



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 10:27 PM EST

PDB ID : 4TUB
Title : Crystal structure of tRNA-Thr bound to Codon ACC-C on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : unknown
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

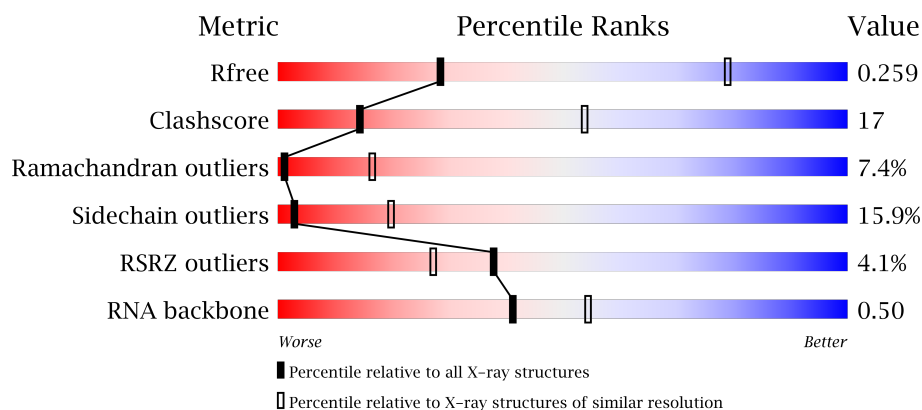
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.













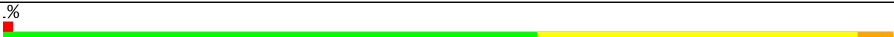


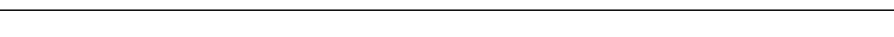
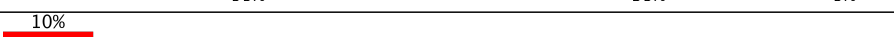
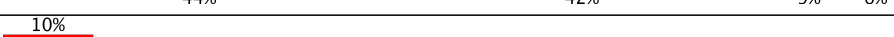



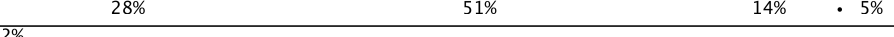





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)
RNA backbone	2435	1002 (4.30-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>0.5%</div> <div>51% 38% 9% ..</div> </div>
1	XA	1522	<div> <div>0.5%</div> <div>50% 38% 9% ..</div> </div>
2	QB	256	<div> <div>10%</div> <div>48% 36% 7% • 7%</div> </div>
2	XB	256	<div> <div>3%</div> <div>46% 36% 10% • 7%</div> </div>





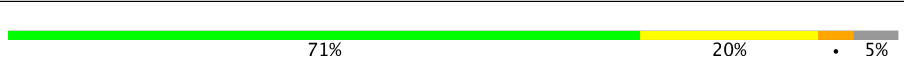
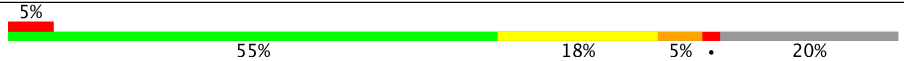
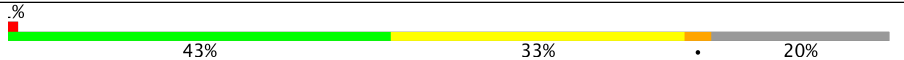
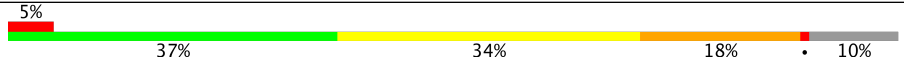
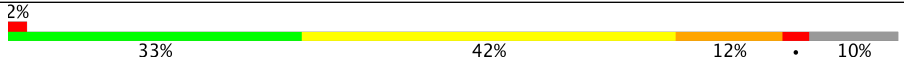
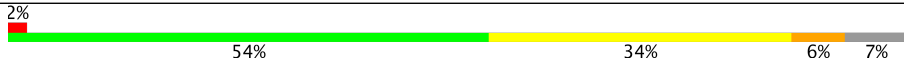
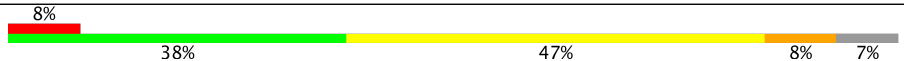
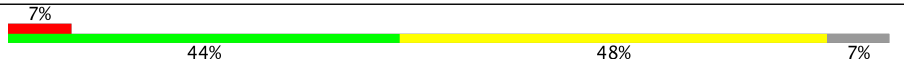

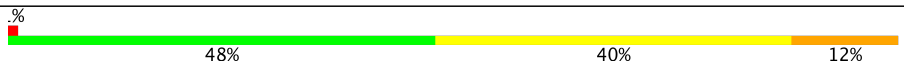
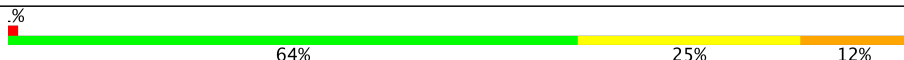

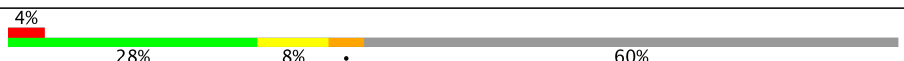
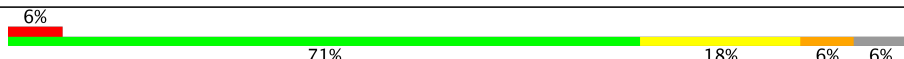



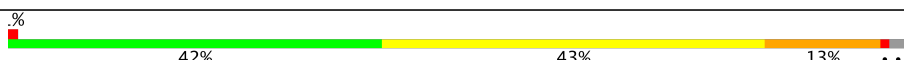
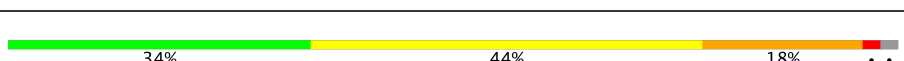
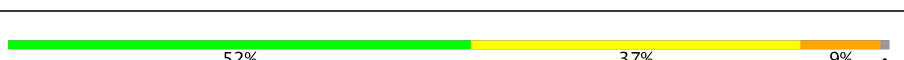
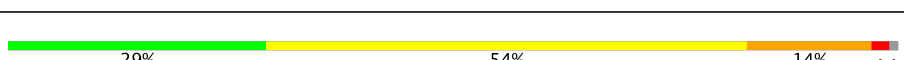
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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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



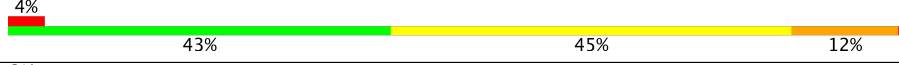

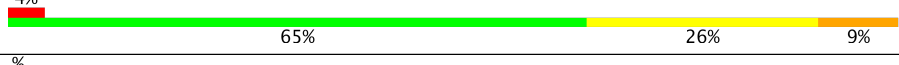
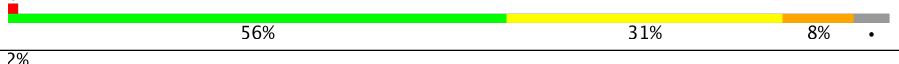
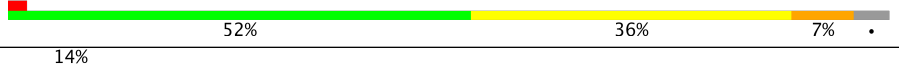
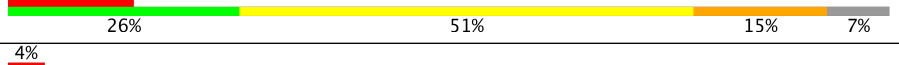
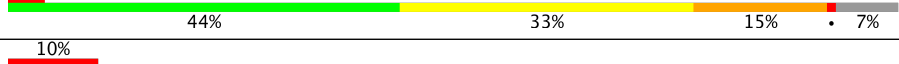


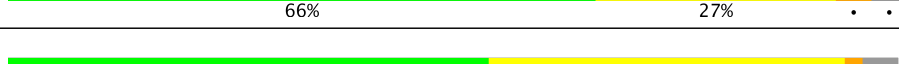
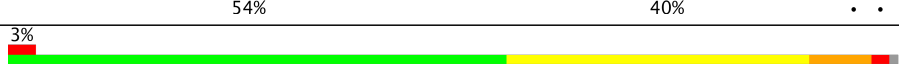
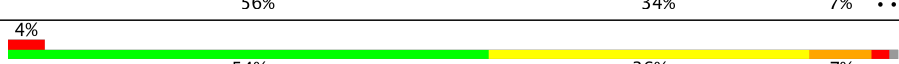

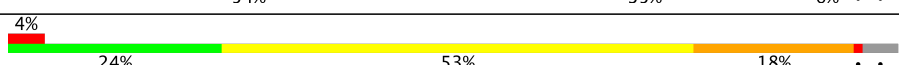
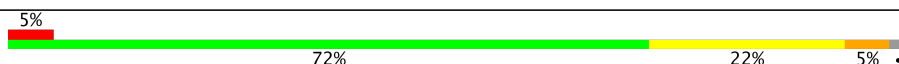
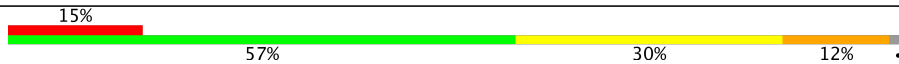

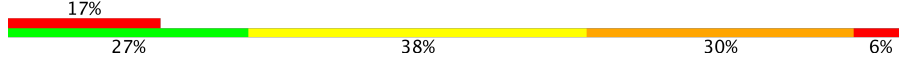

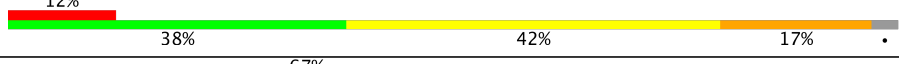

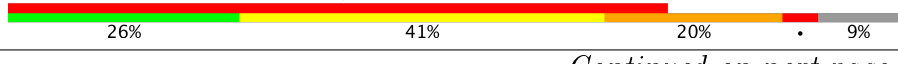

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Mol	Chain	Length	Quality of chain
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	
39	YT	146	
40	RU	118	

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

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z5	3	
56	Z6	3	

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	1602	-	-	-	X
57	MG	QA	1605	-	-	-	X
57	MG	QA	1610	-	-	-	X
57	MG	QA	1612	-	-	-	X
57	MG	QA	1613	-	-	-	X
57	MG	QA	1617	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1629	-	-	-	X
57	MG	QA	1640	-	-	-	X
57	MG	QA	1644	-	-	-	X
57	MG	QA	1650	-	-	-	X
57	MG	QA	1651	-	-	-	X
57	MG	QA	1653	-	-	-	X
57	MG	QA	1654	-	-	-	X
57	MG	QA	1655	-	-	-	X
57	MG	QA	1656	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1659	-	-	-	X
57	MG	QA	1660	-	-	-	X
57	MG	QA	1672	-	-	-	X
57	MG	QE	201	-	-	-	X
57	MG	R5	101	-	-	-	X
57	MG	RA	3003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3005	-	-	-	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	3020	-	-	-	X
57	MG	RA	3021	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3025	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3038	-	-	-	X
57	MG	RA	3040	-	-	-	X
57	MG	RA	3047	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3057	-	-	-	X
57	MG	RA	3059	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3072	-	-	-	X
57	MG	RA	3077	-	-	-	X
57	MG	RA	3079	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3088	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3106	-	-	-	X
57	MG	RA	3118	-	-	-	X
57	MG	RA	3119	-	-	-	X
57	MG	RA	3123	-	-	-	X
57	MG	RA	3130	-	-	-	X
57	MG	RA	3135	-	-	-	X
57	MG	RA	3142	-	-	-	X
57	MG	RA	3152	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3155	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3160	-	-	-	X
57	MG	RA	3169	-	-	-	X
57	MG	RA	3171	-	-	-	X
57	MG	RA	3176	-	-	-	X
57	MG	RA	3181	-	-	-	X
57	MG	RA	3201	-	-	-	X
57	MG	RA	3214	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3230	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RA	3235	-	-	-	X
57	MG	RA	3236	-	-	-	X
57	MG	RA	3240	-	-	-	X
57	MG	RA	3249	-	-	-	X
57	MG	RA	3251	-	-	-	X
57	MG	RA	3264	-	-	-	X
57	MG	RA	3266	-	-	-	X
57	MG	RA	3268	-	-	-	X
57	MG	RA	3272	-	-	-	X
57	MG	RA	3279	-	-	-	X
57	MG	RA	3280	-	-	-	X
57	MG	RA	3281	-	-	-	X
57	MG	RA	3283	-	-	-	X
57	MG	RA	3285	-	-	-	X
57	MG	RA	3298	-	-	-	X
57	MG	RA	3300	-	-	-	X
57	MG	RA	3315	-	-	-	X
57	MG	RA	3320	-	-	-	X
57	MG	RA	3321	-	-	-	X
57	MG	RA	3326	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	RR	201	-	-	-	X
57	MG	XA	1603	-	-	-	X
57	MG	XA	1606	-	-	-	X
57	MG	XA	1613	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1619	-	-	-	X
57	MG	XA	1621	-	-	-	X
57	MG	XA	1623	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1624	-	-	-	X
57	MG	XA	1627	-	-	-	X
57	MG	XA	1631	-	-	-	X
57	MG	XA	1632	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1634	-	-	-	X
57	MG	XA	1639	-	-	-	X
57	MG	XA	1641	-	-	-	X
57	MG	XA	1642	-	-	-	X
57	MG	XA	1643	-	-	-	X
57	MG	XA	1649	-	-	-	X
57	MG	XA	1652	-	-	-	X
57	MG	XA	1663	-	-	-	X
57	MG	XA	1667	-	-	-	X
57	MG	XA	1679	-	-	-	X
57	MG	XA	1684	-	-	-	X
57	MG	XA	1685	-	-	-	X
57	MG	XA	1688	-	-	-	X
57	MG	XA	1692	-	-	-	X
57	MG	XA	1700	-	-	-	X
57	MG	XA	1705	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3004	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3011	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3016	-	-	-	X
57	MG	YA	3022	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3024	-	-	-	X
57	MG	YA	3025	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3028	-	-	-	X
57	MG	YA	3030	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3032	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3036	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3037	-	-	-	X
57	MG	YA	3040	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3046	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3067	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3069	-	-	-	X
57	MG	YA	3075	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3077	-	-	-	X
57	MG	YA	3078	-	-	-	X
57	MG	YA	3082	-	-	-	X
57	MG	YA	3085	-	-	-	X
57	MG	YA	3086	-	-	-	X
57	MG	YA	3094	-	-	-	X
57	MG	YA	3095	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3102	-	-	-	X
57	MG	YA	3103	-	-	-	X
57	MG	YA	3105	-	-	-	X
57	MG	YA	3108	-	-	-	X
57	MG	YA	3114	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3132	-	-	-	X
57	MG	YA	3134	-	-	-	X
57	MG	YA	3136	-	-	-	X
57	MG	YA	3138	-	-	-	X
57	MG	YA	3140	-	-	-	X
57	MG	YA	3147	-	-	-	X
57	MG	YA	3152	-	-	-	X
57	MG	YA	3156	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3169	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3173	-	-	-	X
57	MG	YA	3174	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3187	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3192	-	-	-	X
57	MG	YA	3194	-	-	-	X
57	MG	YA	3197	-	-	-	X
57	MG	YA	3209	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3216	-	-	-	X
57	MG	YA	3219	-	-	-	X
57	MG	YA	3228	-	-	-	X
57	MG	YA	3230	-	-	-	X
57	MG	YA	3232	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3236	-	-	-	X
57	MG	YA	3238	-	-	-	X
57	MG	YA	3240	-	-	-	X
57	MG	YA	3241	-	-	-	X
57	MG	YA	3246	-	-	-	X
57	MG	YA	3247	-	-	-	X
57	MG	YA	3249	-	-	-	X
57	MG	YA	3251	-	-	-	X
57	MG	YA	3264	-	-	-	X
57	MG	YA	3265	-	-	-	X
57	MG	YA	3268	-	-	-	X
57	MG	YA	3269	-	-	-	X
57	MG	YA	3293	-	-	-	X
57	MG	YA	3297	-	-	-	X
57	MG	YA	3303	-	-	-	X
57	MG	YA	3307	-	-	-	X
57	MG	YA	3309	-	-	-	X
57	MG	YA	3313	-	-	-	X
57	MG	YA	3316	-	-	-	X
57	MG	YA	3319	-	-	-	X
57	MG	YA	3323	-	-	-	X
57	MG	YA	3326	-	-	-	X
57	MG	YA	3327	-	-	-	X
57	MG	YA	3328	-	-	-	X
57	MG	YA	3340	-	-	-	X
57	MG	YA	3347	-	-	-	X
57	MG	YA	3348	-	-	-	X
57	MG	YA	3354	-	-	-	X
57	MG	YA	3355	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3357	-	-	-	X
57	MG	YP	202	-	-	-	X
57	MG	YU	201	-	-	-	X
59	ZN	QD	301	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	9	Total	C	N	O	P	0	0	0
			191	86	36	60	9			
23	XX	10	Total	C	N	O	P	0	0	0
			213	96	41	66	10			

- Molecule 24 is a RNA chain called A-site tRNA Thr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	16	Total	C	N	O	P	0	0	0
			344	153	62	113	16			
24	XY	16	Total	C	N	O	P	0	0	0
			344	153	62	113	16			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
25	YA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

- Molecule 26 is a RNA chain called 5S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
46	Y0	82	Total	C	N	O	S	0	0	0
			647	401	137	108	1			

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

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a RNA chain called CC-Puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z5	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			
56	Z6	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	82	Total	Mg	0	0
			82	82		
57	RP	1	Total	Mg	0	0
			1	1		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	359	Total	Mg	0	0
			359	359		
57	Y5	1	Total	Mg	0	0
			1	1		

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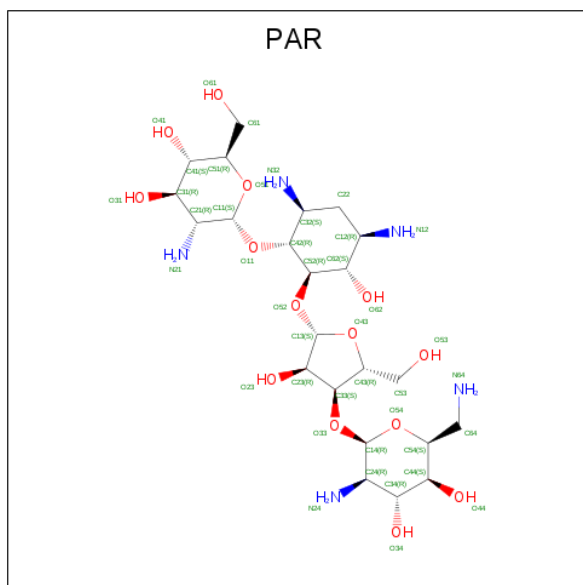
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y1	1	Total 1	Mg 1	0	0
57	XX	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	XA	111	Total 111	Mg 111	0	0
57	YY	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	YU	1	Total 1	Mg 1	0	0
57	Y0	3	Total 3	Mg 3	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	XB	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	327	Total 327	Mg 327	0	0
57	YP	2	Total 2	Mg 2	0	0
57	RE	1	Total 1	Mg 1	0	0
57	YB	4	Total 4	Mg 4	0	0
57	QY	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QE	1	Total	Mg	0	0
			1	1		
57	XD	1	Total	Mg	0	0
			1	1		
57	YE	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

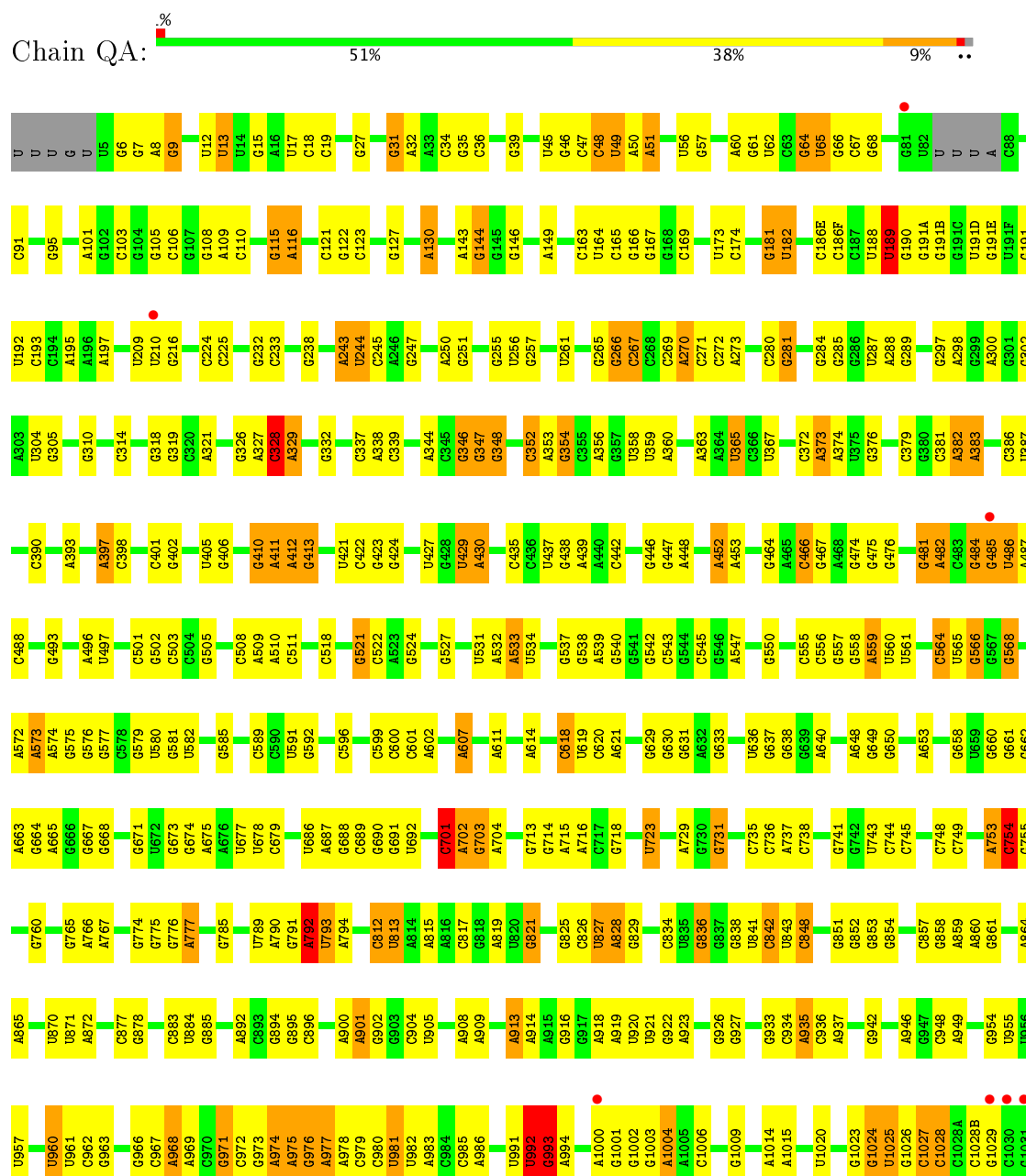
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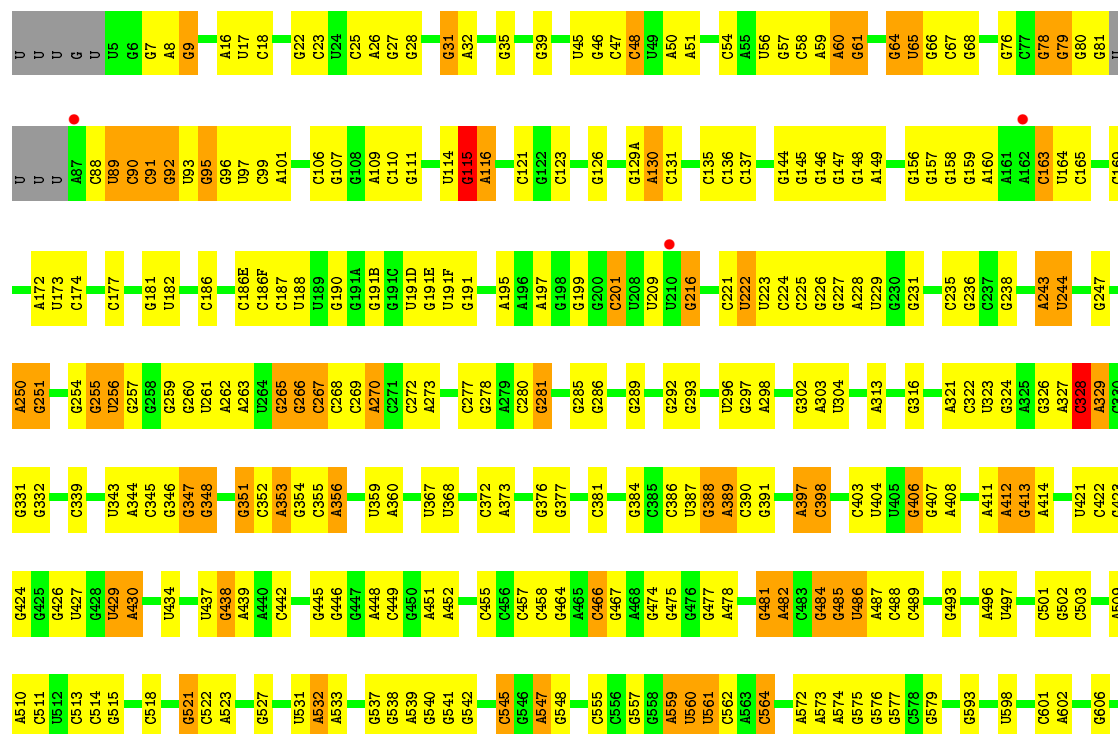
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	Z5	1	Total 37	C 22	N 7	O 7	P 1	0	0
60	Z6	1	Total 37	C 22	N 7	O 7	P 1	0	0

