wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 3, 2024 – 12:41 pm GMT

PDB ID	:	5EL5
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and tRNALys in the A-site with a U-U mismatch in the second position
Authors	:	Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on	:	2015-11-04
Resolution	:	3.15 Å(reported)

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

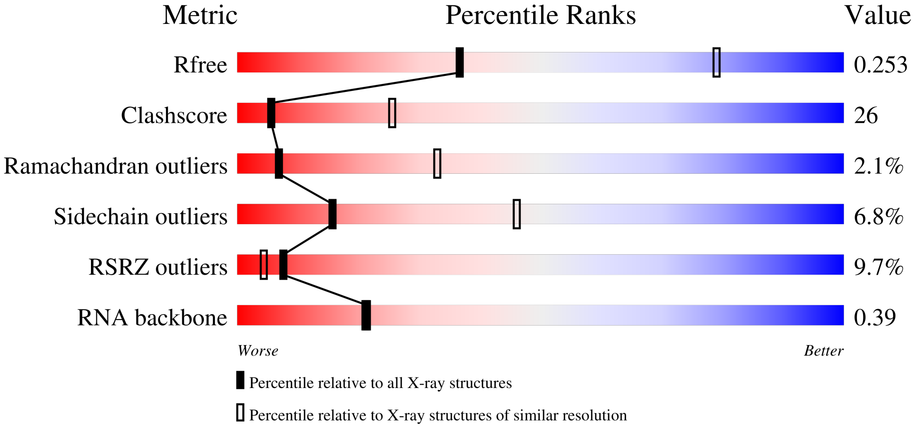
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

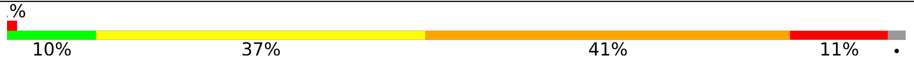
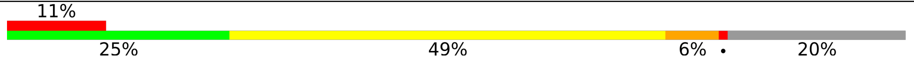
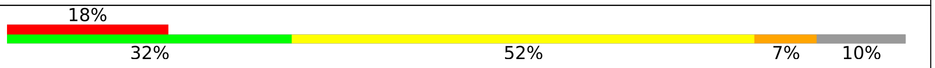
The reported resolution of this entry is 3.15 Å.

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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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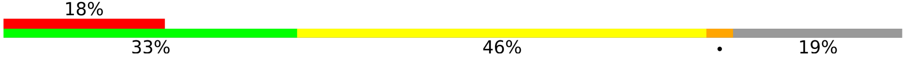
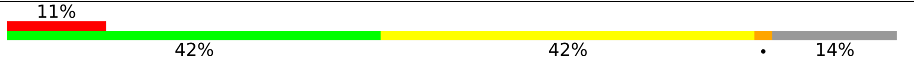
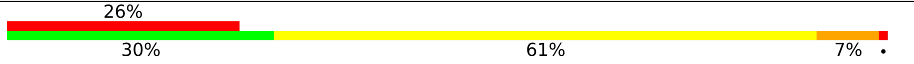
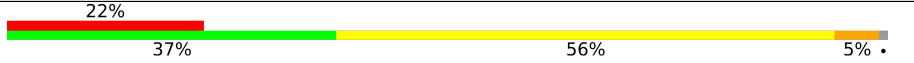
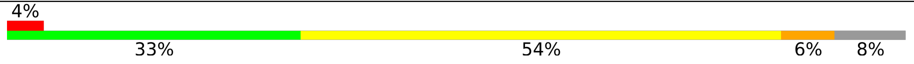
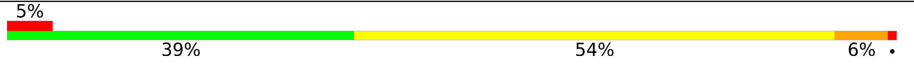
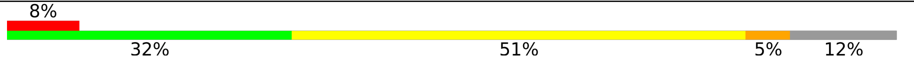
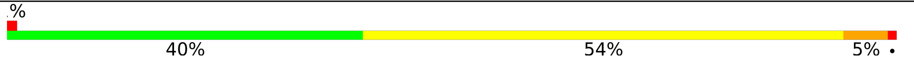
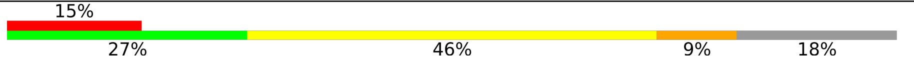
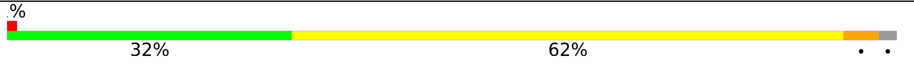
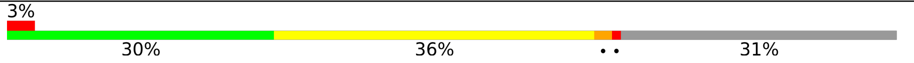
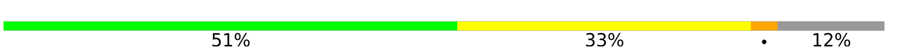
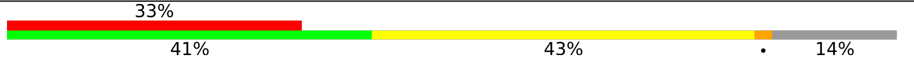
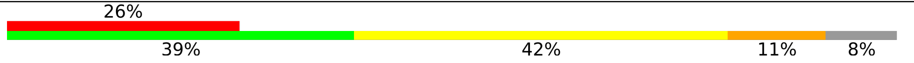
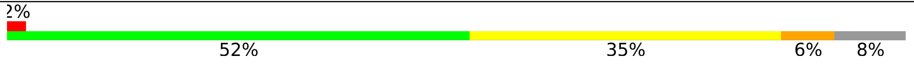
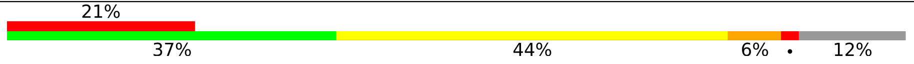
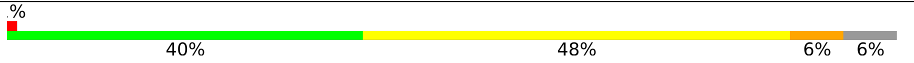
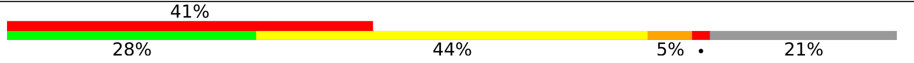
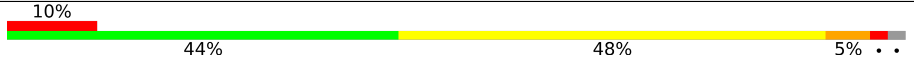
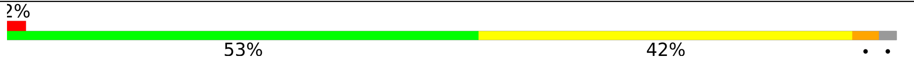
Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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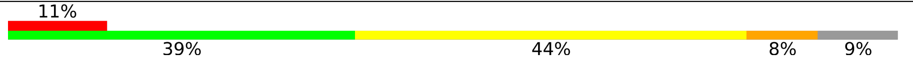
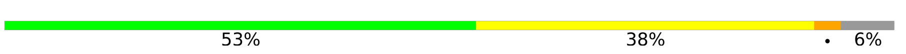
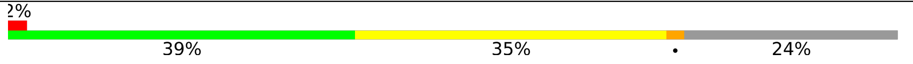
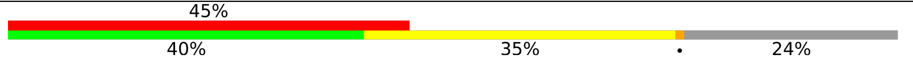
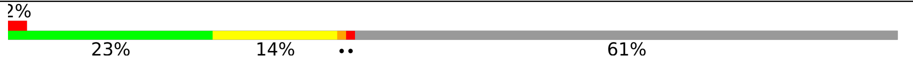
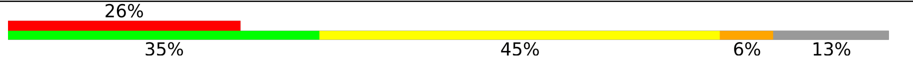
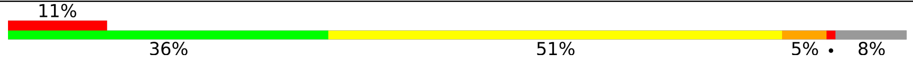
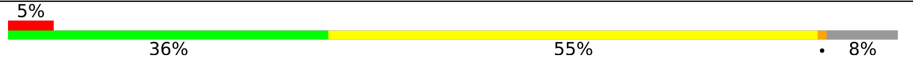
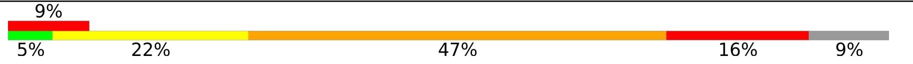
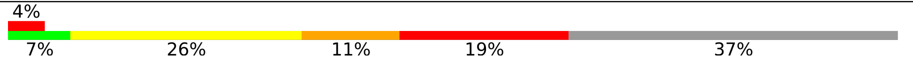
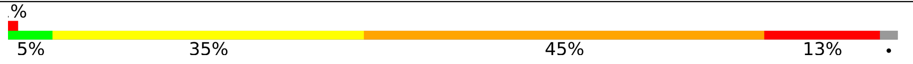
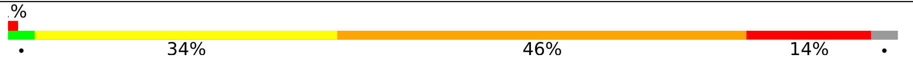
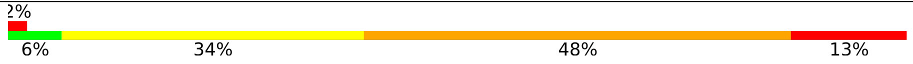
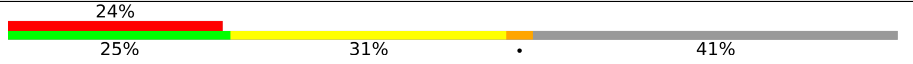
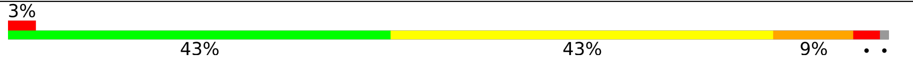
Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	
27	1J	122	
28	71	229	
29	11	276	

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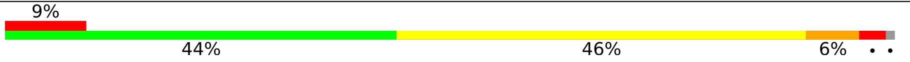
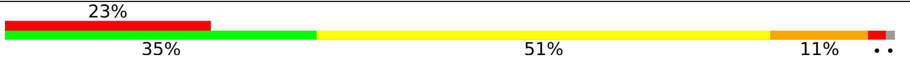
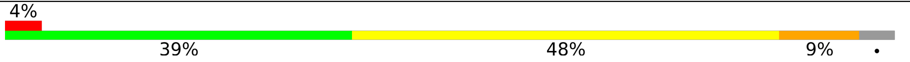
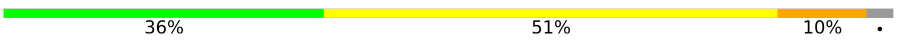
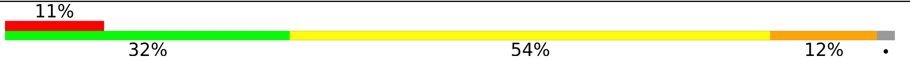
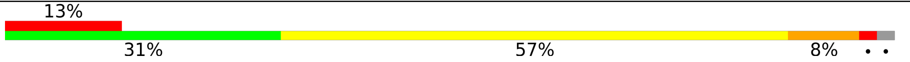
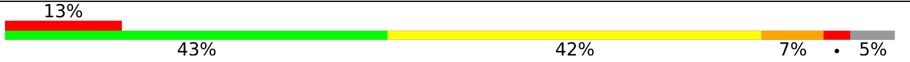
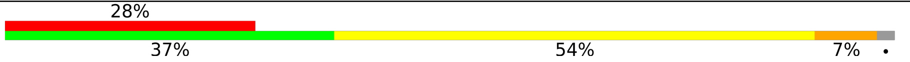
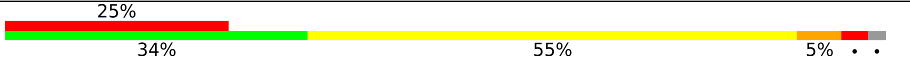
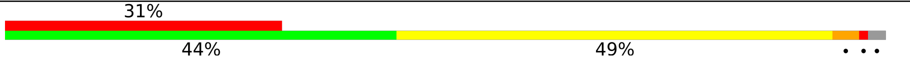
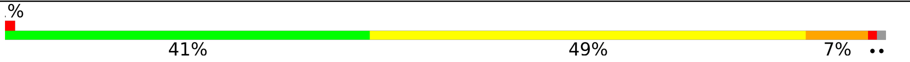
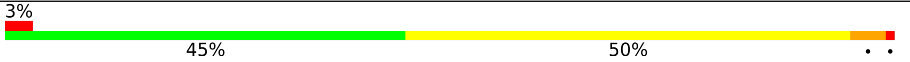
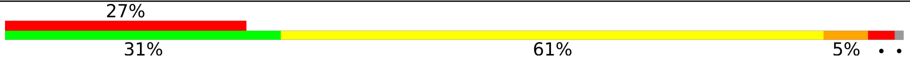
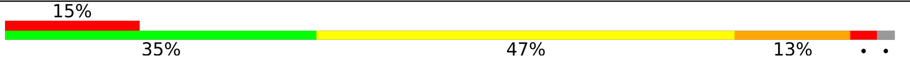
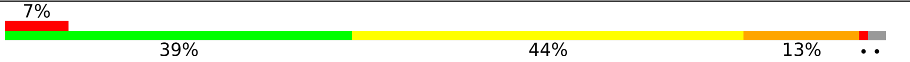
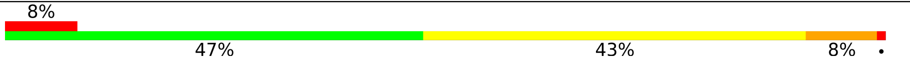
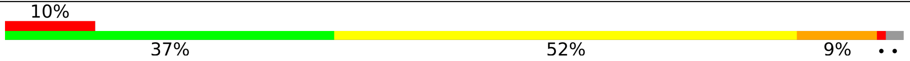
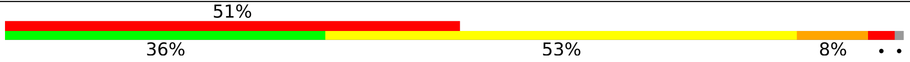
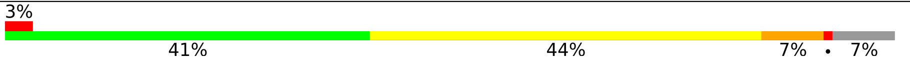
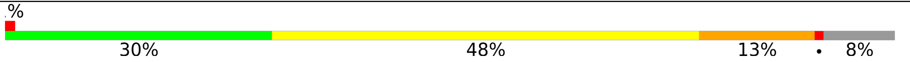
Mol	Chain	Length	Quality of chain
29	19	276	 16% 47% 42% 8% ••
30	21	206	 9% 44% 46% 6% • •
30	29	206	 23% 35% 51% 11% ••
31	31	210	 4% 39% 48% 9% •
31	39	210	 36% 51% 10% •
32	41	182	 11% 32% 54% 12% •
32	49	182	 13% 31% 57% 8% • •
33	51	180	 13% 43% 42% 7% • 5%
33	59	180	 7% 14% 19% 5% 62%
34	61	148	 28% 37% 54% 7% •
34	69	148	 25% 34% 55% 5% • •
35	15	140	 31% 44% 49% • • •
35	58	140	 % 41% 49% 7% ••
36	25	122	 3% 45% 50% • •
36	68	122	 57% 39% 5%
37	35	150	 27% 31% 61% 5% • •
37	78	150	 15% 35% 47% 13% • •
38	45	141	 7% 39% 44% 13% ••
38	88	141	 46% 49% 39% 11% •
39	55	118	 8% 47% 43% 8% •
39	98	118	 63% 42% 55% •
40	65	112	 10% 37% 52% 9% • •
40	A8	112	 51% 36% 53% 8% • •
41	75	146	 3% 41% 44% 7% • 7%
41	B8	146	 % 30% 48% 13% • 8%

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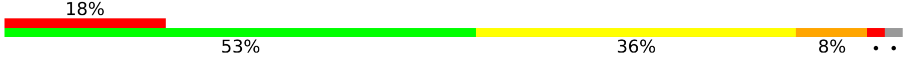
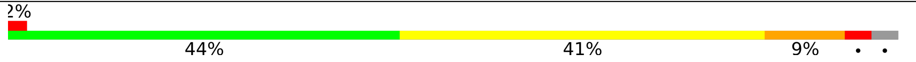
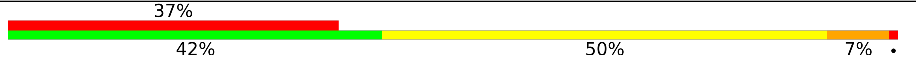
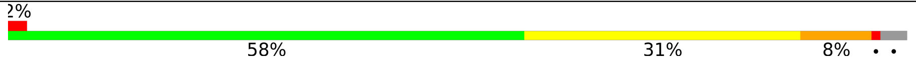
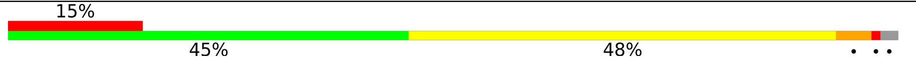
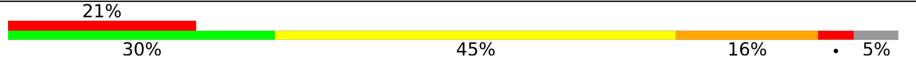
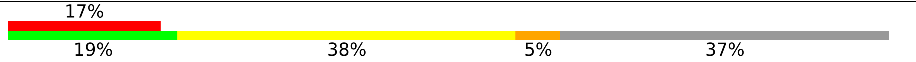
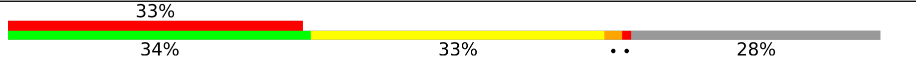
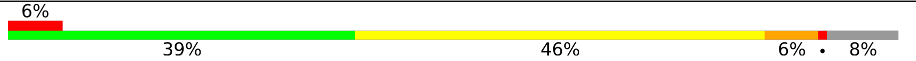
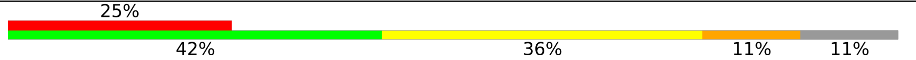
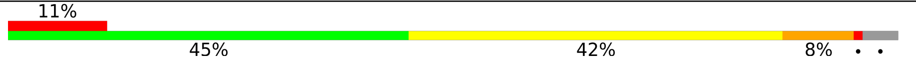
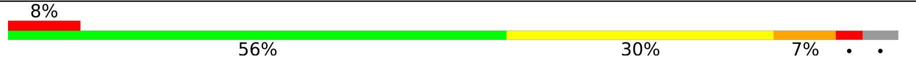
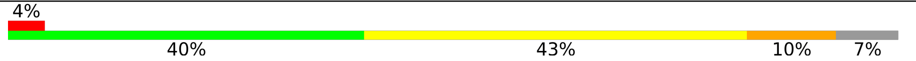
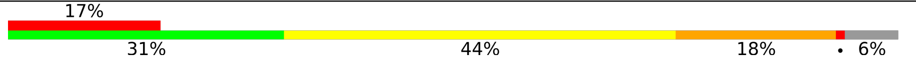
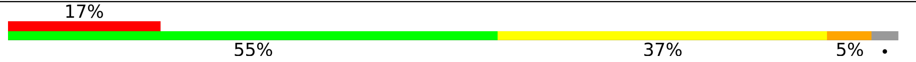
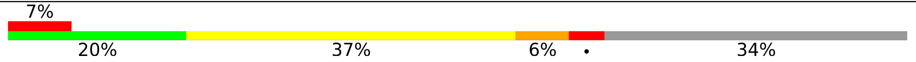
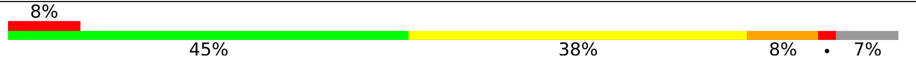
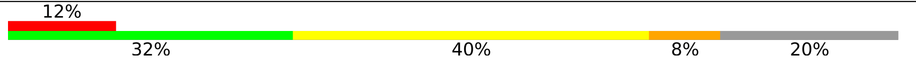
Mol	Chain	Length	Quality of chain
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	

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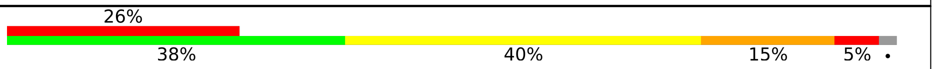
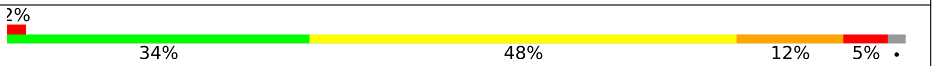
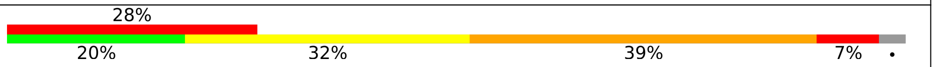
Mol	Chain	Length	Quality of chain
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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	1606	-	-	-	X
58	MG	13	1623	-	-	-	X
58	MG	13	1625	-	-	-	X
58	MG	13	1627	-	-	-	X
58	MG	13	1628	-	-	-	X
58	MG	13	1634	-	-	-	X
58	MG	13	1661	-	-	-	X
58	MG	13	1680	-	-	-	X
58	MG	13	1687	-	-	-	X
58	MG	13	1688	-	-	-	X
58	MG	13	1692	-	-	-	X
58	MG	13	1699	-	-	-	X
58	MG	13	1702	-	-	-	X
58	MG	13	1707	-	-	-	X
58	MG	13	1708	-	-	-	X
58	MG	14	3023	-	-	-	X
58	MG	14	3024	-	-	-	X
58	MG	14	3028	-	-	-	X
58	MG	14	3031	-	-	-	X
58	MG	14	3062	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3109	-	-	-	X
58	MG	14	3132	-	-	-	X
58	MG	14	3149	-	-	-	X
58	MG	14	3150	-	-	-	X
58	MG	14	3159	-	-	-	X
58	MG	14	3171	-	-	-	X
58	MG	14	3179	-	-	-	X
58	MG	14	3192	-	-	-	X
58	MG	14	3195	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3199	-	-	-	X
58	MG	14	3201	-	-	-	X
58	MG	14	3217	-	-	-	X
58	MG	14	3227	-	-	-	X
58	MG	14	3231	-	-	-	X
58	MG	14	3233	-	-	-	X
58	MG	14	3234	-	-	-	X
58	MG	14	3259	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3261	-	-	-	X
58	MG	14	3263	-	-	-	X
58	MG	14	3267	-	-	-	X
58	MG	14	3270	-	-	-	X
58	MG	14	3272	-	-	-	X
58	MG	14	3275	-	-	-	X
58	MG	14	3277	-	-	-	X
58	MG	14	3278	-	-	-	X
58	MG	14	3279	-	-	-	X
58	MG	14	3280	-	-	-	X
58	MG	14	3284	-	-	-	X
58	MG	14	3286	-	-	-	X
58	MG	14	3288	-	-	-	X
58	MG	14	3295	-	-	-	X
58	MG	14	3302	-	-	-	X
58	MG	14	3303	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	14	3315	-	-	-	X
58	MG	14	3321	-	-	-	X
58	MG	14	3325	-	-	-	X
58	MG	14	3328	-	-	-	X
58	MG	14	3331	-	-	-	X
58	MG	16	208	-	-	-	X
58	MG	1G	1602	-	-	-	X
58	MG	1G	1621	-	-	-	X
58	MG	1G	1627	-	-	-	X
58	MG	1G	1635	-	-	-	X
58	MG	1G	1637	-	-	-	X
58	MG	1G	1638	-	-	-	X
58	MG	1G	1639	-	-	-	X
58	MG	1G	1640	-	-	-	X
58	MG	1G	1643	-	-	-	X
58	MG	1G	1644	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1G	1645	-	-	-	X
58	MG	1G	1648	-	-	-	X
58	MG	1G	1660	-	-	-	X
58	MG	1G	1666	-	-	-	X
58	MG	1H	3029	-	-	-	X
58	MG	1H	3030	-	-	-	X
58	MG	1H	3031	-	-	-	X
58	MG	1H	3033	-	-	-	X
58	MG	1H	3077	-	-	-	X
58	MG	1H	3095	-	-	-	X
58	MG	1H	3105	-	-	-	X
58	MG	1H	3128	-	-	-	X
58	MG	1H	3141	-	-	-	X
58	MG	1H	3145	-	-	-	X
58	MG	1H	3146	-	-	-	X
58	MG	1H	3163	-	-	-	X
58	MG	1H	3166	-	-	-	X
58	MG	1H	3187	-	-	-	X
58	MG	1H	3192	-	-	-	X
58	MG	1H	3196	-	-	-	X
58	MG	1H	3199	-	-	-	X
58	MG	1H	3206	-	-	-	X
58	MG	1H	3209	-	-	-	X
58	MG	1H	3235	-	-	-	X
58	MG	1H	3247	-	-	-	X
58	MG	1H	3257	-	-	-	X
58	MG	1H	3263	-	-	-	X
58	MG	1H	3269	-	-	-	X
58	MG	1H	3272	-	-	-	X
58	MG	1H	3286	-	-	-	X
58	MG	1H	3289	-	-	-	X
58	MG	1H	3304	-	-	-	X
58	MG	1H	3309	-	-	-	X
58	MG	1H	3313	-	-	-	X
58	MG	1H	3317	-	-	-	X
58	MG	1H	3319	-	-	-	X
58	MG	1H	3327	-	-	-	X
58	MG	1H	3332	-	-	-	X
58	MG	1H	3337	-	-	-	X
58	MG	1H	3340	-	-	-	X
58	MG	1H	3341	-	-	-	X
58	MG	1H	3342	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3350	-	-	-	X
58	MG	2K	102	-	-	-	X
58	MG	32	301	-	-	-	X
58	MG	45	203	-	-	-	X
58	MG	5E	201	-	-	-	X
58	MG	85	202	-	-	-	X
58	MG	E5	101	-	-	-	X
59	SF4	32	302	-	-	X	-

2 Entry composition ⓘ

There are 61 unique types of molecules in this entry. The entry contains 292607 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1493	Total 32097	C 14286	N 5951	O 10367	P 1493	0	0	0
1	1G	1496	Total 32152	C 14311	N 5953	O 10392	P 1496	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total 1874	C 1199	N 334	O 336	S 5	0	0	0
2	12	206	Total 1695	C 1082	N 305	O 304	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	22	194	Total 1529	C 967	N 296	O 265	S 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 1696	C 1062	N 338	O 289	S 7	0	0	0
4	32	208	Total 1702	C 1066	N 339	O 290	S 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	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1136	716	216	200	4			

- 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	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	151	Total	C	N	O	S	0	0	0
			1229	763	247	213	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

- 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	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			
9	82	105	Total	C	N	O	0	0	0
			820	523	158	139			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	72	Total	C	N	O	S	0	0	0
			593	373	115	104	1			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1A	60	Total C N O 474 298 91 85	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	121	Total C N O S 947 597 191 158 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	48	Total C N O S 388 245 82 57 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 C N O S 729 457 146 124 2	0	0	0
15	6A	87	Total C N O S 729 457 146 124 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	7I	80	Total C N O S 671 427 132 111 1	0	0	0
16	7A	84	Total C N O S 705 446 140 118 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 C N O S 834 534 155 143 2	0	0	0
17	8A	99	Total C N O S 823 528 151 142 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	9I	67	Total C N O 544 349 104 91	0	0	0
18	9A	67	Total C N O 544 349 104 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 C N O S 654 417 122 113 2	0	0	0
19	AA	36	Total C N O S 283 182 49 51 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	BI	97	Total C N O S 746 461 157 126 2	0	0	0
20	BA	98	Total C N O S 757 467 161 127 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	C	N	O	0	0	0
			199	122	48	29			
21	1B	23	Total	C	N	O	0	0	0
			204	126	49	29			

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNALys.

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

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2830	Total	C	N	O	P	0	0	0
			60960	27129	11403	19598	2830			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

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 ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	71	135	Total C N O S 1050 662 197 190 1	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	273	Total C N O S 2120 1338 421 358 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	29	203	Total C N O S 1558 985 298 269 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 1457 931 265 257 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	69	Total C N O 539 339 109 91	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	61	145	Total C N O S 1131 723 200 207 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	137	Total C N O S 1096 707 205 181 3	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	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- 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	0	0	0
			1122	698	229	192	3			
37	35	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			

- 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	0	0	0
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	B8	135	Total C N O S 1123 699 230 193 1	0	0	0
41	75	136	Total C N O 1133 705 233 195	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	C8	115	Total C N O S 950 603 199 147 1	0	0	0
42	85	116	Total C N O S 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
43	D8	101	Total C N O S 778 501 142 134 1	0	0	0
43	95	99	Total C N O 766 494 140 132	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	E8	110	Total C N O S 876 552 171 151 2	0	0	0
44	A5	110	Total C N O S 876 552 171 151 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 740 480 134 126	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	104	Total C N O S 788 507 149 127 5	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	C5	105	Total C N O S 799 513 153 128 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	H8	148	Total C N O S 1218 779 220 217 2	0	0	0
47	D5	130	Total C N O S 1064 685 191 186 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	78	Total C N O S 616 381 130 104 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
50	K8	68	Total C N O S 568 352 115 100 1	0	0	0
50	G5	67	Total C N O S 563 349 114 99 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	L8	58	Total C N O 459 293 89 77	0	0	0
51	H5	58	Total C N O 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
54	L5	45	391	240	97	52	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
			Total	C	N	O	S			
55	M5	64	516	331	102	81	2	0	0	0

- Molecule 56 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	1L	74	1570	702	271	523	74	0	0	0

- Molecule 57 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
57	3L	76	1611	721	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	141	Total Mg 141 141	0	0
58	5E	2	Total Mg 2 2	0	0
58	3I	1	Total Mg 1 1	0	0
58	5I	1	Total Mg 1 1	0	0
58	2K	3	Total Mg 3 3	0	0
58	1H	488	Total Mg 488 488	0	0
58	16	12	Total Mg 12 12	0	0
58	11	1	Total Mg 1 1	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
58	C8	1	Total Mg 1 1	0	0
58	I8	1	Total Mg 1 1	0	0
58	J8	2	Total Mg 2 2	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	78	Total Mg 78 78	0	0
58	32	1	Total Mg 1 1	0	0
58	7A	1	Total Mg 1 1	0	0
58	2L	3	Total Mg 3 3	0	0
58	14	420	Total Mg 420 420	0	0

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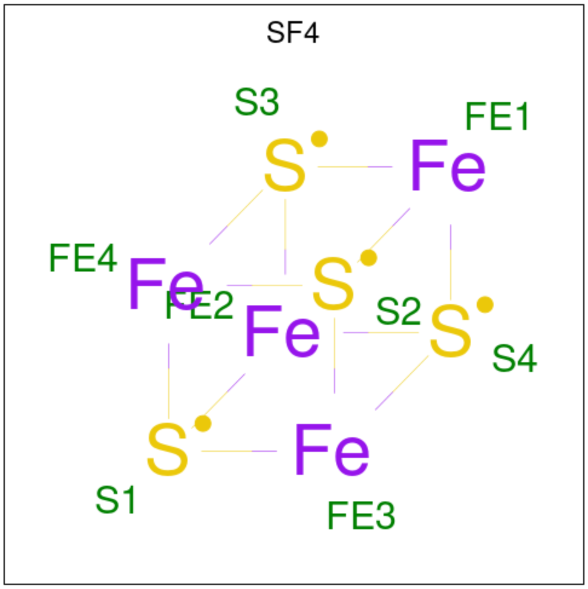
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1J	6	Total Mg 6 6	0	0
58	29	3	Total Mg 3 3	0	0
58	35	1	Total Mg 1 1	0	0
58	45	3	Total Mg 3 3	0	0
58	55	1	Total Mg 1 1	0	0
58	85	2	Total Mg 2 2	0	0
58	C5	1	Total Mg 1 1	0	0
58	E5	1	Total Mg 1 1	0	0
58	L5	1	Total Mg 1 1	0	0

- 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	148	Total O 148 148	0	0
61	3E	2	Total O 2 2	0	0
61	3I	2	Total O 2 2	0	0
61	5I	1	Total O 1 1	0	0
61	6I	1	Total O 1 1	0	0
61	1K	1	Total O 1 1	0	0
61	4K	6	Total O 6 6	0	0
61	1H	670	Total O 670 670	0	0
61	16	18	Total O 18 18	0	0
61	11	9	Total O 9 9	0	0
61	21	5	Total O 5 5	0	0
61	31	6	Total O 6 6	0	0
61	58	2	Total O 2 2	0	0
61	78	3	Total O 3 3	0	0
61	B8	1	Total O 1 1	0	0

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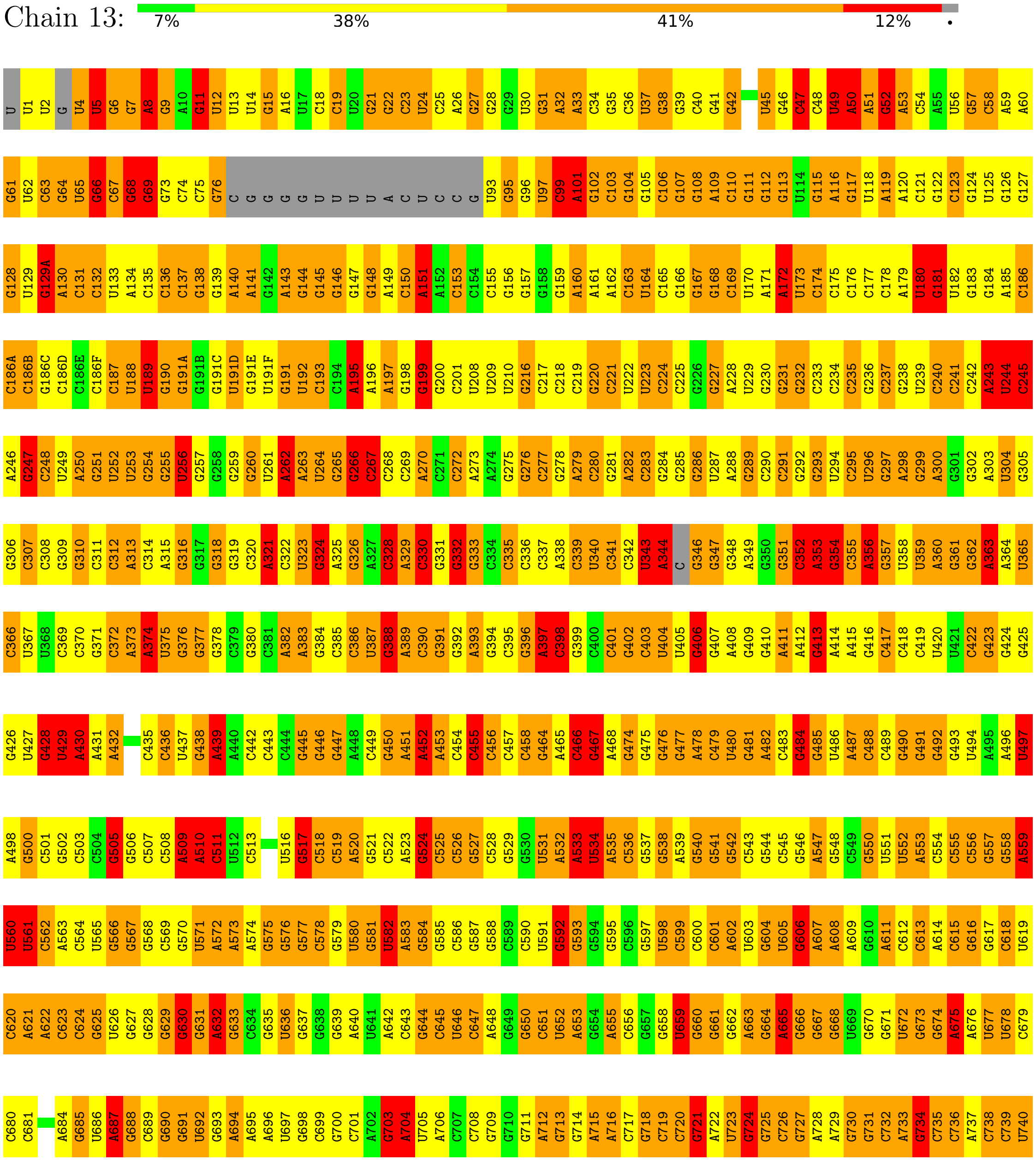
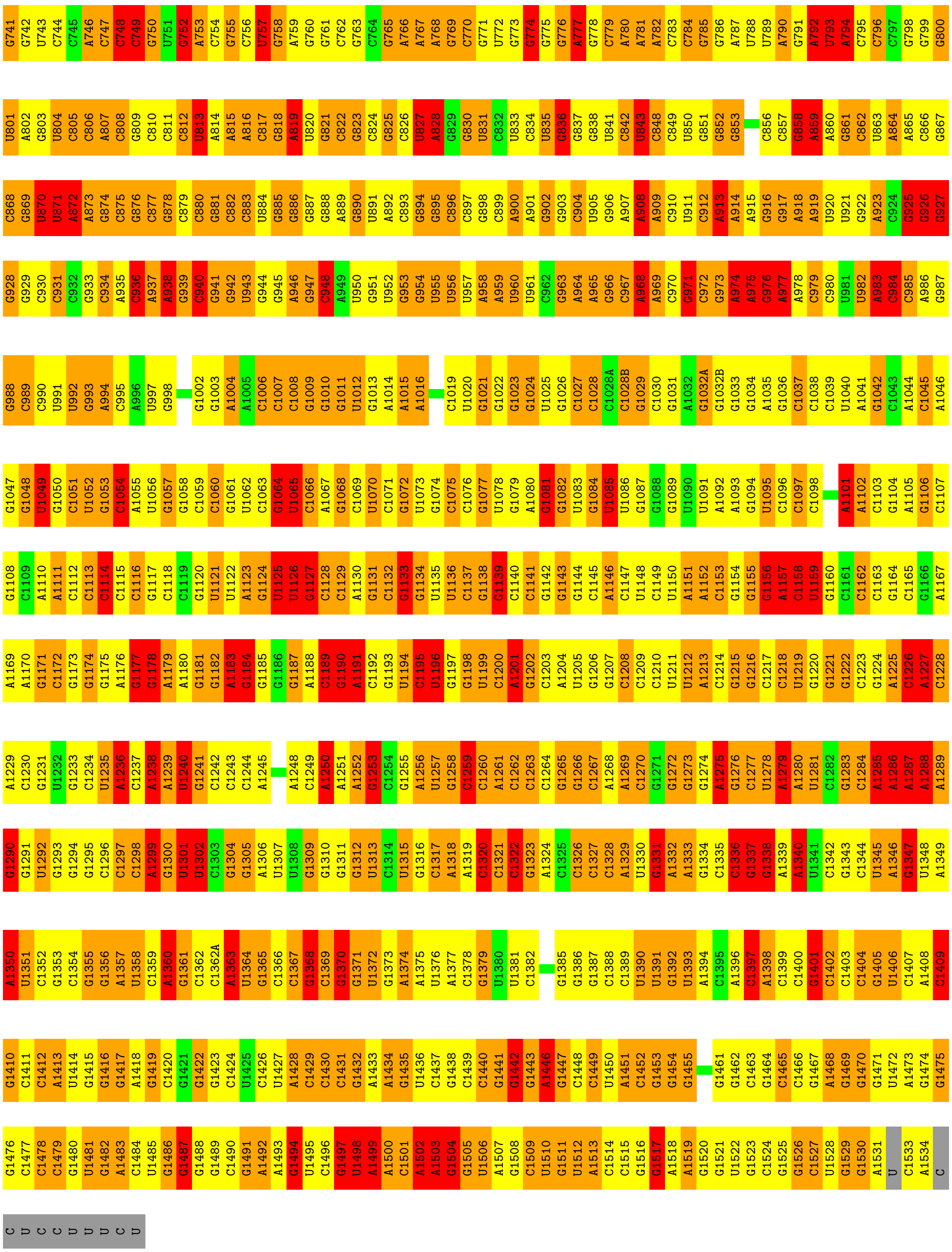
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	D8	1	Total O 1 1	0	0
61	E8	1	Total O 1 1	0	0
61	G8	1	Total O 1 1	0	0
61	I8	1	Total O 1 1	0	0
61	Q8	1	Total O 1 1	0	0
61	1G	44	Total O 44 44	0	0
61	5A	3	Total O 3 3	0	0
61	BA	1	Total O 1 1	0	0
61	14	411	Total O 411 411	0	0
61	1J	11	Total O 11 11	0	0
61	19	4	Total O 4 4	0	0
61	29	3	Total O 3 3	0	0
61	39	8	Total O 8 8	0	0
61	35	2	Total O 2 2	0	0
61	55	1	Total O 1 1	0	0
61	E5	1	Total O 1 1	0	0
61	F5	2	Total O 2 2	0	0
61	L5	1	Total O 1 1	0	0
61	M5	2	Total O 2 2	0	0

