



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:13 PM GMT

PDB ID : 4TUC
Title : Crystal structure of ASL-SufJ bound to Codon ACC-A on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-06-24
Resolution : 3.60 Å(reported)

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

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

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

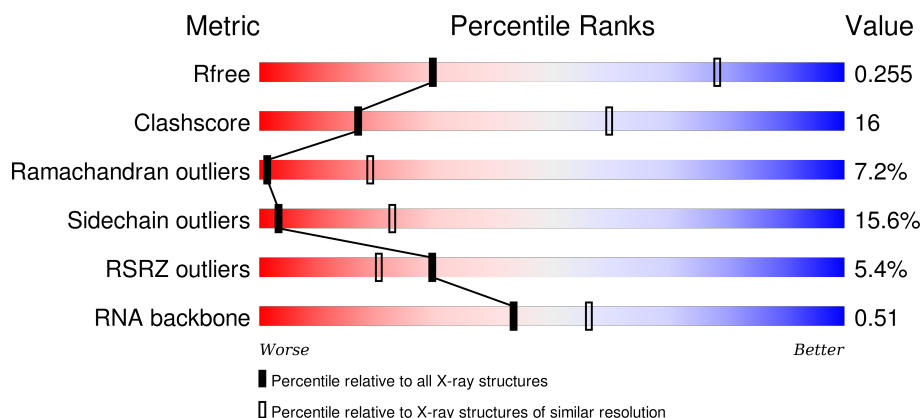
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






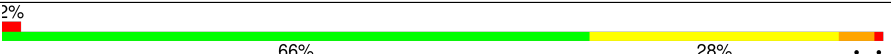
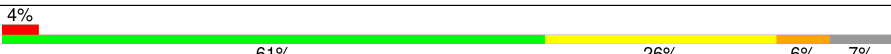
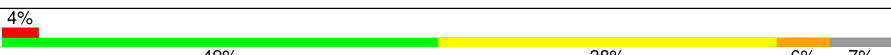
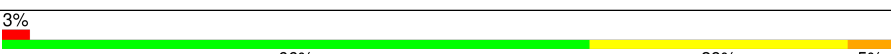
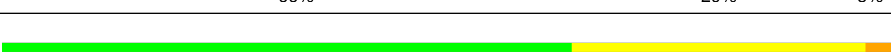

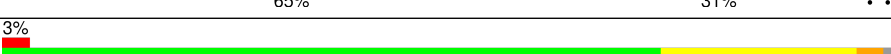
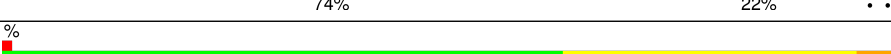
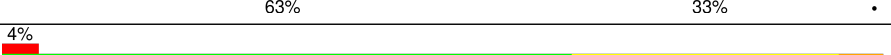
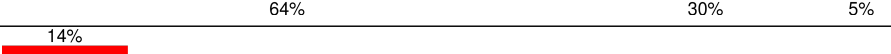
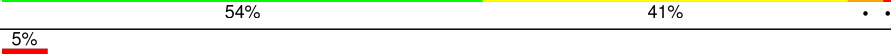

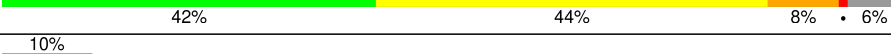
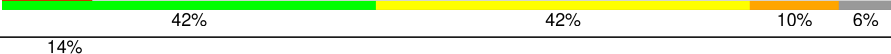



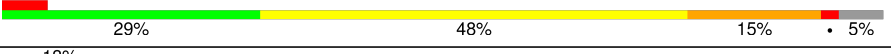
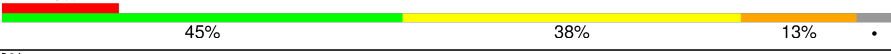



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>7%</div> <div>55%</div> <div>35%</div> <div>8%</div> <div>..</div> </div>
1	XA	1522	<div> <div>4%</div> <div>52%</div> <div>36%</div> <div>10%</div> <div>.</div> </div>
2	QB	256	<div> <div>7%</div> <div>49%</div> <div>36%</div> <div>7%</div> <div>7%</div> </div>
2	XB	256	<div> <div>5%</div> <div>47%</div> <div>35%</div> <div>9%</div> <div>7%</div> </div>







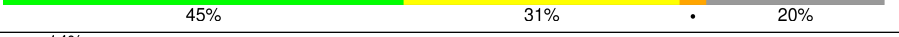

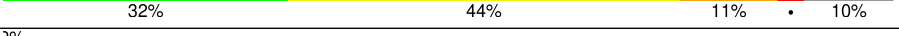

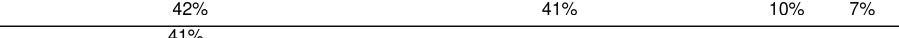
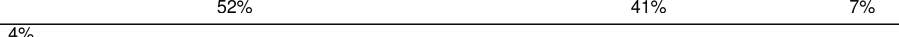

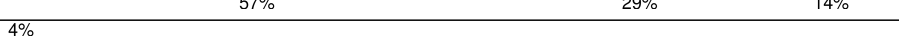


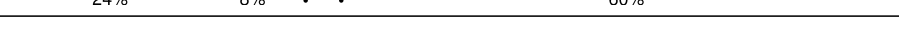

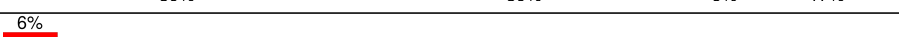




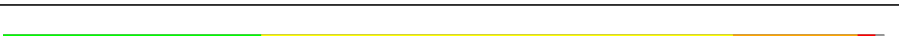

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126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

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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1602	-	-	-	X
57	MG	QA	1605	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1616	-	-	-	X
57	MG	QA	1617	-	-	-	X
57	MG	QA	1619	-	-	-	X
57	MG	QA	1636	-	-	-	X
57	MG	QA	1642	-	-	-	X
57	MG	QA	1652	-	-	-	X
57	MG	QA	1658	-	-	-	X
57	MG	QA	1660	-	-	-	X
57	MG	QA	1664	-	-	-	X
57	MG	QA	1670	-	-	-	X
57	MG	QA	1683	-	-	-	X
57	MG	QA	1684	-	-	-	X
57	MG	QM	201	-	-	-	X
57	MG	QN	102	-	-	-	X
57	MG	QV	102	-	-	-	X
57	MG	R8	101	-	-	-	X
57	MG	RA	3002	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3008	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3009	-	-	-	X
57	MG	RA	3012	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3017	-	-	-	X
57	MG	RA	3024	-	-	-	X
57	MG	RA	3026	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3035	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3038	-	-	-	X
57	MG	RA	3040	-	-	-	X
57	MG	RA	3042	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3050	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3058	-	-	-	X
57	MG	RA	3059	-	-	-	X
57	MG	RA	3062	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3068	-	-	-	X
57	MG	RA	3074	-	-	-	X
57	MG	RA	3076	-	-	-	X
57	MG	RA	3078	-	-	-	X
57	MG	RA	3080	-	-	-	X
57	MG	RA	3083	-	-	-	X
57	MG	RA	3084	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3093	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3096	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3098	-	-	-	X
57	MG	RA	3099	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3105	-	-	-	X
57	MG	RA	3114	-	-	-	X
57	MG	RA	3119	-	-	-	X
57	MG	RA	3123	-	-	-	X
57	MG	RA	3134	-	-	-	X
57	MG	RA	3141	-	-	-	X
57	MG	RA	3144	-	-	-	X
57	MG	RA	3147	-	-	-	X
57	MG	RA	3154	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3159	-	-	-	X
57	MG	RA	3160	-	-	-	X
57	MG	RA	3167	-	-	-	X
57	MG	RA	3171	-	-	-	X
57	MG	RA	3175	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3196	-	-	-	X
57	MG	RA	3198	-	-	-	X
57	MG	RA	3199	-	-	-	X
57	MG	RA	3204	-	-	-	X
57	MG	RA	3210	-	-	-	X
57	MG	RA	3211	-	-	-	X
57	MG	RA	3216	-	-	-	X
57	MG	RA	3218	-	-	-	X
57	MG	RA	3230	-	-	-	X
57	MG	RA	3232	-	-	-	X
57	MG	RA	3233	-	-	-	X
57	MG	RA	3243	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RR	201	-	-	-	X
57	MG	XA	1602	-	-	-	X
57	MG	XA	1603	-	-	-	X
57	MG	XA	1607	-	-	-	X
57	MG	XA	1613	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1618	-	-	-	X
57	MG	XA	1619	-	-	-	X
57	MG	XA	1632	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1634	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1643	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	XA	1648	-	-	-	X
57	MG	XA	1651	-	-	-	X
57	MG	XA	1659	-	-	-	X
57	MG	XA	1665	-	-	-	X
57	MG	XA	1668	-	-	-	X
57	MG	XA	1669	-	-	-	X
57	MG	XA	1693	-	-	-	X
57	MG	XA	1696	-	-	-	X
57	MG	XA	1699	-	-	-	X
57	MG	XA	1700	-	-	-	X
57	MG	XA	1701	-	-	-	X
57	MG	XF	201	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3006	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3015	-	-	-	X
57	MG	YA	3017	-	-	-	X
57	MG	YA	3024	-	-	-	X
57	MG	YA	3025	-	-	-	X
57	MG	YA	3026	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3038	-	-	-	X
57	MG	YA	3041	-	-	-	X
57	MG	YA	3044	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3056	-	-	-	X
57	MG	YA	3057	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3065	-	-	-	X
57	MG	YA	3068	-	-	-	X
57	MG	YA	3073	-	-	-	X
57	MG	YA	3074	-	-	-	X
57	MG	YA	3078	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3080	-	-	-	X
57	MG	YA	3086	-	-	-	X
57	MG	YA	3089	-	-	-	X
57	MG	YA	3090	-	-	-	X
57	MG	YA	3094	-	-	-	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	3110	-	-	-	X
57	MG	YA	3112	-	-	-	X
57	MG	YA	3119	-	-	-	X
57	MG	YA	3131	-	-	-	X
57	MG	YA	3134	-	-	-	X
57	MG	YA	3135	-	-	-	X
57	MG	YA	3137	-	-	-	X
57	MG	YA	3139	-	-	-	X
57	MG	YA	3143	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3175	-	-	-	X
57	MG	YA	3179	-	-	-	X
57	MG	YA	3181	-	-	-	X
57	MG	YA	3187	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3193	-	-	-	X
57	MG	YA	3199	-	-	-	X
57	MG	YA	3204	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3209	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3227	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3238	-	-	-	X
57	MG	YA	3240	-	-	-	X
57	MG	YA	3242	-	-	-	X
57	MG	YA	3243	-	-	-	X
57	MG	YA	3248	-	-	-	X
57	MG	YA	3249	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3250	-	-	-	X
57	MG	YA	3256	-	-	-	X
57	MG	YA	3258	-	-	-	X
57	MG	YA	3261	-	-	-	X
57	MG	YA	3267	-	-	-	X
57	MG	YB	203	-	-	-	X
57	MG	YP	201	-	-	-	X
59	PPU	Z5	101	-	-	-	X
59	PPU	Z6	101	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P-site tRNA 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	QX	11	Total	C	N	O	P	0	0	0
			220	98	43	68	11			
23	XX	10	Total	C	N	O	P	0	0	0
			214	97	43	65	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			
24	XY	15	Total	C	N	O	P	0	0	0
			319	142	55	107	15			

- 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
			62069	27627	11609	19952	2881			
25	YA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	150	Total	C	N	O	S	0	0	0
			1143	711	231	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	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	89	Total	Mg	0	0
			89	89		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	276	Total	Mg	0	0
			276	276		
57	QM	1	Total	Mg	0	0
			1	1		
57	Y1	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	3	Total 3	Mg 3	0	0
57	XA	102	Total 102	Mg 102	0	0
57	R0	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	XF	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	R1	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	Y0	1	Total 1	Mg 1	0	0
57	RA	248	Total 248	Mg 248	0	0
57	YP	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	YB	5	Total 5	Mg 5	0	0
57	QN	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	2	Total 2	Mg 2	0	0

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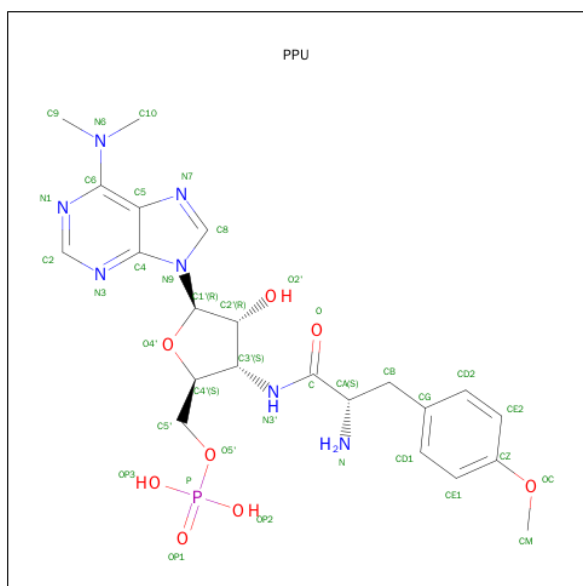
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R8	1	Total	Mg	0	0
			1	1		
57	YE	1	Total	Mg	0	0
			1	1		

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

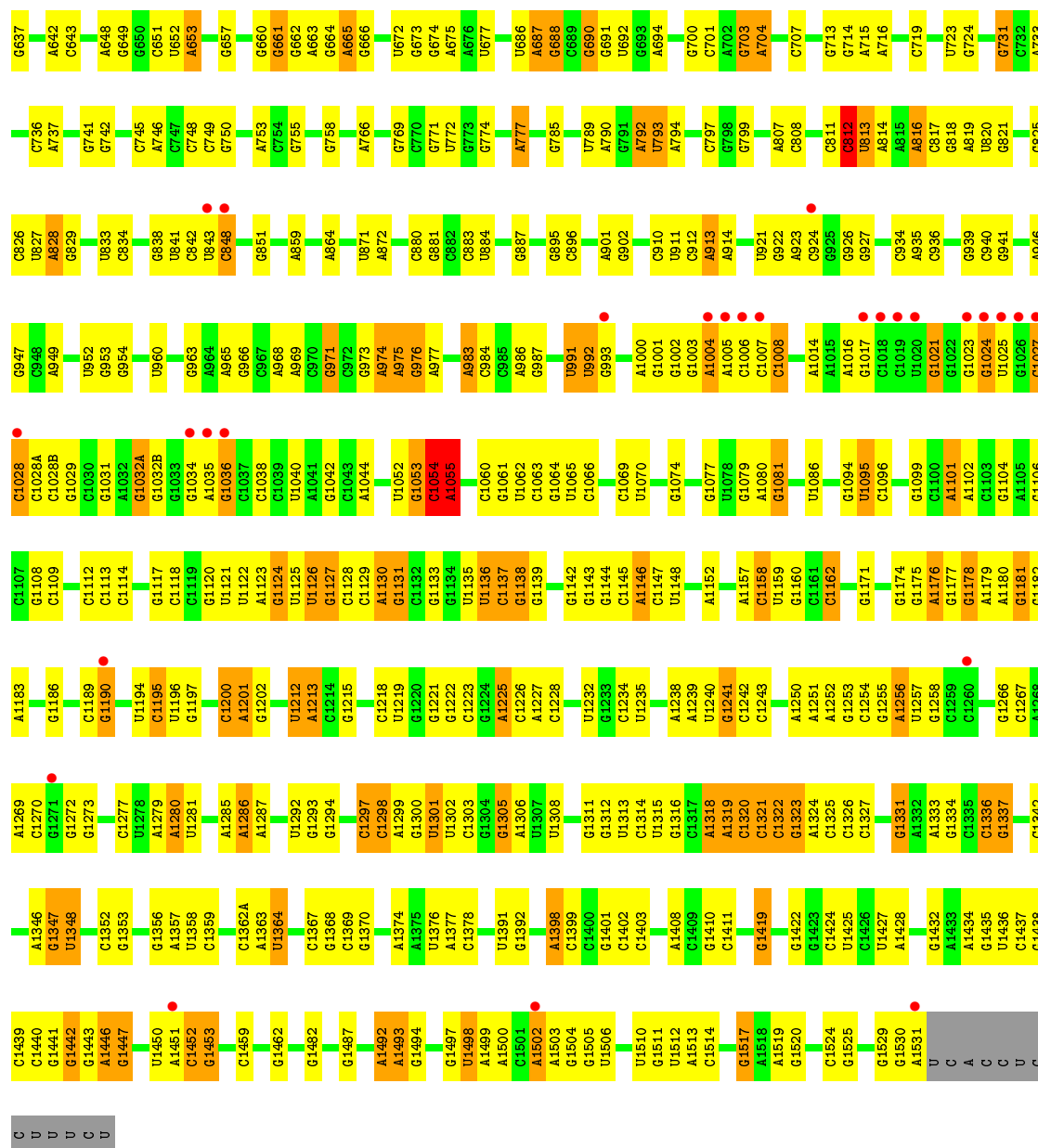
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	XD	1	Total	Zn	0	0
			1	1		
58	QD	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		

- Molecule 59 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: C₂₂H₃₀N₇O₈P).

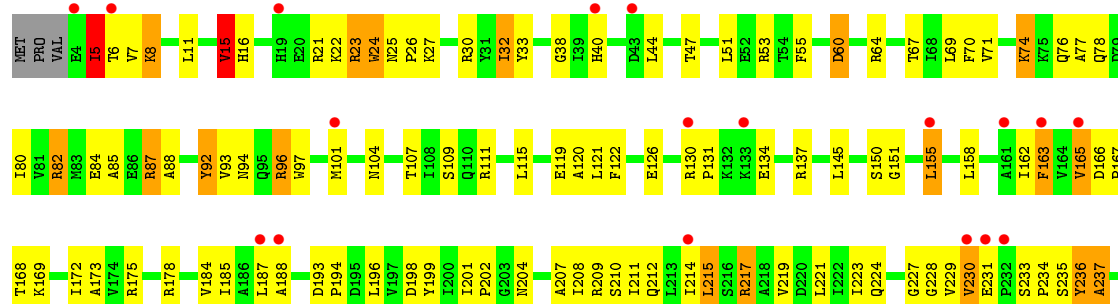


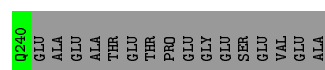
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	Z5	1	Total	C	N	O	P	0	0
			37	22	7	7	1		
59	Z6	1	Total	C	N	O	P	0	0
			37	22	7	7	1		



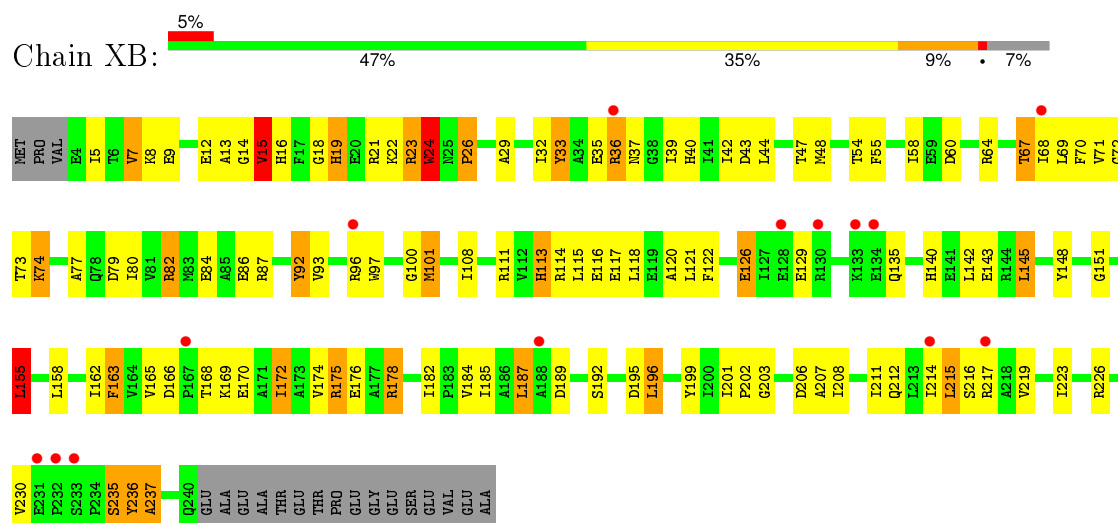


• Molecule 2: 30S ribosomal protein S2

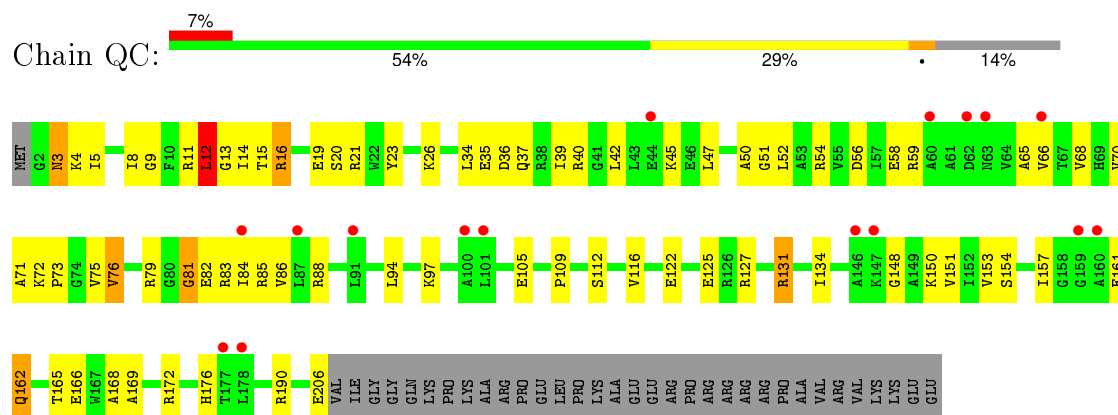




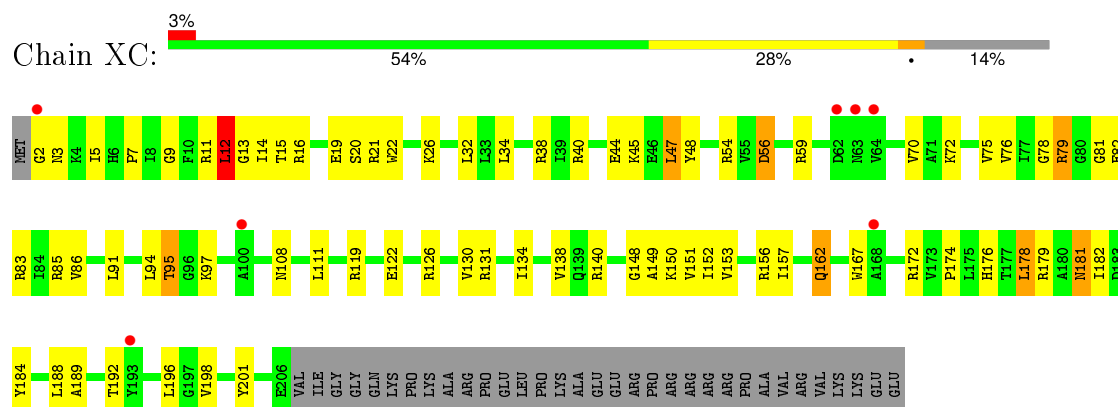
• Molecule 2: 30S ribosomal protein S2



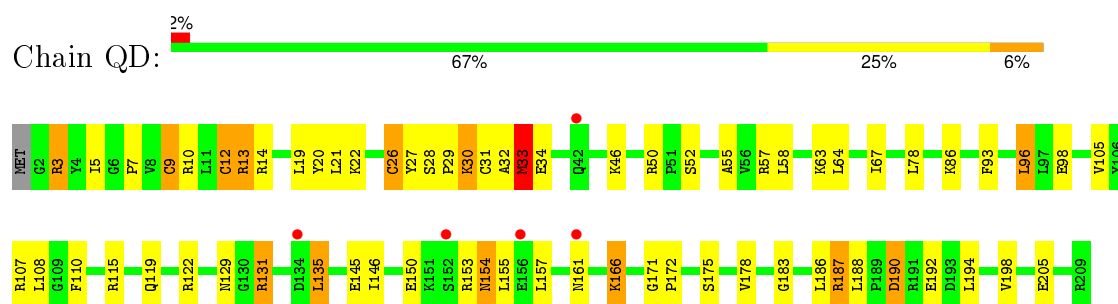
• Molecule 3: 30S ribosomal protein S3



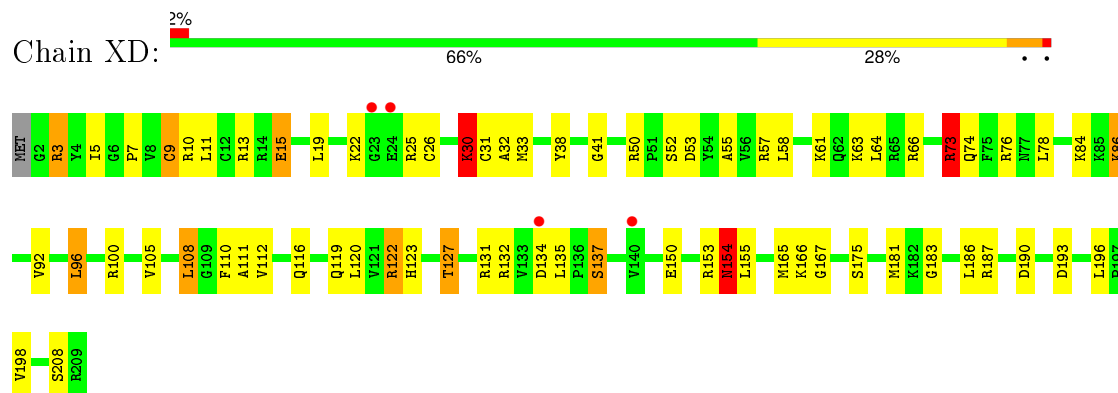
• Molecule 3: 30S ribosomal protein S3



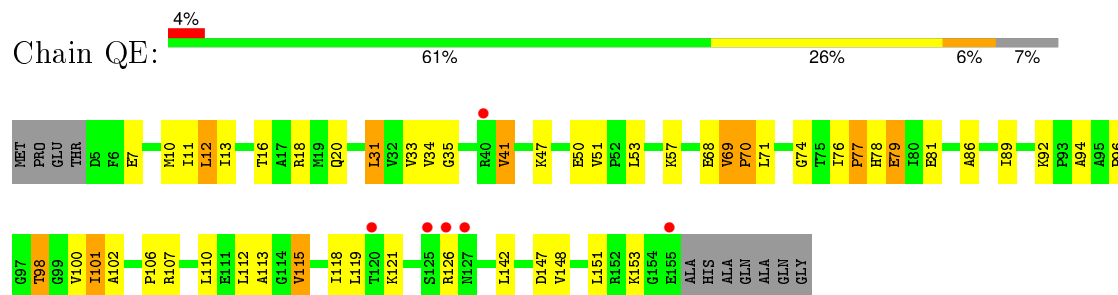
• Molecule 4: 30S ribosomal protein S4



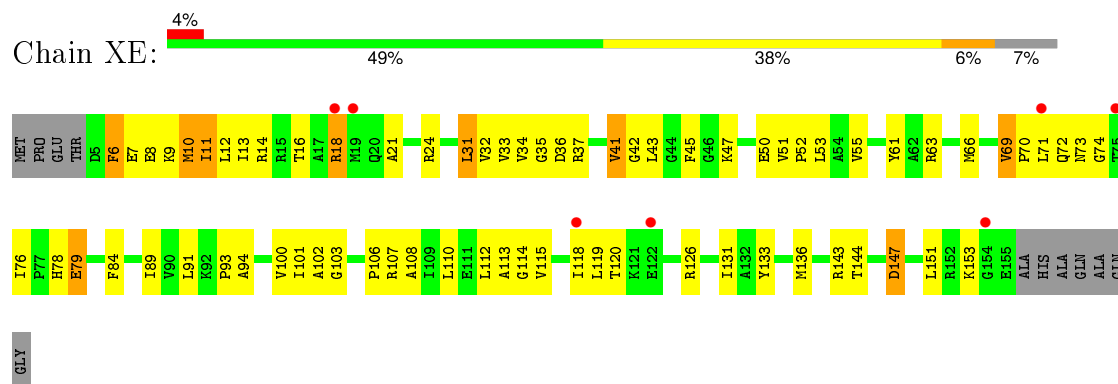
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

