



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 09:50 AM EDT

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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

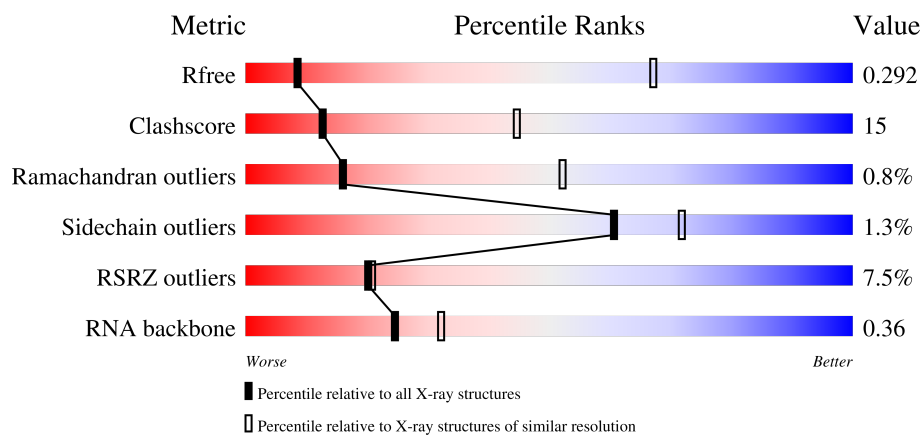
1 Overall quality at a glance

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}	180053	1004 (4.46-3.82)
Clashscore	190562	1004 (4.44-3.84)
Ramachandran outliers	187476	1224 (4.48-3.80)
Sidechain outliers	187428	1211 (4.48-3.80)
RSRZ outliers	180081	1001 (4.46-3.82)
RNA backbone	3983	1026 (5.04-3.10)

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

Mol	Chain	Length	Quality of chain
1	QA	1521	
1	XA	1521	
2	QB	256	
2	XB	256	

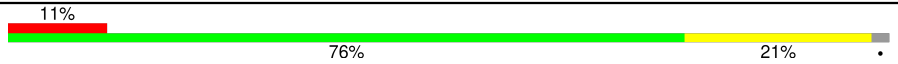
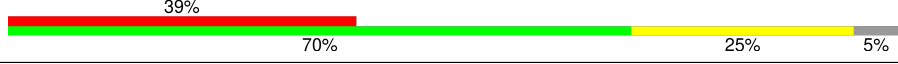
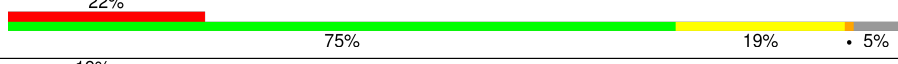
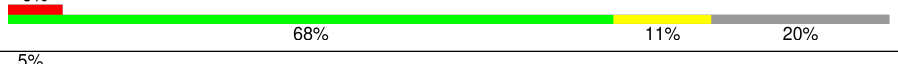
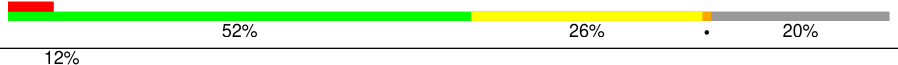
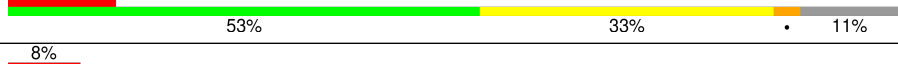
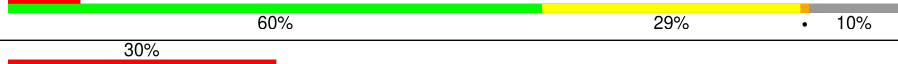
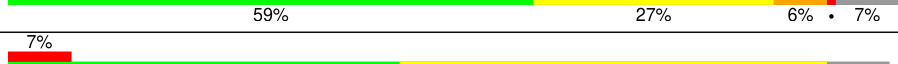
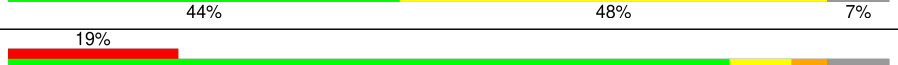
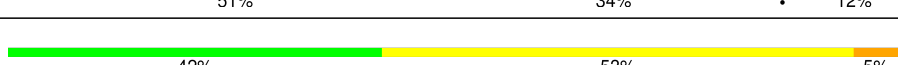
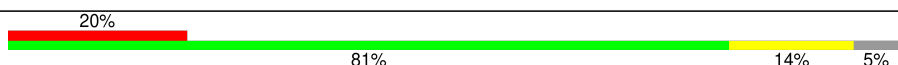
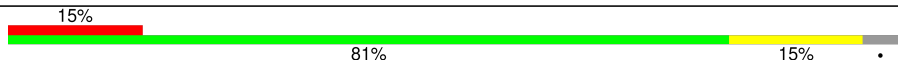
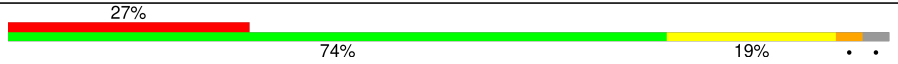
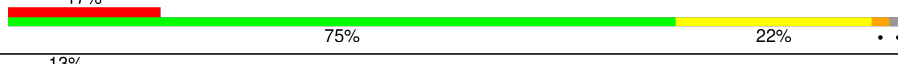
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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	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).

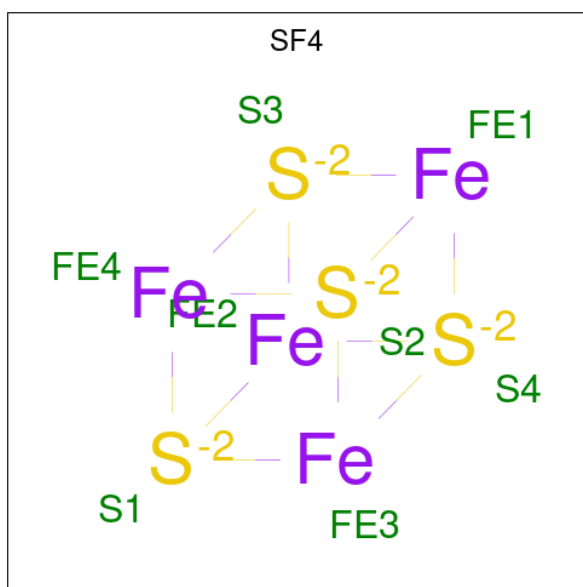
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	70	Total	Mg	0	0
			70	70		
55	QE	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	2	Total	Mg	0	0
			2	2		
55	QL	2	Total	Mg	0	0
			2	2		
55	R0	2	Total	Mg	0	0
			2	2		
55	R3	1	Total	Mg	0	0
			1	1		
55	R8	2	Total	Mg	0	0
			2	2		
55	RA	432	Total	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		

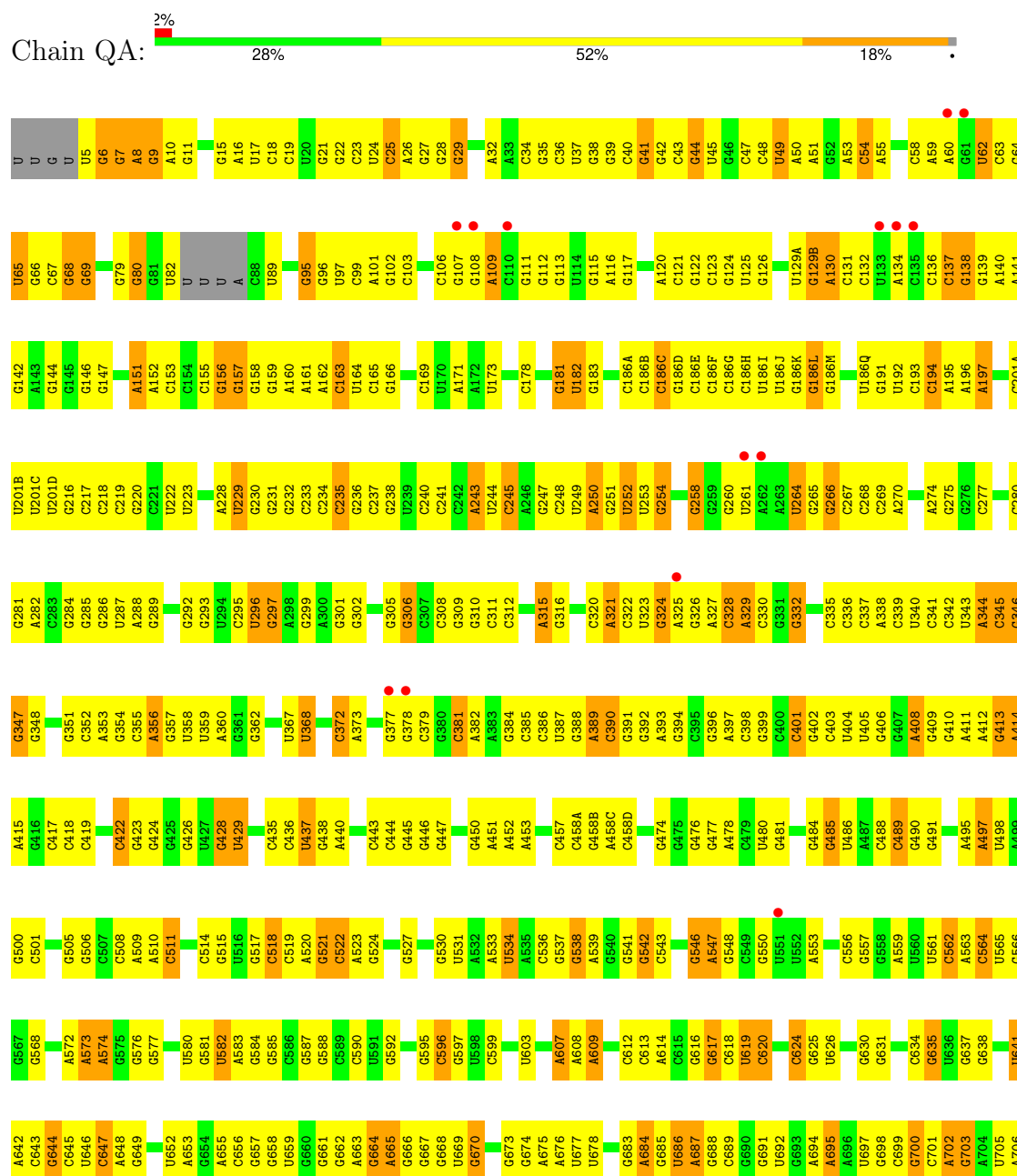
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