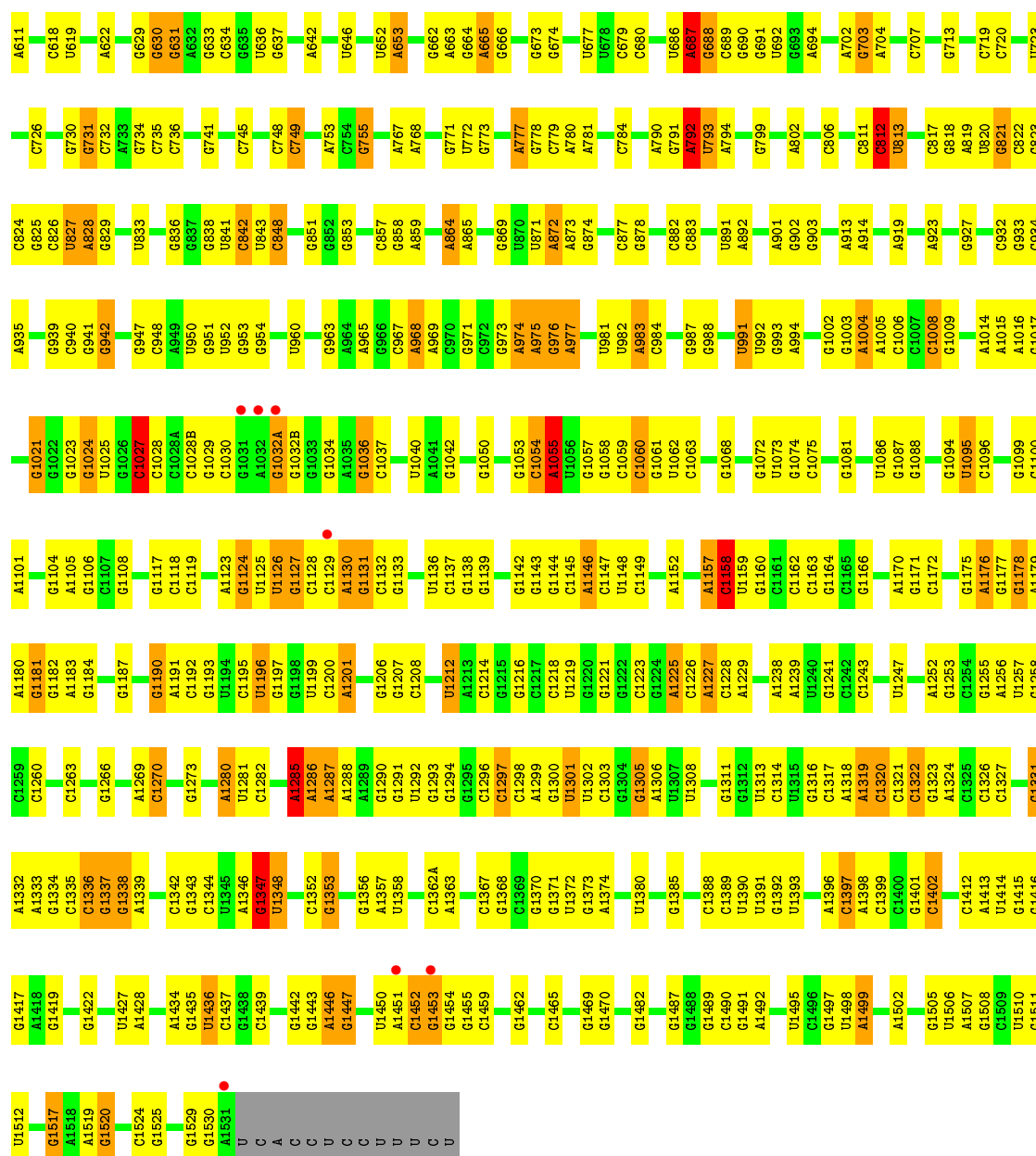
3 Residue-property plots

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

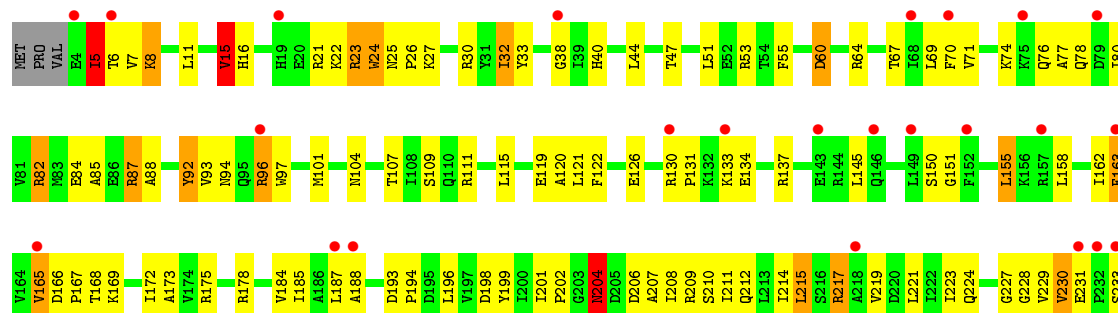
• Molecule 1: 16S rRNA

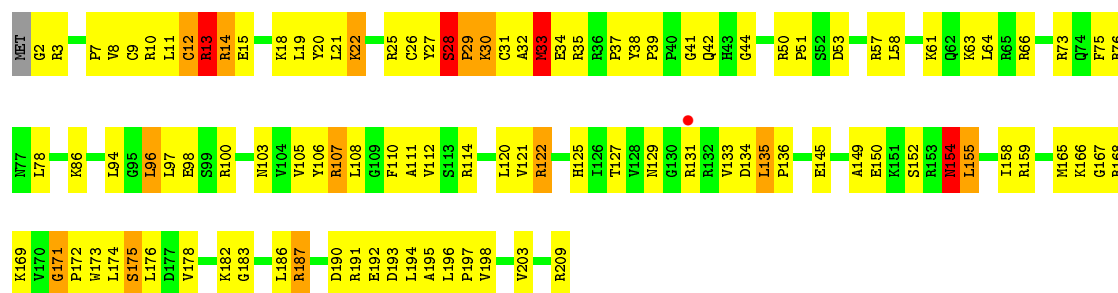






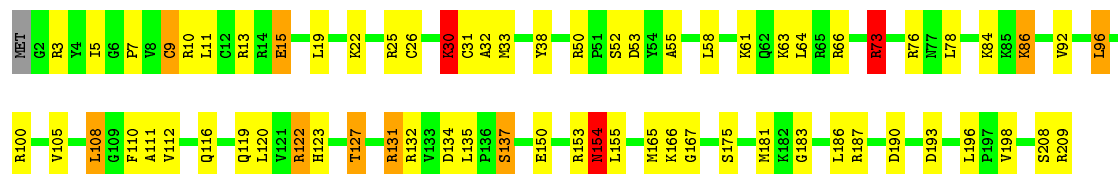
• Molecule 2: 30S ribosomal protein S2





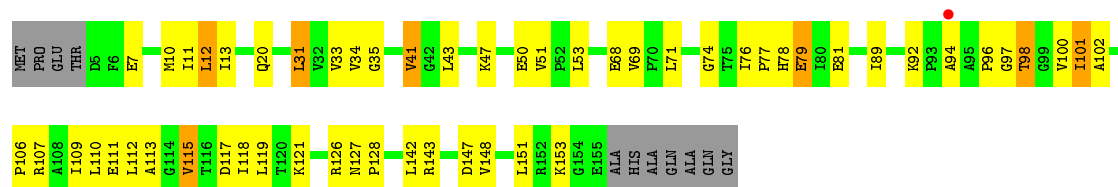
- Molecule 4: 30S ribosomal protein S4

Chain XD: 67% 27% . .



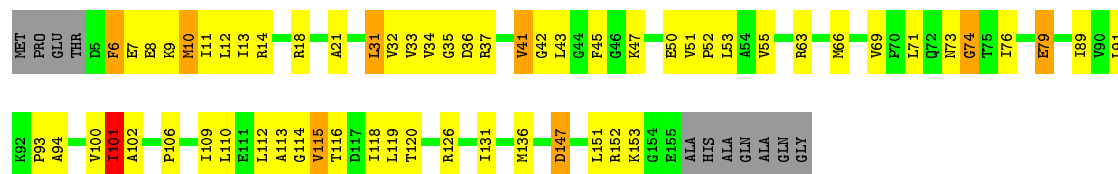
- Molecule 5: 30S ribosomal protein S5

Chain QE: % 59% 30% . 7%



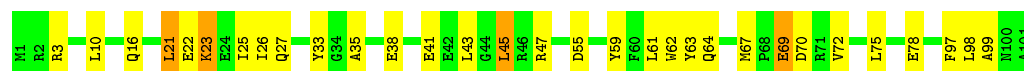
- Molecule 5: 30S ribosomal protein S5

Chain XE: 56% 32% 5% . 7%



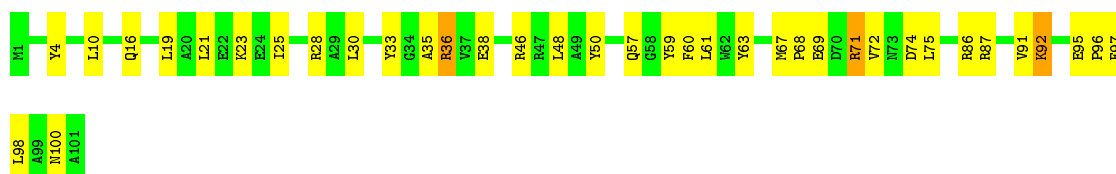
- Molecule 6: 30S ribosomal protein S6

Chain QF: 69% 27% .

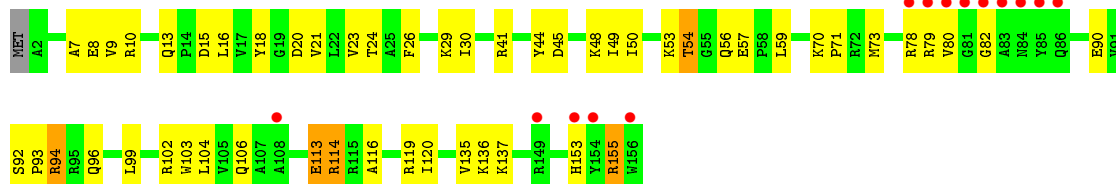


- Molecule 6: 30S ribosomal protein S6

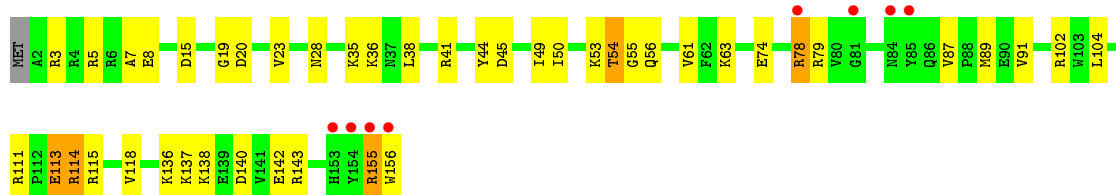
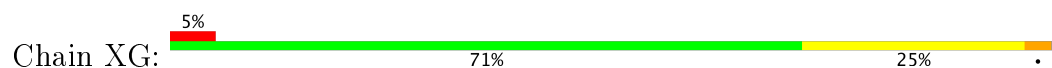
Chain XF: 63% 34% .



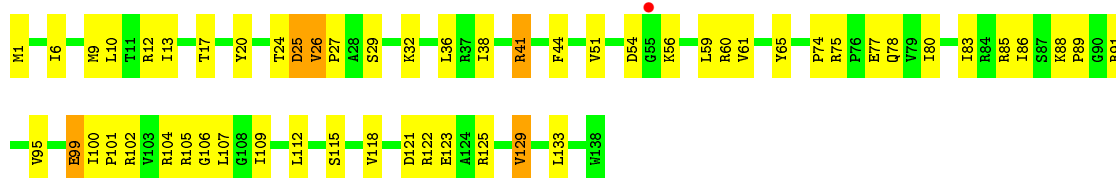
- Molecule 7: 30S ribosomal protein S7



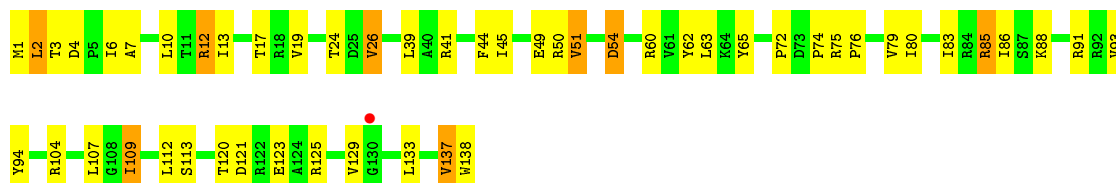
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

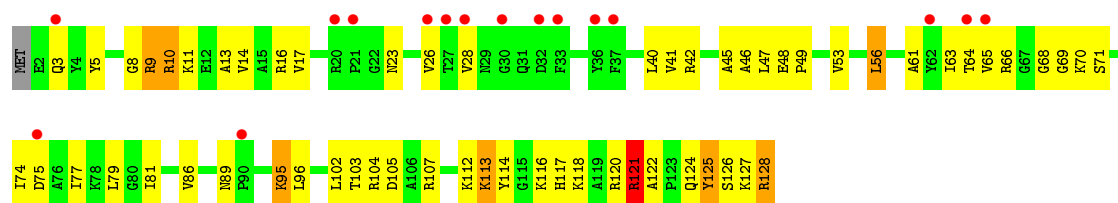


- Molecule 8: 30S ribosomal protein S8



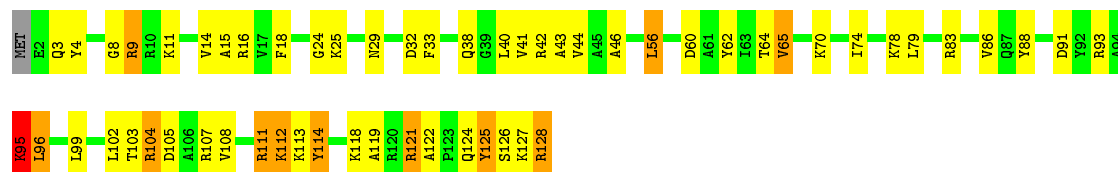
- Molecule 9: 30S ribosomal protein S9





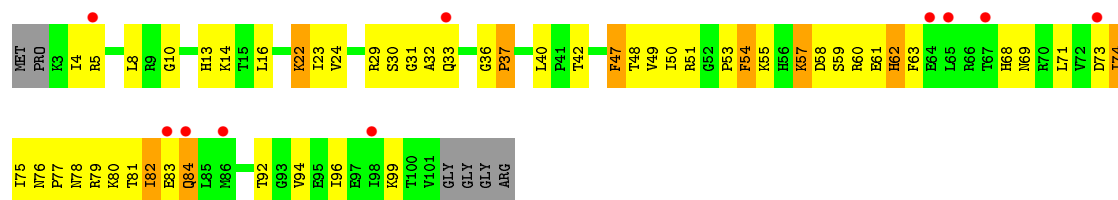
• Molecule 9: 30S ribosomal protein S9

Chain XI: 55% 35% 9% ..



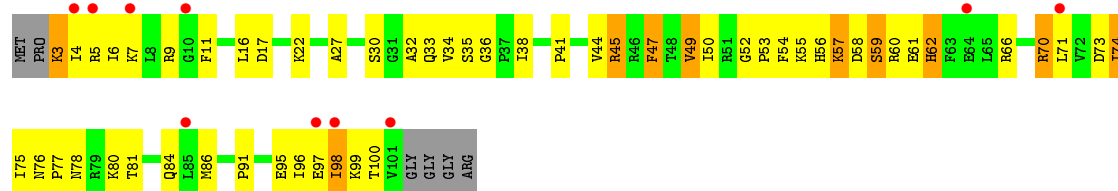
• Molecule 10: 30S ribosomal protein S10

Chain QJ: 10% 44% 42% 9% 6%



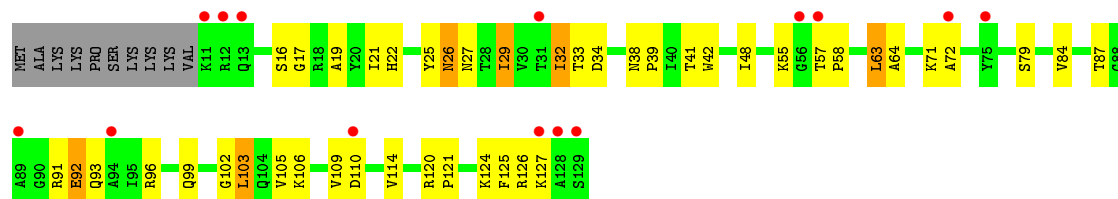
• Molecule 10: 30S ribosomal protein S10

Chain XJ: 10% 42% 43% 10% 6%



• Molecule 11: 30S ribosomal protein S11

Chain QK: 11% 57% 30% 5% 8%



• Molecule 11: 30S ribosomal protein S11

I95	R96	Q99	L103	I108	V109	V114	F115	H116	C119	R120	K127	A128	S129	MET	ALA	LYS	PRO	SER	LYS	LYS	LYS	VAL	K11	R12	R18	A19	Y20	I21	N26	N27	T28	I29	V30	T31	I32	T33	D34	P35	D36	G37	N38	P39	I40	T41	W42	I48	K55	G56	T57	F58	Y59	L63	K71	D81	V82	I83	V84	R85	G86	I87	G88	A89	G90	R91
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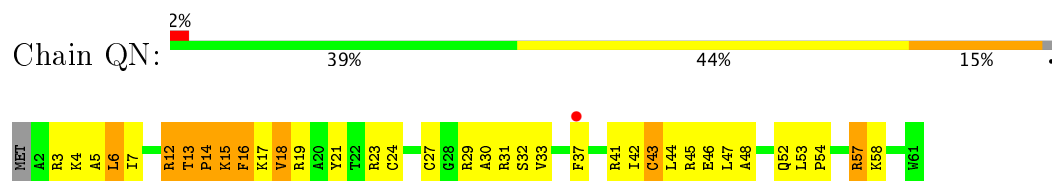
- [illegible]

- [illegible]

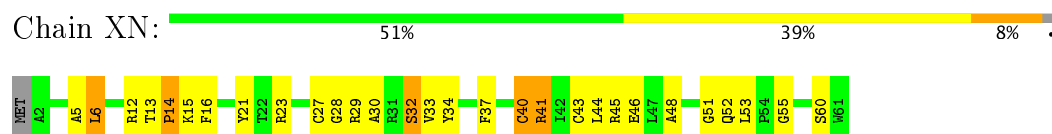
- [illegible]

-
- Figure 1: Schematic representation of the 20 amino acids. The diagram shows two rows of colored blocks representing amino acids. The top row contains MET, R3, I4, A5, G6, V7, B8, I9, M12, K13, R14, V15, D16, V17, A18, L19, T20, Y21, I22, Y23, G24, T25, E32, K36, M40, P41, A42, T43, R44, V45, L48, T49, E52, L56, R57, E58, M62, T63, R64, R65, L66, B67, G68, E69, L70, L81, I84, and R88. The bottom row contains R91, V98, R99, G100, Q101, R102, T103, R104, T105, N106, A107, R108, K111, R114, K115, T116, V117, A118, G119, K120, K121, K122, A123, P124, R125, A126, G127, A128, and L129. Each block is a different color and contains a three-letter code. The blocks are arranged in a grid-like pattern with some gaps.

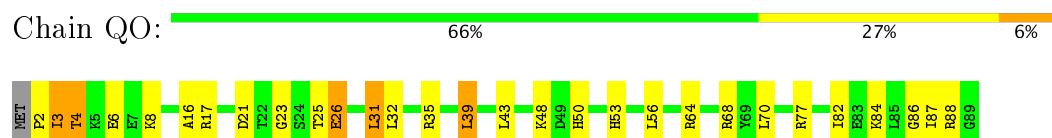
- Molecule 14: 30S ribosomal protein S14 type Z



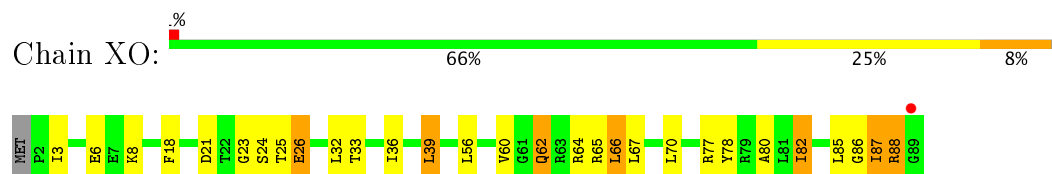
- Molecule 14: 30S ribosomal protein S14 type Z



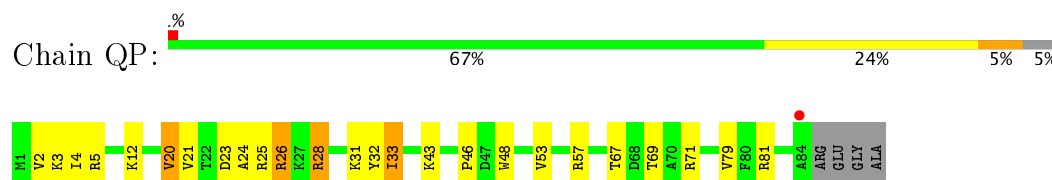
- Molecule 15: 30S ribosomal protein S15



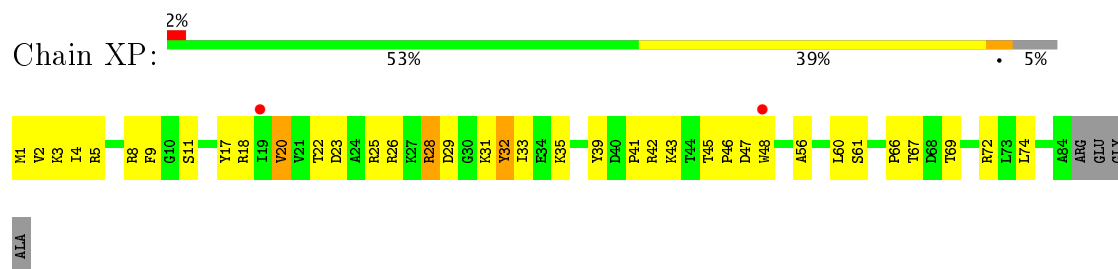
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

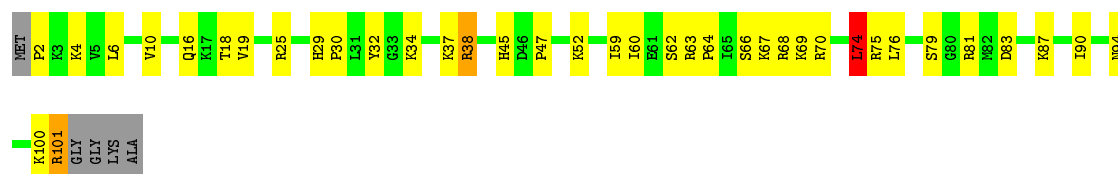


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17





- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



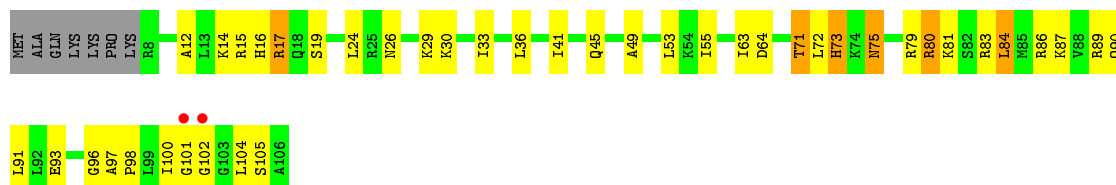
- Molecule 19: 30S ribosomal protein S19



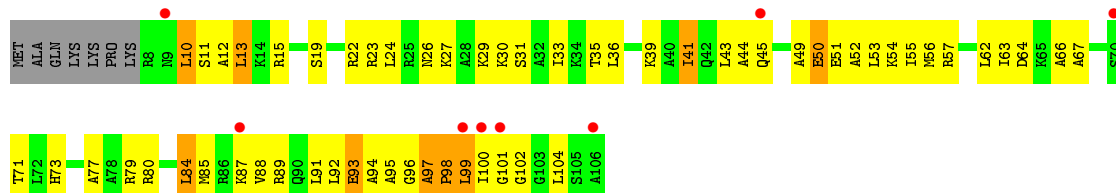
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



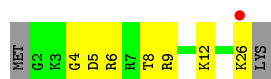
- Molecule 20: 30S ribosomal protein S20



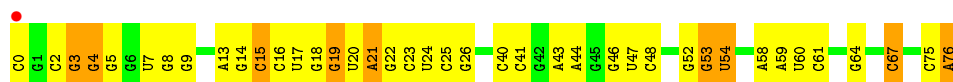
- Molecule 21: 30S ribosomal protein Thx



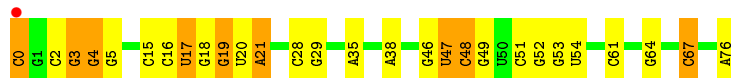
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: P-site tRNA f-Met



- Molecule 22: P-site tRNA f-Met



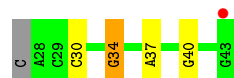
- Molecule 23: messenger RNA



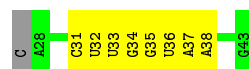
- Chain XX: 



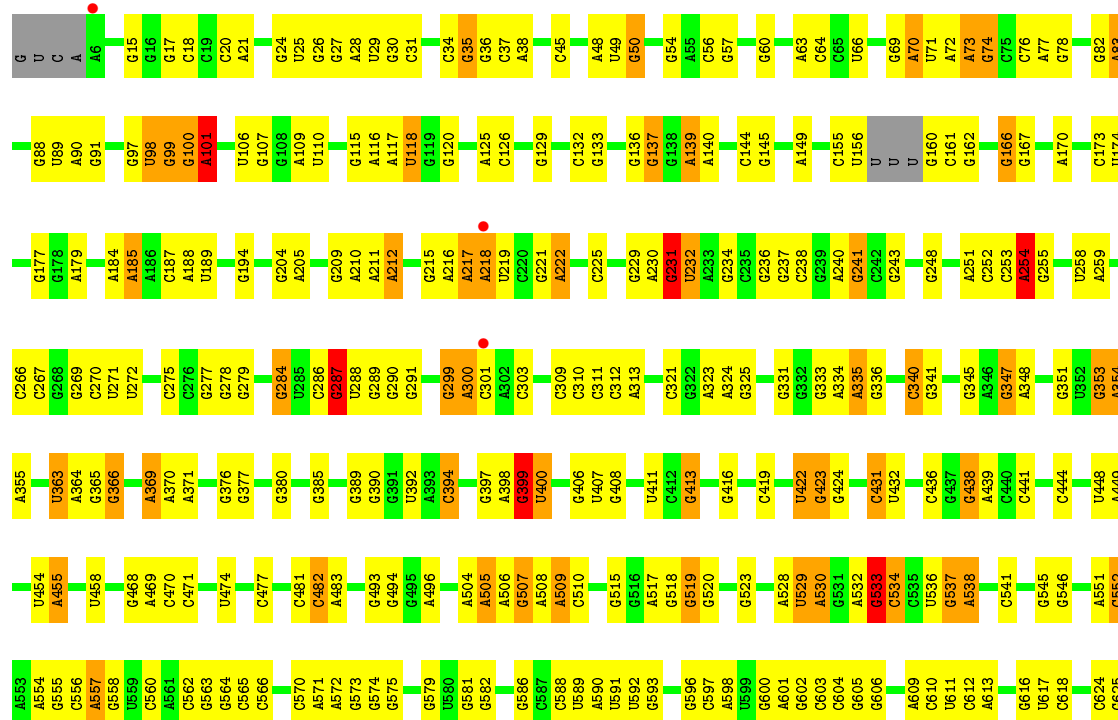
- Chain QY: 



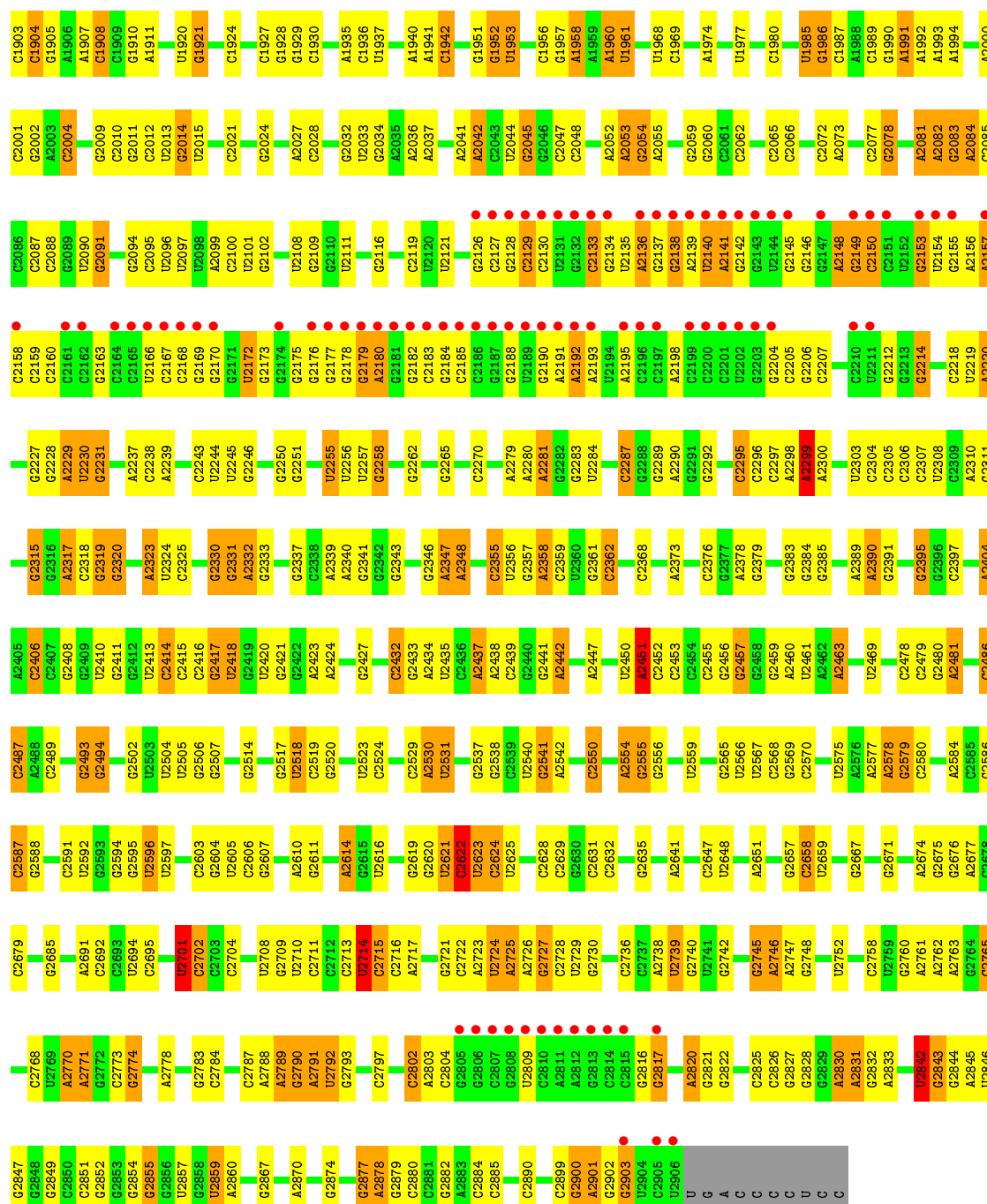
- Chain XY: 



