



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:59 PM GMT

PDB ID : 4LFZ
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-27
Resolution : 3.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

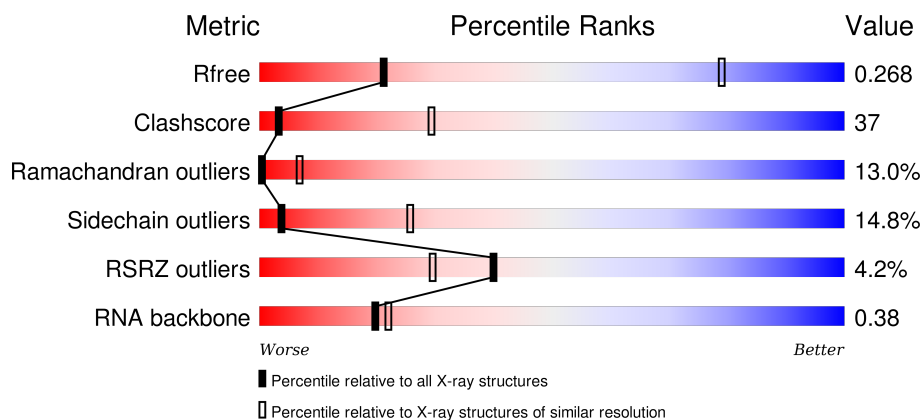
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)
RNA backbone	2183	1079 (5.04-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	25	
23	XX	25	
24	QY	18	
24	XY	18	
25	RA	2916	
25	YA	2916	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	

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

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

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	
56	Z6	3	
56	Z8	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1610	-	-	-	X
57	MG	QA	1611	-	-	-	X
57	MG	QA	1613	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1620	-	-	-	X
57	MG	QA	1622	-	-	-	X
57	MG	QA	1631	-	-	-	X
57	MG	QA	1635	-	-	-	X
57	MG	QA	1646	-	-	-	X
57	MG	QA	1649	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3005	-	-	-	X
57	MG	RA	3008	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3012	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3017	-	-	-	X
57	MG	RA	3019	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3021	-	-	-	X
57	MG	RA	3022	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3024	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3038	-	-	-	X
57	MG	RA	3040	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3055	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3058	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3072	-	-	-	X
57	MG	RA	3075	-	-	-	X
57	MG	RA	3077	-	-	-	X
57	MG	RA	3079	-	-	-	X
57	MG	RA	3081	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3088	-	-	-	X
57	MG	RA	3089	-	-	-	X
57	MG	RA	3093	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3102	-	-	-	X
57	MG	RA	3105	-	-	-	X
57	MG	RA	3106	-	-	-	X
57	MG	RA	3116	-	-	-	X
57	MG	RA	3120	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3122	-	-	-	X
57	MG	RA	3125	-	-	-	X
57	MG	RA	3128	-	-	-	X
57	MG	RA	3130	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3131	-	-	-	X
57	MG	RA	3136	-	-	-	X
57	MG	RA	3140	-	-	-	X
57	MG	RA	3150	-	-	-	X
57	MG	RA	3153	-	-	-	X
57	MG	RA	3158	-	-	-	X
57	MG	RA	3159	-	-	-	X
57	MG	RA	3160	-	-	-	X
57	MG	RA	3164	-	-	-	X
57	MG	RA	3170	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3183	-	-	-	X
57	MG	RA	3184	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3191	-	-	-	X
57	MG	RA	3198	-	-	-	X
57	MG	RA	3204	-	-	-	X
57	MG	RA	3206	-	-	-	X
57	MG	RA	3207	-	-	-	X
57	MG	RA	3208	-	-	-	X
57	MG	RA	3212	-	-	-	X
57	MG	RA	3218	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3222	-	-	-	X
57	MG	RA	3223	-	-	-	X
57	MG	RA	3238	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	XA	1604	-	-	-	X
57	MG	XA	1607	-	-	-	X
57	MG	XA	1615	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1619	-	-	-	X
57	MG	XA	1621	-	-	-	X
57	MG	XA	1628	-	-	-	X
57	MG	XA	1629	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1636	-	-	-	X
57	MG	XA	1637	-	-	-	X
57	MG	XA	1638	-	-	-	X
57	MG	XA	1646	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1651	-	-	-	X
57	MG	XA	1653	-	-	-	X
57	MG	XA	1656	-	-	-	X
57	MG	XA	1664	-	-	-	X
57	MG	XA	1665	-	-	-	X
57	MG	XA	1668	-	-	-	X
57	MG	XV	101	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3004	-	-	-	X
57	MG	YA	3005	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3011	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3024	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3028	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3042	-	-	-	X
57	MG	YA	3044	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3057	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3069	-	-	-	X
57	MG	YA	3070	-	-	-	X
57	MG	YA	3072	-	-	-	X
57	MG	YA	3074	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3078	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3087	-	-	-	X
57	MG	YA	3090	-	-	-	X
57	MG	YA	3091	-	-	-	X
57	MG	YA	3095	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3101	-	-	-	X
57	MG	YA	3107	-	-	-	X
57	MG	YA	3108	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3115	-	-	-	X
57	MG	YA	3116	-	-	-	X
57	MG	YA	3118	-	-	-	X
57	MG	YA	3120	-	-	-	X
57	MG	YA	3126	-	-	-	X
57	MG	YA	3139	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3145	-	-	-	X
57	MG	YA	3155	-	-	-	X
57	MG	YA	3160	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3167	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3171	-	-	-	X
57	MG	YA	3172	-	-	-	X
57	MG	YA	3176	-	-	-	X
57	MG	YA	3179	-	-	-	X
57	MG	YA	3186	-	-	-	X
57	MG	YA	3201	-	-	-	X
57	MG	YA	3206	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3209	-	-	-	X
57	MG	YA	3210	-	-	-	X
57	MG	YA	3212	-	-	-	X
57	MG	YA	3218	-	-	-	X
57	MG	YA	3220	-	-	-	X
57	MG	YA	3229	-	-	-	X
57	MG	YA	3235	-	-	-	X
57	MG	YA	3236	-	-	-	X
57	MG	YA	3245	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3246	-	-	-	X
57	MG	YA	3256	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3262	-	-	-	X
57	MG	YA	3263	-	-	-	X
57	MG	YA	3265	-	-	-	X
57	MG	YA	3266	-	-	-	X
58	ZN	R9	101	-	-	-	X
58	ZN	XD	301	-	-	-	X
58	ZN	Y9	101	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291868 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.

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 S21.

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 fMet.

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 A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
23	XX	7	Total	C	N	O	P	0	0	0
			145	65	23	50	7			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			
24	XY	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

- 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	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
46	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	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	59	Total	C	N	O	S	0	0	0
			459	288	90	76	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 tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	64	Total	Mg	0	0
			64	64		
57	RP	1	Total	Mg	0	0
			1	1		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	269	Total	Mg	0	0
			269	269		
57	QM	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	XB	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	239	Total 239	Mg 239	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	YB	3	Total 3	Mg 3	0	0
57	XV	2	Total 2	Mg 2	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0

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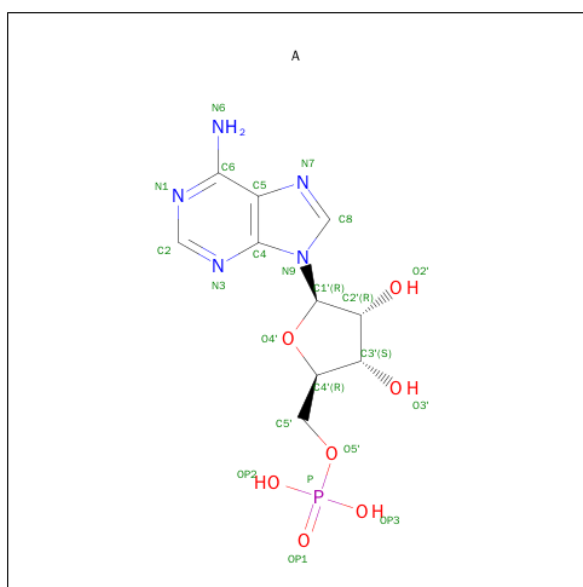
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XM	1	Total	Mg	0	0
			1	1		
57	YE	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y9	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	QD	1	Total	Zn	0	0
			1	1		
58	XD	1	Total	Zn	0	0
			1	1		
58	R9	1	Total	Zn	0	0
			1	1		

- Molecule 59 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C₁₀H₁₄N₅O₇P).

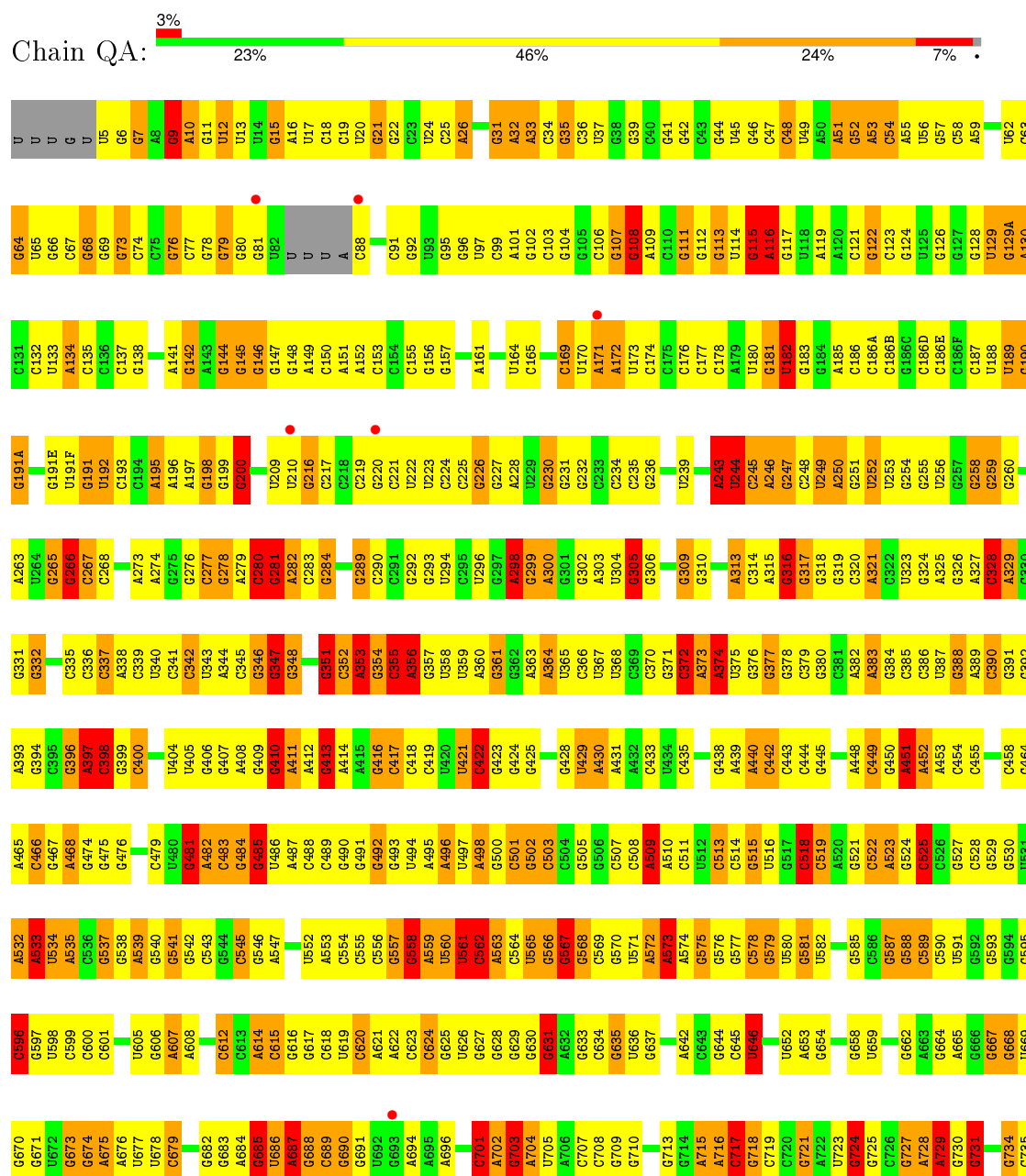


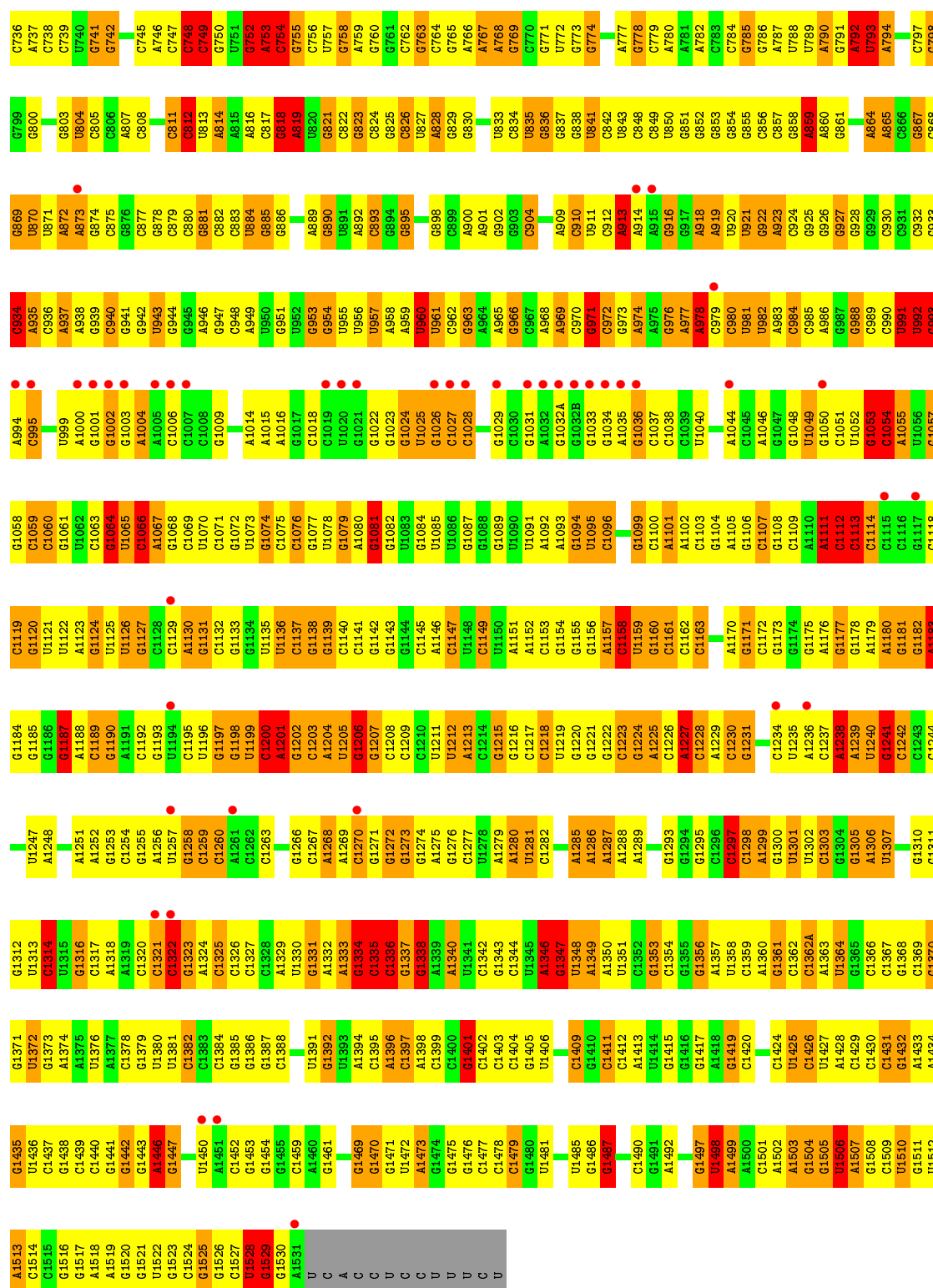
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	XX	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

