



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:16 PM GMT

PDB ID : 4LNT  
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-07-12  
Resolution : 2.94 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](mailto: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.

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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

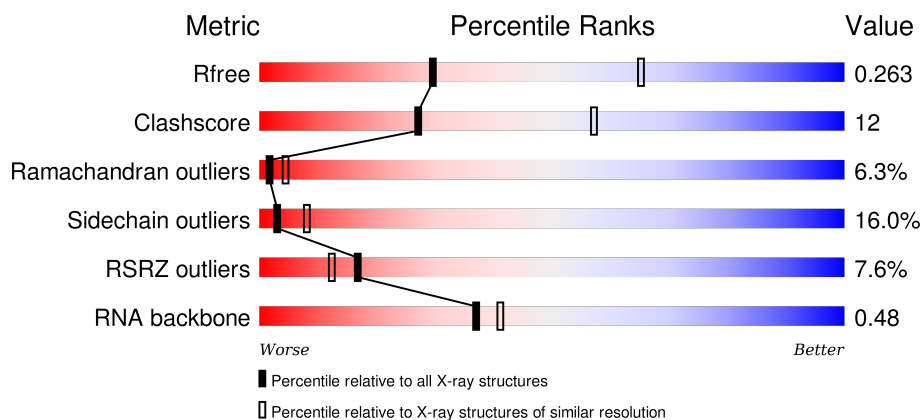
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)
RNA backbone	2183	1014 (3.34-2.54)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>27%</span> <span>51%</span> <span>36%</span> <span>10%</span> <span>..</span> </div> </div>
1	XA	1522	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>50%</span> <span>35%</span> <span>12%</span> <span>..</span> </div> </div>
2	QB	256	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>49%</span> <span>36%</span> <span>7%</span> <span>7%</span> </div> </div>
2	XB	256	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>46%</span> <span>36%</span> <span>9%</span> <span>7%</span> </div> </div>

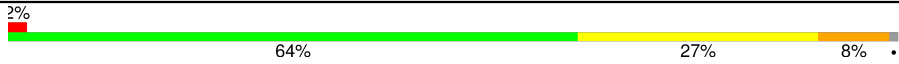





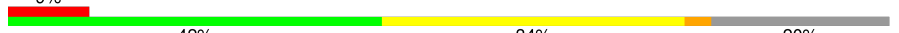
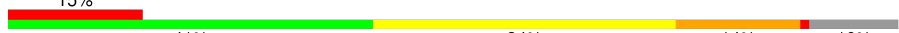







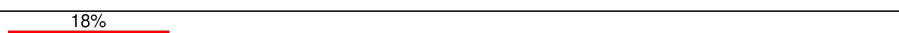
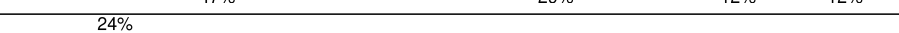





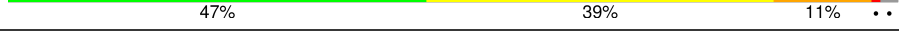


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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QY	17	
23	XY	17	
24	QX	25	
24	XX	25	
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	1604	-	-	-	X
57	MG	QA	1610	-	-	-	X
57	MG	QA	1612	-	-	-	X
57	MG	QA	1613	-	-	-	X
57	MG	QA	1615	-	-	-	X
57	MG	QA	1617	-	-	-	X
57	MG	QA	1661	-	-	-	X
57	MG	QV	101	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3005	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3010	-	-	-	X
57	MG	RA	3013	-	-	-	X
57	MG	RA	3016	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3023	-	-	-	X
57	MG	RA	3025	-	-	-	X
57	MG	RA	3027	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3037	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3039	-	-	-	X
57	MG	RA	3050	-	-	-	X
57	MG	RA	3053	-	-	-	X
57	MG	RA	3055	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3060	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3066	-	-	-	X
57	MG	RA	3076	-	-	-	X
57	MG	RA	3078	-	-	-	X
57	MG	RA	3080	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3088	-	-	-	X
57	MG	RA	3095	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3099	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3124	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RA	3132	-	-	-	X
57	MG	RA	3133	-	-	-	X
57	MG	RA	3137	-	-	-	X
57	MG	RA	3144	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3171	-	-	-	X
57	MG	RA	3177	-	-	-	X
57	MG	RA	3203	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3206	-	-	-	X
57	MG	RA	3214	-	-	-	X
57	MG	RA	3220	-	-	-	X
57	MG	RA	3224	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3237	-	-	-	X
57	MG	RA	3240	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RP	201	-	-	-	X
57	MG	RR	201	-	-	-	X
57	MG	RU	201	-	-	-	X
57	MG	XA	1603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1604	-	-	-	X
57	MG	XA	1607	-	-	-	X
57	MG	XA	1615	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1621	-	-	-	X
57	MG	XA	1629	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1656	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3004	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3011	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3017	-	-	-	X
57	MG	YA	3023	-	-	-	X
57	MG	YA	3024	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3032	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3044	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3057	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3061	-	-	-	X
57	MG	YA	3065	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3070	-	-	-	X
57	MG	YA	3072	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3073	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3081	-	-	-	X
57	MG	YA	3086	-	-	-	X
57	MG	YA	3089	-	-	-	X
57	MG	YA	3090	-	-	-	X
57	MG	YA	3098	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3103	-	-	-	X
57	MG	YA	3107	-	-	-	X
57	MG	YA	3108	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3129	-	-	-	X
57	MG	YA	3132	-	-	-	X
57	MG	YA	3138	-	-	-	X
57	MG	YA	3146	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3171	-	-	-	X
57	MG	YA	3180	-	-	-	X
57	MG	YA	3181	-	-	-	X
57	MG	YA	3182	-	-	-	X
57	MG	YA	3193	-	-	-	X
57	MG	YA	3197	-	-	-	X
57	MG	YA	3198	-	-	-	X
57	MG	YA	3206	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3239	-	-	-	X
57	MG	YA	3251	-	-	-	X
57	MG	YA	3253	-	-	-	X
57	MG	YA	3256	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3263	-	-	-	X
57	MG	YB	203	-	-	-	X
58	PAR	QA	1666	-	-	-	X
58	PAR	XA	1673	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291993 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 messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			
23	XY	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 24 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			
24	XX	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

- 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	65	Total	Mg	0	0
			65	65		
57	RP	2	Total	Mg	0	0
			2	2		
57	QX	1	Total	Mg	0	0
			1	1		
57	YA	268	Total	Mg	0	0
			268	268		
57	QM	1	Total	Mg	0	0
			1	1		

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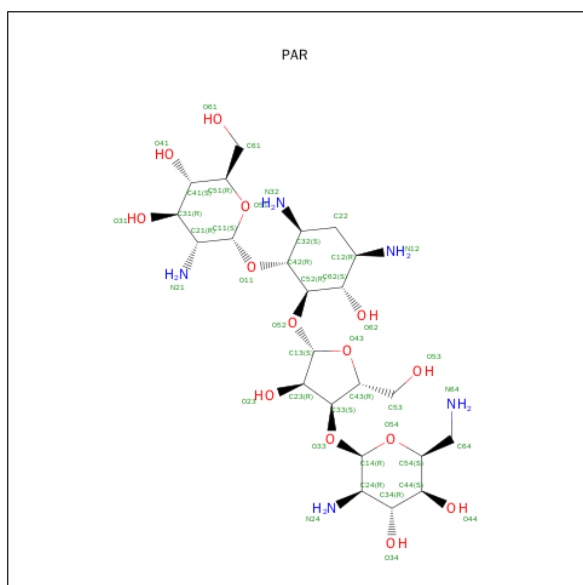
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XX	1	Total 1	Mg 1	0	0
57	QV	1	Total 1	Mg 1	0	0
57	XA	72	Total 72	Mg 72	0	0
57	R0	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	YX	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	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	242	Total 242	Mg 242	0	0
57	YP	2	Total 2	Mg 2	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	1	Total 1	Mg 1	0	0
57	RB	2	Total 2	Mg 2	0	0
57	RF	1	Total 1	Mg 1	0	0

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



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

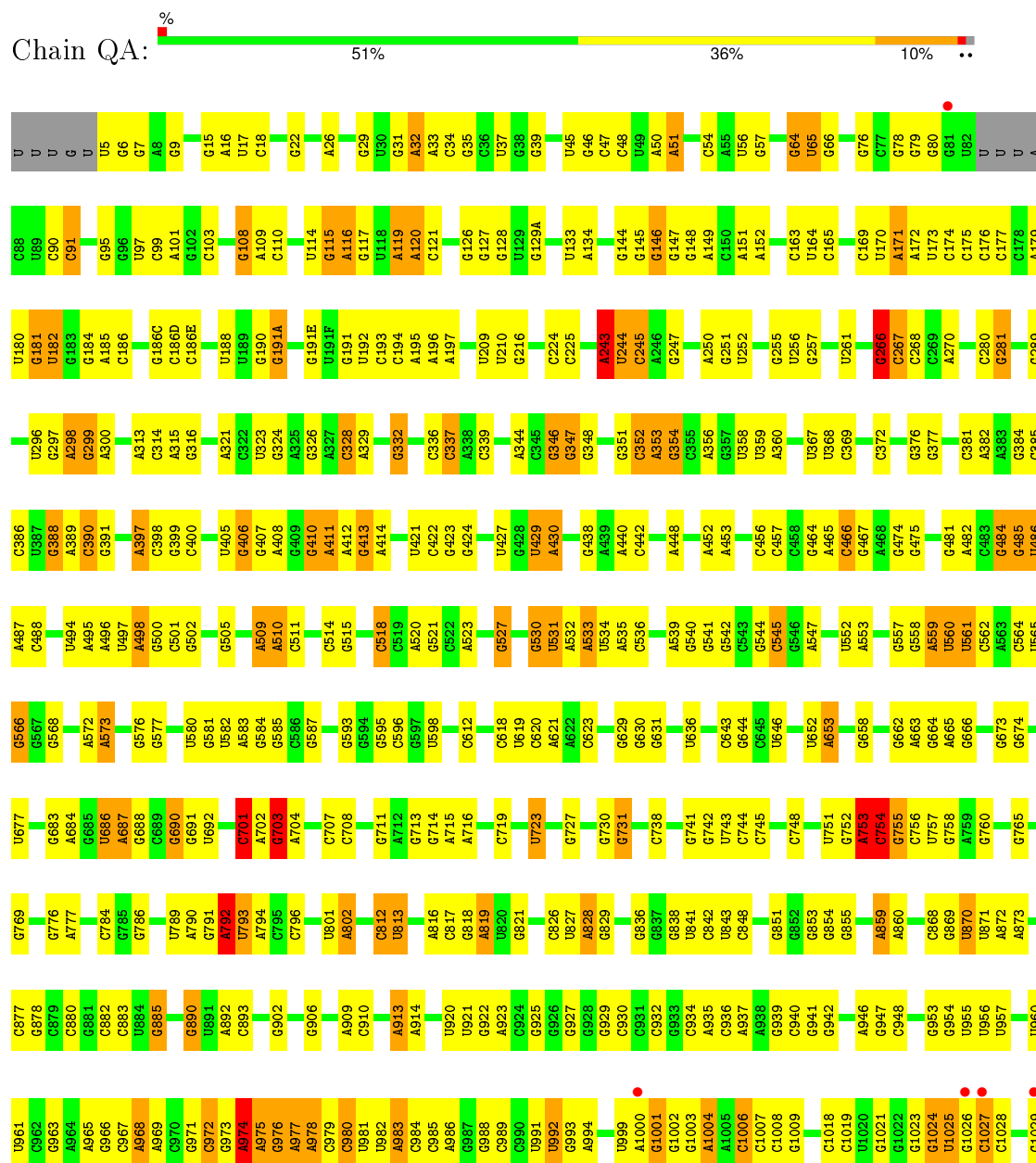
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

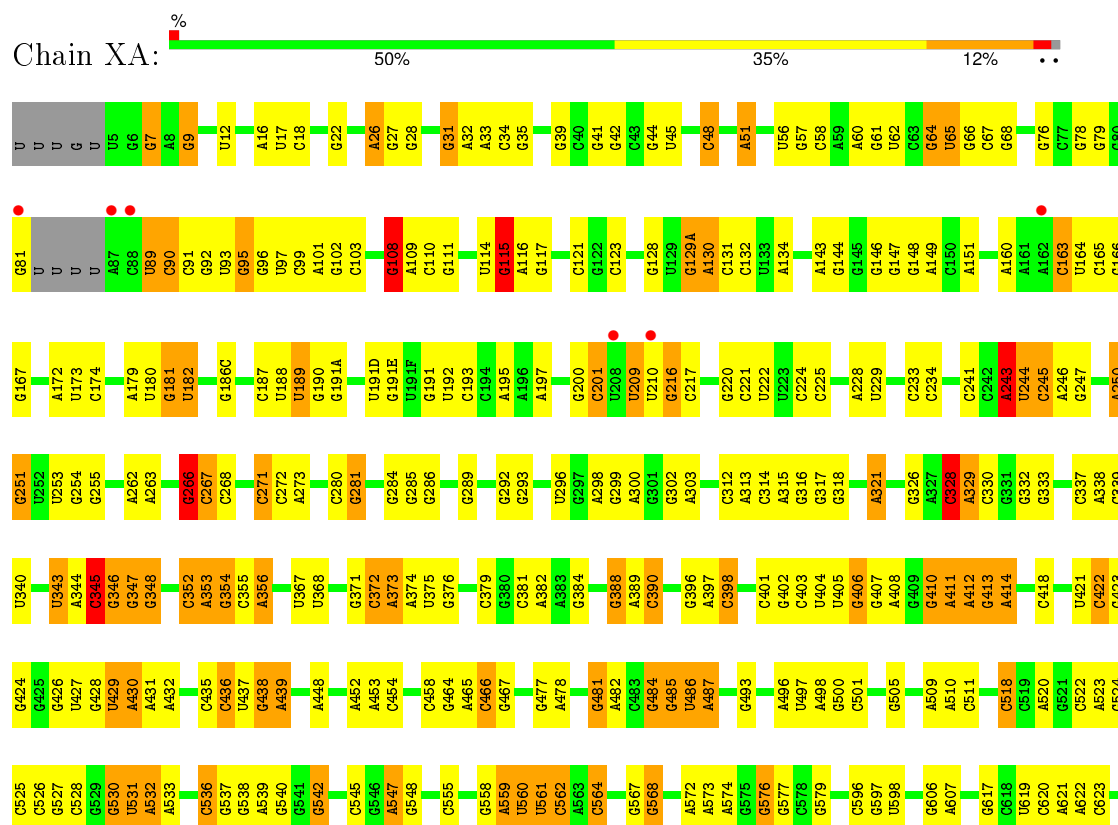
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	XD	1	Total	Zn	0	0
			1	1		
59	QD	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

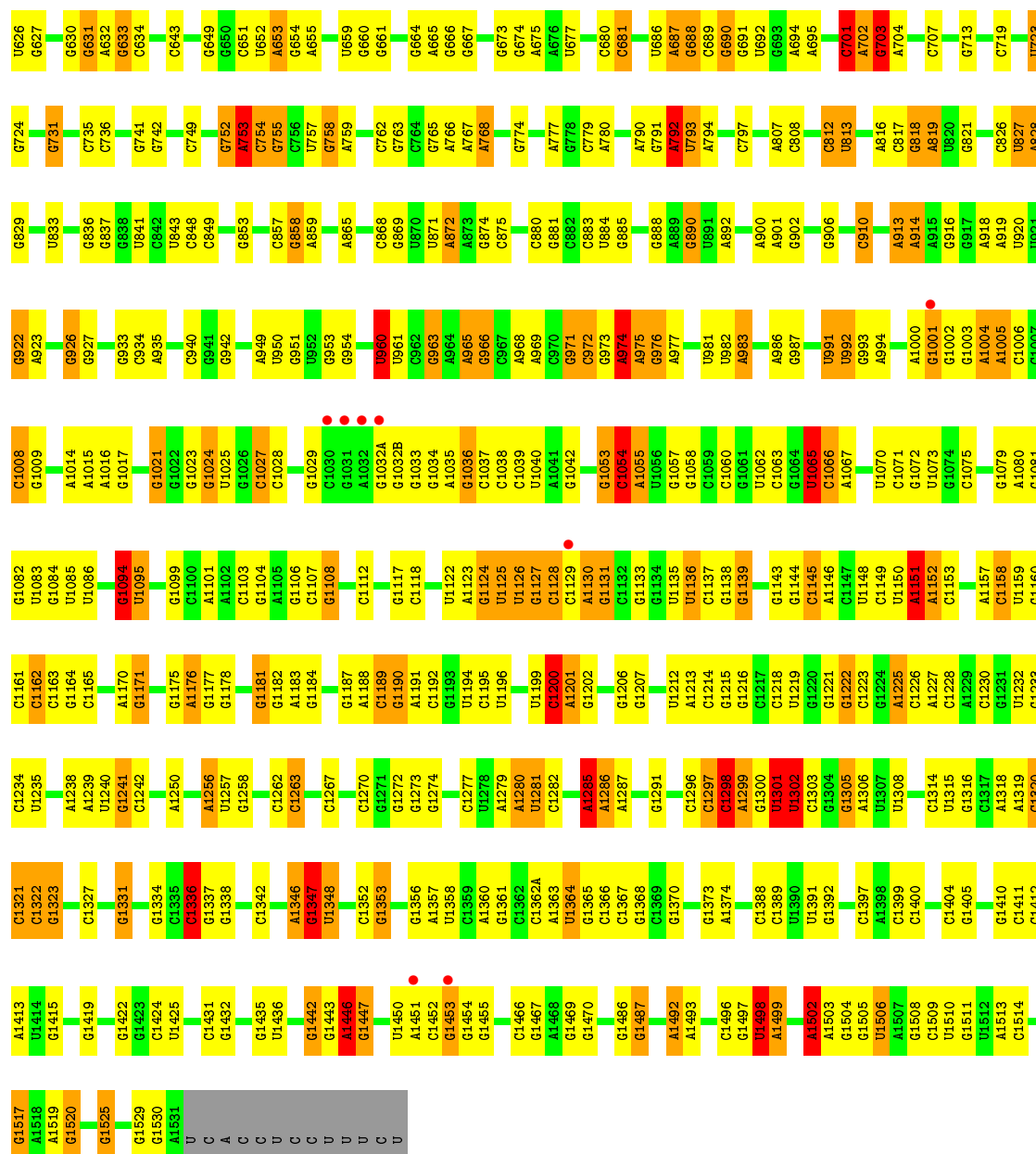
### 3 Residue-property plots

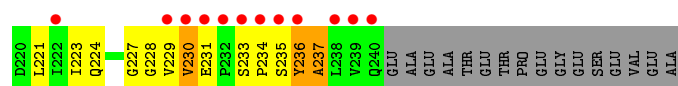
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S rRNA

