wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 01:02 am GMT

PDB ID	:	5IB7
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet, near-cognate tRNALys with U-G mismatch in the A-site and antibiotic paromomycin
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2016-02-22
Resolution	:	2.99 Å(reported)

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

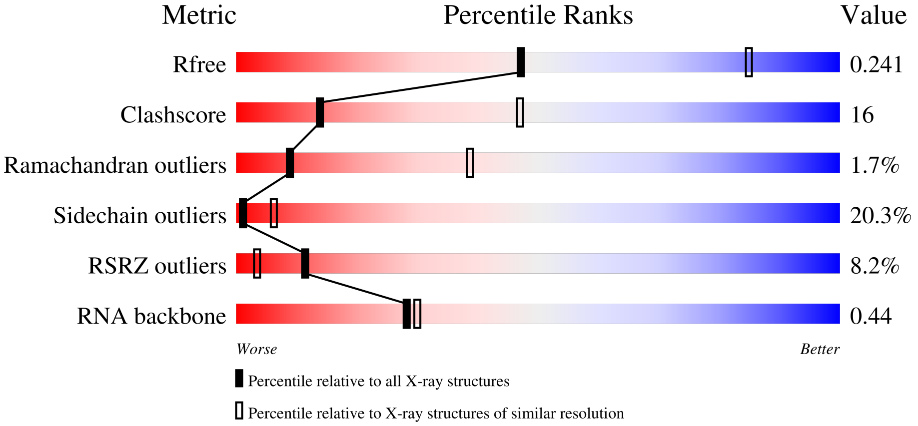
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

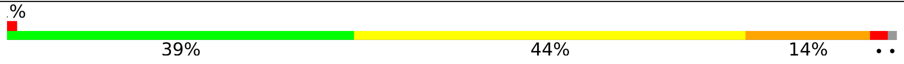
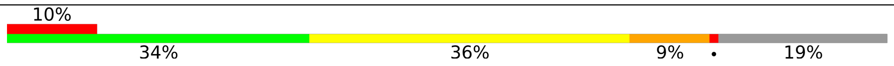
The reported resolution of this entry is 2.99 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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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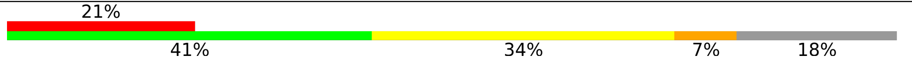
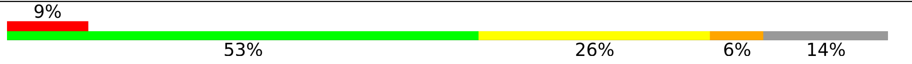
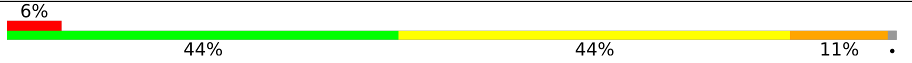
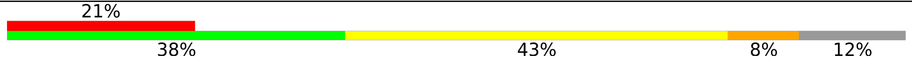
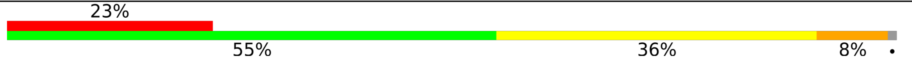
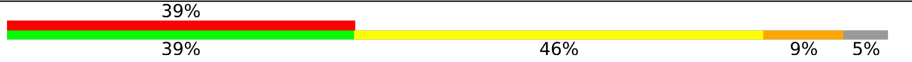
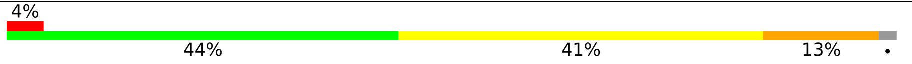
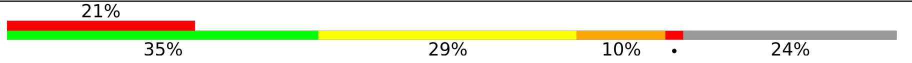
Mol	Chain	Length	Quality of chain
2	1E	256	
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
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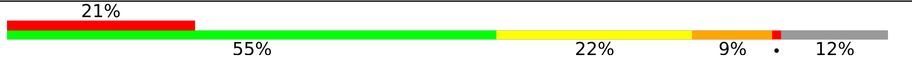
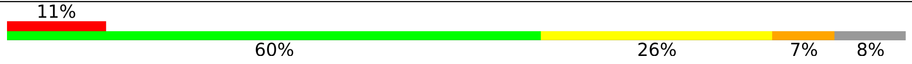
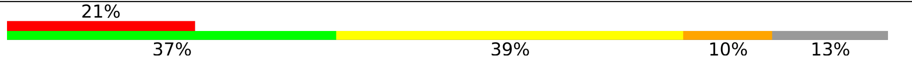
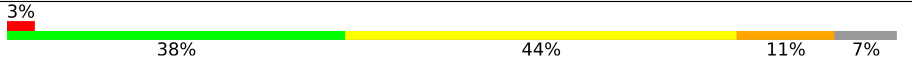
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	

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Mol	Chain	Length	Quality of chain
15	6A	89	3% 61% 35% • •
15	6I	89	3% 55% 35% 8% •
16	7A	88	2% 58% 34% • 5%
16	7I	88	23% 40% 44% 10% 6%
17	8A	105	26% 63% 30% • 6%
17	8I	105	17% 48% 42% 5% 6%
18	9A	88	5% 43% 28% 5% 24%
18	9I	88	2% 44% 27% 6% 23%
19	AA	93	14% 40% 27% • • 30%
19	AI	93	3% 46% 30% 12% 12%
20	BA	106	17% 48% 37% 8% • 7%
20	BI	106	25% 42% 41% 8% 8%
21	1B	27	30% 48% 30% • 19%
21	1F	27	44% 26% 15% 15%
22	1K	76	7% 26% 47% 18% • 5%
23	2K	77	% 42% 40% 14% •
23	2L	77	40% 44% 12% •
24	1L	76	14% 32% 38% 14% • 13%
24	3K	76	13% 17% 37% 36% • 8%
24	3L	76	4% 21% 46% 26% • 5%
25	4K	30	13% 23% 23% 17% 37%
25	4L	30	10% 10% 30% 20% • 37%
26	14	2917	% 34% 41% 18% • •
26	1H	2917	32% 41% 21% • •
27	16	122	% 44% 35% 15% 6%

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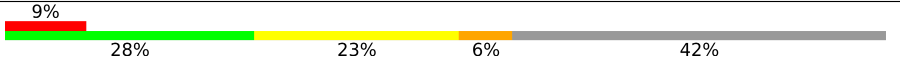
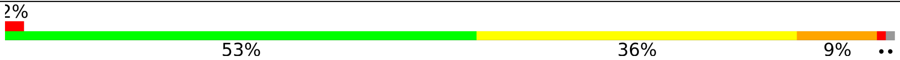
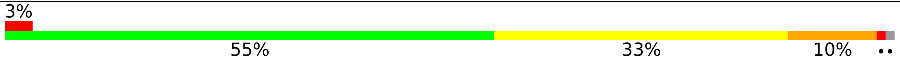
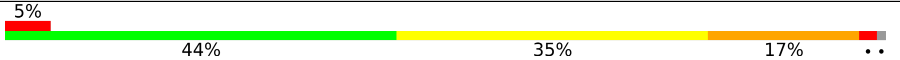
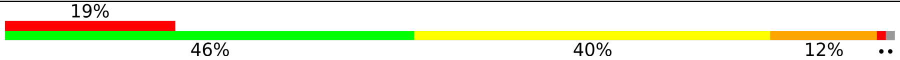
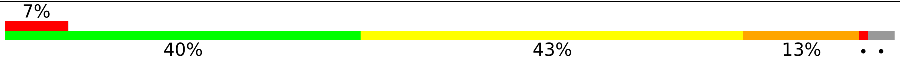
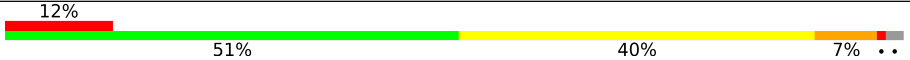
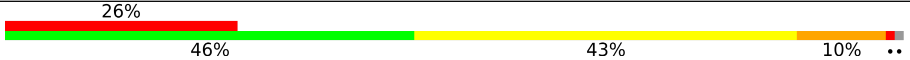
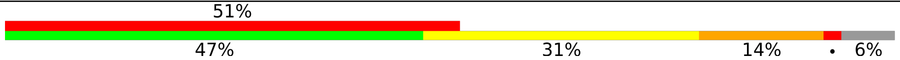
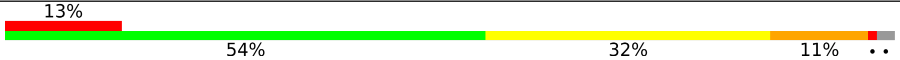
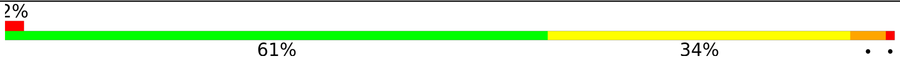
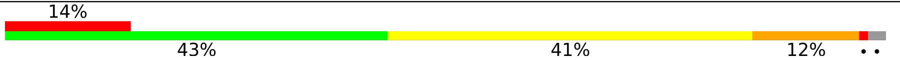
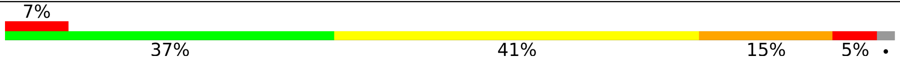
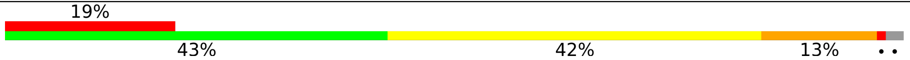
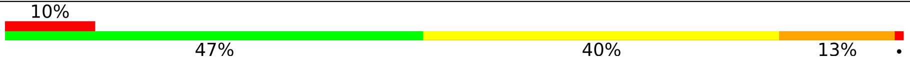
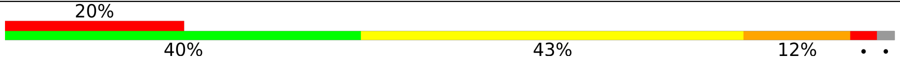
Mol	Chain	Length	Quality of chain
27	1J	122	
28	71	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	

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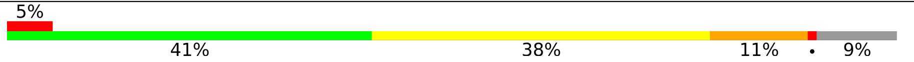
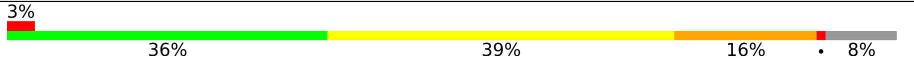
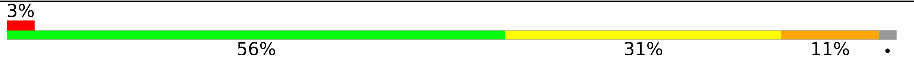
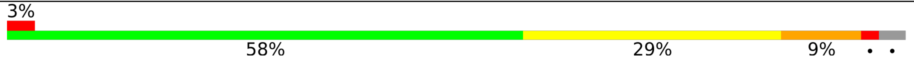
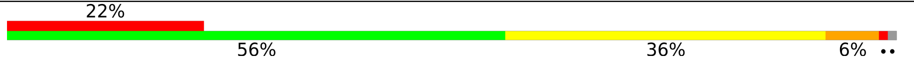
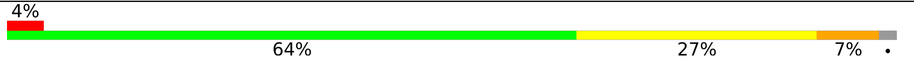
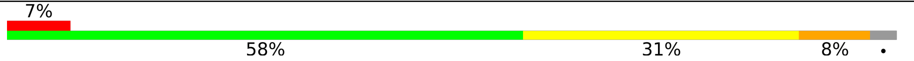
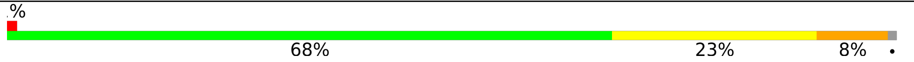
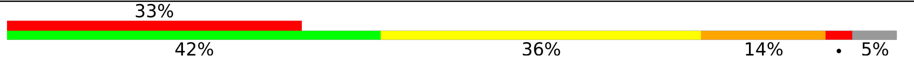
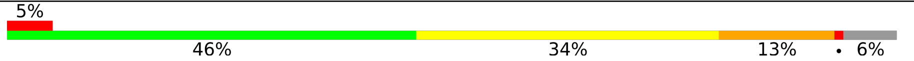
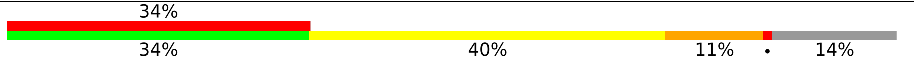
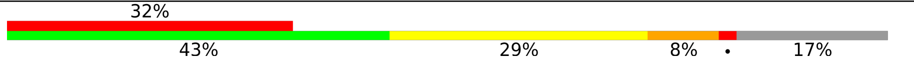
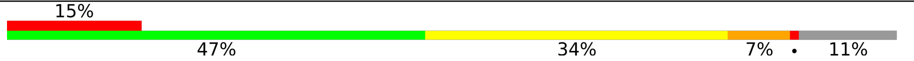
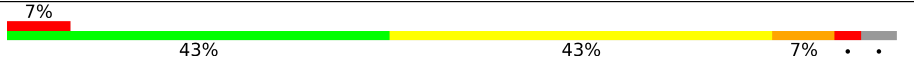
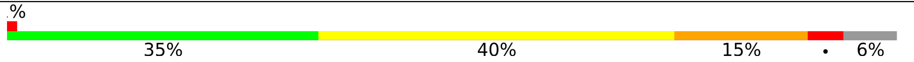
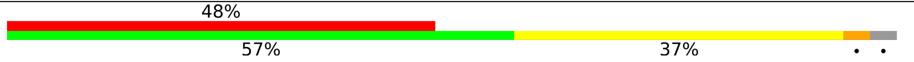
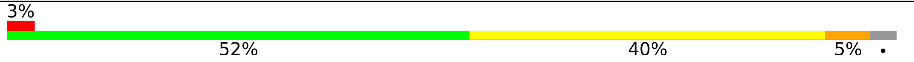
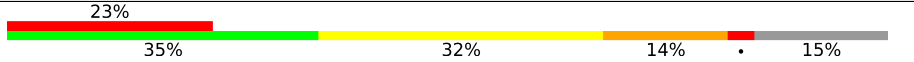
Mol	Chain	Length	Quality of chain
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	

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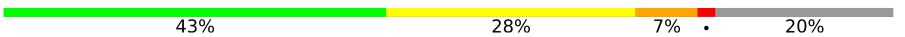
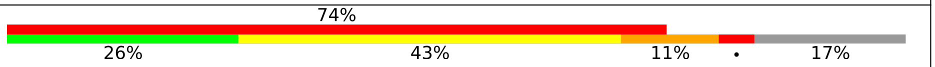
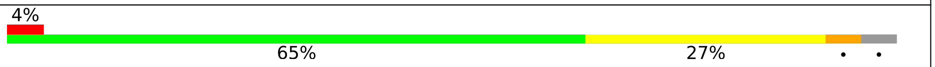
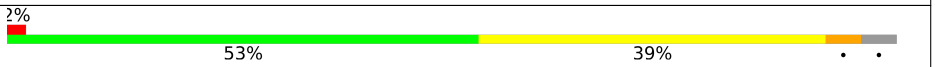
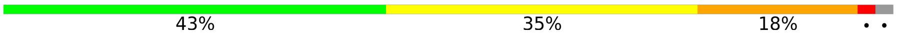
Mol	Chain	Length	Quality of chain
53	N8	60	
54	O8	54	
55	L5	49	
55	P8	49	
56	M5	65	
56	Q8	65	

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	13	1647	-	-	-	X
57	MG	13	1662	-	-	-	X
57	MG	13	1664	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1673	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	14	3064	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3109	-	-	-	X
57	MG	14	3115	-	-	-	X
57	MG	14	3118	-	-	-	X
57	MG	14	3127	-	-	-	X
57	MG	14	3128	-	-	-	X
57	MG	14	3132	-	-	-	X
57	MG	14	3138	-	-	-	X
57	MG	14	3161	-	-	-	X
57	MG	14	3166	-	-	-	X
57	MG	14	3173	-	-	-	X
57	MG	14	3185	-	-	-	X
57	MG	14	3197	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1609	-	-	-	X
57	MG	1G	1618	-	-	-	X
57	MG	1G	1634	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3004	-	-	-	X
57	MG	1H	3053	-	-	-	X
57	MG	1H	3065	-	-	-	X
57	MG	1H	3081	-	-	-	X
57	MG	1H	3111	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3135	-	-	-	X
57	MG	1H	3144	-	-	-	X
57	MG	1H	3145	-	-	-	X
57	MG	1H	3150	-	-	-	X
57	MG	1H	3153	-	-	-	X
57	MG	1H	3163	-	-	-	X
57	MG	1H	3168	-	-	-	X
57	MG	1H	3177	-	-	-	X
57	MG	1H	3180	-	-	-	X
57	MG	1H	3205	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3211	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3237	-	-	-	X
57	MG	E5	101	-	-	-	X
57	MG	P8	101	-	-	-	X
59	SF4	32	302	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	13	1499	Total C N O P 32223 14342 5973 10409 1499	0	0	0
1	1G	1508	Total C N O P 32414 14427 6005 10474 1508	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
2	1E	231	Total C N O S 1874 1199 334 336 5	0	0	0
2	12	207	Total C N O S 1696 1083 306 303 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	2E	205	Total C N O S 1605 1011 313 280 1	0	0	0
3	22	195	Total C N O S 1537 973 297 266 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 1698	C 1064	N 338	O 289	S 7	0	0	0
4	32	208	Total 1702	C 1066	N 339	O 290	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total 1142	C 722	N 216	O 200	S 4	0	0	0
5	42	150	Total 1141	C 719	N 217	O 201	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1I	94	Total C N O S 749 468 147 133 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	121	Total C N O S 947 597 191 158 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	4I	117	Total C N O S 933 577 192 162 2	0	0	0
13	4A	109	Total C N O S 879 544 181 152 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	59	Total C N O S 486 309 103 70 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
			Total	C	N	O	S			
15	6I	87	729	457	146	124	2	0	0	0
15	6A	87	729	457	146	124	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	7I	83	700	443	139	117	1	0	0	0
16	7A	84	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
			Total	C	N	O	S			
17	8I	99	823	528	151	142	2	0	0	0
17	8A	99	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
			Total	C	N	O			
18	9I	68	549	352	105	92	0	0	0
18	9A	67	544	349	104	91	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AI	82	661	422	123	114	2	0	0	0
19	AA	65	510	324	92	92	2	0	0	0

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	1K	72	Total C N O P S 1542 691 269 509 72 1	0	0	0

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	3K	70	Total C N O P 1483 664 260 490 69	0	0	0
24	1L	66	Total C N O P 1401 626 244 465 66	0	0	0
24	3L	72	Total C N O P 1528 684 270 503 71	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	4K	19	Total C N O P 420 188 89 124 19	0	0	0

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2860	Total 61609	C 27418	N 11525	O 19806	P 2860	0	0	0
26	14	2826	Total 60877	C 27092	N 11393	O 19566	P 2826	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	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total 1027	C 648	N 193	O 185	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total 1546	C 978	N 295	O 267	S 6	0	0	0
30	29	204	Total 1563	C 988	N 299	O 270	S 6	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total 1457	C 931	N 265	O 257	S 4	0	0	0
32	49	180	Total 1459	C 931	N 266	O 258	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total 1328	C 842	N 249	O 236	S 1	0	0	0
33	59	169	Total 1295	C 823	N 241	O 230	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	58	137	Total C N O S 1096 706 205 181 4	0	0	0
35	15	137	Total C N O S 1096 707 205 181 3	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	88	141	Total C N O S 1117 712 211 187 7	0	0	0
38	45	138	Total C N O S 1099 702 208 183 6	0	0	0

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	B8	135	1119	697	230	191	1	0	0	0
41	75	133	1109	691	228	189	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	D8	100	774	499	141	133	1	0	0	0
43	95	100	770	496	140	133	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	E8	110	876	552	171	151	2	0	0	0
44	A5	111	886	558	174	152	2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	F8	95	Total C N O S 750 488 135 126 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	103	Total C N O S 783 504 148 126 5	0	0	0
46	C5	104	Total C N O S 794 510 152 127 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	H8	170	Total C N O S 1365 870 246 246 3	0	0	0
47	D5	177	Total C N O S 1411 901 253 255 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	I8	77	Total C N O S 611 378 129 103 1	0	0	0
48	E5	76	Total C N O S 603 372 128 102 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	J8	96	Total C N O S 747 469 148 129 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	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

- 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	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	13	140	140	140	0	0
57	3I	1	1	1	0	0
57	4I	1	1	1	0	0
57	5I	1	1	1	0	0
57	2K	2	2	2	0	0
57	1H	525	525	525	0	0
57	16	11	11	11	0	0
57	21	3	3	3	0	0
57	31	2	2	2	0	0
57	41	1	1	1	0	0
57	78	1	1	1	0	0
57	88	3	3	3	0	0
57	I8	2	2	2	0	0
57	P8	1	1	1	0	0
57	Q8	1	1	1	0	0
57	1G	102	102	102	0	0
57	32	1	1	1	0	0
57	42	1	1	1	0	0

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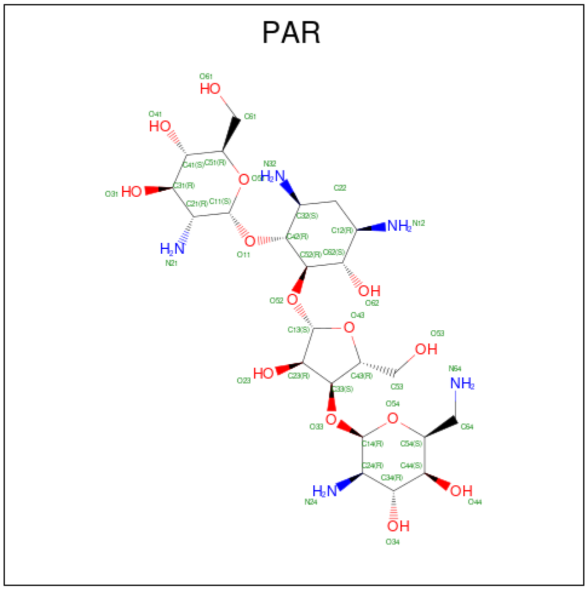
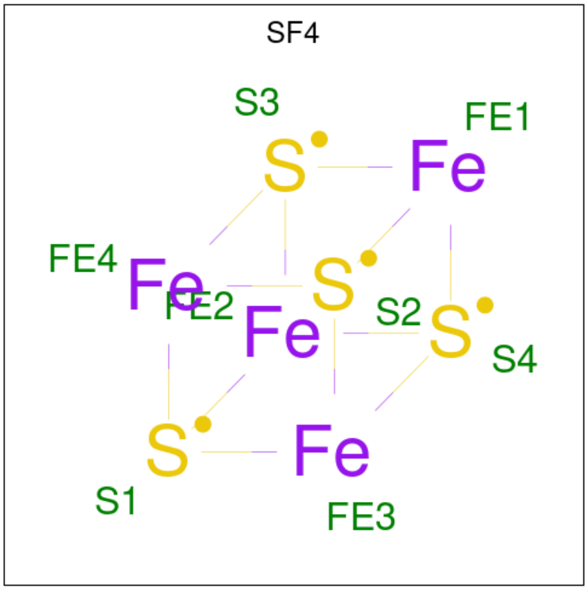
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	52	1	Total Mg 1 1	0	0
57	7A	1	Total Mg 1 1	0	0
57	2L	2	Total Mg 2 2	0	0
57	4L	1	Total Mg 1 1	0	0
57	14	435	Total Mg 435 435	0	0
57	1J	8	Total Mg 8 8	0	0
57	19	1	Total Mg 1 1	0	0
57	29	1	Total Mg 1 1	0	0
57	39	2	Total Mg 2 2	0	0
57	25	1	Total Mg 1 1	0	0
57	35	1	Total Mg 1 1	0	0
57	45	2	Total Mg 2 2	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).

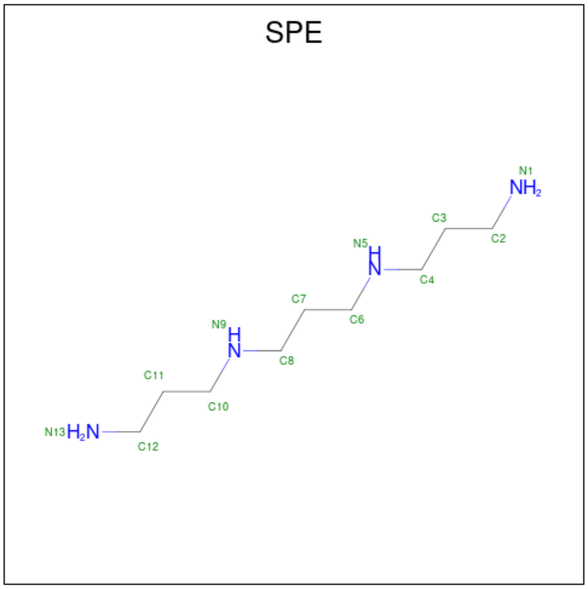


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	3E	1	Total Fe S 8 4 4	0	0
59	32	1	Total Fe S 8 4 4	0	0

- 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 THERMINE (three-letter code: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	13	320	Total O 320 320	0	0
62	4E	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	8E	2	Total O 2 2	0	0
62	1I	2	Total O 2 2	0	0
62	3I	2	Total O 2 2	0	0
62	5I	2	Total O 2 2	0	0
62	6I	3	Total O 3 3	0	0
62	7I	1	Total O 1 1	0	0
62	BI	2	Total O 2 2	0	0
62	1F	1	Total O 1 1	0	0
62	1K	2	Total O 2 2	0	0
62	2K	8	Total O 8 8	0	0
62	4K	5	Total O 5 5	0	0
62	1H	1470	Total O 1470 1470	0	0
62	16	12	Total O 12 12	0	0
62	11	17	Total O 17 17	0	0
62	21	7	Total O 7 7	0	0
62	31	5	Total O 5 5	0	0
62	41	1	Total O 1 1	0	0
62	58	2	Total O 2 2	0	0
62	78	10	Total O 10 10	0	0
62	B8	1	Total O 1 1	0	0
62	C8	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	F8	2	Total O 2 2	0	0
62	G8	2	Total O 2 2	0	0
62	I8	6	Total O 6 6	0	0
62	J8	4	Total O 4 4	0	0
62	L8	3	Total O 3 3	0	0
62	P8	1	Total O 1 1	0	0
62	Q8	5	Total O 5 5	0	0
62	1G	317	Total O 317 317	0	0
62	32	1	Total O 1 1	0	0
62	52	4	Total O 4 4	0	0
62	1A	1	Total O 1 1	0	0
62	6A	2	Total O 2 2	0	0
62	7A	5	Total O 5 5	0	0
62	9A	2	Total O 2 2	0	0
62	BA	2	Total O 2 2	0	0
62	2L	6	Total O 6 6	0	0
62	4L	6	Total O 6 6	0	0
62	14	1144	Total O 1144 1144	0	0
62	1J	12	Total O 12 12	0	0
62	19	15	Total O 15 15	0	0
62	29	4	Total O 4 4	0	0

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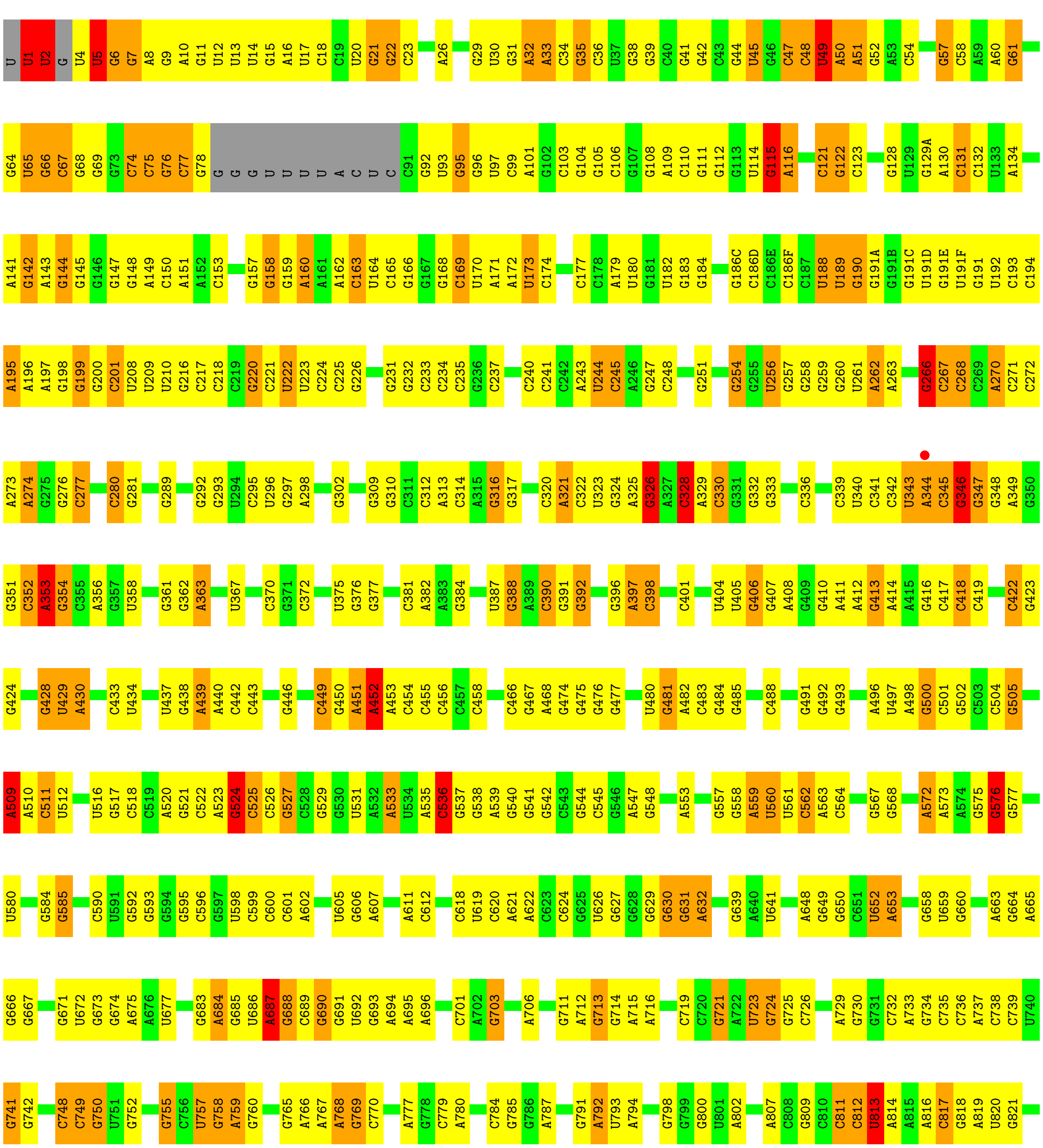
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	39	5	Total O 5 5	0	0
62	15	1	Total O 1 1	0	0
62	25	6	Total O 6 6	0	0
62	35	8	Total O 8 8	0	0
62	55	3	Total O 3 3	0	0
62	85	2	Total O 2 2	0	0
62	A5	1	Total O 1 1	0	0
62	B5	1	Total O 1 1	0	0
62	C5	3	Total O 3 3	0	0
62	F5	1	Total O 1 1	0	0
62	H5	2	Total O 2 2	0	0
62	M5	9	Total O 9 9	0	0

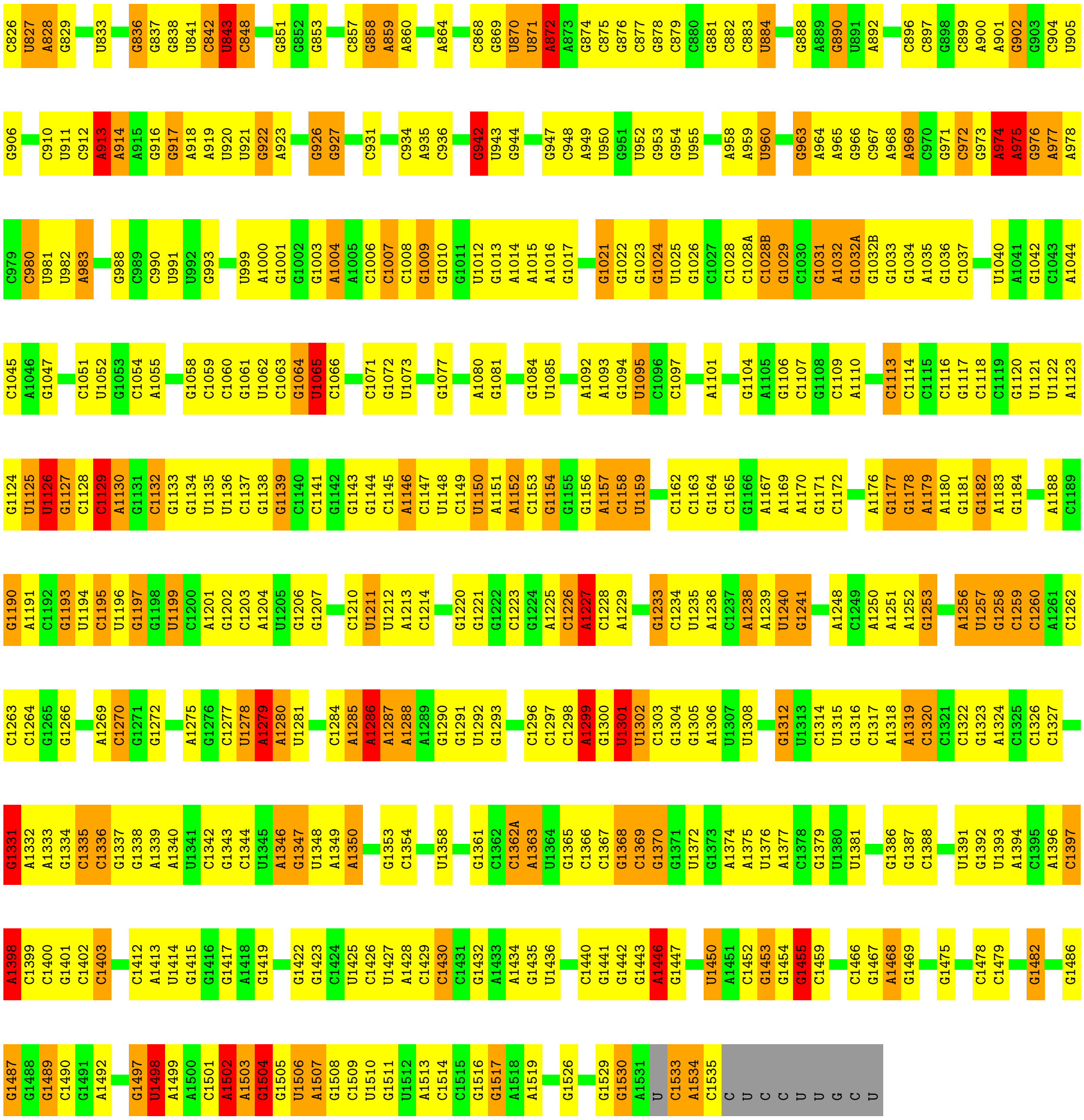
3 Residue-property plots ⓘ

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

- Molecule 1: 16S ribosomal RNA

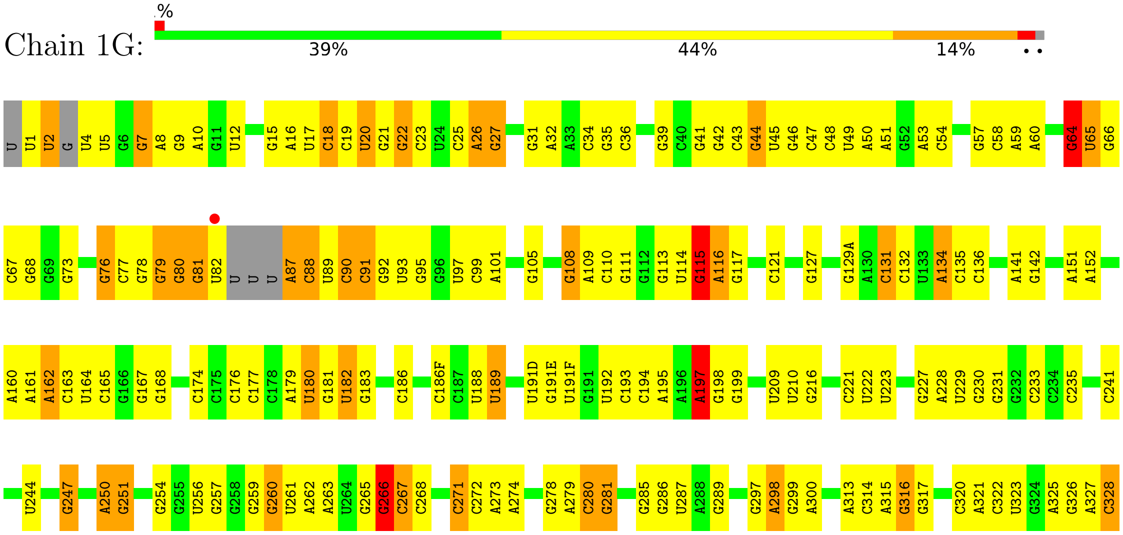
Chain 13:

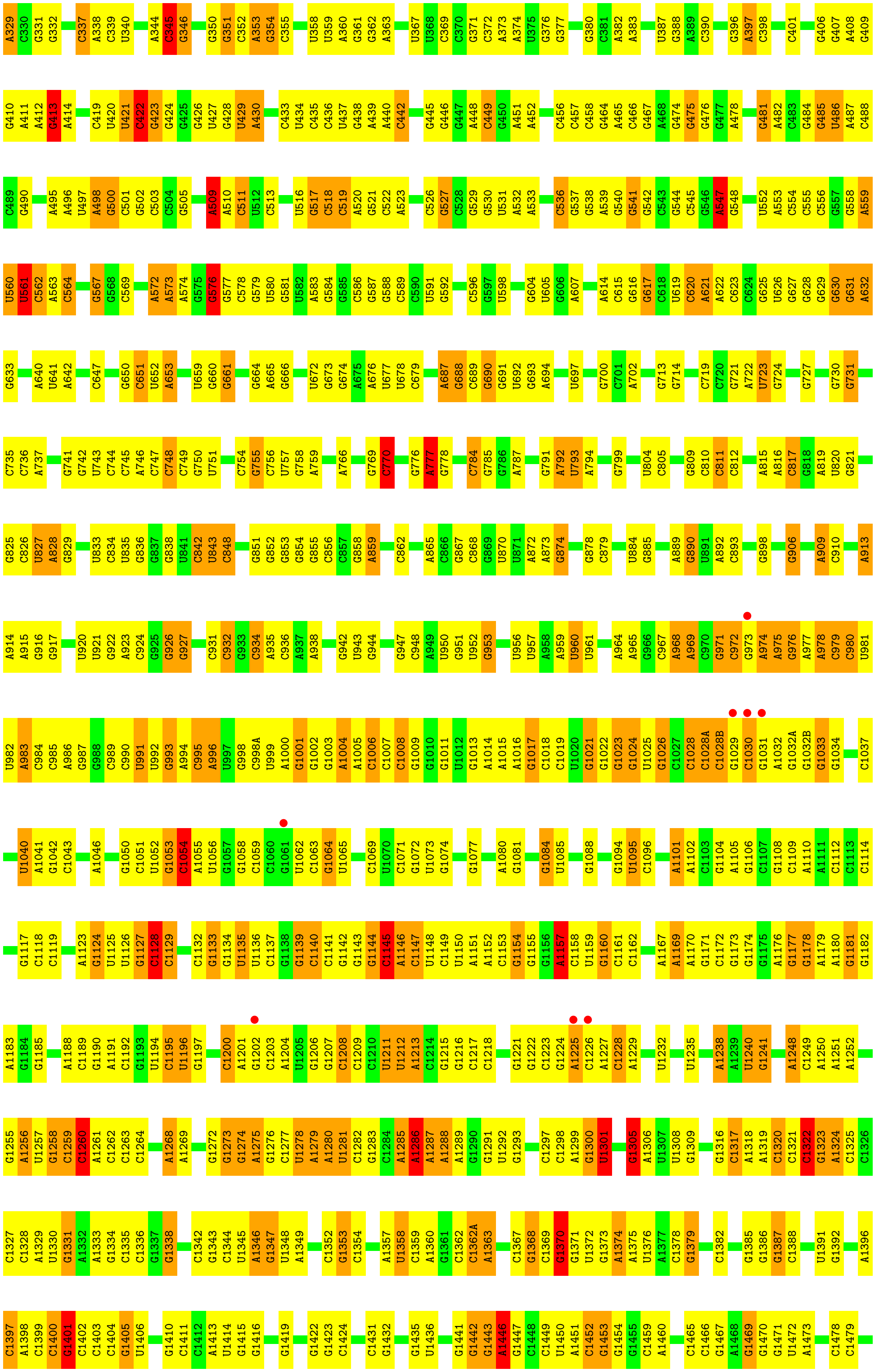




- Molecule 1: 16S ribosomal RNA

Chain 1G:

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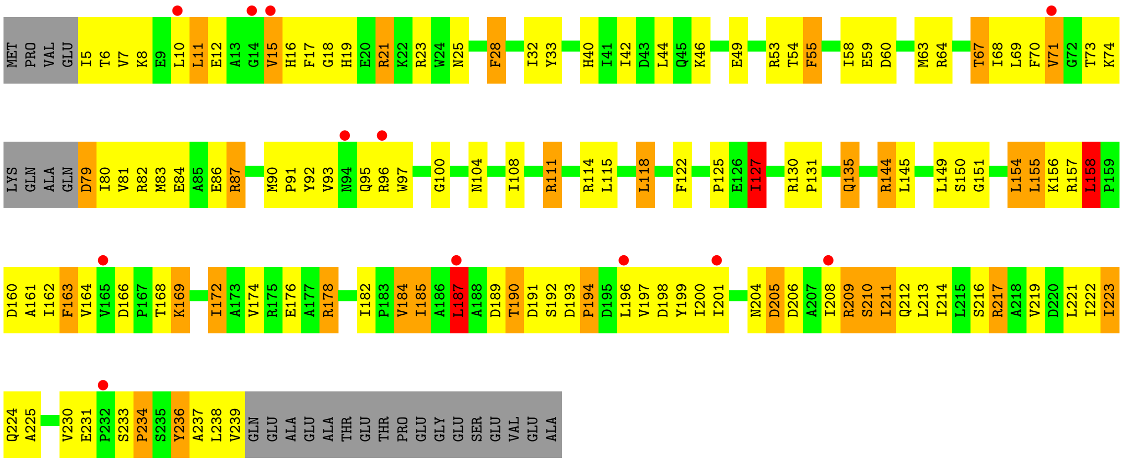
G410 A411 A412 G413 A414 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 C433 U434 C435 C436 U437 G438 A439 A440 C442 G445 G446 G447 A448 C449 G450 A451 A452 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G476 G477 A478 G481 A482 C483 G484 G485 U486 A487 C488
C489 G490 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 U516 G517 C518 C519 A520 G521 C522 A523 C526 G527 C528 G529 G530 U531 A532 A533 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 U552 A553 C554 C555 C556 G557 G558 A559
U560 U561 C562 A563 C564 G567 G568 C569 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 C596 G597 U598 G604 U605 G606 A607 A614 C615 G616 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632
G633 A640 U641 A642 C647 G650 C651 U652 A653 U659 G660 G661 G664 A665 G666 U672 G673 G674 A675 A676 U677 U678 C679 A687 G688 C689 G690 G691 U692 G693 A694 U697 G700 C701 A702 G713 G714 C719 C720 G721 A722 U723 G724 G727 G730 G731
C735 C736 A737 G741 G742 U743 C744 G745 A746 C747 C748 C749 G750 U751 C754 G755 C756 U757 G758 A759 A766 G769 C770 G776 A777 G778 C784 G785 G786 A787 G791 A792 U793 A794 G799 U804 C805 G809 C810 C811 C812 A815 A816 C817 G818 A819 U820 G821
G825 C826 U827 A828 G829 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 G851 G852 G853 G854 G855 C856 C857 G858 A859 C862 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 G878 C879 U884 G885 A889 G890 U891 A892 C893 G898 G906 A909 C910 A913
A914 A915 G916 G917 U920 U921 G922 A923 C924 G925 G926 G927 C931 C932 G933 C934 A935 C936 A937 A938 G942 U943 G944 G947 C948 A949 U950 G951 U952 G953 U956 U957 A958 A959 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981
U982 A983 C984 G985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1034 C1037
U1040 A1041 G1042 C1043 A1046 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1069 U1070 C1071 G1072 U1073 G1074 G1077 A1080 G1081 G1084 U1085 G1088 G1094 U1095 C1096 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114
G1117 C1118 C1119 A1123 G1124 U1125 U1126 G1127 C1128 C1129 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1167 A1169 A1170 C1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182
A1183 G1184 G1185 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 U1232 U1235 A1238 A1239 U1240 G1241 A1248 C1249 A1250 A1251 A1252
G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 A1268 A1269 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 C1297 C1298 A1299 G1300 U1301 G1305 A1306 U1307 U1308 G1309 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326
C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 C1335 C1336 G1337 G1338 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 C1352 G1353 C1354 A1357 U1358 C1359 A1360 G1361 C1362 C1362A A1363 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 C1382 G1385 G1386 G1387 C1388 U1391 G1392 A1396
C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 G1410 C1411 C1412 A1413 U1414 G1415 G1416 G1419 G1422 G1423 C1424 C1431 G1432 G1435 U1436 G1441 G1442 G1443 A1446 C1447 C1448 C1449 U1450 A1451 C1452 G1453 G1454 G1455 C1459 A1460 C1465 C1466 G1467 A1468 G1469 G1470 U1471 U1472 A1473 C1478 C1479

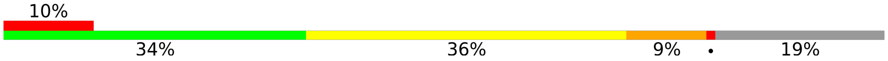
- Molecule 2: 30S ribosomal protein S2

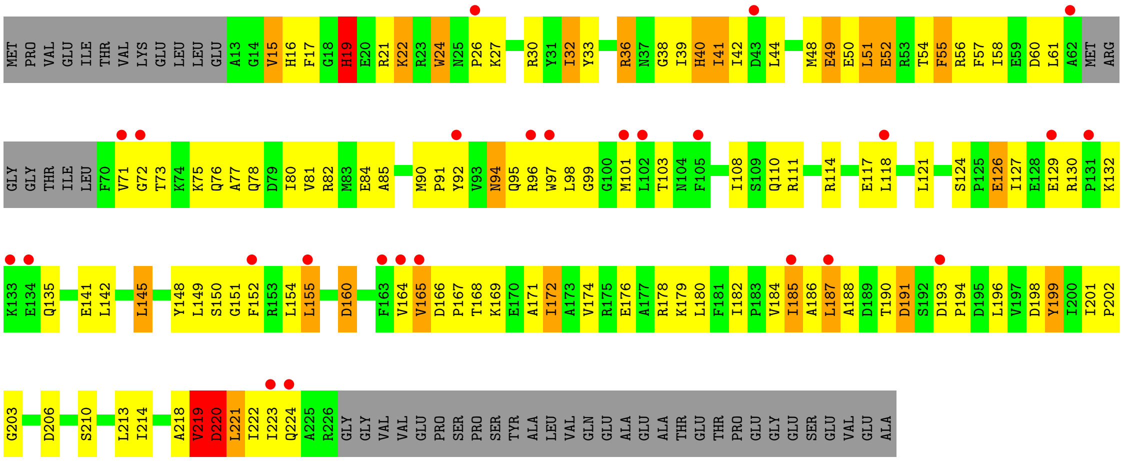
Chain 1E:



- Molecule 2: 30S ribosomal protein S2

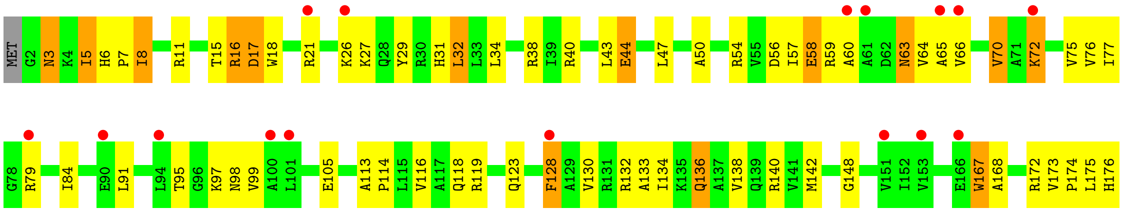
Chain 12:

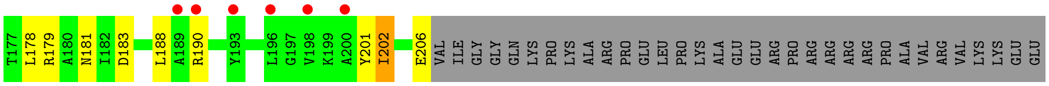




- Molecule 3: 30S ribosomal protein S3

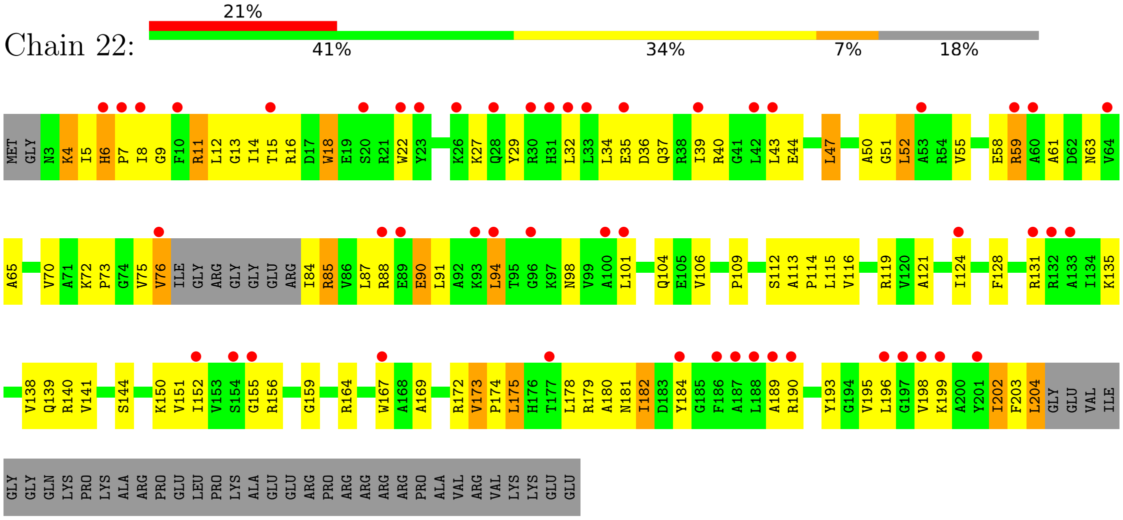
Chain 2E:





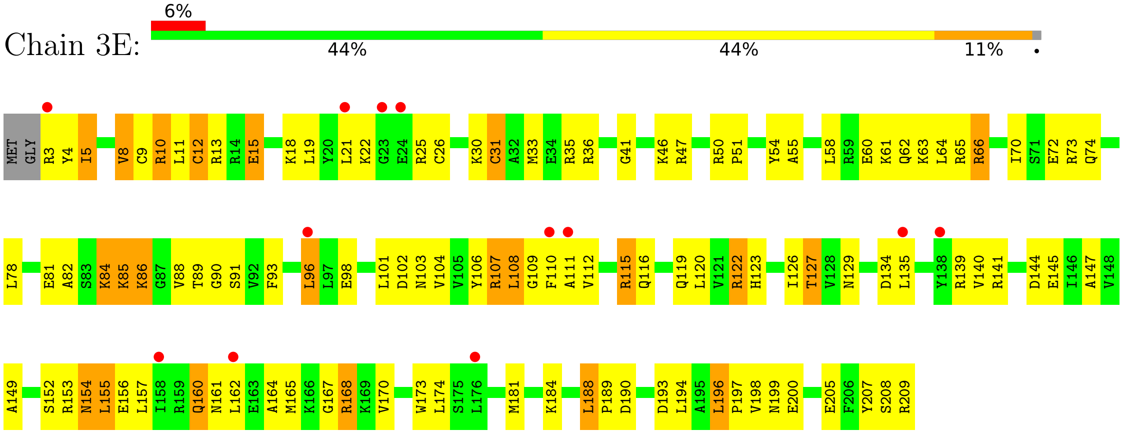
- Molecule 3: 30S ribosomal protein S3

Chain 22:



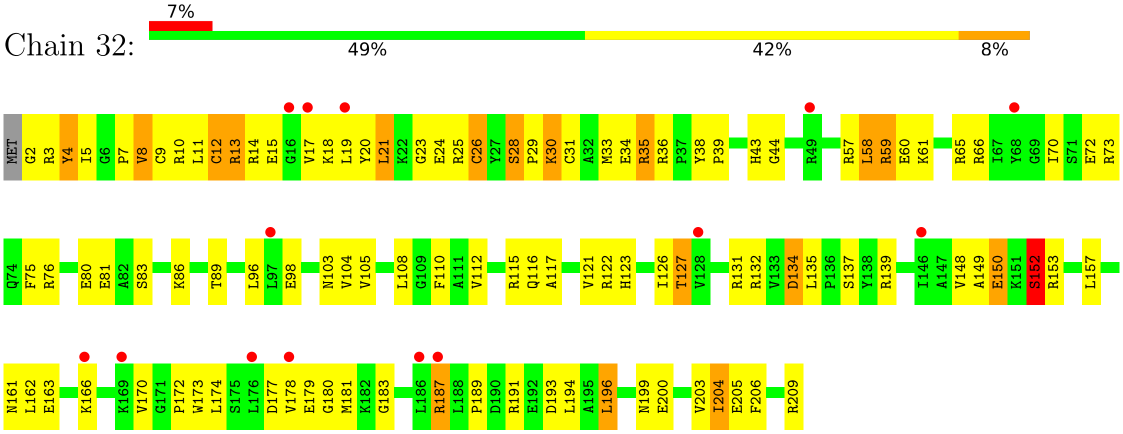
- Molecule 4: 30S ribosomal protein S4

Chain 3E:



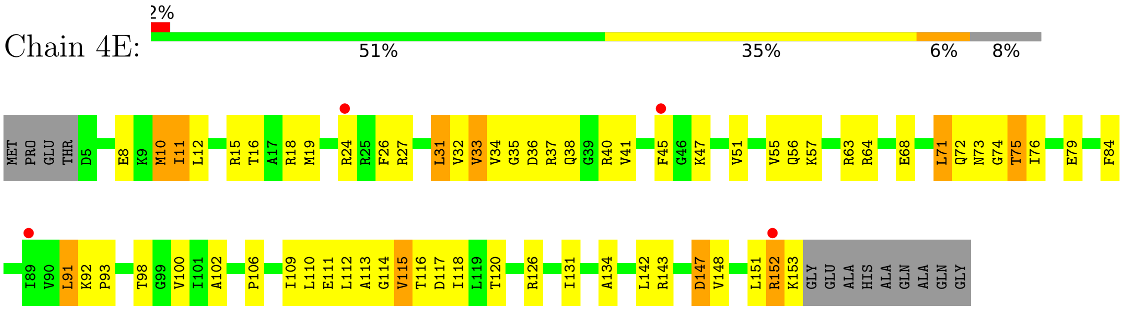
- Molecule 4: 30S ribosomal protein S4

Chain 32:



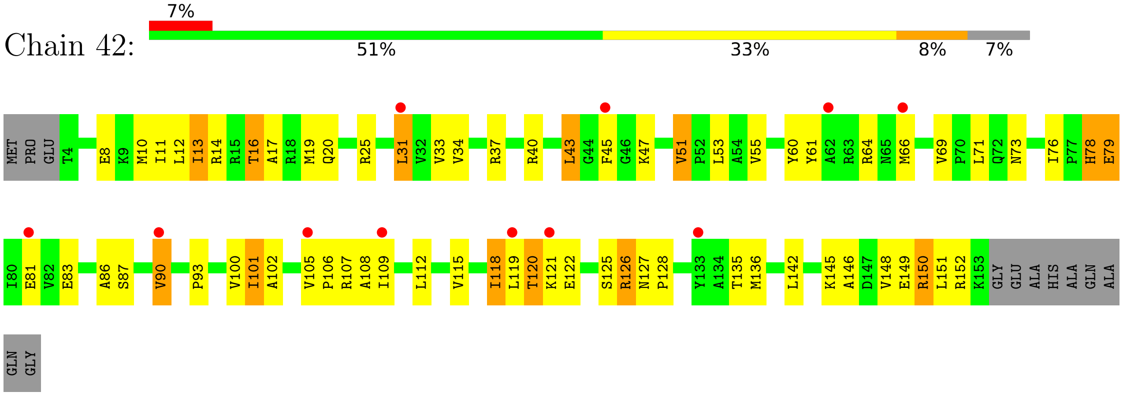
- Molecule 5: 30S ribosomal protein S5

Chain 4E:



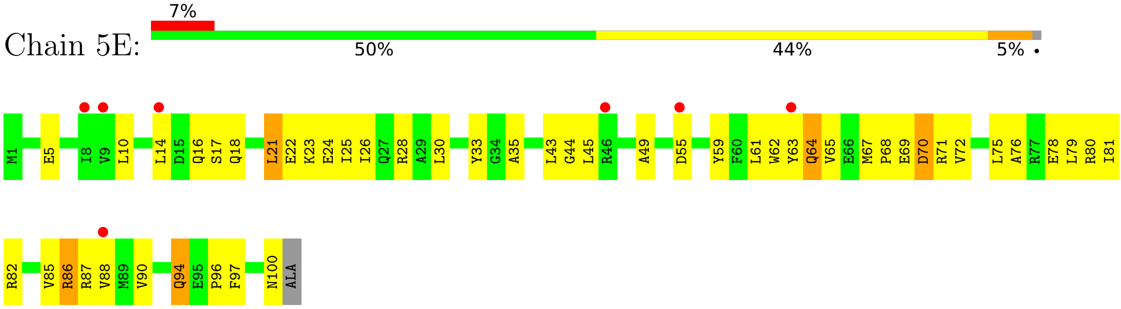
- Molecule 5: 30S ribosomal protein S5

Chain 42:



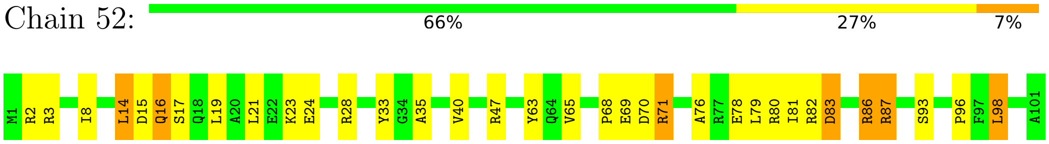
- Molecule 6: 30S ribosomal protein S6

Chain 5E:



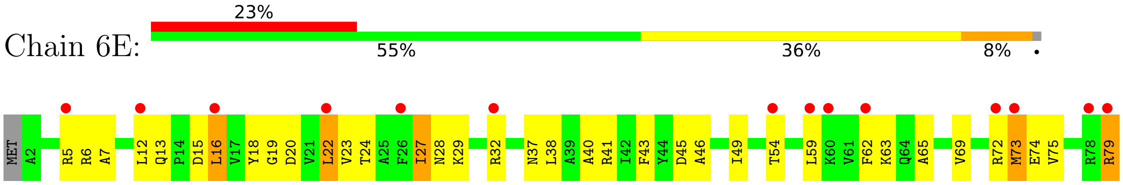
- Molecule 6: 30S ribosomal protein S6

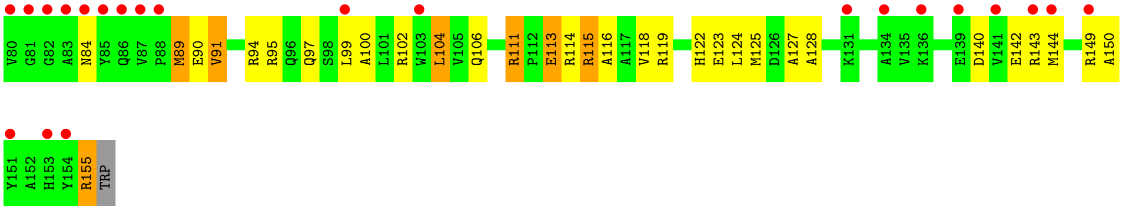
Chain 52:



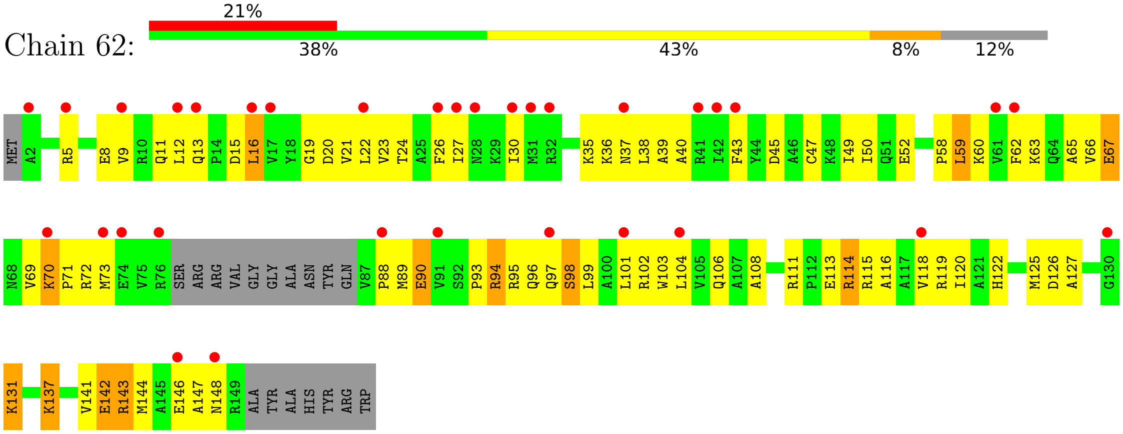
- Molecule 7: 30S ribosomal protein S7

Chain 6E:

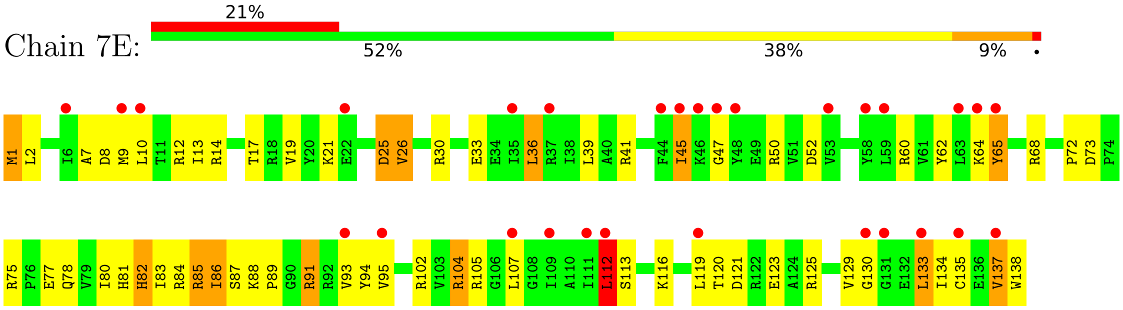




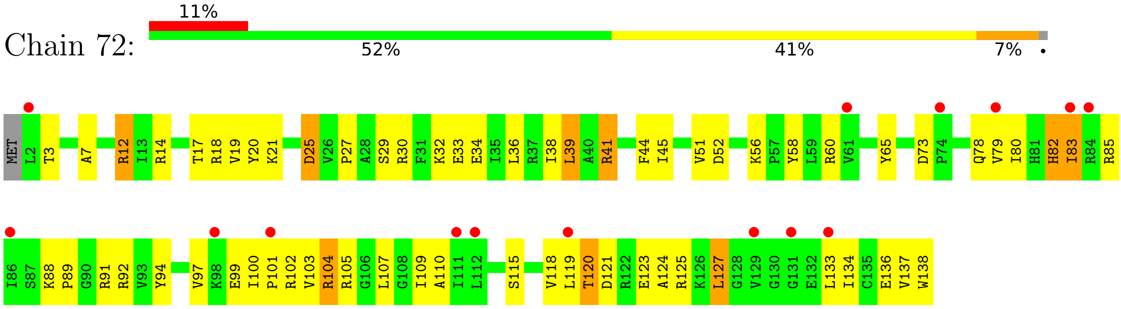
- Molecule 7: 30S ribosomal protein S7



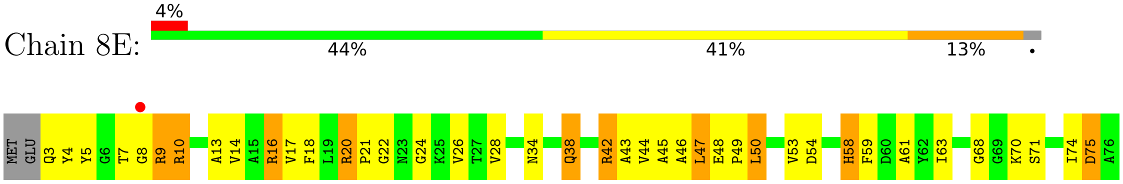
- Molecule 8: 30S ribosomal protein S8

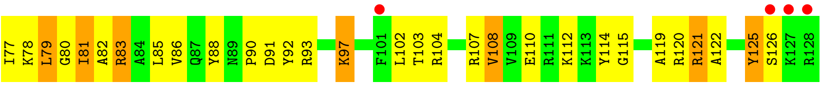


- Molecule 8: 30S ribosomal protein S8

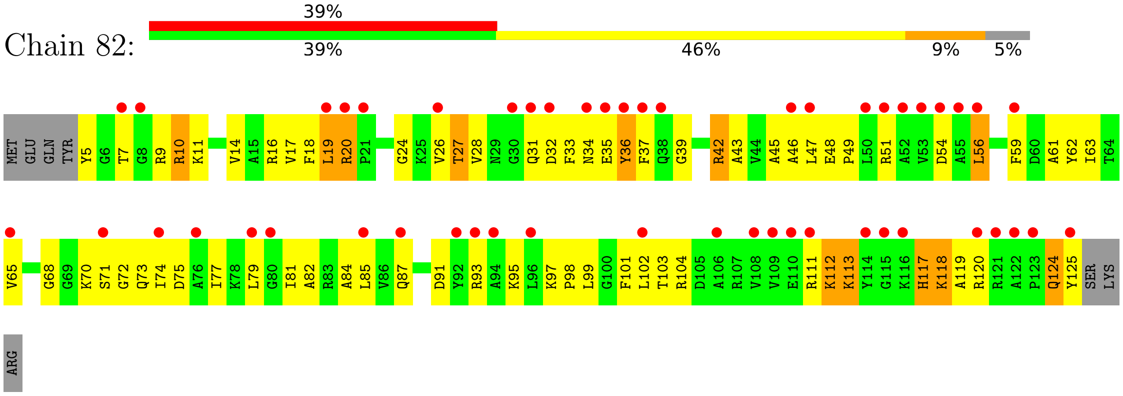


- Molecule 9: 30S ribosomal protein S9

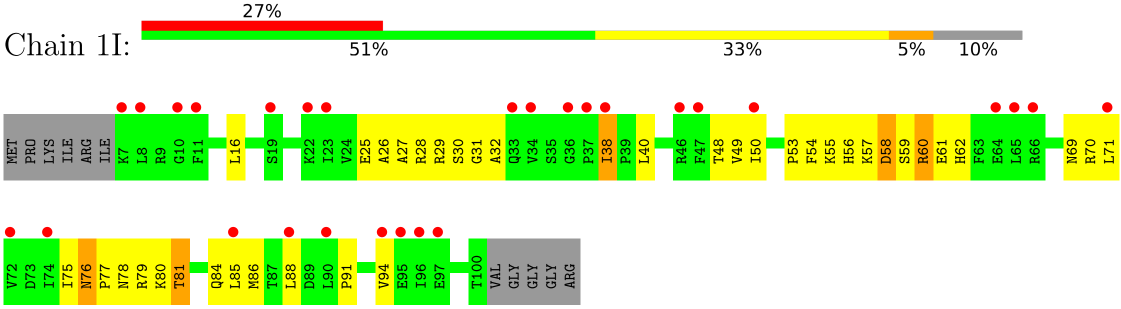




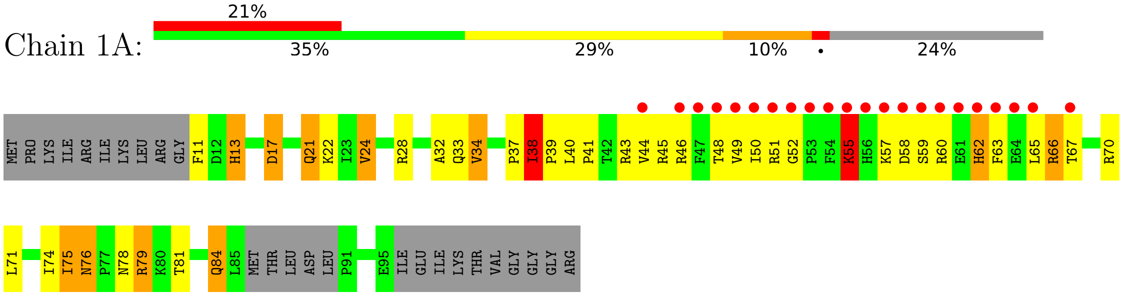
- Molecule 9: 30S ribosomal protein S9



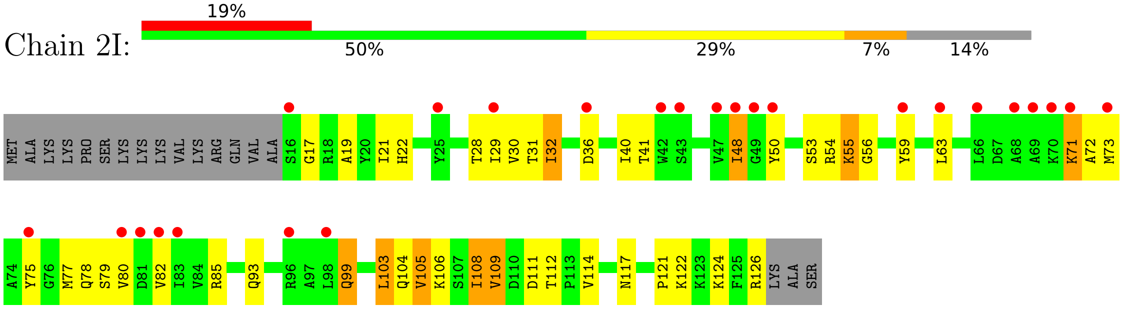
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

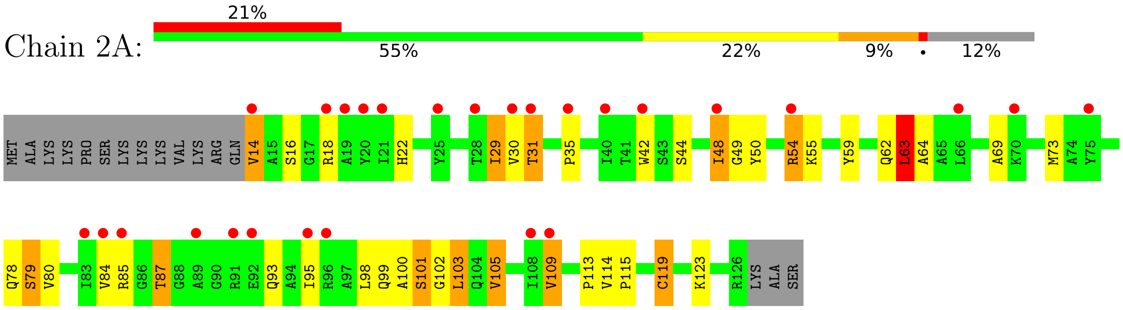


- Molecule 11: 30S ribosomal protein S11



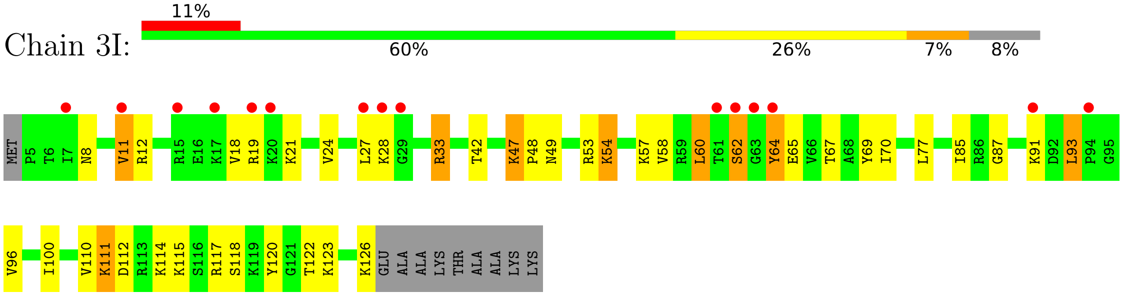
- Molecule 11: 30S ribosomal protein S11

Chain 2A:



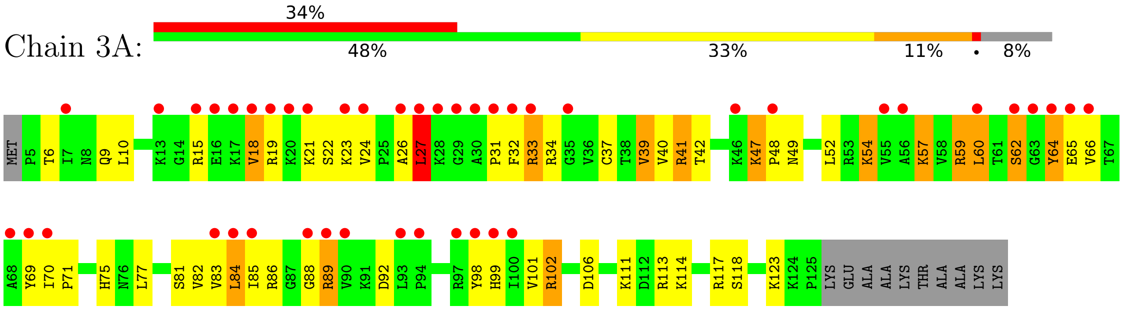
- Molecule 12: 30S ribosomal protein S12

Chain 3I:



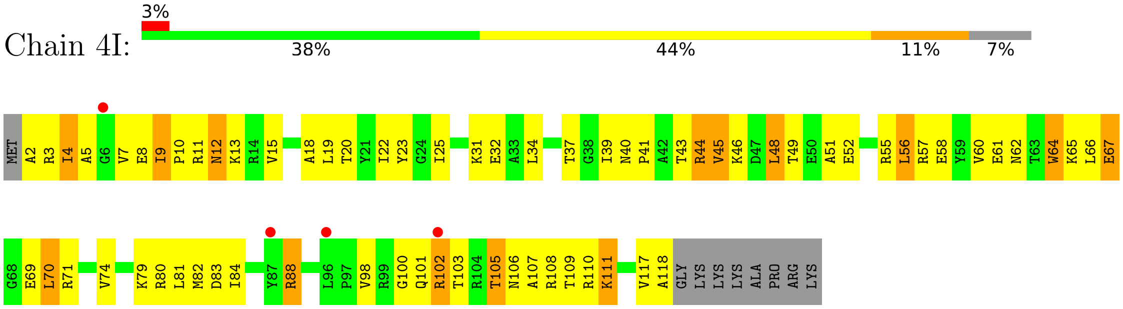
- Molecule 12: 30S ribosomal protein S12

Chain 3A:



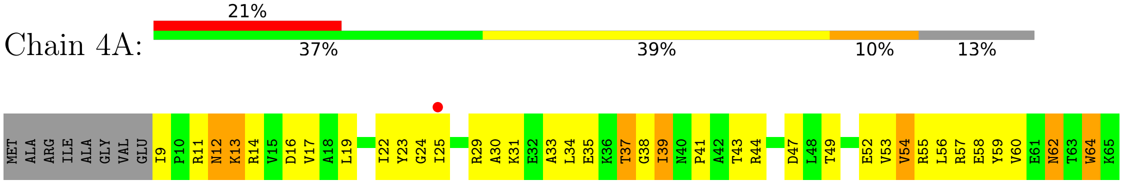
- Molecule 13: 30S ribosomal protein S13

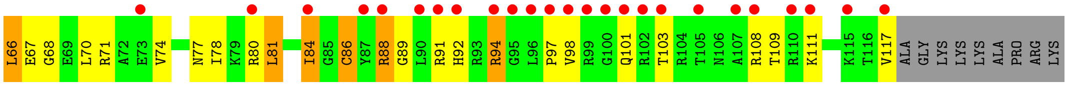
Chain 4I:



- Molecule 13: 30S ribosomal protein S13

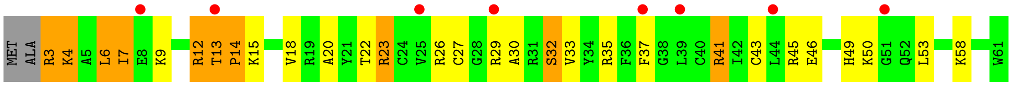
Chain 4A:





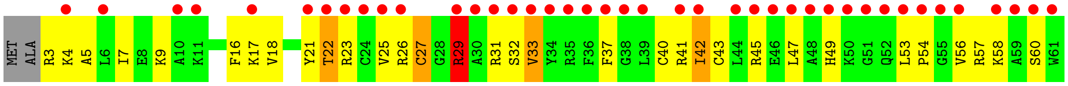
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



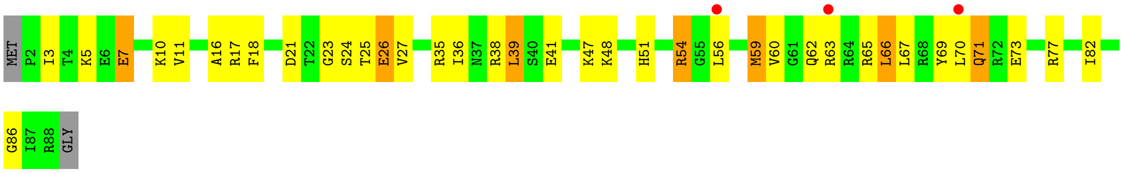
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



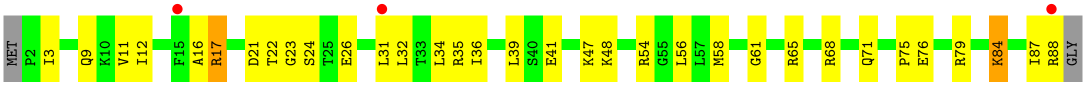
- Molecule 15: 30S ribosomal protein S15

Chain 6I:



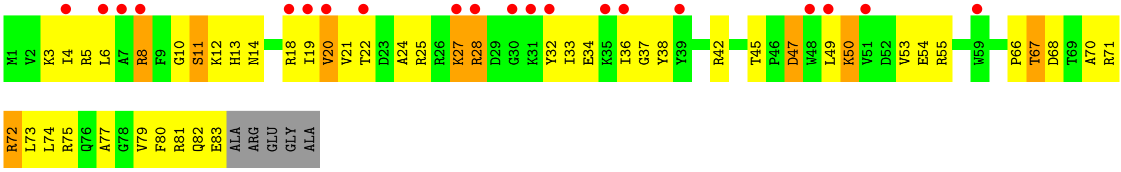
- Molecule 15: 30S ribosomal protein S15

Chain 6A:



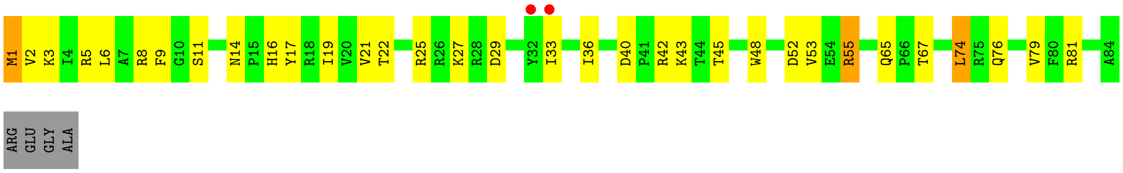
- Molecule 16: 30S ribosomal protein S16

Chain 7I:



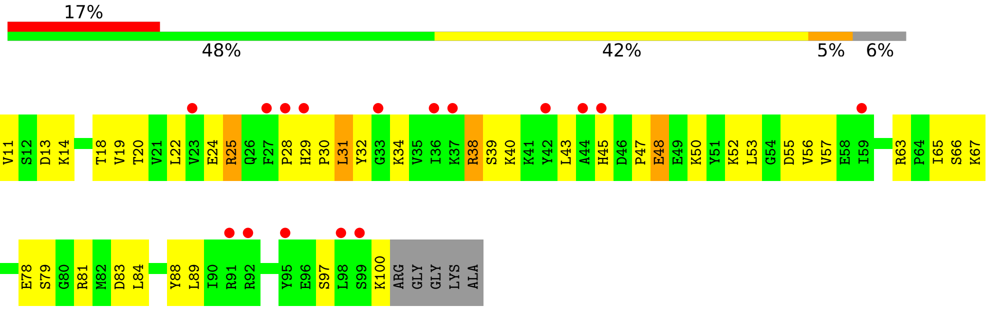
- Molecule 16: 30S ribosomal protein S16

Chain 7A:



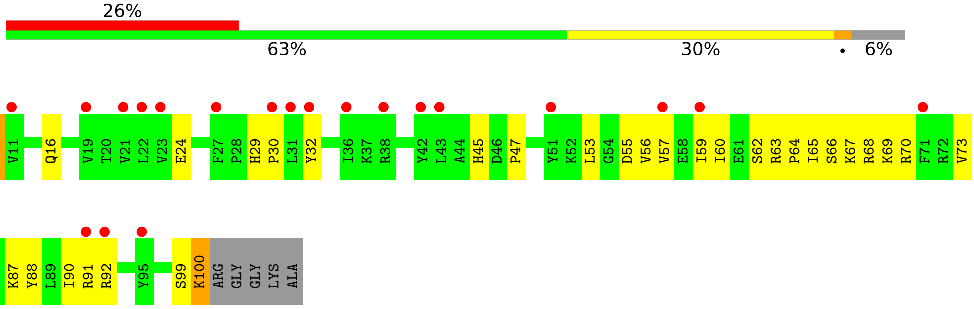
- Molecule 17: 30S ribosomal protein S17

Chain 8I:



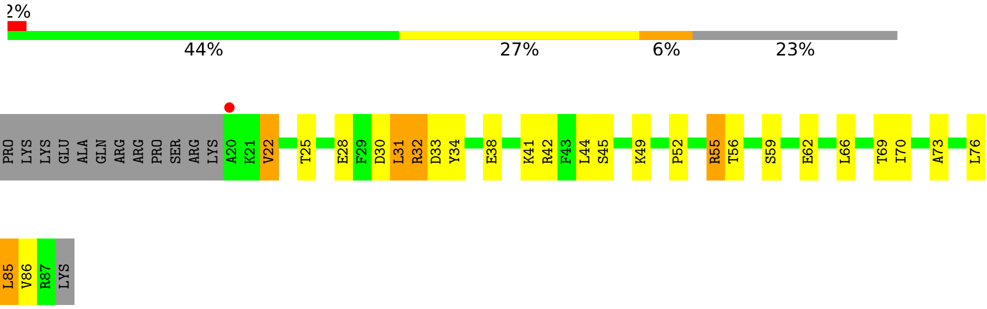
- Molecule 17: 30S ribosomal protein S17

Chain 8A:



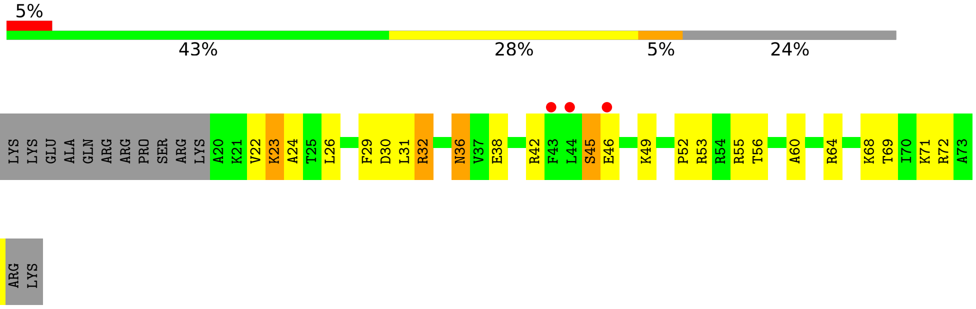
- Molecule 18: 30S ribosomal protein S18

Chain 9I:

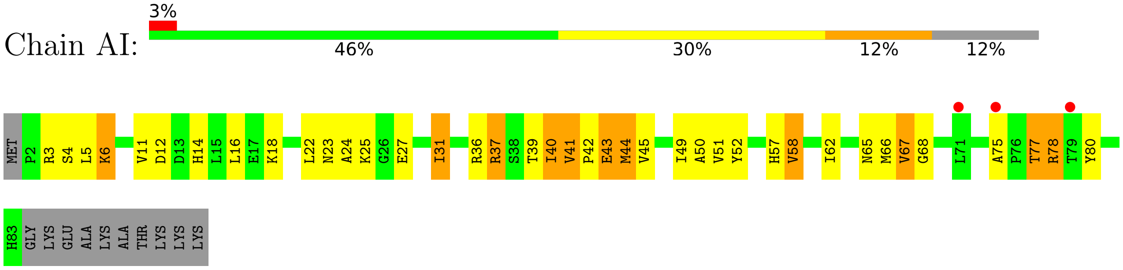


- Molecule 18: 30S ribosomal protein S18

Chain 9A:



- Molecule 19: 30S ribosomal protein S19



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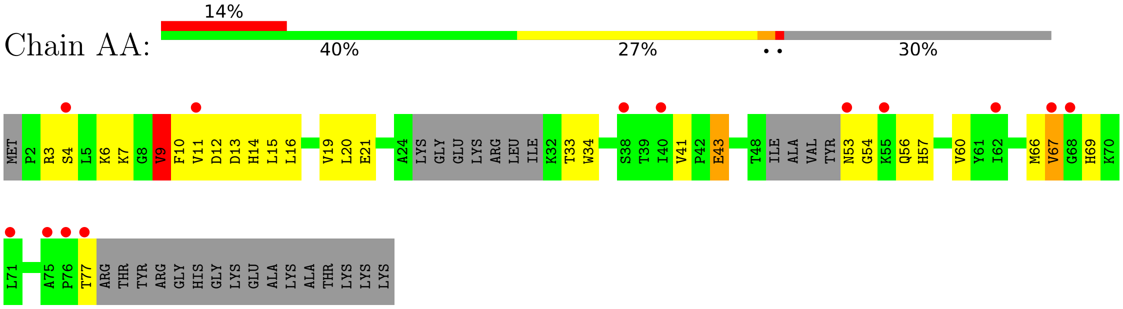

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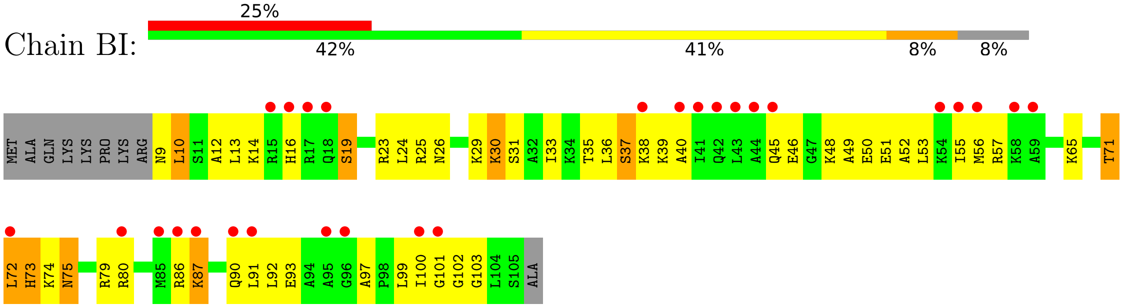

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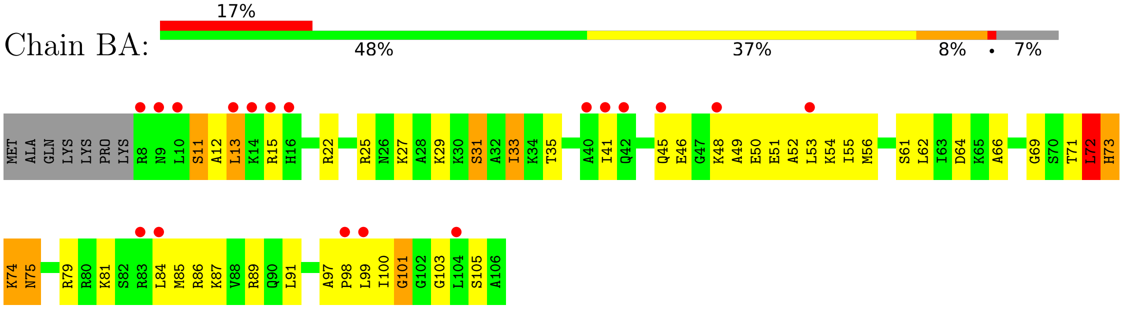
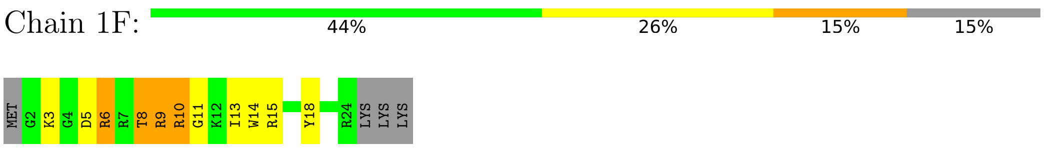


- Molecule 21: 30S ribosomal protein Thx



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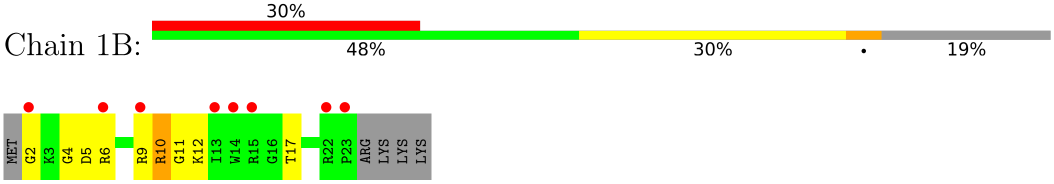

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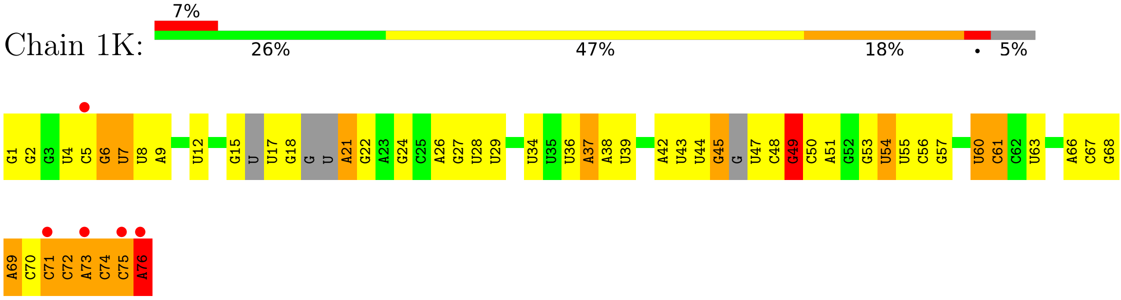

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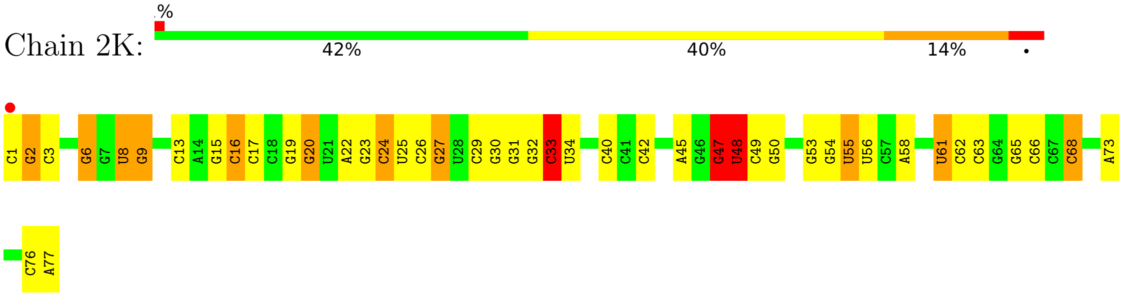

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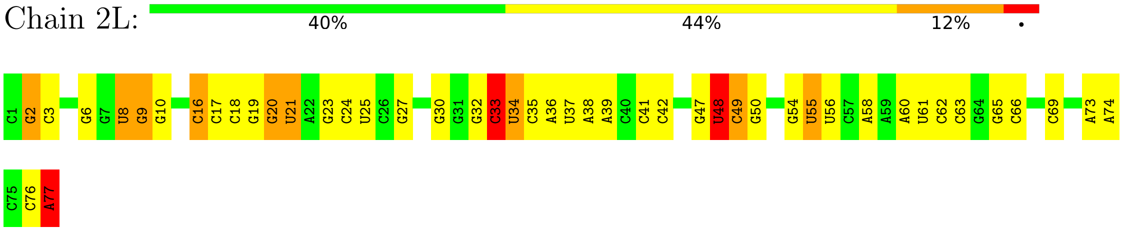

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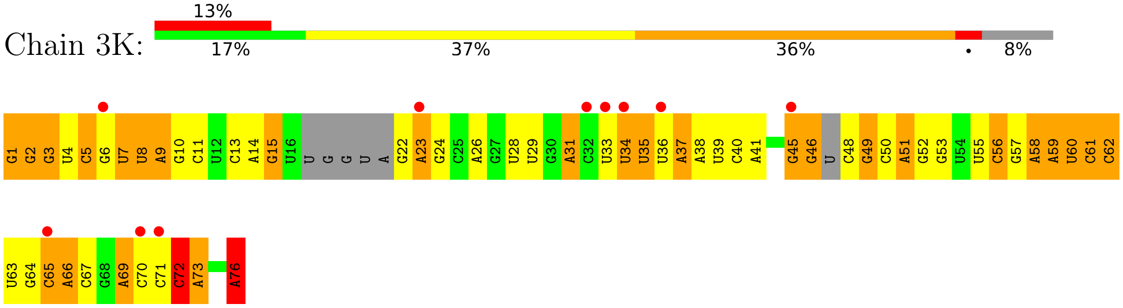

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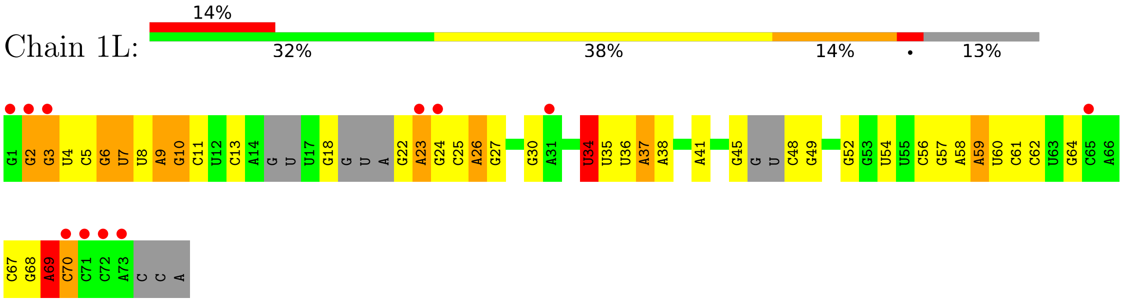

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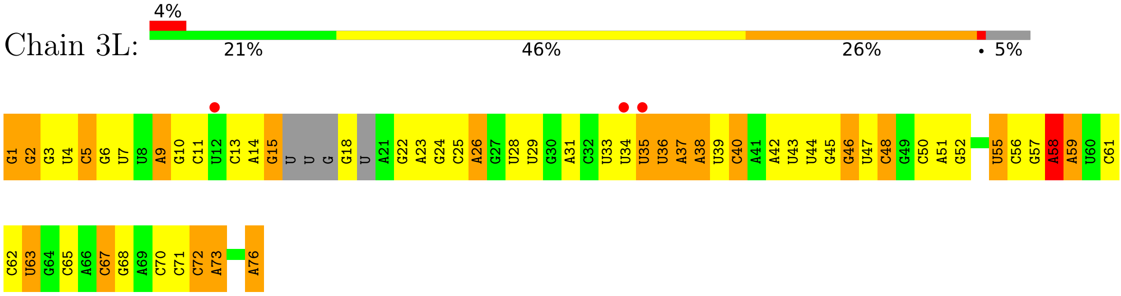

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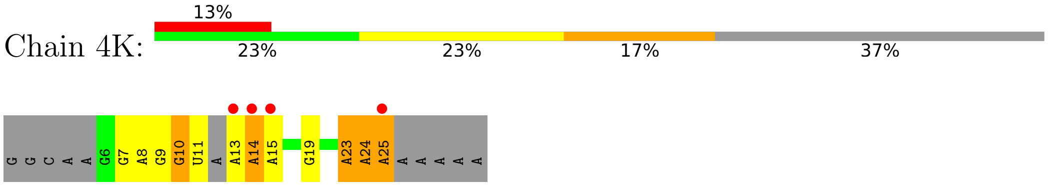

- Molecule 25: mRNA

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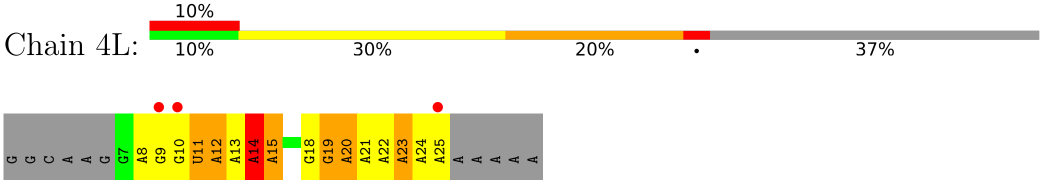

- Molecule 26: 23S ribosomal RNA

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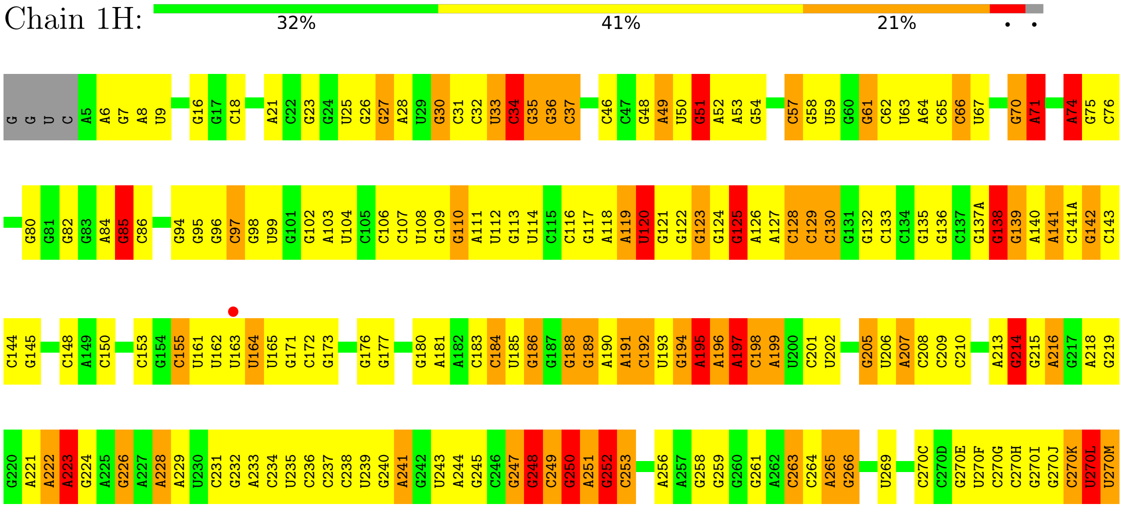

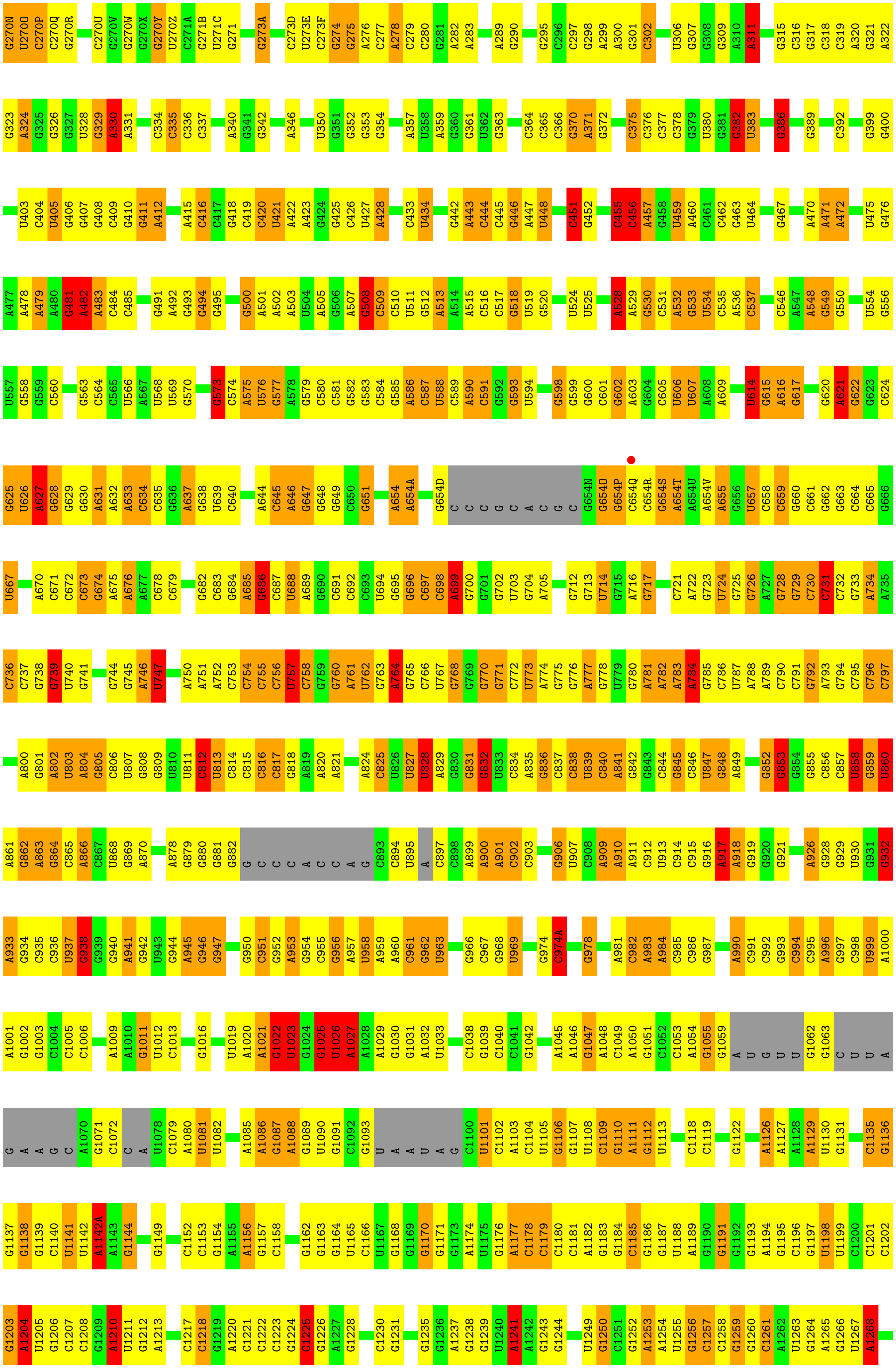
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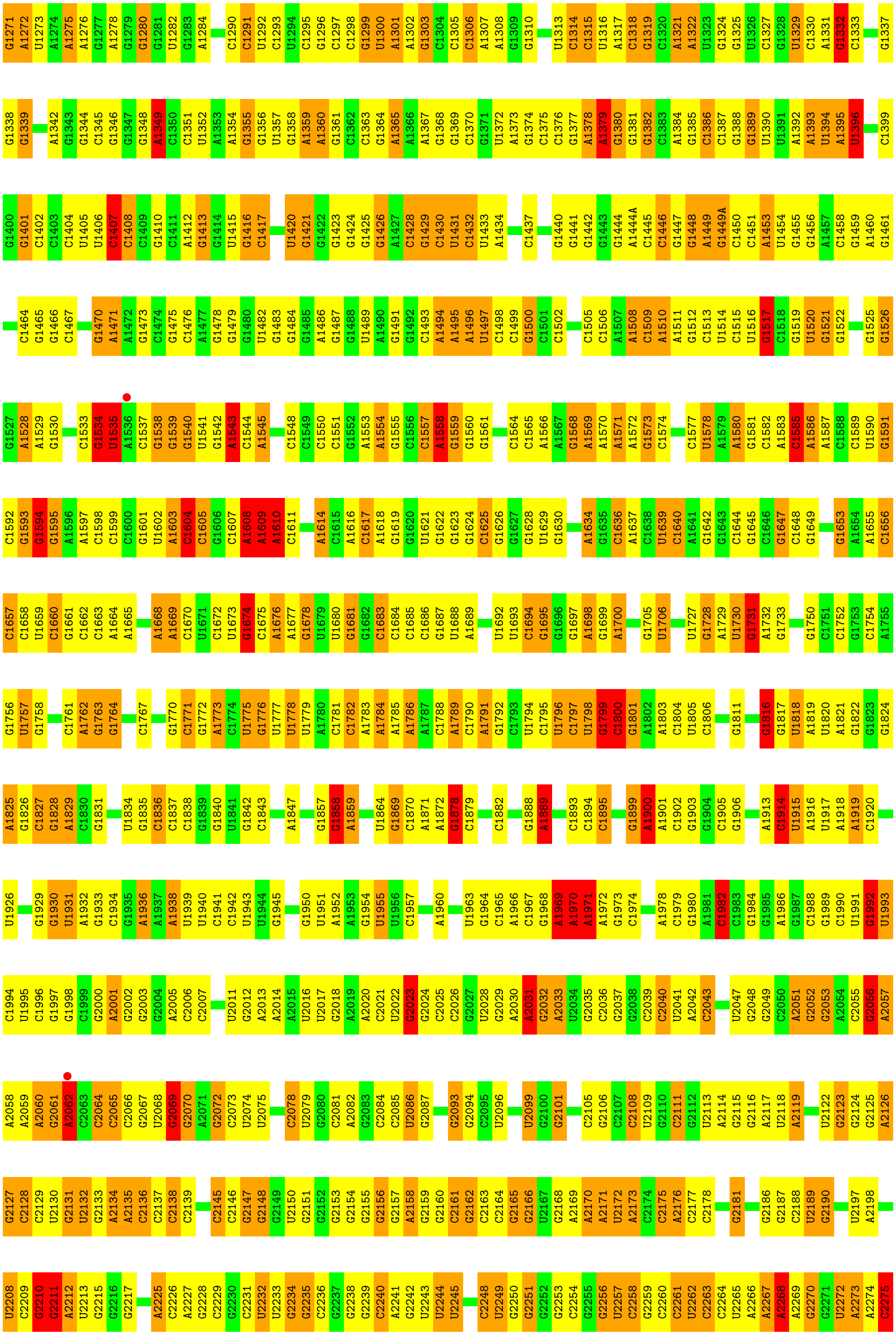
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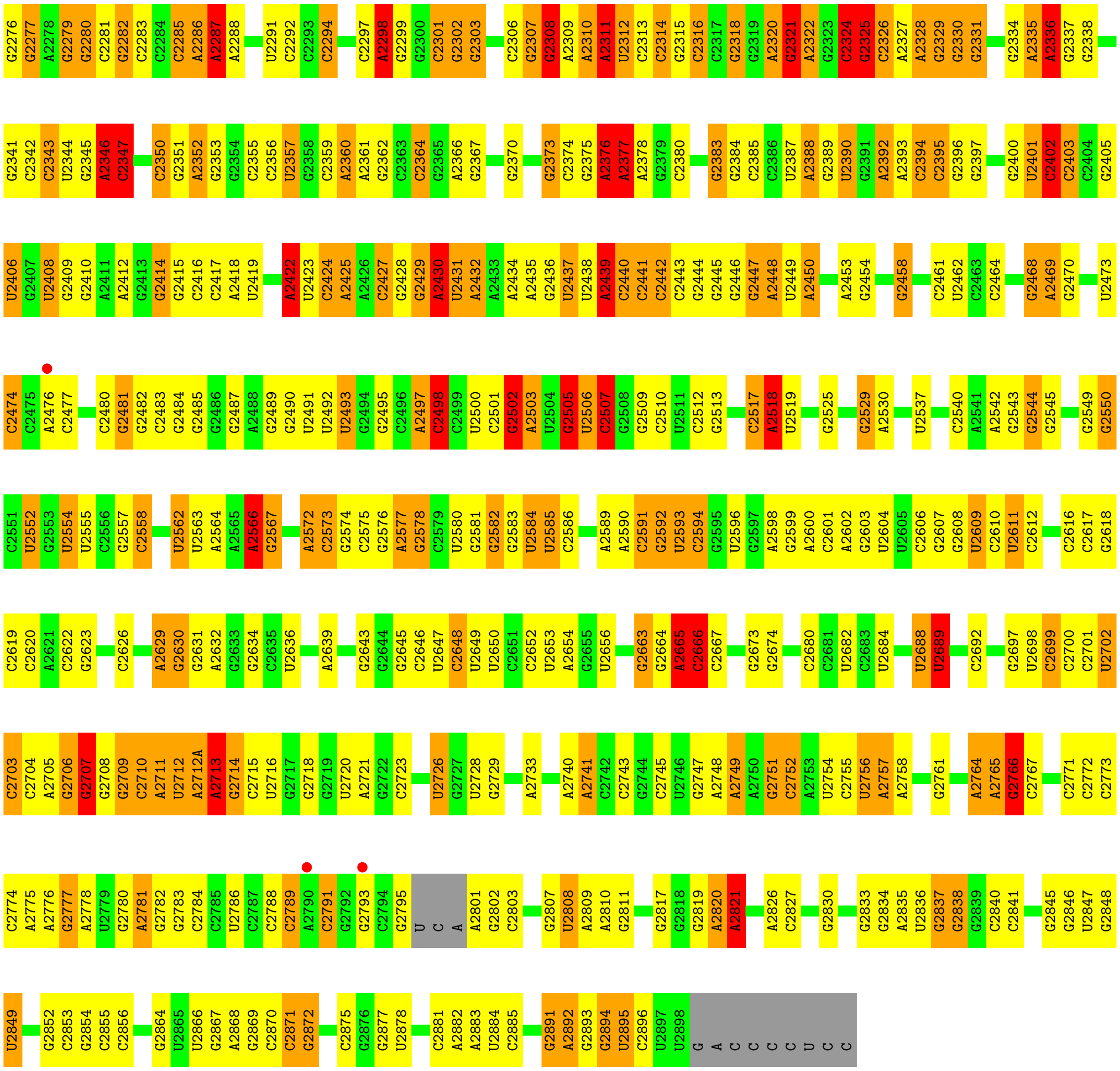
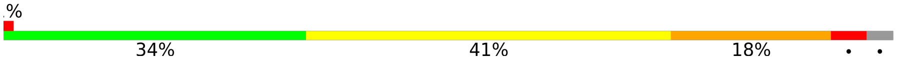
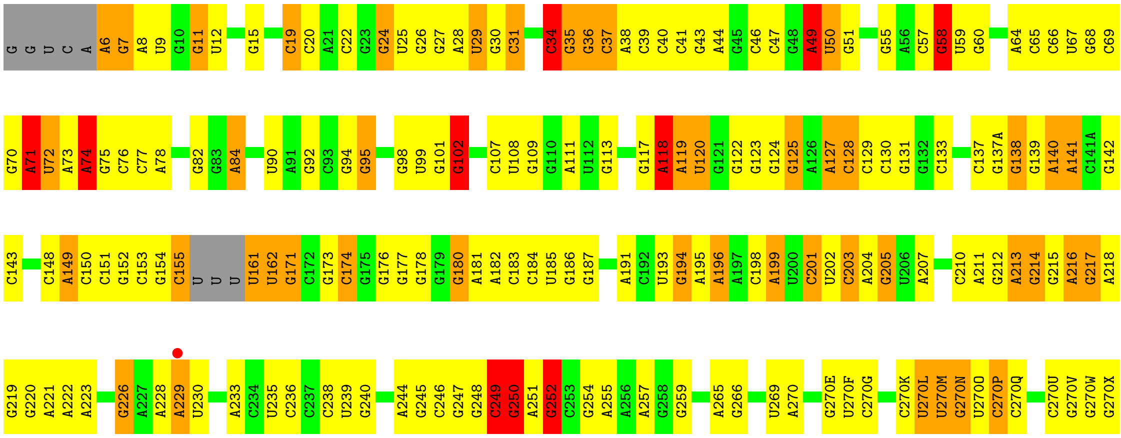
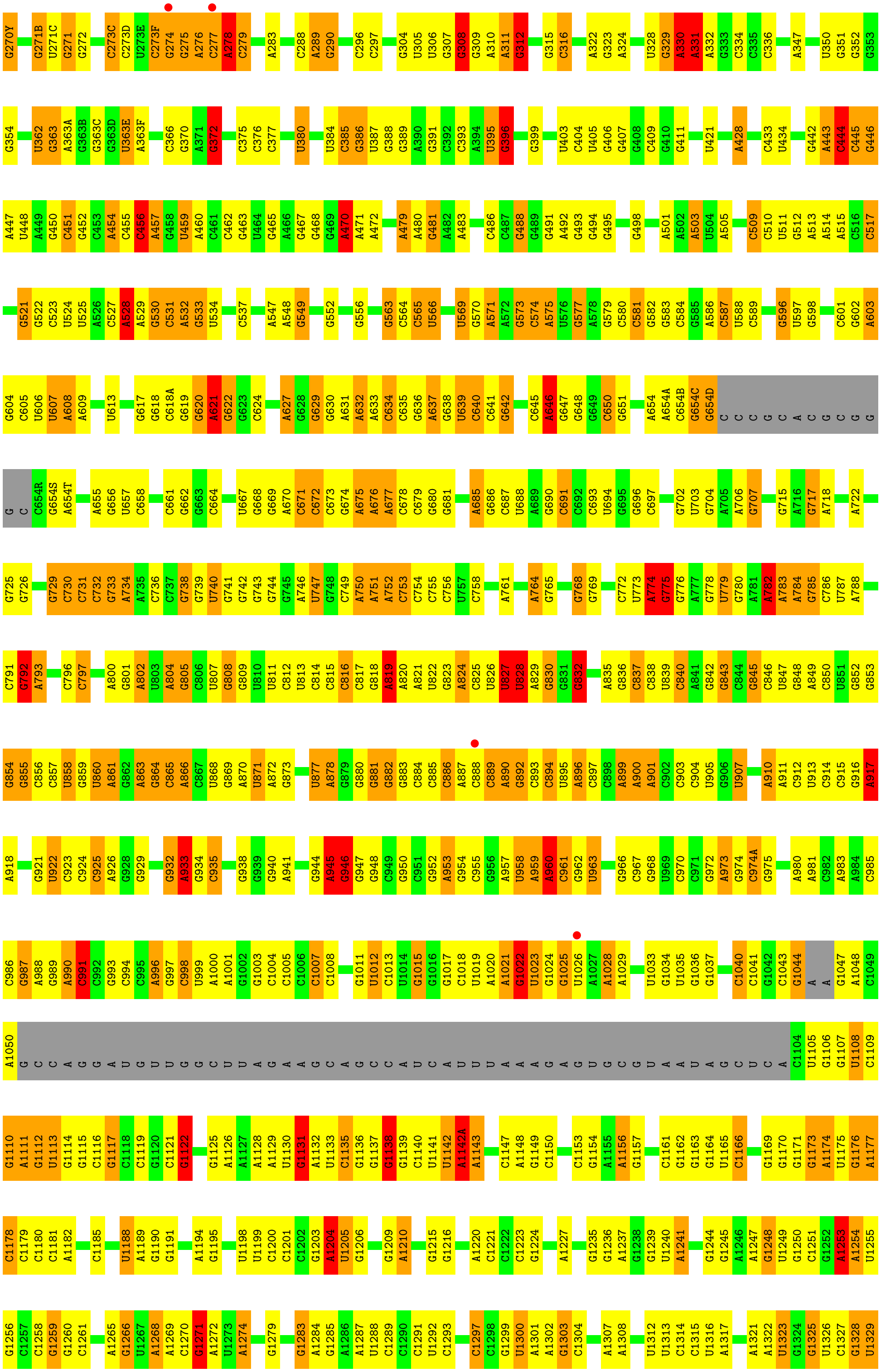


- Molecule 26: 23S ribosomal RNA

Chain 14:



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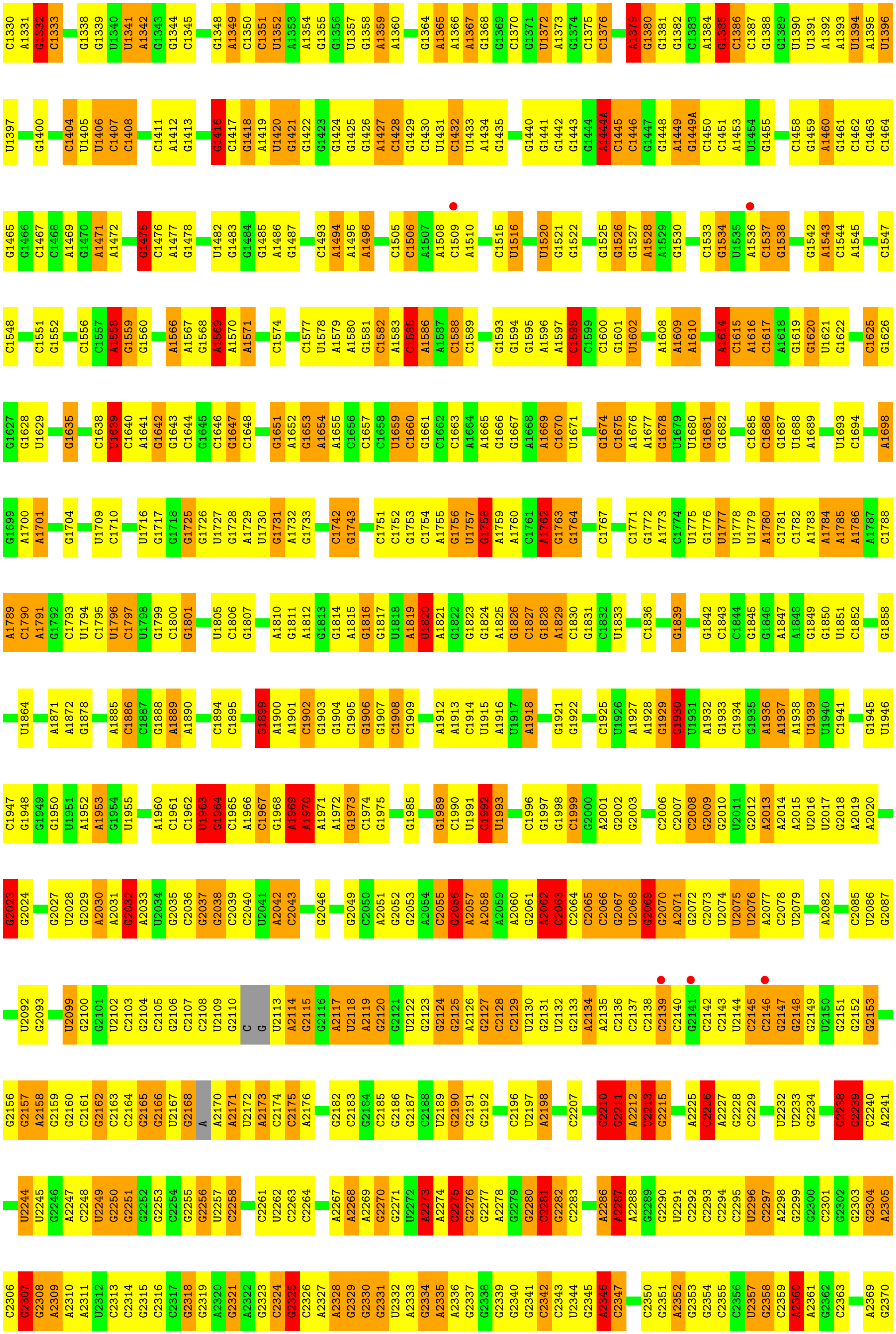
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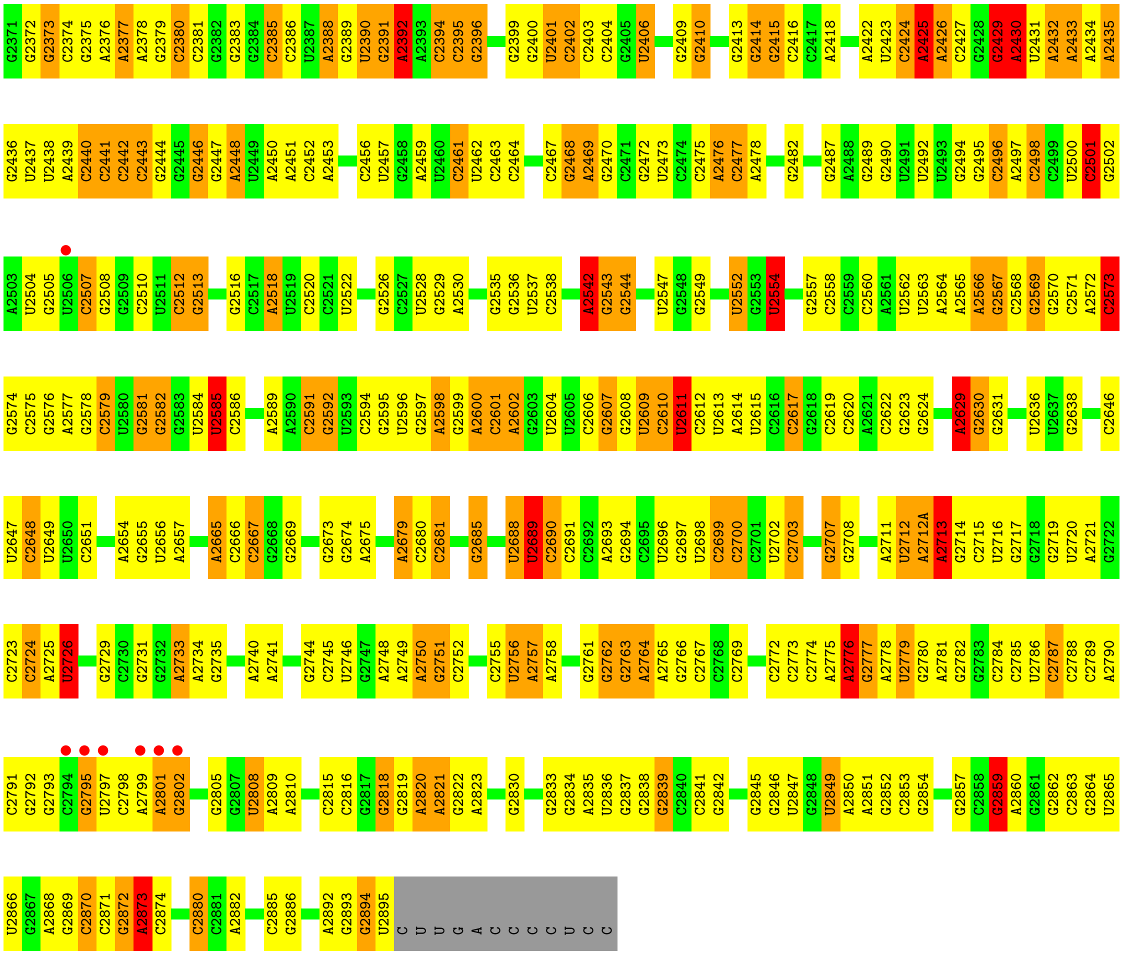

- Molecule 27: 5S ribosomal RNA

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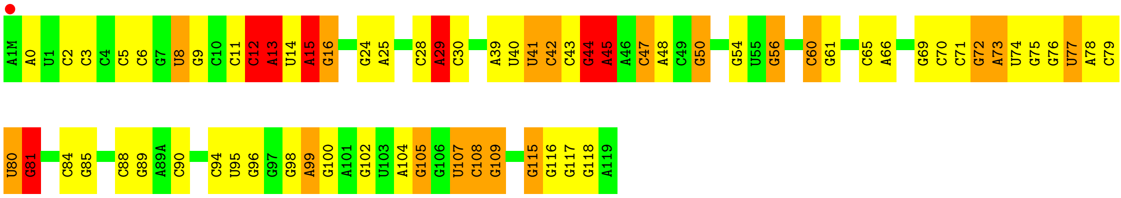

