wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 02:28 pm GMT

PDB ID	:	5EL7
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and tRNALys in the A-site with a U-U mismatch in the second position and antibiotic paromomycin
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:

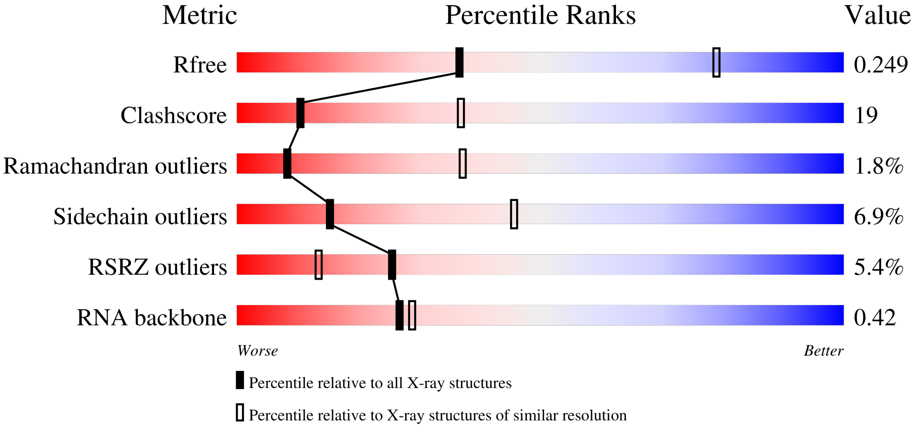
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

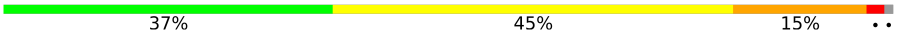
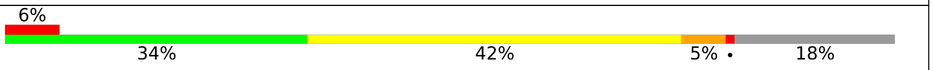
The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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

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

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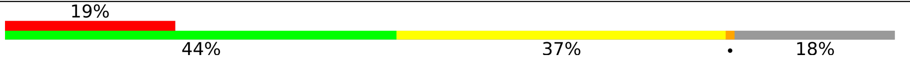
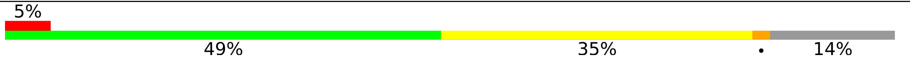
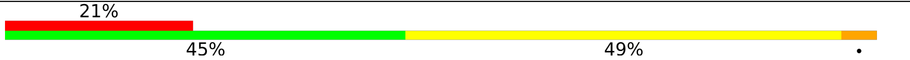
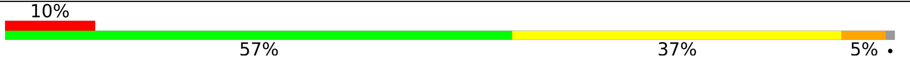
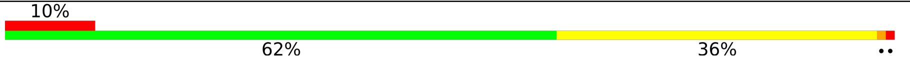
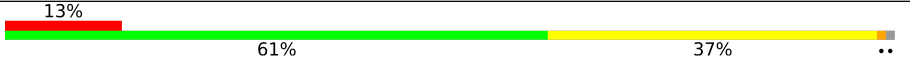
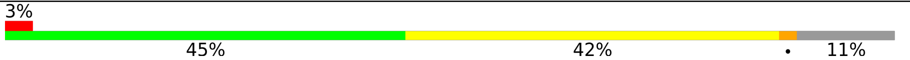
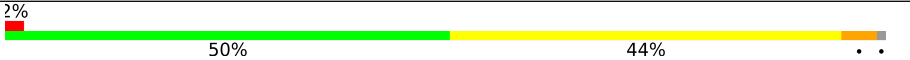
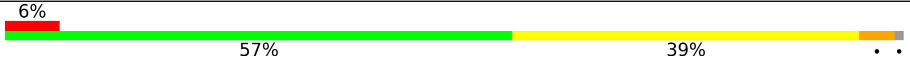
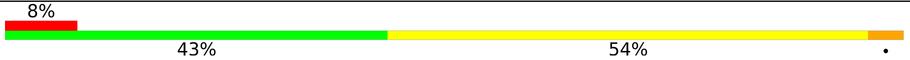
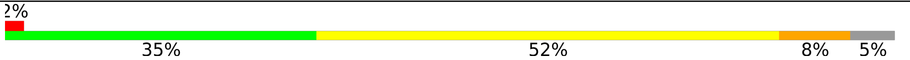
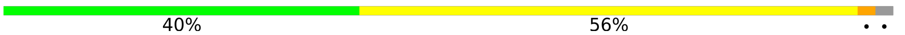
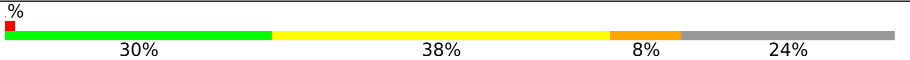
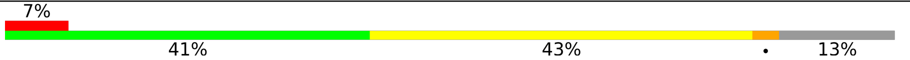
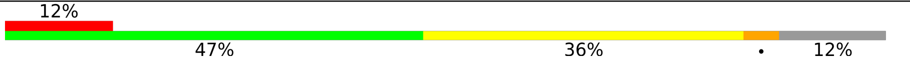
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
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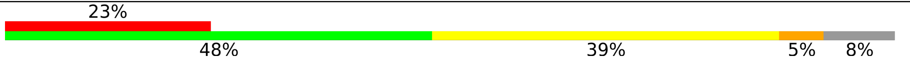
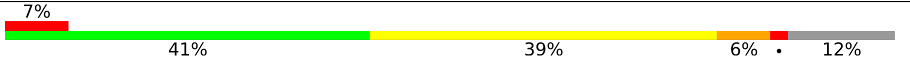
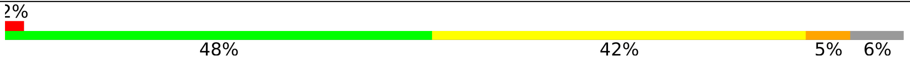
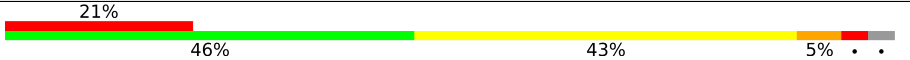
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	

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Mol	Chain	Length	Quality of chain
15	6A	89	3% 53% 43% • •
15	6I	89	% 60% 37% • •
16	7A	88	% 53% 35% 7% 5%
16	7I	88	44% 47% • 6%
17	8A	105	9% 54% 37% • 6%
17	8I	105	5% 46% 43% 7% 5%
18	9A	88	10% 44% 30% • 24%
18	9I	88	25% 44% 30% • 23%
19	AA	93	5% 41% 19% 6% 33%
19	AI	93	3% 41% 41% • • 13%
20	BA	106	2% 53% 36% • • 7%
20	BI	106	% 42% 47% • 8%
21	1B	27	7% 37% 41% • 19%
21	1F	27	41% 44% 15%
22	1K	76	11% 18% 45% 25% • 9%
22	1L	76	25% 28% 41% 24% • •
23	2K	77	49% 40% 8% •
23	2L	77	43% 39% 12% 6%
24	3K	76	4% 13% 36% 46% 5%
25	4K	27	7% 26% 22% 22% • 26%
25	4L	27	7% 22% 26% 19% • 30%
26	14	2917	% 34% 43% 18% • •
26	1H	2917	30% 42% 21% • •
27	16	122	% 39% 37% 20% •
27	1J	122	31% 45% 21% •

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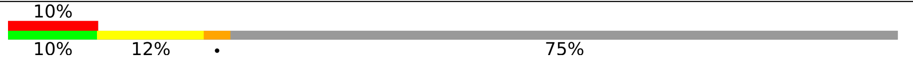
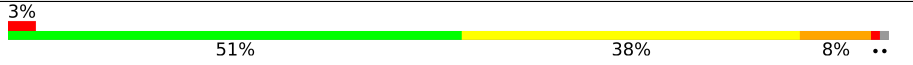
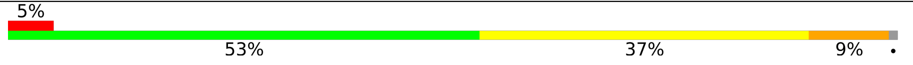
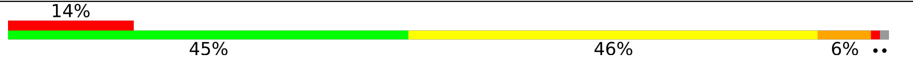
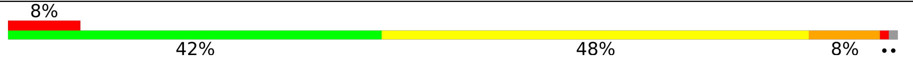
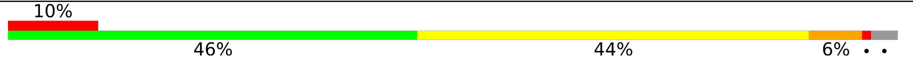
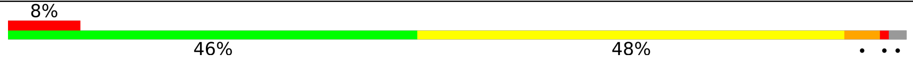
Mol	Chain	Length	Quality of chain
28	71	229	
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
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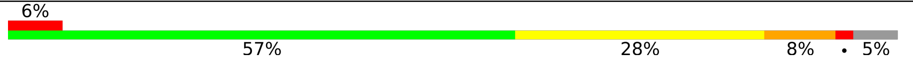
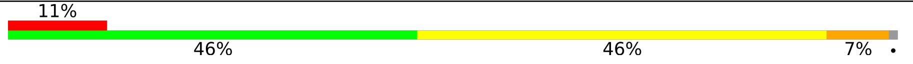
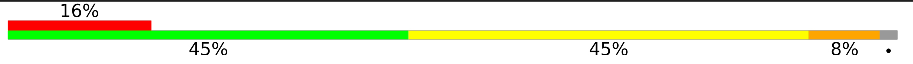
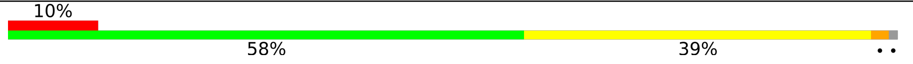
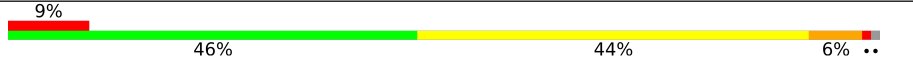
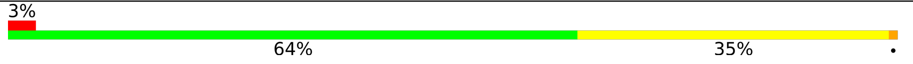
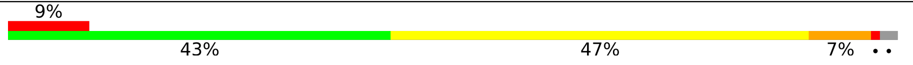
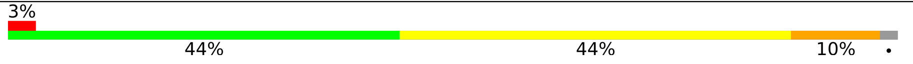
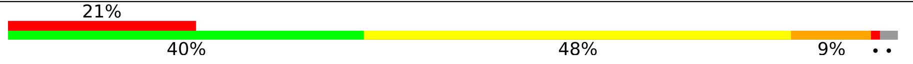
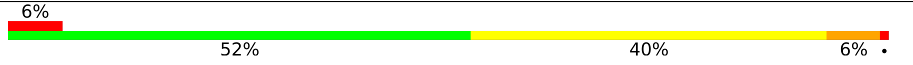
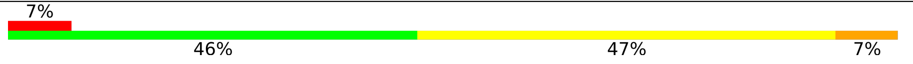
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	

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Mol	Chain	Length	Quality of chain
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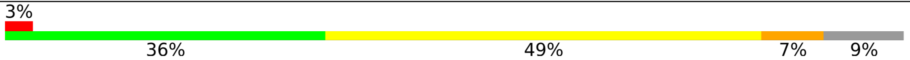
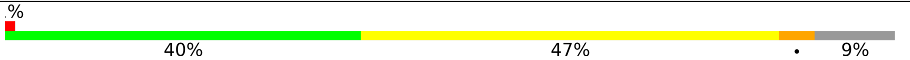
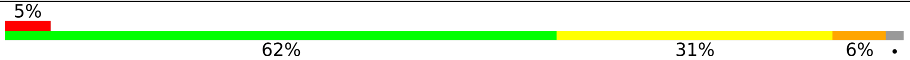
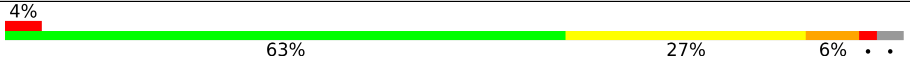
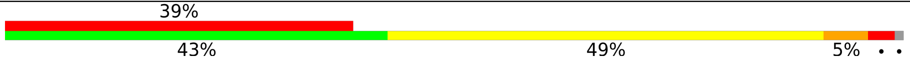
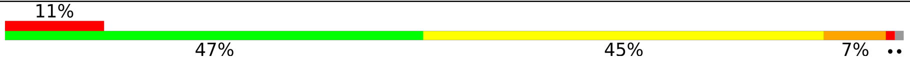
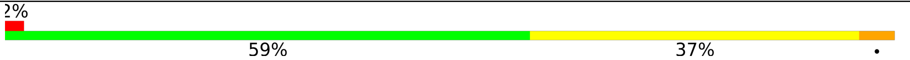
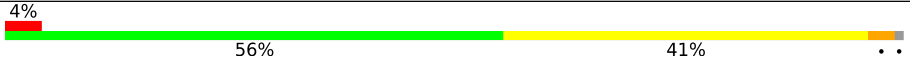
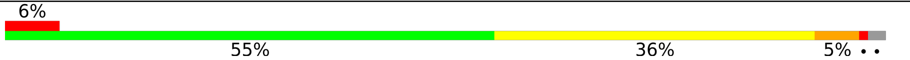
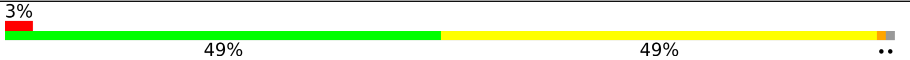
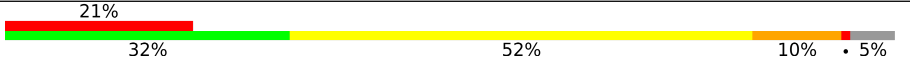
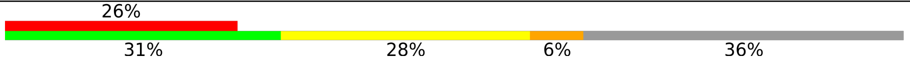
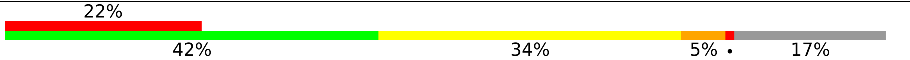
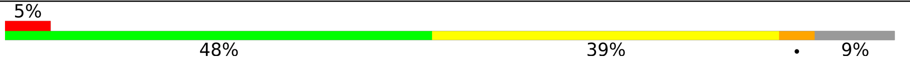
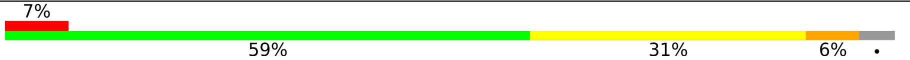
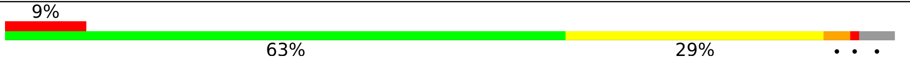
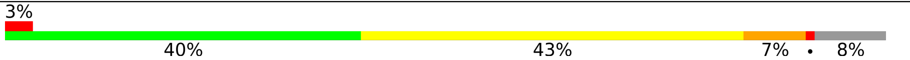
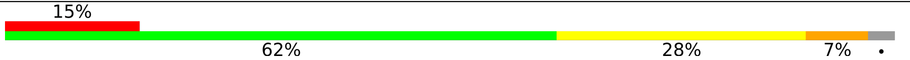
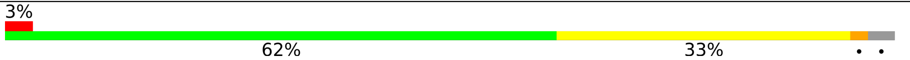
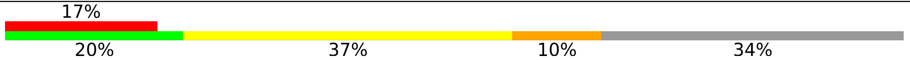
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	

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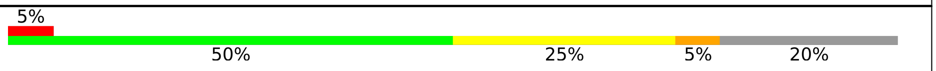
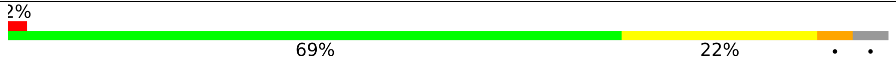
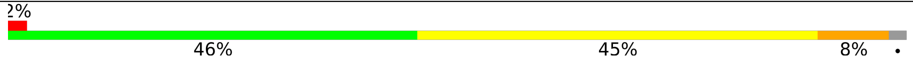
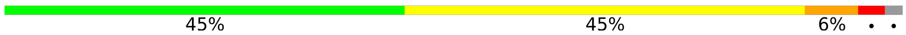
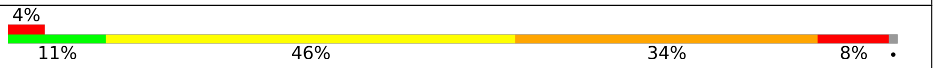
Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	3L	76	

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
57	MG	11	303	-	-	-	X
57	MG	13	1655	-	-	-	X
57	MG	13	1656	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1665	-	-	-	X
57	MG	13	1667	-	-	-	X
57	MG	14	3016	-	-	-	X
57	MG	14	3075	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3190	-	-	-	X
57	MG	14	3191	-	-	-	X
57	MG	14	3206	-	-	-	X
57	MG	14	3223	-	-	-	X
57	MG	14	3237	-	-	-	X
57	MG	14	3243	-	-	-	X
57	MG	14	3257	-	-	-	X
57	MG	14	3265	-	-	-	X
57	MG	14	3268	-	-	-	X
57	MG	16	206	-	-	-	X
57	MG	1G	1620	-	-	-	X
57	MG	1H	3069	-	-	-	X
57	MG	1H	3103	-	-	-	X
57	MG	1H	3108	-	-	-	X
57	MG	1H	3121	-	-	-	X
57	MG	1H	3136	-	-	-	X
57	MG	1H	3144	-	-	-	X
57	MG	1H	3190	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3220	-	-	-	X
57	MG	1H	3244	-	-	-	X
57	MG	1H	3280	-	-	-	X
57	MG	1H	3284	-	-	-	X
57	MG	1H	3289	-	-	-	X
57	MG	29	301	-	-	-	X
57	MG	2L	103	-	-	-	X
57	MG	P8	101	-	-	-	X
59	SF4	32	301	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	13	1496	32157	14313	5960	10388	1496	0	0	0
1	1G	1506	32368	14408	5999	10456	1505	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1690	1058	336	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	139	Total	C	N	O	S	0	0	0
			1115	692	222	195	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total 1477	C 662	N 257	O 488	P 69	S 1	0	0	0
22	1L	73	Total 1563	C 700	N 271	O 518	P 73	S 1	0	0	0

- Molecule 23 is a RNA chain called E. coli tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

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

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total 439	C 197	N 91	O 131	P 20	0	0	0
25	4L	19	Total 417	C 187	N 86	O 125	P 19	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	1H	2833	Total C N O P 61028 27159 11418 19618 2833	0	0	0
26	14	2861	Total C N O P 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 rRNA.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	71	133	Total C N O S 1033 651 194 187 1	0	0	0
28	79	57	Total C N O 456 283 91 82	0	0	0

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

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

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

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

- 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	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	74	Total	C	N	O		0	0	0
			573	359	117	97				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	69	145	Total 1131	C 723	N 200	O 207	S 1	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total 967	C 604	N 203	O 159	S 1	0	0	0
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	C	N	O	0	0	0
			875	550	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
44	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	K8	68	Total C N O S 568 352 115 100 1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	G5	66	Total C N O S 558 346 113 98 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	M8	47	Total C N O S 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
53	N8	48	Total C N O S 369 229 75 60 5	0	0	0
53	J5	56	Total C N O S 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
54	P8	47	Total C N O S 401 246 99 54 2	0	0	0
54	L5	47	Total C N O S 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
55	Q8	64	Total C N O S 516 331 102 81 2	0	0	0
55	M5	64	Total C N O S 516 331 102 81 2	0	0	0

- Molecule 56 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	3L	75	Total C N O P 1601 717 280 530 74	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	13	150	Total Mg 150 150	0	0
57	5E	1	Total Mg 1 1	0	0
57	1I	1	Total Mg 1 1	0	0
57	3I	1	Total Mg 1 1	0	0
57	5I	1	Total Mg 1 1	0	0
57	BI	1	Total Mg 1 1	0	0
57	2K	3	Total Mg 3 3	0	0
57	1H	502	Total Mg 502 502	0	0
57	16	12	Total Mg 12 12	0	0
57	11	3	Total Mg 3 3	0	0
57	21	3	Total Mg 3 3	0	0
57	31	1	Total Mg 1 1	0	0
57	41	2	Total Mg 2 2	0	0
57	78	1	Total Mg 1 1	0	0
57	88	1	Total Mg 1 1	0	0
57	I8	1	Total Mg 1 1	0	0
57	L8	1	Total Mg 1 1	0	0
57	P8	1	Total Mg 1 1	0	0
57	Q8	1	Total Mg 1 1	0	0

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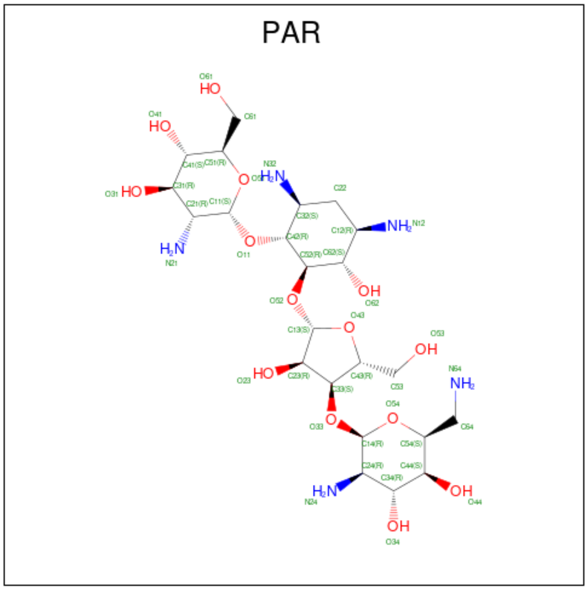
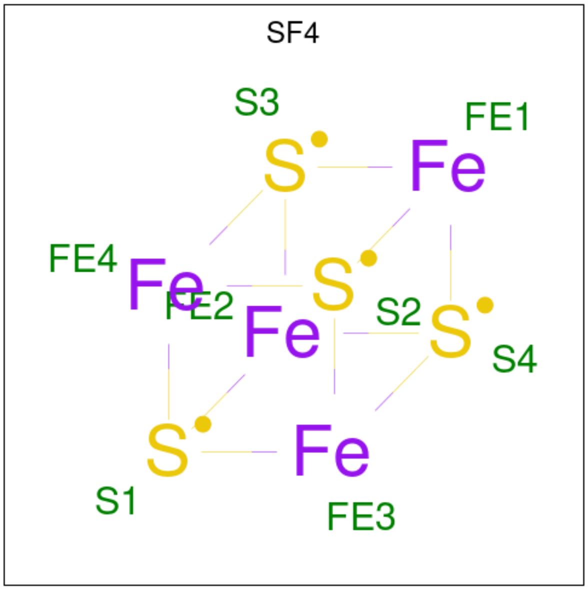
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	93	Total Mg 93 93	0	0
57	7A	1	Total Mg 1 1	0	0
57	2L	4	Total Mg 4 4	0	0
57	14	454	Total Mg 454 454	0	0
57	1J	6	Total Mg 6 6	0	0
57	29	4	Total Mg 4 4	0	0
57	39	2	Total Mg 2 2	0	0
57	35	2	Total Mg 2 2	0	0
57	45	3	Total Mg 3 3	0	0
57	55	1	Total Mg 1 1	0	0
57	85	1	Total Mg 1 1	0	0
57	C5	1	Total Mg 1 1	0	0
57	E5	1	Total Mg 1 1	0	0
57	M5	1	Total Mg 1 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	1	Total C N O 42 23 5 14	0	0
58	1G	1	Total C N O 42 23 5 14	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	319	Total O 319 319	0	0
61	3E	3	Total O 3 3	0	0
61	4E	3	Total O 3 3	0	0
61	8E	1	Total O 1 1	0	0
61	1I	1	Total O 1 1	0	0
61	3I	3	Total O 3 3	0	0
61	5I	1	Total O 1 1	0	0
61	6I	2	Total O 2 2	0	0
61	8I	2	Total O 2 2	0	0
61	BI	5	Total O 5 5	0	0
61	1F	1	Total O 1 1	0	0
61	1K	1	Total O 1 1	0	0
61	2K	7	Total O 7 7	0	0
61	3K	1	Total O 1 1	0	0
61	4K	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1H	1158	Total O 1158 1158	0	0
61	16	26	Total O 26 26	0	0
61	11	12	Total O 12 12	0	0
61	21	6	Total O 6 6	0	0
61	31	9	Total O 9 9	0	0
61	58	1	Total O 1 1	0	0
61	78	6	Total O 6 6	0	0
61	88	2	Total O 2 2	0	0
61	C8	2	Total O 2 2	0	0
61	E8	3	Total O 3 3	0	0
61	F8	2	Total O 2 2	0	0
61	G8	2	Total O 2 2	0	0
61	I8	5	Total O 5 5	0	0
61	J8	3	Total O 3 3	0	0
61	K8	2	Total O 2 2	0	0
61	L8	2	Total O 2 2	0	0
61	P8	1	Total O 1 1	0	0
61	Q8	9	Total O 9 9	0	0
61	1G	226	Total O 226 226	0	0
61	32	3	Total O 3 3	0	0
61	42	1	Total O 1 1	0	0

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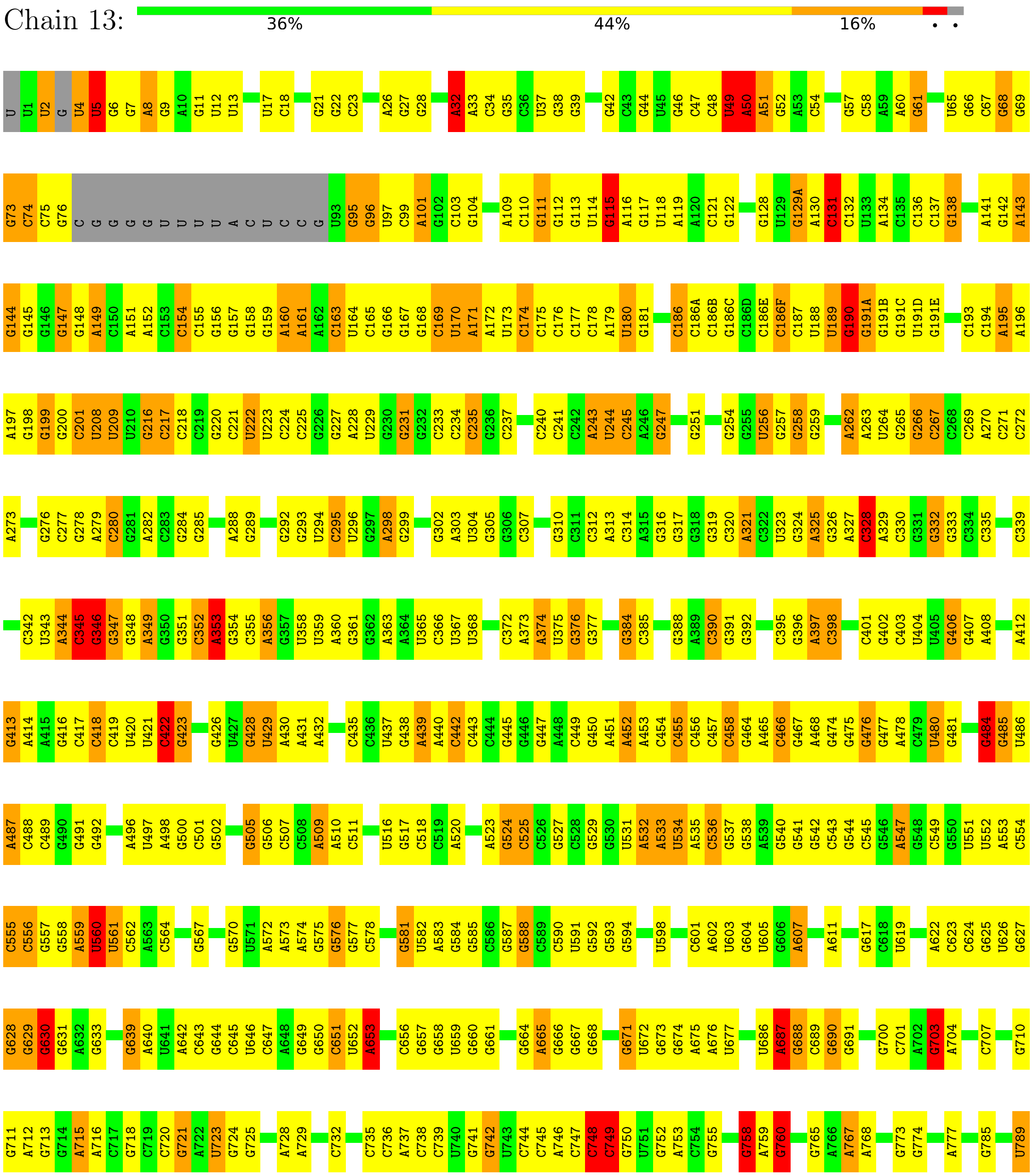
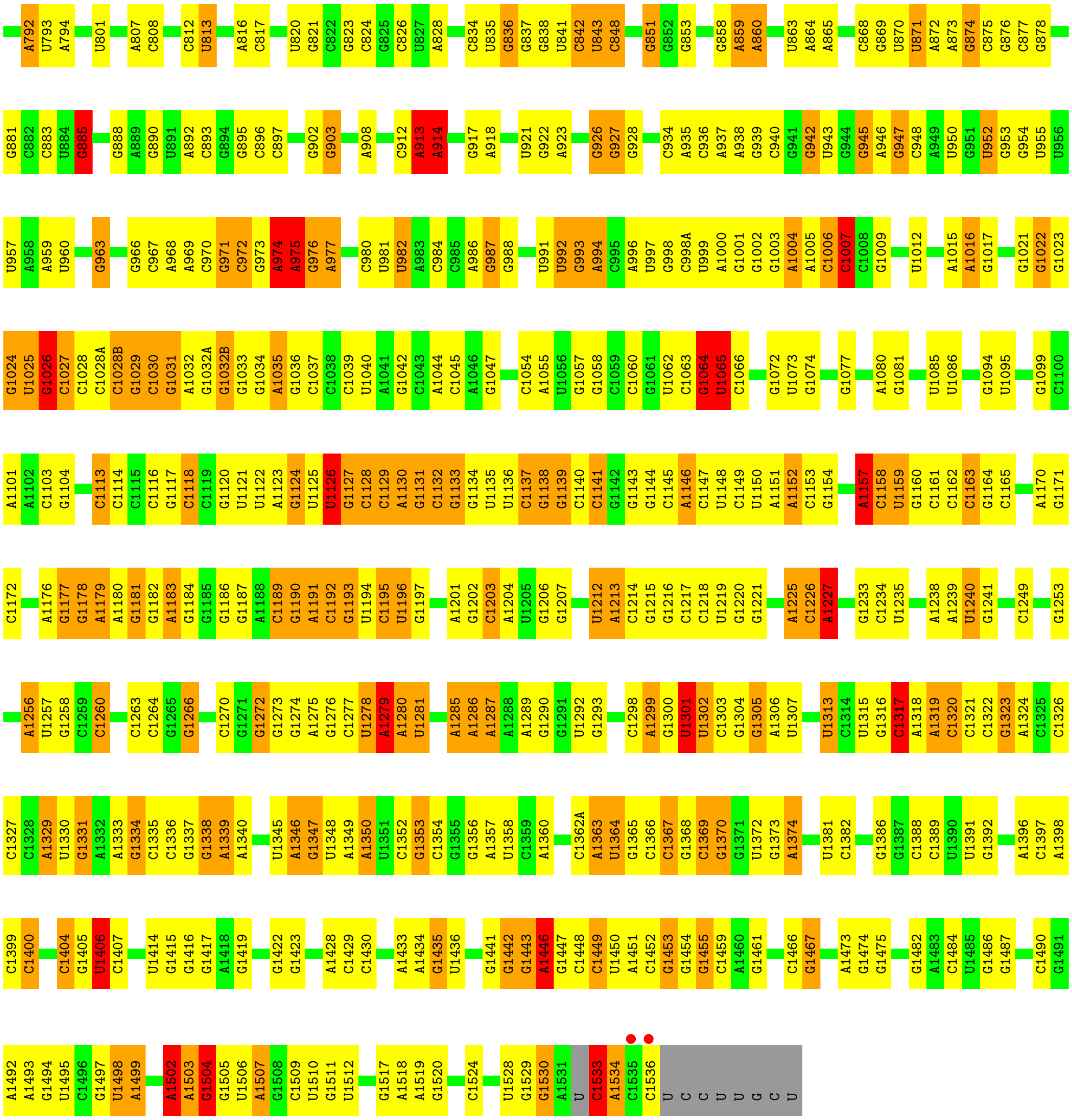
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	3A	1	Total O 1 1	0	0
61	6A	3	Total O 3 3	0	0
61	8A	1	Total O 1 1	0	0
61	BA	3	Total O 3 3	0	0
61	2L	1	Total O 1 1	0	0
61	4L	3	Total O 3 3	0	0
61	14	1015	Total O 1015 1015	0	0
61	1J	18	Total O 18 18	0	0
61	19	12	Total O 12 12	0	0
61	29	6	Total O 6 6	0	0
61	39	8	Total O 8 8	0	0
61	35	5	Total O 5 5	0	0
61	55	1	Total O 1 1	0	0
61	75	1	Total O 1 1	0	0
61	85	2	Total O 2 2	0	0
61	A5	2	Total O 2 2	0	0
61	B5	1	Total O 1 1	0	0
61	C5	4	Total O 4 4	0	0
61	H5	3	Total O 3 3	0	0
61	L5	2	Total O 2 2	0	0
61	M5	10	Total O 10 10	0	0

3 Residue-property plots ⓘ

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

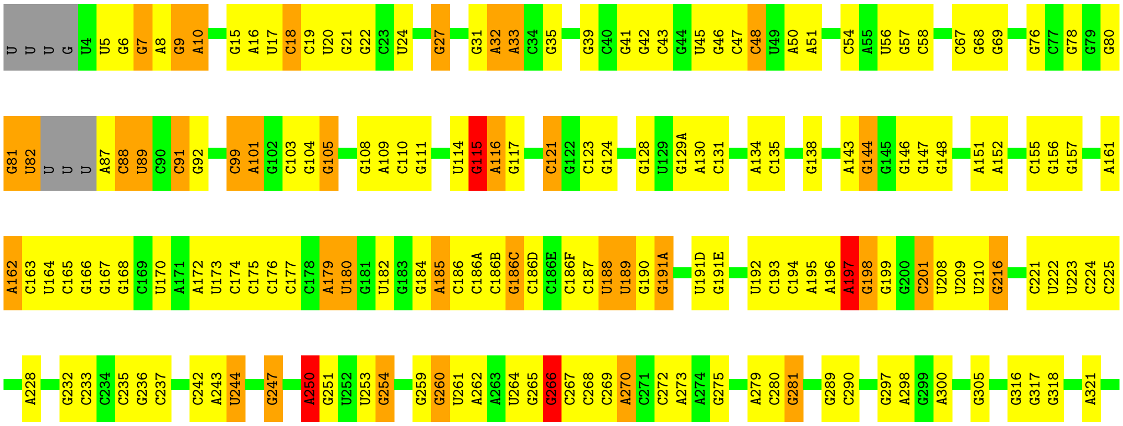
- Molecule 1: 16S rRNA

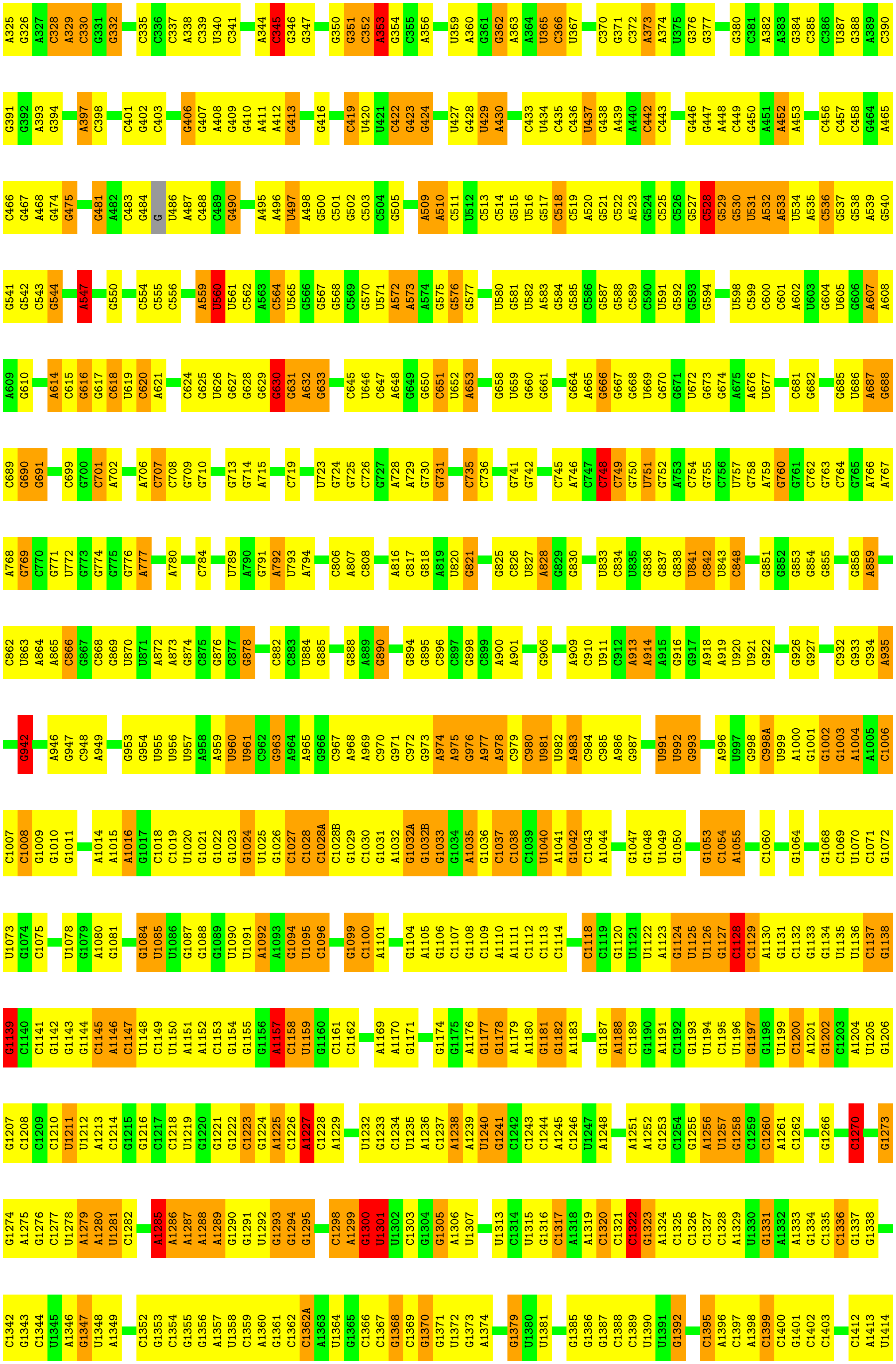


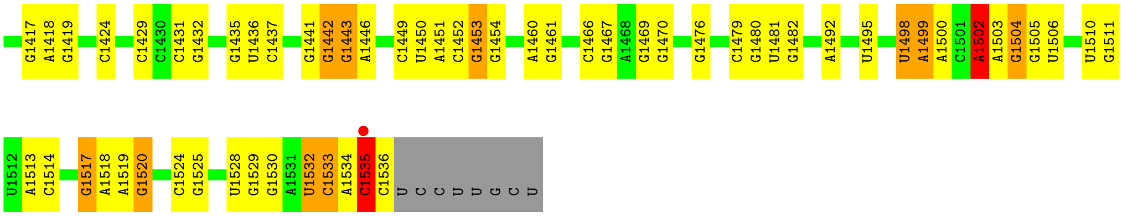


- Molecule 1: 16S rRNA

Chain 1G:

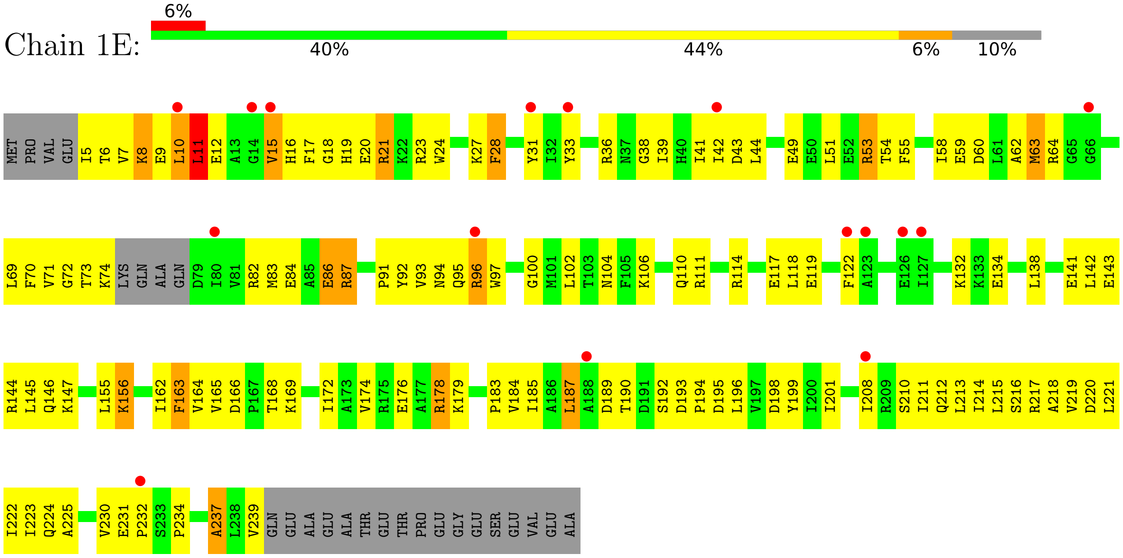



A325 G326 A327 C328 A329 C330 G331 G332 C335 C336 C337 A338 C339 U340 C341 A344 C345 G346 G347 G350 G351 C352 A353 G354 C355 A356 U359 A360 G361 G362 A363 A364 U365 C366 U367 C370 G371 C372 A373 A374 U375 G376 G377 G380 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390
G391 G392 A393 G394 A397 C398 C401 G402 C403 G406 G407 A408 G409 G410 A411 A412 G413 G416 C419 U420 U421 C422 G423 G424 U427 G428 U429 A430 C433 U434 C435 C436 U437 G438 A439 A440 C442 C443 G446 G447 A448 C449 G450 A451 A452 A453 C456 C457 C458 G464 A465
C466 G467 A468 G474 G475 G481 A482 C483 G484 G U486 A487 C488 C489 G490 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 U514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540
G541 G542 C543 G544 A547 G550 C554 C555 C556 A559 U560 U561 C562 A563 C564 U565 G566 G567 C568 C569 G570 U571 A572 A573 A574 G575 G576 G577 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 G593 G594 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608
A609 G610 A614 C615 G616 G617 C618 U619 C620 A621 C624 G625 U626 G627 C628 G629 G630 G631 A632 G633 C645 U646 C647 A648 G649 G650 C651 U652 A653 G658 U659 G660 G661 G664 A665 G666 G667 C668 U669 G670 G671 U672 G673 G674 A675 A676 U677 C681 G682 G685 U686 A687 G688
C689 G690 G691 C699 G700 C701 A702 A706 C707 C708 G709 G710 G713 G714 A715 C719 U723 G724 G725 C726 G727 A728 A729 G730 G731 C735 C736 G741 G742 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G760 G761 C762 G763 C764 G765 A766 A767
A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 A780 C784 U789 A790 G791 A792 U793 A794 C806 A807 C808 A816 C817 G818 A819 U820 G821 G825 C826 U827 A828 G829 G830 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 G851 G852 G853 G854 G855 G858 A859
C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C882 C883 U884 G885 G888 A889 G890 G894 G895 C896 C897 G898 C899 A900 A901 G906 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 G926 G927 C932 G933 C934 A935
G942 A946 G947 C948 A949 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 U991 U992 G993 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006
C1007 C1008 G1009 G1010 G1011 A1014 A1015 A1016 G1017 C1018 C1019 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 G1047 G1048 U1049 G1050 G1053 C1054 A1055 C1060 G1064 G1068 C1069 U1070 C1071 G1072
U1073 G1074 C1075 U1078 G1079 A1080 G1081 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 G1099 C1100 A1101 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138
G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1169 G1170 G1171 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206
G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 G1245 C1246 U1247 A1248 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 G1266 C1270 G1273
G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 C1334 C1335 C1336 G1337 G1338
C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1362A A1363 U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 G1379 U1380 U1381 G1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1412 A1413 U1414



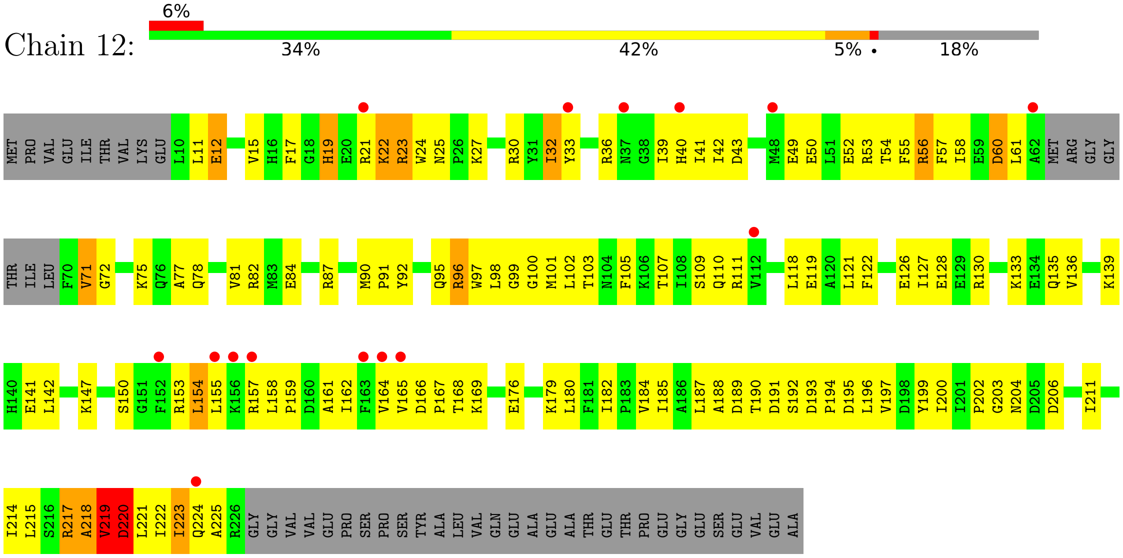
- Molecule 2: 30S ribosomal protein S2

Chain 1E:



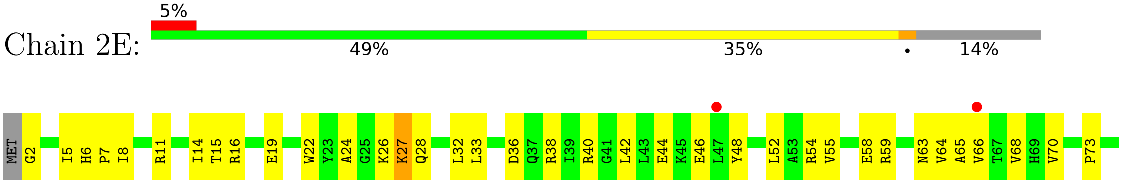
- Molecule 2: 30S ribosomal protein S2

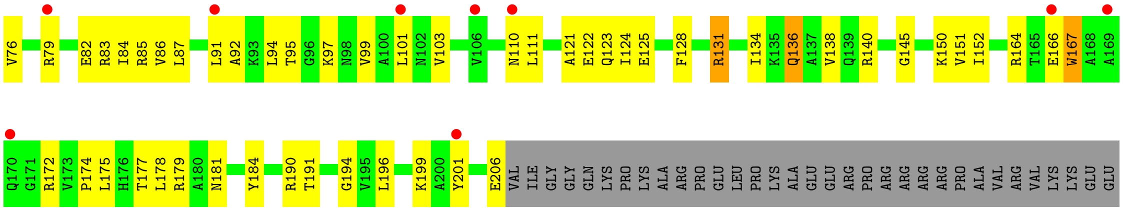
Chain 12:



- Molecule 3: 30S ribosomal protein S3

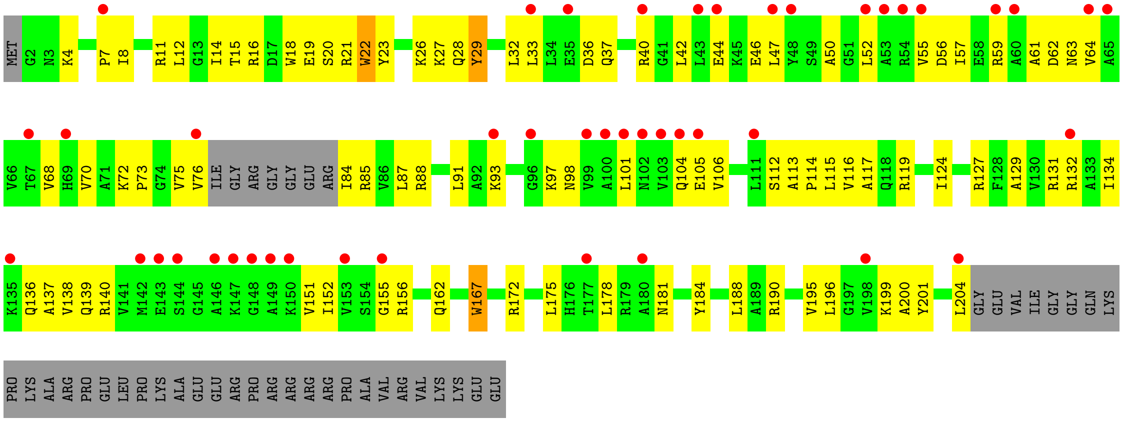
Chain 2E:





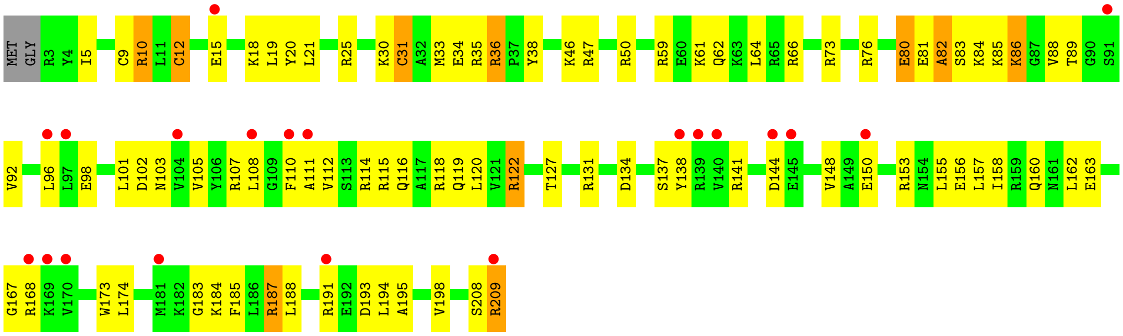
- Molecule 3: 30S ribosomal protein S3

Chain 22:



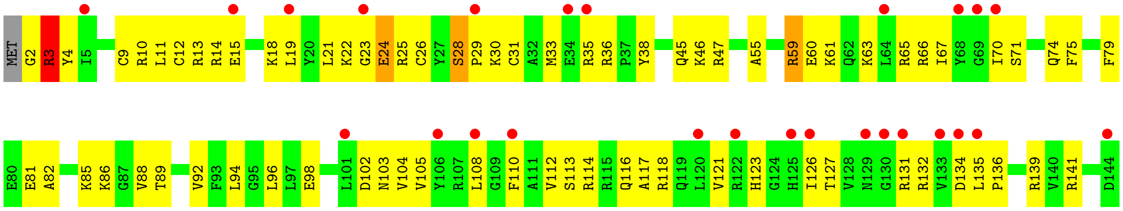
- Molecule 4: 30S ribosomal protein S4

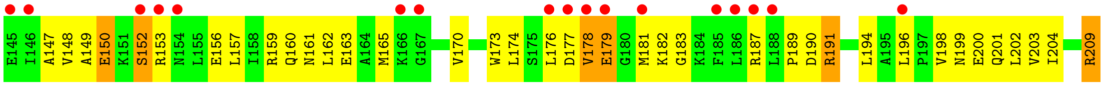
Chain 3E:



- Molecule 4: 30S ribosomal protein S4

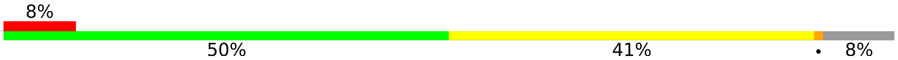
Chain 32:

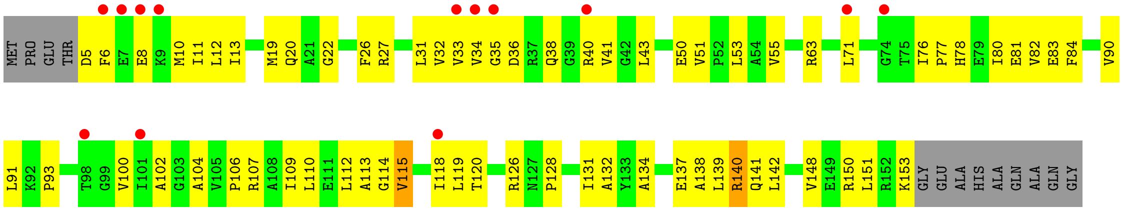




- Molecule 5: 30S ribosomal protein S5

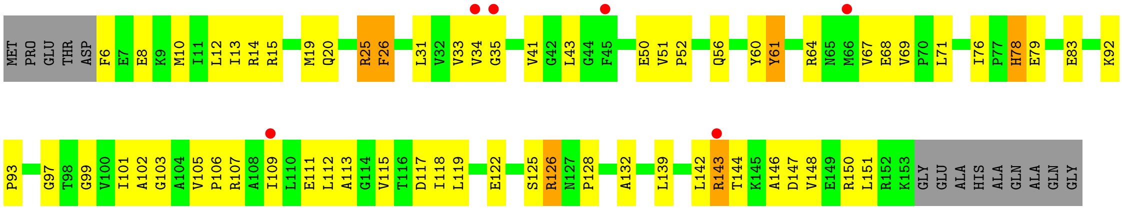
Chain 4E:





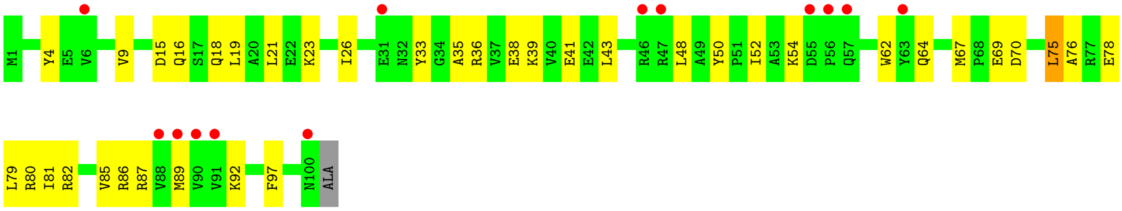
- Molecule 5: 30S ribosomal protein S5

Chain 42:



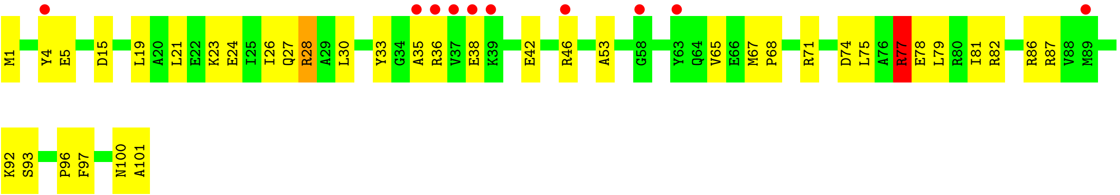
- Molecule 6: 30S ribosomal protein S6

Chain 5E:



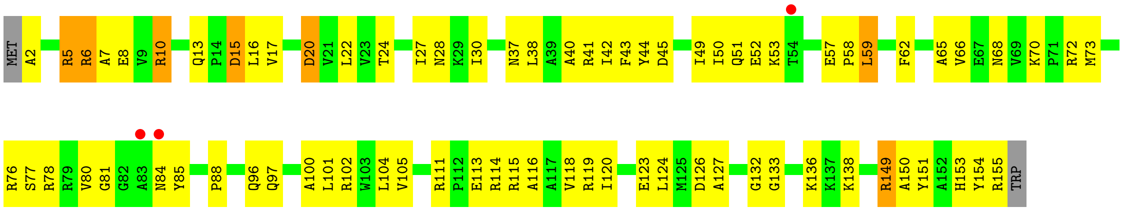
- Molecule 6: 30S ribosomal protein S6

Chain 52:



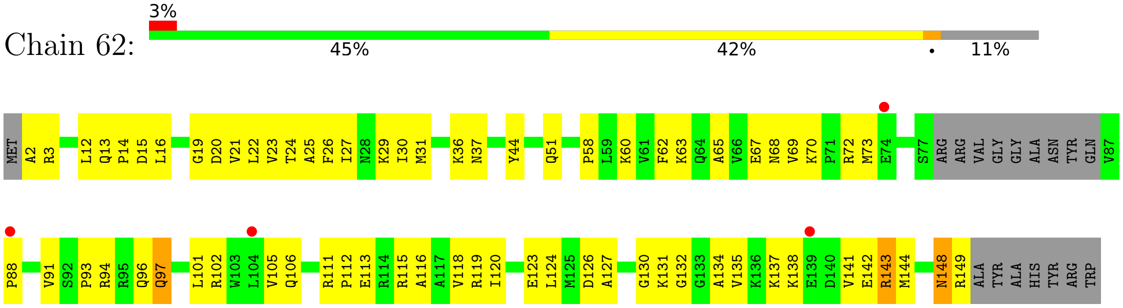
- Molecule 7: 30S ribosomal protein S7

Chain 6E:



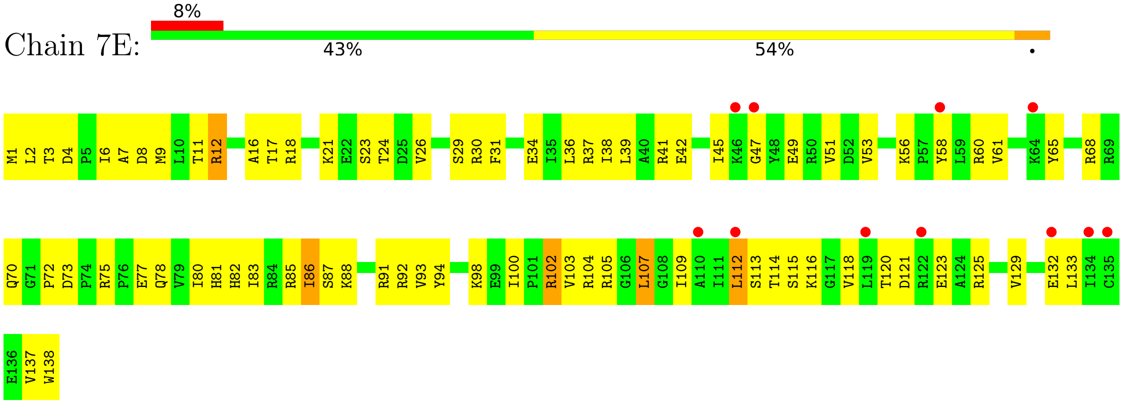
- Molecule 7: 30S ribosomal protein S7

Chain 62:



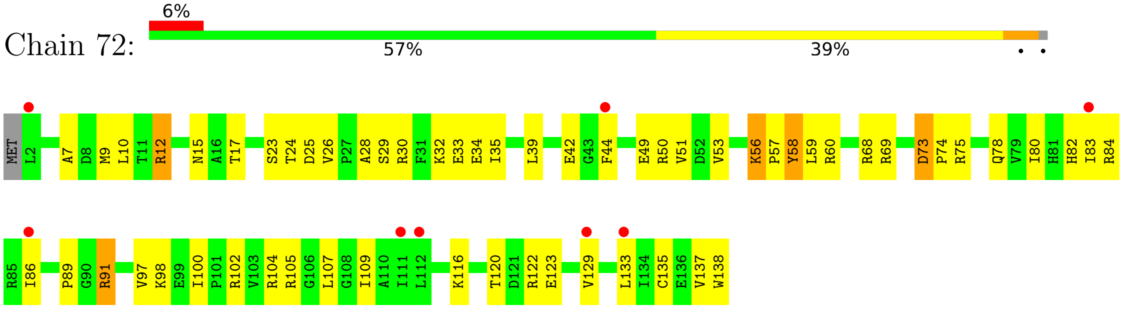
- Molecule 8: 30S ribosomal protein S8

Chain 7E:



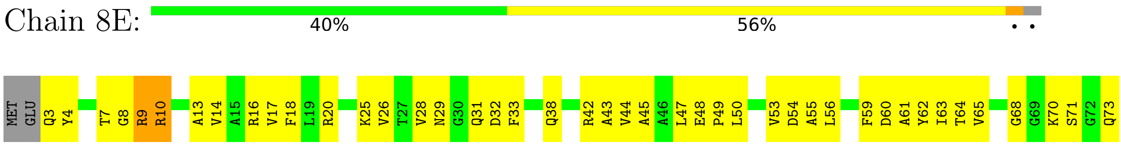
- Molecule 8: 30S ribosomal protein S8

Chain 72:



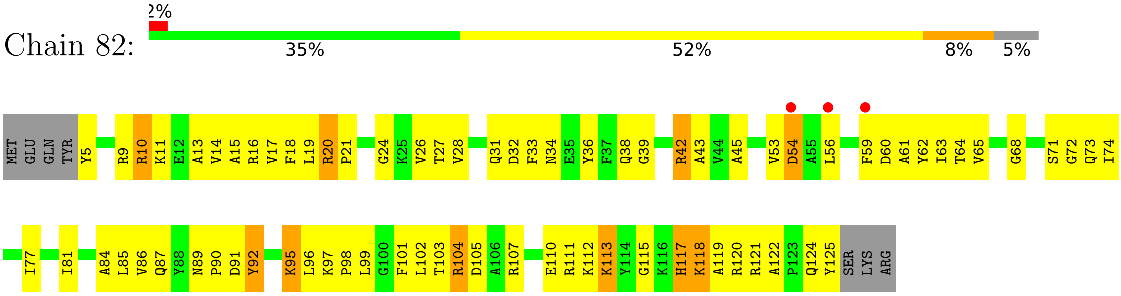
- Molecule 9: 30S ribosomal protein S9

Chain 8E:



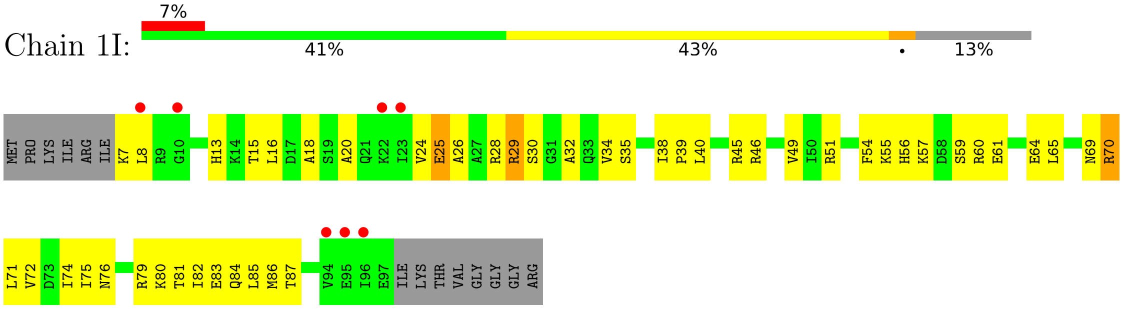
- Molecule 9: 30S ribosomal protein S9

Chain 82:



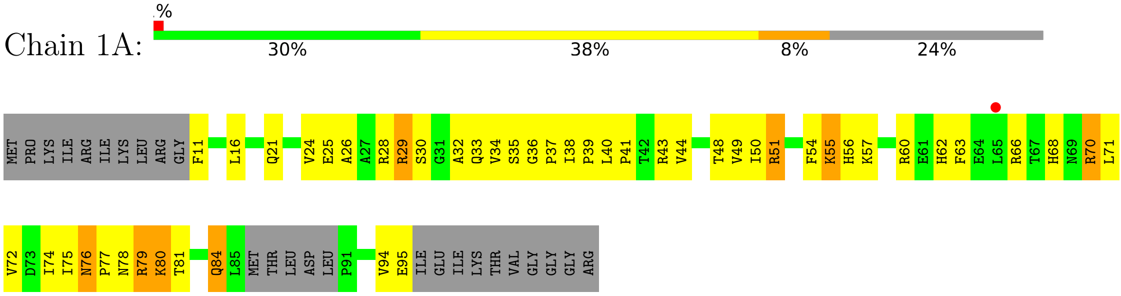
- Molecule 10: 30S ribosomal protein S10

Chain 1I:



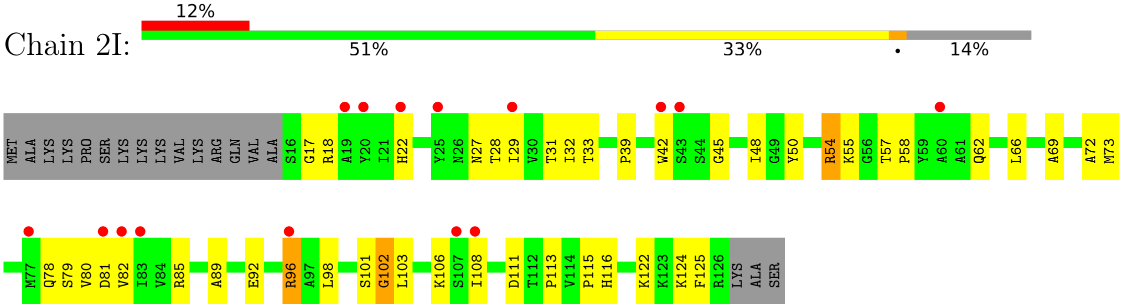
- Molecule 10: 30S ribosomal protein S10

Chain 1A:



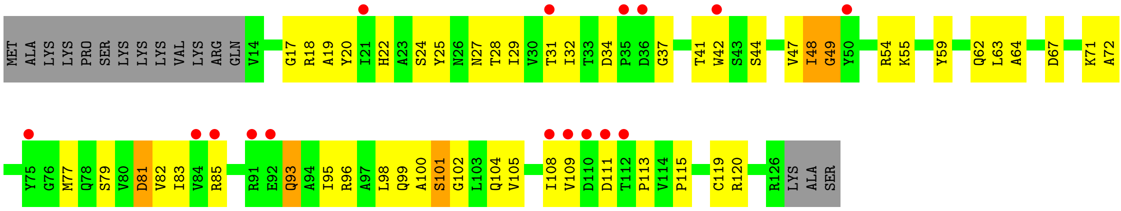
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



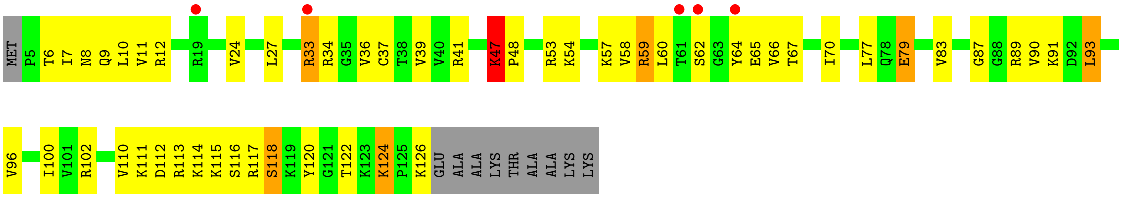
- Molecule 11: 30S ribosomal protein S11

Chain 2A:



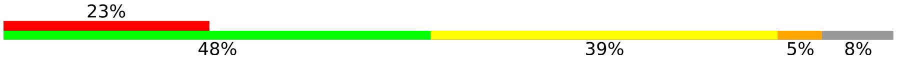
- Molecule 12: 30S ribosomal protein S12

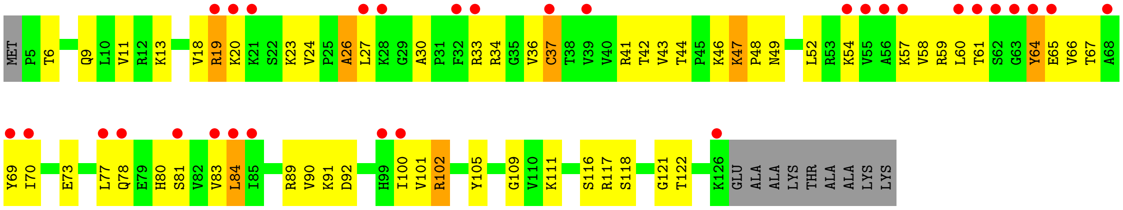
Chain 3I:



- Molecule 12: 30S ribosomal protein S12

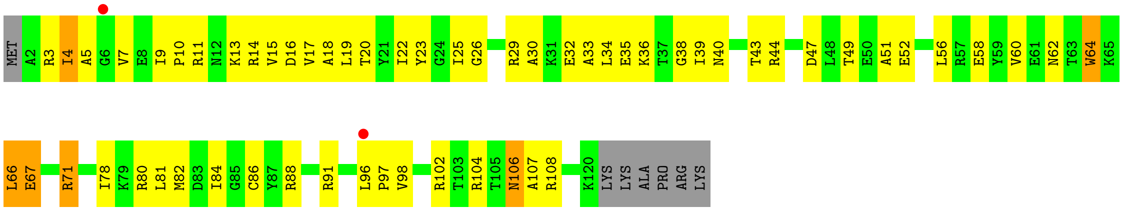
Chain 3A:





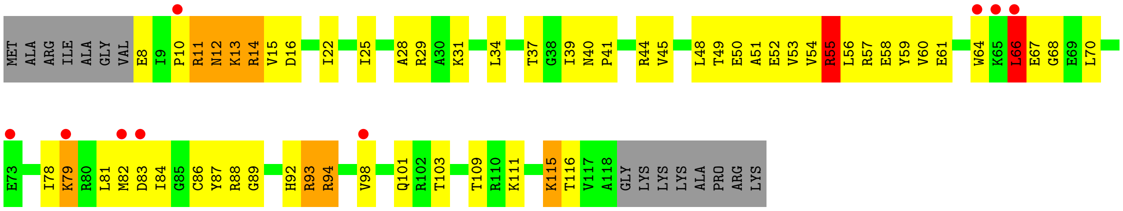
- Molecule 13: 30S ribosomal protein S13

Chain 4I:

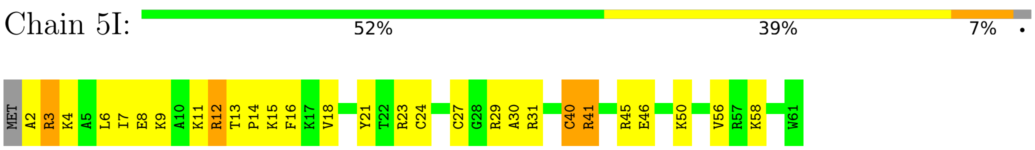


- Molecule 13: 30S ribosomal protein S13

Chain 4A:



- Molecule 14: 30S ribosomal protein S14 type Z



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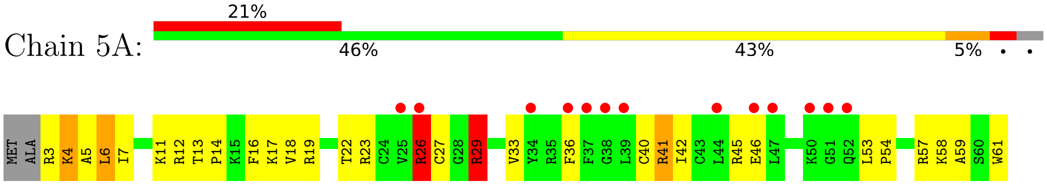

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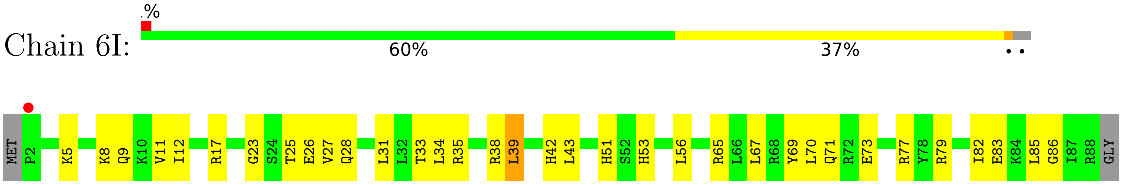

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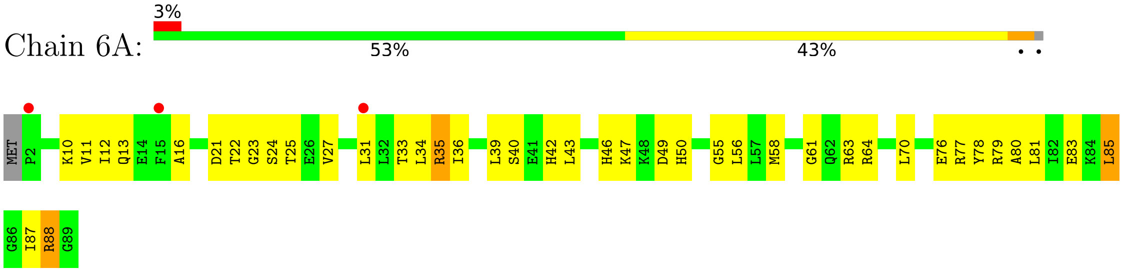

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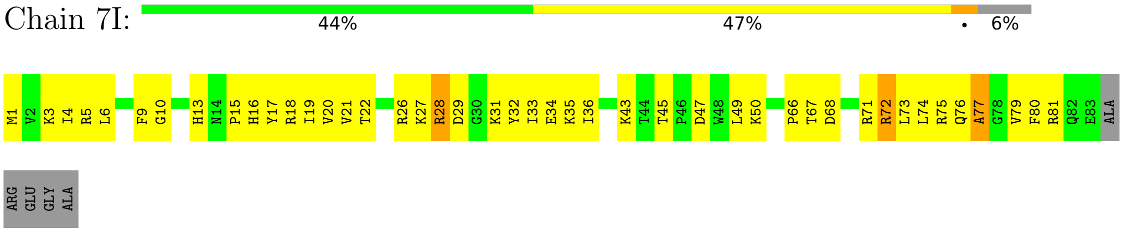

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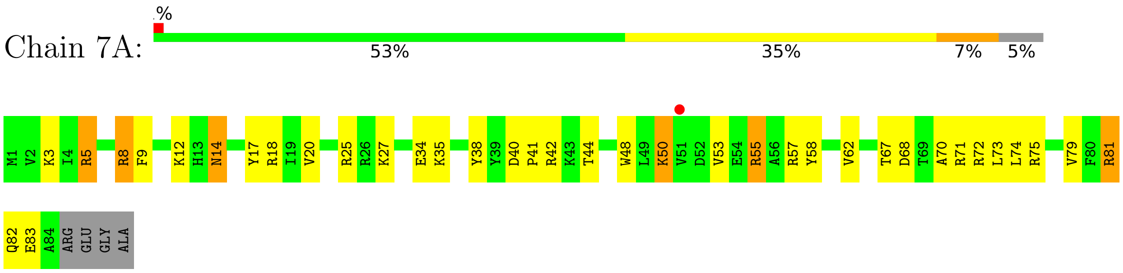
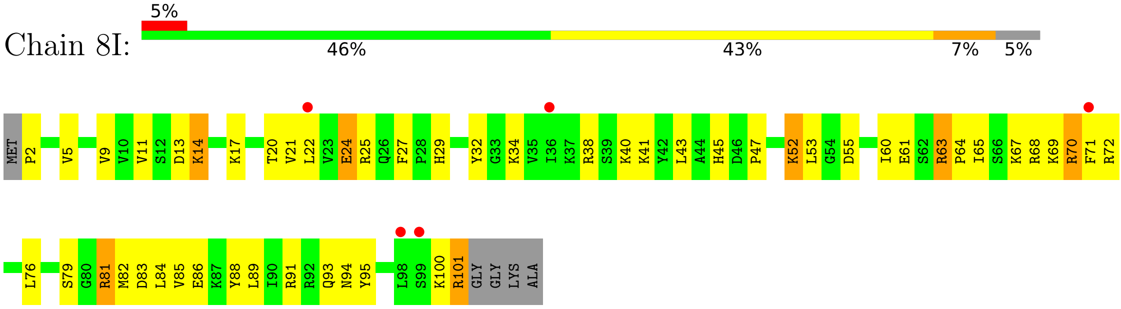


- Molecule 17: 30S ribosomal protein S17

Chain 8I:



- Molecule 17: 30S ribosomal protein S17

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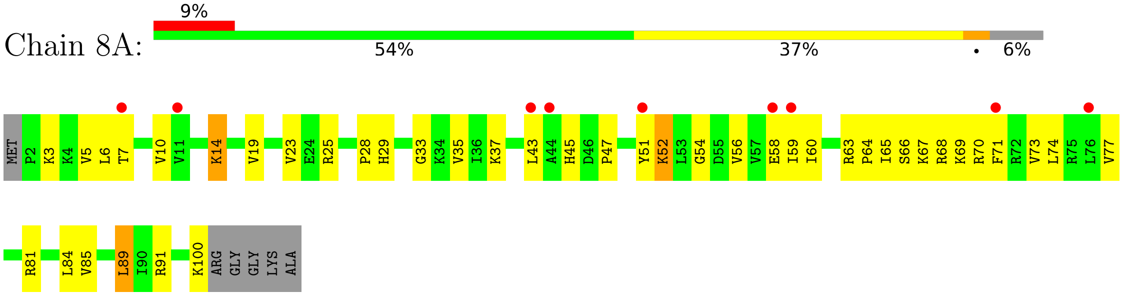

- Molecule 18: 30S ribosomal protein S18

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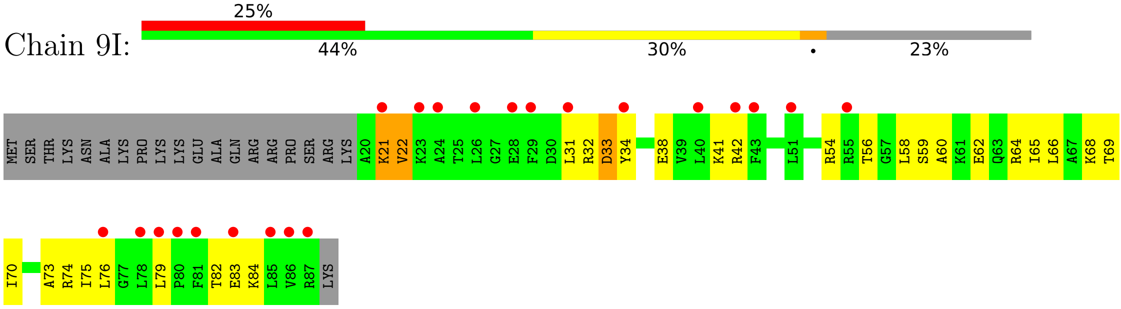

- Molecule 18: 30S ribosomal protein S18

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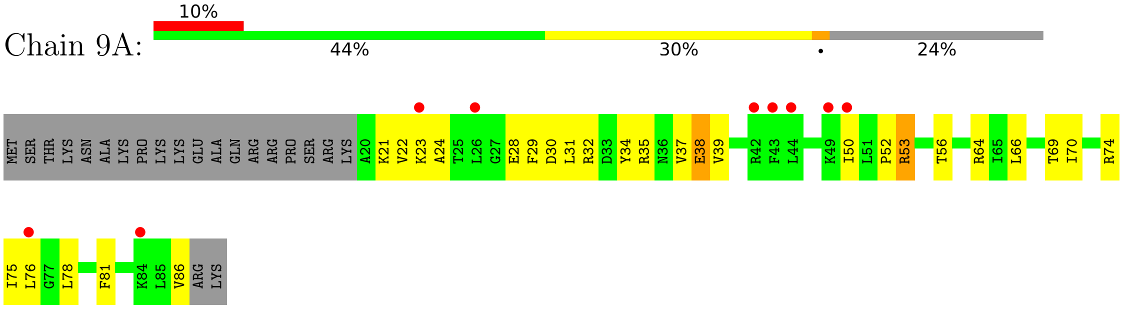

- Molecule 19: 30S ribosomal protein S19

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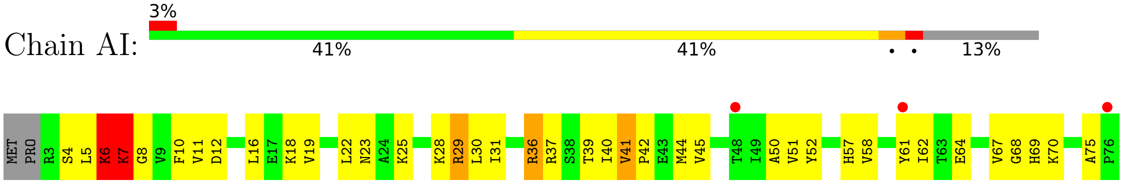

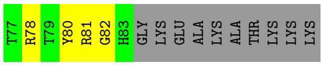

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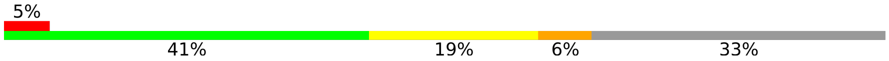

