



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 01:20 PM UTC

PDB ID : 6OSI / pdb_00006osi
Title : Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (near cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-01
Resolution : 4.14 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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

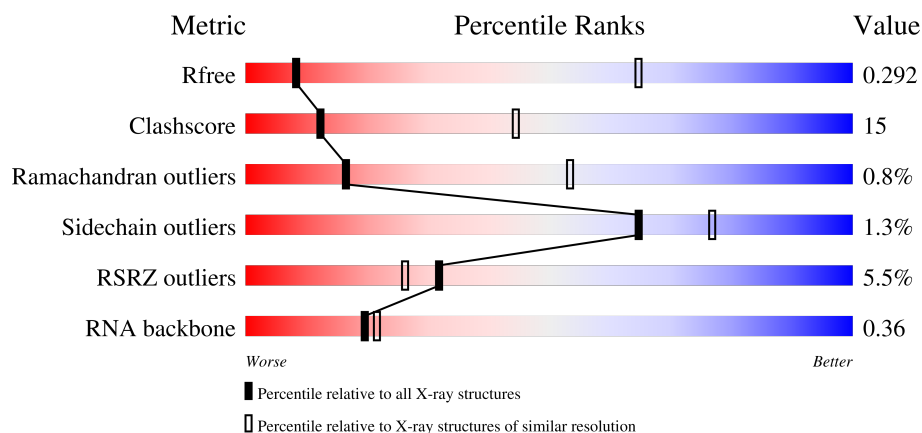
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.14 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}	164625	1166 (4.48-3.80)
Clashscore	180529	1233 (4.48-3.80)
Ramachandran outliers	177936	1158 (4.48-3.80)
Sidechain outliers	177891	1145 (4.48-3.80)
RSRZ outliers	164620	1164 (4.48-3.80)
RNA backbone	3690	1145 (5.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1521	28% 52% 18% •
1	XA	1521	32% 47% 17% •
2	QB	256	4% 61% 30% • 8%
2	XB	256	7% 67% 24% • 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	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

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Mol	Chain	Length	Quality of chain
28	R4	71	
28	Y4	71	
29	R5	60	
29	Y5	60	
30	R6	54	
30	Y6	54	
31	R7	49	
31	Y7	49	
32	R8	65	
32	Y8	65	
33	R9	37	
33	Y9	37	
34	RA	2905	
34	YA	2905	
35	RB	122	
35	YB	122	
36	RD	276	
36	YD	276	
37	RE	206	
37	YE	206	
38	RF	210	
38	YF	210	
39	RG	182	
39	YG	182	
40	RH	180	

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Mol	Chain	Length	Quality of chain
40	YH	180	
41	RI	148	
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	

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Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	

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	1610	-	-	-	X
55	MG	QA	1622	-	-	-	X
55	MG	QE	201	-	-	-	X
55	MG	RA	2912	-	-	-	X
55	MG	RA	2921	-	-	-	X
55	MG	RA	2954	-	-	-	X
55	MG	RA	2970	-	-	-	X
55	MG	RA	2975	-	-	-	X
55	MG	RA	2976	-	-	-	X
55	MG	RA	2999	-	-	-	X
55	MG	RA	3013	-	-	-	X
55	MG	RA	3051	-	-	-	X
55	MG	RA	3057	-	-	-	X
55	MG	RA	3064	-	-	-	X
55	MG	RA	3071	-	-	-	X
55	MG	RA	3075	-	-	-	X
55	MG	RA	3078	-	-	-	X
55	MG	RA	3083	-	-	-	X
55	MG	RA	3101	-	-	-	X
55	MG	RA	3103	-	-	-	X
55	MG	RA	3133	-	-	-	X
55	MG	RA	3139	-	-	-	X
55	MG	RA	3144	-	-	-	X
55	MG	RA	3147	-	-	-	X
55	MG	RA	3152	-	-	-	X
55	MG	RA	3162	-	-	-	X
55	MG	RA	3220	-	-	-	X
55	MG	RA	3221	-	-	-	X
55	MG	RA	3223	-	-	-	X
55	MG	RA	3260	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	RA	3286	-	-	-	X
55	MG	RA	3307	-	-	-	X
55	MG	RA	3310	-	-	-	X
55	MG	RA	3318	-	-	-	X
55	MG	RE	304	-	-	-	X
55	MG	XA	1605	-	-	-	X
55	MG	XA	1610	-	-	-	X
55	MG	XA	1612	-	-	-	X
55	MG	XA	1613	-	-	-	X
55	MG	XA	1621	-	-	-	X
55	MG	XA	1657	-	-	-	X
55	MG	XA	1665	-	-	-	X
55	MG	XA	1688	-	-	X	-
55	MG	Y8	101	-	-	-	X
55	MG	YA	2904	-	-	-	X
55	MG	YA	2905	-	-	-	X
55	MG	YA	2907	-	-	-	X
55	MG	YA	2930	-	-	-	X
55	MG	YA	2932	-	-	-	X
55	MG	YA	2933	-	-	-	X
55	MG	YA	2934	-	-	-	X
55	MG	YA	2936	-	-	-	X
55	MG	YA	2952	-	-	-	X
55	MG	YA	2953	-	-	-	X
55	MG	YA	2955	-	-	-	X
55	MG	YA	2962	-	-	-	X
55	MG	YA	2974	-	-	-	X
55	MG	YA	2983	-	-	-	X
55	MG	YA	2984	-	-	-	X
55	MG	YA	2985	-	-	-	X
55	MG	YA	3004	-	-	-	X
55	MG	YA	3010	-	-	-	X
55	MG	YA	3017	-	-	-	X
55	MG	YA	3018	-	-	-	X
55	MG	YA	3031	-	-	-	X
55	MG	YA	3087	-	-	-	X
55	MG	YA	3097	-	-	-	X
55	MG	YA	3101	-	-	-	X
55	MG	YA	3117	-	-	-	X
55	MG	YA	3120	-	-	-	X
55	MG	YA	3122	-	-	-	X
55	MG	YA	3126	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3153	-	-	-	X
55	MG	YA	3168	-	-	-	X
55	MG	YA	3175	-	-	-	X
55	MG	YA	3192	-	-	X	-
55	MG	YA	3194	-	-	-	X
55	MG	YA	3202	-	-	-	X
55	MG	YA	3205	-	-	-	X
55	MG	YA	3211	-	-	-	X
55	MG	YA	3237	-	-	-	X
55	MG	YA	3239	-	-	-	X
55	MG	YA	3245	-	-	-	X
55	MG	YA	3262	-	-	-	X
55	MG	YA	3263	-	-	-	X
55	MG	YA	3276	-	-	-	X
55	MG	YA	3281	-	-	-	X
55	MG	YA	3288	-	-	-	X
55	MG	YA	3290	-	-	-	X
56	SF4	QD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291185 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	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
1	XA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

- 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	105	Total	C	N	O		0	0	0
			816	519	152	145				
9	XI	107	Total	C	N	O		0	0	0
			834	530	157	147				

- 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	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	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 tRNA(Pro).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			
22	XV	68	Total	C	N	O	P	0	0	0
			1452	647	260	477	68			

- 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
			409	184	81	126	18			
23	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

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

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

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

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	193	Total	C	N	O	S	0	0	0
			1529	973	270	283	3			

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

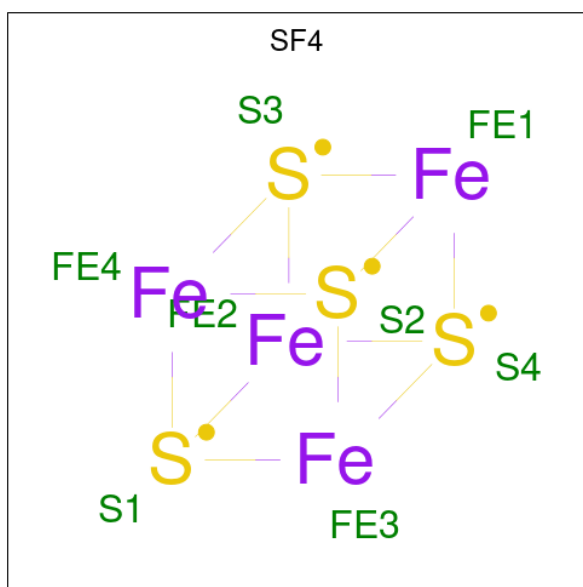
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	70	Total	Mg	0	0
			70	70		
55	QE	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	2	Total	Mg	0	0
			2	2		
55	QL	2	Total	Mg	0	0
			2	2		
55	R0	2	Total	Mg	0	0
			2	2		
55	R3	1	Total	Mg	0	0
			1	1		
55	R8	2	Total	Mg	0	0
			2	2		
55	RA	432	Total	Mg	0	0
			432	432		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	4	Total	Mg	0	0
			4	4		
55	RF	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		
55	RO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XA	88	Total 88	Mg 88	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XO	1	Total 1	Mg 1	0	0
55	Y1	1	Total 1	Mg 1	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	2	Total 2	Mg 2	0	0
55	YA	394	Total 394	Mg 394	0	0
55	YB	1	Total 1	Mg 1	0	0
55	YD	2	Total 2	Mg 2	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YP	1	Total 1	Mg 1	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	YR	2	Total 2	Mg 2	0	0
55	YU	1	Total 1	Mg 1	0	0
55	YX	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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		

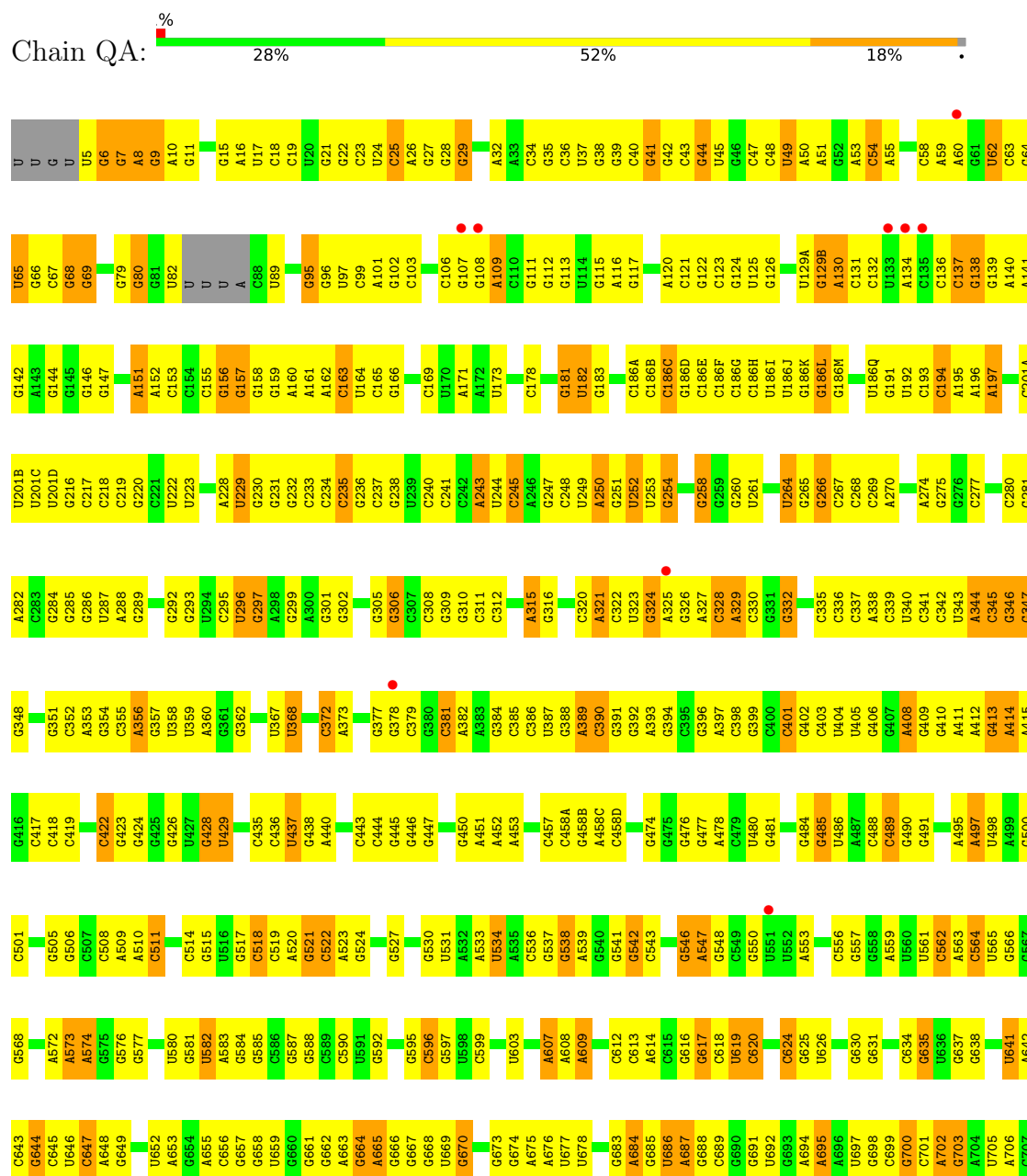
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

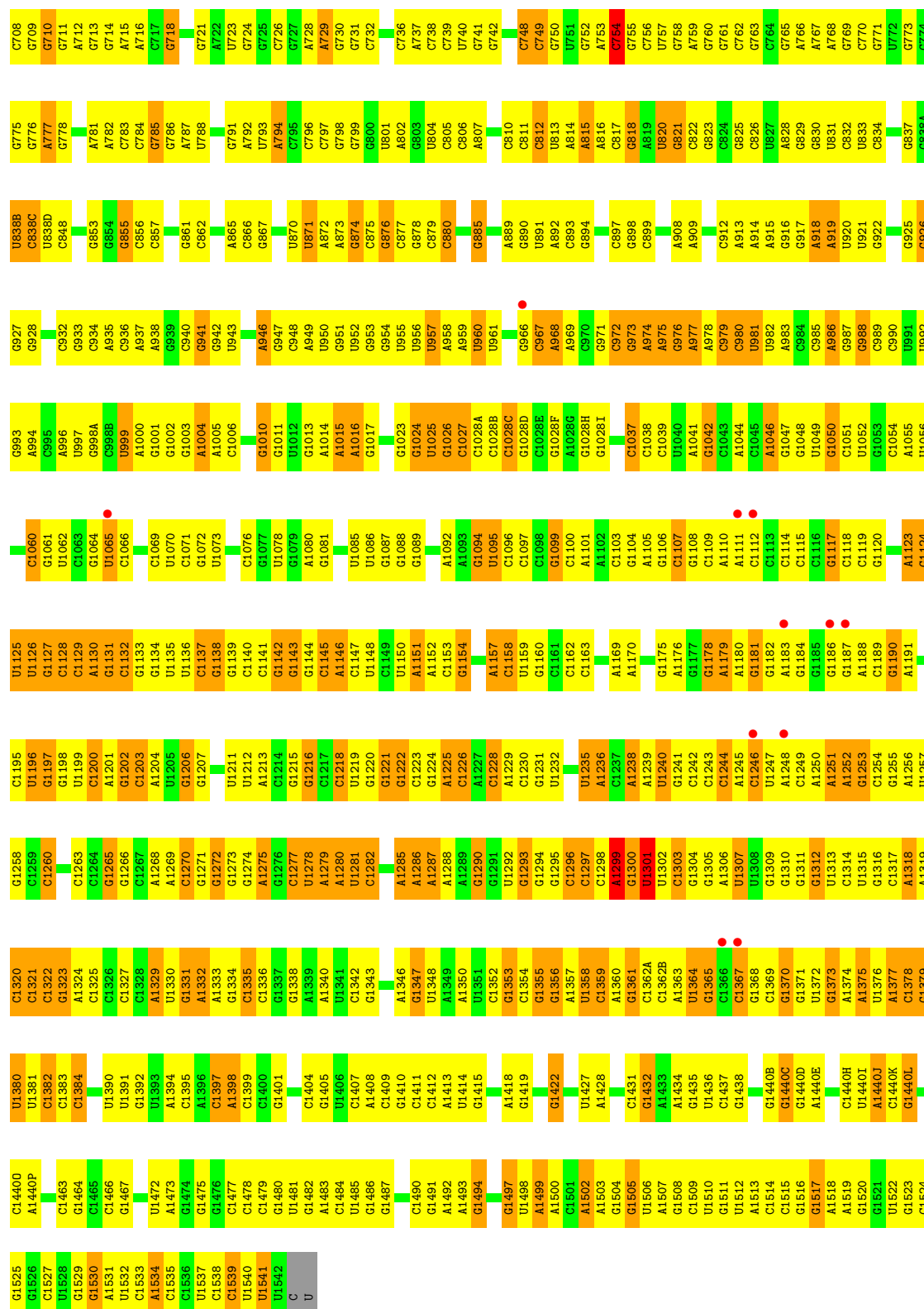
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	Y9	1	Total	Zn	0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

3 Residue-property plots

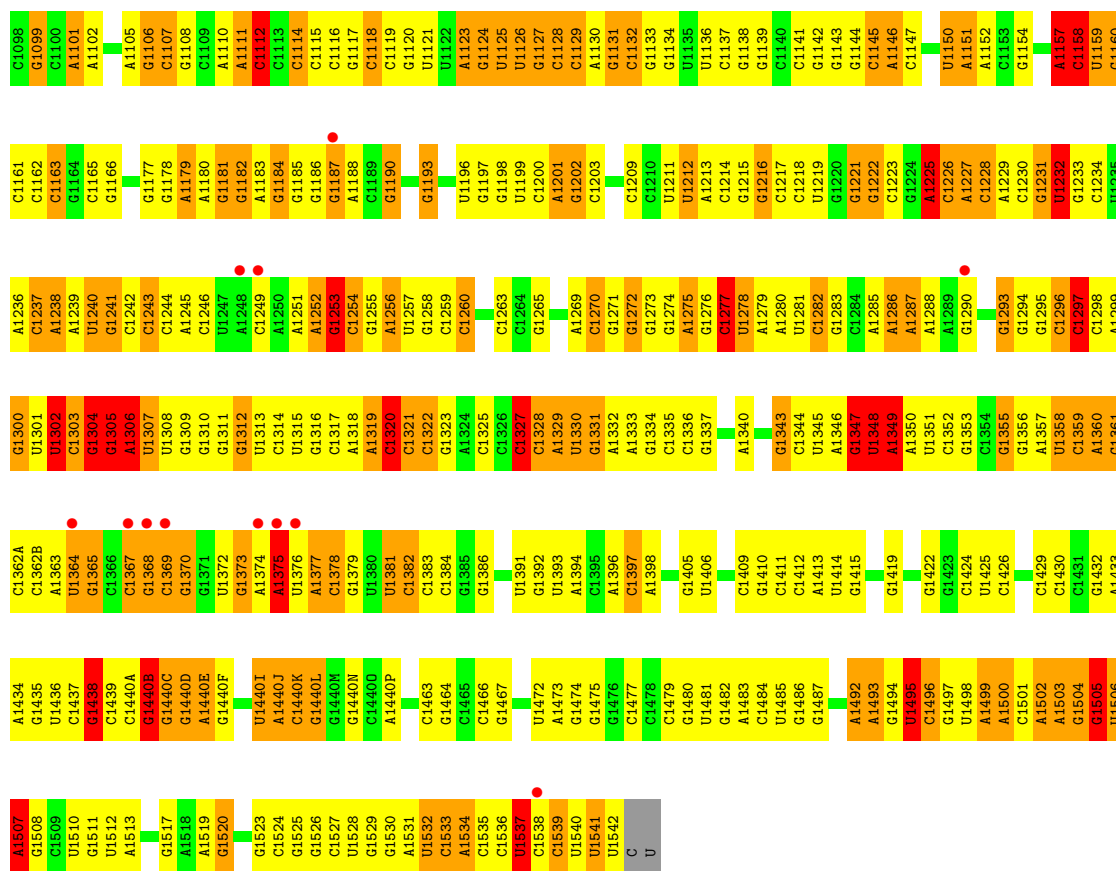
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

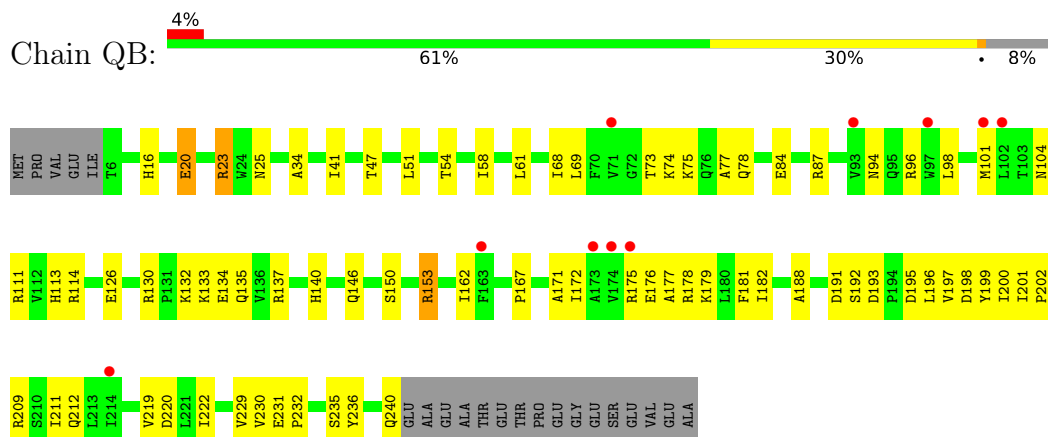




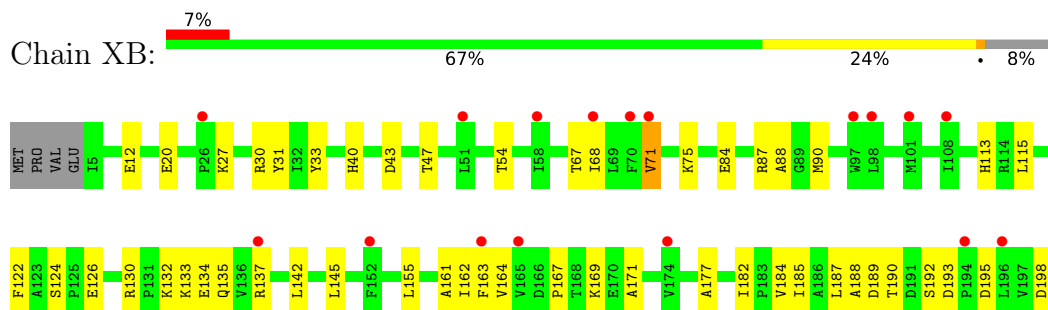


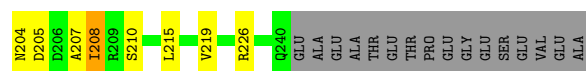


• Molecule 2: 30S ribosomal protein S2

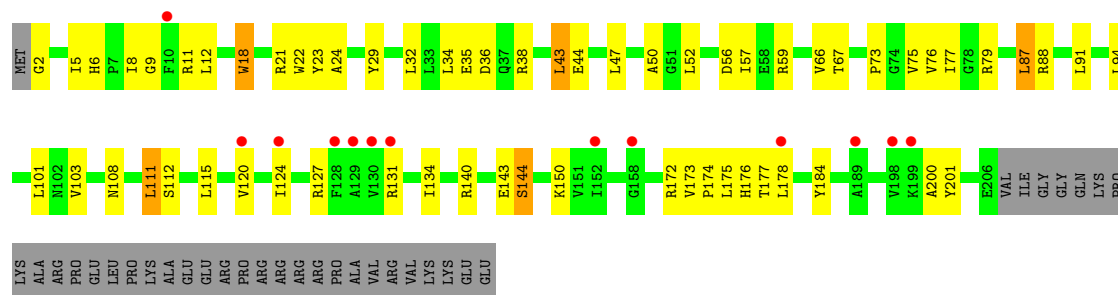


• Molecule 2: 30S ribosomal protein S2

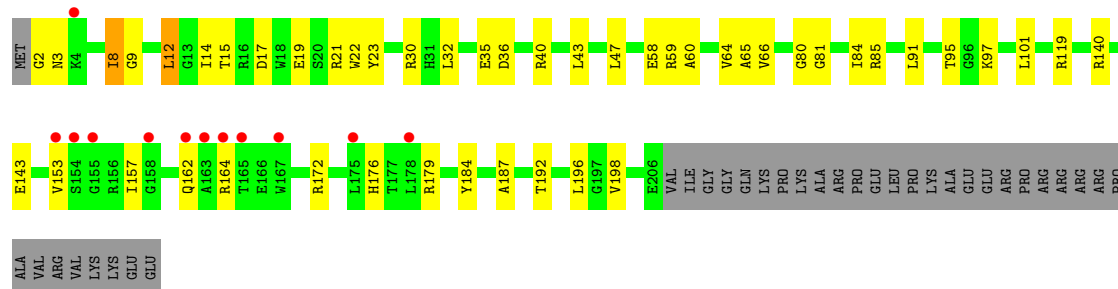




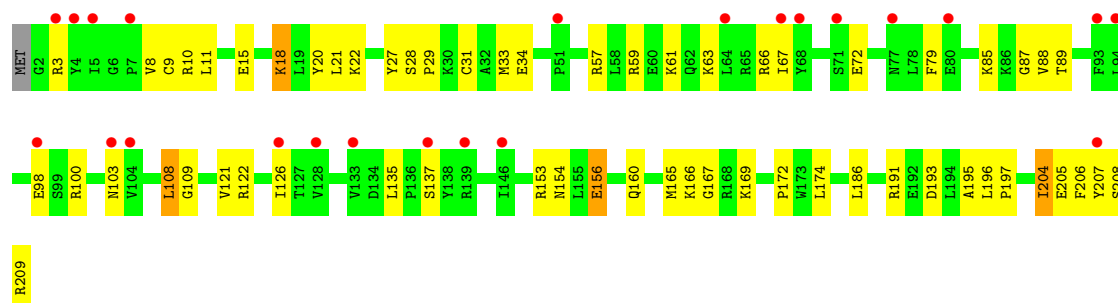
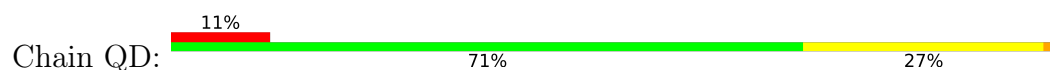
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