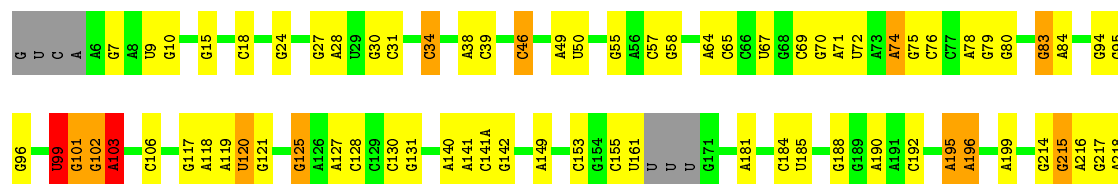
- Chain RA: 



A1817	G1637	U1381	U1211	A1132	G1068	A986	C904	G703	A626
A1818	C1638	A1382	C1212	G1133	U1069	G987	U905	U704	G627
C1821	G1639	G1383		A1134	G1070	G988	G906	G1070	G628
A1822	G1640	G1384	G1215	G1135	G1071	G989	U907	C706	U629
	G1641			U1137	U1072	G990	A908	G707	U630
U1825	C1644	U1387	G1218	G1137	A1073	G991	G909	C708	A631
C1826	C1645	A1388	A1219	G1138	A1074	G992	A910	G709	
U1827	C1646	G1389	G1220	G1139	A1075	G993			G636
U1828	C1652	C1390	G1221	U1140	G1076	G994	G916	G715	U637
U1829	U1562	C1391	A1222	A1141	G1077	G995	A917	G716	U638
G1830	C1564	G1487	G1223	A1142	U1078	G996	U918	A717	G639
C1831	G1564	G1488	C1224	U1143	U1079	G997	A919	A640	A640
G1832	A1654	G1489	C1225	U1144	G1080	G998	G920	G720	G641
A1833	A1655	A1395		G1145	U1081	G999		G721	
A1834	G1557	U1398	G1232	U1146	G1082		G926	A722	G644
	G1568	A1399	U1233	C1148	G1083		G927	A723	G645
C1837	A1660	G1402	U1234	A1149	C1086	A1002	U1002	A726	G647
G1838	C1661	G1316	A1234	G1150	C1087	U1003	G928		
U1839	A1662	U1403	G1235	C1151	G1088	A1004	G929	G733	A652
A1840	C1663	G1404	G1236	U1152	G1089	U1005	G930	C734	G655
G1842	A1664	A1405		G1156	G1090	C1006	G931	U735	A656
			G1240	A1157	A1091	G1011	G932	G739	A657
G1847	G1669	C1579	U1243	G1158	A1092	G1019	G933	C740	A658
G1848	G1672	G1505	C1245	U1159	A1093	G1020	G934		
U1849	G1673	G1506	G1246	G1160	G1094		G935		
G1850	C1674	G1507	C1247	G1161	A1095	A1026	C936	C745	A662
U1851	C1675	G1508	G1248	G1164	G1096	A1029	G937	G749	G663
G1853	C1676	C1511	G1249	C1168	G1097	G1033	G938	U750	C670
		G1514	A1249	G1171	G1098	A1034	G939	G751	A671
G1857	G1684	G1517	U1250	G1172	C1099	G1035	U941	A752	
C1858	C1685	A1518	G1254	A1173	A1100	A1036	A942	G753	C675
G1859	G1686	G1519	U1255	A1174	G1102	G1039	A943	G754	G676
A1860	G1687	G1520	G1257	A1175	G1103	A945	A946	G757	C677
		G1521		U1176	G1104	A947	A947	G764	A678
U1864	G1688	C1423	A1265	G1177	U1055	A1042	G950	A769	A679
U1865	A1699	G1432	C1266	G1178	U1056	G1043	U951	A769	G680
G1866	G1700	G1435	G1269	C1180	G1107	A1046	G952	G770	C681
C1869	A1701	U1436	G1270	G1181	C1110	A1047	U953	G771	G
G1870	A1702	U1437	G1271	G1182	U1111	G1048	G956	G772	G
	C1703	U1528	A1358	G1183	U1112	G1049	A956	G773	C
G1873	C1704	G1529	C1360	G1184	A1113	C1050	G960	G776	C
C1874	C1705	A1532	G1273	C1185	G1114	C1051	G961	C777	G
		A1536	G1276	U1186	A1115	C1052	G962	A781	A
A1876	A1712	C1449	G1277	U1187	G1116	C1053	A963	A793	C
A1878	G1713	U1625		A1188	G1117	C1054	A964	U794	C
A1879	A1715	A1626		A1189	G1120	A1055	G965		G
G1889	G1721	C1453	G1282	G1190		A1056	U968	A798	G
A1890	C1722	C1454	A1283	G1195	A1123	G1057	G969	A799	C
U1895	U1810	C1457	G1284	C1196	U1124	U1058	C892	C800	C
U1896	A1811	U1543	G1370	G1197	C1125	C1059	C893	C801	C
C1897	C1812	C1544	U1286	C1198	U1128		U894	C802	
A1898	U1726	G1462	A1287	G1199	U1129	G1063	G895		G698
C1899	U1727	G1463		G1200	U1130	G1064	A896	G699	
A1899	A1815	A1465	G1290	C1199	U1131	G1065	G977	A700	
G1900	A1816	C1552	A1292	G1206	A1131	A1066	A978	A701	
						A1067	G983	G812	A702

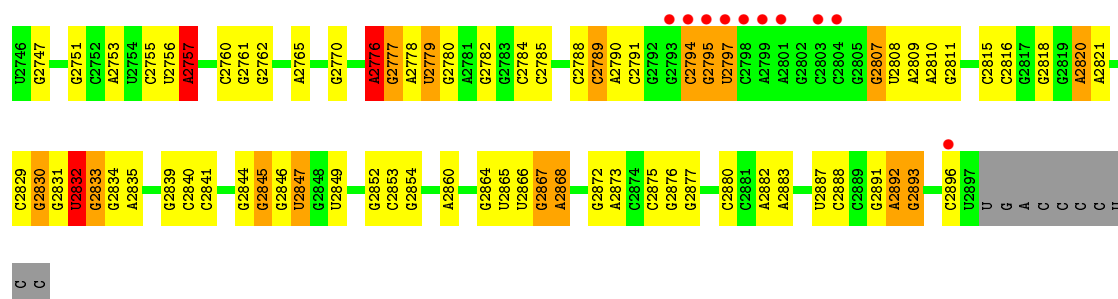


• Molecule 25: 23S rRNA

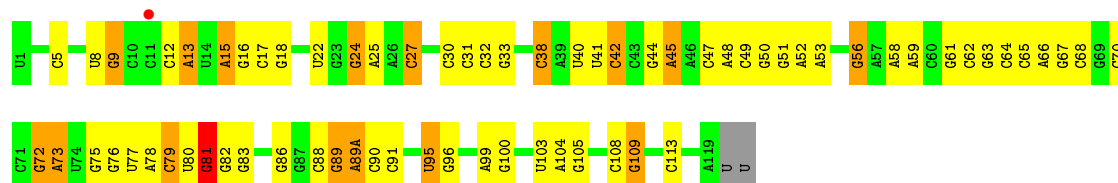


U1312	A1210	U1130	G1063	A983	U905	U813	G729	G	U594	A514	G425	G341	G270V	A221
U1313	U1211	G1131	G1064	A984	G906	C914	C730	C	C595	A515	C426	G342	G270W	A222
U1316	G1216	C1135	U1066	C985	U907	G818	C731	A	U597	C516	U427	A345	U270Z	A223
A1317	G1217	G1137	A1067	C994	A910	A819	A734	C	G598	A518	A428	A346	G271A	G224
G1319	G1218	G1138	G1068	C995	A911	G823	U740	C	G599	U519	A432	A347	G271B	A225
C1320	C1221	G1139	A1069	A996	C914	A824	G741	G	G600	G520	C433	G348	U271C	G256
A1321	C1222	C1140	G1070			C825	G742	C	A603	C527	G442	G349	G271	A227
U1329	U1141	U1141	C1072	G1003	A917	U826	G743	C	G604	A528	C443	G351	U230	A228
C1330	U1142	U1142	U1073	C1004	A918	U827	G744	C	C605	A529	C444	G352	U230	A229
A1331	A1143	A1143A	G1074	C1005	G919	U828			U606	G530	C445	G353	G274	C231
G1332	G1144	G1144	C1075	C1006	G920	U829	U747	C654T	U607	C531	G446	G354	G275	G232
	C1145		C1076	C1007	G921	G831	G748	A654U	A608	A532	A447	G354	G276	A233
U1335	U1336	G1151	U1077	C1008	U922	G832	A752	A654V	A609	G533	U448	A357	C277	C234
G1337	G1236	C1152	U1078	C1009	C923	C833	C753	A655	G609A		U358	U358	C277	U235
G1338	G1237	G1153	G1079	A1010	A926	C834		G656	G612	C537	C451	G363	C279	C236
G1339	G1238	C1154	U1081	U1012	U930	G843	C756	G657	U613	G539	C455	G363	C287	A241
U1340	A1241	A1155	U1082	C1013	G931	C846	U757	G658	U614	G540	C456	G363B	C288	G242
A1342	A1247	A1156	A1084	G1017	A932	U847	G760	C859	G615	C541	G457	G363C	U292	U243
G1343		U1165	U1085	C1018	G933	G848	A761	G660	A616	C542	G458	C364	U293	C246
C1345	G1250	C1166	G1087	U1019	C936	A849	A764	G668	G620	A546	G463	C365	A294	G247
G1346	A1253	G1169	A1088	A1020	U937	G855		G669	A621	G549	A466	C370	G297	G248
G1347	G1256	G1170	U1089	U1023	G938	C856	G771	A670	G622	G550	G467	A371	G298	C249
G1348	C1257	G1171	G1091	G1024	A941	U858	C772	C857	G623	G551	G468	G372	G299	G250
A1349	C1258	G1173	G1092	G1025	G942	G859	U773	G674	G625	G552	G469	U373	A300	A251
U1352	U1263	A1174	U1093	U1026	U943	U860	G775	A675	U626	U564	A471	A374	U305	G252
A1353	G1264	U1175	A1094	A1027	G944	A861		A676	A627	G556	A472	U383	U306	C253
A1354	A1265	G1177	A1095	A1028	A945	G862	G780	G684	G628	G561	G473	U384	G307	G254
U1357	G1266	A1178	U1096	G1030	G946	A863	A781	G685	G629	U562	A479	C385	G308	G259
G1358	U1267	C1179	A1098	U1033	G948	A793	A782	G686	A631	G563	A480	U387	A310	C263
A1359	A1268	C1180	G1100	G1034	G950	U871	A794	G688	A632	U566	G481	G388	A311	C264
A1360	A1269	G1184	U1101	U1035	C951	A878	G786	C691	A633		A482	G389	G312	A265
G1365	C1270	C1185	C1102	G1036	G952	G880	U787	C692	C634	U569	A483	A390	A313	G266
A1365	G1271	G1186	A1103	G1036		G881	A788	C693	A637	G570	G491	U395	A314	
U1368	U1273	U1187	C1104	G1041	C955	G882	C790	G699	U639	A572	G492	G396	C316	U269
	A1278	A1188	G1109	G1042	G956	G883	C791	G700	C640	G573	G494	A401	A320	G270E
U1372	A1287	G1189	G1110	A1045	A957	C884	G792	G701	C645	G574	G498	C404	G323	U270F
A1373		G1190	A1111	A1046	U958	C885	A793	G702	A646	A575	U499	U405	A324	C270G
G1374	G1291	A1194	G1112	G1047	A959	C886	G794		A647	C580	U499	U405	A324	G270H
C1375	U1292	C1196	U1113	A1048	A960	C887	C795	A705	G647	C581	G500	G411	G325	G270I
	C1293		C1114	C1048	G962	A888	C796		G648	C582	A501	A412	G326	G270J
A1379			C1119	A1050		C889	C797	G715	G651	G583	A502	A412		C270K
U1384	G1296	C1201	G1122	A1054	G968	A890	A802	G717			A503	C413	G329	U270L
G1385	G1203	C1202	C1123	G1056	U969	G892		G717	A654	A586	U504	C414	A330	U270M
C1386	U1300	A1204	G1124	A1057	C970	A896	G805	A722	G654B	C587	A505	A415	A331	U270N
C1387	A1301	U1205	C1125	G1058	G972	C997	C806	G723	G	G506	A507	G418	A332	U270O
G1388	G1206	G1207	A1126	G1059	A974	C998	U807	G724	G	G508	C509		G333	C270P
	G1309	C1208	A1127	U1060	G974	A899	G808	G725	G	G509		U421	G334	C270Q
U1394	G1310	G1208	A1128	U1061	C974A	A900	U811	G726	G	G512	A422	A422	G335	G270R
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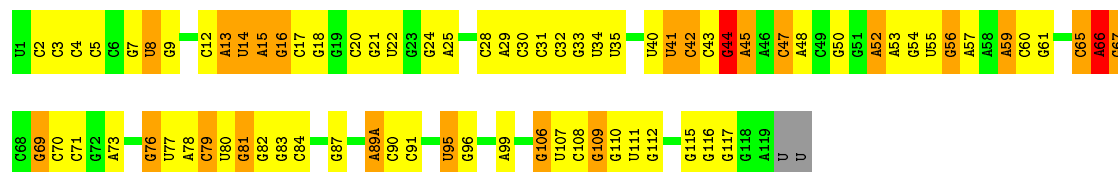




