



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 7, 2024 – 01:37 am GMT

PDB ID : 6GSK  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and near-cognate tRNA<sup>Thr</sup> in the A-site  
Authors : Rozov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2018-06-14  
Resolution : 3.36 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

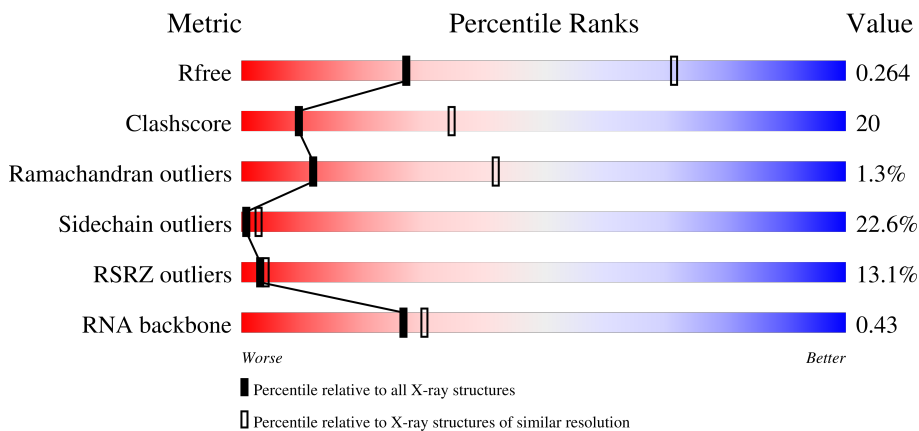
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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.



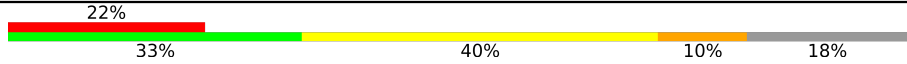

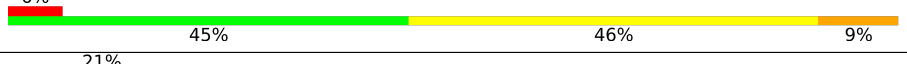
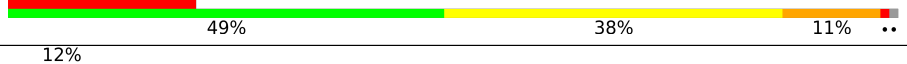
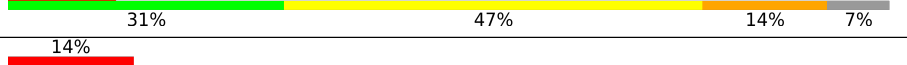


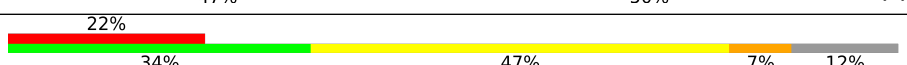
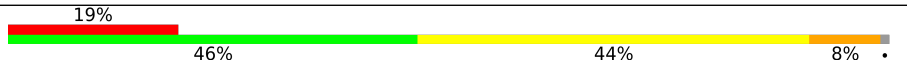

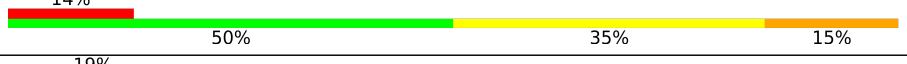
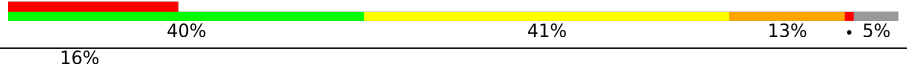
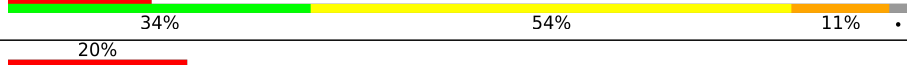

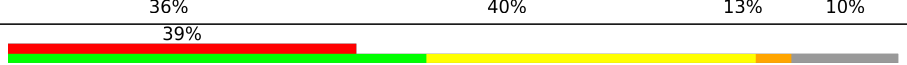
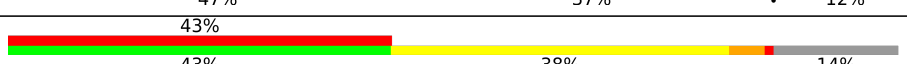
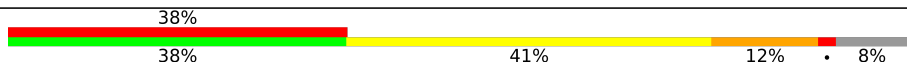
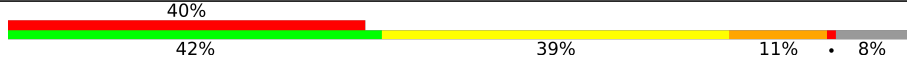
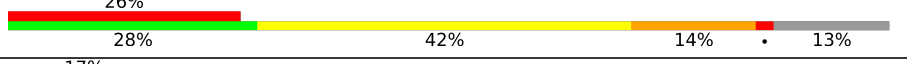






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      30%      49%      17%      . .</p>
1	1G	1522	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      28%      48%      20%      . .</p>
2	12	256	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4%      38%      32%      11%      19%</p>
2	1E	256	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      39%      39%      12%      10%</p>



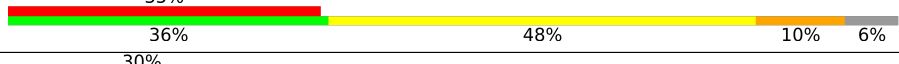
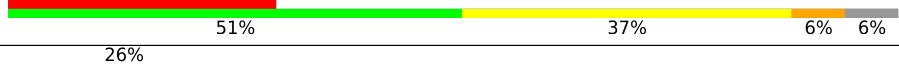
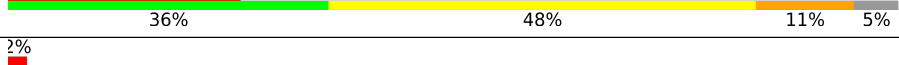
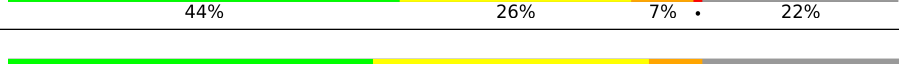
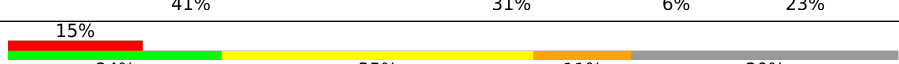
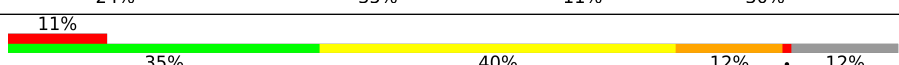


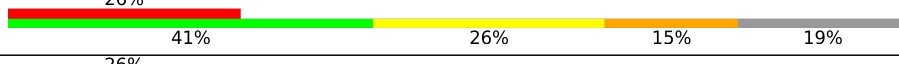
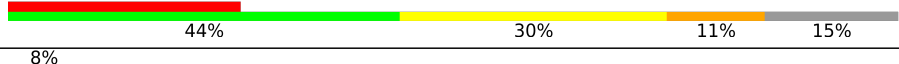
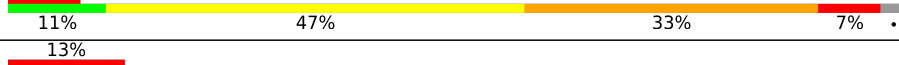
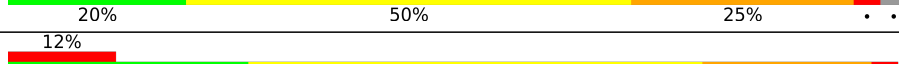
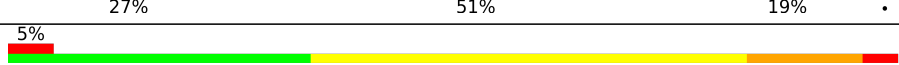
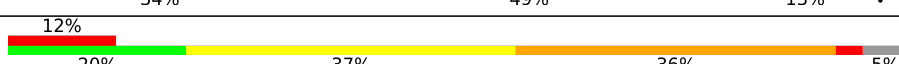
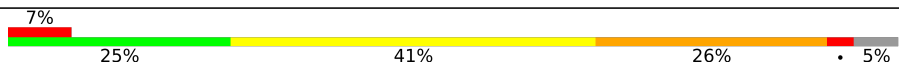
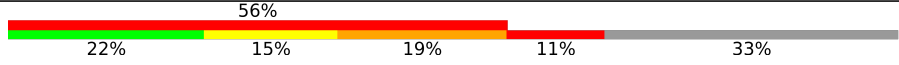
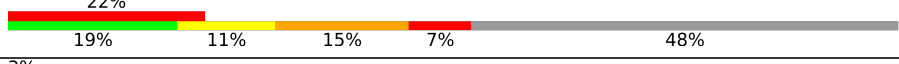
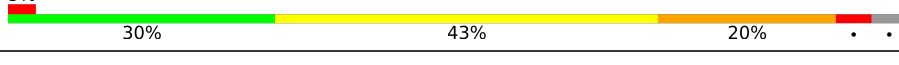
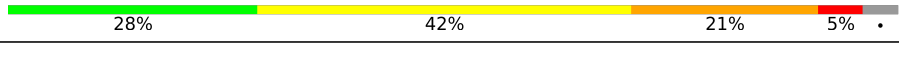

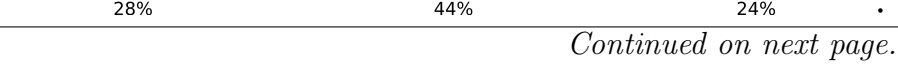


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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

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

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Mol	Chain	Length	Quality of chain
28	11	276	19% 47% 40% 12% ..
28	19	276	35% 51% 36% 12% .
29	21	206	25% 47% 37% 15%
29	29	206	26% 46% 38% 13% ..
30	31	210	14% 44% 40% 12% .
30	39	210	11% 31% 50% 15% ..
31	41	182	8% 48% 37% 12% ..
31	49	182	38% 38% 48% 13% ..
32	51	180	41% 39% 14% . .
32	59	180	44% 39% 41% 14% 6%
33	61	148	45% 35% 14% . .
33	69	148	3% 47% 36% 14% ..
34	15	140	65% 41% 46% 11% ..
34	58	140	19% 37% 41% 10% . 11%
35	25	122	42% 49% 39% 11% .
35	68	122	23% 69% 25% 6%
36	35	150	39% 39% 43% 15% ..
36	78	150	11% 35% 47% 14% ..
37	45	141	60% 45% 40% 11% ..
37	88	141	26% 48% 40% 11% .
38	55	118	26% 39% 47% 14% .
38	98	118	31% 44% 45% 10% .
39	65	112	3% 33% 44% 20% ..
39	A8	112	10% 39% 45% 15% .
40	75	146	9% 40% 42% 12% . .

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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	M8	71	
52	J5	60	
52	N8	60	
53	L5	49	

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Mol	Chain	Length	Quality of chain
53	P8	49	
54	M5	65	
54	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
22	H2U	1L	17	-	-	-	X
55	MG	13	1638	-	-	-	X
55	MG	13	1674	-	-	-	X
55	MG	13	1686	-	-	-	X
55	MG	13	1705	-	-	-	X
55	MG	14	3009	-	-	-	X
55	MG	14	3041	-	-	-	X
55	MG	14	3092	-	-	-	X
55	MG	14	3094	-	-	-	X
55	MG	14	3112	-	-	-	X
55	MG	14	3133	-	-	-	X
55	MG	14	3135	-	-	-	X
55	MG	14	3177	-	-	-	X
55	MG	14	3185	-	-	-	X
55	MG	1G	1618	-	-	-	X
55	MG	1G	1621	-	-	-	X
55	MG	1G	1650	-	-	-	X
55	MG	1G	1662	-	-	-	X
55	MG	1G	1663	-	-	-	X
55	MG	1G	1670	-	-	-	X
55	MG	1H	3045	-	-	-	X
55	MG	1H	3107	-	-	-	X
55	MG	1H	3142	-	-	-	X
55	MG	1H	3149	-	-	-	X
55	MG	1H	3181	-	-	-	X
55	MG	1H	3185	-	-	-	X
55	MG	1H	3212	-	-	-	X
55	MG	1H	3223	-	-	-	X
55	MG	1H	3226	-	-	-	X
55	MG	1H	3229	-	-	-	X
55	MG	1H	3241	-	-	-	X
55	MG	1H	3274	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
55	MG	1H	3275	-	-	-	X
55	MG	35	201	-	-	-	X
55	MG	5I	101	-	-	-	X
55	MG	8I	201	-	-	-	X
56	SF4	32	302	-	-	X	-



## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 292640 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
			Total	C	N	O	P			
1	13	1500	Total 32246	C 14352	N 5978	O 10416	P 1500	0	0	0
1	1G	1490	Total 32028	C 14255	N 5932	O 10351	P 1490	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	231	Total 1874	C 1199	N 334	O 336	S 5	0	0	0
2	12	207	Total 1696	C 1083	N 306	O 303	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	22	197	Total 1546	C 978	N 299	O 268	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3E	207	Total 1698	C 1064	N 338	O 289	S 7	0	0	0

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	8E	126	1000	634	196	170	0	0	0
9	82	121	953	605	186	162	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1I	94	Total 749	C 468	N 147	O 133	S 1	0	0	0
10	1A	99	Total 801	C 504	N 157	O 139	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	119	Total 942	C 582	N 194	O 164	S 2	0	0	0
13	4A	109	Total 879	C 544	N 181	O 152	S 2	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	69	Total	C	N	O	0	0	0
			554	355	106	93			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

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

- Molecule 22 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			
22	1L	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	0	0	0
			1644	733	297	537	77			
23	2L	77	Total	C	N	O	P	0	0	0
			1644	733	297	537	77			

- Molecule 24 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	72	Total	C	N	O	P	0	0	0
			1537	686	276	503	72			
24	3L	72	Total	C	N	O	P	0	0	0
			1537	686	276	503	72			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	18	Total	C	N	O	P	0	0	0
			391	176	79	118	18			
25	4L	14	Total	C	N	O	P	0	0	0
			303	137	62	90	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2811	Total	C	N	O	P	0	0	0
			60546	26946	11325	19464	2811			
26	14	2811	Total	C	N	O	P	0	0	0
			60561	26951	11337	19462	2811			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
28	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1556	984	297	269	6			
29	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
31	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
32	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	125	Total	C	N	O	S	0	0	0
			995	645	183	163	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	15	137	1096	707	205	181	3	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	68	122	932	588	171	169	4	0	0	0
35	25	122	932	588	171	169	4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	78	148	1127	701	230	193	3	0	0	0
36	35	147	1122	698	229	192	3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	88	141	1117	712	211	187	7	0	0	0
37	45	138	1099	702	208	183	6	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	98	118	967	604	203	159	1	0	0	0
38	55	118	967	604	203	159	1	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	A8	111	881	556	176	149	0	0	0
39	65	110	876	553	175	148	0	0	0



- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	B8	136	1128	702	231	194	1	0	0	0
40	75	140	1164	723	238	202	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	C8	115	950	603	199	147	1	0	0	0
41	85	116	959	608	201	149	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	D8	100	774	499	141	133	1	0	0	0
42	95	100	770	496	140	133	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	F8	95	750	488	135	126	1	0	0	0
44	B5	94	735	477	133	125		0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	97	Total	C	N	O	S	0	0	0
			734	472	140	117	5			
45	C5	52	Total	C	N	O	S	0	0	0
			396	258	72	65	1			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
48	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
49	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L31.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	P8	47	401	246	99	54	2	0	0	0
53	L5	48	406	249	100	55	2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	140	Total	Mg	0	0
			140	140		
55	5I	2	Total	Mg	0	0
			2	2		
55	8I	1	Total	Mg	0	0
			1	1		

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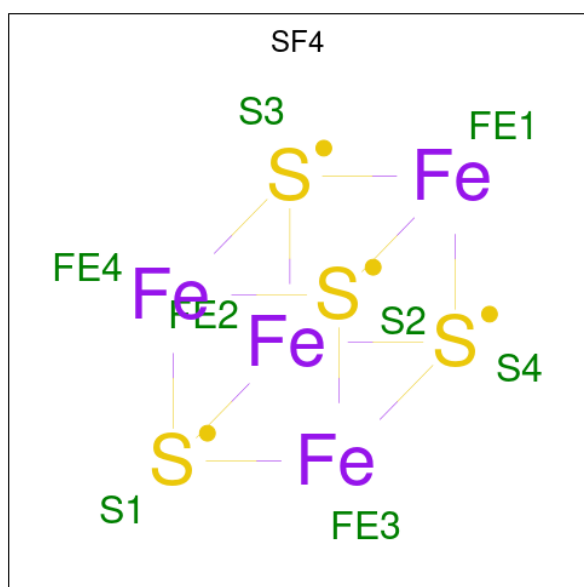
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BI	1	Total Mg 1 1	0	0
55	1F	2	Total Mg 2 2	0	0
55	2K	1	Total Mg 1 1	0	0
55	1H	473	Total Mg 473 473	0	0
55	16	2	Total Mg 2 2	0	0
55	11	1	Total Mg 1 1	0	0
55	21	3	Total Mg 3 3	0	0
55	41	1	Total Mg 1 1	0	0
55	78	2	Total Mg 2 2	0	0
55	88	3	Total Mg 3 3	0	0
55	C8	2	Total Mg 2 2	0	0
55	D8	1	Total Mg 1 1	0	0
55	I8	1	Total Mg 1 1	0	0
55	J8	1	Total Mg 1 1	0	0
55	P8	1	Total Mg 1 1	0	0
55	1G	126	Total Mg 126 126	0	0
55	32	1	Total Mg 1 1	0	0
55	42	2	Total Mg 2 2	0	0
55	2A	1	Total Mg 1 1	0	0
55	4A	1	Total Mg 1 1	0	0
55	7A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	1	Total Mg 1 1	0	0
55	2L	1	Total Mg 1 1	0	0
55	14	300	Total Mg 300 300	0	0
55	1J	2	Total Mg 2 2	0	0
55	29	1	Total Mg 1 1	0	0
55	39	1	Total Mg 1 1	0	0
55	35	1	Total Mg 1 1	0	0
55	45	2	Total Mg 2 2	0	0
55	85	1	Total Mg 1 1	0	0
55	E5	1	Total Mg 1 1	0	0
55	F5	1	Total Mg 1 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	3E	1	Total	Fe	S	0	0
			8	4	4		
56	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	5I	1	Total	Zn	0	0
			1	1		
57	5A	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	274	Total	O	0	0
			274	274		
58	4E	6	Total	O	0	0
			6	6		
58	8E	1	Total	O	0	0
			1	1		
58	1I	2	Total	O	0	0
			2	2		
58	3I	1	Total	O	0	0
			1	1		
58	4I	2	Total	O	0	0
			2	2		
58	5I	1	Total	O	0	0
			1	1		
58	7I	3	Total	O	0	0
			3	3		
58	1F	1	Total	O	0	0
			1	1		
58	1K	1	Total	O	0	0
			1	1		
58	1H	1010	Total	O	0	0
			1010	1010		
58	16	8	Total	O	0	0
			8	8		
58	11	8	Total	O	0	0
			8	8		
58	21	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	31	5	Total 5	O 5	0	0
58	58	1	Total 1	O 1	0	0
58	78	8	Total 8	O 8	0	0
58	98	1	Total 1	O 1	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	1	Total 1	O 1	0	0
58	G8	1	Total 1	O 1	0	0
58	I8	3	Total 3	O 3	0	0
58	J8	2	Total 2	O 2	0	0
58	L8	3	Total 3	O 3	0	0
58	Q8	2	Total 2	O 2	0	0
58	1G	240	Total 240	O 240	0	0
58	32	1	Total 1	O 1	0	0
58	42	1	Total 1	O 1	0	0
58	7A	4	Total 4	O 4	0	0
58	BA	2	Total 2	O 2	0	0
58	2L	6	Total 6	O 6	0	0
58	4L	1	Total 1	O 1	0	0
58	14	586	Total 586	O 586	0	0
58	19	7	Total 7	O 7	0	0
58	29	2	Total 2	O 2	0	0

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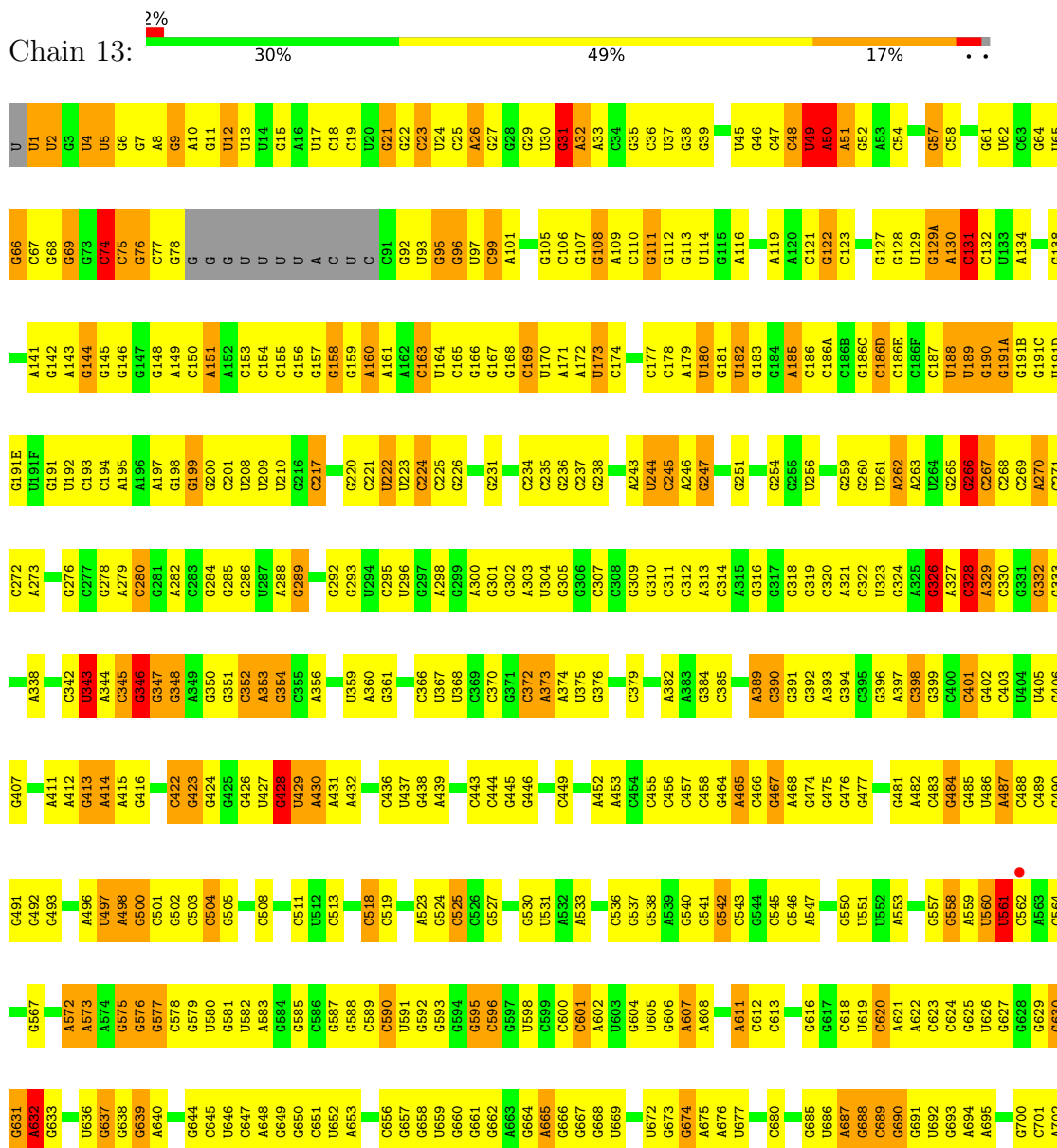
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58	35	5	Total 5	O 5	0	0
58	45	5	Total 5	O 5	0	0
58	B5	2	Total 2	O 2	0	0
58	H5	2	Total 2	O 2	0	0
58	L5	1	Total 1	O 1	0	0

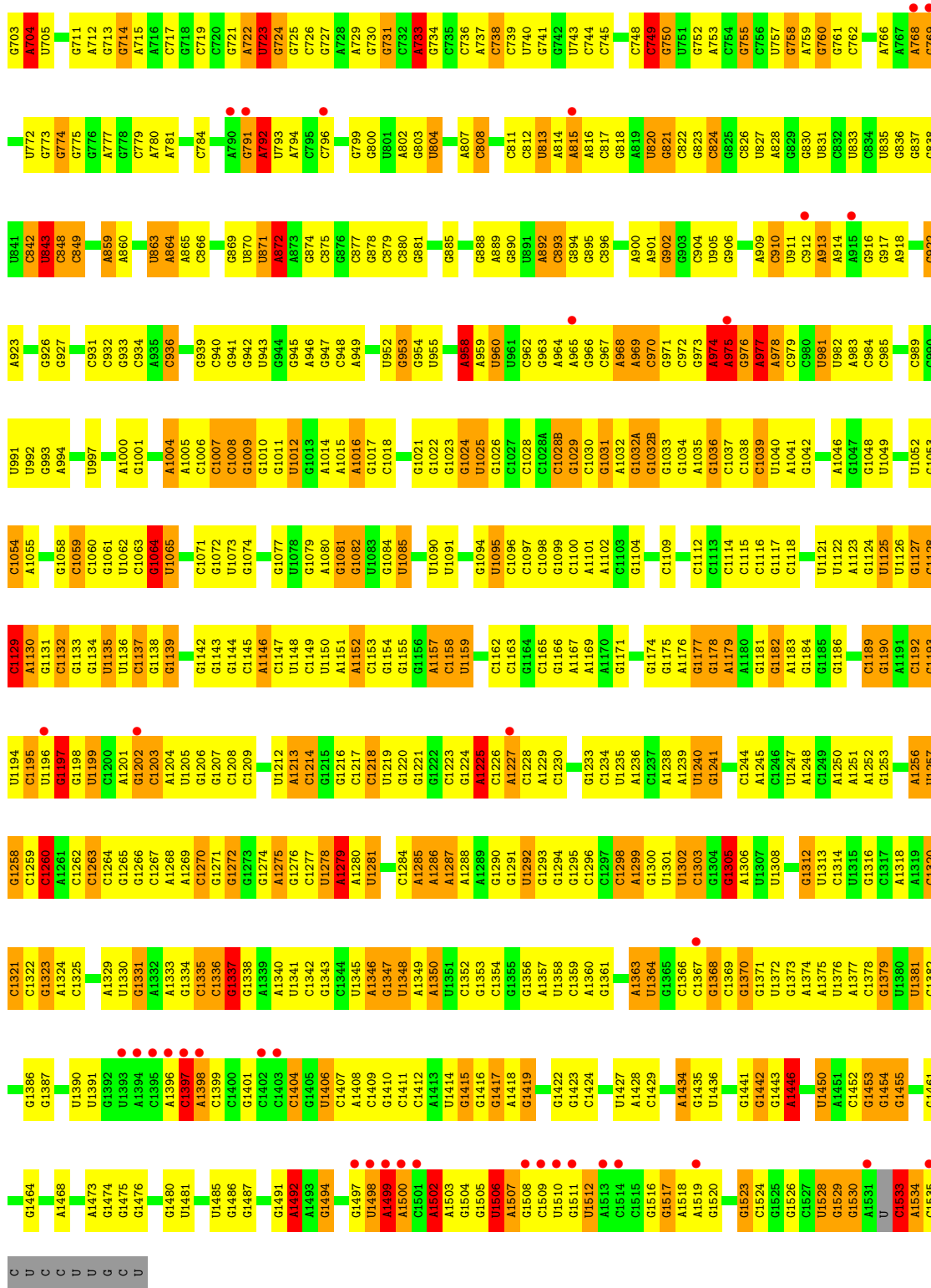


### 3 Residue-property plots

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.