3 Residue-property plots (i)

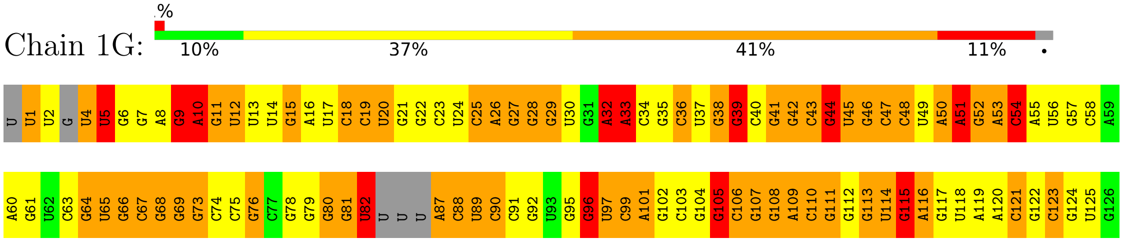
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

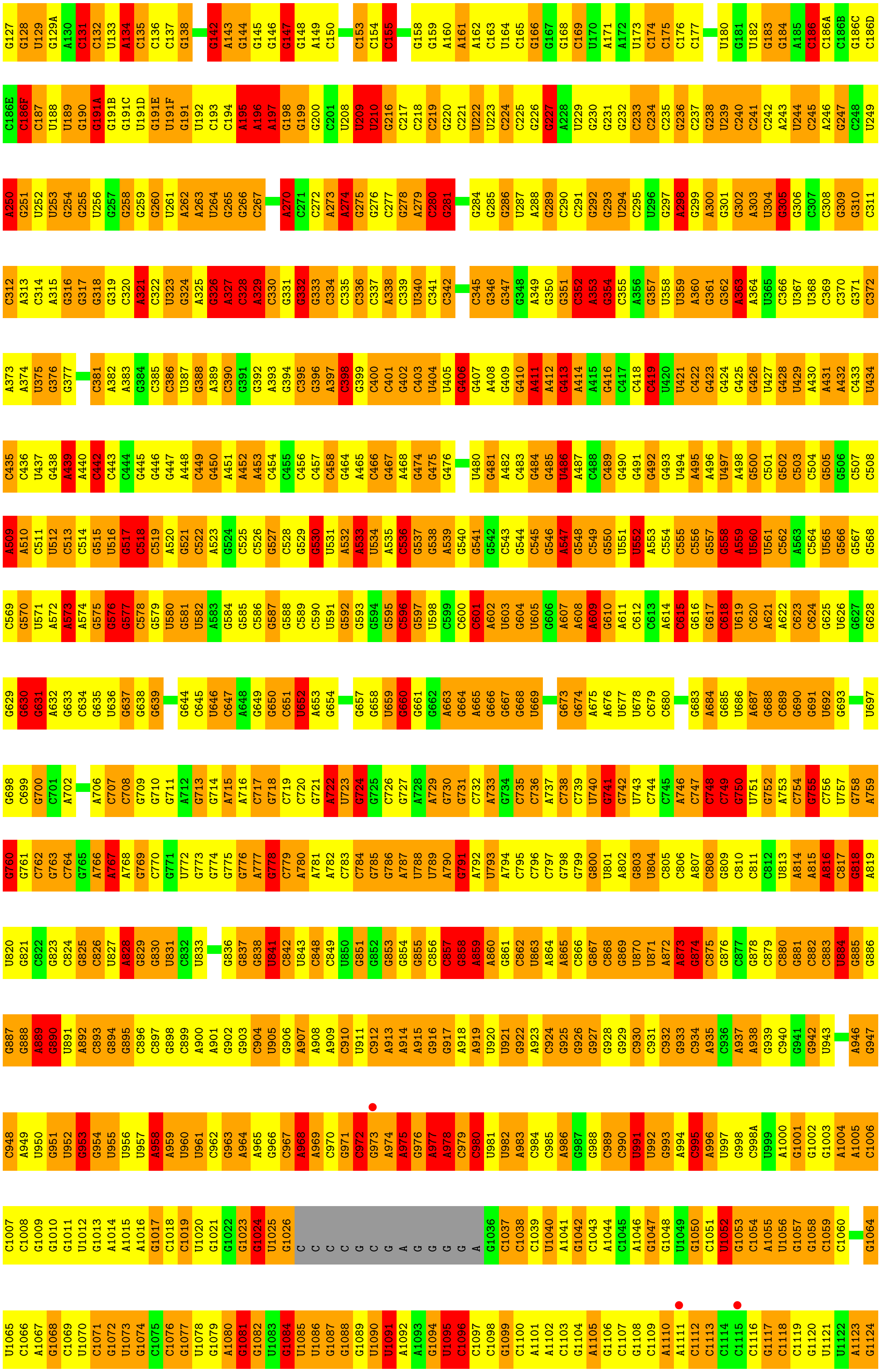
- Molecule 1: 16S ribosomal RNA





- Molecule 1: 16S ribosomal RNA





G127 G128 U129 G129A A130 C131 C132 U133 A134 C135 C136 C137 G138 G142 A143 G144 G145 G146 G147 G148 A149 C150 C153 C154 C155 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 U180 G181 U182 G183 G184 A185 C186 C186A C186B G186C C186D

C186E C186F C187 U188 U189 G190 G191A G191B G191C U191D G191E U191F G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U208 U209 U210 G216 C217 C218 C219 G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 G231 G232 C233 C234 C235 G236 C237 G238 U239 C240 C241 C242 A243 U244 C245 A246 G247 C248 U249

A250 G251 U252 U253 G254 G255 U256 G257 G258 G259 G260 U261 A262 A263 U264 G265 G266 C267 A270 C271 C272 A273 A274 G275 G276 C277 G278 A279 C280 G281 G284 G285 G286 U287 A288 G289 C290 C291 G292 G293 U294 C295 U296 G297 A298 G299 A300 G301 G302 A303 U304 G305 G306 C307 C308 G309 G310 C311

C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 C331 G332 G333 C334 C335 C336 C337 A338 C339 U340 C341 C342 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 A363 A364 U365 C366 U367 U368 G369 C370 G371 C372

A373 A374 U375 G376 G377 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 C398 G399 C400 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434

C435 C436 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 G476 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 G506 C507 C508

A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568

C569 G570 U571 A572 A573 A574 C575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 C588 C589 C590 U591 G592 G593 G594 G595 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 G610 A611 C612 C613 A614 C615 G616 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628

G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G654 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G668 U669 G673 G674 A675 A676 U677 U678 C679 C680 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 U697

G698 C699 G700 C701 A702 A706 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C717 G718 C719 C720 C721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739 U740 G741 G742 U743 C744 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759

G760 G761 C762 G763 C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819

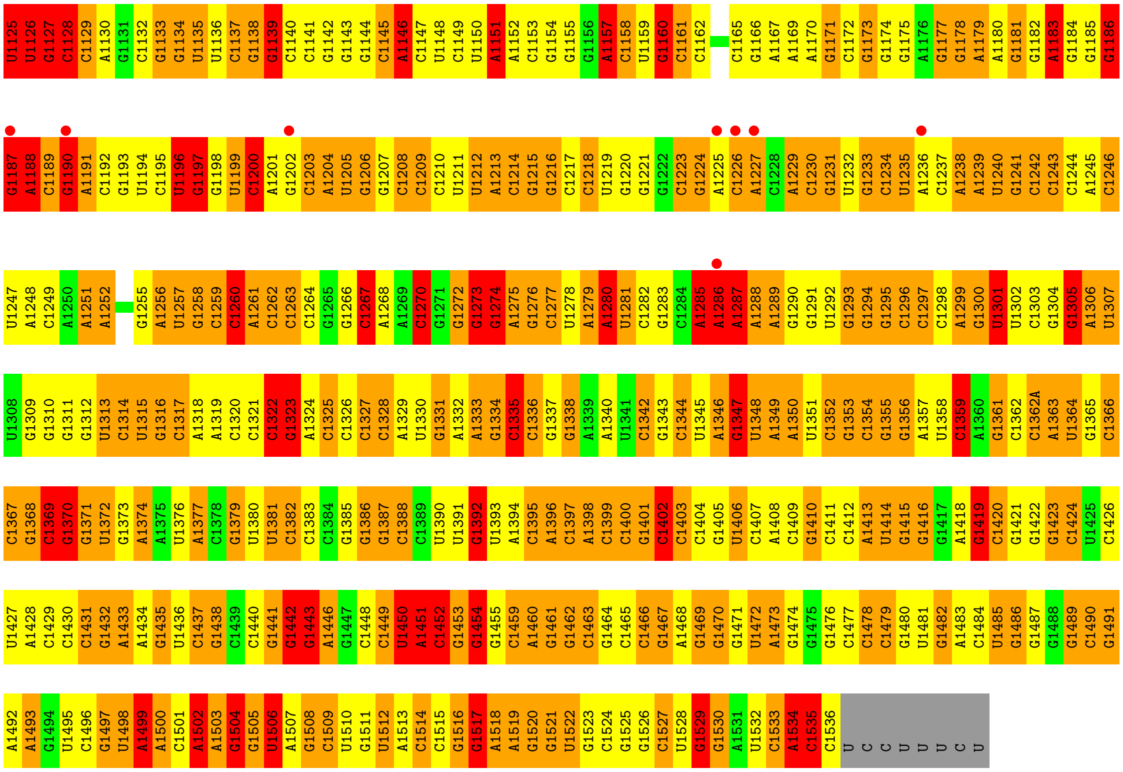
U820 G821 C822 G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 G836 G837 G838 U841 C842 U843 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G886

G887 G888 A889 G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 A946 G947

C948 A949 U950 G951 U952 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 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006

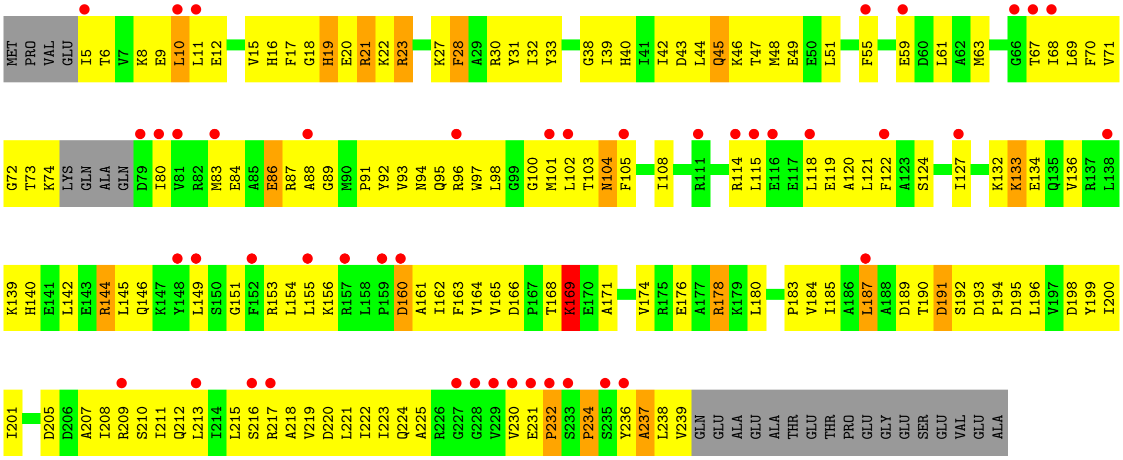
C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C C C C G C G A G G G G A G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1064

U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124



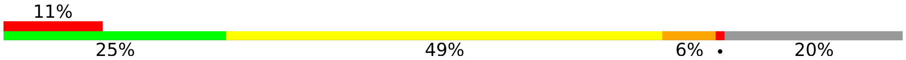
- Molecule 2: 30S ribosomal protein S2

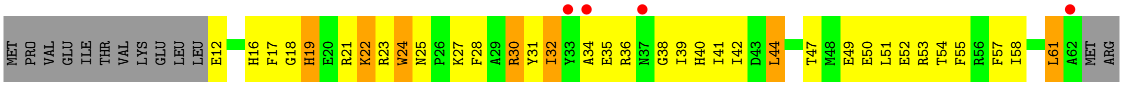
Chain 1E:

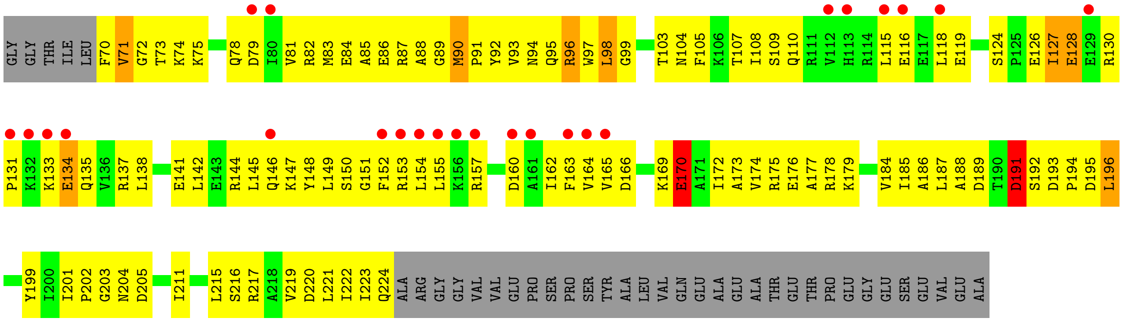


- Molecule 2: 30S ribosomal protein S2

Chain 12:

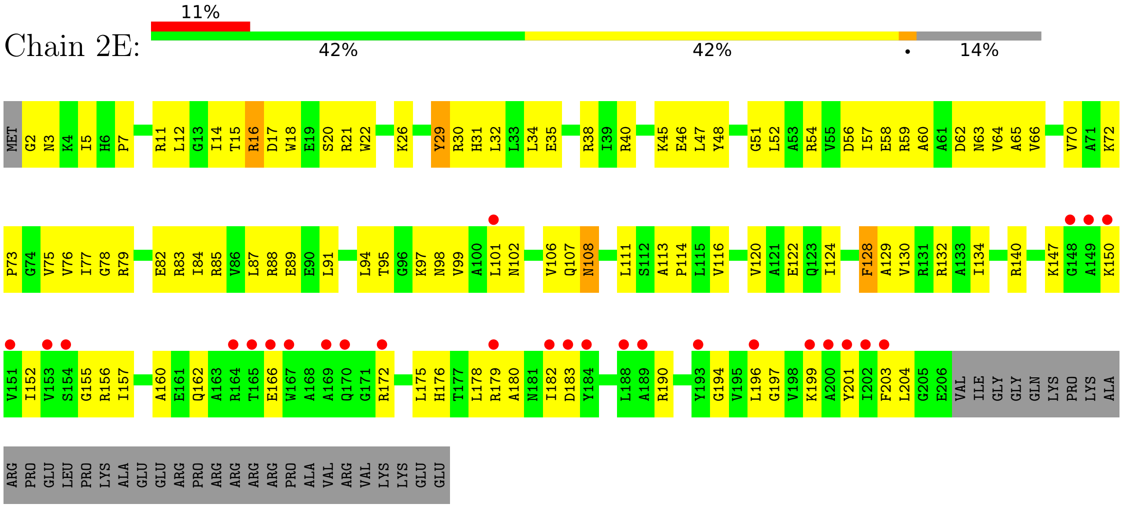






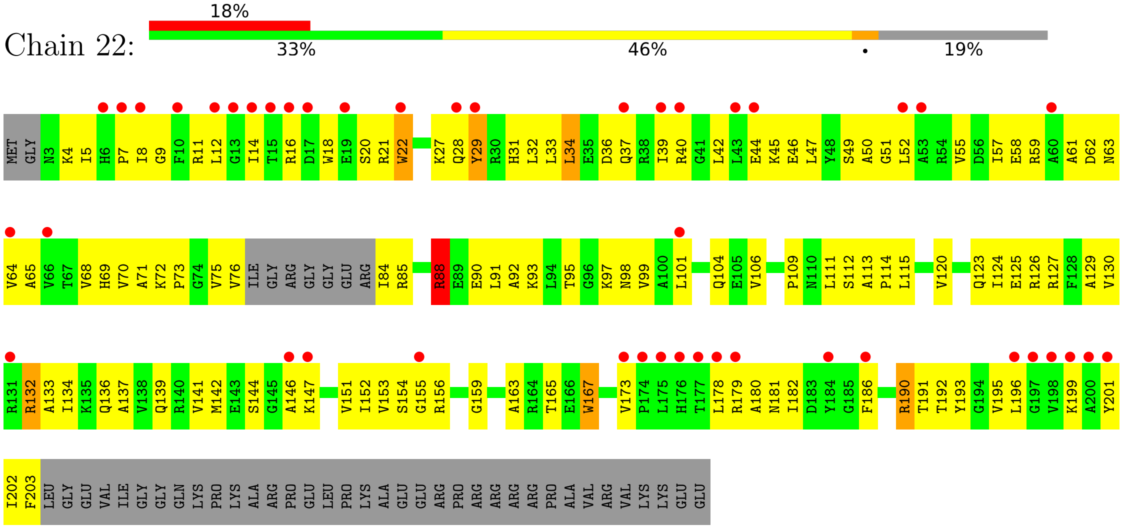
- Molecule 3: 30S ribosomal protein S3

Chain 2E:



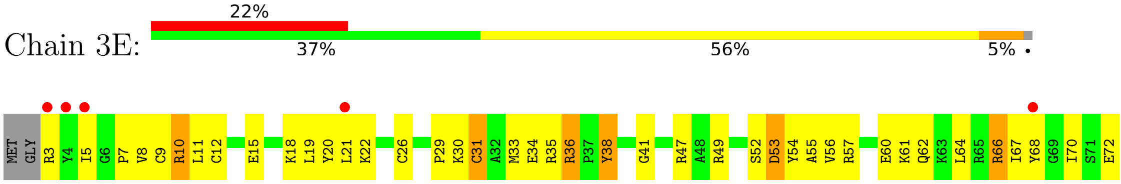
- Molecule 3: 30S ribosomal protein S3

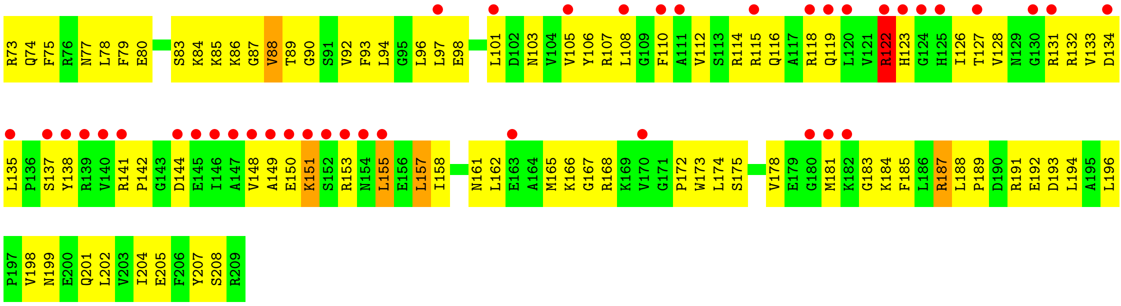
Chain 22:



- Molecule 4: 30S ribosomal protein S4

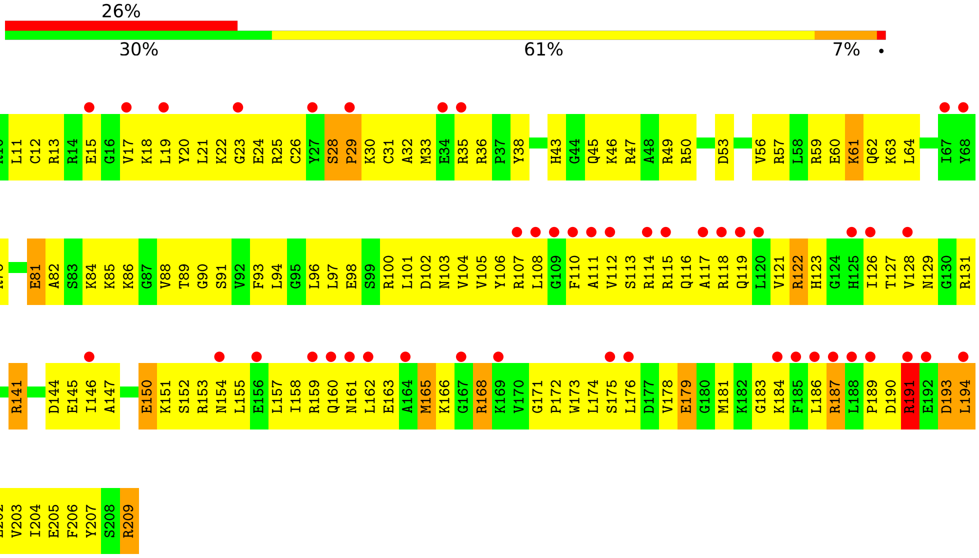
Chain 3E:





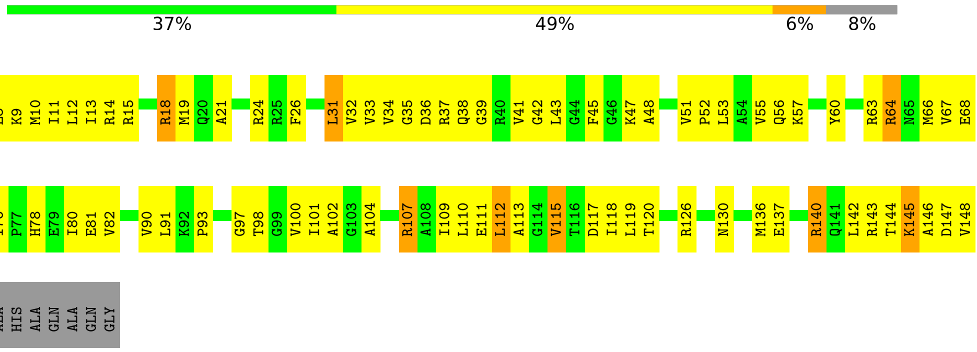
- Molecule 4: 30S ribosomal protein S4

Chain 32:



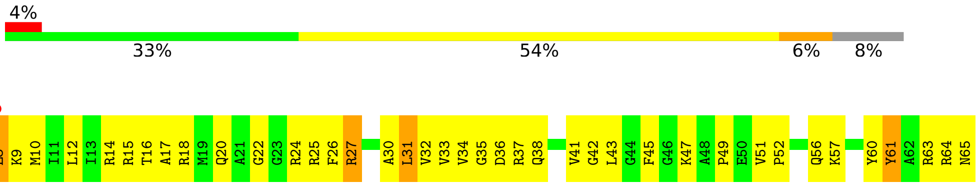
- Molecule 5: 30S ribosomal protein S5

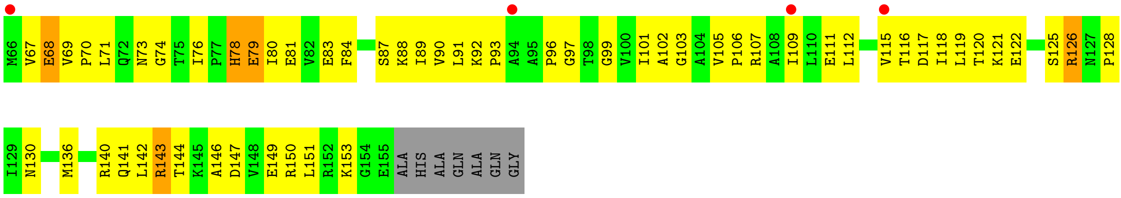
Chain 4E:



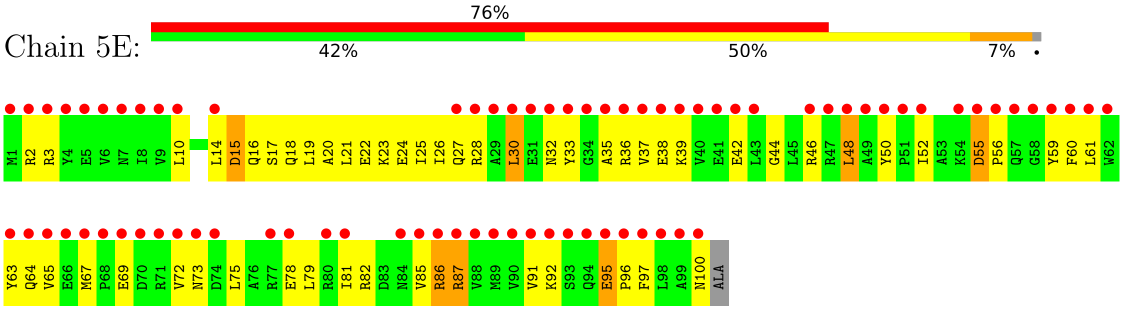
- Molecule 5: 30S ribosomal protein S5

Chain 42:

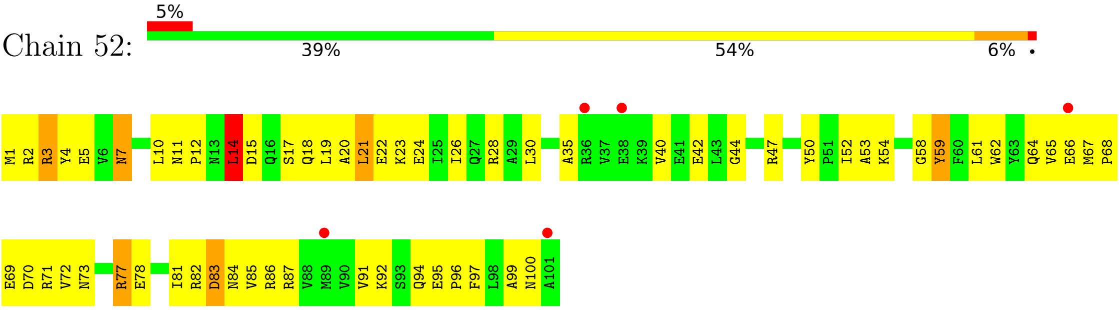




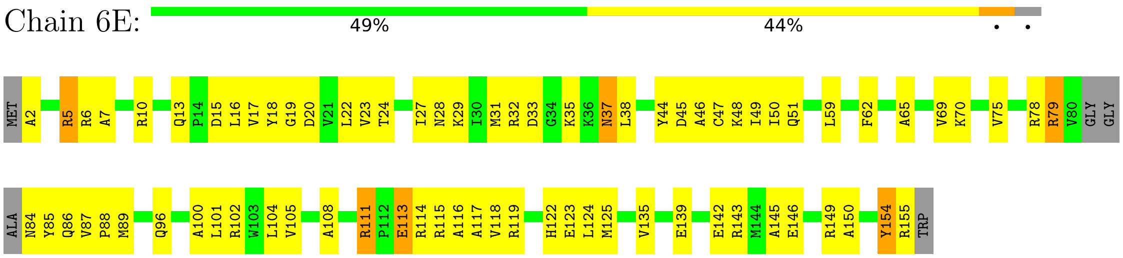
- Molecule 6: 30S ribosomal protein S6



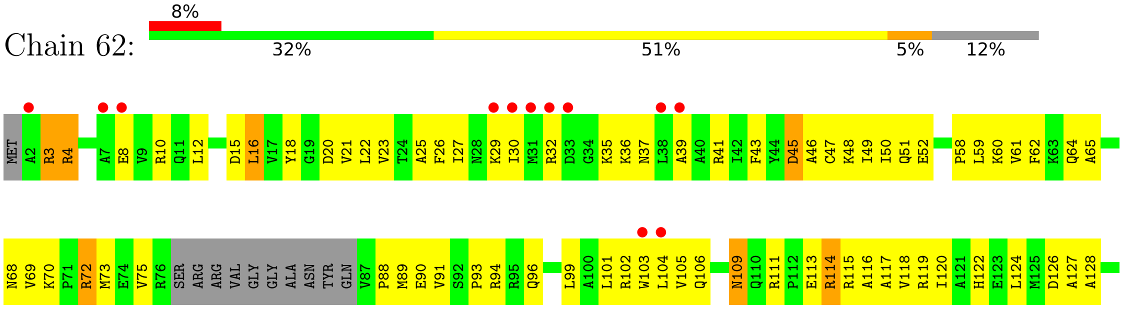
- Molecule 6: 30S ribosomal protein S6

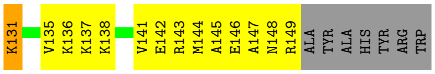


- Molecule 7: 30S ribosomal protein S7



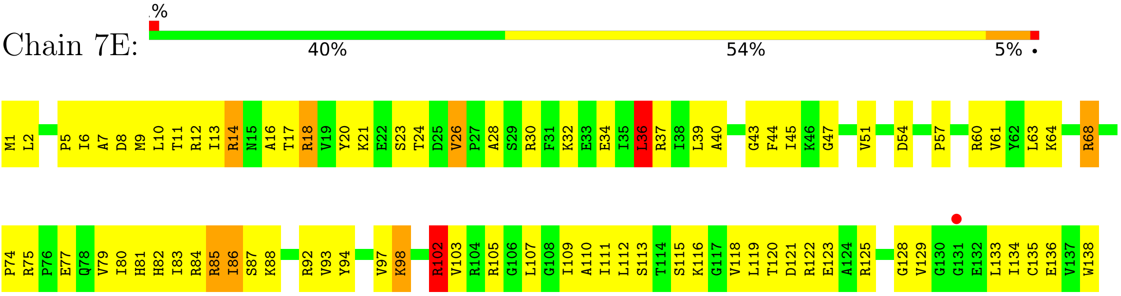
- Molecule 7: 30S ribosomal protein S7





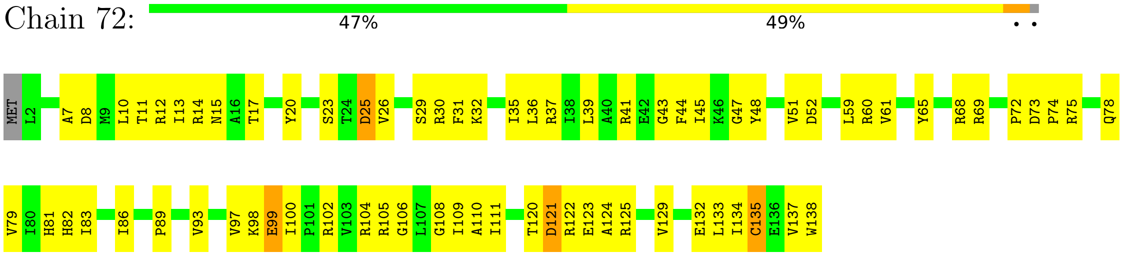
- Molecule 8: 30S ribosomal protein S8

Chain 7E:



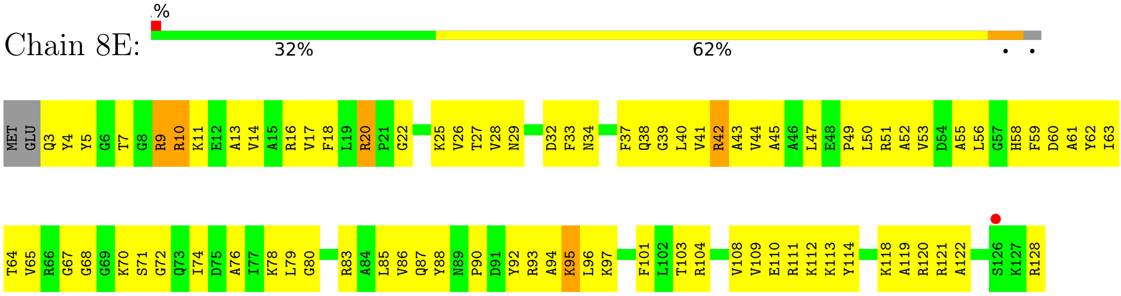
- Molecule 8: 30S ribosomal protein S8

Chain 72:



- Molecule 9: 30S ribosomal protein S9

Chain 8E:



- Molecule 9: 30S ribosomal protein S9

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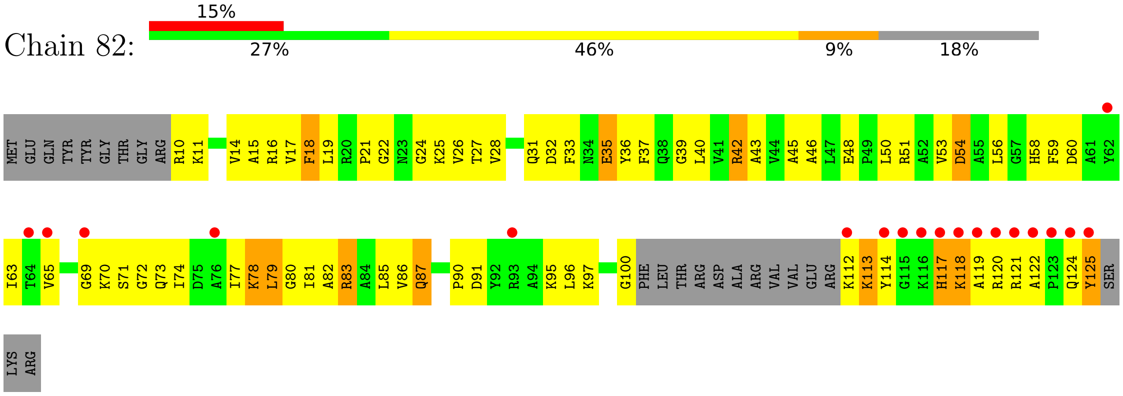
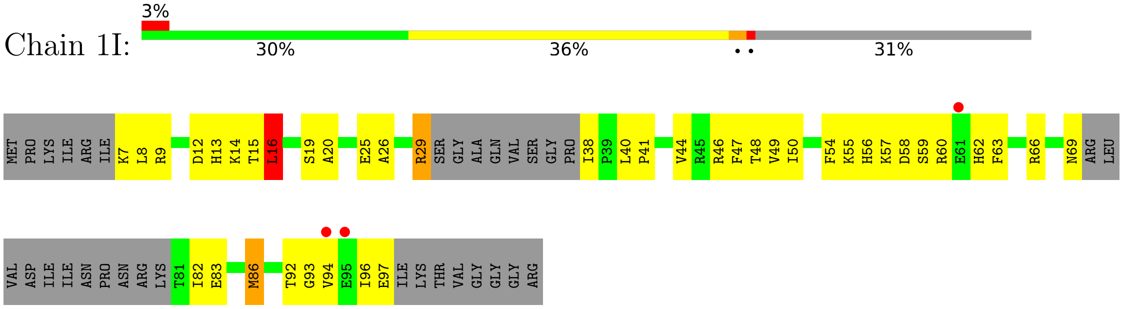


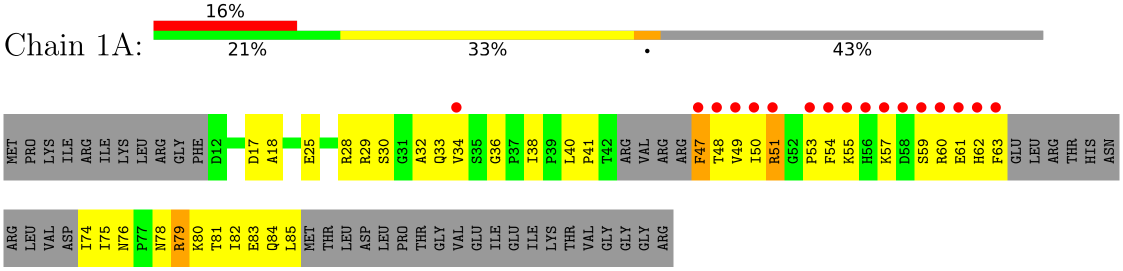
- Molecule 10: 30S ribosomal protein S10

Chain 1I:



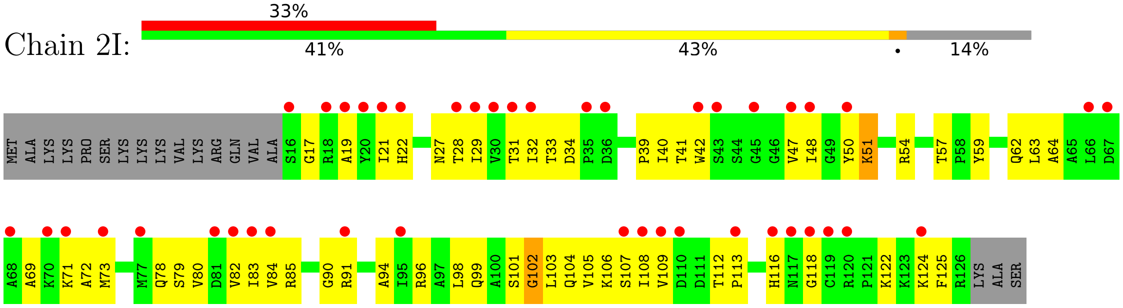
- Molecule 10: 30S ribosomal protein S10

Chain 1A:



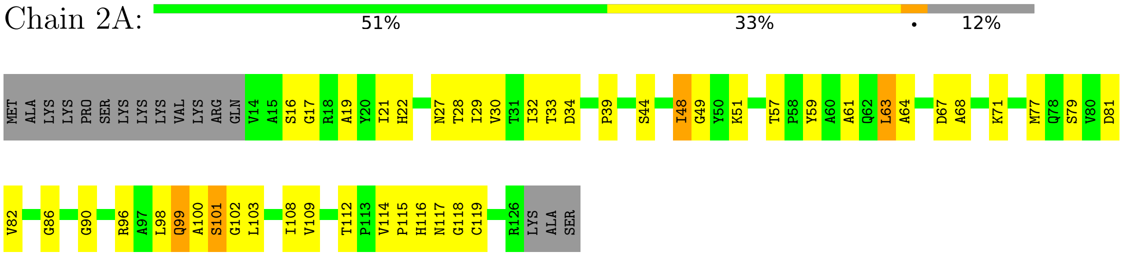
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



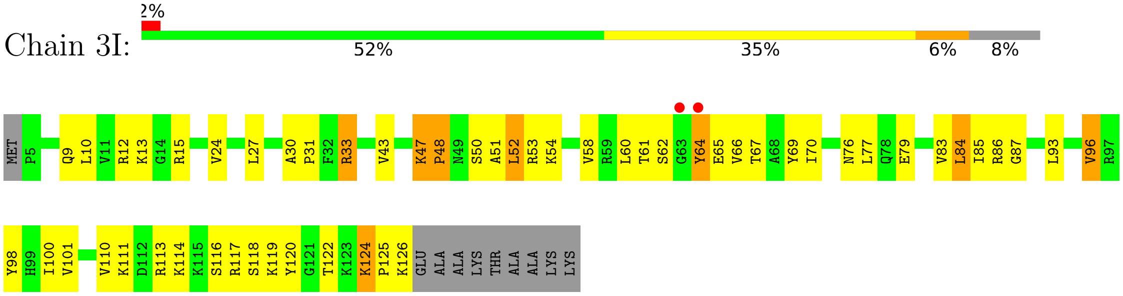
- Molecule 11: 30S ribosomal protein S11

Chain 2A:

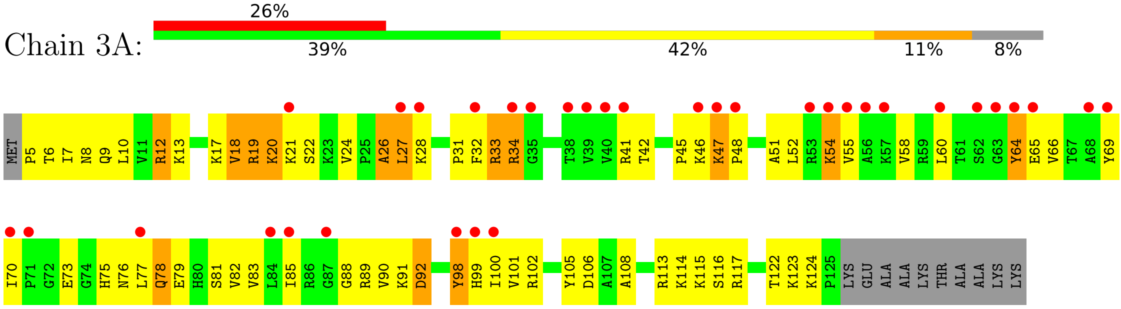


- Molecule 12: 30S ribosomal protein S12

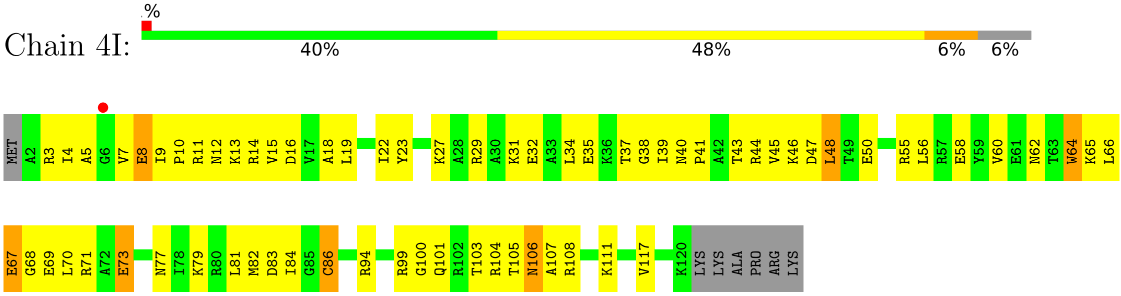
Chain 3I:



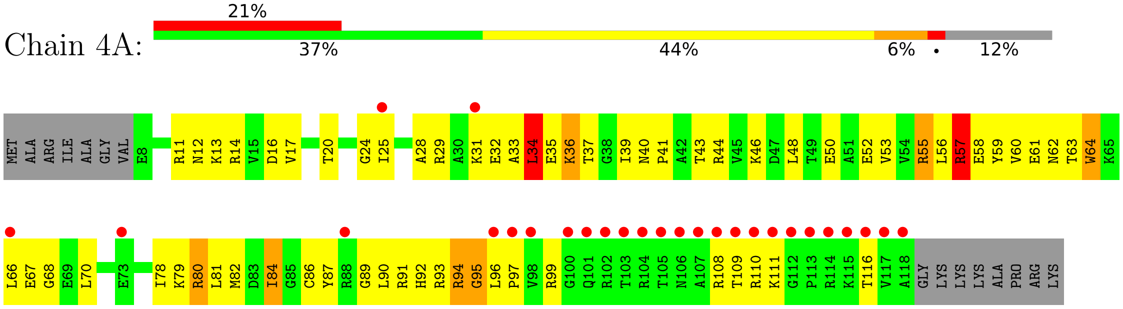
- Molecule 12: 30S ribosomal protein S12



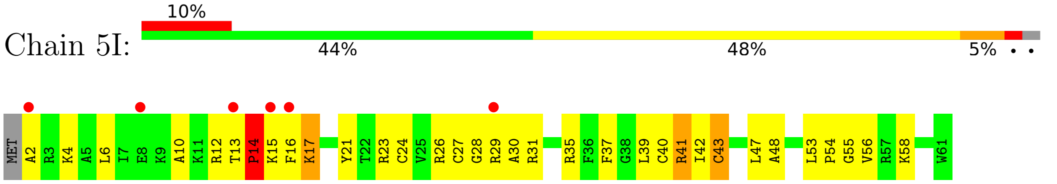
- Molecule 13: 30S ribosomal protein S13



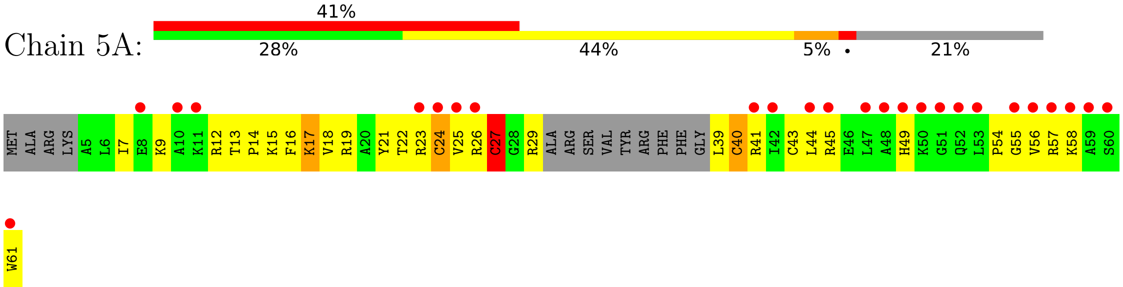
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

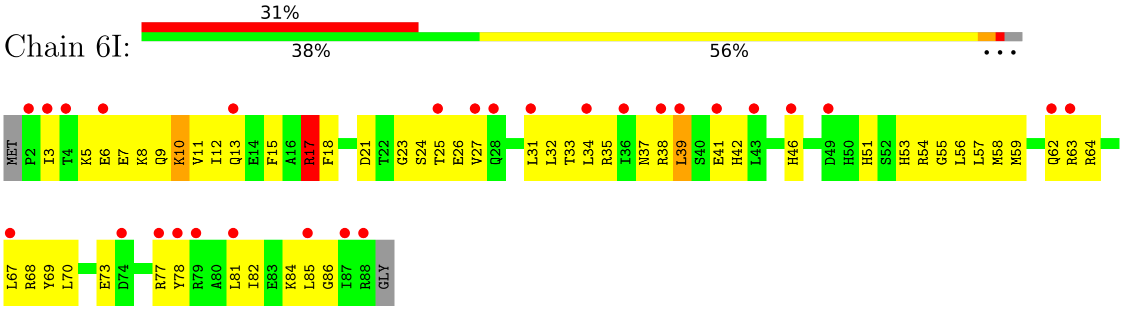


- Molecule 14: 30S ribosomal protein S14 type Z



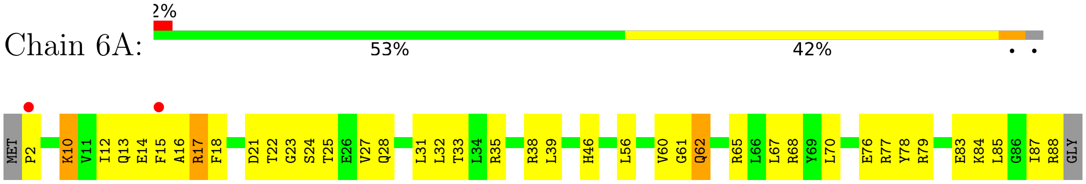
- Molecule 15: 30S ribosomal protein S15

Chain 6I:



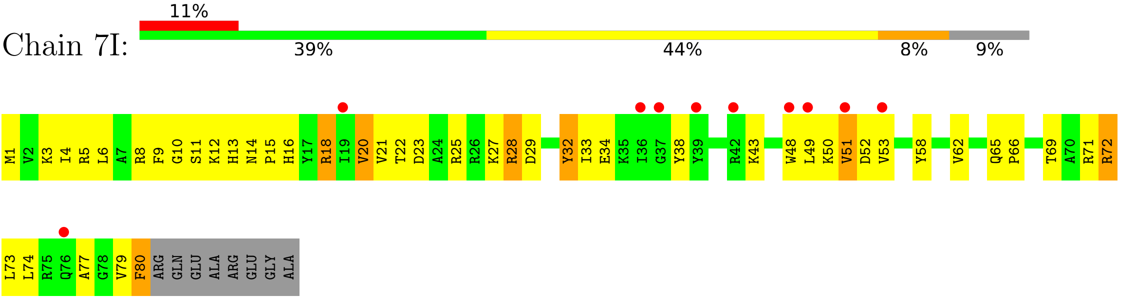
- Molecule 15: 30S ribosomal protein S15

Chain 6A:



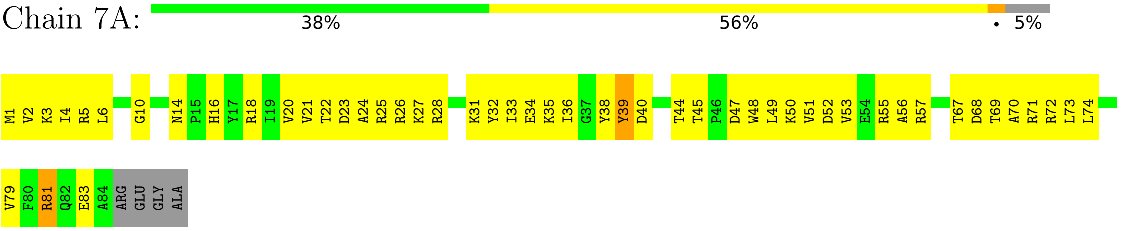
- Molecule 16: 30S ribosomal protein S16

Chain 7I:



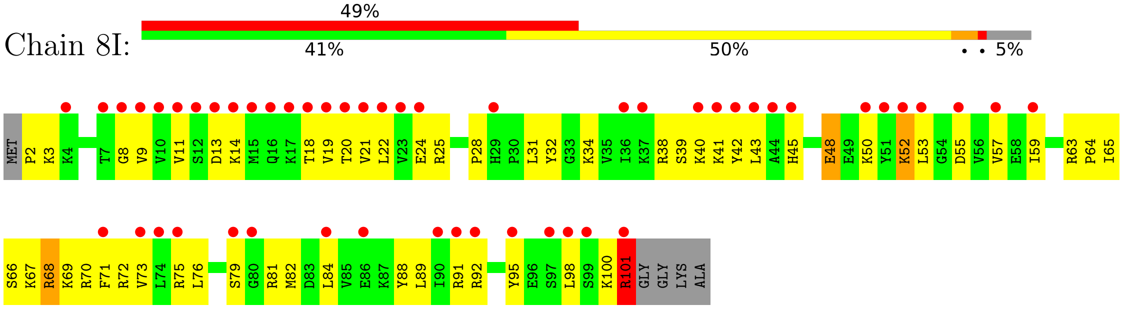
- Molecule 16: 30S ribosomal protein S16

Chain 7A:

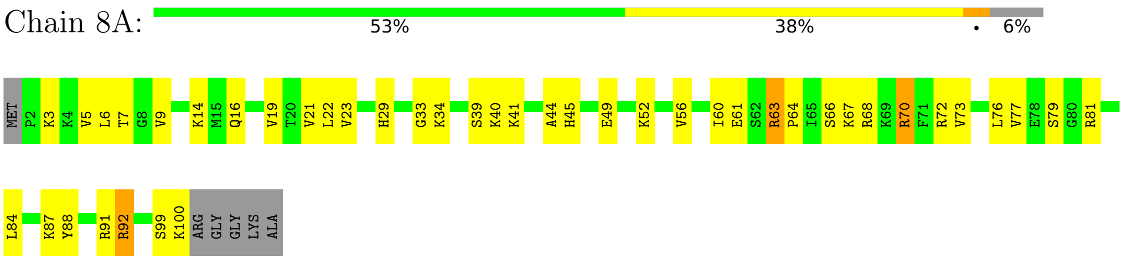


- Molecule 17: 30S ribosomal protein S17

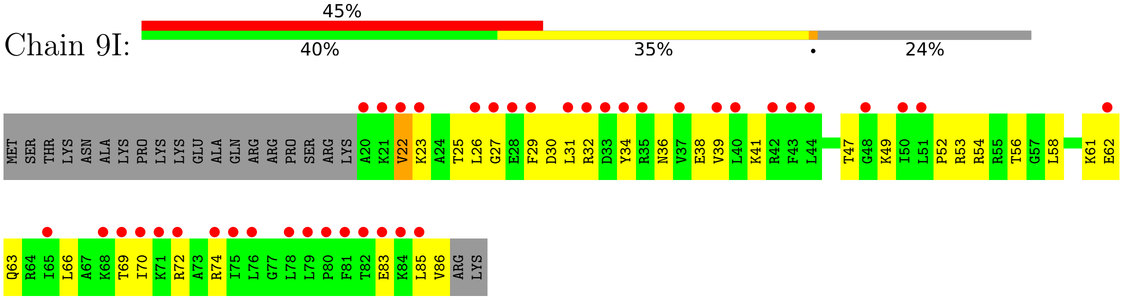
Chain 8I:



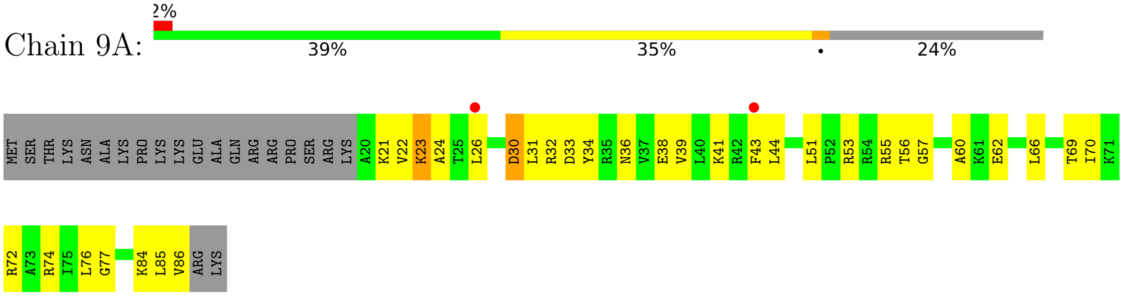
- Molecule 17: 30S ribosomal protein S17



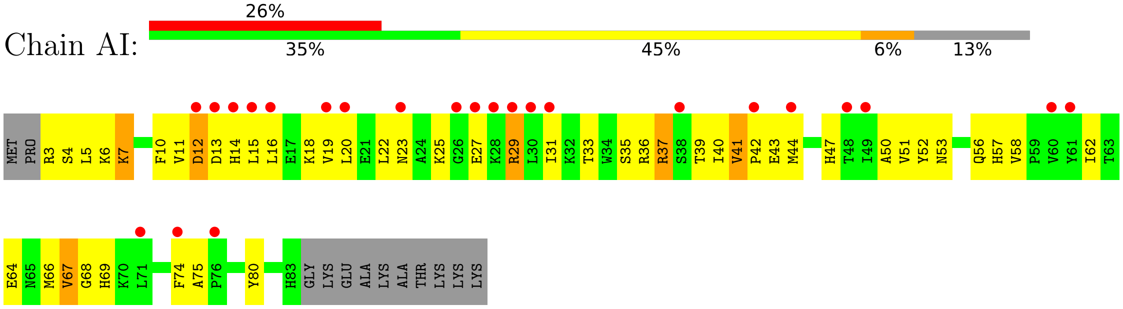
• Molecule 18: 30S ribosomal protein S18



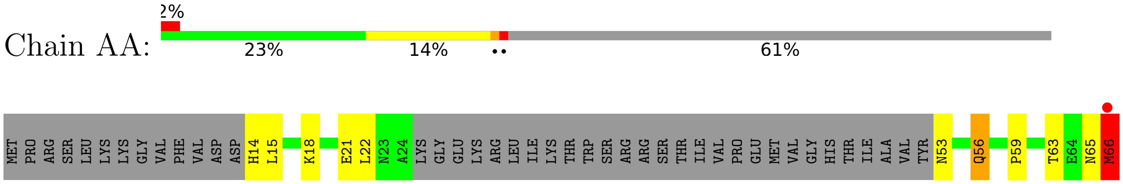
• Molecule 18: 30S ribosomal protein S18

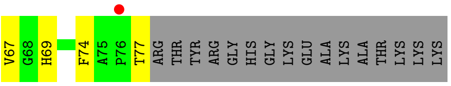


• Molecule 19: 30S ribosomal protein S19

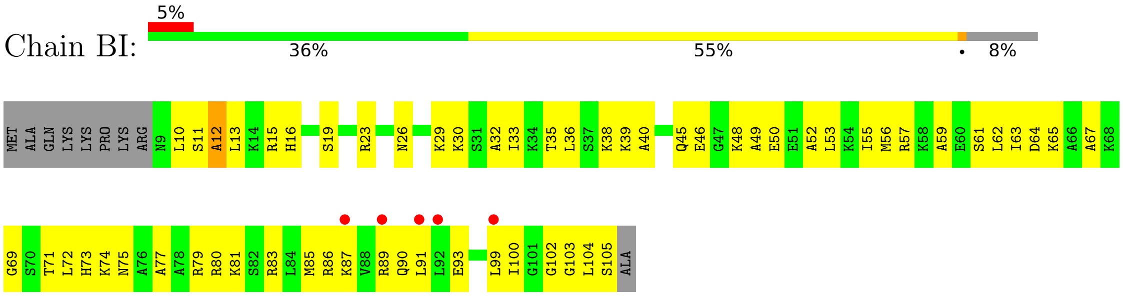


• Molecule 19: 30S ribosomal protein S19

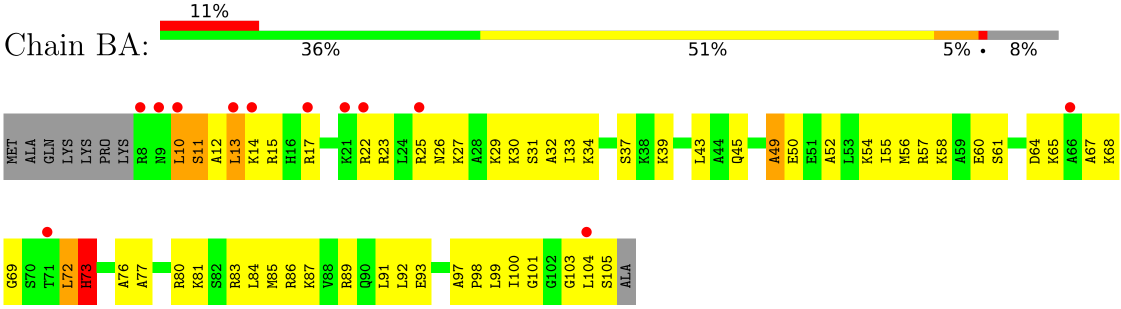




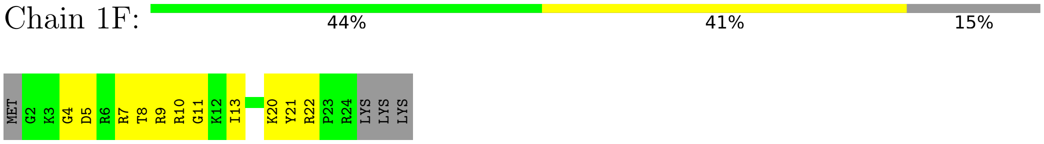
- Molecule 20: 30S ribosomal protein S20



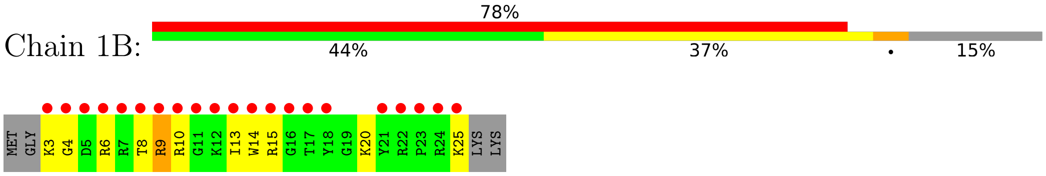
- Molecule 20: 30S ribosomal protein S20



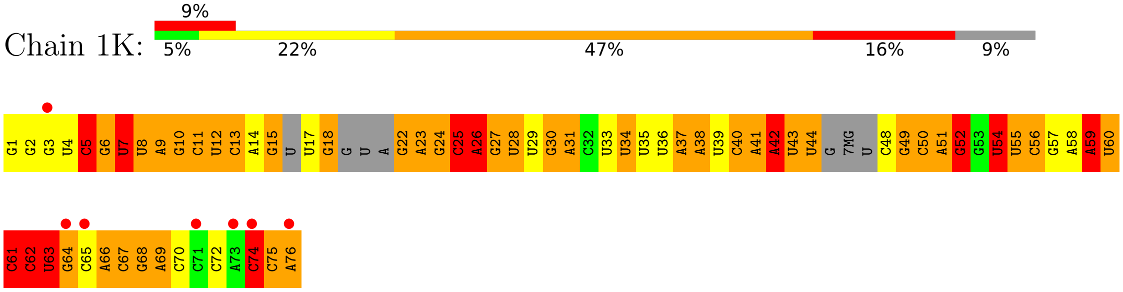
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

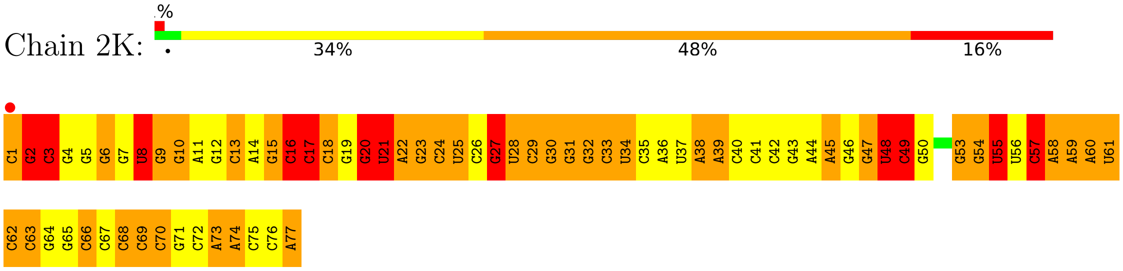


- Molecule 22: tRNALys



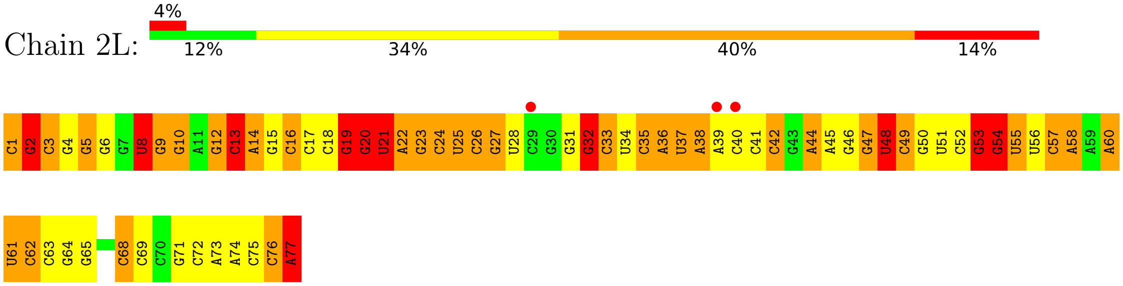
- Molecule 23: tRNAfMet

Chain 2K:



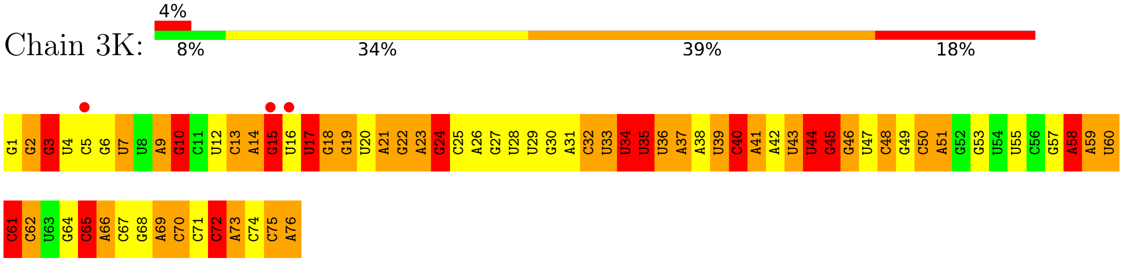
- Molecule 23: tRNAfMet

Chain 2L:



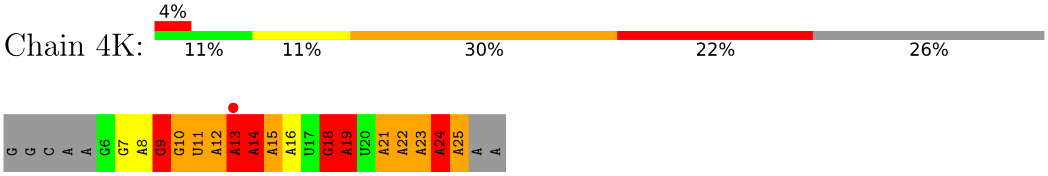
- Molecule 24: tRNALys

Chain 3K:



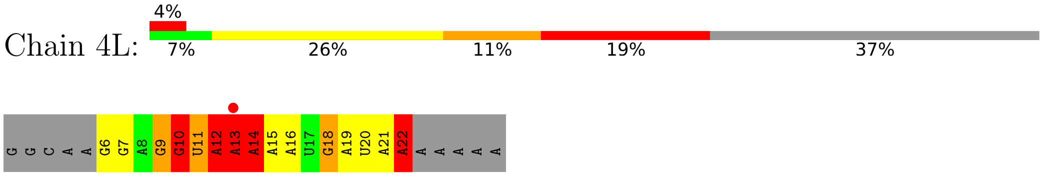
- Molecule 25: mRNA

Chain 4K:



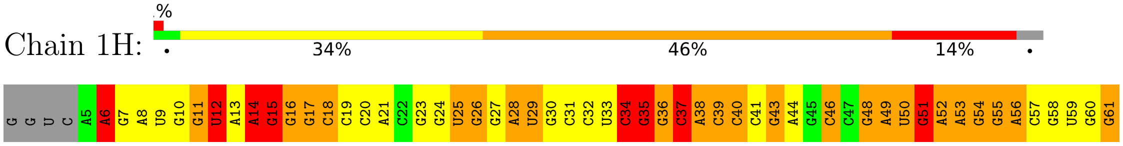
- Molecule 25: mRNA

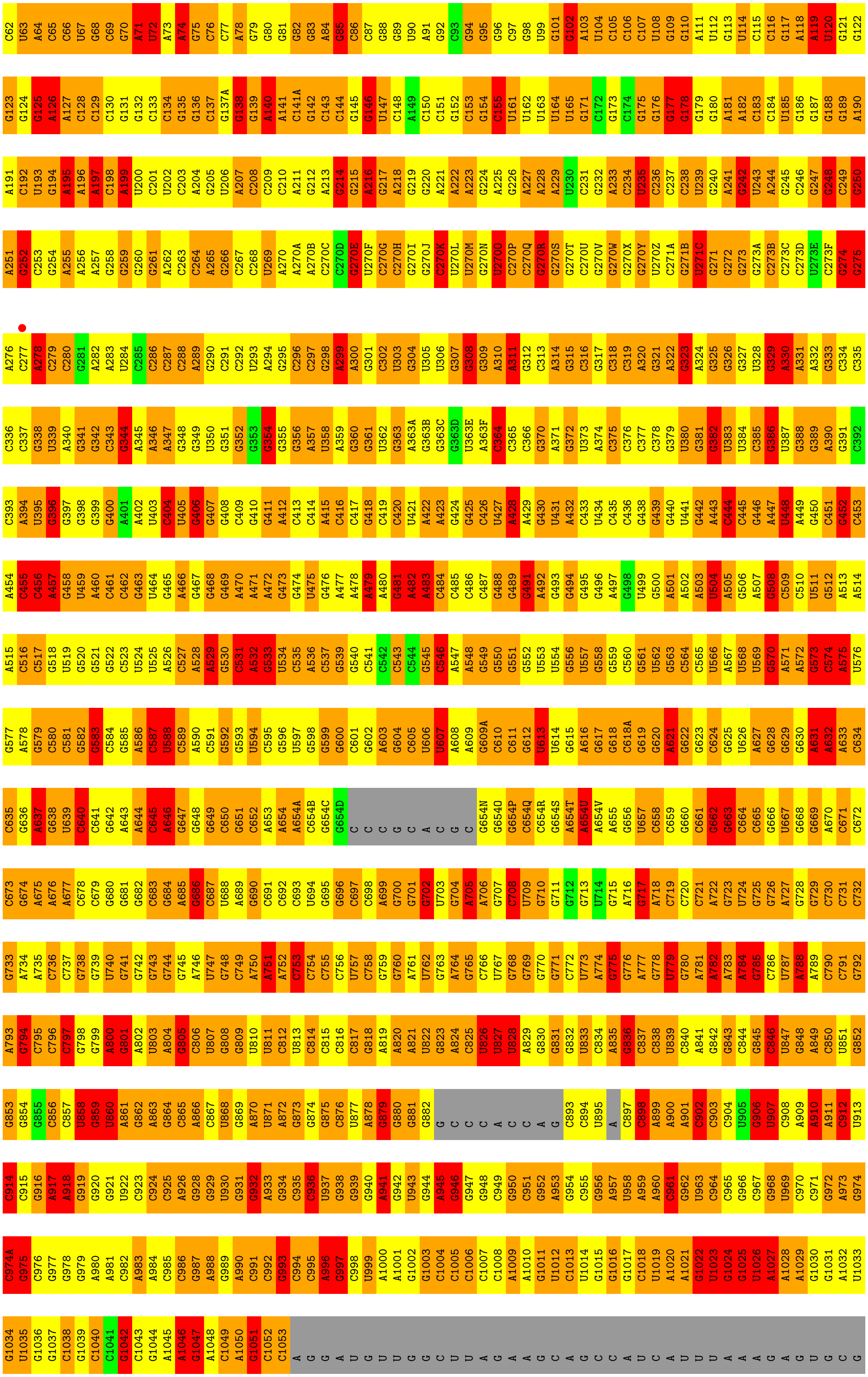
Chain 4L:



- Molecule 26: 23S ribosomal RNA

Chain 1H:

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G123 G124 G125 A126 A127 C128 C129 C130 G131 G132 C133 C134 G135 G136 C137 G137A G138 G139 A140 A141 C141A G142 C143 C144 G145 G146 U147 C148 A149 C150 C151 G152 C153 G154 C155 U161 U162 U163 U164 U165 G171 C172 G173 C174 G175 G176 G177 G178 G179 G180 A181 A182 C183 C184 U185 G186 G187 G188 G189 A190
A191 C192 U193 G194 A195 A196 A197 C198 A199 U200 C201 U202 C203 A204 G205 U206 A207 C208 C209 C210 A211 G212 A213 G214 G215 A216 G217 A218 G219 G220 A221 A222 A223 G224 A225 G226 A227 A228 A229 U230 C231 G232 A233 C234 U235 C236 C237 C238 U239 G240 A241 G242 U243 A244 G245 C246 G247 G248 C249 G250
A251 G252 C253 G254 A255 A256 A257 G258 G259 G260 G261 A262 C263 C264 A265 G266 C267 C268 U269 A270 A270A A270B C270C C270D G270E U270F C270G C270H G270I G270J C270K U270L U270M G270N U270O C270P C270Q G270R G270S G270T C270U C270V G270W G270X G270Y U270Z C271A G271B U271C G271 G272 G273 G273A C273B C273C C273D U273E C273F G274 G275
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G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 U594 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G609A C610 C611 G612 U613 U614 G615 A616 G617 G618 C618A G619 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634
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G733 A734 A735 C736 C737 G738 G739 U740 G741 G742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 G771 C772 U773 A774 C775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792
A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852
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C974A G975 C976 G977 G978 G979 A980 A981 C982 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 C1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033
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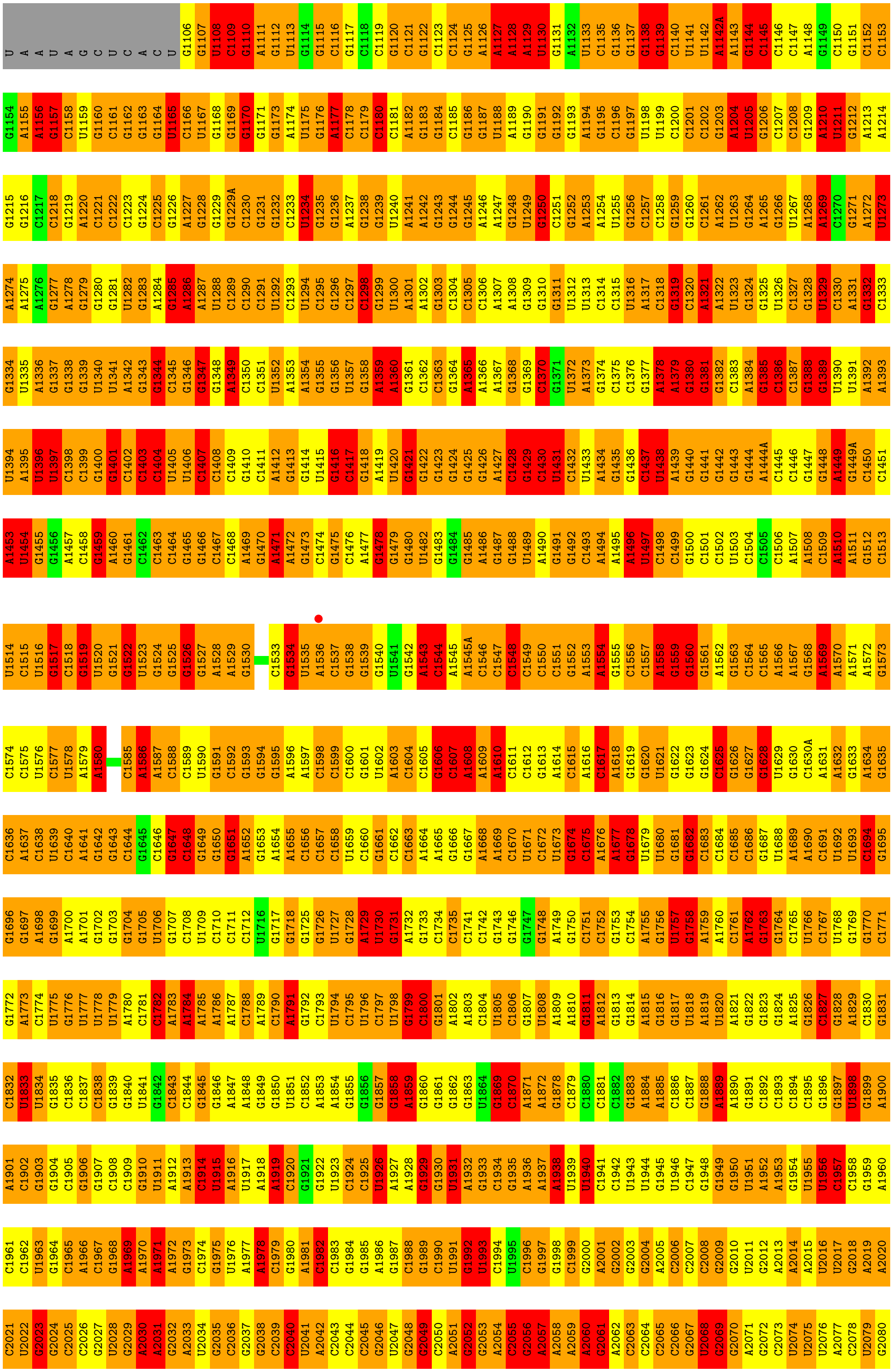

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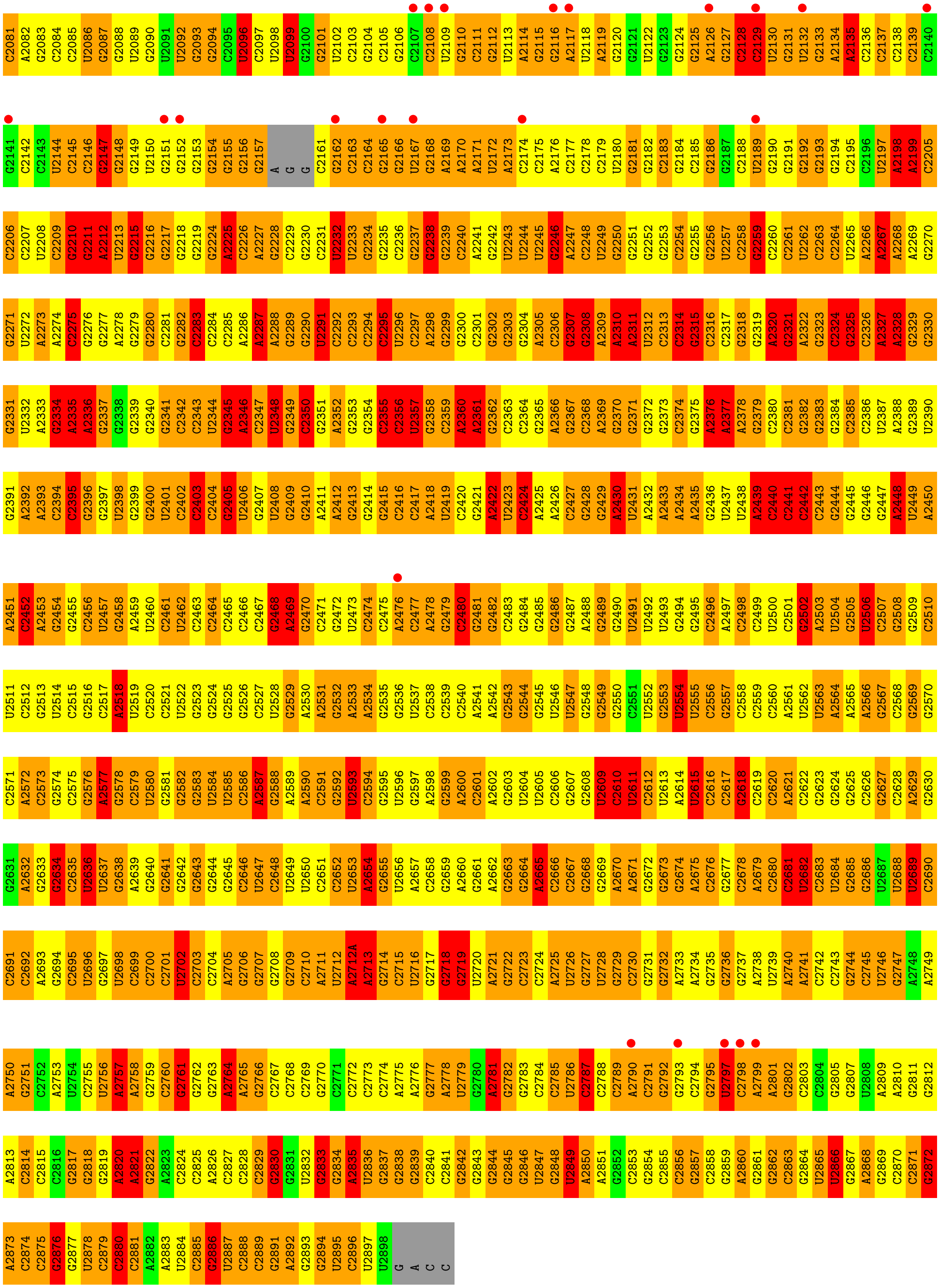

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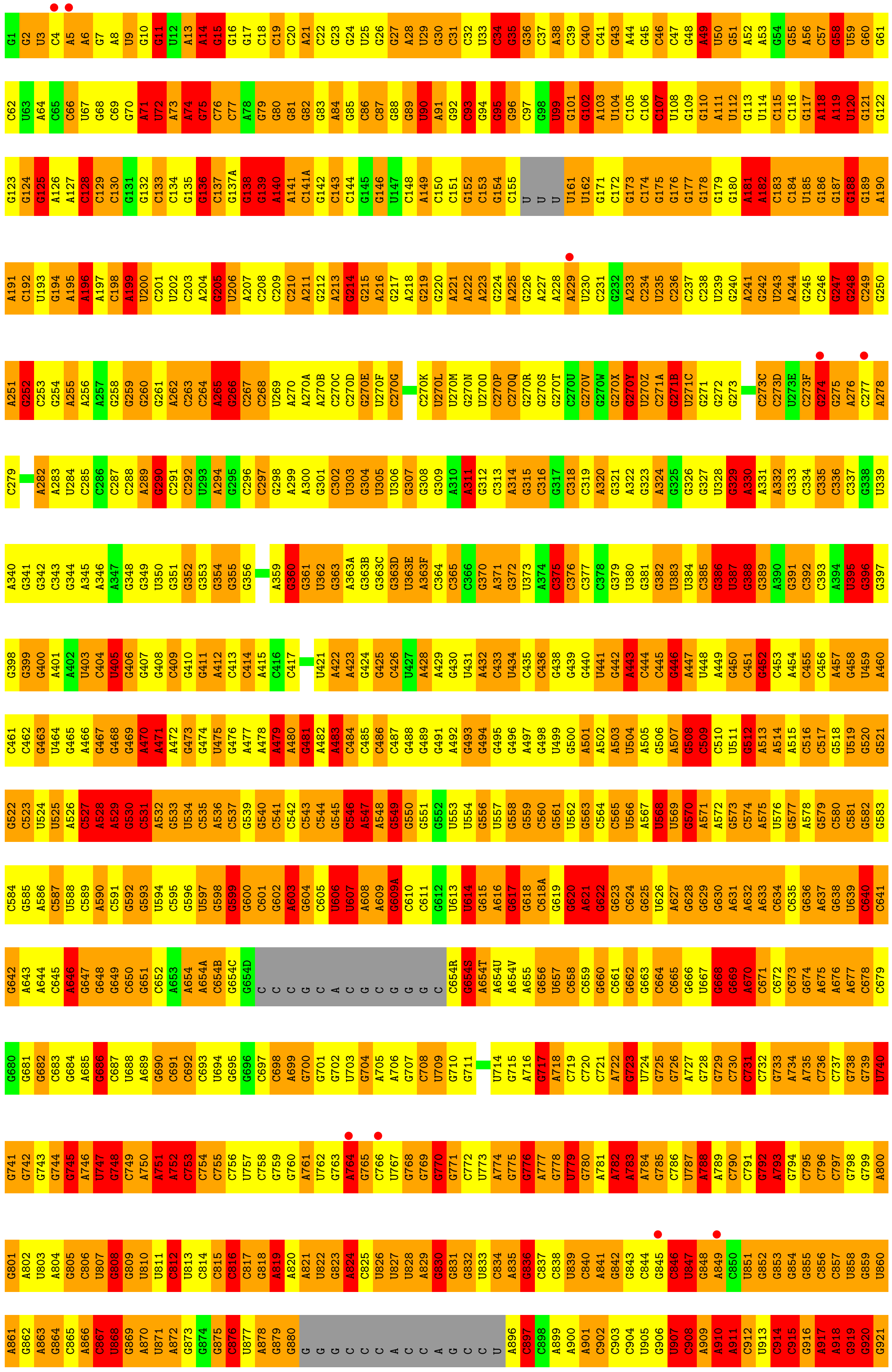
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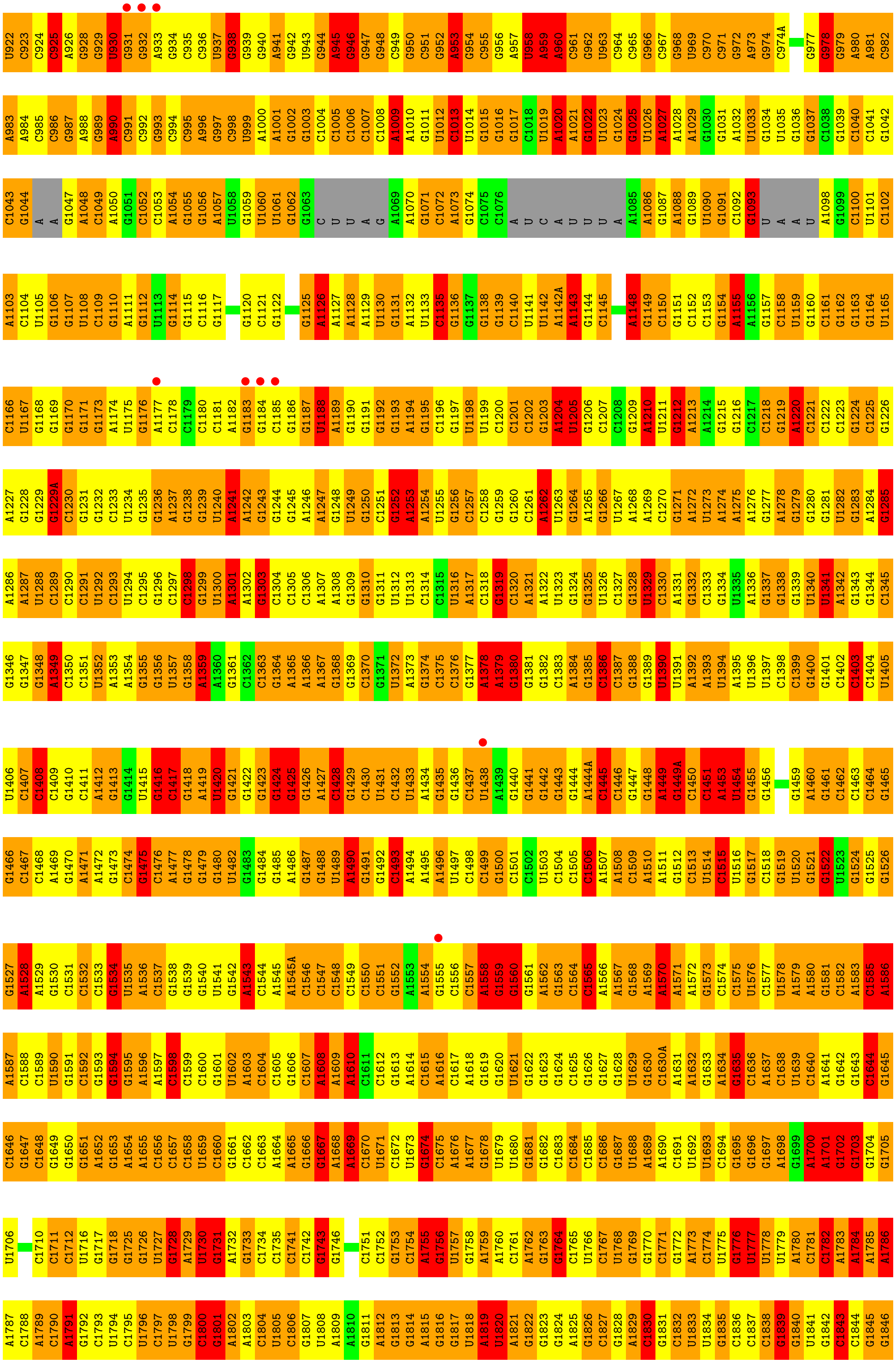

