wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 06:35 pm GMT

PDB ID	:	5E7K
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and cognate tRNALys in the A-site
Authors	:	Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on	:	2015-10-12
Resolution	:	3.20 Å(reported)

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

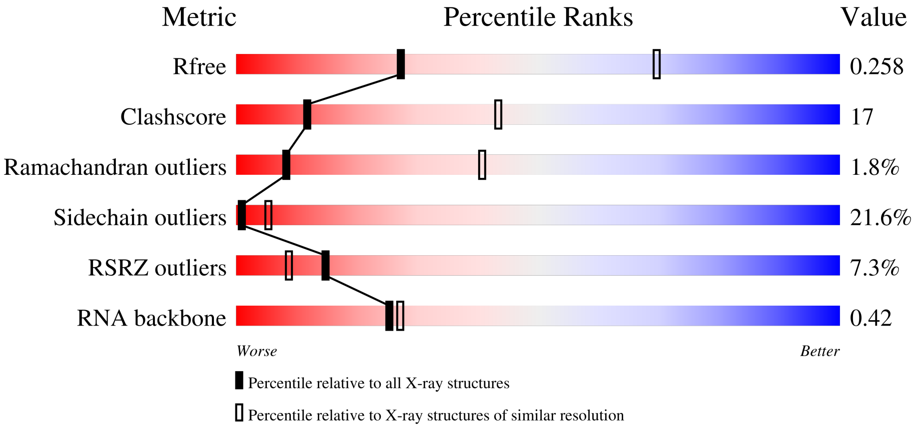
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

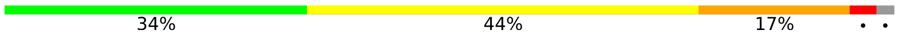
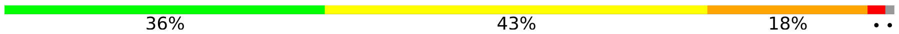
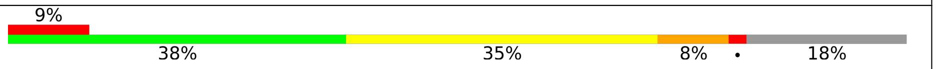
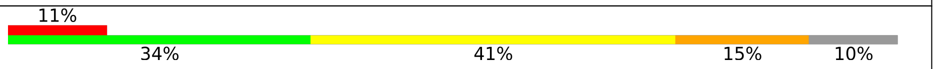
The reported resolution of this entry is 3.20 Å.

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

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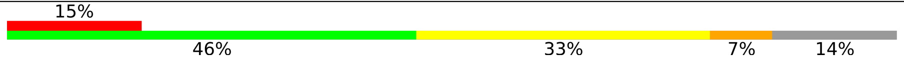
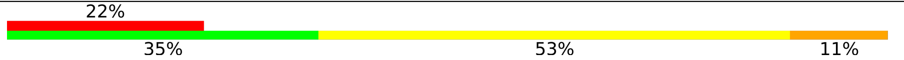
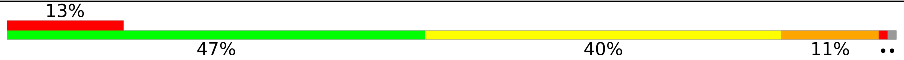
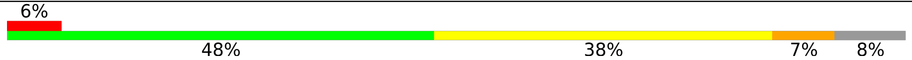
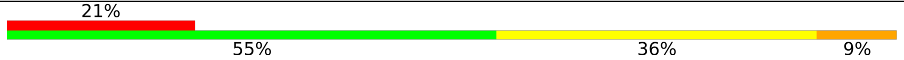
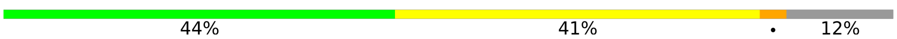
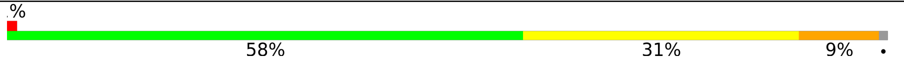
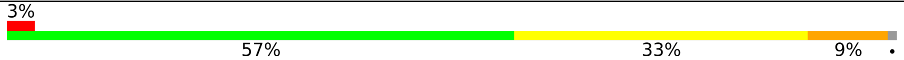
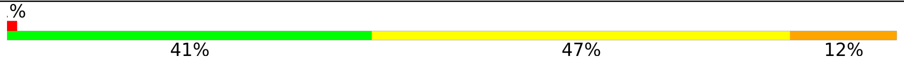
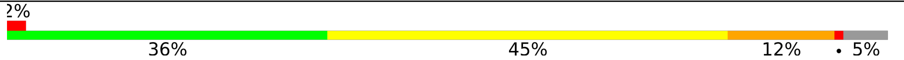
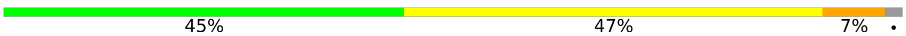
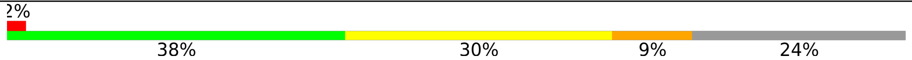
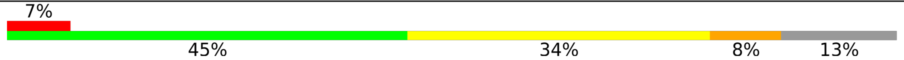
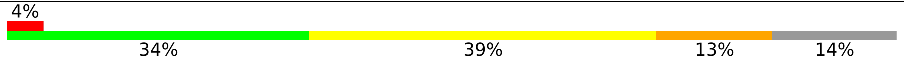
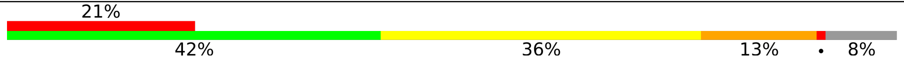
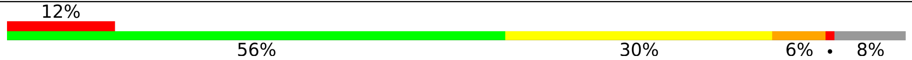
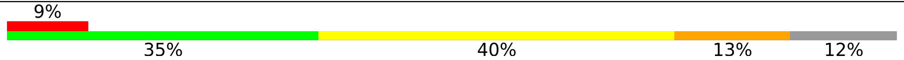
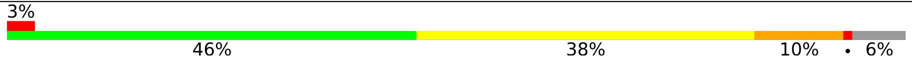
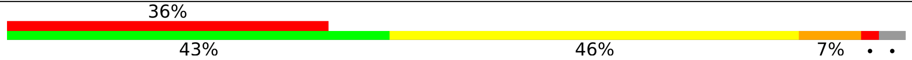
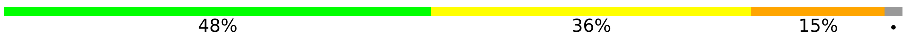
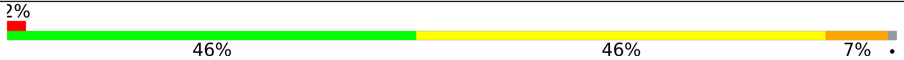
Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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Mol	Chain	Length	Quality of chain
15	6I	89	47% 42% 9% •
16	7A	88	2% 47% 38% 11% 5%
16	7I	88	8% 30% 53% 11% 6%
17	8A	105	3% 53% 32% 9% 6%
17	8I	105	% 48% 37% 10% 5%
18	9A	88	25% 36% 30% 10% 24%
18	9I	88	19% 34% 32% 10% • 23%
19	AA	93	15% 28% 31% 8% 33%
19	AI	93	6% 38% 40% 9% • 13%
20	BA	106	% 54% 32% 6% • 7%
20	BI	106	% 36% 45% 10% 8%
21	1B	27	19% 33% 48% 19%
21	1F	27	52% 33% 15%
22	1K	75	% 21% 49% 20% • 5%
23	2K	77	35% 31% 25% 9%
23	2L	77	32% 42% 21% 5%
24	3K	76	% 16% 47% 32% 5%
25	4K	27	4% 22% 22% 26% 30%
25	4L	27	26% 15% 26% 33%
26	14	2917	% 32% 41% 21% • •
26	1H	2917	27% 40% 24% 6% •
27	16	122	% 44% 33% 16% 7%
27	1J	122	31% 43% 23% •
28	71	229	15% 24% 26% 8% 42%
28	79	229	15% 7% • 75%

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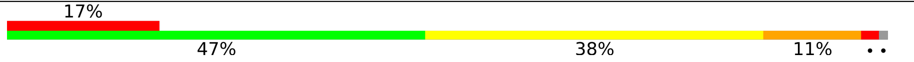
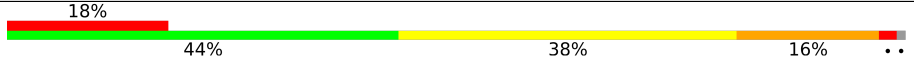
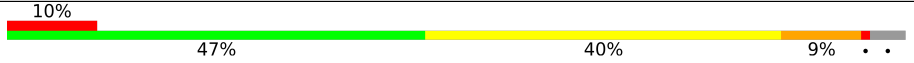
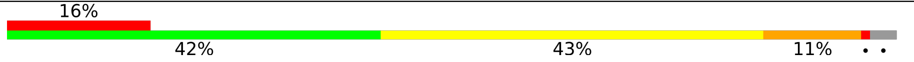
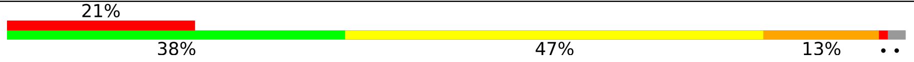
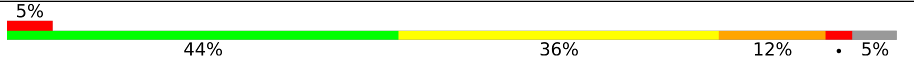
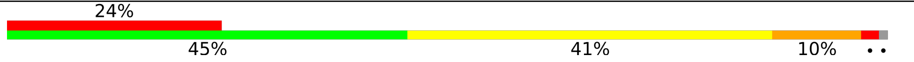
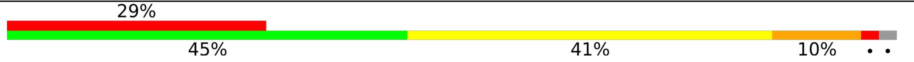
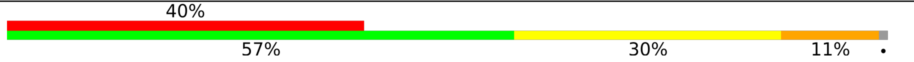
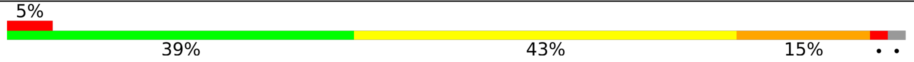
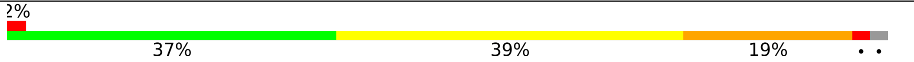
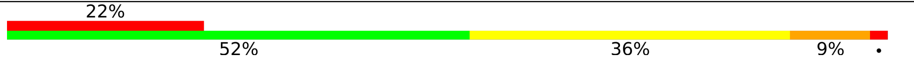
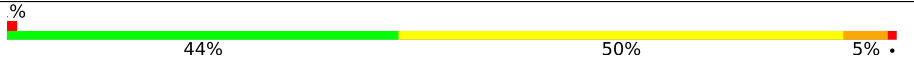
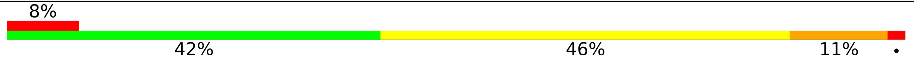
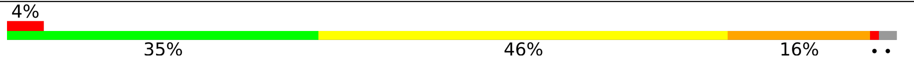
Mol	Chain	Length	Quality of chain
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	

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Mol	Chain	Length	Quality of chain
41	B8	146	% 42% 37% 11% • 9%
42	85	118	28% 49% 41% 7% • •
42	C8	118	3% 56% 28% 12% • •
43	95	101	68% 40% 43% 12% 5% •
43	D8	101	6% 46% 33% 18% • •
44	A5	113	2% 58% 32% 9% •
44	E8	113	4% 57% 31% 12% •
45	B5	96	14% 53% 28% 17% •
45	F8	96	10% 53% 40% 6% •
46	C5	110	8% 28% 46% 17% • 5%
46	G8	110	47% 30% 16% • 5%
47	D5	206	28% 23% 32% 8% 36%
47	H8	206	32% 37% 33% 12% • 17%
48	E5	85	5% 53% 29% 8% 9%
48	I8	85	4% 47% 36% 6% 11%
49	F5	98	2% 47% 38% 11% •
49	J8	98	2% 47% 36% 10% • •
50	G5	72	6% 35% 39% 12% 6% 8%
50	K8	72	3% 43% 36% 11% • 6%
51	H5	60	43% 55% 40% • •
51	L8	60	5% 52% 33% 12% •
52	M8	71	44% 20% 37% 8% • 34%
53	J5	60	55% 32% 7% 7%
53	N8	60	12% 38% 32% 10% 20%
54	L5	49	4% 57% 37% • •

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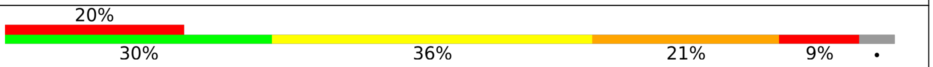
Mol	Chain	Length	Quality of chain
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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
58	MG	13	1603	-	-	-	X
58	MG	13	1630	-	-	-	X
58	MG	13	1641	-	-	-	X
58	MG	13	1644	-	-	-	X
58	MG	13	1653	-	-	-	X
58	MG	13	1659	-	-	-	X
58	MG	13	1672	-	-	-	X
58	MG	13	1689	-	-	-	X
58	MG	13	1694	-	-	-	X
58	MG	13	1695	-	-	-	X
58	MG	13	1704	-	-	-	X
58	MG	14	3017	-	-	-	X
58	MG	14	3018	-	-	-	X
58	MG	14	3019	-	-	-	X
58	MG	14	3029	-	-	-	X
58	MG	14	3034	-	-	-	X
58	MG	14	3037	-	-	-	X
58	MG	14	3052	-	-	-	X
58	MG	14	3068	-	-	-	X
58	MG	14	3073	-	-	-	X
58	MG	14	3080	-	-	-	X
58	MG	14	3085	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3108	-	-	-	X
58	MG	14	3117	-	-	-	X
58	MG	14	3129	-	-	-	X
58	MG	14	3144	-	-	-	X
58	MG	14	3150	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3153	-	-	-	X
58	MG	14	3155	-	-	-	X
58	MG	14	3181	-	-	-	X
58	MG	14	3182	-	-	-	X
58	MG	14	3183	-	-	-	X
58	MG	14	3185	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3188	-	-	-	X
58	MG	14	3190	-	-	-	X
58	MG	14	3191	-	-	-	X
58	MG	14	3227	-	-	-	X
58	MG	14	3229	-	-	-	X
58	MG	14	3234	-	-	-	X
58	MG	14	3243	-	-	-	X
58	MG	14	3250	-	-	-	X
58	MG	14	3251	-	-	-	X
58	MG	14	3257	-	-	-	X
58	MG	14	3259	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3261	-	-	-	X
58	MG	14	3264	-	-	-	X
58	MG	14	3265	-	-	-	X
58	MG	14	3268	-	-	-	X
58	MG	14	3269	-	-	-	X
58	MG	14	3280	-	-	-	X
58	MG	14	3282	-	-	-	X
58	MG	14	3288	-	-	-	X
58	MG	14	3293	-	-	-	X
58	MG	14	3297	-	-	-	X
58	MG	14	3302	-	-	-	X
58	MG	14	3304	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	14	3313	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1604	-	-	-	X
58	MG	1G	1649	-	-	-	X
58	MG	1G	1666	-	-	-	X
58	MG	1G	1672	-	-	-	X
58	MG	1H	3016	-	-	-	X
58	MG	1H	3024	-	-	-	X
58	MG	1H	3031	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3032	-	-	-	X
58	MG	1H	3033	-	-	-	X
58	MG	1H	3035	-	-	-	X
58	MG	1H	3036	-	-	-	X
58	MG	1H	3043	-	-	-	X
58	MG	1H	3087	-	-	-	X
58	MG	1H	3122	-	-	-	X
58	MG	1H	3142	-	-	-	X
58	MG	1H	3154	-	-	-	X
58	MG	1H	3167	-	-	-	X
58	MG	1H	3171	-	-	-	X
58	MG	1H	3175	-	-	-	X
58	MG	1H	3180	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3201	-	-	-	X
58	MG	1H	3207	-	-	-	X
58	MG	1H	3224	-	-	-	X
58	MG	1H	3228	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3268	-	-	-	X
58	MG	1H	3278	-	-	-	X
58	MG	1H	3279	-	-	-	X
58	MG	1H	3282	-	-	-	X
58	MG	1H	3284	-	-	-	X
58	MG	1H	3285	-	-	-	X
58	MG	1H	3288	-	-	-	X
58	MG	1H	3301	-	-	-	X
58	MG	1H	3309	-	-	-	X
58	MG	1H	3315	-	-	-	X
58	MG	1H	3324	-	-	-	X
58	MG	1H	3327	-	-	-	X
58	MG	1H	3328	-	-	-	X
58	MG	1H	3331	-	-	-	X
58	MG	1H	3342	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	2K	102	-	-	-	X
58	MG	2K	103	-	-	-	X
58	MG	2L	102	-	-	-	X
58	MG	E5	101	-	-	-	X
59	SF4	32	301	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 294444 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
			Total	C	N	O	P			
1	13	1496	32157	14313	5960	10388	1496	0	0	0
1	1G	1507	32391	14418	6004	10463	1506	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	231	1874	1199	334	336	5	0	0	0
2	12	210	1721	1100	309	308	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	1605	1011	313	280	1	0	0	0
3	22	196	1541	975	298	267	1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	3E	207	Total C N O S 1698 1064 338 289 7	0	0	0
4	32	208	Total C N O S 1702 1066 339 290 7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	4E	149	Total C N O S 1142 722 216 200 4	0	0	0
5	42	148	Total C N O S 1134 718 215 197 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	5E	100	Total C N O S 837 528 154 152 3	0	0	0
6	52	101	Total C N O S 842 531 155 153 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	6E	154	Total C N O S 1242 770 250 216 6	0	0	0
7	62	138	Total C N O S 1110 689 221 194 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	7E	138	Total C N O S 1115 705 215 192 3	0	0	0
8	72	137	Total C N O S 1107 700 214 191 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	8E	126	Total C N O 1000 634 196 170	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	82	121	Total C N O 953 605 186 162	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1I	91	Total C N O S 734 459 144 130 1	0	0	0
10	1A	80	Total C N O 646 403 129 114	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	2I	111	Total C N O S 823 512 154 154 3	0	0	0
11	2A	113	Total C N O S 835 520 156 156 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	3I	122	Total C N O S 956 603 193 159 1	0	0	0
12	3A	122	Total C N O S 956 603 193 159 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	4I	119	Total C N O S 942 582 194 164 2	0	0	0
13	4A	111	Total C N O S 893 552 183 156 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	5I	60	Total C N O S 491 312 104 71 4	0	0	0
14	5A	59	Total C N O S 486 309 103 70 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total 729	C 457	N 146	O 124	S 2	0	0	0
15	6A	88	Total 733	C 459	N 147	O 125	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total 700	C 443	N 139	O 117	S 1	0	0	0
16	7A	84	Total 705	C 446	N 140	O 118	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total 834	C 534	N 155	O 143	S 2	0	0	0
17	8A	99	Total 823	C 528	N 151	O 142	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total 549	C 352	N 105	O 92	0	0	0
18	9A	67	Total 544	C 349	N 104	O 91	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total 654	C 417	N 122	O 113	S 2	0	0	0
19	AA	62	Total 481	C 306	N 85	O 88	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total 746	C 461	N 157	O 126	S 2	0	0	0
20	BA	99	Total 762	C 470	N 162	O 128	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total 199	C 122	N 48	O 29	0	0	0
21	1B	22	Total 188	C 116	N 44	O 28	0	0	0

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	71	Total 1520	C 681	N 264	O 503	P 71	S 1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1K	?	-	G	deletion	GB 836716955

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total 1646	C 735	N 297	O 536	P 77	S 1	0	0	0
23	2L	77	Total 1646	C 735	N 297	O 536	P 77	S 1	0	0	0

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total 1611	C 721	N 281	O 534	P 75	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total 419	C 188	N 89	O 123	P 19	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	18	Total 397	C 178	N 84	O 117	P 18	0	0	0

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total 61028	C 27159	N 11418	O 19618	P 2833	0	0	0
26	14	2861	Total 61630	C 27429	N 11535	O 19806	P 2860	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total 1033	C 651	N 194	O 187	S 1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	79	57	Total C N O 456 283 91 82	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	11	273	Total C N O S 2120 1338 421 358 3	0	0	0
29	19	274	Total C N O S 2125 1341 422 359 3	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	21	203	Total C N O S 1558 985 298 269 6	0	0	0
30	29	204	Total C N O S 1563 988 299 270 6	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	31	202	Total C N O S 1585 1011 297 275 2	0	0	0
31	39	204	Total C N O S 1602 1022 299 279 2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	41	179	Total C N O S 1457 931 265 257 4	0	0	0
32	49	179	Total C N O S 1458 931 266 257 4	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	51	171	Total C N O S 1312 832 246 233 1	0	0	0
33	59	73	Total C N O 568 356 116 96	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	61	146	Total C N O S 1136 726 201 208 1	0	0	0
34	69	145	Total C N O S 1131 723 200 207 1	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	58	138	Total C N O S 1104 712 206 182 4	0	0	0
35	15	138	Total C N O S 1104 712 206 182 4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	68	122	Total C N O S 932 588 171 169 4	0	0	0
36	25	122	Total C N O S 932 588 171 169 4	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	78	147	Total C N O S 1122 698 229 192 3	0	0	0
37	35	147	Total C N O S 1122 698 229 192 3	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	88	141	Total C N O S 1113 709 210 187 7	0	0	0
38	45	138	Total C N O S 1099 702 208 183 6	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	98	118	967	604	203	159	1	0	0	0
39	55	118	967	604	203	159	1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	A8	111	881	556	176	149	0	0	0
40	65	110	876	553	175	148	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	B8	133	1109	691	228	189	1	0	0	0
41	75	133	1109	691	228	189	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	C8	115	950	603	199	147	1	0	0	0
42	85	116	959	608	201	149	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	D8	100	774	499	141	133	1	0	0	0
43	95	100	774	499	141	133	1	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	E8	112	890	560	175	153	2	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	A5	113	Total C N O S 899 566 177 154 2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	F8	95	Total C N O S 743 482 134 126 1	0	0	0
45	B5	94	Total C N O 735 477 133 125	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	G8	105	Total C N O S 796 513 150 128 5	0	0	0
46	C5	104	Total C N O S 794 510 152 127 5	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	H8	171	Total C N O S 1373 876 247 247 3	0	0	0
47	D5	132	Total C N O S 1074 691 193 188 2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	I8	76	Total C N O S 606 376 128 101 1	0	0	0
48	E5	77	Total C N O S 608 375 129 103 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	J8	94	Total C N O S 737 463 146 127 1	0	0	0
49	F5	94	Total C N O S 737 463 146 127 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	K8	68	568	352	115	100	1	0	0	0
50	G5	66	558	346	113	98	1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	L8	58	459	293	89	77	0	0	0
51	H5	58	459	293	89	77	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M8	47	366	234	61	66	5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	N8	48	369	229	75	60	5	0	0	0
53	J5	56	434	272	87	70	5	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	P8	47	401	246	99	54	2	0	0	0
54	L5	47	401	246	99	54	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	Q8	64	516	331	102	81	2	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	M5	64	Total C N O S 516 331 102 81 2	0	0	0

- Molecule 56 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	1L	73	Total C N O P S 1563 700 271 518 73 1	0	0	0

- Molecule 57 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	3L	76	Total C N O P 1612 722 281 534 75	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	132	Total Mg 132 132	0	0
58	1E	1	Total Mg 1 1	0	0
58	5E	1	Total Mg 1 1	0	0
58	1K	1	Total Mg 1 1	0	0
58	2K	3	Total Mg 3 3	0	0
58	3K	1	Total Mg 1 1	0	0
58	1H	467	Total Mg 467 467	0	0
58	16	9	Total Mg 9 9	0	0
58	21	2	Total Mg 2 2	0	0
58	41	1	Total Mg 1 1	0	0
58	78	1	Total Mg 1 1	0	0
58	88	1	Total Mg 1 1	0	0

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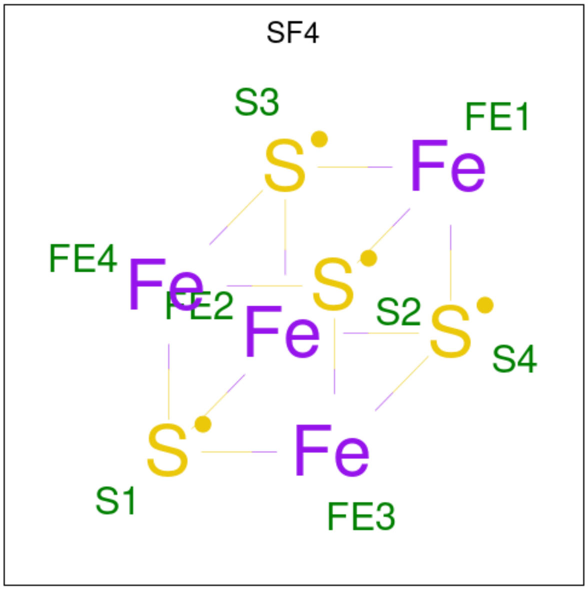
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	98	1	Total Mg 1 1	0	0
58	I8	3	Total Mg 3 3	0	0
58	J8	1	Total Mg 1 1	0	0
58	L8	1	Total Mg 1 1	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	90	Total Mg 90 90	0	0
58	6A	1	Total Mg 1 1	0	0
58	2L	2	Total Mg 2 2	0	0
58	14	399	Total Mg 399 399	0	0
58	1J	5	Total Mg 5 5	0	0
58	29	4	Total Mg 4 4	0	0
58	39	1	Total Mg 1 1	0	0
58	25	1	Total Mg 1 1	0	0
58	35	3	Total Mg 3 3	0	0
58	45	2	Total Mg 2 2	0	0
58	55	1	Total Mg 1 1	0	0
58	E5	1	Total Mg 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	3E	1	Total Fe S 8 4 4	0	0
59	32	1	Total Fe S 8 4 4	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	1	Total Zn 1 1	0	0
60	G8	1	Total Zn 1 1	0	0
60	5A	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	126	Total O 126 126	0	0
61	3I	2	Total O 2 2	0	0
61	5I	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1K	8	Total O 8 8	0	0
61	3K	1	Total O 1 1	0	0
61	4K	2	Total O 2 2	0	0
61	1H	629	Total O 629 629	0	0
61	16	29	Total O 29 29	0	0
61	11	7	Total O 7 7	0	0
61	21	4	Total O 4 4	0	0
61	31	9	Total O 9 9	0	0
61	58	2	Total O 2 2	0	0
61	78	7	Total O 7 7	0	0
61	88	1	Total O 1 1	0	0
61	B8	1	Total O 1 1	0	0
61	E8	2	Total O 2 2	0	0
61	F8	1	Total O 1 1	0	0
61	G8	1	Total O 1 1	0	0
61	I8	3	Total O 3 3	0	0
61	L8	2	Total O 2 2	0	0
61	1G	78	Total O 78 78	0	0
61	32	1	Total O 1 1	0	0
61	5A	2	Total O 2 2	0	0
61	14	417	Total O 417 417	0	0

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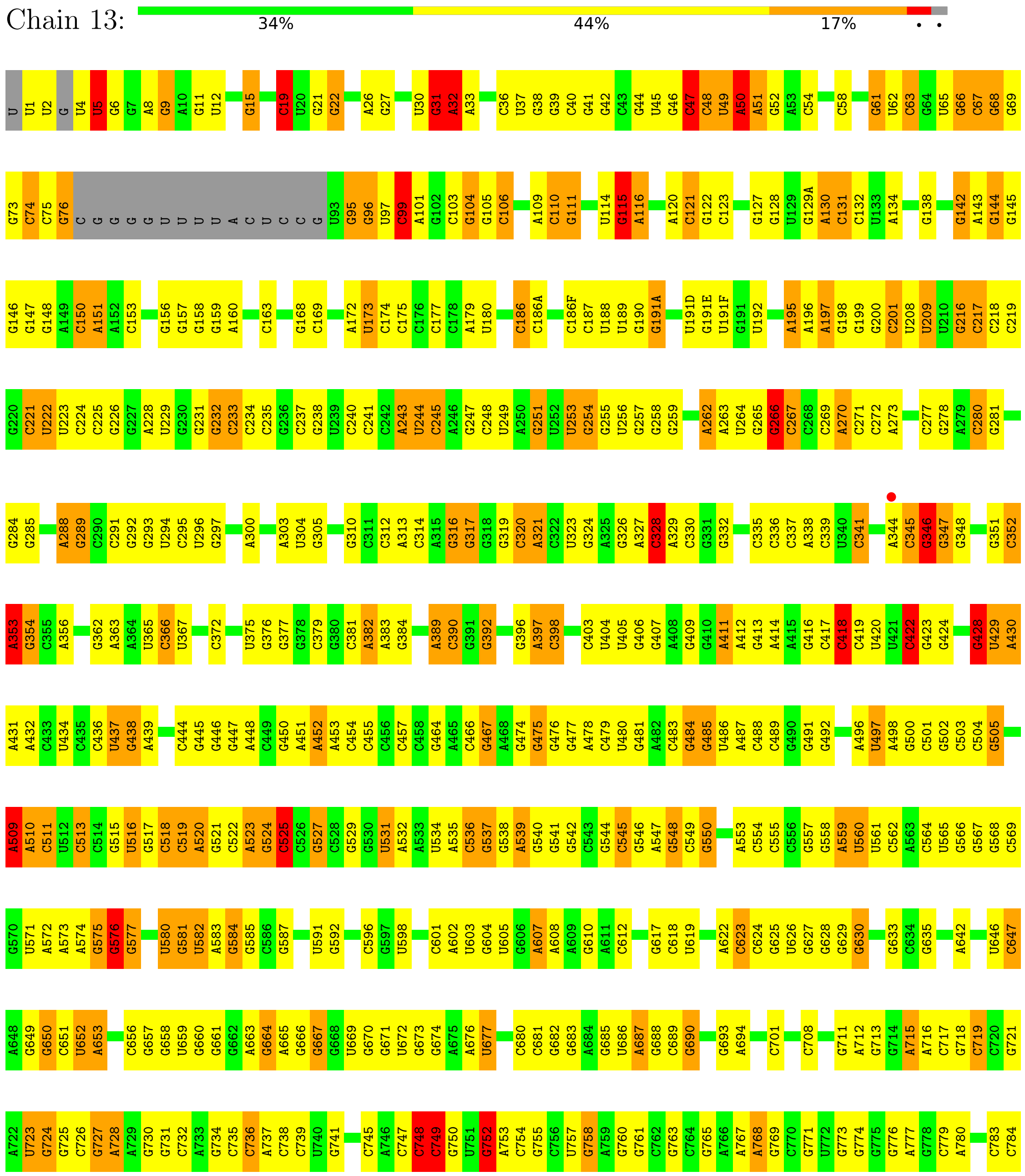
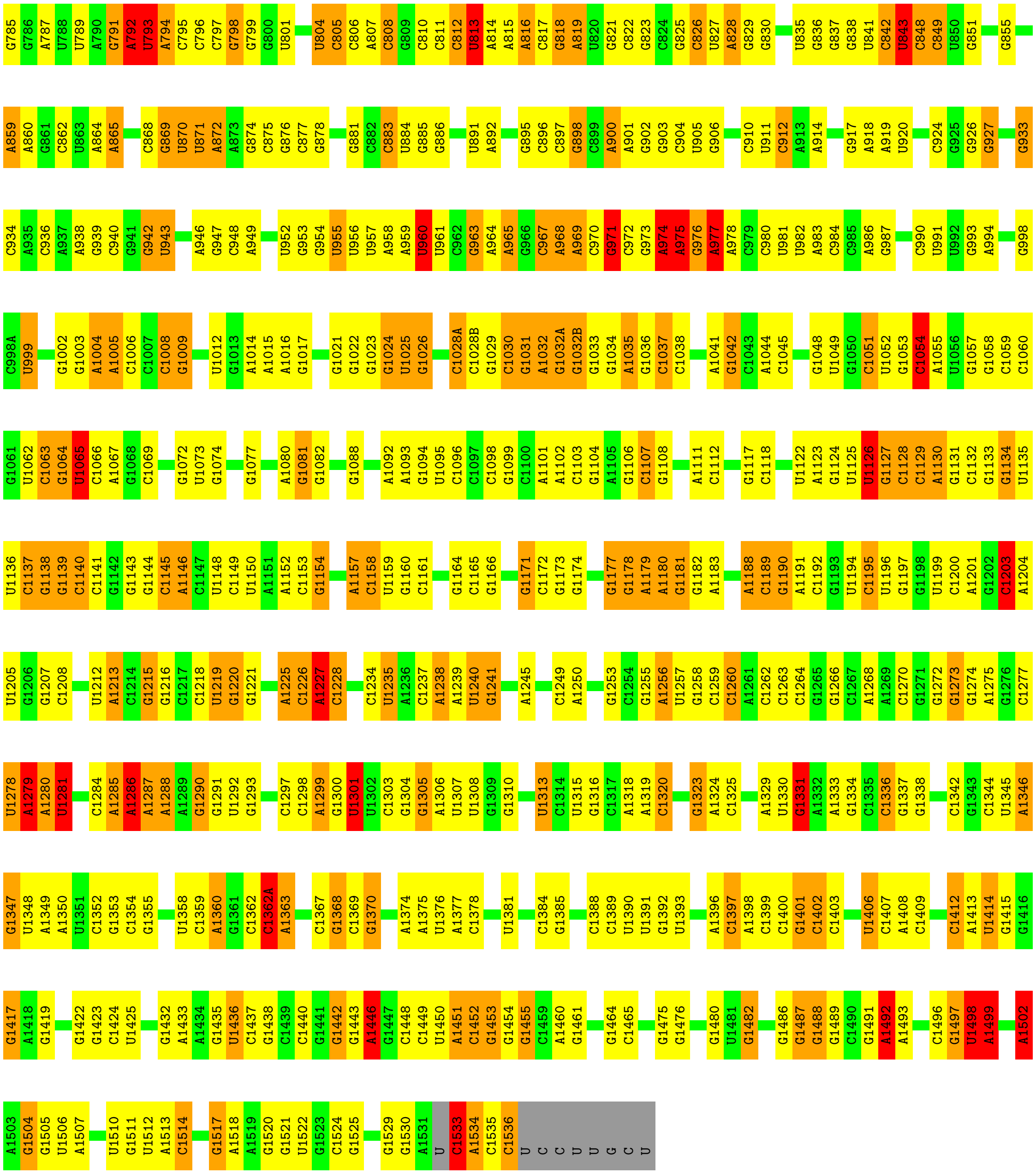
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1J	6	Total O 6 6	0	0
61	19	8	Total O 8 8	0	0
61	29	2	Total O 2 2	0	0
61	39	5	Total O 5 5	0	0
61	35	1	Total O 1 1	0	0
61	55	1	Total O 1 1	0	0
61	A5	1	Total O 1 1	0	0
61	H5	2	Total O 2 2	0	0

3 Residue-property plots ⓘ

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

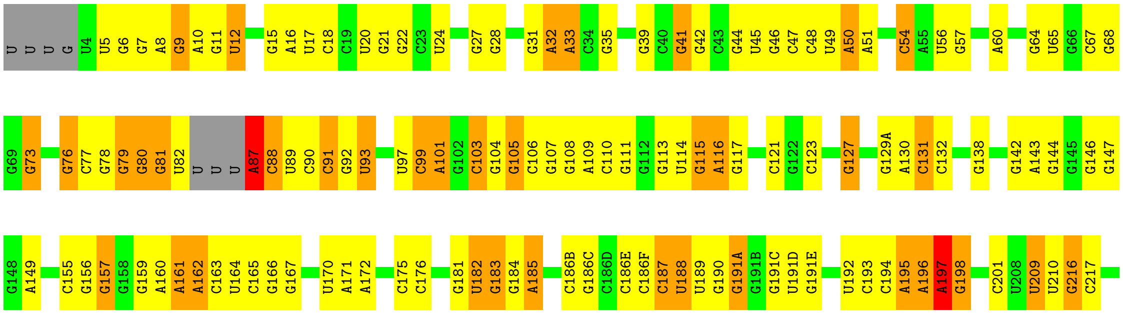
- Molecule 1: 16S rRNA

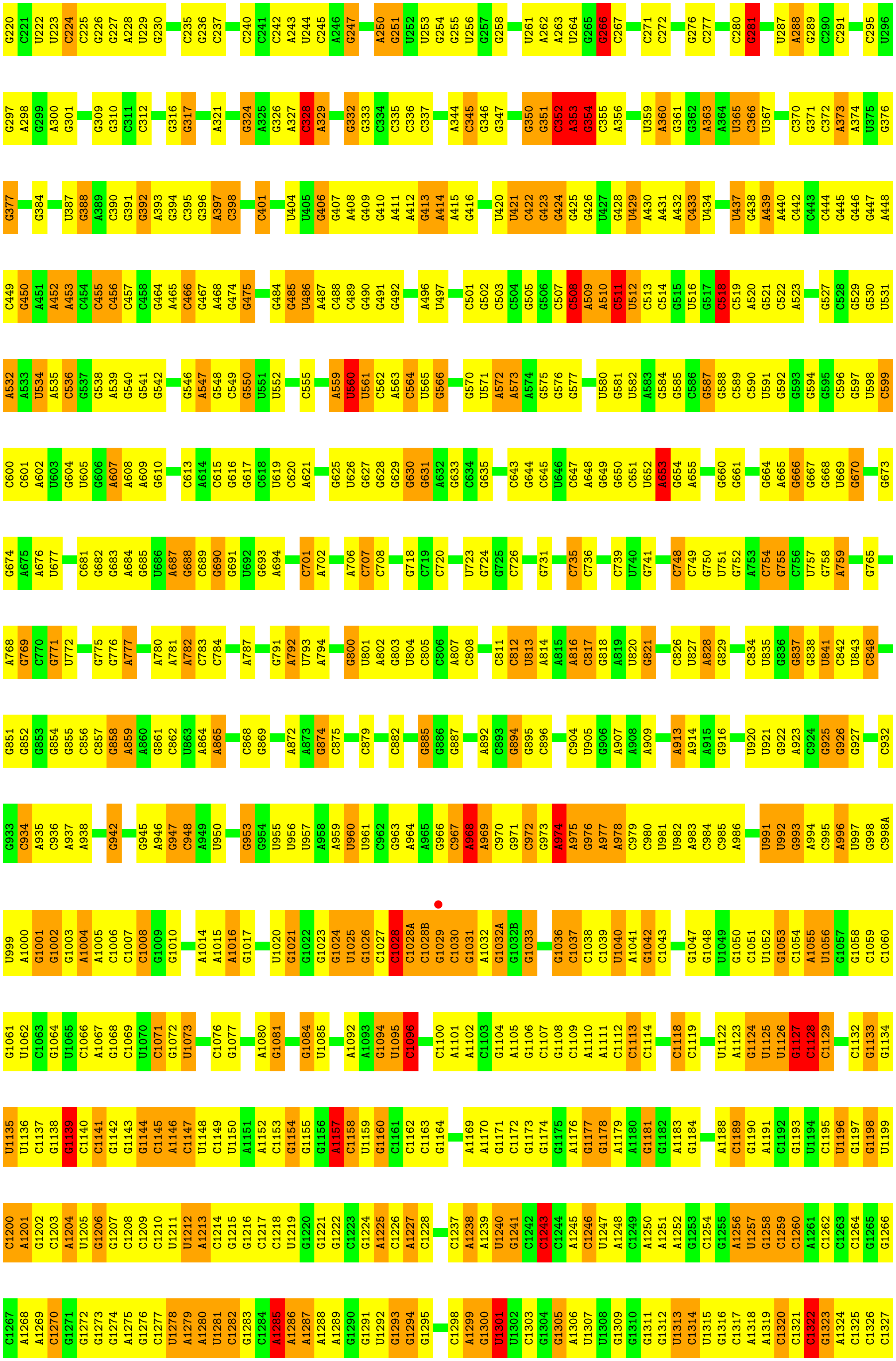




- Molecule 1: 16S rRNA

Chain 1G:

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G297 A298 G299 A300 G301 G309 G310 C311 C312 G316 G317 A321 G324 A325 G326 A327 C328 A329 G332 G333 C334 C335 C336 C337 A344 C345 G346 G347 G350 G351 C352 A353 G354 C355 A356 U359 A360 G361 G362 A363 A364 U365 C366 U367 C370 G371 C372 A373 A374 U375 G376
G377 G384 U387 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 C398 C401 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 U437 G438 A439 A440 C442 C443 C444 G445 G446 G447 A448
C449 G450 A451 A452 A453 C454 C455 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G484 G485 U486 A487 C488 C489 G490 G491 G492 A496 U497 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G527 C528 G529 G530 U531
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C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 G610 C613 A614 C615 G616 G617 C618 U619 C620 A621 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 G660 G661 G664 A665 G666 G667 G668 U669 G670 G673
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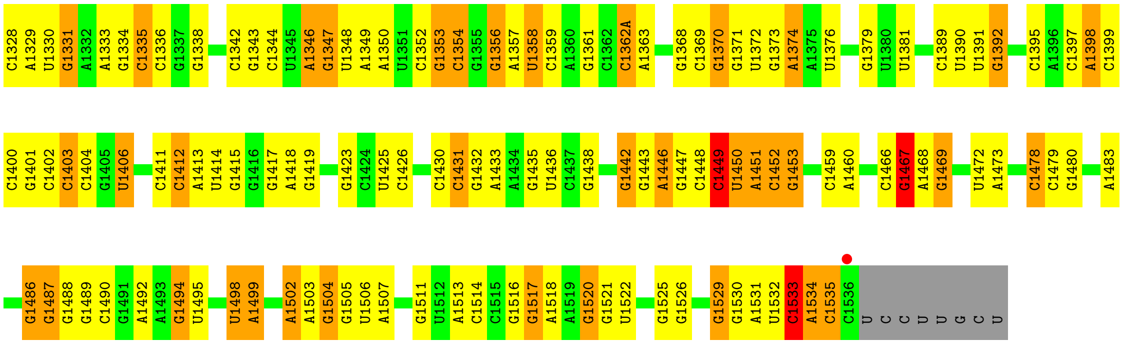
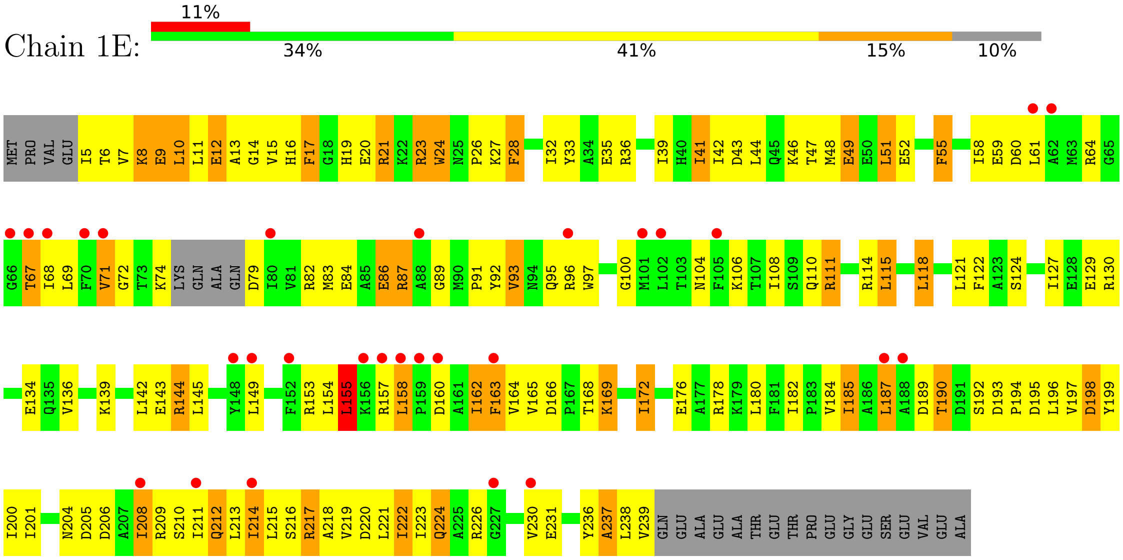
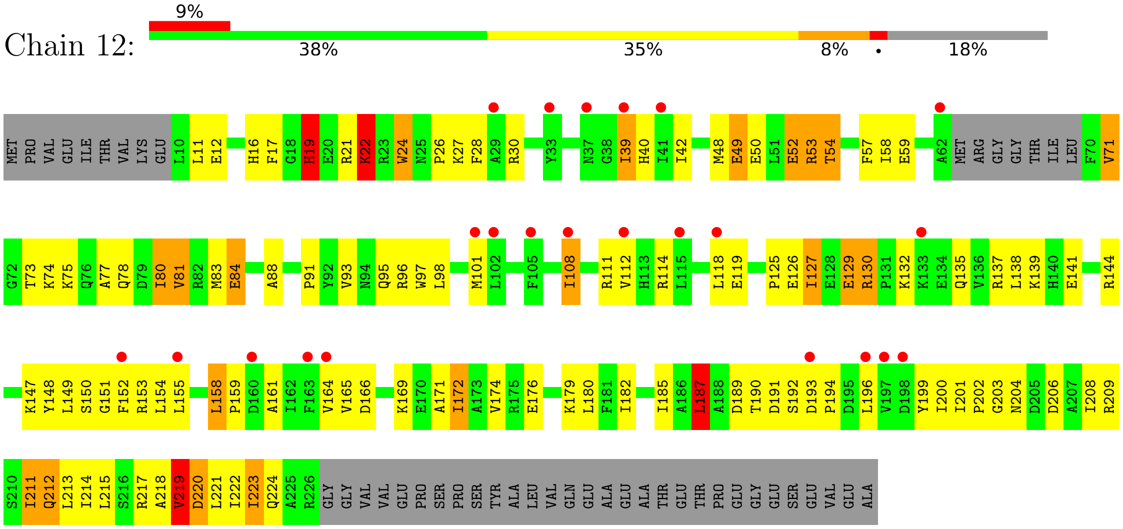
G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C868 G869 A872 A873 G874 C875 C879 C882 G885 G886 G887 A892 C893 G894 G895 C896 C904 U905 G906 A907 A908 A909 A913 A914 A915 G916 U920 U921 G922 A923 C924 G925 G926 G927 C932
G933 C934 A935 C936 A937 A938 G942 G945 A946 G947 C948 A949 U950 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 U991 U992 G993 A994 C995 A996 U997 G998 C998A
U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 A1014 A1015 A1016 G1017 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060
G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 C1076 G1077 A1080 G1081 G1084 U1085 A1092 A1093 G1094 U1095 C1096 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1118 C1119 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 C1132 G1133 G1134
U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199
C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266
C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327



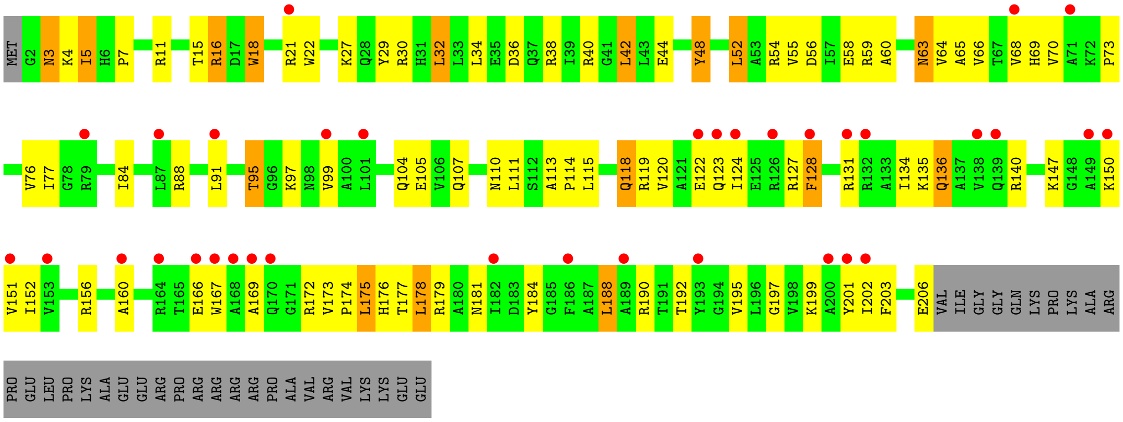
- Molecule 2: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S2

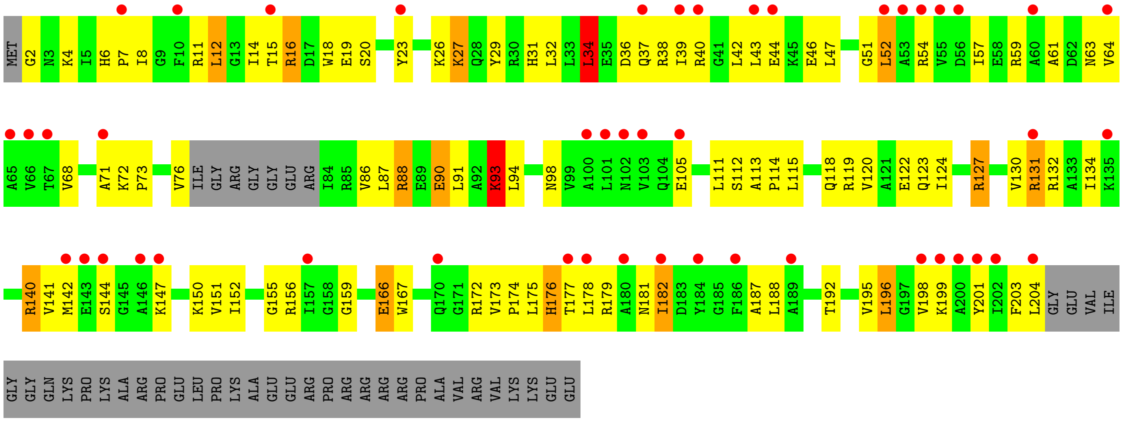


- Molecule 3: 30S ribosomal protein S3



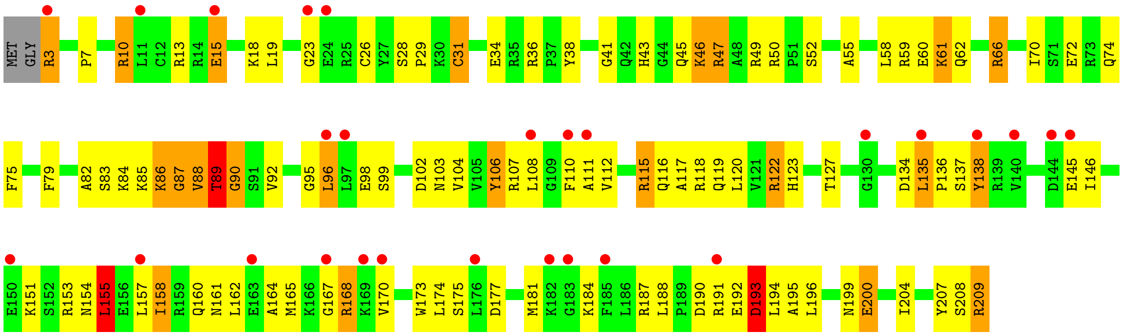
- Molecule 3: 30S ribosomal protein S3

Chain 22:



- Molecule 4: 30S ribosomal protein S4

Chain 3E:



- Molecule 4: 30S ribosomal protein S4

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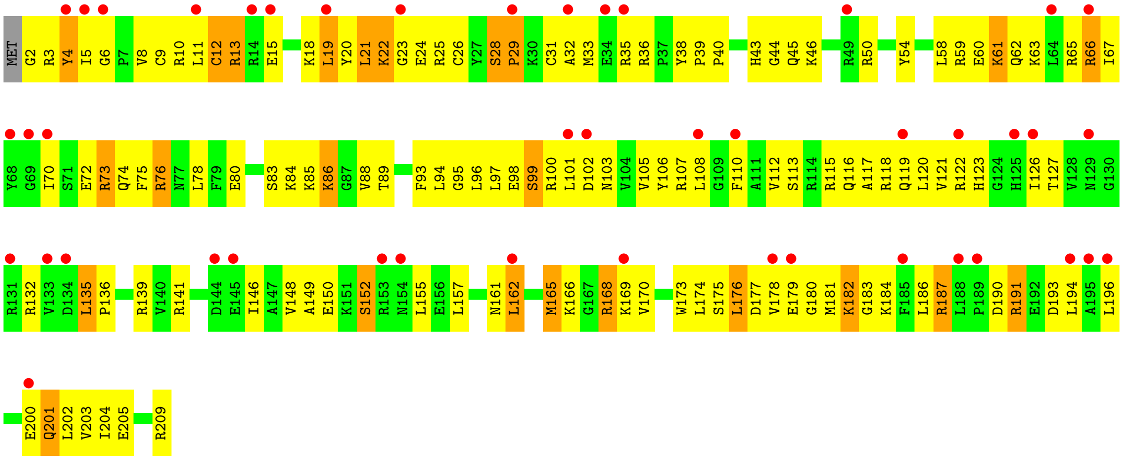
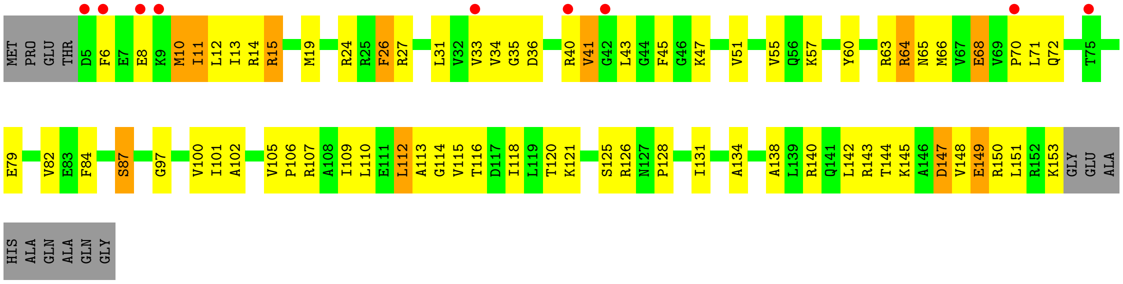


- Molecule 5: 30S ribosomal protein S5

Chain 4E:



- Molecule 5: 30S ribosomal protein S5

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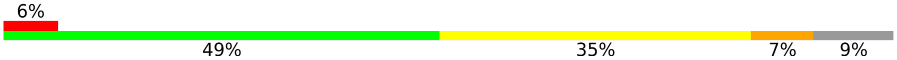
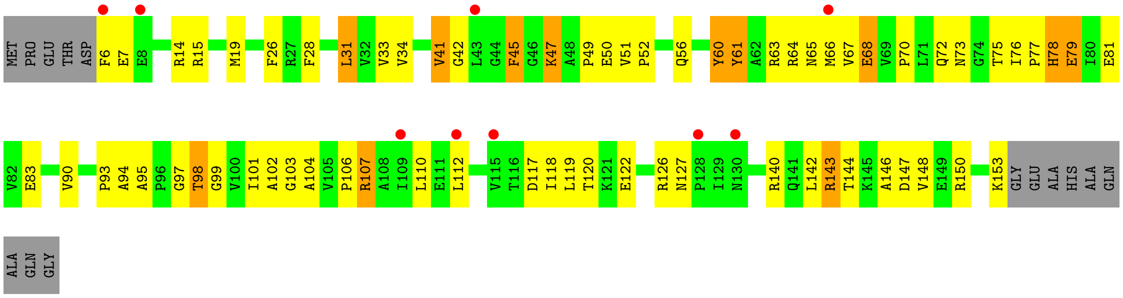
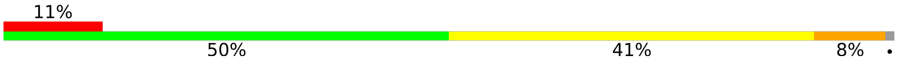
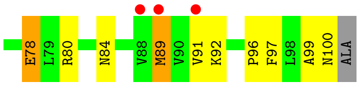




- Molecule 6: 30S ribosomal protein S6

Chain 5E:





- Molecule 6: 30S ribosomal protein S6

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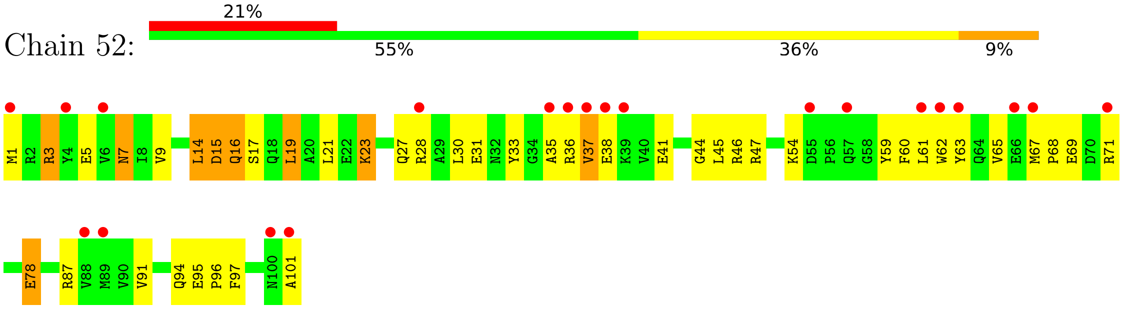
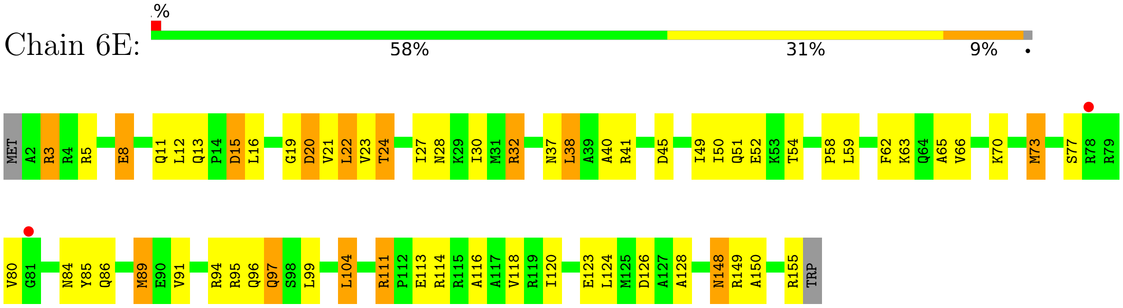


- Molecule 7: 30S ribosomal protein S7

Chain 6E:



- Molecule 7: 30S ribosomal protein S7

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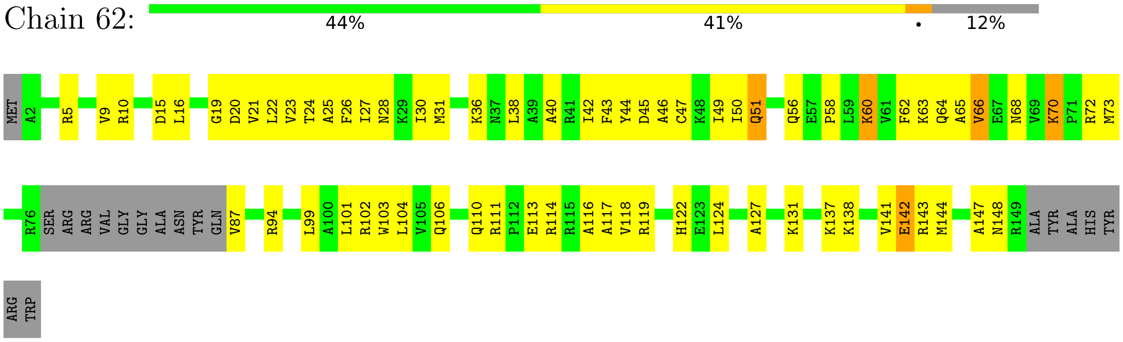
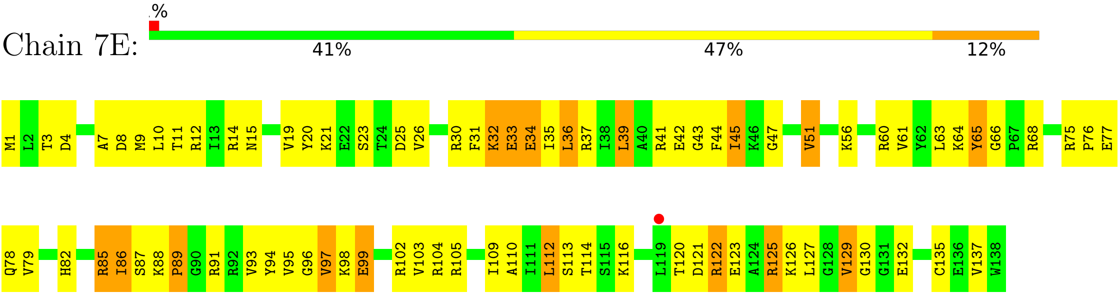
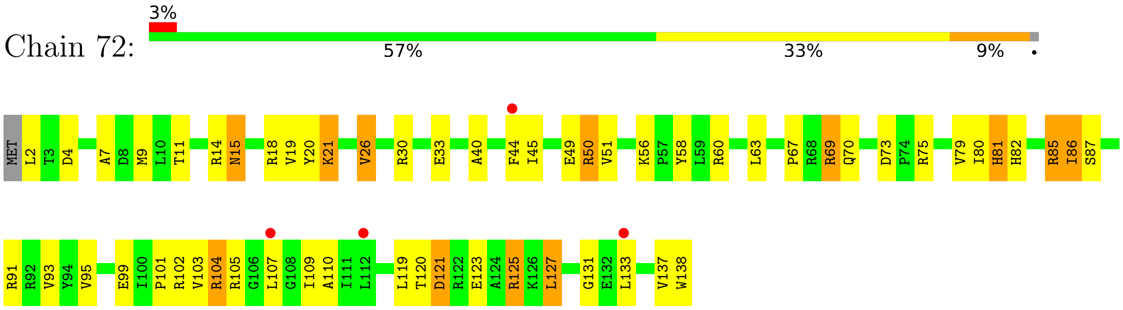


- Molecule 8: 30S ribosomal protein S8

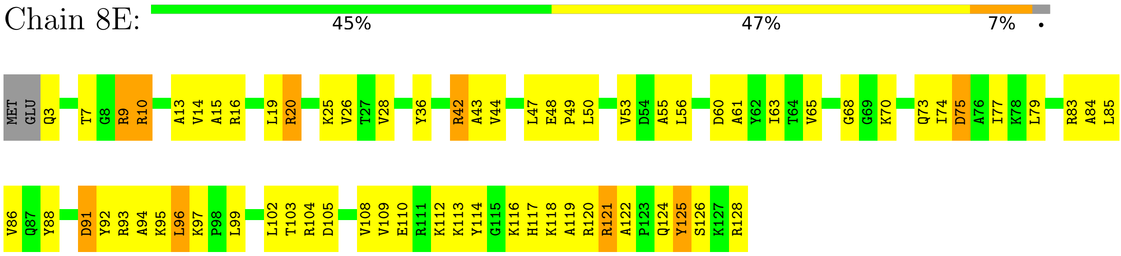
Chain 7E:



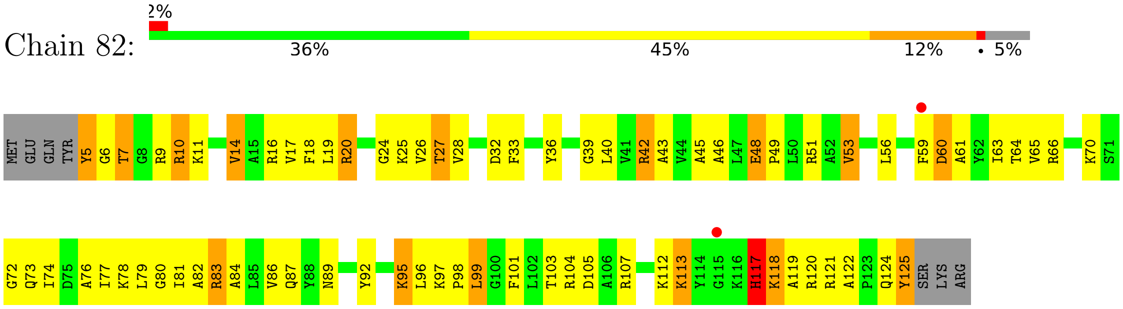
- Molecule 8: 30S ribosomal protein S8



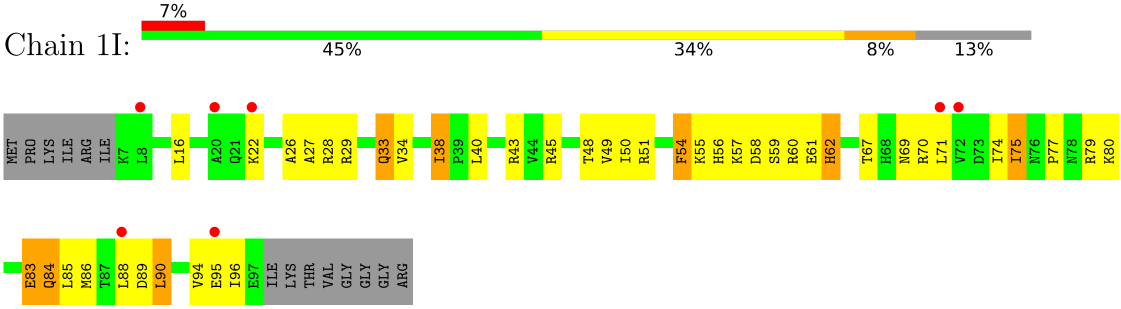
- Molecule 9: 30S ribosomal protein S9



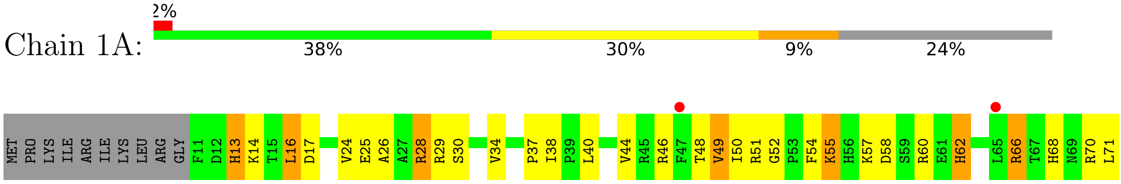
- Molecule 9: 30S ribosomal protein S9

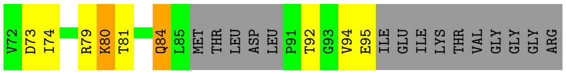


- Molecule 10: 30S ribosomal protein S10



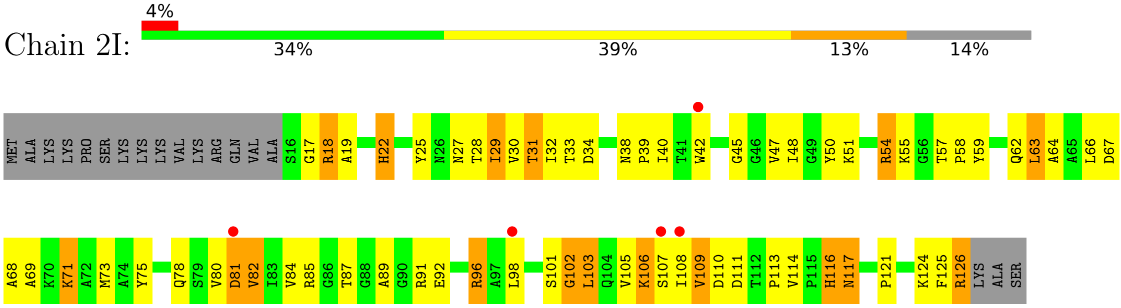
- Molecule 10: 30S ribosomal protein S10





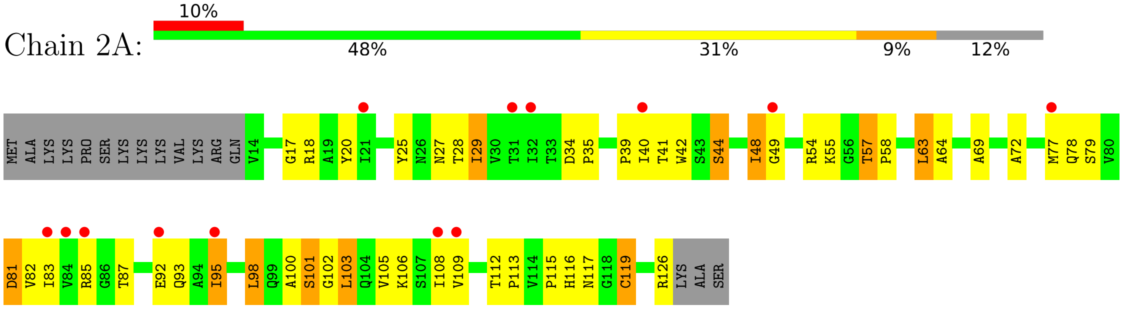
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



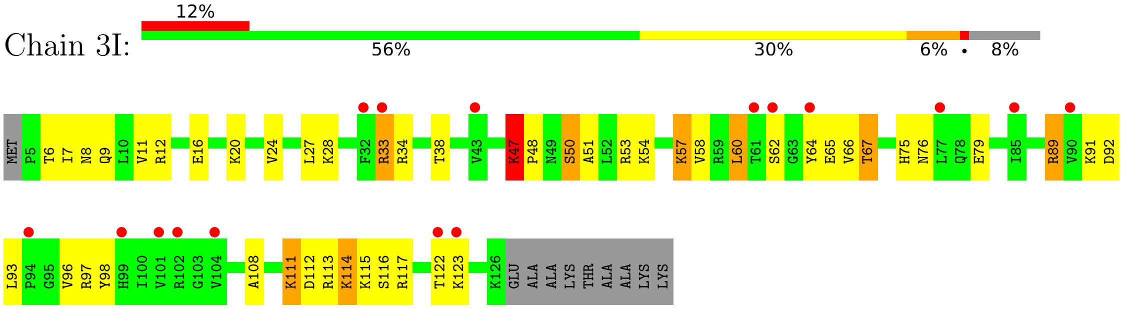
- Molecule 11: 30S ribosomal protein S11

Chain 2A:



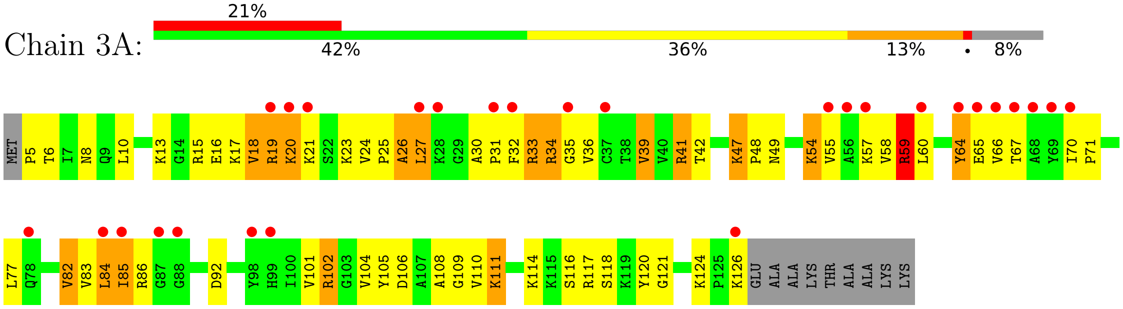
- Molecule 12: 30S ribosomal protein S12

Chain 3I:



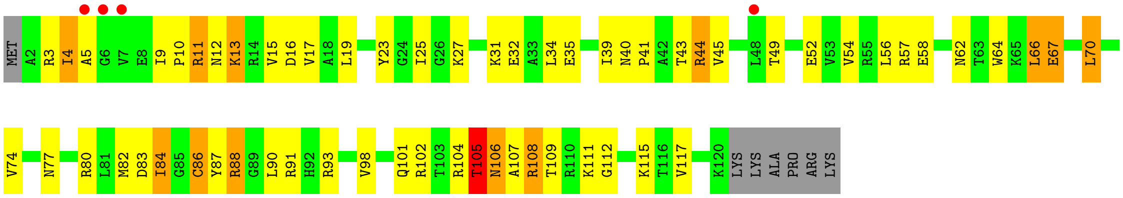
- Molecule 12: 30S ribosomal protein S12

Chain 3A:



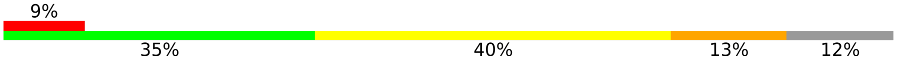
- Molecule 13: 30S ribosomal protein S13

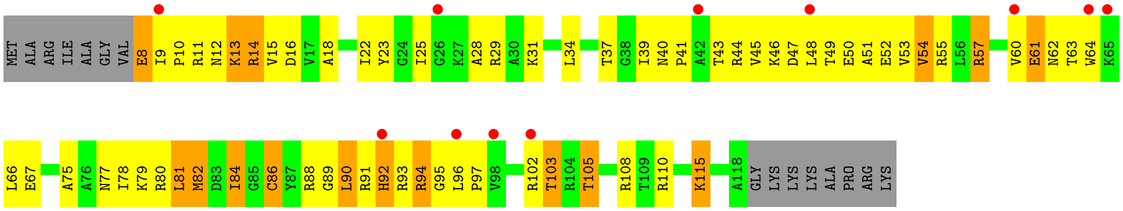
Chain 4I:



- Molecule 13: 30S ribosomal protein S13

Chain 4A:



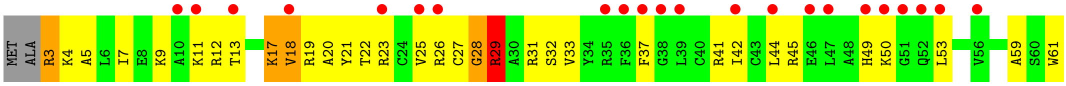


- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:

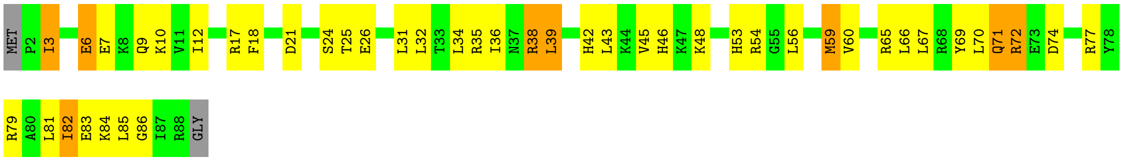
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



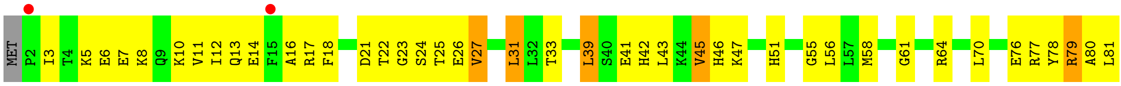
- Molecule 15: 30S ribosomal protein S15

Chain 6I:

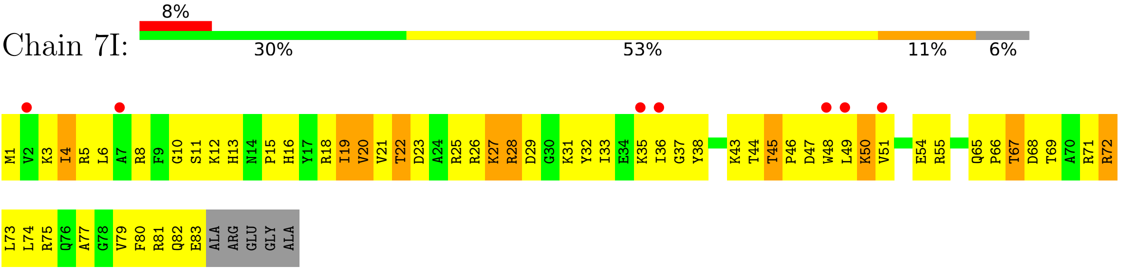


- Molecule 15: 30S ribosomal protein S15

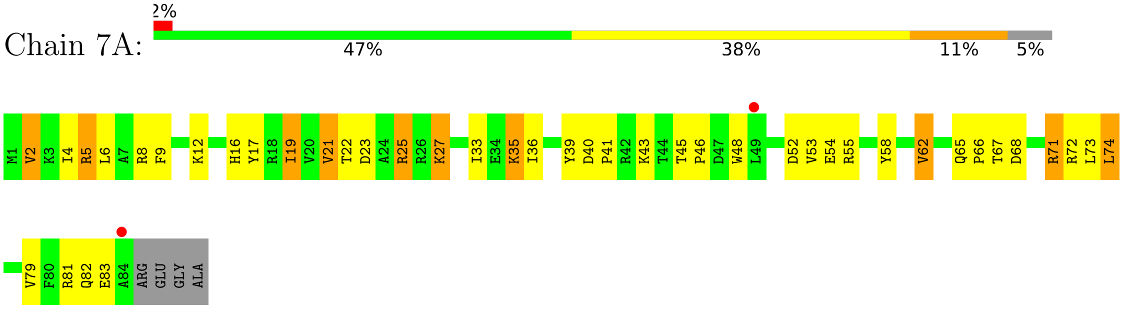
Chain 6A:



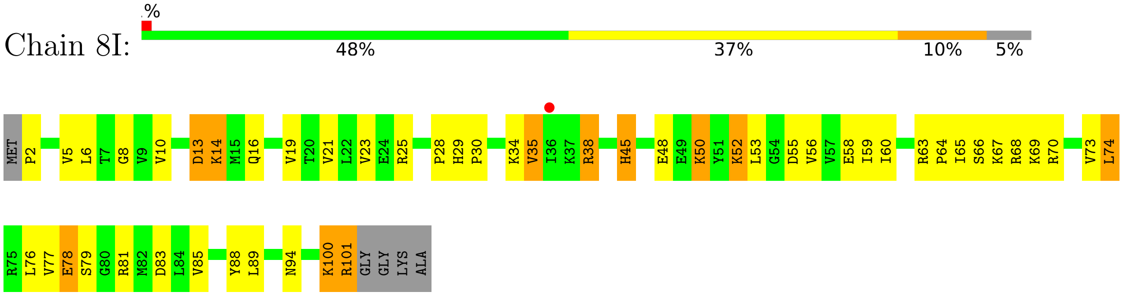
- Molecule 16: 30S ribosomal protein S16



