



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 6OJ2 / pdb_00006oj2
Title : Crystal structure of tRNA^{Ala}(GGC) bound to the near-cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-10
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

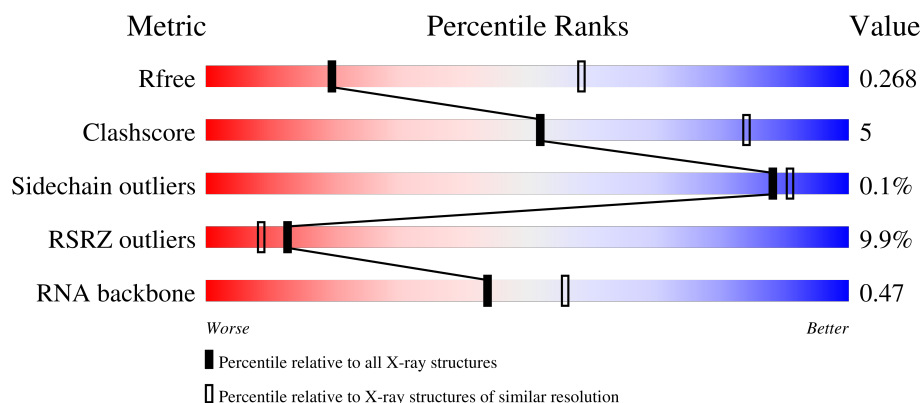
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	2% 66% 28% 5%
1	XA	1522	% 65% 29%
2	QB	256	5% 71% 22% 7%
2	XB	256	10% 72% 20% 7%
3	QC	239	8% 72% 14% 14%

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Mol	Chain	Length	Quality of chain
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	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	

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Mol	Chain	Length	Quality of chain
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	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	
27	Y1	98	
28	R2	72	

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Mol	Chain	Length	Quality of chain
28	Y2	72	
29	R3	60	
29	Y3	60	
30	R4	71	
30	Y4	71	
31	R5	60	
31	Y5	60	
32	R6	54	
32	Y6	54	
33	R7	49	
33	Y7	49	
34	R8	65	
34	Y8	65	
35	R9	37	
35	Y9	37	
36	RA	2915	
36	YA	2915	
37	RB	122	
37	YB	122	
38	RD	276	
38	YD	276	
39	RE	206	
39	YE	206	
40	RF	210	
40	YF	210	

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Mol	Chain	Length	Quality of chain
41	RG	182	
41	YG	182	
42	RH	180	
42	YH	180	
43	RI	148	
43	YI	148	
44	RN	140	
44	YN	140	
45	RO	122	
45	YO	122	
46	RP	150	
46	YP	150	
47	RQ	141	
47	YQ	141	
48	RR	118	
48	YR	118	
49	RS	112	
49	YS	112	
50	RT	146	
50	YT	146	
51	RU	118	
51	YU	118	
52	RV	101	
52	YV	101	
53	RW	113	

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Mol	Chain	Length	Quality of chain
53	YW	113	
54	RX	96	
54	YX	96	
55	RY	110	
55	YY	110	
56	RZ	206	
56	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
57	MG	QA	1601	-	-	-	X
57	MG	QA	1602	-	-	-	X
57	MG	QA	1605	-	-	-	X
57	MG	QA	1606	-	-	-	X
57	MG	QA	1607	-	-	-	X
57	MG	QA	1608	-	-	-	X
57	MG	QA	1609	-	-	-	X
57	MG	QA	1610	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1615	-	-	-	X
57	MG	QA	1616	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1621	-	-	-	X
57	MG	QA	1622	-	-	-	X
57	MG	QA	1627	-	-	-	X
57	MG	QA	1632	-	-	-	X
57	MG	QA	1637	-	-	-	X
57	MG	QA	1641	-	-	-	X
57	MG	QA	1650	-	-	-	X
57	MG	QA	1653	-	-	-	X
57	MG	QA	1668	-	-	-	X
57	MG	QA	1671	-	-	-	X
57	MG	QA	1672	-	-	-	X
57	MG	QA	1674	-	-	-	X
57	MG	QA	1677	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1686	-	-	-	X
57	MG	R8	101	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3010	-	-	-	X
57	MG	RA	3013	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3018	-	-	-	X
57	MG	RA	3019	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3023	-	-	-	X
57	MG	RA	3024	-	-	-	X
57	MG	RA	3025	-	-	-	X
57	MG	RA	3027	-	-	-	X
57	MG	RA	3028	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3040	-	-	-	X
57	MG	RA	3041	-	-	-	X
57	MG	RA	3042	-	-	-	X
57	MG	RA	3043	-	-	-	X
57	MG	RA	3047	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3050	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3053	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3055	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3057	-	-	-	X
57	MG	RA	3059	-	-	-	X
57	MG	RA	3060	-	-	-	X
57	MG	RA	3061	-	-	-	X
57	MG	RA	3063	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3065	-	-	-	X
57	MG	RA	3067	-	-	-	X
57	MG	RA	3068	-	-	-	X
57	MG	RA	3070	-	-	-	X
57	MG	RA	3072	-	-	-	X
57	MG	RA	3073	-	-	-	X
57	MG	RA	3078	-	-	-	X
57	MG	RA	3080	-	-	-	X
57	MG	RA	3081	-	-	-	X
57	MG	RA	3083	-	-	-	X
57	MG	RA	3084	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3089	-	-	-	X
57	MG	RA	3090	-	-	-	X
57	MG	RA	3091	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3096	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3100	-	-	-	X
57	MG	RA	3101	-	-	-	X
57	MG	RA	3103	-	-	-	X
57	MG	RA	3104	-	-	-	X
57	MG	RA	3105	-	-	-	X
57	MG	RA	3107	-	-	-	X
57	MG	RA	3108	-	-	-	X
57	MG	RA	3109	-	-	-	X
57	MG	RA	3111	-	-	-	X
57	MG	RA	3113	-	-	-	X
57	MG	RA	3114	-	-	-	X
57	MG	RA	3115	-	-	-	X
57	MG	RA	3117	-	-	-	X
57	MG	RA	3118	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RA	3134	-	-	-	X
57	MG	RA	3140	-	-	-	X
57	MG	RA	3141	-	-	-	X
57	MG	RA	3144	-	-	-	X
57	MG	RA	3149	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3150	-	-	-	X
57	MG	RA	3152	-	-	-	X
57	MG	RA	3153	-	-	-	X
57	MG	RA	3155	-	-	-	X
57	MG	RA	3156	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3158	-	-	-	X
57	MG	RA	3159	-	-	-	X
57	MG	RA	3162	-	-	-	X
57	MG	RA	3163	-	-	-	X
57	MG	RA	3164	-	-	-	X
57	MG	RA	3166	-	-	-	X
57	MG	RA	3167	-	-	-	X
57	MG	RA	3172	-	-	-	X
57	MG	RA	3174	-	-	-	X
57	MG	RA	3176	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3182	-	-	-	X
57	MG	RA	3186	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3196	-	-	-	X
57	MG	RA	3198	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3214	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3223	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RA	3235	-	-	-	X
57	MG	RA	3236	-	-	-	X
57	MG	RA	3240	-	-	-	X
57	MG	RA	3244	-	-	-	X
57	MG	RA	3246	-	-	-	X
57	MG	RA	3247	-	-	-	X
57	MG	RA	3249	-	-	-	X
57	MG	RA	3250	-	-	-	X
57	MG	RA	3251	-	-	-	X
57	MG	RA	3252	-	-	-	X
57	MG	RA	3253	-	-	-	X
57	MG	RA	3254	-	-	-	X
57	MG	RA	3255	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3256	-	-	-	X
57	MG	RA	3257	-	-	-	X
57	MG	RA	3259	-	-	-	X
57	MG	RA	3261	-	-	-	X
57	MG	RA	3263	-	-	-	X
57	MG	RA	3264	-	-	-	X
57	MG	RA	3266	-	-	-	X
57	MG	RA	3267	-	-	-	X
57	MG	RA	3268	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3271	-	-	-	X
57	MG	RA	3272	-	-	-	X
57	MG	RA	3273	-	-	-	X
57	MG	RA	3276	-	-	-	X
57	MG	RA	3279	-	-	-	X
57	MG	RA	3280	-	-	-	X
57	MG	RA	3282	-	-	-	X
57	MG	RA	3283	-	-	-	X
57	MG	RA	3284	-	-	-	X
57	MG	RA	3285	-	-	-	X
57	MG	RA	3286	-	-	-	X
57	MG	RA	3287	-	-	-	X
57	MG	RA	3288	-	-	-	X
57	MG	RA	3291	-	-	-	X
57	MG	RA	3292	-	-	-	X
57	MG	RA	3295	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	RA	3304	-	-	-	X
57	MG	RA	3307	-	-	-	X
57	MG	RA	3308	-	-	-	X
57	MG	RA	3309	-	-	-	X
57	MG	RA	3312	-	-	-	X
57	MG	RA	3313	-	-	-	X
57	MG	RA	3314	-	-	-	X
57	MG	RA	3315	-	-	-	X
57	MG	RA	3316	-	-	-	X
57	MG	RA	3318	-	-	-	X
57	MG	RA	3319	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RE	301	-	-	-	X
57	MG	RE	302	-	-	-	X
57	MG	RE	303	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1601	-	-	-	X
57	MG	XA	1606	-	-	-	X
57	MG	XA	1609	-	-	-	X
57	MG	XA	1611	-	-	-	X
57	MG	XA	1613	-	-	-	X
57	MG	XA	1614	-	-	-	X
57	MG	XA	1615	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1624	-	-	-	X
57	MG	XA	1625	-	-	-	X
57	MG	XA	1627	-	-	-	X
57	MG	XA	1630	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1639	-	-	-	X
57	MG	XA	1641	-	-	-	X
57	MG	XA	1647	-	-	-	X
57	MG	XA	1648	-	-	-	X
57	MG	XA	1654	-	-	-	X
57	MG	XA	1656	-	-	-	X
57	MG	XA	1659	-	-	-	X
57	MG	XA	1663	-	-	-	X
57	MG	XA	1664	-	-	-	X
57	MG	XA	1665	-	-	-	X
57	MG	XA	1669	-	-	-	X
57	MG	XA	1673	-	-	-	X
57	MG	XA	1674	-	-	-	X
57	MG	XA	1677	-	-	-	X
57	MG	XA	1680	-	-	-	X
57	MG	XA	1681	-	-	-	X
57	MG	XA	1682	-	-	-	X
57	MG	XA	1685	-	-	-	X
57	MG	XA	1687	-	-	-	X
57	MG	XA	1689	-	-	-	X
57	MG	XA	1694	-	-	-	X
57	MG	XA	1695	-	-	-	X
57	MG	XV	101	-	-	-	X
57	MG	Y0	101	-	-	-	X
57	MG	Y7	101	-	-	-	X
57	MG	Y7	102	-	-	-	X
57	MG	Y8	101	-	-	-	X
57	MG	Y8	102	-	-	-	X
57	MG	YA	3001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3002	-	-	-	X
57	MG	YA	3003	-	-	-	X
57	MG	YA	3004	-	-	-	X
57	MG	YA	3005	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3010	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3016	-	-	-	X
57	MG	YA	3020	-	-	-	X
57	MG	YA	3022	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3028	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3038	-	-	-	X
57	MG	YA	3039	-	-	-	X
57	MG	YA	3042	-	-	-	X
57	MG	YA	3046	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3054	-	-	-	X
57	MG	YA	3055	-	-	-	X
57	MG	YA	3056	-	-	-	X
57	MG	YA	3057	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3059	-	-	-	X
57	MG	YA	3060	-	-	-	X
57	MG	YA	3061	-	-	-	X
57	MG	YA	3063	-	-	-	X
57	MG	YA	3064	-	-	-	X
57	MG	YA	3065	-	-	-	X
57	MG	YA	3066	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3067	-	-	-	X
57	MG	YA	3071	-	-	-	X
57	MG	YA	3072	-	-	-	X
57	MG	YA	3073	-	-	-	X
57	MG	YA	3074	-	-	-	X
57	MG	YA	3075	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3077	-	-	-	X
57	MG	YA	3078	-	-	-	X
57	MG	YA	3079	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3081	-	-	-	X
57	MG	YA	3082	-	-	-	X
57	MG	YA	3083	-	-	-	X
57	MG	YA	3086	-	-	-	X
57	MG	YA	3087	-	-	-	X
57	MG	YA	3088	-	-	-	X
57	MG	YA	3089	-	-	-	X
57	MG	YA	3090	-	-	-	X
57	MG	YA	3091	-	-	-	X
57	MG	YA	3092	-	-	-	X
57	MG	YA	3093	-	-	-	X
57	MG	YA	3094	-	-	-	X
57	MG	YA	3095	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3097	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3101	-	-	-	X
57	MG	YA	3102	-	-	-	X
57	MG	YA	3104	-	-	-	X
57	MG	YA	3105	-	-	-	X
57	MG	YA	3106	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3110	-	-	-	X
57	MG	YA	3112	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3116	-	-	-	X
57	MG	YA	3118	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3120	-	-	-	X
57	MG	YA	3121	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3124	-	-	-	X
57	MG	YA	3125	-	-	-	X
57	MG	YA	3126	-	-	-	X
57	MG	YA	3127	-	-	-	X
57	MG	YA	3128	-	-	-	X
57	MG	YA	3129	-	-	-	X
57	MG	YA	3130	-	-	-	X
57	MG	YA	3131	-	-	-	X
57	MG	YA	3136	-	-	-	X
57	MG	YA	3138	-	-	-	X
57	MG	YA	3139	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3142	-	-	-	X
57	MG	YA	3143	-	-	-	X
57	MG	YA	3144	-	-	-	X
57	MG	YA	3146	-	-	-	X
57	MG	YA	3148	-	-	-	X
57	MG	YA	3149	-	-	-	X
57	MG	YA	3150	-	-	-	X
57	MG	YA	3151	-	-	-	X
57	MG	YA	3156	-	-	-	X
57	MG	YA	3158	-	-	-	X
57	MG	YA	3160	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3162	-	-	-	X
57	MG	YA	3163	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3165	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3169	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3171	-	-	-	X
57	MG	YA	3175	-	-	-	X
57	MG	YA	3177	-	-	-	X
57	MG	YA	3179	-	-	-	X
57	MG	YA	3181	-	-	-	X
57	MG	YA	3184	-	-	-	X
57	MG	YA	3185	-	-	-	X
57	MG	YA	3186	-	-	-	X
57	MG	YA	3187	-	-	-	X
57	MG	YA	3191	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3194	-	-	-	X
57	MG	YA	3199	-	-	-	X
57	MG	YA	3202	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3213	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3218	-	-	-	X
57	MG	YA	3220	-	-	-	X
57	MG	YA	3221	-	-	-	X
57	MG	YA	3222	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3224	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3244	-	-	-	X
57	MG	YA	3247	-	-	-	X
57	MG	YA	3252	-	-	-	X
57	MG	YA	3253	-	-	-	X
57	MG	YA	3262	-	-	-	X
57	MG	YA	3263	-	-	-	X
57	MG	YA	3264	-	-	-	X
57	MG	YA	3270	-	-	-	X
57	MG	YA	3271	-	-	-	X
57	MG	YA	3274	-	-	-	X
57	MG	YA	3275	-	-	-	X
57	MG	YA	3279	-	-	-	X
57	MG	YA	3282	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3284	-	-	-	X
57	MG	YA	3285	-	-	-	X
57	MG	YA	3286	-	-	-	X
57	MG	YA	3287	-	-	-	X
57	MG	YA	3288	-	-	-	X
57	MG	YA	3289	-	-	-	X
57	MG	YA	3290	-	-	-	X
57	MG	YA	3291	-	-	-	X
57	MG	YA	3292	-	-	-	X
57	MG	YA	3293	-	-	-	X
57	MG	YA	3294	-	-	-	X
57	MG	YA	3295	-	-	-	X
57	MG	YA	3296	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3297	-	-	-	X
57	MG	YA	3298	-	-	-	X
57	MG	YA	3300	-	-	-	X
57	MG	YA	3301	-	-	-	X
57	MG	YA	3302	-	-	-	X
57	MG	YA	3305	-	-	-	X
57	MG	YA	3309	-	-	-	X
57	MG	YA	3310	-	-	-	X
57	MG	YA	3314	-	-	-	X
57	MG	YA	3315	-	-	-	X
57	MG	YA	3316	-	-	-	X
57	MG	YA	3319	-	-	-	X
57	MG	YA	3321	-	-	-	X
57	MG	YA	3326	-	-	-	X
57	MG	YA	3331	-	-	-	X
57	MG	YA	3334	-	-	-	X
57	MG	YA	3335	-	-	-	X
57	MG	YA	3338	-	-	-	X
57	MG	YA	3339	-	-	-	X
57	MG	YA	3341	-	-	-	X
57	MG	YA	3342	-	-	-	X
57	MG	YA	3344	-	-	-	X
57	MG	YA	3345	-	-	-	X
57	MG	YA	3348	-	-	-	X
57	MG	YA	3349	-	-	-	X
57	MG	YA	3350	-	-	-	X
57	MG	YA	3352	-	-	-	X
57	MG	YA	3357	-	-	-	X
57	MG	YA	3359	-	-	-	X
57	MG	YA	3361	-	-	-	X
57	MG	YA	3362	-	-	-	X
57	MG	YA	3363	-	-	-	X
57	MG	YA	3368	-	-	-	X
57	MG	YA	3369	-	-	-	X
57	MG	YA	3371	-	-	-	X
57	MG	YA	3372	-	-	-	X
57	MG	YA	3373	-	-	-	X
57	MG	YA	3375	-	-	-	X
57	MG	YA	3376	-	-	-	X
57	MG	YB	201	-	-	-	X
57	MG	YB	207	-	-	-	X
57	MG	YD	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YD	302	-	-	-	X
57	MG	YD	303	-	-	-	X
57	MG	YE	3401	-	-	-	X
57	MG	YE	3402	-	-	-	X
57	MG	YE	3403	-	-	-	X
57	MG	YH	201	-	-	-	X
57	MG	YP	201	-	-	-	X
57	MG	YP	203	-	-	-	X
57	MG	YR	201	-	-	-	X
57	MG	YR	202	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298371 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 30S ribosomal protein S14 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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			418	187	87	125	19			
24	XX	17	Total	C	N	O	P	0	0	0
			374	167	77	113	17			

- Molecule 25 is a RNA chain called A-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
30	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
32	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
33	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a RNA chain called 23S rRNA.

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

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a protein called 50S ribosomal protein L2.

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

- Molecule 39 is a protein called 50S ribosomal protein L3.

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

- Molecule 40 is a protein called 50S ribosomal protein L4.

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

- Molecule 41 is a protein called 50S ribosomal protein L5.

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

- Molecule 42 is a protein called 50S ribosomal protein L6.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L9.

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

- Molecule 44 is a protein called 50S ribosomal protein L13.

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

- Molecule 45 is a protein called 50S ribosomal protein L14.

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

- Molecule 46 is a protein called 50S ribosomal protein L15.

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

- Molecule 47 is a protein called 50S ribosomal protein L16.

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

- Molecule 48 is a protein called 50S ribosomal protein L17.

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

- Molecule 49 is a protein called 50S ribosomal protein L18.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L20.

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

- Molecule 52 is a protein called 50S ribosomal protein L21.

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

- Molecule 53 is a protein called 50S ribosomal protein L22.

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

- Molecule 54 is a protein called 50S ribosomal protein L23.

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

- Molecule 55 is a protein called 50S ribosomal protein L24.

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

- Molecule 56 is a protein called 50S ribosomal protein L25.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	85	Total	Mg	0	0
			85	85		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	2	Total	Mg	0	0
			2	2		
57	QV	4	Total	Mg	0	0
			4	4		

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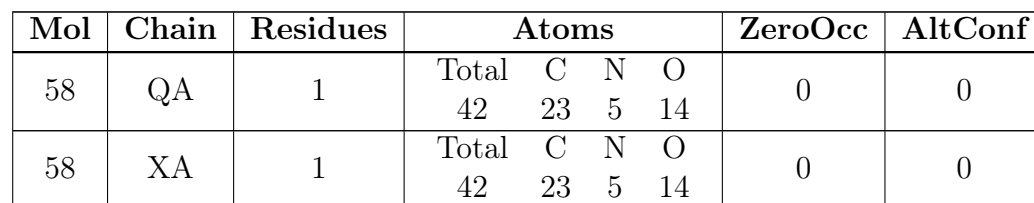
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RA	321	Total 321	Mg 321	0	0
57	RB	4	Total 4	Mg 4	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	3	Total 3	Mg 3	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	XA	94	Total 94	Mg 94	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	XY	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y0	1	Total 1	Mg 1	0	0
57	Y2	1	Total 1	Mg 1	0	0
57	Y5	2	Total 2	Mg 2	0	0
57	Y7	2	Total 2	Mg 2	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	YA	379	Total 379	Mg 379	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	3	Total 3	Mg 3	0	0
57	YE	3	Total 3	Mg 3	0	0
57	YH	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YU	2	Total 2	Mg 2	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YX	3	Total 3	Mg 3	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



-
- Diagram illustrating a cubane cluster, Fe_4S_4 , showing four iron (Fe) atoms and four sulfur (S) atoms arranged in a cube-like structure. The atoms are labeled: SF4, S3, FE1, FE2, S2, S4, S1, and FE3.

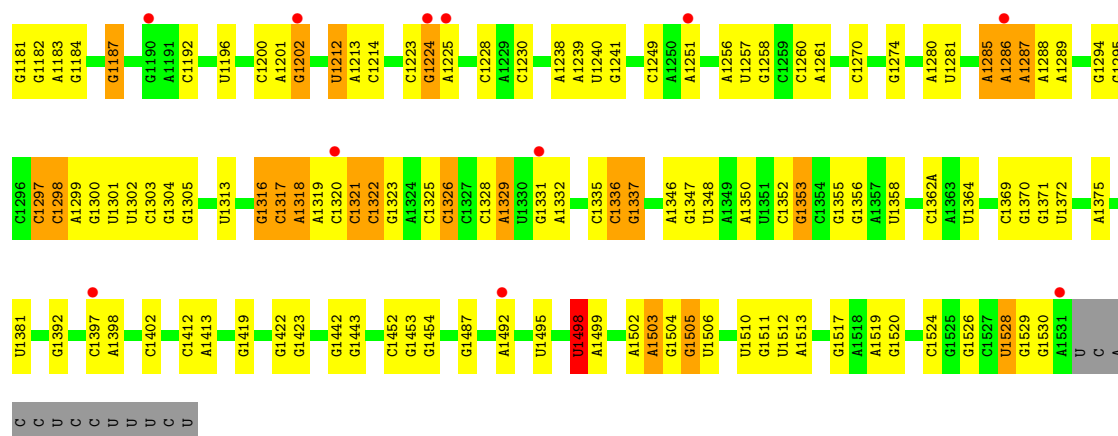
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	QD	1	Total 8	Fe 4	S 4	0	0
59	XD	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

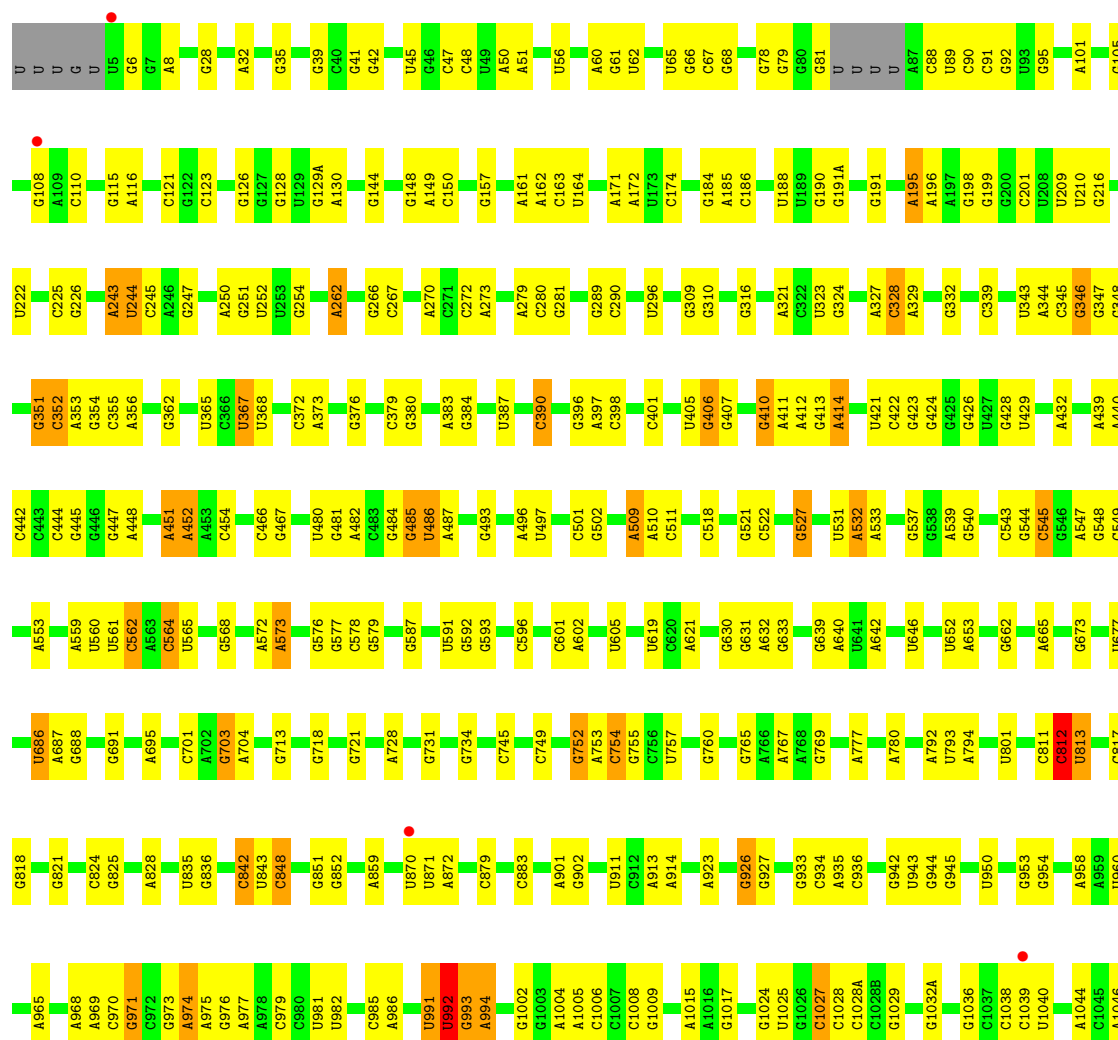
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	XN	1	Total 1	Zn 1	0	0

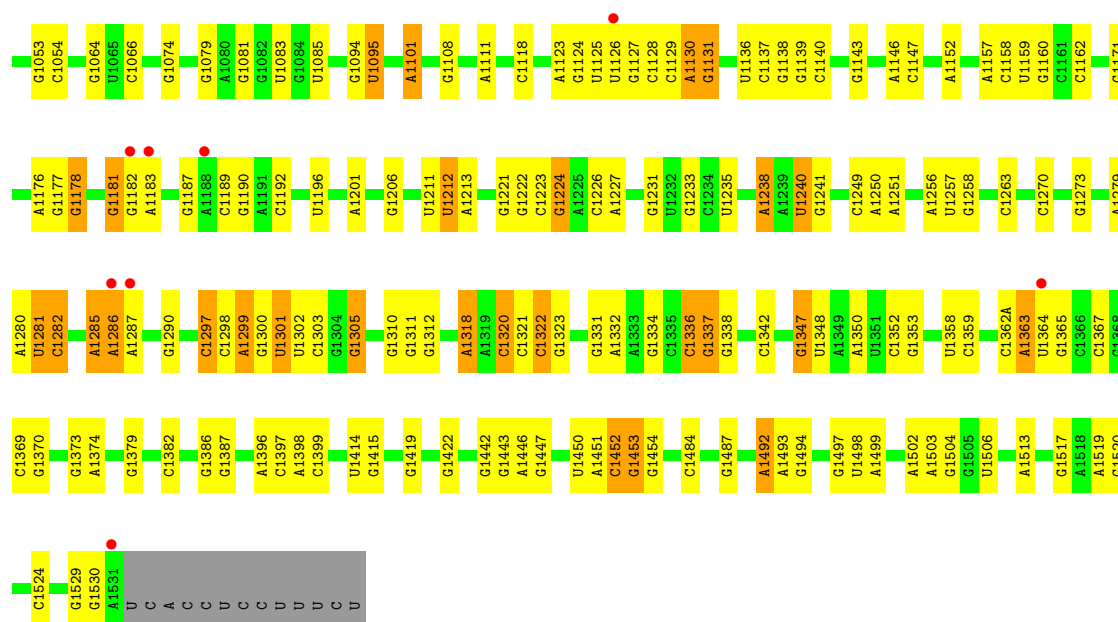
- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	QA	1	Total 1	O 1	0	0
61	QX	1	Total 1	O 1	0	0