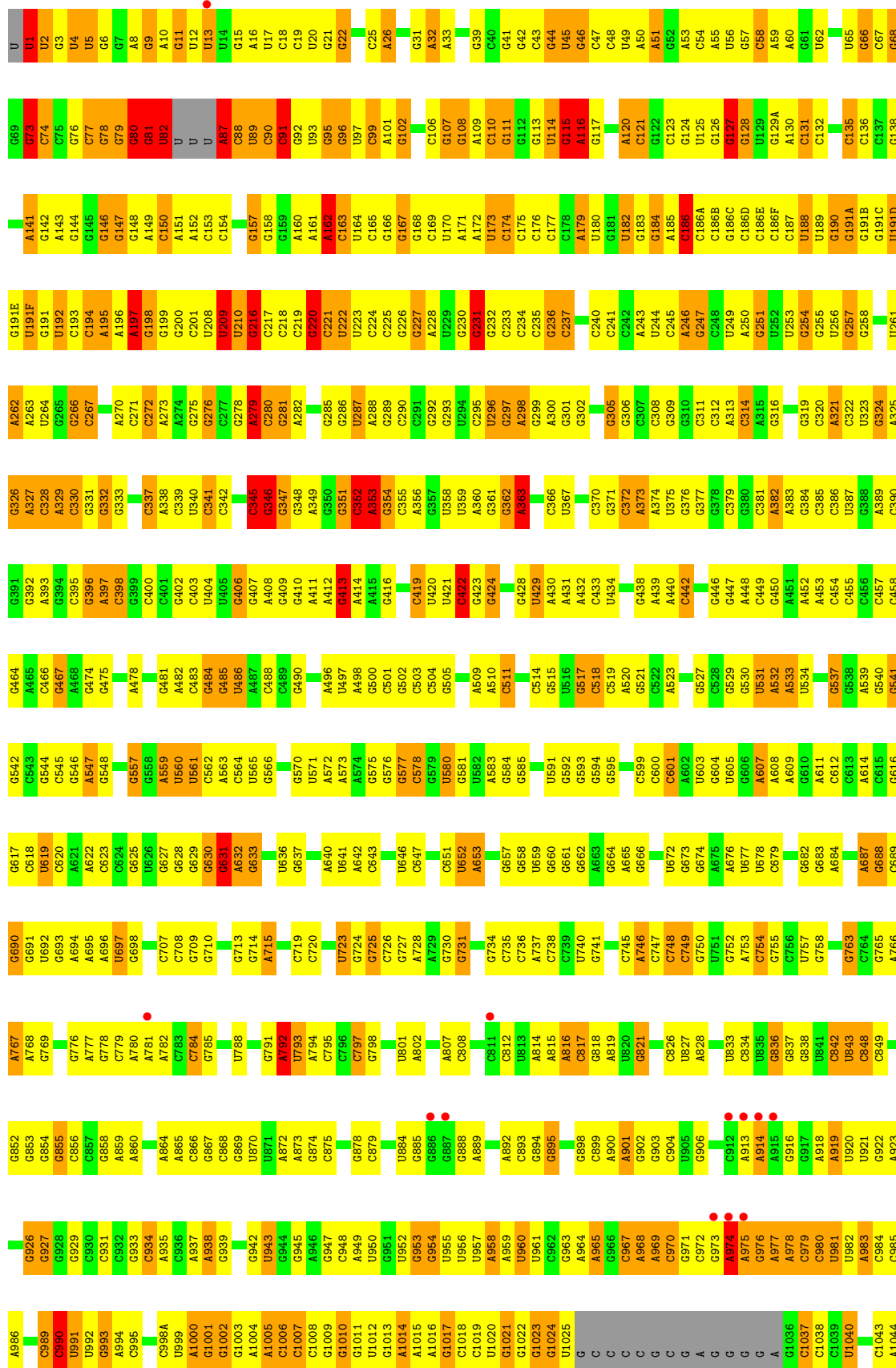
- Molecule 1: 16S ribosomal RNA

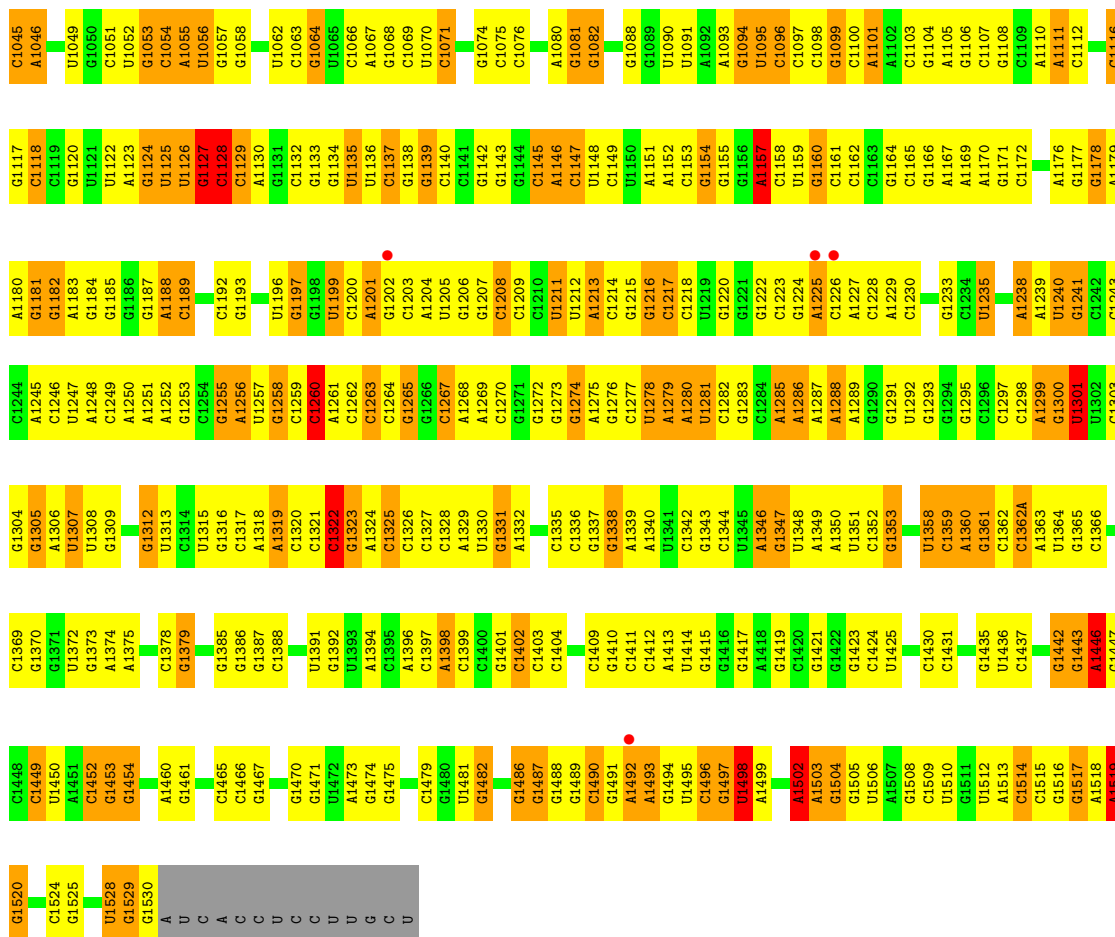




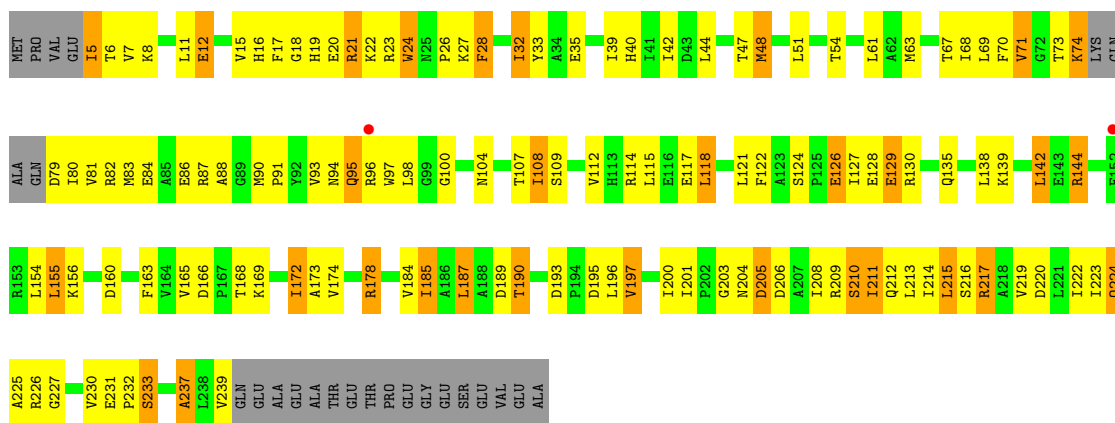
● Molecule 1: 16S ribosomal RNA





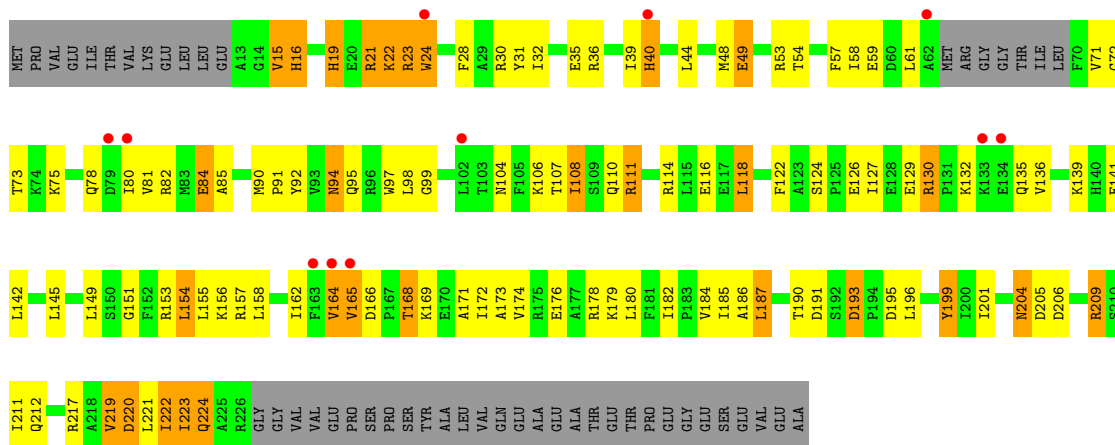


• Molecule 2: 30S ribosomal protein S2

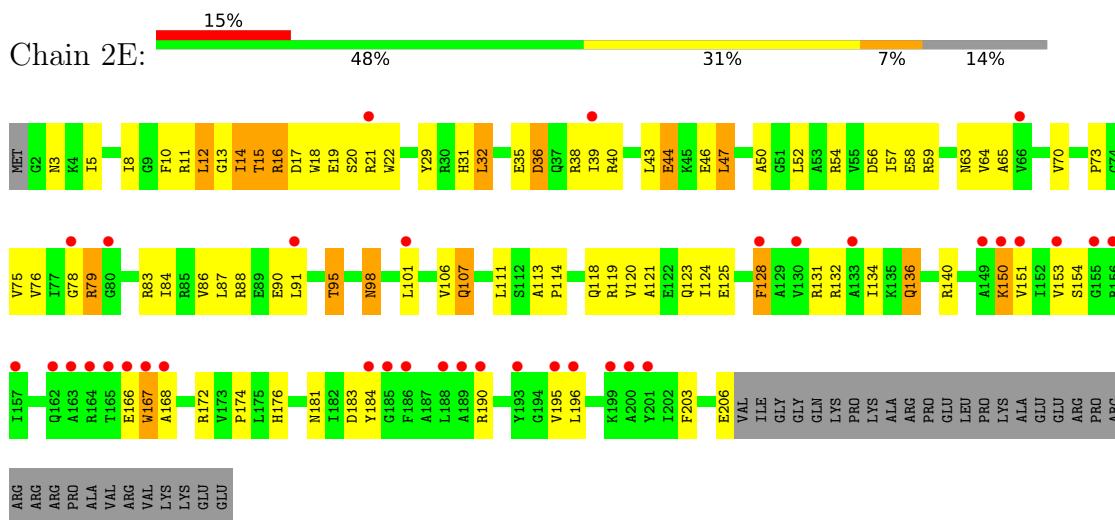


• Molecule 2: 30S ribosomal protein S2

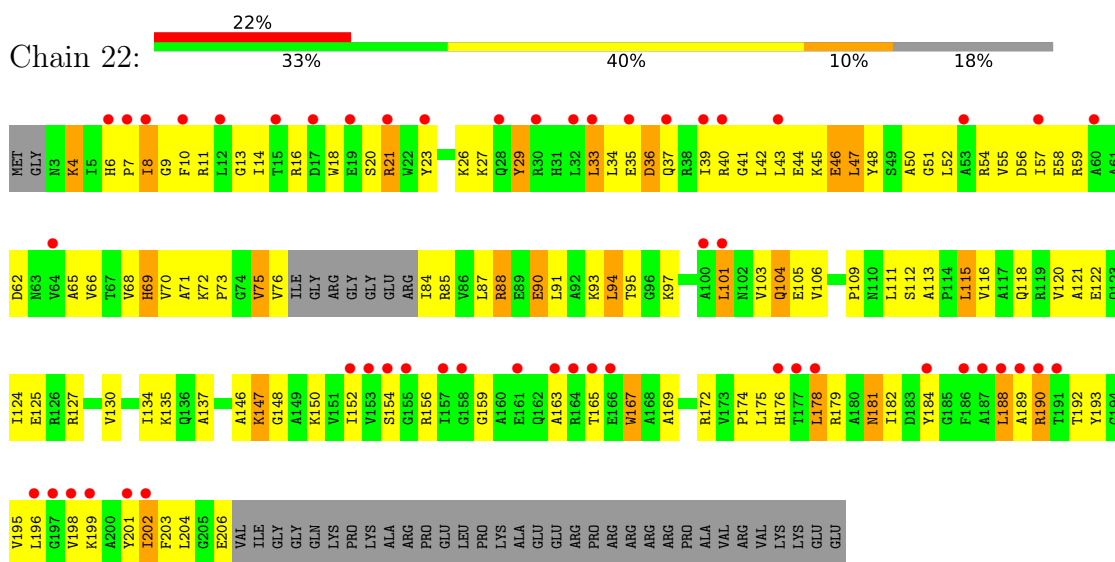




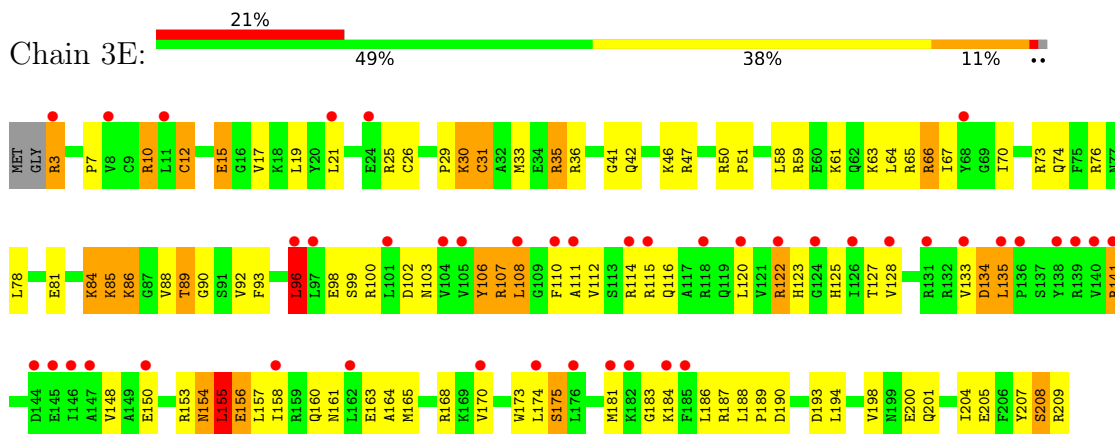
• Molecule 3: 30S ribosomal protein S3



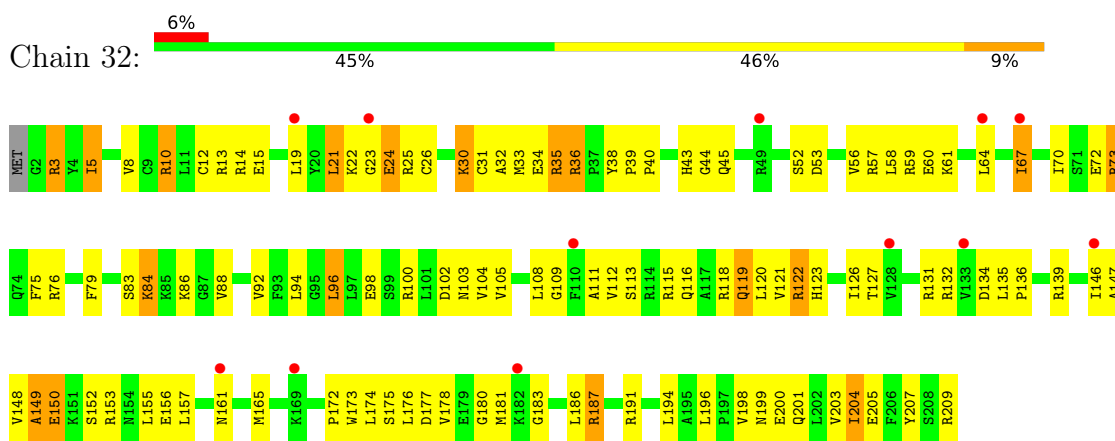
• Molecule 3: 30S ribosomal protein S3



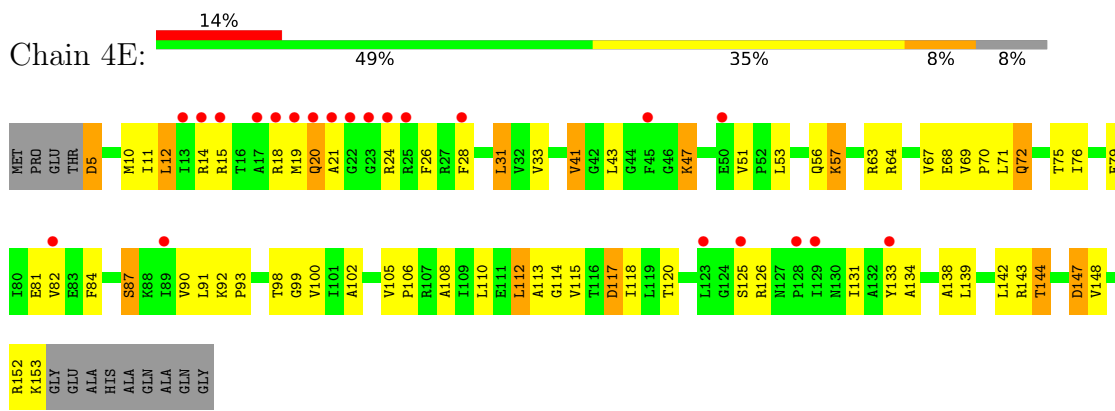
• Molecule 4: 30S ribosomal protein S4



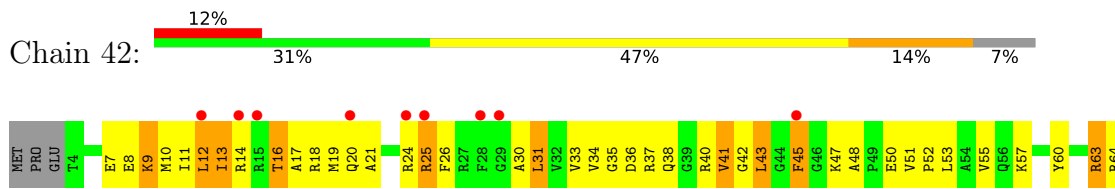
• Molecule 4: 30S ribosomal protein S4

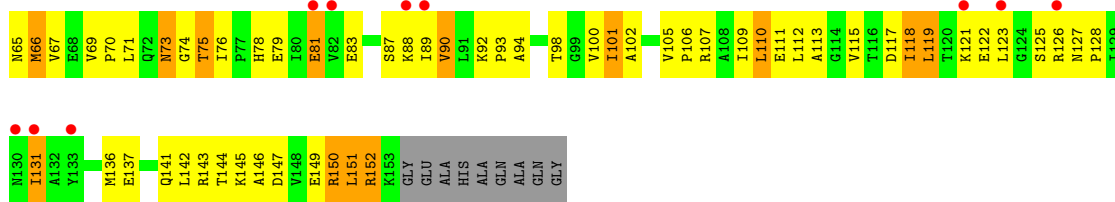


• Molecule 5: 30S ribosomal protein S5

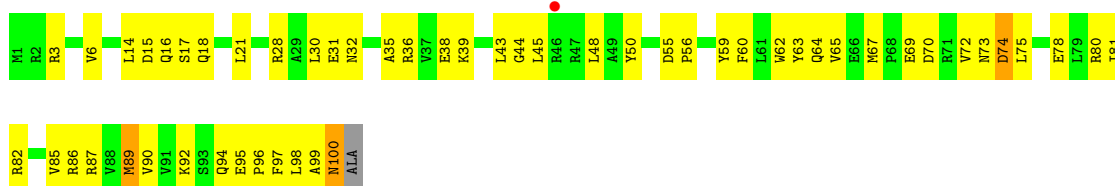


• Molecule 5: 30S ribosomal protein S5

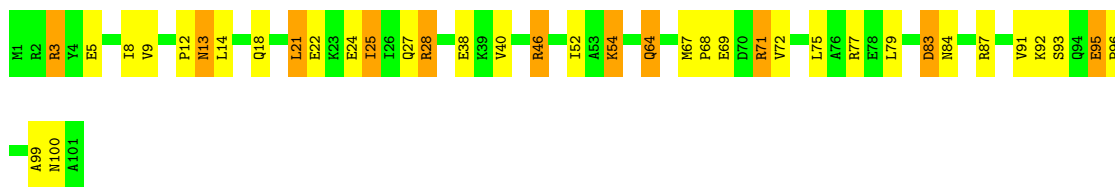




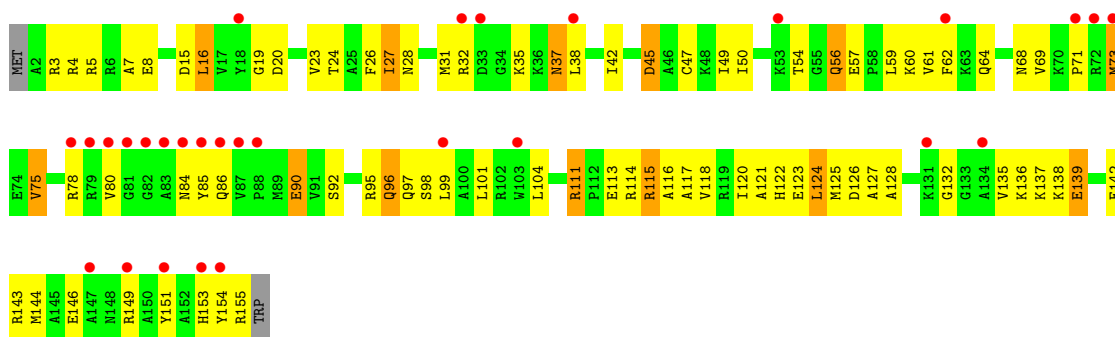
• Molecule 6: 30S ribosomal protein S6



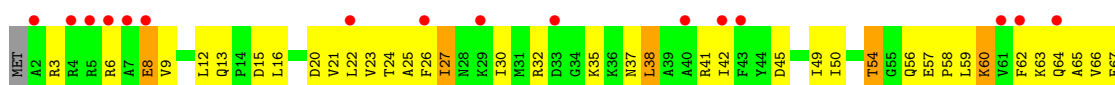
• Molecule 6: 30S ribosomal protein S6

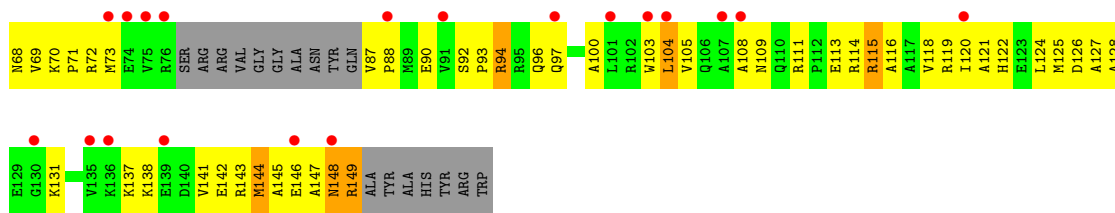


• Molecule 7: 30S ribosomal protein S7

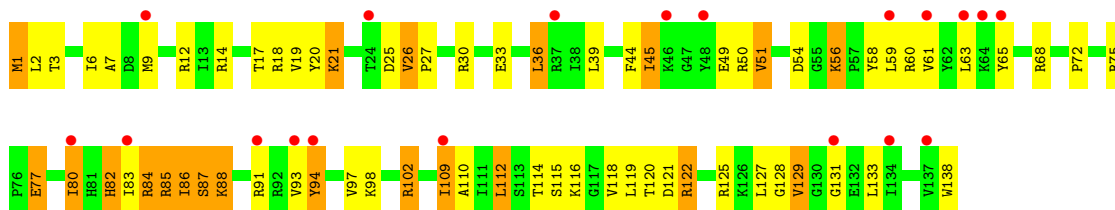


• Molecule 7: 30S ribosomal protein S7

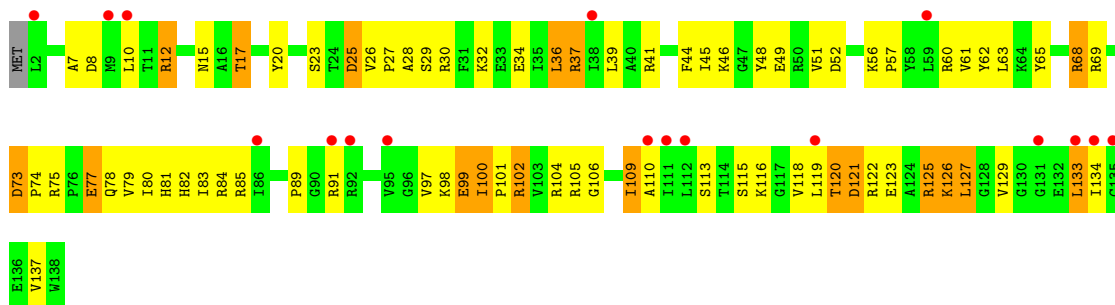
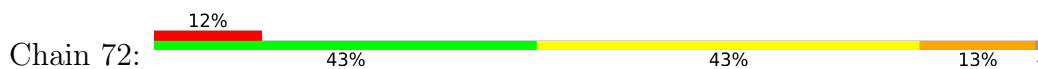




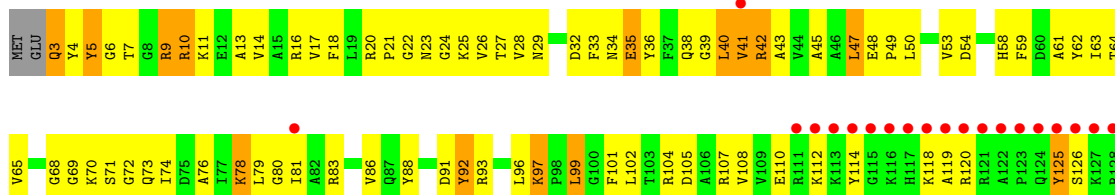
• Molecule 8: 30S ribosomal protein S8



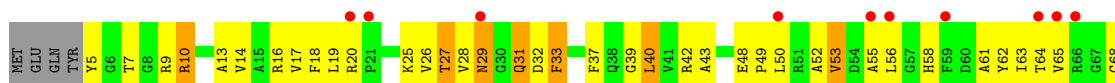
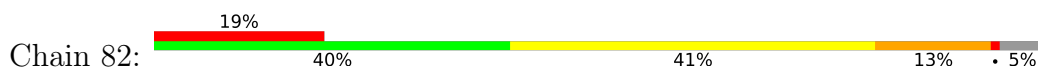
• Molecule 8: 30S ribosomal protein S8



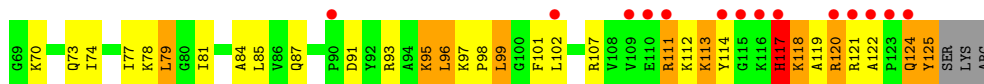
• Molecule 9: 30S ribosomal protein S9



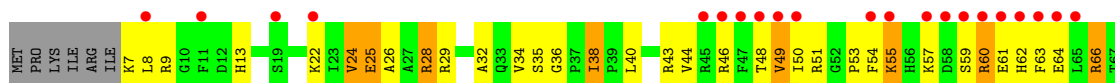
• Molecule 9: 30S ribosomal protein S9



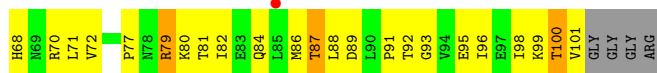
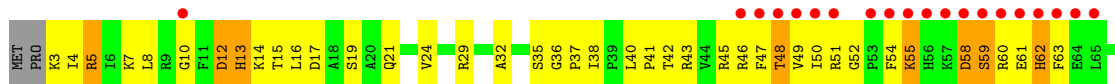




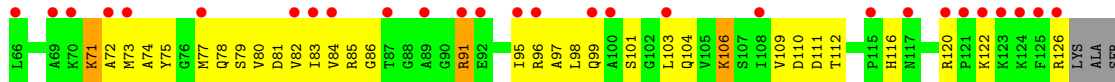
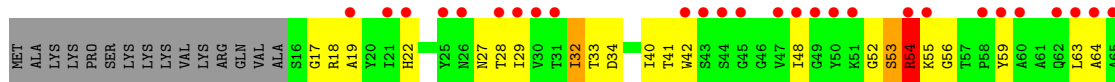
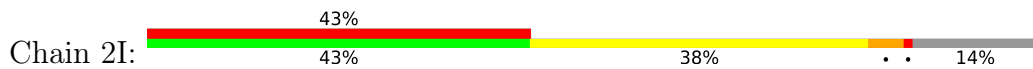
• Molecule 10: 30S ribosomal protein S10



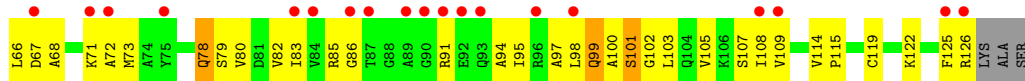
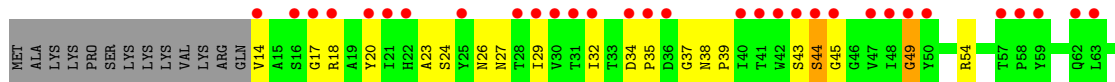
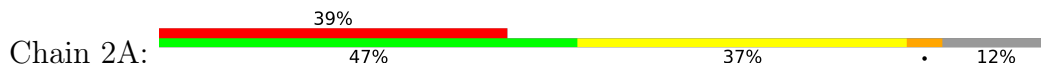
• Molecule 10: 30S ribosomal protein S10



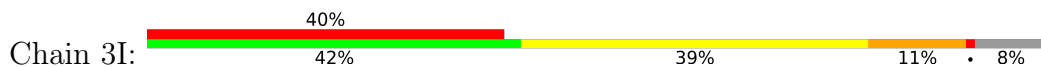
• Molecule 11: 30S ribosomal protein S11

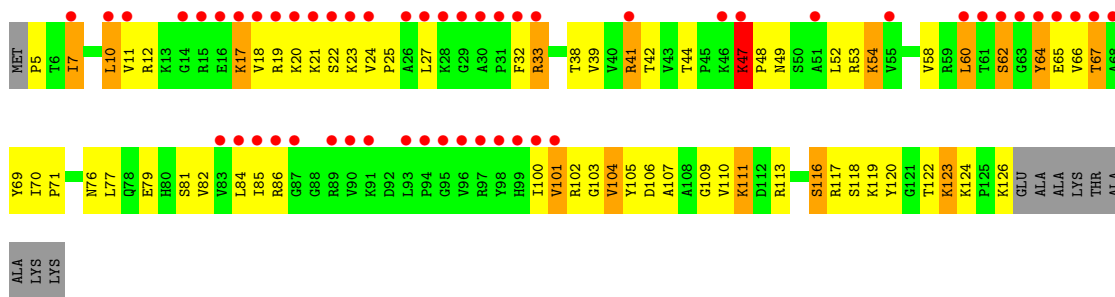


• Molecule 11: 30S ribosomal protein S11

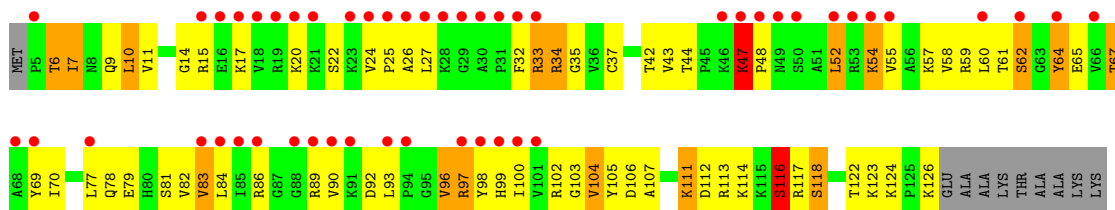
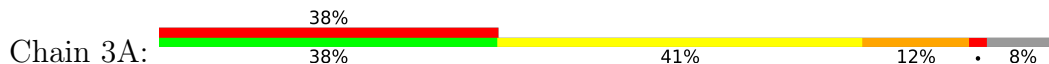


• Molecule 12: 30S ribosomal protein S12

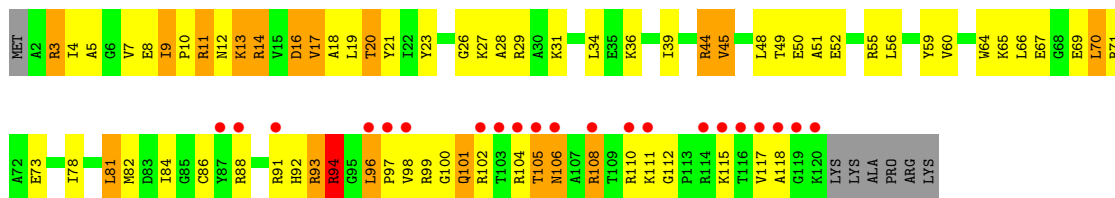
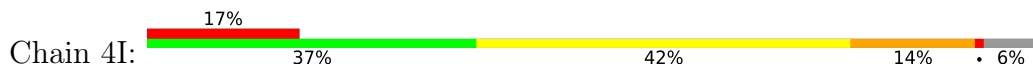




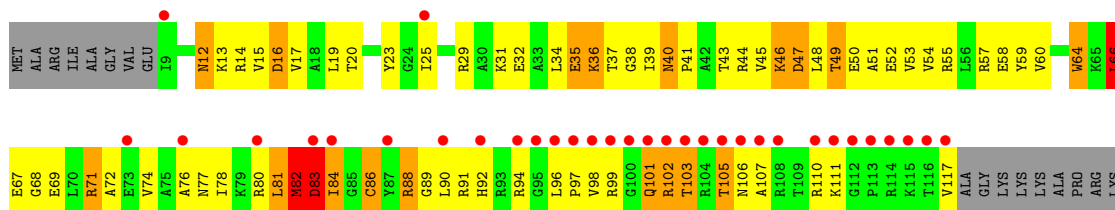
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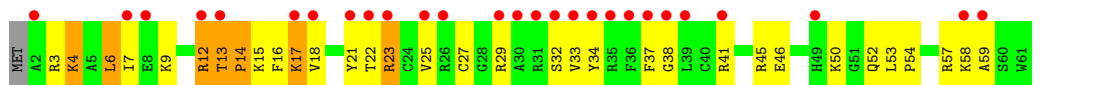
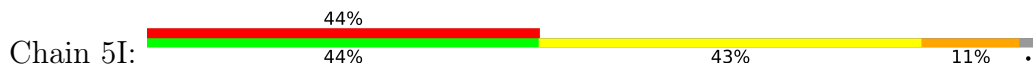
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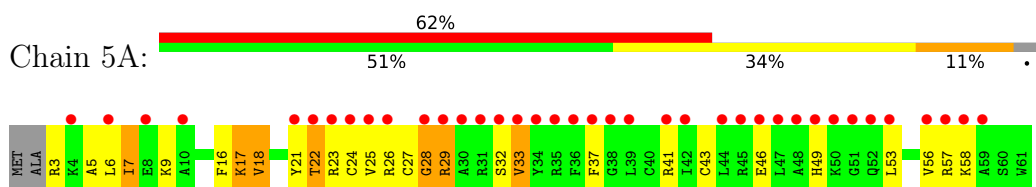
• Molecule 13: 30S ribosomal protein S13