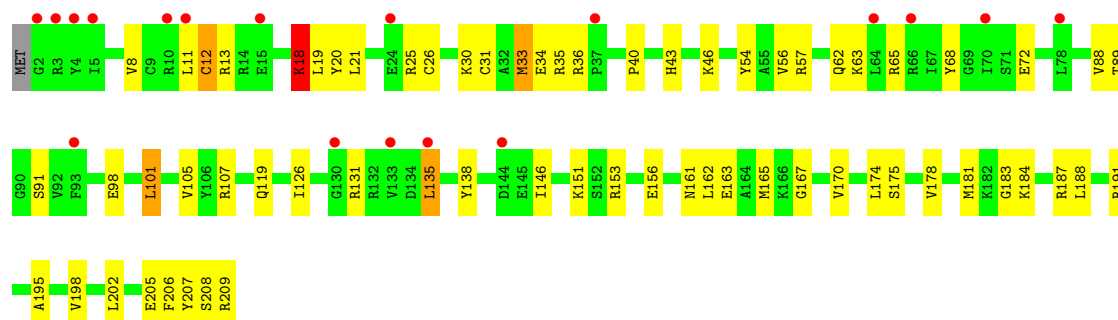


• Molecule 4: 30S ribosomal protein S4

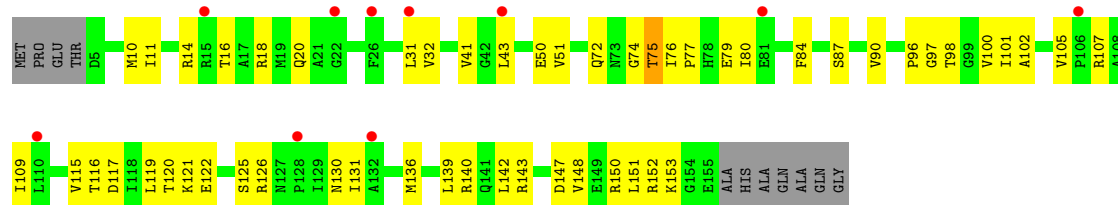


• Molecule 4: 30S ribosomal protein S4

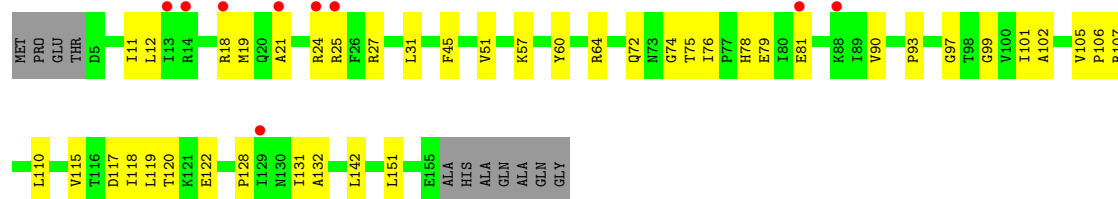




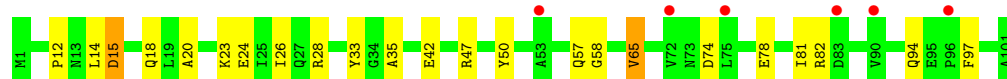
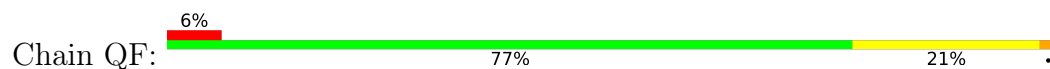
• Molecule 5: 30S ribosomal protein S5



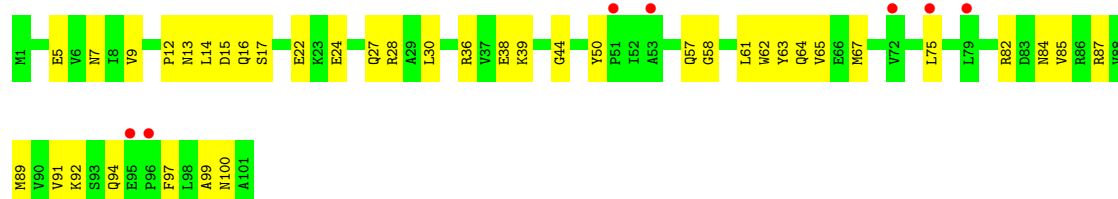
• Molecule 5: 30S ribosomal protein S5



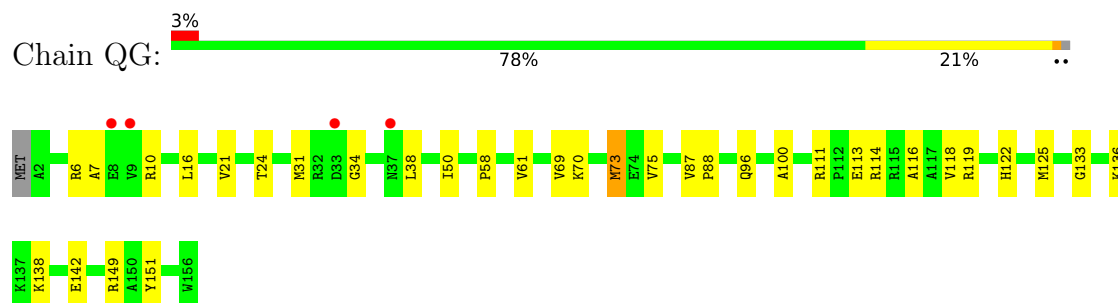
• Molecule 6: 30S ribosomal protein S6



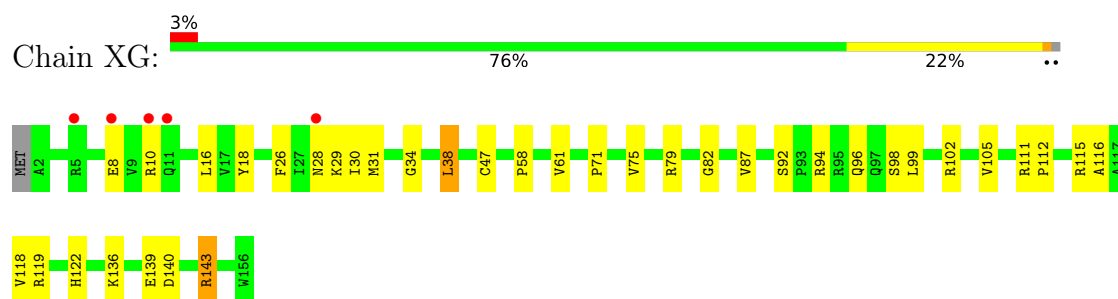
• Molecule 6: 30S ribosomal protein S6



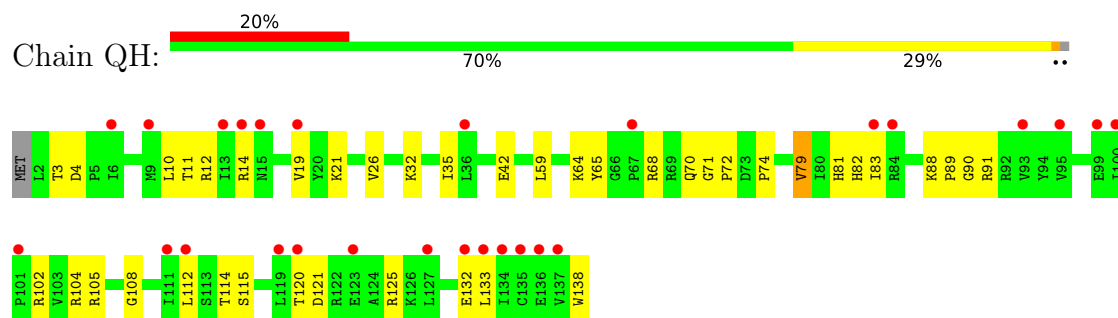
- Molecule 7: 30S ribosomal protein S7



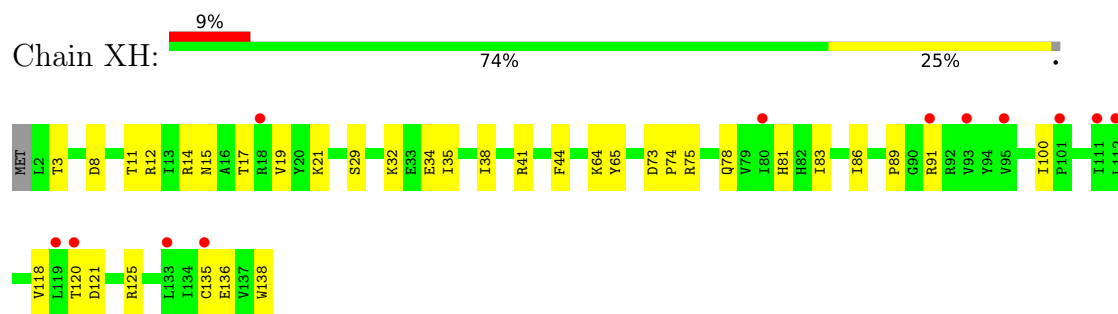
- Molecule 7: 30S ribosomal protein S7



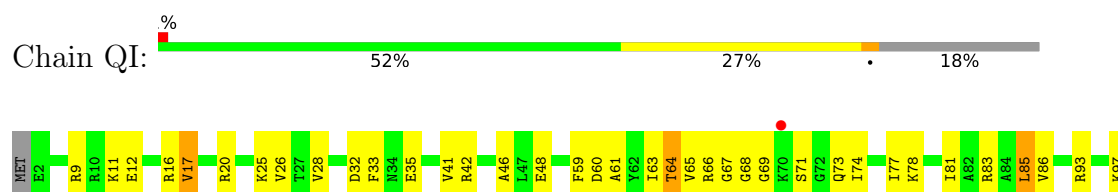
- Molecule 8: 30S ribosomal protein S8

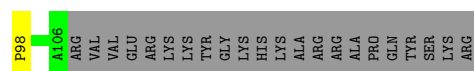


- Molecule 8: 30S ribosomal protein S8

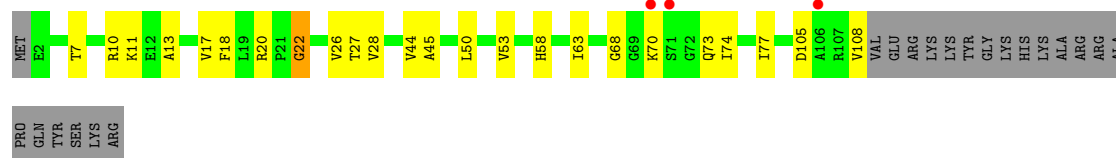


- Molecule 9: 30S ribosomal protein S9

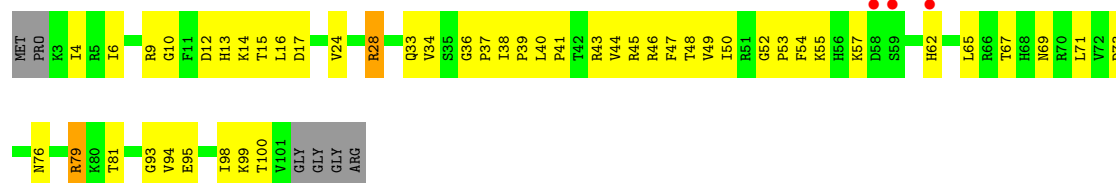




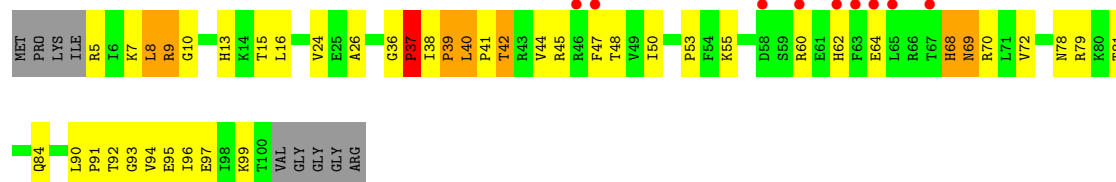
- Molecule 9: 30S ribosomal protein S9



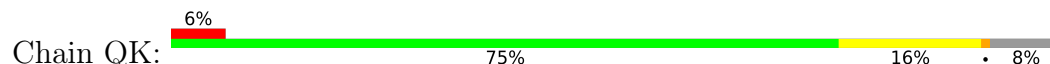
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

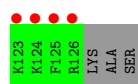


- Molecule 11: 30S ribosomal protein S11

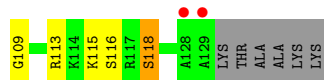
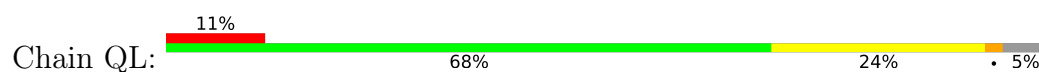


- Molecule 11: 30S ribosomal protein S11

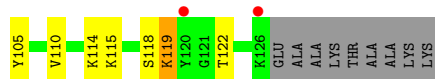
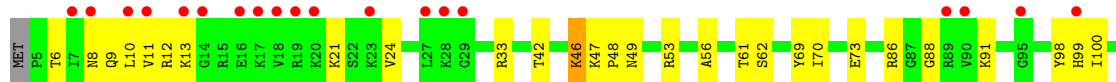




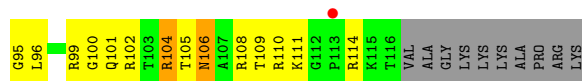
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



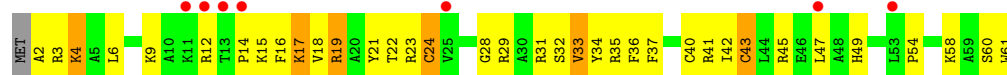
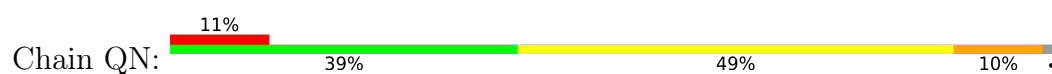
- Molecule 13: 30S ribosomal protein S13



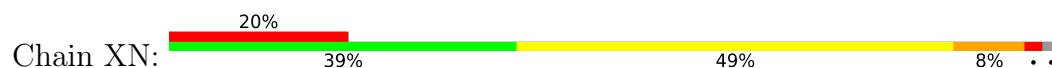
- Molecule 13: 30S ribosomal protein S13



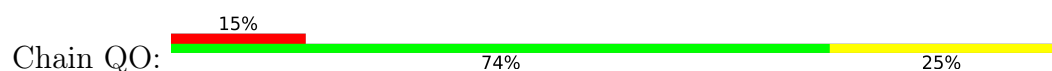
- Molecule 14: 30S ribosomal protein S14 type Z



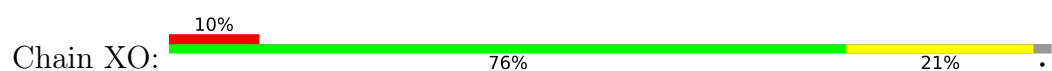
- Molecule 14: 30S ribosomal protein S14 type Z



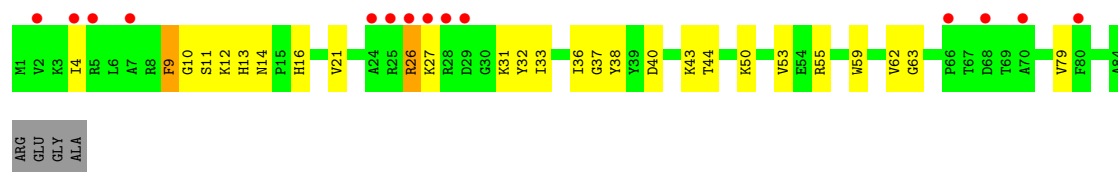
- Molecule 15: 30S ribosomal protein S15



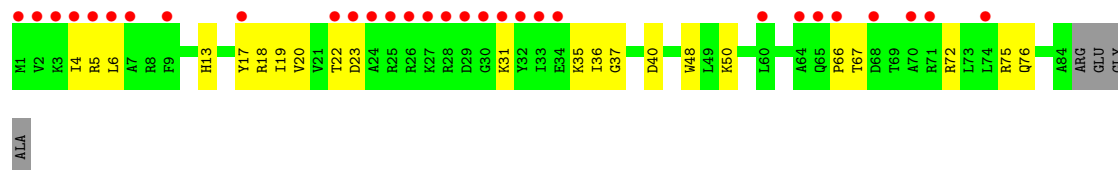
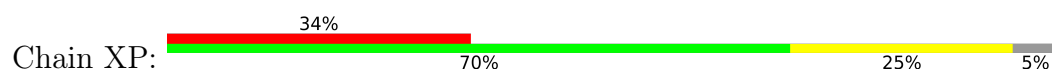
- Molecule 15: 30S ribosomal protein S15



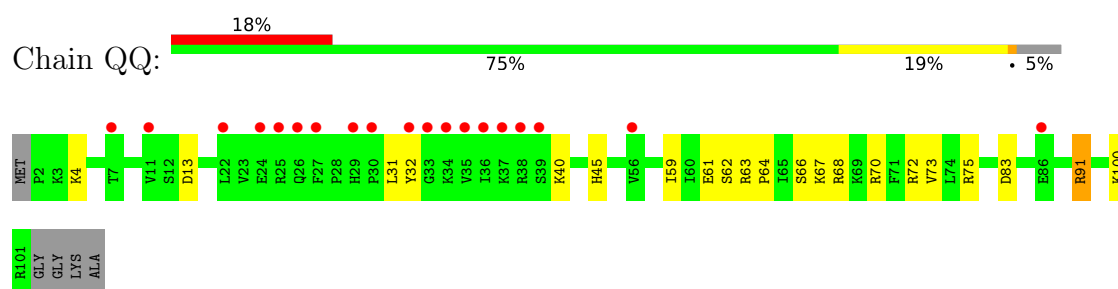
- Molecule 16: 30S ribosomal protein S16



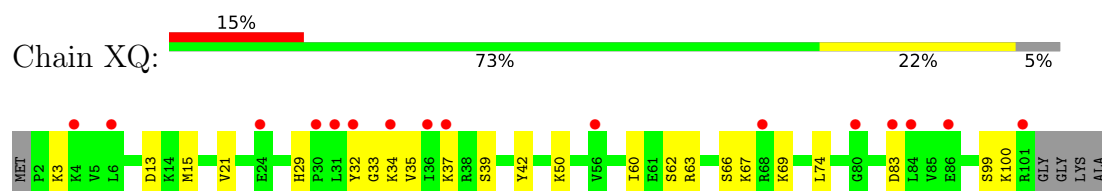
- Molecule 16: 30S ribosomal protein S16



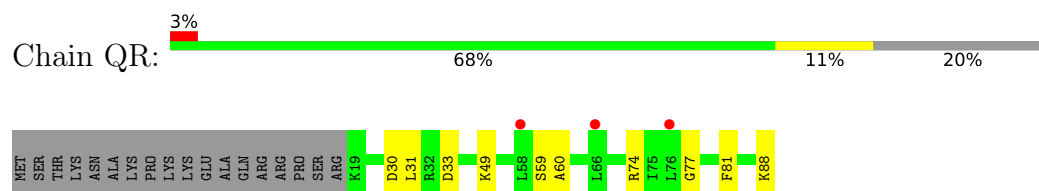
- Molecule 17: 30S ribosomal protein S17



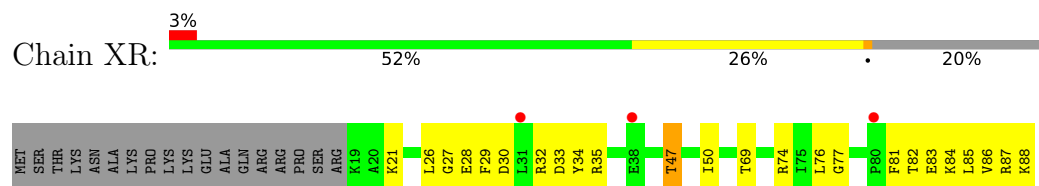
- Molecule 17: 30S ribosomal protein S17



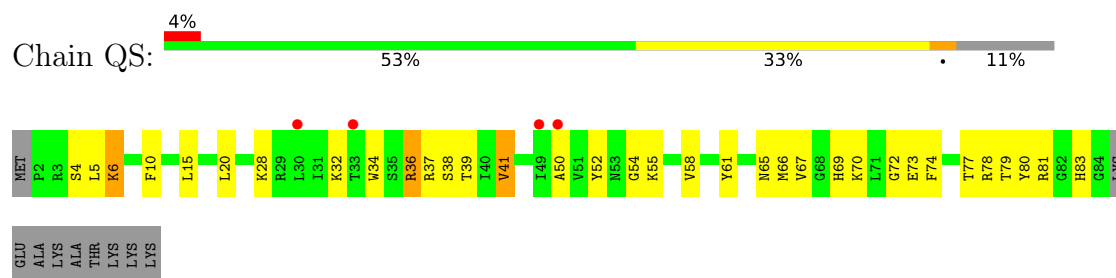
- Molecule 18: 30S ribosomal protein S18



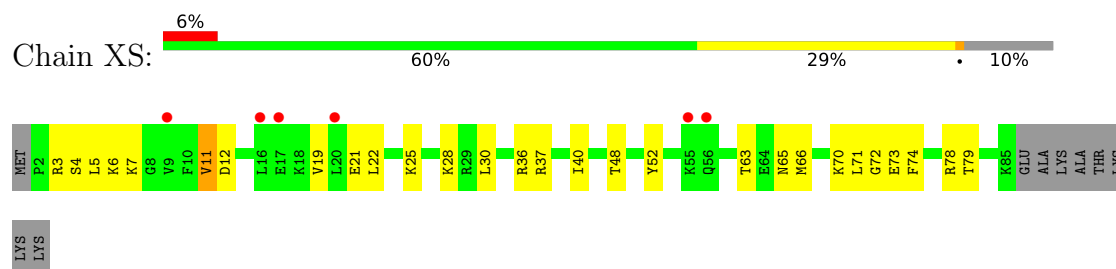
- Molecule 18: 30S ribosomal protein S18



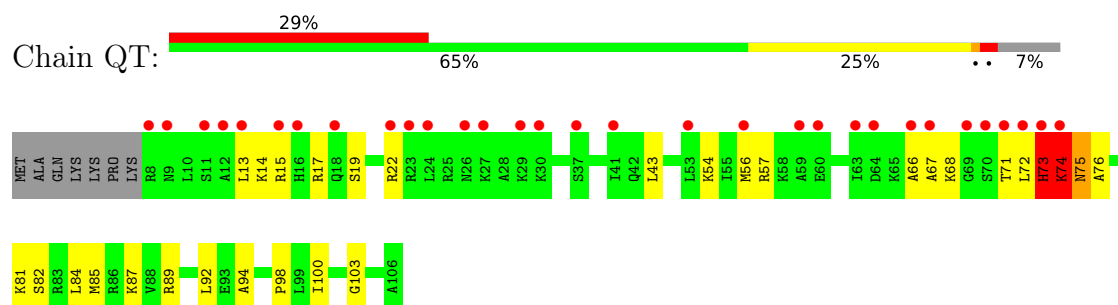
- Molecule 19: 30S ribosomal protein S19



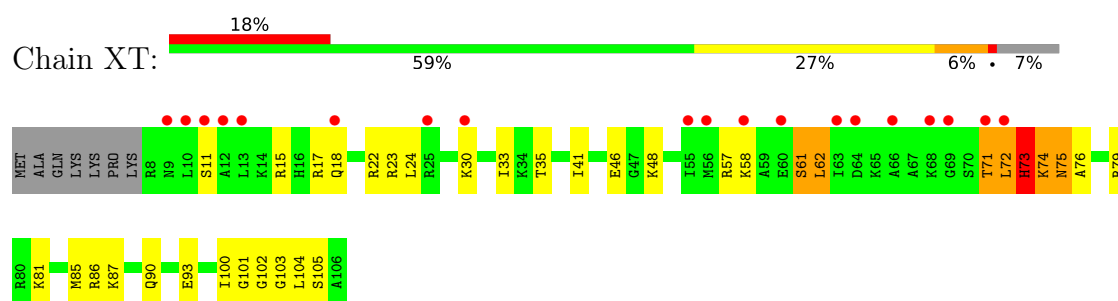
- Molecule 19: 30S ribosomal protein S19



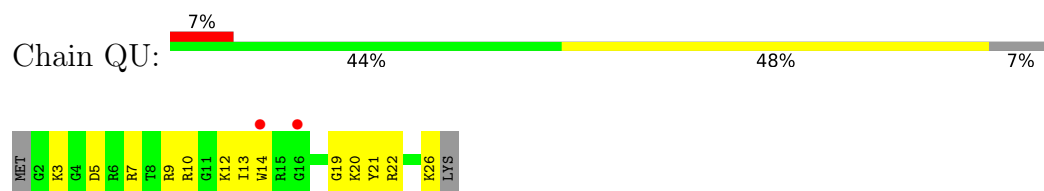
- Molecule 20: 30S ribosomal protein S20



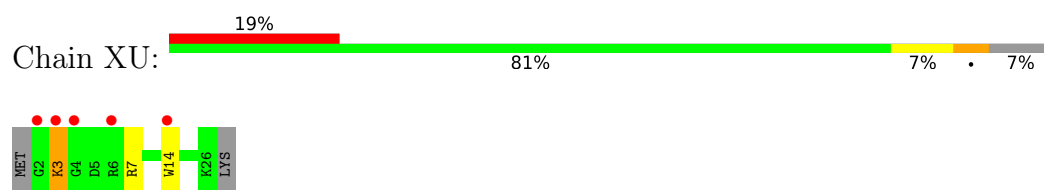
- Molecule 20: 30S ribosomal protein S20



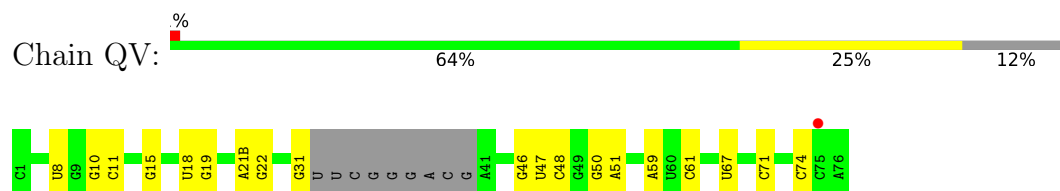
- Molecule 21: 30S ribosomal protein Thx



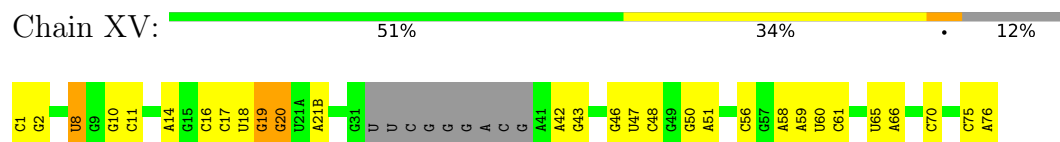
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA(Pro)



- Molecule 22: tRNA(Pro)



- Molecule 23: mRNA

Chain QX:  42% 53% 5%



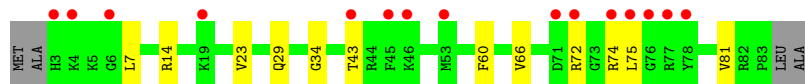
- Molecule 23: mRNA

Chain XX:  47% 26% 26%



- Molecule 24: 50S ribosomal protein L27

Chain R0:  18% 81% 14% 5%



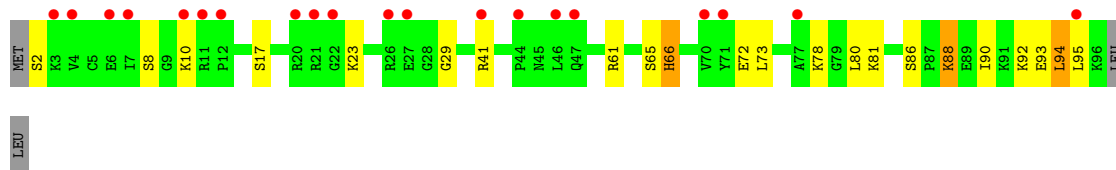
- Molecule 24: 50S ribosomal protein L27

Chain Y0:  7% 81% 15% .