3 Residue-property plots

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

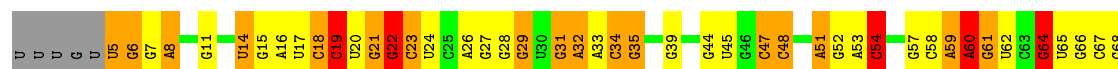
• Molecule 1: 16S rRNA



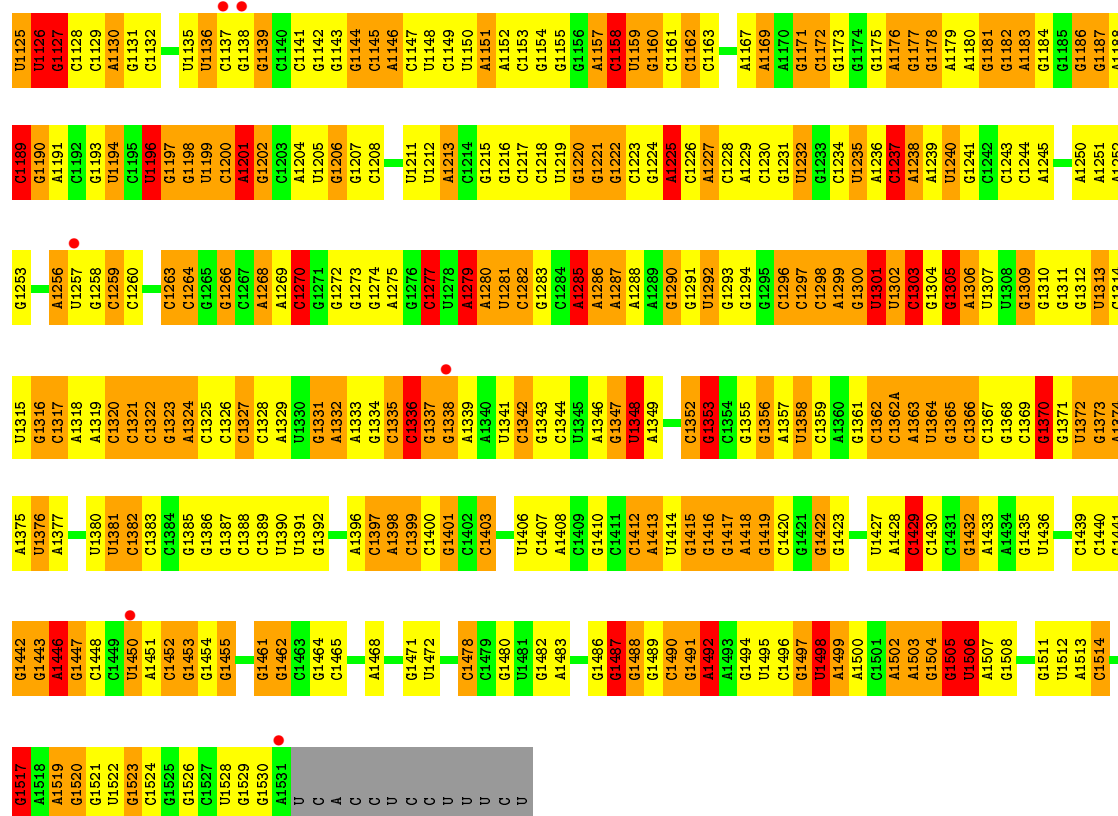


• Molecule 1: 16S rRNA

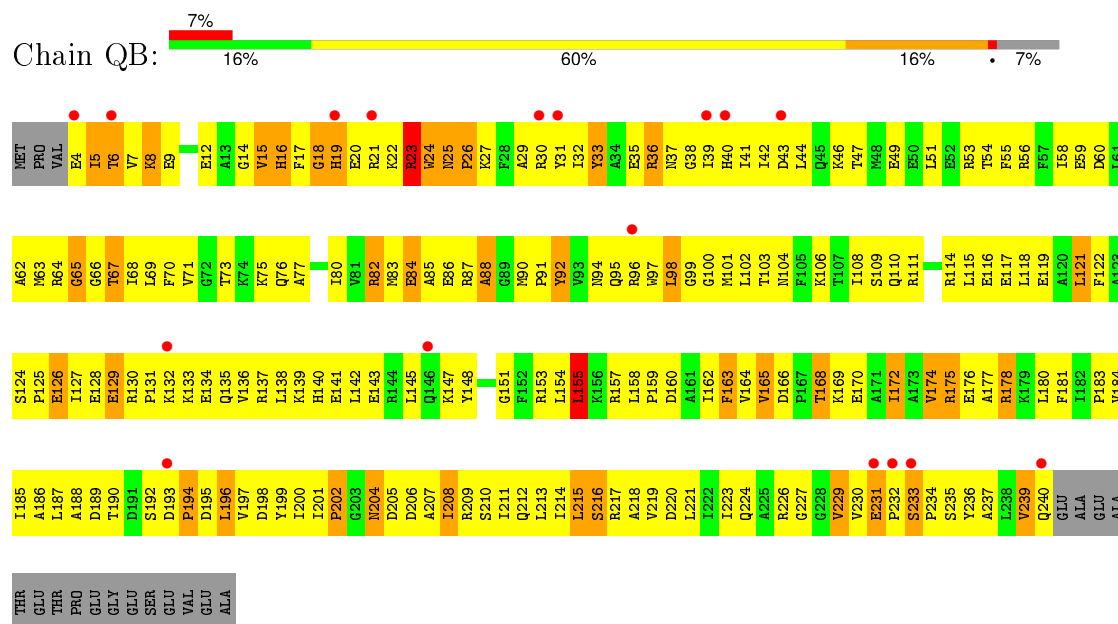
Chain XA: 3% 24% 41% 27% 7%



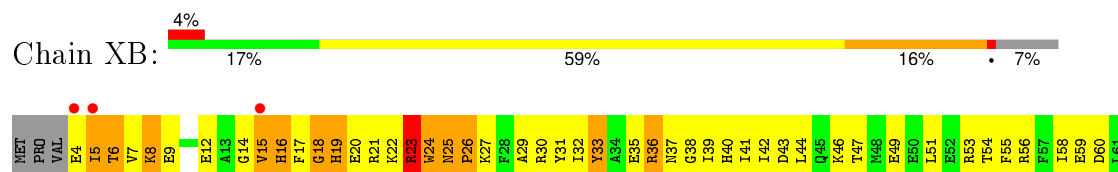


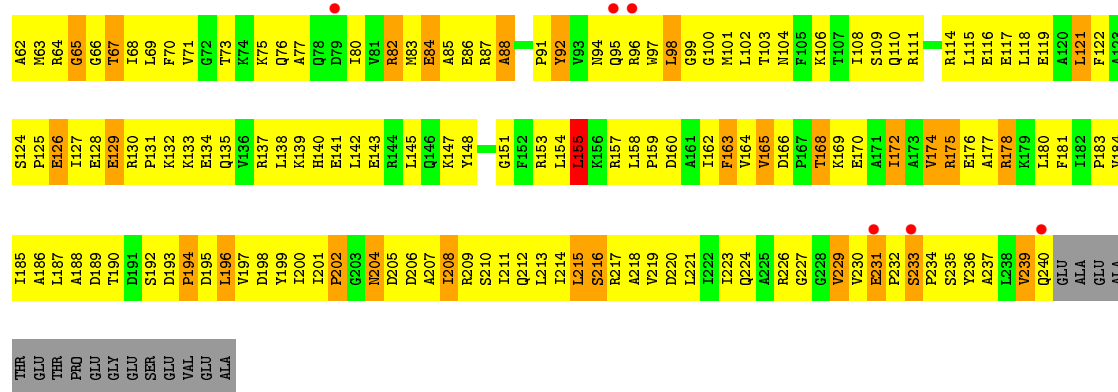


• Molecule 2: 30S ribosomal protein S2

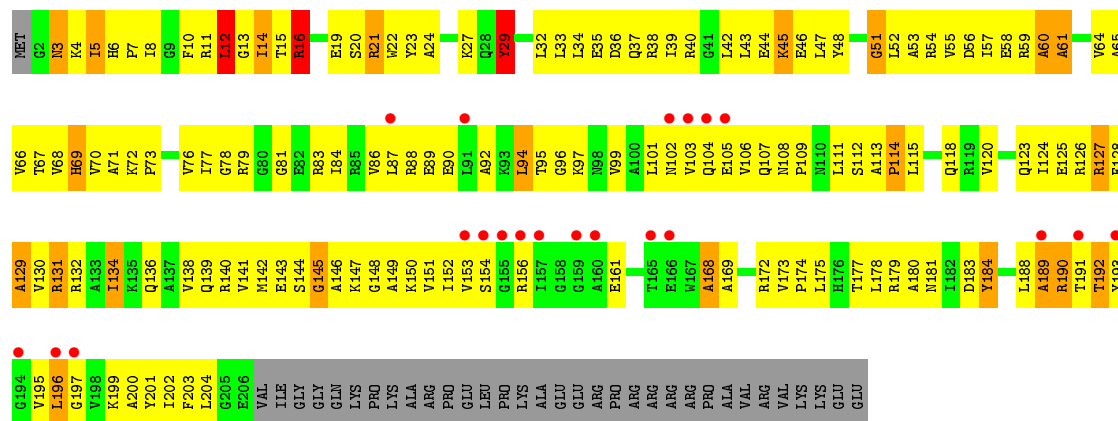


• Molecule 2: 30S ribosomal protein S2

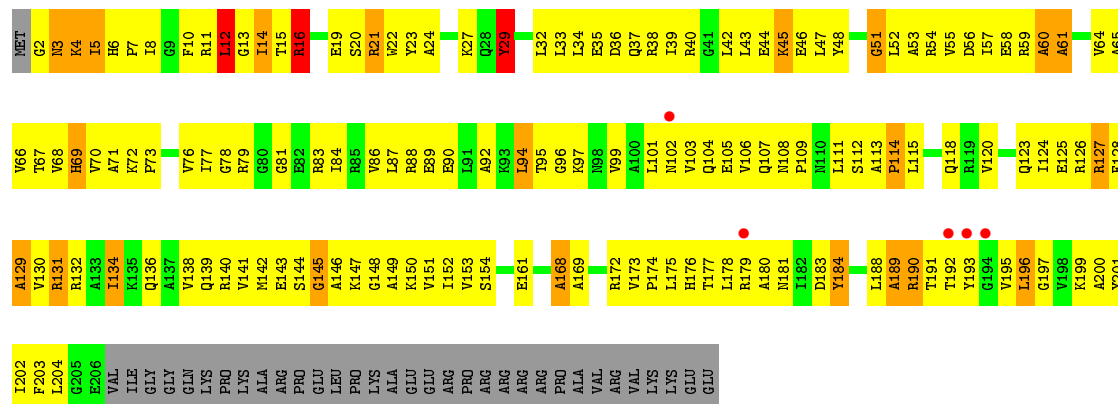




• Molecule 3: 30S ribosomal protein S3

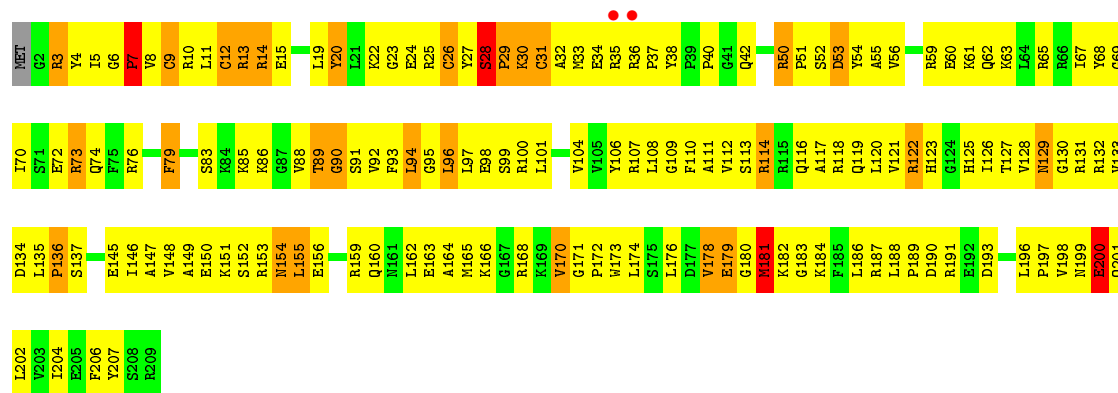


• Molecule 3: 30S ribosomal protein S3

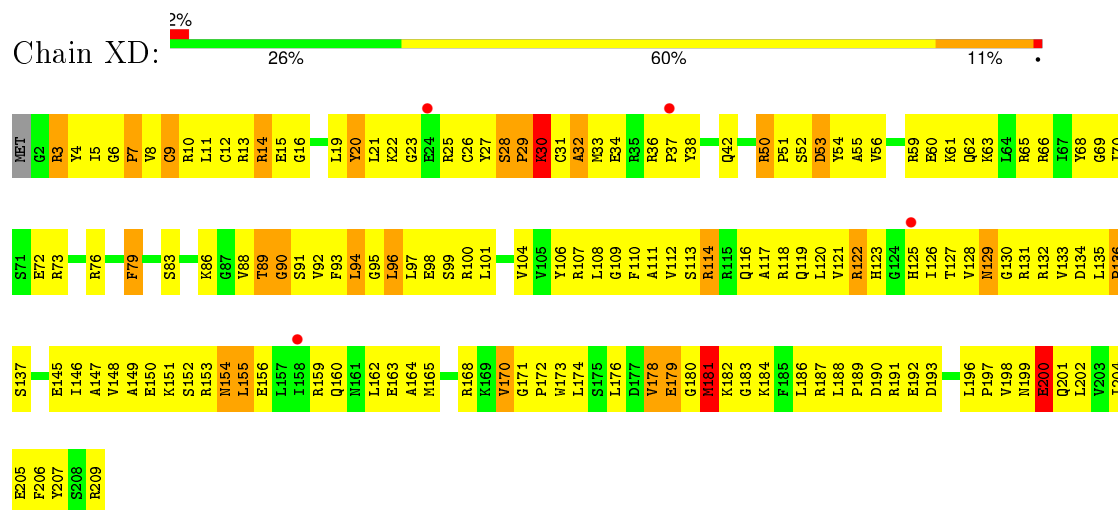


• Molecule 4: 30S ribosomal protein S4

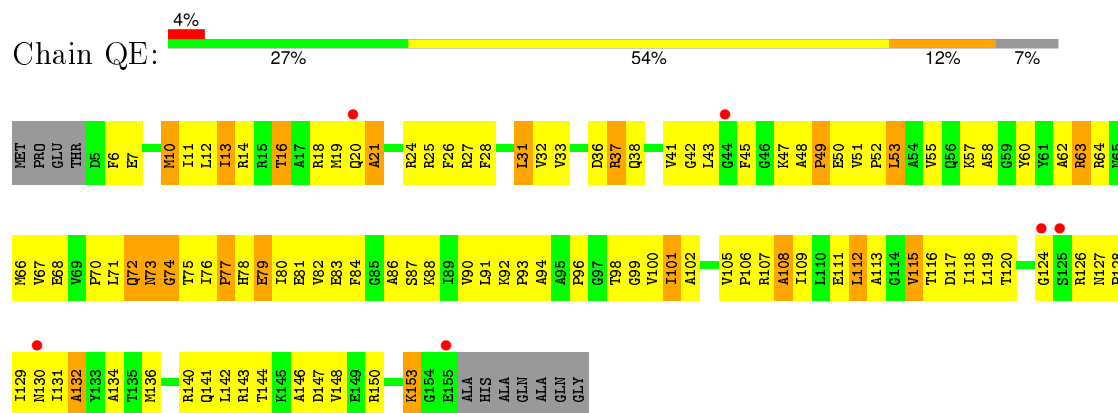




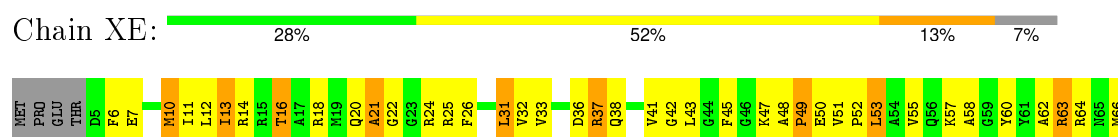
• Molecule 4: 30S ribosomal protein S4

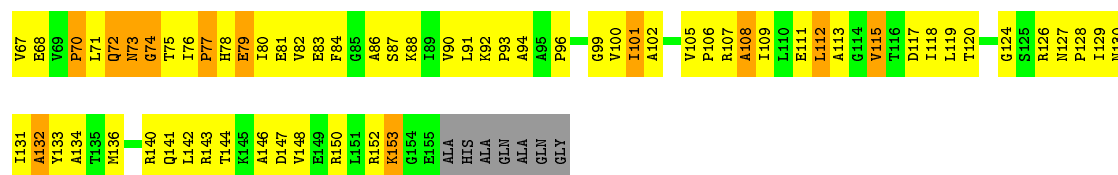


• Molecule 5: 30S ribosomal protein S5

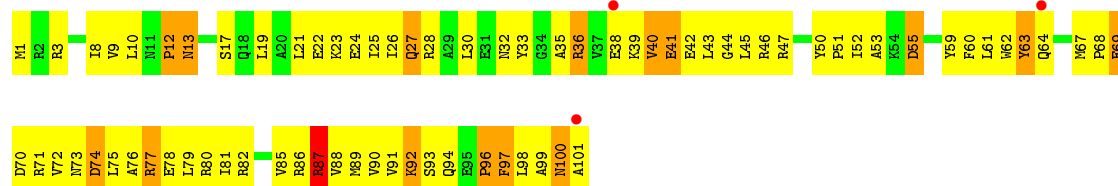


• Molecule 5: 30S ribosomal protein S5

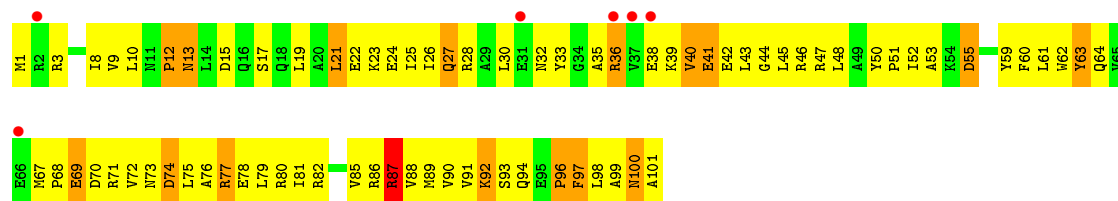




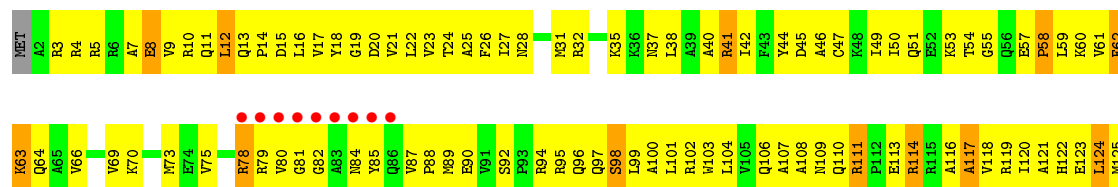
• Molecule 6: 30S ribosomal protein S6



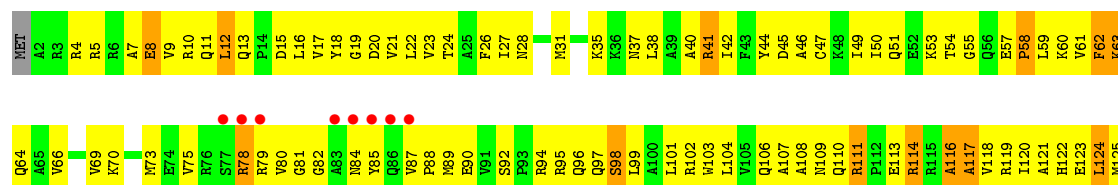
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

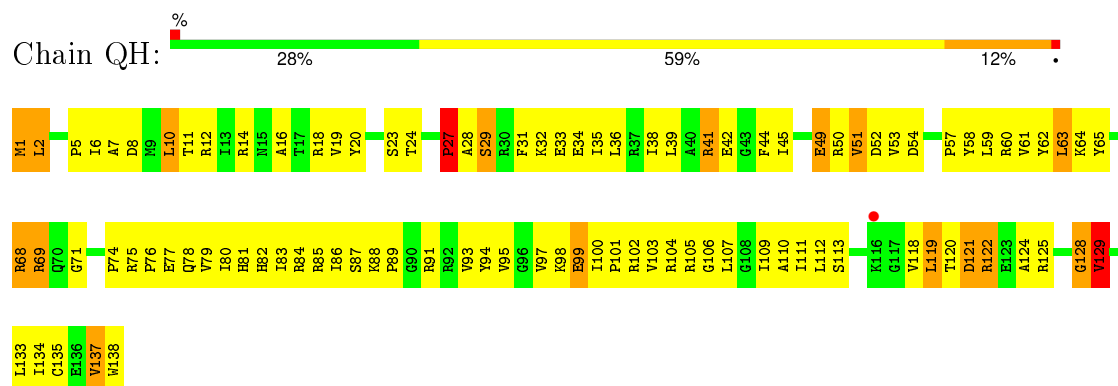


• Molecule 7: 30S ribosomal protein S7

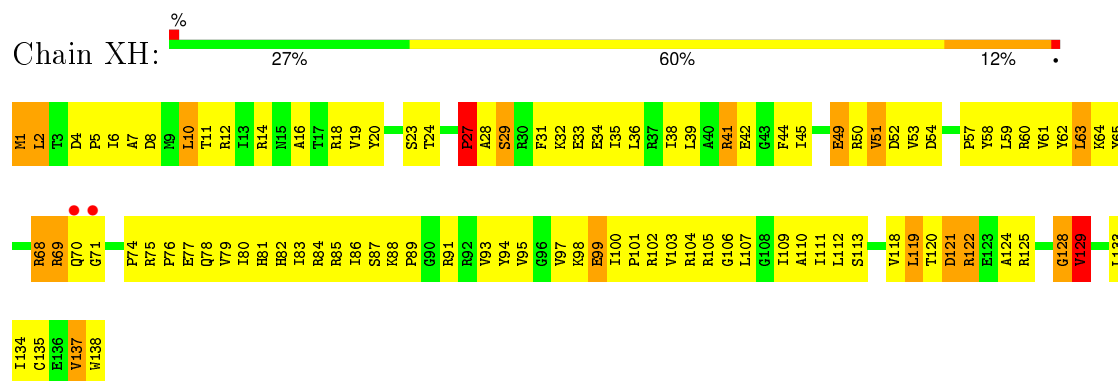




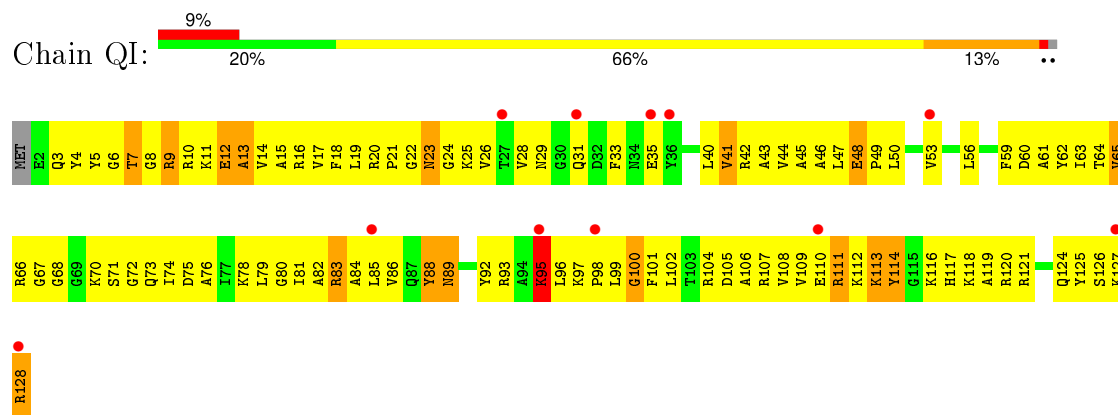
- Molecule 8: 30S ribosomal protein S8



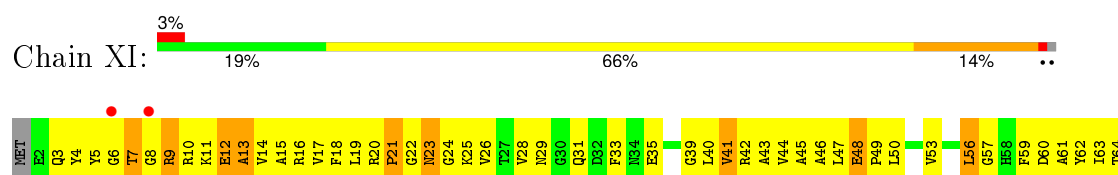
- Molecule 8: 30S ribosomal protein S8

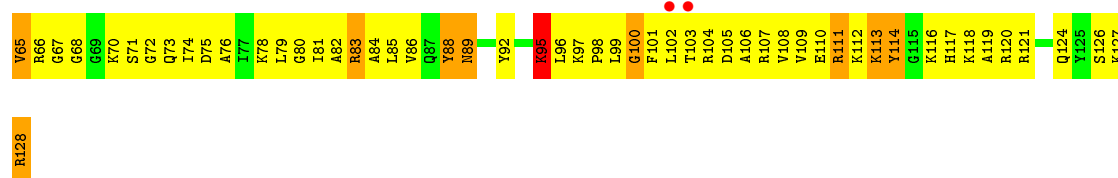


- Molecule 9: 30S ribosomal protein S9

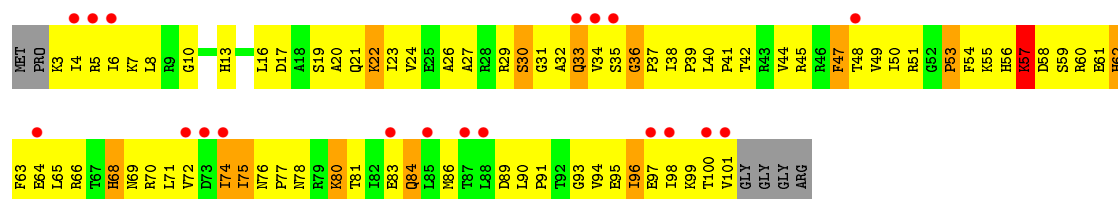


- Molecule 9: 30S ribosomal protein S9

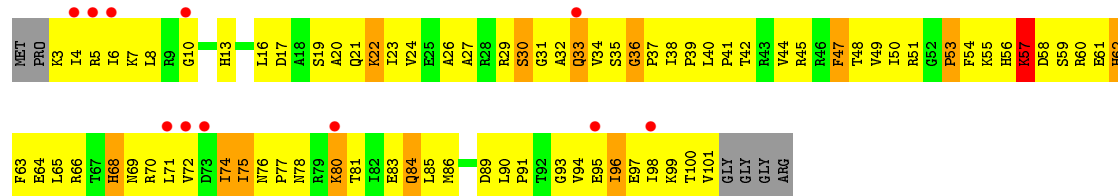




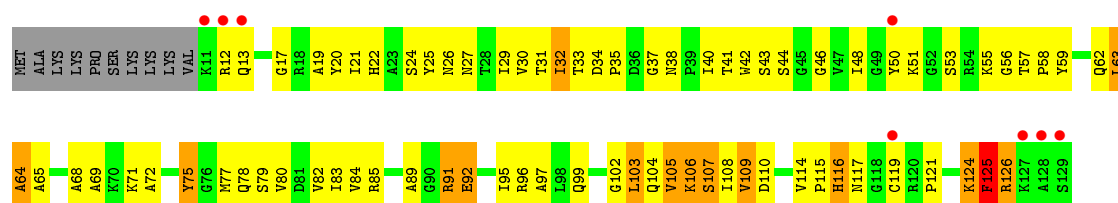
- Molecule 10: 30S ribosomal protein S10



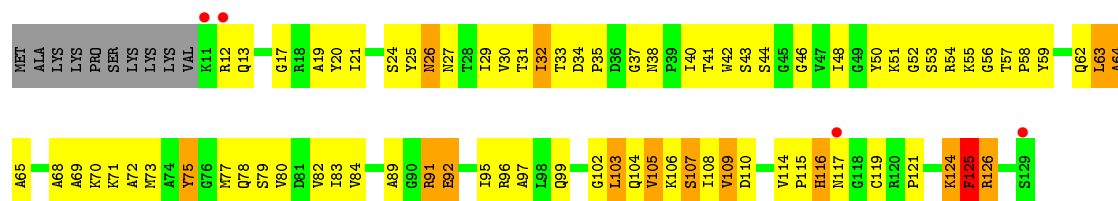
- Molecule 10: 30S ribosomal protein S10



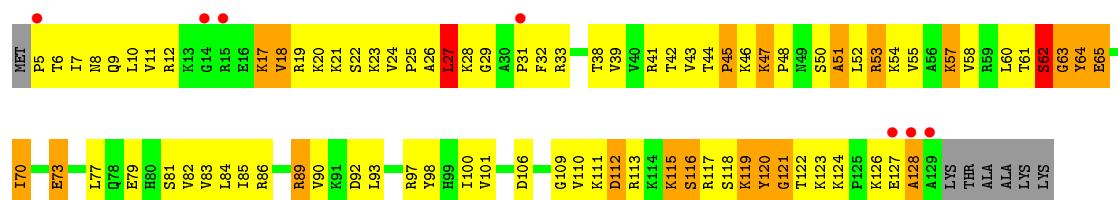
- Molecule 11: 30S ribosomal protein S11



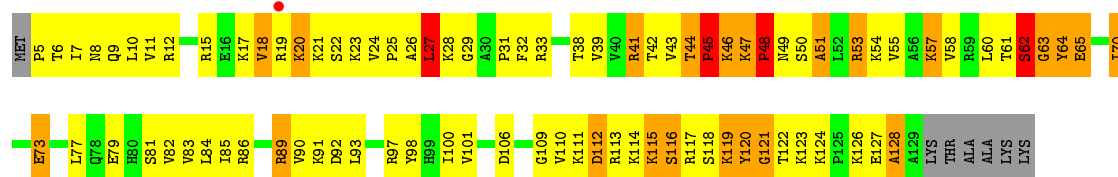
- Molecule 11: 30S ribosomal protein S11



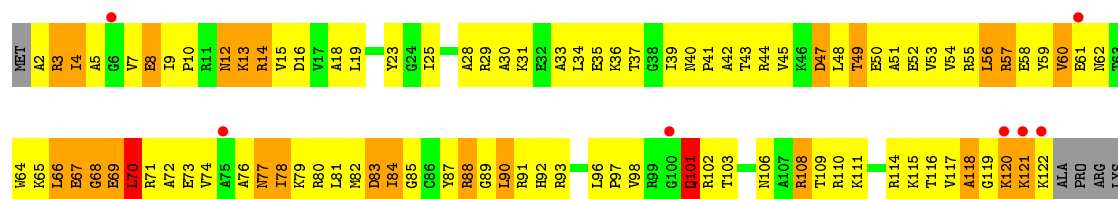
- Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12



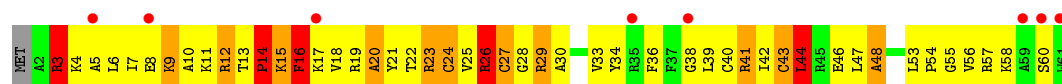
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

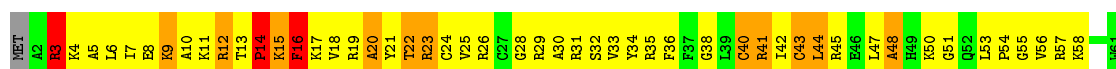


• Molecule 14: 30S ribosomal protein S14

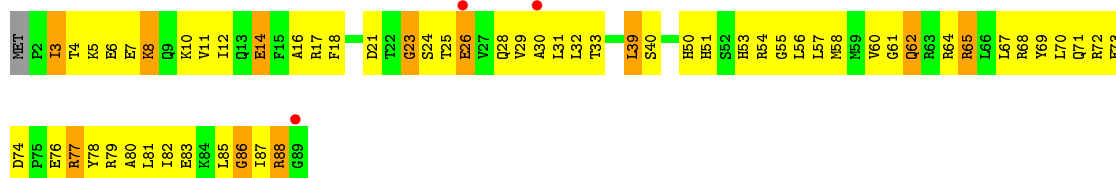


• Molecule 14: 30S ribosomal protein S14

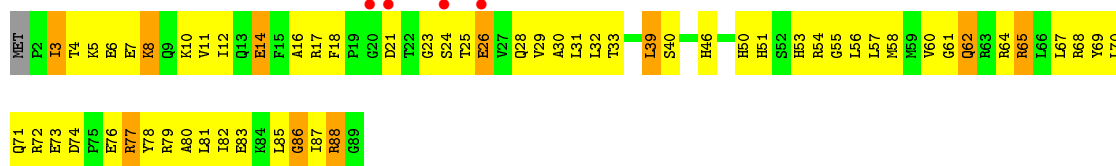




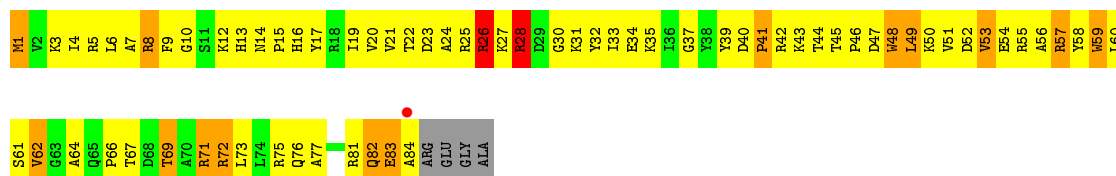
- Molecule 15: 30S ribosomal protein S15