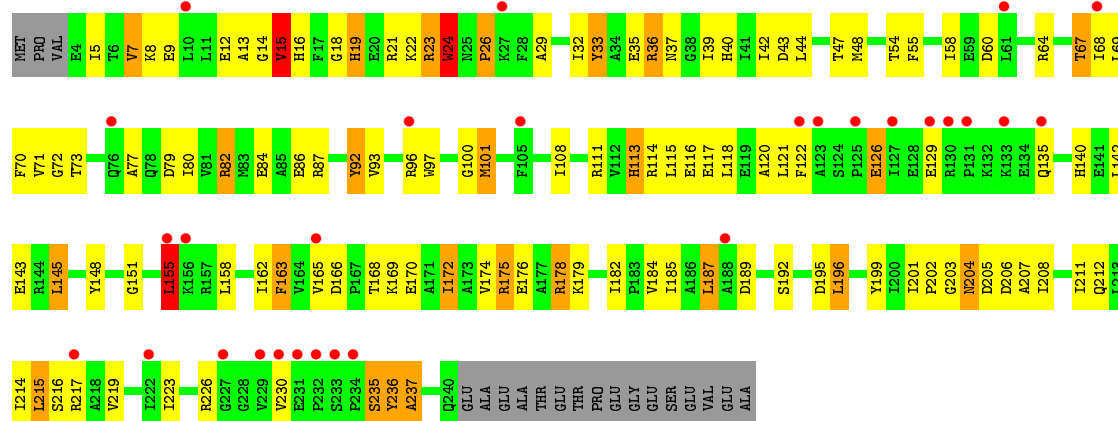




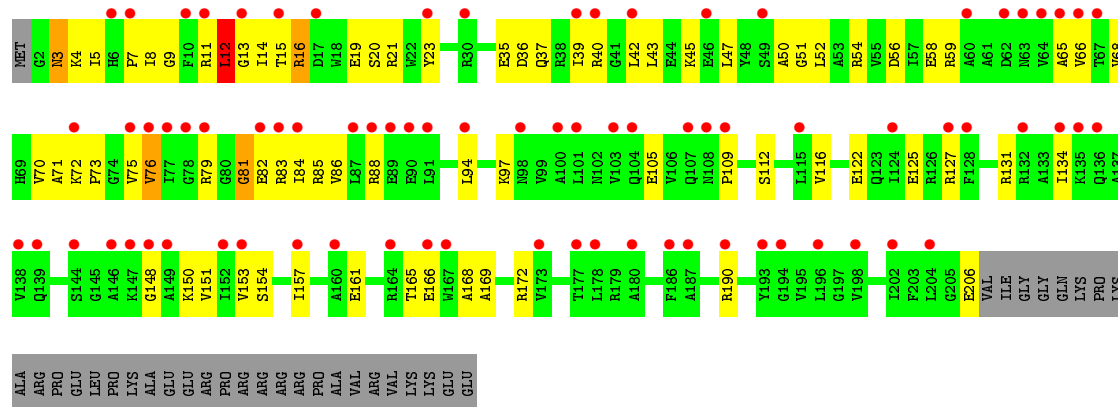




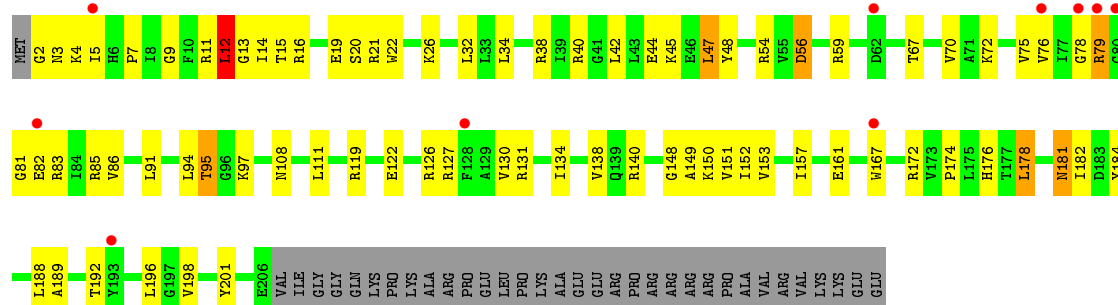
• Molecule 2: 30S ribosomal protein S2



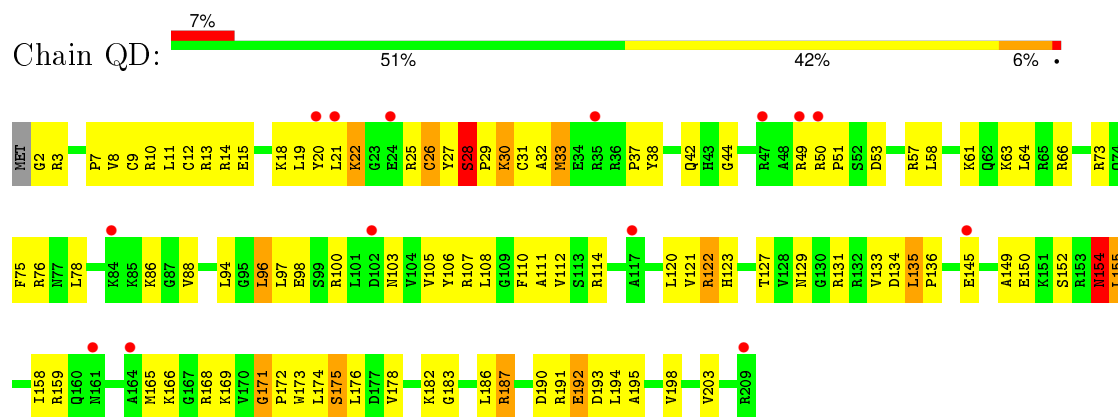
• Molecule 3: 30S ribosomal protein S3



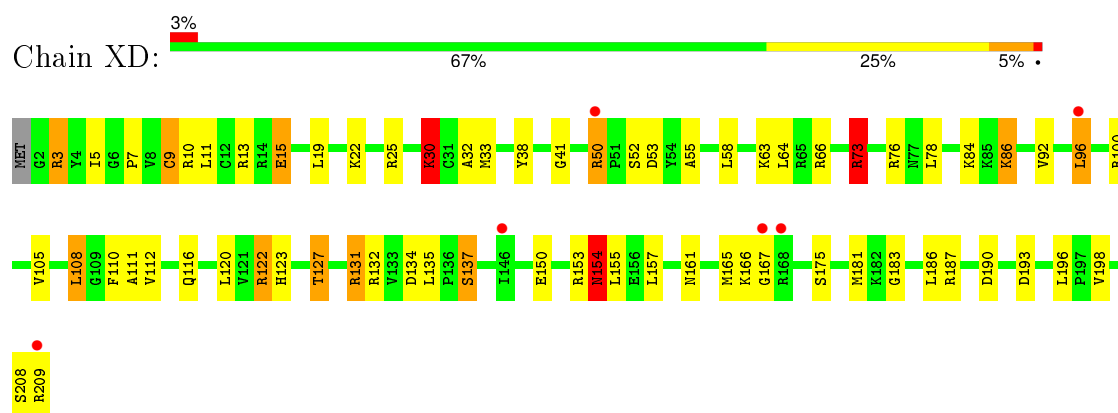
• Molecule 3: 30S ribosomal protein S3



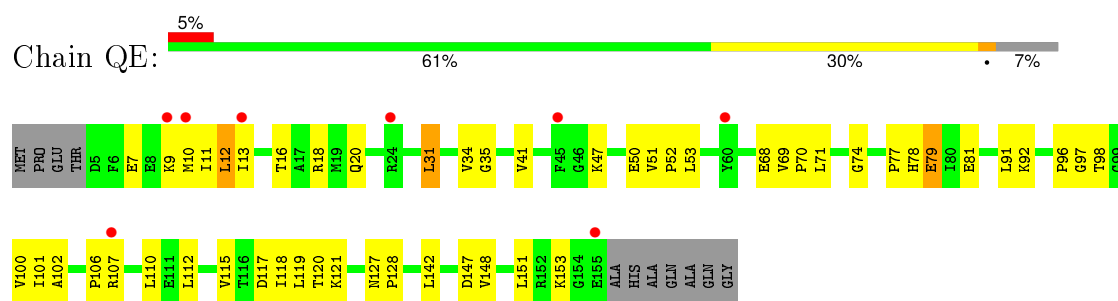
- Molecule 4: 30S ribosomal protein S4



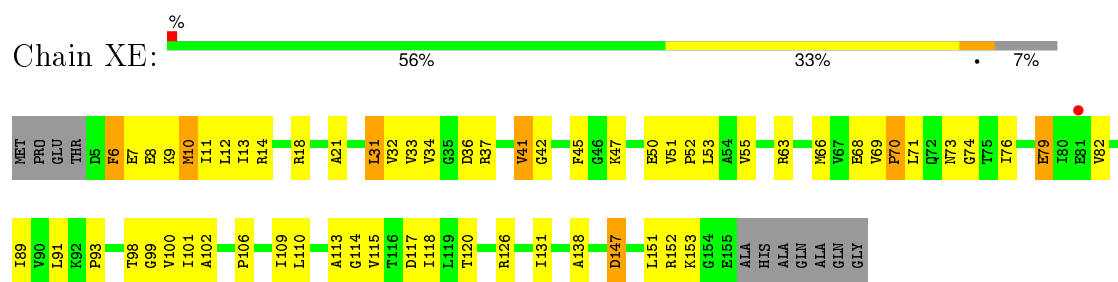
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



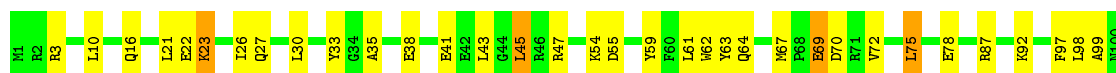
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6



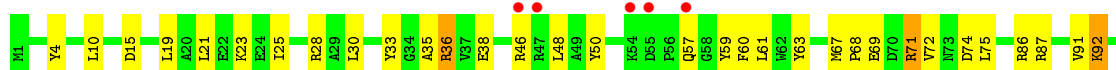
Chain QF:  66% 30% .



A101

- Molecule 6: 30S ribosomal protein S6

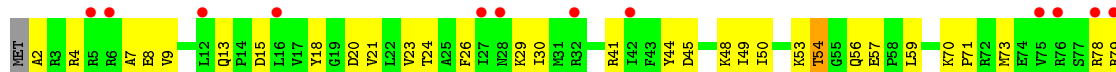
Chain XF:  6% 63% 34% .



E95  
P96  
F97  
L98  
A99  
N100  
A101


- Molecule 7: 30S ribosomal protein S7

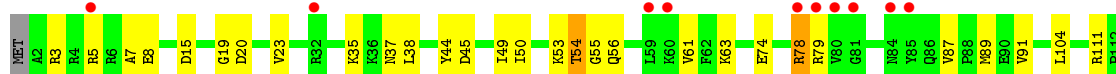
Chain QG:  17% 65% 31% . .



V80  
G81  
G82  
A83  
R84  
R85  
R86  
R87  
R88  
R89  
R90  
R91  
R92  
R93  
R94  
R95  
R96  
L99  
R102  
W103  
L104  
T24  
V105  
Q106  
E113  
R114  
R115  
A116  
A117  
V118  
R119  
I120  
V135  
K136  
K137  
E146  
R149  
A152  
H153  
Y154  
R155  
W156

- Molecule 7: 30S ribosomal protein S7

Chain XG:  9% 73% 23% . .



E113  
R114  
R115  
V118  
K136  
K137  
K138  
D139  
D140  
V141  
E142  
R143  
H153  
Y154  
R155  
W156

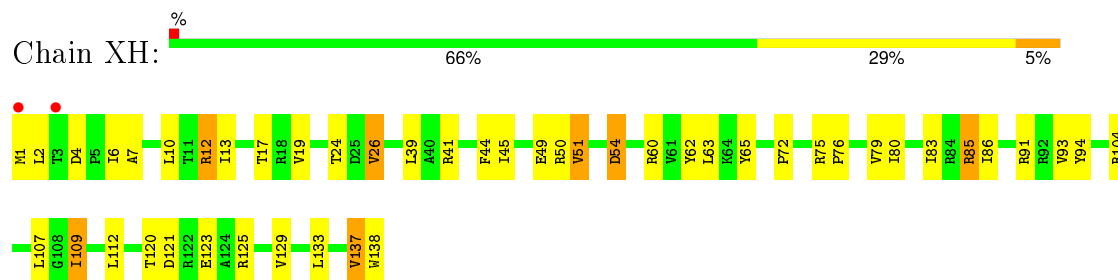
- Molecule 8: 30S ribosomal protein S8

Chain QH:  61% 36% .

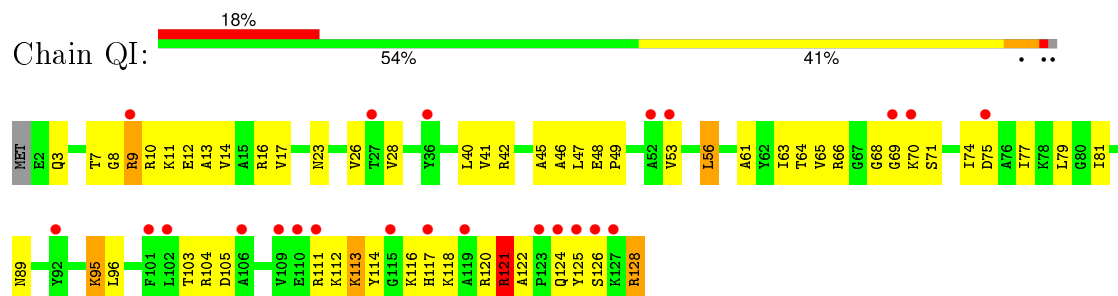


R91  
Y94  
V95  
E99  
I100  
P101  
R104  
R105  
G106  
L107  
G108  
I109  
L112  
V118  
D121  
R122  
E123  
A124  
R125  
V129  
L133  
W138

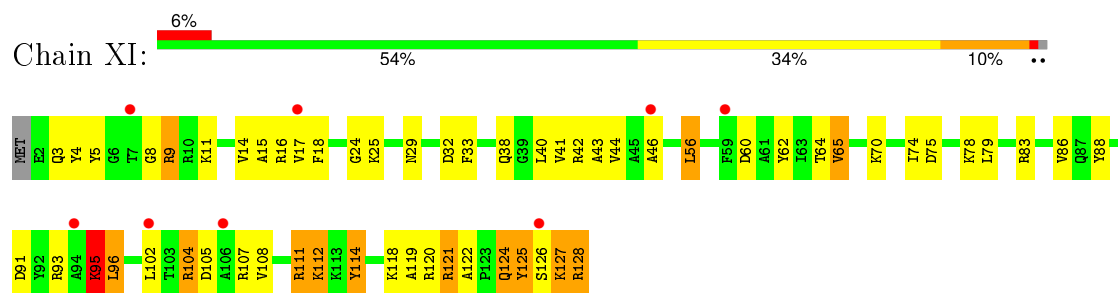
- Molecule 8: 30S ribosomal protein S8



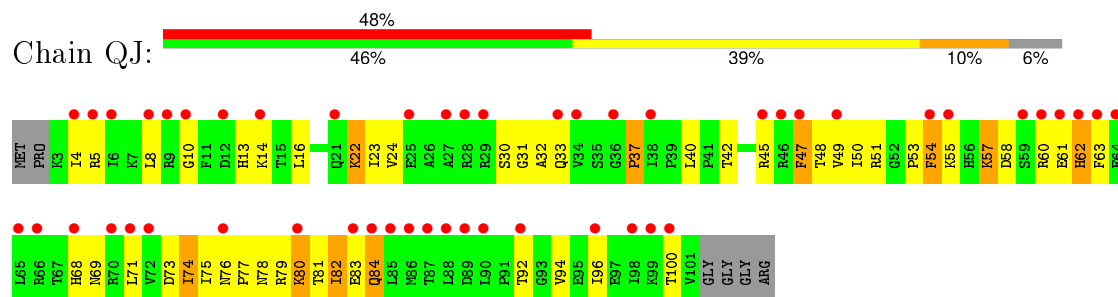
- Molecule 9: 30S ribosomal protein S9



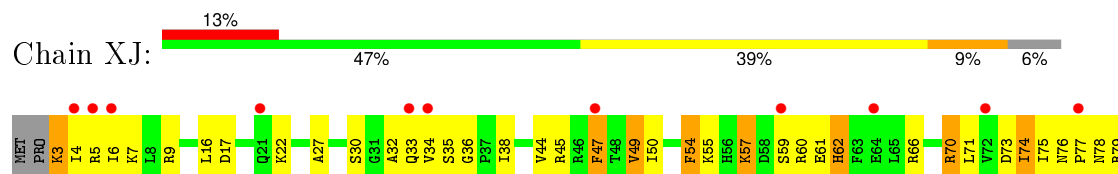
- Molecule 9: 30S ribosomal protein S9

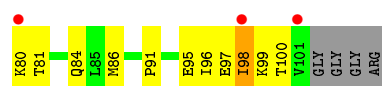


- Molecule 10: 30S ribosomal protein S10

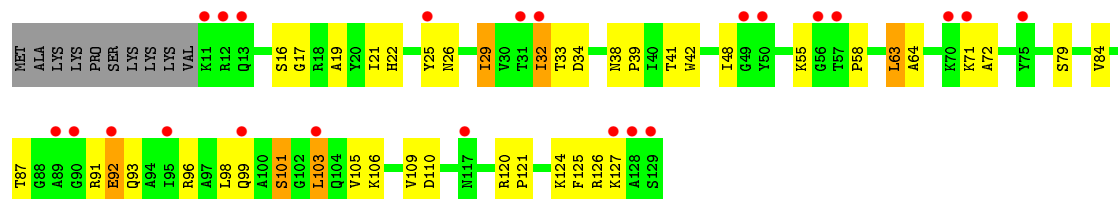


- Molecule 10: 30S ribosomal protein S10

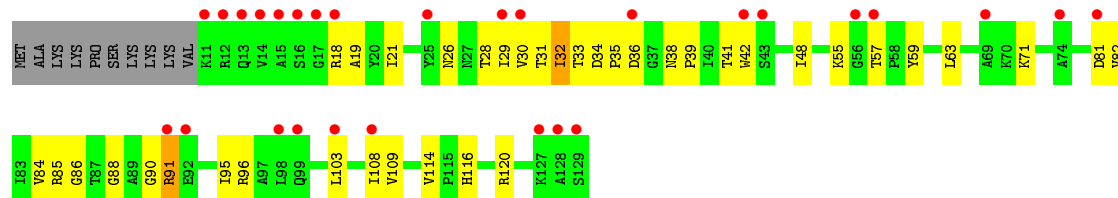




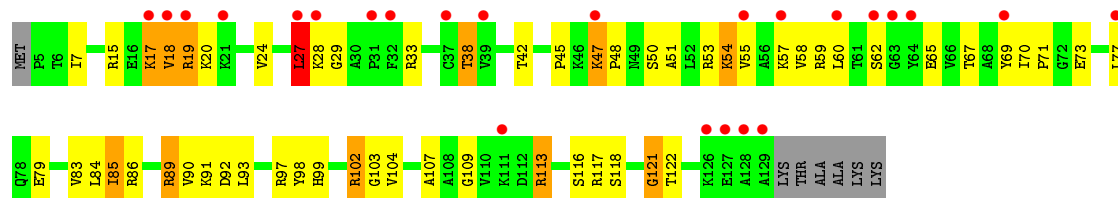
- Molecule 11: 30S ribosomal protein S11



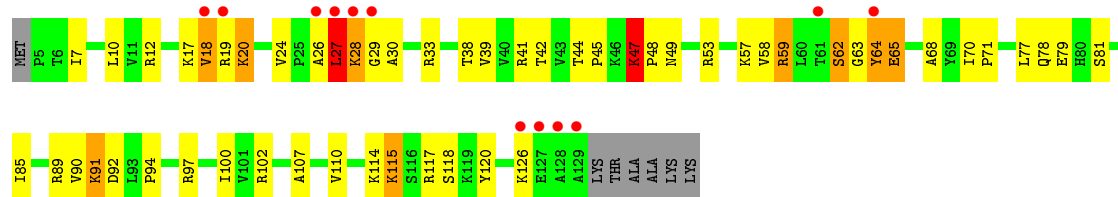
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

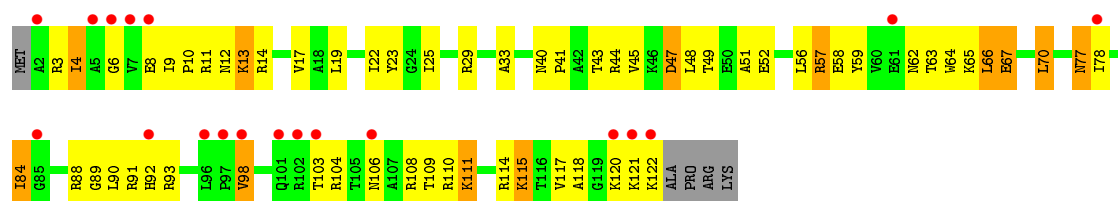


- Molecule 12: 30S ribosomal protein S12

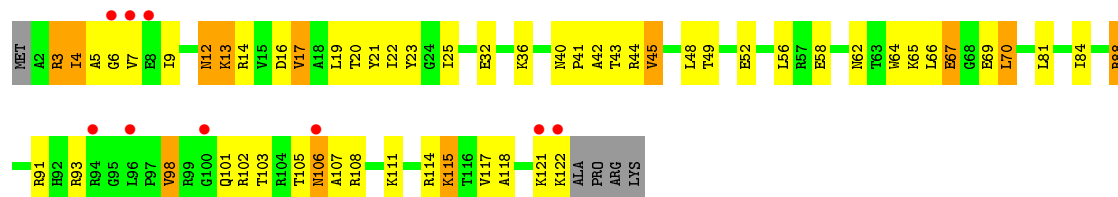


- Molecule 13: 30S ribosomal protein S13

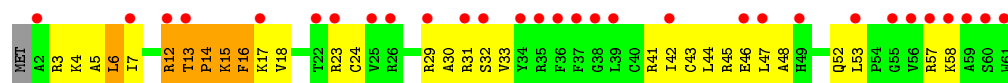




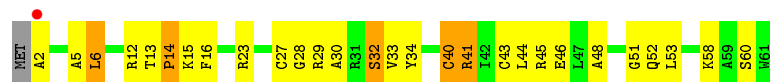
- Molecule 13: 30S ribosomal protein S13



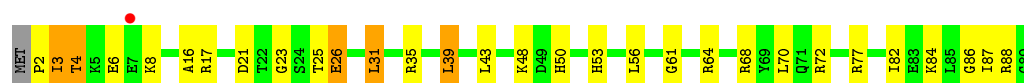
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



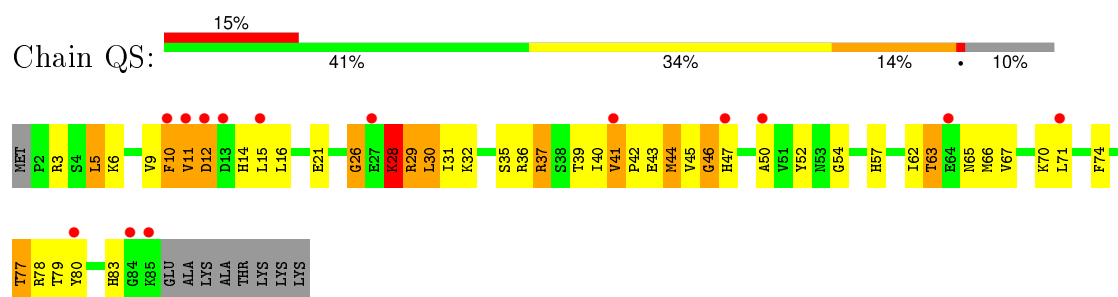
- Molecule 15: 30S ribosomal protein S15



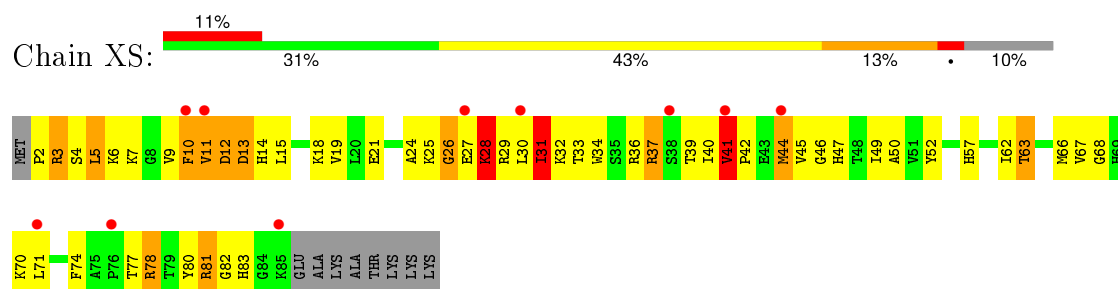
- Molecule 16: 30S ribosomal protein S16



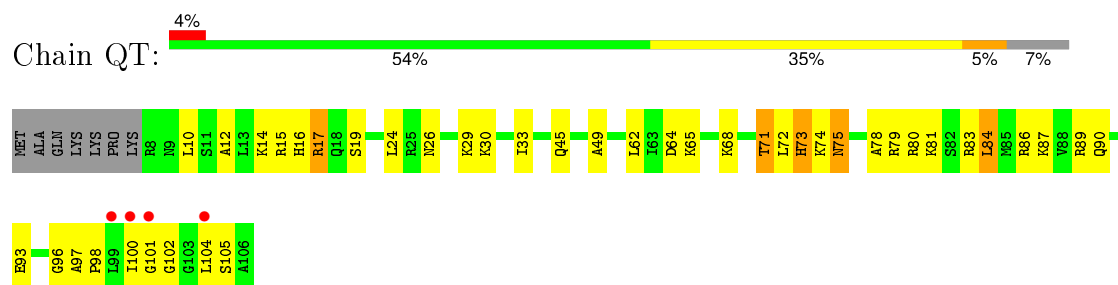




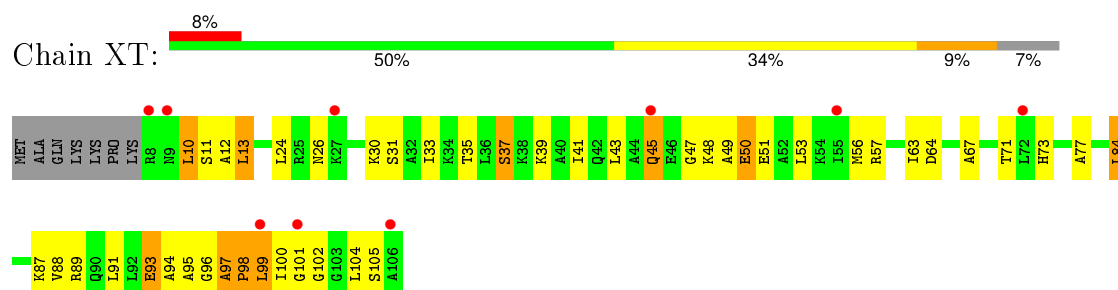
- Molecule 19: 30S ribosomal protein S19



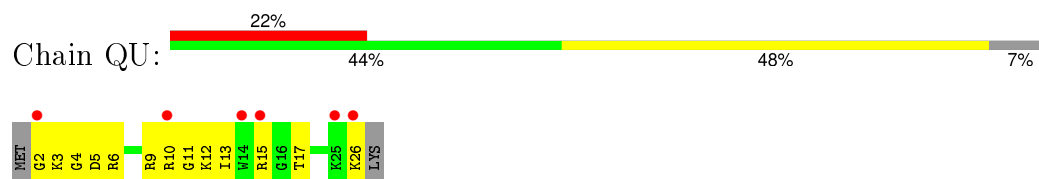
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