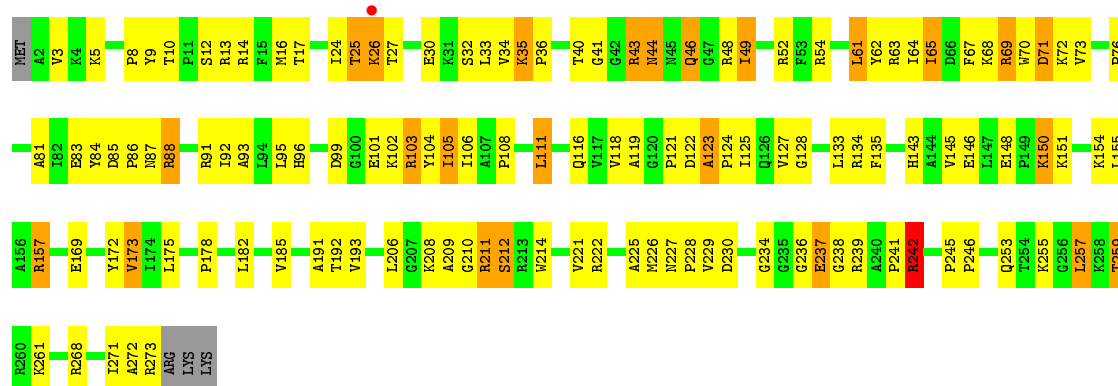
- Molecule 26: 5S rRNA



- Molecule 26: 5S rRNA

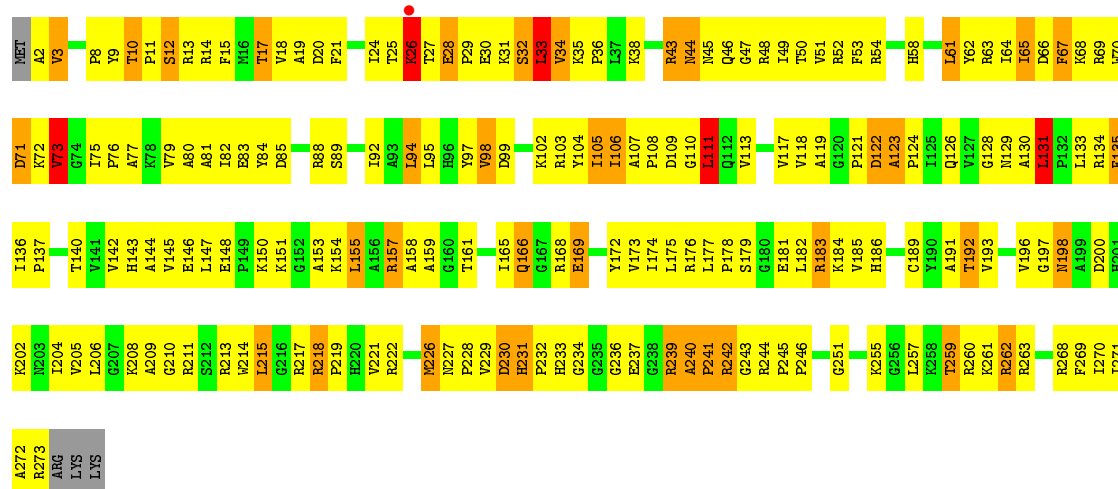


- Molecule 27: 50S ribosomal protein L2

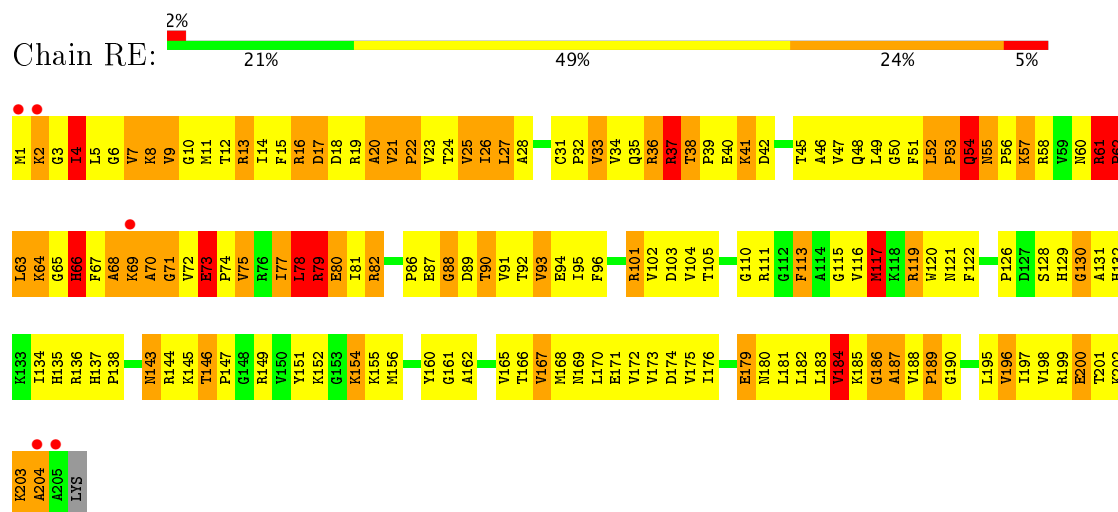


- Molecule 27: 50S ribosomal protein L2

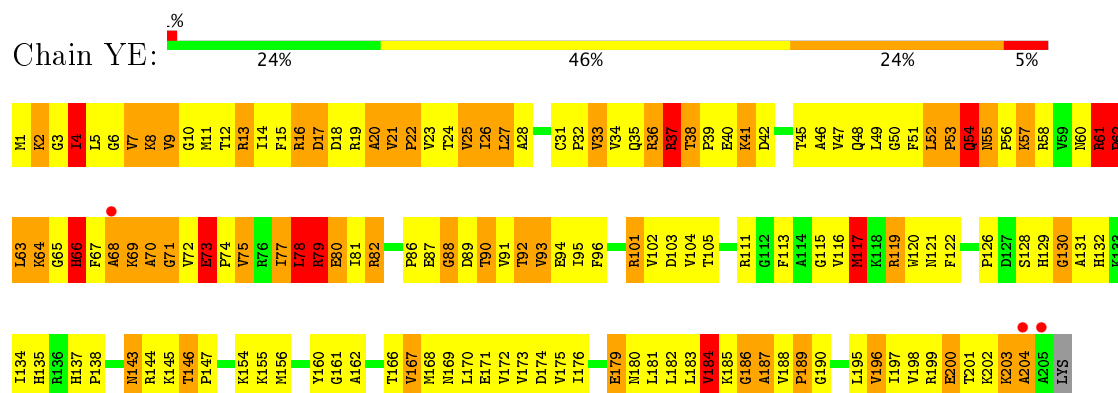




• Molecule 28: 50S ribosomal protein L3

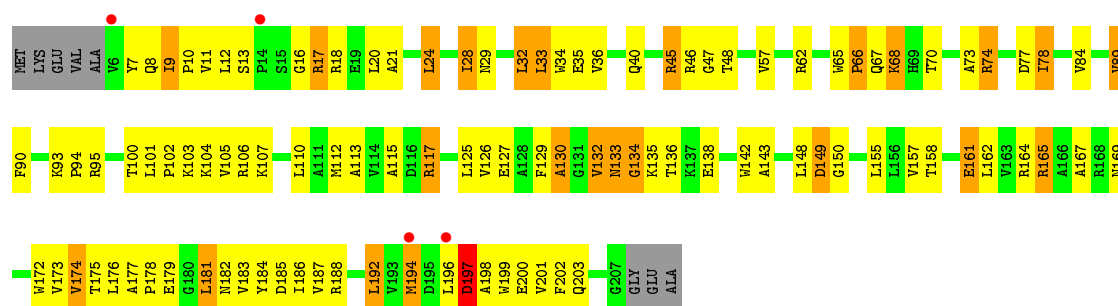


• Molecule 28: 50S ribosomal protein L3

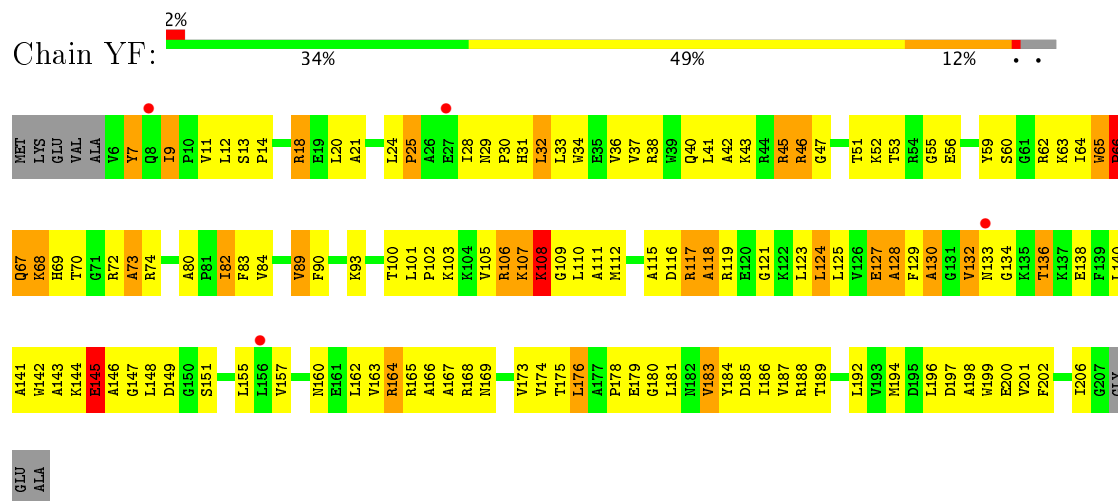


• Molecule 29: 50S ribosomal protein L4

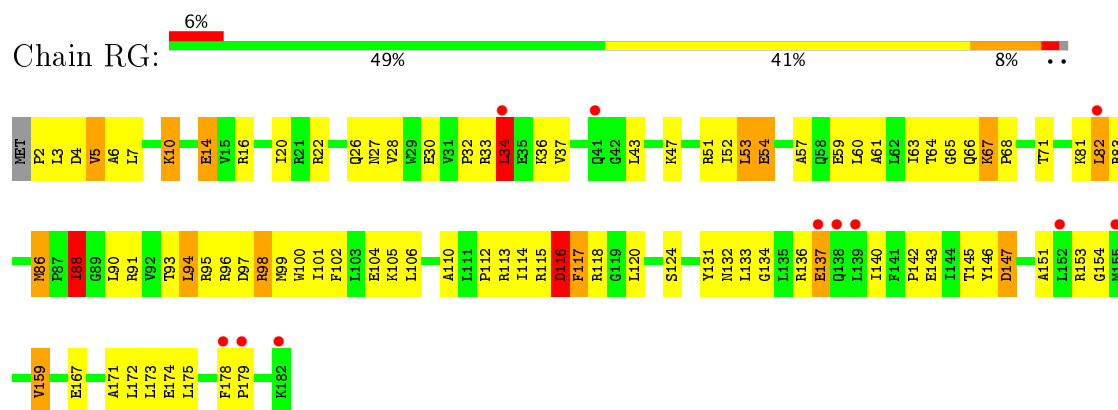




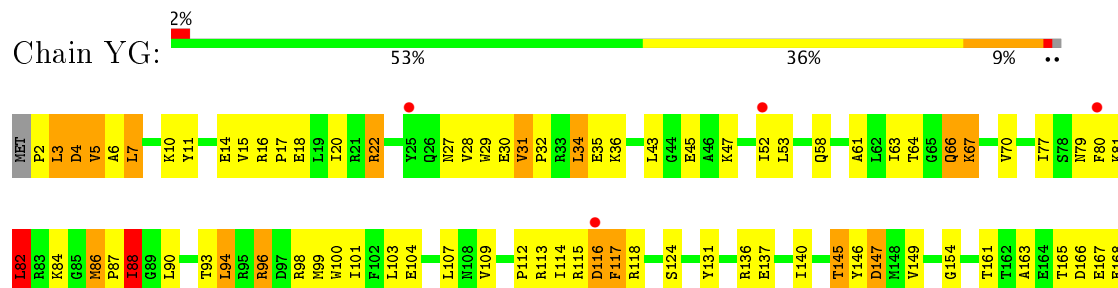
• Molecule 29: 50S ribosomal protein L4

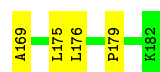


• Molecule 30: 50S ribosomal protein L5

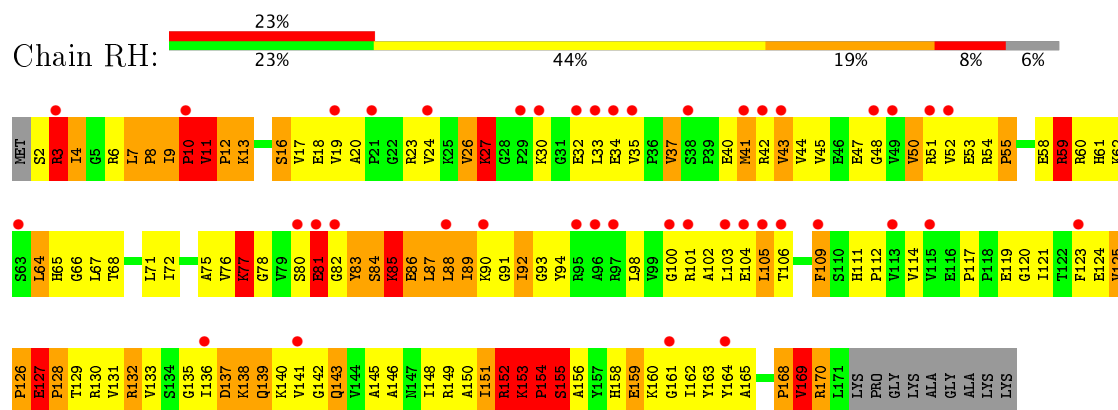


• Molecule 30: 50S ribosomal protein L5

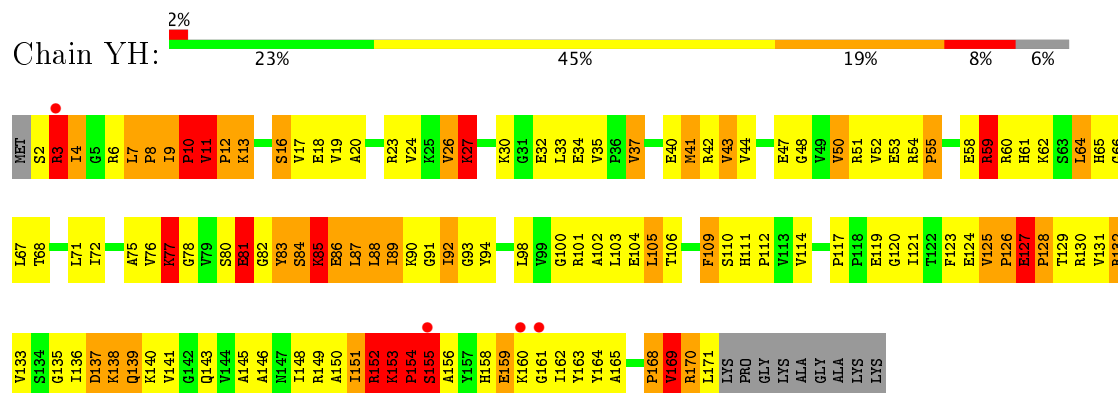




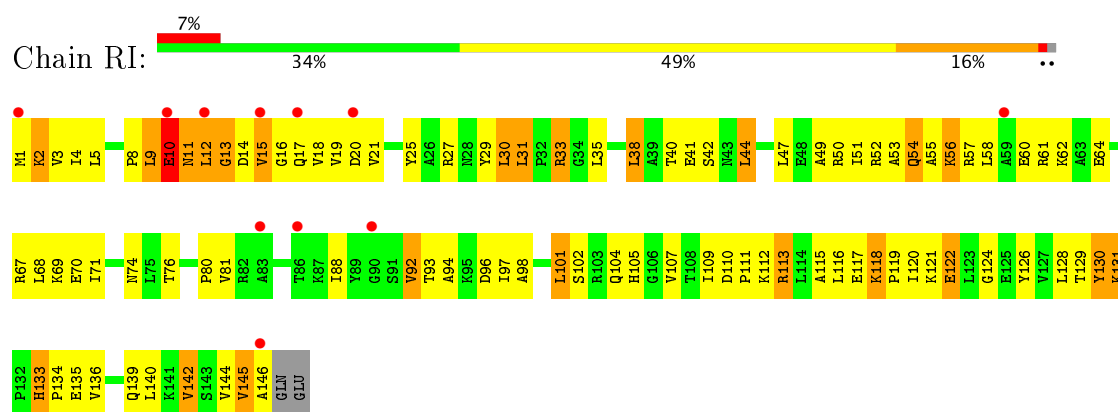
• Molecule 31: 50S ribosomal protein L6



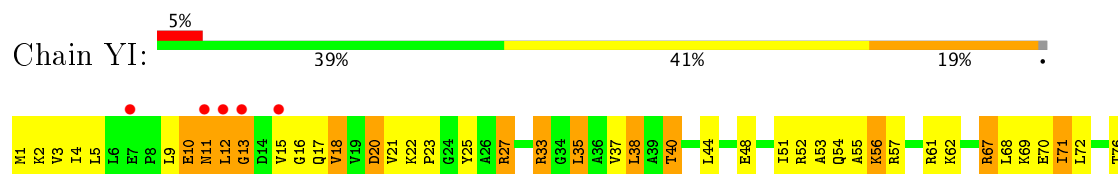
• Molecule 31: 50S ribosomal protein L6

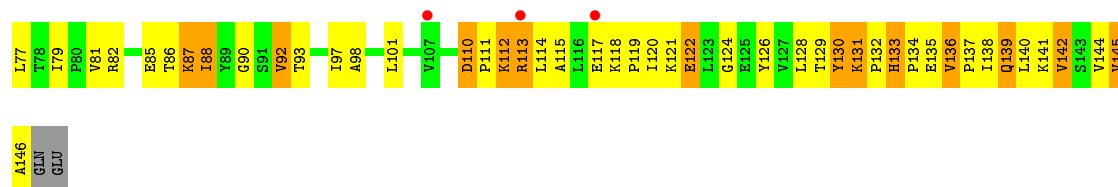


• Molecule 32: 50S ribosomal protein L9

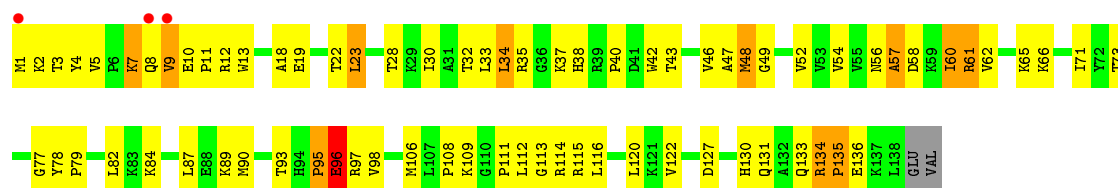


• Molecule 32: 50S ribosomal protein L9

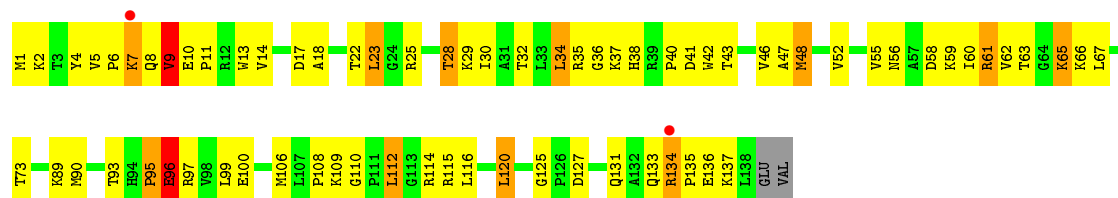




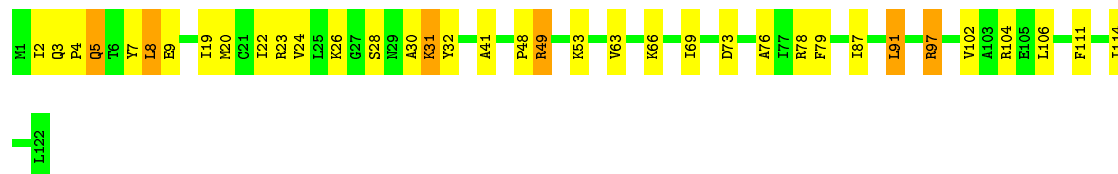
- Molecule 33: 50S ribosomal protein L13



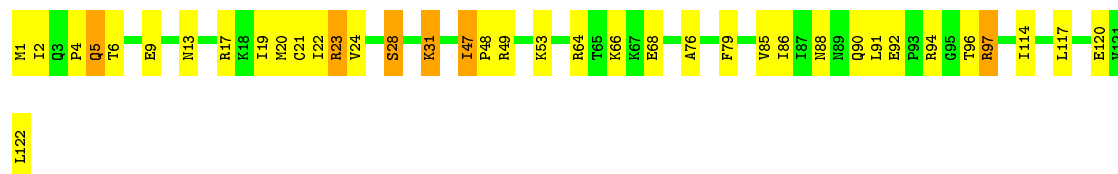
- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14

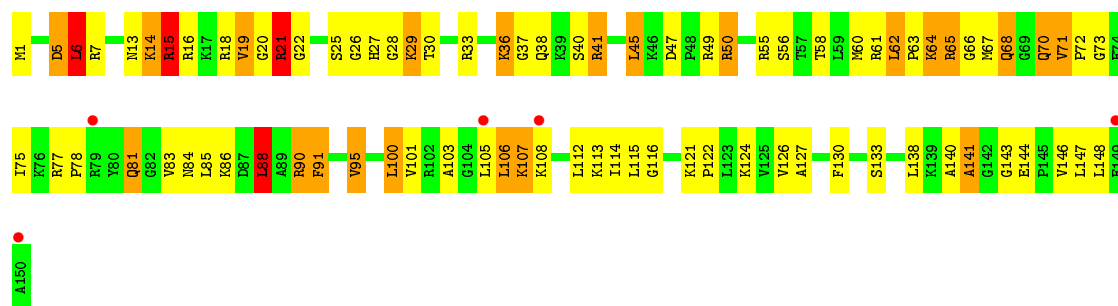


- Molecule 34: 50S ribosomal protein L14

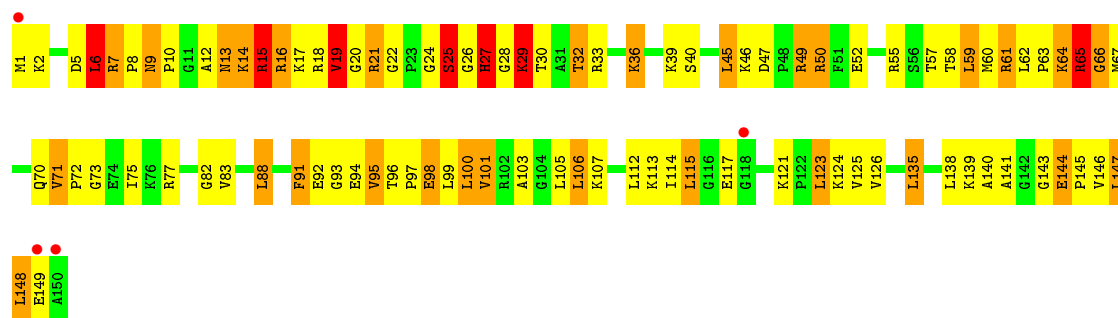


- Molecule 35: 50S ribosomal protein L15

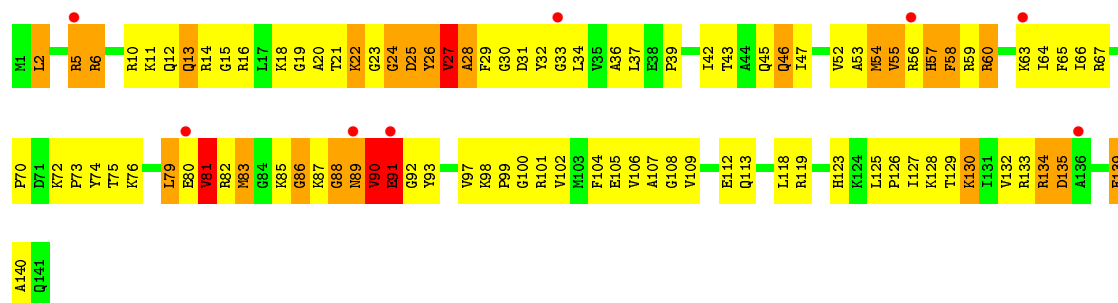




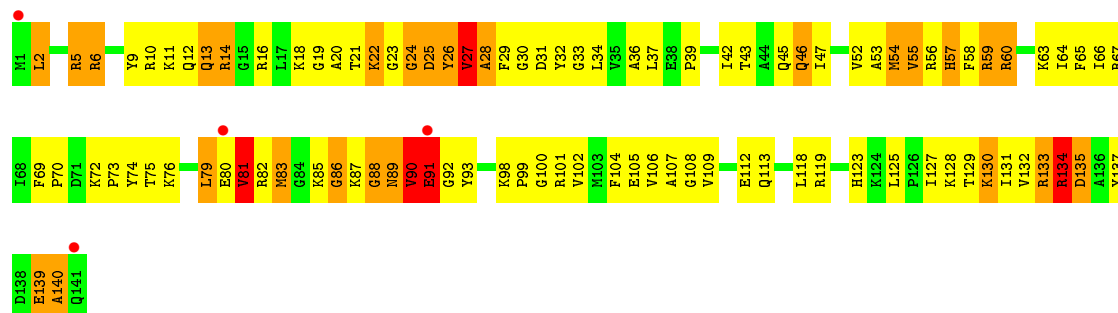
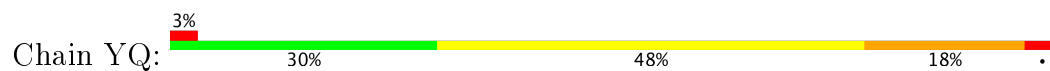
- Molecule 35: 50S ribosomal protein L15



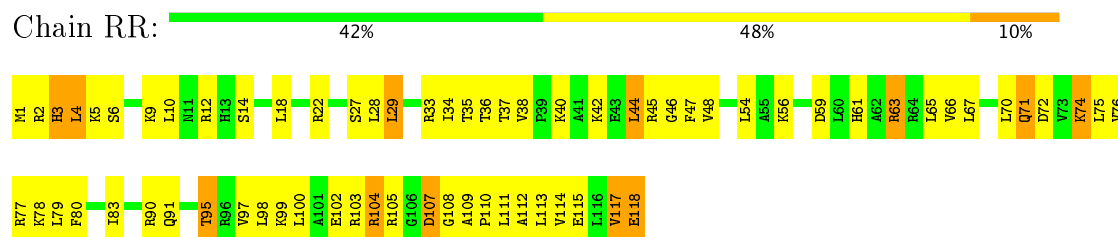
- Molecule 36: 50S ribosomal protein L16



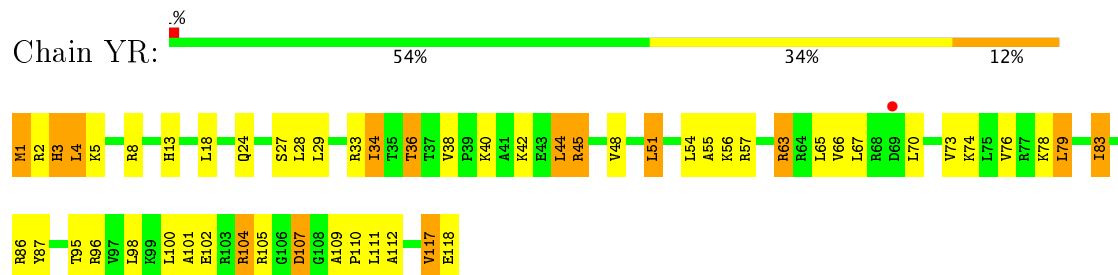
- Molecule 36: 50S ribosomal protein L16



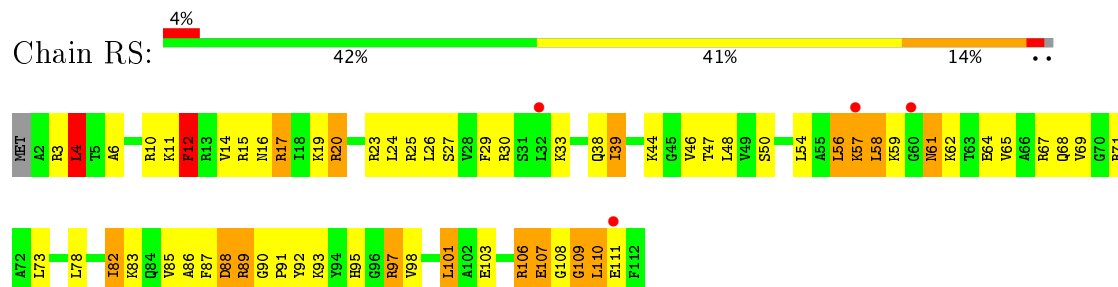
- Molecule 37: 50S ribosomal protein L17



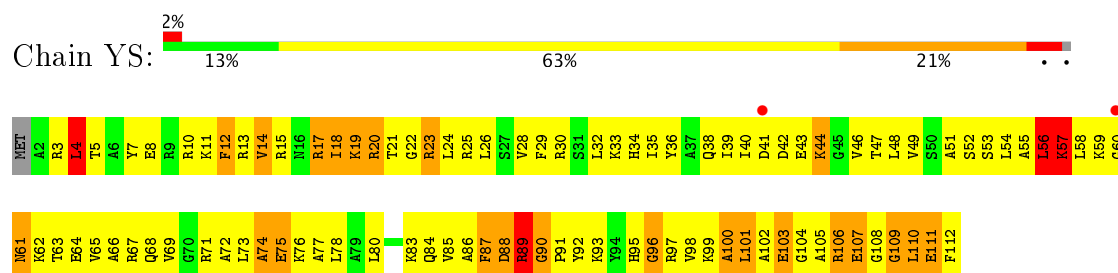
- Molecule 37: 50S ribosomal protein L17



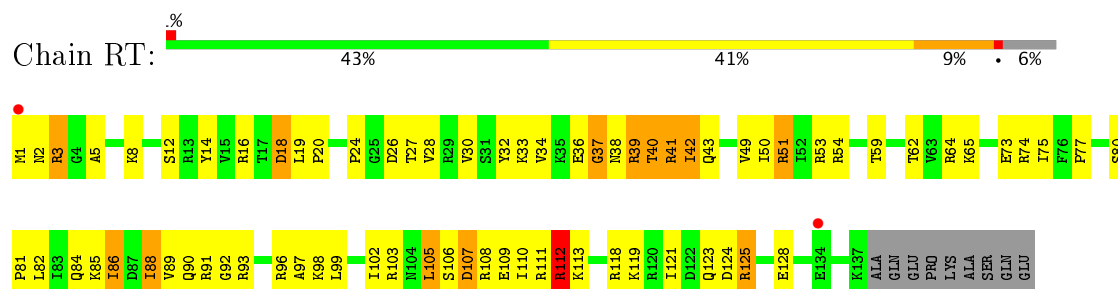
- Molecule 38: 50S ribosomal protein L18



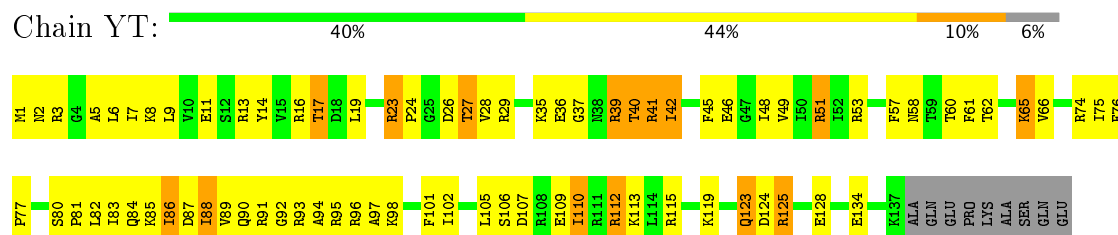
- Molecule 38: 50S ribosomal protein L18



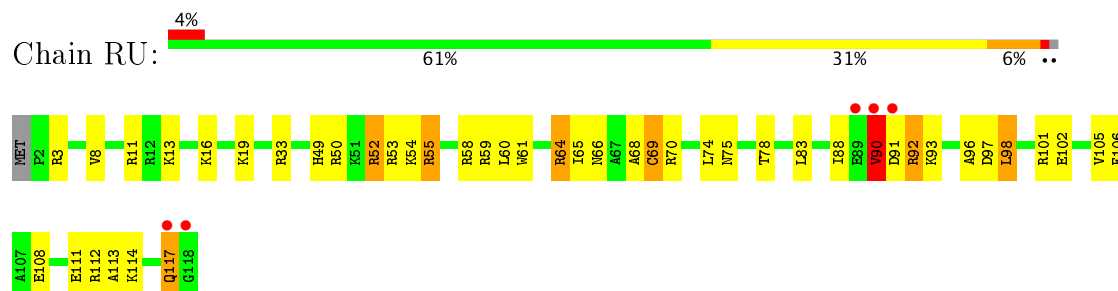
- Molecule 39: 50S ribosomal protein L19



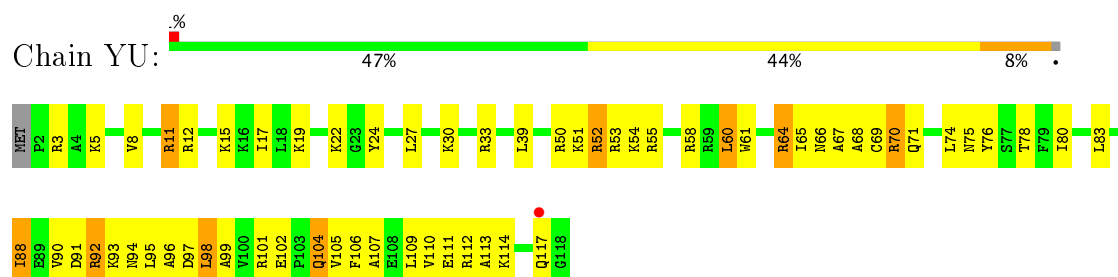
- Molecule 39: 50S ribosomal protein L19



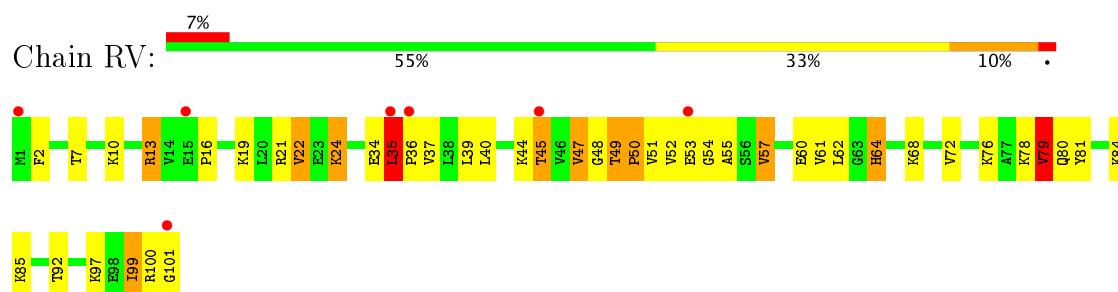
- Molecule 40: 50S ribosomal protein L20



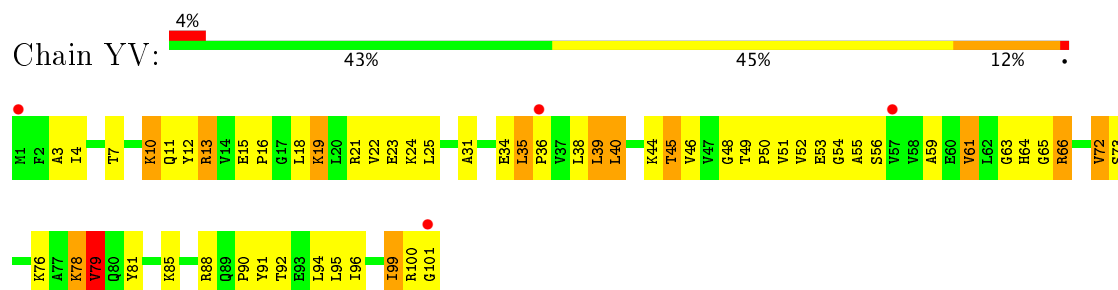
- Molecule 40: 50S ribosomal protein L20



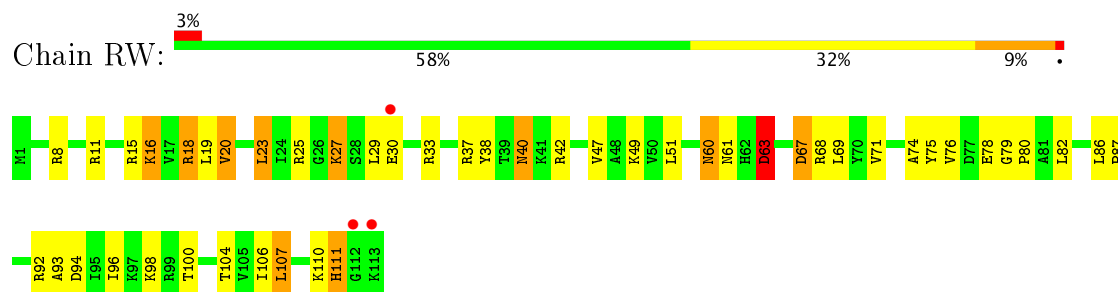
- Molecule 41: 50S ribosomal protein L21



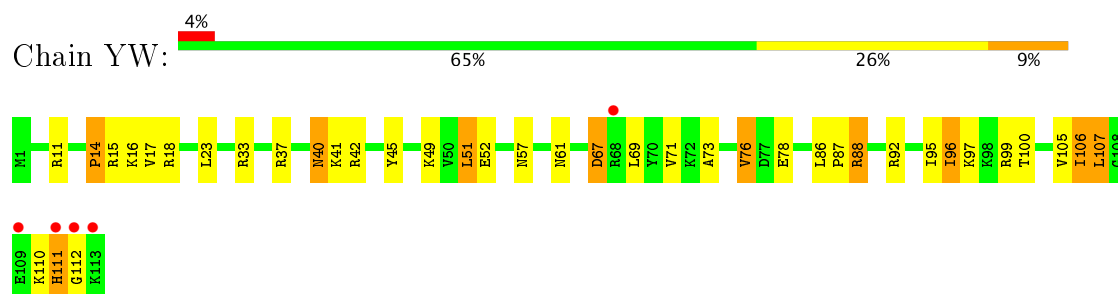
- Molecule 41: 50S ribosomal protein L21



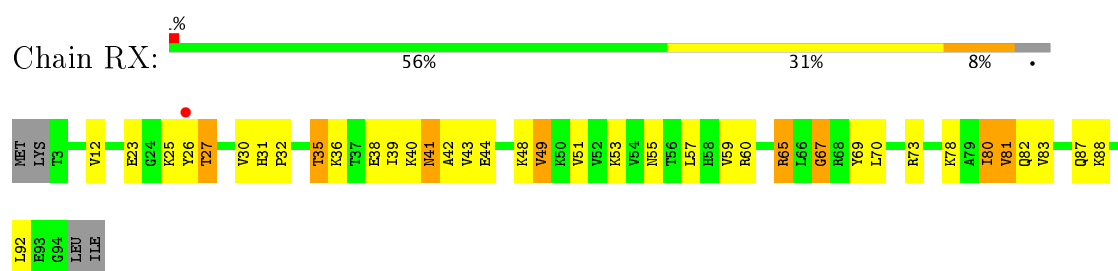
- Molecule 42: 50S ribosomal protein L22



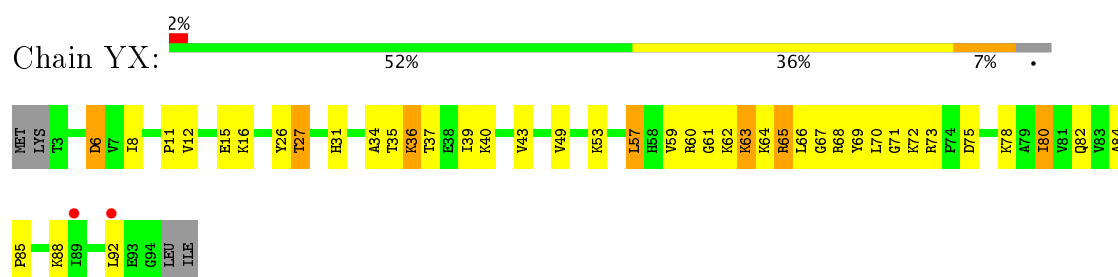
- Molecule 42: 50S ribosomal protein L22



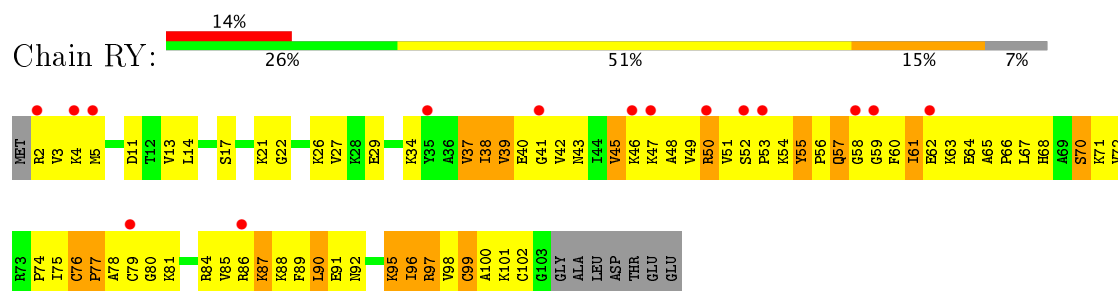
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23



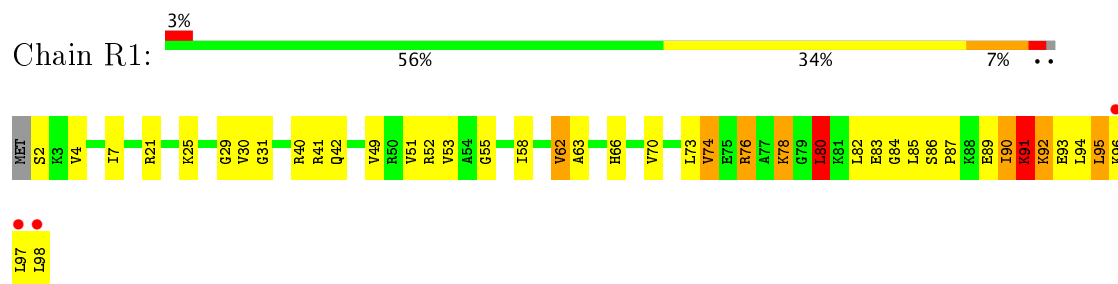
- Molecule 44: 50S ribosomal protein L24



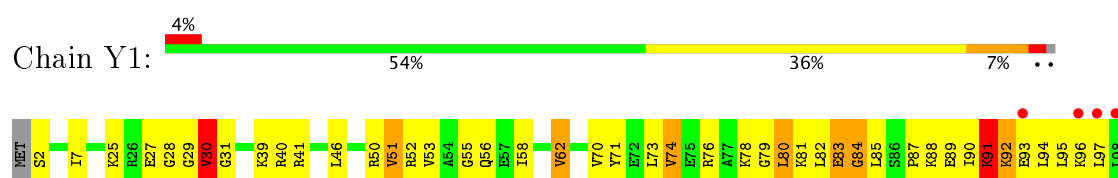
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| K5 |
| G6 |
| L7 |
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| S9 |
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| R11 |
| N12 |
| D15 |
| S16 |
| Q17 |
| A18 |
| K19 |
| R20 |
| V23 |
| K24 |
| R25 |
| Y26 |
| E27 |
| I36 |
| L37 |
| V38 |
| R39 |
| J40 |
| R41 |
| G42 |
| T43 |
| N50 |
| M63 |
| G54 |
| R55 |
| T58 |
| L59 |
| F60 |
| V63 |
| D64 |
| E68 |
| F69 |
| Q70 |
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| G76 |
| R77 |
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| R9V |

