73,73	0
55	MG	QA	1614	1/1	0.90	0.10	80,80,80,80	0
55	MG	YA	3112	1/1	0.90	0.17	60,60,60,60	0
55	MG	RA	3121	1/1	0.90	0.22	64,64,64,64	0
55	MG	RA	3305	1/1	0.90	0.10	59,59,59,59	0
55	MG	YA	3030	1/1	0.90	0.22	55,55,55,55	0
55	MG	QA	1617	1/1	0.90	0.43	79,79,79,79	0
55	MG	RA	3185	1/1	0.90	0.07	44,44,44,44	0
55	MG	YA	3118	1/1	0.90	0.16	47,47,47,47	0
55	MG	YA	3120	1/1	0.90	0.40	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3121	1/1	0.90	0.22	55,55,55,55	0
55	MG	YB	208	1/1	0.90	0.08	66,66,66,66	0
55	MG	YD	301	1/1	0.90	0.10	44,44,44,44	0
55	MG	YA	3420	1/1	0.90	0.13	79,79,79,79	0
55	MG	YA	3123	1/1	0.90	0.33	41,41,41,41	0
55	MG	RA	3371	1/1	0.90	0.15	48,48,48,48	0
55	MG	YA	3036	1/1	0.90	0.22	26,26,26,26	0
55	MG	YA	3346	1/1	0.90	0.11	73,73,73,73	0
55	MG	QA	1619	1/1	0.90	0.10	90,90,90,90	0
55	MG	RA	3277	1/1	0.90	0.42	76,76,76,76	0
55	MG	RA	3374	1/1	0.90	0.05	63,63,63,63	0
55	MG	YA	3044	1/1	0.90	0.20	48,48,48,48	0
55	MG	YA	3171	1/1	0.90	0.10	40,40,40,40	0
55	MG	RA	3164	1/1	0.90	0.21	45,45,45,45	0
55	MG	RA	3078	1/1	0.90	0.07	70,70,70,70	0
55	MG	YA	3051	1/1	0.90	0.29	48,48,48,48	0
55	MG	YA	3435	1/1	0.90	0.18	46,46,46,46	0
55	MG	RA	3127	1/1	0.91	0.13	84,84,84,84	0
55	MG	QA	1642	1/1	0.91	0.10	110,110,110,110	0
55	MG	YA	3060	1/1	0.91	0.22	36,36,36,36	0
55	MG	RA	3169	1/1	0.91	0.23	52,52,52,52	0
55	MG	QA	1655	1/1	0.91	0.08	88,88,88,88	0
55	MG	YA	3404	1/1	0.91	0.08	92,92,92,92	0
55	MG	YA	3107	1/1	0.91	0.09	41,41,41,41	0
55	MG	RA	3053	1/1	0.91	0.14	42,42,42,42	0
55	MG	QA	1630	1/1	0.91	0.30	114,114,114,114	0
55	MG	YA	3365	1/1	0.91	0.14	76,76,76,76	0
55	MG	RA	3023	1/1	0.91	0.18	76,76,76,76	0
55	MG	YA	3149	1/1	0.91	0.12	60,60,60,60	0
55	MG	YA	3221	1/1	0.91	0.20	27,27,27,27	0
55	MG	YA	3152	1/1	0.91	0.10	89,89,89,89	0
55	MG	RA	3202	1/1	0.91	0.21	52,52,52,52	0
55	MG	RA	3174	1/1	0.91	0.14	37,37,37,37	0
55	MG	XA	1648	1/1	0.91	0.26	73,73,73,73	0
55	MG	YA	3035	1/1	0.91	0.19	43,43,43,43	0
55	MG	YA	3007	1/1	0.91	0.10	64,64,64,64	0
55	MG	RA	3024	1/1	0.91	0.10	44,44,44,44	0
55	MG	YA	3038	1/1	0.91	0.14	33,33,33,33	0
55	MG	YA	3122	1/1	0.91	0.33	54,54,54,54	0
55	MG	QA	1651	1/1	0.91	0.07	70,70,70,70	0
55	MG	XA	1619	1/1	0.91	0.09	39,39,39,39	0
