wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 03:23 am GMT

PDB ID	:	5EL4
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and tRNALys in the A-site with a U-U mismatch in the first 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:

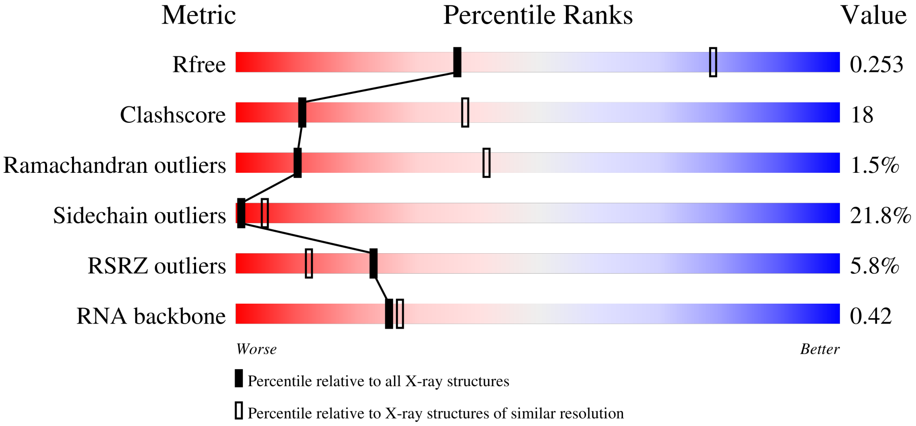
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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
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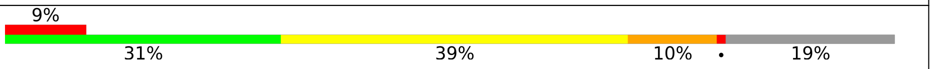
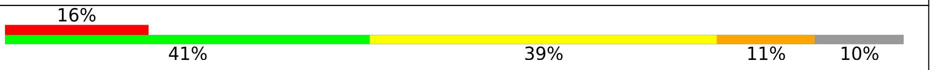
1	1G	1522	
2	12	256	
2	1E	256	

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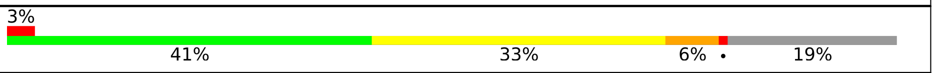
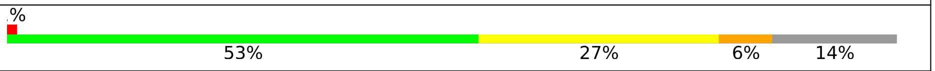
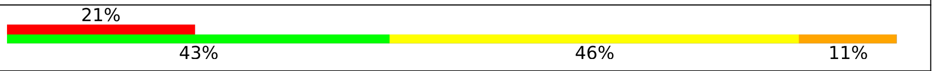
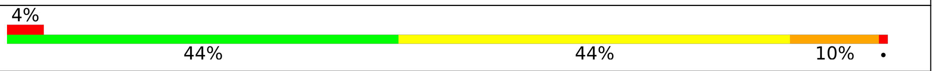
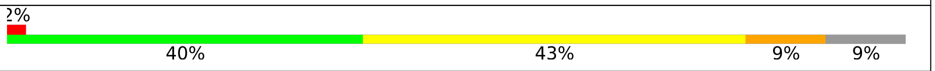
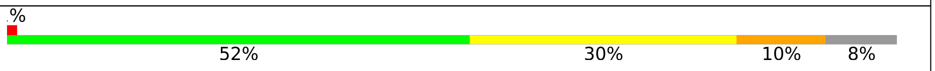
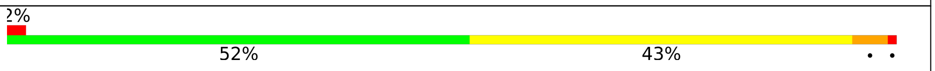
Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
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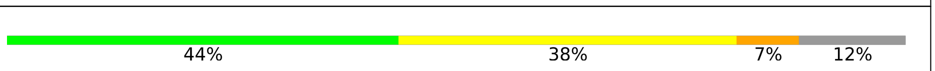
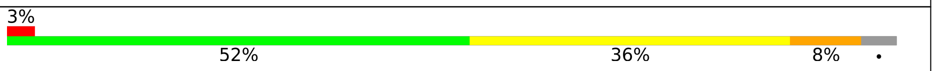
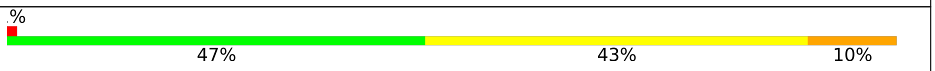
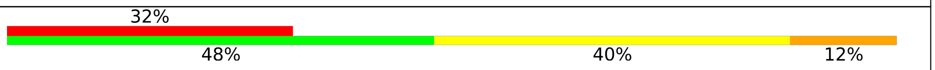
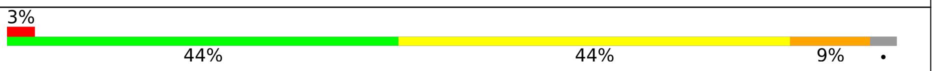
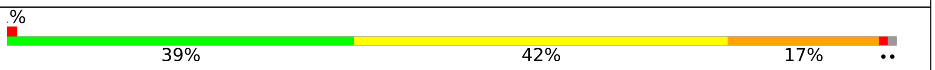
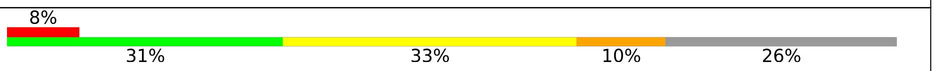
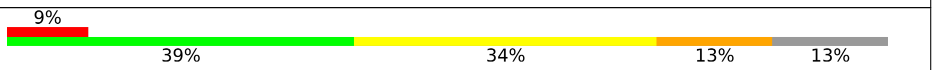
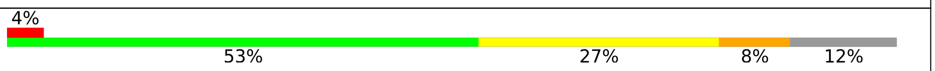
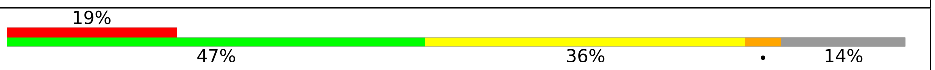
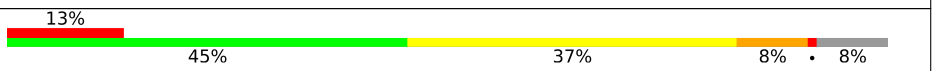
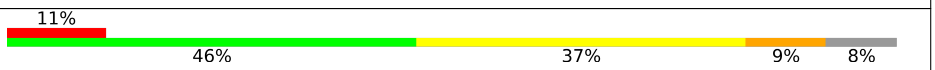
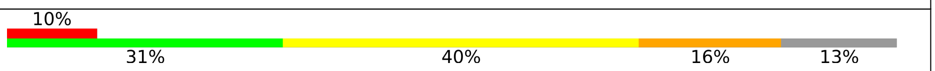
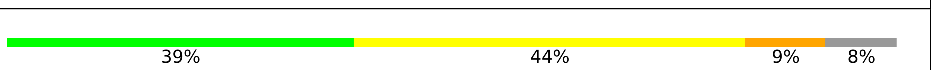
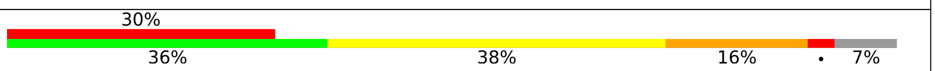
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
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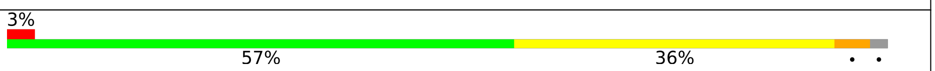
15	6A	89	

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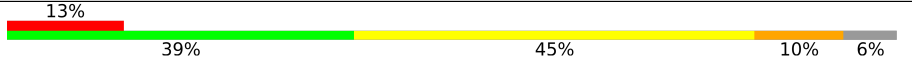
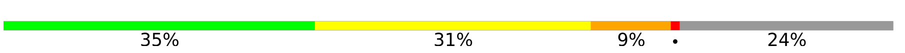
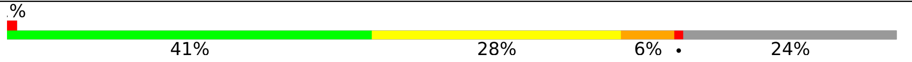
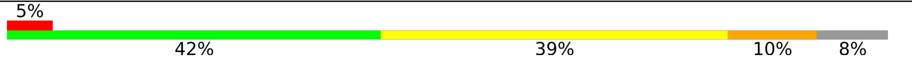
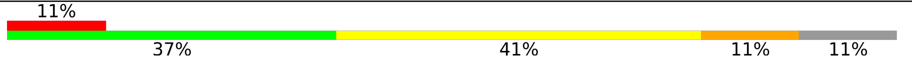
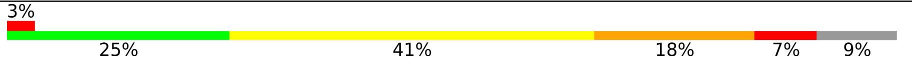
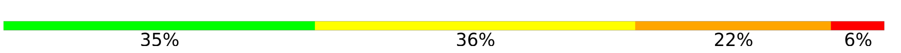
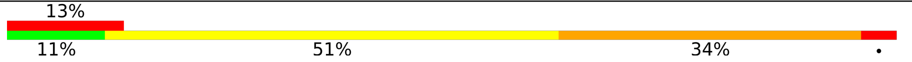
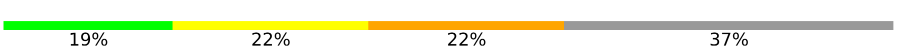
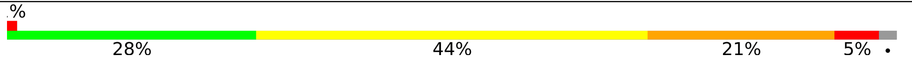
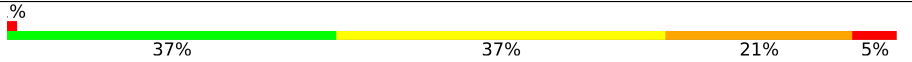
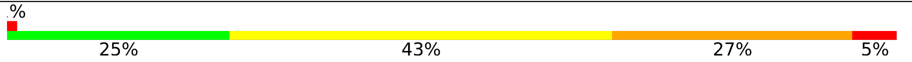
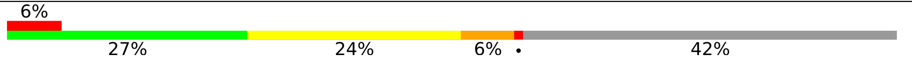
Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	71	229	
29	11	276	

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Mol	Chain	Length	Quality of chain
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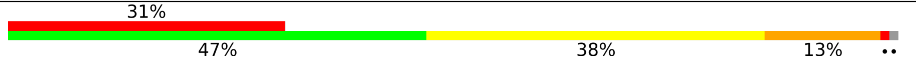
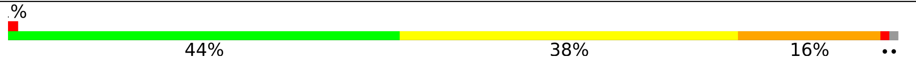
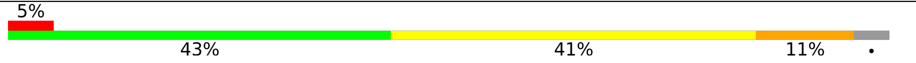
30	21	206	
30	29	206	
31	31	210	
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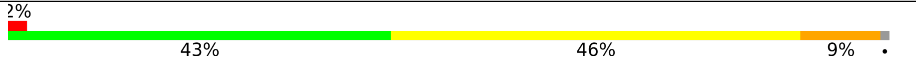
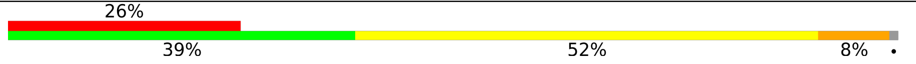
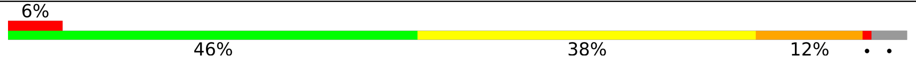
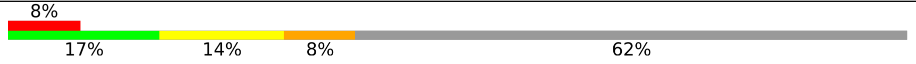
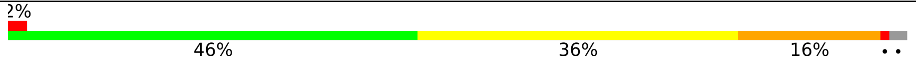
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
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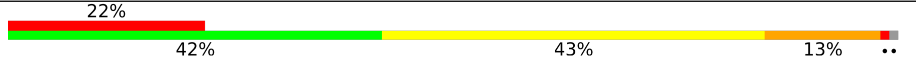
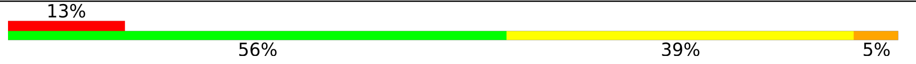
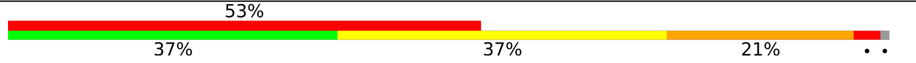
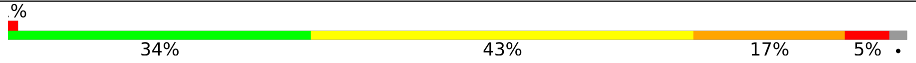
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
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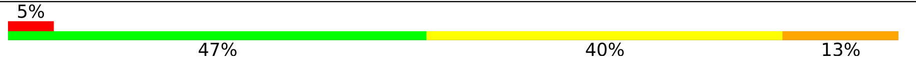
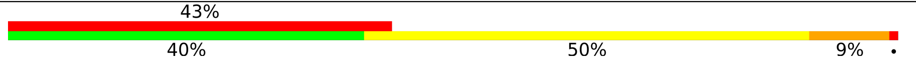
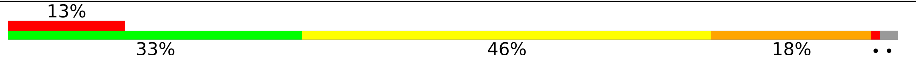
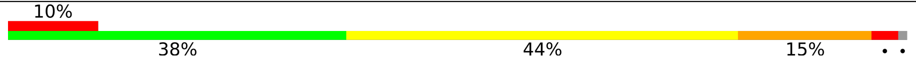
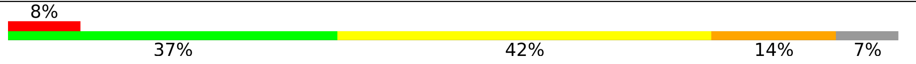
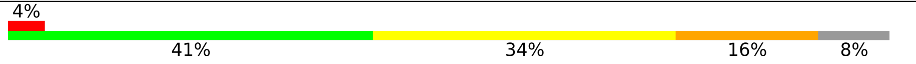
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	
41	B8	146	

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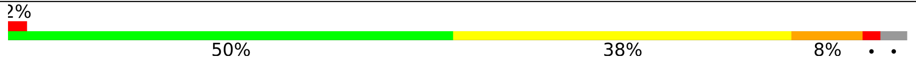
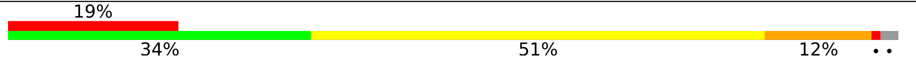
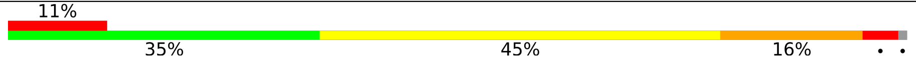
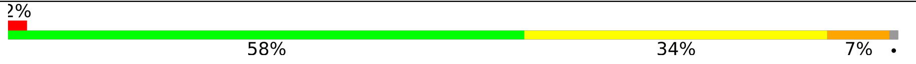
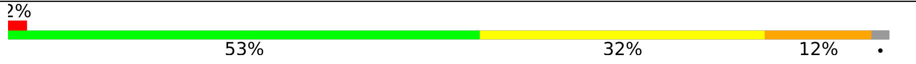
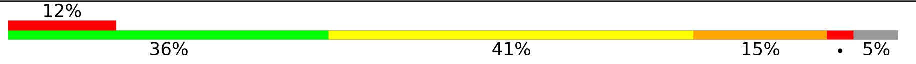
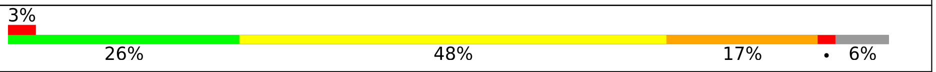
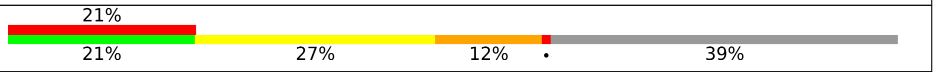
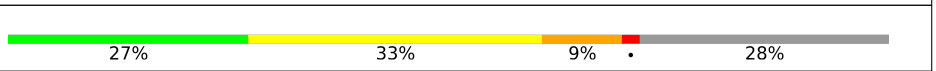
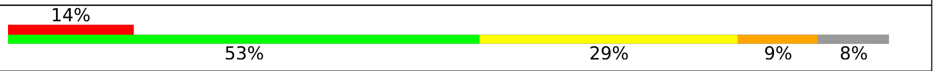
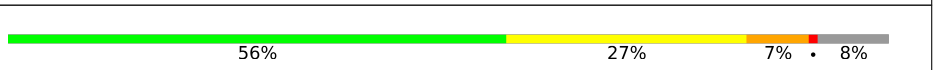
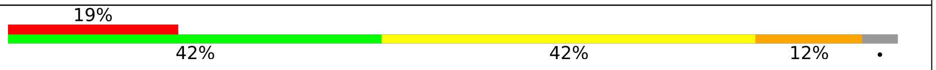
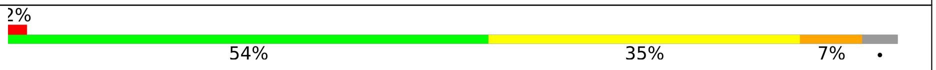
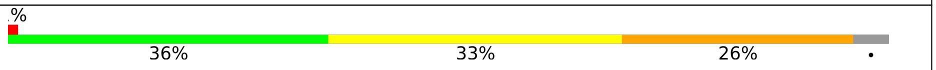
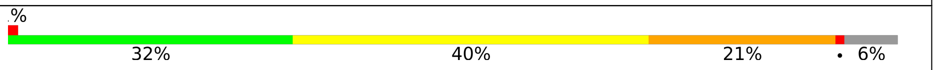
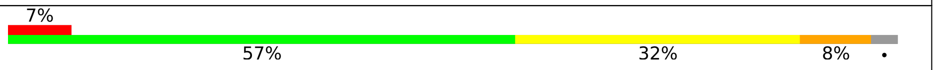
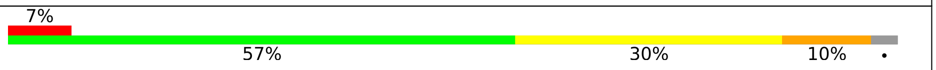
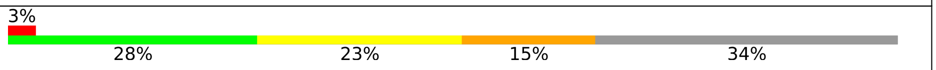
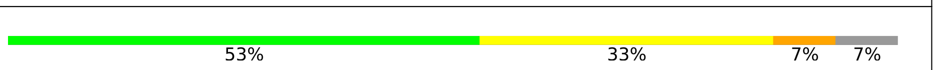
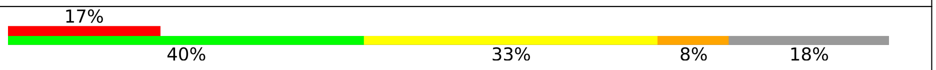
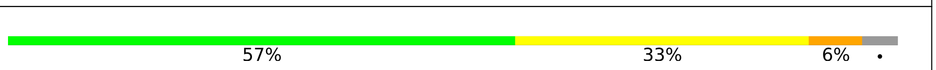
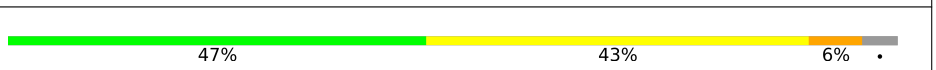
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	

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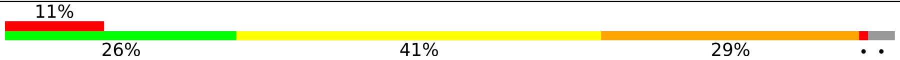
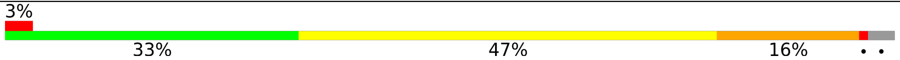
Mol	Chain	Length	Quality of chain
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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	1607	-	-	-	X
58	MG	13	1628	-	-	-	X
58	MG	13	1669	-	-	-	X
58	MG	13	1694	-	-	-	X
58	MG	13	1696	-	-	-	X
58	MG	14	3013	-	-	-	X
58	MG	14	3014	-	-	-	X
58	MG	14	3068	-	-	-	X
58	MG	14	3102	-	-	-	X
58	MG	14	3122	-	-	-	X
58	MG	14	3126	-	-	-	X
58	MG	14	3139	-	-	-	X
58	MG	14	3152	-	-	-	X
58	MG	14	3153	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3216	-	-	-	X
58	MG	14	3221	-	-	-	X
58	MG	14	3222	-	-	-	X
58	MG	14	3225	-	-	-	X
58	MG	14	3229	-	-	-	X
58	MG	14	3240	-	-	-	X
58	MG	14	3246	-	-	-	X
58	MG	14	3254	-	-	-	X
58	MG	14	3257	-	-	-	X
58	MG	14	3263	-	-	-	X
58	MG	14	3273	-	-	-	X
58	MG	14	3277	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1627	-	-	-	X
58	MG	1G	1628	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1G	1635	-	-	-	X
58	MG	1G	1657	-	-	-	X
58	MG	1H	3027	-	-	-	X
58	MG	1H	3035	-	-	-	X
58	MG	1H	3149	-	-	-	X
58	MG	1H	3175	-	-	-	X
58	MG	1H	3184	-	-	-	X
58	MG	1H	3188	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3205	-	-	-	X
58	MG	1H	3207	-	-	-	X
58	MG	1H	3234	-	-	-	X
58	MG	1H	3255	-	-	-	X
58	MG	1H	3264	-	-	-	X
58	MG	1H	3276	-	-	-	X
58	MG	1H	3279	-	-	-	X
58	MG	1H	3301	-	-	-	X
58	MG	1K	101	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	2K	102	-	-	-	X
58	MG	2L	102	-	-	-	X
58	MG	45	203	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 294304 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	1496	Total C N O P 32157 14313 5960 10388 1496	0	0	0
1	1G	1507	Total C N O P 32391 14418 6004 10463 1506	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	1E	231	Total C N O S 1874 1199 334 336 5	0	0	0
2	12	208	Total C N O S 1711 1094 307 306 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 C N O S 1605 1011 313 280 1	0	0	0
3	22	194	Total C N O S 1529 967 296 265 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	4E	149	Total C N O S 1142 722 216 200 4	0	0	0
5	42	147	Total C N O S 1123 709 214 196 4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	6E	149	Total C N O S 1214 754 244 210 6	0	0	0
7	62	138	Total C N O S 1110 689 221 194 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	7E	138	Total C N O S 1115 705 215 192 3	0	0	0
8	72	138	Total C N O S 1115 705 215 192 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	8E	127	Total C N O 1005 637 197 171	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	82	124	Total C N O 983 624 190 169	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1I	91	Total C N O S 734 459 144 130 1	0	0	0
10	1A	78	Total C N O 626 388 126 112	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	116	Total C N O S 928 574 191 161 2	0	0	0
13	4A	110	Total C N O S 888 549 182 155 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	61	Total C N O S 496 315 105 72 4	0	0	0
14	5A	57	Total C N O S 466 297 97 68 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	6I	88	Total C N O S 733 459 147 125 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	99	Total C N O S 823 528 151 142 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	80	Total C N O S 643 411 118 112 2	0	0	0
19	AA	60	Total C N O S 471 300 83 86 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	98	Total	C	N	O	S	0	0	0
			757	467	161	127	2			

- 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	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called tRNA-Lys.

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 tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	295	528	76	1			

- Molecule 24 is a RNA chain called tRNA-Lys.

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
			Total	C	N	O	P			
26	1H	2833	61028	27159	11418	19618	2833	0	0	0
26	14	2861	61630	27429	11535	19806	2860	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	16	122	2617	1166	486	844	121	0	0	0
27	1J	122	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
			Total	C	N	O	S			
28	71	133	1033	651	194	187	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
71	19	ILE	VAL	conflict	UNP Q5SLP7
71	27	HIS	ARG	conflict	UNP Q5SLP7

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	11	274	Total C N O S 2125 1341 422 359 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	204	Total C N O S 1563 988 299 270 6	0	0	0
30	29	204	Total C N O S 1563 988 299 270 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	31	202	Total C N O S 1585 1011 297 275 2	0	0	0
31	39	205	Total C N O S 1606 1024 300 280 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	41	180	Total C N O S 1464 936 266 258 4	0	0	0
32	49	180	Total C N O S 1464 936 266 258 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	51	173	Total C N O S 1327 842 249 235 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
			Total	C	N	O	S			
34	61	145	1131	723	200	207	1	0	0	0
34	69	145	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
			Total	C	N	O	S			
35	58	138	1104	712	206	182	4	0	0	0
35	15	137	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
			Total	C	N	O	S			
36	68	122	932	588	171	169	4	0	0	0
36	25	122	932	588	171	169	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	78	147	1122	698	229	192	3	0	0	0
37	35	148	1130	704	230	193	3	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	134	Total 1118	C 696	N 229	O 192	S 1	0	0	0
41	75	136	Total 1132	C 704	N 232	O 195	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total 774	C 499	N 141	O 133	S 1	0	0	0
43	95	99	Total 763	C 493	N 137	O 132	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total 890	C 560	N 175	O 153	S 2	0	0	0
44	A5	111	Total 886	C 558	N 174	O 152	S 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	F8	96	Total C N O 751 489 135 127	0	0	0
45	B5	94	Total C N O S 738 479 133 125 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	G8	103	Total C N O S 783 504 148 126 5	0	0	0
46	C5	104	Total C N O S 794 510 152 127 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	H8	148	Total C N O S 1222 781 221 217 3	0	0	0
47	D5	126	Total C N O S 1034 667 187 178 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	I8	78	Total C N O S 616 381 130 104 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
			Total	C	N	O	S			
50	K8	68	571	355	115	100	1	0	0	0
50	G5	69	573	355	116	101	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	N8	49	381	238	76	62	5	0	0	0
53	J5	56	434	272	87	70	5	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	Q8	64	516	331	102	81	2	0	0	0
55	M5	64	516	331	102	81	2	0	0	0

- Molecule 56 is a RNA chain called tRNA-Lys.

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 tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
57	3L	74	1571	703	277	518	73	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	13	142	142	142	0	0
58	1I	1	1	1	0	0
58	2I	1	1	1	0	0
58	3I	1	1	1	0	0
58	4I	1	1	1	0	0
58	5I	1	1	1	0	0
58	7I	1	1	1	0	0
58	1K	1	1	1	0	0
58	2K	2	2	2	0	0
58	4K	1	1	1	0	0
58	1H	495	495	495	0	0
58	16	11	11	11	0	0
58	11	1	1	1	0	0
58	21	2	2	2	0	0
58	41	1	1	1	0	0

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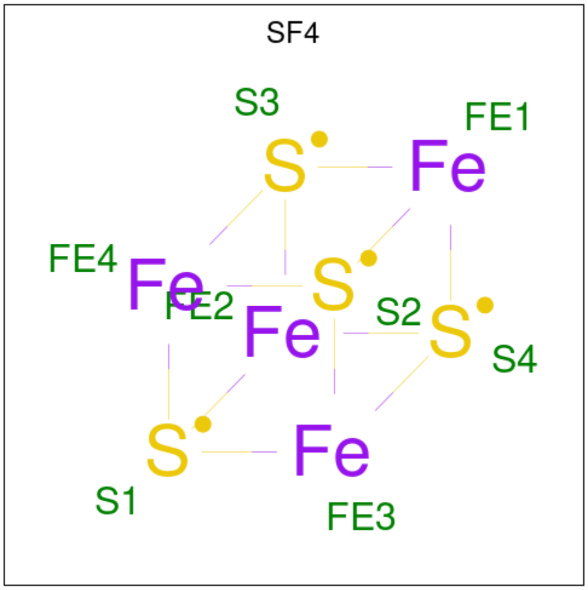
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	78	1	Total Mg 1 1	0	0
58	88	3	Total Mg 3 3	0	0
58	I8	1	Total Mg 1 1	0	0
58	J8	1	Total Mg 1 1	0	0
58	N8	1	Total Mg 1 1	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	95	Total Mg 95 95	0	0
58	2L	2	Total Mg 2 2	0	0
58	3L	1	Total Mg 1 1	0	0
58	14	421	Total Mg 421 421	0	0
58	1J	6	Total Mg 6 6	0	0
58	19	1	Total Mg 1 1	0	0
58	29	3	Total Mg 3 3	0	0
58	39	2	Total Mg 2 2	0	0
58	25	1	Total Mg 1 1	0	0
58	45	3	Total Mg 3 3	0	0
58	E5	1	Total Mg 1 1	0	0

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



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	207	Total O 207 207	0	0
61	3E	2	Total O 2 2	0	0
61	4E	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	8E	1	Total O 1 1	0	0
61	1I	1	Total O 1 1	0	0
61	3I	2	Total O 2 2	0	0
61	5I	2	Total O 2 2	0	0
61	6I	1	Total O 1 1	0	0
61	4K	4	Total O 4 4	0	0
61	1H	819	Total O 819 819	0	0
61	16	22	Total O 22 22	0	0
61	11	9	Total O 9 9	0	0
61	21	6	Total O 6 6	0	0
61	31	4	Total O 4 4	0	0
61	78	1	Total O 1 1	0	0
61	B8	1	Total O 1 1	0	0
61	C8	3	Total O 3 3	0	0
61	F8	1	Total O 1 1	0	0
61	I8	5	Total O 5 5	0	0
61	J8	2	Total O 2 2	0	0
61	L8	3	Total O 3 3	0	0
61	1G	117	Total O 117 117	0	0
61	32	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0

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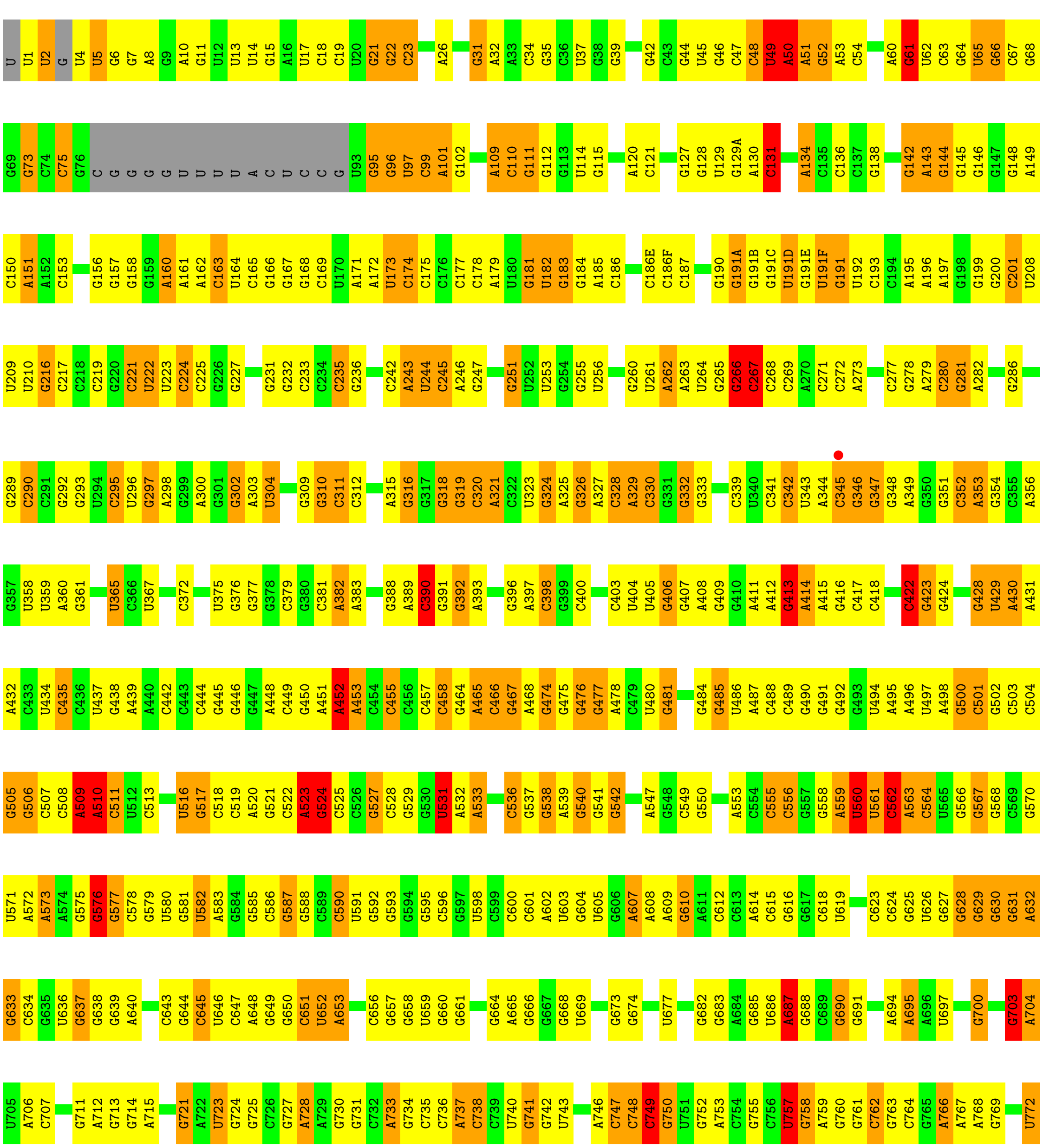
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	6A	2	Total O 2 2	0	0
61	7A	1	Total O 1 1	0	0
61	BA	1	Total O 1 1	0	0
61	14	717	Total O 717 717	0	0
61	1J	6	Total O 6 6	0	0
61	19	10	Total O 10 10	0	0
61	29	3	Total O 3 3	0	0
61	39	3	Total O 3 3	0	0
61	15	1	Total O 1 1	0	0
61	35	3	Total O 3 3	0	0
61	75	2	Total O 2 2	0	0
61	85	3	Total O 3 3	0	0
61	M5	3	Total O 3 3	0	0

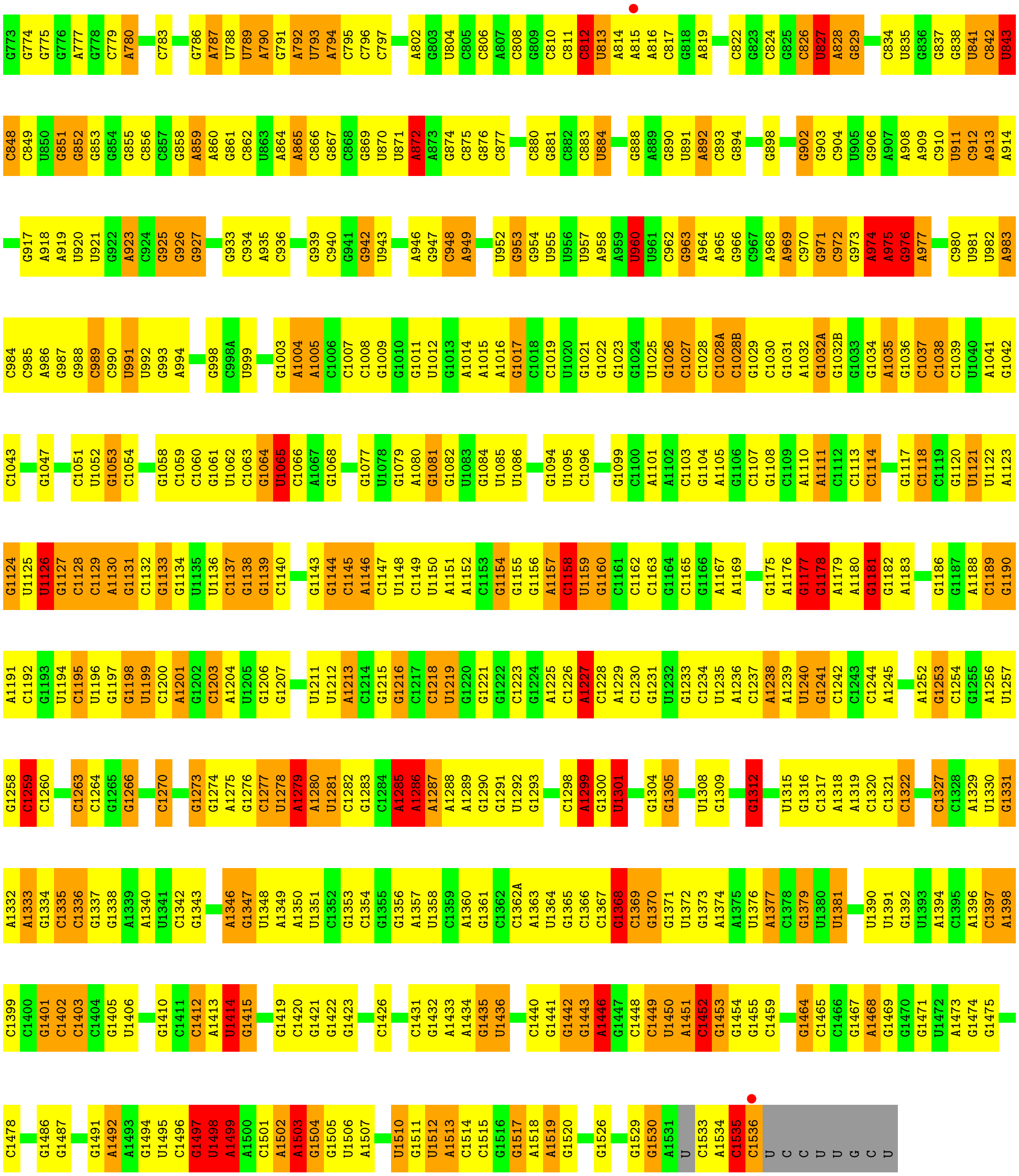
3 Residue-property plots ⓘ

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

- Molecule 1: 16S ribosomal RNA

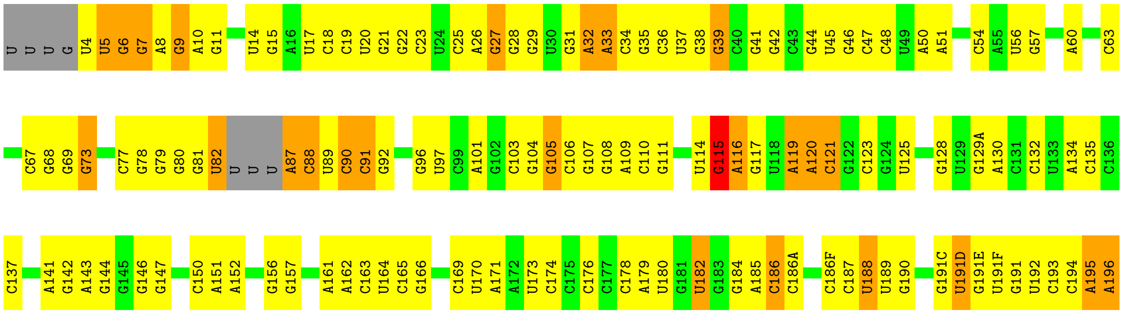
Chain 13:

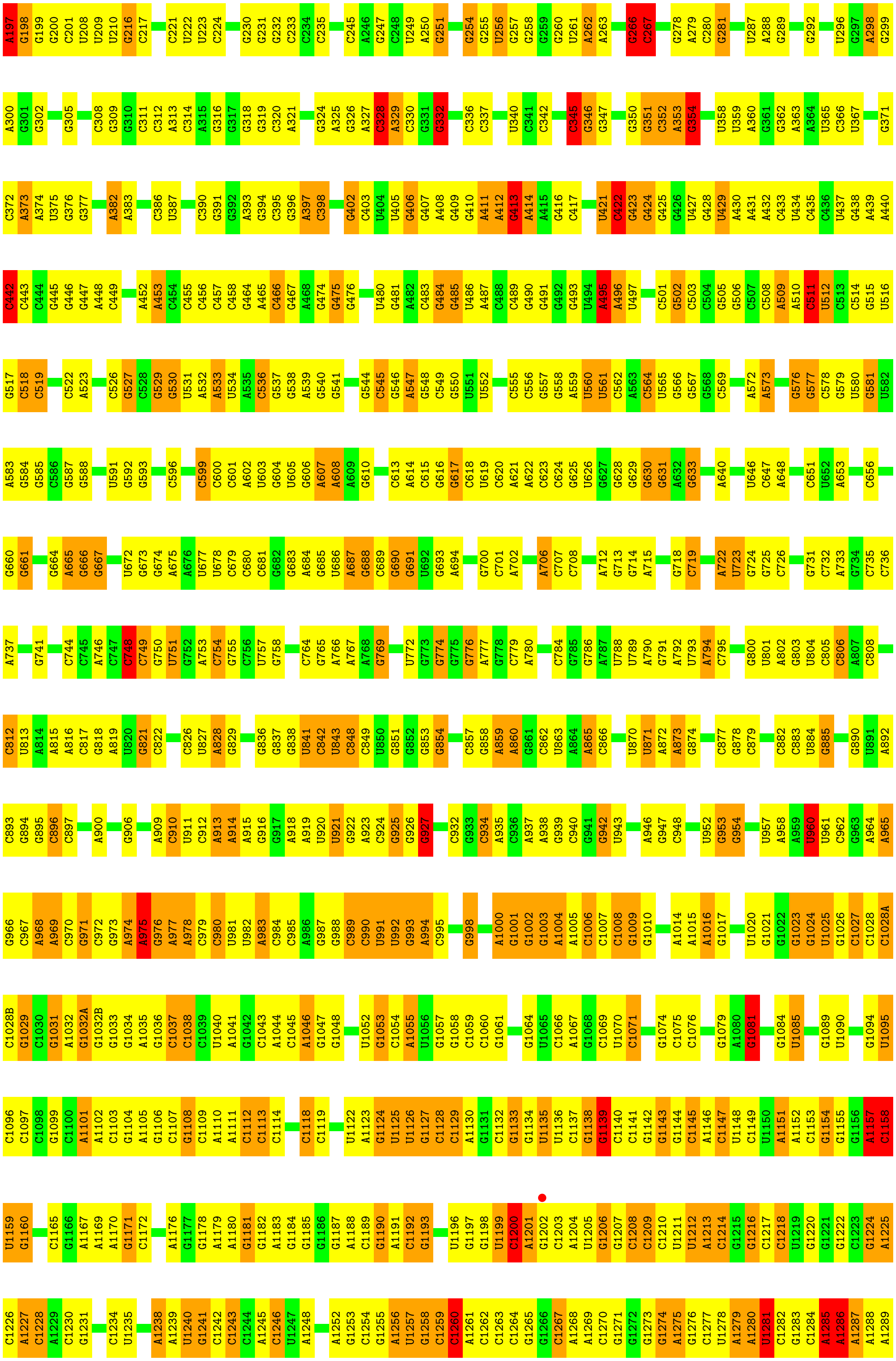


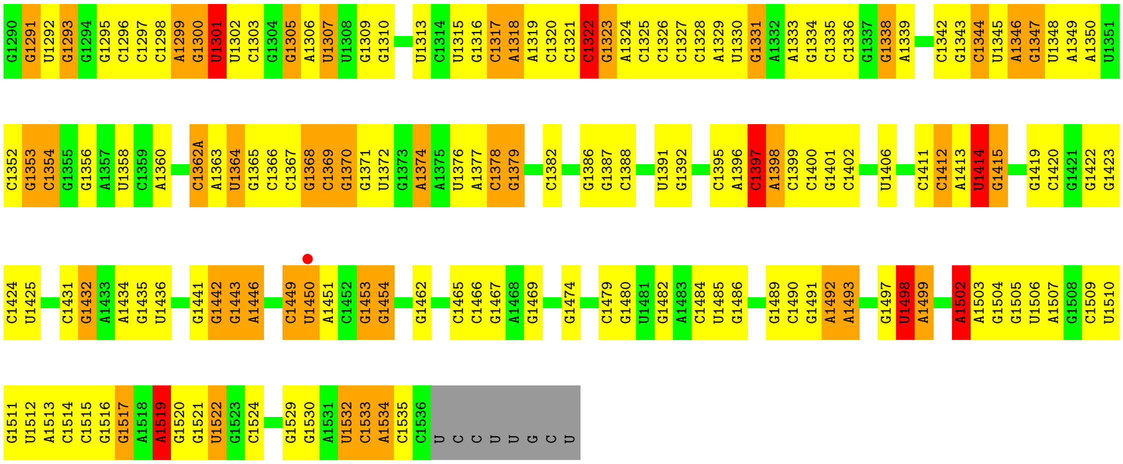


- Molecule 1: 16S ribosomal RNA

Chain 1G:

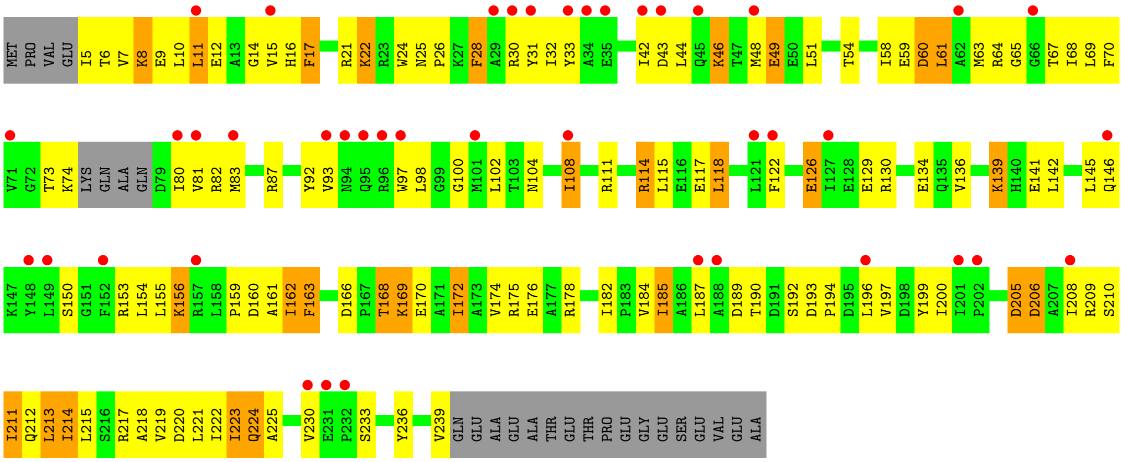



A197 G198 G199 G200 C201 U208 U209 U210 G216 C217 C221 U222 U223 C224 G230 G231 G232 C233 C234 C235 C245 A246 G247 C248 U249 A250 G251 G254 G255 U256 G257 G258 G259 G260 U261 A262 A263 G266 C267 G278 A279 C280 G281 U287 A288 G289 G292 U296 G297 A298 G299
A300 G301 G302 G305 C308 G309 G310 C311 C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 G324 A325 G326 A327 C328 A329 C330 G331 G332 C336 C337 U340 C341 C342 C345 G346 G347 G350 G351 C352 A353 G354 U358 U359 A360 G361 G362 A363 A364 U365 C366 U367 G371
C372 A373 A374 U375 C376 G377 A382 A383 C386 U387 C390 G391 G392 A393 G394 C395 G396 A397 C398 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 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 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 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516
G517 C518 C519 C522 A523 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 C540 G541 G544 C545 G546 A547 G548 C549 G550 U551 U552 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 C569 A572 A573 G576 C577 C578 G579 U580 G581 U582
A583 G584 G585 C586 G587 G588 U591 G592 G593 C596 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 G610 C613 A614 C615 G616 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 A640 U646 C647 A648 C651 U652 A653 C656
G660 G661 G664 A665 G666 G667 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 G700 C701 A702 A706 C707 C708 A712 G713 G714 A715 G718 C719 A722 U723 G724 G725 C726 G731 C732 A733 G734 C735 C736
A737 G741 C744 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 C764 G765 A766 A767 A768 G769 U772 G773 G774 G775 G776 A777 G778 C779 A780 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 G800 U801 A802 G803 U804 C805 C806 A807 C808
C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 C826 U827 A828 G829 G836 G837 G838 U841 C842 U843 C848 C849 U850 G851 G852 G853 G854 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 U870 U871 A872 A873 G874 C877 G878 C879 C882 C883 U884 G885 G890 U891 A892
C893 G894 G895 C896 C897 A900 G906 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 A946 G947 C948 U952 G953 G954 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 G998 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 A1014 A1015 A1016 G1017 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A
C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1074 C1075 C1076 G1079 A1080 G1081 G1084 U1085 G1089 U1090 G1094 U1095
C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1118 C1119 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 C1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158
U1159 G1160 C1165 G1166 A1167 A1169 A1170 G1171 C1172 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 C1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 C1222 C1223 G1224 A1225
C1226 A1227 C1228 A1229 C1230 G1231 C1234 U1235 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 U1247 A1248 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289



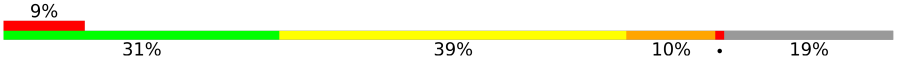
- Molecule 2: 30S ribosomal protein S2

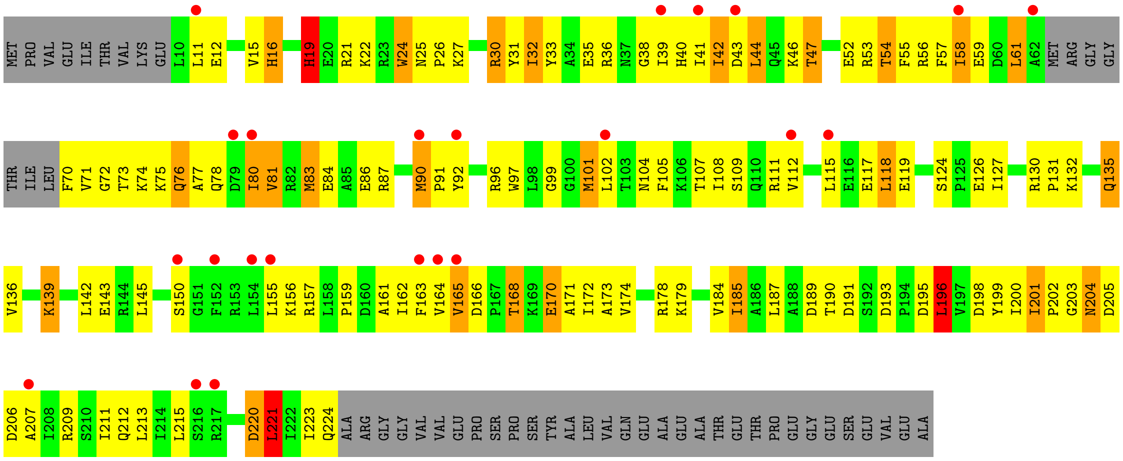
Chain 1E:



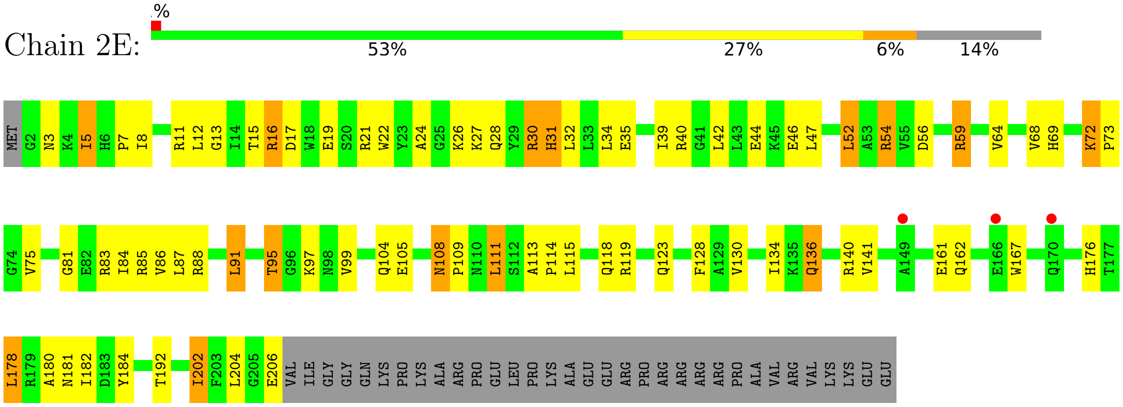
- Molecule 2: 30S ribosomal protein S2

Chain 12:

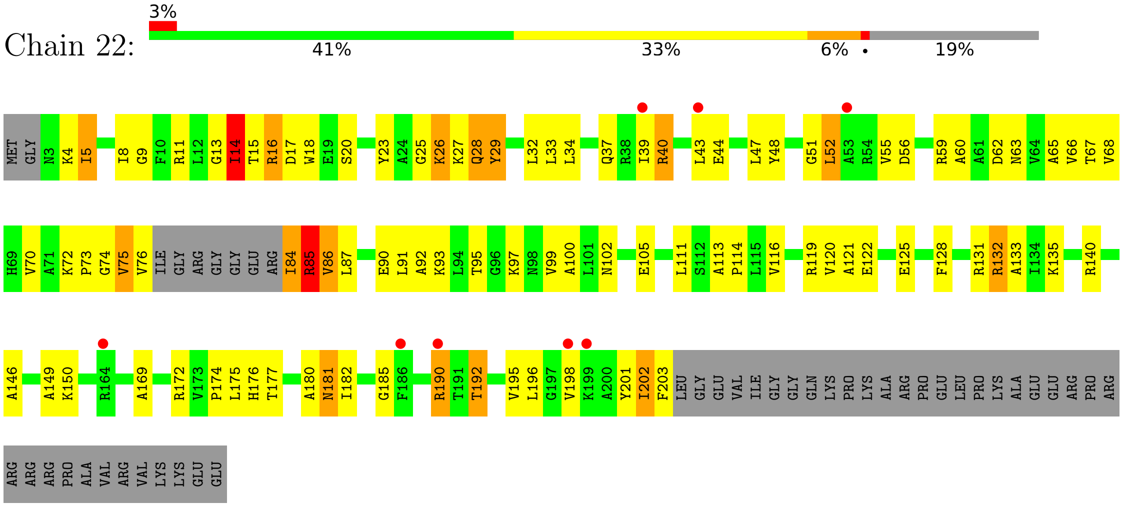




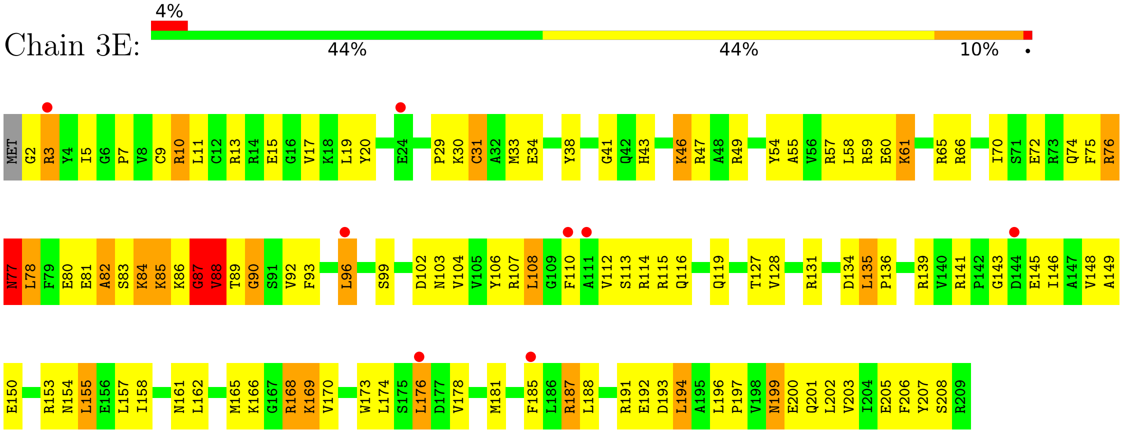
- Molecule 3: 30S ribosomal protein S3



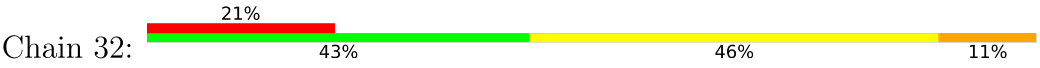
- Molecule 3: 30S ribosomal protein S3

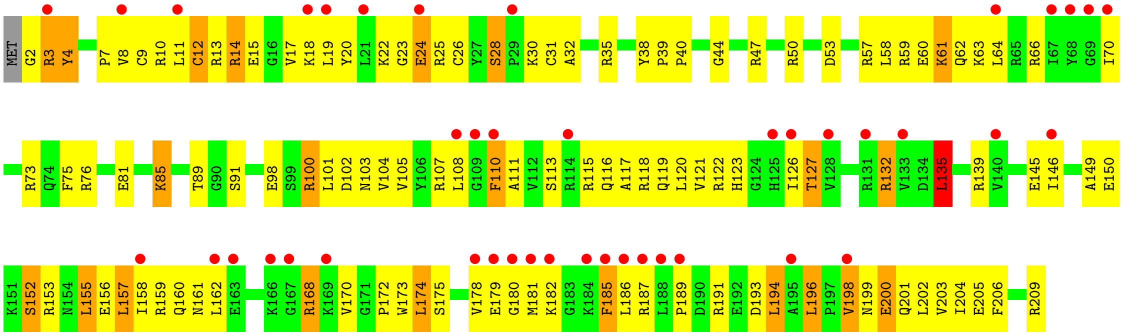


- Molecule 4: 30S ribosomal protein S4



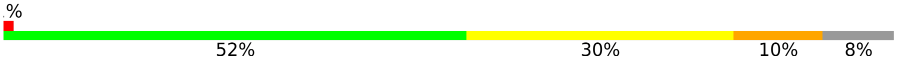
- Molecule 4: 30S ribosomal protein S4

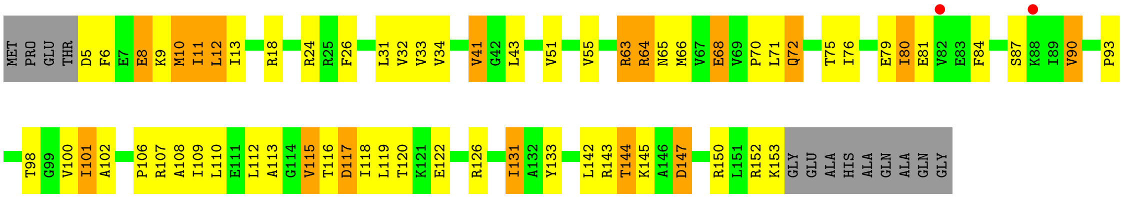




- Molecule 5: 30S ribosomal protein S5

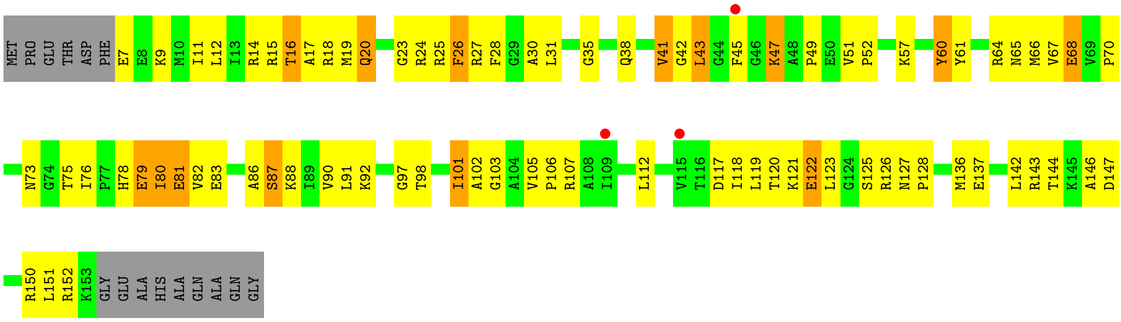
Chain 4E:





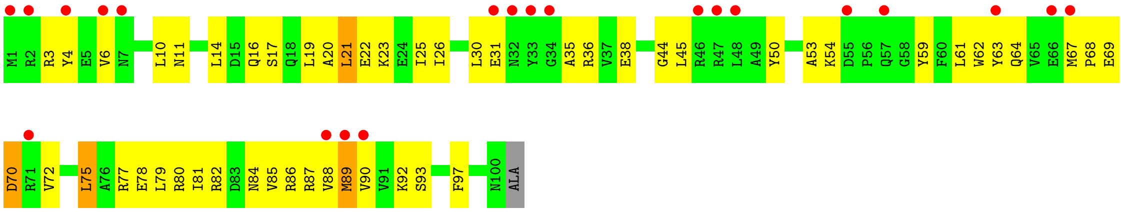
- Molecule 5: 30S ribosomal protein S5

Chain 42:



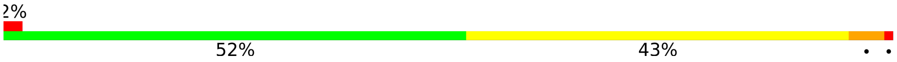
- Molecule 6: 30S ribosomal protein S6

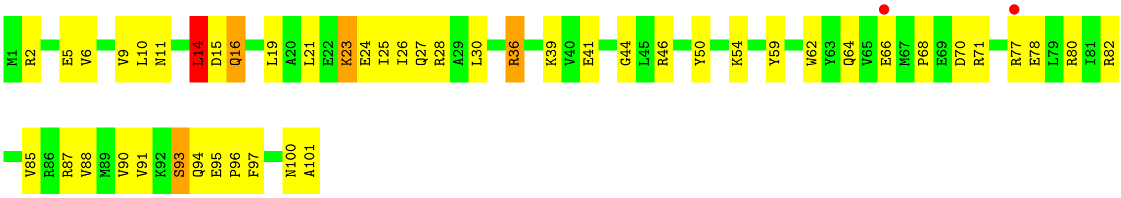
Chain 5E:



- Molecule 6: 30S ribosomal protein S6

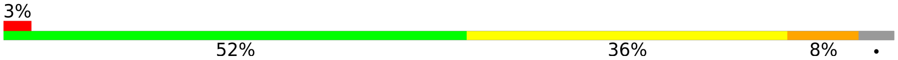
Chain 52:

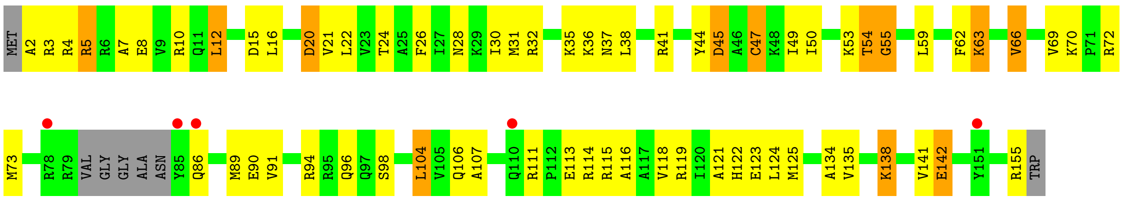




- Molecule 7: 30S ribosomal protein S7

Chain 6E:



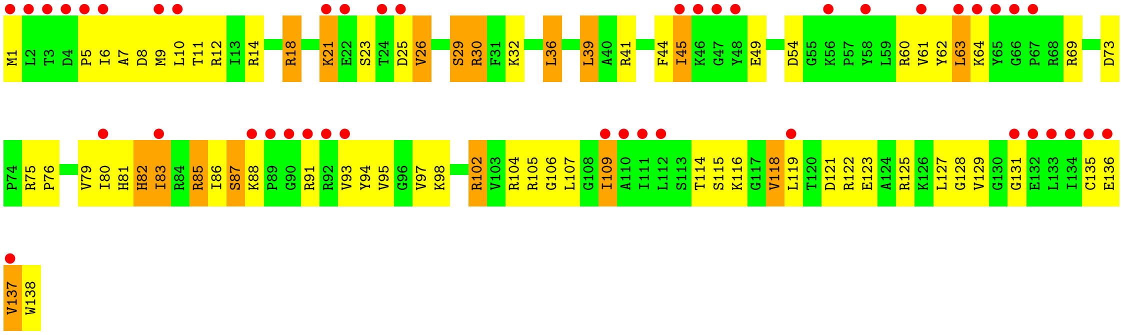


- Molecule 7: 30S ribosomal protein S7

Chain 62:

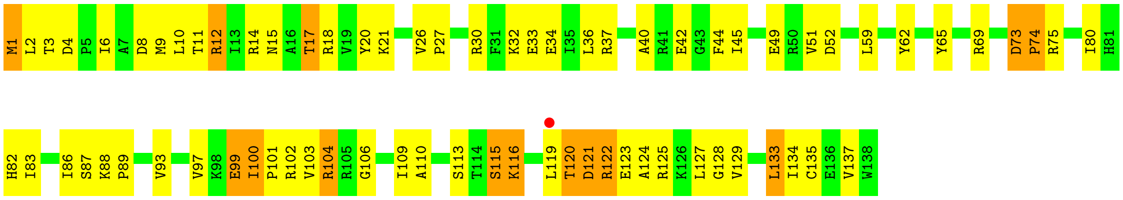
- Molecule 8: 30S ribosomal protein S8

Chain 7E:

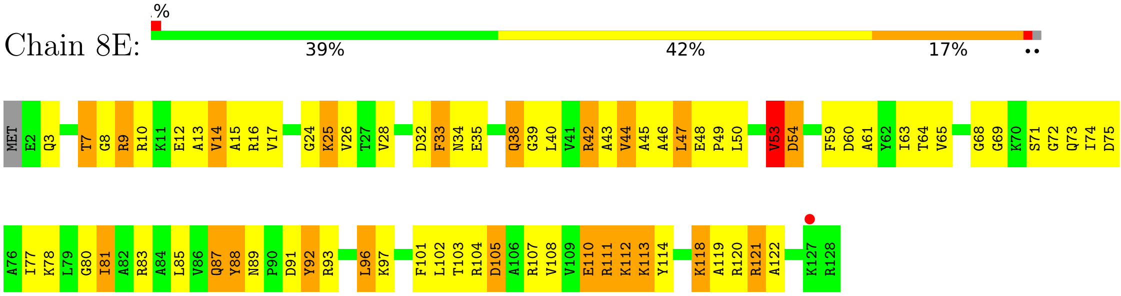


- Molecule 8: 30S ribosomal protein S8

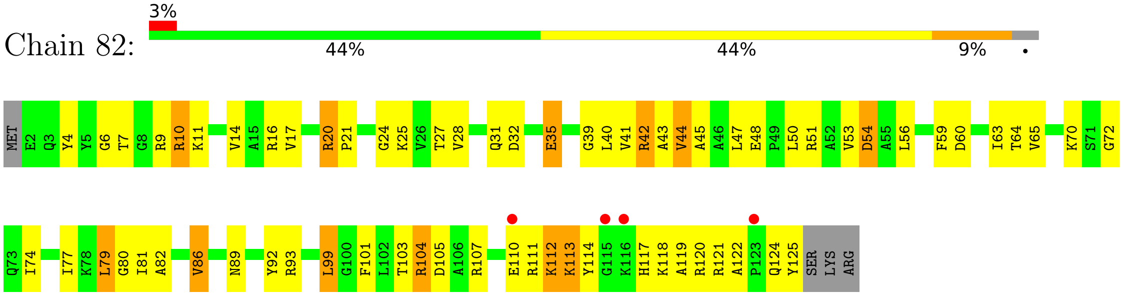
Chain 72:



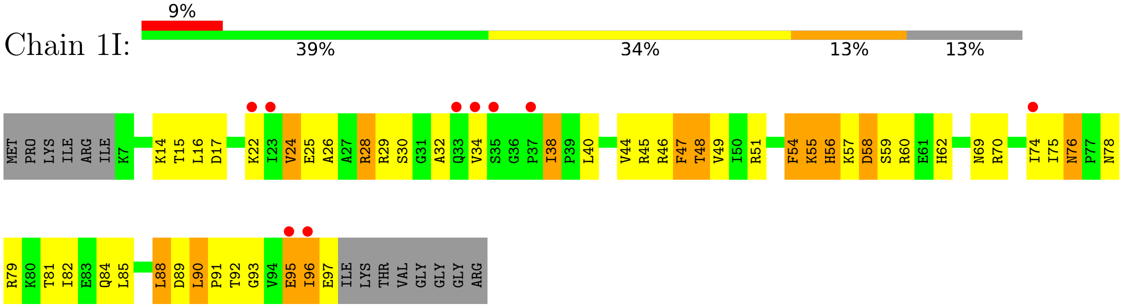
- Molecule 9: 30S ribosomal protein S9



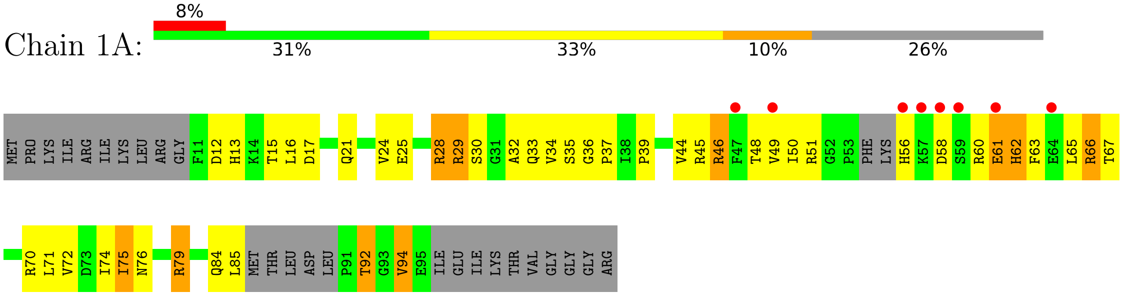
- Molecule 9: 30S ribosomal protein S9



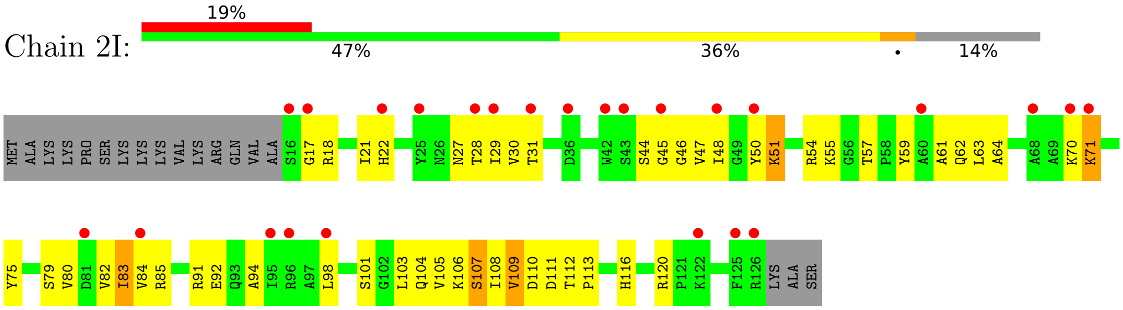
- Molecule 10: 30S ribosomal protein S10



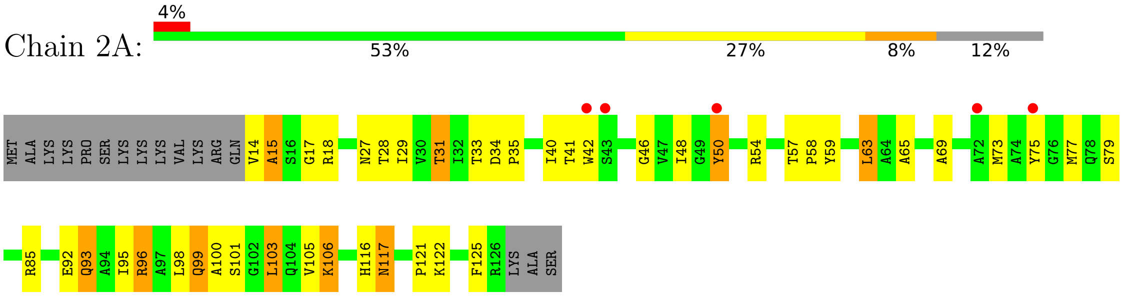
- Molecule 10: 30S ribosomal protein S10



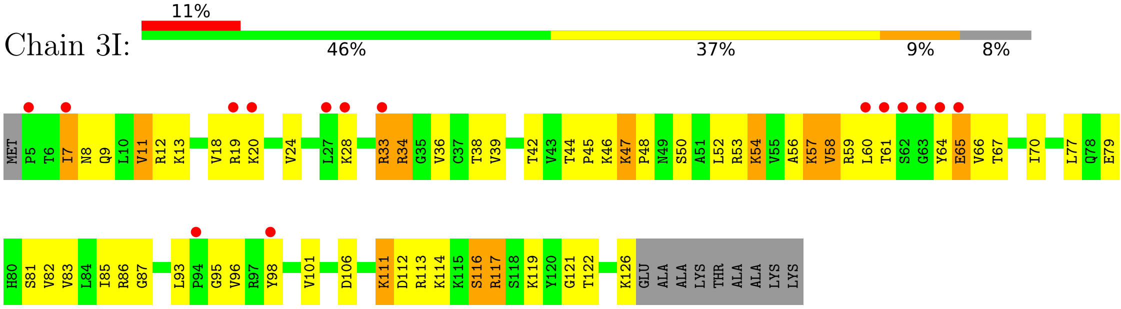
- Molecule 11: 30S ribosomal protein S11



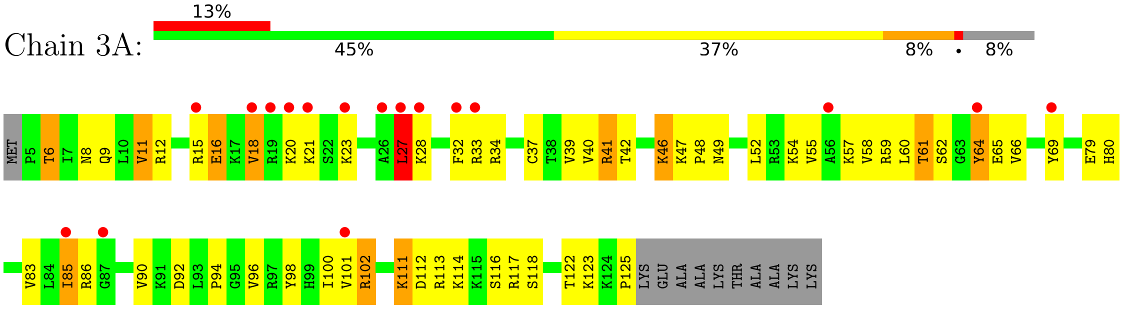
- Molecule 11: 30S ribosomal protein S11



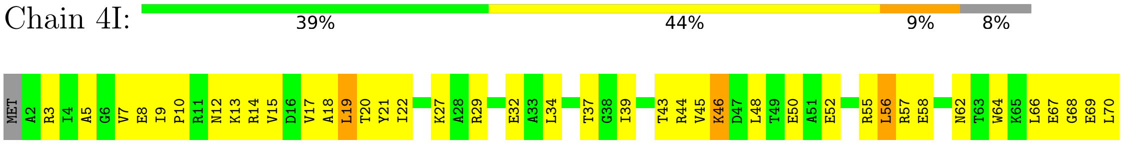
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



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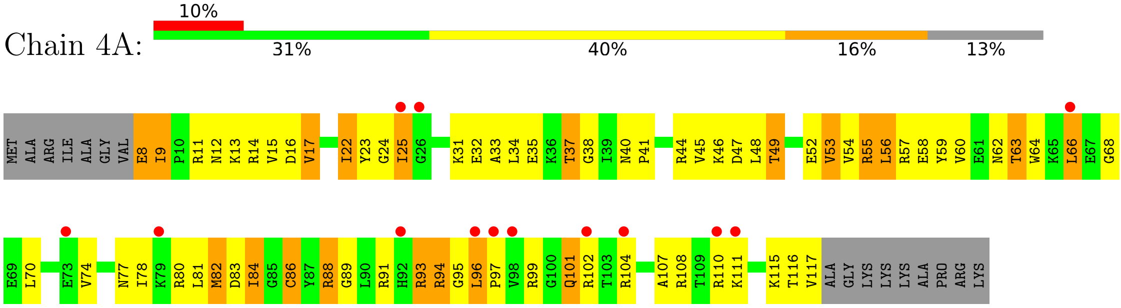
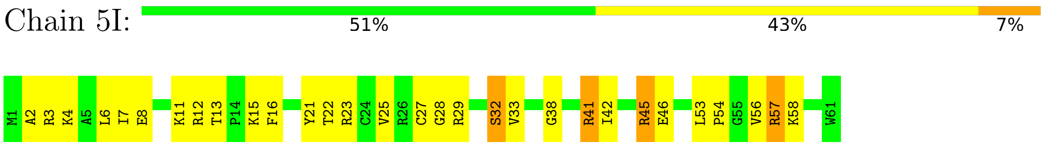
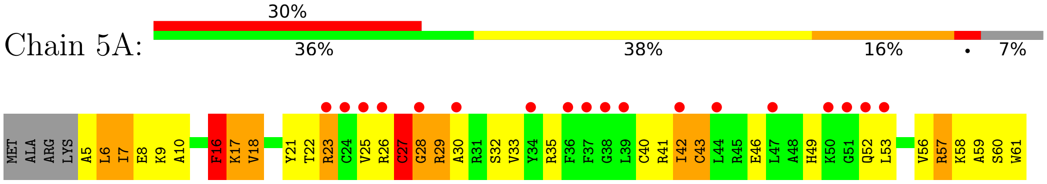


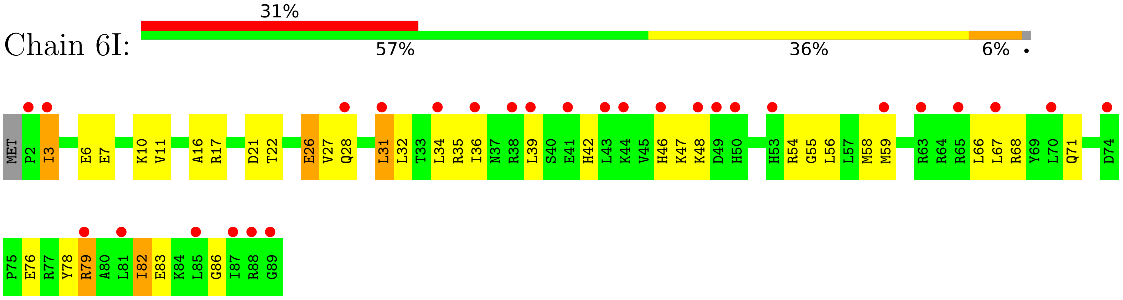
- Molecule 14: 30S ribosomal protein S14 type Z



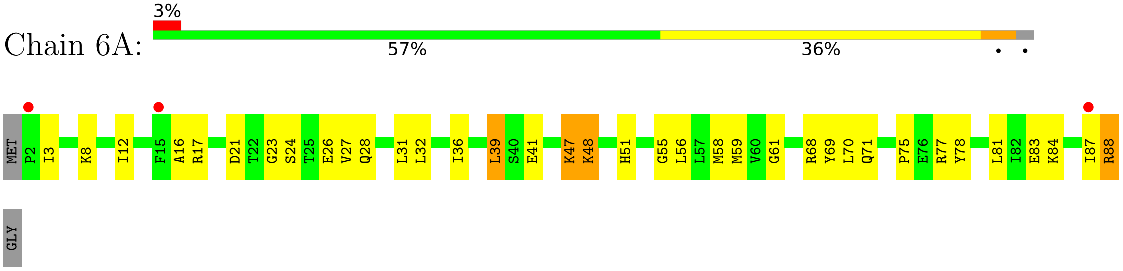
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