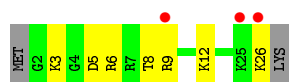


- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

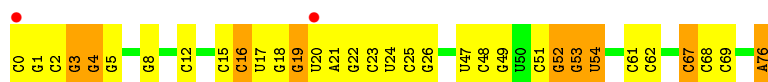




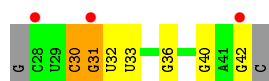
- Molecule 22: P-site tRNA fMet



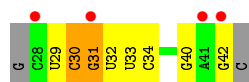
- Molecule 22: P-site tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



- Molecule 24: A-site ASL SufA6



- Molecule 24: A-site ASL SufA6



- Molecule 25: 23S rRNA



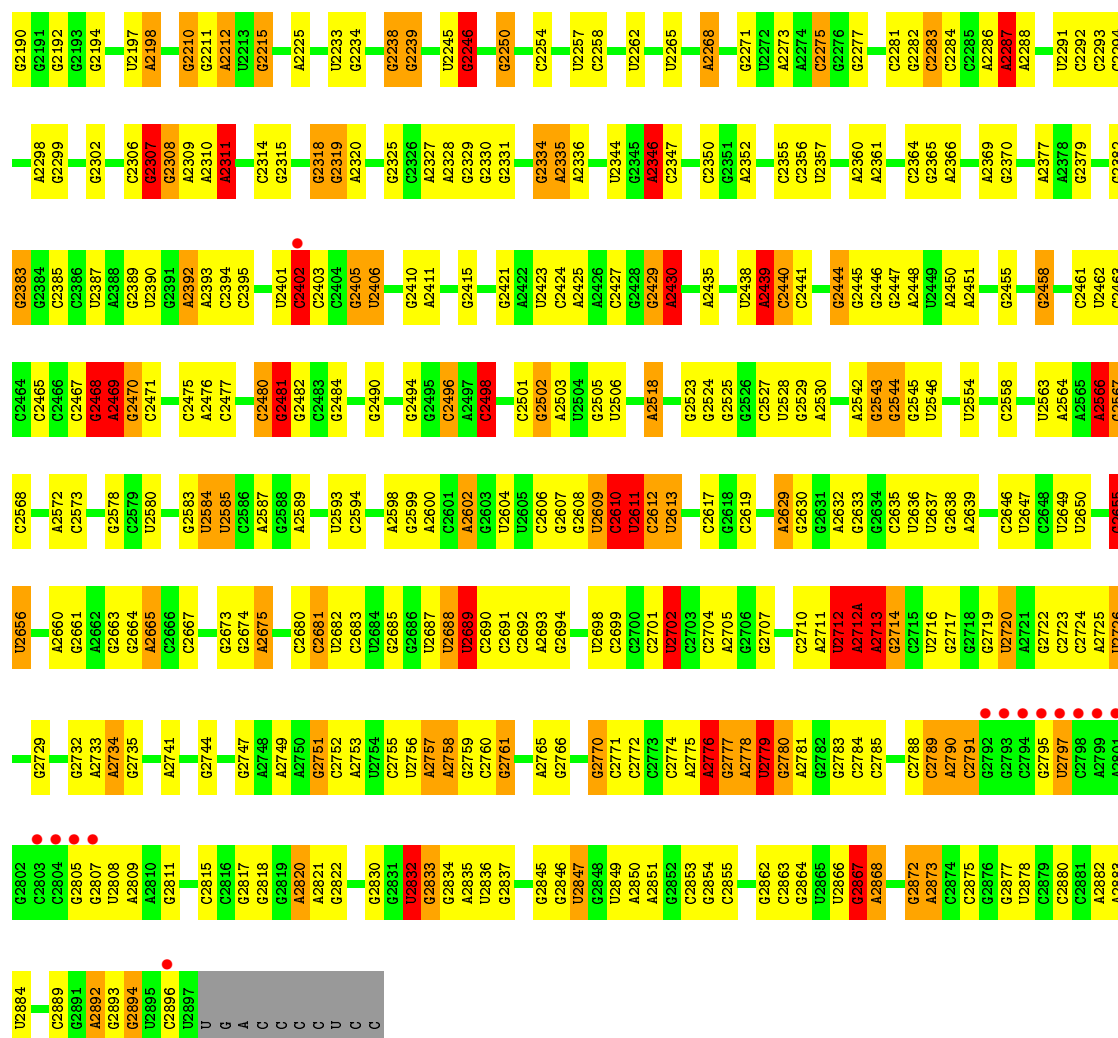




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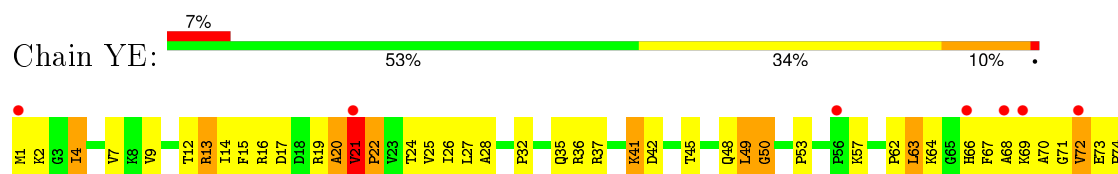


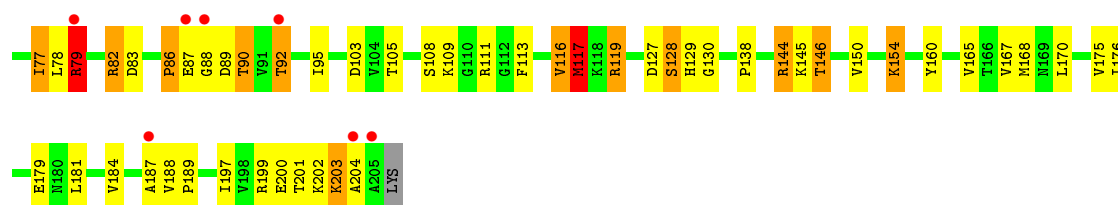


- Molecule 27: 50S ribosomal protein L2

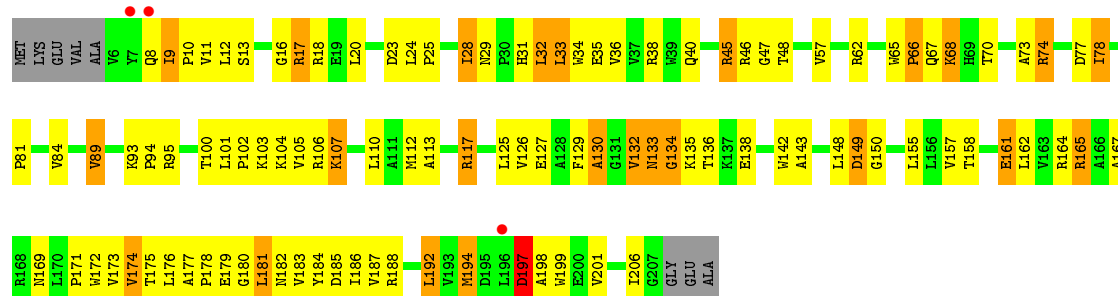
- Molecule 28: 50S ribosomal protein L3

- Molecule 28: 50S ribosomal protein L3

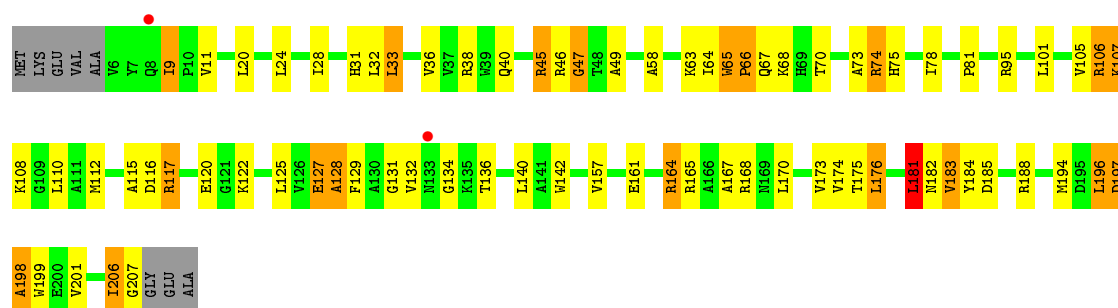




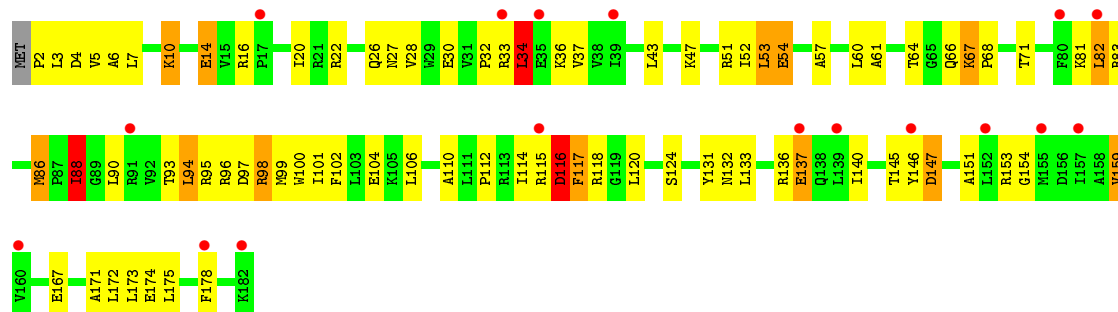
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4

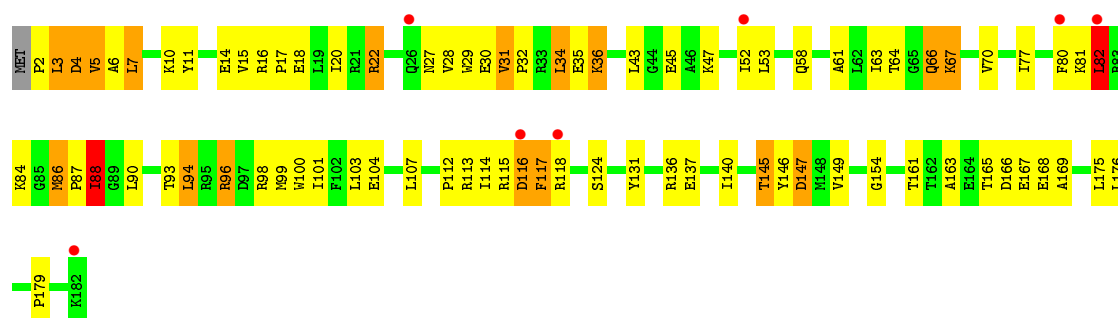


• Molecule 30: 50S ribosomal protein L5

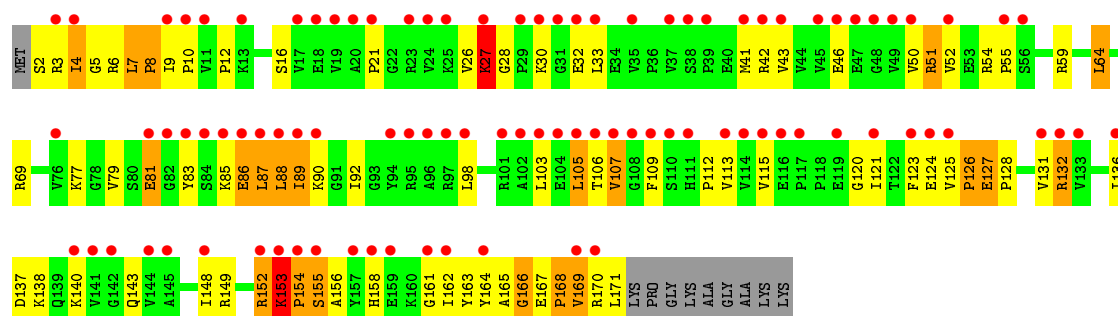


• Molecule 30: 50S ribosomal protein L5

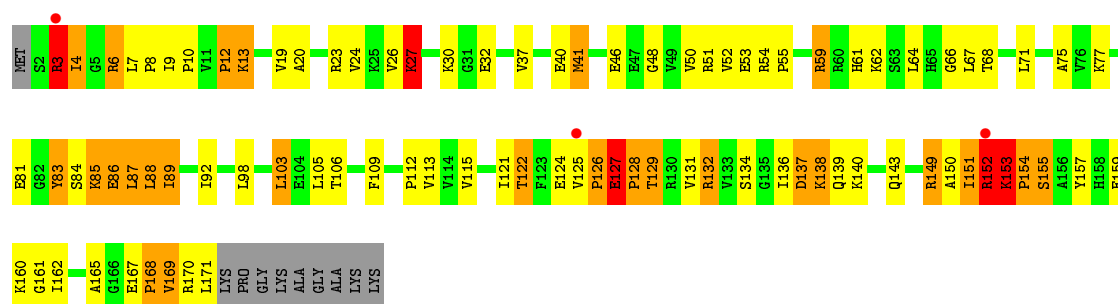




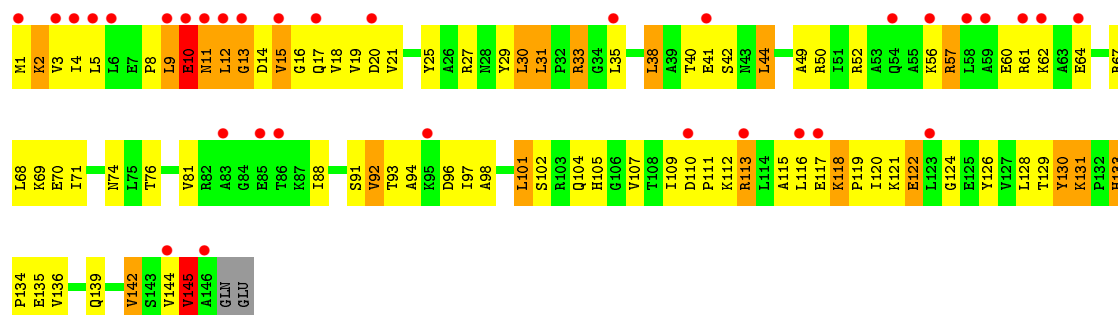
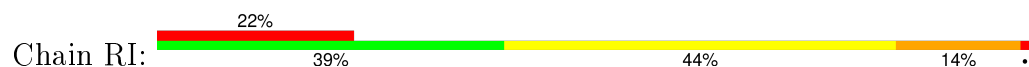
- Molecule 31: 50S ribosomal protein L6



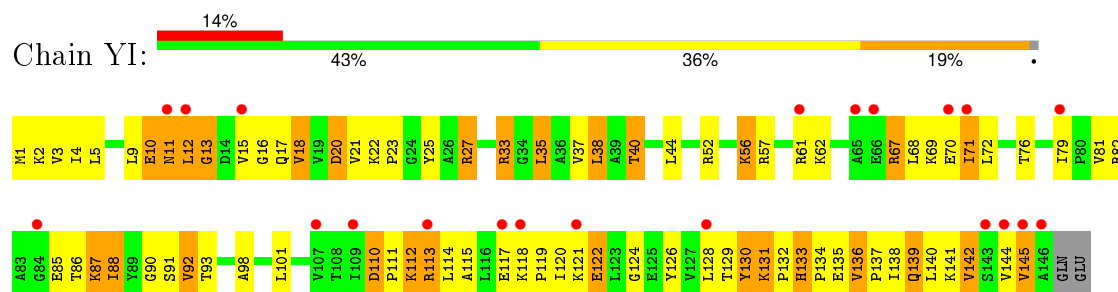
- Molecule 31: 50S ribosomal protein L6



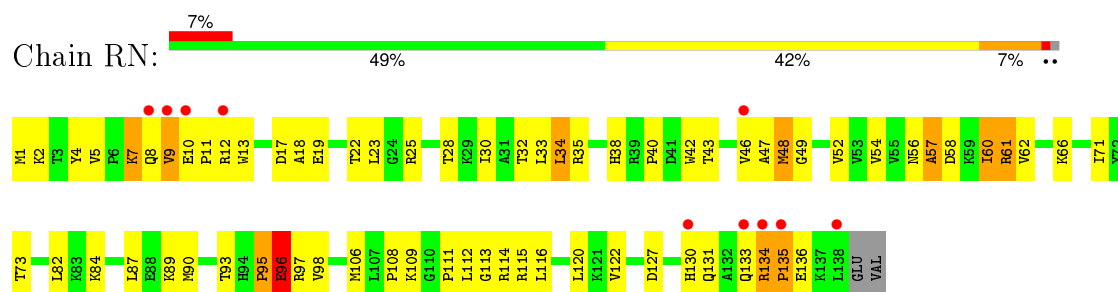
- Molecule 32: 50S ribosomal protein L9



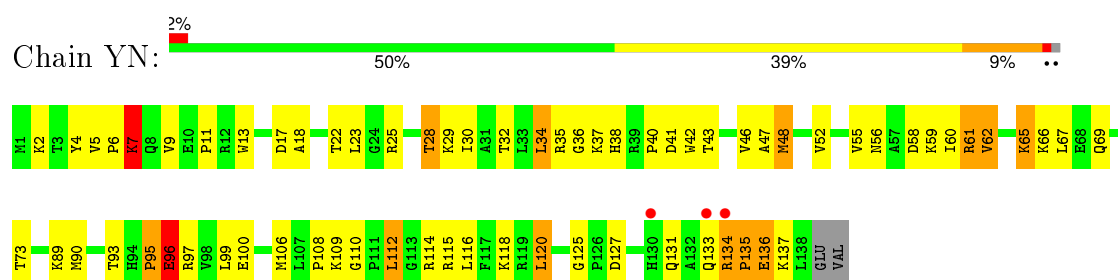
- Molecule 32: 50S ribosomal protein L9



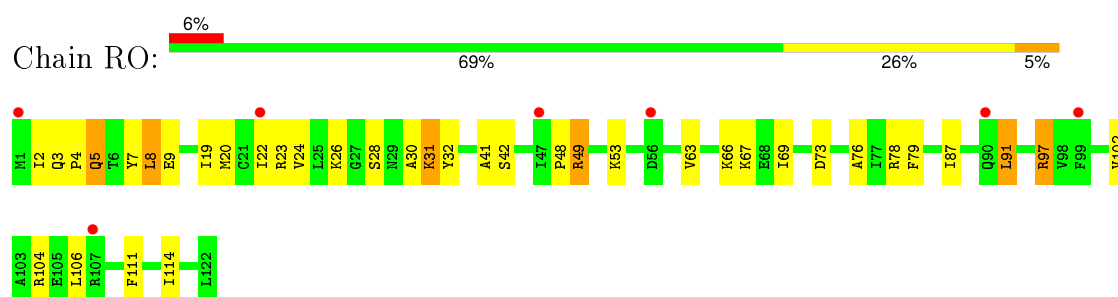
- Molecule 33: 50S ribosomal protein L13



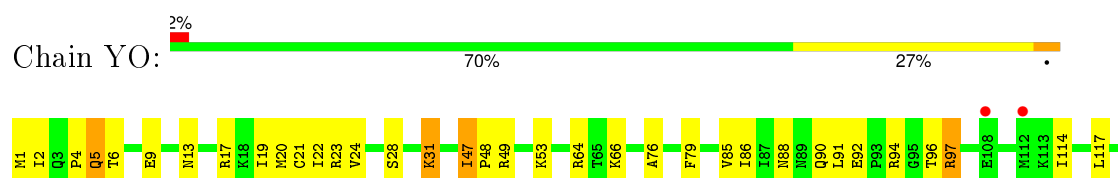
- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14



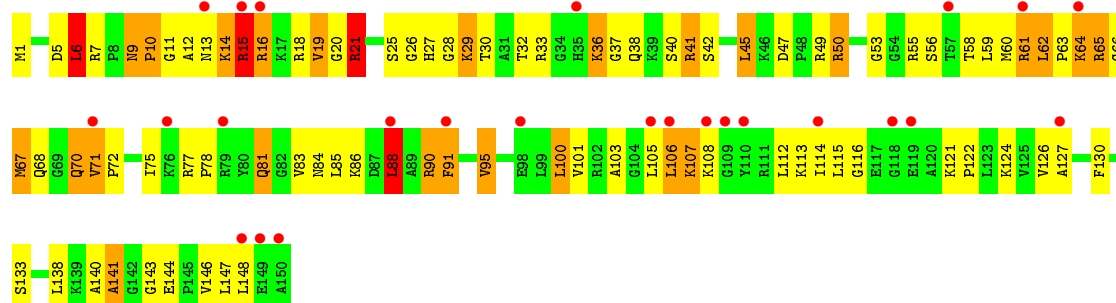
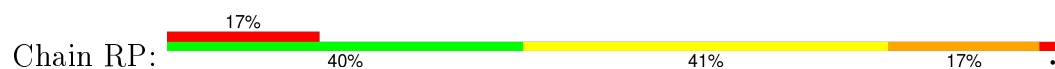
- Molecule 34: 50S ribosomal protein L14



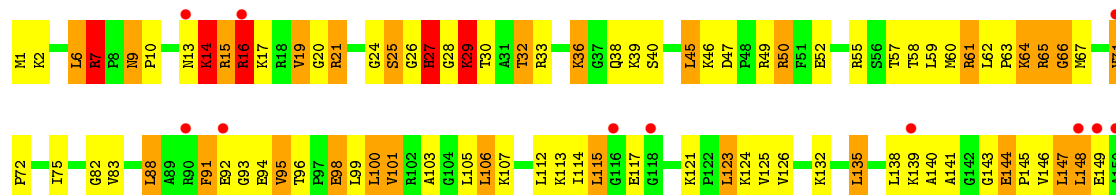
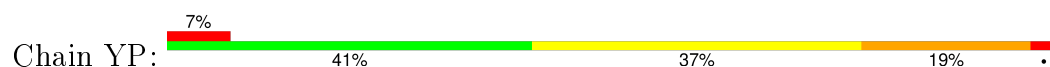




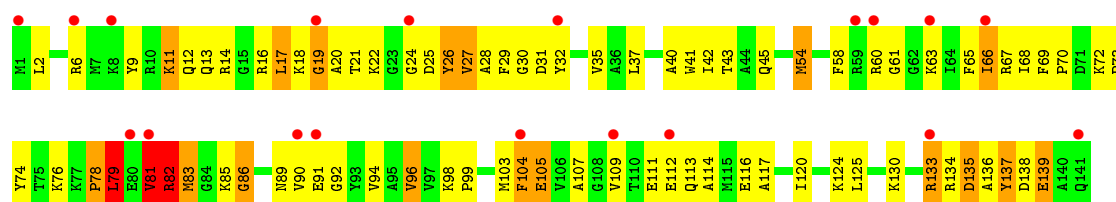
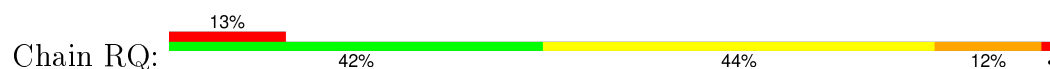
- Molecule 35: 50S ribosomal protein L15