55	MG	YA	3271	1/1	0.91	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3283	1/1	0.91	0.10	63,63,63,63	0
55	MG	RA	3334	1/1	0.91	0.36	75,75,75,75	0
55	MG	YA	3046	1/1	0.91	0.17	37,37,37,37	0
55	MG	XA	1626	1/1	0.91	0.06	88,88,88,88	0
55	MG	QA	1623	1/1	0.91	0.05	92,92,92,92	0
55	MG	YA	3052	1/1	0.91	0.29	52,52,52,52	0
55	MG	YA	3241	1/1	0.91	0.22	54,54,54,54	0
55	MG	RA	3318	1/1	0.91	0.05	66,66,66,66	0
55	MG	QA	1665	1/1	0.91	0.18	82,82,82,82	0
57	ZN	XN	101	1/1	0.91	0.07	237,237,237,237	0
55	MG	YA	3244	1/1	0.91	0.16	57,57,57,57	0
55	MG	RA	3086	1/1	0.91	0.24	72,72,72,72	0
55	MG	YA	3103	1/1	0.92	0.14	54,54,54,54	0
55	MG	XA	1640	1/1	0.92	0.08	79,79,79,79	0
55	MG	RA	3032	1/1	0.92	0.16	52,52,52,52	0
55	MG	RA	3058	1/1	0.92	0.10	65,65,65,65	0
55	MG	RA	3060	1/1	0.92	0.17	61,61,61,61	0
55	MG	QA	1649	1/1	0.92	0.18	95,95,95,95	0
55	MG	XA	1620	1/1	0.92	0.17	63,63,63,63	0
55	MG	YA	3146	1/1	0.92	0.18	41,41,41,41	0
55	MG	QA	1629	1/1	0.92	0.07	83,83,83,83	0
55	MG	XA	1623	1/1	0.92	0.07	95,95,95,95	0
55	MG	RA	3360	1/1	0.92	0.09	94,94,94,94	0
55	MG	YA	3151	1/1	0.92	0.24	51,51,51,51	0
55	MG	RA	3377	1/1	0.92	0.14	42,42,42,42	0
55	MG	XA	1628	1/1	0.92	0.15	76,76,76,76	0
55	MG	YA	3013	1/1	0.92	0.29	38,38,38,38	0
55	MG	QV	101	1/1	0.92	0.23	98,98,98,98	0
55	MG	RA	3167	1/1	0.92	0.22	70,70,70,70	0
55	MG	RA	3036	1/1	0.92	0.16	43,43,43,43	0
55	MG	RA	3207	1/1	0.92	0.33	78,78,78,78	0
55	MG	RA	3145	1/1	0.92	0.22	82,82,82,82	0
55	MG	YA	3261	1/1	0.92	0.10	38,38,38,38	0
55	MG	YA	3092	1/1	0.92	0.06	61,61,61,61	0
55	MG	RA	3336	1/1	0.92	0.08	75,75,75,75	0
55	MG	YA	3095	1/1	0.92	0.10	39,39,39,39	0
55	MG	RA	3158	1/1	0.92	0.12	100,100,100,100	0
55	MG	YA	3056	1/1	0.92	0.10	47,47,47,47	0
57	ZN	QN	101	1/1	0.92	0.12	211,211,211,211	0
55	MG	YA	3166	1/1	0.92	0.20	60,60,60,60	0
55	MG	XA	1636	1/1	0.92	0.07	78,78,78,78	0
55	MG	RA	3010	1/1	0.92	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1605	1/1	0.92	0.06	99,99,99,99	0
55	MG	XE	201	1/1	0.92	0.06	61,61,61,61	0
57	ZN	Y5	101	1/1	0.92	0.07	242,242,242,242	0
55	MG	YA	3394	1/1	0.93	0.16	79,79,79,79	0
55	MG	YA	3068	1/1	0.93	0.08	38,38,38,38	0
55	MG	YA	3288	1/1	0.93	0.16	79,79,79,79	0