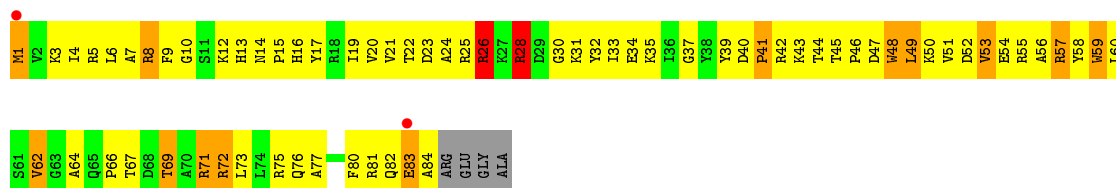
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

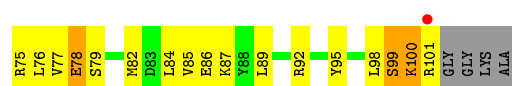


- Molecule 16: 30S ribosomal protein S16

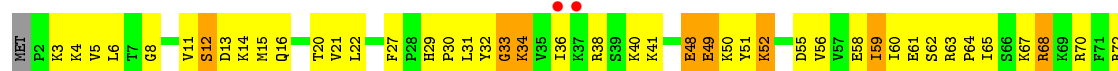


- Molecule 17: 30S ribosomal protein S17





- Molecule 17: 30S ribosomal protein S17



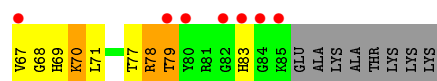
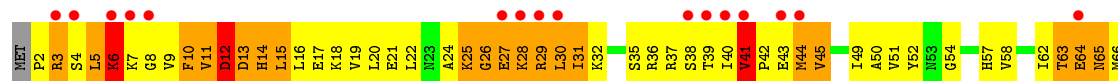
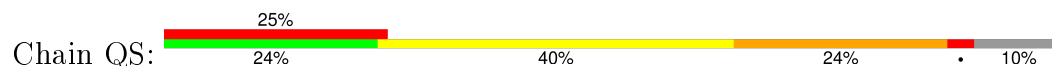
- Molecule 18: 30S ribosomal protein S18



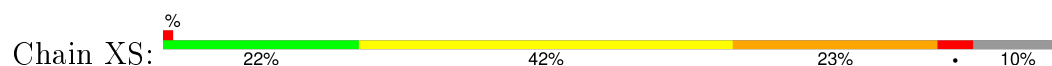
- Molecule 18: 30S ribosomal protein S18

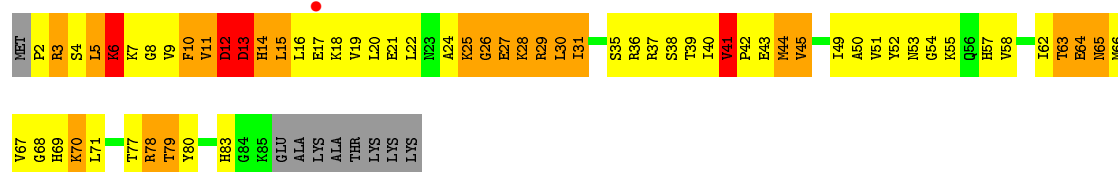


- Molecule 19: 30S ribosomal protein S19

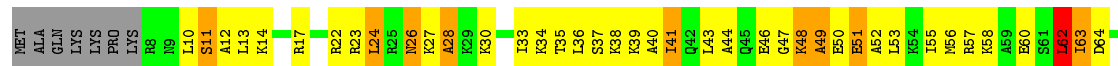


- Molecule 19: 30S ribosomal protein S19

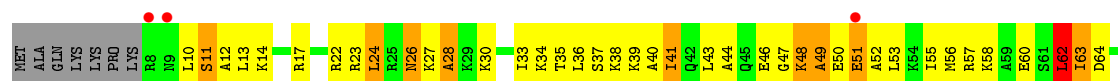




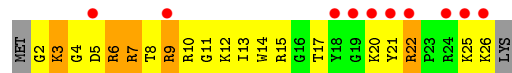
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



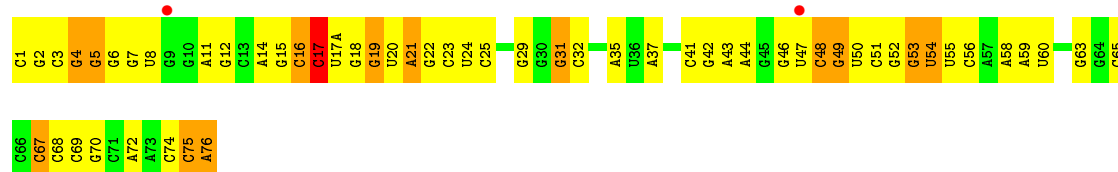
- Molecule 21: 30S ribosomal protein S21



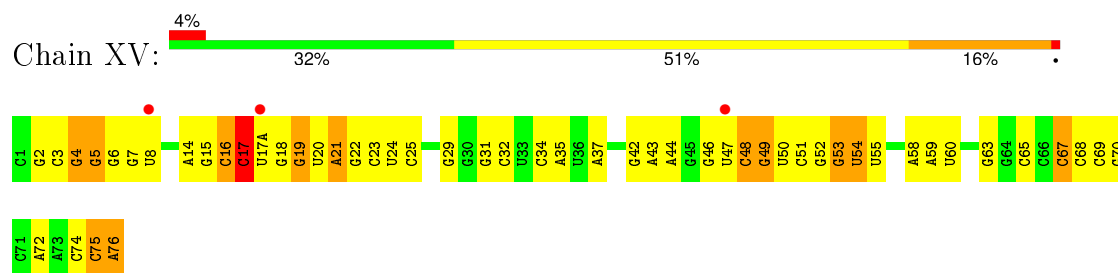
- Molecule 21: 30S ribosomal protein S21



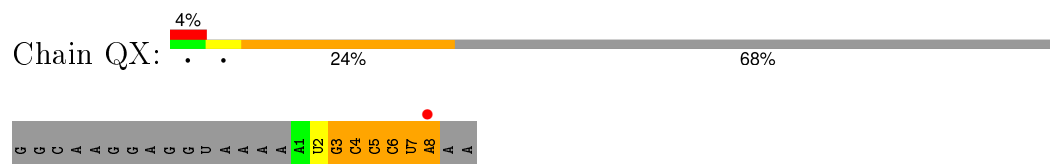
- Molecule 22: P-site tRNA fMet



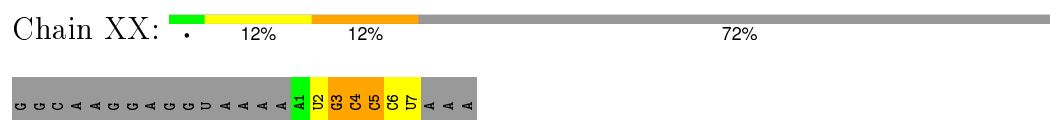
- Molecule 22: P-site tRNA fMet



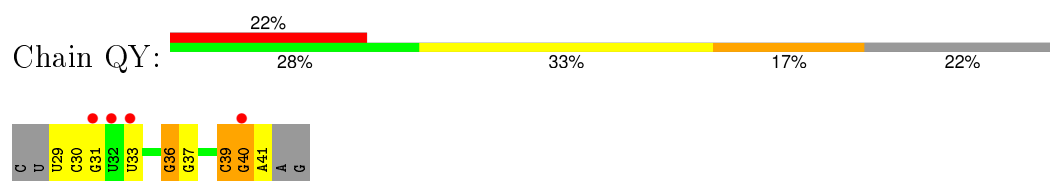
- Molecule 23: A-site ASL SufA6



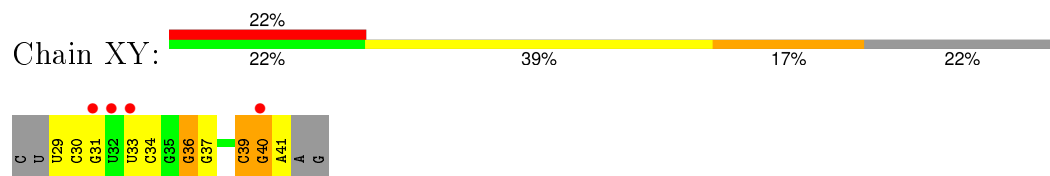
- Molecule 23: A-site ASL SufA6



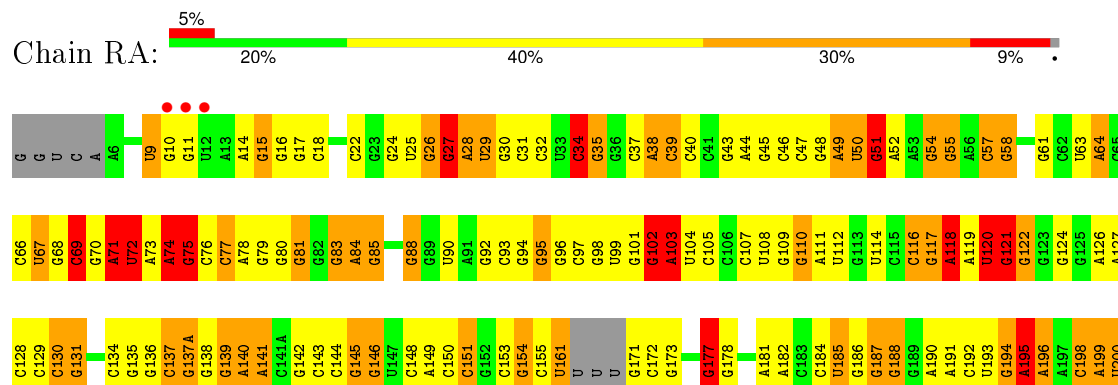
- Molecule 24: messenger RNA



- Molecule 24: messenger RNA

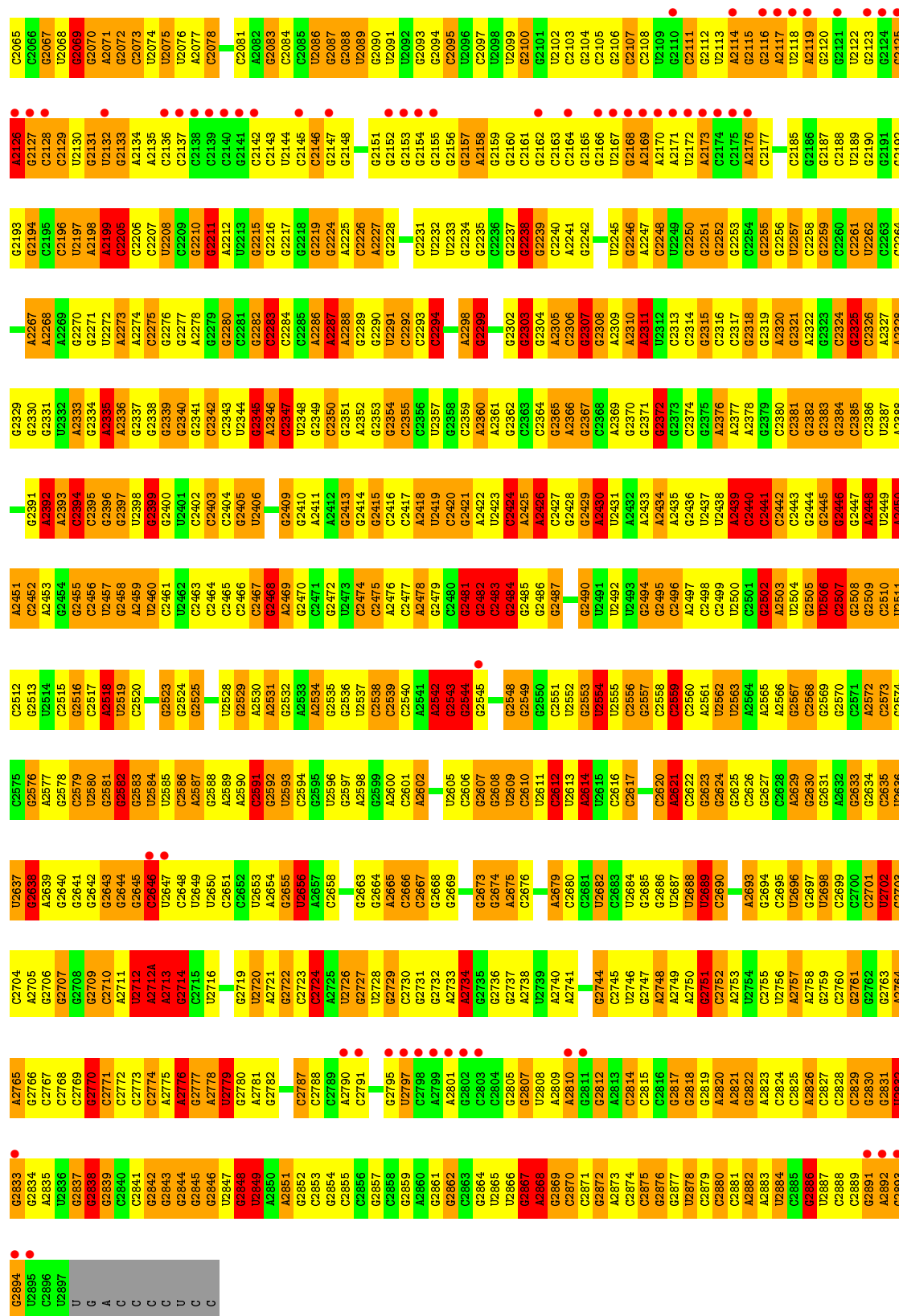


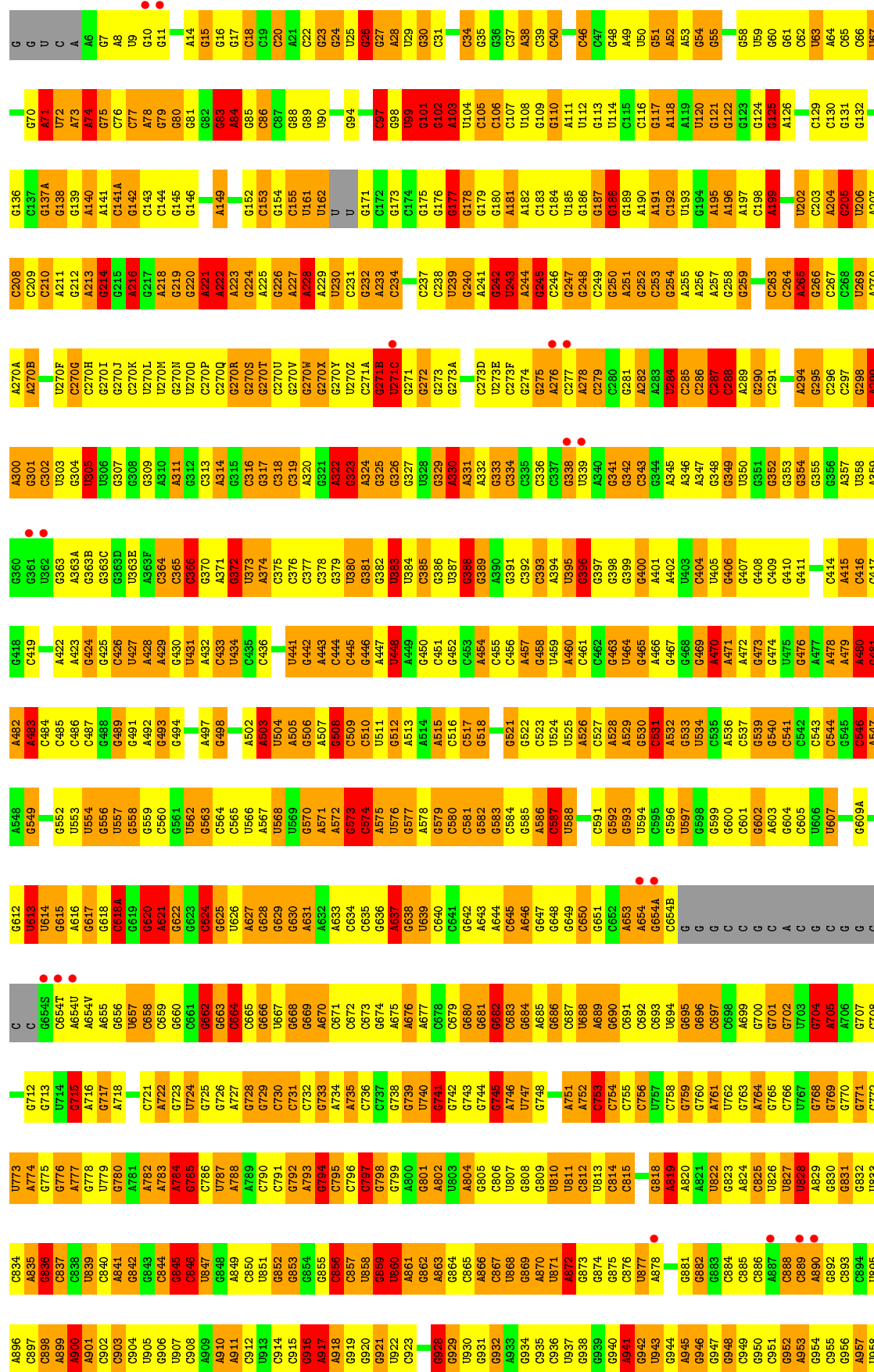
- Molecule 25: 23S rRNA



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G975	G975	C915	G852	C790	G726	C665	G625	U567	A432	G363D	A300	C267	C203
C1038	G976	C915	G853	C791	A727	G666	U626	U568	C433	U363E	G301	C268	A204
C1041	G977	G916	G854	G792	G728	U667	A627	U569	A501	A363F	C302	U269	G205
G1042	G978	A917	G855	G793	G729	G668	G628	G570	A502	G364	U303	U270	U206
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A1045	A981	G920	U858	G796	G732	C871	G631	G573	G506	G367	U306	A270C	C209
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A1048	A984	G923	A861	G735	A736	G674	G636	U576	C444	U373	G309	U270F	G212
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A1050	G986	C925	A863	U803	C737	A676	A637	A578	A447	C375	A311	G270I	G215
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U1061	G998	U937	G874	C814		G687	G649	C589	G458	G388	A322	G270T	G226
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C1067	G1003	G944	G880	A820	C756	U695	G654A	C595	G464	A394	G329	U270Z	G232
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A1069	C1005	G946	G882	U822	C758	G697	G	U597	A466	G396	A331	G271B	C234
C1070	G1006	G947	G883	A824	G759	C698	G	G598	G467	C397	A332	U271C	U235
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G1079	G1015	G956	C893	G832	G769	A706	C	U607	G476	G407	G341	A276	C246
C1080	G1016	A957	C894	U833	G770	G707	G	A608	A477		G342	C277	G247
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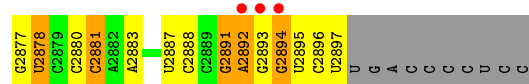
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A2051	U1991	A1931	C1852	A1791	C1713	G1648	C1587	G1522	A1398	A1275	A1212	C1150
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A2058	G1998	U1798	A1859	G1798	G1728	A1654	G1594	U1529	U1405	U1282	C1222	G1157
A2059	G1999	G1799	G1860	A1799	A1729	A1655	G1595	G1530	C1406	U1283	C1223	C1158
A2060	G2000	C1800	C1861	C1800	U1730	C1656	A1596	C1531	C1407	A1284	G1224	G1159
G2061	A2001	G1801	C1862	G1801	G1731	C1657	A1597	C1532	C1408	G1285	C1225	C1161
A2062	G2002	A1802	C1863	A1802	A1732	C1658	C1598	G1470	C1409	A1286	G1226	G1162
C2063	G2003	G1733	U1659	C1533	G1734	C1660	C1600	G1534	G1410	G1348		
C2064	G2004	C1804										



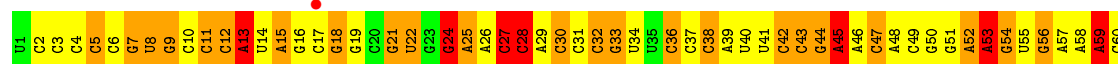
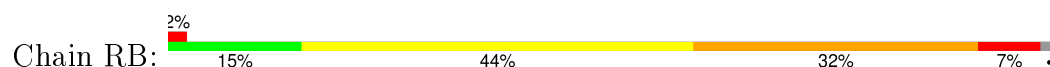




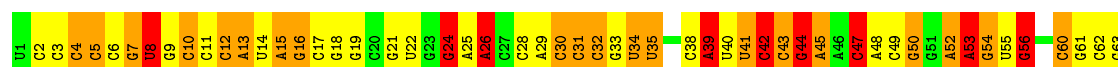
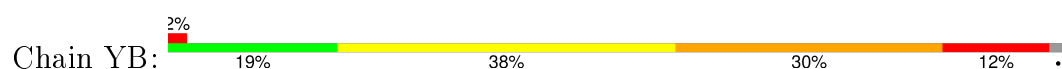




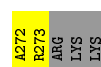
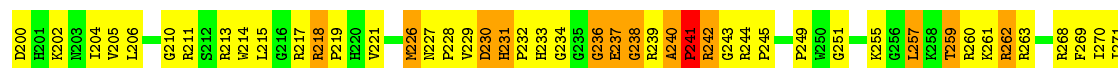
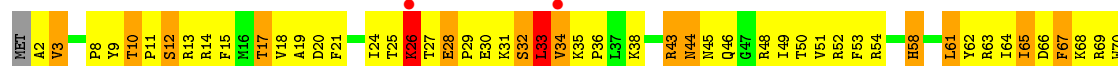
• Molecule 26: 5S rRNA



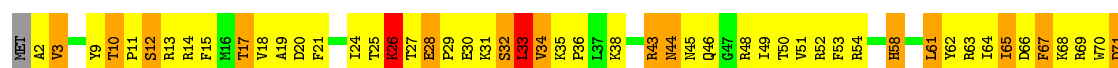
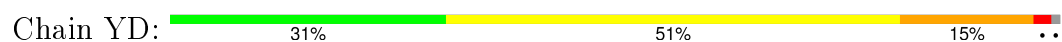
• Molecule 26: 5S rRNA