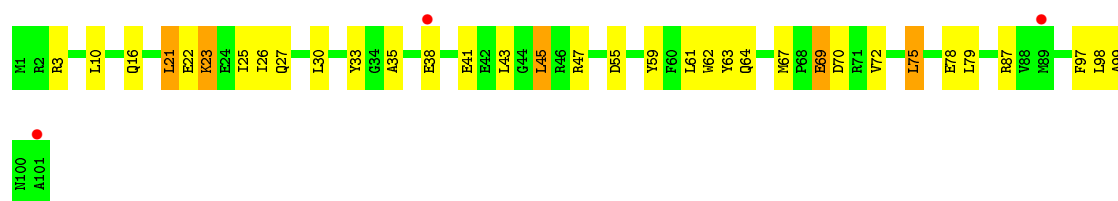


- Molecule 5: 30S ribosomal protein S5



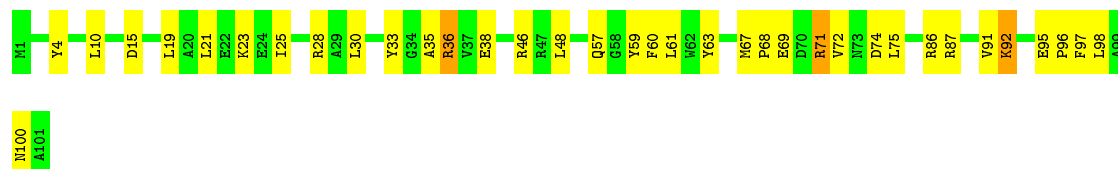
- Molecule 6: 30S ribosomal protein S6





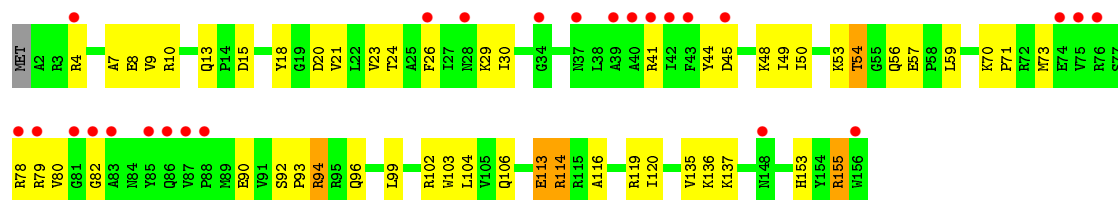
• Molecule 6: 30S ribosomal protein S6

Chain XF: 64% 33%



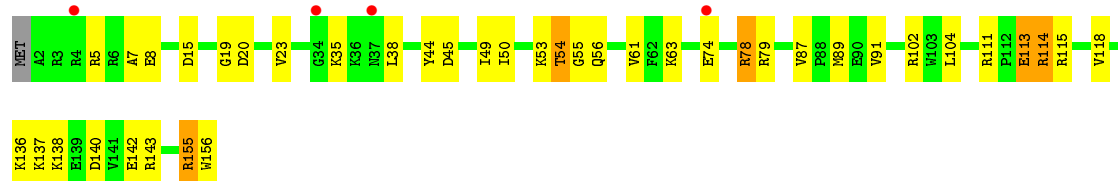
• Molecule 7: 30S ribosomal protein S7

Chain QG: 16% 65% 31%



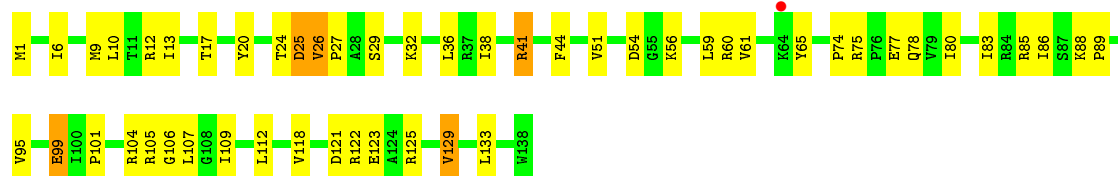
• Molecule 7: 30S ribosomal protein S7

Chain XG: 3% 74% 22%



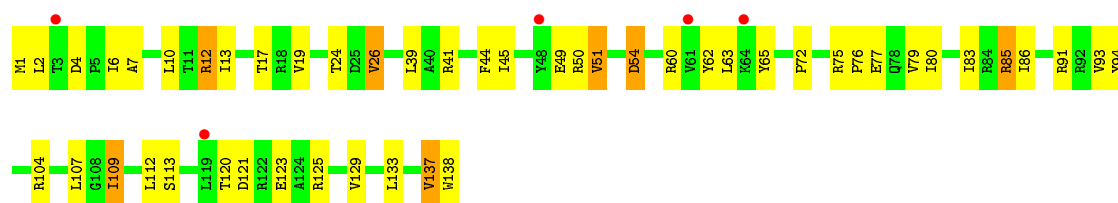
• Molecule 8: 30S ribosomal protein S8

Chain QH: 63% 33%

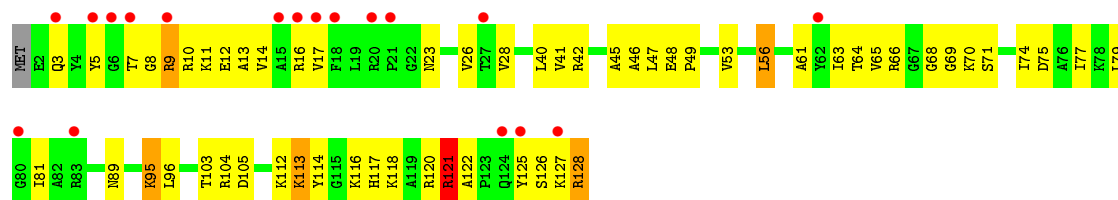


• Molecule 8: 30S ribosomal protein S8

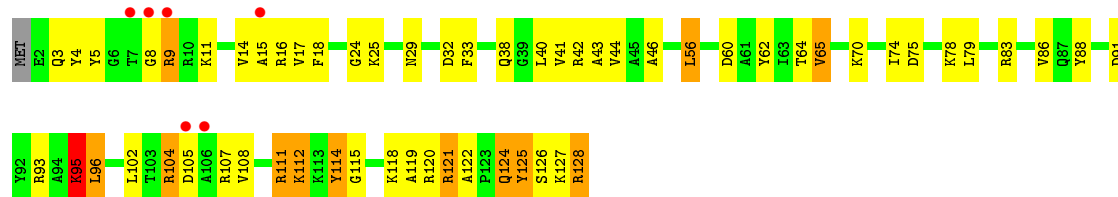
Chain XH: 4% 64% 30% 5%



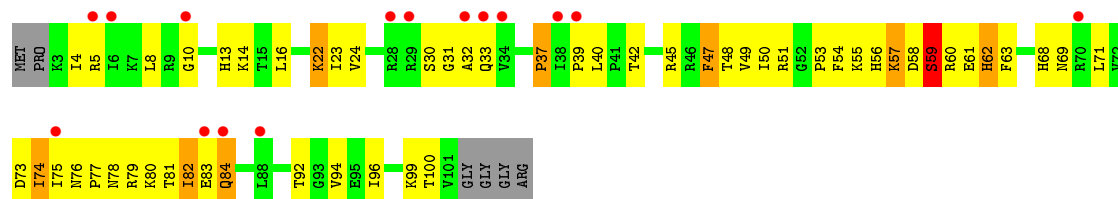
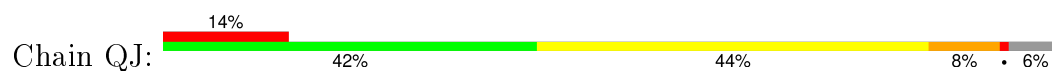
• Molecule 9: 30S ribosomal protein S9



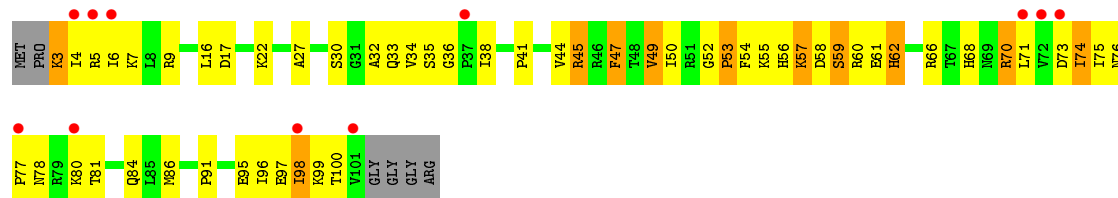
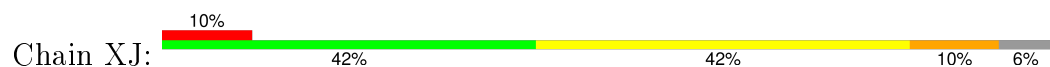
• Molecule 9: 30S ribosomal protein S9



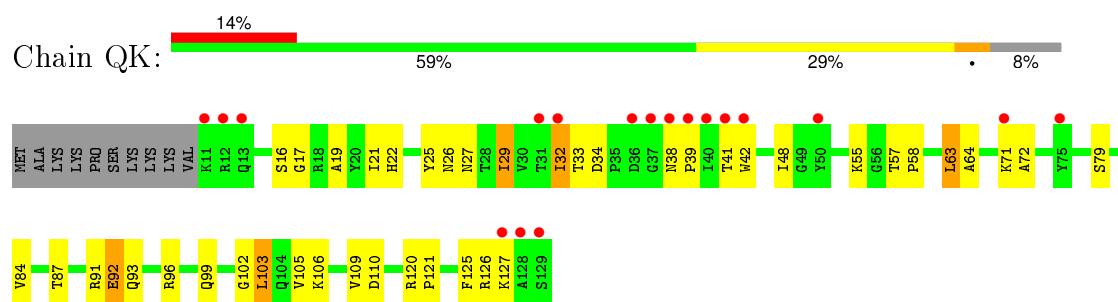
• Molecule 10: 30S ribosomal protein S10



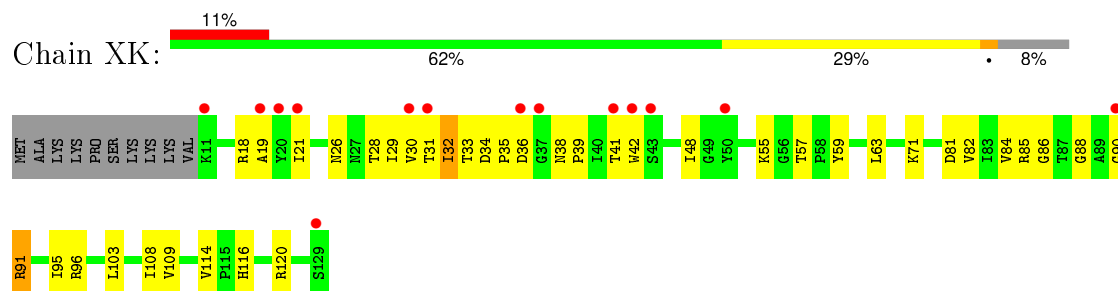
• Molecule 10: 30S ribosomal protein S10



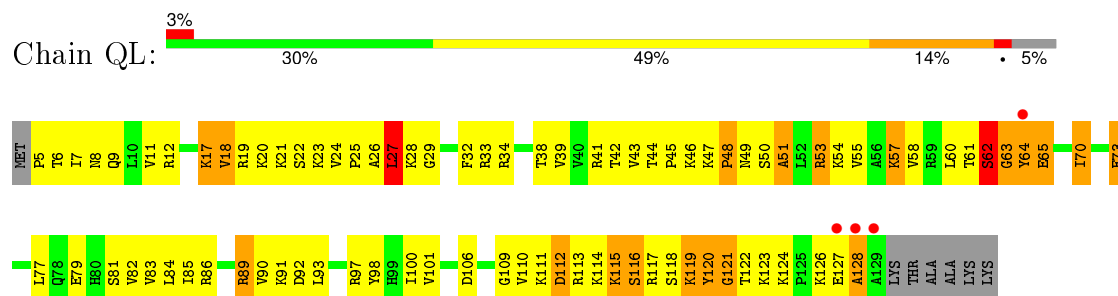
• Molecule 11: 30S ribosomal protein S11



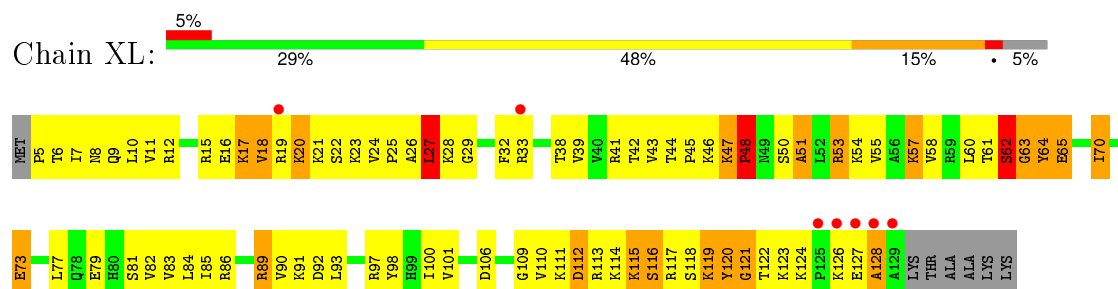
- Molecule 11: 30S ribosomal protein S11



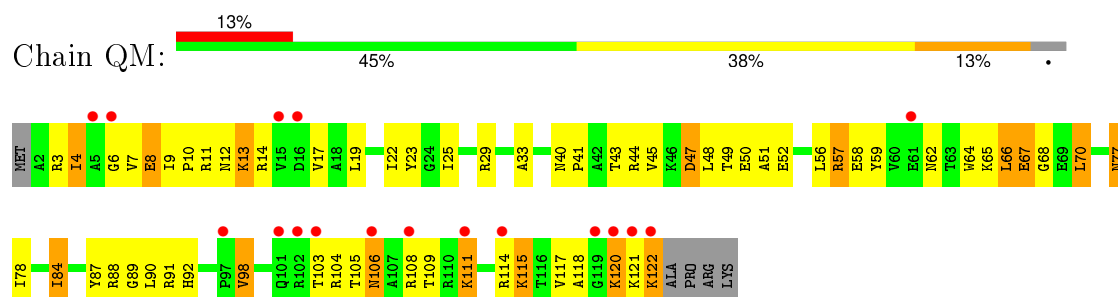
- Molecule 12: 30S ribosomal protein S12



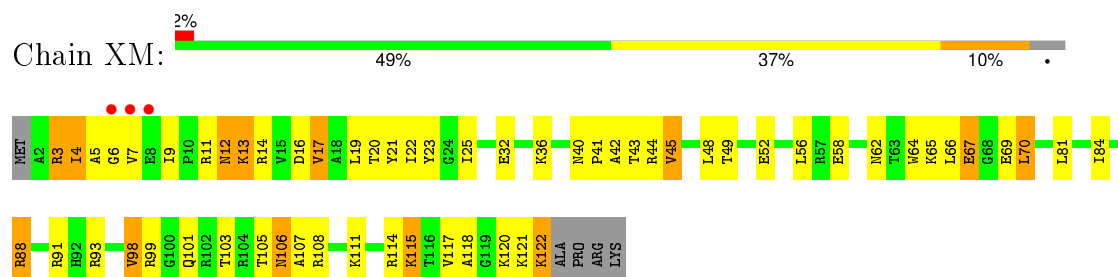
- Molecule 12: 30S ribosomal protein S12



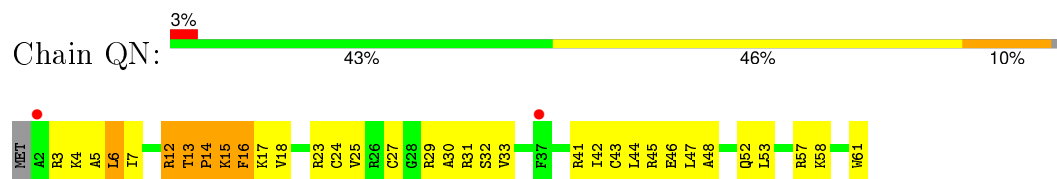
- Molecule 13: 30S ribosomal protein S13



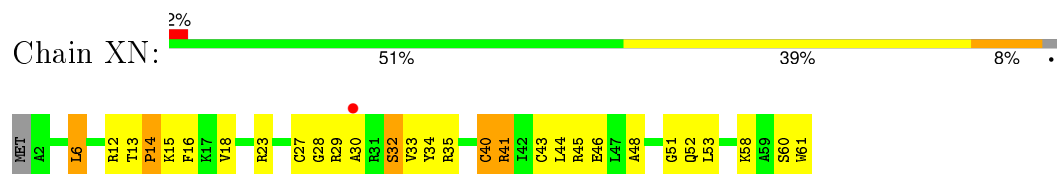
- Molecule 13: 30S ribosomal protein S13



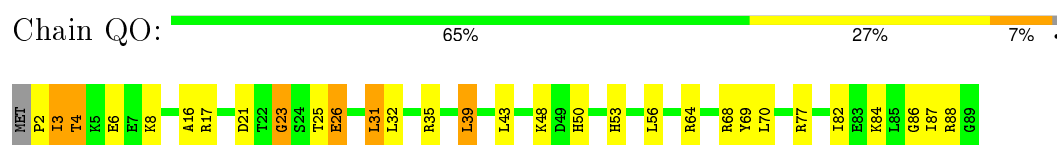
- Molecule 14: 30S ribosomal protein S14 type Z



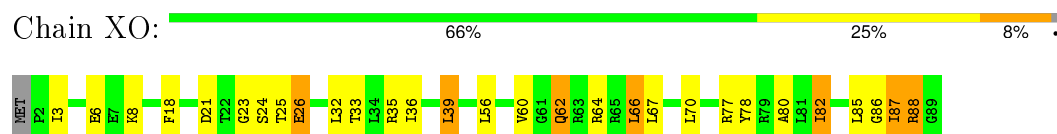
- Molecule 14: 30S ribosomal protein S14 type Z



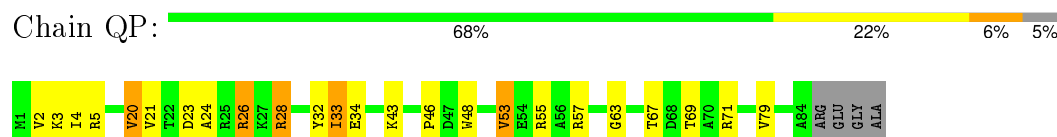
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16





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|------|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met1 | P2 | K3 | K4 | V5 | L6 | V10 | K14 | M15 | Q16 | R17 | T18 | V19 | H29 | P30 | K37 | R38 | H45 | D46 | P47 | K52 | I59 | I60 | E61 | S62 | S63 | R64 | P64 | I65 | S66 | K67 | R68 | K69 | R70 | F71 | R72 | L74 | R75 | L76 | S79 | G80 | R81 | M82 | D83 | K87 | I90 | N94 | Y95 |
|------|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



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|-----|----|----|----|----|----|--|-----|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|--|--|-----|--|--|--|-----|--|--|--|------|--|------|--|-----|--|-----|--|-----|
| Met | P2 | K3 | K4 | V5 | L6 | | V11 | S12 | | K17 | | Y32 | | R38 | | L43 | | K52 | | D55 | | E58 | | I59 | | | S62 | | R63 | | P64 | | I65 | | S66 | | K67 | | R68 | | K69 | | R70 | | F71 | | R72 | | V73 | | L74 | | S79 | | | | V85 | | | | R92 | | | | K100 | | R101 | | GLY | | LVS | | ALA |
|-----|----|----|----|----|----|--|-----|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|--|--|-----|--|--|--|-----|--|--|--|------|--|------|--|-----|--|-----|--|-----|

- | MET |
|---------|
| SER THR |
| LYS |
| ASV |
| ALA |
| LYS LYS |
| PRO |
| GLU |
| GLN |
| ARG ARG |
| PRO |
| SER SER |
| ARG |
| R19 |
| A20 |
| K21 |
| V22 |
| K23 |
| D24 |
| T25 |
| I26 |
| F29 |
| D30 |
| L31 |
| K32 |
| N36 |
| V37 |
| K42 |
| F43 |
| E46 |
| K49 |
| R53 |
| R54 |
| R55 |
| T56 |
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| L76 |
| G77 |
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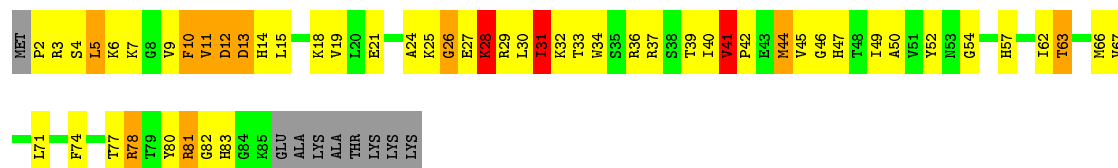
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| NET | SER | THR | LYS | ASN | ALA | LYS | PRO | LYS | GLU | ALA | GLN | ARG | ARG | PRO | SER | ARG | K19 | A20 | T25 | L26 | G27 | E28 | P29 | D30 | L31 | R32 | M36 | V37 | E38 | K41 | R42 | F43 | R44 | E46 | K49 | P52 | M53 | R54 | R55 | T56 | G57 | L58 | E62 | L66 | T69 | I70 | A73 | L76 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



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|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PET | P2 | R3 | S4 | L5 | V9 | F10 | V11 | D12 | D13 | H14 | L15 | L16 | E21 | G26 | E27 | R28 | R29 | L30 | I31 | K32 | T33 | R34 | S35 | S36 | R37 | R38 | T39 | I40 | V41 | P42 | E43 | M44 | V45 | G46 | H47 | A50 | V51 | V52 | H57 | I62 | T63 | E64 | M65 | M66 | V67 | L71 | G72 | E73 | F74 | T77 | R78 |
|-----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

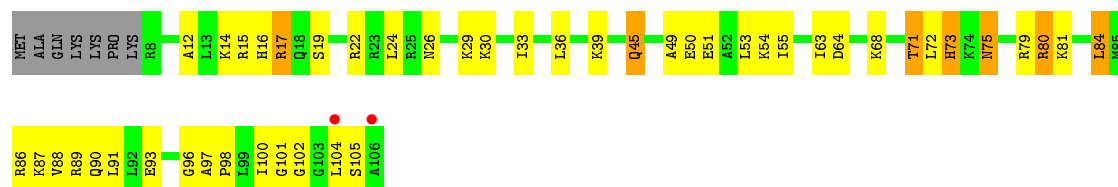
- Molecule 19: 30S ribosomal protein S19

Chain XS: 



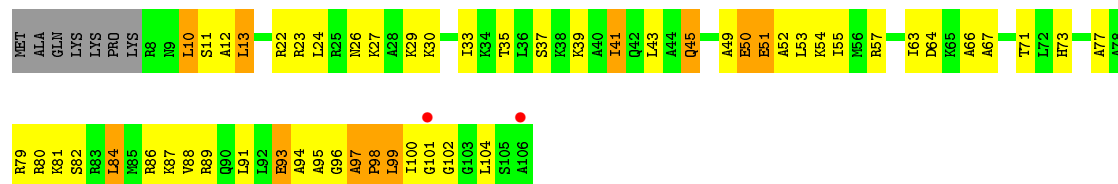
- Molecule 20: 30S ribosomal protein S20

Chain QT: 

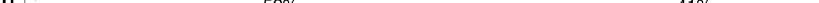


- Molecule 20: 30S ribosomal protein S20

Chain XT: 



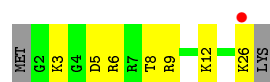
- Molecule 21: 30S ribosomal protein Thx

Chain QU: 



- Molecule 21: 30S ribosomal protein Thx

Chain XU: 



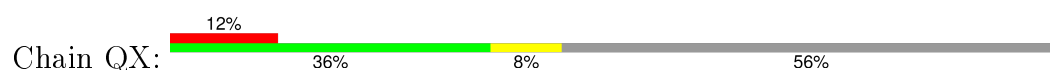
- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



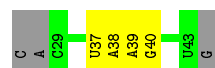
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