- Molecule 27: 5S ribosomal RNA

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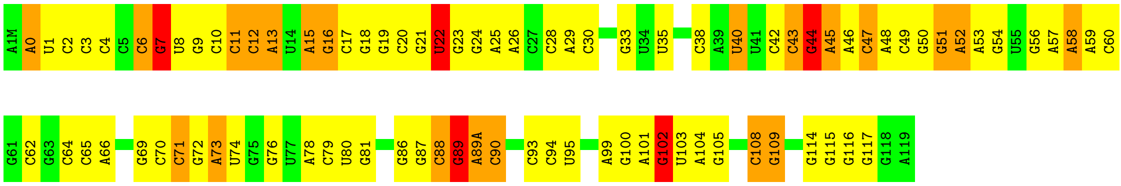
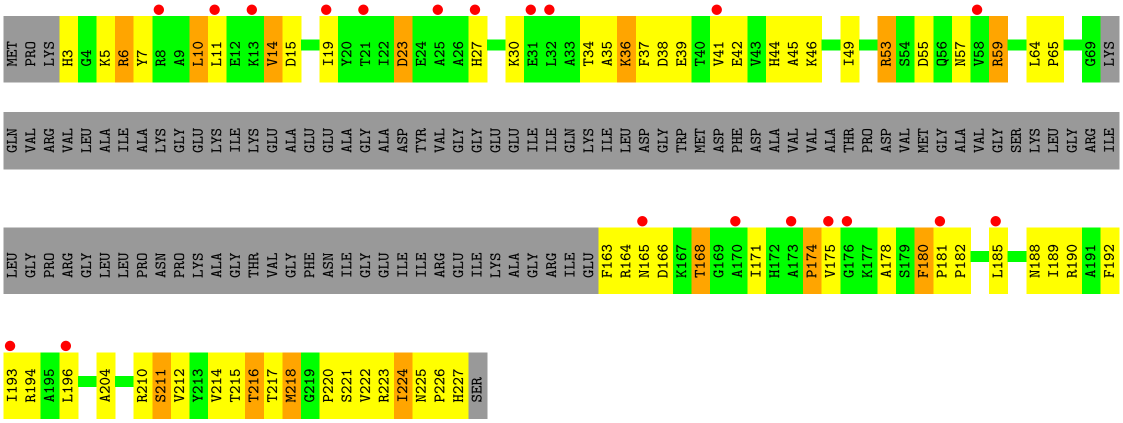


- Molecule 28: 50S ribosomal protein L1

Chain 71:



- Molecule 29: 50S ribosomal protein L2

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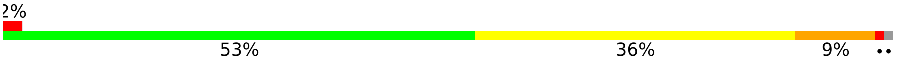

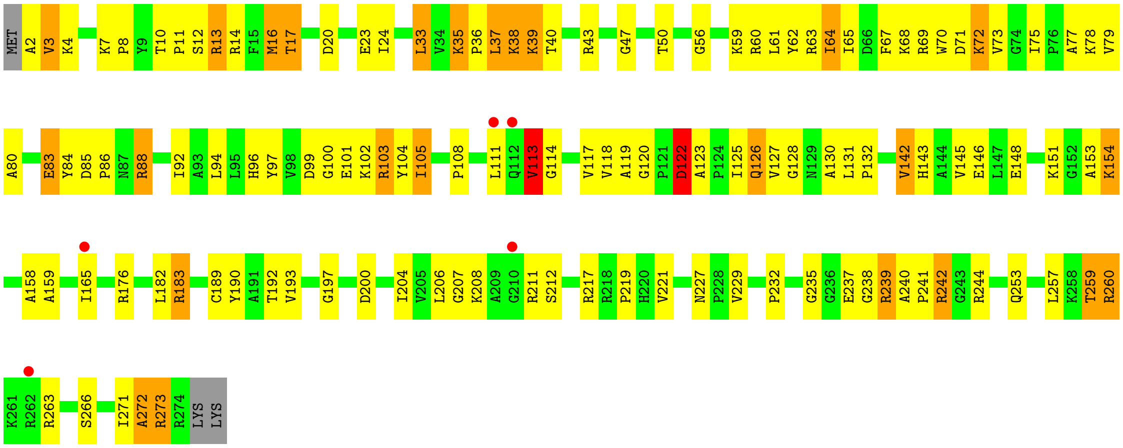

- Molecule 29: 50S ribosomal protein L2

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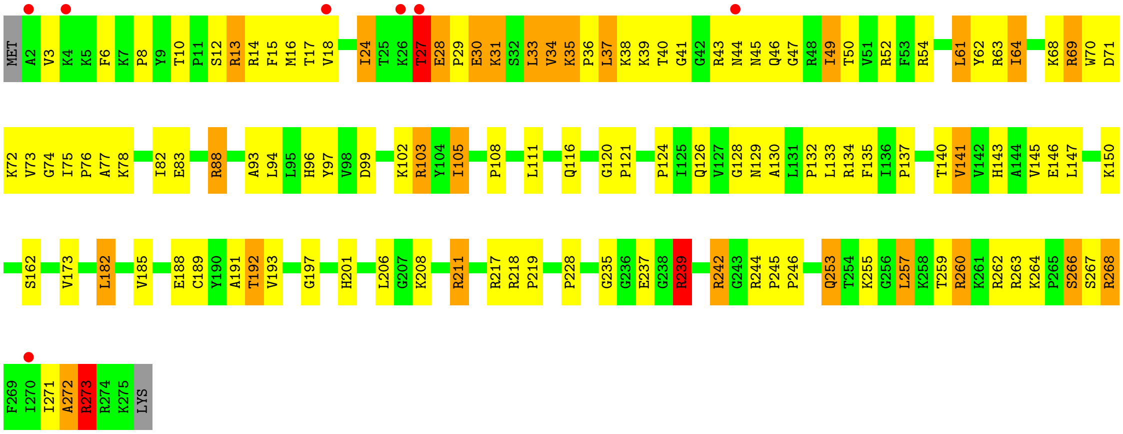

- Molecule 30: 50S ribosomal protein L3

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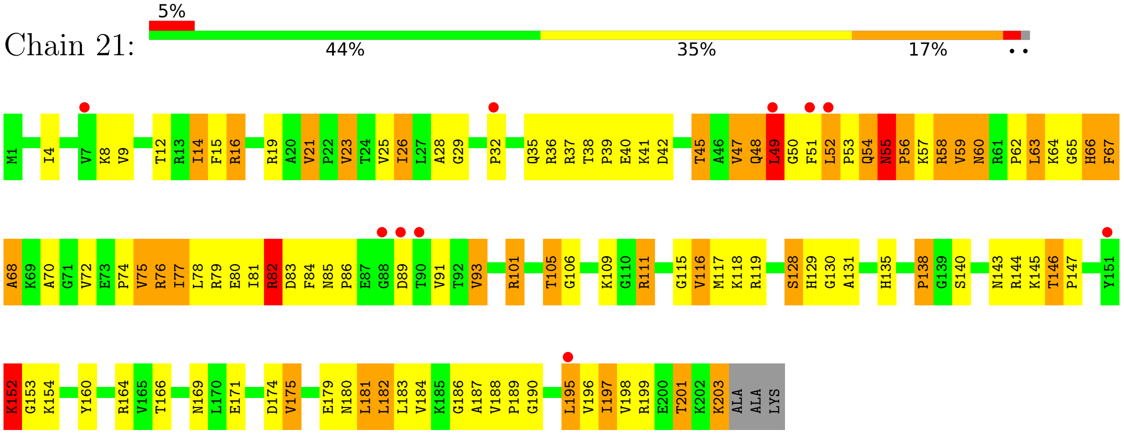

- Molecule 30: 50S ribosomal protein L3

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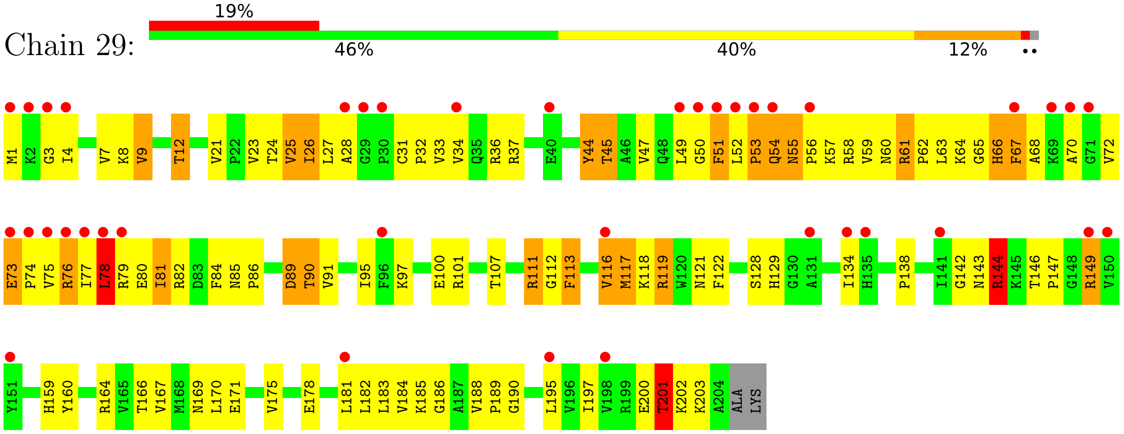
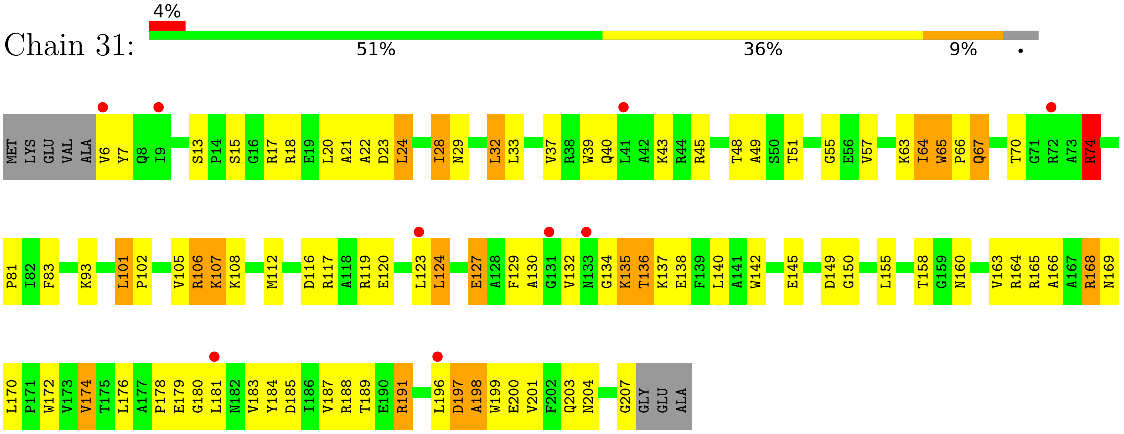


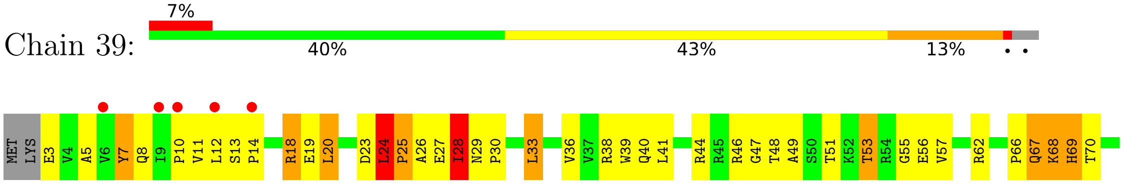
- Molecule 31: 50S ribosomal protein L4

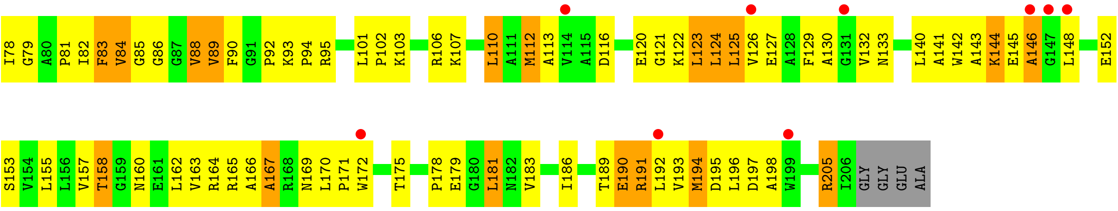
Chain 31:



- Molecule 31: 50S ribosomal protein L4

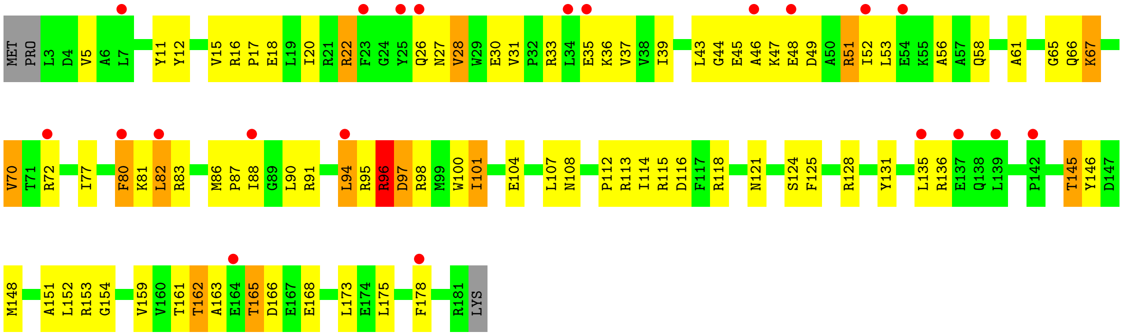
Chain 39:





- Molecule 32: 50S ribosomal protein L5

Chain 41:



- Molecule 32: 50S ribosomal protein L5

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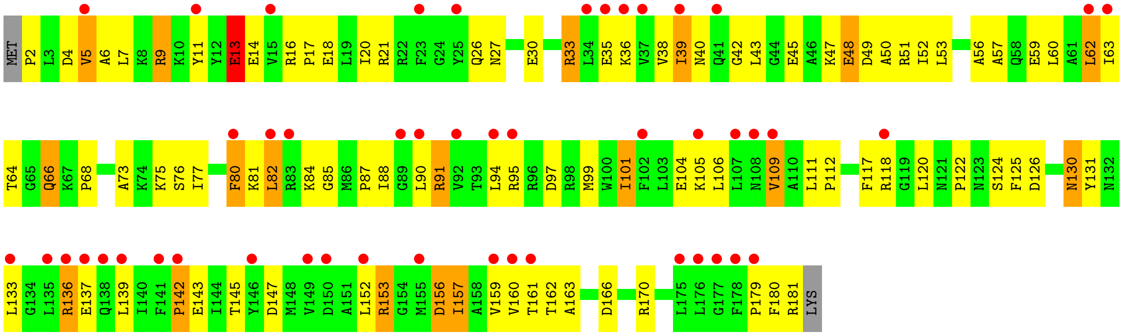
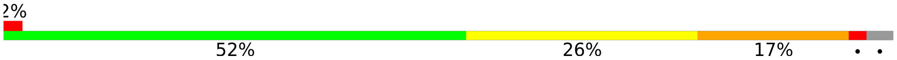
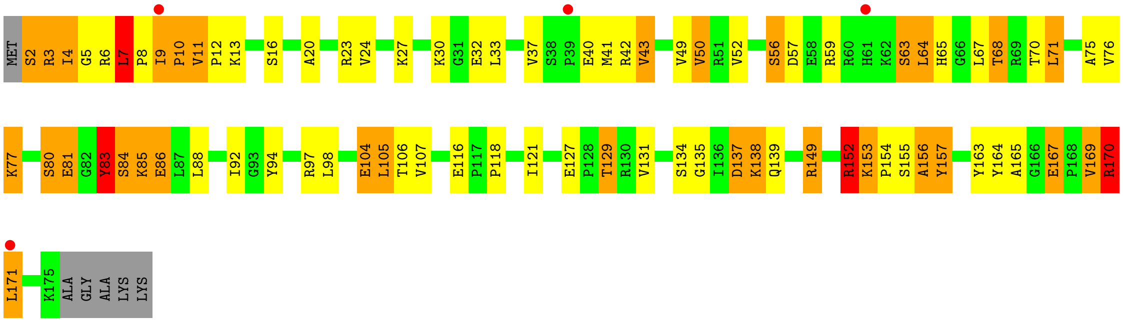


- Molecule 33: 50S ribosomal protein L6

Chain 51:





- Molecule 33: 50S ribosomal protein L6

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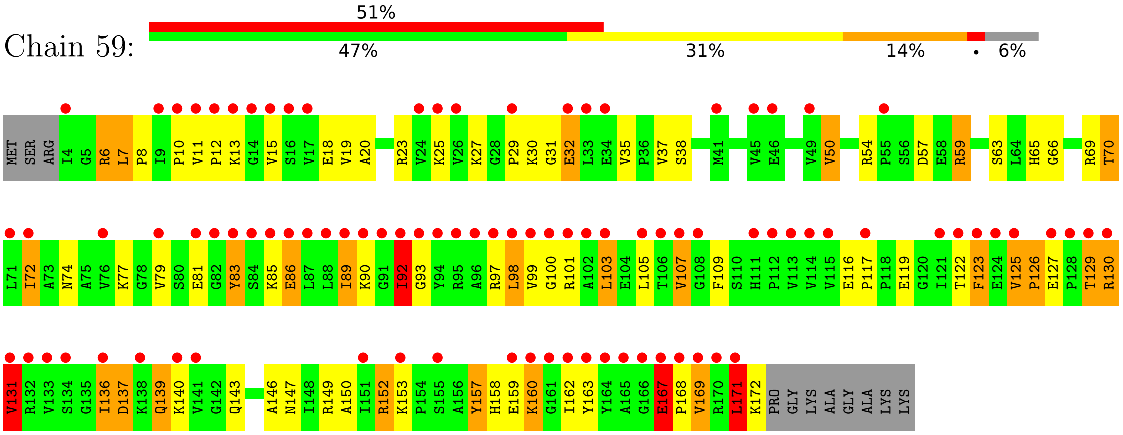

- Molecule 34: 50S ribosomal protein L9

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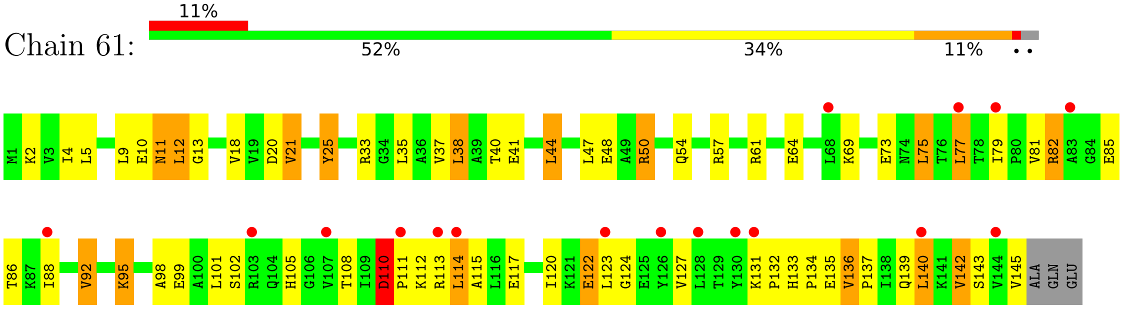

- Molecule 34: 50S ribosomal protein L9

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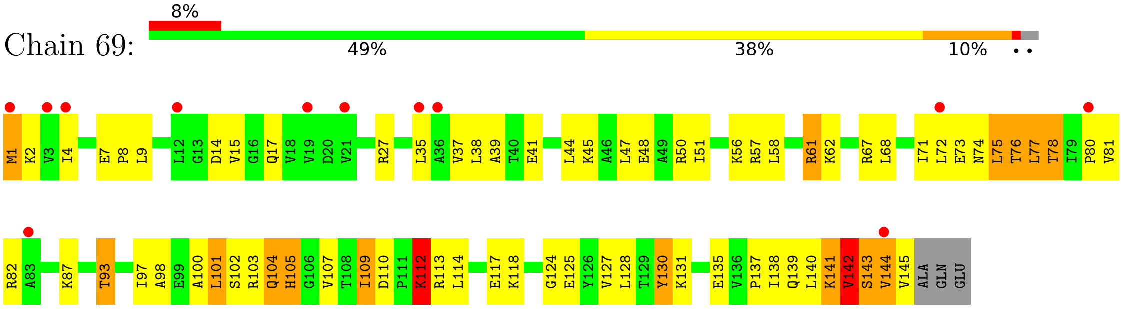

- Molecule 35: 50S ribosomal protein L13

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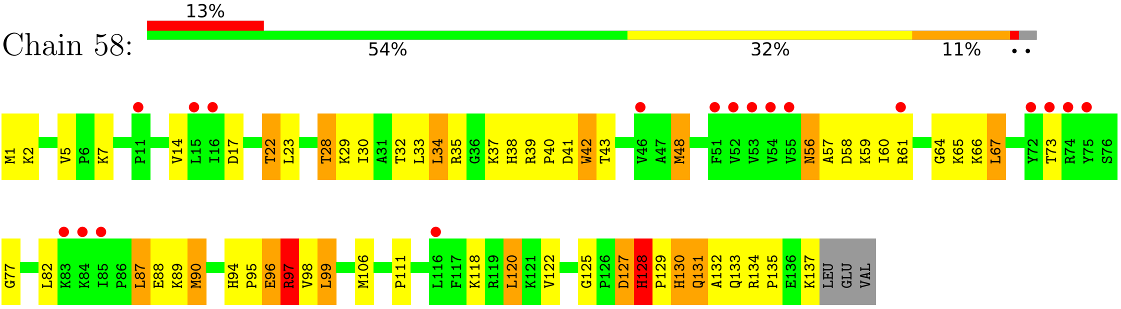

- Molecule 35: 50S ribosomal protein L13

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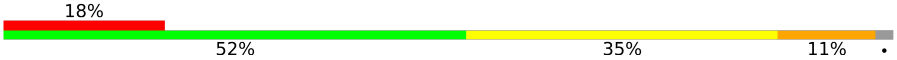
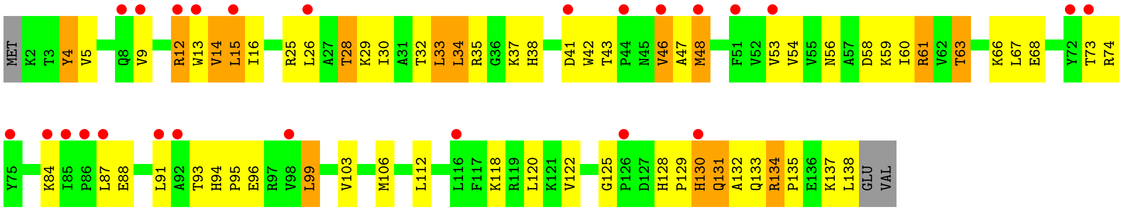
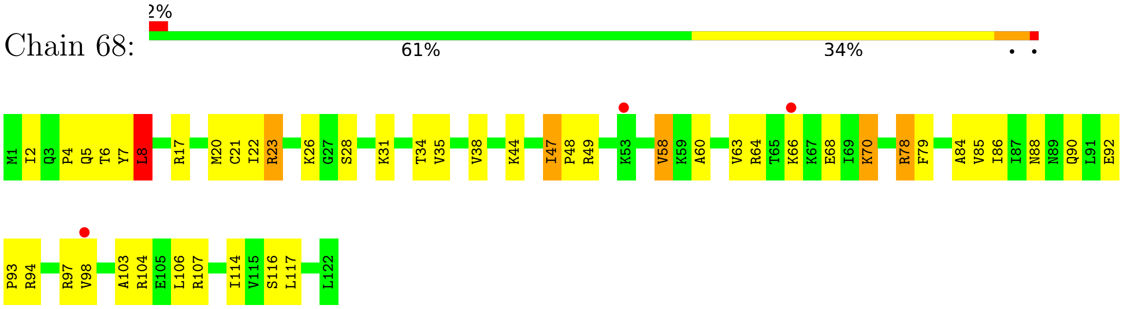
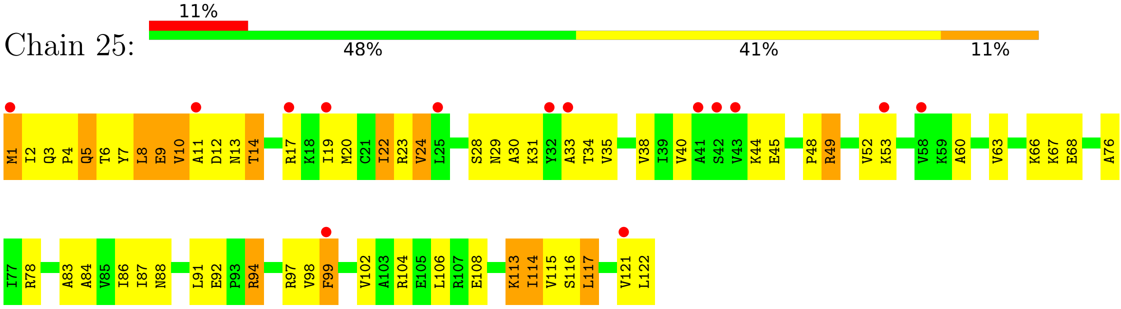




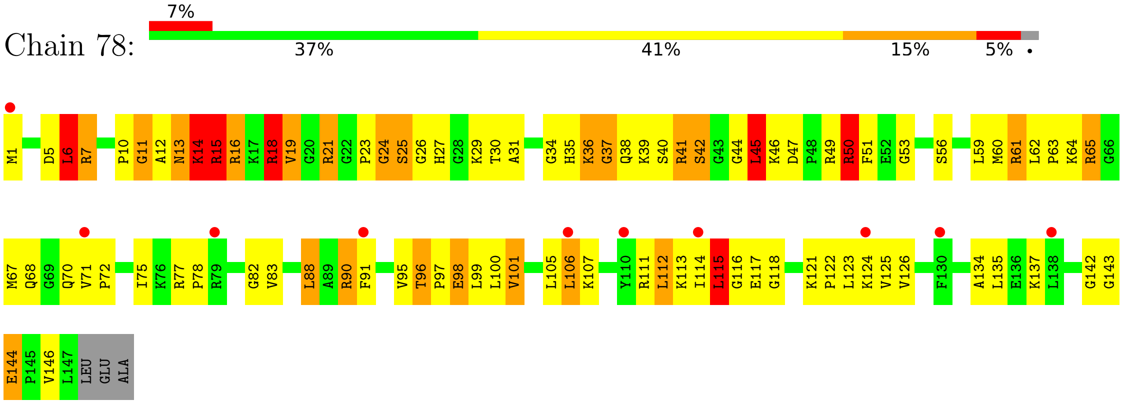
- Molecule 36: 50S ribosomal protein L14



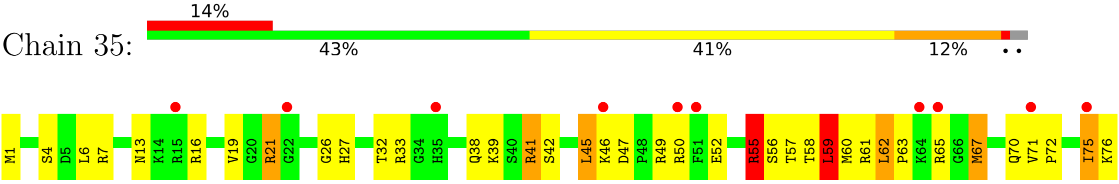
- Molecule 36: 50S ribosomal protein L14

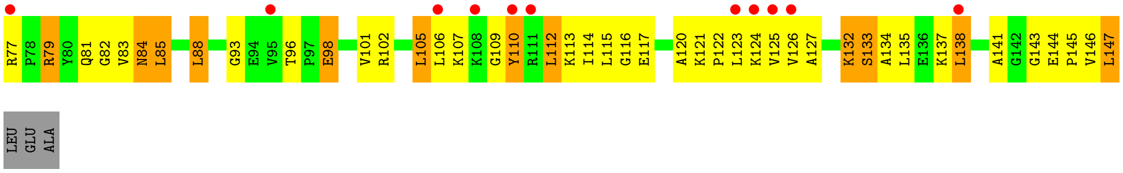


- Molecule 37: 50S ribosomal protein L15



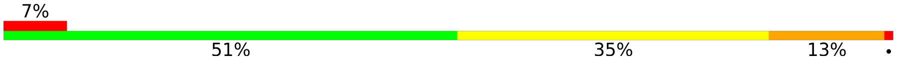
- Molecule 37: 50S ribosomal protein L15

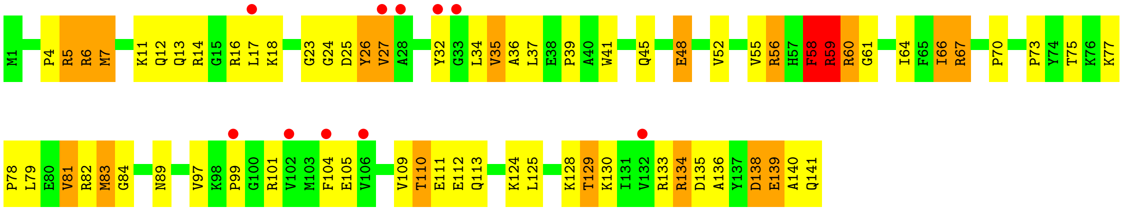




- Molecule 38: 50S ribosomal protein L16

Chain 88:





- Molecule 38: 50S ribosomal protein L16

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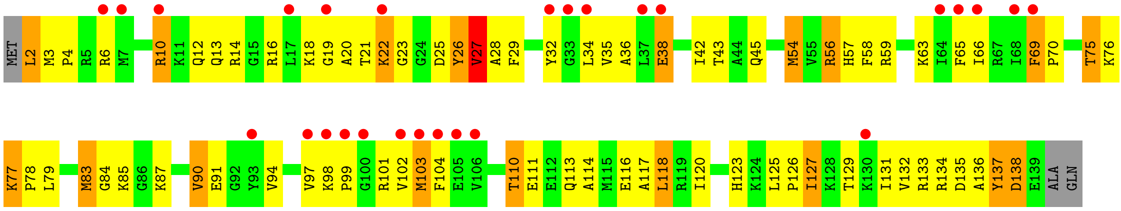
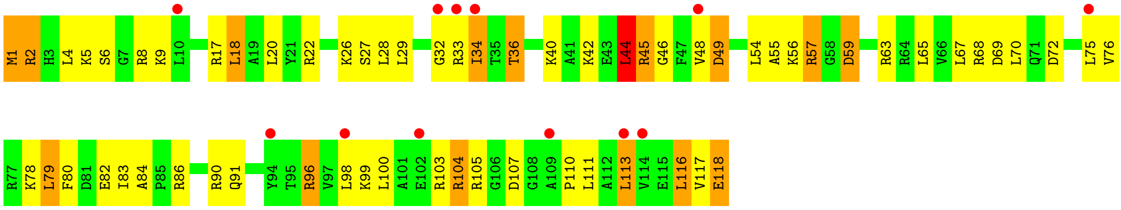


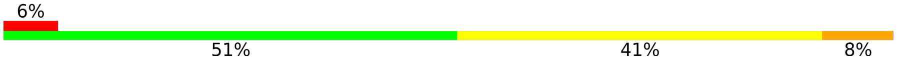
- Molecule 39: 50S ribosomal protein L17

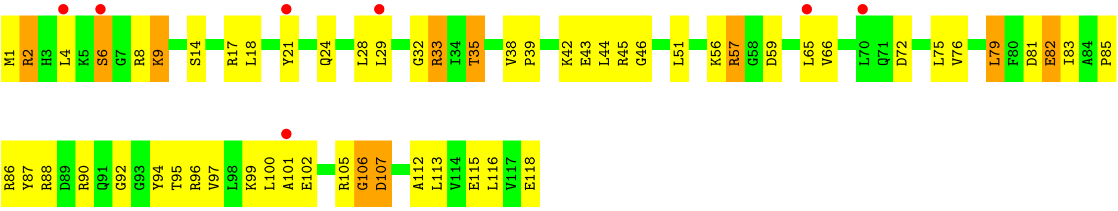
Chain 98:



- Molecule 39: 50S ribosomal protein L17

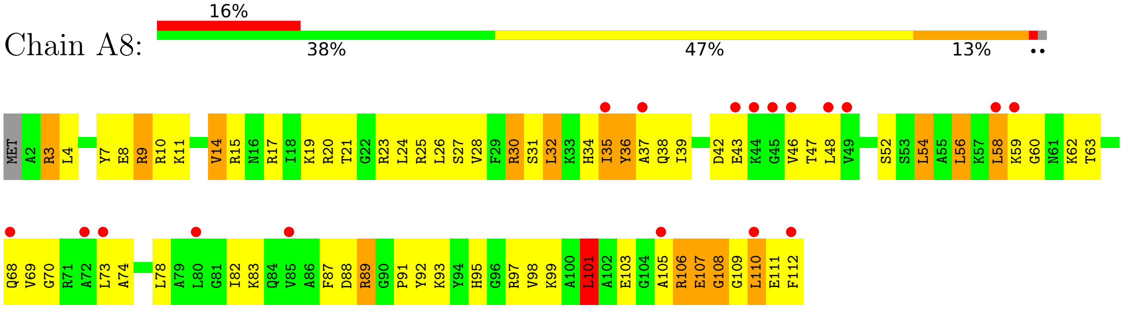
Chain 55:





- Molecule 40: 50S ribosomal protein L18

Chain A8:



- Molecule 40: 50S ribosomal protein L18

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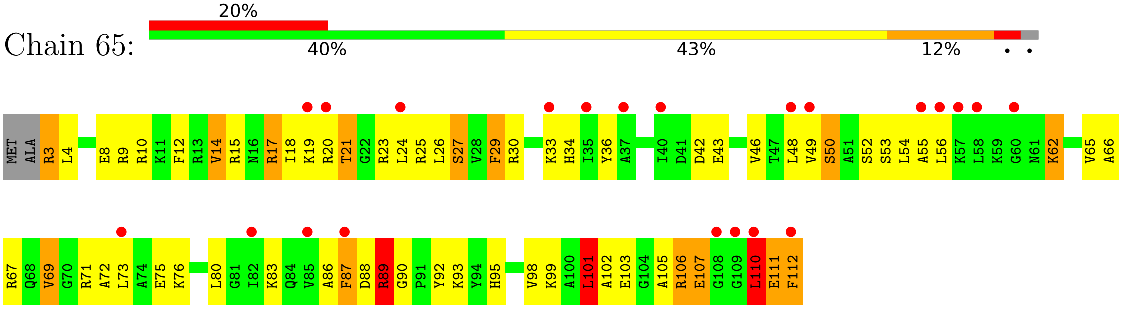
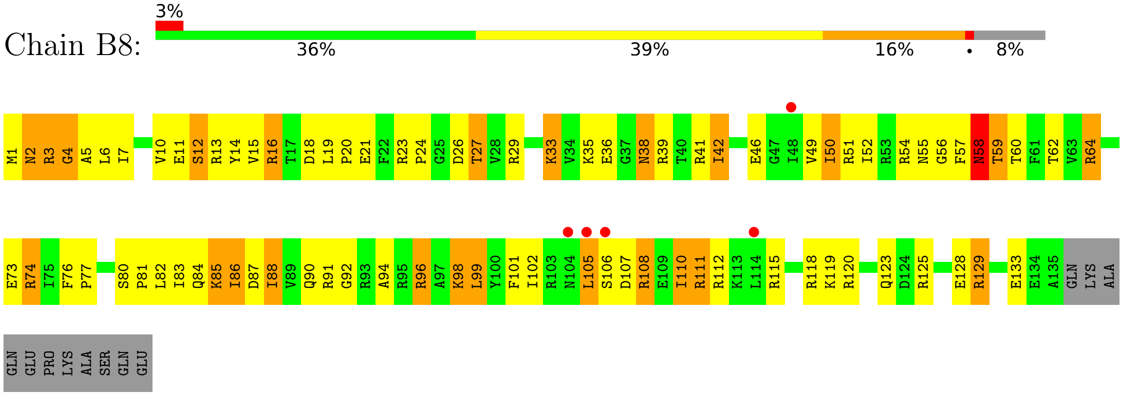


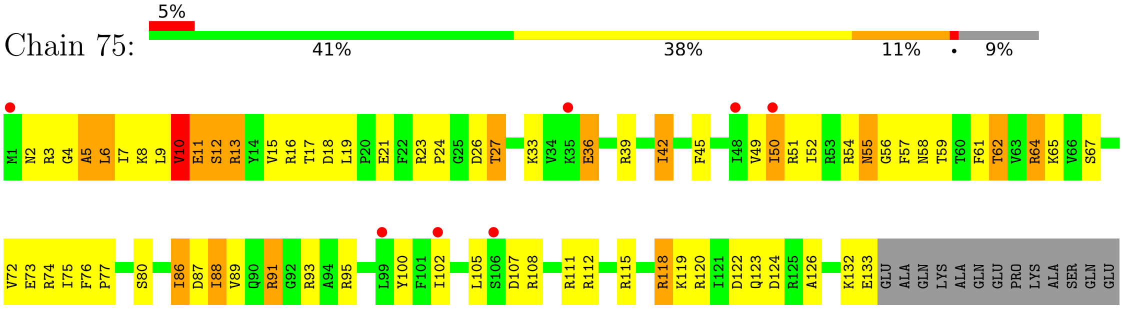
- Molecule 41: 50S ribosomal protein L19

Chain B8:



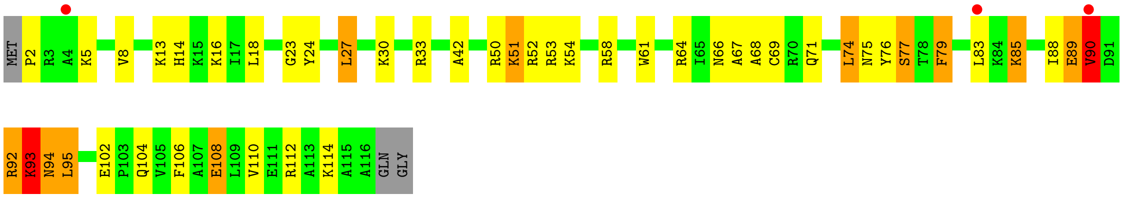
- Molecule 41: 50S ribosomal protein L19

Chain 75:



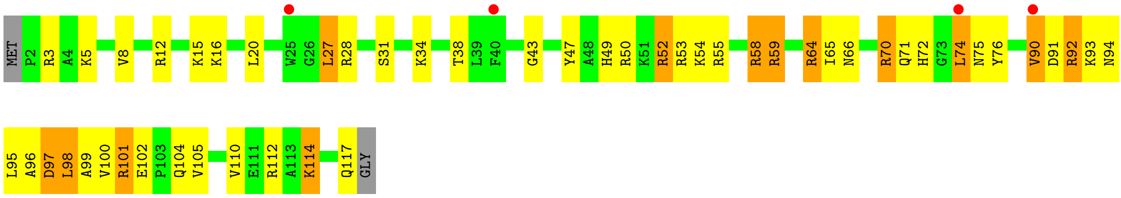
- Molecule 42: 50S ribosomal protein L20

Chain C8:



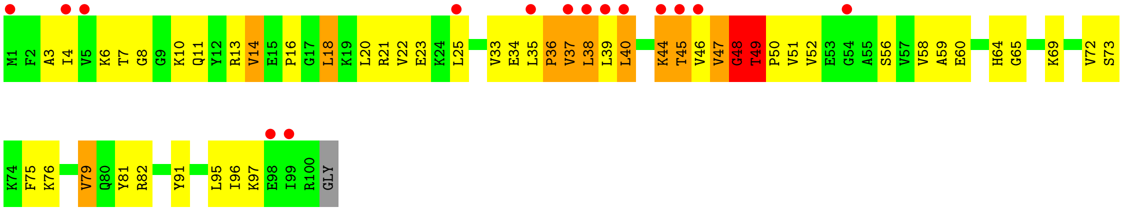
- Molecule 42: 50S ribosomal protein L20

Chain 85:



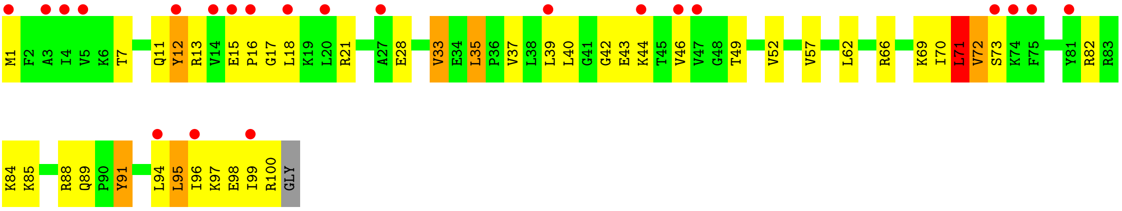
- Molecule 43: 50S ribosomal protein L21

Chain D8:



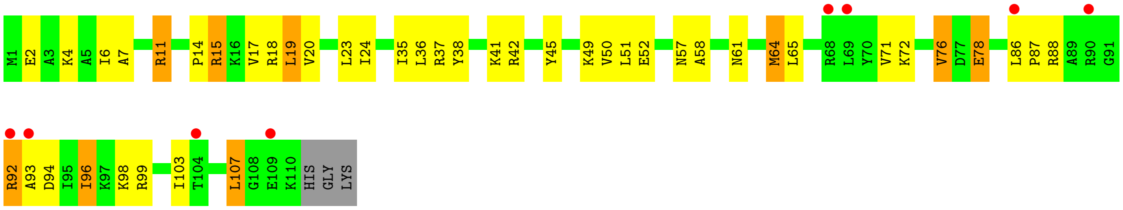
- Molecule 43: 50S ribosomal protein L21

Chain 95:



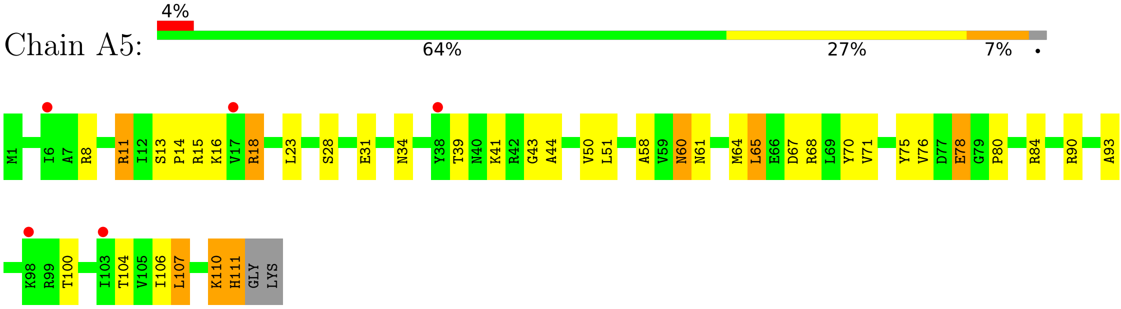
- Molecule 44: 50S ribosomal protein L22

Chain E8:



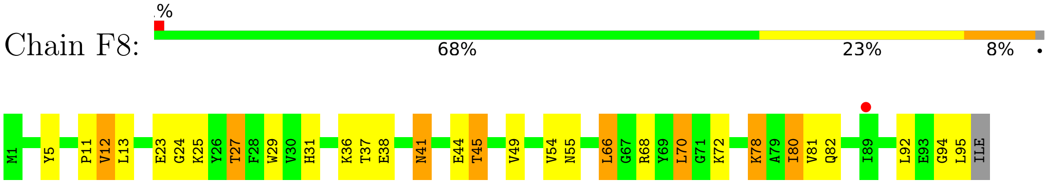
- Molecule 44: 50S ribosomal protein L22

Chain A5:



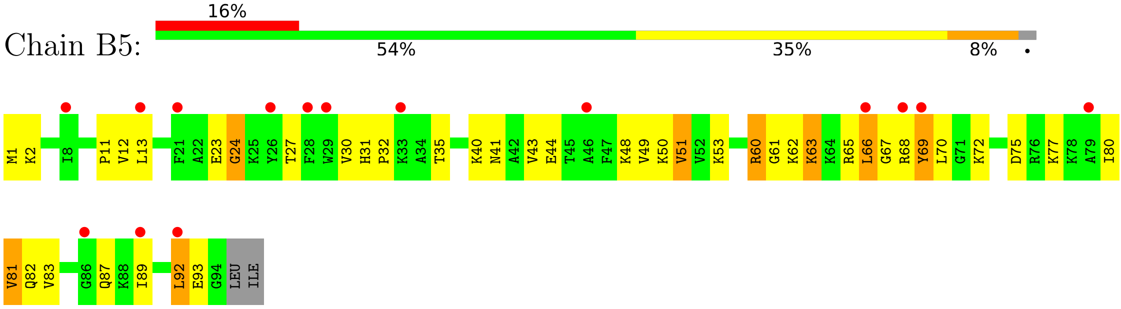
- Molecule 45: 50S ribosomal protein L23

Chain F8:



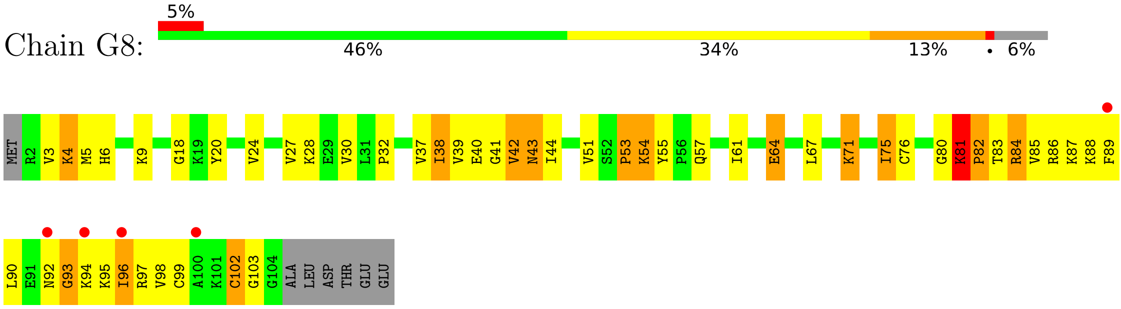
- Molecule 45: 50S ribosomal protein L23

Chain B5:



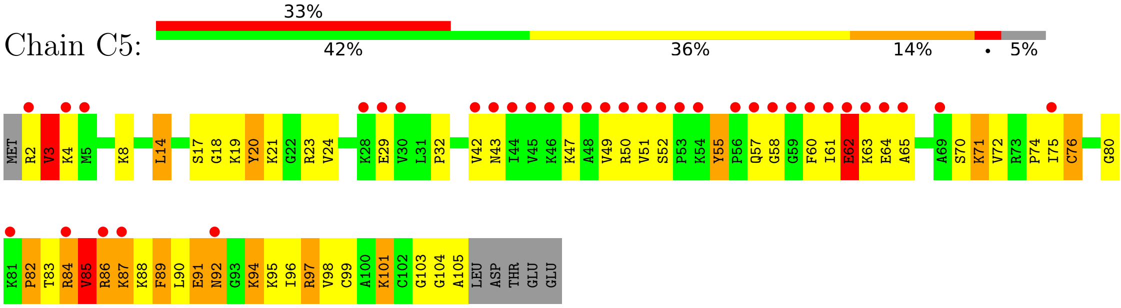
- Molecule 46: 50S ribosomal protein L24

Chain G8:

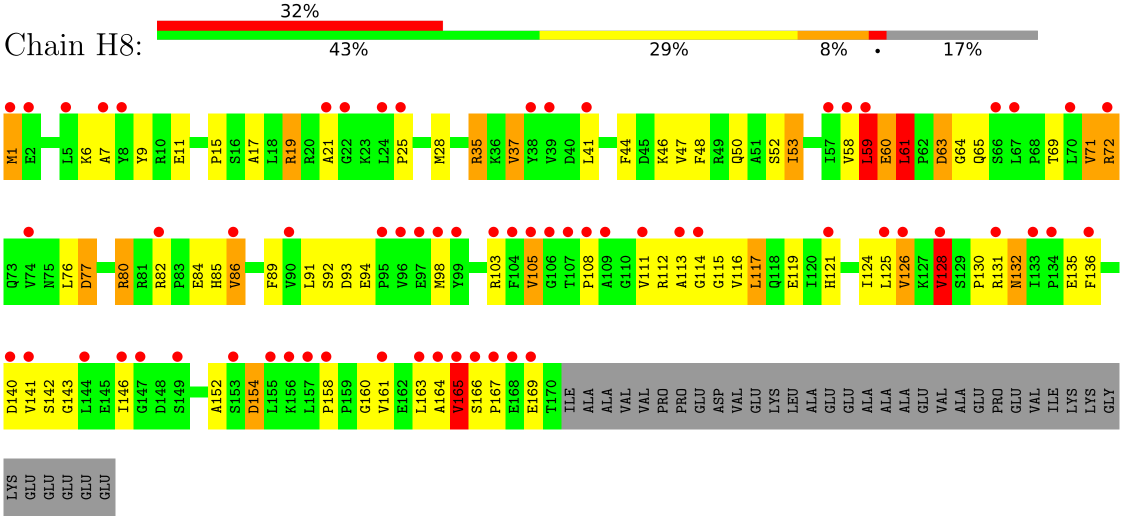


- Molecule 46: 50S ribosomal protein L24

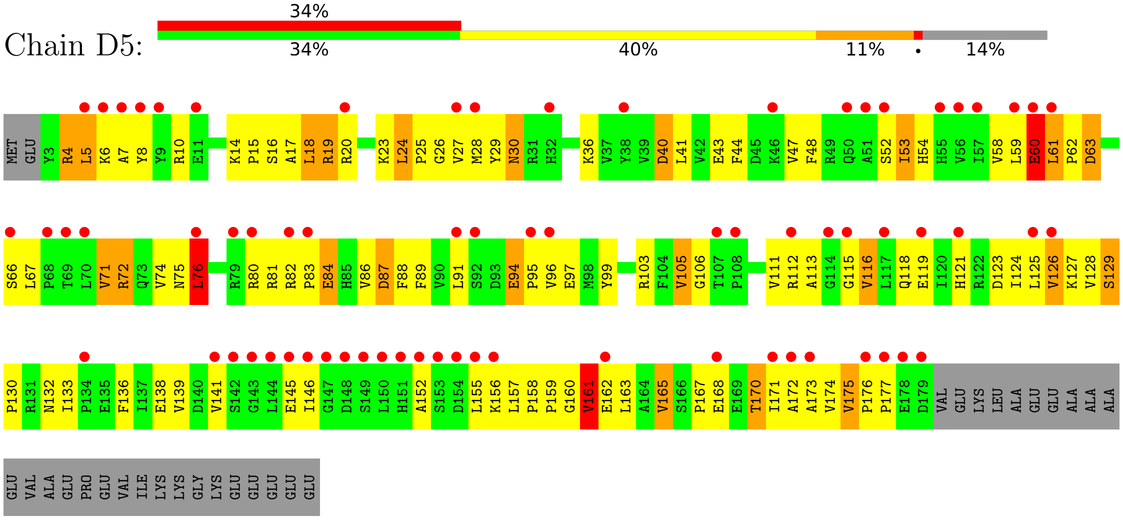
Chain C5:



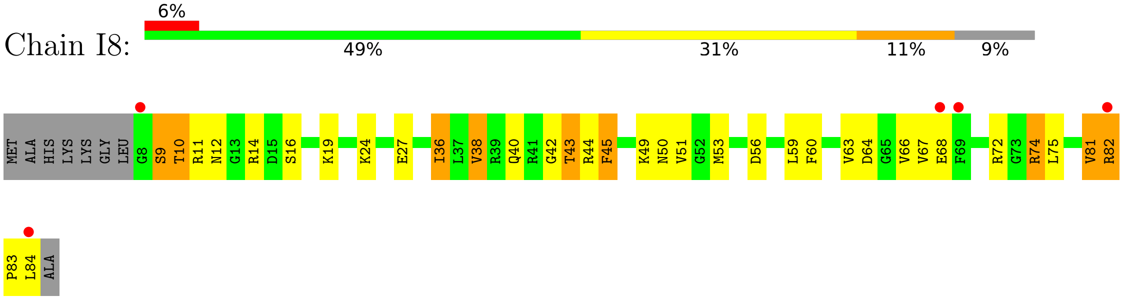
- Molecule 47: 50S ribosomal protein L25



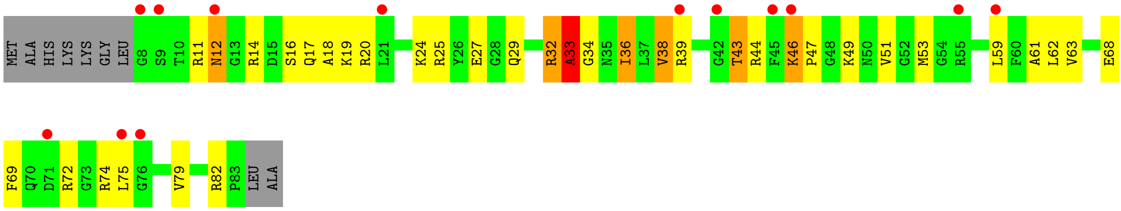
- Molecule 47: 50S ribosomal protein L25



- Molecule 48: 50S ribosomal protein L27

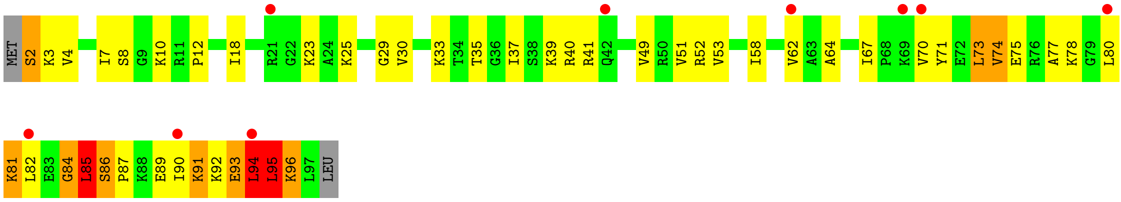


- Molecule 48: 50S ribosomal protein L27



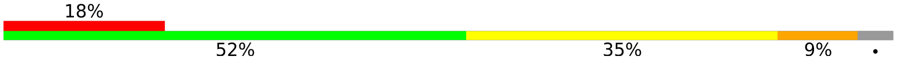
- Molecule 49: 50S ribosomal protein L28

Chain J8:



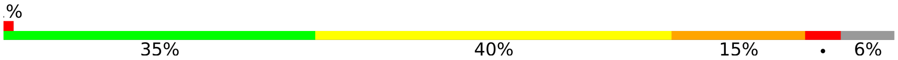
- Molecule 49: 50S ribosomal protein L28

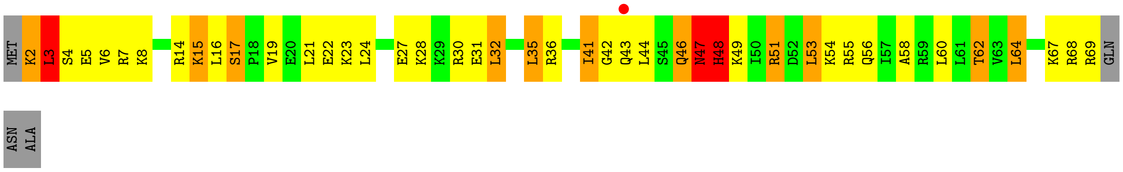
Chain F5:



- Molecule 50: 50S ribosomal protein L29

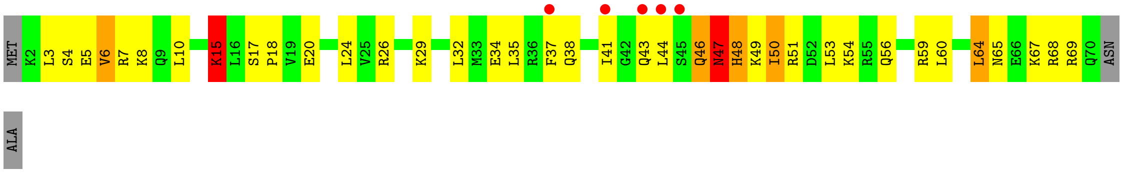
Chain K8:



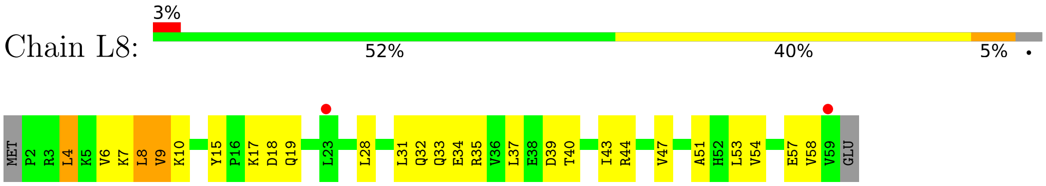


- Molecule 50: 50S ribosomal protein L29

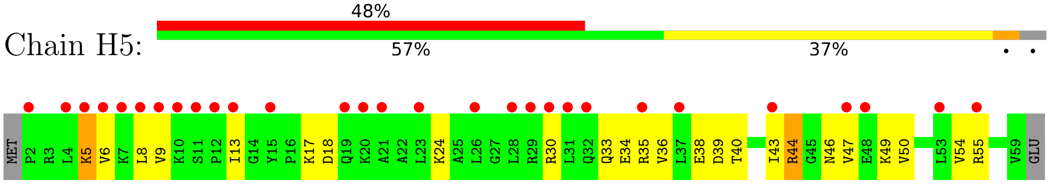
Chain G5:



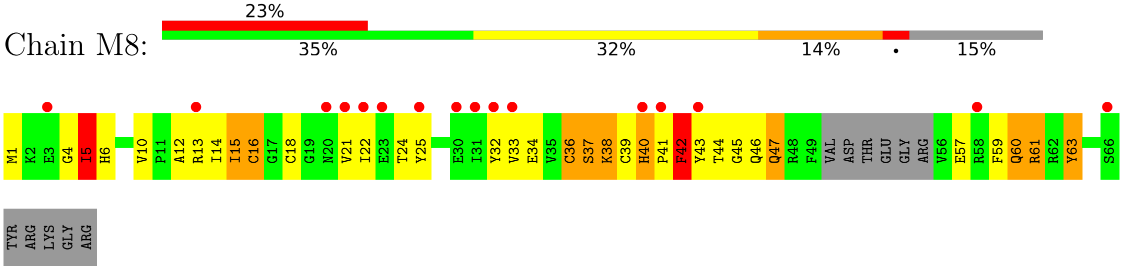
- Molecule 51: 50S ribosomal protein L30



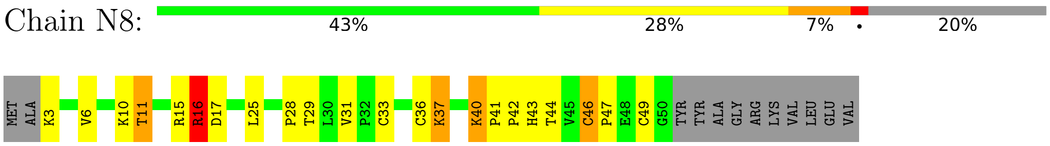
- Molecule 51: 50S ribosomal protein L30



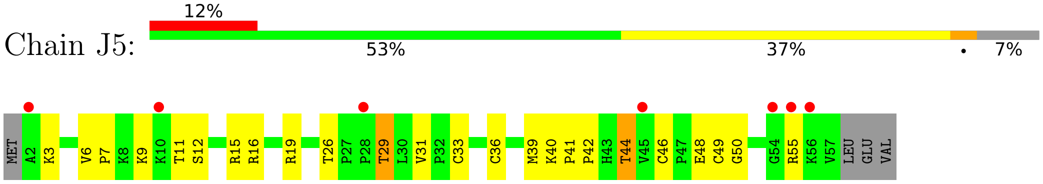
- Molecule 52: 50S ribosomal protein L31



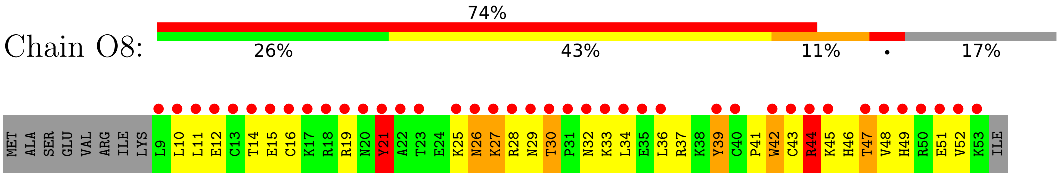
- Molecule 53: 50S ribosomal protein L32



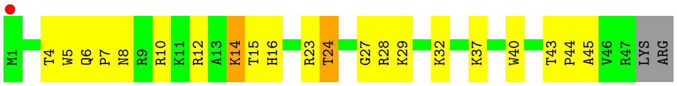
- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33

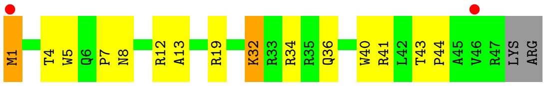


- Molecule 55: 50S ribosomal protein L34



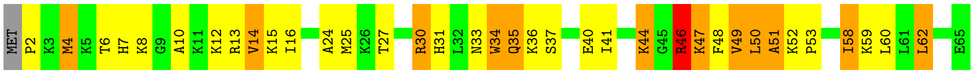
- Molecule 55: 50S ribosomal protein L34

Chain L5:



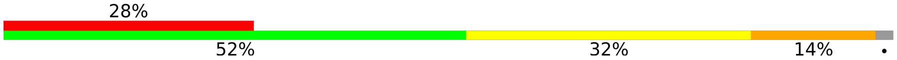
- Molecule 56: 50S ribosomal protein L35

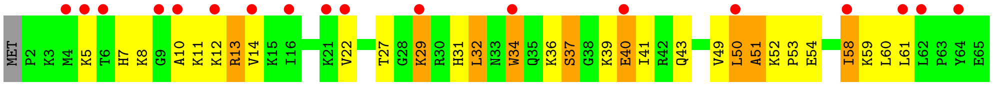
Chain Q8:



- Molecule 56: 50S ribosomal protein L35

Chain M5:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.30Å 448.80Å 620.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 161.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (161.81-2.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.241 0.202 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.7	EDS
L-test for twinning[2]	$< \|L\| >= 0.48$, $< L^2 >= 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: ZN, PAR, 5MU, OMC, PSU, 4SU, SF4, 7MG, U8U, T6A, MG, SPE

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	0.70	1/36068 (0.0%)	1.35	292/56287 (0.5%)
1	1G	0.61	0/36282	1.22	170/56623 (0.3%)
2	12	0.37	0/1727	0.61	1/2326 (0.0%)
2	1E	0.40	0/1908	0.63	2/2573 (0.1%)
3	22	0.43	1/1560 (0.1%)	0.56	0/2104
3	2E	0.47	1/1629 (0.1%)	0.62	1/2195 (0.0%)
4	32	0.45	1/1732 (0.1%)	0.64	0/2318
4	3E	0.48	1/1728 (0.1%)	0.62	1/2313 (0.0%)
5	42	0.38	0/1156	0.60	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.49	0/855	0.66	1/1154 (0.1%)
6	5E	0.46	0/850	0.61	0/1147
7	62	0.39	0/1122	0.61	0/1500
7	6E	0.39	0/1259	0.54	0/1686
8	72	0.37	0/1127	0.57	0/1517
8	7E	0.41	0/1135	0.64	1/1527 (0.1%)
9	82	0.36	0/971	0.62	0/1304
9	8E	0.39	0/1019	0.61	0/1367
10	1A	1.00	2/658 (0.3%)	0.56	0/885
10	1I	0.40	0/762	0.62	0/1027
11	2A	0.40	0/850	0.61	1/1150 (0.1%)
11	2I	0.47	0/838	0.65	0/1133
12	3A	0.44	0/963	0.66	1/1290 (0.1%)
12	3I	0.63	0/972	0.80	1/1301 (0.1%)
13	4A	0.35	0/889	0.59	0/1192
13	4I	0.50	0/943	0.67	0/1265
14	5A	0.34	0/495	0.65	0/657
14	5I	0.47	0/495	0.69	1/657 (0.2%)
15	6A	0.40	0/740	0.58	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.43	0/721	0.65	0/970
16	7I	0.43	0/716	0.68	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.51	0/836	0.65	0/1117
18	9A	0.46	0/549	0.67	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.67	0/700
19	AI	0.42	0/676	0.72	0/910
20	BA	0.35	0/764	0.67	1/1007 (0.1%)
20	BI	0.50	1/748 (0.1%)	0.63	0/986
21	1B	0.40	0/192	0.61	0/252
21	1F	0.42	0/203	0.71	0/266
22	1K	0.56	0/1589	1.11	6/2464 (0.2%)
23	2K	0.77	0/1721	1.42	16/2682 (0.6%)
23	2L	0.66	1/1721 (0.1%)	1.22	7/2682 (0.3%)
24	1L	0.39	0/1560	0.96	3/2418 (0.1%)
24	3K	0.52	0/1654	1.19	13/2570 (0.5%)
24	3L	0.52	0/1705	1.12	9/2650 (0.3%)
25	4K	0.74	0/473	1.15	0/735
25	4L	0.69	0/473	1.29	3/737 (0.4%)
26	14	0.84	45/68181 (0.1%)	1.54	1291/106432 (1.2%)
26	1H	1.01	117/68997 (0.2%)	1.75	2061/107696 (1.9%)
27	16	0.83	0/2928	1.57	59/4568 (1.3%)
27	1J	0.70	0/2928	1.37	32/4568 (0.7%)
28	71	0.29	0/1049	0.54	0/1417
29	11	0.66	1/2170 (0.0%)	0.90	4/2926 (0.1%)
29	19	0.64	1/2175 (0.0%)	0.85	2/2933 (0.1%)
30	21	0.57	0/1579	0.92	3/2131 (0.1%)
30	29	0.53	0/1596	0.80	3/2153 (0.1%)
31	31	0.63	1/1620 (0.1%)	0.90	3/2194 (0.1%)
31	39	0.51	0/1637	0.80	1/2218 (0.0%)
32	41	0.47	0/1481	0.68	0/1994
32	49	0.38	0/1483	0.63	1/1997 (0.1%)
33	51	0.53	0/1354	0.86	4/1833 (0.2%)
33	59	0.35	0/1320	0.69	3/1787 (0.2%)
34	61	0.41	0/1146	0.71	1/1551 (0.1%)
34	69	0.41	0/1146	0.70	1/1551 (0.1%)
35	15	0.41	0/1123	0.61	0/1515
35	58	0.52	0/1123	0.75	0/1514
36	25	0.48	0/942	0.71	1/1269 (0.1%)
36	68	0.55	0/942	0.76	2/1269 (0.2%)
37	35	0.53	0/1139	0.83	2/1514 (0.1%)
37	78	0.61	0/1139	1.04	8/1514 (0.5%)
38	45	0.61	2/1120 (0.2%)	0.81	0/1498
38	88	0.69	0/1138	0.92	1/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	55	0.51	0/981	0.83	0/1312
39	98	0.49	0/981	0.81	1/1312 (0.1%)
40	65	0.47	0/886	0.83	3/1180 (0.3%)
40	A8	0.59	0/891	0.83	2/1187 (0.2%)
41	75	0.51	0/1123	0.74	2/1500 (0.1%)
41	B8	0.58	0/1133	0.83	2/1514 (0.1%)
42	85	0.50	0/977	0.67	0/1301
42	C8	0.61	0/968	0.82	2/1289 (0.2%)
43	95	0.47	0/781	0.76	0/1048
43	D8	0.53	0/785	0.74	1/1052 (0.1%)
44	A5	0.55	0/897	0.77	1/1204 (0.1%)
44	E8	0.57	0/886	0.81	0/1189
45	B5	0.57	0/749	0.71	0/1007
45	F8	0.64	0/764	0.80	1/1025 (0.1%)
46	C5	0.52	0/807	0.81	1/1076 (0.1%)
46	G8	0.65	0/796	0.95	2/1062 (0.2%)
47	D5	0.54	1/1443 (0.1%)	0.64	1/1960 (0.1%)
47	H8	0.44	0/1395	0.73	1/1890 (0.1%)
48	E5	0.52	0/611	0.77	0/814
48	I8	0.76	1/619 (0.2%)	0.94	1/825 (0.1%)
49	F5	0.52	0/744	0.90	1/989 (0.1%)
49	J8	0.69	0/754	0.96	4/1003 (0.4%)
50	G5	0.53	0/578	0.73	0/766
50	K8	0.69	0/577	1.02	3/763 (0.4%)
51	H5	0.46	0/464	0.64	0/623
51	L8	0.50	0/464	0.73	0/623
52	M8	0.47	0/485	0.83	0/652
53	J5	0.58	0/448	0.76	0/606
53	N8	0.61	0/381	0.83	1/516 (0.2%)
54	O8	0.63	1/396 (0.3%)	0.90	1/529 (0.2%)
55	L5	0.57	0/409	0.78	0/540
55	P8	0.75	0/409	0.98	2/540 (0.4%)
56	M5	0.65	0/524	0.87	1/691 (0.1%)
56	Q8	0.69	0/524	1.02	3/691 (0.4%)
All	All	0.76	179/317928 (0.1%)	1.36	4051/476129 (0.9%)

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	2
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AA	0	2
19	AI	0	1
20	BA	0	2
29	11	0	5
29	19	0	3
30	21	0	8
30	29	0	5
31	39	0	7
32	41	0	1
32	49	0	2
33	51	0	5
33	59	0	1
34	61	0	3
34	69	0	4
35	58	0	1
37	35	0	2
37	78	0	6
38	45	0	2
38	88	0	4
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	2
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	2
43	D8	0	3
44	A5	0	1
45	B5	0	2
46	C5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	G8	0	5
47	D5	0	3
47	H8	0	6
48	E5	0	2
48	I8	0	1
49	F5	0	1
49	J8	0	1
50	G5	0	2
50	K8	0	2
52	M8	0	3
54	O8	0	1
55	P8	0	1
56	M5	0	2
56	Q8	0	3
All	All	0	145

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1A	38	ILE	C-N	19.47	1.71	1.34
47	D5	94	GLU	C-N	14.46	1.61	1.34
10	1A	76	ASN	C-N	14.15	1.61	1.34
26	1H	774	A	N9-C4	-13.65	1.29	1.37
26	14	783	A	N9-C4	-12.02	1.30	1.37

The worst 5 of 4051 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-23.89	111.67	126.00
26	1H	945	A	C6-C5-N7	-20.89	117.67	132.30
26	1H	945	A	N1-C6-N6	20.76	131.05	118.60
26	1H	1899	G	N3-C4-C5	20.42	138.81	128.60
26	1H	2430	A	C2-N3-C4	-20.30	100.45	110.60

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	234	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	1E	236	TYR	Peptide
9	8E	4	TYR	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	32223	0	16267	692	0
1	1G	32414	0	16360	752	0
2	12	1696	0	1730	89	0
2	1E	1874	0	1926	95	0
3	22	1537	0	1603	84	0
3	2E	1605	0	1668	54	0
4	32	1702	0	1765	93	0
4	3E	1698	0	1759	84	0
5	42	1141	0	1199	40	0
5	4E	1142	0	1204	40	0
6	52	842	0	857	19	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	53	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	62	0
9	8E	1000	0	1031	63	0
10	1A	646	0	662	45	0
10	1I	749	0	767	42	0
11	2A	835	0	847	25	0
11	2I	823	0	833	29	0
12	3A	947	0	1033	45	0
12	3I	956	0	1046	35	0
13	4A	879	0	935	46	0
13	4I	933	0	992	57	0
14	5A	486	0	525	35	0
14	5I	486	0	524	29	0
15	6A	729	0	768	26	0
15	6I	729	0	768	23	0
16	7A	705	0	725	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7I	700	0	720	45	0
17	8A	823	0	891	22	0
17	8I	823	0	891	34	0
18	9A	544	0	605	19	0
18	9I	549	0	607	21	0
19	AA	510	0	507	21	0
19	AI	661	0	683	43	0
20	BA	762	0	861	43	0
20	BI	746	0	843	44	0
21	1B	188	0	195	8	0
21	1F	199	0	208	9	0
22	1K	1542	0	790	25	0
23	2K	1646	0	845	18	0
23	2L	1646	0	845	25	0
24	1L	1401	0	713	22	0
24	3K	1483	0	756	50	0
24	3L	1528	0	778	42	0
25	4K	420	0	209	7	0
25	4L	419	0	208	17	0
26	14	60877	0	30690	1171	0
26	1H	61609	0	31058	1189	0
27	16	2617	0	1328	50	0
27	1J	2617	0	1328	76	0
28	71	1027	0	1043	57	0
29	11	2120	0	2197	100	0
29	19	2125	0	2199	105	0
30	21	1546	0	1602	86	0
30	29	1563	0	1629	93	0
31	31	1585	0	1632	70	0
31	39	1602	0	1649	88	0
32	41	1457	0	1514	68	0
32	49	1459	0	1507	65	0
33	51	1328	0	1396	64	0
33	59	1295	0	1366	58	0
34	61	1131	0	1218	36	0
34	69	1131	0	1218	49	0
35	15	1096	0	1168	47	0
35	58	1096	0	1169	48	0
36	25	932	0	996	46	0
36	68	932	0	996	41	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	45	1099	0	1154	73	0
38	88	1117	0	1168	58	0
39	55	967	0	1033	42	0
39	98	967	0	1033	45	0
40	65	876	0	938	63	0
40	A8	881	0	943	54	0
41	75	1109	0	1170	61	0
41	B8	1119	0	1177	72	0
42	85	959	0	1019	40	0
42	C8	950	0	1011	58	0
43	95	770	0	838	32	0
43	D8	774	0	849	40	0
44	A5	886	0	948	23	0
44	E8	876	0	941	30	0
45	B5	735	0	785	30	0
45	F8	750	0	814	19	0
46	C5	794	0	885	52	0
46	G8	783	0	869	49	0
47	D5	1411	0	1436	82	0
47	H8	1365	0	1391	57	0
48	E5	603	0	620	33	0
48	I8	611	0	631	34	0
49	F5	737	0	813	32	0
49	J8	747	0	817	42	0
50	G5	576	0	625	27	0
50	K8	575	0	634	42	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	475	0	465	34	0
53	J5	434	0	454	22	0
53	N8	369	0	388	21	0
54	O8	389	0	404	26	0
55	L5	401	0	436	10	0
55	P8	401	0	436	11	0
56	M5	516	0	582	25	0
56	Q8	516	0	582	37	0
57	13	140	0	0	0	0
57	14	435	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	102	0	0	0	0
57	1H	525	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1J	8	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	31	2	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	2	0	0	0	0
57	4I	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	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	88	3	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	2	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	43	0	0
58	1G	42	0	45	1	0
59	32	8	0	0	3	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	14	26	0	45	8	0
61	1G	13	0	24	0	0
62	11	17	0	0	4	0
62	13	320	0	0	12	0
62	14	1144	0	0	65	0
62	15	1	0	0	0	0
62	16	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	19	15	0	0	3	0
62	1A	1	0	0	0	0
62	1F	1	0	0	0	0
62	1G	317	0	0	21	0
62	1H	1470	0	0	90	0
62	1I	2	0	0	0	0
62	1J	12	0	0	1	0
62	1K	2	0	0	0	0
62	21	7	0	0	1	0
62	25	6	0	0	0	0
62	29	4	0	0	0	0
62	2K	8	0	0	1	0
62	2L	6	0	0	0	0
62	31	5	0	0	0	0
62	32	1	0	0	0	0
62	35	8	0	0	1	0
62	39	5	0	0	1	0
62	3I	2	0	0	0	0
62	41	1	0	0	0	0
62	4E	3	0	0	0	0
62	4K	5	0	0	0	0
62	4L	6	0	0	0	0
62	52	4	0	0	0	0
62	55	3	0	0	0	0
62	58	2	0	0	0	0
62	5I	2	0	0	0	0
62	6A	2	0	0	0	0
62	6I	3	0	0	0	0
62	78	10	0	0	0	0
62	7A	5	0	0	0	0
62	7I	1	0	0	0	0
62	85	2	0	0	0	0
62	8E	2	0	0	0	0
62	9A	2	0	0	0	0
62	A5	1	0	0	0	0
62	B5	1	0	0	0	0
62	B8	1	0	0	0	0
62	BA	2	0	0	0	0
62	BI	2	0	0	1	0
62	C5	3	0	0	0	0
62	C8	3	0	0	0	0
62	F5	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	F8	2	0	0	0	0
62	G8	2	0	0	0	0
62	H5	2	0	0	1	0
62	I8	6	0	0	1	0
62	J8	4	0	0	0	0
62	L8	3	0	0	1	0
62	M5	9	0	0	1	0
62	P8	1	0	0	0	0
62	Q8	5	0	0	2	0
All	All	297444	0	197360	7486	0

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

The worst 5 of 7486 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)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.44
38:45:27:VAL:HB	38:45:28:ALA:HA	1.19	1.13
29:11:182:LEU:H	29:11:272:ALA:HB3	1.23	1.02
37:78:63:PRO:HB2	56:Q8:30:ARG:HH21	1.23	1.01
26:1H:1496:A:H8	26:1H:1577:C:HO2’	1.00	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	173 (85%)	25 (12%)	5 (2%)	5	28
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	191/239 (80%)	171 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	32	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	29	68
4	3E	205/209 (98%)	192 (94%)	12 (6%)	1 (0%)	29	68
5	42	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	22	60
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22	60
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	42
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	60
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	19	57
9	8E	124/128 (97%)	108 (87%)	16 (13%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	85 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	8	37
11	2I	109/129 (84%)	94 (86%)	12 (11%)	3 (3%)	5	25
12	3A	119/132 (90%)	100 (84%)	15 (13%)	4 (3%)	3	20
12	3I	120/132 (91%)	107 (89%)	12 (10%)	1 (1%)	19	57
13	4A	107/126 (85%)	88 (82%)	18 (17%)	1 (1%)	17	55
13	4I	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	17	55
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	37
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	20
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	53
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9I	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	42
19	AA	59/93 (63%)	49 (83%)	8 (14%)	2 (3%)	3	20
19	AI	80/93 (86%)	68 (85%)	9 (11%)	3 (4%)	3	18
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	15	53
20	BI	95/106 (90%)	84 (88%)	10 (10%)	1 (1%)	14	50
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	128/229 (56%)	120 (94%)	8 (6%)	0	100	100
29	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	37
29	19	272/276 (99%)	246 (90%)	23 (8%)	3 (1%)	14	50
30	21	201/206 (98%)	158 (79%)	33 (16%)	10 (5%)	2	12
30	29	202/206 (98%)	149 (74%)	42 (21%)	11 (5%)	2	11
31	31	200/210 (95%)	181 (90%)	17 (8%)	2 (1%)	15	53
31	39	202/210 (96%)	162 (80%)	34 (17%)	6 (3%)	4	24
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	9	39
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	25	64
33	51	172/180 (96%)	141 (82%)	20 (12%)	11 (6%)	1	7
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	3	19
34	61	143/148 (97%)	122 (85%)	19 (13%)	2 (1%)	11	43
34	69	143/148 (97%)	111 (78%)	29 (20%)	3 (2%)	7	33
35	15	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
35	58	135/140 (96%)	114 (84%)	17 (13%)	4 (3%)	4	24
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	119 (82%)	26 (18%)	0	100	100
37	78	145/150 (97%)	114 (79%)	22 (15%)	9 (6%)	1	8
38	45	136/141 (96%)	115 (85%)	19 (14%)	2 (2%)	10	42
38	88	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	3	19
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	55
39	98	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	17	55
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	117 (89%)	12 (9%)	2 (2%)	10	42
41	B8	133/146 (91%)	118 (89%)	15 (11%)	0	100	100
42	85	114/118 (97%)	104 (91%)	9 (8%)	1 (1%)	17	55
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	26
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	4	23
43	D8	98/101 (97%)	88 (90%)	6 (6%)	4 (4%)	3	16
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	17	55
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	6	31
45	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	6
46	G8	101/110 (92%)	81 (80%)	16 (16%)	4 (4%)	3	17
47	D5	175/206 (85%)	136 (78%)	31 (18%)	8 (5%)	2	14
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	16
48	E5	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	5	26
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	45
49	F5	92/98 (94%)	79 (86%)	12 (13%)	1 (1%)	14	50
49	J8	94/98 (96%)	83 (88%)	9 (10%)	2 (2%)	7	33
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	4	24
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	14
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	40 (71%)	15 (27%)	1 (2%)	8	37
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	O8	43/54 (80%)	30 (70%)	12 (28%)	1 (2%)	6	30
55	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
56	M5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	9	40
56	Q8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11128/12158 (92%)	9762 (88%)	1180 (11%)	186 (2%)	9 39

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
30	21	83	ASP

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	179/220 (81%)	143 (80%)	36 (20%)	1 6
2	1E	200/220 (91%)	154 (77%)	46 (23%)	1 4
3	22	154/188 (82%)	128 (83%)	26 (17%)	2 11
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2 10
4	32	180/181 (99%)	151 (84%)	29 (16%)	2 12
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1 8
5	42	114/123 (93%)	87 (76%)	27 (24%)	1 3
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1 8
6	52	90/90 (100%)	74 (82%)	16 (18%)	2 9
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6 25
7	62	114/127 (90%)	88 (77%)	26 (23%)	1 4
7	6E	125/127 (98%)	105 (84%)	20 (16%)	2 12
8	72	118/119 (99%)	101 (86%)	17 (14%)	3 15
8	7E	119/119 (100%)	99 (83%)	20 (17%)	2 11
9	82	92/99 (93%)	73 (79%)	19 (21%)	1 6
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	2
10	1I	81/92 (88%)	73 (90%)	8 (10%)	8	30
11	2A	85/99 (86%)	67 (79%)	18 (21%)	1	5
11	2I	84/99 (85%)	70 (83%)	14 (17%)	2	11
12	3A	102/109 (94%)	79 (78%)	23 (22%)	1	4
12	3I	103/109 (94%)	91 (88%)	12 (12%)	5	22
13	4A	90/101 (89%)	68 (76%)	22 (24%)	0	3
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	29
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	7A	72/74 (97%)	61 (85%)	11 (15%)	2	13
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	19
17	8I	94/97 (97%)	82 (87%)	12 (13%)	4	19
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	8
18	9I	58/77 (75%)	49 (84%)	9 (16%)	2	13
19	AA	56/80 (70%)	47 (84%)	9 (16%)	2	12
19	AI	72/80 (90%)	61 (85%)	11 (15%)	2	13
20	BA	76/82 (93%)	66 (87%)	10 (13%)	4	18
20	BI	75/82 (92%)	61 (81%)	14 (19%)	1	8
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	71	108/181 (60%)	87 (81%)	21 (19%)	1	7
29	11	214/218 (98%)	173 (81%)	41 (19%)	1	8
29	19	214/218 (98%)	171 (80%)	43 (20%)	1	6
30	21	162/166 (98%)	118 (73%)	44 (27%)	0	2
30	29	165/166 (99%)	135 (82%)	30 (18%)	1	9
31	31	161/166 (97%)	128 (80%)	33 (20%)	1	6
31	39	163/166 (98%)	126 (77%)	37 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	126 (82%)	27 (18%)	2	10
32	49	152/156 (97%)	125 (82%)	27 (18%)	2	9
33	51	143/148 (97%)	106 (74%)	37 (26%)	0	2
33	59	140/148 (95%)	106 (76%)	34 (24%)	0	3
34	61	122/124 (98%)	86 (70%)	36 (30%)	0	1
34	69	122/124 (98%)	89 (73%)	33 (27%)	0	2
35	15	116/119 (98%)	90 (78%)	26 (22%)	1	4
35	58	116/119 (98%)	87 (75%)	29 (25%)	0	3
36	25	100/100 (100%)	76 (76%)	24 (24%)	0	3
36	68	100/100 (100%)	90 (90%)	10 (10%)	7	29
37	35	114/116 (98%)	82 (72%)	32 (28%)	0	2
37	78	114/116 (98%)	78 (68%)	36 (32%)	0	1
38	45	109/111 (98%)	88 (81%)	21 (19%)	1	8
38	88	110/111 (99%)	90 (82%)	20 (18%)	1	9
39	55	101/101 (100%)	80 (79%)	21 (21%)	1	5
39	98	101/101 (100%)	72 (71%)	29 (29%)	0	2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	A8	87/88 (99%)	66 (76%)	21 (24%)	0	3
41	75	117/127 (92%)	95 (81%)	22 (19%)	1	8
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0	2
42	85	93/94 (99%)	73 (78%)	20 (22%)	1	5
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10
43	95	81/82 (99%)	68 (84%)	13 (16%)	2	12
43	D8	82/82 (100%)	63 (77%)	19 (23%)	1	4
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	8
44	E8	90/92 (98%)	73 (81%)	17 (19%)	1	8
45	B5	74/78 (95%)	56 (76%)	18 (24%)	0	3
45	F8	77/78 (99%)	64 (83%)	13 (17%)	2	11
46	C5	85/91 (93%)	63 (74%)	22 (26%)	0	2
46	G8	84/91 (92%)	66 (79%)	18 (21%)	1	5
47	D5	156/179 (87%)	124 (80%)	32 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	124 (82%)	27 (18%)	2	9
48	E5	61/67 (91%)	55 (90%)	6 (10%)	8	30
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3	15
49	F5	79/83 (95%)	63 (80%)	16 (20%)	1	6
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	14
50	G5	63/67 (94%)	46 (73%)	17 (27%)	0	2
50	K8	64/67 (96%)	43 (67%)	21 (33%)	0	1
51	H5	50/52 (96%)	38 (76%)	12 (24%)	0	3
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1	7
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	2
53	J5	48/52 (92%)	41 (85%)	7 (15%)	3	15
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	O8	44/52 (85%)	29 (66%)	15 (34%)	0	1
55	L5	38/42 (90%)	32 (84%)	6 (16%)	2	12
55	P8	38/42 (90%)	31 (82%)	7 (18%)	1	9
56	M5	54/55 (98%)	43 (80%)	11 (20%)	1	6
56	Q8	54/55 (98%)	44 (82%)	10 (18%)	1	8
All	All	9397/10064 (93%)	7493 (80%)	1904 (20%)	1	6