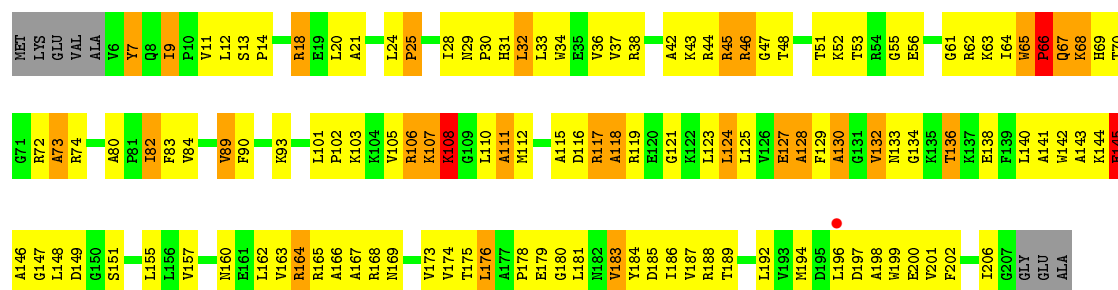


• Molecule 27: 50S ribosomal protein L2

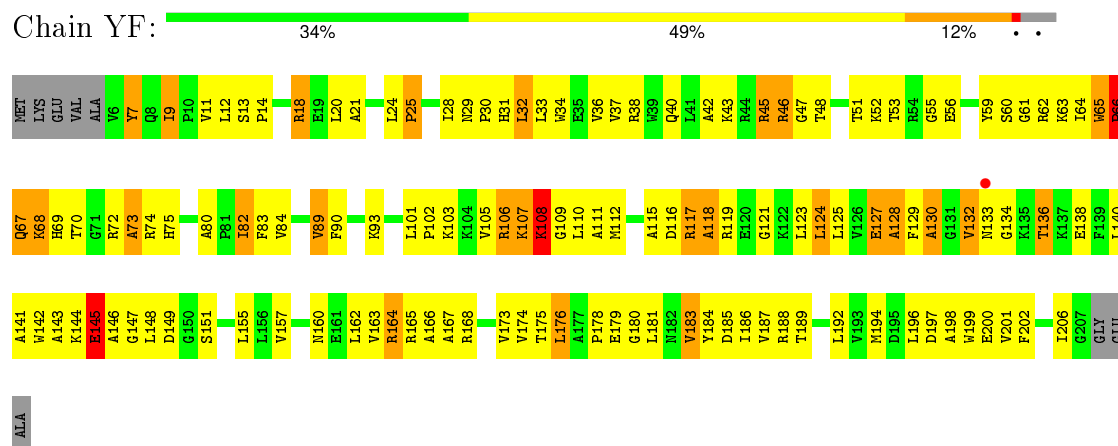


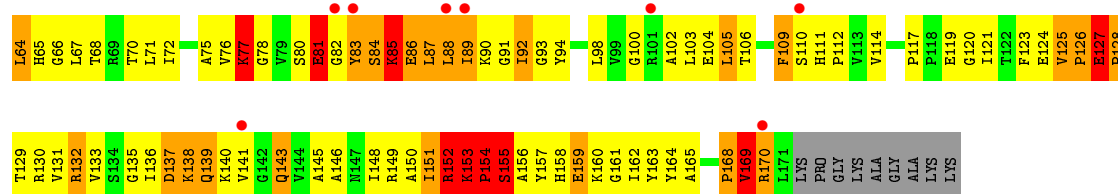
• Molecule 27: 50S ribosomal protein L2



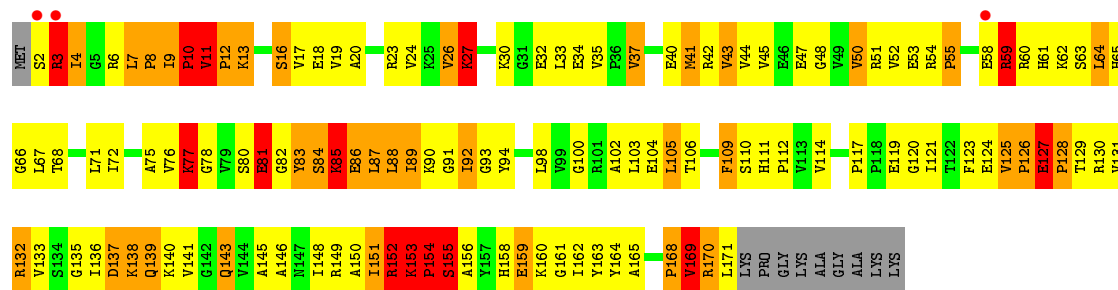
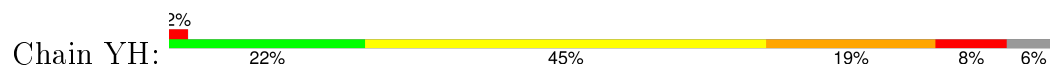


- Molecule 29: 50S ribosomal protein L4

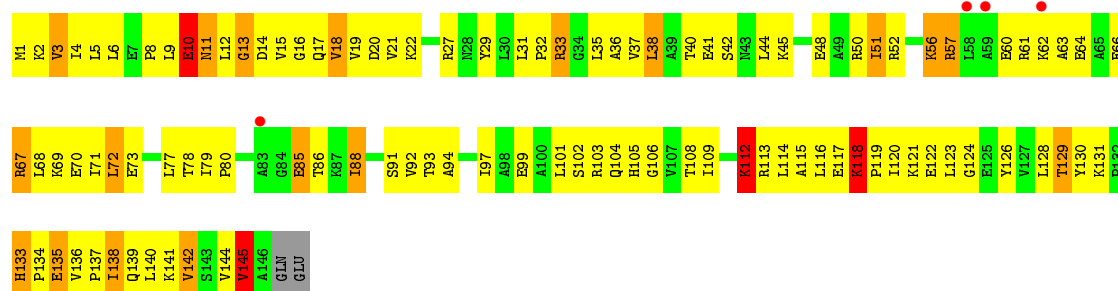




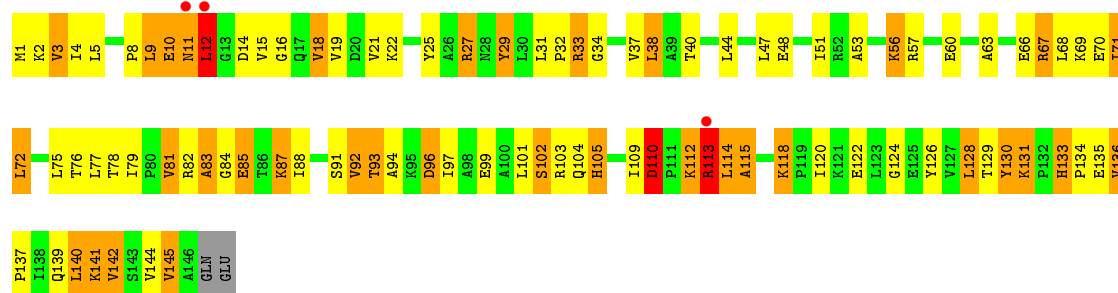
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

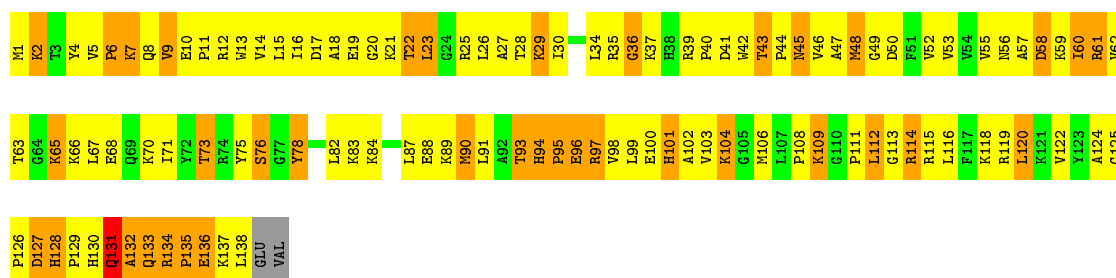


• Molecule 32: 50S ribosomal protein L9



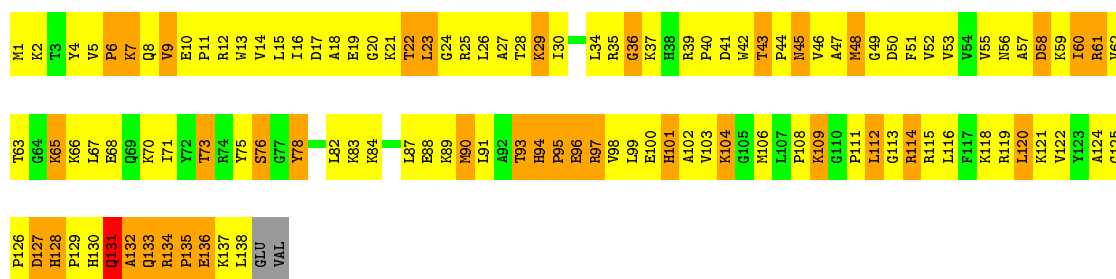
• Molecule 33: 50S ribosomal protein L13





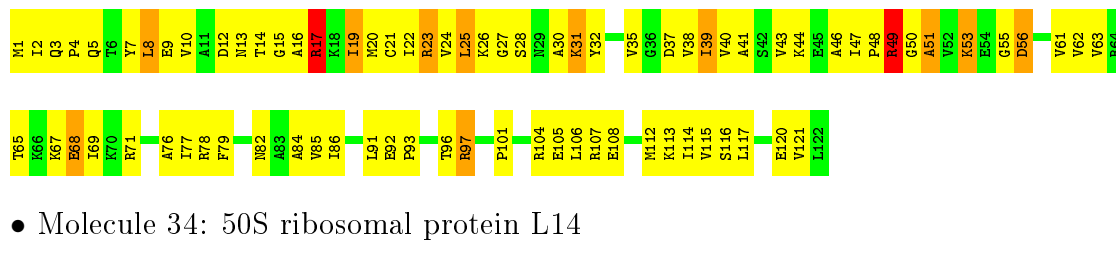
• Molecule 33: 50S ribosomal protein L13

Chain YN: 16% 56% 26% ..



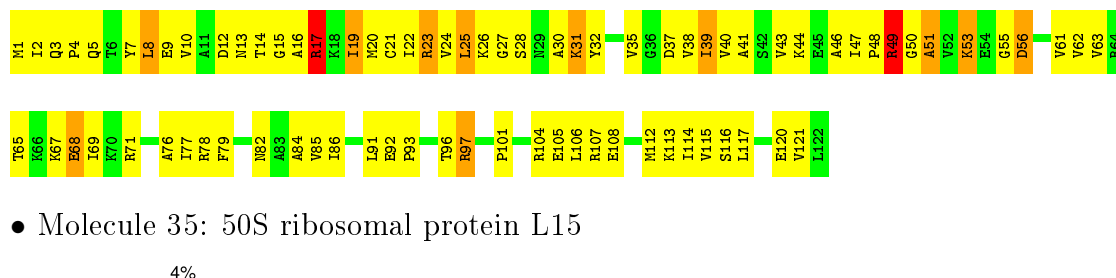
• Molecule 34: 50S ribosomal protein L14

Chain RO: 34% 55% 9% .



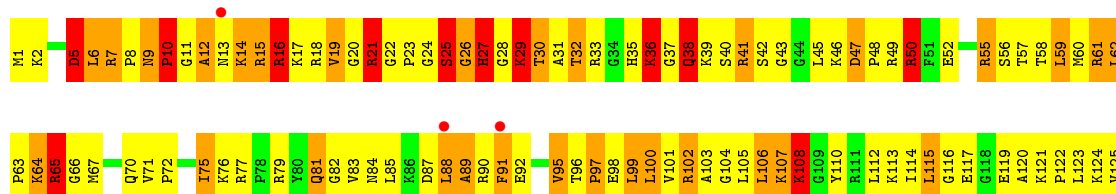
• Molecule 34: 50S ribosomal protein L14

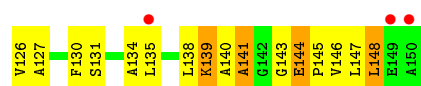
Chain YO: 34% 55% 9% .



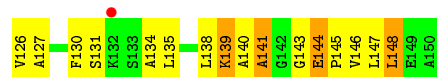
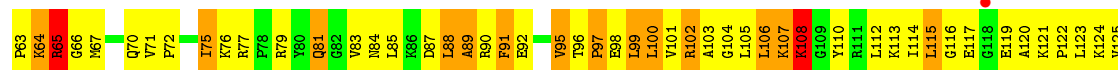
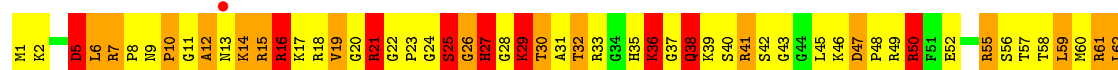
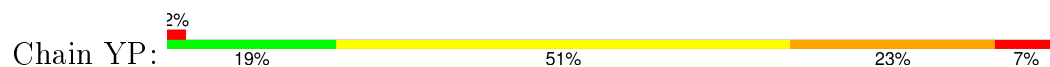
• Molecule 35: 50S ribosomal protein L15

Chain RP: 4% 19% 51% 23% 8%

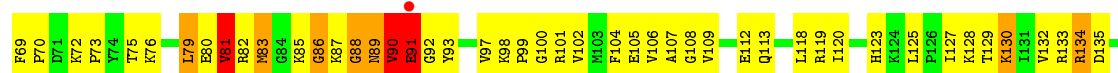
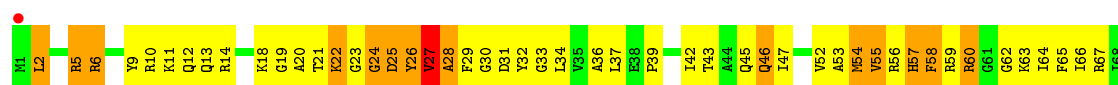




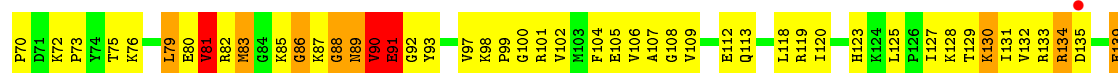
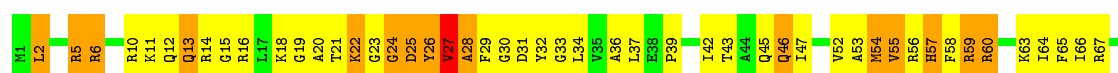
• Molecule 35: 50S ribosomal protein L15



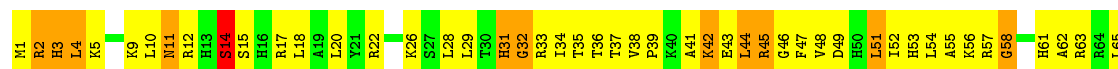
• Molecule 36: 50S ribosomal protein L16



• Molecule 36: 50S ribosomal protein L16

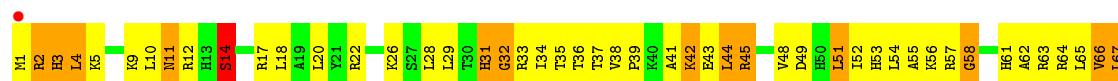


• Molecule 37: 50S ribosomal protein L17

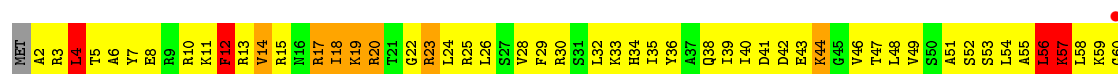
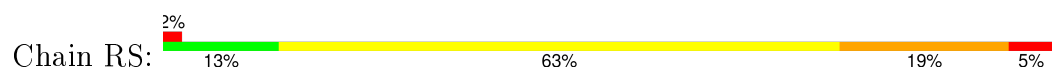




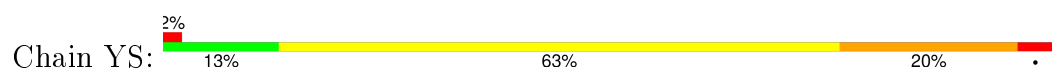
- Molecule 37: 50S ribosomal protein L17



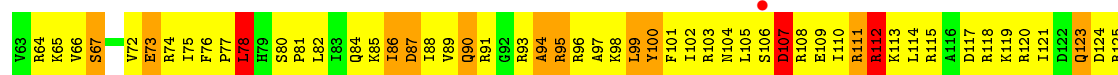
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18



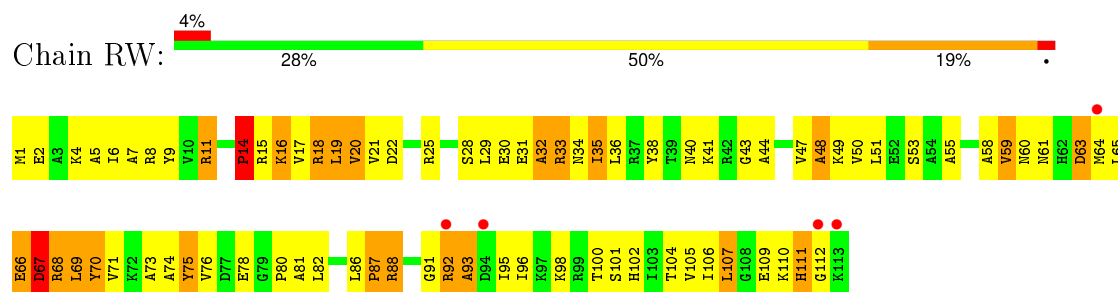
- Molecule 39: 50S ribosomal protein L19



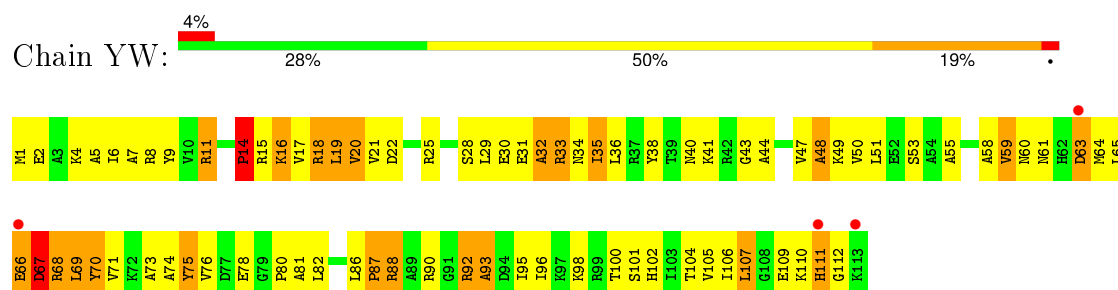
- Molecule 39: 50S ribosomal protein L19



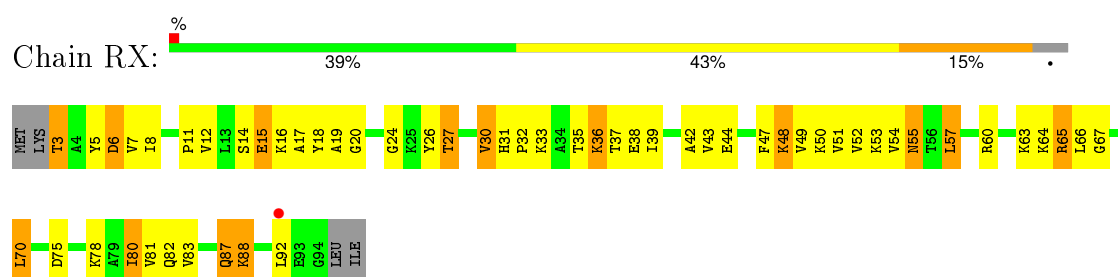
- Molecule 42: 50S ribosomal protein L22



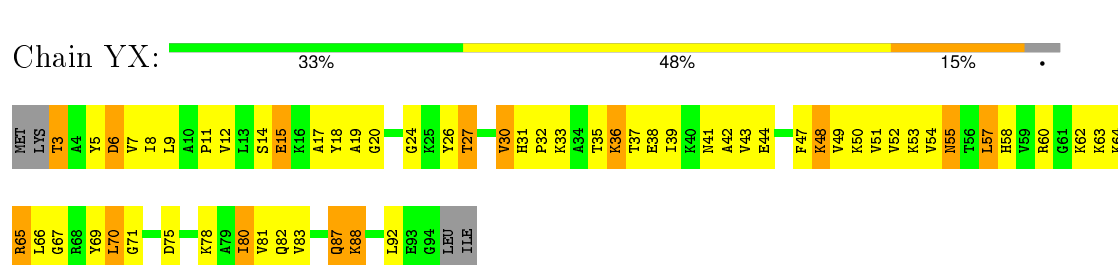
- Molecule 42: 50S ribosomal protein L22



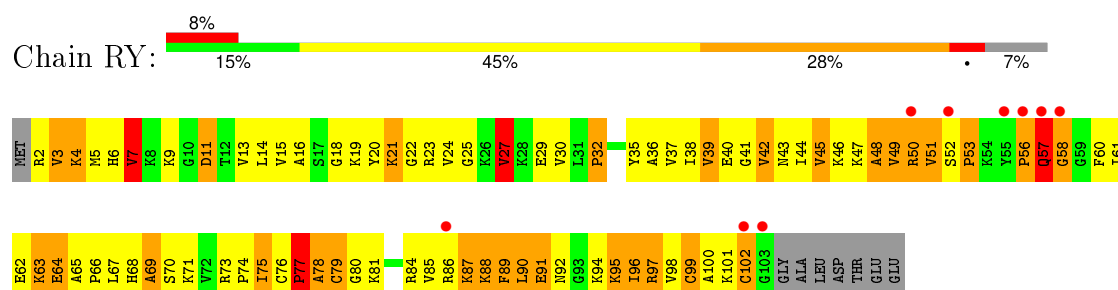
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23



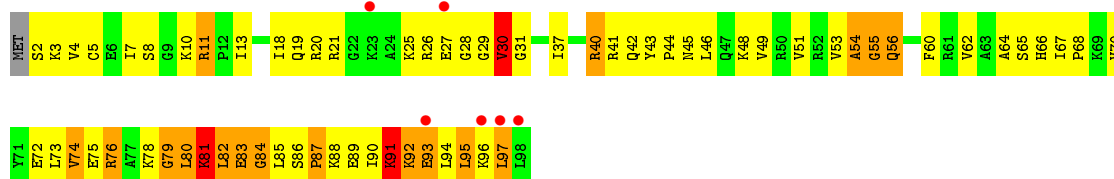
- Molecule 44: 50S ribosomal protein L24



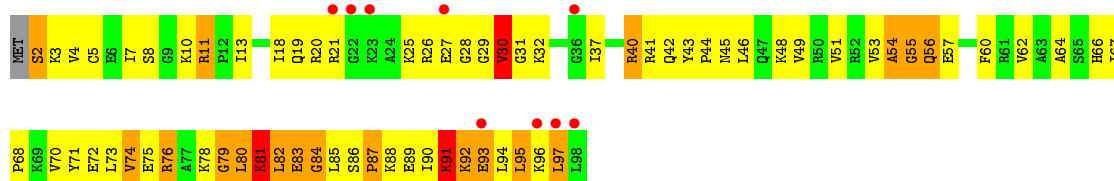
- Chain Y0:  51% 33% 12% . .