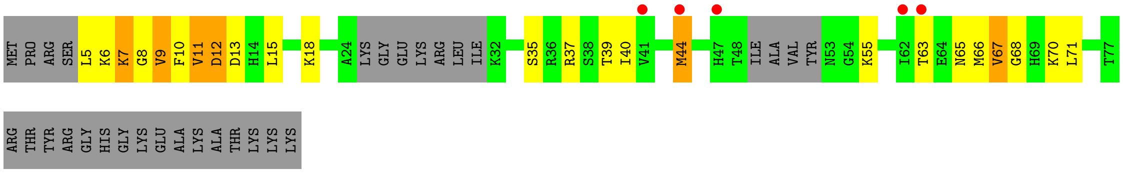

- Molecule 20: 30S ribosomal protein S20

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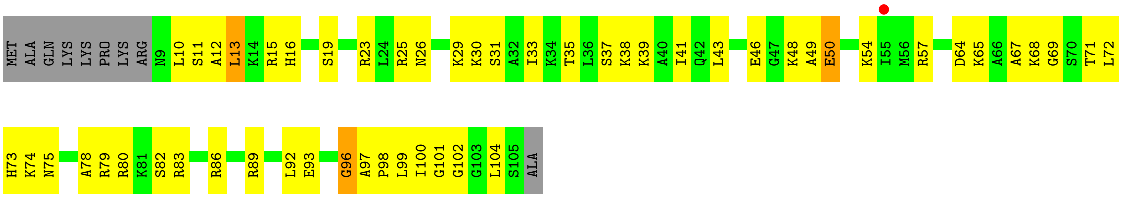

- Molecule 20: 30S ribosomal protein S20

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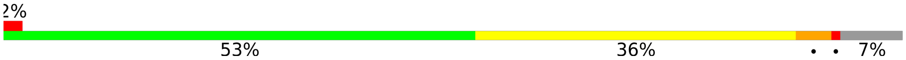
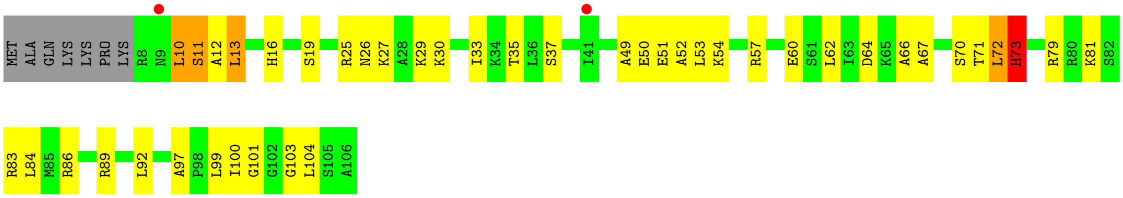
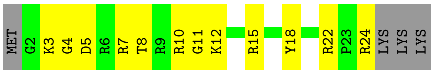




- Molecule 21: 30S ribosomal protein Thx

Chain 1F:



- Molecule 21: 30S ribosomal protein Thx

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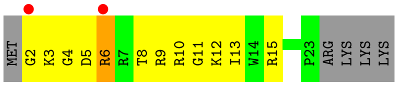
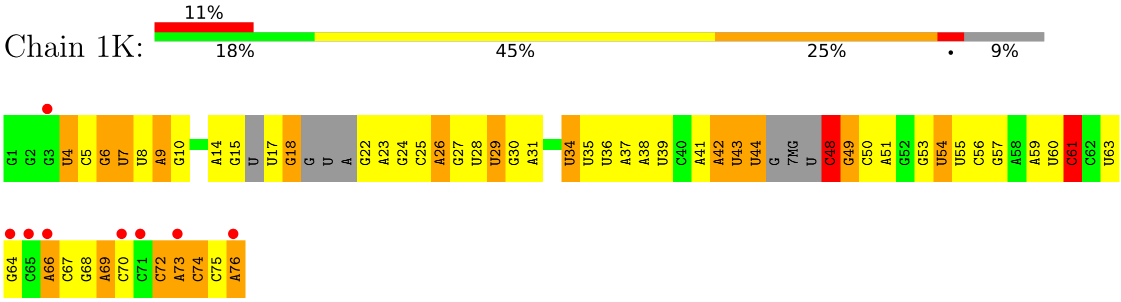


- Molecule 22: tRNALys



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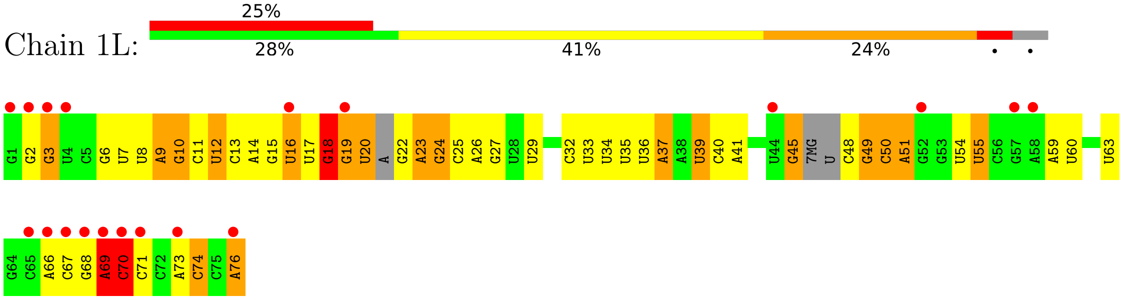
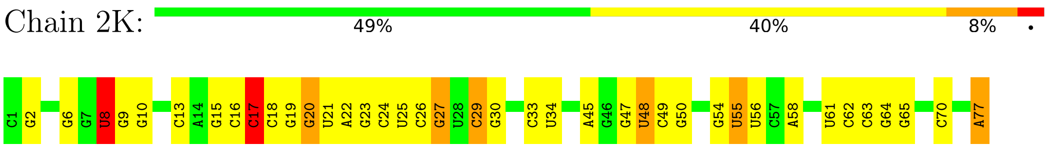
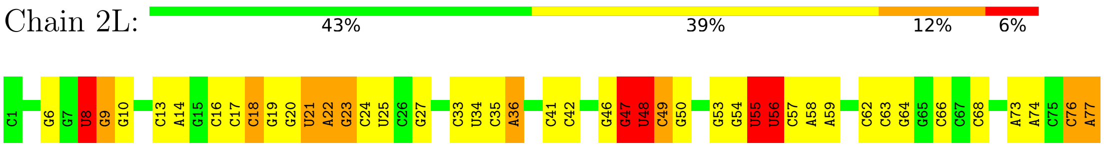


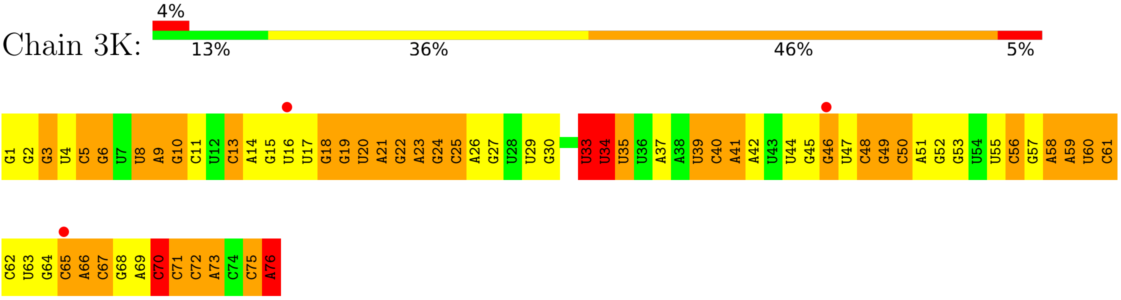
- Molecule 23: E. coli tRNAfMet



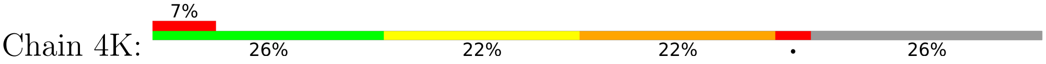
- Molecule 23: E. coli tRNAfMet

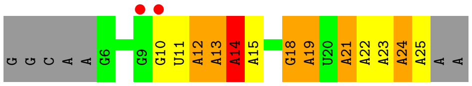


- Molecule 24: tRNALys

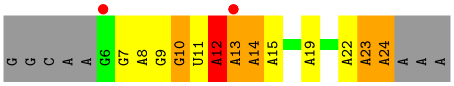


- Molecule 25: mRNA

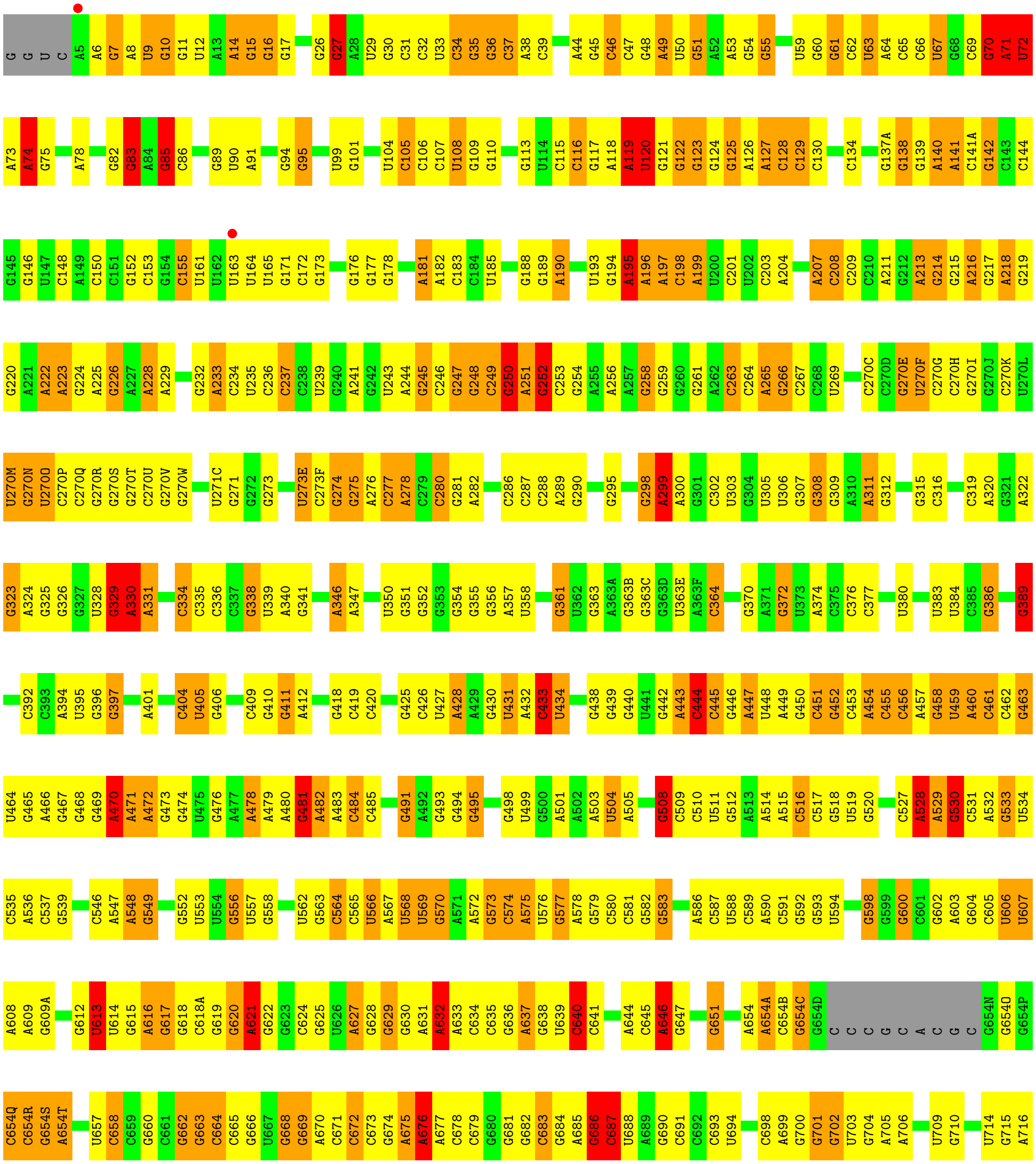


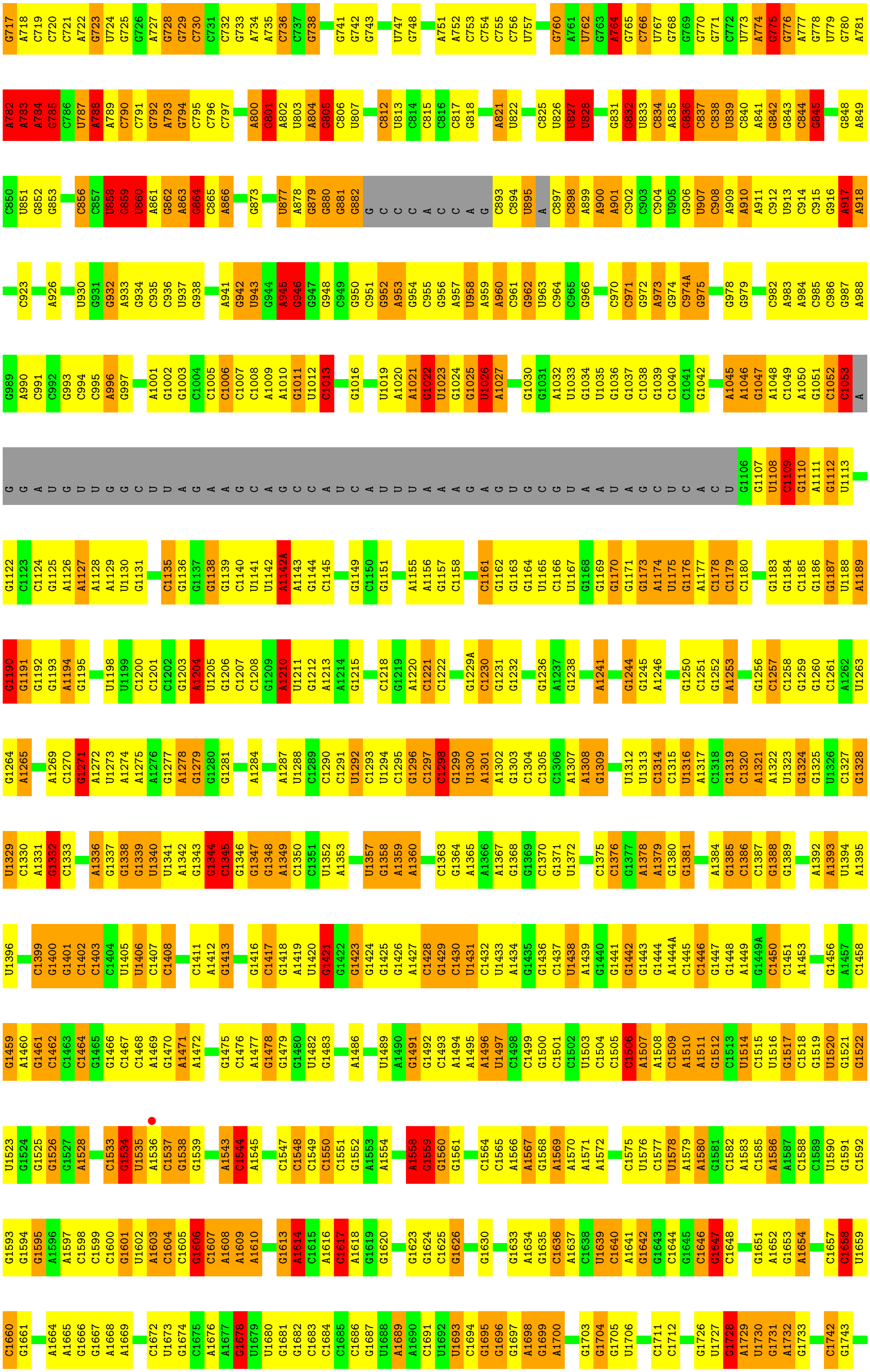


- Molecule 25: mRNA



- Molecule 26: 23S rRNA

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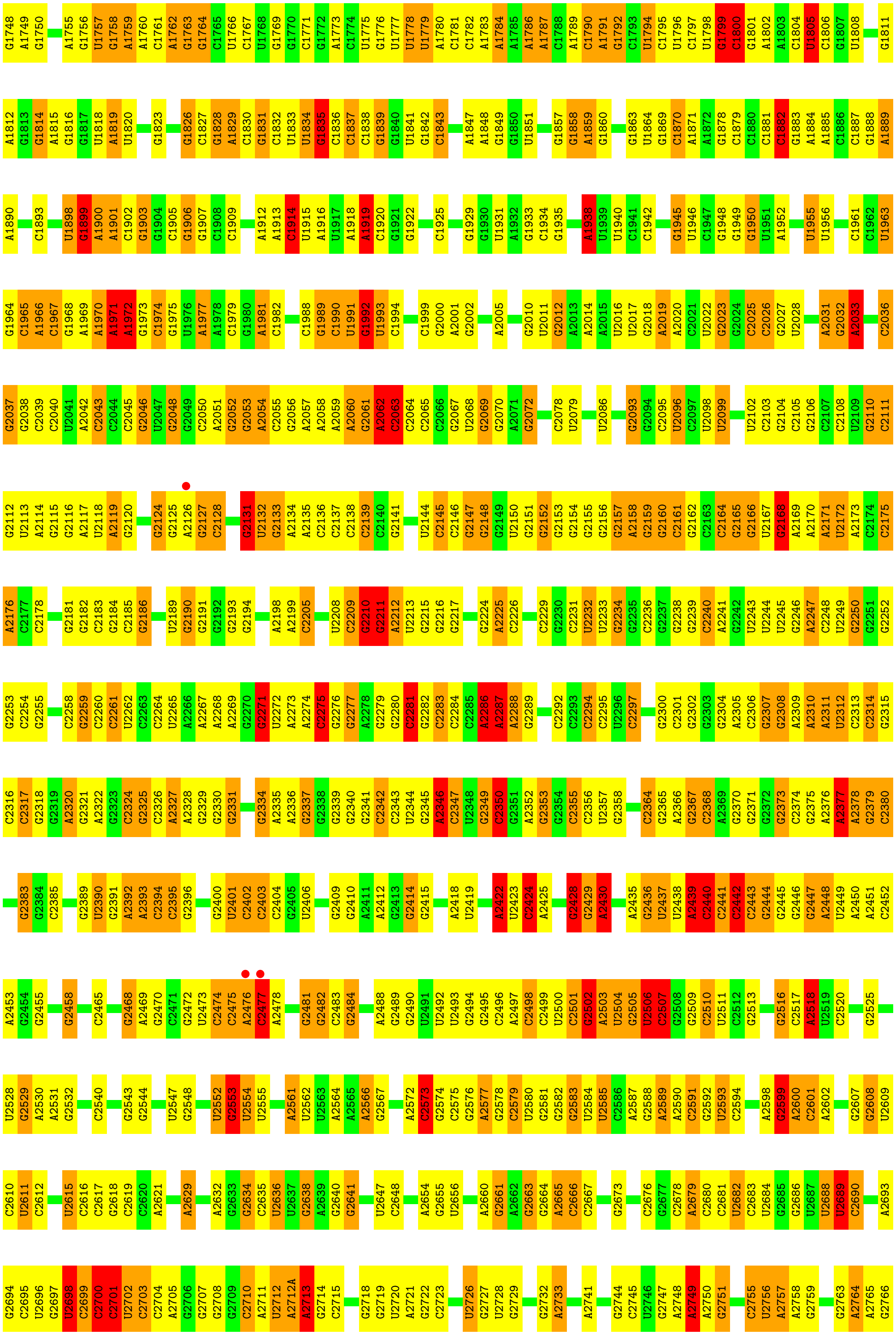
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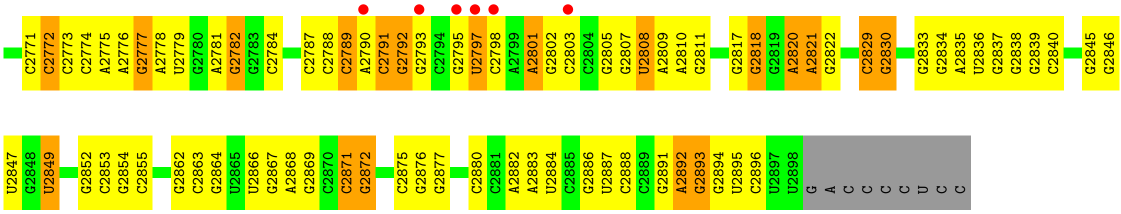
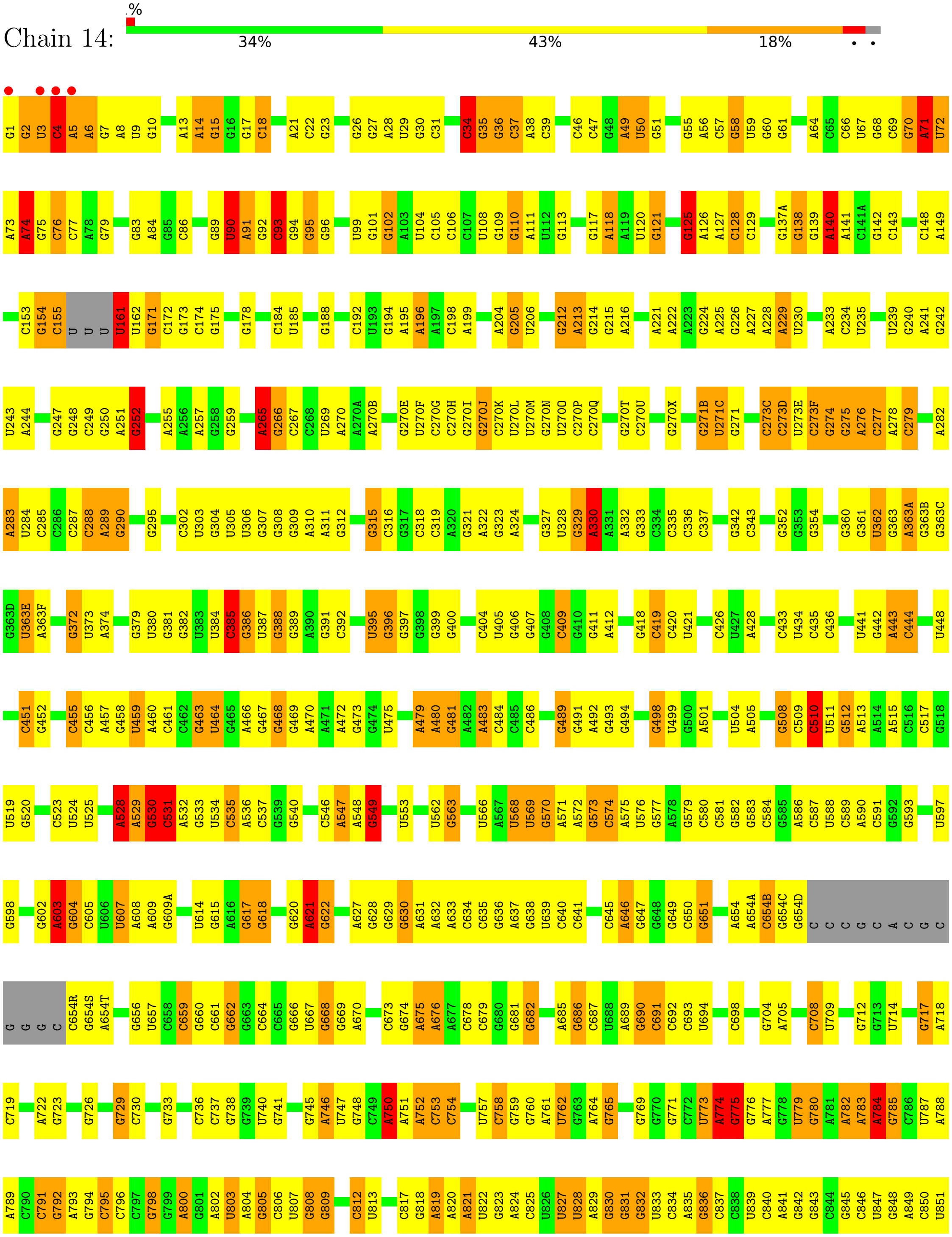
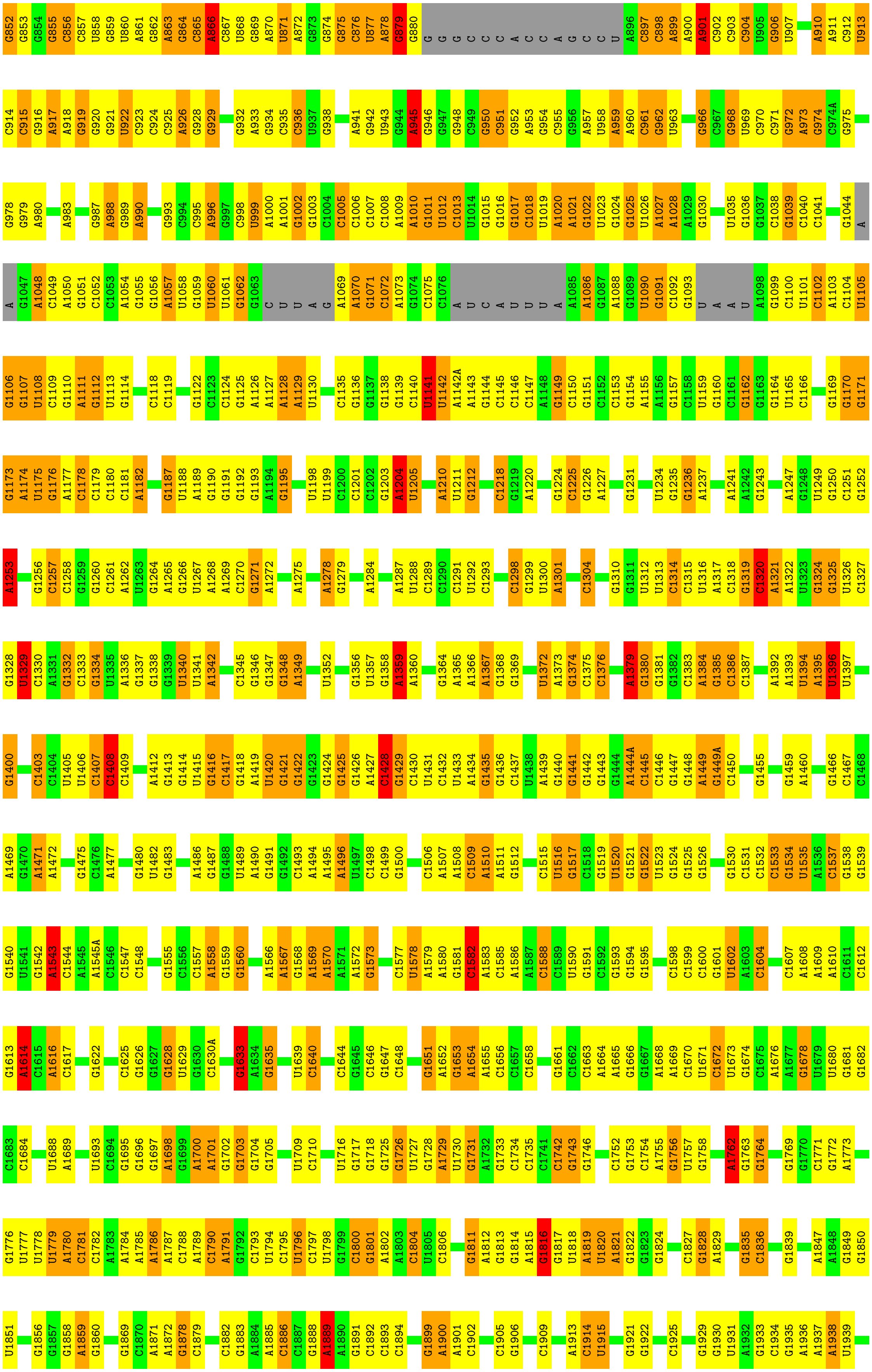


- Molecule 26: 23S rRNA

Chain 14:

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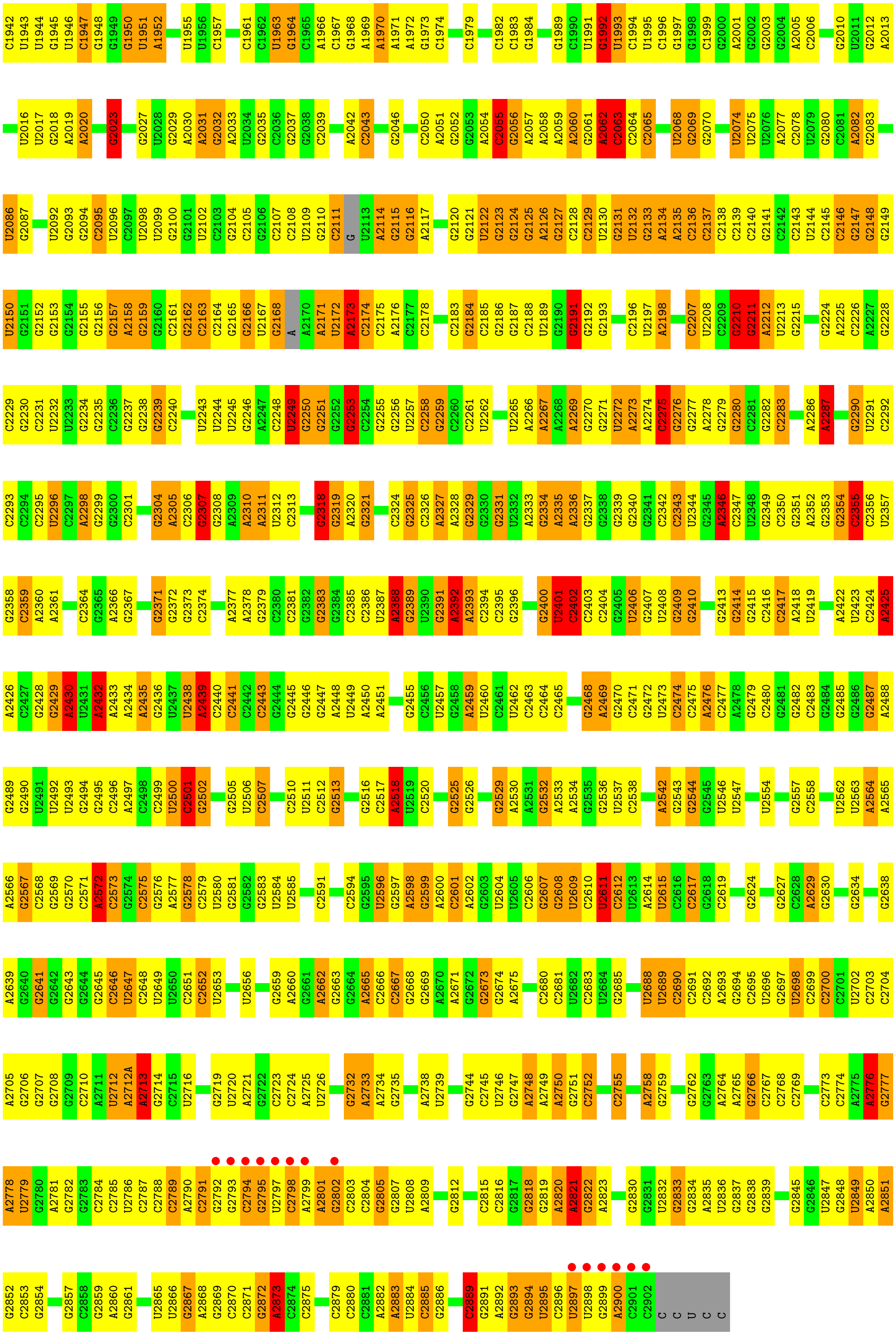
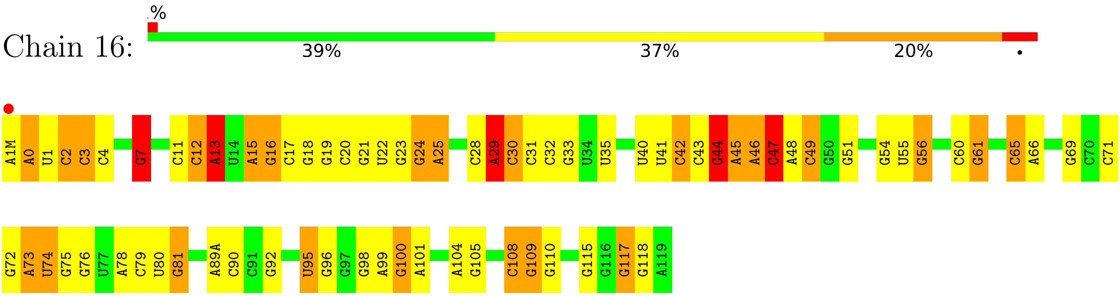


- Molecule 27: 5S rRNA

Chain 16:



- Molecule 27: 5S rRNA

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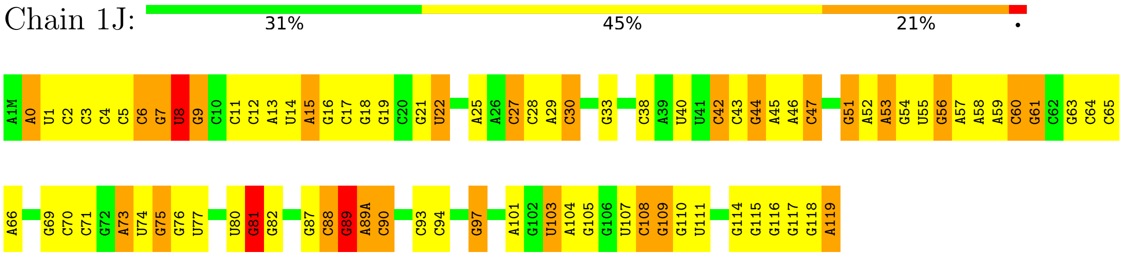
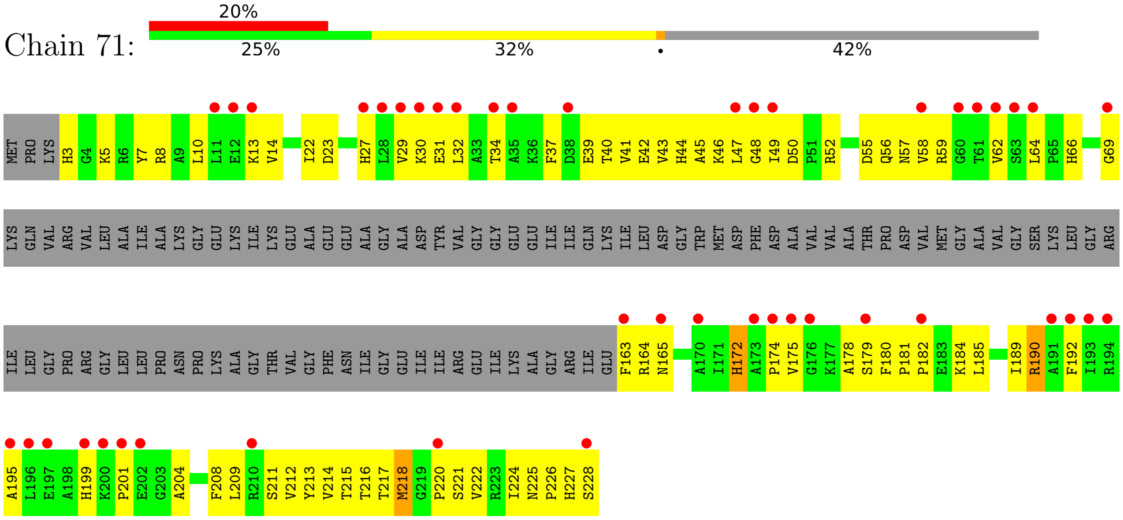


- Molecule 28: 50S ribosomal protein L1

Chain 71:



- Molecule 28: 50S ribosomal protein L1

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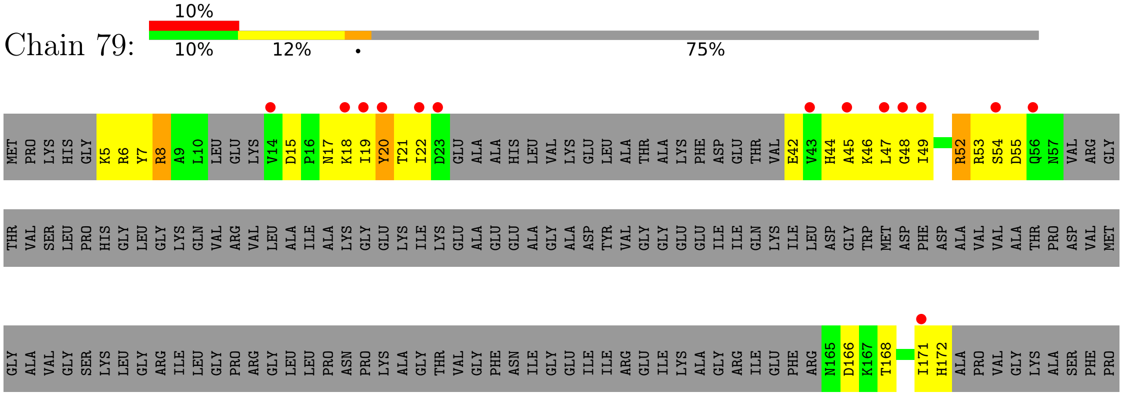
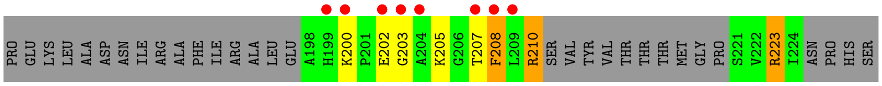
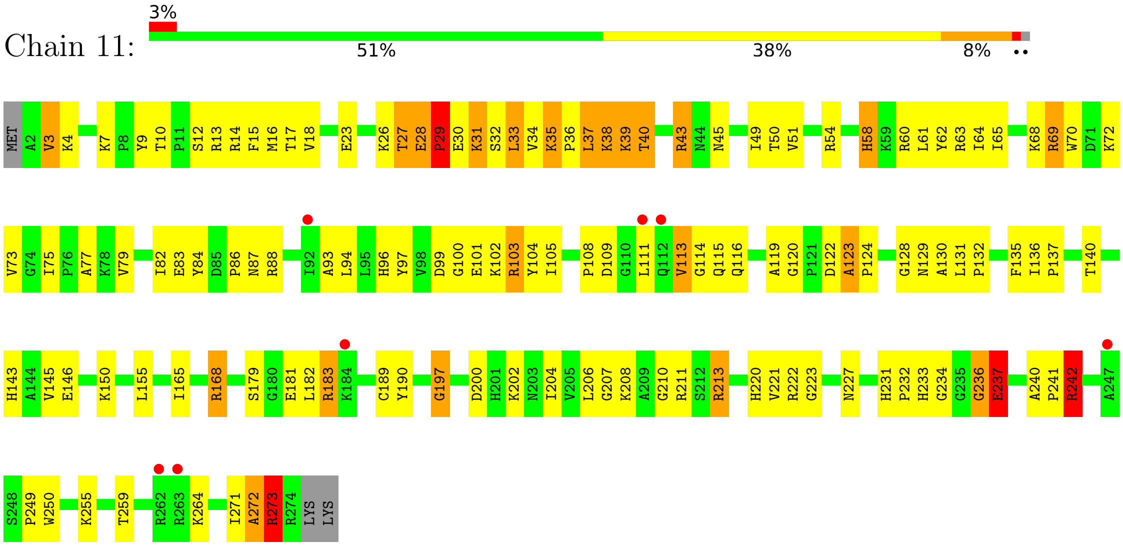
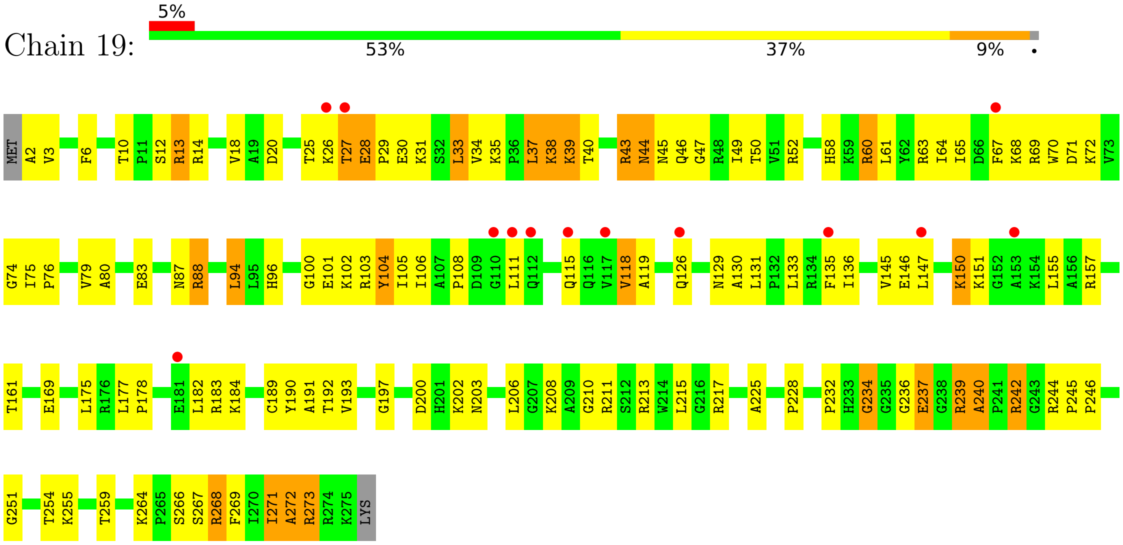