- Molecule 25: 50S ribosomal protein L28

Chain R1:  20% 74% 19% . .



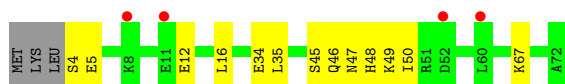
- Molecule 25: 50S ribosomal protein L28

Chain Y1:  15% 78% 17% 5%

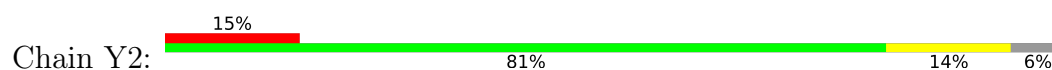


- Molecule 26: 50S ribosomal protein L29

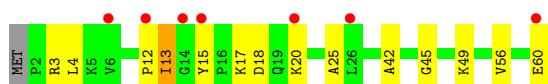
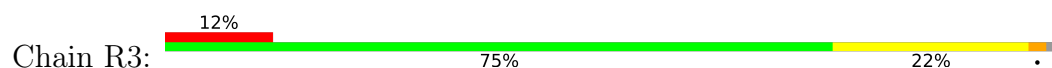
Chain R2:  6% 78% 18% .



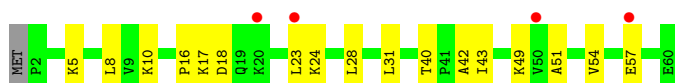
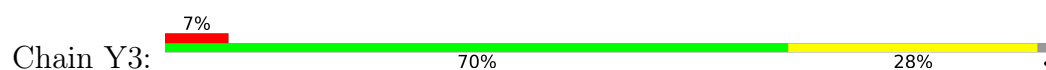
- Molecule 26: 50S ribosomal protein L29



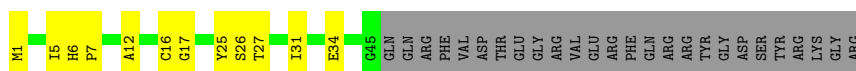
- Molecule 27: 50S ribosomal protein L30



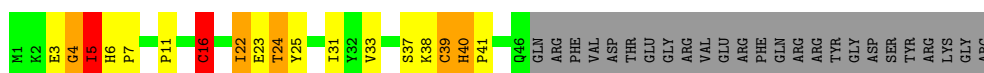
- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



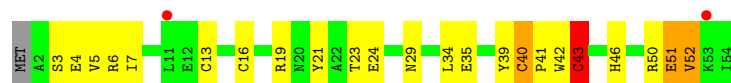
- Molecule 29: 50S ribosomal protein L32



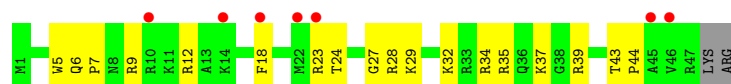
- Molecule 30: 50S ribosomal protein L33



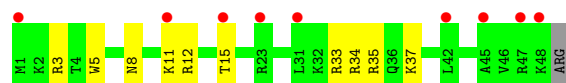
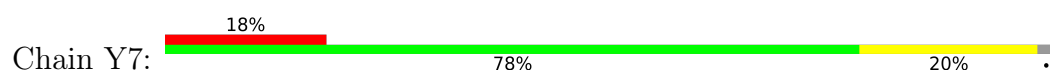
- Molecule 30: 50S ribosomal protein L33



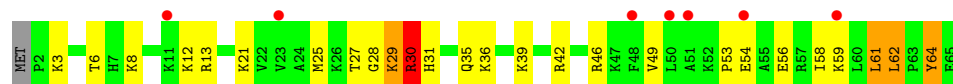
- Molecule 31: 50S ribosomal protein L34



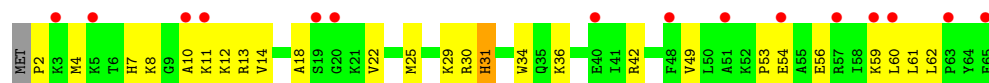
- Molecule 31: 50S ribosomal protein L34



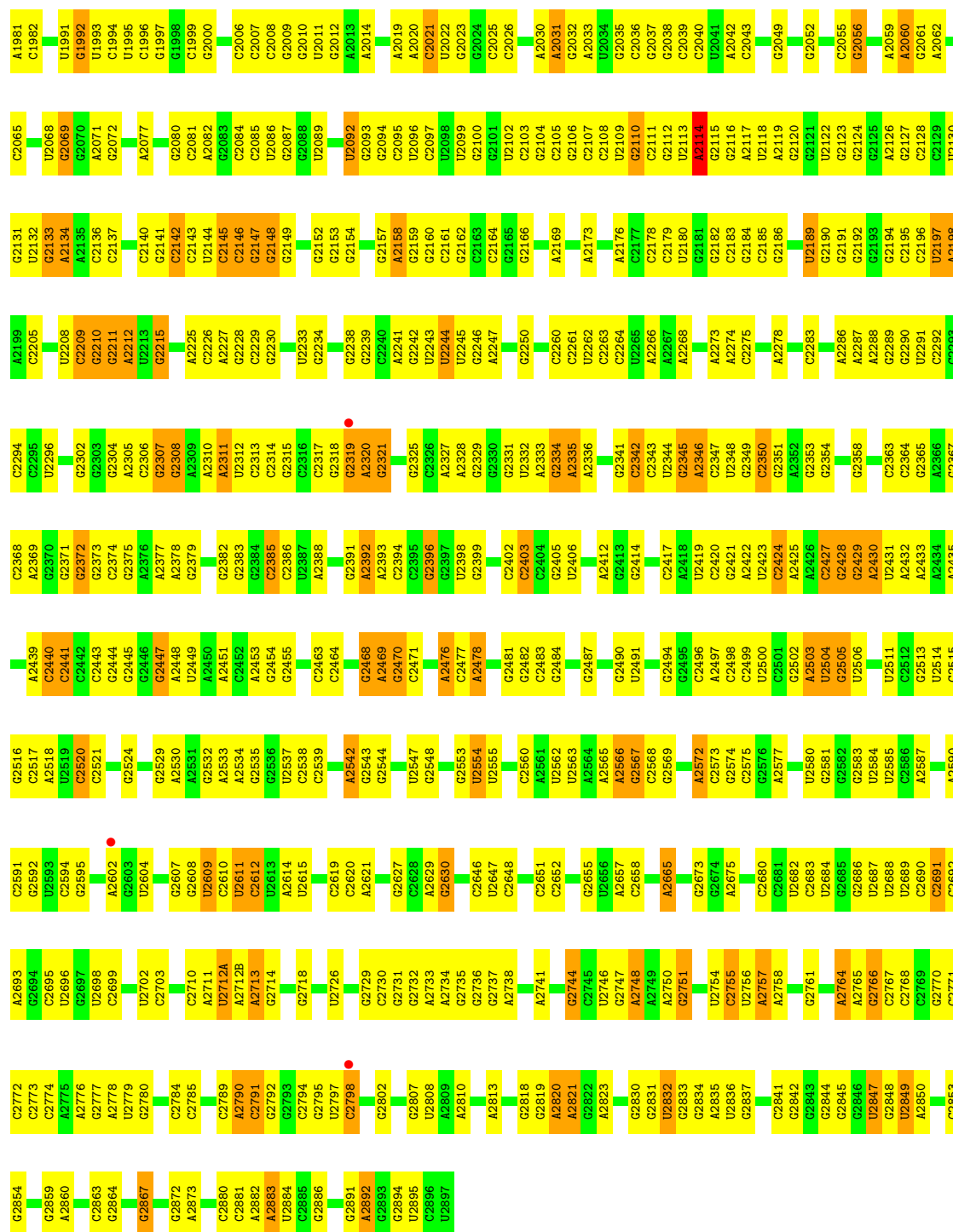
- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35

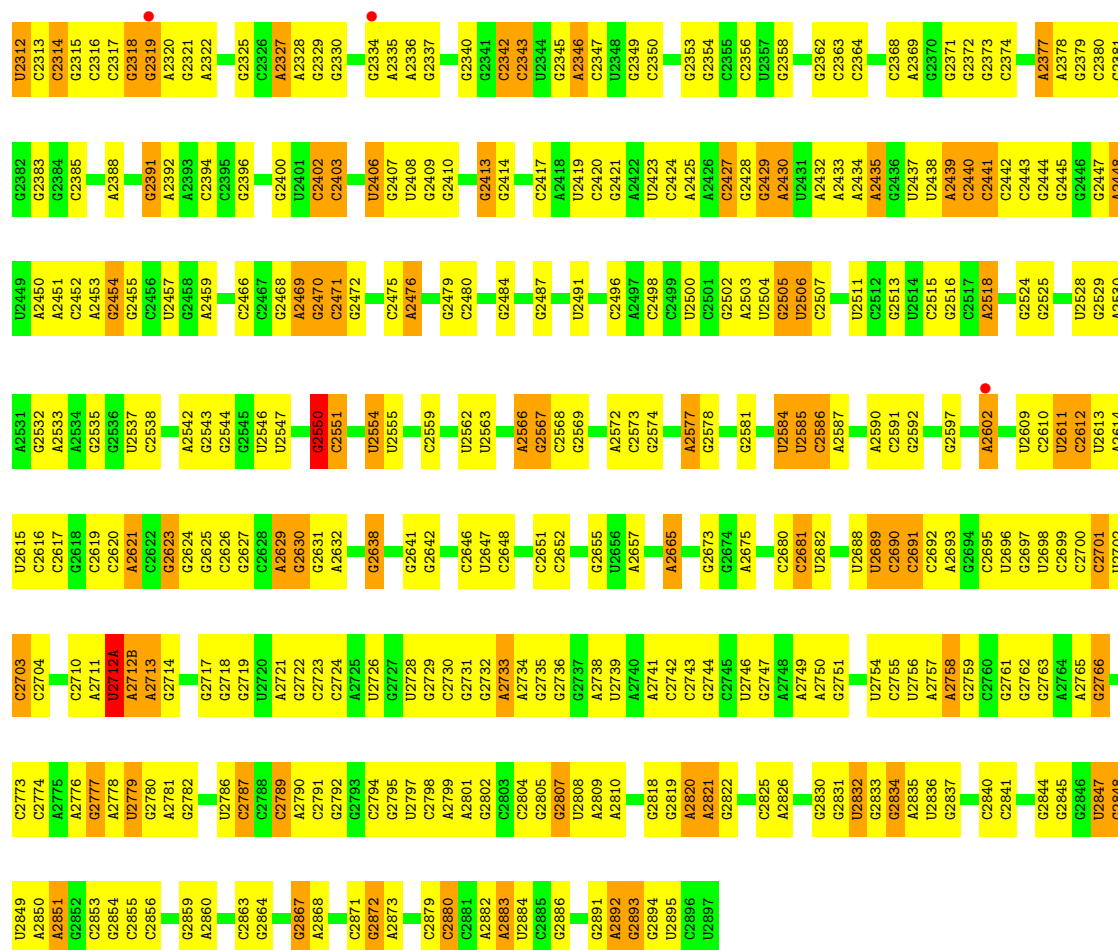


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U1808	A1809	A1810	G1811	A1812	G1813	G1814	A1815	G1816	G1817	U1818	A1819	U1820	A1821	A1822	A1823	A1824	A1825	A1826	C1827	A1828	U1829	U1834	G1835	C1838	A1846	A1847	A1848	G1849	G1850	A1853	A1854	G1857	G1858	U1859	G1864	G1869	C1871	A1872	A1878	C1881	C1882	G1883	A1884	A1885	C1886	C1887	G1888	A1889	C1892	A1893	G1896								
C1712	G1718	G1725	G1728	A1729	U1730	G1731	A1732	G1733	C1742	G1743	C1752	G1753	C1754	A1755	G1756	A1759	A1762	G1763	G1764	U1768	G1769	G1770	C1771	A1772	A1773	G1774	U1775	G1776	A1780	C1781	C1782	A1783	A1784	A1787	C1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	U1796	C1797	G1798	U1799	G1800	G1801	A1802	A1803									
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U1060	A988	A989	C991	A1142B	U1066	A1067	G1068	A1069	A981	A996	G997	C998	U999	A1000	C1005	U1068	U1083	U1089	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	G1030	G1031	U1032	A1033	U958	A960	C961	C967	G968	C884	A887	C970	C971	G972	A973	C974A	C974B	A980	A983	C904	U905	G906	A907	C908	A909	C989	C990	C992		
C753	C754	C755	C756	C757	C758	C759	A764	G765	G769	G775	G776	A777	G778	U779	G780	A781	A782	A783	A784	G785	G786	U787	A788	A789	C790	C791	G792	C795	C796	C797	C798	G799	A800	A804	G805	C806	U807	G808	G809	C812	U813	C814	C815	C816	C817	A818	A819	C903	A821	U822	G823	A824	C825						



G1093	A1028	C949	U877	C806	C730	G	U607	C530	G458	C377	U306	A270B	A197	G97
U1094	A1029	C949	A878	U807	C731	C	A808	C531	U459	U380	G307	A270C	C198	G98
A1095	G1030	A953	A879	G808		C	G609B	A532	A460	C461		C270D	A199	U99
U1096	U1033	G956	G880	U811	G738	C	C654U	G533	C461	G382	A311	C270E	G204	G101
A1097	G1034	A957	G881	C812	U740	G654U	C654U	U534	C462	U383	G312	U270F	A205	G102
A1098	U1035	U958	C882	U813	G741	A654V	C654V	C535	U463	U384		C270G	G205	A103
A1099	G1036	U958	G883	C814	G742	A654W	C654W	A536	G463		C316	C270H		
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C1102	C1038	C886	C887	G816	G745	A655	G655	G539	G467	C386	C318	C270J	C209	C107
A1103	A1039	A960	A887	C817	U746	U657	A616	G540	G468	U387	C319	G270K	C210	
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G1114	A1047	C974A	G823	G625	C755	C665	G625	G556	A479	C404	A331	G270S	A222	C129
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C1119	G1051	C984	A901	G831	G759		G629	G563	C486	C409	G338	G270X	A228	G135
G1120		C985						C564	C487			G270Y	U230	
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G1122	G1055	G987	U905	A835	G765	A675	A633	U588	G491	C411	G342	G271C	G231	G138
C1123	G1056	A988	G906		C766	A676	C634			A412	G343	U271D	A233	G139
G1124	A1057	G989	U907	U839			C635			C413	G344	G271E	A140	
G1125	G1058			C840	G770	C679	G636	G573	G494	C414	G345		C236	C141B
A1126	U1060	C992	A910	A841	C771	C680	A637	C574	G495	A415	G346	C273E	C237	G142
C1127	C1061	G993	A911	G842	U772	G690	G638	A575	G496	C416	A347	U273F	C238	C143
A1128	U1062	C994		C843	G773		U639	U576	A497	C417	G348	G273G		
A1129		G995	C914	G844	A774	A685	C840	G577	G498			G274	A241	G144
U1130	U1065	A996	C915	G845	G775	C687	G642	A578		C420	G352	G275	G242	G145
G1131	G1066	G997	G916	C846	G776	U688	G642	G579	A503	A423		A276	U243	C151
U1132	A1067	C998	A917	U847	A777	A689	C645	C581	U504	C277	G356	C277	A244	
U1133	U1068	U999	A918	G848	G778	G690	A646	C582	A505	C278	A357	C279	G245	
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G1136	A1069		G920	C850	G780	C692	G647	C584	A507	A428	U389	C280	G247	U161
	U1070	C1005	G921	U851	A781	G695	G649	G585	C509	A429	G360		G248	U162
G1139	G1071		U922	C852	A782		C650	C510	U511	G361	U362	U284	C249	U
C1140	C1072	C1008	C923	C853	A783	A699	G651	A586	G512	U362	G363A	C285	G250	U
U1141	A1073	A1009	C924	G854	G784	G700	C652	C589	A513	G438	A363B	C286	A251	G171
U1142A	G1074	A1010	G925	G855	G785	G701	A653	A890	A514		G363C	C287	G252	C172
A1142B	C1075	G1011	A926	C856	U787		A654B	C591	A515	G442	G363D	C288	C253	G173
A1143	U1076	U1012	G928	C857	U787	G704	G654B	G592		C443	G363E	A289	G254	
G1144	A1077	C1013	G929	U858	A788		C654C	G593	G518	C444	U363F	G290	G177	
	U1078	U1014	G932	G859	A789	U709	G	U594	U519	C445	A363G	C291	G178	
G1149	C1079	G1015	G933	U860	C790	G710	G	C595	G520	G446	C364	C292	G259	G260
C1150	U1080	C1016	A933	A861	C791	G710	G	G596	G521	A447		C296	G261	
G1151	U1081	G1017	G934	G862	A792		C	U597	G522	U448	C365	C297	A262	C184
C1152	U1082		C935	A863	A793	G713	C	G598	C523		C366	C297	G188	
C1153	U1083	C936	C936	G864		U714	G	G599	U524	C451	G370	G298	C264	G189
G1154	A1084	C936	C936	C865	C797	G714	G	G600	U525	G452	A299	C299	A265	A190
A1155	A1085	A941	G942	A866	G799	C721	C	G601	A526	G453	G372	A300	C267	A191
C1156	U1086	U1022	G942			A722	A	G602	A527	C455	U373		C268	C192
G1157	G1087	U1023	U943	G869	A800	G726	C	A603	C527	A456	A374	U303	G269	A195
C1158	U1088	U1024	G944	A870	A804	A727	G	G604	A528		C375	G304	U269	
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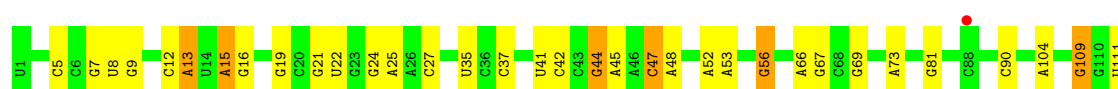
• Molecule 35: 5S rRNA

Chain RB: 68% 27%



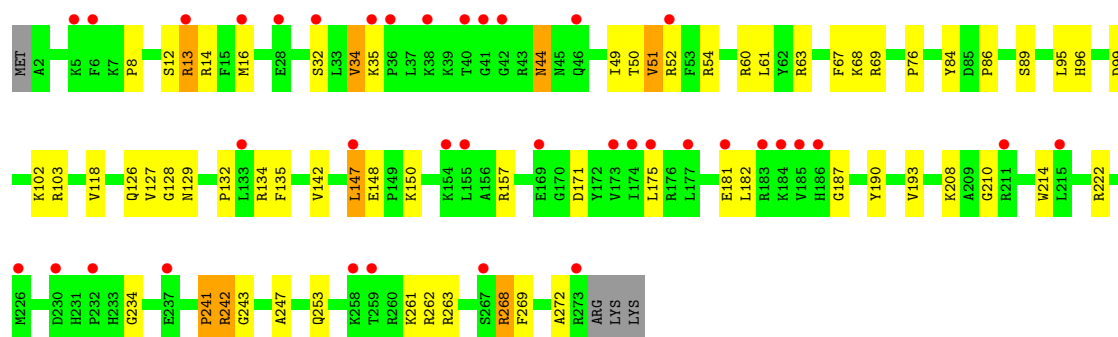
• Molecule 35: 5S rRNA

Chain YB: 70% 24%



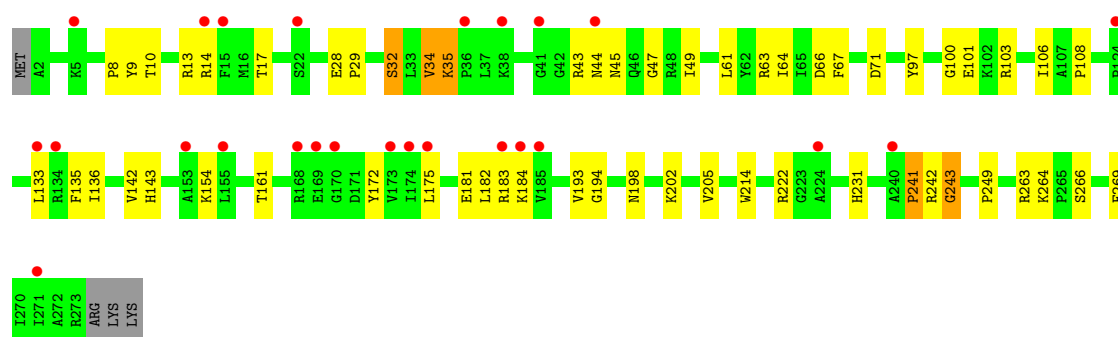
• Molecule 36: 50S ribosomal protein L2

Chain RD: 



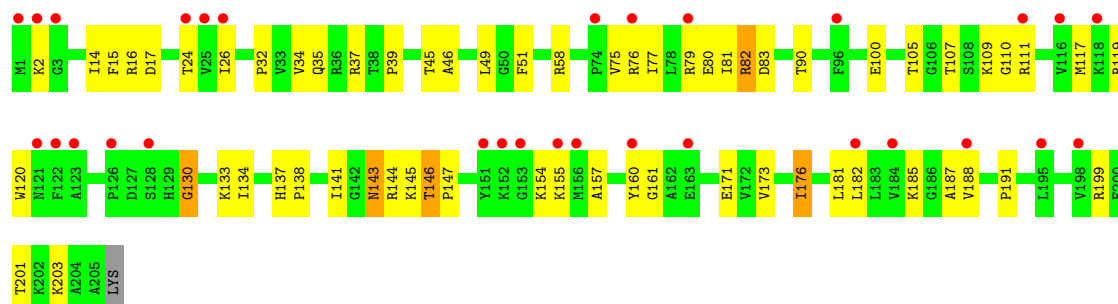
• Molecule 36: 50S ribosomal protein L2

Chain YD: 



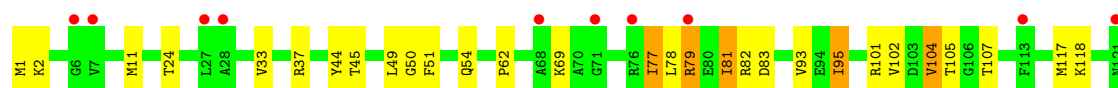
• Molecule 37: 50S ribosomal protein L3

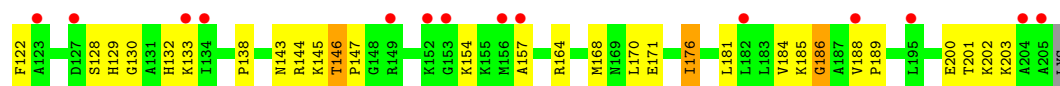
Chain RE: 



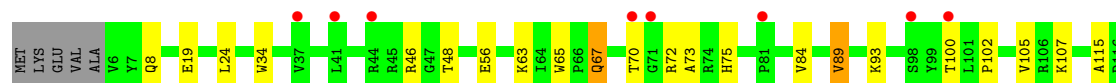
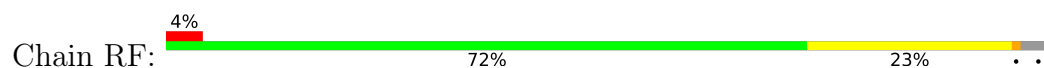
• Molecule 37: 50S ribosomal protein L3

Chain YE: 

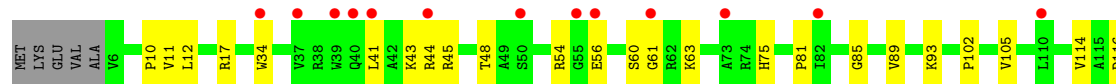
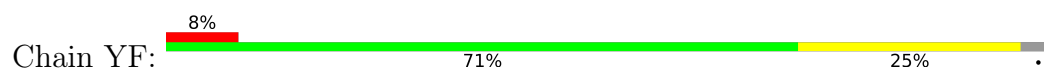




- Molecule 38: 50S ribosomal protein L4



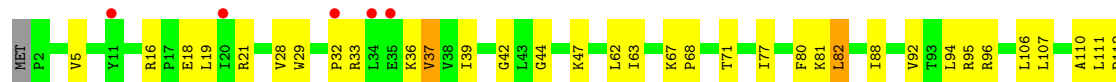
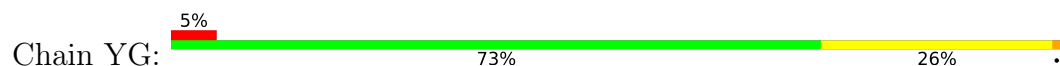
- Molecule 38: 50S ribosomal protein L4