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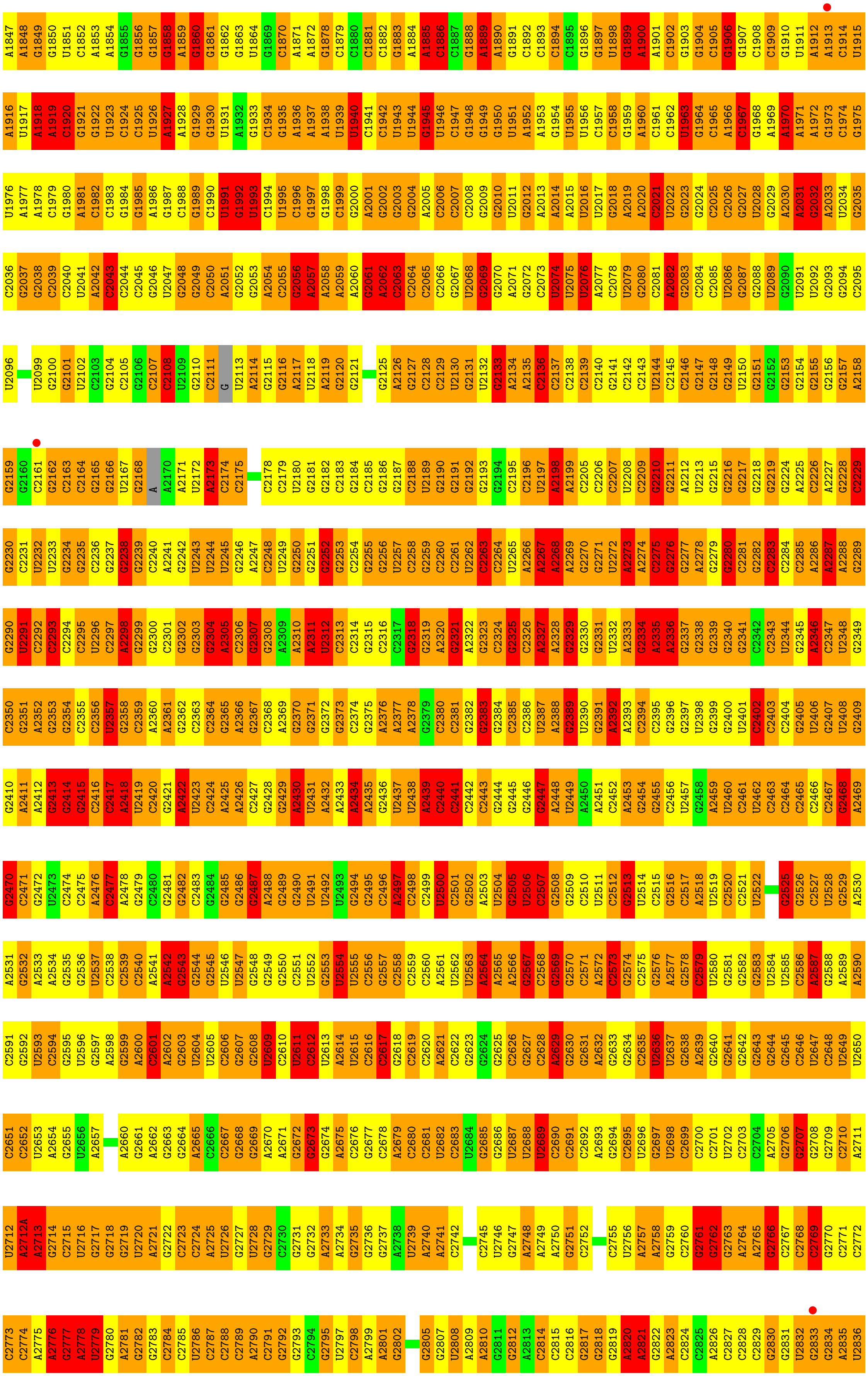
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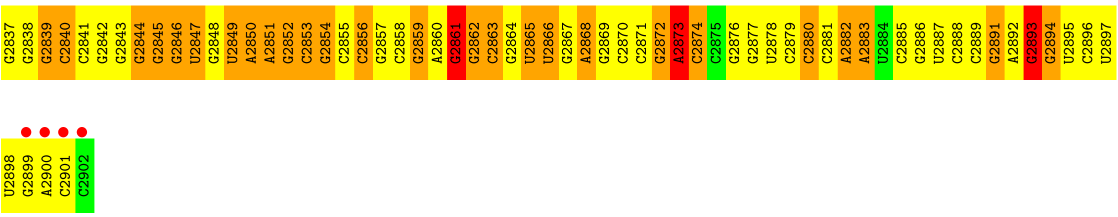
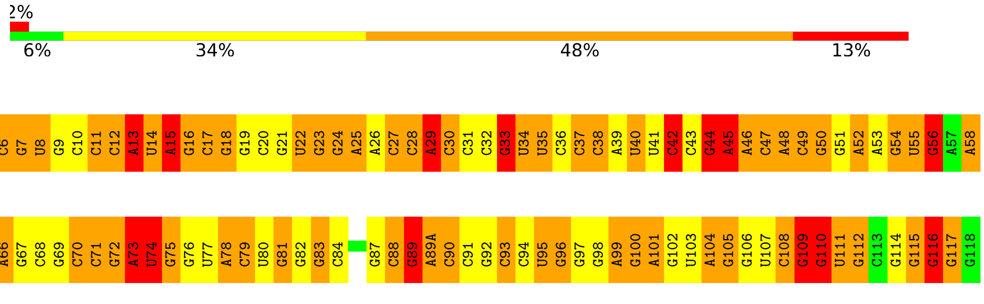


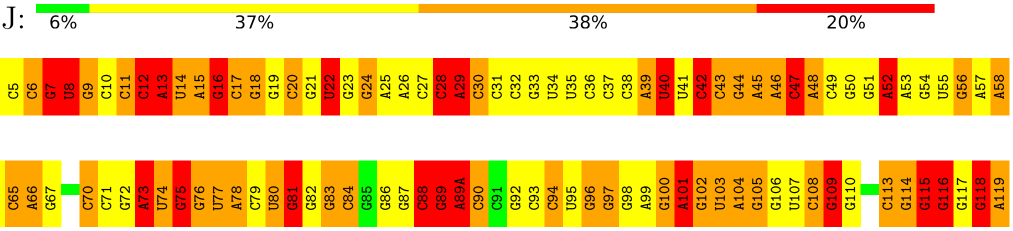
- Molecule 27: 5S ribosomal RNA

Chain 16:



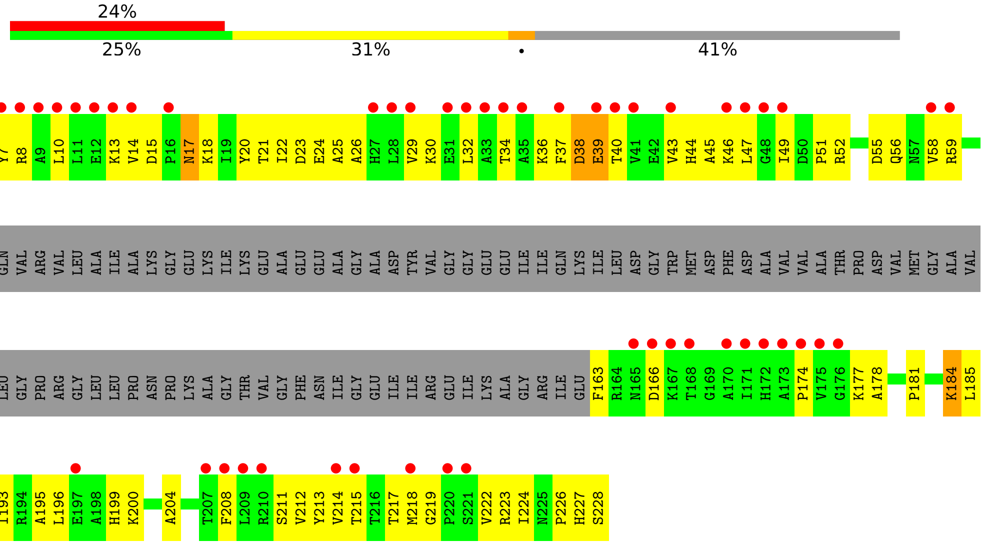
- Molecule 27: 5S ribosomal RNA

Chain 1J:



- Molecule 28: 50S ribosomal protein L1

Chain 71:



- Molecule 29: 50S ribosomal protein L2

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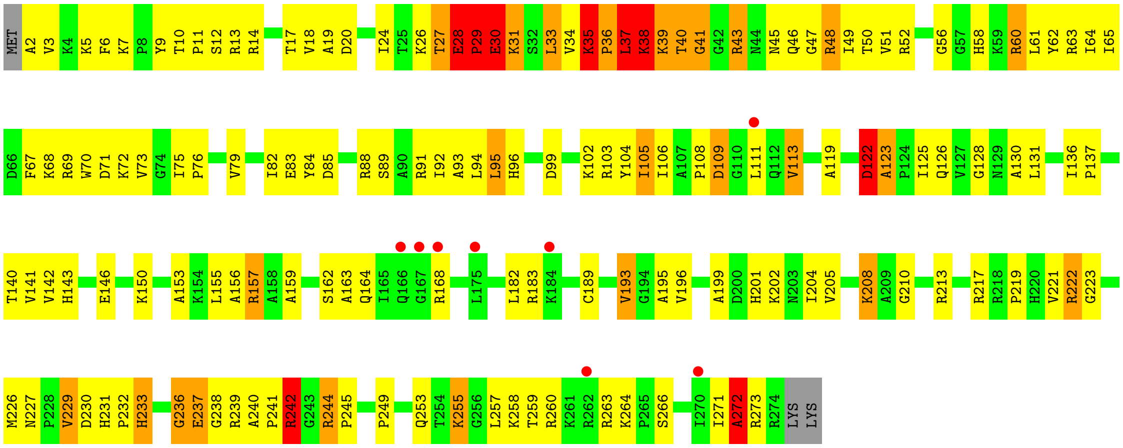

- Molecule 29: 50S ribosomal protein L2

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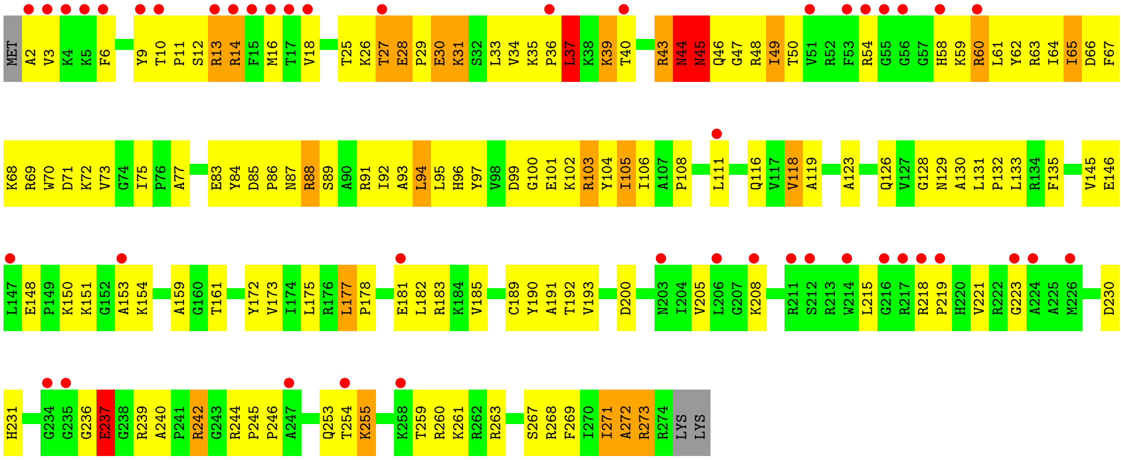

- Molecule 30: 50S ribosomal protein L3

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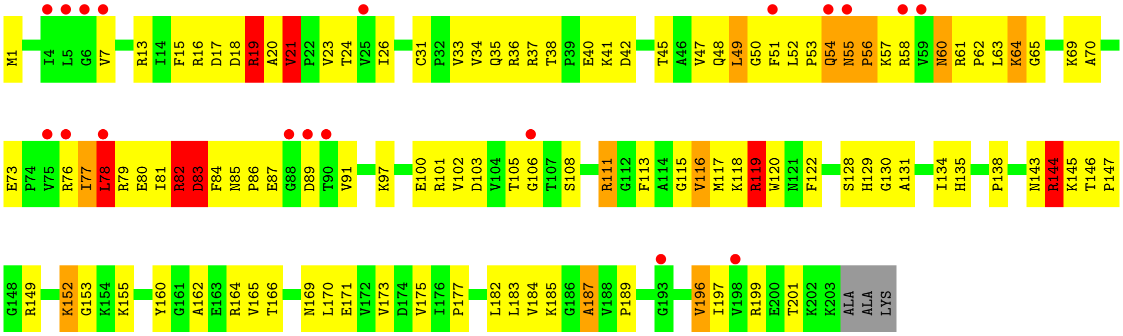

- Molecule 30: 50S ribosomal protein L3

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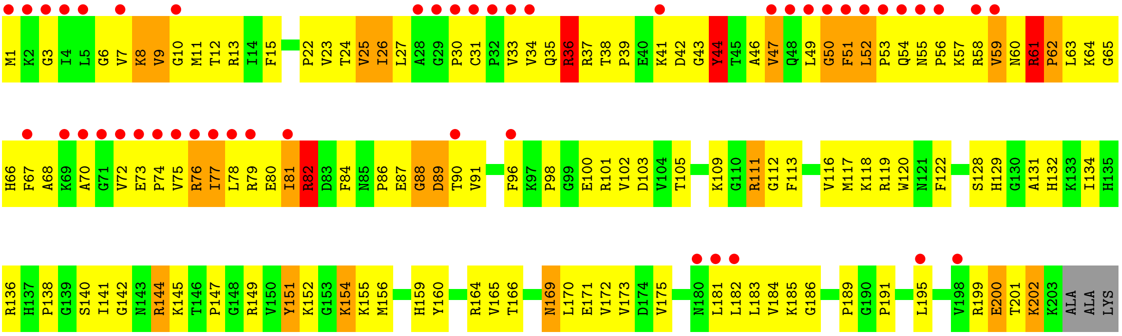
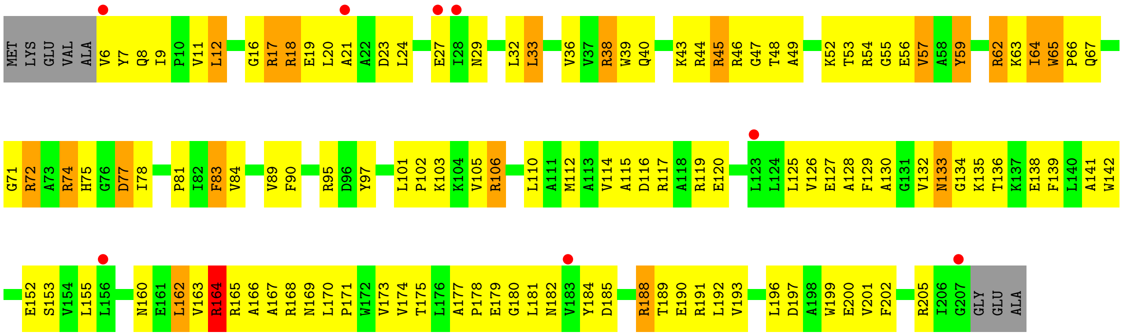


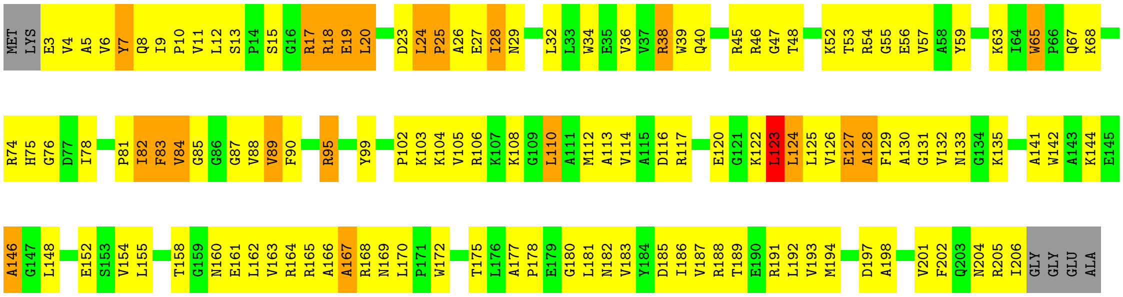
- Molecule 31: 50S ribosomal protein L4

Chain 31:



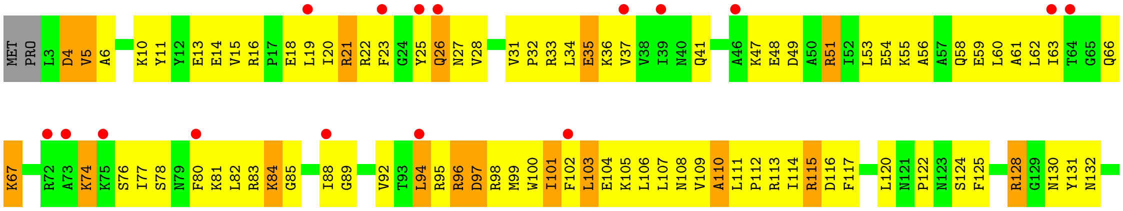
- Molecule 31: 50S ribosomal protein L4

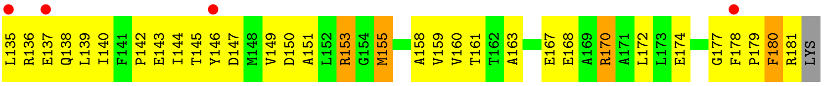
Chain 39:



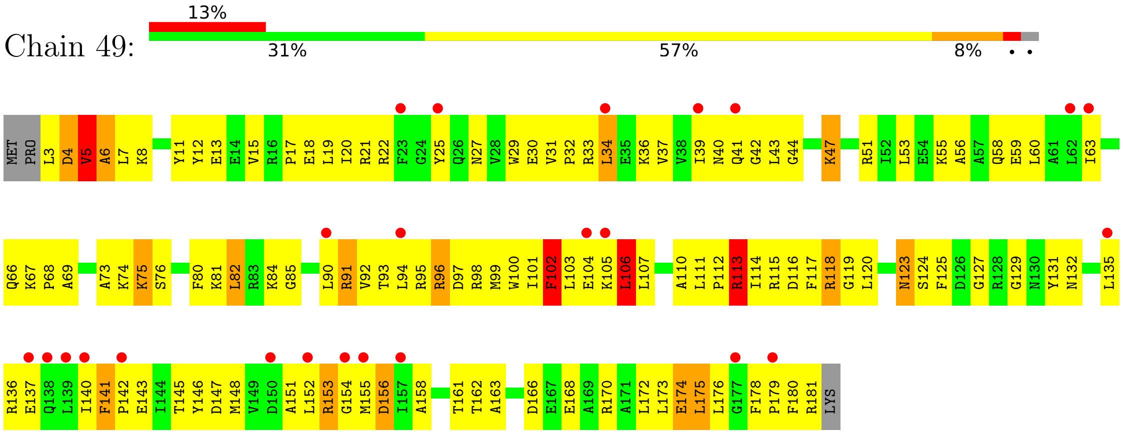
- Molecule 32: 50S ribosomal protein L5

Chain 41:

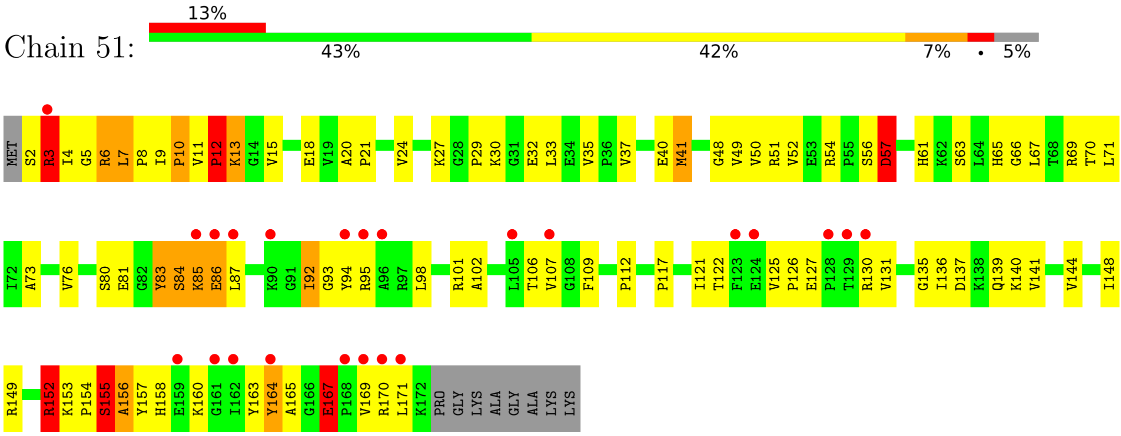




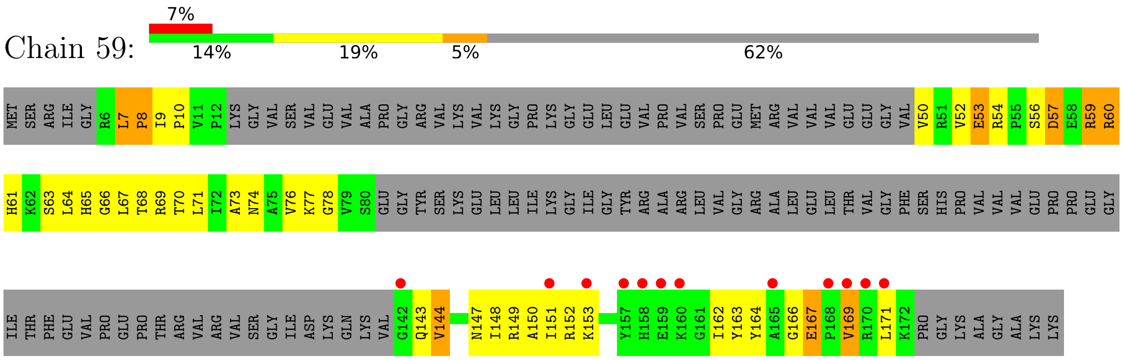
- Molecule 32: 50S ribosomal protein L5



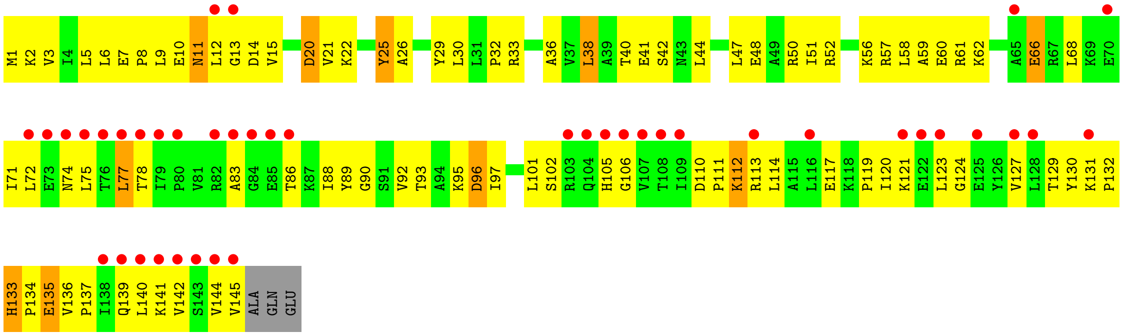
- Molecule 33: 50S ribosomal protein L6



- Molecule 33: 50S ribosomal protein L6

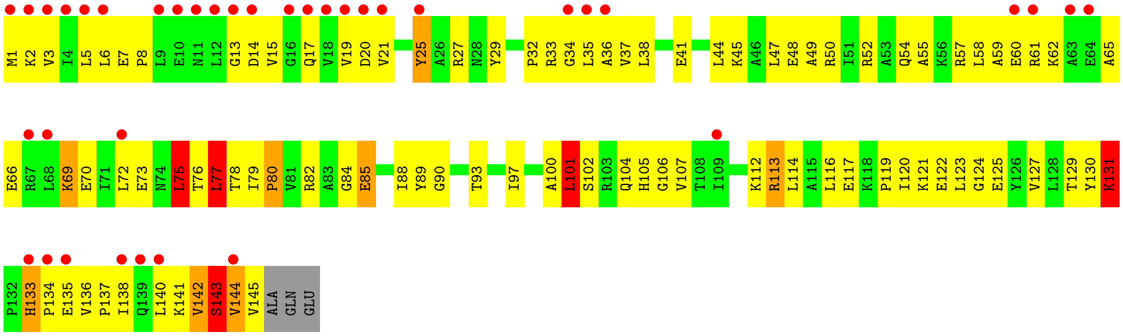


- Molecule 34: 50S ribosomal protein L9



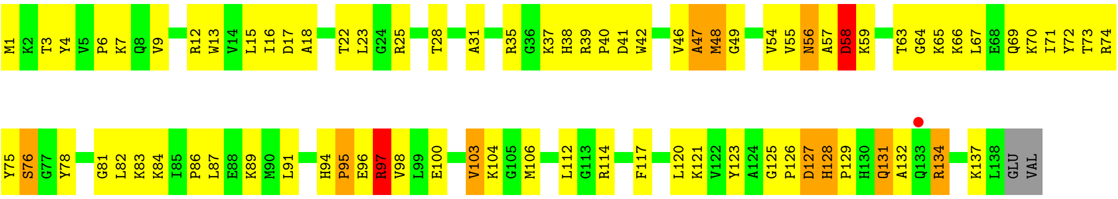
- Molecule 34: 50S ribosomal protein L9

Chain 69:



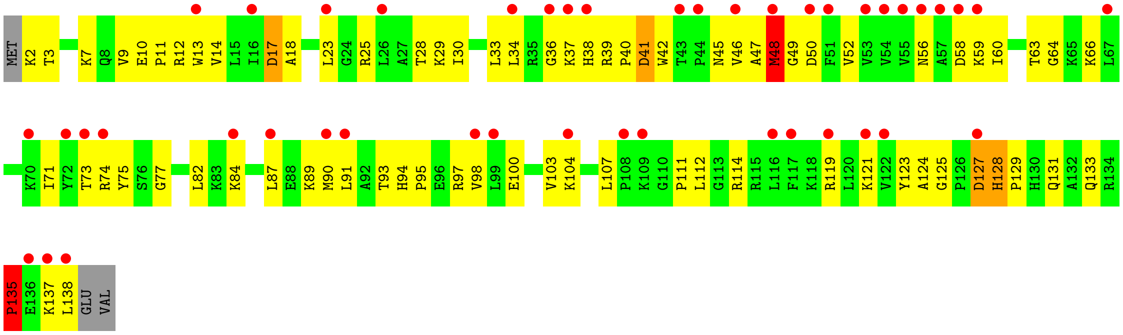
- Molecule 35: 50S ribosomal protein L13

Chain 58:

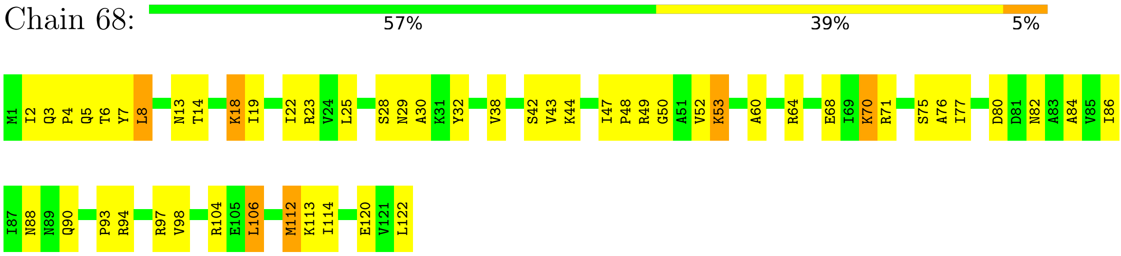


- Molecule 35: 50S ribosomal protein L13

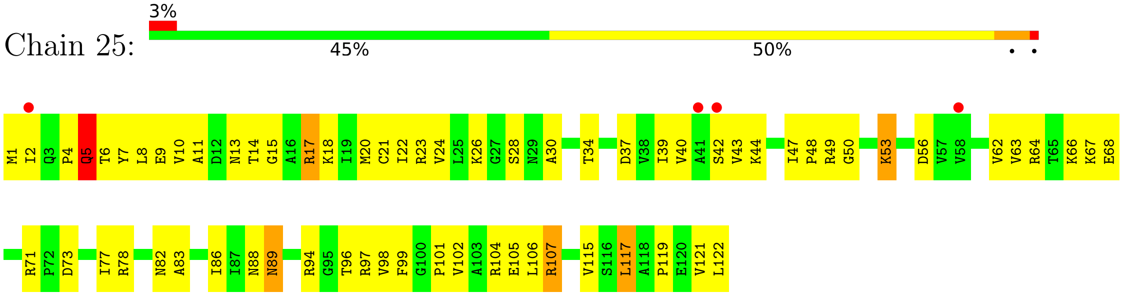
Chain 15:



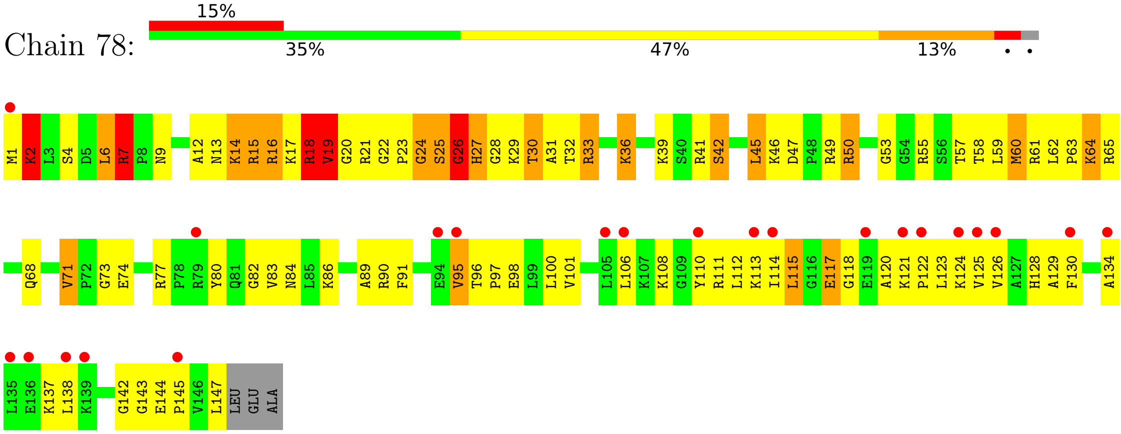
- Molecule 36: 50S ribosomal protein L14



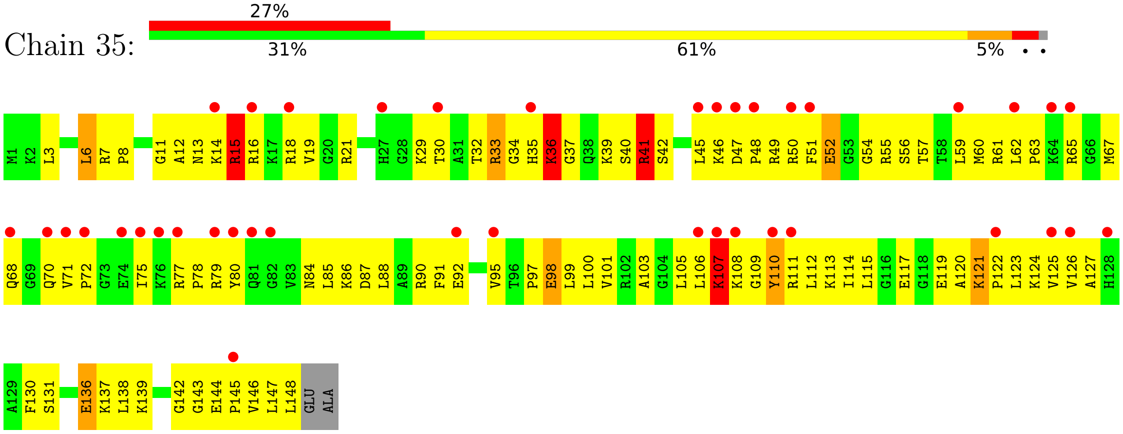
- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15

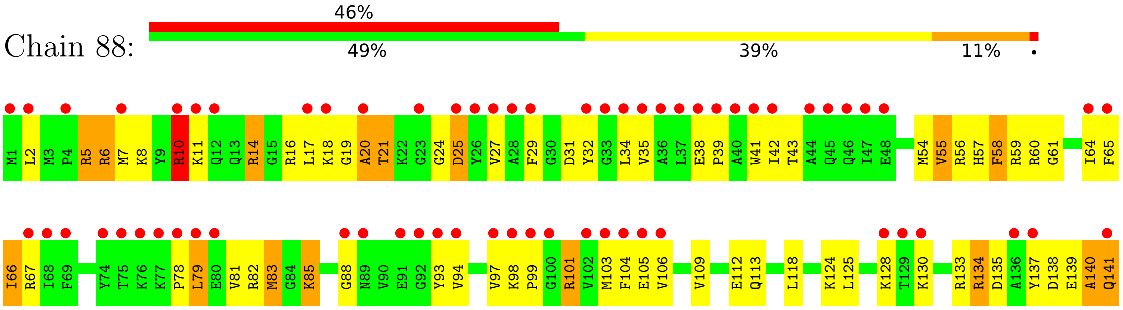


- Molecule 37: 50S ribosomal protein L15



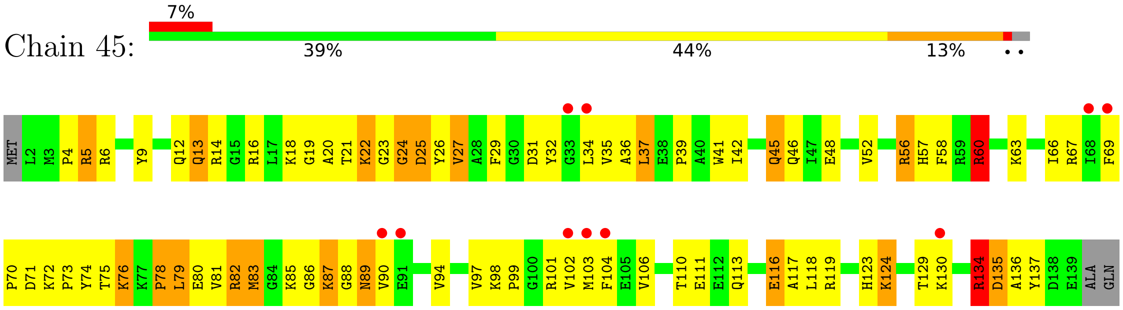
- Molecule 38: 50S ribosomal protein L16

Chain 88:



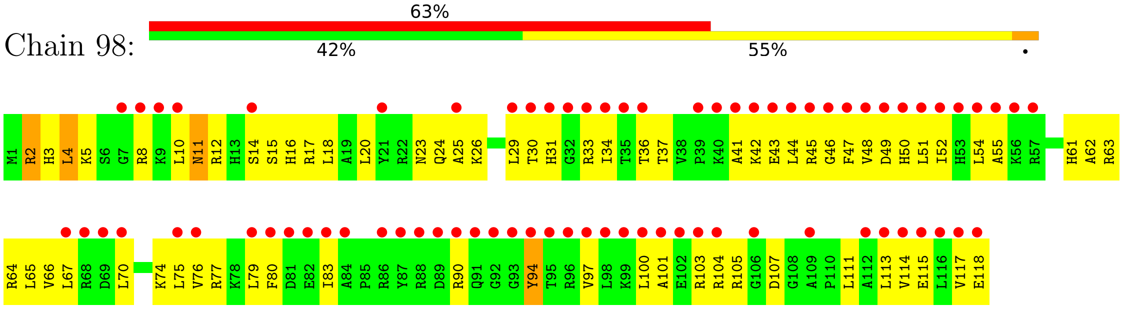
- Molecule 38: 50S ribosomal protein L16

Chain 45:



- Molecule 39: 50S ribosomal protein L17

Chain 98:



- Molecule 39: 50S ribosomal protein L17

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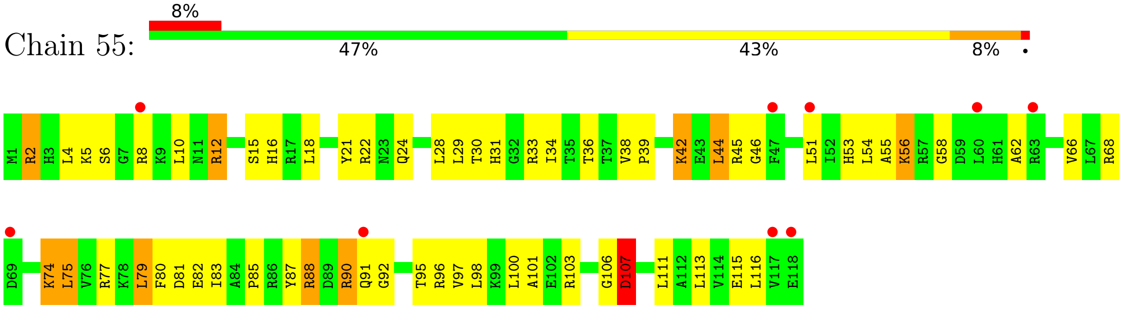
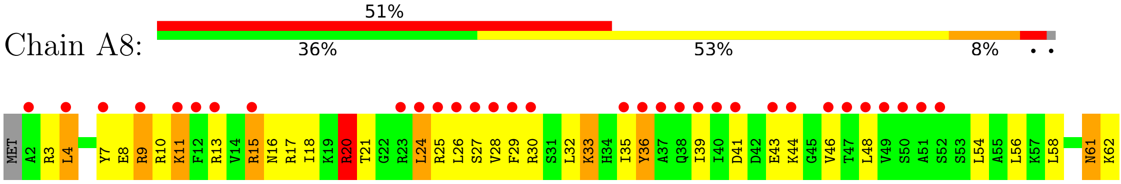


- Molecule 40: 50S ribosomal protein L18

Chain A8:



- Molecule 40: 50S ribosomal protein L18

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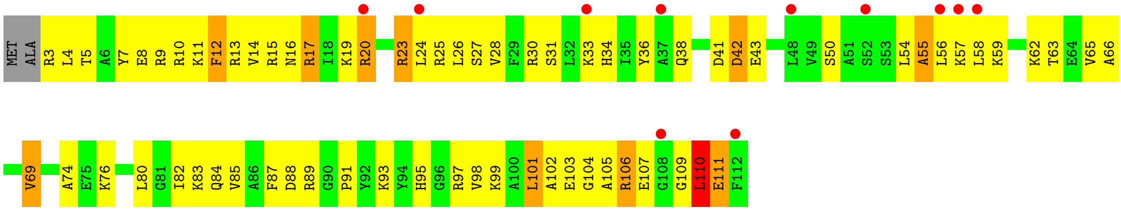
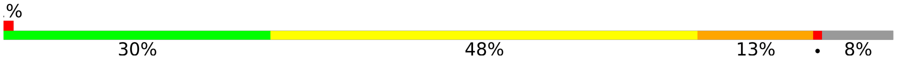
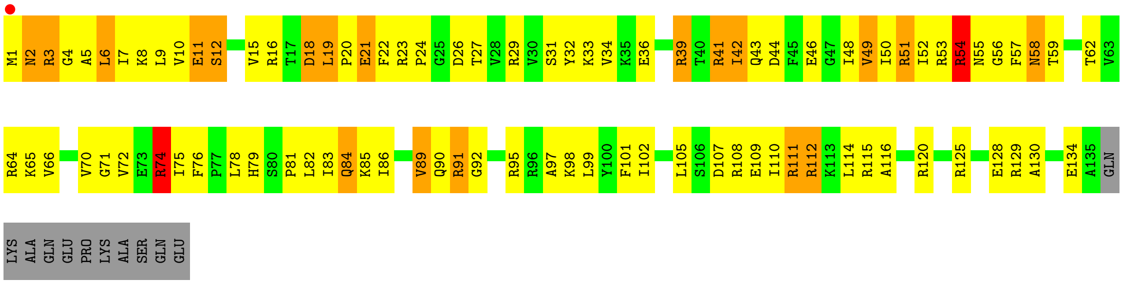