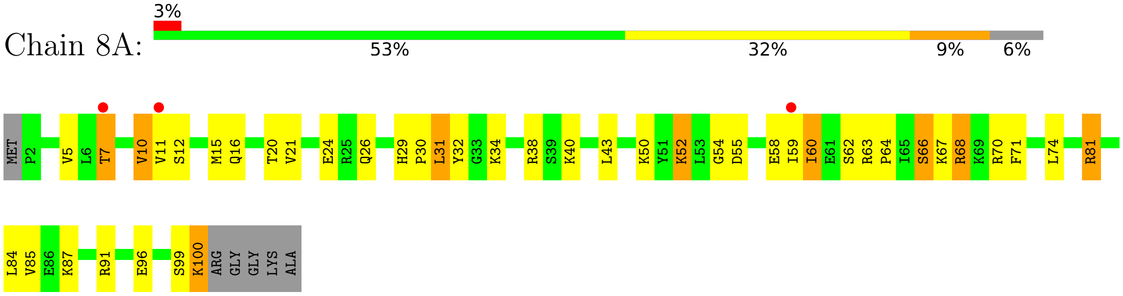
- Molecule 16: 30S ribosomal protein S16



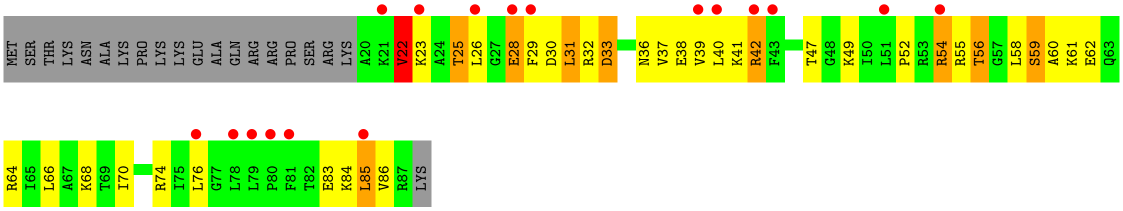
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

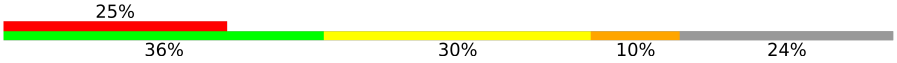


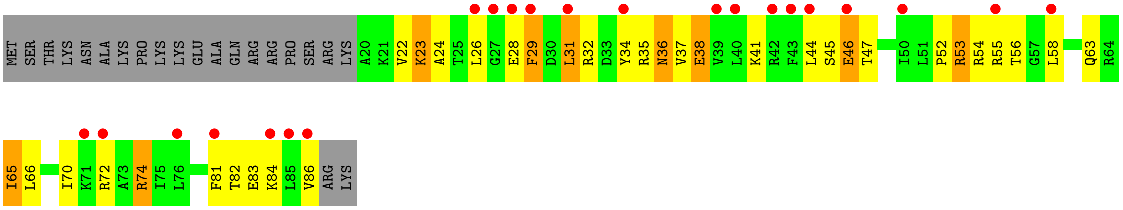
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

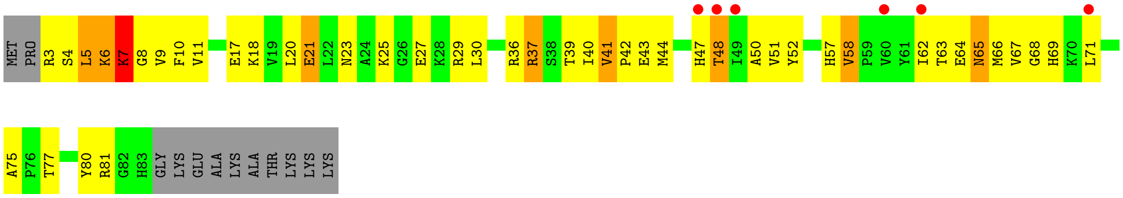
Chain 9A:





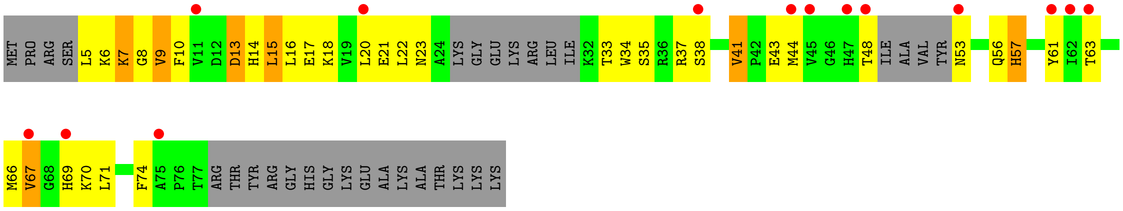
- Molecule 19: 30S ribosomal protein S19

Chain AI:



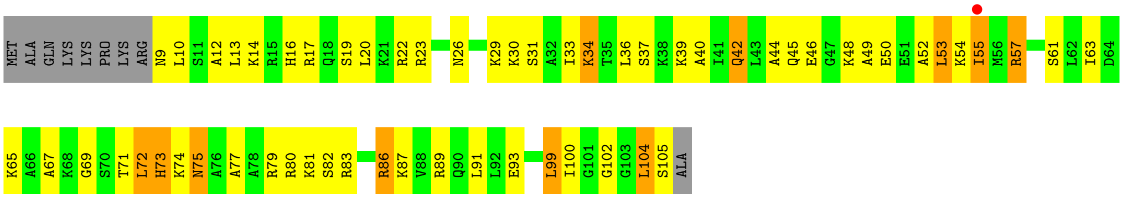
- Molecule 19: 30S ribosomal protein S19

Chain AA:



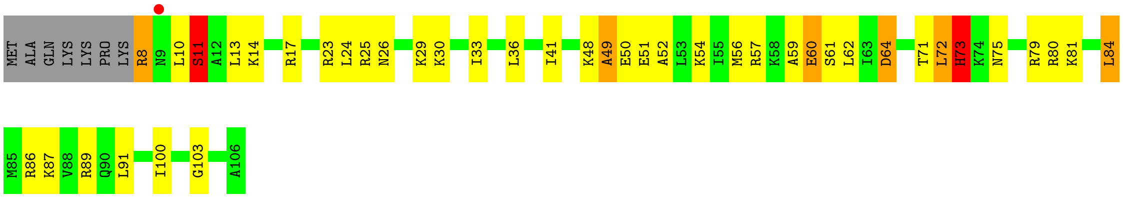
- Molecule 20: 30S ribosomal protein S20

Chain BI:



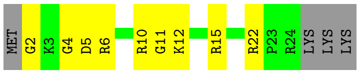
- Molecule 20: 30S ribosomal protein S20

Chain BA:



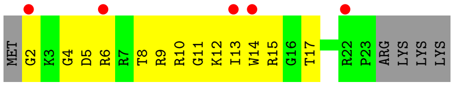
- Molecule 21: 30S ribosomal protein Thx

Chain 1F:



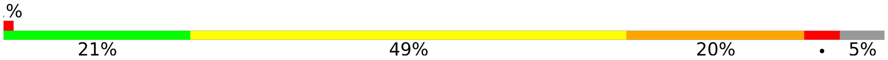
- Molecule 21: 30S ribosomal protein Thx

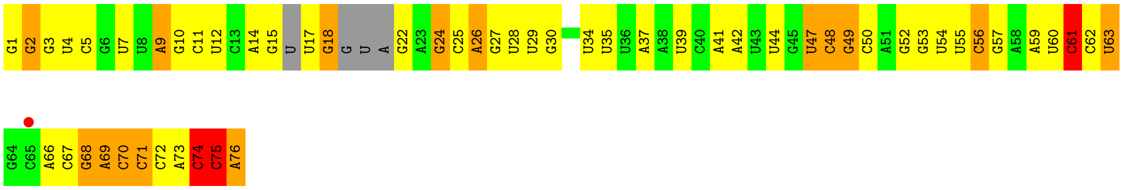
Chain 1B:



- Molecule 22: tRNALys

Chain 1K:





- Molecule 23: tRNAfMet

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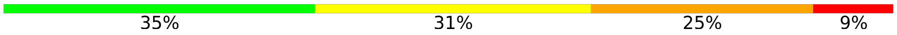

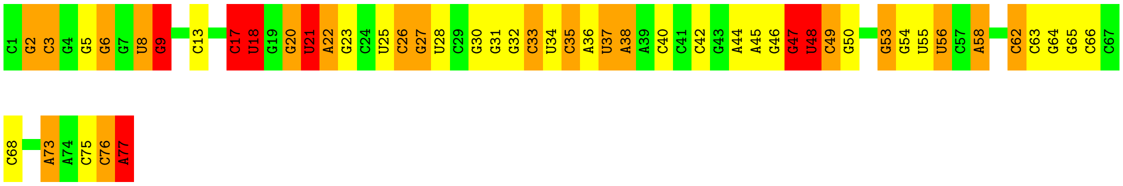

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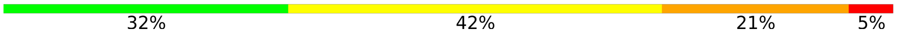

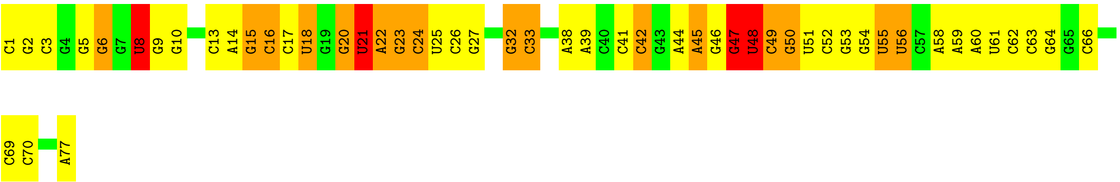

- Molecule 24: tRNALys

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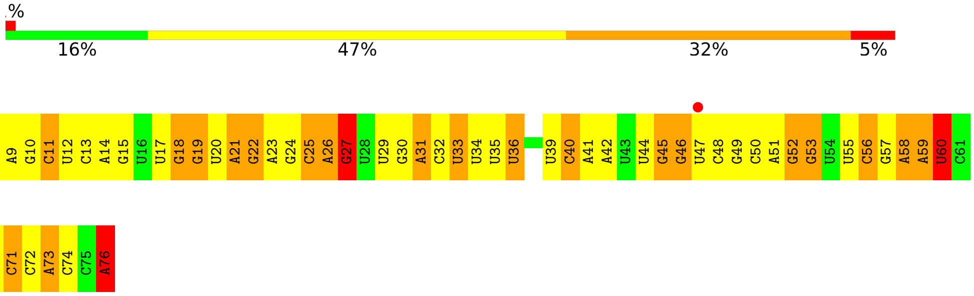

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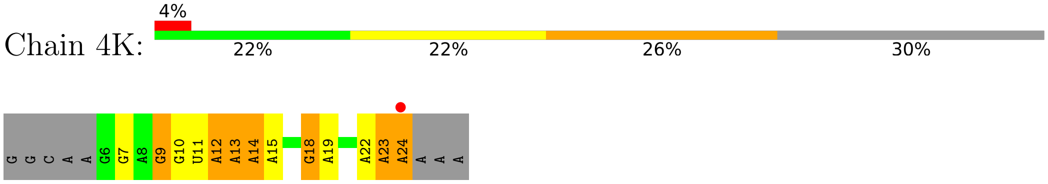

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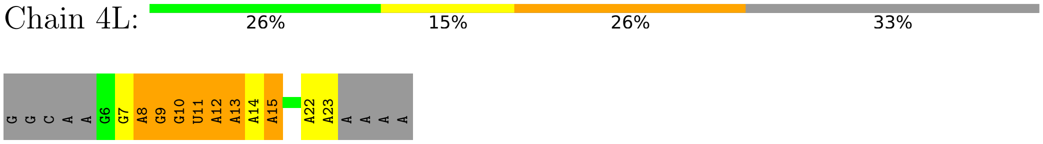

- Molecule 26: 23S rRNA

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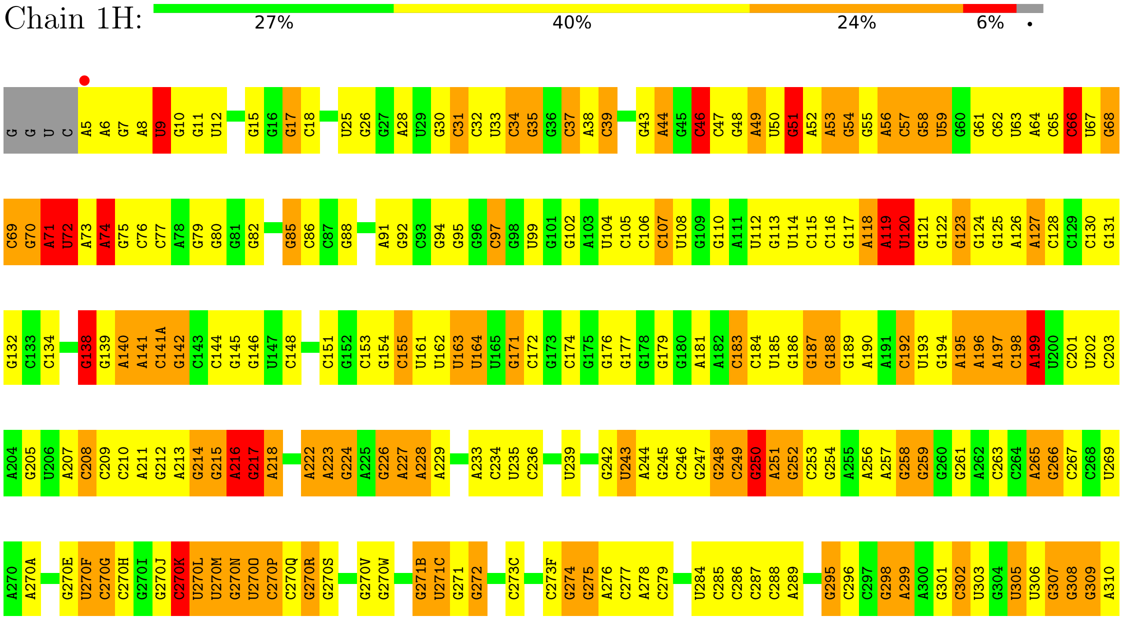

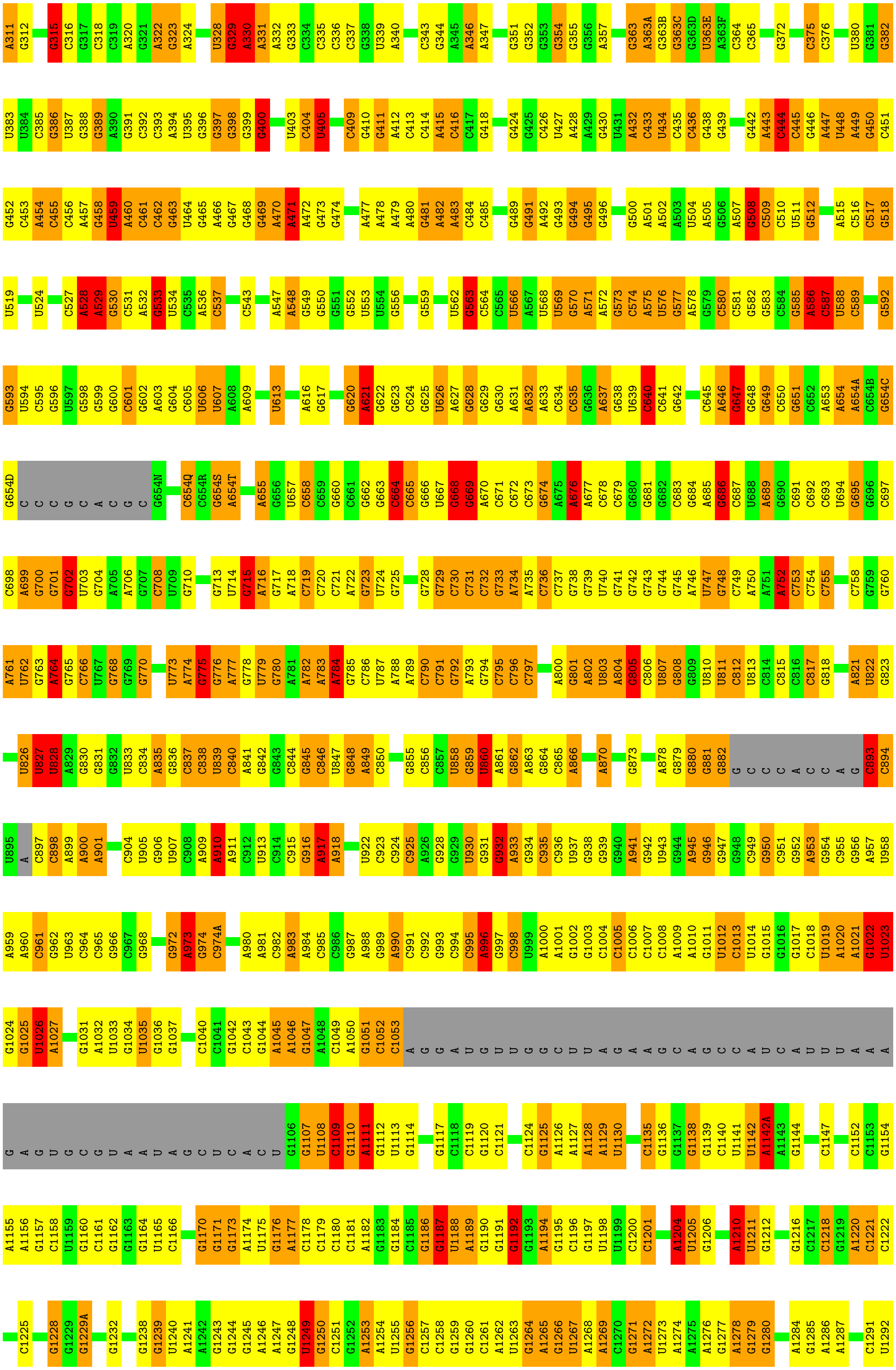
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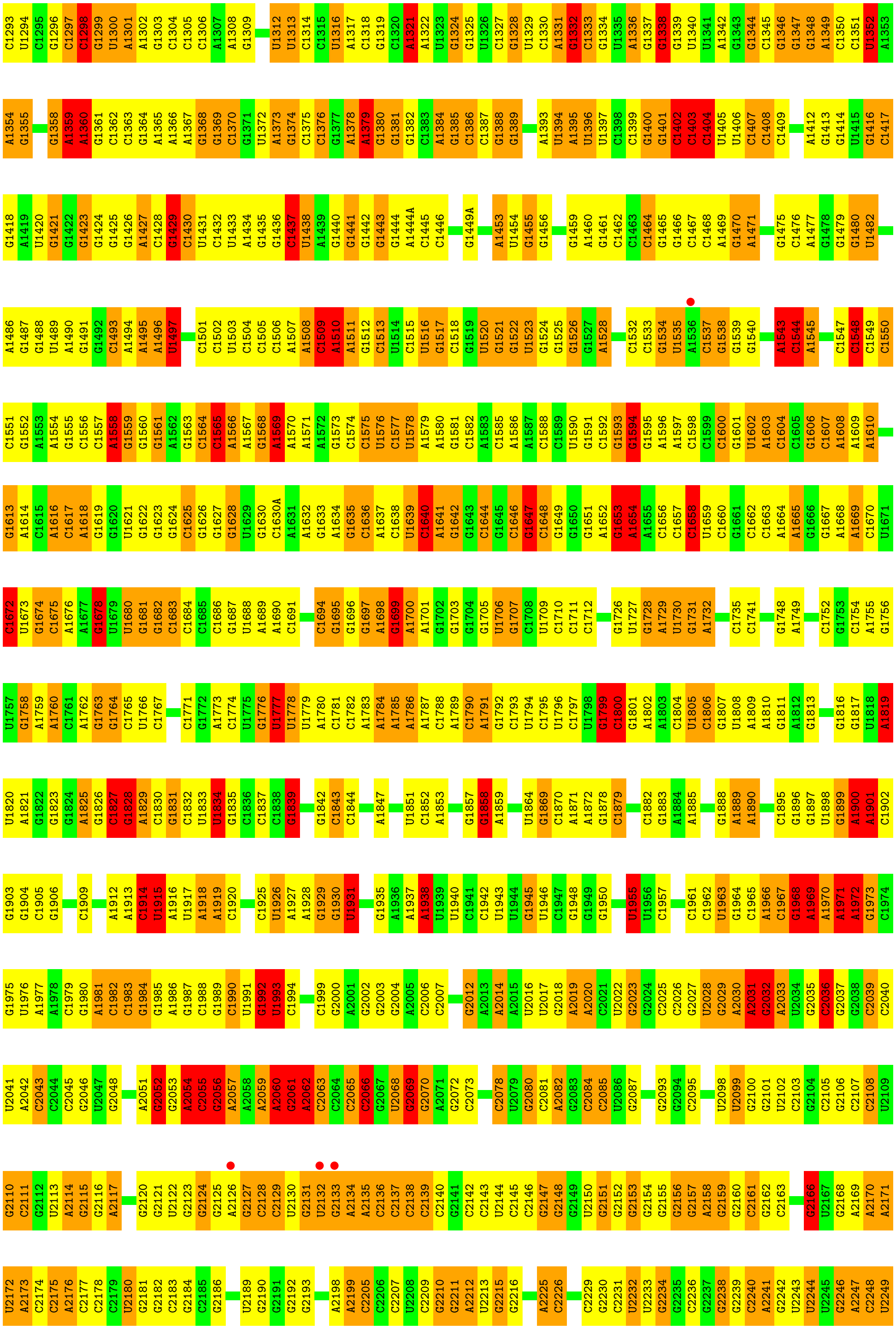
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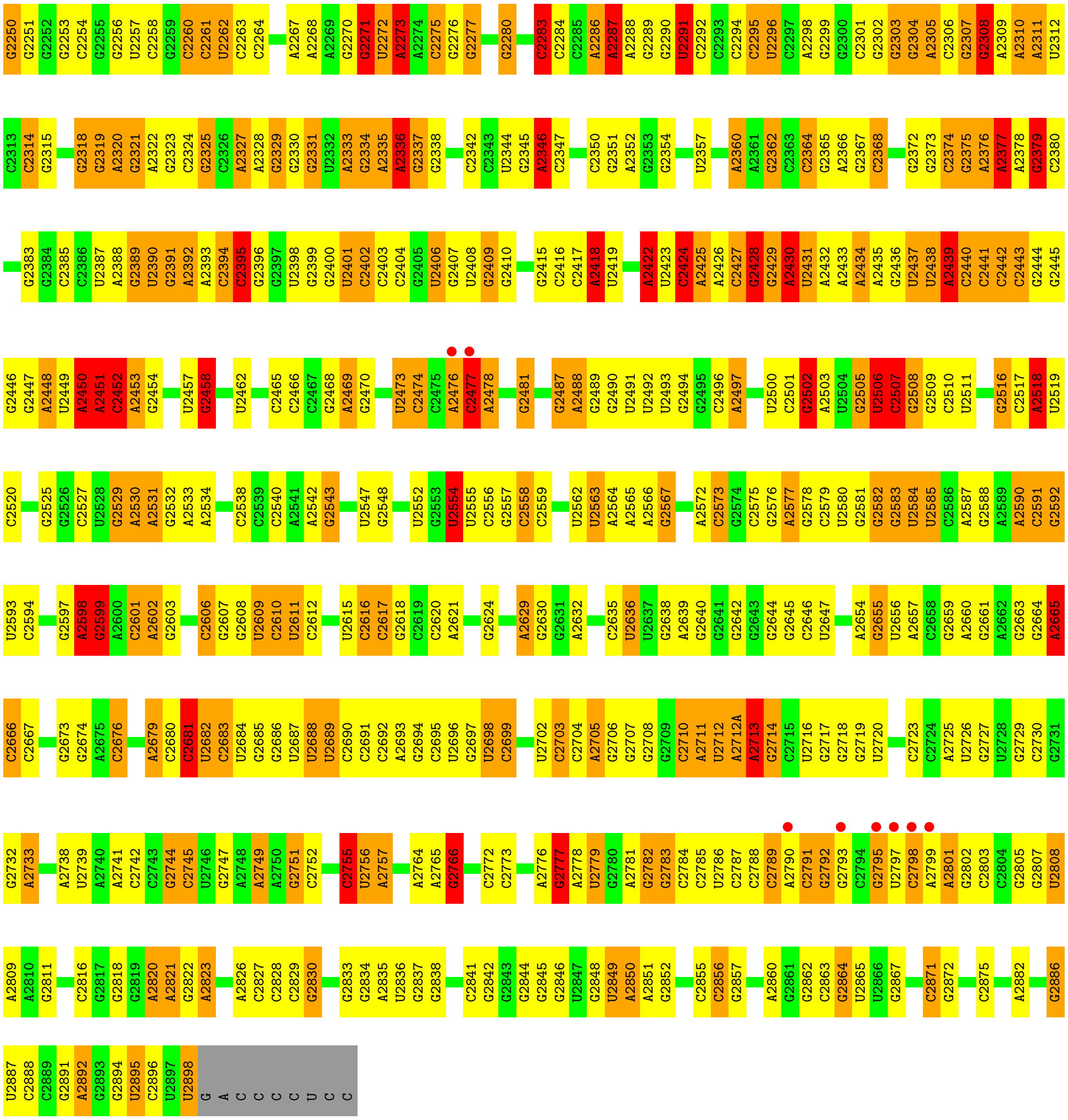

- Molecule 26: 23S rRNA

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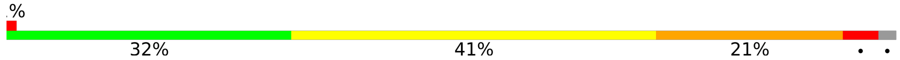

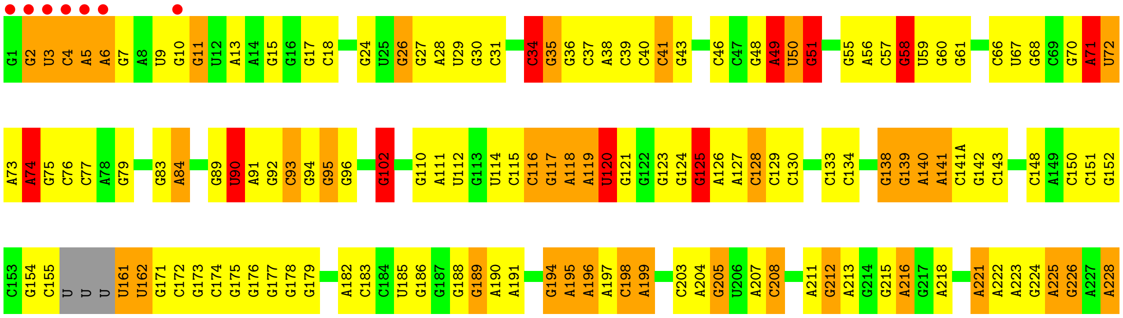

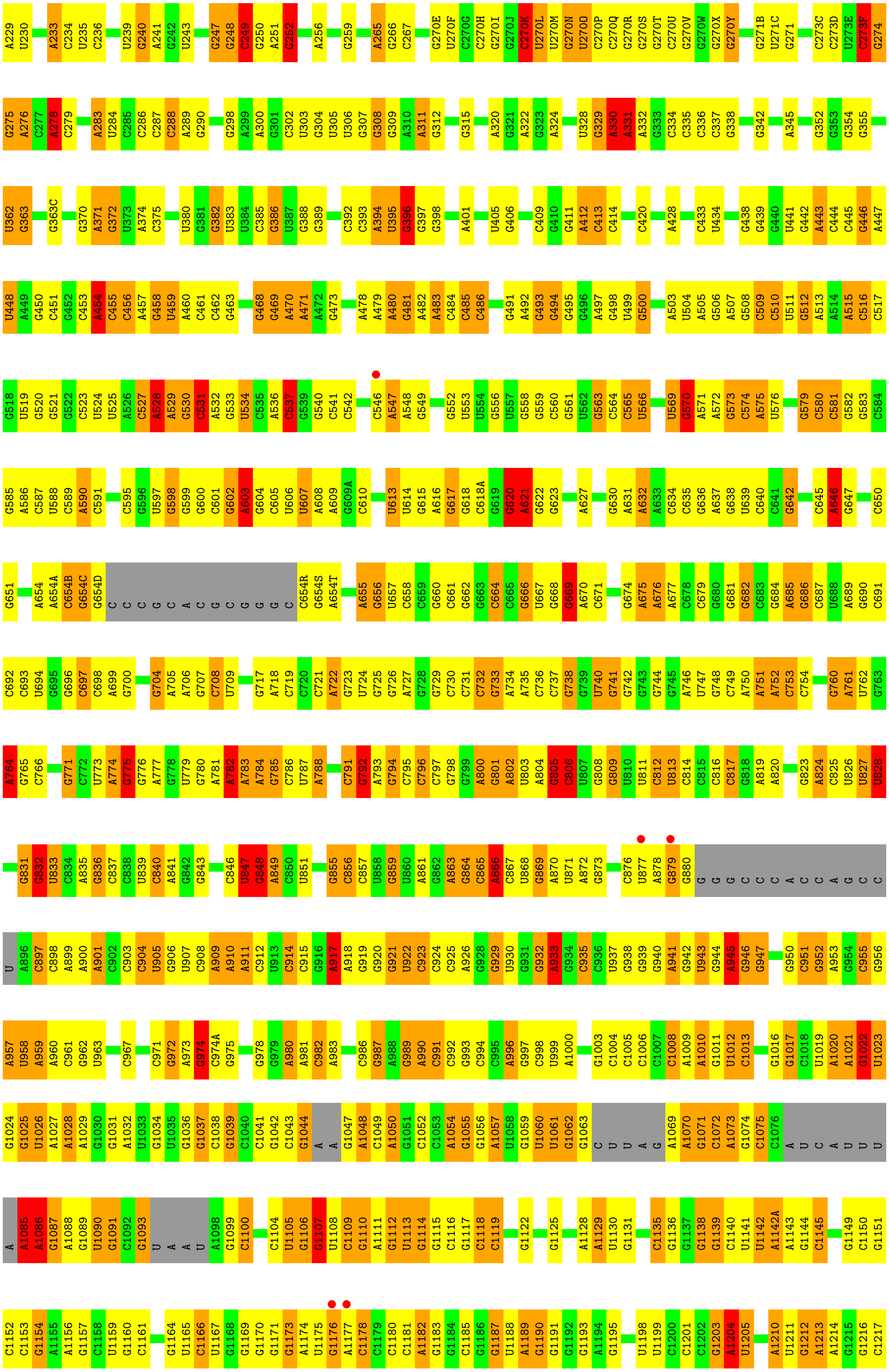
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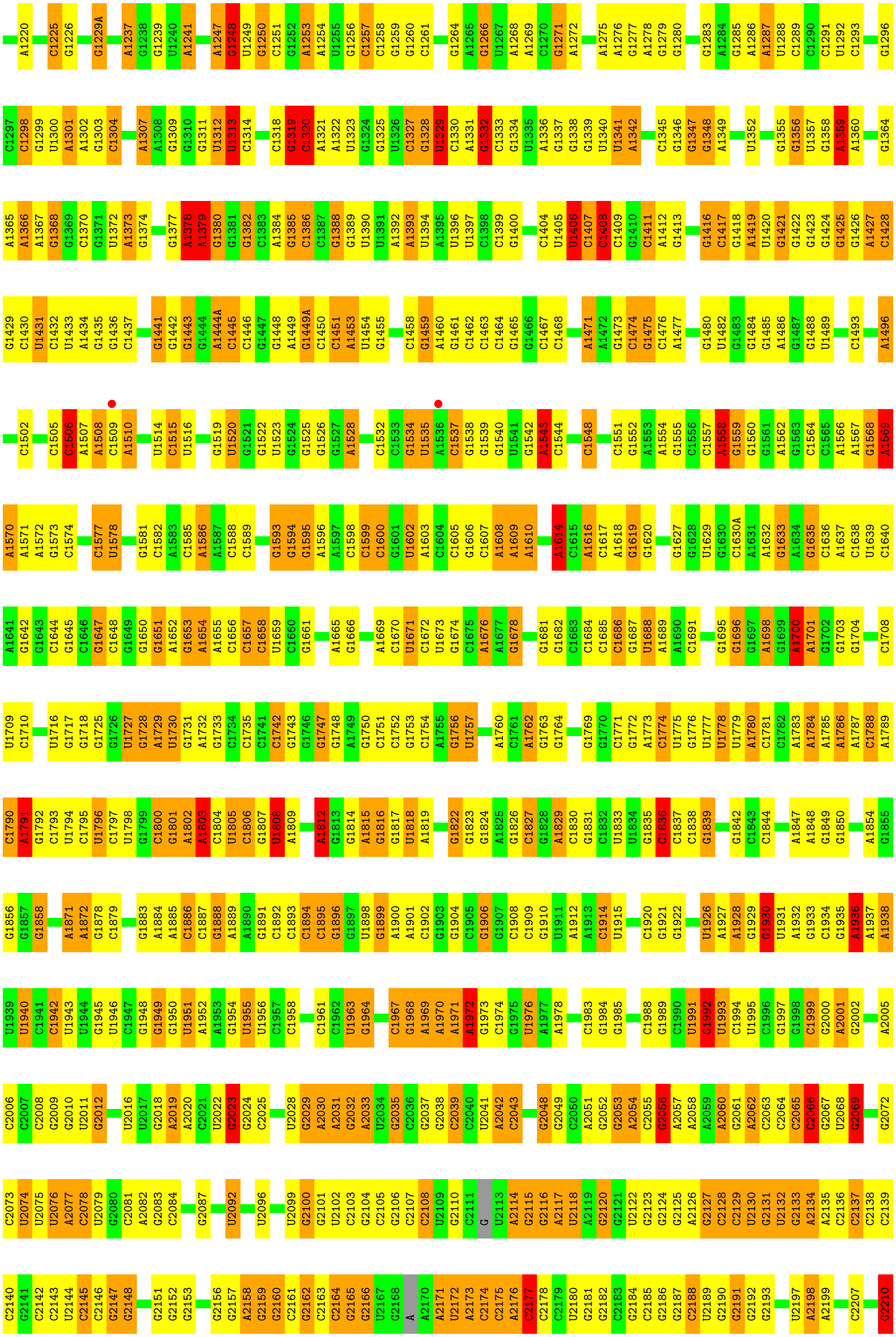

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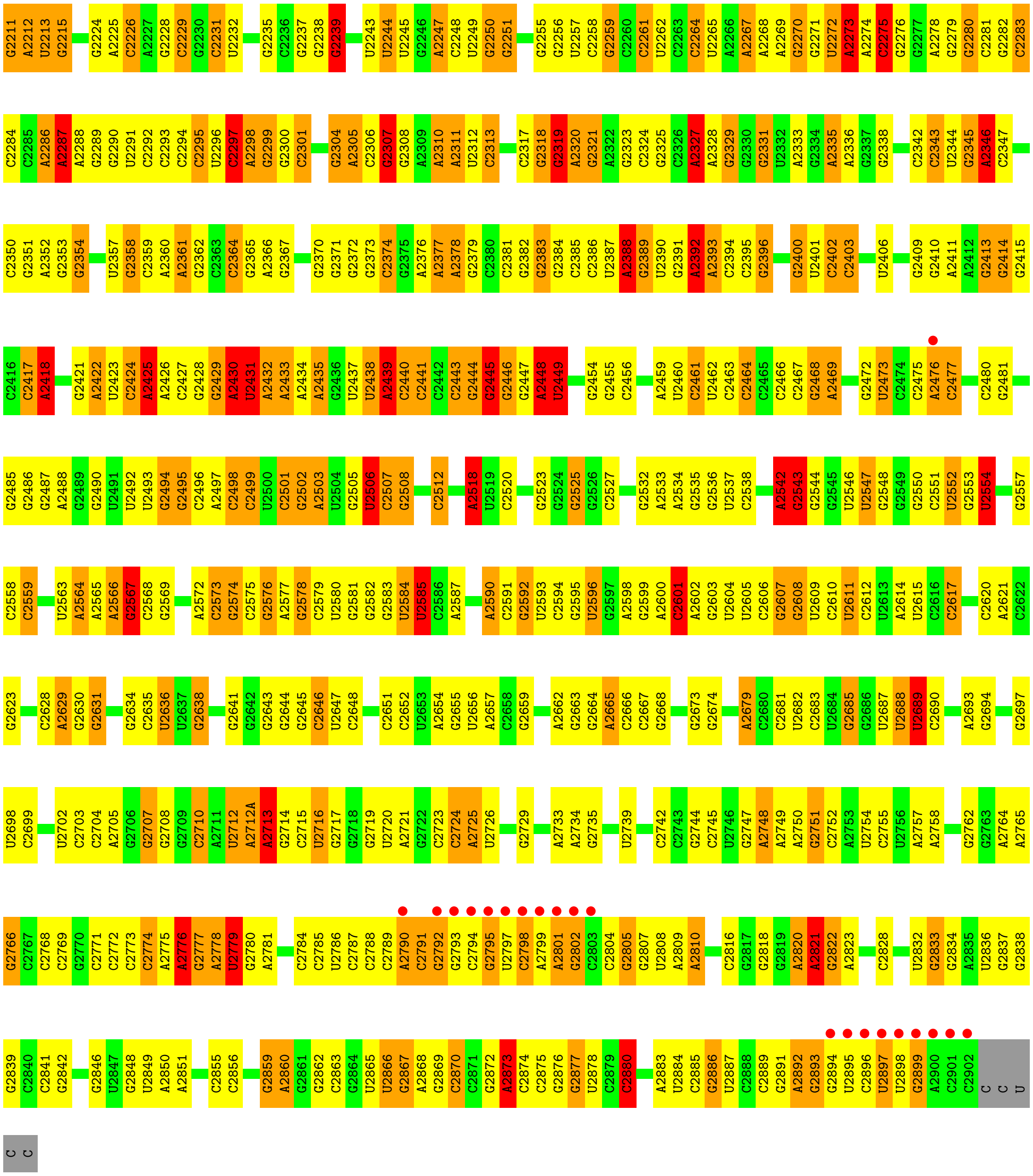

- Molecule 27: 5S rRNA

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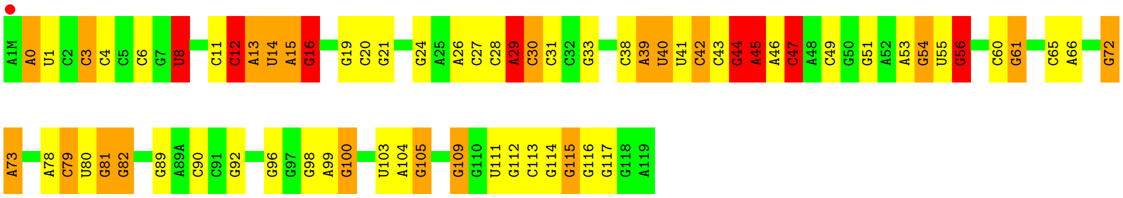