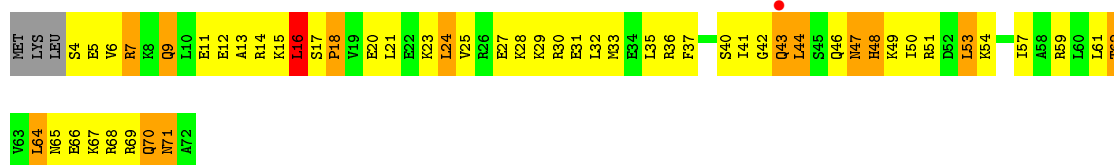
- Molecule 47: 50S ribosomal protein L28



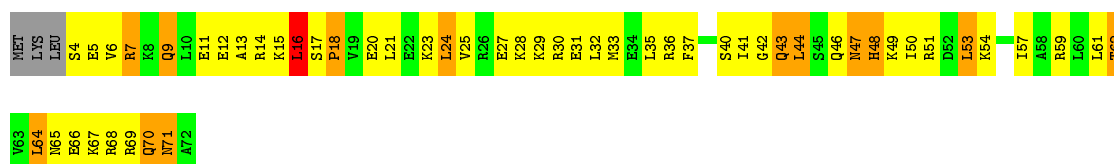
- Molecule 47: 50S ribosomal protein L28



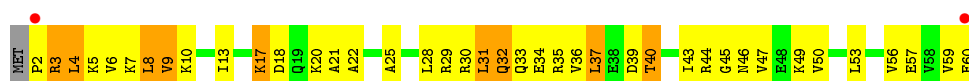
- Molecule 48: 50S ribosomal protein L29



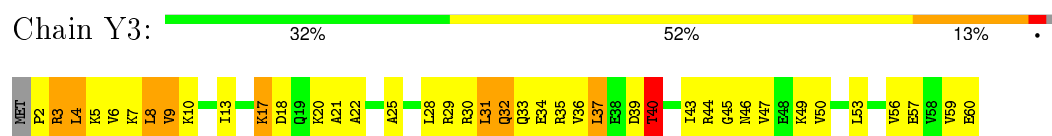
- Molecule 48: 50S ribosomal protein L29



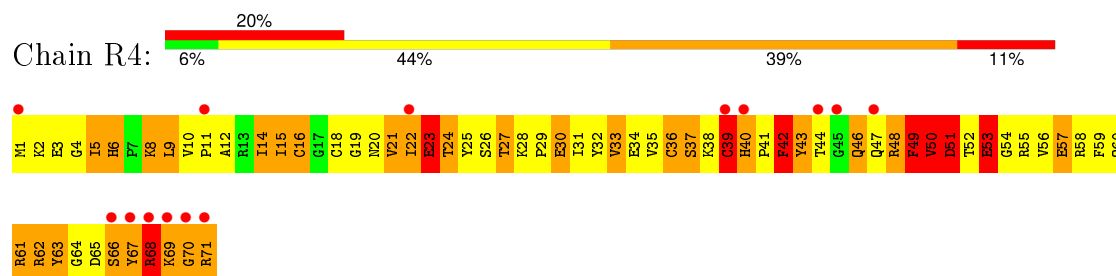
- Molecule 49: 50S ribosomal protein L30



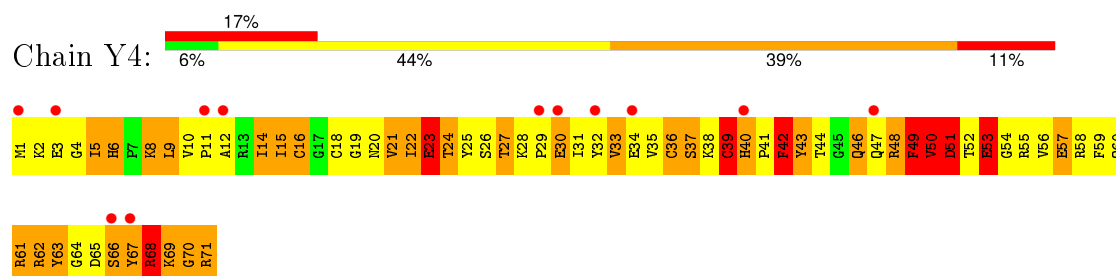
- Molecule 49: 50S ribosomal protein L30



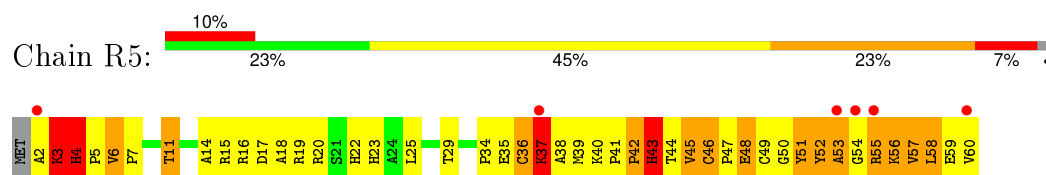
- Molecule 50: 50S ribosomal protein L31



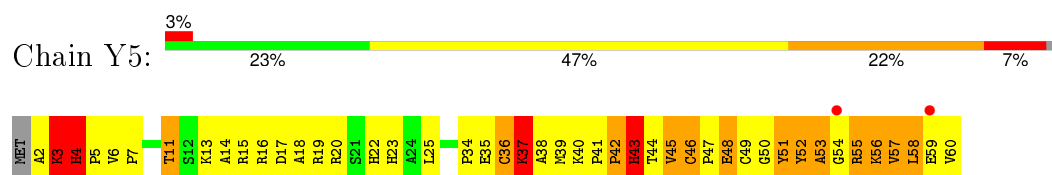
- Molecule 50: 50S ribosomal protein L31



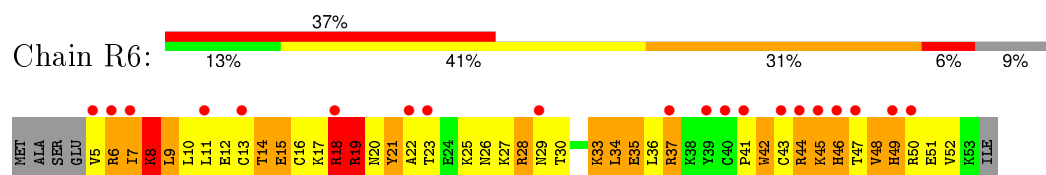
- Molecule 51: 50S ribosomal protein L32



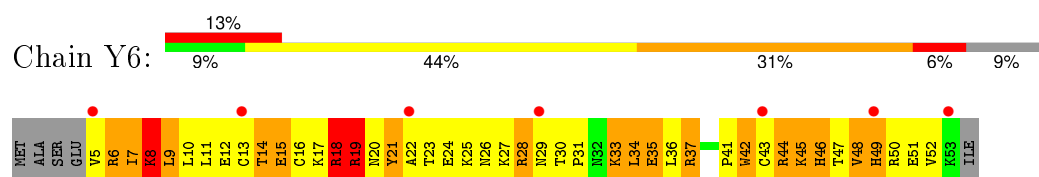
- Molecule 51: 50S ribosomal protein L32



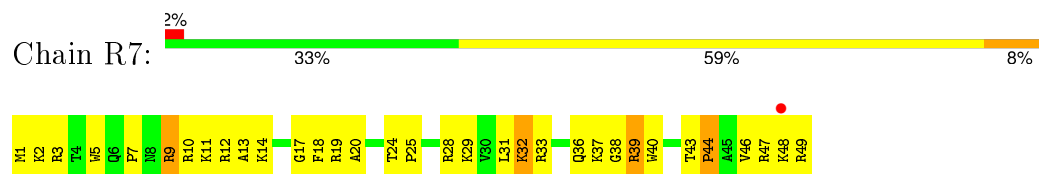
- Molecule 52: 50S ribosomal protein L33



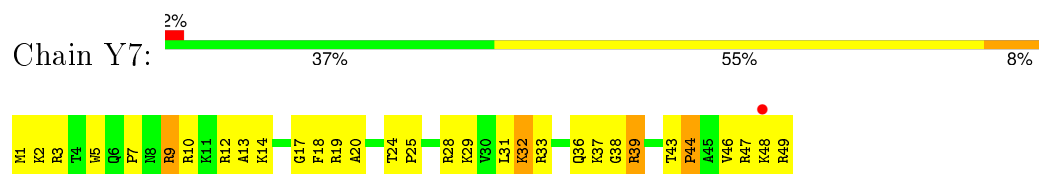
- Molecule 52: 50S ribosomal protein L33



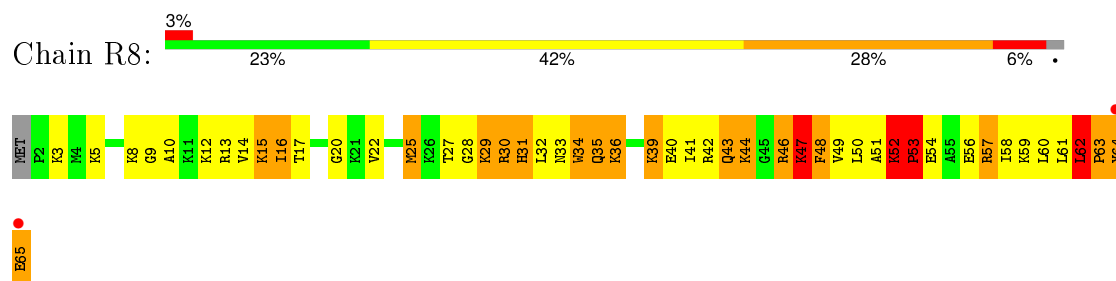
- Molecule 53: 50S ribosomal protein L34



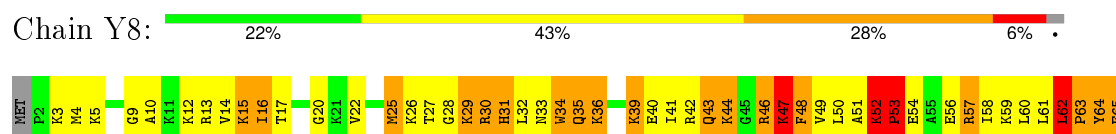
- Molecule 53: 50S ribosomal protein L34



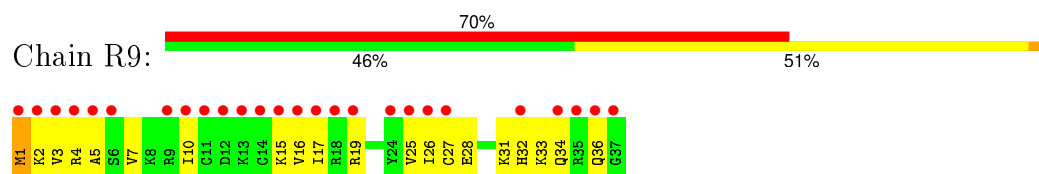
- Molecule 54: 50S ribosomal protein L35



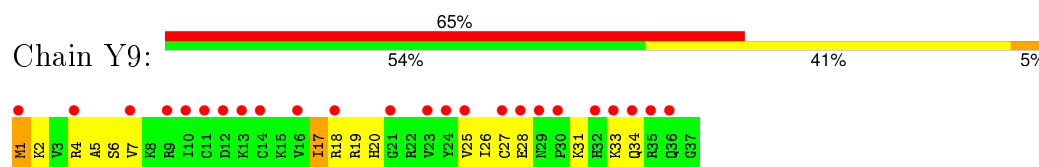
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic

Chain Z6:  33% 33% 33%


C74
C75
A76

- Molecule 56: tRNA acceptor end mimic

Chain Z8:  33% 67%


C74
C75
A76

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92 34.83 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.77-3.92) 99.8 (34.83-3.80)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.214 , 0.268	Depositor DCC
R_{free} test set	23130 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 573835 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	291868	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, 1MG, 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	0.84	19/36098 (0.1%)	1.59	747/56341 (1.3%)
1	XA	0.89	21/36101 (0.1%)	1.65	830/56346 (1.5%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.36	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.36	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.37	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.47	0/991	0.79	2/1327 (0.2%)
12	XL	0.52	1/991 (0.1%)	0.83	4/1327 (0.3%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.35	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.40	0/745	0.67	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.70	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	QV	0.51	0/1836	1.00	6/2859 (0.2%)
22	XV	0.52	0/1836	0.99	6/2859 (0.2%)
23	QX	0.39	0/185	0.71	0/285
23	XX	0.51	0/160	0.76	0/246
24	QY	0.52	0/311	0.87	0/483
24	XY	0.52	0/311	0.89	0/483
25	RA	1.03	104/69521 (0.1%)	1.85	2693/108529 (2.5%)
25	YA	1.19	254/69543 (0.4%)	1.98	3497/108563 (3.2%)
26	RB	0.82	1/2878 (0.0%)	1.59	60/4490 (1.3%)
26	YB	0.86	1/2878 (0.0%)	1.72	76/4490 (1.7%)
27	RD	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
27	YD	0.56	1/2165 (0.0%)	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	0.50	0/1620	0.76	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.40	0/1499	0.66	0/2016
30	YG	0.40	0/1499	0.66	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	0.44	0/1151	0.77	1/1558 (0.1%)
32	YI	0.44	0/1151	0.76	0/1558
33	RN	0.46	0/1131	0.78	1/1525 (0.1%)
33	YN	0.46	0/1131	0.78	1/1525 (0.1%)
34	RO	0.54	0/943	0.71	0/1269
34	YO	0.53	0/943	0.71	0/1269
35	RP	0.50	0/1162	0.95	3/1544 (0.2%)
35	YP	0.49	0/1162	0.95	3/1544 (0.2%)
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.90	3/1527 (0.2%)
37	RR	0.45	0/982	0.80	1/1312 (0.1%)
37	YR	0.45	0/982	0.80	1/1312 (0.1%)
38	RS	0.46	0/892	0.82	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YS	0.45	0/892	0.82	1/1187 (0.1%)
39	RT	0.47	0/1155	0.73	2/1542 (0.1%)
39	YT	0.47	0/1155	0.73	2/1542 (0.1%)
40	RU	0.48	0/982	0.78	0/1306
40	YU	0.48	0/982	0.78	0/1306
41	RV	0.47	0/790	0.82	0/1057
41	YV	0.47	0/790	0.82	0/1057
42	RW	0.45	0/911	0.75	0/1220
42	YW	0.45	0/911	0.75	0/1220
43	RX	0.56	0/739	0.77	0/993
43	YX	0.56	0/739	0.77	0/993
44	RY	0.52	0/798	0.80	0/1064
44	YY	0.52	0/798	0.80	0/1064
45	RZ	0.44	0/1493	0.70	0/2026
45	YZ	0.43	0/1493	0.70	0/2026
46	R0	0.52	0/657	0.73	0/874
46	Y0	0.55	0/657	0.80	1/874 (0.1%)
47	R1	0.49	0/770	0.85	1/1022 (0.1%)
47	Y1	0.49	0/770	0.85	1/1022 (0.1%)
48	R2	0.51	0/583	0.84	1/771 (0.1%)
48	Y2	0.51	0/583	0.83	1/771 (0.1%)
49	R3	0.47	0/474	0.71	0/635
49	Y3	0.43	0/474	0.71	0/635
50	R4	0.38	0/594	0.78	1/795 (0.1%)
50	Y4	0.38	0/594	0.78	1/795 (0.1%)
51	R5	0.51	0/473	0.74	0/639
51	Y5	0.51	0/473	0.74	0/639
52	R6	0.42	0/431	0.76	0/575
52	Y6	0.42	0/431	0.76	0/575
53	R7	0.56	0/438	0.76	0/575
53	Y7	0.56	0/438	0.76	0/575
54	R8	0.62	0/525	0.93	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.35	0/310	0.59	0/407
55	Y9	0.37	0/310	0.61	0/407
56	Z6	0.78	0/40	1.78	1/60 (1.7%)
56	Z8	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.89	404/316298 (0.1%)	1.59	7980/472872 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
45	YZ	0	1

The worst 5 of 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1201	A	C3'-C2'	12.06	1.66	1.52
1	XA	1054	C	C4'-C3'	11.40	1.65	1.53
25	YA	783	A	N7-C5	-11.18	1.32	1.39
25	YA	793	A	N7-C5	-10.74	1.32	1.39
25	YA	783	A	C5-C6	-10.48	1.31	1.41

The worst 5 of 7980 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	761	A	N1-C6-N6	19.13	130.07	118.60
25	RA	2490	G	C6-C5-N7	-18.87	119.08	130.40
25	RA	783	A	C6-C5-N7	-17.19	120.27	132.30
25	RA	783	A	N1-C6-N6	16.89	128.74	118.60
25	YA	783	A	N1-C6-N6	16.68	128.61	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	YZ	181	GLU	Peptide

5.2 Too-close contacts [i](#)

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	1130	0
1	XA	32249	0	16279	1064	1
2	QB	1924	0	1975	289	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	205	0
3	XC	1605	0	1668	211	0
4	QD	1703	0	1764	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1765	214	0
5	QE	1155	0	1213	182	0
5	XE	1155	0	1213	147	0
6	QF	843	0	857	94	0
6	XF	843	0	857	99	0
7	QG	1257	0	1296	151	0
7	XG	1257	0	1294	142	0
8	QH	1116	0	1175	167	0
8	XH	1116	0	1177	150	0
9	QI	1010	0	1037	144	0
9	XI	1010	0	1037	152	0
10	QJ	801	0	849	150	0
10	XJ	801	0	849	132	0
11	QK	885	0	904	103	0
11	XK	885	0	904	107	0
12	QL	975	0	1062	100	0
12	XL	975	0	1062	111	0
13	QM	964	0	1034	169	0
13	XM	964	0	1034	163	0
14	QN	492	0	530	102	0
14	XN	492	0	530	99	0
15	QO	734	0	771	76	0
15	XO	734	0	771	78	0
16	QP	705	0	725	120	0
16	XP	705	0	725	113	0
17	QQ	834	0	904	84	0
17	XQ	834	0	904	81	0
18	QR	574	0	644	66	0
18	XR	574	0	644	66	0
19	QS	674	0	699	109	0
19	XS	674	0	699	132	0
20	QT	763	0	860	108	0
20	XT	763	0	861	108	0
21	QU	217	0	234	30	0
21	XU	217	0	234	26	0
22	QV	1644	0	836	44	0
22	XV	1644	0	836	29	0
23	QX	167	0	87	13	0
23	XX	145	0	75	9	0
24	QY	303	0	154	11	0
24	XY	303	0	154	11	0
25	RA	62071	0	31285	1926	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YA	62091	0	31293	1989	0
26	RB	2573	0	1306	121	0
26	YB	2573	0	1306	103	0
27	RD	2115	0	2195	324	0
27	YD	2115	0	2195	332	0
28	RE	1568	0	1634	270	0
28	YE	1568	0	1634	263	0
29	RF	1585	0	1632	178	0
29	YF	1585	0	1632	178	0
30	RG	1474	0	1535	201	0
30	YG	1474	0	1535	194	0
31	RH	1307	0	1382	226	0
31	YH	1307	0	1382	228	0
32	RI	1136	0	1223	79	1
32	YI	1136	0	1223	72	0
33	RN	1104	0	1180	200	0
33	YN	1104	0	1180	189	0
34	RO	933	0	996	126	0
34	YO	933	0	996	125	0
35	RP	1145	0	1228	256	0
35	YP	1145	0	1228	244	0
36	RQ	1122	0	1179	157	0
36	YQ	1122	0	1178	165	0
37	RR	968	0	1033	115	0
37	YR	968	0	1033	117	0
38	RS	882	0	943	166	0
38	YS	882	0	943	159	0
39	RT	1141	0	1202	151	0
39	YT	1141	0	1202	155	0
40	RU	964	0	1022	130	0
40	YU	964	0	1022	142	0
41	RV	779	0	852	130	0
41	YV	779	0	852	131	0
42	RW	900	0	964	100	0
42	YW	900	0	964	108	0
43	RX	725	0	778	70	0
43	YX	725	0	778	74	0
44	RY	785	0	878	167	0
44	YY	785	0	878	160	0
45	RZ	1461	0	1493	81	0
45	YZ	1461	0	1493	86	0
46	R0	648	0	671	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Y0	648	0	672	51	0
47	R1	763	0	848	142	0
47	Y1	763	0	848	142	0
48	R2	581	0	629	83	0
48	Y2	581	0	629	78	0
49	R3	469	0	518	41	0
49	Y3	469	0	518	46	0
50	R4	581	0	574	159	0
50	Y4	581	0	574	167	0
51	R5	459	0	480	73	0
51	Y5	459	0	480	76	0
52	R6	424	0	450	90	0
52	Y6	424	0	450	97	0
53	R7	430	0	480	42	0
53	Y7	430	0	480	40	0
54	R8	517	0	582	104	0
54	Y8	517	0	582	105	0
55	R9	307	0	335	23	0
55	Y9	307	0	336	24	0
56	Z6	74	0	51	10	0
56	Z8	74	0	51	10	0
57	QA	64	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	239	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	2	0	0	0	0
57	XA	72	0	0	1	0
57	XB	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	269	0	0	1	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	R9	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y9	1	0	0	0	0
59	XX	22	0	12	1	0
All	All	291868	0	198240	17856	1

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 37.

The worst 5 of 17856 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)
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.54
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.28	1.54
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
4:XD:22:LYS:CG	4:XD:26:CYS:SG	2.01	1.49

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	7
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	7
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1	15
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	1	15
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	14
4	XD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	11
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	13
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	11
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	16
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	16
7	QG	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	14
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	16
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	10
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	10
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	7
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	15
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	1	12
11	QK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	20
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	23
12	QL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	8
12	XL	123/132 (93%)	83 (68%)	24 (20%)	16 (13%)	0	7
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	5
13	XM	119/126 (94%)	72 (60%)	25 (21%)	22 (18%)	0	3
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	32 (55%)	14 (24%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	23
15	XO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	23
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	6
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	18
18	QR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	8
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	8
19	QS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	3
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
21	XU	23/27 (85%)	16 (70%)	3 (13%)	4 (17%)	0	3
27	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	23
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	23
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%)	144 (72%)	36 (18%)	20 (10%)	1	13
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	13
30	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	8
30	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	8
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%)	32 (22%)	13 (9%)	1	16
32	YI	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	5
33	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
33	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	5
34	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	20
34	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	2
35	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	2
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	13
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	13
37	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	8
37	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	8
38	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
38	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
39	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	5
39	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	5
40	RU	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	19
40	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	19
41	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	13
41	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	13
42	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	7
42	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	7
43	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	29
43	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	29
44	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
44	YY	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
45	RZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	8
45	YZ	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	1	15
46	R0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	31
46	Y0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	31
47	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	9
47	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	9
48	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	6
48	Y2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	6
49	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	30
49	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	30
50	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
51	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
51	Y5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
52	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
52	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
53	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	26
53	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	26
54	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
55	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	7621 (66%)	2356 (20%)	1493 (13%)	0	7

5 of 1493 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	181 (88%)	24 (12%)	7	35
2	XB	205/220 (93%)	181 (88%)	24 (12%)	7	35
3	QC	159/188 (85%)	143 (90%)	16 (10%)	9	41
3	XC	159/188 (85%)	143 (90%)	16 (10%)	9	41
4	QD	180/181 (99%)	160 (89%)	20 (11%)	8	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	165 (92%)	15 (8%)	14	51
5	QE	116/123 (94%)	107 (92%)	9 (8%)	16	54
5	XE	116/123 (94%)	107 (92%)	9 (8%)	16	54
6	QF	90/90 (100%)	76 (84%)	14 (16%)	3	24
6	XF	90/90 (100%)	76 (84%)	14 (16%)	3	24
7	QG	126/127 (99%)	115 (91%)	11 (9%)	13	49
7	XG	126/127 (99%)	115 (91%)	11 (9%)	13	49
8	QH	119/119 (100%)	106 (89%)	13 (11%)	8	38
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	38
9	QI	98/99 (99%)	87 (89%)	11 (11%)	7	37
9	XI	98/99 (99%)	87 (89%)	11 (11%)	7	37
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	12	47
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	12	47
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	42
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	42
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5	30
12	XL	104/109 (95%)	89 (86%)	15 (14%)	4	27
13	QM	97/101 (96%)	81 (84%)	16 (16%)	3	21
13	XM	97/101 (96%)	81 (84%)	16 (16%)	3	21
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	15
14	XN	49/50 (98%)	44 (90%)	5 (10%)	9	41
15	QO	79/80 (99%)	73 (92%)	6 (8%)	16	56
15	XO	79/80 (99%)	73 (92%)	6 (8%)	16	56
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	32
16	XP	72/74 (97%)	63 (88%)	9 (12%)	6	32
17	QQ	95/97 (98%)	89 (94%)	6 (6%)	22	61
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	61
18	QR	61/77 (79%)	54 (88%)	7 (12%)	7	36
18	XR	61/77 (79%)	54 (88%)	7 (12%)	7	36
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	25
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	68 (90%)	8 (10%)	8	40
20	XT	76/82 (93%)	68 (90%)	8 (10%)	8	40
21	QU	20/22 (91%)	19 (95%)	1 (5%)	30	68
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	68
27	RD	214/218 (98%)	177 (83%)	37 (17%)	2	18
27	YD	214/218 (98%)	178 (83%)	36 (17%)	2	20
28	RE	165/166 (99%)	128 (78%)	37 (22%)	1	9
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	8
29	RF	161/166 (97%)	140 (87%)	21 (13%)	5	31
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	31
30	RG	155/156 (99%)	130 (84%)	25 (16%)	3	22
30	YG	155/156 (99%)	130 (84%)	25 (16%)	3	22
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	13
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	13
32	RI	122/124 (98%)	94 (77%)	28 (23%)	1	8
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1	7
33	RN	117/119 (98%)	98 (84%)	19 (16%)	3	22
33	YN	117/119 (98%)	98 (84%)	19 (16%)	3	22
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	42
34	YO	100/100 (100%)	90 (90%)	10 (10%)	9	42
35	RP	116/116 (100%)	89 (77%)	27 (23%)	1	8
35	YP	116/116 (100%)	89 (77%)	27 (23%)	1	8
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	22
36	YQ	111/111 (100%)	93 (84%)	18 (16%)	3	22
37	RR	101/101 (100%)	84 (83%)	17 (17%)	2	20
37	YR	101/101 (100%)	84 (83%)	17 (17%)	2	20
38	RS	87/88 (99%)	74 (85%)	13 (15%)	4	25
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	25
39	RT	120/127 (94%)	97 (81%)	23 (19%)	2	14
39	YT	120/127 (94%)	97 (81%)	23 (19%)	2	14
40	RU	93/94 (99%)	80 (86%)	13 (14%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YU	93/94 (99%)	80 (86%)	13 (14%)	4	28
41	RV	82/82 (100%)	71 (87%)	11 (13%)	5	30
41	YV	82/82 (100%)	71 (87%)	11 (13%)	5	30
42	RW	92/92 (100%)	77 (84%)	15 (16%)	3	21
42	YW	92/92 (100%)	77 (84%)	15 (16%)	3	21
43	RX	74/78 (95%)	63 (85%)	11 (15%)	4	25
43	YX	74/78 (95%)	63 (85%)	11 (15%)	4	25
44	RY	85/91 (93%)	70 (82%)	15 (18%)	2	18
44	YY	85/91 (93%)	70 (82%)	15 (18%)	2	18
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	2	17
45	YZ	162/179 (90%)	131 (81%)	31 (19%)	2	14
46	R0	65/67 (97%)	58 (89%)	7 (11%)	8	39
46	Y0	65/67 (97%)	58 (89%)	7 (11%)	8	39
47	R1	82/83 (99%)	67 (82%)	15 (18%)	2	16
47	Y1	82/83 (99%)	67 (82%)	15 (18%)	2	16
48	R2	64/67 (96%)	57 (89%)	7 (11%)	8	38
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	38
49	R3	51/52 (98%)	40 (78%)	11 (22%)	1	10
49	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	10
50	R4	63/63 (100%)	44 (70%)	19 (30%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	4
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	8
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	8
52	R6	48/52 (92%)	38 (79%)	10 (21%)	1	11
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	11
53	R7	42/42 (100%)	39 (93%)	3 (7%)	18	58
53	Y7	42/42 (100%)	39 (93%)	3 (7%)	18	58
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	4
54	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	4
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	64
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9702/10066 (96%)	8266 (85%)	1436 (15%)	4 26