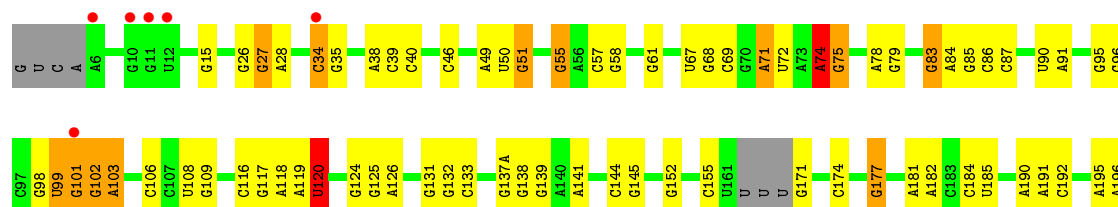
- Molecule 24: A-site ASL-SufJ

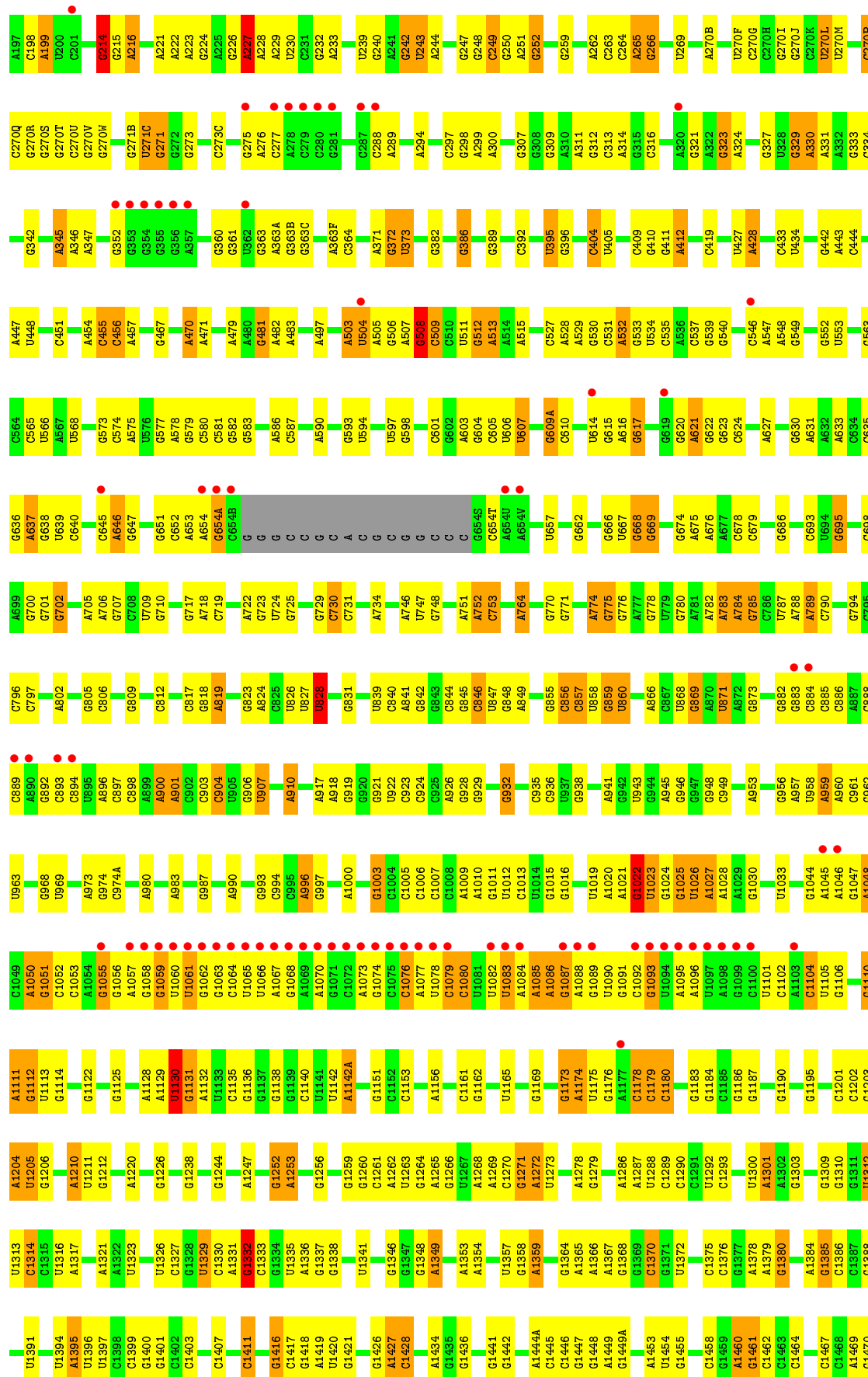


- Molecule 24: A-site ASL-SufJ

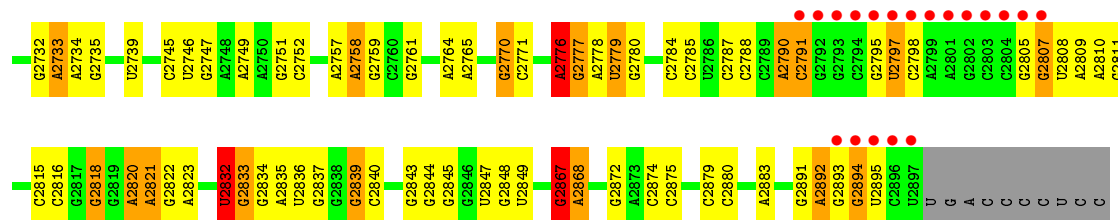


- Molecule 25: 23S rRNA

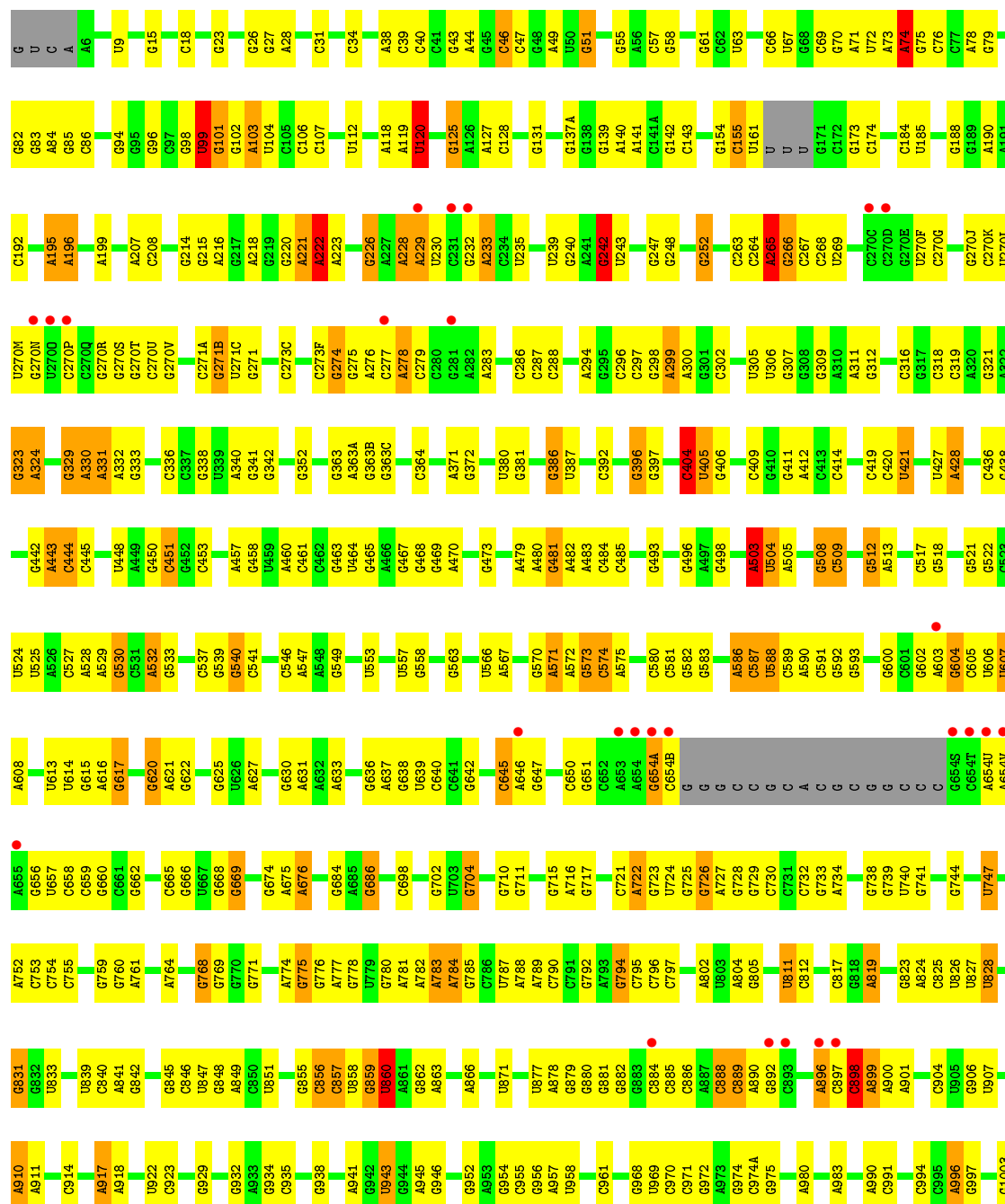




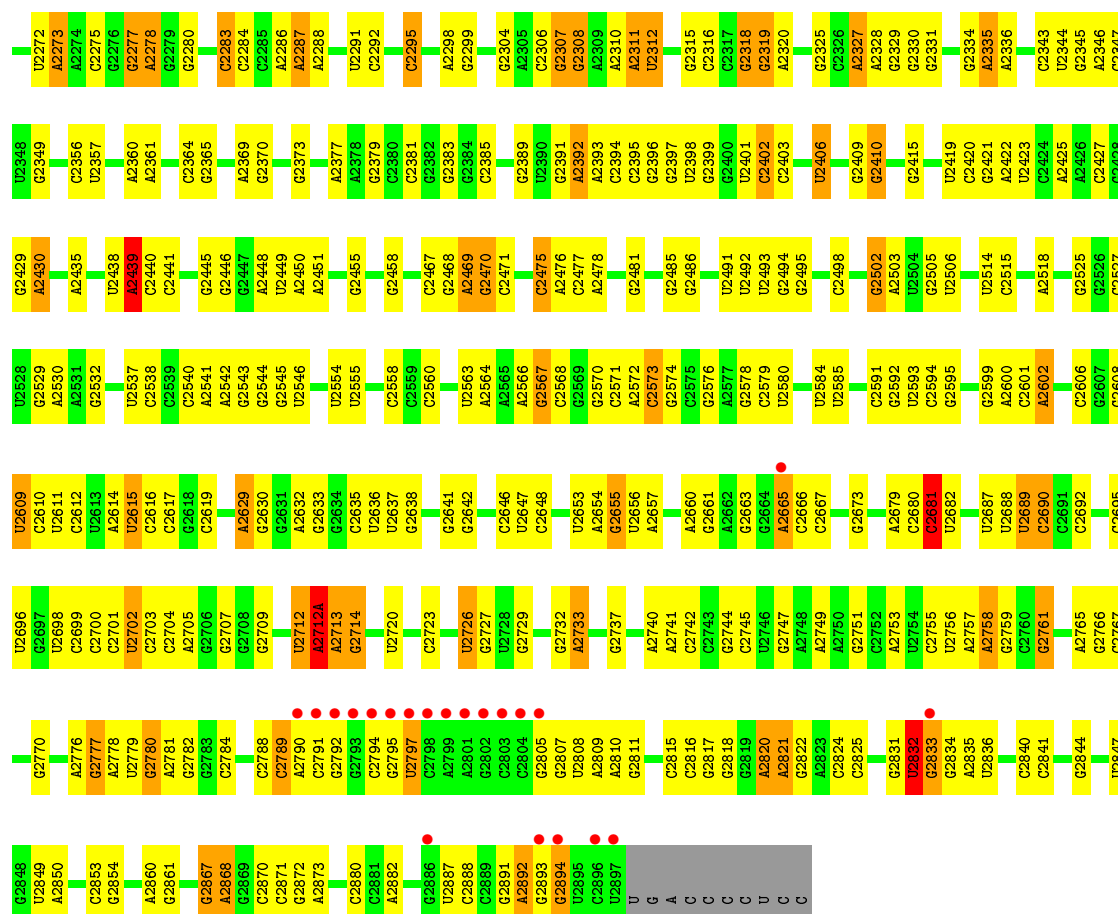
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U2650	G2567	C2469	U2386	A2199	U2122	A2033	A1927	C1837	A1759	G1649	A1566	A1477
G2655	C2568	A2470	U2387	G2209	G2123	G2037	A1928	C1838	A1760	G1651	A1567	G1478
G2656	G2569	G2471	A2388	G2210	G2124	G2038	A1929	G1839	G1761	A1652	A1568	G1479
G2657	G2570	G2472	U2389	G2211	G2125	G2039	U1930	C1844	A1762	A1653	A1569	G1480
G2658	G2571	A2473	U2390	G2212	G2126	C2040	U1931	G1845	G1763	A1654	A1570	U1482
A2662	A2572	C2474	G2391	G2213	G2127	U2041	C1934	G1846	G1764	A1655	A1571	G1483
G2663	G2573	G2475	A2392	G2214	G2128	A2042	C1935	G1847				
A2664	A2574	G2476	A2393	G2215	U2129	U2043	A1936	A1848				
G2665	G2575	U2477	C2394	G2216	G2130	G2044	C1937	A1849				
G2666	G2576	G2478	U2395	G2217	G2131	G2045	A1938	A1850				
G2667	A2577	G2479	G2396	G2218	U2132	G2046	U1939	G1851				
	G2578	U2480	A2397	G2219	G2133	G2047	A1940	A1852				
		U2481	A2398	G2220	G2134	G2048	C1941	A1853				
G2673	G2579	U2482	G2399	G2221	A2135	G2049	A1942	A1854				
G2674	U2580	C2402	C2402	G2222	C2136	A2050	C1943	A1855				
A2675	G2581	C2403	C2403	G2223	G2137	G2051	A1944	G1856				
G2676	G2582	G2404	C2404	G2224	G2138	G2052	G1945	G1857				
G2677	G2583	G2405	G2405	G2225	G2139	G2053	G1946	G1858				
G2678	G2584	U2406	U2406	G2226		G2054	A1947	G1859				
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			G2346	G2255	G2168	G2083	U1984	G1798				
			G2347	G2256	G2169	G2084	U1985	A1608				
			G2348	G2257	G2170	G2085	U1986	A1609				
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			G2353	G2262	G2175	G2090	U1991	A1614				
			G2354	G2263	G2176	G2091	U1992	A1615				
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			G2373	G2282	G2195	G2110	U2011	A1634				
			G2374	G2283	G2196	G2111	U2012	A1635				
			G2375	G2284	G2197	G2112	U2013	A1636				
			G2376	G2285	G2198	G2113	U2014	A1637				
			G2377	G2286	G2199	G2114	U2015	A1638				
			G2378	G2287	G2200	G2115	U2016	A1639				
			G2379	G2288	G2201	G2116	U2017	A1640				
			G2380	G2289	G2202	G2117	U2018	A1641				
			G2381	G2290	G2203	G2118	U2019	A1642				
			G2382	G2291	G2204	G2119	U2020	A1643				
			G2383	G2292	G2205	G2120	U2021	A1644				
			G2384	G2293	G2206	G2121	U2022	A1645				
			G2385	G2294	G2207	G2122	U2023	A1646				
			G2386	G2295	G2208	G2123	G2023	A1647				
			G2387	G2296	G2209	G2124		A1648				
			G2388	G2297	G2210	G2125		A1649				
			G2389	G2298	G2211	G2126		A1650				
			G2390	G2299	G2212	G2127		A1651				
			G2391	G2300	G2213	G2128		A1652				
			G2392	G2301	G2214	G2129		A1653				
			G2393	G2302	G2215	G2130		A1654				
			G2394	G2303	G2216	G2131		A1655				
			G2395	G2304	G2217	G2132		A1656				
			G2396	G2305	G2218	G2133		A1657				
			G2397	G2306	G2219	G2134		A1658				
			G2398	G2307	G2220	G2135		A1659				
			G2399	G2308	G2221	G2136		A1660				
			G2400	G2309	G2222	G2137		A1661				
			G2401	G2310	G2223	G2138		A1662				
			G2402	G2311	G2224	G2139		A1663				
			G2403	G2312	G2225	G2140		A1664				
			G2404	G2313	G2226	G2141		A1665				
			G2405	G2314	G2227	G2142		A1666				
			G2406	G2315	G2228	G2143		A1667				
			G2407	G2316	G2229	G2144		A1668				
			G2408	G2317	G2230	G2145		A1669				
			G2409	G2318	G2231	G2146		A1670				
			G2410	G2319	G2232	G2147		A1671				
			G2411	G2320	G2233	G2148		A1672				
			G2412	G2321	G2234	G2149		A1673				
			G2413	G2322	G2235	G2150		A1674				
			G2414	G2323	G2236	G2151		A1675				
			G2415	G2324	G2237	G2152		A1676				
			G2416	G2325	G2238	G2153		A1677				
			G2417	G2326	G2239	G2154		A1678				
			G2418	G2327	G2240	G2155		A1679				
			G2419	G2328	G2241	G2156		A1680				
			G2420	G2329	G2242	G2157		A1681				
			G2421	G2330	G2243	G2158		A1682				
			G2422	G2331	G2244	G2159		A1683				
			G2423	G2332	G2245	G2160		A1684				
			G2424	G2333	G2246	G2161		A1685				
			G2425	G2334	G2247	G2162		A1686				
			G2426	G2335	G2248	G2163		A1687				
			G2427	G2336	G2249	G2164		A1688				
			G2428	G2337	G2250	G2165		A1689				
			G2429	G2338	G2251	G2166		A1690				
			G2430	G2339	G2252	G2167		A1691				
			G2431	G2340	G2253	G2168		A1692				
			G2432	G2341	G2254	G2169		A1693				
			G2433	G2342	G2255	G2170		A1694				
			G2434	G2343	G2256	G2171		A1695				
			G2435									



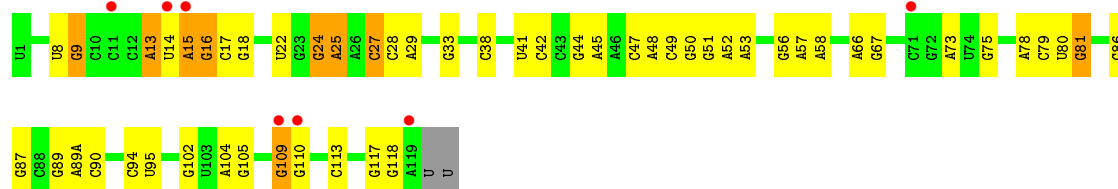
• Molecule 25: 23S rRNA



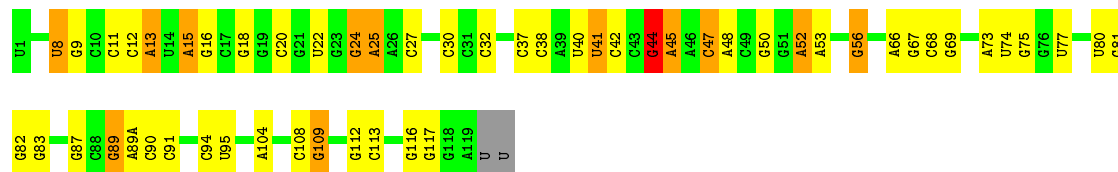




- Molecule 26: 5S rRNA

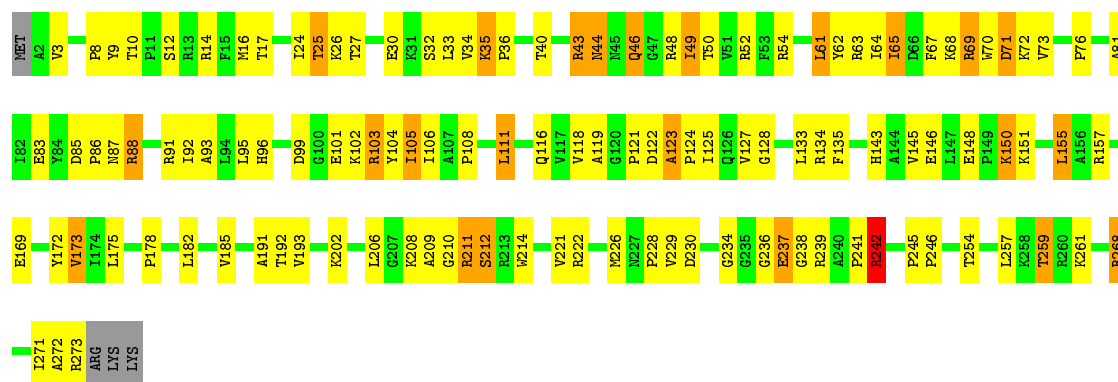


- Molecule 26: 5S rRNA



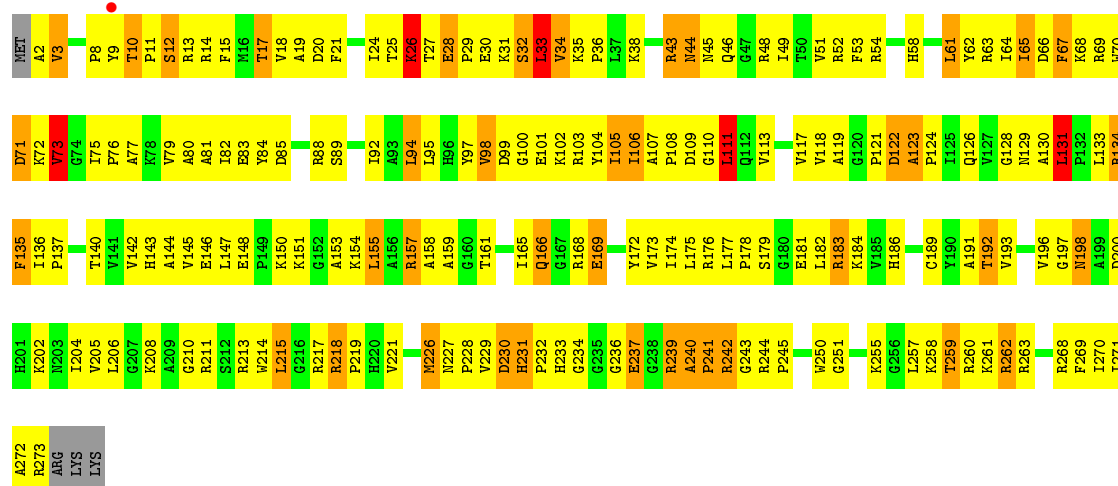
- Molecule 27: 50S ribosomal protein L2





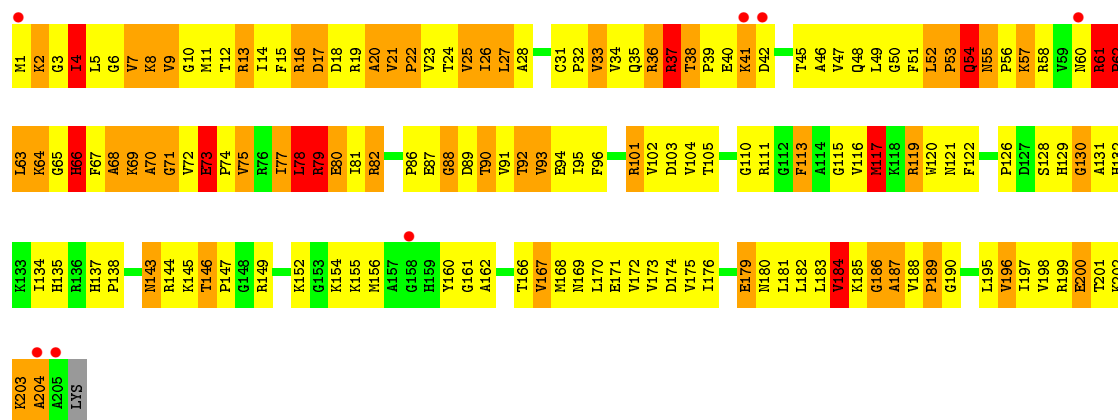
• Molecule 27: 50S ribosomal protein L2

Chain YD: 29% 53% 14% ..



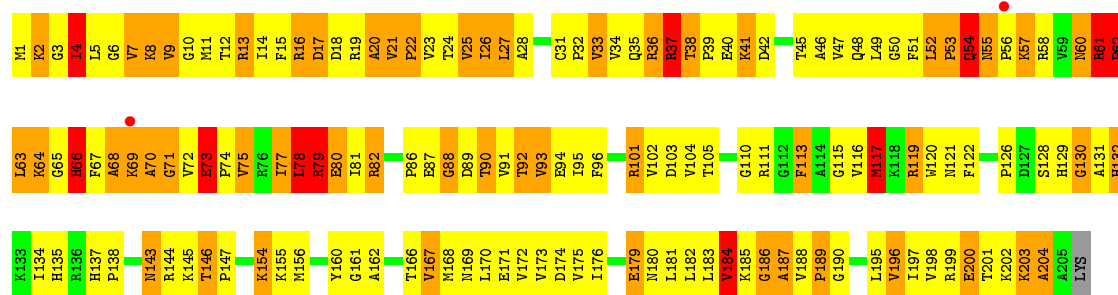
• Molecule 28: 50S ribosomal protein L3

Chain RE: 3% 23% 47% 24% 5%

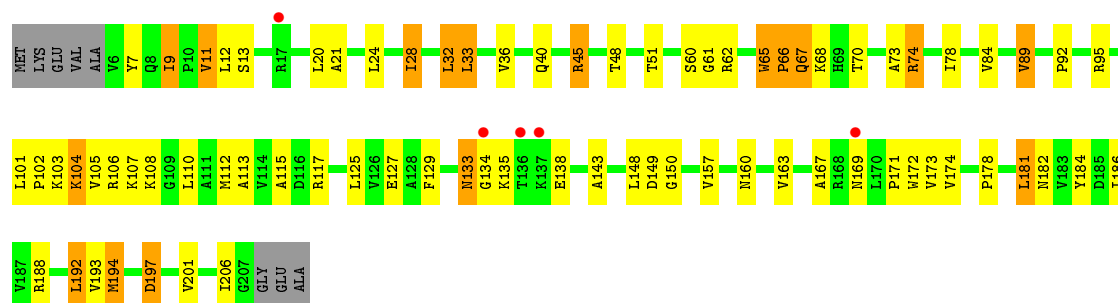


• Molecule 28: 50S ribosomal protein L3

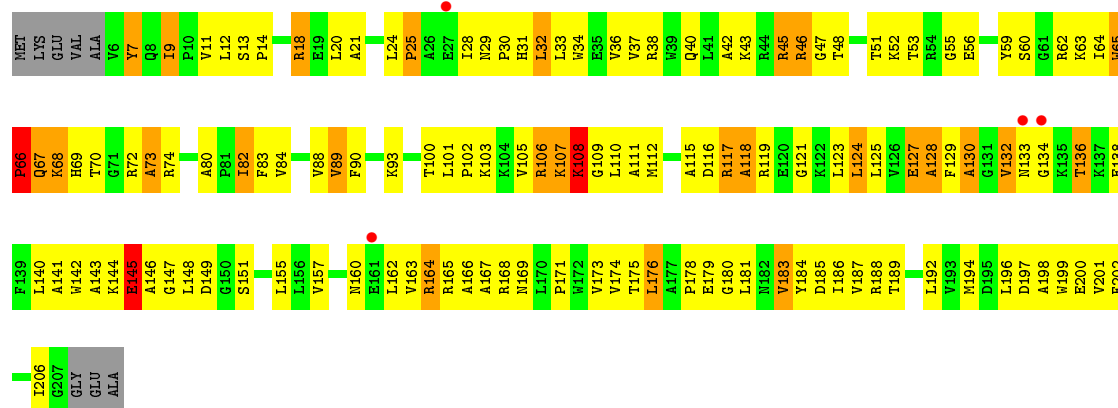
Chain YE: 24% 45% 26% 5%



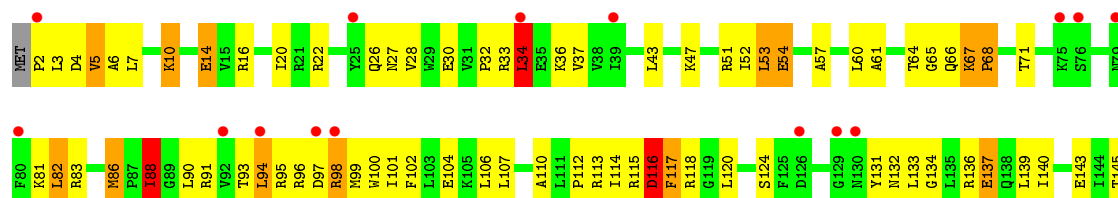
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4