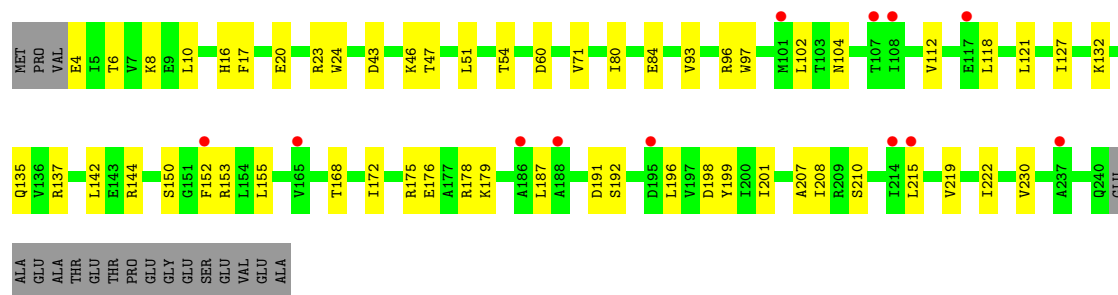
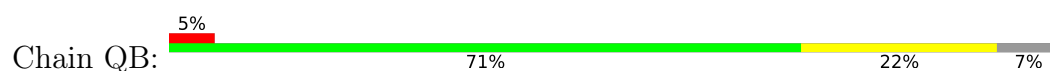


• Molecule 1: 16S rRNA

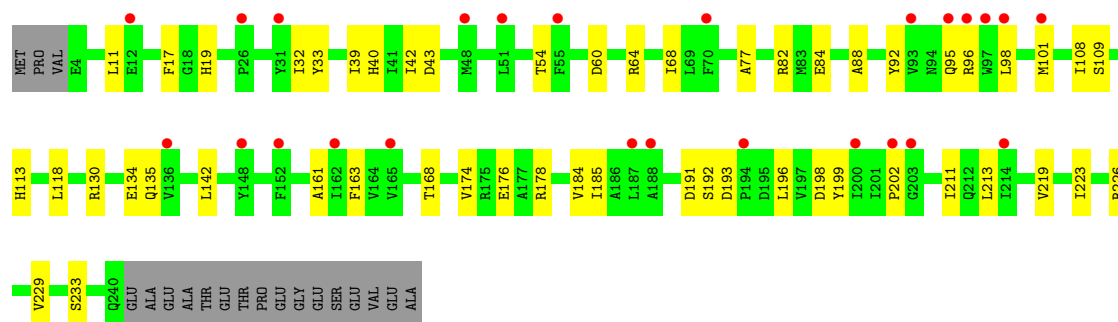
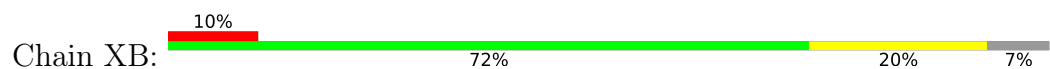




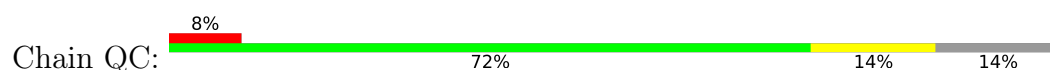
• Molecule 2: 30S ribosomal protein S2

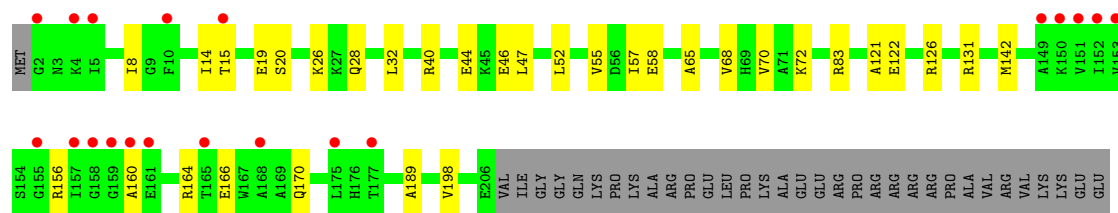


• Molecule 2: 30S ribosomal protein S2

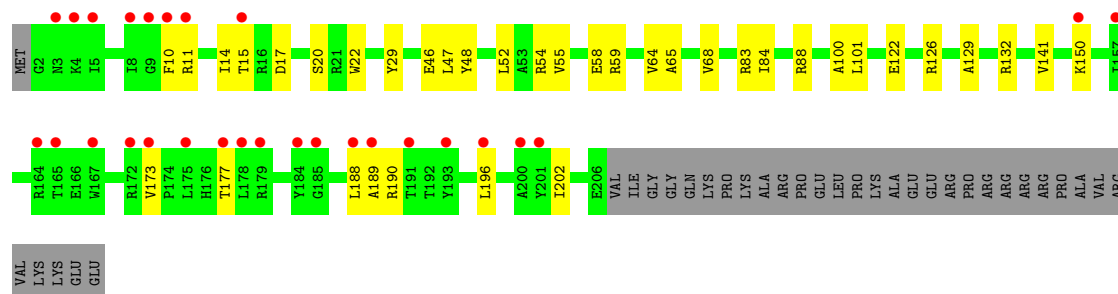
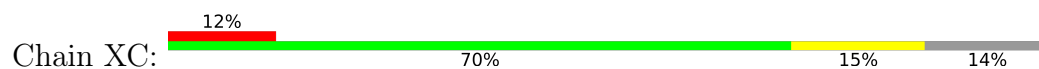


• Molecule 3: 30S ribosomal protein S3

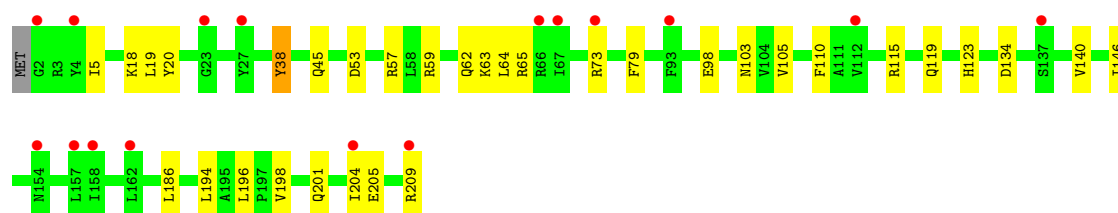
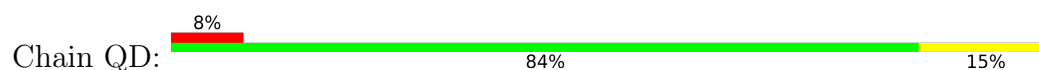




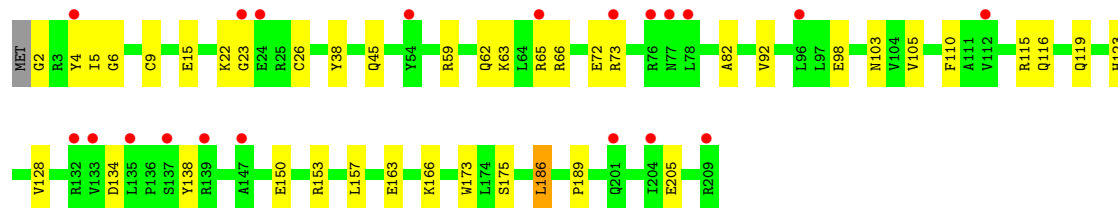
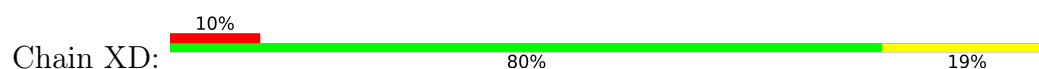
• Molecule 3: 30S ribosomal protein S3



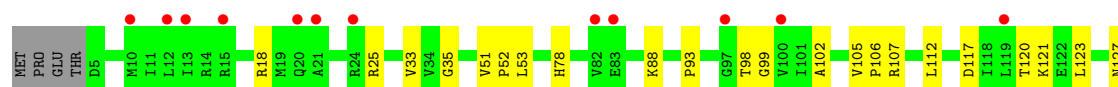
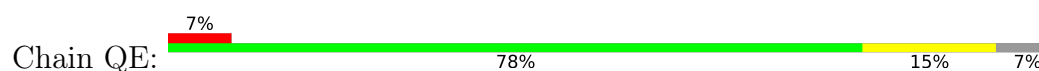
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

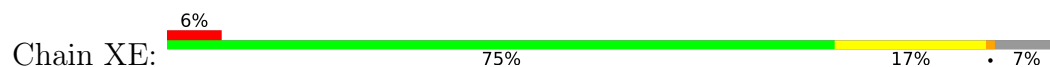


• Molecule 5: 30S ribosomal protein S5

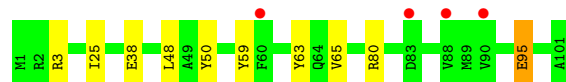




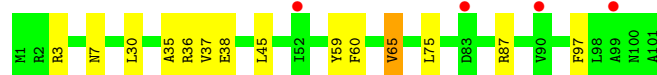
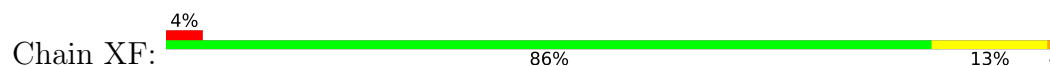
- Molecule 5: 30S ribosomal protein S5



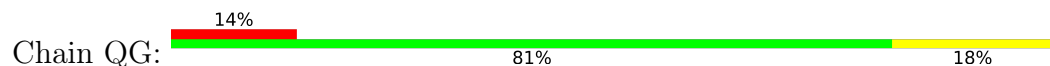
- Molecule 6: 30S ribosomal protein S6



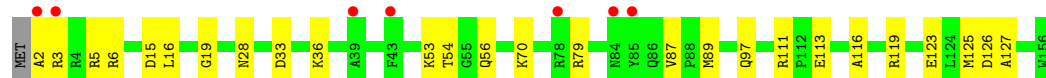
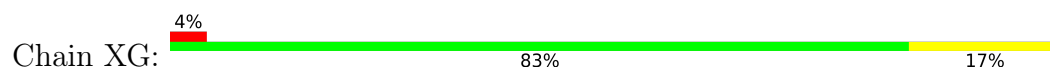
- Molecule 6: 30S ribosomal protein S6



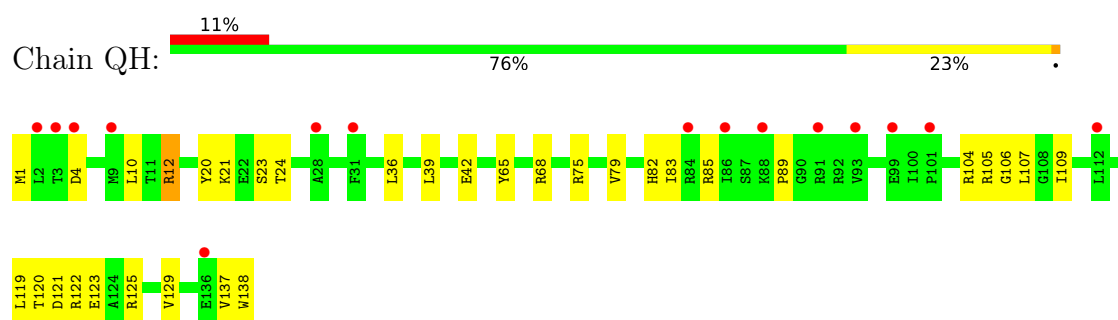
- Molecule 7: 30S ribosomal protein S7



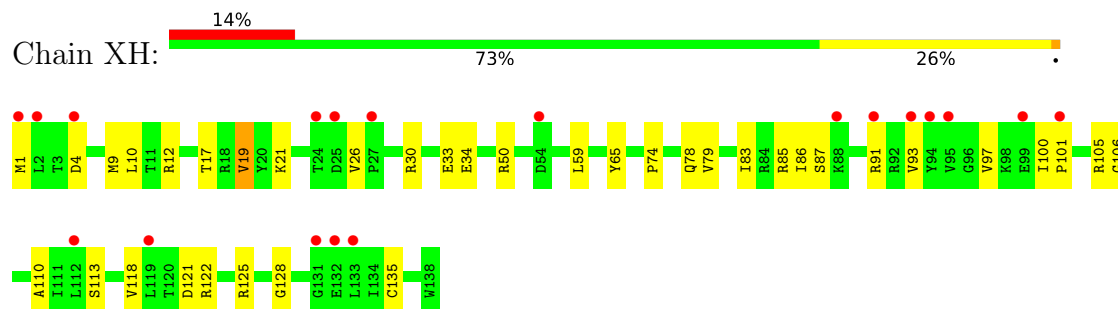
- Molecule 7: 30S ribosomal protein S7



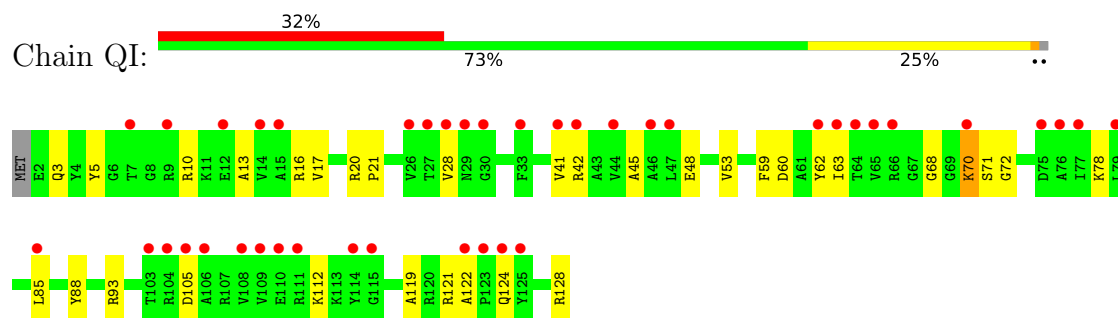
- Molecule 8: 30S ribosomal protein S8



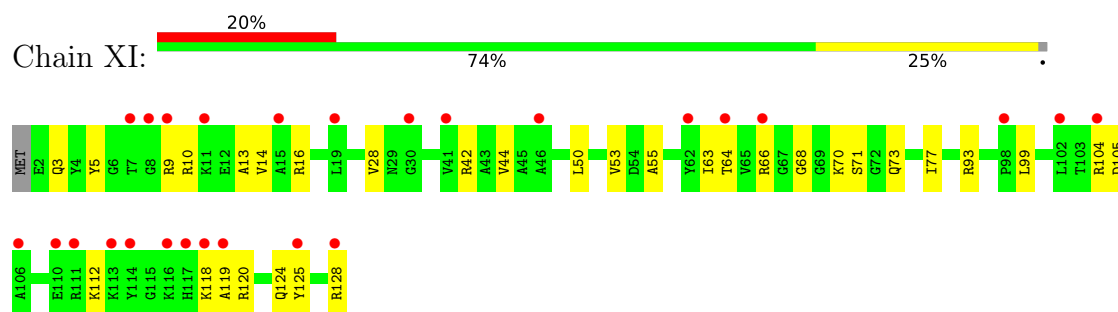
• Molecule 8: 30S ribosomal protein S8



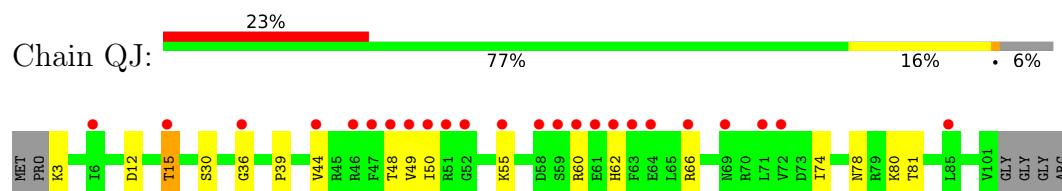
• Molecule 9: 30S ribosomal protein S9



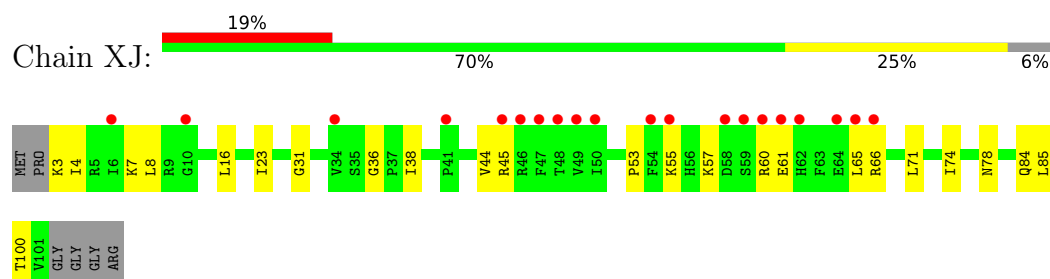
• Molecule 9: 30S ribosomal protein S9



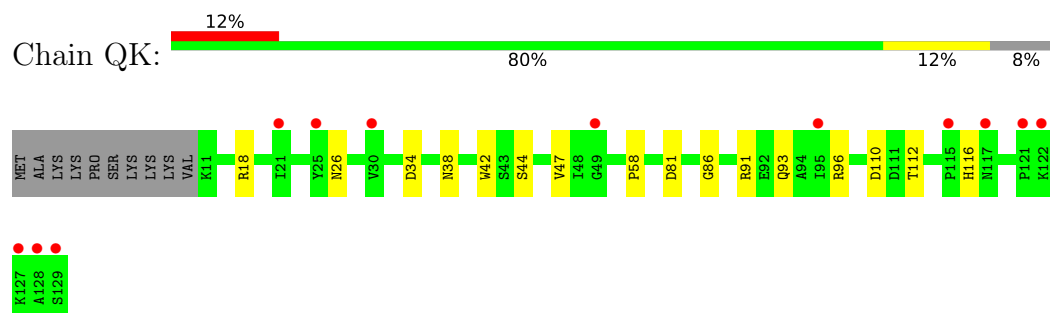
• Molecule 10: 30S ribosomal protein S10



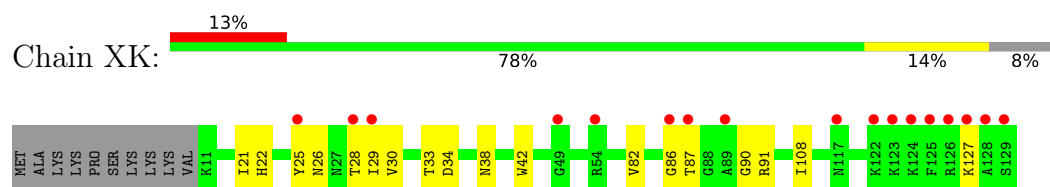
- Molecule 10: 30S ribosomal protein S10



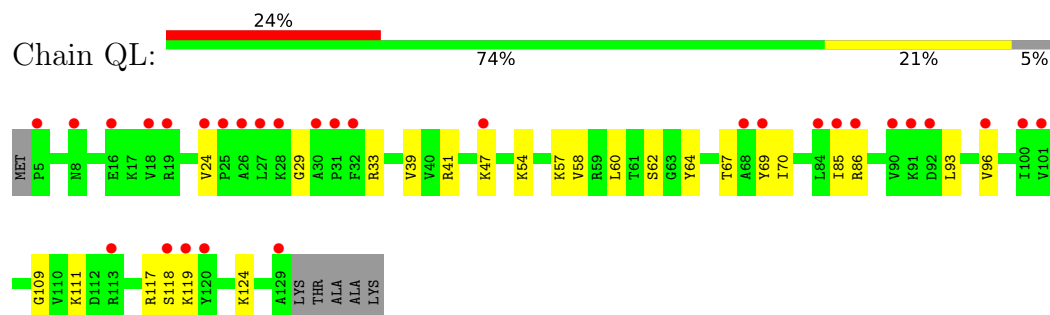
- Molecule 11: 30S ribosomal protein S11



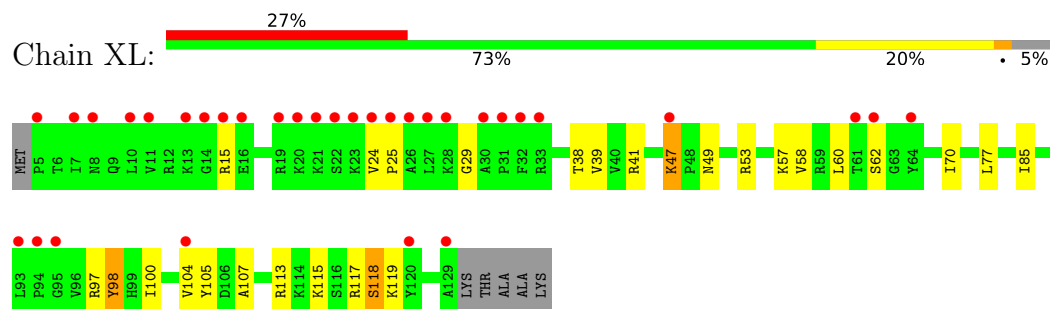
- Molecule 11: 30S ribosomal protein S11



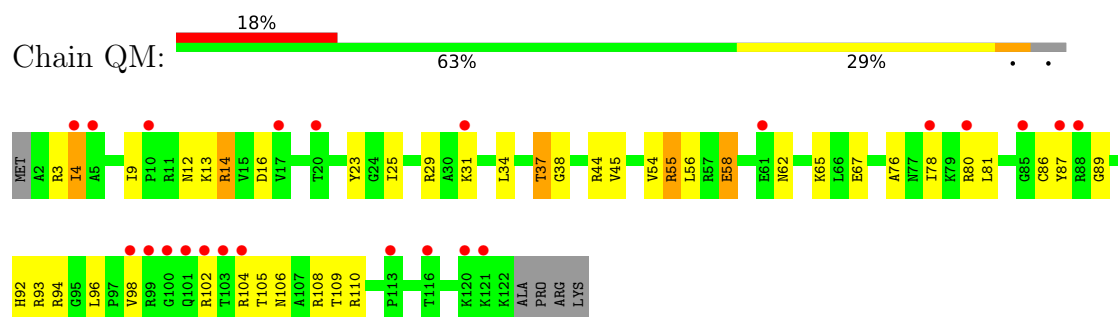
- Molecule 12: 30S ribosomal protein S12



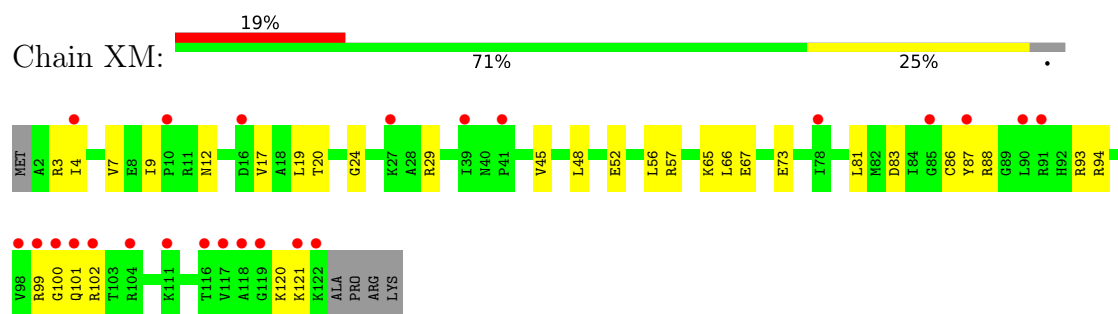
- Molecule 12: 30S ribosomal protein S12



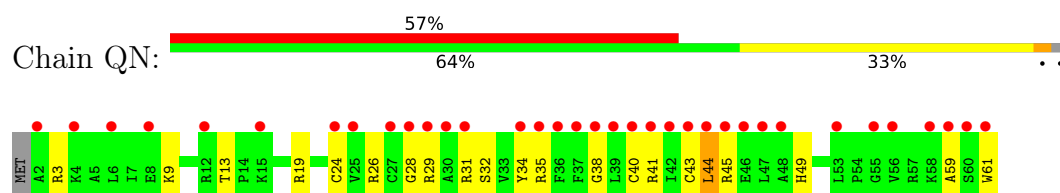
- Molecule 13: 30S ribosomal protein S13



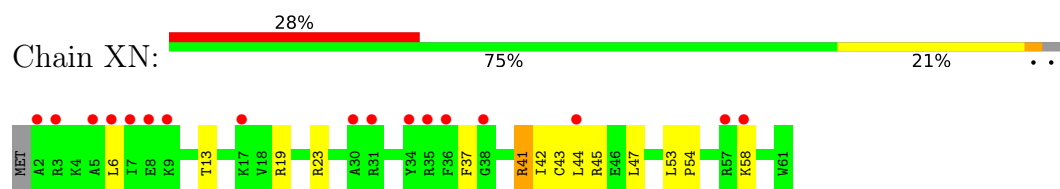
- Molecule 13: 30S ribosomal protein S13



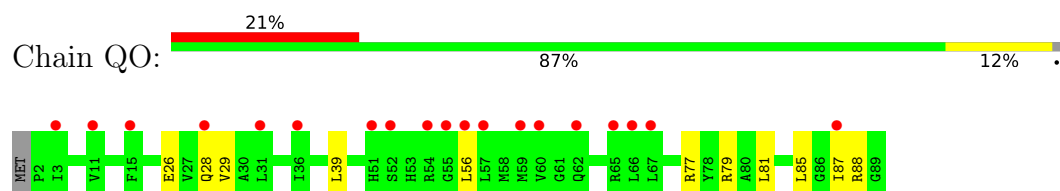
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

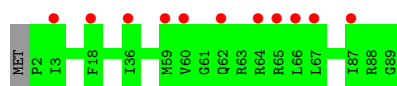


- Molecule 15: 30S ribosomal protein S15

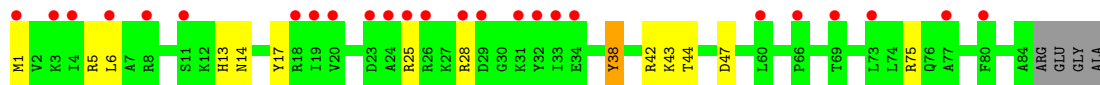
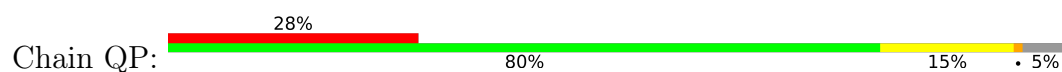


- Molecule 15: 30S ribosomal protein S15

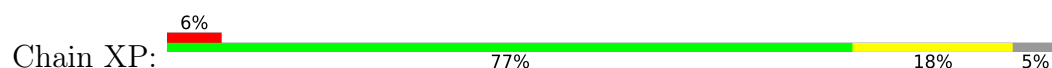




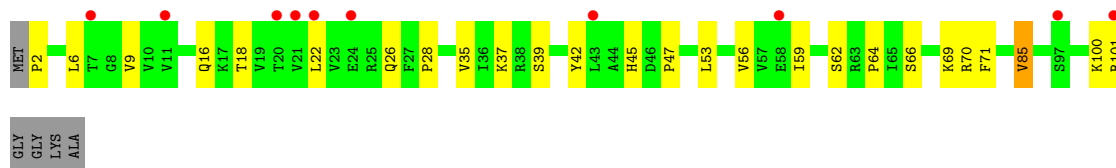
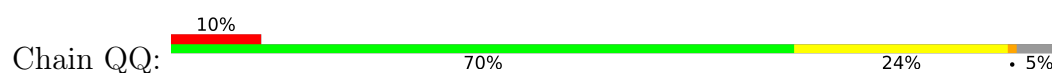
- Molecule 16: 30S ribosomal protein S16



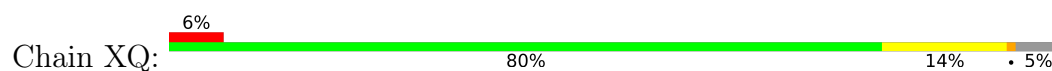
- Molecule 16: 30S ribosomal protein S16



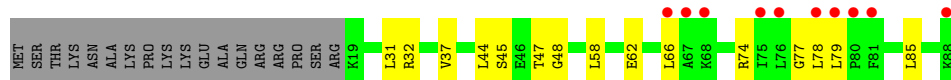
- Molecule 17: 30S ribosomal protein S17



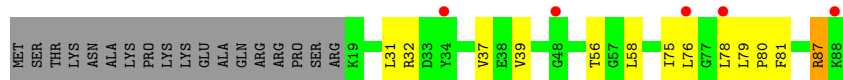
- Molecule 17: 30S ribosomal protein S17



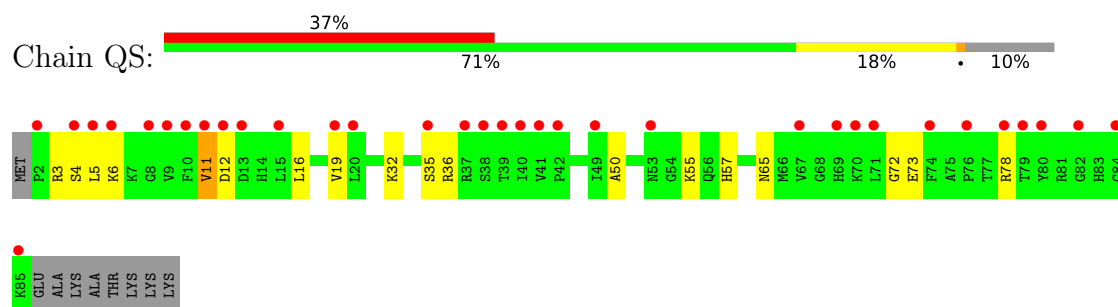
- Molecule 18: 30S ribosomal protein S18