- Molecule 27: 5S rRNA

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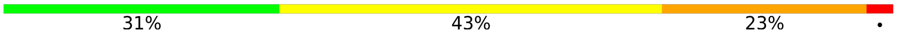

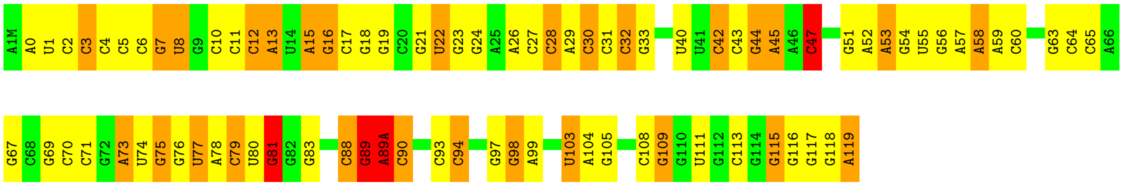

- Molecule 28: 50S ribosomal protein L1

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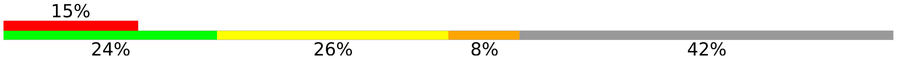

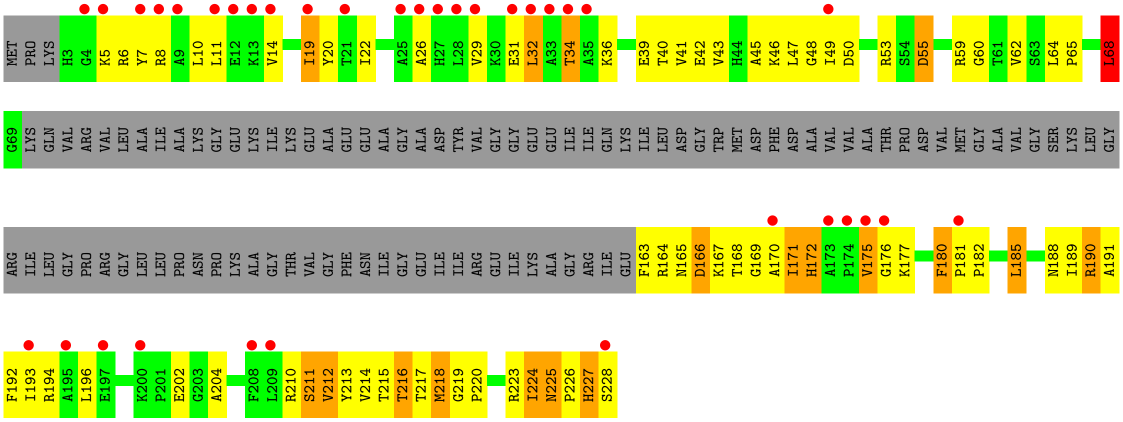

- Molecule 28: 50S ribosomal protein L1

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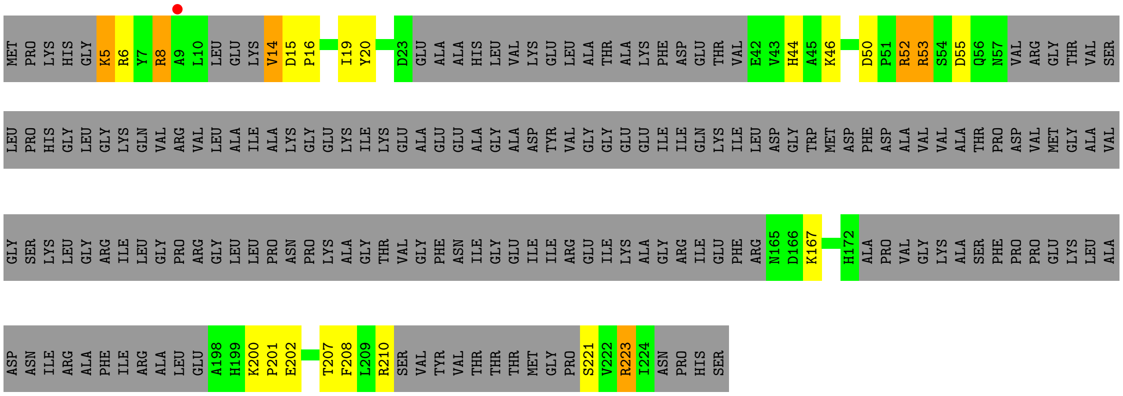

- Molecule 29: 50S ribosomal protein L2

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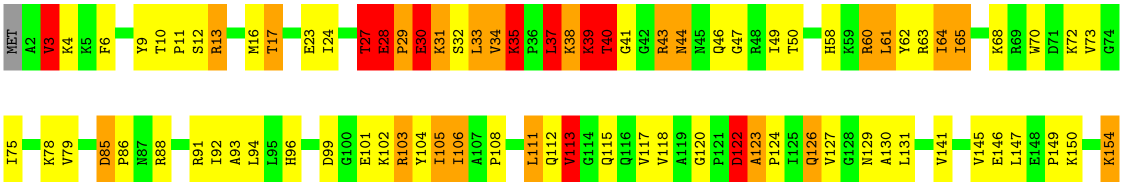

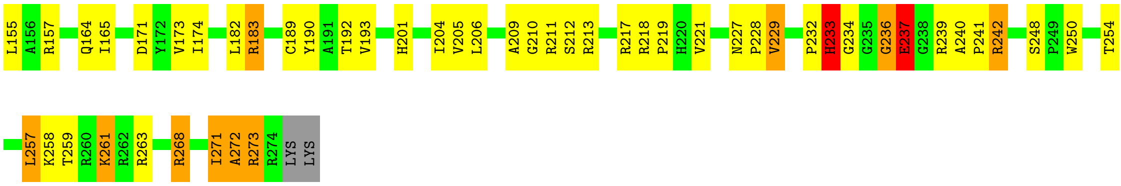

- Molecule 29: 50S ribosomal protein L2

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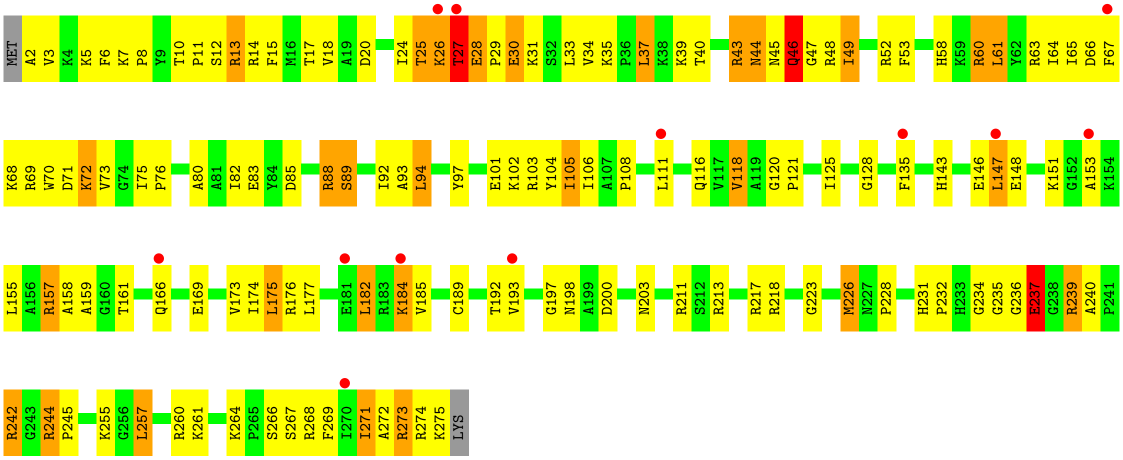

- Molecule 30: 50S ribosomal protein L3

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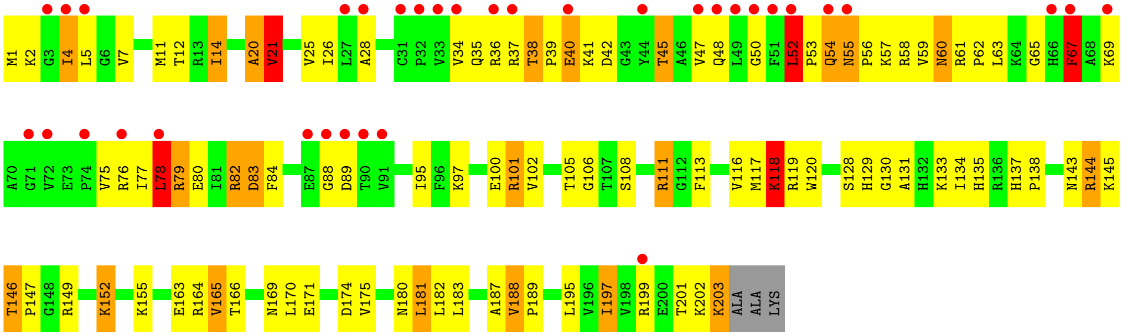
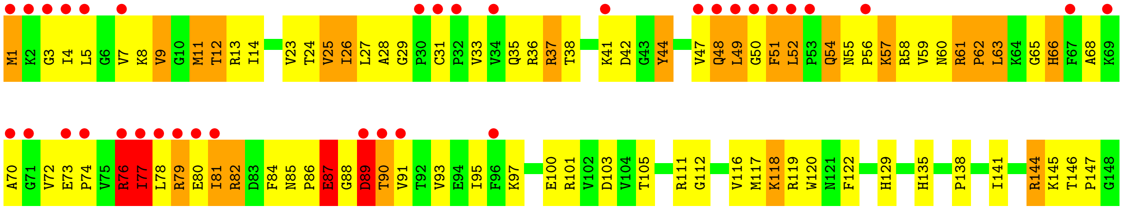
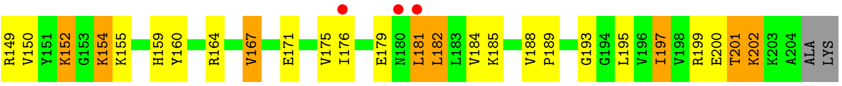


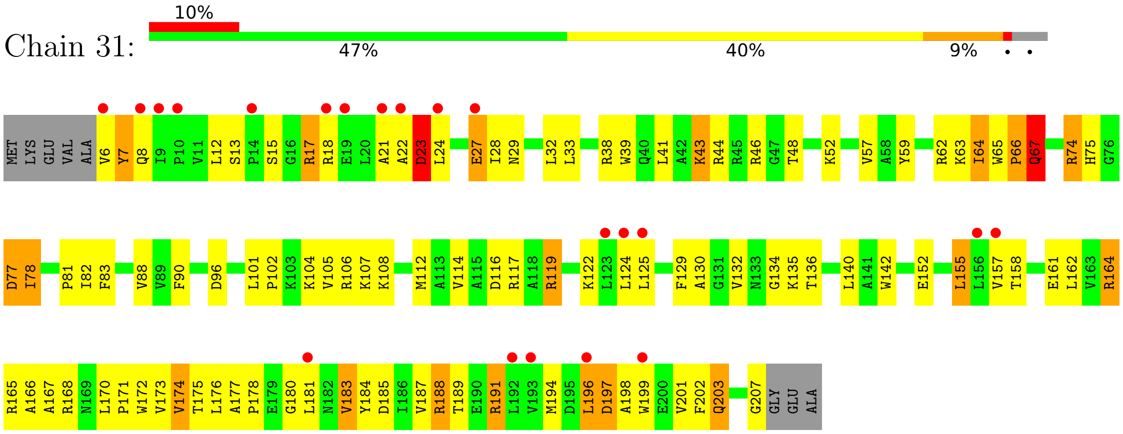
- Molecule 30: 50S ribosomal protein L3

Chain 29:

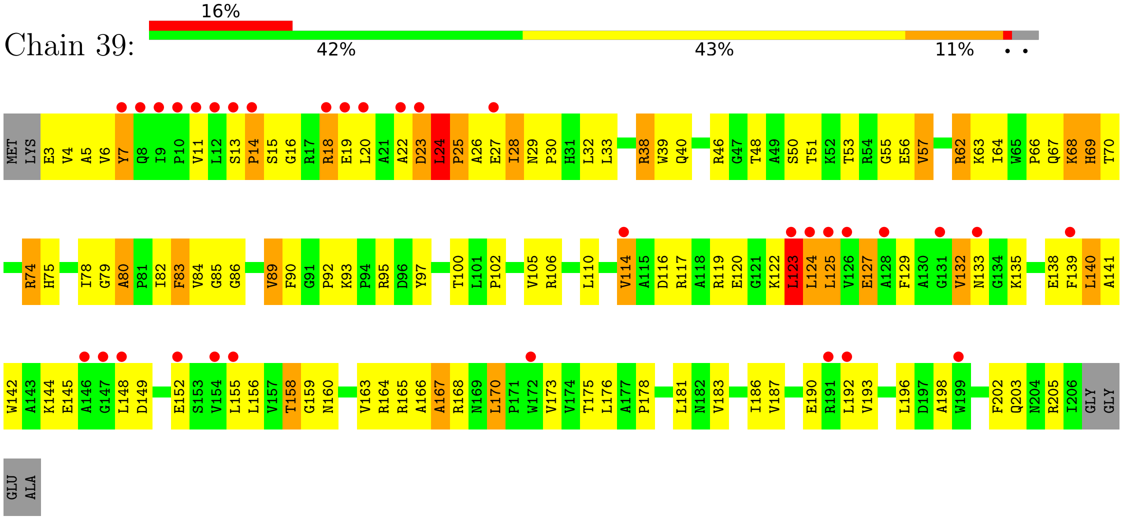




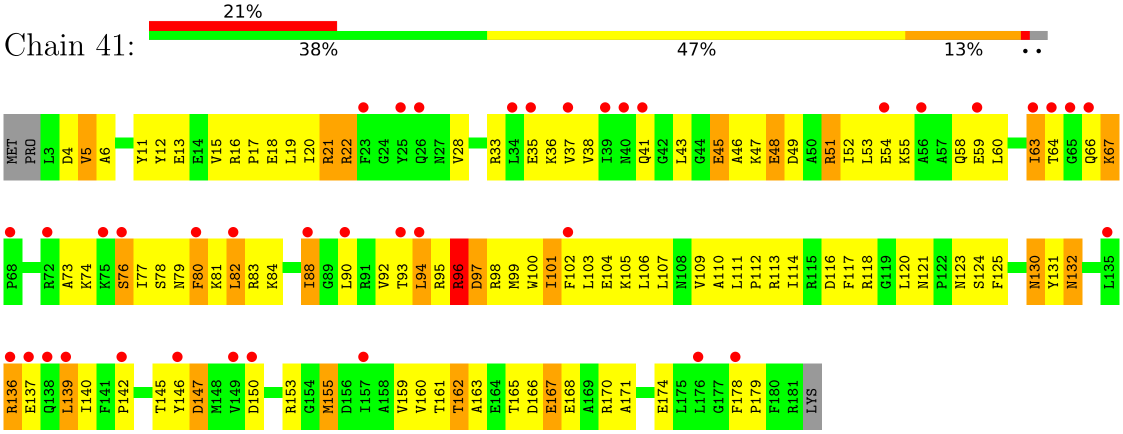
- Molecule 31: 50S ribosomal protein L4



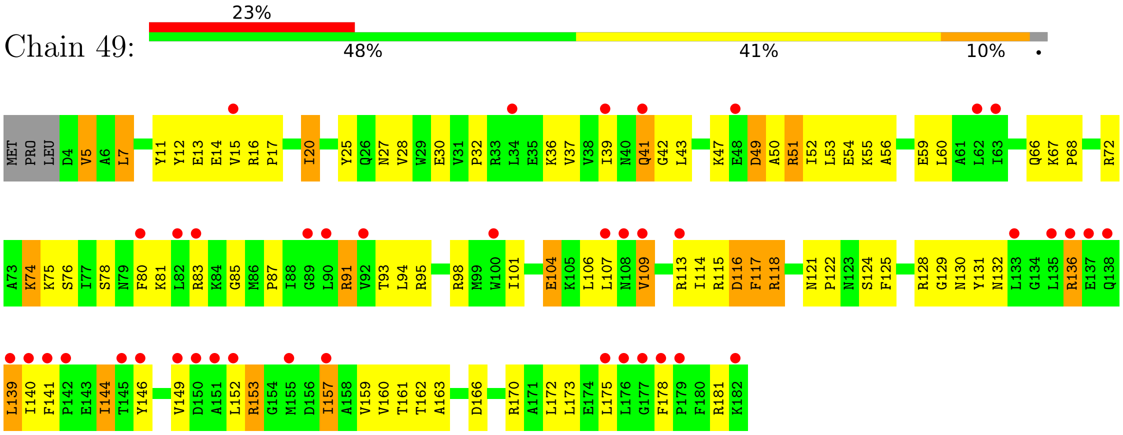
- Molecule 31: 50S ribosomal protein L4



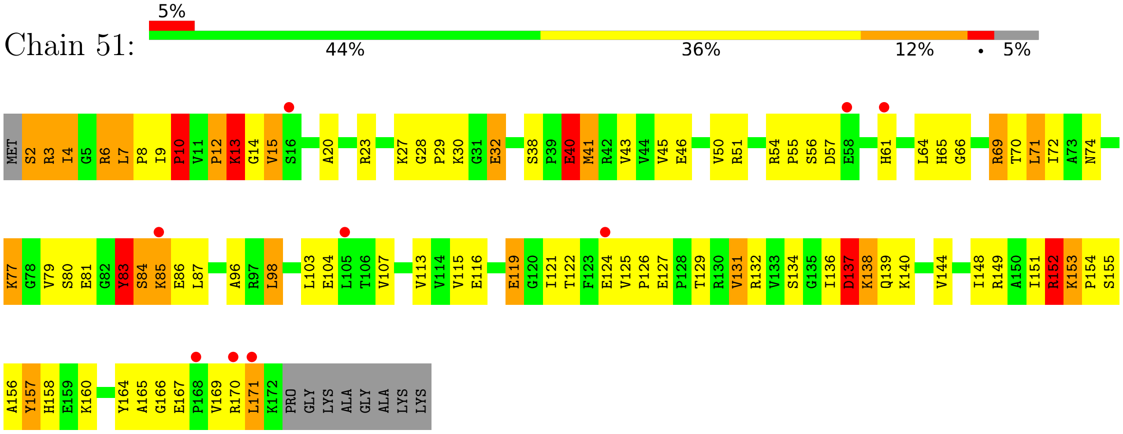
- Molecule 32: 50S ribosomal protein L5



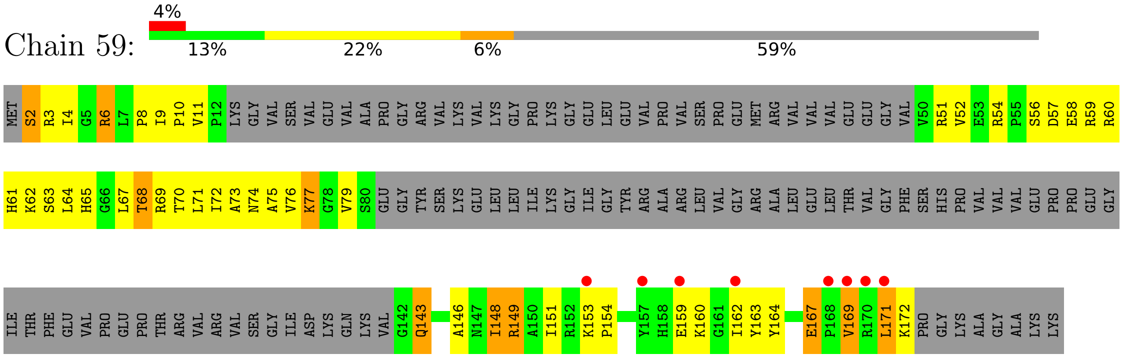
- Molecule 32: 50S ribosomal protein L5



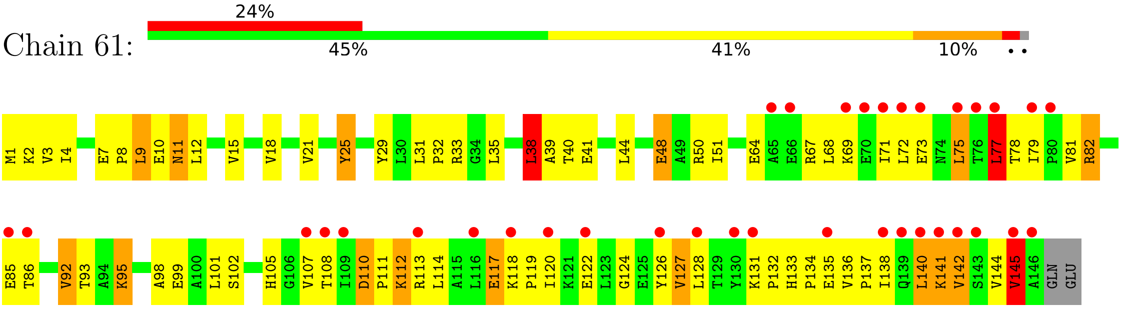
- Molecule 33: 50S ribosomal protein L6



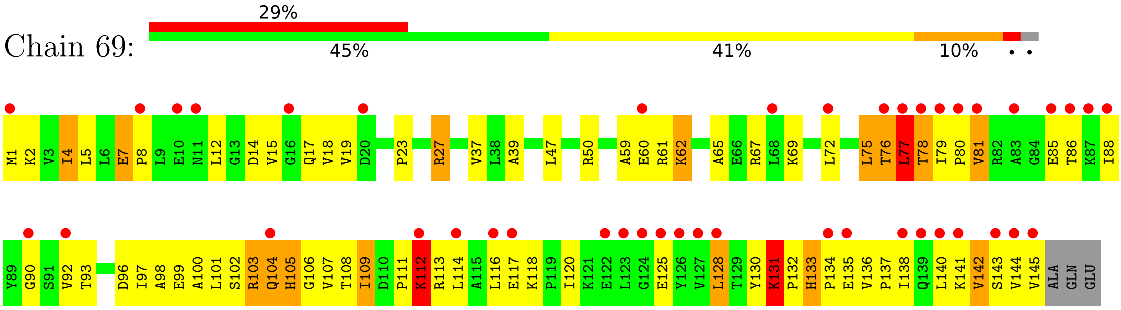
- Molecule 33: 50S ribosomal protein L6



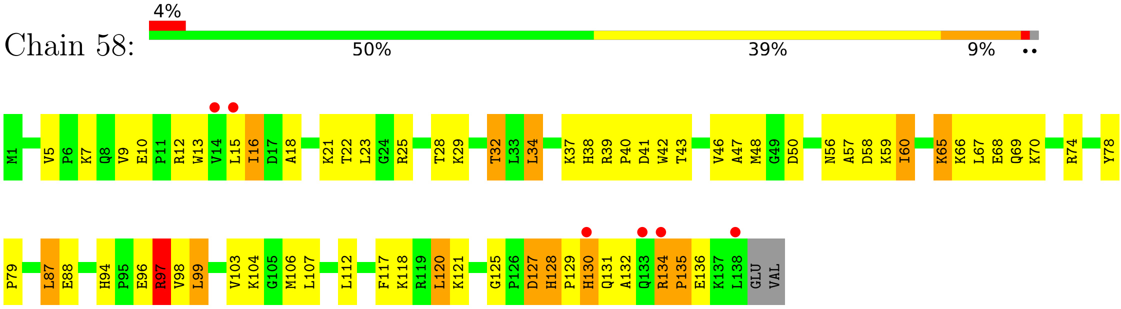
- Molecule 34: 50S ribosomal protein L9



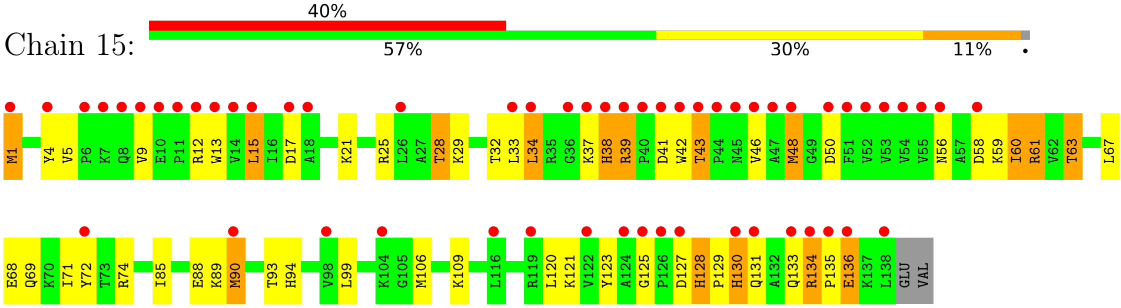
- Molecule 34: 50S ribosomal protein L9



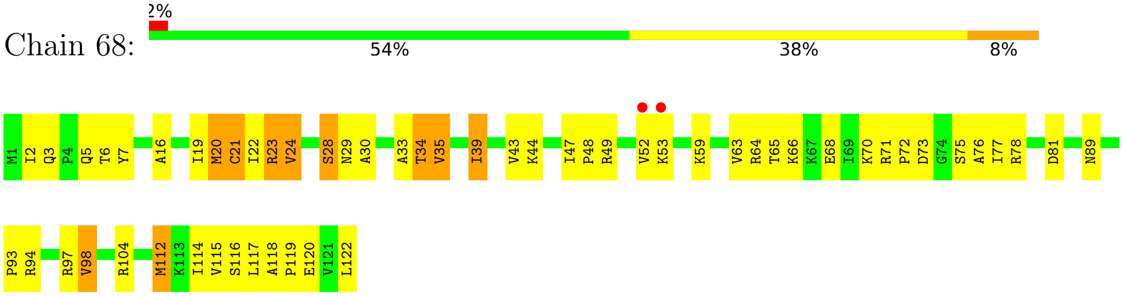
- Molecule 35: 50S ribosomal protein L13



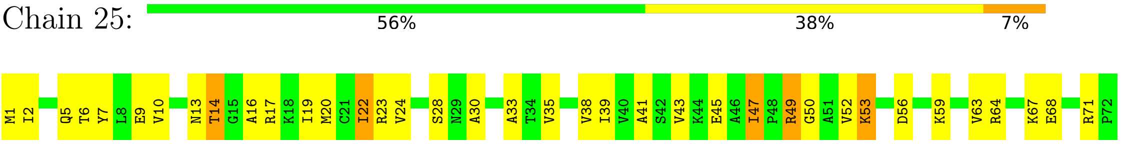
- Molecule 35: 50S ribosomal protein L13

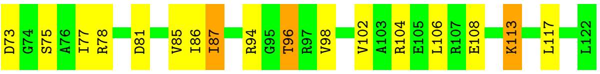


- Molecule 36: 50S ribosomal protein L14

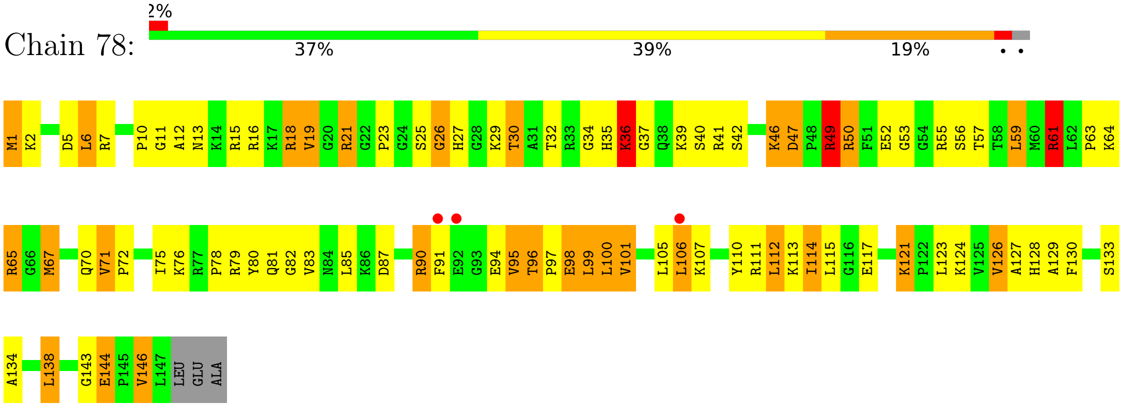


- Molecule 36: 50S ribosomal protein L14

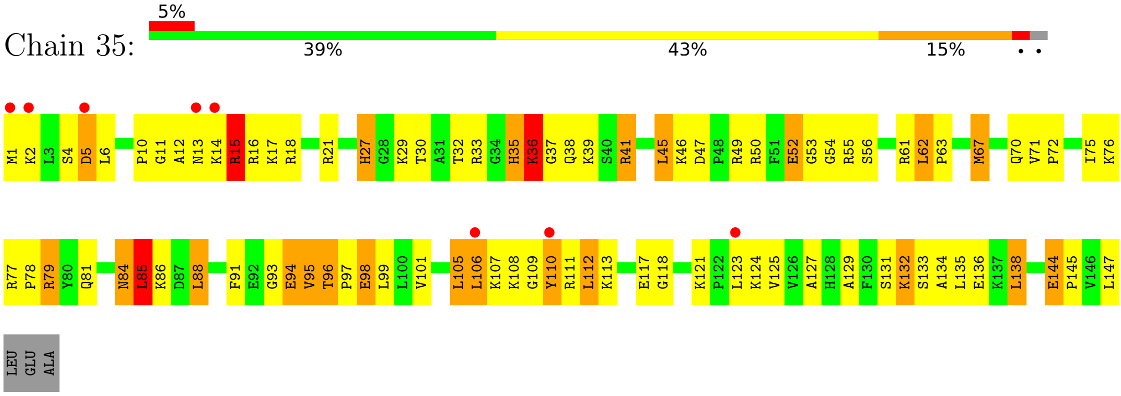




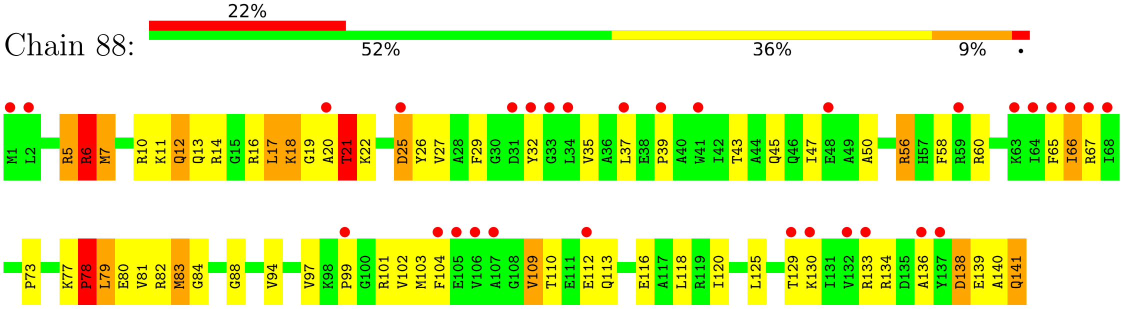
- Molecule 37: 50S ribosomal protein L15



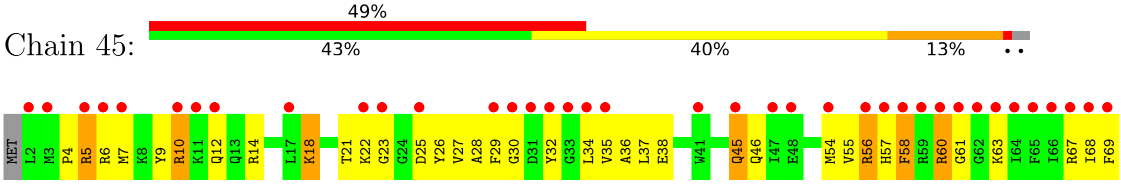
- Molecule 37: 50S ribosomal protein L15

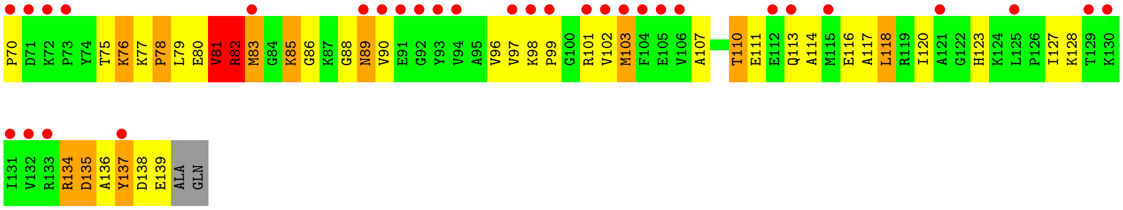


- Molecule 38: 50S ribosomal protein L16



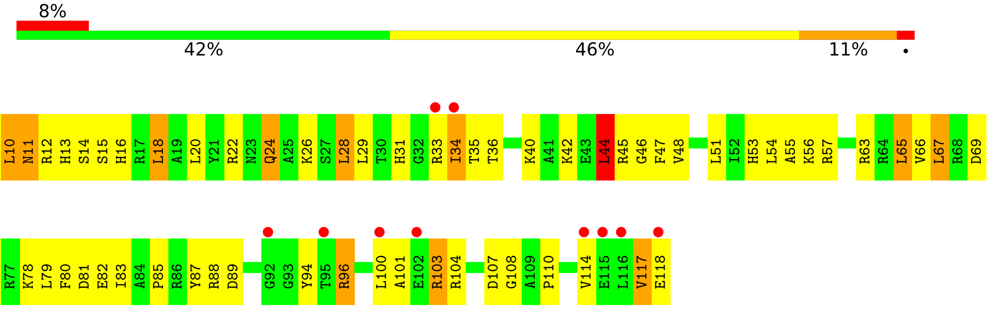
- Molecule 38: 50S ribosomal protein L16





- Molecule 39: 50S ribosomal protein L17

Chain 98:



- Molecule 39: 50S ribosomal protein L17

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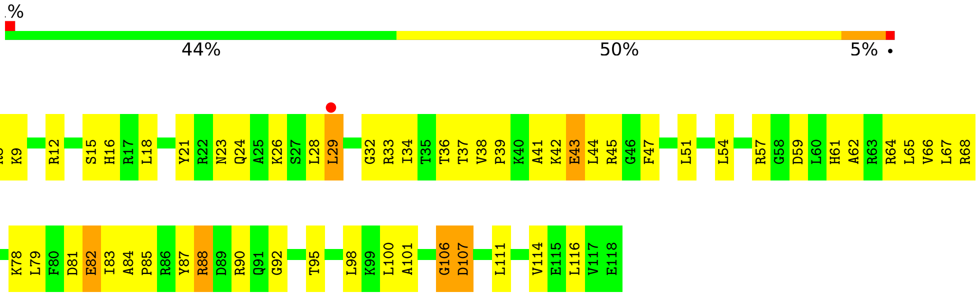
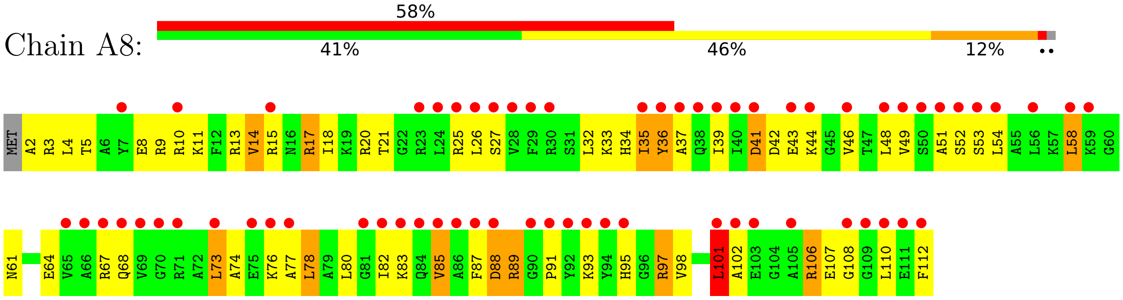


- Molecule 40: 50S ribosomal protein L18

Chain A8:



- Molecule 40: 50S ribosomal protein L18

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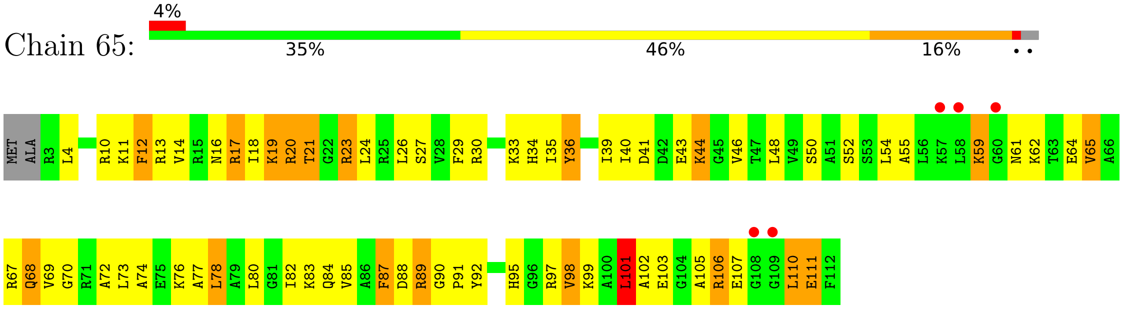
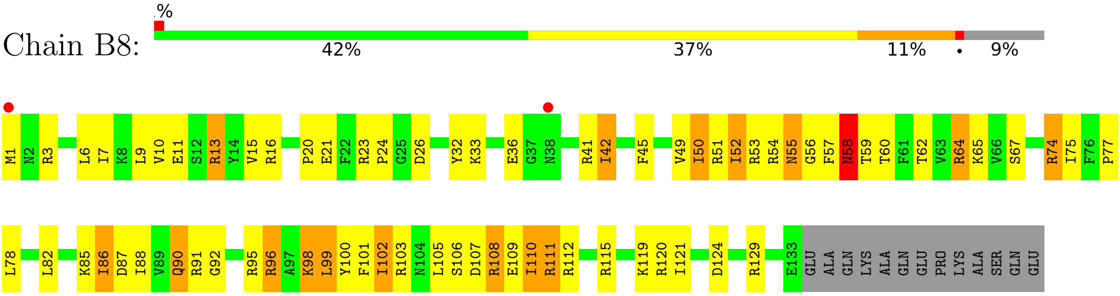


- Molecule 41: 50S ribosomal protein L19

Chain B8:



- Molecule 41: 50S ribosomal protein L19

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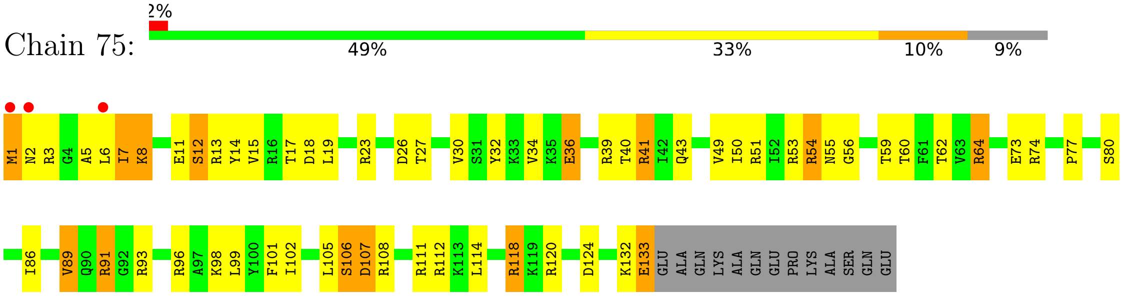
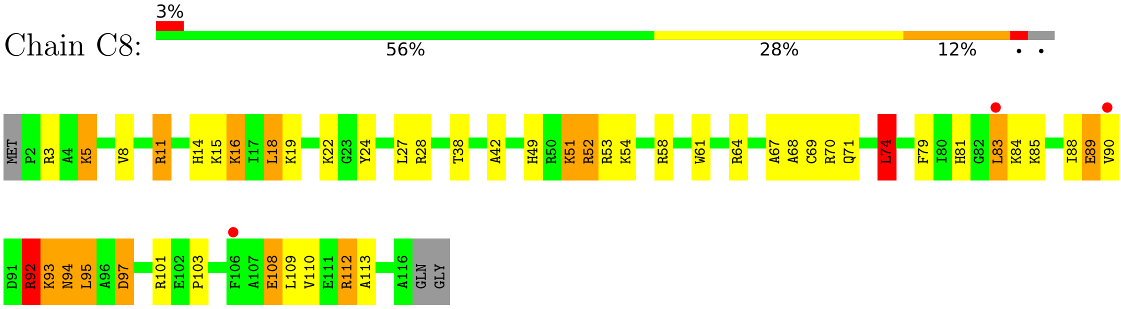