ALA

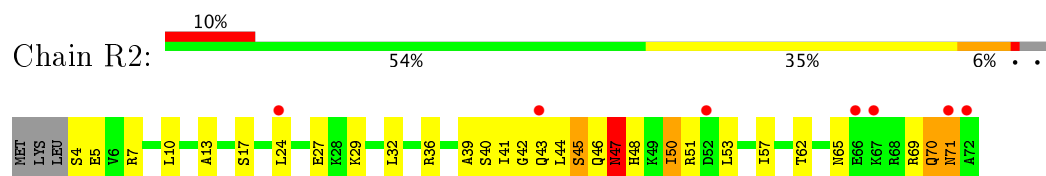
- Molecule 47: 50S ribosomal protein L28



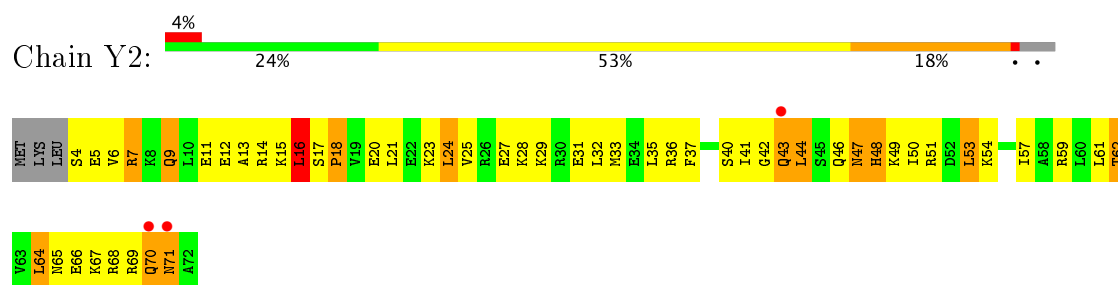
- Molecule 47: 50S ribosomal protein L28



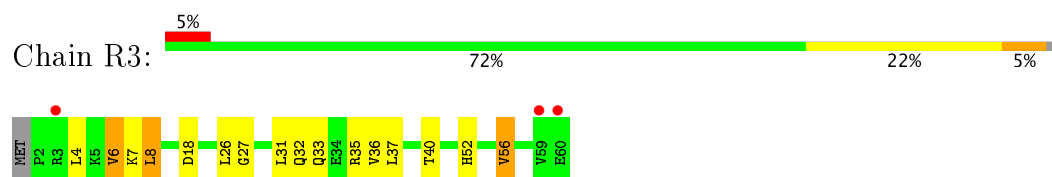
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

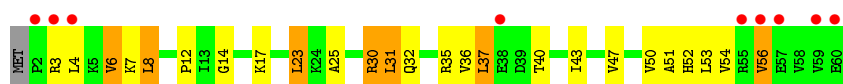


- Molecule 49: 50S ribosomal protein L30

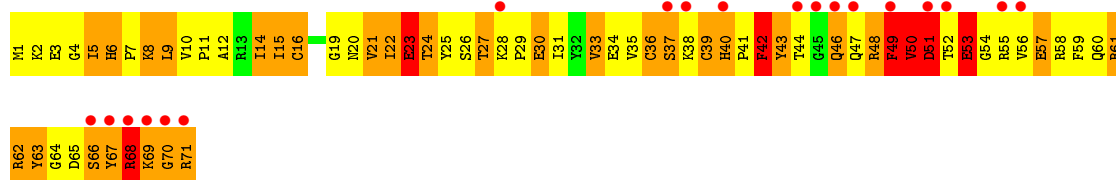


- Molecule 49: 50S ribosomal protein L30

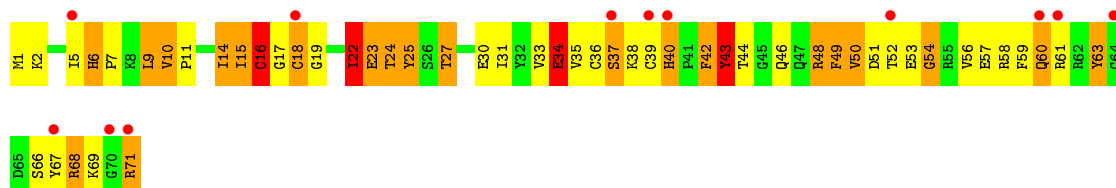




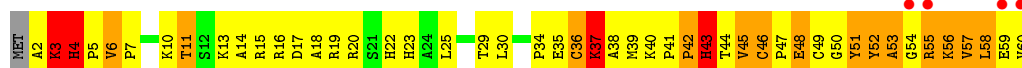
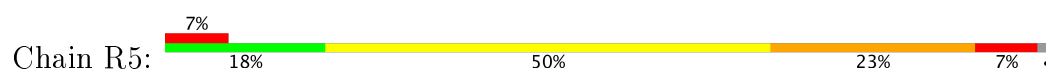
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



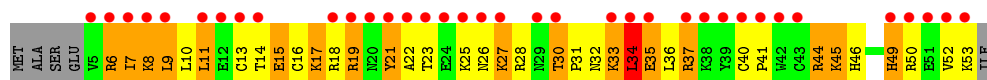
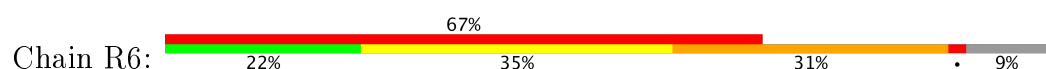
- Molecule 51: 50S ribosomal protein L32



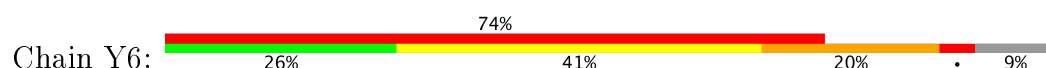
- Molecule 51: 50S ribosomal protein L32

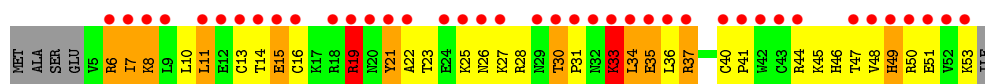


- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33





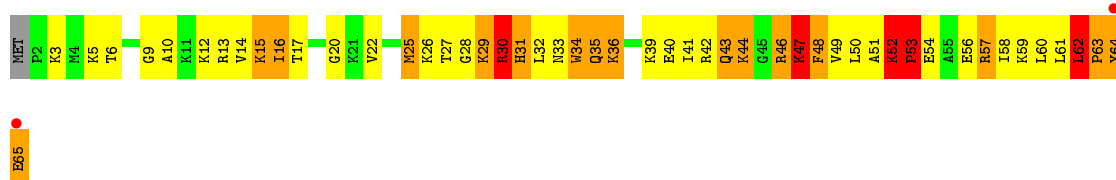
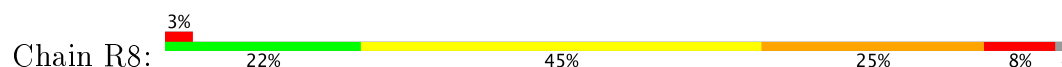
- Molecule 53: 50S ribosomal protein L34



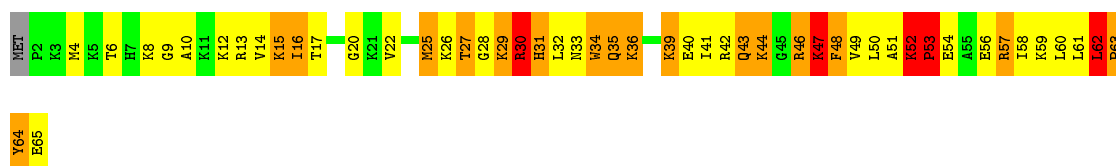
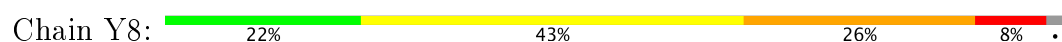
- Molecule 53: 50S ribosomal protein L34



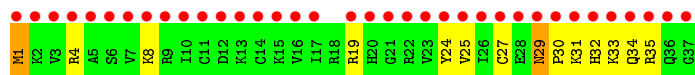
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro

Chain Z5:  33% 33% 33%



- Molecule 56: CC-Puro

Chain Z6:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.99Å 444.57Å 616.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.39 – 3.60 69.39 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (69.39-3.60) 97.2 (69.39-3.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.259 0.218 , 0.259	Depositor DCC
R_{free} test set	28849 reflections (4.53%)	DCC
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 95.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	292320	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.32	0/36098	0.87	44/56341 (0.1%)
1	XA	0.36	0/36101	0.88	26/56346 (0.0%)
2	QB	0.32	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.41	0/1733	0.60	2/2318 (0.1%)
4	XD	0.40	0/1733	0.59	0/2318
5	QE	0.38	0/1171	0.60	0/1576
5	XE	0.43	1/1171 (0.1%)	0.63	2/1576 (0.1%)
6	QF	0.38	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.34	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.56	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.38	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.50	0/991	0.85	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.40	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.36	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.34	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.65	0/1007
20	XT	0.32	0/765	0.61	0/1007
21	QU	0.30	0/221	0.55	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.38	1/1836 (0.1%)	0.80	0/2859
22	XV	0.41	1/1836 (0.1%)	0.83	0/2859
23	QX	0.33	0/213	0.81	0/329
23	XX	0.67	0/238	0.86	0/368
24	QY	0.43	0/384	0.83	0/597
24	XY	0.36	0/384	0.85	0/597
25	RA	0.39	2/69521 (0.0%)	0.91	59/108529 (0.1%)
25	YA	0.42	1/69521 (0.0%)	0.94	81/108529 (0.1%)
26	RB	0.51	0/2878	1.17	11/4490 (0.2%)
26	YB	0.62	1/2878 (0.0%)	1.28	24/4490 (0.5%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.44	0/1620	0.70	3/2194 (0.1%)
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.45	0/1332	0.85	4/1802 (0.2%)
32	RI	0.38	0/1151	0.67	0/1558
32	YI	0.38	0/1151	0.65	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.46	0/1131	0.66	1/1525 (0.1%)
34	RO	0.41	0/943	0.63	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.41	0/1162	0.79	1/1544 (0.1%)
35	YP	0.53	0/1162	0.89	2/1544 (0.1%)
36	RQ	0.54	0/1143	0.90	3/1527 (0.2%)
36	YQ	0.53	0/1143	0.87	3/1527 (0.2%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.65	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.43	0/1155	0.66	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.70	0/1064
45	RZ	0.30	0/1493	0.52	0/2026
45	YZ	0.29	0/1493	0.55	0/2026
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.49	0/656	0.70	0/872
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.64	0/771
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.50	0/468	0.72	0/632
52	R6	0.34	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.56	0/438	0.71	0/575
54	R8	0.61	0/525	0.92	1/691 (0.1%)
54	Y8	0.62	0/525	0.92	1/691 (0.1%)
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.33	0/310	0.48	0/407
56	Z5	0.80	0/40	1.79	1/60 (1.7%)
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
All	All	0.40	9/316522 (0.0%)	0.86	296/473223 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.63	1.48	1.61
22	XV	0	C	OP3-P	-10.58	1.48	1.61
5	XE	101	ILE	C-N	5.68	1.47	1.34
25	RA	2299	A	N9-C4	-5.68	1.34	1.37
25	YA	1021	A	N9-C4	-5.59	1.34	1.37

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	YE	21	VAL	C-N-CD	-10.10	98.37	120.60
28	RE	21	VAL	C-N-CD	-10.10	98.39	120.60
1	XA	1054	C	C6-N1-C2	-9.78	116.39	120.30
1	XA	1495	U	N1-C2-O2	9.30	129.31	122.80
25	RA	2432	C	O5'-P-OP1	-9.29	97.34	105.70

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	16278	544	0
1	XA	32249	0	16279	566	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	88	0
3	QC	1605	0	1668	51	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1765	106	0
4	XD	1703	0	1762	47	0
5	QE	1155	0	1213	48	0
5	XE	1155	0	1213	52	0
6	QF	843	0	857	17	0
6	XF	843	0	857	33	0
7	QG	1257	0	1296	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	27	0
8	QH	1116	0	1177	42	0
8	XH	1116	0	1177	33	0
9	QI	1010	0	1037	49	0
9	XI	1010	0	1037	51	0
10	QJ	801	0	849	52	0
10	XJ	801	0	849	63	0
11	QK	885	0	904	32	0
11	XK	885	0	904	29	0
12	QL	975	0	1062	98	0
12	XL	975	0	1062	95	0
13	QM	964	0	1034	66	0
13	XM	964	0	1034	47	0
14	QN	492	0	529	33	0
14	XN	492	0	529	20	0
15	QO	734	0	771	19	0
15	XO	734	0	771	18	0
16	QP	705	0	725	17	0
16	XP	705	0	725	24	0
17	QQ	834	0	904	25	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	11	0
18	XR	574	0	644	23	0
19	QS	674	0	699	95	0
19	XS	674	0	699	43	0
20	QT	763	0	861	31	0
20	XT	763	0	861	68	0
21	QU	217	0	234	13	0
21	XU	217	0	234	5	0
22	QV	1644	0	835	20	0
22	XV	1644	0	836	18	0
23	QX	191	0	99	1	0
23	XX	213	0	110	3	0
24	QY	344	0	173	3	0
24	XY	344	0	173	14	0
25	RA	62071	0	31290	1016	0
25	YA	62071	0	31290	988	0
26	RB	2573	0	1306	57	0
26	YB	2573	0	1306	79	0
27	RD	2115	0	2195	104	0
27	YD	2115	0	2195	327	0
28	RE	1568	0	1634	282	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	273	0
29	RF	1585	0	1632	78	0
29	YF	1585	0	1632	179	0
30	RG	1474	0	1535	111	0
30	YG	1474	0	1535	69	0
31	RH	1307	0	1382	228	0
31	YH	1307	0	1382	227	0
32	RI	1136	0	1223	106	0
32	YI	1136	0	1223	68	0
33	RN	1104	0	1180	45	0
33	YN	1104	0	1180	53	0
34	RO	933	0	996	26	0
34	YO	933	0	996	27	0
35	RP	1145	0	1228	117	0
35	YP	1145	0	1227	113	0
36	RQ	1122	0	1179	168	0
36	YQ	1122	0	1179	176	0
37	RR	968	0	1033	53	0
37	YR	968	0	1033	41	0
38	RS	882	0	943	54	0
38	YS	882	0	943	164	0
39	RT	1141	0	1202	72	0
39	YT	1141	0	1202	59	0
40	RU	964	0	1022	38	0
40	YU	964	0	1021	59	0
41	RV	779	0	852	26	0
41	YV	779	0	852	45	0
42	RW	900	0	964	29	0
42	YW	900	0	964	27	0
43	RX	725	0	778	31	0
43	YX	725	0	778	26	0
44	RY	785	0	878	53	0
44	YY	785	0	878	39	0
45	RZ	1461	0	1493	43	0
45	YZ	1461	0	1493	63	0
46	R0	648	0	672	26	0
46	Y0	647	0	668	41	0
47	R1	763	0	848	33	0
47	Y1	763	0	848	36	0
48	R2	581	0	629	24	0
48	Y2	581	0	629	73	0
49	R3	469	0	518	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	16	0
50	R4	581	0	575	230	0
50	Y4	581	0	577	63	0
51	R5	459	0	480	76	0
51	Y5	454	0	475	40	0
52	R6	424	0	450	41	0
52	Y6	424	0	450	38	0
53	R7	430	0	480	18	0
53	Y7	430	0	480	22	0
54	R8	517	0	582	132	0
54	Y8	517	0	582	103	0
55	R9	307	0	338	11	0
55	Y9	307	0	338	17	0
56	Z5	37	0	23	2	0
56	Z6	37	0	23	3	0
57	QA	82	0	0	0	0
57	QE	1	0	0	0	0
57	QF	1	0	0	0	0
57	QV	3	0	0	0	0
57	QX	1	0	0	0	0
57	QY	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	RA	327	0	0	0	0
57	RB	5	0	0	0	0
57	RE	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	111	0	0	0	0
57	XB	1	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	Y0	3	0	0	0	0
57	Y1	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	359	0	0	0	0
57	YB	4	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YU	1	0	0	0	0
57	YY	1	0	0	0	0
58	QA	42	0	45	4	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
60	Z5	37	0	28	12	0
60	Z6	37	0	28	7	0
All	All	292320	0	198405	8425	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 17.

The worst 5 of 8425 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)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
32:RI:144:VAL:O	32:RI:145:VAL:HG12	1.22	1.36
4:QD:9:CYS:SG	4:QD:22:LYS:CE	2.22	1.28
32:YI:144:VAL:O	32:YI:145:VAL:HG22	1.22	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1 17
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	5	40
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	12	55
4	QD	206/209 (99%)	178 (86%)	19 (9%)	9 (4%)	3	30
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	7	45
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	6	42
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	14	57
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	15 (10%)	2 (1%)	14	57
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	14	57
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	25	68
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	5	41
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	32
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5	38
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	5	40
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	25
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	52
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	52
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	8
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	8
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	15
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	15
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	19
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	10
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15	59
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	7	46
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	15	59
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	15	59
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9	49
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	12	55
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	5
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0	7
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2	22
20	XT	97/106 (92%)	75 (77%)	17 (18%)	5 (5%)	2	25
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	30
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	30
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	30
27	YD	270/276 (98%)	205 (76%)	46 (17%)	19 (7%)	1	18
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	171 (86%)	19 (10%)	10 (5%)	2	26
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1	10
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	15
30	YG	179/182 (98%)	143 (80%)	24 (13%)	12 (7%)	1	20
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
32	RI	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	1	11
32	YI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0	7
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	12
33	YN	136/140 (97%)	109 (80%)	16 (12%)	11 (8%)	1	14
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	52
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	52
35	RP	148/150 (99%)	112 (76%)	25 (17%)	11 (7%)	1	16
35	YP	148/150 (99%)	111 (75%)	22 (15%)	15 (10%)	1	10
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	10
36	YQ	139/141 (99%)	98 (70%)	25 (18%)	16 (12%)	0	8
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3	30
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	25
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	10
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	12
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	16
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4	37
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	11	52
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	22
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	14
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4	36
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	10	51
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	47
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8	47
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	4
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	7
45	RZ	181/206 (88%)	128 (71%)	33 (18%)	20 (11%)	0	8
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1	10
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	14	57
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1	11
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	21
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	2	22
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	5
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4	37
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	10	51
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	4	36
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	3
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	8	48
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	8	48
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Y8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	9009 (79%)	1610 (14%)	850 (7%)	1	16

5 of 850 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
4	QD	33	MET

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%)	172 (84%)	33 (16%)	3	19
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6	31
3	QC	159/188 (85%)	145 (91%)	14 (9%)	12	47
3	XC	159/188 (85%)	145 (91%)	14 (9%)	12	47
4	QD	180/181 (99%)	155 (86%)	25 (14%)	4	27
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4	25
5	QE	116/123 (94%)	104 (90%)	12 (10%)	8	40
5	XE	116/123 (94%)	104 (90%)	12 (10%)	8	40
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	28
6	XF	90/90 (100%)	82 (91%)	8 (9%)	11	46
7	QG	126/127 (99%)	114 (90%)	12 (10%)	10	44
7	XG	126/127 (99%)	114 (90%)	12 (10%)	10	44
8	QH	119/119 (100%)	109 (92%)	10 (8%)	13	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	XH	119/119 (100%)	106 (89%)	13 (11%)	7	37
9	QI	98/99 (99%)	80 (82%)	18 (18%)	2	12
9	XI	98/99 (99%)	79 (81%)	19 (19%)	1	11
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	28
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	3	21
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	41
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	41
12	QL	104/109 (95%)	90 (86%)	14 (14%)	4	28
12	XL	104/109 (95%)	89 (86%)	15 (14%)	4	25
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	5
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	11
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	12
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	26
15	QO	79/80 (99%)	72 (91%)	7 (9%)	11	46
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5	30
16	QP	72/74 (97%)	64 (89%)	8 (11%)	7	37
16	XP	72/74 (97%)	64 (89%)	8 (11%)	7	37
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	13	49
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	21	60
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	13
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	24
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	11
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	7
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6	33
20	XT	76/82 (93%)	67 (88%)	9 (12%)	6	33
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	28	66
27	RD	214/218 (98%)	174 (81%)	40 (19%)	2	12
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	17
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	7
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	RF	161/166 (97%)	131 (81%)	30 (19%)	2	12
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	29
30	RG	155/156 (99%)	134 (86%)	21 (14%)	4	28
30	YG	155/156 (99%)	133 (86%)	22 (14%)	4	26
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	10
31	YH	142/148 (96%)	115 (81%)	27 (19%)	2	11
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2	13
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1	5
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	16
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1	10
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	41
34	YO	100/100 (100%)	88 (88%)	12 (12%)	6	32
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	5
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0	2
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	19
36	YQ	111/111 (100%)	91 (82%)	20 (18%)	2	13
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	14
37	YR	101/101 (100%)	81 (80%)	20 (20%)	1	10
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	9
38	YS	87/88 (99%)	74 (85%)	13 (15%)	3	23
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	23
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	15
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	23
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	16
41	RV	82/82 (100%)	66 (80%)	16 (20%)	1	11
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	12
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	9
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	15
43	RX	74/78 (95%)	64 (86%)	10 (14%)	4	28
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2	11
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	YY	85/91 (93%)	64 (75%)	21 (25%)	1	5
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	3	24
45	YZ	162/179 (90%)	145 (90%)	17 (10%)	8	39
46	R0	65/67 (97%)	60 (92%)	5 (8%)	15	52
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	11	45
47	R1	82/83 (99%)	73 (89%)	9 (11%)	7	37
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	3	24
48	R2	64/67 (96%)	55 (86%)	9 (14%)	4	26
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	7	37
49	R3	51/52 (98%)	45 (88%)	6 (12%)	6	33
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	3	21
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	3
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	6
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	6
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	4
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	9
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2	11
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	2	17
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	23	62
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	23	62
All	All	9702/10066 (96%)	8159 (84%)	1543 (16%)	3	20

5 of 1543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	R2	53	LEU
7	XG	78	ARG
44	YY	97	ARG
50	R4	62	ARG
2	XB	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
50	R4	6	HIS
2	XB	19	HIS
28	YE	48	GLN
55	R9	29	ASN
2	XB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	279 (18%)	43 (2%)
1	XA	1498/1522 (98%)	282 (18%)	37 (2%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	13 (17%)	1 (1%)
23	QX	8/25 (32%)	2 (25%)	0
23	XX	9/25 (36%)	1 (11%)	0
24	QY	15/17 (88%)	2 (13%)	0
24	XY	15/17 (88%)	1 (6%)	0
25	RA	2879/2915 (98%)	606 (21%)	50 (1%)
25	YA	2879/2915 (98%)	607 (21%)	56 (1%)
26	RB	119/122 (97%)	22 (18%)	2 (1%)
26	YB	119/122 (97%)	27 (22%)	1 (0%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9193/9362 (98%)	1863 (20%)	191 (2%)

5 of 1863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C

5 of 191 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2530	A
1	XA	266	G
25	YA	1955	U

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Mol	Chain	Res	Type
25	RA	2622	C
1	XA	31	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 926 ligands modelled in this entry, 922 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	QA	1681	-	45,45,45	1.46	8 (17%)	60,67,67	1.39	6 (10%)
58	PAR	XA	1710	-	45,45,45	1.46	7 (15%)	60,67,67	1.30	5 (8%)
60	PPU	Z5	101	56	31,40,41	2.57	6 (19%)	34,57,60	2.55	6 (17%)
60	PPU	Z6	101	56	31,40,41	2.57	6 (19%)	34,57,60	2.55	6 (17%)

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	QA	1681	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1710	-	-	0/18/94/94	0/4/4/4
60	PPU	Z5	101	56	-	0/21/43/44	0/4/4/4
60	PPU	Z6	101	56	-	0/21/43/44	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Z6	101	PPU	C9-N6	-5.76	1.31	1.45
60	Z5	101	PPU	C9-N6	-5.75	1.32	1.45
60	Z6	101	PPU	C10-N6	-5.41	1.32	1.45
60	Z5	101	PPU	C10-N6	-5.38	1.32	1.45
60	Z5	101	PPU	C5-N7	-2.04	1.32	1.39