55	MG	YA	3071	1/1	0.93	0.15	63,63,63,63	0
55	MG	XA	1624	1/1	0.93	0.07	106,106,106,106	0
55	MG	YA	3073	1/1	0.93	0.12	40,40,40,40	0
55	MG	RA	3188	1/1	0.93	0.07	48,48,48,48	0
55	MG	YA	3245	1/1	0.93	0.19	33,33,33,33	0
55	MG	QA	1601	1/1	0.93	0.26	49,49,49,49	0
55	MG	XA	1642	1/1	0.93	0.08	59,59,59,59	0
55	MG	YA	3150	1/1	0.93	0.11	59,59,59,59	0
55	MG	RA	3364	1/1	0.93	0.07	50,50,50,50	0
55	MG	RA	3128	1/1	0.93	0.05	67,67,67,67	0
55	MG	YA	3434	1/1	0.93	0.20	29,29,29,29	0
55	MG	YA	3130	1/1	0.93	0.09	41,41,41,41	0
55	MG	YA	3154	1/1	0.93	0.08	51,51,51,51	0
55	MG	QA	1632	1/1	0.93	0.04	88,88,88,88	0
55	MG	YR	202	1/1	0.93	0.11	15,15,15,15	0
55	MG	RA	3043	1/1	0.93	0.17	49,49,49,49	0
55	MG	RA	3280	1/1	0.93	0.26	86,86,86,86	0
55	MG	RA	3261	1/1	0.93	0.07	50,50,50,50	0
55	MG	YA	3059	1/1	0.93	0.16	47,47,47,47	0
55	MG	XA	1651	1/1	0.93	0.05	93,93,93,93	0
55	MG	RA	3157	1/1	0.93	0.12	93,93,93,93	0
55	MG	RA	3337	1/1	0.93	0.06	83,83,83,83	0
55	MG	RA	3059	1/1	0.93	0.09	25,25,25,25	0
55	MG	YA	3448	1/1	0.93	0.07	47,47,47,47	0
55	MG	RA	3076	1/1	0.93	0.09	43,43,43,43	0
55	MG	YA	3393	1/1	0.93	0.20	67,67,67,67	0
57	ZN	Y9	101	1/1	0.93	0.09	102,102,102,102	0
55	MG	YA	3210	1/1	0.94	0.13	44,44,44,44	0
55	MG	RA	3075	1/1	0.94	0.29	62,62,62,62	0
55	MG	YA	3386	1/1	0.94	0.18	50,50,50,50	0
55	MG	RA	3012	1/1	0.94	0.07	38,38,38,38	0
55	MG	RA	3021	1/1	0.94	0.13	57,57,57,57	0
55	MG	YA	3178	1/1	0.94	0.18	79,79,79,79	0
55	MG	YA	3094	1/1	0.94	0.13	11,11,11,11	0
55	MG	YA	3034	1/1	0.94	0.16	36,36,36,36	0
55	MG	RB	202	1/1	0.94	0.05	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3125	1/1	0.94	0.07	53,53,53,53	0
55	MG	YA	3237	1/1	0.94	0.32	52,52,52,52	0
55	MG	YA	3111	1/1	0.94	0.11	37,37,37,37	0
55	MG	YA	3202	1/1	0.94	0.04	52,52,52,52	0
55	MG	YA	3141	1/1	0.94	0.08	54,54,54,54	0
55	MG	YA	3333	1/1	0.94	0.07	91,91,91,91	0
55	MG	YA	3047	1/1	0.94	0.25	39,39,39,39	0
55	MG	YA	3377	1/1	0.94	0.09	69,69,69,69	0
57	ZN	RY	201	1/1	0.94	0.07	169,169,169,169	0
55	MG	YA	3378	1/1	0.94	0.10	65,65,65,65	0
55	MG	YA	3379	1/1	0.94	0.10	58,58,58,58	0
57	ZN	R9	101	1/1	0.94	0.11	137,137,137,137	0
55	MG	XA	1644	1/1	0.94	0.06	85,85,85,85	0
55	MG	YA	3018	1/1	0.94	0.13	47,47,47,47	0