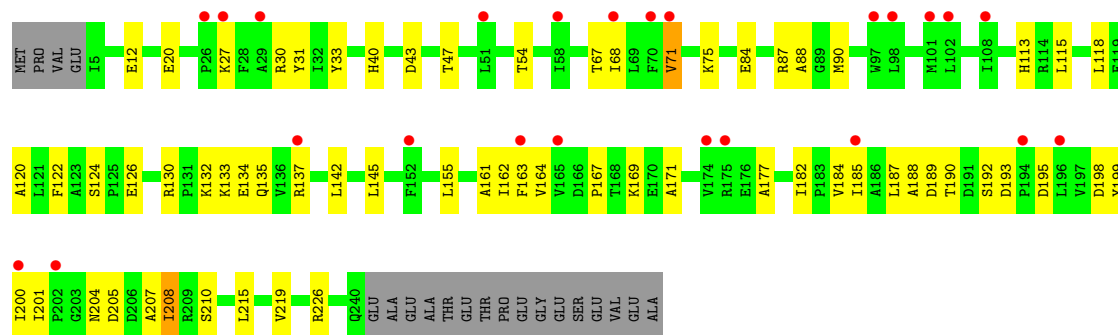


C1524	C14400	G1379	A1319	U1257	C1195	G1124	U1086	U992	C938A	G774	C707
G1525	A1440P	U1380	C1320	G1258	U1196	U1125	C1060	G993	U838B	G775	C708
G1526		U1381	C1321	C1259	U1126	U1126		A994	C338C	G776	C709
C1527		C1382	C1322	C1260	G1197	G1127	G1061	G928	U838D	A777	G710
C1463	C1463	C1383	G1323		G1198	C1128	U1062	G932	C948	G778	G711
U1528	G1464	C1384	A1324	C1263	U1199	C1129	C1063	U997			A712
G1529	G1465		C1325	C1264	C1200	A1130	G1064	G934	G853	A761	G713
A1530	C1466	U1390	G1326	G1265	A1201	G1131	U1065	C998A	G853	A761	G714
U1531	C1467	U1391	C1327	G1266	G1202	C1132	U1066	G999	G954	A762	G715
C1533		G1392	C1328	C1267	C1203	G1133		A1000	G855	C784	A716
A1534	U1472	U1393	A1329	A1268	A1204	G1134	C1069	G1001	A938	G785	C717
C1535	A1473	A1394	U1330	A1269	U1205	U1135	U1070	G1002	C957	G786	G718
A1536	G1474	C1395	G1331	C1270	G1206	U1136	C1071	G1003	G861	A787	G719
G1537	G1475	A1396	A1332	G1271	G1207		U1072	G1004	C862	U788	
C1538	G1476	C1397	A1333	G1272		U1211	G1076	A1005	A865		G721
U1539	C1477	A1398	G1334	G1273	U1121	G1138	U1077	G942	C866	A791	U723
U1540	C1478	C1399	C1335	G1274	U1212	G1139	G1078	U943	G724	A792	U724
U1541	C1479	G1400	C1336	A1275	A1213	C1141	U1079		G867	U793	C726
U1542	G1480	G1401	C1337	G1276	G1214	G1142	G1077	A846	U870	A794	C727
C	U1481	C1404	G1338	C1277	G1215	G1143	G1078	G947	C948	C795	G727
U	U1482	G1405	A1339	A1278	G1216	C1144	U1079	A949	U871	C796	A728
	A1483	C1406	A1340	A1279	C1217	C1145	G1081	U950	A872	C797	A729
	C1484	U1406	C1341	A1280	G1218	A1146		G951	G873	G798	G730
	U1485	C1407	U1342	U1281	U1219	C1147	U1085	U952	A874	G799	G731
	G1486	A1408	G1343	C1282	G1220	U1148	U1086	G953	C875	G800	C732
	G1487	C1409			G1221	C1149	G1087	G954	C876	U801	
		G1410	A1346	C1285	U1222	U1150	U1088	U955	A802	G377	C736
	C1490	C1411	G1347	A1286	G1223	C1151	G1089	U956	G803	C378	A737
	G1491	C1412	U1348	A1287	G1224	A1152		U957	U804	G379	C738
	A1492	A1413	A1349	A1288	C1225	C1153	A1092	A958	C805	C739	C739
	U1493	U1414	C1350	A1289	C1226	G1194	U1093	U959	C806	U740	
	G1494	G1415	U1351	G1290	A1227		A1094	U960	A807	G741	G742
			C1352	G1291	C1228	A1157	C1095	C1028A	C810		
	G1497	A1418	G1353	U1292	A1229	C1158	C1096	C1028B	C811		C748
	U1498	G1419	C1354	G1293	U1230	U1159	C1097	G1028D	C812		C749
	A1499		G1355	G1294	G1231	G1160	C1098	C1028E	U891		C750
	A1500	G1422	G1356	G1295	U1232		C1099	G1028F	U892		
	C1501		A1357	C1296	C1161		C1100	A1028G	A814		
	A1502	U1427	U1358	C1297	C1162	C1163	A1101	G1028H	C815		G752
	A1503	A1428	C1359	C1298	A1236		C1102	G1028I	A816		A753
	G1504		A1360	A1299	G1237	A1169	C1103		C817		C754
	C1431	C1431	G1361	G1300	A1238	A1170	G1104	C1037	G972		G755
	A1432		C1362A	U1301	A1239		A1105	C1038	G973		G756
	A1433		C1362B	C1302	U1240	G1175	G1106	A975	A819		C756
	A1434		A1363	C1303	G1241	A1176	C1107	G1039	U821		U757
	C1508	G1435	U1364	G1304	C1242	G1177	U1040	A908	G822		G758
	C1509	U1436	G1365	G1305	C1243	G1178	C1109	A909	G823		A759
	U1510	C1437	C1366	A1306	C1244	A1179	G1042	A978	G824		G760
	G1511						C1043	C979	C824		G761
	U1512	G1438	C1367	U1307	A1245	A1180	A1044	C980	C912		C762
	A1513		G1368	C1308	C1246	A1181	C1112	U981	A913		C763
	C1514	G1440B	C1369	G1309	U1247	G1182	C1113	A982	U827		G764
	A1515	A1440C	G1370	C1310	A1248	A1183	C1114	A983	A828		C765
	C1516	G1440D	G1371	G1311	C1249	G1184	C1115	G917	G916		A766
	G1517	A1440E	U1372	G1312	A1250	G1185	C1116	C984	G829		A767
	A1518		G1373	U1313	A1251	G1186	G1117	C985	A918		C768
	U1519	C1440H	A1374	C1314	A1252	G1187	C1118	A986	U919		A769
	G1520	A1440I	U1375	U1315	G1253	C1189	G1119	G987	U920		C770
	C1521	A1440J	C1376	G1316	C1254	C1189	G1120	C988	U921		G771
	U1522		C1377	C1317	G1255	G1190	G1053	C989	G922		C772
	C1523	C1440K	A1378	C1318	A1256	A1191	A1192	C990	C834		U773
		C1440L	C1379	C1319	C1257	A1192		U991	C935		C774

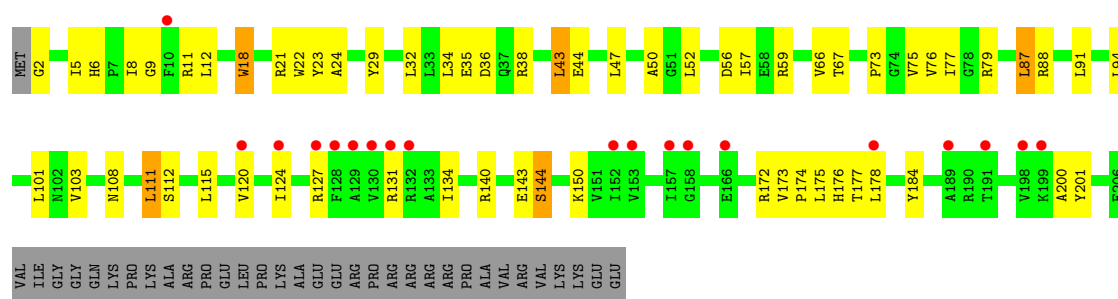
• Molecule 1: 16S rRNA



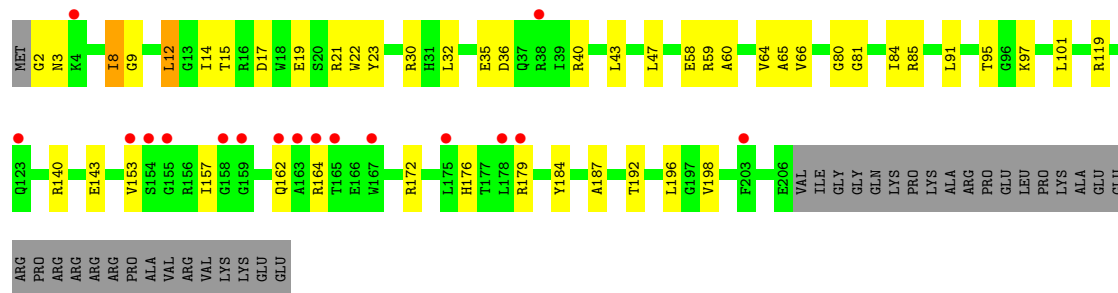




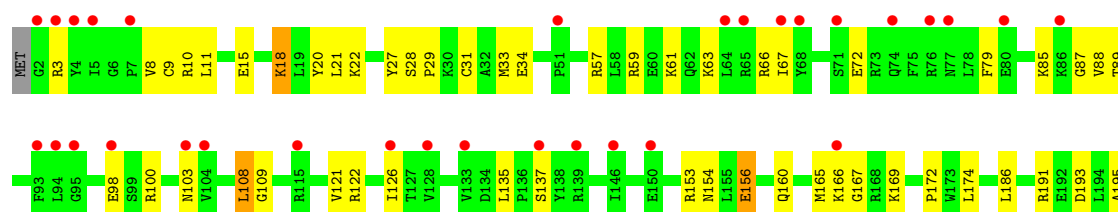
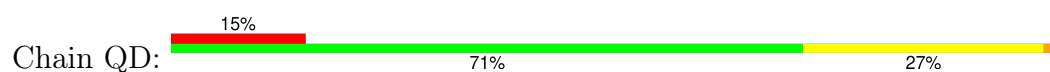
• Molecule 3: 30S ribosomal protein S3

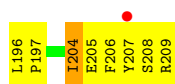


• Molecule 3: 30S ribosomal protein S3

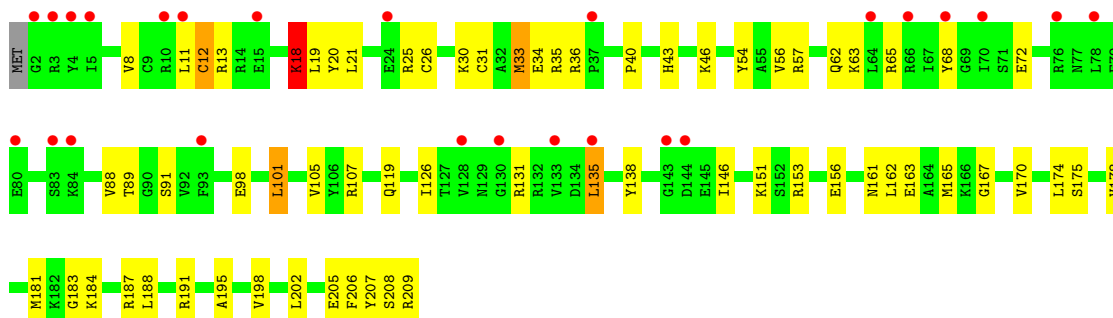


• Molecule 4: 30S ribosomal protein S4

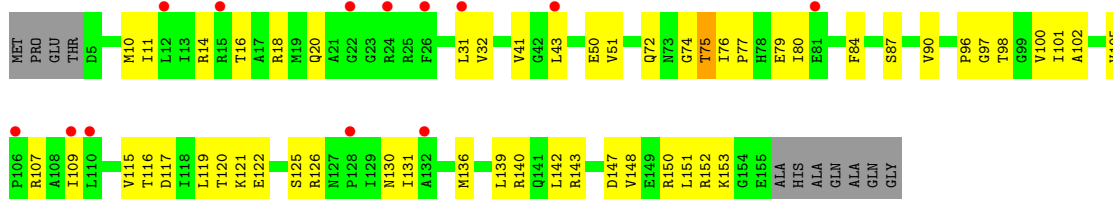




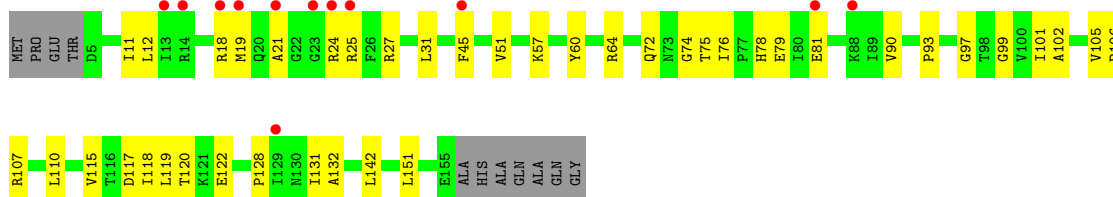
• Molecule 4: 30S ribosomal protein S4



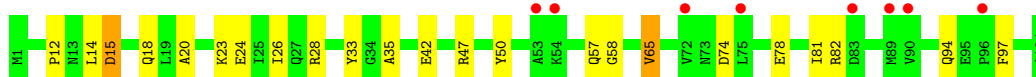
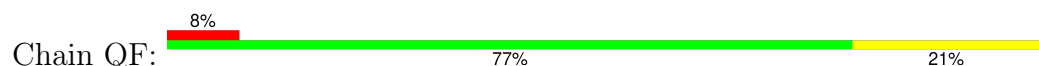
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

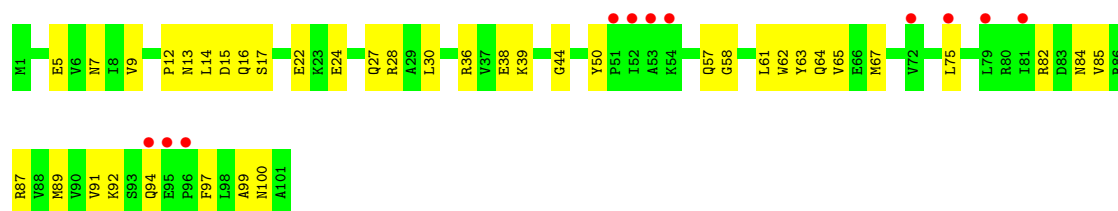


• Molecule 6: 30S ribosomal protein S6

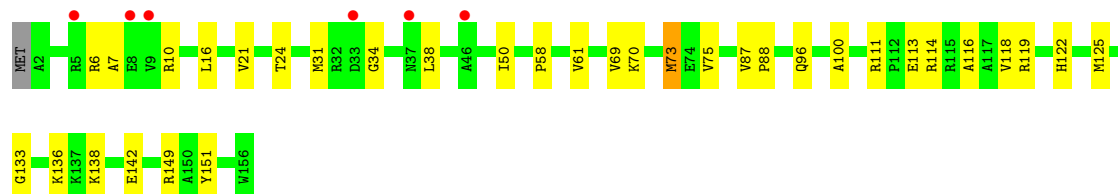
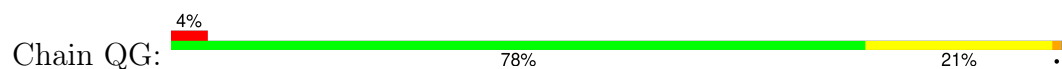


• Molecule 6: 30S ribosomal protein S6

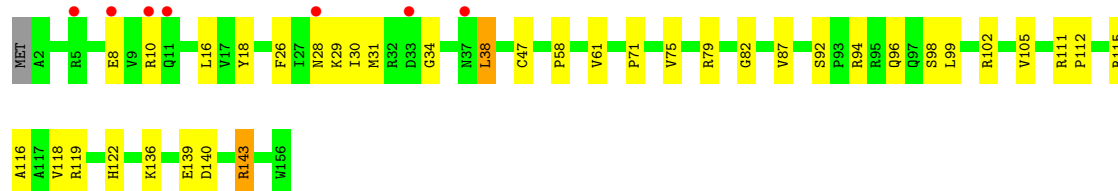
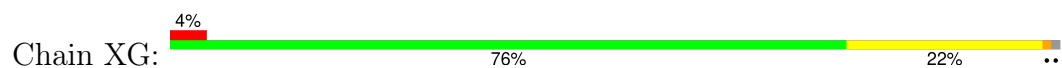