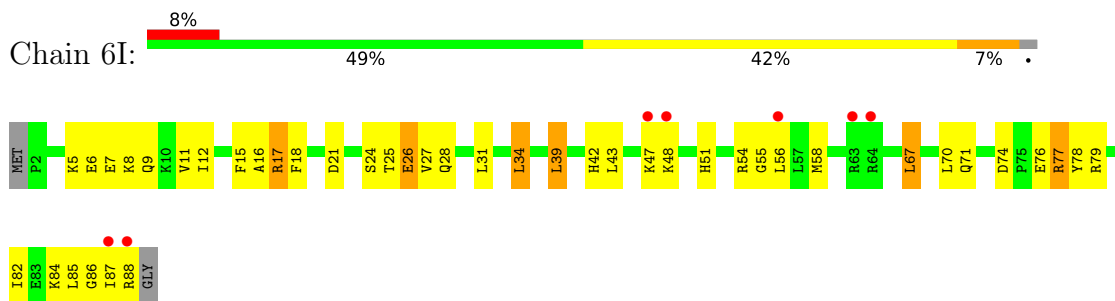
• Molecule 14: 30S ribosomal protein S14 type Z



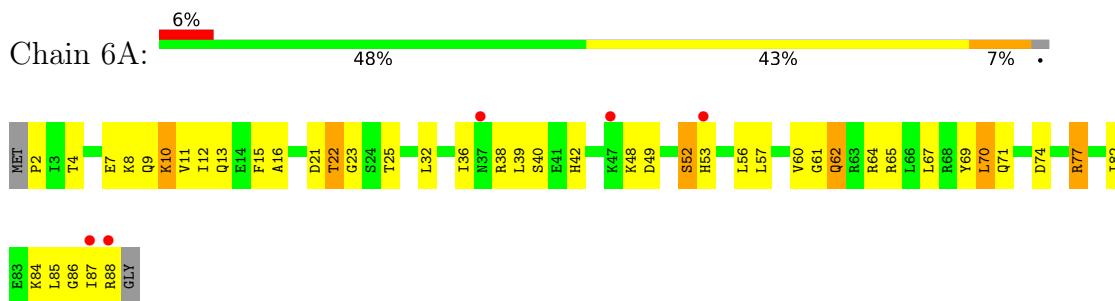
• Molecule 14: 30S ribosomal protein S14 type Z



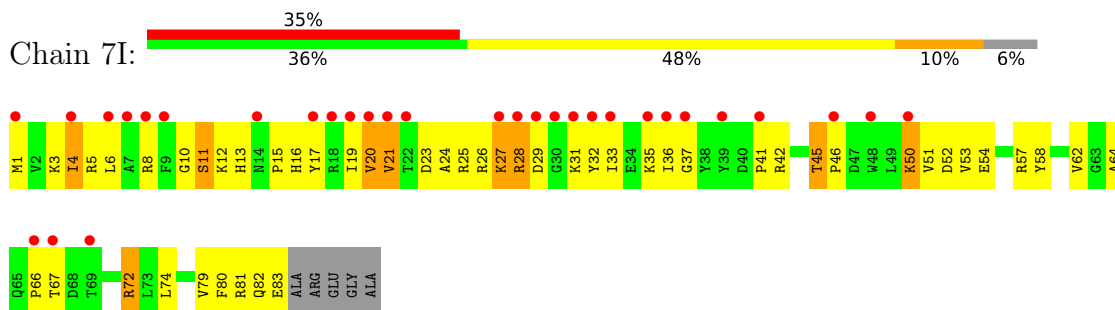
- Molecule 15: 30S ribosomal protein S15



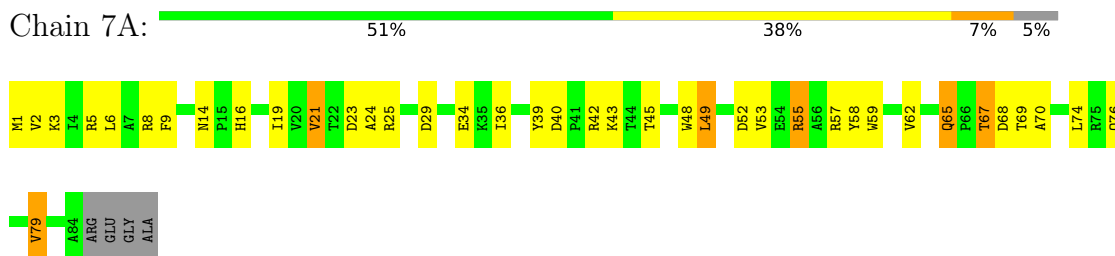
- Molecule 15: 30S ribosomal protein S15



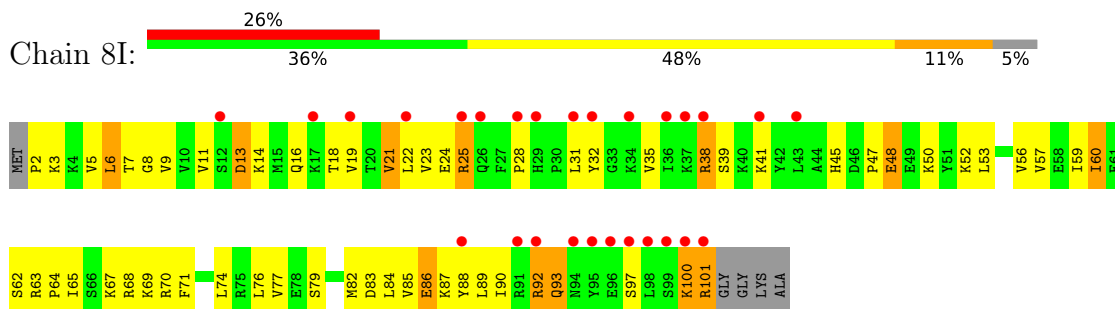
- Molecule 16: 30S ribosomal protein S16



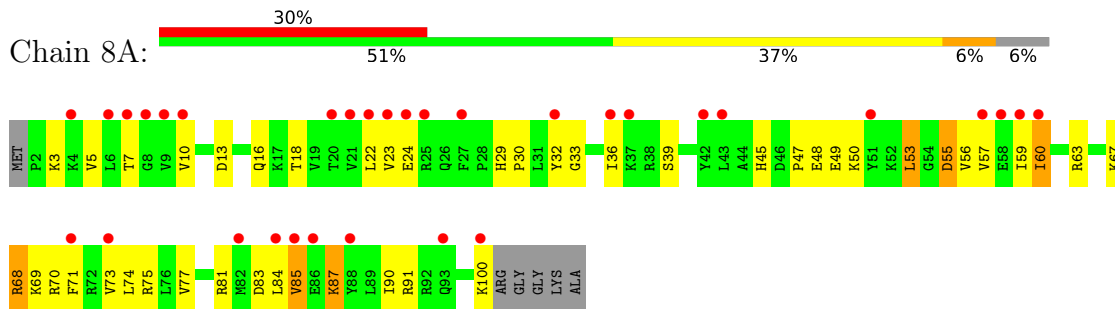
- Molecule 16: 30S ribosomal protein S16



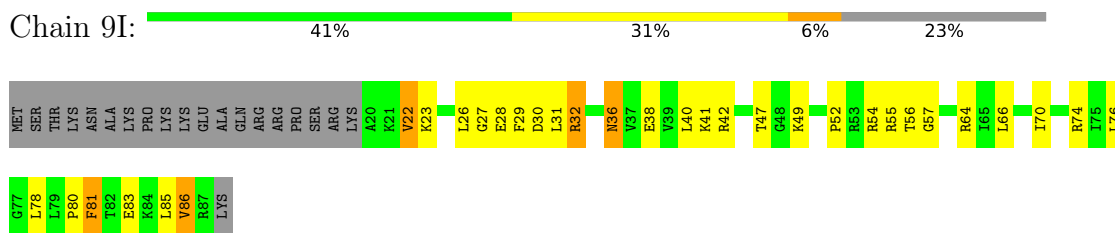
- Molecule 17: 30S ribosomal protein S17



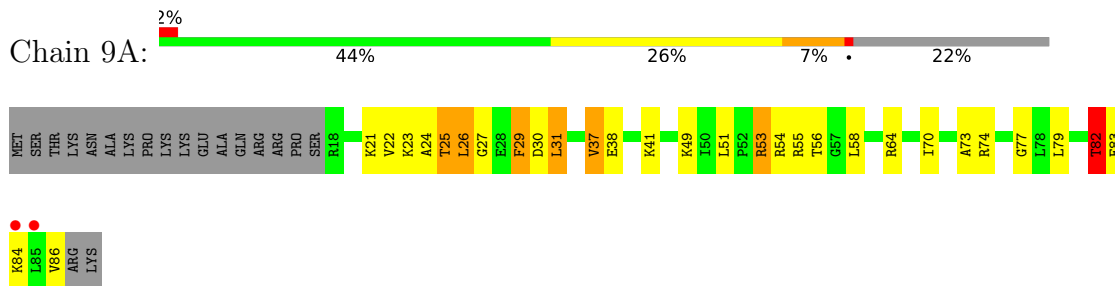
● Molecule 17: 30S ribosomal protein S17



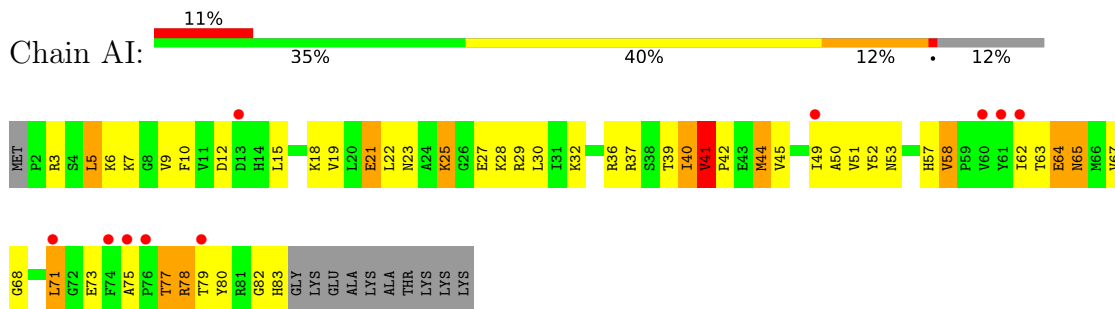
● Molecule 18: 30S ribosomal protein S18



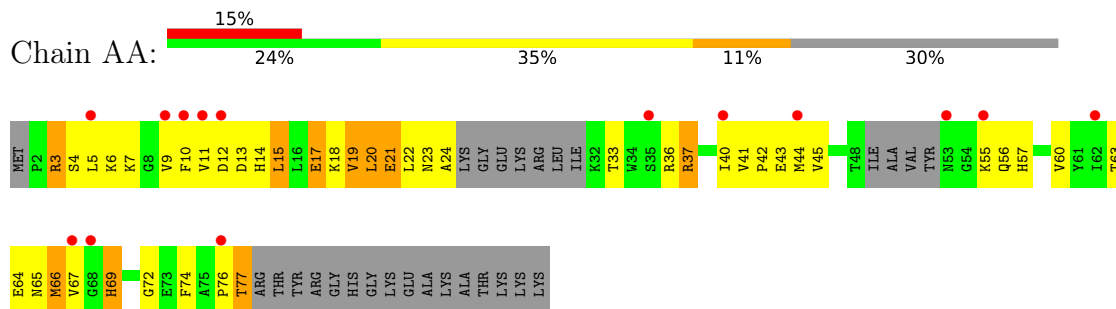
● Molecule 18: 30S ribosomal protein S18



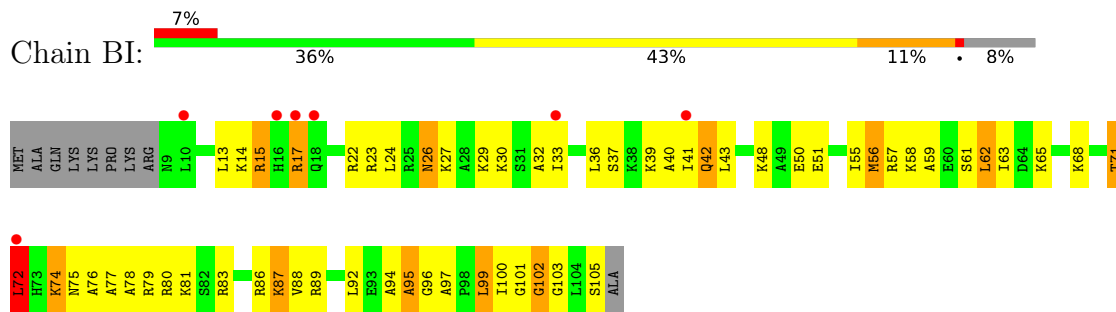
● Molecule 19: 30S ribosomal protein S19



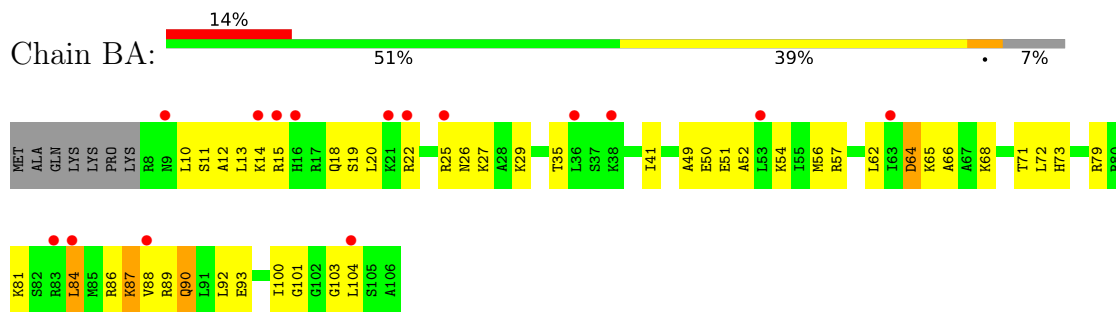
- Molecule 19: 30S ribosomal protein S19



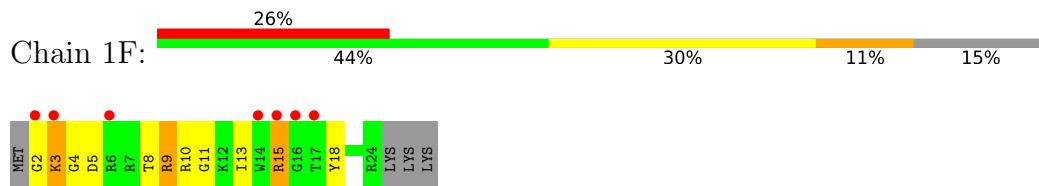
- Molecule 20: 30S ribosomal protein S20



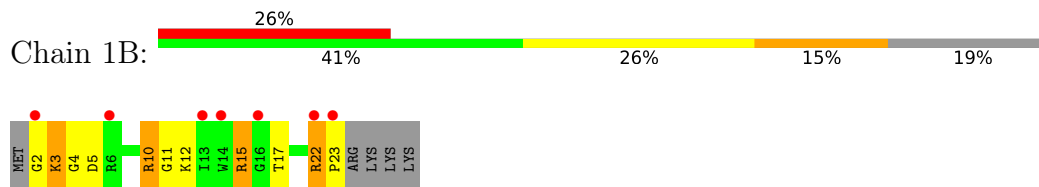
- Molecule 20: 30S ribosomal protein S20



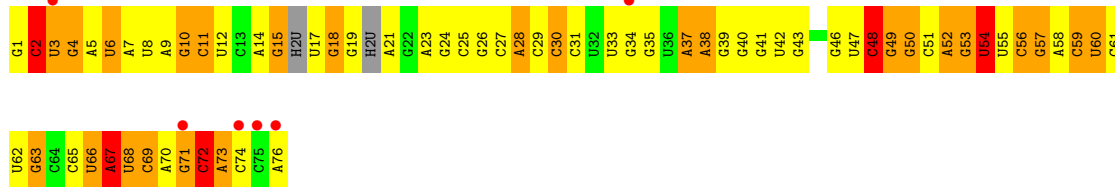
- Molecule 21: 30S ribosomal protein Thx



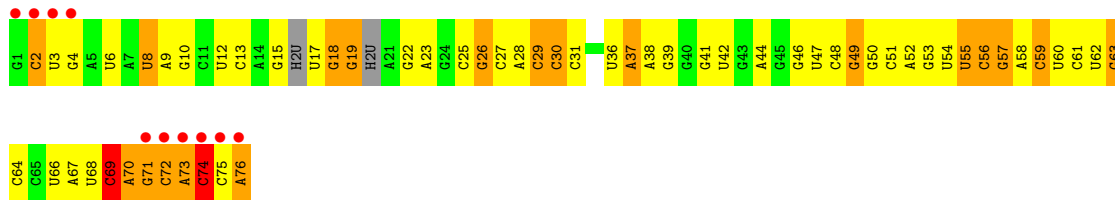
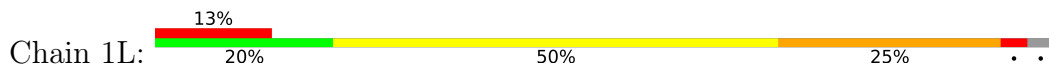
- Molecule 21: 30S ribosomal protein Thx



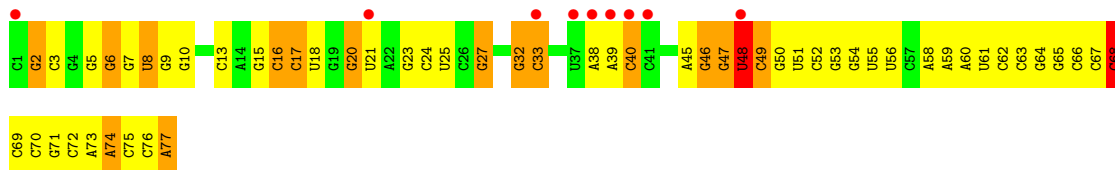
- Molecule 22: tRNAThr



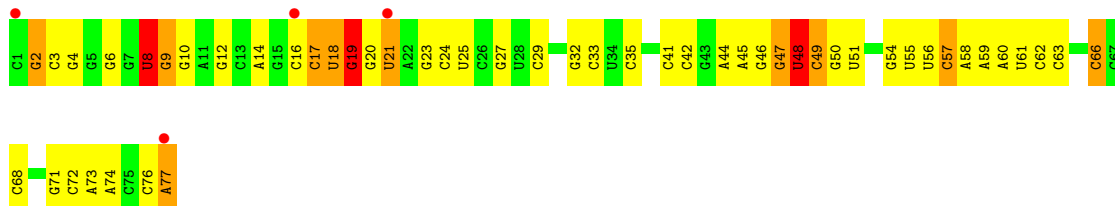
• Molecule 22: tRNAThr



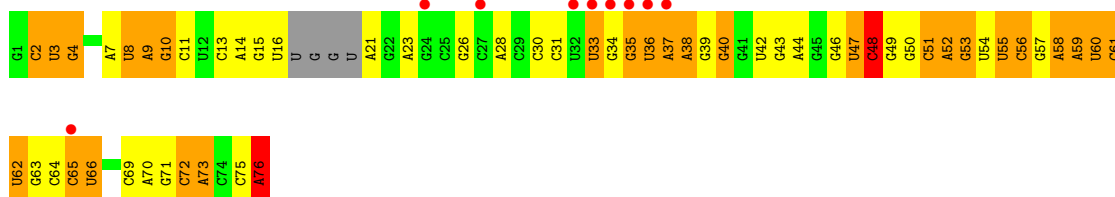
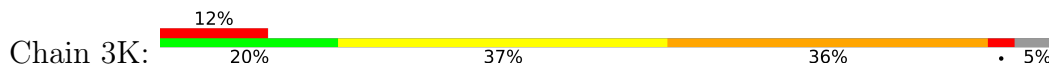
• Molecule 23: tRNAfMet