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	L8	58	VAL
45	B5	82	GLN
8	72	41	ARG
44	A5	107	LEU
55	L5	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
18	9A	36	ASN
29	19	227	ASN
51	H5	33	GLN
40	65	95	HIS

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Mol	Chain	Res	Type
50	G5	47	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	331 (22%)	33 (2%)
1	1G	1506/1522 (98%)	352 (23%)	33 (2%)
22	1K	68/76 (89%)	27 (39%)	4 (5%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	15 (19%)	2 (2%)
24	1L	61/76 (80%)	24 (39%)	2 (3%)
24	3K	67/76 (88%)	37 (55%)	2 (2%)
24	3L	69/76 (90%)	30 (43%)	2 (2%)
25	4K	17/30 (56%)	9 (52%)	1 (5%)
25	4L	18/30 (60%)	12 (66%)	1 (5%)
26	14	2821/2917 (96%)	675 (23%)	42 (1%)
26	1H	2850/2917 (97%)	630 (22%)	52 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	32 (26%)	3 (2%)
All	All	9368/9640 (97%)	2219 (23%)	180 (1%)

5 of 2219 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G

5 of 180 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	992	U
26	14	503	A
1	1G	1145	C
23	2L	33	OMC
26	14	960	A

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

15 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	7MG	2K	47	23	22,26,27	2.88	7 (31%)	29,39,42	2.89	10 (34%)
23	PSU	2K	56	23	18,21,22	1.32	2 (11%)	22,30,33	1.79	3 (13%)
23	4SU	2L	8	23	18,21,22	1.95	4 (22%)	26,30,33	2.36	5 (19%)
23	PSU	2L	56	23	18,21,22	1.25	2 (11%)	22,30,33	1.45	2 (9%)
22	U8U	1K	34	25,22	19,24,25	2.61	7 (36%)	23,34,37	1.18	2 (8%)
22	T6A	1K	37	22	27,34,35	2.48	5 (18%)	29,49,52	2.41	7 (24%)
23	4SU	2K	8	23	18,21,22	1.66	3 (16%)	26,30,33	2.38	4 (15%)
23	5MU	2L	55	23	19,22,23	4.00	5 (26%)	28,32,35	3.11	8 (28%)
23	5MU	2K	55	23	19,22,23	3.89	5 (26%)	28,32,35	3.15	9 (32%)
23	7MG	2L	47	23	22,26,27	3.01	8 (36%)	29,39,42	2.86	10 (34%)
22	5MU	1K	54	22	19,22,23	3.94	5 (26%)	28,32,35	2.92	7 (25%)
23	OMC	2L	33	23	19,22,23	1.78	4 (21%)	26,31,34	1.26	2 (7%)
22	PSU	1K	39	22	18,21,22	1.02	1 (5%)	22,30,33	1.53	4 (18%)
22	PSU	1K	55	22	18,21,22	1.28	1 (5%)	22,30,33	1.56	4 (18%)
23	OMC	2K	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.03	2 (7%)

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	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	3/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	0/9/28/29	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	T6A	1K	37	22	-	6/19/41/42	0/3/3/3
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.89	1.59	1.38
22	1K	54	5MU	C2-N1	12.63	1.58	1.38
23	2K	55	5MU	C2-N1	12.52	1.58	1.38
23	2L	47	7MG	C5-N7	8.90	1.45	1.35
23	2K	47	7MG	C5-N7	8.03	1.44	1.35

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2L	55	5MU	C5-C4-N3	9.89	123.75	115.31
23	2K	55	5MU	C5-C4-N3	9.69	123.58	115.31
22	1K	54	5MU	C5-C4-N3	9.41	123.34	115.31
23	2L	8	4SU	C4-N3-C2	-8.13	119.44	127.34
23	2K	8	4SU	C4-N3-C2	-7.63	119.93	127.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2K	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1269 ligands modelled in this entry, 1262 are monoatomic - leaving 7 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	#$\lvert Z\rvert > 2$
61	SPE	14	3437	26	12,12,12	0.83	0	11,11,11	0.96	1 (9%)
58	PAR	13	1741	1	45,45,45	0.68	0	64,67,67	1.48	10 (15%)
59	SF4	32	302	4	0,12,12	-	-	-		
59	SF4	3E	301	4	0,12,12	-	-	-		
61	SPE	1G	1703	-	12,12,12	0.35	0	11,11,11	0.76	0
58	PAR	1G	1702	-	45,45,45	0.67	1 (2%)	64,67,67	1.39	9 (14%)
61	SPE	14	3436	-	12,12,12	0.43	0	11,11,11	0.65	0

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
61	SPE	14	3437	26	-	5/10/10/10	-
58	PAR	13	1741	1	-	5/18/94/94	0/4/4/4
59	SF4	32	302	4	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5
61	SPE	1G	1703	-	-	3/10/10/10	-
58	PAR	1G	1702	-	-	1/18/94/94	0/4/4/4
61	SPE	14	3436	-	-	5/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.22	1.43	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	13	1741	PAR	C32-C22-C12	3.69	118.76	111.18
58	13	1741	PAR	C11-O51-C51	3.65	120.85	113.69
58	1G	1702	PAR	C14-O33-C33	-3.57	109.14	117.96
58	13	1741	PAR	C22-C12-C62	3.28	115.00	110.04
58	1G	1702	PAR	C13-O52-C52	-3.28	109.84	117.96

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	13	1741	PAR	C44-C54-C64-N64
58	13	1741	PAR	O54-C54-C64-N64
61	1G	1703	SPE	C2-C3-C4-N5
61	14	3437	SPE	C6-C7-C8-N9
61	14	3437	SPE	N9-C10-C11-C12

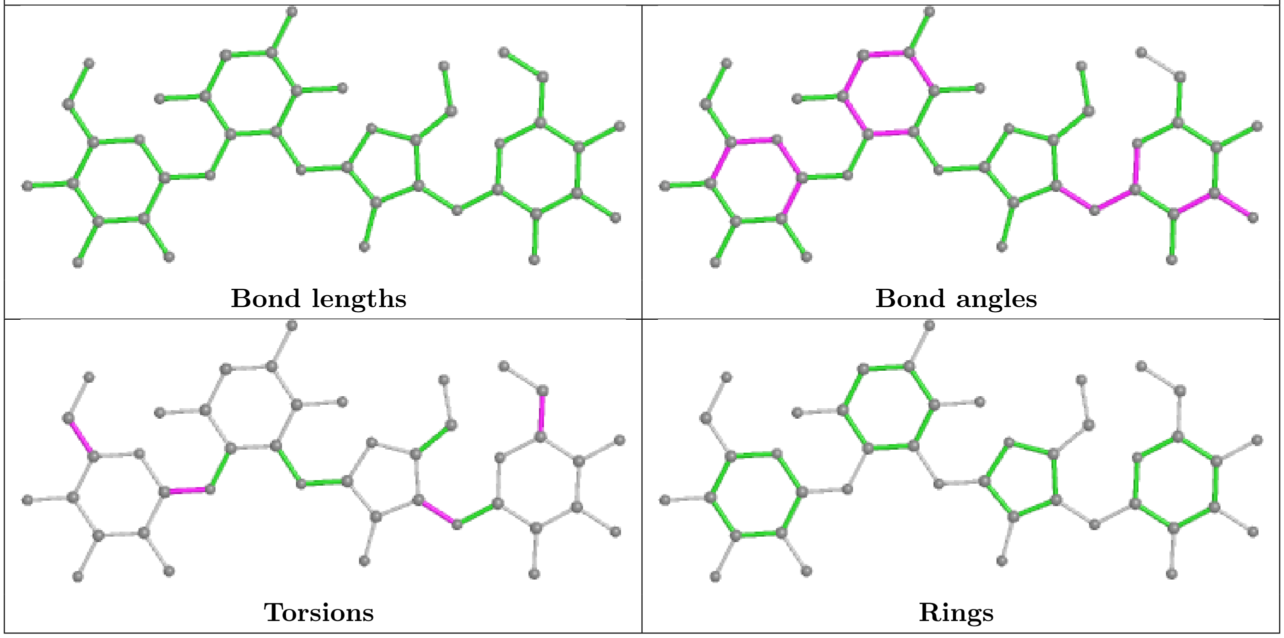
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	14	3437	SPE	6	0
59	32	302	SF4	3	0
59	3E	301	SF4	1	0
58	1G	1702	PAR	1	0
61	14	3436	SPE	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 1741

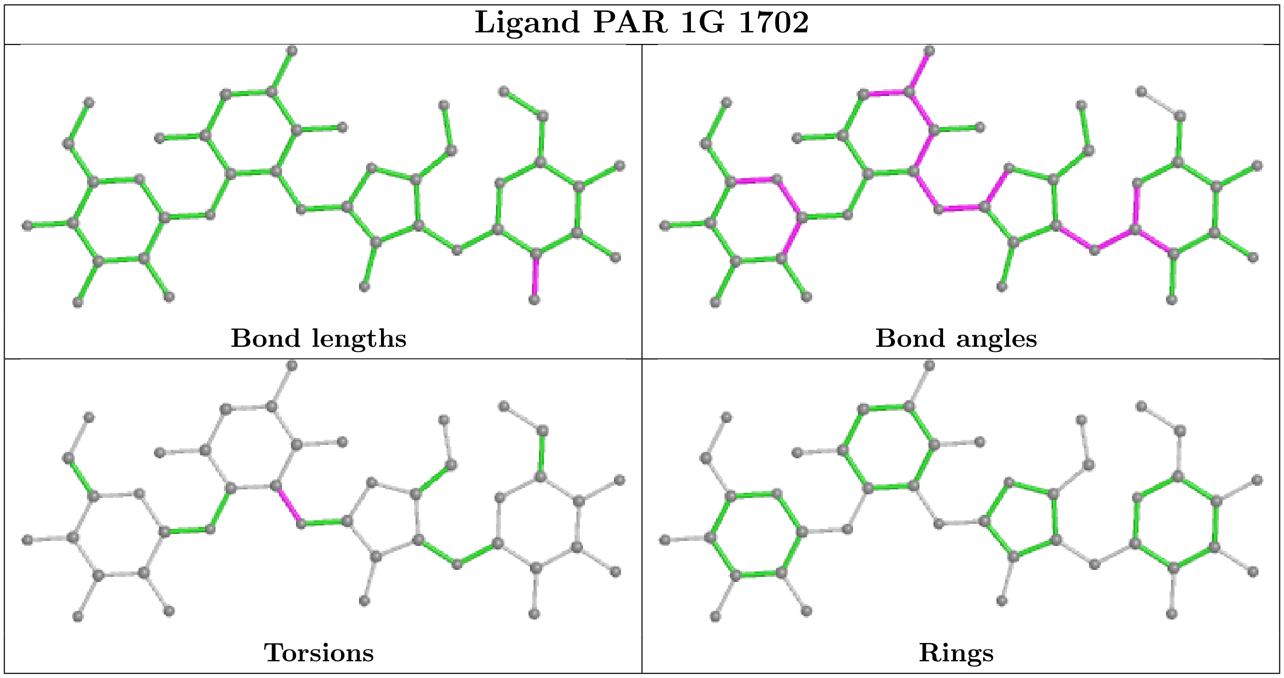


Bond lengths

Bond angles

Torsions

Rings



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
10	1A	2
26	1H	1
24	1L	1
47	D5	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13	1499/1522 (98%)	-0.23	1 (0%)	95	89	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.17	10 (0%)	87	69	71, 119, 192, 267	0
2	12	207/256 (80%)	0.75	26 (12%)	3	1	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.24	12 (5%)	27	10	112, 143, 169, 174	0
3	22	195/239 (81%)	1.21	50 (25%)	0	0	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.67	22 (10%)	6	2	88, 111, 143, 151	0
4	32	208/209 (99%)	0.66	14 (6%)	17	5	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.31	12 (5%)	23	7	84, 108, 132, 144	0
5	42	150/162 (92%)	0.49	11 (7%)	15	4	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.30	4 (2%)	54	26	82, 103, 121, 131	0
6	52	101/101 (100%)	0.02	0	100	100	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.52	7 (7%)	16	5	85, 105, 120, 132	0
7	62	138/156 (88%)	1.18	33 (23%)	0	0	116, 130, 141, 147	0
7	6E	154/156 (98%)	1.23	36 (23%)	0	0	102, 120, 150, 171	0
8	72	137/138 (99%)	0.73	15 (10%)	5	2	100, 131, 142, 149	0
8	7E	138/138 (100%)	1.07	29 (21%)	1	0	93, 110, 122, 134	0
9	82	121/128 (94%)	1.87	50 (41%)	0	0	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.24	5 (3%)	38	15	87, 138, 157, 163	0
10	1A	80/105 (76%)	1.02	22 (27%)	0	0	133, 156, 169, 174	0
10	1I	94/105 (89%)	1.42	28 (29%)	0	0	81, 131, 168, 173	0
11	2A	113/129 (87%)	1.33	27 (23%)	0	0	84, 109, 124, 135	0
11	2I	111/129 (86%)	1.14	25 (22%)	0	0	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.72	45 (37%)	0	0	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.72	15 (12%)	4	1	66, 76, 102, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	109/126 (86%)	0.85	26 (23%) 0 0	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.32	4 (3%) 45 19	88, 116, 131, 138	0
14	5A	59/61 (96%)	3.90	41 (69%) 0 0	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.83	8 (13%) 3 1	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.13	3 (3%) 45 19	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.35	3 (3%) 45 19	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.26	2 (2%) 59 30	92, 105, 129, 155	0
16	7I	83/88 (94%)	1.13	20 (24%) 0 0	96, 111, 137, 155	0
17	8A	99/105 (94%)	1.30	27 (27%) 0 0	97, 113, 130, 135	0
17	8I	99/105 (94%)	1.10	18 (18%) 1 0	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.35	4 (5%) 21 7	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.20	2 (2%) 51 23	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.17	13 (20%) 1 0	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.24	3 (3%) 41 17	96, 117, 138, 151	0
20	BA	99/106 (93%)	1.15	18 (18%) 1 0	90, 114, 140, 152	0
20	BI	97/106 (91%)	1.37	27 (27%) 0 0	106, 119, 145, 151	0
21	1B	22/27 (81%)	1.72	8 (36%) 0 0	127, 141, 145, 148	0
21	1F	23/27 (85%)	0.24	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	0.54	5 (7%) 14 4	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.03	1 (1%) 75 49	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.07	0 100 100	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.06	11 (16%) 1 0	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.91	10 (14%) 2 1	76, 229, 251, 253	0
24	3L	72/76 (94%)	0.16	3 (4%) 36 14	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.97	4 (21%) 1 0	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.35	3 (15%) 2 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.06	17 (0%) 89 72	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.10	7 (0%) 95 87	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.35	1 (0%) 86 65	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.45	0 100 100	85, 119, 145, 205	0
28	71	132/229 (57%)	0.80	20 (15%) 2 1	146, 210, 235, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
29	11	273/276 (98%)	0.46	5 (1%)	68	40	41, 63, 79, 93	0
29	19	274/276 (99%)	0.59	7 (2%)	56	27	47, 73, 88, 107	0
30	21	203/206 (98%)	0.63	10 (4%)	29	11	48, 84, 120, 130	0
30	29	204/206 (99%)	1.03	39 (19%)	1	0	60, 95, 134, 149	0
31	31	202/210 (96%)	0.63	9 (4%)	33	12	46, 76, 112, 127	0
31	39	204/210 (97%)	0.56	14 (6%)	16	5	57, 101, 148, 177	0
32	41	179/182 (98%)	0.77	21 (11%)	4	1	79, 100, 134, 146	0
32	49	180/182 (98%)	1.22	48 (26%)	0	0	117, 138, 156, 174	0
33	51	174/180 (96%)	0.30	4 (2%)	60	31	77, 102, 119, 130	0
33	59	169/180 (93%)	2.48	92 (54%)	0	0	152, 196, 220, 233	0
34	61	145/148 (97%)	0.52	17 (11%)	4	1	76, 131, 149, 157	0
34	69	145/148 (97%)	0.46	12 (8%)	11	3	86, 122, 149, 156	0
35	15	137/140 (97%)	1.16	25 (18%)	1	0	81, 108, 135, 151	0
35	58	137/140 (97%)	0.86	18 (13%)	3	1	63, 85, 121, 138	0
36	25	122/122 (100%)	0.91	14 (11%)	4	1	69, 88, 105, 117	0
36	68	122/122 (100%)	0.39	3 (2%)	57	29	56, 72, 90, 99	0
37	35	147/150 (98%)	0.86	21 (14%)	2	1	58, 102, 135, 152	0
37	78	147/150 (98%)	0.57	10 (6%)	17	5	47, 80, 104, 115	0
38	45	138/141 (97%)	0.95	27 (19%)	1	0	76, 105, 124, 155	0
38	88	141/141 (100%)	0.71	10 (7%)	16	5	54, 75, 95, 123	0
39	55	118/118 (100%)	0.60	7 (5%)	22	7	65, 80, 97, 112	0
39	98	118/118 (100%)	0.81	12 (10%)	6	2	60, 78, 94, 106	0
40	65	110/112 (98%)	1.06	22 (20%)	1	0	89, 112, 132, 137	0
40	A8	111/112 (99%)	1.09	18 (16%)	1	0	72, 85, 105, 116	0
41	75	133/146 (91%)	0.40	7 (5%)	26	10	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.14	5 (3%)	41	17	67, 84, 128, 139	0
42	85	116/118 (98%)	0.54	4 (3%)	45	19	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.31	3 (2%)	56	27	53, 77, 102, 108	0
43	95	100/101 (99%)	1.08	22 (22%)	0	0	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.89	15 (15%)	2	1	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.79	5 (4%)	33	12	57, 75, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	E8	110/113 (97%)	0.49	8 (7%) 15 4	53, 70, 94, 106	0
45	B5	94/96 (97%)	1.09	15 (15%) 1 1	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.21	1 (1%) 80 56	49, 66, 97, 110	0
46	C5	104/110 (94%)	2.12	36 (34%) 0 0	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.26	5 (4%) 29 11	73, 95, 122, 130	0
47	D5	177/206 (85%)	1.81	70 (39%) 0 0	108, 148, 226, 236	0
47	H8	170/206 (82%)	1.81	65 (38%) 0 0	80, 116, 202, 210	0
48	E5	76/85 (89%)	1.15	13 (17%) 1 0	66, 88, 102, 115	0
48	I8	77/85 (90%)	0.58	5 (6%) 18 5	54, 69, 91, 102	0
49	F5	94/98 (95%)	1.21	18 (19%) 1 0	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.85	9 (9%) 8 3	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.44	5 (7%) 15 4	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.12	1 (1%) 73 46	59, 79, 96, 120	0
51	H5	58/60 (96%)	2.04	29 (50%) 0 0	77, 99, 122, 135	0
51	L8	58/60 (96%)	0.54	2 (3%) 45 19	60, 77, 103, 110	0
52	M8	60/71 (84%)	1.54	16 (26%) 0 0	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.72	7 (12%) 3 1	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.36	0 100 100	46, 78, 119, 127	0
54	O8	45/54 (83%)	4.57	40 (88%) 0 0	117, 153, 171, 177	0
55	L5	47/49 (95%)	0.47	2 (4%) 35 13	47, 60, 87, 97	0
55	P8	47/49 (95%)	0.09	1 (2%) 63 34	42, 50, 72, 87	0
56	M5	64/65 (98%)	1.47	18 (28%) 0 0	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.36	0 100 100	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.42	1700 (8%) 11 3	40, 99, 184, 267	0

The worst 5 of 1700 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	C5	59	GLY	14.7
14	5A	38	GLY	12.9
33	59	96	ALA	12.6
46	C5	49	VAL	12.1
52	M8	40	HIS	11.7