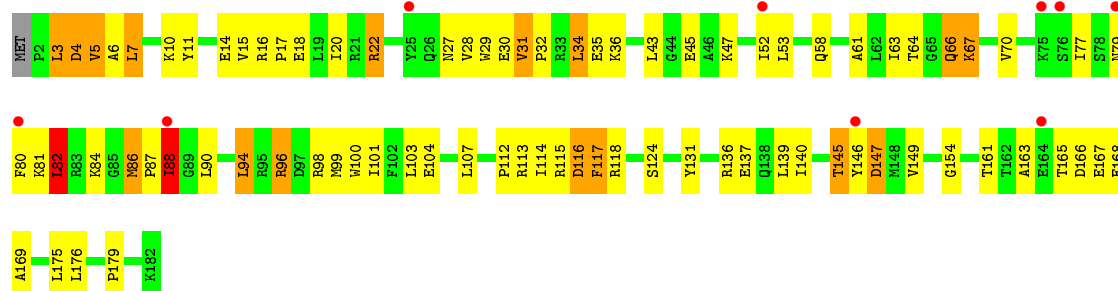


• Molecule 30: 50S ribosomal protein L5

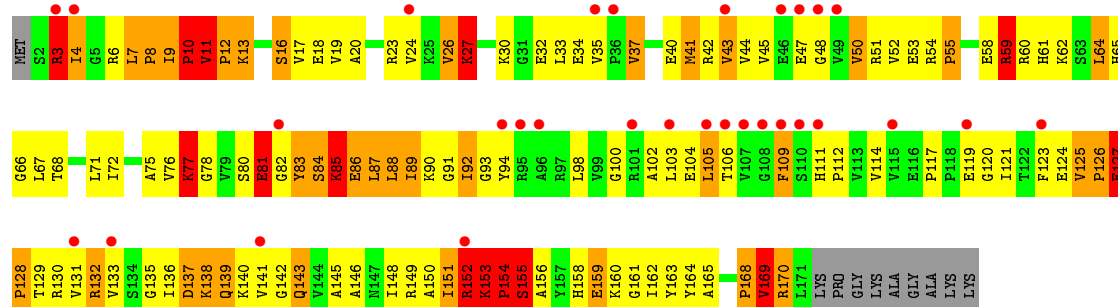




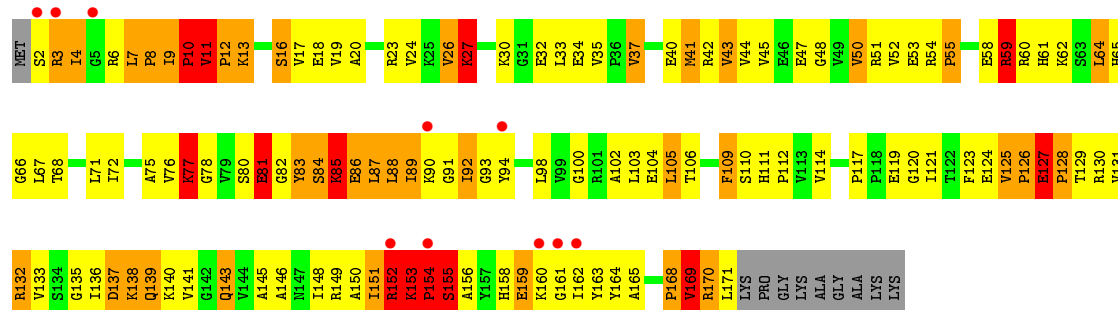
- Molecule 30: 50S ribosomal protein L5



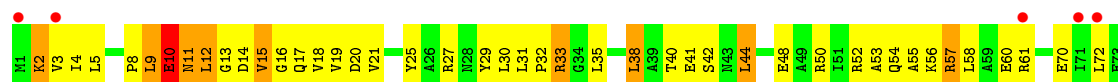
- Molecule 31: 50S ribosomal protein L6

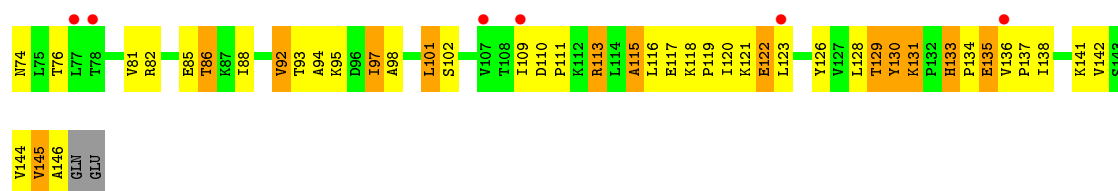


- Molecule 31: 50S ribosomal protein L6

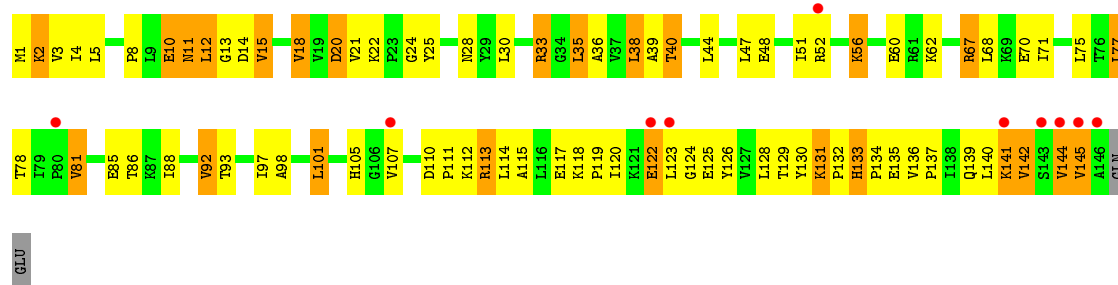


- Molecule 32: 50S ribosomal protein L9

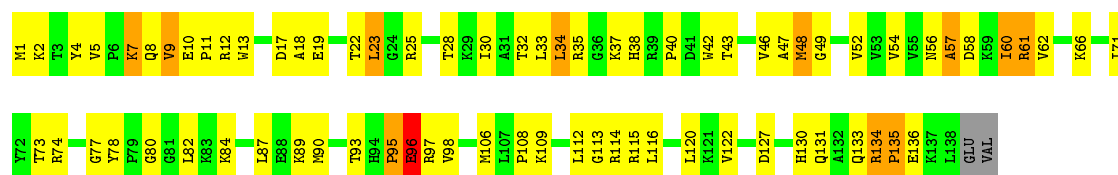




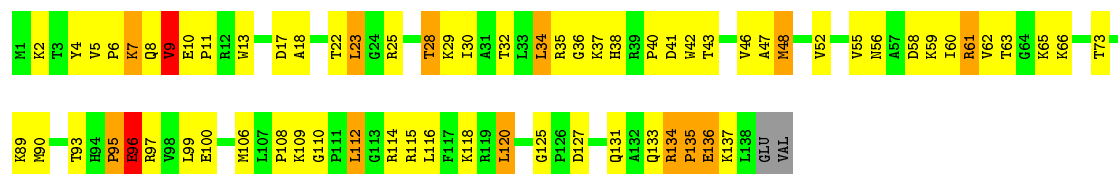
- Molecule 32: 50S ribosomal protein L9



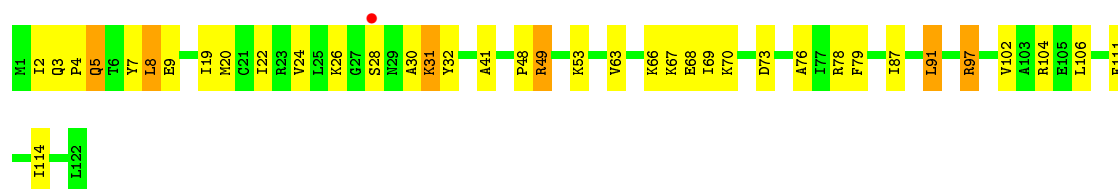
- Molecule 33: 50S ribosomal protein L13



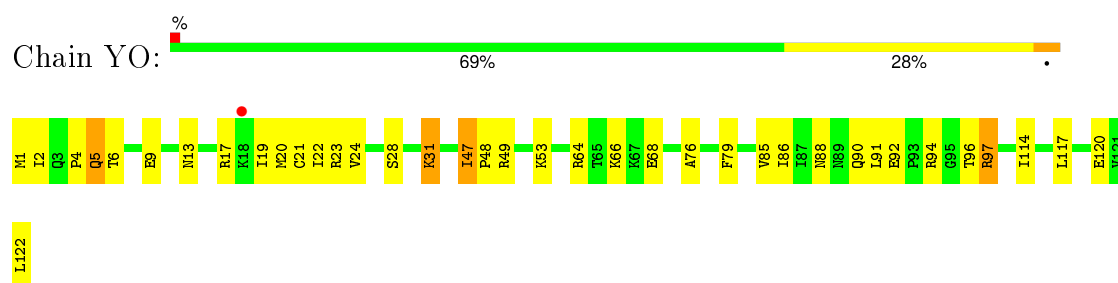
- Molecule 33: 50S ribosomal protein L13



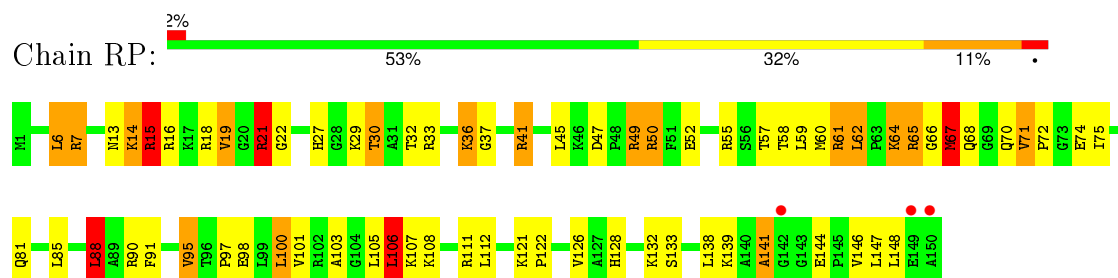
- Molecule 34: 50S ribosomal protein L14



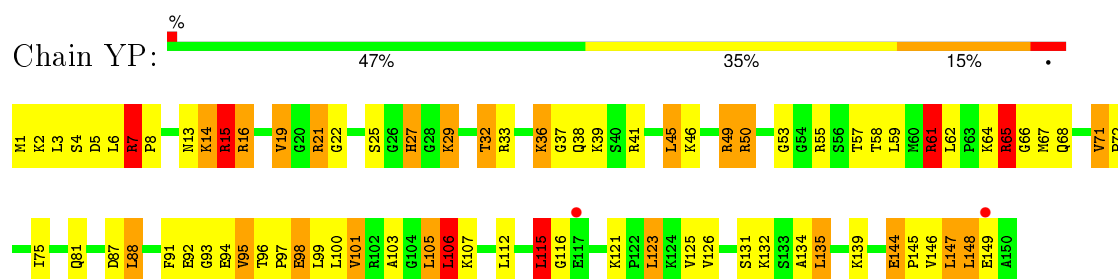
- Molecule 34: 50S ribosomal protein L14



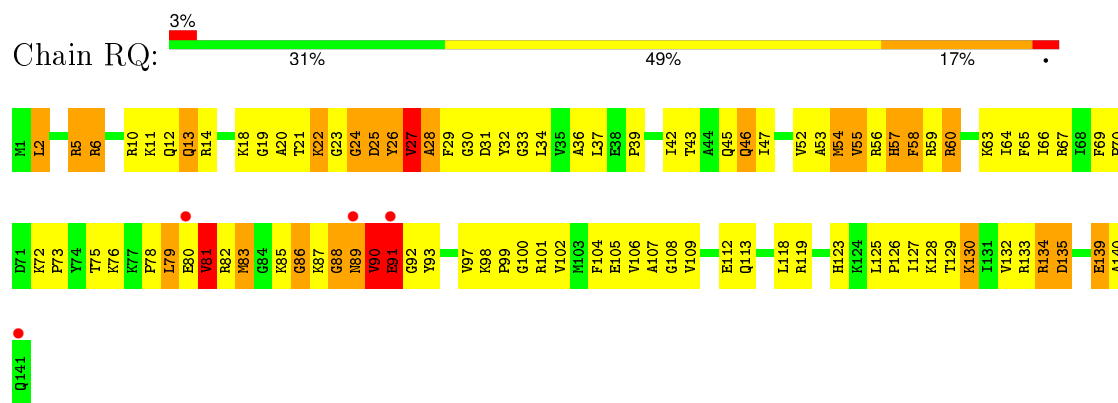
• Molecule 35: 50S ribosomal protein L15



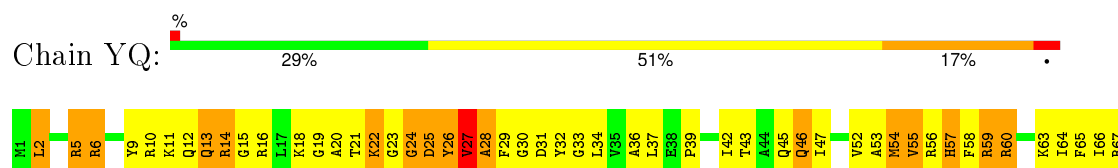
• Molecule 35: 50S ribosomal protein L15

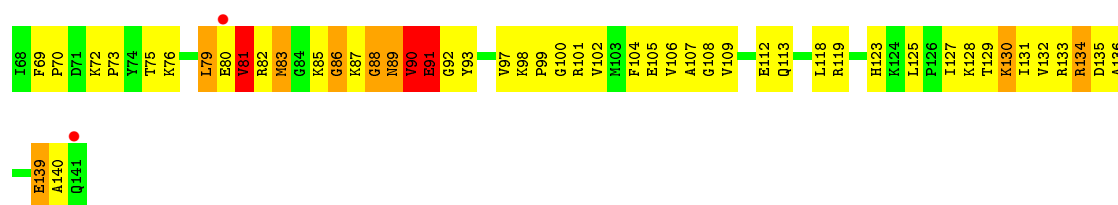


• Molecule 36: 50S ribosomal protein L16



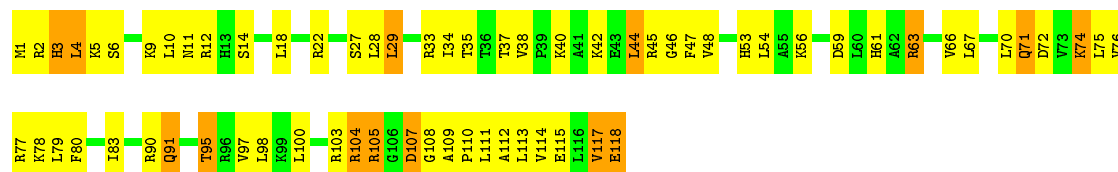
• Molecule 36: 50S ribosomal protein L16





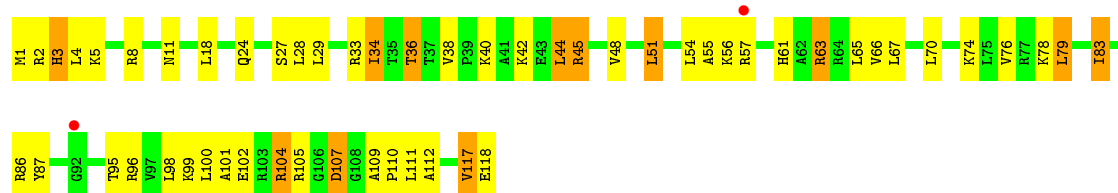
• Molecule 37: 50S ribosomal protein L17

Chain RR: 43% 45% 12%



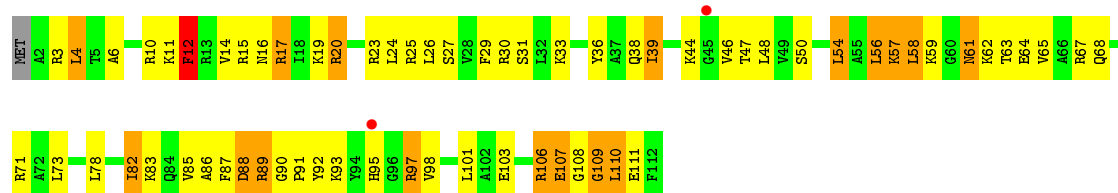
• Molecule 37: 50S ribosomal protein L17

Chain YR: 2% 53% 36% 10%



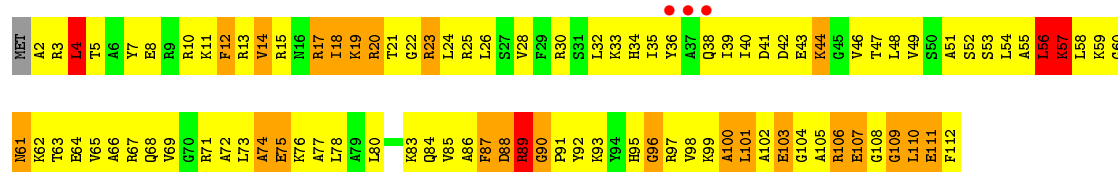
• Molecule 38: 50S ribosomal protein L18

Chain RS: 2% 40% 43% 15% ..



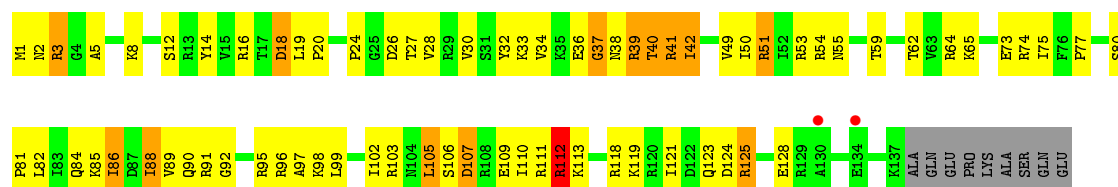
• Molecule 38: 50S ribosomal protein L18

Chain YS: 3% 13% 63% 21% ..

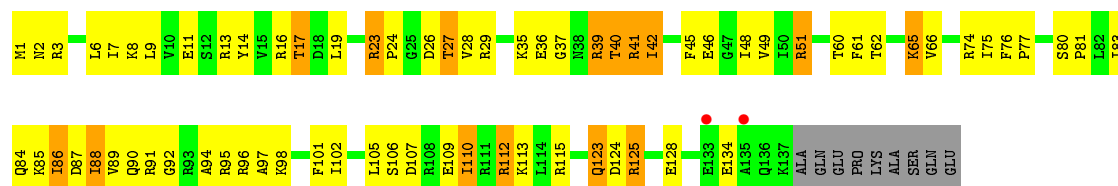


• Molecule 39: 50S ribosomal protein L19

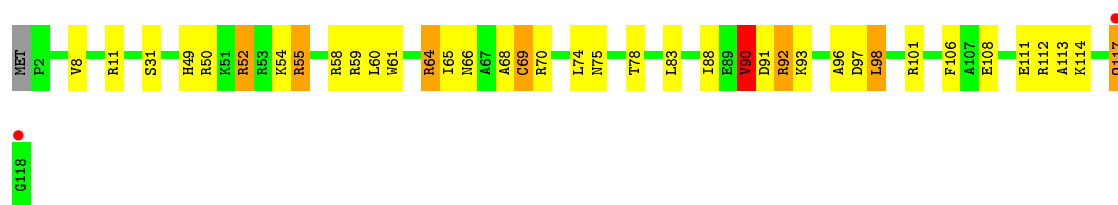
Chain RT: % 44% 40% 9% 6%



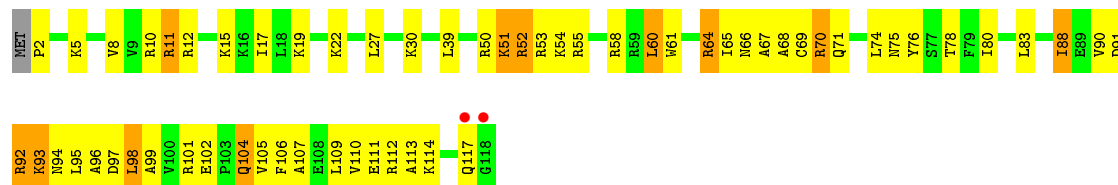
• Molecule 39: 50S ribosomal protein L19



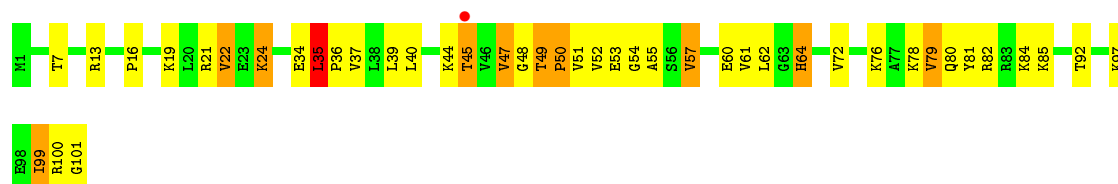
• Molecule 40: 50S ribosomal protein L20



• Molecule 40: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L21

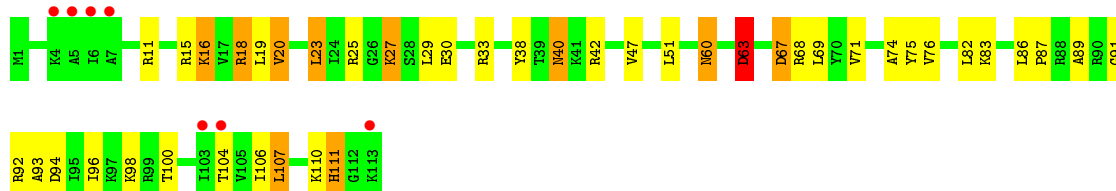


• Molecule 41: 50S ribosomal protein L21

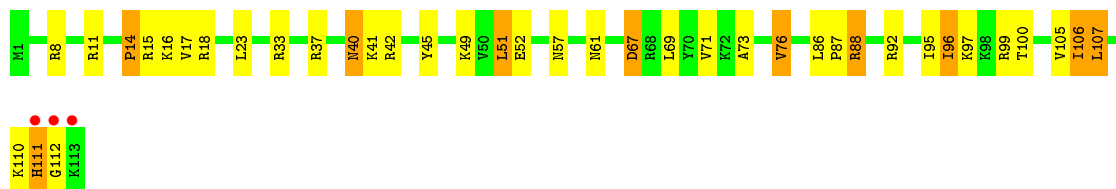




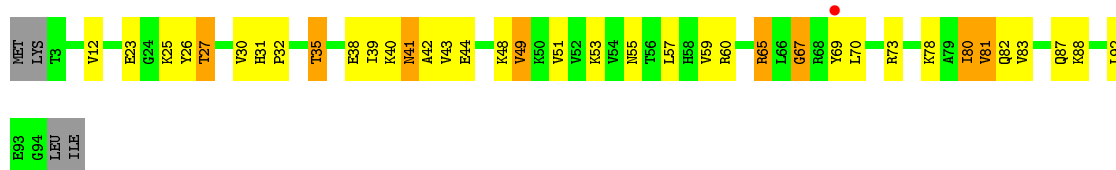
- Molecule 42: 50S ribosomal protein L22



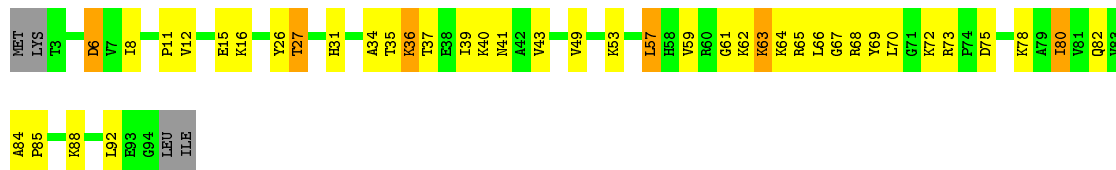
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23

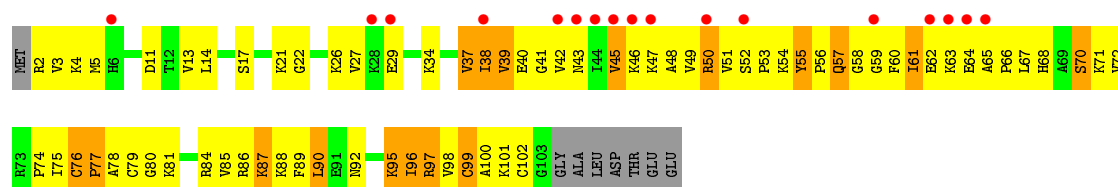


- Molecule 43: 50S ribosomal protein L23

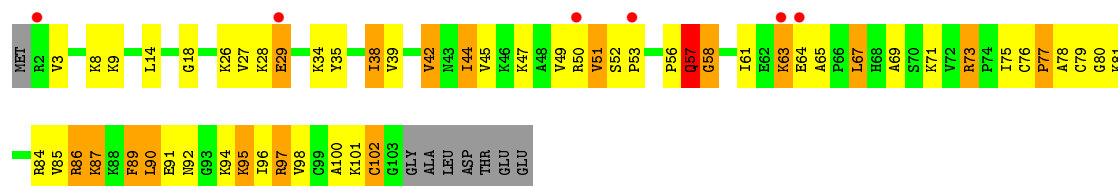
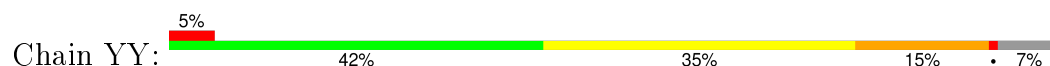


- Molecule 44: 50S ribosomal protein L24

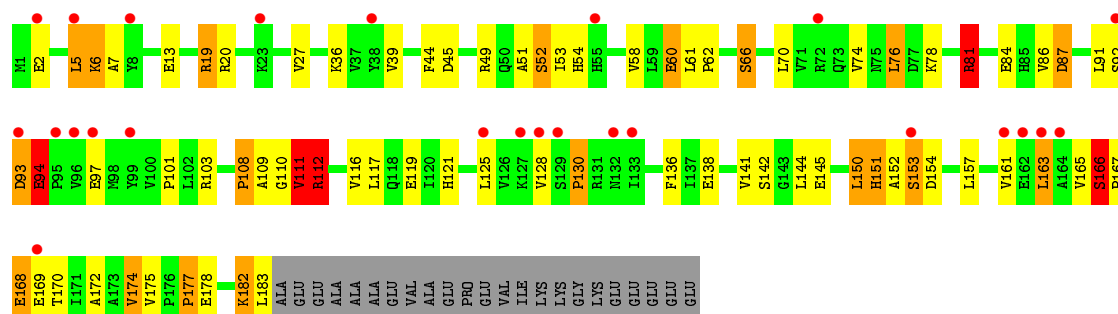




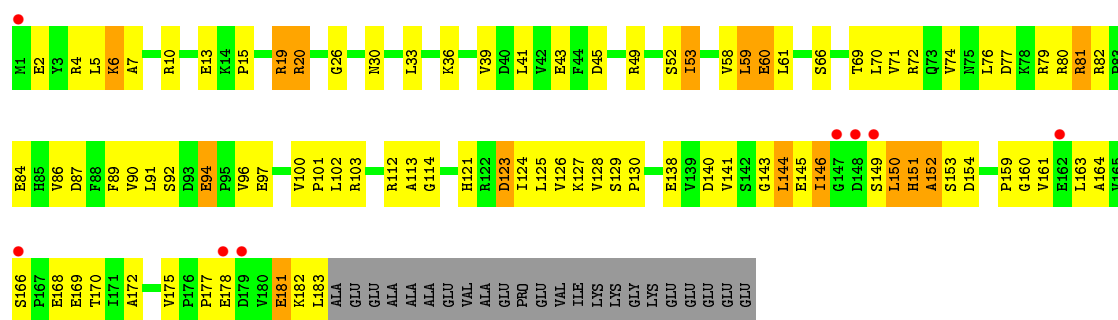
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25



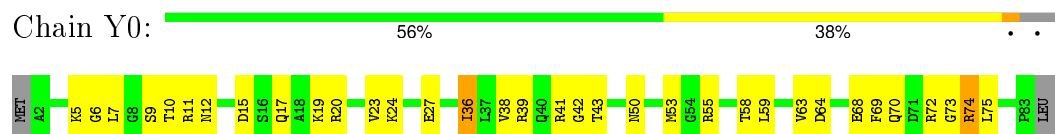
• Molecule 45: 50S ribosomal protein L25



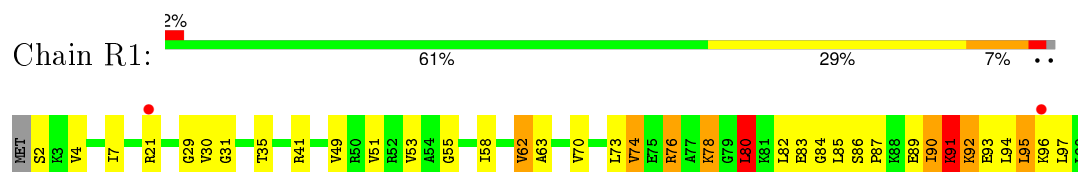
• Molecule 46: 50S ribosomal protein L27



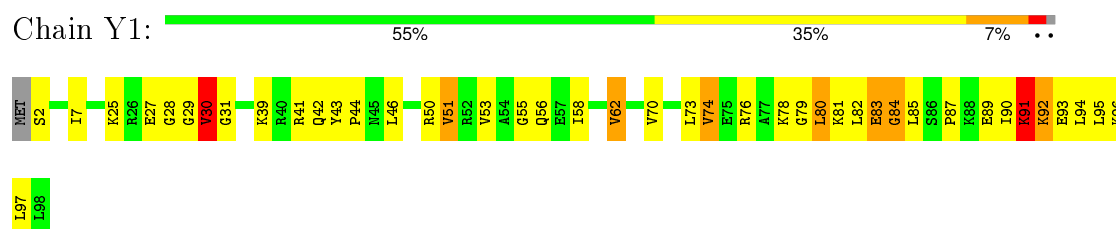
- Molecule 46: 50S ribosomal protein L27