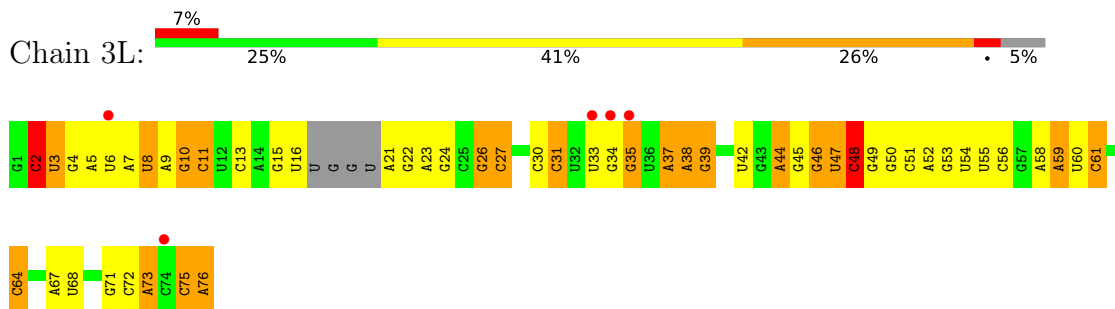
• Molecule 23: tRNAfMet



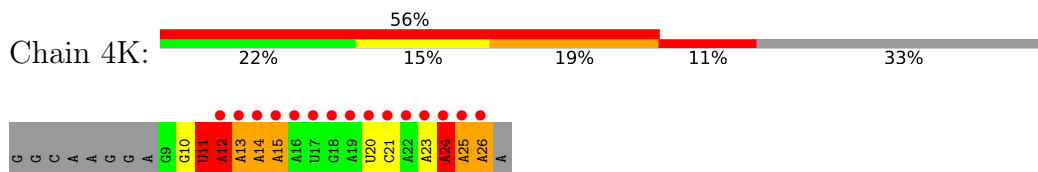
• Molecule 24: tRNAThr



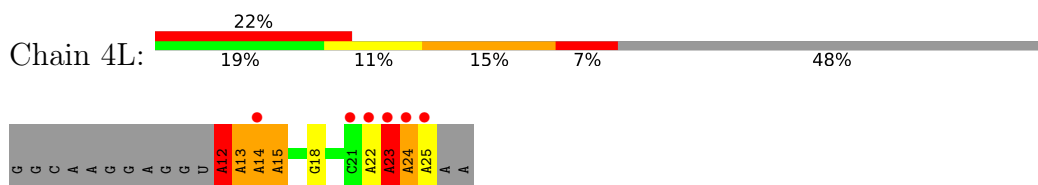
• Molecule 24: tRNAThr



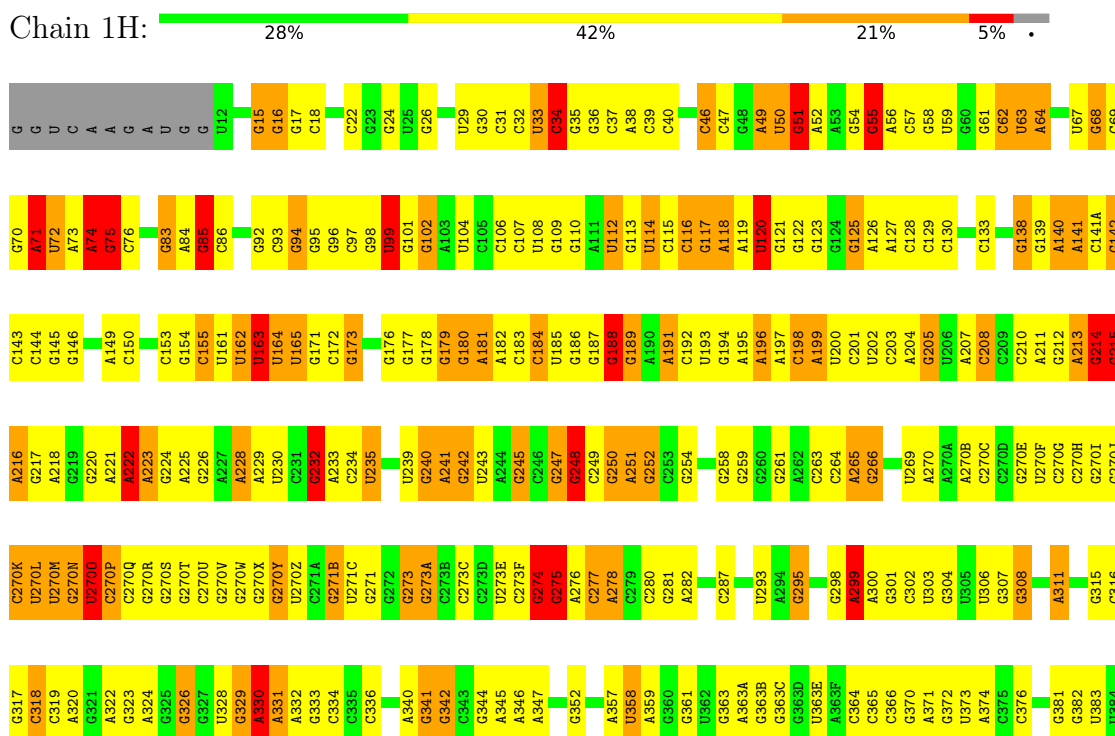
• Molecule 25: mRNA

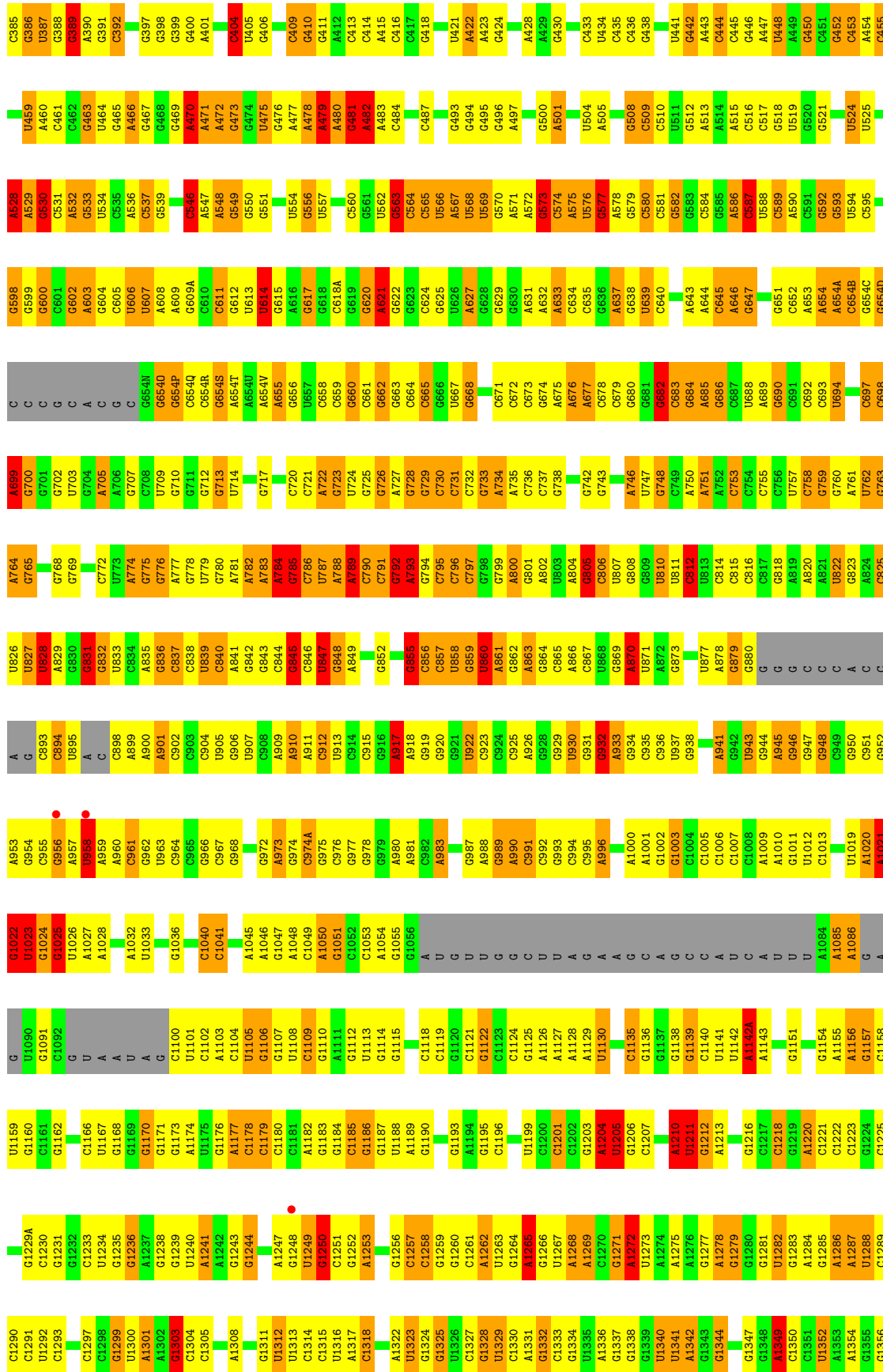


• Molecule 25: mRNA



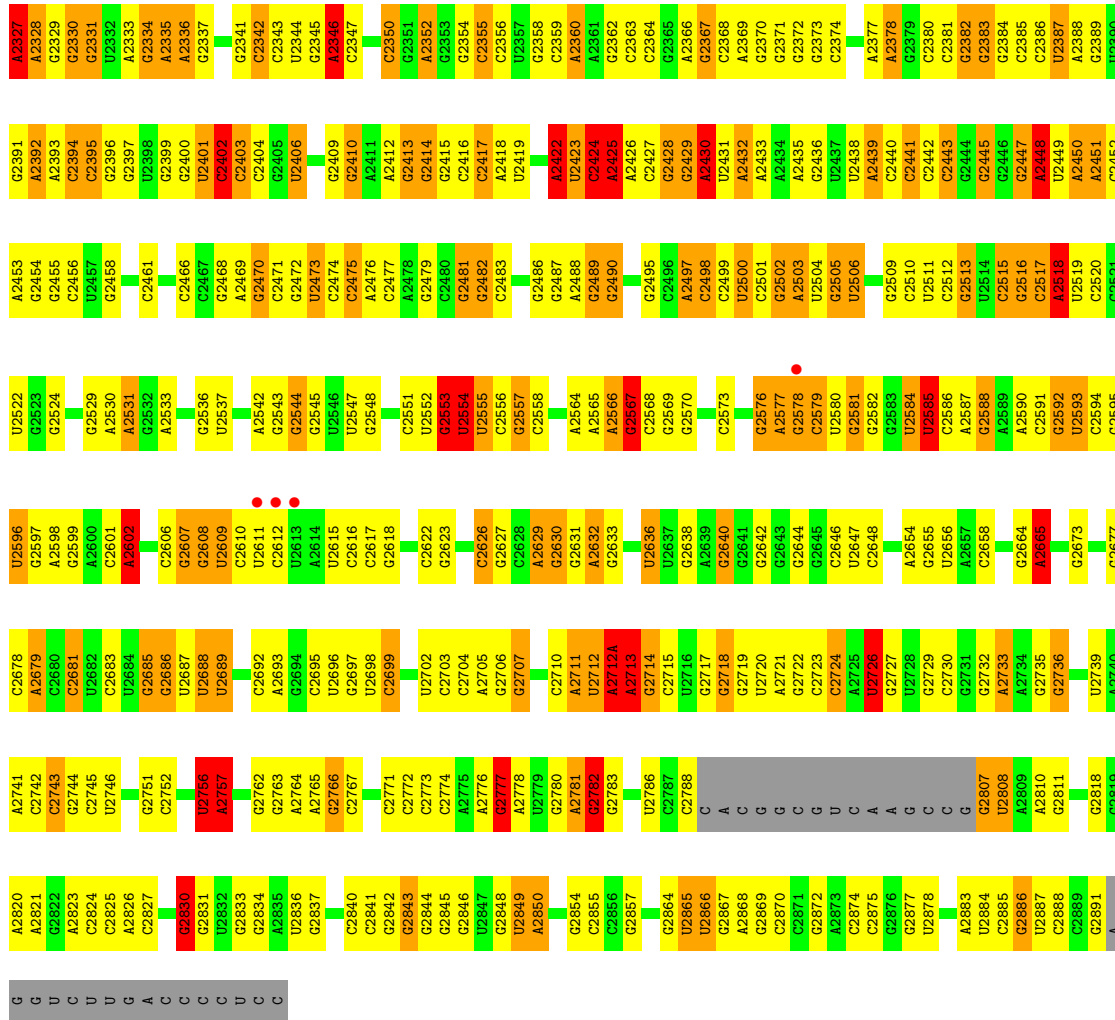
• Molecule 26: 23S ribosomal RNA



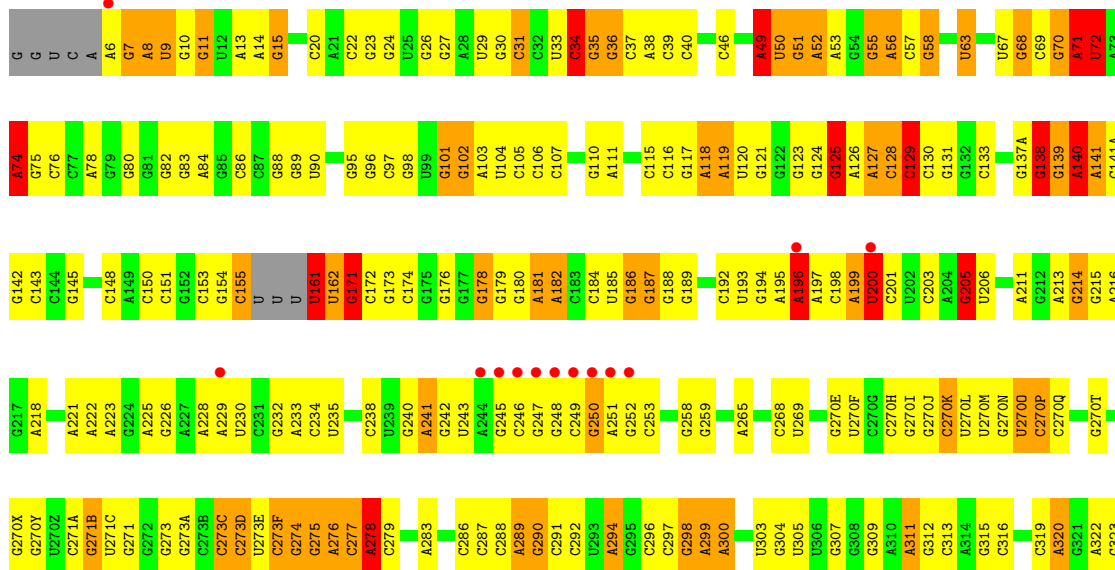


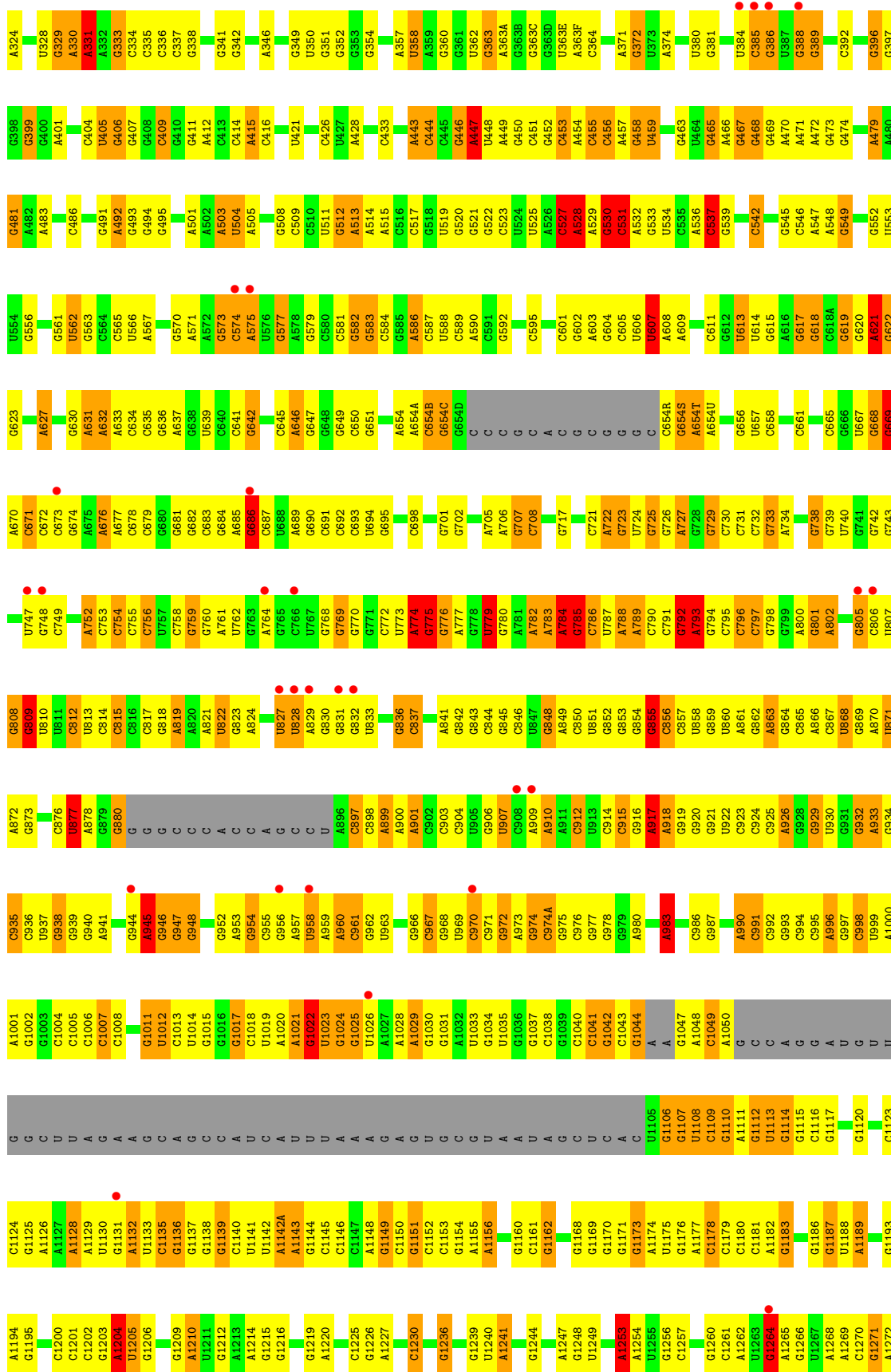


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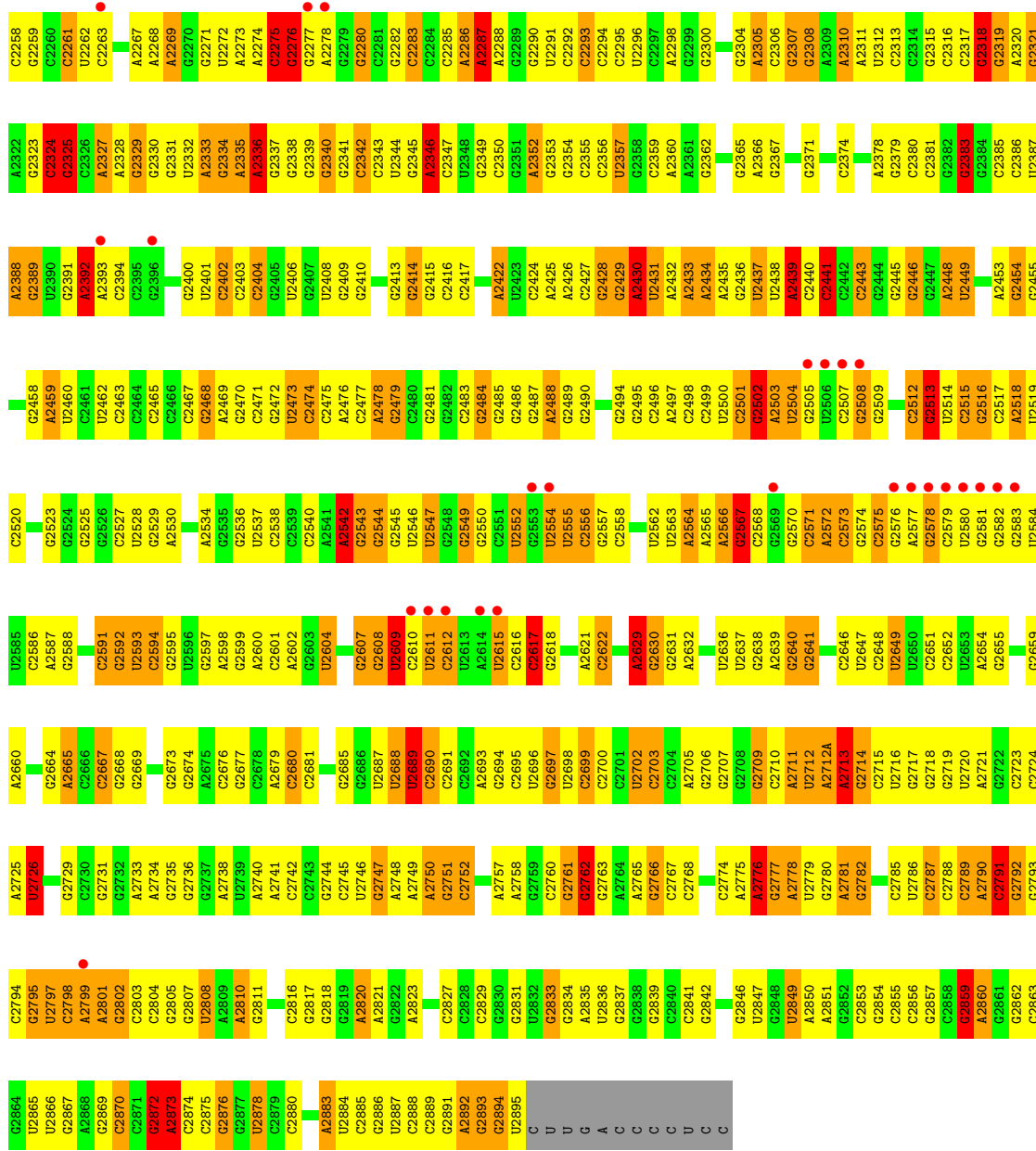


• Molecule 26: 23S ribosomal RNA

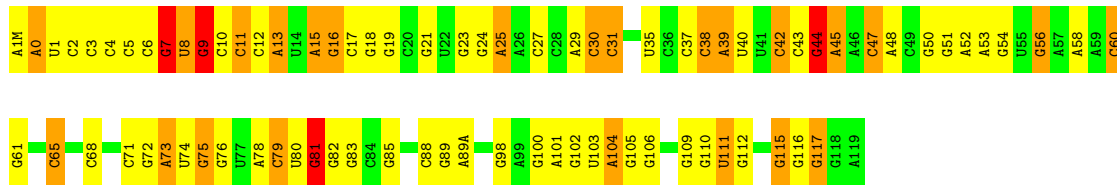




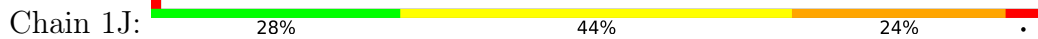
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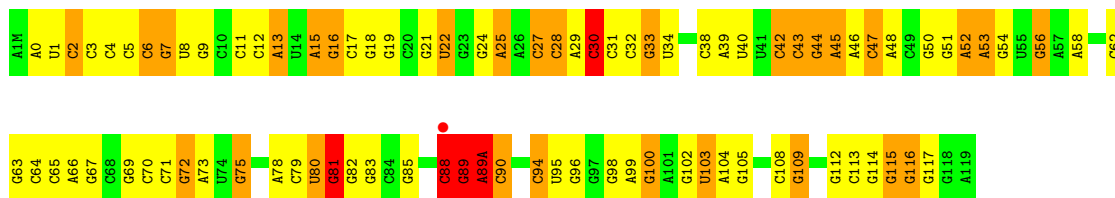


• Molecule 27: 5S ribosomal RNA

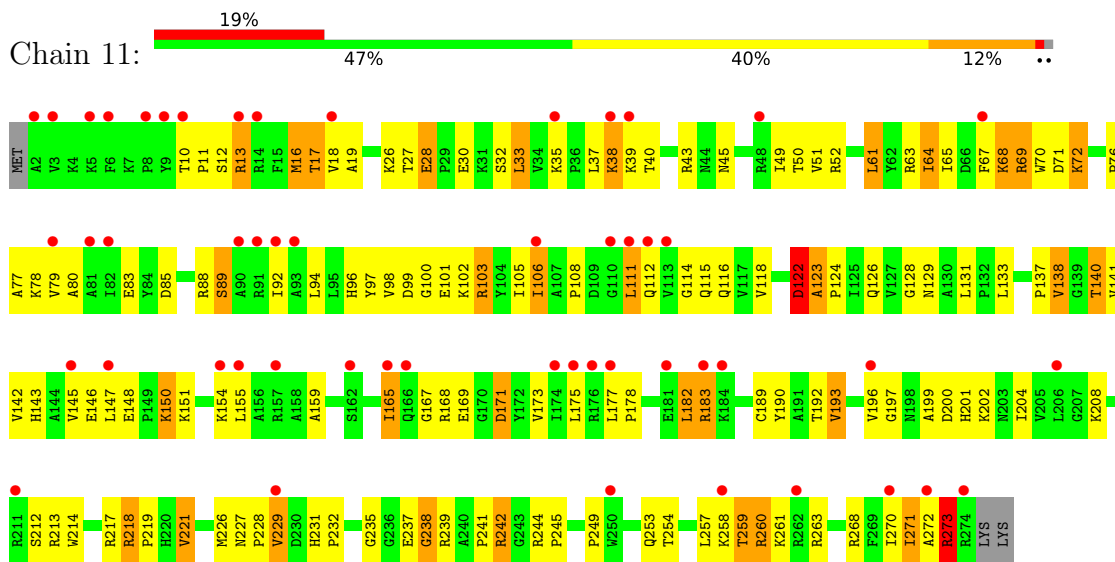


• Molecule 27: 5S ribosomal RNA

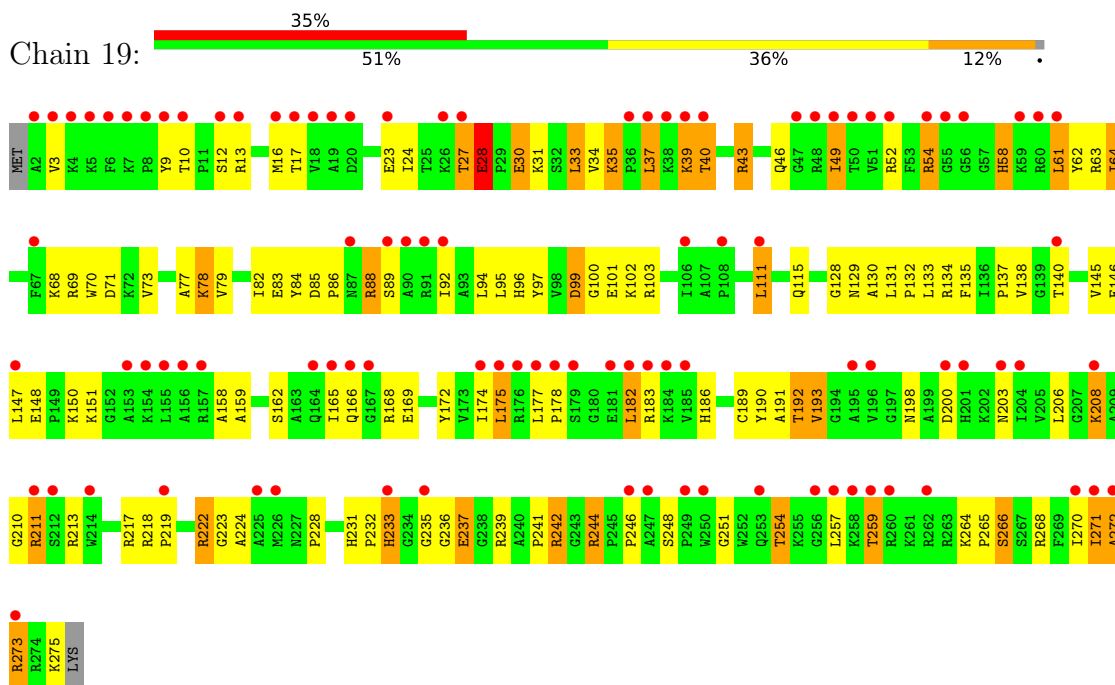




• Molecule 28: 50S ribosomal protein L2

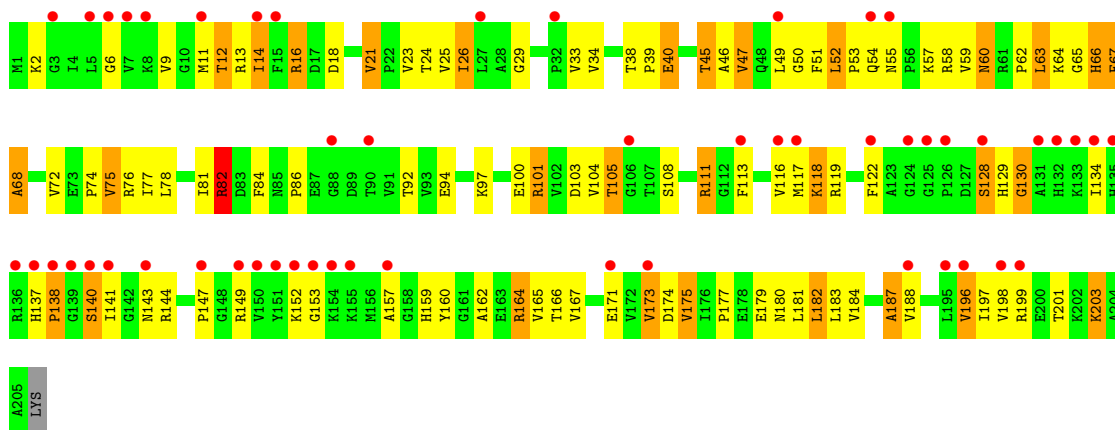


• Molecule 28: 50S ribosomal protein L2

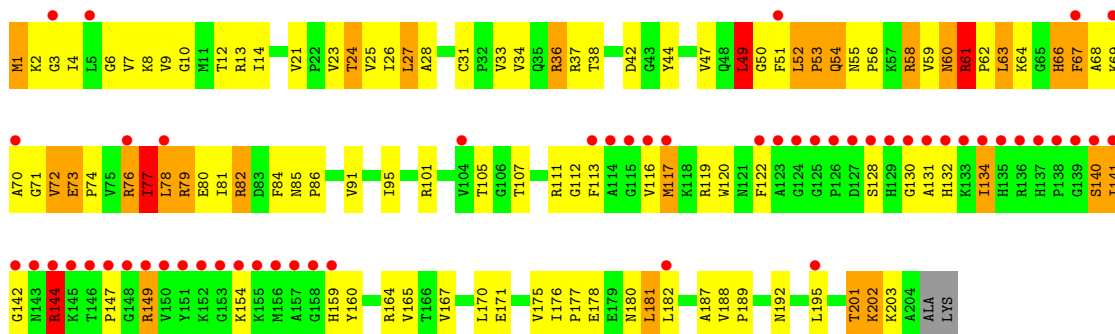


• Molecule 29: 50S ribosomal protein L3

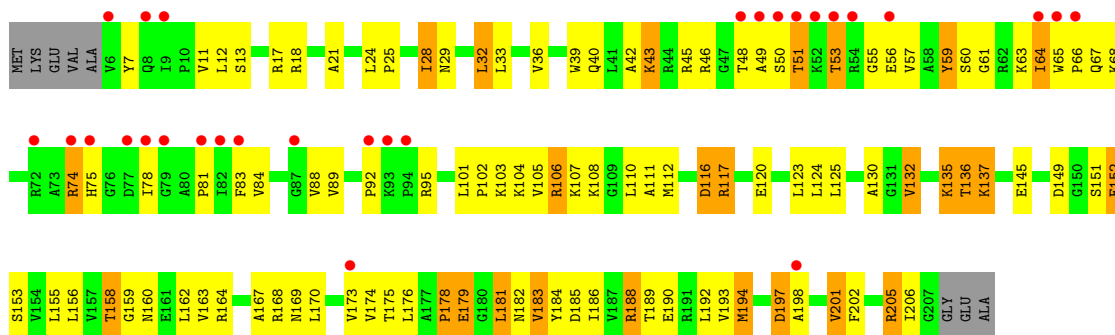
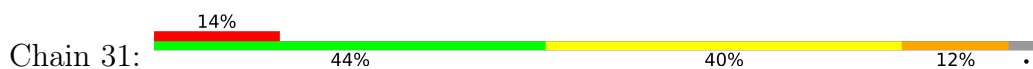




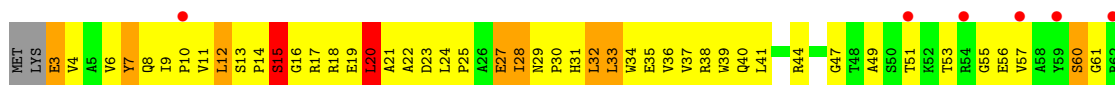
• Molecule 29: 50S ribosomal protein L3

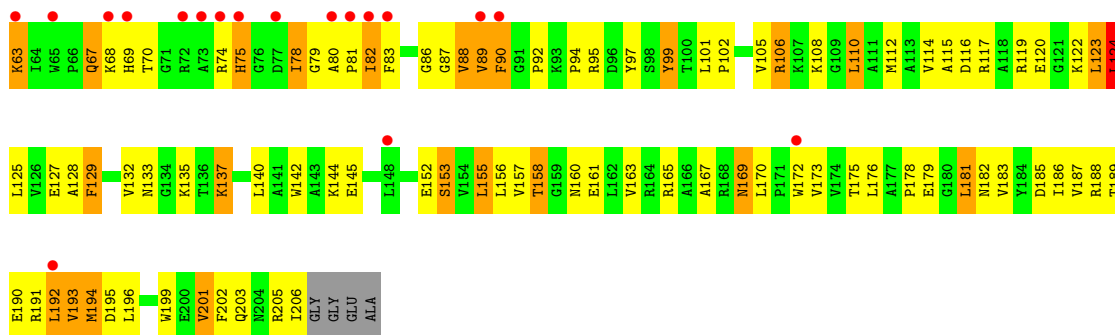


• Molecule 30: 50S ribosomal protein L4

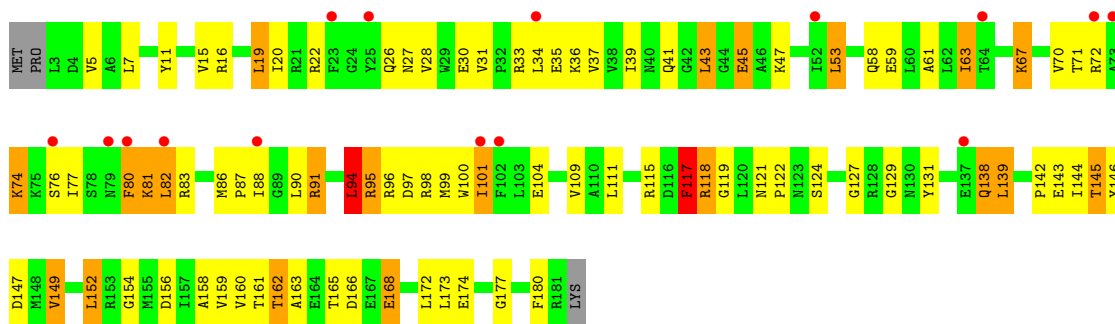


• Molecule 30: 50S ribosomal protein L4

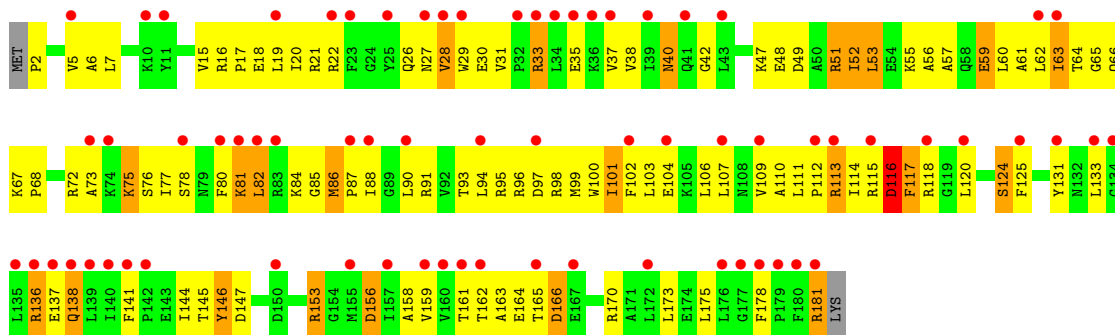




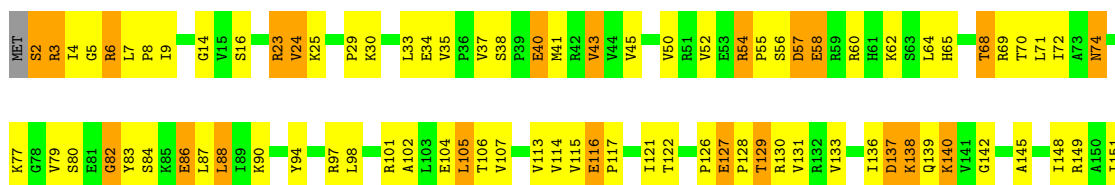
• Molecule 31: 50S ribosomal protein L5



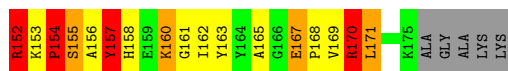
• Molecule 31: 50S ribosomal protein L5



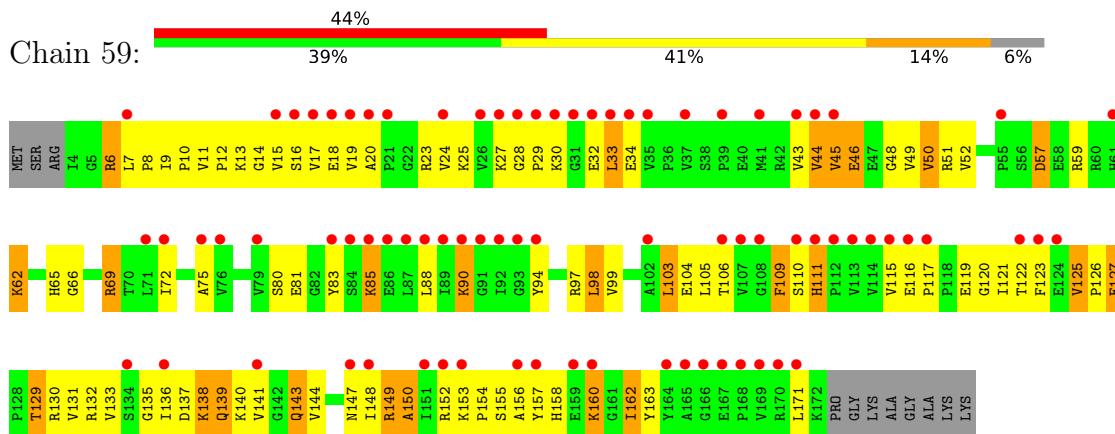
• Molecule 32: 50S ribosomal protein L6



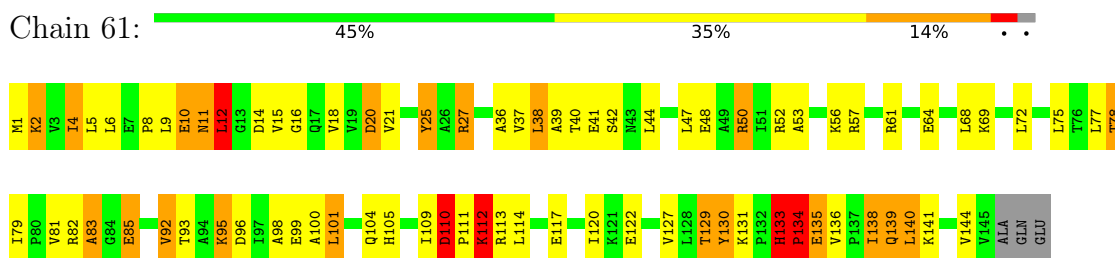




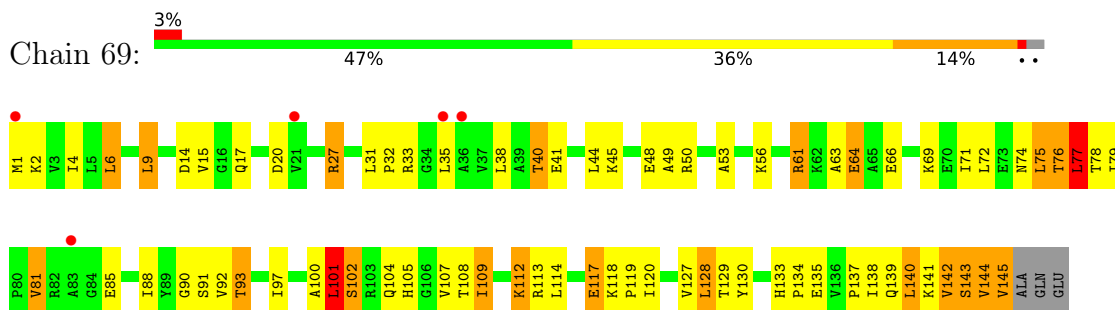
- Molecule 32: 50S ribosomal protein L6



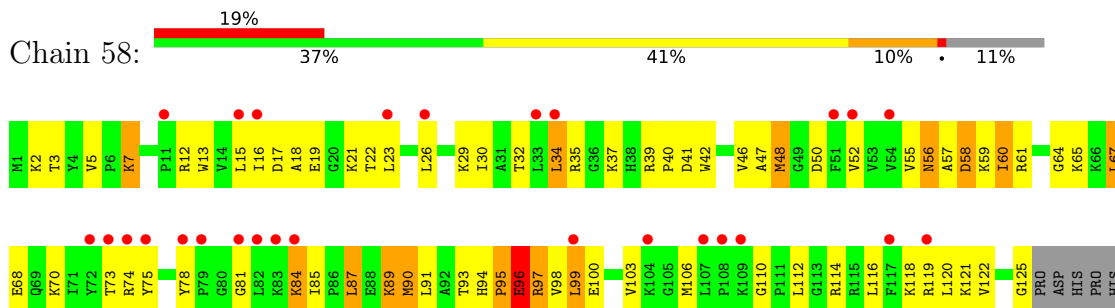
- Molecule 33: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L9

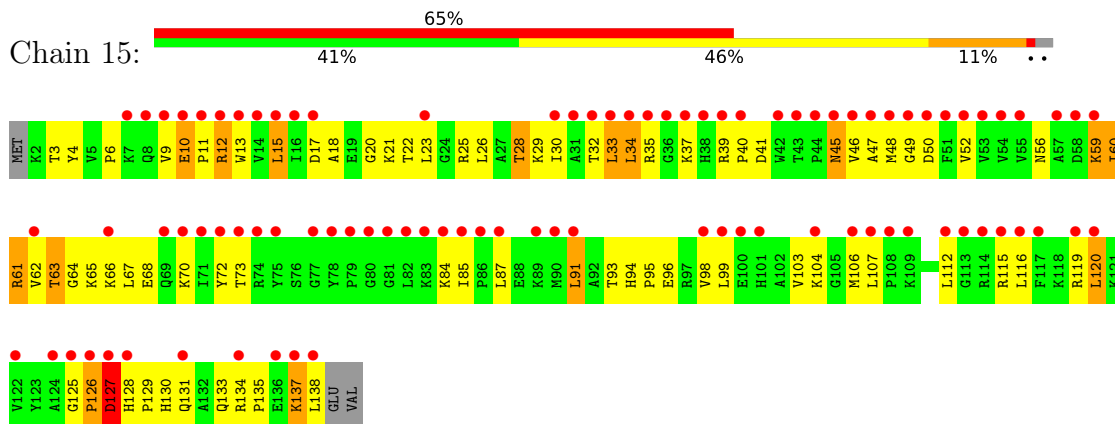


- Molecule 34: 50S ribosomal protein L13

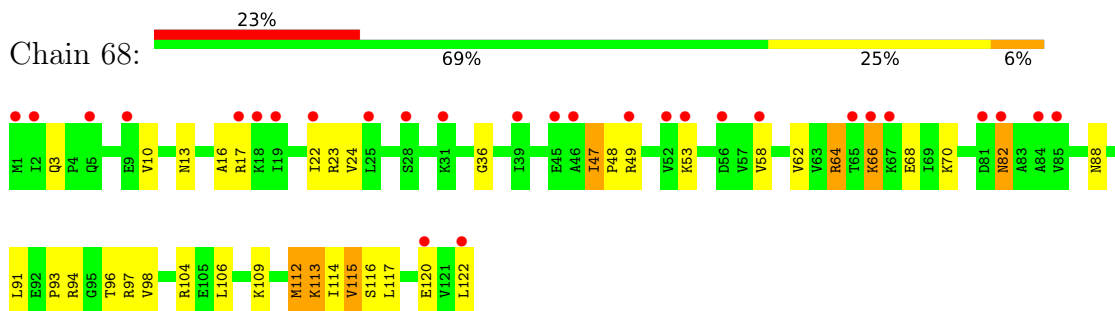


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GLN  
ARG  
PRO  
GLU  
LYS  
LEU  
GLU  
VAL