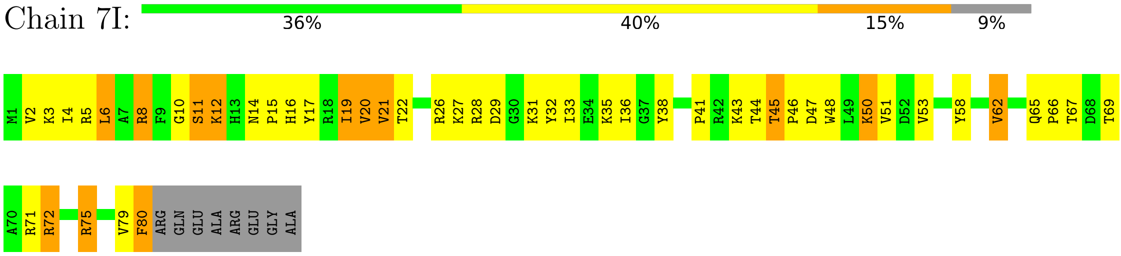


- Molecule 15: 30S ribosomal protein S15



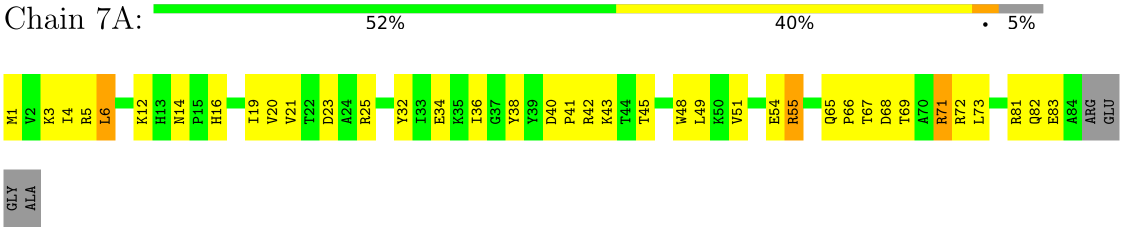
- Molecule 16: 30S ribosomal protein S16

Chain 7I:



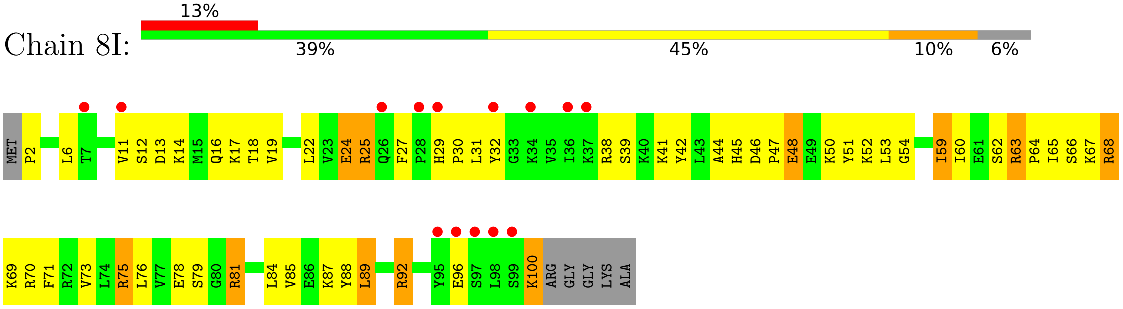
- Molecule 16: 30S ribosomal protein S16

Chain 7A:



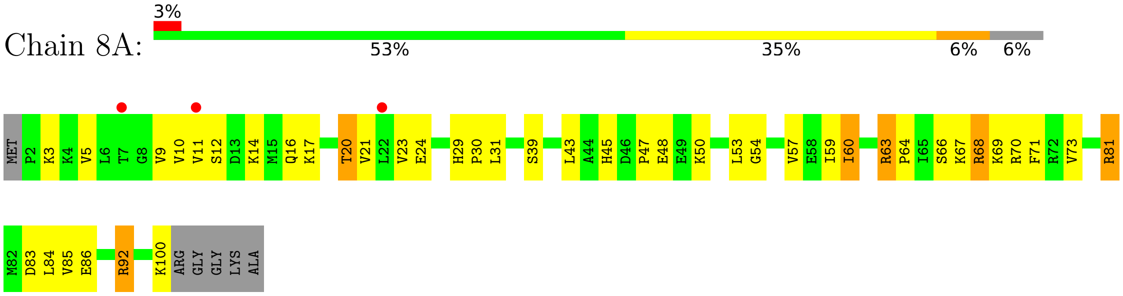
- Molecule 17: 30S ribosomal protein S17

Chain 8I:



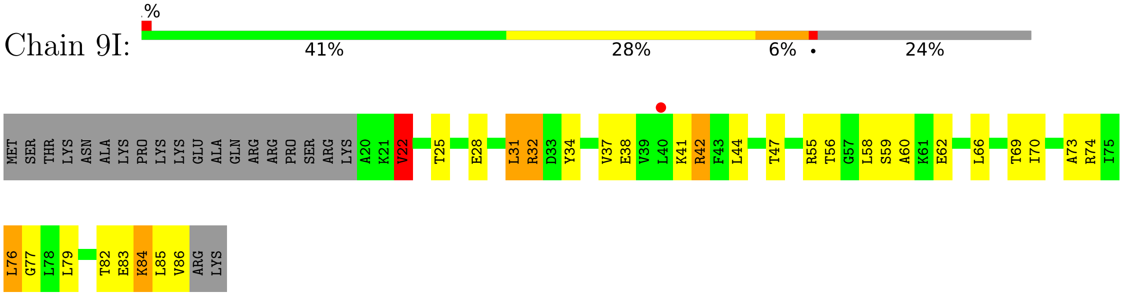
- Molecule 17: 30S ribosomal protein S17

Chain 8A:

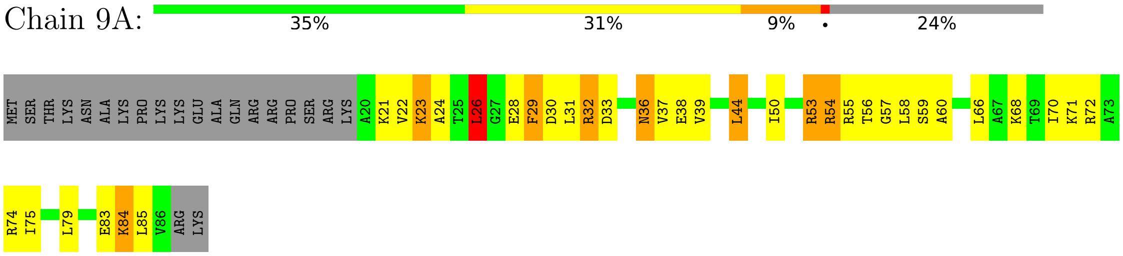


- Molecule 18: 30S ribosomal protein S18

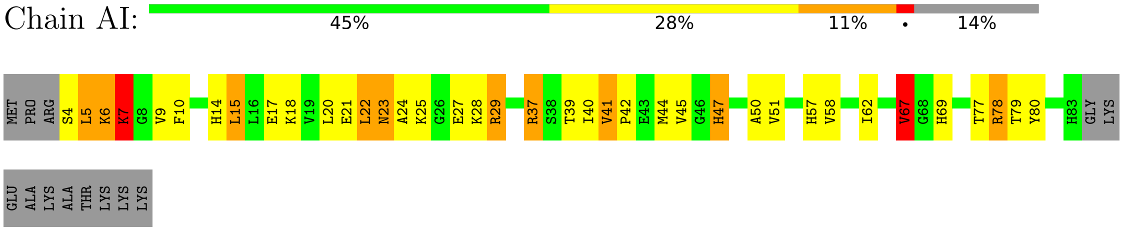
Chain 9I:



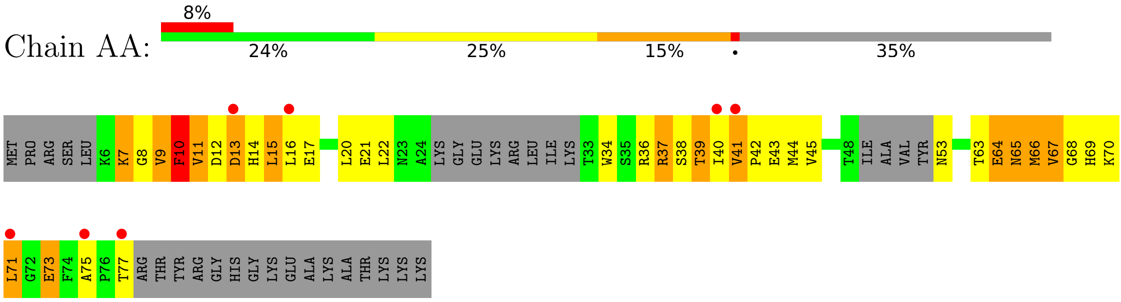
- Molecule 18: 30S ribosomal protein S18



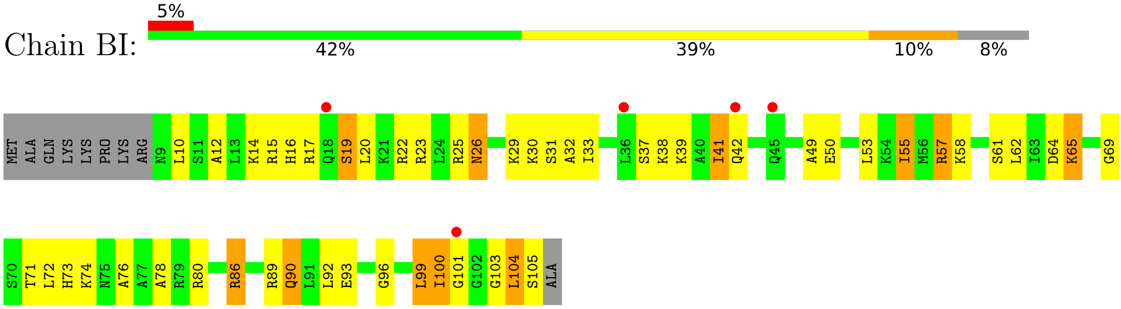
- Molecule 19: 30S ribosomal protein S19



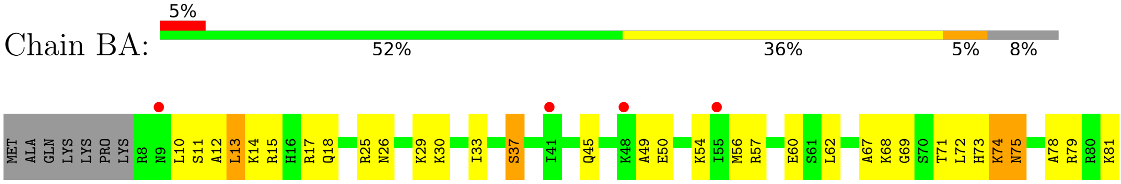
- Molecule 19: 30S ribosomal protein S19

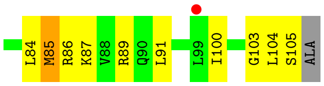


- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



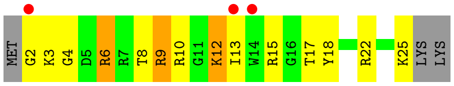


- Molecule 21: 30S ribosomal protein Thx

Chain 1F:

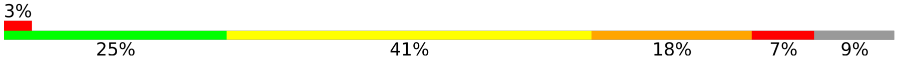
- Molecule 21: 30S ribosomal protein Thx

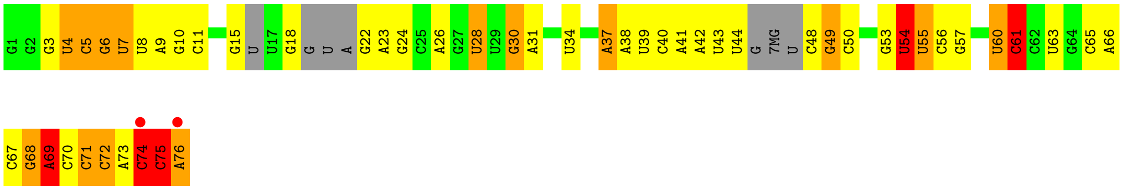
Chain 1B:



- Molecule 22: tRNA-Lys

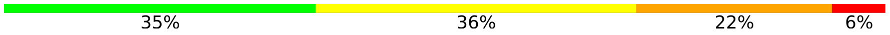
Chain 1K:

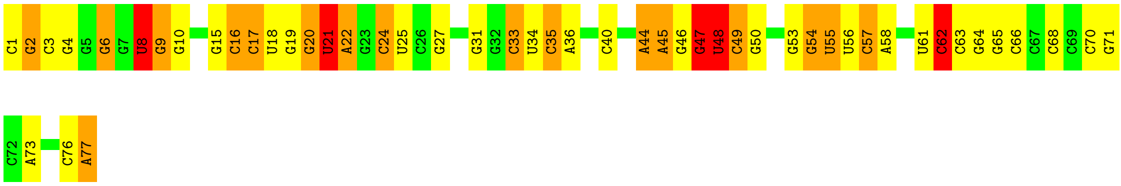




- Molecule 23: tRNA-fMet

Chain 2K:



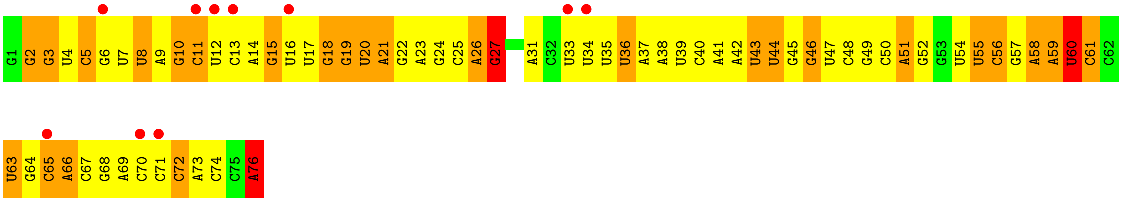


- Molecule 23: tRNA-fMet

Chain 2L:

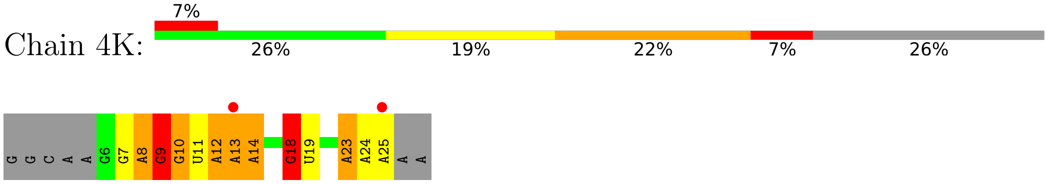
- Molecule 24: tRNA-Lys

Chain 3K:



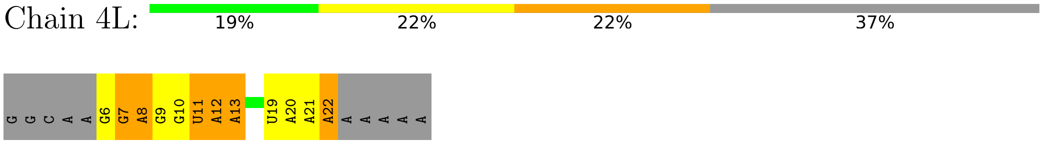
- Molecule 25: mRNA

Chain 4K:



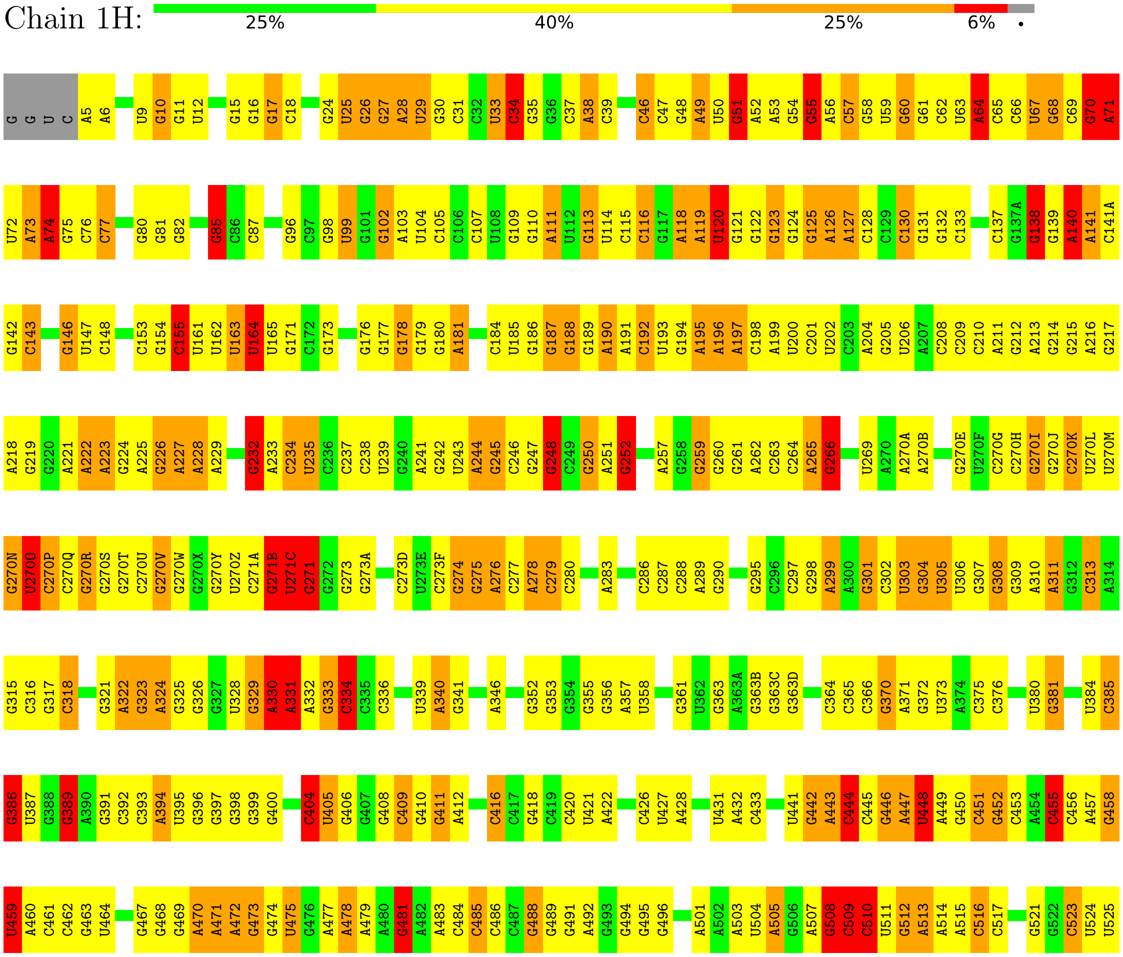
- Molecule 25: mRNA

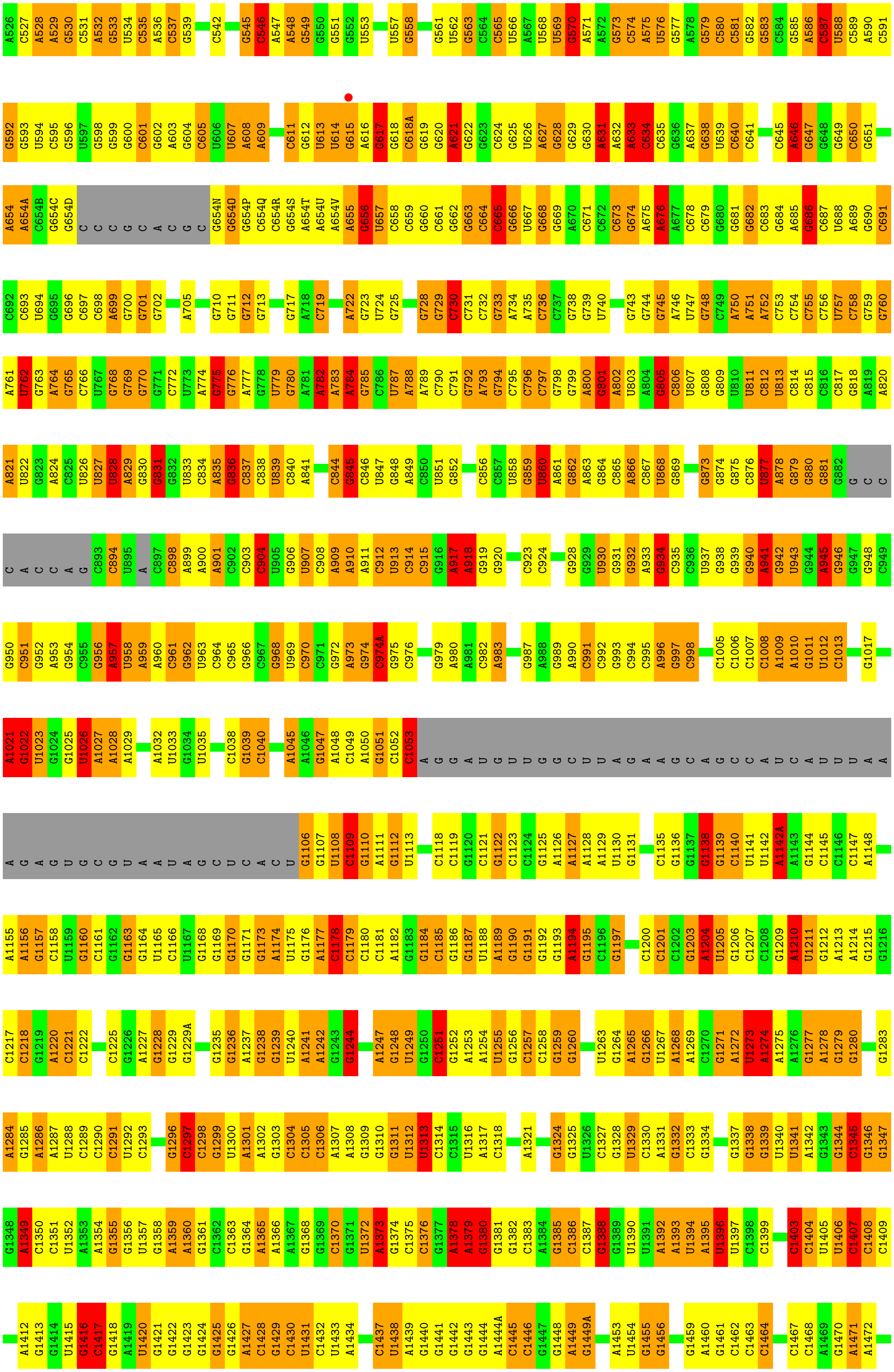
Chain 4L:



- Molecule 26: 23S ribosomal RNA

Chain 1H:

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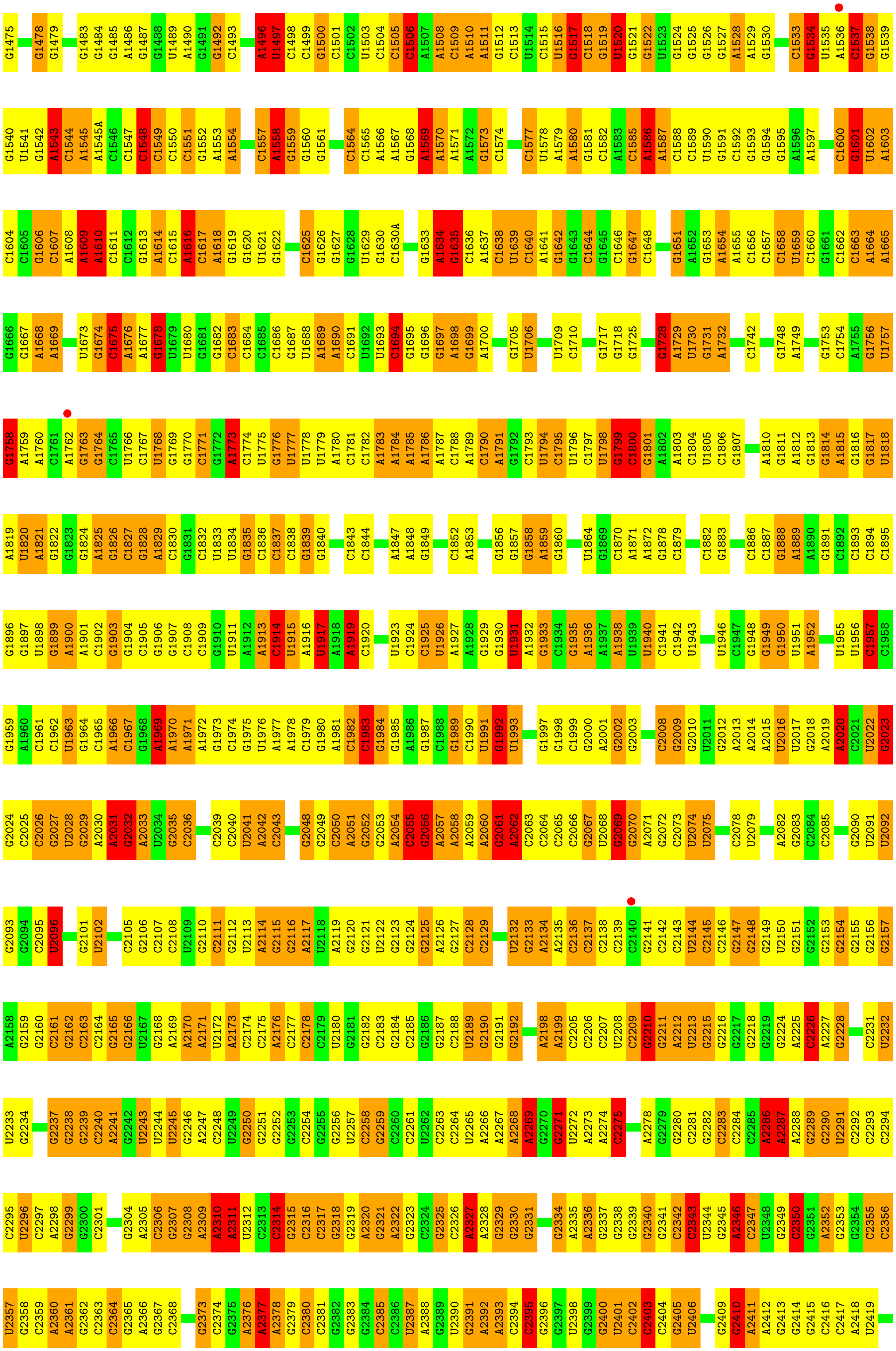
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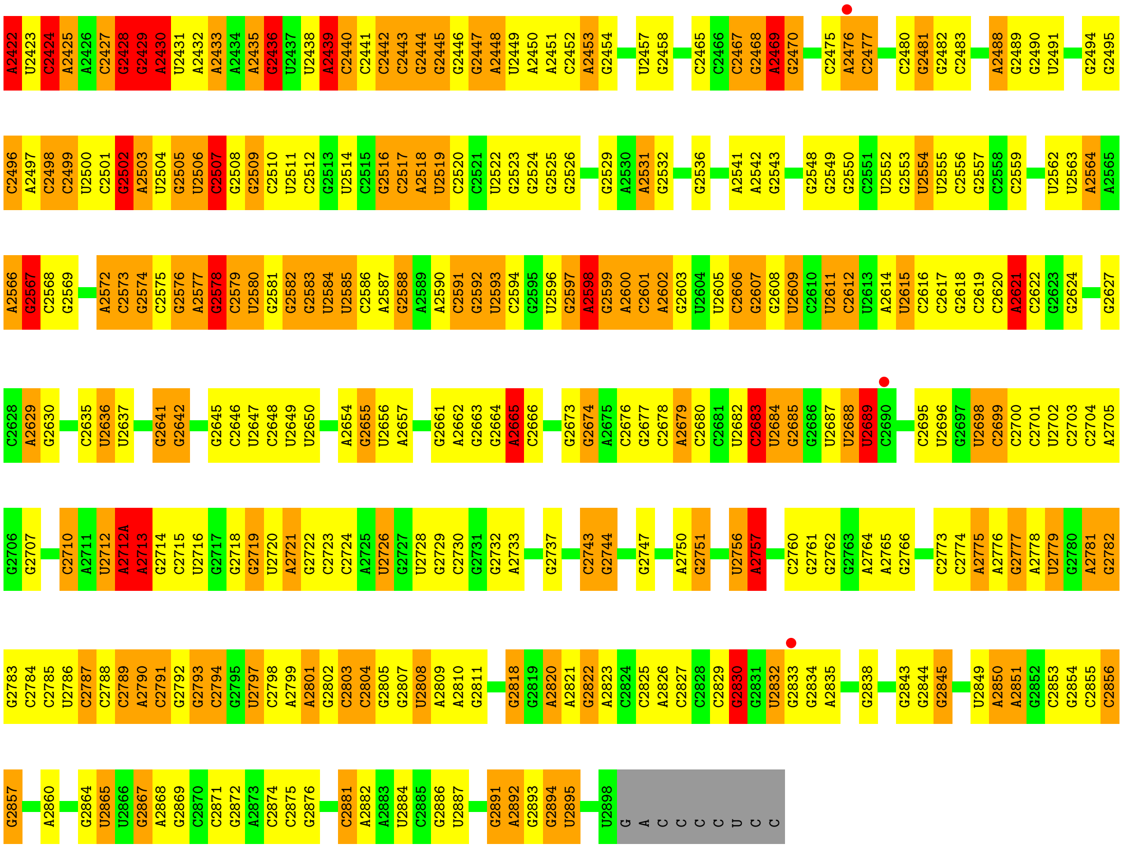
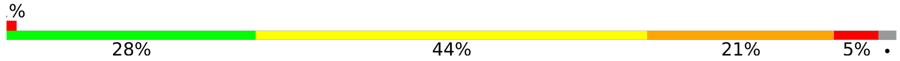
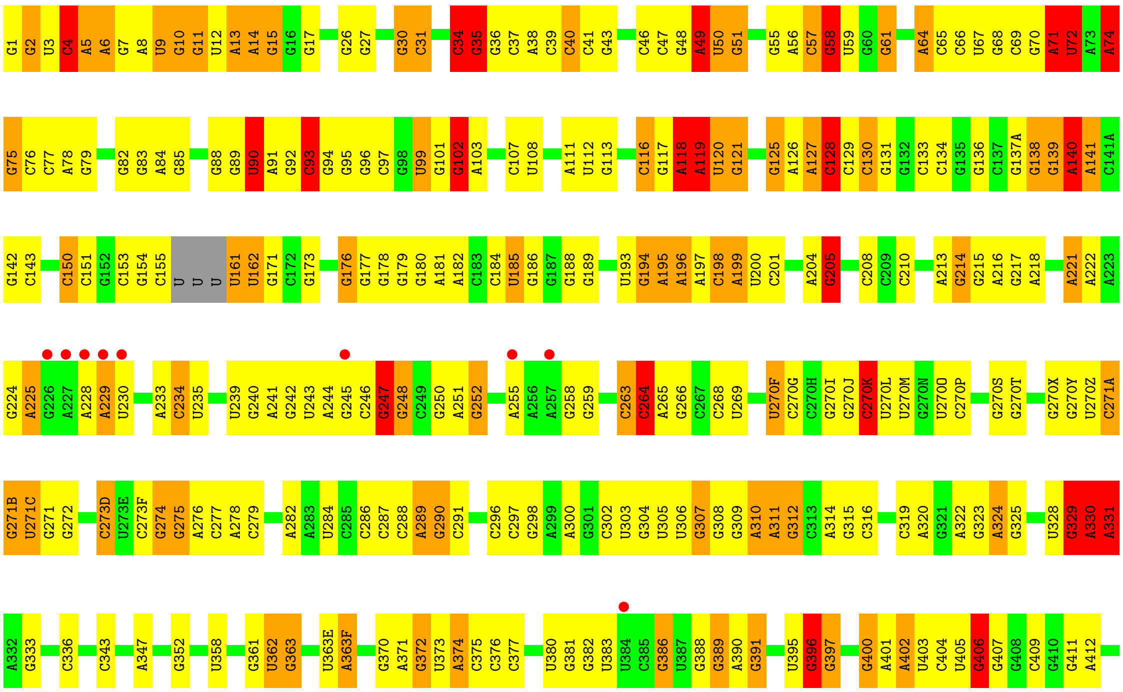
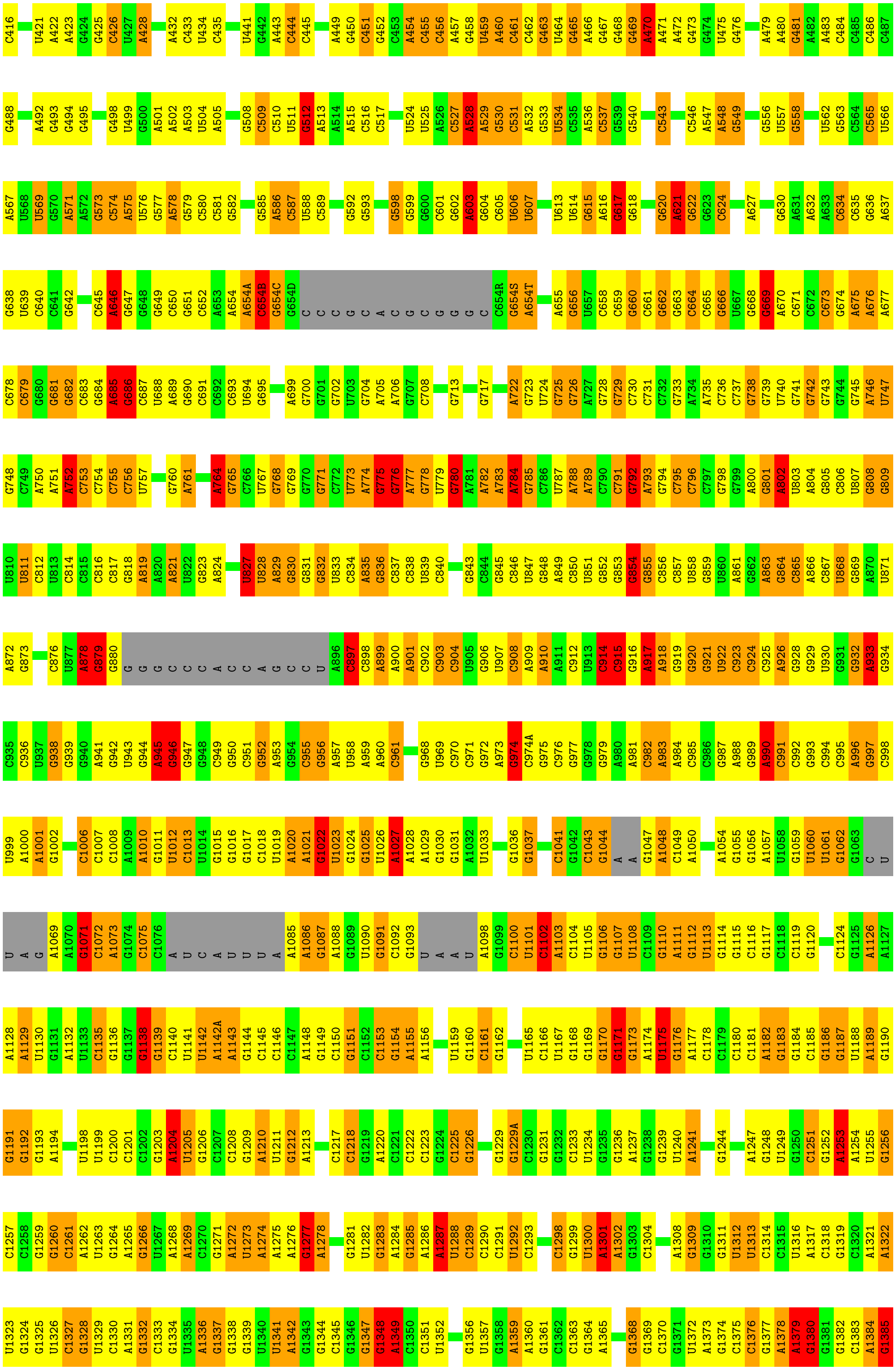


- Molecule 26: 23S ribosomal RNA

Chain 14:



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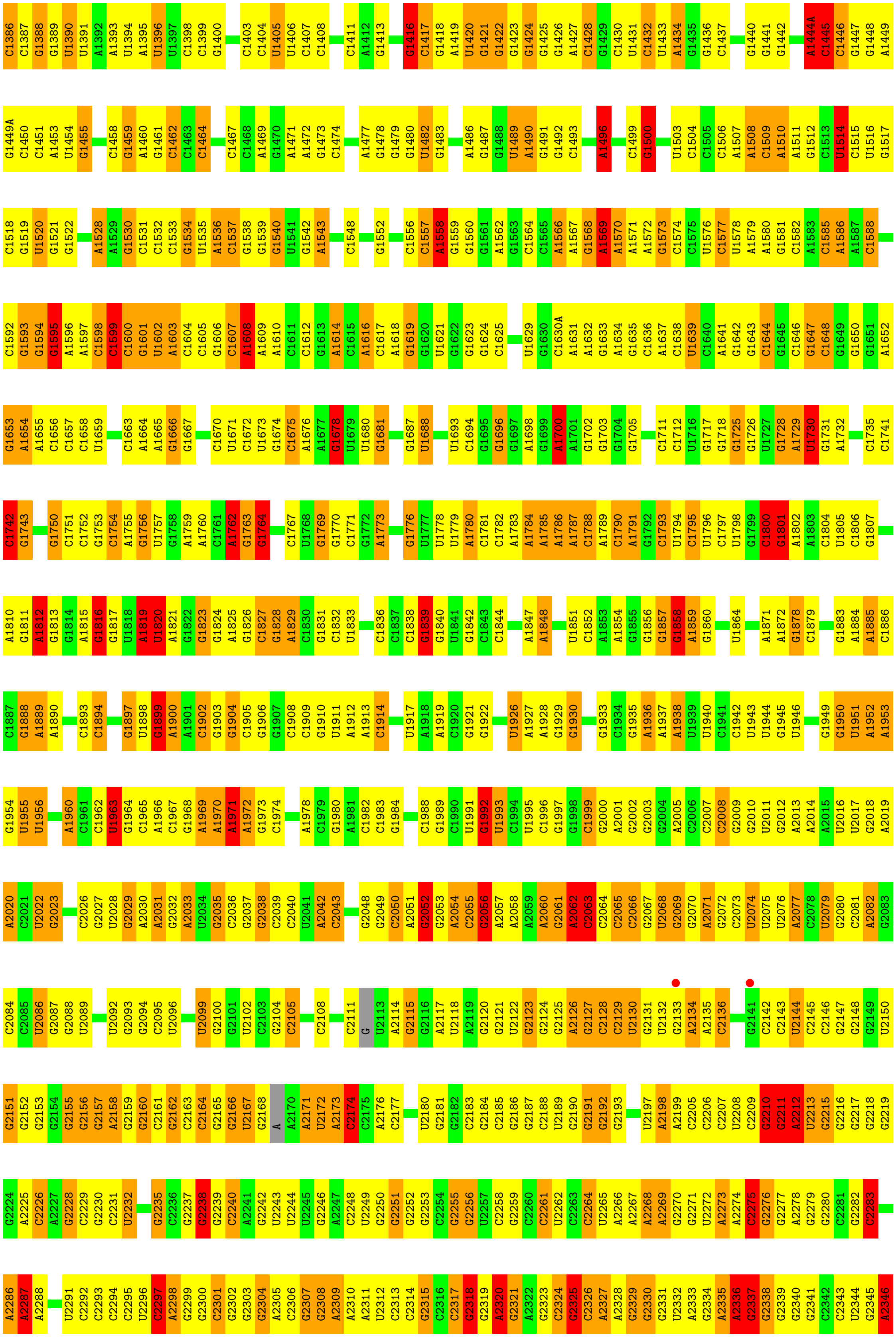
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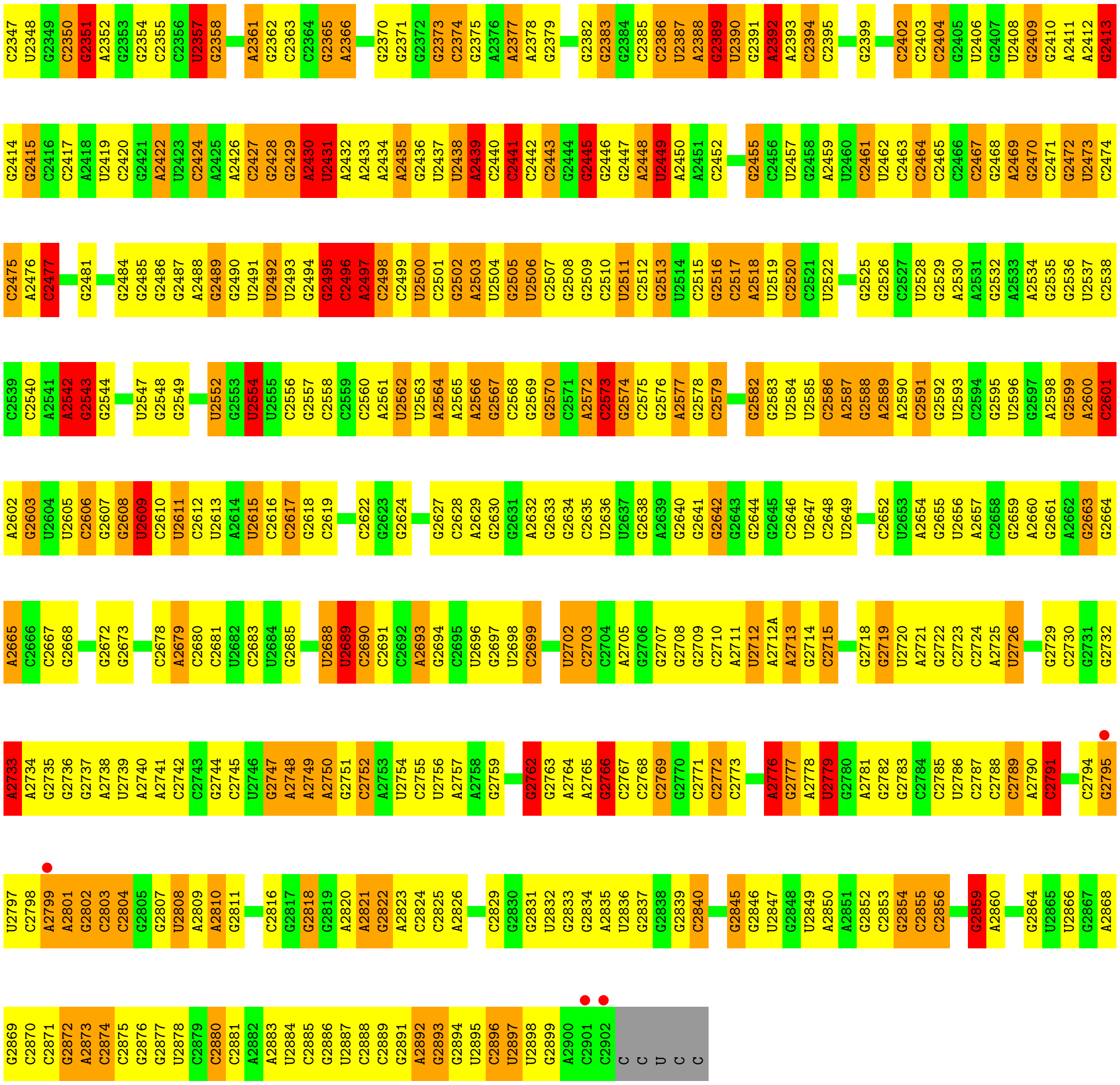