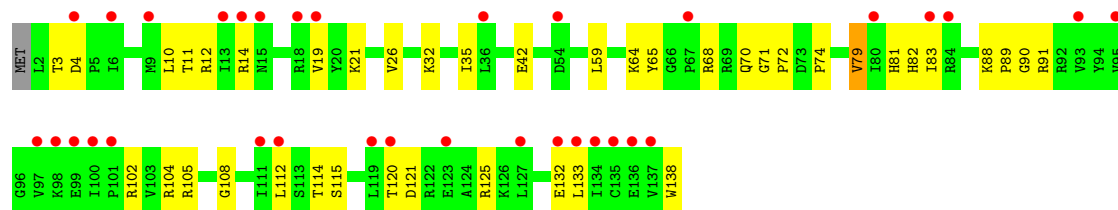
• Molecule 7: 30S ribosomal protein S7



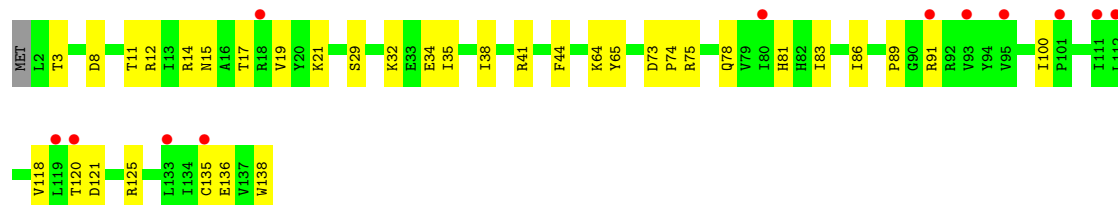
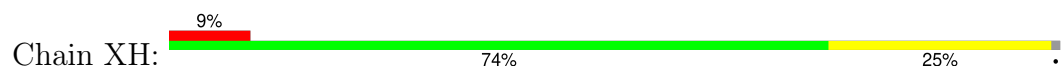
• Molecule 7: 30S ribosomal protein S7



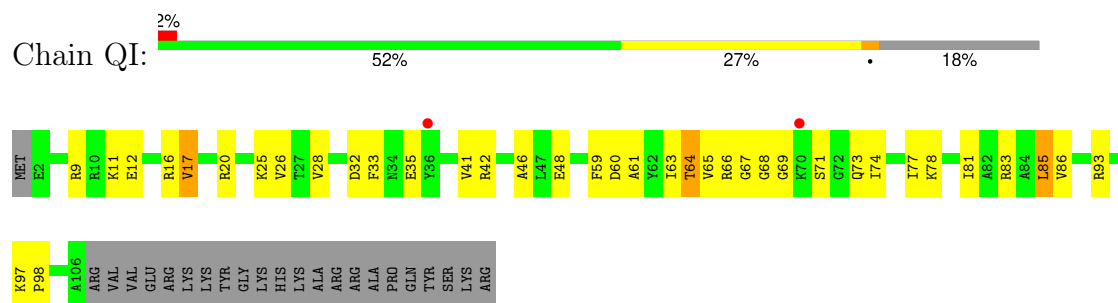
• Molecule 8: 30S ribosomal protein S8



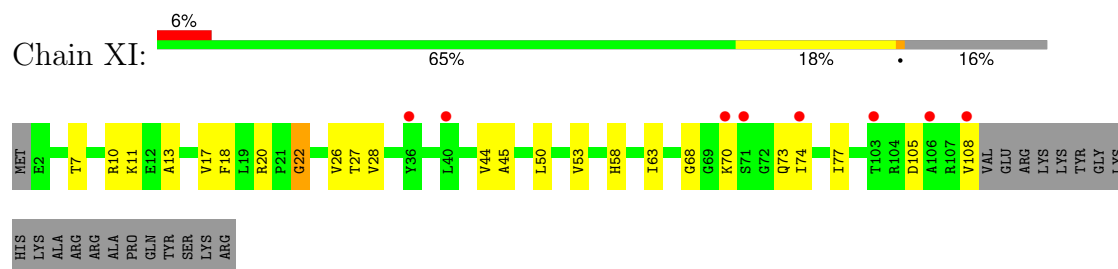
• Molecule 8: 30S ribosomal protein S8



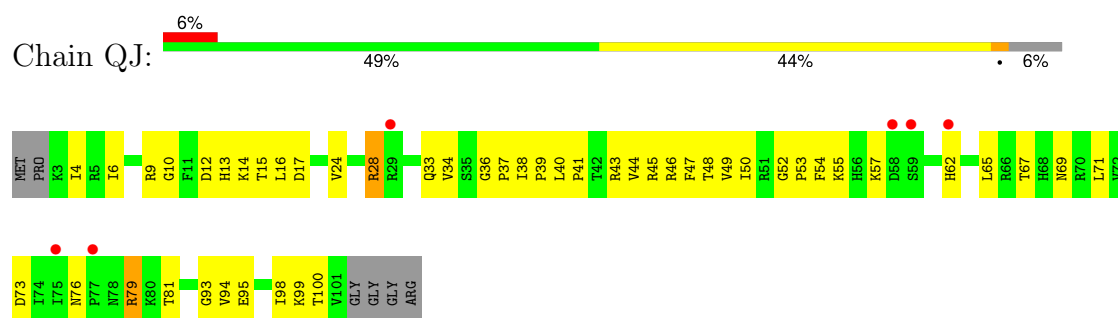
- Molecule 9: 30S ribosomal protein S9



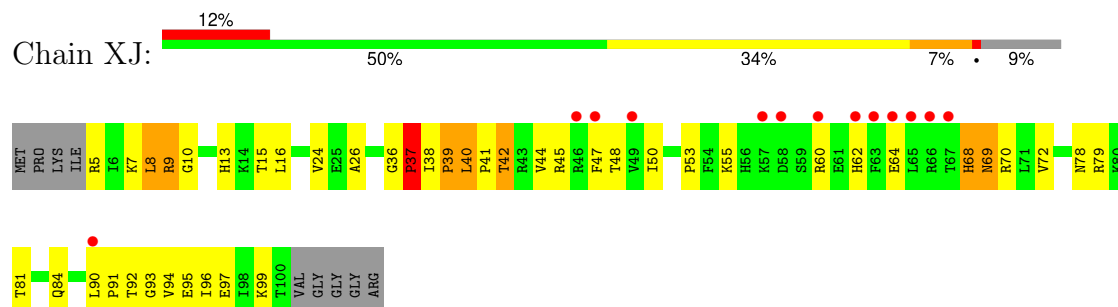
- Molecule 9: 30S ribosomal protein S9



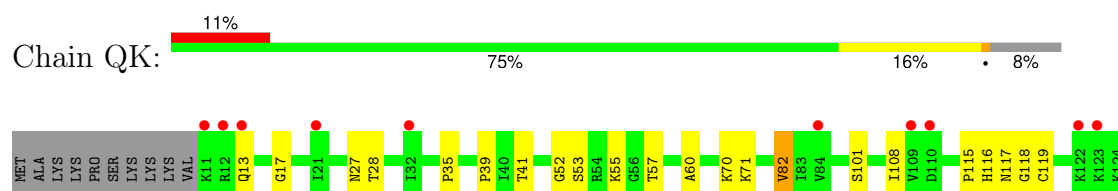
- Molecule 10: 30S ribosomal protein S10

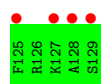


- Molecule 10: 30S ribosomal protein S10

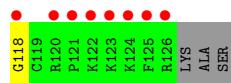


- Molecule 11: 30S ribosomal protein S11

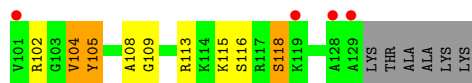




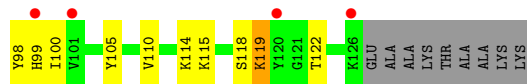
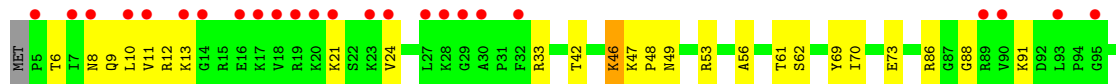
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



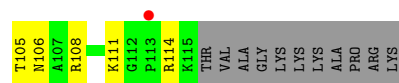
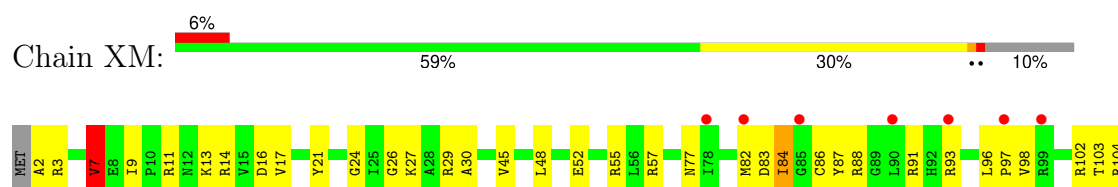
• Molecule 12: 30S ribosomal protein S12



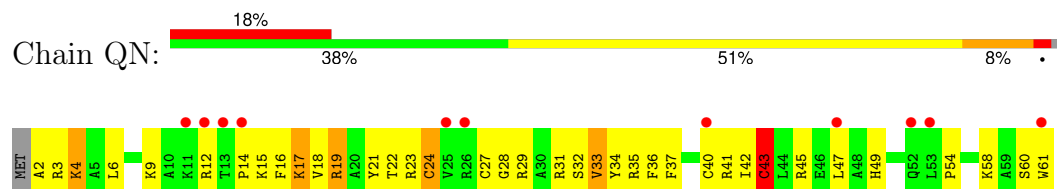
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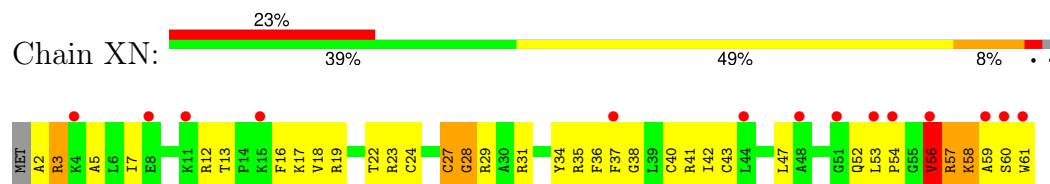
• Molecule 13: 30S ribosomal protein S13



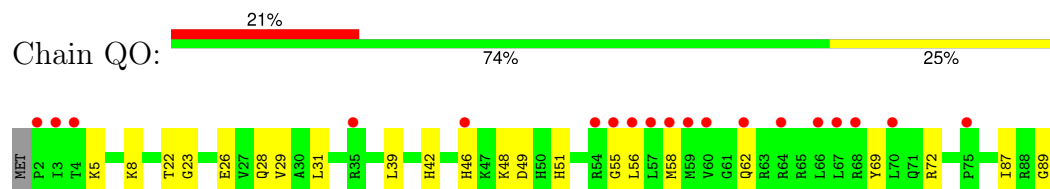
- Molecule 14: 30S ribosomal protein S14 type Z



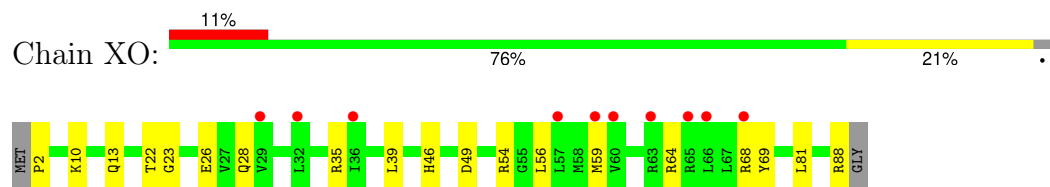
- Molecule 14: 30S ribosomal protein S14 type Z



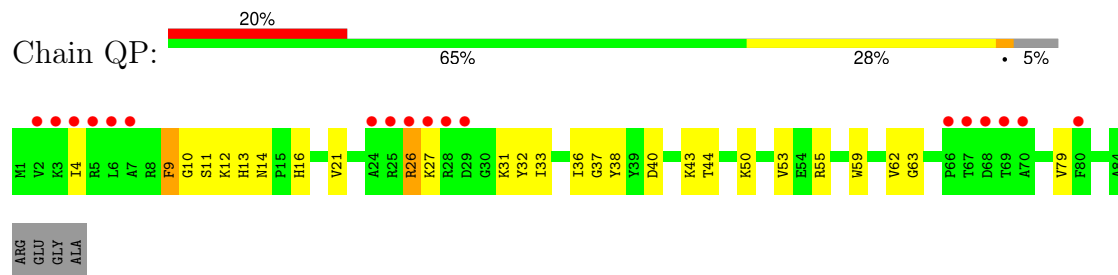
- Molecule 15: 30S ribosomal protein S15



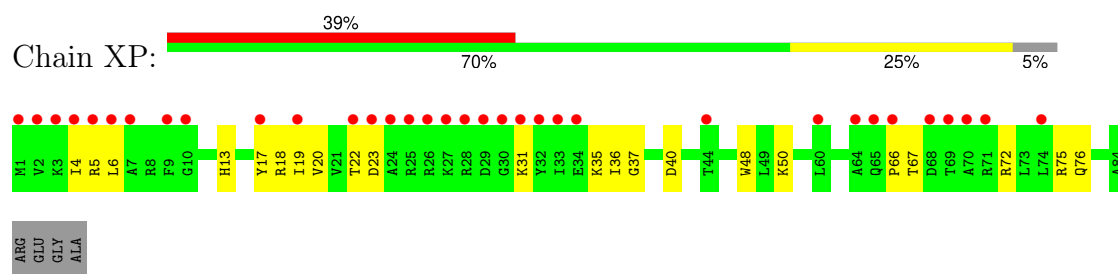
- Molecule 15: 30S ribosomal protein S15



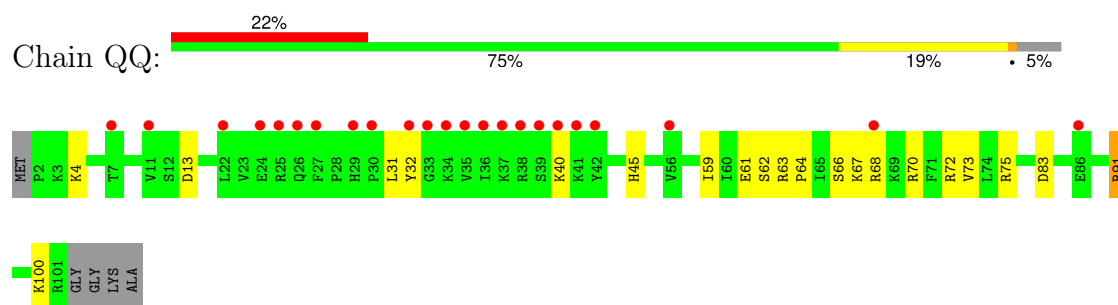
- Molecule 16: 30S ribosomal protein S16