55	MG	YA	3428	1/1	0.94	0.08	38,38,38,38	0
55	MG	YA	3075	1/1	0.94	0.15	45,45,45,45	0
55	MG	QA	1641	1/1	0.94	0.08	113,113,113,113	0
55	MG	YA	3140	1/1	0.95	0.10	35,35,35,35	0
55	MG	RA	3065	1/1	0.95	0.05	54,54,54,54	0
55	MG	RA	3118	1/1	0.95	0.11	59,59,59,59	0
55	MG	RA	3323	1/1	0.95	0.06	64,64,64,64	0
55	MG	YA	3005	1/1	0.95	0.13	57,57,57,57	0
55	MG	YA	3101	1/1	0.95	0.14	20,20,20,20	0
55	MG	RA	3272	1/1	0.95	0.04	64,64,64,64	0
55	MG	RA	3220	1/1	0.95	0.15	64,64,64,64	0
55	MG	YA	3040	1/1	0.95	0.07	48,48,48,48	0
55	MG	YA	3041	1/1	0.95	0.09	22,22,22,22	0
55	MG	RA	3125	1/1	0.95	0.05	66,66,66,66	0
55	MG	YA	3327	1/1	0.95	0.09	47,47,47,47	0
55	MG	YA	3043	1/1	0.95	0.29	47,47,47,47	0
55	MG	YA	3108	1/1	0.95	0.07	48,48,48,48	0
55	MG	YA	3063	1/1	0.95	0.17	51,51,51,51	0
55	MG	RA	3148	1/1	0.95	0.14	60,60,60,60	0
55	MG	RA	3242	1/1	0.95	0.06	66,66,66,66	0
55	MG	RA	3232	1/1	0.95	0.25	56,56,56,56	0
55	MG	RA	3108	1/1	0.95	0.10	90,90,90,90	0
55	MG	RA	3073	1/1	0.95	0.10	52,52,52,52	0
55	MG	YA	3269	1/1	0.95	0.18	49,49,49,49	0
55	MG	RA	3009	1/1	0.95	0.10	55,55,55,55	0
55	MG	RA	3100	1/1	0.95	0.05	89,89,89,89	0
55	MG	RA	3045	1/1	0.96	0.05	36,36,36,36	0
55	MG	RA	3135	1/1	0.96	0.08	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1654	1/1	0.96	0.06	88,88,88,88	0
55	MG	RA	3302	1/1	0.96	0.06	59,59,59,59	0
55	MG	YA	3080	1/1	0.96	0.17	68,68,68,68	0
55	MG	XA	1601	1/1	0.96	0.16	81,81,81,81	0
55	MG	YA	3208	1/1	0.96	0.12	61,61,61,61	0
55	MG	XA	1661	1/1	0.96	0.15	51,51,51,51	0
55	MG	XA	1602	1/1	0.96	0.09	81,81,81,81	0
55	MG	RA	3303	1/1	0.96	0.08	79,79,79,79	0
55	MG	YA	3185	1/1	0.96	0.09	84,84,84,84	0
55	MG	YA	3349	1/1	0.96	0.07	49,49,49,49	0
55	MG	QA	1611	1/1	0.96	0.14	46,46,46,46	0
55	MG	YA	3087	1/1	0.96	0.20	21,21,21,21	0
55	MG	XA	1645	1/1	0.96	0.21	111,111,111,111	0
55	MG	RA	3092	1/1	0.96	0.18	62,62,62,62	0
55	MG	RA	3104	1/1	0.96	0.16	58,58,58,58	0
55	MG	RA	3093	1/1	0.96	0.06	60,60,60,60	0
55	MG	RA	3189	1/1	0.96	0.07	85,85,85,85	0
55	MG	RA	3048	1/1	0.96	0.04	46,46,46,46	0
55	MG	YA	3070	1/1	0.96	0.14	38,38,38,38	0
55	MG	RA	3031	1/1	0.96	0.08	50,50,50,50	0
55	MG	YA	3223	1/1	0.96	0.28	45,45,45,45	0
55	MG	QA	1622	1/1	0.96	0.10	68,68,68,68	0