- Molecule 41: 50S ribosomal protein L19

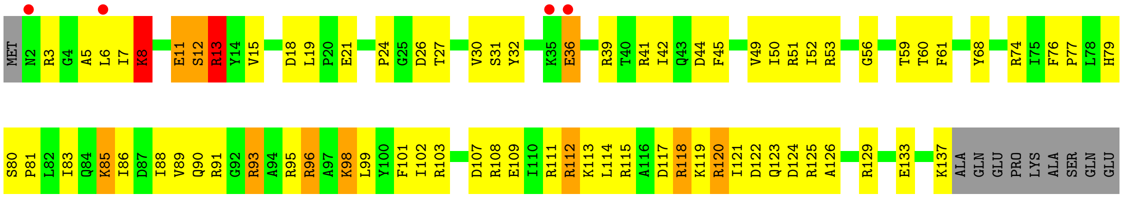
Chain B8:





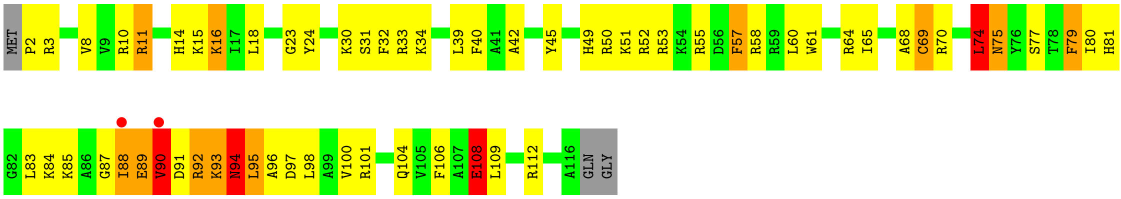
- Molecule 41: 50S ribosomal protein L19

Chain 75:



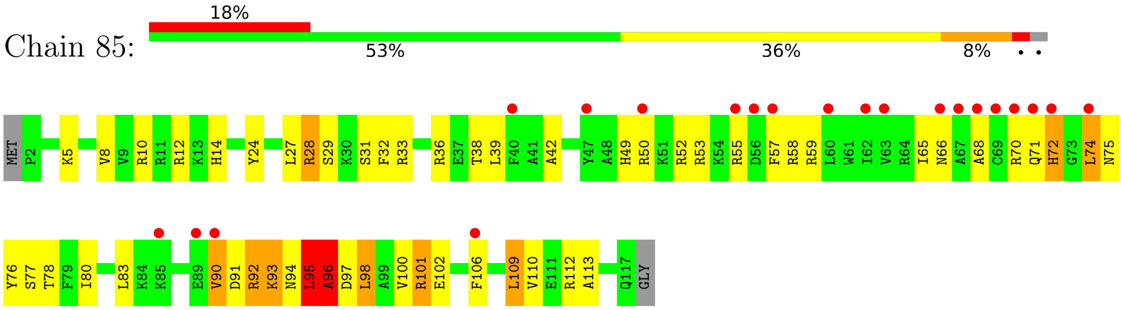
- Molecule 42: 50S ribosomal protein L20

Chain C8:



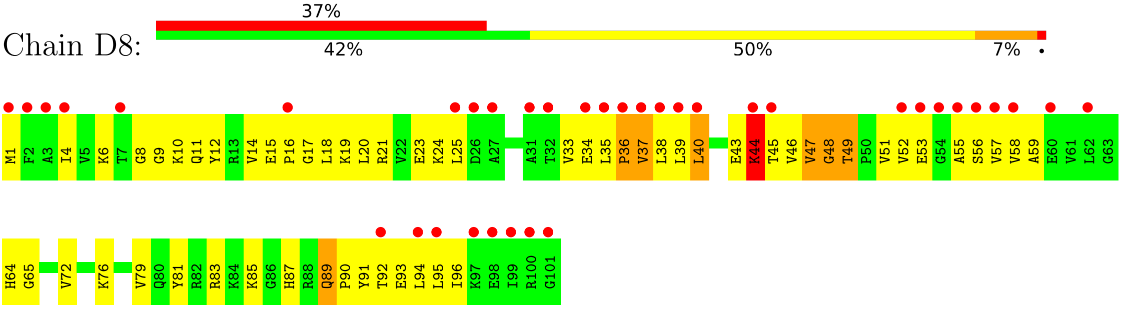
- Molecule 42: 50S ribosomal protein L20

Chain 85:



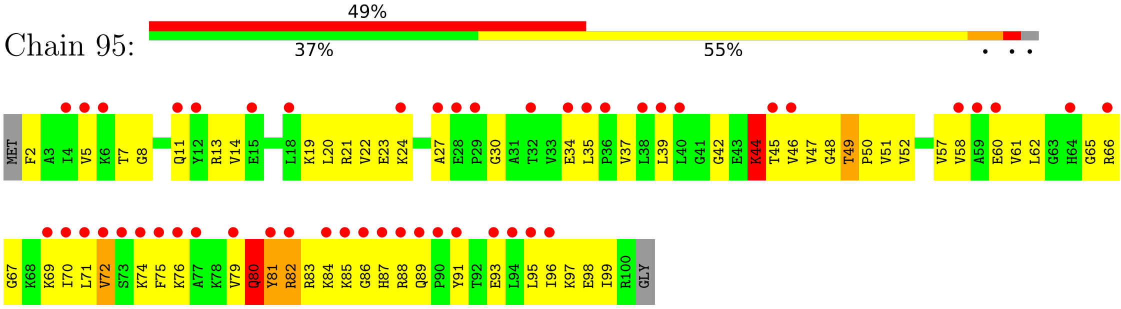
- Molecule 43: 50S ribosomal protein L21

Chain D8:



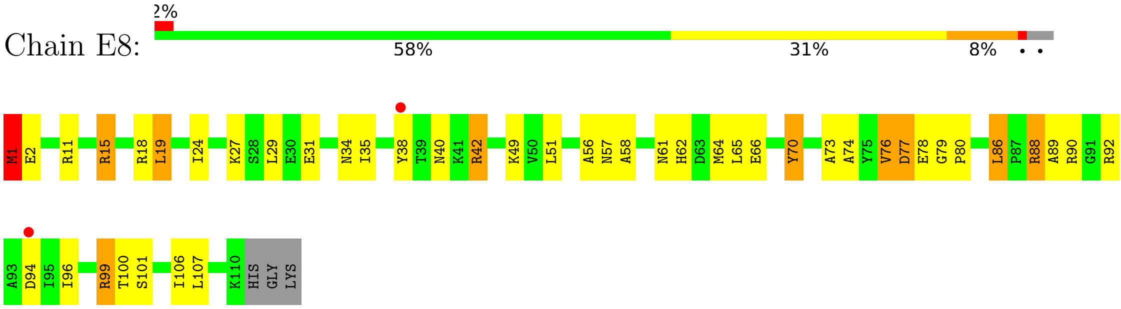
- Molecule 43: 50S ribosomal protein L21

Chain 95:



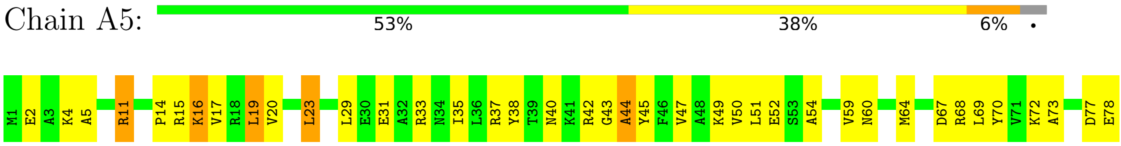
- Molecule 44: 50S ribosomal protein L22

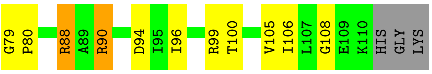
Chain E8:



- Molecule 44: 50S ribosomal protein L22

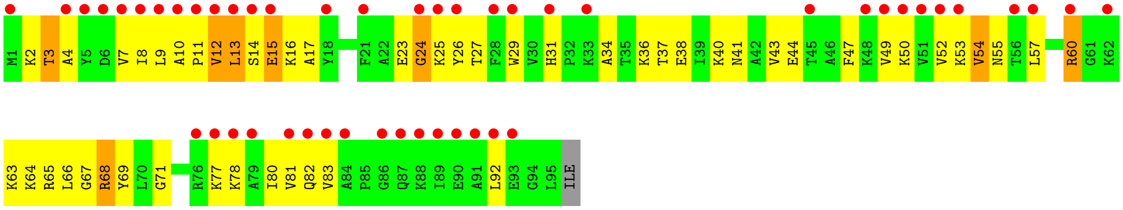
Chain A5:





- Molecule 45: 50S ribosomal protein L23

Chain F8:



- Molecule 45: 50S ribosomal protein L23

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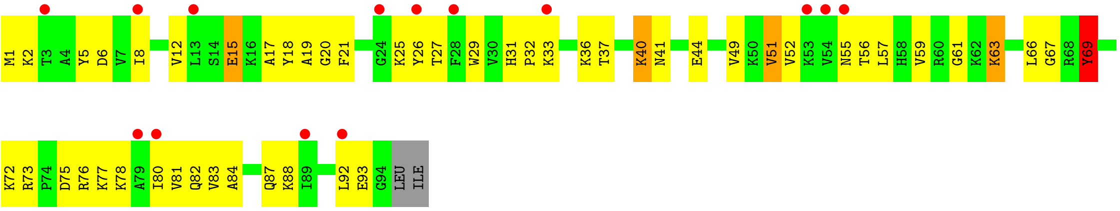
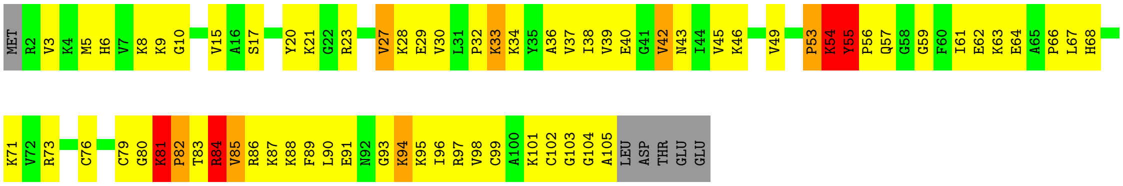


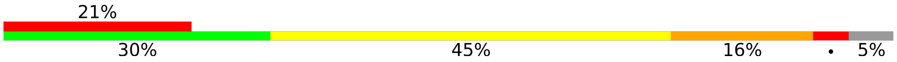
- Molecule 46: 50S ribosomal protein L24

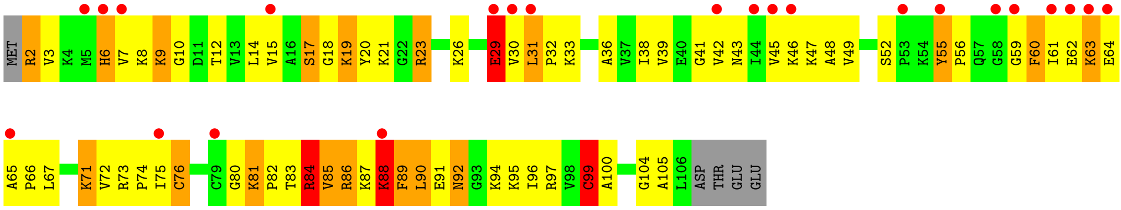
Chain G8:



- Molecule 46: 50S ribosomal protein L24

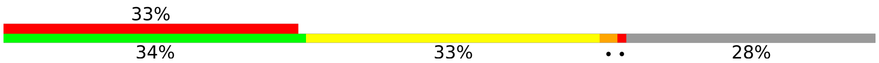
Chain C5:

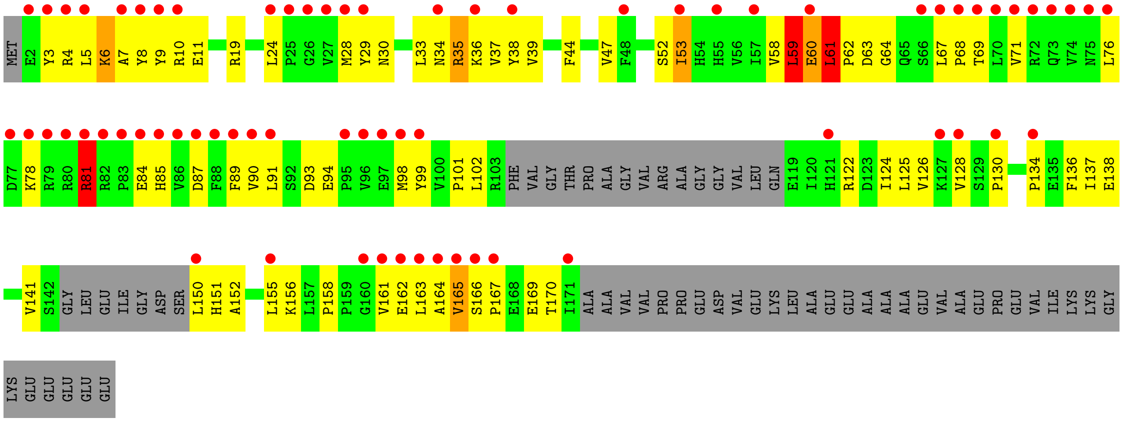




- Molecule 47: 50S ribosomal protein L25

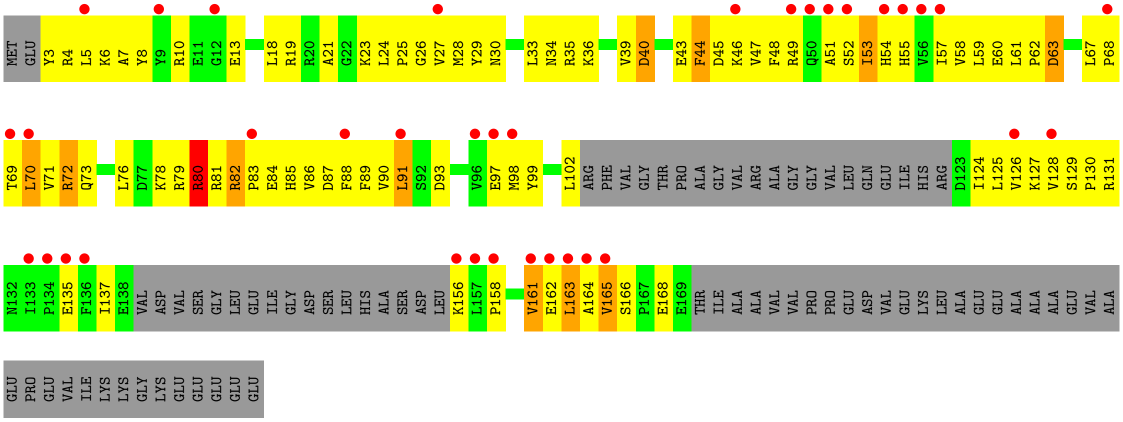
Chain H8:





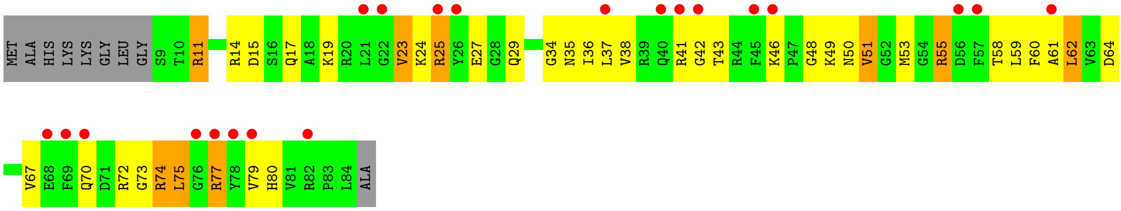
- Molecule 47: 50S ribosomal protein L25

Chain D5:



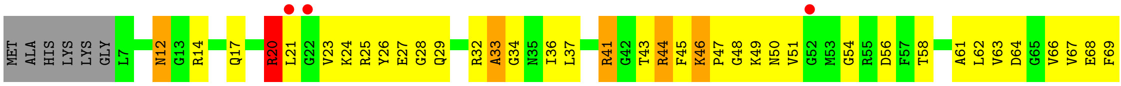
- Molecule 48: 50S ribosomal protein L27

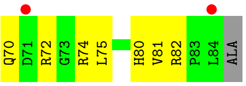
Chain I8:



- Molecule 48: 50S ribosomal protein L27

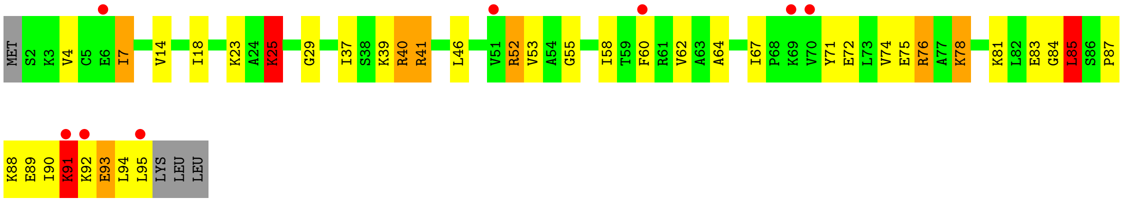
Chain E5:





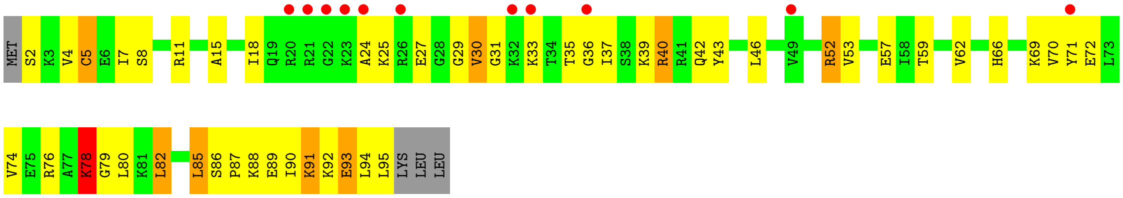
- Molecule 49: 50S ribosomal protein L28

Chain J8:



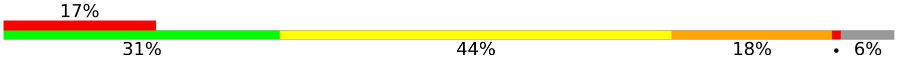
- Molecule 49: 50S ribosomal protein L28

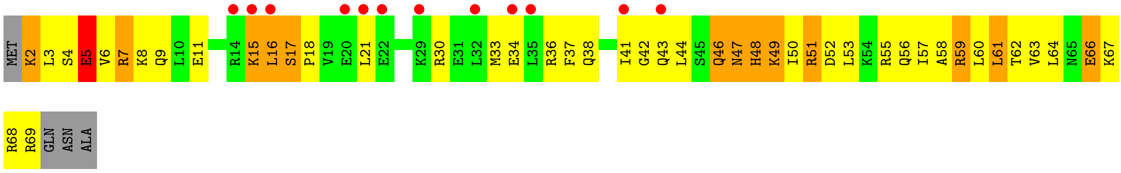
Chain F5:



- Molecule 50: 50S ribosomal protein L29

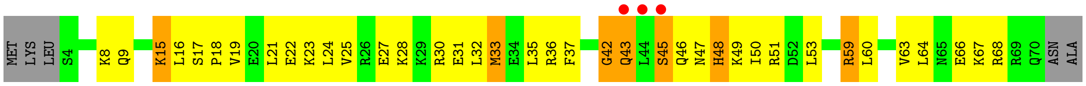
Chain K8:





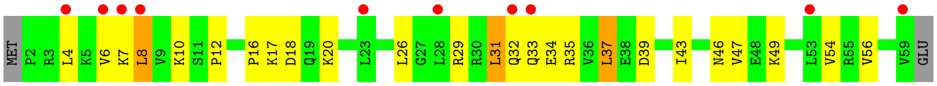
- Molecule 50: 50S ribosomal protein L29

Chain G5:



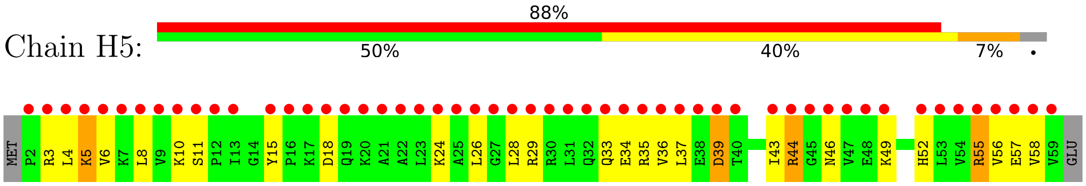
- Molecule 51: 50S ribosomal protein L30

Chain L8:



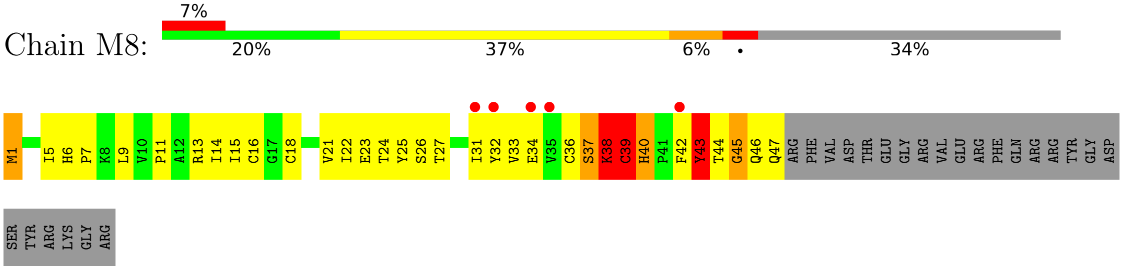
- Molecule 51: 50S ribosomal protein L30

Chain H5:



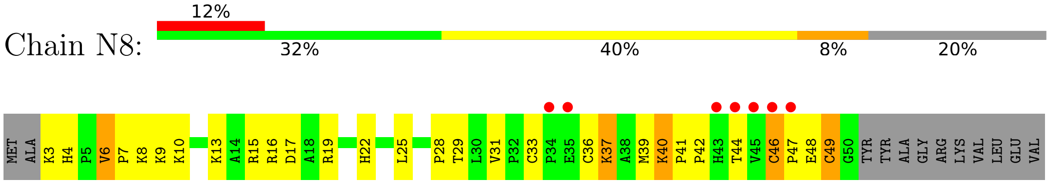
- Molecule 52: 50S ribosomal protein L31

Chain M8:



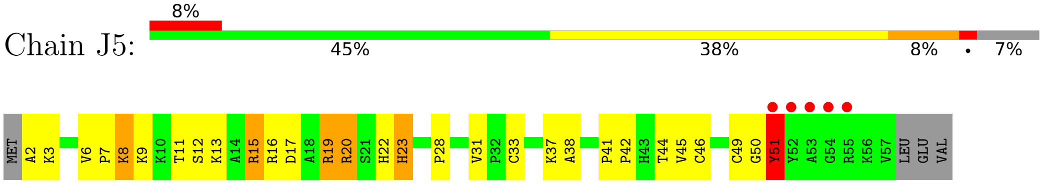
- Molecule 53: 50S ribosomal protein L32

Chain N8:



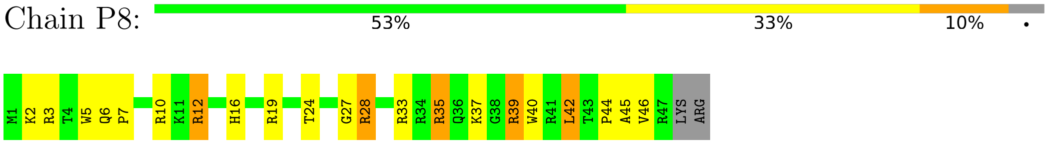
- Molecule 53: 50S ribosomal protein L32

Chain J5:



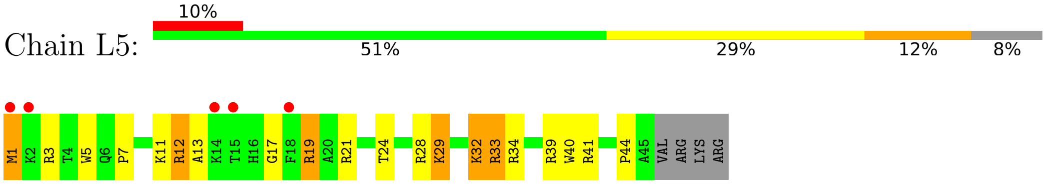
- Molecule 54: 50S ribosomal protein L34

Chain P8:



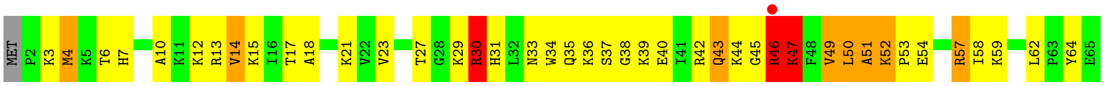
- Molecule 54: 50S ribosomal protein L34

Chain L5:



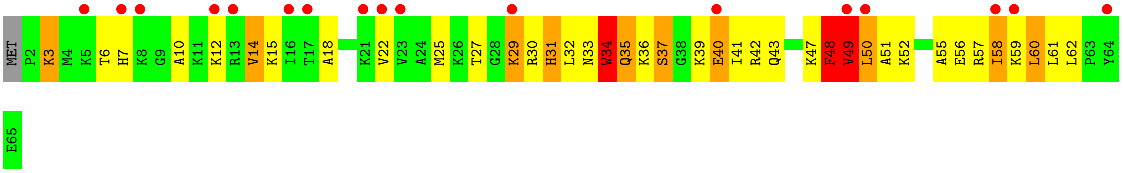
- Molecule 55: 50S ribosomal protein L35

Chain Q8:



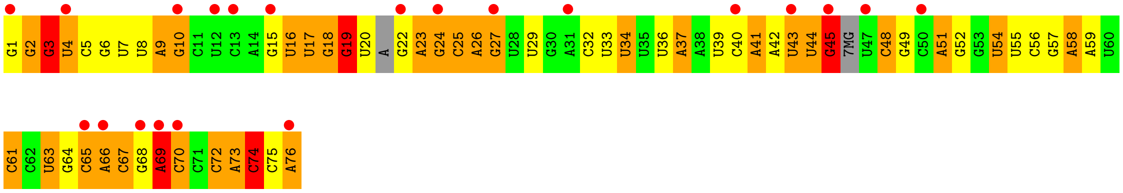
- Molecule 55: 50S ribosomal protein L35

Chain M5:



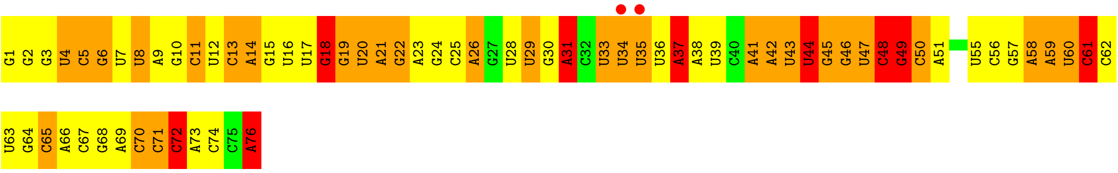
- Molecule 56: tRNALys

Chain 1L:



- 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	208.40Å 447.10Å 616.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.44 – 3.15 152.44 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (152.44-3.15) 92.0 (152.44-3.15)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.254 0.193 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å^2)	107.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 87.5	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	0.95	EDS
Total number of atoms	292607	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: ZN, U8U, 4SU, PSU, SF4, G7M, T6A, OMC, 5MU, MG

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	1.35	176/35927 (0.5%)	2.42	3309/56065 (5.9%)
1	1G	1.15	83/35987 (0.2%)	2.10	2179/56159 (3.9%)
2	12	0.54	2/1726 (0.1%)	0.74	0/2324
2	1E	0.60	0/1908	0.80	2/2573 (0.1%)
3	22	0.50	1/1552 (0.1%)	0.72	2/2093 (0.1%)
3	2E	0.80	0/1629	0.87	2/2195 (0.1%)
4	32	0.72	1/1732 (0.1%)	0.89	3/2318 (0.1%)
4	3E	0.86	2/1726 (0.1%)	0.90	3/2310 (0.1%)
5	42	0.75	3/1151 (0.3%)	0.76	1/1549 (0.1%)
5	4E	0.85	1/1158 (0.1%)	0.91	1/1559 (0.1%)
6	52	0.75	0/855	0.85	2/1154 (0.2%)
6	5E	0.77	1/850 (0.1%)	0.97	4/1147 (0.3%)
7	62	0.66	1/1122 (0.1%)	0.78	1/1500 (0.1%)
7	6E	0.64	0/1245	0.72	0/1666
8	72	0.57	1/1127 (0.1%)	0.74	1/1517 (0.1%)
8	7E	0.94	4/1135 (0.4%)	0.93	3/1527 (0.2%)
9	82	0.64	1/835 (0.1%)	0.84	1/1120 (0.1%)
9	8E	0.61	0/1019	0.77	0/1367
10	1A	0.56	0/482	0.73	0/647
10	1I	0.73	0/602	0.84	1/806 (0.1%)
11	2A	0.70	1/850 (0.1%)	0.80	1/1150 (0.1%)
11	2I	0.71	0/838	0.88	0/1133
12	3A	0.69	0/963	0.95	3/1290 (0.2%)
12	3I	0.99	2/972 (0.2%)	1.12	2/1301 (0.2%)
13	4A	0.61	0/903	0.87	2/1211 (0.2%)
13	4I	0.79	2/952 (0.2%)	0.89	2/1277 (0.2%)
14	5A	0.63	1/393 (0.3%)	0.91	1/521 (0.2%)
14	5I	0.83	1/500 (0.2%)	0.98	1/664 (0.2%)
15	6A	0.75	2/740 (0.3%)	0.81	0/987
15	6I	0.81	1/740 (0.1%)	0.87	0/987
16	7A	0.77	0/721	0.90	0/970
16	7I	0.74	1/687 (0.1%)	0.86	0/925

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\lvert Z\rvert >5$	RMSZ	$\#\lvert Z\rvert >5$
17	8A	0.65	0/836	0.75	0/1117
17	8I	0.85	3/847 (0.4%)	0.89	0/1131
18	9A	0.80	0/549	0.81	1/732 (0.1%)
18	9I	0.68	0/549	0.88	0/732
19	AA	0.54	0/288	0.90	1/388 (0.3%)
19	AI	0.80	0/668	0.93	0/899
20	BA	0.64	0/759	0.86	1/1000 (0.1%)
20	BI	0.57	0/748	0.80	0/986
21	1B	0.57	0/208	0.76	0/272
21	1F	0.56	0/203	0.79	0/266
22	1K	1.14	11/1516 (0.7%)	1.96	70/2350 (3.0%)
23	2K	1.63	25/1721 (1.5%)	2.75	223/2682 (8.3%)
23	2L	1.15	2/1721 (0.1%)	2.03	86/2682 (3.2%)
24	3K	1.13	5/1799 (0.3%)	1.94	76/2801 (2.7%)
25	4K	1.74	7/494 (1.4%)	2.28	40/767 (5.2%)
25	4L	1.44	3/420 (0.7%)	2.11	26/654 (4.0%)
26	14	1.58	825/69023 (1.2%)	2.76	8688/107740 (8.1%)
26	1H	1.84	1510/68273 (2.2%)	3.14	11225/106575 (10.5%)
27	16	1.49	22/2928 (0.8%)	2.87	390/4568 (8.5%)
27	1J	1.26	10/2928 (0.3%)	2.37	253/4568 (5.5%)
28	71	0.68	0/1073	0.78	0/1447
29	11	1.14	8/2170 (0.4%)	1.34	30/2926 (1.0%)
29	19	1.05	3/2170 (0.1%)	1.24	22/2926 (0.8%)
30	21	1.06	9/1591 (0.6%)	1.16	8/2146 (0.4%)
30	29	0.99	5/1591 (0.3%)	1.13	5/2146 (0.2%)
31	31	1.11	8/1620 (0.5%)	1.23	15/2194 (0.7%)
31	39	0.88	2/1637 (0.1%)	1.08	6/2218 (0.3%)
32	41	0.85	4/1481 (0.3%)	1.01	3/1994 (0.2%)
32	49	0.63	0/1481	0.91	4/1994 (0.2%)
33	51	0.96	2/1337 (0.1%)	1.17	6/1809 (0.3%)
33	59	0.67	1/548 (0.2%)	0.82	0/738
34	61	0.70	0/1146	0.89	0/1551
34	69	0.70	2/1146 (0.2%)	0.89	3/1551 (0.2%)
35	15	0.78	0/1123	0.93	2/1515 (0.1%)
35	58	0.90	1/1131 (0.1%)	1.00	3/1525 (0.2%)
36	25	0.90	0/942	1.00	1/1269 (0.1%)
36	68	0.97	0/942	1.11	4/1269 (0.3%)
37	35	1.11	1/1147 (0.1%)	1.16	6/1525 (0.4%)
37	78	1.08	3/1139 (0.3%)	1.33	14/1514 (0.9%)
38	45	0.98	4/1120 (0.4%)	1.06	2/1498 (0.1%)
38	88	1.13	6/1134 (0.5%)	1.22	7/1519 (0.5%)
39	55	0.89	1/981 (0.1%)	1.20	10/1312 (0.8%)
39	98	0.81	0/981	1.13	4/1312 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	65	0.76	1/886 (0.1%)	1.04	4/1180 (0.3%)
40	A8	0.95	1/891 (0.1%)	1.26	6/1187 (0.5%)
41	75	0.98	4/1147 (0.3%)	1.10	3/1532 (0.2%)
41	B8	1.10	7/1137 (0.6%)	1.11	5/1519 (0.3%)
42	85	0.83	0/977	1.01	4/1301 (0.3%)
42	C8	1.02	4/968 (0.4%)	1.08	2/1289 (0.2%)
43	95	1.01	4/777 (0.5%)	1.02	0/1042
43	D8	0.93	1/789 (0.1%)	1.08	1/1057 (0.1%)
44	A5	1.05	1/886 (0.1%)	1.15	6/1189 (0.5%)
44	E8	1.03	1/886 (0.1%)	1.21	8/1189 (0.7%)
45	B5	1.08	2/749 (0.3%)	1.09	2/1007 (0.2%)
45	F8	1.17	5/754 (0.7%)	1.27	6/1014 (0.6%)
46	C5	1.09	5/812 (0.6%)	1.08	4/1083 (0.4%)
46	G8	1.33	8/801 (1.0%)	1.34	6/1069 (0.6%)
47	D5	0.84	4/1088 (0.4%)	0.85	2/1473 (0.1%)
47	H8	0.78	1/1244 (0.1%)	0.96	3/1683 (0.2%)
48	E5	0.87	0/624	1.08	1/832 (0.1%)
48	I8	1.12	1/614 (0.2%)	1.28	8/819 (1.0%)
49	F5	0.94	2/744 (0.3%)	1.09	3/989 (0.3%)
49	J8	1.09	4/744 (0.5%)	1.18	5/989 (0.5%)
50	G5	0.80	0/565	0.99	1/748 (0.1%)
50	K8	1.09	0/570	1.43	11/755 (1.5%)
51	H5	0.80	0/464	0.90	0/623
51	L8	0.92	1/464 (0.2%)	1.13	1/623 (0.2%)
52	M8	0.77	0/375	1.08	3/507 (0.6%)
53	J5	0.92	2/448 (0.4%)	1.08	4/606 (0.7%)
53	N8	1.02	1/381 (0.3%)	1.08	0/516
54	L5	0.99	0/399	1.23	3/526 (0.6%)
54	P8	1.17	0/409	1.62	9/540 (1.7%)
55	M5	1.10	5/524 (1.0%)	1.18	4/691 (0.6%)
55	Q8	1.13	1/524 (0.2%)	1.41	9/691 (1.3%)
56	1L	0.76	1/1683 (0.1%)	1.38	20/2615 (0.8%)
57	3L	0.96	7/1777 (0.4%)	1.72	50/2767 (1.8%)
All	All	1.39	2845/315237 (0.9%)	2.39	26956/472471 (5.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	3
3	22	0	2
3	2E	0	2
4	32	0	4
4	3E	0	1
5	4E	0	1
7	6E	0	1
9	82	0	1
9	8E	0	1
11	2A	0	1
11	2I	0	1
12	3A	0	1
12	3I	0	5
13	4A	0	2
13	4I	0	3
14	5A	0	1
14	5I	0	1
15	6A	0	1
16	7I	0	1
17	8I	0	1
19	AA	0	1
19	AI	0	2
20	BA	0	4
20	BI	0	1
26	14	0	1
28	71	0	1
29	11	0	6
29	19	0	6
30	21	0	11
30	29	0	6
31	31	0	3
31	39	0	11
32	41	0	3
32	49	0	6
33	51	0	3
33	59	0	3
34	61	0	4
34	69	0	6
35	15	0	4
35	58	0	3
37	35	0	4
37	78	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	45	0	7
38	88	0	3
40	A8	0	2
41	75	0	2
41	B8	0	4
42	85	0	5
42	C8	0	3
43	95	0	3
43	D8	0	4
44	A5	0	1
45	B5	0	2
45	F8	0	2
46	C5	0	1
46	G8	0	6
47	D5	0	1
47	H8	0	2
48	E5	0	1
49	F5	0	3
49	J8	0	2
50	G5	0	4
50	K8	0	4
52	M8	0	5
54	P8	0	1
55	M5	0	3
55	Q8	0	2
All	All	0	209

The worst 5 of 2845 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	35	121	LYS	C-N	22.50	1.76	1.34
26	1H	783	A	N3-C4	-21.39	1.22	1.34
26	1H	676	A	N9-C4	-19.81	1.25	1.37
26	14	783	A	N9-C4	-18.75	1.26	1.37
26	1H	2346	A	N3-C4	-16.77	1.24	1.34

The worst 5 of 26956 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	14	783	A	C2-N3-C4	-38.22	91.49	110.60
26	1H	783	A	C2-N3-C4	-32.53	94.33	110.60
26	1H	1899	G	C2-N3-C4	-29.93	96.93	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	676	A	C2-N3-C4	-28.68	96.26	110.60
26	14	929	G	N1-C6-O6	25.84	135.40	119.90

There are no chirality outliers.