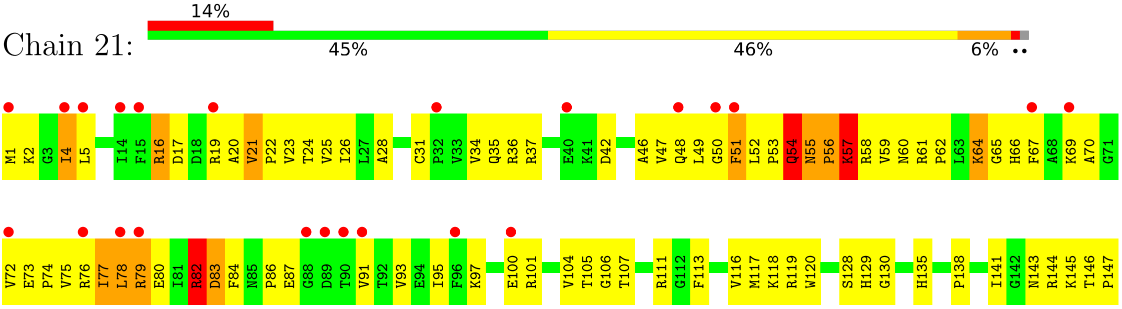
- Molecule 29: 50S ribosomal protein L2

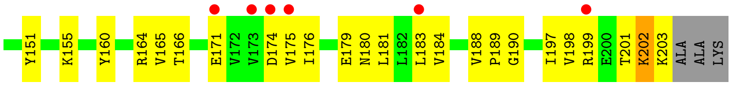


- Molecule 29: 50S ribosomal protein L2



- Molecule 30: 50S ribosomal protein L3





- Molecule 30: 50S ribosomal protein L3

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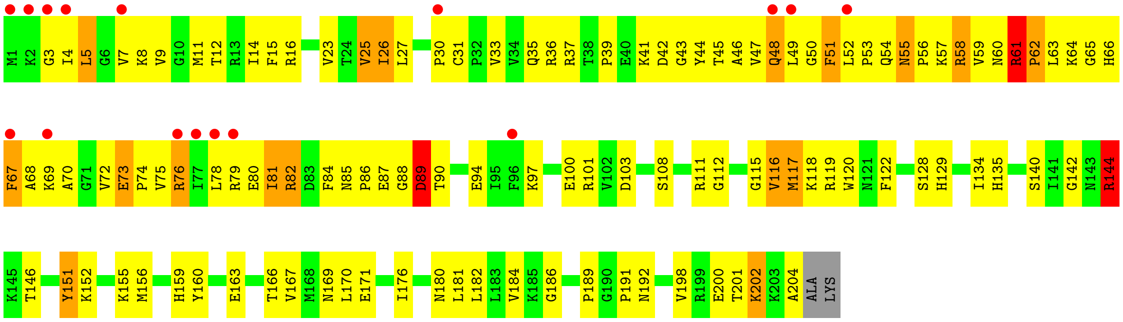
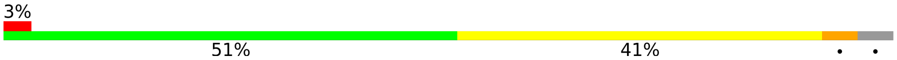
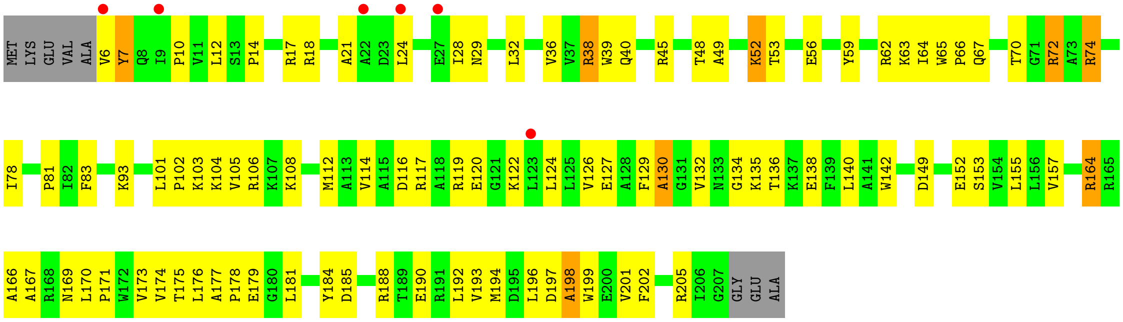


- Molecule 31: 50S ribosomal protein L4

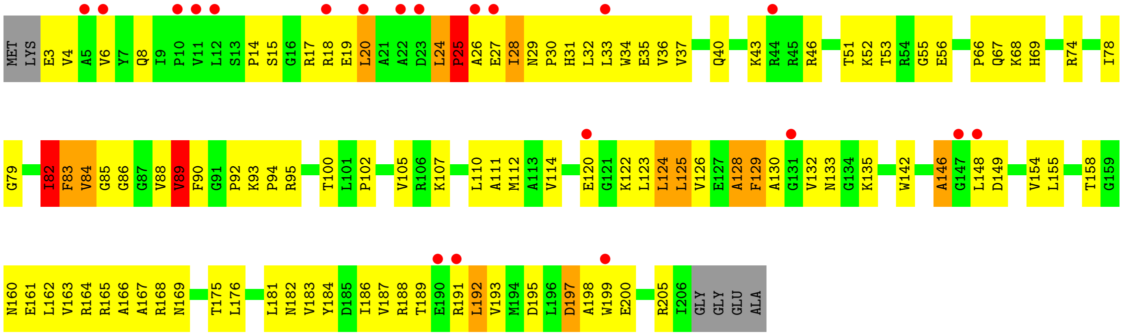
Chain 31:





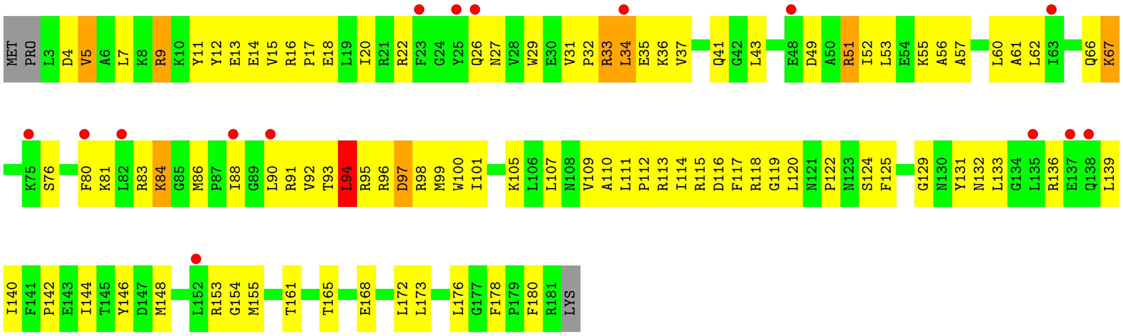
- Molecule 31: 50S ribosomal protein L4

Chain 39:



- Molecule 32: 50S ribosomal protein L5

Chain 41:



- Molecule 32: 50S ribosomal protein L5

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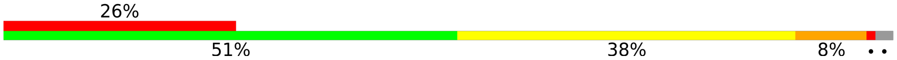
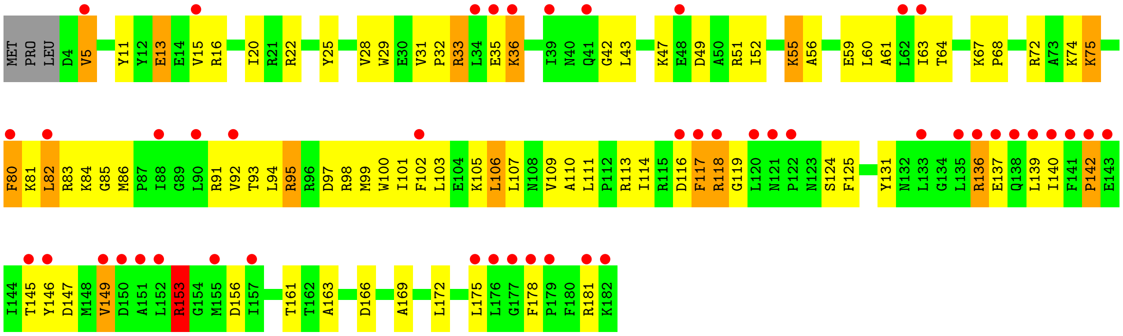
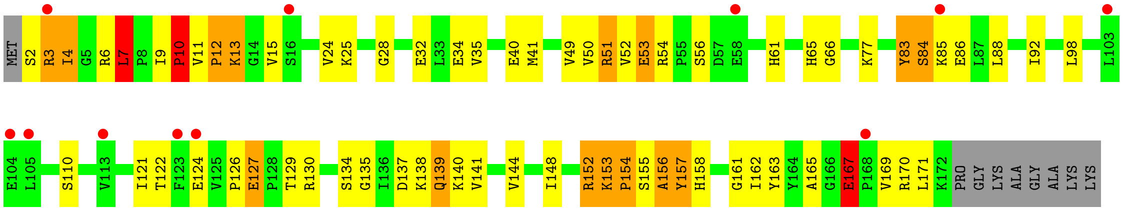




- Molecule 33: 50S ribosomal protein L6

Chain 51:



- Molecule 33: 50S ribosomal protein L6

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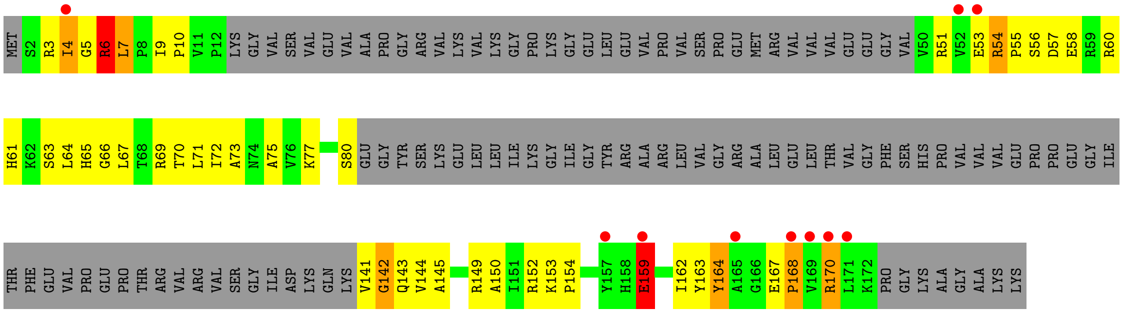
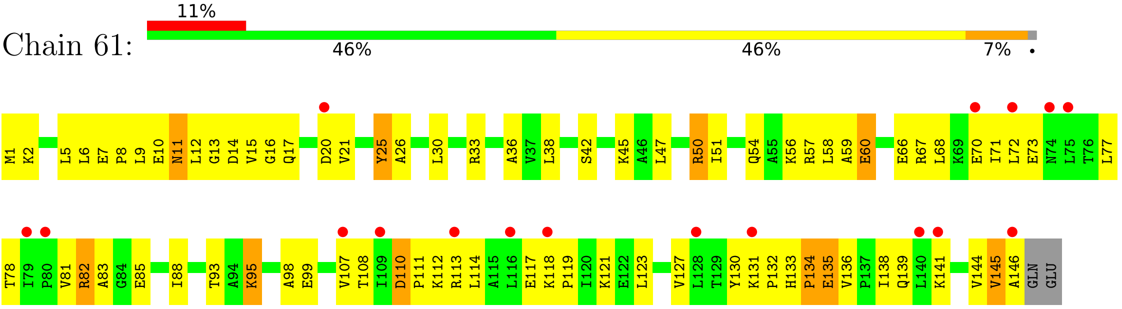
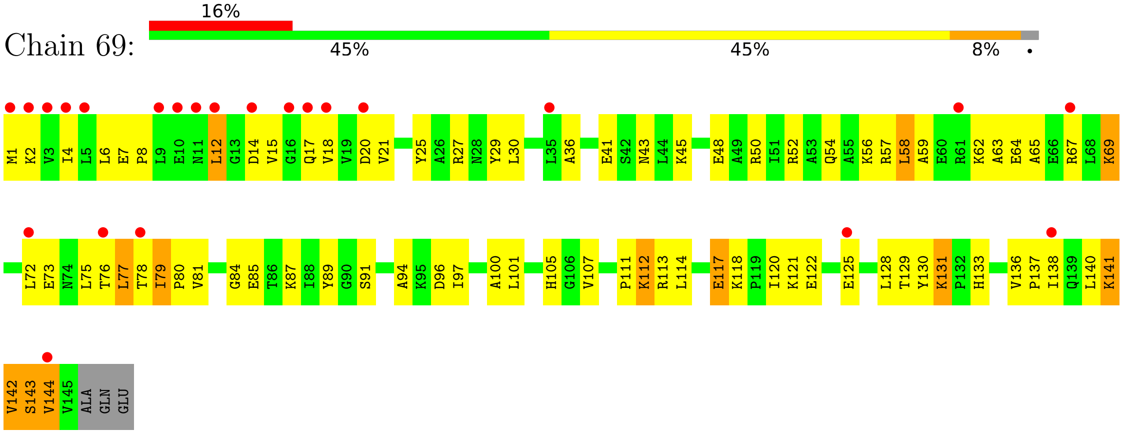


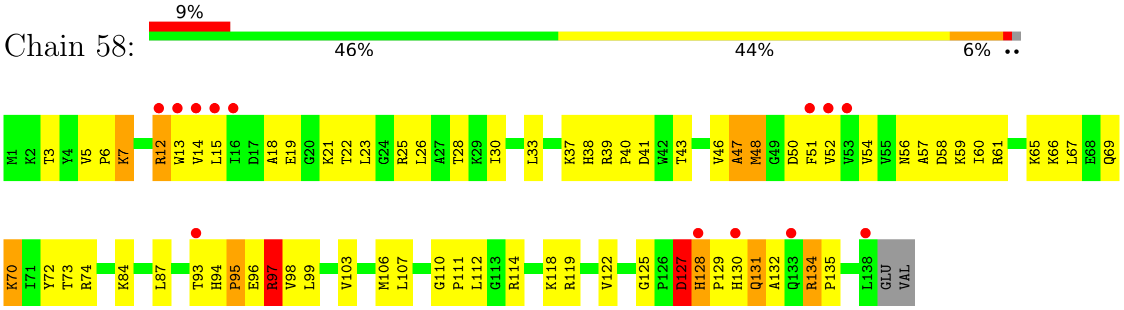
- Molecule 34: 50S ribosomal protein L9



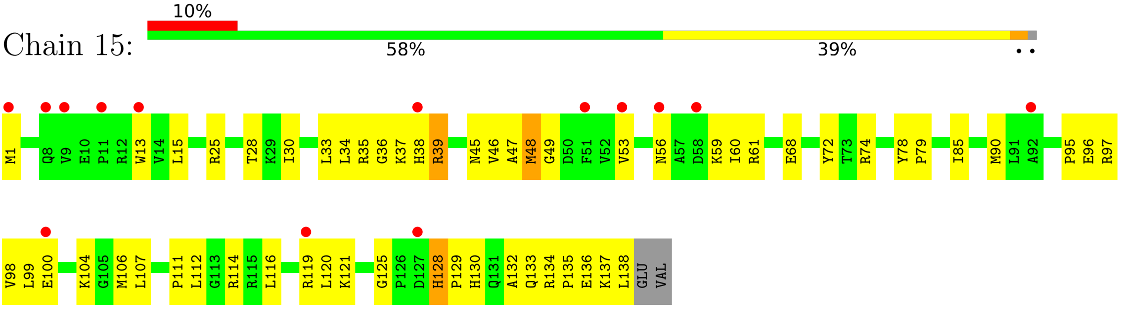
- Molecule 34: 50S ribosomal protein L9



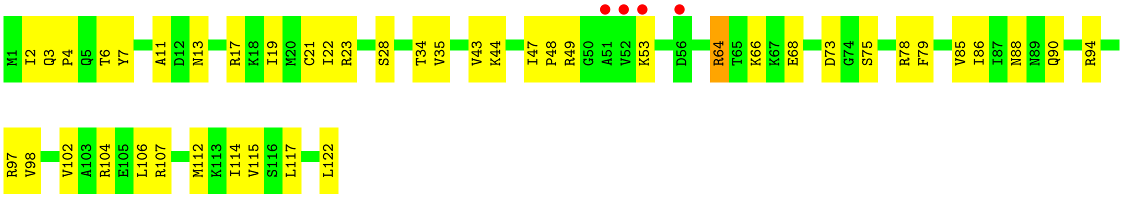
- Molecule 35: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L13

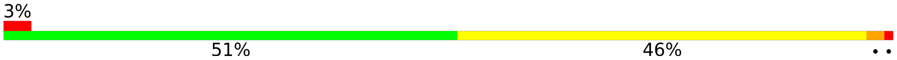


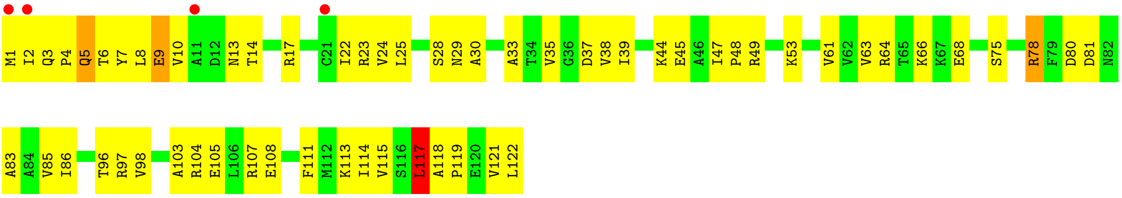
- Molecule 36: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L14

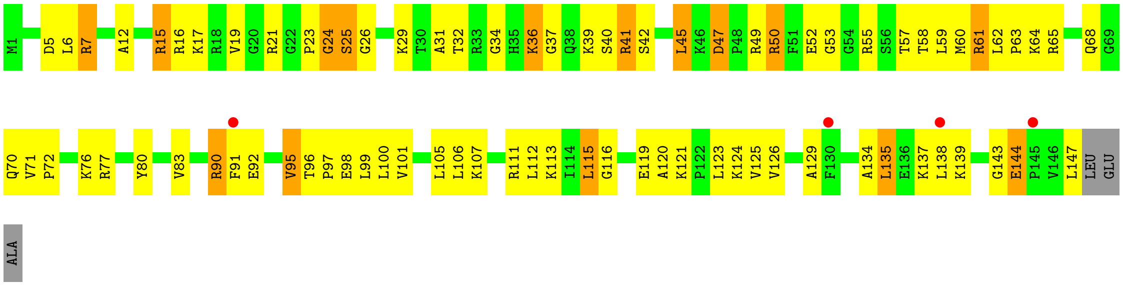
Chain 25:





- Molecule 37: 50S ribosomal protein L15

Chain 78:



- Molecule 37: 50S ribosomal protein L15

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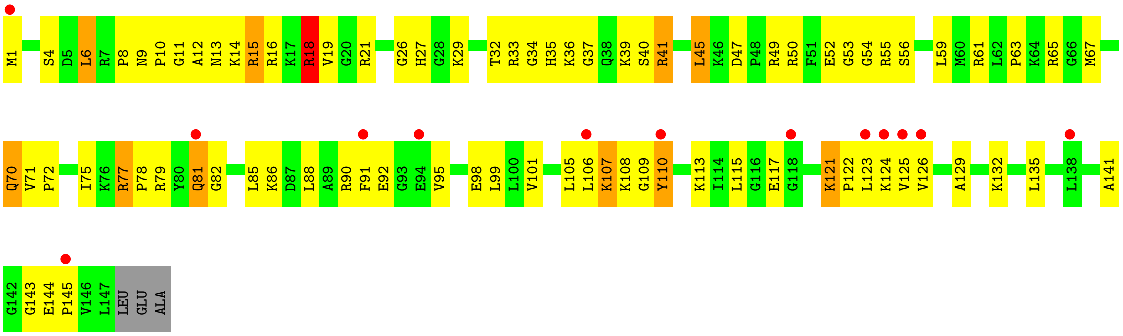
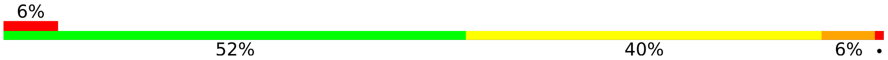
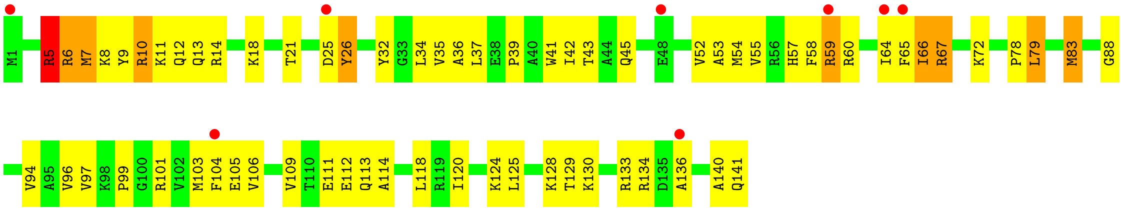


- Molecule 38: 50S ribosomal protein L16

Chain 88:





- Molecule 38: 50S ribosomal protein L16

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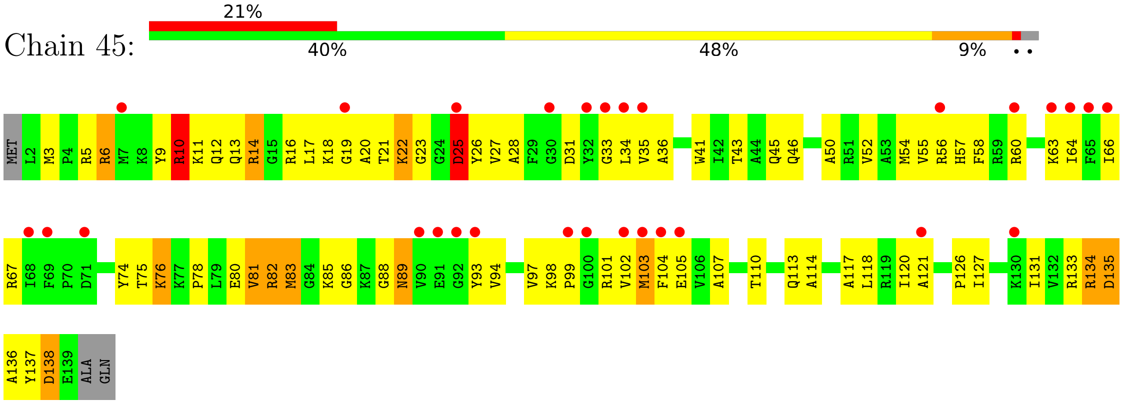
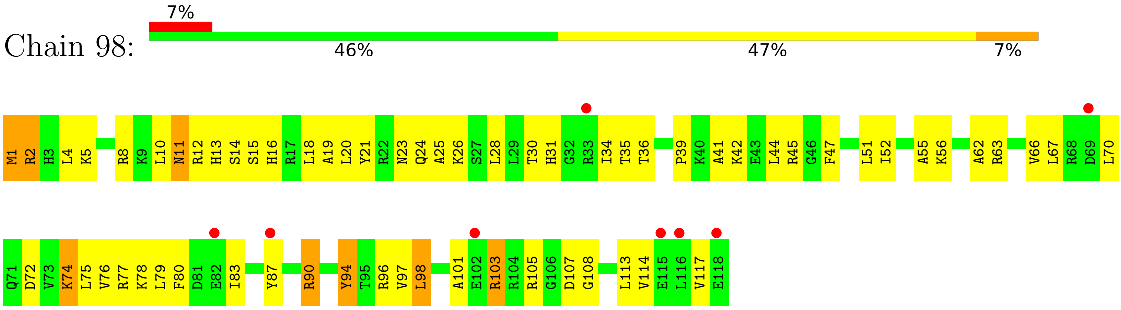


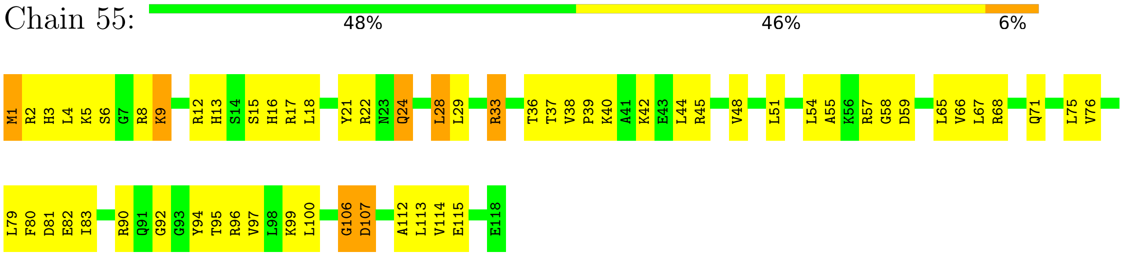
- Molecule 39: 50S ribosomal protein L17

Chain 98:



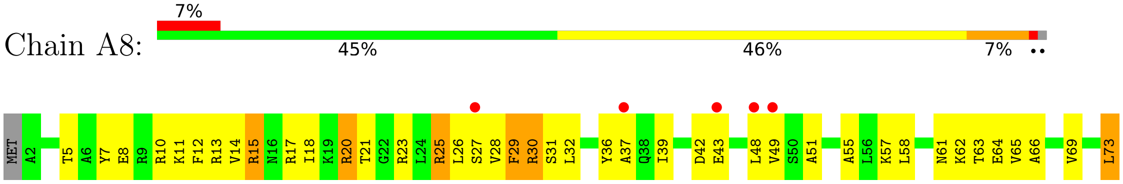
- Molecule 39: 50S ribosomal protein L17

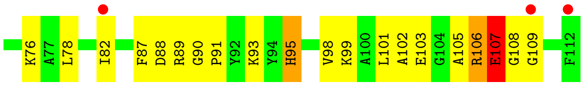
Chain 55:



- Molecule 40: 50S ribosomal protein L18

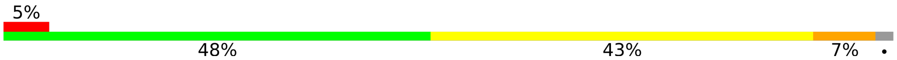
Chain A8:

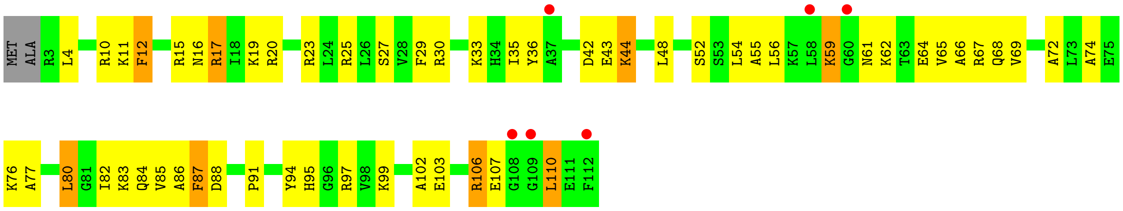




- Molecule 40: 50S ribosomal protein L18

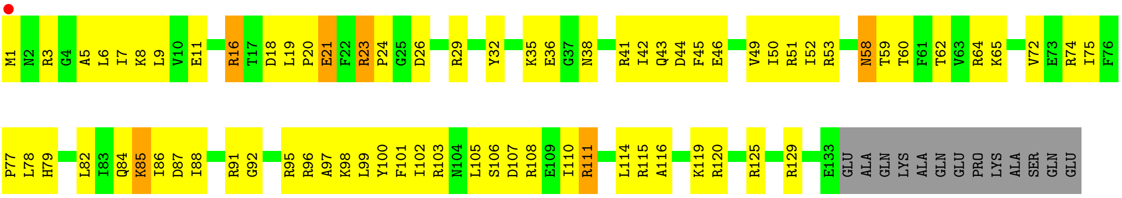
Chain 65:





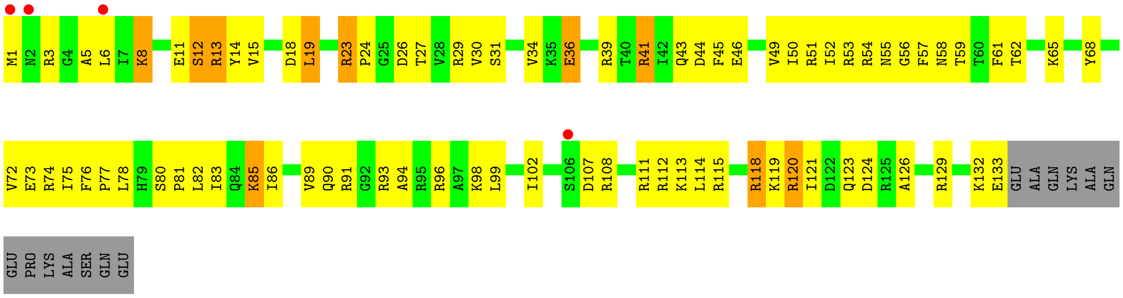
- Molecule 41: 50S ribosomal protein L19

Chain B8:



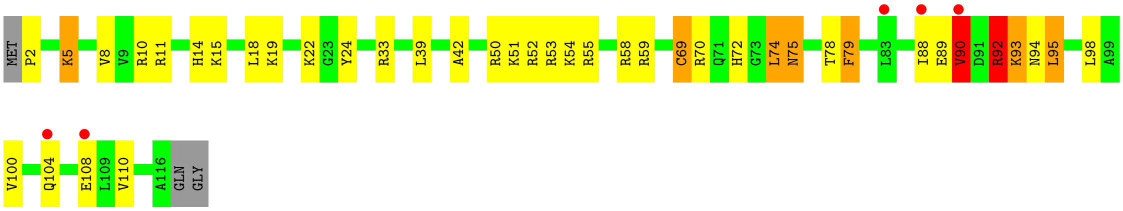
- Molecule 41: 50S ribosomal protein L19

Chain 75:



- Molecule 42: 50S ribosomal protein L20

Chain C8:



- Molecule 42: 50S ribosomal protein L20

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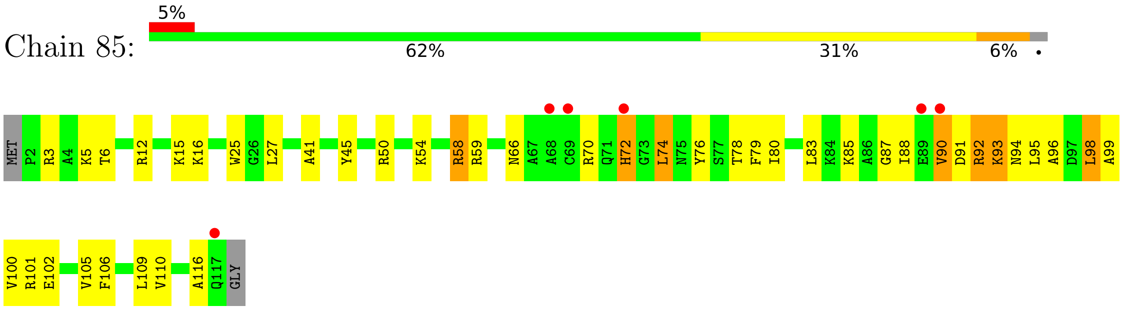
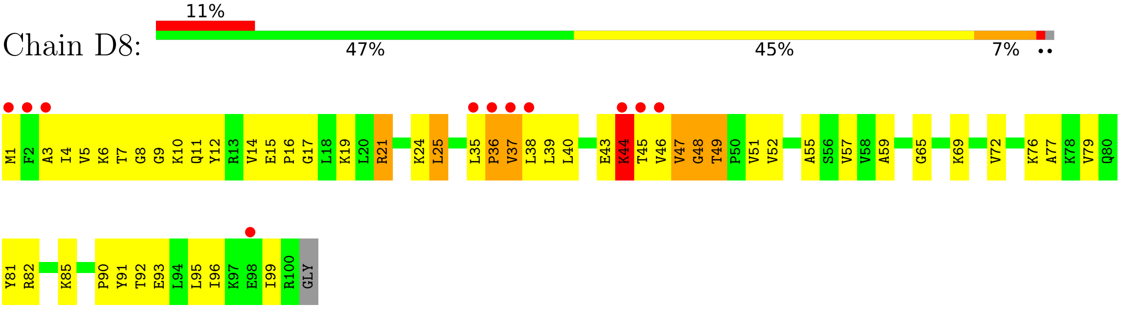


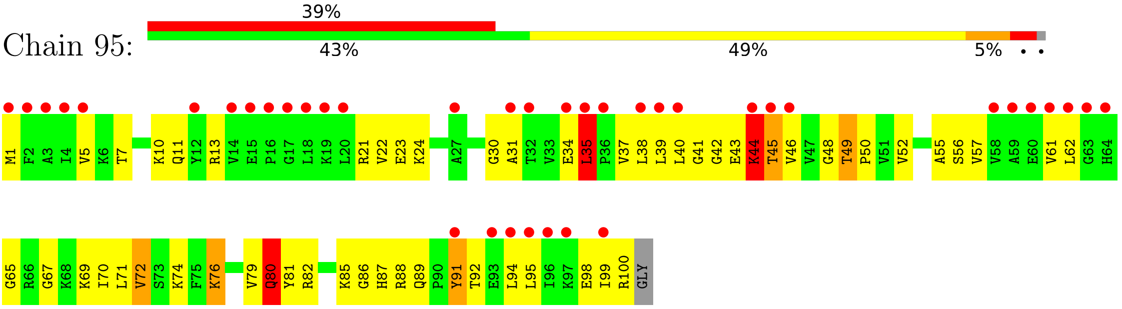
- Molecule 43: 50S ribosomal protein L21

Chain D8:



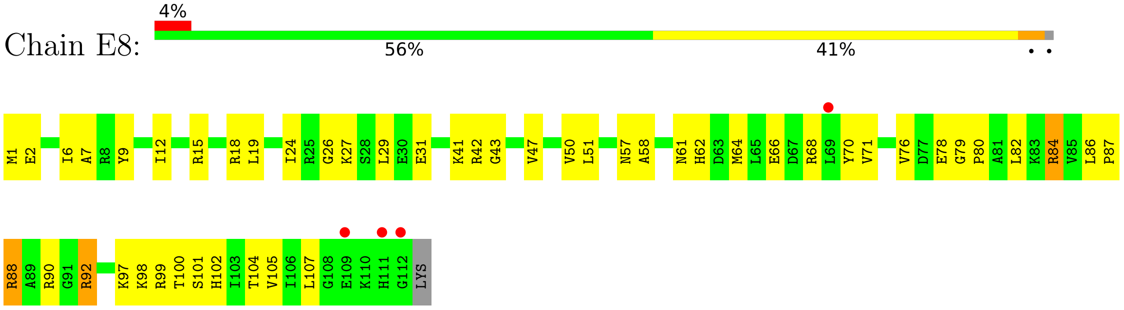
- Molecule 43: 50S ribosomal protein L21

Chain 95:



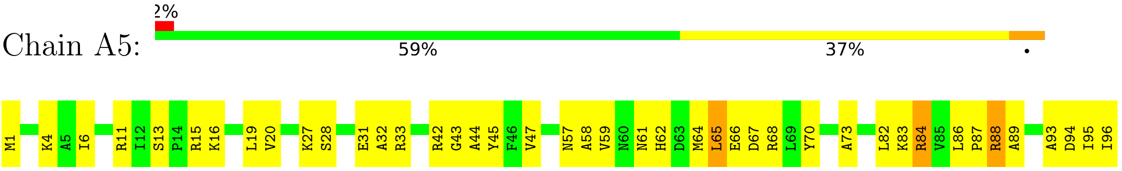
- Molecule 44: 50S ribosomal protein L22

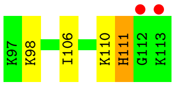
Chain E8:



- Molecule 44: 50S ribosomal protein L22

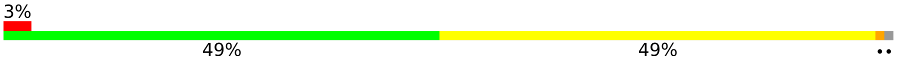
Chain A5:

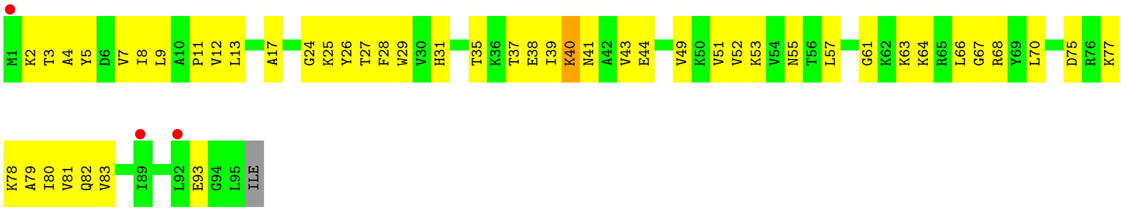




- Molecule 45: 50S ribosomal protein L23

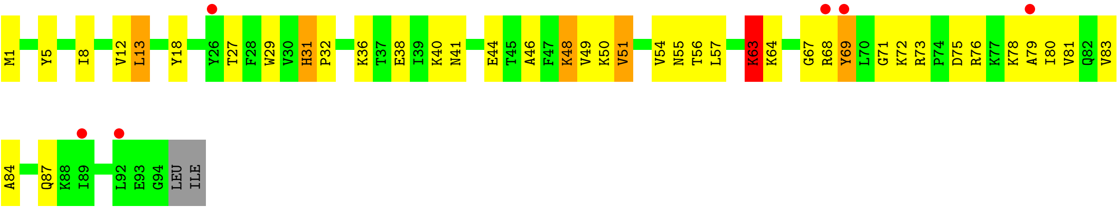
Chain F8:





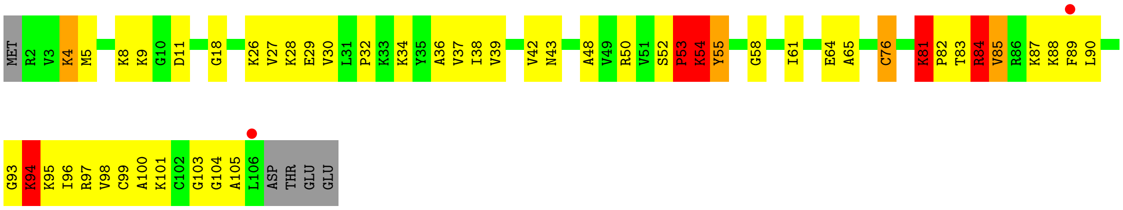
- Molecule 45: 50S ribosomal protein L23

Chain B5:



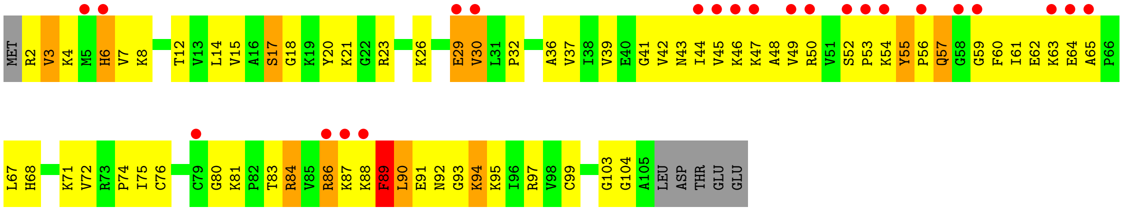
- Molecule 46: 50S ribosomal protein L24

Chain G8:



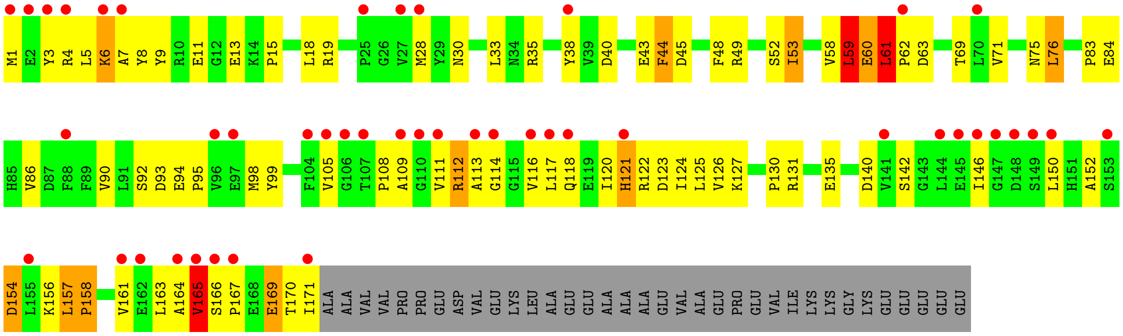
- Molecule 46: 50S ribosomal protein L24

Chain C5:



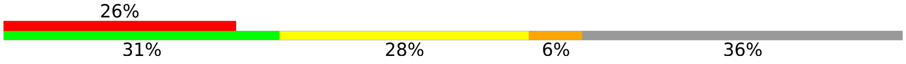
- Molecule 47: 50S ribosomal protein L25

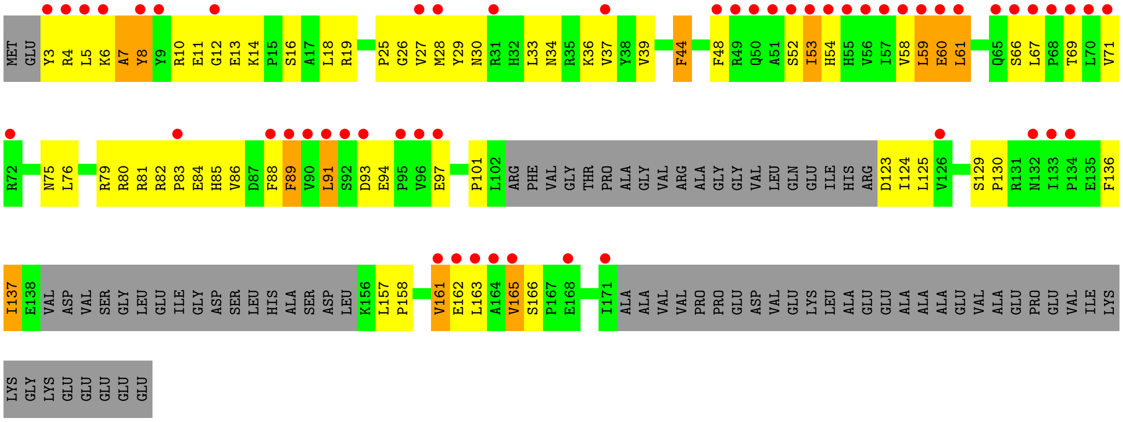
Chain H8:



- Molecule 47: 50S ribosomal protein L25

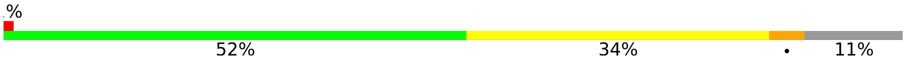
Chain D5:

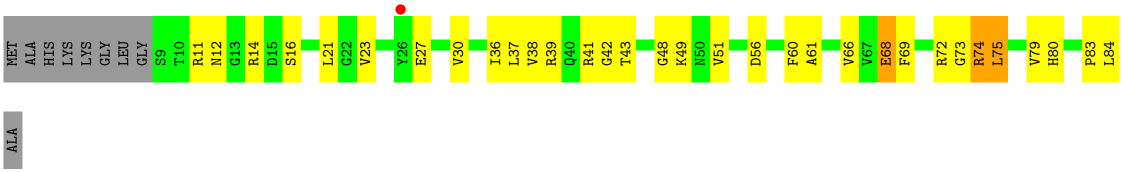




- Molecule 48: 50S ribosomal protein L27

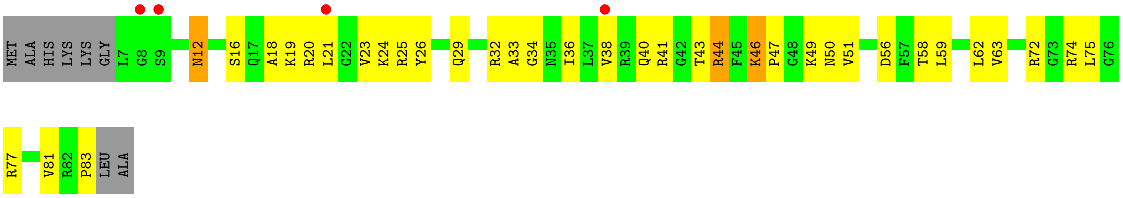
Chain I8:





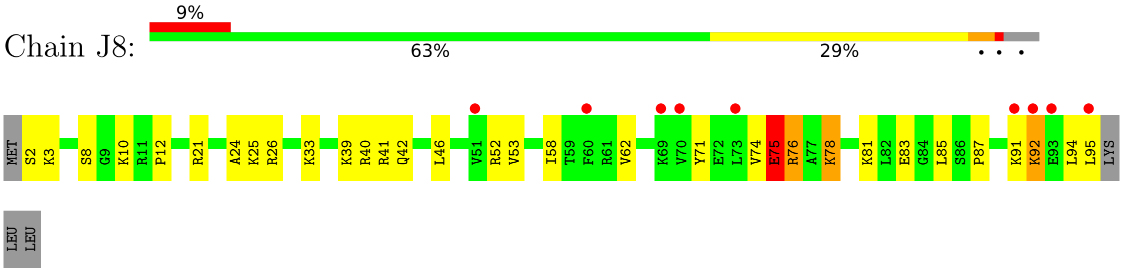
- Molecule 48: 50S ribosomal protein L27

Chain E5:



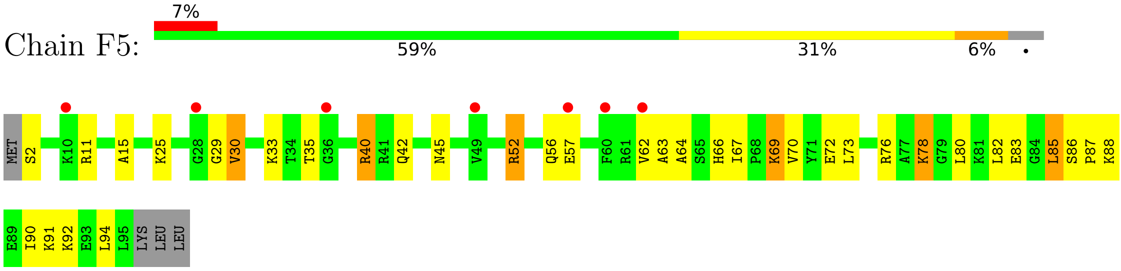
- Molecule 49: 50S ribosomal protein L28

Chain J8:



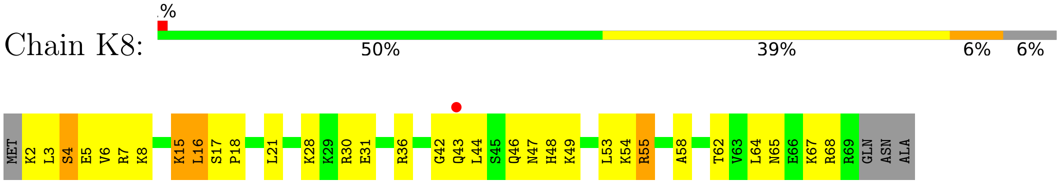
- Molecule 49: 50S ribosomal protein L28

Chain F5:



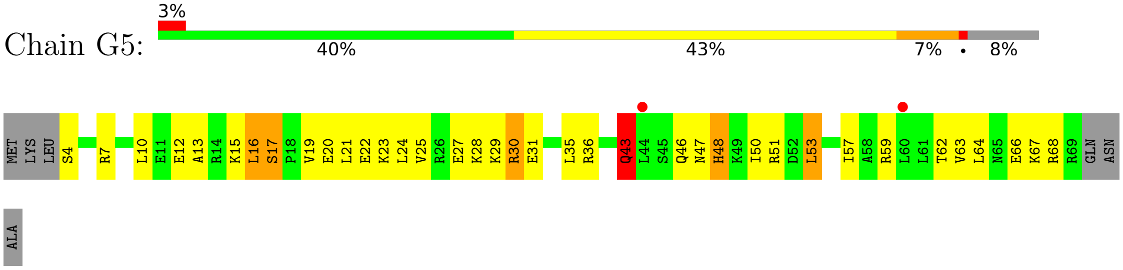
- Molecule 50: 50S ribosomal protein L29

Chain K8:



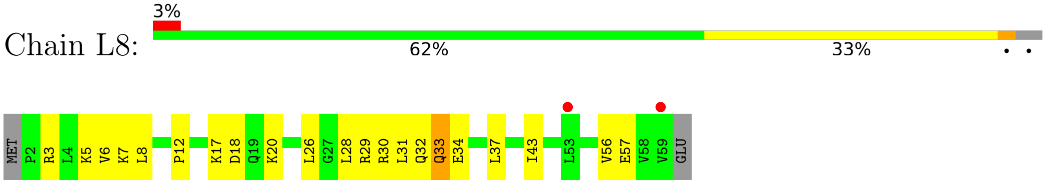
- Molecule 50: 50S ribosomal protein L29

Chain G5:



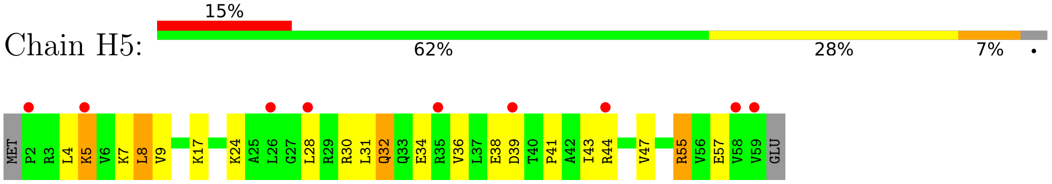
- Molecule 51: 50S ribosomal protein L30

Chain L8:



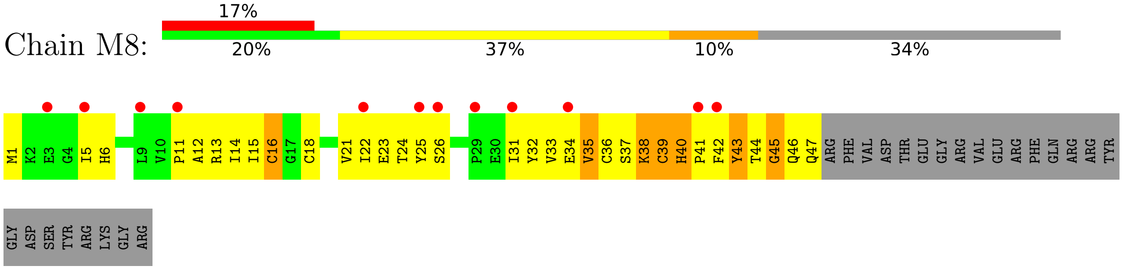
- Molecule 51: 50S ribosomal protein L30

Chain H5:



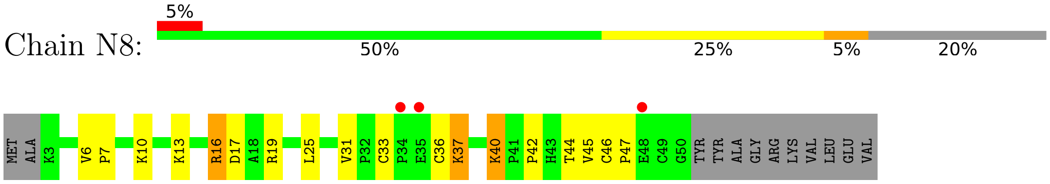
- Molecule 52: 50S ribosomal protein L31

Chain M8:



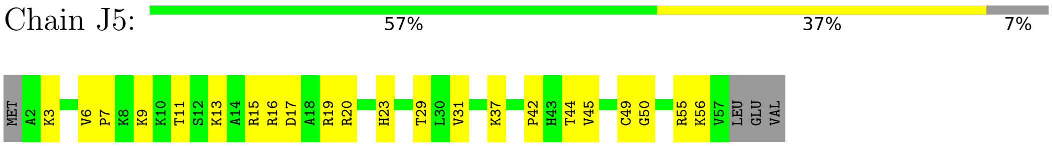
- Molecule 53: 50S ribosomal protein L32

Chain N8:



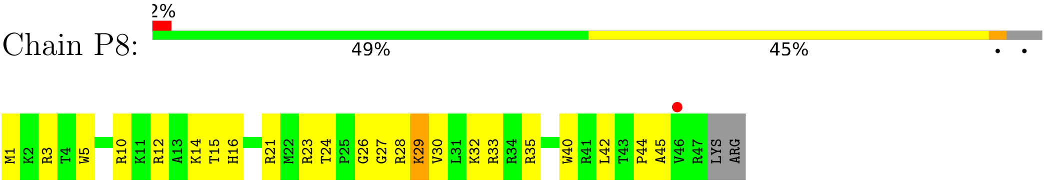
- Molecule 53: 50S ribosomal protein L32

Chain J5:



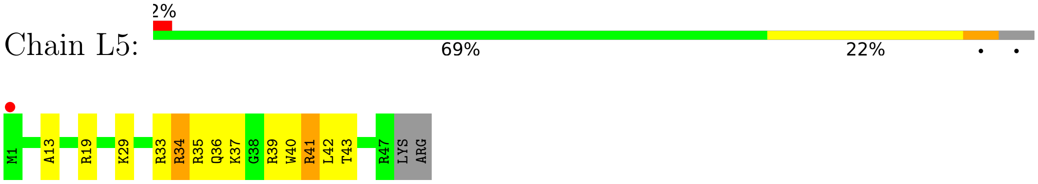
- Molecule 54: 50S ribosomal protein L34

Chain P8:



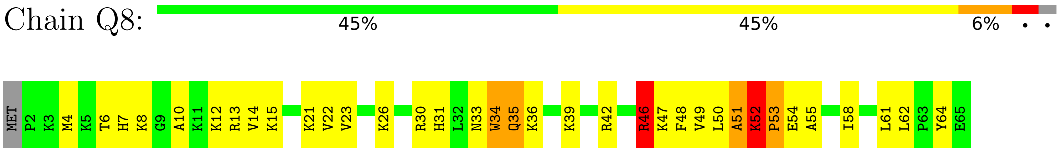
- Molecule 54: 50S ribosomal protein L34

Chain L5:



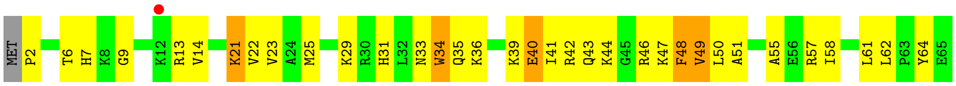
- Molecule 55: 50S ribosomal protein L35

Chain Q8:



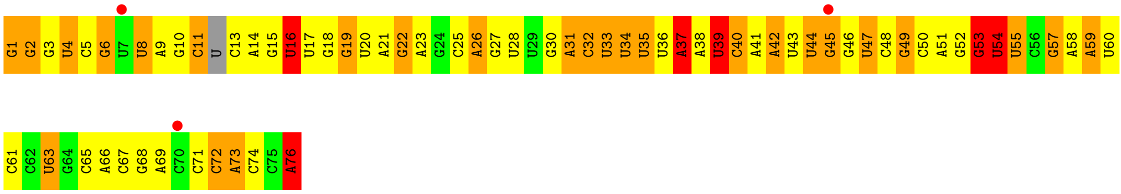
- Molecule 55: 50S ribosomal protein L35

Chain M5:



- Molecule 56: tRNALys

Chain 3L:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.70Å 449.50Å 620.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.17 – 3.15 152.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.17-3.15) 91.9 (152.17-3.15)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.247 0.194 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å^2)	80.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.9	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	296184	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.67	2/35994 (0.0%)	1.31	276/56171 (0.5%)
1	1G	0.58	0/36231	1.17	128/56544 (0.2%)
2	12	0.39	0/1752	0.71	0/2360
2	1E	0.46	1/1908 (0.1%)	0.69	3/2573 (0.1%)
3	22	0.39	0/1564	0.62	0/2109
3	2E	0.51	2/1629 (0.1%)	0.64	1/2195 (0.0%)
4	32	0.50	1/1732 (0.1%)	0.70	3/2318 (0.1%)
4	3E	0.54	2/1720 (0.1%)	0.69	0/2305
5	42	0.44	0/1150	0.66	1/1548 (0.1%)
5	4E	0.47	0/1158	0.68	1/1559 (0.1%)
6	52	0.52	0/855	0.66	1/1154 (0.1%)
6	5E	0.48	0/850	0.68	1/1147 (0.1%)
7	62	0.50	0/1127	0.67	0/1507
7	6E	0.39	0/1259	0.57	0/1686
8	72	0.36	0/1127	0.57	0/1517
8	7E	0.45	0/1135	0.72	2/1527 (0.1%)
9	82	0.37	0/971	0.71	0/1304
9	8E	0.42	0/1019	0.66	0/1367
10	1A	0.66	1/658 (0.2%)	0.63	0/885
10	1I	0.47	0/747	0.68	1/1006 (0.1%)
11	2A	0.38	0/850	0.58	0/1150
11	2I	0.40	0/838	0.62	0/1133
12	3A	0.44	0/972	0.70	0/1301
12	3I	0.55	0/972	0.78	1/1301 (0.1%)
13	4A	0.40	0/903	0.68	1/1211 (0.1%)
13	4I	0.49	0/952	0.67	0/1277
14	5A	0.40	0/495	0.71	1/657 (0.2%)
14	5I	0.45	0/500	0.73	1/664 (0.2%)
15	6A	0.42	0/744	0.58	0/992
15	6I	0.41	0/740	0.60	0/987
16	7A	0.48	1/721 (0.1%)	0.66	0/970
16	7I	0.44	0/716	0.69	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.41	0/836	0.59	0/1117
17	8I	0.48	2/847 (0.2%)	0.68	1/1131 (0.1%)
18	9A	0.44	0/549	0.63	0/732
18	9I	0.42	0/554	0.69	1/739 (0.1%)
19	AA	0.43	0/490	0.69	0/662
19	AI	0.49	0/668	0.73	0/899
20	BA	0.37	0/764	0.69	1/1007 (0.1%)
20	BI	0.40	0/748	0.76	1/986 (0.1%)
21	1B	0.44	0/192	0.63	0/252
21	1F	0.45	0/203	0.66	0/266
22	1K	0.58	0/1516	1.24	17/2350 (0.7%)
22	1L	0.48	0/1613	1.08	10/2504 (0.4%)
23	2K	0.74	0/1721	1.38	13/2682 (0.5%)
23	2L	0.63	0/1721	1.22	8/2682 (0.3%)
24	3K	0.49	0/1777	1.21	15/2767 (0.5%)
25	4K	0.77	0/495	1.38	6/771 (0.8%)
25	4L	0.69	0/470	1.27	2/732 (0.3%)
26	14	0.79	24/69023 (0.0%)	1.44	778/107740 (0.7%)
26	1H	0.88	50/68351 (0.1%)	1.58	1425/106700 (1.3%)
27	16	0.72	0/2928	1.46	42/4568 (0.9%)
27	1J	0.63	0/2928	1.30	18/4568 (0.4%)
28	71	0.34	0/1055	0.63	0/1425
28	79	0.31	0/459	0.57	0/608
29	11	0.75	6/2170 (0.3%)	0.93	4/2926 (0.1%)
29	19	0.58	0/2175	0.84	4/2933 (0.1%)
30	21	0.54	0/1591	0.86	2/2146 (0.1%)
30	29	0.68	5/1596 (0.3%)	1.00	7/2153 (0.3%)
31	31	0.55	0/1620	0.79	0/2194
31	39	0.48	0/1637	0.78	2/2218 (0.1%)
32	41	0.43	0/1481	0.74	1/1994 (0.1%)
32	49	0.53	3/1482 (0.2%)	0.72	1/1994 (0.1%)
33	51	0.56	1/1337 (0.1%)	0.85	4/1809 (0.2%)
33	59	0.50	1/582 (0.2%)	0.77	1/783 (0.1%)
34	61	0.42	0/1151	0.77	2/1558 (0.1%)
34	69	0.49	1/1146 (0.1%)	0.76	3/1551 (0.2%)
35	15	0.40	0/1131	0.65	1/1525 (0.1%)
35	58	0.49	1/1131 (0.1%)	0.73	1/1525 (0.1%)
36	25	0.56	2/942 (0.2%)	0.72	1/1269 (0.1%)
36	68	0.48	0/942	0.72	0/1269
37	35	0.61	1/1139 (0.1%)	0.90	1/1514 (0.1%)
37	78	0.54	0/1139	0.89	4/1514 (0.3%)
38	45	0.72	4/1120 (0.4%)	0.84	1/1498 (0.1%)
38	88	0.72	2/1134 (0.2%)	0.90	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	55	0.50	0/981	0.80	1/1312 (0.1%)
39	98	0.45	0/981	0.80	1/1312 (0.1%)
40	65	0.49	0/886	0.83	2/1180 (0.2%)
40	A8	0.56	0/884	0.76	0/1178
41	75	0.61	3/1123 (0.3%)	0.72	0/1500
41	B8	0.62	2/1123 (0.2%)	0.76	1/1500 (0.1%)
42	85	0.49	0/977	0.70	0/1301
42	C8	0.55	1/968 (0.1%)	0.76	1/1289 (0.1%)
43	95	0.57	0/785	0.85	2/1052 (0.2%)
43	D8	0.52	0/785	0.81	2/1052 (0.2%)
44	A5	0.56	0/910	0.73	0/1220
44	E8	0.51	0/901	0.77	0/1209
45	B5	0.55	0/749	0.77	1/1007 (0.1%)
45	F8	0.60	0/757	0.81	2/1017 (0.2%)
46	C5	0.51	0/807	0.89	2/1076 (0.2%)
46	G8	0.68	2/809 (0.2%)	1.05	4/1080 (0.4%)
47	D5	0.49	0/1098	0.75	0/1487
47	H8	0.46	0/1403	0.75	2/1901 (0.1%)
48	E5	0.50	0/616	0.77	0/821
48	I8	0.75	2/614 (0.3%)	0.86	1/819 (0.1%)
49	F5	0.52	0/744	0.81	0/989
49	J8	0.59	0/744	0.83	1/989 (0.1%)
50	G5	0.52	0/560	0.75	0/741
50	K8	0.84	4/570 (0.7%)	0.86	0/755
51	H5	0.42	0/464	0.65	1/623 (0.2%)
51	L8	0.53	0/464	0.73	0/623
52	M8	0.41	0/375	0.86	2/507 (0.4%)
53	J5	0.49	0/448	0.70	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.54	0/409	0.84	1/540 (0.2%)
54	P8	0.62	0/409	0.88	0/540
55	M5	0.66	1/524 (0.2%)	0.81	1/691 (0.1%)
55	Q8	0.56	0/524	1.02	2/691 (0.3%)
56	3L	0.54	0/1729	1.28	17/2690 (0.6%)
All	All	0.70	128/317045 (0.0%)	1.28	2847/474982 (0.6%)

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	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	3
4	3E	0	1
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	4
13	4A	0	3
13	4I	0	2
14	5A	0	3
14	5I	0	1
16	7I	0	2
18	9I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	3
20	BI	0	1
29	11	0	7
29	19	0	5
30	21	0	8
30	29	0	7
31	31	0	2
31	39	0	8
32	41	0	1
32	49	0	6
33	51	0	5
33	59	0	5
34	61	0	4
34	69	0	3
35	58	0	2
37	35	0	4
37	78	0	4
38	45	0	4
39	55	0	1
40	65	0	1
40	A8	0	1
41	75	0	1
42	85	0	4
42	C8	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	95	0	3
43	D8	0	3
44	A5	0	1
45	F8	0	1
46	C5	0	3
46	G8	0	4
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	4
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	169

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	2572	A	N7-C5	24.38	1.53	1.39
26	14	2572	A	N9-C8	-21.02	1.21	1.37
26	14	2572	A	C5-C4	-18.45	1.25	1.38
26	14	2572	A	C5-C6	-15.84	1.26	1.41
26	1H	774	A	N9-C4	-12.29	1.30	1.37

The worst 5 of 2847 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	14	2572	A	N9-C4-C5	28.35	117.14	105.80
26	14	2572	A	C4-C5-C6	24.01	129.00	117.00
26	14	2572	A	C4-C5-N7	-20.90	100.25	110.70
26	1H	1899	G	N3-C4-N9	-19.20	114.48	126.00
26	14	2572	A	N7-C8-N9	18.60	123.10	113.80

There are no chirality outliers.

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
4	3E	82	ALA	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	16234	754	0
1	1G	32368	0	16343	752	1
2	12	1721	0	1758	119	0
2	1E	1874	0	1926	112	0
3	22	1541	0	1606	76	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1765	101	0
4	3E	1690	0	1738	92	0
5	42	1134	0	1200	69	0
5	4E	1142	0	1204	51	0
6	52	842	0	857	28	0
6	5E	837	0	852	29	0
7	62	1115	0	1165	57	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	54	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	72	0
9	8E	1000	0	1031	69	0
10	1A	646	0	662	48	0
10	1I	734	0	761	53	0
11	2A	835	0	847	47	0
11	2I	823	0	833	37	0
12	3A	956	0	1046	54	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	55	0
13	4I	942	0	997	48	0
14	5A	486	0	524	28	0
14	5I	491	0	530	36	0
15	6A	733	0	771	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	26	0
16	7A	705	0	725	37	0
16	7I	700	0	720	51	0
17	8A	823	0	891	41	0
17	8I	834	0	904	59	0
18	9A	544	0	605	25	0
18	9I	549	0	607	22	0
19	AA	481	0	468	19	0
19	AI	654	0	675	52	0
20	BA	762	0	861	39	0
20	BI	746	0	843	50	0
21	1B	188	0	195	17	0
21	1F	199	0	208	15	0
22	1K	1477	0	758	30	0
22	1L	1563	0	799	31	0
23	2K	1646	0	844	19	0
23	2L	1646	0	844	33	0
24	3K	1611	0	817	74	0
25	4K	439	0	218	10	0
25	4L	417	0	207	11	0
26	14	61630	0	31072	1406	1
26	1H	61028	0	30762	1443	0
27	16	2617	0	1328	70	0
27	1J	2617	0	1328	79	0
28	71	1033	0	1048	71	0
28	79	456	0	460	31	0
29	11	2120	0	2197	151	0
29	19	2125	0	2199	133	0
30	21	1558	0	1624	96	0
30	29	1563	0	1629	134	0
31	31	1585	0	1632	94	0
31	39	1602	0	1649	96	0
32	41	1457	0	1514	91	0
32	49	1458	0	1516	72	0
33	51	1312	0	1384	64	0
33	59	573	0	597	43	0
34	61	1136	0	1223	60	0
34	69	1131	0	1218	73	0
35	15	1104	0	1180	51	0
35	58	1104	0	1180	58	0
36	25	932	0	996	55	0
36	68	932	0	996	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	35	1122	0	1206	93	0
37	78	1122	0	1206	109	0
38	45	1099	0	1154	94	0
38	88	1113	0	1157	56	0
39	55	967	0	1033	56	0
39	98	967	0	1033	64	0
40	65	876	0	938	57	0
40	A8	875	0	936	54	0
41	75	1109	0	1169	74	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	54	0
42	C8	950	0	1011	53	0
43	95	774	0	849	82	0
43	D8	774	0	849	58	0
44	A5	899	0	964	34	0
44	E8	890	0	951	33	0
45	B5	735	0	785	43	0
45	F8	743	0	794	39	0
46	C5	794	0	886	74	0
46	G8	796	0	886	53	0
47	D5	1074	0	1086	63	0
47	H8	1373	0	1402	81	0
48	E5	608	0	622	37	0
48	I8	606	0	625	31	0
49	F5	737	0	813	41	0
49	J8	737	0	813	28	0
50	G5	558	0	610	33	0
50	K8	568	0	614	31	0
51	H5	459	0	512	15	0
51	L8	459	0	512	18	0
52	M8	366	0	370	31	0
53	J5	434	0	454	24	0
53	N8	369	0	388	22	0
54	L5	401	0	436	13	0
54	P8	401	0	436	17	0
55	M5	516	0	582	34	0
55	Q8	516	0	582	49	0
56	3L	1601	0	814	69	0
57	11	3	0	0	0	0
57	13	150	0	0	0	0
57	14	454	0	0	0	0
57	16	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	93	0	0	0	0
57	1H	502	0	0	0	0
57	1I	1	0	0	0	0
57	1J	6	0	0	0	0
57	21	3	0	0	0	0
57	29	4	0	0	0	0
57	2K	3	0	0	0	0
57	2L	4	0	0	0	0
57	31	1	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	41	2	0	0	0	0
57	45	3	0	0	0	0
57	55	1	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	88	1	0	0	0	0
57	BI	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	45	3	0
58	1G	42	0	45	2	0
59	32	8	0	0	2	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	12	0	0	1	0
61	13	319	0	0	23	0
61	14	1015	0	0	117	0
61	16	26	0	0	6	0
61	19	12	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1F	1	0	0	0	0
61	1G	226	0	0	16	0
61	1H	1158	0	0	132	0
61	1I	1	0	0	0	0
61	1J	18	0	0	2	0
61	1K	1	0	0	0	0
61	21	6	0	0	1	0
61	29	6	0	0	0	0
61	2K	7	0	0	0	0
61	2L	1	0	0	0	0
61	31	9	0	0	0	0
61	32	3	0	0	0	0
61	35	5	0	0	1	0
61	39	8	0	0	1	0
61	3A	1	0	0	0	0
61	3E	3	0	0	0	0
61	3I	3	0	0	1	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4E	3	0	0	1	0
61	4K	4	0	0	0	0
61	4L	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	1	0	0	1	0
61	6A	3	0	0	0	0
61	6I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	6	0	0	1	0
61	85	2	0	0	0	0
61	88	2	0	0	0	0
61	8A	1	0	0	0	0
61	8E	1	0	0	0	0
61	8I	2	0	0	0	0
61	A5	2	0	0	0	0
61	B5	1	0	0	0	0
61	BA	3	0	0	1	0
61	BI	5	0	0	0	0
61	C5	4	0	0	0	0
61	C8	2	0	0	0	0
61	E8	3	0	0	0	0
61	F8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	G8	2	0	0	0	0
61	H5	3	0	0	0	0
61	I8	5	0	0	1	0
61	J8	3	0	0	0	0
61	K8	2	0	0	0	0
61	L5	2	0	0	0	0
61	L8	2	0	0	0	0
61	M5	10	0	0	0	0
61	P8	1	0	0	0	0
61	Q8	9	0	0	2	0
All	All	296184	0	196367	8846	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 19.

The worst 5 of 8846 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)
37:35:81:GLN:NE2	37:35:106:LEU:HA	1.45	1.29
15:6A:27:VAL:O	15:6A:31:LEU:HD13	1.26	1.27
26:14:2572:A:C5	30:29:144:ARG:NH1	2.04	1.25
37:35:81:GLN:CD	37:35:106:LEU:HA	1.58	1.24
29:19:69:ARG:NH2	29:19:130:ALA:H	1.33	1.21

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]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	206/256 (80%)	175 (85%)	24 (12%)	7 (3%)	3	21
2	1E	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	17	53
3	22	192/239 (80%)	169 (88%)	23 (12%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	15	51
4	3E	205/209 (98%)	188 (92%)	16 (8%)	1 (0%)	29	65
5	42	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	22	59
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	135/156 (86%)	122 (90%)	12 (9%)	1 (1%)	22	59
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	10	41
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	59
9	82	119/128 (93%)	108 (91%)	9 (8%)	2 (2%)	9	38
9	8E	124/128 (97%)	105 (85%)	18 (14%)	1 (1%)	19	55
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	89/105 (85%)	82 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	98 (88%)	11 (10%)	2 (2%)	8	37
11	2I	109/129 (84%)	95 (87%)	12 (11%)	2 (2%)	8	37
12	3A	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	4	22
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	55
13	4A	109/126 (86%)	92 (84%)	15 (14%)	2 (2%)	8	37
13	4I	117/126 (93%)	98 (84%)	18 (15%)	1 (1%)	17	53
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	8	37
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	21
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10	41
19	AA	56/93 (60%)	49 (88%)	4 (7%)	3 (5%)	2	12
19	AI	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	5	29
20	BA	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	7	33
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	244 (90%)	17 (6%)	10 (4%)	3	19
29	19	272/276 (99%)	245 (90%)	21 (8%)	6 (2%)	6	32
30	21	201/206 (98%)	156 (78%)	36 (18%)	9 (4%)	2	16
30	29	202/206 (98%)	154 (76%)	39 (19%)	9 (4%)	2	16
31	31	200/210 (95%)	179 (90%)	20 (10%)	1 (0%)	29	65
31	39	202/210 (96%)	161 (80%)	31 (15%)	10 (5%)	2	14
32	41	177/182 (97%)	153 (86%)	21 (12%)	3 (2%)	9	38
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	14	48
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	11
33	59	68/180 (38%)	49 (72%)	14 (21%)	5 (7%)	1	6
34	61	144/148 (97%)	116 (81%)	26 (18%)	2 (1%)	11	43
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	7	33
35	15	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	22	59
35	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	4	25
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	55
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	116 (80%)	25 (17%)	4 (3%)	5	26
37	78	145/150 (97%)	115 (79%)	26 (18%)	4 (3%)	5	26
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	4	25
38	88	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	20
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	102 (88%)	13 (11%)	1 (1%)	17	53
40	65	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	8	36
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	116 (88%)	15 (12%)	0	100	100
41	B8	131/146 (90%)	118 (90%)	12 (9%)	1 (1%)	19	55
42	85	114/118 (97%)	101 (89%)	12 (10%)	1 (1%)	17	53
42	C8	113/118 (96%)	100 (88%)	10 (9%)	3 (3%)	5	27
43	95	98/101 (97%)	75 (76%)	19 (19%)	4 (4%)	3	18
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	3	18
44	A5	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	17	53
44	E8	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
45	B5	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	32
45	F8	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	14	48
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	7
46	G8	103/110 (94%)	85 (82%)	13 (13%)	5 (5%)	2	14
47	D5	126/206 (61%)	99 (79%)	20 (16%)	7 (6%)	2	12
47	H8	169/206 (82%)	132 (78%)	31 (18%)	6 (4%)	3	20
48	E5	75/85 (88%)	64 (85%)	9 (12%)	2 (3%)	5	27
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	14	48
49	J8	92/98 (94%)	85 (92%)	4 (4%)	3 (3%)	4	22
50	G5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	9	40
50	K8	66/72 (92%)	58 (88%)	6 (9%)	2 (3%)	4	24
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
52	M8	45/71 (63%)	30 (67%)	14 (31%)	1 (2%)	6	32
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	15
All	All	10975/12333 (89%)	9578 (87%)	1200 (11%)	197 (2%)	8	37

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU
29	11	273	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%)	172 (94%)	10 (6%)	21	54
2	1E	200/220 (91%)	183 (92%)	17 (8%)	10	36
3	22	154/188 (82%)	147 (96%)	7 (4%)	27	61
3	2E	159/188 (85%)	151 (95%)	8 (5%)	24	57
4	32	180/181 (99%)	167 (93%)	13 (7%)	14	43
4	3E	178/181 (98%)	166 (93%)	12 (7%)	16	47
5	42	114/123 (93%)	104 (91%)	10 (9%)	10	34
5	4E	115/123 (94%)	112 (97%)	3 (3%)	46	74
6	52	90/90 (100%)	86 (96%)	4 (4%)	28	61
6	5E	90/90 (100%)	85 (94%)	5 (6%)	21	53
7	62	114/127 (90%)	105 (92%)	9 (8%)	12	40
7	6E	125/127 (98%)	109 (87%)	16 (13%)	4	18
8	72	118/119 (99%)	107 (91%)	11 (9%)	9	31
8	7E	119/119 (100%)	111 (93%)	8 (7%)	16	47
9	82	92/99 (93%)	80 (87%)	12 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	91 (94%)	6 (6%)	18	50
10	1A	71/92 (77%)	63 (89%)	8 (11%)	6	23
10	1I	81/92 (88%)	79 (98%)	2 (2%)	47	75
11	2A	85/99 (86%)	82 (96%)	3 (4%)	36	67
11	2I	84/99 (85%)	82 (98%)	2 (2%)	49	76
12	3A	103/109 (94%)	92 (89%)	11 (11%)	6	25
12	3I	103/109 (94%)	97 (94%)	6 (6%)	20	52
13	4A	91/101 (90%)	81 (89%)	10 (11%)	6	24
13	4I	94/101 (93%)	85 (90%)	9 (10%)	8	29
14	5A	49/50 (98%)	43 (88%)	6 (12%)	5	20
14	5I	49/50 (98%)	47 (96%)	2 (4%)	30	63
15	6A	79/80 (99%)	74 (94%)	5 (6%)	18	49
15	6I	79/80 (99%)	75 (95%)	4 (5%)	24	56
16	7A	72/74 (97%)	66 (92%)	6 (8%)	11	37
16	7I	72/74 (97%)	69 (96%)	3 (4%)	30	62
17	8A	94/97 (97%)	89 (95%)	5 (5%)	22	55
17	8I	95/97 (98%)	87 (92%)	8 (8%)	11	37
18	9A	58/77 (75%)	56 (97%)	2 (3%)	37	68
18	9I	58/77 (75%)	55 (95%)	3 (5%)	23	55
19	AA	52/80 (65%)	49 (94%)	3 (6%)	20	52
19	AI	71/80 (89%)	64 (90%)	7 (10%)	8	28
20	BA	76/82 (93%)	72 (95%)	4 (5%)	22	55
20	BI	75/82 (92%)	72 (96%)	3 (4%)	31	64
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	51
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	71	109/181 (60%)	104 (95%)	5 (5%)	27	60
28	79	48/181 (26%)	41 (85%)	7 (15%)	3	14
29	11	214/218 (98%)	194 (91%)	20 (9%)	9	31
29	19	214/218 (98%)	198 (92%)	16 (8%)	13	42
30	21	165/166 (99%)	158 (96%)	7 (4%)	30	62
30	29	165/166 (99%)	155 (94%)	10 (6%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	151 (94%)	10 (6%)	18	50
31	39	163/166 (98%)	159 (98%)	4 (2%)	47	75
32	41	153/156 (98%)	142 (93%)	11 (7%)	14	43
32	49	153/156 (98%)	141 (92%)	12 (8%)	12	40
33	51	142/148 (96%)	134 (94%)	8 (6%)	21	53
33	59	59/148 (40%)	54 (92%)	5 (8%)	10	36
34	61	122/124 (98%)	114 (93%)	8 (7%)	16	47
34	69	122/124 (98%)	115 (94%)	7 (6%)	20	53
35	15	117/119 (98%)	112 (96%)	5 (4%)	29	62
35	58	117/119 (98%)	107 (92%)	10 (8%)	10	36
36	25	100/100 (100%)	96 (96%)	4 (4%)	31	64
36	68	100/100 (100%)	98 (98%)	2 (2%)	55	79
37	35	114/116 (98%)	106 (93%)	8 (7%)	15	45
37	78	114/116 (98%)	109 (96%)	5 (4%)	28	61
38	45	109/111 (98%)	98 (90%)	11 (10%)	7	27
38	88	109/111 (98%)	99 (91%)	10 (9%)	9	31
39	55	101/101 (100%)	96 (95%)	5 (5%)	24	57
39	98	101/101 (100%)	93 (92%)	8 (8%)	12	40
40	65	87/88 (99%)	79 (91%)	8 (9%)	9	31
40	A8	86/88 (98%)	75 (87%)	11 (13%)	4	18
41	75	117/127 (92%)	104 (89%)	13 (11%)	6	24
41	B8	117/127 (92%)	105 (90%)	12 (10%)	7	26
42	85	93/94 (99%)	86 (92%)	7 (8%)	13	42
42	C8	92/94 (98%)	83 (90%)	9 (10%)	8	28
43	95	82/82 (100%)	75 (92%)	7 (8%)	10	36
43	D8	82/82 (100%)	79 (96%)	3 (4%)	34	66
44	A5	92/92 (100%)	84 (91%)	8 (9%)	10	34
44	E8	91/92 (99%)	81 (89%)	10 (11%)	6	24
45	B5	74/78 (95%)	69 (93%)	5 (7%)	16	46
45	F8	75/78 (96%)	72 (96%)	3 (4%)	31	64
46	C5	85/91 (93%)	77 (91%)	8 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	85/91 (93%)	77 (91%)	8 (9%)	8	30
47	D5	118/179 (66%)	111 (94%)	7 (6%)	19	51
47	H8	152/179 (85%)	143 (94%)	9 (6%)	19	51
48	E5	61/67 (91%)	59 (97%)	2 (3%)	38	69
48	I8	61/67 (91%)	60 (98%)	1 (2%)	62	83
49	F5	79/83 (95%)	74 (94%)	5 (6%)	18	49
49	J8	79/83 (95%)	76 (96%)	3 (4%)	33	65
50	G5	62/67 (92%)	57 (92%)	5 (8%)	11	39
50	K8	62/67 (92%)	58 (94%)	4 (6%)	17	48
51	H5	50/52 (96%)	45 (90%)	5 (10%)	7	28
51	L8	50/52 (96%)	47 (94%)	3 (6%)	19	51
52	M8	42/63 (67%)	38 (90%)	4 (10%)	8	30
53	J5	48/52 (92%)	46 (96%)	2 (4%)	30	62
53	N8	43/52 (83%)	40 (93%)	3 (7%)	15	45
54	L5	38/42 (90%)	35 (92%)	3 (8%)	12	40
54	P8	38/42 (90%)	34 (90%)	4 (10%)	7	26
55	M5	54/55 (98%)	52 (96%)	2 (4%)	34	66
55	Q8	54/55 (98%)	52 (96%)	2 (4%)	34	66
All	All	9274/10193 (91%)	8636 (93%)	638 (7%)	15	46

5 of 638 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	79	223	ARG
42	85	12	ARG
29	19	169	GLU
28	79	210	ARG
35	15	48	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
6	52	27	GLN
18	9A	63	GLN
10	1A	84	GLN

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Mol	Chain	Res	Type
29	19	44	ASN
29	11	231	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	362 (24%)	32 (2%)
1	1G	1503/1522 (98%)	365 (24%)	35 (2%)
22	1K	65/76 (85%)	32 (49%)	3 (4%)
22	1L	69/76 (90%)	37 (53%)	3 (4%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	75/76 (98%)	49 (65%)	3 (4%)
25	4K	19/27 (70%)	10 (52%)	1 (5%)
25	4L	18/27 (66%)	10 (55%)	1 (5%)
26	14	2852/2917 (97%)	745 (26%)	45 (1%)
26	1H	2828/2917 (96%)	684 (24%)	52 (1%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
56	3L	73/76 (96%)	44 (60%)	5 (6%)
All	All	9389/9634 (97%)	2432 (25%)	189 (2%)

5 of 2432 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	28	G

5 of 189 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	913	A
26	14	71	A
1	1G	1126	U
1	1G	1533	C
26	14	479	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PSU	2K	56	23	18,21,22	1.15	1 (5%)	22,30,33	1.89	5 (22%)
22	T6A	1K	37	22	27,34,35	2.77	6 (22%)	29,49,52	2.48	9 (31%)
22	U8U	1K	34	22,25	19,24,25	2.52	7 (36%)	23,34,37	1.09	2 (8%)
22	U8U	1L	34	22,25	19,24,25	2.59	7 (36%)	23,34,37	1.27	3 (13%)
23	OMC	2K	33	23	19,22,23	1.81	3 (15%)	26,31,34	0.80	0
23	4SU	2L	8	23	18,21,22	1.83	3 (16%)	26,30,33	2.71	6 (23%)
22	PSU	1K	55	22	18,21,22	1.15	1 (5%)	22,30,33	1.83	4 (18%)
56	PSU	3L	39	56	18,21,22	1.14	2 (11%)	22,30,33	1.99	5 (22%)
22	PSU	1K	39	22	18,21,22	1.10	1 (5%)	22,30,33	1.73	4 (18%)
23	PSU	2L	56	23	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
23	5MU	2L	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.41	10 (35%)
23	G7M	2K	47	23	20,26,27	2.39	6 (30%)	17,39,42	0.85	1 (5%)
22	PSU	1L	55	22	18,21,22	1.09	1 (5%)	22,30,33	1.70	5 (22%)
22	PSU	1L	39	22	18,21,22	1.01	1 (5%)	22,30,33	1.73	3 (13%)
22	5MU	1K	54	22	19,22,23	3.80	5 (26%)	28,32,35	3.18	9 (32%)
23	G7M	2L	47	23	20,26,27	2.38	6 (30%)	17,39,42	1.05	1 (5%)
23	4SU	2K	8	23	18,21,22	1.89	5 (27%)	26,30,33	2.54	5 (19%)
24	PSU	3K	39	24	18,21,22	1.28	1 (5%)	22,30,33	1.72	4 (18%)
23	5MU	2K	55	23	19,22,23	3.81	5 (26%)	28,32,35	3.40	6 (21%)
23	OMC	2L	33	23	19,22,23	1.97	4 (21%)	26,31,34	1.07	1 (3%)
56	T6A	3L	37	56	27,34,35	2.60	5 (18%)	29,49,52	2.24	11 (37%)
22	5MU	1L	54	22	19,22,23	3.90	5 (26%)	28,32,35	3.27	8 (28%)
22	T6A	1L	37	22	27,34,35	2.57	6 (22%)	29,49,52	2.37	8 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	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	U8U	1K	34	22,25	-	2/9/28/29	0/2/2/2
22	U8U	1L	34	22,25	-	2/9/28/29	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	PSU	3L	39	56	-	2/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
22	PSU	1L	55	22	-	3/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	3/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
56	T6A	3L	37	56	-	10/19/41/42	0/3/3/3
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	7/19/41/42	0/3/3/3

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	12.57	1.58	1.38
23	2L	55	5MU	C2-N1	12.55	1.58	1.38
23	2K	55	5MU	C2-N1	12.48	1.58	1.38
22	1K	54	5MU	C2-N1	12.00	1.57	1.38
56	3L	37	T6A	C6-N6	8.37	1.51	1.36

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	11.43	125.06	115.31
23	2L	55	5MU	C5-C4-N3	11.29	124.95	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	54	5MU	C5-C4-N3	10.66	124.41	115.31
22	1K	54	5MU	C5-C4-N3	10.55	124.32	115.31
23	2L	8	4SU	C4-N3-C2	-9.01	118.59	127.34

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	3K	39	PSU	C3'-C4'-C5'-O5'
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	N-C-C5-C6
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	34	U8U	1	0
23	2L	8	4SU	2	0
56	3L	39	PSU	1	0
23	2L	56	PSU	3	0
23	2L	55	5MU	3	0
22	1K	54	5MU	1	0
23	2L	47	G7M	4	0
23	2K	8	4SU	1	0
23	2K	55	5MU	2	0
56	3L	37	T6A	2	0
22	1L	37	T6A	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1269 ligands modelled in this entry, 1265 are monoatomic - leaving 4 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
59	SF4	3E	301	4	0,12,12	-	-	-		
58	PAR	13	1749	-	45,45,45	0.85	0	64,67,67	2.01	16 (25%)
59	SF4	32	301	-	0,12,12	-	-	-		
58	PAR	1G	1691	-	45,45,45	0.71	0	64,67,67	1.73	17 (26%)

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	3E	301	4	-	-	0/6/5/5
58	PAR	13	1749	-	-	4/18/94/94	0/4/4/4
59	SF4	32	301	-	-	-	0/6/5/5
58	PAR	1G	1691	-	-	6/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	C22-C12-C62	-4.86	102.69	110.04
58	13	1749	PAR	C14-O33-C33	-4.70	106.32	117.96
58	1G	1691	PAR	O11-C11-C21	-4.60	100.30	108.22
58	13	1749	PAR	C11-O51-C51	4.53	122.58	113.69
58	13	1749	PAR	C14-O54-C54	4.32	122.17	113.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	13	1749	PAR	C41-C51-C61-O61
58	1G	1691	PAR	C33-C43-C53-O53
58	1G	1691	PAR	O43-C43-C53-O53
58	13	1749	PAR	O51-C51-C61-O61
58	1G	1691	PAR	O43-C13-O52-C52

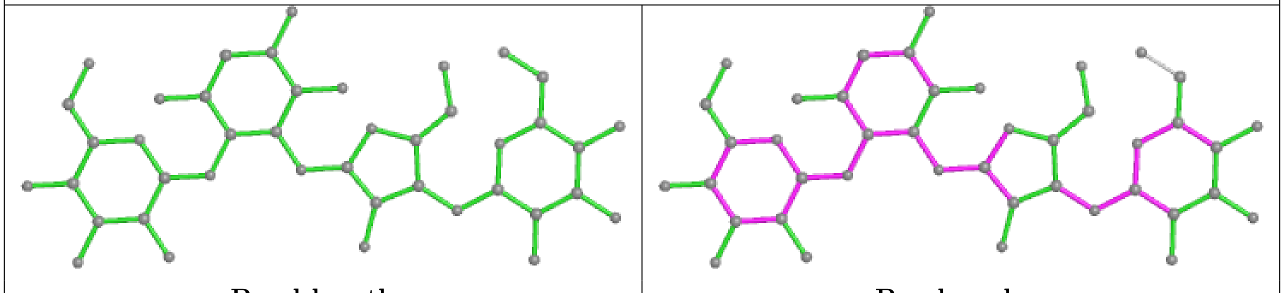
There are no ring outliers.