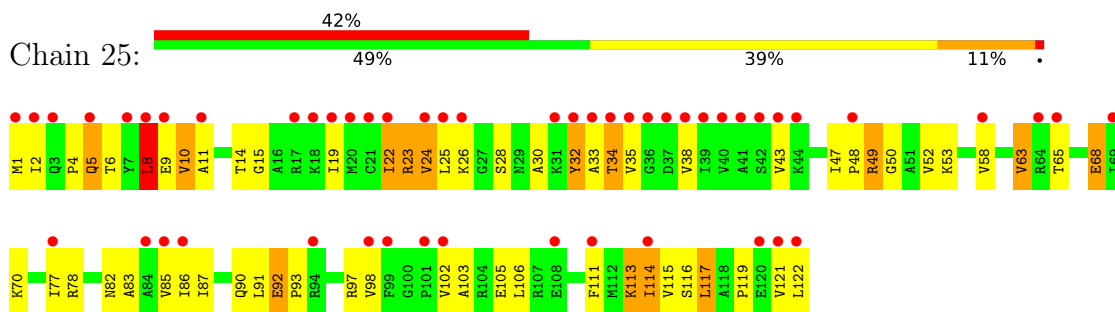
• Molecule 34: 50S ribosomal protein L13



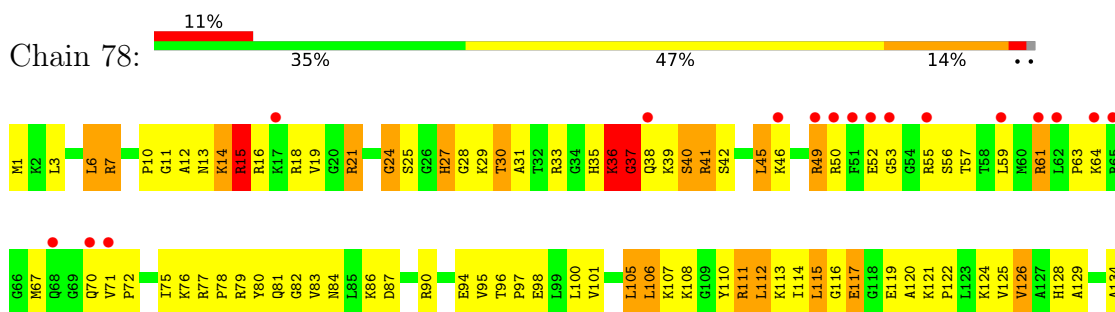
• Molecule 35: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L14

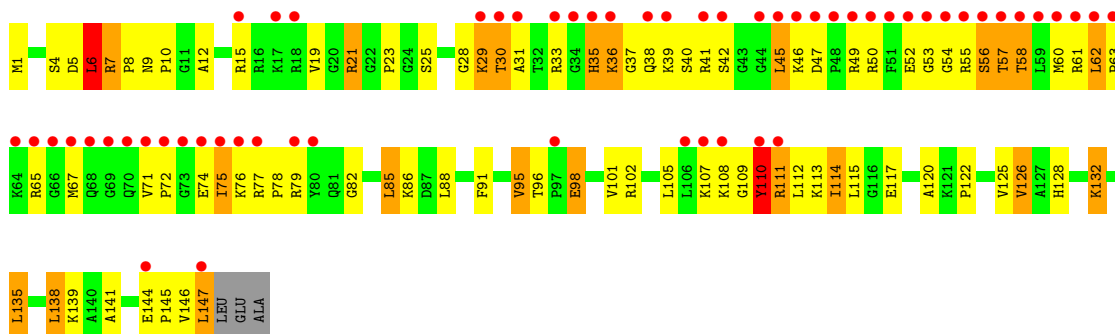


• Molecule 36: 50S ribosomal protein L15





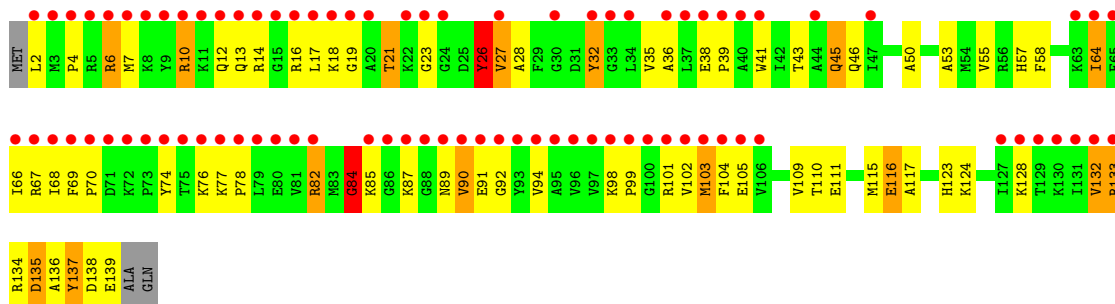
- Molecule 36: 50S ribosomal protein L15



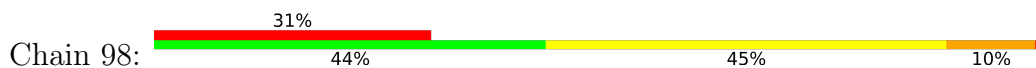
- Molecule 37: 50S ribosomal protein L16

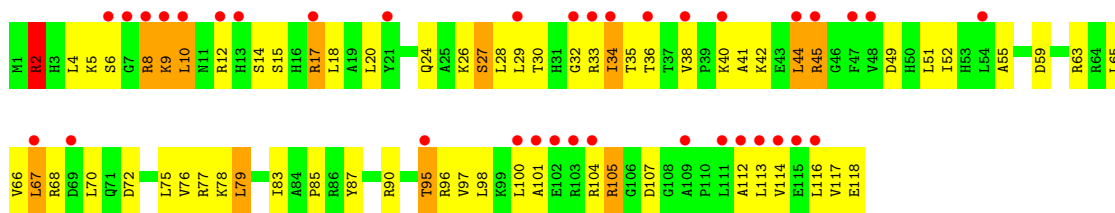


- Molecule 37: 50S ribosomal protein L16

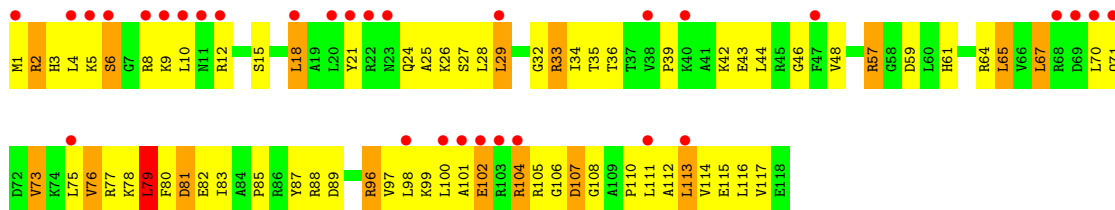


- Molecule 38: 50S ribosomal protein L17

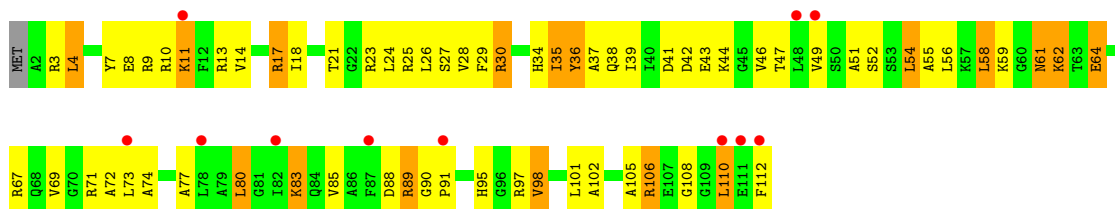




• Molecule 38: 50S ribosomal protein L17



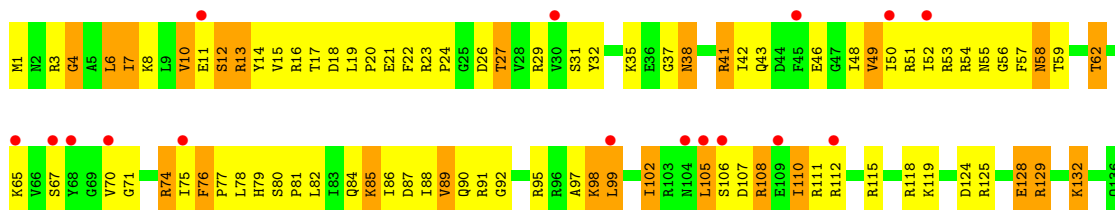
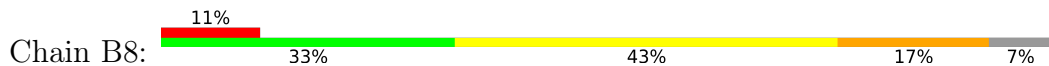
• Molecule 39: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L18

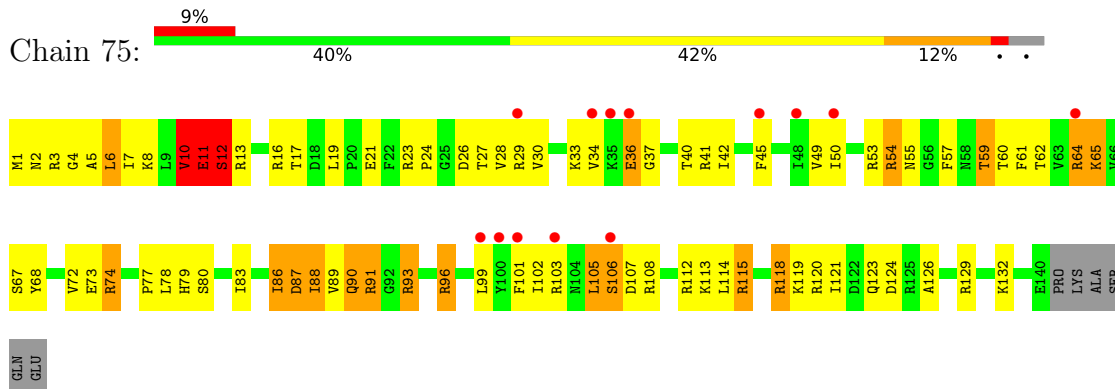


• Molecule 40: 50S ribosomal protein L19

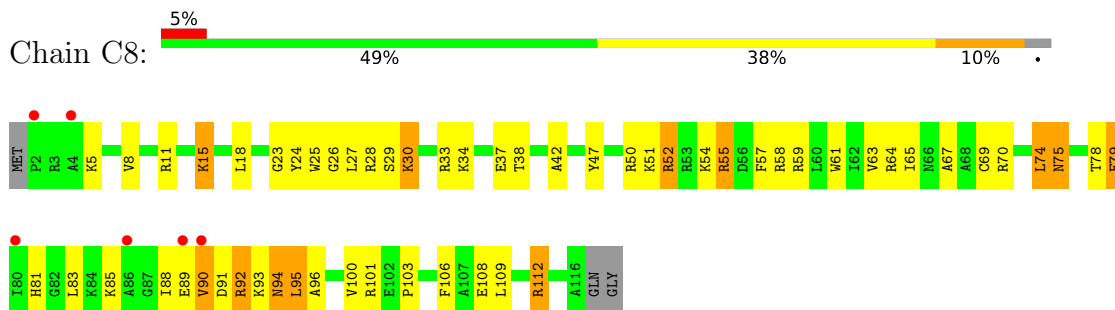


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GLN  
GLU  
PRO  
LYS  
ALA  
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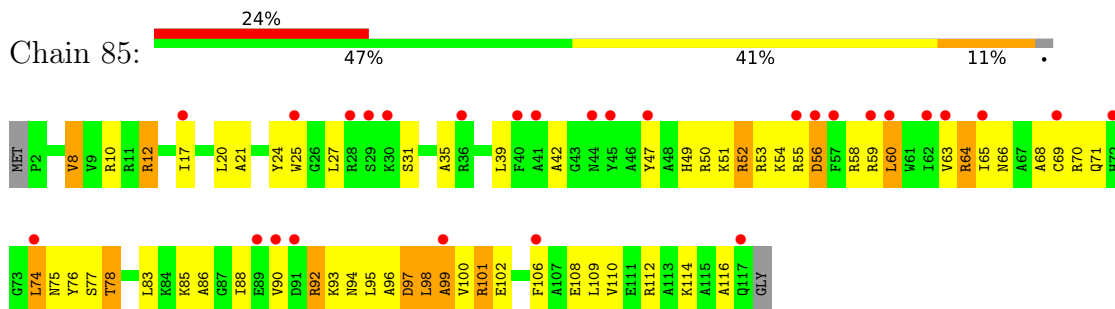
• Molecule 40: 50S ribosomal protein L19



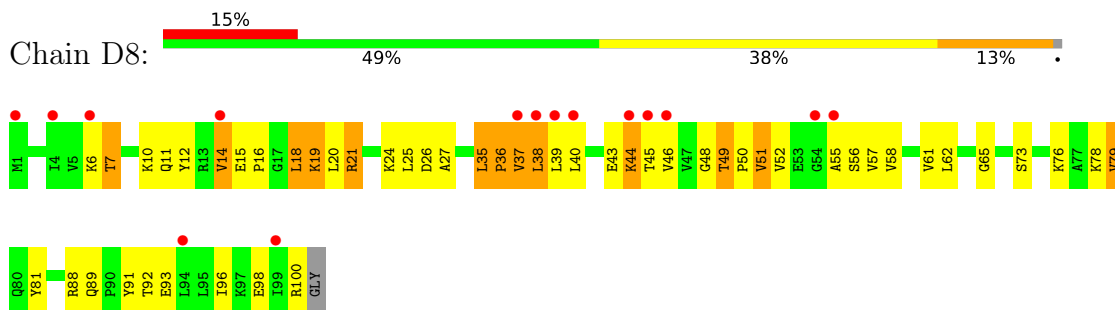
• Molecule 41: 50S ribosomal protein L20



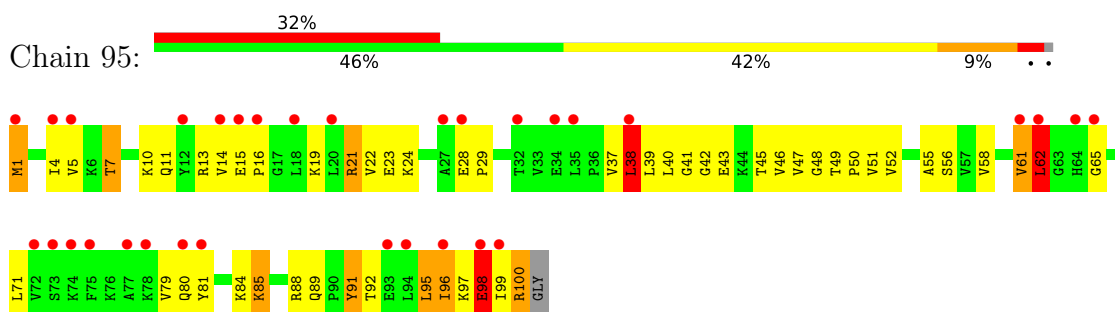
• Molecule 41: 50S ribosomal protein L20



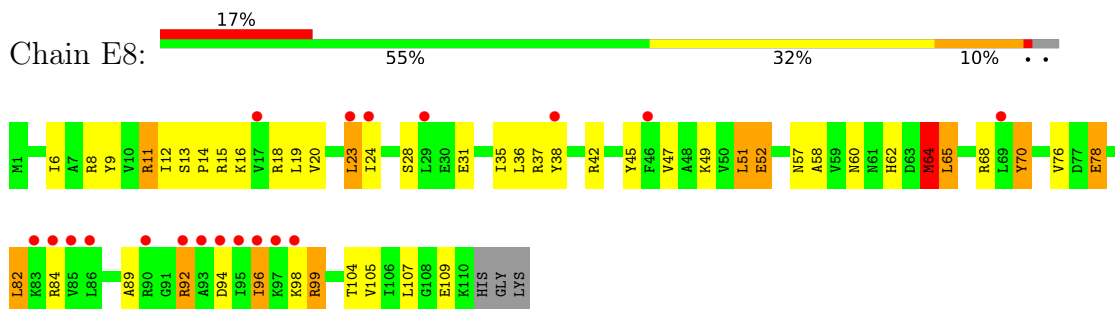
• Molecule 42: 50S ribosomal protein L21



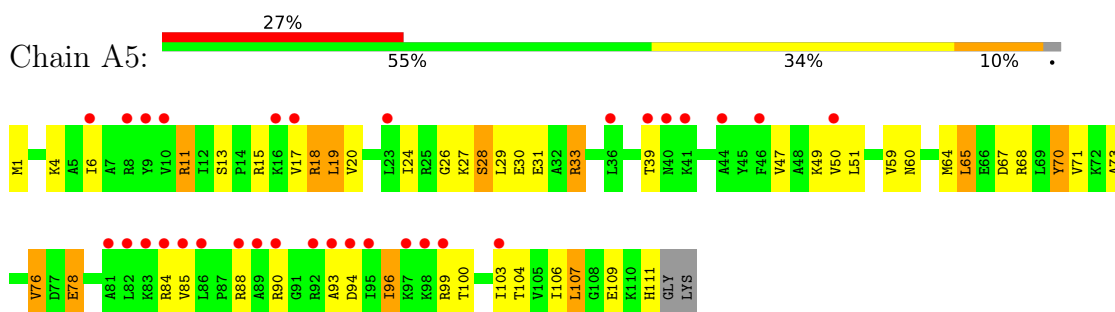
• Molecule 42: 50S ribosomal protein L21



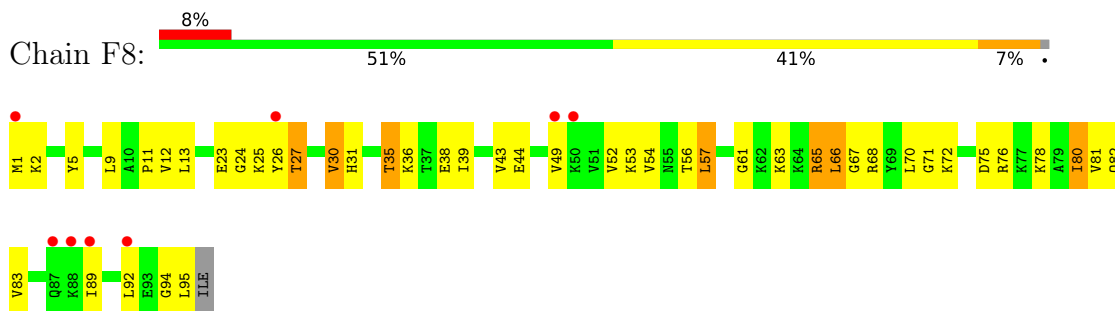
- Molecule 43: 50S ribosomal protein L22



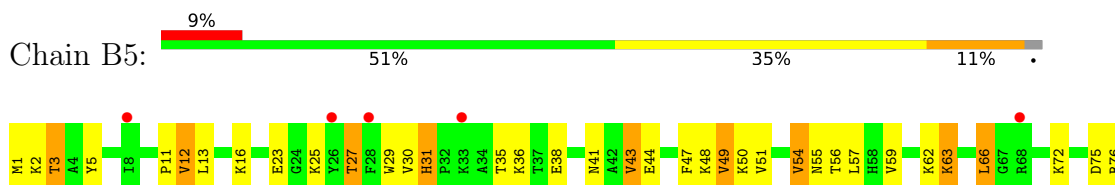
- Molecule 43: 50S ribosomal protein L22

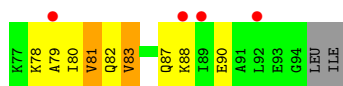


- Molecule 44: 50S ribosomal protein L23

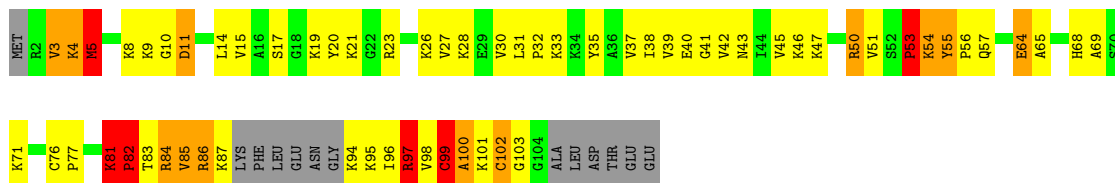
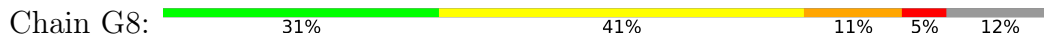


- Molecule 44: 50S ribosomal protein L23

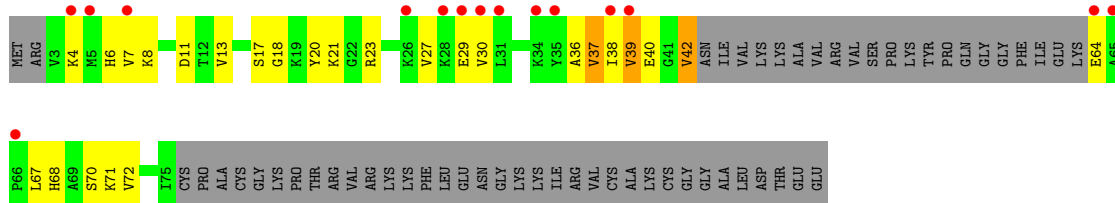




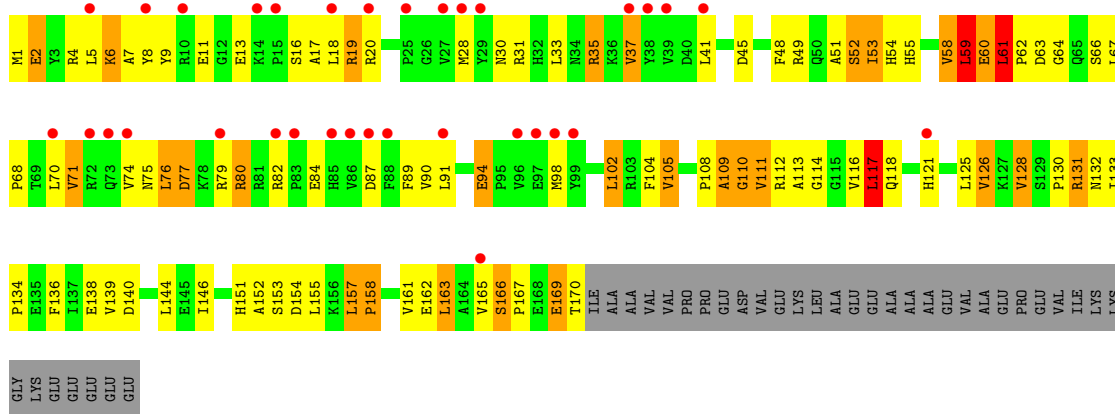
● Molecule 45: 50S ribosomal protein L24



● Molecule 45: 50S ribosomal protein L24

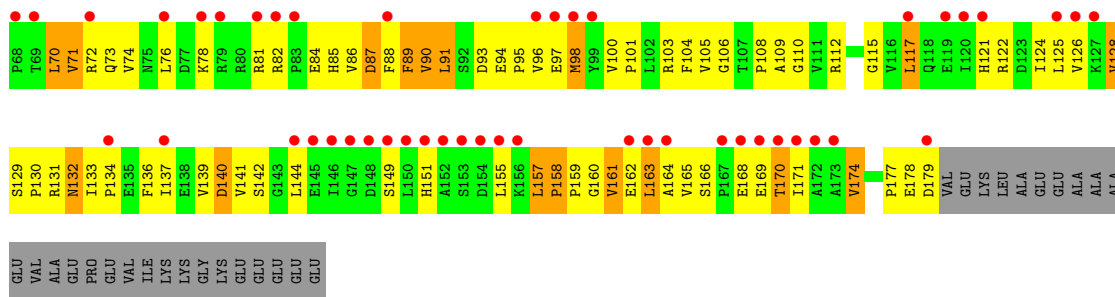


● Molecule 46: 50S ribosomal protein L25

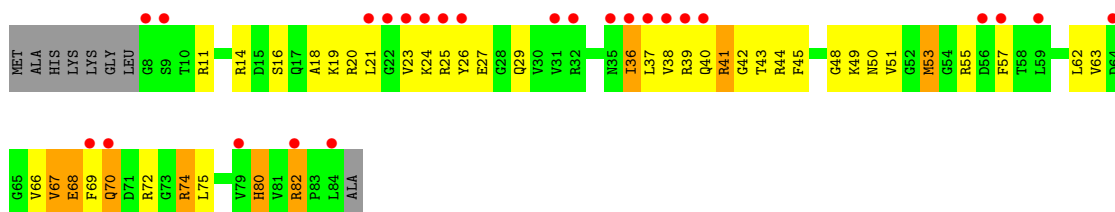


● Molecule 46: 50S ribosomal protein L25

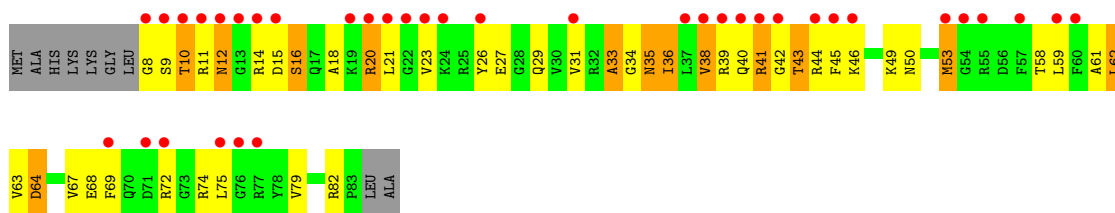




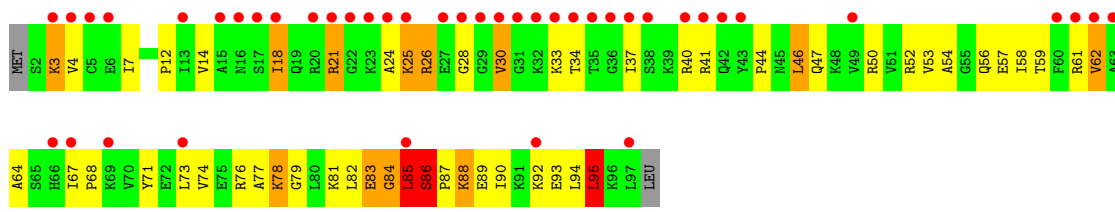
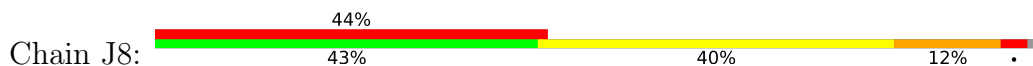
• Molecule 47: 50S ribosomal protein L27



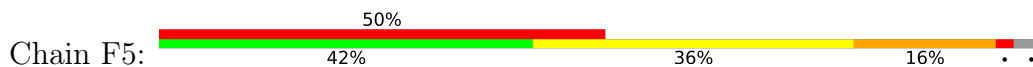
• Molecule 47: 50S ribosomal protein L27



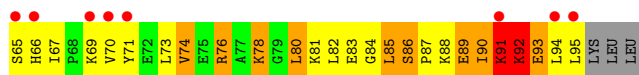
• Molecule 48: 50S ribosomal protein L28



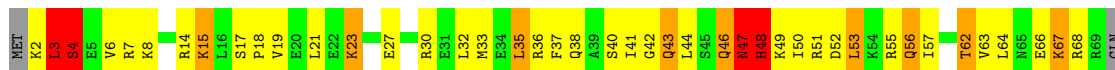
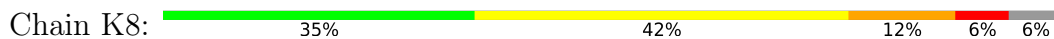
• Molecule 48: 50S ribosomal protein L28







• Molecule 49: 50S ribosomal protein L29



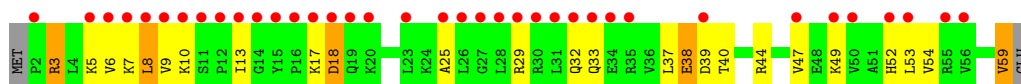
• Molecule 49: 50S ribosomal protein L29



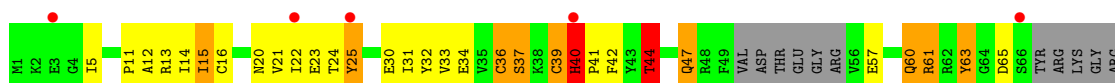
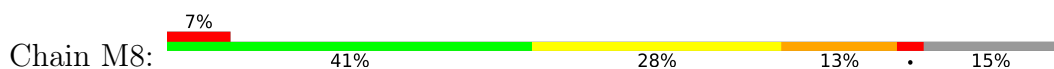
• Molecule 50: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L30



• Molecule 51: 50S ribosomal protein L31

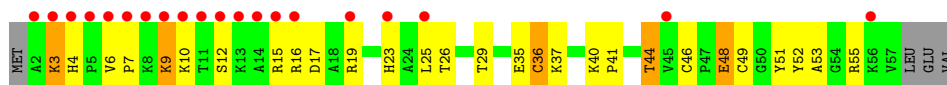


• Molecule 52: 50S ribosomal protein L32

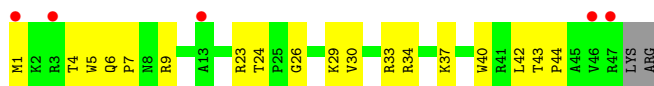




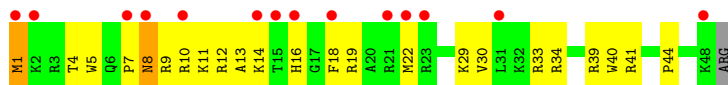
• Molecule 52: 50S ribosomal protein L32



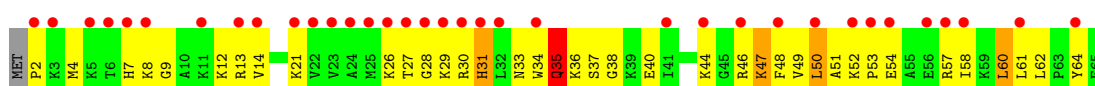
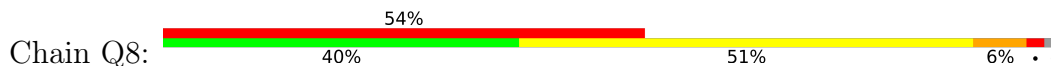
• Molecule 53: 50S ribosomal protein L34



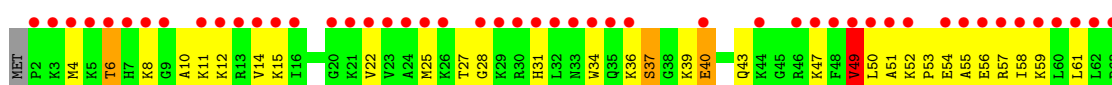
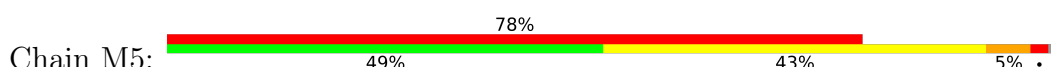
• Molecule 53: 50S ribosomal protein L34



• Molecule 54: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.82Å 449.75Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.88 – 3.36 309.36 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (224.88-3.36) 91.0 (309.36-3.36)	Depositor EDS
$R_{merge}$	0.36	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.88 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.200 , 0.264 0.200 , 0.264	Depositor DCC
$R_{free}$ test set	1998 reflections (0.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.0	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 75.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	292640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: H2U, PSU, AET, ZN, SF4, MG, 5MU