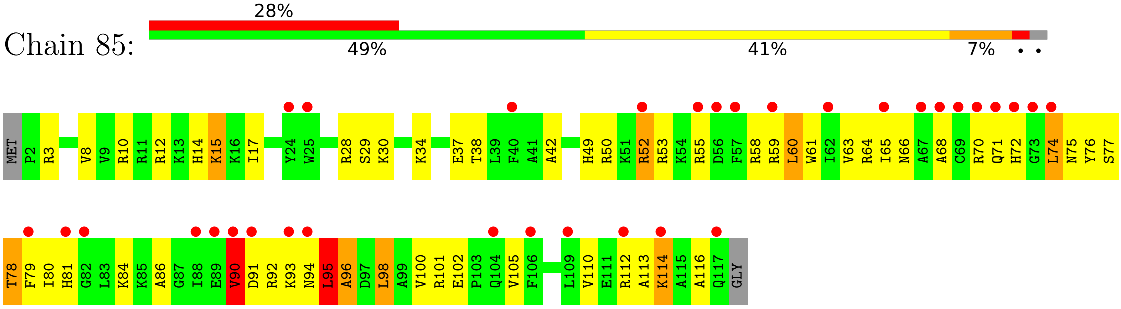
- Molecule 42: 50S ribosomal protein L20

Chain C8:



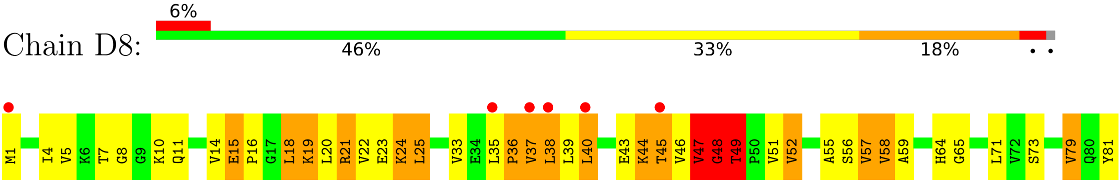
- Molecule 42: 50S ribosomal protein L20

Chain 85:

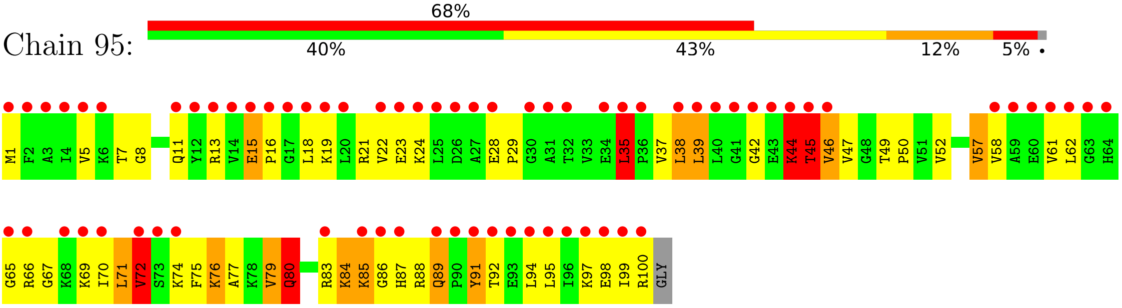


- Molecule 43: 50S ribosomal protein L21

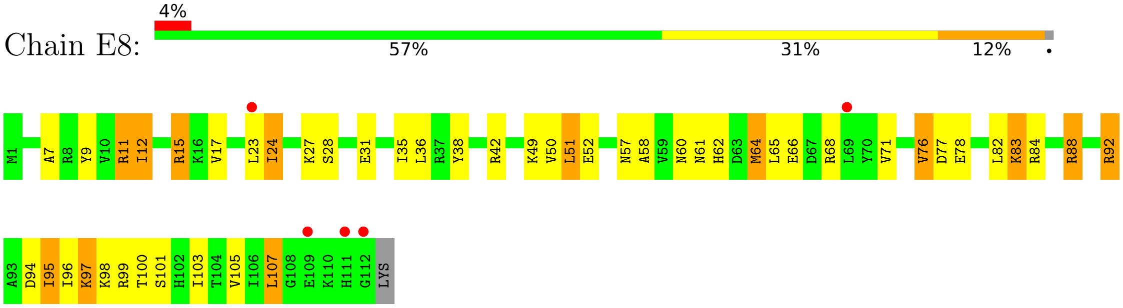
Chain D8:



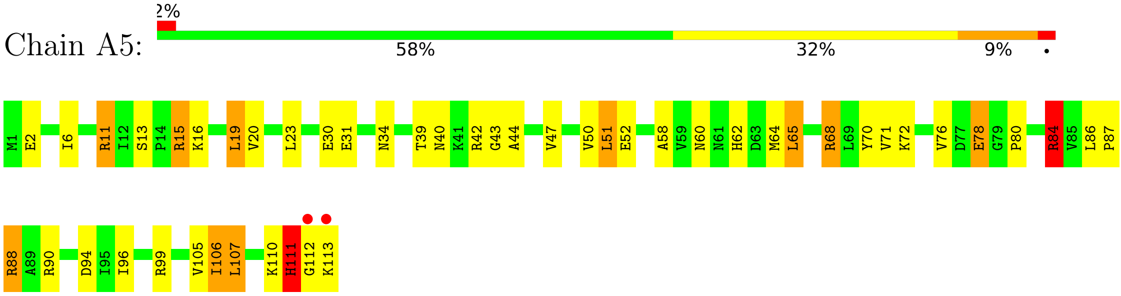
- Molecule 43: 50S ribosomal protein L21



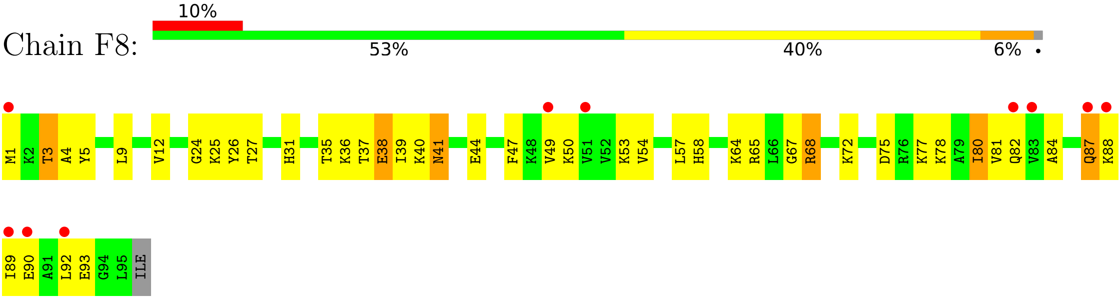
- Molecule 44: 50S ribosomal protein L22



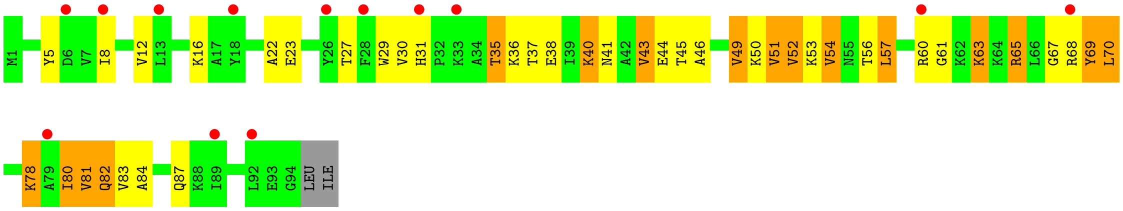
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23

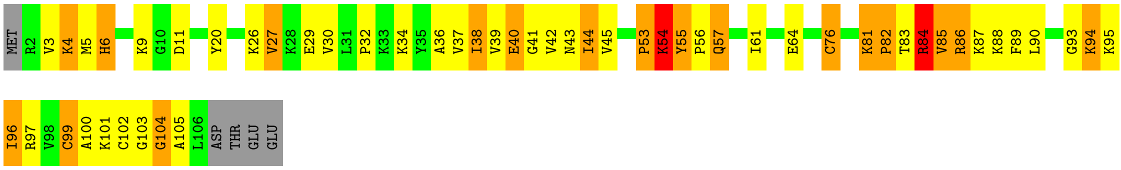


- Molecule 45: 50S ribosomal protein L23



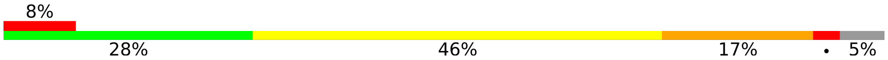
- Molecule 46: 50S ribosomal protein L24

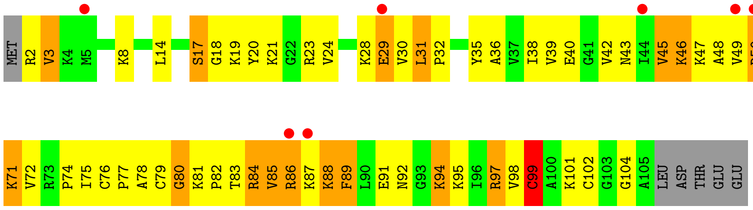
Chain G8:



- Molecule 46: 50S ribosomal protein L24

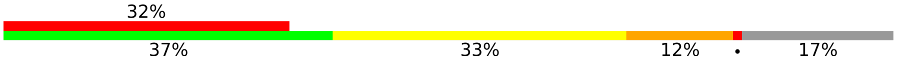
Chain C5:

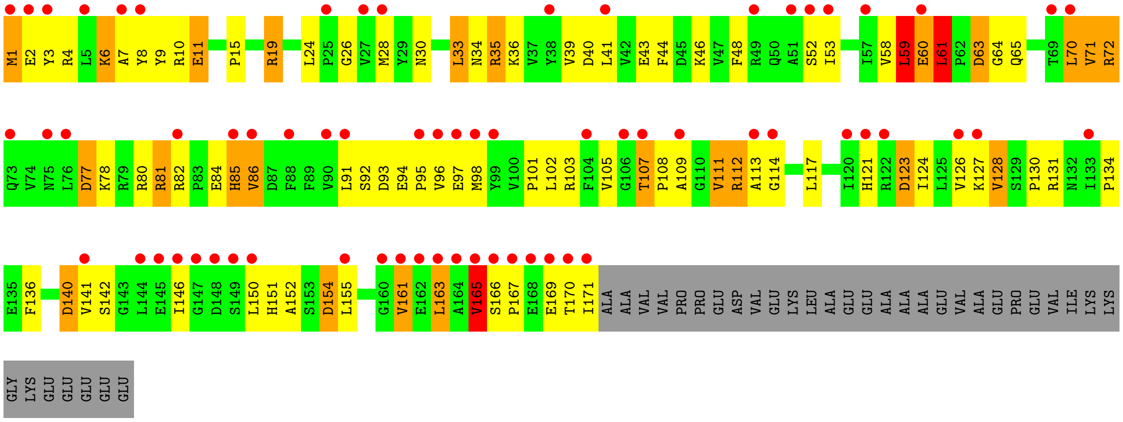




- Molecule 47: 50S ribosomal protein L25

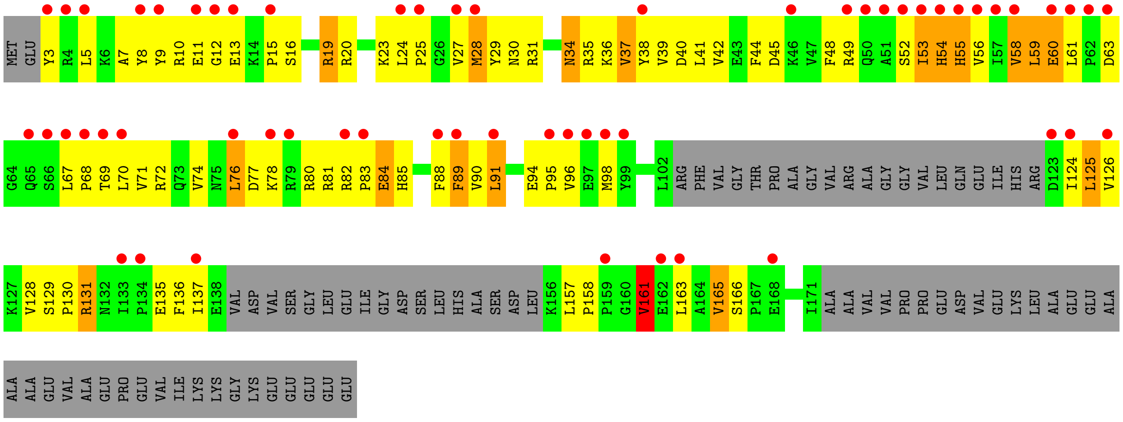
Chain H8:





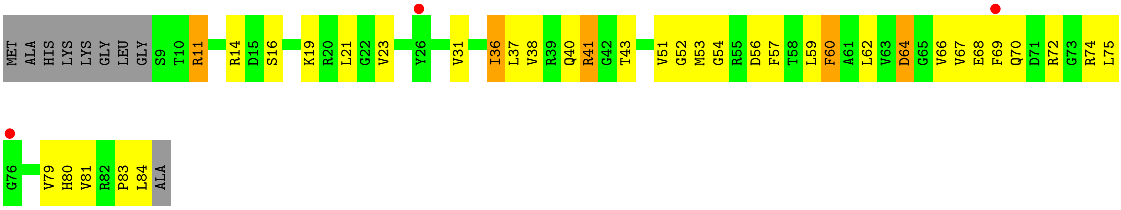
- Molecule 47: 50S ribosomal protein L25

Chain D5:



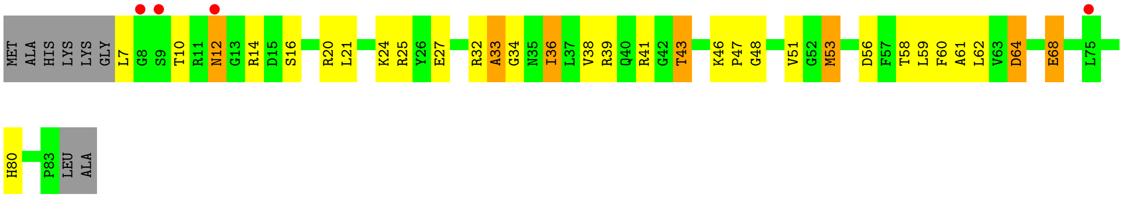
- Molecule 48: 50S ribosomal protein L27

Chain I8:



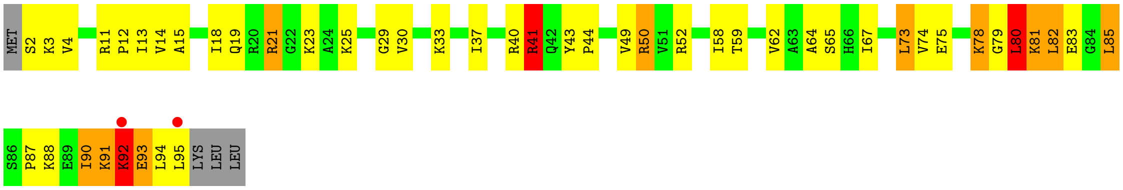
- Molecule 48: 50S ribosomal protein L27

Chain E5:



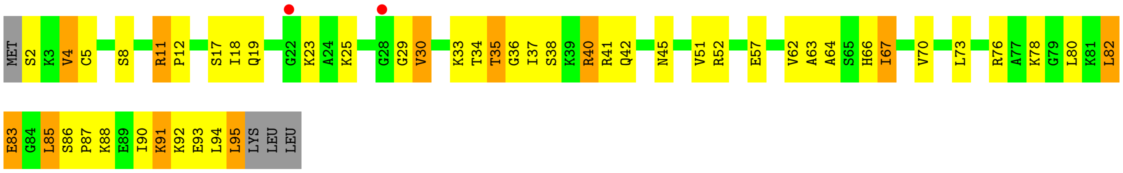
- Molecule 49: 50S ribosomal protein L28

Chain J8:



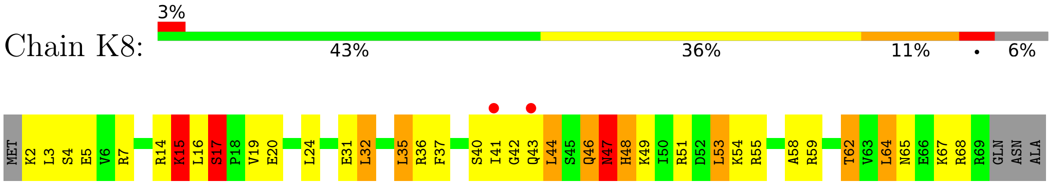
- Molecule 49: 50S ribosomal protein L28

Chain F5:



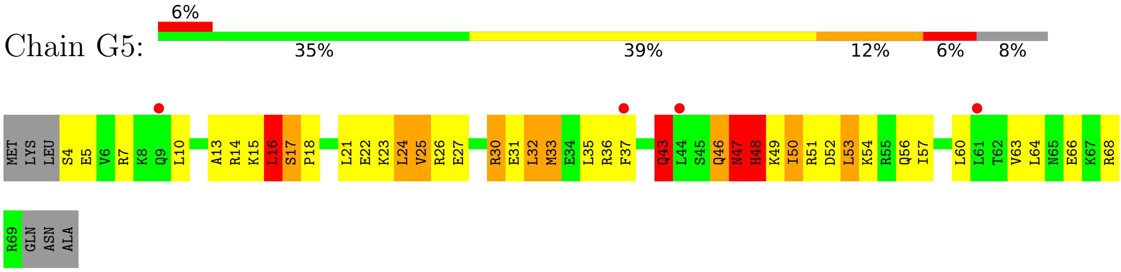
- Molecule 50: 50S ribosomal protein L29

Chain K8:



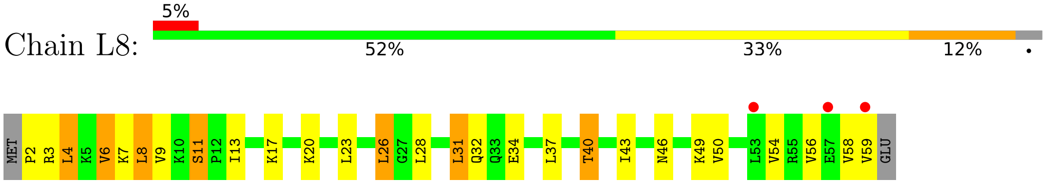
- Molecule 50: 50S ribosomal protein L29

Chain G5:



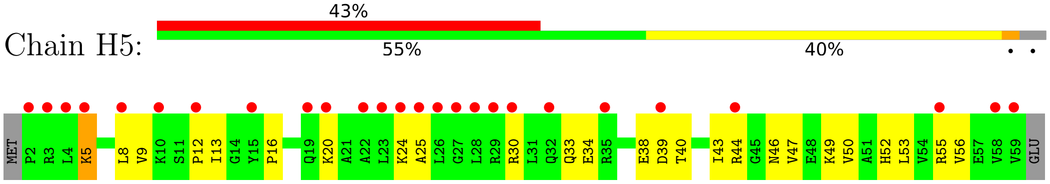
- Molecule 51: 50S ribosomal protein L30

Chain L8:



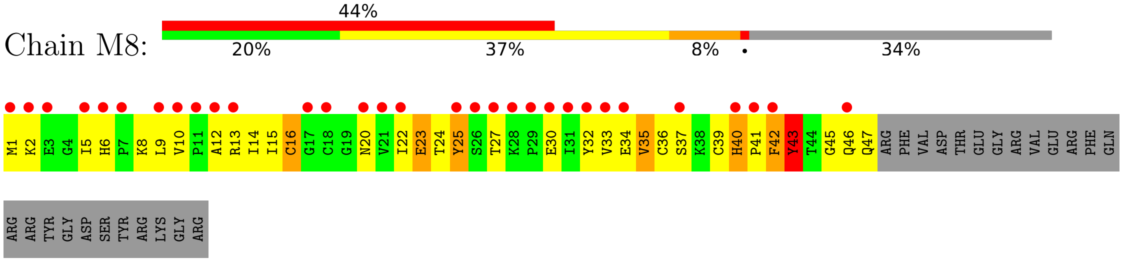
- Molecule 51: 50S ribosomal protein L30

Chain H5:

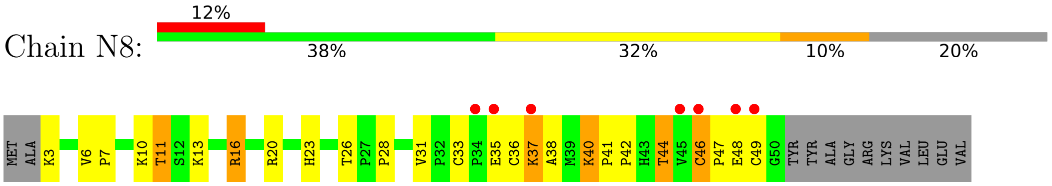


- Molecule 52: 50S ribosomal protein L31

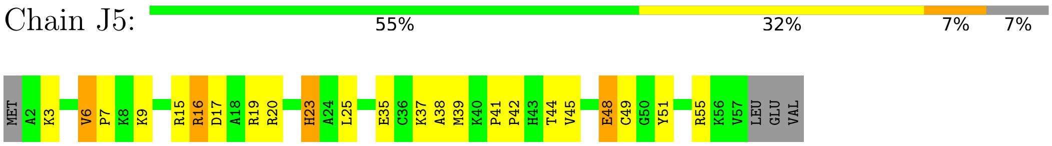
Chain M8:



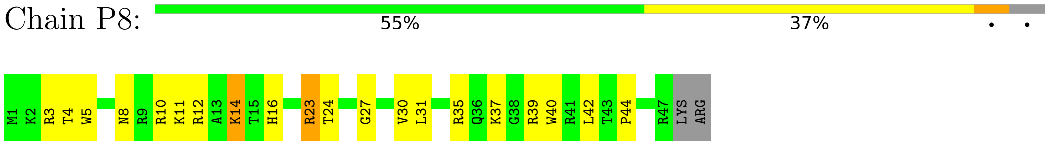
- Molecule 53: 50S ribosomal protein L32



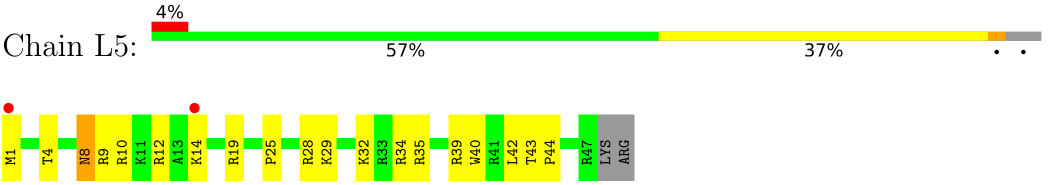
- Molecule 53: 50S ribosomal protein L32



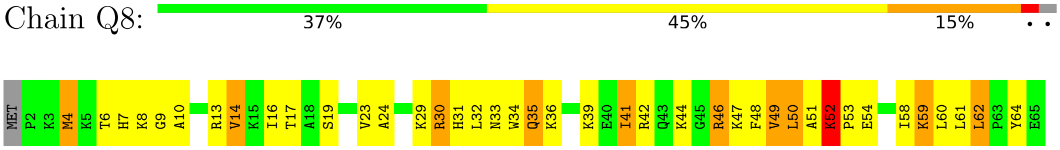
- Molecule 54: 50S ribosomal protein L34



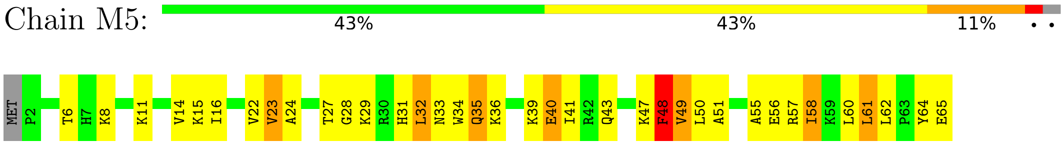
- Molecule 54: 50S ribosomal protein L34



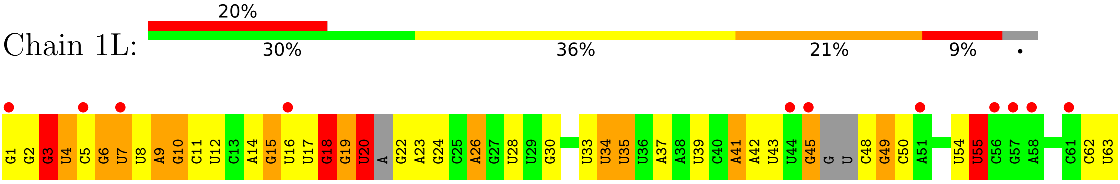
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35

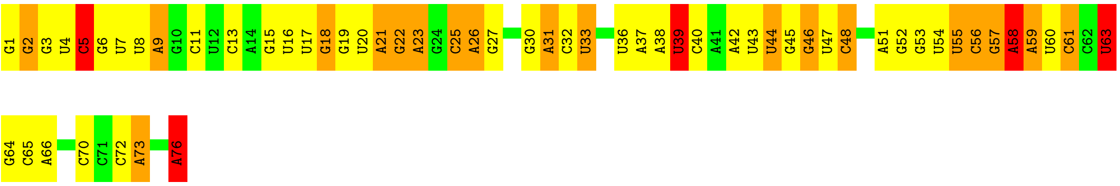


- Molecule 56: tRNALys



- Molecule 57: tRNALys

Chain 3L:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.50Å 450.10Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.72 – 3.20 173.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.72-3.20) 93.8 (173.72-3.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.258 0.192 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 77.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	294444	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, G7M, PSU, SF4, U8U, 5MU, T6A, MG, ZN, OMC

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	13	0.75	5/35994 (0.0%)	1.39	368/56171 (0.7%)
1	1G	0.64	1/36258 (0.0%)	1.26	191/56589 (0.3%)
2	12	0.44	0/1752	0.74	1/2360 (0.0%)
2	1E	0.46	0/1908	0.74	4/2573 (0.2%)
3	22	0.40	0/1564	0.64	1/2109 (0.0%)
3	2E	0.49	0/1629	0.67	0/2195
4	32	0.48	0/1732	0.74	1/2318 (0.0%)
4	3E	0.52	0/1728	0.74	1/2313 (0.0%)
5	42	0.45	0/1150	0.69	0/1548
5	4E	0.53	0/1158	0.71	0/1559
6	52	0.51	0/855	0.68	0/1154
6	5E	0.57	0/850	0.72	0/1147
7	62	0.43	0/1122	0.65	0/1500
7	6E	0.43	0/1259	0.59	0/1686
8	72	0.41	0/1127	0.65	0/1517
8	7E	0.47	0/1135	0.74	1/1527 (0.1%)
9	82	0.42	0/971	0.71	0/1304
9	8E	0.44	0/1019	0.66	0/1367
10	1A	0.42	0/658	0.60	0/885
10	1I	0.51	0/747	0.75	1/1006 (0.1%)
11	2A	0.45	0/850	0.63	0/1150
11	2I	0.49	0/838	0.69	0/1133
12	3A	0.55	0/972	0.83	2/1301 (0.2%)
12	3I	0.72	0/972	0.87	0/1301
13	4A	0.42	0/903	0.72	1/1211 (0.1%)
13	4I	0.53	0/952	0.73	0/1277
14	5A	0.47	0/495	0.72	1/657 (0.2%)
14	5I	0.62	0/500	0.75	0/664
15	6A	0.44	0/744	0.59	0/992
15	6I	0.52	0/740	0.71	0/987
16	7A	0.49	0/721	0.74	0/970
16	7I	0.47	0/716	0.73	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.45	0/836	0.64	0/1117
17	8I	0.52	0/847	0.70	0/1131
18	9A	0.46	0/549	0.70	0/732
18	9I	0.53	0/554	0.77	0/739
19	AA	0.44	0/490	0.70	0/662
19	AI	0.53	0/668	0.79	0/899
20	BA	0.43	0/764	0.73	0/1007
20	BI	0.43	0/748	0.65	1/986 (0.1%)
21	1B	0.47	0/192	0.70	0/252
21	1F	0.52	0/203	0.68	0/266
22	1K	0.66	0/1565	1.29	14/2429 (0.6%)
23	2K	0.84	1/1721 (0.1%)	1.50	32/2682 (1.2%)
23	2L	0.66	1/1721 (0.1%)	1.24	10/2682 (0.4%)
24	3K	0.67	0/1799	1.31	17/2801 (0.6%)
25	4K	0.91	0/473	1.34	1/737 (0.1%)
25	4L	0.67	0/448	1.13	0/698
26	14	0.90	57/69023 (0.1%)	1.59	1407/107740 (1.3%)
26	1H	1.06	113/68351 (0.2%)	1.80	2304/106700 (2.2%)
27	16	0.84	0/2928	1.55	47/4568 (1.0%)
27	1J	0.70	0/2928	1.36	28/4568 (0.6%)
28	71	0.46	0/1055	0.72	1/1425 (0.1%)
28	79	0.43	0/459	0.90	3/608 (0.5%)
29	11	0.82	2/2170 (0.1%)	1.01	7/2926 (0.2%)
29	19	0.71	1/2175 (0.0%)	0.93	3/2933 (0.1%)
30	21	0.67	0/1591	0.96	2/2146 (0.1%)
30	29	0.63	0/1596	0.92	2/2153 (0.1%)
31	31	0.73	1/1620 (0.1%)	0.91	1/2194 (0.0%)
31	39	0.62	0/1637	0.90	3/2218 (0.1%)
32	41	0.52	0/1481	0.78	1/1994 (0.1%)
32	49	0.43	0/1482	0.68	0/1994
33	51	0.68	0/1337	1.00	9/1809 (0.5%)
33	59	0.46	0/577	0.88	2/776 (0.3%)
34	61	0.52	0/1151	0.80	2/1558 (0.1%)
34	69	0.46	0/1146	0.77	3/1551 (0.2%)
35	15	0.46	0/1131	0.68	0/1525
35	58	0.60	0/1131	0.82	0/1525
36	25	0.58	0/942	0.74	0/1269
36	68	0.67	0/942	0.81	0/1269
37	35	0.61	0/1139	0.98	2/1514 (0.1%)
37	78	0.70	0/1139	1.12	8/1514 (0.5%)
38	45	0.69	0/1120	0.97	4/1498 (0.3%)
38	88	0.78	0/1134	0.98	2/1519 (0.1%)
39	55	0.64	0/981	0.85	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	98	0.56	0/981	0.85	1/1312 (0.1%)
40	65	0.51	0/886	0.86	3/1180 (0.3%)
40	A8	0.63	0/891	0.85	1/1187 (0.1%)
41	75	0.56	0/1123	0.72	0/1500
41	B8	0.66	0/1123	0.82	0/1500
42	85	0.59	0/977	0.75	1/1301 (0.1%)
42	C8	0.67	0/968	0.82	1/1289 (0.1%)
43	95	0.70	0/785	0.87	1/1052 (0.1%)
43	D8	0.58	0/785	0.90	4/1052 (0.4%)
44	A5	0.62	0/910	0.84	1/1220 (0.1%)
44	E8	0.66	0/901	0.87	0/1209
45	B5	0.68	0/749	0.79	0/1007
45	F8	0.76	0/757	0.87	0/1017
46	C5	0.63	0/807	0.93	2/1076 (0.2%)
46	G8	0.82	1/809 (0.1%)	1.08	4/1080 (0.4%)
47	D5	0.51	0/1098	0.73	0/1487
47	H8	0.53	0/1403	0.81	1/1901 (0.1%)
48	E5	0.57	0/616	0.84	0/821
48	I8	0.76	0/614	0.94	0/819
49	F5	0.66	0/744	0.88	1/989 (0.1%)
49	J8	0.73	0/744	0.93	4/989 (0.4%)
50	G5	0.59	0/560	0.82	2/741 (0.3%)
50	K8	0.72	0/570	0.97	0/755
51	H5	0.49	0/464	0.66	0/623
51	L8	0.63	0/464	0.84	0/623
52	M8	0.53	0/375	0.95	2/507 (0.4%)
53	J5	0.61	0/448	0.81	0/606
53	N8	0.69	1/381 (0.3%)	0.86	0/516
54	L5	0.69	0/409	0.89	0/540
54	P8	0.85	0/409	1.07	2/540 (0.4%)
55	M5	0.75	0/524	1.00	3/691 (0.4%)
55	Q8	0.79	0/524	1.17	4/691 (0.6%)
56	1L	0.61	1/1613 (0.1%)	1.18	11/2504 (0.4%)
57	3L	0.65	0/1733	1.28	14/2699 (0.5%)
All	All	0.81	185/317108 (0.1%)	1.41	4553/475084 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	13	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	4
2	1E	0	4
3	22	0	2
4	32	0	1
4	3E	0	1
9	82	0	1
9	8E	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	1
13	4A	0	2
13	4I	0	3
14	5A	0	1
18	9I	0	1
19	AI	0	2
20	BA	0	2
28	71	0	3
29	11	0	4
29	19	0	4
30	21	0	5
30	29	0	5
31	31	0	4
31	39	0	7
32	41	0	1
32	49	0	1
33	51	0	6
34	61	0	4
34	69	0	2
37	35	0	3
37	78	0	5
38	45	0	6
38	88	0	1
39	55	0	1
39	98	0	1
40	65	0	1
41	75	0	1
41	B8	0	1
42	85	0	4
42	C8	0	2
43	95	0	2
43	D8	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	A5	0	2
45	B5	0	1
45	F8	0	2
46	C5	0	3
46	G8	0	7
47	D5	0	2
47	H8	0	4
49	J8	0	2
50	G5	0	4
50	K8	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	1
All	All	1	141

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-11.99	1.30	1.37
26	1H	2430	A	N9-C4	-11.47	1.30	1.37
26	1H	783	A	N3-C4	-11.40	1.28	1.34
26	14	2430	A	N9-C4	-10.71	1.31	1.37
26	14	528	A	N9-C4	-10.24	1.31	1.37

The worst 5 of 4553 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-19.34	114.40	126.00
26	1H	783	A	C8-N9-C4	-17.08	98.97	105.80
26	14	2518	A	N1-C6-N6	17.07	128.84	118.60
26	1H	676	A	C2-N3-C4	-16.88	102.16	110.60
26	14	774	A	C2-N3-C4	-16.75	102.23	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	A	C1’