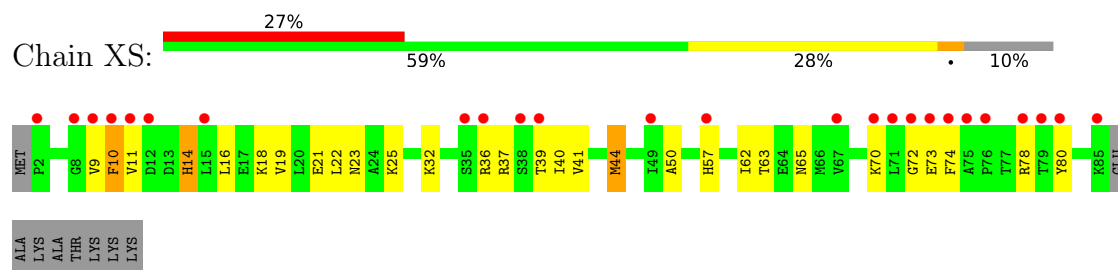
- Molecule 18: 30S ribosomal protein S18



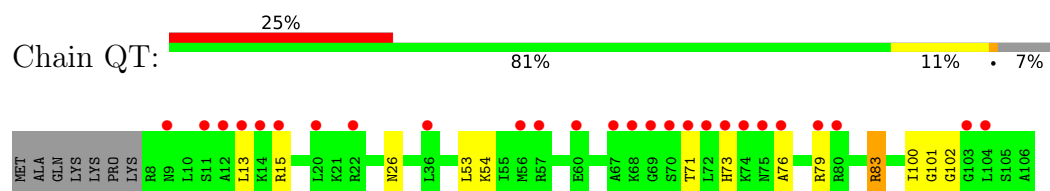
- Molecule 19: 30S ribosomal protein S19



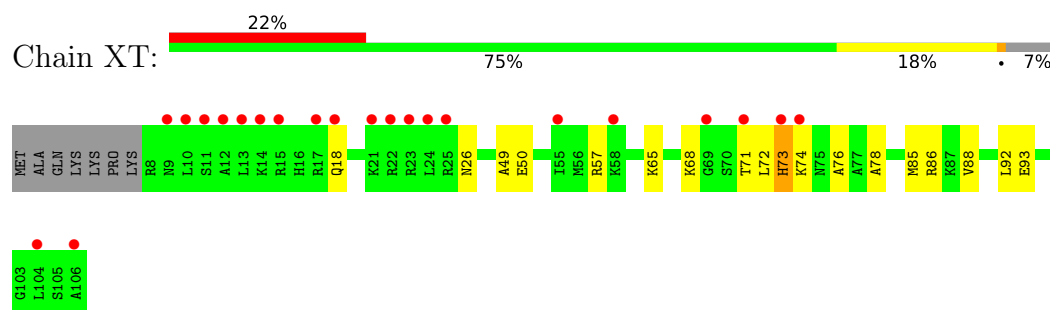
- Molecule 19: 30S ribosomal protein S19



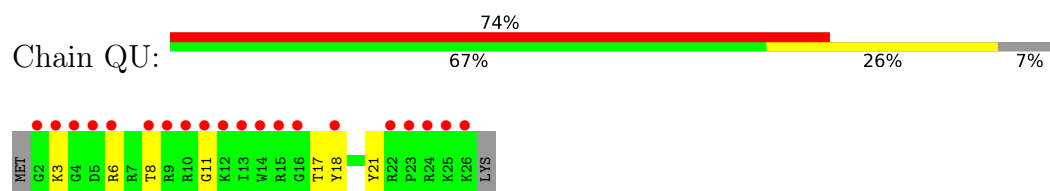
- Molecule 20: 30S ribosomal protein S20



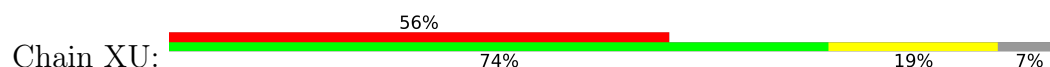
- Molecule 20: 30S ribosomal protein S20

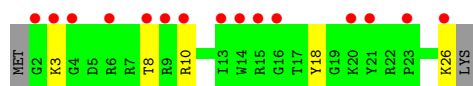


- Molecule 21: 30S ribosomal protein Thx

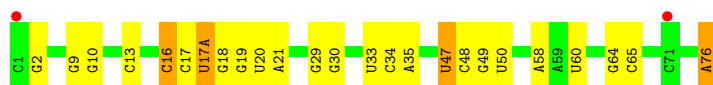


- Molecule 21: 30S ribosomal protein Thx

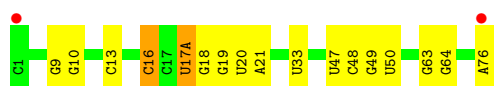
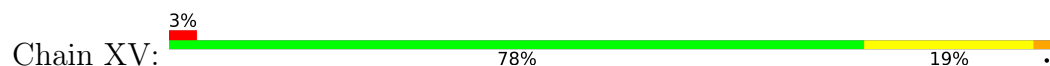




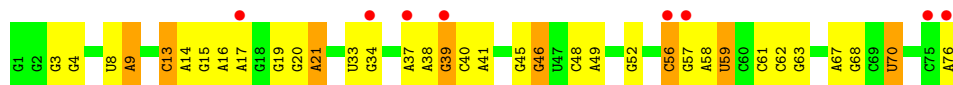
- Molecule 22: P-site tRNA^{fMet}



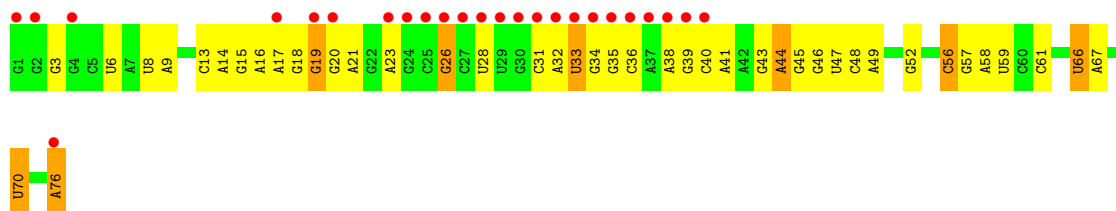
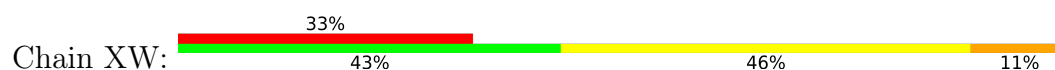
- Molecule 22: P-site tRNA^{fMet}



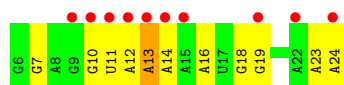
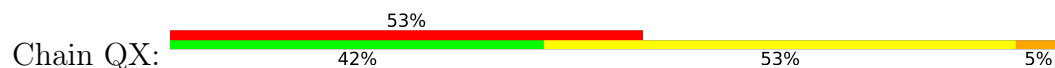
- Molecule 23: E-site tRNA^{Ala}(GGC)



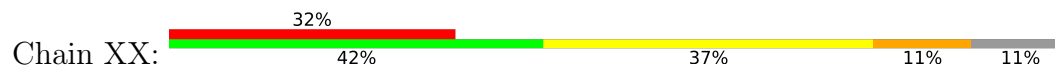
- Molecule 23: E-site tRNA^{Ala}(GGC)

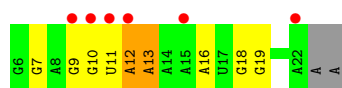


- Molecule 24: mRNA

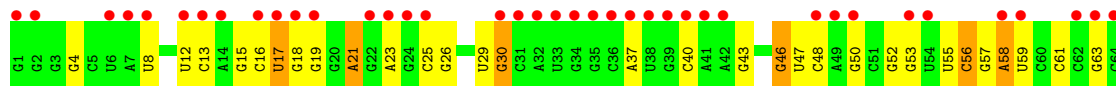


- Molecule 24: mRNA

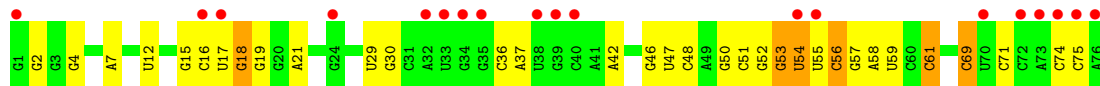




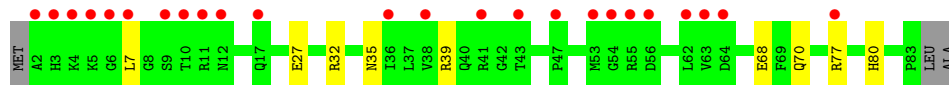
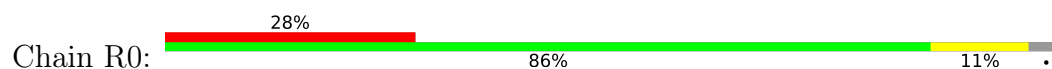
- Molecule 25: A-site tRNAAla(GGC)



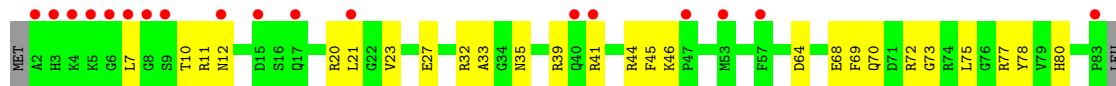
- Molecule 25: A-site tRNAAla(GGC)



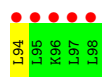
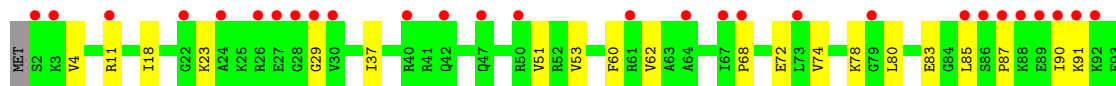
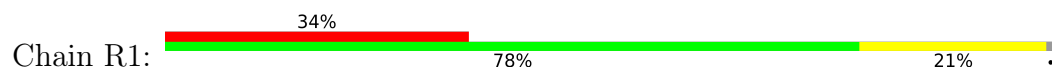
- Molecule 26: 50S ribosomal protein L27



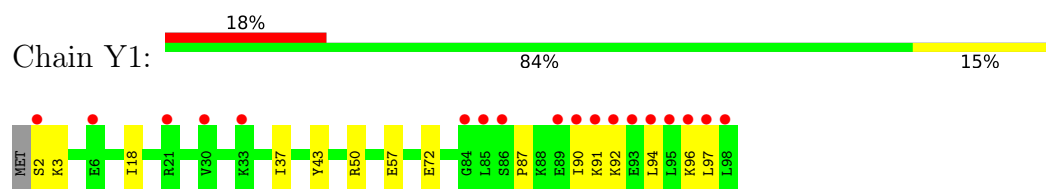
- Molecule 26: 50S ribosomal protein L27



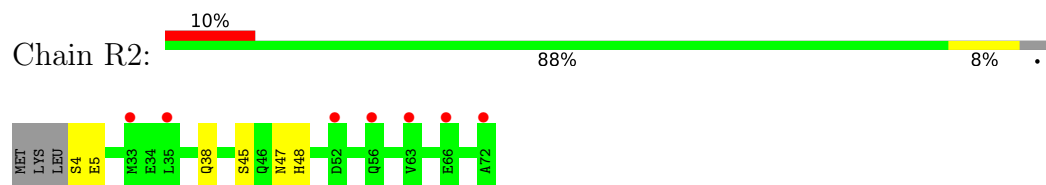
- Molecule 27: 50S ribosomal protein L28



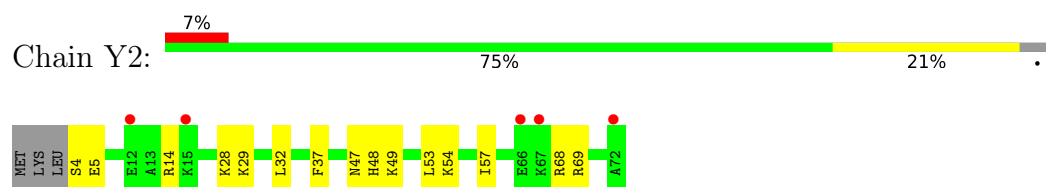
- Molecule 27: 50S ribosomal protein L28



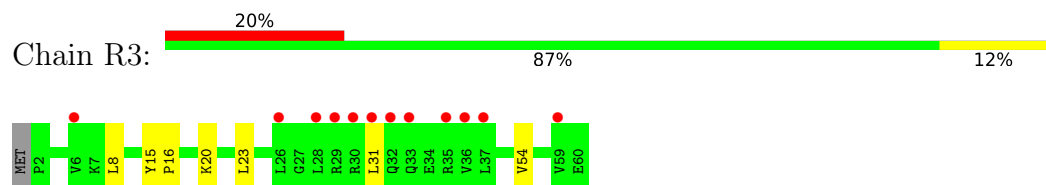
- Molecule 28: 50S ribosomal protein L29



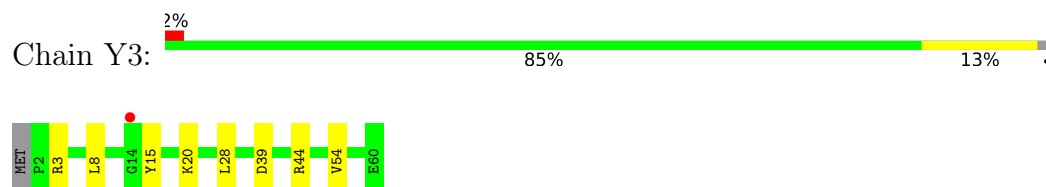
- Molecule 28: 50S ribosomal protein L29



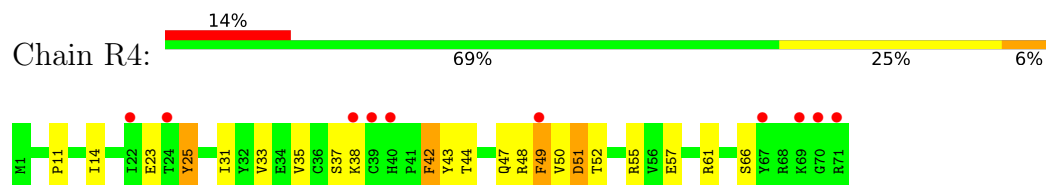
- Molecule 29: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L30

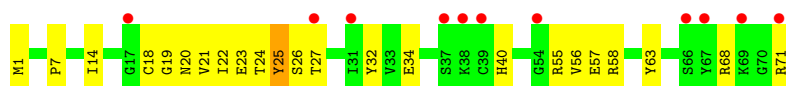


- Molecule 30: 50S ribosomal protein L31

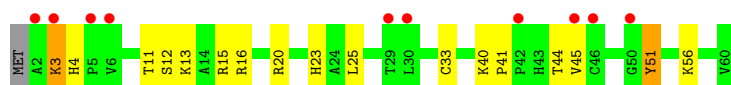
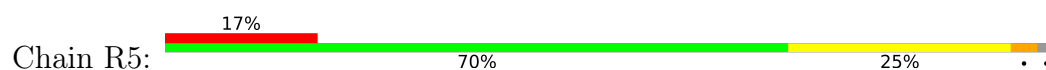


- Molecule 30: 50S ribosomal protein L31

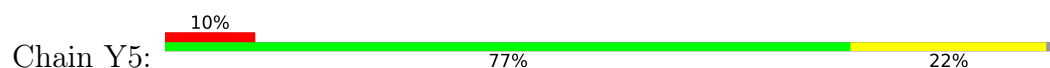




- Molecule 31: 50S ribosomal protein L32



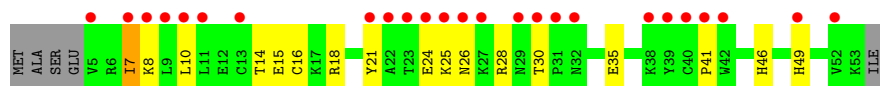
- Molecule 31: 50S ribosomal protein L32



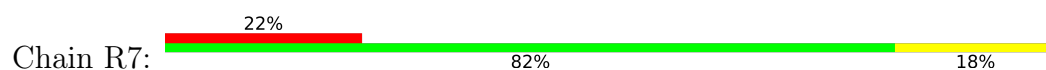
- Molecule 32: 50S ribosomal protein L33



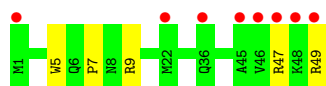
- Molecule 32: 50S ribosomal protein L33



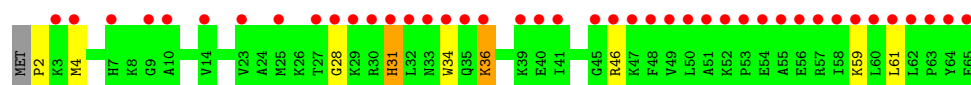
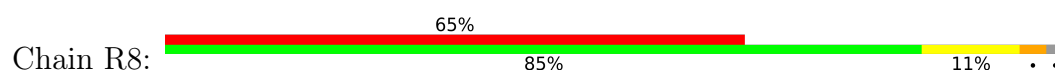
- Molecule 33: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L34



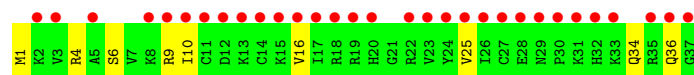
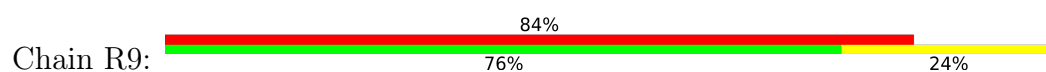
- Molecule 34: 50S ribosomal protein L35



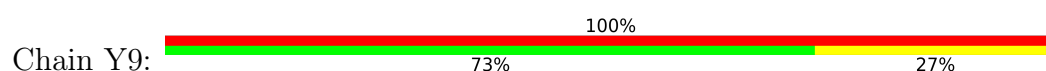
- Molecule 34: 50S ribosomal protein L35



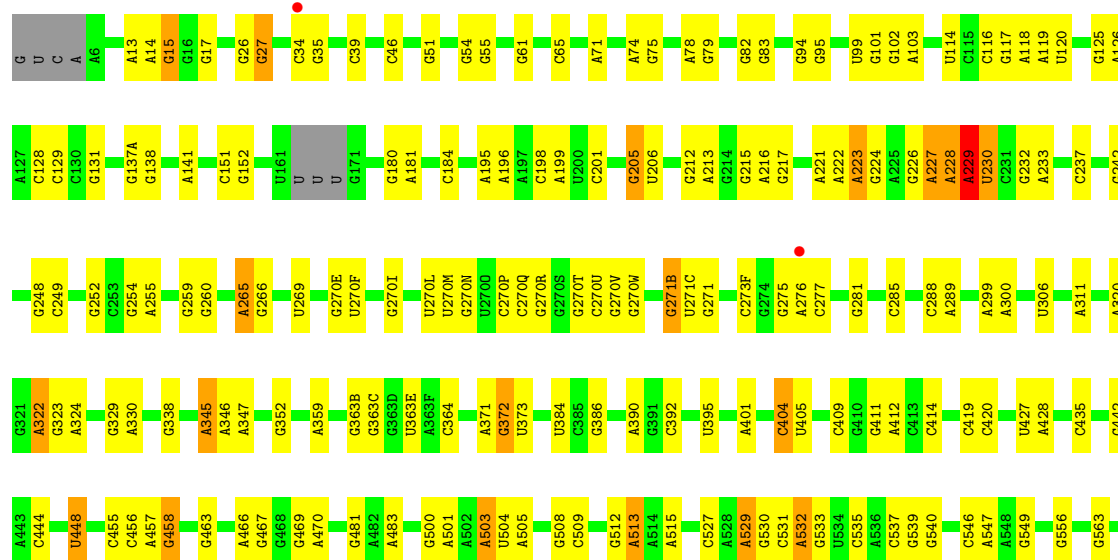
- Molecule 35: 50S ribosomal protein L36



- Molecule 35: 50S ribosomal protein L36

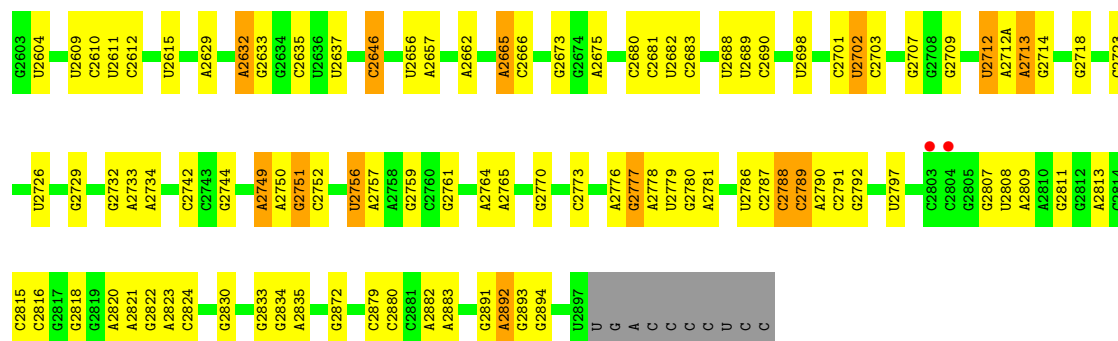


- Molecule 36: 23S rRNA



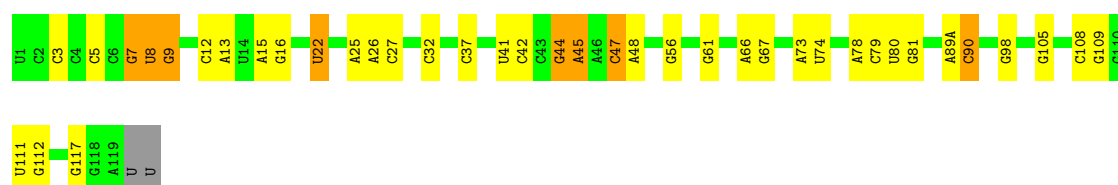
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G2131	G2010	A1698	G1568	C1458	C1327	A1177	A1084	A901	A781	A654	C574
U2132	U2011	A1569	A1569	G1458	G1328	C1178	A1085	G906	A782	G654A	A575
G2133	G2012	G1703	A1570	G1459	G1329	C1179	A1086	U907	A783	G	A578
A2134	A2013	G1858	U1576	A1460	U1329	G1184	G1087	A910	A784	G	G579
A2135	G1725	G1725	C1577	G1461	C1330	U1184	A1088	A910	G785	C	C580
C2136	G1728	G1728	U1578	C1462	U1341	A1189	G1091	C915	C790	C	C581
C2146	A1729	A1729	U1579	C1467	A1342	G1190	G1092	G915	C791	C	G582
G2147	C1870	C1870	A1580	G1467	G1343	G1191	G1093	A917	G792	C	G583
G2148	A1871	A1871	G1581	A1471	U1349	G1192	U1019	A918	A793	C	A586
A2154	G1878	G1878	A1586	U1479	U1352	G1195	A1095	G919	A800	A	A587
G2155	C1882	C1882	A1587	G1480	A1353	U1204	G1023	G932	A800	C	C587
G2156	G1756	G1756	U1595	U1482	A1365	A1205	U1023	G932	G805	C	C591
A2158	G1756	G1756	G1595	G1483	A1365	U1205	G1024	G938	G806	C	G592
C2164	A1762	A1762	C1598	U1486	G1368	G1206	U1026	A941	U907	C	G593
G2165	G1763	G1763	G1599	A1486	U1368	U1210	A1104	G942	C812	C	U697
C2166	G1764	G1764	C1600	A1490	A1378	U1211	U1105	G942	C812	C	G598
G2167	A1773	A1773	A1603	G1491	A1379	A1111	U1033	A946	A819	G654S	A603
G2168	G1779	G1779	C1493	G1492	A1384	C1217	G1036	A946	U827	U657	G604
A2169	U1779	U1779	C1493	A1494	A1384	A1220	G1039	G947	U828	C658	C605
G2170	A1780	A1780	A1608	U1497	G1385	G1236	G1043	G948	A829	C659	U606
A2170	C1781	C1781	A1609	U1497	G1388	A1237	C1044	A953	G830	G660	U607
C2171	A1936	A1936	A1610	G1500	U1391	G1237	A1045	A954	G831	C661	A608
A2172	A1937	A1937	C1617	C1506	U1391	A1238	A1046	C955	G832	G662	A609
G2173	A1938	A1938	A1618	A1507	U1394	G1252	A1047	U958	C946	G666	U614
A2176	C1788	C1788	G1622	A1508	A1395	A1253	G1123	A959	U847	U616	G615
G2187	A1791	A1791	G1622	A1510	C1403	A1254	C1124	C961	C856	G669	G617
C2188	C1795	C1795	C1636	A1511	C1407	U1255	A1049	U969	U858	G686	A621
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G2190	G1800	G1800	C1638	U1522	G1416	A1263	A1054	A973	U860	C693	U626
C2191	A1801	A1801	U1639	G1522	C1417	G1264	A1057	G974	G862	G702	A627
G2192	G1802	G1802	C1640	G1525	G1418	A1265	G1059	C974A	A863	G702	G629
A2198	A1811	A1811	C1648	G1525	A1419	G1270	U1061	A980	A966	A705	G630
A2199	G1815	G1815	G1651	G1525	U1420	C1271	U1065	A983	G869	G717	A631
G2210	A1816	A1816	A1652	G1533	G1421	A1272	U1066	A984	G880	A722	A633
C2211	G1817	G1817	G1653	G1534	U1422	U1273	G1068	C985	G881	G730	C634
U2213	A1818	A1818	A1654	U1535	G1423	U1286	A1069	G987	G882	A705	A637
G2215	U1818	U1818	C1662	A1536	G1423	A1287	A1070	A988	G883	G730	U637
C2216	A1819	A1819	G1667	C1537	A1427	U1288	G1071	G989	C884	A752	U639
A2225	U1820	U1820	A1668	G1539	C1428	G1286	G1072	C992	C885	C753	G642
G2233	G1824	G1824	G1674	G1542	G1441	U1300	U1073	C993	C886	G753	U642
U2233	A1825	A1825	C1675	A1543	G1442	A1301	G1074	C994	A887	U762	C645
G2238	C1827	C1827	A1544	A1545	A1444A	U1314	C1075	C995	C888	G763	C645
C2239	A1828	A1828	G1681	A1545	C1445	C1314	G1076	A996	C889	A764	A646
G2240	U1829	U1829	U1681	A1558	C1445	C1314	C1077	A996	A896	G765	G649
C2241	A1833	A1833	A1689	G1559	A1449	G1315	U1078	A1000	C897	G769	C650
U2244	G1834	G1834	C1694	C1565	G1449A	U1316	G1171	A1000	C898	G769	C651
G2245	U1835	U1835	G1695	A1566	U1454	A1317	C1079	G1003	A899	G776	C652





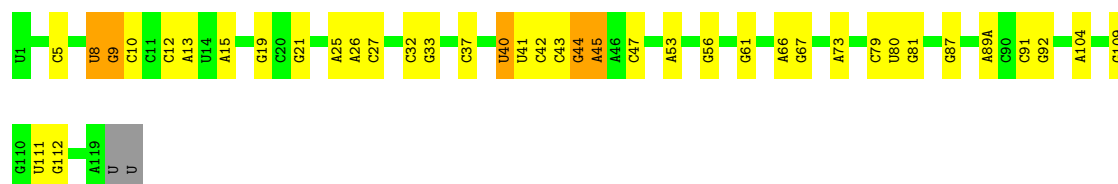
• Molecule 37: 5S rRNA

Chain RB: 66% 26% 7%



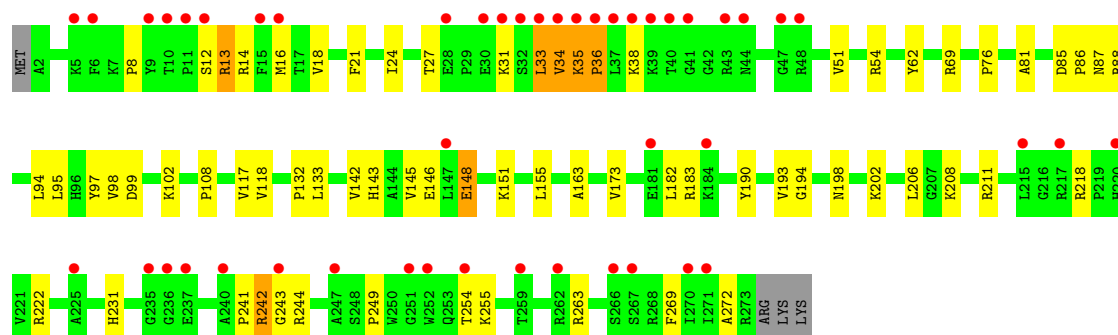
• Molecule 37: 5S rRNA

Chain YB: 66% 28%



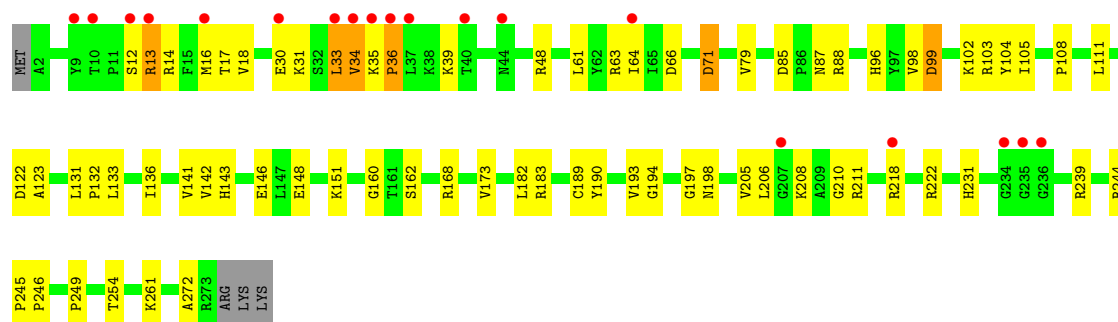
• Molecule 38: 50S ribosomal protein L2

Chain RD: 17% 74% 22%

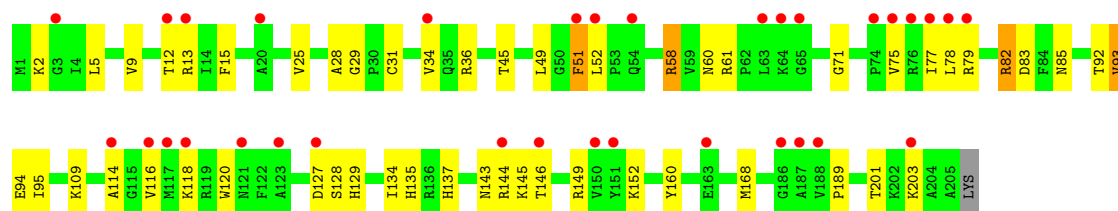
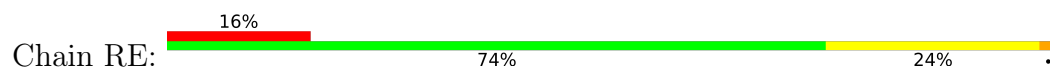