3 monomers are involved in 7 short contacts:

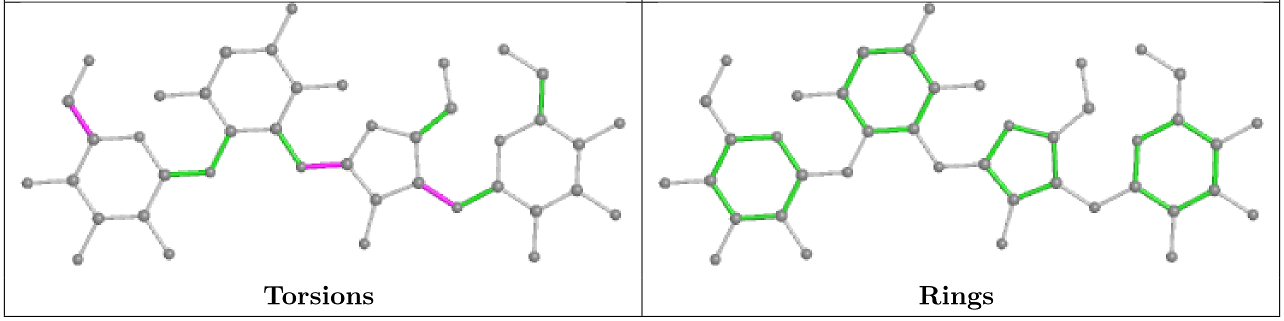
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	13	1749	PAR	3	0
59	32	301	SF4	2	0
58	1G	1691	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR 13 1749

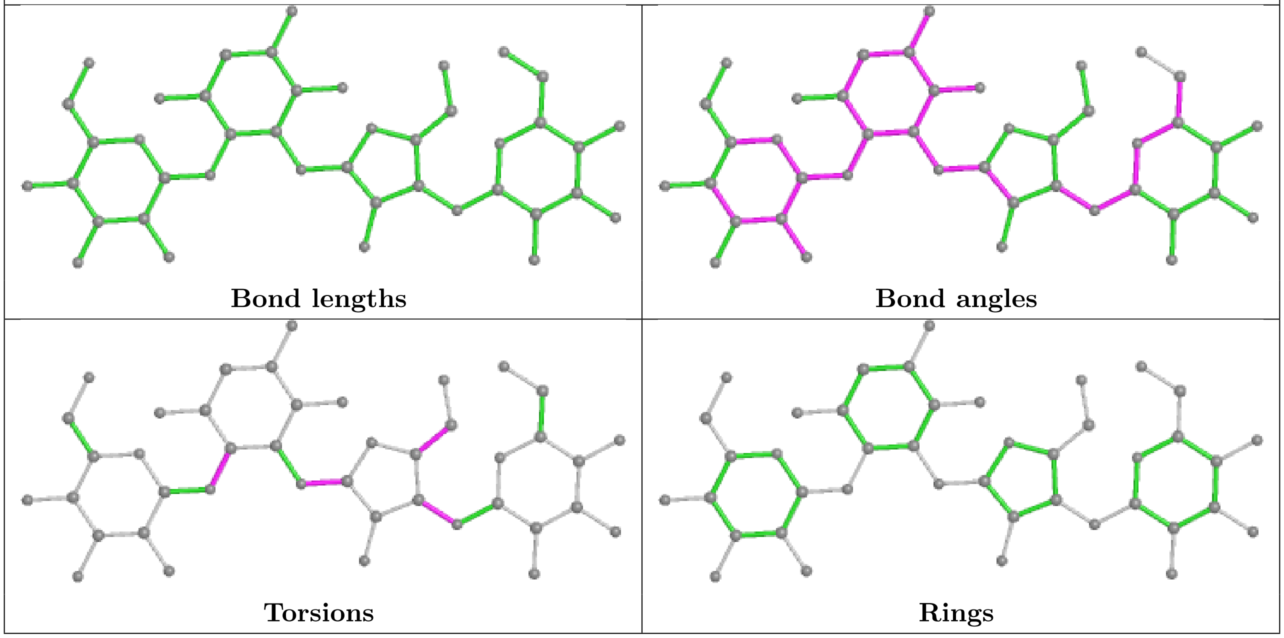


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PAR 1G 1691



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	3E	1
34	69	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3E	36:ARG	C	37:PRO	N	1.17
1	69	79:ILE	C	80:PRO	N	1.16
1	1A	76:ASN	C	77:PRO	N	1.12

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13	1496/1522 (98%)	-0.82	2 (0%)	95	95	58, 99, 162, 246	0
1	1G	1506/1522 (98%)	-0.86	1 (0%)	95	95	73, 114, 168, 253	0
2	12	210/256 (82%)	0.45	15 (7%)	16	8	127, 152, 169, 182	0
2	1E	231/256 (90%)	0.44	16 (6%)	16	9	105, 136, 157, 168	0
3	22	196/239 (82%)	1.11	45 (22%)	0	0	122, 138, 165, 170	0
3	2E	205/239 (85%)	0.46	11 (5%)	25	13	81, 103, 128, 138	0
4	32	208/209 (99%)	0.99	43 (20%)	1	0	98, 118, 136, 144	0
4	3E	207/209 (99%)	0.54	20 (9%)	7	4	80, 101, 121, 129	0
5	42	148/162 (91%)	0.40	6 (4%)	37	22	104, 121, 137, 147	0
5	4E	149/162 (91%)	0.55	13 (8%)	10	5	79, 96, 112, 121	0
6	52	101/101 (100%)	0.58	10 (9%)	7	4	83, 101, 118, 131	0
6	5E	100/101 (99%)	0.88	13 (13%)	3	2	83, 100, 115, 121	0
7	62	139/156 (89%)	0.17	4 (2%)	51	35	111, 124, 135, 141	0
7	6E	154/156 (98%)	-0.07	3 (1%)	66	53	101, 115, 132, 141	0
8	72	137/138 (99%)	0.41	8 (5%)	23	12	104, 124, 136, 142	0
8	7E	138/138 (100%)	0.57	11 (7%)	12	6	91, 106, 118, 127	0
9	82	121/128 (94%)	0.20	3 (2%)	57	42	110, 151, 165, 175	0
9	8E	126/128 (98%)	-0.18	0	100	100	89, 128, 147, 153	0
10	1A	80/105 (76%)	-0.01	1 (1%)	77	66	116, 145, 154, 156	0
10	1I	91/105 (86%)	0.24	7 (7%)	13	6	80, 121, 156, 161	0
11	2A	113/129 (87%)	0.82	16 (14%)	2	1	86, 110, 123, 130	0
11	2I	111/129 (86%)	0.91	15 (13%)	3	2	77, 102, 118, 125	0
12	3A	122/132 (92%)	1.17	31 (25%)	0	0	84, 102, 126, 145	0
12	3I	122/132 (92%)	0.40	5 (4%)	37	22	67, 77, 99, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	0.61	9 (8%) 12 6	109, 138, 154, 162	0
13	4I	119/126 (94%)	0.12	2 (1%) 70 57	84, 113, 128, 142	0
14	5A	59/61 (96%)	0.79	13 (22%) 0 0	122, 135, 145, 150	0
14	5I	60/61 (98%)	-0.33	0 100 100	82, 92, 108, 112	0
15	6A	88/89 (98%)	0.07	3 (3%) 45 28	89, 109, 128, 132	0
15	6I	87/89 (97%)	0.29	1 (1%) 80 70	83, 99, 116, 124	0
16	7A	84/88 (95%)	0.07	1 (1%) 79 68	92, 107, 125, 140	0
16	7I	83/88 (94%)	-0.26	0 100 100	97, 106, 136, 155	0
17	8A	99/105 (94%)	0.48	9 (9%) 9 5	95, 114, 127, 134	0
17	8I	100/105 (95%)	0.32	5 (5%) 28 15	88, 104, 115, 121	0
18	9A	67/88 (76%)	0.90	9 (13%) 3 2	93, 111, 130, 132	0
18	9I	68/88 (77%)	1.64	22 (32%) 0 0	87, 102, 124, 127	0
19	AA	62/93 (66%)	0.43	5 (8%) 12 6	123, 142, 153, 156	0
19	AI	81/93 (87%)	0.41	3 (3%) 41 25	91, 110, 132, 138	0
20	BA	99/106 (93%)	-0.06	2 (2%) 65 50	90, 110, 133, 142	0
20	BI	97/106 (91%)	-0.12	1 (1%) 82 73	104, 121, 147, 152	0
21	1B	22/27 (81%)	0.04	2 (9%) 9 5	119, 130, 141, 145	0
21	1F	23/27 (85%)	-0.35	0 100 100	89, 102, 110, 112	0
22	1K	64/76 (84%)	0.37	8 (12%) 3 2	84, 173, 191, 198	0
22	1L	68/76 (89%)	1.45	19 (27%) 0 0	115, 198, 216, 220	0
23	2K	72/77 (93%)	-0.54	0 100 100	74, 96, 123, 139	0
23	2L	72/77 (93%)	-0.48	0 100 100	81, 109, 138, 153	0
24	3K	75/76 (98%)	-0.33	3 (4%) 38 23	76, 207, 224, 234	0
25	4K	20/27 (74%)	0.14	2 (10%) 7 4	73, 133, 219, 222	0
25	4L	19/27 (70%)	0.29	2 (10%) 6 3	92, 146, 215, 217	0
26	14	2861/2917 (98%)	-0.59	18 (0%) 89 84	54, 86, 192, 250	0
26	1H	2833/2917 (97%)	-0.61	12 (0%) 92 89	44, 76, 171, 250	0
27	16	122/122 (100%)	-0.83	1 (0%) 86 78	69, 93, 114, 188	0
27	1J	122/122 (100%)	-0.87	0 100 100	87, 113, 134, 182	0
28	71	133/229 (58%)	1.48	45 (33%) 0 0	135, 198, 223, 231	0
28	79	57/229 (24%)	1.56	22 (38%) 0 0	141, 174, 199, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	11	273/276 (98%)	0.32	7 (2%) 56 40	43, 68, 86, 96	0
29	19	274/276 (99%)	0.45	13 (4%) 31 17	52, 75, 91, 115	0
30	21	203/206 (98%)	0.66	29 (14%) 2 1	55, 93, 129, 137	0
30	29	204/206 (99%)	0.40	16 (7%) 13 6	63, 94, 125, 142	0
31	31	202/210 (96%)	0.11	6 (2%) 50 33	49, 80, 114, 128	0
31	39	204/210 (97%)	0.52	20 (9%) 7 4	60, 101, 144, 170	0
32	41	179/182 (98%)	0.45	15 (8%) 11 5	80, 101, 132, 143	0
32	49	179/182 (98%)	1.36	47 (26%) 0 0	107, 123, 144, 167	0
33	51	171/180 (95%)	0.34	11 (6%) 19 10	84, 103, 118, 126	0
33	59	74/180 (41%)	0.50	10 (13%) 3 2	127, 155, 176, 191	0
34	61	146/148 (98%)	0.68	17 (11%) 4 2	80, 125, 142, 155	0
34	69	145/148 (97%)	0.86	23 (15%) 1 1	86, 121, 142, 152	0
35	15	138/140 (98%)	0.74	14 (10%) 7 3	80, 104, 132, 141	0
35	58	138/140 (98%)	0.65	13 (9%) 8 4	67, 94, 126, 137	0
36	25	122/122 (100%)	0.37	4 (3%) 46 29	69, 87, 103, 112	0
36	68	122/122 (100%)	0.25	4 (3%) 46 29	61, 79, 95, 103	0
37	35	147/150 (98%)	0.52	13 (8%) 10 5	60, 102, 129, 139	0
37	78	147/150 (98%)	0.03	4 (2%) 54 38	50, 84, 111, 117	0
38	45	138/141 (97%)	1.28	29 (21%) 1 0	74, 100, 118, 130	0
38	88	141/141 (100%)	0.47	8 (5%) 23 12	61, 80, 100, 123	0
39	55	118/118 (100%)	-0.11	0 100 100	64, 80, 96, 107	0
39	98	118/118 (100%)	0.51	8 (6%) 17 9	66, 89, 106, 118	0
40	65	110/112 (98%)	0.55	6 (5%) 25 13	84, 106, 121, 127	0
40	A8	111/112 (99%)	0.58	8 (7%) 15 8	76, 88, 107, 116	0
41	75	133/146 (91%)	0.03	4 (3%) 50 33	76, 95, 122, 143	0
41	B8	133/146 (91%)	-0.17	1 (0%) 86 78	71, 94, 126, 141	0
42	85	116/118 (98%)	0.27	6 (5%) 27 14	67, 90, 121, 132	0
42	C8	115/118 (97%)	0.19	5 (4%) 35 21	60, 84, 111, 120	0
43	95	100/101 (99%)	1.72	39 (39%) 0 0	68, 117, 131, 142	0
43	D8	100/101 (99%)	0.82	11 (11%) 5 3	62, 103, 123, 129	0
44	A5	113/113 (100%)	0.18	2 (1%) 68 55	61, 75, 104, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	E8	112/113 (99%)	0.44	4 (3%)	42	26	60, 76, 104, 136	0
45	B5	94/96 (97%)	0.35	6 (6%)	19	10	72, 83, 104, 119	0
45	F8	95/96 (98%)	0.21	3 (3%)	47	30	59, 74, 97, 107	0
46	C5	104/110 (94%)	1.12	23 (22%)	0	0	89, 114, 147, 154	0
46	G8	105/110 (95%)	0.11	2 (1%)	66	53	72, 94, 124, 135	0
47	D5	132/206 (64%)	1.65	54 (40%)	0	0	104, 132, 155, 163	0
47	H8	171/206 (83%)	1.27	45 (26%)	0	0	87, 118, 188, 193	0
48	E5	77/85 (90%)	0.66	4 (5%)	27	14	69, 87, 102, 123	0
48	I8	76/85 (89%)	-0.12	1 (1%)	77	66	59, 72, 85, 100	0
49	F5	94/98 (95%)	0.57	7 (7%)	14	8	66, 84, 115, 128	0
49	J8	94/98 (95%)	0.41	9 (9%)	8	4	54, 77, 114, 120	0
50	G5	66/72 (91%)	0.25	2 (3%)	50	33	81, 101, 121, 132	0
50	K8	68/72 (94%)	0.29	1 (1%)	73	61	67, 84, 98, 115	0
51	H5	58/60 (96%)	0.94	9 (15%)	2	1	77, 98, 128, 136	0
51	L8	58/60 (96%)	0.33	2 (3%)	45	28	65, 83, 107, 123	0
52	M8	47/71 (66%)	1.16	12 (25%)	0	0	102, 135, 150, 157	0
53	J5	56/60 (93%)	-0.10	0	100	100	59, 87, 127, 134	0
53	N8	48/60 (80%)	0.21	3 (6%)	20	10	55, 86, 128, 132	0
54	L5	47/49 (95%)	-0.19	1 (2%)	63	49	54, 62, 83, 88	0
54	P8	47/49 (95%)	-0.39	1 (2%)	63	49	49, 55, 72, 81	0
55	M5	64/65 (98%)	0.18	1 (1%)	72	59	68, 78, 93, 111	0
55	Q8	64/65 (98%)	-0.14	0	100	100	62, 70, 84, 97	0
56	3L	73/76 (96%)	0.11	3 (4%)	37	22	84, 205, 228, 235	0
All	All	20602/21967 (93%)	-0.02	1104 (5%)	25	13	43, 99, 165, 253	0