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	9	GLU	Peptide
4	3E	193	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16233	755	0
1	1G	32391	0	16353	749	0
2	12	1721	0	1758	101	0
2	1E	1874	0	1926	103	0
3	22	1541	0	1606	69	0
3	2E	1605	0	1668	58	0
4	32	1702	0	1765	110	0
4	3E	1698	0	1761	83	0
5	42	1134	0	1200	45	0
5	4E	1142	0	1204	62	0
6	52	842	0	857	30	0
6	5E	837	0	852	35	0
7	62	1110	0	1163	49	0
7	6E	1242	0	1286	44	0
8	72	1107	0	1165	39	0
8	7E	1115	0	1177	58	0
9	82	953	0	983	70	0
9	8E	1000	0	1031	58	0
10	1A	646	0	662	33	0
10	1I	734	0	761	43	0
11	2A	835	0	847	31	0
11	2I	823	0	833	49	0
12	3A	956	0	1046	56	0
12	3I	956	0	1046	33	0
13	4A	893	0	946	61	0
13	4I	942	0	997	53	0
14	5A	486	0	525	25	0
14	5I	491	0	529	26	0
15	6A	733	0	771	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	29	0
16	7A	705	0	725	29	0
16	7I	700	0	720	47	0
17	8A	823	0	891	35	0
17	8I	834	0	904	42	0
18	9A	544	0	605	26	0
18	9I	549	0	607	36	0
19	AA	481	0	468	32	0
19	AI	654	0	675	44	0
20	BA	762	0	861	32	0
20	BI	746	0	843	49	0
21	1B	188	0	195	13	0
21	1F	199	0	208	5	0
22	1K	1520	0	778	41	0
23	2K	1646	0	843	30	0
23	2L	1646	0	843	40	0
24	3K	1611	0	817	48	0
25	4K	419	0	208	6	0
25	4L	397	0	197	12	0
26	14	61630	0	31073	1315	0
26	1H	61028	0	30763	1351	0
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	65	0
28	71	1033	0	1048	77	0
28	79	456	0	460	22	0
29	11	2120	0	2197	131	0
29	19	2125	0	2199	104	0
30	21	1558	0	1624	83	0
30	29	1563	0	1629	117	0
31	31	1585	0	1632	89	0
31	39	1602	0	1649	80	0
32	41	1457	0	1514	94	0
32	49	1458	0	1516	59	0
33	51	1312	0	1384	66	0
33	59	568	0	595	48	0
34	61	1136	0	1223	57	0
34	69	1131	0	1218	48	0
35	15	1104	0	1180	38	0
35	58	1104	0	1180	54	0
36	25	932	0	996	36	0
36	68	932	0	996	42	0
37	35	1122	0	1206	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	78	1122	0	1206	94	0
38	45	1099	0	1154	79	0
38	88	1113	0	1157	51	0
39	55	967	0	1033	49	0
39	98	967	0	1033	49	0
40	65	876	0	938	65	0
40	A8	881	0	943	52	0
41	75	1109	0	1170	55	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	53	0
42	C8	950	0	1011	52	0
43	95	774	0	849	63	0
43	D8	774	0	849	43	0
44	A5	899	0	964	28	0
44	E8	890	0	951	25	0
45	B5	735	0	785	35	0
45	F8	743	0	794	36	0
46	C5	794	0	886	68	0
46	G8	796	0	886	45	0
47	D5	1074	0	1086	53	0
47	H8	1373	0	1402	59	0
48	E5	608	0	622	26	0
48	I8	606	0	625	30	0
49	F5	737	0	813	32	0
49	J8	737	0	813	39	0
50	G5	558	0	610	33	0
50	K8	568	0	614	36	0
51	H5	459	0	512	10	0
51	L8	459	0	512	18	0
52	M8	366	0	370	37	0
53	J5	434	0	454	22	0
53	N8	369	0	388	22	0
54	L5	401	0	436	14	0
54	P8	401	0	436	14	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1563	0	799	42	0
57	3L	1612	0	819	41	0
58	13	132	0	0	0	0
58	14	399	0	0	0	0
58	16	9	0	0	0	0
58	1E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1G	90	0	0	0	0
58	1H	467	0	0	0	0
58	1J	5	0	0	0	0
58	1K	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	4	0	0	0	0
58	2K	3	0	0	0	0
58	2L	2	0	0	0	0
58	35	3	0	0	0	0
58	39	1	0	0	0	0
58	3K	1	0	0	0	0
58	41	1	0	0	0	0
58	45	2	0	0	0	0
58	55	1	0	0	0	0
58	5E	1	0	0	0	0
58	6A	1	0	0	0	0
58	78	1	0	0	0	0
58	88	1	0	0	0	0
58	98	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	3	0	0	0	0
58	J8	1	0	0	0	0
58	L8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	2	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	7	0	0	5	0
61	13	126	0	0	21	0
61	14	417	0	0	73	0
61	16	29	0	0	6	0
61	19	8	0	0	1	0
61	1G	78	0	0	9	0
61	1H	629	0	0	101	0
61	1J	6	0	0	1	0
61	1K	8	0	0	0	0
61	21	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	2	0	0	0	0
61	31	9	0	0	0	0
61	32	1	0	0	0	0
61	35	1	0	0	0	0
61	39	5	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	4K	2	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	2	0	0	0	0
61	5I	2	0	0	0	0
61	78	7	0	0	2	0
61	88	1	0	0	0	0
61	A5	1	0	0	0	0
61	B8	1	0	0	0	0
61	E8	2	0	0	0	0
61	F8	1	0	0	0	0
61	G8	1	0	0	0	0
61	H5	2	0	0	1	0
61	I8	3	0	0	1	0
61	L8	2	0	0	1	0
All	All	294444	0	196318	8229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8229 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)
46:G8:100:ALA:HB1	46:G8:101:LYS:HG2	1.34	1.09
55:M5:48:PHE:HB2	55:M5:49:VAL:HG22	1.31	1.07
26:14:161:U:H5’	26:14:171:G:H21	1.18	1.06
26:1H:2711:A:OP2	61:1H:3501:HOH:O	1.73	1.05
26:14:2002:G:N7	61:14:3505:HOH:O	1.91	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	206/256 (80%)	168 (82%)	31 (15%)	7 (3%)	3	24
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12	47
3	22	192/239 (80%)	169 (88%)	22 (12%)	1 (0%)	29	67
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29	67
4	3E	205/209 (98%)	188 (92%)	14 (7%)	3 (2%)	10	44
5	42	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22	61
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	22	61
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22	61
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	22	61
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22	61
9	82	119/128 (93%)	107 (90%)	11 (9%)	1 (1%)	19	58
9	8E	124/128 (97%)	104 (84%)	19 (15%)	1 (1%)	19	58
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	89/105 (85%)	83 (93%)	6 (7%)	0	100	100
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	8	41
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	17	56
12	3A	120/132 (91%)	102 (85%)	13 (11%)	5 (4%)	3	20
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	58
13	4A	109/126 (86%)	95 (87%)	13 (12%)	1 (1%)	17	56
13	4I	117/126 (93%)	97 (83%)	19 (16%)	1 (1%)	17	56
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	24
15	6A	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	2 (3%)	1 (2%)	10	44
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	44
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	3	23
19	AI	79/93 (85%)	67 (85%)	10 (13%)	2 (2%)	5	32
20	BA	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	7	37
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	119 (92%)	10 (8%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	243 (90%)	17 (6%)	11 (4%)	3	21
29	19	272/276 (99%)	241 (89%)	25 (9%)	6 (2%)	6	35
30	21	201/206 (98%)	157 (78%)	36 (18%)	8 (4%)	3	21
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	21
31	31	200/210 (95%)	175 (88%)	25 (12%)	0	100	100
31	39	202/210 (96%)	157 (78%)	36 (18%)	9 (4%)	2	18
32	41	177/182 (97%)	155 (88%)	19 (11%)	3 (2%)	9	42
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	14	51
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	12
33	59	67/180 (37%)	50 (75%)	14 (21%)	3 (4%)	2	18
34	61	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	11	46
34	69	143/148 (97%)	116 (81%)	26 (18%)	1 (1%)	22	61
35	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	61
35	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
36	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	35	145/150 (97%)	114 (79%)	29 (20%)	2 (1%)	11	46
37	78	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3	24
38	45	136/141 (96%)	112 (82%)	21 (15%)	3 (2%)	6	35
38	88	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	23
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	56
39	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	17	56
40	65	108/112 (96%)	86 (80%)	20 (18%)	2 (2%)	8	39
40	A8	109/112 (97%)	92 (84%)	14 (13%)	3 (3%)	5	29
41	75	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
41	B8	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
42	85	114/118 (97%)	101 (89%)	11 (10%)	2 (2%)	8	41
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	30
43	95	98/101 (97%)	77 (79%)	14 (14%)	7 (7%)	1	8
43	D8	98/101 (97%)	87 (89%)	6 (6%)	5 (5%)	2	15
44	A5	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	17	56
44	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	4 (4%)	3 (3%)	4	25
45	F8	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	51
46	C5	102/110 (93%)	75 (74%)	17 (17%)	10 (10%)	0	3
46	G8	103/110 (94%)	86 (84%)	13 (13%)	4 (4%)	3	22
47	D5	126/206 (61%)	100 (79%)	21 (17%)	5 (4%)	3	21
47	H8	169/206 (82%)	136 (80%)	25 (15%)	8 (5%)	2	17
48	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	12	47
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	85 (92%)	6 (6%)	1 (1%)	14	51
49	J8	92/98 (94%)	83 (90%)	8 (9%)	1 (1%)	14	51
50	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	4	26
50	K8	66/72 (92%)	58 (88%)	5 (8%)	3 (4%)	2	18
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	M8	45/71 (63%)	29 (64%)	15 (33%)	1 (2%)	6	35
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	P8	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
55	M5	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	26
55	Q8	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	17
All	All	10973/12333 (89%)	9576 (87%)	1201 (11%)	196 (2%)	8	41

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	13	THR
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	154 (85%)	28 (15%)	2	13
2	1E	200/220 (91%)	143 (72%)	57 (28%)	0	1
3	22	154/188 (82%)	123 (80%)	31 (20%)	1	6
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	5
4	32	180/181 (99%)	143 (79%)	37 (21%)	1	6
4	3E	180/181 (99%)	137 (76%)	43 (24%)	0	3
5	42	114/123 (93%)	91 (80%)	23 (20%)	1	6
5	4E	115/123 (94%)	98 (85%)	17 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	6
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1	8
7	62	114/127 (90%)	95 (83%)	19 (17%)	2	10
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1	8
8	72	118/119 (99%)	98 (83%)	20 (17%)	2	10
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	92/99 (93%)	71 (77%)	21 (23%)	1	4
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	6
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	1
10	1I	81/92 (88%)	65 (80%)	16 (20%)	1	7
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	9
11	2I	84/99 (85%)	61 (73%)	23 (27%)	0	1
12	3A	103/109 (94%)	81 (79%)	22 (21%)	1	5
12	3I	103/109 (94%)	87 (84%)	16 (16%)	2	12
13	4A	91/101 (90%)	70 (77%)	21 (23%)	1	3
13	4I	94/101 (93%)	75 (80%)	19 (20%)	1	6
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1	4
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	13
15	6I	79/80 (99%)	62 (78%)	17 (22%)	1	5
16	7A	72/74 (97%)	52 (72%)	20 (28%)	0	1
16	7I	72/74 (97%)	51 (71%)	21 (29%)	0	1
17	8A	94/97 (97%)	79 (84%)	15 (16%)	2	11
17	8I	95/97 (98%)	79 (83%)	16 (17%)	2	10
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0	1
18	9I	58/77 (75%)	44 (76%)	14 (24%)	0	3
19	AA	52/80 (65%)	40 (77%)	12 (23%)	1	3
19	AI	71/80 (89%)	58 (82%)	13 (18%)	1	8
20	BA	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	BI	75/82 (92%)	59 (79%)	16 (21%)	1	5
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1F	18/22 (82%)	17 (94%)	1 (6%)	21	57
28	71	109/181 (60%)	87 (80%)	22 (20%)	1	6
28	79	48/181 (26%)	38 (79%)	10 (21%)	1	6
29	11	214/218 (98%)	161 (75%)	53 (25%)	0	2
29	19	214/218 (98%)	169 (79%)	45 (21%)	1	6
30	21	165/166 (99%)	128 (78%)	37 (22%)	1	4
30	29	165/166 (99%)	126 (76%)	39 (24%)	1	3
31	31	161/166 (97%)	126 (78%)	35 (22%)	1	5
31	39	163/166 (98%)	130 (80%)	33 (20%)	1	6
32	41	153/156 (98%)	121 (79%)	32 (21%)	1	6
32	49	153/156 (98%)	125 (82%)	28 (18%)	1	8
33	51	142/148 (96%)	109 (77%)	33 (23%)	1	3
33	59	59/148 (40%)	50 (85%)	9 (15%)	2	13
34	61	122/124 (98%)	95 (78%)	27 (22%)	1	4
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	117/119 (98%)	87 (74%)	30 (26%)	0	2
35	58	117/119 (98%)	90 (77%)	27 (23%)	1	3
36	25	100/100 (100%)	82 (82%)	18 (18%)	1	9
36	68	100/100 (100%)	85 (85%)	15 (15%)	3	14
37	35	114/116 (98%)	78 (68%)	36 (32%)	0	0
37	78	114/116 (98%)	80 (70%)	34 (30%)	0	1
38	45	109/111 (98%)	89 (82%)	20 (18%)	1	8
38	88	109/111 (98%)	87 (80%)	22 (20%)	1	6
39	55	101/101 (100%)	83 (82%)	18 (18%)	2	9
39	98	101/101 (100%)	76 (75%)	25 (25%)	0	2
40	65	87/88 (99%)	64 (74%)	23 (26%)	0	2
40	A8	87/88 (99%)	67 (77%)	20 (23%)	1	3
41	75	117/127 (92%)	91 (78%)	26 (22%)	1	4
41	B8	117/127 (92%)	87 (74%)	30 (26%)	0	2
42	85	93/94 (99%)	83 (89%)	10 (11%)	6	27
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	95	82/82 (100%)	61 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	59 (72%)	23 (28%)	0	1
44	A5	92/92 (100%)	73 (79%)	19 (21%)	1	6
44	E8	91/92 (99%)	65 (71%)	26 (29%)	0	1
45	B5	74/78 (95%)	52 (70%)	22 (30%)	0	1
45	F8	75/78 (96%)	64 (85%)	11 (15%)	3	14
46	C5	85/91 (93%)	60 (71%)	25 (29%)	0	1
46	G8	85/91 (93%)	70 (82%)	15 (18%)	2	9
47	D5	118/179 (66%)	93 (79%)	25 (21%)	1	5
47	H8	152/179 (85%)	113 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	4	19
48	I8	61/67 (91%)	51 (84%)	10 (16%)	2	11
49	F5	79/83 (95%)	61 (77%)	18 (23%)	1	4
49	J8	79/83 (95%)	60 (76%)	19 (24%)	0	3
50	G5	62/67 (92%)	47 (76%)	15 (24%)	0	2
50	K8	62/67 (92%)	44 (71%)	18 (29%)	0	1
51	H5	50/52 (96%)	40 (80%)	10 (20%)	1	6
51	L8	50/52 (96%)	38 (76%)	12 (24%)	0	3
52	M8	42/63 (67%)	31 (74%)	11 (26%)	0	2
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	8
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	6
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4	19
54	P8	38/42 (90%)	34 (90%)	4 (10%)	7	28
55	M5	54/55 (98%)	44 (82%)	10 (18%)	1	8
55	Q8	54/55 (98%)	39 (72%)	15 (28%)	0	1
All	All	9277/10193 (91%)	7277 (78%)	2000 (22%)	1	5

5 of 2000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	2	GLU
40	65	89	ARG
4	32	152	SER

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Mol	Chain	Res	Type
40	65	4	LEU
46	C5	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
10	1A	84	GLN
18	9A	36	ASN
44	A5	60	ASN
14	5A	49	HIS
19	AA	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	361 (24%)	29 (1%)
1	1G	1506/1522 (98%)	367 (24%)	27 (1%)
22	1K	67/75 (89%)	27 (40%)	2 (2%)
23	2K	76/77 (98%)	22 (28%)	1 (1%)
23	2L	76/77 (98%)	14 (18%)	2 (2%)
24	3K	75/76 (98%)	42 (56%)	4 (5%)
25	4K	18/27 (66%)	12 (66%)	2 (11%)
25	4L	17/27 (62%)	9 (52%)	0
26	14	2853/2917 (97%)	731 (25%)	38 (1%)
26	1H	2829/2917 (96%)	722 (25%)	50 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	1 (0%)
56	1L	69/76 (90%)	27 (39%)	4 (5%)
57	3L	75/76 (98%)	35 (46%)	1 (1%)
All	All	9396/9633 (97%)	2428 (25%)	162 (1%)

5 of 2428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	9	G
1	13	15	G

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1533	C
26	14	1558	A
56	1L	69	A
26	14	528	A
26	14	2275	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PSU	3L	39	57	18,21,22	1.24	1 (5%)	22,30,33	1.46	4 (18%)
56	T6A	1L	37	56	27,34,35	2.48	6 (22%)	29,49,52	2.37	8 (27%)
57	5MU	3L	54	57	19,22,23	4.05	6 (31%)	28,32,35	2.95	10 (35%)
22	T6A	1K	37	22	27,34,35	2.37	7 (25%)	29,49,52	1.98	5 (17%)
56	U8U	1L	34	25,56	19,24,25	2.68	7 (36%)	23,34,37	0.94	1 (4%)
56	PSU	1L	55	56	18,21,22	1.09	1 (5%)	22,30,33	1.60	4 (18%)
22	PSU	1K	39	22	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
23	4SU	2K	8	23	18,21,22	1.82	4 (22%)	26,30,33	2.30	5 (19%)
23	5MU	2K	55	23	19,22,23	3.79	5 (26%)	28,32,35	3.53	9 (32%)
23	G7M	2L	47	23	20,26,27	4.82	5 (25%)	17,39,42	1.15	1 (5%)
56	PSU	1L	39	56	18,21,22	1.14	1 (5%)	22,30,33	1.57	3 (13%)
23	OMC	2L	33	23	19,22,23	1.71	3 (15%)	26,31,34	1.06	3 (11%)
57	PSU	3L	55	57	18,21,22	1.20	1 (5%)	22,30,33	1.73	5 (22%)
22	U8U	1K	34	22,25	19,24,25	2.42	6 (31%)	23,34,37	0.91	1 (4%)
23	PSU	2K	56	23	18,21,22	1.21	2 (11%)	22,30,33	1.91	3 (13%)
23	5MU	2L	55	23	19,22,23	3.80	5 (26%)	28,32,35	3.40	8 (28%)
22	5MU	1K	54	22	19,22,23	3.69	5 (26%)	28,32,35	3.13	6 (21%)
23	G7M	2K	47	23	20,26,27	4.75	6 (30%)	17,39,42	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	OMC	2K	33	23	19,22,23	1.72	4 (21%)	26,31,34	0.95	2 (7%)
56	5MU	1L	54	56	19,22,23	3.84	5 (26%)	28,32,35	3.25	8 (28%)
22	PSU	1K	55	22	18,21,22	1.08	1 (5%)	22,30,33	1.56	4 (18%)
23	PSU	2L	56	23	18,21,22	1.28	1 (5%)	22,30,33	1.73	4 (18%)
23	4SU	2L	8	23	18,21,22	1.76	3 (16%)	26,30,33	2.66	4 (15%)

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
57	PSU	3L	39	57	-	2/7/25/26	0/2/2/2
56	T6A	1L	37	56	-	5/19/41/42	0/3/3/3
57	5MU	3L	54	57	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/19/41/42	0/3/3/3
56	U8U	1L	34	25,56	-	2/9/28/29	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
57	PSU	3L	55	57	-	4/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	2/9/28/29	0/2/2/2
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	3/3/25/26	0/3/3/3
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	17.70	1.65	1.33
23	2K	47	G7M	C8-N7	17.48	1.65	1.33
57	3L	54	5MU	C2-N1	12.59	1.58	1.38
56	1L	54	5MU	C2-N1	12.47	1.58	1.38
23	2L	55	5MU	C2-N1	12.19	1.58	1.38

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	11.30	124.95	115.31
22	1K	54	5MU	C5-C4-N3	10.92	124.63	115.31
23	2L	55	5MU	C5-C4-N3	10.89	124.61	115.31
56	1L	54	5MU	C5-C4-N3	10.30	124.10	115.31
57	3L	54	5MU	C5-C4-N3	8.97	122.97	115.31

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
56	1L	37	T6A	C13-C12-C14-C15
57	3L	55	PSU	C2'-C1'-C5-C4
56	1L	34	U8U	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	3L	39	PSU	1	0
56	1L	34	U8U	2	0
56	1L	55	PSU	1	0
23	2L	47	G7M	2	0
23	2L	33	OMC	1	0
57	3L	55	PSU	1	0
23	2K	56	PSU	1	0
23	2L	55	5MU	1	0
23	2K	47	G7M	1	0
23	2K	33	OMC	2	0
23	2L	56	PSU	1	0
23	2L	8	4SU	2	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1144 ligands modelled in this entry, 1142 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	SF4	32	301	-	0,12,12	-	-	-		
59	SF4	3E	301	4	0,12,12	-	-	-		

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	SF4	32	301	-	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	301	SF4	2	0
59	3E	301	SF4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	13	1496/1522 (98%)	-0.66	1 (0%) 95 95	62, 109, 164, 193	0
1	1G	1507/1522 (99%)	-0.64	2 (0%) 95 95	80, 127, 170, 197	0
2	12	210/256 (82%)	0.46	23 (10%) 5 3	127, 152, 162, 177	0
2	1E	231/256 (90%)	0.62	29 (12%) 3 2	117, 141, 159, 166	0
3	22	196/239 (82%)	1.21	47 (23%) 0 0	129, 143, 156, 164	0
3	2E	205/239 (85%)	0.92	35 (17%) 1 1	94, 114, 136, 145	0
4	32	208/209 (99%)	1.20	45 (21%) 0 1	108, 128, 145, 152	0
4	3E	207/209 (99%)	0.82	27 (13%) 3 2	92, 114, 134, 139	0
5	42	148/162 (91%)	0.60	9 (6%) 21 12	114, 129, 143, 152	0
5	4E	149/162 (91%)	0.53	9 (6%) 21 12	89, 108, 124, 140	0
6	52	101/101 (100%)	1.28	21 (20%) 1 1	95, 111, 129, 137	0
6	5E	100/101 (99%)	0.77	11 (11%) 5 3	87, 107, 126, 136	0
7	62	138/156 (88%)	-0.42	0 100 100	121, 134, 144, 148	0
7	6E	154/156 (98%)	-0.23	2 (1%) 77 65	109, 125, 148, 166	0
8	72	137/138 (99%)	0.07	4 (2%) 51 36	111, 133, 142, 145	0
8	7E	138/138 (100%)	-0.05	1 (0%) 87 81	97, 117, 128, 138	0
9	82	121/128 (94%)	-0.34	2 (1%) 70 57	117, 149, 158, 163	0
9	8E	126/128 (98%)	-0.44	0 100 100	96, 135, 152, 157	0
10	1A	80/105 (76%)	0.04	2 (2%) 57 43	129, 146, 156, 161	0
10	1I	91/105 (86%)	0.47	7 (7%) 13 7	87, 128, 159, 165	0
11	2A	113/129 (87%)	0.76	13 (11%) 4 3	94, 117, 130, 138	0
11	2I	111/129 (86%)	0.35	5 (4%) 33 21	85, 113, 127, 142	0
12	3A	122/132 (92%)	1.10	28 (22%) 0 0	89, 107, 130, 146	0
12	3I	122/132 (92%)	1.08	16 (13%) 3 2	73, 82, 106, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	0.72	11 (9%) 7 4	125, 145, 156, 160	0
13	4I	119/126 (94%)	0.18	4 (3%) 45 29	93, 123, 136, 147	0
14	5A	59/61 (96%)	1.75	22 (37%) 0 0	134, 143, 153, 154	0
14	5I	60/61 (98%)	-0.16	0 100 100	92, 103, 118, 131	0
15	6A	88/89 (98%)	0.30	2 (2%) 60 47	96, 119, 135, 139	0
15	6I	87/89 (97%)	-0.07	0 100 100	88, 104, 122, 127	0
16	7A	84/88 (95%)	0.19	2 (2%) 59 44	102, 117, 135, 152	0
16	7I	83/88 (94%)	0.53	7 (8%) 11 6	110, 119, 143, 150	0
17	8A	99/105 (94%)	0.19	3 (3%) 50 34	105, 120, 132, 133	0
17	8I	100/105 (95%)	0.32	1 (1%) 82 72	98, 114, 124, 126	0
18	9A	67/88 (76%)	1.36	22 (32%) 0 0	106, 121, 135, 142	0
18	9I	68/88 (77%)	1.17	17 (25%) 0 0	94, 109, 133, 136	0
19	AA	62/93 (66%)	1.29	14 (22%) 0 0	134, 149, 156, 158	0
19	AI	81/93 (87%)	0.54	6 (7%) 14 8	102, 122, 138, 151	0
20	BA	99/106 (93%)	-0.19	1 (1%) 82 72	100, 118, 141, 152	0
20	BI	97/106 (91%)	-0.10	1 (1%) 82 72	112, 125, 148, 157	0
21	1B	22/27 (81%)	1.15	5 (22%) 0 0	129, 137, 145, 148	0
21	1F	23/27 (85%)	-0.33	0 100 100	94, 112, 118, 122	0
22	1K	66/75 (88%)	0.07	1 (1%) 73 61	85, 153, 177, 183	0
23	2K	72/77 (93%)	-0.44	0 100 100	77, 104, 132, 146	0
23	2L	72/77 (93%)	-0.30	0 100 100	85, 122, 151, 162	0
24	3K	76/76 (100%)	-0.28	1 (1%) 77 65	79, 178, 191, 196	0
25	4K	19/27 (70%)	-0.20	1 (5%) 26 14	79, 152, 184, 184	0
25	4L	18/27 (66%)	0.10	0 100 100	101, 161, 187, 187	0
26	14	2861/2917 (98%)	-0.36	35 (1%) 79 67	55, 92, 180, 204	0
26	1H	2833/2917 (97%)	-0.42	13 (0%) 91 86	49, 79, 168, 203	0
27	16	122/122 (100%)	-0.12	1 (0%) 86 78	74, 98, 119, 179	0
27	1J	122/122 (100%)	-0.73	0 100 100	93, 125, 145, 177	0
28	71	133/229 (58%)	1.28	35 (26%) 0 0	143, 174, 185, 189	0
28	79	57/229 (24%)	-0.24	1 (1%) 68 55	140, 165, 176, 179	0
29	11	273/276 (98%)	-0.20	0 100 100	48, 71, 89, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
29	19	274/276 (99%)	0.53	12 (4%)	34	21	58, 82, 101, 117	0
30	21	203/206 (98%)	0.81	35 (17%)	1	1	55, 93, 139, 153	0
30	29	204/206 (99%)	0.63	38 (18%)	1	1	60, 99, 134, 144	0
31	31	202/210 (96%)	0.39	21 (10%)	6	4	54, 84, 118, 142	0
31	39	204/210 (97%)	0.79	33 (16%)	1	1	62, 111, 151, 168	0
32	41	179/182 (98%)	1.18	39 (21%)	0	0	85, 107, 140, 156	0
32	49	179/182 (98%)	0.97	41 (22%)	0	0	122, 139, 155, 171	0
33	51	171/180 (95%)	0.46	9 (5%)	26	14	89, 110, 127, 139	0
33	59	73/180 (40%)	0.25	8 (10%)	5	3	136, 154, 165, 177	0
34	61	146/148 (98%)	1.08	35 (23%)	0	0	83, 130, 143, 150	0
34	69	145/148 (97%)	1.35	43 (29%)	0	0	93, 129, 147, 152	0
35	15	138/140 (98%)	1.92	56 (40%)	0	0	86, 114, 139, 155	0
35	58	138/140 (98%)	0.27	6 (4%)	35	22	68, 97, 130, 145	0
36	25	122/122 (100%)	0.04	0	100	100	77, 94, 114, 120	0
36	68	122/122 (100%)	0.03	2 (1%)	72	59	64, 81, 99, 104	0
37	35	147/150 (98%)	0.31	8 (5%)	25	14	65, 111, 138, 144	0
37	78	147/150 (98%)	0.05	3 (2%)	65	51	53, 88, 113, 120	0
38	45	138/141 (97%)	2.27	69 (50%)	0	0	78, 108, 128, 142	0
38	88	141/141 (100%)	1.23	31 (21%)	0	0	63, 83, 108, 129	0
39	55	118/118 (100%)	-0.03	1 (0%)	86	78	69, 86, 108, 127	0
39	98	118/118 (100%)	0.49	10 (8%)	10	6	67, 90, 109, 122	0
40	65	110/112 (98%)	0.34	5 (4%)	33	21	92, 117, 135, 142	0
40	A8	111/112 (99%)	2.42	65 (58%)	0	0	71, 93, 115, 123	0
41	75	133/146 (91%)	-0.35	3 (2%)	60	47	87, 101, 129, 141	0
41	B8	133/146 (91%)	-0.43	2 (1%)	73	61	78, 98, 133, 149	0
42	85	116/118 (98%)	1.37	33 (28%)	0	0	73, 100, 132, 138	0
42	C8	115/118 (97%)	-0.16	3 (2%)	56	40	59, 86, 114, 118	0
43	95	100/101 (99%)	2.98	69 (69%)	0	0	69, 121, 139, 153	0
43	D8	100/101 (99%)	0.14	6 (6%)	21	12	62, 106, 126, 144	0
44	A5	113/113 (100%)	0.01	2 (1%)	68	55	68, 82, 112, 158	0
44	E8	112/113 (99%)	0.36	5 (4%)	33	21	63, 79, 106, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	B5	94/96 (97%)	0.94	13 (13%) 2 2	77, 91, 118, 128	0
45	F8	95/96 (98%)	0.67	10 (10%) 6 3	60, 76, 104, 118	0
46	C5	104/110 (94%)	0.44	9 (8%) 10 5	91, 122, 149, 154	0
46	G8	105/110 (95%)	-0.23	0 100 100	75, 101, 131, 139	0
47	D5	132/206 (64%)	1.81	58 (43%) 0 0	115, 135, 150, 158	0
47	H8	171/206 (83%)	1.74	66 (38%) 0 0	90, 122, 167, 172	0
48	E5	77/85 (90%)	0.12	4 (5%) 27 15	72, 94, 111, 131	0
48	I8	76/85 (89%)	0.49	3 (3%) 39 25	61, 75, 90, 102	0
49	F5	94/98 (95%)	0.15	2 (2%) 63 49	67, 88, 121, 136	0
49	J8	94/98 (95%)	0.10	2 (2%) 63 49	62, 77, 120, 122	0
50	G5	66/72 (91%)	0.52	4 (6%) 21 12	87, 108, 126, 145	0
50	K8	68/72 (94%)	0.15	2 (2%) 51 36	68, 84, 102, 124	0
51	H5	58/60 (96%)	1.89	26 (44%) 0 0	81, 106, 128, 135	0
51	L8	58/60 (96%)	0.37	3 (5%) 27 15	63, 85, 115, 127	0
52	M8	47/71 (66%)	2.74	31 (65%) 0 0	109, 143, 158, 163	0
53	J5	56/60 (93%)	-0.11	0 100 100	66, 86, 141, 148	0
53	N8	48/60 (80%)	0.41	7 (14%) 2 1	56, 84, 140, 142	0
54	L5	47/49 (95%)	0.14	2 (4%) 35 22	58, 66, 85, 91	0
54	P8	47/49 (95%)	-0.44	0 100 100	52, 57, 77, 88	0
55	M5	64/65 (98%)	0.14	0 100 100	76, 85, 101, 117	0
55	Q8	64/65 (98%)	0.15	0 100 100	61, 71, 88, 99	0
56	1L	68/76 (89%)	1.09	15 (22%) 0 0	118, 173, 181, 188	0
57	3L	73/76 (96%)	-0.60	0 100 100	87, 172, 185, 190	0
All	All	20602/21966 (93%)	0.11	1495 (7%) 15 9	48, 107, 162, 204	0

The worst 5 of 1495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2899	G	12.6
26	14	2901	C	10.8
26	14	2799	A	10.4
26	14	2902	C	9.9
43	95	45	THR	9.5