- Molecule 27: 5S ribosomal RNA

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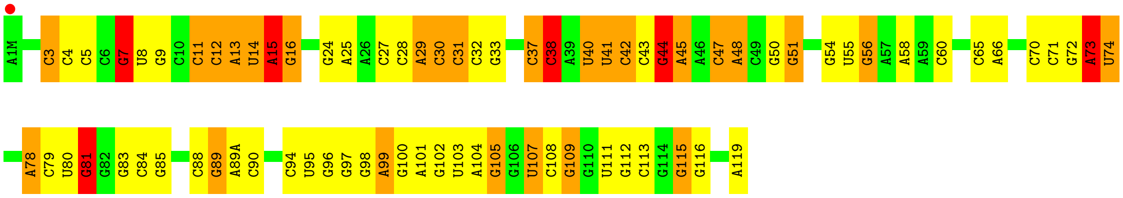

- Molecule 27: 5S ribosomal RNA

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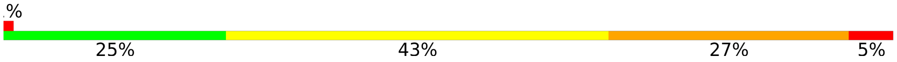

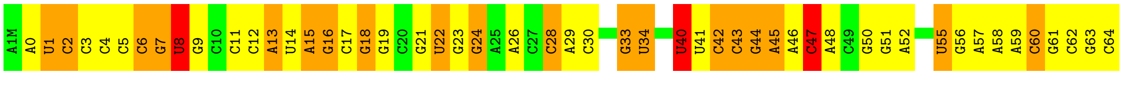

- Molecule 28: 50S ribosomal protein L1

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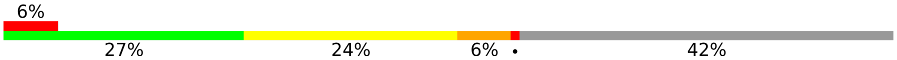

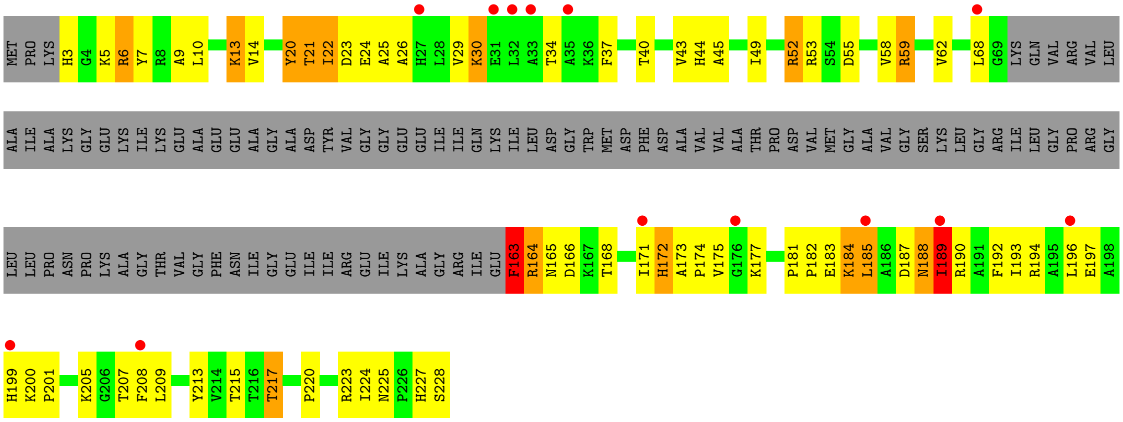

- Molecule 29: 50S ribosomal protein L2

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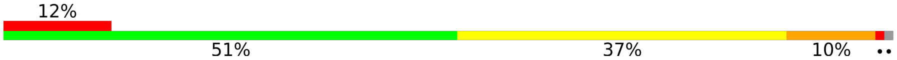

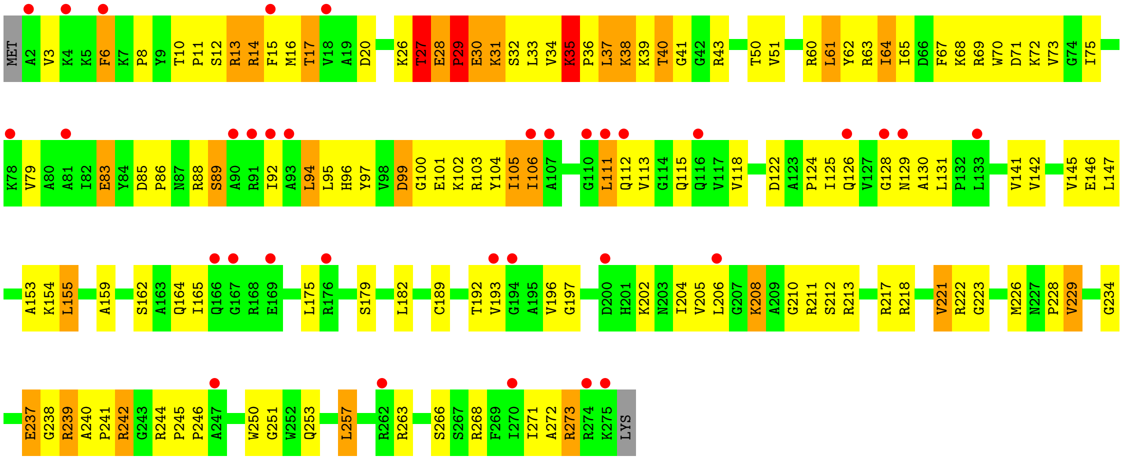

- Molecule 29: 50S ribosomal protein L2

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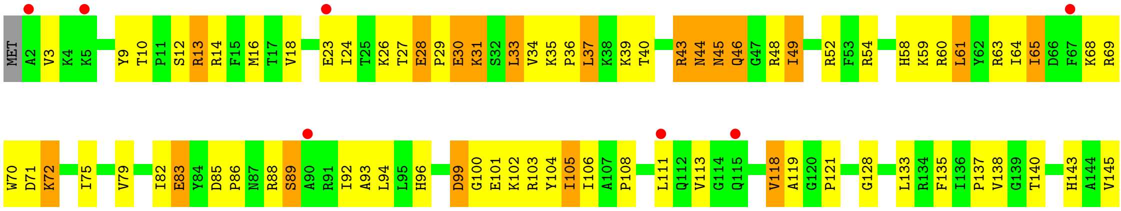
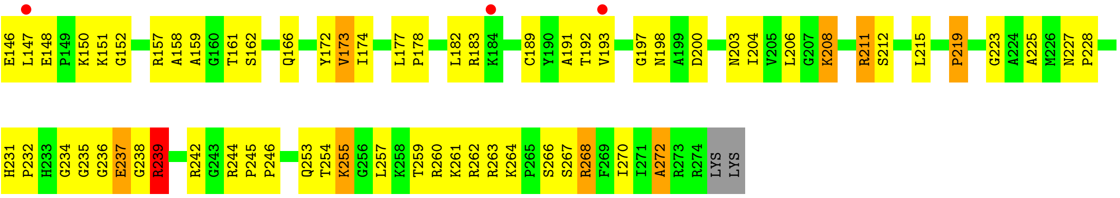
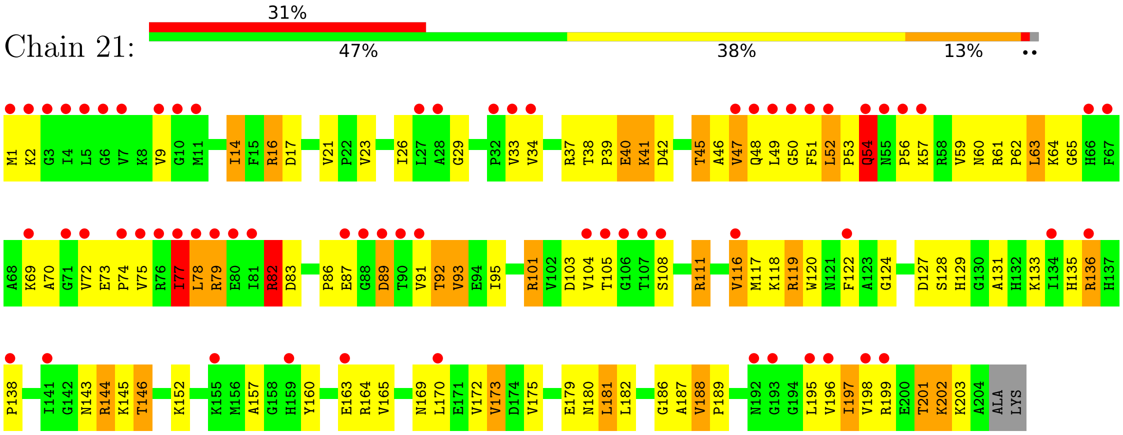




- Molecule 30: 50S ribosomal protein L3

Chain 21:



- Molecule 30: 50S ribosomal protein L3

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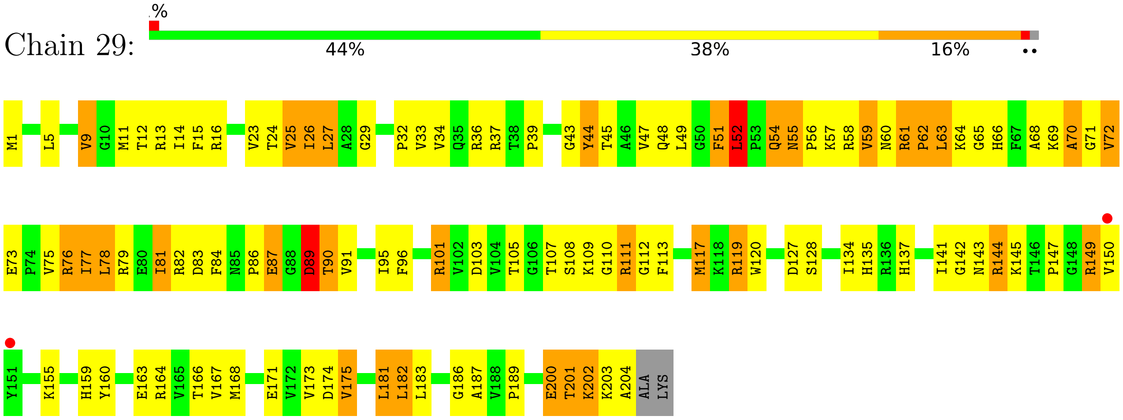
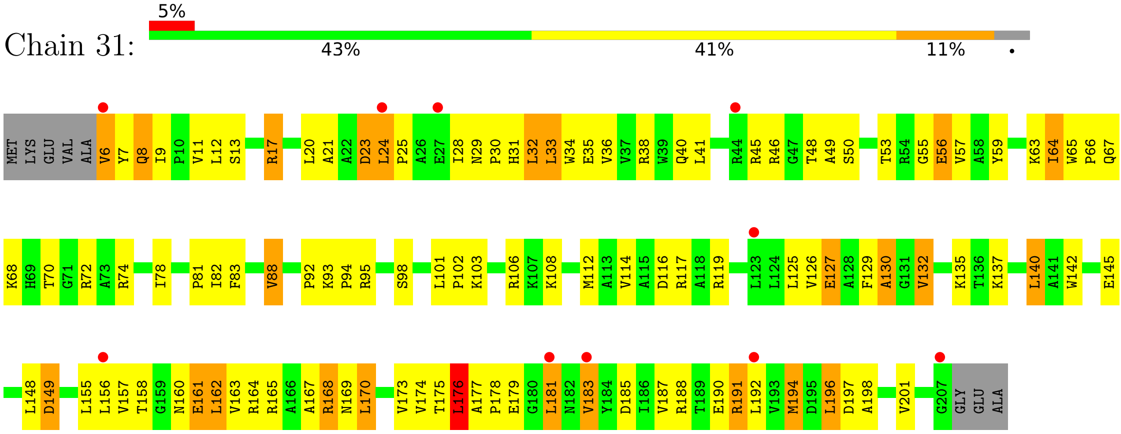
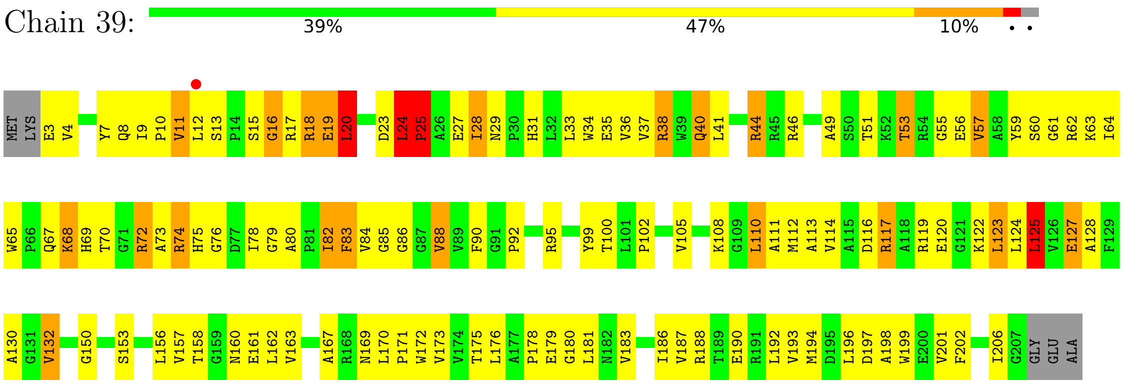


- Molecule 31: 50S ribosomal protein L4

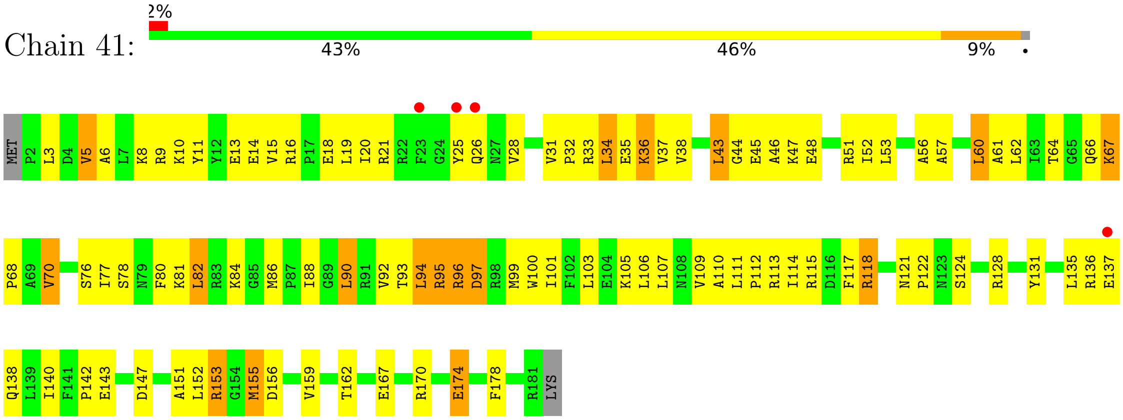
Chain 31:



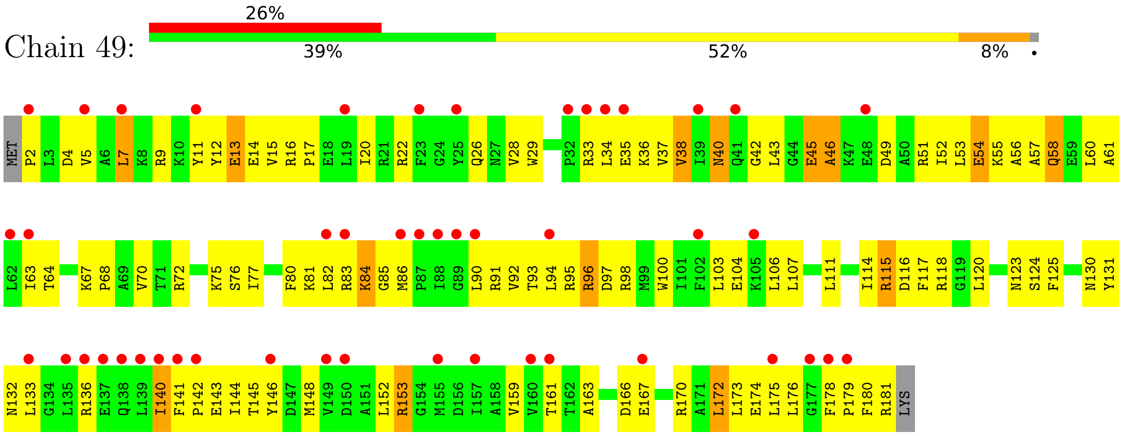
- Molecule 31: 50S ribosomal protein L4



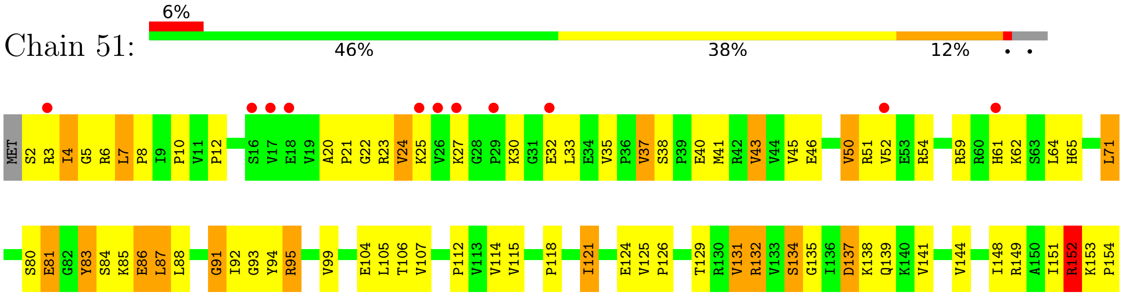
- Molecule 32: 50S ribosomal protein L5

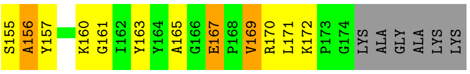


- Molecule 32: 50S ribosomal protein L5

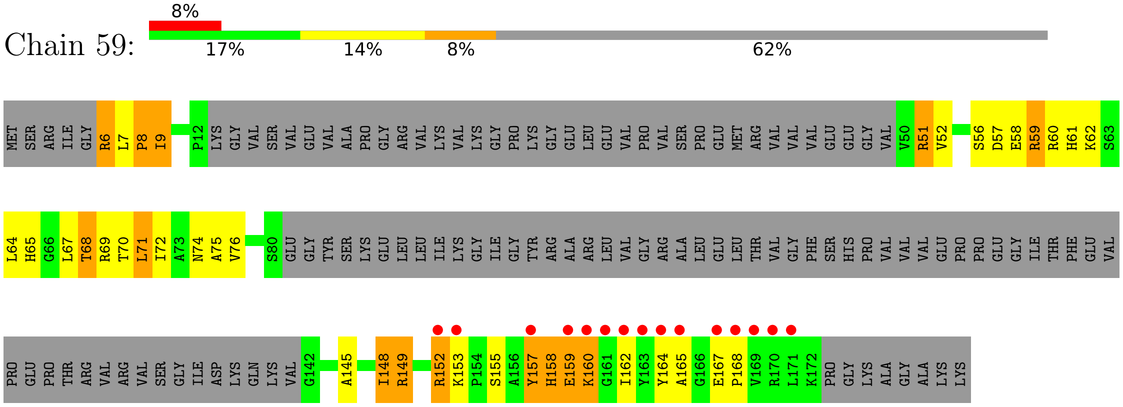


- Molecule 33: 50S ribosomal protein L6

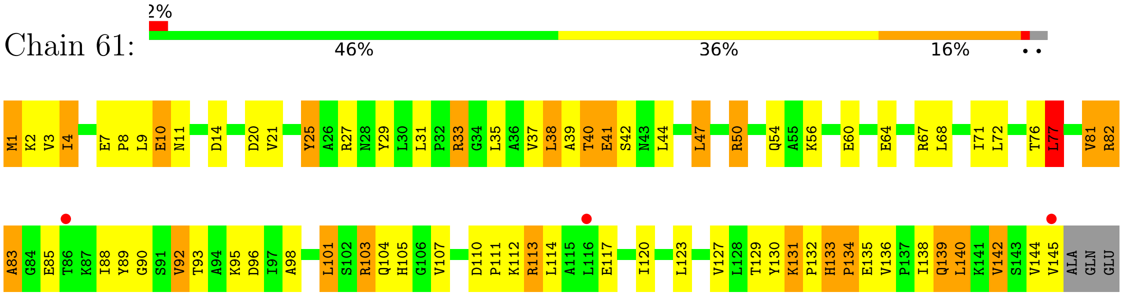




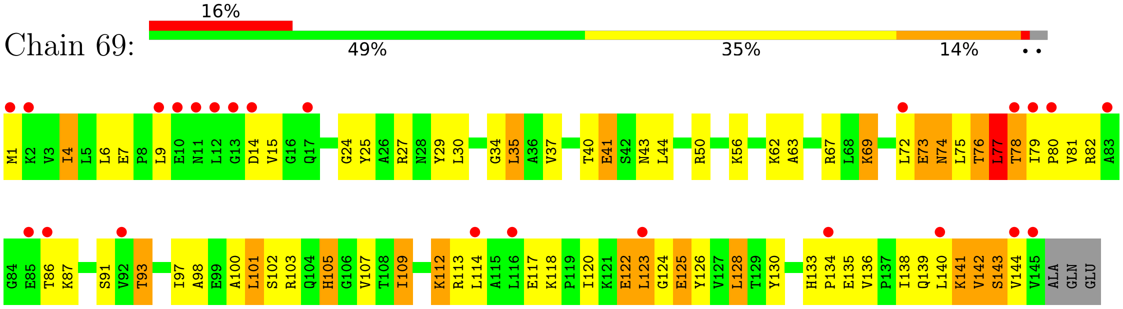
- Molecule 33: 50S ribosomal protein L6



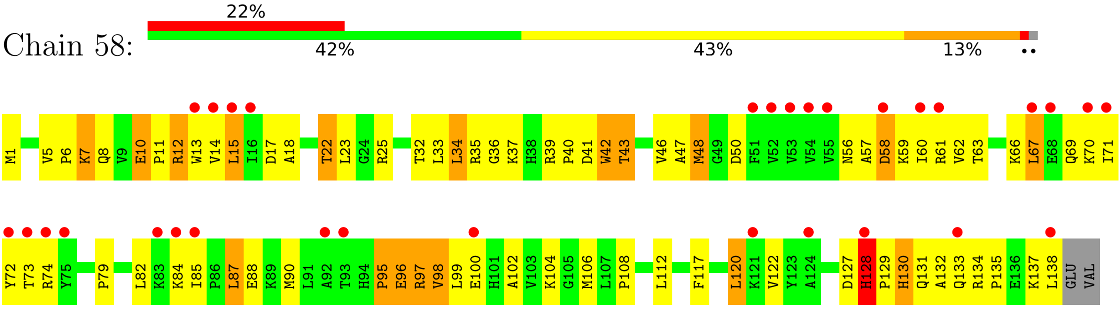
- Molecule 34: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L9

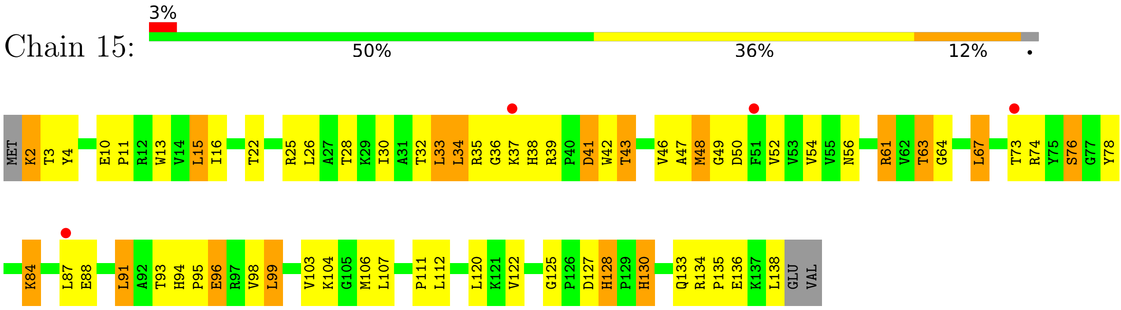


- Molecule 35: 50S ribosomal protein L13



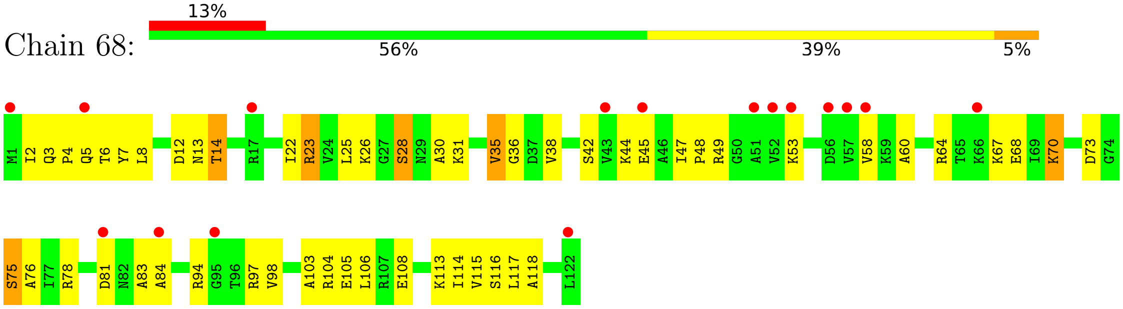
- Molecule 35: 50S ribosomal protein L13

Chain 15:



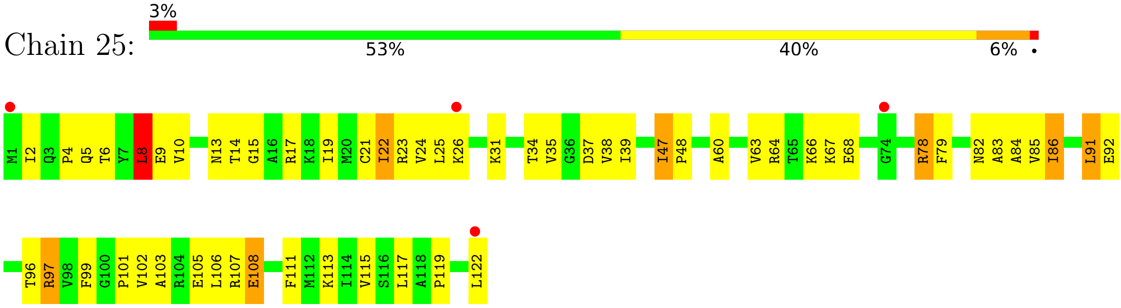
- Molecule 36: 50S ribosomal protein L14

Chain 68:



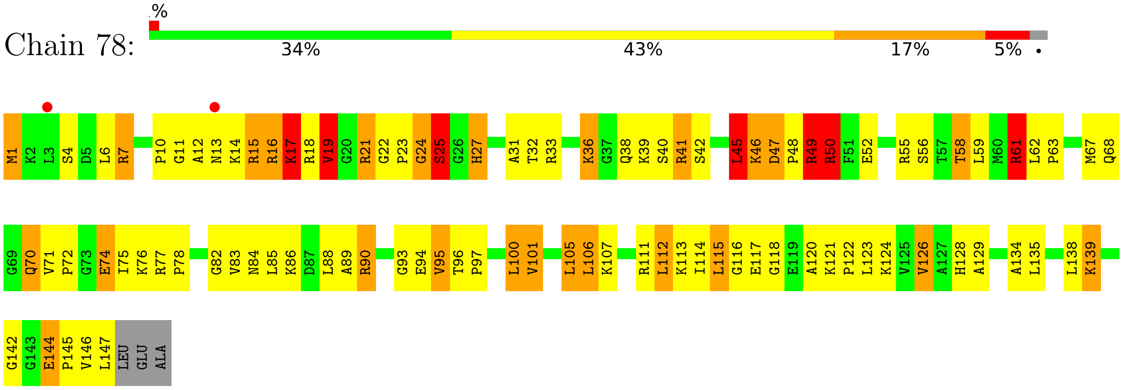
- Molecule 36: 50S ribosomal protein L14

Chain 25:



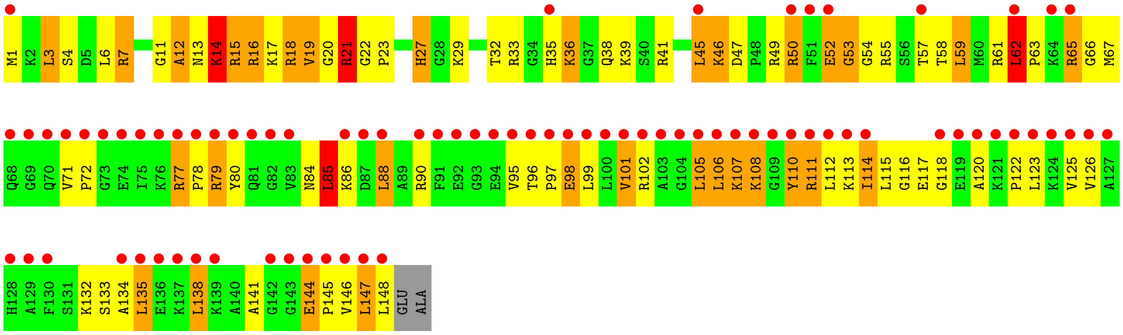
- Molecule 37: 50S ribosomal protein L15

Chain 78:



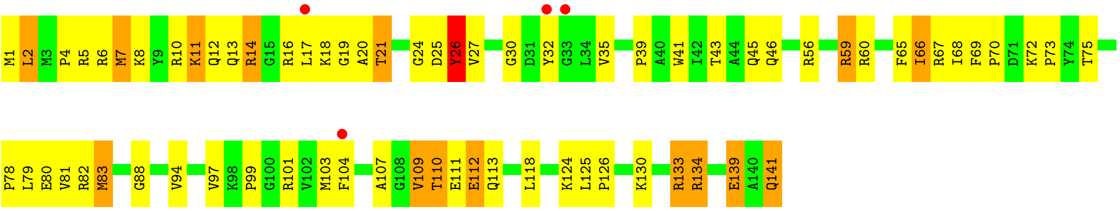
- Molecule 37: 50S ribosomal protein L15

Chain 35:



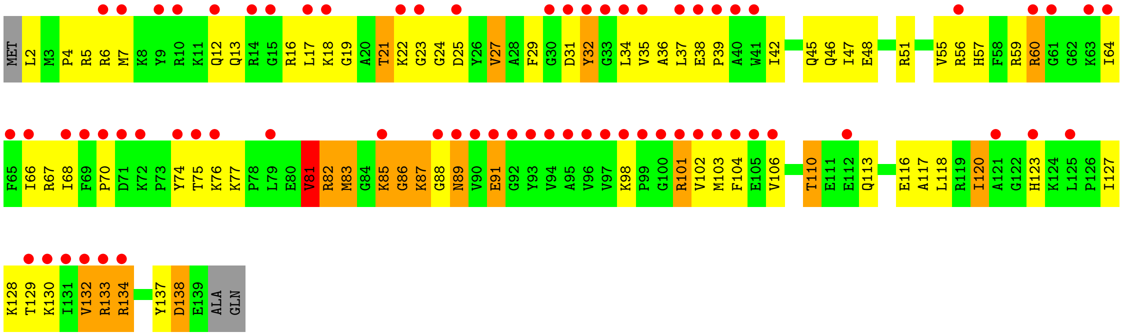
- Molecule 38: 50S ribosomal protein L16

Chain 88:



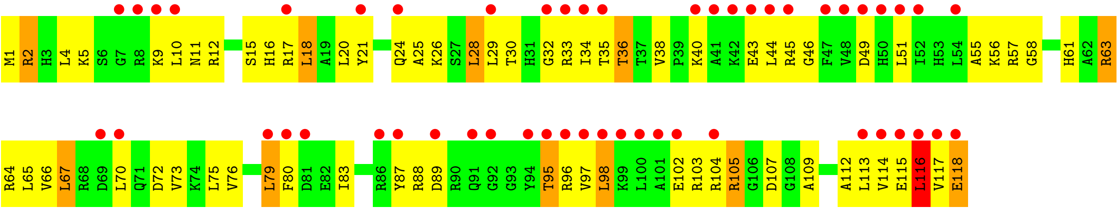
- Molecule 38: 50S ribosomal protein L16

Chain 45:



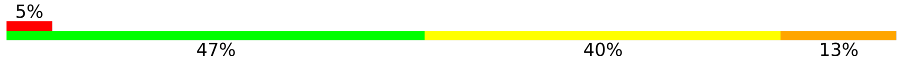
- Molecule 39: 50S ribosomal protein L17

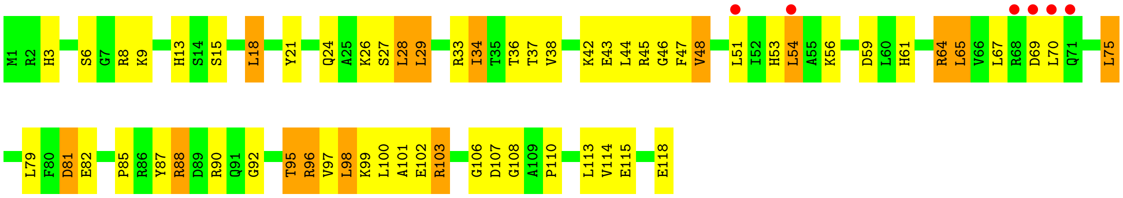
Chain 98:



- Molecule 39: 50S ribosomal protein L17

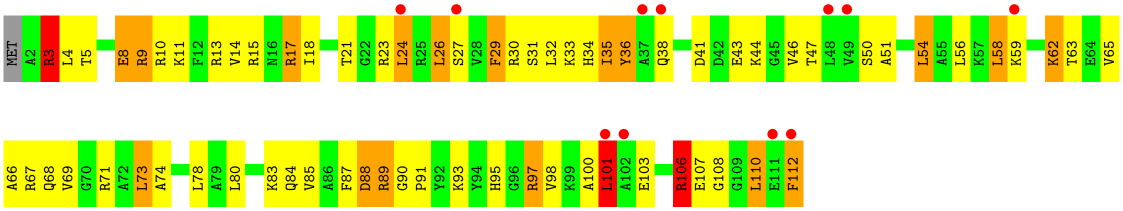
Chain 55:





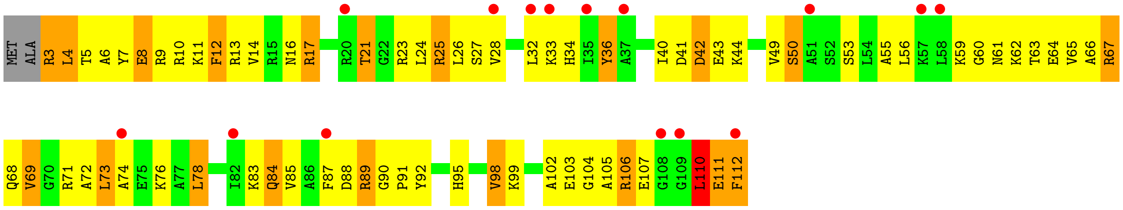
- Molecule 40: 50S ribosomal protein L18

Chain A8:



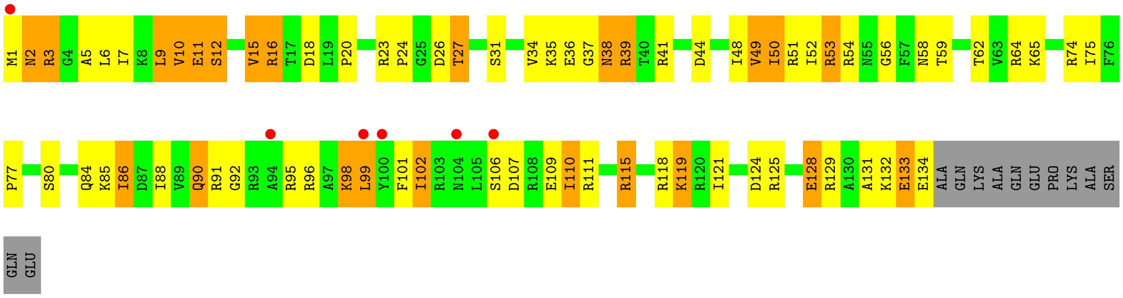
- Molecule 40: 50S ribosomal protein L18

Chain 65:



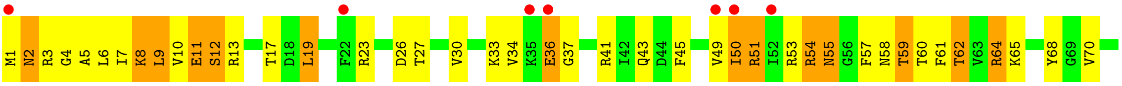
- Molecule 41: 50S ribosomal protein L19

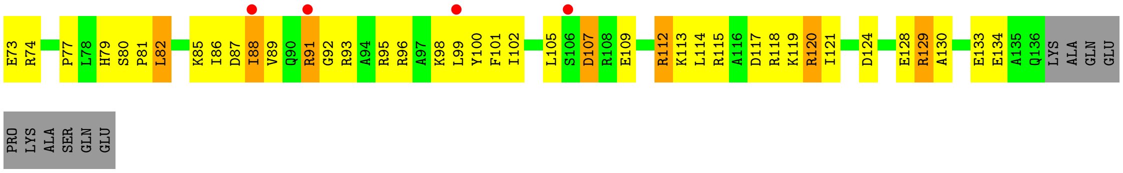
Chain B8:



- Molecule 41: 50S ribosomal protein L19

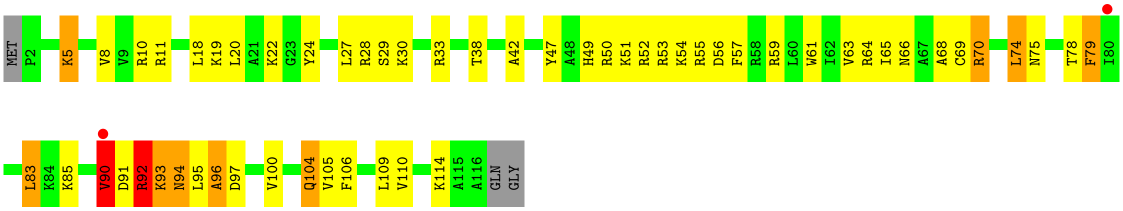
Chain 75:





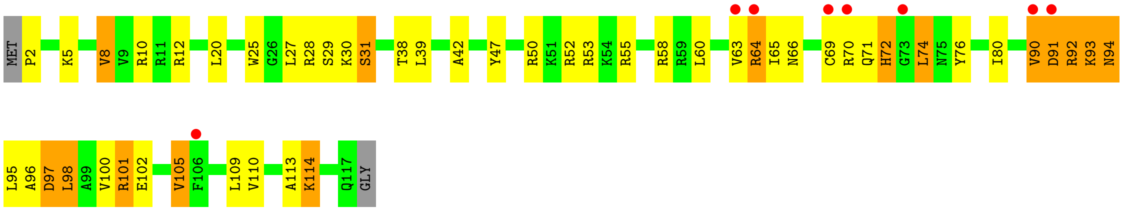
- Molecule 42: 50S ribosomal protein L20