• Molecule 38: 50S ribosomal protein L2

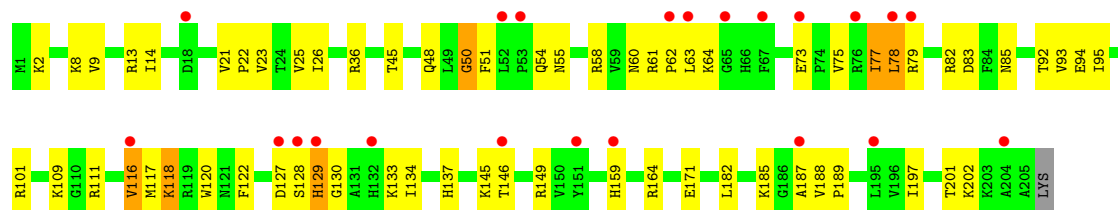
Chain YD: 7% 72% 24%



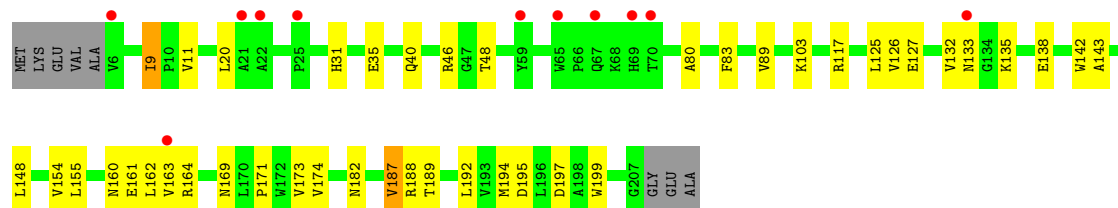
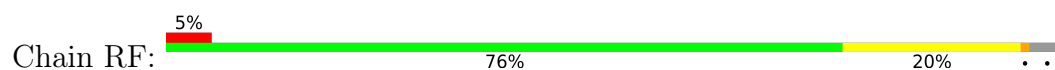
• Molecule 39: 50S ribosomal protein L3



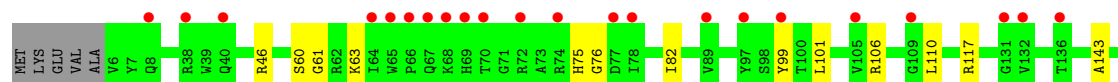
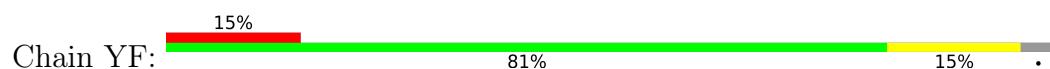
• Molecule 39: 50S ribosomal protein L3

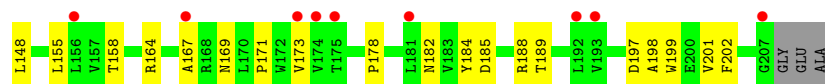


• Molecule 40: 50S ribosomal protein L4

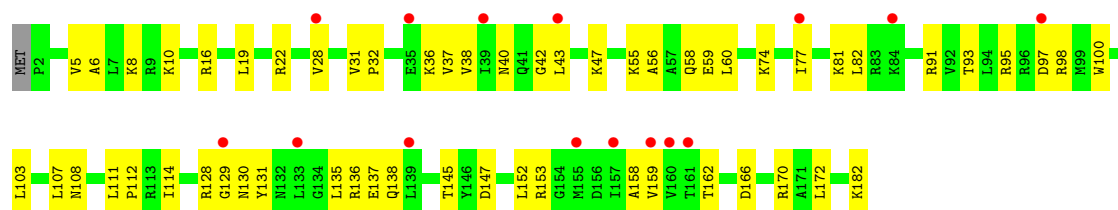


• Molecule 40: 50S ribosomal protein L4

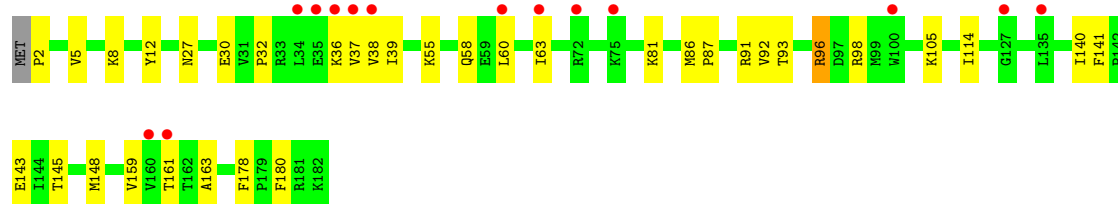
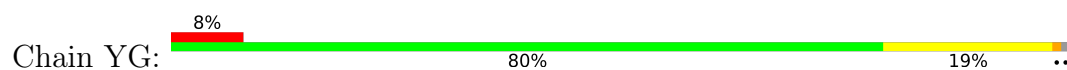




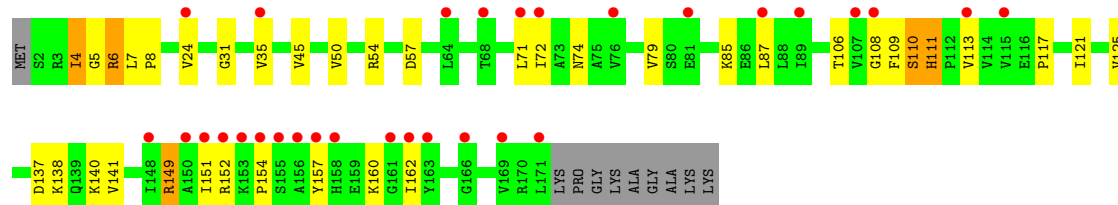
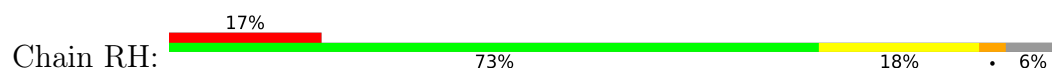
• Molecule 41: 50S ribosomal protein L5



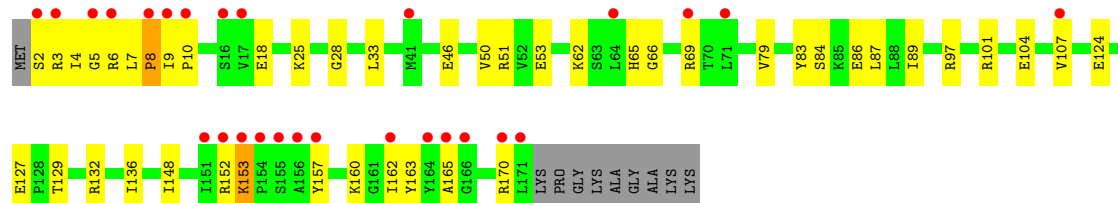
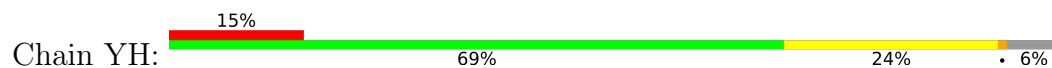
• Molecule 41: 50S ribosomal protein L5



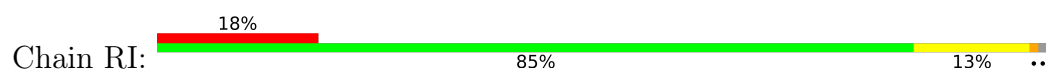
• Molecule 42: 50S ribosomal protein L6

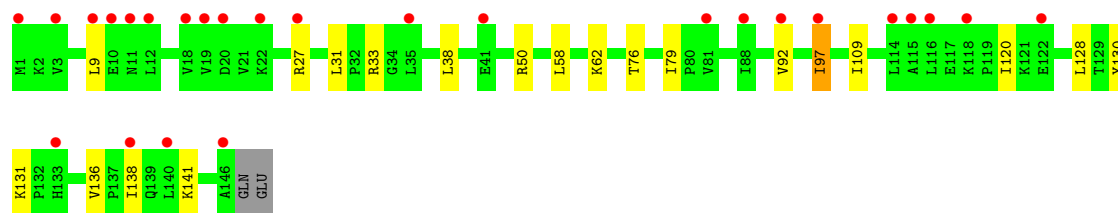


• Molecule 42: 50S ribosomal protein L6

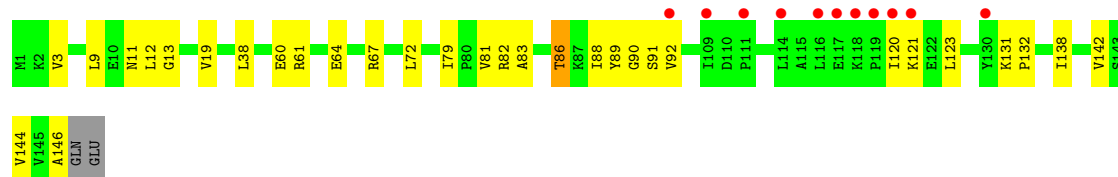
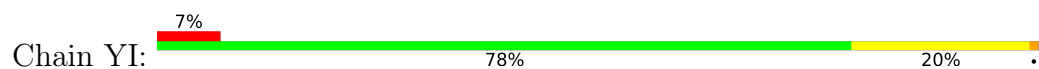


• Molecule 43: 50S ribosomal protein L9

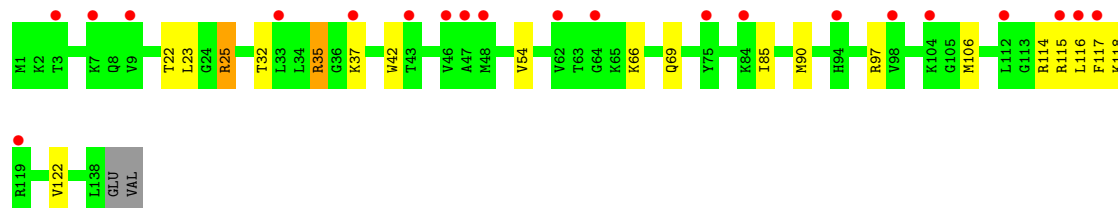
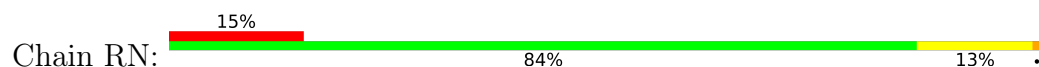




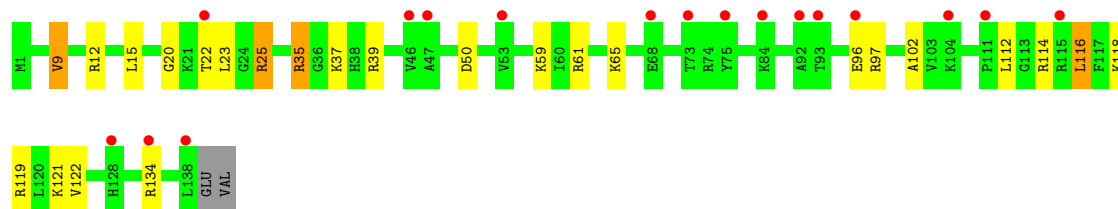
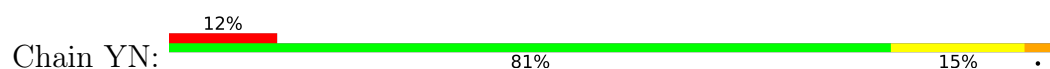
- Molecule 43: 50S ribosomal protein L9



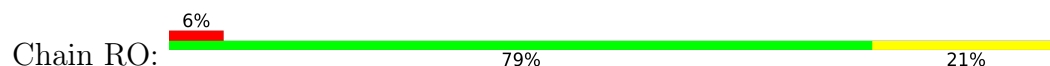
- Molecule 44: 50S ribosomal protein L13



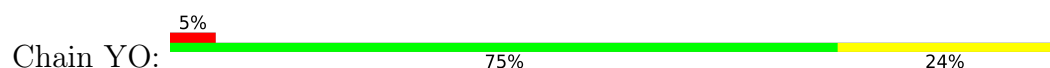
- Molecule 44: 50S ribosomal protein L13



- Molecule 45: 50S ribosomal protein L14

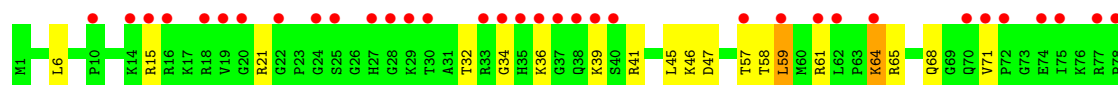
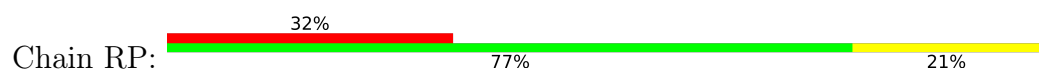


- Molecule 45: 50S ribosomal protein L14

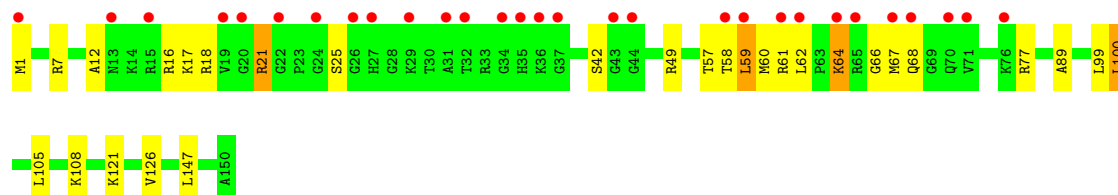
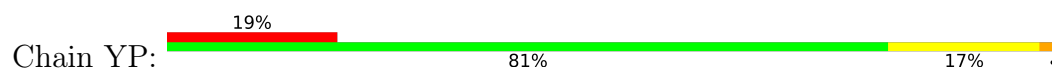




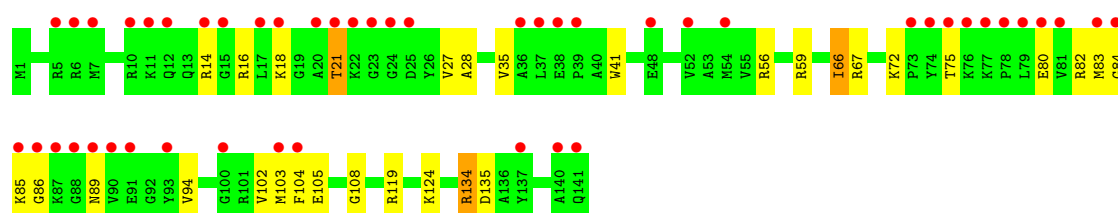
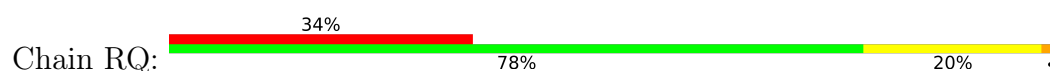
- Molecule 46: 50S ribosomal protein L15



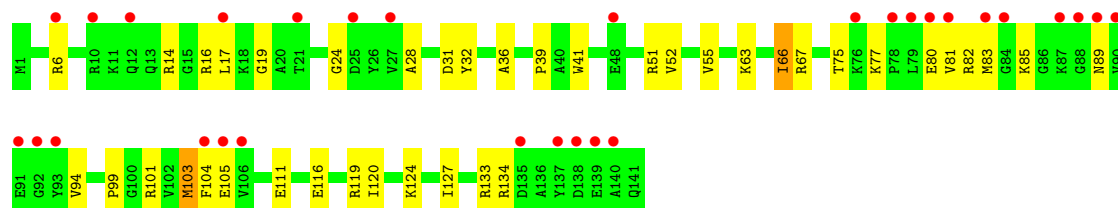
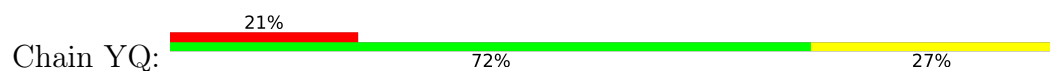
- Molecule 46: 50S ribosomal protein L15



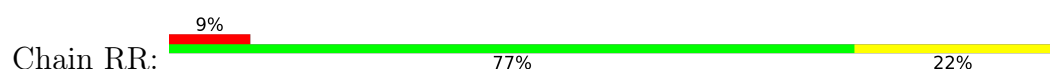
- Molecule 47: 50S ribosomal protein L16

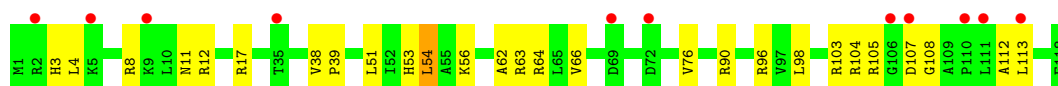


- Molecule 47: 50S ribosomal protein L16

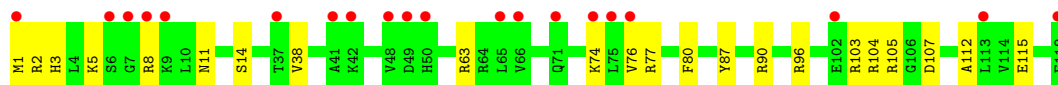
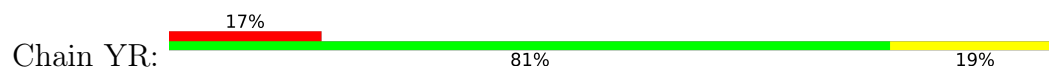


- Molecule 48: 50S ribosomal protein L17

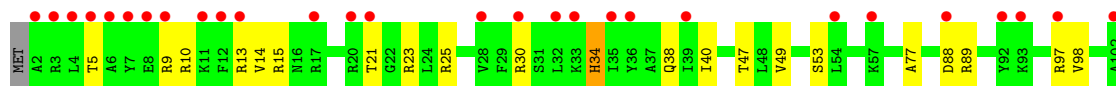
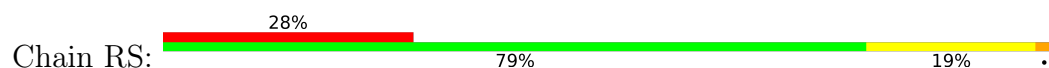




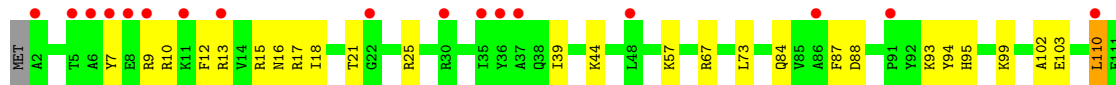
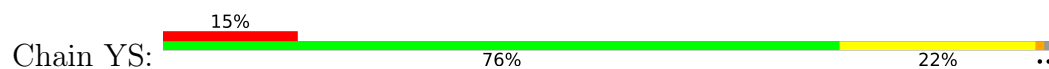
- Molecule 48: 50S ribosomal protein L17



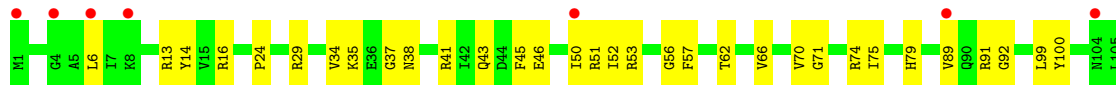
- Molecule 49: 50S ribosomal protein L18



- Molecule 49: 50S ribosomal protein L18

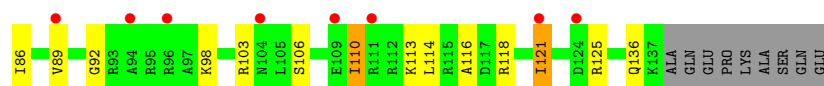


- Molecule 50: 50S ribosomal protein L19

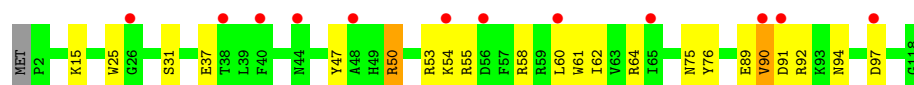
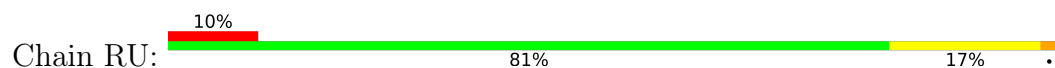


- Molecule 50: 50S ribosomal protein L19

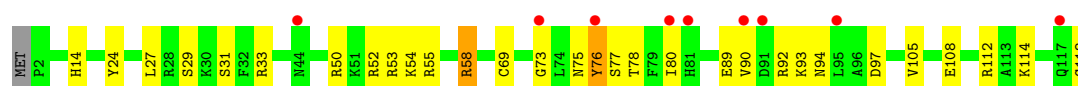
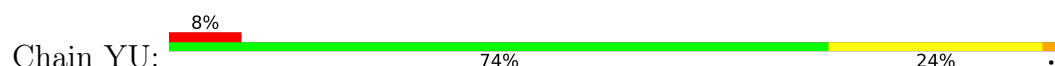




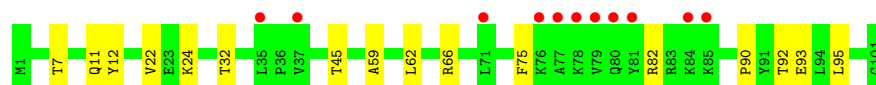
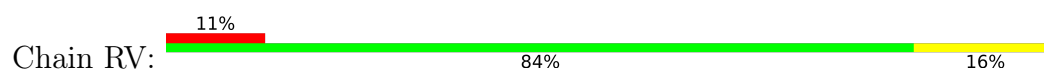
- Molecule 51: 50S ribosomal protein L20



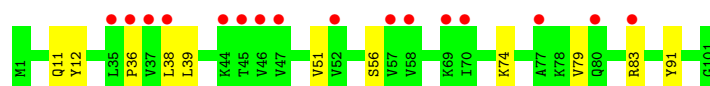
- Molecule 51: 50S ribosomal protein L20



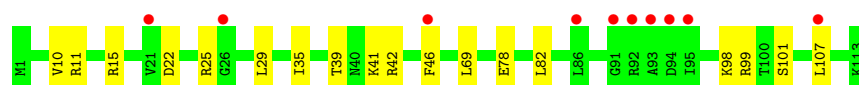
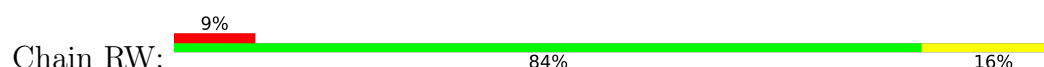
- Molecule 52: 50S ribosomal protein L21



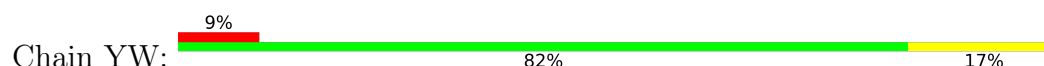
- Molecule 52: 50S ribosomal protein L21



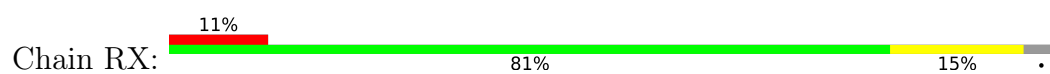
- Molecule 53: 50S ribosomal protein L22



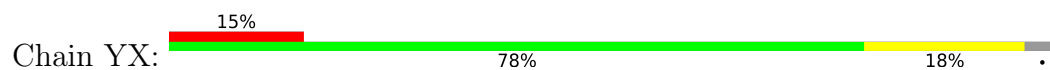
- Molecule 53: 50S ribosomal protein L22



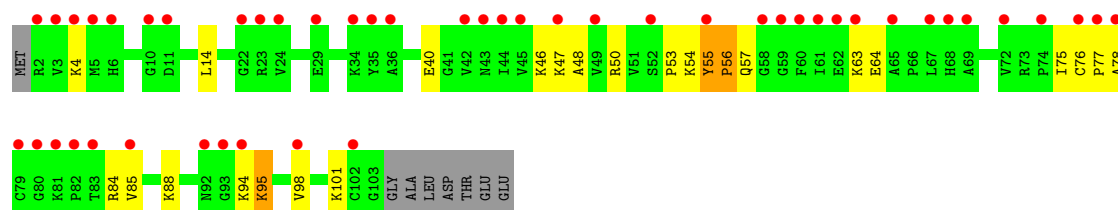
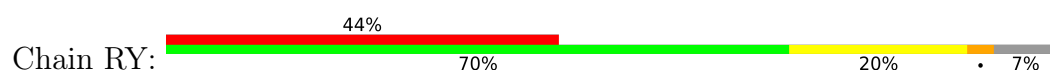
- Molecule 54: 50S ribosomal protein L23



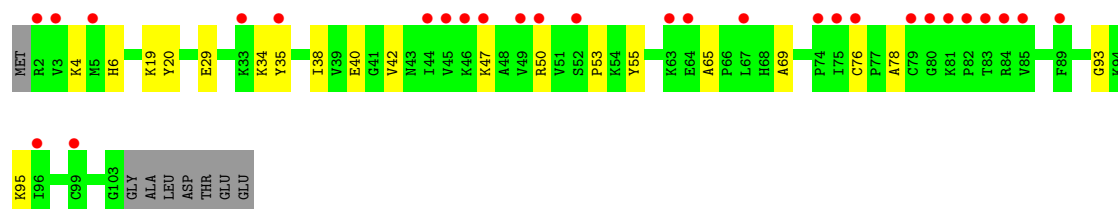
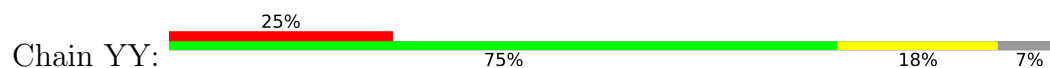
- Molecule 54: 50S ribosomal protein L23



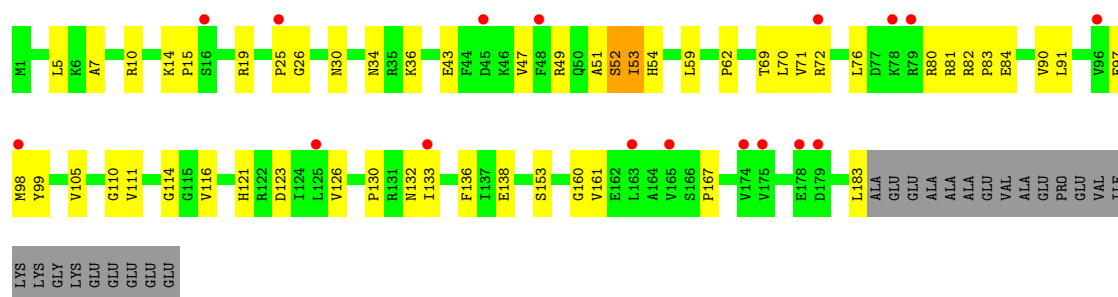
- Molecule 55: 50S ribosomal protein L24