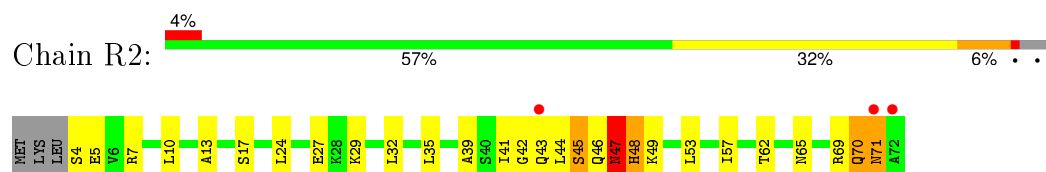
- Molecule 47: 50S ribosomal protein L28



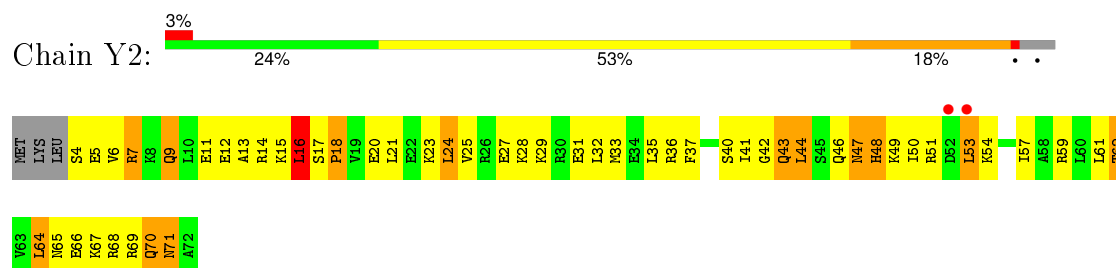
- Molecule 47: 50S ribosomal protein L28



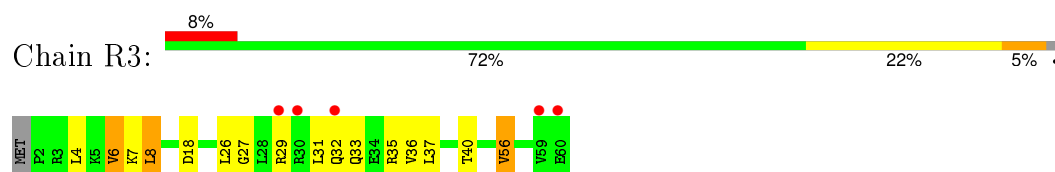
- Molecule 48: 50S ribosomal protein L29



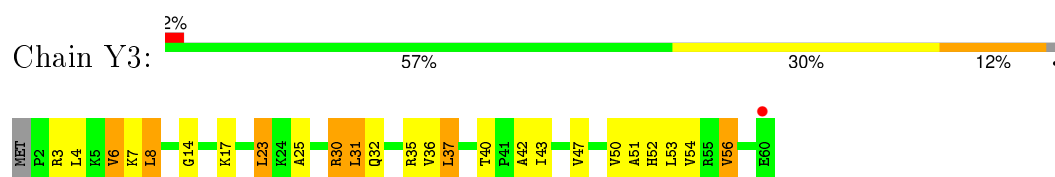
- Molecule 48: 50S ribosomal protein L29



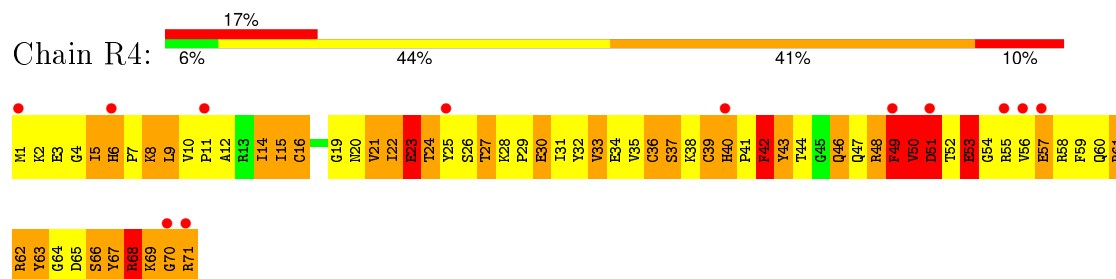
- Molecule 49: 50S ribosomal protein L30



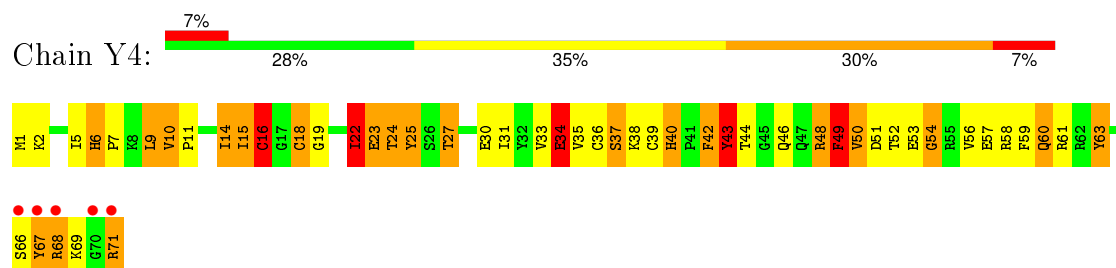
- Molecule 49: 50S ribosomal protein L30



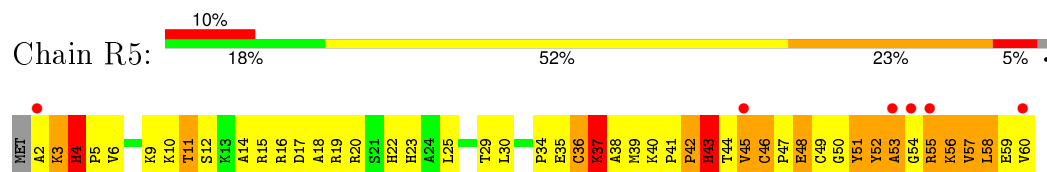
- Molecule 50: 50S ribosomal protein L31



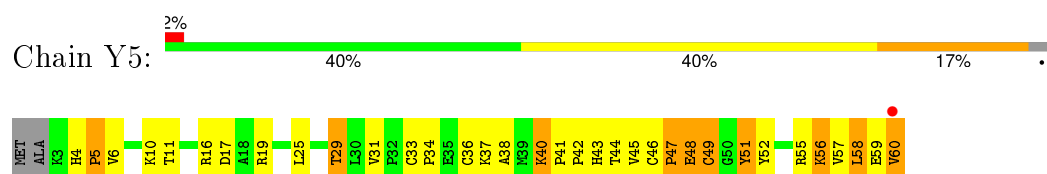
- Molecule 50: 50S ribosomal protein L31



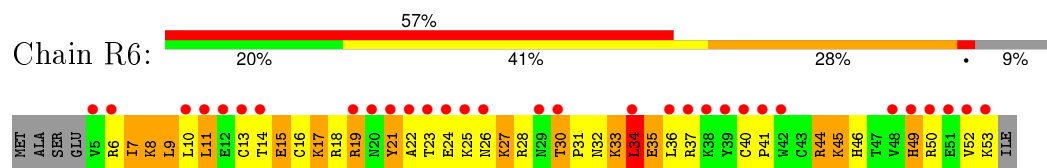
- Molecule 51: 50S ribosomal protein L32



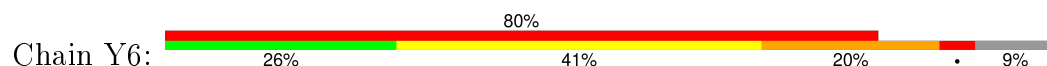
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

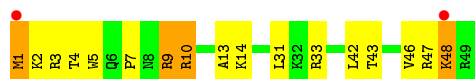


- Molecule 52: 50S ribosomal protein L33





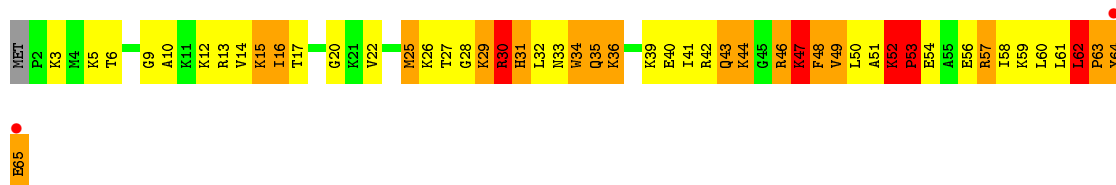
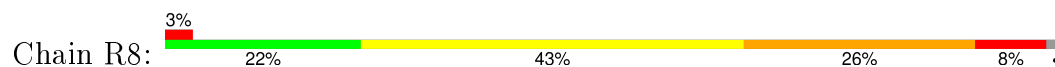
- Molecule 53: 50S ribosomal protein L34



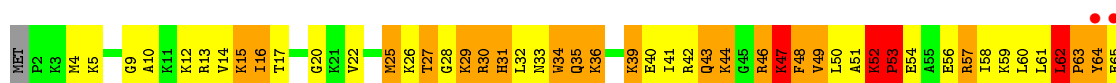
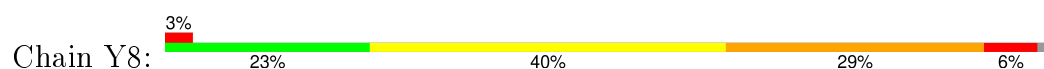
- Molecule 53: 50S ribosomal protein L34



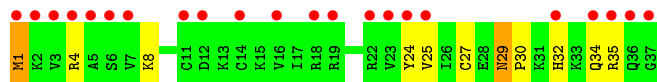
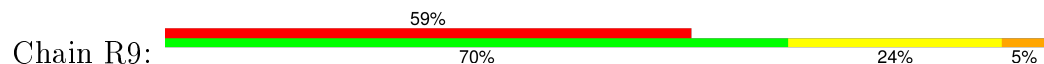
- Molecule 54: 50S ribosomal protein L35



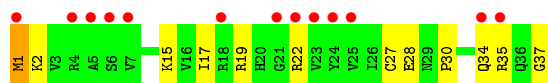
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro

Chain Z5:  33% 33% 33%



● Molecule 56: CC-Puro

Chain Z6:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.35Å 450.71Å 622.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.60 49.51 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.51-3.60) 96.6 (49.51-3.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.214 , 0.253 0.219 , 0.255	Depositor DCC
R_{free} test set	30328 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	5 of 772080 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	292042	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.28	0/36098	0.79	27/56341 (0.0%)
1	XA	0.31	0/36101	0.82	20/56346 (0.0%)
2	QB	0.32	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.32	0/1629	0.54	0/2195
3	XC	0.36	0/1629	0.56	0/2195
4	QD	0.27	0/1733	0.45	0/2318
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.40	1/1171 (0.1%)	0.60	1/1576 (0.1%)
5	XE	0.41	0/1171	0.70	3/1576 (0.2%)
6	QF	0.38	0/856	0.55	0/1154
6	XF	0.39	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.51	0/1709
8	QH	0.34	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.36	0/814	0.62	2/1095 (0.2%)
10	XJ	0.39	1/814 (0.1%)	0.63	1/1095 (0.1%)
11	QK	0.38	0/900	0.59	1/1213 (0.1%)
11	XK	0.39	0/900	0.59	0/1213
12	QL	0.49	1/991 (0.1%)	0.80	1/1327 (0.1%)
12	XL	0.49	0/991	0.83	3/1327 (0.2%)
13	QM	0.32	0/974	0.58	0/1303
13	XM	0.37	0/974	0.62	0/1303
14	QN	0.37	0/501	0.62	0/664
14	XN	0.43	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.39	0/745	0.55	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.36	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.35	0/765	0.62	0/1007
20	XT	0.32	0/765	0.59	0/1007
21	QU	0.30	0/221	0.54	0/288
21	XU	0.31	0/221	0.62	0/288
22	QV	0.36	1/1836 (0.1%)	0.76	0/2859
22	XV	0.41	1/1836 (0.1%)	0.80	0/2859
23	QX	0.44	0/246	0.80	0/381
23	XX	0.67	0/238	1.19	3/369 (0.8%)
24	QY	0.47	0/355	0.87	0/551
24	XY	0.45	0/355	1.03	0/551
25	RA	0.36	0/69518	0.87	51/108523 (0.0%)
25	YA	0.42	1/69520 (0.0%)	0.92	68/108527 (0.1%)
26	RB	0.30	0/2878	0.82	0/4490
26	YB	0.36	0/2878	0.88	3/4490 (0.1%)
27	RD	0.51	0/2165	0.70	0/2919
27	YD	0.56	0/2165	0.90	4/2919 (0.1%)
28	RE	0.52	0/1601	0.91	2/2160 (0.1%)
28	YE	0.52	0/1601	0.91	2/2160 (0.1%)
29	RF	0.30	0/1620	0.48	0/2194
29	YF	0.50	0/1620	0.76	0/2194
30	RG	0.32	0/1499	0.57	1/2016 (0.0%)
30	YG	0.40	0/1499	0.60	0/2016
31	RH	0.45	0/1332	0.85	3/1802 (0.2%)
31	YH	0.44	0/1332	0.85	3/1802 (0.2%)
32	RI	0.27	0/1151	0.56	0/1558
32	YI	0.28	0/1151	0.54	0/1558
33	RN	0.41	0/1131	0.62	0/1525
33	YN	0.43	0/1131	0.63	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	0.29	0/1162	0.60	1/1544 (0.1%)
35	YP	0.32	0/1158	0.64	0/1535
36	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
36	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
37	RR	0.43	0/982	0.69	0/1312
37	YR	0.45	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	0.46	0/892	0.83	1/1187 (0.1%)
39	RT	0.42	0/1155	0.63	0/1542
39	YT	0.43	0/1155	0.66	0/1542
40	RU	0.40	0/982	0.65	0/1306
40	YU	0.51	0/982	0.70	0/1306
41	RV	0.38	0/790	0.61	1/1057 (0.1%)
41	YV	0.46	0/790	0.73	1/1057 (0.1%)
42	RW	0.49	0/911	0.67	0/1220
42	YW	0.45	0/911	0.68	0/1220
43	RX	0.47	0/739	0.62	0/993
43	YX	0.48	0/739	0.65	0/993
44	RY	0.44	0/798	0.69	0/1064
44	YY	0.46	0/798	0.70	0/1064
45	RZ	0.26	0/1493	0.52	0/2026
45	YZ	0.28	0/1493	0.55	0/2026
46	R0	0.46	0/657	0.68	0/874
46	Y0	0.48	0/657	0.69	0/874
47	R1	0.44	0/770	0.65	0/1022
47	Y1	0.46	0/770	0.69	0/1022
48	R2	0.38	0/583	0.63	0/771
48	Y2	0.50	0/583	0.83	1/771 (0.1%)
49	R3	0.35	0/474	0.57	0/635
49	Y3	0.42	0/474	0.59	0/635
50	R4	0.39	0/594	0.78	1/795 (0.1%)
50	Y4	0.37	0/594	0.68	0/795
51	R5	0.49	0/473	0.74	0/639
51	Y5	0.49	0/468	0.72	0/632
52	R6	0.34	0/431	0.69	0/575
52	Y6	0.37	0/431	0.67	0/575
53	R7	0.49	0/438	0.67	0/575
53	Y7	0.56	0/438	0.70	0/575
54	R8	0.61	0/525	0.92	1/691 (0.1%)
54	Y8	0.62	0/525	0.93	1/691 (0.1%)
55	R9	0.27	0/310	0.46	0/407
55	Y9	0.32	0/310	0.48	0/407
56	Z5	0.79	0/40	1.80	1/60 (1.7%)
56	Z6	0.79	0/40	1.81	1/60 (1.7%)
All	All	0.38	6/316490 (0.0%)	0.81	218/473169 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	0	C	OP3-P	-10.53	1.48	1.61
22	XV	0	C	OP3-P	-10.40	1.48	1.61
25	YA	1888	G	O3'-P	-5.78	1.54	1.61
12	QL	48	PRO	N-CD	5.49	1.55	1.47
5	QE	70	PRO	N-CD	5.34	1.55	1.47

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1884	A	P-O3'-C3'	22.15	146.28	119.70
25	YA	1884	A	OP1-P-O3'	11.40	130.28	105.20
5	XE	69	VAL	O-C-N	10.41	140.88	121.10
28	YE	21	VAL	C-N-CD	-10.12	98.33	120.60
28	RE	21	VAL	C-N-CD	-10.08	98.42	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	458	0
1	XA	32249	0	16278	462	0
2	QB	1924	0	1975	61	0
2	XB	1924	0	1975	82	0
3	QC	1605	0	1668	49	0
3	XC	1605	0	1668	60	0
4	QD	1703	0	1764	58	0
4	XD	1703	0	1764	50	0
5	QE	1155	0	1213	69	0
5	XE	1155	0	1213	78	0
6	QF	843	0	857	21	0
6	XF	843	0	857	21	0
7	QG	1257	0	1296	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	22	0
8	QH	1116	0	1175	35	0
8	XH	1116	0	1177	29	0
9	QI	1010	0	1037	36	0
9	XI	1010	0	1037	49	0
10	QJ	801	0	849	68	0
10	XJ	801	0	849	61	0
11	QK	885	0	904	25	0
11	XK	885	0	904	28	0
12	QL	975	0	1062	98	0
12	XL	975	0	1062	102	0
13	QM	964	0	1034	67	0
13	XM	964	0	1034	46	0
14	QN	492	0	529	25	0
14	XN	492	0	529	18	0
15	QO	734	0	771	21	0
15	XO	734	0	771	17	0
16	QP	705	0	725	15	0
16	XP	705	0	725	23	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	19	0
19	QS	674	0	699	53	0
19	XS	674	0	699	43	0
20	QT	763	0	860	38	0
20	XT	763	0	861	63	0
21	QU	217	0	234	10	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	21	0
22	XV	1644	0	836	15	0
23	QX	220	0	109	1	0
23	XX	214	0	111	3	0
24	QY	319	0	162	2	0
24	XY	319	0	162	5	0
25	RA	62069	0	31285	904	0
25	YA	62070	0	31285	984	0
26	RB	2573	0	1306	42	0
26	YB	2573	0	1306	48	0
27	RD	2115	0	2195	96	0
27	YD	2115	0	2195	342	0
28	RE	1568	0	1634	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YE	1568	0	1634	291	0
29	RF	1585	0	1632	58	0
29	YF	1585	0	1632	181	0
30	RG	1474	0	1535	105	0
30	YG	1474	0	1535	58	0
31	RH	1307	0	1382	231	0
31	YH	1307	0	1382	239	0
32	RI	1136	0	1223	70	0
32	YI	1136	0	1223	51	0
33	RN	1104	0	1180	47	0
33	YN	1104	0	1180	55	0
34	RO	933	0	996	24	0
34	YO	933	0	996	28	0
35	RP	1145	0	1227	68	0
35	YP	1143	0	1224	85	0
36	RQ	1122	0	1179	166	0
36	YQ	1122	0	1179	179	0
37	RR	968	0	1033	51	0
37	YR	968	0	1033	36	0
38	RS	882	0	943	55	0
38	YS	882	0	943	167	0
39	RT	1141	0	1202	73	0
39	YT	1141	0	1202	55	0
40	RU	964	0	1022	28	0
40	YU	964	0	1022	61	0
41	RV	779	0	852	21	0
41	YV	779	0	852	45	0
42	RW	900	0	964	26	0
42	YW	900	0	964	24	0
43	RX	725	0	778	27	0
43	YX	725	0	778	22	0
44	RY	785	0	878	51	0
44	YY	785	0	878	46	0
45	RZ	1461	0	1493	46	0
45	YZ	1461	0	1493	64	0
46	R0	648	0	672	29	0
46	Y0	648	0	672	39	0
47	R1	763	0	848	27	0
47	Y1	763	0	848	35	0
48	R2	581	0	629	18	0
48	Y2	581	0	629	75	0
49	R3	469	0	518	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y3	469	0	518	18	0
50	R4	581	0	575	189	0
50	Y4	581	0	577	53	0
51	R5	459	0	480	73	0
51	Y5	454	0	475	39	0
52	R6	424	0	450	28	0
52	Y6	424	0	450	33	0
53	R7	430	0	480	20	0
53	Y7	430	0	480	20	0
54	R8	517	0	582	116	0
54	Y8	517	0	582	118	0
55	R9	307	0	338	9	0
55	Y9	307	0	338	10	0
56	Z5	37	0	23	3	0
56	Z6	37	0	23	1	0
57	QA	89	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	QN	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	248	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	1	0	0	0	0
57	RP	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	102	0	0	0	0
57	XF	1	0	0	0	0
57	XV	3	0	0	0	0
57	XX	1	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y1	1	0	0	0	0
57	Y5	1	0	0	0	0
57	YA	276	0	0	0	0
57	YB	5	0	0	0	0
57	YE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YP	1	0	0	0	0
58	QD	1	0	0	0	0
58	QN	1	0	0	0	0
58	XD	1	0	0	0	0
58	XN	1	0	0	0	0
59	Z5	37	0	28	10	0
59	Z6	37	0	28	9	0
All	All	292042	0	198293	7833	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7833 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:RH:127:GLU:CG	31:RH:128:PRO:HD3	1.35	1.53
31:YH:127:GLU:CG	31:YH:128:PRO:HD3	1.36	1.52
30:RG:67:LYS:HE2	50:R4:6:HIS:CE1	1.69	1.26
51:Y5:49:CYS:SG	51:Y5:60:VAL:HG12	1.75	1.26
19:QS:5:LEU:CD2	50:R4:67:TYR:CZ	2.18	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	174 (74%)	44 (19%)	17 (7%)	1	19
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	2	23
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	5	44
3	XC	203/239 (85%)	172 (85%)	28 (14%)	3 (2%)	13	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	QD	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	13	57
4	XD	206/209 (99%)	176 (85%)	25 (12%)	5 (2%)	7	49
5	QE	149/162 (92%)	137 (92%)	8 (5%)	4 (3%)	6	46
5	XE	149/162 (92%)	134 (90%)	13 (9%)	2 (1%)	15	60
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	136 (89%)	15 (10%)	2 (1%)	15	60
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	15	60
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	26	72
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	6	44
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	4	35
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	5	42
10	QJ	97/105 (92%)	77 (79%)	16 (16%)	4 (4%)	3	34
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	27
11	QK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	55
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	11	55
12	QL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	9
12	XL	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	0	9
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	17
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	17
14	QN	58/61 (95%)	50 (86%)	4 (7%)	4 (7%)	1	20
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	1	11
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16	62
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	50
16	QP	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	16	62
16	XP	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	16	62
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	9	53
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	3	32
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	13	57
19	QS	82/93 (88%)	55 (67%)	16 (20%)	11 (13%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	6
20	QT	97/106 (92%)	77 (79%)	14 (14%)	6 (6%)	2	24
20	XT	97/106 (92%)	77 (79%)	16 (16%)	4 (4%)	3	34
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	33
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	33
27	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	32
27	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	20
28	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
28	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
29	RF	200/210 (95%)	181 (90%)	13 (6%)	6 (3%)	5	44
29	YF	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	11
30	RG	179/182 (98%)	139 (78%)	25 (14%)	15 (8%)	1	15
30	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	21
31	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
31	YH	168/180 (93%)	94 (56%)	37 (22%)	37 (22%)	0	1
32	RI	144/148 (97%)	109 (76%)	24 (17%)	11 (8%)	1	17
32	YI	144/148 (97%)	107 (74%)	23 (16%)	14 (10%)	1	12
33	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	14
33	YN	136/140 (97%)	107 (79%)	16 (12%)	13 (10%)	1	12
34	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	11	55
34	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	11	55
35	RP	148/150 (99%)	109 (74%)	26 (18%)	13 (9%)	1	14
35	YP	146/150 (97%)	100 (68%)	35 (24%)	11 (8%)	1	17
36	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	11
36	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	11
37	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	3	33
37	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	27
38	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	11
38	YS	109/112 (97%)	62 (57%)	29 (27%)	18 (16%)	0	4
39	RT	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	13
39	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	4	40
40	YU	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	11	55
41	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	24
41	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	15
42	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	4	39
42	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	11	54
43	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	8	51
43	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	8	51
44	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	4
44	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	8
45	RZ	181/206 (88%)	127 (70%)	34 (19%)	20 (11%)	0	9
45	YZ	181/206 (88%)	135 (75%)	28 (16%)	18 (10%)	1	12
46	R0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	15	60
46	Y0	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
47	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	1	12
47	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	23
48	R2	67/72 (93%)	54 (81%)	9 (13%)	4 (6%)	2	24
48	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	6
49	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	4	40
49	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	11	54
50	R4	69/71 (97%)	22 (32%)	21 (30%)	26 (38%)	0	0
50	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
51	R5	57/60 (95%)	33 (58%)	10 (18%)	14 (25%)	0	1
51	Y5	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	4	39
52	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
52	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	3
53	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	9	52
53	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9	52
54	R8	62/65 (95%)	36 (58%)	14 (23%)	12 (19%)	0	2
54	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	3
55	R9	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11467/12128 (94%)	9027 (79%)	1609 (14%)	831 (7%)	1	19

5 of 831 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	33	MET
12	QL	18	VAL