The worst 5 of 1104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	12.8
26	14	2901	C	9.8
32	49	138	GLN	8.4
44	A5	113	LYS	8.2
22	1L	71	C	8.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PSU	3L	39	20/21	0.85	0.17	118,132,140,141	0
22	T6A	1K	37	32/33	0.87	0.28	66,85,127,129	0
22	PSU	1L	55	20/21	0.88	0.21	126,149,158,158	0
22	T6A	1L	37	32/33	0.88	0.23	104,115,143,144	0
56	T6A	3L	37	32/33	0.89	0.19	121,132,147,147	0
22	5MU	1K	54	21/22	0.91	0.18	118,126,140,143	0
22	U8U	1L	34	23/24	0.91	0.17	115,123,131,134	0
22	PSU	1K	55	20/21	0.92	0.14	107,132,143,147	0
23	PSU	2L	56	20/21	0.92	0.10	106,110,116,120	0
23	4SU	2L	8	20/21	0.93	0.14	100,111,114,121	0
23	G7M	2K	47	24/25	0.93	0.12	90,101,110,116	0
22	PSU	1L	39	20/21	0.93	0.13	104,123,128,130	0
23	5MU	2L	55	21/22	0.94	0.10	105,114,119,125	0
23	OMC	2L	33	21/22	0.94	0.15	96,100,104,113	0
22	U8U	1K	34	23/24	0.95	0.14	81,89,100,107	0
22	5MU	1L	54	21/22	0.95	0.20	131,141,157,158	0
23	5MU	2K	55	21/22	0.95	0.09	90,103,110,112	0
23	4SU	2K	8	20/21	0.95	0.13	87,92,97,98	0
24	PSU	3K	39	20/21	0.95	0.09	109,116,128,137	0
22	PSU	1K	39	20/21	0.96	0.11	79,97,103,106	0
23	OMC	2K	33	21/22	0.96	0.14	73,80,83,87	0
23	PSU	2K	56	20/21	0.96	0.08	95,100,104,111	0
23	G7M	2L	47	24/25	0.96	0.12	114,121,128,132	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3031	1/1	0.32	0.26	105,105,105,105	0
57	MG	13	1646	1/1	0.44	0.17	109,109,109,109	0
57	MG	1H	3282	1/1	0.45	0.25	96,96,96,96	0
57	MG	1H	3183	1/1	0.46	0.35	92,92,92,92	0
57	MG	14	3266	1/1	0.53	0.24	84,84,84,84	0
57	MG	13	1643	1/1	0.57	0.21	89,89,89,89	0
57	MG	1H	3277	1/1	0.59	0.18	77,77,77,77	0
57	MG	13	1689	1/1	0.59	0.40	99,99,99,99	0
57	MG	55	201	1/1	0.59	0.33	83,83,83,83	0
57	MG	13	1661	1/1	0.62	0.11	102,102,102,102	0
57	MG	35	202	1/1	0.62	0.22	75,75,75,75	0
57	MG	13	1635	1/1	0.62	0.07	85,85,85,85	0
57	MG	14	3116	1/1	0.63	0.39	87,87,87,87	0
57	MG	14	3206	1/1	0.64	0.55	95,95,95,95	0
57	MG	1G	1620	1/1	0.64	0.77	79,79,79,79	0
57	MG	1G	1621	1/1	0.65	0.18	103,103,103,103	0
57	MG	14	3162	1/1	0.65	0.30	67,67,67,67	0
57	MG	1H	3210	1/1	0.65	0.32	74,74,74,74	0
57	MG	14	3267	1/1	0.66	0.15	83,83,83,83	0
57	MG	14	3272	1/1	0.66	0.30	77,77,77,77	0
57	MG	14	3237	1/1	0.66	0.50	72,72,72,72	0
57	MG	1H	3496	1/1	0.66	0.06	94,94,94,94	0
57	MG	14	3268	1/1	0.67	0.44	60,60,60,60	0
57	MG	14	3120	1/1	0.67	0.35	67,67,67,67	0
57	MG	1H	3180	1/1	0.67	0.38	76,76,76,76	0
57	MG	14	3016	1/1	0.67	0.56	73,73,73,73	0
57	MG	14	3155	1/1	0.68	0.26	66,66,66,66	0
57	MG	14	3157	1/1	0.68	0.32	99,99,99,99	0
57	MG	16	206	1/1	0.68	0.41	81,81,81,81	0
57	MG	14	3179	1/1	0.68	0.35	74,74,74,74	0
57	MG	2L	103	1/1	0.68	0.57	80,80,80,80	0
57	MG	13	1667	1/1	0.68	0.43	97,97,97,97	0
57	MG	14	3224	1/1	0.69	0.38	80,80,80,80	0
57	MG	1H	3129	1/1	0.69	0.31	76,76,76,76	0
57	MG	14	3243	1/1	0.69	0.41	86,86,86,86	0
57	MG	29	304	1/1	0.69	0.23	71,71,71,71	0
57	MG	14	3265	1/1	0.69	0.51	79,79,79,79	0
57	MG	13	1628	1/1	0.69	0.37	96,96,96,96	0
57	MG	13	1665	1/1	0.70	0.46	82,82,82,82	0
57	MG	1H	3207	1/1	0.70	0.16	56,56,56,56	0
57	MG	14	3013	1/1	0.70	0.24	74,74,74,74	0
57	MG	14	3248	1/1	0.70	0.35	75,75,75,75	0
57	MG	14	3063	1/1	0.71	0.31	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	13	1650	1/1	0.71	0.38	100,100,100,100	0
57	MG	13	1625	1/1	0.72	0.27	96,96,96,96	0
57	MG	1H	3493	1/1	0.72	0.19	94,94,94,94	0
57	MG	13	1655	1/1	0.72	0.46	71,71,71,71	0
57	MG	16	203	1/1	0.72	0.16	79,79,79,79	0
57	MG	14	3202	1/1	0.72	0.23	90,90,90,90	0
57	MG	16	205	1/1	0.72	0.20	81,81,81,81	0
57	MG	14	3171	1/1	0.73	0.22	73,73,73,73	0
57	MG	1H	3284	1/1	0.73	0.62	75,75,75,75	0
57	MG	1H	3190	1/1	0.73	0.47	74,74,74,74	0
57	MG	1H	3205	1/1	0.73	0.17	77,77,77,77	0
57	MG	1H	3289	1/1	0.74	0.40	82,82,82,82	0
57	MG	1H	3278	1/1	0.74	0.20	82,82,82,82	0
57	MG	14	3374	1/1	0.74	0.07	96,96,96,96	0
57	MG	29	301	1/1	0.74	0.44	80,80,80,80	0
57	MG	14	3223	1/1	0.74	0.42	75,75,75,75	0
57	MG	1H	3019	1/1	0.74	0.27	78,78,78,78	0
57	MG	1H	3020	1/1	0.74	0.19	107,107,107,107	0
57	MG	1H	3121	1/1	0.75	0.42	79,79,79,79	0
57	MG	14	3190	1/1	0.75	0.88	82,82,82,82	0
57	MG	14	3075	1/1	0.75	0.46	70,70,70,70	0
57	MG	1H	3198	1/1	0.75	0.26	76,76,76,76	0
57	MG	7A	101	1/1	0.75	0.23	89,89,89,89	0
57	MG	14	3357	1/1	0.75	0.11	84,84,84,84	0
57	MG	13	1684	1/1	0.75	0.22	85,85,85,85	0
57	MG	1J	203	1/1	0.75	0.30	93,93,93,93	0
57	MG	5I	101	1/1	0.75	0.08	88,88,88,88	0
57	MG	1H	3069	1/1	0.75	0.46	65,65,65,65	0
57	MG	11	303	1/1	0.75	0.51	65,65,65,65	0
57	MG	14	3257	1/1	0.75	0.58	87,87,87,87	0
57	MG	1H	3220	1/1	0.76	0.40	73,73,73,73	0
57	MG	1H	3233	1/1	0.76	0.34	70,70,70,70	0
57	MG	1H	3287	1/1	0.76	0.37	80,80,80,80	0
57	MG	14	3236	1/1	0.76	0.21	88,88,88,88	0
57	MG	1G	1641	1/1	0.76	0.34	78,78,78,78	0
57	MG	1H	3244	1/1	0.77	0.41	84,84,84,84	0
57	MG	1H	3128	1/1	0.77	0.22	64,64,64,64	0
57	MG	16	207	1/1	0.77	0.26	77,77,77,77	0
57	MG	14	3037	1/1	0.77	0.21	63,63,63,63	0
57	MG	14	3241	1/1	0.77	0.33	84,84,84,84	0
57	MG	1G	1626	1/1	0.78	0.29	73,73,73,73	0
57	MG	13	1659	1/1	0.78	0.42	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2K	101	1/1	0.78	0.29	95,95,95,95	0
57	MG	13	1656	1/1	0.78	0.50	62,62,62,62	0
57	MG	14	3443	1/1	0.78	0.07	108,108,108,108	0
57	MG	14	3097	1/1	0.78	0.51	65,65,65,65	0
57	MG	14	3005	1/1	0.78	0.37	70,70,70,70	0
57	MG	1H	3125	1/1	0.78	0.34	61,61,61,61	0
57	MG	14	3143	1/1	0.78	0.24	73,73,73,73	0
57	MG	1H	3249	1/1	0.78	0.22	61,61,61,61	0
57	MG	1I	201	1/1	0.79	0.12	100,100,100,100	0
57	MG	1H	3103	1/1	0.79	0.43	82,82,82,82	0
57	MG	1H	3107	1/1	0.79	0.19	64,64,64,64	0
57	MG	14	3423	1/1	0.79	0.06	144,144,144,144	0
57	MG	1H	3136	1/1	0.79	0.84	73,73,73,73	0
57	MG	1H	3108	1/1	0.79	0.41	82,82,82,82	0
57	MG	1H	3280	1/1	0.79	0.42	80,80,80,80	0
57	MG	1H	3054	1/1	0.79	0.34	59,59,59,59	0
57	MG	14	3226	1/1	0.79	0.27	78,78,78,78	0
57	MG	1G	1657	1/1	0.79	0.13	105,105,105,105	0
57	MG	14	3232	1/1	0.80	0.26	130,130,130,130	0
57	MG	14	3191	1/1	0.80	0.44	73,73,73,73	0
57	MG	1G	1609	1/1	0.80	0.19	108,108,108,108	0
57	MG	1H	3139	1/1	0.80	0.35	71,71,71,71	0
57	MG	1H	3144	1/1	0.80	0.48	75,75,75,75	0
57	MG	35	201	1/1	0.80	0.33	71,71,71,71	0
57	MG	1H	3199	1/1	0.80	0.38	75,75,75,75	0
57	MG	P8	101	1/1	0.80	0.44	66,66,66,66	0
57	MG	1H	3066	1/1	0.81	0.21	57,57,57,57	0
57	MG	1G	1618	1/1	0.81	0.19	86,86,86,86	0
57	MG	14	3180	1/1	0.81	0.31	69,69,69,69	0
57	MG	1G	1692	1/1	0.81	0.36	105,105,105,105	0
57	MG	29	303	1/1	0.81	0.16	67,67,67,67	0
57	MG	14	3036	1/1	0.81	0.24	76,76,76,76	0
57	MG	1H	3208	1/1	0.81	0.23	76,76,76,76	0
57	MG	1H	3242	1/1	0.81	0.27	80,80,80,80	0
57	MG	13	1603	1/1	0.81	0.36	76,76,76,76	0
57	MG	14	3258	1/1	0.82	0.77	83,83,83,83	0
57	MG	13	1618	1/1	0.82	0.33	64,64,64,64	0
57	MG	1G	1631	1/1	0.82	0.29	107,107,107,107	0
57	MG	1H	3036	1/1	0.82	0.20	78,78,78,78	0
57	MG	14	3192	1/1	0.82	0.36	100,100,100,100	0
57	MG	21	303	1/1	0.82	0.22	69,69,69,69	0
57	MG	14	3108	1/1	0.82	0.11	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1648	1/1	0.82	0.30	90,90,90,90	0
57	MG	1H	3192	1/1	0.82	0.32	82,82,82,82	0
57	MG	14	3427	1/1	0.82	0.08	102,102,102,102	0
57	MG	1G	1613	1/1	0.82	0.52	73,73,73,73	0
57	MG	14	3454	1/1	0.82	0.20	79,79,79,79	0
57	MG	14	3144	1/1	0.82	0.52	80,80,80,80	0
57	MG	14	3154	1/1	0.82	0.69	74,74,74,74	0
57	MG	1G	1616	1/1	0.82	0.23	86,86,86,86	0
57	MG	1H	3018	1/1	0.82	0.45	80,80,80,80	0
57	MG	13	1645	1/1	0.82	0.23	93,93,93,93	0
57	MG	1H	3200	1/1	0.82	0.35	73,73,73,73	0
57	MG	1G	1623	1/1	0.82	0.31	77,77,77,77	0
57	MG	1H	3291	1/1	0.83	0.46	88,88,88,88	0
57	MG	14	3204	1/1	0.83	0.19	90,90,90,90	0
57	MG	14	3129	1/1	0.83	0.16	69,69,69,69	0
57	MG	14	3212	1/1	0.83	0.43	80,80,80,80	0
57	MG	14	3213	1/1	0.83	0.46	87,87,87,87	0
57	MG	1H	3471	1/1	0.83	0.12	82,82,82,82	0
57	MG	14	3421	1/1	0.83	0.15	75,75,75,75	0
57	MG	1H	3246	1/1	0.83	0.38	85,85,85,85	0
57	MG	1H	3188	1/1	0.83	0.38	74,74,74,74	0
57	MG	1H	3120	1/1	0.83	0.16	63,63,63,63	0
57	MG	16	204	1/1	0.83	0.27	90,90,90,90	0
57	MG	13	1663	1/1	0.83	0.35	71,71,71,71	0
57	MG	1H	3023	1/1	0.83	0.39	81,81,81,81	0
57	MG	1H	3177	1/1	0.83	0.25	81,81,81,81	0
57	MG	1G	1639	1/1	0.83	0.18	97,97,97,97	0
57	MG	1H	3241	1/1	0.83	0.55	71,71,71,71	0
57	MG	1H	3093	1/1	0.83	0.63	71,71,71,71	0
57	MG	1H	3115	1/1	0.83	0.29	82,82,82,82	0
57	MG	14	3135	1/1	0.84	0.37	71,71,71,71	0
57	MG	14	3199	1/1	0.84	0.38	84,84,84,84	0
57	MG	14	3435	1/1	0.84	0.08	103,103,103,103	0
57	MG	14	3264	1/1	0.84	0.32	90,90,90,90	0
57	MG	14	3229	1/1	0.84	0.29	74,74,74,74	0
57	MG	1H	3083	1/1	0.84	0.21	74,74,74,74	0
57	MG	13	1682	1/1	0.84	0.68	90,90,90,90	0
57	MG	1H	3269	1/1	0.84	0.22	73,73,73,73	0
57	MG	14	3185	1/1	0.84	0.28	89,89,89,89	0
57	MG	1G	1688	1/1	0.84	0.06	100,100,100,100	0
57	MG	14	3244	1/1	0.84	0.68	77,77,77,77	0
57	MG	1H	3275	1/1	0.84	0.21	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3455	1/1	0.85	0.06	103,103,103,103	0
57	MG	1H	3087	1/1	0.85	0.16	68,68,68,68	0
57	MG	14	3211	1/1	0.85	0.38	78,78,78,78	0
57	MG	1H	3092	1/1	0.85	0.34	57,57,57,57	0
57	MG	1H	3238	1/1	0.85	0.34	78,78,78,78	0
57	MG	1H	3279	1/1	0.85	0.99	71,71,71,71	0
57	MG	1H	3133	1/1	0.85	0.42	80,80,80,80	0
57	MG	13	1670	1/1	0.85	0.33	78,78,78,78	0
57	MG	13	1649	1/1	0.85	0.37	78,78,78,78	0
57	MG	1H	3086	1/1	0.85	0.07	71,71,71,71	0
57	MG	14	3173	1/1	0.85	0.28	69,69,69,69	0
57	MG	1G	1627	1/1	0.85	0.25	86,86,86,86	0
57	MG	14	3044	1/1	0.85	0.81	76,76,76,76	0
57	MG	16	211	1/1	0.85	0.08	84,84,84,84	0
57	MG	1G	1638	1/1	0.85	0.58	88,88,88,88	0
57	MG	1H	3209	1/1	0.85	0.23	78,78,78,78	0
57	MG	1H	3194	1/1	0.85	0.45	66,66,66,66	0
57	MG	1G	1655	1/1	0.85	0.07	120,120,120,120	0
57	MG	14	3259	1/1	0.85	0.19	97,97,97,97	0
57	MG	41	202	1/1	0.85	0.26	82,82,82,82	0
57	MG	14	3238	1/1	0.86	0.55	69,69,69,69	0
57	MG	1H	3286	1/1	0.86	0.23	82,82,82,82	0
57	MG	14	3242	1/1	0.86	0.11	95,95,95,95	0
57	MG	1H	3131	1/1	0.86	0.52	67,67,67,67	0
57	MG	14	3163	1/1	0.86	0.64	72,72,72,72	0
57	MG	14	3164	1/1	0.86	0.33	65,65,65,65	0
57	MG	14	3168	1/1	0.86	0.21	89,89,89,89	0
57	MG	1G	1604	1/1	0.86	0.17	87,87,87,87	0
57	MG	1H	3119	1/1	0.86	0.20	71,71,71,71	0
57	MG	14	3260	1/1	0.86	0.13	117,117,117,117	0
57	MG	1H	3077	1/1	0.86	0.55	74,74,74,74	0
57	MG	1H	3411	1/1	0.86	0.07	81,81,81,81	0
57	MG	1H	3428	1/1	0.86	0.08	87,87,87,87	0
57	MG	14	3188	1/1	0.86	0.40	66,66,66,66	0
57	MG	1H	3138	1/1	0.86	0.41	55,55,55,55	0
57	MG	1H	3255	1/1	0.86	0.14	88,88,88,88	0
57	MG	1H	3487	1/1	0.86	0.08	91,91,91,91	0
57	MG	1H	3259	1/1	0.86	0.36	74,74,74,74	0
57	MG	13	1741	1/1	0.86	0.14	79,79,79,79	0
57	MG	14	3107	1/1	0.86	0.42	81,81,81,81	0
57	MG	1H	3212	1/1	0.86	0.35	77,77,77,77	0
57	MG	14	3113	1/1	0.86	0.41	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	1H	3195	1/1	0.86	0.28	73,73,73,73	0
57	MG	1H	3226	1/1	0.86	0.15	64,64,64,64	0
57	MG	1H	3229	1/1	0.86	0.34	73,73,73,73	0
57	MG	1G	1646	1/1	0.86	0.67	84,84,84,84	0
57	MG	1H	3059	1/1	0.86	0.21	66,66,66,66	0
57	MG	1H	3281	1/1	0.86	0.52	69,69,69,69	0
57	MG	14	3152	1/1	0.86	0.32	67,67,67,67	0
57	MG	13	1626	1/1	0.86	0.14	87,87,87,87	0
57	MG	13	1668	1/1	0.86	0.23	95,95,95,95	0
57	MG	1H	3501	1/1	0.87	0.05	72,72,72,72	0
57	MG	13	1679	1/1	0.87	0.22	86,86,86,86	0
57	MG	14	3053	1/1	0.87	0.30	77,77,77,77	0
57	MG	1H	3007	1/1	0.87	0.29	68,68,68,68	0
57	MG	14	3069	1/1	0.87	0.42	67,67,67,67	0
57	MG	1G	1628	1/1	0.87	0.24	124,124,124,124	0
57	MG	14	3444	1/1	0.87	0.12	87,87,87,87	0
57	MG	1H	3452	1/1	0.87	0.09	89,89,89,89	0
57	MG	1H	3285	1/1	0.87	0.55	87,87,87,87	0
57	MG	1H	3011	1/1	0.87	0.68	72,72,72,72	0
57	MG	1H	3014	1/1	0.87	0.50	75,75,75,75	0
57	MG	13	1748	1/1	0.87	0.09	115,115,115,115	0
57	MG	1H	3272	1/1	0.87	0.73	95,95,95,95	0
57	MG	14	3121	1/1	0.87	0.31	77,77,77,77	0
57	MG	14	3366	1/1	0.87	0.12	76,76,76,76	0
57	MG	13	1674	1/1	0.88	0.36	78,78,78,78	0
57	MG	1H	3489	1/1	0.88	0.08	125,125,125,125	0
57	MG	1G	1633	1/1	0.88	0.41	100,100,100,100	0
57	MG	1G	1636	1/1	0.88	0.22	89,89,89,89	0
57	MG	1H	3271	1/1	0.88	0.20	74,74,74,74	0
57	MG	1H	3495	1/1	0.88	0.07	98,98,98,98	0
57	MG	14	3146	1/1	0.88	0.44	76,76,76,76	0
57	MG	14	3147	1/1	0.88	0.29	72,72,72,72	0
57	MG	1H	3047	1/1	0.88	0.28	61,61,61,61	0
57	MG	1H	3273	1/1	0.88	0.26	57,57,57,57	0
57	MG	13	1677	1/1	0.88	0.22	76,76,76,76	0
57	MG	13	1636	1/1	0.88	0.21	75,75,75,75	0
57	MG	13	1642	1/1	0.88	0.26	107,107,107,107	0
57	MG	13	1666	1/1	0.88	0.41	77,77,77,77	0
57	MG	1H	3186	1/1	0.88	0.24	57,57,57,57	0
57	MG	13	1620	1/1	0.88	0.35	58,58,58,58	0
57	MG	1H	3122	1/1	0.88	0.52	73,73,73,73	0
57	MG	14	3010	1/1	0.88	0.31	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3015	1/1	0.88	0.24	72,72,72,72	0
57	MG	1H	3193	1/1	0.88	0.61	84,84,84,84	0
57	MG	14	3324	1/1	0.88	0.09	107,107,107,107	0
57	MG	L8	101	1/1	0.88	0.39	72,72,72,72	0
57	MG	13	1713	1/1	0.88	0.08	89,89,89,89	0
57	MG	1H	3243	1/1	0.88	0.24	62,62,62,62	0
57	MG	13	1739	1/1	0.88	0.06	104,104,104,104	0
57	MG	13	1660	1/1	0.88	0.55	83,83,83,83	0
57	MG	14	3198	1/1	0.88	0.21	81,81,81,81	0
57	MG	14	3054	1/1	0.88	0.40	67,67,67,67	0
57	MG	14	3441	1/1	0.88	0.08	72,72,72,72	0
57	MG	1H	3247	1/1	0.88	0.61	77,77,77,77	0
57	MG	13	1622	1/1	0.88	0.21	81,81,81,81	0
57	MG	1H	3439	1/1	0.88	0.14	81,81,81,81	0
57	MG	1J	201	1/1	0.88	0.20	85,85,85,85	0
57	MG	14	3096	1/1	0.88	0.34	65,65,65,65	0
57	MG	1H	3134	1/1	0.88	0.31	76,76,76,76	0
57	MG	1H	3098	1/1	0.88	0.33	63,63,63,63	0
57	MG	14	3216	1/1	0.88	0.23	74,74,74,74	0
57	MG	39	301	1/1	0.88	0.14	95,95,95,95	0
57	MG	1G	1624	1/1	0.88	0.19	87,87,87,87	0
57	MG	1H	3466	1/1	0.88	0.05	83,83,83,83	0
57	MG	1H	3263	1/1	0.88	1.00	93,93,93,93	0
57	MG	14	3269	1/1	0.89	0.30	102,102,102,102	0
57	MG	13	1735	1/1	0.89	0.07	118,118,118,118	0
57	MG	14	3303	1/1	0.89	0.13	63,63,63,63	0
57	MG	14	3308	1/1	0.89	0.08	96,96,96,96	0
57	MG	14	3310	1/1	0.89	0.09	68,68,68,68	0
57	MG	1H	3114	1/1	0.89	0.41	78,78,78,78	0
57	MG	14	3227	1/1	0.89	0.34	83,83,83,83	0
57	MG	1H	3021	1/1	0.89	0.16	90,90,90,90	0
57	MG	1H	3116	1/1	0.89	0.30	63,63,63,63	0
57	MG	14	3380	1/1	0.89	0.12	93,93,93,93	0
57	MG	14	3416	1/1	0.89	0.07	66,66,66,66	0
57	MG	1G	1637	1/1	0.89	0.20	77,77,77,77	0
57	MG	14	3123	1/1	0.89	0.49	70,70,70,70	0
57	MG	1H	3148	1/1	0.89	0.23	65,65,65,65	0
57	MG	1H	3213	1/1	0.89	0.14	92,92,92,92	0
57	MG	1H	3171	1/1	0.89	0.43	68,68,68,68	0
57	MG	1G	1619	1/1	0.89	0.21	92,92,92,92	0
57	MG	1H	3176	1/1	0.89	0.33	67,67,67,67	0
57	MG	14	3055	1/1	0.89	0.35	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3058	1/1	0.89	0.25	66,66,66,66	0
57	MG	1H	3084	1/1	0.89	0.14	82,82,82,82	0
57	MG	1G	1683	1/1	0.89	0.09	96,96,96,96	0
57	MG	1H	3178	1/1	0.89	0.12	93,93,93,93	0
57	MG	1H	3006	1/1	0.89	0.14	86,86,86,86	0
57	MG	1H	3075	1/1	0.89	0.12	60,60,60,60	0
57	MG	14	3215	1/1	0.89	0.30	64,64,64,64	0
57	MG	78	201	1/1	0.89	0.24	75,75,75,75	0
57	MG	14	3165	1/1	0.89	0.11	78,78,78,78	0
57	MG	14	3102	1/1	0.90	0.20	86,86,86,86	0
57	MG	1G	1635	1/1	0.90	0.45	97,97,97,97	0
57	MG	14	3225	1/1	0.90	0.36	80,80,80,80	0
57	MG	1H	3211	1/1	0.90	0.34	80,80,80,80	0
57	MG	1H	3254	1/1	0.90	0.62	82,82,82,82	0
57	MG	1H	3149	1/1	0.90	0.15	61,61,61,61	0
57	MG	1H	3157	1/1	0.90	0.28	64,64,64,64	0
57	MG	14	3233	1/1	0.90	0.26	79,79,79,79	0
57	MG	1H	3262	1/1	0.90	0.17	68,68,68,68	0
57	MG	1G	1642	1/1	0.90	0.30	82,82,82,82	0
57	MG	1G	1643	1/1	0.90	0.39	67,67,67,67	0
57	MG	16	212	1/1	0.90	0.08	88,88,88,88	0
57	MG	14	3139	1/1	0.90	0.22	58,58,58,58	0
57	MG	14	3142	1/1	0.90	0.31	82,82,82,82	0
57	MG	1H	3376	1/1	0.90	0.06	88,88,88,88	0
57	MG	1H	3159	1/1	0.90	0.37	56,56,56,56	0
57	MG	1G	1666	1/1	0.90	0.05	106,106,106,106	0
57	MG	41	201	1/1	0.90	0.14	75,75,75,75	0
57	MG	14	3149	1/1	0.90	0.29	96,96,96,96	0
57	MG	1G	1686	1/1	0.90	0.07	92,92,92,92	0
57	MG	14	3261	1/1	0.90	0.21	102,102,102,102	0
57	MG	1H	3267	1/1	0.90	0.17	67,67,67,67	0
57	MG	1H	3434	1/1	0.90	0.10	73,73,73,73	0
57	MG	1H	3221	1/1	0.90	0.21	60,60,60,60	0
57	MG	1H	3097	1/1	0.90	0.16	51,51,51,51	0
57	MG	14	3001	1/1	0.90	0.05	103,103,103,103	0
57	MG	1H	3196	1/1	0.90	0.56	88,88,88,88	0
57	MG	14	3271	1/1	0.90	0.45	80,80,80,80	0
57	MG	14	3009	1/1	0.90	0.20	68,68,68,68	0
57	MG	1G	1607	1/1	0.90	0.22	91,91,91,91	0
57	MG	1H	3231	1/1	0.90	0.42	65,65,65,65	0
57	MG	1H	3470	1/1	0.90	0.08	100,100,100,100	0
57	MG	14	3318	1/1	0.90	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3176	1/1	0.90	0.08	88,88,88,88	0
57	MG	14	3326	1/1	0.90	0.09	74,74,74,74	0
57	MG	14	3330	1/1	0.90	0.06	113,113,113,113	0
57	MG	14	3027	1/1	0.90	0.31	83,83,83,83	0
57	MG	13	1658	1/1	0.90	0.12	88,88,88,88	0
57	MG	14	3182	1/1	0.90	0.57	67,67,67,67	0
57	MG	14	3183	1/1	0.90	0.59	74,74,74,74	0
57	MG	1G	1617	1/1	0.90	0.22	61,61,61,61	0
57	MG	1H	3476	1/1	0.90	0.07	93,93,93,93	0
57	MG	14	3038	1/1	0.90	0.08	76,76,76,76	0
57	MG	14	3424	1/1	0.90	0.05	107,107,107,107	0
57	MG	1H	3484	1/1	0.90	0.07	90,90,90,90	0
57	MG	13	1631	1/1	0.90	0.10	73,73,73,73	0
57	MG	14	3194	1/1	0.90	0.21	68,68,68,68	0
57	MG	1H	3488	1/1	0.90	0.05	113,113,113,113	0
57	MG	1H	3105	1/1	0.90	0.24	79,79,79,79	0
57	MG	14	3448	1/1	0.90	0.06	92,92,92,92	0
57	MG	14	3057	1/1	0.90	0.36	41,41,41,41	0
57	MG	13	1722	1/1	0.90	0.05	92,92,92,92	0
57	MG	1H	3091	1/1	0.90	0.26	57,57,57,57	0
57	MG	1H	3143	1/1	0.90	0.45	89,89,89,89	0
57	MG	1H	3498	1/1	0.90	0.12	85,85,85,85	0
57	MG	13	1612	1/1	0.90	0.26	85,85,85,85	0
57	MG	13	1738	1/1	0.90	0.09	97,97,97,97	0
57	MG	39	302	1/1	0.90	0.10	63,63,63,63	0
57	MG	14	3098	1/1	0.90	0.22	67,67,67,67	0
57	MG	14	3219	1/1	0.90	0.29	64,64,64,64	0
57	MG	14	3221	1/1	0.90	0.51	73,73,73,73	0
57	MG	1H	3265	1/1	0.91	0.12	89,89,89,89	0
57	MG	14	3175	1/1	0.91	0.24	90,90,90,90	0
57	MG	13	1736	1/1	0.91	0.06	95,95,95,95	0
57	MG	14	3178	1/1	0.91	0.09	71,71,71,71	0
57	MG	1H	3189	1/1	0.91	0.31	87,87,87,87	0
57	MG	88	201	1/1	0.91	0.18	82,82,82,82	0
57	MG	14	3086	1/1	0.91	0.22	61,61,61,61	0
57	MG	14	3089	1/1	0.91	0.22	56,56,56,56	0
57	MG	BI	201	1/1	0.91	0.03	103,103,103,103	0
57	MG	1H	3228	1/1	0.91	0.49	69,69,69,69	0
57	MG	13	1672	1/1	0.91	0.11	96,96,96,96	0
57	MG	1H	3230	1/1	0.91	0.37	78,78,78,78	0
57	MG	1H	3109	1/1	0.91	0.33	65,65,65,65	0
57	MG	14	3193	1/1	0.91	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1610	1/1	0.91	0.13	114,114,114,114	0
57	MG	14	3296	1/1	0.91	0.09	59,59,59,59	0
57	MG	14	3111	1/1	0.91	0.15	79,79,79,79	0
57	MG	1G	1689	1/1	0.91	0.06	126,126,126,126	0
57	MG	14	3200	1/1	0.91	0.21	69,69,69,69	0
57	MG	1H	3482	1/1	0.91	0.06	72,72,72,72	0
57	MG	1H	3110	1/1	0.91	0.15	84,84,84,84	0
57	MG	1H	3112	1/1	0.91	0.39	66,66,66,66	0
57	MG	14	3207	1/1	0.91	0.10	71,71,71,71	0
57	MG	14	3208	1/1	0.91	0.31	75,75,75,75	0
57	MG	13	1662	1/1	0.91	0.21	119,119,119,119	0
57	MG	14	3124	1/1	0.91	0.27	64,64,64,64	0
57	MG	1H	3022	1/1	0.91	0.18	81,81,81,81	0
57	MG	13	1637	1/1	0.91	0.26	86,86,86,86	0
57	MG	1H	3283	1/1	0.91	0.47	82,82,82,82	0
57	MG	1H	3008	1/1	0.91	0.26	57,57,57,57	0
57	MG	14	3015	1/1	0.91	0.27	77,77,77,77	0
57	MG	14	3425	1/1	0.91	0.06	122,122,122,122	0
57	MG	14	3222	1/1	0.91	0.41	64,64,64,64	0
57	MG	14	3428	1/1	0.91	0.09	104,104,104,104	0
57	MG	1H	3090	1/1	0.91	0.48	57,57,57,57	0
57	MG	14	3436	1/1	0.91	0.07	108,108,108,108	0
57	MG	14	3017	1/1	0.91	0.23	97,97,97,97	0
57	MG	14	3442	1/1	0.91	0.07	95,95,95,95	0
57	MG	14	3024	1/1	0.91	0.26	58,58,58,58	0
57	MG	1H	3010	1/1	0.91	0.47	59,59,59,59	0
57	MG	1H	3053	1/1	0.91	0.47	56,56,56,56	0
57	MG	14	3452	1/1	0.91	0.09	113,113,113,113	0
57	MG	13	1664	1/1	0.91	0.30	81,81,81,81	0
57	MG	1H	3290	1/1	0.91	0.23	62,62,62,62	0
57	MG	1H	3126	1/1	0.91	0.45	70,70,70,70	0
57	MG	14	3234	1/1	0.91	0.16	64,64,64,64	0
57	MG	1H	3334	1/1	0.91	0.10	82,82,82,82	0
57	MG	14	3045	1/1	0.91	0.23	64,64,64,64	0
57	MG	1H	3371	1/1	0.91	0.05	85,85,85,85	0
57	MG	14	3239	1/1	0.91	0.36	87,87,87,87	0
57	MG	1H	3057	1/1	0.91	0.40	53,53,53,53	0
57	MG	13	1750	1/1	0.91	0.18	76,76,76,76	0
57	MG	45	202	1/1	0.91	0.10	102,102,102,102	0
57	MG	13	1652	1/1	0.91	0.48	89,89,89,89	0
57	MG	E5	101	1/1	0.91	0.43	72,72,72,72	0
57	MG	M5	101	1/1	0.91	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3315	1/1	0.92	0.05	81,81,81,81	0
57	MG	1H	3222	1/1	0.92	0.11	68,68,68,68	0
57	MG	1H	3481	1/1	0.92	0.06	92,92,92,92	0
57	MG	1H	3258	1/1	0.92	0.21	79,79,79,79	0
57	MG	14	3228	1/1	0.92	0.15	81,81,81,81	0
57	MG	14	3351	1/1	0.92	0.06	72,72,72,72	0
57	MG	1H	3140	1/1	0.92	0.22	62,62,62,62	0
57	MG	14	3181	1/1	0.92	0.20	63,63,63,63	0
57	MG	13	1678	1/1	0.92	0.21	83,83,83,83	0
57	MG	13	1724	1/1	0.92	0.08	114,114,114,114	0
57	MG	14	3383	1/1	0.92	0.07	101,101,101,101	0
57	MG	14	3400	1/1	0.92	0.06	86,86,86,86	0
57	MG	14	3407	1/1	0.92	0.10	74,74,74,74	0
57	MG	1H	3181	1/1	0.92	0.53	77,77,77,77	0
57	MG	14	3033	1/1	0.92	0.14	74,74,74,74	0
57	MG	14	3422	1/1	0.92	0.09	84,84,84,84	0
57	MG	1H	3182	1/1	0.92	0.44	72,72,72,72	0
57	MG	1H	3206	1/1	0.92	0.21	56,56,56,56	0
57	MG	1G	1653	1/1	0.92	0.08	110,110,110,110	0
57	MG	1H	3236	1/1	0.92	0.32	75,75,75,75	0
57	MG	1H	3035	1/1	0.92	0.24	57,57,57,57	0
57	MG	14	3429	1/1	0.92	0.05	98,98,98,98	0
57	MG	14	3195	1/1	0.92	0.23	105,105,105,105	0
57	MG	13	1704	1/1	0.92	0.13	105,105,105,105	0
57	MG	14	3255	1/1	0.92	0.13	87,87,87,87	0
57	MG	1G	1668	1/1	0.92	0.07	111,111,111,111	0
57	MG	1G	1674	1/1	0.92	0.06	107,107,107,107	0
57	MG	1G	1679	1/1	0.92	0.05	91,91,91,91	0
57	MG	16	201	1/1	0.92	0.17	87,87,87,87	0
57	MG	1H	3096	1/1	0.92	0.15	67,67,67,67	0
57	MG	14	3263	1/1	0.92	0.44	80,80,80,80	0
57	MG	13	1686	1/1	0.92	0.21	96,96,96,96	0
57	MG	1H	3162	1/1	0.92	0.15	61,61,61,61	0
57	MG	14	3158	1/1	0.92	0.12	70,70,70,70	0
57	MG	1H	3245	1/1	0.92	0.57	69,69,69,69	0
57	MG	1H	3170	1/1	0.92	0.73	72,72,72,72	0
57	MG	1H	3459	1/1	0.92	0.10	91,91,91,91	0
57	MG	14	3270	1/1	0.92	0.28	83,83,83,83	0
57	MG	1H	3052	1/1	0.92	0.32	57,57,57,57	0
57	MG	1H	3467	1/1	0.92	0.08	77,77,77,77	0
57	MG	14	3169	1/1	0.92	0.18	65,65,65,65	0
57	MG	1H	3174	1/1	0.92	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3105	1/1	0.92	0.26	55,55,55,55	0
57	MG	1H	3101	1/1	0.92	0.18	58,58,58,58	0
57	MG	1H	3168	1/1	0.93	0.27	80,80,80,80	0
57	MG	14	3184	1/1	0.93	0.33	60,60,60,60	0
57	MG	1H	3046	1/1	0.93	0.56	73,73,73,73	0
57	MG	1G	1670	1/1	0.93	0.08	108,108,108,108	0
57	MG	13	1671	1/1	0.93	0.32	71,71,71,71	0
57	MG	1G	1678	1/1	0.93	0.03	115,115,115,115	0
57	MG	1H	3123	1/1	0.93	0.21	71,71,71,71	0
57	MG	14	3104	1/1	0.93	0.36	81,81,81,81	0
57	MG	1H	3215	1/1	0.93	0.27	65,65,65,65	0
57	MG	14	3280	1/1	0.93	0.12	54,54,54,54	0
57	MG	1H	3218	1/1	0.93	0.74	70,70,70,70	0
57	MG	1H	3248	1/1	0.93	0.14	79,79,79,79	0
57	MG	14	3110	1/1	0.93	0.18	86,86,86,86	0
57	MG	1H	3065	1/1	0.93	0.17	56,56,56,56	0
57	MG	14	3112	1/1	0.93	0.37	88,88,88,88	0
57	MG	1H	3480	1/1	0.93	0.08	78,78,78,78	0
57	MG	13	1621	1/1	0.93	0.23	67,67,67,67	0
57	MG	2L	102	1/1	0.93	0.36	96,96,96,96	0
57	MG	1H	3099	1/1	0.93	0.13	60,60,60,60	0
57	MG	14	3210	1/1	0.93	0.34	80,80,80,80	0
57	MG	13	1630	1/1	0.93	0.28	92,92,92,92	0
57	MG	14	3004	1/1	0.93	0.88	77,77,77,77	0
57	MG	14	3370	1/1	0.93	0.08	81,81,81,81	0
57	MG	1H	3130	1/1	0.93	0.23	67,67,67,67	0
57	MG	14	3007	1/1	0.93	0.29	50,50,50,50	0
57	MG	1H	3288	1/1	0.93	0.38	80,80,80,80	0
57	MG	14	3387	1/1	0.93	0.05	97,97,97,97	0
57	MG	1H	3073	1/1	0.93	0.20	36,36,36,36	0
57	MG	14	3220	1/1	0.93	0.53	88,88,88,88	0
57	MG	1G	1622	1/1	0.93	0.35	76,76,76,76	0
57	MG	1H	3203	1/1	0.93	0.28	64,64,64,64	0
57	MG	13	1714	1/1	0.93	0.10	93,93,93,93	0
57	MG	1H	3325	1/1	0.93	0.11	69,69,69,69	0
57	MG	1H	3266	1/1	0.93	0.15	75,75,75,75	0
57	MG	14	3150	1/1	0.93	0.46	68,68,68,68	0
57	MG	14	3151	1/1	0.93	0.23	72,72,72,72	0
57	MG	1H	3500	1/1	0.93	0.06	71,71,71,71	0
57	MG	1H	3185	1/1	0.93	0.36	90,90,90,90	0
57	MG	14	3434	1/1	0.93	0.06	82,82,82,82	0
57	MG	14	3230	1/1	0.93	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	1H	3235	1/1	0.93	0.14	65,65,65,65	0
57	MG	14	3439	1/1	0.93	0.06	96,96,96,96	0
57	MG	16	202	1/1	0.93	0.28	73,73,73,73	0
57	MG	1H	3380	1/1	0.93	0.14	55,55,55,55	0
57	MG	14	3235	1/1	0.93	0.50	69,69,69,69	0
57	MG	1H	3385	1/1	0.93	0.08	57,57,57,57	0
57	MG	1H	3395	1/1	0.93	0.11	59,59,59,59	0
57	MG	1H	3076	1/1	0.93	0.25	76,76,76,76	0
57	MG	14	3049	1/1	0.93	0.27	63,63,63,63	0
57	MG	14	3240	1/1	0.93	0.30	85,85,85,85	0
57	MG	14	3166	1/1	0.93	0.24	61,61,61,61	0
57	MG	1H	3187	1/1	0.93	0.08	88,88,88,88	0
57	MG	1H	3431	1/1	0.93	0.16	52,52,52,52	0
57	MG	1H	3163	1/1	0.93	0.28	59,59,59,59	0
57	MG	1H	3435	1/1	0.93	0.05	94,94,94,94	0
57	MG	1G	1648	1/1	0.93	0.23	86,86,86,86	0
57	MG	1H	3438	1/1	0.93	0.05	75,75,75,75	0
57	MG	14	3067	1/1	0.93	0.34	68,68,68,68	0
57	MG	1H	3274	1/1	0.93	0.29	70,70,70,70	0
57	MG	14	3074	1/1	0.93	0.27	62,62,62,62	0
57	MG	C5	201	1/1	0.93	0.04	110,110,110,110	0
57	MG	1H	3451	1/1	0.93	0.04	95,95,95,95	0
57	MG	14	3082	1/1	0.93	0.40	55,55,55,55	0
57	MG	14	3088	1/1	0.94	0.29	65,65,65,65	0
57	MG	1G	1634	1/1	0.94	0.18	93,93,93,93	0
57	MG	14	3090	1/1	0.94	0.13	60,60,60,60	0
57	MG	14	3095	1/1	0.94	0.22	85,85,85,85	0
57	MG	13	1669	1/1	0.94	0.46	74,74,74,74	0
57	MG	1H	3472	1/1	0.94	0.07	93,93,93,93	0
57	MG	13	1651	1/1	0.94	0.21	68,68,68,68	0
57	MG	1H	3478	1/1	0.94	0.06	85,85,85,85	0
57	MG	1H	3224	1/1	0.94	0.28	63,63,63,63	0
57	MG	1G	1640	1/1	0.94	0.18	100,100,100,100	0
57	MG	14	3106	1/1	0.94	0.49	82,82,82,82	0
57	MG	1H	3225	1/1	0.94	0.40	67,67,67,67	0
57	MG	13	1719	1/1	0.94	0.15	72,72,72,72	0
57	MG	1H	3483	1/1	0.94	0.05	106,106,106,106	0
57	MG	1G	1644	1/1	0.94	0.35	67,67,67,67	0
57	MG	1H	3227	1/1	0.94	0.11	70,70,70,70	0
57	MG	1G	1647	1/1	0.94	0.25	115,115,115,115	0
57	MG	13	1680	1/1	0.94	0.36	75,75,75,75	0
57	MG	1G	1649	1/1	0.94	0.12	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3048	1/1	0.94	0.06	80,80,80,80	0
57	MG	14	3245	1/1	0.94	0.36	79,79,79,79	0
57	MG	1H	3049	1/1	0.94	0.28	68,68,68,68	0
57	MG	14	3253	1/1	0.94	0.18	63,63,63,63	0
57	MG	14	3254	1/1	0.94	0.21	81,81,81,81	0
57	MG	2K	102	1/1	0.94	0.06	92,92,92,92	0
57	MG	14	3128	1/1	0.94	0.12	60,60,60,60	0
57	MG	1G	1665	1/1	0.94	0.13	97,97,97,97	0
57	MG	14	3131	1/1	0.94	0.22	78,78,78,78	0
57	MG	14	3132	1/1	0.94	0.17	58,58,58,58	0
57	MG	14	3134	1/1	0.94	0.26	98,98,98,98	0
57	MG	13	1640	1/1	0.94	0.24	71,71,71,71	0
57	MG	14	3136	1/1	0.94	0.37	59,59,59,59	0
57	MG	1G	1667	1/1	0.94	0.06	100,100,100,100	0
57	MG	1H	3135	1/1	0.94	0.34	81,81,81,81	0
57	MG	13	1733	1/1	0.94	0.06	73,73,73,73	0
57	MG	1G	1671	1/1	0.94	0.07	117,117,117,117	0
57	MG	1H	3191	1/1	0.94	0.13	95,95,95,95	0
57	MG	1H	3055	1/1	0.94	0.33	72,72,72,72	0
57	MG	13	1734	1/1	0.94	0.06	86,86,86,86	0
57	MG	1H	3104	1/1	0.94	0.20	62,62,62,62	0
57	MG	1H	3323	1/1	0.94	0.06	61,61,61,61	0
57	MG	1G	1687	1/1	0.94	0.06	95,95,95,95	0
57	MG	1H	3142	1/1	0.94	0.52	85,85,85,85	0
57	MG	1H	3326	1/1	0.94	0.07	49,49,49,49	0
57	MG	14	3309	1/1	0.94	0.14	73,73,73,73	0
57	MG	1G	1690	1/1	0.94	0.07	118,118,118,118	0
57	MG	1H	3058	1/1	0.94	0.28	53,53,53,53	0
57	MG	14	3159	1/1	0.94	0.18	71,71,71,71	0
57	MG	14	3319	1/1	0.94	0.11	91,91,91,91	0
57	MG	14	3321	1/1	0.94	0.06	89,89,89,89	0
57	MG	1H	3337	1/1	0.94	0.07	73,73,73,73	0
57	MG	14	3325	1/1	0.94	0.05	78,78,78,78	0
57	MG	1H	3360	1/1	0.94	0.09	60,60,60,60	0
57	MG	1H	3366	1/1	0.94	0.08	65,65,65,65	0
57	MG	2L	104	1/1	0.94	0.40	72,72,72,72	0
57	MG	1H	3369	1/1	0.94	0.16	74,74,74,74	0
57	MG	21	301	1/1	0.94	0.36	66,66,66,66	0
57	MG	21	302	1/1	0.94	0.32	50,50,50,50	0
57	MG	14	3372	1/1	0.94	0.09	73,73,73,73	0
57	MG	13	1619	1/1	0.94	0.12	90,90,90,90	0
57	MG	1H	3372	1/1	0.94	0.07	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3174	1/1	0.94	0.16	71,71,71,71	0
57	MG	1H	3062	1/1	0.94	0.42	66,66,66,66	0
57	MG	14	3390	1/1	0.94	0.06	82,82,82,82	0
57	MG	13	1617	1/1	0.94	0.23	53,53,53,53	0
57	MG	14	3405	1/1	0.94	0.04	83,83,83,83	0
57	MG	14	3406	1/1	0.94	0.15	76,76,76,76	0
57	MG	1H	3202	1/1	0.94	0.39	58,58,58,58	0
57	MG	1H	3386	1/1	0.94	0.06	84,84,84,84	0
57	MG	1H	3393	1/1	0.94	0.09	56,56,56,56	0
57	MG	1G	1601	1/1	0.94	0.46	86,86,86,86	0
57	MG	1H	3252	1/1	0.94	0.32	80,80,80,80	0
57	MG	14	3030	1/1	0.94	0.22	68,68,68,68	0
57	MG	1G	1606	1/1	0.94	0.27	67,67,67,67	0
57	MG	1H	3397	1/1	0.94	0.07	85,85,85,85	0
57	MG	14	3034	1/1	0.94	0.36	57,57,57,57	0
57	MG	1H	3403	1/1	0.94	0.18	89,89,89,89	0
57	MG	1H	3154	1/1	0.94	0.18	75,75,75,75	0
57	MG	13	1737	1/1	0.94	0.10	147,147,147,147	0
57	MG	14	3043	1/1	0.94	0.27	75,75,75,75	0
57	MG	14	3438	1/1	0.94	0.07	93,93,93,93	0
57	MG	1G	1614	1/1	0.94	0.27	99,99,99,99	0
57	MG	1H	3111	1/1	0.94	0.31	80,80,80,80	0
57	MG	14	3048	1/1	0.94	0.75	75,75,75,75	0
57	MG	1H	3068	1/1	0.94	0.61	69,69,69,69	0
57	MG	14	3052	1/1	0.94	0.32	62,62,62,62	0
57	MG	14	3446	1/1	0.94	0.04	109,109,109,109	0
57	MG	13	1688	1/1	0.94	0.25	90,90,90,90	0
57	MG	14	3449	1/1	0.94	0.09	95,95,95,95	0
57	MG	1H	3436	1/1	0.94	0.10	65,65,65,65	0
57	MG	1H	3165	1/1	0.94	0.32	72,72,72,72	0
57	MG	14	3056	1/1	0.94	0.67	82,82,82,82	0
57	MG	1H	3017	1/1	0.94	0.18	55,55,55,55	0
57	MG	1J	205	1/1	0.94	0.05	95,95,95,95	0
57	MG	1H	3450	1/1	0.94	0.04	87,87,87,87	0
57	MG	13	1676	1/1	0.94	0.26	101,101,101,101	0
57	MG	13	1616	1/1	0.94	0.31	48,48,48,48	0
57	MG	14	3068	1/1	0.94	0.32	67,67,67,67	0
57	MG	13	1742	1/1	0.94	0.08	100,100,100,100	0
57	MG	14	3071	1/1	0.94	0.15	73,73,73,73	0
57	MG	14	3217	1/1	0.94	0.30	76,76,76,76	0
57	MG	1H	3270	1/1	0.94	0.10	71,71,71,71	0
57	MG	13	1744	1/1	0.94	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3076	1/1	0.94	0.20	77,77,77,77	0
57	MG	13	1708	1/1	0.94	0.07	76,76,76,76	0
57	MG	13	1710	1/1	0.94	0.12	108,108,108,108	0
57	MG	1H	3141	1/1	0.95	0.21	67,67,67,67	0
57	MG	1H	3033	1/1	0.95	0.26	62,62,62,62	0
57	MG	14	3039	1/1	0.95	0.19	73,73,73,73	0
57	MG	14	3041	1/1	0.95	0.20	64,64,64,64	0
57	MG	1G	1632	1/1	0.95	0.15	132,132,132,132	0
57	MG	14	3262	1/1	0.95	0.14	72,72,72,72	0
57	MG	1H	3067	1/1	0.95	0.33	52,52,52,52	0
57	MG	1H	3197	1/1	0.95	0.34	67,67,67,67	0
57	MG	1H	3106	1/1	0.95	0.43	74,74,74,74	0
57	MG	1H	3004	1/1	0.95	0.23	54,54,54,54	0
57	MG	13	1609	1/1	0.95	0.25	58,58,58,58	0
57	MG	14	3170	1/1	0.95	0.31	86,86,86,86	0
57	MG	1H	3348	1/1	0.95	0.11	65,65,65,65	0
57	MG	1H	3359	1/1	0.95	0.12	52,52,52,52	0
57	MG	1H	3201	1/1	0.95	0.37	65,65,65,65	0
57	MG	1H	3251	1/1	0.95	0.22	78,78,78,78	0
57	MG	1H	3072	1/1	0.95	0.69	73,73,73,73	0
57	MG	14	3177	1/1	0.95	0.35	79,79,79,79	0
57	MG	1H	3156	1/1	0.95	0.33	61,61,61,61	0
57	MG	1H	3037	1/1	0.95	0.17	55,55,55,55	0
57	MG	1H	3374	1/1	0.95	0.07	55,55,55,55	0
57	MG	1H	3038	1/1	0.95	0.23	53,53,53,53	0
57	MG	14	3311	1/1	0.95	0.07	66,66,66,66	0
57	MG	14	3312	1/1	0.95	0.06	77,77,77,77	0
57	MG	14	3313	1/1	0.95	0.07	72,72,72,72	0
57	MG	1H	3042	1/1	0.95	0.17	79,79,79,79	0
57	MG	14	3316	1/1	0.95	0.07	102,102,102,102	0
57	MG	1H	3260	1/1	0.95	0.25	65,65,65,65	0
57	MG	1H	3045	1/1	0.95	0.29	54,54,54,54	0
57	MG	1H	3078	1/1	0.95	0.35	60,60,60,60	0
57	MG	1H	3080	1/1	0.95	0.72	82,82,82,82	0
57	MG	14	3081	1/1	0.95	0.74	74,74,74,74	0
57	MG	1G	1663	1/1	0.95	0.07	87,87,87,87	0
57	MG	14	3328	1/1	0.95	0.07	93,93,93,93	0
57	MG	16	210	1/1	0.95	0.09	88,88,88,88	0
57	MG	14	3336	1/1	0.95	0.05	83,83,83,83	0
57	MG	14	3338	1/1	0.95	0.06	72,72,72,72	0
57	MG	1H	3082	1/1	0.95	0.23	49,49,49,49	0
57	MG	14	3353	1/1	0.95	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3400	1/1	0.95	0.21	67,67,67,67	0
57	MG	14	3365	1/1	0.95	0.09	88,88,88,88	0
57	MG	13	1712	1/1	0.95	0.08	75,75,75,75	0
57	MG	14	3091	1/1	0.95	0.23	85,85,85,85	0
57	MG	14	3371	1/1	0.95	0.05	83,83,83,83	0
57	MG	1H	3409	1/1	0.95	0.08	69,69,69,69	0
57	MG	1H	3173	1/1	0.95	0.15	63,63,63,63	0
57	MG	14	3378	1/1	0.95	0.04	93,93,93,93	0
57	MG	1H	3427	1/1	0.95	0.04	88,88,88,88	0
57	MG	1G	1675	1/1	0.95	0.07	88,88,88,88	0
57	MG	14	3099	1/1	0.95	0.17	57,57,57,57	0
57	MG	1G	1677	1/1	0.95	0.05	105,105,105,105	0
57	MG	13	1632	1/1	0.95	0.13	77,77,77,77	0
57	MG	14	3403	1/1	0.95	0.08	76,76,76,76	0
57	MG	14	3209	1/1	0.95	0.79	64,64,64,64	0
57	MG	13	1687	1/1	0.95	0.23	70,70,70,70	0
57	MG	1H	3433	1/1	0.95	0.11	86,86,86,86	0
57	MG	14	3408	1/1	0.95	0.08	78,78,78,78	0
57	MG	14	3412	1/1	0.95	0.04	120,120,120,120	0
57	MG	1G	1684	1/1	0.95	0.08	121,121,121,121	0
57	MG	13	1673	1/1	0.95	0.14	90,90,90,90	0
57	MG	1H	3124	1/1	0.95	0.24	74,74,74,74	0
57	MG	1H	3179	1/1	0.95	0.25	49,49,49,49	0
57	MG	1H	3088	1/1	0.95	0.34	53,53,53,53	0
57	MG	13	1743	1/1	0.95	0.05	87,87,87,87	0
57	MG	14	3114	1/1	0.95	0.39	63,63,63,63	0
57	MG	14	3115	1/1	0.95	0.39	71,71,71,71	0
57	MG	1G	1605	1/1	0.95	0.29	92,92,92,92	0
57	MG	14	3431	1/1	0.95	0.06	90,90,90,90	0
57	MG	14	3118	1/1	0.95	0.30	66,66,66,66	0
57	MG	1G	1694	1/1	0.95	0.48	98,98,98,98	0
57	MG	1H	3442	1/1	0.95	0.11	86,86,86,86	0
57	MG	2L	101	1/1	0.95	0.36	70,70,70,70	0
57	MG	1H	3448	1/1	0.95	0.09	62,62,62,62	0
57	MG	1G	1608	1/1	0.95	0.23	91,91,91,91	0
57	MG	13	1721	1/1	0.95	0.07	70,70,70,70	0
57	MG	13	1657	1/1	0.95	0.43	73,73,73,73	0
57	MG	14	3231	1/1	0.95	0.44	76,76,76,76	0
57	MG	1G	1611	1/1	0.95	0.39	74,74,74,74	0
57	MG	1G	1612	1/1	0.95	0.34	67,67,67,67	0
57	MG	13	1692	1/1	0.95	0.07	81,81,81,81	0
57	MG	1H	3454	1/1	0.95	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3138	1/1	0.95	0.08	68,68,68,68	0
57	MG	1G	1615	1/1	0.95	0.20	92,92,92,92	0
57	MG	1H	3095	1/1	0.95	0.36	65,65,65,65	0
57	MG	1H	3457	1/1	0.95	0.10	82,82,82,82	0
57	MG	1J	206	1/1	0.95	0.05	94,94,94,94	0
57	MG	13	1729	1/1	0.95	0.05	91,91,91,91	0
57	MG	1H	3463	1/1	0.95	0.07	82,82,82,82	0
57	MG	13	1698	1/1	0.95	0.04	93,93,93,93	0
57	MG	1H	3232	1/1	0.95	0.31	65,65,65,65	0
57	MG	13	1699	1/1	0.95	0.06	73,73,73,73	0
57	MG	1H	3061	1/1	0.95	0.29	68,68,68,68	0
57	MG	13	1681	1/1	0.95	0.40	86,86,86,86	0
57	MG	45	201	1/1	0.95	0.15	72,72,72,72	0
57	MG	14	3251	1/1	0.95	0.23	82,82,82,82	0
57	MG	1H	3102	1/1	0.95	0.46	70,70,70,70	0
57	MG	13	1624	1/1	0.95	0.12	81,81,81,81	0
57	MG	14	3156	1/1	0.95	0.41	75,75,75,75	0
57	MG	14	3256	1/1	0.95	0.12	91,91,91,91	0
57	MG	14	3026	1/1	0.96	0.32	72,72,72,72	0
57	MG	1H	3146	1/1	0.96	0.25	51,51,51,51	0
57	MG	1H	3147	1/1	0.96	0.16	51,51,51,51	0
57	MG	1H	3240	1/1	0.96	0.25	72,72,72,72	0
57	MG	13	1627	1/1	0.96	0.29	64,64,64,64	0
57	MG	13	1696	1/1	0.96	0.03	86,86,86,86	0
57	MG	1H	3458	1/1	0.96	0.11	87,87,87,87	0
57	MG	13	1605	1/1	0.96	0.31	68,68,68,68	0
57	MG	1H	3301	1/1	0.96	0.15	49,49,49,49	0
57	MG	1H	3313	1/1	0.96	0.11	72,72,72,72	0
57	MG	14	3276	1/1	0.96	0.11	62,62,62,62	0
57	MG	1H	3315	1/1	0.96	0.10	73,73,73,73	0
57	MG	1H	3316	1/1	0.96	0.14	63,63,63,63	0
57	MG	1G	1630	1/1	0.96	0.22	113,113,113,113	0
57	MG	1H	3322	1/1	0.96	0.04	82,82,82,82	0
57	MG	14	3172	1/1	0.96	0.19	63,63,63,63	0
57	MG	13	1751	1/1	0.96	0.14	87,87,87,87	0
57	MG	1H	3474	1/1	0.96	0.09	89,89,89,89	0
57	MG	13	1641	1/1	0.96	0.43	69,69,69,69	0
57	MG	1H	3158	1/1	0.96	0.58	68,68,68,68	0
57	MG	1H	3479	1/1	0.96	0.04	89,89,89,89	0
57	MG	13	1730	1/1	0.96	0.15	82,82,82,82	0
57	MG	14	3317	1/1	0.96	0.09	59,59,59,59	0
57	MG	1H	3335	1/1	0.96	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	1H	3161	1/1	0.96	0.29	72,72,72,72	0
57	MG	1H	3345	1/1	0.96	0.15	56,56,56,56	0
57	MG	14	3062	1/1	0.96	0.25	85,85,85,85	0
57	MG	13	1701	1/1	0.96	0.07	70,70,70,70	0
57	MG	1H	3485	1/1	0.96	0.05	76,76,76,76	0
57	MG	13	1633	1/1	0.96	0.13	85,85,85,85	0
57	MG	14	3186	1/1	0.96	0.24	84,84,84,84	0
57	MG	1H	3164	1/1	0.96	0.22	47,47,47,47	0
57	MG	1G	1645	1/1	0.96	0.55	88,88,88,88	0
57	MG	14	3344	1/1	0.96	0.09	72,72,72,72	0
57	MG	14	3348	1/1	0.96	0.05	88,88,88,88	0
57	MG	1H	3363	1/1	0.96	0.09	61,61,61,61	0
57	MG	13	1685	1/1	0.96	0.12	101,101,101,101	0
57	MG	14	3354	1/1	0.96	0.15	78,78,78,78	0
57	MG	1H	3166	1/1	0.96	0.12	70,70,70,70	0
57	MG	14	3361	1/1	0.96	0.09	69,69,69,69	0
57	MG	1H	3034	1/1	0.96	0.19	54,54,54,54	0
57	MG	1G	1650	1/1	0.96	0.21	87,87,87,87	0
57	MG	1H	3003	1/1	0.96	0.19	57,57,57,57	0
57	MG	1H	3127	1/1	0.96	0.34	56,56,56,56	0
57	MG	13	1629	1/1	0.96	0.29	98,98,98,98	0
57	MG	1H	3377	1/1	0.96	0.11	76,76,76,76	0
57	MG	14	3203	1/1	0.96	0.18	89,89,89,89	0
57	MG	1H	3378	1/1	0.96	0.06	84,84,84,84	0
57	MG	14	3205	1/1	0.96	0.17	77,77,77,77	0
57	MG	14	3092	1/1	0.96	0.27	56,56,56,56	0
57	MG	14	3388	1/1	0.96	0.07	82,82,82,82	0
57	MG	14	3094	1/1	0.96	0.28	85,85,85,85	0
57	MG	14	3391	1/1	0.96	0.09	86,86,86,86	0
57	MG	1H	3379	1/1	0.96	0.11	86,86,86,86	0
57	MG	14	3402	1/1	0.96	0.08	88,88,88,88	0
57	MG	1H	3100	1/1	0.96	0.19	44,44,44,44	0
57	MG	1H	3264	1/1	0.96	0.18	74,74,74,74	0
57	MG	1G	1669	1/1	0.96	0.08	114,114,114,114	0
57	MG	1H	3175	1/1	0.96	0.31	65,65,65,65	0
57	MG	14	3100	1/1	0.96	0.32	43,43,43,43	0
57	MG	14	3411	1/1	0.96	0.05	74,74,74,74	0
57	MG	14	3101	1/1	0.96	0.47	64,64,64,64	0
57	MG	1H	3214	1/1	0.96	0.43	92,92,92,92	0
57	MG	16	209	1/1	0.96	0.10	73,73,73,73	0
57	MG	1H	3005	1/1	0.96	0.34	74,74,74,74	0
57	MG	13	1711	1/1	0.96	0.05	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	1H	3132	1/1	0.96	0.23	75,75,75,75	0
57	MG	1H	3040	1/1	0.96	0.15	60,60,60,60	0
57	MG	14	3426	1/1	0.96	0.04	80,80,80,80	0
57	MG	1G	1682	1/1	0.96	0.10	127,127,127,127	0
57	MG	1H	3406	1/1	0.96	0.05	87,87,87,87	0
57	MG	1H	3074	1/1	0.96	0.21	48,48,48,48	0
57	MG	14	3430	1/1	0.96	0.04	90,90,90,90	0
57	MG	1H	3410	1/1	0.96	0.10	56,56,56,56	0
57	MG	31	301	1/1	0.96	0.06	61,61,61,61	0
57	MG	13	1613	1/1	0.96	0.28	65,65,65,65	0
57	MG	1H	3418	1/1	0.96	0.05	69,69,69,69	0
57	MG	14	3117	1/1	0.96	0.36	66,66,66,66	0
57	MG	1H	3421	1/1	0.96	0.05	78,78,78,78	0
57	MG	1H	3422	1/1	0.96	0.07	79,79,79,79	0
57	MG	1G	1693	1/1	0.96	0.09	92,92,92,92	0
57	MG	1H	3425	1/1	0.96	0.07	83,83,83,83	0
57	MG	1H	3044	1/1	0.96	0.28	62,62,62,62	0
57	MG	Q8	101	1/1	0.96	0.15	73,73,73,73	0
57	MG	14	3447	1/1	0.96	0.06	101,101,101,101	0
57	MG	1H	3137	1/1	0.96	0.09	72,72,72,72	0
57	MG	14	3130	1/1	0.96	0.32	71,71,71,71	0
57	MG	1H	3276	1/1	0.96	0.12	98,98,98,98	0
57	MG	1H	3184	1/1	0.96	0.41	67,67,67,67	0
57	MG	13	1653	1/1	0.96	0.15	66,66,66,66	0
57	MG	1J	202	1/1	0.96	0.22	94,94,94,94	0
57	MG	14	3003	1/1	0.96	0.19	65,65,65,65	0
57	MG	13	1654	1/1	0.96	0.32	75,75,75,75	0
57	MG	13	1691	1/1	0.96	0.12	79,79,79,79	0
57	MG	1H	3012	1/1	0.96	0.41	42,42,42,42	0
57	MG	1H	3013	1/1	0.96	0.34	60,60,60,60	0
57	MG	1H	3440	1/1	0.96	0.04	87,87,87,87	0
57	MG	14	3011	1/1	0.96	0.47	72,72,72,72	0
57	MG	14	3145	1/1	0.96	0.44	74,74,74,74	0
57	MG	14	3012	1/1	0.96	0.20	68,68,68,68	0
57	MG	13	1720	1/1	0.96	0.07	86,86,86,86	0
57	MG	14	3148	1/1	0.96	0.37	69,69,69,69	0
57	MG	14	3014	1/1	0.96	0.17	72,72,72,72	0
57	MG	45	203	1/1	0.96	0.48	71,71,71,71	0
57	MG	1H	3444	1/1	0.96	0.07	77,77,77,77	0
57	MG	1H	3447	1/1	0.96	0.12	97,97,97,97	0
57	MG	1H	3234	1/1	0.96	0.19	72,72,72,72	0
57	MG	1H	3113	1/1	0.96	0.36	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	PAR	13	1749	42/42	0.96	0.20	64,70,78,81	0
58	PAR	1G	1691	42/42	0.96	0.16	70,82,88,95	0
60	ZN	C5	202	1/1	0.96	0.15	169,169,169,169	0
57	MG	1H	3432	1/1	0.97	0.09	75,75,75,75	0
57	MG	13	1638	1/1	0.97	0.46	58,58,58,58	0
57	MG	1H	3250	1/1	0.97	0.19	67,67,67,67	0
57	MG	14	3006	1/1	0.97	0.24	66,66,66,66	0
57	MG	1H	3321	1/1	0.97	0.09	77,77,77,77	0
57	MG	14	3141	1/1	0.97	0.36	50,50,50,50	0
57	MG	14	3008	1/1	0.97	0.11	72,72,72,72	0
57	MG	1H	3028	1/1	0.97	0.26	51,51,51,51	0
57	MG	1H	3437	1/1	0.97	0.04	57,57,57,57	0
57	MG	13	1731	1/1	0.97	0.05	86,86,86,86	0
57	MG	1H	3253	1/1	0.97	0.69	76,76,76,76	0
57	MG	13	1707	1/1	0.97	0.04	90,90,90,90	0
57	MG	1H	3441	1/1	0.97	0.10	94,94,94,94	0
57	MG	1H	3330	1/1	0.97	0.12	57,57,57,57	0
57	MG	1H	3333	1/1	0.97	0.16	75,75,75,75	0
57	MG	13	1639	1/1	0.97	0.10	84,84,84,84	0
57	MG	14	3279	1/1	0.97	0.09	62,62,62,62	0
57	MG	14	3018	1/1	0.97	0.26	49,49,49,49	0
57	MG	14	3021	1/1	0.97	0.32	53,53,53,53	0
57	MG	14	3022	1/1	0.97	0.41	60,60,60,60	0
57	MG	14	3304	1/1	0.97	0.07	59,59,59,59	0
57	MG	1H	3001	1/1	0.97	0.16	53,53,53,53	0
57	MG	14	3025	1/1	0.97	0.19	58,58,58,58	0
57	MG	1H	3070	1/1	0.97	0.29	45,45,45,45	0
57	MG	1H	3340	1/1	0.97	0.11	54,54,54,54	0
57	MG	14	3161	1/1	0.97	0.30	73,73,73,73	0
57	MG	1H	3344	1/1	0.97	0.08	49,49,49,49	0
57	MG	14	3314	1/1	0.97	0.06	75,75,75,75	0
57	MG	1H	3453	1/1	0.97	0.04	83,83,83,83	0
57	MG	14	3032	1/1	0.97	0.18	47,47,47,47	0
57	MG	13	1615	1/1	0.97	0.24	91,91,91,91	0
57	MG	1H	3347	1/1	0.97	0.10	69,69,69,69	0
57	MG	14	3167	1/1	0.97	0.14	65,65,65,65	0
57	MG	14	3320	1/1	0.97	0.09	83,83,83,83	0
57	MG	14	3035	1/1	0.97	0.39	83,83,83,83	0
57	MG	14	3323	1/1	0.97	0.08	72,72,72,72	0
57	MG	13	1608	1/1	0.97	0.23	75,75,75,75	0
57	MG	1H	3350	1/1	0.97	0.12	69,69,69,69	0
57	MG	1H	3352	1/1	0.97	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	1H	3461	1/1	0.97	0.05	85,85,85,85	0
57	MG	14	3329	1/1	0.97	0.06	90,90,90,90	0
57	MG	1H	3354	1/1	0.97	0.10	62,62,62,62	0
57	MG	1H	3464	1/1	0.97	0.08	62,62,62,62	0
57	MG	1H	3465	1/1	0.97	0.26	53,53,53,53	0
57	MG	14	3340	1/1	0.97	0.11	73,73,73,73	0
57	MG	14	3342	1/1	0.97	0.09	58,58,58,58	0
57	MG	14	3343	1/1	0.97	0.09	63,63,63,63	0
57	MG	1H	3357	1/1	0.97	0.09	68,68,68,68	0
57	MG	14	3047	1/1	0.97	0.33	42,42,42,42	0
57	MG	14	3350	1/1	0.97	0.11	56,56,56,56	0
57	MG	1H	3216	1/1	0.97	0.21	57,57,57,57	0
57	MG	1H	3469	1/1	0.97	0.04	100,100,100,100	0
57	MG	1H	3217	1/1	0.97	0.16	59,59,59,59	0
57	MG	1H	3362	1/1	0.97	0.07	60,60,60,60	0
57	MG	13	1675	1/1	0.97	0.41	79,79,79,79	0
57	MG	14	3363	1/1	0.97	0.11	68,68,68,68	0
57	MG	1H	3473	1/1	0.97	0.07	85,85,85,85	0
57	MG	1H	3364	1/1	0.97	0.03	106,106,106,106	0
57	MG	1H	3475	1/1	0.97	0.13	88,88,88,88	0
57	MG	1H	3041	1/1	0.97	0.28	72,72,72,72	0
57	MG	14	3187	1/1	0.97	0.15	80,80,80,80	0
57	MG	1H	3477	1/1	0.97	0.10	65,65,65,65	0
57	MG	14	3376	1/1	0.97	0.11	52,52,52,52	0
57	MG	14	3377	1/1	0.97	0.16	67,67,67,67	0
57	MG	14	3189	1/1	0.97	0.48	69,69,69,69	0
57	MG	1H	3367	1/1	0.97	0.09	54,54,54,54	0
57	MG	14	3066	1/1	0.97	0.18	53,53,53,53	0
57	MG	14	3384	1/1	0.97	0.06	95,95,95,95	0
57	MG	1H	3368	1/1	0.97	0.15	60,60,60,60	0
57	MG	13	1604	1/1	0.97	0.14	112,112,112,112	0
57	MG	13	1611	1/1	0.97	0.24	79,79,79,79	0
57	MG	14	3070	1/1	0.97	0.38	52,52,52,52	0
57	MG	14	3392	1/1	0.97	0.06	87,87,87,87	0
57	MG	14	3393	1/1	0.97	0.09	79,79,79,79	0
57	MG	14	3394	1/1	0.97	0.05	78,78,78,78	0
57	MG	14	3396	1/1	0.97	0.08	62,62,62,62	0
57	MG	14	3398	1/1	0.97	0.13	83,83,83,83	0
57	MG	14	3399	1/1	0.97	0.09	78,78,78,78	0
57	MG	14	3196	1/1	0.97	0.17	90,90,90,90	0
57	MG	14	3197	1/1	0.97	0.14	56,56,56,56	0
57	MG	13	1740	1/1	0.97	0.04	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3404	1/1	0.97	0.09	94,94,94,94	0
57	MG	14	3072	1/1	0.97	0.25	69,69,69,69	0
57	MG	14	3073	1/1	0.97	0.23	57,57,57,57	0
57	MG	14	3201	1/1	0.97	0.47	58,58,58,58	0
57	MG	1H	3373	1/1	0.97	0.14	66,66,66,66	0
57	MG	14	3410	1/1	0.97	0.05	85,85,85,85	0
57	MG	13	1644	1/1	0.97	0.20	80,80,80,80	0
57	MG	1H	3375	1/1	0.97	0.18	57,57,57,57	0
57	MG	14	3413	1/1	0.97	0.10	97,97,97,97	0
57	MG	14	3414	1/1	0.97	0.06	85,85,85,85	0
57	MG	14	3415	1/1	0.97	0.06	77,77,77,77	0
57	MG	14	3077	1/1	0.97	0.41	80,80,80,80	0
57	MG	14	3078	1/1	0.97	0.28	86,86,86,86	0
57	MG	1H	3486	1/1	0.97	0.18	61,61,61,61	0
57	MG	1H	3145	1/1	0.97	0.24	46,46,46,46	0
57	MG	14	3083	1/1	0.97	0.21	61,61,61,61	0
57	MG	1G	1652	1/1	0.97	0.11	82,82,82,82	0
57	MG	14	3087	1/1	0.97	0.09	97,97,97,97	0
57	MG	1H	3081	1/1	0.97	0.19	47,47,47,47	0
57	MG	13	1693	1/1	0.97	0.13	72,72,72,72	0
57	MG	1H	3490	1/1	0.97	0.07	83,83,83,83	0
57	MG	1G	1662	1/1	0.97	0.11	76,76,76,76	0
57	MG	13	1601	1/1	0.97	0.21	68,68,68,68	0
57	MG	14	3433	1/1	0.97	0.05	71,71,71,71	0
57	MG	14	3218	1/1	0.97	0.28	54,54,54,54	0
57	MG	14	3093	1/1	0.97	0.39	51,51,51,51	0
57	MG	1H	3494	1/1	0.97	0.03	126,126,126,126	0
57	MG	13	1606	1/1	0.97	0.28	52,52,52,52	0
57	MG	1H	3382	1/1	0.97	0.04	70,70,70,70	0
57	MG	14	3440	1/1	0.97	0.04	94,94,94,94	0
57	MG	1H	3150	1/1	0.97	0.09	50,50,50,50	0
57	MG	1H	3151	1/1	0.97	0.18	91,91,91,91	0
57	MG	1H	3387	1/1	0.97	0.10	64,64,64,64	0
57	MG	1H	3502	1/1	0.97	0.32	59,59,59,59	0
57	MG	14	3445	1/1	0.97	0.03	87,87,87,87	0
57	MG	1G	1672	1/1	0.97	0.03	91,91,91,91	0
57	MG	1H	3153	1/1	0.97	0.18	59,59,59,59	0
57	MG	1H	3118	1/1	0.97	0.12	60,60,60,60	0
57	MG	1H	3050	1/1	0.97	0.32	66,66,66,66	0
57	MG	13	1745	1/1	0.97	0.05	117,117,117,117	0
57	MG	1H	3237	1/1	0.97	0.18	61,61,61,61	0
57	MG	1G	1680	1/1	0.97	0.03	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3109	1/1	0.97	0.32	60,60,60,60	0
57	MG	13	1747	1/1	0.97	0.13	72,72,72,72	0
57	MG	13	1723	1/1	0.97	0.06	84,84,84,84	0
57	MG	13	1647	1/1	0.97	0.21	104,104,104,104	0
57	MG	1G	1685	1/1	0.97	0.06	109,109,109,109	0
57	MG	1H	3056	1/1	0.97	0.28	52,52,52,52	0
57	MG	1H	3413	1/1	0.97	0.08	78,78,78,78	0
57	MG	1H	3414	1/1	0.97	0.13	53,53,53,53	0
57	MG	1H	3416	1/1	0.97	0.16	48,48,48,48	0
57	MG	13	1727	1/1	0.97	0.07	110,110,110,110	0
57	MG	1H	3094	1/1	0.97	0.12	52,52,52,52	0
57	MG	5E	201	1/1	0.97	0.20	81,81,81,81	0
57	MG	14	3247	1/1	0.97	0.25	67,67,67,67	0
57	MG	1H	3204	1/1	0.97	0.22	86,86,86,86	0
57	MG	14	3250	1/1	0.97	0.18	65,65,65,65	0
57	MG	13	1614	1/1	0.97	0.59	64,64,64,64	0
57	MG	1H	3303	1/1	0.97	0.11	63,63,63,63	0
57	MG	1H	3429	1/1	0.97	0.11	75,75,75,75	0
57	MG	1H	3430	1/1	0.97	0.06	85,85,85,85	0
57	MG	I8	101	1/1	0.97	0.04	65,65,65,65	0
60	ZN	G8	201	1/1	0.97	0.18	146,146,146,146	0
57	MG	3I	201	1/1	0.97	0.16	57,57,57,57	0
57	MG	14	3290	1/1	0.98	0.09	64,64,64,64	0
57	MG	14	3292	1/1	0.98	0.13	61,61,61,61	0
57	MG	1H	3298	1/1	0.98	0.10	61,61,61,61	0
57	MG	14	3300	1/1	0.98	0.14	57,57,57,57	0
57	MG	14	3302	1/1	0.98	0.10	68,68,68,68	0
57	MG	1H	3381	1/1	0.98	0.11	95,95,95,95	0
57	MG	1H	3299	1/1	0.98	0.06	50,50,50,50	0
57	MG	1H	3384	1/1	0.98	0.11	73,73,73,73	0
57	MG	1H	3085	1/1	0.98	0.29	71,71,71,71	0
57	MG	14	3160	1/1	0.98	0.30	51,51,51,51	0
57	MG	14	3040	1/1	0.98	0.33	64,64,64,64	0
57	MG	1H	3024	1/1	0.98	0.31	45,45,45,45	0
57	MG	14	3042	1/1	0.98	0.24	58,58,58,58	0
57	MG	1H	3310	1/1	0.98	0.10	58,58,58,58	0
57	MG	1H	3391	1/1	0.98	0.13	49,49,49,49	0
57	MG	1H	3392	1/1	0.98	0.06	69,69,69,69	0
57	MG	1H	3117	1/1	0.98	0.51	72,72,72,72	0
57	MG	1H	3394	1/1	0.98	0.14	70,70,70,70	0
57	MG	1H	3314	1/1	0.98	0.13	75,75,75,75	0
57	MG	14	3050	1/1	0.98	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3051	1/1	0.98	0.39	62,62,62,62	0
57	MG	1H	3025	1/1	0.98	0.32	56,56,56,56	0
57	MG	1H	3398	1/1	0.98	0.12	50,50,50,50	0
57	MG	1H	3399	1/1	0.98	0.13	61,61,61,61	0
57	MG	1H	3256	1/1	0.98	0.34	71,71,71,71	0
57	MG	1H	3402	1/1	0.98	0.09	73,73,73,73	0
57	MG	1H	3320	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3404	1/1	0.98	0.09	76,76,76,76	0
57	MG	14	3332	1/1	0.98	0.07	63,63,63,63	0
57	MG	14	3333	1/1	0.98	0.14	59,59,59,59	0
57	MG	14	3334	1/1	0.98	0.11	61,61,61,61	0
57	MG	14	3335	1/1	0.98	0.07	87,87,87,87	0
57	MG	14	3060	1/1	0.98	0.30	74,74,74,74	0
57	MG	14	3337	1/1	0.98	0.05	76,76,76,76	0
57	MG	14	3061	1/1	0.98	0.34	61,61,61,61	0
57	MG	1H	3405	1/1	0.98	0.11	69,69,69,69	0
57	MG	1H	3257	1/1	0.98	0.25	84,84,84,84	0
57	MG	14	3064	1/1	0.98	0.36	58,58,58,58	0
57	MG	14	3065	1/1	0.98	0.28	54,54,54,54	0
57	MG	14	3345	1/1	0.98	0.08	68,68,68,68	0
57	MG	14	3346	1/1	0.98	0.11	75,75,75,75	0
57	MG	14	3347	1/1	0.98	0.13	67,67,67,67	0
57	MG	1G	1651	1/1	0.98	0.08	81,81,81,81	0
57	MG	14	3349	1/1	0.98	0.08	81,81,81,81	0
57	MG	1H	3492	1/1	0.98	0.06	105,105,105,105	0
57	MG	1H	3407	1/1	0.98	0.06	50,50,50,50	0
57	MG	14	3352	1/1	0.98	0.06	65,65,65,65	0
57	MG	1G	1654	1/1	0.98	0.09	93,93,93,93	0
57	MG	1H	3219	1/1	0.98	0.14	62,62,62,62	0
57	MG	14	3356	1/1	0.98	0.13	61,61,61,61	0
57	MG	1H	3026	1/1	0.98	0.44	40,40,40,40	0
57	MG	14	3358	1/1	0.98	0.12	54,54,54,54	0
57	MG	14	3359	1/1	0.98	0.11	67,67,67,67	0
57	MG	14	3360	1/1	0.98	0.06	83,83,83,83	0
57	MG	1G	1658	1/1	0.98	0.05	94,94,94,94	0
57	MG	1G	1659	1/1	0.98	0.13	79,79,79,79	0
57	MG	14	3364	1/1	0.98	0.05	73,73,73,73	0
57	MG	1G	1661	1/1	0.98	0.05	111,111,111,111	0
57	MG	1H	3324	1/1	0.98	0.13	47,47,47,47	0
57	MG	14	3368	1/1	0.98	0.07	72,72,72,72	0
57	MG	14	3369	1/1	0.98	0.19	56,56,56,56	0
57	MG	1H	3497	1/1	0.98	0.07	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	1G	1664	1/1	0.98	0.05	91,91,91,91	0
57	MG	1H	3412	1/1	0.98	0.13	66,66,66,66	0
57	MG	14	3373	1/1	0.98	0.06	93,93,93,93	0
57	MG	14	3079	1/1	0.98	0.30	64,64,64,64	0
57	MG	14	3375	1/1	0.98	0.05	91,91,91,91	0
57	MG	14	3080	1/1	0.98	0.38	46,46,46,46	0
57	MG	13	1725	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3261	1/1	0.98	0.22	67,67,67,67	0
57	MG	14	3379	1/1	0.98	0.10	94,94,94,94	0
57	MG	1H	3328	1/1	0.98	0.08	52,52,52,52	0
57	MG	14	3381	1/1	0.98	0.05	52,52,52,52	0
57	MG	14	3382	1/1	0.98	0.09	91,91,91,91	0
57	MG	14	3084	1/1	0.98	0.34	56,56,56,56	0
57	MG	14	3085	1/1	0.98	0.31	65,65,65,65	0
57	MG	14	3385	1/1	0.98	0.07	70,70,70,70	0
57	MG	14	3386	1/1	0.98	0.07	56,56,56,56	0
57	MG	1H	3329	1/1	0.98	0.13	55,55,55,55	0
57	MG	1H	3420	1/1	0.98	0.07	64,64,64,64	0
57	MG	14	3389	1/1	0.98	0.07	81,81,81,81	0
57	MG	1H	3031	1/1	0.98	0.38	53,53,53,53	0
57	MG	1H	3332	1/1	0.98	0.07	63,63,63,63	0
57	MG	1G	1673	1/1	0.98	0.09	84,84,84,84	0
57	MG	1H	3424	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3223	1/1	0.98	0.18	64,64,64,64	0
57	MG	14	3395	1/1	0.98	0.04	78,78,78,78	0
57	MG	1G	1676	1/1	0.98	0.04	86,86,86,86	0
57	MG	14	3397	1/1	0.98	0.14	64,64,64,64	0
57	MG	1H	3426	1/1	0.98	0.08	57,57,57,57	0
57	MG	14	3214	1/1	0.98	0.15	73,73,73,73	0
57	MG	1H	3152	1/1	0.98	0.19	87,87,87,87	0
57	MG	1H	3032	1/1	0.98	0.14	61,61,61,61	0
57	MG	1H	3336	1/1	0.98	0.13	61,61,61,61	0
57	MG	13	1726	1/1	0.98	0.08	85,85,85,85	0
57	MG	11	301	1/1	0.98	0.10	46,46,46,46	0
57	MG	11	302	1/1	0.98	0.11	57,57,57,57	0
57	MG	1H	3155	1/1	0.98	0.18	75,75,75,75	0
57	MG	1H	3341	1/1	0.98	0.09	57,57,57,57	0
57	MG	14	3103	1/1	0.98	0.52	68,68,68,68	0
57	MG	1H	3342	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3268	1/1	0.98	0.25	81,81,81,81	0
57	MG	1H	3063	1/1	0.98	0.27	52,52,52,52	0
57	MG	13	1610	1/1	0.98	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	13	1728	1/1	0.98	0.08	91,91,91,91	0
57	MG	13	1746	1/1	0.98	0.08	83,83,83,83	0
57	MG	14	3419	1/1	0.98	0.05	70,70,70,70	0
57	MG	1H	3160	1/1	0.98	0.46	67,67,67,67	0
57	MG	13	1702	1/1	0.98	0.12	76,76,76,76	0
57	MG	1H	3356	1/1	0.98	0.10	58,58,58,58	0
57	MG	1H	3009	1/1	0.98	0.25	54,54,54,54	0
57	MG	13	1703	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3445	1/1	0.98	0.03	97,97,97,97	0
57	MG	1G	1602	1/1	0.98	0.28	72,72,72,72	0
57	MG	1G	1603	1/1	0.98	0.20	81,81,81,81	0
57	MG	1H	3446	1/1	0.98	0.04	93,93,93,93	0
57	MG	14	3119	1/1	0.98	0.50	63,63,63,63	0
57	MG	1H	3071	1/1	0.98	0.43	54,54,54,54	0
57	MG	13	1623	1/1	0.98	0.35	61,61,61,61	0
57	MG	14	3122	1/1	0.98	0.07	104,104,104,104	0
57	MG	1H	3449	1/1	0.98	0.12	69,69,69,69	0
57	MG	13	1715	1/1	0.98	0.09	110,110,110,110	0
57	MG	14	3437	1/1	0.98	0.03	93,93,93,93	0
57	MG	14	3125	1/1	0.98	0.17	54,54,54,54	0
57	MG	14	3246	1/1	0.98	0.23	76,76,76,76	0
57	MG	14	3126	1/1	0.98	0.43	64,64,64,64	0
57	MG	13	1716	1/1	0.98	0.08	66,66,66,66	0
57	MG	1H	3169	1/1	0.98	0.20	85,85,85,85	0
57	MG	13	1718	1/1	0.98	0.09	78,78,78,78	0
57	MG	13	1705	1/1	0.98	0.07	76,76,76,76	0
57	MG	13	1706	1/1	0.98	0.12	71,71,71,71	0
57	MG	1H	3456	1/1	0.98	0.05	72,72,72,72	0
57	MG	1H	3370	1/1	0.98	0.11	70,70,70,70	0
57	MG	13	1607	1/1	0.98	0.27	74,74,74,74	0
57	MG	14	3137	1/1	0.98	0.22	72,72,72,72	0
57	MG	14	3450	1/1	0.98	0.10	63,63,63,63	0
57	MG	14	3451	1/1	0.98	0.14	77,77,77,77	0
57	MG	1H	3079	1/1	0.98	0.30	47,47,47,47	0
57	MG	1H	3460	1/1	0.98	0.14	62,62,62,62	0
57	MG	14	3140	1/1	0.98	0.31	81,81,81,81	0
57	MG	14	3020	1/1	0.98	0.38	51,51,51,51	0
57	MG	13	1634	1/1	0.98	0.70	71,71,71,71	0
57	MG	1J	204	1/1	0.98	0.06	82,82,82,82	0
57	MG	1H	3462	1/1	0.98	0.07	54,54,54,54	0
57	MG	13	1709	1/1	0.98	0.09	75,75,75,75	0
57	MG	2K	103	1/1	0.98	0.36	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1700	1/1	0.98	0.07	93,93,93,93	0
57	MG	1H	3002	1/1	0.98	0.31	39,39,39,39	0
57	MG	14	3029	1/1	0.98	0.26	59,59,59,59	0
57	MG	1G	1625	1/1	0.98	0.20	89,89,89,89	0
57	MG	1H	3292	1/1	0.98	0.10	50,50,50,50	0
57	MG	1H	3468	1/1	0.98	0.11	71,71,71,71	0
57	MG	14	3273	1/1	0.98	0.19	58,58,58,58	0
57	MG	1H	3293	1/1	0.98	0.06	63,63,63,63	0
57	MG	14	3277	1/1	0.98	0.08	67,67,67,67	0
57	MG	14	3278	1/1	0.98	0.05	65,65,65,65	0
57	MG	14	3153	1/1	0.98	0.09	79,79,79,79	0
57	MG	1G	1629	1/1	0.98	0.67	83,83,83,83	0
57	MG	14	3282	1/1	0.98	0.09	58,58,58,58	0
57	MG	14	3283	1/1	0.98	0.09	74,74,74,74	0
57	MG	14	3285	1/1	0.98	0.05	59,59,59,59	0
57	MG	14	3286	1/1	0.98	0.05	63,63,63,63	0
60	ZN	5A	101	1/1	0.98	0.09	128,128,128,128	0
57	MG	14	3289	1/1	0.98	0.12	58,58,58,58	0
57	MG	14	3275	1/1	0.99	0.09	61,61,61,61	0
57	MG	1H	3317	1/1	0.99	0.20	45,45,45,45	0
57	MG	14	3127	1/1	0.99	0.34	48,48,48,48	0
57	MG	1H	3318	1/1	0.99	0.15	54,54,54,54	0
57	MG	1H	3319	1/1	0.99	0.13	67,67,67,67	0
57	MG	13	1694	1/1	0.99	0.17	79,79,79,79	0
57	MG	14	3281	1/1	0.99	0.16	66,66,66,66	0
57	MG	14	3059	1/1	0.99	0.41	69,69,69,69	0
57	MG	1H	3039	1/1	0.99	0.12	90,90,90,90	0
57	MG	14	3284	1/1	0.99	0.07	57,57,57,57	0
57	MG	14	3133	1/1	0.99	0.33	71,71,71,71	0
57	MG	1H	3089	1/1	0.99	0.44	51,51,51,51	0
57	MG	14	3287	1/1	0.99	0.17	56,56,56,56	0
57	MG	14	3288	1/1	0.99	0.14	50,50,50,50	0
57	MG	1H	3491	1/1	0.99	0.13	75,75,75,75	0
57	MG	1H	3027	1/1	0.99	0.40	63,63,63,63	0
57	MG	14	3291	1/1	0.99	0.12	66,66,66,66	0
57	MG	13	1695	1/1	0.99	0.11	76,76,76,76	0
57	MG	14	3295	1/1	0.99	0.11	58,58,58,58	0
57	MG	1H	3029	1/1	0.99	0.35	49,49,49,49	0
57	MG	14	3297	1/1	0.99	0.08	74,74,74,74	0
57	MG	14	3298	1/1	0.99	0.03	79,79,79,79	0
57	MG	14	3299	1/1	0.99	0.06	60,60,60,60	0
57	MG	1H	3043	1/1	0.99	0.28	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3301	1/1	0.99	0.15	56,56,56,56	0
57	MG	1H	3327	1/1	0.99	0.05	55,55,55,55	0
57	MG	14	3401	1/1	0.99	0.10	66,66,66,66	0
57	MG	1H	3030	1/1	0.99	0.23	45,45,45,45	0
57	MG	1H	3167	1/1	0.99	0.16	63,63,63,63	0
57	MG	14	3305	1/1	0.99	0.17	57,57,57,57	0
57	MG	14	3306	1/1	0.99	0.10	55,55,55,55	0
57	MG	14	3307	1/1	0.99	0.12	79,79,79,79	0
57	MG	1H	3499	1/1	0.99	0.26	67,67,67,67	0
57	MG	1H	3060	1/1	0.99	0.37	55,55,55,55	0
57	MG	14	3409	1/1	0.99	0.14	80,80,80,80	0
57	MG	1H	3331	1/1	0.99	0.07	66,66,66,66	0
57	MG	14	3002	1/1	0.99	0.12	49,49,49,49	0
57	MG	13	1602	1/1	0.99	0.41	88,88,88,88	0
57	MG	13	1697	1/1	0.99	0.10	90,90,90,90	0
57	MG	1H	3443	1/1	0.99	0.08	67,67,67,67	0
57	MG	1H	3383	1/1	0.99	0.05	78,78,78,78	0
57	MG	1H	3294	1/1	0.99	0.13	56,56,56,56	0
57	MG	14	3417	1/1	0.99	0.07	87,87,87,87	0
57	MG	14	3418	1/1	0.99	0.05	75,75,75,75	0
57	MG	1H	3295	1/1	0.99	0.11	52,52,52,52	0
57	MG	14	3420	1/1	0.99	0.12	65,65,65,65	0
57	MG	1H	3296	1/1	0.99	0.18	49,49,49,49	0
57	MG	1H	3297	1/1	0.99	0.14	49,49,49,49	0
57	MG	16	208	1/1	0.99	0.05	67,67,67,67	0
57	MG	1H	3388	1/1	0.99	0.14	57,57,57,57	0
57	MG	14	3322	1/1	0.99	0.14	74,74,74,74	0
57	MG	1H	3389	1/1	0.99	0.16	59,59,59,59	0
57	MG	1H	3338	1/1	0.99	0.18	53,53,53,53	0
57	MG	1H	3339	1/1	0.99	0.09	50,50,50,50	0
57	MG	13	1683	1/1	0.99	0.21	67,67,67,67	0
57	MG	14	3327	1/1	0.99	0.06	67,67,67,67	0
57	MG	1H	3172	1/1	0.99	0.14	73,73,73,73	0
57	MG	14	3432	1/1	0.99	0.10	83,83,83,83	0
57	MG	1H	3300	1/1	0.99	0.11	54,54,54,54	0
57	MG	14	3019	1/1	0.99	0.33	58,58,58,58	0
57	MG	14	3331	1/1	0.99	0.09	66,66,66,66	0
57	MG	1H	3396	1/1	0.99	0.08	60,60,60,60	0
57	MG	1H	3343	1/1	0.99	0.07	74,74,74,74	0
57	MG	1H	3064	1/1	0.99	0.23	54,54,54,54	0
57	MG	14	3023	1/1	0.99	0.30	54,54,54,54	0
57	MG	1H	3302	1/1	0.99	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	1H	3346	1/1	0.99	0.11	58,58,58,58	0
57	MG	1G	1656	1/1	0.99	0.19	105,105,105,105	0
57	MG	14	3339	1/1	0.99	0.07	86,86,86,86	0
57	MG	1H	3401	1/1	0.99	0.10	52,52,52,52	0
57	MG	14	3341	1/1	0.99	0.07	62,62,62,62	0
57	MG	14	3028	1/1	0.99	0.21	60,60,60,60	0
57	MG	13	1717	1/1	0.99	0.10	66,66,66,66	0
57	MG	1H	3304	1/1	0.99	0.11	55,55,55,55	0
57	MG	1G	1660	1/1	0.99	0.03	96,96,96,96	0
57	MG	14	3249	1/1	0.99	0.28	60,60,60,60	0
57	MG	1H	3349	1/1	0.99	0.17	53,53,53,53	0
57	MG	1H	3305	1/1	0.99	0.09	53,53,53,53	0
57	MG	14	3453	1/1	0.99	0.04	88,88,88,88	0
57	MG	14	3252	1/1	0.99	0.19	67,67,67,67	0
57	MG	1H	3351	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3306	1/1	0.99	0.09	60,60,60,60	0
57	MG	1H	3408	1/1	0.99	0.11	50,50,50,50	0
57	MG	1H	3353	1/1	0.99	0.09	57,57,57,57	0
57	MG	1H	3307	1/1	0.99	0.06	57,57,57,57	0
57	MG	14	3355	1/1	0.99	0.12	59,59,59,59	0
57	MG	1H	3355	1/1	0.99	0.10	68,68,68,68	0
57	MG	29	302	1/1	0.99	0.29	40,40,40,40	0
57	MG	1H	3309	1/1	0.99	0.12	48,48,48,48	0
57	MG	13	1732	1/1	0.99	0.08	108,108,108,108	0
57	MG	1H	3358	1/1	0.99	0.12	67,67,67,67	0
57	MG	1H	3415	1/1	0.99	0.10	52,52,52,52	0
57	MG	1H	3311	1/1	0.99	0.10	53,53,53,53	0
57	MG	14	3362	1/1	0.99	0.05	62,62,62,62	0
57	MG	1H	3417	1/1	0.99	0.11	56,56,56,56	0
57	MG	14	3046	1/1	0.99	0.41	58,58,58,58	0
57	MG	13	1690	1/1	0.99	0.14	68,68,68,68	0
57	MG	1H	3419	1/1	0.99	0.06	63,63,63,63	0
57	MG	85	201	1/1	0.99	0.20	72,72,72,72	0
57	MG	14	3367	1/1	0.99	0.05	60,60,60,60	0
57	MG	1H	3361	1/1	0.99	0.08	53,53,53,53	0
57	MG	1H	3051	1/1	0.99	0.16	93,93,93,93	0
57	MG	1H	3016	1/1	0.99	0.40	49,49,49,49	0
57	MG	1H	3239	1/1	0.99	0.09	67,67,67,67	0
59	SF4	3E	301	8/8	0.99	0.19	71,78,87,91	0
59	SF4	32	301	8/8	0.99	0.17	100,111,117,118	0
60	ZN	5I	102	1/1	0.99	0.13	88,88,88,88	0
57	MG	1G	1681	1/1	0.99	0.04	85,85,85,85	0