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

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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	PSU	3L	55	20/21	0.83	0.08	166,169,175,175	0
57	5MU	3L	54	21/22	0.87	0.09	162,169,172,173	0
56	PSU	1L	55	20/21	0.87	0.30	134,150,156,159	0
56	PSU	1L	39	20/21	0.88	0.18	105,127,133,134	0
23	PSU	2L	56	20/21	0.88	0.12	116,129,133,137	0
22	PSU	1K	55	20/21	0.90	0.17	109,120,133,134	0
57	PSU	3L	39	20/21	0.91	0.13	153,162,166,168	0
23	4SU	2L	8	20/21	0.91	0.17	112,125,130,135	0
56	U8U	1L	34	23/24	0.91	0.18	110,126,134,138	0
23	4SU	2K	8	20/21	0.92	0.17	93,98,102,106	0
56	T6A	1L	37	32/33	0.93	0.18	102,120,127,130	0
23	G7M	2L	47	24/25	0.93	0.12	129,137,150,151	0
22	5MU	1K	54	21/22	0.94	0.22	114,122,134,142	0
23	G7M	2K	47	24/25	0.94	0.12	104,115,129,135	0
23	PSU	2K	56	20/21	0.94	0.14	104,113,121,127	0
23	5MU	2L	55	21/22	0.94	0.13	128,133,141,143	0
22	PSU	1K	39	20/21	0.95	0.15	79,98,105,108	0
56	5MU	1L	54	21/22	0.95	0.25	138,147,154,155	0
22	T6A	1K	37	32/33	0.96	0.16	76,86,103,106	0
23	OMC	2L	33	21/22	0.96	0.15	109,114,117,125	0
22	U8U	1K	34	23/24	0.96	0.15	78,88,93,105	0
23	5MU	2K	55	21/22	0.96	0.12	112,118,125,127	0
23	OMC	2K	33	21/22	0.97	0.14	82,87,92,96	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	13	1698	1/1	0.08	0.21	138,138,138,138	0
58	MG	13	1699	1/1	0.28	0.31	94,94,94,94	0
58	MG	14	3282	1/1	0.32	0.42	109,109,109,109	0
58	MG	14	3303	1/1	0.32	0.18	106,106,106,106	0
58	MG	13	1603	1/1	0.33	0.47	92,92,92,92	0
58	MG	1H	3016	1/1	0.34	0.56	75,75,75,75	0
58	MG	1H	3297	1/1	0.39	0.24	99,99,99,99	0
58	MG	14	3258	1/1	0.41	0.38	92,92,92,92	0
58	MG	14	3311	1/1	0.42	0.36	100,100,100,100	0
58	MG	1H	3219	1/1	0.43	0.37	103,103,103,103	0
58	MG	1G	1638	1/1	0.44	0.30	93,93,93,93	0
58	MG	14	3108	1/1	0.46	0.73	92,92,92,92	0
58	MG	1H	3283	1/1	0.48	0.24	92,92,92,92	0
58	MG	13	1697	1/1	0.49	0.22	92,92,92,92	0
58	MG	1H	3152	1/1	0.51	0.34	100,100,100,100	0
58	MG	14	3224	1/1	0.51	0.38	90,90,90,90	0
58	MG	1G	1664	1/1	0.51	0.30	100,100,100,100	0
58	MG	2K	102	1/1	0.52	0.69	94,94,94,94	0
58	MG	13	1700	1/1	0.52	0.33	94,94,94,94	0
58	MG	14	3034	1/1	0.52	0.97	88,88,88,88	0
58	MG	39	301	1/1	0.52	0.21	96,96,96,96	0
58	MG	14	3399	1/1	0.53	0.28	107,107,107,107	0
58	MG	13	1672	1/1	0.54	0.45	109,109,109,109	0
58	MG	1H	3249	1/1	0.54	0.37	80,80,80,80	0
58	MG	13	1653	1/1	0.54	0.41	72,72,72,72	0
58	MG	13	1696	1/1	0.55	0.32	92,92,92,92	0
58	MG	1H	3171	1/1	0.56	0.43	83,83,83,83	0
58	MG	14	3037	1/1	0.56	0.46	106,106,106,106	0
58	MG	1H	3309	1/1	0.56	0.51	90,90,90,90	0
58	MG	1H	3036	1/1	0.56	0.74	100,100,100,100	0
58	MG	1H	3284	1/1	0.56	0.48	81,81,81,81	0
58	MG	14	3294	1/1	0.57	0.26	87,87,87,87	0
58	MG	14	3304	1/1	0.58	0.71	92,92,92,92	0
58	MG	13	1688	1/1	0.58	0.34	101,101,101,101	0
58	MG	1H	3035	1/1	0.59	0.45	83,83,83,83	0
58	MG	1H	3279	1/1	0.59	0.49	67,67,67,67	0
58	MG	25	201	1/1	0.59	0.34	102,102,102,102	0
58	MG	14	3316	1/1	0.60	0.35	122,122,122,122	0
58	MG	1H	3336	1/1	0.60	0.24	104,104,104,104	0
58	MG	14	3283	1/1	0.60	0.32	69,69,69,69	0
58	MG	14	3184	1/1	0.60	0.24	98,98,98,98	0
58	MG	14	3197	1/1	0.61	0.34	116,116,116,116	0
58	MG	14	3180	1/1	0.61	0.30	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3229	1/1	0.61	0.76	88,88,88,88	0
58	MG	1H	3164	1/1	0.61	0.21	64,64,64,64	0
58	MG	14	3185	1/1	0.61	0.51	82,82,82,82	0
58	MG	14	3190	1/1	0.61	0.58	86,86,86,86	0
58	MG	14	3191	1/1	0.61	0.58	96,96,96,96	0
58	MG	1H	3264	1/1	0.62	0.18	76,76,76,76	0
58	MG	1H	3278	1/1	0.62	0.48	95,95,95,95	0
58	MG	14	3017	1/1	0.62	0.51	90,90,90,90	0
58	MG	1H	3024	1/1	0.62	0.69	82,82,82,82	0
58	MG	1H	3331	1/1	0.62	0.62	73,73,73,73	0
58	MG	13	1605	1/1	0.62	0.24	76,76,76,76	0
58	MG	14	3129	1/1	0.62	0.69	73,73,73,73	0
58	MG	14	3140	1/1	0.62	0.33	82,82,82,82	0
58	MG	1G	1603	1/1	0.62	0.59	102,102,102,102	0
58	MG	1G	1635	1/1	0.63	0.28	107,107,107,107	0
58	MG	14	3269	1/1	0.63	0.50	88,88,88,88	0
58	MG	1H	3160	1/1	0.63	0.28	72,72,72,72	0
58	MG	1G	1646	1/1	0.63	0.24	100,100,100,100	0
58	MG	14	3068	1/1	0.63	0.65	100,100,100,100	0
58	MG	1G	1616	1/1	0.63	0.31	87,87,87,87	0
58	MG	14	3302	1/1	0.64	0.46	66,66,66,66	0
58	MG	14	3085	1/1	0.64	0.47	67,67,67,67	0
58	MG	14	3089	1/1	0.64	0.88	79,79,79,79	0
58	MG	13	1630	1/1	0.64	0.48	80,80,80,80	0
58	MG	1H	3285	1/1	0.65	0.47	68,68,68,68	0
58	MG	14	3261	1/1	0.65	0.49	77,77,77,77	0
58	MG	14	3026	1/1	0.66	0.34	89,89,89,89	0
58	MG	1J	203	1/1	0.66	0.23	103,103,103,103	0
58	MG	14	3153	1/1	0.66	0.44	89,89,89,89	0
58	MG	1E	301	1/1	0.66	0.20	106,106,106,106	0
58	MG	1H	3194	1/1	0.67	0.40	84,84,84,84	0
58	MG	1H	3207	1/1	0.67	0.48	84,84,84,84	0
58	MG	14	3264	1/1	0.67	0.57	85,85,85,85	0
58	MG	1H	3167	1/1	0.67	0.54	93,93,93,93	0
58	MG	14	3275	1/1	0.67	0.37	91,91,91,91	0
58	MG	14	3277	1/1	0.67	0.34	85,85,85,85	0
58	MG	35	202	1/1	0.67	0.24	87,87,87,87	0
58	MG	14	3262	1/1	0.68	0.34	96,96,96,96	0
58	MG	1H	3122	1/1	0.68	0.63	79,79,79,79	0
58	MG	14	3135	1/1	0.68	0.24	95,95,95,95	0
58	MG	13	1695	1/1	0.68	0.43	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3392	1/1	0.68	0.06	128,128,128,128	0
58	MG	1H	3292	1/1	0.68	0.30	77,77,77,77	0
58	MG	14	3227	1/1	0.68	0.44	76,76,76,76	0
58	MG	2L	102	1/1	0.68	0.64	83,83,83,83	0
58	MG	1H	3253	1/1	0.68	0.37	66,66,66,66	0
58	MG	1H	3254	1/1	0.68	0.57	99,99,99,99	0
58	MG	1H	3459	1/1	0.69	0.06	106,106,106,106	0
58	MG	13	1632	1/1	0.69	0.40	107,107,107,107	0
58	MG	1H	3293	1/1	0.69	0.35	84,84,84,84	0
58	MG	14	3308	1/1	0.69	0.70	106,106,106,106	0
58	MG	14	3186	1/1	0.69	0.45	82,82,82,82	0
58	MG	1H	3079	1/1	0.69	0.38	79,79,79,79	0
58	MG	1H	3277	1/1	0.70	0.32	68,68,68,68	0
58	MG	1H	3314	1/1	0.70	0.30	85,85,85,85	0
58	MG	1H	3178	1/1	0.70	0.38	71,71,71,71	0
58	MG	1G	1648	1/1	0.70	0.32	117,117,117,117	0
58	MG	1G	1649	1/1	0.70	0.41	83,83,83,83	0
58	MG	13	1646	1/1	0.70	0.29	75,75,75,75	0
58	MG	1H	3301	1/1	0.70	0.44	84,84,84,84	0
58	MG	1H	3305	1/1	0.70	0.39	67,67,67,67	0
58	MG	1H	3306	1/1	0.70	0.31	91,91,91,91	0
58	MG	14	3030	1/1	0.70	0.39	86,86,86,86	0
58	MG	14	3257	1/1	0.70	1.14	86,86,86,86	0
58	MG	1H	3315	1/1	0.71	0.53	76,76,76,76	0
58	MG	1H	3328	1/1	0.71	0.58	80,80,80,80	0
58	MG	1H	3302	1/1	0.71	0.22	92,92,92,92	0
58	MG	13	1705	1/1	0.71	0.35	90,90,90,90	0
58	MG	14	3313	1/1	0.71	0.49	92,92,92,92	0
58	MG	13	1728	1/1	0.71	0.11	118,118,118,118	0
58	MG	16	204	1/1	0.71	0.32	73,73,73,73	0
58	MG	14	3255	1/1	0.71	0.25	78,78,78,78	0
58	MG	1H	3251	1/1	0.71	0.39	71,71,71,71	0
58	MG	1H	3217	1/1	0.71	0.34	71,71,71,71	0
58	MG	14	3295	1/1	0.71	0.20	85,85,85,85	0
58	MG	14	3259	1/1	0.71	0.75	98,98,98,98	0
58	MG	14	3231	1/1	0.72	0.34	86,86,86,86	0
58	MG	13	1656	1/1	0.72	0.15	103,103,103,103	0
58	MG	13	1659	1/1	0.72	0.62	97,97,97,97	0
58	MG	1J	201	1/1	0.72	0.30	94,94,94,94	0
58	MG	1H	3224	1/1	0.72	0.58	73,73,73,73	0
58	MG	1H	3368	1/1	0.72	0.24	74,74,74,74	0
58	MG	1H	3324	1/1	0.72	0.57	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3058	1/1	0.72	0.18	84,84,84,84	0
58	MG	E5	101	1/1	0.72	0.47	89,89,89,89	0
58	MG	1H	3139	1/1	0.73	0.36	71,71,71,71	0
58	MG	13	1641	1/1	0.73	0.44	93,93,93,93	0
58	MG	1H	3101	1/1	0.73	0.26	59,59,59,59	0
58	MG	1H	3180	1/1	0.73	0.43	75,75,75,75	0
58	MG	1H	3032	1/1	0.73	0.49	79,79,79,79	0
58	MG	14	3234	1/1	0.73	0.89	70,70,70,70	0
58	MG	14	3155	1/1	0.73	0.71	64,64,64,64	0
58	MG	14	3251	1/1	0.74	0.50	69,69,69,69	0
58	MG	1H	3288	1/1	0.74	0.87	93,93,93,93	0
58	MG	14	3194	1/1	0.74	0.34	81,81,81,81	0
58	MG	14	3019	1/1	0.74	0.67	90,90,90,90	0
58	MG	14	3181	1/1	0.74	0.41	89,89,89,89	0
58	MG	14	3260	1/1	0.74	0.78	72,72,72,72	0
58	MG	14	3300	1/1	0.74	0.24	117,117,117,117	0
58	MG	29	301	1/1	0.74	0.34	77,77,77,77	0
58	MG	13	1689	1/1	0.74	0.52	107,107,107,107	0
58	MG	1H	3222	1/1	0.74	0.33	98,98,98,98	0
58	MG	14	3143	1/1	0.74	0.30	102,102,102,102	0
58	MG	1H	3342	1/1	0.74	0.63	92,92,92,92	0
58	MG	1H	3031	1/1	0.75	0.53	76,76,76,76	0
58	MG	1H	3080	1/1	0.75	0.21	65,65,65,65	0
58	MG	I8	101	1/1	0.75	0.32	73,73,73,73	0
58	MG	14	3144	1/1	0.75	0.41	71,71,71,71	0
58	MG	2K	103	1/1	0.75	0.42	114,114,114,114	0
58	MG	1H	3228	1/1	0.75	0.45	83,83,83,83	0
58	MG	14	3250	1/1	0.75	0.41	78,78,78,78	0
58	MG	1H	3457	1/1	0.75	0.06	141,141,141,141	0
58	MG	1H	3313	1/1	0.76	0.26	98,98,98,98	0
58	MG	14	3147	1/1	0.76	0.23	95,95,95,95	0
58	MG	14	3310	1/1	0.76	0.23	114,114,114,114	0
58	MG	14	3052	1/1	0.76	0.50	113,113,113,113	0
58	MG	1H	3199	1/1	0.76	0.25	69,69,69,69	0
58	MG	1H	3247	1/1	0.76	0.21	81,81,81,81	0
58	MG	1G	1666	1/1	0.76	0.50	84,84,84,84	0
58	MG	1H	3154	1/1	0.76	0.54	84,84,84,84	0
58	MG	13	1681	1/1	0.76	0.19	116,116,116,116	0
58	MG	14	3288	1/1	0.76	0.74	86,86,86,86	0
58	MG	13	1662	1/1	0.76	0.36	118,118,118,118	0
58	MG	14	3188	1/1	0.76	0.56	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3043	1/1	0.76	0.76	81,81,81,81	0
58	MG	1H	3197	1/1	0.76	0.63	80,80,80,80	0
58	MG	35	203	1/1	0.76	0.24	75,75,75,75	0
58	MG	1H	3291	1/1	0.76	0.31	73,73,73,73	0
58	MG	14	3291	1/1	0.77	0.35	87,87,87,87	0
58	MG	14	3293	1/1	0.77	0.51	91,91,91,91	0
58	MG	14	3345	1/1	0.77	0.10	90,90,90,90	0
58	MG	1G	1672	1/1	0.77	0.43	99,99,99,99	0
58	MG	14	3268	1/1	0.77	0.41	94,94,94,94	0
58	MG	1H	3087	1/1	0.77	0.57	70,70,70,70	0
58	MG	14	3301	1/1	0.77	0.21	109,109,109,109	0
58	MG	14	3117	1/1	0.77	0.44	81,81,81,81	0
58	MG	29	302	1/1	0.77	0.45	65,65,65,65	0
58	MG	1H	3296	1/1	0.77	0.22	57,57,57,57	0
58	MG	1H	3136	1/1	0.77	0.34	49,49,49,49	0
58	MG	13	1621	1/1	0.77	0.21	90,90,90,90	0
58	MG	1H	3142	1/1	0.77	0.45	68,68,68,68	0
58	MG	14	3290	1/1	0.77	0.22	92,92,92,92	0
58	MG	14	3306	1/1	0.78	0.29	88,88,88,88	0
58	MG	1G	1643	1/1	0.78	0.24	132,132,132,132	0
58	MG	1H	3263	1/1	0.78	0.25	76,76,76,76	0
58	MG	1H	3439	1/1	0.78	0.07	99,99,99,99	0
58	MG	13	1644	1/1	0.78	0.43	96,96,96,96	0
58	MG	1H	3271	1/1	0.78	0.39	76,76,76,76	0
58	MG	14	3247	1/1	0.78	0.28	67,67,67,67	0
58	MG	14	3073	1/1	0.78	1.32	83,83,83,83	0
58	MG	14	3183	1/1	0.78	0.77	79,79,79,79	0
58	MG	1H	3327	1/1	0.78	0.79	82,82,82,82	0
58	MG	1H	3175	1/1	0.78	0.53	65,65,65,65	0
58	MG	1H	3022	1/1	0.78	0.39	62,62,62,62	0
58	MG	1G	1604	1/1	0.78	0.44	87,87,87,87	0
58	MG	1H	3201	1/1	0.78	0.69	92,92,92,92	0
58	MG	13	1706	1/1	0.78	0.39	109,109,109,109	0
58	MG	35	201	1/1	0.78	0.26	74,74,74,74	0
58	MG	14	3029	1/1	0.78	0.72	78,78,78,78	0
58	MG	1H	3364	1/1	0.78	0.10	98,98,98,98	0
58	MG	14	3265	1/1	0.78	0.52	98,98,98,98	0
58	MG	13	1694	1/1	0.79	0.55	64,64,64,64	0
58	MG	14	3018	1/1	0.79	0.61	72,72,72,72	0
58	MG	14	3353	1/1	0.79	0.09	118,118,118,118	0
58	MG	1G	1606	1/1	0.79	0.22	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3243	1/1	0.79	0.47	81,81,81,81	0
58	MG	1H	3414	1/1	0.79	0.19	80,80,80,80	0
58	MG	1G	1618	1/1	0.79	0.33	109,109,109,109	0
58	MG	16	209	1/1	0.79	0.10	100,100,100,100	0
58	MG	14	3252	1/1	0.79	0.39	84,84,84,84	0
58	MG	14	3253	1/1	0.79	0.26	94,94,94,94	0
58	MG	14	3280	1/1	0.79	0.91	86,86,86,86	0
58	MG	1H	3045	1/1	0.79	0.33	82,82,82,82	0
58	MG	1G	1680	1/1	0.79	0.06	140,140,140,140	0
58	MG	14	3182	1/1	0.79	0.74	75,75,75,75	0
58	MG	1H	3083	1/1	0.79	0.33	67,67,67,67	0
58	MG	14	3023	1/1	0.80	0.29	83,83,83,83	0
58	MG	13	1675	1/1	0.80	0.30	73,73,73,73	0
58	MG	1H	3268	1/1	0.80	0.42	85,85,85,85	0
58	MG	14	3221	1/1	0.80	0.20	69,69,69,69	0
58	MG	1H	3196	1/1	0.80	0.44	83,83,83,83	0
58	MG	1H	3033	1/1	0.80	0.58	88,88,88,88	0
58	MG	14	3150	1/1	0.80	0.40	87,87,87,87	0
58	MG	1H	3021	1/1	0.80	0.30	83,83,83,83	0
58	MG	1H	3298	1/1	0.80	0.35	74,74,74,74	0
58	MG	14	3179	1/1	0.80	0.24	60,60,60,60	0
58	MG	14	3391	1/1	0.80	0.13	104,104,104,104	0
58	MG	1G	1667	1/1	0.80	0.28	109,109,109,109	0
58	MG	1H	3173	1/1	0.80	0.47	84,84,84,84	0
58	MG	1G	1678	1/1	0.80	0.06	128,128,128,128	0
58	MG	14	3080	1/1	0.80	0.46	82,82,82,82	0
58	MG	1J	204	1/1	0.80	0.27	101,101,101,101	0
58	MG	14	3292	1/1	0.80	0.14	113,113,113,113	0
58	MG	1H	3282	1/1	0.80	0.60	88,88,88,88	0
58	MG	1H	3205	1/1	0.80	0.19	81,81,81,81	0
58	MG	13	1704	1/1	0.80	0.41	82,82,82,82	0
58	MG	14	3297	1/1	0.80	0.69	70,70,70,70	0
58	MG	14	3187	1/1	0.80	0.45	80,80,80,80	0
58	MG	13	1678	1/1	0.80	0.27	93,93,93,93	0
58	MG	13	1679	1/1	0.80	0.28	100,100,100,100	0
58	MG	1G	1663	1/1	0.81	0.10	94,94,94,94	0
58	MG	1H	3307	1/1	0.81	0.52	94,94,94,94	0
58	MG	98	201	1/1	0.81	0.41	72,72,72,72	0
58	MG	1H	3337	1/1	0.81	0.22	89,89,89,89	0
58	MG	P8	101	1/1	0.81	0.58	77,77,77,77	0
58	MG	13	1637	1/1	0.81	0.38	56,56,56,56	0
58	MG	1G	1679	1/1	0.81	0.11	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1670	1/1	0.81	0.19	97,97,97,97	0
58	MG	1G	1686	1/1	0.81	0.08	125,125,125,125	0
58	MG	1H	3179	1/1	0.81	0.35	83,83,83,83	0
58	MG	1H	3097	1/1	0.81	0.44	71,71,71,71	0
58	MG	14	3271	1/1	0.81	0.21	81,81,81,81	0
58	MG	1H	3246	1/1	0.81	0.23	54,54,54,54	0
58	MG	1H	3441	1/1	0.81	0.13	89,89,89,89	0
58	MG	14	3395	1/1	0.81	0.10	103,103,103,103	0
58	MG	14	3146	1/1	0.81	0.43	57,57,57,57	0
58	MG	14	3228	1/1	0.81	0.17	101,101,101,101	0
58	MG	13	1661	1/1	0.81	0.48	103,103,103,103	0
58	MG	1H	3209	1/1	0.81	0.42	90,90,90,90	0
58	MG	16	203	1/1	0.81	0.14	90,90,90,90	0
58	MG	1H	3019	1/1	0.81	0.49	92,92,92,92	0
58	MG	14	3245	1/1	0.81	0.47	77,77,77,77	0
58	MG	14	3170	1/1	0.81	0.37	83,83,83,83	0
58	MG	14	3177	1/1	0.81	0.46	72,72,72,72	0
58	MG	16	205	1/1	0.81	0.11	81,81,81,81	0
58	MG	1G	1657	1/1	0.81	0.36	92,92,92,92	0
58	MG	1G	1659	1/1	0.81	0.18	142,142,142,142	0
58	MG	14	3109	1/1	0.82	0.38	73,73,73,73	0
58	MG	1G	1636	1/1	0.82	0.32	101,101,101,101	0
58	MG	14	3125	1/1	0.82	0.75	72,72,72,72	0
58	MG	1G	1668	1/1	0.82	0.36	116,116,116,116	0
58	MG	3K	101	1/1	0.82	0.34	162,162,162,162	0
58	MG	13	1682	1/1	0.82	0.45	88,88,88,88	0
58	MG	1H	3151	1/1	0.82	0.20	55,55,55,55	0
58	MG	14	3393	1/1	0.82	0.06	127,127,127,127	0
58	MG	1H	3128	1/1	0.82	0.22	62,62,62,62	0
58	MG	1G	1684	1/1	0.82	0.11	109,109,109,109	0
58	MG	14	3193	1/1	0.82	0.40	77,77,77,77	0
58	MG	1J	202	1/1	0.82	0.27	95,95,95,95	0
58	MG	14	3059	1/1	0.82	0.32	86,86,86,86	0
58	MG	14	3060	1/1	0.82	0.23	73,73,73,73	0
58	MG	13	1685	1/1	0.82	0.24	121,121,121,121	0
58	MG	14	3222	1/1	0.82	0.23	97,97,97,97	0
58	MG	1H	3413	1/1	0.82	0.08	102,102,102,102	0
58	MG	14	3074	1/1	0.82	0.81	79,79,79,79	0
58	MG	1G	1615	1/1	0.82	0.23	125,125,125,125	0
58	MG	1H	3280	1/1	0.82	0.33	77,77,77,77	0
58	MG	1H	3438	1/1	0.82	0.11	83,83,83,83	0
58	MG	78	201	1/1	0.82	0.36	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3287	1/1	0.83	0.29	104,104,104,104	0
58	MG	1H	3018	1/1	0.83	0.55	71,71,71,71	0
58	MG	1G	1609	1/1	0.83	0.18	94,94,94,94	0
58	MG	13	1715	1/1	0.83	0.10	109,109,109,109	0
58	MG	1H	3190	1/1	0.83	0.32	73,73,73,73	0
58	MG	1H	3159	1/1	0.83	0.42	67,67,67,67	0
58	MG	1G	1620	1/1	0.83	0.31	82,82,82,82	0
58	MG	14	3107	1/1	0.83	0.51	77,77,77,77	0
58	MG	1G	1630	1/1	0.83	0.41	103,103,103,103	0
58	MG	6A	101	1/1	0.83	0.26	93,93,93,93	0
58	MG	13	1650	1/1	0.83	0.30	94,94,94,94	0
58	MG	14	3012	1/1	0.83	0.81	80,80,80,80	0
58	MG	13	1604	1/1	0.83	0.27	87,87,87,87	0
58	MG	13	1634	1/1	0.83	1.02	93,93,93,93	0
58	MG	14	3201	1/1	0.83	0.27	59,59,59,59	0
58	MG	1H	3335	1/1	0.83	0.68	74,74,74,74	0
58	MG	14	3273	1/1	0.83	0.46	101,101,101,101	0
58	MG	14	3022	1/1	0.83	0.38	64,64,64,64	0
58	MG	1H	3137	1/1	0.83	0.61	88,88,88,88	0
58	MG	13	1668	1/1	0.83	0.09	90,90,90,90	0
58	MG	21	302	1/1	0.83	0.33	77,77,77,77	0
58	MG	1G	1650	1/1	0.83	0.30	114,114,114,114	0
58	MG	14	3230	1/1	0.83	0.41	64,64,64,64	0
58	MG	1H	3338	1/1	0.83	0.37	65,65,65,65	0
58	MG	1H	3341	1/1	0.83	0.21	79,79,79,79	0
58	MG	14	3236	1/1	0.83	0.51	89,89,89,89	0
58	MG	14	3238	1/1	0.83	0.33	99,99,99,99	0
58	MG	13	1669	1/1	0.83	0.30	68,68,68,68	0
58	MG	13	1708	1/1	0.83	0.13	89,89,89,89	0
58	MG	1H	3262	1/1	0.83	0.37	94,94,94,94	0
58	MG	1H	3184	1/1	0.84	0.26	82,82,82,82	0
58	MG	14	3248	1/1	0.84	0.21	79,79,79,79	0
58	MG	1H	3233	1/1	0.84	0.59	62,62,62,62	0
58	MG	1H	3187	1/1	0.84	0.25	69,69,69,69	0
58	MG	1H	3316	1/1	0.84	0.88	92,92,92,92	0
58	MG	1H	3089	1/1	0.84	0.44	59,59,59,59	0
58	MG	14	3021	1/1	0.84	0.45	52,52,52,52	0
58	MG	14	3278	1/1	0.84	0.34	75,75,75,75	0
58	MG	14	3256	1/1	0.84	0.54	83,83,83,83	0
58	MG	5E	201	1/1	0.84	0.26	89,89,89,89	0
58	MG	14	3067	1/1	0.84	0.31	87,87,87,87	0
58	MG	29	304	1/1	0.84	0.22	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3125	1/1	0.84	0.50	69,69,69,69	0
58	MG	14	3237	1/1	0.84	0.37	83,83,83,83	0
58	MG	1H	3308	1/1	0.84	0.51	90,90,90,90	0
58	MG	14	3027	1/1	0.84	0.39	96,96,96,96	0
58	MG	1H	3226	1/1	0.84	0.38	85,85,85,85	0
58	MG	14	3363	1/1	0.84	0.19	72,72,72,72	0
58	MG	1G	1633	1/1	0.85	0.31	98,98,98,98	0
58	MG	1H	3252	1/1	0.85	0.50	66,66,66,66	0
58	MG	1H	3071	1/1	0.85	0.38	61,61,61,61	0
58	MG	1G	1637	1/1	0.85	0.55	87,87,87,87	0
58	MG	41	201	1/1	0.85	0.07	78,78,78,78	0
58	MG	14	3061	1/1	0.85	0.12	81,81,81,81	0
58	MG	14	3205	1/1	0.85	0.34	96,96,96,96	0
58	MG	1H	3322	1/1	0.85	0.65	81,81,81,81	0
58	MG	1H	3108	1/1	0.85	0.33	74,74,74,74	0
58	MG	1H	3072	1/1	0.85	0.30	77,77,77,77	0
58	MG	1H	3422	1/1	0.85	0.16	112,112,112,112	0
58	MG	1H	3227	1/1	0.85	0.68	85,85,85,85	0
58	MG	13	1703	1/1	0.85	0.78	77,77,77,77	0
58	MG	1H	3332	1/1	0.85	0.32	74,74,74,74	0
58	MG	1H	3096	1/1	0.85	0.33	60,60,60,60	0
58	MG	1H	3193	1/1	0.85	0.50	73,73,73,73	0
58	MG	14	3266	1/1	0.85	0.53	85,85,85,85	0
58	MG	1G	1665	1/1	0.85	0.26	113,113,113,113	0
58	MG	1H	3463	1/1	0.85	0.08	112,112,112,112	0
58	MG	1H	3213	1/1	0.85	0.38	74,74,74,74	0
58	MG	14	3309	1/1	0.85	0.44	110,110,110,110	0
58	MG	1H	3130	1/1	0.85	0.32	74,74,74,74	0
58	MG	1H	3020	1/1	0.85	0.32	66,66,66,66	0
58	MG	1H	3290	1/1	0.86	0.22	70,70,70,70	0
58	MG	1G	1619	1/1	0.86	0.21	101,101,101,101	0
58	MG	1H	3321	1/1	0.86	0.25	67,67,67,67	0
58	MG	1H	3157	1/1	0.86	0.47	73,73,73,73	0
58	MG	13	1692	1/1	0.86	0.16	122,122,122,122	0
58	MG	1G	1634	1/1	0.86	0.29	112,112,112,112	0
58	MG	13	1606	1/1	0.86	0.46	94,94,94,94	0
58	MG	1H	3141	1/1	0.86	0.40	61,61,61,61	0
58	MG	14	3013	1/1	0.86	0.23	78,78,78,78	0
58	MG	14	3199	1/1	0.86	0.50	69,69,69,69	0
58	MG	14	3118	1/1	0.86	0.45	69,69,69,69	0
58	MG	1H	3329	1/1	0.86	0.77	81,81,81,81	0
58	MG	1H	3203	1/1	0.86	0.37	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1G	1641	1/1	0.86	0.34	113,113,113,113	0
58	MG	1H	3276	1/1	0.86	0.68	75,75,75,75	0
58	MG	1H	3185	1/1	0.86	0.40	95,95,95,95	0
58	MG	1H	3234	1/1	0.86	0.08	66,66,66,66	0
58	MG	1H	3303	1/1	0.86	0.77	78,78,78,78	0
58	MG	1H	3242	1/1	0.86	0.36	52,52,52,52	0
58	MG	1G	1654	1/1	0.86	0.53	83,83,83,83	0
58	MG	1H	3340	1/1	0.86	0.50	78,78,78,78	0
58	MG	1H	3206	1/1	0.86	0.35	77,77,77,77	0
58	MG	14	3163	1/1	0.86	0.27	90,90,90,90	0
58	MG	1H	3126	1/1	0.86	0.23	58,58,58,58	0
58	MG	1H	3188	1/1	0.86	0.38	73,73,73,73	0
58	MG	13	1647	1/1	0.86	0.23	89,89,89,89	0
58	MG	1H	3216	1/1	0.86	0.40	67,67,67,67	0
58	MG	13	1707	1/1	0.86	0.15	76,76,76,76	0
58	MG	1H	3015	1/1	0.86	0.27	63,63,63,63	0
58	MG	14	3296	1/1	0.86	0.41	84,84,84,84	0
58	MG	1G	1671	1/1	0.86	0.38	88,88,88,88	0
58	MG	55	201	1/1	0.86	0.30	74,74,74,74	0
58	MG	1H	3426	1/1	0.86	0.13	58,58,58,58	0
58	MG	1H	3452	1/1	0.87	0.13	104,104,104,104	0
58	MG	14	3263	1/1	0.87	0.24	75,75,75,75	0
58	MG	14	3169	1/1	0.87	0.40	58,58,58,58	0
58	MG	1H	3168	1/1	0.87	0.38	69,69,69,69	0
58	MG	14	3084	1/1	0.87	0.56	80,80,80,80	0
58	MG	1G	1662	1/1	0.87	0.68	72,72,72,72	0
58	MG	13	1686	1/1	0.87	0.50	76,76,76,76	0
58	MG	1H	3156	1/1	0.87	0.31	67,67,67,67	0
58	MG	14	3272	1/1	0.87	0.38	76,76,76,76	0
58	MG	16	202	1/1	0.87	0.25	64,64,64,64	0
58	MG	14	3274	1/1	0.87	0.15	76,76,76,76	0
58	MG	13	1680	1/1	0.87	0.28	96,96,96,96	0
58	MG	1H	3176	1/1	0.87	0.46	76,76,76,76	0
58	MG	1H	3158	1/1	0.87	0.49	74,74,74,74	0
58	MG	1H	3066	1/1	0.87	0.33	59,59,59,59	0
58	MG	14	3281	1/1	0.87	0.38	86,86,86,86	0
58	MG	14	3246	1/1	0.87	0.22	69,69,69,69	0
58	MG	1H	3281	1/1	0.87	0.20	88,88,88,88	0
58	MG	14	3284	1/1	0.87	0.78	78,78,78,78	0
58	MG	14	3131	1/1	0.87	0.33	95,95,95,95	0
58	MG	1H	3376	1/1	0.87	0.23	76,76,76,76	0
58	MG	1J	205	1/1	0.87	0.09	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3326	1/1	0.87	0.56	83,83,83,83	0
58	MG	13	1639	1/1	0.87	0.56	82,82,82,82	0
58	MG	1H	3182	1/1	0.87	0.20	78,78,78,78	0
58	MG	1H	3258	1/1	0.87	0.27	59,59,59,59	0
58	MG	1H	3135	1/1	0.87	0.12	65,65,65,65	0
58	MG	1K	101	1/1	0.87	0.09	145,145,145,145	0
58	MG	1H	3186	1/1	0.87	0.34	75,75,75,75	0
58	MG	14	3211	1/1	0.87	0.37	91,91,91,91	0
58	MG	14	3154	1/1	0.87	0.25	69,69,69,69	0
58	MG	1H	3445	1/1	0.87	0.07	110,110,110,110	0
58	MG	13	1608	1/1	0.88	0.75	90,90,90,90	0
58	MG	13	1624	1/1	0.88	0.23	103,103,103,103	0
58	MG	1H	3286	1/1	0.88	0.32	94,94,94,94	0
58	MG	I8	102	1/1	0.88	0.24	70,70,70,70	0
58	MG	14	3286	1/1	0.88	0.38	80,80,80,80	0
58	MG	14	3364	1/1	0.88	0.16	85,85,85,85	0
58	MG	14	3386	1/1	0.88	0.16	90,90,90,90	0
58	MG	14	3100	1/1	0.88	0.38	76,76,76,76	0
58	MG	L8	101	1/1	0.88	0.62	84,84,84,84	0
58	MG	1H	3140	1/1	0.88	0.27	58,58,58,58	0
58	MG	Q8	101	1/1	0.88	0.33	70,70,70,70	0
58	MG	1G	1677	1/1	0.88	0.12	96,96,96,96	0
58	MG	14	3032	1/1	0.88	0.45	75,75,75,75	0
58	MG	14	3232	1/1	0.88	0.21	81,81,81,81	0
58	MG	1H	3041	1/1	0.88	0.22	76,76,76,76	0
58	MG	1H	3467	1/1	0.88	0.10	84,84,84,84	0
58	MG	14	3299	1/1	0.88	0.20	98,98,98,98	0
58	MG	13	1677	1/1	0.88	0.16	104,104,104,104	0
58	MG	14	3055	1/1	0.88	0.10	81,81,81,81	0
58	MG	1H	3333	1/1	0.88	0.34	100,100,100,100	0
58	MG	1G	1613	1/1	0.88	0.21	98,98,98,98	0
58	MG	1H	3320	1/1	0.88	0.46	77,77,77,77	0
58	MG	1H	3170	1/1	0.88	0.46	65,65,65,65	0
58	MG	1H	3269	1/1	0.88	0.32	65,65,65,65	0
58	MG	1H	3323	1/1	0.88	0.45	80,80,80,80	0
58	MG	1H	3144	1/1	0.88	0.40	77,77,77,77	0
58	MG	1G	1628	1/1	0.88	0.44	95,95,95,95	0
58	MG	1G	1689	1/1	0.89	0.17	121,121,121,121	0
58	MG	14	3126	1/1	0.89	0.39	67,67,67,67	0
58	MG	13	1652	1/1	0.89	0.24	99,99,99,99	0
58	MG	1H	3334	1/1	0.89	0.30	76,76,76,76	0
58	MG	14	3244	1/1	0.89	0.59	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3007	1/1	0.89	0.48	54,54,54,54	0
58	MG	14	3324	1/1	0.89	0.06	99,99,99,99	0
58	MG	1G	1631	1/1	0.89	0.25	96,96,96,96	0
58	MG	1H	3388	1/1	0.89	0.07	77,77,77,77	0
58	MG	13	1691	1/1	0.89	0.48	90,90,90,90	0
58	MG	1H	3325	1/1	0.89	0.44	71,71,71,71	0
58	MG	14	3195	1/1	0.89	0.37	68,68,68,68	0
58	MG	14	3285	1/1	0.89	0.25	68,68,68,68	0
58	MG	1H	3417	1/1	0.89	0.22	94,94,94,94	0
58	MG	14	3287	1/1	0.89	0.22	82,82,82,82	0
58	MG	1H	3419	1/1	0.89	0.06	101,101,101,101	0
58	MG	1H	3131	1/1	0.89	0.56	73,73,73,73	0
58	MG	14	3203	1/1	0.89	0.34	56,56,56,56	0
58	MG	1H	3232	1/1	0.89	0.17	52,52,52,52	0
58	MG	14	3024	1/1	0.89	0.57	77,77,77,77	0
58	MG	14	3220	1/1	0.89	0.43	76,76,76,76	0
58	MG	14	3160	1/1	0.89	0.37	72,72,72,72	0
58	MG	1H	3042	1/1	0.89	0.85	90,90,90,90	0
58	MG	14	3090	1/1	0.89	0.29	74,74,74,74	0
58	MG	1H	3221	1/1	0.89	0.40	89,89,89,89	0
58	MG	14	3104	1/1	0.89	0.65	86,86,86,86	0
58	MG	1G	1647	1/1	0.89	0.80	83,83,83,83	0
58	MG	13	1687	1/1	0.89	0.27	99,99,99,99	0
58	MG	1H	3353	1/1	0.89	0.16	57,57,57,57	0
58	MG	13	1620	1/1	0.89	0.28	73,73,73,73	0
58	MG	1G	1622	1/1	0.89	1.19	92,92,92,92	0
58	MG	14	3307	1/1	0.89	0.48	101,101,101,101	0
58	MG	13	1655	1/1	0.90	0.46	87,87,87,87	0
58	MG	1H	3034	1/1	0.90	0.45	80,80,80,80	0
58	MG	1H	3446	1/1	0.90	0.09	84,84,84,84	0
58	MG	14	3033	1/1	0.90	0.26	77,77,77,77	0
58	MG	14	3149	1/1	0.90	0.54	73,73,73,73	0
58	MG	1H	3238	1/1	0.90	0.14	65,65,65,65	0
58	MG	14	3035	1/1	0.90	0.22	93,93,93,93	0
58	MG	13	1651	1/1	0.90	0.41	88,88,88,88	0
58	MG	14	3049	1/1	0.90	0.21	70,70,70,70	0
58	MG	14	3157	1/1	0.90	0.25	57,57,57,57	0
58	MG	1H	3155	1/1	0.90	0.34	74,74,74,74	0
58	MG	1H	3003	1/1	0.90	0.26	64,64,64,64	0
58	MG	14	3165	1/1	0.90	0.51	77,77,77,77	0
58	MG	14	3168	1/1	0.90	0.53	106,106,106,106	0
58	MG	1H	3464	1/1	0.90	0.14	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3249	1/1	0.90	0.24	80,80,80,80	0
58	MG	1H	3039	1/1	0.90	0.32	68,68,68,68	0
58	MG	14	3172	1/1	0.90	0.70	70,70,70,70	0
58	MG	14	3176	1/1	0.90	0.47	79,79,79,79	0
58	MG	1H	3085	1/1	0.90	0.42	63,63,63,63	0
58	MG	1H	3215	1/1	0.90	0.28	63,63,63,63	0
58	MG	14	3312	1/1	0.90	0.54	80,80,80,80	0
58	MG	1H	3132	1/1	0.90	0.65	85,85,85,85	0
58	MG	1H	3318	1/1	0.90	0.42	79,79,79,79	0
58	MG	16	207	1/1	0.90	0.07	80,80,80,80	0
58	MG	14	3325	1/1	0.90	0.14	63,63,63,63	0
58	MG	14	3333	1/1	0.90	0.17	74,74,74,74	0
58	MG	1H	3362	1/1	0.90	0.11	53,53,53,53	0
58	MG	1G	1687	1/1	0.90	0.06	139,139,139,139	0
58	MG	1H	3319	1/1	0.90	0.52	110,110,110,110	0
58	MG	1H	3009	1/1	0.90	0.27	62,62,62,62	0
58	MG	14	3378	1/1	0.90	0.07	100,100,100,100	0
58	MG	1G	1639	1/1	0.90	0.51	74,74,74,74	0
58	MG	14	3389	1/1	0.90	0.09	102,102,102,102	0
58	MG	1G	1640	1/1	0.90	0.48	87,87,87,87	0
58	MG	14	3096	1/1	0.90	0.34	73,73,73,73	0
58	MG	1H	3088	1/1	0.90	0.34	68,68,68,68	0
58	MG	13	1702	1/1	0.90	0.27	98,98,98,98	0
58	MG	1H	3027	1/1	0.90	0.32	81,81,81,81	0
58	MG	13	1631	1/1	0.90	0.37	93,93,93,93	0
58	MG	1H	3267	1/1	0.90	0.49	73,73,73,73	0
58	MG	14	3111	1/1	0.90	0.14	81,81,81,81	0
58	MG	14	3200	1/1	0.90	0.46	74,74,74,74	0
58	MG	14	3115	1/1	0.90	0.40	80,80,80,80	0
58	MG	1H	3063	1/1	0.90	0.13	78,78,78,78	0
58	MG	14	3204	1/1	0.90	0.19	77,77,77,77	0
58	MG	13	1629	1/1	0.90	0.39	96,96,96,96	0
58	MG	1H	3119	1/1	0.90	0.20	69,69,69,69	0
58	MG	14	3212	1/1	0.90	0.39	70,70,70,70	0
58	MG	1H	3272	1/1	0.90	0.18	64,64,64,64	0
58	MG	14	3025	1/1	0.90	0.62	84,84,84,84	0
58	MG	1H	3200	1/1	0.90	0.49	81,81,81,81	0
58	MG	45	201	1/1	0.90	0.16	108,108,108,108	0
58	MG	1G	1661	1/1	0.90	0.23	123,123,123,123	0
58	MG	14	3028	1/1	0.90	0.25	69,69,69,69	0
58	MG	1H	3460	1/1	0.91	0.09	104,104,104,104	0
58	MG	14	3305	1/1	0.91	0.49	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3047	1/1	0.91	0.32	47,47,47,47	0
58	MG	1G	1614	1/1	0.91	0.30	107,107,107,107	0
58	MG	1H	3002	1/1	0.91	0.25	38,38,38,38	0
58	MG	1H	3367	1/1	0.91	0.09	71,71,71,71	0
58	MG	13	1654	1/1	0.91	0.38	74,74,74,74	0
58	MG	14	3215	1/1	0.91	0.22	72,72,72,72	0
58	MG	14	3217	1/1	0.91	0.43	83,83,83,83	0
58	MG	1H	3095	1/1	0.91	0.33	65,65,65,65	0
58	MG	1H	3220	1/1	0.91	0.27	82,82,82,82	0
58	MG	1H	3004	1/1	0.91	0.32	57,57,57,57	0
58	MG	14	3223	1/1	0.91	0.35	86,86,86,86	0