Chain C8:



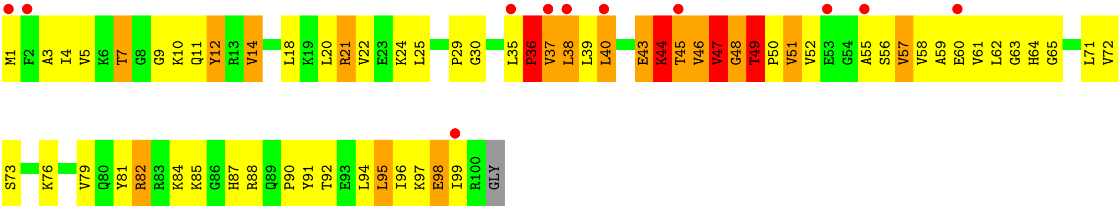
- Molecule 42: 50S ribosomal protein L20

Chain 85:



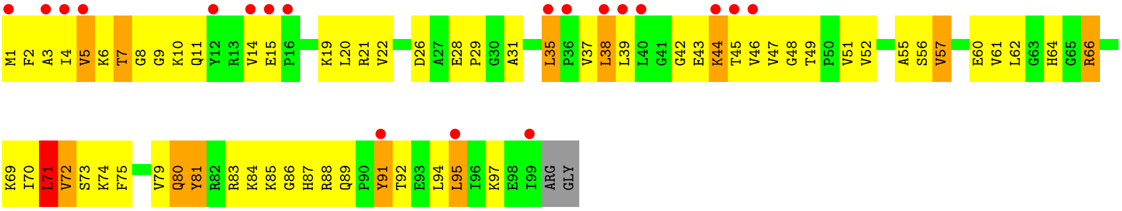
- Molecule 43: 50S ribosomal protein L21

Chain D8:



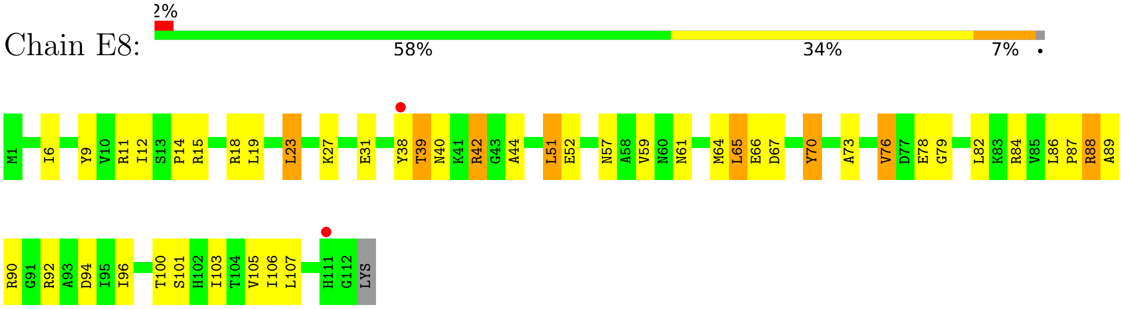
- Molecule 43: 50S ribosomal protein L21

Chain 95:



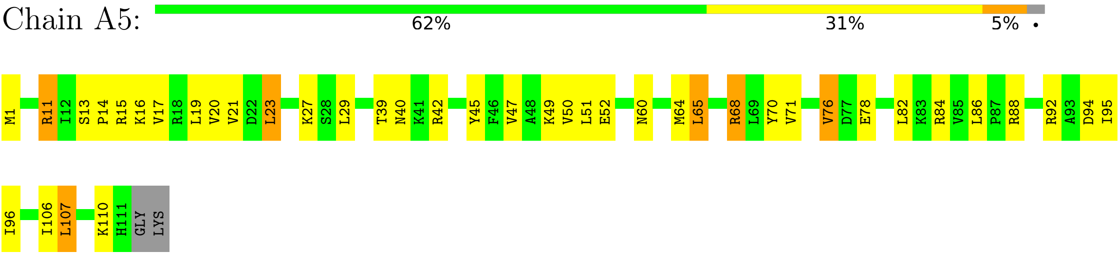
- Molecule 44: 50S ribosomal protein L22

Chain E8:



- Molecule 44: 50S ribosomal protein L22

Chain A5:

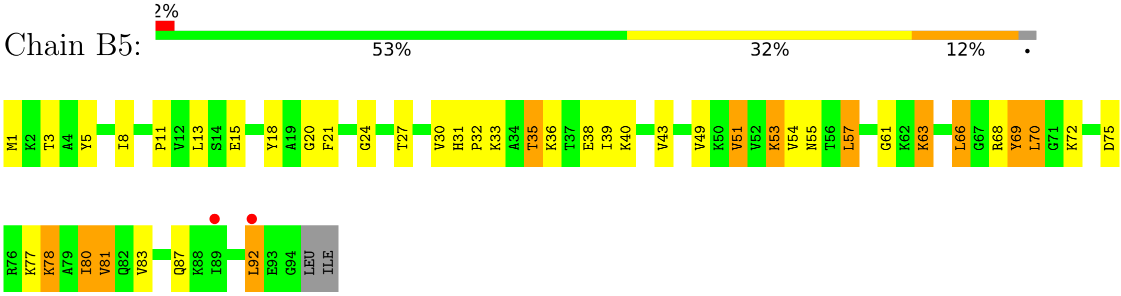


- Molecule 45: 50S ribosomal protein L23

Chain F8:

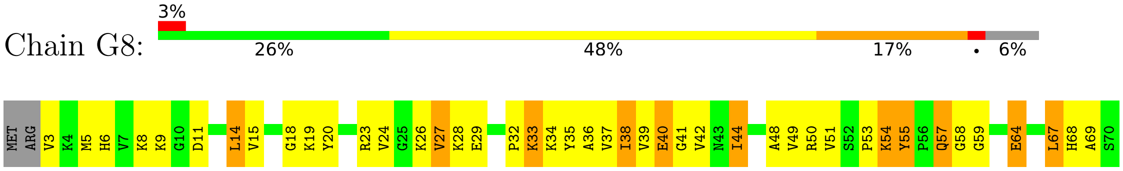
- Molecule 45: 50S ribosomal protein L23

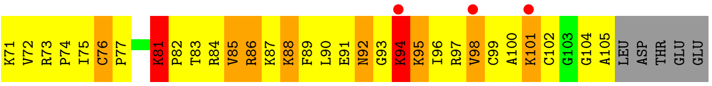
Chain B5:



- Molecule 46: 50S ribosomal protein L24

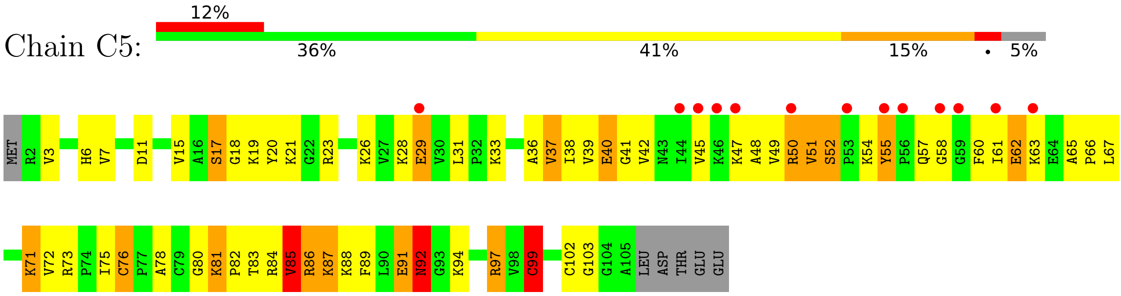
Chain G8:





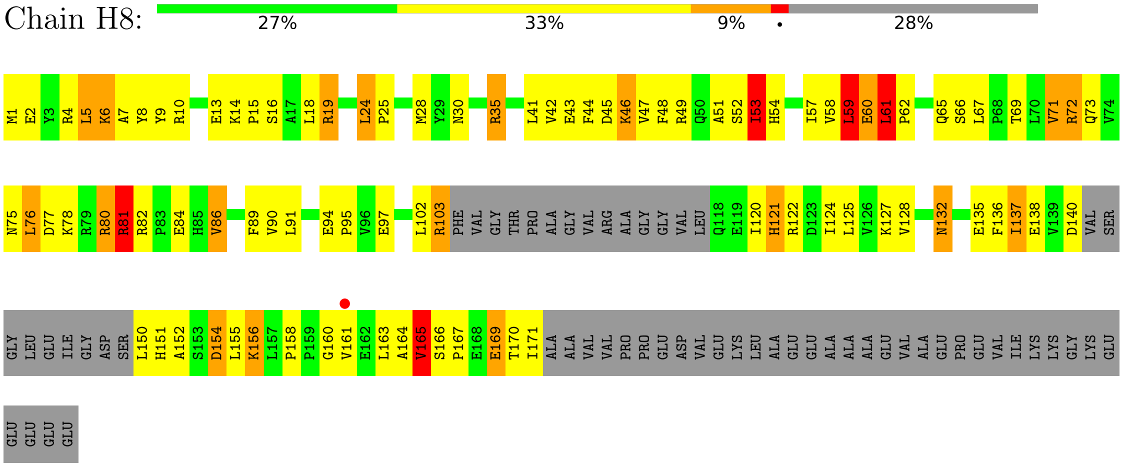
• Molecule 46: 50S ribosomal protein L24

Chain C5:



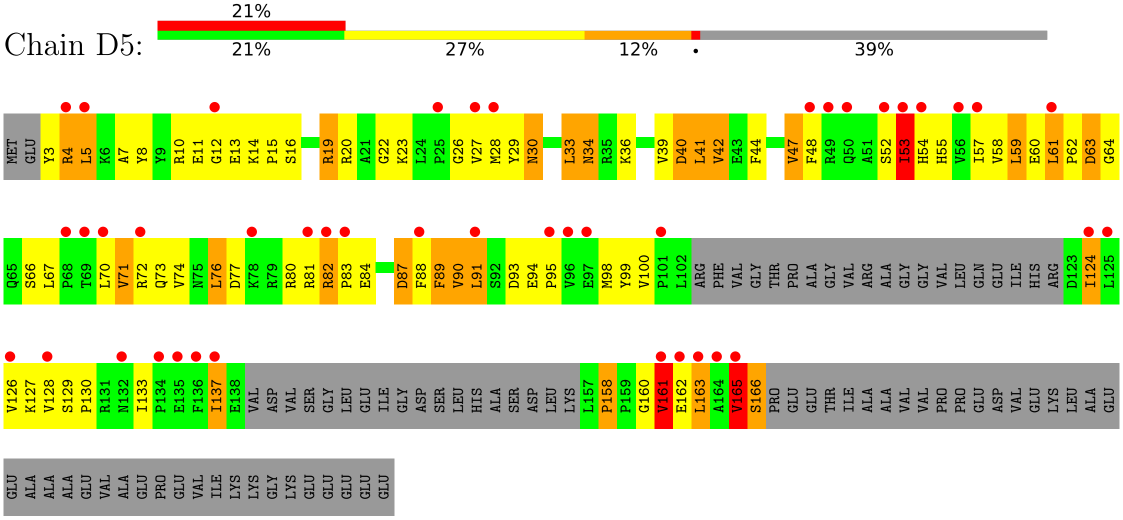
• Molecule 47: 50S ribosomal protein L25

Chain H8:



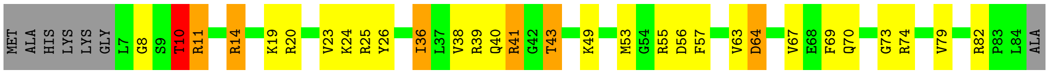
• Molecule 47: 50S ribosomal protein L25

Chain D5:



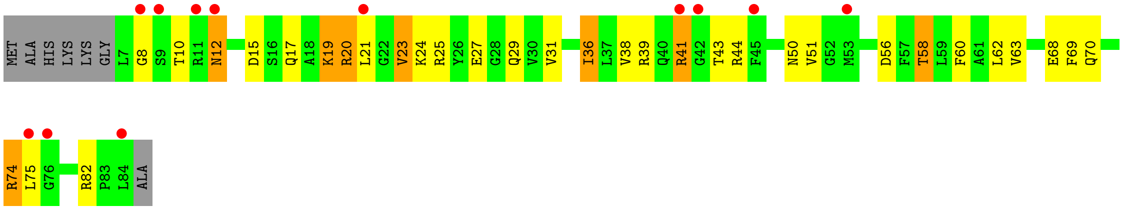
• Molecule 48: 50S ribosomal protein L27

Chain I8:



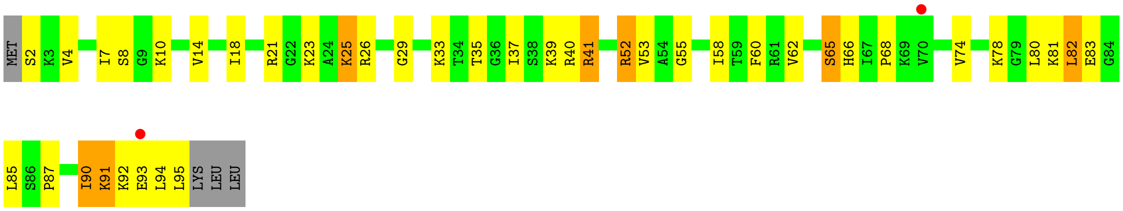
- Molecule 48: 50S ribosomal protein L27

Chain E5:



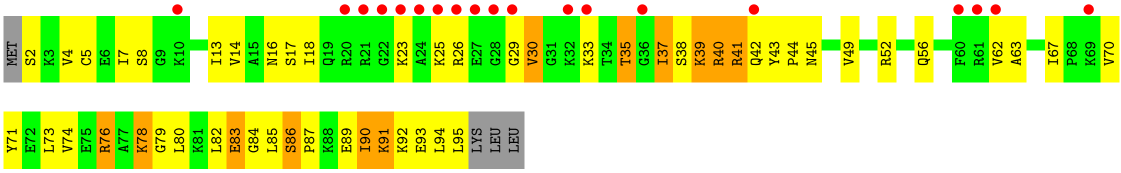
- Molecule 49: 50S ribosomal protein L28

Chain J8:



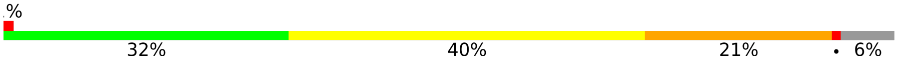
- Molecule 49: 50S ribosomal protein L28

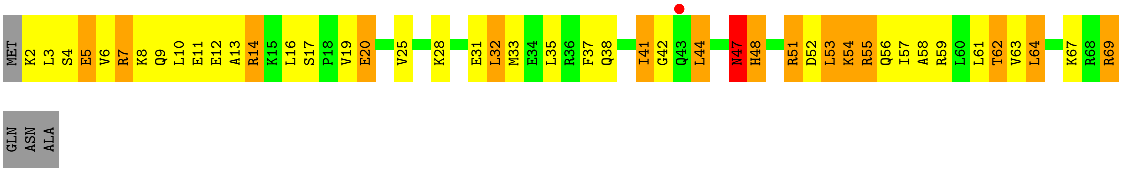
Chain F5:



- Molecule 50: 50S ribosomal protein L29

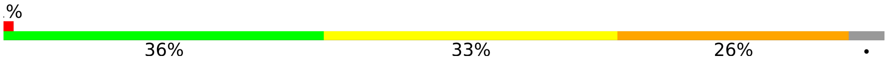
Chain K8:

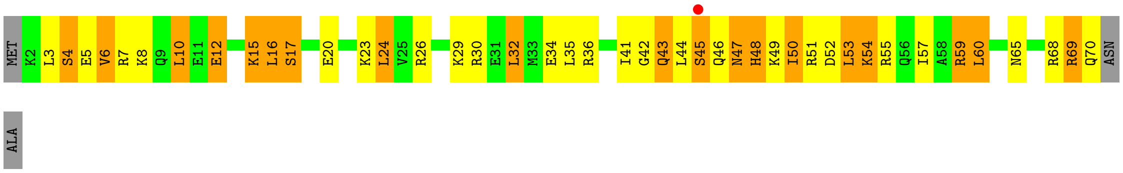




- Molecule 50: 50S ribosomal protein L29

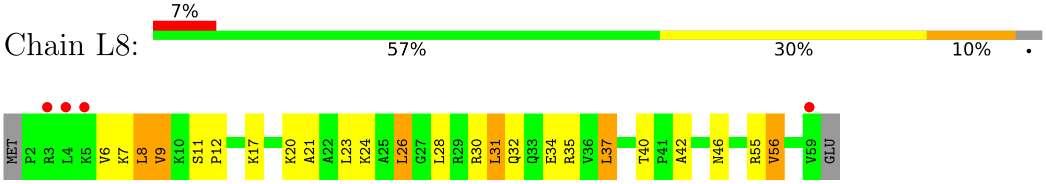
Chain G5:





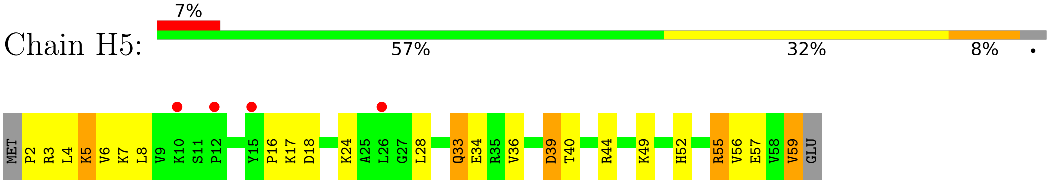
- Molecule 51: 50S ribosomal protein L30

Chain L8:



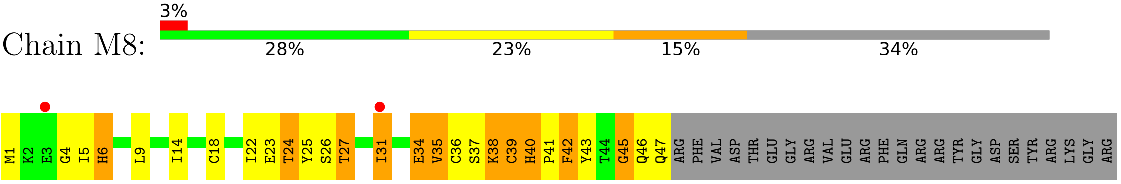
- Molecule 51: 50S ribosomal protein L30

Chain H5:



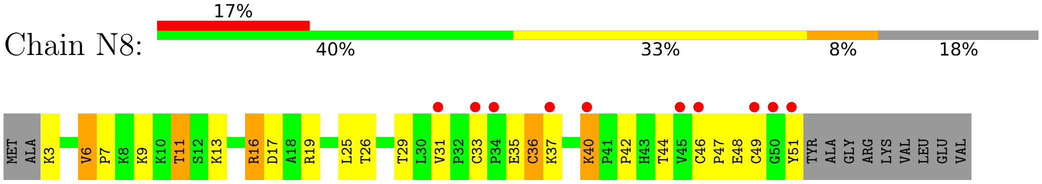
- Molecule 52: 50S ribosomal protein L31

Chain M8:



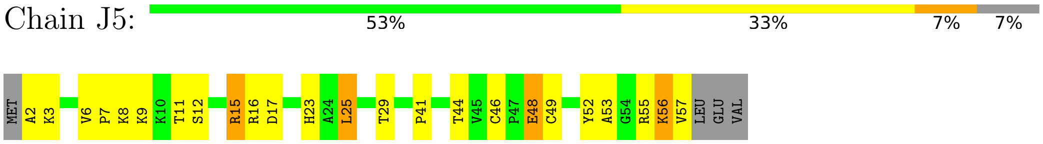
- Molecule 53: 50S ribosomal protein L32

Chain N8:



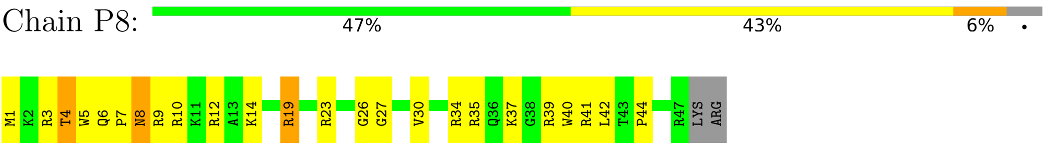
- Molecule 53: 50S ribosomal protein L32

Chain J5:



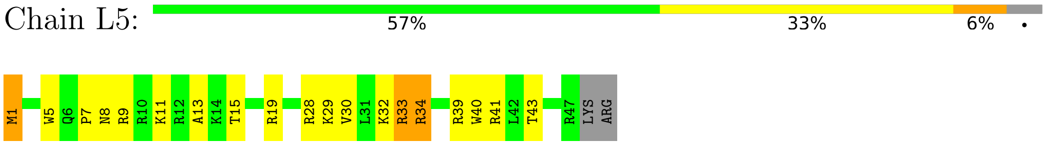
- Molecule 54: 50S ribosomal protein L34

Chain P8:



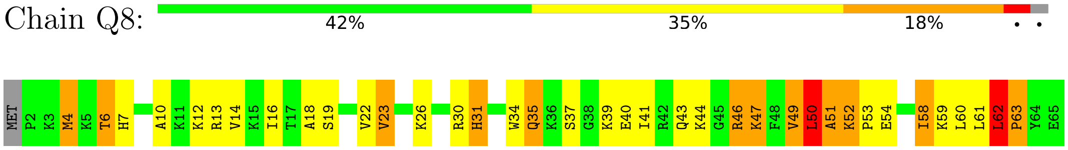
- Molecule 54: 50S ribosomal protein L34

Chain L5:



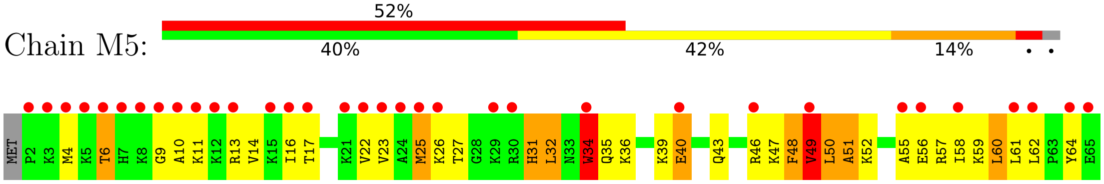
- Molecule 55: 50S ribosomal protein L35

Chain Q8:



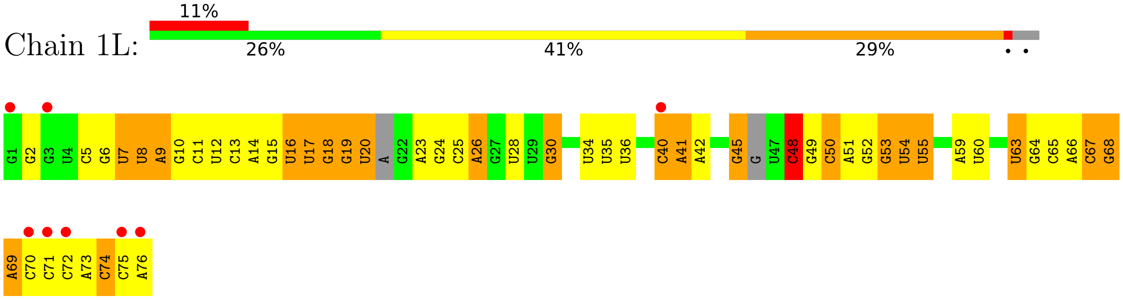
- Molecule 55: 50S ribosomal protein L35

Chain M5:



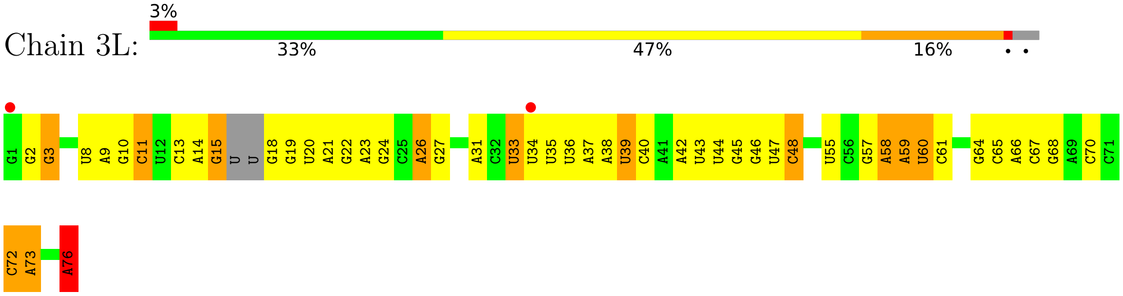
- Molecule 56: tRNA-Lys

Chain 1L:



- Molecule 57: tRNA-Lys

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	208.90Å 447.80Å 617.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.53 – 3.15 161.39 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.53-3.15) 93.3 (161.39-3.15)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.79 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.251 0.194 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	294304	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: SF4, 7MG, ZN, 4SU, 5MU, T6A, MG, PSU, U8U, OMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	13	0.78	5/35994 (0.0%)	1.45	459/56171 (0.8%)
1	1G	0.66	0/36258	1.30	243/56589 (0.4%)
2	12	0.49	0/1742	0.74	1/2346 (0.0%)
2	1E	0.46	0/1908	0.69	0/2573
3	22	0.43	0/1552	0.70	2/2093 (0.1%)
3	2E	0.53	0/1629	0.72	0/2195
4	32	0.47	0/1732	0.72	2/2318 (0.1%)
4	3E	0.61	0/1732	0.79	2/2318 (0.1%)
5	42	0.52	0/1138	0.73	1/1532 (0.1%)
5	4E	0.57	0/1158	0.75	0/1559
6	52	0.52	0/855	0.69	1/1154 (0.1%)
6	5E	0.53	0/850	0.70	0/1147
7	62	0.45	0/1122	0.68	0/1500
7	6E	0.47	0/1230	0.65	0/1645
8	72	0.42	0/1135	0.61	0/1527
8	7E	0.51	0/1135	0.74	0/1527
9	82	0.44	0/1002	0.65	0/1346
9	8E	0.48	0/1024	0.70	1/1374 (0.1%)
10	1A	0.43	0/636	0.65	0/855
10	1I	0.47	0/747	0.71	2/1006 (0.2%)
11	2A	0.47	0/850	0.67	0/1150
11	2I	0.54	0/838	0.73	0/1133
12	3A	0.54	0/963	0.76	1/1290 (0.1%)
12	3I	0.74	0/972	0.92	0/1301
13	4A	0.47	0/898	0.69	1/1204 (0.1%)
13	4I	0.54	0/938	0.76	1/1258 (0.1%)
14	5A	0.46	0/475	0.76	1/632 (0.2%)
14	5I	0.58	0/505	0.76	0/671
15	6A	0.46	0/740	0.65	1/987 (0.1%)
15	6I	0.51	0/744	0.69	0/992
16	7A	0.49	0/721	0.69	0/970
16	7I	0.48	0/687	0.74	0/925

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.49	0/836	0.63	0/1117
17	8I	0.64	2/836 (0.2%)	0.77	0/1117
18	9A	0.51	0/549	0.72	1/732 (0.1%)
18	9I	0.54	0/549	0.74	0/732
19	AA	0.45	0/480	0.76	0/648
19	AI	0.58	0/657	0.86	0/885
20	BA	0.46	0/759	0.69	0/1000
20	BI	0.44	0/748	0.63	0/986
21	1B	0.43	0/212	0.60	0/277
21	1F	0.44	0/203	0.67	0/266
22	1K	0.64	0/1516	1.28	12/2350 (0.5%)
23	2K	0.83	0/1721	1.52	28/2682 (1.0%)
23	2L	0.68	0/1698	1.29	10/2644 (0.4%)
24	3K	0.62	0/1799	1.27	16/2801 (0.6%)
25	4K	0.90	0/495	1.40	4/771 (0.5%)
25	4L	0.70	0/420	1.09	0/654
26	14	0.94	73/69023 (0.1%)	1.67	1714/107740 (1.6%)
26	1H	1.08	148/68351 (0.2%)	1.86	2473/106700 (2.3%)
27	16	0.83	0/2928	1.65	60/4568 (1.3%)
27	1J	0.74	1/2928 (0.0%)	1.45	28/4568 (0.6%)
28	71	0.56	1/1055 (0.1%)	0.80	3/1425 (0.2%)
29	11	0.83	2/2175 (0.1%)	1.03	7/2933 (0.2%)
29	19	0.83	1/2170 (0.0%)	0.97	4/2926 (0.1%)
30	21	0.70	0/1596	0.93	3/2153 (0.1%)
30	29	0.66	0/1596	0.93	1/2153 (0.0%)
31	31	0.76	0/1620	0.93	3/2194 (0.1%)
31	39	0.65	0/1641	0.90	1/2223 (0.0%)
32	41	0.55	0/1489	0.74	0/2005
32	49	0.43	0/1489	0.71	0/2005
33	51	0.60	0/1353	0.89	3/1830 (0.2%)
33	59	0.51	0/548	0.78	0/738
34	61	0.51	0/1146	0.74	1/1551 (0.1%)
34	69	0.50	0/1146	0.78	2/1551 (0.1%)
35	15	0.47	0/1123	0.72	0/1515
35	58	0.62	0/1131	0.84	1/1525 (0.1%)
36	25	0.61	0/942	0.79	1/1269 (0.1%)
36	68	0.67	0/942	0.82	1/1269 (0.1%)
37	35	0.69	0/1147	1.06	4/1525 (0.3%)
37	78	0.76	0/1139	1.14	8/1514 (0.5%)
38	45	0.66	0/1120	0.90	2/1498 (0.1%)
38	88	0.79	0/1134	0.95	2/1519 (0.1%)
39	55	0.65	0/981	0.83	0/1312
39	98	0.61	0/981	0.85	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	65	0.55	0/886	0.83	2/1180 (0.2%)
40	A8	0.67	0/891	0.94	3/1187 (0.3%)
41	75	0.64	0/1146	0.88	0/1531
41	B8	0.70	0/1132	0.88	0/1512
42	85	0.59	0/977	0.75	0/1301
42	C8	0.71	0/968	0.84	1/1289 (0.1%)
43	95	0.74	0/774	0.91	2/1038 (0.2%)
43	D8	0.69	0/785	0.88	3/1052 (0.3%)
44	A5	0.63	0/897	0.82	0/1204
44	E8	0.75	0/901	0.91	0/1209
45	B5	0.76	0/752	0.87	1/1010 (0.1%)
45	F8	0.83	0/765	0.91	2/1029 (0.2%)
46	C5	0.65	0/807	0.88	1/1076 (0.1%)
46	G8	0.82	0/796	1.08	2/1062 (0.2%)
47	D5	0.49	0/1057	0.76	0/1430
47	H8	0.51	0/1248	0.78	1/1687 (0.1%)
48	E5	0.61	0/624	0.83	0/832
48	I8	0.78	0/624	0.94	1/832 (0.1%)
49	F5	0.67	0/744	0.83	0/989
49	J8	0.73	0/744	0.97	1/989 (0.1%)
50	G5	0.61	0/575	0.81	0/762
50	K8	0.87	2/573 (0.3%)	0.84	0/759
51	H5	0.51	0/464	0.69	0/623
51	L8	0.59	0/464	0.80	0/623
52	M8	0.52	0/375	0.86	1/507 (0.2%)
53	J5	0.65	1/448 (0.2%)	0.83	0/606
53	N8	0.74	0/394	0.92	0/534
54	L5	0.71	0/409	0.93	1/540 (0.2%)
54	P8	0.88	0/409	1.05	0/540
55	M5	0.85	1/524 (0.2%)	0.92	1/691 (0.1%)
55	Q8	0.80	0/524	1.05	3/691 (0.4%)
56	1L	0.62	0/1705	1.20	6/2649 (0.2%)
57	3L	0.60	0/1732	1.14	8/2695 (0.3%)
All	All	0.84	237/316396 (0.1%)	1.46	5154/474130 (1.1%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	32	0	2
4	3E	0	4
7	62	0	1
7	6E	0	1
10	1A	0	1
12	3A	0	2
12	3I	0	2
13	4I	0	2
14	5A	0	1
19	AA	0	1
19	AI	0	3
28	71	0	1
29	11	0	4
29	19	0	2
30	21	0	2
30	29	0	6
31	31	0	2
31	39	0	6
32	41	0	1
32	49	0	2
33	51	0	3
33	59	0	1
34	61	0	3
34	69	0	1
35	58	0	1
37	35	0	10
37	78	0	7
38	45	0	4
38	88	0	1
40	65	0	1
40	A8	0	1
41	75	0	3
41	B8	0	4
42	85	0	2
42	C8	0	3
43	D8	0	3
45	B5	0	3
45	F8	0	1
46	C5	0	4
46	G8	0	2
47	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	H8	0	2
50	G5	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	2
All	All	0	119

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-13.80	1.29	1.37
26	1H	676	A	N9-C4	-13.67	1.29	1.37
26	14	783	A	N9-C4	-10.88	1.31	1.37
26	1H	472	A	N3-C4	-10.55	1.28	1.34
26	1H	783	A	N3-C4	-10.35	1.28	1.34

The worst 5 of 5154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-22.91	112.25	126.00
26	1H	676	A	C2-N3-C4	-20.00	100.60	110.60
26	1H	945	A	N1-C6-N6	19.59	130.36	118.60
26	1H	945	A	C6-C5-N7	-18.66	119.24	132.30
26	1H	1332	G	C2-N3-C4	-18.37	102.72	111.90

There are no chirality outliers.

5 of 119 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
4	3E	77	ASN	Peptide
4	3E	82	ALA	Peptide
4	3E	87	GLY	Peptide
4	3E	88	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16233	797	0
1	1G	32391	0	16352	818	1
2	12	1711	0	1751	90	0
2	1E	1874	0	1926	86	0
3	22	1529	0	1592	72	0
3	2E	1605	0	1668	50	0
4	32	1702	0	1766	96	0
4	3E	1702	0	1762	103	0
5	42	1123	0	1191	56	0
5	4E	1142	0	1204	44	0
6	52	842	0	857	31	0
6	5E	837	0	852	47	0
7	62	1110	0	1163	53	0
7	6E	1214	0	1259	41	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	53	0
9	82	983	0	1006	57	0
9	8E	1005	0	1033	76	0
10	1A	626	0	639	34	0
10	1I	734	0	761	51	0
11	2A	835	0	847	38	0
11	2I	823	0	833	33	0
12	3A	947	0	1033	50	0
12	3I	956	0	1046	43	0
13	4A	888	0	941	64	0
13	4I	928	0	987	50	0
14	5A	466	0	499	38	0
14	5I	496	0	535	25	0
15	6A	729	0	768	29	0
15	6I	733	0	771	23	0
16	7A	705	0	725	31	0
16	7I	671	0	693	40	0
17	8A	823	0	891	34	0
17	8I	823	0	891	48	0
18	9A	544	0	605	30	0
18	9I	544	0	605	28	0
19	AA	471	0	464	35	0
19	AI	643	0	662	36	0
20	BA	757	0	856	34	0
20	BI	746	0	843	42	0
21	1B	208	0	221	26	0
21	1F	199	0	208	7	0
22	1K	1477	0	758	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	844	30	0
23	2L	1626	0	835	30	0
24	3K	1611	0	817	57	0
25	4K	439	0	218	14	0
25	4L	373	0	185	9	0
26	14	61630	0	31070	1393	1
26	1H	61028	0	30763	1409	0
27	16	2617	0	1328	71	0
27	1J	2617	0	1328	87	0
28	71	1033	0	1048	54	0
29	11	2125	0	2199	118	0
29	19	2120	0	2197	118	0
30	21	1563	0	1629	92	0
30	29	1563	0	1629	110	0
31	31	1585	0	1632	101	0
31	39	1606	0	1652	93	0
32	41	1464	0	1522	74	0
32	49	1464	0	1522	73	0
33	51	1327	0	1405	62	0
33	59	539	0	563	34	0
34	61	1131	0	1218	51	0
34	69	1131	0	1218	55	0
35	15	1096	0	1168	61	0
35	58	1104	0	1180	69	0
36	25	932	0	996	42	0
36	68	932	0	996	41	0
37	35	1130	0	1217	98	0
37	78	1122	0	1206	91	0
38	45	1099	0	1154	67	0
38	88	1113	0	1157	54	0
39	55	967	0	1033	46	0
39	98	967	0	1033	48	0
40	65	876	0	938	81	0
40	A8	881	0	943	61	0
41	75	1132	0	1189	75	0
41	B8	1118	0	1176	62	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	54	0
43	95	763	0	836	71	0
43	D8	774	0	849	52	0
44	A5	886	0	948	23	0
44	E8	890	0	951	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B5	738	0	792	36	0
45	F8	751	0	807	40	0
46	C5	794	0	886	53	0
46	G8	783	0	873	67	0
47	D5	1034	0	1061	68	0
47	H8	1222	0	1247	80	0
48	E5	616	0	633	38	0
48	I8	616	0	633	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	39	0
50	G5	573	0	616	33	0
50	K8	571	0	623	37	0
51	H5	459	0	512	17	0
51	L8	459	0	512	18	0
52	M8	366	0	370	31	0
53	J5	434	0	454	18	0
53	N8	381	0	397	27	0
54	L5	401	0	436	18	0
54	P8	401	0	436	21	0
55	M5	516	0	582	36	0
55	Q8	516	0	582	34	0
56	1L	1570	0	798	34	0
57	3L	1571	0	798	34	0
58	11	1	0	0	0	0
58	13	142	0	0	0	0
58	14	421	0	0	0	0
58	16	11	0	0	0	0
58	19	1	0	0	0	0
58	1G	95	0	0	0	0
58	1H	495	0	0	0	0
58	1I	1	0	0	0	0
58	1J	6	0	0	0	0
58	1K	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	3	0	0	0	0
58	2I	1	0	0	0	0
58	2K	2	0	0	0	0
58	2L	2	0	0	0	0
58	39	2	0	0	0	0
58	3I	1	0	0	0	0
58	3L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	41	1	0	0	0	0
58	45	3	0	0	0	0
58	4I	1	0	0	0	0
58	4K	1	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7I	1	0	0	0	0
58	88	3	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	1	0	0	0	0
58	N8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	0	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	2	0
61	13	207	0	0	37	0
61	14	717	0	0	118	0
61	15	1	0	0	0	0
61	16	22	0	0	3	0
61	19	10	0	0	4	0
61	1G	117	0	0	23	0
61	1H	819	0	0	163	0
61	1I	1	0	0	0	0
61	1J	6	0	0	0	0
61	21	6	0	0	3	0
61	29	3	0	0	0	0
61	2A	1	0	0	0	0
61	31	4	0	0	1	0
61	32	2	0	0	0	0
61	35	3	0	0	0	0
61	39	3	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	4E	2	0	0	0	0
61	4K	4	0	0	0	0
61	5I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	6A	2	0	0	1	0
61	6I	1	0	0	0	0
61	75	2	0	0	0	0
61	78	1	0	0	0	0
61	7A	1	0	0	0	0
61	85	3	0	0	1	0
61	8E	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	C8	3	0	0	1	0
61	F8	1	0	0	0	0
61	I8	5	0	0	0	0
61	J8	2	0	0	0	0
61	L8	3	0	0	0	0
61	M5	3	0	0	0	0
All	All	294304	0	195547	8554	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8554 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)
1:13:788:U:H2’	1:13:789:U:H5’	1.29	1.06
30:21:135:HIS:NE2	61:21:401:HOH:O	1.87	1.06
26:1H:511:U:OP2	61:1H:3501:HOH:O	1.72	1.05
47:H8:5:LEU:HD11	47:H8:44:PHE:HA	1.40	1.02
26:14:1899:G:H21	26:14:1902:C:N4	1.56	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2’	26:14:271(C):U:O4[3_545]	2.15	0.05

