wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:07 PM GMT

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	:	2014-06-24
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

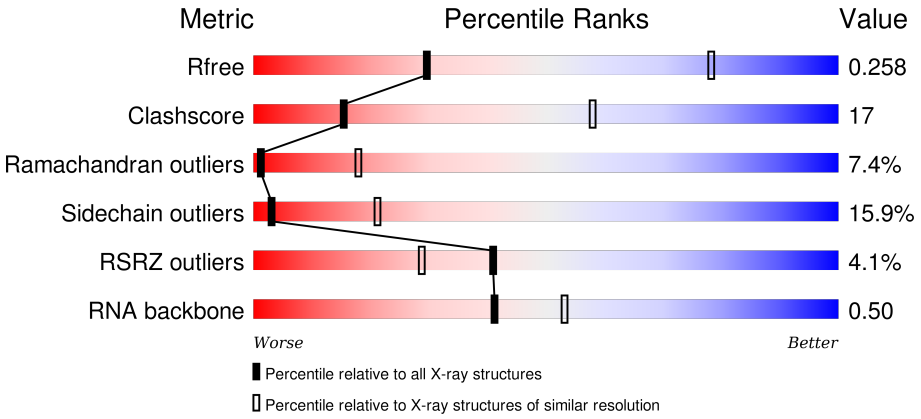
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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 <=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	51% 38% 9%
1	XA	1522	50% 38% 9%
2	QB	256	10% 48% 36% 7% 7%
2	XB	256	3% 46% 36% 10% 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	53% 30% 14%
3	XC	239	54% 29% 14%
4	QD	209	48% 43% 6%
4	XD	209	67% 27%
5	QE	162	59% 30% 7%
5	XE	162	56% 32% 5% 7%
6	QF	101	69% 27%
6	XF	101	63% 34%
7	QG	156	8% 65% 31%
7	XG	156	6% 71% 25%
8	QH	138	60% 36%
8	XH	138	63% 31% 6%
9	QI	128	13% 52% 41% 5%
9	XI	128	55% 35% 9%
10	QJ	105	10% 44% 42% 9% 6%
10	XJ	105	9% 42% 43% 10% 6%
11	QK	129	12% 57% 30% 5% 8%
11	XK	129	5% 60% 30% 8%
12	QL	132	3% 28% 51% 14% 5%
12	XL	132	2% 30% 48% 14% 5%
13	QM	126	10% 49% 35% 11%
13	XM	126	2% 51% 35% 10%
14	QN	61	2% 39% 44% 15%
14	XN	61	51% 39% 8%
15	QO	89	66% 27% 6%

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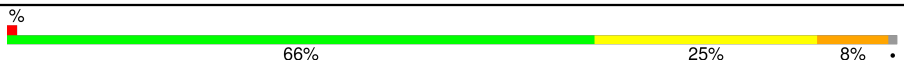
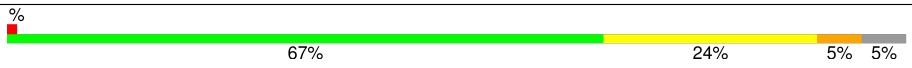
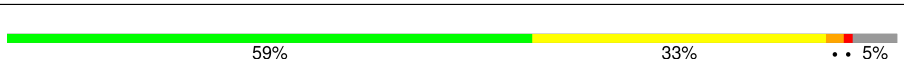
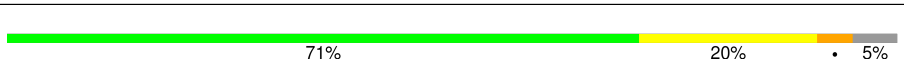
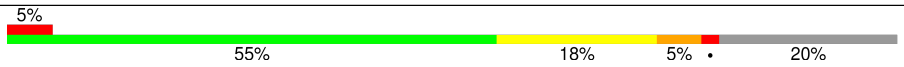
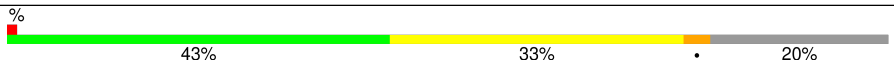
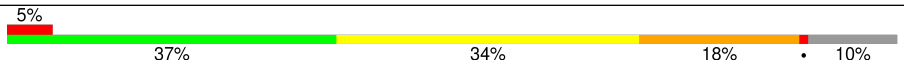
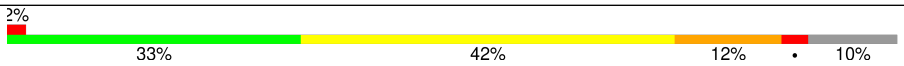
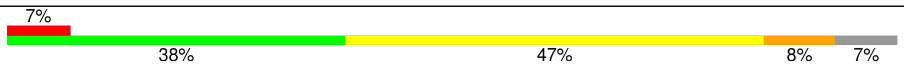
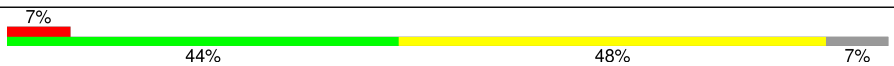
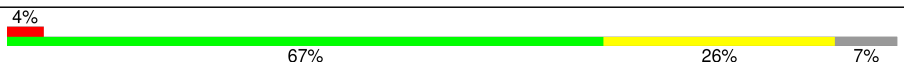
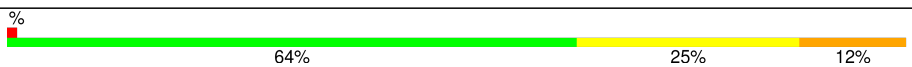
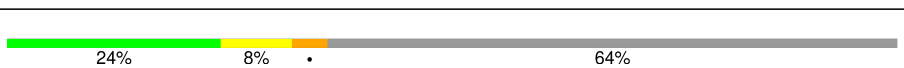
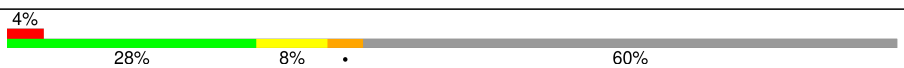
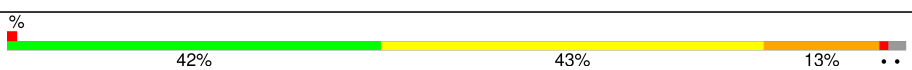
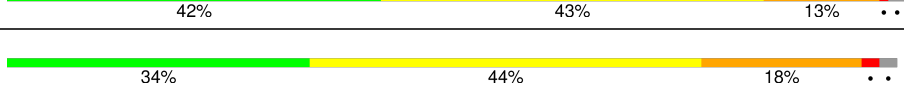
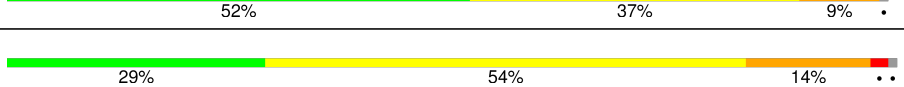
Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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Mol	Chain	Length	Quality of chain
28	RE	206	2% 21% 49% 24% 5%
28	YE	206	% 24% 46% 24% 5%
29	RF	210	2% 46% 39% 11%
29	YF	210	2% 34% 49% 12%
30	RG	182	6% 49% 41% 8%
30	YG	182	2% 53% 36% 9%
31	RH	180	24% 23% 44% 19% 8% 6%
31	YH	180	3% 23% 45% 19% 8% 6%
32	RI	148	7% 34% 49% 16%
32	YI	148	5% 39% 41% 19%
33	RN	140	2% 46% 44% 8%
33	YN	140	2% 48% 41% 8%
34	RO	122	% 70% 25% 5%
34	YO	122	69% 26% 5%
35	RP	150	4% 44% 39% 15%
35	YP	150	3% 37% 39% 19% 5%
36	RQ	141	6% 30% 50% 17%
36	YQ	141	3% 30% 48% 18%
37	RR	118	42% 48% 10%
37	YR	118	% 54% 34% 12%
38	RS	112	4% 42% 41% 14%
38	YS	112	2% 13% 63% 21%
39	RT	146	% 43% 41% 9% 6%
39	YT	146	40% 44% 10% 6%
40	RU	118	4% 61% 31% 6%

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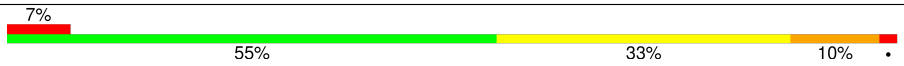
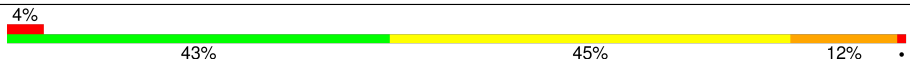
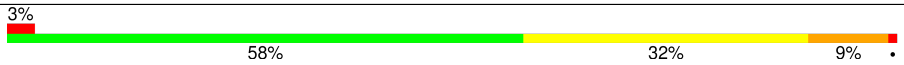
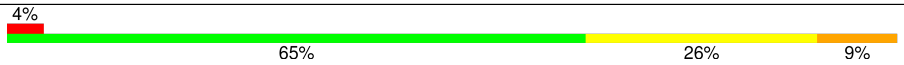
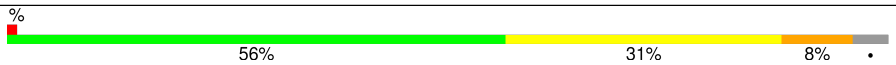
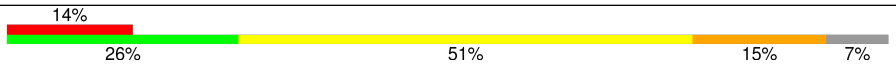
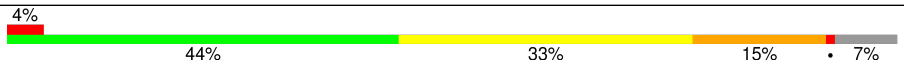
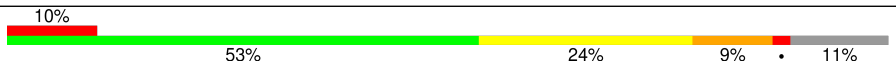
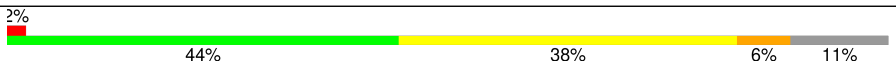
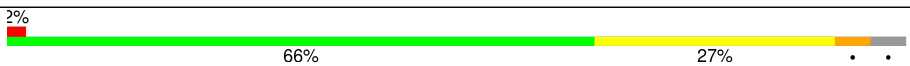
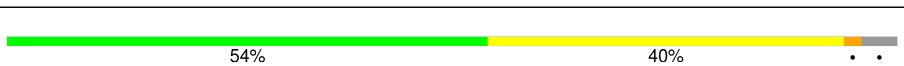
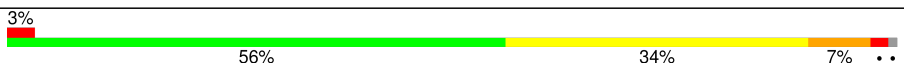
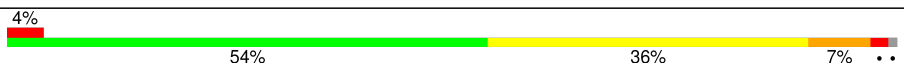
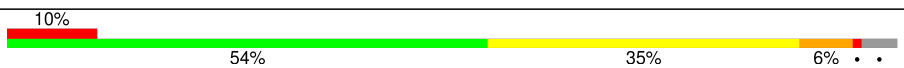
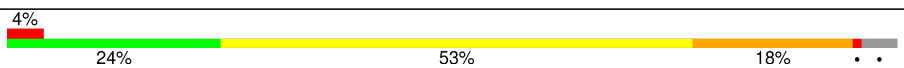
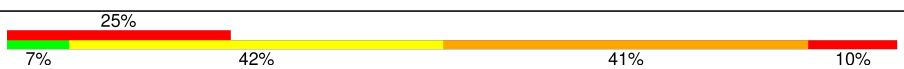
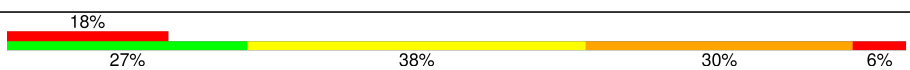
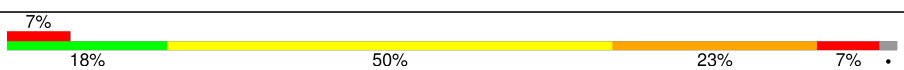
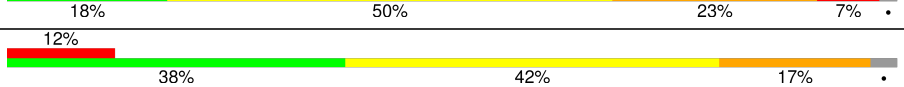
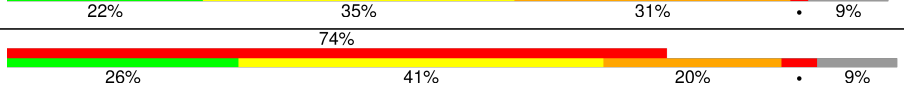
Mol	Chain	Length	Quality of chain
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	

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Mol	Chain	Length	Quality of chain
53	R7	49	2% 65% 29% 6%
53	Y7	49	2% 61% 31% 8%
54	R8	65	3% 22% 45% 25% 8%
54	Y8	65	22% 43% 26% 8%
55	R9	37	97% 62% 32% 5%
55	Y9	37	95% 68% 27% 5%
56	Z5	3	33% 33% 33%
56	Z6	3	33% 33% 33%

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	0	0	0
			882	556	176	150			
38	YS	111	Total	C	N	O	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 Mg 1 1	0	0
57	XX	1	Total Mg 1 1	0	0
57	QV	3	Total Mg 3 3	0	0
57	XA	111	Total Mg 111 111	0	0
57	YY	1	Total Mg 1 1	0	0
57	R0	1	Total Mg 1 1	0	0
57	YU	1	Total Mg 1 1	0	0
57	Y0	3	Total Mg 3 3	0	0
57	XF	1	Total Mg 1 1	0	0
57	RR	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	XB	1	Total Mg 1 1	0	0
57	QF	1	Total Mg 1 1	0	0
57	R5	1	Total Mg 1 1	0	0
57	RA	327	Total Mg 327 327	0	0
57	YP	2	Total Mg 2 2	0	0
57	RE	1	Total Mg 1 1	0	0
57	YB	4	Total Mg 4 4	0	0
57	QY	1	Total Mg 1 1	0	0
57	XV	3	Total Mg 3 3	0	0
57	RB	5	Total Mg 5 5	0	0

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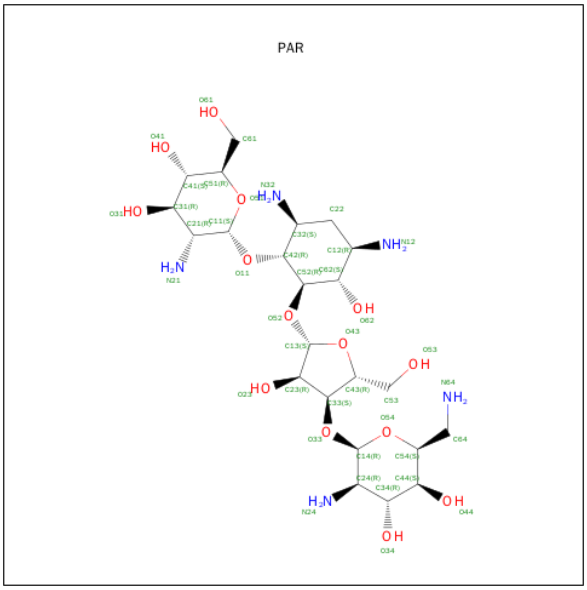
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QE	1	Total Mg 1 1	0	0
57	XD	1	Total Mg 1 1	0	0
57	YE	1	Total Mg 1 1	0	0

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

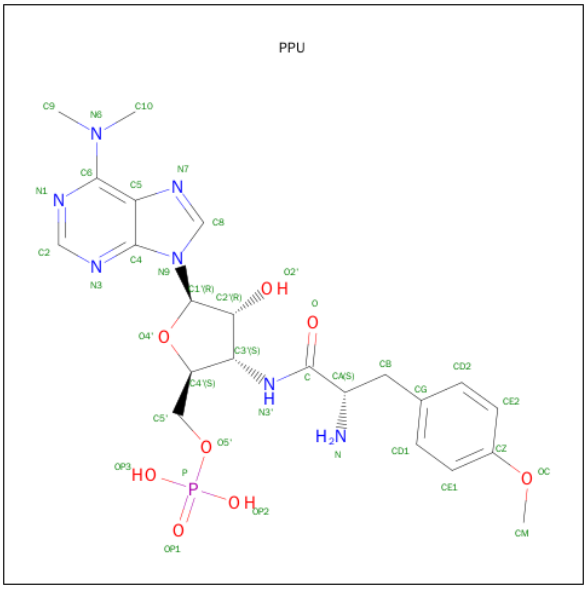


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QA	1	Total C N O 42 23 5 14	0	0
58	XA	1	Total C N O 42 23 5 14	0	0

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

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

- Molecule 60 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



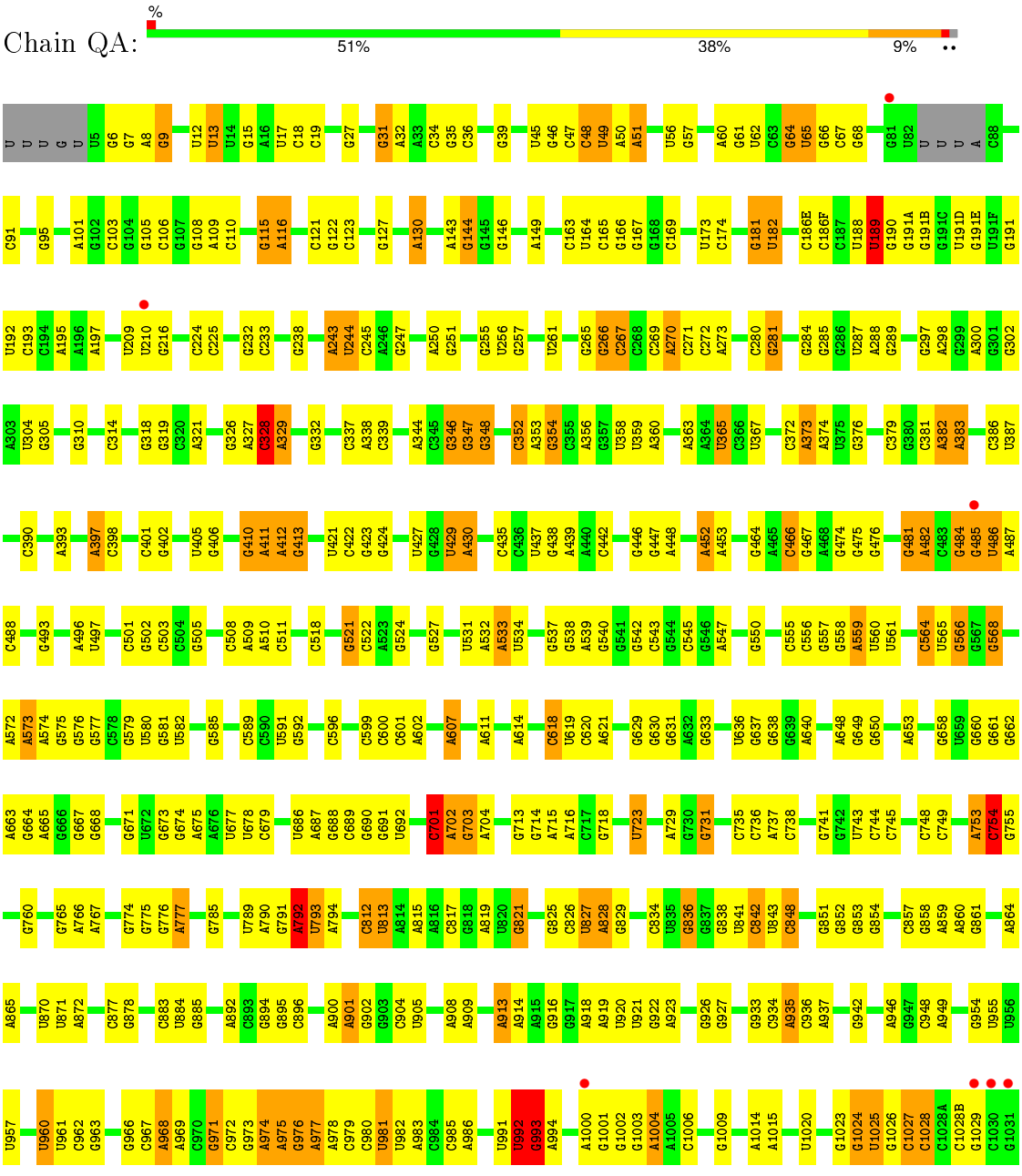
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	Z5	1	Total	C	N	O	P	0	0
			37	22	7	7	1		
60	Z6	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