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Z5	101	PPU	C3'-N3'-C	-8.61	110.23	123.21
60	Z6	101	PPU	C3'-N3'-C	-8.59	110.26	123.21
60	Z5	101	PPU	N3-C2-N1	-8.55	121.42	128.86
60	Z6	101	PPU	N3-C2-N1	-8.51	121.45	128.86
60	Z6	101	PPU	C4'-O4'-C1'	-4.18	105.32	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1681	PAR	4	0
58	XA	1710	PAR	2	0
60	Z5	101	PPU	12	0
60	Z6	101	PPU	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.05	16 (1%) 80 67	40, 98, 191, 460	0
1	XA	1500/1522 (98%)	0.05	10 (0%) 87 78	37, 88, 192, 384	0
2	QB	237/256 (92%)	0.69	26 (10%) 6 6	91, 151, 229, 303	0
2	XB	237/256 (92%)	0.37	7 (2%) 51 37	71, 131, 209, 300	0
3	QC	205/239 (85%)	0.32	1 (0%) 90 84	79, 138, 213, 261	0
3	XC	205/239 (85%)	-0.02	0 100 100	53, 95, 150, 275	0
4	QD	208/209 (99%)	0.12	1 (0%) 90 84	59, 105, 170, 323	0
4	XD	208/209 (99%)	-0.12	0 100 100	43, 92, 156, 208	0
5	QE	151/162 (93%)	0.12	1 (0%) 87 78	66, 112, 178, 228	0
5	XE	151/162 (93%)	-0.16	0 100 100	44, 86, 140, 204	0
6	QF	101/101 (100%)	-0.14	0 100 100	48, 92, 135, 211	0
6	XF	101/101 (100%)	-0.06	0 100 100	47, 96, 150, 271	0
7	QG	155/156 (99%)	0.58	14 (9%) 10 8	86, 136, 192, 401	0
7	XG	155/156 (99%)	0.35	8 (5%) 28 20	63, 118, 165, 229	0
8	QH	138/138 (100%)	0.16	1 (0%) 87 78	66, 110, 155, 279	0
8	XH	138/138 (100%)	-0.00	1 (0%) 87 78	62, 104, 145, 170	0
9	QI	127/128 (99%)	0.84	16 (12%) 4 4	82, 153, 208, 251	0
9	XI	127/128 (99%)	0.25	0 100 100	56, 131, 179, 246	0
10	QJ	99/105 (94%)	0.81	10 (10%) 8 7	101, 158, 246, 398	0
10	XJ	99/105 (94%)	0.61	10 (10%) 8 7	60, 121, 205, 240	0
11	QK	119/129 (92%)	0.89	14 (11%) 5 5	60, 100, 188, 269	0
11	XK	119/129 (92%)	0.51	5 (4%) 37 26	37, 93, 164, 272	0
12	QL	125/132 (94%)	0.30	4 (3%) 48 35	47, 91, 145, 263	0
12	XL	125/132 (94%)	0.17	3 (2%) 59 45	42, 72, 139, 285	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.63	12 (9%) 8 7	91, 151, 204, 320	0
13	XM	121/126 (96%)	0.19	3 (2%) 58 43	58, 116, 178, 305	0
14	QN	60/61 (98%)	0.61	1 (1%) 70 57	88, 128, 188, 195	0
14	XN	60/61 (98%)	-0.00	0 100 100	49, 90, 129, 159	0
15	QO	88/89 (98%)	-0.00	0 100 100	41, 92, 137, 169	0
15	XO	88/89 (98%)	0.09	1 (1%) 80 67	56, 97, 143, 170	0
16	QP	84/88 (95%)	0.32	1 (1%) 79 66	62, 95, 137, 206	0
16	XP	84/88 (95%)	0.57	2 (2%) 59 45	74, 110, 158, 267	0
17	QQ	100/105 (95%)	0.26	0 100 100	57, 99, 132, 165	0
17	XQ	100/105 (95%)	0.24	0 100 100	68, 112, 143, 168	0
18	QR	70/88 (79%)	0.19	4 (5%) 24 17	64, 101, 147, 191	0
18	XR	70/88 (79%)	0.20	1 (1%) 75 62	62, 104, 164, 181	0
19	QS	84/93 (90%)	0.71	5 (5%) 23 16	100, 157, 204, 241	0
19	XS	84/93 (90%)	0.56	2 (2%) 59 45	66, 121, 190, 335	0
20	QT	99/106 (93%)	0.39	2 (2%) 65 51	55, 101, 164, 255	0
20	XT	99/106 (93%)	0.73	8 (8%) 13 10	80, 141, 215, 265	0
21	QU	25/27 (92%)	0.69	2 (8%) 13 10	95, 140, 198, 248	0
21	XU	25/27 (92%)	0.28	1 (4%) 39 28	76, 110, 159, 180	0
22	QV	77/77 (100%)	0.14	1 (1%) 77 64	38, 106, 168, 231	0
22	XV	77/77 (100%)	0.20	1 (1%) 77 64	42, 84, 137, 180	0
23	QX	9/25 (36%)	0.42	0 100 100	63, 86, 158, 171	0
23	XX	10/25 (40%)	0.50	1 (10%) 8 7	47, 69, 148, 219	0
24	QY	16/17 (94%)	0.41	1 (6%) 21 15	87, 115, 167, 175	0
24	XY	16/17 (94%)	0.18	0 100 100	68, 95, 153, 191	0
25	RA	2882/2915 (98%)	0.11	117 (4%) 38 27	27, 74, 249, 510	0
25	YA	2882/2915 (98%)	0.13	107 (3%) 42 31	27, 69, 246, 557	0
26	RB	120/122 (98%)	0.04	1 (0%) 86 75	90, 127, 170, 210	0
26	YB	120/122 (98%)	-0.17	0 100 100	61, 90, 124, 152	0
27	RD	272/276 (98%)	-0.14	1 (0%) 92 87	22, 61, 105, 222	0
27	YD	272/276 (98%)	-0.07	1 (0%) 92 87	22, 61, 105, 185	0
28	RE	205/206 (99%)	0.24	5 (2%) 59 45	39, 83, 168, 336	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	0.12	3 (1%) 74 61	31, 91, 177, 273	0
29	RF	202/210 (96%)	0.27	4 (1%) 65 51	23, 99, 171, 216	0
29	YF	202/210 (96%)	0.09	4 (1%) 65 51	32, 78, 149, 227	0
30	RG	181/182 (99%)	0.67	11 (6%) 22 16	92, 150, 197, 231	0
30	YG	181/182 (99%)	0.22	4 (2%) 62 48	61, 98, 160, 244	0
31	RH	170/180 (94%)	1.43	42 (24%) 1 1	102, 193, 270, 361	0
31	YH	170/180 (94%)	0.43	4 (2%) 59 45	53, 105, 164, 210	0
32	RI	146/148 (98%)	0.53	11 (7%) 15 11	67, 125, 195, 258	0
32	YI	146/148 (98%)	0.50	8 (5%) 26 18	48, 123, 189, 271	0
33	RN	138/140 (98%)	0.19	3 (2%) 62 48	51, 93, 154, 202	0
33	YN	138/140 (98%)	0.26	2 (1%) 75 62	47, 92, 157, 220	0
34	RO	122/122 (100%)	0.16	0 100 100	48, 80, 114, 148	0
34	YO	122/122 (100%)	0.05	0 100 100	27, 64, 103, 120	0
35	RP	150/150 (100%)	0.50	5 (3%) 47 35	28, 99, 159, 288	0
35	YP	150/150 (100%)	0.20	4 (2%) 55 41	31, 90, 162, 231	0
36	RQ	141/141 (100%)	0.61	8 (5%) 24 17	54, 102, 180, 226	0
36	YQ	141/141 (100%)	0.18	4 (2%) 53 40	35, 73, 140, 222	0
37	RR	118/118 (100%)	-0.14	0 100 100	29, 70, 104, 138	0
37	YR	118/118 (100%)	0.10	1 (0%) 86 75	51, 91, 139, 190	0
38	RS	111/112 (99%)	0.50	4 (3%) 43 32	81, 120, 204, 273	0
38	YS	111/112 (99%)	0.13	2 (1%) 69 55	67, 101, 156, 201	0
39	RT	137/146 (93%)	0.07	2 (1%) 74 61	50, 91, 188, 276	0
39	YT	137/146 (93%)	0.03	0 100 100	51, 89, 212, 242	0
40	RU	117/118 (99%)	0.23	5 (4%) 36 25	35, 81, 155, 298	0
40	YU	117/118 (99%)	-0.04	1 (0%) 84 72	40, 81, 152, 243	0
41	RV	101/101 (100%)	0.74	7 (6%) 18 13	55, 114, 183, 398	0
41	YV	101/101 (100%)	0.39	4 (3%) 39 28	44, 111, 174, 335	0
42	RW	113/113 (100%)	0.10	3 (2%) 55 41	36, 63, 115, 296	0
42	YW	113/113 (100%)	0.14	5 (4%) 35 25	37, 74, 134, 258	0
43	RX	92/96 (95%)	0.34	1 (1%) 80 67	51, 77, 128, 164	0
43	YX	92/96 (95%)	0.32	2 (2%) 62 48	37, 73, 112, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.93	15 (14%) 3 2	55, 119, 185, 325	0
44	YY	102/110 (92%)	0.20	4 (3%) 40 29	42, 92, 162, 273	0
45	RZ	183/206 (88%)	0.89	21 (11%) 5 5	104, 153, 230, 292	0
45	YZ	183/206 (88%)	0.49	4 (2%) 62 48	55, 116, 202, 300	0
46	R0	82/85 (96%)	0.44	2 (2%) 59 45	48, 88, 127, 238	0
46	Y0	82/85 (96%)	0.11	0 100 100	44, 71, 99, 142	0
47	R1	97/98 (98%)	0.43	3 (3%) 49 36	37, 80, 161, 290	0
47	Y1	97/98 (98%)	0.38	4 (4%) 38 27	39, 75, 176, 210	0
48	R2	69/72 (95%)	0.67	7 (10%) 8 7	63, 105, 160, 274	0
48	Y2	69/72 (95%)	0.17	3 (4%) 36 25	47, 80, 151, 219	0
49	R3	59/60 (98%)	0.60	3 (5%) 29 20	63, 97, 155, 205	0
49	Y3	59/60 (98%)	0.73	9 (15%) 2 2	55, 89, 162, 293	0
50	R4	71/71 (100%)	1.66	19 (26%) 1 1	150, 244, 350, 423	0
50	Y4	71/71 (100%)	0.85	12 (16%) 2 2	69, 162, 340, 411	0
51	R5	59/60 (98%)	0.24	4 (6%) 18 13	40, 77, 216, 261	0
51	Y5	58/60 (96%)	0.47	7 (12%) 5 5	44, 97, 231, 342	0
52	R6	49/54 (90%)	3.45	36 (73%) 0 0	119, 194, 264, 286	0
52	Y6	49/54 (90%)	3.17	40 (81%) 0 0	115, 171, 260, 295	0
53	R7	49/49 (100%)	-0.21	1 (2%) 65 51	27, 54, 110, 166	0
53	Y7	49/49 (100%)	-0.23	1 (2%) 65 51	32, 51, 111, 180	0
54	R8	64/65 (98%)	0.24	2 (3%) 49 36	42, 82, 134, 223	0
54	Y8	64/65 (98%)	-0.03	0 100 100	35, 68, 120, 229	0
55	R9	37/37 (100%)	5.80	36 (97%) 0 0	134, 200, 317, 510	0
55	Y9	37/37 (100%)	5.50	36 (97%) 0 0	134, 206, 322, 404	0
56	Z5	2/3 (66%)	0.18	0 100 100	50, 50, 50, 60	0
56	Z6	2/3 (66%)	0.04	0 100 100	38, 38, 38, 41	0
All	All	20878/21490 (97%)	0.25	852 (4%) 38 27	22, 92, 205, 557	0

The worst 5 of 852 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	17.4
25	YA	2165	G	14.4