- Molecule 39: 50S ribosomal protein L5

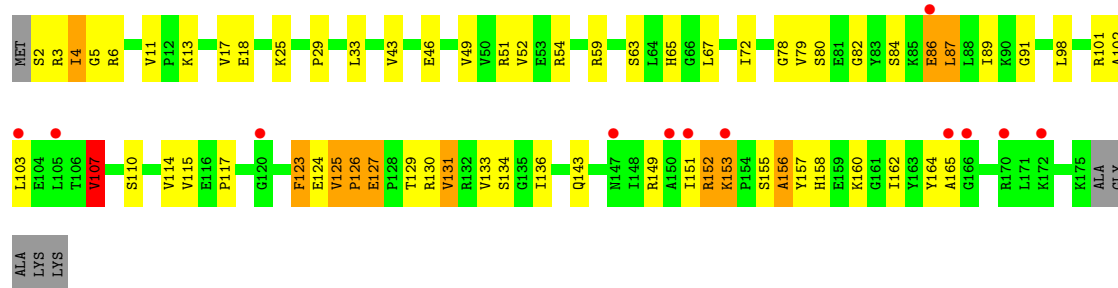


- Molecule 39: 50S ribosomal protein L5

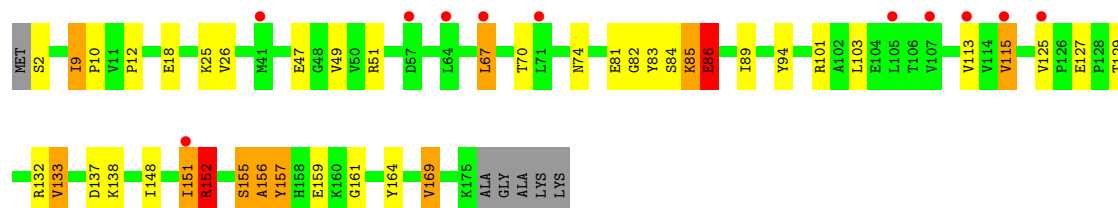
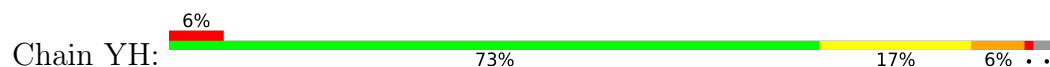


- Molecule 40: 50S ribosomal protein L6

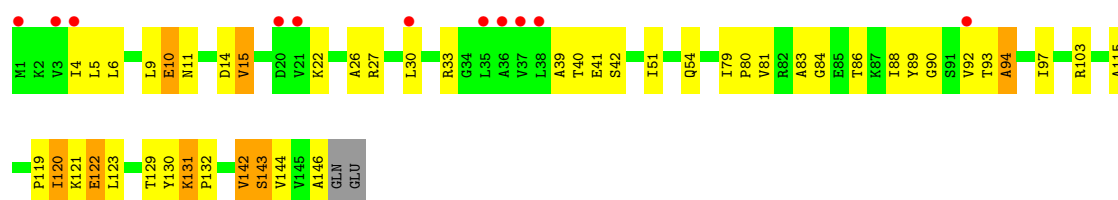




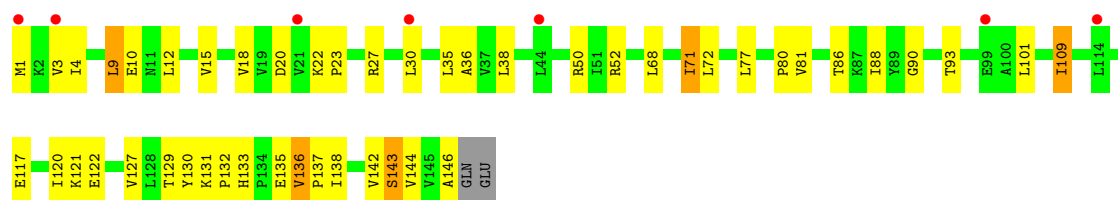
- Molecule 40: 50S ribosomal protein L6



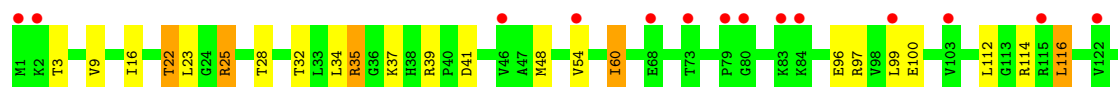
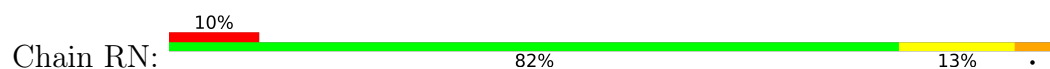
- Molecule 41: 50S ribosomal protein L9



- Molecule 41: 50S ribosomal protein L9



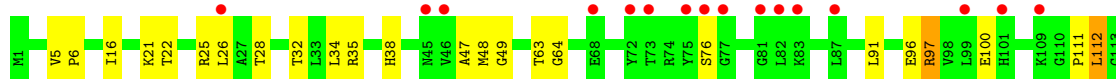
- Molecule 42: 50S ribosomal protein L13





- Molecule 42: 50S ribosomal protein L13

Chain YN: 13% 76% 21% ..



- Molecule 43: 50S ribosomal protein L14

Chain RO: 7% 74% 25% .



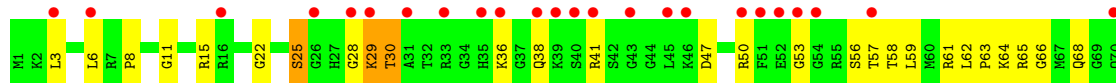
- Molecule 43: 50S ribosomal protein L14

Chain YO: 83% 17%



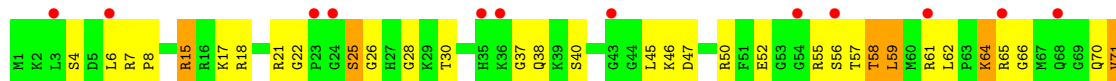
- Molecule 44: 50S ribosomal protein L15

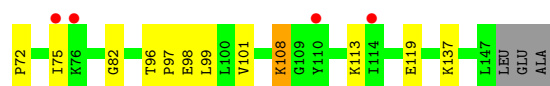
Chain RP: 18% 71% 27% .



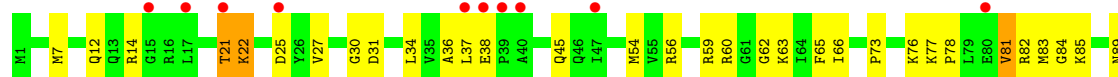
- Molecule 44: 50S ribosomal protein L15

Chain YP: 11% 68% 25% 5% .

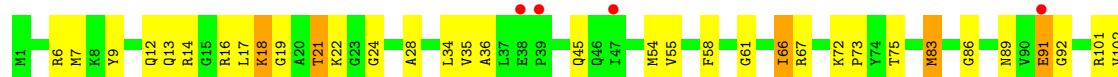
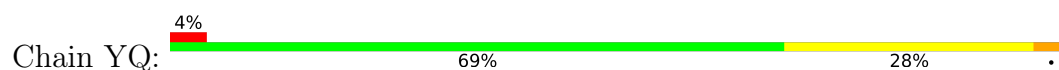




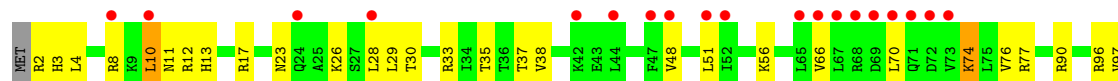
- Molecule 45: 50S ribosomal protein L16



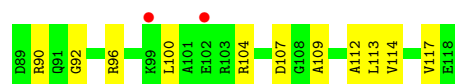
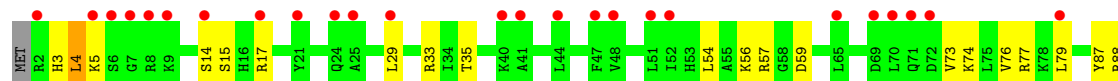
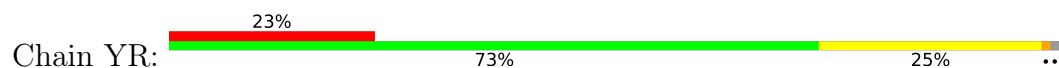
- Molecule 45: 50S ribosomal protein L16



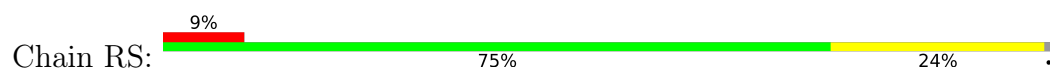
- Molecule 46: 50S ribosomal protein L17

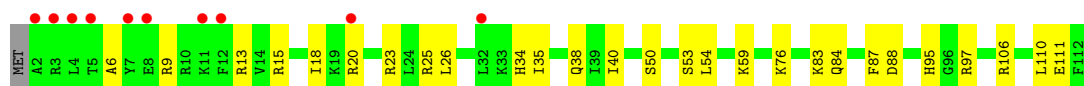


- Molecule 46: 50S ribosomal protein L17

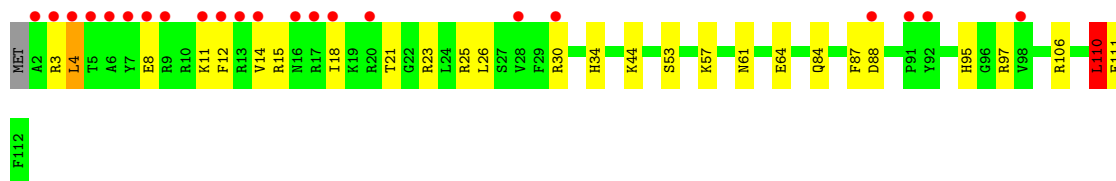
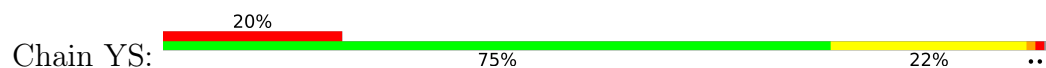


- Molecule 47: 50S ribosomal protein L18

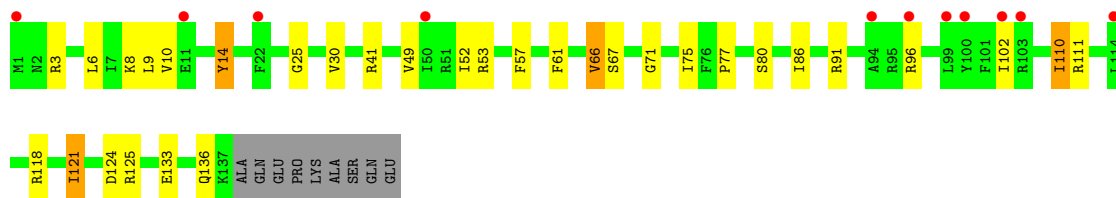
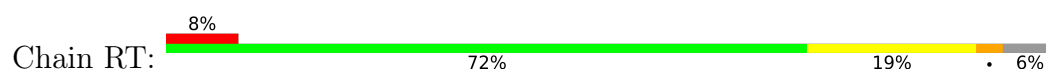




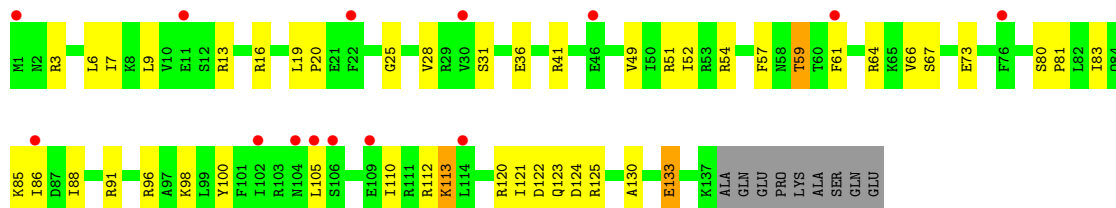
- Molecule 47: 50S ribosomal protein L18



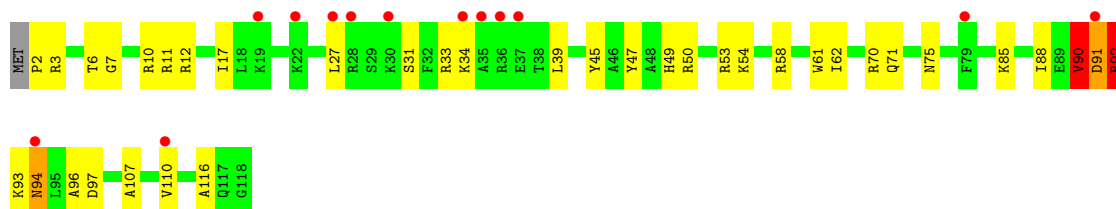
- Molecule 48: 50S ribosomal protein L19



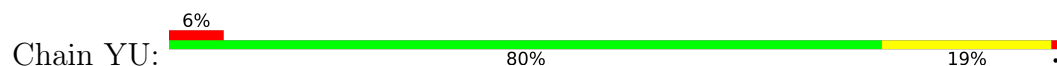
- Molecule 48: 50S ribosomal protein L19

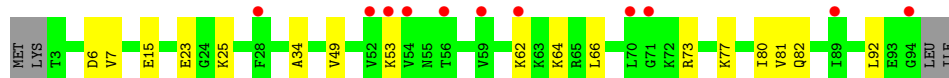


- Molecule 49: 50S ribosomal protein L20

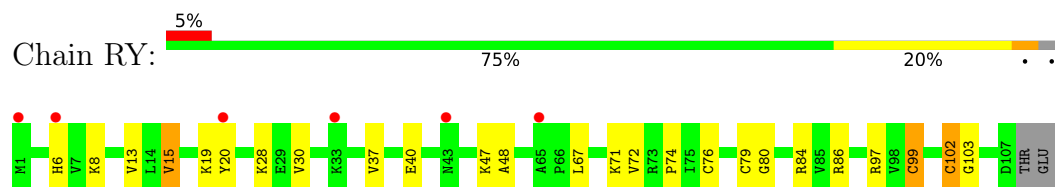


- Molecule 49: 50S ribosomal protein L20

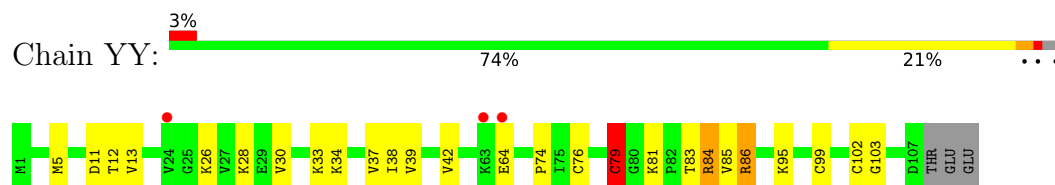




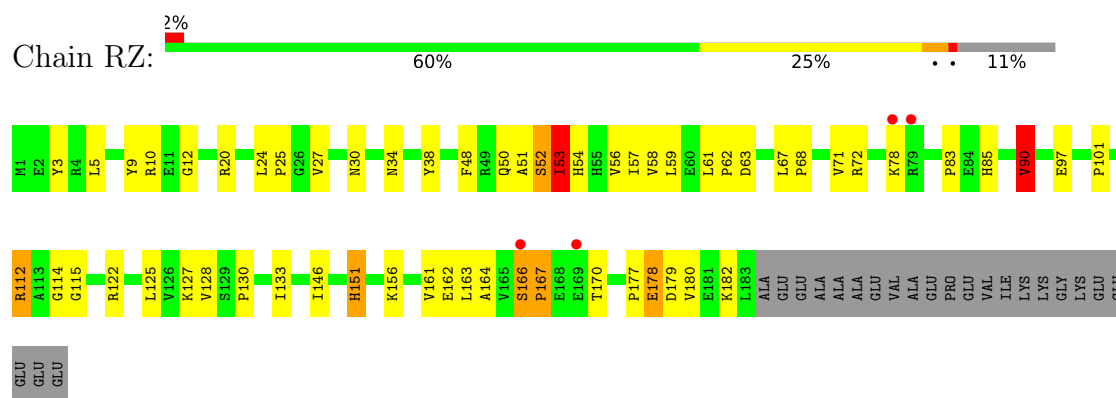
- Molecule 53: 50S ribosomal protein L24



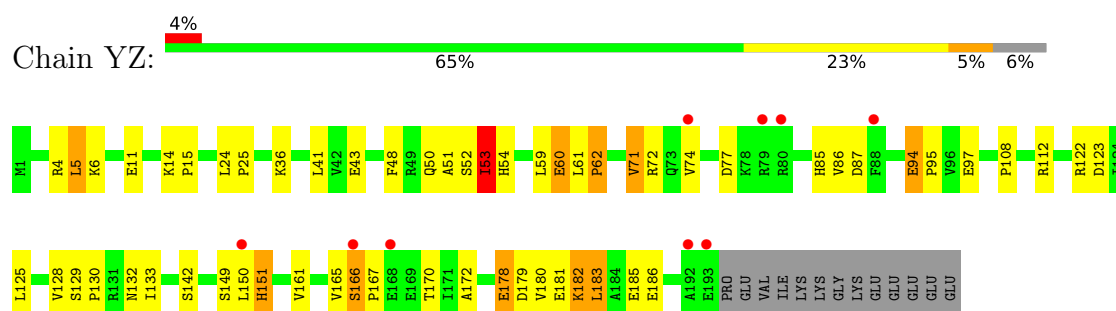
- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



- Molecule 54: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.09Å 450.32Å 622.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 4.14 49.85 – 4.14	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.85-4.14) 98.4 (49.85-4.14)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.248 , 0.294 0.246 , 0.292	Depositor DCC
R_{free} test set	19049 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	171.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 97.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	291185	wwPDB-VP
Average B, all atoms (Å ²)	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	0.30	0/36343	0.61	8/56720 (0.0%)
1	XA	0.41	19/36435 (0.1%)	0.77	138/56865 (0.2%)
2	QB	0.33	0/1942	0.98	12/2619 (0.5%)
2	XB	0.33	0/1950	0.93	6/2630 (0.2%)
3	QC	0.32	0/1629	0.94	7/2195 (0.3%)
3	XC	0.32	0/1629	0.86	3/2195 (0.1%)
4	QD	0.39	0/1733	0.98	6/2318 (0.3%)
4	XD	0.43	1/1733 (0.1%)	0.96	6/2318 (0.3%)
5	QE	0.35	0/1171	0.96	11/1576 (0.7%)
5	XE	0.43	1/1171 (0.1%)	0.84	4/1576 (0.3%)
6	QF	0.34	0/856	0.94	6/1154 (0.5%)
6	XF	0.36	0/856	0.81	2/1154 (0.2%)
7	QG	0.32	0/1276	0.93	2/1709 (0.1%)
7	XG	0.32	0/1276	0.83	3/1709 (0.2%)
8	QH	0.37	0/1128	0.90	2/1517 (0.1%)
8	XH	0.40	0/1128	0.93	2/1517 (0.1%)
9	QI	0.44	1/831 (0.1%)	1.10	9/1120 (0.8%)
9	XI	0.34	0/849	1.02	5/1144 (0.4%)
10	QJ	0.34	0/814	1.01	4/1095 (0.4%)
10	XJ	0.98	2/790 (0.3%)	1.29	3/1063 (0.3%)
11	QK	0.34	0/900	0.81	0/1213
11	XK	0.36	0/879	0.84	4/1187 (0.3%)
12	QL	0.39	0/991	1.00	5/1327 (0.4%)
12	XL	0.43	0/972	1.08	6/1301 (0.5%)
13	QM	0.33	0/931	1.06	7/1248 (0.6%)
13	XM	0.32	0/924	0.98	2/1238 (0.2%)
14	QN	0.55	1/501 (0.2%)	1.14	7/664 (1.1%)
14	XN	0.58	1/501 (0.2%)	1.22	5/664 (0.8%)
15	QO	0.35	0/745	0.77	0/992
15	XO	0.37	0/740	0.75	0/987
16	QP	0.38	0/721	0.92	4/970 (0.4%)
16	XP	0.34	0/721	0.92	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.33	0/847	0.87	3/1131 (0.3%)
17	XQ	0.46	0/847	0.93	3/1131 (0.3%)
18	QR	0.36	0/579	0.81	0/768
18	XR	0.36	0/579	0.78	1/768 (0.1%)
19	QS	0.32	0/680	1.05	6/915 (0.7%)
19	XS	0.34	0/689	1.00	3/926 (0.3%)
20	QT	1.05	3/765 (0.4%)	1.53	12/1007 (1.2%)
20	XT	0.37	0/765	1.14	10/1007 (1.0%)
21	QU	0.28	0/221	0.75	0/288
21	XU	0.75	0/221	0.99	0/288
22	QV	0.19	0/1621	0.37	0/2523
22	XV	0.22	0/1621	0.41	0/2523
23	QX	0.21	0/459	0.44	0/715
23	XX	0.33	0/459	0.53	0/715
24	R0	0.38	0/652	0.83	0/867
24	Y0	0.58	0/657	0.86	0/874
25	R1	0.58	0/753	0.99	6/1000 (0.6%)
25	Y1	0.61	1/736 (0.1%)	1.07	3/978 (0.3%)
26	R2	0.35	0/583	0.94	2/771 (0.3%)
26	Y2	0.48	0/577	0.89	1/764 (0.1%)
27	R3	0.38	0/474	0.93	0/635
27	Y3	0.65	1/474 (0.2%)	0.86	1/635 (0.2%)
28	R4	0.25	0/357	0.85	0/483
28	Y4	2.19	2/366 (0.5%)	2.01	17/495 (3.4%)
29	R5	0.87	2/473 (0.4%)	1.26	7/639 (1.1%)
29	Y5	1.10	2/473 (0.4%)	1.33	4/639 (0.6%)
30	R6	0.69	2/460 (0.4%)	0.97	2/613 (0.3%)
30	Y6	1.20	7/460 (1.5%)	1.54	9/613 (1.5%)
31	R7	0.55	0/417	0.89	1/550 (0.2%)
31	Y7	0.64	0/426	0.83	0/561
32	R8	0.47	0/525	1.19	8/691 (1.2%)
32	Y8	0.61	0/525	1.19	5/691 (0.7%)
33	R9	0.86	1/310 (0.3%)	1.33	3/407 (0.7%)
33	Y9	0.63	0/310	1.00	1/407 (0.2%)
34	RA	0.25	0/69520	0.53	16/108527 (0.0%)
34	YA	0.27	1/69543 (0.0%)	0.57	26/108563 (0.0%)
35	RB	0.24	0/2878	0.40	0/4490
35	YB	0.31	0/2878	0.46	0/4490
36	RD	0.52	0/2165	0.99	9/2919 (0.3%)
36	YD	0.64	0/2165	1.03	11/2919 (0.4%)
37	RE	0.51	0/1601	1.44	13/2160 (0.6%)
37	YE	0.63	0/1601	1.50	16/2160 (0.7%)
38	RF	0.45	0/1620	1.00	10/2194 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.62	0/1620	0.96	8/2194 (0.4%)
39	RG	0.36	0/1499	1.01	9/2016 (0.4%)
39	YG	0.42	0/1499	0.97	7/2016 (0.3%)
40	RH	0.41	0/1362	1.19	15/1841 (0.8%)
40	YH	0.68	1/1362 (0.1%)	1.25	21/1841 (1.1%)
41	RI	0.52	1/1151 (0.1%)	1.18	16/1558 (1.0%)
41	YI	0.48	1/1151 (0.1%)	1.10	10/1558 (0.6%)
42	RN	0.44	0/1131	0.99	5/1525 (0.3%)
42	YN	0.62	0/1131	1.05	7/1525 (0.5%)
43	RO	0.46	0/943	0.87	1/1269 (0.1%)
43	YO	0.59	0/943	0.86	0/1269
44	RP	0.47	0/1162	1.05	6/1544 (0.4%)
44	YP	0.59	0/1139	1.19	12/1514 (0.8%)
45	RQ	0.42	0/1143	1.00	9/1527 (0.6%)
45	YQ	0.57	0/1143	1.10	10/1527 (0.7%)
46	RR	0.49	0/974	1.00	6/1302 (0.5%)
46	YR	0.59	0/974	1.01	3/1302 (0.2%)
47	RS	0.37	0/892	0.94	1/1187 (0.1%)
47	YS	0.50	0/892	0.98	4/1187 (0.3%)
48	RT	0.41	0/1155	1.09	8/1542 (0.5%)
48	YT	0.51	0/1155	1.06	9/1542 (0.6%)
49	RU	0.45	0/982	0.99	6/1306 (0.5%)
49	YU	0.65	0/982	0.95	6/1306 (0.5%)
50	RV	0.44	0/790	1.08	8/1057 (0.8%)
50	YV	0.61	0/790	1.01	4/1057 (0.4%)
51	RW	0.50	0/911	0.88	1/1220 (0.1%)
51	YW	0.64	0/911	0.88	2/1220 (0.2%)
52	RX	0.48	0/739	0.84	1/993 (0.1%)
52	YX	0.61	0/739	0.95	2/993 (0.2%)
53	RY	0.51	1/831 (0.1%)	0.93	1/1108 (0.1%)
53	YY	0.61	1/831 (0.1%)	0.99	6/1108 (0.5%)
54	RZ	0.42	0/1493	1.55	19/2026 (0.9%)
54	YZ	0.50	0/1561	1.46	14/2119 (0.7%)
All	All	0.38	53/315379 (0.0%)	0.74	726/471694 (0.2%)

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
1	XA	1	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y4	1	1
34	RA	0	1
34	YA	0	6
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	2	30

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-36.28	1.05	1.54
20	QT	73	HIS	N-CA	-19.12	1.21	1.46
28	Y4	4	GLY	N-CA	-18.89	1.18	1.45
20	QT	74	LYS	CA-CB	-17.55	1.23	1.53
29	Y5	32	PRO	N-CA	17.49	1.69	1.47

The worst 5 of 726 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	YE	146	THR	CA-C-N	33.70	161.97	119.84
37	YE	146	THR	C-N-CA	33.70	161.97	119.84
54	RZ	166	SER	CA-C-N	32.45	160.40	119.84
54	RZ	166	SER	C-N-CA	32.45	160.40	119.84
54	YZ	166	SER	CA-C-N	30.23	157.62	119.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	XA	617	G	C2'
28	Y4	5	ILE	CA

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	RA	1649	G	Sidechain
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
1	XA	308	C	Sidechain