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	204/256 (80%)	170 (83%)	32 (16%)	2 (1%)	15	51
2	1E	227/256 (89%)	191 (84%)	34 (15%)	2 (1%)	17	53
3	22	190/239 (80%)	173 (91%)	15 (8%)	2 (1%)	14	48
3	2E	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29	65
4	3E	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	6	30
5	42	145/162 (90%)	136 (94%)	8 (6%)	1 (1%)	22	59
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	22	59
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	62	134/156 (86%)	126 (94%)	8 (6%)	0	100	100
7	6E	145/156 (93%)	136 (94%)	9 (6%)	0	100	100
8	72	136/138 (99%)	126 (93%)	8 (6%)	2 (2%)	10	41
8	7E	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	82	122/128 (95%)	111 (91%)	11 (9%)	0	100	100
9	8E	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	55
10	1A	72/105 (69%)	64 (89%)	8 (11%)	0	100	100
10	1I	89/105 (85%)	81 (91%)	7 (8%)	1 (1%)	14	48
11	2A	111/129 (86%)	99 (89%)	11 (10%)	1 (1%)	17	53
11	2I	109/129 (84%)	99 (91%)	8 (7%)	2 (2%)	8	37
12	3A	119/132 (90%)	99 (83%)	19 (16%)	1 (1%)	19	55
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	55
13	4A	108/126 (86%)	87 (81%)	20 (18%)	1 (1%)	17	53
13	4I	114/126 (90%)	93 (82%)	19 (17%)	2 (2%)	8	37
14	5A	55/61 (90%)	46 (84%)	8 (14%)	1 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	59/61 (97%)	51 (86%)	8 (14%)	0	100	100
15	6A	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
15	6I	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	13	46
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	78/88 (89%)	76 (97%)	2 (3%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	10	41
19	AA	54/93 (58%)	45 (83%)	5 (9%)	4 (7%)	1	6
19	AI	78/93 (84%)	68 (87%)	6 (8%)	4 (5%)	2	13
20	BA	96/106 (91%)	88 (92%)	8 (8%)	0	100	100
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	71	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
29	11	272/276 (99%)	247 (91%)	16 (6%)	9 (3%)	4	22
29	19	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	37
30	21	202/206 (98%)	173 (86%)	25 (12%)	4 (2%)	7	34
30	29	202/206 (98%)	153 (76%)	36 (18%)	13 (6%)	1	9
31	31	200/210 (95%)	179 (90%)	19 (10%)	2 (1%)	15	51
31	39	203/210 (97%)	174 (86%)	24 (12%)	5 (2%)	5	29
32	41	178/182 (98%)	152 (85%)	23 (13%)	3 (2%)	9	38
32	49	178/182 (98%)	158 (89%)	18 (10%)	2 (1%)	14	48
33	51	171/180 (95%)	132 (77%)	35 (20%)	4 (2%)	6	31
33	59	63/180 (35%)	45 (71%)	17 (27%)	1 (2%)	9	40
34	61	143/148 (97%)	116 (81%)	25 (18%)	2 (1%)	11	43
34	69	143/148 (97%)	116 (81%)	27 (19%)	0	100	100
35	15	135/140 (96%)	123 (91%)	11 (8%)	1 (1%)	22	59
35	58	136/140 (97%)	116 (85%)	17 (12%)	3 (2%)	6	32
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
37	35	146/150 (97%)	112 (77%)	27 (18%)	7 (5%)	2	15
37	78	145/150 (97%)	118 (81%)	20 (14%)	7 (5%)	2	15
38	45	136/141 (96%)	111 (82%)	22 (16%)	3 (2%)	6	32
38	88	139/141 (99%)	114 (82%)	19 (14%)	6 (4%)	2	17
39	55	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
39	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
40	65	108/112 (96%)	92 (85%)	14 (13%)	2 (2%)	8	36
40	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	8	37
41	75	134/146 (92%)	115 (86%)	18 (13%)	1 (1%)	22	59
41	B8	132/146 (90%)	118 (89%)	14 (11%)	0	100	100
42	85	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	17	53
42	C8	113/118 (96%)	105 (93%)	6 (5%)	2 (2%)	8	37
43	95	97/101 (96%)	78 (80%)	15 (16%)	4 (4%)	3	18
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	23
44	A5	109/113 (96%)	99 (91%)	10 (9%)	0	100	100
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	6 (6%)	1 (1%)	14	48
45	F8	94/96 (98%)	83 (88%)	8 (8%)	3 (3%)	4	22
46	C5	102/110 (93%)	69 (68%)	26 (26%)	7 (7%)	1	7
46	G8	101/110 (92%)	90 (89%)	9 (9%)	2 (2%)	7	34
47	D5	120/206 (58%)	92 (77%)	24 (20%)	4 (3%)	4	22
47	H8	142/206 (69%)	120 (84%)	15 (11%)	7 (5%)	2	14
48	E5	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
48	I8	76/85 (89%)	67 (88%)	8 (10%)	1 (1%)	12	44
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	6	32
49	J8	92/98 (94%)	88 (96%)	3 (3%)	1 (1%)	14	48
50	G5	67/72 (93%)	60 (90%)	5 (8%)	2 (3%)	4	24
50	K8	66/72 (92%)	62 (94%)	3 (4%)	1 (2%)	10	41
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	M8	45/71 (63%)	26 (58%)	18 (40%)	1 (2%)	6	32
53	J5	54/60 (90%)	47 (87%)	7 (13%)	0	100	100
53	N8	47/60 (78%)	43 (92%)	4 (8%)	0	100	100
54	L5	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
54	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	15
55	Q8	62/65 (95%)	54 (87%)	4 (6%)	4 (6%)	1	8
All	All	10880/12104 (90%)	9578 (88%)	1134 (10%)	168 (2%)	10	41

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3E	88	VAL
18	9I	22	VAL
29	11	40	THR
29	11	237	GLU
37	78	16	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	138 (76%)	44 (24%)	0	2
2	1E	200/220 (91%)	152 (76%)	48 (24%)	0	3
3	22	153/188 (81%)	126 (82%)	27 (18%)	2	9
3	2E	159/188 (85%)	129 (81%)	30 (19%)	1	7
4	32	180/181 (99%)	145 (81%)	35 (19%)	1	7
4	3E	180/181 (99%)	149 (83%)	31 (17%)	2	9
5	42	113/123 (92%)	85 (75%)	28 (25%)	0	2
5	4E	115/123 (94%)	91 (79%)	24 (21%)	1	5
6	52	90/90 (100%)	80 (89%)	10 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6	24
7	62	114/127 (90%)	94 (82%)	20 (18%)	2	9
7	6E	123/127 (97%)	91 (74%)	32 (26%)	0	2
8	72	119/119 (100%)	98 (82%)	21 (18%)	2	9
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	6
9	82	95/99 (96%)	75 (79%)	20 (21%)	1	5
9	8E	97/99 (98%)	70 (72%)	27 (28%)	0	1
10	1A	69/92 (75%)	53 (77%)	16 (23%)	1	3
10	1I	81/92 (88%)	62 (76%)	19 (24%)	1	3
11	2A	85/99 (86%)	73 (86%)	12 (14%)	3	15
11	2I	84/99 (85%)	68 (81%)	16 (19%)	1	7
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	7
12	3I	103/109 (94%)	81 (79%)	22 (21%)	1	5
13	4A	91/101 (90%)	65 (71%)	26 (29%)	0	1
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	47/50 (94%)	31 (66%)	16 (34%)	0	0
14	5I	49/50 (98%)	40 (82%)	9 (18%)	1	8
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	27
15	6I	79/80 (99%)	68 (86%)	11 (14%)	3	15
16	7A	72/74 (97%)	62 (86%)	10 (14%)	3	15
16	7I	69/74 (93%)	50 (72%)	19 (28%)	0	1
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	18
17	8I	94/97 (97%)	73 (78%)	21 (22%)	1	4
18	9A	58/77 (75%)	45 (78%)	13 (22%)	1	4
18	9I	58/77 (75%)	48 (83%)	10 (17%)	2	9
19	AA	52/80 (65%)	34 (65%)	18 (35%)	0	0
19	AI	70/80 (88%)	57 (81%)	13 (19%)	1	8
20	BA	76/82 (93%)	65 (86%)	11 (14%)	3	14
20	BI	75/82 (92%)	62 (83%)	13 (17%)	2	9
21	1B	19/22 (86%)	16 (84%)	3 (16%)	2	11
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	71	109/181 (60%)	76 (70%)	33 (30%)	0	1
29	11	214/218 (98%)	169 (79%)	45 (21%)	1	5
29	19	214/218 (98%)	164 (77%)	50 (23%)	1	3
30	21	165/166 (99%)	128 (78%)	37 (22%)	1	4
30	29	165/166 (99%)	134 (81%)	31 (19%)	1	7
31	31	161/166 (97%)	126 (78%)	35 (22%)	1	5
31	39	163/166 (98%)	128 (78%)	35 (22%)	1	5
32	41	154/156 (99%)	118 (77%)	36 (23%)	1	3
32	49	154/156 (99%)	123 (80%)	31 (20%)	1	6
33	51	144/148 (97%)	113 (78%)	31 (22%)	1	5
33	59	56/148 (38%)	41 (73%)	15 (27%)	0	1
34	61	122/124 (98%)	93 (76%)	29 (24%)	0	3
34	69	122/124 (98%)	90 (74%)	32 (26%)	0	2
35	15	116/119 (98%)	92 (79%)	24 (21%)	1	5
35	58	117/119 (98%)	91 (78%)	26 (22%)	1	4
36	25	100/100 (100%)	85 (85%)	15 (15%)	3	13
36	68	100/100 (100%)	82 (82%)	18 (18%)	1	8
37	35	115/116 (99%)	82 (71%)	33 (29%)	0	1
37	78	114/116 (98%)	79 (69%)	35 (31%)	0	1
38	45	109/111 (98%)	85 (78%)	24 (22%)	1	4
38	88	109/111 (98%)	89 (82%)	20 (18%)	1	8
39	55	101/101 (100%)	81 (80%)	20 (20%)	1	6
39	98	101/101 (100%)	76 (75%)	25 (25%)	0	2
40	65	87/88 (99%)	66 (76%)	21 (24%)	0	2
40	A8	87/88 (99%)	60 (69%)	27 (31%)	0	1
41	75	119/127 (94%)	88 (74%)	31 (26%)	0	2
41	B8	118/127 (93%)	87 (74%)	31 (26%)	0	2
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	9
42	C8	92/94 (98%)	77 (84%)	15 (16%)	2	10
43	95	81/82 (99%)	61 (75%)	20 (25%)	0	2
43	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	8
44	E8	91/92 (99%)	71 (78%)	20 (22%)	1	4
45	B5	75/78 (96%)	60 (80%)	15 (20%)	1	6
45	F8	76/78 (97%)	63 (83%)	13 (17%)	2	9
46	C5	85/91 (93%)	62 (73%)	23 (27%)	0	1
46	G8	84/91 (92%)	59 (70%)	25 (30%)	0	1
47	D5	115/179 (64%)	82 (71%)	33 (29%)	0	1
47	H8	137/179 (76%)	103 (75%)	34 (25%)	0	2
48	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
48	I8	62/67 (92%)	50 (81%)	12 (19%)	1	7
49	F5	79/83 (95%)	56 (71%)	23 (29%)	0	1
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	8
50	G5	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	K8	63/67 (94%)	43 (68%)	20 (32%)	0	0
51	H5	50/52 (96%)	42 (84%)	8 (16%)	2	10
51	L8	50/52 (96%)	42 (84%)	8 (16%)	2	10
52	M8	42/63 (67%)	34 (81%)	8 (19%)	1	7
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	7
53	N8	44/52 (85%)	32 (73%)	12 (27%)	0	1
54	L5	38/42 (90%)	32 (84%)	6 (16%)	2	11
54	P8	38/42 (90%)	31 (82%)	7 (18%)	1	8
55	M5	54/55 (98%)	37 (68%)	17 (32%)	0	0
55	Q8	54/55 (98%)	40 (74%)	14 (26%)	0	2
All	All	9210/10012 (92%)	7199 (78%)	2011 (22%)	1	5

5 of 2011 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	G8	98	VAL
41	75	57	PHE
4	32	120	LEU
40	65	84	GLN
47	D5	54	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
32	49	58	GLN
43	95	87	HIS
50	G5	43	GLN
40	65	95	HIS
2	12	135	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	374 (25%)	34 (2%)
1	1G	1505/1522 (98%)	376 (24%)	30 (1%)
22	1K	64/76 (84%)	31 (48%)	3 (4%)
23	2K	76/77 (98%)	22 (28%)	3 (3%)
23	2L	74/77 (96%)	19 (25%)	3 (4%)
24	3K	75/76 (98%)	43 (57%)	2 (2%)
25	4K	19/27 (70%)	9 (47%)	2 (10%)
25	4L	16/27 (59%)	7 (43%)	0
26	14	2852/2917 (97%)	732 (25%)	47 (1%)
26	1H	2828/2917 (96%)	709 (25%)	52 (1%)
27	16	121/122 (99%)	25 (20%)	2 (1%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	31 (43%)	4 (5%)
57	3L	72/76 (94%)	21 (29%)	2 (2%)
All	All	9387/9634 (97%)	2440 (25%)	186 (1%)

5 of 2440 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	11	G
1	13	31	G

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	913	A
26	14	278	A
1	1G	1145	C

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Mol	Chain	Res	Type
56	1L	67	C
26	14	784	A

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

18 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	$\#\|Z\| > 2$
56	PSU	1L	55	56	18,21,22	1.14	1 (5%)	22,30,33	1.63	4 (18%)
23	OMC	2L	33	23	19,22,23	1.83	4 (21%)	26,31,34	1.09	1 (3%)
23	4SU	2L	8	23	18,21,22	1.92	5 (27%)	26,30,33	2.32	6 (23%)
23	OMC	2K	33	23	19,22,23	1.73	3 (15%)	26,31,34	0.95	2 (7%)
56	5MU	1L	54	56	19,22,23	3.87	5 (26%)	28,32,35	3.09	11 (39%)
23	5MU	2K	55	23	19,22,23	3.88	5 (26%)	28,32,35	3.36	9 (32%)
23	PSU	2K	56	23	18,21,22	1.25	1 (5%)	22,30,33	1.89	4 (18%)
22	T6A	1K	37	22	27,34,35	2.52	6 (22%)	29,49,52	2.40	9 (31%)
22	5MU	1K	54	22	19,22,23	3.81	5 (26%)	28,32,35	3.23	6 (21%)
23	PSU	2L	56	23	18,21,22	1.29	1 (5%)	22,30,33	1.62	3 (13%)
22	PSU	1K	55	22	18,21,22	1.30	1 (5%)	22,30,33	1.69	5 (22%)
23	5MU	2L	55	23	19,22,23	3.96	5 (26%)	28,32,35	3.19	9 (32%)
22	U8U	1K	34	22,25	19,24,25	2.50	6 (31%)	23,34,37	1.27	3 (13%)
57	PSU	3L	39	57	18,21,22	1.17	1 (5%)	22,30,33	1.45	2 (9%)
23	7MG	2L	47	23	22,26,27	3.03	6 (27%)	29,39,42	2.88	11 (37%)
22	PSU	1K	39	22	18,21,22	1.15	1 (5%)	22,30,33	1.55	3 (13%)
23	4SU	2K	8	23	18,21,22	1.75	3 (16%)	26,30,33	2.38	5 (19%)
23	7MG	2K	47	23	22,26,27	3.33	6 (27%)	29,39,42	2.57	10 (34%)

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
56	PSU	1L	55	56	-	3/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	4/9/27/28	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
56	5MU	1L	54	56	-	3/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/19/41/42	0/3/3/3
22	5MU	1K	54	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	2/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	2/9/28/29	0/2/2/2
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.72	1.58	1.38
23	2K	55	5MU	C2-N1	12.43	1.58	1.38
22	1K	54	5MU	C2-N1	12.32	1.58	1.38
56	1L	54	5MU	C2-N1	12.12	1.57	1.38
23	2K	47	7MG	C5-N7	10.13	1.47	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1K	54	5MU	C5-C4-N3	10.96	124.67	115.31
23	2L	55	5MU	C5-C4-N3	10.30	124.10	115.31
23	2K	55	5MU	C5-C4-N3	10.20	124.02	115.31
56	1L	54	5MU	C5-C4-N3	9.93	123.78	115.31
23	2K	8	4SU	C4-N3-C2	-7.76	119.80	127.34

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	O4'-C4'-C5'-O5'
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	N11-C12-C14-C15
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	33	OMC	1	0
23	2L	8	4SU	2	0
23	2K	33	OMC	1	0
23	2K	55	5MU	3	0
22	1K	37	T6A	1	0
22	1K	54	5MU	3	0
22	1K	55	PSU	1	0
23	2L	55	5MU	1	0
57	3L	39	PSU	1	0
23	2L	47	7MG	1	0
23	2K	8	4SU	1	0
23	2K	47	7MG	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SF4	32	301	-	0,12,12	-	-	-		
59	SF4	3E	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	32	301	-	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13	1496/1522 (98%)	-0.52	3 (0%)	95	94	61, 106, 170, 196	0
1	1G	1507/1522 (99%)	-0.58	2 (0%)	95	95	74, 126, 175, 200	0
2	12	208/256 (81%)	0.59	23 (11%)	5	3	134, 156, 168, 176	0
2	1E	231/256 (90%)	1.07	42 (18%)	1	1	116, 144, 162, 166	0
3	22	194/239 (81%)	0.03	8 (4%)	37	22	129, 148, 164, 167	0
3	2E	205/239 (85%)	-0.25	3 (1%)	73	61	89, 111, 139, 148	0
4	32	208/209 (99%)	1.12	43 (20%)	1	0	105, 125, 146, 151	0
4	3E	208/209 (99%)	0.18	8 (3%)	40	25	85, 106, 126, 135	0
5	42	147/162 (90%)	0.04	3 (2%)	65	50	112, 126, 138, 145	0
5	4E	149/162 (91%)	0.22	2 (1%)	77	66	81, 103, 122, 131	0
6	52	101/101 (100%)	0.14	2 (1%)	65	50	92, 111, 128, 134	0
6	5E	100/101 (99%)	1.07	21 (21%)	1	0	90, 109, 127, 132	0
7	62	138/156 (88%)	-0.15	0	100	100	122, 133, 142, 148	0
7	6E	149/156 (95%)	0.04	5 (3%)	45	28	107, 124, 143, 149	0
8	72	138/138 (100%)	-0.22	1 (0%)	87	81	112, 131, 141, 149	0
8	7E	138/138 (100%)	1.36	44 (31%)	0	0	92, 115, 130, 139	0
9	82	124/128 (96%)	-0.06	4 (3%)	47	30	121, 153, 162, 166	0
9	8E	127/128 (99%)	-0.38	1 (0%)	86	78	91, 137, 154, 159	0
10	1A	78/105 (74%)	-0.26	8 (10%)	6	3	119, 148, 159, 161	0
10	1I	91/105 (86%)	0.39	9 (9%)	7	4	87, 128, 157, 163	0
11	2A	113/129 (87%)	0.46	5 (4%)	34	20	89, 115, 135, 141	0
11	2I	111/129 (86%)	1.18	25 (22%)	0	0	82, 110, 127, 140	0
12	3A	121/132 (91%)	0.62	17 (14%)	2	1	93, 113, 129, 148	0
12	3I	122/132 (92%)	0.91	15 (12%)	4	2	72, 80, 103, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	110/126 (87%)	0.35	13 (11%) 4 2	135, 149, 160, 164	0
13	4I	116/126 (92%)	-0.27	0 100 100	94, 127, 141, 150	0
14	5A	57/61 (93%)	1.33	18 (31%) 0 0	134, 146, 155, 158	0
14	5I	61/61 (100%)	-0.57	0 100 100	86, 100, 118, 123	0
15	6A	87/89 (97%)	0.27	3 (3%) 45 28	93, 119, 139, 144	0
15	6I	88/89 (98%)	1.54	28 (31%) 0 0	81, 104, 125, 134	0
16	7A	84/88 (95%)	0.03	0 100 100	95, 114, 137, 148	0
16	7I	80/88 (90%)	-0.18	0 100 100	101, 115, 133, 142	0
17	8A	99/105 (94%)	0.39	3 (3%) 50 33	102, 119, 130, 135	0
17	8I	99/105 (94%)	0.86	14 (14%) 2 1	93, 109, 125, 130	0
18	9A	67/88 (76%)	-0.19	0 100 100	101, 118, 136, 139	0
18	9I	67/88 (76%)	0.18	1 (1%) 73 61	94, 112, 132, 136	0
19	AA	60/93 (64%)	0.57	7 (11%) 4 2	133, 161, 167, 171	0
19	AI	80/93 (86%)	-0.85	0 100 100	105, 121, 143, 150	0
20	BA	98/106 (92%)	0.51	5 (5%) 28 15	87, 115, 141, 154	0
20	BI	97/106 (91%)	0.33	5 (5%) 27 14	114, 126, 152, 156	0
21	1B	24/27 (88%)	0.66	3 (12%) 3 2	128, 144, 156, 160	0
21	1F	23/27 (85%)	-0.07	0 100 100	106, 114, 122, 128	0
22	1K	64/76 (84%)	0.02	2 (3%) 49 32	96, 170, 182, 184	0
23	2K	72/77 (93%)	-0.29	0 100 100	74, 103, 134, 154	0
23	2L	71/77 (92%)	-0.16	0 100 100	84, 121, 153, 157	0
24	3K	76/76 (100%)	0.35	10 (13%) 3 2	79, 183, 195, 202	0
25	4K	20/27 (74%)	0.37	2 (10%) 7 4	78, 145, 186, 186	0
25	4L	17/27 (62%)	0.47	0 100 100	104, 160, 189, 189	0
26	14	2861/2917 (98%)	-0.29	15 (0%) 91 86	54, 88, 183, 207	0
26	1H	2833/2917 (97%)	-0.37	7 (0%) 95 94	45, 77, 169, 200	0
27	16	122/122 (100%)	-0.63	1 (0%) 86 78	70, 97, 122, 187	0
27	1J	122/122 (100%)	-0.55	1 (0%) 86 78	94, 131, 151, 186	0
28	71	133/229 (58%)	0.49	13 (9%) 7 4	126, 158, 171, 177	0
29	11	274/276 (99%)	1.01	34 (12%) 4 2	47, 69, 89, 99	0
29	19	273/276 (98%)	0.53	10 (3%) 41 25	51, 76, 92, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($\AA^2$)	Q<0.9
30	21	204/206 (99%)	1.43	64 (31%) 0 0	52, 92, 133, 150	0
30	29	204/206 (99%)	0.09	2 (0%) 82 73	59, 96, 131, 135	0
31	31	202/210 (96%)	0.48	10 (4%) 28 15	51, 81, 113, 135	0
31	39	205/210 (97%)	0.10	1 (0%) 91 86	61, 104, 144, 171	0
32	41	180/182 (98%)	0.11	4 (2%) 62 47	90, 110, 144, 155	0
32	49	180/182 (98%)	1.40	47 (26%) 0 0	124, 143, 162, 169	0
33	51	173/180 (96%)	0.30	11 (6%) 19 10	87, 109, 124, 137	0
33	59	69/180 (38%)	0.41	15 (21%) 0 0	136, 158, 168, 170	0
34	61	145/148 (97%)	-0.18	3 (2%) 63 49	84, 133, 147, 158	0
34	69	145/148 (97%)	0.70	24 (16%) 1 1	87, 127, 146, 152	0
35	15	137/140 (97%)	0.45	4 (2%) 51 35	78, 109, 138, 155	0
35	58	138/140 (98%)	1.14	31 (22%) 0 0	69, 92, 132, 145	0
36	25	122/122 (100%)	0.53	4 (3%) 46 29	70, 92, 109, 116	0
36	68	122/122 (100%)	0.86	16 (13%) 3 2	60, 81, 99, 113	0
37	35	148/150 (98%)	2.27	80 (54%) 0 0	59, 105, 140, 156	0
37	78	147/150 (98%)	-0.09	2 (1%) 75 63	52, 84, 108, 119	0
38	45	138/141 (97%)	2.25	69 (50%) 0 0	75, 110, 134, 149	0
38	88	141/141 (100%)	0.12	4 (2%) 53 36	58, 85, 105, 122	0
39	55	118/118 (100%)	0.49	6 (5%) 28 15	64, 84, 102, 119	0
39	98	118/118 (100%)	1.89	51 (43%) 0 0	66, 87, 108, 130	0
40	65	110/112 (98%)	0.80	15 (13%) 3 2	92, 120, 137, 142	0
40	A8	111/112 (99%)	0.64	11 (9%) 7 4	75, 93, 115, 135	0
41	75	136/146 (93%)	0.70	11 (8%) 12 6	80, 100, 138, 155	0
41	B8	134/146 (91%)	0.17	6 (4%) 33 19	74, 95, 137, 155	0
42	85	116/118 (98%)	0.47	8 (6%) 16 9	68, 97, 129, 138	0
42	C8	115/118 (97%)	-0.12	2 (1%) 70 57	57, 83, 110, 117	0
43	95	99/101 (98%)	1.11	19 (19%) 1 0	65, 123, 136, 145	0
43	D8	100/101 (99%)	0.69	11 (11%) 5 3	59, 102, 124, 139	0
44	A5	111/113 (98%)	0.09	0 100 100	65, 77, 107, 135	0
44	E8	112/113 (99%)	0.15	2 (1%) 68 55	61, 75, 105, 140	0
45	B5	94/96 (97%)	0.29	2 (2%) 63 49	69, 90, 111, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
45	F8	96/96 (100%)	0.25	0	100	100	53, 74, 112, 125	0
46	C5	104/110 (94%)	0.62	13 (12%)	3	2	91, 119, 148, 157	0
46	G8	103/110 (93%)	0.36	3 (2%)	51	35	74, 93, 127, 130	0
47	D5	126/206 (61%)	1.43	43 (34%)	0	0	117, 137, 159, 164	0
47	H8	148/206 (71%)	0.08	1 (0%)	87	81	86, 121, 154, 160	0
48	E5	78/85 (91%)	0.89	12 (15%)	2	1	73, 93, 110, 138	0
48	I8	78/85 (91%)	-0.07	0	100	100	62, 77, 98, 110	0
49	F5	94/98 (95%)	1.07	19 (20%)	1	0	65, 86, 123, 133	0
49	J8	94/98 (95%)	0.18	2 (2%)	63	49	57, 79, 115, 126	0
50	G5	69/72 (95%)	-0.20	1 (1%)	75	63	89, 109, 131, 150	0
50	K8	68/72 (94%)	0.11	1 (1%)	73	61	64, 81, 98, 126	0
51	H5	58/60 (96%)	0.74	4 (6%)	16	9	77, 103, 128, 137	0
51	L8	58/60 (96%)	0.49	4 (6%)	16	9	66, 81, 110, 129	0
52	M8	47/71 (66%)	0.51	2 (4%)	35	21	114, 147, 163, 171	0
53	J5	56/60 (93%)	-0.01	0	100	100	61, 87, 134, 143	0
53	N8	49/60 (81%)	0.96	10 (20%)	1	0	55, 82, 140, 150	0
54	L5	47/49 (95%)	-0.05	0	100	100	57, 62, 79, 91	0
54	P8	47/49 (95%)	-0.17	0	100	100	49, 55, 78, 89	0
55	M5	64/65 (98%)	2.11	34 (53%)	0	0	72, 82, 97, 124	0
55	Q8	64/65 (98%)	0.27	0	100	100	56, 73, 86, 101	0
56	1L	72/76 (94%)	0.39	8 (11%)	5	3	127, 184, 195, 204	0
57	3L	73/76 (96%)	-0.16	2 (2%)	54	38	84, 172, 185, 193	0
All	All	20506/21738 (94%)	0.10	1183 (5%)	23	12	45, 104, 163, 207	0