55	MG	YA	3048	1/1	0.96	0.17	10,10,10,10	0
55	MG	YA	3124	1/1	0.96	0.13	48,48,48,48	0
55	MG	YA	3452	1/1	0.96	0.06	41,41,41,41	0
55	MG	RA	3087	1/1	0.96	0.08	33,33,33,33	0
55	MG	QA	1657	1/1	0.96	0.09	81,81,81,81	0
55	MG	YA	3069	1/1	0.97	0.10	30,30,30,30	0
55	MG	QA	1669	1/1	0.97	0.09	116,116,116,116	0
55	MG	RA	3066	1/1	0.97	0.05	80,80,80,80	0
55	MG	QA	1618	1/1	0.97	0.04	72,72,72,72	0
55	MG	YA	3090	1/1	0.97	0.10	47,47,47,47	0
55	MG	YA	3446	1/1	0.97	0.08	43,43,43,43	0
55	MG	RA	3098	1/1	0.97	0.06	56,56,56,56	0
55	MG	XA	1617	1/1	0.97	0.09	57,57,57,57	0
55	MG	XA	1637	1/1	0.97	0.06	90,90,90,90	0
55	MG	RB	208	1/1	0.97	0.08	67,67,67,67	0
55	MG	YA	3023	1/1	0.97	0.13	52,52,52,52	0
56	SF4	XD	301	8/8	0.97	0.06	128,182,257,300	0
55	MG	XA	1667	1/1	0.97	0.05	82,82,82,82	0
55	MG	YA	3050	1/1	0.97	0.08	51,51,51,51	0
55	MG	QA	1608	1/1	0.97	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3374	1/1	0.97	0.11	66,66,66,66	0
55	MG	YA	3065	1/1	0.97	0.15	43,43,43,43	0
55	MG	YA	3336	1/1	0.97	0.07	27,27,27,27	0
55	MG	YA	3066	1/1	0.97	0.13	50,50,50,50	0
55	MG	YA	3119	1/1	0.97	0.08	42,42,42,42	0
55	MG	XA	1658	1/1	0.97	0.06	89,89,89,89	0
55	MG	RA	3019	1/1	0.97	0.07	49,49,49,49	0
55	MG	XA	1615	1/1	0.98	0.08	51,51,51,51	0
56	SF4	QD	301	8/8	0.98	0.05	161,182,293,373	0
55	MG	XA	1627	1/1	0.98	0.04	118,118,118,118	0
55	MG	XA	1621	1/1	0.98	0.11	54,54,54,54	0
55	MG	YA	3352	1/1	0.98	0.07	35,35,35,35	0
55	MG	YA	3180	1/1	0.98	0.05	65,65,65,65	0
55	MG	RA	3304	1/1	0.98	0.07	82,82,82,82	0
57	ZN	R6	101	1/1	0.98	0.04	109,109,109,109	0
55	MG	QA	1627	1/1	0.98	0.04	60,60,60,60	0
55	MG	YB	203	1/1	0.98	0.05	44,44,44,44	0
55	MG	XA	1618	1/1	0.98	0.07	46,46,46,46	0
55	MG	YA	3447	1/1	0.98	0.27	15,15,15,15	0
55	MG	YA	3029	1/1	0.98	0.08	38,38,38,38	0
57	ZN	Y6	101	1/1	0.98	0.06	98,98,98,98	0
55	MG	RA	3107	1/1	0.98	0.07	43,43,43,43	0
55	MG	YA	3195	1/1	0.99	0.04	74,74,74,74	0
55	MG	YA	3085	1/1	0.99	0.03	24,24,24,24	0
55	MG	RA	3044	1/1	0.99	0.04	46,46,46,46	0
55	MG	YA	3019	1/1	0.99	0.07	48,48,48,48	0
55	MG	RA	3013	1/1	0.99	0.03	52,52,52,52	0
55	MG	YA	3109	1/1	0.99	0.03	45,45,45,45	0
55	MG	YA	3020	1/1	1.00	0.09	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.