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	PSU	1K	55	20/21	0.87	0.16	107,127,140,145	0
23	4SU	2L	8	20/21	0.88	0.16	107,118,124,125	0
23	OMC	2L	33	21/22	0.90	0.19	94,103,107,109	0
23	PSU	2L	56	20/21	0.91	0.10	109,121,126,126	0
23	7MG	2L	47	24/25	0.92	0.14	118,128,137,141	0
23	PSU	2K	56	20/21	0.92	0.12	91,101,110,117	0
22	5MU	1K	54	21/22	0.92	0.16	104,125,133,143	0
22	PSU	1K	39	20/21	0.93	0.21	94,112,118,120	0
22	T6A	1K	37	32/33	0.94	0.20	81,92,114,116	0
23	5MU	2L	55	21/22	0.94	0.14	115,122,127,130	0
23	4SU	2K	8	20/21	0.94	0.17	89,95,101,103	0
23	7MG	2K	47	24/25	0.94	0.15	96,101,113,116	0
23	5MU	2K	55	21/22	0.95	0.14	98,105,112,114	0
23	OMC	2K	33	21/22	0.96	0.21	73,79,82,94	0
22	U8U	1K	34	23/24	0.96	0.17	83,98,108,110	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1678	1/1	0.02	0.16	112,112,112,112	0
57	MG	1H	3445	1/1	0.18	0.12	92,92,92,92	0
57	MG	1H	3081	1/1	0.19	0.45	83,83,83,83	0
57	MG	13	1704	1/1	0.32	0.13	106,106,106,106	0
57	MG	14	3393	1/1	0.32	0.08	165,165,165,165	0
57	MG	1G	1673	1/1	0.34	0.14	115,115,115,115	0
57	MG	1H	3180	1/1	0.34	0.42	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	14	3350	1/1	0.39	0.16	101,101,101,101	0
57	MG	14	3115	1/1	0.40	0.78	87,87,87,87	0
57	MG	14	3377	1/1	0.47	0.10	131,131,131,131	0
57	MG	1H	3113	1/1	0.48	0.26	81,81,81,81	0
57	MG	1G	1609	1/1	0.50	0.87	92,92,92,92	0
57	MG	14	3163	1/1	0.51	0.38	93,93,93,93	0
57	MG	14	3422	1/1	0.52	0.24	108,108,108,108	0
57	MG	1H	3154	1/1	0.53	0.23	58,58,58,58	0
57	MG	13	1709	1/1	0.54	0.26	99,99,99,99	0
57	MG	1H	3157	1/1	0.54	0.38	89,89,89,89	0
57	MG	1H	3454	1/1	0.54	0.07	111,111,111,111	0
57	MG	1H	3520	1/1	0.54	0.10	105,105,105,105	0
57	MG	1G	1642	1/1	0.55	0.28	99,99,99,99	0
57	MG	1H	3145	1/1	0.56	0.53	80,80,80,80	0
57	MG	14	3127	1/1	0.56	1.02	87,87,87,87	0
57	MG	14	3355	1/1	0.56	0.10	104,104,104,104	0
57	MG	1G	1686	1/1	0.57	0.13	106,106,106,106	0
57	MG	13	1679	1/1	0.57	0.30	99,99,99,99	0
57	MG	1H	3237	1/1	0.57	0.46	81,81,81,81	0
57	MG	1G	1678	1/1	0.58	0.11	111,111,111,111	0
57	MG	14	3154	1/1	0.58	0.40	95,95,95,95	0
57	MG	13	1643	1/1	0.59	0.23	101,101,101,101	0
57	MG	13	1739	1/1	0.59	0.06	121,121,121,121	0
57	MG	1H	3141	1/1	0.59	0.29	83,83,83,83	0
57	MG	1H	3007	1/1	0.59	0.31	81,81,81,81	0
57	MG	1H	3050	1/1	0.59	0.38	72,72,72,72	0
57	MG	1H	3230	1/1	0.60	0.36	82,82,82,82	0
57	MG	1H	3120	1/1	0.60	0.18	88,88,88,88	0
57	MG	14	3008	1/1	0.60	0.21	77,77,77,77	0
57	MG	E5	101	1/1	0.60	0.58	89,89,89,89	0
57	MG	1H	3150	1/1	0.61	0.70	98,98,98,98	0
57	MG	14	3208	1/1	0.61	0.95	88,88,88,88	0
57	MG	14	3132	1/1	0.61	0.44	82,82,82,82	0
57	MG	14	3430	1/1	0.61	0.19	107,107,107,107	0
57	MG	1H	3339	1/1	0.61	0.12	106,106,106,106	0
57	MG	1H	3205	1/1	0.62	0.60	79,79,79,79	0
57	MG	1H	3500	1/1	0.62	0.14	94,94,94,94	0
57	MG	14	3384	1/1	0.63	0.14	78,78,78,78	0
57	MG	1H	3442	1/1	0.64	0.09	103,103,103,103	0
57	MG	14	3114	1/1	0.64	0.22	70,70,70,70	0
57	MG	1H	3503	1/1	0.64	0.12	91,91,91,91	0
57	MG	14	3347	1/1	0.64	0.10	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1685	1/1	0.64	0.16	90,90,90,90	0
57	MG	14	3433	1/1	0.64	0.26	114,114,114,114	0
57	MG	13	1738	1/1	0.64	0.10	133,133,133,133	0
57	MG	14	3332	1/1	0.65	0.09	102,102,102,102	0
57	MG	14	3064	1/1	0.65	0.48	63,63,63,63	0
57	MG	14	3166	1/1	0.65	0.46	79,79,79,79	0
57	MG	14	3426	1/1	0.65	0.16	104,104,104,104	0
57	MG	1H	3451	1/1	0.65	0.08	102,102,102,102	0
57	MG	14	3376	1/1	0.65	0.23	102,102,102,102	0
57	MG	1J	208	1/1	0.65	0.10	103,103,103,103	0
57	MG	C5	201	1/1	0.65	0.10	113,113,113,113	0
57	MG	14	3266	1/1	0.65	0.08	107,107,107,107	0
57	MG	1H	3079	1/1	0.66	0.34	63,63,63,63	0
57	MG	1H	3204	1/1	0.66	0.20	91,91,91,91	0
57	MG	1H	3388	1/1	0.66	0.13	55,55,55,55	0
57	MG	14	3344	1/1	0.66	0.09	93,93,93,93	0
57	MG	14	3135	1/1	0.66	0.32	79,79,79,79	0
57	MG	14	3152	1/1	0.66	0.17	78,78,78,78	0
57	MG	14	3434	1/1	0.66	0.12	110,110,110,110	0
57	MG	13	1671	1/1	0.66	0.51	79,79,79,79	0
57	MG	1H	3211	1/1	0.66	0.46	78,78,78,78	0
57	MG	13	1723	1/1	0.66	0.07	128,128,128,128	0
57	MG	1H	3423	1/1	0.67	0.18	84,84,84,84	0
57	MG	14	3429	1/1	0.67	0.30	95,95,95,95	0
57	MG	1H	3496	1/1	0.67	0.16	89,89,89,89	0
57	MG	14	3176	1/1	0.67	0.20	82,82,82,82	0
57	MG	14	3387	1/1	0.67	0.14	83,83,83,83	0
57	MG	14	3122	1/1	0.67	0.37	75,75,75,75	0
57	MG	14	3395	1/1	0.67	0.10	118,118,118,118	0
57	MG	1H	3004	1/1	0.67	0.51	89,89,89,89	0
57	MG	14	3277	1/1	0.68	0.16	84,84,84,84	0
57	MG	1H	3511	1/1	0.68	0.16	101,101,101,101	0
57	MG	13	1729	1/1	0.68	0.11	110,110,110,110	0
57	MG	1H	3499	1/1	0.68	0.09	112,112,112,112	0
57	MG	14	3017	1/1	0.68	0.34	119,119,119,119	0
57	MG	1H	3234	1/1	0.68	0.20	79,79,79,79	0
57	MG	1H	3487	1/1	0.68	0.11	85,85,85,85	0
57	MG	31	301	1/1	0.69	0.13	63,63,63,63	0
57	MG	1H	3085	1/1	0.69	0.28	70,70,70,70	0
57	MG	1H	3065	1/1	0.69	0.53	65,65,65,65	0
57	MG	13	1662	1/1	0.69	0.50	89,89,89,89	0
57	MG	13	1673	1/1	0.69	0.40	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3216	1/1	0.69	0.27	82,82,82,82	0
57	MG	35	201	1/1	0.69	0.22	75,75,75,75	0
57	MG	14	3407	1/1	0.69	0.12	123,123,123,123	0
57	MG	1H	3422	1/1	0.69	0.33	65,65,65,65	0
57	MG	14	3173	1/1	0.70	0.45	79,79,79,79	0
57	MG	1H	3177	1/1	0.70	0.90	82,82,82,82	0
57	MG	16	208	1/1	0.70	0.39	85,85,85,85	0
57	MG	14	3212	1/1	0.70	0.32	75,75,75,75	0
57	MG	1H	3428	1/1	0.70	0.09	89,89,89,89	0
57	MG	14	3385	1/1	0.70	0.16	67,67,67,67	0
57	MG	14	3435	1/1	0.70	0.20	92,92,92,92	0
57	MG	1H	3130	1/1	0.70	0.47	63,63,63,63	0
57	MG	4I	200	1/1	0.70	0.23	95,95,95,95	0
57	MG	1H	3419	1/1	0.70	0.15	86,86,86,86	0
57	MG	13	1668	1/1	0.70	0.29	66,66,66,66	0
57	MG	14	3110	1/1	0.71	0.24	69,69,69,69	0
57	MG	14	3161	1/1	0.71	0.41	78,78,78,78	0
57	MG	14	3264	1/1	0.71	0.14	93,93,93,93	0
57	MG	1G	1635	1/1	0.71	0.20	105,105,105,105	0
57	MG	14	3164	1/1	0.71	0.33	78,78,78,78	0
57	MG	14	3330	1/1	0.71	0.14	94,94,94,94	0
57	MG	1H	3135	1/1	0.71	0.49	79,79,79,79	0
57	MG	14	3138	1/1	0.71	0.67	78,78,78,78	0
57	MG	14	3109	1/1	0.71	0.43	67,67,67,67	0
57	MG	14	3207	1/1	0.71	0.37	70,70,70,70	0
57	MG	1H	3168	1/1	0.72	0.49	80,80,80,80	0
57	MG	1H	3195	1/1	0.72	0.31	55,55,55,55	0
57	MG	14	3291	1/1	0.72	0.21	85,85,85,85	0
57	MG	1G	1682	1/1	0.72	0.05	123,123,123,123	0
57	MG	1H	3006	1/1	0.72	0.28	74,74,74,74	0
57	MG	1H	3225	1/1	0.72	0.43	71,71,71,71	0
57	MG	1H	3227	1/1	0.72	0.28	72,72,72,72	0
57	MG	14	3252	1/1	0.72	0.18	90,90,90,90	0
57	MG	14	3409	1/1	0.72	0.22	88,88,88,88	0
57	MG	1G	1671	1/1	0.72	0.17	112,112,112,112	0
57	MG	14	3406	1/1	0.73	0.12	101,101,101,101	0
57	MG	13	1669	1/1	0.73	0.53	95,95,95,95	0
57	MG	14	3181	1/1	0.73	0.30	75,75,75,75	0
57	MG	14	3417	1/1	0.73	0.12	108,108,108,108	0
57	MG	14	3185	1/1	0.73	0.41	86,86,86,86	0
57	MG	1H	3171	1/1	0.73	0.38	73,73,73,73	0
57	MG	14	3023	1/1	0.73	0.27	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	14	3366	1/1	0.73	0.23	82,82,82,82	0
57	MG	1H	3172	1/1	0.73	0.30	83,83,83,83	0
57	MG	13	1737	1/1	0.73	0.11	99,99,99,99	0
57	MG	1H	3458	1/1	0.73	0.10	82,82,82,82	0
57	MG	16	205	1/1	0.73	0.18	69,69,69,69	0
57	MG	1H	3075	1/1	0.73	0.29	76,76,76,76	0
57	MG	1H	3267	1/1	0.73	0.10	56,56,56,56	0
57	MG	7A	101	1/1	0.73	0.26	114,114,114,114	0
57	MG	4L	101	1/1	0.74	0.32	131,131,131,131	0
57	MG	1H	3444	1/1	0.74	0.11	74,74,74,74	0
57	MG	14	3151	1/1	0.74	0.29	70,70,70,70	0
57	MG	1H	3396	1/1	0.74	0.22	59,59,59,59	0
57	MG	13	1660	1/1	0.74	0.23	88,88,88,88	0
57	MG	1G	1644	1/1	0.74	0.20	106,106,106,106	0
57	MG	14	3073	1/1	0.74	0.31	78,78,78,78	0
57	MG	1G	1668	1/1	0.74	0.09	124,124,124,124	0
57	MG	13	1637	1/1	0.74	0.32	74,74,74,74	0
57	MG	1H	3226	1/1	0.74	0.31	71,71,71,71	0
57	MG	1H	3476	1/1	0.74	0.21	82,82,82,82	0
57	MG	14	3118	1/1	0.74	0.44	61,61,61,61	0
57	MG	13	1714	1/1	0.74	0.09	122,122,122,122	0
57	MG	13	1674	1/1	0.74	0.36	92,92,92,92	0
57	MG	14	3128	1/1	0.74	0.41	89,89,89,89	0
57	MG	14	3211	1/1	0.74	0.09	81,81,81,81	0
57	MG	P8	101	1/1	0.74	0.56	71,71,71,71	0
57	MG	1H	3217	1/1	0.75	0.64	82,82,82,82	0
57	MG	1H	3395	1/1	0.75	0.14	68,68,68,68	0
57	MG	1H	3522	1/1	0.75	0.14	110,110,110,110	0
57	MG	16	203	1/1	0.75	0.21	82,82,82,82	0
57	MG	1G	1699	1/1	0.75	0.07	133,133,133,133	0
57	MG	1H	3063	1/1	0.75	0.27	100,100,100,100	0
57	MG	1H	3415	1/1	0.75	0.14	72,72,72,72	0
57	MG	1H	3118	1/1	0.75	0.15	69,69,69,69	0
61	SPE	14	3436	13/13	0.75	0.25	83,88,93,94	0
57	MG	1G	1675	1/1	0.76	0.08	103,103,103,103	0
57	MG	1H	3479	1/1	0.76	0.10	83,83,83,83	0
57	MG	1G	1618	1/1	0.76	0.69	78,78,78,78	0
57	MG	14	3197	1/1	0.76	0.61	77,77,77,77	0
57	MG	14	3080	1/1	0.76	0.25	68,68,68,68	0
57	MG	14	3098	1/1	0.76	0.35	77,77,77,77	0
57	MG	14	3100	1/1	0.76	0.27	71,71,71,71	0
57	MG	14	3432	1/1	0.76	0.13	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3103	1/1	0.76	0.43	96,96,96,96	0
57	MG	13	1727	1/1	0.76	0.13	90,90,90,90	0
57	MG	1H	3374	1/1	0.76	0.11	83,83,83,83	0
57	MG	1H	3053	1/1	0.76	0.46	75,75,75,75	0
57	MG	1H	3243	1/1	0.76	0.17	82,82,82,82	0
57	MG	1H	3196	1/1	0.76	0.38	77,77,77,77	0
57	MG	14	3398	1/1	0.76	0.13	76,76,76,76	0
57	MG	1H	3414	1/1	0.76	0.14	105,105,105,105	0
57	MG	1H	3516	1/1	0.77	0.14	102,102,102,102	0
57	MG	1H	3153	1/1	0.77	0.44	77,77,77,77	0
57	MG	14	3060	1/1	0.77	0.30	98,98,98,98	0
57	MG	1H	3277	1/1	0.77	0.16	71,71,71,71	0
57	MG	13	1706	1/1	0.77	0.08	117,117,117,117	0
57	MG	1H	3352	1/1	0.77	0.12	57,57,57,57	0
57	MG	14	3428	1/1	0.77	0.29	119,119,119,119	0
57	MG	1H	3363	1/1	0.77	0.12	96,96,96,96	0
57	MG	1H	3488	1/1	0.77	0.28	105,105,105,105	0
57	MG	13	1676	1/1	0.77	0.47	93,93,93,93	0
57	MG	1H	3123	1/1	0.77	0.37	65,65,65,65	0
57	MG	14	3379	1/1	0.77	0.14	84,84,84,84	0
57	MG	14	3156	1/1	0.77	0.17	87,87,87,87	0
57	MG	14	3258	1/1	0.77	0.07	79,79,79,79	0
57	MG	1H	3389	1/1	0.77	0.14	88,88,88,88	0
57	MG	1H	3003	1/1	0.77	0.37	65,65,65,65	0
57	MG	14	3274	1/1	0.77	0.05	85,85,85,85	0
57	MG	1H	3203	1/1	0.77	0.24	74,74,74,74	0
57	MG	1H	3129	1/1	0.78	0.20	76,76,76,76	0
57	MG	14	3342	1/1	0.78	0.09	113,113,113,113	0
57	MG	1H	3163	1/1	0.78	0.44	91,91,91,91	0
57	MG	1H	3518	1/1	0.78	0.11	96,96,96,96	0
57	MG	14	3348	1/1	0.78	0.11	96,96,96,96	0
57	MG	14	3067	1/1	0.78	0.23	78,78,78,78	0
57	MG	1H	3206	1/1	0.78	0.56	93,93,93,93	0
57	MG	1H	3309	1/1	0.78	0.23	54,54,54,54	0
57	MG	14	3257	1/1	0.78	0.16	69,69,69,69	0
57	MG	1H	3089	1/1	0.78	0.20	38,38,38,38	0
57	MG	1H	3105	1/1	0.78	0.23	72,72,72,72	0
57	MG	14	3382	1/1	0.78	0.12	66,66,66,66	0
57	MG	14	3168	1/1	0.78	0.24	89,89,89,89	0
57	MG	14	3134	1/1	0.78	0.33	85,85,85,85	0
57	MG	13	1661	1/1	0.78	0.19	90,90,90,90	0
57	MG	1H	3241	1/1	0.78	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3326	1/1	0.78	0.09	77,77,77,77	0
57	MG	14	3139	1/1	0.78	0.31	68,68,68,68	0
57	MG	13	1647	1/1	0.79	0.47	88,88,88,88	0
57	MG	14	3421	1/1	0.79	0.10	97,97,97,97	0
57	MG	1G	1680	1/1	0.79	0.07	123,123,123,123	0
57	MG	14	3276	1/1	0.79	0.10	120,120,120,120	0
57	MG	1H	3170	1/1	0.79	0.34	80,80,80,80	0
57	MG	14	3381	1/1	0.79	0.31	79,79,79,79	0
57	MG	14	3187	1/1	0.79	0.25	117,117,117,117	0
57	MG	1H	3198	1/1	0.79	0.23	79,79,79,79	0
57	MG	1G	1688	1/1	0.79	0.24	113,113,113,113	0
57	MG	1G	1694	1/1	0.79	0.12	113,113,113,113	0
57	MG	1H	3434	1/1	0.79	0.17	95,95,95,95	0
57	MG	1J	207	1/1	0.79	0.15	97,97,97,97	0
57	MG	52	201	1/1	0.79	0.15	129,129,129,129	0
57	MG	19	301	1/1	0.79	0.42	48,48,48,48	0
57	MG	1H	3111	1/1	0.79	0.61	79,79,79,79	0
57	MG	1G	1632	1/1	0.79	0.09	91,91,91,91	0
57	MG	1G	1634	1/1	0.79	0.72	85,85,85,85	0
57	MG	14	3175	1/1	0.79	0.21	88,88,88,88	0
57	MG	13	1711	1/1	0.80	0.16	74,74,74,74	0
57	MG	1G	1663	1/1	0.80	0.23	98,98,98,98	0
57	MG	1H	3043	1/1	0.80	0.40	75,75,75,75	0
57	MG	1H	3421	1/1	0.80	0.06	82,82,82,82	0
57	MG	14	3142	1/1	0.80	0.29	80,80,80,80	0
57	MG	14	3146	1/1	0.80	0.28	75,75,75,75	0
57	MG	14	3271	1/1	0.80	0.06	94,94,94,94	0
57	MG	1H	3368	1/1	0.80	0.12	69,69,69,69	0
57	MG	1H	3224	1/1	0.80	0.33	85,85,85,85	0
57	MG	14	3069	1/1	0.80	0.46	86,86,86,86	0
57	MG	13	1664	1/1	0.80	0.46	78,78,78,78	0
57	MG	1H	3497	1/1	0.80	0.10	107,107,107,107	0
57	MG	1H	3329	1/1	0.80	0.08	85,85,85,85	0
57	MG	1H	3391	1/1	0.80	0.13	89,89,89,89	0
57	MG	14	3339	1/1	0.80	0.10	107,107,107,107	0
57	MG	1H	3332	1/1	0.80	0.16	102,102,102,102	0
57	MG	14	3108	1/1	0.80	0.28	72,72,72,72	0
57	MG	1G	1690	1/1	0.80	0.06	117,117,117,117	0
57	MG	1G	1693	1/1	0.80	0.07	129,129,129,129	0
57	MG	1H	3144	1/1	0.80	0.61	102,102,102,102	0
57	MG	1H	3405	1/1	0.80	0.09	66,66,66,66	0
57	MG	1G	1704	1/1	0.80	0.20	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	1G	1636	1/1	0.80	0.33	90,90,90,90	0
57	MG	1G	1637	1/1	0.80	0.16	103,103,103,103	0
57	MG	1H	3350	1/1	0.80	0.11	74,74,74,74	0
57	MG	14	3007	1/1	0.80	0.26	60,60,60,60	0
57	MG	14	3133	1/1	0.80	1.00	88,88,88,88	0
57	MG	1G	1605	1/1	0.81	0.39	104,104,104,104	0
57	MG	14	3285	1/1	0.81	0.06	108,108,108,108	0
57	MG	1H	3074	1/1	0.81	0.38	64,64,64,64	0
57	MG	1H	3386	1/1	0.81	0.18	42,42,42,42	0
57	MG	14	3131	1/1	0.81	0.29	64,64,64,64	0
57	MG	1H	3106	1/1	0.81	0.23	87,87,87,87	0
57	MG	14	3183	1/1	0.81	0.30	103,103,103,103	0
57	MG	1H	3470	1/1	0.81	0.08	83,83,83,83	0
57	MG	1H	3125	1/1	0.81	0.20	56,56,56,56	0
57	MG	1H	3341	1/1	0.81	0.12	78,78,78,78	0
57	MG	14	3202	1/1	0.81	0.49	84,84,84,84	0
57	MG	14	3074	1/1	0.81	0.27	69,69,69,69	0
57	MG	1H	3486	1/1	0.81	0.07	95,95,95,95	0
57	MG	14	3091	1/1	0.81	0.09	78,78,78,78	0
57	MG	1H	3083	1/1	0.81	0.84	83,83,83,83	0
57	MG	1G	1697	1/1	0.81	0.09	128,128,128,128	0
57	MG	13	1675	1/1	0.81	0.47	101,101,101,101	0
57	MG	1H	3401	1/1	0.81	0.09	64,64,64,64	0
57	MG	1H	3308	1/1	0.81	0.14	50,50,50,50	0
57	MG	1G	1669	1/1	0.81	0.09	105,105,105,105	0
57	MG	1G	1670	1/1	0.81	0.06	134,134,134,134	0
57	MG	41	201	1/1	0.81	0.12	69,69,69,69	0
57	MG	1H	3055	1/1	0.81	0.18	48,48,48,48	0
57	MG	14	3404	1/1	0.82	0.16	97,97,97,97	0
57	MG	1H	3367	1/1	0.82	0.08	66,66,66,66	0
57	MG	14	3221	1/1	0.82	0.20	62,62,62,62	0
57	MG	1H	3197	1/1	0.82	0.51	77,77,77,77	0
57	MG	14	3412	1/1	0.82	0.10	97,97,97,97	0
57	MG	14	3345	1/1	0.82	0.16	99,99,99,99	0
57	MG	1H	3408	1/1	0.82	0.12	67,67,67,67	0
57	MG	13	1628	1/1	0.82	0.32	91,91,91,91	0
57	MG	14	3262	1/1	0.82	0.14	83,83,83,83	0
57	MG	1H	3201	1/1	0.82	0.75	104,104,104,104	0
57	MG	1H	3222	1/1	0.82	0.14	69,69,69,69	0
57	MG	1H	3456	1/1	0.82	0.06	94,94,94,94	0
57	MG	13	1649	1/1	0.82	0.42	75,75,75,75	0
57	MG	1H	3119	1/1	0.82	0.39	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3072	1/1	0.82	0.27	94,94,94,94	0
57	MG	1H	3020	1/1	0.82	0.14	73,73,73,73	0
57	MG	1J	205	1/1	0.82	0.15	73,73,73,73	0
57	MG	14	3155	1/1	0.82	0.16	78,78,78,78	0
57	MG	14	3295	1/1	0.82	0.10	60,60,60,60	0
57	MG	14	3386	1/1	0.82	0.09	74,74,74,74	0
57	MG	39	302	1/1	0.82	0.20	74,74,74,74	0
57	MG	14	3298	1/1	0.82	0.11	86,86,86,86	0
57	MG	1H	3038	1/1	0.82	0.32	50,50,50,50	0
57	MG	14	3075	1/1	0.82	0.16	73,73,73,73	0
57	MG	1H	3431	1/1	0.82	0.09	98,98,98,98	0
61	SPE	14	3437	13/13	0.82	0.29	59,68,73,74	0
57	MG	14	3368	1/1	0.83	0.09	88,88,88,88	0
57	MG	13	1670	1/1	0.83	0.30	82,82,82,82	0
57	MG	14	3204	1/1	0.83	0.22	72,72,72,72	0
57	MG	1H	3483	1/1	0.83	0.17	91,91,91,91	0
57	MG	1H	3485	1/1	0.83	0.06	77,77,77,77	0
57	MG	1H	3066	1/1	0.83	0.26	60,60,60,60	0
57	MG	1H	3347	1/1	0.83	0.10	67,67,67,67	0
57	MG	14	3214	1/1	0.83	0.70	80,80,80,80	0
57	MG	14	3003	1/1	0.83	0.27	78,78,78,78	0
57	MG	14	3225	1/1	0.83	0.07	73,73,73,73	0
57	MG	14	3391	1/1	0.83	0.23	99,99,99,99	0
57	MG	14	3230	1/1	0.83	0.17	63,63,63,63	0
57	MG	14	3243	1/1	0.83	0.15	58,58,58,58	0
57	MG	14	3005	1/1	0.83	0.26	54,54,54,54	0
57	MG	1H	3229	1/1	0.83	0.49	90,90,90,90	0
57	MG	1H	3071	1/1	0.83	0.22	79,79,79,79	0
57	MG	1H	3176	1/1	0.83	0.14	83,83,83,83	0
57	MG	1H	3236	1/1	0.83	0.31	67,67,67,67	0
57	MG	1H	3134	1/1	0.83	0.14	57,57,57,57	0
57	MG	1H	3156	1/1	0.83	0.15	83,83,83,83	0
57	MG	1H	3504	1/1	0.83	0.07	109,109,109,109	0
57	MG	1H	3376	1/1	0.83	0.15	66,66,66,66	0
57	MG	1H	3191	1/1	0.83	0.27	58,58,58,58	0
57	MG	14	3278	1/1	0.83	0.09	102,102,102,102	0
57	MG	1H	3517	1/1	0.83	0.07	91,91,91,91	0
57	MG	5I	101	1/1	0.83	0.10	79,79,79,79	0
57	MG	1G	1674	1/1	0.83	0.08	107,107,107,107	0
57	MG	1H	3220	1/1	0.83	0.45	89,89,89,89	0
57	MG	1H	3298	1/1	0.83	0.11	51,51,51,51	0
57	MG	1H	3523	1/1	0.83	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3453	1/1	0.83	0.12	93,93,93,93	0
57	MG	1G	1683	1/1	0.83	0.13	121,121,121,121	0
57	MG	1H	3161	1/1	0.83	0.38	67,67,67,67	0
57	MG	1H	3223	1/1	0.83	0.43	85,85,85,85	0
57	MG	13	1728	1/1	0.83	0.05	117,117,117,117	0
57	MG	14	3184	1/1	0.83	0.26	78,78,78,78	0
57	MG	1H	3049	1/1	0.83	0.25	62,62,62,62	0
57	MG	88	203	1/1	0.83	0.33	79,79,79,79	0
57	MG	1H	3407	1/1	0.83	0.09	72,72,72,72	0
57	MG	14	3198	1/1	0.83	0.43	81,81,81,81	0
57	MG	1G	1657	1/1	0.84	0.06	121,121,121,121	0
57	MG	1H	3178	1/1	0.84	0.43	63,63,63,63	0
57	MG	1H	3162	1/1	0.84	0.29	60,60,60,60	0
57	MG	1H	3420	1/1	0.84	0.12	69,69,69,69	0
57	MG	14	3099	1/1	0.84	0.18	78,78,78,78	0
57	MG	14	3318	1/1	0.84	0.12	89,89,89,89	0
57	MG	1H	3147	1/1	0.84	0.39	84,84,84,84	0
57	MG	14	3153	1/1	0.84	0.59	90,90,90,90	0
57	MG	1H	3274	1/1	0.84	0.14	97,97,97,97	0
57	MG	14	3414	1/1	0.84	0.12	97,97,97,97	0
57	MG	14	3213	1/1	0.84	0.71	87,87,87,87	0
57	MG	14	3418	1/1	0.84	0.07	90,90,90,90	0
57	MG	14	3107	1/1	0.84	0.36	54,54,54,54	0
57	MG	14	3343	1/1	0.84	0.06	80,80,80,80	0
57	MG	14	3215	1/1	0.84	1.26	86,86,86,86	0
57	MG	14	3427	1/1	0.84	0.08	65,65,65,65	0
57	MG	1H	3506	1/1	0.84	0.08	106,106,106,106	0
57	MG	13	1724	1/1	0.84	0.11	117,117,117,117	0
57	MG	1H	3136	1/1	0.84	0.41	116,116,116,116	0
57	MG	1G	1610	1/1	0.84	0.23	91,91,91,91	0
57	MG	1H	3140	1/1	0.84	0.20	54,54,54,54	0
57	MG	14	3256	1/1	0.84	0.13	83,83,83,83	0
57	MG	1H	3084	1/1	0.84	0.20	62,62,62,62	0
57	MG	1H	3406	1/1	0.84	0.08	85,85,85,85	0
57	MG	14	3063	1/1	0.84	0.24	67,67,67,67	0
57	MG	1H	3373	1/1	0.84	0.09	80,80,80,80	0
57	MG	13	1627	1/1	0.84	0.48	71,71,71,71	0
57	MG	14	3267	1/1	0.84	0.06	82,82,82,82	0
57	MG	1H	3525	1/1	0.84	0.22	68,68,68,68	0
57	MG	1G	1691	1/1	0.84	0.05	133,133,133,133	0
57	MG	16	201	1/1	0.84	0.25	62,62,62,62	0
57	MG	13	1732	1/1	0.84	0.08	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	14	3389	1/1	0.84	0.07	93,93,93,93	0
57	MG	14	3157	1/1	0.85	0.32	92,92,92,92	0
57	MG	1H	3482	1/1	0.85	0.09	94,94,94,94	0
57	MG	1H	3242	1/1	0.85	0.47	90,90,90,90	0
57	MG	1G	1641	1/1	0.85	0.59	103,103,103,103	0
57	MG	13	1733	1/1	0.85	0.11	101,101,101,101	0
57	MG	32	301	1/1	0.85	0.47	113,113,113,113	0
57	MG	14	3170	1/1	0.85	0.58	81,81,81,81	0
57	MG	1H	3433	1/1	0.85	0.14	72,72,72,72	0
57	MG	1G	1647	1/1	0.85	0.10	97,97,97,97	0
57	MG	14	3399	1/1	0.85	0.09	123,123,123,123	0
57	MG	14	3111	1/1	0.85	0.19	58,58,58,58	0
57	MG	1G	1654	1/1	0.85	0.30	108,108,108,108	0
57	MG	14	3286	1/1	0.85	0.11	73,73,73,73	0
57	MG	13	1650	1/1	0.85	0.41	75,75,75,75	0
57	MG	14	3117	1/1	0.85	0.47	64,64,64,64	0
57	MG	1H	3058	1/1	0.85	0.17	60,60,60,60	0
57	MG	14	3006	1/1	0.85	0.32	75,75,75,75	0
57	MG	14	3323	1/1	0.85	0.11	81,81,81,81	0
57	MG	14	3419	1/1	0.85	0.06	110,110,110,110	0
57	MG	14	3196	1/1	0.85	0.51	71,71,71,71	0
57	MG	14	3328	1/1	0.85	0.08	81,81,81,81	0
57	MG	14	3425	1/1	0.85	0.13	91,91,91,91	0
57	MG	1H	3489	1/1	0.85	0.32	73,73,73,73	0
57	MG	16	206	1/1	0.85	0.12	77,77,77,77	0
57	MG	14	3130	1/1	0.85	0.24	66,66,66,66	0
57	MG	1H	3061	1/1	0.85	0.28	53,53,53,53	0
57	MG	1H	3128	1/1	0.85	0.42	85,85,85,85	0
57	MG	13	1665	1/1	0.85	0.69	82,82,82,82	0
57	MG	14	3061	1/1	0.85	0.31	61,61,61,61	0
57	MG	13	1654	1/1	0.85	0.41	101,101,101,101	0
57	MG	1H	3502	1/1	0.85	0.18	141,141,141,141	0
57	MG	1H	3194	1/1	0.85	0.10	63,63,63,63	0
57	MG	1G	1606	1/1	0.85	0.13	73,73,73,73	0
57	MG	1H	3164	1/1	0.85	0.41	69,69,69,69	0
57	MG	1H	3148	1/1	0.85	0.37	83,83,83,83	0
57	MG	13	1659	1/1	0.85	0.15	126,126,126,126	0
57	MG	1G	1621	1/1	0.85	0.42	82,82,82,82	0
57	MG	1H	3346	1/1	0.85	0.10	92,92,92,92	0
57	MG	14	3380	1/1	0.85	0.08	78,78,78,78	0
60	ZN	C5	202	1/1	0.85	0.06	165,165,165,165	0
57	MG	1H	3394	1/1	0.85	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3481	1/1	0.85	0.11	103,103,103,103	0
57	MG	1H	3235	1/1	0.86	0.20	71,71,71,71	0
57	MG	14	3025	1/1	0.86	0.12	80,80,80,80	0
57	MG	14	3049	1/1	0.86	1.18	83,83,83,83	0
57	MG	I8	101	1/1	0.86	0.09	85,85,85,85	0
57	MG	14	3401	1/1	0.86	0.15	110,110,110,110	0
57	MG	1H	3320	1/1	0.86	0.08	58,58,58,58	0
57	MG	14	3312	1/1	0.86	0.16	92,92,92,92	0
57	MG	1H	3457	1/1	0.86	0.16	84,84,84,84	0
57	MG	14	3408	1/1	0.86	0.13	92,92,92,92	0
57	MG	1H	3383	1/1	0.86	0.10	68,68,68,68	0
57	MG	13	1710	1/1	0.86	0.07	96,96,96,96	0
57	MG	14	3137	1/1	0.86	0.53	99,99,99,99	0
57	MG	1H	3174	1/1	0.86	0.23	55,55,55,55	0
57	MG	1H	3512	1/1	0.86	0.13	87,87,87,87	0
57	MG	1H	3513	1/1	0.86	0.15	53,53,53,53	0
57	MG	1H	3240	1/1	0.86	0.38	73,73,73,73	0
57	MG	1H	3046	1/1	0.86	0.13	33,33,33,33	0
57	MG	14	3077	1/1	0.86	0.22	52,52,52,52	0
57	MG	1H	3392	1/1	0.86	0.15	48,48,48,48	0
57	MG	13	1740	1/1	0.86	0.06	98,98,98,98	0
57	MG	1G	1695	1/1	0.86	0.23	107,107,107,107	0
57	MG	13	1622	1/1	0.86	0.26	63,63,63,63	0
57	MG	1H	3133	1/1	0.86	0.23	55,55,55,55	0
57	MG	14	3254	1/1	0.86	0.10	77,77,77,77	0
57	MG	14	3255	1/1	0.86	0.13	79,79,79,79	0
57	MG	14	3373	1/1	0.86	0.12	65,65,65,65	0
57	MG	1H	3271	1/1	0.86	0.19	51,51,51,51	0
57	MG	1J	202	1/1	0.86	0.28	92,92,92,92	0
57	MG	1H	3443	1/1	0.86	0.10	75,75,75,75	0
57	MG	1J	206	1/1	0.86	0.24	94,94,94,94	0
57	MG	1H	3005	1/1	0.86	0.21	68,68,68,68	0
57	MG	14	3165	1/1	0.86	0.66	77,77,77,77	0
57	MG	1H	3492	1/1	0.86	0.15	78,78,78,78	0
57	MG	1H	3101	1/1	0.86	0.41	78,78,78,78	0
57	MG	1H	3080	1/1	0.86	0.17	80,80,80,80	0
57	MG	1G	1667	1/1	0.86	0.11	103,103,103,103	0
57	MG	21	302	1/1	0.86	0.25	72,72,72,72	0
57	MG	1H	3498	1/1	0.86	0.20	98,98,98,98	0
57	MG	1H	3137	1/1	0.86	0.43	70,70,70,70	0
57	MG	78	201	1/1	0.86	0.10	66,66,66,66	0
57	MG	1H	3384	1/1	0.87	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	1H	3455	1/1	0.87	0.15	76,76,76,76	0
57	MG	14	3336	1/1	0.87	0.09	94,94,94,94	0
57	MG	1H	3192	1/1	0.87	0.34	75,75,75,75	0
57	MG	14	3411	1/1	0.87	0.04	105,105,105,105	0
57	MG	13	1610	1/1	0.87	0.38	82,82,82,82	0
57	MG	1H	3213	1/1	0.87	0.29	71,71,71,71	0
57	MG	14	3416	1/1	0.87	0.13	102,102,102,102	0
57	MG	1H	3348	1/1	0.87	0.10	111,111,111,111	0
57	MG	1H	3008	1/1	0.87	0.39	82,82,82,82	0
57	MG	14	3125	1/1	0.87	0.21	81,81,81,81	0
57	MG	1H	3477	1/1	0.87	0.14	83,83,83,83	0
57	MG	1H	3001	1/1	0.87	0.39	84,84,84,84	0
57	MG	1H	3002	1/1	0.87	0.21	48,48,48,48	0
57	MG	14	3177	1/1	0.87	0.45	101,101,101,101	0
57	MG	1G	1656	1/1	0.87	0.08	100,100,100,100	0
57	MG	1H	3108	1/1	0.87	0.24	64,64,64,64	0
57	MG	1G	1659	1/1	0.87	0.04	115,115,115,115	0
57	MG	14	3268	1/1	0.87	0.15	82,82,82,82	0
57	MG	14	3076	1/1	0.87	0.45	81,81,81,81	0
57	MG	1H	3314	1/1	0.87	0.08	68,68,68,68	0
57	MG	14	3275	1/1	0.87	0.10	65,65,65,65	0
57	MG	13	1616	1/1	0.87	0.48	74,74,74,74	0
57	MG	14	3084	1/1	0.87	0.27	79,79,79,79	0
57	MG	14	3088	1/1	0.87	0.49	87,87,87,87	0
57	MG	14	3200	1/1	0.87	0.15	89,89,89,89	0
57	MG	13	1683	1/1	0.87	0.05	93,93,93,93	0
57	MG	1H	3375	1/1	0.87	0.10	79,79,79,79	0
57	MG	13	1651	1/1	0.87	0.29	98,98,98,98	0
57	MG	1H	3521	1/1	0.87	0.12	82,82,82,82	0
57	MG	14	3209	1/1	0.87	0.17	83,83,83,83	0
57	MG	1G	1611	1/1	0.87	0.65	76,76,76,76	0
57	MG	1G	1615	1/1	0.87	0.21	86,86,86,86	0
57	MG	1H	3412	1/1	0.87	0.10	75,75,75,75	0
57	MG	14	3403	1/1	0.87	0.12	84,84,84,84	0
57	MG	13	1726	1/1	0.87	0.08	74,74,74,74	0
57	MG	1H	3362	1/1	0.88	0.13	100,100,100,100	0
57	MG	1H	3515	1/1	0.88	0.19	58,58,58,58	0
57	MG	1H	3410	1/1	0.88	0.10	83,83,83,83	0
57	MG	1H	3010	1/1	0.88	0.37	39,39,39,39	0
57	MG	1H	3212	1/1	0.88	0.27	65,65,65,65	0
57	MG	1H	3069	1/1	0.88	0.41	69,69,69,69	0
57	MG	1H	3142	1/1	0.88	0.29	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1696	1/1	0.88	0.05	93,93,93,93	0
57	MG	14	3143	1/1	0.88	0.17	57,57,57,57	0
57	MG	14	3210	1/1	0.88	0.29	91,91,91,91	0
57	MG	14	3413	1/1	0.88	0.15	107,107,107,107	0
57	MG	13	1700	1/1	0.88	0.12	102,102,102,102	0
57	MG	1H	3296	1/1	0.88	0.08	91,91,91,91	0
57	MG	1H	3379	1/1	0.88	0.09	73,73,73,73	0
57	MG	13	1620	1/1	0.88	0.53	86,86,86,86	0
57	MG	1G	1646	1/1	0.88	0.10	86,86,86,86	0
57	MG	16	204	1/1	0.88	0.06	59,59,59,59	0
57	MG	1G	1649	1/1	0.88	0.14	113,113,113,113	0
57	MG	14	3424	1/1	0.88	0.09	109,109,109,109	0
57	MG	13	1615	1/1	0.88	0.24	88,88,88,88	0
57	MG	14	3236	1/1	0.88	0.28	44,44,44,44	0
57	MG	14	3159	1/1	0.88	0.11	79,79,79,79	0
57	MG	2L	102	1/1	0.88	0.18	132,132,132,132	0
57	MG	13	1613	1/1	0.88	0.13	87,87,87,87	0
57	MG	13	1617	1/1	0.88	0.14	51,51,51,51	0
57	MG	14	3431	1/1	0.88	0.25	116,116,116,116	0
57	MG	1H	3126	1/1	0.88	0.43	86,86,86,86	0
57	MG	1H	3082	1/1	0.88	0.27	71,71,71,71	0
57	MG	14	3167	1/1	0.88	0.32	78,78,78,78	0
57	MG	13	1730	1/1	0.88	0.09	94,94,94,94	0
57	MG	13	1731	1/1	0.88	0.05	112,112,112,112	0
57	MG	14	3172	1/1	0.88	0.39	77,77,77,77	0
57	MG	1H	3057	1/1	0.88	0.38	75,75,75,75	0
57	MG	1H	3452	1/1	0.88	0.10	72,72,72,72	0
57	MG	13	1635	1/1	0.88	0.24	81,81,81,81	0
57	MG	14	3273	1/1	0.88	0.09	86,86,86,86	0
57	MG	13	1712	1/1	0.88	0.07	89,89,89,89	0
57	MG	1H	3165	1/1	0.88	0.29	64,64,64,64	0
57	MG	14	3390	1/1	0.88	0.22	94,94,94,94	0
57	MG	13	1713	1/1	0.88	0.08	86,86,86,86	0
57	MG	14	3129	1/1	0.88	0.42	118,118,118,118	0
61	SPE	1G	1703	13/13	0.88	0.09	90,107,113,114	0
57	MG	13	1694	1/1	0.88	0.14	82,82,82,82	0
57	MG	1G	1679	1/1	0.88	0.09	94,94,94,94	0
57	MG	13	1655	1/1	0.89	0.50	82,82,82,82	0
57	MG	14	3223	1/1	0.89	0.10	87,87,87,87	0
57	MG	1H	3181	1/1	0.89	0.24	65,65,65,65	0
57	MG	1H	3221	1/1	0.89	0.24	73,73,73,73	0
57	MG	1G	1648	1/1	0.89	0.16	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	14	3241	1/1	0.89	0.05	78,78,78,78	0
57	MG	13	1684	1/1	0.89	0.08	85,85,85,85	0
57	MG	14	3070	1/1	0.89	0.22	52,52,52,52	0
57	MG	13	1719	1/1	0.89	0.04	81,81,81,81	0
57	MG	14	3346	1/1	0.89	0.08	99,99,99,99	0
57	MG	1H	3086	1/1	0.89	0.18	53,53,53,53	0
57	MG	13	1658	1/1	0.89	0.25	82,82,82,82	0
57	MG	1H	3371	1/1	0.89	0.10	56,56,56,56	0
57	MG	1H	3149	1/1	0.89	0.24	55,55,55,55	0
57	MG	1G	1664	1/1	0.89	0.05	80,80,80,80	0
57	MG	1H	3424	1/1	0.89	0.04	101,101,101,101	0
57	MG	1H	3246	1/1	0.89	0.09	55,55,55,55	0
57	MG	14	3374	1/1	0.89	0.12	92,92,92,92	0
57	MG	1H	3460	1/1	0.89	0.06	96,96,96,96	0
57	MG	16	202	1/1	0.89	0.23	82,82,82,82	0
57	MG	14	3001	1/1	0.89	0.17	57,57,57,57	0
57	MG	14	3144	1/1	0.89	0.32	102,102,102,102	0
57	MG	1G	1625	1/1	0.89	0.08	99,99,99,99	0
57	MG	14	3148	1/1	0.89	0.39	85,85,85,85	0
57	MG	1G	1629	1/1	0.89	0.52	85,85,85,85	0
57	MG	14	3203	1/1	0.89	0.53	79,79,79,79	0
57	MG	1H	3256	1/1	0.89	0.13	47,47,47,47	0
57	MG	1J	204	1/1	0.89	0.09	89,89,89,89	0
57	MG	14	3282	1/1	0.89	0.06	90,90,90,90	0
57	MG	14	3388	1/1	0.89	0.07	85,85,85,85	0
57	MG	1H	3098	1/1	0.89	0.41	46,46,46,46	0
57	MG	1G	1676	1/1	0.89	0.09	93,93,93,93	0
57	MG	1H	3215	1/1	0.89	0.13	63,63,63,63	0
57	MG	1H	3435	1/1	0.89	0.06	62,62,62,62	0
57	MG	14	3024	1/1	0.89	0.07	81,81,81,81	0
57	MG	14	3299	1/1	0.89	0.11	79,79,79,79	0
57	MG	1H	3480	1/1	0.89	0.07	87,87,87,87	0
57	MG	14	3160	1/1	0.89	0.18	65,65,65,65	0
57	MG	14	3402	1/1	0.89	0.08	78,78,78,78	0
57	MG	1H	3509	1/1	0.89	0.12	47,47,47,47	0
57	MG	13	1629	1/1	0.89	0.21	72,72,72,72	0
57	MG	14	3354	1/1	0.90	0.14	60,60,60,60	0
57	MG	13	1708	1/1	0.90	0.16	65,65,65,65	0
57	MG	14	3358	1/1	0.90	0.15	86,86,86,86	0
57	MG	1G	1639	1/1	0.90	0.54	78,78,78,78	0
57	MG	13	1725	1/1	0.90	0.04	115,115,115,115	0
57	MG	1H	3409	1/1	0.90	0.07	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	1G	1643	1/1	0.90	0.54	83,83,83,83	0
57	MG	1H	3244	1/1	0.90	0.42	74,74,74,74	0
57	MG	13	1626	1/1	0.90	0.33	84,84,84,84	0
57	MG	1H	3062	1/1	0.90	0.13	38,38,38,38	0
57	MG	1H	3013	1/1	0.90	0.27	40,40,40,40	0
57	MG	14	3009	1/1	0.90	0.34	57,57,57,57	0
57	MG	1H	3416	1/1	0.90	0.06	89,89,89,89	0
57	MG	14	3227	1/1	0.90	0.15	58,58,58,58	0
57	MG	14	3022	1/1	0.90	0.13	81,81,81,81	0
57	MG	1H	3268	1/1	0.90	0.17	59,59,59,59	0
57	MG	1H	3127	1/1	0.90	0.12	91,91,91,91	0
57	MG	1H	3484	1/1	0.90	0.09	105,105,105,105	0
57	MG	14	3245	1/1	0.90	0.14	63,63,63,63	0
57	MG	14	3042	1/1	0.90	0.19	65,65,65,65	0
57	MG	1H	3088	1/1	0.90	0.42	80,80,80,80	0
57	MG	14	3057	1/1	0.90	0.25	49,49,49,49	0
57	MG	13	1656	1/1	0.90	0.38	74,74,74,74	0
57	MG	14	3397	1/1	0.90	0.17	96,96,96,96	0
57	MG	1H	3294	1/1	0.90	0.16	54,54,54,54	0
57	MG	1H	3037	1/1	0.90	0.54	75,75,75,75	0
57	MG	14	3260	1/1	0.90	0.11	106,106,106,106	0
57	MG	13	1657	1/1	0.90	0.15	68,68,68,68	0
57	MG	14	3263	1/1	0.90	0.09	71,71,71,71	0
57	MG	1H	3490	1/1	0.90	0.07	89,89,89,89	0
57	MG	14	3405	1/1	0.90	0.07	108,108,108,108	0
57	MG	1H	3429	1/1	0.90	0.10	88,88,88,88	0
57	MG	88	202	1/1	0.90	0.32	66,66,66,66	0
57	MG	14	3158	1/1	0.90	0.24	66,66,66,66	0
57	MG	1H	3303	1/1	0.90	0.17	48,48,48,48	0
57	MG	1H	3103	1/1	0.90	0.32	61,61,61,61	0
57	MG	13	1695	1/1	0.90	0.10	106,106,106,106	0
57	MG	13	1618	1/1	0.90	0.20	48,48,48,48	0
57	MG	13	1640	1/1	0.90	0.28	92,92,92,92	0
57	MG	1H	3321	1/1	0.90	0.46	86,86,86,86	0
57	MG	1H	3109	1/1	0.90	0.31	59,59,59,59	0
57	MG	14	3279	1/1	0.90	0.08	58,58,58,58	0
57	MG	14	3083	1/1	0.90	0.15	72,72,72,72	0
57	MG	14	3420	1/1	0.90	0.07	107,107,107,107	0
57	MG	1H	3331	1/1	0.90	0.12	70,70,70,70	0
57	MG	14	3169	1/1	0.90	0.31	85,85,85,85	0
57	MG	1G	1612	1/1	0.90	0.15	106,106,106,106	0
57	MG	1G	1614	1/1	0.90	0.60	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	14	3296	1/1	0.90	0.12	72,72,72,72	0
57	MG	1G	1687	1/1	0.90	0.08	111,111,111,111	0
57	MG	1H	3505	1/1	0.90	0.14	100,100,100,100	0
57	MG	14	3307	1/1	0.90	0.15	66,66,66,66	0
57	MG	13	1641	1/1	0.90	0.19	81,81,81,81	0
57	MG	14	3316	1/1	0.90	0.13	69,69,69,69	0
57	MG	1G	1619	1/1	0.90	0.10	102,102,102,102	0
57	MG	14	3319	1/1	0.90	0.07	95,95,95,95	0
57	MG	1G	1692	1/1	0.90	0.12	101,101,101,101	0
57	MG	1H	3508	1/1	0.90	0.10	117,117,117,117	0
57	MG	1J	201	1/1	0.90	0.29	73,73,73,73	0
57	MG	14	3327	1/1	0.90	0.09	82,82,82,82	0
57	MG	1H	3334	1/1	0.90	0.10	77,77,77,77	0
57	MG	1G	1628	1/1	0.90	0.31	113,113,113,113	0
57	MG	14	3186	1/1	0.90	0.16	108,108,108,108	0
57	MG	1H	3336	1/1	0.90	0.14	62,62,62,62	0
57	MG	14	3193	1/1	0.90	0.13	45,45,45,45	0
57	MG	13	1722	1/1	0.90	0.09	87,87,87,87	0
57	MG	1H	3404	1/1	0.90	0.13	71,71,71,71	0
57	MG	25	201	1/1	0.90	0.05	115,115,115,115	0
57	MG	1H	3115	1/1	0.90	0.10	61,61,61,61	0
57	MG	42	201	1/1	0.90	0.21	120,120,120,120	0
57	MG	14	3119	1/1	0.90	0.20	81,81,81,81	0
57	MG	14	3120	1/1	0.90	0.18	78,78,78,78	0
57	MG	14	3121	1/1	0.90	0.12	61,61,61,61	0
57	MG	14	3349	1/1	0.90	0.13	83,83,83,83	0
57	MG	13	1631	1/1	0.90	0.09	78,78,78,78	0
57	MG	13	1677	1/1	0.91	0.47	77,77,77,77	0
57	MG	14	3396	1/1	0.91	0.03	126,126,126,126	0
57	MG	14	3297	1/1	0.91	0.17	71,71,71,71	0
57	MG	13	1701	1/1	0.91	0.12	108,108,108,108	0
57	MG	13	1720	1/1	0.91	0.15	109,109,109,109	0
57	MG	16	209	1/1	0.91	0.47	76,76,76,76	0
57	MG	14	3309	1/1	0.91	0.14	55,55,55,55	0
57	MG	1G	1696	1/1	0.91	0.07	128,128,128,128	0
57	MG	14	3313	1/1	0.91	0.05	105,105,105,105	0
57	MG	2K	101	1/1	0.91	0.11	100,100,100,100	0
57	MG	1H	3093	1/1	0.91	0.09	56,56,56,56	0
57	MG	13	1735	1/1	0.91	0.07	100,100,100,100	0
57	MG	1H	3447	1/1	0.91	0.24	70,70,70,70	0
57	MG	14	3090	1/1	0.91	0.35	86,86,86,86	0
57	MG	1H	3151	1/1	0.91	0.55	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3095	1/1	0.91	0.18	62,62,62,62	0
57	MG	1G	1652	1/1	0.91	0.15	81,81,81,81	0
57	MG	1H	3132	1/1	0.91	0.23	65,65,65,65	0
57	MG	1H	3116	1/1	0.91	0.16	53,53,53,53	0
57	MG	1H	3251	1/1	0.91	0.16	48,48,48,48	0
57	MG	14	3237	1/1	0.91	0.26	51,51,51,51	0
57	MG	1G	1604	1/1	0.91	0.17	127,127,127,127	0
57	MG	1H	3185	1/1	0.91	0.49	64,64,64,64	0
57	MG	1H	3190	1/1	0.91	0.38	91,91,91,91	0
57	MG	14	3251	1/1	0.91	0.09	80,80,80,80	0
57	MG	14	3423	1/1	0.91	0.07	120,120,120,120	0
57	MG	1H	3351	1/1	0.91	0.09	68,68,68,68	0
57	MG	1H	3117	1/1	0.91	0.18	60,60,60,60	0
57	MG	1H	3270	1/1	0.91	0.15	50,50,50,50	0
57	MG	13	1645	1/1	0.91	0.28	92,92,92,92	0
57	MG	14	3011	1/1	0.91	0.18	44,44,44,44	0
57	MG	14	3015	1/1	0.91	0.29	63,63,63,63	0
57	MG	1H	3193	1/1	0.91	0.26	61,61,61,61	0
57	MG	14	3359	1/1	0.91	0.08	93,93,93,93	0
57	MG	13	1672	1/1	0.91	0.15	88,88,88,88	0
57	MG	1H	3104	1/1	0.91	0.13	43,43,43,43	0
57	MG	14	3369	1/1	0.91	0.10	91,91,91,91	0
57	MG	1H	3138	1/1	0.91	0.14	54,54,54,54	0
57	MG	14	3180	1/1	0.91	0.41	91,91,91,91	0
57	MG	1H	3122	1/1	0.91	0.09	52,52,52,52	0
57	MG	14	3039	1/1	0.91	0.71	89,89,89,89	0
57	MG	1G	1624	1/1	0.91	0.13	95,95,95,95	0
57	MG	1H	3301	1/1	0.91	0.17	45,45,45,45	0
57	MG	1H	3228	1/1	0.91	0.15	60,60,60,60	0
57	MG	13	1697	1/1	0.91	0.07	84,84,84,84	0
57	MG	14	3188	1/1	0.91	0.50	72,72,72,72	0
57	MG	39	301	1/1	0.91	0.18	89,89,89,89	0
57	MG	1G	1630	1/1	0.91	0.37	72,72,72,72	0
57	MG	1H	3427	1/1	0.91	0.10	67,67,67,67	0
57	MG	1H	3124	1/1	0.91	0.21	61,61,61,61	0
57	MG	45	202	1/1	0.91	0.44	64,64,64,64	0
57	MG	1H	3310	1/1	0.91	0.18	70,70,70,70	0
57	MG	1G	1689	1/1	0.91	0.06	116,116,116,116	0
57	MG	14	3201	1/1	0.91	0.20	88,88,88,88	0
57	MG	1H	3231	1/1	0.91	0.49	66,66,66,66	0
57	MG	14	3392	1/1	0.91	0.07	63,63,63,63	0
57	MG	1H	3202	1/1	0.91	0.45	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	3095	1/1	0.92	0.17	70,70,70,70	0
57	MG	Q8	300	1/1	0.92	0.12	80,80,80,80	0
57	MG	14	3259	1/1	0.92	0.10	71,71,71,71	0
57	MG	1G	1602	1/1	0.92	0.33	106,106,106,106	0
57	MG	14	3383	1/1	0.92	0.07	90,90,90,90	0
57	MG	1H	3370	1/1	0.92	0.08	68,68,68,68	0
57	MG	1H	3494	1/1	0.92	0.08	72,72,72,72	0
57	MG	1H	3189	1/1	0.92	0.35	68,68,68,68	0
57	MG	1G	1608	1/1	0.92	0.37	93,93,93,93	0
57	MG	1H	3425	1/1	0.92	0.07	64,64,64,64	0
57	MG	13	1682	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3100	1/1	0.92	0.54	68,68,68,68	0
57	MG	1H	3299	1/1	0.92	0.13	48,48,48,48	0
57	MG	1H	3501	1/1	0.92	0.07	90,90,90,90	0
57	MG	13	1686	1/1	0.92	0.17	76,76,76,76	0
57	MG	1H	3432	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3102	1/1	0.92	0.21	60,60,60,60	0
57	MG	1H	3077	1/1	0.92	0.42	80,80,80,80	0
57	MG	1H	3078	1/1	0.92	0.28	58,58,58,58	0
57	MG	14	3178	1/1	0.92	0.73	78,78,78,78	0
57	MG	14	3400	1/1	0.92	0.05	108,108,108,108	0
57	MG	1H	3158	1/1	0.92	0.17	71,71,71,71	0
57	MG	1H	3312	1/1	0.92	0.15	44,44,44,44	0
57	MG	14	3289	1/1	0.92	0.13	74,74,74,74	0
57	MG	1H	3023	1/1	0.92	0.17	50,50,50,50	0
57	MG	1G	1701	1/1	0.92	0.03	111,111,111,111	0
57	MG	1H	3390	1/1	0.92	0.20	64,64,64,64	0
57	MG	14	3113	1/1	0.92	0.18	52,52,52,52	0
57	MG	1H	3446	1/1	0.92	0.06	98,98,98,98	0
57	MG	1H	3034	1/1	0.92	0.21	46,46,46,46	0
57	MG	14	3302	1/1	0.92	0.11	58,58,58,58	0
57	MG	14	3303	1/1	0.92	0.07	74,74,74,74	0
57	MG	14	3306	1/1	0.92	0.08	58,58,58,58	0
57	MG	14	3190	1/1	0.92	0.37	59,59,59,59	0
57	MG	13	1707	1/1	0.92	0.10	56,56,56,56	0
57	MG	3I	201	1/1	0.92	0.24	60,60,60,60	0
57	MG	13	1698	1/1	0.92	0.11	83,83,83,83	0
57	MG	1H	3519	1/1	0.92	0.18	116,116,116,116	0
57	MG	1G	1640	1/1	0.92	0.39	108,108,108,108	0
57	MG	1H	3167	1/1	0.92	0.53	98,98,98,98	0
57	MG	1H	3397	1/1	0.92	0.19	51,51,51,51	0
57	MG	1H	3064	1/1	0.92	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3403	1/1	0.92	0.07	99,99,99,99	0
57	MG	1H	3524	1/1	0.92	0.18	81,81,81,81	0
57	MG	13	1717	1/1	0.92	0.11	99,99,99,99	0
57	MG	1H	3209	1/1	0.92	0.60	76,76,76,76	0
57	MG	14	3333	1/1	0.92	0.17	50,50,50,50	0
57	MG	1H	3340	1/1	0.92	0.05	76,76,76,76	0
57	MG	14	3337	1/1	0.92	0.14	104,104,104,104	0
57	MG	13	1638	1/1	0.92	0.07	85,85,85,85	0
57	MG	14	3020	1/1	0.92	0.12	75,75,75,75	0
57	MG	1H	3345	1/1	0.92	0.06	102,102,102,102	0
57	MG	1H	3087	1/1	0.92	0.21	71,71,71,71	0
57	MG	13	1612	1/1	0.92	0.12	86,86,86,86	0
57	MG	16	207	1/1	0.92	0.33	74,74,74,74	0
57	MG	14	3141	1/1	0.92	0.28	95,95,95,95	0
57	MG	14	3224	1/1	0.92	0.24	45,45,45,45	0
57	MG	1G	1660	1/1	0.92	0.14	74,74,74,74	0
57	MG	14	3041	1/1	0.92	0.20	55,55,55,55	0
57	MG	1G	1662	1/1	0.92	0.13	91,91,91,91	0
57	MG	1H	3253	1/1	0.92	0.08	42,42,42,42	0
57	MG	14	3357	1/1	0.92	0.08	105,105,105,105	0
57	MG	1H	3051	1/1	0.92	0.11	60,60,60,60	0
57	MG	14	3149	1/1	0.92	0.28	72,72,72,72	0
57	MG	14	3360	1/1	0.92	0.07	96,96,96,96	0
57	MG	14	3361	1/1	0.92	0.05	79,79,79,79	0
57	MG	1H	3092	1/1	0.92	0.24	61,61,61,61	0
57	MG	1H	3146	1/1	0.92	0.16	52,52,52,52	0
57	MG	1H	3417	1/1	0.92	0.18	83,83,83,83	0
60	ZN	G8	201	1/1	0.92	0.14	139,139,139,139	0
57	MG	1H	3418	1/1	0.92	0.10	46,46,46,46	0
57	MG	1H	3219	1/1	0.92	0.20	71,71,71,71	0
57	MG	1H	3073	1/1	0.92	0.21	66,66,66,66	0
57	MG	1H	3094	1/1	0.92	0.15	33,33,33,33	0
57	MG	1H	3076	1/1	0.93	0.24	72,72,72,72	0
57	MG	14	3331	1/1	0.93	0.20	90,90,90,90	0
57	MG	1H	3293	1/1	0.93	0.14	73,73,73,73	0
57	MG	14	3071	1/1	0.93	0.19	74,74,74,74	0
57	MG	14	3335	1/1	0.93	0.08	81,81,81,81	0
57	MG	13	1639	1/1	0.93	0.58	70,70,70,70	0
57	MG	1H	3462	1/1	0.93	0.10	94,94,94,94	0
57	MG	14	3338	1/1	0.93	0.05	107,107,107,107	0
57	MG	1H	3468	1/1	0.93	0.24	82,82,82,82	0
57	MG	2L	101	1/1	0.93	0.40	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3160	1/1	0.93	0.18	71,71,71,71	0
57	MG	14	3410	1/1	0.93	0.06	85,85,85,85	0
57	MG	1H	3436	1/1	0.93	0.10	70,70,70,70	0
57	MG	14	3079	1/1	0.93	0.30	48,48,48,48	0
57	MG	1H	3438	1/1	0.93	0.04	62,62,62,62	0
57	MG	1H	3478	1/1	0.93	0.06	101,101,101,101	0
57	MG	14	3415	1/1	0.93	0.15	103,103,103,103	0
57	MG	1G	1677	1/1	0.93	0.17	92,92,92,92	0
57	MG	1H	3378	1/1	0.93	0.09	50,50,50,50	0
57	MG	13	1667	1/1	0.93	0.67	89,89,89,89	0
57	MG	14	3352	1/1	0.93	0.07	82,82,82,82	0
57	MG	1H	3261	1/1	0.93	0.08	63,63,63,63	0
57	MG	14	3094	1/1	0.93	0.65	73,73,73,73	0
57	MG	1G	1681	1/1	0.93	0.06	96,96,96,96	0
57	MG	1G	1645	1/1	0.93	0.14	81,81,81,81	0
57	MG	1H	3300	1/1	0.93	0.19	62,62,62,62	0
57	MG	1G	1685	1/1	0.93	0.14	110,110,110,110	0
57	MG	1H	3048	1/1	0.93	0.13	45,45,45,45	0
57	MG	14	3365	1/1	0.93	0.13	78,78,78,78	0
57	MG	14	3284	1/1	0.93	0.14	72,72,72,72	0
57	MG	1G	1613	1/1	0.93	0.76	89,89,89,89	0
57	MG	1H	3028	1/1	0.93	0.10	67,67,67,67	0
57	MG	14	3371	1/1	0.93	0.10	107,107,107,107	0
57	MG	1G	1650	1/1	0.93	0.16	101,101,101,101	0
57	MG	1H	3155	1/1	0.93	0.15	55,55,55,55	0
57	MG	1H	3067	1/1	0.93	0.21	58,58,58,58	0
57	MG	14	3112	1/1	0.93	0.20	83,83,83,83	0
57	MG	14	3378	1/1	0.93	0.13	92,92,92,92	0
57	MG	14	3220	1/1	0.93	0.12	54,54,54,54	0
57	MG	1G	1655	1/1	0.93	0.12	110,110,110,110	0
57	MG	16	210	1/1	0.93	0.11	73,73,73,73	0
57	MG	14	3043	1/1	0.93	0.29	71,71,71,71	0
57	MG	1G	1620	1/1	0.93	0.19	91,91,91,91	0
57	MG	14	3051	1/1	0.93	0.27	61,61,61,61	0
57	MG	1H	3232	1/1	0.93	0.22	48,48,48,48	0
57	MG	14	3233	1/1	0.93	0.26	65,65,65,65	0
57	MG	14	3311	1/1	0.93	0.11	67,67,67,67	0
57	MG	1H	3343	1/1	0.93	0.07	78,78,78,78	0
57	MG	1H	3430	1/1	0.93	0.08	73,73,73,73	0
57	MG	1H	3393	1/1	0.93	0.11	50,50,50,50	0
57	MG	14	3317	1/1	0.93	0.08	82,82,82,82	0
57	MG	14	3124	1/1	0.93	0.18	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	M5	101	1/1	0.93	0.18	88,88,88,88	0
57	MG	1G	1700	1/1	0.93	0.06	109,109,109,109	0
57	MG	14	3249	1/1	0.93	0.15	52,52,52,52	0
57	MG	14	3250	1/1	0.93	0.08	79,79,79,79	0
57	MG	88	201	1/1	0.93	0.19	76,76,76,76	0
57	MG	14	3068	1/1	0.93	0.41	53,53,53,53	0
57	MG	14	3238	1/1	0.94	0.20	50,50,50,50	0
57	MG	14	3362	1/1	0.94	0.06	114,114,114,114	0
57	MG	1H	3475	1/1	0.94	0.12	97,97,97,97	0
57	MG	13	1644	1/1	0.94	0.45	85,85,85,85	0
57	MG	14	3367	1/1	0.94	0.08	106,106,106,106	0
57	MG	14	3244	1/1	0.94	0.15	54,54,54,54	0
57	MG	1H	3218	1/1	0.94	0.21	37,37,37,37	0
57	MG	14	3029	1/1	0.94	0.21	57,57,57,57	0
57	MG	14	3033	1/1	0.94	0.33	80,80,80,80	0
57	MG	14	3035	1/1	0.94	0.41	58,58,58,58	0
57	MG	14	3038	1/1	0.94	0.21	52,52,52,52	0
57	MG	21	301	1/1	0.94	0.14	59,59,59,59	0
57	MG	1H	3259	1/1	0.94	0.17	54,54,54,54	0
57	MG	14	3145	1/1	0.94	0.21	90,90,90,90	0
57	MG	13	1681	1/1	0.94	0.14	59,59,59,59	0
57	MG	1G	1666	1/1	0.94	0.14	100,100,100,100	0
57	MG	14	3046	1/1	0.94	0.45	79,79,79,79	0
57	MG	14	3150	1/1	0.94	0.12	63,63,63,63	0
57	MG	1H	3266	1/1	0.94	0.08	54,54,54,54	0
57	MG	14	3050	1/1	0.94	0.20	57,57,57,57	0
57	MG	1H	3184	1/1	0.94	0.24	70,70,70,70	0
57	MG	14	3265	1/1	0.94	0.07	91,91,91,91	0
57	MG	14	3054	1/1	0.94	0.25	79,79,79,79	0
57	MG	1H	3009	1/1	0.94	0.54	71,71,71,71	0
57	MG	13	1666	1/1	0.94	0.20	85,85,85,85	0
57	MG	14	3269	1/1	0.94	0.05	78,78,78,78	0
57	MG	13	1653	1/1	0.94	0.33	73,73,73,73	0
57	MG	13	1633	1/1	0.94	0.22	73,73,73,73	0
57	MG	1H	3356	1/1	0.94	0.11	54,54,54,54	0
57	MG	1H	3357	1/1	0.94	0.12	52,52,52,52	0
57	MG	1H	3358	1/1	0.94	0.18	45,45,45,45	0
57	MG	14	3162	1/1	0.94	0.40	74,74,74,74	0
57	MG	1H	3276	1/1	0.94	0.10	78,78,78,78	0
57	MG	1H	3131	1/1	0.94	0.50	83,83,83,83	0
57	MG	1H	3491	1/1	0.94	0.10	70,70,70,70	0
57	MG	1H	3365	1/1	0.94	0.16	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	3366	1/1	0.94	0.17	68,68,68,68	0
57	MG	1H	3279	1/1	0.94	0.15	48,48,48,48	0
57	MG	1H	3283	1/1	0.94	0.15	71,71,71,71	0
57	MG	1G	1684	1/1	0.94	0.06	96,96,96,96	0
57	MG	14	3292	1/1	0.94	0.12	74,74,74,74	0
57	MG	1H	3285	1/1	0.94	0.14	55,55,55,55	0
57	MG	1H	3288	1/1	0.94	0.08	54,54,54,54	0
57	MG	1H	3372	1/1	0.94	0.08	89,89,89,89	0
57	MG	1H	3021	1/1	0.94	0.17	49,49,49,49	0
57	MG	1H	3107	1/1	0.94	0.12	60,60,60,60	0
57	MG	1H	3295	1/1	0.94	0.09	89,89,89,89	0
57	MG	13	1634	1/1	0.94	0.36	75,75,75,75	0
57	MG	14	3304	1/1	0.94	0.10	74,74,74,74	0
57	MG	1H	3026	1/1	0.94	0.39	55,55,55,55	0
57	MG	1G	1623	1/1	0.94	0.21	115,115,115,115	0
57	MG	13	1715	1/1	0.94	0.06	76,76,76,76	0
57	MG	14	3097	1/1	0.94	0.26	97,97,97,97	0
57	MG	1H	3507	1/1	0.94	0.08	57,57,57,57	0
57	MG	1G	1626	1/1	0.94	0.19	83,83,83,83	0
57	MG	1H	3441	1/1	0.94	0.06	105,105,105,105	0
57	MG	1H	3030	1/1	0.94	0.10	39,39,39,39	0
57	MG	14	3104	1/1	0.94	0.18	78,78,78,78	0
57	MG	14	3105	1/1	0.94	0.14	73,73,73,73	0
57	MG	14	3321	1/1	0.94	0.08	69,69,69,69	0
57	MG	14	3106	1/1	0.94	0.41	57,57,57,57	0
57	MG	1H	3510	1/1	0.94	0.14	39,39,39,39	0
57	MG	1H	3114	1/1	0.94	0.15	71,71,71,71	0
57	MG	13	1716	1/1	0.94	0.10	71,71,71,71	0
57	MG	1H	3035	1/1	0.94	0.11	40,40,40,40	0
57	MG	13	1642	1/1	0.94	0.13	103,103,103,103	0
57	MG	13	1718	1/1	0.94	0.09	90,90,90,90	0
57	MG	14	3205	1/1	0.94	0.45	59,59,59,59	0
57	MG	1H	3449	1/1	0.94	0.10	80,80,80,80	0
57	MG	1H	3238	1/1	0.94	0.34	80,80,80,80	0
57	MG	1H	3313	1/1	0.94	0.17	47,47,47,47	0
57	MG	1H	3239	1/1	0.94	0.10	67,67,67,67	0
57	MG	1H	3041	1/1	0.94	0.28	51,51,51,51	0
57	MG	14	3340	1/1	0.94	0.09	107,107,107,107	0
57	MG	1H	3173	1/1	0.94	0.22	59,59,59,59	0
57	MG	13	1687	1/1	0.94	0.06	103,103,103,103	0
57	MG	1H	3175	1/1	0.94	0.29	64,64,64,64	0
57	MG	13	1691	1/1	0.94	0.12	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	3218	1/1	0.94	0.09	65,65,65,65	0
57	MG	14	3123	1/1	0.94	0.28	83,83,83,83	0
57	MG	1H	3245	1/1	0.94	0.11	47,47,47,47	0
57	MG	13	1625	1/1	0.94	0.16	82,82,82,82	0
57	MG	14	3010	1/1	0.94	0.25	57,57,57,57	0
57	MG	1H	3337	1/1	0.94	0.05	86,86,86,86	0
57	MG	1H	3469	1/1	0.94	0.14	58,58,58,58	0
58	PAR	1G	1702	42/42	0.94	0.22	83,92,100,103	0
57	MG	1H	3099	1/1	0.94	0.44	56,56,56,56	0
57	MG	14	3232	1/1	0.94	0.14	66,66,66,66	0
57	MG	14	3018	1/1	0.94	0.14	44,44,44,44	0
57	MG	1H	3473	1/1	0.94	0.13	95,95,95,95	0
57	MG	1H	3474	1/1	0.94	0.09	93,93,93,93	0
57	MG	13	1611	1/1	0.95	0.25	70,70,70,70	0
57	MG	14	3174	1/1	0.95	0.08	89,89,89,89	0
57	MG	14	3370	1/1	0.95	0.06	97,97,97,97	0
57	MG	1G	1665	1/1	0.95	0.05	91,91,91,91	0
57	MG	1H	3159	1/1	0.95	0.13	80,80,80,80	0
57	MG	13	1636	1/1	0.95	0.28	74,74,74,74	0
57	MG	14	3272	1/1	0.95	0.09	71,71,71,71	0
57	MG	1H	3459	1/1	0.95	0.13	75,75,75,75	0
57	MG	14	3179	1/1	0.95	0.32	77,77,77,77	0
57	MG	14	3021	1/1	0.95	0.35	38,38,38,38	0
57	MG	1H	3139	1/1	0.95	0.35	71,71,71,71	0
57	MG	1H	3047	1/1	0.95	0.15	55,55,55,55	0
57	MG	1H	3467	1/1	0.95	0.03	84,84,84,84	0
57	MG	13	1721	1/1	0.95	0.17	106,106,106,106	0
57	MG	14	3281	1/1	0.95	0.16	69,69,69,69	0
57	MG	14	3028	1/1	0.95	0.33	45,45,45,45	0
57	MG	14	3283	1/1	0.95	0.07	68,68,68,68	0
57	MG	1H	3514	1/1	0.95	0.05	98,98,98,98	0
57	MG	14	3030	1/1	0.95	0.36	57,57,57,57	0
57	MG	14	3189	1/1	0.95	0.33	51,51,51,51	0
57	MG	14	3288	1/1	0.95	0.19	49,49,49,49	0
57	MG	1G	1616	1/1	0.95	0.13	94,94,94,94	0
57	MG	14	3290	1/1	0.95	0.22	59,59,59,59	0
57	MG	14	3192	1/1	0.95	0.28	74,74,74,74	0
57	MG	1G	1617	1/1	0.95	0.11	116,116,116,116	0
57	MG	14	3195	1/1	0.95	0.25	78,78,78,78	0
57	MG	14	3036	1/1	0.95	0.27	85,85,85,85	0
57	MG	1H	3249	1/1	0.95	0.13	63,63,63,63	0
57	MG	1H	3250	1/1	0.95	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3472	1/1	0.95	0.04	83,83,83,83	0
57	MG	14	3300	1/1	0.95	0.09	89,89,89,89	0
57	MG	2K	102	1/1	0.95	0.17	78,78,78,78	0
57	MG	1H	3143	1/1	0.95	0.37	50,50,50,50	0
57	MG	14	3126	1/1	0.95	0.28	72,72,72,72	0
57	MG	13	1646	1/1	0.95	0.17	71,71,71,71	0
57	MG	1H	3257	1/1	0.95	0.14	43,43,43,43	0
57	MG	1H	3068	1/1	0.95	0.40	72,72,72,72	0
57	MG	1H	3316	1/1	0.95	0.07	78,78,78,78	0
57	MG	14	3053	1/1	0.95	0.07	95,95,95,95	0
57	MG	1H	3260	1/1	0.95	0.19	42,42,42,42	0
57	MG	14	3315	1/1	0.95	0.12	68,68,68,68	0
57	MG	1H	3377	1/1	0.95	0.09	76,76,76,76	0
57	MG	14	3058	1/1	0.95	0.34	84,84,84,84	0
57	MG	13	1703	1/1	0.95	0.13	70,70,70,70	0
57	MG	14	3136	1/1	0.95	0.46	92,92,92,92	0
57	MG	14	3320	1/1	0.95	0.09	53,53,53,53	0
57	MG	1H	3326	1/1	0.95	0.10	62,62,62,62	0
57	MG	14	3062	1/1	0.95	0.25	59,59,59,59	0
57	MG	1H	3381	1/1	0.95	0.11	74,74,74,74	0
57	MG	1H	3052	1/1	0.95	0.18	59,59,59,59	0
57	MG	14	3065	1/1	0.95	0.10	47,47,47,47	0
57	MG	14	3329	1/1	0.95	0.06	105,105,105,105	0
57	MG	1H	3200	1/1	0.95	0.26	71,71,71,71	0
57	MG	1G	1638	1/1	0.95	0.14	127,127,127,127	0
57	MG	1H	3072	1/1	0.95	0.20	58,58,58,58	0
57	MG	1H	3269	1/1	0.95	0.16	41,41,41,41	0
57	MG	14	3334	1/1	0.95	0.10	60,60,60,60	0
57	MG	13	1624	1/1	0.95	0.32	59,59,59,59	0
57	MG	1H	3110	1/1	0.95	0.23	79,79,79,79	0
57	MG	1H	3054	1/1	0.95	0.35	52,52,52,52	0
57	MG	1H	3233	1/1	0.95	0.08	93,93,93,93	0
57	MG	1H	3017	1/1	0.95	0.29	62,62,62,62	0
57	MG	1H	3493	1/1	0.95	0.05	101,101,101,101	0
57	MG	31	302	1/1	0.95	0.16	77,77,77,77	0
57	MG	1H	3019	1/1	0.95	0.23	32,32,32,32	0
57	MG	1H	3344	1/1	0.95	0.08	103,103,103,103	0
57	MG	14	3246	1/1	0.95	0.13	61,61,61,61	0
57	MG	1J	203	1/1	0.95	0.26	73,73,73,73	0
57	MG	14	3247	1/1	0.95	0.09	52,52,52,52	0
57	MG	14	3248	1/1	0.95	0.29	47,47,47,47	0
57	MG	1H	3282	1/1	0.95	0.04	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3039	1/1	0.95	0.20	33,33,33,33	0
57	MG	14	3085	1/1	0.95	0.25	88,88,88,88	0
57	MG	14	3351	1/1	0.95	0.11	78,78,78,78	0
57	MG	14	3087	1/1	0.95	0.27	76,76,76,76	0
57	MG	14	3353	1/1	0.95	0.08	83,83,83,83	0
57	MG	1G	1653	1/1	0.95	0.11	97,97,97,97	0
57	MG	1H	3284	1/1	0.95	0.07	83,83,83,83	0
57	MG	45	201	1/1	0.95	0.13	101,101,101,101	0
57	MG	1H	3179	1/1	0.95	0.14	80,80,80,80	0
57	MG	14	3092	1/1	0.95	0.26	66,66,66,66	0
57	MG	I8	102	1/1	0.95	0.05	62,62,62,62	0
57	MG	1H	3096	1/1	0.95	0.15	64,64,64,64	0
58	PAR	13	1741	42/42	0.95	0.24	64,71,75,82	0
57	MG	1G	1658	1/1	0.95	0.06	104,104,104,104	0
57	MG	1H	3289	1/1	0.95	0.12	59,59,59,59	0
57	MG	14	3363	1/1	0.95	0.09	107,107,107,107	0
57	MG	13	1688	1/1	0.95	0.10	109,109,109,109	0
57	MG	1H	3355	1/1	0.95	0.09	59,59,59,59	0
57	MG	1H	3182	1/1	0.95	0.57	60,60,60,60	0
57	MG	1H	3323	1/1	0.96	0.17	57,57,57,57	0
57	MG	1H	3324	1/1	0.96	0.08	70,70,70,70	0
57	MG	1H	3070	1/1	0.96	0.34	75,75,75,75	0
57	MG	14	3089	1/1	0.96	0.24	54,54,54,54	0
57	MG	13	1689	1/1	0.96	0.07	88,88,88,88	0
57	MG	14	3372	1/1	0.96	0.12	86,86,86,86	0
57	MG	1H	3330	1/1	0.96	0.10	71,71,71,71	0
57	MG	13	1690	1/1	0.96	0.05	70,70,70,70	0
57	MG	1H	3199	1/1	0.96	0.12	61,61,61,61	0
57	MG	13	1604	1/1	0.96	0.15	62,62,62,62	0
57	MG	14	3096	1/1	0.96	0.20	65,65,65,65	0
57	MG	1H	3335	1/1	0.96	0.14	48,48,48,48	0
57	MG	1H	3272	1/1	0.96	0.09	63,63,63,63	0
57	MG	1H	3461	1/1	0.96	0.06	45,45,45,45	0
57	MG	14	3280	1/1	0.96	0.14	61,61,61,61	0
57	MG	1H	3399	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3182	1/1	0.96	0.36	74,74,74,74	0
57	MG	14	3102	1/1	0.96	0.56	85,85,85,85	0
57	MG	1H	3463	1/1	0.96	0.09	81,81,81,81	0
57	MG	1H	3464	1/1	0.96	0.08	63,63,63,63	0
57	MG	1H	3465	1/1	0.96	0.09	67,67,67,67	0
57	MG	14	3287	1/1	0.96	0.11	88,88,88,88	0
57	MG	1H	3400	1/1	0.96	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	14	3012	1/1	0.96	0.32	57,57,57,57	0
57	MG	13	1705	1/1	0.96	0.17	97,97,97,97	0
57	MG	14	3016	1/1	0.96	0.38	74,74,74,74	0
57	MG	14	3394	1/1	0.96	0.05	91,91,91,91	0
57	MG	1H	3402	1/1	0.96	0.05	85,85,85,85	0
57	MG	1H	3338	1/1	0.96	0.11	66,66,66,66	0
57	MG	14	3194	1/1	0.96	0.22	80,80,80,80	0
57	MG	1H	3471	1/1	0.96	0.12	90,90,90,90	0
57	MG	1H	3275	1/1	0.96	0.18	57,57,57,57	0
57	MG	1H	3022	1/1	0.96	0.19	49,49,49,49	0
57	MG	13	1692	1/1	0.96	0.18	72,72,72,72	0
57	MG	14	3116	1/1	0.96	0.13	88,88,88,88	0
57	MG	1H	3342	1/1	0.96	0.06	86,86,86,86	0
57	MG	1H	3024	1/1	0.96	0.24	83,83,83,83	0
57	MG	14	3027	1/1	0.96	0.14	66,66,66,66	0
57	MG	1H	3025	1/1	0.96	0.35	75,75,75,75	0
57	MG	13	1693	1/1	0.96	0.07	85,85,85,85	0
57	MG	14	3310	1/1	0.96	0.15	54,54,54,54	0
57	MG	1H	3207	1/1	0.96	0.24	92,92,92,92	0
57	MG	14	3031	1/1	0.96	0.28	73,73,73,73	0
57	MG	1H	3208	1/1	0.96	0.15	72,72,72,72	0
57	MG	14	3314	1/1	0.96	0.16	69,69,69,69	0
57	MG	1H	3286	1/1	0.96	0.12	40,40,40,40	0
57	MG	1H	3287	1/1	0.96	0.08	71,71,71,71	0
57	MG	13	1608	1/1	0.96	0.08	76,76,76,76	0
57	MG	1H	3029	1/1	0.96	0.32	77,77,77,77	0
57	MG	1H	3290	1/1	0.96	0.12	55,55,55,55	0
57	MG	13	1736	1/1	0.96	0.12	101,101,101,101	0
57	MG	14	3217	1/1	0.96	0.20	56,56,56,56	0
57	MG	1H	3033	1/1	0.96	0.25	70,70,70,70	0
57	MG	14	3324	1/1	0.96	0.15	48,48,48,48	0
57	MG	14	3219	1/1	0.96	0.10	57,57,57,57	0
57	MG	14	3044	1/1	0.96	0.18	57,57,57,57	0
57	MG	1G	1603	1/1	0.96	0.14	88,88,88,88	0
57	MG	1H	3214	1/1	0.96	0.47	77,77,77,77	0
57	MG	13	1652	1/1	0.96	0.62	71,71,71,71	0
57	MG	1H	3297	1/1	0.96	0.14	49,49,49,49	0
57	MG	1H	3183	1/1	0.96	0.21	70,70,70,70	0
57	MG	1H	3426	1/1	0.96	0.05	74,74,74,74	0
57	MG	1H	3248	1/1	0.96	0.11	44,44,44,44	0
57	MG	14	3140	1/1	0.96	0.13	51,51,51,51	0
57	MG	14	3234	1/1	0.96	0.18	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	13	1614	1/1	0.96	0.34	84,84,84,84	0
57	MG	14	3059	1/1	0.96	0.23	89,89,89,89	0
57	MG	1H	3495	1/1	0.96	0.05	97,97,97,97	0
57	MG	14	3240	1/1	0.96	0.12	73,73,73,73	0
57	MG	13	1632	1/1	0.96	0.22	78,78,78,78	0
57	MG	1H	3369	1/1	0.96	0.08	44,44,44,44	0
57	MG	1H	3188	1/1	0.96	0.41	49,49,49,49	0
57	MG	1H	3305	1/1	0.96	0.14	63,63,63,63	0
57	MG	1H	3307	1/1	0.96	0.14	44,44,44,44	0
57	MG	1H	3112	1/1	0.96	0.26	55,55,55,55	0
57	MG	13	1680	1/1	0.96	0.16	64,64,64,64	0
57	MG	13	1699	1/1	0.96	0.09	83,83,83,83	0
57	MG	1H	3258	1/1	0.96	0.11	47,47,47,47	0
57	MG	1H	3440	1/1	0.96	0.09	92,92,92,92	0
57	MG	13	1623	1/1	0.96	0.22	76,76,76,76	0
57	MG	1H	3042	1/1	0.96	0.26	65,65,65,65	0
57	MG	1H	3014	1/1	0.96	0.17	53,53,53,53	0
57	MG	1H	3317	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3318	1/1	0.96	0.15	59,59,59,59	0
57	MG	1G	1698	1/1	0.96	0.10	123,123,123,123	0
57	MG	14	3078	1/1	0.96	0.29	56,56,56,56	0
57	MG	1H	3263	1/1	0.96	0.19	46,46,46,46	0
57	MG	14	3261	1/1	0.96	0.17	59,59,59,59	0
57	MG	1G	1631	1/1	0.96	0.56	92,92,92,92	0
57	MG	14	3082	1/1	0.96	0.49	79,79,79,79	0
57	MG	14	3364	1/1	0.96	0.07	92,92,92,92	0
57	MG	1H	3166	1/1	0.96	0.43	78,78,78,78	0
57	MG	1H	3387	1/1	0.96	0.10	33,33,33,33	0
57	MG	1H	3056	1/1	0.97	0.31	49,49,49,49	0
57	MG	1H	3439	1/1	0.97	0.07	67,67,67,67	0
57	MG	14	3081	1/1	0.97	0.15	56,56,56,56	0
57	MG	1G	1601	1/1	0.97	0.20	77,77,77,77	0
57	MG	1H	3018	1/1	0.97	0.18	41,41,41,41	0
57	MG	14	3026	1/1	0.97	0.29	56,56,56,56	0
57	MG	13	1663	1/1	0.97	0.10	107,107,107,107	0
57	MG	14	3199	1/1	0.97	0.38	76,76,76,76	0
57	MG	14	3086	1/1	0.97	0.23	56,56,56,56	0
57	MG	1H	3262	1/1	0.97	0.18	43,43,43,43	0
57	MG	14	3270	1/1	0.97	0.13	67,67,67,67	0
57	MG	13	1606	1/1	0.97	0.26	72,72,72,72	0
57	MG	1H	3315	1/1	0.97	0.10	63,63,63,63	0
57	MG	1H	3411	1/1	0.97	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	14	3032	1/1	0.97	0.41	64,64,64,64	0
57	MG	1G	1651	1/1	0.97	0.11	76,76,76,76	0
57	MG	14	3093	1/1	0.97	0.42	84,84,84,84	0
57	MG	1H	3264	1/1	0.97	0.25	50,50,50,50	0
57	MG	1H	3413	1/1	0.97	0.10	78,78,78,78	0
57	MG	14	3037	1/1	0.97	0.26	65,65,65,65	0
57	MG	1H	3448	1/1	0.97	0.07	80,80,80,80	0
57	MG	1H	3265	1/1	0.97	0.08	46,46,46,46	0
57	MG	13	1602	1/1	0.97	0.14	120,120,120,120	0
57	MG	1H	3382	1/1	0.97	0.09	49,49,49,49	0
57	MG	14	3101	1/1	0.97	0.33	87,87,87,87	0
57	MG	1H	3011	1/1	0.97	0.30	56,56,56,56	0
57	MG	1H	3090	1/1	0.97	0.21	42,42,42,42	0
57	MG	14	3045	1/1	0.97	0.20	53,53,53,53	0
57	MG	1H	3012	1/1	0.97	0.42	58,58,58,58	0
57	MG	14	3048	1/1	0.97	0.47	51,51,51,51	0
57	MG	1G	1661	1/1	0.97	0.08	95,95,95,95	0
57	MG	1H	3353	1/1	0.97	0.14	48,48,48,48	0
57	MG	14	3226	1/1	0.97	0.16	51,51,51,51	0
57	MG	14	3293	1/1	0.97	0.10	63,63,63,63	0
57	MG	1H	3354	1/1	0.97	0.17	60,60,60,60	0
57	MG	14	3052	1/1	0.97	0.23	54,54,54,54	0
57	MG	14	3231	1/1	0.97	0.23	55,55,55,55	0
57	MG	1H	3247	1/1	0.97	0.14	36,36,36,36	0
57	MG	1H	3036	1/1	0.97	0.16	37,37,37,37	0
57	MG	1H	3328	1/1	0.97	0.13	47,47,47,47	0
57	MG	13	1609	1/1	0.97	0.15	70,70,70,70	0
57	MG	14	3171	1/1	0.97	0.34	56,56,56,56	0
57	MG	1H	3361	1/1	0.97	0.07	52,52,52,52	0
57	MG	14	3239	1/1	0.97	0.17	77,77,77,77	0
57	MG	14	3375	1/1	0.97	0.07	93,93,93,93	0
57	MG	14	3002	1/1	0.97	0.37	57,57,57,57	0
57	MG	14	3308	1/1	0.97	0.10	94,94,94,94	0
57	MG	1H	3273	1/1	0.97	0.14	78,78,78,78	0
57	MG	14	3004	1/1	0.97	0.28	63,63,63,63	0
57	MG	16	211	1/1	0.97	0.11	73,73,73,73	0
57	MG	13	1605	1/1	0.97	0.20	71,71,71,71	0
57	MG	1G	1672	1/1	0.97	0.12	110,110,110,110	0
57	MG	1H	3364	1/1	0.97	0.09	44,44,44,44	0
57	MG	21	303	1/1	0.97	0.09	46,46,46,46	0
57	MG	1H	3466	1/1	0.97	0.05	72,72,72,72	0
57	MG	1H	3169	1/1	0.97	0.45	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1734	1/1	0.97	0.10	94,94,94,94	0
57	MG	14	3014	1/1	0.97	0.25	59,59,59,59	0
57	MG	14	3253	1/1	0.97	0.07	58,58,58,58	0
57	MG	1H	3304	1/1	0.97	0.10	58,58,58,58	0
57	MG	1H	3186	1/1	0.97	0.26	62,62,62,62	0
57	MG	1H	3306	1/1	0.97	0.09	75,75,75,75	0
57	MG	1H	3040	1/1	0.97	0.31	44,44,44,44	0
57	MG	1H	3027	1/1	0.97	0.19	52,52,52,52	0
57	MG	1H	3437	1/1	0.97	0.09	92,92,92,92	0
57	MG	14	3147	1/1	0.98	0.40	69,69,69,69	0
57	MG	14	3191	1/1	0.98	0.26	67,67,67,67	0
57	MG	1H	3255	1/1	0.98	0.08	49,49,49,49	0
57	MG	14	3294	1/1	0.98	0.05	75,75,75,75	0
57	MG	13	1648	1/1	0.98	0.16	67,67,67,67	0
57	MG	1H	3319	1/1	0.98	0.18	57,57,57,57	0
57	MG	14	3066	1/1	0.98	0.57	61,61,61,61	0
57	MG	1G	1622	1/1	0.98	0.20	125,125,125,125	0
57	MG	13	1619	1/1	0.98	0.21	52,52,52,52	0
57	MG	14	3356	1/1	0.98	0.06	75,75,75,75	0
57	MG	1H	3349	1/1	0.98	0.12	50,50,50,50	0
57	MG	14	3301	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3380	1/1	0.98	0.18	55,55,55,55	0
57	MG	1H	3015	1/1	0.98	0.31	51,51,51,51	0
57	MG	1G	1627	1/1	0.98	0.41	87,87,87,87	0
57	MG	14	3305	1/1	0.98	0.12	49,49,49,49	0
57	MG	1H	3322	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3187	1/1	0.98	0.42	44,44,44,44	0
57	MG	1H	3016	1/1	0.98	0.19	44,44,44,44	0
57	MG	1H	3385	1/1	0.98	0.15	25,25,25,25	0
57	MG	14	3206	1/1	0.98	0.27	85,85,85,85	0
57	MG	1H	3278	1/1	0.98	0.09	75,75,75,75	0
57	MG	14	3034	1/1	0.98	0.48	40,40,40,40	0
57	MG	1G	1633	1/1	0.98	0.21	118,118,118,118	0
57	MG	1H	3327	1/1	0.98	0.08	50,50,50,50	0
57	MG	1H	3152	1/1	0.98	0.41	70,70,70,70	0
57	MG	1H	3302	1/1	0.98	0.13	51,51,51,51	0
57	MG	1H	3280	1/1	0.98	0.15	36,36,36,36	0
57	MG	14	3040	1/1	0.98	0.25	68,68,68,68	0
57	MG	1H	3359	1/1	0.98	0.17	44,44,44,44	0
57	MG	14	3216	1/1	0.98	0.21	52,52,52,52	0
57	MG	1H	3281	1/1	0.98	0.15	61,61,61,61	0
57	MG	14	3322	1/1	0.98	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	13	1601	1/1	0.98	0.42	80,80,80,80	0
57	MG	1H	3333	1/1	0.98	0.13	77,77,77,77	0
57	MG	14	3325	1/1	0.98	0.04	79,79,79,79	0
57	MG	1H	3097	1/1	0.98	0.06	65,65,65,65	0
57	MG	1G	1607	1/1	0.98	0.20	86,86,86,86	0
57	MG	14	3222	1/1	0.98	0.20	59,59,59,59	0
57	MG	14	3047	1/1	0.98	0.34	65,65,65,65	0
57	MG	1H	3044	1/1	0.98	0.36	67,67,67,67	0
57	MG	29	301	1/1	0.98	0.35	58,58,58,58	0
57	MG	1H	3045	1/1	0.98	0.28	46,46,46,46	0
57	MG	1H	3398	1/1	0.98	0.07	78,78,78,78	0
57	MG	13	1621	1/1	0.98	0.09	85,85,85,85	0
57	MG	14	3228	1/1	0.98	0.14	56,56,56,56	0
57	MG	14	3229	1/1	0.98	0.13	59,59,59,59	0
57	MG	13	1702	1/1	0.98	0.13	85,85,85,85	0
57	MG	1H	3311	1/1	0.98	0.09	53,53,53,53	0
57	MG	14	3013	1/1	0.98	0.23	47,47,47,47	0
57	MG	13	1603	1/1	0.98	0.24	74,74,74,74	0
57	MG	1H	3252	1/1	0.98	0.09	65,65,65,65	0
57	MG	14	3341	1/1	0.98	0.12	66,66,66,66	0
57	MG	14	3235	1/1	0.98	0.24	48,48,48,48	0
60	ZN	5A	101	1/1	0.98	0.09	146,146,146,146	0
57	MG	1H	3210	1/1	0.98	0.18	56,56,56,56	0
57	MG	1H	3292	1/1	0.98	0.21	43,43,43,43	0
57	MG	1H	3254	1/1	0.98	0.08	46,46,46,46	0
57	MG	14	3019	1/1	0.98	0.35	57,57,57,57	0
57	MG	13	1607	1/1	0.99	0.20	72,72,72,72	0
57	MG	1H	3059	1/1	0.99	0.27	56,56,56,56	0
57	MG	1H	3060	1/1	0.99	0.16	35,35,35,35	0
57	MG	14	3242	1/1	0.99	0.10	62,62,62,62	0
57	MG	1H	3091	1/1	0.99	0.15	41,41,41,41	0
57	MG	1H	3031	1/1	0.99	0.14	51,51,51,51	0
57	MG	1H	3325	1/1	0.99	0.15	46,46,46,46	0
57	MG	1H	3121	1/1	0.99	0.24	39,39,39,39	0
59	SF4	3E	301	8/8	0.99	0.21	82,91,95,98	0
59	SF4	32	302	8/8	0.99	0.17	100,109,118,124	0
60	ZN	5I	102	1/1	0.99	0.13	86,86,86,86	0
57	MG	1H	3032	1/1	0.99	0.25	47,47,47,47	0
57	MG	1H	3291	1/1	0.99	0.13	59,59,59,59	0
57	MG	13	1630	1/1	0.99	0.34	96,96,96,96	0
57	MG	1H	3360	1/1	0.99	0.09	78,78,78,78	0
57	MG	14	3055	1/1	0.99	0.30	60,60,60,60	0