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	32469	0	16385	1581	0
1	XA	32551	0	16418	1289	0
2	QB	1907	0	1958	101	0
2	XB	1915	0	1966	41	0
3	QC	1605	0	1667	136	0
3	XC	1605	0	1668	96	18
4	QD	1703	0	1762	107	0
4	XD	1703	0	1763	59	7
5	QE	1155	0	1213	79	0
5	XE	1155	0	1213	33	0
6	QF	843	0	857	10	5
6	XF	843	0	855	92	0
7	QG	1257	0	1296	57	18
7	XG	1257	0	1295	62	0
8	QH	1108	0	1165	53	0
8	XH	1108	0	1165	26	0
9	QI	816	0	822	52	6
9	XI	834	0	847	23	0
10	QJ	801	0	843	199	0
10	XJ	777	0	816	117	6
11	QK	885	0	904	35	0
11	XK	864	0	880	74	0
12	QL	975	0	1062	46	0
12	XL	956	0	1046	30	0
13	QM	921	0	974	138	0
13	XM	914	0	966	128	0
14	QN	492	0	528	285	0
14	XN	492	0	521	172	0
15	QO	734	0	770	57	0
15	XO	729	0	767	46	0
16	QP	705	0	725	71	0
16	XP	705	0	725	16	0
17	QQ	834	0	904	43	0
17	XQ	834	0	902	23	0
18	QR	574	0	644	8	0
18	XR	574	0	643	105	0
19	QS	665	0	678	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	695	112	0
20	QT	763	0	861	27	0
20	XT	763	0	861	40	0
21	QU	217	0	223	45	0
21	XU	217	0	234	10	0
22	QV	1452	0	736	3	0
22	XV	1452	0	736	16	0
23	QX	409	0	209	5	0
23	XX	409	0	209	23	0
24	R0	643	0	667	12	0
24	Y0	648	0	672	11	0
25	R1	746	0	826	26	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	5	1
26	Y2	575	0	624	6	0
27	R3	469	0	518	13	2
27	Y3	469	0	518	12	0
28	R4	348	0	354	26	0
28	Y4	357	0	362	10	0
29	R5	459	0	477	20	0
29	Y5	459	0	476	25	1
30	R6	453	0	474	11	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	12	0
31	Y7	418	0	467	19	0
32	R8	517	0	582	31	0
32	Y8	517	0	582	27	0
33	R9	307	0	335	24	0
33	Y9	307	0	336	19	0
34	RA	62070	0	31282	996	0
34	YA	62091	0	31289	1257	1
35	RB	2573	0	1306	22	0
35	YB	2573	0	1306	14	0
36	RD	2115	0	2195	53	2
36	YD	2115	0	2195	65	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	33	0
38	RF	1585	0	1632	33	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	50	0
39	YG	1474	0	1535	27	0
40	RH	1336	0	1418	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YH	1336	0	1418	25	0
41	RI	1136	0	1223	42	0
41	YI	1136	0	1223	30	0
42	RN	1104	0	1180	13	0
42	YN	1104	0	1180	18	0
43	RO	933	0	996	23	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	39	0
44	YP	1122	0	1206	45	2
45	RQ	1122	0	1179	42	0
45	YQ	1122	0	1179	35	0
46	RR	960	0	1021	22	0
46	YR	960	0	1021	24	0
47	RS	882	0	943	19	0
47	YS	882	0	943	17	0
48	RT	1141	0	1202	19	0
48	YT	1141	0	1202	30	0
49	RU	964	0	1022	39	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	16	0
50	YV	779	0	852	12	1
51	RW	900	0	964	21	0
51	YW	900	0	964	19	0
52	RX	725	0	778	11	0
52	YX	725	0	778	9	0
53	RY	818	0	911	26	0
53	YY	818	0	910	20	0
54	RZ	1461	0	1493	37	0
54	YZ	1529	0	1551	33	0
55	QA	70	0	0	0	0
55	QE	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	2	0	0	0	0
55	R0	2	0	0	0	0
55	R3	1	0	0	0	0
55	R8	2	0	0	0	0
55	RA	432	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	RO	1	0	0	0	0
55	XA	88	0	0	2	0
55	XE	1	0	0	0	0
55	XO	1	0	0	0	0
55	Y1	1	0	0	0	0
55	Y2	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	394	0	0	3	0
55	YB	1	0	0	0	0
55	YD	2	0	0	0	0
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YP	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	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	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	1	0
All	All	291185	0	197034	7054	35

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 15.

The worst 5 of 7054 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)
10:QJ:47:PHE:CZ	14:QN:36:PHE:HB3	1.21	1.72
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:980:C:C1'	14:QN:19:ARG:HG2	1.23	1.68
1:QA:1049:U:C5	14:QN:3:ARG:HB3	1.26	1.66
1:XA:1190:G:H5'	3:XC:176:HIS:CE1	1.30	1.64

The worst 5 of 35 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)
7:QG:149:ARG:NE	3:XC:81:GLY:O[4_555]	0.51	1.69
7:QG:149:ARG:NH1	3:XC:85:ARG:N[4_555]	1.02	1.18
7:QG:149:ARG:NH1	3:XC:85:ARG:CA[4_555]	1.16	1.04
7:QG:149:ARG:CZ	3:XC:85:ARG:N[4_555]	1.35	0.85
7:QG:149:ARG:NH1	3:XC:85:ARG:CB[4_555]	1.52	0.68

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	67
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	25	62
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	25	62
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	19	56
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	19	56
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	103/128 (80%)	91 (88%)	12 (12%)	0	100	100
9	XI	105/128 (82%)	97 (92%)	8 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	13	47
10	XJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	5	32
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	16	53
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	113/126 (90%)	96 (85%)	16 (14%)	1 (1%)	14	50
13	XM	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	14	50
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	37
14	XN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	24
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	25
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	3	25
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	12	45
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	12 (27%)	4 (9%)	0	10
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	3	25
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	19	56
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	30	67
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4	29
37	YE	203/206 (98%)	162 (80%)	39 (19%)	2 (1%)	13	47
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	13	47
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	25	62
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	22	59
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	37
40	YH	172/180 (96%)	147 (86%)	21 (12%)	4 (2%)	5	31
41	RI	144/148 (97%)	114 (79%)	24 (17%)	6 (4%)	2	21
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	19	56
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	19	56
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
43	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	6	34
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	19	56
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	19	56
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	19	56
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14	50
47	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	14	50
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	4	29
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	13	47
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	13	47
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	5	32
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	2	23
All	All	11368/12128 (94%)	10080 (89%)	1202 (11%)	86 (1%)	16	53

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN

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Mol	Chain	Res	Type
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR

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%)	86	90
2	XB	204/220 (93%)	203 (100%)	1 (0%)	86	90
3	QC	159/188 (85%)	158 (99%)	1 (1%)	84	88
3	XC	159/188 (85%)	157 (99%)	2 (1%)	65	77
4	QD	180/181 (99%)	179 (99%)	1 (1%)	84	88
4	XD	180/181 (99%)	177 (98%)	3 (2%)	56	72
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	75	83
6	QF	90/90 (100%)	89 (99%)	1 (1%)	70	80
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	79	84
8	QH	118/119 (99%)	117 (99%)	1 (1%)	79	84
8	XH	118/119 (99%)	117 (99%)	1 (1%)	79	84
9	QI	79/99 (80%)	76 (96%)	3 (4%)	28	51
9	XI	81/99 (82%)	79 (98%)	2 (2%)	42	62
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	81 (94%)	5 (6%)	17	40
11	QK	90/99 (91%)	88 (98%)	2 (2%)	47	65
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	101 (98%)	2 (2%)	52	69
13	QM	93/101 (92%)	93 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	26	49
14	XN	49/50 (98%)	47 (96%)	2 (4%)	26	49
15	QO	79/80 (99%)	77 (98%)	2 (2%)	42	62
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%)	93 (98%)	2 (2%)	48	66
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%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	72 (99%)	1 (1%)	62	75
20	QT	76/82 (93%)	75 (99%)	1 (1%)	65	77
20	XT	76/82 (93%)	75 (99%)	1 (1%)	65	77
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	20	44
24	R0	65/67 (97%)	65 (100%)	0	100	100
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	42	62
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	64 (100%)	0	100	100
27	R3	51/52 (98%)	50 (98%)	1 (2%)	50	68
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	40 (98%)	1 (2%)	44	63
29	R5	51/52 (98%)	50 (98%)	1 (2%)	50	68
29	Y5	51/52 (98%)	49 (96%)	2 (4%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R6	51/52 (98%)	50 (98%)	1 (2%)	50	68
30	Y6	51/52 (98%)	50 (98%)	1 (2%)	50	68
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	33 (97%)	1 (3%)	37	58
36	RD	214/218 (98%)	211 (99%)	3 (1%)	62	75
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	162 (98%)	3 (2%)	54	71
37	YE	165/166 (99%)	160 (97%)	5 (3%)	36	57
38	RF	161/166 (97%)	158 (98%)	3 (2%)	52	69
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	154 (99%)	1 (1%)	84	88
39	YG	155/156 (99%)	152 (98%)	3 (2%)	52	69
40	RH	145/148 (98%)	137 (94%)	8 (6%)	18	42
40	YH	145/148 (98%)	139 (96%)	6 (4%)	26	49
41	RI	122/124 (98%)	120 (98%)	2 (2%)	58	74
41	YI	122/124 (98%)	118 (97%)	4 (3%)	33	55
42	RN	117/119 (98%)	114 (97%)	3 (3%)	41	61
42	YN	117/119 (98%)	116 (99%)	1 (1%)	75	83
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	99 (99%)	1 (1%)	73	81
44	RP	116/116 (100%)	116 (100%)	0	100	100
44	YP	114/116 (98%)	113 (99%)	1 (1%)	75	83
45	RQ	111/111 (100%)	109 (98%)	2 (2%)	54	71
45	YQ	111/111 (100%)	111 (100%)	0	100	100
46	RR	100/101 (99%)	99 (99%)	1 (1%)	73	81
46	YR	100/101 (99%)	100 (100%)	0	100	100
47	RS	87/88 (99%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	YS	87/88 (99%)	85 (98%)	2 (2%)	45	64
48	RT	120/127 (94%)	118 (98%)	2 (2%)	56	72
48	YT	120/127 (94%)	118 (98%)	2 (2%)	56	72
49	RU	93/94 (99%)	92 (99%)	1 (1%)	70	80
49	YU	93/94 (99%)	92 (99%)	1 (1%)	70	80
50	RV	82/82 (100%)	80 (98%)	2 (2%)	44	63
50	YV	82/82 (100%)	78 (95%)	4 (5%)	21	44
51	RW	92/92 (100%)	91 (99%)	1 (1%)	70	80
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	73 (99%)	1 (1%)	62	75
52	YX	74/78 (95%)	72 (97%)	2 (3%)	40	60
53	RY	88/91 (97%)	87 (99%)	1 (1%)	70	80
53	YY	88/91 (97%)	87 (99%)	1 (1%)	70	80
54	RZ	162/179 (90%)	161 (99%)	1 (1%)	84	88
54	YZ	167/179 (93%)	164 (98%)	3 (2%)	54	71
All	All	9610/10066 (96%)	9488 (99%)	122 (1%)	65	77

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	XC	12	LEU
48	YT	105	LEU
10	XJ	96	ILE
48	YT	66	VAL
53	YY	79	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
4	XD	123	HIS
12	XL	8	ASN
6	XF	57	GLN
10	XJ	56	HIS
14	XN	49	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	532 (35%)	14 (0%)
1	XA	1514/1521 (99%)	469 (30%)	27 (1%)
22	QV	66/77 (85%)	15 (22%)	1 (1%)
22	XV	66/77 (85%)	16 (24%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	0
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2877/2905 (99%)	706 (24%)	40 (1%)
34	YA	2880/2905 (99%)	754 (26%)	40 (1%)
35	RB	119/122 (97%)	20 (16%)	1 (0%)
35	YB	119/122 (97%)	23 (19%)	1 (0%)
All	All	9186/9288 (98%)	2545 (27%)	125 (1%)

5 of 2545 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	7	G
1	QA	8	A
1	QA	9	G
1	QA	15	G

5 of 125 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	266	G
34	YA	1653	G
1	XA	1304	G
34	YA	1608	A
34	YA	2566	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1038 ligands modelled in this entry, 1036 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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1511/1521 (99%)	-0.06	20 (1%) 74 60	186, 276, 733, 884	0
1	XA	1515/1521 (99%)	-0.17	16 (1%) 77 64	158, 261, 672, 775	0
2	QB	235/256 (91%)	0.03	10 (4%) 40 32	230, 330, 393, 429	0
2	XB	236/256 (92%)	0.28	18 (7%) 21 19	237, 291, 340, 364	0
3	QC	205/239 (85%)	0.26	13 (6%) 27 24	271, 379, 421, 449	0
3	XC	205/239 (85%)	0.35	12 (5%) 29 25	275, 359, 467, 497	0
4	QD	208/209 (99%)	0.70	23 (11%) 12 12	231, 275, 325, 369	0
4	XD	208/209 (99%)	0.60	18 (8%) 17 16	216, 258, 306, 370	0
5	QE	151/162 (93%)	0.44	10 (6%) 26 23	208, 268, 318, 333	0
5	XE	151/162 (93%)	0.12	9 (5%) 29 24	174, 222, 277, 313	0
6	QF	101/101 (100%)	0.32	6 (5%) 29 25	224, 285, 333, 355	0
6	XF	101/101 (100%)	0.46	7 (6%) 24 21	278, 343, 376, 406	0
7	QG	155/156 (99%)	-0.05	4 (2%) 57 43	332, 425, 492, 522	0
7	XG	155/156 (99%)	0.08	5 (3%) 50 38	327, 458, 559, 580	0
8	QH	137/138 (99%)	1.15	27 (19%) 3 6	230, 290, 341, 368	0
8	XH	137/138 (99%)	0.61	12 (8%) 17 16	197, 259, 299, 342	0
9	QI	105/128 (82%)	0.07	1 (0%) 79 65	289, 373, 413, 449	0
9	XI	107/128 (83%)	0.21	3 (2%) 55 41	364, 448, 487, 522	0
10	QJ	99/105 (94%)	0.41	3 (3%) 52 40	354, 404, 458, 476	0
10	XJ	96/105 (91%)	0.73	9 (9%) 15 15	340, 397, 495, 509	0
11	QK	119/129 (92%)	0.45	8 (6%) 25 22	172, 269, 315, 333	0
11	XK	116/129 (89%)	0.55	9 (7%) 20 19	213, 279, 334, 364	0
12	QL	125/132 (94%)	0.79	14 (11%) 11 12	183, 237, 288, 334	0
12	XL	122/132 (92%)	0.87	21 (17%) 5 7	168, 221, 289, 338	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	115/126 (91%)	0.02	2 (1%) 69 53	298, 386, 443, 469	0
13	XM	114/126 (90%)	0.34	7 (6%) 28 24	317, 414, 450, 463	0
14	QN	60/61 (98%)	0.74	7 (11%) 10 11	295, 353, 479, 493	0
14	XN	60/61 (98%)	1.00	12 (20%) 3 6	312, 556, 587, 612	0
15	QO	88/89 (98%)	0.73	13 (14%) 7 9	196, 272, 314, 335	0
15	XO	87/89 (97%)	0.57	9 (10%) 13 13	182, 221, 267, 284	0
16	QP	84/88 (95%)	0.97	14 (16%) 5 7	189, 247, 303, 348	0
16	XP	84/88 (95%)	1.56	30 (35%) 1 2	264, 358, 461, 493	0
17	QQ	100/105 (95%)	1.19	19 (19%) 4 6	199, 251, 286, 319	0
17	XQ	100/105 (95%)	0.61	16 (16%) 6 8	174, 231, 273, 307	0
18	QR	70/88 (79%)	0.20	3 (4%) 40 32	240, 297, 336, 375	0
18	XR	70/88 (79%)	0.21	3 (4%) 40 32	168, 247, 321, 337	0
19	QS	83/93 (89%)	0.81	4 (4%) 36 30	308, 459, 605, 672	0
19	XS	84/93 (90%)	0.77	6 (7%) 23 21	341, 414, 456, 474	0
20	QT	99/106 (93%)	1.29	31 (31%) 1 3	205, 271, 358, 377	0
20	XT	99/106 (93%)	1.14	19 (19%) 4 6	198, 242, 278, 302	0
21	QU	25/27 (92%)	0.81	2 (8%) 20 18	300, 347, 463, 563	0
21	XU	25/27 (92%)	1.18	5 (20%) 3 6	336, 374, 530, 549	0
22	QV	68/77 (88%)	-0.19	1 (1%) 71 57	294, 387, 435, 446	0
22	XV	68/77 (88%)	-0.34	0 100 100	281, 411, 474, 504	0
23	QX	19/19 (100%)	0.21	0 100 100	368, 432, 461, 464	0
23	XX	19/19 (100%)	0.29	0 100 100	356, 422, 471, 476	0
24	R0	81/85 (95%)	0.79	15 (18%) 4 6	166, 206, 296, 364	0
24	Y0	82/85 (96%)	0.57	6 (7%) 22 20	120, 168, 274, 329	0
25	R1	95/98 (96%)	1.23	20 (21%) 3 5	162, 201, 262, 291	0
25	Y1	93/98 (94%)	1.06	15 (16%) 5 8	117, 176, 219, 232	0
26	R2	69/72 (95%)	0.38	4 (5%) 30 25	124, 192, 238, 283	0
26	Y2	68/72 (94%)	0.88	11 (16%) 5 8	124, 171, 214, 231	0
27	R3	59/60 (98%)	0.51	7 (11%) 10 11	175, 228, 281, 338	0
27	Y3	59/60 (98%)	0.49	4 (6%) 25 22	115, 168, 241, 269	0
28	R4	45/71 (63%)	-0.29	0 100 100	237, 382, 418, 429	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	Y4	46/71 (64%)	-0.31	0	100	100	206, 273, 315, 322	0
29	R5	59/60 (98%)	0.19	1 (1%)	69	53	142, 193, 225, 291	0
29	Y5	59/60 (98%)	0.15	1 (1%)	69	53	122, 172, 225, 300	0
30	R6	53/54 (98%)	-0.27	1 (1%)	66	50	175, 230, 267, 357	0
30	Y6	53/54 (98%)	0.22	2 (3%)	44	35	144, 194, 248, 260	0
31	R7	47/49 (95%)	0.96	7 (14%)	7	9	138, 167, 186, 207	0
31	Y7	48/49 (97%)	0.75	9 (18%)	4	6	111, 146, 192, 224	0
32	R8	64/65 (98%)	0.75	7 (10%)	12	13	154, 201, 248, 284	0
32	Y8	64/65 (98%)	1.21	15 (23%)	2	4	120, 172, 209, 259	0
33	R9	37/37 (100%)	1.48	10 (27%)	2	4	260, 289, 340, 357	0
33	Y9	37/37 (100%)	1.25	6 (16%)	5	8	174, 205, 233, 250	0
34	RA	2882/2905 (99%)	-0.31	3 (0%)	92	89	123, 197, 357, 505	0
34	YA	2883/2905 (99%)	-0.32	13 (0%)	87	76	96, 149, 276, 493	0
35	RB	120/122 (98%)	-0.35	0	100	100	205, 256, 303, 350	0
35	YB	120/122 (98%)	-0.41	1 (0%)	82	69	135, 175, 210, 248	0
36	RD	272/276 (98%)	0.71	38 (13%)	7	10	127, 186, 231, 284	0
36	YD	272/276 (98%)	0.62	25 (9%)	16	15	107, 159, 207, 243	0
37	RE	205/206 (99%)	0.78	30 (14%)	7	9	128, 211, 265, 310	0
37	YE	205/206 (99%)	0.68	24 (11%)	10	11	102, 157, 205, 254	0
38	RF	202/210 (96%)	0.25	9 (4%)	39	31	143, 199, 272, 328	0
38	YF	202/210 (96%)	0.47	16 (7%)	20	18	101, 160, 215, 256	0
39	RG	181/182 (99%)	-0.04	5 (2%)	55	41	231, 307, 360, 388	0
39	YG	181/182 (99%)	0.06	9 (4%)	35	29	178, 226, 291, 327	0
40	RH	174/180 (96%)	0.23	12 (6%)	24	21	189, 269, 313, 358	0
40	YH	174/180 (96%)	0.36	11 (6%)	27	24	123, 175, 217, 258	0
41	RI	146/148 (98%)	0.29	11 (7%)	22	20	188, 254, 300, 327	0
41	YI	146/148 (98%)	0.06	7 (4%)	36	30	158, 226, 271, 293	0
42	RN	138/140 (98%)	0.49	14 (10%)	14	13	139, 219, 260, 268	0
42	YN	138/140 (98%)	0.71	18 (13%)	9	10	94, 160, 205, 231	0
43	RO	122/122 (100%)	0.34	8 (6%)	26	23	158, 202, 247, 286	0
43	YO	122/122 (100%)	0.11	1 (0%)	82	69	113, 159, 199, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.72	27 (18%) 4 7	160, 228, 287, 331	0
44	YP	147/150 (98%)	0.66	16 (10%) 12 13	128, 166, 217, 255	0
45	RQ	141/141 (100%)	0.36	13 (9%) 16 15	194, 231, 267, 309	0
45	YQ	141/141 (100%)	0.37	5 (3%) 47 36	132, 174, 238, 314	0
46	RR	117/118 (99%)	0.94	19 (16%) 5 8	121, 180, 224, 257	0
46	YR	117/118 (99%)	0.99	27 (23%) 2 4	104, 155, 212, 237	0
47	RS	111/112 (99%)	0.40	10 (9%) 17 15	191, 262, 311, 357	0
47	YS	111/112 (99%)	0.70	22 (19%) 3 6	146, 196, 282, 328	0
48	RT	137/146 (93%)	0.33	11 (8%) 20 18	158, 225, 307, 320	0
48	YT	137/146 (93%)	0.46	14 (10%) 13 13	127, 185, 257, 282	0
49	RU	117/118 (99%)	0.70	13 (11%) 12 12	149, 243, 286, 304	0
49	YU	117/118 (99%)	0.56	7 (5%) 29 24	101, 147, 194, 223	0
50	RV	101/101 (100%)	0.19	10 (9%) 14 14	165, 222, 278, 288	0
50	YV	101/101 (100%)	0.35	12 (11%) 10 11	118, 170, 240, 280	0
51	RW	113/113 (100%)	0.59	10 (8%) 17 16	117, 160, 226, 339	0
51	YW	113/113 (100%)	0.62	12 (10%) 13 13	92, 137, 192, 239	0
52	RX	92/96 (95%)	0.58	6 (6%) 26 23	127, 177, 212, 235	0
52	YX	92/96 (95%)	0.76	11 (11%) 10 11	110, 146, 190, 259	0
53	RY	107/110 (97%)	0.50	6 (5%) 31 26	170, 219, 264, 315	0
53	YY	107/110 (97%)	0.29	3 (2%) 55 41	107, 170, 205, 244	0
54	RZ	183/206 (88%)	-0.07	4 (2%) 62 47	211, 258, 298, 354	0
54	YZ	193/206 (93%)	0.14	9 (4%) 37 30	124, 196, 287, 350	0
All	All	20769/21416 (96%)	0.16	1144 (5%) 32 26	92, 221, 460, 884	0

The worst 5 of 1144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	XD	4	TYR	11.2
17	QQ	24	GLU	9.4
2	XB	101	MET	9.1
8	QH	111	ILE	9.0
12	XL	28	LYS	8.6