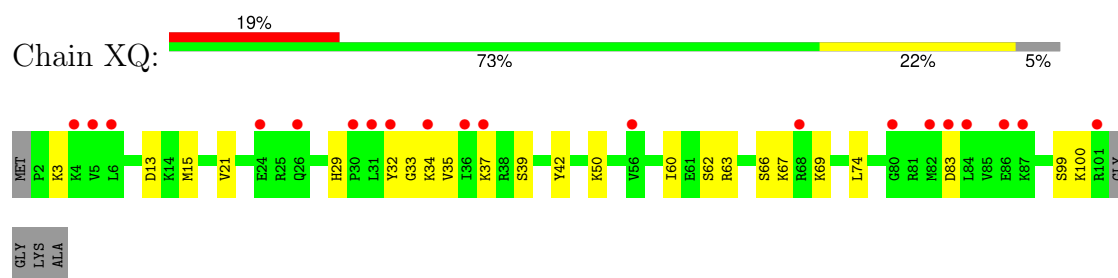
- Molecule 16: 30S ribosomal protein S16



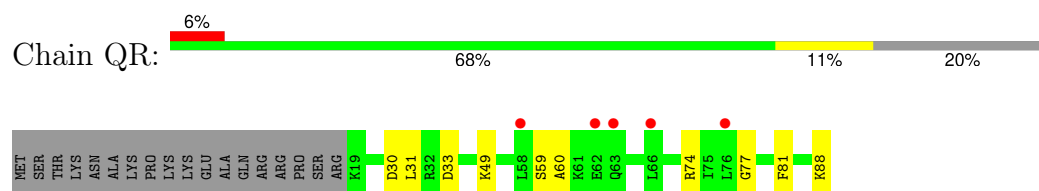
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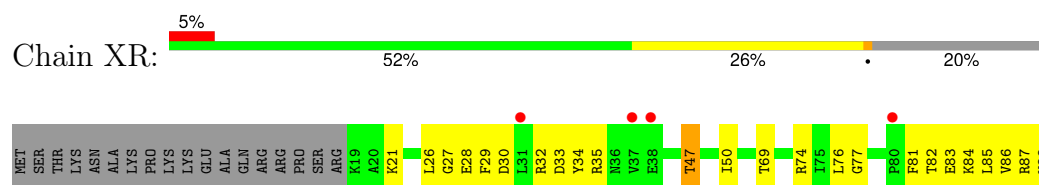
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

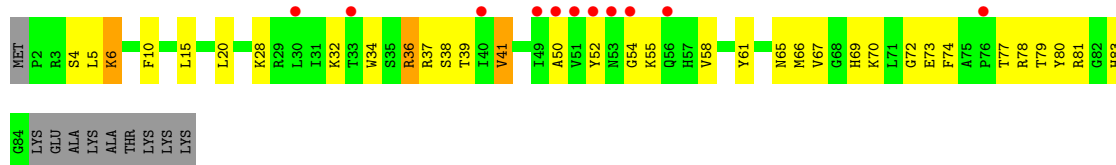


- Molecule 18: 30S ribosomal protein S18

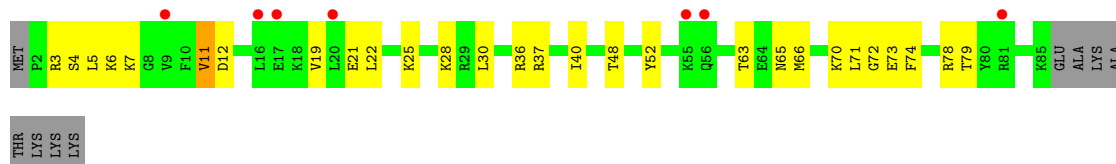


- Molecule 19: 30S ribosomal protein S19

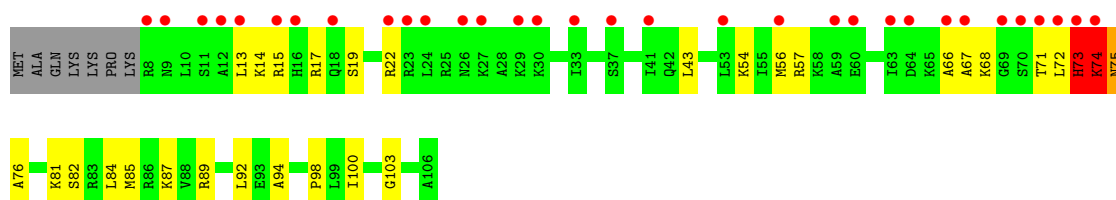




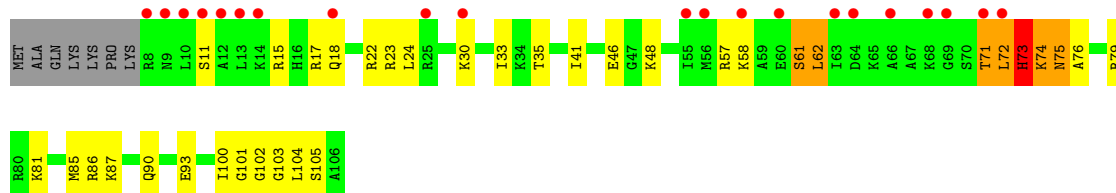
- Molecule 19: 30S ribosomal protein S19



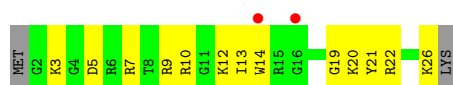
- Molecule 20: 30S ribosomal protein S20



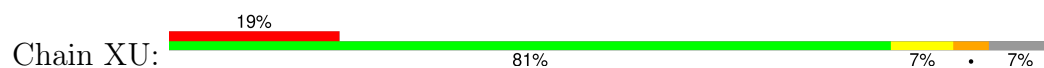
- Molecule 20: 30S ribosomal protein S20

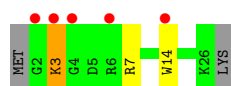


- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx





• Molecule 22: tRNA(Pro)



• Molecule 22: tRNA(Pro)



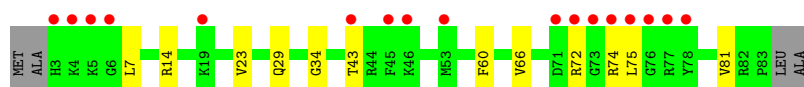
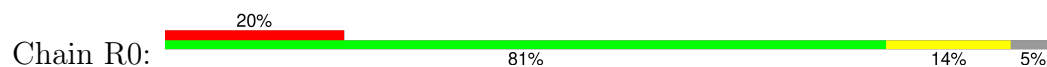
• Molecule 23: mRNA



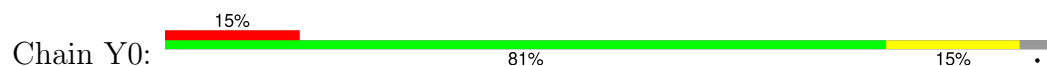
• Molecule 23: mRNA



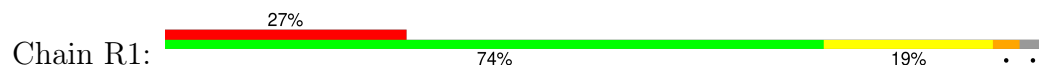
• Molecule 24: 50S ribosomal protein L27

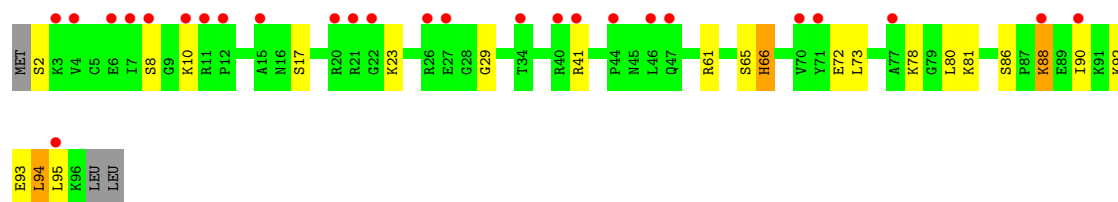


• Molecule 24: 50S ribosomal protein L27

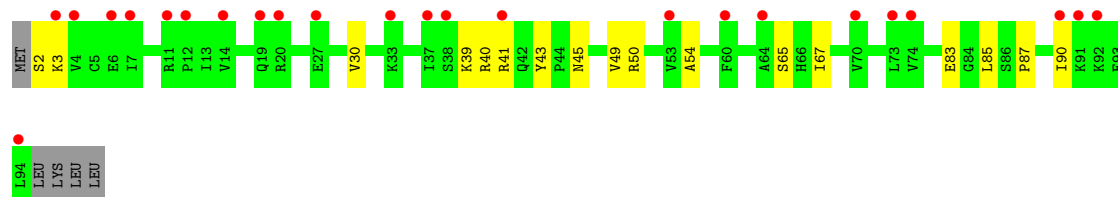
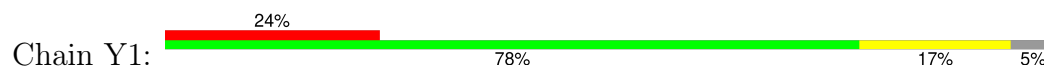


• Molecule 25: 50S ribosomal protein L28

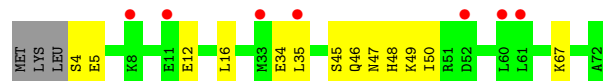
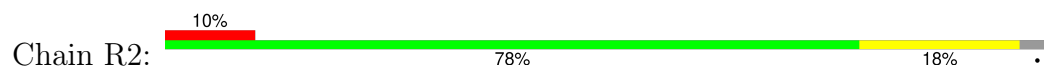




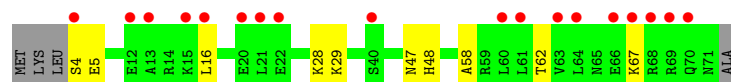
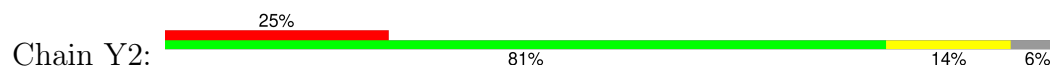
- Molecule 25: 50S ribosomal protein L28



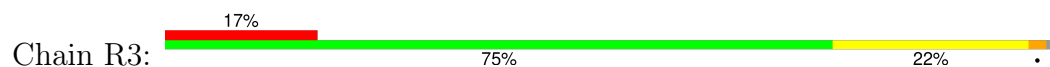
- Molecule 26: 50S ribosomal protein L29



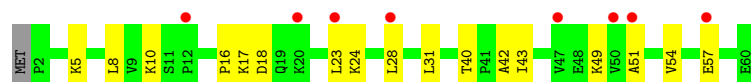
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

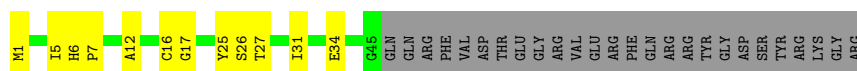


- Molecule 27: 50S ribosomal protein L30

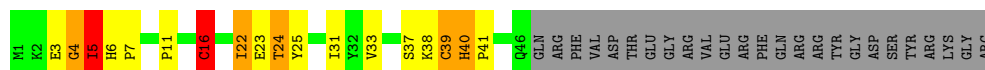


- Molecule 28: 50S ribosomal protein L31





- Molecule 28: 50S ribosomal protein L31



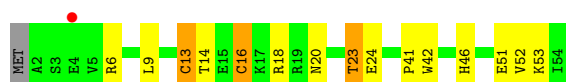
- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



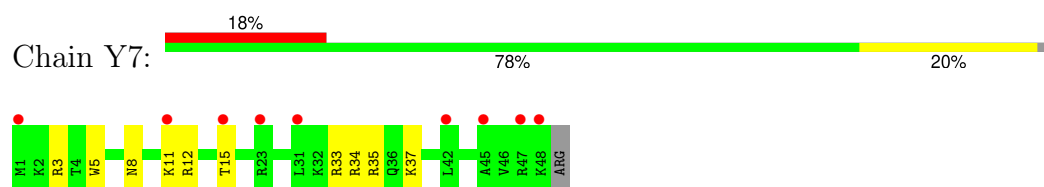
- Molecule 30: 50S ribosomal protein L33



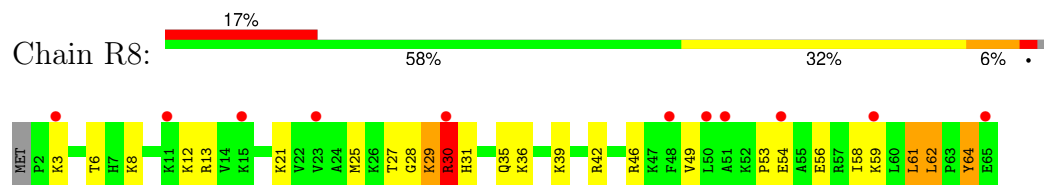
- Molecule 31: 50S ribosomal protein L34



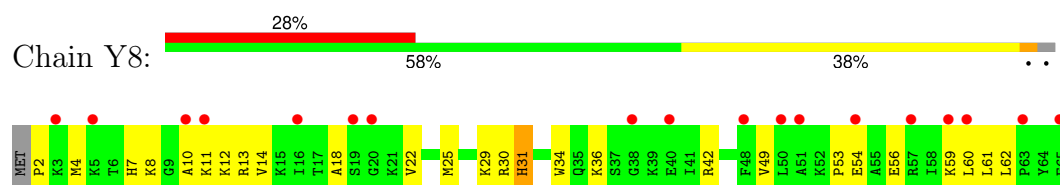
- Molecule 31: 50S ribosomal protein L34



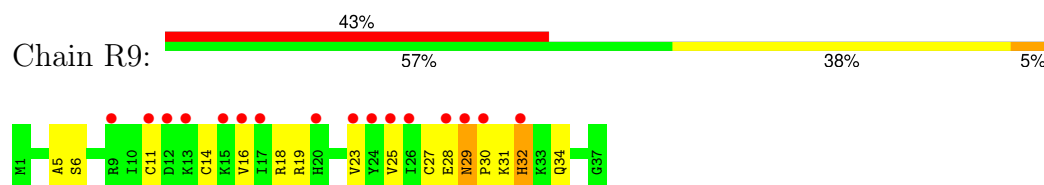
- Molecule 32: 50S ribosomal protein L35