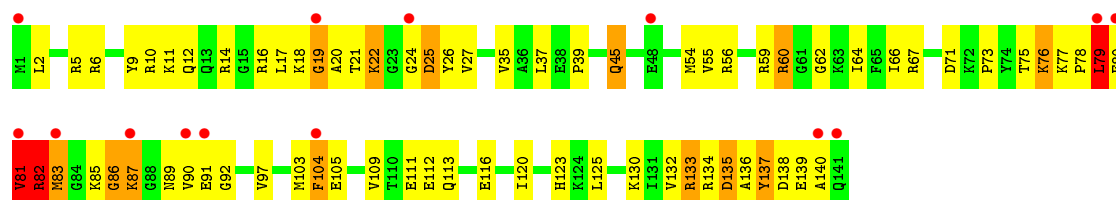
- Molecule 35: 50S ribosomal protein L15



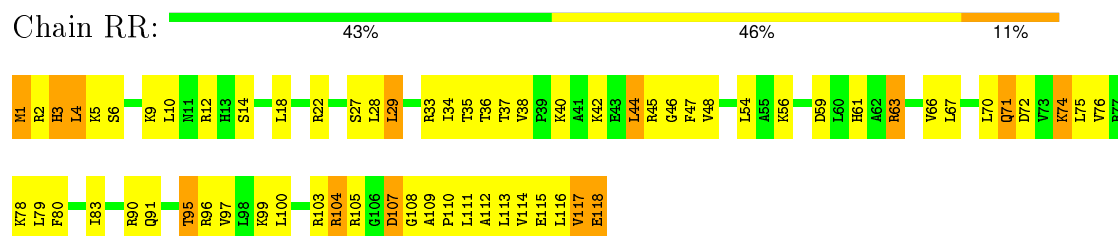
- Molecule 36: 50S ribosomal protein L16



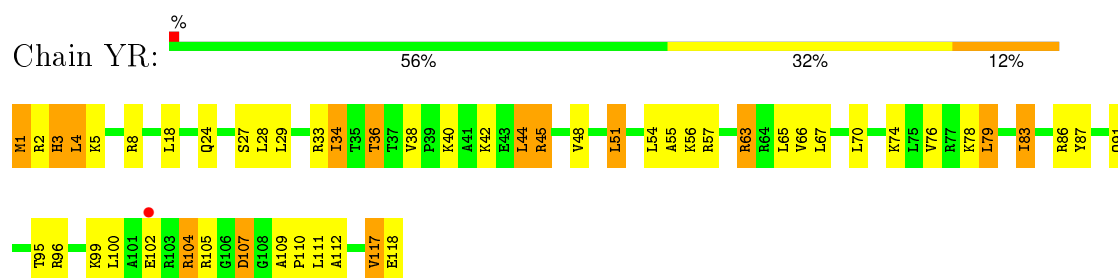
- Molecule 36: 50S ribosomal protein L16



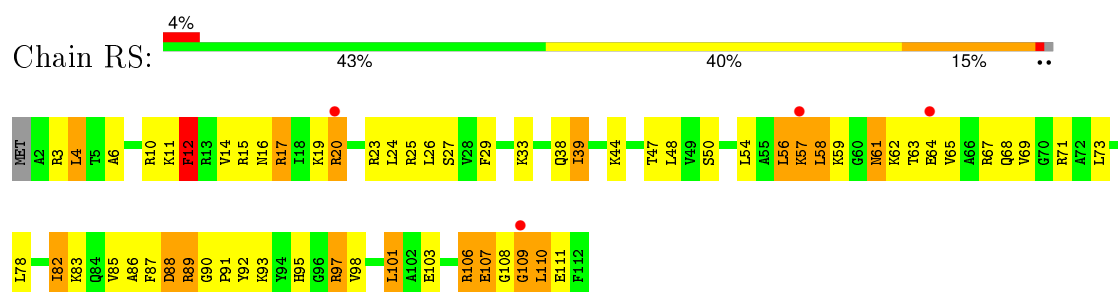
- Molecule 37: 50S ribosomal protein L17



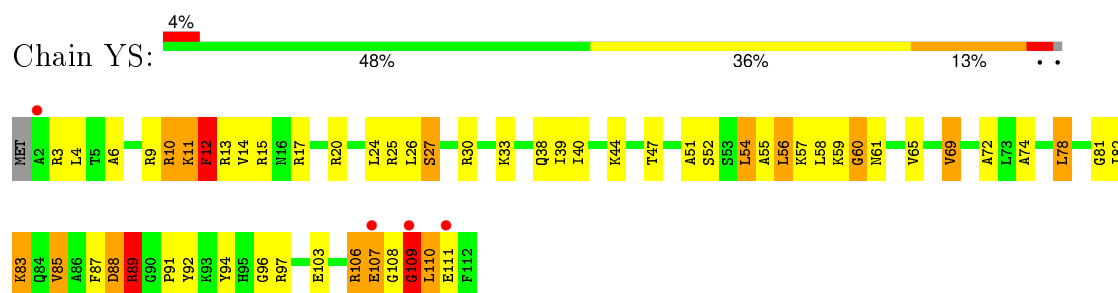
- Molecule 37: 50S ribosomal protein L17



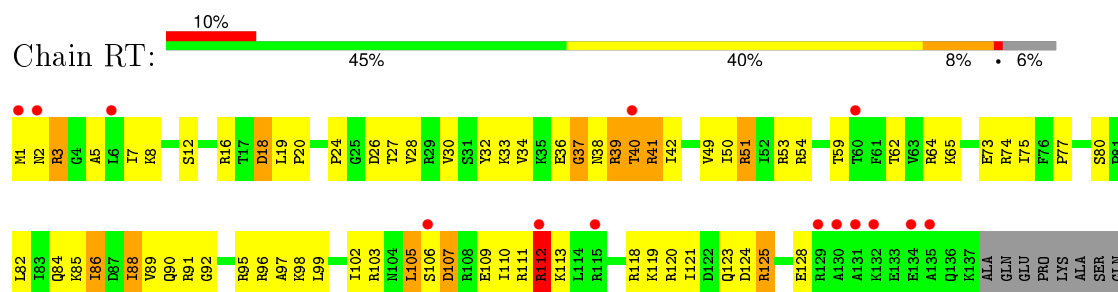
- Molecule 38: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L18

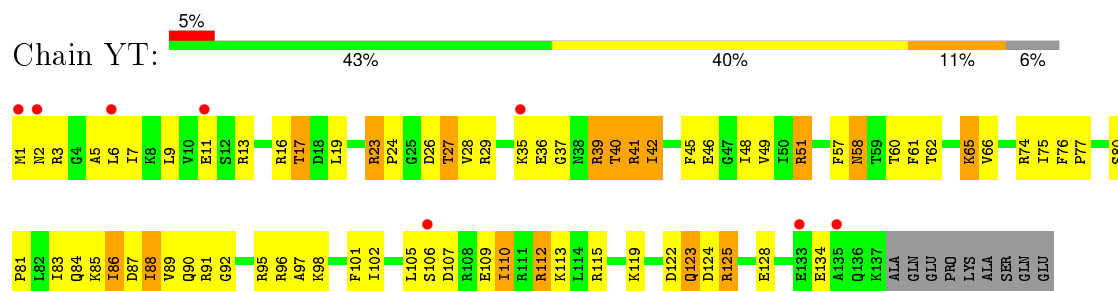


- Molecule 39: 50S ribosomal protein L19

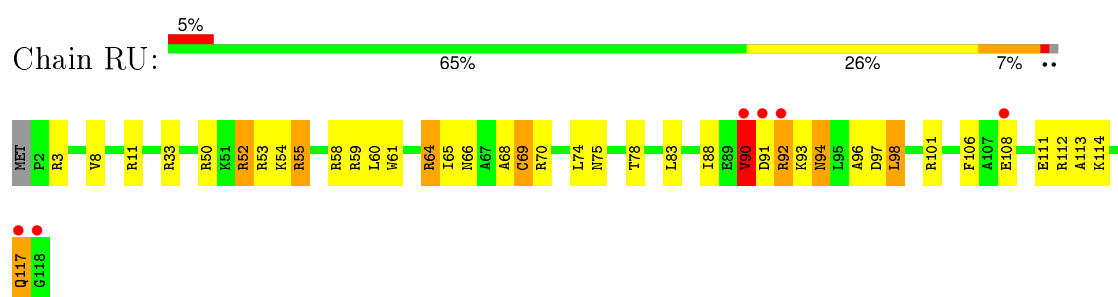


GLU

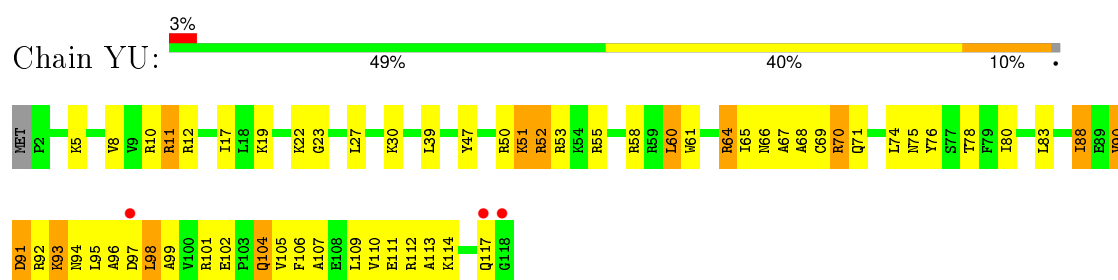
- Molecule 39: 50S ribosomal protein L19



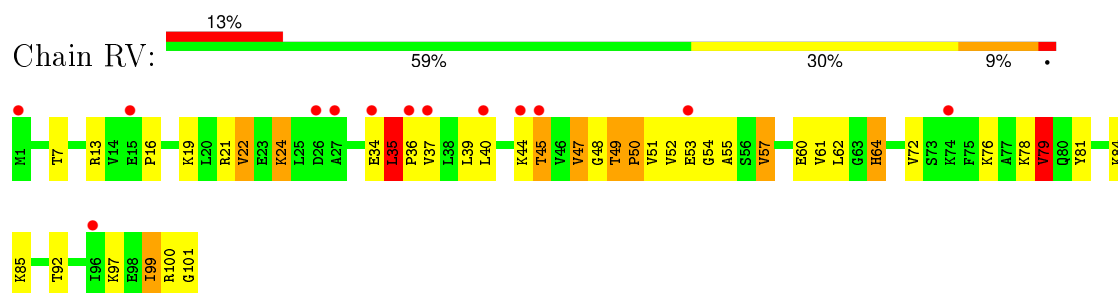
- Molecule 40: 50S ribosomal protein L20



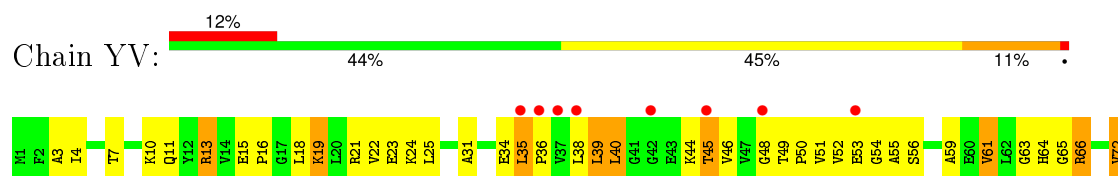
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21





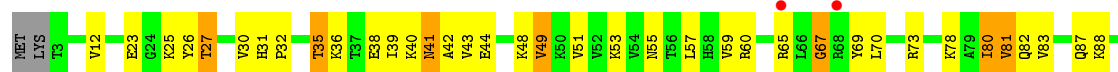
- Molecule 42: 50S ribosomal protein L22



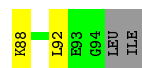
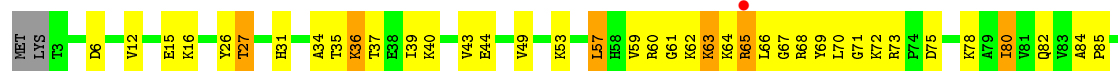
- Molecule 42: 50S ribosomal protein L22



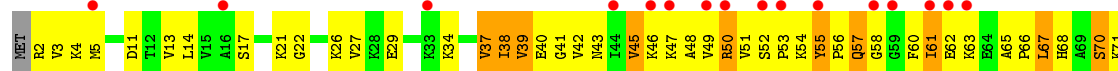
- Molecule 43: 50S ribosomal protein L23

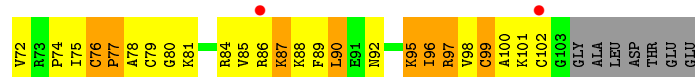


- Molecule 43: 50S ribosomal protein L23

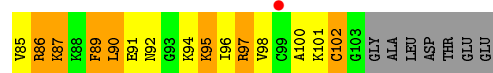
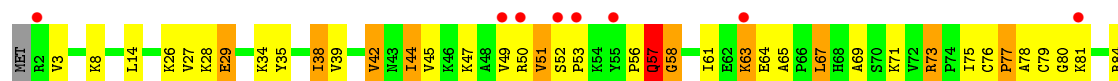


- Molecule 44: 50S ribosomal protein L24

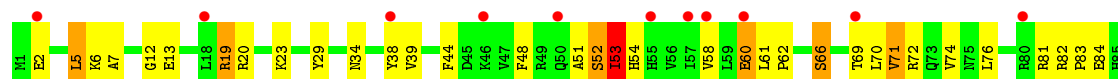




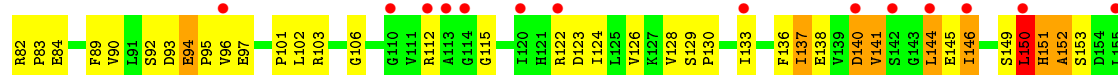
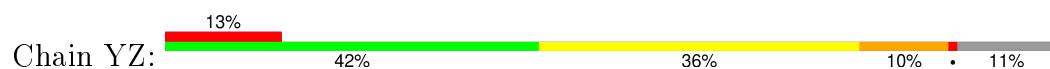
- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25



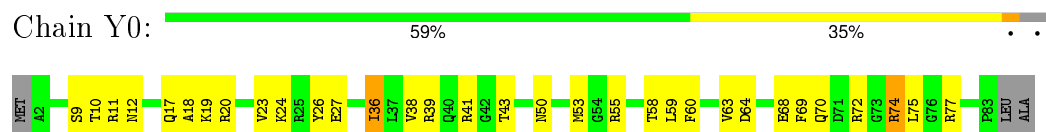
- Molecule 45: 50S ribosomal protein L25



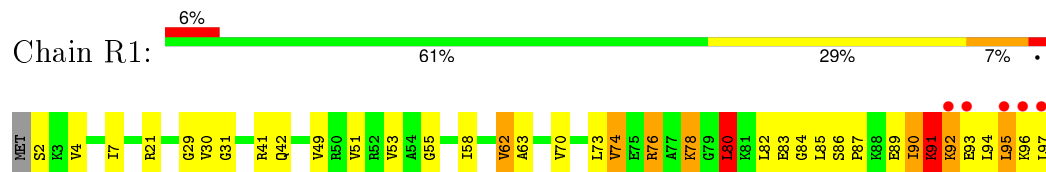
- Molecule 46: 50S ribosomal protein L27



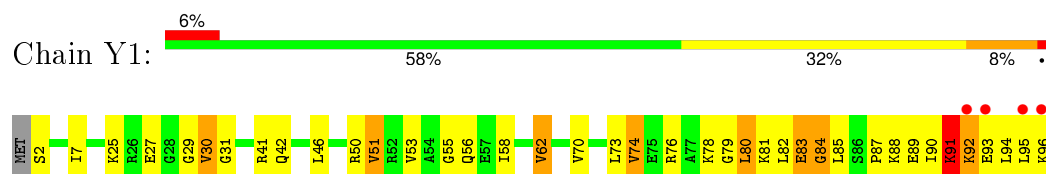
- Molecule 46: 50S ribosomal protein L27



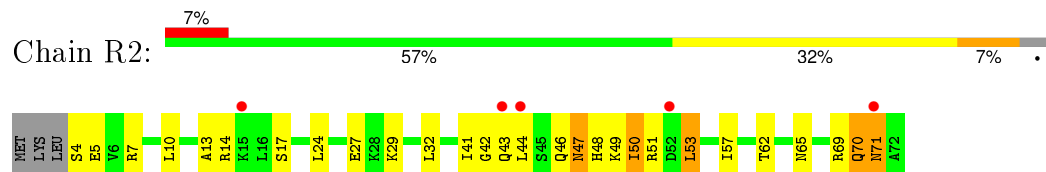
- Molecule 47: 50S ribosomal protein L28



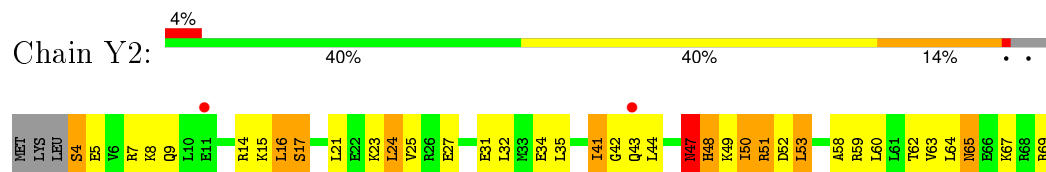
- Molecule 47: 50S ribosomal protein L28



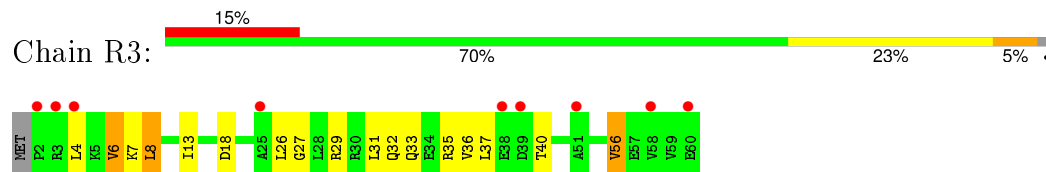
- Molecule 48: 50S ribosomal protein L29



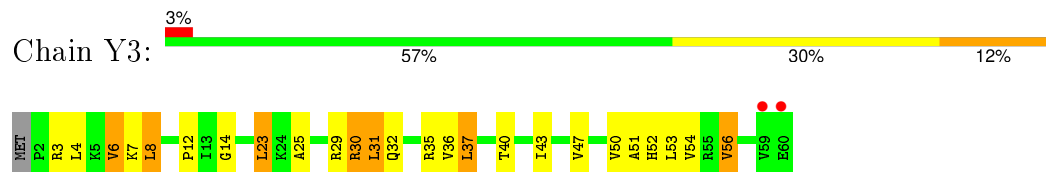
- Molecule 48: 50S ribosomal protein L29



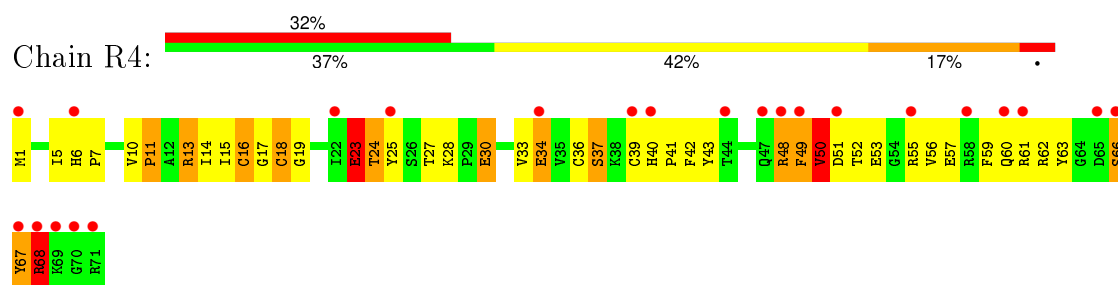
- Molecule 49: 50S ribosomal protein L30



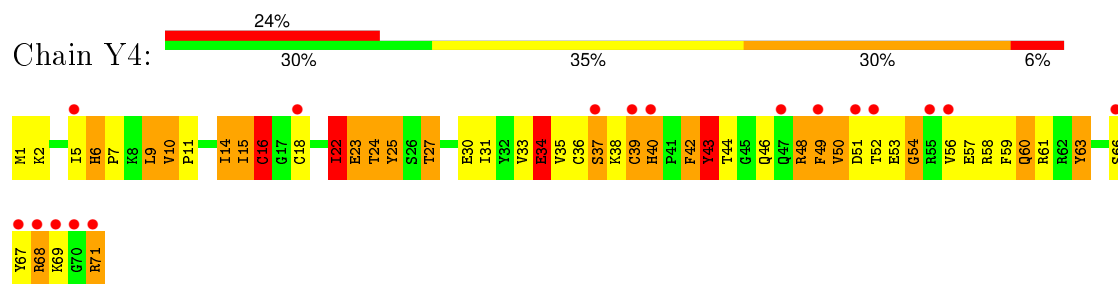
- Molecule 49: 50S ribosomal protein L30



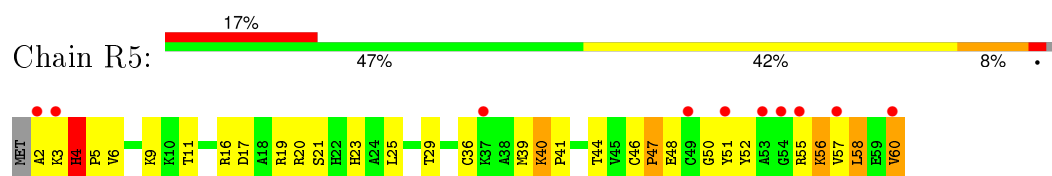
- Molecule 50: 50S ribosomal protein L31



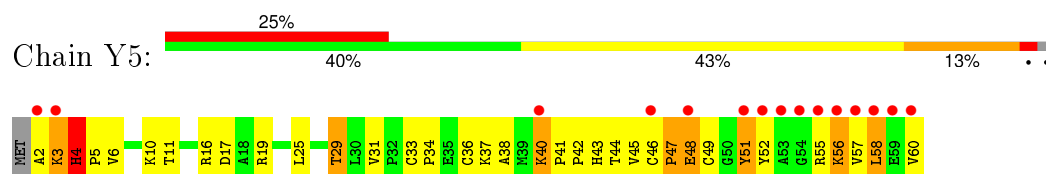
- Molecule 50: 50S ribosomal protein L31



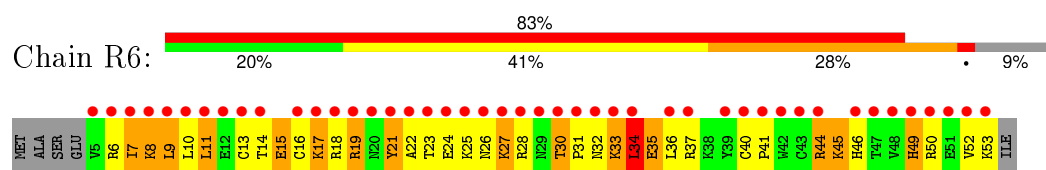
- Molecule 51: 50S ribosomal protein L32



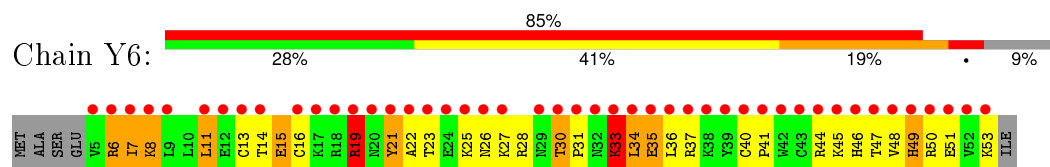
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