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	21
2	XB	205/220 (93%)	180 (88%)	25 (12%)	6	32
3	QC	159/188 (85%)	144 (91%)	15 (9%)	11	47
3	XC	159/188 (85%)	145 (91%)	14 (9%)	12	50
4	QD	180/181 (99%)	161 (89%)	19 (11%)	8	40
4	XD	180/181 (99%)	154 (86%)	26 (14%)	4	26
5	QE	116/123 (94%)	104 (90%)	12 (10%)	9	42
5	XE	116/123 (94%)	104 (90%)	12 (10%)	9	42
6	QF	90/90 (100%)	78 (87%)	12 (13%)	5	30
6	XF	90/90 (100%)	82 (91%)	8 (9%)	12	50
7	QG	126/127 (99%)	114 (90%)	12 (10%)	11	46
7	XG	126/127 (99%)	114 (90%)	12 (10%)	11	46
8	QH	119/119 (100%)	109 (92%)	10 (8%)	14	52
8	XH	119/119 (100%)	106 (89%)	13 (11%)	8	39
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	XI	98/99 (99%)	80 (82%)	18 (18%)	2	14
10	QJ	89/92 (97%)	79 (89%)	10 (11%)	7	38
10	XJ	89/92 (97%)	75 (84%)	14 (16%)	3	22
11	QK	90/99 (91%)	81 (90%)	9 (10%)	9	43
11	XK	90/99 (91%)	81 (90%)	9 (10%)	9	43
12	QL	104/109 (95%)	90 (86%)	14 (14%)	5	29
12	XL	104/109 (95%)	89 (86%)	15 (14%)	4	26
13	QM	97/101 (96%)	73 (75%)	24 (25%)	1	6
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	12
14	QN	49/50 (98%)	40 (82%)	9 (18%)	2	14
14	XN	49/50 (98%)	42 (86%)	7 (14%)	4	27
15	QO	79/80 (99%)	72 (91%)	7 (9%)	12	50
15	XO	79/80 (99%)	69 (87%)	10 (13%)	5	31
16	QP	72/74 (97%)	63 (88%)	9 (12%)	6	32
16	XP	72/74 (97%)	64 (89%)	8 (11%)	8	38
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	14	52
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	22	64
18	QR	61/77 (79%)	50 (82%)	11 (18%)	2	15
18	XR	61/77 (79%)	52 (85%)	9 (15%)	4	25
19	QS	73/80 (91%)	59 (81%)	14 (19%)	2	12
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	9
20	QT	76/82 (93%)	67 (88%)	9 (12%)	6	34
20	XT	76/82 (93%)	66 (87%)	10 (13%)	5	30
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	30	70
27	RD	214/218 (98%)	175 (82%)	39 (18%)	2	14
27	YD	214/218 (98%)	177 (83%)	37 (17%)	2	17
28	RE	165/166 (99%)	127 (77%)	38 (23%)	1	7
28	YE	165/166 (99%)	127 (77%)	38 (23%)	1	7
29	RF	161/166 (97%)	142 (88%)	19 (12%)	6	34
29	YF	161/166 (97%)	140 (87%)	21 (13%)	5	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	RG	155/156 (99%)	134 (86%)	21 (14%)	5	29
30	YG	155/156 (99%)	133 (86%)	22 (14%)	4	27
31	RH	142/148 (96%)	114 (80%)	28 (20%)	1	12
31	YH	142/148 (96%)	114 (80%)	28 (20%)	1	12
32	RI	122/124 (98%)	101 (83%)	21 (17%)	2	17
32	YI	122/124 (98%)	97 (80%)	25 (20%)	1	11
33	RN	117/119 (98%)	97 (83%)	20 (17%)	2	18
33	YN	117/119 (98%)	96 (82%)	21 (18%)	2	15
34	RO	100/100 (100%)	90 (90%)	10 (10%)	9	43
34	YO	100/100 (100%)	89 (89%)	11 (11%)	8	39
35	RP	116/116 (100%)	86 (74%)	30 (26%)	0	5
35	YP	115/116 (99%)	79 (69%)	36 (31%)	0	3
36	RQ	111/111 (100%)	93 (84%)	18 (16%)	3	20
36	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	18
37	RR	101/101 (100%)	83 (82%)	18 (18%)	2	16
37	YR	101/101 (100%)	82 (81%)	19 (19%)	2	13
38	RS	87/88 (99%)	69 (79%)	18 (21%)	1	10
38	YS	87/88 (99%)	74 (85%)	13 (15%)	4	25
39	RT	120/127 (94%)	102 (85%)	18 (15%)	3	25
39	YT	120/127 (94%)	99 (82%)	21 (18%)	2	16
40	RU	93/94 (99%)	79 (85%)	14 (15%)	3	24
40	YU	93/94 (99%)	77 (83%)	16 (17%)	2	17
41	RV	82/82 (100%)	66 (80%)	16 (20%)	2	12
41	YV	82/82 (100%)	67 (82%)	15 (18%)	2	14
42	RW	92/92 (100%)	73 (79%)	19 (21%)	1	10
42	YW	92/92 (100%)	76 (83%)	16 (17%)	2	17
43	RX	74/78 (95%)	64 (86%)	10 (14%)	5	29
43	YX	74/78 (95%)	60 (81%)	14 (19%)	2	13
44	RY	85/91 (93%)	63 (74%)	22 (26%)	0	5
44	YY	85/91 (93%)	64 (75%)	21 (25%)	1	6
45	RZ	162/179 (90%)	138 (85%)	24 (15%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	YZ	162/179 (90%)	144 (89%)	18 (11%)	8	38
46	R0	65/67 (97%)	60 (92%)	5 (8%)	16	56
46	Y0	65/67 (97%)	59 (91%)	6 (9%)	11	48
47	R1	82/83 (99%)	73 (89%)	9 (11%)	8	39
47	Y1	82/83 (99%)	70 (85%)	12 (15%)	4	26
48	R2	64/67 (96%)	55 (86%)	9 (14%)	4	28
48	Y2	64/67 (96%)	57 (89%)	7 (11%)	8	39
49	R3	51/52 (98%)	45 (88%)	6 (12%)	6	34
49	Y3	51/52 (98%)	43 (84%)	8 (16%)	3	22
50	R4	63/63 (100%)	46 (73%)	17 (27%)	0	4
50	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	3
51	R5	51/52 (98%)	39 (76%)	12 (24%)	1	7
51	Y5	51/52 (98%)	39 (76%)	12 (24%)	1	7
52	R6	48/52 (92%)	35 (73%)	13 (27%)	0	4
52	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	10
53	R7	42/42 (100%)	34 (81%)	8 (19%)	2	12
53	Y7	42/42 (100%)	35 (83%)	7 (17%)	3	19
54	R8	54/55 (98%)	39 (72%)	15 (28%)	0	4
54	Y8	54/55 (98%)	38 (70%)	16 (30%)	0	3
55	R9	34/34 (100%)	32 (94%)	2 (6%)	24	66
55	Y9	34/34 (100%)	32 (94%)	2 (6%)	24	66
All	All	9701/10066 (96%)	8186 (84%)	1515 (16%)	3	23

5 of 1515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	R3	56	VAL
7	XG	137	LYS
45	YZ	19	ARG
51	R5	6	VAL
2	XB	163	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	212	GLN
5	XE	72	GLN
31	YH	147	ASN
3	XC	162	GLN
3	XC	176	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	264 (17%)	39 (2%)
1	XA	1498/1522 (98%)	283 (18%)	36 (2%)
22	QV	76/77 (98%)	16 (21%)	1 (1%)
22	XV	76/77 (98%)	14 (18%)	1 (1%)
23	QX	9/25 (36%)	1 (11%)	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	14/18 (77%)	1 (7%)	0
24	XY	14/18 (77%)	3 (21%)	0
25	RA	2879/2915 (98%)	590 (20%)	51 (1%)
25	YA	2879/2915 (98%)	606 (21%)	53 (1%)
26	RB	119/122 (97%)	15 (12%)	2 (1%)
26	YB	119/122 (97%)	22 (18%)	2 (1%)
56	Z5	1/3 (33%)	0	0
56	Z6	1/3 (33%)	0	0
All	All	9192/9364 (98%)	1818 (19%)	185 (2%)

5 of 1818 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	2518	A
1	XA	328	C
25	YA	1930	G
25	RA	2712	U
1	XA	31	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 754 ligands modelled in this entry, 752 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	$\# Z > 2$
59	PPU	Z5	101	56	30,40,41	2.58	6 (20%)	37,57,60	3.24	11 (29%)
59	PPU	Z6	101	56	30,40,41	2.58	5 (16%)	37,57,60	3.24	11 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PPU	Z5	101	56	-	0/21/43/44	0/4/4/4
59	PPU	Z6	101	56	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Z6	101	PPU	C9-N6	-5.66	1.31	1.45
59	Z5	101	PPU	C9-N6	-5.61	1.32	1.45
59	Z5	101	PPU	C10-N6	-5.32	1.32	1.45
59	Z6	101	PPU	C10-N6	-5.25	1.32	1.45
59	Z5	101	PPU	C5-N7	-2.01	1.32	1.39

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Z6	101	PPU	C2'-C1'-N9	-10.33	98.52	114.29
59	Z5	101	PPU	C2'-C1'-N9	-10.33	98.52	114.29
59	Z5	101	PPU	N3-C2-N1	-9.72	121.45	128.89
59	Z6	101	PPU	N3-C2-N1	-9.68	121.48	128.89
59	Z6	101	PPU	C3'-N3'-C	-8.23	110.22	123.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	Z5	101	PPU	10	0
59	Z6	101	PPU	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	0.45	112 (7%) 17 12	68, 119, 216, 326	0
1	XA	1500/1522 (98%)	0.23	55 (3%) 45 32	51, 103, 202, 332	0
2	QB	237/256 (92%)	0.48	18 (7%) 17 11	120, 181, 240, 264	0
2	XB	237/256 (92%)	0.29	14 (5%) 26 17	99, 157, 210, 239	0
3	QC	205/239 (85%)	0.45	16 (7%) 16 10	121, 172, 216, 250	0
3	XC	205/239 (85%)	0.25	7 (3%) 49 35	79, 131, 185, 239	0
4	QD	208/209 (99%)	-0.01	5 (2%) 62 47	92, 126, 170, 212	0
4	XD	208/209 (99%)	0.19	4 (1%) 70 56	83, 131, 180, 211	0
5	QE	151/162 (93%)	0.16	6 (3%) 42 29	93, 140, 182, 216	0
5	XE	151/162 (93%)	0.25	7 (4%) 36 26	77, 121, 174, 245	0
6	QF	101/101 (100%)	-0.04	3 (2%) 54 38	76, 116, 161, 205	0
6	XF	101/101 (100%)	-0.27	0 100 100	77, 120, 162, 198	0
7	QG	155/156 (99%)	0.79	25 (16%) 3 2	92, 148, 197, 212	0
7	XG	155/156 (99%)	-0.05	4 (2%) 59 44	82, 123, 165, 203	0
8	QH	138/138 (100%)	-0.09	1 (0%) 89 81	86, 140, 178, 207	0
8	XH	138/138 (100%)	0.06	5 (3%) 46 33	84, 119, 161, 178	0
9	QI	127/128 (99%)	0.78	18 (14%) 4 3	122, 188, 231, 267	0
9	XI	127/128 (99%)	0.14	6 (4%) 35 25	76, 150, 201, 226	0
10	QJ	99/105 (94%)	1.02	15 (15%) 3 3	122, 205, 256, 279	0
10	XJ	99/105 (94%)	0.66	11 (11%) 7 6	82, 158, 223, 244	0
11	QK	119/129 (92%)	0.48	18 (15%) 3 3	80, 122, 188, 209	0
11	XK	119/129 (92%)	0.55	14 (11%) 6 5	64, 104, 171, 198	0
12	QL	125/132 (94%)	-0.04	4 (3%) 51 37	67, 114, 162, 222	0
12	XL	125/132 (94%)	0.07	7 (5%) 28 19	50, 90, 150, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	0.55	17 (14%) 4 3	106, 172, 212, 249	0
13	XM	121/126 (96%)	0.07	3 (2%) 61 46	67, 128, 184, 225	0
14	QN	60/61 (98%)	0.27	2 (3%) 50 36	135, 164, 205, 221	0
14	XN	60/61 (98%)	0.21	1 (1%) 73 59	88, 114, 157, 184	0
15	QO	88/89 (98%)	0.10	0 100 100	78, 118, 156, 167	0
15	XO	88/89 (98%)	-0.04	0 100 100	62, 104, 151, 183	0
16	QP	84/88 (95%)	-0.31	0 100 100	70, 109, 154, 202	0
16	XP	84/88 (95%)	0.05	2 (2%) 62 47	92, 122, 167, 209	0
17	QQ	100/105 (95%)	0.08	3 (3%) 54 38	74, 116, 157, 175	0
17	XQ	100/105 (95%)	-0.08	0 100 100	70, 114, 154, 184	0
18	QR	70/88 (79%)	0.54	7 (10%) 9 7	83, 124, 172, 203	0
18	XR	70/88 (79%)	0.39	3 (4%) 39 27	72, 116, 171, 191	0
19	QS	84/93 (90%)	0.70	13 (15%) 3 2	118, 184, 216, 227	0
19	XS	84/93 (90%)	-0.13	0 100 100	74, 141, 182, 215	0
20	QT	99/106 (93%)	-0.20	2 (2%) 68 54	72, 121, 165, 219	0
20	XT	99/106 (93%)	0.06	2 (2%) 68 54	85, 134, 187, 220	0
21	QU	25/27 (92%)	1.94	11 (44%) 0 0	132, 164, 200, 248	0
21	XU	25/27 (92%)	0.32	1 (4%) 42 29	98, 126, 181, 218	0
22	QV	77/77 (100%)	0.12	4 (5%) 31 22	66, 116, 162, 216	0
22	XV	77/77 (100%)	0.40	3 (3%) 43 31	62, 90, 128, 178	0
23	QX	11/25 (44%)	1.26	3 (27%) 1 1	93, 112, 226, 253	0
23	XX	10/25 (40%)	0.73	1 (10%) 9 7	70, 95, 186, 197	0
24	QY	15/18 (83%)	0.21	0 100 100	107, 141, 236, 256	0
24	XY	15/18 (83%)	0.93	1 (6%) 21 13	89, 117, 219, 223	0
25	RA	2882/2915 (98%)	0.36	161 (5%) 28 19	43, 86, 233, 352	0
25	YA	2882/2915 (98%)	0.29	133 (4%) 36 26	31, 70, 224, 366	0
26	RB	120/122 (98%)	0.38	7 (5%) 26 18	103, 157, 198, 227	0
26	YB	120/122 (98%)	-0.08	0 100 100	68, 118, 143, 176	0
27	RD	272/276 (98%)	-0.18	0 100 100	43, 78, 129, 207	0
27	YD	272/276 (98%)	-0.04	1 (0%) 93 88	33, 69, 112, 205	0
28	RE	205/206 (99%)	0.25	7 (3%) 49 35	50, 100, 166, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YE	205/206 (99%)	-0.14	2 (0%) 84 73	37, 93, 167, 230	0
29	RF	202/210 (96%)	-0.01	5 (2%) 61 46	38, 104, 162, 221	0
29	YF	202/210 (96%)	-0.06	4 (1%) 68 54	32, 84, 147, 201	0
30	RG	181/182 (99%)	0.50	19 (10%) 8 6	125, 179, 223, 250	0
30	YG	181/182 (99%)	0.20	9 (4%) 32 22	81, 135, 183, 245	0
31	RH	170/180 (94%)	0.84	30 (17%) 2 2	108, 184, 228, 277	0
31	YH	170/180 (94%)	0.30	10 (5%) 26 17	83, 119, 170, 234	0
32	RI	146/148 (98%)	0.66	11 (7%) 17 12	67, 164, 206, 249	0
32	YI	146/148 (98%)	0.20	10 (6%) 20 13	63, 158, 202, 226	0
33	RN	138/140 (98%)	-0.08	0 100 100	60, 111, 165, 197	0
33	YN	138/140 (98%)	-0.25	0 100 100	49, 91, 148, 194	0
34	RO	122/122 (100%)	-0.12	1 (0%) 87 78	56, 85, 126, 144	0
34	YO	122/122 (100%)	-0.06	1 (0%) 87 78	47, 77, 118, 145	0
35	RP	150/150 (100%)	0.16	3 (2%) 68 54	45, 109, 175, 219	0
35	YP	150/150 (100%)	-0.13	2 (1%) 79 66	33, 86, 155, 210	0
36	RQ	141/141 (100%)	0.22	4 (2%) 56 42	76, 118, 174, 231	0
36	YQ	141/141 (100%)	0.07	2 (1%) 78 65	46, 85, 138, 230	0
37	RR	118/118 (100%)	-0.18	0 100 100	52, 84, 121, 150	0
37	YR	118/118 (100%)	-0.01	2 (1%) 73 59	48, 83, 127, 171	0
38	RS	111/112 (99%)	0.05	2 (1%) 71 58	126, 160, 218, 229	0
38	YS	111/112 (99%)	0.12	3 (2%) 58 43	93, 124, 171, 199	0
39	RT	137/146 (93%)	-0.09	2 (1%) 76 64	60, 95, 190, 262	0
39	YT	137/146 (93%)	-0.19	2 (1%) 76 64	59, 92, 179, 223	0
40	RU	117/118 (99%)	-0.12	2 (1%) 73 59	52, 104, 157, 243	0
40	YU	117/118 (99%)	0.04	2 (1%) 73 59	46, 83, 151, 203	0
41	RV	101/101 (100%)	0.03	1 (0%) 84 73	62, 125, 186, 258	0
41	YV	101/101 (100%)	0.05	3 (2%) 54 38	42, 106, 174, 235	0
42	RW	113/113 (100%)	0.10	7 (6%) 24 16	48, 81, 135, 217	0
42	YW	113/113 (100%)	0.03	3 (2%) 58 43	40, 74, 140, 199	0
43	RX	92/96 (95%)	-0.16	1 (1%) 82 70	61, 93, 139, 182	0
43	YX	92/96 (95%)	-0.32	0 100 100	49, 74, 115, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RY	102/110 (92%)	0.83	17 (16%) 2 2	84, 131, 189, 225	0
44	YY	102/110 (92%)	0.38	6 (5%) 26 17	69, 107, 159, 251	0
45	RZ	183/206 (88%)	0.54	25 (13%) 4 4	99, 165, 224, 280	0
45	YZ	183/206 (88%)	0.08	8 (4%) 38 27	82, 124, 202, 240	0
46	R0	82/85 (96%)	0.16	1 (1%) 81 69	64, 104, 143, 168	0
46	Y0	82/85 (96%)	-0.10	0 100 100	46, 79, 114, 140	0
47	R1	97/98 (98%)	0.17	2 (2%) 67 52	55, 89, 182, 204	0
47	Y1	97/98 (98%)	-0.11	0 100 100	36, 73, 178, 200	0
48	R2	69/72 (95%)	-0.09	3 (4%) 39 27	83, 120, 172, 193	0
48	Y2	69/72 (95%)	-0.06	2 (2%) 55 40	65, 84, 157, 226	0
49	R3	59/60 (98%)	0.58	5 (8%) 13 10	79, 111, 172, 193	0
49	Y3	59/60 (98%)	0.13	1 (1%) 73 59	57, 89, 148, 197	0
50	R4	71/71 (100%)	0.70	12 (16%) 2 2	158, 229, 303, 319	0
50	Y4	71/71 (100%)	0.39	5 (7%) 19 13	127, 173, 251, 269	0
51	R5	59/60 (98%)	0.59	6 (10%) 9 7	48, 92, 214, 226	0
51	Y5	58/60 (96%)	-0.05	1 (1%) 73 59	41, 85, 195, 229	0
52	R6	49/54 (90%)	3.63	31 (63%) 0 0	142, 185, 226, 245	0
52	Y6	49/54 (90%)	4.07	43 (87%) 0 0	115, 172, 221, 241	0
53	R7	49/49 (100%)	0.16	2 (4%) 41 29	41, 66, 126, 203	0
53	Y7	49/49 (100%)	-0.14	2 (4%) 41 29	31, 53, 115, 183	0
54	R8	64/65 (98%)	0.17	2 (3%) 52 38	56, 99, 146, 240	0
54	Y8	64/65 (98%)	-0.05	2 (3%) 52 38	43, 78, 132, 225	0
55	R9	37/37 (100%)	3.15	22 (59%) 0 0	128, 172, 212, 231	0
55	Y9	37/37 (100%)	1.66	13 (35%) 0 0	103, 149, 207, 229	0
56	Z5	2/3 (66%)	0.59	0 100 100	77, 77, 77, 85	0
56	Z6	2/3 (66%)	0.74	0 100 100	51, 51, 51, 59	0
All	All	20878/21492 (97%)	0.26	1117 (5%) 29 20	31, 107, 207, 366	0

The worst 5 of 1117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R6	13	CYS	21.9
25	YA	2119	A	13.3

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Mol	Chain	Res	Type	RSRZ
25	YA	654	A	13.0
25	YA	2117	A	12.9
25	YA	1536	A	11.9