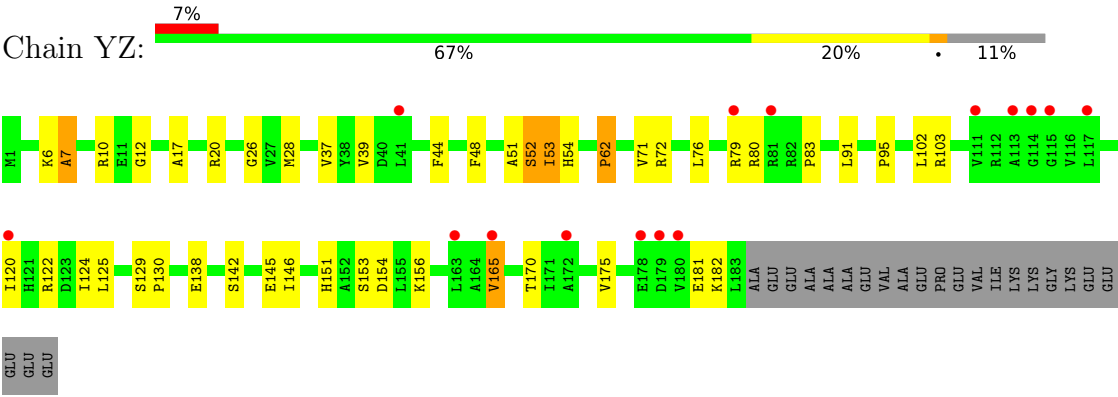
- Molecule 55: 50S ribosomal protein L24



- Molecule 56: 50S ribosomal protein L25



- Molecule 56: 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	211.00Å 453.48Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.20 49.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.99-3.20) 99.5 (49.99-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.237 , 0.270 (Not available) , 0.268	Depositor DCC
R_{free} test set	45370 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298371	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: PAR, ZN, SF4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.28	0/36098	0.44	14/56341 (0.0%)
1	XA	0.29	0/36101	0.43	10/56346 (0.0%)
2	QB	0.35	0/1959	0.94	12/2642 (0.5%)
2	XB	0.29	0/1959	0.89	1/2642 (0.0%)
3	QC	0.35	1/1629 (0.1%)	0.91	4/2195 (0.2%)
3	XC	0.27	0/1629	0.83	0/2195
4	QD	0.37	0/1704	0.85	2/2284 (0.1%)
4	XD	0.35	0/1704	0.85	3/2284 (0.1%)
5	QE	0.29	0/1171	0.79	1/1576 (0.1%)
5	XE	0.33	0/1171	0.90	5/1576 (0.3%)
6	QF	0.32	0/856	0.91	5/1154 (0.4%)
6	XF	0.31	0/856	0.83	1/1154 (0.1%)
7	QG	0.28	0/1276	0.82	2/1709 (0.1%)
7	XG	0.28	0/1276	0.82	0/1709
8	QH	0.29	0/1136	0.84	3/1527 (0.2%)
8	XH	0.28	0/1136	0.81	2/1527 (0.1%)
9	QI	0.31	0/1029	0.97	4/1379 (0.3%)
9	XI	0.32	0/1029	1.00	5/1379 (0.4%)
10	QJ	0.30	0/814	0.86	1/1095 (0.1%)
10	XJ	0.29	0/814	0.84	1/1095 (0.1%)
11	QK	0.32	0/900	0.76	0/1213
11	XK	0.31	0/900	0.83	2/1213 (0.2%)
12	QL	0.35	0/991	0.99	6/1327 (0.5%)
12	XL	0.36	0/991	1.00	10/1327 (0.8%)
13	QM	0.36	0/974	1.18	10/1303 (0.8%)
13	XM	0.31	0/974	1.04	6/1303 (0.5%)
14	QN	0.37	0/501	0.99	3/664 (0.5%)
14	XN	0.43	0/501	1.13	6/664 (0.9%)
15	QO	0.29	0/745	0.76	0/992
15	XO	0.29	0/745	0.74	0/992
16	QP	0.37	0/721	0.94	1/970 (0.1%)
16	XP	0.33	0/721	0.96	3/970 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.33	0/847	0.84	2/1131 (0.2%)
17	XQ	0.27	0/847	0.79	1/1131 (0.1%)
18	QR	0.27	0/579	0.80	0/768
18	XR	0.32	0/579	0.89	4/768 (0.5%)
19	QS	0.28	0/689	0.95	2/926 (0.2%)
19	XS	0.52	1/689 (0.1%)	1.22	10/926 (1.1%)
20	QT	0.28	0/765	0.93	3/1007 (0.3%)
20	XT	0.29	0/765	1.03	6/1007 (0.6%)
21	QU	0.38	0/221	0.74	1/288 (0.3%)
21	XU	0.37	0/221	0.84	1/288 (0.3%)
22	QV	0.26	0/1832	0.37	0/2855
22	XV	0.28	0/1832	0.35	0/2855
23	QW	0.21	0/1826	0.39	0/2845
23	XW	0.22	0/1826	0.46	0/2845
24	QX	0.24	0/471	0.48	0/734
24	XX	0.27	0/421	0.51	0/656
25	QY	0.20	0/1791	0.38	0/2791
25	XY	0.20	0/1816	0.38	0/2830
26	R0	0.29	0/657	0.77	0/874
26	Y0	0.38	0/657	0.82	1/874 (0.1%)
27	R1	0.36	0/770	0.95	5/1022 (0.5%)
27	Y1	0.46	0/770	0.92	3/1022 (0.3%)
28	R2	0.33	0/583	0.92	0/771
28	Y2	0.35	0/583	1.07	5/771 (0.6%)
29	R3	0.25	0/474	0.77	0/635
29	Y3	0.30	0/474	0.82	1/635 (0.2%)
30	R4	0.46	0/594	1.27	9/795 (1.1%)
30	Y4	0.41	0/594	1.21	7/795 (0.9%)
31	R5	0.36	0/473	1.19	3/639 (0.5%)
31	Y5	0.48	0/473	1.00	2/639 (0.3%)
32	R6	0.78	0/431	1.63	9/575 (1.6%)
32	Y6	0.43	0/431	1.24	6/575 (1.0%)
33	R7	0.43	0/438	0.85	1/575 (0.2%)
33	Y7	0.36	0/438	0.86	0/575
34	R8	0.41	0/525	1.03	3/691 (0.4%)
34	Y8	0.43	0/525	0.99	5/691 (0.7%)
35	R9	0.25	0/310	0.90	0/407
35	Y9	0.24	0/310	0.72	0/407
36	RA	0.31	0/69521	0.43	17/108529 (0.0%)
36	YA	0.33	0/69543	0.43	11/108563 (0.0%)
37	RB	0.27	0/2878	0.39	0/4490
37	YB	0.28	0/2878	0.41	0/4490
38	RD	0.49	2/2165 (0.1%)	1.00	13/2919 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YD	0.45	0/2165	0.97	7/2919 (0.2%)
39	RE	0.55	3/1601 (0.2%)	1.09	11/2160 (0.5%)
39	YE	0.51	0/1601	1.18	20/2160 (0.9%)
40	RF	0.36	0/1620	0.91	8/2194 (0.4%)
40	YF	0.38	0/1620	0.92	4/2194 (0.2%)
41	RG	0.39	0/1499	0.99	5/2016 (0.2%)
41	YG	0.33	0/1499	0.88	3/2016 (0.1%)
42	RH	0.33	0/1332	1.08	12/1802 (0.7%)
42	YH	0.42	0/1332	1.07	9/1802 (0.5%)
43	RI	0.50	0/1151	1.10	9/1558 (0.6%)
43	YI	0.47	0/1151	1.14	10/1558 (0.6%)
44	RN	0.32	0/1131	0.96	8/1525 (0.5%)
44	YN	0.39	0/1131	1.04	8/1525 (0.5%)
45	RO	0.38	0/943	0.83	0/1269
45	YO	0.38	0/943	0.88	2/1269 (0.2%)
46	RP	0.39	0/1162	1.01	4/1544 (0.3%)
46	YP	0.42	0/1162	1.06	8/1544 (0.5%)
47	RQ	0.38	0/1143	1.09	8/1527 (0.5%)
47	YQ	0.39	0/1143	1.09	6/1527 (0.4%)
48	RR	0.33	0/982	0.92	3/1312 (0.2%)
48	YR	0.33	0/982	0.94	4/1312 (0.3%)
49	RS	0.43	0/892	1.11	9/1187 (0.8%)
49	YS	0.38	0/892	1.11	8/1187 (0.7%)
50	RT	0.36	0/1155	1.03	8/1542 (0.5%)
50	YT	0.33	0/1155	1.03	10/1542 (0.6%)
51	RU	0.35	0/982	1.01	7/1306 (0.5%)
51	YU	0.40	0/982	1.01	5/1306 (0.4%)
52	RV	0.33	0/790	0.93	2/1057 (0.2%)
52	YV	0.38	0/790	0.99	2/1057 (0.2%)
53	RW	0.37	0/911	0.87	1/1220 (0.1%)
53	YW	0.32	0/911	0.83	3/1220 (0.2%)
54	RX	0.33	0/739	0.88	1/993 (0.1%)
54	YX	0.39	0/739	0.88	2/993 (0.2%)
55	RY	0.41	0/798	1.19	11/1064 (1.0%)
55	YY	0.41	0/798	1.16	4/1064 (0.4%)
56	RZ	0.33	0/1493	1.01	11/2026 (0.5%)
56	YZ	0.36	0/1493	1.09	13/2026 (0.6%)
All	All	0.33	7/323336 (0.0%)	0.62	500/483880 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	RE	58	ARG	CD-NE	7.70	1.57	1.46
39	RE	58	ARG	CZ-NH1	6.52	1.41	1.32
39	RE	58	ARG	NE-CZ	6.47	1.40	1.33
38	RD	35	LYS	C-N	6.28	1.48	1.33
3	QC	160	ALA	N-CA	-5.99	1.38	1.45

The worst 5 of 500 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	YH	9	ILE	N-CA-C	12.68	120.81	109.02
1	QA	1317	C	O5'-P-OP1	-11.77	72.70	108.00
38	RD	242	ARG	CG-CD-NE	10.98	136.16	112.00
38	YD	13	ARG	N-CA-C	-10.86	100.14	113.50
1	XA	367	U	C2'-C3'-O3'	10.46	125.19	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16273	214	0
1	XA	32249	0	16278	207	0
2	QB	1924	0	1975	28	0
2	XB	1924	0	1975	33	0
3	QC	1605	0	1668	18	0
3	XC	1605	0	1668	25	0
4	QD	1674	0	1718	27	0
4	XD	1674	0	1718	30	0
5	QE	1155	0	1213	19	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	17	0
8	QH	1116	0	1177	21	0
8	XH	1116	0	1177	23	0
9	QI	1010	0	1037	26	0
9	XI	1010	0	1037	23	0
10	QJ	801	0	849	12	0
10	XJ	801	0	848	16	0
11	QK	885	0	904	11	0
11	XK	885	0	904	11	0
12	QL	975	0	1062	18	0
12	XL	975	0	1062	21	0
13	QM	964	0	1034	28	0
13	XM	964	0	1034	21	0
14	QN	492	0	533	18	0
14	XN	492	0	530	8	0
15	QO	734	0	771	7	0
15	XO	734	0	771	0	0
16	QP	705	0	725	11	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	11	0
18	QR	574	0	644	11	0
18	XR	574	0	644	8	0
19	QS	674	0	699	15	0
19	XS	674	0	699	21	0
20	QT	763	0	861	10	0
20	XT	763	0	861	12	0
21	QU	217	0	234	6	0
21	XU	217	0	234	4	0
22	QV	1640	0	837	10	0
22	XV	1640	0	837	6	0
23	QW	1632	0	824	12	0
23	XW	1632	0	824	10	0
24	QX	418	0	207	4	0
24	XX	374	0	186	2	0
25	QY	1603	0	811	12	0
25	XY	1625	0	822	7	0
26	R0	648	0	672	6	0
26	Y0	648	0	672	21	0
27	R1	763	0	848	11	0
27	Y1	763	0	848	7	0
28	R2	581	0	629	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Y2	581	0	628	7	0
29	R3	469	0	518	5	0
29	Y3	469	0	518	4	0
30	R4	581	0	577	23	0
30	Y4	581	0	577	13	0
31	R5	459	0	480	12	0
31	Y5	459	0	480	9	0
32	R6	424	0	450	16	0
32	Y6	424	0	450	11	0
33	R7	430	0	480	7	0
33	Y7	430	0	480	5	0
34	R8	517	0	582	7	0
34	Y8	517	0	582	13	0
35	R9	307	0	338	6	0
35	Y9	307	0	338	8	0
36	RA	62071	0	31280	324	0
36	YA	62091	0	31292	307	0
37	RB	2573	0	1306	19	0
37	YB	2573	0	1306	23	0
38	RD	2115	0	2195	54	0
38	YD	2115	0	2195	63	0
39	RE	1568	0	1634	36	0
39	YE	1568	0	1634	40	0
40	RF	1585	0	1632	27	0
40	YF	1585	0	1632	18	0
41	RG	1474	0	1535	40	0
41	YG	1474	0	1535	21	0
42	RH	1307	0	1382	26	0
42	YH	1307	0	1382	38	0
43	RI	1136	0	1223	16	0
43	YI	1136	0	1223	13	0
44	RN	1104	0	1180	9	0
44	YN	1104	0	1180	13	0
45	RO	933	0	996	22	0
45	YO	933	0	996	21	0
46	RP	1145	0	1226	24	0
46	YP	1145	0	1228	23	0
47	RQ	1122	0	1179	24	0
47	YQ	1122	0	1179	30	0
48	RR	968	0	1033	21	0
48	YR	968	0	1033	13	0
49	RS	882	0	943	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	YS	882	0	943	16	0
50	RT	1141	0	1202	24	0
50	YT	1141	0	1202	25	0
51	RU	964	0	1022	17	0
51	YU	964	0	1022	26	0
52	RV	779	0	852	9	0
52	YV	779	0	852	7	0
53	RW	900	0	964	11	0
53	YW	900	0	964	13	0
54	RX	725	0	777	11	0
54	YX	725	0	778	14	0
55	RY	785	0	878	13	0
55	YY	785	0	878	11	0
56	RZ	1461	0	1493	31	0
56	YZ	1461	0	1493	24	0
57	QA	85	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	2	0	0	0	0
57	QV	4	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	321	0	0	0	0
57	RB	4	0	0	0	0
57	RD	1	0	0	0	0
57	RE	3	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RU	1	0	0	0	0
57	RX	1	0	0	0	0
57	XA	94	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y2	1	0	0	0	0
57	Y5	2	0	0	0	0
57	Y7	2	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	379	0	0	0	0
57	YB	8	0	0	0	0
57	YD	3	0	0	0	0
57	YE	3	0	0	0	0
57	YH	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	2	0	0	0	0
57	YU	2	0	0	0	0
57	YV	1	0	0	0	0
57	YX	3	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	XN	1	0	0	0	0
61	QA	1	0	0	0	0
61	QX	1	0	0	0	0
All	All	298371	0	201333	2272	0

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 5.

The worst 5 of 2272 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)
36:YA:1112:G:H5'	42:YH:3:ARG:HD3	1.20	1.19
36:YA:1112:G:H5'	42:YH:3:ARG:CD	1.79	1.12
43:RI:92:VAL:CG1	43:RI:120:ILE:HG23	1.82	1.09
42:RH:6:ARG:HD3	42:RH:6:ARG:H	1.19	1.07
38:YD:33:LEU:H	38:YD:33:LEU:HD23	1.19	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	205 (100%)	0	100	100
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	89/99 (90%)	89 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	58/92 (63%)	58 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100
12	QL	104/108 (96%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	97 (100%)	0	100	100
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	R0	65/67 (97%)	65 (100%)	0	100	100
26	Y0	65/67 (97%)	65 (100%)	0	100	100
27	R1	68/83 (82%)	68 (100%)	0	100	100
27	Y1	82/83 (99%)	82 (100%)	0	100	100
28	Y2	64/67 (96%)	64 (100%)	0	100	100
29	Y3	51/52 (98%)	51 (100%)	0	100	100
30	Y4	63/63 (100%)	63 (100%)	0	100	100
31	Y5	51/52 (98%)	51 (100%)	0	100	100
32	R6	46/52 (88%)	46 (100%)	0	100	100
32	Y6	48/52 (92%)	48 (100%)	0	100	100
33	R7	42/42 (100%)	42 (100%)	0	100	100
33	Y7	42/42 (100%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	R8	54/55 (98%)	54 (100%)	0	100	100
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	34 (100%)	0	100	100
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	214 (100%)	0	100	100
38	YD	214/218 (98%)	211 (99%)	3 (1%)	59	77
39	RE	165/166 (99%)	165 (100%)	0	100	100
39	YE	165/166 (99%)	165 (100%)	0	100	100
40	RF	161/166 (97%)	161 (100%)	0	100	100
40	YF	161/166 (97%)	161 (100%)	0	100	100
41	RG	155/156 (99%)	155 (100%)	0	100	100
41	YG	155/156 (99%)	155 (100%)	0	100	100
42	RH	142/148 (96%)	141 (99%)	1 (1%)	76	83
42	YH	142/148 (96%)	140 (99%)	2 (1%)	59	77
43	RI	122/124 (98%)	122 (100%)	0	100	100
43	YI	122/124 (98%)	122 (100%)	0	100	100
44	RN	117/119 (98%)	117 (100%)	0	100	100
44	YN	117/119 (98%)	117 (100%)	0	100	100
45	RO	100/100 (100%)	100 (100%)	0	100	100
45	YO	100/100 (100%)	100 (100%)	0	100	100
46	RP	116/116 (100%)	116 (100%)	0	100	100
46	YP	116/116 (100%)	116 (100%)	0	100	100
47	RQ	111/111 (100%)	111 (100%)	0	100	100
47	YQ	111/111 (100%)	111 (100%)	0	100	100
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100
49	RS	87/88 (99%)	87 (100%)	0	100	100
49	YS	87/88 (99%)	87 (100%)	0	100	100
50	RT	120/127 (94%)	120 (100%)	0	100	100
50	YT	120/127 (94%)	120 (100%)	0	100	100
51	RU	93/94 (99%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	YU	93/94 (99%)	93 (100%)	0	100	100
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	82 (100%)	0	100	100
53	RW	92/92 (100%)	92 (100%)	0	100	100
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	74 (100%)	0	100	100
54	YX	74/78 (95%)	74 (100%)	0	100	100
55	RY	85/91 (93%)	85 (100%)	0	100	100
55	YY	85/91 (93%)	85 (100%)	0	100	100
56	RZ	162/179 (90%)	162 (100%)	0	100	100
56	YZ	162/179 (90%)	162 (100%)	0	100	100
All	All	9403/9830 (96%)	9397 (100%)	6 (0%)	88	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	YD	36	PRO
42	YH	4	ILE
42	YH	8	PRO
38	YD	33	LEU
42	RH	4	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
20	XT	42	GLN
40	YF	40	GLN
20	XT	90	GLN
32	Y6	26	ASN
46	YP	70	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	275 (18%)	34 (2%)
1	XA	1498/1522 (98%)	287 (19%)	30 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	24 (32%)	1 (1%)
23	XW	75/76 (98%)	38 (50%)	2 (2%)
24	QX	18/19 (94%)	8 (44%)	1 (5%)
24	XX	16/19 (84%)	7 (43%)	1 (6%)
25	QY	74/76 (97%)	28 (37%)	0
25	XY	75/76 (98%)	31 (41%)	0
36	RA	2879/2915 (98%)	609 (21%)	47 (1%)
36	YA	2880/2915 (98%)	579 (20%)	44 (1%)
37	RB	119/122 (97%)	24 (20%)	1 (0%)
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1956 (20%)	162 (1%)

5 of 1956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	XW	58	A
36	YA	1558	A
36	YA	222	A
36	YA	827	U
36	YA	1980	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 955 ligands modelled in this entry, 951 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	XA	1679	-	44,45,45	0.65	0	63,67,67	1.43	6 (9%)
59	SF4	QD	501	4	0,12,12	-	-	-		
58	PAR	QA	1667	-	44,45,45	0.69	0	63,67,67	1.18	5 (7%)
59	SF4	XD	501	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
58	PAR	XA	1679	-	-	6/18/94/94	0/4/4/4
59	SF4	QD	501	4	-	-	0/6/5/5
58	PAR	QA	1667	-	-	4/18/94/94	0/4/4/4
59	SF4	XD	501	4	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1679	PAR	C14-O33-C33	-4.31	107.75	117.98
58	QA	1667	PAR	C13-O52-C52	-3.77	109.04	117.98
58	XA	1679	PAR	O33-C14-C24	3.64	114.03	108.08
58	XA	1679	PAR	C13-O52-C52	-3.64	109.35	117.98
58	XA	1679	PAR	C44-C34-C24	3.40	116.63	110.99

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

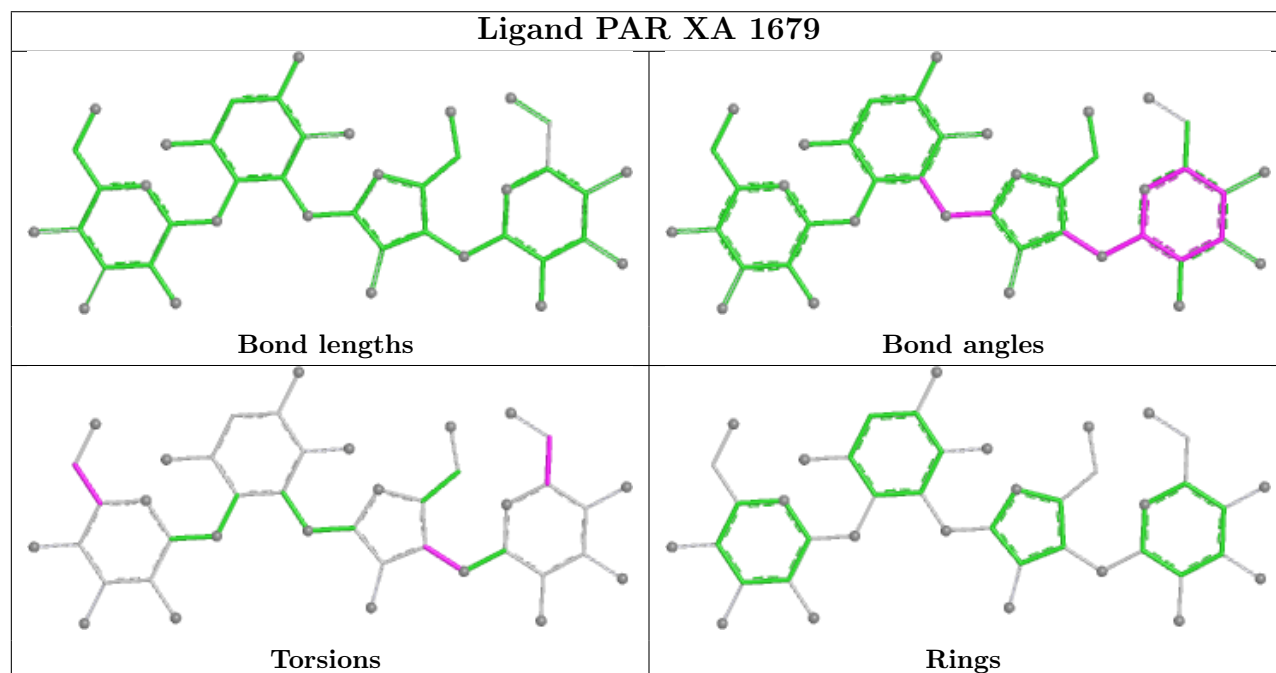
Mol	Chain	Res	Type	Atoms
58	QA	1667	PAR	O54-C54-C64-N64
58	XA	1679	PAR	C44-C54-C64-N64
58	XA	1679	PAR	O54-C54-C64-N64
58	XA	1679	PAR	O51-C51-C61-O61
58	QA	1667	PAR	O51-C51-C61-O61