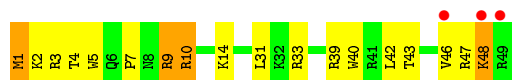


- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

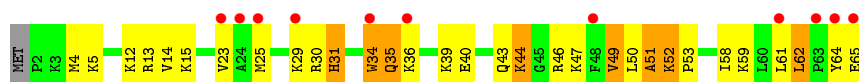




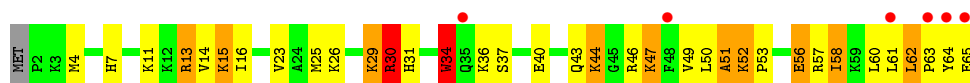
- Molecule 53: 50S ribosomal protein L34



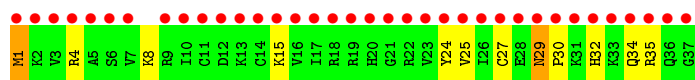
- Molecule 54: 50S ribosomal protein L35



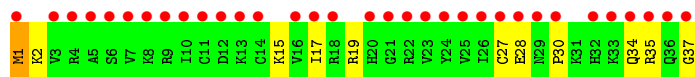
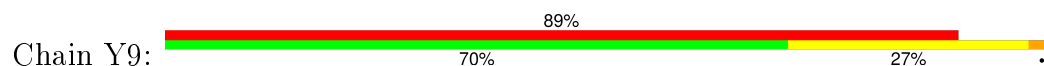
- Molecule 54: 50S ribosomal protein L35



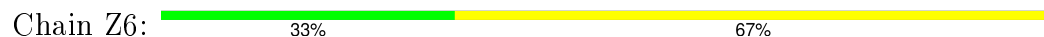
- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA acceptor end mimic



- Molecule 56: tRNA acceptor end mimic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94 181.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (155.22-2.94) 97.9 (181.78-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.265 0.219 , 0.263	Depositor DCC
$R_{free}$ test set	57063 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 1394065 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	291993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PAR, 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	0.46	0/36098	1.01	71/56341 (0.1%)
1	XA	0.54	0/36101	1.09	114/56346 (0.2%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.31	0/1629	0.53	0/2195
3	XC	0.36	0/1629	0.56	0/2195
4	QD	0.38	0/1733	0.58	1/2318 (0.0%)
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.38	0/856	0.54	0/1154
6	XF	0.38	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.50	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.33	0/1029	0.57	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.59	0/1095
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.38	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.45	0/991	0.74	1/1327 (0.1%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.36	0/974	0.63	0/1303
14	QN	0.41	0/501	0.60	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.53	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.56	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	QQ	0.35	0/847	0.53	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.60	0/926
19	XS	0.37	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.63	0/1007
20	XT	0.31	0/765	0.59	0/1007
21	QU	0.30	0/221	0.54	0/288
21	XU	0.31	0/221	0.61	0/288
22	QV	0.52	1/1836 (0.1%)	0.98	4/2859 (0.1%)
22	XV	0.59	1/1836 (0.1%)	1.06	4/2859 (0.1%)
23	QY	0.34	0/333	0.91	0/517
23	XY	0.40	0/333	0.94	0/517
24	QX	0.44	0/185	1.15	2/285 (0.7%)
24	XX	0.67	0/185	1.08	0/285
25	RA	0.63	8/69521 (0.0%)	1.16	318/108529 (0.3%)
25	YA	0.72	19/69543 (0.0%)	1.26	504/108563 (0.5%)
26	RB	0.49	0/2878	1.05	6/4490 (0.1%)
26	YB	0.56	0/2878	1.15	18/4490 (0.4%)
27	RD	0.50	0/2165	0.70	0/2919
27	YD	0.58	0/2165	0.78	1/2919 (0.0%)
28	RE	0.43	0/1601	0.73	3/2160 (0.1%)
28	YE	0.46	0/1601	0.75	2/2160 (0.1%)
29	RF	0.42	0/1620	0.62	0/2194
29	YF	0.48	0/1620	0.71	1/2194 (0.0%)
30	RG	0.31	0/1499	0.57	1/2016 (0.0%)
30	YG	0.39	0/1499	0.60	0/2016
31	RH	0.28	0/1332	0.58	0/1802
31	YH	0.45	0/1332	0.73	0/1802
32	RI	0.35	0/1151	0.67	0/1558
32	YI	0.35	0/1151	0.66	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.64	0/1525
34	RO	0.41	0/943	0.62	1/1269 (0.1%)
34	YO	0.49	0/943	0.65	0/1269
35	RP	0.43	0/1162	0.81	1/1544 (0.1%)
35	YP	0.49	0/1162	0.90	2/1544 (0.1%)
36	RQ	0.47	0/1143	0.73	2/1527 (0.1%)
36	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
37	RR	0.42	0/982	0.69	0/1312
37	YR	0.44	0/982	0.73	0/1312
38	RS	0.36	0/892	0.64	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	YS	0.40	0/892	0.75	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.44	0/1155	0.67	0/1542
40	RU	0.39	0/982	0.65	0/1306
40	YU	0.50	0/982	0.68	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.45	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.50	0/739	0.66	0/993
44	RY	0.44	0/798	0.68	0/1064
44	YY	0.46	0/798	0.69	0/1064
45	RZ	0.34	0/1493	0.59	0/2026
45	YZ	0.37	0/1493	0.64	2/2026 (0.1%)
46	R0	0.45	0/657	0.65	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.66	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.39	0/583	0.65	0/771
48	Y2	0.52	0/583	0.73	0/771
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.41	0/474	0.59	0/635
50	R4	0.33	0/594	0.68	0/795
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.43	0/473	0.73	0/639
51	Y5	0.43	0/473	0.77	1/639 (0.2%)
52	R6	0.35	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.68	0/575
53	Y7	0.57	0/438	0.71	0/575
54	R8	0.55	0/525	0.79	0/691
54	Y8	0.58	0/525	0.82	0/691
55	R9	0.26	0/310	0.45	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z6	0.80	0/40	1.80	1/60 (1.7%)
56	Z8	0.78	0/40	1.81	1/60 (1.7%)
All	All	0.56	29/316367 (0.0%)	1.04	1068/472979 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	QL	0	1
12	XL	0	1
28	RE	0	1
28	YE	0	1
29	YF	0	1
31	RH	0	2
31	YH	0	2
38	YS	0	1
45	YZ	0	1
48	Y2	0	1
54	R8	0	2
54	Y8	0	2
All	All	0	16

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.50	1.48	1.61
22	XV	0	C	OP3-P	-10.49	1.48	1.61
25	YA	528	A	N9-C4	-9.10	1.32	1.37
25	YA	783	A	N9-C4	-7.66	1.33	1.37
25	YA	783	A	N3-C4	-7.55	1.30	1.34

The worst 5 of 1068 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1786	A	N7-C8-N9	13.21	120.41	113.80
25	YA	528	A	C2-N3-C4	-13.10	104.05	110.60
25	YA	783	A	C2-N3-C4	-12.39	104.41	110.60
25	YA	1786	A	C5-N7-C8	-12.26	97.77	103.90
25	YA	1786	A	C2-N3-C4	-11.73	104.73	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
54	R8	30	ARG	Peptide
28	RE	21	VAL	Peptide
31	RH	127	GLU	Peptide
31	RH	153	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	492	0
1	XA	32249	0	16279	529	1
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	80	0
3	QC	1605	0	1668	41	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1763	63	0
4	XD	1703	0	1764	47	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	42	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	37	0
7	XG	1257	0	1296	24	0
8	QH	1116	0	1175	37	0
8	XH	1116	0	1177	25	0
9	QI	1010	0	1037	34	0
9	XI	1010	0	1037	50	0
10	QJ	801	0	849	48	0
10	XJ	801	0	849	42	0
11	QK	885	0	904	25	0
11	XK	885	0	904	28	0
12	QL	975	0	1062	35	0
12	XL	975	0	1062	46	0
13	QM	964	0	1034	40	0
13	XM	964	0	1034	39	0
14	QN	492	0	529	24	0
14	XN	492	0	529	17	0
15	QO	734	0	771	21	0
15	XO	734	0	771	19	0
16	QP	705	0	725	18	0
16	XP	705	0	725	26	0
17	QQ	834	0	904	19	0
17	XQ	834	0	904	19	0
18	QR	574	0	644	11	0
18	XR	574	0	644	21	0
19	QS	674	0	699	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	44	0
20	QT	763	0	860	26	0
20	XT	763	0	861	36	0
21	QU	217	0	234	11	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	26	0
22	XV	1644	0	836	18	0
23	QY	323	0	165	3	0
23	XY	323	0	165	4	0
24	QX	167	0	87	0	0
24	XX	167	0	87	0	0
25	RA	62071	0	31288	921	1
25	YA	62091	0	31295	872	0
26	RB	2573	0	1306	40	1
26	YB	2573	0	1306	32	0
27	RD	2115	0	2195	96	0
27	YD	2115	0	2195	97	0
28	RE	1568	0	1634	72	0
28	YE	1568	0	1634	64	0
29	RF	1585	0	1632	80	0
29	YF	1585	0	1632	64	0
30	RG	1474	0	1535	54	0
30	YG	1474	0	1535	57	0
31	RH	1307	0	1382	61	0
31	YH	1307	0	1382	66	0
32	RI	1136	0	1223	59	1
32	YI	1136	0	1223	49	0
33	RN	1104	0	1180	40	0
33	YN	1104	0	1180	50	0
34	RO	933	0	996	26	0
34	YO	933	0	996	25	0
35	RP	1145	0	1227	87	0
35	YP	1145	0	1227	94	0
36	RQ	1122	0	1179	61	0
36	YQ	1122	0	1178	48	0
37	RR	968	0	1033	48	0
37	YR	968	0	1033	36	0
38	RS	882	0	943	48	0
38	YS	882	0	943	40	0
39	RT	1141	0	1202	53	0
39	YT	1141	0	1202	50	0
40	RU	964	0	1022	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YU	964	0	1022	58	0
41	RV	779	0	852	20	0
41	YV	779	0	852	42	0
42	RW	900	0	964	27	0
42	YW	900	0	964	28	0
43	RX	725	0	778	28	0
43	YX	725	0	778	25	0
44	RY	785	0	878	52	0
44	YY	785	0	878	39	0
45	RZ	1461	0	1493	59	0
45	YZ	1461	0	1493	56	0
46	R0	648	0	672	20	0
46	Y0	648	0	672	27	0
47	R1	763	0	848	26	0
47	Y1	763	0	848	28	0
48	R2	581	0	629	19	0
48	Y2	581	0	629	26	0
49	R3	469	0	518	7	0
49	Y3	469	0	518	17	0
50	R4	581	0	574	25	0
50	Y4	581	0	574	45	0
51	R5	459	0	480	25	0
51	Y5	459	0	480	33	0
52	R6	424	0	450	27	0
52	Y6	424	0	450	30	0
53	R7	430	0	480	14	0
53	Y7	430	0	480	17	0
54	R8	517	0	582	30	0
54	Y8	517	0	582	40	0
55	R9	307	0	338	9	0
55	Y9	307	0	338	7	0
56	Z6	74	0	51	6	0
56	Z8	74	0	51	5	0
57	QA	65	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RA	242	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	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XV	1	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	268	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YX	1	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291993	0	198359	5830	2

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 12.

The worst 5 of 5830 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)
4:QD:22:LYS:HG3	4:QD:26:CYS:SG	1.85	1.16
25:RA:2701:C:H3'	25:RA:2702:U:H5''	1.30	1.13
25:YA:2701:C:H3'	25:YA:2702:U:H5''	1.32	1.07
25:RA:1359:A:N6	25:RA:1372:U:O4	1.87	1.07
27:YD:43:ARG:NH1	27:YD:44:ASN:OD1	1.86	1.06

All (2) 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)
25:RA:1593:G:O2'	26:RB:54:G:OP1[1_655]	2.12	0.08
32:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	175 (74%)	43 (18%)	17 (7%)	1	3
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	2	4
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	5	21
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	13	41
4	QD	206/209 (99%)	175 (85%)	25 (12%)	6 (3%)	6	22
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	7	28
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	5	18
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	9	33
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	15	45
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	15	45
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	26	62
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	6	22
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	4	13
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5	19
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	5	20
10	XJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2	7
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	7	25
11	XK	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	11	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	2	6
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	2
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	3
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	3
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	3
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	1	1
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16	47
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	29
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	16	47
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	16	47
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9	33
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3	11
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	13	41
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	1
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	1
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	2	5
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	2	5
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	12
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	12
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	11
27	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	5	18
28	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	1	1
28	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	1	1
29	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	4
29	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	4	13
30	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	3
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	4
31	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	1
31	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	0
32	RI	144/148 (97%)	101 (70%)	30 (21%)	13 (9%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	YI	144/148 (97%)	104 (72%)	23 (16%)	17 (12%)	0	1
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	2
33	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	1	1
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	37
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	37
35	RP	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	1	2
35	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	1
36	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	1
36	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	0
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3	12
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	7
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	1
38	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	1
39	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	1	2
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	3
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4	17
40	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	4	17
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	5
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	2
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4	16
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	11	36
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	30
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8	30
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	0
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	1
45	RZ	181/206 (88%)	124 (68%)	32 (18%)	25 (14%)	0	0
45	YZ	181/206 (88%)	124 (68%)	40 (22%)	17 (9%)	1	2
46	R0	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	15	45
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1	2
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	3
48	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	2
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4	17
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	11	36
50	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	4	17
51	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	4	17
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	0
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	9	32
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9	32
54	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	2
54	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	4
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9215 (80%)	1533 (13%)	722 (6%)	2	4

5 of 722 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
13	QM	67	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	172 (84%)	33 (16%)	3	8
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6	18
3	QC	159/188 (85%)	145 (91%)	14 (9%)	12	34
3	XC	159/188 (85%)	146 (92%)	13 (8%)	14	38
4	QD	180/181 (99%)	157 (87%)	23 (13%)	5	16
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4	11
5	QE	116/123 (94%)	104 (90%)	12 (10%)	9	26
5	XE	116/123 (94%)	104 (90%)	12 (10%)	9	26
6	QF	90/90 (100%)	78 (87%)	12 (13%)	5	14
6	XF	90/90 (100%)	82 (91%)	8 (9%)	12	34
7	QG	126/127 (99%)	114 (90%)	12 (10%)	11	30
7	XG	126/127 (99%)	114 (90%)	12 (10%)	11	30
8	QH	119/119 (100%)	109 (92%)	10 (8%)	14	36
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	23
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	7
9	XI	98/99 (99%)	80 (82%)	18 (18%)	2	5
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	5	13
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	7
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	28
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	28
12	QL	104/109 (95%)	87 (84%)	17 (16%)	3	8
12	XL	104/109 (95%)	93 (89%)	11 (11%)	8	24
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	2
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	4
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	5
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	11
15	QO	79/80 (99%)	72 (91%)	7 (9%)	12	34
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5	16
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	16
16	XP	72/74 (97%)	64 (89%)	8 (11%)	8	22
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	14	36
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	6
18	XR	61/77 (79%)	52 (85%)	9 (15%)	4	10
19	QS	73/80 (91%)	59 (81%)	14 (19%)	2	4
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	3
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6	19
20	XT	76/82 (93%)	66 (87%)	10 (13%)	5	14
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	64
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	5
27	YD	214/218 (98%)	181 (85%)	33 (15%)	3	9
28	RE	165/166 (99%)	126 (76%)	39 (24%)	1	2
28	YE	165/166 (99%)	137 (83%)	28 (17%)	2	7
29	RF	161/166 (97%)	132 (82%)	29 (18%)	2	6
29	YF	161/166 (97%)	137 (85%)	24 (15%)	4	10
30	RG	155/156 (99%)	134 (86%)	21 (14%)	5	13
30	YG	155/156 (99%)	133 (86%)	22 (14%)	4	12
31	RH	142/148 (96%)	121 (85%)	21 (15%)	4	10
31	YH	142/148 (96%)	115 (81%)	27 (19%)	2	5
32	RI	122/124 (98%)	99 (81%)	23 (19%)	2	5
32	YI	122/124 (98%)	92 (75%)	30 (25%)	1	2
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	7
33	YN	117/119 (98%)	96 (82%)	21 (18%)	2	6
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	28
34	YO	100/100 (100%)	89 (89%)	11 (11%)	8	22
35	RP	116/116 (100%)	85 (73%)	31 (27%)	0	1
35	YP	116/116 (100%)	82 (71%)	34 (29%)	0	1
36	RQ	111/111 (100%)	95 (86%)	16 (14%)	4	11
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	7
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	6
37	YR	101/101 (100%)	80 (79%)	21 (21%)	1	3
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	YS	87/88 (99%)	68 (78%)	19 (22%)	1	3
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	10
39	YT	120/127 (94%)	98 (82%)	22 (18%)	2	5
40	RU	93/94 (99%)	78 (84%)	15 (16%)	3	8
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	7
41	RV	82/82 (100%)	66 (80%)	16 (20%)	2	4
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	5
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	4
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	6
43	RX	74/78 (95%)	64 (86%)	10 (14%)	5	13
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2	5
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	2
44	YY	85/91 (93%)	64 (75%)	21 (25%)	1	2
45	RZ	162/179 (90%)	133 (82%)	29 (18%)	2	6
45	YZ	162/179 (90%)	130 (80%)	32 (20%)	1	4
46	R0	65/67 (97%)	60 (92%)	5 (8%)	16	41
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	11	32
47	R1	82/83 (99%)	73 (89%)	9 (11%)	8	22
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	4	11
48	R2	64/67 (96%)	57 (89%)	7 (11%)	8	23
48	Y2	64/67 (96%)	47 (73%)	17 (27%)	0	1
49	R3	51/52 (98%)	45 (88%)	6 (12%)	6	19
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	3	9
50	R4	63/63 (100%)	45 (71%)	18 (29%)	0	1
50	Y4	63/63 (100%)	43 (68%)	20 (32%)	0	0
51	R5	51/52 (98%)	37 (72%)	14 (28%)	0	1
51	Y5	51/52 (98%)	37 (72%)	14 (28%)	0	1
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	1
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	3
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2	5
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	R8	54/55 (98%)	44 (82%)	10 (18%)	2	5
54	Y8	54/55 (98%)	41 (76%)	13 (24%)	1	2
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	57
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24	57
All	All	9702/10066 (96%)	8152 (84%)	1550 (16%)	3	8

5 of 1550 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	40	THR
8	XH	24	THR
45	YZ	141	VAL
51	R5	4	HIS
2	XB	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
28	RE	55	ASN
45	RZ	73	GLN
11	XK	26	ASN
38	RS	34	HIS
45	RZ	54	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	304 (20%)	48 (3%)
1	XA	1498/1522 (98%)	311 (20%)	50 (3%)
22	QV	76/77 (98%)	21 (27%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QY	14/17 (82%)	5 (35%)	1 (7%)
23	XY	14/17 (82%)	6 (42%)	1 (7%)
24	QX	7/25 (28%)	3 (42%)	2 (28%)
24	XX	7/25 (28%)	1 (14%)	0
25	RA	2879/2916 (98%)	659 (22%)	74 (2%)
25	YA	2880/2916 (98%)	623 (21%)	75 (2%)
26	RB	119/122 (97%)	29 (24%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	YB	119/122 (97%)	29 (24%)	3 (2%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9190/9364 (98%)	2008 (21%)	258 (2%)

5 of 2008 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	29	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2506	U
1	XA	412	A
25	YA	2126	A
25	RA	2689	U
1	XA	78	G