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	RA	3062	1/1	0.89	1.16	64.81	72,72,72,72	0
57	MG	RA	3063	1/1	0.94	1.20	57.07	82,82,82,82	0
57	MG	XA	1633	1/1	0.93	1.31	50.97	96,96,96,96	0
57	MG	RA	3096	1/1	0.97	0.70	42.68	44,44,44,44	0
57	MG	RA	3097	1/1	0.97	0.65	38.92	50,50,50,50	0
57	MG	XA	1651	1/1	0.77	0.80	36.58	78,78,78,78	0
57	MG	YA	3261	1/1	0.96	1.22	35.17	86,86,86,86	0
57	MG	YA	3015	1/1	0.90	0.85	35.03	63,63,63,63	0
57	MG	RA	3026	1/1	0.85	0.78	33.27	74,74,74,74	0
57	MG	QA	1617	1/1	0.87	0.86	31.30	96,96,96,96	0
57	MG	YA	3057	1/1	0.98	0.87	28.29	69,69,69,69	0
57	MG	RA	3059	1/1	0.96	0.64	27.39	38,38,38,38	0
57	MG	YA	3223	1/1	0.94	0.57	27.25	57,57,57,57	0
57	MG	YA	3103	1/1	0.93	0.85	26.94	34,34,34,34	0
57	MG	YA	3248	1/1	0.92	1.10	26.44	49,49,49,49	0
57	MG	YA	3031	1/1	0.97	0.91	26.25	63,63,63,63	0
57	MG	YA	3037	1/1	0.87	0.57	26.12	60,60,60,60	0
57	MG	QA	1642	1/1	0.62	1.35	25.92	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3107	1/1	0.92	0.60	25.62	65,65,65,65	0
57	MG	YA	3256	1/1	0.95	0.52	25.13	62,62,62,62	0
57	MG	RA	3084	1/1	0.97	0.68	24.76	59,59,59,59	0
57	MG	RA	3141	1/1	0.93	0.68	23.14	46,46,46,46	0
57	MG	YA	3006	1/1	0.88	0.66	22.89	62,62,62,62	0
57	MG	RA	3094	1/1	0.99	0.56	22.04	39,39,39,39	0
57	MG	RA	3167	1/1	0.86	0.99	21.94	77,77,77,77	0
57	MG	QA	1664	1/1	0.35	0.95	21.73	88,88,88,88	0
57	MG	RA	3015	1/1	0.96	0.50	21.49	38,38,38,38	0
57	MG	RA	3154	1/1	0.92	0.51	21.22	80,80,80,80	0
57	MG	RA	3078	1/1	0.95	0.64	20.19	48,48,48,48	0
57	MG	YA	3099	1/1	0.93	0.64	20.02	44,44,44,44	0
57	MG	XA	1602	1/1	0.96	0.48	19.54	47,47,47,47	0
57	MG	RA	3049	1/1	0.87	0.60	18.62	51,51,51,51	0
57	MG	RA	3233	1/1	0.62	1.04	18.33	60,60,60,60	0
57	MG	RA	3052	1/1	0.90	0.63	18.21	41,41,41,41	0
57	MG	YA	3049	1/1	0.95	0.67	18.04	42,42,42,42	0
57	MG	QA	1602	1/1	0.87	1.25	18.01	75,75,75,75	0
57	MG	RA	3123	1/1	0.86	0.60	17.77	56,56,56,56	0
57	MG	XA	1669	1/1	0.87	0.64	17.67	66,66,66,66	0
57	MG	YA	3179	1/1	0.87	0.66	17.63	66,66,66,66	0
57	MG	XA	1619	1/1	0.94	0.62	17.32	63,63,63,63	0
57	MG	YA	3240	1/1	0.98	0.71	17.12	31,31,31,31	0
57	MG	RA	3002	1/1	0.88	0.60	16.78	53,53,53,53	0
57	MG	YA	3242	1/1	0.92	0.81	16.76	39,39,39,39	0
57	MG	YA	3227	1/1	0.95	0.42	16.29	98,98,98,98	0
57	MG	YA	3108	1/1	0.96	0.45	16.11	32,32,32,32	0
57	MG	RA	3199	1/1	0.92	0.39	15.14	93,93,93,93	0
57	MG	YA	3068	1/1	0.89	0.58	15.08	52,52,52,52	0
57	MG	RA	3033	1/1	0.97	0.64	14.97	44,44,44,44	0
57	MG	RA	3031	1/1	0.96	0.57	14.71	59,59,59,59	0
57	MG	YA	3050	1/1	0.92	0.72	14.67	58,58,58,58	0
57	MG	RA	3119	1/1	0.84	0.77	14.64	76,76,76,76	0
57	MG	YA	3044	1/1	0.90	0.45	14.48	32,32,32,32	0
57	MG	YA	3166	1/1	0.86	0.69	14.40	41,41,41,41	0
57	MG	XA	1603	1/1	0.96	0.90	14.32	61,61,61,61	0
57	MG	QN	102	1/1	0.16	1.76	13.73	143,143,143,143	0
57	MG	YA	3238	1/1	0.79	0.55	13.69	47,47,47,47	0
57	MG	YA	3100	1/1	0.98	0.44	13.41	31,31,31,31	0
57	MG	RA	3009	1/1	0.72	0.51	13.28	79,79,79,79	0
57	MG	QA	1660	1/1	0.85	0.51	13.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3006	1/1	0.98	0.45	13.06	41,41,41,41	0
57	MG	XA	1700	1/1	0.89	0.53	12.73	90,90,90,90	0
57	MG	XA	1665	1/1	0.87	0.28	12.57	64,64,64,64	0
57	MG	RA	3204	1/1	0.94	0.45	12.29	46,46,46,46	0
57	MG	YA	3204	1/1	0.91	0.36	12.04	51,51,51,51	0
57	MG	YA	3033	1/1	0.97	0.58	12.02	35,35,35,35	0
57	MG	RA	3230	1/1	0.96	0.42	11.88	52,52,52,52	0
57	MG	YA	3086	1/1	0.98	0.46	11.75	43,43,43,43	0
57	MG	QA	1670	1/1	0.72	0.37	11.62	65,65,65,65	0
57	MG	YA	3199	1/1	0.76	0.55	10.97	61,61,61,61	0
57	MG	YA	3041	1/1	0.90	0.71	10.93	62,62,62,62	0
57	MG	RA	3232	1/1	0.97	0.43	10.75	50,50,50,50	0
57	MG	RA	3210	1/1	0.60	0.41	10.56	65,65,65,65	0
57	MG	RA	3093	1/1	0.98	0.58	10.25	41,41,41,41	0
57	MG	YA	3181	1/1	0.92	0.52	10.25	44,44,44,44	0
57	MG	RA	3035	1/1	0.99	0.52	10.24	42,42,42,42	0
57	MG	YA	3175	1/1	0.88	0.46	10.23	67,67,67,67	0
57	MG	YA	3026	1/1	0.92	0.59	10.09	37,37,37,37	0
57	MG	YA	3017	1/1	0.97	0.36	10.05	28,28,28,28	0
57	MG	YA	3036	1/1	0.97	0.28	9.90	29,29,29,29	0
57	MG	YA	3209	1/1	0.92	0.48	9.85	48,48,48,48	0
57	MG	RA	3098	1/1	0.85	0.49	9.46	55,55,55,55	0
57	MG	QA	1658	1/1	0.94	0.60	9.41	80,80,80,80	0
57	MG	XA	1648	1/1	0.87	0.44	9.32	59,59,59,59	0
57	MG	XA	1613	1/1	0.97	0.50	9.05	52,52,52,52	0
57	MG	RA	3144	1/1	0.96	0.43	9.02	52,52,52,52	0
57	MG	RA	3008	1/1	0.97	0.51	9.01	43,43,43,43	0
57	MG	YA	3080	1/1	0.92	0.58	8.78	29,29,29,29	0
57	MG	QA	1616	1/1	0.93	0.58	8.56	93,93,93,93	0
57	MG	QA	1683	1/1	0.87	0.30	8.48	80,80,80,80	0
57	MG	YA	3058	1/1	0.94	0.41	8.19	32,32,32,32	0
57	MG	XA	1616	1/1	0.86	0.52	8.05	67,67,67,67	0
57	MG	RA	3196	1/1	0.77	0.42	7.83	57,57,57,57	0
57	MG	YA	3135	1/1	0.97	0.37	7.79	46,46,46,46	0
57	MG	YP	201	1/1	0.93	0.96	7.74	162,162,162,162	0
57	MG	RA	3004	1/1	0.97	0.44	7.71	42,42,42,42	0
57	MG	YA	3048	1/1	0.95	0.55	7.65	69,69,69,69	0
57	MG	XA	1696	1/1	0.96	0.33	7.52	65,65,65,65	0
57	MG	RA	3024	1/1	0.94	0.29	7.51	44,44,44,44	0
57	MG	RA	3099	1/1	0.65	0.35	7.45	67,67,67,67	0
57	MG	YA	3074	1/1	0.67	0.29	7.43	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3040	1/1	0.99	0.34	7.29	42,42,42,42	0
57	MG	YA	3110	1/1	0.98	0.34	7.23	61,61,61,61	0
57	MG	YA	3207	1/1	0.91	0.25	7.21	88,88,88,88	0
57	MG	RA	3114	1/1	0.88	0.35	7.21	39,39,39,39	0
57	MG	RA	3218	1/1	0.96	0.56	7.15	47,47,47,47	0
57	MG	RA	3056	1/1	0.98	0.44	7.00	44,44,44,44	0
57	MG	YA	3053	1/1	0.93	0.39	6.94	28,28,28,28	0
57	MG	RA	3012	1/1	0.96	0.56	6.92	43,43,43,43	0
57	MG	RA	3058	1/1	0.82	0.41	6.46	38,38,38,38	0
57	MG	QA	1684	1/1	0.82	0.88	6.45	83,83,83,83	0
57	MG	RA	3087	1/1	0.96	0.50	6.43	59,59,59,59	0
57	MG	YA	3009	1/1	0.96	0.40	6.43	33,33,33,33	0
57	MG	RA	3198	1/1	0.97	0.37	6.36	47,47,47,47	0
57	MG	YA	3094	1/1	0.94	0.51	6.30	71,71,71,71	0
57	MG	YB	203	1/1	0.89	0.36	6.26	125,125,125,125	0
57	MG	YA	3193	1/1	0.93	0.37	6.26	47,47,47,47	0
57	MG	YA	3243	1/1	0.91	0.55	6.22	69,69,69,69	0
57	MG	RA	3036	1/1	0.97	0.38	6.12	41,41,41,41	0
57	MG	RA	3157	1/1	0.73	0.40	6.11	48,48,48,48	0
57	MG	RA	3080	1/1	0.92	0.45	5.96	85,85,85,85	0
57	MG	YA	3119	1/1	0.96	0.51	5.93	53,53,53,53	0
57	MG	RA	3050	1/1	0.97	0.36	5.93	60,60,60,60	0
57	MG	RA	3076	1/1	0.96	0.38	5.93	38,38,38,38	0
57	MG	QA	1636	1/1	0.94	0.37	5.79	73,73,73,73	0
57	MG	YA	3056	1/1	0.97	0.39	5.77	37,37,37,37	0
57	MG	YA	3038	1/1	0.94	0.27	5.64	31,31,31,31	0
57	MG	XA	1607	1/1	0.92	0.30	5.58	93,93,93,93	0
57	MG	QA	1605	1/1	0.93	0.54	5.50	69,69,69,69	0
57	MG	YA	3233	1/1	0.94	0.33	5.44	46,46,46,46	0
57	MG	RR	201	1/1	0.89	0.60	5.43	52,52,52,52	0
57	MG	YA	3143	1/1	0.91	0.29	5.37	66,66,66,66	0
57	MG	RA	3068	1/1	0.73	0.21	5.23	58,58,58,58	0
57	MG	XA	1632	1/1	0.91	0.23	5.18	51,51,51,51	0
57	MG	YA	3187	1/1	0.92	0.41	5.10	84,84,84,84	0
57	MG	YA	3250	1/1	0.95	0.37	5.08	32,32,32,32	0
57	MG	RA	3054	1/1	0.93	0.33	5.05	45,45,45,45	0
57	MG	RA	3083	1/1	0.95	0.30	4.99	46,46,46,46	0
57	MG	XA	1659	1/1	0.91	0.32	4.93	84,84,84,84	0
57	MG	YA	3139	1/1	0.91	0.36	4.92	51,51,51,51	0
57	MG	RA	3105	1/1	0.97	0.28	4.75	46,46,46,46	0
57	MG	YA	3013	1/1	0.97	0.47	4.70	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3024	1/1	0.92	0.43	4.55	62,62,62,62	0
57	MG	RA	3065	1/1	0.83	0.58	4.54	74,74,74,74	0
57	MG	RA	3034	1/1	0.90	0.36	4.46	49,49,49,49	0
57	MG	YA	3089	1/1	0.95	0.39	4.40	39,39,39,39	0
57	MG	QV	102	1/1	0.97	0.31	4.34	45,45,45,45	0
57	MG	XA	1668	1/1	0.96	0.27	4.31	70,70,70,70	0
57	MG	RA	3085	1/1	0.92	0.36	4.30	64,64,64,64	0
57	MG	YA	3249	1/1	0.95	0.38	4.21	32,32,32,32	0
57	MG	RA	3216	1/1	0.66	0.42	4.12	88,88,88,88	0
57	MG	QA	1619	1/1	0.97	0.48	4.08	74,74,74,74	0
57	MG	YA	3025	1/1	0.94	0.26	3.99	40,40,40,40	0
57	MG	YA	3073	1/1	0.98	0.37	3.93	38,38,38,38	0
57	MG	RA	3014	1/1	0.95	0.28	3.88	44,44,44,44	0
57	MG	RA	3086	1/1	0.97	0.54	3.65	37,37,37,37	0
57	MG	XA	1618	1/1	0.94	0.52	3.62	69,69,69,69	0
57	MG	QA	1614	1/1	0.86	0.41	3.62	60,60,60,60	0
57	MG	RA	3038	1/1	1.00	0.33	3.50	39,39,39,39	0
57	MG	RA	3092	1/1	0.97	0.43	3.49	38,38,38,38	0
57	MG	YA	3137	1/1	0.93	0.28	3.44	33,33,33,33	0
57	MG	YA	3191	1/1	0.94	0.27	3.41	69,69,69,69	0
57	MG	YA	3131	1/1	0.83	0.29	3.41	62,62,62,62	0
57	MG	YA	3267	1/1	0.94	0.19	3.38	71,71,71,71	0
57	MG	RA	3178	1/1	0.73	0.36	3.38	66,66,66,66	0
57	MG	YA	3002	1/1	0.98	0.38	3.36	32,32,32,32	0
57	MG	YA	3078	1/1	0.97	0.31	3.34	30,30,30,30	0
57	MG	RA	3160	1/1	0.97	0.32	3.29	62,62,62,62	0
57	MG	YA	3170	1/1	0.64	0.30	3.28	51,51,51,51	0
57	MG	RA	3134	1/1	0.94	0.34	3.28	42,42,42,42	0
57	MG	XA	1699	1/1	0.97	0.27	3.19	87,87,87,87	0
57	MG	YA	3258	1/1	0.97	0.26	3.15	33,33,33,33	0
57	MG	YA	3134	1/1	0.85	0.34	3.07	63,63,63,63	0
57	MG	RD	301	1/1	0.87	0.29	3.04	73,73,73,73	0
57	MG	RA	3017	1/1	0.94	0.24	3.03	47,47,47,47	0
57	MG	RA	3175	1/1	0.97	0.24	2.95	42,42,42,42	0
57	MG	XA	1634	1/1	0.93	0.37	2.95	67,67,67,67	0
57	MG	XA	1643	1/1	0.74	0.34	2.88	79,79,79,79	0
57	MG	RA	3074	1/1	0.96	0.24	2.84	40,40,40,40	0
57	MG	QA	1652	1/1	0.72	0.45	2.84	115,115,115,115	0
57	MG	RA	3042	1/1	0.97	0.26	2.81	46,46,46,46	0
57	MG	YA	3112	1/1	0.81	0.32	2.71	50,50,50,50	0
59	PPU	Z6	101	37/38	0.95	0.33	2.65	52,54,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3035	1/1	0.97	0.31	2.64	32,32,32,32	0
57	MG	YA	3065	1/1	0.96	0.23	2.59	40,40,40,40	0
57	MG	XF	201	1/1	0.88	0.34	2.57	104,104,104,104	0
57	MG	XA	1635	1/1	0.95	0.35	2.49	91,91,91,91	0
57	MG	YA	3226	1/1	0.91	0.26	2.46	57,57,57,57	0
57	MG	XA	1693	1/1	0.95	0.31	2.45	51,51,51,51	0
59	PPU	Z5	101	37/38	0.94	0.32	2.38	74,76,77,78	0
57	MG	XA	1701	1/1	0.88	0.30	2.36	151,151,151,151	0
57	MG	RA	3159	1/1	0.76	0.21	2.29	56,56,56,56	0
57	MG	RA	3211	1/1	0.91	0.30	2.29	68,68,68,68	0
57	MG	RA	3147	1/1	0.91	0.25	2.27	96,96,96,96	0
57	MG	YA	3008	1/1	0.96	0.22	2.26	39,39,39,39	0
57	MG	R8	101	1/1	0.75	0.35	2.18	50,50,50,50	0
57	MG	YA	3090	1/1	0.90	0.29	2.17	42,42,42,42	0
57	MG	RA	3243	1/1	0.96	0.32	2.15	88,88,88,88	0
57	MG	RA	3171	1/1	0.97	0.24	2.08	51,51,51,51	0
57	MG	YA	3161	1/1	0.79	0.28	2.01	68,68,68,68	0
57	MG	YA	3229	1/1	0.96	0.25	1.96	57,57,57,57	0
57	MG	RA	3116	1/1	0.98	0.25	1.92	91,91,91,91	0
57	MG	RA	3156	1/1	0.66	0.25	1.90	49,49,49,49	0
57	MG	YA	3173	1/1	0.79	0.24	1.89	40,40,40,40	0
57	MG	YA	3072	1/1	0.76	0.26	1.85	64,64,64,64	0
57	MG	YA	3032	1/1	0.96	0.33	1.85	47,47,47,47	0
57	MG	QA	1678	1/1	0.87	0.37	1.67	109,109,109,109	0
57	MG	RA	3181	1/1	0.89	0.21	1.66	88,88,88,88	0
57	MG	XV	102	1/1	0.98	0.31	1.65	32,32,32,32	0
57	MG	RA	3202	1/1	0.90	0.23	1.56	56,56,56,56	0
57	MG	XA	1631	1/1	0.93	0.28	1.53	67,67,67,67	0
58	ZN	QD	301	1/1	0.93	0.32	1.53	115,115,115,115	0
57	MG	RA	3193	1/1	0.92	0.25	1.51	75,75,75,75	0
57	MG	YA	3042	1/1	0.92	0.33	1.50	39,39,39,39	0
57	MG	YA	3214	1/1	0.88	0.26	1.50	73,73,73,73	0
57	MG	RA	3021	1/1	0.99	0.29	1.48	39,39,39,39	0
57	MG	RA	3213	1/1	0.83	0.27	1.40	55,55,55,55	0
57	MG	RA	3191	1/1	0.92	0.24	1.27	54,54,54,54	0
57	MG	RA	3238	1/1	0.96	0.30	1.25	55,55,55,55	0
57	MG	YA	3014	1/1	0.98	0.33	1.05	34,34,34,34	0
57	MG	XA	1623	1/1	0.82	0.21	1.04	73,73,73,73	0
57	MG	RA	3120	1/1	0.98	0.26	1.02	57,57,57,57	0
57	MG	QM	201	1/1	0.56	0.69	0.98	113,113,113,113	0
57	MG	YA	3098	1/1	0.93	0.31	0.89	31,31,31,31	0
57	MG	YA	3023	1/1	0.97	0.25	0.87	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1651	1/1	0.94	0.35	0.83	102,102,102,102	0
57	MG	QA	1648	1/1	0.84	0.30	0.76	94,94,94,94	0
57	MG	RA	3019	1/1	0.98	0.27	0.74	38,38,38,38	0
57	MG	YA	3027	1/1	0.99	0.22	0.71	30,30,30,30	0
57	MG	QA	1629	1/1	0.96	0.17	0.62	60,60,60,60	0
57	MG	QA	1663	1/1	0.95	0.26	0.60	73,73,73,73	0
57	MG	YA	3034	1/1	0.88	0.34	0.59	64,64,64,64	0
57	MG	QA	1612	1/1	0.91	0.31	0.53	61,61,61,61	0
57	MG	YA	3276	1/1	0.95	0.24	0.45	39,39,39,39	0
57	MG	YA	3059	1/1	0.97	0.23	0.44	65,65,65,65	0
57	MG	QA	1675	1/1	0.91	0.22	0.43	72,72,72,72	0
57	MG	RA	3122	1/1	0.95	0.16	0.42	92,92,92,92	0
58	ZN	XD	301	1/1	0.97	0.32	0.35	103,103,103,103	0
57	MG	XA	1621	1/1	0.96	0.23	0.33	63,63,63,63	0
57	MG	YA	3180	1/1	0.74	0.23	0.22	109,109,109,109	0
57	MG	QA	1620	1/1	0.93	0.28	0.21	75,75,75,75	0
57	MG	RP	201	1/1	0.88	0.24	0.18	132,132,132,132	0
57	MG	RA	3126	1/1	0.98	0.22	0.16	51,51,51,51	0
57	MG	YA	3251	1/1	0.98	0.20	0.15	43,43,43,43	0
57	MG	RA	3187	1/1	0.90	0.14	0.13	94,94,94,94	0
57	MG	RA	3228	1/1	0.97	0.29	0.12	50,50,50,50	0
57	MG	XA	1624	1/1	0.97	0.20	0.09	66,66,66,66	0
57	MG	XA	1654	1/1	0.97	0.23	0.08	58,58,58,58	0
57	MG	YA	3136	1/1	0.75	0.21	0.01	60,60,60,60	0
57	MG	YA	3011	1/1	0.96	0.25	-0.02	26,26,26,26	0
57	MG	YA	3071	1/1	0.55	0.16	-0.13	46,46,46,46	0
57	MG	YA	3257	1/1	0.97	0.20	-0.15	48,48,48,48	0
57	MG	QA	1613	1/1	0.93	0.23	-0.16	75,75,75,75	0
57	MG	RA	3207	1/1	0.94	0.19	-0.30	52,52,52,52	0
57	MG	QA	1647	1/1	0.94	0.18	-0.32	118,118,118,118	0
57	MG	RA	3246	1/1	0.91	0.19	-0.35	39,39,39,39	0
57	MG	RA	3110	1/1	0.94	0.20	-0.37	67,67,67,67	0
57	MG	RA	3158	1/1	0.98	0.20	-0.37	68,68,68,68	0
57	MG	YA	3208	1/1	0.56	0.21	-0.37	80,80,80,80	0
57	MG	YA	3269	1/1	0.87	0.18	-0.38	59,59,59,59	0
57	MG	QA	1659	1/1	0.94	0.22	-0.39	66,66,66,66	0
57	MG	YA	3259	1/1	0.94	0.24	-0.40	39,39,39,39	0
57	MG	RA	3101	1/1	0.80	0.22	-0.40	61,61,61,61	0
57	MG	QA	1685	1/1	0.93	0.27	-0.42	127,127,127,127	0
57	MG	RA	3104	1/1	0.95	0.17	-0.53	42,42,42,42	0
57	MG	RA	3129	1/1	0.91	0.28	-0.56	42,42,42,42	0
57	MG	RA	3106	1/1	0.98	0.21	-0.60	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3124	1/1	0.96	0.21	-0.63	39,39,39,39	0
57	MG	QA	1640	1/1	0.82	0.20	-0.66	91,91,91,91	0
57	MG	QA	1650	1/1	0.83	0.13	-0.69	65,65,65,65	0
57	MG	RA	3064	1/1	0.94	0.18	-0.75	42,42,42,42	0
57	MG	YA	3225	1/1	0.68	0.16	-0.81	67,67,67,67	0
57	MG	YA	3151	1/1	0.97	0.19	-0.82	32,32,32,32	0
57	MG	RA	3151	1/1	0.50	0.19	-0.88	62,62,62,62	0
57	MG	RA	3183	1/1	0.94	0.19	-0.89	40,40,40,40	0
57	MG	RA	3071	1/1	0.97	0.20	-0.90	49,49,49,49	0
57	MG	RA	3130	1/1	0.90	0.11	-0.91	64,64,64,64	0
57	MG	RA	3162	1/1	0.77	0.13	-0.91	82,82,82,82	0
57	MG	XA	1641	1/1	0.98	0.17	-0.91	71,71,71,71	0
57	MG	RA	3234	1/1	0.96	0.16	-0.96	71,71,71,71	0
57	MG	RA	3200	1/1	0.65	0.17	-1.00	70,70,70,70	0
57	MG	XA	1620	1/1	0.99	0.17	-1.08	55,55,55,55	0
57	MG	QA	1686	1/1	0.86	0.23	-1.08	129,129,129,129	0
57	MG	QA	1687	1/1	0.82	0.23	-1.10	154,154,154,154	0
57	MG	QA	1631	1/1	0.82	0.14	-1.10	63,63,63,63	0
57	MG	R1	101	1/1	0.94	0.18	-1.11	58,58,58,58	0
58	ZN	QN	101	1/1	0.98	0.13	-1.12	149,149,149,149	0
57	MG	XA	1655	1/1	0.95	0.27	-1.12	63,63,63,63	0
57	MG	YA	3165	1/1	0.85	0.14	-1.15	72,72,72,72	0
57	MG	XA	1702	1/1	0.92	0.17	-1.15	74,74,74,74	0
57	MG	YA	3005	1/1	0.98	0.16	-1.15	38,38,38,38	0
57	MG	YA	3275	1/1	0.88	0.14	-1.18	32,32,32,32	0
57	MG	XA	1656	1/1	0.97	0.13	-1.19	92,92,92,92	0
58	ZN	XN	101	1/1	1.00	0.12	-1.27	115,115,115,115	0
57	MG	RA	3139	1/1	0.85	0.20	-1.30	74,74,74,74	0
57	MG	YA	3113	1/1	0.94	0.20	-1.31	35,35,35,35	0
57	MG	YB	201	1/1	0.86	0.09	-1.35	100,100,100,100	0
57	MG	RA	3127	1/1	0.98	0.14	-1.40	44,44,44,44	0
57	MG	RA	3247	1/1	0.79	0.20	-1.43	88,88,88,88	0
57	MG	Y1	101	1/1	0.91	0.14	-1.51	58,58,58,58	0
57	MG	YA	3163	1/1	0.96	0.15	-1.73	67,67,67,67	0
57	MG	XA	1636	1/1	0.87	0.14	-1.75	73,73,73,73	0
57	MG	RA	3152	1/1	0.80	0.13	-1.76	80,80,80,80	0
57	MG	RA	3022	1/1	0.95	0.17	-1.86	40,40,40,40	0
57	MG	YA	3156	1/1	0.96	0.17	-1.90	37,37,37,37	0
57	MG	XA	1611	1/1	0.96	0.12	-2.02	51,51,51,51	0
57	MG	XA	1627	1/1	0.85	0.12	-2.05	54,54,54,54	0
57	MG	QA	1615	1/1	0.88	0.13	-2.13	100,100,100,100	0
57	MG	RA	3148	1/1	0.94	0.15	-2.26	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3111	1/1	0.99	0.11	-2.52	33,33,33,33	0
57	MG	XA	1609	1/1	0.94	0.17	-2.56	46,46,46,46	0
57	MG	XA	1690	1/1	0.92	0.11	-2.60	98,98,98,98	0
57	MG	QA	1609	1/1	0.96	0.12	-2.62	61,61,61,61	0
57	MG	YA	3172	1/1	0.93	0.12	-2.69	65,65,65,65	0
57	MG	YA	3070	1/1	0.92	0.14	-2.80	30,30,30,30	0
57	MG	YA	3184	1/1	0.90	0.13	-2.88	57,57,57,57	0
57	MG	YA	3004	1/1	0.97	0.11	-2.91	37,37,37,37	0
57	MG	RA	3079	1/1	0.96	0.11	-3.00	62,62,62,62	0
57	MG	YA	3016	1/1	0.89	0.15	-3.13	30,30,30,30	0
57	MG	QA	1656	1/1	0.97	0.10	-3.21	78,78,78,78	0
57	MG	RA	3025	1/1	0.80	0.16	-3.23	39,39,39,39	0
57	MG	RA	3133	1/1	0.92	0.12	-3.37	46,46,46,46	0
57	MG	QA	1644	1/1	0.98	0.09	-3.56	62,62,62,62	0
57	MG	QA	1630	1/1	0.91	0.12	-3.82	111,111,111,111	0
57	MG	QA	1607	1/1	0.98	0.13	-3.91	71,71,71,71	0
57	MG	XA	1626	1/1	0.82	0.13	-4.04	49,49,49,49	0
57	MG	RA	3073	1/1	0.96	0.11	-4.13	49,49,49,49	0
57	MG	XA	1646	1/1	0.92	0.10	-4.51	97,97,97,97	0
57	MG	YA	3079	1/1	0.93	0.10	-5.13	53,53,53,53	0
57	MG	YA	3162	1/1	0.97	0.09	-5.20	67,67,67,67	0
57	MG	YA	3104	1/1	0.91	0.09	-6.06	41,41,41,41	0
57	MG	YA	3141	1/1	0.94	0.11	-6.22	38,38,38,38	0
57	MG	XA	1663	1/1	0.93	0.17	-	127,127,127,127	0
57	MG	QA	1666	1/1	0.94	0.22	-	97,97,97,97	0
57	MG	QA	1674	1/1	0.06	1.19	-	97,97,97,97	0
57	MG	XA	1645	1/1	0.92	0.40	-	51,51,51,51	0
57	MG	YA	3177	1/1	0.77	0.77	-	48,48,48,48	0
57	MG	YA	3142	1/1	0.93	0.14	-	42,42,42,42	0
57	MG	YA	3122	1/1	0.92	0.26	-	42,42,42,42	0
57	MG	YA	3123	1/1	0.94	0.57	-	31,31,31,31	0
57	MG	QA	1653	1/1	0.94	0.15	-	115,115,115,115	0
57	MG	YA	3154	1/1	0.96	0.33	-	53,53,53,53	0
57	MG	YA	3149	1/1	0.89	0.10	-	84,84,84,84	0
57	MG	YA	3018	1/1	0.90	0.75	-	71,71,71,71	0
57	MG	RA	3214	1/1	0.96	0.42	-	65,65,65,65	0
57	MG	YA	3092	1/1	0.96	0.44	-	46,46,46,46	0
57	MG	YA	3045	1/1	0.81	0.74	-	69,69,69,69	0
57	MG	YA	3085	1/1	0.95	0.35	-	37,37,37,37	0
57	MG	YA	3030	1/1	0.74	0.64	-	70,70,70,70	0
57	MG	RA	3223	1/1	0.68	0.47	-	60,60,60,60	0
57	MG	RA	3180	1/1	0.96	0.12	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1668	1/1	0.80	0.24	-	67,67,67,67	0
57	MG	XA	1678	1/1	0.90	0.97	-	79,79,79,79	0
57	MG	RA	3107	1/1	0.94	0.28	-	51,51,51,51	0
57	MG	XA	1687	1/1	0.93	0.23	-	104,104,104,104	0
57	MG	YA	3043	1/1	0.97	0.65	-	33,33,33,33	0
57	MG	YB	202	1/1	0.94	0.89	-	79,79,79,79	0
57	MG	YA	3176	1/1	0.96	0.16	-	47,47,47,47	0
57	MG	YA	3064	1/1	0.98	0.35	-	56,56,56,56	0
57	MG	QV	103	1/1	0.93	0.22	-	42,42,42,42	0
57	MG	RA	3190	1/1	0.88	0.13	-	81,81,81,81	0
57	MG	YA	3052	1/1	0.98	0.33	-	44,44,44,44	0
57	MG	XX	101	1/1	0.90	0.45	-	56,56,56,56	0
57	MG	QA	1657	1/1	0.75	0.80	-	89,89,89,89	0
57	MG	YA	3197	1/1	0.86	0.21	-	89,89,89,89	0