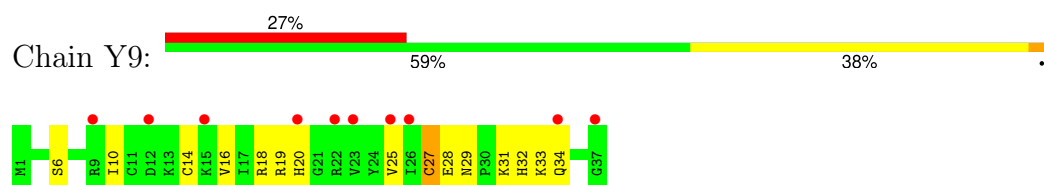
- Molecule 32: 50S ribosomal protein L35



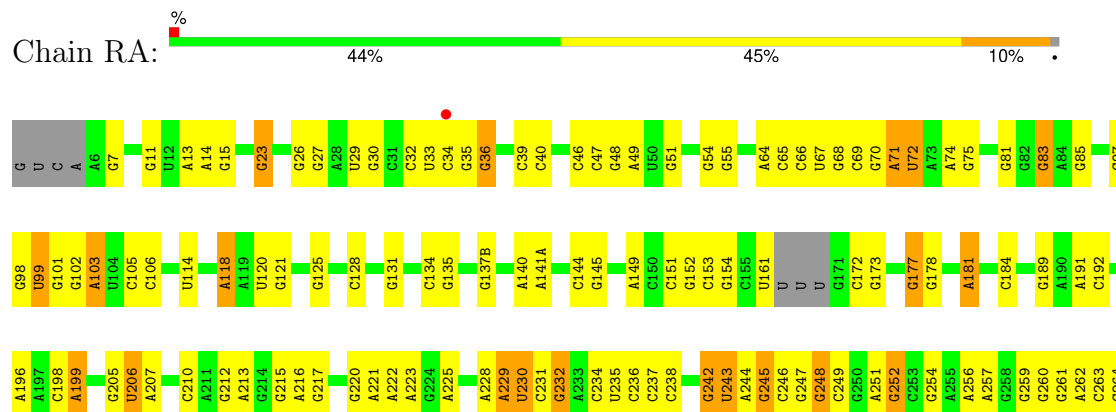
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36



- Molecule 34: 23S rRNA



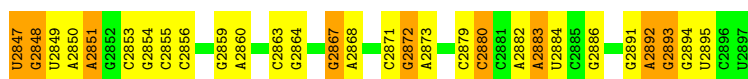


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A2503	A2426	G2352	G2121	U2122	C1965	A1885	U1793	C1612	G1613	G1539	G1464
U2504	G2427	G2353	U2123	G2124	A1966	G1886	U1796	A1701	A1614	G1540	G1465
G2505	G2428	G2354	G2124	G2125	C1967	G1887	C1797	C1708	A1615	A1543	C1467
U2506	G2429	G2358	G2125	G2127	G1968	A1889	U1798	U1709			
	A2430	C2363	U2126		A1969		G1799				
	U2511	C2364	G2127		A1971		C1800				



A1654	G1484	C1403	A1329	A1237	C1161	G1093	A1028	G949	C906	C730	G
A1655	G1485	C1404	U1329	G1238	G1162	G1094	A1029	U877	U807	C731	C
C1657	G1486	C1407	C1330	G1239	G1163	A1094	A1094	A878	C808	C738	C
C1658	G1487	C1408	A1331	G1240	G1164	A1095	A1095	G880	U811	G739	G654T
U1659	A1490	C1409	G1332	A1241	C1165	A1096	U1033	G881	C812	U740	C654U
C1660	C1493	C1409	C1333	G1243	C1166	A1097	U1035	G882	U813	G741	A654V
G1661	C1494	C1411	G1334	G1244	U1167	A1098	U1036	G883	C814	G742	A654W
C1662	C1495	C1412	U1335	G1245	G1168	G1099	G1037	U958	C815		A655
C1663	A1496	G1416	A1336	A1247	G1169	C1102	C1038	C886	C916	G745	
A1570	G1497	G1417	G1337	G1248	G1170	A1103	C1039	A887	C917	A746	U657
A1571	U1498	G1418	G1338	A1173	G1171	A1103	U1039	C888	G818	U747	C658
A1572	C1499	G1419	U1340	A1174	U1175	C1104	C1040	C889	G819	G748	C659
G1573	G1500	A1420	U1341	U1176	U1175	G1110	C1041	A890	A820	C749	G660
C1574	C1501	G1421	A1349	A1177	G1176	A1111	G1043	G971	A821		C661
C1575	C1502	A1427	U1352	U1255	A1177	G1112	G1044	G972	U822	A752	G662
U1576	U1503	C1428	A1353	G1256	C1178	U1113	A1045	G973	G823	C753	G663
C1577	C1504	G1429	A1354	A1265	C1179	G1114	A1046	A896	A824	C754	C664
U1578	C1505	G1430	A1354	G1266	C1180	G1115	G1047	C974A	G818	C755	C665
A1579	C1506	U1431	A1359	U1267	C1181	G1116	A1048	C974B	G819	C756	G666
G1581	A1507	U1437	A1360	U1268	G1183	G1117	C1049	G975	U827	U757	
C1582	U1508	C1437	G1361	G1271	G1183	C1118	A1050	A983	U828		C671
C1583	A1509	A1444B	C1362	A1272	G1186	G1119	G1051	A984	C831	C758	C672
C1585	A1510	C1445	C1363	U1273	G1187	G1120	A1054	C985	C834	A764	C673
A1586	A1511	C1446	C1364	A1274	U1188	G1122	G1055	C987	A835	G765	A675
A1603	U1514	C1447	A1365	A1275	A1189	C1123	G1056	A988	U907	C766	A676
C1604	G1521	G1448	A1366	G1278	G1191	C1124	A1057	C989	U839	G770	C679
C1605	G1522	A1449A	A1367	G1279	A1126	G1125	G1058	A910	C840	G771	G680
G1606	U1523	G1449B	G1368	G1280	G1195	A1127	U1060	A911	G842	C772	
C1607	G1524	C1370	C1370	G1281	U1198	A1128	U1061	C994	C843	U773	A685
A1608	G1525	U1372	U1372	U1288	U1199	G1130	U1062	C995	C844	U774	G686
A1609	A1528	C1375	C1375	U1292	A1204	G1131	U1065	A996	C845	G775	C687
C1610	G1529	C1376	C1376	U1293	U1205	U1132	U1066	G997	G846	G776	U688
G1612	U1534	G1377	G1377	U1294	G1206	U1133	U1067	C998	U847	A777	A689
G1613	U1535	C1378	C1378	C1295	A1210	C1135	G1068	G919	A849	U779	G690
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C1638	U1541	G1466	A1386	A1301	C1217	U1142A	G1074	A1009	G855	A784	A699
U1639	C1542	C1467	C1387	A1302	C1218	A1142B	C1075	A1010	C856	G785	G700
C1640	A1543	A1469	G1387	G1303	G1219	A1143	U1076	G1011	C857	C786	G701
A1641	C1544	G1470	G1388	C1304	A1220	G1144	A1077	U1012	U858	U787	
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G1646	C1547	A1472	A1393	G1311	C1222	G1150	C1079	G1015	U860	C790	U709
C1647	C1547	G1475	U1394	U1312	C1223	G1151	U1081	G1016	A861	G791	G710
G1648	A1554	C1476	U1395	U1313	C1224	C1152	U1082	G1017	G862	G792	
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C1651	C1556	G1478	U1397	G1317	A1156	A1156	A1084	A941	G865	C797	U714
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G1756	A1558	G1480	G1400	G1319	C1158	G1087	G1087	U943	G869	G799	A722
	A1652	U1482	A1401	G1326	U1159	A1088	U1026	G944	A870	A800	G726
	G1653	G1483	C1402	U1326	G1160	U1090	A1027	A945	A872	A804	A727

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G2529	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2554	G2555	G2556	G2557	G2558	G2559	G2562	G2563	G2566	G2567	G2568	G2569	G2572	G2573	G2574	G2577	G2578	G2581	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2597	G2598	G2599	G2602	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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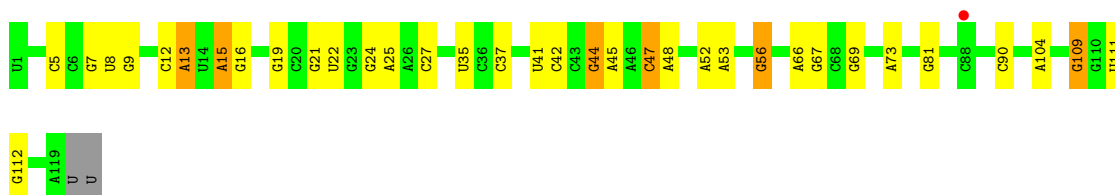
• Molecule 35: 5S rRNA

Chain RB: 68% 27% 5%



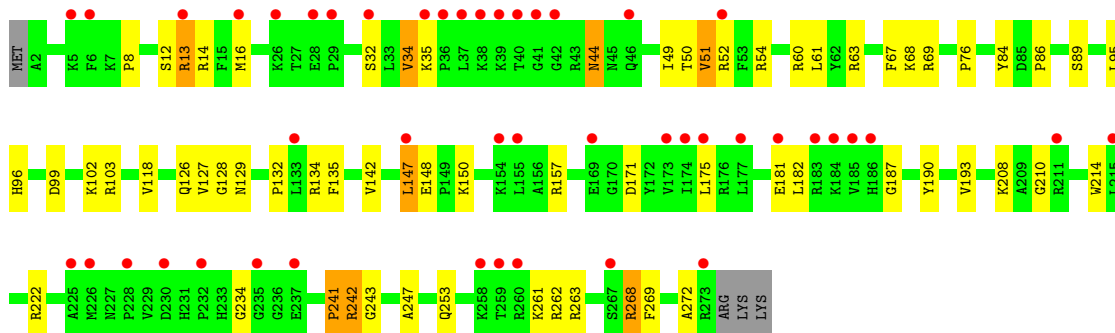
• Molecule 35: 5S rRNA

Chain YB: 70% 24% 5%



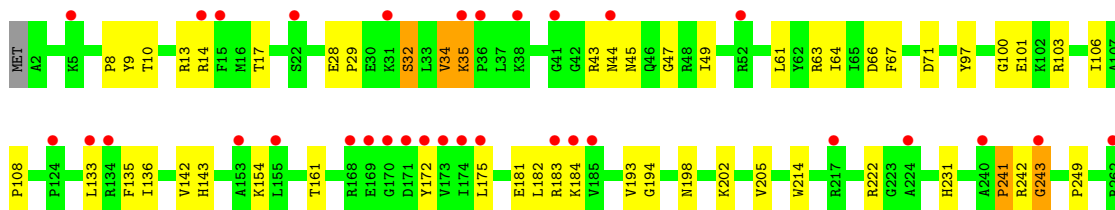
• Molecule 36: 50S ribosomal protein L2

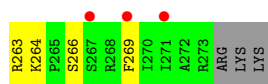
Chain RD: 17% 75% 8%



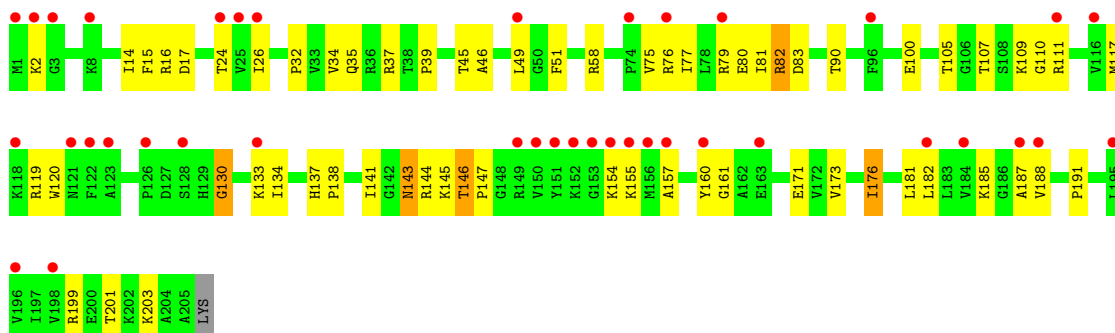
• Molecule 36: 50S ribosomal protein L2

Chain YD: 13% 78% 9%

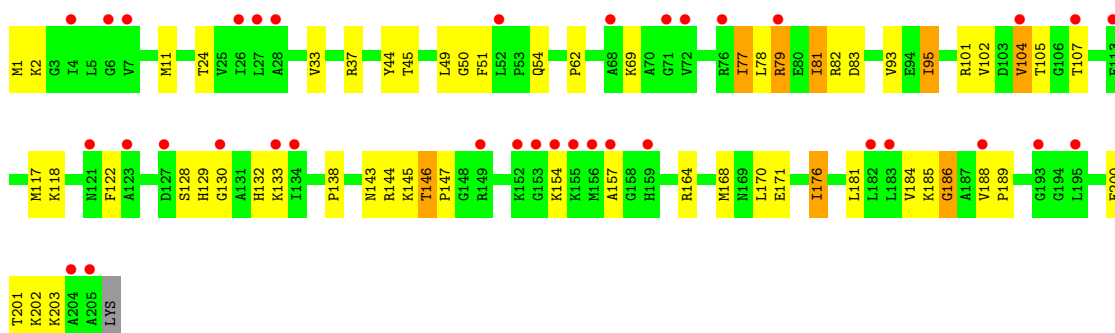
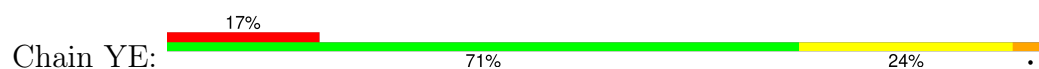