5 of 1436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	8	LEU
7	XG	111	ARG
45	YZ	141	VAL
50	R4	50	VAL
2	XB	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
43	RX	55	ASN
2	XB	135	GLN
43	YX	55	ASN
43	RX	87	GLN
48	R2	47	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	385 (25%)	49 (3%)
1	XA	1498/1522 (98%)	378 (25%)	60 (4%)
22	QV	76/77 (98%)	30 (39%)	1 (1%)
22	XV	76/77 (98%)	30 (39%)	1 (1%)
23	QX	7/25 (28%)	5 (71%)	1 (14%)
23	XX	6/25 (24%)	3 (50%)	0
24	QY	13/18 (72%)	5 (38%)	1 (7%)
24	XY	13/18 (72%)	5 (38%)	1 (7%)
25	RA	2879/2916 (98%)	835 (29%)	82 (2%)
25	YA	2880/2916 (98%)	865 (30%)	93 (3%)
26	RB	119/122 (97%)	32 (26%)	3 (2%)
26	YB	119/122 (97%)	42 (35%)	2 (1%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9366 (98%)	2615 (28%)	294 (3%)

5 of 2615 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	10	A
1	QA	22	G
1	QA	32	A

5 of 294 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2848	G
1	XA	595	G
25	YA	2238	G
26	RB	108	C
1	XA	328	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
24	1MG	QY	37	24	16,26,27	2.89	3 (18%)	19,39,42	1.58	4 (21%)
24	1MG	XY	37	24	16,26,27	2.91	3 (18%)	19,39,42	1.59	4 (21%)
56	PPU	Z6	76	25,56	30,40,41	2.58	6 (20%)	37,57,60	3.25	11 (29%)
56	PPU	Z8	76	25,56	30,40,41	2.57	5 (16%)	37,57,60	3.25	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
24	1MG	QY	37	24	-	0/3/25/26	0/3/3/3
24	1MG	XY	37	24	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	76	25,56	-	0/21/43/44	0/4/4/4
56	PPU	Z8	76	25,56	-	0/21/43/44	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	C9-N6	-5.56	1.32	1.45
56	Z8	76	PPU	C9-N6	-5.55	1.32	1.45
56	Z8	76	PPU	C10-N6	-5.32	1.32	1.45
56	Z6	76	PPU	C10-N6	-5.31	1.32	1.45
56	Z6	76	PPU	C5-N7	-2.02	1.32	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	C2'-C1'-N9	-10.40	98.40	114.29
56	Z6	76	PPU	C2'-C1'-N9	-10.31	98.53	114.29
56	Z8	76	PPU	N3-C2-N1	-9.82	121.38	128.89
56	Z6	76	PPU	N3-C2-N1	-9.80	121.39	128.89
56	Z6	76	PPU	C3'-N3'-C	-8.26	110.17	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	QY	37	1MG	1	0
24	XY	37	1MG	1	0
56	Z6	76	PPU	7	0
56	Z8	76	PPU	10	0

5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 681 ligands modelled in this entry, 680 are monoatomic - leaving 1 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	$\# Z > 2$
59	A	XX	101	-	15,24,25	0.65	0	16,35,38	1.08	1 (6%)

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
59	A	XX	101	-	-	0/3/25/26	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	XX	101	A	C1'-N9-C4	3.55	132.29	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	XX	101	A	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.10	50 (3%) 50 38	3, 59, 153, 236	0
1	XA	1500/1522 (98%)	0.06	42 (2%) 56 44	1, 53, 148, 240	0
2	QB	237/256 (92%)	0.34	17 (7%) 18 12	41, 113, 151, 177	0
2	XB	237/256 (92%)	0.14	9 (3%) 44 33	21, 96, 142, 157	0
3	QC	205/239 (85%)	0.38	21 (10%) 9 7	22, 104, 139, 161	0
3	XC	205/239 (85%)	-0.10	5 (2%) 62 50	22, 79, 122, 161	0
4	QD	208/209 (99%)	-0.11	2 (0%) 84 77	8, 69, 116, 153	0
4	XD	208/209 (99%)	0.04	4 (1%) 70 59	16, 74, 114, 159	0
5	QE	151/162 (93%)	0.38	6 (3%) 42 31	32, 95, 133, 161	0
5	XE	151/162 (93%)	-0.18	0 100 100	20, 63, 108, 140	0
6	QF	101/101 (100%)	-0.07	3 (2%) 54 40	15, 68, 105, 139	0
6	XF	101/101 (100%)	0.20	6 (5%) 26 17	4, 66, 107, 134	0
7	QG	155/156 (99%)	0.19	10 (6%) 22 14	26, 89, 133, 154	0
7	XG	155/156 (99%)	0.13	9 (5%) 26 18	28, 83, 124, 148	0
8	QH	138/138 (100%)	-0.07	1 (0%) 89 84	21, 79, 122, 132	0
8	XH	138/138 (100%)	-0.15	2 (1%) 78 68	14, 68, 108, 133	0
9	QI	127/128 (99%)	0.50	11 (8%) 13 9	49, 102, 138, 161	0
9	XI	127/128 (99%)	0.12	4 (3%) 52 40	13, 91, 134, 162	0
10	QJ	99/105 (94%)	0.89	19 (19%) 2 2	57, 108, 148, 192	0
10	XJ	99/105 (94%)	0.55	11 (11%) 7 6	40, 94, 140, 165	0
11	QK	119/129 (92%)	0.33	8 (6%) 21 14	25, 72, 127, 150	0
11	XK	119/129 (92%)	0.01	4 (3%) 49 37	4, 59, 109, 129	0
12	QL	125/132 (94%)	0.17	7 (5%) 28 20	15, 64, 124, 159	0
12	XL	125/132 (94%)	-0.08	1 (0%) 87 82	6, 48, 102, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.21	7 (5%) 26 18	48, 101, 151, 159	0
13	XM	121/126 (96%)	-0.02	1 (0%) 87 82	38, 85, 119, 158	0
14	QN	60/61 (98%)	0.69	8 (13%) 4 4	52, 108, 148, 159	0
14	XN	60/61 (98%)	-0.06	0 100 100	33, 72, 116, 130	0
15	QO	88/89 (98%)	-0.08	3 (3%) 49 37	17, 71, 119, 151	0
15	XO	88/89 (98%)	0.05	4 (4%) 37 27	7, 59, 102, 127	0
16	QP	84/88 (95%)	-0.11	1 (1%) 81 72	14, 59, 114, 134	0
16	XP	84/88 (95%)	-0.10	2 (2%) 62 50	28, 68, 122, 176	0
17	QQ	100/105 (95%)	0.09	3 (3%) 54 40	30, 70, 116, 148	0
17	XQ	100/105 (95%)	0.06	3 (3%) 54 40	19, 71, 106, 144	0
18	QR	70/88 (79%)	0.05	1 (1%) 78 68	22, 70, 125, 150	0
18	XR	70/88 (79%)	-0.04	1 (1%) 78 68	9, 65, 106, 140	0
19	QS	84/93 (90%)	1.06	23 (27%) 1 1	69, 116, 148, 161	0
19	XS	84/93 (90%)	0.11	1 (1%) 81 72	48, 87, 132, 145	0
20	QT	99/106 (93%)	0.15	2 (2%) 68 57	16, 73, 113, 135	0
20	XT	99/106 (93%)	0.26	4 (4%) 42 31	23, 77, 124, 157	0
21	QU	25/27 (92%)	1.62	10 (40%) 0 1	31, 92, 141, 158	0
21	XU	25/27 (92%)	0.90	2 (8%) 15 10	32, 83, 121, 143	0
22	QV	77/77 (100%)	0.33	2 (2%) 59 47	21, 85, 147, 180	0
22	XV	77/77 (100%)	0.31	3 (3%) 43 32	6, 64, 119, 169	0
23	QX	8/25 (32%)	0.74	1 (12%) 5 5	50, 74, 138, 138	0
23	XX	7/25 (28%)	0.88	0 100 100	18, 51, 81, 90	0
24	QY	13/18 (72%)	1.87	4 (30%) 1 1	106, 175, 223, 238	0
24	XY	13/18 (72%)	2.21	4 (30%) 1 1	55, 149, 189, 217	0
25	RA	2882/2916 (98%)	0.07	136 (4%) 35 26	0, 30, 174, 252	0
25	YA	2883/2916 (98%)	-0.02	108 (3%) 45 34	0, 20, 159, 242	0
26	RB	120/122 (98%)	0.28	3 (2%) 61 48	39, 82, 133, 170	0
26	YB	120/122 (98%)	0.14	3 (2%) 61 48	16, 68, 104, 146	0
27	RD	272/276 (98%)	-0.22	2 (0%) 89 84	0, 34, 82, 147	0
27	YD	272/276 (98%)	-0.34	0 100 100	0, 18, 64, 125	0
28	RE	205/206 (99%)	-0.16	2 (0%) 84 77	1, 49, 112, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	-0.15	4 (1%) 68 57	0, 47, 104, 155	0
29	RF	202/210 (96%)	-0.26	1 (0%) 91 88	0, 55, 108, 143	0
29	YF	202/210 (96%)	-0.30	1 (0%) 91 88	0, 32, 96, 124	0
30	RG	181/182 (99%)	0.84	23 (12%) 5 5	39, 113, 160, 177	0
30	YG	181/182 (99%)	0.26	11 (6%) 25 16	18, 92, 131, 177	0
31	RH	170/180 (94%)	0.91	24 (14%) 4 3	45, 112, 156, 177	0
31	YH	170/180 (94%)	-0.07	3 (1%) 71 61	11, 66, 116, 131	0
32	RI	146/148 (98%)	-0.09	4 (2%) 58 46	3, 77, 124, 177	0
32	YI	146/148 (98%)	-0.18	3 (2%) 67 55	3, 64, 125, 140	0
33	RN	138/140 (98%)	-0.02	0 100 100	6, 61, 118, 144	0
33	YN	138/140 (98%)	-0.30	0 100 100	4, 45, 98, 131	0
34	RO	122/122 (100%)	-0.25	0 100 100	2, 42, 80, 107	0
34	YO	122/122 (100%)	-0.25	0 100 100	2, 41, 82, 126	0
35	RP	150/150 (100%)	0.00	6 (4%) 42 31	1, 58, 130, 158	0
35	YP	150/150 (100%)	-0.13	3 (2%) 68 57	1, 46, 101, 160	0
36	RQ	141/141 (100%)	-0.06	3 (2%) 67 55	3, 58, 103, 133	0
36	YQ	141/141 (100%)	-0.24	1 (0%) 89 84	0, 47, 97, 115	0
37	RR	118/118 (100%)	-0.35	0 100 100	1, 34, 87, 136	0
37	YR	118/118 (100%)	-0.29	1 (0%) 87 82	2, 38, 98, 136	0
38	RS	111/112 (99%)	-0.00	2 (1%) 71 61	23, 83, 117, 138	0
38	YS	111/112 (99%)	0.06	2 (1%) 71 61	13, 73, 115, 168	0
39	RT	137/146 (93%)	0.00	4 (2%) 55 42	8, 58, 130, 152	0
39	YT	137/146 (93%)	-0.10	6 (4%) 38 27	9, 56, 122, 170	0
40	RU	117/118 (99%)	-0.11	2 (1%) 73 62	1, 49, 113, 166	0
40	YU	117/118 (99%)	-0.39	2 (1%) 73 62	1, 31, 97, 145	0
41	RV	101/101 (100%)	-0.07	3 (2%) 54 40	1, 68, 120, 193	0
41	YV	101/101 (100%)	-0.16	1 (0%) 84 77	1, 45, 97, 171	0
42	RW	113/113 (100%)	-0.04	5 (4%) 38 27	2, 34, 95, 131	0
42	YW	113/113 (100%)	-0.13	4 (3%) 48 36	1, 24, 84, 155	0
43	RX	92/96 (95%)	-0.16	1 (1%) 82 75	4, 44, 91, 131	0
43	YX	92/96 (95%)	-0.07	0 100 100	1, 25, 64, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.42	9 (8%) 12 9	10, 84, 138, 174	0
44	YY	102/110 (92%)	-0.28	2 (1%) 68 57	2, 50, 106, 160	0
45	RZ	183/206 (88%)	0.05	3 (1%) 74 63	20, 88, 136, 160	0
45	YZ	183/206 (88%)	-0.05	6 (3%) 50 38	20, 78, 137, 167	0
46	R0	82/85 (96%)	-0.36	1 (1%) 81 72	6, 44, 83, 137	0
46	Y0	82/85 (96%)	-0.36	0 100 100	2, 32, 70, 88	0
47	R1	97/98 (98%)	0.30	6 (6%) 24 16	2, 47, 126, 202	0
47	Y1	97/98 (98%)	0.16	9 (9%) 11 8	0, 32, 114, 142	0
48	R2	69/72 (95%)	-0.14	1 (1%) 78 68	8, 72, 116, 128	0
48	Y2	69/72 (95%)	-0.28	0 100 100	0, 39, 97, 137	0
49	R3	59/60 (98%)	-0.08	2 (3%) 49 37	7, 60, 126, 152	0
49	Y3	59/60 (98%)	-0.38	0 100 100	3, 40, 87, 128	0
50	R4	71/71 (100%)	1.04	14 (19%) 1 2	78, 145, 193, 235	0
50	Y4	71/71 (100%)	0.54	12 (16%) 2 2	69, 122, 166, 194	0
51	R5	59/60 (98%)	0.18	6 (10%) 9 7	4, 39, 139, 166	0
51	Y5	59/60 (98%)	0.09	2 (3%) 49 37	1, 40, 132, 156	0
52	R6	49/54 (90%)	1.96	20 (40%) 0 1	48, 122, 152, 191	0
52	Y6	49/54 (90%)	1.02	7 (14%) 4 3	47, 108, 148, 175	0
53	R7	49/49 (100%)	-0.18	1 (2%) 68 57	1, 27, 75, 161	0
53	Y7	49/49 (100%)	-0.10	1 (2%) 68 57	1, 15, 84, 140	0
54	R8	64/65 (98%)	0.02	2 (3%) 52 40	4, 41, 94, 153	0
54	Y8	64/65 (98%)	-0.07	0 100 100	2, 34, 85, 138	0
55	R9	37/37 (100%)	3.11	26 (70%) 0 1	53, 103, 154, 162	0
55	Y9	37/37 (100%)	2.81	24 (64%) 0 1	60, 98, 136, 154	0
56	Z6	2/3 (66%)	0.68	0 100 100	17, 17, 17, 30	0
56	Z8	2/3 (66%)	0.72	0 100 100	19, 19, 19, 22	0
All	All	20870/21494 (97%)	0.06	870 (4%) 40 29	0, 55, 139, 252	0

The worst 5 of 870 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	RA	2173	A	13.8
25	RA	1084	A	12.1