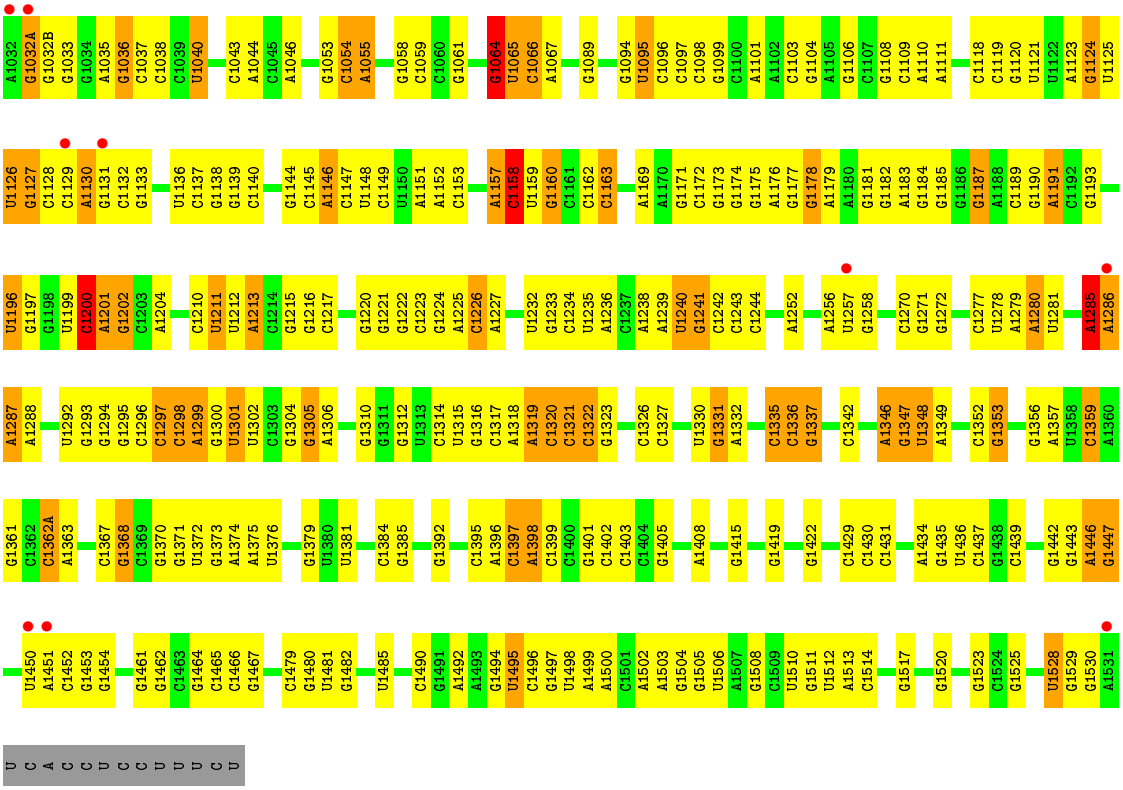
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

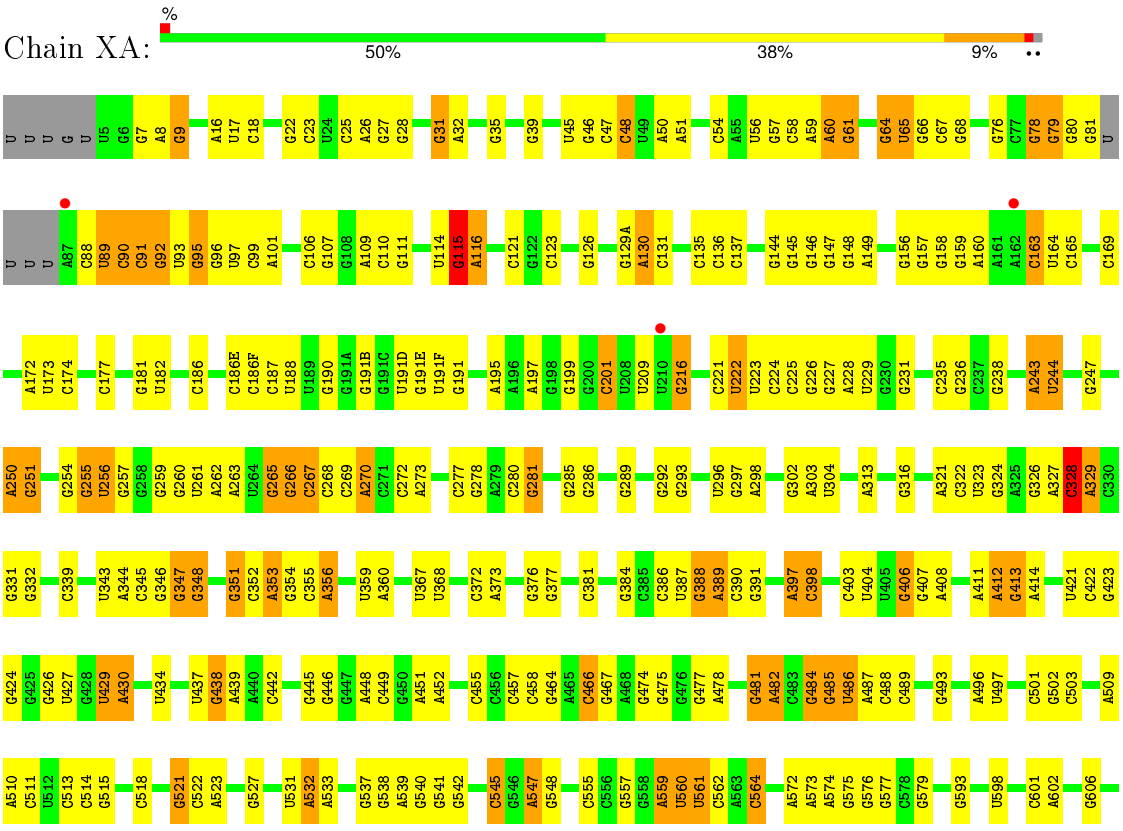
Chain QA:

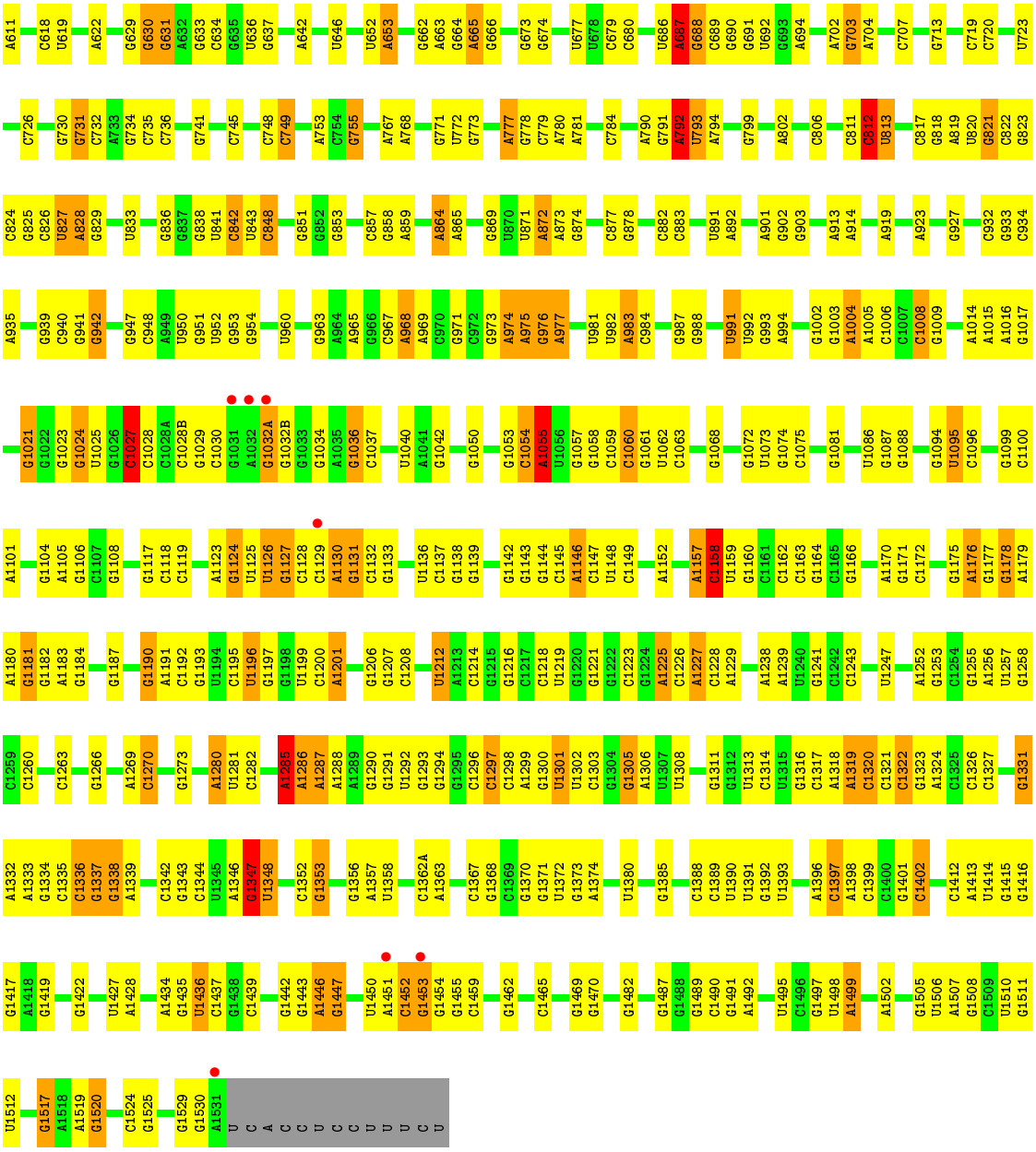




- Molecule 1: 16S rRNA

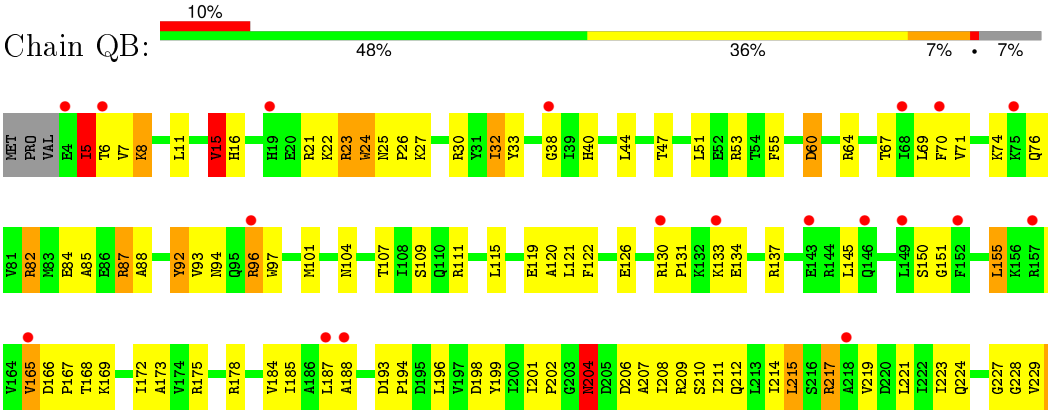
Chain XA:

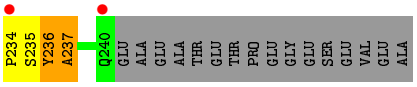




• Molecule 2: 30S ribosomal protein S2

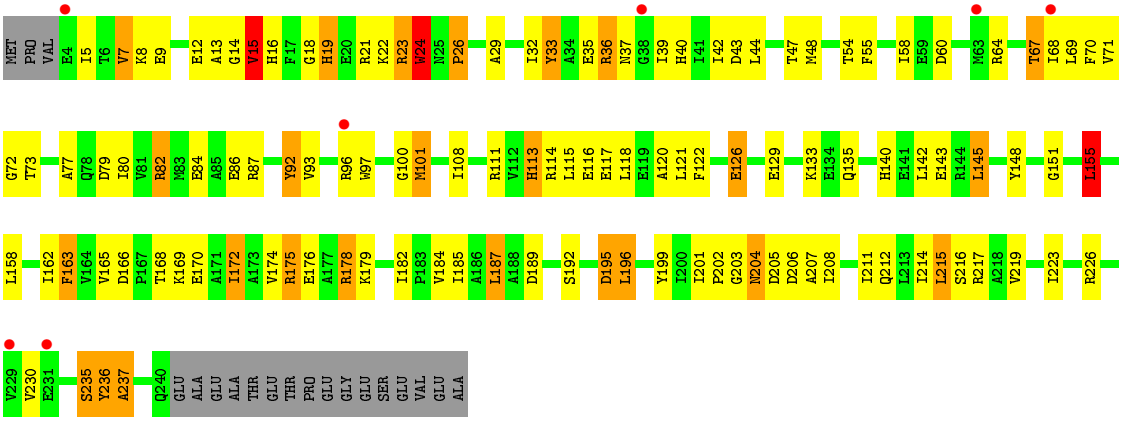
Chain QB:





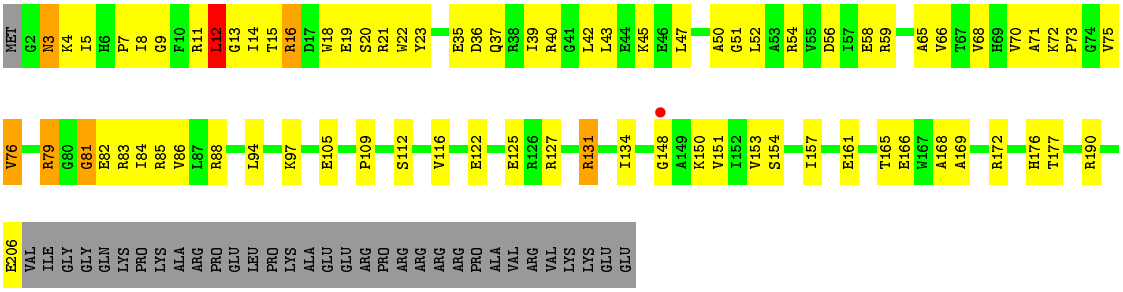
• Molecule 2: 30S ribosomal protein S2

Chain XB:



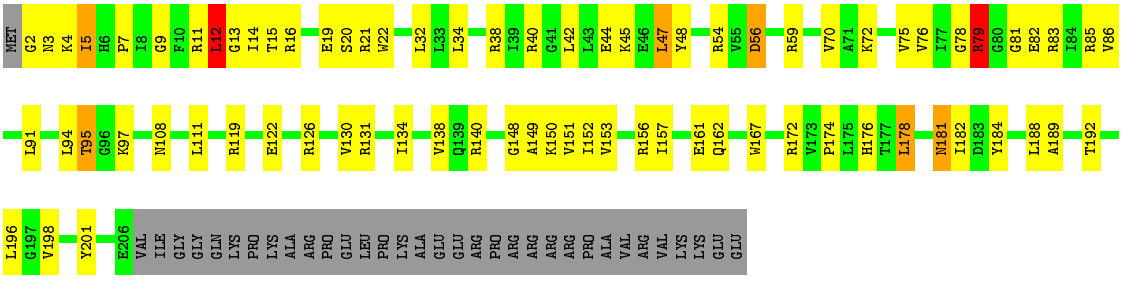
• Molecule 3: 30S ribosomal protein S3

Chain QC:



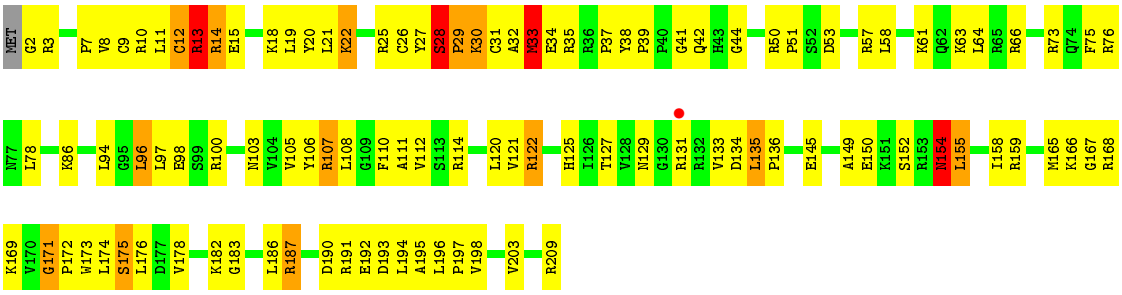
• Molecule 3: 30S ribosomal protein S3

Chain XC:



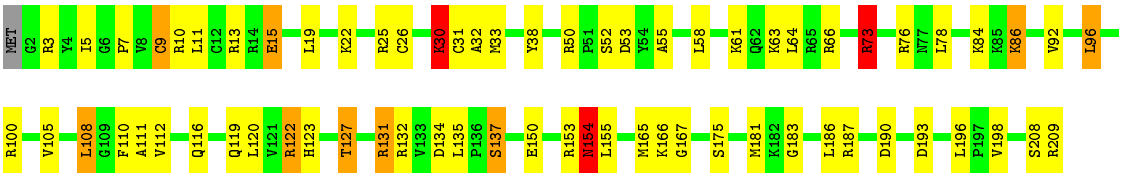
• Molecule 4: 30S ribosomal protein S4

Chain QD:



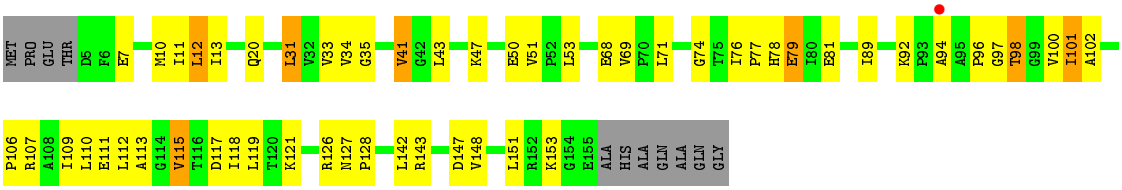
• Molecule 4: 30S ribosomal protein S4

Chain XD:



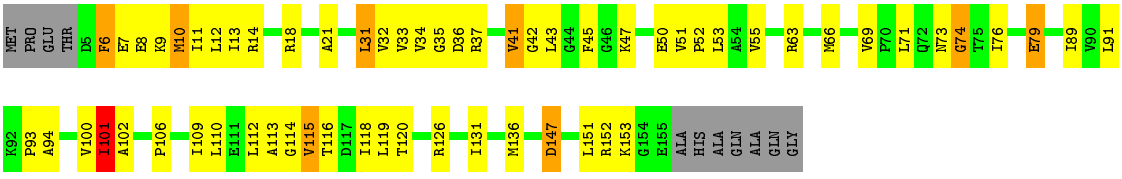
• Molecule 5: 30S ribosomal protein S5

Chain QE:



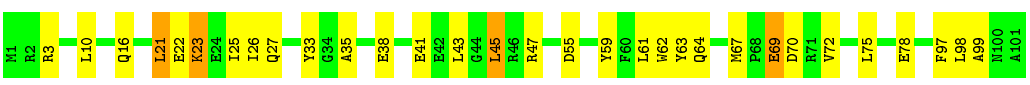
• Molecule 5: 30S ribosomal protein S5

Chain XE:



• Molecule 6: 30S ribosomal protein S6

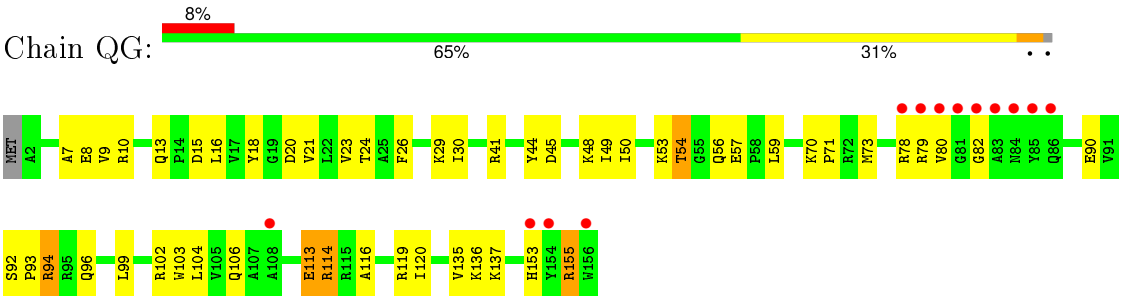
Chain QF:



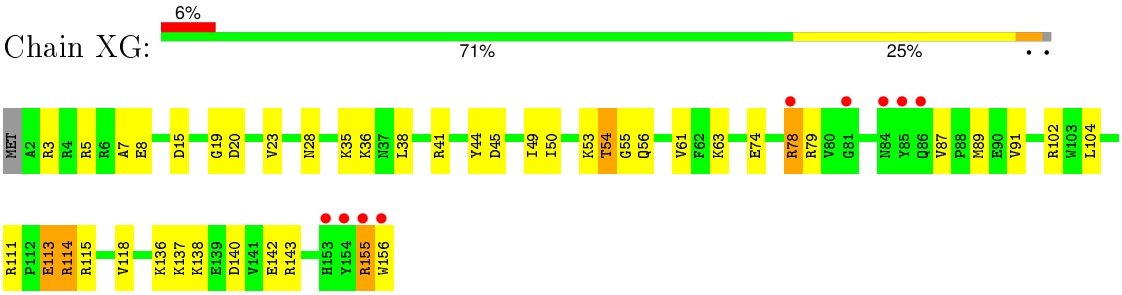
• Molecule 6: 30S ribosomal protein S6

Chain XF:

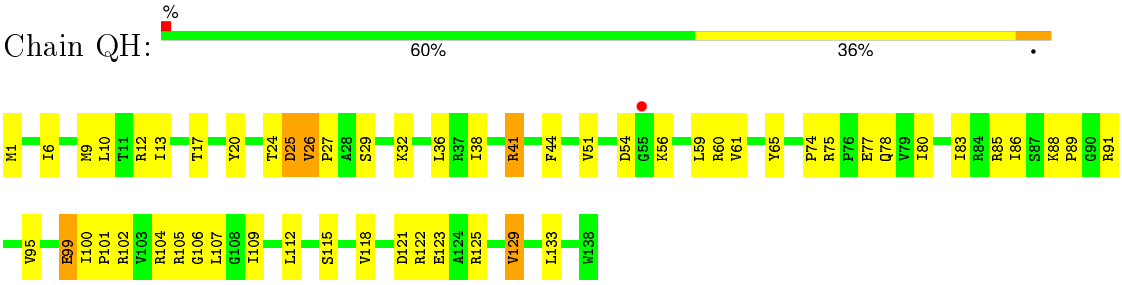
• Molecule 7: 30S ribosomal protein S7



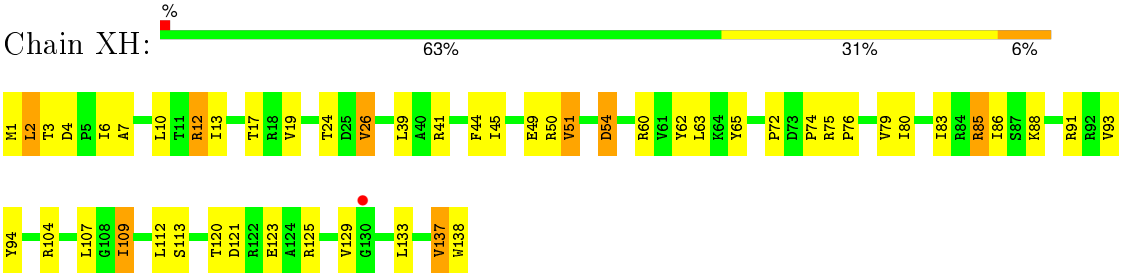
• Molecule 7: 30S ribosomal protein S7



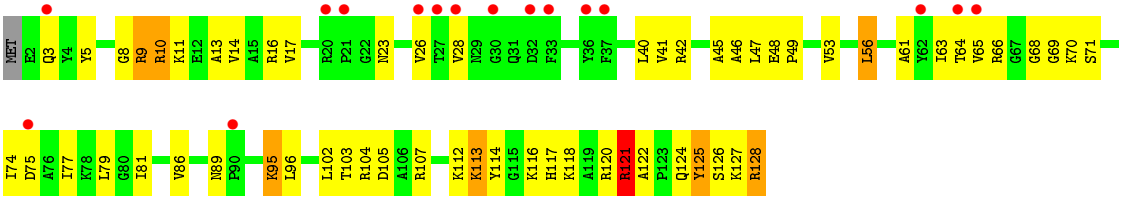
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

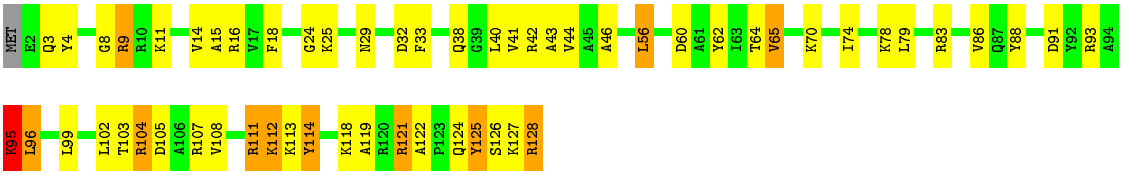


• Molecule 9: 30S ribosomal protein S9



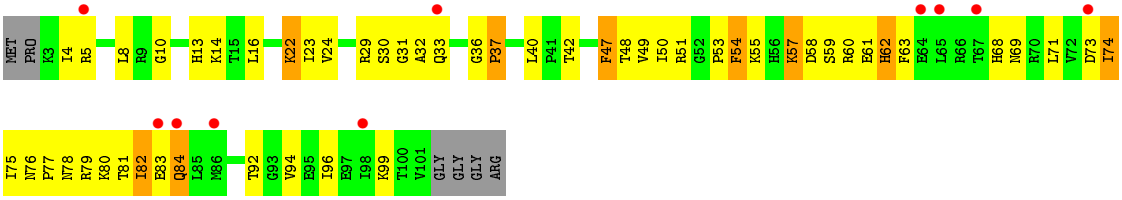
• Molecule 9: 30S ribosomal protein S9

Chain XI:



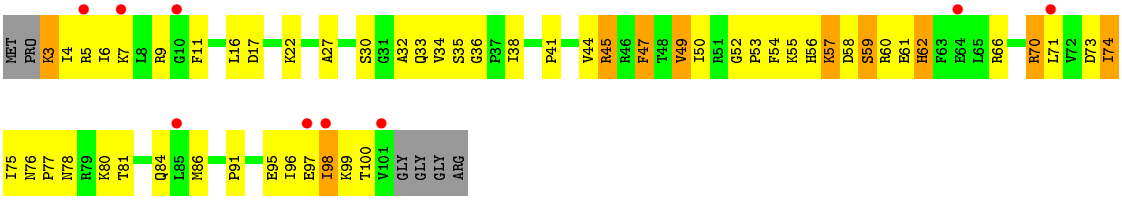
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



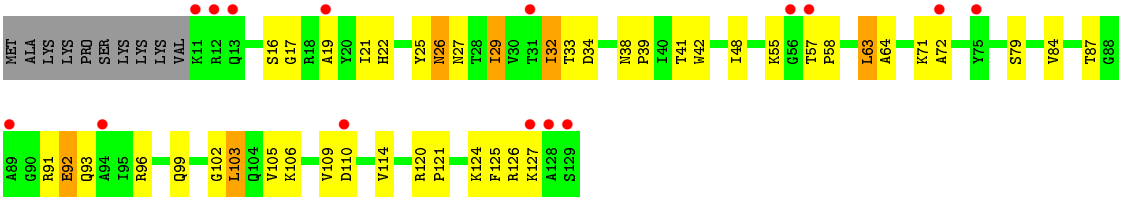
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



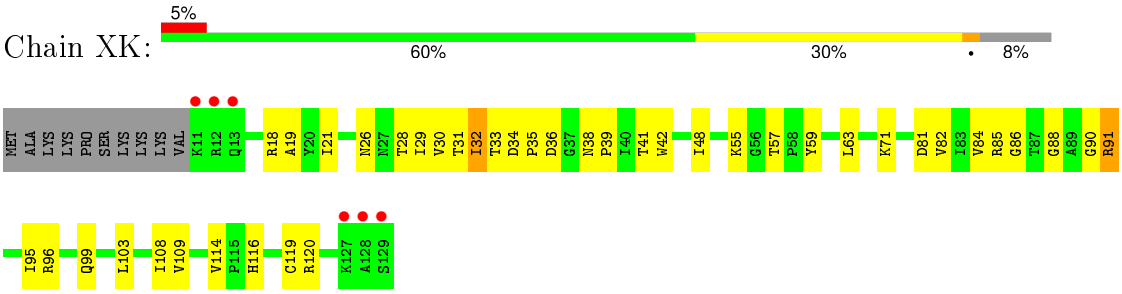
• Molecule 11: 30S ribosomal protein S11

Chain QK:



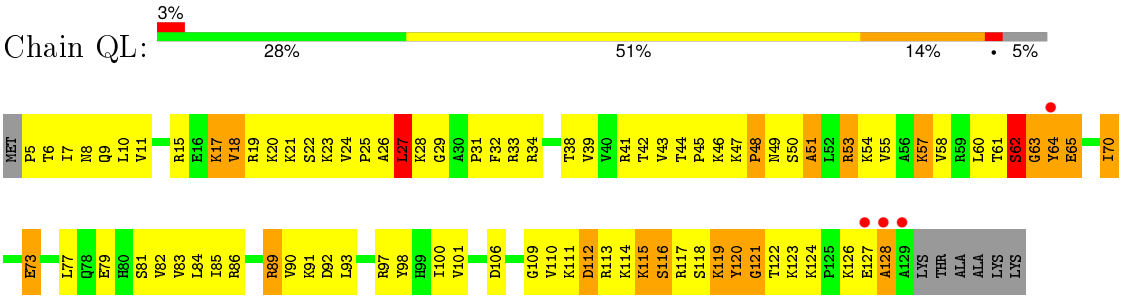
• Molecule 11: 30S ribosomal protein S11

Chain XK:



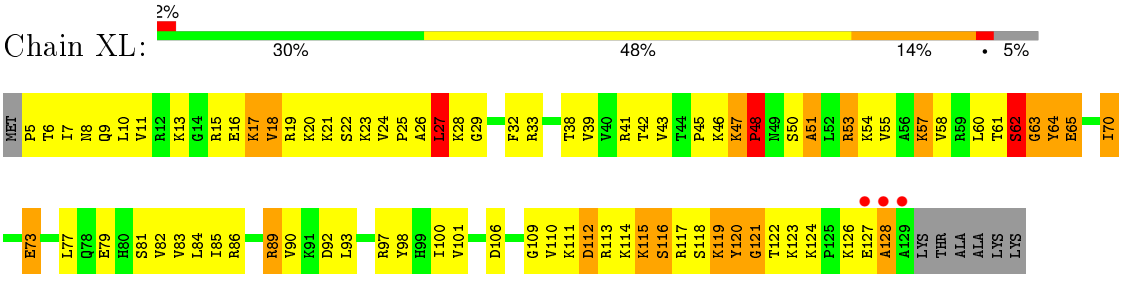
• Molecule 12: 30S ribosomal protein S12

Chain QL:



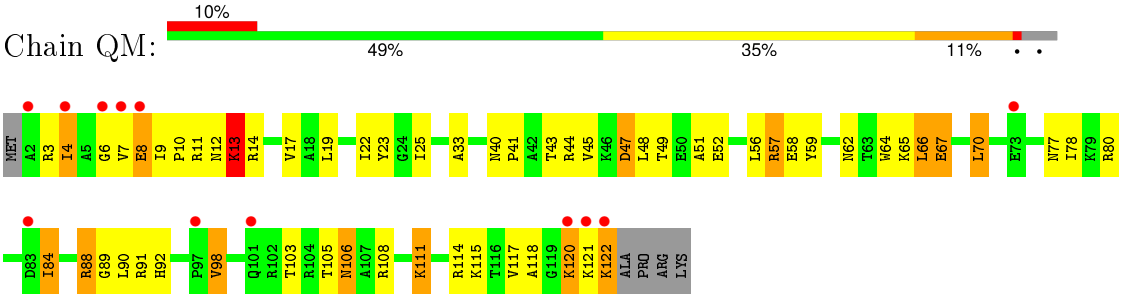
• Molecule 12: 30S ribosomal protein S12

Chain XL:



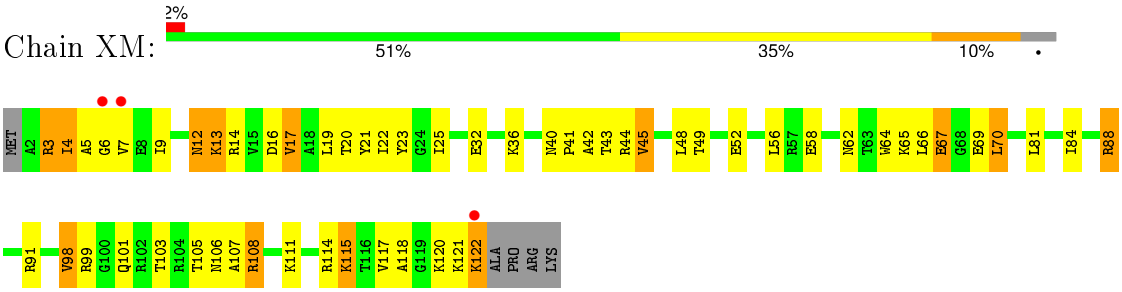
• Molecule 13: 30S ribosomal protein S13

Chain QM:



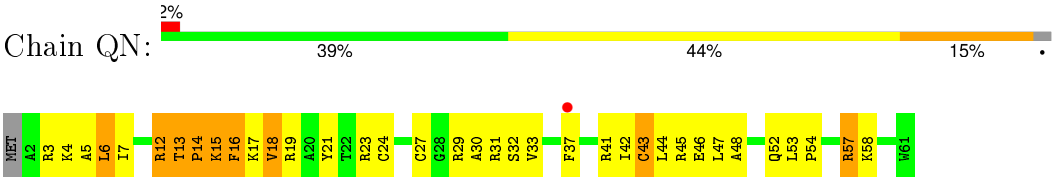
• Molecule 13: 30S ribosomal protein S13

Chain XM:



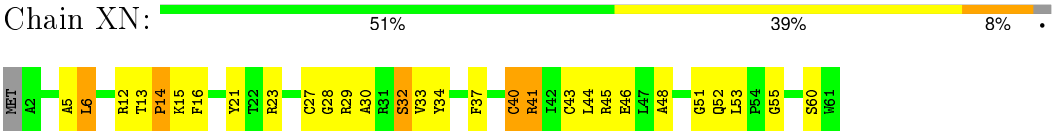
• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



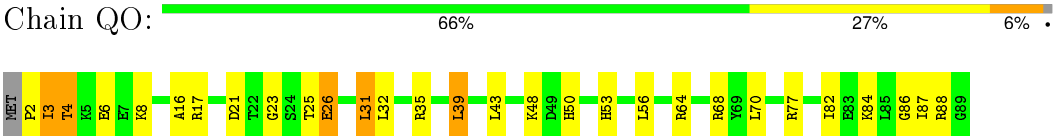
• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



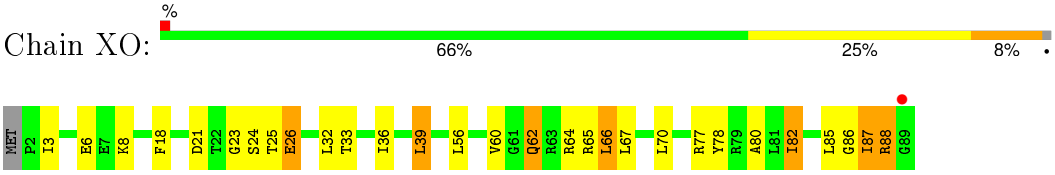
• Molecule 15: 30S ribosomal protein S15

Chain QO:



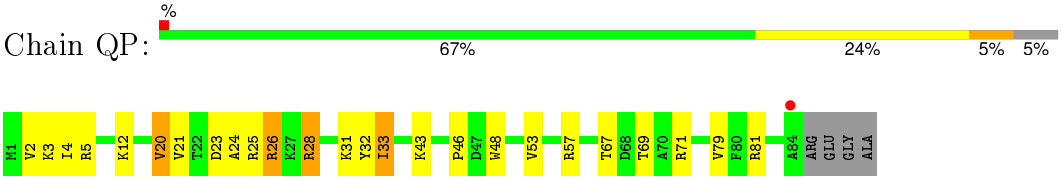
• Molecule 15: 30S ribosomal protein S15

Chain XO:



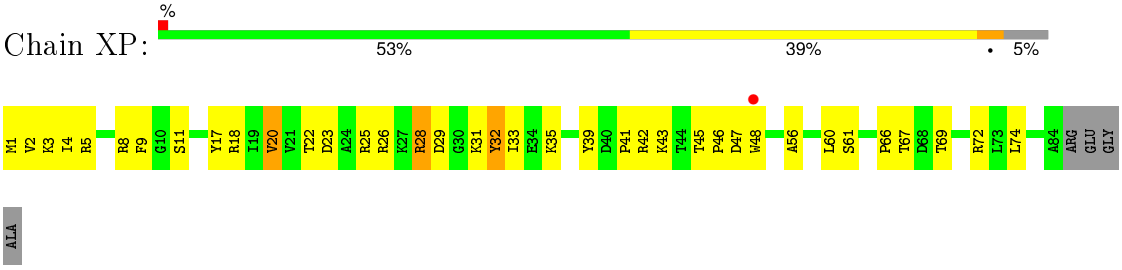
• Molecule 16: 30S ribosomal protein S16

Chain QP:



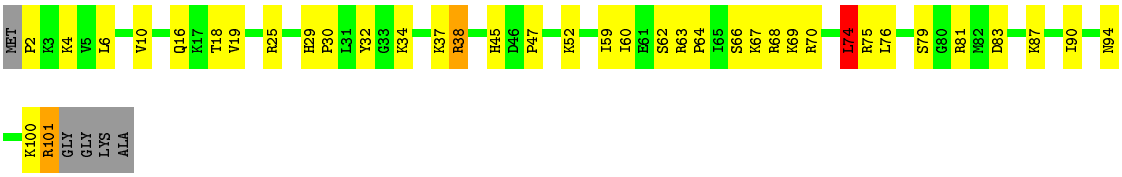
• Molecule 16: 30S ribosomal protein S16

Chain XP:

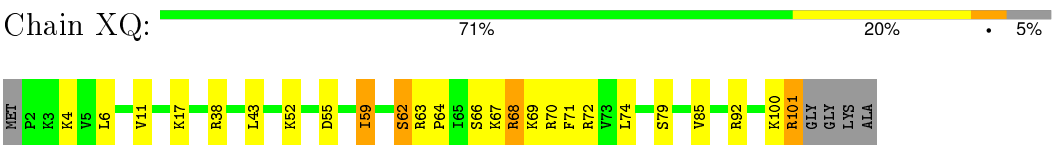


• Molecule 17: 30S ribosomal protein S17

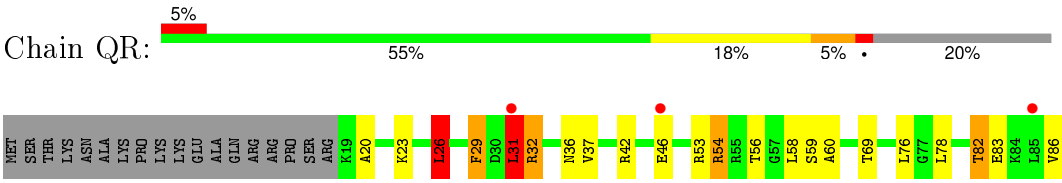
Chain QQ:



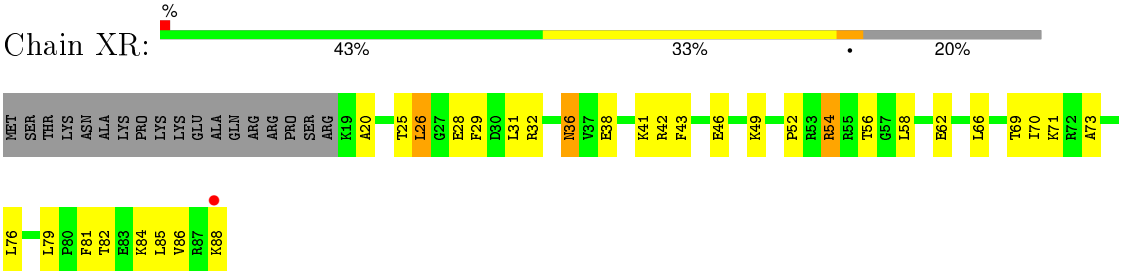
• Molecule 17: 30S ribosomal protein S17



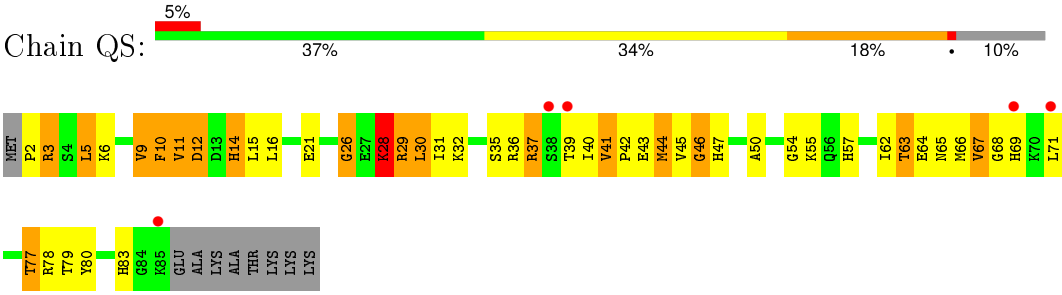
• Molecule 18: 30S ribosomal protein S18



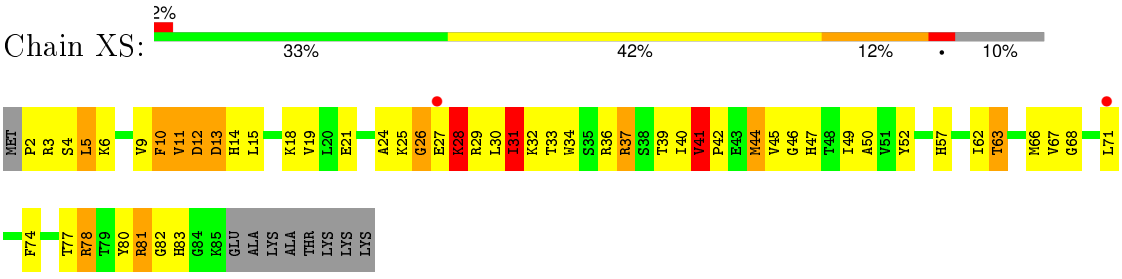
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