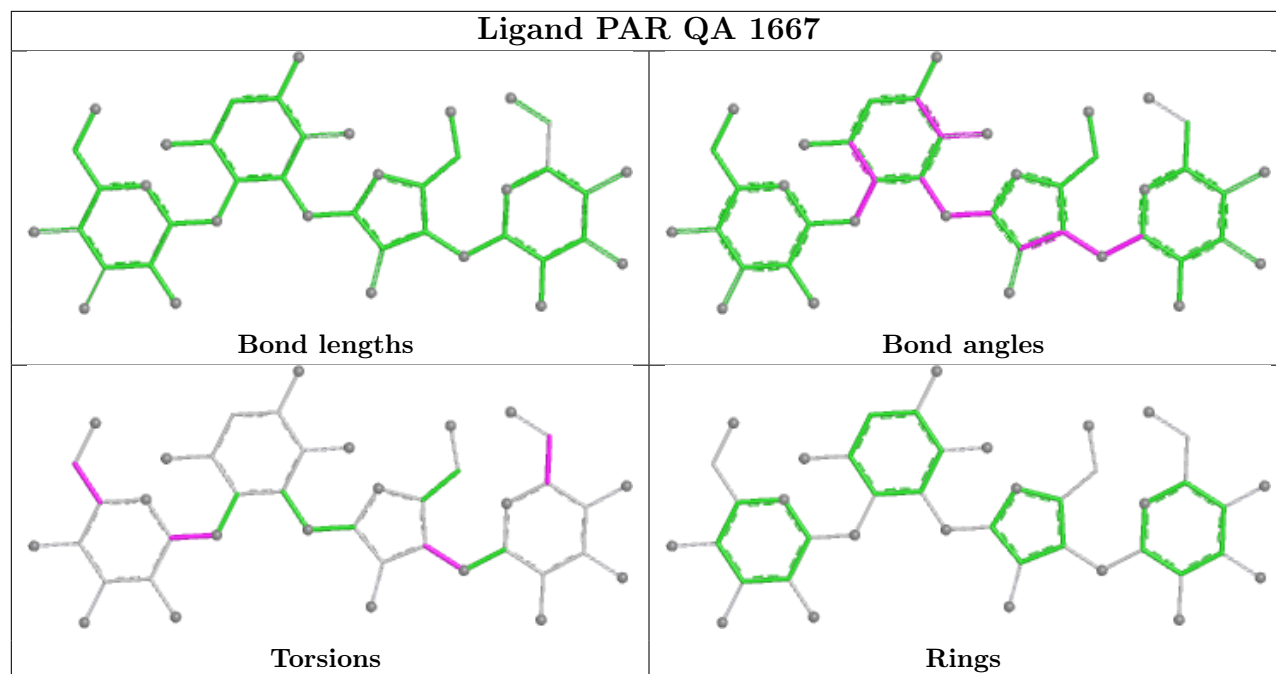
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XA	1679	PAR	1	0
58	QA	1667	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.01	24 (1%) 70 51	91, 119, 221, 344	0
1	XA	1500/1522 (98%)	-0.07	12 (0%) 82 67	78, 119, 208, 371	0
2	QB	237/256 (92%)	0.61	12 (5%) 33 21	136, 160, 215, 232	0
2	XB	237/256 (92%)	0.70	25 (10%) 11 8	133, 174, 202, 213	0
3	QC	205/239 (85%)	0.59	20 (9%) 13 9	146, 175, 209, 223	0
3	XC	205/239 (85%)	0.64	28 (13%) 6 5	135, 159, 212, 215	0
4	QD	208/209 (99%)	0.63	16 (7%) 19 13	89, 115, 156, 179	0
4	XD	208/209 (99%)	0.80	20 (9%) 13 9	103, 127, 142, 172	0
5	QE	151/162 (93%)	0.60	12 (7%) 18 12	117, 152, 181, 191	0
5	XE	151/162 (93%)	0.43	9 (5%) 27 17	105, 128, 166, 194	0
6	QF	101/101 (100%)	0.48	4 (3%) 42 26	106, 134, 184, 207	0
6	XF	101/101 (100%)	0.32	4 (3%) 42 26	113, 134, 156, 173	0
7	QG	155/156 (99%)	0.85	22 (14%) 6 5	141, 164, 201, 215	0
7	XG	155/156 (99%)	0.42	7 (4%) 38 24	126, 138, 175, 192	0
8	QH	138/138 (100%)	0.75	15 (10%) 10 7	110, 135, 162, 181	0
8	XH	138/138 (100%)	0.84	19 (13%) 6 5	105, 133, 184, 184	0
9	QI	127/128 (99%)	1.61	41 (32%) 1 1	149, 193, 215, 221	0
9	XI	127/128 (99%)	1.22	26 (20%) 2 2	121, 155, 185, 207	0
10	QJ	99/105 (94%)	1.45	24 (24%) 2 2	172, 197, 243, 250	0
10	XJ	99/105 (94%)	1.15	20 (20%) 3 2	136, 174, 184, 191	0
11	QK	119/129 (92%)	1.12	16 (13%) 7 6	111, 144, 184, 206	0
11	XK	119/129 (92%)	1.02	17 (14%) 6 5	104, 126, 158, 209	0
12	QL	125/131 (95%)	1.42	32 (25%) 1 2	111, 137, 179, 214	0
12	XL	125/131 (95%)	1.39	36 (28%) 1 1	92, 124, 179, 211	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	QM	121/126 (96%)	1.12	23 (19%)	3	2	141, 158, 209, 241	0
13	XM	121/126 (96%)	1.18	24 (19%)	3	2	137, 151, 189, 206	0
14	QN	60/61 (98%)	2.33	35 (58%)	0	0	171, 188, 213, 213	0
14	XN	60/61 (98%)	1.62	17 (28%)	1	1	119, 158, 186, 190	0
15	QO	88/89 (98%)	1.45	19 (21%)	2	2	123, 148, 179, 191	0
15	XO	88/89 (98%)	0.85	11 (12%)	8	6	93, 111, 168, 169	0
16	QP	84/88 (95%)	1.49	25 (29%)	1	1	111, 134, 174, 181	0
16	XP	84/88 (95%)	0.84	5 (5%)	27	17	116, 136, 210, 210	0
17	QQ	100/105 (95%)	0.87	10 (10%)	12	8	100, 123, 187, 188	0
17	XQ	100/105 (95%)	0.74	6 (6%)	27	17	108, 129, 151, 162	0
18	QR	70/88 (79%)	0.94	10 (14%)	6	5	124, 149, 201, 204	0
18	XR	70/88 (79%)	0.60	5 (7%)	22	14	90, 128, 171, 184	0
19	QS	84/93 (90%)	1.89	34 (40%)	0	1	199, 211, 225, 240	0
19	XS	84/93 (90%)	1.62	25 (29%)	1	1	175, 185, 204, 225	0
20	QT	99/106 (93%)	1.65	26 (26%)	1	2	97, 141, 204, 232	0
20	XT	99/106 (93%)	1.49	23 (23%)	2	2	120, 127, 190, 207	0
21	QU	25/27 (92%)	3.09	20 (80%)	0	0	179, 188, 223, 224	0
21	XU	25/27 (92%)	2.41	15 (60%)	0	0	159, 161, 175, 176	0
22	QV	77/77 (100%)	0.03	2 (2%)	57	37	116, 142, 201, 236	0
22	XV	77/77 (100%)	-0.09	2 (2%)	57	37	95, 131, 165, 239	0
23	QW	76/76 (100%)	0.50	8 (10%)	11	8	221, 257, 335, 357	0
23	XW	76/76 (100%)	1.57	25 (32%)	1	1	194, 394, 520, 525	0
24	QX	19/19 (100%)	2.33	10 (52%)	0	1	143, 241, 288, 293	0
24	XX	17/19 (89%)	1.72	6 (35%)	1	1	109, 259, 304, 304	0
25	QY	75/76 (98%)	2.80	47 (62%)	0	0	400, 613, 641, 644	0
25	XY	76/76 (100%)	1.45	19 (25%)	2	2	331, 415, 498, 499	0
26	R0	82/85 (96%)	1.39	24 (29%)	1	1	109, 129, 207, 214	0
26	Y0	82/85 (96%)	1.27	18 (21%)	2	2	83, 106, 152, 230	0
27	R1	97/98 (98%)	1.57	33 (34%)	1	1	75, 113, 219, 219	0
27	Y1	97/98 (98%)	1.17	18 (18%)	3	3	66, 87, 164, 193	0
28	R2	69/72 (95%)	1.12	7 (10%)	12	8	101, 139, 188, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y2	69/72 (95%)	0.74	5 (7%) 21 14	76, 95, 138, 165	0
29	R3	59/60 (98%)	1.31	12 (20%) 3 2	106, 150, 215, 239	0
29	Y3	59/60 (98%)	0.52	1 (1%) 69 49	74, 99, 137, 173	0
30	R4	71/71 (100%)	1.15	10 (14%) 6 5	180, 219, 253, 272	0
30	Y4	71/71 (100%)	1.18	11 (15%) 5 4	156, 178, 248, 248	0
31	R5	59/60 (98%)	1.18	10 (16%) 4 3	78, 114, 187, 222	0
31	Y5	59/60 (98%)	0.99	6 (10%) 12 8	65, 95, 240, 264	0
32	R6	49/54 (90%)	2.29	25 (51%) 0 1	234, 260, 264, 279	0
32	Y6	49/54 (90%)	2.15	25 (51%) 0 1	220, 239, 254, 273	0
33	R7	49/49 (100%)	1.79	11 (22%) 2 2	74, 100, 228, 229	0
33	Y7	49/49 (100%)	0.98	8 (16%) 4 3	55, 75, 221, 221	0
34	R8	64/65 (98%)	2.86	42 (65%) 0 0	104, 142, 187, 215	0
34	Y8	64/65 (98%)	1.79	23 (35%) 1 1	75, 92, 157, 184	0
35	R9	37/37 (100%)	4.39	31 (83%) 0 0	281, 356, 357, 358	0
35	Y9	37/37 (100%)	5.65	37 (100%) 0 0	299, 302, 385, 386	0
36	RA	2882/2915 (98%)	-0.23	18 (0%) 85 73	57, 94, 225, 392	0
36	YA	2883/2915 (98%)	-0.17	16 (0%) 85 73	57, 87, 209, 343	0
37	RB	120/122 (98%)	0.24	0 100 100	130, 158, 184, 201	0
37	YB	120/122 (98%)	0.20	0 100 100	116, 131, 153, 208	0
38	RD	272/276 (98%)	0.88	47 (17%) 4 3	71, 86, 126, 199	0
38	YD	272/276 (98%)	0.64	19 (6%) 22 14	57, 82, 107, 172	0
39	RE	205/206 (99%)	0.95	33 (16%) 4 3	71, 106, 159, 190	0
39	YE	205/206 (99%)	0.77	22 (10%) 11 7	65, 96, 161, 186	0
40	RF	202/210 (96%)	0.62	11 (5%) 31 20	69, 119, 165, 217	0
40	YF	202/210 (96%)	0.99	31 (15%) 5 4	65, 105, 146, 193	0
41	RG	181/182 (99%)	0.63	15 (8%) 17 11	133, 160, 188, 204	0
41	YG	181/182 (99%)	0.66	14 (7%) 19 13	119, 147, 183, 212	0
42	RH	170/180 (94%)	1.13	30 (17%) 4 3	161, 202, 225, 265	0
42	YH	170/180 (94%)	0.98	27 (15%) 5 3	90, 136, 171, 237	0
43	RI	146/148 (98%)	1.08	26 (17%) 4 3	115, 169, 192, 196	0
43	YI	146/148 (98%)	0.74	11 (7%) 20 13	101, 145, 187, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RN	138/140 (98%)	1.04	21 (15%) 5 4	91, 124, 177, 190	0
44	YN	138/140 (98%)	0.92	17 (12%) 8 6	73, 102, 186, 218	0
45	RO	122/122 (100%)	0.60	7 (5%) 29 19	73, 100, 128, 166	0
45	YO	122/122 (100%)	0.48	6 (4%) 35 22	67, 93, 148, 153	0
46	RP	150/150 (100%)	1.60	48 (32%) 1 1	91, 129, 191, 201	0
46	YP	150/150 (100%)	1.05	29 (19%) 3 2	68, 103, 146, 214	0
47	RQ	141/141 (100%)	1.59	48 (34%) 1 1	99, 138, 176, 202	0
47	YQ	141/141 (100%)	1.25	30 (21%) 2 2	75, 103, 154, 196	0
48	RR	118/118 (100%)	0.98	11 (9%) 14 9	67, 100, 144, 156	0
48	YR	118/118 (100%)	1.12	20 (16%) 4 3	81, 108, 127, 166	0
49	RS	111/112 (99%)	1.54	31 (27%) 1 1	139, 162, 208, 223	0
49	YS	111/112 (99%)	1.07	17 (15%) 5 4	116, 137, 195, 229	0
50	RT	137/146 (93%)	0.64	10 (7%) 21 13	78, 110, 184, 198	0
50	YT	137/146 (93%)	0.75	16 (11%) 9 6	85, 111, 173, 204	0
51	RU	117/118 (99%)	0.91	12 (10%) 12 8	80, 130, 170, 203	0
51	YU	117/118 (99%)	0.74	9 (7%) 19 13	72, 98, 136, 180	0
52	RV	101/101 (100%)	0.74	11 (10%) 10 7	105, 143, 188, 242	0
52	YV	101/101 (100%)	0.98	16 (15%) 5 4	73, 131, 167, 231	0
53	RW	113/113 (100%)	0.79	10 (8%) 15 10	76, 95, 156, 184	0
53	YW	113/113 (100%)	0.64	10 (8%) 15 10	69, 83, 130, 194	0
54	RX	92/96 (95%)	0.84	11 (11%) 9 6	87, 99, 132, 161	0
54	YX	92/96 (95%)	1.00	14 (15%) 5 4	65, 89, 140, 141	0
55	RY	102/110 (92%)	2.07	48 (47%) 0 1	111, 161, 208, 240	0
55	YY	102/110 (92%)	1.53	28 (27%) 1 1	81, 144, 167, 192	0
56	RZ	183/206 (88%)	0.79	17 (9%) 14 9	149, 173, 241, 270	0
56	YZ	183/206 (88%)	0.64	15 (8%) 17 11	114, 149, 199, 231	0
All	All	21164/21740 (97%)	0.53	2102 (9%) 13 8	55, 121, 223, 644	0

The worst 5 of 2102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	Y9	26	ILE	12.7
11	XK	129	SER	12.6

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Mol	Chain	Res	Type	RSRZ
31	R5	2	ALA	11.0
35	Y9	25	VAL	10.6
35	R9	26	ILE	10.1