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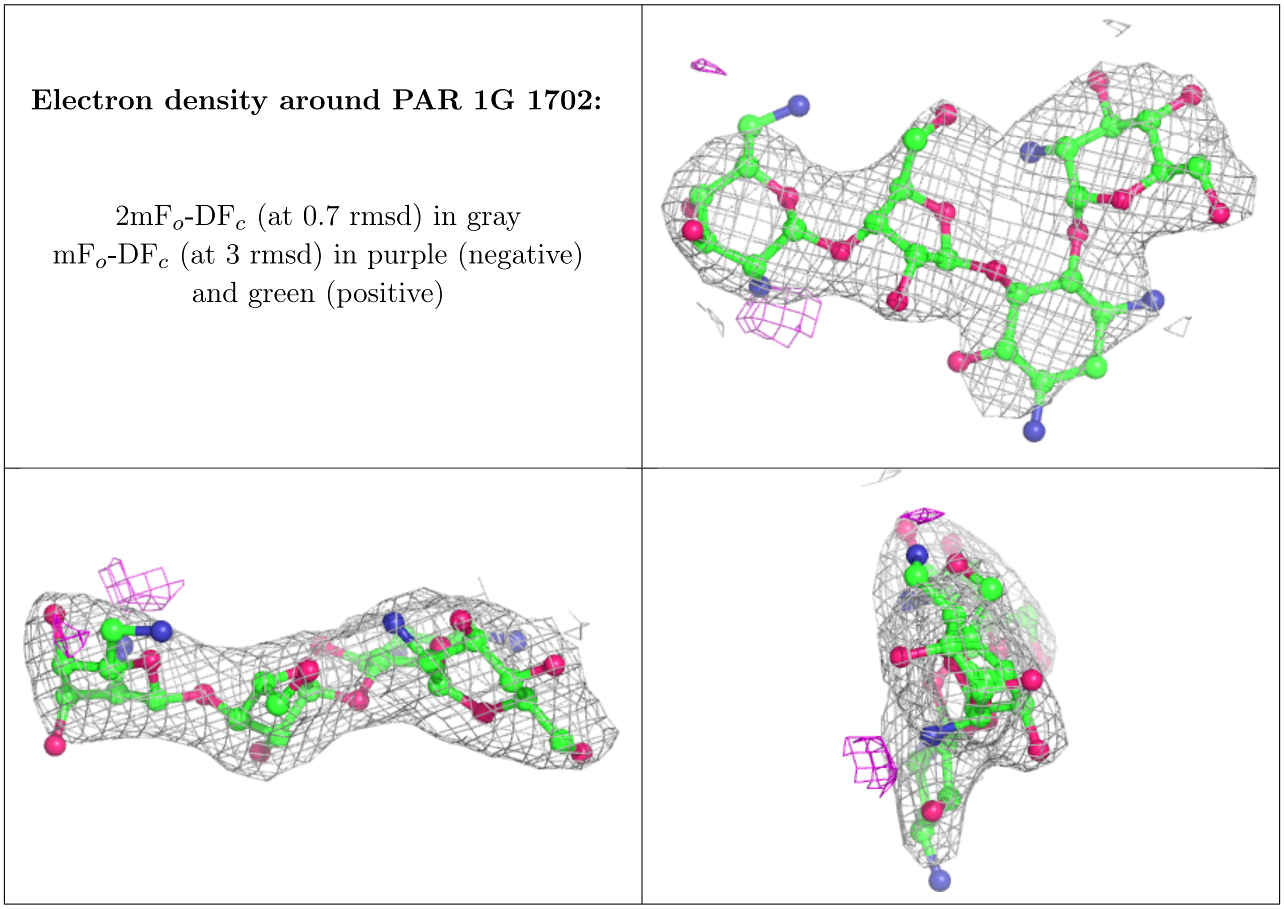
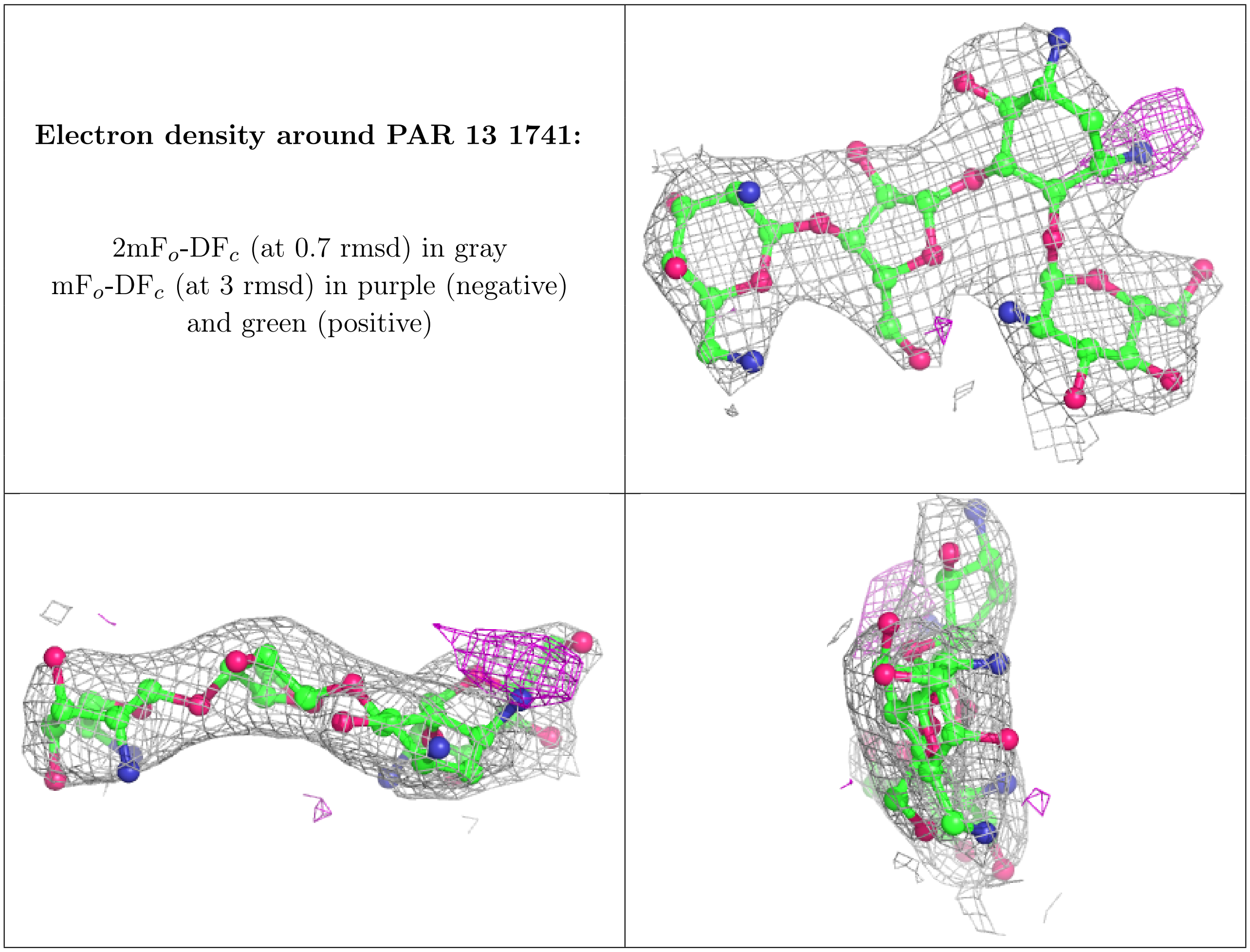
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	14	3056	1/1	0.99	0.11	54,54,54,54	0
57	MG	1H	3450	1/1	1.00	0.06	44,44,44,44	0

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 1G 1702:

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 13 1741:

$2mF_o$-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.