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z  > 2$
23	1MG	QY	37	23	16,26,27	2.88	3 (18%)	19,39,42	1.36	3 (15%)
23	1MG	XY	37	23	16,26,27	2.80	3 (18%)	19,39,42	1.39	3 (15%)
56	PPU	Z6	76	25,56	30,40,41	2.59	6 (20%)	37,57,60	3.25	11 (29%)
56	PPU	Z8	76	25,56	30,40,41	2.57	6 (20%)	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
23	1MG	QY	37	23	-	0/3/25/26	0/3/3/3
23	1MG	XY	37	23	-	0/3/25/26	0/3/3/3
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 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	C9-N6	-5.63	1.31	1.45
56	Z8	76	PPU	C9-N6	-5.62	1.32	1.45
56	Z8	76	PPU	C10-N6	-5.27	1.32	1.45
56	Z6	76	PPU	C10-N6	-5.27	1.32	1.45
56	Z8	76	PPU	C5-N7	-2.01	1.32	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	C2'-C1'-N9	-10.35	98.49	114.29
56	Z6	76	PPU	C2'-C1'-N9	-10.32	98.53	114.29
56	Z8	76	PPU	N3-C2-N1	-9.82	121.37	128.89
56	Z6	76	PPU	N3-C2-N1	-9.77	121.41	128.89
56	Z6	76	PPU	C3'-N3'-C	-8.24	110.19	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	6	0
56	Z8	76	PPU	5	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 683 ligands modelled in this entry, 681 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PAR	QA	1666	-	45,45,45	1.31	7 (15%)	59,67,67	1.41	7 (11%)
58	PAR	XA	1673	-	45,45,45	1.35	7 (15%)	59,67,67	1.35	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	QA	1666	-	-	0/18/94/94	0/4/4/4
58	PAR	XA	1673	-	-	0/18/94/94	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	XA	1673	PAR	C31-C21	2.02	1.56	1.53
58	QA	1666	PAR	C14-C24	2.05	1.56	1.52
58	QA	1666	PAR	C31-C21	2.16	1.56	1.53
58	QA	1666	PAR	C11-C21	2.20	1.56	1.52
58	XA	1673	PAR	C14-C24	2.24	1.56	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1666	PAR	O11-C42-C32	-2.98	101.70	108.92
58	QA	1666	PAR	O54-C54-C44	-2.07	105.79	109.68
58	XA	1673	PAR	C11-O51-C51	2.59	118.76	113.75
58	XA	1673	PAR	O54-C54-C64	2.67	111.32	106.10
58	QA	1666	PAR	O54-C54-C64	2.79	111.54	106.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1666	PAR	2	0
58	XA	1673	PAR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	QA	1500/1522 (98%)	0.03	18 (1%) 81 80	14, 55, 134, 294	0
1	XA	1500/1522 (98%)	0.00	14 (0%) 85 85	7, 42, 133, 270	0
2	QB	237/256 (92%)	1.53	68 (28%) 1 0	42, 98, 171, 216	0
2	XB	237/256 (92%)	0.76	29 (12%) 5 4	27, 78, 141, 206	0
3	QC	205/239 (85%)	1.89	79 (38%) 0 0	37, 91, 139, 193	0
3	XC	205/239 (85%)	0.46	10 (4%) 33 29	11, 53, 103, 148	0
4	QD	208/209 (99%)	0.52	14 (6%) 21 16	23, 54, 106, 136	0
4	XD	208/209 (99%)	0.42	6 (2%) 55 51	17, 51, 103, 175	0
5	QE	151/162 (93%)	0.40	8 (5%) 30 26	29, 65, 114, 172	0
5	XE	151/162 (93%)	0.18	1 (0%) 89 89	15, 43, 86, 138	0
6	QF	101/101 (100%)	-0.07	0 100 100	13, 48, 78, 119	0
6	XF	101/101 (100%)	0.35	6 (5%) 26 21	13, 46, 76, 153	0
7	QG	155/156 (99%)	0.94	26 (16%) 2 1	23, 73, 121, 172	0
7	XG	155/156 (99%)	0.82	14 (9%) 12 8	18, 62, 109, 143	0
8	QH	138/138 (100%)	0.09	2 (1%) 78 77	30, 67, 99, 116	0
8	XH	138/138 (100%)	-0.04	2 (1%) 78 77	13, 48, 84, 127	0
9	QI	127/128 (99%)	1.12	23 (18%) 2 1	33, 89, 129, 180	0
9	XI	127/128 (99%)	0.50	8 (6%) 23 18	19, 69, 124, 167	0
10	QJ	99/105 (94%)	2.13	50 (50%) 0 0	27, 98, 176, 200	0
10	XJ	99/105 (94%)	0.84	14 (14%) 4 2	5, 72, 131, 162	0
11	QK	119/129 (92%)	1.46	23 (19%) 2 1	22, 55, 110, 180	0
11	XK	119/129 (92%)	1.49	28 (23%) 1 1	16, 43, 106, 177	0
12	QL	125/132 (94%)	1.06	24 (19%) 2 1	14, 47, 100, 195	0
12	XL	125/132 (94%)	0.51	12 (9%) 10 7	7, 30, 103, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	QM	121/126 (96%)	0.80	19 (15%) 3 2	27, 84, 121, 226	0
13	XM	121/126 (96%)	0.50	9 (7%) 17 13	24, 57, 113, 211	0
14	QN	60/61 (98%)	1.97	30 (50%) 0 0	38, 80, 105, 122	0
14	XN	60/61 (98%)	0.31	1 (1%) 73 72	22, 43, 76, 100	0
15	QO	88/89 (98%)	0.02	1 (1%) 82 81	15, 52, 101, 137	0
15	XO	88/89 (98%)	0.10	2 (2%) 64 61	10, 42, 80, 97	0
16	QP	84/88 (95%)	-0.23	0 100 100	26, 50, 96, 135	0
16	XP	84/88 (95%)	0.18	1 (1%) 81 80	25, 57, 102, 179	0
17	QQ	100/105 (95%)	0.19	1 (1%) 84 83	27, 56, 100, 119	0
17	XQ	100/105 (95%)	0.49	4 (4%) 42 38	23, 55, 94, 109	0
18	QR	70/88 (79%)	0.35	4 (5%) 27 23	18, 55, 97, 111	0
18	XR	70/88 (79%)	0.76	8 (11%) 7 5	16, 50, 102, 113	0
19	QS	84/93 (90%)	1.07	14 (16%) 2 1	50, 96, 144, 180	0
19	XS	84/93 (90%)	0.82	10 (11%) 6 4	20, 65, 113, 176	0
20	QT	99/106 (93%)	0.28	4 (4%) 42 38	20, 59, 117, 189	0
20	XT	99/106 (93%)	0.58	9 (9%) 11 8	30, 68, 122, 151	0
21	QU	25/27 (92%)	0.78	6 (24%) 1 1	30, 73, 126, 140	0
21	XU	25/27 (92%)	0.75	3 (12%) 6 4	31, 45, 98, 136	0
22	QV	77/77 (100%)	0.23	1 (1%) 79 79	13, 59, 116, 149	0
22	XV	77/77 (100%)	0.25	2 (2%) 59 56	3, 42, 86, 154	0
23	QY	14/17 (82%)	1.60	3 (21%) 1 1	60, 101, 150, 155	0
23	XY	14/17 (82%)	1.60	4 (28%) 1 0	24, 79, 120, 138	0
24	QX	8/25 (32%)	0.35	0 100 100	30, 49, 70, 98	0
24	XX	8/25 (32%)	0.20	0 100 100	15, 25, 40, 55	0
25	RA	2882/2916 (98%)	0.20	115 (3%) 42 38	1, 31, 175, 318	0
25	YA	2883/2916 (98%)	0.11	104 (3%) 46 42	0, 21, 170, 311	0
26	RB	120/122 (98%)	-0.17	0 100 100	29, 55, 88, 110	0
26	YB	120/122 (98%)	-0.16	0 100 100	14, 37, 58, 106	0
27	RD	272/276 (98%)	0.05	3 (1%) 82 81	0, 24, 63, 135	0
27	YD	272/276 (98%)	-0.04	4 (1%) 76 75	0, 14, 46, 168	0
28	RE	205/206 (99%)	0.41	13 (6%) 23 18	1, 36, 109, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	YE	205/206 (99%)	0.32	14 (6%) 20 16	0, 32, 113, 183	0
29	RF	202/210 (96%)	0.06	3 (1%) 76 75	2, 41, 94, 154	0
29	YF	202/210 (96%)	-0.14	2 (0%) 84 83	0, 27, 83, 144	0
30	RG	181/182 (99%)	0.54	17 (9%) 11 7	26, 79, 130, 185	0
30	YG	181/182 (99%)	0.09	7 (3%) 43 39	14, 43, 93, 158	0
31	RH	170/180 (94%)	2.62	95 (55%) 0 0	42, 117, 172, 219	0
31	YH	170/180 (94%)	-0.01	3 (1%) 71 70	12, 50, 96, 160	0
32	RI	146/148 (98%)	1.25	33 (22%) 1 1	22, 74, 128, 179	0
32	YI	146/148 (98%)	0.79	21 (14%) 3 2	16, 74, 128, 161	0
33	RN	138/140 (98%)	0.62	10 (7%) 18 14	16, 43, 86, 151	0
33	YN	138/140 (98%)	0.25	3 (2%) 65 63	10, 35, 87, 139	0
34	RO	122/122 (100%)	0.61	7 (5%) 27 23	10, 34, 75, 103	0
34	YO	122/122 (100%)	0.12	3 (2%) 61 58	1, 25, 48, 76	0
35	RP	150/150 (100%)	1.31	25 (16%) 2 1	3, 48, 112, 222	0
35	YP	150/150 (100%)	0.51	11 (7%) 18 13	2, 32, 95, 190	0
36	RQ	141/141 (100%)	0.97	19 (13%) 4 3	4, 47, 104, 139	0
36	YQ	141/141 (100%)	0.55	14 (9%) 9 6	1, 27, 82, 153	0
37	RR	118/118 (100%)	-0.17	0 100 100	3, 30, 55, 88	0
37	YR	118/118 (100%)	0.27	1 (0%) 87 87	6, 31, 58, 113	0
38	RS	111/112 (99%)	0.35	4 (3%) 46 42	23, 58, 109, 127	0
38	YS	111/112 (99%)	0.21	4 (3%) 46 42	13, 40, 93, 150	0
39	RT	137/146 (93%)	0.69	14 (10%) 9 6	16, 42, 124, 206	0
39	YT	137/146 (93%)	0.26	8 (5%) 26 22	9, 35, 131, 196	0
40	RU	117/118 (99%)	0.52	6 (5%) 32 27	6, 34, 96, 165	0
40	YU	117/118 (99%)	0.11	3 (2%) 59 56	2, 21, 85, 144	0
41	RV	101/101 (100%)	0.92	13 (12%) 5 3	7, 53, 108, 198	0
41	YV	101/101 (100%)	0.54	12 (11%) 6 4	0, 46, 93, 208	0
42	RW	113/113 (100%)	0.12	5 (4%) 38 34	3, 25, 69, 172	0
42	YW	113/113 (100%)	0.15	4 (3%) 48 43	1, 25, 79, 174	0
43	RX	92/96 (95%)	0.07	2 (2%) 65 63	0, 33, 64, 106	0
43	YX	92/96 (95%)	-0.09	1 (1%) 82 81	0, 22, 59, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	RY	102/110 (92%)	0.99	18 (17%) 2 1	10, 65, 132, 205	0
44	YY	102/110 (92%)	0.27	9 (8%) 12 9	8, 46, 109, 201	0
45	RZ	183/206 (88%)	1.12	35 (19%) 2 1	28, 81, 152, 203	0
45	YZ	183/206 (88%)	1.10	27 (14%) 3 2	16, 59, 135, 195	0
46	R0	82/85 (96%)	0.64	3 (3%) 45 41	13, 36, 60, 83	0
46	Y0	82/85 (96%)	0.21	0 100 100	2, 22, 41, 74	0
47	R1	97/98 (98%)	0.92	6 (6%) 24 19	5, 33, 134, 196	0
47	Y1	97/98 (98%)	0.21	6 (6%) 24 19	1, 29, 123, 178	0
48	R2	69/72 (95%)	0.38	5 (7%) 18 14	15, 51, 121, 133	0
48	Y2	69/72 (95%)	0.18	3 (4%) 39 35	8, 32, 85, 167	0
49	R3	59/60 (98%)	1.26	9 (15%) 3 2	15, 41, 78, 134	0
49	Y3	59/60 (98%)	0.36	2 (3%) 49 44	10, 30, 81, 142	0
50	R4	71/71 (100%)	1.88	23 (32%) 1 0	59, 140, 202, 292	0
50	Y4	71/71 (100%)	1.10	17 (23%) 1 1	39, 97, 174, 227	0
51	R5	59/60 (98%)	0.63	10 (16%) 2 1	2, 33, 145, 188	0
51	Y5	59/60 (98%)	1.34	15 (25%) 1 0	1, 39, 172, 198	0
52	R6	49/54 (90%)	6.08	45 (91%) 0 0	68, 125, 194, 221	0
52	Y6	49/54 (90%)	5.18	46 (93%) 0 0	70, 113, 183, 206	0
53	R7	49/49 (100%)	0.29	3 (6%) 25 20	2, 12, 67, 170	0
53	Y7	49/49 (100%)	-0.04	2 (4%) 41 37	0, 7, 50, 140	0
54	R8	64/65 (98%)	1.23	11 (17%) 2 1	8, 31, 93, 151	0
54	Y8	64/65 (98%)	0.58	6 (9%) 11 7	0, 25, 81, 172	0
55	R9	37/37 (100%)	6.37	36 (97%) 0 0	55, 105, 158, 176	0
55	Y9	37/37 (100%)	4.84	33 (89%) 0 0	47, 87, 153, 202	0
56	Z6	2/3 (66%)	0.53	0 100 100	21, 21, 21, 24	0
56	Z8	2/3 (66%)	0.48	0 100 100	5, 5, 5, 14	0
All	All	20873/21492 (97%)	0.42	1588 (7%) 17 12	0, 43, 135, 318	0

The worst 5 of 1588 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R6	6	ARG	23.8
52	R6	5	VAL	22.7