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Mol	Chain	Res	Type	RSRZ
25	YA	2179	C	13.3
55	Y9	34	GLN	12.6
25	RA	2138	G	11.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
57	MG	YA	3319	1/1	0.76	0.80	123.14	34,34,34,34	0
57	MG	YA	3192	1/1	0.41	0.76	48.89	60,60,60,60	0
57	MG	R5	101	1/1	0.80	1.07	40.76	162,162,162,162	0
57	MG	YA	3140	1/1	0.92	0.60	39.84	58,58,58,58	0
57	MG	YA	3268	1/1	0.88	0.51	37.82	43,43,43,43	0
57	MG	YA	3030	1/1	0.99	0.52	36.44	9,9,9,9	0
57	MG	QA	1655	1/1	0.98	0.69	33.07	19,19,19,19	0
57	MG	RA	3033	1/1	0.98	0.46	32.67	16,16,16,16	0
57	MG	RA	3034	1/1	0.95	0.72	30.23	49,49,49,49	0
57	MG	YA	3232	1/1	0.85	0.56	30.00	25,25,25,25	0
57	MG	YA	3354	1/1	0.87	0.54	28.17	61,61,61,61	0
57	MG	RA	3169	1/1	0.80	0.42	25.55	35,35,35,35	0
57	MG	RA	3298	1/1	0.85	0.36	24.86	53,53,53,53	0
57	MG	XA	1688	1/1	0.96	0.61	24.46	60,60,60,60	0
57	MG	RA	3272	1/1	0.88	0.58	23.89	30,30,30,30	0
57	MG	RA	3320	1/1	0.88	0.48	23.52	32,32,32,32	0
57	MG	YA	3134	1/1	0.83	0.55	23.35	30,30,30,30	0
57	MG	YA	3230	1/1	0.98	0.56	23.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1659	1/1	0.91	0.51	22.53	40,40,40,40	0
57	MG	YA	3077	1/1	0.95	0.50	22.50	21,21,21,21	0
57	MG	YA	3138	1/1	0.88	0.42	22.40	50,50,50,50	0
57	MG	YA	3326	1/1	0.90	0.36	21.94	49,49,49,49	0
57	MG	YA	3046	1/1	0.95	0.39	21.67	18,18,18,18	0
57	MG	RA	3235	1/1	0.94	0.62	21.64	71,71,71,71	0
57	MG	RA	3283	1/1	0.94	0.53	21.27	32,32,32,32	0
57	MG	YA	3048	1/1	0.95	0.43	20.06	21,21,21,21	0
57	MG	YA	3173	1/1	0.78	0.51	19.93	63,63,63,63	0
57	MG	RA	3123	1/1	0.84	0.40	19.85	33,33,33,33	0
57	MG	RA	3321	1/1	0.82	0.53	19.38	40,40,40,40	0
57	MG	YA	3187	1/1	0.98	0.51	19.24	51,51,51,51	0
57	MG	YA	3233	1/1	0.95	0.46	19.15	16,16,16,16	0
57	MG	YA	3033	1/1	0.93	0.55	19.09	27,27,27,27	0
57	MG	YA	3303	1/1	0.92	0.49	19.05	53,53,53,53	0
57	MG	QA	1656	1/1	0.50	0.40	18.74	63,63,63,63	0
57	MG	RA	3285	1/1	0.94	0.62	18.26	57,57,57,57	0
57	MG	YA	3238	1/1	0.90	0.67	18.23	43,43,43,43	0
57	MG	XA	1667	1/1	0.91	0.50	18.22	23,23,23,23	0
57	MG	YA	3025	1/1	0.98	0.58	18.20	39,39,39,39	0
57	MG	XA	1649	1/1	0.76	0.49	17.74	39,39,39,39	0
57	MG	XA	1619	1/1	0.90	0.60	17.29	40,40,40,40	0
57	MG	RA	3279	1/1	0.79	0.48	17.26	54,54,54,54	0
57	MG	YA	3022	1/1	0.96	0.41	16.82	28,28,28,28	0
57	MG	YA	3327	1/1	0.82	0.47	16.76	56,56,56,56	0
57	MG	YA	3009	1/1	0.94	0.46	16.72	30,30,30,30	0
57	MG	RA	3057	1/1	0.96	0.43	16.52	19,19,19,19	0
57	MG	RA	3059	1/1	0.96	0.37	16.52	15,15,15,15	0
57	MG	YA	3251	1/1	0.96	0.37	16.34	37,37,37,37	0
57	MG	QA	1640	1/1	0.66	0.84	16.34	63,63,63,63	0
57	MG	RA	3155	1/1	0.96	0.47	16.22	55,55,55,55	0
57	MG	YA	3169	1/1	0.93	0.66	16.12	85,85,85,85	0
57	MG	YA	3264	1/1	0.94	0.53	15.70	65,65,65,65	0
57	MG	YA	3323	1/1	0.94	0.49	15.67	42,42,42,42	0
57	MG	RA	3005	1/1	0.96	0.55	15.54	10,10,10,10	0
57	MG	YA	3095	1/1	0.95	0.38	15.23	30,30,30,30	0
57	MG	YA	3214	1/1	0.70	0.40	15.08	40,40,40,40	0
57	MG	YA	3170	1/1	0.92	0.44	14.99	52,52,52,52	0
57	MG	YA	3240	1/1	0.99	0.43	14.90	21,21,21,21	0
57	MG	YA	3307	1/1	0.95	0.37	14.57	37,37,37,37	0
57	MG	RA	3003	1/1	0.99	0.44	14.56	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	RA	3118	1/1	0.97	0.46	14.38	40,40,40,40	0
57	MG	YA	3076	1/1	0.94	0.53	14.23	15,15,15,15	0
57	MG	QA	1660	1/1	0.89	0.41	14.01	31,31,31,31	0
57	MG	XA	1692	1/1	0.92	0.29	13.83	58,58,58,58	0
57	MG	RA	3227	1/1	0.81	0.34	13.61	23,23,23,23	0
57	MG	XA	1643	1/1	0.77	0.40	13.60	59,59,59,59	0
57	MG	XA	1634	1/1	0.92	0.41	13.49	38,38,38,38	0
57	MG	RA	3160	1/1	0.94	0.42	13.28	55,55,55,55	0
57	MG	XA	1632	1/1	0.52	0.35	13.11	58,58,58,58	0
57	MG	RA	3031	1/1	0.98	0.36	13.08	40,40,40,40	0
57	MG	QA	1613	1/1	0.95	0.48	12.92	40,40,40,40	0
57	MG	YA	3161	1/1	0.91	0.41	12.83	39,39,39,39	0
57	MG	YA	3156	1/1	0.83	0.44	12.82	76,76,76,76	0
57	MG	RA	3119	1/1	0.93	0.54	12.76	50,50,50,50	0
57	MG	RA	3062	1/1	0.97	0.46	12.34	3,3,3,3	0
57	MG	XA	1633	1/1	0.93	0.77	12.31	47,47,47,47	0
57	MG	RA	3052	1/1	0.97	0.34	12.25	5,5,5,5	0
57	MG	RA	3098	1/1	0.97	0.41	12.16	14,14,14,14	0
57	MG	YA	3102	1/1	0.98	0.36	11.89	16,16,16,16	0
57	MG	QA	1672	1/1	0.93	0.35	11.73	41,41,41,41	0
57	MG	RA	3049	1/1	0.92	0.41	11.43	14,14,14,14	0
57	MG	RA	3007	1/1	0.93	0.55	11.33	12,12,12,12	0
57	MG	RA	3315	1/1	0.95	0.74	11.30	42,42,42,42	0
57	MG	RA	3232	1/1	0.82	0.40	11.24	46,46,46,46	0
57	MG	XA	1679	1/1	0.96	0.57	11.12	27,27,27,27	0
57	MG	RA	3264	1/1	0.90	0.45	11.02	58,58,58,58	0
57	MG	RA	3040	1/1	0.99	0.31	10.29	24,24,24,24	0
57	MG	YA	3082	1/1	0.96	0.34	9.91	12,12,12,12	0
57	MG	RA	3142	1/1	0.92	0.45	9.77	19,19,19,19	0
57	MG	RA	3009	1/1	0.87	0.31	9.72	39,39,39,39	0
57	MG	QA	1629	1/1	0.68	0.32	9.69	52,52,52,52	0
57	MG	YA	3114	1/1	0.93	0.39	9.62	40,40,40,40	0
57	MG	QA	1612	1/1	0.95	0.45	9.60	39,39,39,39	0
57	MG	RA	3063	1/1	0.96	0.51	9.56	9,9,9,9	0
57	MG	YA	3096	1/1	0.98	0.44	9.54	21,21,21,21	0
57	MG	QA	1605	1/1	0.97	0.47	9.52	30,30,30,30	0
57	MG	YA	3014	1/1	0.93	0.30	9.47	6,6,6,6	0
57	MG	YA	3103	1/1	0.97	0.32	9.26	11,11,11,11	0
57	MG	XA	1700	1/1	0.89	0.57	9.13	50,50,50,50	0
57	MG	YA	3347	1/1	0.84	0.41	9.03	46,46,46,46	0
57	MG	YA	3013	1/1	0.96	0.51	8.84	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3088	1/1	0.96	0.30	8.77	18,18,18,18	0
57	MG	YA	3023	1/1	0.92	0.41	8.74	23,23,23,23	0
57	MG	RA	3087	1/1	0.97	0.44	8.74	23,23,23,23	0
57	MG	YA	3313	1/1	0.64	0.39	8.49	50,50,50,50	0
57	MG	RA	3097	1/1	0.97	0.35	8.47	5,5,5,5	0
57	MG	RA	3047	1/1	0.97	0.43	8.41	12,12,12,12	0
57	MG	YA	3085	1/1	0.93	0.38	8.37	31,31,31,31	0
57	MG	YA	3219	1/1	0.95	0.27	8.33	37,37,37,37	0
57	MG	XA	1639	1/1	0.97	0.44	8.16	43,43,43,43	0
57	MG	RA	3280	1/1	0.83	0.45	8.13	53,53,53,53	0
57	MG	YA	3249	1/1	0.96	0.37	7.97	44,44,44,44	0
57	MG	XA	1624	1/1	0.97	0.44	7.95	41,41,41,41	0
57	MG	RA	3249	1/1	0.86	0.32	7.92	57,57,57,57	0
57	MG	RA	3135	1/1	0.92	0.39	7.73	15,15,15,15	0
57	MG	YA	3246	1/1	0.97	0.31	7.67	34,34,34,34	0
57	MG	RA	3013	1/1	0.95	0.38	7.65	23,23,23,23	0
57	MG	YA	3075	1/1	0.93	0.34	7.53	21,21,21,21	0
57	MG	YA	3209	1/1	0.62	0.33	7.41	50,50,50,50	0
57	MG	RA	3026	1/1	0.93	0.41	7.40	27,27,27,27	0
57	MG	RA	3085	1/1	0.97	0.33	7.39	9,9,9,9	0
57	MG	RA	3079	1/1	0.97	0.40	7.32	36,36,36,36	0
57	MG	YA	3086	1/1	0.95	0.42	7.32	56,56,56,56	0
57	MG	RA	3130	1/1	0.94	0.39	7.28	21,21,21,21	0
57	MG	YA	3236	1/1	0.90	0.40	7.13	28,28,28,28	0
57	MG	XA	1616	1/1	0.98	0.37	7.09	29,29,29,29	0
57	MG	QA	1650	1/1	0.94	0.37	6.98	41,41,41,41	0
57	MG	RA	3054	1/1	0.79	0.24	6.71	15,15,15,15	0
57	MG	YA	3094	1/1	0.91	0.51	6.66	26,26,26,26	0
57	MG	XA	1613	1/1	0.98	0.36	6.63	17,17,17,17	0
57	MG	RA	3038	1/1	0.99	0.28	6.59	13,13,13,13	0
57	MG	RA	3010	1/1	0.80	0.33	6.53	46,46,46,46	0
57	MG	YA	3297	1/1	0.98	0.34	6.53	32,32,32,32	0
57	MG	QA	1617	1/1	0.88	0.28	6.52	38,38,38,38	0
57	MG	YA	3197	1/1	0.80	0.29	6.35	55,55,55,55	0
57	MG	QA	1644	1/1	0.93	0.55	6.32	54,54,54,54	0
57	MG	QA	1654	1/1	0.96	0.34	6.29	68,68,68,68	0
57	MG	XA	1685	1/1	0.98	0.28	6.27	21,21,21,21	0
57	MG	RA	3251	1/1	0.90	0.28	6.23	47,47,47,47	0
57	MG	YA	3049	1/1	0.99	0.29	6.21	8,8,8,8	0
57	MG	YA	3152	1/1	0.96	0.23	6.20	18,18,18,18	0
57	MG	YA	3328	1/1	0.91	0.36	6.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3340	1/1	0.81	0.29	6.18	56,56,56,56	0
57	MG	QA	1651	1/1	0.97	0.29	6.12	29,29,29,29	0
57	MG	XA	1642	1/1	0.98	0.38	6.11	27,27,27,27	0
57	MG	YA	3011	1/1	0.98	0.31	6.06	13,13,13,13	0
57	MG	RA	3006	1/1	0.99	0.38	6.05	7,7,7,7	0
57	MG	YA	3164	1/1	0.77	0.27	5.96	51,51,51,51	0
57	MG	RA	3240	1/1	0.98	0.28	5.90	35,35,35,35	0
57	MG	YA	3191	1/1	0.74	0.32	5.87	56,56,56,56	0
57	MG	YU	201	1/1	0.81	0.34	5.85	62,62,62,62	0
57	MG	RA	3300	1/1	0.86	0.31	5.80	48,48,48,48	0
57	MG	RA	3025	1/1	0.85	0.29	5.79	11,11,11,11	0
57	MG	QE	201	1/1	0.92	0.71	5.75	59,59,59,59	0
57	MG	YA	3293	1/1	0.64	0.53	5.57	47,47,47,47	0
57	MG	XA	1606	1/1	0.91	0.40	5.57	40,40,40,40	0
57	MG	XA	1705	1/1	0.69	0.30	5.56	52,52,52,52	0
57	MG	YA	3357	1/1	0.76	0.42	5.56	66,66,66,66	0
57	MG	RA	3234	1/1	0.96	0.28	5.56	18,18,18,18	0
57	MG	QA	1618	1/1	0.90	0.30	5.51	58,58,58,58	0
57	MG	YA	3132	1/1	0.96	0.31	5.48	21,21,21,21	0
57	MG	QA	1602	1/1	0.97	0.52	5.48	22,22,22,22	0
57	MG	XA	1623	1/1	0.76	0.28	5.43	48,48,48,48	0
57	MG	RA	3326	1/1	0.97	0.34	5.43	24,24,24,24	0
57	MG	YA	3309	1/1	0.92	0.58	5.29	69,69,69,69	0
57	MG	YA	3040	1/1	0.97	0.45	5.22	11,11,11,11	0
57	MG	YA	3316	1/1	0.94	0.31	4.97	34,34,34,34	0
57	MG	YA	3016	1/1	0.97	0.27	4.97	28,28,28,28	0
57	MG	RA	3022	1/1	0.97	0.34	4.91	14,14,14,14	0
57	MG	YA	3043	1/1	0.88	0.30	4.80	9,9,9,9	0
57	MG	YA	3037	1/1	0.97	0.26	4.76	12,12,12,12	0
57	MG	YA	3027	1/1	0.92	0.27	4.74	17,17,17,17	0
57	MG	RA	3268	1/1	0.89	0.27	4.70	67,67,67,67	0
57	MG	XA	1621	1/1	0.98	0.29	4.66	25,25,25,25	0
57	MG	YA	3004	1/1	0.90	0.28	4.62	22,22,22,22	0
57	MG	YA	3047	1/1	0.93	0.32	4.59	15,15,15,15	0
57	MG	XA	1652	1/1	0.93	0.34	4.54	72,72,72,72	0
57	MG	QA	1658	1/1	0.60	0.73	4.53	62,62,62,62	0
57	MG	YA	3265	1/1	0.92	0.28	4.46	42,42,42,42	0
57	MG	YA	3174	1/1	0.56	0.26	4.41	89,89,89,89	0
57	MG	YA	3068	1/1	0.90	0.25	4.40	29,29,29,29	0
57	MG	YA	3216	1/1	0.94	0.28	4.35	25,25,25,25	0
57	MG	RR	201	1/1	0.72	0.60	4.32	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1641	1/1	0.97	0.27	4.32	21,21,21,21	0
57	MG	RA	3021	1/1	0.98	0.27	4.25	4,4,4,4	0
57	MG	YA	3078	1/1	0.84	0.22	4.23	17,17,17,17	0
57	MG	RA	3152	1/1	0.92	0.25	4.19	34,34,34,34	0
57	MG	YA	3024	1/1	0.96	0.28	4.15	15,15,15,15	0
57	MG	RA	3157	1/1	0.87	0.25	4.15	26,26,26,26	0
57	MG	YA	3136	1/1	0.78	0.26	4.10	40,40,40,40	0
57	MG	XA	1631	1/1	0.91	0.25	4.07	63,63,63,63	0
57	MG	YA	3069	1/1	0.97	0.34	4.02	8,8,8,8	0
57	MG	RA	3181	1/1	0.84	0.27	4.01	48,48,48,48	0
57	MG	RA	3230	1/1	0.99	0.37	3.97	22,22,22,22	0
57	MG	QA	1653	1/1	0.96	0.41	3.73	30,30,30,30	0
57	MG	RA	3072	1/1	0.98	0.30	3.72	26,26,26,26	0
57	MG	RA	3094	1/1	0.98	0.35	3.72	18,18,18,18	0
57	MG	YA	3006	1/1	0.93	0.45	3.56	33,33,33,33	0
57	MG	YA	3028	1/1	0.97	0.31	3.48	17,17,17,17	0
57	MG	YA	3034	1/1	0.98	0.27	3.48	19,19,19,19	0
57	MG	RA	3281	1/1	0.94	0.33	3.36	39,39,39,39	0
57	MG	YA	3269	1/1	0.97	0.28	3.32	51,51,51,51	0
57	MG	YA	3031	1/1	0.95	0.29	3.30	11,11,11,11	0
57	MG	RA	3020	1/1	0.96	0.31	3.27	2,2,2,2	0
57	MG	RA	3201	1/1	0.62	0.27	3.26	55,55,55,55	0
57	MG	RA	3236	1/1	0.97	0.28	3.19	21,21,21,21	0
57	MG	XA	1663	1/1	0.95	0.28	3.17	26,26,26,26	0
57	MG	YA	3105	1/1	0.96	0.25	3.13	45,45,45,45	0
57	MG	YA	3002	1/1	0.95	0.30	3.12	14,14,14,14	0
57	MG	YA	3099	1/1	0.98	0.26	3.11	5,5,5,5	0
57	MG	RA	3106	1/1	0.97	0.26	3.04	21,21,21,21	0
57	MG	YA	3041	1/1	0.98	0.38	3.04	31,31,31,31	0
57	MG	YA	3036	1/1	0.99	0.25	2.99	10,10,10,10	0
57	MG	YA	3355	1/1	0.95	0.32	2.89	19,19,19,19	0
57	MG	QA	1610	1/1	0.98	0.31	2.70	20,20,20,20	0
57	MG	YA	3348	1/1	0.95	0.24	2.69	40,40,40,40	0
57	MG	YA	3194	1/1	0.66	0.20	2.67	90,90,90,90	0
57	MG	YA	3147	1/1	0.86	0.22	2.65	27,27,27,27	0
57	MG	XA	1627	1/1	0.85	0.19	2.60	98,98,98,98	0
57	MG	RA	3266	1/1	0.85	0.23	2.58	40,40,40,40	0
57	MG	YA	3119	1/1	0.91	0.24	2.58	20,20,20,20	0
57	MG	RA	3036	1/1	0.99	0.24	2.56	12,12,12,12	0
57	MG	XA	1603	1/1	0.97	0.32	2.55	16,16,16,16	0
57	MG	YA	3108	1/1	0.97	0.27	2.51	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3241	1/1	0.98	0.21	2.46	45,45,45,45	0
57	MG	YA	3067	1/1	0.98	0.22	2.42	10,10,10,10	0
57	MG	RA	3176	1/1	0.72	0.23	2.42	31,31,31,31	0
57	MG	YP	202	1/1	0.93	0.33	2.42	32,32,32,32	0
59	ZN	QD	301	1/1	0.75	0.34	2.33	77,77,77,77	0
57	MG	YA	3032	1/1	0.98	0.32	2.19	16,16,16,16	0
57	MG	YA	3228	1/1	0.82	0.35	2.18	43,43,43,43	0
57	MG	RA	3214	1/1	0.71	0.20	2.16	33,33,33,33	0
57	MG	RA	3077	1/1	0.92	0.25	2.14	7,7,7,7	0
57	MG	XA	1684	1/1	0.78	0.30	2.12	56,56,56,56	0
57	MG	RA	3171	1/1	0.91	0.29	2.11	34,34,34,34	0
57	MG	YA	3247	1/1	0.98	0.41	2.08	70,70,70,70	0
57	MG	RP	201	1/1	0.98	0.38	2.06	31,31,31,31	0
57	MG	YA	3026	1/1	0.98	0.24	2.03	6,6,6,6	0
57	MG	RA	3220	1/1	0.99	0.34	1.96	23,23,23,23	0
57	MG	YA	3090	1/1	0.95	0.28	1.92	45,45,45,45	0
58	PAR	XA	1710	42/42	0.95	0.24	1.91	56,56,57,57	0
57	MG	RA	3015	1/1	0.97	0.23	1.87	15,15,15,15	0
60	PPU	Z6	101	37/38	0.94	0.26	1.84	36,37,38,38	0
57	MG	YA	3199	1/1	0.83	0.20	1.80	63,63,63,63	0
58	PAR	QA	1681	42/42	0.91	0.27	1.80	71,71,72,72	0
57	MG	YA	3112	1/1	0.87	0.24	1.79	39,39,39,39	0
59	ZN	XD	301	1/1	0.98	0.31	1.72	49,49,49,49	0
57	MG	RA	3093	1/1	0.97	0.32	1.62	45,45,45,45	0
60	PPU	Z5	101	37/38	0.95	0.27	1.57	45,47,48,48	0
57	MG	RA	3167	1/1	0.92	0.20	1.52	26,26,26,26	0
57	MG	YA	3184	1/1	0.96	0.20	1.51	22,22,22,22	0
57	MG	YA	3288	1/1	0.99	0.22	1.32	28,28,28,28	0
57	MG	QA	1616	1/1	0.96	0.34	1.32	35,35,35,35	0
57	MG	RA	3260	1/1	0.90	0.30	1.30	56,56,56,56	0
57	MG	RA	3173	1/1	0.83	0.25	1.29	19,19,19,19	0
57	MG	YA	3008	1/1	0.97	0.22	1.22	11,11,11,11	0
57	MG	YA	3259	1/1	0.91	0.23	1.20	43,43,43,43	0
57	MG	RA	3217	1/1	0.43	0.19	1.19	48,48,48,48	0
57	MG	XA	1617	1/1	0.98	0.22	1.18	41,41,41,41	0
57	MG	YA	3130	1/1	0.90	0.26	1.17	37,37,37,37	0
57	MG	YA	3356	1/1	0.95	0.25	1.17	28,28,28,28	0
57	MG	XD	302	1/1	0.95	0.26	1.16	82,82,82,82	0
57	MG	YA	3137	1/1	0.90	0.20	1.14	76,76,76,76	0
57	MG	RA	3024	1/1	0.98	0.23	1.14	6,6,6,6	0
57	MG	QA	1666	1/1	0.83	0.22	1.06	50,50,50,50	0
57	MG	YA	3087	1/1	0.97	0.26	1.03	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1626	1/1	0.80	0.26	0.95	31,31,31,31	0
57	MG	RA	3185	1/1	0.90	0.25	0.89	28,28,28,28	0
57	MG	RA	3075	1/1	0.97	0.22	0.88	4,4,4,4	0
57	MG	RA	3086	1/1	0.99	0.21	0.86	30,30,30,30	0
57	MG	RA	3114	1/1	0.94	0.20	0.80	12,12,12,12	0
57	MG	RA	3134	1/1	0.91	0.19	0.80	64,64,64,64	0
57	MG	YA	3252	1/1	0.98	0.21	0.70	11,11,11,11	0
57	MG	RA	3120	1/1	0.98	0.18	0.67	40,40,40,40	0
57	MG	YA	3060	1/1	0.97	0.24	0.65	17,17,17,17	0
57	MG	YA	3129	1/1	0.86	0.20	0.60	39,39,39,39	0
57	MG	RA	3081	1/1	0.96	0.24	0.59	39,39,39,39	0
57	MG	QV	102	1/1	0.96	0.19	0.50	27,27,27,27	0
57	MG	RA	3042	1/1	0.98	0.20	0.40	12,12,12,12	0
57	MG	RA	3064	1/1	0.98	0.19	0.23	13,13,13,13	0
57	MG	YA	3200	1/1	0.87	0.20	0.17	32,32,32,32	0
57	MG	RA	3058	1/1	0.65	0.20	0.12	10,10,10,10	0
57	MG	YA	3074	1/1	0.96	0.22	0.08	22,22,22,22	0
57	MG	QA	1642	1/1	0.93	0.21	0.07	62,62,62,62	0
57	MG	RA	3019	1/1	0.99	0.18	0.05	9,9,9,9	0
57	MG	YA	3057	1/1	0.88	0.20	-0.01	12,12,12,12	0
57	MG	YA	3181	1/1	0.88	0.17	-0.05	47,47,47,47	0
57	MG	QA	1628	1/1	0.94	0.20	-0.10	64,64,64,64	0
57	MG	Y7	101	1/1	0.89	0.24	-0.15	33,33,33,33	0
57	MG	YA	3358	1/1	0.74	0.21	-0.20	61,61,61,61	0
57	MG	XA	1653	1/1	0.92	0.19	-0.21	42,42,42,42	0
57	MG	YA	3158	1/1	0.94	0.17	-0.23	18,18,18,18	0
57	MG	RA	3065	1/1	0.97	0.24	-0.24	3,3,3,3	0
57	MG	RA	3148	1/1	0.80	0.16	-0.27	41,41,41,41	0
57	MG	RA	3243	1/1	0.91	0.17	-0.30	47,47,47,47	0
57	MG	YA	3070	1/1	0.84	0.18	-0.38	27,27,27,27	0
57	MG	RA	3189	1/1	0.52	0.17	-0.43	69,69,69,69	0
57	MG	YA	3058	1/1	0.97	0.18	-0.47	33,33,33,33	0
57	MG	QA	1619	1/1	0.92	0.21	-0.51	40,40,40,40	0
57	MG	RA	3104	1/1	0.97	0.18	-0.51	19,19,19,19	0
57	MG	YA	3248	1/1	0.94	0.18	-0.51	27,27,27,27	0
57	MG	RA	3080	1/1	0.96	0.17	-0.52	24,24,24,24	0
57	MG	YA	3305	1/1	0.95	0.23	-0.53	12,12,12,12	0
57	MG	YA	3298	1/1	0.92	0.17	-0.57	45,45,45,45	0
57	MG	QA	1682	1/1	0.86	0.19	-0.63	104,104,104,104	0
57	MG	QA	1620	1/1	0.95	0.20	-0.63	66,66,66,66	0
57	MG	XA	1618	1/1	0.87	0.21	-0.64	37,37,37,37	0
57	MG	QA	1662	1/1	0.88	0.19	-0.67	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3109	1/1	0.93	0.19	-0.67	26,26,26,26	0
57	MG	XV	102	1/1	0.98	0.18	-0.68	14,14,14,14	0
57	MG	RA	3203	1/1	0.88	0.16	-0.69	47,47,47,47	0
57	MG	YA	3160	1/1	0.85	0.14	-0.69	70,70,70,70	0
57	MG	RA	3017	1/1	0.98	0.17	-0.72	24,24,24,24	0
57	MG	RA	3145	1/1	0.95	0.17	-0.76	41,41,41,41	0
57	MG	XA	1636	1/1	0.75	0.18	-0.78	66,66,66,66	0
57	MG	YA	3123	1/1	0.93	0.20	-0.86	54,54,54,54	0
57	MG	YA	3239	1/1	0.95	0.20	-0.86	19,19,19,19	0
59	ZN	XN	101	1/1	0.95	0.16	-0.87	81,81,81,81	0
57	MG	YA	3005	1/1	0.95	0.16	-0.93	16,16,16,16	0
57	MG	XA	1647	1/1	0.92	0.21	-0.93	82,82,82,82	0
57	MG	RA	3149	1/1	0.96	0.17	-0.95	37,37,37,37	0
57	MG	QA	1638	1/1	0.79	0.17	-0.96	53,53,53,53	0
57	MG	XA	1612	1/1	0.89	0.15	-0.96	68,68,68,68	0
57	MG	RA	3121	1/1	0.93	0.16	-1.05	24,24,24,24	0
57	MG	RA	3110	1/1	0.96	0.15	-1.19	33,33,33,33	0
57	MG	RA	3105	1/1	0.98	0.17	-1.26	12,12,12,12	0
57	MG	RA	3116	1/1	0.95	0.13	-1.27	65,65,65,65	0
57	MG	YA	3310	1/1	0.90	0.16	-1.29	26,26,26,26	0
57	MG	YB	202	1/1	0.98	0.17	-1.30	51,51,51,51	0
57	MG	YA	3107	1/1	0.86	0.18	-1.34	42,42,42,42	0
57	MG	RA	3131	1/1	0.91	0.13	-1.35	52,52,52,52	0
59	ZN	QN	101	1/1	0.94	0.14	-1.41	135,135,135,135	0
57	MG	RA	3074	1/1	0.86	0.15	-1.50	58,58,58,58	0
57	MG	XA	1620	1/1	0.96	0.16	-1.53	52,52,52,52	0
57	MG	RA	3101	1/1	0.91	0.14	-1.58	38,38,38,38	0
57	MG	YA	3106	1/1	0.96	0.16	-1.61	32,32,32,32	0
57	MG	QA	1607	1/1	0.97	0.16	-1.64	35,35,35,35	0
57	MG	YA	3179	1/1	0.76	0.12	-1.66	52,52,52,52	0
57	MG	YA	3055	1/1	0.95	0.17	-1.67	13,13,13,13	0
57	MG	Y1	101	1/1	0.97	0.10	-1.70	35,35,35,35	0
57	MG	YA	3218	1/1	0.98	0.15	-1.71	55,55,55,55	0
57	MG	RA	3179	1/1	0.95	0.14	-1.71	28,28,28,28	0
57	MG	RA	3309	1/1	0.93	0.17	-1.71	39,39,39,39	0
57	MG	RA	3314	1/1	0.80	0.14	-1.79	67,67,67,67	0
57	MG	RA	3126	1/1	0.92	0.15	-1.89	24,24,24,24	0
57	MG	XA	1610	1/1	0.98	0.15	-1.99	21,21,21,21	0
57	MG	RA	3205	1/1	0.94	0.15	-2.15	51,51,51,51	0
57	MG	YA	3157	1/1	0.94	0.15	-2.16	44,44,44,44	0
57	MG	RA	3327	1/1	0.95	0.07	-2.18	62,62,62,62	0
57	MG	QA	1609	1/1	0.98	0.16	-2.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1632	1/1	0.96	0.16	-2.22	28,28,28,28	0
57	MG	YA	3100	1/1	0.88	0.16	-2.30	20,20,20,20	0
57	MG	XA	1683	1/1	0.93	0.11	-2.31	48,48,48,48	0
57	MG	YA	3064	1/1	0.96	0.13	-2.52	9,9,9,9	0
57	MG	RA	3310	1/1	0.74	0.12	-2.55	56,56,56,56	0
57	MG	XA	1646	1/1	0.81	0.17	-2.62	72,72,72,72	0
57	MG	RA	3183	1/1	0.93	0.13	-2.64	49,49,49,49	0
57	MG	XA	1654	1/1	0.96	0.08	-2.69	78,78,78,78	0
57	MG	RA	3245	1/1	0.99	0.11	-2.73	68,68,68,68	0
57	MG	RA	3014	1/1	0.92	0.12	-2.81	16,16,16,16	0
57	MG	RA	3182	1/1	0.92	0.13	-2.89	37,37,37,37	0
57	MG	YA	3126	1/1	0.86	0.11	-2.98	43,43,43,43	0
57	MG	RA	3153	1/1	0.91	0.11	-2.98	26,26,26,26	0
57	MG	YA	3318	1/1	0.97	0.11	-3.13	63,63,63,63	0
57	MG	RA	3209	1/1	0.92	0.15	-3.16	68,68,68,68	0
57	MG	RA	3035	1/1	0.98	0.12	-3.38	10,10,10,10	0
57	MG	RA	3068	1/1	0.87	0.13	-3.38	39,39,39,39	0
57	MG	XA	1691	1/1	0.93	0.11	-3.42	105,105,105,105	0
57	MG	RB	201	1/1	0.97	0.12	-3.44	99,99,99,99	0
57	MG	YA	3167	1/1	0.95	0.12	-3.60	49,49,49,49	0
57	MG	XA	1677	1/1	0.75	0.12	-4.15	81,81,81,81	0
57	MG	RA	3140	1/1	0.97	0.09	-4.23	36,36,36,36	0
57	MG	YA	3185	1/1	0.93	0.14	-4.70	87,87,87,87	0
57	MG	QA	1674	1/1	0.96	0.09	-5.06	56,56,56,56	0
57	MG	YA	3195	1/1	0.96	0.08	-5.48	53,53,53,53	0
57	MG	YA	3035	1/1	0.97	0.16	-5.53	23,23,23,23	0
57	MG	XA	1608	1/1	0.97	0.13	-5.60	21,21,21,21	0
57	MG	RA	3231	1/1	0.88	0.42	-	36,36,36,36	0
57	MG	XA	1708	1/1	0.91	0.28	-	33,33,33,33	0
57	MG	RA	3028	1/1	0.94	0.30	-	18,18,18,18	0
57	MG	YB	204	1/1	0.96	0.36	-	27,27,27,27	0
57	MG	RA	3313	1/1	0.86	0.34	-	59,59,59,59	0
57	MG	RA	3225	1/1	0.79	0.35	-	60,60,60,60	0
57	MG	YA	3317	1/1	0.89	0.38	-	45,45,45,45	0
57	MG	RA	3096	1/1	0.95	0.46	-	31,31,31,31	0
57	MG	RA	3301	1/1	0.87	0.46	-	37,37,37,37	0
57	MG	QA	1679	1/1	0.86	0.33	-	52,52,52,52	0
57	MG	RA	3143	1/1	0.95	0.34	-	60,60,60,60	0
57	MG	RA	3168	1/1	0.95	0.28	-	26,26,26,26	0
57	MG	RA	3247	1/1	0.97	0.44	-	46,46,46,46	0
57	MG	YA	3296	1/1	0.73	0.46	-	55,55,55,55	0
57	MG	YA	3144	1/1	0.73	0.27	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1647	1/1	0.90	0.34	-	35,35,35,35	0
57	MG	RA	3195	1/1	0.93	0.36	-	56,56,56,56	0
57	MG	RA	3276	1/1	0.86	0.59	-	59,59,59,59	0
57	MG	YA	3217	1/1	0.88	0.52	-	83,83,83,83	0
57	MG	QA	1608	1/1	0.99	0.08	-	18,18,18,18	0
57	MG	QA	1665	1/1	0.92	0.26	-	55,55,55,55	0
57	MG	RA	3055	1/1	0.97	0.40	-	14,14,14,14	0
57	MG	YA	3295	1/1	0.80	0.53	-	61,61,61,61	0
57	MG	RA	3291	1/1	0.96	0.23	-	37,37,37,37	0
57	MG	RA	3206	1/1	0.86	0.19	-	45,45,45,45	0
57	MG	YA	3224	1/1	0.79	0.48	-	41,41,41,41	0
57	MG	YA	3280	1/1	0.88	0.23	-	43,43,43,43	0
57	MG	XA	1630	1/1	0.96	0.45	-	47,47,47,47	0
57	MG	RA	3286	1/1	0.95	0.35	-	26,26,26,26	0
57	MG	RA	3125	1/1	0.98	0.26	-	51,51,51,51	0
57	MG	RA	3212	1/1	0.75	0.80	-	57,57,57,57	0
57	MG	QY	101	1/1	0.57	0.27	-	66,66,66,66	0
57	MG	XA	1615	1/1	0.96	0.26	-	25,25,25,25	0
57	MG	YA	3073	1/1	0.97	0.28	-	10,10,10,10	0
57	MG	RA	3275	1/1	0.94	0.34	-	44,44,44,44	0
57	MG	YA	3324	1/1	0.88	0.40	-	34,34,34,34	0
57	MG	QA	1643	1/1	0.85	0.26	-	23,23,23,23	0
57	MG	RA	3128	1/1	0.89	0.25	-	42,42,42,42	0
57	MG	YE	301	1/1	0.82	0.30	-	49,49,49,49	0
57	MG	RA	3150	1/1	0.89	0.36	-	37,37,37,37	0
57	MG	YA	3117	1/1	0.91	0.24	-	42,42,42,42	0
57	MG	RA	3292	1/1	0.96	0.16	-	58,58,58,58	0
57	MG	RA	3122	1/1	0.94	0.20	-	74,74,74,74	0
57	MG	YA	3151	1/1	0.54	0.27	-	52,52,52,52	0
57	MG	QA	1604	1/1	0.89	0.60	-	47,47,47,47	0
57	MG	RA	3256	1/1	0.97	1.02	-	52,52,52,52	0
57	MG	YA	3286	1/1	0.82	0.53	-	58,58,58,58	0
57	MG	YA	3304	1/1	0.93	0.44	-	50,50,50,50	0
57	MG	YA	3335	1/1	0.69	0.83	-	57,57,57,57	0
57	MG	RA	3293	1/1	0.87	0.22	-	39,39,39,39	0
57	MG	RA	3100	1/1	0.94	0.20	-	32,32,32,32	0
57	MG	YA	3244	1/1	0.95	0.60	-	38,38,38,38	0
57	MG	XA	1698	1/1	0.89	0.79	-	76,76,76,76	0
57	MG	QA	1657	1/1	0.94	0.27	-	29,29,29,29	0
57	MG	YA	3038	1/1	0.94	0.18	-	8,8,8,8	0
57	MG	RA	3166	1/1	0.83	0.67	-	57,57,57,57	0
57	MG	RA	3289	1/1	0.88	0.35	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1609	1/1	0.94	0.32	-	25,25,25,25	0
57	MG	YA	3021	1/1	0.97	0.32	-	17,17,17,17	0
57	MG	RA	3137	1/1	0.62	0.28	-	61,61,61,61	0
57	MG	RA	3056	1/1	0.93	0.29	-	48,48,48,48	0
57	MG	YA	3271	1/1	0.87	0.88	-	32,32,32,32	0
57	MG	YB	203	1/1	0.91	0.30	-	37,37,37,37	0
57	MG	YA	3054	1/1	0.94	0.27	-	11,11,11,11	0
57	MG	YA	3207	1/1	0.94	0.63	-	28,28,28,28	0
57	MG	YA	3089	1/1	0.96	0.48	-	17,17,17,17	0
57	MG	YA	3283	1/1	0.96	0.16	-	46,46,46,46	0
57	MG	YA	3256	1/1	0.92	0.54	-	52,52,52,52	0
57	MG	RA	3297	1/1	0.68	0.31	-	53,53,53,53	0
57	MG	YA	3149	1/1	0.89	0.58	-	69,69,69,69	0