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Mol	Chain	Res	Type	RSRZ
25	RA	1094	U	11.7
25	RA	1058	G	11.1
40	RU	118	GLY	10.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	1MG	QY	37	24/25	0.88	0.23	-	130,130,130,130	0
24	1MG	XY	37	24/25	0.90	0.26	-	56,56,56,56	0
56	PPU	Z8	76	37/38	0.91	0.39	-	10,10,10,10	0
56	PPU	Z6	76	37/38	0.95	0.32	-	14,14,14,14	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	YA	3207	1/1	0.55	0.99	69.63	7,7,7,7	0
57	MG	YA	3263	1/1	0.89	0.76	64.70	4,4,4,4	0
57	MG	YA	3265	1/1	0.91	1.06	61.99	4,4,4,4	0
57	MG	XA	1656	1/1	0.80	1.10	54.80	10,10,10,10	0
57	MG	RA	3034	1/1	0.97	0.86	52.92	9,9,9,9	0
57	MG	RA	3049	1/1	0.76	1.01	52.28	13,13,13,13	0
57	MG	RA	3002	1/1	0.97	0.88	51.17	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3055	1/1	0.92	0.94	41.69	5,5,5,5	0
57	MG	YA	3080	1/1	0.80	1.47	39.45	50,50,50,50	0
57	MG	YA	3068	1/1	0.96	0.51	36.88	2,2,2,2	0
57	MG	YA	3047	1/1	0.97	0.61	36.67	3,3,3,3	0
57	MG	YA	3015	1/1	0.94	1.11	36.04	50,50,50,50	0
57	MG	XA	1604	1/1	0.98	0.97	35.72	10,10,10,10	0
57	MG	RA	3062	1/1	0.51	1.85	35.47	50,50,50,50	0
57	MG	YA	3049	1/1	0.85	0.89	34.01	50,50,50,50	0
57	MG	RA	3097	1/1	0.97	0.47	29.21	2,2,2,2	0
57	MG	YA	3100	1/1	0.72	0.92	29.12	6,6,6,6	0
57	MG	YA	3087	1/1	0.97	0.68	28.73	11,11,11,11	0
57	MG	XA	1628	1/1	0.95	0.54	28.15	10,10,10,10	0
57	MG	YA	3259	1/1	0.92	0.71	28.05	8,8,8,8	0
57	MG	RA	3052	1/1	0.89	0.87	27.35	50,50,50,50	0
57	MG	RA	3170	1/1	0.90	1.02	26.60	5,5,5,5	0
57	MG	YA	3220	1/1	0.98	0.66	25.70	33,33,33,33	0
57	MG	YA	3012	1/1	0.83	1.55	24.91	50,50,50,50	0
57	MG	RA	3130	1/1	0.81	0.61	24.83	2,2,2,2	0
57	MG	YA	3057	1/1	0.98	0.87	23.74	4,4,4,4	0
57	MG	RA	3058	1/1	0.95	0.74	23.07	3,3,3,3	0
57	MG	RA	3036	1/1	0.92	0.78	22.35	6,6,6,6	0
57	MG	RA	3079	1/1	0.93	0.68	21.87	5,5,5,5	0
57	MG	YA	3009	1/1	0.98	0.73	21.70	8,8,8,8	0
57	MG	YA	3053	1/1	0.93	0.53	21.67	4,4,4,4	0
57	MG	RA	3004	1/1	0.94	0.96	21.52	10,10,10,10	0
57	MG	RA	3219	1/1	0.42	0.73	21.41	40,40,40,40	0
57	MG	RA	3008	1/1	0.96	0.47	21.21	0,0,0,0	0
57	MG	RP	201	1/1	0.78	1.36	21.02	21,21,21,21	0
57	MG	YA	3206	1/1	0.98	0.34	20.83	26,26,26,26	0
57	MG	RA	3131	1/1	0.92	0.68	20.55	9,9,9,9	0
57	MG	RA	3015	1/1	0.95	0.69	20.31	5,5,5,5	0
57	MG	YA	3002	1/1	0.92	1.06	20.17	50,50,50,50	0
57	MG	YA	3014	1/1	0.84	1.26	19.96	50,50,50,50	0
57	MG	RA	3105	1/1	0.98	0.47	19.65	11,11,11,11	0
57	MG	YA	3172	1/1	0.77	1.40	19.56	1,1,1,1	0
57	MG	YA	3108	1/1	0.98	0.49	19.37	1,1,1,1	0
57	MG	QA	1613	1/1	0.92	0.69	19.28	15,15,15,15	0
57	MG	YA	3186	1/1	0.93	0.62	19.08	11,11,11,11	0
57	MG	QA	1618	1/1	0.84	0.51	18.06	3,3,3,3	0
57	MG	RA	3098	1/1	0.98	0.63	17.60	14,14,14,14	0
57	MG	YA	3013	1/1	0.98	0.55	17.16	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3212	1/1	0.98	0.51	17.09	1,1,1,1	0
57	MG	YA	3160	1/1	0.90	0.51	16.80	1,1,1,1	0
57	MG	RA	3089	1/1	0.93	0.57	16.49	11,11,11,11	0
57	MG	YA	3176	1/1	0.70	0.51	16.37	6,6,6,6	0
57	MG	YA	3120	1/1	0.95	0.61	15.87	8,8,8,8	0
57	MG	RA	3122	1/1	0.96	0.56	15.24	5,5,5,5	0
57	MG	RA	3106	1/1	0.97	0.36	15.20	13,13,13,13	0
57	MG	YA	3201	1/1	0.91	0.57	15.20	9,9,9,9	0
57	MG	RA	3178	1/1	0.89	0.25	15.02	1,1,1,1	0
57	MG	RA	3085	1/1	0.88	0.82	14.88	5,5,5,5	0
57	MG	YA	3034	1/1	0.96	0.54	14.83	2,2,2,2	0
57	MG	YA	3026	1/1	0.95	1.12	14.66	1,1,1,1	0
57	MG	YA	3031	1/1	0.98	0.60	14.43	0,0,0,0	0
57	MG	RA	3031	1/1	0.96	0.74	14.23	5,5,5,5	0
57	MG	YA	3262	1/1	0.97	0.56	14.13	8,8,8,8	0
57	MG	RA	3019	1/1	0.96	0.38	13.95	8,8,8,8	0
57	MG	RA	3077	1/1	0.96	0.55	13.63	0,0,0,0	0
57	MG	YA	3024	1/1	0.92	0.55	13.51	50,50,50,50	0
57	MG	YA	3004	1/1	0.94	0.40	13.47	12,12,12,12	0
57	MG	RA	3140	1/1	0.90	0.73	13.40	9,9,9,9	0
57	MG	YA	3210	1/1	0.80	0.51	13.03	3,3,3,3	0
57	MG	YA	3070	1/1	0.96	0.40	12.94	15,15,15,15	0
57	MG	RA	3116	1/1	0.92	0.46	12.76	9,9,9,9	0
57	MG	YA	3139	1/1	0.96	0.40	12.69	7,7,7,7	0
57	MG	RA	3087	1/1	0.98	0.93	12.16	11,11,11,11	0
57	MG	RA	3040	1/1	0.97	0.37	12.15	14,14,14,14	0
57	MG	YA	3095	1/1	0.96	0.48	11.88	2,2,2,2	0
57	MG	YA	3107	1/1	0.98	0.46	11.58	15,15,15,15	0
57	MG	RA	3121	1/1	0.87	0.77	11.51	5,5,5,5	0
57	MG	RA	3125	1/1	0.89	0.53	11.43	1,1,1,1	0
57	MG	RA	3063	1/1	0.81	0.81	11.40	3,3,3,3	0
57	MG	YA	3099	1/1	0.91	0.76	11.27	10,10,10,10	0
57	MG	YA	3069	1/1	0.93	0.51	11.11	2,2,2,2	0
57	MG	RA	3081	1/1	0.98	0.71	11.02	1,1,1,1	0
57	MG	XA	1665	1/1	0.87	0.49	10.98	7,7,7,7	0
57	MG	RA	3183	1/1	0.94	0.33	10.93	57,57,57,57	0
57	MG	RA	3022	1/1	0.83	0.36	10.69	4,4,4,4	0
57	MG	RA	3005	1/1	0.90	0.63	10.46	12,12,12,12	0
57	MG	YA	3090	1/1	0.98	0.43	10.40	1,1,1,1	0
57	MG	RA	3153	1/1	0.70	0.35	10.18	15,15,15,15	0
57	MG	QA	1646	1/1	0.86	0.53	9.71	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3020	1/1	0.95	0.73	9.59	50,50,50,50	0
57	MG	RA	3094	1/1	0.95	0.47	9.27	0,0,0,0	0
57	MG	YA	3035	1/1	0.96	0.33	9.25	9,9,9,9	0
57	MG	YA	3212	1/1	0.86	0.25	9.25	8,8,8,8	0
57	MG	YA	3167	1/1	0.81	0.52	9.15	2,2,2,2	0
57	MG	RA	3220	1/1	0.86	0.28	9.12	26,26,26,26	0
57	MG	RA	3222	1/1	0.86	0.34	9.12	14,14,14,14	0
57	MG	YA	3218	1/1	0.88	0.36	9.09	5,5,5,5	0
57	MG	RA	3088	1/1	0.89	0.62	9.02	15,15,15,15	0
57	MG	XA	1618	1/1	0.96	0.50	8.84	3,3,3,3	0
57	MG	QA	1635	1/1	0.97	0.41	8.65	13,13,13,13	0
57	MG	RA	3026	1/1	0.90	0.63	8.21	50,50,50,50	0
57	MG	YA	3050	1/1	0.92	0.45	8.14	50,50,50,50	0
57	MG	YA	3091	1/1	0.98	0.39	8.04	13,13,13,13	0
57	MG	RA	3223	1/1	0.91	0.30	7.97	47,47,47,47	0
57	MG	YA	3145	1/1	0.82	0.33	7.94	9,9,9,9	0
57	MG	XV	101	1/1	0.94	0.45	7.91	14,14,14,14	0
57	MG	RA	3218	1/1	0.93	0.34	7.89	23,23,23,23	0
57	MG	XA	1651	1/1	0.94	0.27	7.70	25,25,25,25	0
57	MG	YA	3041	1/1	0.96	0.73	7.65	0,0,0,0	0
57	MG	RA	3206	1/1	0.76	0.37	7.60	3,3,3,3	0
57	MG	YA	3101	1/1	0.90	0.59	7.58	2,2,2,2	0
57	MG	YA	3036	1/1	0.98	0.32	7.54	2,2,2,2	0
57	MG	XA	1636	1/1	0.90	0.38	7.50	3,3,3,3	0
57	MG	RA	3056	1/1	0.98	0.36	7.43	5,5,5,5	0
57	MG	QA	1614	1/1	0.92	0.51	7.42	9,9,9,9	0
57	MG	RA	3033	1/1	0.89	0.59	7.30	50,50,50,50	0
57	MG	YA	3023	1/1	0.99	0.32	7.20	2,2,2,2	0
57	MG	QA	1649	1/1	0.84	0.42	7.18	6,6,6,6	0
57	MG	YA	3008	1/1	0.98	0.32	7.09	10,10,10,10	0
57	MG	XA	1615	1/1	0.98	0.28	7.07	6,6,6,6	0
57	MG	RA	3009	1/1	0.82	0.36	6.99	10,10,10,10	0
57	MG	RA	3158	1/1	0.99	0.28	6.99	15,15,15,15	0
57	MG	XA	1619	1/1	0.98	0.28	6.97	5,5,5,5	0
57	MG	RA	3208	1/1	0.86	0.65	6.96	15,15,15,15	0
57	MG	YA	3229	1/1	0.93	0.24	6.95	3,3,3,3	0
57	MG	RA	3093	1/1	0.95	0.59	6.81	10,10,10,10	0
57	MG	YA	3042	1/1	0.98	0.57	6.77	2,2,2,2	0
57	MG	YA	3141	1/1	0.92	0.53	6.77	0,0,0,0	0
57	MG	YA	3209	1/1	0.89	0.28	6.63	15,15,15,15	0
57	MG	YA	3246	1/1	0.84	0.35	6.46	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3058	1/1	0.97	0.52	6.46	15,15,15,15	0
57	MG	XA	1653	1/1	0.91	0.35	6.43	8,8,8,8	0
57	MG	YA	3109	1/1	0.98	0.30	6.36	2,2,2,2	0
57	MG	RA	3038	1/1	0.99	0.32	6.28	8,8,8,8	0
57	MG	RA	3035	1/1	0.96	0.41	6.01	11,11,11,11	0
57	MG	YA	3033	1/1	0.95	0.45	5.87	4,4,4,4	0
57	MG	YA	3171	1/1	0.92	0.40	5.85	13,13,13,13	0
57	MG	RA	3012	1/1	0.97	0.49	5.84	4,4,4,4	0
57	MG	YA	3116	1/1	0.96	0.42	5.76	3,3,3,3	0
57	MG	YA	3006	1/1	0.92	0.57	5.75	3,3,3,3	0
57	MG	YA	3011	1/1	0.94	0.32	5.63	0,0,0,0	0
57	MG	RA	3072	1/1	0.98	0.40	5.53	3,3,3,3	0
57	MG	RA	3159	1/1	0.86	0.26	5.47	6,6,6,6	0
57	MG	QA	1622	1/1	0.93	0.33	5.39	14,14,14,14	0
57	MG	YA	3078	1/1	0.95	0.36	5.39	2,2,2,2	0
57	MG	RA	3164	1/1	0.94	0.16	5.39	4,4,4,4	0
57	MG	RA	3017	1/1	0.96	0.39	5.19	11,11,11,11	0
57	MG	QA	1631	1/1	0.69	0.43	5.06	26,26,26,26	0
57	MG	RA	3065	1/1	0.97	0.37	4.90	7,7,7,7	0
57	MG	XA	1646	1/1	0.81	0.28	4.89	7,7,7,7	0
57	MG	YA	3126	1/1	0.97	0.35	4.81	7,7,7,7	0
57	MG	YA	3168	1/1	0.94	0.29	4.80	41,41,41,41	0
57	MG	XA	1621	1/1	0.92	0.33	4.79	3,3,3,3	0
57	MG	QA	1620	1/1	0.60	0.32	4.77	6,6,6,6	0
57	MG	YA	3037	1/1	0.99	0.25	4.75	13,13,13,13	0
57	MG	YA	3074	1/1	0.89	0.18	4.71	11,11,11,11	0
57	MG	YA	3044	1/1	0.98	0.30	4.60	6,6,6,6	0
57	MG	XA	1638	1/1	0.85	0.32	4.59	20,20,20,20	0
57	MG	XA	1664	1/1	0.88	0.29	4.52	8,8,8,8	0
57	MG	YA	3236	1/1	0.62	0.28	4.33	5,5,5,5	0
57	MG	YA	3118	1/1	0.95	0.28	4.28	14,14,14,14	0
57	MG	YA	3028	1/1	0.93	0.37	4.20	6,6,6,6	0
57	MG	YA	3115	1/1	0.93	0.33	4.15	4,4,4,4	0
57	MG	YA	3235	1/1	0.98	0.36	4.07	3,3,3,3	0
57	MG	RA	3238	1/1	0.93	0.49	4.03	16,16,16,16	0
57	MG	RA	3120	1/1	0.95	0.22	3.87	1,1,1,1	0
57	MG	XA	1637	1/1	0.94	0.43	3.77	25,25,25,25	0
57	MG	XA	1635	1/1	0.91	0.57	3.60	4,4,4,4	0
57	MG	QA	1610	1/1	0.99	0.23	3.54	7,7,7,7	0
57	MG	YA	3266	1/1	0.94	0.27	3.52	2,2,2,2	0
57	MG	RA	3128	1/1	0.99	0.43	3.43	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3054	1/1	0.97	0.28	3.38	3,3,3,3	0
57	MG	YA	3005	1/1	0.97	0.25	3.35	3,3,3,3	0
57	MG	RA	3150	1/1	0.96	0.33	3.34	37,37,37,37	0
57	MG	RA	3191	1/1	0.78	0.30	3.09	67,67,67,67	0
57	MG	RA	3160	1/1	0.96	0.34	3.09	4,4,4,4	0
57	MG	RA	3187	1/1	0.89	0.48	3.07	3,3,3,3	0
57	MG	YA	3245	1/1	0.88	0.30	3.04	2,2,2,2	0
57	MG	RA	3204	1/1	0.95	0.27	3.03	18,18,18,18	0
57	MG	YA	3256	1/1	0.90	0.39	2.91	7,7,7,7	0
57	MG	YA	3155	1/1	0.88	0.34	2.85	7,7,7,7	0
57	MG	RA	3136	1/1	0.96	0.37	2.82	0,0,0,0	0
57	MG	YA	3179	1/1	0.92	0.24	2.81	0,0,0,0	0
57	MG	YA	3072	1/1	0.95	0.21	2.80	2,2,2,2	0
57	MG	XA	1668	1/1	0.94	0.23	2.70	18,18,18,18	0
57	MG	RA	3024	1/1	0.96	0.23	2.64	16,16,16,16	0
57	MG	XA	1607	1/1	0.86	0.37	2.58	16,16,16,16	0
57	MG	RA	3064	1/1	0.96	0.18	2.55	5,5,5,5	0
57	MG	XA	1629	1/1	0.82	0.17	2.53	8,8,8,8	0
57	MG	RA	3102	1/1	0.95	0.28	2.49	4,4,4,4	0
57	MG	YA	3166	1/1	0.77	0.30	2.49	4,4,4,4	0
57	MG	RA	3198	1/1	0.92	0.17	2.44	12,12,12,12	0
57	MG	RA	3207	1/1	0.81	0.28	2.31	11,11,11,11	0
57	MG	RA	3075	1/1	0.98	0.19	2.27	3,3,3,3	0
57	MG	RA	3021	1/1	0.97	0.22	2.26	2,2,2,2	0
57	MG	RA	3184	1/1	0.96	0.26	2.23	8,8,8,8	0
57	MG	QA	1611	1/1	0.95	0.31	2.02	6,6,6,6	0
57	MG	RA	3185	1/1	0.90	0.18	1.96	9,9,9,9	0
57	MG	YA	3079	1/1	0.98	0.23	1.90	4,4,4,4	0
57	MG	XA	1659	1/1	0.95	0.32	1.83	0,0,0,0	0
57	MG	RA	3080	1/1	0.98	0.34	1.83	21,21,21,21	0
57	MG	YA	3032	1/1	0.94	0.28	1.82	1,1,1,1	0
57	MG	YA	3114	1/1	0.82	0.34	1.71	13,13,13,13	0
57	MG	XA	1645	1/1	0.97	0.24	1.64	1,1,1,1	0
57	MG	RA	3210	1/1	0.99	0.17	1.63	45,45,45,45	0
57	MG	RF	301	1/1	0.96	0.39	1.62	2,2,2,2	0
57	MG	YA	3241	1/1	0.98	0.18	1.58	5,5,5,5	0
57	MG	RA	3014	1/1	0.95	0.28	1.55	13,13,13,13	0
57	MG	QV	101	1/1	0.98	0.26	1.52	1,1,1,1	0
58	ZN	XD	301	1/1	0.99	0.42	1.51	50,50,50,50	0
57	MG	RA	3141	1/1	0.87	0.24	1.51	2,2,2,2	0
57	MG	RA	3129	1/1	0.91	0.21	1.45	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1671	1/1	0.88	0.22	1.45	3,3,3,3	0
57	MG	XA	1666	1/1	0.91	0.32	1.41	50,50,50,50	0
57	MG	YA	3165	1/1	0.86	0.23	1.38	11,11,11,11	0
57	MG	XA	1610	1/1	0.97	0.23	1.38	3,3,3,3	0
57	MG	RA	3086	1/1	0.97	0.24	1.36	0,0,0,0	0
57	MG	QA	1639	1/1	0.94	0.18	1.35	3,3,3,3	0
57	MG	XA	1611	1/1	0.95	0.31	1.35	7,7,7,7	0
57	MG	YA	3073	1/1	0.98	0.25	1.34	1,1,1,1	0
57	MG	QA	1643	1/1	0.92	0.29	1.30	33,33,33,33	0
57	MG	RD	301	1/1	0.81	0.47	1.27	1,1,1,1	0
57	MG	RA	3149	1/1	0.96	0.15	1.23	20,20,20,20	0
57	MG	YA	3105	1/1	0.98	0.18	1.13	4,4,4,4	0
57	MG	QA	1604	1/1	0.96	0.28	1.08	0,0,0,0	0
57	MG	RA	3099	1/1	0.98	0.24	1.06	10,10,10,10	0
57	MG	RA	3118	1/1	0.97	0.22	1.05	2,2,2,2	0
57	MG	YA	3159	1/1	0.82	0.21	1.01	6,6,6,6	0
57	MG	YA	3113	1/1	0.97	0.20	0.99	1,1,1,1	0
57	MG	RE	302	1/1	0.90	0.25	0.95	1,1,1,1	0
57	MG	YA	3111	1/1	0.95	0.21	0.91	15,15,15,15	0
57	MG	YA	3071	1/1	0.90	0.20	0.90	28,28,28,28	0
57	MG	QA	1659	1/1	0.97	0.23	0.89	4,4,4,4	0
57	MG	RR	201	1/1	0.98	0.24	0.83	13,13,13,13	0
57	MG	RA	3107	1/1	0.99	0.19	0.77	10,10,10,10	0
57	MG	YA	3169	1/1	0.91	0.17	0.69	6,6,6,6	0
57	MG	YA	3225	1/1	0.92	0.25	0.60	10,10,10,10	0
57	MG	YA	3198	1/1	0.92	0.25	0.56	51,51,51,51	0
57	MG	YA	3219	1/1	0.72	0.17	0.55	7,7,7,7	0
57	MG	YA	3025	1/1	0.98	0.19	0.53	4,4,4,4	0
57	MG	YA	3178	1/1	0.96	0.12	0.52	2,2,2,2	0
57	MG	YA	3239	1/1	0.90	0.20	0.46	5,5,5,5	0
57	MG	XA	1612	1/1	0.98	0.18	0.46	19,19,19,19	0
57	MG	YA	3130	1/1	0.97	0.21	0.42	20,20,20,20	0
57	MG	YA	3038	1/1	0.98	0.17	0.34	7,7,7,7	0
58	ZN	QD	301	1/1	0.91	0.35	0.32	50,50,50,50	0
57	MG	RA	3196	1/1	0.98	0.17	0.30	0,0,0,0	0
57	MG	YA	3154	1/1	0.92	0.23	0.15	1,1,1,1	0
57	MG	YA	3194	1/1	0.92	0.17	0.13	0,0,0,0	0
57	MG	RA	3215	1/1	0.94	0.17	0.10	27,27,27,27	0
57	MG	RA	3135	1/1	0.95	0.17	0.09	7,7,7,7	0
57	MG	YA	3240	1/1	0.94	0.17	0.08	72,72,72,72	0
57	MG	YA	3016	1/1	0.92	0.22	0.03	6,6,6,6	0
57	MG	RA	3042	1/1	0.98	0.18	0.02	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XB	301	1/1	0.83	0.33	0.01	2,2,2,2	0
57	MG	QA	1617	1/1	0.97	0.20	-0.02	4,4,4,4	0
57	MG	YB	203	1/1	0.92	0.23	-0.12	37,37,37,37	0
57	MG	RA	3068	1/1	0.95	0.12	-0.12	6,6,6,6	0
57	MG	YA	3143	1/1	0.96	0.15	-0.12	8,8,8,8	0
57	MG	YA	3216	1/1	0.98	0.16	-0.13	19,19,19,19	0
57	MG	XA	1649	1/1	0.91	0.20	-0.19	0,0,0,0	0
57	MG	XA	1661	1/1	0.93	0.16	-0.35	2,2,2,2	0
57	MG	QA	1657	1/1	0.91	0.14	-0.46	7,7,7,7	0
57	MG	RA	3074	1/1	0.96	0.13	-0.53	8,8,8,8	0
57	MG	RA	3154	1/1	0.96	0.18	-0.54	11,11,11,11	0
57	MG	XA	1644	1/1	0.97	0.14	-0.62	5,5,5,5	0
57	MG	QA	1632	1/1	0.80	0.14	-0.63	42,42,42,42	0
57	MG	XA	1625	1/1	0.93	0.17	-0.63	5,5,5,5	0
58	ZN	XN	101	1/1	0.98	0.20	-0.71	84,84,84,84	0
57	MG	YA	3264	1/1	0.95	0.17	-0.76	9,9,9,9	0
57	MG	YA	3056	1/1	0.97	0.18	-0.86	5,5,5,5	0
57	MG	RA	3161	1/1	0.96	0.13	-0.92	1,1,1,1	0
57	MG	YA	3136	1/1	0.95	0.12	-0.92	21,21,21,21	0
57	MG	QA	1606	1/1	0.98	0.13	-0.93	16,16,16,16	0
57	MG	YA	3017	1/1	0.98	0.17	-0.94	1,1,1,1	0
57	MG	YA	3138	1/1	0.97	0.12	-1.03	0,0,0,0	0
57	MG	RA	3112	1/1	0.94	0.18	-1.05	6,6,6,6	0
57	MG	YA	3112	1/1	0.97	0.13	-1.06	21,21,21,21	0
57	MG	XA	1614	1/1	0.97	0.15	-1.09	26,26,26,26	0
57	MG	QA	1645	1/1	0.96	0.13	-1.09	38,38,38,38	0
57	MG	RA	3132	1/1	0.87	0.16	-1.11	3,3,3,3	0
57	MG	XA	1660	1/1	0.95	0.13	-1.12	24,24,24,24	0
57	MG	QM	201	1/1	0.99	0.14	-1.22	44,44,44,44	0
57	MG	XA	1608	1/1	0.92	0.13	-1.22	37,37,37,37	0
57	MG	YA	3185	1/1	0.90	0.14	-1.26	2,2,2,2	0
58	ZN	QN	101	1/1	0.87	0.13	-1.33	104,104,104,104	0
57	MG	YA	3187	1/1	0.98	0.13	-1.33	2,2,2,2	0
57	MG	RA	3045	1/1	0.93	0.13	-1.36	1,1,1,1	0
58	ZN	R9	101	1/1	0.92	0.41	-1.36	145,145,145,145	0
57	MG	XA	1626	1/1	0.97	0.16	-1.36	6,6,6,6	0
57	MG	YP	201	1/1	0.83	0.16	-1.37	94,94,94,94	0
58	ZN	Y9	101	1/1	0.91	0.47	-1.41	138,138,138,138	0
57	MG	YA	3231	1/1	0.98	0.11	-1.41	45,45,45,45	0
57	MG	RA	3100	1/1	0.98	0.14	-1.41	2,2,2,2	0
57	MG	RA	3123	1/1	0.98	0.12	-1.44	7,7,7,7	0
57	MG	QA	1654	1/1	0.97	0.13	-1.49	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3144	1/1	0.94	0.12	-1.62	4,4,4,4	0
57	MG	QA	1616	1/1	0.96	0.09	-1.73	29,29,29,29	0
57	MG	YA	3133	1/1	0.92	0.13	-1.85	1,1,1,1	0
57	MG	RA	3146	1/1	0.97	0.13	-1.85	5,5,5,5	0
57	MG	RA	3156	1/1	0.98	0.13	-2.05	9,9,9,9	0
57	MG	YA	3065	1/1	0.99	0.15	-2.07	5,5,5,5	0
57	MG	RB	201	1/1	0.93	0.13	-2.11	8,8,8,8	0
57	MG	YA	3027	1/1	0.98	0.11	-2.32	1,1,1,1	0
57	MG	YA	3205	1/1	0.94	0.14	-2.53	10,10,10,10	0
57	MG	YA	3061	1/1	0.97	0.12	-2.75	17,17,17,17	0
57	MG	QA	1630	1/1	0.98	0.15	-3.19	7,7,7,7	0
57	MG	YA	3199	1/1	0.97	0.11	-3.22	55,55,55,55	0
57	MG	YA	3191	1/1	0.97	0.05	-4.57	7,7,7,7	0
57	MG	QA	1619	1/1	0.93	0.45	-	4,4,4,4	0
57	MG	R5	101	1/1	0.89	0.52	-	5,5,5,5	0
57	MG	XA	1657	1/1	0.89	0.42	-	8,8,8,8	0
57	MG	YA	3161	1/1	0.95	0.20	-	1,1,1,1	0
57	MG	RA	3092	1/1	0.95	0.54	-	7,7,7,7	0
57	MG	YA	3248	1/1	0.85	0.44	-	0,0,0,0	0
57	MG	XA	1654	1/1	0.93	0.29	-	26,26,26,26	0
57	MG	YA	3255	1/1	0.95	1.31	-	0,0,0,0	0
57	MG	YA	3177	1/1	0.99	0.22	-	3,3,3,3	0
57	MG	YA	3122	1/1	0.86	0.40	-	3,3,3,3	0
57	MG	RA	3041	1/1	0.93	0.44	-	4,4,4,4	0
57	MG	YA	3158	1/1	0.96	0.27	-	6,6,6,6	0
57	MG	XA	1667	1/1	0.75	0.27	-	17,17,17,17	0
57	MG	YA	3001	1/1	0.86	1.21	-	50,50,50,50	0