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Mol	Chain	Res	Type	RSRZ
52	Y6	42	TRP	19.1
52	R6	13	CYS	18.2
55	Y9	1	MET	18.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	1MG	XY	37	24/25	0.96	0.18	-	30,30,30,30	0
23	1MG	QY	37	24/25	0.95	0.18	-	53,53,53,53	0
56	PPU	Z6	76	37/38	0.93	0.30	-	27,27,27,27	0
56	PPU	Z8	76	37/38	0.94	0.27	-	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	YA	3171	1/1	0.95	0.51	53.97	29,29,29,29	0
57	MG	RA	3099	1/1	0.97	0.37	46.21	12,12,12,12	0
57	MG	YA	3009	1/1	0.99	0.38	41.47	2,2,2,2	0
57	MG	YA	3256	1/1	0.99	0.35	41.31	3,3,3,3	0
57	MG	RA	3132	1/1	0.94	0.35	26.24	24,24,24,24	0
57	MG	YA	3239	1/1	0.91	0.37	25.68	38,38,38,38	0
57	MG	YA	3263	1/1	0.95	0.38	22.43	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3259	1/1	0.98	0.38	22.29	13,13,13,13	0
57	MG	YA	3198	1/1	0.87	0.32	22.26	69,69,69,69	0
57	MG	YA	3090	1/1	0.98	0.41	21.87	39,39,39,39	0
57	MG	RA	3177	1/1	0.89	0.35	20.99	24,24,24,24	0
57	MG	RA	3098	1/1	0.96	0.31	20.32	7,7,7,7	0
57	MG	RA	3005	1/1	0.97	0.41	20.06	9,9,9,9	0
57	MG	YA	3166	1/1	0.95	0.76	19.94	156,156,156,156	0
57	MG	XA	1603	1/1	0.97	0.41	18.51	13,13,13,13	0
57	MG	YA	3119	1/1	0.81	0.30	17.87	23,23,23,23	0
57	MG	RA	3003	1/1	0.98	0.34	17.49	4,4,4,4	0
57	MG	YA	3050	1/1	0.97	0.28	17.17	2,2,2,2	0
57	MG	RA	3025	1/1	0.98	0.29	16.99	12,12,12,12	0
57	MG	YA	3068	1/1	0.93	0.27	16.85	12,12,12,12	0
57	MG	RA	3124	1/1	0.95	0.39	15.67	24,24,24,24	0
57	MG	YA	3026	1/1	0.98	0.33	15.27	2,2,2,2	0
57	MG	RA	3237	1/1	0.92	0.42	14.95	28,28,28,28	0
57	MG	YA	3146	1/1	0.94	0.31	14.93	37,37,37,37	0
57	MG	RA	3240	1/1	0.94	0.33	14.85	14,14,14,14	0
57	MG	XA	1629	1/1	0.90	0.27	14.66	32,32,32,32	0
57	MG	RA	3205	1/1	0.96	0.28	14.43	5,5,5,5	0
57	MG	YA	3031	1/1	0.98	0.35	14.05	1,1,1,1	0
57	MG	YA	3251	1/1	0.89	0.40	13.82	38,38,38,38	0
57	MG	RA	3126	1/1	0.95	0.30	13.16	33,33,33,33	0
57	MG	YA	3181	1/1	0.96	0.29	12.92	36,36,36,36	0
57	MG	YA	3034	1/1	0.96	0.28	12.88	13,13,13,13	0
57	MG	YA	3015	1/1	0.94	0.32	12.74	15,15,15,15	0
57	MG	YA	3004	1/1	0.98	0.23	12.67	0,0,0,0	0
57	MG	XA	1621	1/1	0.94	0.32	12.41	23,23,23,23	0
57	MG	RA	3086	1/1	0.99	0.34	12.26	13,13,13,13	0
57	MG	YA	3080	1/1	0.98	0.30	12.24	1,1,1,1	0
57	MG	YA	3206	1/1	0.89	0.23	12.11	14,14,14,14	0
57	MG	YA	3008	1/1	0.98	0.27	11.68	2,2,2,2	0
57	MG	RA	3063	1/1	0.99	0.36	11.49	1,1,1,1	0
57	MG	RA	3006	1/1	0.95	0.41	11.01	17,17,17,17	0
57	MG	YA	3048	1/1	0.97	0.27	10.98	11,11,11,11	0
57	MG	YA	3117	1/1	0.97	0.34	10.84	24,24,24,24	0
57	MG	RA	3053	1/1	0.90	0.32	10.69	12,12,12,12	0
57	MG	RA	3137	1/1	0.94	0.29	10.41	7,7,7,7	0
57	MG	YA	3180	1/1	0.93	0.26	10.21	41,41,41,41	0
57	MG	RA	3016	1/1	0.98	0.29	10.13	1,1,1,1	0
57	MG	YA	3108	1/1	0.96	0.30	10.12	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3024	1/1	0.94	0.30	9.93	1,1,1,1	0
57	MG	YA	3253	1/1	0.99	0.32	9.87	2,2,2,2	0
57	MG	XA	1656	1/1	0.94	0.30	9.67	31,31,31,31	0
57	MG	RA	3010	1/1	0.85	0.30	9.56	38,38,38,38	0
57	MG	YA	3061	1/1	0.92	0.22	9.43	17,17,17,17	0
57	MG	QA	1613	1/1	0.95	0.21	9.25	37,37,37,37	0
57	MG	QA	1610	1/1	0.95	0.33	9.20	14,14,14,14	0
57	MG	YA	3057	1/1	0.99	0.30	9.03	1,1,1,1	0
57	MG	RA	3206	1/1	0.90	0.25	8.92	44,44,44,44	0
57	MG	QA	1661	1/1	0.70	0.33	8.92	138,138,138,138	0
57	MG	RA	3032	1/1	0.96	0.33	8.88	27,27,27,27	0
57	MG	RA	3050	1/1	0.91	0.28	8.85	30,30,30,30	0
57	MG	YA	3049	1/1	0.97	0.29	8.53	8,8,8,8	0
57	MG	YA	3197	1/1	0.90	0.22	8.51	42,42,42,42	0
57	MG	RA	3056	1/1	0.99	0.27	8.31	1,1,1,1	0
57	MG	RA	3066	1/1	0.95	0.33	8.28	17,17,17,17	0
57	MG	YA	3100	1/1	0.91	0.30	8.13	1,1,1,1	0
57	MG	YA	3047	1/1	0.96	0.26	8.05	4,4,4,4	0
57	MG	RA	3060	1/1	0.98	0.28	7.93	0,0,0,0	0
57	MG	RP	201	1/1	0.98	0.67	7.93	144,144,144,144	0
57	MG	YA	3011	1/1	0.97	0.27	7.93	14,14,14,14	0
57	MG	RA	3214	1/1	0.98	0.23	7.83	13,13,13,13	0
57	MG	RA	3121	1/1	0.98	0.27	7.78	36,36,36,36	0
57	MG	YA	3103	1/1	0.95	0.25	7.56	8,8,8,8	0
57	MG	RA	3064	1/1	0.91	0.30	7.55	13,13,13,13	0
57	MG	YA	3099	1/1	0.95	0.24	7.52	9,9,9,9	0
57	MG	YA	3002	1/1	0.99	0.29	7.38	1,1,1,1	0
57	MG	YA	3037	1/1	0.97	0.24	7.35	0,0,0,0	0
57	MG	YA	3098	1/1	0.98	0.30	7.25	2,2,2,2	0
57	MG	QA	1604	1/1	0.94	0.23	7.21	4,4,4,4	0
57	MG	RA	3035	1/1	0.99	0.27	7.11	0,0,0,0	0
57	MG	RA	3065	1/1	0.96	0.26	7.03	9,9,9,9	0
57	MG	YA	3023	1/1	0.99	0.28	7.01	6,6,6,6	0
58	PAR	QA	1666	42/42	0.90	0.29	6.99	43,43,43,43	0
57	MG	YA	3107	1/1	0.98	0.28	6.87	2,2,2,2	0
57	MG	RA	3203	1/1	0.78	0.25	6.72	47,47,47,47	0
57	MG	RA	3220	1/1	0.77	0.24	6.65	31,31,31,31	0
57	MG	RA	3227	1/1	0.70	0.25	6.65	32,32,32,32	0
57	MG	YA	3032	1/1	0.92	0.32	6.59	4,4,4,4	0
57	MG	YA	3013	1/1	0.96	0.26	6.36	7,7,7,7	0
57	MG	RA	3013	1/1	0.95	0.23	6.34	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3080	1/1	0.96	0.22	6.25	17,17,17,17	0
57	MG	YA	3041	1/1	0.94	0.26	6.06	2,2,2,2	0
57	MG	YA	3132	1/1	0.96	0.19	6.06	5,5,5,5	0
57	MG	XA	1615	1/1	0.97	0.24	5.98	2,2,2,2	0
57	MG	QA	1617	1/1	0.88	0.27	5.97	31,31,31,31	0
57	MG	RA	3088	1/1	0.93	0.35	5.75	25,25,25,25	0
57	MG	RA	3037	1/1	0.98	0.24	5.67	11,11,11,11	0
57	MG	YA	3033	1/1	0.96	0.31	5.60	9,9,9,9	0
57	MG	YA	3006	1/1	0.97	0.34	5.59	0,0,0,0	0
57	MG	RA	3157	1/1	0.89	0.20	5.49	25,25,25,25	0
57	MG	YA	3070	1/1	0.95	0.22	5.44	18,18,18,18	0
57	MG	YA	3014	1/1	0.96	0.27	5.42	4,4,4,4	0
57	MG	YA	3089	1/1	0.97	0.25	5.39	16,16,16,16	0
57	MG	YA	3193	1/1	0.90	0.28	5.37	18,18,18,18	0
57	MG	YA	3168	1/1	0.98	0.19	5.22	0,0,0,0	0
57	MG	RA	3171	1/1	0.93	0.28	5.15	33,33,33,33	0
57	MG	YA	3073	1/1	0.97	0.31	5.14	8,8,8,8	0
57	MG	RA	3027	1/1	0.96	0.31	5.12	1,1,1,1	0
57	MG	RA	3022	1/1	0.98	0.24	5.09	3,3,3,3	0
57	MG	YA	3065	1/1	0.97	0.20	4.96	0,0,0,0	0
57	MG	YA	3086	1/1	0.99	0.25	4.84	10,10,10,10	0
57	MG	XA	1604	1/1	0.97	0.30	4.78	19,19,19,19	0
57	MG	RA	3133	1/1	0.92	0.22	4.76	6,6,6,6	0
57	MG	YA	3237	1/1	0.94	0.24	4.76	25,25,25,25	0
57	MG	RA	3036	1/1	0.98	0.24	4.64	2,2,2,2	0
57	MG	RA	3076	1/1	0.99	0.23	4.63	0,0,0,0	0
57	MG	RA	3023	1/1	0.94	0.23	4.56	5,5,5,5	0
57	MG	YA	3129	1/1	0.91	0.22	4.52	28,28,28,28	0
57	MG	QA	1612	1/1	0.97	0.24	4.39	9,9,9,9	0
57	MG	RA	3078	1/1	0.97	0.26	4.33	23,23,23,23	0
57	MG	YA	3044	1/1	0.95	0.21	4.25	4,4,4,4	0
57	MG	RA	3055	1/1	0.96	0.19	4.06	8,8,8,8	0
58	PAR	XA	1673	42/42	0.93	0.27	3.92	31,31,31,31	0
57	MG	QV	101	1/1	0.98	0.24	3.91	9,9,9,9	0
57	MG	YB	203	1/1	0.96	0.18	3.79	18,18,18,18	0
57	MG	YA	3138	1/1	0.99	0.20	3.78	0,0,0,0	0
57	MG	YA	3081	1/1	0.96	0.22	3.53	10,10,10,10	0
57	MG	RA	3144	1/1	0.98	0.24	3.53	8,8,8,8	0
57	MG	QA	1615	1/1	0.95	0.15	3.50	28,28,28,28	0
57	MG	RA	3224	1/1	0.93	0.20	3.40	18,18,18,18	0
57	MG	YA	3058	1/1	0.98	0.25	3.36	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1618	1/1	0.91	0.24	3.27	11,11,11,11	0
57	MG	RD	301	1/1	0.86	0.24	3.14	35,35,35,35	0
57	MG	YA	3035	1/1	0.98	0.20	3.04	1,1,1,1	0
57	MG	RA	3039	1/1	0.95	0.22	2.96	10,10,10,10	0
57	MG	RA	3034	1/1	0.95	0.30	2.86	17,17,17,17	0
57	MG	XA	1607	1/1	0.93	0.22	2.59	22,22,22,22	0
57	MG	YA	3182	1/1	0.87	0.21	2.59	18,18,18,18	0
57	MG	YA	3017	1/1	0.96	0.22	2.50	18,18,18,18	0
57	MG	YA	3072	1/1	0.98	0.20	2.50	9,9,9,9	0
57	MG	XA	1633	1/1	0.92	0.22	2.44	16,16,16,16	0
57	MG	RA	3095	1/1	0.96	0.27	2.42	6,6,6,6	0
57	MG	RR	201	1/1	0.97	0.25	2.36	20,20,20,20	0
57	MG	RU	201	1/1	0.97	0.29	2.23	117,117,117,117	0
57	MG	XA	1635	1/1	0.98	0.27	2.13	12,12,12,12	0
57	MG	YA	3027	1/1	0.95	0.24	2.09	9,9,9,9	0
57	MG	YA	3104	1/1	0.60	0.18	1.89	3,3,3,3	0
57	MG	RA	3221	1/1	0.89	0.19	1.89	39,39,39,39	0
57	MG	RA	3041	1/1	0.97	0.22	1.88	22,22,22,22	0
57	MG	YA	3124	1/1	0.98	0.21	1.88	9,9,9,9	0
57	MG	QX	101	1/1	0.94	0.23	1.87	26,26,26,26	0
57	MG	QA	1629	1/1	0.82	0.20	1.87	30,30,30,30	0
57	MG	RA	3020	1/1	0.98	0.23	1.84	8,8,8,8	0
57	MG	RE	302	1/1	0.94	0.23	1.84	5,5,5,5	0
57	MG	YA	3005	1/1	0.98	0.19	1.83	6,6,6,6	0
57	MG	RA	3058	1/1	0.92	0.18	1.75	34,34,34,34	0
57	MG	YA	3056	1/1	0.97	0.22	1.69	1,1,1,1	0
57	MG	RA	3043	1/1	0.95	0.20	1.68	7,7,7,7	0
57	MG	RA	3089	1/1	0.99	0.18	1.67	2,2,2,2	0
57	MG	RA	3188	1/1	0.92	0.22	1.42	29,29,29,29	0
57	MG	YA	3242	1/1	0.86	0.18	1.40	33,33,33,33	0
57	MG	YA	3234	1/1	0.95	0.17	1.39	25,25,25,25	0
57	MG	YA	3264	1/1	0.94	0.18	1.36	7,7,7,7	0
57	MG	YA	3038	1/1	0.96	0.19	1.30	4,4,4,4	0
57	MG	YA	3112	1/1	0.92	0.18	1.27	11,11,11,11	0
57	MG	YA	3125	1/1	0.97	0.19	1.26	9,9,9,9	0
57	MG	YA	3262	1/1	0.98	0.21	1.19	4,4,4,4	0
57	MG	YA	3042	1/1	0.97	0.21	1.13	4,4,4,4	0
57	MG	YA	3184	1/1	0.90	0.17	1.04	26,26,26,26	0
57	MG	YA	3177	1/1	0.93	0.18	0.99	12,12,12,12	0
57	MG	YA	3091	1/1	0.96	0.18	0.99	29,29,29,29	0
57	MG	YA	3159	1/1	0.96	0.17	0.91	16,16,16,16	0
57	MG	QA	1639	1/1	0.96	0.16	0.89	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3241	1/1	0.97	0.24	0.83	13,13,13,13	0
57	MG	YA	3190	1/1	0.97	0.17	0.80	0,0,0,0	0
57	MG	XA	1650	1/1	0.85	0.16	0.76	27,27,27,27	0
57	MG	RA	3222	1/1	0.89	0.16	0.60	36,36,36,36	0
57	MG	YA	3175	1/1	0.95	0.16	0.52	23,23,23,23	0
57	MG	RA	3018	1/1	0.96	0.18	0.52	17,17,17,17	0
57	MG	RA	3021	1/1	0.96	0.24	0.50	2,2,2,2	0
57	MG	RA	3117	1/1	0.95	0.17	0.49	2,2,2,2	0
59	ZN	XD	301	1/1	0.97	0.27	0.44	39,39,39,39	0
57	MG	YA	3094	1/1	0.98	0.18	0.42	4,4,4,4	0
57	MG	RA	3082	1/1	0.98	0.20	0.37	35,35,35,35	0
57	MG	RA	3238	1/1	0.87	0.24	0.32	14,14,14,14	0
57	MG	RA	3087	1/1	0.98	0.17	0.26	25,25,25,25	0
57	MG	YX	101	1/1	0.89	0.18	0.24	46,46,46,46	0
57	MG	XA	1626	1/1	0.99	0.17	0.18	9,9,9,9	0
57	MG	YA	3113	1/1	0.99	0.18	0.11	11,11,11,11	0
57	MG	XA	1622	1/1	0.97	0.17	0.10	33,33,33,33	0
57	MG	XA	1636	1/1	0.94	0.16	0.08	24,24,24,24	0
57	MG	YA	3059	1/1	0.87	0.15	-0.04	19,19,19,19	0
57	MG	YA	3028	1/1	0.98	0.18	-0.04	2,2,2,2	0
57	MG	RA	3090	1/1	0.99	0.17	-0.07	8,8,8,8	0
57	MG	QA	1638	1/1	0.98	0.14	-0.10	27,27,27,27	0
57	MG	XV	101	1/1	0.99	0.18	-0.14	0,0,0,0	0
57	MG	RA	3210	1/1	0.94	0.16	-0.17	18,18,18,18	0
57	MG	RA	3015	1/1	0.98	0.18	-0.21	5,5,5,5	0
57	MG	RA	3208	1/1	0.97	0.15	-0.23	7,7,7,7	0
57	MG	QA	1606	1/1	0.97	0.15	-0.24	11,11,11,11	0
57	MG	YA	3185	1/1	0.92	0.14	-0.31	8,8,8,8	0
57	MG	RB	201	1/1	0.93	0.16	-0.32	41,41,41,41	0
57	MG	XA	1655	1/1	0.71	0.18	-0.41	39,39,39,39	0
59	ZN	QD	301	1/1	0.99	0.22	-0.48	58,58,58,58	0
57	MG	QA	1616	1/1	0.94	0.13	-0.66	28,28,28,28	0
57	MG	RP	202	1/1	0.76	0.18	-0.72	85,85,85,85	0
57	MG	RF	301	1/1	0.93	0.18	-0.84	24,24,24,24	0
57	MG	RA	3108	1/1	0.98	0.16	-0.91	8,8,8,8	0
57	MG	QA	1665	1/1	0.85	0.14	-0.92	31,31,31,31	0
57	MG	QM	201	1/1	0.85	0.14	-0.92	58,58,58,58	0
57	MG	R8	101	1/1	0.90	0.16	-0.93	25,25,25,25	0
57	MG	RA	3142	1/1	0.89	0.16	-0.93	32,32,32,32	0
57	MG	YA	3016	1/1	0.85	0.16	-0.97	0,0,0,0	0
57	MG	RA	3123	1/1	0.96	0.16	-1.00	28,28,28,28	0
57	MG	YA	3205	1/1	0.95	0.16	-1.02	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3025	1/1	0.94	0.16	-1.03	6,6,6,6	0
57	MG	YA	3142	1/1	0.89	0.15	-1.05	8,8,8,8	0
57	MG	XA	1643	1/1	0.98	0.14	-1.13	12,12,12,12	0
57	MG	QA	1646	1/1	0.95	0.12	-1.15	38,38,38,38	0
57	MG	YA	3238	1/1	0.87	0.16	-1.16	26,26,26,26	0
57	MG	XA	1661	1/1	0.85	0.11	-1.16	23,23,23,23	0
57	MG	QA	1620	1/1	0.98	0.12	-1.27	16,16,16,16	0
57	MG	XA	1637	1/1	0.97	0.14	-1.30	20,20,20,20	0
57	MG	YA	3167	1/1	0.95	0.15	-1.33	1,1,1,1	0
57	MG	RA	3136	1/1	0.98	0.16	-1.33	14,14,14,14	0
57	MG	YA	3153	1/1	0.98	0.13	-1.37	13,13,13,13	0
57	MG	RA	3159	1/1	0.92	0.14	-1.38	24,24,24,24	0
57	MG	YA	3228	1/1	0.90	0.14	-1.44	11,11,11,11	0
59	ZN	XN	101	1/1	0.99	0.11	-1.47	42,42,42,42	0
57	MG	YA	3162	1/1	0.93	0.13	-1.47	16,16,16,16	0
57	MG	YA	3135	1/1	0.94	0.13	-1.48	3,3,3,3	0
59	ZN	QN	101	1/1	0.98	0.07	-1.56	95,95,95,95	0
57	MG	XA	1666	1/1	0.96	0.06	-1.56	13,13,13,13	0
57	MG	YA	3074	1/1	0.97	0.12	-1.60	2,2,2,2	0
57	MG	QA	1619	1/1	0.97	0.14	-1.61	1,1,1,1	0
57	MG	RA	3059	1/1	0.98	0.15	-1.64	4,4,4,4	0
57	MG	XA	1614	1/1	0.92	0.11	-1.66	7,7,7,7	0
57	MG	XA	1610	1/1	0.97	0.16	-1.80	7,7,7,7	0
57	MG	XA	1620	1/1	0.98	0.13	-1.83	10,10,10,10	0
57	MG	YA	3137	1/1	0.95	0.14	-1.86	1,1,1,1	0
57	MG	XA	1645	1/1	0.98	0.14	-1.88	15,15,15,15	0
57	MG	YA	3195	1/1	0.89	0.13	-1.94	26,26,26,26	0
57	MG	RA	3073	1/1	0.98	0.12	-1.97	10,10,10,10	0
57	MG	QA	1649	1/1	0.95	0.12	-1.99	31,31,31,31	0
57	MG	YP	202	1/1	0.84	0.15	-1.99	5,5,5,5	0
57	MG	YP	201	1/1	0.96	0.09	-2.01	96,96,96,96	0
57	MG	QA	1657	1/1	0.85	0.13	-2.03	37,37,37,37	0
57	MG	RA	3081	1/1	0.96	0.12	-2.03	10,10,10,10	0
57	MG	RA	3170	1/1	0.92	0.11	-2.05	33,33,33,33	0
57	MG	QA	1630	1/1	0.77	0.12	-2.07	48,48,48,48	0
57	MG	RA	3119	1/1	0.95	0.10	-2.14	30,30,30,30	0
57	MG	QA	1608	1/1	0.80	0.08	-2.16	22,22,22,22	0
57	MG	RA	3103	1/1	0.96	0.13	-2.25	2,2,2,2	0
57	MG	RA	3185	1/1	0.98	0.14	-2.28	16,16,16,16	0
57	MG	QA	1653	1/1	0.98	0.07	-2.30	88,88,88,88	0
57	MG	RA	3184	1/1	0.92	0.14	-2.35	26,26,26,26	0
57	MG	YA	3071	1/1	0.93	0.14	-2.35	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1612	1/1	0.99	0.13	-2.42	3,3,3,3	0
57	MG	RA	3106	1/1	0.94	0.15	-2.44	4,4,4,4	0
57	MG	YA	3036	1/1	0.98	0.14	-2.45	4,4,4,4	0
57	MG	RA	3162	1/1	0.93	0.12	-2.57	2,2,2,2	0
57	MG	QA	1645	1/1	0.93	0.08	-2.81	20,20,20,20	0
57	MG	YA	3178	1/1	0.88	0.14	-2.91	29,29,29,29	0
57	MG	XA	1659	1/1	0.96	0.11	-2.93	43,43,43,43	0
57	MG	YA	3170	1/1	0.96	0.07	-3.08	15,15,15,15	0
57	MG	XA	1608	1/1	0.90	0.09	-3.10	34,34,34,34	0
57	MG	YA	3082	1/1	0.97	0.14	-3.18	0,0,0,0	0
57	MG	QA	1654	1/1	0.97	0.08	-3.27	36,36,36,36	0
57	MG	XA	1634	1/1	0.96	0.12	-3.30	6,6,6,6	0
57	MG	RA	3100	1/1	0.98	0.12	-3.49	6,6,6,6	0
57	MG	RA	3179	1/1	0.93	0.11	-3.54	2,2,2,2	0
57	MG	XA	1638	1/1	0.92	0.10	-3.58	20,20,20,20	0
57	MG	RA	3125	1/1	0.98	0.09	-3.61	13,13,13,13	0
57	MG	QA	1643	1/1	0.92	0.07	-3.66	21,21,21,21	0
57	MG	RA	3131	1/1	0.97	0.12	-3.67	13,13,13,13	0
57	MG	RA	3175	1/1	0.84	0.10	-3.68	19,19,19,19	0
57	MG	RA	3147	1/1	0.94	0.13	-3.81	14,14,14,14	0
57	MG	XA	1625	1/1	0.99	0.10	-3.87	6,6,6,6	0
57	MG	YA	3218	1/1	0.98	0.12	-3.90	1,1,1,1	0
57	MG	RA	3150	1/1	0.92	0.10	-3.91	25,25,25,25	0
57	MG	YA	3224	1/1	0.94	0.08	-3.94	14,14,14,14	0
57	MG	XA	1671	1/1	0.94	0.12	-4.23	18,18,18,18	0
57	MG	RA	3160	1/1	0.94	0.14	-4.26	12,12,12,12	0
57	MG	RA	3155	1/1	0.87	0.13	-4.31	10,10,10,10	0
57	MG	RA	3161	1/1	0.95	0.13	-4.36	17,17,17,17	0
57	MG	XA	1619	1/1	0.97	0.12	-4.44	7,7,7,7	0
57	MG	QA	1631	1/1	0.85	0.08	-4.56	39,39,39,39	0
57	MG	XA	1648	1/1	0.98	0.10	-4.62	14,14,14,14	0
57	MG	RA	3186	1/1	0.93	0.08	-4.71	14,14,14,14	0
57	MG	RA	3215	1/1	0.93	0.07	-4.76	24,24,24,24	0
57	MG	RA	3101	1/1	0.88	0.11	-4.79	2,2,2,2	0
57	MG	XA	1660	1/1	0.96	0.08	-4.82	6,6,6,6	0
57	MG	QA	1635	1/1	0.97	0.12	-4.87	18,18,18,18	0
57	MG	RA	3151	1/1	0.99	0.06	-5.10	0,0,0,0	0
57	MG	QA	1609	1/1	0.97	0.14	-5.17	13,13,13,13	0
57	MG	YA	3201	1/1	0.98	0.13	-5.33	2,2,2,2	0
57	MG	YA	3217	1/1	0.94	0.11	-5.72	9,9,9,9	0
57	MG	XA	1628	1/1	0.95	0.08	-5.95	1,1,1,1	0
57	MG	RA	3191	1/1	0.95	0.07	-6.19	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3199	1/1	0.94	0.09	-6.20	10,10,10,10	0
57	MG	RA	3165	1/1	0.92	0.07	-6.33	14,14,14,14	0
57	MG	RA	3075	1/1	0.96	0.08	-6.45	6,6,6,6	0
57	MG	QA	1621	1/1	0.97	0.07	-6.60	30,30,30,30	0
57	MG	YA	3211	1/1	0.99	0.06	-6.73	0,0,0,0	0
57	MG	YA	3154	1/1	0.95	0.11	-8.99	3,3,3,3	0
57	MG	RA	3212	1/1	0.96	0.08	-9.42	13,13,13,13	0
57	MG	YA	3144	1/1	0.97	0.09	-9.78	11,11,11,11	0
57	MG	YA	3233	1/1	0.96	0.09	-10.86	6,6,6,6	0
57	MG	YA	3111	1/1	0.98	0.08	-17.45	8,8,8,8	0
57	MG	YA	3079	1/1	0.98	0.11	-18.66	2,2,2,2	0
57	MG	RA	3235	1/1	0.94	0.31	-	28,28,28,28	0
57	MG	YA	3118	1/1	0.99	0.31	-	22,22,22,22	0
57	MG	XA	1602	1/1	0.98	0.14	-	18,18,18,18	0
57	MG	YA	3169	1/1	0.99	0.32	-	12,12,12,12	0
57	MG	YA	3187	1/1	0.94	0.17	-	25,25,25,25	0
57	MG	YB	202	1/1	0.95	0.26	-	16,16,16,16	0
57	MG	RA	3128	1/1	0.98	0.23	-	4,4,4,4	0
57	MG	YA	3084	1/1	0.80	0.24	-	2,2,2,2	0
57	MG	RA	3127	1/1	0.91	0.23	-	12,12,12,12	0
57	MG	RA	3111	1/1	0.93	0.28	-	14,14,14,14	0
57	MG	QA	1626	1/1	0.98	0.10	-	21,21,21,21	0
57	MG	QA	1632	1/1	0.96	0.11	-	88,88,88,88	0
57	MG	RA	3232	1/1	0.95	0.28	-	10,10,10,10	0
57	MG	YA	3165	1/1	0.73	0.23	-	40,40,40,40	0
57	MG	YA	3258	1/1	0.95	0.14	-	2,2,2,2	0
57	MG	RA	3231	1/1	0.94	0.32	-	1,1,1,1	0
57	MG	QA	1651	1/1	0.96	0.16	-	18,18,18,18	0
57	MG	YA	3022	1/1	0.94	0.26	-	1,1,1,1	0