57	MG	YA	3091	1/1	0.99	0.38	-	76,76,76,76	0
57	MG	XA	1680	1/1	0.92	0.22	-	47,47,47,47	0
57	MG	YA	3189	1/1	0.62	1.07	-	62,62,62,62	0
57	MG	YA	3217	1/1	0.98	0.39	-	48,48,48,48	0
57	MG	QA	1641	1/1	0.95	0.18	-	57,57,57,57	0
57	MG	RA	3153	1/1	0.91	0.28	-	48,48,48,48	0
57	MG	RA	3102	1/1	0.94	0.12	-	50,50,50,50	0
57	MG	XA	1671	1/1	0.86	0.48	-	89,89,89,89	0
57	MG	RA	3220	1/1	0.88	0.51	-	36,36,36,36	0
57	MG	YA	3221	1/1	0.90	0.29	-	90,90,90,90	0
57	MG	YA	3190	1/1	0.94	0.21	-	60,60,60,60	0
57	MG	YA	3160	1/1	0.96	0.47	-	47,47,47,47	0
57	MG	RA	3248	1/1	0.91	0.66	-	69,69,69,69	0
57	MG	YA	3138	1/1	0.80	0.33	-	66,66,66,66	0
57	MG	YA	3167	1/1	0.91	0.27	-	69,69,69,69	0
57	MG	QA	1606	1/1	0.94	0.95	-	62,62,62,62	0
57	MG	XA	1644	1/1	0.87	0.31	-	84,84,84,84	0
57	MG	RA	3137	1/1	0.92	0.42	-	53,53,53,53	0
57	MG	RA	3131	1/1	0.94	0.23	-	65,65,65,65	0
57	MG	YA	3228	1/1	0.88	0.22	-	74,74,74,74	0
57	MG	YA	3054	1/1	0.91	0.40	-	46,46,46,46	0
57	MG	RA	3192	1/1	0.90	0.29	-	73,73,73,73	0
57	MG	YA	3039	1/1	0.92	0.14	-	26,26,26,26	0
57	MG	YA	3128	1/1	0.96	0.12	-	73,73,73,73	0
57	MG	QA	1655	1/1	0.65	0.91	-	93,93,93,93	0
57	MG	YA	3021	1/1	0.95	0.72	-	66,66,66,66	0
57	MG	YA	3271	1/1	0.96	0.35	-	54,54,54,54	0
57	MG	RA	3163	1/1	0.96	0.23	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3224	1/1	0.83	0.16	-	71,71,71,71	0
57	MG	YA	3047	1/1	0.89	0.77	-	76,76,76,76	0
57	MG	XA	1666	1/1	0.91	0.22	-	62,62,62,62	0
57	MG	YA	3183	1/1	0.97	0.14	-	82,82,82,82	0
57	MG	RA	3174	1/1	0.56	0.91	-	56,56,56,56	0
57	MG	RA	3027	1/1	0.98	0.30	-	46,46,46,46	0
57	MG	RA	3149	1/1	0.81	0.28	-	58,58,58,58	0
57	MG	XA	1670	1/1	0.93	0.49	-	67,67,67,67	0
57	MG	RA	3240	1/1	0.98	0.38	-	56,56,56,56	0
57	MG	RA	3188	1/1	0.76	0.16	-	97,97,97,97	0
57	MG	YA	3236	1/1	0.83	0.54	-	54,54,54,54	0
57	MG	YA	3169	1/1	0.94	0.15	-	44,44,44,44	0
57	MG	QA	1671	1/1	0.90	0.37	-	134,134,134,134	0
57	MG	YA	3244	1/1	0.96	0.89	-	64,64,64,64	0
57	MG	YA	3051	1/1	0.94	0.38	-	32,32,32,32	0
57	MG	YA	3093	1/1	0.91	0.56	-	32,32,32,32	0
57	MG	RA	3070	1/1	0.92	0.40	-	67,67,67,67	0
57	MG	XA	1664	1/1	0.80	0.34	-	100,100,100,100	0
57	MG	RA	3124	1/1	0.95	0.28	-	87,87,87,87	0
57	MG	XA	1647	1/1	0.52	0.66	-	94,94,94,94	0
57	MG	XA	1682	1/1	0.72	0.56	-	114,114,114,114	0
57	MG	QA	1677	1/1	0.95	0.21	-	69,69,69,69	0
57	MG	YA	3069	1/1	0.92	0.60	-	53,53,53,53	0
57	MG	YA	3129	1/1	0.59	0.31	-	33,33,33,33	0
57	MG	RA	3060	1/1	0.97	0.48	-	38,38,38,38	0
57	MG	XA	1698	1/1	0.64	0.58	-	64,64,64,64	0
57	MG	YA	3260	1/1	0.93	0.29	-	34,34,34,34	0
57	MG	XA	1691	1/1	0.95	0.12	-	145,145,145,145	0
57	MG	YA	3132	1/1	0.90	0.40	-	60,60,60,60	0
57	MG	YA	3075	1/1	0.94	0.41	-	41,41,41,41	0
57	MG	RA	3237	1/1	0.90	0.28	-	43,43,43,43	0
57	MG	QA	1662	1/1	0.93	0.33	-	62,62,62,62	0
57	MG	YA	3222	1/1	0.84	0.41	-	69,69,69,69	0
57	MG	YA	3061	1/1	0.96	0.37	-	39,39,39,39	0
57	MG	YA	3088	1/1	0.97	0.35	-	41,41,41,41	0
57	MG	RA	3113	1/1	0.96	0.53	-	48,48,48,48	0
57	MG	XA	1622	1/1	0.90	0.82	-	79,79,79,79	0
57	MG	RA	3030	1/1	0.98	0.64	-	47,47,47,47	0
57	MG	YA	3265	1/1	0.97	0.42	-	33,33,33,33	0
57	MG	RA	3235	1/1	0.93	0.20	-	80,80,80,80	0
57	MG	QA	1649	1/1	0.77	0.40	-	76,76,76,76	0
57	MG	XA	1652	1/1	0.82	0.17	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3148	1/1	0.88	0.29	-	51,51,51,51	0
57	MG	XA	1674	1/1	0.96	0.20	-	64,64,64,64	0
57	MG	RA	3128	1/1	0.94	0.30	-	68,68,68,68	0
57	MG	YA	3115	1/1	0.95	0.19	-	37,37,37,37	0
57	MG	RA	3227	1/1	0.83	0.57	-	50,50,50,50	0
57	MG	XA	1617	1/1	0.95	0.26	-	50,50,50,50	0
57	MG	RA	3061	1/1	0.94	0.21	-	70,70,70,70	0
57	MG	RA	3245	1/1	0.98	0.12	-	69,69,69,69	0
57	MG	RA	3143	1/1	0.99	0.56	-	54,54,54,54	0
57	MG	QA	1625	1/1	0.95	0.24	-	90,90,90,90	0
57	MG	RA	3132	1/1	0.80	0.19	-	79,79,79,79	0
57	MG	RA	3048	1/1	0.96	0.18	-	40,40,40,40	0
57	MG	RA	3053	1/1	0.95	0.60	-	49,49,49,49	0
57	MG	QA	1635	1/1	0.82	0.54	-	69,69,69,69	0
57	MG	RA	3184	1/1	0.86	0.31	-	66,66,66,66	0
57	MG	YA	3270	1/1	0.93	0.37	-	58,58,58,58	0
57	MG	RA	3242	1/1	0.79	0.45	-	57,57,57,57	0
57	MG	RA	3082	1/1	0.87	0.36	-	62,62,62,62	0
57	MG	QA	1638	1/1	0.97	0.20	-	71,71,71,71	0
57	MG	RA	3047	1/1	0.96	0.50	-	42,42,42,42	0
57	MG	RE	301	1/1	0.85	0.34	-	41,41,41,41	0
57	MG	YA	3125	1/1	0.91	0.24	-	32,32,32,32	0
57	MG	RA	3150	1/1	0.97	0.08	-	74,74,74,74	0
57	MG	YA	3147	1/1	0.93	0.14	-	64,64,64,64	0
57	MG	XA	1628	1/1	0.89	0.58	-	67,67,67,67	0
57	MG	RA	3208	1/1	0.87	0.20	-	79,79,79,79	0
57	MG	YA	3255	1/1	0.90	0.51	-	57,57,57,57	0
57	MG	XA	1689	1/1	0.90	0.50	-	89,89,89,89	0
57	MG	XA	1614	1/1	0.97	0.40	-	50,50,50,50	0
57	MG	RA	3121	1/1	0.98	0.13	-	85,85,85,85	0
57	MG	QA	1608	1/1	0.95	0.10	-	71,71,71,71	0
57	MG	RA	3005	1/1	0.91	1.03	-	81,81,81,81	0
57	MG	YA	3232	1/1	0.87	0.27	-	48,48,48,48	0
57	MG	YA	3159	1/1	0.90	0.29	-	37,37,37,37	0
57	MG	YA	3095	1/1	0.98	0.49	-	32,32,32,32	0
57	MG	XA	1672	1/1	0.96	0.85	-	69,69,69,69	0
57	MG	YA	3263	1/1	0.74	0.28	-	62,62,62,62	0
57	MG	YA	3152	1/1	0.75	0.35	-	68,68,68,68	0
57	MG	QV	101	1/1	0.52	1.41	-	119,119,119,119	0
57	MG	YA	3212	1/1	0.93	0.45	-	59,59,59,59	0
57	MG	YA	3040	1/1	0.96	0.86	-	63,63,63,63	0
57	MG	XA	1686	1/1	0.80	0.62	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3007	1/1	0.89	0.26	-	38,38,38,38	0
57	MG	RA	3146	1/1	0.96	0.25	-	71,71,71,71	0
57	MG	RA	3195	1/1	0.89	0.97	-	52,52,52,52	0
57	MG	XA	1684	1/1	0.84	1.13	-	91,91,91,91	0
57	MG	RA	3176	1/1	0.89	0.52	-	52,52,52,52	0
57	MG	YA	3195	1/1	0.93	0.10	-	51,51,51,51	0
57	MG	RA	3215	1/1	0.91	0.53	-	76,76,76,76	0
57	MG	QA	1637	1/1	0.90	0.20	-	79,79,79,79	0
57	MG	QA	1665	1/1	0.92	1.15	-	84,84,84,84	0
57	MG	YA	3126	1/1	0.76	0.62	-	68,68,68,68	0
57	MG	RA	3209	1/1	0.87	0.32	-	53,53,53,53	0
57	MG	RA	3241	1/1	0.98	0.21	-	71,71,71,71	0
57	MG	YA	3022	1/1	0.98	0.53	-	29,29,29,29	0
57	MG	QA	1643	1/1	0.78	0.39	-	89,89,89,89	0
57	MG	YA	3082	1/1	0.94	0.54	-	41,41,41,41	0
57	MG	RA	3201	1/1	0.90	0.78	-	55,55,55,55	0
57	MG	QA	1654	1/1	0.97	0.11	-	86,86,86,86	0
57	MG	YA	3253	1/1	0.94	0.94	-	58,58,58,58	0
57	MG	YA	3268	1/1	0.85	0.42	-	74,74,74,74	0
57	MG	QA	1623	1/1	0.71	0.67	-	79,79,79,79	0
57	MG	QA	1603	1/1	0.90	0.63	-	69,69,69,69	0
57	MG	YA	3106	1/1	0.95	0.53	-	52,52,52,52	0
57	MG	YA	3192	1/1	0.97	0.90	-	31,31,31,31	0
57	MG	RA	3091	1/1	0.92	0.58	-	54,54,54,54	0
57	MG	QA	1621	1/1	0.96	0.66	-	102,102,102,102	0
57	MG	YB	205	1/1	0.97	0.19	-	170,170,170,170	0
57	MG	RA	3186	1/1	0.75	0.25	-	60,60,60,60	0
57	MG	YA	3231	1/1	0.74	0.26	-	43,43,43,43	0
57	MG	YA	3109	1/1	0.99	0.22	-	36,36,36,36	0
57	MG	QF	201	1/1	0.89	0.15	-	77,77,77,77	0
57	MG	YA	3245	1/1	0.89	0.34	-	35,35,35,35	0
57	MG	RA	3164	1/1	0.90	0.27	-	60,60,60,60	0
57	MG	XA	1605	1/1	0.79	0.90	-	60,60,60,60	0
57	MG	RA	3115	1/1	0.95	0.14	-	56,56,56,56	0
57	MG	YA	3105	1/1	0.97	0.20	-	60,60,60,60	0
57	MG	QA	1681	1/1	0.89	0.45	-	64,64,64,64	0
57	MG	YA	3188	1/1	0.98	0.22	-	61,61,61,61	0
57	MG	RA	3173	1/1	0.93	0.22	-	77,77,77,77	0
57	MG	XA	1612	1/1	0.98	0.08	-	50,50,50,50	0
57	MG	QA	1669	1/1	0.92	0.26	-	94,94,94,94	0
57	MG	R5	101	1/1	0.81	0.33	-	38,38,38,38	0
57	MG	YA	3120	1/1	0.74	0.45	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1606	1/1	0.91	0.48	-	85,85,85,85	0
57	MG	RA	3125	1/1	0.97	0.14	-	52,52,52,52	0
57	MG	YA	3114	1/1	0.88	0.46	-	75,75,75,75	0
57	MG	RA	3055	1/1	0.93	0.40	-	40,40,40,40	0
57	MG	XA	1625	1/1	0.88	0.23	-	53,53,53,53	0
57	MG	RA	3168	1/1	0.97	0.16	-	60,60,60,60	0
57	MG	XA	1601	1/1	0.95	0.78	-	74,74,74,74	0
57	MG	RA	3161	1/1	0.74	0.79	-	38,38,38,38	0
57	MG	QA	1646	1/1	0.89	0.11	-	91,91,91,91	0
57	MG	YA	3081	1/1	0.98	0.40	-	37,37,37,37	0
57	MG	XA	1604	1/1	0.91	0.81	-	83,83,83,83	0
57	MG	RA	3028	1/1	0.88	0.28	-	46,46,46,46	0
57	MG	YA	3246	1/1	0.95	0.40	-	44,44,44,44	0
57	MG	XA	1697	1/1	0.76	0.55	-	61,61,61,61	0
57	MG	YA	3234	1/1	0.94	0.50	-	45,45,45,45	0
57	MG	YA	3206	1/1	0.95	0.26	-	53,53,53,53	0
57	MG	QA	1634	1/1	0.92	0.09	-	62,62,62,62	0
57	MG	RA	3088	1/1	0.97	0.61	-	51,51,51,51	0
57	MG	QA	1639	1/1	0.96	0.14	-	59,59,59,59	0
57	MG	QA	1672	1/1	0.98	0.18	-	56,56,56,56	0
57	MG	XA	1681	1/1	0.58	1.69	-	98,98,98,98	0
57	MG	RA	3239	1/1	0.99	0.21	-	52,52,52,52	0
57	MG	RA	3229	1/1	0.93	0.20	-	60,60,60,60	0
57	MG	QA	1611	1/1	0.93	0.29	-	60,60,60,60	0
57	MG	RA	3075	1/1	0.95	0.52	-	52,52,52,52	0
57	MG	YA	3066	1/1	0.90	0.56	-	45,45,45,45	0
57	MG	YA	3203	1/1	0.93	0.23	-	43,43,43,43	0
57	MG	YA	3252	1/1	0.94	0.56	-	29,29,29,29	0
57	MG	YE	301	1/1	0.92	0.47	-	35,35,35,35	0
57	MG	XA	1679	1/1	0.89	0.70	-	47,47,47,47	0
57	MG	RA	3219	1/1	0.85	1.04	-	78,78,78,78	0
57	MG	YA	3155	1/1	0.91	0.40	-	46,46,46,46	0
57	MG	YA	3117	1/1	0.97	0.12	-	32,32,32,32	0
57	MG	RA	3072	1/1	0.95	0.49	-	58,58,58,58	0
57	MG	XA	1630	1/1	0.92	0.48	-	57,57,57,57	0
57	MG	YA	3164	1/1	0.96	0.47	-	76,76,76,76	0
57	MG	YA	3116	1/1	0.84	0.66	-	70,70,70,70	0
57	MG	RA	3203	1/1	0.94	0.28	-	52,52,52,52	0
57	MG	YA	3230	1/1	0.97	0.29	-	43,43,43,43	0
57	MG	YA	3213	1/1	0.76	0.63	-	72,72,72,72	0
57	MG	RA	3037	1/1	0.93	0.37	-	56,56,56,56	0
57	MG	XA	1660	1/1	0.78	0.26	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	XA	1692	1/1	0.87	0.39	-	66,66,66,66	0
57	MG	RA	3225	1/1	0.79	0.38	-	44,44,44,44	0
57	MG	YA	3062	1/1	0.98	0.56	-	72,72,72,72	0
57	MG	YA	3247	1/1	0.90	0.53	-	31,31,31,31	0
57	MG	RA	3090	1/1	0.99	0.39	-	53,53,53,53	0
57	MG	YA	3218	1/1	0.96	0.14	-	60,60,60,60	0
57	MG	RA	3172	1/1	0.91	0.24	-	66,66,66,66	0
57	MG	RA	3221	1/1	0.88	0.11	-	62,62,62,62	0
57	MG	YA	3046	1/1	0.91	0.52	-	59,59,59,59	0
57	MG	RA	3222	1/1	0.89	0.73	-	50,50,50,50	0
57	MG	RA	3140	1/1	0.59	0.50	-	83,83,83,83	0
57	MG	XA	1677	1/1	0.90	0.99	-	103,103,103,103	0
57	MG	RA	3032	1/1	0.94	1.09	-	77,77,77,77	0
57	MG	Y0	101	1/1	0.38	0.52	-	49,49,49,49	0
57	MG	XA	1639	1/1	0.95	0.26	-	49,49,49,49	0
57	MG	XV	101	1/1	0.91	0.27	-	49,49,49,49	0
57	MG	RA	3044	1/1	0.93	0.43	-	42,42,42,42	0
57	MG	RA	3182	1/1	0.89	0.34	-	62,62,62,62	0
57	MG	YA	3146	1/1	0.94	0.19	-	43,43,43,43	0
57	MG	RA	3165	1/1	0.89	0.34	-	42,42,42,42	0
57	MG	RA	3007	1/1	0.81	0.70	-	62,62,62,62	0
57	MG	YA	3157	1/1	0.88	0.18	-	67,67,67,67	0
57	MG	YA	3144	1/1	0.77	0.81	-	49,49,49,49	0
57	MG	Y5	101	1/1	0.94	0.15	-	31,31,31,31	0
57	MG	YA	3178	1/1	0.89	0.66	-	48,48,48,48	0
57	MG	RA	3217	1/1	0.91	0.55	-	58,58,58,58	0
57	MG	XA	1640	1/1	0.99	0.56	-	73,73,73,73	0
57	MG	YA	3012	1/1	0.77	0.86	-	63,63,63,63	0
57	MG	RA	3003	1/1	0.86	0.74	-	96,96,96,96	0
57	MG	RA	3136	1/1	0.45	0.42	-	81,81,81,81	0
57	MG	QA	1645	1/1	0.92	0.34	-	58,58,58,58	0
57	MG	YA	3254	1/1	0.94	0.65	-	34,34,34,34	0
57	MG	XA	1657	1/1	0.87	0.54	-	52,52,52,52	0
57	MG	RA	3100	1/1	0.97	0.40	-	41,41,41,41	0
57	MG	RA	3185	1/1	0.95	0.48	-	84,84,84,84	0
57	MG	YA	3194	1/1	0.89	0.24	-	45,45,45,45	0
57	MG	XV	103	1/1	0.93	0.44	-	30,30,30,30	0
57	MG	YA	3168	1/1	0.80	0.16	-	65,65,65,65	0
57	MG	XA	1667	1/1	0.75	0.38	-	54,54,54,54	0
57	MG	XA	1683	1/1	0.97	0.16	-	57,57,57,57	0
57	MG	XA	1675	1/1	0.85	0.59	-	57,57,57,57	0
57	MG	YA	3133	1/1	0.96	0.38	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3210	1/1	0.96	0.22	-	81,81,81,81	0
57	MG	YA	3153	1/1	0.87	0.33	-	80,80,80,80	0
57	MG	XA	1658	1/1	0.94	0.42	-	123,123,123,123	0
57	MG	YA	3216	1/1	0.94	0.38	-	33,33,33,33	0
57	MG	QH	201	1/1	0.46	0.15	-	94,94,94,94	0
57	MG	QA	1661	1/1	0.86	0.94	-	72,72,72,72	0
57	MG	RA	3194	1/1	0.83	0.35	-	59,59,59,59	0
57	MG	RA	3197	1/1	0.67	0.88	-	81,81,81,81	0
57	MG	RA	3166	1/1	0.91	0.27	-	60,60,60,60	0
57	MG	RA	3046	1/1	0.95	0.82	-	53,53,53,53	0
57	MG	RA	3069	1/1	0.91	0.75	-	49,49,49,49	0
57	MG	RA	3066	1/1	0.96	0.49	-	46,46,46,46	0
57	MG	YA	3055	1/1	0.97	0.35	-	43,43,43,43	0
57	MG	QA	1679	1/1	0.90	0.94	-	106,106,106,106	0
57	MG	XA	1662	1/1	0.96	0.89	-	80,80,80,80	0
57	MG	XA	1629	1/1	0.88	0.14	-	67,67,67,67	0
57	MG	XA	1642	1/1	0.91	0.69	-	90,90,90,90	0
57	MG	QA	1673	1/1	0.76	0.45	-	65,65,65,65	0
57	MG	YA	3001	1/1	0.95	0.61	-	31,31,31,31	0
57	MG	RA	3013	1/1	0.91	0.87	-	73,73,73,73	0
57	MG	QA	1632	1/1	0.88	0.71	-	62,62,62,62	0
57	MG	RA	3103	1/1	0.91	0.17	-	54,54,54,54	0
57	MG	RA	3117	1/1	0.90	0.30	-	41,41,41,41	0
57	MG	RA	3231	1/1	0.96	0.73	-	45,45,45,45	0
57	MG	YA	3264	1/1	0.76	0.49	-	81,81,81,81	0
57	MG	YA	3200	1/1	0.73	0.28	-	63,63,63,63	0
57	MG	YA	3028	1/1	0.97	0.21	-	31,31,31,31	0
57	MG	RA	3039	1/1	0.92	0.37	-	36,36,36,36	0
57	MG	YA	3020	1/1	0.90	0.55	-	42,42,42,42	0
57	MG	XA	1695	1/1	0.87	0.31	-	57,57,57,57	0
57	MG	RA	3051	1/1	0.95	0.51	-	39,39,39,39	0
57	MG	RA	3057	1/1	0.99	0.48	-	47,47,47,47	0
57	MG	YA	3272	1/1	0.88	0.31	-	51,51,51,51	0
57	MG	QA	1624	1/1	0.91	0.39	-	83,83,83,83	0
57	MG	RA	3108	1/1	0.93	0.70	-	70,70,70,70	0
57	MG	YA	3077	1/1	0.92	0.40	-	35,35,35,35	0
57	MG	YA	3201	1/1	0.86	0.38	-	66,66,66,66	0
57	MG	YA	3121	1/1	0.90	0.34	-	61,61,61,61	0
57	MG	YA	3096	1/1	0.97	0.35	-	29,29,29,29	0
57	MG	RA	3045	1/1	0.98	0.50	-	47,47,47,47	0
57	MG	RA	3016	1/1	0.96	0.31	-	43,43,43,43	0
57	MG	QA	1626	1/1	0.91	0.25	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	QA	1628	1/1	0.86	0.56	-	84,84,84,84	0
57	MG	YA	3063	1/1	0.73	0.32	-	75,75,75,75	0
57	MG	RA	3177	1/1	0.78	0.36	-	62,62,62,62	0
57	MG	YA	3158	1/1	0.39	1.08	-	105,105,105,105	0
57	MG	YA	3019	1/1	0.92	0.31	-	35,35,35,35	0
57	MG	RA	3029	1/1	0.95	0.53	-	42,42,42,42	0
57	MG	RA	3170	1/1	0.77	0.68	-	100,100,100,100	0
57	MG	YA	3010	1/1	0.94	0.39	-	37,37,37,37	0
57	MG	YA	3174	1/1	0.75	0.10	-	70,70,70,70	0
57	MG	QA	1682	1/1	0.82	0.77	-	77,77,77,77	0
57	MG	RA	3236	1/1	0.91	0.65	-	39,39,39,39	0
57	MG	XA	1608	1/1	0.94	0.54	-	46,46,46,46	0
57	MG	YA	3102	1/1	0.94	0.26	-	79,79,79,79	0
57	MG	RA	3081	1/1	0.99	0.25	-	38,38,38,38	0
57	MG	QA	1622	1/1	0.86	0.55	-	104,104,104,104	0
57	MG	RA	3077	1/1	0.99	0.43	-	67,67,67,67	0
57	MG	QA	1610	1/1	0.93	0.41	-	66,66,66,66	0
57	MG	XA	1676	1/1	0.84	0.96	-	73,73,73,73	0
57	MG	YA	3182	1/1	0.95	0.17	-	79,79,79,79	0
57	MG	XA	1661	1/1	0.87	0.48	-	54,54,54,54	0
57	MG	YA	3237	1/1	0.84	0.49	-	41,41,41,41	0
57	MG	YA	3198	1/1	0.91	0.19	-	40,40,40,40	0
57	MG	XA	1653	1/1	0.89	0.38	-	56,56,56,56	0
57	MG	XA	1673	1/1	0.63	0.40	-	58,58,58,58	0
57	MG	RA	3138	1/1	0.89	0.87	-	78,78,78,78	0
57	MG	YB	204	1/1	0.93	0.46	-	82,82,82,82	0
57	MG	RA	3244	1/1	0.94	0.60	-	64,64,64,64	0
57	MG	YA	3273	1/1	0.58	0.49	-	68,68,68,68	0
57	MG	RA	3145	1/1	0.96	0.30	-	58,58,58,58	0
57	MG	XA	1685	1/1	0.97	0.13	-	92,92,92,92	0
57	MG	YA	3205	1/1	0.95	0.22	-	58,58,58,58	0
57	MG	RA	3179	1/1	0.82	0.20	-	69,69,69,69	0
57	MG	QA	1688	1/1	0.93	0.30	-	96,96,96,96	0
57	MG	QA	1680	1/1	0.86	0.27	-	123,123,123,123	0
57	MG	XA	1615	1/1	0.96	0.27	-	58,58,58,58	0
57	MG	YA	3118	1/1	0.94	0.56	-	50,50,50,50	0
57	MG	RA	3089	1/1	0.81	0.45	-	61,61,61,61	0
57	MG	RA	3018	1/1	0.98	0.45	-	39,39,39,39	0
57	MG	YA	3097	1/1	0.96	0.40	-	68,68,68,68	0
57	MG	YA	3101	1/1	0.99	0.80	-	58,58,58,58	0
57	MG	RB	201	1/1	0.92	0.12	-	166,166,166,166	0
57	MG	XA	1637	1/1	0.99	0.20	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	YA	3186	1/1	0.84	0.28	-	74,74,74,74	0
57	MG	YA	3150	1/1	0.93	1.17	-	30,30,30,30	0
57	MG	YA	3076	1/1	0.97	0.51	-	28,28,28,28	0
57	MG	YA	3202	1/1	0.92	0.24	-	64,64,64,64	0
57	MG	QA	1601	1/1	0.76	0.82	-	67,67,67,67	0
57	MG	RA	3095	1/1	0.97	0.37	-	44,44,44,44	0
57	MG	QA	1618	1/1	0.90	1.12	-	119,119,119,119	0
57	MG	XA	1694	1/1	0.76	0.69	-	74,74,74,74	0
57	MG	RA	3043	1/1	0.96	0.40	-	62,62,62,62	0
57	MG	XA	1688	1/1	0.55	0.39	-	66,66,66,66	0
57	MG	YA	3145	1/1	0.89	0.59	-	49,49,49,49	0
57	MG	RA	3212	1/1	0.45	0.33	-	84,84,84,84	0
57	MG	YA	3235	1/1	0.85	0.31	-	31,31,31,31	0
57	MG	QA	1667	1/1	0.84	0.46	-	102,102,102,102	0
57	MG	YA	3130	1/1	0.97	0.19	-	78,78,78,78	0
57	MG	RA	3226	1/1	0.81	0.33	-	48,48,48,48	0
57	MG	YA	3083	1/1	0.93	0.43	-	51,51,51,51	0
57	MG	YA	3274	1/1	0.89	0.40	-	75,75,75,75	0
57	MG	RA	3041	1/1	0.96	0.33	-	44,44,44,44	0
57	MG	RA	3189	1/1	0.89	0.18	-	45,45,45,45	0
57	MG	RA	3109	1/1	0.88	0.61	-	89,89,89,89	0
57	MG	YA	3266	1/1	0.90	1.28	-	67,67,67,67	0
57	MG	QA	1676	1/1	0.78	0.52	-	111,111,111,111	0
57	MG	RB	202	1/1	0.91	0.99	-	118,118,118,118	0
57	MG	XA	1638	1/1	0.92	0.62	-	48,48,48,48	0
57	MG	YA	3029	1/1	0.91	0.37	-	32,32,32,32	0
57	MG	RA	3001	1/1	0.85	0.85	-	48,48,48,48	0
57	MG	RA	3111	1/1	0.96	0.27	-	75,75,75,75	0
57	MG	YA	3171	1/1	0.98	0.68	-	46,46,46,46	0
57	MG	YA	3185	1/1	0.82	0.38	-	88,88,88,88	0
57	MG	QA	1633	1/1	0.93	0.52	-	128,128,128,128	0
57	MG	YA	3060	1/1	0.88	0.66	-	65,65,65,65	0
57	MG	RA	3023	1/1	0.98	0.30	-	55,55,55,55	0
57	MG	YA	3087	1/1	0.88	0.57	-	43,43,43,43	0
57	MG	RA	3142	1/1	0.92	0.36	-	62,62,62,62	0
57	MG	RA	3118	1/1	0.92	0.20	-	59,59,59,59	0
57	MG	YA	3196	1/1	0.99	0.09	-	46,46,46,46	0
57	MG	QA	1627	1/1	0.98	0.13	-	62,62,62,62	0
57	MG	RA	3169	1/1	0.83	0.17	-	38,38,38,38	0
57	MG	YA	3241	1/1	0.99	0.27	-	38,38,38,38	0
57	MG	QA	1689	1/1	0.86	0.18	-	93,93,93,93	0
57	MG	YA	3239	1/1	0.94	1.16	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	RA	3135	1/1	0.92	0.46	-	44,44,44,44	0
57	MG	RA	3155	1/1	0.92	0.27	-	63,63,63,63	0
57	MG	R0	101	1/1	0.56	0.43	-	68,68,68,68	0
57	MG	XA	1649	1/1	0.93	0.34	-	82,82,82,82	0
57	MG	YA	3067	1/1	0.98	0.18	-	43,43,43,43	0
57	MG	YA	3219	1/1	0.87	0.35	-	57,57,57,57	0
57	MG	RA	3205	1/1	0.58	0.63	-	76,76,76,76	0
57	MG	XA	1610	1/1	0.94	0.60	-	72,72,72,72	0
57	MG	RA	3206	1/1	0.91	0.35	-	68,68,68,68	0
57	MG	RA	3011	1/1	0.87	0.38	-	39,39,39,39	0
57	MG	RA	3112	1/1	0.85	0.17	-	37,37,37,37	0
57	MG	YA	3215	1/1	0.91	0.34	-	50,50,50,50	0
57	MG	YA	3262	1/1	0.98	0.18	-	30,30,30,30	0
57	MG	RA	3010	1/1	0.82	0.62	-	43,43,43,43	0
57	MG	YA	3084	1/1	0.74	0.38	-	63,63,63,63	0
57	MG	YA	3127	1/1	0.95	0.43	-	73,73,73,73	0
57	MG	YA	3003	1/1	0.94	0.34	-	30,30,30,30	0
57	MG	XA	1650	1/1	0.81	0.90	-	80,80,80,80	0
57	MG	RA	3020	1/1	0.97	0.48	-	38,38,38,38	0
57	MG	QA	1604	1/1	0.70	0.80	-	74,74,74,74	0
57	MG	RA	3224	1/1	0.93	0.85	-	64,64,64,64	0
57	MG	XY	101	1/1	0.75	0.16	-	53,53,53,53	0
57	MG	YA	3220	1/1	0.90	0.31	-	37,37,37,37	0
57	MG	RA	3067	1/1	0.85	0.15	-	61,61,61,61	0
57	MG	YA	3140	1/1	0.96	0.32	-	58,58,58,58	0
57	MG	YA	3211	1/1	0.89	0.18	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.