5 of 209 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
2	1E	9	GLU	Peptide
3	2E	128	PHE	Peptide
3	2E	166	GLU	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	32097	0	16197	1109	0
1	1G	32152	0	16231	1228	2
2	12	1695	0	1729	133	0
2	1E	1874	0	1926	143	0
3	22	1529	0	1592	134	0
3	2E	1605	0	1668	83	0
4	32	1702	0	1764	160	0
4	3E	1696	0	1752	134	0
5	42	1136	0	1200	105	0
5	4E	1142	0	1204	90	0
6	52	842	0	857	50	0
6	5E	837	0	852	48	0
7	62	1110	0	1163	82	0
7	6E	1229	0	1274	76	0
8	72	1107	0	1165	73	0
8	7E	1115	0	1177	78	0
9	82	820	0	848	83	0
9	8E	1000	0	1031	93	0
10	1A	474	0	484	43	0
10	1I	593	0	610	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	2A	835	0	847	31	0
11	2I	823	0	833	53	0
12	3A	947	0	1033	81	0
12	3I	956	0	1046	47	0
13	4A	893	0	946	85	0
13	4I	942	0	997	66	0
14	5A	388	0	424	47	0
14	5I	491	0	530	37	0
15	6A	729	0	768	35	0
15	6I	729	0	768	52	0
16	7A	705	0	725	55	0
16	7I	671	0	693	60	0
17	8A	823	0	891	37	0
17	8I	834	0	904	56	0
18	9A	544	0	605	35	0
18	9I	544	0	605	33	0
19	AA	283	0	284	22	0
19	AI	654	0	675	55	0
20	BA	757	0	856	56	0
20	BI	746	0	843	56	0
21	1B	204	0	218	18	0
21	1F	199	0	208	10	0
22	1K	1477	0	758	66	0
23	2K	1646	0	844	42	0
23	2L	1646	0	844	59	0
24	3K	1611	0	817	93	0
25	4K	439	0	219	17	0
25	4L	373	0	185	10	0
26	14	61630	0	31047	1916	1
26	1H	60960	0	30668	1946	0
27	16	2617	0	1328	91	0
27	1J	2617	0	1328	133	0
28	71	1050	0	1071	88	0
29	11	2120	0	2197	169	0
29	19	2120	0	2197	169	0
30	21	1558	0	1624	120	0
30	29	1558	0	1622	186	0
31	31	1585	0	1632	121	0
31	39	1602	0	1649	122	0
32	41	1457	0	1514	130	0
32	49	1457	0	1514	161	0
33	51	1312	0	1384	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	59	539	0	563	41	0
34	61	1131	0	1218	80	1
34	69	1131	0	1218	86	0
35	15	1096	0	1168	60	0
35	58	1104	0	1180	75	0
36	25	932	0	996	65	0
36	68	932	0	996	50	0
37	35	1130	0	1217	140	0
37	78	1122	0	1206	122	0
38	45	1099	0	1153	112	0
38	88	1113	0	1156	82	0
39	55	967	0	1033	57	0
39	98	967	0	1033	62	0
40	65	876	0	938	85	0
40	A8	881	0	943	86	0
41	75	1133	0	1190	80	0
41	B8	1123	0	1181	105	0
42	85	959	0	1019	68	0
42	C8	950	0	1011	82	0
43	95	766	0	837	77	0
43	D8	778	0	851	80	0
44	A5	876	0	941	41	0
44	E8	876	0	941	46	0
45	B5	735	0	785	54	0
45	F8	740	0	787	50	0
46	C5	799	0	888	79	0
46	G8	788	0	875	88	0
47	D5	1064	0	1082	88	0
47	H8	1218	0	1241	75	0
48	E5	616	0	633	49	0
48	I8	606	0	625	40	0
49	F5	737	0	813	60	0
49	J8	737	0	813	50	0
50	G5	563	0	612	35	0
50	K8	568	0	614	47	0
51	H5	459	0	512	19	0
51	L8	459	0	512	20	0
52	M8	366	0	370	49	0
53	J5	434	0	454	33	0
53	N8	369	0	388	44	0
54	L5	391	0	432	22	0
54	P8	401	0	436	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	M5	516	0	582	50	0
55	Q8	516	0	582	54	0
56	1L	1570	0	798	39	0
57	3L	1611	0	817	69	0
58	11	1	0	0	0	0
58	13	141	0	0	0	0
58	14	420	0	0	0	0
58	16	12	0	0	0	0
58	1G	78	0	0	0	0
58	1H	488	0	0	0	0
58	1J	6	0	0	0	0
58	21	2	0	0	0	0
58	29	3	0	0	0	0
58	2K	3	0	0	0	0
58	2L	3	0	0	0	0
58	32	1	0	0	0	0
58	35	1	0	0	0	0
58	3I	1	0	0	0	0
58	41	1	0	0	0	0
58	45	3	0	0	0	0
58	55	1	0	0	0	0
58	5E	2	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7A	1	0	0	0	0
58	85	2	0	0	0	0
58	88	1	0	0	0	0
58	C5	1	0	0	0	0
58	C8	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	2	0	0	0	0
58	L5	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	4	0
59	3E	8	0	0	0	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	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	13	148	0	0	21	0
61	14	411	0	0	57	0
61	16	18	0	0	4	0
61	19	4	0	0	2	0
61	1G	44	0	0	6	0
61	1H	670	0	0	78	0
61	1J	11	0	0	2	0
61	1K	1	0	0	0	0
61	21	5	0	0	2	0
61	29	3	0	0	0	0
61	31	6	0	0	0	0
61	35	2	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	1	0
61	3I	2	0	0	0	0
61	4K	6	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	3	0	0	2	0
61	5I	1	0	0	0	0
61	6I	1	0	0	0	0
61	78	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	D8	1	0	0	0	0
61	E5	1	0	0	0	0
61	E8	1	0	0	0	0
61	F5	2	0	0	0	0
61	G8	1	0	0	0	0
61	I8	1	0	0	0	0
61	L5	1	0	0	0	0
61	M5	2	0	0	0	0
61	Q8	1	0	0	0	0
All	All	292607	0	194505	12060	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

The worst 5 of 12060 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:G8:84:ARG:CB	46:G8:84:ARG:CG	1.75	1.63
46:G8:84:ARG:CG	46:G8:84:ARG:CD	1.76	1.61
29:19:246:PRO:N	29:19:255:LYS:HZ1	1.10	1.44
3:22:29:TYR:CE1	3:22:33:LEU:HD22	1.61	1.35
37:35:121:LYS:C	37:35:122:PRO:N	1.77	1.35

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	1.99	0.21
34:61:89:TYR:O	1:1G:357:G:O2'[4_555]	2.19	0.01

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	202/256 (79%)	170 (84%)	26 (13%)	6 (3%)	4	24
2	1E	227/256 (89%)	194 (86%)	28 (12%)	5 (2%)	6	32
3	22	190/239 (80%)	167 (88%)	22 (12%)	1 (0%)	29	65
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	181 (88%)	22 (11%)	3 (2%)	10	41
4	3E	205/209 (98%)	189 (92%)	14 (7%)	2 (1%)	15	51
5	42	147/162 (91%)	136 (92%)	11 (8%)	0	100	100
5	4E	147/162 (91%)	137 (93%)	9 (6%)	1 (1%)	22	59
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	121 (90%)	13 (10%)	0	100	100
7	6E	147/156 (94%)	141 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	59
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	59
9	82	101/128 (79%)	88 (87%)	11 (11%)	2 (2%)	7	34
9	8E	124/128 (97%)	103 (83%)	20 (16%)	1 (1%)	19	55
10	1A	54/105 (51%)	46 (85%)	8 (15%)	0	100	100
10	1I	66/105 (63%)	58 (88%)	6 (9%)	2 (3%)	4	24
11	2A	111/129 (86%)	97 (87%)	12 (11%)	2 (2%)	8	37
11	2I	109/129 (84%)	94 (86%)	13 (12%)	2 (2%)	8	37
12	3A	119/132 (90%)	97 (82%)	17 (14%)	5 (4%)	3	17
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	55
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	17	53
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	44/61 (72%)	37 (84%)	7 (16%)	0	100	100
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	21
15	6A	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
15	6I	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	78/88 (89%)	73 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	10	41
19	AA	32/93 (34%)	25 (78%)	6 (19%)	1 (3%)	4	23
19	AI	79/93 (85%)	66 (84%)	11 (14%)	2 (2%)	5	29
20	BA	96/106 (91%)	81 (84%)	12 (12%)	3 (3%)	4	23
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	21/27 (78%)	21 (100%)	0	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	131/229 (57%)	121 (92%)	9 (7%)	1 (1%)	19	55
29	11	271/276 (98%)	233 (86%)	26 (10%)	12 (4%)	2	16
29	19	271/276 (98%)	245 (90%)	19 (7%)	7 (3%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	21	201/206 (98%)	158 (79%)	34 (17%)	9 (4%)	2	16
30	29	201/206 (98%)	153 (76%)	37 (18%)	11 (6%)	2	12
31	31	200/210 (95%)	176 (88%)	22 (11%)	2 (1%)	15	51
31	39	202/210 (96%)	158 (78%)	36 (18%)	8 (4%)	3	18
32	41	177/182 (97%)	154 (87%)	18 (10%)	5 (3%)	5	26
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	14	48
33	51	169/180 (94%)	135 (80%)	20 (12%)	14 (8%)	1	4
33	59	63/180 (35%)	44 (70%)	13 (21%)	6 (10%)	0	3
34	61	143/148 (97%)	118 (82%)	24 (17%)	1 (1%)	22	59
34	69	143/148 (97%)	111 (78%)	27 (19%)	5 (4%)	3	21
35	15	135/140 (96%)	119 (88%)	13 (10%)	3 (2%)	6	32
35	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	4	25
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	55
36	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
37	35	146/150 (97%)	111 (76%)	31 (21%)	4 (3%)	5	27
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	2	12
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	4	25
38	88	139/141 (99%)	115 (83%)	17 (12%)	7 (5%)	2	14
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	53
39	98	116/118 (98%)	93 (80%)	22 (19%)	1 (1%)	17	53
40	65	108/112 (96%)	87 (81%)	18 (17%)	3 (3%)	5	26
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	53
41	75	134/146 (92%)	121 (90%)	13 (10%)	0	100	100
41	B8	133/146 (91%)	117 (88%)	14 (10%)	2 (2%)	10	41
42	85	114/118 (97%)	99 (87%)	13 (11%)	2 (2%)	8	37
42	C8	113/118 (96%)	104 (92%)	5 (4%)	4 (4%)	3	21
43	95	97/101 (96%)	77 (79%)	16 (16%)	4 (4%)	3	18
43	D8	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	4	24
44	A5	108/113 (96%)	100 (93%)	7 (6%)	1 (1%)	17	53
44	E8	108/113 (96%)	97 (90%)	11 (10%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	5 (5%)	2 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	F8	93/96 (97%)	82 (88%)	10 (11%)	1 (1%)	14	48
46	C5	103/110 (94%)	70 (68%)	26 (25%)	7 (7%)	1	7
46	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	1	11
47	D5	124/206 (60%)	96 (77%)	25 (20%)	3 (2%)	6	30
47	H8	142/206 (69%)	112 (79%)	22 (16%)	8 (6%)	2	12
48	E5	76/85 (89%)	66 (87%)	8 (10%)	2 (3%)	5	28
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	6	32
49	J8	92/98 (94%)	84 (91%)	6 (6%)	2 (2%)	6	32
50	G5	65/72 (90%)	61 (94%)	3 (5%)	1 (2%)	10	41
50	K8	66/72 (92%)	55 (83%)	7 (11%)	4 (6%)	1	10
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
52	M8	45/71 (63%)	28 (62%)	15 (33%)	2 (4%)	2	16
53	J5	54/60 (90%)	46 (85%)	8 (15%)	0	100	100
53	N8	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
54	L5	43/49 (88%)	39 (91%)	4 (9%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	6	32
55	M5	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	2	15
55	Q8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	8
All	All	10778/12104 (89%)	9303 (86%)	1246 (12%)	229 (2%)	7	33

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	91	ARG
18	9I	22	VAL
19	AI	67	VAL
29	11	28	GLU
29	11	40	THR

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	180/220 (82%)	164 (91%)	16 (9%)	9	33
2	1E	200/220 (91%)	181 (90%)	19 (10%)	8	30
3	22	153/188 (81%)	143 (94%)	10 (6%)	17	48
3	2E	159/188 (85%)	148 (93%)	11 (7%)	15	46
4	32	180/181 (99%)	165 (92%)	15 (8%)	11	37
4	3E	179/181 (99%)	167 (93%)	12 (7%)	16	47
5	42	114/123 (93%)	106 (93%)	8 (7%)	15	45
5	4E	115/123 (94%)	106 (92%)	9 (8%)	12	40
6	52	90/90 (100%)	81 (90%)	9 (10%)	7	28
6	5E	90/90 (100%)	87 (97%)	3 (3%)	38	69
7	62	114/127 (90%)	101 (89%)	13 (11%)	5	23
7	6E	125/127 (98%)	118 (94%)	7 (6%)	21	53
8	72	118/119 (99%)	112 (95%)	6 (5%)	24	56
8	7E	119/119 (100%)	111 (93%)	8 (7%)	16	47
9	82	79/99 (80%)	69 (87%)	10 (13%)	4	19
9	8E	97/99 (98%)	90 (93%)	7 (7%)	14	43
10	1A	52/92 (56%)	48 (92%)	4 (8%)	13	41
10	1I	65/92 (71%)	62 (95%)	3 (5%)	27	60
11	2A	85/99 (86%)	82 (96%)	3 (4%)	36	67
11	2I	84/99 (85%)	81 (96%)	3 (4%)	35	67
12	3A	102/109 (94%)	95 (93%)	7 (7%)	15	46
12	3I	103/109 (94%)	95 (92%)	8 (8%)	12	40
13	4A	91/101 (90%)	85 (93%)	6 (7%)	16	47
13	4I	94/101 (93%)	87 (93%)	7 (7%)	13	43
14	5A	40/50 (80%)	36 (90%)	4 (10%)	7	28
14	5I	49/50 (98%)	48 (98%)	1 (2%)	55	79
15	6A	79/80 (99%)	75 (95%)	4 (5%)	24	56
15	6I	79/80 (99%)	75 (95%)	4 (5%)	24	56
16	7A	72/74 (97%)	70 (97%)	2 (3%)	43	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	7I	69/74 (93%)	63 (91%)	6 (9%)	10	34
17	8A	94/97 (97%)	90 (96%)	4 (4%)	29	62
17	8I	95/97 (98%)	91 (96%)	4 (4%)	30	62
18	9A	58/77 (75%)	56 (97%)	2 (3%)	37	68
18	9I	58/77 (75%)	57 (98%)	1 (2%)	60	82
19	AA	31/80 (39%)	28 (90%)	3 (10%)	8	29
19	AI	71/80 (89%)	66 (93%)	5 (7%)	15	45
20	BA	76/82 (93%)	74 (97%)	2 (3%)	46	74
20	BI	75/82 (92%)	72 (96%)	3 (4%)	31	64
21	1B	19/22 (86%)	18 (95%)	1 (5%)	22	55
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	71	111/181 (61%)	106 (96%)	5 (4%)	27	61
29	11	214/218 (98%)	205 (96%)	9 (4%)	30	62
29	19	214/218 (98%)	204 (95%)	10 (5%)	26	60
30	21	165/166 (99%)	159 (96%)	6 (4%)	35	67
30	29	165/166 (99%)	155 (94%)	10 (6%)	18	50
31	31	161/166 (97%)	153 (95%)	8 (5%)	24	57
31	39	163/166 (98%)	153 (94%)	10 (6%)	18	50
32	41	153/156 (98%)	136 (89%)	17 (11%)	6	24
32	49	153/156 (98%)	134 (88%)	19 (12%)	4	20
33	51	142/148 (96%)	134 (94%)	8 (6%)	21	53
33	59	56/148 (38%)	53 (95%)	3 (5%)	22	55
34	61	122/124 (98%)	112 (92%)	10 (8%)	11	38
34	69	122/124 (98%)	114 (93%)	8 (7%)	16	47
35	15	116/119 (98%)	112 (97%)	4 (3%)	37	68
35	58	117/119 (98%)	109 (93%)	8 (7%)	16	46
36	25	100/100 (100%)	92 (92%)	8 (8%)	12	39
36	68	100/100 (100%)	96 (96%)	4 (4%)	31	64
37	35	115/116 (99%)	110 (96%)	5 (4%)	29	62
37	78	114/116 (98%)	107 (94%)	7 (6%)	18	50
38	45	109/111 (98%)	96 (88%)	13 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	88	109/111 (98%)	104 (95%)	5 (5%)	27	60
39	55	101/101 (100%)	94 (93%)	7 (7%)	15	46
39	98	101/101 (100%)	98 (97%)	3 (3%)	41	71
40	65	87/88 (99%)	81 (93%)	6 (7%)	15	46
40	A8	87/88 (99%)	78 (90%)	9 (10%)	7	26
41	75	119/127 (94%)	105 (88%)	14 (12%)	5	21
41	B8	118/127 (93%)	106 (90%)	12 (10%)	7	27
42	85	93/94 (99%)	85 (91%)	8 (9%)	10	35
42	C8	92/94 (98%)	82 (89%)	10 (11%)	6	24
43	95	81/82 (99%)	76 (94%)	5 (6%)	18	50
43	D8	82/82 (100%)	76 (93%)	6 (7%)	14	43
44	A5	90/92 (98%)	84 (93%)	6 (7%)	16	47
44	E8	90/92 (98%)	84 (93%)	6 (7%)	16	47
45	B5	74/78 (95%)	72 (97%)	2 (3%)	44	73
45	F8	74/78 (95%)	70 (95%)	4 (5%)	22	55
46	C5	85/91 (93%)	72 (85%)	13 (15%)	2	12
46	G8	84/91 (92%)	79 (94%)	5 (6%)	19	51
47	D5	118/179 (66%)	107 (91%)	11 (9%)	9	31
47	H8	137/179 (76%)	133 (97%)	4 (3%)	42	72
48	E5	62/67 (92%)	56 (90%)	6 (10%)	8	29
48	I8	61/67 (91%)	58 (95%)	3 (5%)	25	59
49	F5	79/83 (95%)	76 (96%)	3 (4%)	33	65
49	J8	79/83 (95%)	75 (95%)	4 (5%)	24	56
50	G5	62/67 (92%)	60 (97%)	2 (3%)	39	70
50	K8	62/67 (92%)	56 (90%)	6 (10%)	8	29
51	H5	50/52 (96%)	44 (88%)	6 (12%)	5	21
51	L8	50/52 (96%)	48 (96%)	2 (4%)	31	64
52	M8	42/63 (67%)	40 (95%)	2 (5%)	25	59
53	J5	48/52 (92%)	44 (92%)	4 (8%)	11	37
53	N8	43/52 (83%)	38 (88%)	5 (12%)	5	22
54	L5	38/42 (90%)	32 (84%)	6 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	P8	38/42 (90%)	38 (100%)	0	100	100
55	M5	54/55 (98%)	49 (91%)	5 (9%)	9	31
55	Q8	54/55 (98%)	49 (91%)	5 (9%)	9	31
All	All	9127/10012 (91%)	8510 (93%)	617 (7%)	16	46

5 of 617 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	49	116	ASP
46	C5	99	CYS
34	69	25	TYR
32	49	113	ARG
40	65	12	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
40	65	38	GLN
50	G5	9	GLN
50	G5	56	GLN
47	H8	85	HIS
44	E8	34	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1488/1522 (97%)	386 (25%)	35 (2%)
1	1G	1492/1522 (98%)	427 (28%)	39 (2%)
22	1K	64/76 (84%)	41 (64%)	2 (3%)
23	2K	76/77 (98%)	23 (30%)	2 (2%)
23	2L	76/77 (98%)	21 (27%)	2 (2%)
24	3K	75/76 (98%)	40 (53%)	4 (5%)
25	4K	18/27 (66%)	9 (50%)	2 (11%)
25	4L	16/27 (59%)	9 (56%)	1 (6%)
26	14	2852/2912 (97%)	788 (27%)	58 (2%)
26	1H	2824/2912 (96%)	736 (26%)	78 (2%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	40 (56%)	5 (7%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	3L	75/76 (98%)	40 (53%)	1 (1%)
All	All	9369/9624 (97%)	2628 (28%)	232 (2%)

5 of 2628 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2481	G
26	14	2611	U
1	1G	889	A
26	14	2447	G
26	14	1420	U

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

19 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	$\#\|Z\| > 2$
22	PSU	1K	39	22	18,21,22	1.11	2 (11%)	22,30,33	1.78	5 (22%)
22	PSU	1K	55	22	18,21,22	1.23	1 (5%)	22,30,33	1.83	4 (18%)
22	U8U	1K	34	25,22	19,24,25	2.66	6 (31%)	23,34,37	1.52	4 (17%)
23	G7M	2K	47	23	20,26,27	2.46	6 (30%)	17,39,42	1.21	2 (11%)
23	5MU	2L	55	23	19,22,23	4.07	5 (26%)	28,32,35	3.14	11 (39%)
23	G7M	2L	47	23	20,26,27	2.29	7 (35%)	17,39,42	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PSU	1L	39	56	18,21,22	1.11	2 (11%)	22,30,33	1.50	4 (18%)
22	T6A	1K	37	22	27,34,35	2.84	9 (33%)	29,49,52	3.63	10 (34%)
23	PSU	2L	56	23	18,21,22	1.28	2 (11%)	22,30,33	1.83	4 (18%)
22	5MU	1K	54	22	19,22,23	3.95	5 (26%)	28,32,35	2.86	9 (32%)
56	5MU	1L	54	56	19,22,23	3.81	5 (26%)	28,32,35	3.23	11 (39%)
23	4SU	2L	8	23	18,21,22	1.87	4 (22%)	26,30,33	2.83	7 (26%)
23	PSU	2K	56	23	18,21,22	1.37	2 (11%)	22,30,33	2.43	5 (22%)
23	OMC	2K	33	23	19,22,23	1.67	3 (15%)	26,31,34	1.39	3 (11%)
56	PSU	1L	55	56	18,21,22	1.32	1 (5%)	22,30,33	1.82	4 (18%)
23	5MU	2K	55	23	19,22,23	3.95	5 (26%)	28,32,35	3.43	9 (32%)
57	PSU	3L	39	57	18,21,22	1.11	1 (5%)	22,30,33	1.53	3 (13%)
23	4SU	2K	8	23	18,21,22	1.84	3 (16%)	26,30,33	2.38	7 (26%)
23	OMC	2L	33	23	19,22,23	1.96	3 (15%)	26,31,34	1.56	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
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	4/9/28/29	0/2/2/2
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
23	5MU	2L	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	-	2/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/19/41/42	0/3/3/3
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	2/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	3/9/27/28	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	2/7/25/26	0/2/2/2
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2L	33	23	-	2/9/27/28	0/2/2/2

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	13.10	1.59	1.38
23	2K	55	5MU	C2-N1	12.95	1.59	1.38
22	1K	54	5MU	C2-N1	12.38	1.58	1.38
56	1L	54	5MU	C2-N1	11.97	1.57	1.38
22	1K	37	T6A	C10-N11	7.71	1.52	1.35

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1L	54	5MU	C5-C4-N3	10.94	124.65	115.31
22	1K	37	T6A	N3-C2-N1	-9.86	113.27	128.68
23	2K	55	5MU	C5-C4-N3	9.59	123.50	115.31
22	1K	54	5MU	C5-C4-N3	9.15	123.12	115.31
23	2L	8	4SU	C4-N3-C2	-9.09	118.50	127.34

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	N-C-C5-C4
22	1K	34	U8U	N-C-C5-C6
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2L	47	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	55	PSU	1	0
22	1K	34	U8U	3	0
23	2K	47	G7M	2	0
23	2L	55	5MU	4	0
23	2L	47	G7M	3	0
22	1K	37	T6A	1	0
22	1K	54	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1L	54	5MU	2	0
23	2L	8	4SU	1	0
23	2K	33	OMC	3	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1188 ligands modelled in this entry, 1186 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	302	4	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	302	4	-	-	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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	302	SF4	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1
37	35	1
38	45	1
5	4E	1
38	88	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3’	25:A	P	4.44
1	35	121:LYS	C	122:PRO	N	1.77
1	45	124:LYS	C	125:LEU	N	1.15
1	4E	69:VAL	C	70:PRO	N	1.12
1	88	124:LYS	C	125:LEU	N	1.12

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	1493/1522 (98%)	-0.64	0 100 100	83, 129, 202, 287	0
1	1G	1496/1522 (98%)	-0.44	11 (0%) 87 81	100, 152, 223, 279	0
2	12	206/256 (80%)	0.24	28 (13%) 3 2	173, 206, 218, 228	0
2	1E	231/256 (90%)	0.85	46 (19%) 1 0	140, 173, 197, 207	0
3	22	194/239 (81%)	1.00	44 (22%) 0 0	172, 196, 209, 214	0
3	2E	205/239 (85%)	0.59	27 (13%) 3 2	115, 136, 165, 176	0
4	32	208/209 (99%)	1.17	55 (26%) 0 0	129, 152, 173, 183	0
4	3E	207/209 (99%)	0.77	46 (22%) 0 0	104, 131, 154, 164	0
5	42	149/162 (91%)	0.15	6 (4%) 38 23	138, 160, 177, 190	0
5	4E	149/162 (91%)	-0.19	0 100 100	104, 125, 147, 155	0
6	52	101/101 (100%)	0.21	5 (4%) 28 15	119, 135, 156, 163	0
6	5E	100/101 (99%)	3.74	77 (77%) 0 0	103, 129, 149, 159	0
7	62	138/156 (88%)	0.04	12 (8%) 10 5	150, 164, 173, 181	0
7	6E	151/156 (96%)	-0.83	0 100 100	134, 150, 170, 179	0
8	72	137/138 (99%)	-0.74	0 100 100	136, 164, 180, 190	0
8	7E	138/138 (100%)	-0.47	1 (0%) 87 81	112, 138, 152, 161	0
9	82	105/128 (82%)	0.72	19 (18%) 1 1	149, 196, 209, 221	0
9	8E	126/128 (98%)	-0.64	1 (0%) 86 78	111, 170, 192, 200	0
10	1A	60/105 (57%)	1.66	17 (28%) 0 0	166, 193, 204, 205	0
10	1I	72/105 (68%)	0.12	3 (4%) 36 21	112, 150, 193, 204	0
11	2A	113/129 (87%)	-0.40	0 100 100	118, 143, 157, 167	0
11	2I	111/129 (86%)	1.72	43 (38%) 0 0	102, 136, 151, 164	0
12	3A	121/132 (91%)	1.11	34 (28%) 0 0	119, 142, 165, 179	0
12	3I	122/132 (92%)	0.14	2 (1%) 72 59	91, 102, 126, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	1.08	27 (24%) 0 0	162, 187, 202, 212	0
13	4I	119/126 (94%)	-0.36	1 (0%) 86 78	111, 146, 162, 173	0
14	5A	48/61 (78%)	2.62	25 (52%) 0 0	170, 191, 208, 218	0
14	5I	60/61 (98%)	0.65	6 (10%) 7 4	107, 124, 141, 155	0
15	6A	87/89 (97%)	-0.17	2 (2%) 60 46	123, 148, 167, 174	0
15	6I	87/89 (97%)	1.61	28 (32%) 0 0	106, 127, 148, 153	0
16	7A	84/88 (95%)	-0.32	0 100 100	120, 139, 161, 184	0
16	7I	80/88 (90%)	0.56	10 (12%) 3 2	127, 140, 169, 180	0
17	8A	99/105 (94%)	-0.81	0 100 100	121, 143, 156, 159	0
17	8I	100/105 (95%)	2.24	51 (51%) 0 0	117, 136, 148, 154	0
18	9A	67/88 (76%)	0.12	2 (2%) 50 33	128, 145, 163, 171	0
18	9I	67/88 (76%)	2.73	40 (59%) 0 0	115, 134, 159, 164	0
19	AA	36/93 (38%)	-0.13	2 (5%) 24 12	191, 209, 217, 223	0
19	AI	81/93 (87%)	1.21	24 (29%) 0 0	125, 148, 173, 183	0
20	BA	98/106 (92%)	0.53	12 (12%) 4 2	107, 139, 163, 176	0
20	BI	97/106 (91%)	-0.13	5 (5%) 27 14	135, 152, 181, 193	0
21	1B	23/27 (85%)	3.95	21 (91%) 0 0	157, 179, 187, 189	0
21	1F	23/27 (85%)	-0.90	0 100 100	119, 134, 143, 145	0
22	1K	64/76 (84%)	0.39	7 (10%) 5 3	112, 226, 251, 253	0
23	2K	72/77 (93%)	-0.38	1 (1%) 75 63	94, 125, 153, 169	0
23	2L	72/77 (93%)	0.10	3 (4%) 36 21	100, 151, 178, 198	0
24	3K	76/76 (100%)	-0.22	3 (3%) 39 24	96, 189, 207, 218	0
25	4K	20/27 (74%)	0.12	1 (5%) 28 15	96, 156, 196, 199	0
25	4L	17/27 (62%)	0.43	1 (5%) 22 12	131, 170, 208, 211	0
26	14	2861/2912 (98%)	-0.35	25 (0%) 84 75	72, 111, 235, 276	0
26	1H	2830/2912 (97%)	-0.37	25 (0%) 84 75	65, 97, 204, 287	0
27	16	122/122 (100%)	-0.17	3 (2%) 57 42	92, 117, 143, 228	0
27	1J	122/122 (100%)	-0.74	0 100 100	117, 155, 179, 225	0
28	71	135/229 (58%)	1.87	56 (41%) 0 0	149, 167, 190, 202	0
29	11	273/276 (98%)	0.09	8 (2%) 51 35	65, 90, 111, 122	0
29	19	273/276 (98%)	0.92	45 (16%) 1 1	74, 100, 121, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
30	21	203/206 (98%)	0.50	19 (9%) 8 4	73, 112, 157, 172	0
30	29	203/206 (98%)	1.06	47 (23%) 0 0	79, 116, 162, 178	0
31	31	202/210 (96%)	0.17	8 (3%) 38 23	70, 102, 136, 155	0
31	39	204/210 (97%)	-0.30	0 100 100	83, 128, 181, 201	0
32	41	179/182 (98%)	0.49	20 (11%) 5 3	107, 128, 164, 174	0
32	49	179/182 (98%)	0.64	24 (13%) 3 2	151, 171, 195, 204	0
33	51	171/180 (95%)	0.31	23 (13%) 3 2	102, 128, 146, 157	0
33	59	69/180 (38%)	0.77	12 (17%) 1 1	170, 198, 213, 220	0
34	61	145/148 (97%)	1.26	42 (28%) 0 0	102, 163, 188, 199	0
34	69	145/148 (97%)	1.05	37 (25%) 0 0	111, 152, 176, 189	0
35	15	137/140 (97%)	1.44	44 (32%) 0 0	106, 134, 162, 179	0
35	58	138/140 (98%)	-0.27	1 (0%) 87 81	86, 112, 154, 172	0
36	25	122/122 (100%)	0.44	4 (3%) 46 29	92, 113, 132, 142	0
36	68	122/122 (100%)	-0.18	0 100 100	81, 98, 118, 131	0
37	35	148/150 (98%)	1.18	40 (27%) 0 0	84, 135, 174, 190	0
37	78	147/150 (98%)	0.45	22 (14%) 2 1	72, 104, 136, 144	0
38	45	138/141 (97%)	0.21	10 (7%) 15 8	99, 131, 151, 168	0
38	88	141/141 (100%)	1.78	65 (46%) 0 0	76, 101, 123, 153	0
39	55	118/118 (100%)	0.59	9 (7%) 13 7	87, 102, 118, 138	0
39	98	118/118 (100%)	2.89	74 (62%) 0 0	87, 109, 131, 147	0
40	65	110/112 (98%)	0.58	11 (10%) 7 4	116, 145, 164, 172	0
40	A8	111/112 (99%)	2.30	57 (51%) 0 0	93, 112, 135, 144	0
41	75	136/146 (93%)	-0.40	4 (2%) 51 35	102, 120, 169, 198	0
41	B8	135/146 (92%)	-0.49	1 (0%) 87 81	92, 116, 166, 185	0
42	85	116/118 (98%)	1.01	21 (18%) 1 1	90, 121, 154, 166	0
42	C8	115/118 (97%)	-0.12	2 (1%) 70 57	77, 102, 130, 141	0
43	95	99/101 (98%)	1.95	49 (49%) 0 0	91, 152, 166, 174	0
43	D8	101/101 (100%)	1.67	37 (36%) 0 0	78, 124, 149, 160	0
44	A5	110/113 (97%)	-0.37	0 100 100	84, 96, 127, 133	0
44	E8	110/113 (97%)	0.03	2 (1%) 68 55	79, 95, 125, 140	0
45	B5	94/96 (97%)	0.77	14 (14%) 2 1	94, 110, 134, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
45	F8	95/96 (98%)	2.16	49 (51%)	0	0	78, 93, 120, 133	0
46	C5	105/110 (95%)	1.16	23 (21%)	0	0	110, 143, 175, 185	0
46	G8	104/110 (94%)	-0.66	0	100	100	88, 116, 148, 161	0
47	D5	130/206 (63%)	1.18	36 (27%)	0	0	138, 163, 188, 194	0
47	H8	148/206 (71%)	2.00	69 (46%)	0	0	106, 140, 195, 207	0
48	E5	78/85 (91%)	0.60	5 (6%)	19	10	99, 116, 136, 149	0
48	I8	76/85 (89%)	1.40	21 (27%)	0	0	79, 95, 111, 130	0
49	F5	94/98 (95%)	0.72	11 (11%)	4	2	86, 109, 144, 159	0
49	J8	94/98 (95%)	0.40	8 (8%)	10	5	79, 96, 143, 153	0
50	G5	67/72 (93%)	0.23	3 (4%)	33	19	113, 134, 152, 171	0
50	K8	68/72 (94%)	1.05	12 (17%)	1	1	82, 105, 124, 151	0
51	H5	58/60 (96%)	3.97	53 (91%)	0	0	103, 128, 155, 180	0
51	L8	58/60 (96%)	0.96	10 (17%)	1	1	83, 104, 140, 152	0
52	M8	47/71 (66%)	0.58	5 (10%)	6	3	131, 172, 183, 188	0
53	J5	56/60 (93%)	-0.18	5 (8%)	9	5	82, 108, 155, 165	0
53	N8	48/60 (80%)	0.59	7 (14%)	2	1	72, 108, 153, 164	0
54	L5	45/49 (91%)	0.55	5 (11%)	5	3	75, 83, 95, 107	0
54	P8	47/49 (95%)	-0.22	0	100	100	68, 74, 98, 108	0
55	M5	64/65 (98%)	1.41	17 (26%)	0	0	90, 105, 123, 143	0
55	Q8	64/65 (98%)	0.18	1 (1%)	72	59	80, 91, 108, 123	0
56	1L	71/76 (93%)	1.63	21 (29%)	0	0	140, 257, 274, 277	0
57	3L	75/76 (98%)	-0.09	2 (2%)	54	38	107, 259, 277, 285	0
All	All	20395/21728 (93%)	0.17	1973 (9%)	7	4	65, 127, 204, 287	0

The worst 5 of 1973 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	71	1	PRO	15.3
43	D8	101	GLY	10.4
10	1A	59	SER	10.3
21	1B	14	TRP	9.7
32	49	137	GLU	9.6