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	0.73	4/36095 (0.0%)	1.32	286/56332 (0.5%)
1	1G	0.74	5/35850 (0.0%)	1.34	316/55949 (0.6%)
2	12	0.37	0/1727	0.60	1/2326 (0.0%)
2	1E	0.38	0/1908	0.58	1/2573 (0.0%)
3	22	0.38	0/1569	0.63	1/2116 (0.0%)
3	2E	0.42	0/1629	0.62	0/2195
4	32	0.41	0/1732	0.64	0/2318
4	3E	0.44	0/1728	0.61	1/2313 (0.0%)
5	42	0.42	0/1156	0.58	0/1557
5	4E	0.43	0/1158	0.64	0/1559
6	52	0.47	0/855	0.60	0/1154
6	5E	0.42	0/850	0.59	0/1147
7	62	0.40	0/1122	0.58	0/1500
7	6E	0.42	0/1259	0.55	0/1686
8	72	0.36	0/1127	0.58	0/1517
8	7E	0.40	0/1135	0.62	0/1527
9	82	0.35	0/971	0.59	0/1304
9	8E	0.41	0/1019	0.63	0/1367
10	1A	0.32	0/814	0.57	0/1095
10	1I	0.38	0/762	0.60	0/1027
11	2A	0.43	0/850	0.58	0/1150
11	2I	0.45	0/838	0.68	0/1133
12	3A	0.46	0/972	0.68	0/1301
12	3I	0.52	0/972	0.73	0/1301
13	4A	0.37	0/889	0.71	1/1192 (0.1%)
13	4I	0.47	0/952	0.70	0/1277
14	5A	0.42	0/495	0.64	0/657
14	5I	0.53	0/500	0.70	1/664 (0.2%)
15	6A	0.41	0/740	0.57	0/987
15	6I	0.41	0/740	0.58	0/987
16	7A	0.41	0/721	0.68	0/970
16	7I	0.43	0/716	0.60	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.49	0/836	0.62	0/1117
17	8I	0.46	0/847	0.63	0/1131
18	9A	0.44	0/559	0.67	1/746 (0.1%)
18	9I	0.43	0/554	0.60	0/739
19	AA	0.41	0/520	0.74	0/700
19	AI	0.44	0/676	0.70	0/910
20	BA	0.37	0/764	0.57	0/1007
20	BI	0.38	0/748	0.62	1/986 (0.1%)
21	1B	0.32	0/192	0.57	0/252
21	1F	0.40	0/203	0.57	0/266
22	1K	0.59	0/1675	1.31	16/2608 (0.6%)
22	1L	0.50	0/1675	1.10	5/2608 (0.2%)
23	2K	0.77	0/1791	1.35	13/2791 (0.5%)
23	2L	0.68	0/1791	1.30	12/2791 (0.4%)
24	3K	0.59	0/1716	1.22	7/2668 (0.3%)
24	3L	0.53	0/1716	1.20	9/2668 (0.3%)
25	4K	0.96	1/440 (0.2%)	1.40	5/684 (0.7%)
25	4L	0.90	0/341	1.59	4/529 (0.8%)
26	14	0.91	46/67828 (0.1%)	1.54	1168/105880 (1.1%)
26	1H	1.07	92/67804 (0.1%)	1.69	1740/105829 (1.6%)
27	16	0.82	1/2928 (0.0%)	1.57	51/4568 (1.1%)
27	1J	0.67	1/2928 (0.0%)	1.34	26/4568 (0.6%)
28	11	0.60	0/2170	0.81	3/2926 (0.1%)
28	19	0.66	3/2175 (0.1%)	0.77	1/2933 (0.0%)
29	21	0.56	0/1589	0.82	0/2145
29	29	0.51	0/1596	0.78	2/2153 (0.1%)
30	31	0.62	0/1620	0.76	1/2194 (0.0%)
30	39	0.50	0/1637	0.71	1/2218 (0.0%)
31	41	0.46	0/1481	0.70	2/1994 (0.1%)
31	49	0.41	0/1483	0.63	1/1997 (0.1%)
32	51	0.48	0/1354	0.84	2/1833 (0.1%)
32	59	0.38	0/1320	0.67	0/1787
33	61	0.43	0/1146	0.77	4/1551 (0.3%)
33	69	0.41	0/1146	0.69	0/1551
34	15	0.43	0/1123	0.64	0/1515
34	58	0.55	0/1017	0.74	0/1369
35	25	0.53	0/942	0.72	1/1269 (0.1%)
35	68	0.56	0/942	0.69	0/1269
36	35	0.54	0/1139	0.81	1/1514 (0.1%)
36	78	0.60	0/1144	0.93	2/1521 (0.1%)
37	45	0.52	0/1120	0.78	0/1498
37	88	0.60	0/1138	0.83	0/1523
38	55	0.45	0/981	0.74	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	98	0.51	0/981	0.74	1/1312 (0.1%)
39	65	0.43	0/886	0.71	2/1180 (0.2%)
39	A8	0.51	0/891	0.73	0/1187
40	75	0.60	1/1178 (0.1%)	0.71	1/1573 (0.1%)
40	B8	0.51	0/1142	0.74	1/1526 (0.1%)
41	85	0.50	0/977	0.69	0/1301
41	C8	0.59	0/968	0.74	1/1289 (0.1%)
42	95	0.46	0/781	0.80	2/1048 (0.2%)
42	D8	0.56	0/785	0.81	2/1052 (0.2%)
43	A5	0.51	0/897	0.69	0/1204
43	E8	0.61	0/886	0.75	1/1189 (0.1%)
44	B5	0.54	0/749	0.70	0/1007
44	F8	0.64	0/764	0.76	0/1025
45	C5	0.60	0/401	0.74	0/535
45	G8	0.65	0/745	0.89	2/993 (0.2%)
46	D5	0.40	0/1443	0.69	2/1960 (0.1%)
46	H8	0.44	0/1395	0.76	1/1890 (0.1%)
47	E5	0.50	0/611	0.77	0/814
47	I8	0.70	1/619 (0.2%)	0.81	0/825
48	F5	0.56	0/744	0.81	0/989
48	J8	0.62	0/754	0.91	2/1003 (0.2%)
49	G5	0.52	0/578	0.73	1/766 (0.1%)
49	K8	0.64	0/577	0.89	2/763 (0.3%)
50	H5	0.45	0/464	0.62	0/623
50	L8	0.51	0/464	0.77	0/623
51	M8	0.53	0/485	0.78	0/652
52	J5	0.52	0/448	0.71	0/606
52	N8	0.59	0/381	0.71	0/516
53	L5	0.56	0/414	0.75	0/547
53	P8	0.70	0/409	0.84	1/540 (0.2%)
54	M5	0.64	1/524 (0.2%)	0.83	0/691
54	Q8	0.61	0/524	0.84	1/691 (0.1%)
All	All	0.80	156/314511 (0.0%)	1.35	3711/471182 (0.8%)

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
2	1E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	2E	0	1
4	32	0	1
4	3E	0	2
5	4E	0	1
9	82	0	1
9	8E	0	3
10	1A	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	2
12	3A	0	4
12	3I	0	2
13	4A	0	6
13	4I	0	3
14	5A	0	1
18	9A	0	1
19	AA	0	4
19	AI	0	1
20	BA	0	1
20	BI	0	1
28	11	0	4
28	19	0	2
29	21	0	7
29	29	0	10
30	31	0	1
30	39	0	4
31	41	0	1
31	49	0	1
32	51	0	5
32	59	0	1
33	61	0	5
33	69	0	5
34	15	0	1
34	58	0	2
35	68	0	1
36	35	0	3
36	78	0	9
37	45	0	5
37	88	0	3
38	98	0	2
39	65	0	1
39	A8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	4
42	95	0	4
42	D8	0	2
43	E8	0	1
44	B5	0	1
45	C5	0	2
45	G8	0	7
46	D5	0	5
46	H8	0	7
47	I8	0	1
48	F5	0	3
48	J8	0	2
49	G5	0	4
49	K8	0	4
51	M8	0	4
52	N8	0	1
54	M5	0	2
54	Q8	0	2
All	All	0	180

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	75	106	SER	CA-CB	11.86	1.70	1.52
26	14	2593	U	C4-O4	11.75	1.33	1.23
26	1H	676	A	N9-C4	-10.05	1.31	1.37
26	1H	774	A	N9-C4	-10.02	1.31	1.37
26	1H	783	A	N7-C5	-8.90	1.33	1.39

The worst 5 of 3711 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-20.44	113.73	126.00
26	1H	1962	C	N1-C2-O2	17.31	129.29	118.90
26	1H	774	A	C2-N3-C4	-16.57	102.32	110.60
26	1H	34	C	O5'-P-OP1	-15.77	91.51	105.70
26	1H	1899	G	N9-C4-C5	15.75	111.70	105.40

There are no chirality outliers.



5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	210	SER	Peptide
3	2E	14	ILE	Peptide
4	3E	155	LEU	Peptide
4	3E	29	PRO	Peptide
5	4E	114	GLY	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	32246	0	16277	909	0
1	1G	32028	0	16164	936	0
2	12	1696	0	1730	80	0
2	1E	1874	0	1926	92	0
3	22	1546	0	1608	104	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1765	95	0
4	3E	1698	0	1761	78	0
5	42	1141	0	1198	66	0
5	4E	1142	0	1204	43	0
6	52	842	0	857	23	0
6	5E	837	0	852	33	0
7	62	1110	0	1163	67	0
7	6E	1242	0	1286	65	0
8	72	1107	0	1165	69	0
8	7E	1115	0	1177	53	0
9	82	953	0	983	59	0
9	8E	1000	0	1031	73	0
10	1A	801	0	849	52	0
10	1I	749	0	767	54	0
11	2A	835	0	847	33	0
11	2I	823	0	833	42	0
12	3A	956	0	1046	48	0
12	3I	956	0	1046	47	0
13	4A	879	0	935	81	0
13	4I	942	0	997	60	0
14	5A	486	0	525	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	5I	491	0	530	28	0
15	6A	729	0	768	35	0
15	6I	729	0	768	41	0
16	7A	705	0	725	34	0
16	7I	700	0	720	43	0
17	8A	823	0	891	37	0
17	8I	834	0	904	53	0
18	9A	554	0	609	22	0
18	9I	549	0	607	28	0
19	AA	510	0	507	36	0
19	AI	661	0	683	42	0
20	BA	762	0	861	34	0
20	BI	746	0	843	56	0
21	1B	188	0	195	9	0
21	1F	199	0	208	10	0
22	1K	1593	0	813	52	0
22	1L	1593	0	813	28	0
23	2K	1644	0	838	34	0
23	2L	1644	0	838	32	0
24	3K	1537	0	779	55	0
24	3L	1537	0	779	32	0
25	4K	391	0	196	12	0
25	4L	303	0	153	10	0
26	14	60561	0	30528	1446	0
26	1H	60546	0	30528	1548	0
27	16	2617	0	1328	57	0
27	1J	2617	0	1328	89	0
28	11	2120	0	2197	108	0
28	19	2125	0	2199	115	0
29	21	1556	0	1612	90	0
29	29	1563	0	1629	94	0
30	31	1585	0	1632	88	0
30	39	1602	0	1649	119	0
31	41	1457	0	1514	76	0
31	49	1459	0	1507	91	0
32	51	1328	0	1396	69	0
32	59	1295	0	1366	85	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	56	0
34	15	1096	0	1168	69	0
34	58	995	0	1077	61	0
35	25	932	0	996	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	68	932	0	996	21	0
36	35	1122	0	1206	84	0
36	78	1127	0	1208	87	0
37	45	1099	0	1154	77	0
37	88	1117	0	1168	79	0
38	55	967	0	1033	56	0
38	98	967	0	1033	42	0
39	65	876	0	938	74	0
39	A8	881	0	943	53	0
40	75	1164	0	1221	69	0
40	B8	1128	0	1183	78	0
41	85	959	0	1019	61	0
41	C8	950	0	1011	58	0
42	95	770	0	838	43	0
42	D8	774	0	849	32	0
43	A5	886	0	948	33	0
43	E8	876	0	941	35	0
44	B5	735	0	785	33	0
44	F8	750	0	814	30	0
45	C5	396	0	444	15	0
45	G8	734	0	820	48	0
46	D5	1411	0	1436	92	0
46	H8	1365	0	1391	77	0
47	E5	603	0	620	45	0
47	I8	611	0	631	43	0
48	F5	737	0	813	53	0
48	J8	747	0	817	45	0
49	G5	576	0	625	28	0
49	K8	575	0	634	37	0
50	H5	459	0	512	15	0
50	L8	459	0	512	21	0
51	M8	475	0	465	27	0
52	J5	434	0	454	22	0
52	N8	369	0	388	36	0
53	L5	406	0	438	28	0
53	P8	401	0	436	10	0
54	M5	516	0	582	26	0
54	Q8	516	0	582	38	0
55	11	1	0	0	0	0
55	13	140	0	0	0	0
55	14	300	0	0	0	0
55	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1F	2	0	0	0	0
55	1G	126	0	0	0	0
55	1H	473	0	0	0	0
55	1J	2	0	0	0	0
55	2I	3	0	0	0	0
55	29	1	0	0	0	0
55	2A	1	0	0	0	0
55	2K	1	0	0	0	0
55	2L	1	0	0	0	0
55	32	1	0	0	0	0
55	35	1	0	0	0	0
55	39	1	0	0	0	0
55	41	1	0	0	0	0
55	42	2	0	0	0	0
55	45	2	0	0	0	0
55	4A	1	0	0	0	0
55	5I	2	0	0	0	0
55	78	2	0	0	0	0
55	7A	1	0	0	0	0
55	85	1	0	0	0	0
55	88	3	0	0	0	0
55	8I	1	0	0	0	0
55	BA	1	0	0	0	0
55	BI	1	0	0	0	0
55	C8	2	0	0	0	0
55	D8	1	0	0	0	0
55	E5	1	0	0	0	0
55	F5	1	0	0	0	0
55	I8	1	0	0	0	0
55	J8	1	0	0	0	0
55	P8	1	0	0	0	0
56	32	8	0	0	2	0
56	3E	8	0	0	1	0
57	5A	1	0	0	0	0
57	5I	1	0	0	0	0
58	11	8	0	0	1	0
58	13	274	0	0	53	0
58	14	586	0	0	117	0
58	16	8	0	0	0	0
58	19	7	0	0	2	0
58	1F	1	0	0	0	0
58	1G	240	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1H	1010	0	0	224	0
58	1I	2	0	0	0	0
58	1K	1	0	0	0	0
58	2I	4	0	0	0	0
58	29	2	0	0	0	0
58	2L	6	0	0	0	0
58	3I	5	0	0	0	0
58	32	1	0	0	0	0
58	35	5	0	0	0	0
58	39	6	0	0	0	0
58	3I	1	0	0	0	0
58	42	1	0	0	0	0
58	45	5	0	0	0	0
58	4E	6	0	0	0	0
58	4I	2	0	0	0	0
58	4L	1	0	0	0	0
58	58	1	0	0	0	0
58	5I	1	0	0	0	0
58	78	8	0	0	0	0
58	7A	4	0	0	0	0
58	7I	3	0	0	0	0
58	8E	1	0	0	0	0
58	98	1	0	0	0	0
58	B5	2	0	0	0	0
58	BA	2	0	0	0	0
58	D8	1	0	0	0	0
58	E8	1	0	0	0	0
58	G8	1	0	0	0	0
58	H5	2	0	0	1	0
58	I8	3	0	0	1	0
58	J8	2	0	0	0	0
58	L5	1	0	0	0	0
58	L8	3	0	0	1	0
58	Q8	2	0	0	1	0
All	All	292640	0	194666	9118	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 20.

The worst 5 of 9118 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)
26:1H:2714:G:OP2	58:1H:3519:HOH:O	1.69	1.07
26:1H:452:G:OP2	58:1H:3521:HOH:O	1.74	1.05
26:1H:1665:A:OP2	58:1H:3520:HOH:O	1.72	1.05
26:14:2499:C:OP2	58:14:3407:HOH:O	1.75	1.04
26:1H:990:A:OP2	58:1H:3522:HOH:O	1.76	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	156 (77%)	46 (23%)	1 (0%)	29	63
2	1E	227/256 (89%)	184 (81%)	42 (18%)	1 (0%)	34	68
3	22	193/239 (81%)	165 (86%)	27 (14%)	1 (0%)	29	63
3	2E	203/239 (85%)	165 (81%)	36 (18%)	2 (1%)	15	49
4	32	206/209 (99%)	166 (81%)	39 (19%)	1 (0%)	29	63
4	3E	205/209 (98%)	178 (87%)	26 (13%)	1 (0%)	29	63
5	42	148/162 (91%)	137 (93%)	11 (7%)	0	100	100
5	4E	147/162 (91%)	137 (93%)	10 (7%)	0	100	100
6	52	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
6	5E	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
7	62	134/156 (86%)	123 (92%)	11 (8%)	0	100	100
7	6E	152/156 (97%)	135 (89%)	17 (11%)	0	100	100
8	72	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	22	56
8	7E	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	10	39
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	9	36
9	8E	124/128 (97%)	103 (83%)	21 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1A	97/105 (92%)	81 (84%)	16 (16%)	0	100	100
10	1I	92/105 (88%)	80 (87%)	10 (11%)	2 (2%)	6	32
11	2A	111/129 (86%)	96 (86%)	13 (12%)	2 (2%)	8	35
11	2I	109/129 (84%)	91 (84%)	17 (16%)	1 (1%)	17	51
12	3A	120/132 (91%)	94 (78%)	24 (20%)	2 (2%)	9	36
12	3I	120/132 (91%)	96 (80%)	23 (19%)	1 (1%)	19	53
13	4A	107/126 (85%)	79 (74%)	27 (25%)	1 (1%)	17	51
13	4I	117/126 (93%)	90 (77%)	25 (21%)	2 (2%)	9	36
14	5A	57/61 (93%)	44 (77%)	12 (21%)	1 (2%)	8	35
14	5I	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	23
15	6A	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
15	6I	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
16	7I	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	8A	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
17	8I	98/105 (93%)	81 (83%)	17 (17%)	0	100	100
18	9A	67/88 (76%)	60 (90%)	7 (10%)	0	100	100
18	9I	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
19	AA	59/93 (63%)	46 (78%)	13 (22%)	0	100	100
19	AI	80/93 (86%)	67 (84%)	12 (15%)	1 (1%)	12	42
20	BA	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
20	BI	95/106 (90%)	72 (76%)	21 (22%)	2 (2%)	7	32
21	1B	20/27 (74%)	19 (95%)	0	1 (5%)	2	15
21	1F	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	16
28	11	271/276 (98%)	231 (85%)	35 (13%)	5 (2%)	8	35
28	19	272/276 (99%)	233 (86%)	39 (14%)	0	100	100
29	21	203/206 (98%)	157 (77%)	42 (21%)	4 (2%)	7	33
29	29	202/206 (98%)	145 (72%)	52 (26%)	5 (2%)	5	29
30	31	200/210 (95%)	172 (86%)	25 (12%)	3 (2%)	10	39
30	39	202/210 (96%)	155 (77%)	42 (21%)	5 (2%)	5	29
31	41	177/182 (97%)	152 (86%)	24 (14%)	1 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	49	178/182 (98%)	151 (85%)	24 (14%)	3 (2%)	9	36
32	51	172/180 (96%)	132 (77%)	30 (17%)	10 (6%)	1	12
32	59	167/180 (93%)	129 (77%)	38 (23%)	0	100	100
33	61	143/148 (97%)	110 (77%)	30 (21%)	3 (2%)	7	32
33	69	143/148 (97%)	109 (76%)	30 (21%)	4 (3%)	5	26
34	15	135/140 (96%)	115 (85%)	19 (14%)	1 (1%)	22	56
34	58	123/140 (88%)	101 (82%)	20 (16%)	2 (2%)	9	38
35	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
35	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	35	145/150 (97%)	117 (81%)	25 (17%)	3 (2%)	7	32
36	78	146/150 (97%)	104 (71%)	35 (24%)	7 (5%)	2	16
37	45	136/141 (96%)	104 (76%)	29 (21%)	3 (2%)	6	32
37	88	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	6	32
38	55	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	51
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
39	65	108/112 (96%)	83 (77%)	24 (22%)	1 (1%)	17	51
39	A8	109/112 (97%)	84 (77%)	24 (22%)	1 (1%)	17	51
40	75	138/146 (94%)	118 (86%)	18 (13%)	2 (1%)	11	40
40	B8	134/146 (92%)	104 (78%)	30 (22%)	0	100	100
41	85	114/118 (97%)	92 (81%)	22 (19%)	0	100	100
41	C8	113/118 (96%)	100 (88%)	11 (10%)	2 (2%)	8	35
42	95	98/101 (97%)	78 (80%)	16 (16%)	4 (4%)	3	19
42	D8	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
43	A5	109/113 (96%)	96 (88%)	13 (12%)	0	100	100
43	E8	108/113 (96%)	97 (90%)	11 (10%)	0	100	100
44	B5	92/96 (96%)	79 (86%)	13 (14%)	0	100	100
44	F8	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
45	C5	48/110 (44%)	36 (75%)	12 (25%)	0	100	100
45	G8	93/110 (84%)	67 (72%)	19 (20%)	7 (8%)	1	7
46	D5	175/206 (85%)	122 (70%)	48 (27%)	5 (3%)	4	26
46	H8	168/206 (82%)	123 (73%)	38 (23%)	7 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	E5	74/85 (87%)	58 (78%)	15 (20%)	1 (1%)	11	40
47	I8	75/85 (88%)	63 (84%)	12 (16%)	0	100	100
48	F5	92/98 (94%)	77 (84%)	12 (13%)	3 (3%)	4	24
48	J8	94/98 (96%)	76 (81%)	13 (14%)	5 (5%)	2	14
49	G5	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10	39
49	K8	66/72 (92%)	56 (85%)	7 (11%)	3 (4%)	2	17
50	H5	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
50	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
51	M8	56/71 (79%)	36 (64%)	18 (32%)	2 (4%)	3	22
52	J5	54/60 (90%)	46 (85%)	8 (15%)	0	100	100
52	N8	46/60 (77%)	41 (89%)	5 (11%)	0	100	100
53	L5	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	P8	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
54	M5	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
54	Q8	62/65 (95%)	45 (73%)	14 (23%)	3 (5%)	2	16
All	All	10925/11875 (92%)	9065 (83%)	1719 (16%)	141 (1%)	12	42

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	51	157	TYR
33	61	134	PRO
34	58	96	GLU
36	78	36	LYS
36	78	37	GLY

### 5.3.2 Protein sidechains [i](#)

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%)	139 (78%)	40 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	200/220 (91%)	151 (76%)	49 (24%)	0	2
3	22	154/188 (82%)	115 (75%)	39 (25%)	0	2
3	2E	159/188 (85%)	132 (83%)	27 (17%)	2	9
4	32	180/181 (99%)	147 (82%)	33 (18%)	1	6
4	3E	180/181 (99%)	135 (75%)	45 (25%)	0	2
5	42	114/123 (93%)	78 (68%)	36 (32%)	0	1
5	4E	115/123 (94%)	87 (76%)	28 (24%)	0	2
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	4
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	11
7	62	114/127 (90%)	95 (83%)	19 (17%)	2	9
7	6E	125/127 (98%)	100 (80%)	25 (20%)	1	4
8	72	118/119 (99%)	93 (79%)	25 (21%)	1	3
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	3
9	82	92/99 (93%)	67 (73%)	25 (27%)	0	1
9	8E	97/99 (98%)	74 (76%)	23 (24%)	1	2
10	1A	89/92 (97%)	66 (74%)	23 (26%)	0	2
10	1I	81/92 (88%)	64 (79%)	17 (21%)	1	4
11	2A	85/99 (86%)	76 (89%)	9 (11%)	6	26
11	2I	84/99 (85%)	71 (84%)	13 (16%)	2	12
12	3A	103/109 (94%)	72 (70%)	31 (30%)	0	1
12	3I	103/109 (94%)	76 (74%)	27 (26%)	0	2
13	4A	90/101 (89%)	64 (71%)	26 (29%)	0	1
13	4I	94/101 (93%)	70 (74%)	24 (26%)	0	2
14	5A	49/50 (98%)	38 (78%)	11 (22%)	1	3
14	5I	49/50 (98%)	41 (84%)	8 (16%)	2	10
15	6A	79/80 (99%)	72 (91%)	7 (9%)	9	34
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	7
16	7A	72/74 (97%)	61 (85%)	11 (15%)	2	12
16	7I	72/74 (97%)	54 (75%)	18 (25%)	0	2
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	18
17	8I	95/97 (98%)	73 (77%)	22 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	49 (84%)	9 (16%)	2	12
18	9I	58/77 (75%)	51 (88%)	7 (12%)	5	20
19	AA	56/80 (70%)	42 (75%)	14 (25%)	0	2
19	AI	72/80 (90%)	51 (71%)	21 (29%)	0	1
20	BA	76/82 (93%)	69 (91%)	7 (9%)	9	32
20	BI	75/82 (92%)	60 (80%)	15 (20%)	1	4
21	1B	17/22 (77%)	14 (82%)	3 (18%)	2	7
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	9
28	11	214/218 (98%)	161 (75%)	53 (25%)	0	2
28	19	214/218 (98%)	164 (77%)	50 (23%)	1	2
29	21	162/166 (98%)	127 (78%)	35 (22%)	1	3
29	29	165/166 (99%)	134 (81%)	31 (19%)	1	6
30	31	161/166 (97%)	125 (78%)	36 (22%)	1	3
30	39	163/166 (98%)	120 (74%)	43 (26%)	0	1
31	41	153/156 (98%)	117 (76%)	36 (24%)	1	2
31	49	152/156 (97%)	114 (75%)	38 (25%)	0	2
32	51	143/148 (97%)	108 (76%)	35 (24%)	0	2
32	59	140/148 (95%)	98 (70%)	42 (30%)	0	1
33	61	122/124 (98%)	84 (69%)	38 (31%)	0	1
33	69	122/124 (98%)	96 (79%)	26 (21%)	1	3
34	15	116/119 (98%)	89 (77%)	27 (23%)	1	2
34	58	105/119 (88%)	80 (76%)	25 (24%)	0	2
35	25	100/100 (100%)	80 (80%)	20 (20%)	1	4
35	68	100/100 (100%)	82 (82%)	18 (18%)	1	7
36	35	114/116 (98%)	80 (70%)	34 (30%)	0	1
36	78	114/116 (98%)	85 (75%)	29 (25%)	0	2
37	45	109/111 (98%)	85 (78%)	24 (22%)	1	3
37	88	110/111 (99%)	91 (83%)	19 (17%)	2	8
38	55	101/101 (100%)	74 (73%)	27 (27%)	0	1
38	98	101/101 (100%)	79 (78%)	22 (22%)	1	3
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	A8	87/88 (99%)	64 (74%)	23 (26%)	0	1
40	75	122/127 (96%)	89 (73%)	33 (27%)	0	1
40	B8	118/127 (93%)	88 (75%)	30 (25%)	0	2
41	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
41	C8	92/94 (98%)	77 (84%)	15 (16%)	2	10
42	95	81/82 (99%)	64 (79%)	17 (21%)	1	4
42	D8	82/82 (100%)	54 (66%)	28 (34%)	0	1
43	A5	91/92 (99%)	72 (79%)	19 (21%)	1	4
43	E8	90/92 (98%)	74 (82%)	16 (18%)	2	7
44	B5	74/78 (95%)	57 (77%)	17 (23%)	1	2
44	F8	77/78 (99%)	61 (79%)	16 (21%)	1	4
45	C5	43/91 (47%)	32 (74%)	11 (26%)	0	2
45	G8	79/91 (87%)	60 (76%)	19 (24%)	0	2
46	D5	156/179 (87%)	115 (74%)	41 (26%)	0	2
46	H8	151/179 (84%)	117 (78%)	34 (22%)	1	3
47	E5	61/67 (91%)	45 (74%)	16 (26%)	0	2
47	I8	62/67 (92%)	54 (87%)	8 (13%)	4	17
48	F5	79/83 (95%)	59 (75%)	20 (25%)	0	2
48	J8	79/83 (95%)	60 (76%)	19 (24%)	0	2
49	G5	63/67 (94%)	44 (70%)	19 (30%)	0	1
49	K8	64/67 (96%)	44 (69%)	20 (31%)	0	1
50	H5	50/52 (96%)	38 (76%)	12 (24%)	0	2
50	L8	50/52 (96%)	35 (70%)	15 (30%)	0	1
51	M8	52/63 (82%)	40 (77%)	12 (23%)	1	2
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	2
52	N8	43/52 (83%)	37 (86%)	6 (14%)	3	15
53	L5	38/42 (90%)	34 (90%)	4 (10%)	7	26
53	P8	38/42 (90%)	33 (87%)	5 (13%)	4	17
54	M5	54/55 (98%)	45 (83%)	9 (17%)	2	9
54	Q8	54/55 (98%)	45 (83%)	9 (17%)	2	9
All	All	9213/9831 (94%)	7134 (77%)	2079 (23%)	1	3

5 of 2079 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	75	64	ARG
43	A5	51	LEU
40	75	61	PHE
39	A8	30	ARG
38	98	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	32	161	ASN
40	75	79	HIS
13	4A	101	GLN
49	G5	48	HIS
32	59	139	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1498/1522 (98%)	346 (23%)	28 (1%)
1	1G	1489/1522 (97%)	369 (24%)	32 (2%)
22	1K	71/76 (93%)	37 (52%)	2 (2%)
22	1L	71/76 (93%)	41 (57%)	3 (4%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	76/77 (98%)	19 (25%)	3 (3%)
24	3K	69/76 (90%)	38 (55%)	2 (2%)
24	3L	69/76 (90%)	36 (52%)	2 (2%)
25	4K	17/27 (62%)	10 (58%)	3 (17%)
25	4L	14/27 (51%)	6 (42%)	3 (21%)
26	14	2804/2917 (96%)	688 (24%)	36 (1%)
26	1H	2800/2917 (95%)	623 (22%)	41 (1%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	34 (28%)	1 (0%)
All	All	9296/9634 (96%)	2294 (24%)	158 (1%)

5 of 2294 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	4	U
1	13	5	U

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Mol	Chain	Res	Type
1	13	6	G
1	13	9	G

5 of 158 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	2L	48	U
26	14	1963	U
25	4L	22	A
26	14	774	A
26	14	2611	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	PSU	2K	56	23	18,21,22	1.19	2 (11%)	22,30,33	2.23	5 (22%)
23	5MU	2K	55	23	19,22,23	3.90	5 (26%)	28,32,35	3.24	8 (28%)
22	H2U	1K	17	22	18,21,22	2.18	4 (22%)	21,30,33	2.01	4 (19%)
22	AET	1K	37	22	28,35,36	3.10	4 (14%)	31,51,54	2.17	8 (25%)
23	5MU	2L	55	23	19,22,23	3.83	5 (26%)	28,32,35	3.23	10 (35%)
22	PSU	1K	55	22	18,21,22	1.24	1 (5%)	22,30,33	1.87	4 (18%)
23	PSU	2L	56	23	18,21,22	1.25	2 (11%)	22,30,33	1.78	3 (13%)
22	H2U	1L	17	22	18,21,22	2.26	4 (22%)	21,30,33	1.88	4 (19%)
22	PSU	1L	55	22	18,21,22	1.18	1 (5%)	22,30,33	1.67	4 (18%)
22	5MU	1K	54	22	19,22,23	3.95	5 (26%)	28,32,35	3.34	9 (32%)
22	5MU	1L	54	22	19,22,23	4.02	5 (26%)	28,32,35	3.19	8 (28%)
22	AET	1L	37	22	28,35,36	2.77	5 (17%)	31,51,54	1.89	6 (19%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	H2U	1K	17	22	-	4/7/38/39	0/2/2/2
22	AET	1K	37	22	-	7/23/45/46	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
22	PSU	1L	55	22	-	4/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	4/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
22	AET	1L	37	22	-	8/23/45/46	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	13.01	1.59	1.38
22	1K	54	5MU	C2-N1	12.84	1.59	1.38
22	1K	37	AET	C10-N6	12.68	1.55	1.37
23	2K	55	5MU	C2-N1	12.61	1.58	1.38
23	2L	55	5MU	C2-N1	11.94	1.57	1.38

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	54	5MU	C5-C4-N3	11.07	124.76	115.31
23	2L	55	5MU	C5-C4-N3	10.88	124.60	115.31
22	1L	54	5MU	C5-C4-N3	9.85	123.72	115.31
23	2K	55	5MU	C5-C4-N3	9.39	123.33	115.31
23	2K	55	5MU	C6-C5-C4	6.91	123.81	118.03

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	17	H2U	O4'-C1'-N1-C6
22	1K	17	H2U	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
22	1K	17	H2U	C2'-C1'-N1-C6
22	1L	17	H2U	O4'-C1'-N1-C2
22	1L	17	H2U	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	AET	4	0
22	1K	54	5MU	1	0
22	1L	37	AET	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1086 ligands modelled in this entry, 1084 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	SF4	3E	301	-	0,12,12	-	-	-		
56	SF4	32	302	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	3E	301	-	-	-	0/6/5/5
56	SF4	32	302	4	-	-	0/6/5/5



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	3E	301	SF4	1	0
56	32	302	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	3L	1
24	3K	1
26	1H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	48:C	O3'	49:G	P	5.47
1	3K	48:C	O3'	49:G	P	4.84
1	1H	1053:C	O3'	1054:A	P	3.77