58	MG	14	3099	1/1	0.91	0.56	87,87,87,87	0
58	MG	13	1710	1/1	0.91	0.09	97,97,97,97	0
58	MG	14	3352	1/1	0.91	0.07	97,97,97,97	0
58	MG	14	3171	1/1	0.91	0.32	99,99,99,99	0
58	MG	1H	3100	1/1	0.91	0.24	61,61,61,61	0
58	MG	1H	3418	1/1	0.91	0.08	92,92,92,92	0
58	MG	14	3365	1/1	0.91	0.05	94,94,94,94	0
58	MG	13	1657	1/1	0.91	0.28	103,103,103,103	0
58	MG	14	3384	1/1	0.91	0.14	83,83,83,83	0
58	MG	14	3279	1/1	0.91	0.09	104,104,104,104	0
58	MG	14	3178	1/1	0.91	0.50	84,84,84,84	0
58	MG	1G	1670	1/1	0.91	0.43	86,86,86,86	0
58	MG	1H	3104	1/1	0.91	0.58	69,69,69,69	0
58	MG	14	3031	1/1	0.91	0.42	68,68,68,68	0
58	MG	1H	3204	1/1	0.91	0.42	69,69,69,69	0
58	MG	14	3397	1/1	0.91	0.50	73,73,73,73	0
58	MG	14	3239	1/1	0.91	0.17	80,80,80,80	0
58	MG	14	3241	1/1	0.91	0.35	56,56,56,56	0
58	MG	14	3242	1/1	0.91	0.52	67,67,67,67	0
58	MG	1G	1674	1/1	0.91	0.44	102,102,102,102	0
58	MG	14	3122	1/1	0.91	0.28	88,88,88,88	0
58	MG	1H	3265	1/1	0.91	0.40	78,78,78,78	0
58	MG	13	1720	1/1	0.91	0.10	90,90,90,90	0
58	MG	J8	101	1/1	0.91	0.19	66,66,66,66	0
58	MG	1H	3162	1/1	0.91	0.39	88,88,88,88	0
58	MG	1H	3118	1/1	0.91	0.84	77,77,77,77	0
58	MG	1H	3270	1/1	0.91	0.86	80,80,80,80	0
58	MG	1G	1602	1/1	0.91	0.42	79,79,79,79	0
58	MG	1G	1645	1/1	0.91	0.52	74,74,74,74	0
58	MG	13	1627	1/1	0.91	0.55	69,69,69,69	0
58	MG	1H	3294	1/1	0.91	0.34	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3148	1/1	0.91	0.31	77,77,77,77	0
58	MG	13	1731	1/1	0.91	0.14	84,84,84,84	0
60	ZN	G8	201	1/1	0.91	0.11	149,149,149,149	0
58	MG	14	3056	1/1	0.92	0.34	55,55,55,55	0
58	MG	1H	3038	1/1	0.92	0.34	92,92,92,92	0
58	MG	1H	3304	1/1	0.92	0.33	86,86,86,86	0
58	MG	1G	1681	1/1	0.92	0.10	78,78,78,78	0
58	MG	13	1625	1/1	0.92	0.33	86,86,86,86	0
58	MG	13	1626	1/1	0.92	0.37	69,69,69,69	0
58	MG	14	3314	1/1	0.92	0.32	94,94,94,94	0
58	MG	14	3267	1/1	0.92	0.25	92,92,92,92	0
58	MG	13	1636	1/1	0.92	0.28	64,64,64,64	0
58	MG	1H	3198	1/1	0.92	0.43	69,69,69,69	0
58	MG	1H	3177	1/1	0.92	0.23	74,74,74,74	0
58	MG	14	3340	1/1	0.92	0.09	79,79,79,79	0
58	MG	14	3343	1/1	0.92	0.08	82,82,82,82	0
58	MG	14	3076	1/1	0.92	0.34	62,62,62,62	0
58	MG	14	3347	1/1	0.92	0.06	108,108,108,108	0
58	MG	1H	3078	1/1	0.92	0.51	67,67,67,67	0
58	MG	13	1623	1/1	0.92	0.23	108,108,108,108	0
58	MG	14	3355	1/1	0.92	0.10	102,102,102,102	0
58	MG	14	3362	1/1	0.92	0.12	77,77,77,77	0
58	MG	1H	3044	1/1	0.92	0.27	82,82,82,82	0
58	MG	14	3086	1/1	0.92	0.43	83,83,83,83	0
58	MG	1H	3161	1/1	0.92	0.30	84,84,84,84	0
58	MG	14	3374	1/1	0.92	0.07	76,76,76,76	0
58	MG	14	3175	1/1	0.92	0.16	92,92,92,92	0
58	MG	14	3381	1/1	0.92	0.14	81,81,81,81	0
58	MG	14	3233	1/1	0.92	0.15	86,86,86,86	0
58	MG	1H	3317	1/1	0.92	0.38	68,68,68,68	0
58	MG	1G	1653	1/1	0.92	0.15	97,97,97,97	0
58	MG	13	1729	1/1	0.92	0.07	113,113,113,113	0
58	MG	1G	1655	1/1	0.92	0.25	100,100,100,100	0
58	MG	1G	1656	1/1	0.92	0.41	78,78,78,78	0
58	MG	14	3394	1/1	0.92	0.05	109,109,109,109	0
58	MG	14	3240	1/1	0.92	0.21	83,83,83,83	0
58	MG	1H	3149	1/1	0.92	0.34	60,60,60,60	0
58	MG	1H	3355	1/1	0.92	0.20	48,48,48,48	0
58	MG	1H	3166	1/1	0.92	0.27	71,71,71,71	0
58	MG	1H	3150	1/1	0.92	0.23	72,72,72,72	0
58	MG	16	201	1/1	0.92	0.11	85,85,85,85	0
58	MG	1H	3239	1/1	0.92	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3028	1/1	0.92	0.28	68,68,68,68	0
58	MG	14	3119	1/1	0.92	0.37	62,62,62,62	0
58	MG	1H	3371	1/1	0.92	0.12	59,59,59,59	0
58	MG	1G	1629	1/1	0.92	0.63	104,104,104,104	0
58	MG	1H	3273	1/1	0.92	0.22	68,68,68,68	0
58	MG	1H	3387	1/1	0.92	0.07	80,80,80,80	0
58	MG	1G	1632	1/1	0.92	0.43	75,75,75,75	0
58	MG	1H	3244	1/1	0.92	0.28	62,62,62,62	0
58	MG	1G	1673	1/1	0.92	0.33	93,93,93,93	0
58	MG	14	3047	1/1	0.92	0.18	74,74,74,74	0
58	MG	45	202	1/1	0.92	0.41	72,72,72,72	0
58	MG	1H	3392	1/1	0.92	0.11	68,68,68,68	0
58	MG	1H	3214	1/1	0.92	0.63	76,76,76,76	0
58	MG	1H	3105	1/1	0.92	0.33	66,66,66,66	0
58	MG	1G	1688	1/1	0.93	0.07	138,138,138,138	0
58	MG	13	1660	1/1	0.93	0.24	103,103,103,103	0
58	MG	1H	3070	1/1	0.93	0.47	58,58,58,58	0
58	MG	1G	1644	1/1	0.93	0.67	92,92,92,92	0
58	MG	1H	3395	1/1	0.93	0.07	77,77,77,77	0
58	MG	1H	3407	1/1	0.93	0.12	116,116,116,116	0
58	MG	1H	3410	1/1	0.93	0.10	58,58,58,58	0
58	MG	13	1645	1/1	0.93	0.42	64,64,64,64	0
58	MG	13	1693	1/1	0.93	0.21	55,55,55,55	0
58	MG	14	3105	1/1	0.93	0.31	67,67,67,67	0
58	MG	14	3106	1/1	0.93	0.40	61,61,61,61	0
58	MG	1H	3225	1/1	0.93	0.35	78,78,78,78	0
58	MG	1G	1651	1/1	0.93	0.20	104,104,104,104	0
58	MG	1H	3107	1/1	0.93	0.28	71,71,71,71	0
58	MG	14	3326	1/1	0.93	0.09	90,90,90,90	0
58	MG	1H	3040	1/1	0.93	0.44	70,70,70,70	0
58	MG	1H	3111	1/1	0.93	0.53	74,74,74,74	0
58	MG	1H	3172	1/1	0.93	0.41	87,87,87,87	0
58	MG	1H	3145	1/1	0.93	0.14	73,73,73,73	0
58	MG	1G	1658	1/1	0.93	0.23	92,92,92,92	0
58	MG	1H	3116	1/1	0.93	0.44	55,55,55,55	0
58	MG	1G	1660	1/1	0.93	0.45	85,85,85,85	0
58	MG	1H	3274	1/1	0.93	0.18	59,59,59,59	0
58	MG	13	1713	1/1	0.93	0.05	101,101,101,101	0
58	MG	1H	3012	1/1	0.93	0.80	83,83,83,83	0
58	MG	1H	3447	1/1	0.93	0.04	86,86,86,86	0
58	MG	13	1607	1/1	0.93	0.19	116,116,116,116	0
58	MG	14	3208	1/1	0.93	0.15	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3141	1/1	0.93	0.21	93,93,93,93	0
58	MG	14	3142	1/1	0.93	0.41	76,76,76,76	0
58	MG	14	3383	1/1	0.93	0.12	86,86,86,86	0
58	MG	1H	3456	1/1	0.93	0.07	97,97,97,97	0
58	MG	14	3276	1/1	0.93	0.37	92,92,92,92	0
58	MG	14	3387	1/1	0.93	0.10	96,96,96,96	0
58	MG	14	3216	1/1	0.93	0.31	77,77,77,77	0
58	MG	1H	3243	1/1	0.93	0.50	65,65,65,65	0
58	MG	14	3219	1/1	0.93	0.31	48,48,48,48	0
58	MG	1H	3311	1/1	0.93	0.29	75,75,75,75	0
58	MG	13	1665	1/1	0.93	0.09	82,82,82,82	0
58	MG	1H	3343	1/1	0.93	0.15	54,54,54,54	0
58	MG	14	3396	1/1	0.93	0.06	108,108,108,108	0
58	MG	14	3054	1/1	0.93	0.37	70,70,70,70	0
58	MG	13	1724	1/1	0.93	0.09	102,102,102,102	0
58	MG	14	3225	1/1	0.93	0.41	82,82,82,82	0
58	MG	1H	3466	1/1	0.93	0.30	56,56,56,56	0
58	MG	1H	3211	1/1	0.93	0.24	83,83,83,83	0
58	MG	1G	1676	1/1	0.93	0.11	90,90,90,90	0
58	MG	14	3289	1/1	0.93	0.76	83,83,83,83	0
58	MG	14	3156	1/1	0.93	0.61	63,63,63,63	0
58	MG	1H	3127	1/1	0.93	0.14	59,59,59,59	0
58	MG	13	1725	1/1	0.93	0.08	94,94,94,94	0
58	MG	14	3162	1/1	0.93	0.54	70,70,70,70	0
58	MG	1H	3050	1/1	0.93	0.39	60,60,60,60	0
58	MG	14	3164	1/1	0.93	0.79	74,74,74,74	0
58	MG	1H	3056	1/1	0.93	0.50	56,56,56,56	0
58	MG	14	3166	1/1	0.93	0.21	60,60,60,60	0
58	MG	1H	3370	1/1	0.93	0.16	71,71,71,71	0
58	MG	13	1726	1/1	0.93	0.05	126,126,126,126	0
58	MG	1H	3064	1/1	0.93	0.32	65,65,65,65	0
58	MG	14	3077	1/1	0.93	0.45	68,68,68,68	0
58	MG	1H	3261	1/1	0.93	0.19	69,69,69,69	0
58	MG	1G	1624	1/1	0.94	0.62	65,65,65,65	0
58	MG	1G	1626	1/1	0.94	0.29	82,82,82,82	0
58	MG	14	3112	1/1	0.94	0.48	65,65,65,65	0
58	MG	14	3114	1/1	0.94	0.42	58,58,58,58	0
58	MG	1H	3098	1/1	0.94	0.24	53,53,53,53	0
58	MG	1H	3065	1/1	0.94	0.35	61,61,61,61	0
58	MG	14	3002	1/1	0.94	0.37	57,57,57,57	0
58	MG	14	3003	1/1	0.94	0.24	62,62,62,62	0
58	MG	13	1712	1/1	0.94	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3443	1/1	0.94	0.19	76,76,76,76	0
58	MG	13	1663	1/1	0.94	0.26	82,82,82,82	0
58	MG	14	3014	1/1	0.94	0.47	57,57,57,57	0
58	MG	1H	3208	1/1	0.94	0.51	88,88,88,88	0
58	MG	14	3132	1/1	0.94	0.27	68,68,68,68	0
58	MG	1H	3023	1/1	0.94	0.46	56,56,56,56	0
58	MG	14	3136	1/1	0.94	0.17	62,62,62,62	0
58	MG	1H	3449	1/1	0.94	0.12	106,106,106,106	0
58	MG	14	3020	1/1	0.94	0.47	75,75,75,75	0
58	MG	1H	3451	1/1	0.94	0.13	114,114,114,114	0
58	MG	1H	3106	1/1	0.94	0.41	63,63,63,63	0
58	MG	13	1664	1/1	0.94	0.12	89,89,89,89	0
58	MG	1H	3073	1/1	0.94	0.50	81,81,81,81	0
58	MG	1H	3458	1/1	0.94	0.07	73,73,73,73	0
58	MG	14	3315	1/1	0.94	1.07	93,93,93,93	0
58	MG	1H	3299	1/1	0.94	0.17	74,74,74,74	0
58	MG	14	3322	1/1	0.94	0.22	65,65,65,65	0
58	MG	14	3323	1/1	0.94	0.14	64,64,64,64	0
58	MG	1H	3300	1/1	0.94	0.42	87,87,87,87	0
58	MG	1H	3461	1/1	0.94	0.04	92,92,92,92	0
58	MG	14	3151	1/1	0.94	0.77	79,79,79,79	0
58	MG	1H	3110	1/1	0.94	0.51	55,55,55,55	0
58	MG	1H	3146	1/1	0.94	0.39	72,72,72,72	0
58	MG	13	1719	1/1	0.94	0.13	71,71,71,71	0
58	MG	1H	3266	1/1	0.94	0.25	81,81,81,81	0
58	MG	1H	3181	1/1	0.94	0.25	61,61,61,61	0
58	MG	14	3348	1/1	0.94	0.17	70,70,70,70	0
58	MG	14	3350	1/1	0.94	0.11	85,85,85,85	0
58	MG	14	3159	1/1	0.94	0.47	63,63,63,63	0
58	MG	1H	3361	1/1	0.94	0.13	63,63,63,63	0
58	MG	1H	3112	1/1	0.94	0.41	56,56,56,56	0
58	MG	1G	1652	1/1	0.94	0.54	71,71,71,71	0
58	MG	1H	3115	1/1	0.94	0.26	43,43,43,43	0
58	MG	1H	3014	1/1	0.94	0.33	70,70,70,70	0
58	MG	1H	3117	1/1	0.94	0.23	48,48,48,48	0
58	MG	14	3053	1/1	0.94	0.23	61,61,61,61	0
58	MG	13	1640	1/1	0.94	0.35	74,74,74,74	0
58	MG	13	1676	1/1	0.94	0.51	76,76,76,76	0
58	MG	1H	3189	1/1	0.94	0.57	67,67,67,67	0
58	MG	14	3057	1/1	0.94	0.27	101,101,101,101	0
58	MG	14	3385	1/1	0.94	0.07	116,116,116,116	0
58	MG	1H	3379	1/1	0.94	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3381	1/1	0.94	0.14	63,63,63,63	0
58	MG	1H	3275	1/1	0.94	0.37	75,75,75,75	0
58	MG	14	3390	1/1	0.94	0.10	89,89,89,89	0
58	MG	1H	3017	1/1	0.94	0.44	71,71,71,71	0
58	MG	14	3063	1/1	0.94	0.28	58,58,58,58	0
58	MG	1H	3229	1/1	0.94	0.27	48,48,48,48	0
58	MG	1H	3393	1/1	0.94	0.20	54,54,54,54	0
58	MG	14	3069	1/1	0.94	0.38	70,70,70,70	0
58	MG	1H	3123	1/1	0.94	0.39	69,69,69,69	0
58	MG	13	1683	1/1	0.94	0.23	94,94,94,94	0
58	MG	1H	3055	1/1	0.94	0.34	49,49,49,49	0
58	MG	13	1619	1/1	0.94	0.13	91,91,91,91	0
58	MG	1H	3091	1/1	0.94	0.46	65,65,65,65	0
58	MG	14	3082	1/1	0.94	0.47	61,61,61,61	0
58	MG	14	3189	1/1	0.94	0.33	82,82,82,82	0
58	MG	1H	3415	1/1	0.94	0.06	73,73,73,73	0
58	MG	1G	1607	1/1	0.94	0.34	73,73,73,73	0
58	MG	1H	3240	1/1	0.94	0.30	74,74,74,74	0
58	MG	1G	1611	1/1	0.94	0.38	104,104,104,104	0
58	MG	1G	1612	1/1	0.94	0.36	81,81,81,81	0
58	MG	1H	3061	1/1	0.94	0.30	48,48,48,48	0
58	MG	14	3198	1/1	0.94	0.18	107,107,107,107	0
58	MG	1H	3165	1/1	0.94	0.52	78,78,78,78	0
58	MG	1H	3420	1/1	0.94	0.06	92,92,92,92	0
58	MG	1H	3421	1/1	0.94	0.06	64,64,64,64	0
58	MG	13	1601	1/1	0.94	0.34	68,68,68,68	0
58	MG	1H	3037	1/1	0.94	0.46	121,121,121,121	0
58	MG	1H	3431	1/1	0.94	0.13	70,70,70,70	0
58	MG	1H	3436	1/1	0.94	0.17	73,73,73,73	0
58	MG	1H	3455	1/1	0.95	0.08	59,59,59,59	0
58	MG	13	1616	1/1	0.95	0.04	88,88,88,88	0
58	MG	1H	3223	1/1	0.95	0.52	78,78,78,78	0
58	MG	14	3016	1/1	0.95	0.40	61,61,61,61	0
58	MG	1H	3250	1/1	0.95	0.27	74,74,74,74	0
58	MG	14	3336	1/1	0.95	0.17	62,62,62,62	0
58	MG	14	3338	1/1	0.95	0.23	60,60,60,60	0
58	MG	1H	3048	1/1	0.95	0.30	56,56,56,56	0
58	MG	1H	3113	1/1	0.95	0.44	51,51,51,51	0
58	MG	1H	3394	1/1	0.95	0.20	53,53,53,53	0
58	MG	14	3346	1/1	0.95	0.09	85,85,85,85	0
58	MG	1H	3153	1/1	0.95	0.20	62,62,62,62	0
58	MG	1H	3049	1/1	0.95	0.50	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3256	1/1	0.95	0.17	61,61,61,61	0
58	MG	14	3351	1/1	0.95	0.12	85,85,85,85	0
58	MG	14	3087	1/1	0.95	0.35	40,40,40,40	0
58	MG	1H	3310	1/1	0.95	0.17	75,75,75,75	0
58	MG	14	3158	1/1	0.95	0.42	75,75,75,75	0
58	MG	14	3358	1/1	0.95	0.09	91,91,91,91	0
58	MG	13	1628	1/1	0.95	0.41	65,65,65,65	0
58	MG	14	3094	1/1	0.95	0.64	60,60,60,60	0
58	MG	14	3095	1/1	0.95	0.41	71,71,71,71	0
58	MG	13	1671	1/1	0.95	0.31	87,87,87,87	0
58	MG	14	3371	1/1	0.95	0.12	53,53,53,53	0
58	MG	1H	3230	1/1	0.95	0.41	43,43,43,43	0
58	MG	1H	3192	1/1	0.95	0.23	80,80,80,80	0
58	MG	14	3380	1/1	0.95	0.10	96,96,96,96	0
58	MG	1H	3005	1/1	0.95	0.34	54,54,54,54	0
58	MG	1H	3345	1/1	0.95	0.18	61,61,61,61	0
58	MG	16	208	1/1	0.95	0.16	86,86,86,86	0
58	MG	1H	3346	1/1	0.95	0.14	45,45,45,45	0
58	MG	1H	3058	1/1	0.95	0.43	46,46,46,46	0
58	MG	1G	1675	1/1	0.95	0.33	91,91,91,91	0
58	MG	14	3388	1/1	0.95	0.10	68,68,68,68	0
58	MG	14	3173	1/1	0.95	0.30	66,66,66,66	0
58	MG	14	3174	1/1	0.95	0.27	101,101,101,101	0
58	MG	14	3110	1/1	0.95	0.37	57,57,57,57	0
58	MG	1H	3235	1/1	0.95	0.16	53,53,53,53	0
58	MG	1H	3428	1/1	0.95	0.19	51,51,51,51	0
58	MG	1H	3357	1/1	0.95	0.23	71,71,71,71	0
58	MG	1H	3432	1/1	0.95	0.11	50,50,50,50	0
58	MG	14	3051	1/1	0.95	0.11	81,81,81,81	0
58	MG	1H	3236	1/1	0.95	0.18	99,99,99,99	0
58	MG	1H	3237	1/1	0.95	0.28	84,84,84,84	0
58	MG	14	3121	1/1	0.95	0.48	78,78,78,78	0
58	MG	1H	3007	1/1	0.95	0.34	54,54,54,54	0
58	MG	14	3124	1/1	0.95	0.40	54,54,54,54	0
58	MG	1H	3084	1/1	0.95	0.20	94,94,94,94	0
58	MG	13	1633	1/1	0.95	0.63	62,62,62,62	0
58	MG	1H	3444	1/1	0.95	0.16	69,69,69,69	0
58	MG	1H	3218	1/1	0.95	0.25	56,56,56,56	0
58	MG	1H	3011	1/1	0.95	0.38	51,51,51,51	0
58	MG	14	3133	1/1	0.95	0.19	107,107,107,107	0
58	MG	14	3134	1/1	0.95	0.28	74,74,74,74	0
58	MG	1H	3375	1/1	0.95	0.29	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1673	1/1	0.95	0.53	70,70,70,70	0
58	MG	14	3137	1/1	0.95	0.09	57,57,57,57	0
58	MG	1H	3377	1/1	0.95	0.13	70,70,70,70	0
58	MG	14	3066	1/1	0.95	0.41	62,62,62,62	0
58	MG	14	3317	1/1	0.95	0.70	89,89,89,89	0
58	MG	14	3319	1/1	0.95	0.10	59,59,59,59	0
58	MG	13	1643	1/1	0.95	0.11	99,99,99,99	0
60	ZN	C5	201	1/1	0.95	0.07	165,165,165,165	0
58	MG	1H	3183	1/1	0.96	0.52	67,67,67,67	0
58	MG	1G	1617	1/1	0.96	0.14	135,135,135,135	0
58	MG	1H	3121	1/1	0.96	0.38	62,62,62,62	0
58	MG	1H	3090	1/1	0.96	0.36	71,71,71,71	0
58	MG	13	1714	1/1	0.96	0.10	73,73,73,73	0
58	MG	13	1658	1/1	0.96	0.24	83,83,83,83	0
58	MG	14	3078	1/1	0.96	0.38	64,64,64,64	0
58	MG	1G	1683	1/1	0.96	0.13	89,89,89,89	0
58	MG	14	3321	1/1	0.96	0.09	78,78,78,78	0
58	MG	2K	101	1/1	0.96	0.36	68,68,68,68	0
58	MG	14	3083	1/1	0.96	0.63	72,72,72,72	0
58	MG	14	3167	1/1	0.96	0.29	87,87,87,87	0
58	MG	1G	1625	1/1	0.96	0.32	93,93,93,93	0
58	MG	13	1666	1/1	0.96	0.13	78,78,78,78	0
58	MG	14	3328	1/1	0.96	0.06	74,74,74,74	0
58	MG	14	3330	1/1	0.96	0.14	77,77,77,77	0
58	MG	1G	1627	1/1	0.96	0.22	94,94,94,94	0
58	MG	13	1615	1/1	0.96	0.40	77,77,77,77	0
58	MG	1H	3454	1/1	0.96	0.07	96,96,96,96	0
58	MG	1H	3260	1/1	0.96	0.37	72,72,72,72	0
58	MG	14	3093	1/1	0.96	0.42	42,42,42,42	0
58	MG	1H	3382	1/1	0.96	0.06	77,77,77,77	0
58	MG	1H	3129	1/1	0.96	0.52	85,85,85,85	0
58	MG	1H	3067	1/1	0.96	0.32	55,55,55,55	0
58	MG	14	3008	1/1	0.96	0.36	65,65,65,65	0
58	MG	14	3349	1/1	0.96	0.15	83,83,83,83	0
58	MG	1H	3389	1/1	0.96	0.10	38,38,38,38	0
58	MG	14	3101	1/1	0.96	0.43	64,64,64,64	0
58	MG	1H	3391	1/1	0.96	0.09	61,61,61,61	0
58	MG	1H	3295	1/1	0.96	0.46	93,93,93,93	0
58	MG	14	3015	1/1	0.96	0.44	49,49,49,49	0
58	MG	13	1722	1/1	0.96	0.08	103,103,103,103	0
58	MG	14	3360	1/1	0.96	0.06	83,83,83,83	0
58	MG	13	1723	1/1	0.96	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1610	1/1	0.96	0.25	80,80,80,80	0
58	MG	1H	3397	1/1	0.96	0.07	71,71,71,71	0
58	MG	1H	3399	1/1	0.96	0.15	62,62,62,62	0
58	MG	14	3366	1/1	0.96	0.04	86,86,86,86	0
58	MG	14	3368	1/1	0.96	0.21	62,62,62,62	0
58	MG	14	3369	1/1	0.96	0.12	59,59,59,59	0
58	MG	1H	3405	1/1	0.96	0.09	63,63,63,63	0
58	MG	1H	3406	1/1	0.96	0.07	76,76,76,76	0
58	MG	14	3376	1/1	0.96	0.07	94,94,94,94	0
58	MG	14	3377	1/1	0.96	0.20	52,52,52,52	0
58	MG	13	1618	1/1	0.96	0.36	80,80,80,80	0
58	MG	1H	3025	1/1	0.96	0.40	64,64,64,64	0
58	MG	1H	3412	1/1	0.96	0.10	78,78,78,78	0
58	MG	14	3382	1/1	0.96	0.07	87,87,87,87	0
58	MG	1H	3231	1/1	0.96	0.20	58,58,58,58	0
58	MG	14	3120	1/1	0.96	0.38	82,82,82,82	0
58	MG	1H	3046	1/1	0.96	0.32	47,47,47,47	0
58	MG	21	301	1/1	0.96	0.38	54,54,54,54	0
58	MG	14	3123	1/1	0.96	0.30	64,64,64,64	0
58	MG	13	1649	1/1	0.96	0.37	72,72,72,72	0
58	MG	1H	3081	1/1	0.96	0.39	87,87,87,87	0
58	MG	1H	3082	1/1	0.96	0.26	78,78,78,78	0
58	MG	1H	3174	1/1	0.96	0.36	88,88,88,88	0
58	MG	14	3206	1/1	0.96	0.09	80,80,80,80	0
58	MG	13	1727	1/1	0.96	0.08	112,112,112,112	0
58	MG	14	3209	1/1	0.96	0.24	66,66,66,66	0
58	MG	1H	3114	1/1	0.96	0.54	74,74,74,74	0
58	MG	I8	103	1/1	0.96	0.04	73,73,73,73	0
58	MG	14	3213	1/1	0.96	0.36	64,64,64,64	0
58	MG	14	3214	1/1	0.96	0.34	88,88,88,88	0
58	MG	13	1690	1/1	0.96	0.13	74,74,74,74	0
58	MG	14	3039	1/1	0.96	0.23	50,50,50,50	0
58	MG	1H	3423	1/1	0.96	0.10	66,66,66,66	0
58	MG	13	1711	1/1	0.96	0.11	97,97,97,97	0
58	MG	13	1730	1/1	0.96	0.17	86,86,86,86	0
58	MG	1H	3429	1/1	0.96	0.12	71,71,71,71	0
58	MG	1H	3430	1/1	0.96	0.17	49,49,49,49	0
58	MG	1H	3354	1/1	0.96	0.13	49,49,49,49	0
58	MG	1G	1605	1/1	0.96	0.38	101,101,101,101	0
58	MG	1H	3312	1/1	0.96	0.24	67,67,67,67	0
58	MG	1H	3433	1/1	0.96	0.17	87,87,87,87	0
58	MG	1H	3434	1/1	0.96	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1610	1/1	0.96	0.31	98,98,98,98	0
58	MG	1H	3212	1/1	0.96	0.43	76,76,76,76	0
58	MG	13	1612	1/1	0.96	0.33	63,63,63,63	0
58	MG	13	1614	1/1	0.96	0.20	78,78,78,78	0
58	MG	1H	3120	1/1	0.96	0.34	74,74,74,74	0
58	MG	1H	3442	1/1	0.96	0.08	69,69,69,69	0
58	MG	14	3235	1/1	0.96	0.66	72,72,72,72	0
58	MG	14	3038	1/1	0.97	0.33	71,71,71,71	0
58	MG	13	1701	1/1	0.97	0.14	114,114,114,114	0
58	MG	1G	1601	1/1	0.97	0.29	91,91,91,91	0
58	MG	14	3226	1/1	0.97	0.41	73,73,73,73	0
58	MG	13	1613	1/1	0.97	0.22	81,81,81,81	0
58	MG	1H	3257	1/1	0.97	0.30	70,70,70,70	0
58	MG	1H	3195	1/1	0.97	0.50	62,62,62,62	0
58	MG	1H	3259	1/1	0.97	0.48	79,79,79,79	0
58	MG	1H	3057	1/1	0.97	0.41	66,66,66,66	0
58	MG	14	3318	1/1	0.97	0.24	64,64,64,64	0
58	MG	13	1684	1/1	0.97	0.14	128,128,128,128	0
58	MG	1H	3440	1/1	0.97	0.05	58,58,58,58	0
58	MG	1H	3380	1/1	0.97	0.11	59,59,59,59	0
58	MG	13	1667	1/1	0.97	0.47	71,71,71,71	0
58	MG	1H	3086	1/1	0.97	0.37	70,70,70,70	0
58	MG	1H	3384	1/1	0.97	0.06	58,58,58,58	0
58	MG	14	3152	1/1	0.97	0.33	92,92,92,92	0
58	MG	1H	3062	1/1	0.97	0.20	64,64,64,64	0
58	MG	14	3062	1/1	0.97	0.17	68,68,68,68	0
58	MG	14	3332	1/1	0.97	0.10	53,53,53,53	0
58	MG	1H	3330	1/1	0.97	0.34	102,102,102,102	0
58	MG	14	3334	1/1	0.97	0.05	64,64,64,64	0
58	MG	14	3335	1/1	0.97	0.09	61,61,61,61	0
58	MG	14	3064	1/1	0.97	0.19	78,78,78,78	0
58	MG	14	3065	1/1	0.97	0.32	67,67,67,67	0
58	MG	13	1717	1/1	0.97	0.08	92,92,92,92	0
58	MG	14	3341	1/1	0.97	0.08	68,68,68,68	0
58	MG	1H	3448	1/1	0.97	0.08	82,82,82,82	0
58	MG	14	3344	1/1	0.97	0.15	81,81,81,81	0
58	MG	1H	3202	1/1	0.97	0.82	70,70,70,70	0
58	MG	14	3161	1/1	0.97	0.52	70,70,70,70	0
58	MG	1H	3450	1/1	0.97	0.10	54,54,54,54	0
58	MG	14	3070	1/1	0.97	0.51	60,60,60,60	0
58	MG	14	3072	1/1	0.97	0.22	45,45,45,45	0
58	MG	13	1718	1/1	0.97	0.04	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1621	1/1	0.97	0.12	92,92,92,92	0
58	MG	14	3075	1/1	0.97	0.29	68,68,68,68	0
58	MG	14	3254	1/1	0.97	0.19	111,111,111,111	0
58	MG	1G	1682	1/1	0.97	0.13	97,97,97,97	0
58	MG	1H	3148	1/1	0.97	0.24	50,50,50,50	0
58	MG	14	3359	1/1	0.97	0.06	79,79,79,79	0
58	MG	13	1732	1/1	0.97	0.20	65,65,65,65	0
58	MG	1G	1685	1/1	0.97	0.09	87,87,87,87	0
58	MG	1H	3010	1/1	0.97	0.36	63,63,63,63	0
58	MG	1H	3396	1/1	0.97	0.10	78,78,78,78	0
58	MG	1H	3026	1/1	0.97	0.47	56,56,56,56	0
58	MG	1H	3398	1/1	0.97	0.16	66,66,66,66	0
58	MG	14	3367	1/1	0.97	0.09	65,65,65,65	0
58	MG	1G	1690	1/1	0.97	0.16	93,93,93,93	0
58	MG	1H	3068	1/1	0.97	0.28	86,86,86,86	0
58	MG	14	3370	1/1	0.97	0.10	64,64,64,64	0
58	MG	14	3088	1/1	0.97	0.45	52,52,52,52	0
58	MG	1H	3401	1/1	0.97	0.18	69,69,69,69	0
58	MG	14	3001	1/1	0.97	0.16	46,46,46,46	0
58	MG	1H	3403	1/1	0.97	0.14	76,76,76,76	0
58	MG	1H	3462	1/1	0.97	0.04	97,97,97,97	0
58	MG	14	3379	1/1	0.97	0.12	60,60,60,60	0
58	MG	14	3270	1/1	0.97	0.30	63,63,63,63	0
58	MG	14	3004	1/1	0.97	0.37	67,67,67,67	0
58	MG	14	3005	1/1	0.97	0.45	48,48,48,48	0
58	MG	14	3098	1/1	0.97	0.17	93,93,93,93	0
58	MG	14	3006	1/1	0.97	0.63	56,56,56,56	0
58	MG	1H	3404	1/1	0.97	0.13	48,48,48,48	0
58	MG	1H	3069	1/1	0.97	0.42	90,90,90,90	0
58	MG	14	3103	1/1	0.97	0.28	51,51,51,51	0
58	MG	1H	3465	1/1	0.97	0.15	71,71,71,71	0
58	MG	1H	3210	1/1	0.97	0.47	71,71,71,71	0
58	MG	14	3192	1/1	0.97	0.51	63,63,63,63	0
58	MG	13	1622	1/1	0.97	0.37	74,74,74,74	0
58	MG	1H	3408	1/1	0.97	0.12	82,82,82,82	0
58	MG	1H	3409	1/1	0.97	0.07	85,85,85,85	0
58	MG	14	3196	1/1	0.97	0.55	75,75,75,75	0
58	MG	13	1635	1/1	0.97	0.52	74,74,74,74	0
58	MG	1H	3030	1/1	0.97	0.22	67,67,67,67	0
58	MG	1G	1642	1/1	0.97	0.48	91,91,91,91	0
58	MG	14	3398	1/1	0.97	0.07	108,108,108,108	0
58	MG	1H	3103	1/1	0.97	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	16	206	1/1	0.97	0.05	73,73,73,73	0
58	MG	1H	3347	1/1	0.97	0.28	51,51,51,51	0
58	MG	14	3116	1/1	0.97	0.20	64,64,64,64	0
58	MG	1H	3350	1/1	0.97	0.12	48,48,48,48	0
58	MG	1H	3416	1/1	0.97	0.08	69,69,69,69	0
58	MG	1H	3245	1/1	0.97	0.70	62,62,62,62	0
58	MG	13	1648	1/1	0.97	0.50	95,95,95,95	0
58	MG	14	3210	1/1	0.97	0.17	80,80,80,80	0
58	MG	1H	3075	1/1	0.97	0.48	43,43,43,43	0
58	MG	1H	3356	1/1	0.97	0.17	42,42,42,42	0
58	MG	88	201	1/1	0.97	0.21	81,81,81,81	0
58	MG	13	1642	1/1	0.97	0.27	74,74,74,74	0
58	MG	1H	3358	1/1	0.97	0.14	45,45,45,45	0
58	MG	1H	3359	1/1	0.97	0.12	59,59,59,59	0
58	MG	13	1609	1/1	0.97	0.37	75,75,75,75	0
58	MG	1H	3133	1/1	0.97	0.34	71,71,71,71	0
58	MG	1H	3163	1/1	0.97	0.35	50,50,50,50	0
58	MG	14	3036	1/1	0.97	0.74	96,96,96,96	0
58	MG	13	1617	1/1	0.97	0.24	83,83,83,83	0
58	MG	1H	3077	1/1	0.98	0.23	60,60,60,60	0
58	MG	14	3337	1/1	0.98	0.06	66,66,66,66	0
58	MG	1H	3008	1/1	0.98	0.26	81,81,81,81	0
58	MG	1H	3385	1/1	0.98	0.20	47,47,47,47	0
58	MG	1H	3386	1/1	0.98	0.11	57,57,57,57	0
58	MG	14	3342	1/1	0.98	0.07	80,80,80,80	0
58	MG	1H	3001	1/1	0.98	0.32	43,43,43,43	0
58	MG	13	1716	1/1	0.98	0.07	76,76,76,76	0
58	MG	1H	3344	1/1	0.98	0.13	58,58,58,58	0
58	MG	1H	3437	1/1	0.98	0.09	58,58,58,58	0
58	MG	14	3127	1/1	0.98	0.27	69,69,69,69	0
58	MG	1H	3390	1/1	0.98	0.09	50,50,50,50	0
58	MG	14	3130	1/1	0.98	0.53	86,86,86,86	0
58	MG	1H	3289	1/1	0.98	0.17	49,49,49,49	0
58	MG	1H	3029	1/1	0.98	0.35	42,42,42,42	0
58	MG	14	3202	1/1	0.98	0.31	63,63,63,63	0
58	MG	1H	3143	1/1	0.98	0.14	56,56,56,56	0
58	MG	1H	3348	1/1	0.98	0.19	50,50,50,50	0
58	MG	14	3356	1/1	0.98	0.17	58,58,58,58	0
58	MG	1H	3349	1/1	0.98	0.18	64,64,64,64	0
58	MG	1H	3102	1/1	0.98	0.39	35,35,35,35	0
58	MG	14	3207	1/1	0.98	0.37	80,80,80,80	0
58	MG	14	3361	1/1	0.98	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1H	3191	1/1	0.98	0.50	90,90,90,90	0
58	MG	14	3139	1/1	0.98	0.34	99,99,99,99	0
58	MG	14	3009	1/1	0.98	0.46	52,52,52,52	0
58	MG	14	3010	1/1	0.98	0.48	41,41,41,41	0
58	MG	14	3071	1/1	0.98	0.58	68,68,68,68	0
58	MG	14	3011	1/1	0.98	0.59	48,48,48,48	0
58	MG	13	1721	1/1	0.98	0.12	66,66,66,66	0
58	MG	14	3145	1/1	0.98	0.32	65,65,65,65	0
58	MG	1H	3241	1/1	0.98	0.35	66,66,66,66	0
58	MG	1H	3400	1/1	0.98	0.11	72,72,72,72	0
58	MG	14	3372	1/1	0.98	0.09	70,70,70,70	0
58	MG	14	3373	1/1	0.98	0.19	61,61,61,61	0
58	MG	14	3218	1/1	0.98	0.56	62,62,62,62	0
58	MG	14	3375	1/1	0.98	0.07	97,97,97,97	0
58	MG	1H	3169	1/1	0.98	0.21	85,85,85,85	0
58	MG	1H	3402	1/1	0.98	0.15	51,51,51,51	0
58	MG	1H	3051	1/1	0.98	0.35	45,45,45,45	0
58	MG	14	3079	1/1	0.98	0.46	70,70,70,70	0
58	MG	1H	3124	1/1	0.98	0.36	46,46,46,46	0
58	MG	14	3081	1/1	0.98	0.32	76,76,76,76	0
58	MG	1H	3453	1/1	0.98	0.10	84,84,84,84	0
58	MG	1H	3052	1/1	0.98	0.33	53,53,53,53	0
58	MG	1H	3360	1/1	0.98	0.10	61,61,61,61	0
58	MG	13	1602	1/1	0.98	0.28	86,86,86,86	0
58	MG	1H	3013	1/1	0.98	0.29	82,82,82,82	0
58	MG	13	1674	1/1	0.98	0.09	91,91,91,91	0
58	MG	1H	3365	1/1	0.98	0.14	74,74,74,74	0
58	MG	1H	3366	1/1	0.98	0.14	76,76,76,76	0
58	MG	1H	3109	1/1	0.98	0.30	47,47,47,47	0
58	MG	14	3092	1/1	0.98	0.32	76,76,76,76	0
58	MG	1G	1669	1/1	0.98	0.36	107,107,107,107	0
58	MG	1H	3006	1/1	0.98	0.36	46,46,46,46	0
58	MG	1H	3369	1/1	0.98	0.18	49,49,49,49	0
58	MG	1H	3060	1/1	0.98	0.40	61,61,61,61	0
58	MG	1H	3074	1/1	0.98	0.29	64,64,64,64	0
58	MG	1H	3373	1/1	0.98	0.12	51,51,51,51	0
58	MG	1H	3374	1/1	0.98	0.16	53,53,53,53	0
58	MG	13	1611	1/1	0.98	0.24	72,72,72,72	0
58	MG	14	3102	1/1	0.98	0.26	61,61,61,61	0
58	MG	1H	3255	1/1	0.98	0.39	73,73,73,73	0
58	MG	1H	3134	1/1	0.98	0.08	69,69,69,69	0
58	MG	1H	3093	1/1	0.98	0.36	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3424	1/1	0.98	0.10	48,48,48,48	0
58	MG	14	3040	1/1	0.98	0.35	59,59,59,59	0
58	MG	14	3041	1/1	0.98	0.35	54,54,54,54	0
58	MG	29	303	1/1	0.98	0.40	52,52,52,52	0
58	MG	14	3043	1/1	0.98	0.38	57,57,57,57	0
58	MG	14	3044	1/1	0.98	0.51	64,64,64,64	0
58	MG	14	3046	1/1	0.98	0.28	66,66,66,66	0
58	MG	1H	3425	1/1	0.98	0.12	63,63,63,63	0
58	MG	14	3327	1/1	0.98	0.16	59,59,59,59	0
58	MG	14	3113	1/1	0.98	0.41	73,73,73,73	0
58	MG	14	3048	1/1	0.98	0.29	90,90,90,90	0
58	MG	14	3331	1/1	0.98	0.14	63,63,63,63	0
58	MG	1H	3076	1/1	0.98	0.41	65,65,65,65	0
58	MG	14	3050	1/1	0.98	0.51	59,59,59,59	0
59	SF4	3E	301	8/8	0.98	0.17	86,99,103,105	0
58	MG	1H	3427	1/1	0.98	0.07	72,72,72,72	0
60	ZN	5A	101	1/1	0.98	0.08	142,142,142,142	0
58	MG	1H	3339	1/1	0.98	0.43	48,48,48,48	0
58	MG	14	3354	1/1	0.99	0.10	70,70,70,70	0
58	MG	1H	3054	1/1	0.99	0.24	52,52,52,52	0
58	MG	1H	3059	1/1	0.99	0.24	49,49,49,49	0
58	MG	14	3357	1/1	0.99	0.22	76,76,76,76	0
58	MG	1H	3372	1/1	0.99	0.11	62,62,62,62	0
58	MG	13	1638	1/1	0.99	0.26	59,59,59,59	0
58	MG	14	3128	1/1	0.99	0.45	58,58,58,58	0
58	MG	1H	3147	1/1	0.99	0.31	64,64,64,64	0
58	MG	14	3298	1/1	0.99	0.90	64,64,64,64	0
58	MG	14	3329	1/1	0.99	0.17	56,56,56,56	0
58	MG	1H	3248	1/1	0.99	0.50	74,74,74,74	0
58	MG	1H	3138	1/1	0.99	0.41	58,58,58,58	0
58	MG	1H	3411	1/1	0.99	0.12	69,69,69,69	0
58	MG	13	1709	1/1	0.99	0.07	92,92,92,92	0
58	MG	1H	3378	1/1	0.99	0.16	53,53,53,53	0
58	MG	1H	3363	1/1	0.99	0.06	68,68,68,68	0
58	MG	1H	3099	1/1	0.99	0.20	55,55,55,55	0
58	MG	1H	3351	1/1	0.99	0.08	46,46,46,46	0
58	MG	14	3138	1/1	0.99	0.32	45,45,45,45	0
58	MG	14	3339	1/1	0.99	0.11	82,82,82,82	0
58	MG	1G	1623	1/1	0.99	0.50	62,62,62,62	0
58	MG	1H	3435	1/1	0.99	0.13	56,56,56,56	0
58	MG	1H	3352	1/1	0.99	0.12	61,61,61,61	0
58	MG	1H	3383	1/1	0.99	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3092	1/1	0.99	0.26	49,49,49,49	0
58	MG	14	3042	1/1	0.99	0.54	70,70,70,70	0
58	MG	14	3091	1/1	0.99	0.43	86,86,86,86	0
58	MG	1H	3053	1/1	0.99	0.34	50,50,50,50	0
58	MG	2L	101	1/1	0.99	0.56	73,73,73,73	0
58	MG	14	3045	1/1	0.99	0.33	58,58,58,58	0
58	MG	1G	1608	1/1	0.99	0.18	89,89,89,89	0
59	SF4	32	301	8/8	0.99	0.15	115,123,133,136	0
60	ZN	5I	101	1/1	0.99	0.13	102,102,102,102	0
58	MG	1H	3094	1/1	0.99	0.37	64,64,64,64	0
58	MG	14	3320	1/1	0.99	0.18	64,64,64,64	0
58	MG	14	3097	1/1	0.99	0.22	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.