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
22	PSU	1K	55	20/21	0.86	0.16	143,175,183,183	0
23	PSU	2L	56	20/21	0.87	0.15	143,152,158,162	0
56	PSU	1L	55	20/21	0.88	0.12	176,201,207,207	0
23	4SU	2L	8	20/21	0.88	0.16	131,155,165,169	0
22	5MU	1K	54	21/22	0.88	0.21	155,171,185,188	0
22	T6A	1K	37	32/33	0.89	0.25	100,113,152,156	0
56	PSU	1L	39	20/21	0.90	0.31	155,179,185,187	0
23	5MU	2L	55	21/22	0.91	0.15	146,159,164,166	0
23	G7M	2L	47	24/25	0.92	0.13	161,169,178,179	0
23	4SU	2K	8	20/21	0.92	0.15	111,120,124,128	0
56	5MU	1L	54	21/22	0.92	0.17	184,194,212,217	0
23	OMC	2L	33	21/22	0.93	0.23	132,140,144,151	0
57	PSU	3L	39	20/21	0.93	0.12	160,164,169,170	0
23	PSU	2K	56	20/21	0.94	0.12	122,127,139,140	0
23	5MU	2K	55	21/22	0.94	0.15	122,135,144,159	0
23	G7M	2K	47	24/25	0.95	0.10	124,132,139,146	0
22	PSU	1K	39	20/21	0.95	0.17	98,124,139,139	0
23	OMC	2K	33	21/22	0.96	0.12	95,105,111,117	0
22	U8U	1K	34	23/24	0.96	0.12	116,123,130,131	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	1H	3033	1/1	0.15	0.55	109,109,109,109	0
58	MG	13	1705	1/1	0.17	0.30	150,150,150,150	0
58	MG	1H	3331	1/1	0.23	0.23	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	5E	201	1/1	0.25	0.83	107,107,107,107	0
58	MG	1H	3313	1/1	0.32	0.68	114,114,114,114	0
58	MG	29	303	1/1	0.33	0.24	106,106,106,106	0
58	MG	1H	3340	1/1	0.35	0.60	101,101,101,101	0
58	MG	1H	3155	1/1	0.36	0.21	86,86,86,86	0
58	MG	13	1627	1/1	0.37	0.42	105,105,105,105	0
58	MG	2K	102	1/1	0.37	0.63	109,109,109,109	0
58	MG	14	3028	1/1	0.39	0.41	124,124,124,124	0
58	MG	14	3319	1/1	0.39	0.17	128,128,128,128	0
58	MG	1H	3262	1/1	0.39	0.26	100,100,100,100	0
58	MG	1H	3316	1/1	0.40	0.38	91,91,91,91	0
58	MG	1H	3264	1/1	0.42	0.24	122,122,122,122	0
58	MG	1G	1645	1/1	0.43	0.56	122,122,122,122	0
58	MG	1G	1628	1/1	0.44	0.40	120,120,120,120	0
58	MG	1H	3146	1/1	0.46	0.46	103,103,103,103	0
58	MG	1H	3256	1/1	0.47	0.39	104,104,104,104	0
58	MG	1G	1640	1/1	0.47	0.42	115,115,115,115	0
58	MG	32	301	1/1	0.48	0.61	128,128,128,128	0
58	MG	13	1625	1/1	0.48	0.55	102,102,102,102	0
58	MG	14	3234	1/1	0.49	0.49	85,85,85,85	0
58	MG	14	3263	1/1	0.49	0.49	102,102,102,102	0
58	MG	13	1703	1/1	0.49	0.37	128,128,128,128	0
58	MG	14	3227	1/1	0.49	1.17	104,104,104,104	0
58	MG	1H	3317	1/1	0.50	0.45	106,106,106,106	0
58	MG	1H	3350	1/1	0.51	0.61	113,113,113,113	0
58	MG	1H	3176	1/1	0.51	0.29	110,110,110,110	0
58	MG	14	3279	1/1	0.51	0.59	103,103,103,103	0
58	MG	14	3150	1/1	0.51	0.86	102,102,102,102	0
58	MG	1G	1668	1/1	0.51	0.27	138,138,138,138	0
58	MG	13	1680	1/1	0.52	0.59	125,125,125,125	0
58	MG	13	1689	1/1	0.52	0.24	182,182,182,182	0
58	MG	1H	3285	1/1	0.53	0.23	115,115,115,115	0
58	MG	1H	3036	1/1	0.54	0.15	118,118,118,118	0
58	MG	14	3303	1/1	0.55	0.54	115,115,115,115	0
58	MG	13	1603	1/1	0.55	0.40	102,102,102,102	0
58	MG	1H	3032	1/1	0.55	0.35	110,110,110,110	0
58	MG	14	3299	1/1	0.56	0.36	118,118,118,118	0
58	MG	1G	1641	1/1	0.56	0.18	131,131,131,131	0
58	MG	16	203	1/1	0.56	0.16	112,112,112,112	0
58	MG	14	3417	1/1	0.56	0.08	140,140,140,140	0
58	MG	14	3026	1/1	0.56	0.36	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3295	1/1	0.57	0.77	96,96,96,96	0
58	MG	1H	3347	1/1	0.57	0.18	102,102,102,102	0
58	MG	14	3301	1/1	0.58	0.17	115,115,115,115	0
58	MG	13	1678	1/1	0.58	0.19	121,121,121,121	0
58	MG	13	1687	1/1	0.58	1.49	100,100,100,100	0
58	MG	14	3296	1/1	0.58	0.32	110,110,110,110	0
58	MG	14	3179	1/1	0.58	0.45	102,102,102,102	0
58	MG	1H	3199	1/1	0.59	0.69	87,87,87,87	0
58	MG	1H	3276	1/1	0.59	0.28	91,91,91,91	0
58	MG	14	3316	1/1	0.59	0.29	111,111,111,111	0
58	MG	14	3062	1/1	0.60	0.56	129,129,129,129	0
58	MG	1G	1621	1/1	0.60	0.76	110,110,110,110	0
58	MG	1H	3322	1/1	0.60	0.30	121,121,121,121	0
58	MG	1H	3105	1/1	0.60	0.90	86,86,86,86	0
58	MG	14	3267	1/1	0.61	0.59	104,104,104,104	0
58	MG	14	3324	1/1	0.61	0.27	104,104,104,104	0
58	MG	14	3277	1/1	0.62	0.50	111,111,111,111	0
58	MG	1H	3263	1/1	0.62	0.68	92,92,92,92	0
58	MG	13	1688	1/1	0.62	0.51	96,96,96,96	0
58	MG	2K	103	1/1	0.62	0.21	134,134,134,134	0
58	MG	14	3171	1/1	0.62	0.95	91,91,91,91	0
58	MG	14	3174	1/1	0.62	0.38	98,98,98,98	0
58	MG	85	202	1/1	0.62	0.65	100,100,100,100	0
58	MG	1G	1643	1/1	0.63	0.57	102,102,102,102	0
58	MG	1H	3337	1/1	0.63	0.52	140,140,140,140	0
58	MG	14	3024	1/1	0.63	1.13	106,106,106,106	0
58	MG	13	1702	1/1	0.64	0.45	114,114,114,114	0
58	MG	1G	1602	1/1	0.64	0.75	133,133,133,133	0
58	MG	1H	3341	1/1	0.64	0.61	110,110,110,110	0
58	MG	14	3233	1/1	0.64	0.63	108,108,108,108	0
58	MG	1H	3351	1/1	0.64	0.33	122,122,122,122	0
58	MG	1H	3187	1/1	0.65	0.53	105,105,105,105	0
58	MG	1H	3336	1/1	0.65	0.12	93,93,93,93	0
58	MG	13	1634	1/1	0.65	0.52	104,104,104,104	0
58	MG	1H	3338	1/1	0.65	0.21	112,112,112,112	0
58	MG	14	3030	1/1	0.65	0.34	104,104,104,104	0
58	MG	1H	3286	1/1	0.65	0.42	109,109,109,109	0
58	MG	1H	3289	1/1	0.65	1.02	86,86,86,86	0
58	MG	14	3260	1/1	0.66	1.01	115,115,115,115	0
58	MG	1G	1644	1/1	0.66	0.70	110,110,110,110	0
58	MG	1H	3332	1/1	0.66	0.81	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	13	1708	1/1	0.66	0.82	102,102,102,102	0
58	MG	14	3183	1/1	0.66	0.34	89,89,89,89	0
58	MG	13	1650	1/1	0.66	0.30	134,134,134,134	0
58	MG	14	3110	1/1	0.66	0.33	94,94,94,94	0
58	MG	1H	3288	1/1	0.66	0.31	99,99,99,99	0
58	MG	14	3059	1/1	0.67	0.17	92,92,92,92	0
58	MG	13	1606	1/1	0.67	1.05	119,119,119,119	0
58	MG	13	1699	1/1	0.67	0.49	97,97,97,97	0
58	MG	1G	1632	1/1	0.68	0.40	130,130,130,130	0
58	MG	1G	1647	1/1	0.68	0.27	101,101,101,101	0
58	MG	1G	1635	1/1	0.68	0.81	111,111,111,111	0
58	MG	16	207	1/1	0.68	0.27	92,92,92,92	0
58	MG	1H	3323	1/1	0.68	0.31	122,122,122,122	0
58	MG	1H	3269	1/1	0.68	0.71	99,99,99,99	0
58	MG	1H	3126	1/1	0.68	0.26	83,83,83,83	0
58	MG	C5	201	1/1	0.68	0.35	137,137,137,137	0
58	MG	1H	3128	1/1	0.69	0.42	90,90,90,90	0
58	MG	16	208	1/1	0.69	0.43	111,111,111,111	0
58	MG	14	3192	1/1	0.69	0.44	104,104,104,104	0
58	MG	14	3201	1/1	0.69	0.49	91,91,91,91	0
58	MG	1H	3297	1/1	0.69	0.21	133,133,133,133	0
58	MG	13	1621	1/1	0.69	0.33	99,99,99,99	0
58	MG	14	3315	1/1	0.69	0.49	114,114,114,114	0
58	MG	13	1679	1/1	0.69	0.25	122,122,122,122	0
58	MG	14	3235	1/1	0.69	0.36	102,102,102,102	0
58	MG	1H	3030	1/1	0.69	0.67	85,85,85,85	0
58	MG	14	3261	1/1	0.69	0.43	101,101,101,101	0
58	MG	13	1659	1/1	0.69	0.27	116,116,116,116	0
58	MG	45	203	1/1	0.69	0.78	104,104,104,104	0
58	MG	1G	1636	1/1	0.69	0.34	111,111,111,111	0
58	MG	1G	1639	1/1	0.69	0.81	93,93,93,93	0
58	MG	1H	3327	1/1	0.70	0.76	120,120,120,120	0
58	MG	1H	3144	1/1	0.70	0.27	89,89,89,89	0
58	MG	1H	3095	1/1	0.70	0.87	95,95,95,95	0
58	MG	13	1684	1/1	0.70	0.26	141,141,141,141	0
58	MG	1H	3230	1/1	0.70	0.12	104,104,104,104	0
58	MG	1H	3163	1/1	0.70	0.49	84,84,84,84	0
58	MG	1H	3257	1/1	0.70	1.55	97,97,97,97	0
58	MG	1H	3175	1/1	0.70	0.15	92,92,92,92	0
58	MG	14	3182	1/1	0.70	0.21	105,105,105,105	0
58	MG	14	3034	1/1	0.71	0.29	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3272	1/1	0.71	0.48	96,96,96,96	0
58	MG	1J	202	1/1	0.71	0.33	110,110,110,110	0
58	MG	13	1673	1/1	0.71	0.40	106,106,106,106	0
58	MG	45	202	1/1	0.71	0.15	122,122,122,122	0
58	MG	14	3023	1/1	0.71	0.47	103,103,103,103	0
58	MG	14	3089	1/1	0.71	1.15	104,104,104,104	0
58	MG	1H	3206	1/1	0.71	0.58	100,100,100,100	0
58	MG	1G	1652	1/1	0.72	0.31	110,110,110,110	0
58	MG	14	3321	1/1	0.72	0.43	109,109,109,109	0
58	MG	14	3284	1/1	0.72	0.67	112,112,112,112	0
58	MG	1G	1666	1/1	0.72	0.77	121,121,121,121	0
58	MG	1H	3212	1/1	0.72	0.40	93,93,93,93	0
58	MG	1H	3272	1/1	0.72	0.63	118,118,118,118	0
58	MG	1H	3166	1/1	0.72	0.42	95,95,95,95	0
58	MG	1H	3303	1/1	0.72	0.24	102,102,102,102	0
58	MG	1H	3235	1/1	0.72	0.68	112,112,112,112	0
58	MG	13	1649	1/1	0.72	0.15	118,118,118,118	0
58	MG	14	3404	1/1	0.73	0.29	101,101,101,101	0
58	MG	1G	1633	1/1	0.73	0.25	137,137,137,137	0
58	MG	1H	3292	1/1	0.73	0.28	82,82,82,82	0
58	MG	14	3194	1/1	0.73	0.30	93,93,93,93	0
58	MG	1G	1660	1/1	0.73	0.93	111,111,111,111	0
58	MG	14	3262	1/1	0.73	0.16	109,109,109,109	0
58	MG	13	1707	1/1	0.73	0.43	114,114,114,114	0
58	MG	14	3132	1/1	0.73	0.69	86,86,86,86	0
58	MG	14	3217	1/1	0.74	0.74	89,89,89,89	0
58	MG	13	1644	1/1	0.74	0.38	120,120,120,120	0
58	MG	1H	3141	1/1	0.74	0.93	83,83,83,83	0
58	MG	1G	1662	1/1	0.74	0.14	118,118,118,118	0
58	MG	14	3108	1/1	0.74	0.35	88,88,88,88	0
58	MG	14	3195	1/1	0.74	0.54	107,107,107,107	0
58	MG	14	3196	1/1	0.74	0.29	98,98,98,98	0
58	MG	13	1628	1/1	0.74	0.68	94,94,94,94	0
58	MG	13	1653	1/1	0.75	0.29	144,144,144,144	0
58	MG	1G	1648	1/1	0.75	0.40	128,128,128,128	0
58	MG	1H	3054	1/1	0.75	0.13	110,110,110,110	0
58	MG	13	1661	1/1	0.75	0.50	90,90,90,90	0
58	MG	14	3310	1/1	0.75	0.38	124,124,124,124	0
58	MG	1H	3483	1/1	0.75	0.11	119,119,119,119	0
58	MG	1H	3343	1/1	0.75	0.12	137,137,137,137	0
58	MG	14	3286	1/1	0.75	0.63	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3109	1/1	0.75	0.57	94,94,94,94	0
58	MG	E5	101	1/1	0.75	0.66	100,100,100,100	0
58	MG	13	1623	1/1	0.76	0.72	88,88,88,88	0
58	MG	14	3149	1/1	0.76	0.58	94,94,94,94	0
58	MG	14	3275	1/1	0.76	0.47	90,90,90,90	0
58	MG	1H	3209	1/1	0.76	0.53	99,99,99,99	0
58	MG	14	3224	1/1	0.76	0.35	105,105,105,105	0
58	MG	14	3280	1/1	0.76	0.61	98,98,98,98	0
58	MG	1H	3319	1/1	0.76	0.62	102,102,102,102	0
58	MG	1H	3140	1/1	0.76	0.29	89,89,89,89	0
58	MG	5E	202	1/1	0.76	0.18	111,111,111,111	0
58	MG	13	1692	1/1	0.76	0.41	99,99,99,99	0
58	MG	1H	3330	1/1	0.76	0.14	105,105,105,105	0
58	MG	14	3018	1/1	0.76	0.39	111,111,111,111	0
58	MG	1H	3304	1/1	0.76	0.49	94,94,94,94	0
58	MG	1H	3287	1/1	0.76	0.31	96,96,96,96	0
58	MG	14	3278	1/1	0.77	0.45	86,86,86,86	0
58	MG	1H	3243	1/1	0.77	0.09	96,96,96,96	0
58	MG	14	3246	1/1	0.77	0.36	95,95,95,95	0
58	MG	1H	3334	1/1	0.77	0.29	77,77,77,77	0
58	MG	13	1674	1/1	0.77	0.27	121,121,121,121	0
58	MG	14	3288	1/1	0.77	0.79	120,120,120,120	0
58	MG	1H	3479	1/1	0.77	0.20	91,91,91,91	0
58	MG	1H	3069	1/1	0.77	0.16	101,101,101,101	0
58	MG	1H	3486	1/1	0.77	0.31	106,106,106,106	0
58	MG	14	3231	1/1	0.77	0.79	107,107,107,107	0
58	MG	14	3302	1/1	0.77	0.81	95,95,95,95	0
58	MG	14	3031	1/1	0.77	0.47	89,89,89,89	0
58	MG	14	3308	1/1	0.77	0.54	104,104,104,104	0
58	MG	7A	101	1/1	0.77	0.23	104,104,104,104	0
58	MG	14	3199	1/1	0.78	0.61	91,91,91,91	0
58	MG	1H	3344	1/1	0.78	0.32	81,81,81,81	0
58	MG	1H	3031	1/1	0.78	0.71	115,115,115,115	0
58	MG	14	3331	1/1	0.78	0.52	108,108,108,108	0
58	MG	1H	3247	1/1	0.78	0.43	101,101,101,101	0
58	MG	1G	1638	1/1	0.78	0.43	102,102,102,102	0
58	MG	1H	3309	1/1	0.78	0.48	126,126,126,126	0
58	MG	1H	3270	1/1	0.78	0.25	87,87,87,87	0
58	MG	1H	3342	1/1	0.78	0.48	105,105,105,105	0
58	MG	1G	1631	1/1	0.78	0.40	97,97,97,97	0
58	MG	14	3240	1/1	0.78	0.21	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3192	1/1	0.78	0.45	85,85,85,85	0
58	MG	14	3259	1/1	0.78	0.54	111,111,111,111	0
58	MG	1G	1627	1/1	0.79	0.49	142,142,142,142	0
58	MG	14	3325	1/1	0.79	0.53	110,110,110,110	0
58	MG	14	3328	1/1	0.79	1.40	107,107,107,107	0
58	MG	1H	3333	1/1	0.79	0.34	93,93,93,93	0
58	MG	1H	3145	1/1	0.79	0.56	117,117,117,117	0
58	MG	1H	3077	1/1	0.79	0.46	65,65,65,65	0
58	MG	14	3146	1/1	0.79	0.35	77,77,77,77	0
58	MG	13	1710	1/1	0.79	0.33	118,118,118,118	0
58	MG	13	1704	1/1	0.79	0.08	134,134,134,134	0
58	MG	1G	1646	1/1	0.79	0.17	126,126,126,126	0
58	MG	1H	3196	1/1	0.79	0.45	102,102,102,102	0
58	MG	14	3175	1/1	0.79	0.19	93,93,93,93	0
58	MG	13	1660	1/1	0.79	0.12	104,104,104,104	0
58	MG	1H	3154	1/1	0.80	0.49	106,106,106,106	0
58	MG	1G	1653	1/1	0.80	0.14	118,118,118,118	0
58	MG	14	3140	1/1	0.80	0.09	79,79,79,79	0
58	MG	1H	3181	1/1	0.80	0.20	92,92,92,92	0
58	MG	1H	3186	1/1	0.80	0.39	96,96,96,96	0
58	MG	1G	1664	1/1	0.80	0.34	122,122,122,122	0
58	MG	14	3159	1/1	0.80	0.43	81,81,81,81	0
58	MG	13	1709	1/1	0.80	0.36	112,112,112,112	0
58	MG	14	3270	1/1	0.80	0.50	97,97,97,97	0
58	MG	1H	3076	1/1	0.80	0.36	78,78,78,78	0
58	MG	13	1641	1/1	0.80	0.14	112,112,112,112	0
58	MG	1H	3173	1/1	0.80	0.23	108,108,108,108	0
58	MG	14	3313	1/1	0.80	0.35	107,107,107,107	0
58	MG	1G	1637	1/1	0.80	0.42	101,101,101,101	0
58	MG	1H	3029	1/1	0.80	0.42	92,92,92,92	0
58	MG	1G	1618	1/1	0.81	0.13	131,131,131,131	0
58	MG	13	1686	1/1	0.81	0.17	79,79,79,79	0
58	MG	13	1637	1/1	0.81	0.43	123,123,123,123	0
58	MG	1H	3208	1/1	0.81	0.92	99,99,99,99	0
58	MG	14	3165	1/1	0.81	0.45	102,102,102,102	0
58	MG	14	3322	1/1	0.81	0.96	117,117,117,117	0
58	MG	14	3058	1/1	0.81	0.26	107,107,107,107	0
58	MG	1H	3039	1/1	0.81	0.54	100,100,100,100	0
58	MG	1G	1677	1/1	0.81	0.06	185,185,185,185	0
58	MG	14	3330	1/1	0.81	0.67	104,104,104,104	0
58	MG	14	3085	1/1	0.81	0.44	85,85,85,85	0
58	MG	14	3339	1/1	0.81	0.63	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1638	1/1	0.81	0.53	82,82,82,82	0
58	MG	1H	3109	1/1	0.81	0.70	102,102,102,102	0
58	MG	1H	3346	1/1	0.81	0.32	113,113,113,113	0
58	MG	1J	204	1/1	0.81	0.07	119,119,119,119	0
58	MG	1H	3012	1/1	0.81	0.40	93,93,93,93	0
58	MG	35	201	1/1	0.81	0.51	90,90,90,90	0
58	MG	41	201	1/1	0.81	0.10	102,102,102,102	0
58	MG	1H	3349	1/1	0.81	0.16	119,119,119,119	0
58	MG	14	3143	1/1	0.81	0.41	110,110,110,110	0
58	MG	14	3200	1/1	0.81	0.55	94,94,94,94	0
58	MG	14	3311	1/1	0.81	0.34	105,105,105,105	0
60	ZN	C5	202	1/1	0.81	0.13	183,183,183,183	0
58	MG	14	3082	1/1	0.82	0.34	92,92,92,92	0
58	MG	14	3155	1/1	0.82	0.35	101,101,101,101	0
58	MG	1H	3011	1/1	0.82	0.47	71,71,71,71	0
58	MG	14	3160	1/1	0.82	0.37	98,98,98,98	0
58	MG	1H	3295	1/1	0.82	0.53	110,110,110,110	0
58	MG	14	3266	1/1	0.82	0.47	99,99,99,99	0
58	MG	14	3202	1/1	0.82	0.33	79,79,79,79	0
58	MG	1H	3085	1/1	0.82	0.46	92,92,92,92	0
58	MG	13	1666	1/1	0.82	0.18	99,99,99,99	0
58	MG	1H	3251	1/1	0.82	0.13	75,75,75,75	0
58	MG	1H	3178	1/1	0.82	0.53	93,93,93,93	0
58	MG	13	1735	1/1	0.82	0.09	146,146,146,146	0
58	MG	1H	3142	1/1	0.82	0.45	89,89,89,89	0
58	MG	14	3185	1/1	0.82	0.71	113,113,113,113	0
58	MG	14	3282	1/1	0.82	0.33	96,96,96,96	0
58	MG	13	1698	1/1	0.82	0.46	96,96,96,96	0
58	MG	1H	3189	1/1	0.82	0.80	93,93,93,93	0
58	MG	1H	3134	1/1	0.83	0.23	103,103,103,103	0
58	MG	16	205	1/1	0.83	0.37	106,106,106,106	0
58	MG	1H	3123	1/1	0.83	0.09	85,85,85,85	0
58	MG	1H	3174	1/1	0.83	0.54	99,99,99,99	0
58	MG	14	3271	1/1	0.83	0.27	101,101,101,101	0
58	MG	1H	3016	1/1	0.83	0.44	105,105,105,105	0
58	MG	13	1612	1/1	0.83	0.36	108,108,108,108	0
58	MG	1H	3217	1/1	0.83	0.22	81,81,81,81	0
58	MG	14	3032	1/1	0.83	0.18	109,109,109,109	0
58	MG	1H	3279	1/1	0.83	0.30	106,106,106,106	0
58	MG	1G	1667	1/1	0.83	0.30	111,111,111,111	0
58	MG	14	3248	1/1	0.83	0.52	89,89,89,89	0
58	MG	1H	3468	1/1	0.83	0.15	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1H	3282	1/1	0.83	0.47	106,106,106,106	0
58	MG	1H	3328	1/1	0.83	0.46	119,119,119,119	0
58	MG	1H	3133	1/1	0.83	0.11	83,83,83,83	0
58	MG	1H	3250	1/1	0.84	0.13	94,94,94,94	0
58	MG	13	1690	1/1	0.84	0.69	113,113,113,113	0
58	MG	1H	3254	1/1	0.84	1.18	91,91,91,91	0
58	MG	1H	3202	1/1	0.84	0.33	95,95,95,95	0
58	MG	14	3257	1/1	0.84	0.16	143,143,143,143	0
58	MG	14	3168	1/1	0.84	0.29	122,122,122,122	0
58	MG	14	3314	1/1	0.84	1.12	99,99,99,99	0
58	MG	1H	3037	1/1	0.84	0.25	87,87,87,87	0
58	MG	1H	3261	1/1	0.84	0.52	115,115,115,115	0
58	MG	1H	3158	1/1	0.84	0.34	105,105,105,105	0
58	MG	1H	3162	1/1	0.84	0.39	106,106,106,106	0
58	MG	16	209	1/1	0.84	0.14	106,106,106,106	0
58	MG	1H	3211	1/1	0.84	0.54	90,90,90,90	0
58	MG	J8	101	1/1	0.84	0.29	89,89,89,89	0
58	MG	13	1738	1/1	0.84	0.05	106,106,106,106	0
58	MG	1H	3305	1/1	0.84	0.57	96,96,96,96	0
58	MG	13	1694	1/1	0.84	0.18	114,114,114,114	0
58	MG	14	3090	1/1	0.84	0.24	83,83,83,83	0
58	MG	14	3381	1/1	0.84	0.12	116,116,116,116	0
58	MG	1H	3311	1/1	0.84	0.18	77,77,77,77	0
58	MG	1H	3168	1/1	0.84	0.40	82,82,82,82	0
58	MG	1H	3275	1/1	0.84	0.12	83,83,83,83	0
58	MG	1H	3010	1/1	0.84	0.21	98,98,98,98	0
58	MG	14	3137	1/1	0.84	0.27	119,119,119,119	0
58	MG	1H	3108	1/1	0.84	0.73	92,92,92,92	0
58	MG	1H	3280	1/1	0.84	0.15	114,114,114,114	0
58	MG	1H	3198	1/1	0.84	0.35	119,119,119,119	0
58	MG	14	3232	1/1	0.84	0.41	89,89,89,89	0
58	MG	14	3297	1/1	0.84	0.55	91,91,91,91	0
58	MG	1H	3324	1/1	0.84	0.11	97,97,97,97	0
58	MG	14	3019	1/1	0.84	0.39	87,87,87,87	0
58	MG	14	3252	1/1	0.85	0.19	106,106,106,106	0
58	MG	14	3254	1/1	0.85	0.45	83,83,83,83	0
58	MG	13	1652	1/1	0.85	0.32	138,138,138,138	0
58	MG	14	3258	1/1	0.85	0.27	93,93,93,93	0
58	MG	14	3022	1/1	0.85	0.57	101,101,101,101	0
58	MG	1H	3226	1/1	0.85	0.32	88,88,88,88	0
58	MG	1G	1651	1/1	0.85	0.14	128,128,128,128	0
58	MG	14	3189	1/1	0.85	0.46	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	1H	3345	1/1	0.85	0.18	79,79,79,79	0
58	MG	1H	3315	1/1	0.85	0.22	99,99,99,99	0
58	MG	1H	3227	1/1	0.85	0.52	92,92,92,92	0
58	MG	1H	3117	1/1	0.85	0.30	75,75,75,75	0
58	MG	14	3148	1/1	0.85	0.40	94,94,94,94	0
58	MG	1H	3093	1/1	0.85	0.88	88,88,88,88	0
58	MG	1H	3302	1/1	0.85	0.42	89,89,89,89	0
58	MG	14	3276	1/1	0.85	0.10	130,130,130,130	0
58	MG	14	3154	1/1	0.85	0.17	84,84,84,84	0
58	MG	1G	1611	1/1	0.85	0.33	129,129,129,129	0
58	MG	14	3341	1/1	0.85	0.36	105,105,105,105	0
58	MG	14	3157	1/1	0.85	0.15	81,81,81,81	0
58	MG	1G	1614	1/1	0.85	0.26	127,127,127,127	0
58	MG	1G	1675	1/1	0.85	0.11	150,150,150,150	0
58	MG	1J	201	1/1	0.85	0.31	100,100,100,100	0
58	MG	14	3163	1/1	0.85	0.57	104,104,104,104	0
58	MG	1H	3075	1/1	0.85	0.93	82,82,82,82	0
58	MG	14	3084	1/1	0.85	0.48	92,92,92,92	0
58	MG	14	3291	1/1	0.85	0.26	96,96,96,96	0
58	MG	14	3292	1/1	0.85	0.99	83,83,83,83	0
58	MG	14	3169	1/1	0.85	0.42	69,69,69,69	0
58	MG	85	201	1/1	0.85	0.20	85,85,85,85	0
58	MG	1H	3161	1/1	0.85	0.46	115,115,115,115	0
58	MG	13	1739	1/1	0.85	0.17	113,113,113,113	0
58	MG	14	3247	1/1	0.85	0.90	104,104,104,104	0
58	MG	1H	3024	1/1	0.85	0.28	99,99,99,99	0
58	MG	1G	1612	1/1	0.86	0.36	105,105,105,105	0
58	MG	14	3178	1/1	0.86	0.25	94,94,94,94	0
58	MG	1H	3131	1/1	0.86	0.33	88,88,88,88	0
58	MG	14	3029	1/1	0.86	0.95	90,90,90,90	0
58	MG	14	3335	1/1	0.86	0.24	124,124,124,124	0
58	MG	1H	3185	1/1	0.86	0.22	68,68,68,68	0
58	MG	14	3101	1/1	0.86	0.27	108,108,108,108	0
58	MG	1H	3147	1/1	0.86	0.75	93,93,93,93	0
58	MG	13	1662	1/1	0.86	0.29	116,116,116,116	0
58	MG	13	1670	1/1	0.86	0.27	119,119,119,119	0
58	MG	14	3274	1/1	0.86	0.14	97,97,97,97	0
58	MG	14	3117	1/1	0.86	0.67	91,91,91,91	0
58	MG	1H	3312	1/1	0.86	0.38	103,103,103,103	0
58	MG	14	3197	1/1	0.86	0.51	124,124,124,124	0
58	MG	14	3250	1/1	0.86	0.47	79,79,79,79	0
58	MG	14	3251	1/1	0.86	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3299	1/1	0.86	0.31	94,94,94,94	0
58	MG	1G	1604	1/1	0.86	0.29	119,119,119,119	0
58	MG	14	3320	1/1	0.86	0.21	119,119,119,119	0
58	MG	14	3080	1/1	0.86	0.41	105,105,105,105	0
58	MG	1H	3035	1/1	0.86	0.64	123,123,123,123	0
58	MG	14	3208	1/1	0.86	0.21	93,93,93,93	0
58	MG	14	3020	1/1	0.87	0.31	93,93,93,93	0
58	MG	1H	3326	1/1	0.87	0.42	97,97,97,97	0
58	MG	14	3287	1/1	0.87	0.20	101,101,101,101	0
58	MG	1H	3278	1/1	0.87	0.41	90,90,90,90	0
58	MG	14	3166	1/1	0.87	0.58	79,79,79,79	0
58	MG	1H	3354	1/1	0.87	0.33	98,98,98,98	0
58	MG	14	3332	1/1	0.87	0.25	98,98,98,98	0
58	MG	14	3294	1/1	0.87	0.80	100,100,100,100	0
58	MG	14	3336	1/1	0.87	0.31	120,120,120,120	0
58	MG	1G	1658	1/1	0.87	0.75	99,99,99,99	0
58	MG	1H	3188	1/1	0.87	0.40	84,84,84,84	0
58	MG	14	3366	1/1	0.87	0.12	114,114,114,114	0
58	MG	1G	1661	1/1	0.87	0.06	169,169,169,169	0
58	MG	14	3264	1/1	0.87	0.51	106,106,106,106	0
58	MG	1H	3119	1/1	0.87	0.59	81,81,81,81	0
58	MG	14	3420	1/1	0.87	0.07	118,118,118,118	0
58	MG	1H	3290	1/1	0.87	0.51	103,103,103,103	0
58	MG	13	1734	1/1	0.87	0.08	131,131,131,131	0
58	MG	1H	3205	1/1	0.87	0.65	114,114,114,114	0
58	MG	14	3055	1/1	0.87	0.32	77,77,77,77	0
58	MG	1H	3169	1/1	0.87	0.21	95,95,95,95	0
58	MG	1G	1623	1/1	0.87	0.65	100,100,100,100	0
58	MG	16	206	1/1	0.87	0.06	89,89,89,89	0
58	MG	1H	3298	1/1	0.87	0.49	95,95,95,95	0
58	MG	1H	3348	1/1	0.87	0.36	111,111,111,111	0
58	MG	1H	3325	1/1	0.87	0.23	100,100,100,100	0
58	MG	1G	1650	1/1	0.87	0.32	98,98,98,98	0
58	MG	L5	101	1/1	0.87	0.89	96,96,96,96	0
58	MG	14	3253	1/1	0.87	0.27	90,90,90,90	0
58	MG	14	3207	1/1	0.88	0.15	107,107,107,107	0
58	MG	1H	3318	1/1	0.88	0.36	116,116,116,116	0
58	MG	14	3273	1/1	0.88	0.15	110,110,110,110	0
58	MG	14	3054	1/1	0.88	0.26	99,99,99,99	0
58	MG	1H	3232	1/1	0.88	0.44	98,98,98,98	0
58	MG	1H	3265	1/1	0.88	1.01	100,100,100,100	0
58	MG	1H	3267	1/1	0.88	0.48	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1693	1/1	0.88	0.54	108,108,108,108	0
58	MG	1H	3183	1/1	0.88	0.93	94,94,94,94	0
58	MG	Q8	101	1/1	0.88	0.39	89,89,89,89	0
58	MG	1H	3246	1/1	0.88	0.33	87,87,87,87	0
58	MG	14	3333	1/1	0.88	0.67	102,102,102,102	0
58	MG	14	3334	1/1	0.88	0.73	92,92,92,92	0
58	MG	14	3283	1/1	0.88	0.67	98,98,98,98	0
58	MG	1H	3124	1/1	0.88	0.42	77,77,77,77	0
58	MG	2L	102	1/1	0.88	1.72	95,95,95,95	0
58	MG	14	3004	1/1	0.88	0.70	76,76,76,76	0
58	MG	14	3342	1/1	0.88	0.35	120,120,120,120	0
58	MG	14	3177	1/1	0.88	0.53	87,87,87,87	0
58	MG	14	3013	1/1	0.88	0.20	98,98,98,98	0
58	MG	14	3382	1/1	0.88	0.14	112,112,112,112	0
58	MG	1H	3100	1/1	0.88	0.85	82,82,82,82	0
58	MG	14	3412	1/1	0.88	0.12	128,128,128,128	0
58	MG	1H	3027	1/1	0.88	0.17	95,95,95,95	0
58	MG	1H	3252	1/1	0.88	0.26	75,75,75,75	0
58	MG	14	3021	1/1	0.88	0.40	73,73,73,73	0
58	MG	14	3186	1/1	0.88	0.69	100,100,100,100	0
58	MG	1H	3129	1/1	0.88	0.60	85,85,85,85	0
58	MG	29	302	1/1	0.88	0.54	94,94,94,94	0
58	MG	13	1683	1/1	0.88	0.77	119,119,119,119	0
58	MG	1H	3472	1/1	0.88	0.08	108,108,108,108	0
58	MG	13	1668	1/1	0.88	0.22	117,117,117,117	0
58	MG	1H	3259	1/1	0.88	0.12	106,106,106,106	0
58	MG	14	3309	1/1	0.88	0.20	109,109,109,109	0
58	MG	13	1723	1/1	0.88	0.15	134,134,134,134	0
58	MG	1G	1659	1/1	0.88	0.31	142,142,142,142	0
58	MG	1H	3139	1/1	0.88	0.18	75,75,75,75	0
58	MG	14	3152	1/1	0.88	0.58	102,102,102,102	0
58	MG	1H	3020	1/1	0.88	0.38	84,84,84,84	0
58	MG	1H	3488	1/1	0.89	0.09	92,92,92,92	0
58	MG	1H	3339	1/1	0.89	0.38	104,104,104,104	0
58	MG	1H	3148	1/1	0.89	0.21	92,92,92,92	0
58	MG	14	3255	1/1	0.89	0.39	105,105,105,105	0
58	MG	1H	3086	1/1	0.89	0.59	89,89,89,89	0
58	MG	1H	3234	1/1	0.89	1.04	90,90,90,90	0
58	MG	14	3051	1/1	0.89	0.37	158,158,158,158	0
58	MG	13	1696	1/1	0.89	0.43	95,95,95,95	0
58	MG	1H	3240	1/1	0.89	0.49	96,96,96,96	0
58	MG	1H	3156	1/1	0.89	0.05	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1635	1/1	0.89	0.36	111,111,111,111	0
58	MG	13	1626	1/1	0.89	0.33	113,113,113,113	0
58	MG	14	3068	1/1	0.89	0.78	108,108,108,108	0
58	MG	14	3411	1/1	0.89	0.05	134,134,134,134	0
58	MG	1H	3248	1/1	0.89	1.57	93,93,93,93	0
58	MG	14	3269	1/1	0.89	0.29	115,115,115,115	0
58	MG	1H	3101	1/1	0.89	0.33	59,59,59,59	0
58	MG	14	3005	1/1	0.89	0.34	101,101,101,101	0
58	MG	13	1614	1/1	0.89	0.20	97,97,97,97	0
58	MG	1H	3164	1/1	0.89	0.24	86,86,86,86	0
58	MG	13	1669	1/1	0.89	0.12	120,120,120,120	0
58	MG	14	3173	1/1	0.89	0.14	96,96,96,96	0
58	MG	1H	3213	1/1	0.89	0.17	81,81,81,81	0
58	MG	1H	3284	1/1	0.89	0.19	97,97,97,97	0
58	MG	13	1695	1/1	0.89	0.30	122,122,122,122	0
58	MG	1H	3481	1/1	0.89	0.15	133,133,133,133	0
58	MG	14	3323	1/1	0.89	0.07	159,159,159,159	0
58	MG	1H	3110	1/1	0.89	0.35	83,83,83,83	0
58	MG	14	3123	1/1	0.89	0.20	109,109,109,109	0
58	MG	1G	1630	1/1	0.89	0.42	120,120,120,120	0
58	MG	1H	3170	1/1	0.89	0.07	92,92,92,92	0
58	MG	13	1740	1/1	0.90	0.20	107,107,107,107	0
58	MG	1G	1609	1/1	0.90	0.09	113,113,113,113	0
58	MG	1H	3066	1/1	0.90	0.53	86,86,86,86	0
58	MG	1H	3237	1/1	0.90	0.15	88,88,88,88	0
58	MG	1H	3151	1/1	0.90	0.13	90,90,90,90	0
58	MG	1G	1616	1/1	0.90	0.34	118,118,118,118	0
58	MG	1H	3242	1/1	0.90	0.41	90,90,90,90	0
58	MG	13	1648	1/1	0.90	0.60	108,108,108,108	0
58	MG	14	3337	1/1	0.90	0.51	125,125,125,125	0
58	MG	1H	3471	1/1	0.90	0.04	128,128,128,128	0
58	MG	1H	3274	1/1	0.90	0.53	105,105,105,105	0
58	MG	1H	3074	1/1	0.90	0.40	94,94,94,94	0
58	MG	14	3298	1/1	0.90	0.29	104,104,104,104	0
58	MG	14	3372	1/1	0.90	0.08	134,134,134,134	0
58	MG	13	1663	1/1	0.90	0.66	86,86,86,86	0
58	MG	5I	101	1/1	0.90	0.14	110,110,110,110	0
58	MG	1H	3159	1/1	0.90	0.38	89,89,89,89	0
58	MG	14	3405	1/1	0.90	0.17	89,89,89,89	0
58	MG	1H	3023	1/1	0.90	0.45	92,92,92,92	0
58	MG	14	3304	1/1	0.90	0.67	87,87,87,87	0
58	MG	13	1681	1/1	0.90	0.49	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3214	1/1	0.90	0.31	94,94,94,94	0
58	MG	1H	3314	1/1	0.90	0.23	107,107,107,107	0
58	MG	14	3221	1/1	0.90	0.68	80,80,80,80	0
58	MG	1H	3215	1/1	0.90	0.24	69,69,69,69	0
58	MG	1J	205	1/1	0.90	0.26	122,122,122,122	0
58	MG	1J	206	1/1	0.90	0.05	130,130,130,130	0
58	MG	1H	3120	1/1	0.90	0.57	107,107,107,107	0
58	MG	14	3229	1/1	0.90	0.46	93,93,93,93	0
58	MG	1H	3143	1/1	0.90	0.35	101,101,101,101	0
58	MG	13	1677	1/1	0.90	0.52	113,113,113,113	0
58	MG	11	301	1/1	0.90	0.31	73,73,73,73	0
58	MG	21	302	1/1	0.90	0.12	91,91,91,91	0
58	MG	1H	3229	1/1	0.90	0.76	89,89,89,89	0
58	MG	1H	3321	1/1	0.90	0.42	84,84,84,84	0
58	MG	1H	3038	1/1	0.90	0.23	102,102,102,102	0
58	MG	13	1672	1/1	0.90	0.15	133,133,133,133	0
58	MG	14	3327	1/1	0.90	0.46	83,83,83,83	0
58	MG	1H	3112	1/1	0.91	0.72	101,101,101,101	0
58	MG	14	3317	1/1	0.91	0.16	122,122,122,122	0
58	MG	1H	3116	1/1	0.91	0.39	88,88,88,88	0
58	MG	1H	3204	1/1	0.91	0.25	87,87,87,87	0
58	MG	14	3181	1/1	0.91	1.18	91,91,91,91	0
58	MG	1H	3167	1/1	0.91	0.62	96,96,96,96	0
58	MG	1H	3034	1/1	0.91	0.33	145,145,145,145	0
58	MG	1H	3320	1/1	0.91	0.47	107,107,107,107	0
58	MG	13	1706	1/1	0.91	0.24	91,91,91,91	0
58	MG	13	1701	1/1	0.91	0.46	103,103,103,103	0
58	MG	14	3191	1/1	0.91	0.53	93,93,93,93	0
58	MG	1H	3121	1/1	0.91	0.37	93,93,93,93	0
58	MG	1H	3355	1/1	0.91	0.54	88,88,88,88	0
58	MG	1H	3398	1/1	0.91	0.19	76,76,76,76	0
58	MG	1H	3457	1/1	0.91	0.30	89,89,89,89	0
58	MG	1H	3465	1/1	0.91	0.07	112,112,112,112	0
58	MG	13	1676	1/1	0.91	0.29	130,130,130,130	0
58	MG	14	3122	1/1	0.91	0.44	95,95,95,95	0
58	MG	1H	3089	1/1	0.91	0.33	83,83,83,83	0
58	MG	14	3129	1/1	0.91	0.40	84,84,84,84	0
58	MG	1H	3149	1/1	0.91	0.42	102,102,102,102	0
58	MG	14	3007	1/1	0.91	0.50	81,81,81,81	0
58	MG	1H	3026	1/1	0.91	0.40	80,80,80,80	0
58	MG	14	3015	1/1	0.91	0.66	82,82,82,82	0
58	MG	14	3375	1/1	0.91	0.11	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3480	1/1	0.91	0.07	114,114,114,114	0
58	MG	14	3223	1/1	0.91	0.19	116,116,116,116	0
58	MG	1H	3153	1/1	0.91	0.13	86,86,86,86	0
58	MG	13	1617	1/1	0.91	0.29	97,97,97,97	0
58	MG	13	1604	1/1	0.91	0.47	90,90,90,90	0
58	MG	1H	3487	1/1	0.91	0.14	96,96,96,96	0
58	MG	13	1717	1/1	0.91	0.06	123,123,123,123	0
58	MG	1H	3157	1/1	0.91	0.94	88,88,88,88	0
58	MG	14	3156	1/1	0.91	0.70	88,88,88,88	0
58	MG	14	3025	1/1	0.91	0.80	87,87,87,87	0
58	MG	16	204	1/1	0.91	0.10	106,106,106,106	0
58	MG	14	3300	1/1	0.91	0.10	118,118,118,118	0
58	MG	1H	3014	1/1	0.91	0.15	65,65,65,65	0
58	MG	14	3162	1/1	0.91	0.67	90,90,90,90	0
58	MG	1H	3073	1/1	0.91	0.60	84,84,84,84	0
58	MG	1H	3307	1/1	0.91	0.56	97,97,97,97	0
58	MG	1H	3308	1/1	0.91	0.24	81,81,81,81	0
58	MG	1H	3136	1/1	0.91	0.25	80,80,80,80	0
58	MG	1H	3195	1/1	0.91	0.74	96,96,96,96	0
58	MG	13	1609	1/1	0.91	0.24	99,99,99,99	0
58	MG	14	3312	1/1	0.91	0.39	97,97,97,97	0
58	MG	1H	3277	1/1	0.91	0.18	122,122,122,122	0
58	MG	1H	3017	1/1	0.91	0.49	79,79,79,79	0
58	MG	1G	1655	1/1	0.91	0.04	176,176,176,176	0
58	MG	1H	3152	1/1	0.92	0.60	108,108,108,108	0
58	MG	14	3176	1/1	0.92	0.37	96,96,96,96	0
58	MG	14	3120	1/1	0.92	0.25	94,94,94,94	0
58	MG	14	3242	1/1	0.92	0.10	92,92,92,92	0
58	MG	14	3245	1/1	0.92	0.43	97,97,97,97	0
58	MG	1H	3062	1/1	0.92	0.44	103,103,103,103	0
58	MG	1H	3092	1/1	0.92	0.36	76,76,76,76	0
58	MG	14	3293	1/1	0.92	0.69	109,109,109,109	0
58	MG	1H	3137	1/1	0.92	0.35	93,93,93,93	0