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	3277	1/1	-0.50	0.38	213,213,213,213	0
55	MG	QA	1634	1/1	-0.34	0.28	175,175,175,175	0
55	MG	RA	3139	1/1	-0.29	0.42	290,290,290,290	0
55	MG	RA	3164	1/1	-0.24	0.31	199,199,199,199	0
55	MG	YA	3192	1/1	-0.23	0.25	219,219,219,219	0
55	MG	RA	3186	1/1	-0.18	0.20	205,205,205,205	0
55	MG	YA	3142	1/1	-0.17	0.39	158,158,158,158	0
55	MG	QH	201	1/1	-0.16	0.17	188,188,188,188	0
55	MG	YA	3145	1/1	-0.16	0.29	84,84,84,84	0
55	MG	QE	201	1/1	-0.14	0.42	198,198,198,198	0
55	MG	RA	3011	1/1	-0.13	0.23	129,129,129,129	0
55	MG	RA	3169	1/1	-0.10	0.37	131,131,131,131	0
55	MG	RA	3163	1/1	-0.09	0.23	165,165,165,165	0
55	MG	YA	3091	1/1	-0.09	0.29	145,145,145,145	0
55	MG	RA	3224	1/1	-0.07	0.23	181,181,181,181	0
55	MG	QA	1654	1/1	-0.06	0.31	189,189,189,189	0
55	MG	RA	3075	1/1	-0.04	0.49	147,147,147,147	0
55	MG	RA	3272	1/1	-0.03	0.27	188,188,188,188	0
55	MG	YA	3254	1/1	0.02	0.23	181,181,181,181	0
55	MG	RA	3211	1/1	0.03	0.27	145,145,145,145	0
55	MG	RA	2989	1/1	0.04	0.27	136,136,136,136	0
55	MG	RA	2907	1/1	0.05	0.22	158,158,158,158	0
55	MG	YA	3202	1/1	0.05	0.41	164,164,164,164	0
55	MG	RA	3078	1/1	0.07	0.45	208,208,208,208	0
55	MG	RA	3326	1/1	0.10	0.22	165,165,165,165	0
55	MG	RA	3030	1/1	0.10	0.22	157,157,157,157	0
55	MG	YA	3250	1/1	0.11	0.34	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1675	1/1	0.11	0.17	137,137,137,137	0
55	MG	RA	2921	1/1	0.11	0.43	136,136,136,136	0
55	MG	YA	3126	1/1	0.12	0.52	84,84,84,84	0
55	MG	RA	3223	1/1	0.12	0.41	122,122,122,122	0
55	MG	XA	1647	1/1	0.13	0.14	199,199,199,199	0
55	MG	RA	3013	1/1	0.14	0.42	143,143,143,143	0
55	MG	RA	2909	1/1	0.14	0.30	186,186,186,186	0
55	MG	RA	3122	1/1	0.14	0.21	97,97,97,97	0
55	MG	RA	3008	1/1	0.15	0.29	150,150,150,150	0
55	MG	XA	1651	1/1	0.15	0.25	162,162,162,162	0
55	MG	YA	3093	1/1	0.16	0.26	127,127,127,127	0
55	MG	YA	3117	1/1	0.16	0.88	120,120,120,120	0
55	MG	YA	2962	1/1	0.17	0.41	124,124,124,124	0
55	MG	RA	3138	1/1	0.17	0.18	185,185,185,185	0
55	MG	RA	3275	1/1	0.17	0.26	156,156,156,156	0
55	MG	RA	3023	1/1	0.18	0.36	98,98,98,98	0
55	MG	RA	3005	1/1	0.18	0.31	174,174,174,174	0
55	MG	RA	3035	1/1	0.18	0.23	113,113,113,113	0
55	MG	YA	3234	1/1	0.19	0.32	123,123,123,123	0
55	MG	QA	1627	1/1	0.20	0.21	173,173,173,173	0
55	MG	RA	3193	1/1	0.20	0.22	141,141,141,141	0
55	MG	QA	1605	1/1	0.20	0.31	188,188,188,188	0
55	MG	QA	1647	1/1	0.20	0.23	225,225,225,225	0
55	MG	RA	2937	1/1	0.20	0.28	119,119,119,119	0
55	MG	YA	3262	1/1	0.20	0.44	150,150,150,150	0
55	MG	RA	3172	1/1	0.20	0.24	107,107,107,107	0
55	MG	YA	3176	1/1	0.21	0.21	111,111,111,111	0
55	MG	RA	3179	1/1	0.21	0.32	121,121,121,121	0
55	MG	XA	1680	1/1	0.22	0.36	144,144,144,144	0
55	MG	RA	3206	1/1	0.23	0.28	101,101,101,101	0
55	MG	YA	2965	1/1	0.23	0.34	94,94,94,94	0
55	MG	XA	1620	1/1	0.24	0.23	138,138,138,138	0
55	MG	XA	1676	1/1	0.25	0.35	143,143,143,143	0
55	MG	QA	1662	1/1	0.25	0.30	151,151,151,151	0
55	MG	QA	1615	1/1	0.25	0.27	139,139,139,139	0
55	MG	QA	1624	1/1	0.26	0.23	92,92,92,92	0
55	MG	YA	2951	1/1	0.26	0.34	101,101,101,101	0
55	MG	XA	1679	1/1	0.26	0.25	124,124,124,124	0
55	MG	RA	3286	1/1	0.27	0.51	126,126,126,126	0
55	MG	RA	2938	1/1	0.27	0.37	159,159,159,159	0
55	MG	YA	3213	1/1	0.28	0.20	169,169,169,169	0
55	MG	RA	3217	1/1	0.28	0.12	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	2905	1/1	0.28	0.56	175,175,175,175	0
55	MG	YA	3175	1/1	0.29	0.50	117,117,117,117	0
55	MG	QA	1636	1/1	0.29	0.26	134,134,134,134	0
55	MG	YA	3281	1/1	0.29	0.45	151,151,151,151	0
55	MG	QA	1602	1/1	0.30	0.21	148,148,148,148	0
55	MG	RA	2935	1/1	0.30	0.24	132,132,132,132	0
55	MG	YA	3015	1/1	0.30	0.25	123,123,123,123	0
55	MG	XA	1657	1/1	0.30	0.48	236,236,236,236	0
55	MG	YA	3039	1/1	0.31	0.10	123,123,123,123	0
55	MG	YA	2980	1/1	0.31	0.21	84,84,84,84	0
55	MG	QA	1664	1/1	0.31	0.13	156,156,156,156	0
55	MG	YA	3245	1/1	0.32	0.49	84,84,84,84	0
55	MG	XA	1660	1/1	0.32	0.32	114,114,114,114	0
55	MG	YA	3290	1/1	0.32	0.41	211,211,211,211	0
55	MG	YA	3178	1/1	0.33	0.40	84,84,84,84	0
55	MG	YA	3233	1/1	0.33	0.17	153,153,153,153	0
55	MG	RA	3294	1/1	0.34	0.14	143,143,143,143	0
55	MG	RA	2906	1/1	0.34	0.40	150,150,150,150	0
55	MG	RA	2963	1/1	0.34	0.20	256,256,256,256	0
55	MG	RA	3140	1/1	0.35	0.37	88,88,88,88	0
55	MG	RA	3083	1/1	0.35	0.66	150,150,150,150	0
55	MG	YA	2916	1/1	0.35	0.37	121,121,121,121	0
55	MG	YA	3162	1/1	0.37	0.13	112,112,112,112	0
55	MG	YA	2955	1/1	0.37	0.48	110,110,110,110	0
55	MG	QA	1613	1/1	0.37	0.35	127,127,127,127	0
55	MG	XA	1672	1/1	0.37	0.23	160,160,160,160	0
55	MG	YA	2948	1/1	0.37	0.33	84,84,84,84	0
55	MG	YA	3137	1/1	0.37	0.31	110,110,110,110	0
55	MG	RA	3029	1/1	0.37	0.34	100,100,100,100	0
55	MG	YA	2954	1/1	0.37	0.39	135,135,135,135	0
55	MG	YA	2904	1/1	0.38	0.47	122,122,122,122	0
55	MG	YA	3164	1/1	0.38	0.37	84,84,84,84	0
55	MG	YA	3171	1/1	0.38	0.26	84,84,84,84	0
55	MG	RA	3161	1/1	0.38	0.28	116,116,116,116	0
55	MG	YA	3068	1/1	0.38	0.21	158,158,158,158	0
55	MG	YA	3120	1/1	0.38	0.41	84,84,84,84	0
55	MG	RA	2930	1/1	0.39	0.32	136,136,136,136	0
55	MG	YA	2972	1/1	0.39	0.31	100,100,100,100	0
55	MG	RA	3117	1/1	0.39	0.12	243,243,243,243	0
55	MG	RA	2923	1/1	0.39	0.28	174,174,174,174	0
55	MG	YA	3060	1/1	0.40	0.18	177,177,177,177	0
55	MG	YA	3148	1/1	0.40	0.18	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3279	1/1	0.40	0.21	122,122,122,122	0
55	MG	XA	1650	1/1	0.40	0.19	189,189,189,189	0
55	MG	QA	1655	1/1	0.40	0.17	121,121,121,121	0
55	MG	YA	3115	1/1	0.41	0.30	148,148,148,148	0
55	MG	RA	3170	1/1	0.41	0.18	132,132,132,132	0
55	MG	RA	3127	1/1	0.41	0.14	132,132,132,132	0
55	MG	RA	3018	1/1	0.41	0.11	136,136,136,136	0
55	MG	YA	3179	1/1	0.41	0.32	84,84,84,84	0
55	MG	XA	1613	1/1	0.41	0.50	171,171,171,171	0
55	MG	YB	201	1/1	0.41	0.35	104,104,104,104	0
55	MG	XA	1628	1/1	0.42	0.20	109,109,109,109	0
55	MG	XA	1601	1/1	0.42	0.25	174,174,174,174	0
55	MG	RA	2962	1/1	0.42	0.27	124,124,124,124	0
55	MG	QA	1663	1/1	0.42	0.28	128,128,128,128	0
55	MG	YA	3127	1/1	0.42	0.24	84,84,84,84	0
55	MG	RA	3289	1/1	0.43	0.28	125,125,125,125	0
55	MG	RA	3238	1/1	0.43	0.29	157,157,157,157	0
55	MG	YA	3205	1/1	0.43	0.42	152,152,152,152	0
55	MG	RA	3028	1/1	0.43	0.24	96,96,96,96	0
55	MG	YA	3059	1/1	0.43	0.15	189,189,189,189	0
55	MG	YA	3194	1/1	0.44	0.53	163,163,163,163	0
55	MG	YA	3186	1/1	0.44	0.24	187,187,187,187	0
55	MG	QA	1643	1/1	0.44	0.24	180,180,180,180	0
55	MG	RA	3137	1/1	0.45	0.10	177,177,177,177	0
55	MG	RA	2929	1/1	0.45	0.20	211,211,211,211	0
55	MG	RA	3302	1/1	0.45	0.19	116,116,116,116	0
55	MG	XA	1649	1/1	0.45	0.17	123,123,123,123	0
55	MG	RA	3074	1/1	0.46	0.16	149,149,149,149	0
55	MG	RA	3173	1/1	0.46	0.25	130,130,130,130	0
55	MG	RA	3162	1/1	0.46	0.55	139,139,139,139	0
55	MG	YA	2956	1/1	0.46	0.29	114,114,114,114	0
55	MG	RA	3106	1/1	0.46	0.23	90,90,90,90	0
55	MG	RA	3332	1/1	0.46	0.40	120,120,120,120	0
55	MG	YA	3109	1/1	0.46	0.28	95,95,95,95	0
55	MG	RA	2947	1/1	0.46	0.24	118,118,118,118	0
55	MG	QA	1670	1/1	0.46	0.20	190,190,190,190	0
55	MG	RA	3124	1/1	0.46	0.13	115,115,115,115	0
55	MG	QA	1604	1/1	0.47	0.29	153,153,153,153	0
55	MG	RA	3213	1/1	0.47	0.12	157,157,157,157	0
55	MG	YA	3003	1/1	0.47	0.28	97,97,97,97	0
55	MG	RA	3314	1/1	0.47	0.38	137,137,137,137	0
55	MG	RA	3132	1/1	0.48	0.36	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3199	1/1	0.48	0.36	186,186,186,186	0
55	MG	YA	3131	1/1	0.48	0.20	141,141,141,141	0
55	MG	QA	1628	1/1	0.48	0.12	238,238,238,238	0
55	MG	XA	1678	1/1	0.49	0.15	173,173,173,173	0
55	MG	XA	1612	1/1	0.49	0.50	191,191,191,191	0
55	MG	RA	3039	1/1	0.49	0.16	256,256,256,256	0
55	MG	YA	3239	1/1	0.49	0.41	84,84,84,84	0
55	MG	RA	3190	1/1	0.49	0.18	143,143,143,143	0
55	MG	RA	3034	1/1	0.49	0.19	111,111,111,111	0
55	MG	XA	1630	1/1	0.49	0.24	180,180,180,180	0
55	MG	YA	3140	1/1	0.49	0.16	84,84,84,84	0
55	MG	YA	3141	1/1	0.49	0.32	102,102,102,102	0
55	MG	RA	3183	1/1	0.49	0.33	201,201,201,201	0
55	MG	YA	3097	1/1	0.49	0.67	135,135,135,135	0
55	MG	XA	1606	1/1	0.49	0.15	165,165,165,165	0
55	MG	YA	3004	1/1	0.49	0.48	84,84,84,84	0
55	MG	YA	3267	1/1	0.50	0.14	84,84,84,84	0
55	MG	XA	1652	1/1	0.50	0.09	143,143,143,143	0
55	MG	RA	3026	1/1	0.50	0.36	84,84,84,84	0
55	MG	RA	3086	1/1	0.50	0.35	84,84,84,84	0
55	MG	RA	3171	1/1	0.50	0.39	115,115,115,115	0
55	MG	RA	3293	1/1	0.50	0.13	121,121,121,121	0
55	MG	RA	3104	1/1	0.51	0.36	84,84,84,84	0
55	MG	RA	2953	1/1	0.51	0.32	101,101,101,101	0
55	MG	YA	3174	1/1	0.51	0.26	94,94,94,94	0
55	MG	XA	1634	1/1	0.52	0.26	107,107,107,107	0
55	MG	RA	3129	1/1	0.52	0.29	126,126,126,126	0
55	MG	YA	3258	1/1	0.52	0.35	88,88,88,88	0
55	MG	YA	3259	1/1	0.52	0.17	84,84,84,84	0
55	MG	RA	3052	1/1	0.52	0.23	84,84,84,84	0
55	MG	YA	3211	1/1	0.52	0.42	101,101,101,101	0
55	MG	XA	1618	1/1	0.52	0.28	103,103,103,103	0
55	MG	RA	3134	1/1	0.52	0.25	117,117,117,117	0
55	MG	RA	2943	1/1	0.52	0.38	132,132,132,132	0
55	MG	RA	3092	1/1	0.52	0.28	98,98,98,98	0
55	MG	YA	3011	1/1	0.52	0.30	84,84,84,84	0
55	MG	YU	201	1/1	0.52	0.13	97,97,97,97	0
55	MG	YA	2982	1/1	0.53	0.32	84,84,84,84	0
55	MG	YA	2989	1/1	0.53	0.15	120,120,120,120	0
55	MG	RA	2916	1/1	0.53	0.27	97,97,97,97	0
55	MG	QA	1637	1/1	0.53	0.26	126,126,126,126	0
55	MG	RA	3073	1/1	0.53	0.22	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3090	1/1	0.53	0.22	84,84,84,84	0
55	MG	RA	3328	1/1	0.54	0.26	145,145,145,145	0
55	MG	YA	3050	1/1	0.54	0.29	84,84,84,84	0
55	MG	QA	1632	1/1	0.54	0.10	84,84,84,84	0
55	MG	YA	3288	1/1	0.54	0.47	84,84,84,84	0
55	MG	XA	1632	1/1	0.54	0.19	104,104,104,104	0
55	MG	RA	3281	1/1	0.54	0.28	105,105,105,105	0
55	MG	RA	3118	1/1	0.54	0.11	186,186,186,186	0
55	MG	XA	1674	1/1	0.55	0.17	159,159,159,159	0
55	MG	YA	2940	1/1	0.55	0.23	84,84,84,84	0
55	MG	RA	3057	1/1	0.55	0.70	180,180,180,180	0
55	MG	RA	3226	1/1	0.55	0.30	84,84,84,84	0
55	MG	RA	3088	1/1	0.55	0.29	101,101,101,101	0
55	MG	YA	3253	1/1	0.55	0.36	84,84,84,84	0
55	MG	YA	3256	1/1	0.56	0.23	94,94,94,94	0
55	MG	RA	3220	1/1	0.56	0.78	166,166,166,166	0
55	MG	RA	2941	1/1	0.56	0.39	167,167,167,167	0
55	MG	YA	3049	1/1	0.56	0.27	84,84,84,84	0
55	MG	RA	2905	1/1	0.56	0.29	184,184,184,184	0
55	MG	RA	3174	1/1	0.56	0.22	142,142,142,142	0
55	MG	YA	3183	1/1	0.56	0.14	89,89,89,89	0
55	MG	RA	3144	1/1	0.56	0.47	126,126,126,126	0
55	MG	YA	3187	1/1	0.56	0.26	117,117,117,117	0
55	MG	QA	1618	1/1	0.56	0.34	176,176,176,176	0
55	MG	XA	1665	1/1	0.56	0.45	123,123,123,123	0
55	MG	RA	2969	1/1	0.56	0.26	104,104,104,104	0
55	MG	XA	1642	1/1	0.57	0.38	128,128,128,128	0
55	MG	RA	2912	1/1	0.57	0.49	132,132,132,132	0
55	MG	RA	3180	1/1	0.57	0.20	168,168,168,168	0
55	MG	RA	2924	1/1	0.57	0.33	98,98,98,98	0
55	MG	XA	1688	1/1	0.57	0.15	122,122,122,122	0
55	MG	RA	3221	1/1	0.57	0.51	182,182,182,182	0
55	MG	RA	2913	1/1	0.57	0.15	107,107,107,107	0
57	ZN	QN	101	1/1	0.57	0.18	439,439,439,439	0
55	MG	RA	3324	1/1	0.58	0.31	120,120,120,120	0
55	MG	YA	3122	1/1	0.58	0.40	84,84,84,84	0
55	MG	YA	3057	1/1	0.58	0.29	105,105,105,105	0
55	MG	XA	1621	1/1	0.58	0.53	128,128,128,128	0
55	MG	RA	3308	1/1	0.58	0.25	161,161,161,161	0
55	MG	YA	3044	1/1	0.58	0.30	84,84,84,84	0
55	MG	QA	1614	1/1	0.58	0.33	120,120,120,120	0
55	MG	RA	3167	1/1	0.59	0.27	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3151	1/1	0.59	0.28	94,94,94,94	0
55	MG	YA	3155	1/1	0.59	0.36	99,99,99,99	0
55	MG	YA	3237	1/1	0.59	0.41	115,115,115,115	0
55	MG	YA	3010	1/1	0.59	0.41	84,84,84,84	0
55	MG	YA	2974	1/1	0.59	0.43	84,84,84,84	0
55	MG	YA	3114	1/1	0.59	0.29	116,116,116,116	0
55	MG	RA	3065	1/1	0.59	0.24	105,105,105,105	0
55	MG	RA	3208	1/1	0.59	0.30	84,84,84,84	0
55	MG	RA	3064	1/1	0.59	0.47	110,110,110,110	0
55	MG	RA	3304	1/1	0.59	0.28	155,155,155,155	0
55	MG	RA	3076	1/1	0.60	0.26	114,114,114,114	0
55	MG	XA	1619	1/1	0.60	0.32	111,111,111,111	0
55	MG	YA	3017	1/1	0.60	0.44	107,107,107,107	0
55	MG	YA	3032	1/1	0.60	0.21	84,84,84,84	0
55	MG	RA	3002	1/1	0.60	0.27	132,132,132,132	0
55	MG	YA	2961	1/1	0.60	0.27	117,117,117,117	0
55	MG	RA	3095	1/1	0.60	0.14	258,258,258,258	0
55	MG	YA	2964	1/1	0.60	0.36	115,115,115,115	0
55	MG	YA	3055	1/1	0.60	0.12	92,92,92,92	0
55	MG	RA	3101	1/1	0.60	0.68	120,120,120,120	0
55	MG	Y5	102	1/1	0.60	0.24	84,84,84,84	0
55	MG	RE	304	1/1	0.60	0.53	96,96,96,96	0
55	MG	RA	3242	1/1	0.60	0.22	101,101,101,101	0
55	MG	XA	1669	1/1	0.60	0.09	187,187,187,187	0
55	MG	YA	3282	1/1	0.60	0.14	116,116,116,116	0
55	MG	YA	3287	1/1	0.60	0.35	84,84,84,84	0
55	MG	YA	2931	1/1	0.60	0.39	84,84,84,84	0
55	MG	RA	2965	1/1	0.60	0.20	211,211,211,211	0
55	MG	YA	3228	1/1	0.60	0.28	115,115,115,115	0
55	MG	RA	2992	1/1	0.60	0.15	123,123,123,123	0
55	MG	RA	3198	1/1	0.60	0.17	144,144,144,144	0
55	MG	RA	3260	1/1	0.61	0.41	104,104,104,104	0
55	MG	YA	3061	1/1	0.61	0.14	146,146,146,146	0
55	MG	QA	1617	1/1	0.61	0.36	159,159,159,159	0
55	MG	YA	3128	1/1	0.61	0.38	134,134,134,134	0
55	MG	YA	3276	1/1	0.61	0.51	115,115,115,115	0
55	MG	RA	2942	1/1	0.61	0.25	109,109,109,109	0
55	MG	YA	3135	1/1	0.61	0.32	84,84,84,84	0
55	MG	YA	2952	1/1	0.61	0.41	101,101,101,101	0
55	MG	Y8	101	1/1	0.61	0.58	197,197,197,197	0
55	MG	YA	3048	1/1	0.61	0.37	84,84,84,84	0
55	MG	XA	1616	1/1	0.61	0.35	291,291,291,291	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3093	1/1	0.61	0.17	131,131,131,131	0
55	MG	QA	1625	1/1	0.61	0.21	104,104,104,104	0
55	MG	R0	101	1/1	0.61	0.26	147,147,147,147	0
55	MG	YA	2935	1/1	0.61	0.39	84,84,84,84	0
55	MG	R8	102	1/1	0.62	0.13	109,109,109,109	0
55	MG	YA	3069	1/1	0.62	0.26	176,176,176,176	0
55	MG	QA	1619	1/1	0.62	0.28	123,123,123,123	0
55	MG	YA	3018	1/1	0.62	0.95	120,120,120,120	0
55	MG	YA	3144	1/1	0.62	0.31	93,93,93,93	0
55	MG	RA	3320	1/1	0.62	0.25	84,84,84,84	0
55	MG	RA	2952	1/1	0.62	0.17	143,143,143,143	0
55	MG	YA	3107	1/1	0.62	0.31	204,204,204,204	0
55	MG	YA	3232	1/1	0.62	0.26	91,91,91,91	0
55	MG	RA	3123	1/1	0.62	0.28	115,115,115,115	0
55	MG	RA	3252	1/1	0.62	0.30	121,121,121,121	0
55	MG	RA	3059	1/1	0.63	0.36	153,153,153,153	0
55	MG	RA	3313	1/1	0.63	0.23	203,203,203,203	0
55	MG	XA	1646	1/1	0.63	0.20	148,148,148,148	0
55	MG	XA	1682	1/1	0.63	0.20	95,95,95,95	0
55	MG	QA	1609	1/1	0.63	0.10	120,120,120,120	0
55	MG	QA	1669	1/1	0.63	0.27	158,158,158,158	0
55	MG	QA	1629	1/1	0.63	0.24	142,142,142,142	0
55	MG	QA	1601	1/1	0.63	0.26	123,123,123,123	0
55	MG	RA	3020	1/1	0.63	0.33	126,126,126,126	0
55	MG	RA	3295	1/1	0.64	0.28	129,129,129,129	0
55	MG	YA	2959	1/1	0.64	0.32	84,84,84,84	0
55	MG	YA	3024	1/1	0.64	0.24	84,84,84,84	0
55	MG	YA	3224	1/1	0.64	0.35	84,84,84,84	0
55	MG	YA	2984	1/1	0.64	0.52	84,84,84,84	0
55	MG	YA	3077	1/1	0.64	0.21	87,87,87,87	0
55	MG	YA	3134	1/1	0.65	0.17	120,120,120,120	0
55	MG	XA	1607	1/1	0.65	0.23	108,108,108,108	0
55	MG	YA	2957	1/1	0.65	0.18	84,84,84,84	0
55	MG	RA	3094	1/1	0.65	0.10	106,106,106,106	0
55	MG	RA	2910	1/1	0.65	0.18	149,149,149,149	0
55	MG	RA	3048	1/1	0.65	0.25	168,168,168,168	0
55	MG	YA	3085	1/1	0.65	0.29	84,84,84,84	0
55	MG	RA	3051	1/1	0.65	0.46	170,170,170,170	0
55	MG	YA	3180	1/1	0.66	0.29	90,90,90,90	0
55	MG	YA	3242	1/1	0.66	0.13	84,84,84,84	0
55	MG	XA	1633	1/1	0.66	0.26	99,99,99,99	0
55	MG	QA	1638	1/1	0.66	0.27	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3218	1/1	0.66	0.32	84,84,84,84	0
55	MG	RA	3143	1/1	0.66	0.19	109,109,109,109	0
55	MG	RA	3103	1/1	0.66	0.42	84,84,84,84	0
55	MG	RA	3210	1/1	0.66	0.17	121,121,121,121	0
55	MG	YA	3196	1/1	0.66	0.20	84,84,84,84	0
55	MG	QA	1645	1/1	0.66	0.17	101,101,101,101	0
55	MG	RA	3071	1/1	0.66	0.64	288,288,288,288	0
55	MG	YA	2933	1/1	0.67	0.46	97,97,97,97	0
55	MG	YA	3273	1/1	0.67	0.23	102,102,102,102	0
55	MG	YA	2981	1/1	0.67	0.32	103,103,103,103	0
55	MG	RA	2918	1/1	0.67	0.27	176,176,176,176	0
55	MG	R0	102	1/1	0.67	0.10	120,120,120,120	0
55	MG	YA	3035	1/1	0.67	0.27	122,122,122,122	0
55	MG	QA	1606	1/1	0.67	0.22	116,116,116,116	0
55	MG	RA	3079	1/1	0.67	0.32	135,135,135,135	0
55	MG	RA	2931	1/1	0.67	0.19	125,125,125,125	0
55	MG	YA	3086	1/1	0.67	0.31	84,84,84,84	0
55	MG	YA	2953	1/1	0.67	0.44	113,113,113,113	0
55	MG	RA	3147	1/1	0.67	0.51	104,104,104,104	0