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(Å ²)	Q<0.9
57	MG	YA	3184	1/1	-0.20	0.52	130,130,130,130	0
57	MG	RA	3234	1/1	-0.16	0.41	130,130,130,130	0
57	MG	YA	3198	1/1	-0.12	0.39	130,130,130,130	0
57	MG	RA	3216	1/1	-0.11	0.31	130,130,130,130	0
57	MG	QA	1601	1/1	-0.10	0.46	130,130,130,130	0
57	MG	YA	3147	1/1	-0.10	0.36	130,130,130,130	0
57	MG	RA	3231	1/1	-0.09	0.27	130,130,130,130	0
57	MG	YA	3261	1/1	-0.09	0.30	130,130,130,130	0
57	MG	RA	3180	1/1	-0.06	0.37	130,130,130,130	0
57	MG	RA	3177	1/1	0.01	0.35	130,130,130,130	0
57	MG	YA	3223	1/1	0.03	0.41	130,130,130,130	0
57	MG	XA	1637	1/1	0.03	0.28	130,130,130,130	0
57	MG	YA	3125	1/1	0.04	0.65	130,130,130,130	0
57	MG	YB	207	1/1	0.05	0.43	130,130,130,130	0
57	MG	XA	1663	1/1	0.06	0.60	130,130,130,130	0
57	MG	YA	3199	1/1	0.07	0.49	130,130,130,130	0
57	MG	RA	3201	1/1	0.08	0.36	130,130,130,130	0
57	MG	YA	3204	1/1	0.08	0.39	130,130,130,130	0
57	MG	XA	1694	1/1	0.08	0.53	130,130,130,130	0
57	MG	YA	3018	1/1	0.08	0.36	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3027	1/1	0.08	0.41	130,130,130,130	0
57	MG	RA	3035	1/1	0.09	0.37	130,130,130,130	0
57	MG	RA	3153	1/1	0.09	0.74	130,130,130,130	0
57	MG	RA	3182	1/1	0.09	0.71	130,130,130,130	0
57	MG	QA	1637	1/1	0.10	0.44	130,130,130,130	0
57	MG	QA	1621	1/1	0.11	0.47	130,130,130,130	0
57	MG	YA	3353	1/1	0.11	0.26	130,130,130,130	0
57	MG	XA	1633	1/1	0.11	0.46	130,130,130,130	0
57	MG	YA	3238	1/1	0.12	0.27	130,130,130,130	0
57	MG	YA	3004	1/1	0.12	0.58	130,130,130,130	0
57	MG	YA	3302	1/1	0.13	0.69	130,130,130,130	0
57	MG	XA	1678	1/1	0.13	0.26	130,130,130,130	0
57	MG	RA	3144	1/1	0.13	0.53	130,130,130,130	0
57	MG	YA	3237	1/1	0.14	0.70	130,130,130,130	0
57	MG	XA	1630	1/1	0.14	0.52	130,130,130,130	0
57	MG	YA	3176	1/1	0.14	0.31	130,130,130,130	0
57	MG	QA	1606	1/1	0.14	0.61	130,130,130,130	0
57	MG	YA	3208	1/1	0.14	0.22	130,130,130,130	0
57	MG	YA	3194	1/1	0.14	0.50	130,130,130,130	0
57	MG	XA	1640	1/1	0.15	0.27	130,130,130,130	0
57	MG	YA	3112	1/1	0.15	0.53	130,130,130,130	0
57	MG	YA	3019	1/1	0.15	0.40	130,130,130,130	0
57	MG	XA	1652	1/1	0.16	0.37	130,130,130,130	0
57	MG	RA	3173	1/1	0.16	0.37	130,130,130,130	0
57	MG	YA	3201	1/1	0.16	0.30	130,130,130,130	0
57	MG	YA	3109	1/1	0.16	0.55	130,130,130,130	0
57	MG	XA	1617	1/1	0.17	0.38	130,130,130,130	0
57	MG	RA	3229	1/1	0.17	0.28	130,130,130,130	0
57	MG	YA	3263	1/1	0.18	0.49	130,130,130,130	0
57	MG	QA	1644	1/1	0.18	0.35	130,130,130,130	0
57	MG	YA	3330	1/1	0.18	0.39	130,130,130,130	0
57	MG	RA	3081	1/1	0.18	0.58	130,130,130,130	0
57	MG	YA	3173	1/1	0.18	0.20	130,130,130,130	0
57	MG	YR	202	1/1	0.18	0.54	130,130,130,130	0
57	MG	YA	3118	1/1	0.19	0.73	130,130,130,130	0
57	MG	RA	3194	1/1	0.19	0.27	130,130,130,130	0
57	MG	YA	3333	1/1	0.19	0.31	130,130,130,130	0
57	MG	RA	3169	1/1	0.19	0.39	130,130,130,130	0
57	MG	RA	3291	1/1	0.19	0.56	130,130,130,130	0
57	MG	YA	3210	1/1	0.19	0.20	130,130,130,130	0
57	MG	RA	3031	1/1	0.20	0.52	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3225	1/1	0.20	0.23	130,130,130,130	0
57	MG	XA	1680	1/1	0.20	0.52	130,130,130,130	0
57	MG	YA	3213	1/1	0.20	0.54	130,130,130,130	0
57	MG	RA	3070	1/1	0.20	0.60	130,130,130,130	0
57	MG	YA	3331	1/1	0.21	0.48	130,130,130,130	0
57	MG	YA	3075	1/1	0.21	0.63	130,130,130,130	0
57	MG	XA	1610	1/1	0.21	0.30	130,130,130,130	0
57	MG	RA	3279	1/1	0.21	0.59	130,130,130,130	0
57	MG	RA	3274	1/1	0.21	0.27	130,130,130,130	0
57	MG	YA	3015	1/1	0.22	0.39	130,130,130,130	0
57	MG	YA	3090	1/1	0.22	0.53	130,130,130,130	0
57	MG	XA	1606	1/1	0.23	0.58	130,130,130,130	0
57	MG	YA	3011	1/1	0.23	0.38	130,130,130,130	0
57	MG	YA	3175	1/1	0.23	0.52	130,130,130,130	0
57	MG	RA	3032	1/1	0.23	0.58	130,130,130,130	0
57	MG	YA	3130	1/1	0.23	0.64	130,130,130,130	0
57	MG	QA	1630	1/1	0.24	0.18	130,130,130,130	0
57	MG	YE	3401	1/1	0.24	0.67	130,130,130,130	0
57	MG	YA	3371	1/1	0.24	0.67	130,130,130,130	0
57	MG	YA	3200	1/1	0.25	0.39	130,130,130,130	0
57	MG	QA	1641	1/1	0.25	0.58	130,130,130,130	0
57	MG	YA	3325	1/1	0.25	0.20	130,130,130,130	0
57	MG	YA	3097	1/1	0.25	0.46	130,130,130,130	0
57	MG	QA	1632	1/1	0.25	0.56	130,130,130,130	0
57	MG	RA	3172	1/1	0.25	0.45	130,130,130,130	0
57	MG	YA	3181	1/1	0.25	0.65	130,130,130,130	0
57	MG	QX	101	1/1	0.25	0.24	130,130,130,130	0
57	MG	RA	3003	1/1	0.25	0.51	130,130,130,130	0
57	MG	YA	3126	1/1	0.25	0.43	130,130,130,130	0
57	MG	YE	3403	1/1	0.25	0.54	130,130,130,130	0
57	MG	QA	1629	1/1	0.25	0.21	130,130,130,130	0
57	MG	RA	3204	1/1	0.26	0.17	130,130,130,130	0
57	MG	RA	3113	1/1	0.26	0.46	130,130,130,130	0
57	MG	RA	3232	1/1	0.26	0.36	130,130,130,130	0
57	MG	RA	3293	1/1	0.26	0.38	130,130,130,130	0
57	MG	YA	3059	1/1	0.26	0.73	130,130,130,130	0
57	MG	RA	3310	1/1	0.26	0.26	130,130,130,130	0
57	MG	XA	1638	1/1	0.26	0.20	130,130,130,130	0
57	MG	YA	3091	1/1	0.26	0.60	130,130,130,130	0
57	MG	RA	3157	1/1	0.26	0.46	130,130,130,130	0
57	MG	YA	3318	1/1	0.26	0.28	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3362	1/1	0.27	0.43	130,130,130,130	0
57	MG	XA	1672	1/1	0.27	0.14	130,130,130,130	0
57	MG	XA	1673	1/1	0.27	0.46	130,130,130,130	0
57	MG	YA	3297	1/1	0.27	0.94	130,130,130,130	0
57	MG	YA	3169	1/1	0.27	0.52	130,130,130,130	0
57	MG	RA	3041	1/1	0.27	0.72	130,130,130,130	0
57	MG	YA	3264	1/1	0.28	0.45	130,130,130,130	0
57	MG	YA	3296	1/1	0.28	0.62	130,130,130,130	0
57	MG	XA	1615	1/1	0.28	0.53	130,130,130,130	0
57	MG	YA	3074	1/1	0.28	0.52	130,130,130,130	0
57	MG	YA	3337	1/1	0.28	0.37	130,130,130,130	0
57	MG	XA	1627	1/1	0.28	0.65	130,130,130,130	0
57	MG	YA	3378	1/1	0.29	0.37	130,130,130,130	0
57	MG	XA	1614	1/1	0.29	0.63	130,130,130,130	0
57	MG	RA	3019	1/1	0.29	0.64	130,130,130,130	0
57	MG	RA	3116	1/1	0.29	0.37	130,130,130,130	0
57	MG	RA	3061	1/1	0.29	0.48	130,130,130,130	0
57	MG	YA	3254	1/1	0.30	0.24	130,130,130,130	0
57	MG	RA	3198	1/1	0.30	0.52	130,130,130,130	0
57	MG	RA	3139	1/1	0.30	0.39	130,130,130,130	0
57	MG	XA	1647	1/1	0.30	0.75	130,130,130,130	0
57	MG	YA	3089	1/1	0.30	0.41	130,130,130,130	0
57	MG	RA	3312	1/1	0.30	0.46	130,130,130,130	0
57	MG	YA	3193	1/1	0.30	0.32	130,130,130,130	0
57	MG	RA	3304	1/1	0.31	0.47	130,130,130,130	0
57	MG	YA	3121	1/1	0.31	0.62	130,130,130,130	0
57	MG	YA	3222	1/1	0.31	0.50	130,130,130,130	0
57	MG	XA	1665	1/1	0.32	0.56	130,130,130,130	0
57	MG	XA	1667	1/1	0.32	0.21	130,130,130,130	0
57	MG	XA	1669	1/1	0.32	0.51	130,130,130,130	0
57	MG	RA	3163	1/1	0.32	0.42	130,130,130,130	0
57	MG	YA	3212	1/1	0.32	0.23	130,130,130,130	0
57	MG	RA	3308	1/1	0.32	0.59	130,130,130,130	0
57	MG	RA	3233	1/1	0.32	0.28	130,130,130,130	0
57	MG	RA	3149	1/1	0.32	0.43	130,130,130,130	0
57	MG	XA	1681	1/1	0.32	0.42	130,130,130,130	0
57	MG	RA	3270	1/1	0.32	0.71	130,130,130,130	0
57	MG	RA	3220	1/1	0.32	0.20	130,130,130,130	0
57	MG	YA	3007	1/1	0.32	0.40	130,130,130,130	0
57	MG	QA	1624	1/1	0.32	0.22	130,130,130,130	0
57	MG	RA	3086	1/1	0.32	0.85	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YE	3402	1/1	0.32	0.62	130,130,130,130	0
57	MG	YA	3272	1/1	0.32	0.40	130,130,130,130	0
57	MG	RA	3162	1/1	0.32	0.80	130,130,130,130	0
57	MG	YA	3339	1/1	0.33	0.42	130,130,130,130	0
57	MG	YA	3349	1/1	0.33	0.48	130,130,130,130	0
57	MG	XA	1641	1/1	0.33	0.52	130,130,130,130	0
57	MG	RA	3018	1/1	0.33	0.45	130,130,130,130	0
57	MG	YA	3117	1/1	0.33	0.27	130,130,130,130	0
57	MG	XA	1608	1/1	0.33	0.33	130,130,130,130	0
57	MG	XA	1695	1/1	0.33	0.86	130,130,130,130	0
57	MG	RA	3141	1/1	0.33	0.41	130,130,130,130	0
57	MG	YA	3267	1/1	0.33	0.29	130,130,130,130	0
57	MG	YA	3270	1/1	0.33	0.49	130,130,130,130	0
57	MG	RA	3191	1/1	0.33	0.33	130,130,130,130	0
57	MG	XJ	301	1/1	0.34	0.29	130,130,130,130	0
57	MG	YA	3216	1/1	0.34	0.37	130,130,130,130	0
57	MG	YA	3352	1/1	0.34	0.54	130,130,130,130	0
57	MG	RA	3131	1/1	0.34	0.38	130,130,130,130	0
57	MG	XA	1645	1/1	0.34	0.28	130,130,130,130	0
57	MG	RA	3307	1/1	0.34	0.45	130,130,130,130	0
57	MG	XA	1676	1/1	0.34	0.29	130,130,130,130	0
57	MG	YB	206	1/1	0.34	0.36	130,130,130,130	0
57	MG	QA	1614	1/1	0.34	0.43	130,130,130,130	0
57	MG	XA	1656	1/1	0.34	0.41	130,130,130,130	0
57	MG	RA	3120	1/1	0.34	0.26	130,130,130,130	0
57	MG	RA	3300	1/1	0.34	0.32	130,130,130,130	0
57	MG	RE	303	1/1	0.34	0.52	130,130,130,130	0
57	MG	YU	202	1/1	0.34	0.34	130,130,130,130	0
57	MG	YA	3079	1/1	0.35	0.94	130,130,130,130	0
57	MG	YA	3062	1/1	0.35	0.35	130,130,130,130	0
57	MG	YA	3160	1/1	0.35	0.53	130,130,130,130	0
57	MG	XA	1687	1/1	0.35	0.47	130,130,130,130	0
57	MG	RA	3192	1/1	0.35	0.17	130,130,130,130	0
57	MG	YA	3247	1/1	0.35	0.44	130,130,130,130	0
57	MG	QA	1622	1/1	0.36	0.52	130,130,130,130	0
57	MG	RA	3045	1/1	0.36	0.37	130,130,130,130	0
57	MG	RA	3095	1/1	0.36	0.25	130,130,130,130	0
57	MG	QA	1672	1/1	0.36	0.47	130,130,130,130	0
57	MG	RA	3069	1/1	0.36	0.37	130,130,130,130	0
57	MG	YA	3373	1/1	0.36	0.41	130,130,130,130	0
57	MG	RA	3021	1/1	0.36	0.38	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1635	1/1	0.37	0.17	130,130,130,130	0
57	MG	R0	101	1/1	0.37	0.39	130,130,130,130	0
57	MG	RB	203	1/1	0.37	0.36	130,130,130,130	0
57	MG	RA	3090	1/1	0.37	0.42	130,130,130,130	0
57	MG	YA	3252	1/1	0.37	0.42	130,130,130,130	0
57	MG	XA	1601	1/1	0.37	0.83	130,130,130,130	0
57	MG	QA	1674	1/1	0.37	0.44	130,130,130,130	0
57	MG	YA	3083	1/1	0.37	0.48	130,130,130,130	0
57	MG	RA	3024	1/1	0.37	0.71	130,130,130,130	0
57	MG	YA	3323	1/1	0.38	0.28	130,130,130,130	0
57	MG	RA	3227	1/1	0.38	0.42	130,130,130,130	0
57	MG	YA	3053	1/1	0.38	0.81	130,130,130,130	0
57	MG	QA	1677	1/1	0.38	0.43	130,130,130,130	0
57	MG	QA	1679	1/1	0.38	0.26	130,130,130,130	0
57	MG	RA	3036	1/1	0.38	0.49	130,130,130,130	0
57	MG	XA	1646	1/1	0.38	0.16	130,130,130,130	0
57	MG	RA	3122	1/1	0.38	0.35	130,130,130,130	0
57	MG	YA	3351	1/1	0.38	0.38	130,130,130,130	0
57	MG	YA	3255	1/1	0.38	0.34	130,130,130,130	0
57	MG	RA	3147	1/1	0.38	0.34	130,130,130,130	0
57	MG	RA	3058	1/1	0.39	0.40	130,130,130,130	0
57	MG	YA	3262	1/1	0.39	0.56	130,130,130,130	0
57	MG	YA	3195	1/1	0.39	0.36	130,130,130,130	0
57	MG	QA	1634	1/1	0.39	0.32	130,130,130,130	0
57	MG	RA	3063	1/1	0.39	0.47	130,130,130,130	0
57	MG	XA	1616	1/1	0.39	0.66	130,130,130,130	0
57	MG	XA	1639	1/1	0.39	0.41	130,130,130,130	0
57	MG	YA	3002	1/1	0.39	0.91	130,130,130,130	0
57	MG	QA	1608	1/1	0.39	0.52	130,130,130,130	0
57	MG	RA	3056	1/1	0.39	0.42	130,130,130,130	0
57	MG	YA	3131	1/1	0.39	0.43	130,130,130,130	0
57	MG	YA	3313	1/1	0.40	0.27	130,130,130,130	0
57	MG	RA	3289	1/1	0.40	0.21	130,130,130,130	0
57	MG	XA	1653	1/1	0.40	0.31	130,130,130,130	0
57	MG	RA	3145	1/1	0.40	0.35	130,130,130,130	0
57	MG	RA	3253	1/1	0.40	0.61	130,130,130,130	0
57	MG	RA	3151	1/1	0.40	0.34	130,130,130,130	0
57	MG	RA	3135	1/1	0.40	0.31	130,130,130,130	0
57	MG	RA	3167	1/1	0.40	0.51	130,130,130,130	0
57	MG	YA	3056	1/1	0.41	0.71	130,130,130,130	0
57	MG	RA	3159	1/1	0.41	0.57	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	RA	3252	1/1	0.41	0.56	130,130,130,130	0
57	MG	YA	3274	1/1	0.41	0.40	130,130,130,130	0
57	MG	QA	1609	1/1	0.41	0.51	130,130,130,130	0
57	MG	Y7	102	1/1	0.41	0.72	130,130,130,130	0
57	MG	RA	3047	1/1	0.41	0.76	130,130,130,130	0
57	MG	YA	3203	1/1	0.41	0.30	130,130,130,130	0
57	MG	YA	3081	1/1	0.41	0.52	130,130,130,130	0
57	MG	YA	3319	1/1	0.41	0.54	130,130,130,130	0
57	MG	YA	3025	1/1	0.41	0.33	130,130,130,130	0
57	MG	YA	3003	1/1	0.41	0.51	130,130,130,130	0
57	MG	YA	3211	1/1	0.41	0.23	130,130,130,130	0
57	MG	YA	3188	1/1	0.41	0.37	130,130,130,130	0
57	MG	RA	3067	1/1	0.41	0.61	130,130,130,130	0
57	MG	YA	3266	1/1	0.41	0.18	130,130,130,130	0
57	MG	RA	3174	1/1	0.42	0.41	130,130,130,130	0
57	MG	RA	3236	1/1	0.42	0.47	130,130,130,130	0
57	MG	Y7	101	1/1	0.42	0.74	130,130,130,130	0
57	MG	RA	3237	1/1	0.42	0.15	130,130,130,130	0
57	MG	RA	3238	1/1	0.42	0.26	130,130,130,130	0
57	MG	XA	1684	1/1	0.42	0.34	130,130,130,130	0
57	MG	YA	3034	1/1	0.42	0.56	130,130,130,130	0
57	MG	YA	3086	1/1	0.42	0.68	130,130,130,130	0
57	MG	RA	3050	1/1	0.42	0.61	130,130,130,130	0
57	MG	QA	1616	1/1	0.42	0.71	130,130,130,130	0
57	MG	YA	3177	1/1	0.43	0.47	130,130,130,130	0
57	MG	YA	3060	1/1	0.43	0.89	130,130,130,130	0
57	MG	RA	3009	1/1	0.43	0.45	130,130,130,130	0
57	MG	RA	3226	1/1	0.43	0.20	130,130,130,130	0
57	MG	QF	301	1/1	0.43	0.27	130,130,130,130	0
57	MG	R8	101	1/1	0.43	1.22	130,130,130,130	0
57	MG	YA	3290	1/1	0.43	0.47	130,130,130,130	0
57	MG	YA	3355	1/1	0.43	0.33	130,130,130,130	0
57	MG	YA	3022	1/1	0.43	0.58	130,130,130,130	0
57	MG	QA	1671	1/1	0.43	0.54	130,130,130,130	0
57	MG	YA	3301	1/1	0.43	0.65	130,130,130,130	0
57	MG	YA	3244	1/1	0.43	0.52	130,130,130,130	0
57	MG	RA	3203	1/1	0.43	0.29	130,130,130,130	0
57	MG	YA	3028	1/1	0.43	0.44	130,130,130,130	0
57	MG	RA	3181	1/1	0.43	0.39	130,130,130,130	0
57	MG	RA	3156	1/1	0.43	0.56	130,130,130,130	0
57	MG	YA	3095	1/1	0.43	0.74	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3098	1/1	0.43	0.36	130,130,130,130	0
57	MG	RA	3223	1/1	0.43	0.69	130,130,130,130	0
57	MG	RA	3109	1/1	0.44	0.47	130,130,130,130	0
57	MG	RE	301	1/1	0.44	0.60	130,130,130,130	0
57	MG	XA	1660	1/1	0.44	0.28	130,130,130,130	0
57	MG	QA	1650	1/1	0.44	0.44	130,130,130,130	0
57	MG	YA	3206	1/1	0.44	0.33	130,130,130,130	0
57	MG	RA	3030	1/1	0.44	0.28	130,130,130,130	0
57	MG	YA	3304	1/1	0.44	0.37	130,130,130,130	0
57	MG	YA	3311	1/1	0.44	0.25	130,130,130,130	0
57	MG	YA	3260	1/1	0.44	0.39	130,130,130,130	0
57	MG	XA	1642	1/1	0.44	0.37	130,130,130,130	0
57	MG	YA	3128	1/1	0.44	0.45	130,130,130,130	0
57	MG	XA	1605	1/1	0.44	0.26	130,130,130,130	0
57	MG	RA	3055	1/1	0.44	0.74	130,130,130,130	0
57	MG	YA	3136	1/1	0.44	0.77	130,130,130,130	0
57	MG	YA	3140	1/1	0.44	0.38	130,130,130,130	0
57	MG	RA	3259	1/1	0.44	0.76	130,130,130,130	0
57	MG	RA	3268	1/1	0.44	0.56	130,130,130,130	0
57	MG	YA	3196	1/1	0.45	0.36	130,130,130,130	0
57	MG	RA	3314	1/1	0.45	0.59	130,130,130,130	0
57	MG	QA	1675	1/1	0.45	0.35	130,130,130,130	0
57	MG	RA	3016	1/1	0.45	0.21	130,130,130,130	0
57	MG	YA	3367	1/1	0.45	0.27	130,130,130,130	0
57	MG	YA	3087	1/1	0.45	0.44	130,130,130,130	0
57	MG	RA	3073	1/1	0.45	0.92	130,130,130,130	0
57	MG	YA	3327	1/1	0.45	0.30	130,130,130,130	0
57	MG	RA	3028	1/1	0.45	0.69	130,130,130,130	0
57	MG	RA	3251	1/1	0.45	0.49	130,130,130,130	0
57	MG	RA	3309	1/1	0.45	0.43	130,130,130,130	0
57	MG	RA	3054	1/1	0.45	0.60	130,130,130,130	0
57	MG	RA	3043	1/1	0.45	0.88	130,130,130,130	0
57	MG	XA	1655	1/1	0.45	0.15	130,130,130,130	0
57	MG	YA	3157	1/1	0.45	0.37	130,130,130,130	0
57	MG	RA	3114	1/1	0.46	0.88	130,130,130,130	0
57	MG	YA	3285	1/1	0.46	0.62	130,130,130,130	0
57	MG	YA	3341	1/1	0.46	0.79	130,130,130,130	0
57	MG	YA	3202	1/1	0.46	0.55	130,130,130,130	0
57	MG	XV	103	1/1	0.46	0.24	130,130,130,130	0
57	MG	RA	3148	1/1	0.46	0.24	130,130,130,130	0
57	MG	YA	3253	1/1	0.46	0.44	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3065	1/1	0.46	0.53	130,130,130,130	0
57	MG	YA	3185	1/1	0.46	0.48	130,130,130,130	0
57	MG	RA	3311	1/1	0.46	0.24	130,130,130,130	0
57	MG	YA	3312	1/1	0.46	0.27	130,130,130,130	0
57	MG	YA	3104	1/1	0.46	0.54	130,130,130,130	0
57	MG	XA	1682	1/1	0.46	0.63	130,130,130,130	0
57	MG	RA	3130	1/1	0.46	0.32	130,130,130,130	0
57	MG	RA	3112	1/1	0.46	0.36	130,130,130,130	0
57	MG	YA	3265	1/1	0.46	0.35	130,130,130,130	0
57	MG	RA	3108	1/1	0.46	0.52	130,130,130,130	0
57	MG	RD	301	1/1	0.46	0.77	130,130,130,130	0
57	MG	YA	3234	1/1	0.46	0.35	130,130,130,130	0
57	MG	YA	3014	1/1	0.46	0.47	130,130,130,130	0
57	MG	YA	3058	1/1	0.47	0.48	130,130,130,130	0
57	MG	XA	1643	1/1	0.47	0.25	130,130,130,130	0
57	MG	YA	3332	1/1	0.47	0.38	130,130,130,130	0
57	MG	QA	1607	1/1	0.47	0.80	130,130,130,130	0
57	MG	YA	3111	1/1	0.47	0.28	130,130,130,130	0
57	MG	RA	3022	1/1	0.47	0.48	130,130,130,130	0
57	MG	YA	3215	1/1	0.47	0.14	130,130,130,130	0
57	MG	YA	3116	1/1	0.47	0.80	130,130,130,130	0
57	MG	RA	3052	1/1	0.47	0.52	130,130,130,130	0
57	MG	YA	3071	1/1	0.47	0.47	130,130,130,130	0
57	MG	RA	3282	1/1	0.47	0.51	130,130,130,130	0
57	MG	QA	1642	1/1	0.47	0.32	130,130,130,130	0
57	MG	XA	1654	1/1	0.47	0.47	130,130,130,130	0
57	MG	QA	1636	1/1	0.47	0.13	139,139,139,139	0
57	MG	QA	1615	1/1	0.47	0.45	130,130,130,130	0
57	MG	RA	3294	1/1	0.47	0.21	130,130,130,130	0
57	MG	QA	1670	1/1	0.47	0.27	130,130,130,130	0
57	MG	RA	3254	1/1	0.47	0.80	130,130,130,130	0
57	MG	YA	3142	1/1	0.47	0.50	130,130,130,130	0
57	MG	RA	3207	1/1	0.47	0.33	130,130,130,130	0
57	MG	YA	3321	1/1	0.47	0.70	130,130,130,130	0
57	MG	YA	3149	1/1	0.47	0.42	130,130,130,130	0
57	MG	RA	3263	1/1	0.47	0.60	130,130,130,130	0
57	MG	RA	3133	1/1	0.47	0.39	130,130,130,130	0
57	MG	YA	3342	1/1	0.48	0.51	130,130,130,130	0
57	MG	XV	101	1/1	0.48	0.55	130,130,130,130	0
57	MG	YA	3221	1/1	0.48	0.47	130,130,130,130	0
57	MG	XA	1609	1/1	0.48	0.59	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3043	1/1	0.48	0.30	130,130,130,130	0
57	MG	YA	3229	1/1	0.48	0.29	130,130,130,130	0
57	MG	YA	3048	1/1	0.48	0.64	130,130,130,130	0
57	MG	YA	3107	1/1	0.48	0.29	130,130,130,130	0
57	MG	YA	3135	1/1	0.48	0.39	130,130,130,130	0
57	MG	YA	3182	1/1	0.48	0.33	130,130,130,130	0
57	MG	RA	3183	1/1	0.48	0.20	130,130,130,130	0
57	MG	XA	1612	1/1	0.48	0.32	130,130,130,130	0
57	MG	RA	3101	1/1	0.48	0.44	130,130,130,130	0
57	MG	RA	3075	1/1	0.48	0.32	130,130,130,130	0
57	MG	QA	1617	1/1	0.48	0.40	130,130,130,130	0
57	MG	RA	3060	1/1	0.48	0.49	130,130,130,130	0
57	MG	YA	3340	1/1	0.48	0.35	130,130,130,130	0
57	MG	YA	3064	1/1	0.48	0.58	130,130,130,130	0
57	MG	QV	103	1/1	0.49	0.24	130,130,130,130	0
57	MG	YA	3054	1/1	0.49	0.53	130,130,130,130	0
57	MG	XA	1620	1/1	0.49	0.28	130,130,130,130	0
57	MG	XA	1624	1/1	0.49	0.53	130,130,130,130	0
57	MG	YA	3310	1/1	0.49	0.89	130,130,130,130	0
57	MG	RA	3057	1/1	0.49	0.52	130,130,130,130	0
57	MG	QA	1631	1/1	0.49	0.15	130,130,130,130	0
57	MG	YA	3092	1/1	0.49	0.59	130,130,130,130	0
57	MG	RA	3006	1/1	0.49	0.47	130,130,130,130	0
57	MG	YA	3364	1/1	0.49	0.40	130,130,130,130	0
57	MG	YA	3023	1/1	0.49	0.31	130,130,130,130	0
57	MG	Y8	102	1/1	0.49	0.88	130,130,130,130	0
57	MG	YA	3138	1/1	0.49	0.60	130,130,130,130	0
57	MG	YA	3105	1/1	0.49	0.63	130,130,130,130	0
57	MG	YB	201	1/1	0.49	0.46	130,130,130,130	0
57	MG	YA	3001	1/1	0.49	0.49	130,130,130,130	0
57	MG	XA	1683	1/1	0.49	0.17	130,130,130,130	0
57	MG	YA	3231	1/1	0.49	0.38	130,130,130,130	0
57	MG	YA	3110	1/1	0.49	0.60	130,130,130,130	0
57	MG	RA	3271	1/1	0.49	0.69	130,130,130,130	0
57	MG	YH	201	1/1	0.49	0.45	130,130,130,130	0
57	MG	QA	1678	1/1	0.49	0.40	130,130,130,130	0
57	MG	RA	3126	1/1	0.49	0.44	130,130,130,130	0
57	MG	RA	3074	1/1	0.50	0.25	130,130,130,130	0
57	MG	YA	3082	1/1	0.50	0.58	130,130,130,130	0
57	MG	QA	1676	1/1	0.50	0.29	130,130,130,130	0
57	MG	YA	3137	1/1	0.50	0.38	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3079	1/1	0.50	0.35	130,130,130,130	0
57	MG	RA	3199	1/1	0.50	0.39	130,130,130,130	0
57	MG	YA	3141	1/1	0.50	0.59	130,130,130,130	0
57	MG	RA	3272	1/1	0.50	0.45	130,130,130,130	0
57	MG	RA	3105	1/1	0.50	0.66	130,130,130,130	0
57	MG	QA	1686	1/1	0.50	0.51	130,130,130,130	0
57	MG	YA	3072	1/1	0.50	1.33	130,130,130,130	0
57	MG	QA	1618	1/1	0.50	0.42	130,130,130,130	0
57	MG	YA	3162	1/1	0.50	0.46	130,130,130,130	0
57	MG	YA	3348	1/1	0.50	0.45	130,130,130,130	0
57	MG	RA	3186	1/1	0.50	0.42	130,130,130,130	0
57	MG	YA	3077	1/1	0.50	0.91	130,130,130,130	0
57	MG	QA	1620	1/1	0.50	0.29	130,130,130,130	0
57	MG	RA	3196	1/1	0.51	0.77	130,130,130,130	0
57	MG	QA	1658	1/1	0.51	0.39	130,130,130,130	0
57	MG	YA	3375	1/1	0.51	0.50	130,130,130,130	0
57	MG	YA	3155	1/1	0.51	0.40	130,130,130,130	0
57	MG	RA	3078	1/1	0.51	0.55	130,130,130,130	0
57	MG	QV	102	1/1	0.51	0.23	130,130,130,130	0
57	MG	RA	3298	1/1	0.51	0.37	130,130,130,130	0
57	MG	YA	3080	1/1	0.51	0.54	130,130,130,130	0
57	MG	YA	3171	1/1	0.51	0.52	130,130,130,130	0
57	MG	XA	1635	1/1	0.51	0.23	130,130,130,130	0
57	MG	XA	1604	1/1	0.51	0.33	130,130,130,130	0
57	MG	RA	3266	1/1	0.51	0.52	130,130,130,130	0
57	MG	RA	3217	1/1	0.51	0.61	130,130,130,130	0
57	MG	YA	3076	1/1	0.52	0.43	130,130,130,130	0
57	MG	RA	3243	1/1	0.52	0.27	130,130,130,130	0
57	MG	YA	3242	1/1	0.52	0.34	130,130,130,130	0
57	MG	RA	3319	1/1	0.52	0.45	130,130,130,130	0
57	MG	RA	3155	1/1	0.52	0.59	130,130,130,130	0
57	MG	QH	201	1/1	0.52	0.14	130,130,130,130	0
57	MG	YA	3145	1/1	0.52	0.24	130,130,130,130	0
57	MG	YA	3277	1/1	0.52	0.26	130,130,130,130	0
57	MG	RA	3284	1/1	0.52	0.42	130,130,130,130	0
57	MG	RA	3286	1/1	0.52	0.51	130,130,130,130	0
57	MG	YA	3052	1/1	0.52	0.32	130,130,130,130	0
57	MG	QA	1633	1/1	0.52	0.29	130,130,130,130	0
57	MG	YP	203	1/1	0.52	0.48	130,130,130,130	0
57	MG	XA	1603	1/1	0.52	0.38	130,130,130,130	0
57	MG	XA	1677	1/1	0.52	0.45	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3146	1/1	0.53	0.48	130,130,130,130	0
57	MG	RA	3242	1/1	0.53	0.19	130,130,130,130	0
57	MG	YA	3294	1/1	0.53	0.55	130,130,130,130	0
57	MG	RA	3124	1/1	0.53	0.35	130,130,130,130	0
57	MG	QA	1602	1/1	0.53	0.47	130,130,130,130	0
57	MG	XA	1625	1/1	0.53	0.58	130,130,130,130	0
57	MG	XA	1691	1/1	0.53	0.27	130,130,130,130	0
57	MG	XA	1692	1/1	0.53	0.30	130,130,130,130	0
57	MG	YA	3357	1/1	0.53	0.52	130,130,130,130	0
57	MG	YA	3249	1/1	0.53	0.26	130,130,130,130	0
57	MG	YA	3127	1/1	0.53	0.45	130,130,130,130	0
57	MG	YA	3093	1/1	0.53	0.57	130,130,130,130	0
57	MG	YA	3129	1/1	0.53	0.97	130,130,130,130	0
57	MG	YA	3094	1/1	0.53	0.56	130,130,130,130	0
57	MG	XA	1693	1/1	0.53	0.12	130,130,130,130	0
57	MG	RA	3129	1/1	0.53	0.39	130,130,130,130	0
57	MG	YA	3051	1/1	0.53	0.29	130,130,130,130	0
57	MG	YA	3009	1/1	0.53	0.72	130,130,130,130	0
57	MG	YA	3214	1/1	0.53	0.69	130,130,130,130	0
57	MG	YD	302	1/1	0.53	0.54	130,130,130,130	0
57	MG	XA	1628	1/1	0.53	0.27	130,130,130,130	0
57	MG	XD	502	1/1	0.53	0.26	130,130,130,130	0
57	MG	YA	3186	1/1	0.53	0.43	130,130,130,130	0
57	MG	RA	3094	1/1	0.53	0.42	130,130,130,130	0
57	MG	RA	3200	1/1	0.53	0.37	130,130,130,130	0
57	MG	YA	3226	1/1	0.53	0.43	130,130,130,130	0
57	MG	RA	3111	1/1	0.53	0.42	130,130,130,130	0
57	MG	XA	1661	1/1	0.54	0.35	130,130,130,130	0
57	MG	RA	3064	1/1	0.54	0.38	130,130,130,130	0
57	MG	YA	3246	1/1	0.54	0.16	130,130,130,130	0
57	MG	XA	1650	1/1	0.54	0.27	130,130,130,130	0
57	MG	YA	3379	1/1	0.54	0.33	130,130,130,130	0
57	MG	RA	3264	1/1	0.54	0.47	130,130,130,130	0
57	MG	YA	3273	1/1	0.54	0.34	130,130,130,130	0
57	MG	QA	1603	1/1	0.54	0.15	130,130,130,130	0
57	MG	YA	3158	1/1	0.54	0.74	130,130,130,130	0
57	MG	RA	3013	1/1	0.54	0.58	130,130,130,130	0
57	MG	YA	3205	1/1	0.54	0.28	130,130,130,130	0
57	MG	XA	1636	1/1	0.54	0.34	130,130,130,130	0
57	MG	RA	3118	1/1	0.54	0.58	130,130,130,130	0
57	MG	RA	3261	1/1	0.54	0.69	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3144	1/1	0.54	0.50	130,130,130,130	0
57	MG	YA	3042	1/1	0.54	0.61	130,130,130,130	0
57	MG	YD	301	1/1	0.55	0.65	130,130,130,130	0
57	MG	YA	3039	1/1	0.55	0.62	130,130,130,130	0
57	MG	YA	3224	1/1	0.55	0.54	130,130,130,130	0
57	MG	YA	3278	1/1	0.55	0.31	130,130,130,130	0
57	MG	YA	3151	1/1	0.55	0.91	130,130,130,130	0
57	MG	RA	3034	1/1	0.55	0.76	130,130,130,130	0
57	MG	RA	3140	1/1	0.55	0.45	130,130,130,130	0
57	MG	RA	3117	1/1	0.55	0.77	130,130,130,130	0
57	MG	RA	3065	1/1	0.55	0.62	130,130,130,130	0
57	MG	XA	1657	1/1	0.56	0.31	130,130,130,130	0
57	MG	QA	1645	1/1	0.56	0.25	130,130,130,130	0
57	MG	YA	3368	1/1	0.56	0.90	130,130,130,130	0
57	MG	RA	3103	1/1	0.56	0.61	130,130,130,130	0
57	MG	RA	3178	1/1	0.56	0.57	130,130,130,130	0
57	MG	XA	1664	1/1	0.56	0.46	130,130,130,130	0
57	MG	YA	3061	1/1	0.56	0.81	130,130,130,130	0
57	MG	YA	3032	1/1	0.56	0.15	151,151,151,151	0
57	MG	RA	3134	1/1	0.56	0.49	130,130,130,130	0
57	MG	YA	3228	1/1	0.56	0.19	130,130,130,130	0
57	MG	RA	3249	1/1	0.56	0.51	130,130,130,130	0
57	MG	YA	3345	1/1	0.56	0.54	130,130,130,130	0
57	MG	YA	3012	1/1	0.56	0.57	130,130,130,130	0
57	MG	RA	3208	1/1	0.56	0.21	130,130,130,130	0
57	MG	YA	3073	1/1	0.56	0.60	130,130,130,130	0
57	MG	RA	3012	1/1	0.56	0.25	130,130,130,130	0
57	MG	XA	1690	1/1	0.56	0.28	130,130,130,130	0
57	MG	YA	3187	1/1	0.56	0.71	130,130,130,130	0
57	MG	XA	1621	1/1	0.56	0.34	130,130,130,130	0
57	MG	YA	3020	1/1	0.56	0.68	130,130,130,130	0
57	MG	RA	3185	1/1	0.57	0.20	130,130,130,130	0
57	MG	RA	3040	1/1	0.57	0.50	130,130,130,130	0
57	MG	YA	3219	1/1	0.57	0.36	130,130,130,130	0
57	MG	RA	3189	1/1	0.57	0.34	130,130,130,130	0
57	MG	YA	3207	1/1	0.57	0.51	130,130,130,130	0
57	MG	RA	3210	1/1	0.57	0.28	130,130,130,130	0
57	MG	QA	1666	1/1	0.57	0.30	130,130,130,130	0
57	MG	QA	1648	1/1	0.57	0.17	130,130,130,130	0
57	MG	YA	3078	1/1	0.57	0.50	130,130,130,130	0
57	MG	RA	3219	1/1	0.57	0.39	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3271	1/1	0.57	0.41	130,130,130,130	0
57	MG	QA	1662	1/1	0.57	0.20	130,130,130,130	0
57	MG	YA	3166	1/1	0.58	0.48	130,130,130,130	0
57	MG	RA	3290	1/1	0.58	0.32	130,130,130,130	0
57	MG	QA	1605	1/1	0.58	0.51	130,130,130,130	0
57	MG	XA	1671	1/1	0.58	0.37	130,130,130,130	0
57	MG	RA	3091	1/1	0.58	0.47	130,130,130,130	0
57	MG	XA	1688	1/1	0.58	0.37	130,130,130,130	0
57	MG	QA	1623	1/1	0.58	0.20	130,130,130,130	0
57	MG	YB	202	1/1	0.58	0.28	130,130,130,130	0
57	MG	YA	3178	1/1	0.58	0.32	130,130,130,130	0
57	MG	YA	3220	1/1	0.58	0.43	130,130,130,130	0
57	MG	RA	3267	1/1	0.58	0.43	130,130,130,130	0
57	MG	XA	1662	1/1	0.58	0.35	130,130,130,130	0
57	MG	RA	3256	1/1	0.58	0.68	130,130,130,130	0
57	MG	YA	3284	1/1	0.58	0.81	130,130,130,130	0
57	MG	RA	3230	1/1	0.58	0.34	130,130,130,130	0
57	MG	RA	3059	1/1	0.58	0.46	130,130,130,130	0
57	MG	YA	3363	1/1	0.58	0.59	130,130,130,130	0
57	MG	YA	3100	1/1	0.58	0.58	130,130,130,130	0
57	MG	YA	3163	1/1	0.58	0.47	130,130,130,130	0
57	MG	YA	3309	1/1	0.59	0.47	130,130,130,130	0
57	MG	RA	3039	1/1	0.59	0.65	130,130,130,130	0
57	MG	YA	3192	1/1	0.59	0.32	130,130,130,130	0
57	MG	YA	3055	1/1	0.59	0.44	130,130,130,130	0
57	MG	RA	3158	1/1	0.59	0.46	130,130,130,130	0
57	MG	RA	3033	1/1	0.59	0.53	130,130,130,130	0
57	MG	YB	204	1/1	0.59	0.34	130,130,130,130	0
57	MG	RA	3161	1/1	0.59	0.32	130,130,130,130	0
57	MG	YA	3124	1/1	0.59	0.60	130,130,130,130	0
57	MG	RA	3007	1/1	0.59	0.62	130,130,130,130	0
57	MG	YA	3291	1/1	0.59	0.72	130,130,130,130	0
57	MG	RA	3104	1/1	0.59	0.52	130,130,130,130	0
57	MG	YA	3161	1/1	0.59	0.43	130,130,130,130	0
57	MG	RA	3164	1/1	0.59	0.41	130,130,130,130	0
57	MG	RA	3292	1/1	0.59	0.96	130,130,130,130	0
57	MG	RA	3276	1/1	0.59	0.67	130,130,130,130	0
57	MG	YA	3168	1/1	0.59	0.83	130,130,130,130	0
57	MG	YA	3305	1/1	0.59	0.47	130,130,130,130	0
57	MG	RA	3299	1/1	0.60	0.26	130,130,130,130	0
57	MG	YA	3098	1/1	0.60	0.33	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3100	1/1	0.60	0.81	130,130,130,130	0
57	MG	RA	3211	1/1	0.60	0.30	130,130,130,130	0
57	MG	YA	3250	1/1	0.60	0.29	130,130,130,130	0
57	MG	YA	3347	1/1	0.60	0.33	130,130,130,130	0
57	MG	QA	1638	1/1	0.60	0.20	130,130,130,130	0
57	MG	RA	3092	1/1	0.60	0.46	130,130,130,130	0
57	MG	RA	3175	1/1	0.60	0.38	130,130,130,130	0
57	MG	YA	3227	1/1	0.60	0.22	130,130,130,130	0
57	MG	RA	3187	1/1	0.60	0.59	130,130,130,130	0
57	MG	YA	3354	1/1	0.60	0.21	130,130,130,130	0
57	MG	YA	3150	1/1	0.60	0.51	130,130,130,130	0
57	MG	YA	3230	1/1	0.60	0.30	130,130,130,130	0
57	MG	QA	1655	1/1	0.60	0.15	130,130,130,130	0
57	MG	QA	1627	1/1	0.60	0.40	130,130,130,130	0
57	MG	Y0	101	1/1	0.60	0.68	130,130,130,130	0
57	MG	RA	3049	1/1	0.60	0.41	130,130,130,130	0
57	MG	RA	3138	1/1	0.60	0.25	130,130,130,130	0
57	MG	RA	3011	1/1	0.61	0.32	130,130,130,130	0
57	MG	YA	3289	1/1	0.61	0.71	130,130,130,130	0
57	MG	YA	3057	1/1	0.61	0.49	130,130,130,130	0
57	MG	RA	3246	1/1	0.61	0.59	130,130,130,130	0
57	MG	XA	1631	1/1	0.61	0.26	130,130,130,130	0
57	MG	YA	3335	1/1	0.61	0.71	130,130,130,130	0
57	MG	QA	1661	1/1	0.61	0.24	130,130,130,130	0
57	MG	YA	3338	1/1	0.61	0.61	130,130,130,130	0
57	MG	YA	3085	1/1	0.61	0.38	130,130,130,130	0
57	MG	RA	3087	1/1	0.61	0.41	130,130,130,130	0
57	MG	RA	3089	1/1	0.61	0.48	130,130,130,130	0
57	MG	XA	1674	1/1	0.61	0.44	130,130,130,130	0
57	MG	YA	3120	1/1	0.61	0.60	130,130,130,130	0
57	MG	QA	1647	1/1	0.61	0.15	130,130,130,130	0
57	MG	YA	3067	1/1	0.61	0.50	130,130,130,130	0
57	MG	RA	3221	1/1	0.61	0.45	130,130,130,130	0
57	MG	RA	3015	1/1	0.61	0.48	130,130,130,130	0
57	MG	YA	3049	1/1	0.61	0.84	130,130,130,130	0
57	MG	RA	3068	1/1	0.61	0.48	130,130,130,130	0
57	MG	QA	1684	1/1	0.61	0.14	137,137,137,137	0
57	MG	RA	3262	1/1	0.61	0.31	130,130,130,130	0
57	MG	RA	3241	1/1	0.61	0.25	130,130,130,130	0
57	MG	RA	3170	1/1	0.61	0.36	130,130,130,130	0
57	MG	YA	3279	1/1	0.62	0.40	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3101	1/1	0.62	0.57	130,130,130,130	0
57	MG	YA	3366	1/1	0.62	0.38	130,130,130,130	0
57	MG	YA	3190	1/1	0.62	0.18	130,130,130,130	0
57	MG	YA	3191	1/1	0.62	0.55	130,130,130,130	0
57	MG	YA	3370	1/1	0.62	0.37	130,130,130,130	0
57	MG	RA	3115	1/1	0.62	0.47	130,130,130,130	0
57	MG	RA	3283	1/1	0.62	0.45	130,130,130,130	0
57	MG	YA	3132	1/1	0.62	0.39	130,130,130,130	0
57	MG	YA	3376	1/1	0.62	0.46	130,130,130,130	0
57	MG	YA	3106	1/1	0.62	0.51	130,130,130,130	0
57	MG	YA	3041	1/1	0.62	0.27	130,130,130,130	0
57	MG	RB	201	1/1	0.62	0.17	130,130,130,130	0
57	MG	RA	3197	1/1	0.62	0.23	130,130,130,130	0
57	MG	YA	3047	1/1	0.62	0.56	130,130,130,130	0
57	MG	YA	3066	1/1	0.62	0.81	130,130,130,130	0
57	MG	RA	3303	1/1	0.62	0.26	130,130,130,130	0
57	MG	XA	1648	1/1	0.62	0.48	130,130,130,130	0
57	MG	RA	3102	1/1	0.62	0.25	130,130,130,130	0
57	MG	RA	3096	1/1	0.62	0.46	130,130,130,130	0
57	MG	XA	1670	1/1	0.62	0.24	130,130,130,130	0
57	MG	QA	1625	1/1	0.62	0.33	130,130,130,130	0
57	MG	QA	1640	1/1	0.62	0.13	130,130,130,130	0
57	MG	RA	3193	1/1	0.62	0.36	130,130,130,130	0
57	MG	RA	3051	1/1	0.62	0.28	130,130,130,130	0
57	MG	RA	3195	1/1	0.62	0.39	130,130,130,130	0
57	MG	QA	1646	1/1	0.63	0.32	130,130,130,130	0
57	MG	YA	3257	1/1	0.63	0.23	130,130,130,130	0
57	MG	RA	3288	1/1	0.63	0.42	130,130,130,130	0
57	MG	RA	3053	1/1	0.63	0.78	130,130,130,130	0
57	MG	RA	3202	1/1	0.63	0.22	130,130,130,130	0
57	MG	XA	1666	1/1	0.63	0.28	130,130,130,130	0
57	MG	YA	3165	1/1	0.63	0.89	130,130,130,130	0
57	MG	QA	1643	1/1	0.63	0.25	130,130,130,130	0
57	MG	XA	1659	1/1	0.63	0.41	130,130,130,130	0
57	MG	YA	3374	1/1	0.63	0.35	130,130,130,130	0
57	MG	RA	3166	1/1	0.63	0.48	130,130,130,130	0
57	MG	RA	3042	1/1	0.63	0.45	130,130,130,130	0
57	MG	YA	3315	1/1	0.63	0.58	130,130,130,130	0
57	MG	YA	3235	1/1	0.63	0.29	130,130,130,130	0
57	MG	YA	3293	1/1	0.64	0.66	130,130,130,130	0
57	MG	YA	3170	1/1	0.64	0.59	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3268	1/1	0.64	0.38	130,130,130,130	0
57	MG	RA	3062	1/1	0.64	0.40	130,130,130,130	0
57	MG	YA	3328	1/1	0.64	0.26	130,130,130,130	0
57	MG	RA	3209	1/1	0.64	0.16	130,130,130,130	0
57	MG	RA	3023	1/1	0.64	0.48	130,130,130,130	0
57	MG	RA	3154	1/1	0.64	0.33	130,130,130,130	0
57	MG	RA	3239	1/1	0.64	0.20	130,130,130,130	0
57	MG	YA	3361	1/1	0.64	0.55	130,130,130,130	0
57	MG	YA	3259	1/1	0.64	0.20	130,130,130,130	0
57	MG	RA	3273	1/1	0.64	0.84	130,130,130,130	0
57	MG	RA	3084	1/1	0.64	0.99	130,130,130,130	0
57	MG	YA	3243	1/1	0.64	0.27	130,130,130,130	0
57	MG	QA	1663	1/1	0.64	0.09	130,130,130,130	0
57	MG	XF	301	1/1	0.64	0.20	130,130,130,130	0
57	MG	YA	3122	1/1	0.64	0.22	130,130,130,130	0
57	MG	YA	3343	1/1	0.64	0.30	130,130,130,130	0
57	MG	RA	3318	1/1	0.64	0.44	130,130,130,130	0
57	MG	RA	3255	1/1	0.65	0.61	130,130,130,130	0
57	MG	XM	201	1/1	0.65	0.25	153,153,153,153	0
57	MG	YA	3179	1/1	0.65	0.41	130,130,130,130	0
57	MG	RA	3017	1/1	0.65	0.34	130,130,130,130	0
57	MG	RA	3010	1/1	0.65	0.71	130,130,130,130	0
57	MG	YA	3316	1/1	0.65	0.64	130,130,130,130	0
57	MG	YA	3292	1/1	0.65	0.63	130,130,130,130	0
57	MG	RA	3179	1/1	0.65	0.34	130,130,130,130	0
57	MG	YA	3153	1/1	0.65	0.36	130,130,130,130	0
57	MG	RA	3296	1/1	0.65	0.11	130,130,130,130	0
57	MG	RA	3085	1/1	0.65	0.43	130,130,130,130	0
57	MG	YA	3218	1/1	0.65	0.48	130,130,130,130	0
57	MG	QA	1626	1/1	0.65	0.33	130,130,130,130	0
57	MG	YA	3174	1/1	0.65	0.37	130,130,130,130	0
57	MG	RA	3214	1/1	0.65	0.50	130,130,130,130	0
57	MG	RA	3215	1/1	0.65	0.19	130,130,130,130	0
57	MG	RA	3097	1/1	0.66	0.40	130,130,130,130	0
57	MG	RA	3152	1/1	0.66	0.52	130,130,130,130	0
57	MG	YA	3275	1/1	0.66	0.62	130,130,130,130	0
57	MG	RA	3046	1/1	0.66	0.20	130,130,130,130	0
57	MG	YA	3322	1/1	0.66	0.29	130,130,130,130	0
57	MG	YA	3021	1/1	0.66	0.32	130,130,130,130	0
57	MG	YA	3303	1/1	0.66	0.27	130,130,130,130	0
57	MG	RA	3110	1/1	0.66	0.36	130,130,130,130	0
57	MG	RA	3248	1/1	0.66	0.16	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3164	1/1	0.66	0.50	130,130,130,130	0
57	MG	QA	1654	1/1	0.66	0.19	130,130,130,130	0
57	MG	RA	3280	1/1	0.66	0.80	130,130,130,130	0
57	MG	XA	1685	1/1	0.66	0.46	130,130,130,130	0
57	MG	RA	3080	1/1	0.66	0.53	130,130,130,130	0
57	MG	YA	3183	1/1	0.66	0.21	130,130,130,130	0
57	MG	QA	1653	1/1	0.67	0.47	130,130,130,130	0
57	MG	XA	1611	1/1	0.67	0.80	130,130,130,130	0
57	MG	XA	1629	1/1	0.67	0.12	130,130,130,130	0
57	MG	RA	3008	1/1	0.67	0.30	147,147,147,147	0
57	MG	RA	3295	1/1	0.67	0.76	130,130,130,130	0
57	MG	YA	3084	1/1	0.67	0.39	130,130,130,130	0
57	MG	YA	3350	1/1	0.67	0.66	130,130,130,130	0
57	MG	RA	3247	1/1	0.67	0.72	130,130,130,130	0
57	MG	RA	3038	1/1	0.67	0.32	130,130,130,130	0
57	MG	YA	3239	1/1	0.67	0.29	130,130,130,130	0
57	MG	RA	3027	1/1	0.67	0.58	130,130,130,130	0
57	MG	XA	1651	1/1	0.67	0.30	130,130,130,130	0
57	MG	YB	208	1/1	0.67	0.39	130,130,130,130	0
57	MG	RA	3099	1/1	0.67	0.33	130,130,130,130	0
57	MG	YA	3133	1/1	0.67	0.38	130,130,130,130	0
57	MG	YA	3008	1/1	0.67	0.67	130,130,130,130	0
57	MG	YA	3113	1/1	0.67	0.73	130,130,130,130	0
57	MG	YA	3031	1/1	0.67	0.61	130,130,130,130	0
57	MG	RA	3240	1/1	0.67	0.68	130,130,130,130	0
57	MG	YA	3225	1/1	0.67	0.10	130,130,130,130	0
57	MG	YR	201	1/1	0.67	0.55	130,130,130,130	0
57	MG	RA	3188	1/1	0.67	0.26	130,130,130,130	0
57	MG	RA	3125	1/1	0.67	0.27	130,130,130,130	0
57	MG	YA	3099	1/1	0.68	0.53	130,130,130,130	0
57	MG	YA	3356	1/1	0.68	0.40	130,130,130,130	0
57	MG	XA	1649	1/1	0.68	0.30	130,130,130,130	0
57	MG	YA	3044	1/1	0.68	0.33	130,130,130,130	0
57	MG	RA	3287	1/1	0.68	0.78	130,130,130,130	0
57	MG	RA	3082	1/1	0.68	0.12	130,130,130,130	0
57	MG	RA	3083	1/1	0.68	0.93	130,130,130,130	0
57	MG	YA	3050	1/1	0.68	0.42	130,130,130,130	0
57	MG	QA	1668	1/1	0.68	0.60	130,130,130,130	0
57	MG	YA	3326	1/1	0.68	0.70	130,130,130,130	0
57	MG	RA	3072	1/1	0.68	0.62	130,130,130,130	0
57	MG	YA	3288	1/1	0.68	0.49	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3096	1/1	0.68	0.46	130,130,130,130	0
57	MG	RA	3020	1/1	0.68	0.49	130,130,130,130	0
57	MG	YA	3143	1/1	0.68	0.50	130,130,130,130	0
57	MG	YA	3063	1/1	0.68	0.56	130,130,130,130	0
57	MG	YA	3314	1/1	0.68	0.69	130,130,130,130	0
57	MG	RA	3165	1/1	0.69	0.24	130,130,130,130	0
57	MG	YA	3102	1/1	0.69	0.52	130,130,130,130	0
57	MG	YA	3346	1/1	0.69	0.36	130,130,130,130	0
57	MG	YA	3156	1/1	0.69	0.45	130,130,130,130	0
57	MG	RA	3313	1/1	0.69	0.51	130,130,130,130	0
57	MG	RB	202	1/1	0.69	0.13	130,130,130,130	0
57	MG	QA	1657	1/1	0.69	0.16	130,130,130,130	0
57	MG	YA	3245	1/1	0.69	0.33	130,130,130,130	0
57	MG	RB	204	1/1	0.69	0.10	133,133,133,133	0
57	MG	YB	203	1/1	0.69	0.27	130,130,130,130	0
57	MG	RA	3213	1/1	0.69	0.16	130,130,130,130	0
57	MG	YA	3248	1/1	0.69	0.20	130,130,130,130	0
57	MG	RA	3119	1/1	0.70	0.32	130,130,130,130	0
57	MG	Y8	101	1/1	0.70	0.65	130,130,130,130	0
57	MG	RA	3150	1/1	0.70	0.59	130,130,130,130	0
57	MG	RA	3160	1/1	0.70	0.12	130,130,130,130	0
57	MG	RA	3257	1/1	0.70	0.47	130,130,130,130	0
57	MG	RA	3321	1/1	0.70	0.33	130,130,130,130	0
57	MG	YA	3359	1/1	0.70	0.62	130,130,130,130	0
57	MG	RE	302	1/1	0.70	0.54	130,130,130,130	0
57	MG	YA	3197	1/1	0.70	0.39	130,130,130,130	0
57	MG	YA	3209	1/1	0.70	0.29	130,130,130,130	0
57	MG	YQ	201	1/1	0.70	0.24	130,130,130,130	0
57	MG	YA	3069	1/1	0.70	0.40	130,130,130,130	0
57	MG	RA	3029	1/1	0.70	0.23	130,130,130,130	0
57	MG	XA	1686	1/1	0.70	0.26	130,130,130,130	0
57	MG	YA	3344	1/1	0.71	0.57	130,130,130,130	0
57	MG	RA	3245	1/1	0.71	0.29	130,130,130,130	0
57	MG	YA	3232	1/1	0.71	0.25	130,130,130,130	0
57	MG	YA	3334	1/1	0.71	0.65	130,130,130,130	0
57	MG	YA	3286	1/1	0.71	0.59	130,130,130,130	0
57	MG	RA	3121	1/1	0.71	0.57	130,130,130,130	0
57	MG	RA	3320	1/1	0.71	0.37	130,130,130,130	0
57	MG	QA	1628	1/1	0.71	0.27	130,130,130,130	0
57	MG	RA	3190	1/1	0.71	0.24	130,130,130,130	0
57	MG	YA	3329	1/1	0.71	0.35	130,130,130,130	0
57	MG	RA	3244	1/1	0.71	0.59	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3315	1/1	0.71	0.41	130,130,130,130	0
57	MG	YA	3016	1/1	0.72	0.43	130,130,130,130	0
57	MG	RA	3176	1/1	0.72	0.44	130,130,130,130	0
57	MG	RA	3037	1/1	0.72	0.35	130,130,130,130	0
57	MG	YA	3172	1/1	0.72	0.20	130,130,130,130	0
57	MG	RA	3317	1/1	0.72	0.22	130,130,130,130	0
57	MG	YA	3283	1/1	0.72	0.41	130,130,130,130	0
57	MG	RA	3250	1/1	0.72	0.47	130,130,130,130	0
57	MG	YA	3217	1/1	0.72	0.25	130,130,130,130	0
57	MG	YA	3035	1/1	0.72	0.49	130,130,130,130	0
57	MG	QA	1619	1/1	0.72	0.16	130,130,130,130	0
57	MG	XA	1622	1/1	0.72	0.17	130,130,130,130	0
57	MG	YA	3308	1/1	0.72	0.18	130,130,130,130	0
57	MG	XA	1607	1/1	0.72	0.18	130,130,130,130	0
57	MG	RA	3184	1/1	0.73	0.30	130,130,130,130	0
57	MG	RP	202	1/1	0.73	0.28	130,130,130,130	0
57	MG	RQ	201	1/1	0.73	0.25	130,130,130,130	0
57	MG	YA	3139	1/1	0.73	0.57	130,130,130,130	0
57	MG	YA	3299	1/1	0.73	0.31	130,130,130,130	0
57	MG	YA	3154	1/1	0.73	0.19	130,130,130,130	0
57	MG	RA	3107	1/1	0.73	0.67	130,130,130,130	0
57	MG	RA	3066	1/1	0.73	0.36	130,130,130,130	0
57	MG	RA	3275	1/1	0.73	0.26	130,130,130,130	0
57	MG	RA	3088	1/1	0.73	0.27	130,130,130,130	0
57	MG	YA	3119	1/1	0.73	0.65	130,130,130,130	0
57	MG	RA	3316	1/1	0.73	0.45	130,130,130,130	0
57	MG	YA	3108	1/1	0.73	0.18	130,130,130,130	0
57	MG	YA	3038	1/1	0.73	0.45	130,130,130,130	0
57	MG	YA	3148	1/1	0.73	0.66	130,130,130,130	0
57	MG	YA	3033	1/1	0.74	0.52	130,130,130,130	0
57	MG	YD	303	1/1	0.74	0.42	130,130,130,130	0
57	MG	QA	1652	1/1	0.74	0.26	130,130,130,130	0
57	MG	YA	3233	1/1	0.74	0.89	130,130,130,130	0
57	MG	XA	1634	1/1	0.74	0.11	130,130,130,130	0
57	MG	YA	3024	1/1	0.74	0.33	130,130,130,130	0
57	MG	RA	3093	1/1	0.74	0.32	130,130,130,130	0
57	MG	RA	3106	1/1	0.74	0.23	130,130,130,130	0
57	MG	R5	101	1/1	0.74	0.34	130,130,130,130	0
57	MG	RA	3136	1/1	0.74	0.14	130,130,130,130	0
57	MG	RA	3235	1/1	0.74	0.40	130,130,130,130	0
57	MG	XA	1689	1/1	0.75	0.50	130,130,130,130	0
57	MG	YA	3360	1/1	0.75	0.15	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3302	1/1	0.75	0.45	130,130,130,130	0
57	MG	YA	3269	1/1	0.75	0.38	130,130,130,130	0
57	MG	XA	1618	1/1	0.75	0.08	130,130,130,130	0
57	MG	RA	3285	1/1	0.75	0.65	130,130,130,130	0
57	MG	QA	1604	1/1	0.75	0.18	130,130,130,130	0
57	MG	YA	3026	1/1	0.75	0.26	130,130,130,130	0
57	MG	QA	1656	1/1	0.75	0.14	130,130,130,130	0
57	MG	YA	3005	1/1	0.75	0.60	130,130,130,130	0
57	MG	RA	3025	1/1	0.75	0.40	130,130,130,130	0
57	MG	QA	1610	1/1	0.75	0.78	130,130,130,130	0
57	MG	RA	3168	1/1	0.76	0.09	130,130,130,130	0
57	MG	YA	3372	1/1	0.76	0.49	130,130,130,130	0
57	MG	YA	3037	1/1	0.76	0.49	130,130,130,130	0
57	MG	RA	3127	1/1	0.76	0.31	130,130,130,130	0
57	MG	QA	1649	1/1	0.76	0.16	130,130,130,130	0
57	MG	QA	1685	1/1	0.76	0.22	130,130,130,130	0
57	MG	RA	3014	1/1	0.76	0.66	130,130,130,130	0
57	MG	QA	1660	1/1	0.76	0.10	130,130,130,130	0
57	MG	Y8	103	1/1	0.76	0.31	130,130,130,130	0
57	MG	YX	101	1/1	0.76	0.33	130,130,130,130	0
57	MG	RA	3146	1/1	0.77	0.35	130,130,130,130	0
57	MG	RA	3228	1/1	0.77	0.17	130,130,130,130	0
57	MG	RA	3218	1/1	0.77	0.28	130,130,130,130	0
57	MG	QA	1639	1/1	0.77	0.18	130,130,130,130	0
57	MG	YA	3115	1/1	0.77	0.21	130,130,130,130	0
57	MG	YA	3282	1/1	0.77	0.47	130,130,130,130	0
57	MG	YA	3300	1/1	0.77	0.57	130,130,130,130	0
57	MG	RA	3205	1/1	0.77	0.43	130,130,130,130	0
57	MG	YA	3298	1/1	0.78	0.74	130,130,130,130	0
57	MG	YA	3045	1/1	0.78	0.35	130,130,130,130	0
57	MG	QA	1613	1/1	0.78	0.23	130,130,130,130	0
57	MG	XA	1613	1/1	0.78	0.62	130,130,130,130	0
57	MG	XA	1626	1/1	0.78	0.26	130,130,130,130	0
57	MG	YA	3088	1/1	0.78	0.57	130,130,130,130	0
57	MG	YA	3036	1/1	0.78	0.77	130,130,130,130	0
57	MG	YA	3103	1/1	0.78	0.22	130,130,130,130	0
57	MG	XA	1619	1/1	0.78	0.28	130,130,130,130	0
57	MG	YA	3358	1/1	0.78	0.25	130,130,130,130	0
57	MG	RA	3077	1/1	0.78	0.25	130,130,130,130	0
57	MG	XV	102	1/1	0.78	0.21	130,130,130,130	0
57	MG	QA	1659	1/1	0.78	0.14	130,130,130,130	0
57	MG	XA	1668	1/1	0.78	0.12	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	Y2	101	1/1	0.78	0.17	130,130,130,130	0
57	MG	QM	202	1/1	0.78	0.25	130,130,130,130	0
57	MG	YA	3295	1/1	0.79	0.69	130,130,130,130	0
57	MG	YA	3287	1/1	0.79	0.73	130,130,130,130	0
57	MG	Y5	102	1/1	0.79	0.36	130,130,130,130	0
57	MG	QA	1611	1/1	0.79	0.21	130,130,130,130	0
57	MG	YP	201	1/1	0.79	0.41	130,130,130,130	0
57	MG	YA	3046	1/1	0.79	0.58	130,130,130,130	0
57	MG	RA	3048	1/1	0.79	0.38	130,130,130,130	0
57	MG	RA	3142	1/1	0.79	0.23	130,130,130,130	0
57	MG	RA	3071	1/1	0.79	0.35	130,130,130,130	0
57	MG	Y5	101	1/1	0.79	0.34	130,130,130,130	0
57	MG	YA	3336	1/1	0.79	0.31	130,130,130,130	0
57	MG	RA	3132	1/1	0.80	0.20	130,130,130,130	0
57	MG	YA	3013	1/1	0.80	0.65	130,130,130,130	0
57	MG	RA	3305	1/1	0.80	0.26	139,139,139,139	0
57	MG	QA	1669	1/1	0.80	0.24	130,130,130,130	0
57	MG	YA	3281	1/1	0.80	0.49	130,130,130,130	0
57	MG	YA	3306	1/1	0.80	0.26	130,130,130,130	0
57	MG	YA	3068	1/1	0.80	0.42	140,140,140,140	0
57	MG	YA	3010	1/1	0.80	0.57	130,130,130,130	0
57	MG	RA	3044	1/1	0.80	0.20	130,130,130,130	0
57	MG	YA	3369	1/1	0.80	0.43	130,130,130,130	0
57	MG	YA	3189	1/1	0.81	0.22	130,130,130,130	0
57	MG	RA	3143	1/1	0.81	0.19	130,130,130,130	0
57	MG	RA	3269	1/1	0.81	0.55	130,130,130,130	0
57	MG	RA	3212	1/1	0.81	0.26	130,130,130,130	0
57	MG	YA	3167	1/1	0.81	0.20	130,130,130,130	0
57	MG	XA	1632	1/1	0.81	0.09	130,130,130,130	0
57	MG	RA	3222	1/1	0.81	0.47	130,130,130,130	0
57	MG	RA	3123	1/1	0.81	0.29	130,130,130,130	0
57	MG	RA	3224	1/1	0.81	0.33	130,130,130,130	0
57	MG	QA	1673	1/1	0.82	0.41	130,130,130,130	0
57	MG	RF	301	1/1	0.82	0.12	130,130,130,130	0
57	MG	YA	3241	1/1	0.82	0.18	130,130,130,130	0
57	MG	R7	101	1/1	0.82	0.28	130,130,130,130	0
57	MG	YA	3251	1/1	0.82	0.27	130,130,130,130	0
57	MG	RA	3278	1/1	0.82	0.24	130,130,130,130	0
57	MG	XA	1658	1/1	0.82	0.09	130,130,130,130	0
57	MG	RA	3301	1/1	0.82	0.69	130,130,130,130	0
57	MG	RA	3026	1/1	0.82	0.55	130,130,130,130	0
57	MG	YA	3070	1/1	0.83	0.51	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3265	1/1	0.83	0.21	130,130,130,130	0
57	MG	YA	3134	1/1	0.83	0.19	130,130,130,130	0
57	MG	RA	3258	1/1	0.83	0.22	130,130,130,130	0
57	MG	QA	1681	1/1	0.83	0.13	130,130,130,130	0
57	MG	YA	3152	1/1	0.83	0.27	130,130,130,130	0
57	MG	YA	3280	1/1	0.84	0.14	130,130,130,130	0
57	MG	YA	3030	1/1	0.84	0.35	130,130,130,130	0
57	MG	YA	3040	1/1	0.84	0.27	130,130,130,130	0
57	MG	XA	1623	1/1	0.84	0.19	130,130,130,130	0
57	MG	RA	3260	1/1	0.84	0.20	130,130,130,130	0
57	MG	YA	3006	1/1	0.85	0.42	130,130,130,130	0
57	MG	QA	1683	1/1	0.85	0.14	130,130,130,130	0
57	MG	RA	3306	1/1	0.85	0.11	130,130,130,130	0
57	MG	QV	101	1/1	0.85	0.70	130,130,130,130	0
57	MG	QV	104	1/1	0.85	0.26	130,130,130,130	0
57	MG	YV	301	1/1	0.85	0.26	130,130,130,130	0
57	MG	XA	1675	1/1	0.85	0.07	130,130,130,130	0
57	MG	XA	1602	1/1	0.86	0.12	130,130,130,130	0
57	MG	RA	3004	1/1	0.86	0.40	130,130,130,130	0
57	MG	RA	3206	1/1	0.86	0.22	130,130,130,130	0
57	MG	QA	1651	1/1	0.86	0.16	130,130,130,130	0
57	MG	YA	3324	1/1	0.86	0.12	130,130,130,130	0
57	MG	RA	3297	1/1	0.86	0.21	130,130,130,130	0
57	MG	YA	3258	1/1	0.86	0.18	130,130,130,130	0
57	MG	YA	3029	1/1	0.86	0.15	130,130,130,130	0
57	MG	YA	3365	1/1	0.87	0.20	130,130,130,130	0
57	MG	XY	101	1/1	0.87	0.12	130,130,130,130	0
57	MG	QA	1680	1/1	0.87	0.35	130,130,130,130	0
57	MG	YA	3114	1/1	0.87	0.16	130,130,130,130	0
57	MG	RA	3005	1/1	0.88	0.42	130,130,130,130	0
57	MG	RA	3137	1/1	0.88	0.16	130,130,130,130	0
57	MG	RA	3076	1/1	0.88	0.34	130,130,130,130	0
57	MG	YA	3320	1/1	0.88	0.26	130,130,130,130	0
57	MG	QM	201	1/1	0.88	0.07	130,130,130,130	0
57	MG	YA	3180	1/1	0.88	0.26	130,130,130,130	0
57	MG	XA	1644	1/1	0.89	0.12	130,130,130,130	0
57	MG	RA	3002	1/1	0.89	0.32	130,130,130,130	0
57	MG	RA	3277	1/1	0.89	0.19	130,130,130,130	0
57	MG	YA	3276	1/1	0.89	0.18	130,130,130,130	0
57	MG	RA	3171	1/1	0.89	0.20	130,130,130,130	0
57	MG	YA	3159	1/1	0.89	0.09	130,130,130,130	0
57	MG	YA	3256	1/1	0.90	0.17	130,130,130,130	0