57	MG	RA	3032	1/1	0.86	1.18	-	50,50,50,50	0
57	MG	R8	101	1/1	0.73	0.37	-	0,0,0,0	0
57	MG	YA	3097	1/1	0.96	0.65	-	5,5,5,5	0
57	MG	RA	3114	1/1	0.89	0.33	-	1,1,1,1	0
57	MG	YA	3062	1/1	0.99	0.39	-	6,6,6,6	0
57	MG	YA	3196	1/1	0.60	0.51	-	1,1,1,1	0
57	MG	RA	3230	1/1	0.92	0.74	-	5,5,5,5	0
57	MG	YA	3137	1/1	0.97	0.21	-	10,10,10,10	0
57	MG	YA	3224	1/1	0.89	0.38	-	0,0,0,0	0
57	MG	RA	3157	1/1	0.77	0.55	-	0,0,0,0	0
57	MG	XA	1663	1/1	0.81	0.54	-	15,15,15,15	0
57	MG	RA	3235	1/1	0.92	0.62	-	1,1,1,1	0
57	MG	RA	3205	1/1	0.96	0.31	-	12,12,12,12	0
57	MG	YA	3055	1/1	0.97	0.26	-	0,0,0,0	0
57	MG	XA	1630	1/1	0.89	0.64	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3040	1/1	0.97	0.54	-	10,10,10,10	0
57	MG	YA	3254	1/1	0.67	0.63	-	2,2,2,2	0
57	MG	QF	201	1/1	0.44	1.08	-	36,36,36,36	0
57	MG	XA	1633	1/1	0.98	0.21	-	3,3,3,3	0
57	MG	RA	3110	1/1	0.92	0.48	-	3,3,3,3	0
57	MG	RA	3239	1/1	0.65	0.49	-	14,14,14,14	0
57	MG	YA	3067	1/1	0.99	0.34	-	5,5,5,5	0
57	MG	XA	1652	1/1	0.90	0.33	-	66,66,66,66	0
57	MG	QA	1637	1/1	0.84	0.31	-	0,0,0,0	0
57	MG	RA	3225	1/1	0.70	0.25	-	10,10,10,10	0
57	MG	YA	3153	1/1	0.91	0.41	-	20,20,20,20	0
57	MG	RA	3144	1/1	0.97	0.26	-	0,0,0,0	0
57	MG	RA	3016	1/1	0.95	0.39	-	8,8,8,8	0
57	MG	QA	1660	1/1	0.99	0.76	-	2,2,2,2	0
57	MG	RA	3214	1/1	0.92	0.34	-	5,5,5,5	0
57	MG	XA	1631	1/1	0.91	0.20	-	31,31,31,31	0
57	MG	XA	1650	1/1	0.84	0.28	-	18,18,18,18	0
57	MG	RA	3067	1/1	0.93	0.26	-	2,2,2,2	0
57	MG	YA	3007	1/1	0.95	0.17	-	7,7,7,7	0
57	MG	YA	3200	1/1	0.89	0.92	-	4,4,4,4	0
57	MG	RA	3109	1/1	0.98	0.23	-	8,8,8,8	0
57	MG	QA	1625	1/1	0.95	0.30	-	0,0,0,0	0
57	MG	YA	3228	1/1	0.97	0.50	-	17,17,17,17	0
57	MG	YA	3188	1/1	0.88	0.51	-	1,1,1,1	0
57	MG	YA	3195	1/1	0.96	0.39	-	9,9,9,9	0
57	MG	YA	3267	1/1	0.93	0.41	-	4,4,4,4	0
57	MG	RA	3029	1/1	0.95	0.37	-	1,1,1,1	0
57	MG	YA	3102	1/1	0.97	0.47	-	14,14,14,14	0
57	MG	RA	3047	1/1	0.95	0.63	-	5,5,5,5	0
57	MG	QA	1651	1/1	0.94	0.22	-	9,9,9,9	0
57	MG	XA	1603	1/1	0.89	0.62	-	8,8,8,8	0
57	MG	RA	3163	1/1	0.97	1.01	-	12,12,12,12	0
57	MG	YA	3085	1/1	0.86	0.61	-	13,13,13,13	0
57	MG	RA	3233	1/1	0.89	0.64	-	2,2,2,2	0
57	MG	RR	202	1/1	0.90	0.34	-	0,0,0,0	0
57	MG	YA	3140	1/1	0.84	0.25	-	12,12,12,12	0
57	MG	RA	3167	1/1	0.96	0.23	-	3,3,3,3	0
57	MG	XA	1669	1/1	0.97	0.19	-	38,38,38,38	0
57	MG	QA	1650	1/1	0.80	0.61	-	11,11,11,11	0
57	MG	RA	3203	1/1	0.76	0.38	-	24,24,24,24	0
57	MG	XA	1632	1/1	0.97	0.81	-	14,14,14,14	0
59	A	XX	101	22/23	0.78	0.30	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3227	1/1	0.95	0.29	-	0,0,0,0	0
57	MG	YQ	201	1/1	0.96	0.21	-	99,99,99,99	0
57	MG	RA	3050	1/1	0.93	0.56	-	11,11,11,11	0
57	MG	YA	3082	1/1	0.96	0.24	-	3,3,3,3	0
57	MG	RA	3190	1/1	0.95	0.19	-	16,16,16,16	0
57	MG	YA	3088	1/1	0.93	0.58	-	50,50,50,50	0
57	MG	RA	3134	1/1	0.95	0.13	-	25,25,25,25	0
57	MG	XA	1623	1/1	0.98	0.16	-	14,14,14,14	0
57	MG	RA	3236	1/1	0.94	0.45	-	0,0,0,0	0
57	MG	RA	3053	1/1	0.96	0.16	-	2,2,2,2	0
57	MG	RA	3193	1/1	0.88	0.32	-	22,22,22,22	0
57	MG	XA	1624	1/1	0.92	0.59	-	3,3,3,3	0
57	MG	XX	102	1/1	0.96	0.09	-	50,50,50,50	0
57	MG	YA	3208	1/1	0.94	0.21	-	15,15,15,15	0
57	MG	RA	3003	1/1	0.74	0.93	-	5,5,5,5	0
57	MG	RA	3165	1/1	0.99	0.48	-	13,13,13,13	0
57	MG	QA	1605	1/1	0.95	1.07	-	7,7,7,7	0
57	MG	RA	3175	1/1	0.90	0.12	-	1,1,1,1	0
57	MG	YA	3110	1/1	0.99	0.12	-	2,2,2,2	0
57	MG	RA	3194	1/1	0.91	0.28	-	6,6,6,6	0
57	MG	YA	3269	1/1	0.89	0.78	-	1,1,1,1	0
57	MG	YA	3119	1/1	0.88	0.78	-	8,8,8,8	0
57	MG	RA	3082	1/1	0.99	0.31	-	0,0,0,0	0
57	MG	YA	3221	1/1	0.94	0.50	-	18,18,18,18	0
57	MG	RA	3151	1/1	0.96	0.41	-	9,9,9,9	0
57	MG	QA	1621	1/1	0.96	0.11	-	5,5,5,5	0
57	MG	RB	202	1/1	0.94	0.08	-	4,4,4,4	0
57	MG	YA	3086	1/1	0.94	0.78	-	6,6,6,6	0
57	MG	YA	3128	1/1	0.86	0.57	-	12,12,12,12	0
57	MG	XA	1601	1/1	0.93	0.95	-	1,1,1,1	0
57	MG	YA	3223	1/1	0.97	0.42	-	34,34,34,34	0
57	MG	RA	3037	1/1	0.98	0.51	-	5,5,5,5	0
57	MG	Y5	101	1/1	0.98	0.36	-	6,6,6,6	0
57	MG	QA	1655	1/1	0.88	0.66	-	20,20,20,20	0
57	MG	XA	1613	1/1	0.99	0.08	-	0,0,0,0	0
57	MG	RA	3101	1/1	0.92	0.45	-	11,11,11,11	0
57	MG	QA	1653	1/1	0.99	0.08	-	67,67,67,67	0
57	MG	YA	3193	1/1	0.86	0.20	-	3,3,3,3	0
57	MG	RA	3133	1/1	0.98	0.16	-	0,0,0,0	0
57	MG	YA	3064	1/1	0.97	0.35	-	8,8,8,8	0
57	MG	RA	3172	1/1	0.81	0.48	-	4,4,4,4	0
57	MG	YA	3197	1/1	0.97	0.15	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3125	1/1	0.95	0.41	-	12,12,12,12	0
57	MG	Y7	101	1/1	0.88	0.73	-	15,15,15,15	0
57	MG	YA	3018	1/1	0.98	0.69	-	3,3,3,3	0
57	MG	RA	3066	1/1	0.99	0.53	-	6,6,6,6	0
57	MG	RA	3142	1/1	0.87	0.48	-	36,36,36,36	0
57	MG	YA	3182	1/1	0.99	0.13	-	8,8,8,8	0
57	MG	QA	1663	1/1	0.96	0.10	-	47,47,47,47	0
57	MG	RA	3152	1/1	0.93	0.14	-	4,4,4,4	0
57	MG	YA	3127	1/1	0.92	0.29	-	2,2,2,2	0
57	MG	XA	1602	1/1	0.99	0.20	-	7,7,7,7	0
57	MG	RA	3182	1/1	0.89	0.21	-	4,4,4,4	0
57	MG	XA	1606	1/1	0.92	0.56	-	10,10,10,10	0
57	MG	YA	3098	1/1	0.97	0.29	-	1,1,1,1	0
57	MG	YA	3190	1/1	0.95	0.24	-	21,21,21,21	0
57	MG	RA	3011	1/1	0.98	0.18	-	6,6,6,6	0
57	MG	RA	3234	1/1	0.88	0.34	-	9,9,9,9	0
57	MG	RA	3176	1/1	0.84	0.32	-	3,3,3,3	0
57	MG	RA	3237	1/1	0.94	1.23	-	1,1,1,1	0
57	MG	XA	1647	1/1	0.88	0.37	-	1,1,1,1	0
57	MG	RA	3090	1/1	0.96	0.15	-	75,75,75,75	0
57	MG	YA	3204	1/1	0.96	0.10	-	11,11,11,11	0
57	MG	QA	1607	1/1	0.94	0.11	-	13,13,13,13	0
57	MG	RA	3108	1/1	0.97	0.09	-	0,0,0,0	0
57	MG	YA	3170	1/1	0.97	0.20	-	8,8,8,8	0
57	MG	RA	3025	1/1	0.86	0.14	-	3,3,3,3	0
57	MG	RA	3192	1/1	0.87	0.27	-	21,21,21,21	0
57	MG	YA	3180	1/1	0.94	0.41	-	38,38,38,38	0
57	MG	YA	3077	1/1	0.97	0.30	-	2,2,2,2	0
57	MG	R0	101	1/1	0.83	0.29	-	0,0,0,0	0
57	MG	YA	3020	1/1	0.99	0.86	-	0,0,0,0	0
57	MG	QA	1638	1/1	0.82	0.64	-	34,34,34,34	0
57	MG	YA	3244	1/1	1.00	0.10	-	9,9,9,9	0
57	MG	YA	3046	1/1	0.97	0.40	-	3,3,3,3	0
57	MG	QA	1652	1/1	0.97	0.16	-	12,12,12,12	0
57	MG	RA	3124	1/1	0.97	0.34	-	10,10,10,10	0
57	MG	QA	1627	1/1	0.93	0.21	-	10,10,10,10	0
57	MG	YA	3151	1/1	0.88	0.17	-	5,5,5,5	0
57	MG	YA	3237	1/1	0.86	0.32	-	7,7,7,7	0
57	MG	RA	3046	1/1	0.80	0.87	-	50,50,50,50	0
57	MG	RA	3084	1/1	0.96	0.16	-	4,4,4,4	0
57	MG	YA	3148	1/1	0.98	0.14	-	7,7,7,7	0
57	MG	XA	1622	1/1	0.95	0.13	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3093	1/1	0.97	0.36	-	7,7,7,7	0
57	MG	YA	3022	1/1	0.99	0.28	-	1,1,1,1	0
57	MG	RA	3060	1/1	0.98	0.30	-	6,6,6,6	0
57	MG	YA	3156	1/1	0.91	0.58	-	2,2,2,2	0
57	MG	YA	3094	1/1	0.93	0.91	-	11,11,11,11	0
57	MG	YA	3076	1/1	0.69	1.29	-	50,50,50,50	0
57	MG	RA	3018	1/1	0.91	0.73	-	6,6,6,6	0
57	MG	YA	3131	1/1	0.66	0.41	-	3,3,3,3	0
57	MG	RA	3007	1/1	0.76	0.41	-	16,16,16,16	0
57	MG	RA	3095	1/1	0.96	0.80	-	1,1,1,1	0
57	MG	YA	3202	1/1	0.91	0.25	-	1,1,1,1	0
57	MG	RA	3043	1/1	0.95	0.20	-	10,10,10,10	0
57	MG	YA	3174	1/1	0.90	0.22	-	40,40,40,40	0
57	MG	RA	3211	1/1	0.94	0.24	-	2,2,2,2	0
57	MG	YA	3183	1/1	0.66	0.55	-	16,16,16,16	0
57	MG	YA	3051	1/1	0.98	0.44	-	3,3,3,3	0
57	MG	RA	3059	1/1	0.98	0.44	-	11,11,11,11	0
57	MG	YA	3019	1/1	0.95	0.47	-	5,5,5,5	0
57	MG	RA	3111	1/1	0.95	0.47	-	11,11,11,11	0
57	MG	YA	3211	1/1	0.94	0.59	-	7,7,7,7	0
57	MG	YA	3066	1/1	0.89	0.59	-	7,7,7,7	0
57	MG	XA	1640	1/1	0.98	0.12	-	75,75,75,75	0
57	MG	RA	3096	1/1	0.98	0.58	-	4,4,4,4	0
57	MG	RA	3189	1/1	0.96	0.27	-	4,4,4,4	0
57	MG	YA	3030	1/1	0.78	0.95	-	5,5,5,5	0
57	MG	YA	3162	1/1	0.97	0.18	-	0,0,0,0	0
57	MG	XA	1648	1/1	0.88	0.57	-	3,3,3,3	0
57	MG	QA	1641	1/1	0.95	0.23	-	7,7,7,7	0
57	MG	RA	3166	1/1	0.49	0.29	-	34,34,34,34	0
57	MG	RA	3119	1/1	0.96	0.39	-	3,3,3,3	0
57	MG	YA	3163	1/1	0.95	0.21	-	4,4,4,4	0
57	MG	YA	3060	1/1	0.98	0.59	-	10,10,10,10	0
57	MG	RA	3181	1/1	0.95	0.20	-	3,3,3,3	0
57	MG	YA	3203	1/1	0.91	0.15	-	53,53,53,53	0
57	MG	YA	3238	1/1	0.85	0.29	-	11,11,11,11	0
57	MG	XA	1605	1/1	0.90	0.57	-	3,3,3,3	0
57	MG	RA	3177	1/1	0.89	0.79	-	7,7,7,7	0
57	MG	YA	3242	1/1	0.76	0.79	-	4,4,4,4	0
57	MG	RA	3061	1/1	0.96	0.16	-	53,53,53,53	0
57	MG	RA	3174	1/1	0.92	0.52	-	4,4,4,4	0
57	MG	YA	3192	1/1	0.91	0.52	-	11,11,11,11	0
57	MG	YA	3233	1/1	0.97	0.23	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3043	1/1	0.94	1.16	-	2,2,2,2	0
57	MG	YA	3103	1/1	0.90	0.14	-	5,5,5,5	0
57	MG	YA	3010	1/1	0.97	0.40	-	5,5,5,5	0
57	MG	YA	3003	1/1	0.97	0.17	-	2,2,2,2	0
57	MG	RE	301	1/1	0.92	0.27	-	12,12,12,12	0
57	MG	YA	3123	1/1	0.95	0.19	-	18,18,18,18	0
57	MG	YA	3142	1/1	0.93	0.66	-	19,19,19,19	0
57	MG	YA	3104	1/1	0.96	0.59	-	10,10,10,10	0
57	MG	YA	3075	1/1	0.89	0.26	-	0,0,0,0	0
57	MG	QA	1633	1/1	0.94	0.58	-	4,4,4,4	0
57	MG	RA	3231	1/1	0.93	0.30	-	14,14,14,14	0
57	MG	RA	3127	1/1	0.99	0.22	-	0,0,0,0	0
57	MG	YA	3222	1/1	0.92	0.19	-	8,8,8,8	0
57	MG	YA	3252	1/1	0.84	0.76	-	8,8,8,8	0
57	MG	RA	3104	1/1	0.99	0.20	-	3,3,3,3	0
57	MG	RA	3023	1/1	0.98	0.32	-	16,16,16,16	0
57	MG	YA	3117	1/1	0.85	0.99	-	6,6,6,6	0
57	MG	RA	3137	1/1	0.83	0.44	-	10,10,10,10	0
57	MG	QA	1626	1/1	0.87	0.40	-	57,57,57,57	0
57	MG	RA	3076	1/1	0.86	0.53	-	7,7,7,7	0
57	MG	RA	3228	1/1	0.98	0.50	-	11,11,11,11	0
57	MG	RA	3199	1/1	0.77	0.74	-	6,6,6,6	0
57	MG	YA	3134	1/1	0.95	0.78	-	11,11,11,11	0
57	MG	RA	3147	1/1	0.96	0.23	-	9,9,9,9	0
57	MG	XM	201	1/1	0.92	0.11	-	85,85,85,85	0
57	MG	YB	201	1/1	0.81	0.31	-	7,7,7,7	0
57	MG	RA	3229	1/1	0.87	1.51	-	50,50,50,50	0
57	MG	RA	3202	1/1	0.83	0.15	-	16,16,16,16	0
57	MG	YA	3147	1/1	0.98	0.57	-	4,4,4,4	0
57	MG	QA	1636	1/1	0.89	0.12	-	16,16,16,16	0
57	MG	YA	3184	1/1	0.76	0.32	-	7,7,7,7	0
57	MG	RA	3057	1/1	0.99	0.31	-	2,2,2,2	0
57	MG	YA	3243	1/1	0.86	0.42	-	32,32,32,32	0
57	MG	RA	3115	1/1	0.97	0.45	-	6,6,6,6	0
57	MG	YA	3149	1/1	0.92	0.20	-	15,15,15,15	0
57	MG	YA	3258	1/1	0.94	0.52	-	1,1,1,1	0
57	MG	QH	201	1/1	0.90	0.20	-	47,47,47,47	0
57	MG	RA	3224	1/1	0.80	0.39	-	5,5,5,5	0
57	MG	QA	1662	1/1	0.84	0.27	-	37,37,37,37	0
57	MG	QA	1609	1/1	0.92	0.71	-	4,4,4,4	0
57	MG	YA	3135	1/1	0.92	0.25	-	6,6,6,6	0
57	MG	YA	3234	1/1	0.91	0.54	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3215	1/1	0.95	0.18	-	14,14,14,14	0
57	MG	RA	3232	1/1	0.93	0.39	-	13,13,13,13	0
57	MG	YA	3146	1/1	0.89	0.44	-	0,0,0,0	0
57	MG	QA	1603	1/1	0.88	0.94	-	14,14,14,14	0
57	MG	RA	3197	1/1	0.80	0.66	-	3,3,3,3	0
57	MG	RA	3006	1/1	0.86	0.99	-	50,50,50,50	0
57	MG	YA	3261	1/1	0.92	0.30	-	4,4,4,4	0
57	MG	YA	3157	1/1	0.92	0.63	-	0,0,0,0	0
57	MG	YA	3081	1/1	0.97	0.50	-	9,9,9,9	0
57	MG	YA	3059	1/1	0.97	0.32	-	5,5,5,5	0
57	MG	RA	3179	1/1	0.79	0.38	-	4,4,4,4	0
57	MG	YA	3106	1/1	0.94	0.34	-	8,8,8,8	0
57	MG	RA	3113	1/1	0.98	0.11	-	0,0,0,0	0
57	MG	XA	1627	1/1	0.81	0.27	-	14,14,14,14	0
57	MG	RA	3001	1/1	0.91	0.60	-	3,3,3,3	0
57	MG	XA	1616	1/1	0.98	0.31	-	1,1,1,1	0
57	MG	YA	3226	1/1	0.98	0.38	-	1,1,1,1	0
57	MG	YA	3181	1/1	0.92	0.34	-	3,3,3,3	0
57	MG	YA	3054	1/1	0.93	0.31	-	1,1,1,1	0
57	MG	RA	3051	1/1	0.96	0.47	-	7,7,7,7	0
57	MG	YA	3251	1/1	0.94	0.17	-	9,9,9,9	0
57	MG	RA	3073	1/1	0.99	0.35	-	2,2,2,2	0
57	MG	RA	3083	1/1	0.89	0.39	-	6,6,6,6	0
57	MG	RA	3227	1/1	0.59	0.57	-	22,22,22,22	0
57	MG	YA	3232	1/1	0.96	0.42	-	2,2,2,2	0
57	MG	QA	1629	1/1	0.64	0.85	-	0,0,0,0	0
57	MG	RA	3028	1/1	0.92	0.47	-	14,14,14,14	0
57	MG	QA	1658	1/1	0.99	0.24	-	16,16,16,16	0
57	MG	QA	1612	1/1	0.92	0.46	-	7,7,7,7	0
57	MG	RA	3221	1/1	0.81	0.33	-	22,22,22,22	0
57	MG	QX	101	1/1	0.79	0.41	-	4,4,4,4	0
57	MG	QA	1664	1/1	0.85	0.41	-	54,54,54,54	0
57	MG	YA	3253	1/1	0.94	0.59	-	6,6,6,6	0
57	MG	QA	1661	1/1	0.61	0.33	-	64,64,64,64	0
57	MG	YE	301	1/1	0.94	0.18	-	0,0,0,0	0
57	MG	QA	1634	1/1	0.98	0.18	-	7,7,7,7	0
57	MG	YA	3021	1/1	0.97	0.43	-	12,12,12,12	0
57	MG	YA	3260	1/1	0.84	0.97	-	50,50,50,50	0
57	MG	XA	1641	1/1	0.91	1.18	-	21,21,21,21	0
57	MG	YA	3268	1/1	0.90	0.53	-	6,6,6,6	0
57	MG	YA	3121	1/1	0.79	0.42	-	62,62,62,62	0
57	MG	XA	1658	1/1	0.94	0.43	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1642	1/1	0.77	0.72	-	5,5,5,5	0
57	MG	XA	1639	1/1	0.99	0.12	-	5,5,5,5	0
57	MG	XA	1617	1/1	0.98	0.22	-	15,15,15,15	0
57	MG	QA	1648	1/1	0.94	0.32	-	12,12,12,12	0
57	MG	QA	1601	1/1	0.83	0.36	-	9,9,9,9	0
57	MG	YA	3214	1/1	0.99	0.20	-	2,2,2,2	0
57	MG	YA	3257	1/1	0.99	0.23	-	3,3,3,3	0
57	MG	YA	3230	1/1	0.86	0.16	-	8,8,8,8	0
57	MG	RA	3162	1/1	0.90	0.23	-	2,2,2,2	0
57	MG	RA	3044	1/1	0.91	0.86	-	10,10,10,10	0
57	MG	YA	3048	1/1	0.97	0.22	-	4,4,4,4	0
57	MG	QA	1624	1/1	0.85	0.66	-	0,0,0,0	0
57	MG	QA	1647	1/1	0.97	0.26	-	33,33,33,33	0
57	MG	QA	1644	1/1	0.94	0.26	-	4,4,4,4	0
57	MG	RA	3078	1/1	0.99	0.35	-	3,3,3,3	0
57	MG	RA	3027	1/1	0.97	0.49	-	13,13,13,13	0
57	MG	RA	3070	1/1	0.84	0.90	-	0,0,0,0	0
57	MG	XA	1634	1/1	0.94	0.56	-	0,0,0,0	0
57	MG	RA	3039	1/1	0.86	0.36	-	10,10,10,10	0
57	MG	YA	3129	1/1	0.97	0.70	-	15,15,15,15	0
57	MG	YA	3084	1/1	0.89	0.27	-	17,17,17,17	0
57	MG	RA	3171	1/1	0.90	0.19	-	12,12,12,12	0
57	MG	YA	3213	1/1	0.98	0.13	-	19,19,19,19	0
57	MG	YA	3150	1/1	0.94	0.42	-	4,4,4,4	0
57	MG	XA	1655	1/1	0.81	0.29	-	9,9,9,9	0
57	MG	QA	1602	1/1	0.93	0.80	-	12,12,12,12	0
57	MG	RA	3195	1/1	0.88	0.25	-	24,24,24,24	0
57	MG	RA	3186	1/1	0.94	0.23	-	8,8,8,8	0
57	MG	YA	3173	1/1	0.90	0.30	-	35,35,35,35	0
57	MG	XA	1662	1/1	0.86	0.88	-	11,11,11,11	0
57	MG	YA	3189	1/1	0.92	0.55	-	6,6,6,6	0
57	MG	YA	3052	1/1	0.96	0.70	-	14,14,14,14	0
57	MG	YA	3039	1/1	0.84	0.28	-	6,6,6,6	0
57	MG	YA	3124	1/1	0.94	0.21	-	9,9,9,9	0
57	MG	YA	3045	1/1	0.86	0.53	-	13,13,13,13	0
57	MG	RA	3216	1/1	0.92	0.52	-	7,7,7,7	0
57	MG	YA	3250	1/1	0.75	1.17	-	11,11,11,11	0
57	MG	RA	3217	1/1	0.96	0.21	-	74,74,74,74	0
57	MG	RA	3139	1/1	0.96	0.24	-	2,2,2,2	0
57	MG	XA	1670	1/1	0.94	0.16	-	43,43,43,43	0
57	MG	XA	1609	1/1	0.91	0.52	-	10,10,10,10	0
57	MG	XA	1643	1/1	0.96	0.38	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3201	1/1	0.96	0.77	-	10,10,10,10	0
57	MG	RA	3126	1/1	0.96	0.44	-	2,2,2,2	0
57	MG	RA	3091	1/1	0.96	0.44	-	9,9,9,9	0
57	MG	YA	3249	1/1	0.98	0.30	-	10,10,10,10	0
57	MG	RA	3226	1/1	0.54	0.37	-	9,9,9,9	0
57	MG	QA	1642	1/1	0.93	0.49	-	16,16,16,16	0
57	MG	YA	3096	1/1	0.95	0.53	-	3,3,3,3	0
57	MG	RA	3173	1/1	0.78	0.51	-	48,48,48,48	0
57	MG	QA	1640	1/1	0.92	0.35	-	9,9,9,9	0
57	MG	YA	3092	1/1	0.98	0.25	-	12,12,12,12	0
57	MG	YA	3247	1/1	0.86	0.38	-	14,14,14,14	0
57	MG	YB	202	1/1	0.86	0.68	-	24,24,24,24	0
57	MG	RA	3071	1/1	0.86	0.23	-	1,1,1,1	0
57	MG	RA	3010	1/1	0.94	0.51	-	14,14,14,14	0
57	MG	RA	3155	1/1	0.89	0.39	-	10,10,10,10	0
57	MG	QA	1608	1/1	0.98	0.10	-	10,10,10,10	0
57	MG	RA	3169	1/1	0.85	0.24	-	16,16,16,16	0
57	MG	XA	1672	1/1	0.95	0.41	-	0,0,0,0	0
57	MG	YA	3217	1/1	0.97	0.17	-	35,35,35,35	0
57	MG	RA	3180	1/1	0.96	0.11	-	6,6,6,6	0
57	MG	RA	3048	1/1	0.86	0.21	-	3,3,3,3	0
57	MG	RA	3117	1/1	0.90	0.15	-	25,25,25,25	0
57	MG	YA	3164	1/1	0.94	0.46	-	8,8,8,8	0
57	MG	RA	3013	1/1	0.94	0.53	-	4,4,4,4	0
57	MG	YA	3083	1/1	0.97	0.50	-	9,9,9,9	0
57	MG	RA	3213	1/1	0.50	0.50	-	8,8,8,8	0
57	MG	RA	3145	1/1	0.94	0.47	-	3,3,3,3	0
57	MG	RA	3209	1/1	0.88	0.34	-	17,17,17,17	0
57	MG	RA	3188	1/1	0.91	0.33	-	5,5,5,5	0
57	MG	YA	3175	1/1	0.86	0.24	-	9,9,9,9	0
57	MG	QA	1623	1/1	0.80	0.42	-	14,14,14,14	0
57	MG	YA	3089	1/1	0.96	0.43	-	5,5,5,5	0
57	MG	RA	3069	1/1	0.84	0.82	-	4,4,4,4	0
57	MG	RA	3143	1/1	0.94	0.30	-	7,7,7,7	0
57	MG	QA	1615	1/1	0.86	0.79	-	4,4,4,4	0
57	MG	RA	3138	1/1	0.52	0.76	-	29,29,29,29	0
57	MG	RA	3168	1/1	0.84	0.47	-	1,1,1,1	0
57	MG	RA	3103	1/1	0.97	0.48	-	9,9,9,9	0
57	MG	RA	3148	1/1	0.99	0.34	-	5,5,5,5	0
57	MG	YA	3029	1/1	0.98	0.81	-	10,10,10,10	0
57	MG	YA	3132	1/1	0.93	0.10	-	5,5,5,5	0
57	MG	RA	3200	1/1	0.96	0.14	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3030	1/1	0.98	0.36	-	5,5,5,5	0
57	MG	XA	1620	1/1	0.94	0.16	-	2,2,2,2	0
57	MG	QA	1628	1/1	0.91	0.21	-	8,8,8,8	0
57	MG	YA	3152	1/1	0.77	0.66	-	5,5,5,5	0
57	MG	YA	3063	1/1	0.80	0.29	-	11,11,11,11	0
57	MG	XV	102	1/1	0.90	0.65	-	9,9,9,9	0
57	MG	QA	1656	1/1	0.93	0.14	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.