55	MG	RA	3240	1/1	0.67	0.21	89,89,89,89	0
55	MG	RA	3054	1/1	0.68	0.37	84,84,84,84	0
55	MG	RA	2920	1/1	0.68	0.17	113,113,113,113	0
55	MG	YA	3203	1/1	0.68	0.27	84,84,84,84	0
55	MG	RA	2939	1/1	0.68	0.14	84,84,84,84	0
55	MG	YA	3209	1/1	0.68	0.19	111,111,111,111	0
55	MG	YA	2995	1/1	0.68	0.28	116,116,116,116	0
55	MG	RA	3053	1/1	0.68	0.34	122,122,122,122	0
55	MG	YA	3268	1/1	0.68	0.27	89,89,89,89	0
55	MG	RA	3182	1/1	0.68	0.12	150,150,150,150	0
55	MG	RA	3199	1/1	0.68	0.26	84,84,84,84	0
55	MG	XA	1658	1/1	0.69	0.33	179,179,179,179	0
55	MG	RA	2986	1/1	0.69	0.34	84,84,84,84	0
55	MG	XA	1664	1/1	0.69	0.30	84,84,84,84	0
55	MG	YA	3005	1/1	0.69	0.32	84,84,84,84	0
55	MG	YA	3143	1/1	0.69	0.39	84,84,84,84	0
55	MG	YA	2908	1/1	0.69	0.30	84,84,84,84	0
55	MG	QA	1607	1/1	0.69	0.34	84,84,84,84	0
55	MG	RA	2903	1/1	0.69	0.13	100,100,100,100	0
55	MG	XA	1670	1/1	0.69	0.34	136,136,136,136	0
55	MG	RA	3102	1/1	0.69	0.29	102,102,102,102	0
55	MG	YA	3189	1/1	0.69	0.21	93,93,93,93	0
55	MG	YA	2936	1/1	0.69	0.42	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3136	1/1	0.69	0.38	84,84,84,84	0
55	MG	RA	3156	1/1	0.70	0.19	106,106,106,106	0
55	MG	XA	1623	1/1	0.70	0.18	127,127,127,127	0
55	MG	YA	3257	1/1	0.70	0.19	84,84,84,84	0
55	MG	QA	1626	1/1	0.70	0.18	104,104,104,104	0
55	MG	RA	3327	1/1	0.70	0.31	84,84,84,84	0
55	MG	RA	3273	1/1	0.70	0.29	113,113,113,113	0
55	MG	YA	3182	1/1	0.70	0.14	84,84,84,84	0
55	MG	YA	3291	1/1	0.70	0.33	84,84,84,84	0
55	MG	YA	3247	1/1	0.70	0.21	87,87,87,87	0
55	MG	YR	202	1/1	0.70	0.40	119,119,119,119	0
55	MG	YA	2944	1/1	0.70	0.18	106,106,106,106	0
55	MG	RA	3305	1/1	0.70	0.22	134,134,134,134	0
55	MG	XA	1656	1/1	0.71	0.13	98,98,98,98	0
55	MG	YA	3132	1/1	0.71	0.10	124,124,124,124	0
55	MG	YA	3087	1/1	0.71	0.43	84,84,84,84	0
55	MG	XA	1685	1/1	0.71	0.18	113,113,113,113	0
55	MG	YA	3153	1/1	0.71	0.41	84,84,84,84	0
55	MG	YA	3002	1/1	0.71	0.28	132,132,132,132	0
55	MG	RA	3133	1/1	0.71	0.88	169,169,169,169	0
55	MG	YA	2963	1/1	0.71	0.35	84,84,84,84	0
55	MG	YA	3210	1/1	0.71	0.40	121,121,121,121	0
55	MG	YA	2907	1/1	0.71	0.46	151,151,151,151	0
55	MG	QA	1642	1/1	0.71	0.07	157,157,157,157	0
55	MG	YA	3248	1/1	0.71	0.27	134,134,134,134	0
55	MG	YA	3133	1/1	0.72	0.16	84,84,84,84	0
55	MG	RA	3045	1/1	0.72	0.31	169,169,169,169	0
55	MG	RA	3112	1/1	0.72	0.24	84,84,84,84	0
55	MG	YA	3265	1/1	0.72	0.34	107,107,107,107	0
55	MG	RA	3115	1/1	0.72	0.10	130,130,130,130	0
55	MG	RA	3204	1/1	0.72	0.34	167,167,167,167	0
55	MG	YA	3271	1/1	0.72	0.30	92,92,92,92	0
55	MG	RA	2954	1/1	0.72	0.62	306,306,306,306	0
55	MG	RA	2968	1/1	0.72	0.13	176,176,176,176	0
55	MG	YA	3111	1/1	0.72	0.17	119,119,119,119	0
55	MG	RA	2998	1/1	0.72	0.18	84,84,84,84	0
55	MG	QA	1660	1/1	0.72	0.16	127,127,127,127	0
55	MG	YA	3067	1/1	0.72	0.11	102,102,102,102	0
55	MG	RA	2972	1/1	0.72	0.33	84,84,84,84	0
55	MG	RA	3125	1/1	0.72	0.38	174,174,174,174	0
55	MG	XA	1603	1/1	0.72	0.15	189,189,189,189	0
55	MG	YA	3156	1/1	0.72	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3083	1/1	0.72	0.33	84,84,84,84	0
55	MG	YA	2932	1/1	0.72	0.70	84,84,84,84	0
55	MG	RA	2904	1/1	0.72	0.30	219,219,219,219	0
55	MG	YA	3001	1/1	0.72	0.11	84,84,84,84	0
55	MG	RA	3225	1/1	0.73	0.32	93,93,93,93	0
55	MG	YA	3094	1/1	0.73	0.17	104,104,104,104	0
55	MG	YA	3095	1/1	0.73	0.14	84,84,84,84	0
55	MG	QA	1623	1/1	0.73	0.24	84,84,84,84	0
55	MG	YA	2988	1/1	0.73	0.31	84,84,84,84	0
55	MG	RA	3237	1/1	0.73	0.33	84,84,84,84	0
55	MG	YA	3110	1/1	0.73	0.20	177,177,177,177	0
55	MG	YA	3051	1/1	0.73	0.31	84,84,84,84	0
55	MG	YA	3154	1/1	0.73	0.14	138,138,138,138	0
55	MG	RA	2917	1/1	0.73	0.15	100,100,100,100	0
55	MG	QA	1648	1/1	0.73	0.28	139,139,139,139	0
55	MG	RA	2926	1/1	0.73	0.31	124,124,124,124	0
55	MG	XA	1602	1/1	0.73	0.20	96,96,96,96	0
55	MG	RA	3046	1/1	0.73	0.22	150,150,150,150	0
55	MG	YA	3173	1/1	0.73	0.29	84,84,84,84	0
55	MG	YA	2915	1/1	0.73	0.28	107,107,107,107	0
55	MG	XA	1637	1/1	0.73	0.16	84,84,84,84	0
55	MG	YA	3284	1/1	0.73	0.10	128,128,128,128	0
55	MG	YA	2930	1/1	0.73	0.41	84,84,84,84	0
55	MG	RA	3107	1/1	0.73	0.25	94,94,94,94	0
55	MG	QL	201	1/1	0.73	0.19	258,258,258,258	0
55	MG	RA	3222	1/1	0.73	0.36	166,166,166,166	0
55	MG	RA	3031	1/1	0.73	0.14	94,94,94,94	0
55	MG	RA	3166	1/1	0.73	0.23	124,124,124,124	0
55	MG	RA	3322	1/1	0.73	0.23	104,104,104,104	0
55	MG	RA	3285	1/1	0.73	0.17	161,161,161,161	0
55	MG	RA	2957	1/1	0.74	0.32	95,95,95,95	0
55	MG	RA	2964	1/1	0.74	0.17	84,84,84,84	0
55	MG	YA	3104	1/1	0.74	0.28	105,105,105,105	0
55	MG	RA	3157	1/1	0.74	0.19	156,156,156,156	0
55	MG	YA	2934	1/1	0.74	0.56	84,84,84,84	0
55	MG	YA	2976	1/1	0.74	0.28	84,84,84,84	0
55	MG	YA	2906	1/1	0.74	0.28	84,84,84,84	0
55	MG	RA	2908	1/1	0.74	0.12	102,102,102,102	0
55	MG	RA	2999	1/1	0.74	0.41	121,121,121,121	0
55	MG	YA	3054	1/1	0.74	0.14	93,93,93,93	0
55	MG	YA	2983	1/1	0.74	0.56	84,84,84,84	0
55	MG	RA	3280	1/1	0.74	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3001	1/1	0.74	0.16	95,95,95,95	0
55	MG	RA	2966	1/1	0.74	0.14	149,149,149,149	0
57	ZN	XN	101	1/1	0.74	0.14	489,489,489,489	0
55	MG	QA	1651	1/1	0.75	0.25	116,116,116,116	0
55	MG	RA	3152	1/1	0.75	0.47	122,122,122,122	0
55	MG	QA	1622	1/1	0.75	0.49	169,169,169,169	0
55	MG	YA	2912	1/1	0.75	0.30	84,84,84,84	0
55	MG	QA	1621	1/1	0.75	0.32	159,159,159,159	0
55	MG	RA	3214	1/1	0.75	0.29	157,157,157,157	0
55	MG	YA	2926	1/1	0.75	0.22	84,84,84,84	0
55	MG	RA	3111	1/1	0.75	0.32	102,102,102,102	0
55	MG	RA	3330	1/1	0.75	0.22	84,84,84,84	0
55	MG	RA	3066	1/1	0.75	0.22	117,117,117,117	0
55	MG	QA	1666	1/1	0.75	0.13	178,178,178,178	0
55	MG	RA	3200	1/1	0.75	0.25	141,141,141,141	0
55	MG	RA	3307	1/1	0.75	0.40	132,132,132,132	0
55	MG	RA	2936	1/1	0.75	0.12	87,87,87,87	0
55	MG	YA	3066	1/1	0.75	0.24	113,113,113,113	0
55	MG	RA	3205	1/1	0.75	0.27	100,100,100,100	0
55	MG	XA	1668	1/1	0.75	0.13	131,131,131,131	0
55	MG	YA	2979	1/1	0.75	0.38	95,95,95,95	0
55	MG	YQ	201	1/1	0.75	0.08	111,111,111,111	0
55	MG	QA	1649	1/1	0.75	0.24	109,109,109,109	0
55	MG	YA	3082	1/1	0.75	0.38	84,84,84,84	0
55	MG	YA	3123	1/1	0.75	0.23	84,84,84,84	0
55	MG	YA	3161	1/1	0.75	0.23	132,132,132,132	0
55	MG	RA	2975	1/1	0.76	0.51	104,104,104,104	0
55	MG	RA	2933	1/1	0.76	0.16	194,194,194,194	0
55	MG	YA	3158	1/1	0.76	0.30	84,84,84,84	0
55	MG	RA	3299	1/1	0.76	0.10	102,102,102,102	0
55	MG	QA	1658	1/1	0.76	0.10	84,84,84,84	0
55	MG	YA	3240	1/1	0.76	0.25	84,84,84,84	0
55	MG	YA	3195	1/1	0.76	0.16	84,84,84,84	0
55	MG	YA	3243	1/1	0.76	0.28	108,108,108,108	0
55	MG	YA	3038	1/1	0.76	0.25	84,84,84,84	0
55	MG	YA	3168	1/1	0.76	0.50	84,84,84,84	0
55	MG	YA	3286	1/1	0.76	0.32	144,144,144,144	0
55	MG	YA	3118	1/1	0.76	0.33	84,84,84,84	0
55	MG	YA	3119	1/1	0.76	0.39	84,84,84,84	0
55	MG	RA	3282	1/1	0.76	0.28	149,149,149,149	0
55	MG	RA	2950	1/1	0.76	0.09	108,108,108,108	0
55	MG	YA	3292	1/1	0.76	0.13	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3271	1/1	0.76	0.22	102,102,102,102	0
55	MG	YE	302	1/1	0.76	0.24	131,131,131,131	0
55	MG	YA	3124	1/1	0.76	0.36	84,84,84,84	0
55	MG	QA	1631	1/1	0.76	0.10	110,110,110,110	0
55	MG	RA	2928	1/1	0.76	0.17	138,138,138,138	0
55	MG	XA	1671	1/1	0.76	0.08	149,149,149,149	0
55	MG	XE	201	1/1	0.76	0.20	157,157,157,157	0
55	MG	YA	3272	1/1	0.77	0.26	98,98,98,98	0
55	MG	QA	1641	1/1	0.77	0.18	155,155,155,155	0
55	MG	YA	3275	1/1	0.77	0.24	112,112,112,112	0
55	MG	YA	3042	1/1	0.77	0.34	84,84,84,84	0
55	MG	YA	3072	1/1	0.77	0.32	106,106,106,106	0
55	MG	YA	2968	1/1	0.77	0.33	84,84,84,84	0
55	MG	RA	3056	1/1	0.77	0.31	139,139,139,139	0
55	MG	YA	2929	1/1	0.77	0.39	84,84,84,84	0
55	MG	RA	3194	1/1	0.77	0.13	111,111,111,111	0
55	MG	RA	3176	1/1	0.77	0.15	152,152,152,152	0
55	MG	QA	1665	1/1	0.77	0.17	84,84,84,84	0
55	MG	YA	3255	1/1	0.77	0.24	84,84,84,84	0
55	MG	YA	3088	1/1	0.77	0.25	84,84,84,84	0
55	MG	QF	301	1/1	0.77	0.12	145,145,145,145	0
55	MG	RA	3218	1/1	0.77	0.17	196,196,196,196	0
55	MG	RA	2976	1/1	0.77	0.47	139,139,139,139	0
55	MG	RA	3116	1/1	0.77	0.18	89,89,89,89	0
55	MG	YA	3263	1/1	0.77	0.53	88,88,88,88	0
55	MG	RA	3311	1/1	0.77	0.26	84,84,84,84	0
55	MG	YA	3096	1/1	0.77	0.26	92,92,92,92	0
55	MG	RA	3146	1/1	0.77	0.09	84,84,84,84	0
55	MG	YA	2945	1/1	0.77	0.17	86,86,86,86	0
55	MG	RA	3202	1/1	0.78	0.18	134,134,134,134	0
55	MG	YA	3025	1/1	0.78	0.10	98,98,98,98	0
55	MG	YA	3031	1/1	0.78	0.48	84,84,84,84	0
55	MG	RA	3027	1/1	0.78	0.23	92,92,92,92	0
55	MG	XA	1605	1/1	0.78	0.43	161,161,161,161	0
55	MG	RA	3038	1/1	0.78	0.20	119,119,119,119	0
55	MG	RA	3141	1/1	0.78	0.25	84,84,84,84	0
55	MG	XA	1654	1/1	0.78	0.13	118,118,118,118	0
55	MG	XA	1610	1/1	0.78	0.57	237,237,237,237	0
55	MG	RA	3310	1/1	0.78	0.53	116,116,116,116	0
55	MG	YA	2911	1/1	0.78	0.24	84,84,84,84	0
55	MG	RA	3278	1/1	0.78	0.12	113,113,113,113	0
55	MG	RA	3177	1/1	0.78	0.15	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3053	1/1	0.78	0.22	93,93,93,93	0
55	MG	YA	3006	1/1	0.78	0.35	84,84,84,84	0
55	MG	YA	2950	1/1	0.78	0.17	111,111,111,111	0
55	MG	YA	3129	1/1	0.78	0.30	84,84,84,84	0
55	MG	YA	3130	1/1	0.78	0.22	84,84,84,84	0
55	MG	YA	3165	1/1	0.78	0.22	84,84,84,84	0
55	MG	XA	1641	1/1	0.78	0.16	112,112,112,112	0
55	MG	YA	3169	1/1	0.78	0.14	119,119,119,119	0
55	MG	YA	2922	1/1	0.78	0.22	84,84,84,84	0
55	MG	RA	3256	1/1	0.78	0.10	84,84,84,84	0
55	MG	QA	1616	1/1	0.78	0.10	128,128,128,128	0
55	MG	YA	3073	1/1	0.79	0.16	84,84,84,84	0
55	MG	RA	3207	1/1	0.79	0.13	151,151,151,151	0
55	MG	YA	3212	1/1	0.79	0.29	84,84,84,84	0
55	MG	YA	2985	1/1	0.79	0.47	84,84,84,84	0
55	MG	RA	3276	1/1	0.79	0.14	138,138,138,138	0
55	MG	RA	3251	1/1	0.79	0.16	177,177,177,177	0
55	MG	YA	3159	1/1	0.79	0.30	84,84,84,84	0
55	MG	RA	3297	1/1	0.79	0.22	167,167,167,167	0
55	MG	YA	2997	1/1	0.79	0.37	84,84,84,84	0
55	MG	RA	3318	1/1	0.79	0.41	84,84,84,84	0
55	MG	QA	1603	1/1	0.79	0.10	121,121,121,121	0
55	MG	QA	1610	1/1	0.79	1.36	211,211,211,211	0
55	MG	YA	3065	1/1	0.79	0.13	107,107,107,107	0
55	MG	RA	3037	1/1	0.79	0.09	145,145,145,145	0
55	MG	YA	2913	1/1	0.79	0.29	84,84,84,84	0
55	MG	RA	2970	1/1	0.79	0.49	102,102,102,102	0
55	MG	RA	2982	1/1	0.79	0.14	87,87,87,87	0
55	MG	RA	3241	1/1	0.79	0.28	84,84,84,84	0
55	MG	YA	3236	1/1	0.80	0.28	84,84,84,84	0
55	MG	RA	3150	1/1	0.80	0.17	84,84,84,84	0
55	MG	Y2	101	1/1	0.80	0.20	133,133,133,133	0
55	MG	YA	3274	1/1	0.80	0.29	84,84,84,84	0
55	MG	YA	3013	1/1	0.80	0.24	84,84,84,84	0
55	MG	RA	3265	1/1	0.80	0.34	84,84,84,84	0
55	MG	YA	3136	1/1	0.80	0.25	84,84,84,84	0
55	MG	YA	3167	1/1	0.80	0.19	84,84,84,84	0
55	MG	YA	2921	1/1	0.80	0.56	84,84,84,84	0
55	MG	RA	3175	1/1	0.80	0.13	84,84,84,84	0
55	MG	YA	2903	1/1	0.80	0.18	90,90,90,90	0
55	MG	RA	3329	1/1	0.80	0.19	93,93,93,93	0
55	MG	YA	3026	1/1	0.80	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	2969	1/1	0.80	0.37	84,84,84,84	0
55	MG	RA	3010	1/1	0.80	0.14	138,138,138,138	0
55	MG	XA	1629	1/1	0.80	0.08	135,135,135,135	0
55	MG	RA	3243	1/1	0.80	0.18	84,84,84,84	0
55	MG	RA	2914	1/1	0.80	0.14	129,129,129,129	0
55	MG	RA	2987	1/1	0.80	0.23	84,84,84,84	0
55	MG	YA	3231	1/1	0.80	0.19	84,84,84,84	0
55	MG	YA	3101	1/1	0.80	0.69	139,139,139,139	0
55	MG	YA	3043	1/1	0.80	0.29	84,84,84,84	0
55	MG	RA	3017	1/1	0.80	0.18	84,84,84,84	0
55	MG	YA	3270	1/1	0.80	0.26	84,84,84,84	0
55	MG	RA	3203	1/1	0.81	0.14	193,193,193,193	0
55	MG	YA	3150	1/1	0.81	0.67	84,84,84,84	0
55	MG	YA	3021	1/1	0.81	0.56	84,84,84,84	0
55	MG	YA	2967	1/1	0.81	0.09	84,84,84,84	0
55	MG	QA	1620	1/1	0.81	0.21	159,159,159,159	0
55	MG	RA	3025	1/1	0.81	0.13	84,84,84,84	0
55	MG	YA	3191	1/1	0.81	0.26	84,84,84,84	0
55	MG	YA	2999	1/1	0.81	0.19	84,84,84,84	0
55	MG	YA	2971	1/1	0.81	0.25	84,84,84,84	0
55	MG	YA	3062	1/1	0.81	0.20	119,119,119,119	0
55	MG	YA	3034	1/1	0.81	0.23	84,84,84,84	0
55	MG	YA	3197	1/1	0.81	0.14	84,84,84,84	0
55	MG	RA	2974	1/1	0.81	0.38	84,84,84,84	0
55	MG	QH	202	1/1	0.81	0.32	211,211,211,211	0
55	MG	RA	3004	1/1	0.81	0.06	205,205,205,205	0
55	MG	RA	2911	1/1	0.81	0.17	111,111,111,111	0
55	MG	XA	1644	1/1	0.81	0.32	235,235,235,235	0
55	MG	RA	3195	1/1	0.81	0.53	170,170,170,170	0
55	MG	YA	3074	1/1	0.81	0.16	84,84,84,84	0
55	MG	YA	3112	1/1	0.81	0.34	96,96,96,96	0
55	MG	YP	201	1/1	0.81	0.16	113,113,113,113	0
55	MG	RA	2959	1/1	0.81	0.30	84,84,84,84	0
55	MG	YA	3078	1/1	0.81	0.27	140,140,140,140	0
55	MG	RA	3047	1/1	0.81	0.07	139,139,139,139	0
55	MG	RA	3022	1/1	0.81	0.31	84,84,84,84	0
55	MG	RA	3120	1/1	0.81	0.27	129,129,129,129	0
55	MG	RA	2981	1/1	0.82	0.18	109,109,109,109	0
55	MG	XA	1640	1/1	0.82	0.08	101,101,101,101	0
55	MG	XA	1625	1/1	0.82	0.13	190,190,190,190	0
55	MG	YA	3188	1/1	0.82	0.14	124,124,124,124	0
55	MG	QA	1657	1/1	0.82	0.36	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	2927	1/1	0.82	0.09	135,135,135,135	0
55	MG	YA	3030	1/1	0.82	0.26	110,110,110,110	0
55	MG	YA	2942	1/1	0.82	0.26	120,120,120,120	0
55	MG	RA	3323	1/1	0.82	0.31	205,205,205,205	0
55	MG	YA	2958	1/1	0.82	0.40	84,84,84,84	0
55	MG	RA	2994	1/1	0.82	0.12	90,90,90,90	0
55	MG	YA	3056	1/1	0.82	0.25	84,84,84,84	0
55	MG	RA	2995	1/1	0.82	0.30	260,260,260,260	0
55	MG	RF	301	1/1	0.82	0.25	118,118,118,118	0
55	MG	YA	3041	1/1	0.82	0.25	84,84,84,84	0
55	MG	RA	3036	1/1	0.83	0.07	136,136,136,136	0
55	MG	RA	3325	1/1	0.83	0.18	84,84,84,84	0
55	MG	RA	3192	1/1	0.83	0.12	105,105,105,105	0
55	MG	RA	2945	1/1	0.83	0.25	84,84,84,84	0
55	MG	RA	3135	1/1	0.83	0.13	100,100,100,100	0
55	MG	YA	3252	1/1	0.83	0.31	118,118,118,118	0
55	MG	RA	3077	1/1	0.83	0.55	185,185,185,185	0
55	MG	XA	1614	1/1	0.83	0.07	106,106,106,106	0
55	MG	RA	2983	1/1	0.83	0.30	84,84,84,84	0
55	MG	YA	3181	1/1	0.83	0.14	115,115,115,115	0
55	MG	RA	3228	1/1	0.83	0.21	105,105,105,105	0
55	MG	RA	3168	1/1	0.83	0.06	206,206,206,206	0
55	MG	YA	2943	1/1	0.83	0.17	93,93,93,93	0
55	MG	QA	1608	1/1	0.83	0.18	97,97,97,97	0
55	MG	YA	2986	1/1	0.83	0.19	84,84,84,84	0
55	MG	RA	3032	1/1	0.83	0.19	84,84,84,84	0
55	MG	YE	303	1/1	0.83	0.40	124,124,124,124	0
55	MG	YA	3075	1/1	0.83	0.39	84,84,84,84	0
55	MG	YA	3022	1/1	0.83	0.27	84,84,84,84	0
55	MG	YR	201	1/1	0.83	0.14	95,95,95,95	0
55	MG	YA	3052	1/1	0.83	0.10	84,84,84,84	0
55	MG	YA	2946	1/1	0.83	0.15	87,87,87,87	0
55	MG	RA	2901	1/1	0.83	0.14	98,98,98,98	0
55	MG	RA	3003	1/1	0.83	0.18	108,108,108,108	0
55	MG	YA	3206	1/1	0.84	0.11	84,84,84,84	0
55	MG	RA	3298	1/1	0.84	0.17	95,95,95,95	0
55	MG	RA	3098	1/1	0.84	0.41	212,212,212,212	0
55	MG	RA	3042	1/1	0.84	0.07	111,111,111,111	0
55	MG	RA	3160	1/1	0.84	0.11	109,109,109,109	0
55	MG	Y8	102	1/1	0.84	0.32	123,123,123,123	0
55	MG	QL	202	1/1	0.84	0.08	95,95,95,95	0
55	MG	YA	3223	1/1	0.84	0.14	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3103	1/1	0.84	0.46	84,84,84,84	0
55	MG	YA	3227	1/1	0.84	0.30	90,90,90,90	0
55	MG	YA	3177	1/1	0.84	0.11	90,90,90,90	0
55	MG	RA	3306	1/1	0.84	0.12	111,111,111,111	0
55	MG	RA	2967	1/1	0.84	0.10	230,230,230,230	0
55	MG	QA	1656	1/1	0.84	0.17	105,105,105,105	0
55	MG	RA	3058	1/1	0.84	0.30	147,147,147,147	0
55	MG	YA	2996	1/1	0.84	0.12	84,84,84,84	0
55	MG	YA	3070	1/1	0.84	0.23	84,84,84,84	0
55	MG	YA	2937	1/1	0.84	0.21	84,84,84,84	0
55	MG	YA	2938	1/1	0.84	0.20	84,84,84,84	0
55	MG	XA	1631	1/1	0.84	0.30	167,167,167,167	0
55	MG	YA	2910	1/1	0.84	0.20	84,84,84,84	0
55	MG	RA	3012	1/1	0.84	0.13	106,106,106,106	0
55	MG	QA	1635	1/1	0.84	0.11	112,112,112,112	0
55	MG	YA	2970	1/1	0.84	0.42	84,84,84,84	0
55	MG	R8	101	1/1	0.84	0.19	111,111,111,111	0
55	MG	YA	3007	1/1	0.84	0.58	84,84,84,84	0
55	MG	XA	1615	1/1	0.84	0.10	162,162,162,162	0
55	MG	YA	3198	1/1	0.84	0.41	124,124,124,124	0
55	MG	YA	2973	1/1	0.84	0.14	90,90,90,90	0
55	MG	YA	3200	1/1	0.84	0.38	142,142,142,142	0
55	MG	XA	1686	1/1	0.84	0.21	108,108,108,108	0
55	MG	YA	2919	1/1	0.84	0.36	84,84,84,84	0
55	MG	RE	303	1/1	0.84	0.18	109,109,109,109	0
55	MG	RA	2961	1/1	0.85	0.14	101,101,101,101	0
55	MG	RA	3201	1/1	0.85	0.34	125,125,125,125	0
55	MG	RA	3110	1/1	0.85	0.14	108,108,108,108	0
55	MG	RA	3315	1/1	0.85	0.19	100,100,100,100	0
55	MG	RA	2985	1/1	0.85	0.30	139,139,139,139	0
55	MG	YA	3027	1/1	0.85	0.11	102,102,102,102	0
55	MG	YA	3157	1/1	0.85	0.25	84,84,84,84	0
55	MG	RA	3155	1/1	0.85	0.13	95,95,95,95	0