The worst 5 of 1183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	35	110	TYR	11.7
43	95	1	MET	9.4
43	95	45	THR	9.3
37	35	148	LEU	8.7
38	45	91	GLU	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
22	PSU	1K	55	20/21	0.86	0.12	121,129,137,142	0
56	PSU	1L	55	20/21	0.88	0.12	137,155,161,162	0
23	4SU	2L	8	20/21	0.90	0.17	110,128,130,136	0
22	5MU	1K	54	21/22	0.91	0.14	118,129,141,147	0
57	PSU	3L	39	20/21	0.91	0.13	147,156,160,160	0
22	T6A	1K	37	32/33	0.91	0.18	89,102,123,128	0
23	PSU	2K	56	20/21	0.91	0.12	103,115,124,125	0
23	PSU	2L	56	20/21	0.91	0.15	133,136,141,142	0
56	5MU	1L	54	21/22	0.92	0.11	143,156,161,162	0
23	OMC	2L	33	21/22	0.93	0.17	106,117,118,119	0
23	4SU	2K	8	20/21	0.93	0.18	90,100,108,111	0
22	PSU	1K	39	20/21	0.93	0.14	104,124,130,132	0
23	5MU	2L	55	21/22	0.94	0.12	131,139,146,151	0
23	7MG	2K	47	24/25	0.94	0.16	103,111,119,127	0
23	5MU	2K	55	21/22	0.94	0.15	117,123,131,135	0
23	OMC	2K	33	21/22	0.96	0.20	80,86,90,95	0
23	7MG	2L	47	24/25	0.96	0.13	133,141,147,149	0
22	U8U	1K	34	23/24	0.96	0.14	88,99,103,104	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1H	3302	1/1	0.15	0.30	94,94,94,94	0
58	MG	3L	101	1/1	0.17	0.24	160,160,160,160	0
58	MG	13	1696	1/1	0.23	0.41	105,105,105,105	0
58	MG	14	3263	1/1	0.32	0.45	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	13	1686	1/1	0.41	0.36	94,94,94,94	0
58	MG	14	3257	1/1	0.42	0.71	92,92,92,92	0
58	MG	14	3201	1/1	0.45	0.27	91,91,91,91	0
58	MG	1H	3265	1/1	0.46	0.26	115,115,115,115	0
58	MG	14	3346	1/1	0.48	0.09	144,144,144,144	0
58	MG	13	1683	1/1	0.50	0.21	97,97,97,97	0
58	MG	1H	3324	1/1	0.51	0.38	65,65,65,65	0
58	MG	14	3123	1/1	0.52	0.34	79,79,79,79	0
58	MG	14	3014	1/1	0.53	0.65	78,78,78,78	0
58	MG	1G	1643	1/1	0.53	0.29	83,83,83,83	0
58	MG	1H	3255	1/1	0.54	0.45	68,68,68,68	0
58	MG	1H	3286	1/1	0.55	0.26	100,100,100,100	0
58	MG	1G	1603	1/1	0.55	0.63	100,100,100,100	0
58	MG	2I	201	1/1	0.55	0.27	98,98,98,98	0
58	MG	14	3194	1/1	0.55	0.31	74,74,74,74	0
58	MG	1G	1678	1/1	0.57	0.20	120,120,120,120	0
58	MG	1G	1641	1/1	0.57	0.19	102,102,102,102	0
58	MG	1K	101	1/1	0.57	0.45	147,147,147,147	0
58	MG	1H	3205	1/1	0.58	0.43	101,101,101,101	0
58	MG	14	3274	1/1	0.58	0.27	91,91,91,91	0
58	MG	14	3017	1/1	0.58	0.28	87,87,87,87	0
58	MG	7I	101	1/1	0.59	0.19	95,95,95,95	0
58	MG	1H	3162	1/1	0.60	0.39	74,74,74,74	0
58	MG	2L	102	1/1	0.61	0.45	94,94,94,94	0
58	MG	13	1675	1/1	0.62	0.34	97,97,97,97	0
58	MG	1H	3207	1/1	0.62	0.56	84,84,84,84	0
58	MG	1G	1661	1/1	0.62	0.11	96,96,96,96	0
58	MG	1H	3211	1/1	0.62	0.37	83,83,83,83	0
58	MG	1G	1628	1/1	0.62	0.49	102,102,102,102	0
58	MG	1H	3309	1/1	0.63	0.33	77,77,77,77	0
58	MG	1H	3246	1/1	0.64	0.21	75,75,75,75	0
58	MG	14	3225	1/1	0.64	0.72	84,84,84,84	0
58	MG	14	3245	1/1	0.64	0.29	90,90,90,90	0
58	MG	1H	3447	1/1	0.64	0.28	87,87,87,87	0
58	MG	1H	3486	1/1	0.64	0.22	98,98,98,98	0
58	MG	13	1735	1/1	0.64	0.09	124,124,124,124	0
58	MG	13	1694	1/1	0.64	0.48	88,88,88,88	0
58	MG	14	3229	1/1	0.65	0.43	85,85,85,85	0
58	MG	1I	201	1/1	0.65	0.26	79,79,79,79	0
60	ZN	C5	201	1/1	0.65	0.08	153,153,153,153	0
58	MG	13	1607	1/1	0.66	0.65	84,84,84,84	0
58	MG	14	3223	1/1	0.66	0.23	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3068	1/1	0.66	0.83	86,86,86,86	0
58	MG	13	1666	1/1	0.66	0.28	97,97,97,97	0
58	MG	1H	3310	1/1	0.66	0.16	126,126,126,126	0
58	MG	14	3249	1/1	0.67	0.35	93,93,93,93	0
58	MG	1H	3034	1/1	0.67	0.22	91,91,91,91	0
58	MG	14	3021	1/1	0.67	0.35	77,77,77,77	0
58	MG	1H	3249	1/1	0.67	0.25	77,77,77,77	0
58	MG	13	1668	1/1	0.67	0.15	105,105,105,105	0
58	MG	1H	3175	1/1	0.67	0.43	84,84,84,84	0
58	MG	14	3262	1/1	0.68	0.27	78,78,78,78	0
58	MG	13	1680	1/1	0.68	0.18	149,149,149,149	0
58	MG	1H	3313	1/1	0.68	0.38	96,96,96,96	0
58	MG	1H	3264	1/1	0.68	0.47	87,87,87,87	0
58	MG	1J	206	1/1	0.68	0.08	115,115,115,115	0
58	MG	14	3158	1/1	0.68	0.30	69,69,69,69	0
58	MG	13	1628	1/1	0.69	0.51	82,82,82,82	0
58	MG	14	3113	1/1	0.69	0.18	84,84,84,84	0
58	MG	1G	1669	1/1	0.69	0.19	93,93,93,93	0
58	MG	13	1669	1/1	0.69	0.52	81,81,81,81	0
58	MG	1H	3184	1/1	0.69	0.40	81,81,81,81	0
58	MG	14	3273	1/1	0.69	1.01	87,87,87,87	0
58	MG	1H	3289	1/1	0.69	0.17	91,91,91,91	0
58	MG	14	3324	1/1	0.69	0.11	93,93,93,93	0
58	MG	1H	3301	1/1	0.69	0.44	80,80,80,80	0
58	MG	1H	3329	1/1	0.69	0.27	91,91,91,91	0
58	MG	1G	1650	1/1	0.69	0.38	102,102,102,102	0
58	MG	1H	3086	1/1	0.70	0.32	59,59,59,59	0
58	MG	1G	1630	1/1	0.70	0.40	79,79,79,79	0
58	MG	29	302	1/1	0.70	0.49	74,74,74,74	0
58	MG	1H	3268	1/1	0.70	0.29	72,72,72,72	0
58	MG	1G	1674	1/1	0.71	0.33	110,110,110,110	0
58	MG	14	3218	1/1	0.71	0.12	84,84,84,84	0
58	MG	13	1649	1/1	0.71	0.37	92,92,92,92	0
58	MG	1H	3176	1/1	0.71	0.14	76,76,76,76	0
58	MG	13	1701	1/1	0.71	0.30	92,92,92,92	0
58	MG	1H	3236	1/1	0.71	0.24	76,76,76,76	0
58	MG	1H	3245	1/1	0.71	0.21	72,72,72,72	0
58	MG	14	3253	1/1	0.71	0.33	84,84,84,84	0
58	MG	14	3197	1/1	0.71	0.30	146,146,146,146	0
58	MG	1H	3234	1/1	0.72	0.42	78,78,78,78	0
58	MG	14	3246	1/1	0.72	0.41	90,90,90,90	0
58	MG	14	3277	1/1	0.72	0.65	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3330	1/1	0.72	0.25	87,87,87,87	0
58	MG	1H	3027	1/1	0.72	0.56	83,83,83,83	0
58	MG	1H	3288	1/1	0.72	0.28	77,77,77,77	0
58	MG	1H	3159	1/1	0.72	0.26	70,70,70,70	0
58	MG	1H	3035	1/1	0.72	0.51	87,87,87,87	0
58	MG	14	3207	1/1	0.73	0.12	66,66,66,66	0
58	MG	14	3216	1/1	0.73	0.55	58,58,58,58	0
58	MG	14	3044	1/1	0.73	0.33	85,85,85,85	0
58	MG	1H	3015	1/1	0.73	0.26	70,70,70,70	0
58	MG	1H	3197	1/1	0.73	0.46	91,91,91,91	0
58	MG	1G	1657	1/1	0.73	0.59	84,84,84,84	0
58	MG	14	3243	1/1	0.73	0.40	118,118,118,118	0
58	MG	1G	1658	1/1	0.73	0.11	99,99,99,99	0
58	MG	1H	3485	1/1	0.73	0.10	116,116,116,116	0
58	MG	1G	1662	1/1	0.73	0.15	84,84,84,84	0
58	MG	1H	3099	1/1	0.73	0.40	57,57,57,57	0
58	MG	14	3240	1/1	0.74	0.57	82,82,82,82	0
58	MG	14	3140	1/1	0.74	0.30	90,90,90,90	0
58	MG	1H	3149	1/1	0.74	0.47	79,79,79,79	0
58	MG	14	3186	1/1	0.74	0.47	63,63,63,63	0
58	MG	14	3289	1/1	0.74	0.12	99,99,99,99	0
58	MG	14	3221	1/1	0.74	0.55	86,86,86,86	0
58	MG	1H	3151	1/1	0.74	0.36	76,76,76,76	0
58	MG	14	3254	1/1	0.74	0.52	90,90,90,90	0
58	MG	1H	3279	1/1	0.74	0.40	71,71,71,71	0
58	MG	1H	3479	1/1	0.74	0.20	102,102,102,102	0
58	MG	14	3190	1/1	0.75	0.27	106,106,106,106	0
58	MG	1H	3188	1/1	0.75	0.57	90,90,90,90	0
58	MG	1J	203	1/1	0.75	0.29	88,88,88,88	0
58	MG	1H	3124	1/1	0.75	0.30	56,56,56,56	0
58	MG	1H	3332	1/1	0.75	0.17	72,72,72,72	0
58	MG	45	203	1/1	0.75	0.46	70,70,70,70	0
58	MG	13	1673	1/1	0.75	0.34	99,99,99,99	0
58	MG	14	3271	1/1	0.76	0.35	77,77,77,77	0
58	MG	14	3013	1/1	0.76	0.48	83,83,83,83	0
58	MG	2K	102	1/1	0.76	0.45	79,79,79,79	0
58	MG	1H	3182	1/1	0.76	0.24	76,76,76,76	0
58	MG	13	1616	1/1	0.76	0.30	62,62,62,62	0
58	MG	1H	3307	1/1	0.76	0.32	68,68,68,68	0
58	MG	1H	3134	1/1	0.76	0.24	58,58,58,58	0
58	MG	1H	3339	1/1	0.76	0.19	84,84,84,84	0
58	MG	1H	3347	1/1	0.76	0.36	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1662	1/1	0.76	0.13	81,81,81,81	0
58	MG	14	3149	1/1	0.76	0.20	83,83,83,83	0
58	MG	1H	3458	1/1	0.76	0.10	99,99,99,99	0
58	MG	1H	3168	1/1	0.77	0.33	70,70,70,70	0
58	MG	14	3219	1/1	0.77	0.35	107,107,107,107	0
58	MG	14	3126	1/1	0.77	0.56	78,78,78,78	0
58	MG	1G	1635	1/1	0.77	0.51	82,82,82,82	0
58	MG	13	1692	1/1	0.77	0.36	101,101,101,101	0
58	MG	13	1656	1/1	0.77	0.13	83,83,83,83	0
58	MG	14	3159	1/1	0.77	0.25	75,75,75,75	0
58	MG	14	3299	1/1	0.77	0.06	99,99,99,99	0
58	MG	1H	3156	1/1	0.77	0.27	76,76,76,76	0
58	MG	14	3339	1/1	0.77	0.12	109,109,109,109	0
58	MG	13	1739	1/1	0.77	0.05	110,110,110,110	0
58	MG	1H	3293	1/1	0.77	0.32	92,92,92,92	0
58	MG	13	1647	1/1	0.77	0.33	107,107,107,107	0
58	MG	1H	3266	1/1	0.77	0.22	82,82,82,82	0
58	MG	1G	1665	1/1	0.77	0.21	85,85,85,85	0
58	MG	1H	3334	1/1	0.77	0.38	96,96,96,96	0
58	MG	1H	3252	1/1	0.78	0.31	77,77,77,77	0
58	MG	13	1734	1/1	0.78	0.07	130,130,130,130	0
58	MG	14	3334	1/1	0.78	0.13	89,89,89,89	0
58	MG	14	3230	1/1	0.78	0.29	87,87,87,87	0
58	MG	14	3153	1/1	0.78	0.65	77,77,77,77	0
58	MG	14	3350	1/1	0.78	0.10	89,89,89,89	0
58	MG	14	3382	1/1	0.78	0.07	75,75,75,75	0
58	MG	1G	1673	1/1	0.78	0.22	93,93,93,93	0
58	MG	1H	3274	1/1	0.78	0.38	75,75,75,75	0
58	MG	14	3122	1/1	0.78	0.46	71,71,71,71	0
58	MG	14	3016	1/1	0.78	0.21	61,61,61,61	0
58	MG	1H	3379	1/1	0.78	0.12	92,92,92,92	0
58	MG	14	3290	1/1	0.79	0.12	89,89,89,89	0
58	MG	1H	3276	1/1	0.79	0.41	67,67,67,67	0
58	MG	14	3102	1/1	0.79	0.80	76,76,76,76	0
58	MG	14	3222	1/1	0.79	0.41	73,73,73,73	0
58	MG	1H	3128	1/1	0.79	0.37	83,83,83,83	0
58	MG	1H	3468	1/1	0.79	0.19	108,108,108,108	0
58	MG	1H	3267	1/1	0.79	0.15	97,97,97,97	0
58	MG	1H	3193	1/1	0.79	0.39	89,89,89,89	0
58	MG	1H	3147	1/1	0.79	0.28	90,90,90,90	0
58	MG	16	204	1/1	0.79	0.29	80,80,80,80	0
58	MG	14	3152	1/1	0.79	0.40	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3285	1/1	0.79	0.22	70,70,70,70	0
58	MG	88	203	1/1	0.79	0.35	75,75,75,75	0
58	MG	1H	3440	1/1	0.80	0.13	102,102,102,102	0
58	MG	1H	3282	1/1	0.80	0.17	67,67,67,67	0
58	MG	14	3332	1/1	0.80	0.07	103,103,103,103	0
58	MG	14	3236	1/1	0.80	0.14	74,74,74,74	0
58	MG	14	3268	1/1	0.80	0.33	79,79,79,79	0
58	MG	14	3269	1/1	0.80	0.12	86,86,86,86	0
58	MG	13	1651	1/1	0.80	0.38	105,105,105,105	0
58	MG	14	3120	1/1	0.80	0.23	70,70,70,70	0
58	MG	1H	3041	1/1	0.80	0.43	86,86,86,86	0
58	MG	1G	1627	1/1	0.80	0.53	103,103,103,103	0
58	MG	13	1603	1/1	0.80	0.39	76,76,76,76	0
58	MG	14	3139	1/1	0.80	0.49	55,55,55,55	0
58	MG	1H	3290	1/1	0.80	0.30	83,83,83,83	0
58	MG	13	1657	1/1	0.81	0.15	72,72,72,72	0
58	MG	1H	3348	1/1	0.81	0.27	63,63,63,63	0
58	MG	1G	1659	1/1	0.81	0.11	107,107,107,107	0
58	MG	14	3146	1/1	0.81	0.39	71,71,71,71	0
58	MG	1H	3196	1/1	0.81	0.30	72,72,72,72	0
58	MG	13	1682	1/1	0.81	0.30	151,151,151,151	0
58	MG	14	3036	1/1	0.81	0.38	115,115,115,115	0
58	MG	1H	3297	1/1	0.81	0.32	78,78,78,78	0
58	MG	1H	3105	1/1	0.81	0.36	63,63,63,63	0
58	MG	13	1670	1/1	0.81	0.19	103,103,103,103	0
58	MG	1H	3303	1/1	0.81	0.53	99,99,99,99	0
58	MG	1H	3304	1/1	0.81	0.40	94,94,94,94	0
58	MG	1H	3150	1/1	0.81	0.38	62,62,62,62	0
58	MG	14	3282	1/1	0.81	0.33	82,82,82,82	0
58	MG	1G	1654	1/1	0.81	0.28	132,132,132,132	0
58	MG	1H	3285	1/1	0.82	0.33	61,61,61,61	0
58	MG	1G	1671	1/1	0.82	0.28	102,102,102,102	0
58	MG	1H	3084	1/1	0.82	0.25	49,49,49,49	0
58	MG	13	1678	1/1	0.82	0.35	89,89,89,89	0
58	MG	13	1704	1/1	0.82	0.19	72,72,72,72	0
58	MG	1G	1680	1/1	0.82	0.07	127,127,127,127	0
58	MG	13	1608	1/1	0.82	0.27	86,86,86,86	0
58	MG	1G	1651	1/1	0.82	0.37	100,100,100,100	0
58	MG	14	3335	1/1	0.82	0.09	120,120,120,120	0
58	MG	1H	3260	1/1	0.82	0.22	60,60,60,60	0
58	MG	14	3344	1/1	0.82	0.10	96,96,96,96	0
58	MG	1H	3119	1/1	0.82	0.28	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3265	1/1	0.82	0.55	83,83,83,83	0
58	MG	14	3147	1/1	0.82	0.49	91,91,91,91	0
58	MG	14	3409	1/1	0.82	0.08	106,106,106,106	0
58	MG	21	302	1/1	0.82	0.22	69,69,69,69	0
58	MG	1H	3062	1/1	0.82	0.17	88,88,88,88	0
58	MG	1H	3422	1/1	0.82	0.09	83,83,83,83	0
58	MG	25	201	1/1	0.82	0.22	85,85,85,85	0
58	MG	1H	3426	1/1	0.82	0.11	103,103,103,103	0
58	MG	1H	3328	1/1	0.82	0.35	65,65,65,65	0
58	MG	1H	3085	1/1	0.83	0.29	59,59,59,59	0
58	MG	P8	101	1/1	0.83	0.26	68,68,68,68	0
58	MG	14	3276	1/1	0.83	0.60	87,87,87,87	0
58	MG	1H	3204	1/1	0.83	0.66	81,81,81,81	0
58	MG	14	3279	1/1	0.83	0.24	77,77,77,77	0
58	MG	1G	1612	1/1	0.83	0.41	100,100,100,100	0
58	MG	1G	1621	1/1	0.83	0.74	79,79,79,79	0
58	MG	14	3287	1/1	0.83	0.42	83,83,83,83	0
58	MG	13	1711	1/1	0.83	0.09	102,102,102,102	0
58	MG	14	3141	1/1	0.83	0.41	80,80,80,80	0
58	MG	1H	3098	1/1	0.83	0.29	65,65,65,65	0
58	MG	1H	3430	1/1	0.83	0.28	112,112,112,112	0
58	MG	1H	3132	1/1	0.83	0.32	74,74,74,74	0
58	MG	14	3241	1/1	0.83	0.18	115,115,115,115	0
58	MG	14	3008	1/1	0.83	0.39	85,85,85,85	0
58	MG	1H	3443	1/1	0.83	0.23	86,86,86,86	0
58	MG	1H	3221	1/1	0.83	0.13	63,63,63,63	0
58	MG	1H	3158	1/1	0.83	0.42	78,78,78,78	0
58	MG	14	3164	1/1	0.83	0.53	70,70,70,70	0
58	MG	13	1737	1/1	0.83	0.14	111,111,111,111	0
58	MG	1H	3191	1/1	0.83	0.39	67,67,67,67	0
58	MG	1H	3484	1/1	0.83	0.08	104,104,104,104	0
58	MG	1H	3333	1/1	0.83	0.63	88,88,88,88	0
58	MG	13	1684	1/1	0.83	0.16	101,101,101,101	0
58	MG	1H	3278	1/1	0.83	0.15	61,61,61,61	0
58	MG	14	3213	1/1	0.83	0.25	72,72,72,72	0
58	MG	1H	3164	1/1	0.83	0.39	70,70,70,70	0
58	MG	14	3250	1/1	0.84	0.53	87,87,87,87	0
58	MG	1H	3250	1/1	0.84	0.27	69,69,69,69	0
58	MG	1H	3322	1/1	0.84	0.34	78,78,78,78	0
58	MG	14	3303	1/1	0.84	0.06	72,72,72,72	0
58	MG	1H	3072	1/1	0.84	0.27	80,80,80,80	0
58	MG	14	3259	1/1	0.84	0.43	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	1G	1648	1/1	0.84	0.35	90,90,90,90	0
58	MG	1G	1677	1/1	0.84	0.11	130,130,130,130	0
58	MG	1H	3189	1/1	0.84	0.56	71,71,71,71	0
58	MG	14	3227	1/1	0.84	0.24	91,91,91,91	0
58	MG	14	3119	1/1	0.84	0.08	80,80,80,80	0
58	MG	1H	3465	1/1	0.84	0.07	97,97,97,97	0
58	MG	14	3376	1/1	0.84	0.11	117,117,117,117	0
58	MG	14	3235	1/1	0.84	0.24	76,76,76,76	0
58	MG	14	3405	1/1	0.84	0.09	107,107,107,107	0
58	MG	1H	3350	1/1	0.84	0.15	49,49,49,49	0
58	MG	1G	1617	1/1	0.84	0.10	101,101,101,101	0
58	MG	1H	3155	1/1	0.84	0.25	71,71,71,71	0
58	MG	13	1634	1/1	0.84	0.19	81,81,81,81	0
58	MG	1H	3209	1/1	0.84	0.45	87,87,87,87	0
58	MG	13	1685	1/1	0.84	0.05	101,101,101,101	0
58	MG	1G	1631	1/1	0.84	0.52	104,104,104,104	0
58	MG	1H	3345	1/1	0.85	0.23	68,68,68,68	0
58	MG	1H	3319	1/1	0.85	0.26	80,80,80,80	0
58	MG	1G	1660	1/1	0.85	0.41	107,107,107,107	0
58	MG	14	3281	1/1	0.85	0.20	93,93,93,93	0
58	MG	1H	3239	1/1	0.85	0.26	58,58,58,58	0
58	MG	14	3284	1/1	0.85	0.41	81,81,81,81	0
58	MG	13	1667	1/1	0.85	0.14	90,90,90,90	0
58	MG	1H	3284	1/1	0.85	0.38	92,92,92,92	0
58	MG	14	3043	1/1	0.85	0.16	85,85,85,85	0
58	MG	1H	3421	1/1	0.85	0.15	118,118,118,118	0
58	MG	14	3163	1/1	0.85	0.68	65,65,65,65	0
58	MG	14	3052	1/1	0.85	0.36	75,75,75,75	0
58	MG	14	3321	1/1	0.85	0.14	87,87,87,87	0
58	MG	14	3165	1/1	0.85	0.26	47,47,47,47	0
58	MG	14	3327	1/1	0.85	0.06	102,102,102,102	0
58	MG	14	3065	1/1	0.85	0.43	67,67,67,67	0
58	MG	13	1646	1/1	0.85	0.19	93,93,93,93	0
58	MG	14	3191	1/1	0.85	0.54	81,81,81,81	0
58	MG	1H	3488	1/1	0.85	0.05	92,92,92,92	0
58	MG	1H	3161	1/1	0.85	0.36	71,71,71,71	0
58	MG	16	205	1/1	0.85	0.15	88,88,88,88	0
58	MG	1H	3103	1/1	0.85	0.31	75,75,75,75	0
58	MG	14	3208	1/1	0.85	0.78	76,76,76,76	0
58	MG	14	3210	1/1	0.85	0.23	58,58,58,58	0
58	MG	14	3212	1/1	0.85	0.32	63,63,63,63	0
58	MG	1H	3229	1/1	0.85	0.43	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	3412	1/1	0.85	0.13	113,113,113,113	0
58	MG	1G	1682	1/1	0.85	0.05	113,113,113,113	0
58	MG	I8	101	1/1	0.85	0.16	90,90,90,90	0
58	MG	14	3270	1/1	0.85	0.20	90,90,90,90	0
58	MG	1H	3023	1/1	0.85	0.15	78,78,78,78	0
58	MG	14	3220	1/1	0.85	0.12	64,64,64,64	0
58	MG	13	1622	1/1	0.85	0.17	109,109,109,109	0
58	MG	1H	3226	1/1	0.86	0.26	74,74,74,74	0
58	MG	1H	3269	1/1	0.86	0.51	71,71,71,71	0
58	MG	1H	3178	1/1	0.86	0.29	76,76,76,76	0
58	MG	14	3337	1/1	0.86	0.07	78,78,78,78	0
58	MG	1H	3194	1/1	0.86	0.41	79,79,79,79	0
58	MG	1H	3079	1/1	0.86	0.34	51,51,51,51	0
58	MG	14	3345	1/1	0.86	0.12	90,90,90,90	0
58	MG	1H	3296	1/1	0.86	0.14	66,66,66,66	0
58	MG	14	3118	1/1	0.86	0.21	53,53,53,53	0
58	MG	1G	1632	1/1	0.86	0.34	106,106,106,106	0
58	MG	1H	3190	1/1	0.86	0.39	66,66,66,66	0
58	MG	14	3403	1/1	0.86	0.07	119,119,119,119	0
58	MG	1H	3215	1/1	0.86	0.28	67,67,67,67	0
58	MG	1H	3349	1/1	0.86	0.24	89,89,89,89	0
58	MG	1H	3160	1/1	0.86	0.31	93,93,93,93	0
58	MG	14	3134	1/1	0.86	0.48	83,83,83,83	0
58	MG	1H	3469	1/1	0.86	0.12	81,81,81,81	0
58	MG	14	3039	1/1	0.86	0.33	72,72,72,72	0
58	MG	1H	3222	1/1	0.86	0.16	74,74,74,74	0
58	MG	14	3232	1/1	0.86	0.25	84,84,84,84	0
58	MG	14	3205	1/1	0.86	0.40	63,63,63,63	0
58	MG	13	1625	1/1	0.87	0.35	69,69,69,69	0
58	MG	1H	3019	1/1	0.87	0.35	64,64,64,64	0
58	MG	14	3177	1/1	0.87	0.28	75,75,75,75	0
58	MG	13	1659	1/1	0.87	0.25	87,87,87,87	0
58	MG	14	3088	1/1	0.87	0.11	70,70,70,70	0
58	MG	14	3306	1/1	0.87	0.18	64,64,64,64	0
58	MG	13	1741	1/1	0.87	0.43	103,103,103,103	0
58	MG	14	3107	1/1	0.87	0.08	92,92,92,92	0
58	MG	14	3112	1/1	0.87	0.39	83,83,83,83	0
58	MG	1H	3138	1/1	0.87	0.32	83,83,83,83	0
58	MG	1H	3145	1/1	0.87	0.11	53,53,53,53	0
58	MG	1H	3230	1/1	0.87	0.11	85,85,85,85	0
58	MG	13	1705	1/1	0.87	0.07	99,99,99,99	0
58	MG	1H	3341	1/1	0.87	0.24	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	1G	1695	1/1	0.87	0.06	136,136,136,136	0
58	MG	13	1693	1/1	0.87	0.62	77,77,77,77	0
58	MG	1H	3346	1/1	0.87	0.24	80,80,80,80	0
58	MG	1H	3170	1/1	0.87	0.37	70,70,70,70	0
58	MG	1H	3244	1/1	0.87	0.21	100,100,100,100	0
58	MG	16	203	1/1	0.87	0.39	84,84,84,84	0
58	MG	1H	3174	1/1	0.87	0.31	93,93,93,93	0
58	MG	13	1720	1/1	0.87	0.06	111,111,111,111	0
58	MG	13	1679	1/1	0.87	0.21	117,117,117,117	0
58	MG	14	3150	1/1	0.87	0.27	78,78,78,78	0
58	MG	1J	202	1/1	0.87	0.34	84,84,84,84	0
58	MG	14	3278	1/1	0.87	0.23	63,63,63,63	0
58	MG	1J	205	1/1	0.87	0.18	89,89,89,89	0
58	MG	1H	3316	1/1	0.87	0.65	79,79,79,79	0
58	MG	13	1633	1/1	0.87	0.37	91,91,91,91	0
58	MG	1H	3181	1/1	0.87	0.41	74,74,74,74	0
58	MG	1H	3427	1/1	0.87	0.15	84,84,84,84	0
58	MG	14	3051	1/1	0.87	0.34	88,88,88,88	0
58	MG	1H	3449	1/1	0.88	0.07	76,76,76,76	0
58	MG	1H	3030	1/1	0.88	0.26	82,82,82,82	0
58	MG	1H	3464	1/1	0.88	0.07	97,97,97,97	0
58	MG	1H	3263	1/1	0.88	0.51	106,106,106,106	0
58	MG	1H	3294	1/1	0.88	0.42	141,141,141,141	0
58	MG	1H	3295	1/1	0.88	0.53	88,88,88,88	0
58	MG	13	1736	1/1	0.88	0.10	116,116,116,116	0
58	MG	1H	3094	1/1	0.88	0.30	62,62,62,62	0
58	MG	14	3238	1/1	0.88	0.46	82,82,82,82	0
58	MG	1G	1652	1/1	0.88	0.11	81,81,81,81	0
58	MG	13	1718	1/1	0.88	0.10	100,100,100,100	0
58	MG	14	3242	1/1	0.88	1.24	90,90,90,90	0
58	MG	1H	3148	1/1	0.88	0.57	77,77,77,77	0
58	MG	1H	3487	1/1	0.88	0.21	117,117,117,117	0
58	MG	13	1687	1/1	0.88	0.15	96,96,96,96	0
58	MG	14	3248	1/1	0.88	0.71	85,85,85,85	0
58	MG	1H	3235	1/1	0.88	0.52	64,64,64,64	0
58	MG	14	3187	1/1	0.88	0.24	72,72,72,72	0
58	MG	1H	3042	1/1	0.88	0.47	67,67,67,67	0
58	MG	1H	3308	1/1	0.88	0.35	76,76,76,76	0
58	MG	1G	1663	1/1	0.88	0.09	99,99,99,99	0
58	MG	1H	3198	1/1	0.88	0.33	72,72,72,72	0
58	MG	1H	3400	1/1	0.88	0.12	71,71,71,71	0
58	MG	1H	3202	1/1	0.88	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3115	1/1	0.88	0.16	104,104,104,104	0
58	MG	14	3267	1/1	0.88	0.31	94,94,94,94	0
58	MG	13	1724	1/1	0.88	0.16	85,85,85,85	0
58	MG	1H	3425	1/1	0.88	0.06	110,110,110,110	0
58	MG	1H	3107	1/1	0.88	0.30	69,69,69,69	0
58	MG	1H	3070	1/1	0.88	0.36	68,68,68,68	0
58	MG	1J	204	1/1	0.88	0.10	99,99,99,99	0
58	MG	13	1742	1/1	0.88	0.10	85,85,85,85	0
58	MG	13	1645	1/1	0.88	0.37	75,75,75,75	0
58	MG	1G	1686	1/1	0.88	0.09	126,126,126,126	0
58	MG	39	301	1/1	0.88	0.32	66,66,66,66	0
58	MG	14	3136	1/1	0.88	0.31	79,79,79,79	0
58	MG	1H	3254	1/1	0.88	0.11	58,58,58,58	0
58	MG	13	1641	1/1	0.88	0.33	86,86,86,86	0
58	MG	13	1708	1/1	0.89	0.12	76,76,76,76	0
58	MG	1H	3199	1/1	0.89	0.29	68,68,68,68	0
58	MG	14	3237	1/1	0.89	0.51	77,77,77,77	0
58	MG	1H	3463	1/1	0.89	0.31	99,99,99,99	0
58	MG	1H	3065	1/1	0.89	0.20	64,64,64,64	0
58	MG	14	3292	1/1	0.89	0.12	68,68,68,68	0
58	MG	1H	3311	1/1	0.89	0.19	127,127,127,127	0
58	MG	1H	3169	1/1	0.89	0.30	84,84,84,84	0
58	MG	1H	3157	1/1	0.89	0.13	67,67,67,67	0
58	MG	1H	3477	1/1	0.89	0.07	96,96,96,96	0
58	MG	1H	3478	1/1	0.89	0.18	64,64,64,64	0
58	MG	14	3247	1/1	0.89	0.36	75,75,75,75	0
58	MG	13	1615	1/1	0.89	0.14	85,85,85,85	0
58	MG	1H	3482	1/1	0.89	0.08	95,95,95,95	0
58	MG	1G	1681	1/1	0.89	0.10	88,88,88,88	0
58	MG	14	3252	1/1	0.89	0.90	82,82,82,82	0
58	MG	1H	3071	1/1	0.89	0.29	80,80,80,80	0
58	MG	1G	1640	1/1	0.89	0.57	75,75,75,75	0
58	MG	14	3121	1/1	0.89	0.47	83,83,83,83	0
58	MG	1G	1691	1/1	0.89	0.07	123,123,123,123	0
58	MG	14	3260	1/1	0.89	0.22	65,65,65,65	0
58	MG	14	3354	1/1	0.89	0.07	92,92,92,92	0
58	MG	1H	3192	1/1	0.89	0.14	86,86,86,86	0
58	MG	14	3377	1/1	0.89	0.11	105,105,105,105	0
58	MG	4K	101	1/1	0.89	0.23	85,85,85,85	0
58	MG	14	3396	1/1	0.89	0.17	67,67,67,67	0
58	MG	14	3127	1/1	0.89	0.37	69,69,69,69	0
58	MG	14	3128	1/1	0.89	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3130	1/1	0.89	0.60	78,78,78,78	0
58	MG	1G	1646	1/1	0.89	0.51	70,70,70,70	0
58	MG	14	3413	1/1	0.89	0.10	102,102,102,102	0
58	MG	14	3417	1/1	0.89	0.08	113,113,113,113	0
58	MG	13	1707	1/1	0.89	0.13	87,87,87,87	0
58	MG	1H	3299	1/1	0.89	0.16	98,98,98,98	0
58	MG	16	201	1/1	0.89	0.06	99,99,99,99	0
58	MG	1H	3180	1/1	0.89	0.23	71,71,71,71	0
58	MG	14	3145	1/1	0.89	0.13	87,87,87,87	0
58	MG	1H	3225	1/1	0.89	0.32	56,56,56,56	0
58	MG	1H	3281	1/1	0.89	0.51	85,85,85,85	0
58	MG	16	211	1/1	0.89	0.08	88,88,88,88	0
58	MG	1H	3080	1/1	0.89	0.20	65,65,65,65	0
58	MG	1H	3227	1/1	0.89	0.23	77,77,77,77	0
58	MG	1H	3418	1/1	0.90	0.06	74,74,74,74	0
58	MG	13	1698	1/1	0.90	0.28	104,104,104,104	0
58	MG	13	1642	1/1	0.90	0.24	92,92,92,92	0
58	MG	1G	1616	1/1	0.90	0.35	116,116,116,116	0
58	MG	1H	3312	1/1	0.90	0.21	80,80,80,80	0
58	MG	14	3162	1/1	0.90	0.22	75,75,75,75	0
58	MG	14	3266	1/1	0.90	0.42	72,72,72,72	0
58	MG	1H	3283	1/1	0.90	0.44	84,84,84,84	0
58	MG	14	3009	1/1	0.90	0.57	73,73,73,73	0
58	MG	14	3012	1/1	0.90	0.19	58,58,58,58	0
58	MG	14	3167	1/1	0.90	0.24	50,50,50,50	0
58	MG	14	3168	1/1	0.90	0.25	64,64,64,64	0
58	MG	14	3169	1/1	0.90	0.10	63,63,63,63	0
58	MG	14	3176	1/1	0.90	0.42	92,92,92,92	0
58	MG	1H	3314	1/1	0.90	0.30	76,76,76,76	0
58	MG	1H	3315	1/1	0.90	0.39	58,58,58,58	0
58	MG	1H	3167	1/1	0.90	0.24	78,78,78,78	0
58	MG	1H	3024	1/1	0.90	0.21	74,74,74,74	0
58	MG	14	3280	1/1	0.90	0.45	49,49,49,49	0
58	MG	1H	3320	1/1	0.90	0.28	84,84,84,84	0
58	MG	14	3033	1/1	0.90	0.16	68,68,68,68	0
58	MG	1G	1633	1/1	0.90	0.15	102,102,102,102	0
58	MG	14	3200	1/1	0.90	0.22	84,84,84,84	0
58	MG	1H	3108	1/1	0.90	0.25	51,51,51,51	0
58	MG	14	3288	1/1	0.90	0.34	56,56,56,56	0
58	MG	1G	1638	1/1	0.90	0.38	131,131,131,131	0
58	MG	1G	1639	1/1	0.90	0.36	68,68,68,68	0
58	MG	1H	3452	1/1	0.90	0.10	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	14	3209	1/1	0.90	0.24	70,70,70,70	0
58	MG	1H	3258	1/1	0.90	0.57	66,66,66,66	0
58	MG	14	3055	1/1	0.90	0.48	71,71,71,71	0
58	MG	14	3314	1/1	0.90	0.13	63,63,63,63	0
58	MG	1H	3111	1/1	0.90	0.17	39,39,39,39	0
58	MG	1H	3172	1/1	0.90	0.16	76,76,76,76	0
58	MG	14	3085	1/1	0.90	0.27	54,54,54,54	0
58	MG	14	3331	1/1	0.90	0.10	102,102,102,102	0
58	MG	1G	1647	1/1	0.90	0.23	105,105,105,105	0
58	MG	1H	3026	1/1	0.90	0.24	60,60,60,60	0
58	MG	14	3105	1/1	0.90	0.43	91,91,91,91	0
58	MG	1H	3331	1/1	0.90	0.23	84,84,84,84	0
58	MG	1H	3123	1/1	0.90	0.21	63,63,63,63	0
58	MG	1H	3233	1/1	0.90	0.29	77,77,77,77	0
58	MG	13	1676	1/1	0.90	0.19	94,94,94,94	0
58	MG	1G	1655	1/1	0.90	0.71	85,85,85,85	0
58	MG	1H	3335	1/1	0.90	0.12	79,79,79,79	0
58	MG	14	3231	1/1	0.90	0.20	90,90,90,90	0
58	MG	14	3366	1/1	0.90	0.10	68,68,68,68	0
58	MG	1H	3126	1/1	0.90	0.60	77,77,77,77	0
58	MG	1H	3092	1/1	0.90	0.17	69,69,69,69	0
58	MG	1H	3342	1/1	0.90	0.28	82,82,82,82	0
58	MG	14	3390	1/1	0.90	0.13	118,118,118,118	0
58	MG	1H	3344	1/1	0.90	0.47	57,57,57,57	0
58	MG	1H	3272	1/1	0.90	0.08	80,80,80,80	0
58	MG	14	3239	1/1	0.90	0.53	102,102,102,102	0
58	MG	14	3407	1/1	0.90	0.10	98,98,98,98	0
58	MG	1H	3011	1/1	0.90	0.50	62,62,62,62	0
58	MG	1G	1664	1/1	0.90	0.35	122,122,122,122	0
58	MG	1H	3489	1/1	0.90	0.21	83,83,83,83	0
58	MG	14	3414	1/1	0.90	0.12	104,104,104,104	0
58	MG	14	3132	1/1	0.90	0.38	81,81,81,81	0
58	MG	1H	3031	1/1	0.90	0.34	70,70,70,70	0
58	MG	1H	3277	1/1	0.90	0.45	96,96,96,96	0
58	MG	1H	3305	1/1	0.90	0.35	90,90,90,90	0
58	MG	13	1653	1/1	0.90	0.12	86,86,86,86	0
58	MG	1H	3186	1/1	0.90	0.24	58,58,58,58	0
58	MG	1H	3381	1/1	0.90	0.15	47,47,47,47	0
58	MG	78	201	1/1	0.90	0.35	76,76,76,76	0
58	MG	1H	3394	1/1	0.90	0.26	104,104,104,104	0
58	MG	45	201	1/1	0.90	0.12	69,69,69,69	0
58	MG	1H	3280	1/1	0.90	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	14	3255	1/1	0.90	0.52	79,79,79,79	0
58	MG	1H	3474	1/1	0.91	0.11	97,97,97,97	0
58	MG	14	3160	1/1	0.91	0.29	76,76,76,76	0
58	MG	13	1689	1/1	0.91	0.78	80,80,80,80	0
58	MG	14	3302	1/1	0.91	0.11	67,67,67,67	0
58	MG	1H	3039	1/1	0.91	0.35	64,64,64,64	0
58	MG	14	3304	1/1	0.91	0.12	62,62,62,62	0
58	MG	14	3086	1/1	0.91	0.52	74,74,74,74	0
58	MG	1H	3397	1/1	0.91	0.10	79,79,79,79	0
58	MG	13	1690	1/1	0.91	0.27	105,105,105,105	0
58	MG	14	3103	1/1	0.91	0.53	75,75,75,75	0
58	MG	1H	3415	1/1	0.91	0.07	69,69,69,69	0
58	MG	1H	3127	1/1	0.91	0.30	64,64,64,64	0
58	MG	14	3110	1/1	0.91	0.15	66,66,66,66	0
58	MG	14	3180	1/1	0.91	0.10	83,83,83,83	0
58	MG	1G	1636	1/1	0.91	0.46	90,90,90,90	0
58	MG	14	3336	1/1	0.91	0.20	107,107,107,107	0
58	MG	13	1674	1/1	0.91	0.14	102,102,102,102	0
58	MG	1H	3130	1/1	0.91	0.18	67,67,67,67	0
58	MG	14	3342	1/1	0.91	0.04	129,129,129,129	0
58	MG	1G	1687	1/1	0.91	0.13	116,116,116,116	0
58	MG	1H	3045	1/1	0.91	0.25	52,52,52,52	0
58	MG	1G	1692	1/1	0.91	0.13	130,130,130,130	0
58	MG	13	1630	1/1	0.91	0.21	62,62,62,62	0
58	MG	1H	3063	1/1	0.91	0.12	58,58,58,58	0
58	MG	14	3361	1/1	0.91	0.14	70,70,70,70	0
58	MG	14	3202	1/1	0.91	0.25	77,77,77,77	0
58	MG	1H	3338	1/1	0.91	0.44	66,66,66,66	0
58	MG	1H	3257	1/1	0.91	0.24	75,75,75,75	0
58	MG	1H	3139	1/1	0.91	0.15	58,58,58,58	0
58	MG	14	3387	1/1	0.91	0.24	89,89,89,89	0
58	MG	1H	3144	1/1	0.91	0.14	48,48,48,48	0
58	MG	13	1654	1/1	0.91	0.26	76,76,76,76	0
58	MG	1H	3004	1/1	0.91	0.25	54,54,54,54	0
58	MG	1H	3005	1/1	0.91	0.17	52,52,52,52	0
58	MG	1H	3460	1/1	0.91	0.17	87,87,87,87	0
58	MG	14	3408	1/1	0.91	0.17	108,108,108,108	0
58	MG	14	3138	1/1	0.91	0.39	91,91,91,91	0
58	MG	14	3020	1/1	0.91	0.46	78,78,78,78	0
58	MG	13	1606	1/1	0.91	0.15	124,124,124,124	0
58	MG	14	3275	1/1	0.91	0.50	71,71,71,71	0
58	MG	Q8	101	1/1	0.91	0.31	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1602	1/1	0.91	0.43	79,79,79,79	0
58	MG	1H	3033	1/1	0.91	0.38	66,66,66,66	0
58	MG	1H	3012	1/1	0.91	0.28	57,57,57,57	0
58	MG	14	3226	1/1	0.91	0.49	99,99,99,99	0
58	MG	14	3148	1/1	0.91	0.47	84,84,84,84	0
58	MG	1G	1614	1/1	0.91	0.24	120,120,120,120	0
58	MG	1H	3201	1/1	0.91	0.12	67,67,67,67	0
58	MG	1H	3271	1/1	0.91	0.44	72,72,72,72	0
58	MG	14	3054	1/1	0.91	0.39	54,54,54,54	0
58	MG	14	3234	1/1	0.91	0.24	81,81,81,81	0
58	MG	1H	3473	1/1	0.91	0.05	89,89,89,89	0
58	MG	1H	3217	1/1	0.92	0.18	67,67,67,67	0
58	MG	1G	1619	1/1	0.92	0.16	78,78,78,78	0
58	MG	1G	1688	1/1	0.92	0.08	122,122,122,122	0
58	MG	1H	3298	1/1	0.92	0.42	84,84,84,84	0
58	MG	1H	3337	1/1	0.92	0.23	53,53,53,53	0
58	MG	14	3224	1/1	0.92	0.54	59,59,59,59	0
58	MG	1G	1693	1/1	0.92	0.10	123,123,123,123	0
58	MG	1H	3462	1/1	0.92	0.07	91,91,91,91	0
58	MG	13	1695	1/1	0.92	0.24	80,80,80,80	0
58	MG	14	3228	1/1	0.92	0.24	76,76,76,76	0
58	MG	1H	3300	1/1	0.92	0.38	85,85,85,85	0
58	MG	1H	3043	1/1	0.92	0.45	86,86,86,86	0
58	MG	13	1714	1/1	0.92	0.06	106,106,106,106	0
58	MG	14	3318	1/1	0.92	0.08	65,65,65,65	0
58	MG	1H	3056	1/1	0.92	0.35	50,50,50,50	0
58	MG	13	1717	1/1	0.92	0.13	97,97,97,97	0
58	MG	1H	3153	1/1	0.92	0.49	80,80,80,80	0
58	MG	13	1652	1/1	0.92	0.28	93,93,93,93	0
58	MG	1H	3275	1/1	0.92	0.35	69,69,69,69	0
58	MG	14	3019	1/1	0.92	0.30	83,83,83,83	0
58	MG	1H	3064	1/1	0.92	0.20	57,57,57,57	0
58	MG	1G	1642	1/1	0.92	0.40	78,78,78,78	0
58	MG	4I	201	1/1	0.92	0.15	84,84,84,84	0
58	MG	1G	1644	1/1	0.92	0.47	93,93,93,93	0
58	MG	1H	3066	1/1	0.92	0.11	60,60,60,60	0
58	MG	14	3343	1/1	0.92	0.18	72,72,72,72	0
58	MG	14	3244	1/1	0.92	0.20	78,78,78,78	0
58	MG	13	1643	1/1	0.92	0.16	90,90,90,90	0
58	MG	1H	3385	1/1	0.92	0.12	60,60,60,60	0
58	MG	1H	3028	1/1	0.92	0.45	63,63,63,63	0