57	MG	YA	3076	1/1	0.98	0.40	-	15,15,15,15	0
57	MG	YA	3051	1/1	0.86	0.30	-	15,15,15,15	0
57	MG	YA	3141	1/1	0.94	0.10	-	17,17,17,17	0
57	MG	YA	3122	1/1	0.94	0.16	-	3,3,3,3	0
57	MG	R0	101	1/1	0.79	0.19	-	15,15,15,15	0
57	MG	RA	3118	1/1	0.94	0.09	-	22,22,22,22	0
57	MG	RA	3225	1/1	0.93	0.15	-	40,40,40,40	0
57	MG	YA	3020	1/1	0.98	0.30	-	10,10,10,10	0
57	MG	YA	3007	1/1	0.98	0.18	-	9,9,9,9	0
57	MG	YA	3139	1/1	0.03	0.36	-	55,55,55,55	0
57	MG	YA	3110	1/1	0.95	0.23	-	14,14,14,14	0
57	MG	YA	3222	1/1	0.95	0.16	-	27,27,27,27	0
57	MG	YA	3230	1/1	0.93	0.21	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1624	1/1	0.95	0.15	-	30,30,30,30	0
57	MG	RA	3069	1/1	0.95	0.11	-	1,1,1,1	0
57	MG	XA	1617	1/1	0.97	0.17	-	8,8,8,8	0
57	MG	YA	3255	1/1	0.91	0.38	-	20,20,20,20	0
57	MG	YA	3149	1/1	0.96	0.18	-	9,9,9,9	0
57	MG	YA	3186	1/1	0.96	0.18	-	15,15,15,15	0
57	MG	QA	1659	1/1	0.97	0.18	-	21,21,21,21	0
57	MG	YA	3053	1/1	0.96	0.30	-	0,0,0,0	0
57	MG	RA	3173	1/1	0.98	0.13	-	1,1,1,1	0
57	MG	QA	1662	1/1	0.89	0.07	-	58,58,58,58	0
57	MG	YA	3196	1/1	0.88	0.24	-	54,54,54,54	0
57	MG	YA	3101	1/1	0.99	0.23	-	3,3,3,3	0
57	MG	XA	1667	1/1	0.95	0.27	-	29,29,29,29	0
57	MG	YA	3130	1/1	0.71	0.23	-	20,20,20,20	0
57	MG	QA	1655	1/1	0.93	0.17	-	38,38,38,38	0
57	MG	RA	3007	1/1	0.95	0.32	-	5,5,5,5	0
57	MG	YA	3114	1/1	0.96	0.26	-	13,13,13,13	0
57	MG	YA	3147	1/1	0.95	0.15	-	2,2,2,2	0
57	MG	RA	3083	1/1	0.97	0.17	-	17,17,17,17	0
57	MG	RA	3194	1/1	0.73	0.20	-	13,13,13,13	0
57	MG	RA	3026	1/1	0.79	0.17	-	3,3,3,3	0
57	MG	RA	3047	1/1	0.93	0.32	-	12,12,12,12	0
57	MG	YA	3231	1/1	0.90	0.25	-	20,20,20,20	0
57	MG	RA	3092	1/1	0.95	0.30	-	17,17,17,17	0
57	MG	XM	201	1/1	0.79	0.07	-	58,58,58,58	0
57	MG	YA	3029	1/1	0.94	0.25	-	1,1,1,1	0
57	MG	YA	3040	1/1	0.96	0.30	-	0,0,0,0	0
57	MG	QA	1634	1/1	0.99	0.07	-	35,35,35,35	0
57	MG	YA	3240	1/1	0.90	0.20	-	32,32,32,32	0
57	MG	YA	3161	1/1	0.96	0.17	-	34,34,34,34	0
57	MG	QA	1601	1/1	0.94	0.26	-	34,34,34,34	0
57	MG	RA	3180	1/1	0.97	0.14	-	18,18,18,18	0
57	MG	RA	3198	1/1	0.98	0.07	-	27,27,27,27	0
57	MG	RA	3017	1/1	0.99	0.21	-	0,0,0,0	0
57	MG	RA	3061	1/1	0.94	0.26	-	2,2,2,2	0
57	MG	RA	3200	1/1	0.92	0.46	-	23,23,23,23	0
57	MG	XA	1609	1/1	0.98	0.22	-	14,14,14,14	0
57	MG	YA	3157	1/1	0.97	0.20	-	23,23,23,23	0
57	MG	YA	3209	1/1	0.94	0.15	-	11,11,11,11	0
57	MG	RA	3153	1/1	0.97	0.28	-	29,29,29,29	0
57	MG	RA	3135	1/1	0.59	0.25	-	31,31,31,31	0
57	MG	RA	3189	1/1	0.94	0.25	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1631	1/1	0.93	0.17	-	33,33,33,33	0
57	MG	RA	3042	1/1	0.99	0.32	-	10,10,10,10	0
57	MG	QA	1618	1/1	0.95	0.13	-	13,13,13,13	0
57	MG	YA	3225	1/1	0.96	0.19	-	3,3,3,3	0
57	MG	RA	3143	1/1	0.86	0.15	-	35,35,35,35	0
57	MG	YA	3249	1/1	0.88	0.36	-	42,42,42,42	0
57	MG	RA	3030	1/1	0.97	0.31	-	0,0,0,0	0
57	MG	XA	1624	1/1	0.97	0.14	-	16,16,16,16	0
57	MG	RA	3071	1/1	0.98	0.23	-	22,22,22,22	0
57	MG	XA	1670	1/1	0.75	0.14	-	35,35,35,35	0
57	MG	YA	3039	1/1	0.89	0.17	-	10,10,10,10	0
57	MG	RA	3219	1/1	0.96	0.60	-	159,159,159,159	0
57	MG	YA	3212	1/1	0.91	0.11	-	20,20,20,20	0
57	MG	RA	3028	1/1	0.98	0.34	-	2,2,2,2	0
57	MG	YA	3210	1/1	0.93	0.29	-	26,26,26,26	0
57	MG	XA	1669	1/1	0.91	0.12	-	49,49,49,49	0
57	MG	RA	3204	1/1	0.92	0.28	-	33,33,33,33	0
57	MG	RA	3169	1/1	0.97	0.28	-	30,30,30,30	0
57	MG	YA	3152	1/1	0.92	0.22	-	31,31,31,31	0
57	MG	RA	3140	1/1	0.93	0.31	-	17,17,17,17	0
57	MG	QA	1622	1/1	0.95	0.13	-	40,40,40,40	0
57	MG	RA	3014	1/1	0.98	0.27	-	3,3,3,3	0
57	MG	R5	101	1/1	0.94	0.14	-	21,21,21,21	0
57	MG	RA	3239	1/1	0.94	0.44	-	28,28,28,28	0
57	MG	YA	3200	1/1	0.95	0.29	-	12,12,12,12	0
57	MG	XA	1665	1/1	0.42	0.18	-	56,56,56,56	0
57	MG	QA	1656	1/1	0.94	0.09	-	89,89,89,89	0
57	MG	YA	3150	1/1	0.91	0.16	-	62,62,62,62	0
57	MG	RA	3172	1/1	0.79	0.13	-	15,15,15,15	0
57	MG	YA	3250	1/1	0.93	0.35	-	22,22,22,22	0
57	MG	RA	3115	1/1	0.93	0.21	-	5,5,5,5	0
57	MG	RA	3217	1/1	0.96	0.12	-	14,14,14,14	0
57	MG	XA	1613	1/1	0.96	0.07	-	6,6,6,6	0
57	MG	RA	3062	1/1	0.96	0.25	-	29,29,29,29	0
57	MG	RA	3148	1/1	0.99	0.20	-	15,15,15,15	0
57	MG	RA	3174	1/1	0.94	0.14	-	25,25,25,25	0
57	MG	QA	1603	1/1	0.94	0.25	-	22,22,22,22	0
57	MG	YA	3043	1/1	0.97	0.29	-	1,1,1,1	0
57	MG	RA	3038	1/1	0.98	0.22	-	1,1,1,1	0
57	MG	RA	3168	1/1	0.83	0.21	-	19,19,19,19	0
57	MG	RA	3236	1/1	0.93	0.23	-	28,28,28,28	0
57	MG	RA	3213	1/1	0.93	0.35	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	RA	3146	1/1	0.91	0.10	-	27,27,27,27	0
57	MG	YA	3203	1/1	0.98	0.13	-	25,25,25,25	0
57	MG	QA	1607	1/1	0.97	0.10	-	10,10,10,10	0
57	MG	RA	3109	1/1	0.93	0.10	-	3,3,3,3	0
57	MG	YA	3134	1/1	0.97	0.21	-	19,19,19,19	0
57	MG	YA	3243	1/1	0.94	0.16	-	21,21,21,21	0
57	MG	YA	3018	1/1	0.96	0.32	-	16,16,16,16	0
57	MG	YA	3126	1/1	0.96	0.14	-	1,1,1,1	0
57	MG	QA	1602	1/1	0.98	0.28	-	22,22,22,22	0
57	MG	RA	3230	1/1	0.98	0.35	-	7,7,7,7	0
57	MG	QA	1623	1/1	0.99	0.29	-	19,19,19,19	0
57	MG	YA	3204	1/1	0.79	0.14	-	17,17,17,17	0
57	MG	YA	3268	1/1	0.98	0.16	-	17,17,17,17	0
57	MG	RA	3084	1/1	0.82	0.13	-	7,7,7,7	0
57	MG	RA	3233	1/1	0.96	0.15	-	13,13,13,13	0
57	MG	RA	3209	1/1	0.83	0.27	-	47,47,47,47	0
57	MG	YA	3116	1/1	0.88	0.22	-	39,39,39,39	0
57	MG	YA	3229	1/1	0.98	0.12	-	19,19,19,19	0
57	MG	YE	301	1/1	0.97	0.25	-	0,0,0,0	0
57	MG	RA	3154	1/1	0.98	0.26	-	26,26,26,26	0
57	MG	YA	3077	1/1	0.99	0.29	-	6,6,6,6	0
57	MG	RA	3193	1/1	0.69	0.23	-	63,63,63,63	0
57	MG	RA	3049	1/1	0.98	0.09	-	1,1,1,1	0
57	MG	YA	3136	1/1	0.98	0.30	-	14,14,14,14	0
57	MG	QA	1644	1/1	0.95	0.11	-	21,21,21,21	0
57	MG	XA	1644	1/1	0.94	0.16	-	23,23,23,23	0
57	MG	YA	3223	1/1	0.98	0.18	-	20,20,20,20	0
57	MG	XA	1652	1/1	0.90	0.10	-	47,47,47,47	0
57	MG	RA	3158	1/1	0.91	0.44	-	40,40,40,40	0
57	MG	RA	3218	1/1	0.98	0.26	-	17,17,17,17	0
57	MG	RA	3012	1/1	0.96	0.25	-	7,7,7,7	0
57	MG	YA	3247	1/1	0.97	0.32	-	16,16,16,16	0
57	MG	RA	3048	1/1	0.99	0.23	-	1,1,1,1	0
57	MG	XA	1639	1/1	0.94	0.29	-	58,58,58,58	0
57	MG	RA	3114	1/1	0.92	0.24	-	19,19,19,19	0
57	MG	RA	3167	1/1	0.86	0.17	-	22,22,22,22	0
57	MG	XA	1663	1/1	0.95	0.08	-	38,38,38,38	0
57	MG	XA	1616	1/1	0.99	0.22	-	6,6,6,6	0
57	MG	YA	3123	1/1	0.98	0.28	-	4,4,4,4	0
57	MG	RA	3077	1/1	0.97	0.27	-	13,13,13,13	0
57	MG	YA	3246	1/1	0.94	0.16	-	26,26,26,26	0
57	MG	RA	3130	1/1	0.74	0.32	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3227	1/1	0.94	0.14	-	8,8,8,8	0
57	MG	YA	3069	1/1	0.97	0.15	-	6,6,6,6	0
57	MG	YA	3088	1/1	0.99	0.32	-	5,5,5,5	0
57	MG	YA	3148	1/1	0.91	0.16	-	21,21,21,21	0
57	MG	XA	1651	1/1	0.96	0.11	-	95,95,95,95	0
57	MG	YA	3172	1/1	0.94	0.17	-	25,25,25,25	0
57	MG	YA	3097	1/1	0.95	0.20	-	14,14,14,14	0
57	MG	YA	3160	1/1	0.84	0.07	-	18,18,18,18	0
57	MG	RA	3029	1/1	0.98	0.37	-	3,3,3,3	0
57	MG	YA	3121	1/1	0.93	0.20	-	27,27,27,27	0
57	MG	YA	3208	1/1	0.93	0.10	-	29,29,29,29	0
57	MG	YA	3191	1/1	0.95	0.21	-	14,14,14,14	0
57	MG	YA	3012	1/1	0.99	0.32	-	2,2,2,2	0
57	MG	YA	3055	1/1	0.98	0.24	-	11,11,11,11	0
57	MG	QA	1664	1/1	0.92	0.14	-	17,17,17,17	0
57	MG	RA	3196	1/1	0.92	0.13	-	42,42,42,42	0
57	MG	YA	3215	1/1	0.94	0.11	-	18,18,18,18	0
57	MG	YA	3189	1/1	0.94	0.08	-	1,1,1,1	0
57	MG	XA	1657	1/1	0.92	0.22	-	21,21,21,21	0
57	MG	QA	1658	1/1	0.93	0.18	-	39,39,39,39	0
57	MG	RA	3156	1/1	0.87	0.12	-	31,31,31,31	0
57	MG	RA	3166	1/1	0.94	0.29	-	28,28,28,28	0
57	MG	YA	3244	1/1	0.94	0.22	-	30,30,30,30	0
57	MG	YA	3151	1/1	0.93	0.32	-	30,30,30,30	0
57	MG	QA	1636	1/1	0.77	0.20	-	39,39,39,39	0
57	MG	RA	3079	1/1	0.98	0.24	-	11,11,11,11	0
57	MG	RA	3207	1/1	0.98	0.13	-	60,60,60,60	0
57	MG	RA	3202	1/1	0.97	0.22	-	15,15,15,15	0
57	MG	QA	1647	1/1	0.95	0.12	-	32,32,32,32	0
57	MG	XA	1649	1/1	0.98	0.19	-	8,8,8,8	0
57	MG	XA	1668	1/1	0.98	0.22	-	15,15,15,15	0
57	MG	YA	3221	1/1	0.90	0.16	-	29,29,29,29	0
57	MG	RA	3129	1/1	0.99	0.18	-	10,10,10,10	0
57	MG	RA	3192	1/1	0.40	0.19	-	68,68,68,68	0
57	MG	RA	3152	1/1	0.98	0.24	-	11,11,11,11	0
57	MG	RA	3019	1/1	0.99	0.27	-	13,13,13,13	0
57	MG	YA	3078	1/1	0.95	0.17	-	14,14,14,14	0
57	MG	RA	3149	1/1	0.95	0.30	-	22,22,22,22	0
57	MG	YA	3226	1/1	0.98	0.25	-	4,4,4,4	0
57	MG	YA	3019	1/1	0.98	0.34	-	8,8,8,8	0
57	MG	QA	1614	1/1	0.98	0.14	-	20,20,20,20	0
57	MG	QF	201	1/1	0.79	0.24	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3241	1/1	0.86	0.12	-	37,37,37,37	0
57	MG	QA	1627	1/1	0.94	0.24	-	22,22,22,22	0
57	MG	YA	3265	1/1	0.91	0.30	-	17,17,17,17	0
57	MG	RA	3201	1/1	0.98	0.14	-	17,17,17,17	0
57	MG	YA	3102	1/1	0.93	0.20	-	44,44,44,44	0
57	MG	RA	3183	1/1	0.96	0.14	-	1,1,1,1	0
57	MG	YA	3158	1/1	0.93	0.30	-	14,14,14,14	0
57	MG	XA	1658	1/1	0.98	0.26	-	12,12,12,12	0
57	MG	RA	3242	1/1	0.93	0.32	-	31,31,31,31	0
57	MG	YA	3120	1/1	0.41	0.28	-	21,21,21,21	0
57	MG	RA	3216	1/1	0.93	0.12	-	33,33,33,33	0
57	MG	RA	3057	1/1	0.94	0.23	-	6,6,6,6	0
57	MG	RA	3181	1/1	0.94	0.25	-	29,29,29,29	0
57	MG	RB	202	1/1	0.90	0.18	-	46,46,46,46	0
57	MG	YA	3083	1/1	0.98	0.18	-	0,0,0,0	0
57	MG	RA	3046	1/1	0.98	0.17	-	8,8,8,8	0
57	MG	YA	3106	1/1	0.95	0.22	-	12,12,12,12	0
57	MG	YA	3248	1/1	0.96	0.34	-	30,30,30,30	0
57	MG	RA	3107	1/1	0.99	0.18	-	6,6,6,6	0
57	MG	YA	3236	1/1	0.97	0.10	-	24,24,24,24	0
57	MG	RA	3097	1/1	0.93	0.26	-	4,4,4,4	0
57	MG	RA	3002	1/1	0.90	0.24	-	26,26,26,26	0
57	MG	YA	3093	1/1	0.97	0.20	-	9,9,9,9	0
57	MG	YA	3214	1/1	0.95	0.16	-	25,25,25,25	0
57	MG	RA	3164	1/1	0.96	0.24	-	20,20,20,20	0
57	MG	YA	3095	1/1	0.99	0.20	-	5,5,5,5	0
57	MG	XA	1642	1/1	0.99	0.16	-	7,7,7,7	0
57	MG	RA	3091	1/1	0.54	0.34	-	23,23,23,23	0
57	MG	YA	3219	1/1	0.97	0.20	-	31,31,31,31	0
57	MG	YQ	201	1/1	0.95	0.22	-	142,142,142,142	0
57	MG	YA	3064	1/1	0.98	0.17	-	6,6,6,6	0
57	MG	RA	3096	1/1	0.96	0.23	-	18,18,18,18	0
57	MG	YA	3001	1/1	0.99	0.29	-	1,1,1,1	0
57	MG	RA	3145	1/1	0.95	0.21	-	27,27,27,27	0
57	MG	YA	3021	1/1	0.96	0.24	-	1,1,1,1	0
57	MG	QA	1650	1/1	0.90	0.20	-	20,20,20,20	0
57	MG	RA	3094	1/1	0.98	0.14	-	8,8,8,8	0
57	MG	YA	3128	1/1	0.98	0.33	-	3,3,3,3	0
57	MG	YA	3030	1/1	0.98	0.39	-	6,6,6,6	0
57	MG	YA	3163	1/1	0.92	0.19	-	25,25,25,25	0
57	MG	YA	3105	1/1	0.95	0.10	-	24,24,24,24	0
57	MG	RA	3226	1/1	0.95	0.18	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	XA	1623	1/1	0.89	0.14	-	13,13,13,13	0
57	MG	YA	3235	1/1	0.95	0.30	-	30,30,30,30	0
57	MG	RA	3040	1/1	0.95	0.26	-	15,15,15,15	0
57	MG	YA	3254	1/1	0.99	0.20	-	18,18,18,18	0
57	MG	YA	3220	1/1	0.93	0.23	-	32,32,32,32	0
57	MG	YA	3207	1/1	0.75	0.23	-	46,46,46,46	0
57	MG	YA	3173	1/1	0.96	0.19	-	49,49,49,49	0
57	MG	YA	3046	1/1	0.92	0.31	-	20,20,20,20	0
57	MG	YA	3010	1/1	0.99	0.27	-	1,1,1,1	0
57	MG	YA	3245	1/1	0.85	0.47	-	28,28,28,28	0
57	MG	YA	3063	1/1	0.99	0.30	-	3,3,3,3	0
57	MG	QA	1648	1/1	0.97	0.14	-	34,34,34,34	0
57	MG	RA	3045	1/1	0.96	0.27	-	6,6,6,6	0
57	MG	XA	1647	1/1	0.91	0.29	-	23,23,23,23	0
57	MG	RA	3102	1/1	0.97	0.21	-	28,28,28,28	0
57	MG	RA	3176	1/1	0.90	0.21	-	10,10,10,10	0
57	MG	RA	3182	1/1	0.94	0.11	-	6,6,6,6	0
57	MG	RA	3139	1/1	0.10	0.28	-	59,59,59,59	0
57	MG	YA	3143	1/1	0.88	0.19	-	33,33,33,33	0
57	MG	RA	3113	1/1	0.99	0.11	-	29,29,29,29	0
57	MG	YA	3266	1/1	0.85	0.32	-	51,51,51,51	0
57	MG	RA	3122	1/1	0.95	0.21	-	32,32,32,32	0
57	MG	QA	1642	1/1	0.92	0.14	-	43,43,43,43	0
57	MG	RA	3104	1/1	0.97	0.10	-	9,9,9,9	0
57	MG	RA	3110	1/1	0.98	0.21	-	2,2,2,2	0
57	MG	RA	3067	1/1	0.96	0.20	-	3,3,3,3	0
57	MG	QA	1605	1/1	0.96	0.37	-	23,23,23,23	0
57	MG	XA	1641	1/1	0.90	0.18	-	33,33,33,33	0
57	MG	YA	3003	1/1	0.92	0.22	-	1,1,1,1	0
57	MG	RA	3004	1/1	0.98	0.37	-	14,14,14,14	0
57	MG	QA	1641	1/1	0.97	0.17	-	22,22,22,22	0
57	MG	YA	3252	1/1	0.95	0.41	-	17,17,17,17	0
57	MG	YA	3075	1/1	0.97	0.37	-	24,24,24,24	0
57	MG	RA	3051	1/1	0.97	0.22	-	4,4,4,4	0
57	MG	YA	3062	1/1	0.93	0.21	-	7,7,7,7	0
57	MG	YA	3066	1/1	0.97	0.36	-	12,12,12,12	0
57	MG	RA	3033	1/1	0.92	0.34	-	3,3,3,3	0
57	MG	RA	3008	1/1	0.92	0.18	-	30,30,30,30	0
57	MG	YA	3156	1/1	0.95	0.25	-	13,13,13,13	0
57	MG	YA	3213	1/1	0.97	0.13	-	6,6,6,6	0
57	MG	YA	3133	1/1	0.94	0.11	-	26,26,26,26	0
57	MG	RA	3085	1/1	0.92	0.24	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3054	1/1	0.63	0.17	-	48,48,48,48	0
57	MG	YA	3194	1/1	0.98	0.13	-	17,17,17,17	0
57	MG	RA	3031	1/1	0.99	0.20	-	3,3,3,3	0
57	MG	YA	3183	1/1	0.97	0.24	-	13,13,13,13	0
57	MG	RA	3116	1/1	0.97	0.19	-	0,0,0,0	0
57	MG	QA	1633	1/1	0.91	0.29	-	35,35,35,35	0
57	MG	QA	1660	1/1	0.97	0.17	-	38,38,38,38	0
57	MG	YA	3179	1/1	0.96	0.41	-	35,35,35,35	0
57	MG	YA	3127	1/1	0.92	0.16	-	26,26,26,26	0
57	MG	RA	3187	1/1	0.90	0.56	-	66,66,66,66	0
57	MG	RA	3068	1/1	0.83	0.18	-	16,16,16,16	0
57	MG	YA	3176	1/1	0.98	0.15	-	2,2,2,2	0
57	MG	RA	3195	1/1	0.98	0.12	-	1,1,1,1	0
57	MG	RA	3234	1/1	0.97	0.24	-	10,10,10,10	0
57	MG	RA	3141	1/1	0.97	0.11	-	15,15,15,15	0
57	MG	RA	3190	1/1	0.91	0.31	-	27,27,27,27	0
57	MG	YA	3109	1/1	0.96	0.11	-	5,5,5,5	0
57	MG	XA	1611	1/1	0.99	0.25	-	7,7,7,7	0
57	MG	RA	3024	1/1	0.97	0.28	-	7,7,7,7	0
57	MG	YA	3085	1/1	0.99	0.28	-	9,9,9,9	0
57	MG	QA	1652	1/1	0.90	0.19	-	32,32,32,32	0
57	MG	YA	3164	1/1	0.69	0.16	-	45,45,45,45	0
57	MG	RA	3228	1/1	0.92	0.13	-	43,43,43,43	0
57	MG	RE	301	1/1	0.94	0.16	-	1,1,1,1	0
57	MG	RA	3072	1/1	0.97	0.18	-	3,3,3,3	0
57	MG	XA	1601	1/1	0.96	0.24	-	7,7,7,7	0
57	MG	XA	1630	1/1	0.89	0.12	-	13,13,13,13	0
57	MG	YA	3092	1/1	0.98	0.25	-	3,3,3,3	0
57	MG	YA	3115	1/1	0.97	0.27	-	18,18,18,18	0
57	MG	YA	3257	1/1	0.98	0.38	-	3,3,3,3	0
57	MG	XA	1672	1/1	0.86	0.12	-	27,27,27,27	0
57	MG	YA	3261	1/1	0.90	0.33	-	19,19,19,19	0
57	MG	RA	3070	1/1	0.97	0.33	-	13,13,13,13	0
57	MG	RA	3011	1/1	0.93	0.41	-	36,36,36,36	0
57	MG	RA	3197	1/1	0.96	0.12	-	9,9,9,9	0
57	MG	QH	201	1/1	0.20	0.15	-	74,74,74,74	0
57	MG	YA	3188	1/1	0.89	0.26	-	33,33,33,33	0
57	MG	YA	3267	1/1	0.98	0.41	-	24,24,24,24	0
57	MG	YA	3155	1/1	0.96	0.21	-	50,50,50,50	0
57	MG	YB	201	1/1	0.82	0.17	-	39,39,39,39	0
57	MG	RA	3112	1/1	0.94	0.22	-	21,21,21,21	0
57	MG	XA	1605	1/1	0.97	0.29	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	QA	1628	1/1	0.44	0.28	-	37,37,37,37	0
57	MG	YA	3131	1/1	0.93	0.20	-	34,34,34,34	0
57	MG	RA	3052	1/1	0.96	0.28	-	7,7,7,7	0
57	MG	RA	3229	1/1	0.92	0.11	-	26,26,26,26	0
57	MG	XA	1640	1/1	0.96	0.19	-	15,15,15,15	0
57	MG	RA	3009	1/1	0.97	0.06	-	0,0,0,0	0
57	MG	YA	3060	1/1	0.95	0.27	-	1,1,1,1	0
57	MG	QA	1611	1/1	0.97	0.31	-	12,12,12,12	0
57	MG	YA	3052	1/1	0.96	0.27	-	1,1,1,1	0
57	MG	QA	1637	1/1	0.91	0.18	-	16,16,16,16	0
57	MG	RA	3093	1/1	0.97	0.28	-	8,8,8,8	0
57	MG	YA	3096	1/1	0.96	0.22	-	5,5,5,5	0
57	MG	YA	3145	1/1	0.92	0.20	-	18,18,18,18	0
57	MG	YA	3192	1/1	0.93	0.21	-	19,19,19,19	0
57	MG	YA	3087	1/1	0.93	0.25	-	1,1,1,1	0
57	MG	RA	3211	1/1	0.93	0.23	-	30,30,30,30	0
57	MG	YA	3174	1/1	0.94	0.09	-	7,7,7,7	0
57	MG	XA	1664	1/1	0.91	0.09	-	44,44,44,44	0
57	MG	Y5	101	1/1	0.91	0.19	-	12,12,12,12	0
57	MG	YA	3260	1/1	0.91	0.29	-	13,13,13,13	0
57	MG	QA	1663	1/1	0.95	0.10	-	67,67,67,67	0
57	MG	XA	1654	1/1	0.88	0.10	-	37,37,37,37	0
57	MG	YA	3067	1/1	0.98	0.21	-	2,2,2,2	0
57	MG	XA	1653	1/1	0.74	0.13	-	70,70,70,70	0
57	MG	QA	1640	1/1	0.95	0.27	-	24,24,24,24	0
57	MG	XX	101	1/1	0.77	0.29	-	45,45,45,45	0
57	MG	RA	3178	1/1	0.94	0.23	-	26,26,26,26	0
57	MG	YA	3199	1/1	0.94	0.27	-	11,11,11,11	0
57	MG	RA	3223	1/1	0.84	0.35	-	59,59,59,59	0
57	MG	XA	1627	1/1	0.98	0.32	-	28,28,28,28	0
57	MG	QA	1625	1/1	0.33	0.19	-	70,70,70,70	0
57	MG	RA	3001	1/1	0.97	0.14	-	4,4,4,4	0
57	MG	RA	3134	1/1	0.93	0.26	-	23,23,23,23	0
57	MG	YA	3216	1/1	0.95	0.32	-	30,30,30,30	0
57	MG	RA	3074	1/1	0.94	0.22	-	0,0,0,0	0
57	MG	XA	1606	1/1	0.96	0.29	-	12,12,12,12	0
57	MG	RA	3138	1/1	0.83	0.28	-	6,6,6,6	0
57	MG	XA	1632	1/1	0.93	0.23	-	21,21,21,21	0
57	MG	YA	3045	1/1	0.90	0.18	-	1,1,1,1	0
57	MG	YA	3140	1/1	0.92	0.23	-	2,2,2,2	0
57	MG	RA	3044	1/1	0.96	0.20	-	18,18,18,18	0
57	MG	RA	3105	1/1	0.97	0.24	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	YA	3232	1/1	0.88	0.33	-	47,47,47,47	0
57	MG	XA	1662	1/1	0.83	0.26	-	40,40,40,40	0
57	MG	RA	3120	1/1	0.53	0.41	-	80,80,80,80	0
57	MG	XA	1646	1/1	0.94	0.27	-	30,30,30,30	0
57	MG	RA	3163	1/1	0.97	0.25	-	19,19,19,19	0
57	MG	YA	3202	1/1	0.95	0.09	-	13,13,13,13	0
57	MG	RA	3054	1/1	0.96	0.12	-	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.