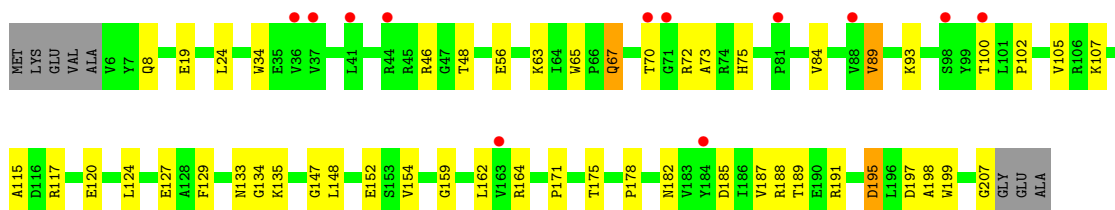
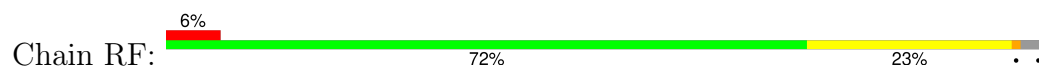
• Molecule 37: 50S ribosomal protein L3



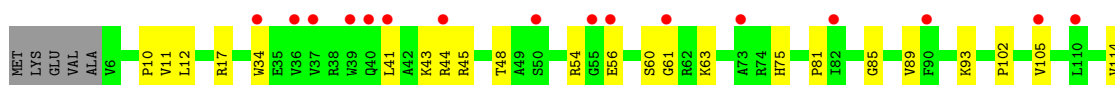
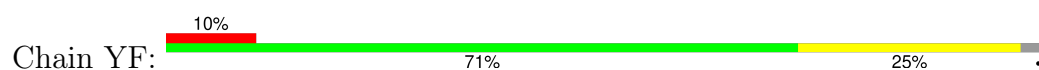
• Molecule 37: 50S ribosomal protein L3



• Molecule 38: 50S ribosomal protein L4



• Molecule 38: 50S ribosomal protein L4

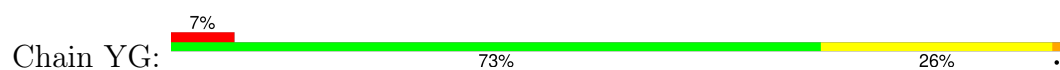




- Molecule 39: 50S ribosomal protein L5



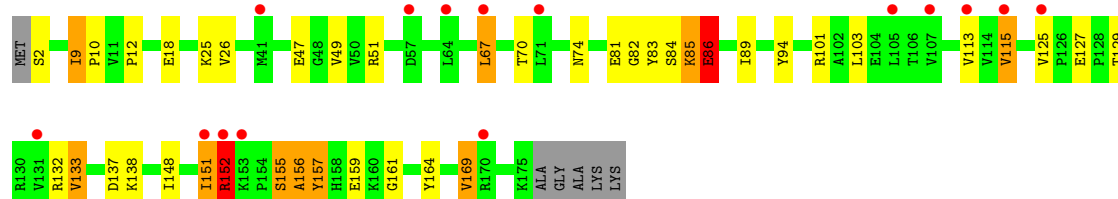
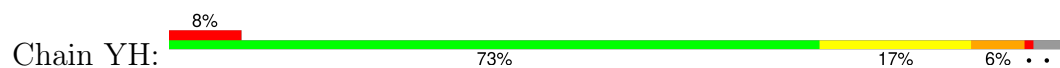
- Molecule 39: 50S ribosomal protein L5



- Molecule 40: 50S ribosomal protein L6

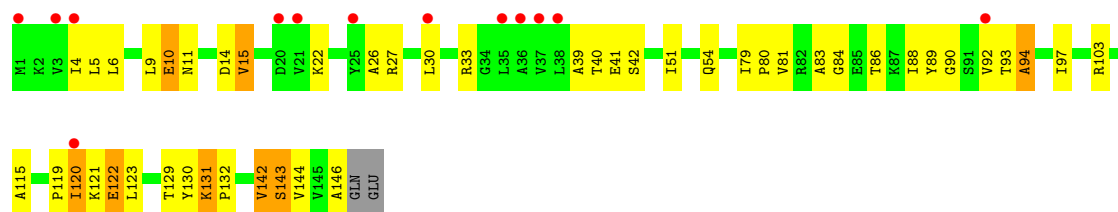


- Molecule 40: 50S ribosomal protein L6



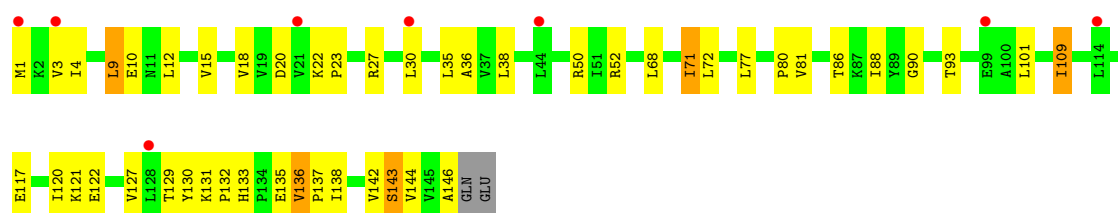
- Molecule 41: 50S ribosomal protein L9

Chain RI: 



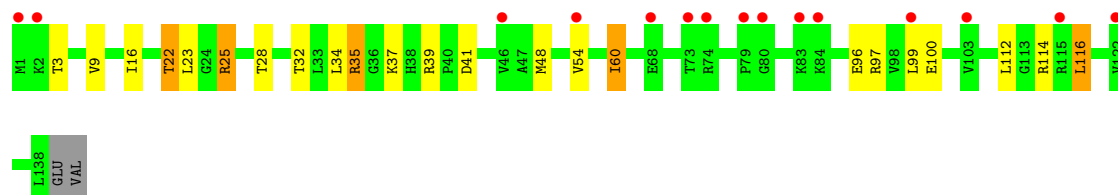
- Molecule 41: 50S ribosomal protein L9

Chain YI: 



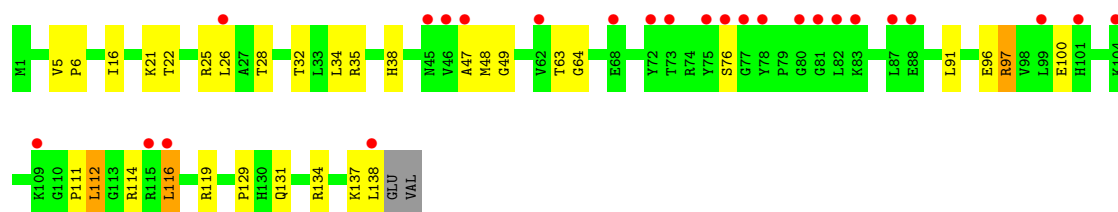
- Molecule 42: 50S ribosomal protein L13

Chain RN: 



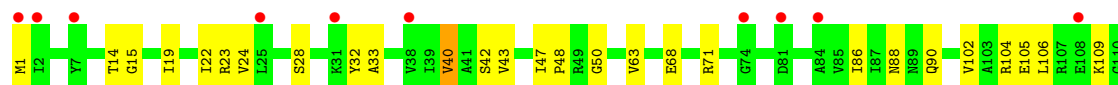
- Molecule 42: 50S ribosomal protein L13

Chain YN: 



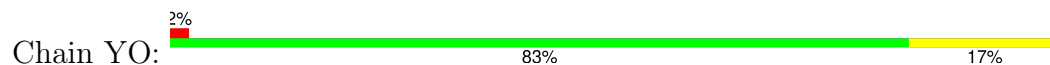
- Molecule 43: 50S ribosomal protein L14

Chain RO: 

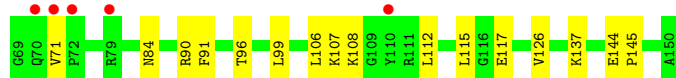
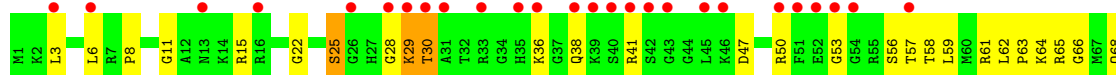




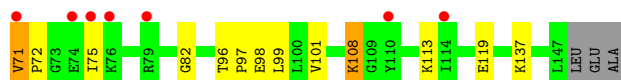
- Molecule 43: 50S ribosomal protein L14



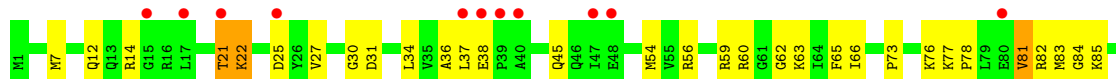
- Molecule 44: 50S ribosomal protein L15



- Molecule 44: 50S ribosomal protein L15

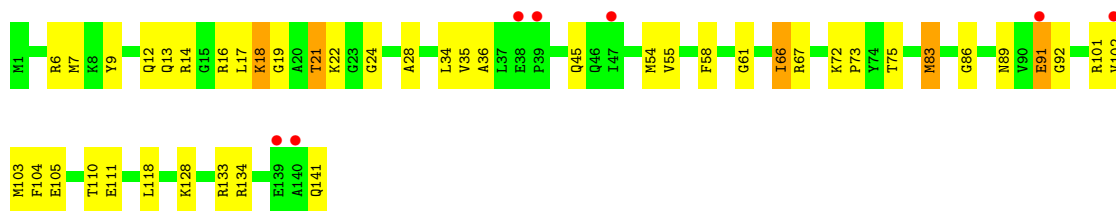


- Molecule 45: 50S ribosomal protein L16

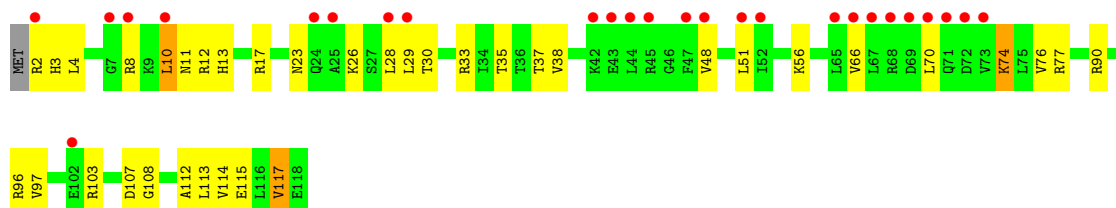


- Molecule 45: 50S ribosomal protein L16

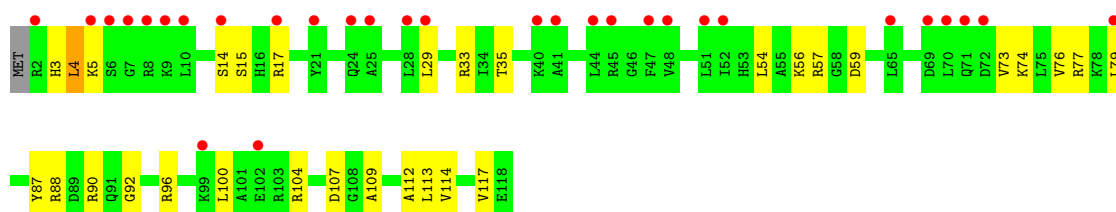
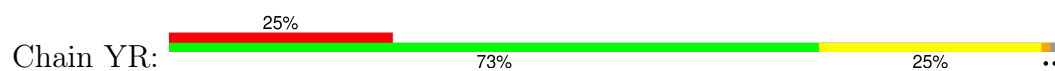




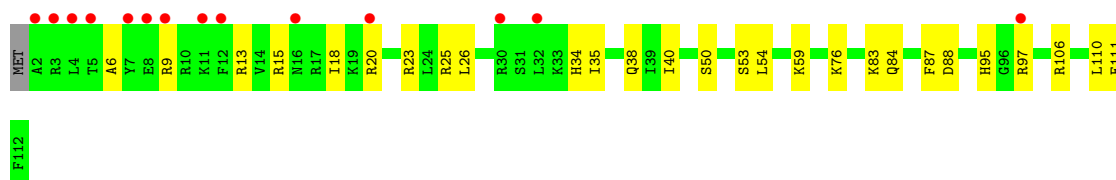
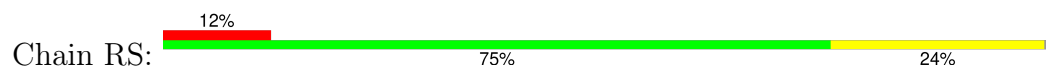
• Molecule 46: 50S ribosomal protein L17



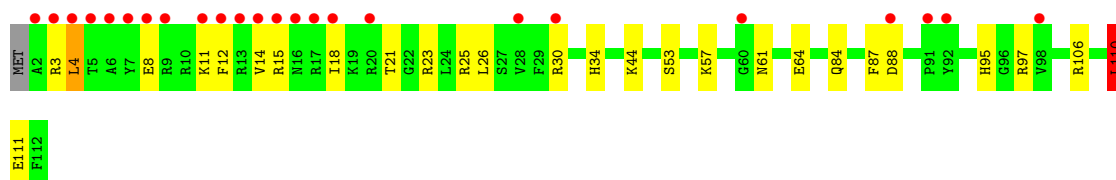
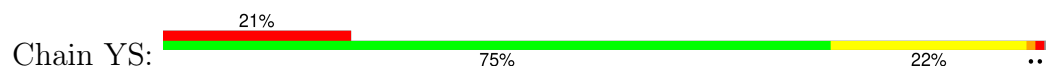
• Molecule 46: 50S ribosomal protein L17



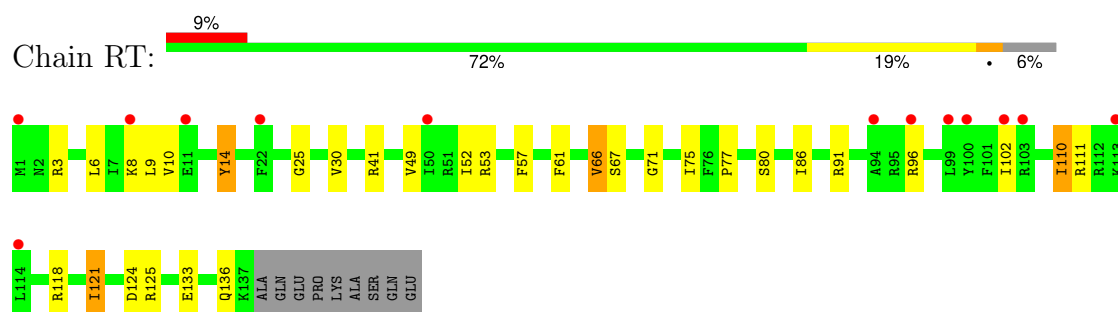
• Molecule 47: 50S ribosomal protein L18