57	MG	RA	3132	1/1	0.95	0.34	-	45,45,45,45	0
57	MG	RA	3109	1/1	0.94	0.48	-	54,54,54,54	0
57	MG	Y0	101	1/1	0.95	0.24	-	10,10,10,10	0
57	MG	RA	3066	1/1	0.97	0.28	-	13,13,13,13	0
57	MG	YA	3215	1/1	0.92	0.15	-	45,45,45,45	0
57	MG	RA	3138	1/1	0.92	0.30	-	26,26,26,26	0
57	MG	YA	3210	1/1	0.94	0.20	-	32,32,32,32	0
57	MG	YA	3330	1/1	0.85	0.58	-	57,57,57,57	0
57	MG	XA	1697	1/1	0.93	0.41	-	47,47,47,47	0
57	MG	XA	1607	1/1	0.94	0.43	-	29,29,29,29	0
57	MG	QA	1636	1/1	0.98	0.14	-	12,12,12,12	0
57	MG	RA	3317	1/1	0.96	0.35	-	40,40,40,40	0
57	MG	QA	1624	1/1	0.73	0.27	-	77,77,77,77	0
57	MG	RA	3198	1/1	0.91	0.91	-	44,44,44,44	0
57	MG	XA	1656	1/1	0.89	0.25	-	56,56,56,56	0
57	MG	YA	3193	1/1	0.95	0.21	-	39,39,39,39	0
57	MG	RA	3252	1/1	0.93	0.34	-	29,29,29,29	0
57	MG	RA	3083	1/1	0.91	0.41	-	26,26,26,26	0
57	MG	YA	3045	1/1	0.97	0.32	-	14,14,14,14	0
57	MG	YA	3196	1/1	0.89	0.49	-	62,62,62,62	0
57	MG	YA	3056	1/1	0.99	0.34	-	21,21,21,21	0
57	MG	YA	3353	1/1	0.66	0.63	-	67,67,67,67	0
57	MG	RA	3103	1/1	0.96	0.20	-	33,33,33,33	0
57	MG	XA	1658	1/1	0.96	0.33	-	30,30,30,30	0
57	MG	RA	3053	1/1	0.97	0.35	-	10,10,10,10	0
57	MG	YA	3044	1/1	0.95	0.34	-	19,19,19,19	0
57	MG	XA	1666	1/1	0.96	0.28	-	48,48,48,48	0
57	MG	XA	1644	1/1	0.91	0.41	-	42,42,42,42	0
57	MG	RA	3127	1/1	0.94	0.25	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3037	1/1	0.98	0.24	-	15,15,15,15	0
57	MG	YA	3176	1/1	0.95	0.17	-	56,56,56,56	0
57	MG	YA	3351	1/1	0.79	0.37	-	66,66,66,66	0
57	MG	RA	3186	1/1	0.92	0.22	-	68,68,68,68	0
57	MG	XA	1689	1/1	0.93	0.63	-	51,51,51,51	0
57	MG	QA	1631	1/1	0.95	0.12	-	69,69,69,69	0
57	MG	QA	1603	1/1	0.76	0.62	-	80,80,80,80	0
57	MG	YA	3281	1/1	0.72	0.56	-	64,64,64,64	0
57	MG	XA	1661	1/1	0.94	0.39	-	44,44,44,44	0
57	MG	RE	301	1/1	0.94	0.32	-	20,20,20,20	0
57	MG	YA	3352	1/1	0.84	0.49	-	50,50,50,50	0
57	MG	YA	3279	1/1	0.94	0.31	-	33,33,33,33	0
57	MG	RA	3324	1/1	0.69	0.21	-	60,60,60,60	0
57	MG	XA	1681	1/1	0.89	0.46	-	21,21,21,21	0
57	MG	YA	3289	1/1	0.84	0.41	-	71,71,71,71	0
57	MG	RA	3117	1/1	0.89	0.27	-	62,62,62,62	0
57	MG	QA	1675	1/1	0.96	0.21	-	36,36,36,36	0
57	MG	XF	201	1/1	0.60	0.25	-	65,65,65,65	0
57	MG	XA	1702	1/1	0.95	0.31	-	43,43,43,43	0
57	MG	YA	3263	1/1	0.91	0.60	-	65,65,65,65	0
57	MG	QA	1601	1/1	0.93	0.15	-	31,31,31,31	0
57	MG	YA	3066	1/1	0.96	0.21	-	36,36,36,36	0
57	MG	QA	1606	1/1	0.97	0.41	-	20,20,20,20	0
57	MG	RA	3190	1/1	0.81	0.22	-	49,49,49,49	0
57	MG	RB	203	1/1	0.92	0.25	-	47,47,47,47	0
57	MG	XA	1669	1/1	0.97	0.25	-	21,21,21,21	0
57	MG	RA	3255	1/1	0.77	1.65	-	78,78,78,78	0
57	MG	RA	3306	1/1	0.90	0.38	-	38,38,38,38	0
57	MG	RA	3188	1/1	0.64	0.21	-	58,58,58,58	0
57	MG	YA	3050	1/1	0.95	0.43	-	22,22,22,22	0
57	MG	RA	3233	1/1	0.91	0.48	-	16,16,16,16	0
57	MG	YA	3165	1/1	0.95	0.38	-	43,43,43,43	0
57	MG	XA	1668	1/1	0.95	0.53	-	48,48,48,48	0
57	MG	YA	3258	1/1	0.64	0.29	-	34,34,34,34	0
57	MG	RA	3115	1/1	0.91	0.23	-	50,50,50,50	0
57	MG	QA	1623	1/1	0.94	0.31	-	54,54,54,54	0
57	MG	YA	3135	1/1	0.83	0.74	-	51,51,51,51	0
57	MG	YA	3182	1/1	0.98	0.18	-	41,41,41,41	0
57	MG	RA	3296	1/1	0.90	0.57	-	48,48,48,48	0
57	MG	XX	101	1/1	0.90	0.47	-	57,57,57,57	0
57	MG	RA	3192	1/1	0.93	0.23	-	46,46,46,46	0
57	MG	YA	3212	1/1	0.88	0.28	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3108	1/1	0.90	0.44	-	34,34,34,34	0
57	MG	RA	3090	1/1	0.79	0.30	-	39,39,39,39	0
57	MG	YA	3148	1/1	0.98	0.29	-	34,34,34,34	0
57	MG	YA	3250	1/1	0.94	0.48	-	27,27,27,27	0
57	MG	QA	1673	1/1	0.75	0.60	-	63,63,63,63	0
57	MG	XA	1601	1/1	0.98	0.88	-	35,35,35,35	0
57	MG	RA	3221	1/1	0.95	0.41	-	4,4,4,4	0
57	MG	RA	3211	1/1	0.96	0.63	-	46,46,46,46	0
57	MG	YB	201	1/1	0.95	0.20	-	46,46,46,46	0
57	MG	YA	3221	1/1	0.93	0.22	-	18,18,18,18	0
57	MG	YA	3229	1/1	0.97	0.45	-	24,24,24,24	0
57	MG	YA	3159	1/1	0.89	0.50	-	51,51,51,51	0
57	MG	RA	3216	1/1	0.88	0.24	-	46,46,46,46	0
57	MG	YA	3208	1/1	0.86	0.41	-	40,40,40,40	0
57	MG	XA	1664	1/1	0.84	0.50	-	38,38,38,38	0
57	MG	QA	1678	1/1	0.95	0.45	-	43,43,43,43	0
57	MG	XA	1670	1/1	0.93	0.47	-	37,37,37,37	0
57	MG	XA	1690	1/1	0.92	0.61	-	50,50,50,50	0
57	MG	YA	3017	1/1	0.91	0.49	-	29,29,29,29	0
57	MG	YA	3116	1/1	0.96	0.41	-	58,58,58,58	0
57	MG	YA	3253	1/1	0.96	0.28	-	32,32,32,32	0
57	MG	RA	3238	1/1	0.92	0.30	-	7,7,7,7	0
57	MG	QA	1669	1/1	0.89	0.34	-	59,59,59,59	0
57	MG	RA	3089	1/1	0.95	0.62	-	31,31,31,31	0
57	MG	QA	1677	1/1	0.84	0.32	-	29,29,29,29	0
57	MG	RA	3004	1/1	0.93	0.27	-	26,26,26,26	0
57	MG	QA	1622	1/1	0.85	0.30	-	70,70,70,70	0
57	MG	RA	3261	1/1	0.84	0.29	-	99,99,99,99	0
57	MG	YA	3124	1/1	0.88	0.17	-	17,17,17,17	0
57	MG	YA	3093	1/1	0.93	0.23	-	42,42,42,42	0
57	MG	YA	3311	1/1	0.87	0.30	-	24,24,24,24	0
57	MG	RA	3107	1/1	0.93	0.17	-	32,32,32,32	0
57	MG	YA	3204	1/1	0.94	0.41	-	70,70,70,70	0
57	MG	RA	3039	1/1	0.98	0.32	-	12,12,12,12	0
57	MG	YA	3299	1/1	0.88	0.64	-	48,48,48,48	0
57	MG	RA	3067	1/1	0.84	0.20	-	47,47,47,47	0
57	MG	XA	1650	1/1	0.94	0.28	-	54,54,54,54	0
57	MG	YA	3059	1/1	0.98	0.21	-	2,2,2,2	0
57	MG	YA	3122	1/1	0.96	0.27	-	38,38,38,38	0
57	MG	XA	1604	1/1	0.90	0.43	-	44,44,44,44	0
57	MG	YA	3083	1/1	0.96	0.36	-	7,7,7,7	0
57	MG	RA	3274	1/1	0.95	0.65	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3070	1/1	0.93	0.26	-	32,32,32,32	0
57	MG	RA	3242	1/1	0.95	0.20	-	84,84,84,84	0
57	MG	YA	3274	1/1	0.93	0.67	-	43,43,43,43	0
57	MG	YA	3345	1/1	0.89	0.20	-	57,57,57,57	0
57	MG	RA	3041	1/1	0.91	0.33	-	9,9,9,9	0
57	MG	YA	3198	1/1	0.95	0.25	-	45,45,45,45	0
57	MG	YA	3202	1/1	0.94	0.20	-	75,75,75,75	0
57	MG	RA	3187	1/1	0.97	0.25	-	53,53,53,53	0
57	MG	QA	1641	1/1	0.86	0.25	-	59,59,59,59	0
57	MG	XA	1696	1/1	0.92	0.78	-	65,65,65,65	0
57	MG	RA	3303	1/1	0.90	0.20	-	44,44,44,44	0
57	MG	YA	3188	1/1	0.87	0.28	-	27,27,27,27	0
57	MG	RA	3129	1/1	0.88	0.97	-	59,59,59,59	0
57	MG	RA	3213	1/1	0.80	0.25	-	46,46,46,46	0
57	MG	RB	204	1/1	0.90	0.28	-	51,51,51,51	0
57	MG	RA	3207	1/1	0.97	0.28	-	22,22,22,22	0
57	MG	YA	3180	1/1	0.80	0.25	-	62,62,62,62	0
57	MG	YA	3139	1/1	0.91	0.39	-	48,48,48,48	0
57	MG	YA	3339	1/1	0.97	0.20	-	39,39,39,39	0
57	MG	QA	1635	1/1	0.91	0.32	-	58,58,58,58	0
57	MG	XA	1703	1/1	0.97	0.35	-	46,46,46,46	0
57	MG	QA	1663	1/1	0.84	0.36	-	55,55,55,55	0
57	MG	RA	3008	1/1	0.85	0.54	-	52,52,52,52	0
57	MG	RA	3172	1/1	0.98	0.33	-	42,42,42,42	0
57	MG	YA	3183	1/1	0.94	0.49	-	37,37,37,37	0
57	MG	XA	1645	1/1	0.94	0.31	-	31,31,31,31	0
57	MG	YA	3091	1/1	0.96	0.24	-	32,32,32,32	0
57	MG	YA	3276	1/1	0.94	0.44	-	50,50,50,50	0
57	MG	YA	3312	1/1	0.94	0.44	-	37,37,37,37	0
57	MG	RA	3284	1/1	0.84	0.32	-	58,58,58,58	0
57	MG	YA	3245	1/1	0.95	0.34	-	45,45,45,45	0
57	MG	RA	3151	1/1	0.91	0.12	-	54,54,54,54	0
57	MG	XA	1659	1/1	0.77	0.21	-	105,105,105,105	0
57	MG	XA	1706	1/1	0.76	0.80	-	66,66,66,66	0
57	MG	RA	3270	1/1	0.69	0.42	-	43,43,43,43	0
57	MG	YA	3237	1/1	0.95	0.51	-	31,31,31,31	0
57	MG	XA	1686	1/1	0.59	0.37	-	72,72,72,72	0
57	MG	YA	3291	1/1	0.86	0.76	-	60,60,60,60	0
57	MG	RA	3210	1/1	0.96	0.12	-	62,62,62,62	0
57	MG	XA	1625	1/1	0.91	0.12	-	32,32,32,32	0
57	MG	RA	3141	1/1	0.86	0.34	-	48,48,48,48	0
57	MG	YA	3350	1/1	0.84	0.43	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3099	1/1	0.86	0.29	-	28,28,28,28	0
57	MG	YA	3302	1/1	0.95	0.54	-	42,42,42,42	0
57	MG	RA	3254	1/1	0.96	0.35	-	35,35,35,35	0
57	MG	QA	1670	1/1	0.87	0.35	-	37,37,37,37	0
57	MG	RA	3200	1/1	0.78	0.41	-	65,65,65,65	0
57	MG	YA	3053	1/1	0.83	0.54	-	52,52,52,52	0
57	MG	RA	3226	1/1	0.95	0.39	-	27,27,27,27	0
57	MG	RA	3304	1/1	0.87	0.40	-	48,48,48,48	0
57	MG	YA	3226	1/1	0.90	0.91	-	57,57,57,57	0
57	MG	XA	1665	1/1	0.90	0.57	-	35,35,35,35	0
57	MG	YA	3104	1/1	0.98	0.15	-	27,27,27,27	0
57	MG	RA	3012	1/1	0.96	0.27	-	16,16,16,16	0
57	MG	YA	3155	1/1	0.94	0.47	-	51,51,51,51	0
57	MG	YA	3015	1/1	0.94	0.09	-	6,6,6,6	0
57	MG	YA	3145	1/1	0.88	0.50	-	34,34,34,34	0
57	MG	RA	3305	1/1	0.91	0.33	-	47,47,47,47	0
57	MG	RA	3224	1/1	0.91	0.55	-	46,46,46,46	0
57	MG	XA	1614	1/1	0.98	0.35	-	13,13,13,13	0
57	MG	YA	3315	1/1	0.91	0.51	-	38,38,38,38	0
57	MG	YA	3349	1/1	0.95	0.40	-	39,39,39,39	0
57	MG	YA	3343	1/1	0.96	0.48	-	67,67,67,67	0
57	MG	RA	3095	1/1	0.96	0.38	-	5,5,5,5	0
57	MG	YA	3261	1/1	0.95	0.34	-	22,22,22,22	0
57	MG	RA	3197	1/1	0.90	0.64	-	49,49,49,49	0
57	MG	RA	3288	1/1	0.83	0.38	-	26,26,26,26	0
57	MG	QA	1637	1/1	0.96	0.22	-	44,44,44,44	0
57	MG	YA	3098	1/1	0.87	0.10	-	59,59,59,59	0
57	MG	RA	3136	1/1	0.95	0.47	-	24,24,24,24	0
57	MG	RA	3044	1/1	0.93	0.28	-	5,5,5,5	0
57	MG	YA	3282	1/1	0.84	0.35	-	59,59,59,59	0
57	MG	QA	1668	1/1	0.74	0.56	-	36,36,36,36	0
57	MG	YA	3051	1/1	0.98	0.34	-	22,22,22,22	0
57	MG	YA	3080	1/1	0.89	0.38	-	51,51,51,51	0
57	MG	RA	3199	1/1	0.82	0.46	-	60,60,60,60	0
57	MG	RA	3078	1/1	0.97	0.39	-	53,53,53,53	0
57	MG	YA	3272	1/1	0.86	0.35	-	60,60,60,60	0
57	MG	RA	3154	1/1	0.86	0.54	-	43,43,43,43	0
57	MG	YA	3110	1/1	0.98	0.32	-	44,44,44,44	0
57	MG	XA	1672	1/1	0.92	0.35	-	36,36,36,36	0
57	MG	RA	3253	1/1	0.89	0.19	-	27,27,27,27	0
57	MG	XA	1699	1/1	0.93	0.44	-	35,35,35,35	0
57	MG	YA	3131	1/1	0.84	0.24	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3225	1/1	0.75	0.66	-	52,52,52,52	0
57	MG	RA	3250	1/1	0.74	0.45	-	46,46,46,46	0
57	MG	YA	3120	1/1	0.86	0.15	-	26,26,26,26	0
57	MG	R0	101	1/1	0.80	0.25	-	14,14,14,14	0
57	MG	RA	3204	1/1	0.92	0.29	-	59,59,59,59	0
57	MG	YA	3125	1/1	0.86	0.12	-	54,54,54,54	0
57	MG	XA	1651	1/1	0.97	0.50	-	62,62,62,62	0
57	MG	YA	3255	1/1	0.79	1.11	-	35,35,35,35	0
57	MG	RA	3177	1/1	0.87	0.36	-	33,33,33,33	0
57	MG	RA	3215	1/1	0.91	0.27	-	51,51,51,51	0
57	MG	YA	3329	1/1	0.95	0.28	-	51,51,51,51	0
57	MG	YA	3172	1/1	0.62	1.16	-	74,74,74,74	0
57	MG	YA	3189	1/1	0.75	0.51	-	62,62,62,62	0
57	MG	YA	3018	1/1	0.92	0.43	-	16,16,16,16	0
57	MG	QA	1667	1/1	0.96	0.39	-	38,38,38,38	0
57	MG	YA	3211	1/1	0.97	0.22	-	31,31,31,31	0
57	MG	YA	3254	1/1	0.97	0.20	-	33,33,33,33	0
57	MG	QA	1627	1/1	0.61	0.31	-	69,69,69,69	0
57	MG	RB	205	1/1	0.86	0.30	-	61,61,61,61	0
57	MG	YA	3266	1/1	0.87	0.28	-	52,52,52,52	0
57	MG	RA	3048	1/1	0.95	0.17	-	7,7,7,7	0
57	MG	RA	3023	1/1	0.96	0.16	-	22,22,22,22	0
57	MG	YA	3308	1/1	0.82	0.56	-	42,42,42,42	0
57	MG	RA	3164	1/1	0.93	0.07	-	36,36,36,36	0
57	MG	QA	1664	1/1	0.95	0.24	-	30,30,30,30	0
57	MG	QV	103	1/1	0.92	0.23	-	27,27,27,27	0
57	MG	YA	3121	1/1	0.94	0.70	-	46,46,46,46	0
57	MG	YA	3097	1/1	0.92	0.43	-	19,19,19,19	0
57	MG	RA	3051	1/1	0.96	0.33	-	4,4,4,4	0
57	MG	YA	3111	1/1	0.74	1.33	-	53,53,53,53	0
57	MG	YA	3084	1/1	0.91	0.30	-	51,51,51,51	0
57	MG	YA	3306	1/1	0.59	0.33	-	72,72,72,72	0
57	MG	RA	3084	1/1	0.96	0.29	-	21,21,21,21	0
57	MG	QA	1683	1/1	0.93	0.11	-	66,66,66,66	0
57	MG	YA	3061	1/1	0.98	0.26	-	12,12,12,12	0
57	MG	YA	3133	1/1	0.83	0.20	-	43,43,43,43	0
57	MG	QA	1680	1/1	0.87	0.58	-	53,53,53,53	0
57	MG	QA	1676	1/1	0.94	0.39	-	63,63,63,63	0
57	MG	QA	1646	1/1	0.94	0.32	-	61,61,61,61	0
57	MG	RA	3060	1/1	0.96	0.33	-	11,11,11,11	0
57	MG	RA	3061	1/1	0.70	0.19	-	61,61,61,61	0
57	MG	YA	3336	1/1	0.67	0.38	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1674	1/1	0.98	0.24	-	4,4,4,4	0
57	MG	YA	3177	1/1	0.85	0.32	-	50,50,50,50	0
57	MG	XA	1687	1/1	0.98	0.57	-	33,33,33,33	0
57	MG	RA	3208	1/1	0.73	0.40	-	59,59,59,59	0
57	MG	RA	3223	1/1	0.94	0.19	-	28,28,28,28	0
57	MG	XA	1673	1/1	0.98	0.51	-	21,21,21,21	0
57	MG	RA	3113	1/1	0.86	0.39	-	21,21,21,21	0
57	MG	QA	1639	1/1	0.89	0.23	-	67,67,67,67	0
57	MG	QA	1661	1/1	0.73	0.45	-	37,37,37,37	0
57	MG	YA	3270	1/1	0.94	0.41	-	32,32,32,32	0
57	MG	RA	3163	1/1	0.90	0.25	-	45,45,45,45	0
57	MG	RA	3323	1/1	0.92	0.41	-	38,38,38,38	0
57	MG	RA	3162	1/1	0.81	0.38	-	27,27,27,27	0
57	MG	YP	201	1/1	0.82	0.19	-	52,52,52,52	0
57	MG	RA	3239	1/1	0.90	0.64	-	17,17,17,17	0
57	MG	RA	3032	1/1	0.96	0.38	-	19,19,19,19	0
57	MG	RA	3156	1/1	0.93	0.38	-	42,42,42,42	0
57	MG	RA	3263	1/1	0.74	0.47	-	63,63,63,63	0
57	MG	YA	3065	1/1	0.96	0.43	-	22,22,22,22	0
57	MG	XA	1711	1/1	0.98	0.12	-	27,27,27,27	0
57	MG	YA	3142	1/1	0.97	0.29	-	33,33,33,33	0
57	MG	XA	1629	1/1	0.86	0.18	-	63,63,63,63	0
57	MG	YA	3062	1/1	0.77	0.19	-	25,25,25,25	0
57	MG	YA	3010	1/1	0.95	0.22	-	6,6,6,6	0
57	MG	QA	1611	1/1	0.90	0.45	-	21,21,21,21	0
57	MG	RA	3287	1/1	0.90	0.28	-	49,49,49,49	0
57	MG	YA	3278	1/1	0.90	0.42	-	25,25,25,25	0
57	MG	RA	3184	1/1	0.83	0.45	-	60,60,60,60	0
57	MG	RA	3295	1/1	0.92	0.30	-	45,45,45,45	0
57	MG	RA	3246	1/1	0.94	0.18	-	55,55,55,55	0
57	MG	YA	3201	1/1	0.85	0.66	-	51,51,51,51	0
57	MG	RA	3180	1/1	0.88	0.33	-	29,29,29,29	0
57	MG	RA	3262	1/1	0.92	0.47	-	33,33,33,33	0
57	MG	YA	3079	1/1	0.99	0.35	-	45,45,45,45	0
57	MG	YA	3338	1/1	0.91	0.62	-	55,55,55,55	0
57	MG	RA	3146	1/1	0.95	0.25	-	27,27,27,27	0
57	MG	QA	1630	1/1	0.88	0.16	-	24,24,24,24	0
57	MG	YA	3341	1/1	0.92	0.27	-	46,46,46,46	0
57	MG	YA	3007	1/1	0.95	0.36	-	10,10,10,10	0
57	MG	XA	1638	1/1	0.88	0.32	-	39,39,39,39	0
57	MG	XA	1660	1/1	0.91	0.93	-	53,53,53,53	0
57	MG	YA	3287	1/1	0.94	0.94	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YY	201	1/1	0.76	0.19	-	45,45,45,45	0
57	MG	YA	3337	1/1	0.65	0.77	-	78,78,78,78	0
57	MG	RA	3043	1/1	0.81	0.41	-	65,65,65,65	0
57	MG	RA	3011	1/1	0.92	0.59	-	27,27,27,27	0
57	MG	YA	3127	1/1	0.87	0.27	-	50,50,50,50	0
57	MG	RA	3316	1/1	0.95	0.76	-	51,51,51,51	0
57	MG	XB	301	1/1	0.94	0.18	-	51,51,51,51	0
57	MG	YA	3222	1/1	0.90	0.34	-	41,41,41,41	0
57	MG	RA	3278	1/1	0.95	0.91	-	40,40,40,40	0
57	MG	YA	3260	1/1	0.84	0.35	-	40,40,40,40	0
57	MG	RA	3082	1/1	0.97	0.21	-	18,18,18,18	0
57	MG	RA	3002	1/1	0.91	0.56	-	42,42,42,42	0
57	MG	YA	3301	1/1	0.82	1.31	-	63,63,63,63	0
57	MG	QA	1648	1/1	0.89	0.23	-	71,71,71,71	0
57	MG	RA	3267	1/1	0.89	0.39	-	45,45,45,45	0
57	MG	RA	3029	1/1	0.96	0.44	-	15,15,15,15	0
57	MG	QA	1652	1/1	0.95	0.49	-	34,34,34,34	0
57	MG	RA	3092	1/1	0.92	0.39	-	18,18,18,18	0
57	MG	YA	3150	1/1	0.96	0.17	-	41,41,41,41	0
57	MG	RA	3193	1/1	0.91	0.16	-	43,43,43,43	0
57	MG	YA	3154	1/1	0.91	0.30	-	67,67,67,67	0
57	MG	RA	3318	1/1	0.94	0.28	-	32,32,32,32	0
57	MG	YA	3223	1/1	0.88	0.45	-	56,56,56,56	0
57	MG	RA	3165	1/1	0.92	0.36	-	36,36,36,36	0
57	MG	YA	3118	1/1	0.96	0.32	-	14,14,14,14	0
57	MG	RA	3277	1/1	0.89	0.23	-	34,34,34,34	0
57	MG	YA	3332	1/1	0.96	0.23	-	67,67,67,67	0
57	MG	QA	1671	1/1	0.94	0.34	-	23,23,23,23	0
57	MG	RA	3302	1/1	0.78	0.64	-	51,51,51,51	0
57	MG	QA	1614	1/1	0.96	0.27	-	30,30,30,30	0
57	MG	QF	201	1/1	0.48	0.34	-	57,57,57,57	0
57	MG	RA	3111	1/1	0.96	0.12	-	58,58,58,58	0
57	MG	YA	3300	1/1	0.71	0.66	-	53,53,53,53	0
57	MG	XA	1709	1/1	0.97	0.23	-	38,38,38,38	0
57	MG	YA	3257	1/1	0.96	0.20	-	54,54,54,54	0
57	MG	YA	3052	1/1	0.92	0.45	-	23,23,23,23	0
57	MG	RA	3158	1/1	0.87	0.35	-	30,30,30,30	0
57	MG	YA	3113	1/1	0.94	0.45	-	23,23,23,23	0
57	MG	RA	3091	1/1	0.96	0.30	-	29,29,29,29	0
57	MG	RA	3307	1/1	0.66	0.52	-	48,48,48,48	0
57	MG	YA	3242	1/1	0.91	0.34	-	33,33,33,33	0
57	MG	RA	3311	1/1	0.81	0.27	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3334	1/1	0.83	0.23	-	60,60,60,60	0
57	MG	YA	3072	1/1	0.97	0.53	-	19,19,19,19	0
57	MG	XA	1682	1/1	0.94	0.35	-	60,60,60,60	0
57	MG	RA	3248	1/1	0.94	0.41	-	41,41,41,41	0
57	MG	YA	3143	1/1	0.96	0.28	-	23,23,23,23	0
57	MG	RA	3282	1/1	0.94	0.46	-	65,65,65,65	0
57	MG	RA	3258	1/1	0.95	0.41	-	50,50,50,50	0
57	MG	QA	1649	1/1	0.96	0.07	-	81,81,81,81	0
57	MG	RA	3229	1/1	0.96	0.36	-	22,22,22,22	0
57	MG	YA	3168	1/1	0.91	0.24	-	54,54,54,54	0
57	MG	YA	3101	1/1	0.92	0.39	-	36,36,36,36	0
57	MG	XA	1657	1/1	0.94	0.63	-	49,49,49,49	0
57	MG	QA	1634	1/1	0.87	0.28	-	58,58,58,58	0
57	MG	XA	1611	1/1	0.96	0.10	-	20,20,20,20	0
57	MG	XA	1694	1/1	0.74	0.22	-	69,69,69,69	0
57	MG	RA	3016	1/1	0.98	0.33	-	15,15,15,15	0
57	MG	YA	3163	1/1	0.85	0.09	-	59,59,59,59	0
57	MG	RA	3218	1/1	0.87	0.27	-	58,58,58,58	0
57	MG	QV	101	1/1	0.92	0.35	-	50,50,50,50	0
57	MG	YA	3178	1/1	0.90	0.21	-	52,52,52,52	0
57	MG	Y0	103	1/1	0.85	0.44	-	46,46,46,46	0
57	MG	YA	3331	1/1	0.57	0.58	-	69,69,69,69	0
57	MG	RA	3299	1/1	0.87	0.25	-	47,47,47,47	0
57	MG	RA	3069	1/1	0.93	0.35	-	9,9,9,9	0
57	MG	QA	1625	1/1	0.86	0.14	-	22,22,22,22	0
57	MG	YA	3290	1/1	0.75	0.67	-	74,74,74,74	0
57	MG	YA	3029	1/1	0.86	0.51	-	36,36,36,36	0
57	MG	RA	3133	1/1	0.80	0.16	-	27,27,27,27	0
57	MG	QA	1621	1/1	0.97	0.52	-	61,61,61,61	0
57	MG	XA	1676	1/1	0.89	0.22	-	41,41,41,41	0
57	MG	RA	3294	1/1	0.96	0.42	-	29,29,29,29	0
57	MG	XA	1635	1/1	0.85	0.45	-	58,58,58,58	0
57	MG	Y0	102	1/1	0.81	0.63	-	45,45,45,45	0
57	MG	RA	3244	1/1	0.98	0.42	-	39,39,39,39	0
57	MG	QA	1645	1/1	0.93	0.19	-	73,73,73,73	0
57	MG	YA	3275	1/1	0.36	0.37	-	80,80,80,80	0
57	MG	XA	1678	1/1	0.95	0.22	-	45,45,45,45	0
57	MG	YA	3001	1/1	0.97	0.45	-	24,24,24,24	0
57	MG	RA	3161	1/1	0.98	0.19	-	18,18,18,18	0
57	MG	XA	1675	1/1	0.51	0.41	-	59,59,59,59	0
57	MG	YA	3220	1/1	0.88	0.20	-	60,60,60,60	0
57	MG	XA	1662	1/1	0.77	0.52	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3231	1/1	0.98	0.38	-	24,24,24,24	0
57	MG	YA	3285	1/1	0.92	0.29	-	44,44,44,44	0
57	MG	RA	3045	1/1	0.98	0.27	-	13,13,13,13	0
57	MG	RA	3175	1/1	0.74	0.32	-	28,28,28,28	0
57	MG	RA	3265	1/1	0.87	1.44	-	53,53,53,53	0
57	MG	YA	3243	1/1	0.86	0.34	-	36,36,36,36	0
57	MG	XA	1648	1/1	0.62	0.35	-	59,59,59,59	0
57	MG	YA	3012	1/1	0.97	0.45	-	8,8,8,8	0
57	MG	YA	3141	1/1	0.91	0.23	-	9,9,9,9	0
57	MG	YA	3115	1/1	0.69	0.62	-	49,49,49,49	0
57	MG	XA	1671	1/1	0.89	0.53	-	39,39,39,39	0
57	MG	RA	3194	1/1	0.94	0.25	-	15,15,15,15	0
57	MG	YA	3063	1/1	0.97	0.20	-	55,55,55,55	0
57	MG	XA	1640	1/1	0.96	0.49	-	41,41,41,41	0
57	MG	XA	1712	1/1	0.97	0.24	-	39,39,39,39	0
57	MG	XA	1605	1/1	0.93	0.60	-	34,34,34,34	0
57	MG	XA	1695	1/1	0.77	0.15	-	78,78,78,78	0
57	MG	YA	3359	1/1	0.94	0.30	-	28,28,28,28	0
57	MG	YA	3262	1/1	0.95	0.39	-	30,30,30,30	0
57	MG	YA	3019	1/1	0.91	0.53	-	24,24,24,24	0
57	MG	YA	3344	1/1	0.96	0.20	-	28,28,28,28	0
57	MG	RA	3027	1/1	0.98	0.34	-	24,24,24,24	0
57	MG	XA	1693	1/1	0.93	0.43	-	40,40,40,40	0
57	MG	YA	3235	1/1	0.94	0.24	-	26,26,26,26	0
57	MG	RA	3191	1/1	0.85	0.27	-	31,31,31,31	0
57	MG	RA	3290	1/1	0.80	0.34	-	45,45,45,45	0
57	MG	RA	3139	1/1	0.85	0.29	-	25,25,25,25	0
57	MG	RA	3271	1/1	0.94	0.61	-	44,44,44,44	0
57	MG	YA	3092	1/1	0.99	0.23	-	23,23,23,23	0
57	MG	YA	3081	1/1	0.97	0.38	-	23,23,23,23	0
57	MG	RA	3001	1/1	0.91	0.26	-	47,47,47,47	0
57	MG	YA	3146	1/1	0.88	0.44	-	39,39,39,39	0
57	MG	RA	3018	1/1	0.95	0.28	-	18,18,18,18	0
57	MG	QA	1633	1/1	0.73	0.34	-	52,52,52,52	0
57	MG	YA	3020	1/1	0.99	0.39	-	16,16,16,16	0
57	MG	XA	1704	1/1	0.85	0.30	-	44,44,44,44	0
57	MG	RA	3071	1/1	0.93	0.51	-	52,52,52,52	0
57	MG	RA	3050	1/1	0.96	0.19	-	22,22,22,22	0
57	MG	RA	3228	1/1	0.87	0.35	-	37,37,37,37	0
57	MG	RA	3322	1/1	0.93	0.66	-	39,39,39,39	0
57	MG	RA	3219	1/1	0.82	0.45	-	75,75,75,75	0
57	MG	QA	1615	1/1	0.96	0.13	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3259	1/1	0.83	0.24	-	45,45,45,45	0
57	MG	YA	3277	1/1	0.87	0.52	-	57,57,57,57	0
57	MG	RA	3241	1/1	0.97	0.24	-	20,20,20,20	0
57	MG	YA	3227	1/1	0.91	0.40	-	19,19,19,19	0
57	MG	YA	3042	1/1	0.97	0.43	-	15,15,15,15	0
57	MG	RA	3112	1/1	0.79	0.21	-	27,27,27,27	0
57	MG	RA	3222	1/1	0.97	0.33	-	6,6,6,6	0
57	MG	RA	3308	1/1	0.93	0.51	-	54,54,54,54	0
57	MG	RA	3030	1/1	0.97	0.31	-	30,30,30,30	0
57	MG	YA	3186	1/1	0.89	0.46	-	19,19,19,19	0
57	MG	RA	3159	1/1	0.89	0.23	-	82,82,82,82	0
57	MG	YA	3003	1/1	0.93	0.21	-	23,23,23,23	0
57	MG	YA	3322	1/1	0.92	0.37	-	40,40,40,40	0
57	MG	XA	1680	1/1	0.85	0.29	-	65,65,65,65	0
57	MG	XA	1602	1/1	0.96	0.56	-	19,19,19,19	0
57	MG	YA	3175	1/1	0.97	0.31	-	19,19,19,19	0
57	MG	YA	3190	1/1	0.88	0.23	-	48,48,48,48	0
57	MG	YA	3267	1/1	0.97	0.37	-	59,59,59,59	0
57	MG	YA	3320	1/1	0.88	0.21	-	39,39,39,39	0
57	MG	YA	3321	1/1	0.96	0.27	-	49,49,49,49	0
57	MG	XA	1655	1/1	0.93	0.50	-	53,53,53,53	0
57	MG	RA	3102	1/1	0.91	0.15	-	25,25,25,25	0
57	MG	YA	3292	1/1	0.84	0.14	-	62,62,62,62	0
57	MG	YA	3294	1/1	0.93	0.53	-	48,48,48,48	0
57	MG	YA	3203	1/1	0.81	0.35	-	73,73,73,73	0
57	MG	YA	3128	1/1	0.93	0.39	-	42,42,42,42	0
57	MG	XA	1628	1/1	0.88	0.48	-	36,36,36,36	0
57	MG	RA	3312	1/1	0.76	0.78	-	68,68,68,68	0
57	MG	YA	3284	1/1	0.93	1.02	-	67,67,67,67	0
57	MG	RA	3170	1/1	0.94	0.23	-	57,57,57,57	0
57	MG	RA	3257	1/1	0.93	0.40	-	48,48,48,48	0
57	MG	RA	3073	1/1	0.98	0.23	-	8,8,8,8	0
57	MG	QX	101	1/1	0.94	0.20	-	43,43,43,43	0
57	MG	XA	1707	1/1	0.89	0.80	-	50,50,50,50	0
57	MG	YA	3213	1/1	0.85	0.32	-	47,47,47,47	0
57	MG	RA	3174	1/1	0.96	0.25	-	31,31,31,31	0
57	MG	YA	3273	1/1	0.78	0.31	-	46,46,46,46	0
57	MG	RA	3147	1/1	0.97	0.21	-	38,38,38,38	0
57	MG	RA	3202	1/1	0.60	0.30	-	70,70,70,70	0
57	MG	YA	3346	1/1	0.96	0.16	-	49,49,49,49	0
57	MG	RA	3124	1/1	0.92	0.29	-	54,54,54,54	0
57	MG	RA	3144	1/1	0.95	0.42	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1701	1/1	0.91	0.23	-	47,47,47,47	0
57	MG	RA	3196	1/1	0.77	0.46	-	44,44,44,44	0
57	MG	YA	3153	1/1	0.92	0.27	-	37,37,37,37	0
57	MG	RA	3325	1/1	0.88	0.99	-	57,57,57,57	0
57	MG	YA	3325	1/1	0.88	0.52	-	51,51,51,51	0
57	MG	YA	3071	1/1	0.85	0.60	-	38,38,38,38	0
57	MG	QA	1626	1/1	0.91	0.20	-	65,65,65,65	0
57	MG	YA	3234	1/1	0.98	0.45	-	10,10,10,10	0
57	MG	RA	3076	1/1	0.95	0.27	-	5,5,5,5	0
57	MG	YA	3205	1/1	0.83	0.27	-	25,25,25,25	0
57	MG	YA	3333	1/1	0.88	0.36	-	59,59,59,59	0
57	MG	YA	3039	1/1	0.98	0.42	-	12,12,12,12	0
57	MG	XA	1622	1/1	0.93	0.59	-	33,33,33,33	0
57	MG	YA	3206	1/1	0.73	0.68	-	49,49,49,49	0
57	MG	YA	3342	1/1	0.92	0.28	-	55,55,55,55	0
57	MG	RB	202	1/1	0.84	0.16	-	69,69,69,69	0
57	MG	YA	3314	1/1	0.82	0.34	-	30,30,30,30	0
57	MG	RA	3178	1/1	0.80	0.49	-	47,47,47,47	0
57	MG	Y5	101	1/1	0.95	0.21	-	17,17,17,17	0
57	MG	YA	3088	1/1	0.98	0.31	-	13,13,13,13	0
57	MG	XA	1637	1/1	0.95	0.13	-	74,74,74,74	0
57	MG	YA	3171	1/1	0.92	0.61	-	43,43,43,43	0
57	MG	RA	3046	1/1	0.97	0.43	-	27,27,27,27	0
57	MG	YA	3166	1/1	0.93	0.45	-	25,25,25,25	0
57	MG	XV	103	1/1	0.92	0.20	-	22,22,22,22	0
57	MG	RA	3269	1/1	0.77	0.68	-	41,41,41,41	0
57	MG	XV	101	1/1	0.91	0.25	-	34,34,34,34	0
57	MG	RA	3237	1/1	0.97	0.09	-	57,57,57,57	0
57	MG	RA	3319	1/1	0.90	0.43	-	62,62,62,62	0
57	MG	YA	3162	1/1	0.92	0.23	-	51,51,51,51	0
57	MG	RA	3273	1/1	0.79	0.49	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.