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	13	1500/1522 (98%)	0.00	37 (2%) 57 59	76, 125, 184, 245	0
1	1G	1490/1522 (97%)	-0.24	16 (1%) 80 84	83, 128, 188, 248	0
2	12	207/256 (80%)	0.14	11 (5%) 26 28	161, 184, 195, 199	0
2	1E	231/256 (90%)	-0.18	2 (0%) 84 87	141, 166, 184, 190	0
3	22	197/239 (82%)	1.16	52 (26%) 0 0	154, 171, 186, 191	0
3	2E	205/239 (85%)	0.79	36 (17%) 1 1	111, 131, 153, 161	0
4	32	208/209 (99%)	0.40	12 (5%) 23 25	120, 138, 152, 159	0
4	3E	207/209 (99%)	1.13	44 (21%) 0 1	110, 133, 148, 155	0
5	42	150/162 (92%)	0.42	19 (12%) 3 4	125, 140, 157, 169	0
5	4E	149/162 (91%)	0.78	22 (14%) 2 2	103, 125, 139, 144	0
6	52	101/101 (100%)	-0.06	0 100 100	115, 130, 143, 149	0
6	5E	100/101 (99%)	0.05	1 (1%) 82 86	111, 130, 143, 148	0
7	62	138/156 (88%)	1.35	35 (25%) 0 0	141, 152, 160, 165	0
7	6E	154/156 (98%)	1.13	29 (18%) 1 1	121, 144, 164, 171	0
8	72	137/138 (99%)	0.59	17 (12%) 4 4	124, 148, 161, 164	0
8	7E	138/138 (100%)	0.77	19 (13%) 2 3	114, 133, 143, 154	0
9	82	121/128 (94%)	1.01	24 (19%) 1 1	136, 172, 180, 189	0
9	8E	126/128 (98%)	0.59	20 (15%) 1 2	113, 159, 175, 182	0
10	1A	99/105 (94%)	0.88	21 (21%) 0 1	151, 177, 186, 190	0
10	1I	94/105 (89%)	0.97	28 (29%) 0 0	108, 151, 170, 173	0
11	2A	113/129 (87%)	2.03	50 (44%) 0 0	107, 132, 147, 153	0
11	2I	111/129 (86%)	2.17	55 (49%) 0 0	100, 132, 150, 165	0
12	3A	122/132 (92%)	1.70	50 (40%) 0 0	112, 126, 140, 147	0
12	3I	122/132 (92%)	1.86	53 (43%) 0 0	89, 102, 123, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	109/126 (86%)	1.07	33 (30%) 0 0	147, 174, 184, 192	0
13	4I	119/126 (94%)	0.56	21 (17%) 1 1	108, 141, 151, 161	0
14	5A	59/61 (96%)	4.09	38 (64%) 0 0	155, 172, 184, 193	0
14	5I	60/61 (98%)	1.83	27 (45%) 0 0	113, 123, 140, 142	0
15	6A	87/89 (97%)	0.23	5 (5%) 23 26	113, 133, 149, 153	0
15	6I	87/89 (97%)	0.43	7 (8%) 12 14	110, 126, 142, 148	0
16	7A	84/88 (95%)	-0.12	0 100 100	110, 128, 147, 175	0
16	7I	83/88 (94%)	1.60	31 (37%) 0 0	127, 142, 164, 175	0
17	8A	99/105 (94%)	1.47	32 (32%) 0 0	116, 127, 141, 145	0
17	8I	100/105 (95%)	1.19	27 (27%) 0 0	111, 128, 138, 139	0
18	9A	69/88 (78%)	0.03	2 (2%) 51 54	118, 135, 151, 160	0
18	9I	68/88 (77%)	0.16	0 100 100	114, 132, 145, 153	0
19	AA	65/93 (69%)	1.08	14 (21%) 0 1	170, 188, 195, 196	0
19	AI	82/93 (88%)	0.53	10 (12%) 4 4	116, 140, 164, 171	0
20	BA	99/106 (93%)	0.87	15 (15%) 2 2	116, 133, 153, 156	0
20	BI	97/106 (91%)	0.59	7 (7%) 15 18	124, 143, 162, 165	0
21	1B	22/27 (81%)	1.34	7 (31%) 0 0	138, 161, 164, 166	0
21	1F	23/27 (85%)	0.93	7 (30%) 0 0	117, 127, 134, 141	0
22	1K	70/76 (92%)	0.28	6 (8%) 10 12	118, 199, 215, 218	0
22	1L	70/76 (92%)	0.65	10 (14%) 2 3	137, 224, 235, 238	0
23	2K	75/77 (97%)	0.79	9 (12%) 4 5	84, 118, 147, 158	0
23	2L	75/77 (97%)	0.38	4 (5%) 26 28	94, 135, 158, 169	0
24	3K	72/76 (94%)	0.65	9 (12%) 3 4	88, 208, 234, 241	0
24	3L	72/76 (94%)	-0.01	5 (6%) 16 19	100, 201, 226, 230	0
25	4K	18/27 (66%)	3.49	15 (83%) 0 0	96, 147, 195, 200	0
25	4L	14/27 (51%)	2.16	6 (42%) 0 0	118, 164, 175, 177	0
26	14	2811/2917 (96%)	0.11	85 (3%) 50 53	64, 104, 193, 248	0
26	1H	2811/2917 (96%)	-0.00	12 (0%) 92 94	56, 89, 174, 260	0
27	16	122/122 (100%)	-0.36	0 100 100	87, 112, 131, 182	0
27	1J	122/122 (100%)	-0.43	1 (0%) 86 89	117, 142, 157, 190	0
28	11	273/276 (98%)	1.06	52 (19%) 1 1	57, 82, 102, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	19	274/276 (99%)	1.58	97 (35%) 0 0	59, 90, 108, 119	0
29	21	205/206 (99%)	1.23	52 (25%) 0 0	66, 100, 134, 144	0
29	29	204/206 (99%)	1.23	54 (26%) 0 0	76, 114, 145, 159	0
30	31	202/210 (96%)	0.84	29 (14%) 2 3	60, 93, 126, 139	0
30	39	204/210 (97%)	0.46	24 (11%) 4 5	74, 123, 157, 170	0
31	41	179/182 (98%)	0.52	15 (8%) 11 13	105, 125, 147, 157	0
31	49	180/182 (98%)	1.87	70 (38%) 0 0	139, 158, 176, 187	0
32	51	174/180 (96%)	0.02	0 100 100	99, 119, 132, 147	0
32	59	169/180 (93%)	2.42	79 (46%) 0 0	174, 207, 224, 229	0
33	61	145/148 (97%)	-0.27	0 100 100	97, 148, 162, 167	0
33	69	145/148 (97%)	0.01	5 (3%) 45 47	100, 142, 160, 165	0
34	15	137/140 (97%)	2.89	91 (66%) 0 0	94, 127, 154, 162	0
34	58	125/140 (89%)	1.12	27 (21%) 0 1	84, 101, 118, 135	0
35	25	122/122 (100%)	1.71	51 (41%) 0 0	82, 104, 119, 128	0
35	68	122/122 (100%)	1.19	28 (22%) 0 0	73, 94, 112, 126	0
36	35	147/150 (98%)	1.68	58 (39%) 0 0	74, 122, 150, 161	0
36	78	148/150 (98%)	0.54	17 (11%) 4 5	63, 98, 121, 128	0
37	45	138/141 (97%)	3.03	84 (60%) 0 0	91, 125, 148, 160	0
37	88	141/141 (100%)	1.28	37 (26%) 0 0	74, 98, 119, 144	0
38	55	118/118 (100%)	1.15	31 (26%) 0 0	79, 101, 115, 124	0
38	98	118/118 (100%)	1.50	36 (30%) 0 0	78, 97, 116, 131	0
39	65	110/112 (98%)	0.14	3 (2%) 54 57	116, 134, 146, 155	0
39	A8	111/112 (99%)	0.78	11 (9%) 7 8	93, 108, 124, 136	0
40	75	140/146 (95%)	0.67	13 (9%) 8 10	97, 114, 166, 177	0
40	B8	136/146 (93%)	0.70	16 (11%) 4 5	89, 108, 150, 175	0
41	85	116/118 (98%)	1.27	28 (24%) 0 0	82, 117, 146, 155	0
41	C8	115/118 (97%)	0.53	6 (5%) 27 29	68, 94, 121, 131	0
42	95	100/101 (99%)	1.53	32 (32%) 0 0	82, 141, 153, 159	0
42	D8	100/101 (99%)	0.92	15 (15%) 2 2	66, 112, 131, 136	0
43	A5	111/113 (98%)	1.38	31 (27%) 0 0	77, 95, 124, 143	0
43	E8	110/113 (97%)	1.04	19 (17%) 1 1	68, 87, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B5	94/96 (97%)	0.76	9 (9%) 8 10	91, 104, 118, 125	0
44	F8	95/96 (98%)	0.63	8 (8%) 11 13	71, 85, 112, 122	0
45	C5	52/110 (47%)	1.51	15 (28%) 0 0	109, 122, 135, 145	0
45	G8	97/110 (88%)	-0.02	0 100 100	91, 107, 131, 142	0
46	D5	177/206 (85%)	1.82	70 (39%) 0 0	132, 166, 217, 221	0
46	H8	170/206 (82%)	0.99	33 (19%) 1 1	105, 137, 187, 195	0
47	E5	76/85 (89%)	2.58	37 (48%) 0 0	95, 109, 124, 131	0
47	I8	77/85 (90%)	1.67	25 (32%) 0 0	76, 88, 110, 120	0
48	F5	94/98 (95%)	2.16	49 (52%) 0 0	78, 104, 133, 138	0
48	J8	96/98 (97%)	1.86	43 (44%) 0 0	72, 94, 142, 152	0
49	G5	69/72 (95%)	0.22	3 (4%) 35 38	107, 128, 145, 156	0
49	K8	68/72 (94%)	0.39	0 100 100	78, 99, 116, 136	0
50	H5	58/60 (96%)	2.74	37 (63%) 0 0	100, 121, 137, 150	0
50	L8	58/60 (96%)	0.67	6 (10%) 6 7	72, 93, 122, 124	0
51	M8	60/71 (84%)	0.19	5 (8%) 11 13	126, 154, 167, 170	0
52	J5	56/60 (93%)	1.52	20 (35%) 0 0	74, 103, 138, 151	0
52	N8	48/60 (80%)	0.91	7 (14%) 2 2	64, 98, 126, 133	0
53	L5	48/49 (97%)	1.70	14 (29%) 0 0	70, 78, 110, 114	0
53	P8	47/49 (95%)	0.69	5 (10%) 6 7	61, 68, 90, 98	0
54	M5	64/65 (98%)	3.63	51 (79%) 0 0	83, 97, 115, 126	0
54	Q8	64/65 (98%)	2.00	35 (54%) 0 0	68, 83, 101, 110	0
All	All	20451/21509 (95%)	0.58	2681 (13%) 3 4	56, 119, 186, 260	0