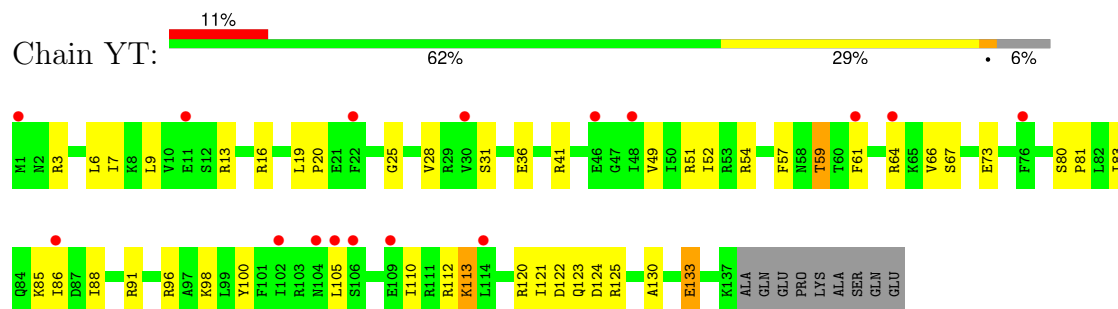
• Molecule 47: 50S ribosomal protein L18



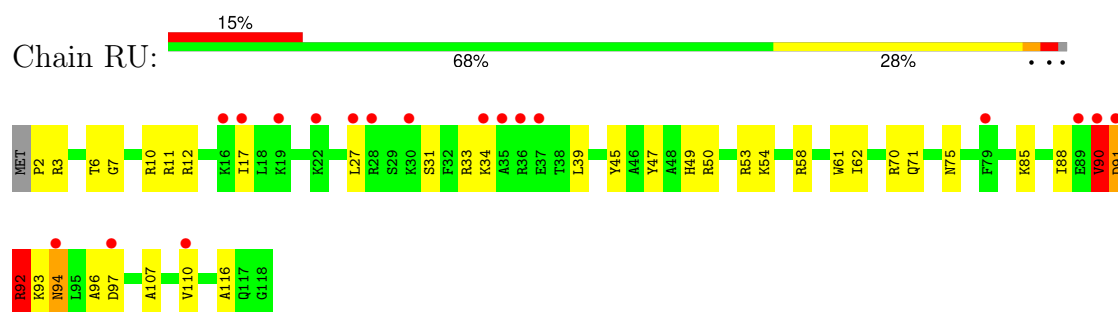
• Molecule 48: 50S ribosomal protein L19



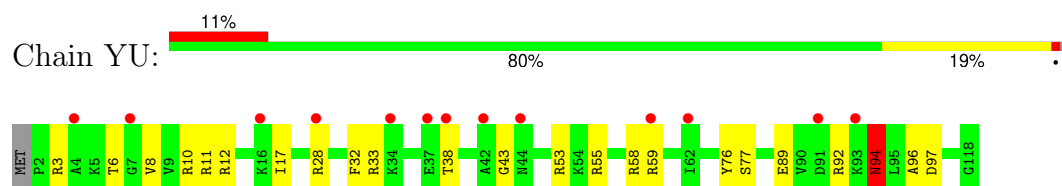
- Molecule 48: 50S ribosomal protein L19



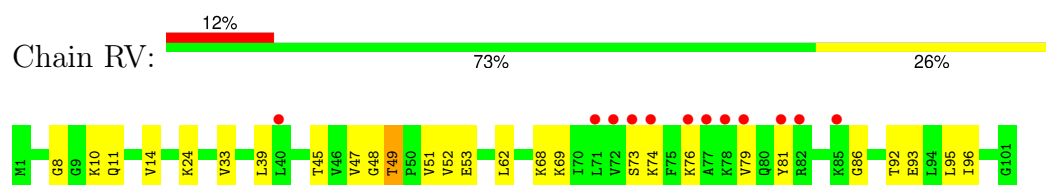
- Molecule 49: 50S ribosomal protein L20



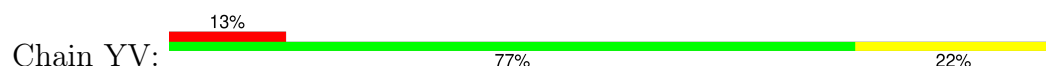
- Molecule 49: 50S ribosomal protein L20



- Molecule 50: 50S ribosomal protein L21

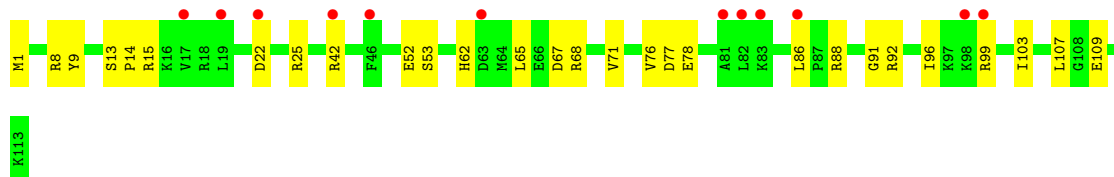
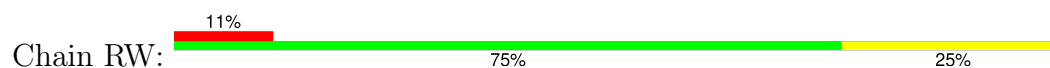


- Molecule 50: 50S ribosomal protein L21

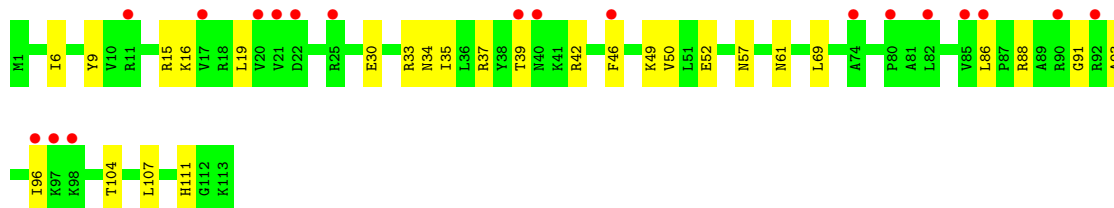
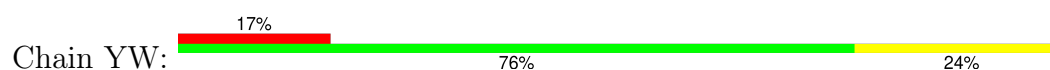




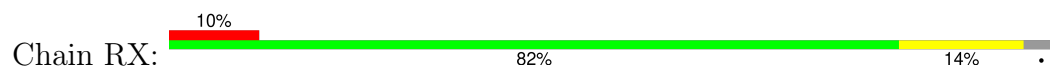
- Molecule 51: 50S ribosomal protein L22



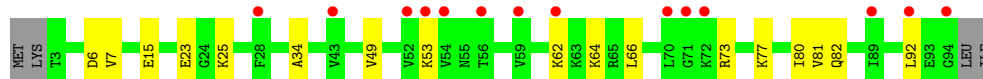
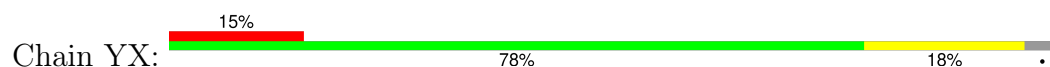
- Molecule 51: 50S ribosomal protein L22



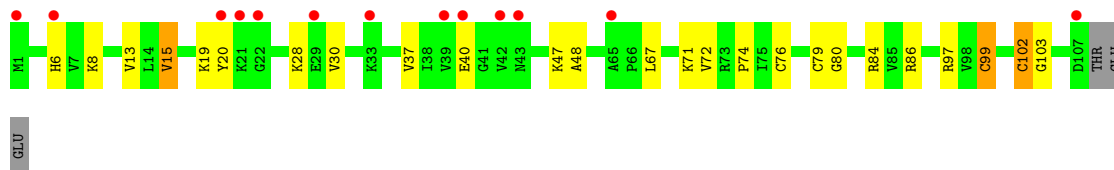
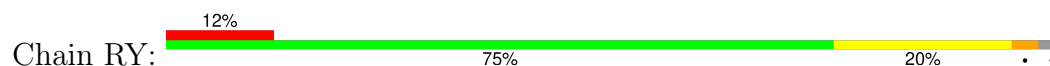
- Molecule 52: 50S ribosomal protein L23



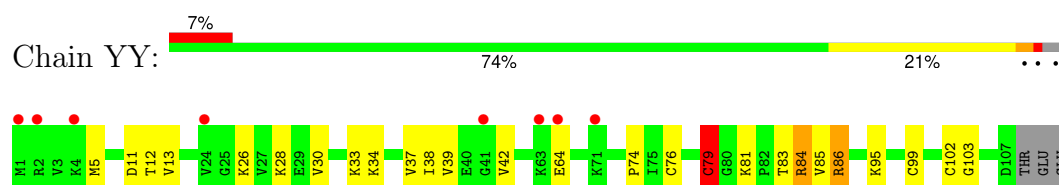
- Molecule 52: 50S ribosomal protein L23



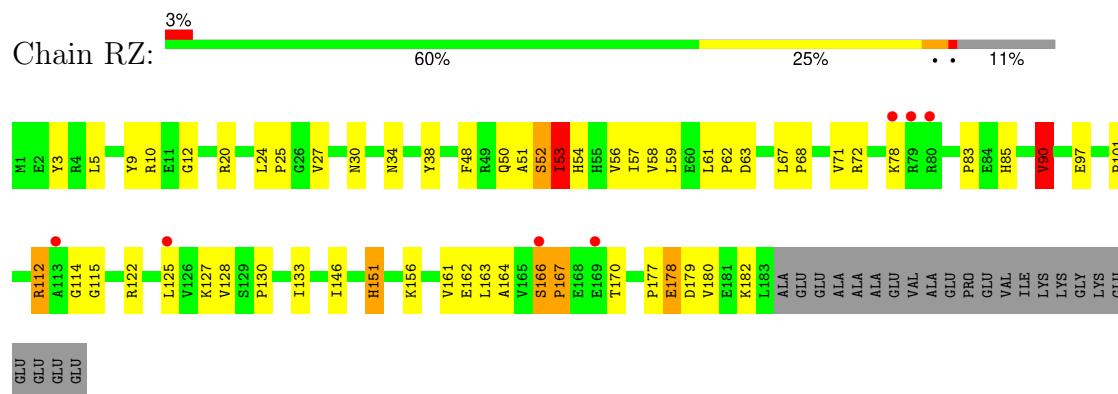
- Molecule 53: 50S ribosomal protein L24



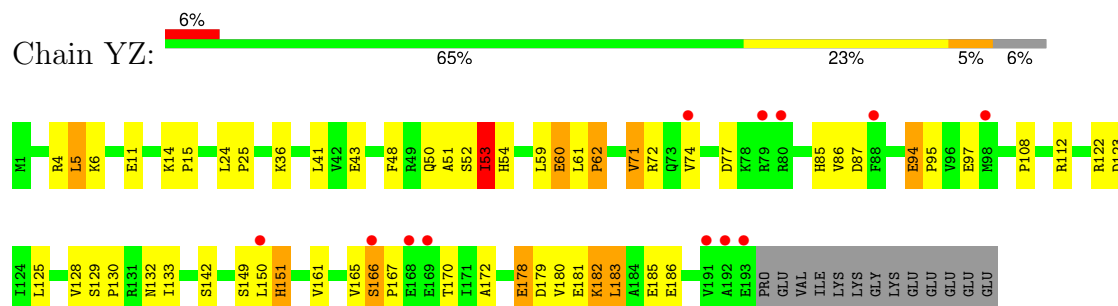
- Molecule 53: 50S ribosomal protein L24



• 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: SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.30	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	286	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	19	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	0	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	65
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%)	24	61
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	61
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	18	54
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	54
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%)	12	46
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	52
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	113/126 (90%)	96 (85%)	16 (14%)	1 (1%)	14	48
13	XM	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	14	48
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	36
14	XN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	23
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%)	11	44
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%)	6	34
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	6	34
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	24
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%)	18	54
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	30	65
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4	29
37	YE	203/206 (98%)	162 (80%)	39 (19%)	2 (1%)	12	46
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	12	46
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	24	61
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	21	58
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	36
40	YH	172/180 (96%)	147 (86%)	21 (12%)	4 (2%)	5	30
41	RI	144/148 (97%)	114 (79%)	24 (17%)	6 (4%)	2	20
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	54
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	18	54
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	33
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	18	54
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	18	54
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	18	54
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14	48
47	RS	109/112 (97%)	95 (87%)	14 (13%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	14	48
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	28
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	46
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	46
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	31
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	2	22
All	All	11368/12128 (94%)	10080 (89%)	1202 (11%)	86 (1%)	16	52