58	MG	1H	3301	1/1	0.92	0.54	99,99,99,99	0
58	MG	13	1618	1/1	0.92	0.22	108,108,108,108	0
58	MG	14	3139	1/1	0.92	0.12	75,75,75,75	0
58	MG	14	3369	1/1	0.92	0.10	105,105,105,105	0
58	MG	1H	3177	1/1	0.92	0.67	93,93,93,93	0
58	MG	1H	3207	1/1	0.92	0.45	93,93,93,93	0
58	MG	1G	1669	1/1	0.92	0.14	151,151,151,151	0
58	MG	14	3045	1/1	0.92	0.21	89,89,89,89	0
58	MG	1G	1673	1/1	0.92	0.17	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	13	1656	1/1	0.92	0.10	105,105,105,105	0
58	MG	14	3151	1/1	0.92	0.29	109,109,109,109	0
58	MG	1H	3374	1/1	0.92	0.13	77,77,77,77	0
58	MG	14	3415	1/1	0.92	0.07	126,126,126,126	0
58	MG	14	3153	1/1	0.92	0.51	102,102,102,102	0
58	MG	14	3418	1/1	0.92	0.08	88,88,88,88	0
58	MG	I8	101	1/1	0.92	0.42	70,70,70,70	0
58	MG	13	1697	1/1	0.92	0.51	98,98,98,98	0
58	MG	14	3061	1/1	0.92	0.12	102,102,102,102	0
58	MG	14	3205	1/1	0.92	0.15	97,97,97,97	0
58	MG	1H	3122	1/1	0.92	0.15	83,83,83,83	0
58	MG	1H	3184	1/1	0.92	0.76	94,94,94,94	0
58	MG	13	1619	1/1	0.92	0.26	81,81,81,81	0
58	MG	1H	3253	1/1	0.92	0.45	84,84,84,84	0
58	MG	13	1630	1/1	0.92	0.14	74,74,74,74	0
58	MG	45	201	1/1	0.92	0.27	101,101,101,101	0
58	MG	1H	3028	1/1	0.92	0.44	82,82,82,82	0
58	MG	1H	3127	1/1	0.92	0.34	79,79,79,79	0
58	MG	55	201	1/1	0.92	0.28	96,96,96,96	0
58	MG	13	1732	1/1	0.92	0.14	127,127,127,127	0
58	MG	14	3228	1/1	0.92	0.29	96,96,96,96	0
58	MG	3I	201	1/1	0.92	0.19	87,87,87,87	0
58	MG	13	1645	1/1	0.92	0.38	113,113,113,113	0
58	MG	1H	3115	1/1	0.92	0.26	70,70,70,70	0
58	MG	1H	3233	1/1	0.92	0.19	93,93,93,93	0
58	MG	13	1633	1/1	0.93	0.57	88,88,88,88	0
58	MG	13	1620	1/1	0.93	0.24	117,117,117,117	0
58	MG	1H	3238	1/1	0.93	0.24	83,83,83,83	0
58	MG	1H	3043	1/1	0.93	0.31	75,75,75,75	0
58	MG	1H	3048	1/1	0.93	0.36	80,80,80,80	0
58	MG	14	3238	1/1	0.93	0.70	83,83,83,83	0
58	MG	1H	3271	1/1	0.93	0.58	87,87,87,87	0
58	MG	1H	3083	1/1	0.93	0.27	74,74,74,74	0
58	MG	14	3244	1/1	0.93	0.12	79,79,79,79	0
58	MG	1H	3482	1/1	0.93	0.06	119,119,119,119	0
58	MG	14	3318	1/1	0.93	0.30	102,102,102,102	0
58	MG	1H	3335	1/1	0.93	0.16	100,100,100,100	0
58	MG	1G	1642	1/1	0.93	0.44	114,114,114,114	0
58	MG	1H	3306	1/1	0.93	0.42	77,77,77,77	0
58	MG	1H	3244	1/1	0.93	0.47	103,103,103,103	0
58	MG	13	1611	1/1	0.93	0.22	91,91,91,91	0
58	MG	1H	3113	1/1	0.93	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3164	1/1	0.93	0.31	93,93,93,93	0
58	MG	14	3044	1/1	0.93	0.28	88,88,88,88	0
58	MG	1H	3310	1/1	0.93	0.54	95,95,95,95	0
58	MG	14	3167	1/1	0.93	0.21	105,105,105,105	0
58	MG	13	1636	1/1	0.93	0.10	123,123,123,123	0
58	MG	1H	3191	1/1	0.93	0.36	95,95,95,95	0
58	MG	1H	3063	1/1	0.93	0.44	57,57,57,57	0
58	MG	14	3057	1/1	0.93	0.22	119,119,119,119	0
58	MG	1H	3222	1/1	0.93	0.25	94,94,94,94	0
58	MG	1H	3225	1/1	0.93	0.33	70,70,70,70	0
58	MG	1H	3090	1/1	0.93	0.43	76,76,76,76	0
58	MG	1H	3255	1/1	0.93	0.79	94,94,94,94	0
58	MG	14	3067	1/1	0.93	0.27	100,100,100,100	0
58	MG	13	1655	1/1	0.93	0.08	106,106,106,106	0
58	MG	14	3351	1/1	0.93	0.06	80,80,80,80	0
58	MG	14	3072	1/1	0.93	0.35	84,84,84,84	0
58	MG	78	201	1/1	0.93	0.26	92,92,92,92	0
58	MG	1H	3197	1/1	0.93	0.49	68,68,68,68	0
58	MG	1H	3258	1/1	0.93	0.33	99,99,99,99	0
58	MG	J8	102	1/1	0.93	0.46	77,77,77,77	0
58	MG	1G	1665	1/1	0.93	0.33	122,122,122,122	0
58	MG	14	3397	1/1	0.93	0.09	103,103,103,103	0
58	MG	13	1647	1/1	0.93	0.28	108,108,108,108	0
58	MG	1H	3353	1/1	0.93	0.53	96,96,96,96	0
58	MG	14	3105	1/1	0.93	0.84	110,110,110,110	0
58	MG	1H	3260	1/1	0.93	1.54	95,95,95,95	0
58	MG	14	3413	1/1	0.93	0.04	92,92,92,92	0
58	MG	1H	3291	1/1	0.93	0.64	116,116,116,116	0
58	MG	14	3416	1/1	0.93	0.04	124,124,124,124	0
58	MG	14	3281	1/1	0.93	0.91	103,103,103,103	0
58	MG	1H	3070	1/1	0.93	0.45	100,100,100,100	0
58	MG	14	3111	1/1	0.93	0.55	82,82,82,82	0
58	MG	14	3113	1/1	0.93	0.49	102,102,102,102	0
58	MG	14	3115	1/1	0.93	0.33	88,88,88,88	0
58	MG	1H	3396	1/1	0.93	0.06	99,99,99,99	0
58	MG	1H	3096	1/1	0.93	0.32	76,76,76,76	0
58	MG	14	3206	1/1	0.93	0.09	88,88,88,88	0
58	MG	1H	3411	1/1	0.93	0.16	94,94,94,94	0
58	MG	1H	3420	1/1	0.93	0.11	81,81,81,81	0
58	MG	14	3213	1/1	0.93	0.27	114,114,114,114	0
58	MG	1G	1620	1/1	0.93	0.58	91,91,91,91	0
58	MG	1H	3432	1/1	0.93	0.12	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3218	1/1	0.93	0.15	97,97,97,97	0
58	MG	14	3134	1/1	0.93	0.39	100,100,100,100	0
58	MG	1H	3433	1/1	0.93	0.28	113,113,113,113	0
58	MG	1H	3438	1/1	0.93	0.10	110,110,110,110	0
58	MG	14	3225	1/1	0.93	0.46	95,95,95,95	0
58	MG	1H	3445	1/1	0.93	0.17	71,71,71,71	0
58	MG	1H	3450	1/1	0.93	0.17	75,75,75,75	0
58	MG	13	1631	1/1	0.93	0.27	82,82,82,82	0
58	MG	16	202	1/1	0.94	0.18	102,102,102,102	0
58	MG	14	3144	1/1	0.94	0.17	112,112,112,112	0
58	MG	1H	3068	1/1	0.94	0.45	70,70,70,70	0
58	MG	14	3147	1/1	0.94	0.34	110,110,110,110	0
58	MG	1H	3409	1/1	0.94	0.12	85,85,85,85	0
58	MG	1H	3410	1/1	0.94	0.08	97,97,97,97	0
58	MG	1H	3114	1/1	0.94	0.15	77,77,77,77	0
58	MG	1H	3300	1/1	0.94	0.86	99,99,99,99	0
58	MG	14	3060	1/1	0.94	0.08	103,103,103,103	0
58	MG	1G	1678	1/1	0.94	0.14	119,119,119,119	0
58	MG	14	3212	1/1	0.94	0.17	105,105,105,105	0
58	MG	1H	3429	1/1	0.94	0.14	82,82,82,82	0
58	MG	1H	3431	1/1	0.94	0.10	111,111,111,111	0
58	MG	1H	3190	1/1	0.94	0.24	108,108,108,108	0
58	MG	14	3338	1/1	0.94	0.07	114,114,114,114	0
58	MG	1H	3160	1/1	0.94	0.40	88,88,88,88	0
58	MG	14	3340	1/1	0.94	0.22	91,91,91,91	0
58	MG	14	3219	1/1	0.94	0.23	83,83,83,83	0
58	MG	14	3158	1/1	0.94	0.36	92,92,92,92	0
58	MG	13	1665	1/1	0.94	0.10	105,105,105,105	0
58	MG	14	3353	1/1	0.94	0.11	73,73,73,73	0
58	MG	14	3358	1/1	0.94	0.17	107,107,107,107	0
58	MG	14	3006	1/1	0.94	0.29	72,72,72,72	0
58	MG	14	3368	1/1	0.94	0.15	87,87,87,87	0
58	MG	14	3083	1/1	0.94	0.28	94,94,94,94	0
58	MG	14	3285	1/1	0.94	0.21	77,77,77,77	0
58	MG	1H	3193	1/1	0.94	0.40	104,104,104,104	0
58	MG	1H	3194	1/1	0.94	0.24	91,91,91,91	0
58	MG	14	3086	1/1	0.94	0.71	95,95,95,95	0
58	MG	14	3289	1/1	0.94	0.34	116,116,116,116	0
58	MG	14	3230	1/1	0.94	0.15	122,122,122,122	0
58	MG	1H	3451	1/1	0.94	0.20	85,85,85,85	0
58	MG	1H	3150	1/1	0.94	0.40	63,63,63,63	0
58	MG	14	3094	1/1	0.94	0.55	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3459	1/1	0.94	0.25	102,102,102,102	0
58	MG	14	3170	1/1	0.94	0.29	119,119,119,119	0
58	MG	14	3237	1/1	0.94	0.21	181,181,181,181	0
58	MG	14	3104	1/1	0.94	0.38	78,78,78,78	0
58	MG	1H	3055	1/1	0.94	0.17	74,74,74,74	0
58	MG	1H	3218	1/1	0.94	0.17	68,68,68,68	0
58	MG	1H	3469	1/1	0.94	0.24	124,124,124,124	0
58	MG	1H	3058	1/1	0.94	0.15	76,76,76,76	0
58	MG	1H	3329	1/1	0.94	0.10	105,105,105,105	0
58	MG	1G	1654	1/1	0.94	0.25	110,110,110,110	0
58	MG	1H	3477	1/1	0.94	0.05	114,114,114,114	0
58	MG	14	3180	1/1	0.94	0.34	81,81,81,81	0
58	MG	1H	3059	1/1	0.94	0.12	110,110,110,110	0
58	MG	1H	3130	1/1	0.94	0.36	79,79,79,79	0
58	MG	13	1671	1/1	0.94	0.20	107,107,107,107	0
58	MG	1H	3203	1/1	0.94	0.22	91,91,91,91	0
58	MG	1H	3006	1/1	0.94	0.27	71,71,71,71	0
58	MG	14	3256	1/1	0.94	0.28	110,110,110,110	0
58	MG	14	3188	1/1	0.94	1.22	93,93,93,93	0
58	MG	1H	3273	1/1	0.94	0.18	85,85,85,85	0
58	MG	14	3041	1/1	0.94	0.39	80,80,80,80	0
58	MG	1H	3385	1/1	0.94	0.07	91,91,91,91	0
58	MG	13	1667	1/1	0.94	0.58	91,91,91,91	0
58	MG	14	3050	1/1	0.94	0.12	87,87,87,87	0
58	MG	14	3204	1/1	0.95	0.25	73,73,73,73	0
58	MG	14	3329	1/1	0.95	1.16	91,91,91,91	0
58	MG	1H	3171	1/1	0.95	0.79	83,83,83,83	0
58	MG	1H	3172	1/1	0.95	0.30	89,89,89,89	0
58	MG	1H	3223	1/1	0.95	0.22	96,96,96,96	0
58	MG	13	1730	1/1	0.95	0.10	108,108,108,108	0
58	MG	14	3211	1/1	0.95	0.21	78,78,78,78	0
58	MG	13	1640	1/1	0.95	0.71	73,73,73,73	0
58	MG	1H	3430	1/1	0.95	0.08	81,81,81,81	0
58	MG	2L	103	1/1	0.95	0.51	128,128,128,128	0
58	MG	14	3069	1/1	0.95	0.32	106,106,106,106	0
58	MG	14	3070	1/1	0.95	0.16	94,94,94,94	0
58	MG	14	3001	1/1	0.95	0.93	97,97,97,97	0
58	MG	1H	3022	1/1	0.95	0.35	69,69,69,69	0
58	MG	1H	3118	1/1	0.95	0.60	104,104,104,104	0
58	MG	14	3347	1/1	0.95	0.05	87,87,87,87	0
58	MG	14	3348	1/1	0.95	0.11	86,86,86,86	0
58	MG	14	3161	1/1	0.95	0.54	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	13	1685	1/1	0.95	0.39	107,107,107,107	0
58	MG	13	1658	1/1	0.95	0.58	89,89,89,89	0
58	MG	1H	3179	1/1	0.95	0.37	101,101,101,101	0
58	MG	1H	3001	1/1	0.95	0.43	66,66,66,66	0
58	MG	14	3088	1/1	0.95	0.40	78,78,78,78	0
58	MG	13	1737	1/1	0.95	0.04	116,116,116,116	0
58	MG	1H	3453	1/1	0.95	0.08	93,93,93,93	0
58	MG	14	3377	1/1	0.95	0.05	106,106,106,106	0
58	MG	14	3378	1/1	0.95	0.09	83,83,83,83	0
58	MG	1H	3042	1/1	0.95	0.34	59,59,59,59	0
58	MG	13	1642	1/1	0.95	0.47	104,104,104,104	0
58	MG	14	3390	1/1	0.95	0.08	114,114,114,114	0
58	MG	14	3395	1/1	0.95	0.06	85,85,85,85	0
58	MG	14	3102	1/1	0.95	0.25	92,92,92,92	0
58	MG	1H	3293	1/1	0.95	0.30	94,94,94,94	0
58	MG	1G	1603	1/1	0.95	0.57	132,132,132,132	0
58	MG	14	3407	1/1	0.95	0.07	121,121,121,121	0
58	MG	1H	3239	1/1	0.95	0.25	71,71,71,71	0
58	MG	14	3241	1/1	0.95	0.47	115,115,115,115	0
58	MG	13	1713	1/1	0.95	0.05	117,117,117,117	0
58	MG	1H	3268	1/1	0.95	0.55	104,104,104,104	0
58	MG	1H	3053	1/1	0.95	0.17	81,81,81,81	0
58	MG	14	3112	1/1	0.95	0.10	108,108,108,108	0
58	MG	1G	1613	1/1	0.95	0.28	114,114,114,114	0
58	MG	13	1716	1/1	0.95	0.10	108,108,108,108	0
58	MG	1G	1615	1/1	0.95	0.22	142,142,142,142	0
58	MG	14	3119	1/1	0.95	0.27	83,83,83,83	0
58	MG	1J	203	1/1	0.95	0.33	124,124,124,124	0
58	MG	1H	3111	1/1	0.95	0.28	64,64,64,64	0
58	MG	14	3033	1/1	0.95	0.79	95,95,95,95	0
58	MG	14	3187	1/1	0.95	0.30	96,96,96,96	0
58	MG	13	1651	1/1	0.95	0.31	96,96,96,96	0
58	MG	1H	3363	1/1	0.95	0.21	81,81,81,81	0
58	MG	14	3043	1/1	0.95	0.38	69,69,69,69	0
58	MG	1H	3214	1/1	0.95	0.28	65,65,65,65	0
58	MG	1H	3375	1/1	0.95	0.16	81,81,81,81	0
58	MG	14	3048	1/1	0.95	0.21	90,90,90,90	0
58	MG	1G	1625	1/1	0.95	0.26	136,136,136,136	0
58	MG	1H	3057	1/1	0.95	0.27	75,75,75,75	0
58	MG	14	3052	1/1	0.95	0.14	83,83,83,83	0
58	MG	1H	3249	1/1	0.95	0.15	83,83,83,83	0
58	MG	1G	1629	1/1	0.95	0.34	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1700	1/1	0.95	0.07	123,123,123,123	0
58	MG	14	3203	1/1	0.95	0.28	84,84,84,84	0
58	MG	1H	3283	1/1	0.96	1.29	95,95,95,95	0
58	MG	14	3236	1/1	0.96	0.09	121,121,121,121	0
58	MG	1H	3060	1/1	0.96	0.57	111,111,111,111	0
58	MG	1H	3061	1/1	0.96	0.84	79,79,79,79	0
58	MG	14	3239	1/1	0.96	0.67	90,90,90,90	0
58	MG	1H	3452	1/1	0.96	0.21	102,102,102,102	0
58	MG	1G	1672	1/1	0.96	0.05	115,115,115,115	0
58	MG	1H	3228	1/1	0.96	0.80	74,74,74,74	0
58	MG	13	1639	1/1	0.96	0.24	87,87,87,87	0
58	MG	14	3079	1/1	0.96	0.25	87,87,87,87	0
58	MG	1H	3200	1/1	0.96	0.29	79,79,79,79	0
58	MG	1G	1617	1/1	0.96	0.05	159,159,159,159	0
58	MG	14	3326	1/1	0.96	0.65	104,104,104,104	0
58	MG	1H	3460	1/1	0.96	0.19	86,86,86,86	0
58	MG	14	3249	1/1	0.96	0.06	102,102,102,102	0
58	MG	1H	3463	1/1	0.96	0.19	103,103,103,103	0
58	MG	1H	3201	1/1	0.96	0.73	97,97,97,97	0
58	MG	1H	3040	1/1	0.96	0.41	71,71,71,71	0
58	MG	14	3087	1/1	0.96	0.42	68,68,68,68	0
58	MG	1G	1624	1/1	0.96	0.58	92,92,92,92	0
58	MG	1H	3005	1/1	0.96	0.33	79,79,79,79	0
58	MG	13	1720	1/1	0.96	0.06	126,126,126,126	0
58	MG	1H	3352	1/1	0.96	0.27	75,75,75,75	0
58	MG	14	3098	1/1	0.96	0.34	86,86,86,86	0
58	MG	14	3099	1/1	0.96	0.25	91,91,91,91	0
58	MG	1H	3236	1/1	0.96	0.19	89,89,89,89	0
58	MG	14	3008	1/1	0.96	0.39	77,77,77,77	0
58	MG	14	3009	1/1	0.96	0.51	74,74,74,74	0
58	MG	14	3184	1/1	0.96	0.26	92,92,92,92	0
58	MG	14	3011	1/1	0.96	0.56	85,85,85,85	0
58	MG	14	3265	1/1	0.96	0.14	110,110,110,110	0
58	MG	14	3106	1/1	0.96	0.36	85,85,85,85	0
58	MG	1H	3182	1/1	0.96	0.52	91,91,91,91	0
58	MG	14	3355	1/1	0.96	0.07	92,92,92,92	0
58	MG	1H	3296	1/1	0.96	0.89	86,86,86,86	0
58	MG	1H	3266	1/1	0.96	0.29	65,65,65,65	0
58	MG	14	3367	1/1	0.96	0.07	86,86,86,86	0
58	MG	14	3190	1/1	0.96	0.22	91,91,91,91	0
58	MG	1H	3372	1/1	0.96	0.07	73,73,73,73	0
58	MG	1H	3047	1/1	0.96	0.56	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3193	1/1	0.96	0.58	79,79,79,79	0
58	MG	1H	3485	1/1	0.96	0.15	83,83,83,83	0
58	MG	14	3114	1/1	0.96	0.57	66,66,66,66	0
58	MG	14	3379	1/1	0.96	0.04	110,110,110,110	0
58	MG	14	3380	1/1	0.96	0.08	94,94,94,94	0
58	MG	1H	3097	1/1	0.96	0.43	72,72,72,72	0
58	MG	14	3116	1/1	0.96	0.45	75,75,75,75	0
58	MG	14	3386	1/1	0.96	0.13	83,83,83,83	0
58	MG	1H	3378	1/1	0.96	0.10	90,90,90,90	0
58	MG	1H	3099	1/1	0.96	0.45	74,74,74,74	0
58	MG	16	201	1/1	0.96	0.11	114,114,114,114	0
58	MG	1H	3390	1/1	0.96	0.12	74,74,74,74	0
58	MG	1H	3392	1/1	0.96	0.17	81,81,81,81	0
58	MG	14	3406	1/1	0.96	0.06	121,121,121,121	0
58	MG	14	3124	1/1	0.96	0.47	90,90,90,90	0
58	MG	1H	3021	1/1	0.96	0.36	86,86,86,86	0
58	MG	1H	3165	1/1	0.96	0.43	99,99,99,99	0
58	MG	1H	3405	1/1	0.96	0.19	75,75,75,75	0
58	MG	14	3136	1/1	0.96	0.42	93,93,93,93	0
58	MG	14	3209	1/1	0.96	0.31	90,90,90,90	0
58	MG	1H	3007	1/1	0.96	0.31	65,65,65,65	0
58	MG	1H	3103	1/1	0.96	0.57	72,72,72,72	0
58	MG	1H	3104	1/1	0.96	0.31	66,66,66,66	0
58	MG	14	3040	1/1	0.96	0.40	72,72,72,72	0
58	MG	1H	3412	1/1	0.96	0.06	84,84,84,84	0
58	MG	14	3145	1/1	0.96	0.26	76,76,76,76	0
58	MG	1H	3009	1/1	0.96	0.27	98,98,98,98	0
58	MG	13	1721	1/1	0.96	0.05	100,100,100,100	0
58	MG	14	3222	1/1	0.96	0.82	95,95,95,95	0
58	MG	1H	3056	1/1	0.96	0.22	89,89,89,89	0
58	MG	C8	201	1/1	0.96	0.20	74,74,74,74	0
58	MG	1H	3219	1/1	0.96	0.16	120,120,120,120	0
58	MG	1G	1657	1/1	0.96	0.16	163,163,163,163	0
58	MG	13	1610	1/1	0.96	0.30	92,92,92,92	0
58	MG	14	3306	1/1	0.96	0.20	129,129,129,129	0
58	MG	14	3307	1/1	0.96	0.10	80,80,80,80	0
58	MG	13	1605	1/1	0.96	0.20	134,134,134,134	0
58	MG	1H	3434	1/1	0.96	0.13	82,82,82,82	0
58	MG	13	1646	1/1	0.96	0.24	129,129,129,129	0
58	MG	1H	3439	1/1	0.96	0.14	72,72,72,72	0
58	MG	1H	3444	1/1	0.96	0.13	85,85,85,85	0
60	ZN	G8	201	1/1	0.96	0.05	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1G	1608	1/1	0.96	0.20	119,119,119,119	0
58	MG	1G	1663	1/1	0.97	0.44	133,133,133,133	0
58	MG	1H	3079	1/1	0.97	0.45	68,68,68,68	0
58	MG	1H	3415	1/1	0.97	0.17	90,90,90,90	0
58	MG	14	3198	1/1	0.97	0.16	109,109,109,109	0
58	MG	16	210	1/1	0.97	0.08	87,87,87,87	0
58	MG	14	3093	1/1	0.97	0.64	71,71,71,71	0
58	MG	16	211	1/1	0.97	0.12	92,92,92,92	0
58	MG	14	3095	1/1	0.97	0.71	75,75,75,75	0
58	MG	16	212	1/1	0.97	0.11	104,104,104,104	0
58	MG	1H	3417	1/1	0.97	0.10	77,77,77,77	0
58	MG	1G	1670	1/1	0.97	0.05	112,112,112,112	0
58	MG	1H	3418	1/1	0.97	0.10	86,86,86,86	0
58	MG	1H	3419	1/1	0.97	0.09	76,76,76,76	0
58	MG	1H	3081	1/1	0.97	0.21	88,88,88,88	0
58	MG	1H	3421	1/1	0.97	0.04	129,129,129,129	0
58	MG	1H	3423	1/1	0.97	0.20	92,92,92,92	0
58	MG	1H	3425	1/1	0.97	0.12	77,77,77,77	0
58	MG	1H	3427	1/1	0.97	0.03	106,106,106,106	0
58	MG	P8	101	1/1	0.97	0.12	101,101,101,101	0
58	MG	14	3215	1/1	0.97	0.37	89,89,89,89	0
58	MG	14	3216	1/1	0.97	0.28	101,101,101,101	0
58	MG	1H	3428	1/1	0.97	0.21	89,89,89,89	0
58	MG	13	1741	1/1	0.97	0.17	88,88,88,88	0
58	MG	14	3003	1/1	0.97	0.34	76,76,76,76	0
58	MG	13	1602	1/1	0.97	0.35	98,98,98,98	0
58	MG	1H	3008	1/1	0.97	0.36	99,99,99,99	0
58	MG	1G	1606	1/1	0.97	0.53	93,93,93,93	0
58	MG	14	3118	1/1	0.97	0.26	73,73,73,73	0
58	MG	1G	1607	1/1	0.97	0.18	109,109,109,109	0
58	MG	14	3226	1/1	0.97	0.28	88,88,88,88	0
58	MG	1H	3088	1/1	0.97	0.22	81,81,81,81	0
58	MG	14	3121	1/1	0.97	0.39	69,69,69,69	0
58	MG	13	1664	1/1	0.97	0.08	105,105,105,105	0
58	MG	1G	1610	1/1	0.97	0.31	118,118,118,118	0
58	MG	13	1675	1/1	0.97	0.29	149,149,149,149	0
58	MG	14	3128	1/1	0.97	0.58	80,80,80,80	0
58	MG	1H	3436	1/1	0.97	0.10	96,96,96,96	0
58	MG	14	3130	1/1	0.97	0.28	93,93,93,93	0
58	MG	14	3016	1/1	0.97	0.43	68,68,68,68	0
58	MG	14	3017	1/1	0.97	0.42	68,68,68,68	0
58	MG	14	3135	1/1	0.97	0.28	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1H	3437	1/1	0.97	0.06	85,85,85,85	0
58	MG	1H	3241	1/1	0.97	0.08	100,100,100,100	0
58	MG	1H	3041	1/1	0.97	0.29	73,73,73,73	0
58	MG	1H	3442	1/1	0.97	0.25	63,63,63,63	0
58	MG	13	1719	1/1	0.97	0.14	94,94,94,94	0
58	MG	14	3243	1/1	0.97	0.24	102,102,102,102	0
58	MG	14	3350	1/1	0.97	0.04	116,116,116,116	0
58	MG	1H	3094	1/1	0.97	0.35	77,77,77,77	0
58	MG	1H	3446	1/1	0.97	0.11	94,94,94,94	0
58	MG	1H	3180	1/1	0.97	0.13	97,97,97,97	0
58	MG	1G	1622	1/1	0.97	0.46	103,103,103,103	0
58	MG	14	3365	1/1	0.97	0.09	96,96,96,96	0
58	MG	14	3027	1/1	0.97	0.45	79,79,79,79	0
58	MG	1H	3210	1/1	0.97	0.47	101,101,101,101	0
58	MG	1H	3064	1/1	0.97	0.26	82,82,82,82	0
58	MG	1H	3065	1/1	0.97	0.34	77,77,77,77	0
58	MG	1H	3454	1/1	0.97	0.25	96,96,96,96	0
58	MG	14	3373	1/1	0.97	0.14	86,86,86,86	0
58	MG	13	1607	1/1	0.97	0.23	101,101,101,101	0
58	MG	1H	3125	1/1	0.97	0.38	75,75,75,75	0
58	MG	1H	3044	1/1	0.97	0.36	68,68,68,68	0
58	MG	14	3038	1/1	0.97	0.35	67,67,67,67	0
58	MG	1H	3462	1/1	0.97	0.15	90,90,90,90	0
58	MG	13	1643	1/1	0.97	0.35	80,80,80,80	0
58	MG	1H	3464	1/1	0.97	0.10	95,95,95,95	0
58	MG	14	3385	1/1	0.97	0.05	92,92,92,92	0
58	MG	1H	3361	1/1	0.97	0.18	72,72,72,72	0
58	MG	1H	3467	1/1	0.97	0.12	115,115,115,115	0
58	MG	14	3394	1/1	0.97	0.20	88,88,88,88	0
58	MG	14	3046	1/1	0.97	0.26	86,86,86,86	0
58	MG	14	3047	1/1	0.97	0.17	102,102,102,102	0
58	MG	14	3402	1/1	0.97	0.14	83,83,83,83	0
58	MG	14	3403	1/1	0.97	0.18	114,114,114,114	0
58	MG	1H	3015	1/1	0.97	0.96	77,77,77,77	0
58	MG	1H	3365	1/1	0.97	0.17	64,64,64,64	0
58	MG	1H	3102	1/1	0.97	0.71	73,73,73,73	0
58	MG	1H	3220	1/1	0.97	0.26	115,115,115,115	0
58	MG	14	3410	1/1	0.97	0.09	91,91,91,91	0
58	MG	14	3268	1/1	0.97	0.30	84,84,84,84	0
58	MG	1H	3474	1/1	0.97	0.05	110,110,110,110	0
58	MG	1H	3476	1/1	0.97	0.03	122,122,122,122	0
58	MG	14	3414	1/1	0.97	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3052	1/1	0.97	0.27	69,69,69,69	0
58	MG	1H	3478	1/1	0.97	0.06	95,95,95,95	0
58	MG	14	3172	1/1	0.97	0.23	75,75,75,75	0
58	MG	13	1622	1/1	0.97	0.30	99,99,99,99	0
58	MG	1H	3380	1/1	0.97	0.10	89,89,89,89	0
58	MG	1H	3381	1/1	0.97	0.15	80,80,80,80	0
58	MG	1H	3002	1/1	0.97	0.45	64,64,64,64	0
58	MG	14	3063	1/1	0.97	0.41	79,79,79,79	0
58	MG	14	3065	1/1	0.97	0.27	80,80,80,80	0
58	MG	1H	3386	1/1	0.97	0.06	109,109,109,109	0
58	MG	1H	3294	1/1	0.97	0.09	103,103,103,103	0
58	MG	1H	3106	1/1	0.97	0.10	82,82,82,82	0
58	MG	1H	3394	1/1	0.97	0.07	89,89,89,89	0
58	MG	14	3071	1/1	0.97	0.34	69,69,69,69	0
58	MG	1H	3135	1/1	0.97	0.12	69,69,69,69	0
58	MG	14	3074	1/1	0.97	0.50	70,70,70,70	0
58	MG	14	3076	1/1	0.97	0.30	83,83,83,83	0
58	MG	14	3078	1/1	0.97	0.44	82,82,82,82	0
58	MG	1H	3107	1/1	0.97	0.35	95,95,95,95	0
58	MG	1H	3401	1/1	0.97	0.15	71,71,71,71	0
58	MG	1H	3004	1/1	0.97	0.26	60,60,60,60	0
58	MG	1H	3406	1/1	0.97	0.08	82,82,82,82	0
58	MG	13	1729	1/1	0.97	0.13	96,96,96,96	0
58	MG	1H	3231	1/1	0.97	0.69	85,85,85,85	0
60	ZN	5A	101	1/1	0.97	0.07	164,164,164,164	0
58	MG	1H	3078	1/1	0.97	0.28	80,80,80,80	0
58	MG	1H	3370	1/1	0.98	0.09	68,68,68,68	0
58	MG	1H	3371	1/1	0.98	0.06	77,77,77,77	0
58	MG	14	3056	1/1	0.98	0.21	109,109,109,109	0
58	MG	13	1629	1/1	0.98	0.50	79,79,79,79	0
58	MG	1H	3443	1/1	0.98	0.24	80,80,80,80	0
58	MG	1H	3373	1/1	0.98	0.15	86,86,86,86	0
58	MG	13	1654	1/1	0.98	0.21	111,111,111,111	0
58	MG	13	1613	1/1	0.98	0.09	109,109,109,109	0
58	MG	1H	3447	1/1	0.98	0.11	115,115,115,115	0
58	MG	1H	3448	1/1	0.98	0.21	88,88,88,88	0
58	MG	1H	3376	1/1	0.98	0.05	106,106,106,106	0
58	MG	14	3066	1/1	0.98	0.33	95,95,95,95	0
58	MG	1H	3377	1/1	0.98	0.05	119,119,119,119	0
58	MG	13	1736	1/1	0.98	0.09	126,126,126,126	0
58	MG	1G	1671	1/1	0.98	0.15	121,121,121,121	0
58	MG	1H	3379	1/1	0.98	0.17	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	13	1624	1/1	0.98	0.55	118,118,118,118	0
58	MG	1G	1674	1/1	0.98	0.06	124,124,124,124	0
58	MG	1H	3455	1/1	0.98	0.13	87,87,87,87	0
58	MG	14	3075	1/1	0.98	0.97	96,96,96,96	0
58	MG	1G	1676	1/1	0.98	0.21	134,134,134,134	0
58	MG	14	3077	1/1	0.98	0.16	83,83,83,83	0
58	MG	13	1714	1/1	0.98	0.11	98,98,98,98	0
58	MG	14	3346	1/1	0.98	0.09	81,81,81,81	0
58	MG	1H	3458	1/1	0.98	0.13	88,88,88,88	0
58	MG	1H	3382	1/1	0.98	0.23	71,71,71,71	0
58	MG	14	3081	1/1	0.98	0.27	89,89,89,89	0
58	MG	1H	3383	1/1	0.98	0.14	75,75,75,75	0
58	MG	14	3352	1/1	0.98	0.05	84,84,84,84	0
58	MG	13	1657	1/1	0.98	0.17	103,103,103,103	0
58	MG	13	1632	1/1	0.98	0.21	83,83,83,83	0
58	MG	14	3356	1/1	0.98	0.18	85,85,85,85	0
58	MG	13	1718	1/1	0.98	0.12	110,110,110,110	0
58	MG	14	3359	1/1	0.98	0.10	94,94,94,94	0
58	MG	14	3361	1/1	0.98	0.11	79,79,79,79	0
58	MG	14	3364	1/1	0.98	0.16	105,105,105,105	0
58	MG	13	1601	1/1	0.98	0.27	86,86,86,86	0
58	MG	13	1691	1/1	0.98	0.81	94,94,94,94	0
58	MG	1G	1619	1/1	0.98	0.27	109,109,109,109	0
58	MG	1H	3395	1/1	0.98	0.17	103,103,103,103	0
58	MG	1H	3098	1/1	0.98	0.66	70,70,70,70	0
58	MG	14	3370	1/1	0.98	0.04	94,94,94,94	0
58	MG	1H	3470	1/1	0.98	0.13	85,85,85,85	0
58	MG	1H	3397	1/1	0.98	0.14	82,82,82,82	0
58	MG	14	3010	1/1	0.98	0.29	73,73,73,73	0
58	MG	14	3376	1/1	0.98	0.03	124,124,124,124	0
58	MG	14	3096	1/1	0.98	0.39	57,57,57,57	0
58	MG	1H	3018	1/1	0.98	0.58	66,66,66,66	0
58	MG	1H	3473	1/1	0.98	0.11	89,89,89,89	0
58	MG	1G	1626	1/1	0.98	0.27	118,118,118,118	0
58	MG	1H	3019	1/1	0.98	0.56	65,65,65,65	0
58	MG	14	3103	1/1	0.98	0.32	81,81,81,81	0
58	MG	14	3383	1/1	0.98	0.11	137,137,137,137	0
58	MG	14	3384	1/1	0.98	0.10	96,96,96,96	0
58	MG	1H	3475	1/1	0.98	0.10	89,89,89,89	0
58	MG	1H	3071	1/1	0.98	0.41	94,94,94,94	0
58	MG	14	3387	1/1	0.98	0.08	88,88,88,88	0
58	MG	14	3389	1/1	0.98	0.11	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1615	1/1	0.98	0.20	90,90,90,90	0
58	MG	14	3391	1/1	0.98	0.09	87,87,87,87	0
58	MG	14	3393	1/1	0.98	0.15	89,89,89,89	0
58	MG	14	3107	1/1	0.98	0.41	80,80,80,80	0
58	MG	13	1722	1/1	0.98	0.06	99,99,99,99	0
58	MG	14	3396	1/1	0.98	0.29	96,96,96,96	0
58	MG	1H	3245	1/1	0.98	0.21	100,100,100,100	0
58	MG	14	3398	1/1	0.98	0.07	111,111,111,111	0
58	MG	14	3401	1/1	0.98	0.10	127,127,127,127	0
58	MG	13	1616	1/1	0.98	0.05	121,121,121,121	0
58	MG	1G	1634	1/1	0.98	0.34	127,127,127,127	0
58	MG	13	1724	1/1	0.98	0.11	99,99,99,99	0
58	MG	1H	3413	1/1	0.98	0.11	90,90,90,90	0
58	MG	1H	3216	1/1	0.98	0.15	65,65,65,65	0
58	MG	1H	3281	1/1	0.98	0.69	108,108,108,108	0
58	MG	14	3408	1/1	0.98	0.07	130,130,130,130	0
58	MG	14	3409	1/1	0.98	0.32	85,85,85,85	0
58	MG	1H	3132	1/1	0.98	0.51	87,87,87,87	0
58	MG	13	1725	1/1	0.98	0.10	101,101,101,101	0
58	MG	13	1727	1/1	0.98	0.08	87,87,87,87	0
58	MG	1H	3003	1/1	0.98	0.58	72,72,72,72	0
58	MG	1H	3221	1/1	0.98	0.27	81,81,81,81	0
58	MG	1H	3080	1/1	0.98	0.27	73,73,73,73	0
58	MG	1H	3426	1/1	0.98	0.25	109,109,109,109	0
58	MG	14	3036	1/1	0.98	0.23	70,70,70,70	0
58	MG	14	3210	1/1	0.98	0.13	113,113,113,113	0
58	MG	13	1682	1/1	0.98	0.17	93,93,93,93	0
58	MG	14	3126	1/1	0.98	0.25	95,95,95,95	0
58	MG	14	3127	1/1	0.98	0.27	67,67,67,67	0
58	MG	1H	3224	1/1	0.98	0.55	76,76,76,76	0
58	MG	1H	3356	1/1	0.98	0.15	67,67,67,67	0
58	MG	1H	3357	1/1	0.98	0.11	79,79,79,79	0
58	MG	14	3131	1/1	0.98	0.33	79,79,79,79	0
58	MG	29	301	1/1	0.98	0.42	69,69,69,69	0
58	MG	14	3305	1/1	0.98	0.24	127,127,127,127	0
58	MG	1H	3138	1/1	0.98	0.17	67,67,67,67	0
58	MG	14	3133	1/1	0.98	0.39	98,98,98,98	0
58	MG	14	3220	1/1	0.98	0.40	97,97,97,97	0
58	MG	1H	3362	1/1	0.98	0.12	71,71,71,71	0
58	MG	13	1608	1/1	0.98	0.19	90,90,90,90	0
58	MG	1H	3364	1/1	0.98	0.20	74,74,74,74	0
58	MG	1H	3084	1/1	0.98	0.59	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	3138	1/1	0.98	0.18	96,96,96,96	0
58	MG	14	3049	1/1	0.98	0.49	74,74,74,74	0
58	MG	1G	1656	1/1	0.98	0.57	102,102,102,102	0
58	MG	14	3142	1/1	0.98	0.13	99,99,99,99	0
60	ZN	5I	102	1/1	0.98	0.14	114,114,114,114	0
58	MG	21	301	1/1	0.98	0.43	69,69,69,69	0
58	MG	1H	3367	1/1	0.98	0.18	84,84,84,84	0
58	MG	14	3053	1/1	0.98	0.56	82,82,82,82	0
58	MG	1H	3369	1/1	0.99	0.16	90,90,90,90	0
58	MG	14	3360	1/1	0.99	0.08	78,78,78,78	0
58	MG	14	3014	1/1	0.99	0.58	82,82,82,82	0
58	MG	14	3362	1/1	0.99	0.08	86,86,86,86	0
58	MG	1H	3407	1/1	0.99	0.15	83,83,83,83	0
58	MG	1H	3408	1/1	0.99	0.23	72,72,72,72	0
58	MG	1H	3051	1/1	0.99	0.32	90,90,90,90	0
58	MG	1H	3067	1/1	0.99	0.22	74,74,74,74	0
58	MG	1H	3456	1/1	0.99	0.23	68,68,68,68	0
58	MG	14	3290	1/1	0.99	0.29	113,113,113,113	0
58	MG	88	201	1/1	0.99	0.23	91,91,91,91	0
58	MG	14	3371	1/1	0.99	0.06	95,95,95,95	0
58	MG	13	1733	1/1	0.99	0.03	102,102,102,102	0
58	MG	1H	3087	1/1	0.99	0.29	69,69,69,69	0
58	MG	14	3374	1/1	0.99	0.17	107,107,107,107	0
58	MG	1G	1649	1/1	0.99	0.37	128,128,128,128	0
58	MG	13	1712	1/1	0.99	0.14	98,98,98,98	0
58	MG	1H	3414	1/1	0.99	0.21	79,79,79,79	0
58	MG	1H	3461	1/1	0.99	0.20	97,97,97,97	0
58	MG	13	1728	1/1	0.99	0.07	105,105,105,105	0
58	MG	14	3091	1/1	0.99	0.37	92,92,92,92	0
58	MG	14	3092	1/1	0.99	0.34	91,91,91,91	0
58	MG	1G	1601	1/1	0.99	0.20	115,115,115,115	0
58	MG	1H	3416	1/1	0.99	0.18	83,83,83,83	0
58	MG	13	1715	1/1	0.99	0.20	113,113,113,113	0
58	MG	1H	3091	1/1	0.99	0.49	58,58,58,58	0
58	MG	14	3097	1/1	0.99	0.29	83,83,83,83	0
58	MG	1G	1605	1/1	0.99	0.37	125,125,125,125	0
58	MG	14	3388	1/1	0.99	0.23	88,88,88,88	0
58	MG	1H	3466	1/1	0.99	0.07	94,94,94,94	0
58	MG	14	3100	1/1	0.99	0.10	107,107,107,107	0
58	MG	1H	3072	1/1	0.99	0.17	120,120,120,120	0
58	MG	14	3392	1/1	0.99	0.05	89,89,89,89	0
58	MG	14	3035	1/1	0.99	0.29	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	13	1711	1/1	0.99	0.18	85,85,85,85	0
58	MG	14	3037	1/1	0.99	0.18	80,80,80,80	0
58	MG	1H	3013	1/1	0.99	0.42	71,71,71,71	0
58	MG	14	3039	1/1	0.99	0.58	86,86,86,86	0
58	MG	1H	3422	1/1	0.99	0.15	102,102,102,102	0
58	MG	14	3399	1/1	0.99	0.03	116,116,116,116	0
58	MG	14	3400	1/1	0.99	0.11	113,113,113,113	0
58	MG	13	1731	1/1	0.99	0.08	108,108,108,108	0
58	MG	14	3042	1/1	0.99	0.26	74,74,74,74	0
58	MG	1H	3424	1/1	0.99	0.12	81,81,81,81	0
58	MG	2K	101	1/1	0.99	0.43	84,84,84,84	0
58	MG	1H	3045	1/1	0.99	0.37	68,68,68,68	0
58	MG	1H	3384	1/1	0.99	0.20	87,87,87,87	0
58	MG	1H	3358	1/1	0.99	0.12	70,70,70,70	0
58	MG	1H	3359	1/1	0.99	0.15	71,71,71,71	0
58	MG	1H	3388	1/1	0.99	0.12	78,78,78,78	0
58	MG	1H	3360	1/1	0.99	0.16	86,86,86,86	0
58	MG	1H	3391	1/1	0.99	0.19	79,79,79,79	0
58	MG	1H	3046	1/1	0.99	0.29	61,61,61,61	0
58	MG	1H	3393	1/1	0.99	0.08	95,95,95,95	0
58	MG	1H	3435	1/1	0.99	0.07	85,85,85,85	0
58	MG	1H	3484	1/1	0.99	0.18	81,81,81,81	0
58	MG	1H	3025	1/1	0.99	0.36	55,55,55,55	0
58	MG	13	1726	1/1	0.99	0.07	91,91,91,91	0
58	MG	14	3125	1/1	0.99	0.30	102,102,102,102	0
58	MG	14	3419	1/1	0.99	0.09	90,90,90,90	0
58	MG	1H	3049	1/1	0.99	0.47	82,82,82,82	0
58	MG	2L	101	1/1	0.99	0.52	97,97,97,97	0
58	MG	1H	3082	1/1	0.99	0.48	79,79,79,79	0
58	MG	1H	3440	1/1	0.99	0.12	70,70,70,70	0
58	MG	1H	3441	1/1	0.99	0.13	92,92,92,92	0
58	MG	14	3002	1/1	0.99	0.12	65,65,65,65	0
58	MG	14	3064	1/1	0.99	0.13	86,86,86,86	0
58	MG	1H	3366	1/1	0.99	0.10	73,73,73,73	0
58	MG	1H	3399	1/1	0.99	0.18	75,75,75,75	0
58	MG	14	3343	1/1	0.99	0.20	87,87,87,87	0
58	MG	14	3344	1/1	0.99	0.08	91,91,91,91	0
58	MG	14	3345	1/1	0.99	0.16	80,80,80,80	0
58	MG	1H	3400	1/1	0.99	0.19	86,86,86,86	0
58	MG	1H	3050	1/1	0.99	0.23	74,74,74,74	0
58	MG	1H	3402	1/1	0.99	0.10	76,76,76,76	0
58	MG	1H	3403	1/1	0.99	0.13	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	3404	1/1	0.99	0.06	84,84,84,84	0
58	MG	1H	3449	1/1	0.99	0.13	89,89,89,89	0
58	MG	14	3141	1/1	0.99	0.29	76,76,76,76	0
58	MG	14	3354	1/1	0.99	0.11	87,87,87,87	0
59	SF4	3E	301	8/8	0.99	0.18	95,111,117,118	0
59	SF4	32	302	8/8	0.99	0.14	127,146,153,155	0
58	MG	14	3073	1/1	0.99	0.15	67,67,67,67	0
58	MG	1H	3368	1/1	0.99	0.21	76,76,76,76	0
58	MG	14	3357	1/1	0.99	0.07	76,76,76,76	0
58	MG	14	3012	1/1	0.99	0.38	67,67,67,67	0
58	MG	1H	3387	1/1	1.00	0.18	60,60,60,60	0
58	MG	14	3363	1/1	1.00	0.23	80,80,80,80	0
58	MG	1H	3389	1/1	1.00	0.12	71,71,71,71	0
58	MG	14	3349	1/1	1.00	0.18	95,95,95,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.