55	MG	XA	1681	1/1	0.85	0.11	171,171,171,171	0
55	MG	YA	2941	1/1	0.85	0.11	106,106,106,106	0
55	MG	RA	3236	1/1	0.85	0.23	84,84,84,84	0
55	MG	YD	302	1/1	0.85	0.35	99,99,99,99	0
55	MG	YA	3269	1/1	0.85	0.23	84,84,84,84	0
55	MG	YA	3185	1/1	0.85	0.12	87,87,87,87	0
55	MG	RA	3097	1/1	0.85	0.04	98,98,98,98	0
55	MG	YA	3098	1/1	0.85	0.26	174,174,174,174	0
55	MG	XA	1655	1/1	0.85	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1643	1/1	0.85	0.18	105,105,105,105	0
55	MG	XA	1673	1/1	0.85	0.12	114,114,114,114	0
55	MG	YA	3222	1/1	0.85	0.15	84,84,84,84	0
55	MG	YA	3020	1/1	0.85	0.18	110,110,110,110	0
55	MG	RA	3055	1/1	0.86	0.24	123,123,123,123	0
55	MG	QA	1646	1/1	0.86	0.07	84,84,84,84	0
55	MG	RA	3119	1/1	0.86	0.11	137,137,137,137	0
55	MG	YA	2990	1/1	0.86	0.08	84,84,84,84	0
55	MG	RA	3089	1/1	0.86	0.17	198,198,198,198	0
55	MG	RA	3283	1/1	0.86	0.41	117,117,117,117	0
55	MG	RA	3181	1/1	0.86	0.14	180,180,180,180	0
55	MG	YA	2966	1/1	0.86	0.28	84,84,84,84	0
55	MG	RA	2934	1/1	0.86	0.21	94,94,94,94	0
55	MG	YA	3285	1/1	0.86	0.13	94,94,94,94	0
55	MG	YA	3108	1/1	0.86	0.12	117,117,117,117	0
55	MG	RA	3288	1/1	0.86	0.13	99,99,99,99	0
55	MG	RA	2977	1/1	0.86	0.11	84,84,84,84	0
55	MG	YA	2914	1/1	0.86	0.45	84,84,84,84	0
55	MG	RA	3185	1/1	0.86	0.24	84,84,84,84	0
55	MG	RA	3033	1/1	0.86	0.16	95,95,95,95	0
55	MG	YA	2918	1/1	0.86	0.20	84,84,84,84	0
55	MG	YA	3009	1/1	0.86	0.24	84,84,84,84	0
55	MG	RA	3062	1/1	0.86	0.26	84,84,84,84	0
55	MG	RA	3191	1/1	0.86	0.39	148,148,148,148	0
55	MG	XA	1635	1/1	0.86	0.11	159,159,159,159	0
55	MG	RA	2919	1/1	0.86	0.10	130,130,130,130	0
55	MG	RA	3230	1/1	0.86	0.17	84,84,84,84	0
55	MG	RA	3043	1/1	0.86	0.09	133,133,133,133	0
55	MG	RA	3303	1/1	0.86	0.20	256,256,256,256	0
55	MG	YA	2901	1/1	0.86	0.32	242,242,242,242	0
55	MG	RA	3006	1/1	0.86	0.17	84,84,84,84	0
55	MG	YA	3081	1/1	0.87	0.18	84,84,84,84	0
55	MG	YA	2939	1/1	0.87	0.11	84,84,84,84	0
55	MG	RA	3100	1/1	0.87	0.60	165,165,165,165	0
55	MG	QA	1661	1/1	0.87	0.12	108,108,108,108	0
55	MG	RA	2979	1/1	0.87	0.11	135,135,135,135	0
55	MG	RA	3215	1/1	0.87	0.11	102,102,102,102	0
55	MG	YA	3149	1/1	0.87	0.15	93,93,93,93	0
55	MG	RA	3151	1/1	0.87	0.13	84,84,84,84	0
55	MG	QA	1652	1/1	0.87	0.09	162,162,162,162	0
55	MG	YA	3063	1/1	0.87	0.17	104,104,104,104	0
55	MG	YA	3040	1/1	0.87	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1659	1/1	0.87	0.15	84,84,84,84	0
55	MG	RA	2951	1/1	0.87	0.24	255,255,255,255	0
55	MG	XA	1661	1/1	0.87	0.20	105,105,105,105	0
55	MG	RA	3292	1/1	0.87	0.15	105,105,105,105	0
55	MG	RA	2956	1/1	0.87	0.28	198,198,198,198	0
55	MG	YA	3071	1/1	0.87	0.22	84,84,84,84	0
55	MG	RA	3087	1/1	0.87	0.29	164,164,164,164	0
55	MG	XA	1687	1/1	0.87	0.54	172,172,172,172	0
55	MG	RA	3041	1/1	0.87	0.07	131,131,131,131	0
55	MG	YA	3235	1/1	0.87	0.25	84,84,84,84	0
55	MG	RA	3121	1/1	0.87	0.31	177,177,177,177	0
55	MG	YA	2975	1/1	0.87	0.12	97,97,97,97	0
55	MG	RA	3246	1/1	0.87	0.20	84,84,84,84	0
55	MG	YA	3080	1/1	0.87	0.13	94,94,94,94	0
55	MG	RE	302	1/1	0.88	0.25	84,84,84,84	0
55	MG	XA	1617	1/1	0.88	0.17	84,84,84,84	0
55	MG	YA	3166	1/1	0.88	0.22	144,144,144,144	0
55	MG	XA	1667	1/1	0.88	0.13	173,173,173,173	0
55	MG	RA	3247	1/1	0.88	0.19	84,84,84,84	0
55	MG	RA	3250	1/1	0.88	0.21	84,84,84,84	0
55	MG	YA	2993	1/1	0.88	0.19	84,84,84,84	0
55	MG	YA	3079	1/1	0.88	0.11	84,84,84,84	0
55	MG	RA	3148	1/1	0.88	0.21	89,89,89,89	0
55	MG	YA	3246	1/1	0.88	0.09	129,129,129,129	0
55	MG	YA	3283	1/1	0.88	0.28	131,131,131,131	0
55	MG	RA	3301	1/1	0.88	0.17	142,142,142,142	0
55	MG	YA	2949	1/1	0.88	0.17	84,84,84,84	0
55	MG	RA	3184	1/1	0.88	0.11	103,103,103,103	0
55	MG	YA	3029	1/1	0.88	0.18	84,84,84,84	0
55	MG	RA	3197	1/1	0.88	0.34	84,84,84,84	0
55	MG	RA	2988	1/1	0.88	0.16	101,101,101,101	0
55	MG	QA	1639	1/1	0.88	0.09	135,135,135,135	0
55	MG	RA	3209	1/1	0.88	0.14	165,165,165,165	0
55	MG	YA	3220	1/1	0.88	0.17	84,84,84,84	0
55	MG	XA	1608	1/1	0.88	0.17	108,108,108,108	0
55	MG	YE	301	1/1	0.88	0.25	113,113,113,113	0
55	MG	YA	3036	1/1	0.88	0.23	84,84,84,84	0
55	MG	XA	1609	1/1	0.88	0.21	96,96,96,96	0
55	MG	YE	304	1/1	0.88	0.33	84,84,84,84	0
55	MG	YA	3226	1/1	0.88	0.06	100,100,100,100	0
55	MG	RA	2960	1/1	0.88	0.21	108,108,108,108	0
55	MG	YA	3266	1/1	0.88	0.23	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3021	1/1	0.88	0.09	96,96,96,96	0
55	MG	RA	3044	1/1	0.88	0.37	156,156,156,156	0
55	MG	RA	3080	1/1	0.88	0.14	108,108,108,108	0
57	ZN	R9	101	1/1	0.88	0.10	314,314,314,314	0
55	MG	RA	3277	1/1	0.88	0.14	182,182,182,182	0
55	MG	YA	2987	1/1	0.89	0.22	84,84,84,84	0
55	MG	YA	3064	1/1	0.89	0.17	84,84,84,84	0
55	MG	RA	3109	1/1	0.89	0.12	84,84,84,84	0
55	MG	YA	3016	1/1	0.89	0.05	84,84,84,84	0
55	MG	RA	3321	1/1	0.89	0.12	88,88,88,88	0
55	MG	RA	3153	1/1	0.89	0.08	117,117,117,117	0
55	MG	QA	1612	1/1	0.89	0.10	141,141,141,141	0
55	MG	RA	3009	1/1	0.89	0.11	101,101,101,101	0
55	MG	YA	3201	1/1	0.89	0.37	139,139,139,139	0
55	MG	RA	3068	1/1	0.89	0.15	113,113,113,113	0
55	MG	RA	3113	1/1	0.89	0.12	84,84,84,84	0
55	MG	XA	1626	1/1	0.89	0.05	112,112,112,112	0
55	MG	XA	1627	1/1	0.89	0.38	165,165,165,165	0
55	MG	YA	2978	1/1	0.89	0.10	90,90,90,90	0
55	MG	RA	3114	1/1	0.89	0.10	84,84,84,84	0
55	MG	RA	3105	1/1	0.89	0.18	107,107,107,107	0
55	MG	QA	1659	1/1	0.89	0.04	125,125,125,125	0
55	MG	RA	3016	1/1	0.89	0.19	84,84,84,84	0
55	MG	YA	3217	1/1	0.89	0.15	104,104,104,104	0
55	MG	RA	3165	1/1	0.89	0.13	197,197,197,197	0
55	MG	RA	3231	1/1	0.89	0.10	141,141,141,141	0
55	MG	RA	3317	1/1	0.89	0.11	84,84,84,84	0
57	ZN	RY	201	1/1	0.89	0.07	344,344,344,344	0
55	MG	RA	3254	1/1	0.89	0.11	130,130,130,130	0
55	MG	YA	3147	1/1	0.90	0.18	84,84,84,84	0
55	MG	RA	3264	1/1	0.90	0.14	148,148,148,148	0
55	MG	YA	2920	1/1	0.90	0.12	84,84,84,84	0
55	MG	RA	3050	1/1	0.90	0.22	110,110,110,110	0
55	MG	RA	3096	1/1	0.90	0.11	122,122,122,122	0
55	MG	YA	2923	1/1	0.90	0.16	84,84,84,84	0
55	MG	YA	3216	1/1	0.90	0.15	84,84,84,84	0
55	MG	YA	3125	1/1	0.90	0.26	89,89,89,89	0
55	MG	RA	3131	1/1	0.90	0.12	117,117,117,117	0
55	MG	RA	2958	1/1	0.90	0.18	91,91,91,91	0
55	MG	YA	3221	1/1	0.90	0.09	84,84,84,84	0
55	MG	RA	2948	1/1	0.90	0.12	84,84,84,84	0
55	MG	YA	2992	1/1	0.90	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3045	1/1	0.90	0.23	84,84,84,84	0
55	MG	YA	3019	1/1	0.90	0.07	84,84,84,84	0
55	MG	RA	3099	1/1	0.90	0.29	84,84,84,84	0
55	MG	RA	3149	1/1	0.90	0.42	85,85,85,85	0
55	MG	YA	3230	1/1	0.90	0.19	84,84,84,84	0
55	MG	XA	1662	1/1	0.90	0.10	141,141,141,141	0
55	MG	XA	1645	1/1	0.90	0.21	106,106,106,106	0
55	MG	YA	2998	1/1	0.90	0.32	84,84,84,84	0
55	MG	RA	2993	1/1	0.90	0.07	141,141,141,141	0
55	MG	XA	1666	1/1	0.90	0.16	113,113,113,113	0
55	MG	QA	1644	1/1	0.90	0.09	84,84,84,84	0
55	MG	RA	2946	1/1	0.90	0.17	96,96,96,96	0
55	MG	RA	2980	1/1	0.90	0.17	84,84,84,84	0
55	MG	QA	1650	1/1	0.90	0.23	108,108,108,108	0
55	MG	RA	3126	1/1	0.90	0.07	137,137,137,137	0
55	MG	QA	1653	1/1	0.91	0.29	130,130,130,130	0
55	MG	RA	2996	1/1	0.91	0.18	177,177,177,177	0
55	MG	RA	3232	1/1	0.91	0.06	99,99,99,99	0
55	MG	YA	3100	1/1	0.91	0.19	84,84,84,84	0
55	MG	YA	3028	1/1	0.91	0.20	84,84,84,84	0
55	MG	YA	2947	1/1	0.91	0.09	84,84,84,84	0
55	MG	RA	3040	1/1	0.91	0.12	89,89,89,89	0
55	MG	YA	3008	1/1	0.91	0.26	84,84,84,84	0
55	MG	YA	3160	1/1	0.91	0.09	112,112,112,112	0
55	MG	YA	2909	1/1	0.91	0.24	84,84,84,84	0
55	MG	YA	3289	1/1	0.91	0.10	84,84,84,84	0
55	MG	RA	3081	1/1	0.91	0.17	84,84,84,84	0
55	MG	YA	3193	1/1	0.91	0.34	176,176,176,176	0
55	MG	RA	3287	1/1	0.91	0.11	123,123,123,123	0
55	MG	RA	3128	1/1	0.91	0.19	187,187,187,187	0
55	MG	YA	3037	1/1	0.91	0.26	84,84,84,84	0
55	MG	YA	3264	1/1	0.91	0.20	84,84,84,84	0
55	MG	YA	3138	1/1	0.91	0.18	98,98,98,98	0
55	MG	RA	3239	1/1	0.91	0.10	84,84,84,84	0
55	MG	RF	302	1/1	0.91	0.08	158,158,158,158	0
55	MG	RA	3291	1/1	0.91	0.15	84,84,84,84	0
55	MG	RA	2915	1/1	0.91	0.10	84,84,84,84	0
55	MG	XA	1636	1/1	0.91	0.12	95,95,95,95	0
55	MG	RA	3178	1/1	0.91	0.41	232,232,232,232	0
55	MG	YA	3238	1/1	0.91	0.10	129,129,129,129	0
55	MG	YX	101	1/1	0.91	0.08	84,84,84,84	0
55	MG	YA	3121	1/1	0.91	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1604	1/1	0.91	0.12	176,176,176,176	0
55	MG	RA	3257	1/1	0.91	0.19	86,86,86,86	0
55	MG	RA	3258	1/1	0.91	0.25	165,165,165,165	0
55	MG	RA	2978	1/1	0.92	0.22	84,84,84,84	0
55	MG	RA	3319	1/1	0.92	0.11	114,114,114,114	0
55	MG	RO	201	1/1	0.92	0.35	186,186,186,186	0
55	MG	XA	1684	1/1	0.92	0.13	210,210,210,210	0
55	MG	RA	3300	1/1	0.92	0.13	117,117,117,117	0
55	MG	XA	1663	1/1	0.92	0.11	115,115,115,115	0
55	MG	RA	3259	1/1	0.92	0.19	97,97,97,97	0
55	MG	RA	3227	1/1	0.92	0.25	123,123,123,123	0
55	MG	RA	3262	1/1	0.92	0.24	194,194,194,194	0
55	MG	RA	3069	1/1	0.92	0.52	189,189,189,189	0
55	MG	RA	3219	1/1	0.92	0.40	143,143,143,143	0
55	MG	XA	1648	1/1	0.92	0.05	137,137,137,137	0
55	MG	RA	3267	1/1	0.92	0.16	143,143,143,143	0
55	MG	YA	3046	1/1	0.92	0.19	124,124,124,124	0
55	MG	YA	3047	1/1	0.92	0.15	84,84,84,84	0
55	MG	RA	2997	1/1	0.92	0.27	161,161,161,161	0
55	MG	YA	2928	1/1	0.92	0.17	103,103,103,103	0
55	MG	RA	3188	1/1	0.92	0.22	140,140,140,140	0
55	MG	RA	3234	1/1	0.92	0.07	101,101,101,101	0
55	MG	RA	3235	1/1	0.92	0.14	84,84,84,84	0
55	MG	RA	3212	1/1	0.92	0.10	170,170,170,170	0
55	MG	YA	3280	1/1	0.92	0.06	120,120,120,120	0
55	MG	RA	2944	1/1	0.92	0.11	84,84,84,84	0
55	MG	QA	1611	1/1	0.92	0.15	124,124,124,124	0
55	MG	RA	3014	1/1	0.92	0.13	84,84,84,84	0
55	MG	RA	2949	1/1	0.93	0.13	96,96,96,96	0
55	MG	YA	3092	1/1	0.93	0.08	149,149,149,149	0
55	MG	RA	3253	1/1	0.93	0.23	84,84,84,84	0
55	MG	YA	2917	1/1	0.93	0.23	98,98,98,98	0
55	MG	RA	3019	1/1	0.93	0.13	84,84,84,84	0
55	MG	RA	3268	1/1	0.93	0.13	84,84,84,84	0
55	MG	YA	3014	1/1	0.93	0.05	84,84,84,84	0
55	MG	RA	3063	1/1	0.93	0.17	84,84,84,84	0
55	MG	YA	3076	1/1	0.93	0.24	158,158,158,158	0
55	MG	RA	3284	1/1	0.93	0.10	108,108,108,108	0
55	MG	RA	3189	1/1	0.93	0.31	174,174,174,174	0
55	MG	YD	301	1/1	0.93	0.14	86,86,86,86	0
55	MG	RA	3091	1/1	0.93	0.28	132,132,132,132	0
55	MG	YA	3106	1/1	0.93	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1622	1/1	0.93	0.10	132,132,132,132	0
55	MG	YA	3000	1/1	0.93	0.10	93,93,93,93	0
55	MG	YA	3241	1/1	0.93	0.18	84,84,84,84	0
55	MG	XA	1653	1/1	0.93	0.11	84,84,84,84	0
55	MG	RA	3249	1/1	0.93	0.10	84,84,84,84	0
55	MG	XA	1624	1/1	0.93	0.06	115,115,115,115	0
55	MG	XA	1611	1/1	0.93	0.41	278,278,278,278	0
55	MG	RA	3216	1/1	0.93	0.12	122,122,122,122	0
55	MG	YA	3190	1/1	0.93	0.28	99,99,99,99	0
55	MG	YA	3249	1/1	0.93	0.07	131,131,131,131	0
55	MG	XO	101	1/1	0.93	0.05	151,151,151,151	0
55	MG	YA	3139	1/1	0.93	0.07	84,84,84,84	0
55	MG	QA	1640	1/1	0.93	0.30	101,101,101,101	0
55	MG	QA	1667	1/1	0.94	0.13	154,154,154,154	0
55	MG	YA	3170	1/1	0.94	0.09	84,84,84,84	0
55	MG	YA	3215	1/1	0.94	0.17	84,84,84,84	0
55	MG	RA	3024	1/1	0.94	0.08	159,159,159,159	0
55	MG	RA	3158	1/1	0.94	0.07	117,117,117,117	0
55	MG	YA	2991	1/1	0.94	0.11	95,95,95,95	0
55	MG	YA	2960	1/1	0.94	0.24	84,84,84,84	0
55	MG	RN	201	1/1	0.94	0.13	98,98,98,98	0
55	MG	RA	3072	1/1	0.94	0.05	142,142,142,142	0
55	MG	RA	3015	1/1	0.94	0.15	141,141,141,141	0
55	MG	YA	3099	1/1	0.94	0.18	84,84,84,84	0
55	MG	YA	3225	1/1	0.94	0.13	100,100,100,100	0
55	MG	RA	3248	1/1	0.94	0.08	105,105,105,105	0
55	MG	RA	3007	1/1	0.94	0.13	87,87,87,87	0
55	MG	RA	3060	1/1	0.94	0.12	106,106,106,106	0
55	MG	RD	301	1/1	0.94	0.18	128,128,128,128	0
55	MG	YA	3204	1/1	0.94	0.13	135,135,135,135	0
55	MG	YA	3105	1/1	0.94	0.16	135,135,135,135	0
55	MG	RE	301	1/1	0.94	0.09	84,84,84,84	0
55	MG	RA	3061	1/1	0.94	0.18	91,91,91,91	0
55	MG	RA	3263	1/1	0.94	0.06	136,136,136,136	0
55	MG	YA	3260	1/1	0.94	0.04	84,84,84,84	0
55	MG	Y1	101	1/1	0.94	0.07	117,117,117,117	0
55	MG	YA	3152	1/1	0.95	0.11	84,84,84,84	0
55	MG	YA	2977	1/1	0.95	0.09	84,84,84,84	0
55	MG	RA	2922	1/1	0.95	0.13	105,105,105,105	0
55	MG	RA	2973	1/1	0.95	0.17	84,84,84,84	0
55	MG	RA	3309	1/1	0.95	0.06	120,120,120,120	0
55	MG	YA	3219	1/1	0.95	0.07	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	Y7	101	1/1	0.95	0.27	208,208,208,208	0
55	MG	RA	3090	1/1	0.95	0.19	138,138,138,138	0
55	MG	RA	3142	1/1	0.95	0.19	152,152,152,152	0
55	MG	XA	1677	1/1	0.95	0.05	147,147,147,147	0
55	MG	RA	3312	1/1	0.95	0.16	115,115,115,115	0
55	MG	RA	3279	1/1	0.95	0.04	169,169,169,169	0
55	MG	YA	3163	1/1	0.95	0.10	104,104,104,104	0
55	MG	YA	3033	1/1	0.95	0.09	84,84,84,84	0
55	MG	YA	3293	1/1	0.95	0.10	102,102,102,102	0
55	MG	YA	2924	1/1	0.95	0.11	84,84,84,84	0
55	MG	RA	3000	1/1	0.95	0.04	109,109,109,109	0
55	MG	RA	2990	1/1	0.95	0.14	103,103,103,103	0
55	MG	YA	3113	1/1	0.95	0.05	84,84,84,84	0
55	MG	YA	3012	1/1	0.95	0.12	84,84,84,84	0
55	MG	RA	3266	1/1	0.95	0.14	305,305,305,305	0
55	MG	YA	3116	1/1	0.95	0.29	133,133,133,133	0
55	MG	YA	3172	1/1	0.95	0.18	84,84,84,84	0
55	MG	RA	3145	1/1	0.95	0.14	112,112,112,112	0
55	MG	RA	2991	1/1	0.95	0.02	110,110,110,110	0
55	MG	RA	3269	1/1	0.95	0.06	200,200,200,200	0
55	MG	YA	2994	1/1	0.95	0.53	84,84,84,84	0
55	MG	RA	3233	1/1	0.95	0.11	84,84,84,84	0
55	MG	RA	3244	1/1	0.95	0.06	144,144,144,144	0
55	MG	RA	2925	1/1	0.95	0.18	84,84,84,84	0
55	MG	RA	3274	1/1	0.95	0.08	149,149,149,149	0
55	MG	YA	3278	1/1	0.95	0.05	85,85,85,85	0
55	MG	RA	3270	1/1	0.96	0.11	84,84,84,84	0
55	MG	RA	3049	1/1	0.96	0.10	84,84,84,84	0
55	MG	RA	3261	1/1	0.96	0.07	191,191,191,191	0
55	MG	RA	3187	1/1	0.96	0.12	130,130,130,130	0
55	MG	YA	3184	1/1	0.96	0.08	95,95,95,95	0
55	MG	YA	3146	1/1	0.96	0.08	84,84,84,84	0
55	MG	YA	3251	1/1	0.96	0.06	99,99,99,99	0
55	MG	YA	3058	1/1	0.96	0.05	84,84,84,84	0
55	MG	RA	3196	1/1	0.96	0.24	168,168,168,168	0
55	MG	RA	3159	1/1	0.96	0.12	104,104,104,104	0
55	MG	RA	2955	1/1	0.96	0.10	192,192,192,192	0
55	MG	RA	3070	1/1	0.96	0.12	181,181,181,181	0
55	MG	RA	3130	1/1	0.96	0.10	119,119,119,119	0
55	MG	YA	2927	1/1	0.96	0.10	103,103,103,103	0
55	MG	RA	3290	1/1	0.96	0.06	95,95,95,95	0
55	MG	RA	2984	1/1	0.96	0.06	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3261	1/1	0.96	0.07	190,190,190,190	0
55	MG	XA	1638	1/1	0.96	0.18	84,84,84,84	0
56	SF4	QD	301	8/8	0.96	0.06	181,237,336,420	0
55	MG	YA	3102	1/1	0.96	0.18	178,178,178,178	0
55	MG	YA	3084	1/1	0.96	0.17	84,84,84,84	0
55	MG	XA	1639	1/1	0.96	0.12	84,84,84,84	0
55	MG	RA	3067	1/1	0.96	0.05	101,101,101,101	0
57	ZN	Y9	101	1/1	0.96	0.05	162,162,162,162	0
55	MG	YA	2925	1/1	0.97	0.11	84,84,84,84	0
55	MG	RA	3084	1/1	0.97	0.11	150,150,150,150	0
55	MG	YF	301	1/1	0.97	0.08	90,90,90,90	0
55	MG	QA	1633	1/1	0.97	0.05	190,190,190,190	0
55	MG	RA	3245	1/1	0.97	0.19	93,93,93,93	0
55	MG	RA	3331	1/1	0.97	0.09	84,84,84,84	0
55	MG	YA	3214	1/1	0.97	0.03	95,95,95,95	0
55	MG	RA	2932	1/1	0.97	0.05	131,131,131,131	0
55	MG	RA	3082	1/1	0.97	0.09	84,84,84,84	0
55	MG	YA	3294	1/1	0.97	0.04	103,103,103,103	0
56	SF4	XD	301	8/8	0.97	0.05	163,216,235,295	0
55	MG	QA	1630	1/1	0.97	0.09	137,137,137,137	0
57	ZN	R5	101	1/1	0.97	0.03	268,268,268,268	0
57	ZN	R6	101	1/1	0.97	0.05	149,149,149,149	0
55	MG	RA	3255	1/1	0.97	0.05	99,99,99,99	0
55	MG	YA	3244	1/1	0.97	0.12	84,84,84,84	0
55	MG	XA	1683	1/1	0.97	0.06	120,120,120,120	0
57	ZN	Y5	101	1/1	0.97	0.07	308,308,308,308	0
55	MG	YA	3207	1/1	0.97	0.06	84,84,84,84	0
55	MG	YA	3208	1/1	0.98	0.09	100,100,100,100	0
55	MG	R3	101	1/1	0.98	0.09	94,94,94,94	0
55	MG	YA	3089	1/1	0.98	0.07	84,84,84,84	0
55	MG	RA	3108	1/1	0.98	0.06	117,117,117,117	0
55	MG	RA	2902	1/1	0.98	0.04	84,84,84,84	0
55	MG	RA	3229	1/1	0.98	0.09	84,84,84,84	0
55	MG	RA	3296	1/1	0.98	0.07	121,121,121,121	0
55	MG	RA	3154	1/1	0.98	0.06	127,127,127,127	0
55	MG	YA	2902	1/1	0.98	0.08	86,86,86,86	0
55	MG	YA	3023	1/1	0.98	0.07	84,84,84,84	0
55	MG	RA	3085	1/1	0.98	0.09	140,140,140,140	0
55	MG	YA	3229	1/1	0.99	0.07	84,84,84,84	0
55	MG	QA	1668	1/1	0.99	0.06	114,114,114,114	0
55	MG	RA	2940	1/1	0.99	0.04	84,84,84,84	0
55	MG	RA	3316	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	Y6	101	1/1	0.99	0.02	144,144,144,144	0
55	MG	RA	2971	1/1	0.99	0.04	84,84,84,84	0
57	ZN	YY	201	1/1	0.99	0.02	193,193,193,193	0

6.5 Other polymers [i](#)

There are no such residues in this entry.