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%)	81	81
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	81
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	80
3	XC	159/188 (85%)	157 (99%)	2 (1%)	61	72
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78	80
4	XD	180/181 (99%)	177 (98%)	3 (2%)	53	68
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	76
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	74
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%)	73	77
8	QH	118/119 (99%)	117 (99%)	1 (1%)	73	77
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	77
9	QI	79/99 (80%)	76 (96%)	3 (4%)	29	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%)	18	42
11	QK	90/99 (91%)	88 (98%)	2 (2%)	45	64
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	103/109 (94%)	101 (98%)	2 (2%)	50	66
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%)	27	49
14	XN	49/50 (98%)	47 (96%)	2 (4%)	27	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%)	47	65
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%)	59	71
20	QT	76/82 (93%)	75 (99%)	1 (1%)	61	72
20	XT	76/82 (93%)	75 (99%)	1 (1%)	61	72
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	22	45
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%)	48	66
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%)	43	63
29	R5	51/52 (98%)	50 (98%)	1 (2%)	48	66
29	Y5	51/52 (98%)	49 (96%)	2 (4%)	28	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	R6	51/52 (98%)	50 (98%)	1 (2%)	48	66
30	Y6	51/52 (98%)	50 (98%)	1 (2%)	48	66
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%)	59	71
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	162 (98%)	3 (2%)	51	67
37	YE	165/166 (99%)	160 (97%)	5 (3%)	36	57
38	RF	161/166 (97%)	158 (98%)	3 (2%)	50	66
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	154 (99%)	1 (1%)	78	80
39	YG	155/156 (99%)	152 (98%)	3 (2%)	50	66
40	RH	145/148 (98%)	137 (94%)	8 (6%)	19	43
40	YH	145/148 (98%)	139 (96%)	6 (4%)	27	49
41	RI	122/124 (98%)	120 (98%)	2 (2%)	55	69
41	YI	122/124 (98%)	118 (97%)	4 (3%)	33	55
42	RN	117/119 (98%)	114 (97%)	3 (3%)	40	60
42	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	99 (99%)	1 (1%)	68	76
44	RP	116/116 (100%)	116 (100%)	0	100	100
44	YP	114/116 (98%)	113 (99%)	1 (1%)	70	76
45	RQ	111/111 (100%)	109 (98%)	2 (2%)	51	67
45	YQ	111/111 (100%)	111 (100%)	0	100	100
46	RR	100/101 (99%)	99 (99%)	1 (1%)	68	76
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%)	44	63
48	RT	120/127 (94%)	118 (98%)	2 (2%)	53	68
48	YT	120/127 (94%)	118 (98%)	2 (2%)	53	68
49	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74
49	YU	93/94 (99%)	92 (99%)	1 (1%)	65	74
50	RV	82/82 (100%)	80 (98%)	2 (2%)	43	63
50	YV	82/82 (100%)	78 (95%)	4 (5%)	22	45
51	RW	92/92 (100%)	91 (99%)	1 (1%)	65	74
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	73 (99%)	1 (1%)	59	71
52	YX	74/78 (95%)	72 (97%)	2 (3%)	39	60
53	RY	88/91 (97%)	87 (99%)	1 (1%)	65	74
53	YY	88/91 (97%)	87 (99%)	1 (1%)	65	74
54	RZ	162/179 (90%)	161 (99%)	1 (1%)	78	80
54	YZ	167/179 (93%)	164 (98%)	3 (2%)	51	67
All	All	9610/10066 (96%)	9488 (99%)	122 (1%)	61	72

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	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	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	QD	301	4	-	-	0/6/5/5
56	SF4	XD	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%)	0.14	37 (2%) 59 46	186, 276, 733, 884	0
1	XA	1515/1521 (99%)	0.01	24 (1%) 70 54	158, 261, 672, 775	0
2	QB	235/256 (91%)	0.18	13 (5%) 30 28	230, 330, 393, 429	0
2	XB	236/256 (92%)	0.45	24 (10%) 12 14	237, 291, 340, 364	0
3	QC	205/239 (85%)	0.42	19 (9%) 14 17	271, 379, 421, 449	0
3	XC	205/239 (85%)	0.53	17 (8%) 17 19	275, 359, 467, 497	0
4	QD	208/209 (99%)	0.90	32 (15%) 5 9	231, 275, 325, 369	0
4	XD	208/209 (99%)	0.80	25 (12%) 9 12	216, 258, 306, 370	0
5	QE	151/162 (93%)	0.62	13 (8%) 16 18	208, 268, 318, 333	0
5	XE	151/162 (93%)	0.27	12 (7%) 18 20	174, 222, 277, 313	0
6	QF	101/101 (100%)	0.49	8 (7%) 18 20	224, 285, 333, 355	0
6	XF	101/101 (100%)	0.65	11 (10%) 10 13	278, 343, 376, 406	0
7	QG	155/156 (99%)	0.09	6 (3%) 43 34	332, 425, 492, 522	0
7	XG	155/156 (99%)	0.24	7 (4%) 38 32	327, 458, 559, 580	0
8	QH	137/138 (99%)	1.40	33 (24%) 2 5	230, 290, 341, 368	0
8	XH	137/138 (99%)	0.81	12 (8%) 15 17	197, 259, 299, 342	0
9	QI	105/128 (82%)	0.22	2 (1%) 66 51	289, 373, 413, 449	0
9	XI	107/128 (83%)	0.38	8 (7%) 20 21	364, 448, 487, 522	0
10	QJ	99/105 (94%)	0.59	6 (6%) 27 26	354, 404, 458, 476	0
10	XJ	96/105 (91%)	0.94	13 (13%) 7 10	340, 397, 495, 509	0
11	QK	119/129 (92%)	0.63	14 (11%) 9 12	172, 269, 315, 333	0
11	XK	116/129 (89%)	0.74	14 (12%) 8 12	213, 279, 334, 364	0
12	QL	125/132 (94%)	1.01	22 (17%) 4 7	183, 237, 288, 334	0
12	XL	122/132 (92%)	1.10	28 (22%) 2 5	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%)	0.17	2 (1%) 69 54	298, 386, 443, 469	0
13	XM	114/126 (90%)	0.52	8 (7%) 22 22	317, 414, 450, 463	0
14	QN	60/61 (98%)	0.95	11 (18%) 3 7	295, 353, 479, 493	0
14	XN	60/61 (98%)	1.23	14 (23%) 2 5	312, 556, 587, 612	0
15	QO	88/89 (98%)	0.95	19 (21%) 2 5	196, 272, 314, 335	0
15	XO	87/89 (97%)	0.77	10 (11%) 9 12	182, 221, 267, 284	0
16	QP	84/88 (95%)	1.21	18 (21%) 2 5	189, 247, 303, 348	0
16	XP	84/88 (95%)	1.86	34 (40%) 0 2	264, 358, 461, 493	0
17	QQ	100/105 (95%)	1.44	23 (23%) 2 5	199, 251, 286, 319	0
17	XQ	100/105 (95%)	0.82	20 (20%) 3 6	174, 231, 273, 307	0
18	QR	70/88 (79%)	0.36	5 (7%) 22 22	240, 297, 336, 375	0
18	XR	70/88 (79%)	0.38	4 (5%) 29 27	168, 247, 321, 337	0
19	QS	83/93 (89%)	1.03	11 (13%) 7 10	308, 459, 605, 672	0
19	XS	84/93 (90%)	0.98	7 (8%) 17 19	341, 414, 456, 474	0
20	QT	99/106 (93%)	1.55	32 (32%) 1 3	205, 271, 358, 377	0
20	XT	99/106 (93%)	1.38	21 (21%) 2 5	198, 242, 278, 302	0
21	QU	25/27 (92%)	1.04	2 (8%) 18 20	300, 347, 463, 563	0
21	XU	25/27 (92%)	1.45	5 (20%) 3 6	336, 374, 530, 549	0
22	QV	68/77 (88%)	-0.00	2 (2%) 53 40	294, 387, 435, 446	0
22	XV	68/77 (88%)	-0.18	0 100 100	281, 411, 474, 504	0
23	QX	19/19 (100%)	0.44	0 100 100	368, 432, 461, 464	0
23	XX	19/19 (100%)	0.53	0 100 100	356, 422, 471, 476	0
24	R0	81/85 (95%)	1.01	17 (20%) 2 5	166, 206, 296, 364	0
24	Y0	82/85 (96%)	0.77	13 (15%) 5 8	120, 168, 274, 329	0
25	R1	95/98 (96%)	1.49	26 (27%) 1 4	162, 201, 262, 291	0
25	Y1	93/98 (94%)	1.30	24 (25%) 1 4	117, 176, 219, 232	0
26	R2	69/72 (95%)	0.56	7 (10%) 12 15	124, 192, 238, 283	0
26	Y2	68/72 (94%)	1.11	18 (26%) 1 4	124, 171, 214, 231	0
27	R3	59/60 (98%)	0.70	10 (16%) 4 8	175, 228, 281, 338	0
27	Y3	59/60 (98%)	0.68	8 (13%) 7 10	115, 168, 241, 269	0
28	R4	45/71 (63%)	-0.17	0 100 100	237, 382, 418, 429	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
28	Y4	46/71 (64%)	-0.19	0	100	100	206, 273, 315, 322	0
29	R5	59/60 (98%)	0.36	4 (6%)	23	23	142, 193, 225, 291	0
29	Y5	59/60 (98%)	0.32	2 (3%)	48	37	122, 172, 225, 300	0
30	R6	53/54 (98%)	-0.14	1 (1%)	66	51	175, 230, 267, 357	0
30	Y6	53/54 (98%)	0.39	2 (3%)	44	35	144, 194, 248, 260	0
31	R7	47/49 (95%)	1.20	10 (21%)	2	5	138, 167, 186, 207	0
31	Y7	48/49 (97%)	0.98	9 (18%)	3	7	111, 146, 192, 224	0
32	R8	64/65 (98%)	0.97	11 (17%)	4	7	154, 201, 248, 284	0
32	Y8	64/65 (98%)	1.47	18 (28%)	1	4	120, 172, 209, 259	0
33	R9	37/37 (100%)	1.76	16 (43%)	0	2	260, 289, 340, 357	0
33	Y9	37/37 (100%)	1.52	10 (27%)	1	4	174, 205, 233, 250	0
34	RA	2882/2905 (99%)	-0.15	16 (0%)	85	71	123, 197, 357, 505	0
34	YA	2883/2905 (99%)	-0.15	20 (0%)	84	69	96, 149, 276, 493	0
35	RB	120/122 (98%)	-0.18	0	100	100	205, 256, 303, 350	0
35	YB	120/122 (98%)	-0.25	1 (0%)	82	67	135, 175, 210, 248	0
36	RD	272/276 (98%)	0.92	46 (16%)	4	8	127, 186, 231, 284	0
36	YD	272/276 (98%)	0.83	35 (12%)	7	11	107, 159, 207, 243	0
37	RE	205/206 (99%)	1.00	39 (19%)	3	7	128, 211, 265, 310	0
37	YE	205/206 (99%)	0.88	36 (17%)	4	7	102, 157, 205, 254	0
38	RF	202/210 (96%)	0.41	12 (5%)	28	26	143, 199, 272, 328	0
38	YF	202/210 (96%)	0.66	20 (9%)	13	15	101, 160, 215, 256	0
39	RG	181/182 (99%)	0.10	8 (4%)	39	32	231, 307, 360, 388	0
39	YG	181/182 (99%)	0.21	13 (7%)	21	21	178, 226, 291, 327	0
40	RH	174/180 (96%)	0.39	13 (7%)	20	21	189, 269, 313, 358	0
40	YH	174/180 (96%)	0.54	15 (8%)	16	18	123, 175, 217, 258	0
41	RI	146/148 (98%)	0.46	13 (8%)	15	17	188, 254, 300, 327	0
41	YI	146/148 (98%)	0.21	8 (5%)	30	28	158, 226, 271, 293	0
42	RN	138/140 (98%)	0.69	15 (10%)	10	13	139, 219, 260, 268	0
42	YN	138/140 (98%)	0.91	25 (18%)	3	7	94, 160, 205, 231	0
43	RO	122/122 (100%)	0.51	11 (9%)	15	17	158, 202, 247, 286	0
43	YO	122/122 (100%)	0.26	2 (1%)	70	54	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%)	0.94	31 (20%) 2 6	160, 228, 287, 331	0
44	YP	147/150 (98%)	0.87	23 (15%) 5 9	128, 166, 217, 255	0
45	RQ	141/141 (100%)	0.54	14 (9%) 13 15	194, 231, 267, 309	0
45	YQ	141/141 (100%)	0.55	7 (4%) 34 29	132, 174, 238, 314	0
46	RR	117/118 (99%)	1.17	26 (22%) 2 5	121, 180, 224, 257	0
46	YR	117/118 (99%)	1.22	30 (25%) 1 4	104, 155, 212, 237	0
47	RS	111/112 (99%)	0.58	14 (12%) 8 11	191, 262, 311, 357	0
47	YS	111/112 (99%)	0.91	24 (21%) 2 5	146, 196, 282, 328	0
48	RT	137/146 (93%)	0.50	13 (9%) 14 16	158, 225, 307, 320	0
48	YT	137/146 (93%)	0.65	16 (11%) 9 12	127, 185, 257, 282	0
49	RU	117/118 (99%)	0.91	18 (15%) 5 9	149, 243, 286, 304	0
49	YU	117/118 (99%)	0.76	13 (11%) 10 13	101, 147, 194, 223	0
50	RV	101/101 (100%)	0.36	12 (11%) 9 12	165, 222, 278, 288	0
50	YV	101/101 (100%)	0.53	13 (12%) 7 11	118, 170, 240, 280	0
51	RW	113/113 (100%)	0.80	12 (10%) 11 14	117, 160, 226, 339	0
51	YW	113/113 (100%)	0.83	19 (16%) 4 8	92, 137, 192, 239	0
52	RX	92/96 (95%)	0.78	10 (10%) 10 13	127, 177, 212, 235	0
52	YX	92/96 (95%)	0.97	14 (15%) 5 9	110, 146, 190, 259	0
53	RY	107/110 (97%)	0.69	13 (12%) 8 12	170, 219, 264, 315	0
53	YY	107/110 (97%)	0.46	8 (7%) 20 21	107, 170, 205, 244	0
54	RZ	183/206 (88%)	0.08	7 (3%) 44 35	211, 258, 298, 354	0
54	YZ	193/206 (93%)	0.30	12 (6%) 26 25	124, 196, 287, 350	0
All	All	20769/21416 (96%)	0.35	1551 (7%) 20 21	92, 221, 460, 884	0

The worst 5 of 1551 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	XD	4	TYR	12.1
17	QQ	24	GLU	10.3
8	QH	111	ILE	9.8
2	XB	101	MET	9.7
12	XL	28	LYS	9.7

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.