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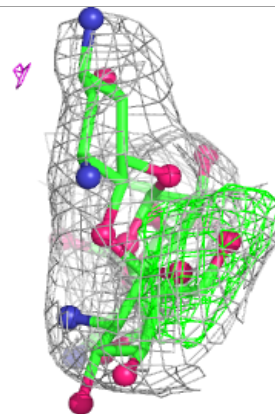
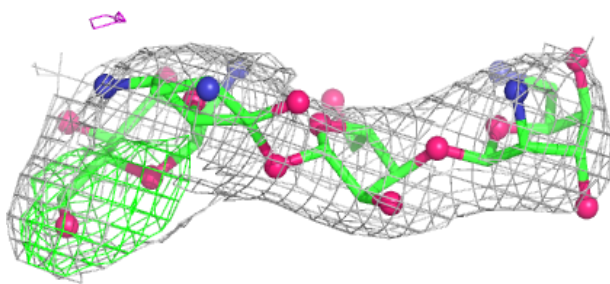
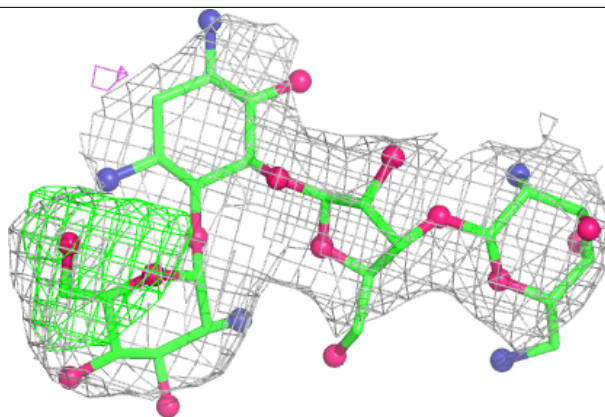
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1612	1/1	0.90	0.14	130,130,130,130	0
57	MG	YP	202	1/1	0.90	0.18	130,130,130,130	0
57	MG	YB	205	1/1	0.90	0.07	130,130,130,130	0
57	MG	QA	1682	1/1	0.90	0.12	130,130,130,130	0
57	MG	YX	103	1/1	0.90	0.15	130,130,130,130	0
58	PAR	QA	1667	42/42	0.90	0.19	130,130,142,148	0
57	MG	RA	3128	1/1	0.91	0.11	130,130,130,130	0
57	MG	YA	3017	1/1	0.91	0.21	130,130,130,130	0
57	MG	RA	3001	1/1	0.91	0.48	130,130,130,130	0
57	MG	YA	3236	1/1	0.92	0.15	130,130,130,130	0
57	MG	QA	1664	1/1	0.92	0.06	130,130,130,130	0
57	MG	QA	1665	1/1	0.93	0.05	130,130,130,130	0
57	MG	YA	3377	1/1	0.93	0.34	130,130,130,130	0
57	MG	RA	3281	1/1	0.93	0.15	130,130,130,130	0
57	MG	YA	3240	1/1	0.93	0.07	130,130,130,130	0
57	MG	YA	3123	1/1	0.93	0.39	130,130,130,130	0
58	PAR	XA	1679	42/42	0.93	0.20	130,130,137,169	0
60	ZN	XN	101	1/1	0.93	0.10	130,130,130,130	0
57	MG	YA	3317	1/1	0.94	0.18	130,130,130,130	0
57	MG	RP	201	1/1	0.94	0.66	196,196,196,196	0
57	MG	RU	201	1/1	0.94	0.22	130,130,130,130	0
57	MG	YX	102	1/1	0.94	0.16	130,130,130,130	0
59	SF4	QD	501	8/8	0.95	0.09	130,130,138,143	0
59	SF4	XD	501	8/8	0.95	0.09	130,130,130,130	0
57	MG	YA	3307	1/1	0.95	0.36	130,130,130,130	0
57	MG	YU	201	1/1	0.96	0.09	130,130,130,130	0
57	MG	RX	101	1/1	0.97	0.06	130,130,130,130	0

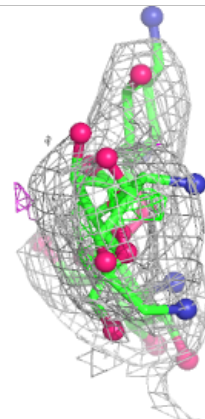
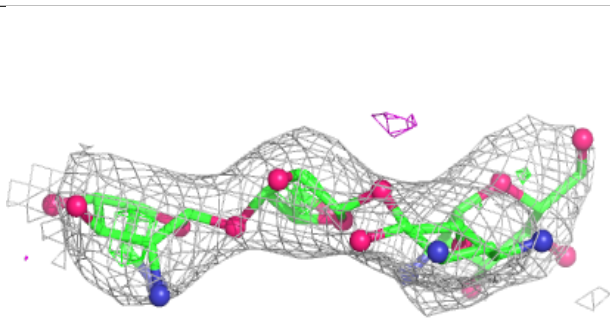
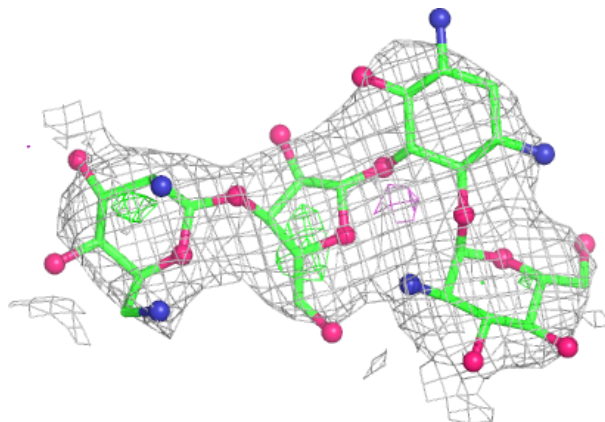
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1667:

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

**Electron density around PAR XA 1679:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.