58	MG	14	3351	1/1	0.92	0.16	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1699	1/1	0.92	0.31	88,88,88,88	0
58	MG	14	3357	1/1	0.92	0.11	83,83,83,83	0
58	MG	1H	3074	1/1	0.92	0.41	44,44,44,44	0
58	MG	1H	3404	1/1	0.92	0.06	78,78,78,78	0
58	MG	14	3064	1/1	0.92	0.42	62,62,62,62	0
58	MG	1H	3406	1/1	0.92	0.09	91,91,91,91	0
58	MG	14	3381	1/1	0.92	0.24	95,95,95,95	0
58	MG	1H	3407	1/1	0.92	0.16	59,59,59,59	0
58	MG	14	3385	1/1	0.92	0.20	86,86,86,86	0
58	MG	1H	3077	1/1	0.92	0.56	62,62,62,62	0
58	MG	14	3389	1/1	0.92	0.08	94,94,94,94	0
58	MG	16	208	1/1	0.92	0.49	82,82,82,82	0
58	MG	1H	3318	1/1	0.92	0.53	71,71,71,71	0
58	MG	14	3399	1/1	0.92	0.09	80,80,80,80	0
58	MG	14	3089	1/1	0.92	0.10	80,80,80,80	0
58	MG	14	3098	1/1	0.92	0.81	57,57,57,57	0
58	MG	14	3192	1/1	0.92	0.32	69,69,69,69	0
58	MG	14	3193	1/1	0.92	0.24	69,69,69,69	0
58	MG	13	1726	1/1	0.92	0.09	122,122,122,122	0
58	MG	14	3195	1/1	0.92	0.28	75,75,75,75	0
58	MG	41	201	1/1	0.92	0.16	86,86,86,86	0
58	MG	14	3199	1/1	0.92	0.41	91,91,91,91	0
58	MG	14	3415	1/1	0.92	0.17	97,97,97,97	0
58	MG	1H	3131	1/1	0.92	0.52	59,59,59,59	0
58	MG	13	1611	1/1	0.92	0.22	85,85,85,85	0
58	MG	13	1691	1/1	0.92	0.23	89,89,89,89	0
58	MG	13	1620	1/1	0.92	0.11	87,87,87,87	0
58	MG	13	1671	1/1	0.92	0.17	121,121,121,121	0
58	MG	1H	3208	1/1	0.92	0.56	71,71,71,71	0
58	MG	13	1672	1/1	0.92	0.20	112,112,112,112	0
58	MG	1G	1608	1/1	0.92	0.17	97,97,97,97	0
58	MG	1H	3446	1/1	0.92	0.07	77,77,77,77	0
58	MG	1H	3093	1/1	0.92	0.46	45,45,45,45	0
58	MG	1G	1615	1/1	0.92	0.13	132,132,132,132	0
58	MG	1H	3146	1/1	0.92	0.49	72,72,72,72	0
58	MG	1H	3413	1/1	0.93	0.11	72,72,72,72	0
58	MG	1H	3480	1/1	0.93	0.09	98,98,98,98	0
58	MG	1H	3166	1/1	0.93	0.27	77,77,77,77	0
58	MG	14	3295	1/1	0.93	0.07	61,61,61,61	0
58	MG	14	3297	1/1	0.93	0.10	55,55,55,55	0
58	MG	14	3131	1/1	0.93	0.49	70,70,70,70	0
58	MG	1H	3416	1/1	0.93	0.18	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	14	3133	1/1	0.93	0.41	66,66,66,66	0
58	MG	1H	3256	1/1	0.93	0.18	70,70,70,70	0
58	MG	1H	3420	1/1	0.93	0.13	80,80,80,80	0
58	MG	14	3137	1/1	0.93	0.21	55,55,55,55	0
58	MG	13	1732	1/1	0.93	0.13	120,120,120,120	0
58	MG	13	1697	1/1	0.93	0.34	95,95,95,95	0
58	MG	1H	3423	1/1	0.93	0.06	71,71,71,71	0
58	MG	1H	3495	1/1	0.93	0.06	70,70,70,70	0
58	MG	13	1626	1/1	0.93	0.21	62,62,62,62	0
58	MG	1H	3195	1/1	0.93	0.40	85,85,85,85	0
58	MG	1H	3287	1/1	0.93	0.21	77,77,77,77	0
58	MG	1H	3429	1/1	0.93	0.09	105,105,105,105	0
58	MG	16	207	1/1	0.93	0.14	84,84,84,84	0
58	MG	13	1713	1/1	0.93	0.09	84,84,84,84	0
58	MG	14	3042	1/1	0.93	0.21	95,95,95,95	0
58	MG	1H	3435	1/1	0.93	0.10	70,70,70,70	0
58	MG	1G	1656	1/1	0.93	0.17	126,126,126,126	0
58	MG	14	3045	1/1	0.93	0.12	83,83,83,83	0
58	MG	1H	3437	1/1	0.93	0.16	82,82,82,82	0
58	MG	1H	3438	1/1	0.93	0.07	79,79,79,79	0
58	MG	1H	3439	1/1	0.93	0.13	80,80,80,80	0
58	MG	13	1665	1/1	0.93	0.14	85,85,85,85	0
58	MG	14	3059	1/1	0.93	0.39	63,63,63,63	0
58	MG	14	3062	1/1	0.93	0.29	72,72,72,72	0
58	MG	1H	3232	1/1	0.93	0.50	75,75,75,75	0
58	MG	14	3363	1/1	0.93	0.09	63,63,63,63	0
58	MG	13	1715	1/1	0.93	0.06	106,106,106,106	0
58	MG	13	1618	1/1	0.93	0.15	107,107,107,107	0
58	MG	14	3070	1/1	0.93	0.40	72,72,72,72	0
58	MG	14	3179	1/1	0.93	0.31	91,91,91,91	0
58	MG	14	3076	1/1	0.93	0.23	88,88,88,88	0
58	MG	14	3184	1/1	0.93	0.40	85,85,85,85	0
58	MG	14	3185	1/1	0.93	0.24	87,87,87,87	0
58	MG	14	3077	1/1	0.93	0.64	84,84,84,84	0
58	MG	13	1702	1/1	0.93	0.21	157,157,157,157	0
58	MG	14	3395	1/1	0.93	0.07	69,69,69,69	0
58	MG	13	1605	1/1	0.93	0.23	79,79,79,79	0
58	MG	1G	1667	1/1	0.93	0.28	81,81,81,81	0
58	MG	14	3400	1/1	0.93	0.12	82,82,82,82	0
58	MG	1H	3352	1/1	0.93	0.11	70,70,70,70	0
58	MG	1G	1610	1/1	0.93	0.18	92,92,92,92	0
58	MG	1H	3371	1/1	0.93	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1631	1/1	0.93	0.21	55,55,55,55	0
58	MG	14	3104	1/1	0.93	0.43	85,85,85,85	0
58	MG	14	3198	1/1	0.93	0.37	69,69,69,69	0
58	MG	1G	1676	1/1	0.93	0.13	91,91,91,91	0
58	MG	3I	201	1/1	0.93	0.18	62,62,62,62	0
58	MG	1H	3327	1/1	0.93	0.34	134,134,134,134	0
58	MG	13	1660	1/1	0.93	0.37	63,63,63,63	0
58	MG	1H	3466	1/1	0.93	0.08	77,77,77,77	0
58	MG	14	3206	1/1	0.93	0.46	71,71,71,71	0
58	MG	1H	3467	1/1	0.93	0.16	101,101,101,101	0
58	MG	5I	101	1/1	0.93	0.18	77,77,77,77	0
58	MG	13	1727	1/1	0.93	0.20	79,79,79,79	0
58	MG	13	1730	1/1	0.93	0.07	95,95,95,95	0
58	MG	29	303	1/1	0.93	0.27	74,74,74,74	0
58	MG	1H	3163	1/1	0.93	0.24	76,76,76,76	0
58	MG	1H	3032	1/1	0.93	0.54	78,78,78,78	0
58	MG	14	3286	1/1	0.93	0.08	103,103,103,103	0
58	MG	1H	3409	1/1	0.93	0.09	58,58,58,58	0
58	MG	E5	101	1/1	0.93	0.24	53,53,53,53	0
58	MG	1G	1694	1/1	0.93	0.09	129,129,129,129	0
58	MG	16	202	1/1	0.94	0.17	90,90,90,90	0
58	MG	14	3188	1/1	0.94	0.15	73,73,73,73	0
58	MG	1H	3068	1/1	0.94	0.44	92,92,92,92	0
58	MG	1H	3102	1/1	0.94	0.31	64,64,64,64	0
58	MG	1H	3200	1/1	0.94	0.41	72,72,72,72	0
58	MG	14	3078	1/1	0.94	0.39	76,76,76,76	0
58	MG	14	3283	1/1	0.94	0.56	78,78,78,78	0
58	MG	1H	3069	1/1	0.94	0.23	62,62,62,62	0
58	MG	1H	3017	1/1	0.94	0.28	54,54,54,54	0
58	MG	1H	3173	1/1	0.94	0.22	66,66,66,66	0
58	MG	11	301	1/1	0.94	0.18	50,50,50,50	0
58	MG	14	3093	1/1	0.94	0.41	52,52,52,52	0
58	MG	1H	3106	1/1	0.94	0.21	46,46,46,46	0
58	MG	1H	3038	1/1	0.94	0.30	72,72,72,72	0
58	MG	1G	1668	1/1	0.94	0.45	141,141,141,141	0
58	MG	13	1623	1/1	0.94	0.18	81,81,81,81	0
58	MG	1G	1670	1/1	0.94	0.44	110,110,110,110	0
58	MG	1H	3177	1/1	0.94	0.17	86,86,86,86	0
58	MG	14	3109	1/1	0.94	0.20	66,66,66,66	0
58	MG	1G	1672	1/1	0.94	0.09	110,110,110,110	0
58	MG	13	1624	1/1	0.94	0.18	75,75,75,75	0
58	MG	14	3211	1/1	0.94	0.08	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	1H	3340	1/1	0.94	0.28	72,72,72,72	0
58	MG	1H	3262	1/1	0.94	0.74	78,78,78,78	0
58	MG	14	3215	1/1	0.94	0.26	73,73,73,73	0
58	MG	13	1738	1/1	0.94	0.13	105,105,105,105	0
58	MG	14	3217	1/1	0.94	0.14	91,91,91,91	0
58	MG	14	3328	1/1	0.94	0.13	105,105,105,105	0
58	MG	1H	3442	1/1	0.94	0.06	64,64,64,64	0
58	MG	1G	1679	1/1	0.94	0.09	103,103,103,103	0
58	MG	1G	1606	1/1	0.94	0.24	88,88,88,88	0
58	MG	1H	3343	1/1	0.94	0.28	77,77,77,77	0
58	MG	1H	3444	1/1	0.94	0.13	50,50,50,50	0
58	MG	14	3124	1/1	0.94	0.42	86,86,86,86	0
58	MG	14	3125	1/1	0.94	0.12	60,60,60,60	0
58	MG	14	3340	1/1	0.94	0.10	72,72,72,72	0
58	MG	14	3341	1/1	0.94	0.05	92,92,92,92	0
58	MG	1G	1611	1/1	0.94	0.39	105,105,105,105	0
58	MG	1H	3216	1/1	0.94	0.11	57,57,57,57	0
58	MG	1H	3120	1/1	0.94	0.09	47,47,47,47	0
58	MG	1H	3219	1/1	0.94	0.23	96,96,96,96	0
58	MG	1H	3154	1/1	0.94	0.34	42,42,42,42	0
58	MG	1H	3121	1/1	0.94	0.12	60,60,60,60	0
58	MG	13	1644	1/1	0.94	0.22	85,85,85,85	0
58	MG	1H	3187	1/1	0.94	0.16	69,69,69,69	0
58	MG	2L	101	1/1	0.94	0.45	81,81,81,81	0
58	MG	1G	1623	1/1	0.94	0.42	80,80,80,80	0
58	MG	1G	1624	1/1	0.94	0.30	100,100,100,100	0
58	MG	14	3365	1/1	0.94	0.07	55,55,55,55	0
58	MG	14	3001	1/1	0.94	0.19	46,46,46,46	0
58	MG	14	3368	1/1	0.94	0.06	79,79,79,79	0
58	MG	14	3370	1/1	0.94	0.08	80,80,80,80	0
58	MG	1G	1625	1/1	0.94	0.36	87,87,87,87	0
58	MG	13	1709	1/1	0.94	0.07	96,96,96,96	0
58	MG	14	3142	1/1	0.94	0.07	89,89,89,89	0
58	MG	1H	3356	1/1	0.94	0.10	56,56,56,56	0
58	MG	1H	3361	1/1	0.94	0.17	47,47,47,47	0
58	MG	1H	3363	1/1	0.94	0.20	53,53,53,53	0
58	MG	1H	3273	1/1	0.94	0.31	80,80,80,80	0
58	MG	1H	3228	1/1	0.94	0.55	68,68,68,68	0
58	MG	14	3391	1/1	0.94	0.15	85,85,85,85	0
58	MG	14	3018	1/1	0.94	0.54	63,63,63,63	0
58	MG	13	1604	1/1	0.94	0.21	86,86,86,86	0
58	MG	1H	3061	1/1	0.94	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3155	1/1	0.94	0.47	69,69,69,69	0
58	MG	14	3402	1/1	0.94	0.07	110,110,110,110	0
58	MG	13	1664	1/1	0.94	0.25	82,82,82,82	0
58	MG	1H	3476	1/1	0.94	0.12	72,72,72,72	0
58	MG	14	3406	1/1	0.94	0.06	100,100,100,100	0
58	MG	1H	3087	1/1	0.94	0.24	46,46,46,46	0
58	MG	1H	3398	1/1	0.94	0.11	48,48,48,48	0
58	MG	1H	3010	1/1	0.94	0.29	57,57,57,57	0
58	MG	14	3411	1/1	0.94	0.04	113,113,113,113	0
58	MG	1H	3401	1/1	0.94	0.10	71,71,71,71	0
58	MG	14	3258	1/1	0.94	0.25	100,100,100,100	0
58	MG	1H	3481	1/1	0.94	0.05	100,100,100,100	0
58	MG	1H	3317	1/1	0.94	0.77	81,81,81,81	0
58	MG	13	1601	1/1	0.94	0.20	72,72,72,72	0
58	MG	14	3420	1/1	0.94	0.10	72,72,72,72	0
58	MG	13	1655	1/1	0.94	0.28	72,72,72,72	0
58	MG	14	3264	1/1	0.94	0.15	86,86,86,86	0
58	MG	14	3171	1/1	0.94	0.30	65,65,65,65	0
58	MG	14	3172	1/1	0.94	0.33	75,75,75,75	0
58	MG	14	3174	1/1	0.94	0.15	53,53,53,53	0
58	MG	19	301	1/1	0.94	0.40	70,70,70,70	0
58	MG	1H	3135	1/1	0.94	0.15	55,55,55,55	0
58	MG	1H	3321	1/1	0.94	0.18	78,78,78,78	0
58	MG	1H	3241	1/1	0.94	0.39	71,71,71,71	0
58	MG	14	3060	1/1	0.94	0.26	67,67,67,67	0
58	MG	14	3183	1/1	0.94	0.29	59,59,59,59	0
58	MG	45	202	1/1	0.94	0.11	102,102,102,102	0
58	MG	1H	3243	1/1	0.94	0.20	65,65,65,65	0
58	MG	13	1617	1/1	0.94	0.27	74,74,74,74	0
58	MG	1H	3419	1/1	0.94	0.10	51,51,51,51	0
58	MG	1H	3253	1/1	0.95	0.28	62,62,62,62	0
58	MG	1H	3118	1/1	0.95	0.26	54,54,54,54	0
58	MG	1H	3292	1/1	0.95	0.06	68,68,68,68	0
58	MG	14	3003	1/1	0.95	0.31	74,74,74,74	0
58	MG	1H	3037	1/1	0.95	0.29	99,99,99,99	0
58	MG	14	3307	1/1	0.95	0.09	67,67,67,67	0
58	MG	14	3310	1/1	0.95	0.13	59,59,59,59	0
58	MG	14	3313	1/1	0.95	0.13	84,84,84,84	0
58	MG	1G	1634	1/1	0.95	0.24	85,85,85,85	0
58	MG	14	3315	1/1	0.95	0.07	81,81,81,81	0
58	MG	13	1637	1/1	0.95	0.32	82,82,82,82	0
58	MG	1H	3414	1/1	0.95	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3323	1/1	0.95	0.10	61,61,61,61	0
58	MG	1H	3483	1/1	0.95	0.05	99,99,99,99	0
58	MG	13	1700	1/1	0.95	0.24	93,93,93,93	0
58	MG	13	1688	1/1	0.95	0.35	85,85,85,85	0
58	MG	13	1619	1/1	0.95	0.22	72,72,72,72	0
58	MG	1H	3336	1/1	0.95	0.20	76,76,76,76	0
58	MG	1H	3095	1/1	0.95	0.50	66,66,66,66	0
58	MG	1H	3029	1/1	0.95	0.54	67,67,67,67	0
58	MG	14	3143	1/1	0.95	0.33	60,60,60,60	0
58	MG	1H	3490	1/1	0.95	0.05	95,95,95,95	0
58	MG	1H	3492	1/1	0.95	0.11	95,95,95,95	0
58	MG	14	3037	1/1	0.95	0.23	55,55,55,55	0
58	MG	1H	3493	1/1	0.95	0.07	96,96,96,96	0
58	MG	14	3040	1/1	0.95	0.26	49,49,49,49	0
58	MG	1G	1649	1/1	0.95	0.25	97,97,97,97	0
58	MG	13	1614	1/1	0.95	0.06	81,81,81,81	0
58	MG	1H	3129	1/1	0.95	0.14	68,68,68,68	0
58	MG	14	3154	1/1	0.95	0.33	66,66,66,66	0
58	MG	1H	3101	1/1	0.95	0.21	47,47,47,47	0
58	MG	14	3157	1/1	0.95	0.43	67,67,67,67	0
58	MG	14	3352	1/1	0.95	0.06	69,69,69,69	0
58	MG	14	3047	1/1	0.95	0.23	56,56,56,56	0
58	MG	14	3049	1/1	0.95	0.22	63,63,63,63	0
58	MG	1H	3014	1/1	0.95	0.35	80,80,80,80	0
58	MG	1H	3060	1/1	0.95	0.19	47,47,47,47	0
58	MG	13	1621	1/1	0.95	0.24	101,101,101,101	0
58	MG	16	206	1/1	0.95	0.33	77,77,77,77	0
58	MG	14	3367	1/1	0.95	0.17	67,67,67,67	0
58	MG	14	3057	1/1	0.95	0.41	64,64,64,64	0
58	MG	14	3251	1/1	0.95	0.12	66,66,66,66	0
58	MG	14	3372	1/1	0.95	0.05	119,119,119,119	0
58	MG	13	1740	1/1	0.95	0.28	93,93,93,93	0
58	MG	1H	3136	1/1	0.95	0.25	63,63,63,63	0
58	MG	14	3379	1/1	0.95	0.37	93,93,93,93	0
58	MG	1H	3137	1/1	0.95	0.47	56,56,56,56	0
58	MG	1H	3081	1/1	0.95	0.25	83,83,83,83	0
58	MG	13	1731	1/1	0.95	0.08	78,78,78,78	0
58	MG	14	3173	1/1	0.95	0.23	92,92,92,92	0
58	MG	1H	3238	1/1	0.95	0.14	63,63,63,63	0
58	MG	1H	3141	1/1	0.95	0.16	47,47,47,47	0
58	MG	14	3261	1/1	0.95	0.22	74,74,74,74	0
58	MG	14	3392	1/1	0.95	0.05	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3394	1/1	0.95	0.09	101,101,101,101	0
58	MG	1H	3240	1/1	0.95	0.25	49,49,49,49	0
58	MG	1G	1666	1/1	0.95	0.24	125,125,125,125	0
58	MG	14	3397	1/1	0.95	0.06	89,89,89,89	0
58	MG	1H	3358	1/1	0.95	0.14	54,54,54,54	0
58	MG	14	3081	1/1	0.95	0.28	56,56,56,56	0
58	MG	14	3084	1/1	0.95	0.42	71,71,71,71	0
58	MG	J8	101	1/1	0.95	0.14	77,77,77,77	0
58	MG	1H	3142	1/1	0.95	0.28	62,62,62,62	0
58	MG	1H	3242	1/1	0.95	0.11	66,66,66,66	0
58	MG	1H	3364	1/1	0.95	0.12	48,48,48,48	0
58	MG	14	3092	1/1	0.95	0.15	74,74,74,74	0
58	MG	1H	3367	1/1	0.95	0.06	59,59,59,59	0
58	MG	1H	3453	1/1	0.95	0.06	98,98,98,98	0
58	MG	1H	3368	1/1	0.95	0.07	53,53,53,53	0
58	MG	1G	1675	1/1	0.95	0.12	78,78,78,78	0
58	MG	1G	1609	1/1	0.95	0.20	98,98,98,98	0
58	MG	1H	3459	1/1	0.95	0.11	85,85,85,85	0
58	MG	14	3106	1/1	0.95	0.23	66,66,66,66	0
58	MG	1H	3171	1/1	0.95	0.14	62,62,62,62	0
58	MG	1H	3376	1/1	0.95	0.11	71,71,71,71	0
58	MG	1H	3143	1/1	0.95	0.19	75,75,75,75	0
58	MG	1H	3203	1/1	0.95	0.16	76,76,76,76	0
58	MG	1H	3382	1/1	0.95	0.07	58,58,58,58	0
58	MG	13	1629	1/1	0.95	0.24	58,58,58,58	0
58	MG	1H	3387	1/1	0.95	0.11	51,51,51,51	0
58	MG	1G	1620	1/1	0.95	0.35	74,74,74,74	0
58	MG	1H	3248	1/1	0.95	0.30	77,77,77,77	0
58	MG	1H	3112	1/1	0.95	0.42	52,52,52,52	0
58	MG	1H	3472	1/1	0.95	0.09	60,60,60,60	0
58	MG	1H	3113	1/1	0.95	0.20	52,52,52,52	0
58	MG	14	3294	1/1	0.95	0.11	65,65,65,65	0
58	MG	1H	3325	1/1	0.95	0.12	82,82,82,82	0
58	MG	14	3296	1/1	0.95	0.08	67,67,67,67	0
58	MG	1H	3114	1/1	0.95	0.59	64,64,64,64	0
58	MG	14	3073	1/1	0.96	0.46	57,57,57,57	0
58	MG	14	3156	1/1	0.96	0.39	66,66,66,66	0
58	MG	14	3074	1/1	0.96	0.49	48,48,48,48	0
58	MG	1H	3388	1/1	0.96	0.15	78,78,78,78	0
58	MG	1G	1683	1/1	0.96	0.05	106,106,106,106	0
58	MG	1H	3390	1/1	0.96	0.10	58,58,58,58	0
58	MG	1H	3445	1/1	0.96	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	14	3338	1/1	0.96	0.17	64,64,64,64	0
58	MG	1H	3006	1/1	0.96	0.18	56,56,56,56	0
58	MG	1G	1690	1/1	0.96	0.08	105,105,105,105	0
58	MG	1H	3116	1/1	0.96	0.29	71,71,71,71	0
58	MG	14	3087	1/1	0.96	0.14	56,56,56,56	0
58	MG	1H	3067	1/1	0.96	0.34	88,88,88,88	0
58	MG	1H	3451	1/1	0.96	0.08	68,68,68,68	0
58	MG	14	3090	1/1	0.96	0.26	64,64,64,64	0
58	MG	14	3091	1/1	0.96	0.21	66,66,66,66	0
58	MG	1H	3165	1/1	0.96	0.24	76,76,76,76	0
58	MG	1H	3021	1/1	0.96	0.28	64,64,64,64	0
58	MG	14	3094	1/1	0.96	0.37	67,67,67,67	0
58	MG	14	3353	1/1	0.96	0.11	80,80,80,80	0
58	MG	14	3095	1/1	0.96	0.30	83,83,83,83	0
58	MG	14	3178	1/1	0.96	0.41	65,65,65,65	0
58	MG	1H	3454	1/1	0.96	0.17	102,102,102,102	0
58	MG	14	3099	1/1	0.96	0.27	69,69,69,69	0
58	MG	14	3181	1/1	0.96	0.19	57,57,57,57	0
58	MG	14	3100	1/1	0.96	0.23	67,67,67,67	0
58	MG	16	209	1/1	0.96	0.11	64,64,64,64	0
58	MG	16	210	1/1	0.96	0.08	80,80,80,80	0
58	MG	1G	1645	1/1	0.96	0.19	96,96,96,96	0
58	MG	14	3371	1/1	0.96	0.09	89,89,89,89	0
58	MG	1H	3223	1/1	0.96	0.15	81,81,81,81	0
58	MG	14	3373	1/1	0.96	0.16	96,96,96,96	0
58	MG	14	3375	1/1	0.96	0.16	49,49,49,49	0
58	MG	1H	3008	1/1	0.96	0.17	90,90,90,90	0
58	MG	1H	3047	1/1	0.96	0.33	43,43,43,43	0
58	MG	14	3378	1/1	0.96	0.09	90,90,90,90	0
58	MG	1H	3461	1/1	0.96	0.06	80,80,80,80	0
58	MG	1H	3408	1/1	0.96	0.10	61,61,61,61	0
58	MG	1H	3048	1/1	0.96	0.33	43,43,43,43	0
58	MG	14	3383	1/1	0.96	0.16	93,93,93,93	0
58	MG	1H	3412	1/1	0.96	0.10	55,55,55,55	0
58	MG	13	1728	1/1	0.96	0.07	76,76,76,76	0
58	MG	14	3388	1/1	0.96	0.08	83,83,83,83	0
58	MG	14	3116	1/1	0.96	0.50	48,48,48,48	0
58	MG	N8	101	1/1	0.96	0.32	67,67,67,67	0
58	MG	1H	3259	1/1	0.96	0.48	82,82,82,82	0
58	MG	1H	3125	1/1	0.96	0.16	79,79,79,79	0
58	MG	14	3393	1/1	0.96	0.12	140,140,140,140	0
58	MG	1H	3059	1/1	0.96	0.26	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	14	3029	1/1	0.96	0.38	49,49,49,49	0
58	MG	14	3204	1/1	0.96	0.36	60,60,60,60	0
58	MG	1H	3417	1/1	0.96	0.08	83,83,83,83	0
58	MG	14	3035	1/1	0.96	0.20	72,72,72,72	0
58	MG	1H	3076	1/1	0.96	0.22	56,56,56,56	0
58	MG	1H	3354	1/1	0.96	0.12	49,49,49,49	0
58	MG	13	1719	1/1	0.96	0.07	95,95,95,95	0
58	MG	14	3404	1/1	0.96	0.04	85,85,85,85	0
58	MG	1H	3475	1/1	0.96	0.09	80,80,80,80	0
58	MG	1H	3078	1/1	0.96	0.39	56,56,56,56	0
58	MG	13	1640	1/1	0.96	0.20	63,63,63,63	0
58	MG	1G	1613	1/1	0.96	0.17	89,89,89,89	0
58	MG	14	3214	1/1	0.96	0.10	82,82,82,82	0
58	MG	14	3410	1/1	0.96	0.09	75,75,75,75	0
58	MG	13	1710	1/1	0.96	0.07	74,74,74,74	0
58	MG	13	1627	1/1	0.96	0.21	97,97,97,97	0
58	MG	14	3048	1/1	0.96	0.08	79,79,79,79	0
58	MG	1H	3082	1/1	0.96	0.30	80,80,80,80	0
58	MG	14	3050	1/1	0.96	0.43	71,71,71,71	0
58	MG	1H	3270	1/1	0.96	0.24	43,43,43,43	0
58	MG	14	3419	1/1	0.96	0.27	62,62,62,62	0
58	MG	1H	3110	1/1	0.96	0.28	60,60,60,60	0
58	MG	14	3421	1/1	0.96	0.05	79,79,79,79	0
58	MG	1J	201	1/1	0.96	0.17	76,76,76,76	0
58	MG	1H	3083	1/1	0.96	0.17	99,99,99,99	0
58	MG	1H	3183	1/1	0.96	0.49	67,67,67,67	0
58	MG	1G	1622	1/1	0.96	0.46	84,84,84,84	0
58	MG	14	3305	1/1	0.96	0.18	51,51,51,51	0
58	MG	14	3144	1/1	0.96	0.20	82,82,82,82	0
58	MG	1H	3436	1/1	0.96	0.07	73,73,73,73	0
58	MG	1H	3040	1/1	0.96	0.12	89,89,89,89	0
58	MG	1H	3185	1/1	0.96	0.33	63,63,63,63	0
58	MG	14	3063	1/1	0.96	0.23	73,73,73,73	0
58	MG	1H	3212	1/1	0.96	0.27	42,42,42,42	0
58	MG	1H	3386	1/1	0.96	0.10	59,59,59,59	0
58	MG	14	3066	1/1	0.96	0.44	47,47,47,47	0
58	MG	14	3233	1/1	0.96	0.30	79,79,79,79	0
58	MG	1H	3441	1/1	0.96	0.17	78,78,78,78	0
58	MG	13	1638	1/1	0.96	0.33	80,80,80,80	0
58	MG	13	1706	1/1	0.97	0.07	80,80,80,80	0
58	MG	14	3034	1/1	0.97	0.38	53,53,53,53	0
58	MG	1H	3494	1/1	0.97	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3325	1/1	0.97	0.06	75,75,75,75	0
58	MG	13	1613	1/1	0.97	0.24	76,76,76,76	0
58	MG	1H	3073	1/1	0.97	0.17	67,67,67,67	0
58	MG	14	3135	1/1	0.97	0.83	71,71,71,71	0
58	MG	1H	3247	1/1	0.97	0.44	76,76,76,76	0
58	MG	14	3333	1/1	0.97	0.11	98,98,98,98	0
58	MG	1H	3432	1/1	0.97	0.12	78,78,78,78	0
58	MG	13	1716	1/1	0.97	0.14	75,75,75,75	0
58	MG	1H	3366	1/1	0.97	0.12	53,53,53,53	0
58	MG	1H	3213	1/1	0.97	0.18	49,49,49,49	0
58	MG	1H	3214	1/1	0.97	0.14	50,50,50,50	0
58	MG	14	3046	1/1	0.97	0.11	74,74,74,74	0
58	MG	1H	3369	1/1	0.97	0.13	49,49,49,49	0
58	MG	1H	3251	1/1	0.97	0.82	78,78,78,78	0
58	MG	1H	3372	1/1	0.97	0.09	73,73,73,73	0
58	MG	1H	3373	1/1	0.97	0.12	76,76,76,76	0
58	MG	1H	3374	1/1	0.97	0.12	63,63,63,63	0
58	MG	1H	3375	1/1	0.97	0.09	50,50,50,50	0
58	MG	14	3053	1/1	0.97	0.30	74,74,74,74	0
58	MG	14	3347	1/1	0.97	0.11	83,83,83,83	0
58	MG	14	3349	1/1	0.97	0.13	47,47,47,47	0
58	MG	1H	3323	1/1	0.97	0.06	77,77,77,77	0
58	MG	14	3151	1/1	0.97	0.53	65,65,65,65	0
58	MG	1H	3378	1/1	0.97	0.12	85,85,85,85	0
58	MG	1H	3075	1/1	0.97	0.47	70,70,70,70	0
58	MG	14	3058	1/1	0.97	0.23	55,55,55,55	0
58	MG	14	3356	1/1	0.97	0.09	61,61,61,61	0
58	MG	1H	3448	1/1	0.97	0.13	67,67,67,67	0
58	MG	1H	3007	1/1	0.97	0.11	83,83,83,83	0
58	MG	14	3362	1/1	0.97	0.11	81,81,81,81	0
58	MG	1H	3104	1/1	0.97	0.36	66,66,66,66	0
58	MG	1H	3383	1/1	0.97	0.13	49,49,49,49	0
58	MG	1H	3384	1/1	0.97	0.11	45,45,45,45	0
58	MG	1G	1601	1/1	0.97	0.23	85,85,85,85	0
58	MG	14	3161	1/1	0.97	0.14	99,99,99,99	0
58	MG	1H	3218	1/1	0.97	0.11	48,48,48,48	0
58	MG	1H	3456	1/1	0.97	0.08	93,93,93,93	0
58	MG	14	3069	1/1	0.97	0.43	64,64,64,64	0
58	MG	14	3256	1/1	0.97	0.52	77,77,77,77	0
58	MG	14	3374	1/1	0.97	0.14	95,95,95,95	0
58	MG	1G	1604	1/1	0.97	0.31	91,91,91,91	0
58	MG	14	3071	1/1	0.97	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	1G	1605	1/1	0.97	0.40	102,102,102,102	0
58	MG	1H	3291	1/1	0.97	0.34	64,64,64,64	0
58	MG	1G	1607	1/1	0.97	0.21	92,92,92,92	0
58	MG	14	3380	1/1	0.97	0.08	85,85,85,85	0
58	MG	1H	3054	1/1	0.97	0.37	45,45,45,45	0
58	MG	13	1729	1/1	0.97	0.08	80,80,80,80	0
58	MG	1H	3009	1/1	0.97	0.32	69,69,69,69	0
58	MG	14	3384	1/1	0.97	0.08	93,93,93,93	0
58	MG	14	3175	1/1	0.97	0.23	88,88,88,88	0
58	MG	14	3082	1/1	0.97	0.34	85,85,85,85	0
58	MG	13	1681	1/1	0.97	0.19	66,66,66,66	0
58	MG	1H	3395	1/1	0.97	0.10	72,72,72,72	0
58	MG	1H	3396	1/1	0.97	0.07	75,75,75,75	0
58	MG	1H	3224	1/1	0.97	0.41	50,50,50,50	0
58	MG	13	1635	1/1	0.97	0.13	97,97,97,97	0
58	MG	1G	1685	1/1	0.97	0.10	109,109,109,109	0
58	MG	1H	3399	1/1	0.97	0.09	40,40,40,40	0
58	MG	13	1703	1/1	0.97	0.12	64,64,64,64	0
58	MG	1G	1618	1/1	0.97	0.19	85,85,85,85	0
58	MG	1G	1689	1/1	0.97	0.07	98,98,98,98	0
58	MG	13	1733	1/1	0.97	0.24	83,83,83,83	0
58	MG	1H	3470	1/1	0.97	0.04	96,96,96,96	0
58	MG	14	3401	1/1	0.97	0.06	83,83,83,83	0
58	MG	1H	3036	1/1	0.97	0.35	126,126,126,126	0
58	MG	1H	3405	1/1	0.97	0.09	70,70,70,70	0
58	MG	13	1650	1/1	0.97	0.14	100,100,100,100	0
58	MG	14	3101	1/1	0.97	0.32	61,61,61,61	0
58	MG	1H	3115	1/1	0.97	0.37	62,62,62,62	0
58	MG	13	1721	1/1	0.97	0.19	63,63,63,63	0
58	MG	13	1723	1/1	0.97	0.05	80,80,80,80	0
58	MG	1H	3410	1/1	0.97	0.07	76,76,76,76	0
58	MG	1H	3089	1/1	0.97	0.36	50,50,50,50	0
58	MG	1H	3306	1/1	0.97	0.24	63,63,63,63	0
58	MG	14	3006	1/1	0.97	0.38	47,47,47,47	0
58	MG	14	3291	1/1	0.97	0.23	55,55,55,55	0
58	MG	1H	3090	1/1	0.97	0.29	48,48,48,48	0
58	MG	14	3293	1/1	0.97	0.19	67,67,67,67	0
58	MG	2K	101	1/1	0.97	0.37	72,72,72,72	0
58	MG	14	3418	1/1	0.97	0.17	52,52,52,52	0
58	MG	14	3010	1/1	0.97	0.29	76,76,76,76	0
58	MG	1H	3122	1/1	0.97	0.29	65,65,65,65	0
58	MG	13	1636	1/1	0.97	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1725	1/1	0.97	0.06	83,83,83,83	0
58	MG	14	3300	1/1	0.97	0.11	57,57,57,57	0
58	MG	14	3301	1/1	0.97	0.10	49,49,49,49	0
58	MG	14	3015	1/1	0.97	0.40	67,67,67,67	0
58	MG	1G	1637	1/1	0.97	0.42	87,87,87,87	0
58	MG	1H	3152	1/1	0.97	0.12	64,64,64,64	0
58	MG	1H	3351	1/1	0.97	0.05	49,49,49,49	0
58	MG	29	301	1/1	0.97	0.26	58,58,58,58	0
58	MG	1H	3206	1/1	0.97	0.47	69,69,69,69	0
58	MG	1H	3353	1/1	0.97	0.12	54,54,54,54	0
58	MG	14	3308	1/1	0.97	0.15	75,75,75,75	0
58	MG	39	302	1/1	0.97	0.25	96,96,96,96	0
58	MG	1H	3179	1/1	0.97	0.32	76,76,76,76	0
58	MG	14	3311	1/1	0.97	0.14	62,62,62,62	0
58	MG	14	3024	1/1	0.97	0.26	58,58,58,58	0
58	MG	14	3025	1/1	0.97	0.27	52,52,52,52	0
58	MG	1H	3355	1/1	0.97	0.13	60,60,60,60	0
60	ZN	G8	201	1/1	0.97	0.16	147,147,147,147	0
60	ZN	5A	101	1/1	0.97	0.11	128,128,128,128	0
58	MG	14	3129	1/1	0.97	0.47	53,53,53,53	0
58	MG	14	3097	1/1	0.98	0.35	49,49,49,49	0
58	MG	1H	3237	1/1	0.98	0.32	72,72,72,72	0
58	MG	1H	3455	1/1	0.98	0.06	65,65,65,65	0
58	MG	14	3348	1/1	0.98	0.09	86,86,86,86	0
58	MG	88	201	1/1	0.98	0.16	75,75,75,75	0
58	MG	88	202	1/1	0.98	0.07	81,81,81,81	0
58	MG	1G	1653	1/1	0.98	0.33	86,86,86,86	0
58	MG	1H	3044	1/1	0.98	0.21	41,41,41,41	0
58	MG	14	3182	1/1	0.98	0.49	89,89,89,89	0
58	MG	1H	3025	1/1	0.98	0.29	41,41,41,41	0
58	MG	1H	3402	1/1	0.98	0.07	60,60,60,60	0
58	MG	1H	3046	1/1	0.98	0.29	55,55,55,55	0
58	MG	14	3358	1/1	0.98	0.05	83,83,83,83	0
58	MG	14	3360	1/1	0.98	0.12	48,48,48,48	0
58	MG	13	1661	1/1	0.98	0.07	86,86,86,86	0
58	MG	14	3030	1/1	0.98	0.26	65,65,65,65	0
58	MG	14	3032	1/1	0.98	0.33	62,62,62,62	0
58	MG	14	3364	1/1	0.98	0.09	98,98,98,98	0
58	MG	14	3189	1/1	0.98	0.28	90,90,90,90	0
58	MG	14	3111	1/1	0.98	0.28	48,48,48,48	0
58	MG	1H	3109	1/1	0.98	0.32	47,47,47,47	0
58	MG	13	1609	1/1	0.98	0.28	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3049	1/1	0.98	0.14	57,57,57,57	0
58	MG	1H	3357	1/1	0.98	0.09	56,56,56,56	0
58	MG	14	3117	1/1	0.98	0.29	62,62,62,62	0
58	MG	14	3196	1/1	0.98	0.09	87,87,87,87	0
58	MG	1H	3050	1/1	0.98	0.31	53,53,53,53	0
58	MG	14	3038	1/1	0.98	0.41	59,59,59,59	0
58	MG	1H	3411	1/1	0.98	0.08	63,63,63,63	0
58	MG	1H	3359	1/1	0.98	0.07	43,43,43,43	0
58	MG	1H	3360	1/1	0.98	0.11	70,70,70,70	0
58	MG	1H	3210	1/1	0.98	0.49	67,67,67,67	0
58	MG	14	3203	1/1	0.98	0.12	71,71,71,71	0
58	MG	1H	3471	1/1	0.98	0.21	92,92,92,92	0
58	MG	1H	3051	1/1	0.98	0.32	45,45,45,45	0
58	MG	1H	3052	1/1	0.98	0.18	57,57,57,57	0
58	MG	1H	3365	1/1	0.98	0.07	60,60,60,60	0
58	MG	13	1663	1/1	0.98	0.46	77,77,77,77	0
58	MG	14	3386	1/1	0.98	0.05	82,82,82,82	0
58	MG	1H	3055	1/1	0.98	0.26	50,50,50,50	0
58	MG	1H	3117	1/1	0.98	0.18	68,68,68,68	0
58	MG	1H	3326	1/1	0.98	0.45	119,119,119,119	0
58	MG	1H	3370	1/1	0.98	0.12	72,72,72,72	0
58	MG	13	1610	1/1	0.98	0.11	66,66,66,66	0
58	MG	1H	3424	1/1	0.98	0.13	66,66,66,66	0
58	MG	1H	3058	1/1	0.98	0.27	54,54,54,54	0
58	MG	14	3056	1/1	0.98	0.33	50,50,50,50	0
58	MG	13	1648	1/1	0.98	0.17	76,76,76,76	0
58	MG	14	3298	1/1	0.98	0.14	69,69,69,69	0
58	MG	13	1602	1/1	0.98	0.32	74,74,74,74	0
58	MG	1H	3220	1/1	0.98	0.25	84,84,84,84	0
58	MG	1H	3088	1/1	0.98	0.28	58,58,58,58	0
58	MG	1G	1684	1/1	0.98	0.08	82,82,82,82	0
58	MG	1H	3377	1/1	0.98	0.14	68,68,68,68	0
58	MG	1H	3433	1/1	0.98	0.19	45,45,45,45	0
58	MG	13	1722	1/1	0.98	0.15	70,70,70,70	0
58	MG	1G	1629	1/1	0.98	0.37	98,98,98,98	0
58	MG	14	3067	1/1	0.98	0.35	60,60,60,60	0
58	MG	1H	3013	1/1	0.98	0.39	67,67,67,67	0
58	MG	14	3309	1/1	0.98	0.18	51,51,51,51	0
58	MG	1H	3491	1/1	0.98	0.03	91,91,91,91	0
58	MG	1H	3380	1/1	0.98	0.09	56,56,56,56	0
58	MG	14	3312	1/1	0.98	0.17	56,56,56,56	0
58	MG	13	1677	1/1	0.98	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	1H	3261	1/1	0.98	0.07	85,85,85,85	0
58	MG	13	1632	1/1	0.98	0.14	57,57,57,57	0
58	MG	14	3317	1/1	0.98	0.10	52,52,52,52	0
58	MG	14	3416	1/1	0.98	0.31	83,83,83,83	0
58	MG	14	3075	1/1	0.98	0.40	60,60,60,60	0
58	MG	14	3319	1/1	0.98	0.18	50,50,50,50	0
58	MG	14	3320	1/1	0.98	0.14	78,78,78,78	0
58	MG	1H	3016	1/1	0.98	0.28	52,52,52,52	0
58	MG	13	1712	1/1	0.98	0.07	66,66,66,66	0
58	MG	13	1658	1/1	0.98	0.15	74,74,74,74	0
58	MG	14	3079	1/1	0.98	0.30	63,63,63,63	0
58	MG	14	3326	1/1	0.98	0.12	77,77,77,77	0
58	MG	1H	3020	1/1	0.98	0.48	52,52,52,52	0
58	MG	1H	3100	1/1	0.98	0.35	38,38,38,38	0
58	MG	14	3330	1/1	0.98	0.06	73,73,73,73	0
58	MG	14	3083	1/1	0.98	0.30	67,67,67,67	0
58	MG	14	3002	1/1	0.98	0.38	53,53,53,53	0
58	MG	1H	3231	1/1	0.98	0.40	75,75,75,75	0
58	MG	14	3004	1/1	0.98	0.42	57,57,57,57	0
58	MG	14	3005	1/1	0.98	0.22	51,51,51,51	0
58	MG	1H	3391	1/1	0.98	0.10	61,61,61,61	0
58	MG	14	3007	1/1	0.98	0.29	52,52,52,52	0
58	MG	1H	3001	1/1	0.98	0.39	52,52,52,52	0
58	MG	1H	3133	1/1	0.98	0.21	60,60,60,60	0
58	MG	14	3170	1/1	0.98	0.46	82,82,82,82	0
58	MG	1H	3450	1/1	0.98	0.13	77,77,77,77	0
60	ZN	5I	102	1/1	0.98	0.16	92,92,92,92	0
58	MG	1H	3022	1/1	0.98	0.33	60,60,60,60	0
58	MG	13	1612	1/1	0.98	0.18	75,75,75,75	0
58	MG	13	1639	1/1	0.98	0.33	80,80,80,80	0
58	MG	14	3359	1/1	0.99	0.08	70,70,70,70	0
58	MG	14	3114	1/1	0.99	0.26	85,85,85,85	0
58	MG	1H	3002	1/1	0.99	0.26	48,48,48,48	0
58	MG	14	3322	1/1	0.99	0.06	69,69,69,69	0
58	MG	1H	3057	1/1	0.99	0.32	51,51,51,51	0
58	MG	14	3026	1/1	0.99	0.33	51,51,51,51	0
58	MG	14	3028	1/1	0.99	0.22	53,53,53,53	0
58	MG	1H	3431	1/1	0.99	0.03	74,74,74,74	0
58	MG	1H	3389	1/1	0.99	0.11	50,50,50,50	0
58	MG	14	3031	1/1	0.99	0.22	75,75,75,75	0
58	MG	14	3369	1/1	0.99	0.13	49,49,49,49	0
58	MG	14	3329	1/1	0.99	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3403	1/1	0.99	0.13	45,45,45,45	0
58	MG	1H	3434	1/1	0.99	0.11	45,45,45,45	0
58	MG	14	3061	1/1	0.99	0.28	56,56,56,56	0
58	MG	1H	3053	1/1	0.99	0.31	54,54,54,54	0
58	MG	1G	1626	1/1	0.99	0.20	93,93,93,93	0
58	MG	1H	3003	1/1	0.99	0.29	38,38,38,38	0
58	MG	21	301	1/1	0.99	0.23	48,48,48,48	0
58	MG	14	3096	1/1	0.99	0.36	65,65,65,65	0
58	MG	14	3011	1/1	0.99	0.43	66,66,66,66	0
58	MG	1H	3392	1/1	0.99	0.10	50,50,50,50	0
58	MG	1H	3393	1/1	0.99	0.06	51,51,51,51	0
58	MG	14	3166	1/1	0.99	0.21	60,60,60,60	0
58	MG	14	3041	1/1	0.99	0.20	81,81,81,81	0
58	MG	1H	3096	1/1	0.99	0.25	51,51,51,51	0
58	MG	1H	3457	1/1	0.99	0.11	75,75,75,75	0
58	MG	14	3272	1/1	0.99	0.10	71,71,71,71	0
58	MG	14	3072	1/1	0.99	0.37	43,43,43,43	0
58	MG	1H	3362	1/1	0.99	0.08	42,42,42,42	0
58	MG	1H	3097	1/1	0.99	0.27	56,56,56,56	0
58	MG	1H	3018	1/1	0.99	0.44	51,51,51,51	0
58	MG	1H	3091	1/1	0.99	0.23	70,70,70,70	0
58	MG	14	3108	1/1	0.99	0.13	77,77,77,77	0
58	MG	1H	3140	1/1	0.99	0.16	61,61,61,61	0
58	MG	1H	3428	1/1	0.99	0.08	64,64,64,64	0
58	MG	14	3316	1/1	0.99	0.06	59,59,59,59	0
58	MG	14	3355	1/1	0.99	0.08	91,91,91,91	0
59	SF4	3E	301	8/8	0.99	0.20	78,90,95,100	0
59	SF4	32	301	8/8	0.99	0.18	119,123,130,133	0
58	MG	14	3022	1/1	0.99	0.38	63,63,63,63	0
58	MG	14	3398	1/1	0.99	0.07	67,67,67,67	0
58	MG	14	3080	1/1	0.99	0.26	62,62,62,62	0
58	MG	14	3023	1/1	0.99	0.26	42,42,42,42	0
58	MG	14	3027	1/1	1.00	0.27	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.