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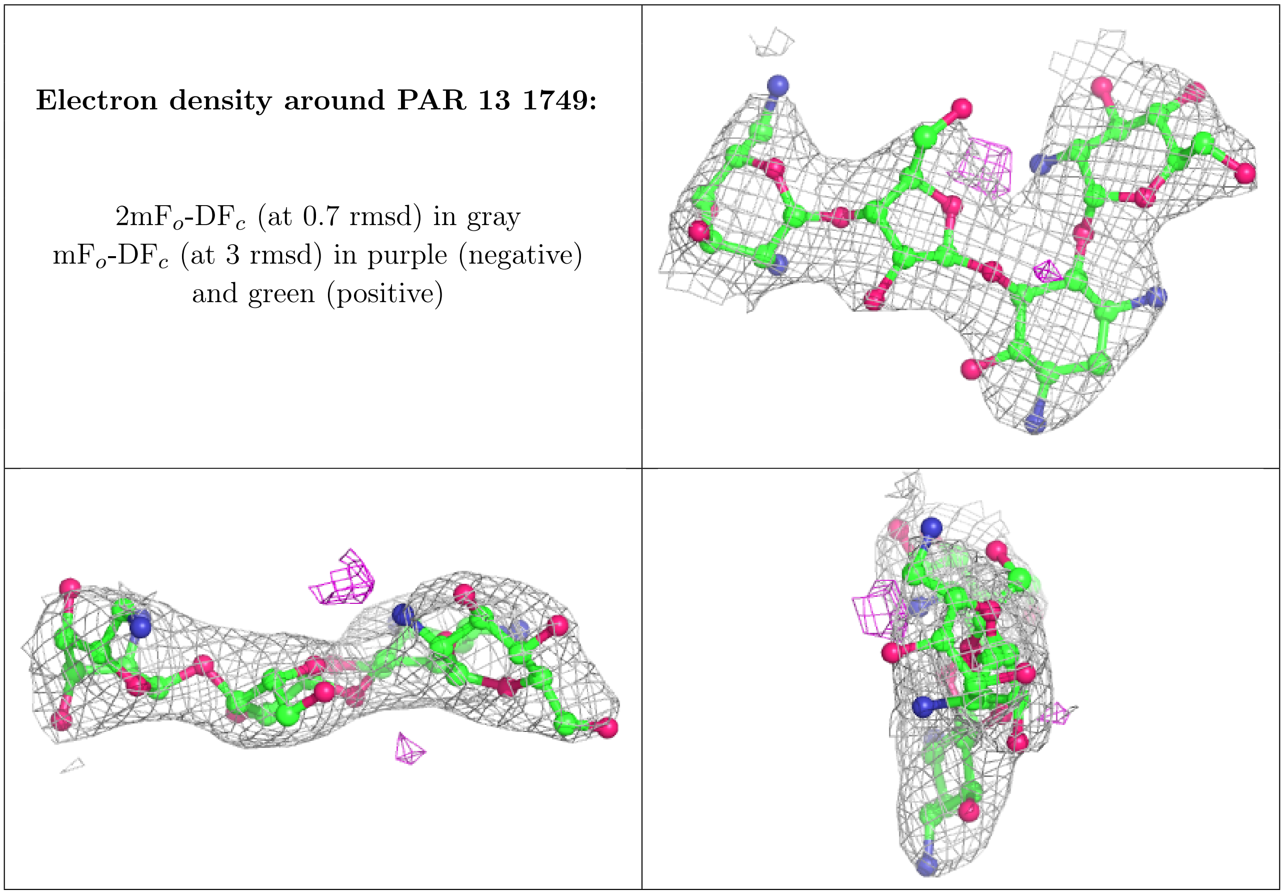
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3365	1/1	0.99	0.10	70,70,70,70	0
57	MG	14	3274	1/1	0.99	0.13	62,62,62,62	0
57	MG	14	3293	1/1	1.00	0.09	51,51,51,51	0
57	MG	14	3294	1/1	1.00	0.11	54,54,54,54	0
57	MG	1H	3390	1/1	1.00	0.08	57,57,57,57	0
57	MG	1H	3312	1/1	1.00	0.05	76,76,76,76	0
57	MG	1H	3308	1/1	1.00	0.08	61,61,61,61	0
57	MG	1H	3423	1/1	1.00	0.10	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

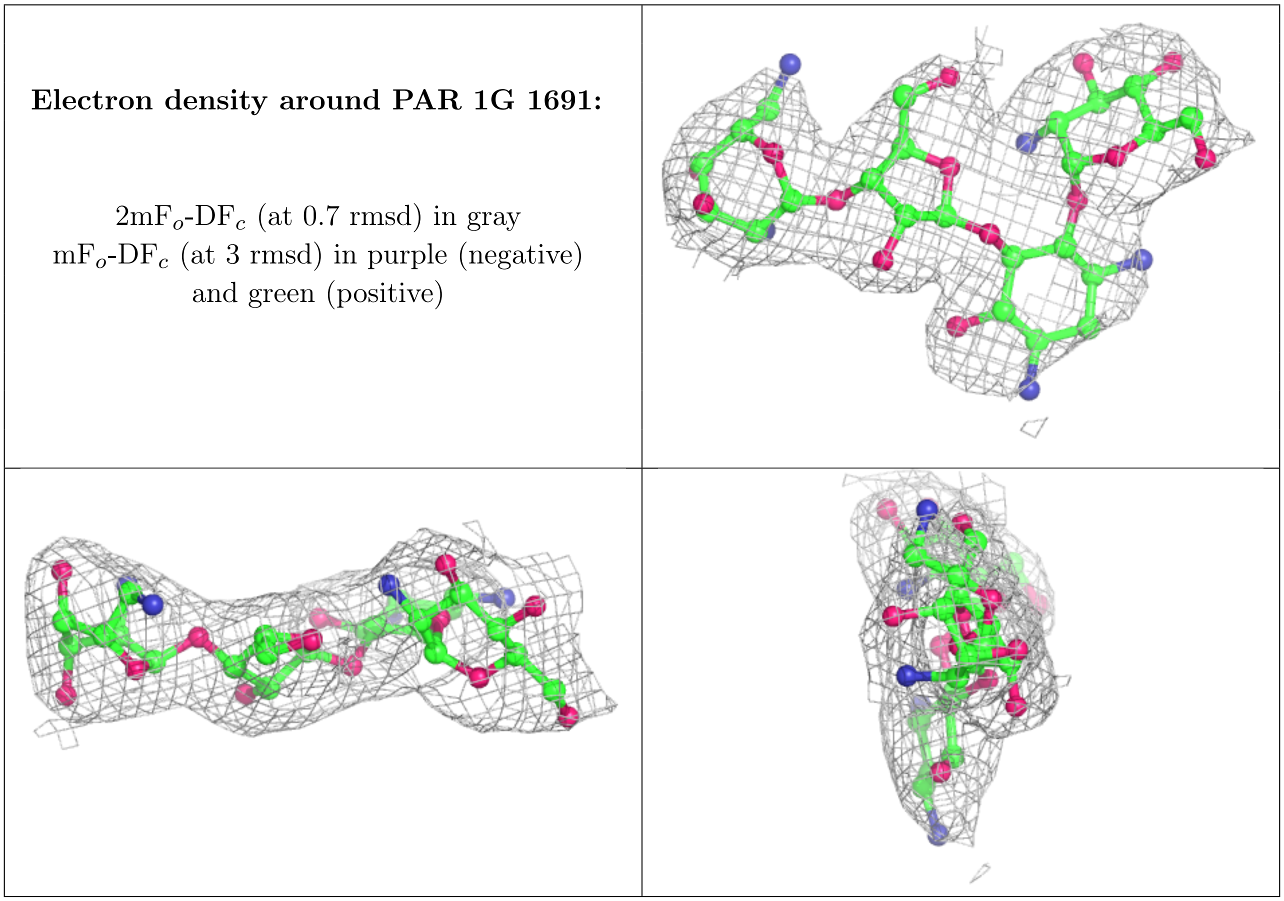


Electron density around PAR 13 1749:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PAR 1G 1691:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.