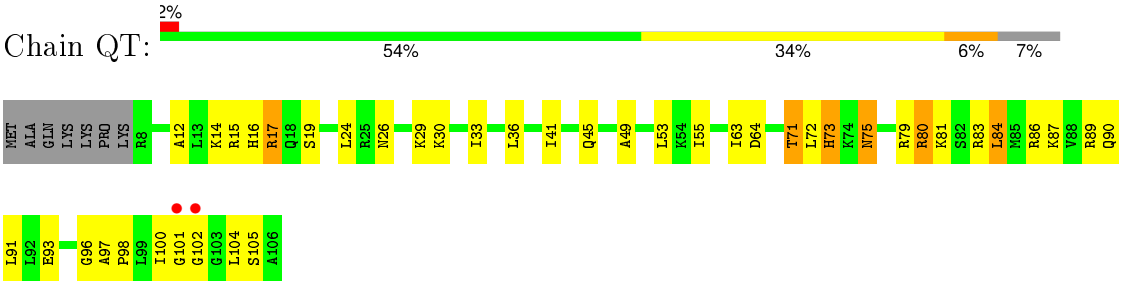


• Molecule 19: 30S ribosomal protein S19



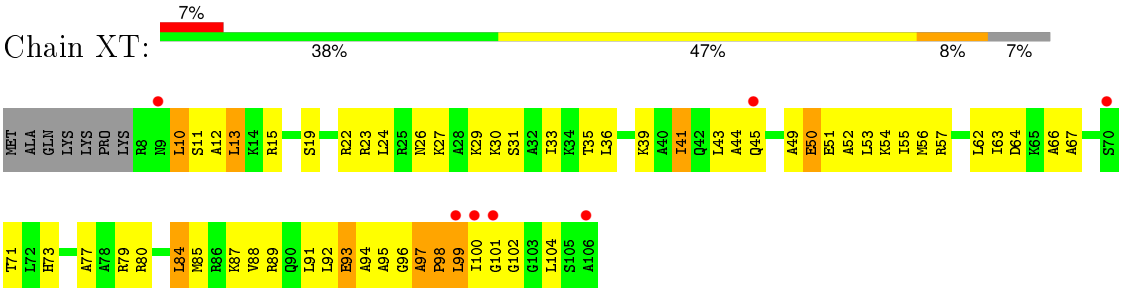
• Molecule 20: 30S ribosomal protein S20

Chain QT:



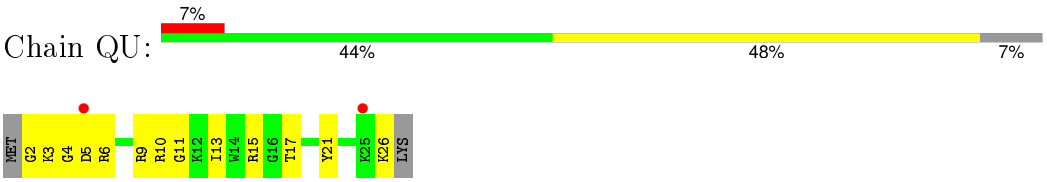
• Molecule 20: 30S ribosomal protein S20

Chain XT:



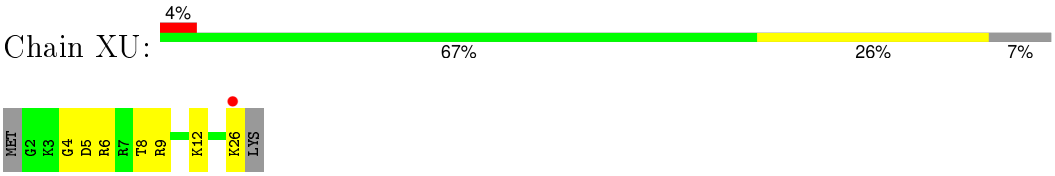
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



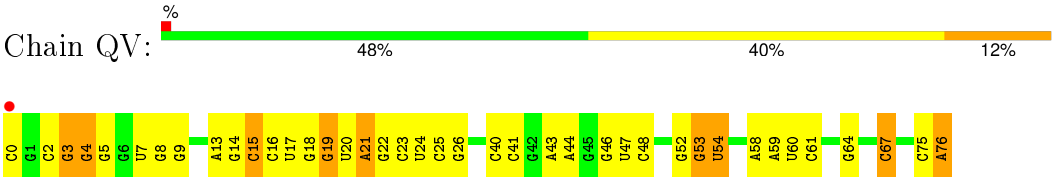
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



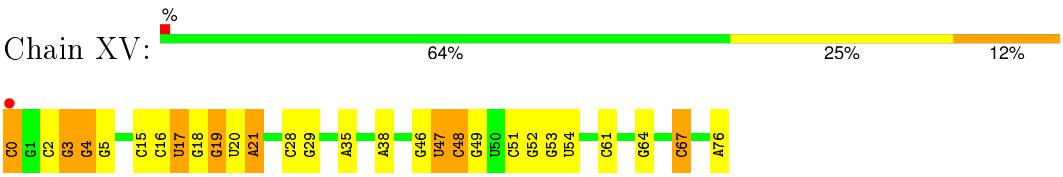
• Molecule 22: P-site tRNA f-Met

Chain QV:



• Molecule 22: P-site tRNA f-Met

Chain XV:

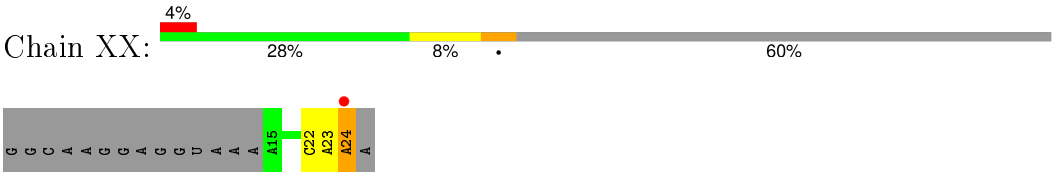


• Molecule 23: messenger RNA

Chain QX:

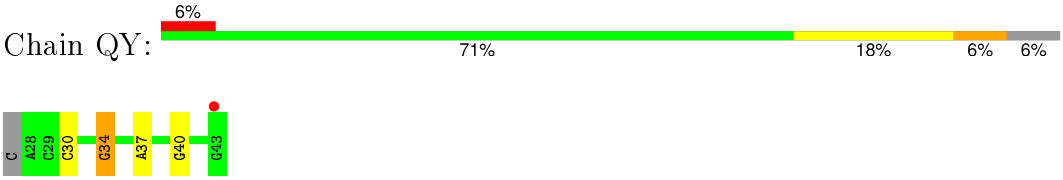
• Molecule 23: messenger RNA

Chain XX:



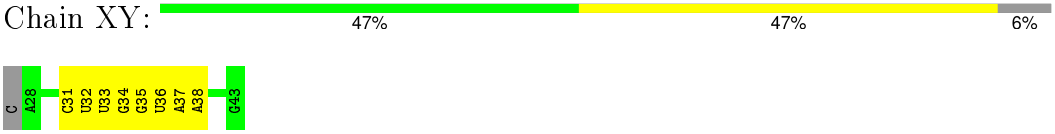
• Molecule 24: A-site tRNA Thr

Chain QY:



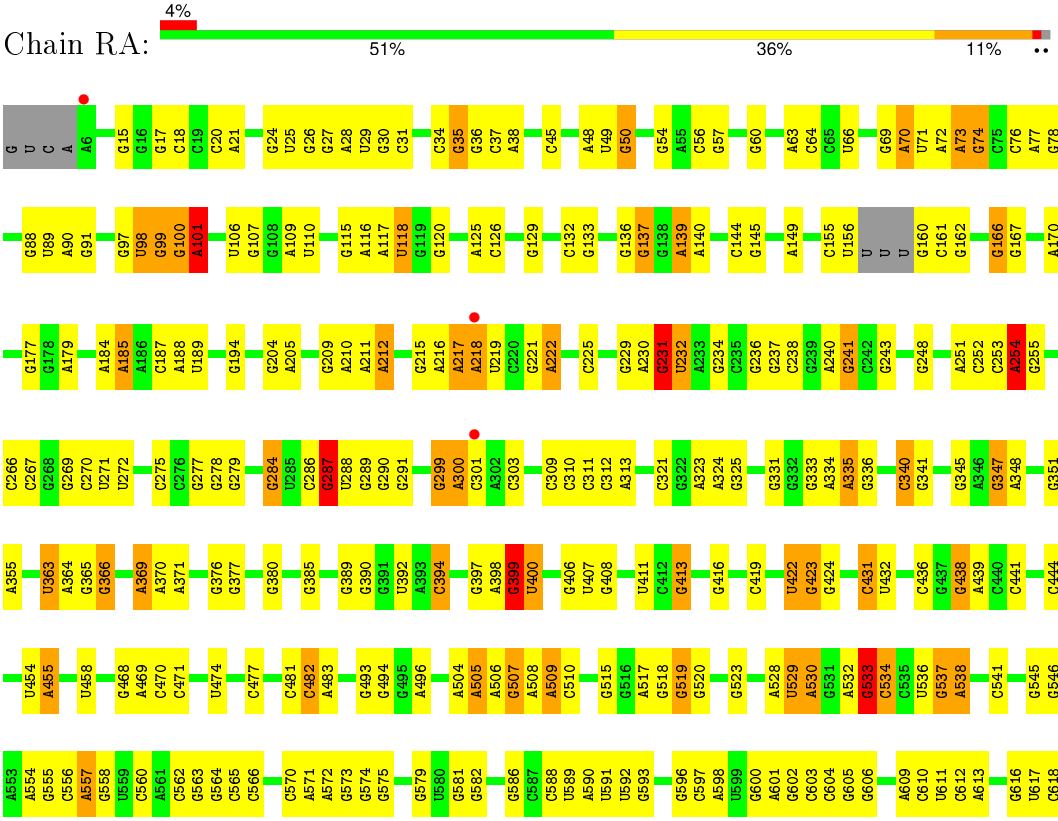
• Molecule 24: A-site tRNA Thr

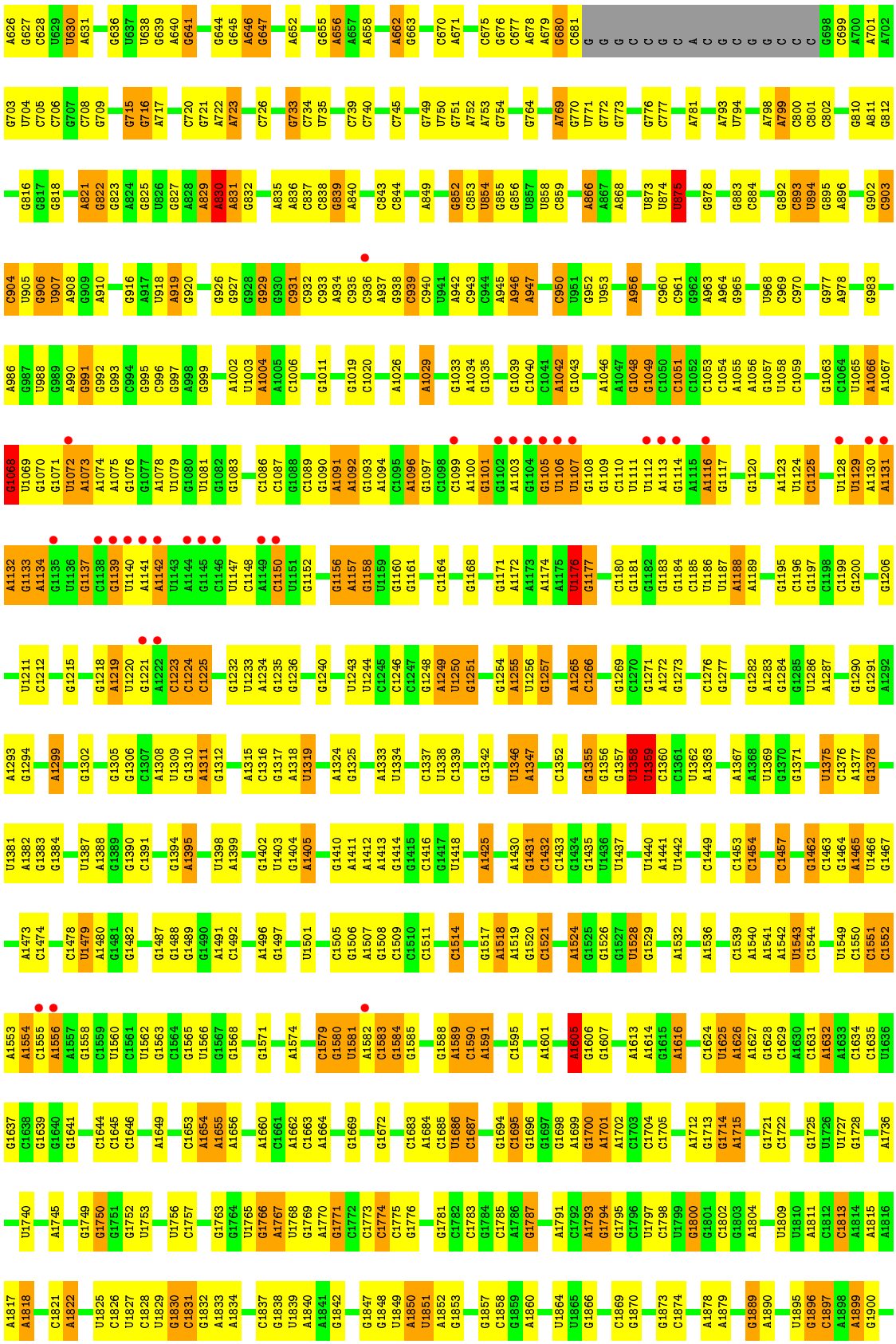
Chain XY:

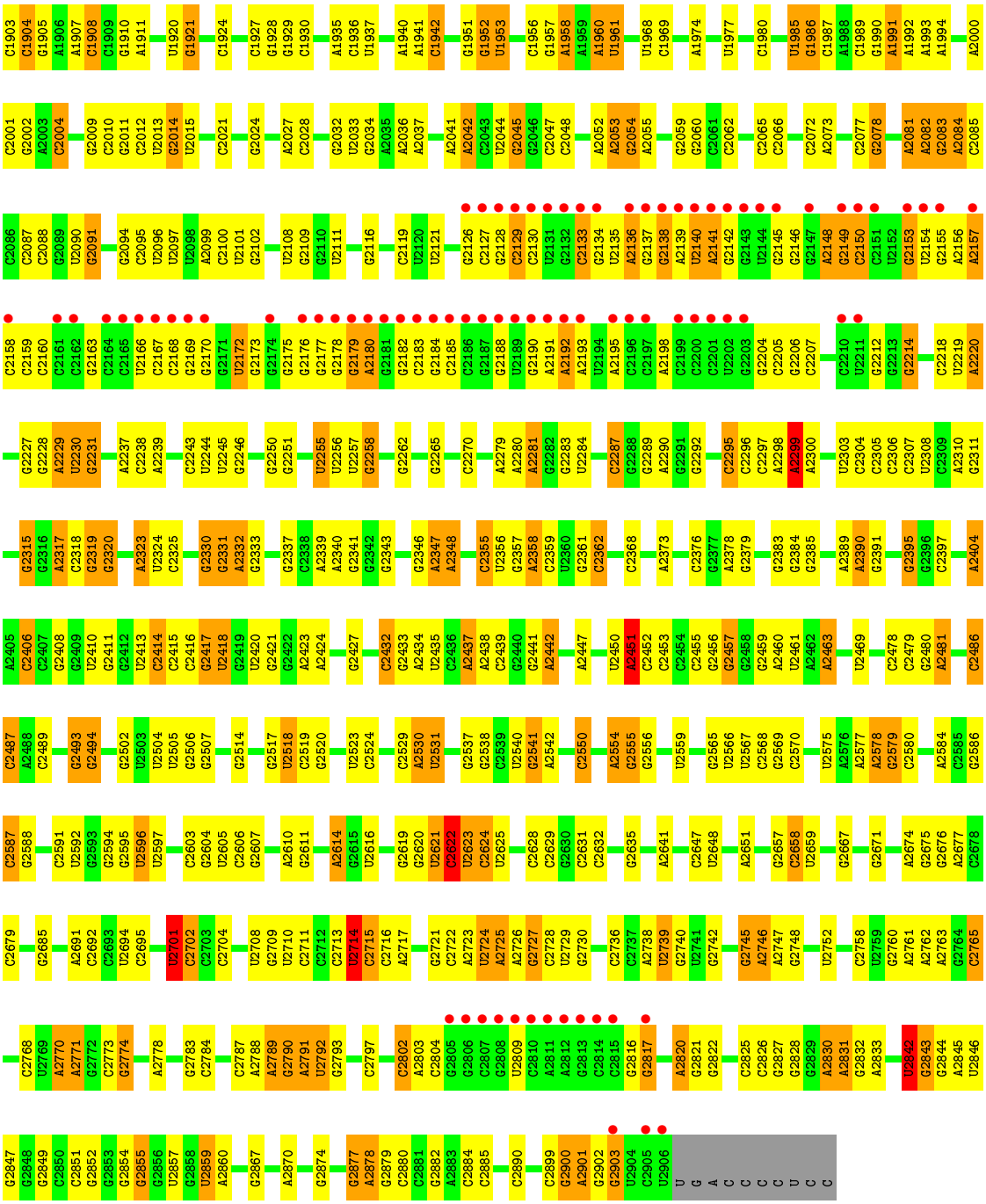


• Molecule 25: 23S rRNA

Chain RA:

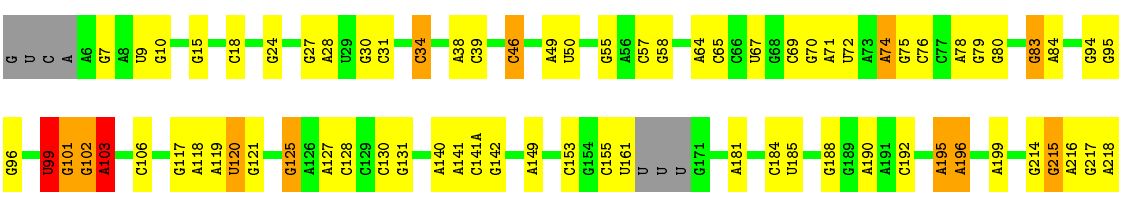


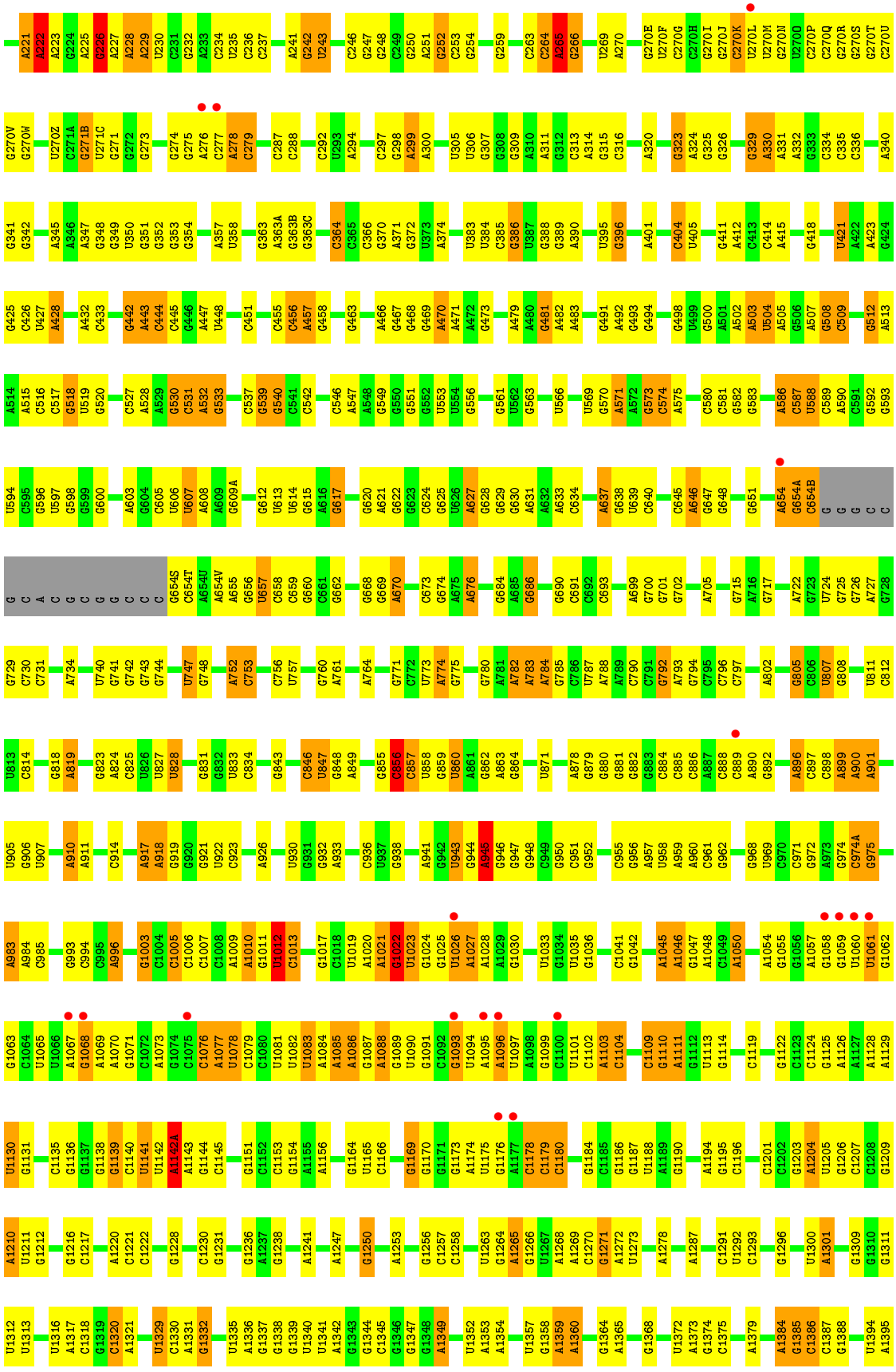


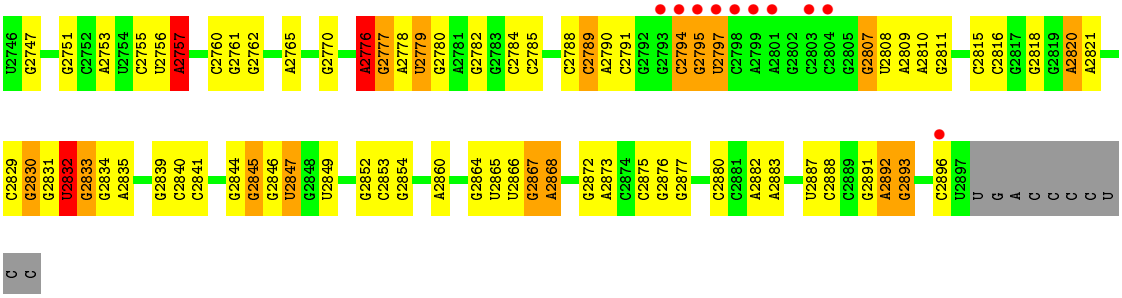


- Molecule 25: 23S rRNA

Chain YA:

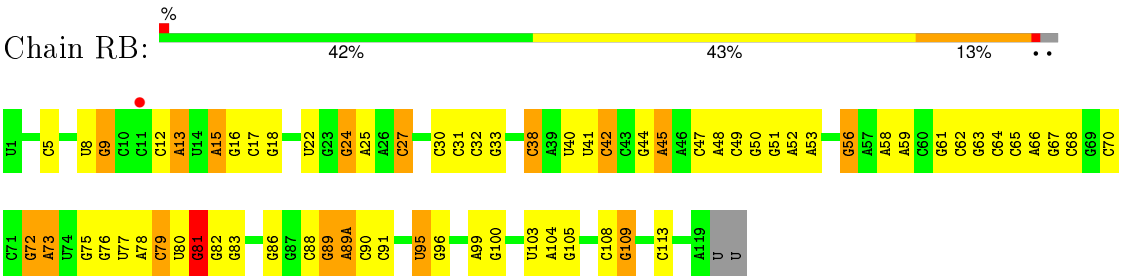






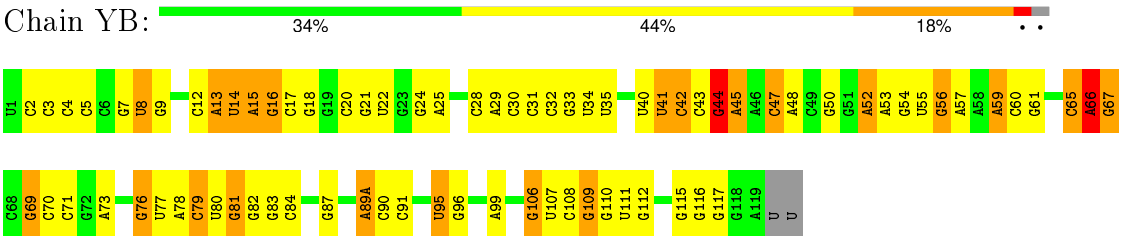
• Molecule 26: 5S rRNA

Chain RB:



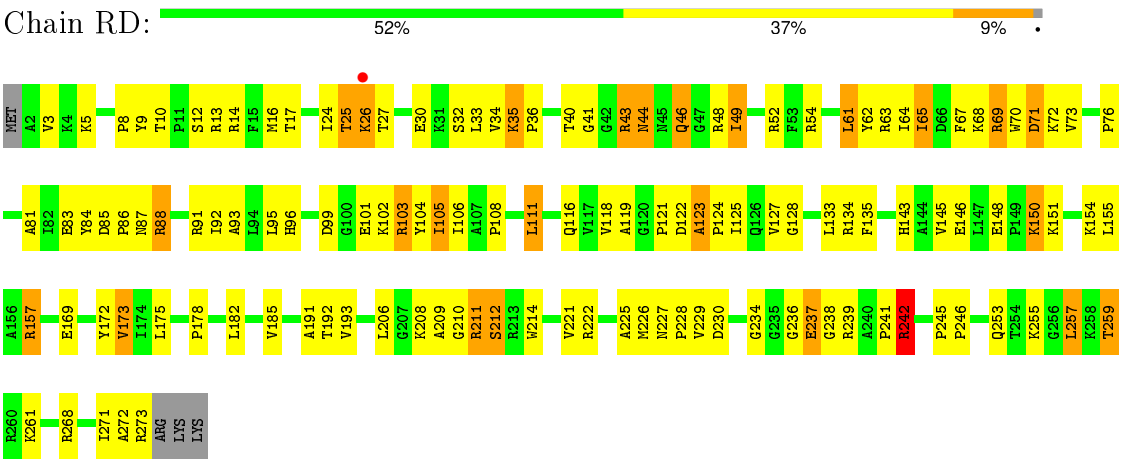
• Molecule 26: 5S rRNA

Chain YB:



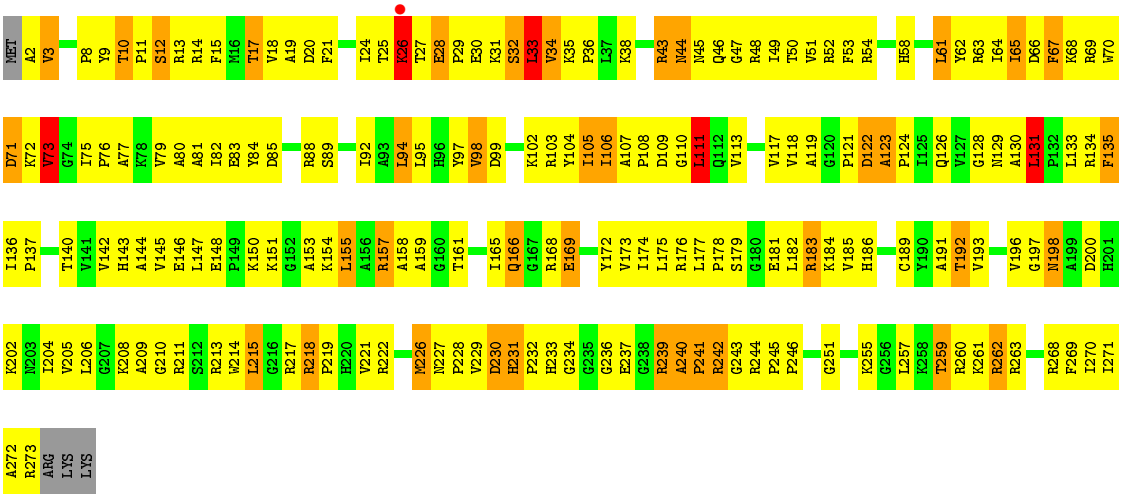
• Molecule 27: 50S ribosomal protein L2

Chain RD:



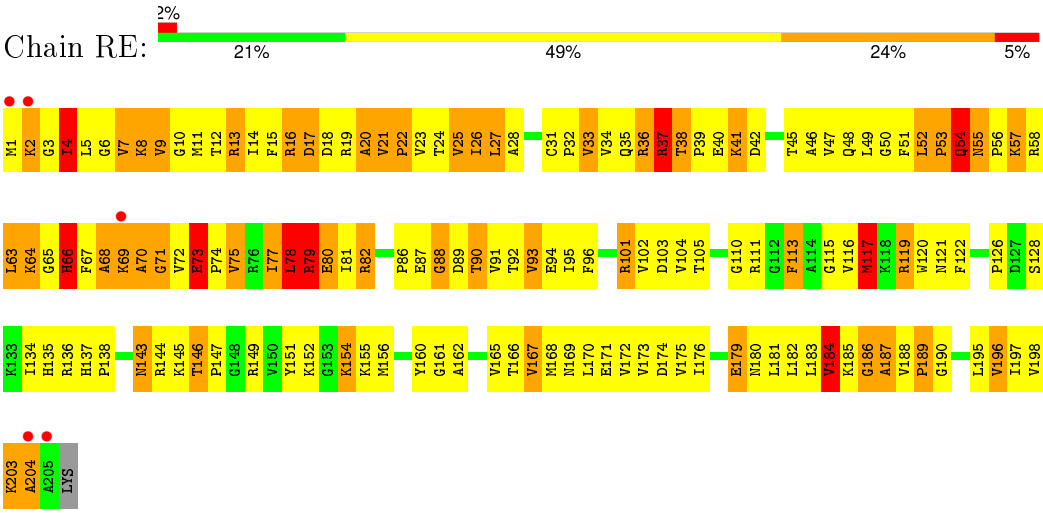
• Molecule 27: 50S ribosomal protein L2

Chain YD:



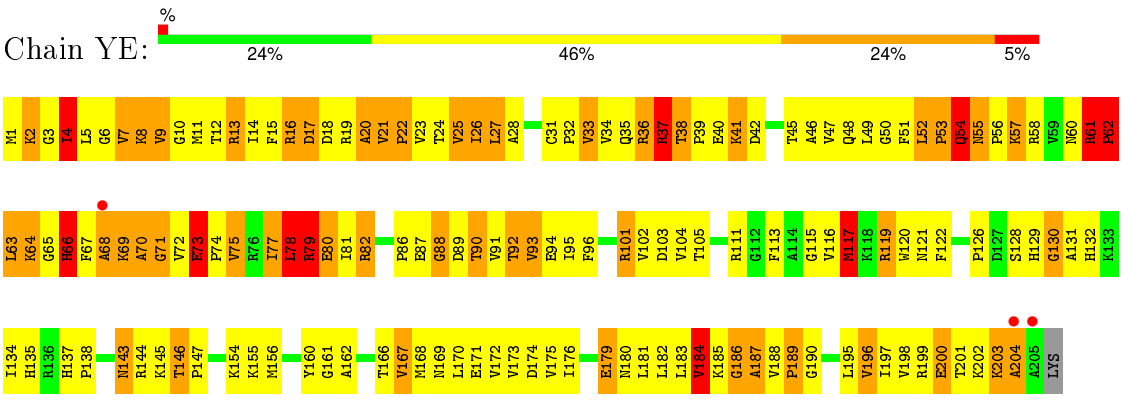
• Molecule 28: 50S ribosomal protein L3

Chain RE:



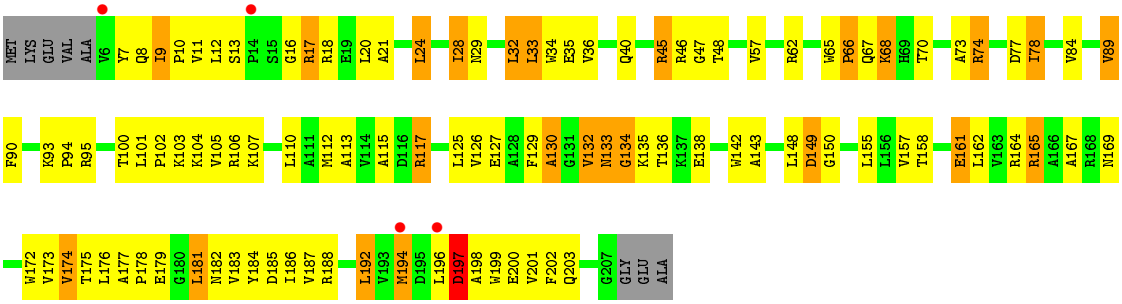
• Molecule 28: 50S ribosomal protein L3

Chain YE:



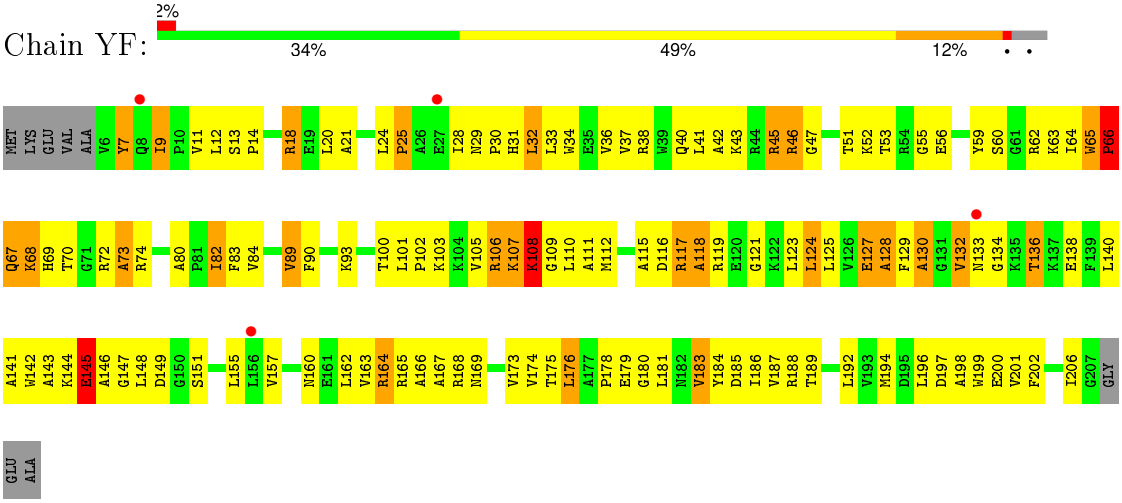
• Molecule 29: 50S ribosomal protein L4

Chain RF:



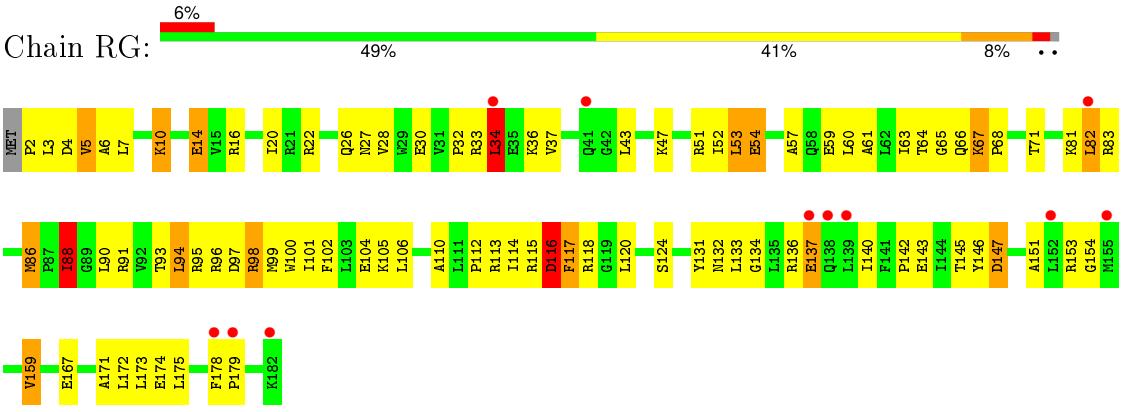
• Molecule 29: 50S ribosomal protein L4

Chain YF:



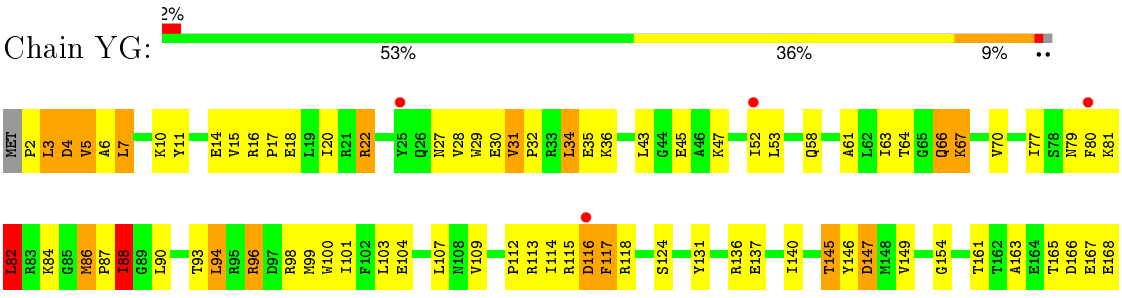
• Molecule 30: 50S ribosomal protein L5

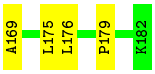
Chain RG:



• Molecule 30: 50S ribosomal protein L5

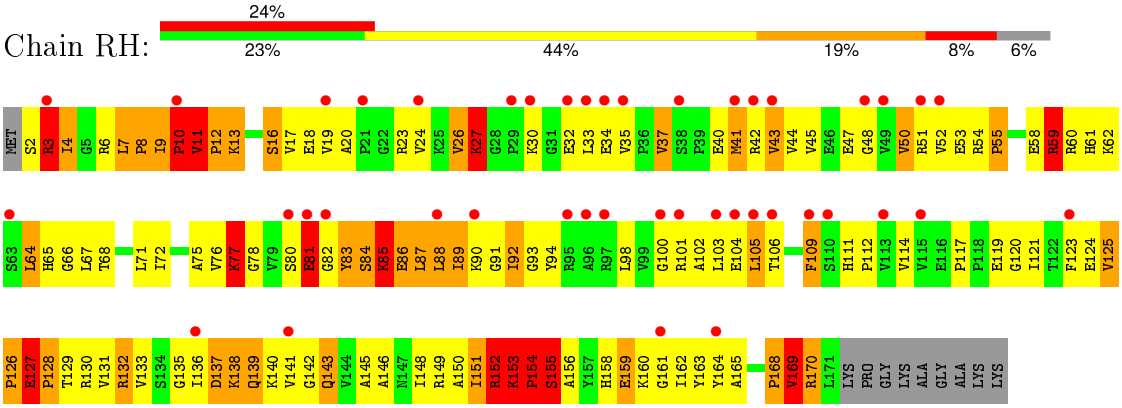
Chain YG:





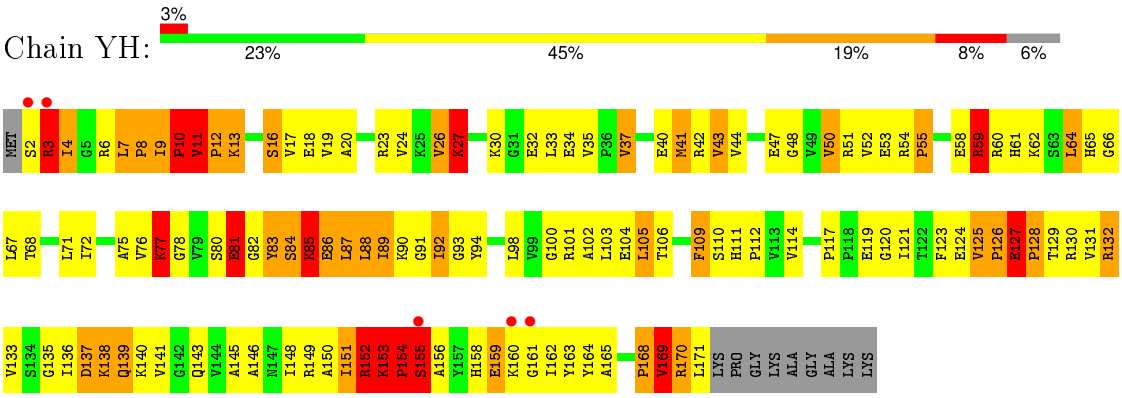
• Molecule 31: 50S ribosomal protein L6

Chain RH:



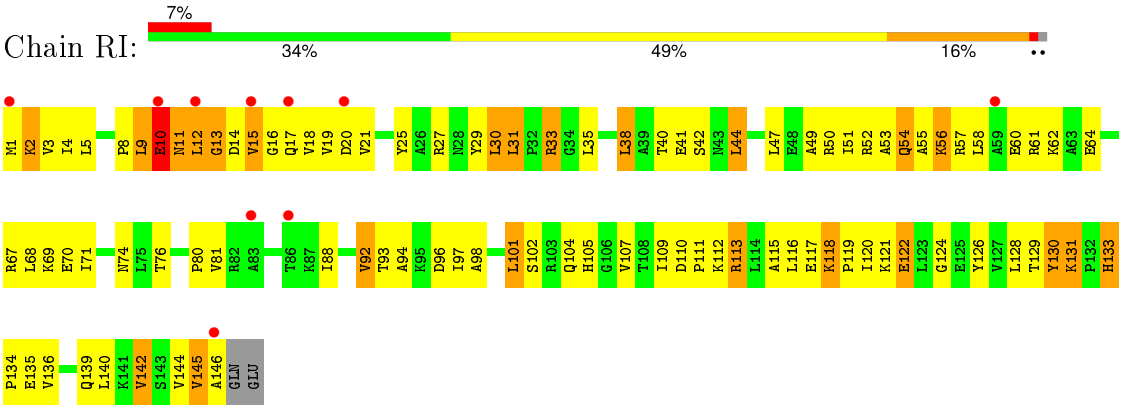
• Molecule 31: 50S ribosomal protein L6

Chain YH:



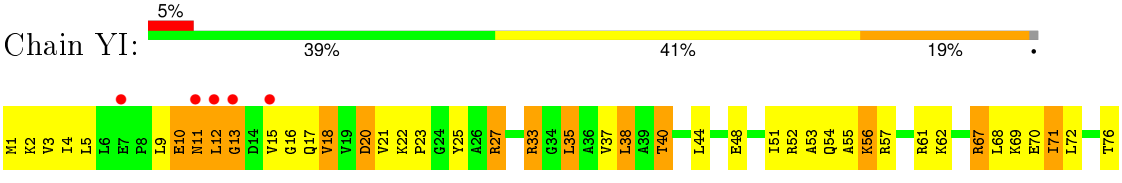
• Molecule 32: 50S ribosomal protein L9

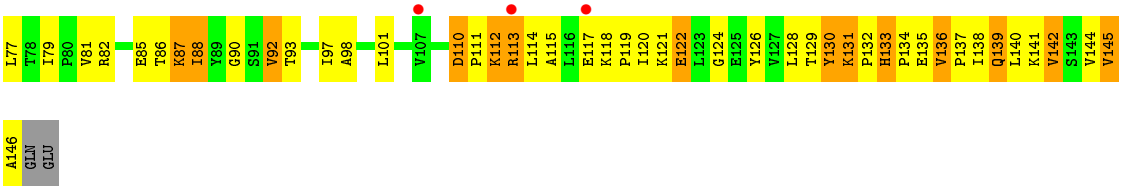
Chain RI:



• Molecule 32: 50S ribosomal protein L9

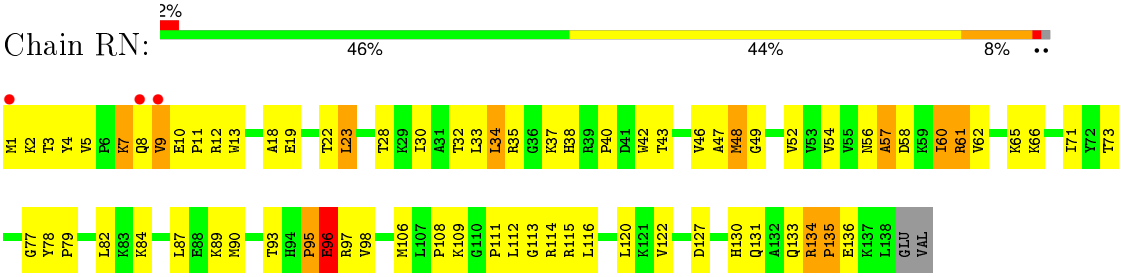
Chain YI:





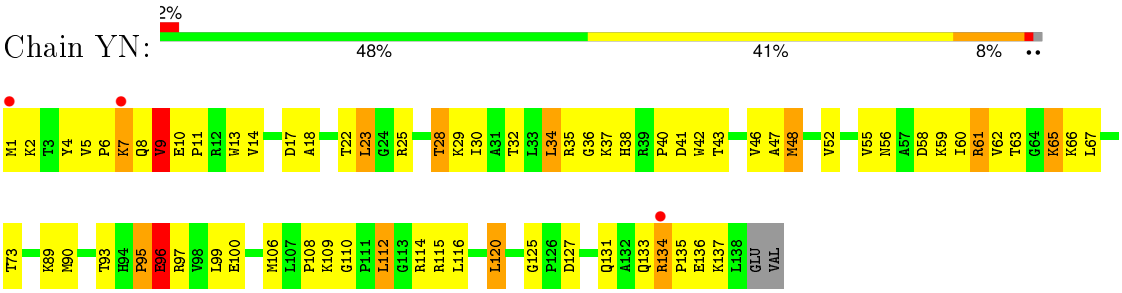
• Molecule 33: 50S ribosomal protein L13

Chain RN:



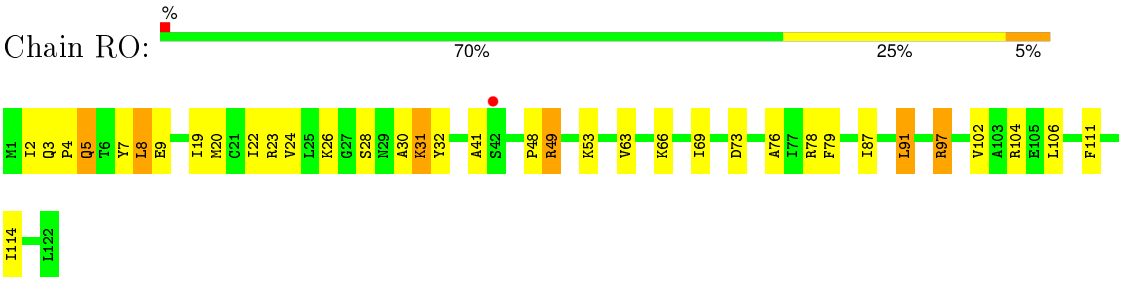
• Molecule 33: 50S ribosomal protein L13

Chain YN:



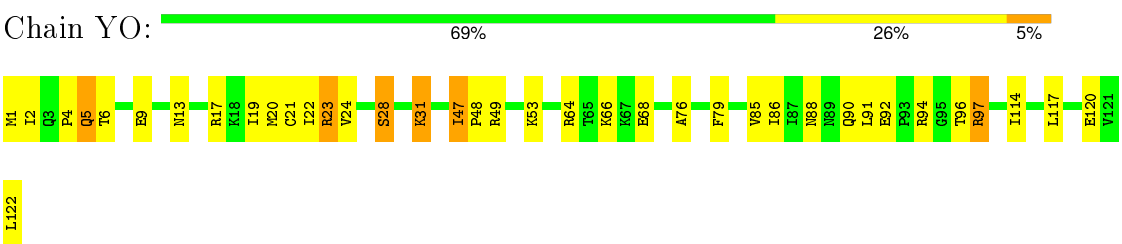
• Molecule 34: 50S ribosomal protein L14

Chain RO:



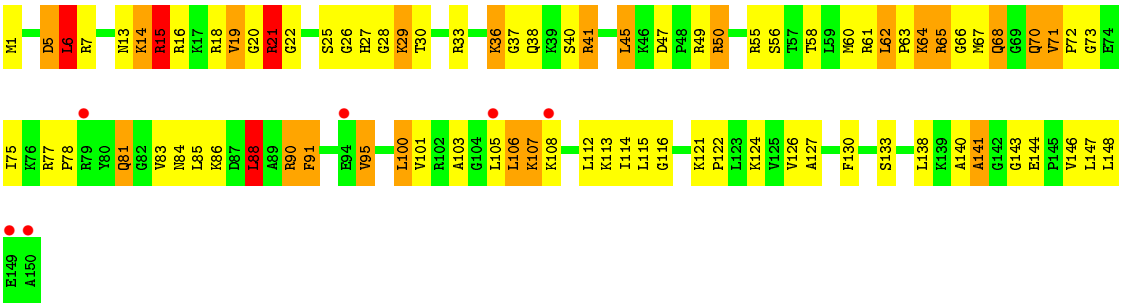
• Molecule 34: 50S ribosomal protein L14

Chain YO:



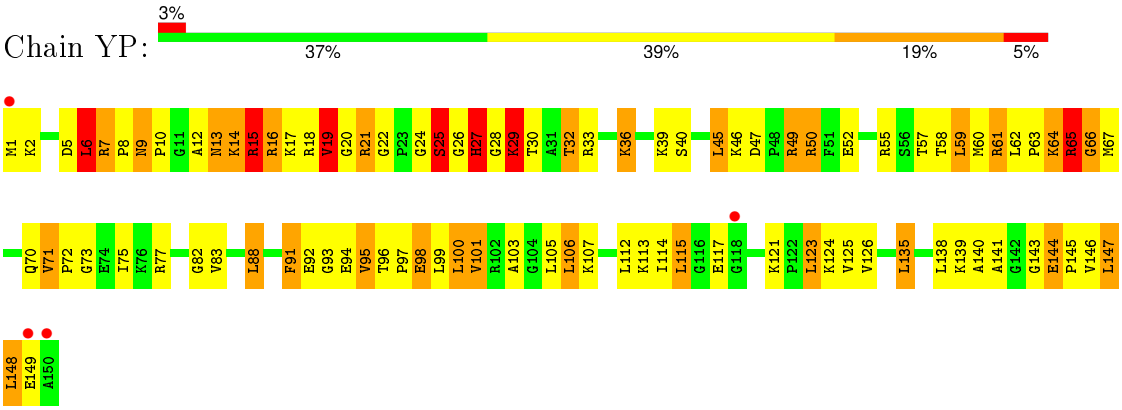
• Molecule 35: 50S ribosomal protein L15

Chain RP:



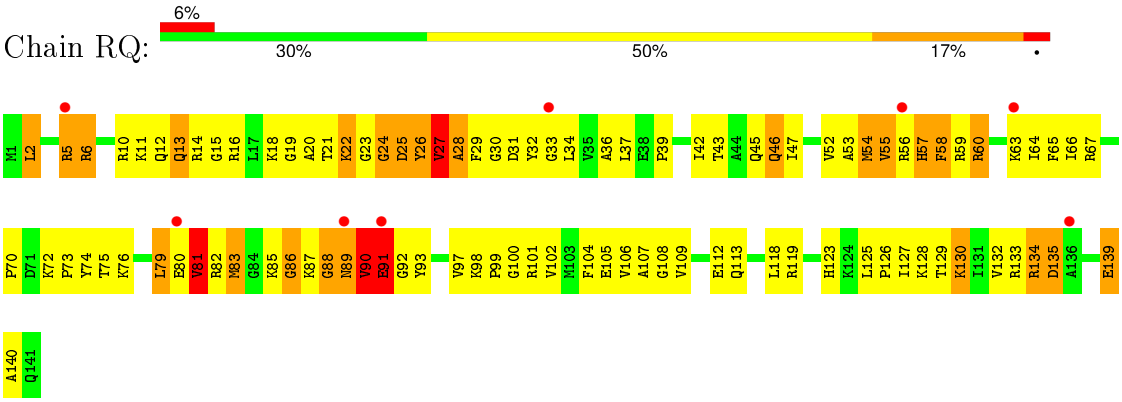
- Molecule 35: 50S ribosomal protein L15

Chain YP:



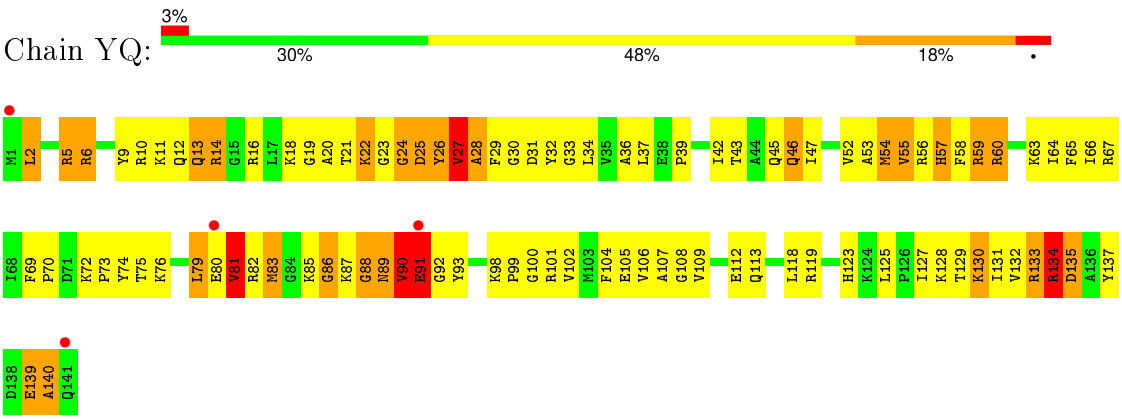
- Molecule 36: 50S ribosomal protein L16

Chain RQ:



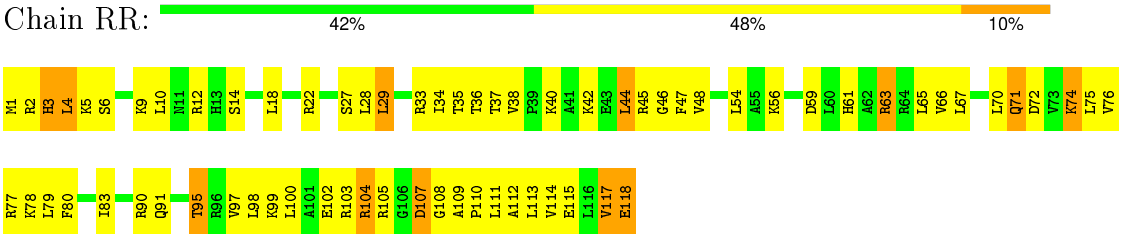
- Molecule 36: 50S ribosomal protein L16

Chain YQ:



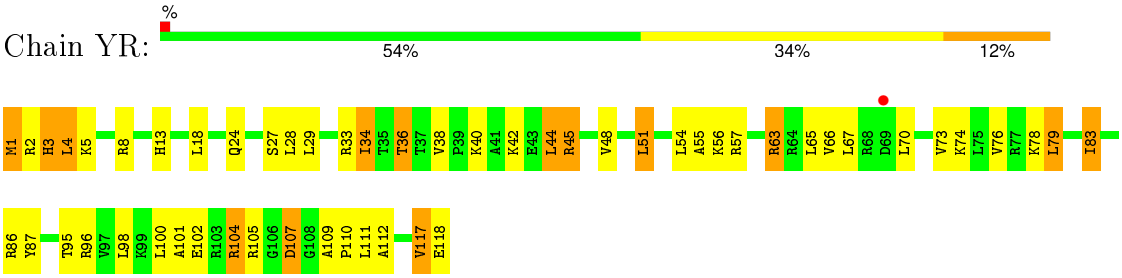
• Molecule 37: 50S ribosomal protein L17

Chain RR:



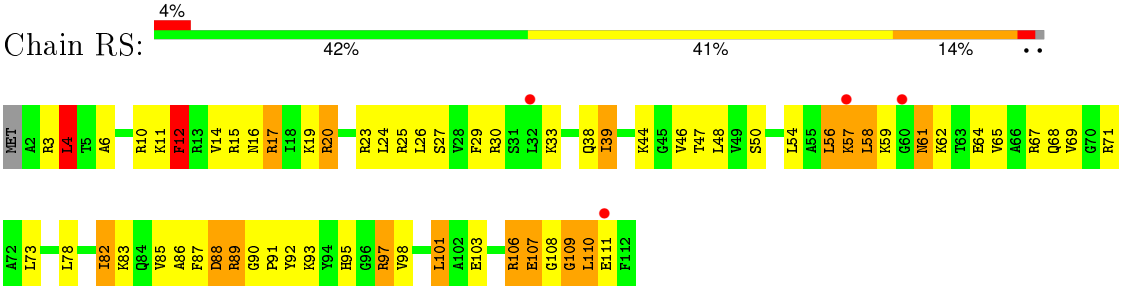
• Molecule 37: 50S ribosomal protein L17

Chain YR:



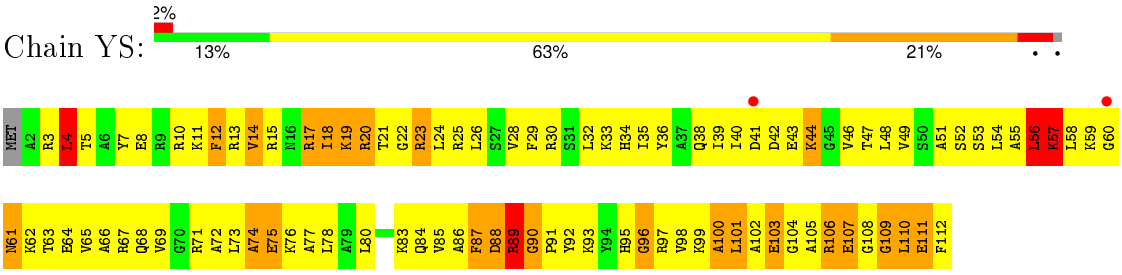
• Molecule 38: 50S ribosomal protein L18

Chain RS:



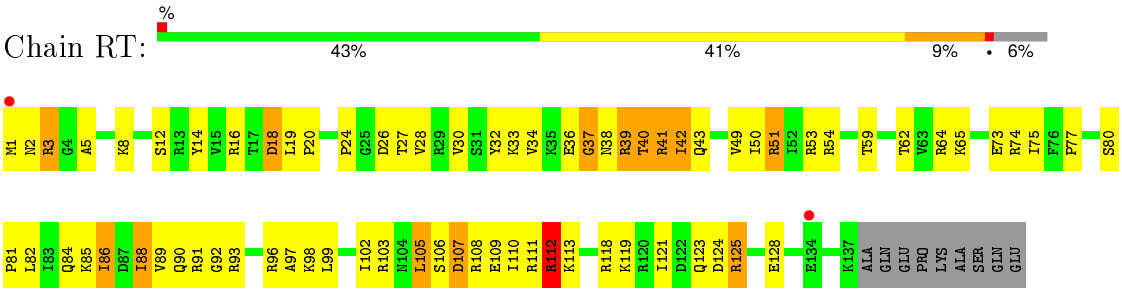
• Molecule 38: 50S ribosomal protein L18

Chain YS:



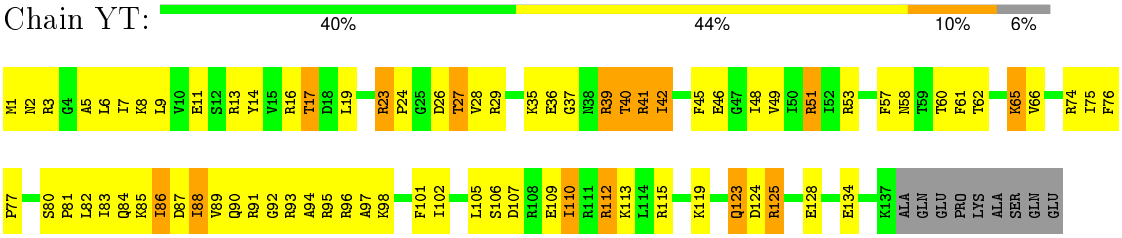
• Molecule 39: 50S ribosomal protein L19

Chain RT:



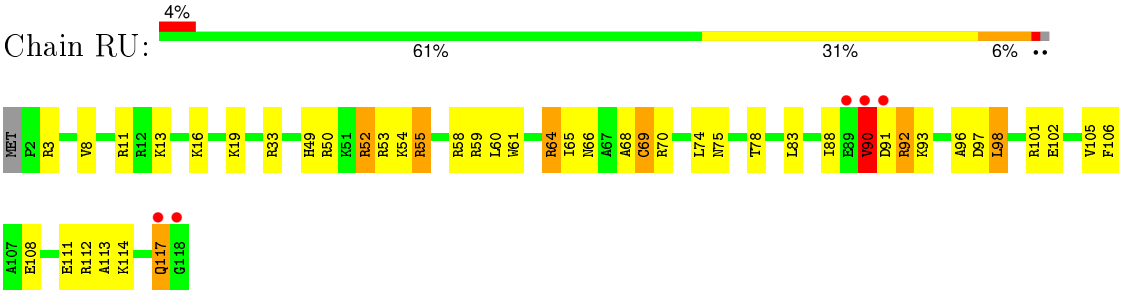
- Molecule 39: 50S ribosomal protein L19

Chain YT:



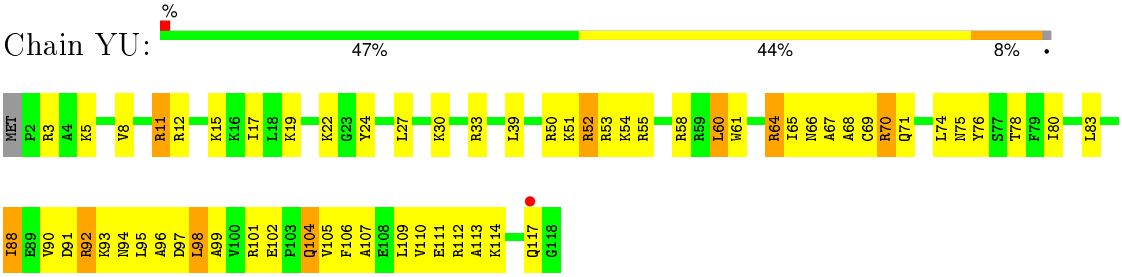
- Molecule 40: 50S ribosomal protein L20

Chain RU:



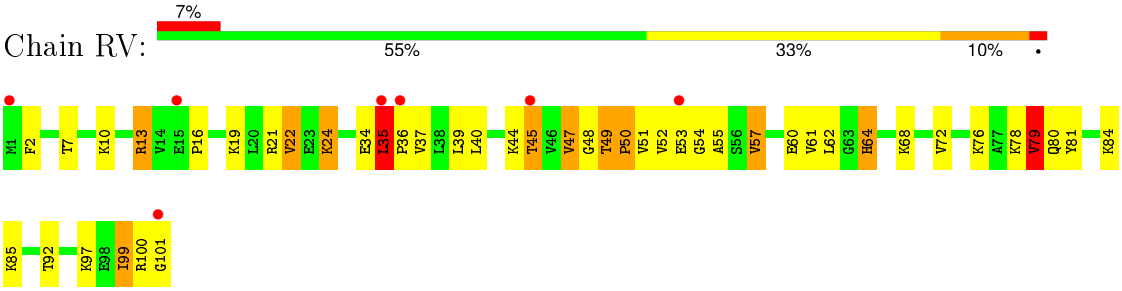
- Molecule 40: 50S ribosomal protein L20

Chain YU:



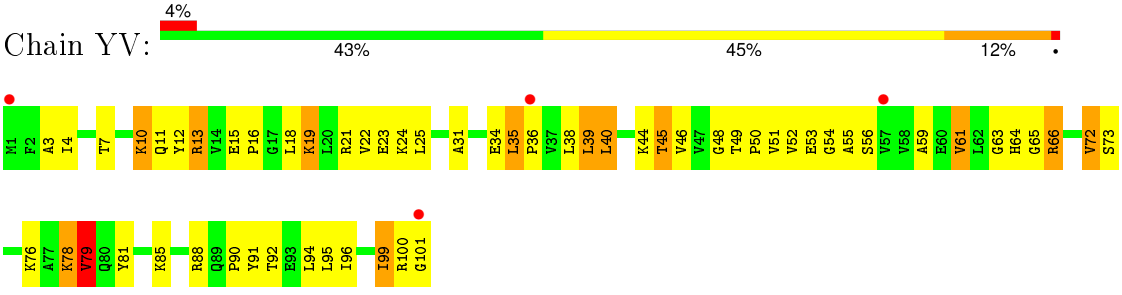
- Molecule 41: 50S ribosomal protein L21

Chain RV:



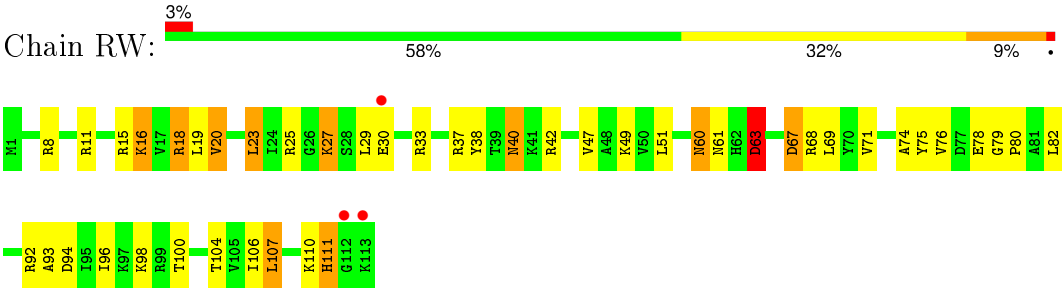
- Molecule 41: 50S ribosomal protein L21

Chain YV:



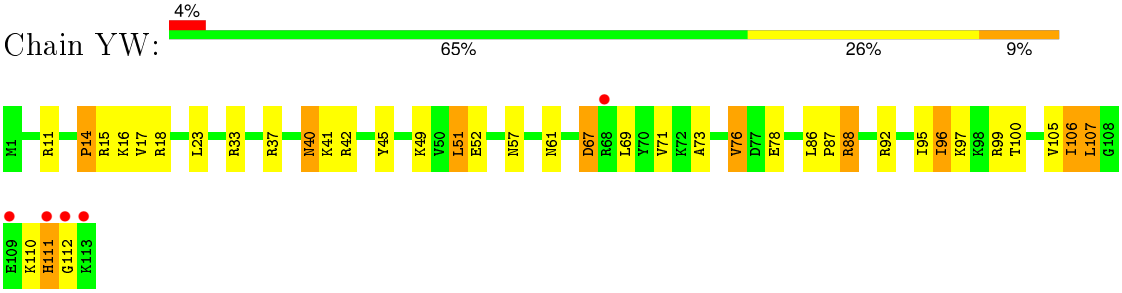
- Molecule 42: 50S ribosomal protein L22

Chain RW:



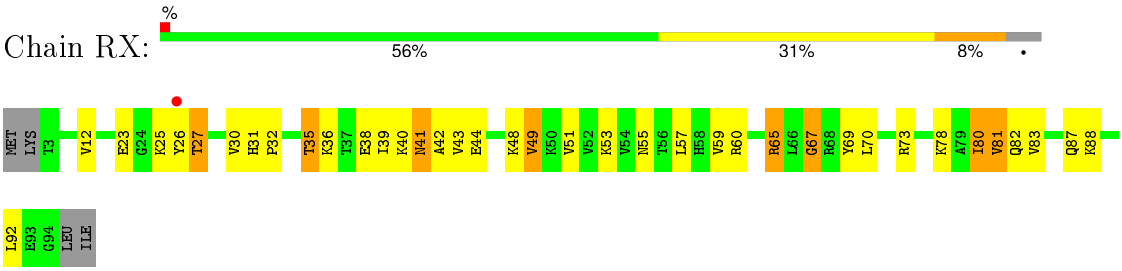
- Molecule 42: 50S ribosomal protein L22

Chain YW:



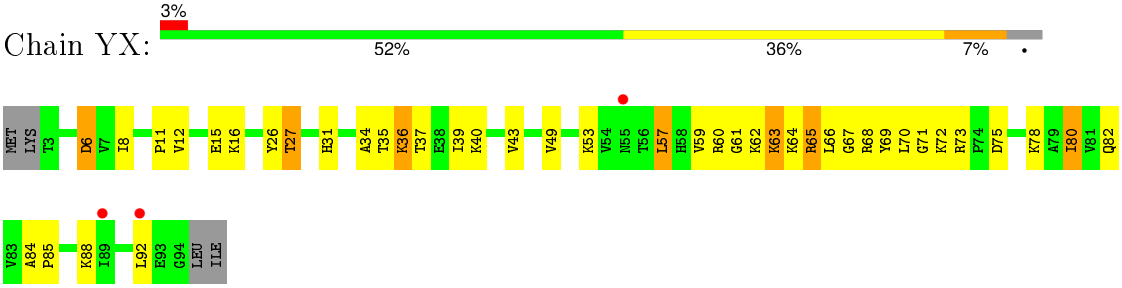
- Molecule 43: 50S ribosomal protein L23

Chain RX:



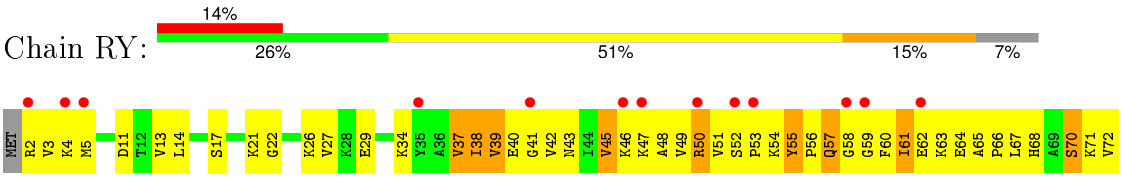
- Molecule 43: 50S ribosomal protein L23

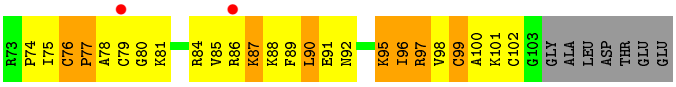
Chain YX:



- Molecule 44: 50S ribosomal protein L24

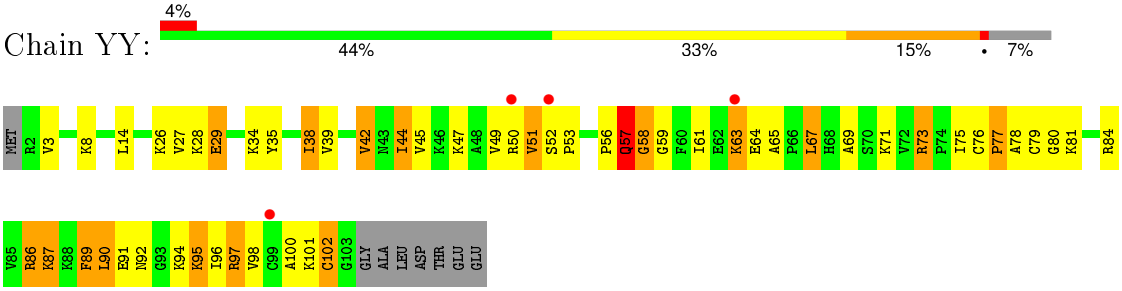
Chain RY:





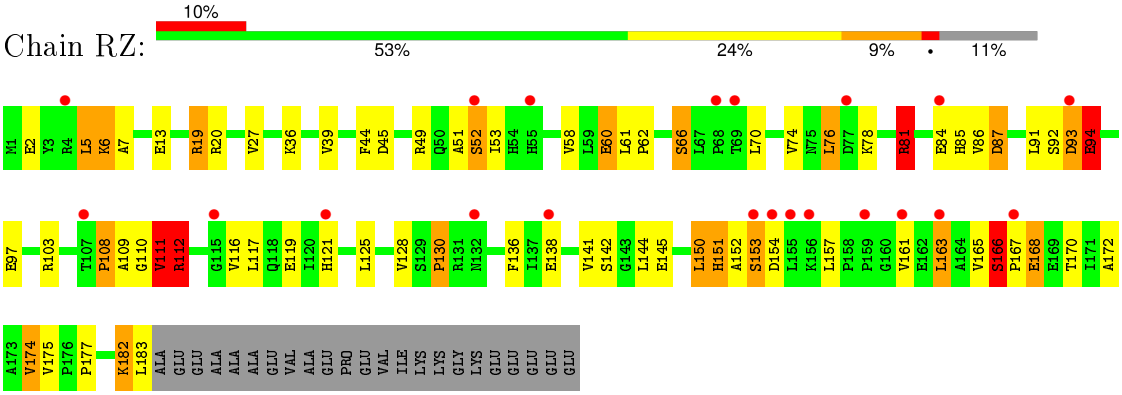
• Molecule 44: 50S ribosomal protein L24

Chain YY:



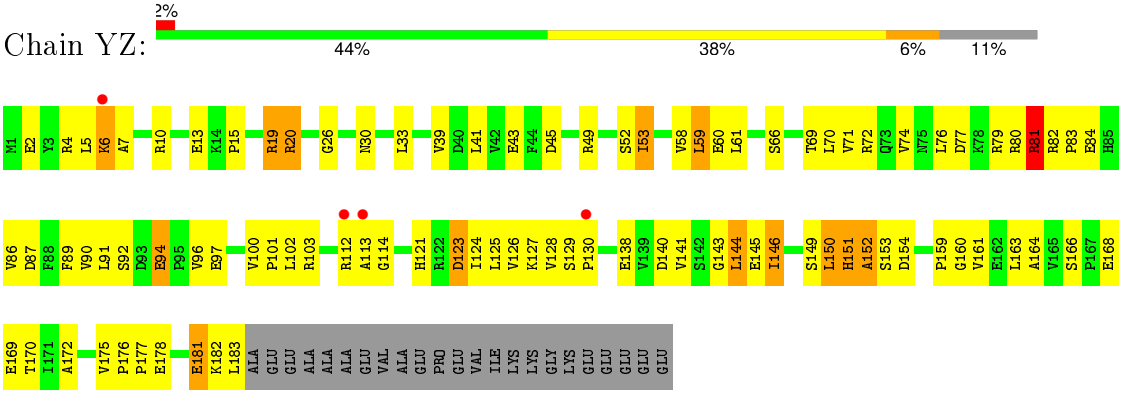
• Molecule 45: 50S ribosomal protein L25

Chain RZ:



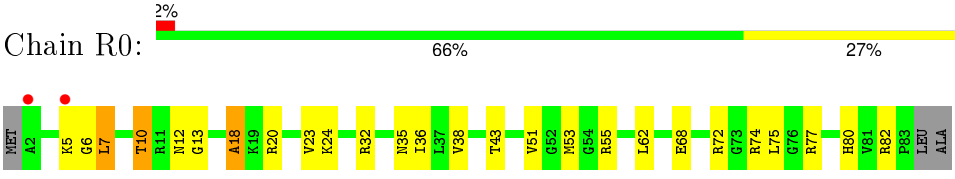
• Molecule 45: 50S ribosomal protein L25

Chain YZ:



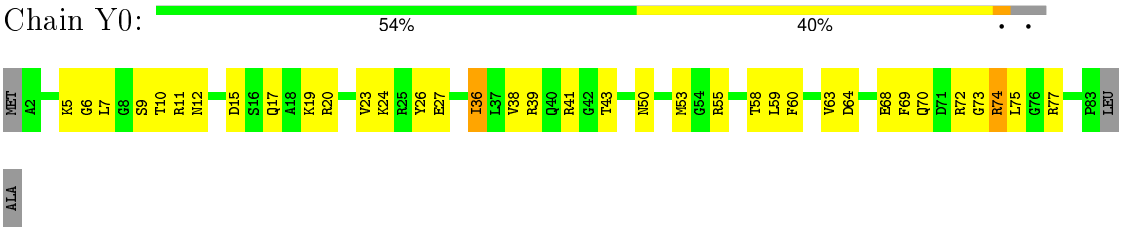
• Molecule 46: 50S ribosomal protein L27

Chain R0:



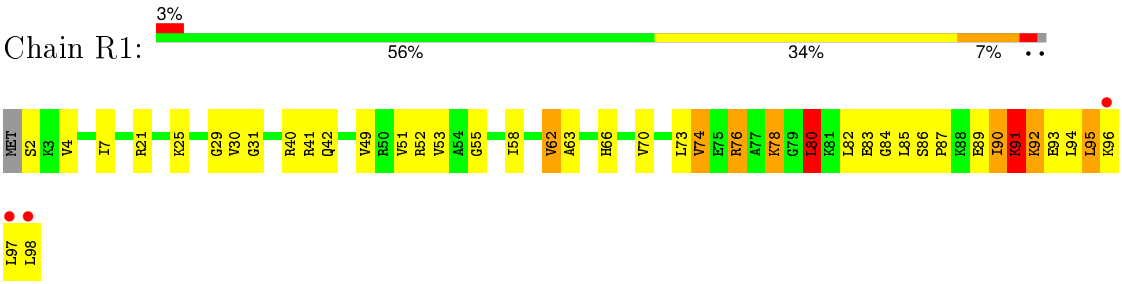
• Molecule 46: 50S ribosomal protein L27

Chain Y0:



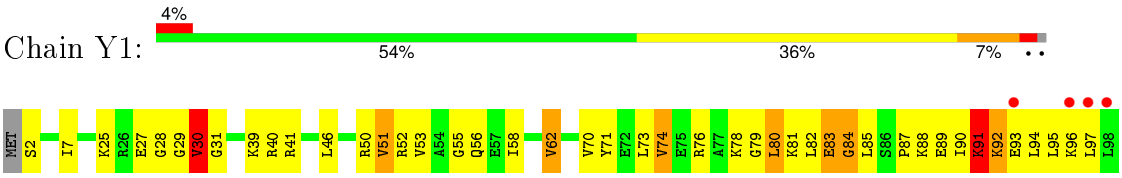
• Molecule 47: 50S ribosomal protein L28

Chain R1:



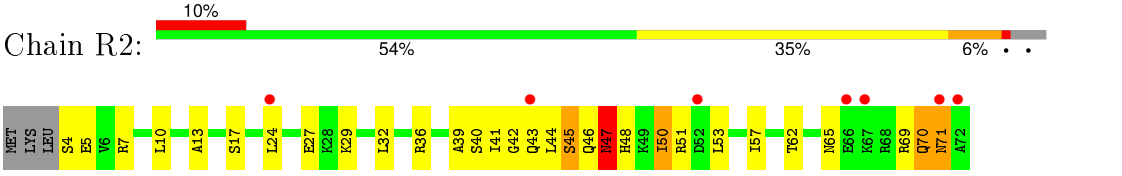
• Molecule 47: 50S ribosomal protein L28

Chain Y1:



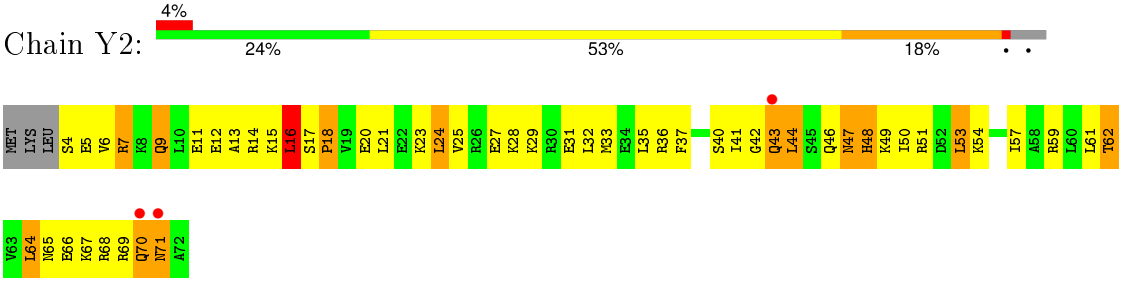
• Molecule 48: 50S ribosomal protein L29

Chain R2:



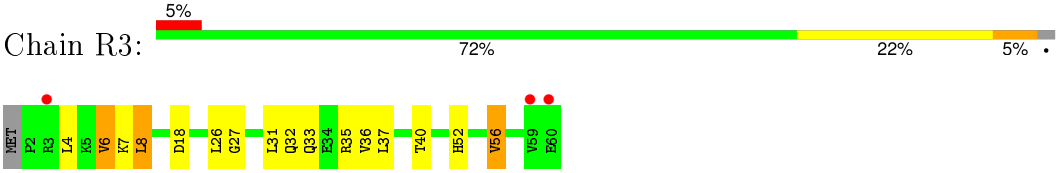
• Molecule 48: 50S ribosomal protein L29

Chain Y2:



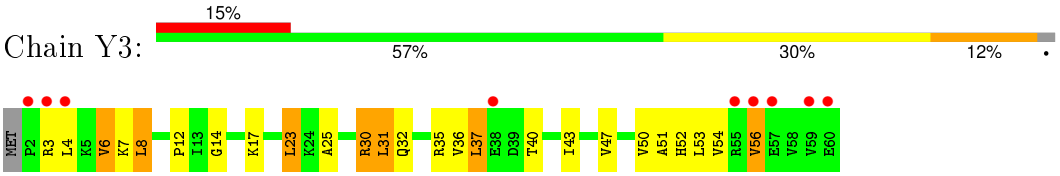
• Molecule 49: 50S ribosomal protein L30

Chain R3:



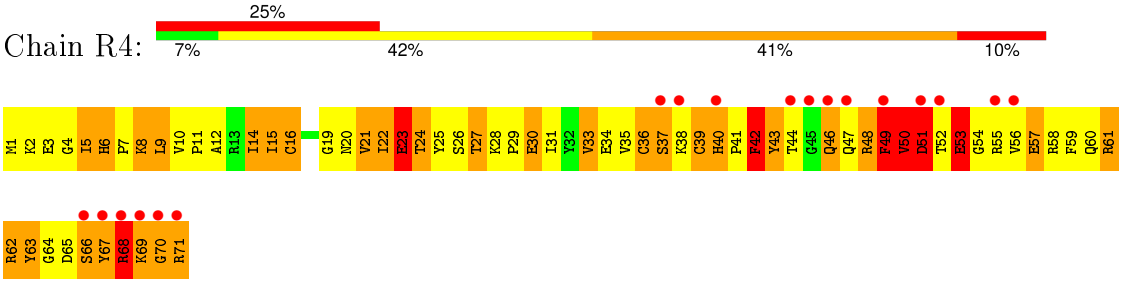
• Molecule 49: 50S ribosomal protein L30

Chain Y3:



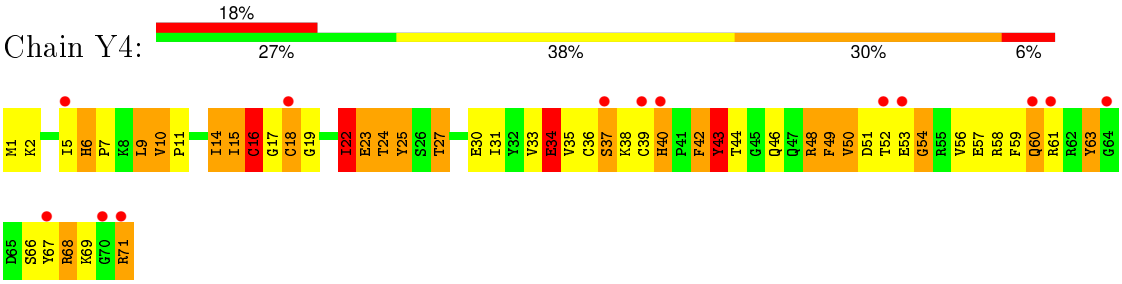
• Molecule 50: 50S ribosomal protein L31

Chain R4:



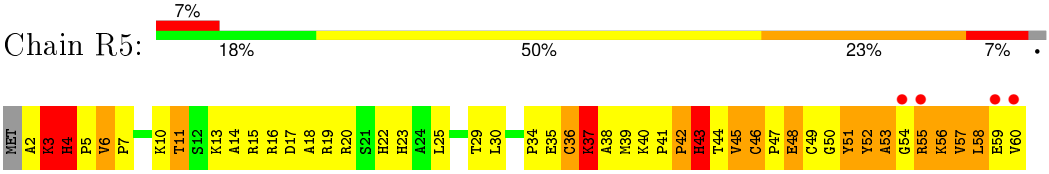
• Molecule 50: 50S ribosomal protein L31

Chain Y4:



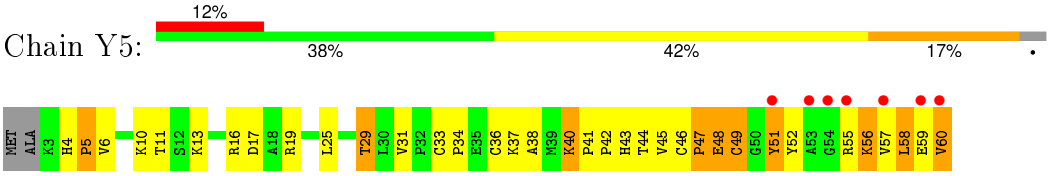
• Molecule 51: 50S ribosomal protein L32

Chain R5:



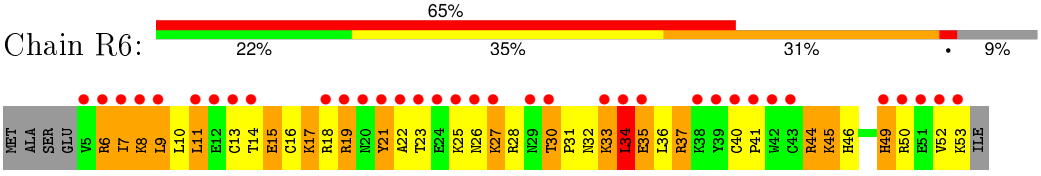
• Molecule 51: 50S ribosomal protein L32

Chain Y5:



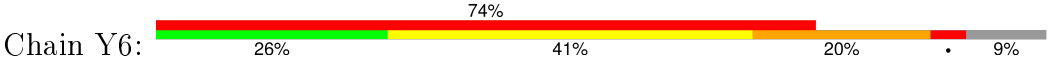
• Molecule 52: 50S ribosomal protein L33

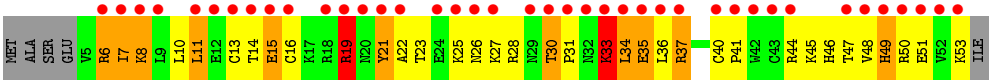
Chain R6:



• Molecule 52: 50S ribosomal protein L33

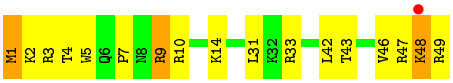
Chain Y6:





• Molecule 53: 50S ribosomal protein L34

Chain R7:

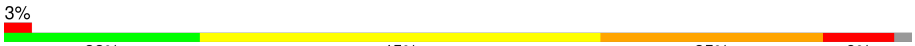


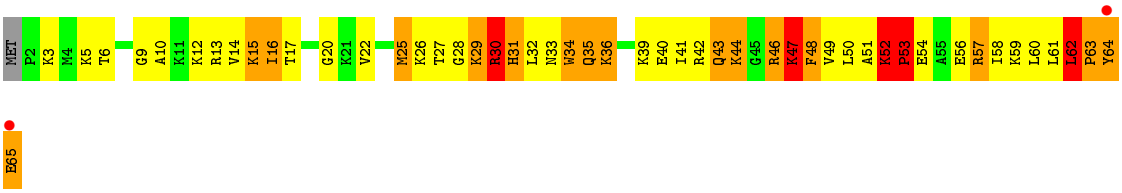
• Molecule 53: 50S ribosomal protein L34

Chain Y7:

• Molecule 54: 50S ribosomal protein L35

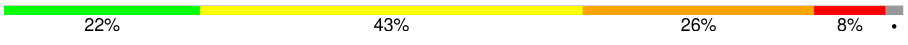
Chain R8:

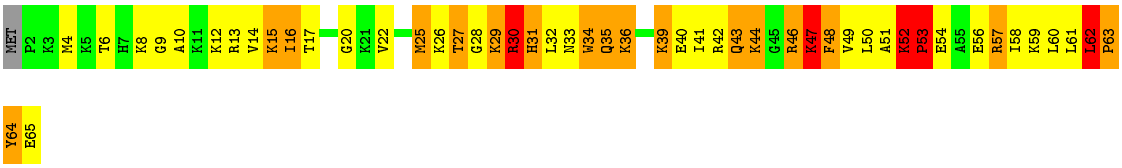




• Molecule 54: 50S ribosomal protein L35

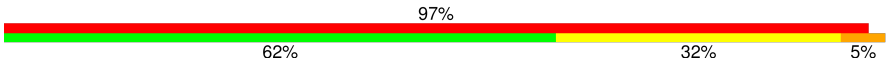
Chain Y8:

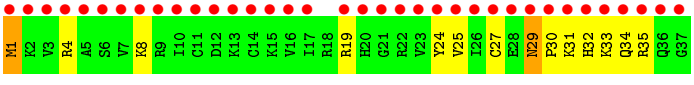




• Molecule 55: 50S ribosomal protein L36

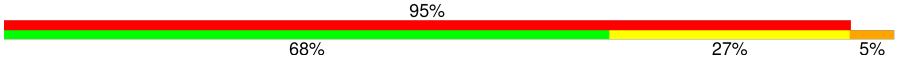
Chain R9:

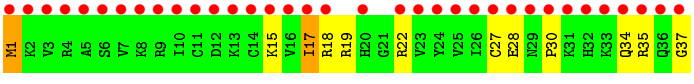




• Molecule 55: 50S ribosomal protein L36

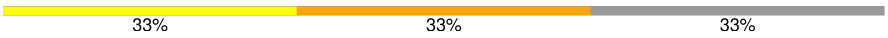
Chain Y9:





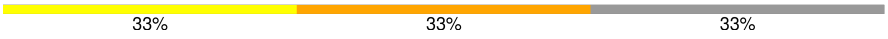
- Molecule 56: CC-Puro

Chain Z5:



- Molecule 56: CC-Puro

Chain Z6:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.40 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.259 0.219 , 0.258	Depositor DCC
R_{free} test set	28875 reflections (4.75%)	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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	2 of 757538 reflections (0.000%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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)

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(^{o})	Ideal(^{o})
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 19
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	2 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	5 44
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	13 57
4	QD	206/209 (99%)	178 (86%)	19 (9%)	9 (4%)	3 32
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	7 49
5	QE	149/162 (92%)	136 (91%)	9 (6%)	4 (3%)	6 46
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	15 60
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%)	15 60
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	15 60
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	26 72
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	6 44
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	4 35
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5 42
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	5 43
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2 27
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11 55
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11 55
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0 9
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0 9
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1 17
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1 17
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1 20
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	1 11
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16 62
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8 50
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	16 62
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	16 62
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9 53
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100 100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	13 57
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0 6
19	XS	82/93 (88%)	54 (66%)	18 (22%)	10 (12%)	0 8
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2 24
20	XT	97/106 (92%)	75 (77%)	17 (18%)	5 (5%)	2 27
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3 33
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3 33
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3 32
27	YD	270/276 (98%)	205 (76%)	46 (17%)	19 (7%)	1 20
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%)	3 29
29	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1 11
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1 16
30	YG	179/182 (98%)	143 (80%)	24 (13%)	12 (7%)	1 21
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 12
32	YI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0 8
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1 14
33	YN	136/140 (97%)	109 (80%)	16 (12%)	11 (8%)	1 15
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11 55
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11 55
35	RP	148/150 (99%)	112 (76%)	25 (17%)	11 (7%)	1 18
35	YP	148/150 (99%)	111 (75%)	22 (15%)	15 (10%)	1 11
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1 11
36	YQ	139/141 (99%)	98 (70%)	25 (18%)	16 (12%)	0 9
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3 33
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2 27
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1 11
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 13
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1 18
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4 40
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	11 55
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2 24
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1 15
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4 39
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	11 54
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8 51
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8 51
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 8
45	RZ	181/206 (88%)	128 (71%)	33 (18%)	20 (11%)	0 9
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1 12
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	15 60
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100 100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1 12
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2 23
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	2 24
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0 6
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4 40
49	Y3	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	11 54
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 39
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%)	9 52
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9 52
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 18

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 (i)

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 21
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6 32
3	QC	159/188 (85%)	145 (91%)	14 (9%)	12 50
3	XC	159/188 (85%)	145 (91%)	14 (9%)	12 50
4	QD	180/181 (99%)	155 (86%)	25 (14%)	4 28
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4 26
5	QE	116/123 (94%)	104 (90%)	12 (10%)	9 42
5	XE	116/123 (94%)	104 (90%)	12 (10%)	9 42
6	QF	90/90 (100%)	78 (87%)	12 (13%)	5 30
6	XF	90/90 (100%)	82 (91%)	8 (9%)	12 50
7	QG	126/127 (99%)	114 (90%)	12 (10%)	11 46
7	XG	126/127 (99%)	114 (90%)	12 (10%)	11 46
8	QH	119/119 (100%)	109 (92%)	10 (8%)	14 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8 39
9	QI	98/99 (99%)	80 (82%)	18 (18%)	2 14
9	XI	98/99 (99%)	79 (81%)	19 (19%)	2 12
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	5 29
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	3 22
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9 43
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9 43
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5 29
12	XL	104/109 (95%)	89 (86%)	15 (14%)	4 26
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1 6
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1 12
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2 14
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4 27
15	QO	79/80 (99%)	72 (91%)	7 (9%)	12 50
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5 31
16	QP	72/74 (97%)	64 (89%)	8 (11%)	8 38
16	XP	72/74 (97%)	64 (89%)	8 (11%)	8 38
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	14 52
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22 64
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2 15
18	XR	61/77 (79%)	52 (85%)	9 (15%)	4 25
19	QS	73/80 (91%)	59 (81%)	14 (19%)	2 12
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1 9
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6 34
20	XT	76/82 (93%)	67 (88%)	9 (12%)	6 34
21	QU	20/22 (91%)	20 (100%)	0	100 100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30 70
27	RD	214/218 (98%)	174 (81%)	40 (19%)	2 13
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2 18
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 13
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5 30
30	RG	155/156 (99%)	134 (86%)	21 (14%)	5 29
30	YG	155/156 (99%)	133 (86%)	22 (14%)	4 27
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1 12
31	YH	142/148 (96%)	115 (81%)	27 (19%)	2 12
32	RI	122/124 (98%)	100 (82%)	22 (18%)	2 15
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1 6
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2 18
33	YN	117/119 (98%)	94 (80%)	23 (20%)	1 12
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9 43
34	YO	100/100 (100%)	88 (88%)	12 (12%)	6 33
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0 5
35	YP	116/116 (100%)	79 (68%)	37 (32%)	0 3
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3 20
36	YQ	111/111 (100%)	91 (82%)	20 (18%)	2 15
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2 16
37	YR	101/101 (100%)	81 (80%)	20 (20%)	1 12
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1 10
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4 25
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3 25
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2 16
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3 24
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2 17
41	RV	82/82 (100%)	66 (80%)	16 (20%)	2 12
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2 14
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1 10
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2 17
43	RX	74/78 (95%)	64 (86%)	10 (14%)	5 29
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2 13
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 6
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	4 25
45	YZ	162/179 (90%)	145 (90%)	17 (10%)	8 41
46	R0	65/67 (97%)	60 (92%)	5 (8%)	16 56
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	11 48
47	R1	82/83 (99%)	73 (89%)	9 (11%)	8 39
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	4 26
48	R2	64/67 (96%)	55 (86%)	9 (14%)	4 28
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8 39
49	R3	51/52 (98%)	45 (88%)	6 (12%)	6 34
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	3 22
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 7
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1 7
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0 4
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1 10
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2 12
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	3 19
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0 4
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0 3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24 66
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24 66
All	All	9702/10066 (96%)	8159 (84%)	1543 (16%)	3 21

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	1.43	8 (17%)	59,67,67	1.37	6 (10%)
58	PAR	XA	1710	-	45,45,45	1.44	7 (15%)	59,67,67	1.28	5 (8%)
60	PPU	Z5	101	56	30,40,41	2.58	6 (20%)	37,57,60	3.24	11 (29%)
60	PPU	Z6	101	56	30,40,41	2.58	6 (20%)	37,57,60	3.24	11 (29%)

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	-5.63	1.31	1.45
60	Z5	101	PPU	C9-N6	-5.62	1.32	1.45
60	Z6	101	PPU	C10-N6	-5.28	1.32	1.45
60	Z5	101	PPU	C10-N6	-5.25	1.32	1.45
60	Z5	101	PPU	C5-N7	-2.04	1.32	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	Z6	101	PPU	C2'-C1'-N9	-10.33	98.51	114.29
60	Z5	101	PPU	C2'-C1'-N9	-10.32	98.52	114.29
60	Z5	101	PPU	N3-C2-N1	-9.77	121.42	128.89
60	Z6	101	PPU	N3-C2-N1	-9.72	121.45	128.89
60	Z5	101	PPU	C3'-N3'-C	-8.22	110.23	123.18

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, 95^{th} 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%)	0.09	16 (1%) 82 70	40, 98, 191, 460	0
1	XA	1500/1522 (98%)	0.09	10 (0%) 89 81	37, 88, 192, 384	0
2	QB	237/256 (92%)	0.71	26 (10%) 7 6	91, 151, 229, 303	0
2	XB	237/256 (92%)	0.40	7 (2%) 54 38	71, 131, 209, 300	0
3	QC	205/239 (85%)	0.34	1 (0%) 91 86	79, 138, 213, 261	0
3	XC	205/239 (85%)	0.01	0 100 100	53, 95, 150, 275	0
4	QD	208/209 (99%)	0.14	1 (0%) 91 86	59, 105, 170, 323	0
4	XD	208/209 (99%)	-0.09	0 100 100	43, 92, 156, 208	0
5	QE	151/162 (93%)	0.14	1 (0%) 89 81	66, 112, 178, 228	0
5	XE	151/162 (93%)	-0.13	0 100 100	44, 86, 140, 204	0
6	QF	101/101 (100%)	-0.12	0 100 100	48, 92, 135, 211	0
6	XF	101/101 (100%)	-0.03	0 100 100	47, 96, 150, 271	0
7	QG	155/156 (99%)	0.60	13 (8%) 14 10	86, 136, 192, 401	0
7	XG	155/156 (99%)	0.37	9 (5%) 26 18	63, 118, 165, 229	0
8	QH	138/138 (100%)	0.18	1 (0%) 89 81	66, 110, 155, 279	0
8	XH	138/138 (100%)	0.02	1 (0%) 89 81	62, 104, 145, 170	0
9	QI	127/128 (99%)	0.86	16 (12%) 5 5	82, 153, 208, 251	0
9	XI	127/128 (99%)	0.27	0 100 100	56, 131, 179, 246	0
10	QJ	99/105 (94%)	0.83	10 (10%) 9 7	101, 158, 246, 398	0
10	XJ	99/105 (94%)	0.63	9 (9%) 11 8	60, 121, 205, 240	0
11	QK	119/129 (92%)	0.91	15 (12%) 5 5	60, 100, 188, 269	0
11	XK	119/129 (92%)	0.53	6 (5%) 32 22	37, 93, 164, 272	0
12	QL	125/132 (94%)	0.33	4 (3%) 51 37	47, 91, 145, 263	0
12	XL	125/132 (94%)	0.19	3 (2%) 62 47	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%)	0.65	12 (9%) 9 7	91, 151, 204, 320	0
13	XM	121/126 (96%)	0.21	3 (2%) 61 46	58, 116, 178, 305	0
14	QN	60/61 (98%)	0.63	1 (1%) 73 59	88, 128, 188, 195	0
14	XN	60/61 (98%)	0.02	0 100 100	49, 90, 129, 159	0
15	QO	88/89 (98%)	0.02	0 100 100	41, 92, 137, 169	0
15	XO	88/89 (98%)	0.12	1 (1%) 82 70	56, 97, 143, 170	0
16	QP	84/88 (95%)	0.35	1 (1%) 81 69	62, 95, 137, 206	0
16	XP	84/88 (95%)	0.59	1 (1%) 81 69	74, 110, 158, 267	0
17	QQ	100/105 (95%)	0.29	0 100 100	57, 99, 132, 165	0
17	XQ	100/105 (95%)	0.27	0 100 100	68, 112, 143, 168	0
18	QR	70/88 (79%)	0.21	4 (5%) 27 19	64, 101, 147, 191	0
18	XR	70/88 (79%)	0.22	1 (1%) 78 65	62, 104, 164, 181	0
19	QS	84/93 (90%)	0.72	5 (5%) 25 17	100, 157, 204, 241	0
19	XS	84/93 (90%)	0.58	2 (2%) 62 47	66, 121, 190, 335	0
20	QT	99/106 (93%)	0.41	2 (2%) 68 54	55, 101, 164, 255	0
20	XT	99/106 (93%)	0.75	7 (7%) 19 12	80, 141, 215, 265	0
21	QU	25/27 (92%)	0.70	2 (8%) 15 10	95, 140, 198, 248	0
21	XU	25/27 (92%)	0.30	1 (4%) 42 29	76, 110, 159, 180	0
22	QV	77/77 (100%)	0.17	1 (1%) 79 66	38, 106, 168, 231	0
22	XV	77/77 (100%)	0.24	1 (1%) 79 66	42, 84, 137, 180	0
23	QX	9/25 (36%)	0.45	0 100 100	63, 86, 158, 171	0
23	XX	10/25 (40%)	0.53	1 (10%) 9 7	47, 69, 148, 219	0
24	QY	16/17 (94%)	0.44	1 (6%) 23 15	87, 115, 167, 175	0
24	XY	16/17 (94%)	0.22	0 100 100	68, 95, 153, 191	0
25	RA	2882/2915 (98%)	0.15	116 (4%) 42 29	27, 74, 249, 510	0
25	YA	2882/2915 (98%)	0.17	105 (3%) 46 33	27, 69, 246, 557	0
26	RB	120/122 (98%)	0.08	1 (0%) 87 78	90, 127, 170, 210	0
26	YB	120/122 (98%)	-0.12	0 100 100	61, 90, 124, 152	0
27	RD	272/276 (98%)	-0.11	1 (0%) 93 88	22, 61, 105, 222	0
27	YD	272/276 (98%)	-0.04	1 (0%) 93 88	22, 61, 105, 185	0
28	RE	205/206 (99%)	0.27	5 (2%) 62 47	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%)	0.14	3 (1%) 76 64	31, 91, 177, 273	0
29	RF	202/210 (96%)	0.30	4 (1%) 68 54	23, 99, 171, 216	0
29	YF	202/210 (96%)	0.11	4 (1%) 68 54	32, 78, 149, 227	0
30	RG	181/182 (99%)	0.69	11 (6%) 25 16	92, 150, 197, 231	0
30	YG	181/182 (99%)	0.25	4 (2%) 65 50	61, 98, 160, 244	0
31	RH	170/180 (94%)	1.44	43 (25%) 1 1	102, 193, 270, 361	0
31	YH	170/180 (94%)	0.45	5 (2%) 55 40	53, 105, 164, 210	0
32	RI	146/148 (98%)	0.55	10 (6%) 20 13	67, 125, 195, 258	0
32	YI	146/148 (98%)	0.52	8 (5%) 29 20	48, 123, 189, 271	0
33	RN	138/140 (98%)	0.22	3 (2%) 65 50	51, 93, 154, 202	0
33	YN	138/140 (98%)	0.28	3 (2%) 65 50	47, 92, 157, 220	0
34	RO	122/122 (100%)	0.18	1 (0%) 87 78	48, 80, 114, 148	0
34	YO	122/122 (100%)	0.08	0 100 100	27, 64, 103, 120	0
35	RP	150/150 (100%)	0.52	6 (4%) 42 29	28, 99, 159, 288	0
35	YP	150/150 (100%)	0.22	4 (2%) 58 43	31, 90, 162, 231	0
36	RQ	141/141 (100%)	0.63	8 (5%) 27 19	54, 102, 180, 226	0
36	YQ	141/141 (100%)	0.20	4 (2%) 56 42	35, 73, 140, 222	0
37	RR	118/118 (100%)	-0.11	0 100 100	29, 70, 104, 138	0
37	YR	118/118 (100%)	0.13	1 (0%) 87 78	51, 91, 139, 190	0
38	RS	111/112 (99%)	0.52	4 (3%) 46 33	81, 120, 204, 273	0
38	YS	111/112 (99%)	0.15	2 (1%) 71 58	67, 101, 156, 201	0
39	RT	137/146 (93%)	0.10	2 (1%) 76 64	50, 91, 188, 276	0
39	YT	137/146 (93%)	0.05	0 100 100	51, 89, 212, 242	0
40	RU	117/118 (99%)	0.26	5 (4%) 39 27	35, 81, 155, 298	0
40	YU	117/118 (99%)	-0.01	1 (0%) 85 75	40, 81, 152, 243	0
41	RV	101/101 (100%)	0.75	7 (6%) 20 13	55, 114, 183, 398	0
41	YV	101/101 (100%)	0.41	4 (3%) 42 29	44, 111, 174, 335	0
42	RW	113/113 (100%)	0.13	3 (2%) 58 43	36, 63, 115, 296	0
42	YW	113/113 (100%)	0.16	5 (4%) 38 27	37, 74, 134, 258	0
43	RX	92/96 (95%)	0.36	1 (1%) 82 70	51, 77, 128, 164	0
43	YX	92/96 (95%)	0.35	3 (3%) 50 36	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%)	0.95	15 (14%) 3 3	55, 119, 185, 325	0
44	YY	102/110 (92%)	0.22	4 (3%) 43 31	42, 92, 162, 273	0
45	RZ	183/206 (88%)	0.91	21 (11%) 6 6	104, 153, 230, 292	0
45	YZ	183/206 (88%)	0.51	4 (2%) 65 50	55, 116, 202, 300	0
46	R0	82/85 (96%)	0.46	2 (2%) 62 47	48, 88, 127, 238	0
46	Y0	82/85 (96%)	0.13	0 100 100	44, 71, 99, 142	0
47	R1	97/98 (98%)	0.45	3 (3%) 52 38	37, 80, 161, 290	0
47	Y1	97/98 (98%)	0.40	4 (4%) 41 29	39, 75, 176, 210	0
48	R2	69/72 (95%)	0.69	7 (10%) 9 7	63, 105, 160, 274	0
48	Y2	69/72 (95%)	0.19	3 (4%) 39 27	47, 80, 151, 219	0
49	R3	59/60 (98%)	0.62	3 (5%) 32 22	63, 97, 155, 205	0
49	Y3	59/60 (98%)	0.75	9 (15%) 3 2	55, 89, 162, 293	0
50	R4	71/71 (100%)	1.66	18 (25%) 1 1	150, 244, 350, 423	0
50	Y4	71/71 (100%)	0.87	13 (18%) 2 1	69, 162, 340, 411	0
51	R5	59/60 (98%)	0.27	4 (6%) 20 13	40, 77, 216, 261	0
51	Y5	58/60 (96%)	0.49	7 (12%) 6 5	44, 97, 231, 342	0
52	R6	49/54 (90%)	3.46	35 (71%) 0 0	119, 194, 264, 286	0
52	Y6	49/54 (90%)	3.18	40 (81%) 0 0	115, 171, 260, 295	0
53	R7	49/49 (100%)	-0.18	1 (2%) 68 54	27, 54, 110, 166	0
53	Y7	49/49 (100%)	-0.21	1 (2%) 68 54	32, 51, 111, 180	0
54	R8	64/65 (98%)	0.26	2 (3%) 52 38	42, 82, 134, 223	0
54	Y8	64/65 (98%)	0.00	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%)	5.49	35 (94%) 0 0	134, 206, 322, 404	0
56	Z5	2/3 (66%)	0.21	0 100 100	50, 50, 50, 60	0
56	Z6	2/3 (66%)	0.08	0 100 100	38, 38, 38, 41	0
All	All	20878/21490 (97%)	0.28	851 (4%) 41 29	22, 92, 205, 557	0

The worst 5 of 851 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	R9	14	CYS	18.4
25	YA	2165	G	14.0

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Mol	Chain	Res	Type	RSRZ
25	YA	2179	C	12.9
55	Y9	34	GLN	12.6
35	RP	149	GLU	11.1

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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.