The worst 5 of 2681 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	5A	38	GLY	16.2
32	59	93	GLY	14.9
22	1L	76	A	14.8
47	E5	9	SER	13.8
14	5A	39	LEU	13.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	H2U	1L	17	20/21	0.26	0.77	213,231,237,237	0
22	H2U	1K	17	20/21	0.45	0.40	199,211,220,220	0
22	PSU	1L	55	20/21	0.79	0.11	169,202,215,222	0
22	5MU	1L	54	21/22	0.85	0.11	171,182,192,193	0
22	AET	1L	37	33/34	0.88	0.42	156,171,176,178	0
22	PSU	1K	55	20/21	0.89	0.12	146,178,188,189	0
22	AET	1K	37	33/34	0.90	0.45	112,124,147,151	0
23	PSU	2L	56	20/21	0.90	0.19	126,136,143,146	0
22	5MU	1K	54	21/22	0.90	0.15	139,156,165,170	0
23	PSU	2K	56	20/21	0.91	0.11	113,119,131,132	0
23	5MU	2L	55	21/22	0.94	0.24	129,139,144,146	0
23	5MU	2K	55	21/22	0.95	0.12	118,124,135,139	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	MG	1H	3180	1/1	0.04	0.26	112,112,112,112	0
55	MG	14	3139	1/1	0.24	0.32	103,103,103,103	0
55	MG	1H	3049	1/1	0.26	0.36	74,74,74,74	0
55	MG	14	3094	1/1	0.27	0.43	108,108,108,108	0
55	MG	1G	1650	1/1	0.37	0.83	107,107,107,107	0
55	MG	1H	3241	1/1	0.39	0.58	110,110,110,110	0
55	MG	13	1675	1/1	0.40	0.33	104,104,104,104	0
55	MG	1H	3045	1/1	0.41	0.42	80,80,80,80	0
55	MG	1H	3223	1/1	0.41	0.70	99,99,99,99	0
55	MG	1G	1656	1/1	0.45	0.36	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3212	1/1	0.48	0.50	91,91,91,91	0
55	MG	14	3177	1/1	0.49	0.57	79,79,79,79	0
55	MG	E5	101	1/1	0.49	0.32	90,90,90,90	0
55	MG	1H	3009	1/1	0.50	0.14	95,95,95,95	0
55	MG	1H	3178	1/1	0.50	0.27	94,94,94,94	0
55	MG	13	1603	1/1	0.50	0.12	85,85,85,85	0
55	MG	1G	1701	1/1	0.51	0.24	137,137,137,137	0
55	MG	14	3116	1/1	0.52	0.17	89,89,89,89	0
55	MG	1G	1663	1/1	0.52	0.47	121,121,121,121	0
55	MG	13	1647	1/1	0.52	0.21	116,116,116,116	0
55	MG	13	1711	1/1	0.52	0.22	154,154,154,154	0
55	MG	14	3144	1/1	0.53	0.38	114,114,114,114	0
55	MG	1G	1668	1/1	0.54	0.38	125,125,125,125	0
55	MG	14	3176	1/1	0.54	0.27	109,109,109,109	0
55	MG	1H	3107	1/1	0.54	0.41	92,92,92,92	0
55	MG	14	3004	1/1	0.54	0.22	66,66,66,66	0
55	MG	14	3184	1/1	0.55	0.30	96,96,96,96	0
55	MG	1H	3229	1/1	0.55	0.70	70,70,70,70	0
55	MG	13	1670	1/1	0.56	0.20	137,137,137,137	0
55	MG	13	1668	1/1	0.56	0.15	121,121,121,121	0
55	MG	1H	3017	1/1	0.56	0.33	75,75,75,75	0
55	MG	1H	3165	1/1	0.56	0.38	90,90,90,90	0
55	MG	1H	3137	1/1	0.57	0.32	75,75,75,75	0
55	MG	14	3069	1/1	0.57	0.35	107,107,107,107	0
55	MG	1G	1693	1/1	0.58	0.09	148,148,148,148	0
55	MG	42	202	1/1	0.58	0.23	135,135,135,135	0
55	MG	1G	1714	1/1	0.59	0.20	133,133,133,133	0
55	MG	14	3185	1/1	0.59	1.15	88,88,88,88	0
55	MG	14	3186	1/1	0.59	0.37	85,85,85,85	0
55	MG	1G	1651	1/1	0.59	0.24	91,91,91,91	0
55	MG	1H	3166	1/1	0.60	0.28	74,74,74,74	0
55	MG	1G	1722	1/1	0.60	0.12	161,161,161,161	0
55	MG	1H	3114	1/1	0.60	0.29	92,92,92,92	0
55	MG	1G	1671	1/1	0.62	0.24	100,100,100,100	0
55	MG	1H	3111	1/1	0.62	0.29	86,86,86,86	0
55	MG	13	1638	1/1	0.62	0.58	80,80,80,80	0
55	MG	1H	3175	1/1	0.63	0.37	114,114,114,114	0
55	MG	1H	3185	1/1	0.63	0.64	72,72,72,72	0
55	MG	1H	3113	1/1	0.63	0.39	83,83,83,83	0
55	MG	14	3190	1/1	0.63	0.30	100,100,100,100	0
55	MG	14	3122	1/1	0.63	0.40	103,103,103,103	0
55	MG	13	1641	1/1	0.64	0.21	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3112	1/1	0.64	1.17	96,96,96,96	0
55	MG	14	3164	1/1	0.64	0.39	95,95,95,95	0
55	MG	1G	1618	1/1	0.64	0.45	98,98,98,98	0
55	MG	35	201	1/1	0.64	0.95	81,81,81,81	0
55	MG	1H	3034	1/1	0.64	0.27	77,77,77,77	0
55	MG	13	1671	1/1	0.65	0.22	117,117,117,117	0
55	MG	1H	3133	1/1	0.65	0.27	85,85,85,85	0
55	MG	13	1629	1/1	0.65	0.24	109,109,109,109	0
55	MG	1H	3096	1/1	0.65	0.19	79,79,79,79	0
55	MG	1G	1662	1/1	0.65	0.49	116,116,116,116	0
55	MG	1H	3181	1/1	0.65	0.52	89,89,89,89	0
55	MG	1G	1683	1/1	0.66	0.26	122,122,122,122	0
55	MG	1H	3121	1/1	0.66	0.23	91,91,91,91	0
55	MG	1G	1667	1/1	0.66	0.23	101,101,101,101	0
55	MG	14	3296	1/1	0.66	0.10	119,119,119,119	0
55	MG	14	3125	1/1	0.66	0.24	97,97,97,97	0
55	MG	14	3099	1/1	0.66	0.30	90,90,90,90	0
55	MG	1H	3179	1/1	0.67	0.32	86,86,86,86	0
55	MG	14	3141	1/1	0.67	0.21	104,104,104,104	0
55	MG	1H	3085	1/1	0.67	0.27	74,74,74,74	0
55	MG	14	3012	1/1	0.67	0.28	95,95,95,95	0
55	MG	14	3170	1/1	0.67	0.26	69,69,69,69	0
55	MG	1H	3214	1/1	0.67	0.17	84,84,84,84	0
55	MG	45	201	1/1	0.67	0.16	121,121,121,121	0
55	MG	1H	3127	1/1	0.67	0.25	87,87,87,87	0
55	MG	1G	1657	1/1	0.68	0.23	98,98,98,98	0
55	MG	13	1663	1/1	0.68	0.21	123,123,123,123	0
55	MG	14	3194	1/1	0.68	0.17	132,132,132,132	0
55	MG	1G	1640	1/1	0.68	0.20	103,103,103,103	0
55	MG	1H	3226	1/1	0.68	1.28	90,90,90,90	0
55	MG	1H	3315	1/1	0.68	0.08	112,112,112,112	0
55	MG	1H	3452	1/1	0.68	0.12	108,108,108,108	0
55	MG	1G	1646	1/1	0.69	0.31	101,101,101,101	0
55	MG	13	1679	1/1	0.69	0.36	111,111,111,111	0
55	MG	14	3016	1/1	0.69	0.27	110,110,110,110	0
55	MG	14	3027	1/1	0.69	0.28	72,72,72,72	0
55	MG	1G	1620	1/1	0.69	0.17	81,81,81,81	0
55	MG	14	3082	1/1	0.69	0.34	78,78,78,78	0
55	MG	1H	3119	1/1	0.69	0.36	105,105,105,105	0
55	MG	13	1705	1/1	0.70	0.53	130,130,130,130	0
55	MG	1H	3149	1/1	0.70	0.44	76,76,76,76	0
55	MG	14	3009	1/1	0.70	0.66	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3244	1/1	0.71	0.31	87,87,87,87	0
55	MG	1H	3088	1/1	0.71	0.34	81,81,81,81	0
55	MG	13	1681	1/1	0.71	0.27	113,113,113,113	0
55	MG	14	3169	1/1	0.71	0.21	97,97,97,97	0
55	MG	1H	3274	1/1	0.72	0.51	78,78,78,78	0
55	MG	1G	1647	1/1	0.72	0.21	120,120,120,120	0
55	MG	1G	1682	1/1	0.72	0.16	101,101,101,101	0
55	MG	14	3029	1/1	0.72	0.13	99,99,99,99	0
55	MG	1H	3148	1/1	0.72	0.31	100,100,100,100	0
55	MG	1H	3340	1/1	0.72	0.18	139,139,139,139	0
55	MG	1H	3024	1/1	0.72	0.20	71,71,71,71	0
55	MG	14	3182	1/1	0.72	0.36	88,88,88,88	0
55	MG	1H	3457	1/1	0.72	0.17	133,133,133,133	0
55	MG	14	3107	1/1	0.72	0.23	88,88,88,88	0
55	MG	14	3110	1/1	0.72	0.37	103,103,103,103	0
55	MG	1G	1659	1/1	0.72	0.14	99,99,99,99	0
55	MG	1H	3164	1/1	0.72	0.24	98,98,98,98	0
55	MG	14	3121	1/1	0.72	0.38	94,94,94,94	0
55	MG	14	3001	1/1	0.72	0.17	94,94,94,94	0
55	MG	1H	3252	1/1	0.72	0.24	69,69,69,69	0
55	MG	1H	3254	1/1	0.72	0.35	97,97,97,97	0
55	MG	5I	101	1/1	0.73	0.75	105,105,105,105	0
55	MG	1G	1644	1/1	0.73	0.27	97,97,97,97	0
55	MG	1G	1660	1/1	0.73	0.17	118,118,118,118	0
55	MG	14	3188	1/1	0.73	0.32	89,89,89,89	0
55	MG	13	1627	1/1	0.73	0.19	94,94,94,94	0
55	MG	13	1708	1/1	0.73	0.32	145,145,145,145	0
55	MG	1H	3145	1/1	0.73	0.34	84,84,84,84	0
55	MG	14	3060	1/1	0.73	0.33	84,84,84,84	0
55	MG	13	1636	1/1	0.73	0.17	91,91,91,91	0
55	MG	1H	3312	1/1	0.73	0.23	105,105,105,105	0
55	MG	1G	1706	1/1	0.74	0.11	138,138,138,138	0
55	MG	1G	1661	1/1	0.74	0.23	77,77,77,77	0
55	MG	13	1639	1/1	0.74	0.18	110,110,110,110	0
55	MG	1G	1621	1/1	0.74	0.50	115,115,115,115	0
55	MG	8I	201	1/1	0.74	1.37	107,107,107,107	0
55	MG	1H	3310	1/1	0.74	0.10	109,109,109,109	0
55	MG	1H	3253	1/1	0.75	0.33	98,98,98,98	0
55	MG	13	1686	1/1	0.75	0.59	73,73,73,73	0
55	MG	1H	3269	1/1	0.75	0.34	55,55,55,55	0
55	MG	14	3041	1/1	0.75	0.56	61,61,61,61	0
55	MG	1H	3337	1/1	0.75	0.08	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3138	1/1	0.75	0.35	98,98,98,98	0
55	MG	1G	1627	1/1	0.75	0.27	122,122,122,122	0
55	MG	14	3083	1/1	0.75	0.27	105,105,105,105	0
55	MG	1G	1629	1/1	0.75	0.11	131,131,131,131	0
55	MG	1H	3141	1/1	0.76	0.34	89,89,89,89	0
55	MG	1H	3142	1/1	0.76	0.43	76,76,76,76	0
55	MG	14	3113	1/1	0.76	0.21	120,120,120,120	0
55	MG	1H	3301	1/1	0.76	0.11	100,100,100,100	0
55	MG	1H	3465	1/1	0.76	0.07	98,98,98,98	0
55	MG	1G	1604	1/1	0.76	0.12	102,102,102,102	0
55	MG	14	3062	1/1	0.76	0.26	87,87,87,87	0
55	MG	1H	3091	1/1	0.76	0.24	70,70,70,70	0
55	MG	13	1630	1/1	0.76	0.23	109,109,109,109	0
55	MG	1G	1669	1/1	0.76	0.33	131,131,131,131	0
55	MG	1G	1670	1/1	0.76	0.59	101,101,101,101	0
55	MG	13	1724	1/1	0.76	0.09	128,128,128,128	0
55	MG	13	1673	1/1	0.76	0.25	113,113,113,113	0
55	MG	1H	3163	1/1	0.77	0.22	82,82,82,82	0
55	MG	21	301	1/1	0.77	0.14	82,82,82,82	0
55	MG	14	3178	1/1	0.77	0.30	98,98,98,98	0
55	MG	1H	3205	1/1	0.77	0.33	80,80,80,80	0
55	MG	14	3298	1/1	0.77	0.12	103,103,103,103	0
55	MG	1H	3279	1/1	0.77	0.31	81,81,81,81	0
55	MG	1H	3300	1/1	0.77	0.32	104,104,104,104	0
55	MG	45	202	1/1	0.77	0.33	116,116,116,116	0
55	MG	14	3079	1/1	0.77	0.22	100,100,100,100	0
55	MG	14	3026	1/1	0.78	0.15	76,76,76,76	0
55	MG	1G	1630	1/1	0.78	0.21	135,135,135,135	0
55	MG	13	1674	1/1	0.78	0.49	109,109,109,109	0
55	MG	14	3108	1/1	0.78	0.20	87,87,87,87	0
55	MG	1H	3419	1/1	0.78	0.09	115,115,115,115	0
55	MG	13	1648	1/1	0.78	0.19	110,110,110,110	0
55	MG	1H	3278	1/1	0.78	0.24	75,75,75,75	0
55	MG	1G	1623	1/1	0.78	0.07	161,161,161,161	0
55	MG	14	3010	1/1	0.78	0.22	78,78,78,78	0
55	MG	1H	3033	1/1	0.78	0.28	60,60,60,60	0
55	MG	1H	3050	1/1	0.78	0.36	79,79,79,79	0
55	MG	14	3133	1/1	0.79	0.43	99,99,99,99	0
55	MG	14	3135	1/1	0.79	1.38	91,91,91,91	0
55	MG	1H	3199	1/1	0.79	0.35	69,69,69,69	0
55	MG	1H	3275	1/1	0.79	0.47	62,62,62,62	0
55	MG	1G	1606	1/1	0.79	0.18	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	13	1701	1/1	0.79	0.26	137,137,137,137	0
55	MG	14	3290	1/1	0.79	0.12	115,115,115,115	0
55	MG	1G	1715	1/1	0.79	0.25	126,126,126,126	0
55	MG	13	1664	1/1	0.79	0.37	87,87,87,87	0
55	MG	1H	3246	1/1	0.79	0.37	117,117,117,117	0
55	MG	14	3092	1/1	0.79	0.69	81,81,81,81	0
55	MG	1G	1685	1/1	0.79	0.33	94,94,94,94	0
55	MG	14	3098	1/1	0.79	0.35	78,78,78,78	0
55	MG	1H	3143	1/1	0.80	0.25	89,89,89,89	0
55	MG	1H	3176	1/1	0.80	0.18	107,107,107,107	0
55	MG	13	1738	1/1	0.80	0.25	134,134,134,134	0
55	MG	1G	1637	1/1	0.80	0.09	125,125,125,125	0
55	MG	13	1652	1/1	0.80	0.27	97,97,97,97	0
55	MG	1H	3208	1/1	0.80	0.22	113,113,113,113	0
55	MG	1G	1645	1/1	0.80	0.27	118,118,118,118	0
55	MG	14	3081	1/1	0.80	0.40	88,88,88,88	0
55	MG	1H	3273	1/1	0.80	0.27	63,63,63,63	0
55	MG	1G	1697	1/1	0.80	0.10	172,172,172,172	0
55	MG	13	1733	1/1	0.80	0.14	92,92,92,92	0
55	MG	1G	1649	1/1	0.80	0.21	151,151,151,151	0
55	MG	1G	1652	1/1	0.81	0.14	105,105,105,105	0
55	MG	13	1624	1/1	0.81	0.17	98,98,98,98	0
55	MG	1H	3067	1/1	0.81	0.34	65,65,65,65	0
55	MG	14	3163	1/1	0.81	0.32	102,102,102,102	0
55	MG	1H	3281	1/1	0.81	0.36	96,96,96,96	0
55	MG	1H	3174	1/1	0.81	0.64	129,129,129,129	0
55	MG	13	1631	1/1	0.81	0.36	132,132,132,132	0
55	MG	88	203	1/1	0.81	0.93	77,77,77,77	0
55	MG	1G	1632	1/1	0.82	0.20	127,127,127,127	0
55	MG	13	1676	1/1	0.82	0.20	104,104,104,104	0
55	MG	13	1602	1/1	0.82	0.18	115,115,115,115	0
55	MG	1G	1641	1/1	0.82	0.13	107,107,107,107	0
55	MG	1G	1614	1/1	0.82	0.27	123,123,123,123	0
55	MG	1H	3202	1/1	0.82	0.50	87,87,87,87	0
55	MG	14	3137	1/1	0.82	0.34	151,151,151,151	0
55	MG	14	3138	1/1	0.82	0.39	134,134,134,134	0
55	MG	1H	3139	1/1	0.82	0.26	60,60,60,60	0
55	MG	13	1606	1/1	0.82	0.31	83,83,83,83	0
55	MG	13	1706	1/1	0.82	0.30	132,132,132,132	0
55	MG	1H	3183	1/1	0.82	0.55	82,82,82,82	0
55	MG	14	3109	1/1	0.82	0.28	102,102,102,102	0
55	MG	1H	3331	1/1	0.82	0.18	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1603	1/1	0.82	0.16	95,95,95,95	0
55	MG	14	3078	1/1	0.82	0.11	100,100,100,100	0
55	MG	1H	3126	1/1	0.83	0.36	78,78,78,78	0
55	MG	1H	3021	1/1	0.83	0.11	78,78,78,78	0
55	MG	1H	3249	1/1	0.83	0.23	70,70,70,70	0
55	MG	1H	3325	1/1	0.83	0.18	122,122,122,122	0
55	MG	1H	3144	1/1	0.83	0.21	106,106,106,106	0
55	MG	1G	1723	1/1	0.83	0.08	113,113,113,113	0
55	MG	1H	3207	1/1	0.83	0.30	77,77,77,77	0
55	MG	1H	3128	1/1	0.83	0.26	92,92,92,92	0
55	MG	1H	3255	1/1	0.83	0.30	78,78,78,78	0
55	MG	1H	3423	1/1	0.83	0.09	102,102,102,102	0
55	MG	1H	3037	1/1	0.83	0.11	76,76,76,76	0
55	MG	13	1637	1/1	0.83	0.18	101,101,101,101	0
55	MG	1H	3216	1/1	0.83	0.36	89,89,89,89	0
55	MG	14	3019	1/1	0.83	0.11	85,85,85,85	0
55	MG	14	3189	1/1	0.83	0.27	99,99,99,99	0
55	MG	1H	3221	1/1	0.83	0.20	100,100,100,100	0
55	MG	1G	1681	1/1	0.83	0.26	92,92,92,92	0
55	MG	1H	3154	1/1	0.83	0.20	61,61,61,61	0
55	MG	1H	3090	1/1	0.83	0.21	88,88,88,88	0
55	MG	1H	3029	1/1	0.83	0.21	68,68,68,68	0
55	MG	1G	1692	1/1	0.83	0.09	118,118,118,118	0
55	MG	1H	3237	1/1	0.83	0.19	79,79,79,79	0
55	MG	14	3076	1/1	0.83	0.44	90,90,90,90	0
55	MG	13	1739	1/1	0.83	0.12	128,128,128,128	0
55	MG	1H	3313	1/1	0.84	0.26	112,112,112,112	0
55	MG	1H	3104	1/1	0.84	0.51	74,74,74,74	0
55	MG	1H	3320	1/1	0.84	0.25	127,127,127,127	0
55	MG	13	1736	1/1	0.84	0.15	137,137,137,137	0
55	MG	1G	1648	1/1	0.84	0.24	115,115,115,115	0
55	MG	1G	1611	1/1	0.84	0.38	112,112,112,112	0
55	MG	1H	3238	1/1	0.84	0.15	94,94,94,94	0
55	MG	1H	3335	1/1	0.84	0.28	134,134,134,134	0
55	MG	14	3111	1/1	0.84	0.46	110,110,110,110	0
55	MG	13	1695	1/1	0.84	0.14	139,139,139,139	0
55	MG	1H	3182	1/1	0.84	0.53	114,114,114,114	0
55	MG	1H	3001	1/1	0.84	0.21	53,53,53,53	0
55	MG	1H	3421	1/1	0.84	0.14	113,113,113,113	0
55	MG	14	3063	1/1	0.84	0.29	82,82,82,82	0
55	MG	1H	3422	1/1	0.84	0.06	121,121,121,121	0
55	MG	1H	3184	1/1	0.84	0.17	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3291	1/1	0.84	0.24	114,114,114,114	0
55	MG	1H	3093	1/1	0.84	0.37	70,70,70,70	0
55	MG	1H	3196	1/1	0.84	0.56	107,107,107,107	0
55	MG	1G	1725	1/1	0.84	0.09	130,130,130,130	0
55	MG	13	1640	1/1	0.84	0.22	99,99,99,99	0
55	MG	1H	3200	1/1	0.84	0.38	88,88,88,88	0
55	MG	14	3088	1/1	0.84	0.17	109,109,109,109	0
55	MG	1H	3040	1/1	0.85	0.23	58,58,58,58	0
55	MG	1H	3071	1/1	0.85	0.55	72,72,72,72	0
55	MG	14	3114	1/1	0.85	0.24	101,101,101,101	0
55	MG	1H	3330	1/1	0.85	0.11	78,78,78,78	0
55	MG	14	3011	1/1	0.85	0.29	66,66,66,66	0
55	MG	1G	1699	1/1	0.85	0.31	121,121,121,121	0
55	MG	14	3013	1/1	0.85	0.18	96,96,96,96	0
55	MG	13	1702	1/1	0.85	0.17	110,110,110,110	0
55	MG	1H	3445	1/1	0.85	0.19	91,91,91,91	0
55	MG	1G	1713	1/1	0.85	0.10	144,144,144,144	0
55	MG	14	3191	1/1	0.85	0.19	102,102,102,102	0
55	MG	1H	3449	1/1	0.85	0.17	99,99,99,99	0
55	MG	14	3284	1/1	0.85	0.10	98,98,98,98	0
55	MG	1H	3027	1/1	0.85	0.12	75,75,75,75	0
55	MG	14	3106	1/1	0.85	1.18	90,90,90,90	0
55	MG	14	3143	1/1	0.85	0.19	97,97,97,97	0
55	MG	1H	3256	1/1	0.85	0.26	53,53,53,53	0
55	MG	1H	3463	1/1	0.85	0.06	110,110,110,110	0
55	MG	13	1656	1/1	0.85	0.13	124,124,124,124	0
55	MG	1G	1684	1/1	0.85	0.37	89,89,89,89	0
55	MG	1G	1622	1/1	0.85	0.18	104,104,104,104	0
55	MG	1H	3311	1/1	0.86	0.32	97,97,97,97	0
55	MG	13	1607	1/1	0.86	0.22	110,110,110,110	0
55	MG	14	3145	1/1	0.86	0.19	86,86,86,86	0
55	MG	4A	201	1/1	0.86	0.15	136,136,136,136	0
55	MG	1H	3451	1/1	0.86	0.23	81,81,81,81	0
55	MG	14	3165	1/1	0.86	0.55	83,83,83,83	0
55	MG	1H	3264	1/1	0.86	0.19	72,72,72,72	0
55	MG	1H	3456	1/1	0.86	0.10	111,111,111,111	0
55	MG	14	3105	1/1	0.86	0.25	81,81,81,81	0
55	MG	1H	3268	1/1	0.86	0.43	74,74,74,74	0
55	MG	1G	1642	1/1	0.86	0.43	154,154,154,154	0
55	MG	1H	3153	1/1	0.86	0.44	91,91,91,91	0
55	MG	13	1653	1/1	0.86	0.46	120,120,120,120	0
55	MG	1H	3328	1/1	0.86	0.21	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3161	1/1	0.86	0.33	86,86,86,86	0
55	MG	1G	1690	1/1	0.86	0.05	144,144,144,144	0
55	MG	13	1634	1/1	0.86	0.26	120,120,120,120	0
55	MG	1H	3055	1/1	0.86	0.39	91,91,91,91	0
55	MG	13	1723	1/1	0.86	0.13	103,103,103,103	0
55	MG	1H	3018	1/1	0.86	0.20	68,68,68,68	0
55	MG	14	3257	1/1	0.86	0.14	99,99,99,99	0
55	MG	1H	3394	1/1	0.86	0.15	75,75,75,75	0
55	MG	1H	3405	1/1	0.86	0.12	108,108,108,108	0
55	MG	1G	1708	1/1	0.86	0.21	100,100,100,100	0
55	MG	1H	3418	1/1	0.86	0.09	99,99,99,99	0
55	MG	14	3136	1/1	0.86	0.40	120,120,120,120	0
55	MG	1H	3168	1/1	0.86	0.23	109,109,109,109	0
55	MG	13	1688	1/1	0.86	0.16	122,122,122,122	0
55	MG	1H	3302	1/1	0.86	0.11	120,120,120,120	0
55	MG	1H	3022	1/1	0.86	0.29	77,77,77,77	0
55	MG	14	3142	1/1	0.87	0.38	105,105,105,105	0
55	MG	13	1617	1/1	0.87	0.22	92,92,92,92	0
55	MG	13	1651	1/1	0.87	0.30	110,110,110,110	0
55	MG	14	3085	1/1	0.87	1.14	94,94,94,94	0
55	MG	14	3146	1/1	0.87	0.25	92,92,92,92	0
55	MG	1H	3134	1/1	0.87	0.38	61,61,61,61	0
55	MG	1H	3346	1/1	0.87	0.12	63,63,63,63	0
55	MG	1H	3373	1/1	0.87	0.12	106,106,106,106	0
55	MG	BI	201	1/1	0.87	0.24	110,110,110,110	0
55	MG	1H	3191	1/1	0.87	0.12	93,93,93,93	0
55	MG	1H	3416	1/1	0.87	0.07	119,119,119,119	0
55	MG	1H	3284	1/1	0.87	0.19	60,60,60,60	0
55	MG	1H	3293	1/1	0.87	0.10	124,124,124,124	0
55	MG	1H	3195	1/1	0.87	0.13	114,114,114,114	0
55	MG	1H	3106	1/1	0.87	0.15	100,100,100,100	0
55	MG	1G	1674	1/1	0.87	0.11	89,89,89,89	0
55	MG	1H	3065	1/1	0.87	0.38	87,87,87,87	0
55	MG	13	1690	1/1	0.87	0.32	123,123,123,123	0
55	MG	1H	3172	1/1	0.87	0.12	101,101,101,101	0
55	MG	13	1709	1/1	0.87	0.35	147,147,147,147	0
55	MG	1H	3074	1/1	0.87	0.27	65,65,65,65	0
55	MG	14	3119	1/1	0.87	0.23	101,101,101,101	0
55	MG	14	3214	1/1	0.87	0.27	96,96,96,96	0
55	MG	14	3254	1/1	0.87	0.10	108,108,108,108	0
55	MG	13	1704	1/1	0.87	0.26	147,147,147,147	0
55	MG	1H	3210	1/1	0.87	0.61	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3462	1/1	0.87	0.08	106,106,106,106	0
55	MG	1H	3322	1/1	0.87	0.53	124,124,124,124	0
55	MG	14	3292	1/1	0.87	0.27	103,103,103,103	0
55	MG	13	1722	1/1	0.87	0.13	106,106,106,106	0
55	MG	1H	3123	1/1	0.87	0.22	79,79,79,79	0
55	MG	1J	201	1/1	0.87	0.16	106,106,106,106	0
55	MG	1H	3019	1/1	0.87	0.31	57,57,57,57	0
55	MG	1G	1601	1/1	0.87	0.12	101,101,101,101	0
55	MG	1G	1711	1/1	0.87	0.07	139,139,139,139	0
55	MG	13	1740	1/1	0.87	0.21	123,123,123,123	0
55	MG	F5	101	1/1	0.87	0.27	82,82,82,82	0
55	MG	1G	1724	1/1	0.88	0.13	120,120,120,120	0
55	MG	1H	3122	1/1	0.88	0.24	98,98,98,98	0
55	MG	1H	3198	1/1	0.88	0.25	68,68,68,68	0
55	MG	13	1735	1/1	0.88	0.10	100,100,100,100	0
55	MG	13	1678	1/1	0.88	0.74	116,116,116,116	0
55	MG	14	3080	1/1	0.88	0.23	90,90,90,90	0
55	MG	1H	3231	1/1	0.88	0.18	65,65,65,65	0
55	MG	14	3006	1/1	0.88	0.16	91,91,91,91	0
55	MG	1H	3115	1/1	0.88	0.32	76,76,76,76	0
55	MG	1H	3204	1/1	0.88	0.28	80,80,80,80	0
55	MG	14	3207	1/1	0.88	0.26	117,117,117,117	0
55	MG	1H	3240	1/1	0.88	0.54	114,114,114,114	0
55	MG	14	3250	1/1	0.88	0.22	99,99,99,99	0
55	MG	14	3090	1/1	0.88	0.31	69,69,69,69	0
55	MG	1G	1666	1/1	0.88	0.48	136,136,136,136	0
55	MG	1H	3118	1/1	0.88	0.15	89,89,89,89	0
55	MG	14	3286	1/1	0.88	0.08	97,97,97,97	0
55	MG	14	3289	1/1	0.88	0.13	84,84,84,84	0
55	MG	1H	3129	1/1	0.88	0.34	92,92,92,92	0
55	MG	14	3018	1/1	0.88	0.72	84,84,84,84	0
55	MG	1H	3189	1/1	0.88	0.26	71,71,71,71	0
55	MG	14	3021	1/1	0.88	0.49	90,90,90,90	0
55	MG	13	1685	1/1	0.88	0.22	107,107,107,107	0
55	MG	1H	3332	1/1	0.88	0.25	125,125,125,125	0
55	MG	14	3028	1/1	0.88	0.27	114,114,114,114	0
55	MG	1H	3192	1/1	0.88	0.15	114,114,114,114	0
55	MG	1G	1720	1/1	0.88	0.09	152,152,152,152	0
55	MG	1H	3193	1/1	0.88	0.27	73,73,73,73	0
55	MG	13	1616	1/1	0.88	0.21	93,93,93,93	0
55	MG	1H	3041	1/1	0.89	0.14	65,65,65,65	0
55	MG	1H	3117	1/1	0.89	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3162	1/1	0.89	0.30	57,57,57,57	0
55	MG	1H	3324	1/1	0.89	0.39	115,115,115,115	0
55	MG	1H	3044	1/1	0.89	0.60	72,72,72,72	0
55	MG	1H	3224	1/1	0.89	0.13	102,102,102,102	0
55	MG	1H	3461	1/1	0.89	0.17	119,119,119,119	0
55	MG	13	1661	1/1	0.89	0.39	117,117,117,117	0
55	MG	14	3172	1/1	0.89	0.29	100,100,100,100	0
55	MG	13	1698	1/1	0.89	0.27	138,138,138,138	0
55	MG	1H	3197	1/1	0.89	0.27	77,77,77,77	0
55	MG	16	202	1/1	0.89	0.14	118,118,118,118	0
55	MG	1H	3334	1/1	0.89	0.17	94,94,94,94	0
55	MG	78	202	1/1	0.89	0.35	55,55,55,55	0
55	MG	1H	3006	1/1	0.89	0.36	49,49,49,49	0
55	MG	1H	3280	1/1	0.89	0.28	73,73,73,73	0
55	MG	14	3003	1/1	0.89	0.11	85,85,85,85	0
55	MG	13	1619	1/1	0.89	0.19	86,86,86,86	0
55	MG	1H	3147	1/1	0.89	0.30	54,54,54,54	0
55	MG	1H	3353	1/1	0.89	0.09	59,59,59,59	0
55	MG	1G	1665	1/1	0.89	0.28	130,130,130,130	0
55	MG	14	3204	1/1	0.89	0.13	106,106,106,106	0
55	MG	1G	1607	1/1	0.89	0.30	94,94,94,94	0
55	MG	1H	3285	1/1	0.89	0.26	89,89,89,89	0
55	MG	14	3217	1/1	0.89	0.09	97,97,97,97	0
55	MG	1G	1612	1/1	0.89	0.24	85,85,85,85	0
55	MG	1H	3383	1/1	0.89	0.11	60,60,60,60	0
55	MG	13	1628	1/1	0.89	0.35	120,120,120,120	0
55	MG	1H	3397	1/1	0.89	0.07	81,81,81,81	0
55	MG	14	3285	1/1	0.89	0.16	99,99,99,99	0
55	MG	13	1666	1/1	0.89	0.10	115,115,115,115	0
55	MG	13	1633	1/1	0.89	0.24	85,85,85,85	0
55	MG	1H	3110	1/1	0.89	0.28	93,93,93,93	0
55	MG	1H	3155	1/1	0.89	0.32	78,78,78,78	0
55	MG	13	1614	1/1	0.89	0.13	100,100,100,100	0
55	MG	1H	3211	1/1	0.89	0.34	93,93,93,93	0
55	MG	1H	3081	1/1	0.89	0.27	72,72,72,72	0
55	MG	1G	1635	1/1	0.89	0.14	139,139,139,139	0
55	MG	14	3140	1/1	0.89	0.17	86,86,86,86	0
55	MG	1H	3436	1/1	0.89	0.31	96,96,96,96	0
55	MG	1G	1639	1/1	0.89	0.12	106,106,106,106	0
55	MG	1H	3083	1/1	0.89	0.40	85,85,85,85	0
55	MG	1H	3447	1/1	0.89	0.08	102,102,102,102	0
55	MG	1H	3243	1/1	0.90	0.20	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1713	1/1	0.90	0.12	81,81,81,81	0
55	MG	13	1622	1/1	0.90	0.17	88,88,88,88	0
55	MG	13	1605	1/1	0.90	0.26	122,122,122,122	0
55	MG	14	3020	1/1	0.90	0.39	81,81,81,81	0
55	MG	1H	3384	1/1	0.90	0.10	76,76,76,76	0
55	MG	1H	3151	1/1	0.90	0.28	100,100,100,100	0
55	MG	1H	3396	1/1	0.90	0.14	64,64,64,64	0
55	MG	1F	101	1/1	0.90	0.12	107,107,107,107	0
55	MG	1H	3131	1/1	0.90	0.24	73,73,73,73	0
55	MG	1H	3410	1/1	0.90	0.13	95,95,95,95	0
55	MG	14	3059	1/1	0.90	0.25	105,105,105,105	0
55	MG	14	3202	1/1	0.90	0.22	106,106,106,106	0
55	MG	1H	3412	1/1	0.90	0.19	128,128,128,128	0
55	MG	14	3132	1/1	0.90	0.96	100,100,100,100	0
55	MG	1H	3031	1/1	0.90	0.25	83,83,83,83	0
55	MG	1H	3156	1/1	0.90	0.31	75,75,75,75	0
55	MG	14	3220	1/1	0.90	0.09	84,84,84,84	0
55	MG	14	3243	1/1	0.90	0.11	116,116,116,116	0
55	MG	14	3246	1/1	0.90	0.12	105,105,105,105	0
55	MG	1H	3260	1/1	0.90	0.23	53,53,53,53	0
55	MG	1H	3160	1/1	0.90	0.21	81,81,81,81	0
55	MG	13	1608	1/1	0.90	0.12	131,131,131,131	0
55	MG	1H	3136	1/1	0.90	0.43	87,87,87,87	0
55	MG	1H	3003	1/1	0.90	0.14	49,49,49,49	0
55	MG	13	1621	1/1	0.90	0.14	117,117,117,117	0
55	MG	42	201	1/1	0.90	0.28	115,115,115,115	0
55	MG	1H	3038	1/1	0.90	0.18	83,83,83,83	0
55	MG	14	3084	1/1	0.90	0.26	91,91,91,91	0
55	MG	13	1680	1/1	0.90	0.21	108,108,108,108	0
55	MG	13	1707	1/1	0.90	0.18	133,133,133,133	0
55	MG	13	1696	1/1	0.90	0.14	117,117,117,117	0
55	MG	1H	3455	1/1	0.90	0.13	85,85,85,85	0
55	MG	13	1697	1/1	0.90	0.06	146,146,146,146	0
55	MG	1G	1679	1/1	0.90	0.23	79,79,79,79	0
55	MG	1H	3336	1/1	0.90	0.08	127,127,127,127	0
55	MG	1H	3283	1/1	0.90	0.41	83,83,83,83	0
55	MG	13	1655	1/1	0.90	0.15	95,95,95,95	0
55	MG	13	1642	1/1	0.91	0.06	149,149,149,149	0
55	MG	1H	3140	1/1	0.91	0.25	80,80,80,80	0
55	MG	1G	1609	1/1	0.91	0.49	105,105,105,105	0
55	MG	1H	3203	1/1	0.91	0.27	81,81,81,81	0
55	MG	1H	3169	1/1	0.91	0.47	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3437	1/1	0.91	0.21	95,95,95,95	0
55	MG	1H	3308	1/1	0.91	0.22	107,107,107,107	0
55	MG	2A	201	1/1	0.91	0.09	101,101,101,101	0
55	MG	1H	3309	1/1	0.91	0.10	108,108,108,108	0
55	MG	1H	3187	1/1	0.91	0.26	99,99,99,99	0
55	MG	1H	3348	1/1	0.91	0.12	54,54,54,54	0
55	MG	13	1714	1/1	0.91	0.07	121,121,121,121	0
55	MG	1G	1626	1/1	0.91	0.13	100,100,100,100	0
55	MG	14	3007	1/1	0.91	0.15	97,97,97,97	0
55	MG	1H	3454	1/1	0.91	0.21	109,109,109,109	0
55	MG	1H	3190	1/1	0.91	0.11	106,106,106,106	0
55	MG	1H	3130	1/1	0.91	0.36	66,66,66,66	0
55	MG	1G	1675	1/1	0.91	0.20	77,77,77,77	0
55	MG	13	1718	1/1	0.91	0.07	113,113,113,113	0
55	MG	1H	3317	1/1	0.91	0.05	106,106,106,106	0
55	MG	13	1643	1/1	0.91	0.23	124,124,124,124	0
55	MG	1G	1638	1/1	0.91	0.11	151,151,151,151	0
55	MG	13	1677	1/1	0.91	0.23	100,100,100,100	0
55	MG	1H	3162	1/1	0.91	0.18	87,87,87,87	0
55	MG	1G	1686	1/1	0.91	0.31	112,112,112,112	0
55	MG	14	3248	1/1	0.91	0.09	86,86,86,86	0
55	MG	1H	3466	1/1	0.91	0.19	111,111,111,111	0
55	MG	1H	3473	1/1	0.91	0.09	74,74,74,74	0
55	MG	13	1604	1/1	0.91	0.26	87,87,87,87	0
55	MG	14	3279	1/1	0.91	0.07	107,107,107,107	0
55	MG	1G	1696	1/1	0.91	0.08	137,137,137,137	0
55	MG	13	1712	1/1	0.91	0.11	96,96,96,96	0
55	MG	41	201	1/1	0.91	0.17	88,88,88,88	0
55	MG	14	3061	1/1	0.91	0.30	92,92,92,92	0
55	MG	1H	3329	1/1	0.91	0.09	119,119,119,119	0
55	MG	88	202	1/1	0.91	0.98	62,62,62,62	0
55	MG	1H	3417	1/1	0.91	0.13	108,108,108,108	0
55	MG	1H	3030	1/1	0.91	0.47	77,77,77,77	0
55	MG	14	3077	1/1	0.91	0.25	89,89,89,89	0
55	MG	1G	1712	1/1	0.91	0.14	131,131,131,131	0
55	MG	1H	3291	1/1	0.91	0.09	98,98,98,98	0
55	MG	14	3152	1/1	0.91	0.24	90,90,90,90	0
55	MG	14	3161	1/1	0.91	0.18	73,73,73,73	0
55	MG	1H	3420	1/1	0.91	0.10	96,96,96,96	0
55	MG	1G	1655	1/1	0.91	0.13	84,84,84,84	0
55	MG	13	1720	1/1	0.92	0.13	117,117,117,117	0
55	MG	1G	1634	1/1	0.92	0.06	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1657	1/1	0.92	0.14	123,123,123,123	0
55	MG	13	1687	1/1	0.92	0.27	88,88,88,88	0
55	MG	1H	3271	1/1	0.92	0.23	82,82,82,82	0
55	MG	14	3104	1/1	0.92	0.12	91,91,91,91	0
55	MG	1H	3272	1/1	0.92	0.37	83,83,83,83	0
55	MG	1H	3135	1/1	0.92	0.26	75,75,75,75	0
55	MG	14	3183	1/1	0.92	0.31	99,99,99,99	0
55	MG	1H	3403	1/1	0.92	0.10	87,87,87,87	0
55	MG	1H	3404	1/1	0.92	0.11	76,76,76,76	0
55	MG	1G	1687	1/1	0.92	0.12	108,108,108,108	0
55	MG	13	1710	1/1	0.92	0.34	143,143,143,143	0
55	MG	1H	3319	1/1	0.92	0.07	123,123,123,123	0
55	MG	13	1726	1/1	0.92	0.21	103,103,103,103	0
55	MG	1G	1694	1/1	0.92	0.08	151,151,151,151	0
55	MG	14	3193	1/1	0.92	0.08	87,87,87,87	0
55	MG	1H	3158	1/1	0.92	0.18	92,92,92,92	0
55	MG	14	3195	1/1	0.92	0.14	67,67,67,67	0
55	MG	14	3198	1/1	0.92	0.34	109,109,109,109	0
55	MG	14	3115	1/1	0.92	0.23	103,103,103,103	0
55	MG	13	1601	1/1	0.92	0.15	77,77,77,77	0
55	MG	14	3206	1/1	0.92	0.32	131,131,131,131	0
55	MG	14	3117	1/1	0.92	0.17	91,91,91,91	0
55	MG	1H	3028	1/1	0.92	0.15	80,80,80,80	0
55	MG	14	3216	1/1	0.92	0.10	68,68,68,68	0
55	MG	14	3120	1/1	0.92	0.22	106,106,106,106	0
55	MG	13	1618	1/1	0.92	0.17	115,115,115,115	0
55	MG	14	3237	1/1	0.92	0.22	96,96,96,96	0
55	MG	14	3241	1/1	0.92	0.08	86,86,86,86	0
55	MG	14	3036	1/1	0.92	0.18	80,80,80,80	0
55	MG	14	3244	1/1	0.92	0.08	105,105,105,105	0
55	MG	13	1644	1/1	0.92	0.14	109,109,109,109	0
55	MG	14	3044	1/1	0.92	0.17	85,85,85,85	0
55	MG	1H	3248	1/1	0.92	0.33	86,86,86,86	0
55	MG	14	3253	1/1	0.92	0.16	83,83,83,83	0
55	MG	1H	3103	1/1	0.92	0.18	77,77,77,77	0
55	MG	1H	3064	1/1	0.92	0.30	85,85,85,85	0
55	MG	14	3265	1/1	0.92	0.09	65,65,65,65	0
55	MG	14	3270	1/1	0.92	0.17	85,85,85,85	0
55	MG	14	3272	1/1	0.92	0.08	93,93,93,93	0
55	MG	1H	3431	1/1	0.92	0.10	62,62,62,62	0
55	MG	1H	3292	1/1	0.92	0.07	103,103,103,103	0
55	MG	1H	3105	1/1	0.92	0.16	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	14	3072	1/1	0.92	0.18	91,91,91,91	0
55	MG	1G	1716	1/1	0.92	0.08	123,123,123,123	0
55	MG	1G	1615	1/1	0.92	0.21	141,141,141,141	0
55	MG	1H	3296	1/1	0.92	0.17	122,122,122,122	0
55	MG	1H	3167	1/1	0.92	0.40	93,93,93,93	0
55	MG	1H	3448	1/1	0.92	0.10	72,72,72,72	0
55	MG	1H	3007	1/1	0.92	0.23	62,62,62,62	0
55	MG	14	3300	1/1	0.92	0.14	140,140,140,140	0
55	MG	14	3151	1/1	0.92	0.22	96,96,96,96	0
55	MG	1J	202	1/1	0.92	0.13	129,129,129,129	0
55	MG	1H	3341	1/1	0.92	0.09	129,129,129,129	0
55	MG	1H	3344	1/1	0.92	0.07	72,72,72,72	0
55	MG	13	1610	1/1	0.92	0.08	130,130,130,130	0
55	MG	1H	3305	1/1	0.92	0.21	110,110,110,110	0
55	MG	13	1620	1/1	0.92	0.14	70,70,70,70	0
55	MG	14	3014	1/1	0.93	0.18	78,78,78,78	0
55	MG	1H	3206	1/1	0.93	0.23	108,108,108,108	0
55	MG	13	1734	1/1	0.93	0.33	133,133,133,133	0
55	MG	13	1700	1/1	0.93	0.07	151,151,151,151	0
55	MG	1G	1698	1/1	0.93	0.23	176,176,176,176	0
55	MG	1H	3321	1/1	0.93	0.24	123,123,123,123	0
55	MG	1G	1700	1/1	0.93	0.20	142,142,142,142	0
55	MG	1H	3450	1/1	0.93	0.10	132,132,132,132	0
55	MG	1H	3188	1/1	0.93	0.17	91,91,91,91	0
55	MG	1H	3014	1/1	0.93	0.25	64,64,64,64	0
55	MG	14	3030	1/1	0.93	0.25	110,110,110,110	0
55	MG	14	3118	1/1	0.93	0.15	99,99,99,99	0
55	MG	1H	3401	1/1	0.93	0.15	72,72,72,72	0
55	MG	1H	3087	1/1	0.93	0.30	74,74,74,74	0
55	MG	1H	3170	1/1	0.93	0.51	80,80,80,80	0
55	MG	14	3047	1/1	0.93	0.37	83,83,83,83	0
55	MG	14	3123	1/1	0.93	0.23	99,99,99,99	0
55	MG	14	3048	1/1	0.93	0.26	94,94,94,94	0
55	MG	14	3130	1/1	0.93	0.08	106,106,106,106	0
55	MG	13	1669	1/1	0.93	0.09	100,100,100,100	0
55	MG	14	3236	1/1	0.93	0.11	98,98,98,98	0
55	MG	1H	3458	1/1	0.93	0.06	126,126,126,126	0
55	MG	1H	3173	1/1	0.93	0.14	94,94,94,94	0
55	MG	1G	1717	1/1	0.93	0.07	137,137,137,137	0
55	MG	1G	1718	1/1	0.93	0.14	112,112,112,112	0
55	MG	14	3245	1/1	0.93	0.07	117,117,117,117	0
55	MG	14	3064	1/1	0.93	0.32	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3258	1/1	0.93	0.22	73,73,73,73	0
55	MG	14	3071	1/1	0.93	0.13	84,84,84,84	0
55	MG	1H	3051	1/1	0.93	0.19	95,95,95,95	0
55	MG	1H	3052	1/1	0.93	0.16	64,64,64,64	0
55	MG	1H	3267	1/1	0.93	0.31	67,67,67,67	0
55	MG	14	3258	1/1	0.93	0.06	97,97,97,97	0
55	MG	1G	1673	1/1	0.93	0.42	93,93,93,93	0
55	MG	14	3268	1/1	0.93	0.06	82,82,82,82	0
55	MG	32	301	1/1	0.93	0.12	138,138,138,138	0
55	MG	13	1737	1/1	0.93	0.20	111,111,111,111	0
55	MG	14	3149	1/1	0.93	0.12	61,61,61,61	0
55	MG	1F	102	1/1	0.93	0.92	125,125,125,125	0
55	MG	1G	1676	1/1	0.93	0.10	83,83,83,83	0
55	MG	1H	3099	1/1	0.93	0.34	79,79,79,79	0
55	MG	14	3287	1/1	0.93	0.10	110,110,110,110	0
55	MG	2L	101	1/1	0.93	0.15	147,147,147,147	0
55	MG	13	1635	1/1	0.93	0.40	82,82,82,82	0
55	MG	13	1719	1/1	0.93	0.08	107,107,107,107	0
55	MG	88	201	1/1	0.93	0.10	94,94,94,94	0
55	MG	14	3293	1/1	0.93	0.11	130,130,130,130	0
55	MG	14	3294	1/1	0.93	0.09	117,117,117,117	0
55	MG	14	3168	1/1	0.93	0.22	72,72,72,72	0
55	MG	1H	3426	1/1	0.93	0.27	97,97,97,97	0
55	MG	1H	3427	1/1	0.93	0.15	68,68,68,68	0
55	MG	1H	3069	1/1	0.93	0.23	77,77,77,77	0
55	MG	1H	3004	1/1	0.93	0.21	64,64,64,64	0
55	MG	13	1654	1/1	0.93	0.26	81,81,81,81	0
55	MG	1H	3438	1/1	0.93	0.13	93,93,93,93	0
55	MG	14	3179	1/1	0.93	0.21	70,70,70,70	0
55	MG	14	3181	1/1	0.93	0.65	71,71,71,71	0
55	MG	1H	3440	1/1	0.93	0.14	54,54,54,54	0
55	MG	D8	201	1/1	0.94	0.40	84,84,84,84	0
55	MG	14	3091	1/1	0.94	0.19	105,105,105,105	0
55	MG	1H	3232	1/1	0.94	0.28	76,76,76,76	0
55	MG	14	3093	1/1	0.94	0.12	94,94,94,94	0
55	MG	1H	3318	1/1	0.94	0.12	93,93,93,93	0
55	MG	1H	3057	1/1	0.94	0.25	57,57,57,57	0
55	MG	13	1665	1/1	0.94	0.20	115,115,115,115	0
55	MG	14	3103	1/1	0.94	0.26	113,113,113,113	0
55	MG	1H	3277	1/1	0.94	0.38	103,103,103,103	0
55	MG	1H	3100	1/1	0.94	0.28	65,65,65,65	0
55	MG	1H	3201	1/1	0.94	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3242	1/1	0.94	0.27	94,94,94,94	0
55	MG	1H	3102	1/1	0.94	0.30	105,105,105,105	0
55	MG	14	3192	1/1	0.94	0.06	104,104,104,104	0
55	MG	1H	3282	1/1	0.94	0.41	101,101,101,101	0
55	MG	1H	3005	1/1	0.94	0.18	51,51,51,51	0
55	MG	1H	3066	1/1	0.94	0.33	78,78,78,78	0
55	MG	14	3197	1/1	0.94	0.29	114,114,114,114	0
55	MG	1H	3247	1/1	0.94	0.17	101,101,101,101	0
55	MG	1H	3286	1/1	0.94	0.26	67,67,67,67	0
55	MG	1H	3132	1/1	0.94	0.25	79,79,79,79	0
55	MG	14	3205	1/1	0.94	0.22	118,118,118,118	0
55	MG	13	1662	1/1	0.94	0.08	99,99,99,99	0
55	MG	1H	3026	1/1	0.94	0.72	82,82,82,82	0
55	MG	1H	3295	1/1	0.94	0.29	83,83,83,83	0
55	MG	14	3215	1/1	0.94	0.10	111,111,111,111	0
55	MG	1H	3042	1/1	0.94	0.25	96,96,96,96	0
55	MG	14	3022	1/1	0.94	0.47	91,91,91,91	0
55	MG	14	3024	1/1	0.94	0.12	51,51,51,51	0
55	MG	14	3224	1/1	0.94	0.09	84,84,84,84	0
55	MG	14	3227	1/1	0.94	0.11	79,79,79,79	0
55	MG	14	3233	1/1	0.94	0.10	89,89,89,89	0
55	MG	1G	1689	1/1	0.94	0.19	125,125,125,125	0
55	MG	1H	3297	1/1	0.94	0.19	86,86,86,86	0
55	MG	1G	1633	1/1	0.94	0.41	96,96,96,96	0
55	MG	1H	3345	1/1	0.94	0.10	63,63,63,63	0
55	MG	14	3129	1/1	0.94	0.16	90,90,90,90	0
55	MG	1H	3043	1/1	0.94	0.14	72,72,72,72	0
55	MG	14	3032	1/1	0.94	0.16	62,62,62,62	0
55	MG	14	3247	1/1	0.94	0.15	125,125,125,125	0
55	MG	1G	1636	1/1	0.94	0.17	123,123,123,123	0
55	MG	14	3134	1/1	0.94	0.59	105,105,105,105	0
55	MG	14	3251	1/1	0.94	0.11	65,65,65,65	0
55	MG	1H	3347	1/1	0.94	0.18	65,65,65,65	0
55	MG	13	1691	1/1	0.94	0.16	113,113,113,113	0
55	MG	1H	3350	1/1	0.94	0.14	71,71,71,71	0
55	MG	1H	3352	1/1	0.94	0.09	55,55,55,55	0
55	MG	13	1692	1/1	0.94	0.17	107,107,107,107	0
55	MG	1H	3360	1/1	0.94	0.20	62,62,62,62	0
55	MG	1G	1707	1/1	0.94	0.20	122,122,122,122	0
55	MG	1H	3303	1/1	0.94	0.11	98,98,98,98	0
55	MG	14	3278	1/1	0.94	0.11	109,109,109,109	0
55	MG	1H	3375	1/1	0.94	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3382	1/1	0.94	0.12	93,93,93,93	0
55	MG	1H	3304	1/1	0.94	0.16	96,96,96,96	0
55	MG	13	1672	1/1	0.94	0.15	123,123,123,123	0
55	MG	1H	3385	1/1	0.94	0.09	63,63,63,63	0
55	MG	14	3288	1/1	0.94	0.40	86,86,86,86	0
55	MG	1H	3467	1/1	0.94	0.05	106,106,106,106	0
55	MG	13	1609	1/1	0.94	0.12	99,99,99,99	0
55	MG	14	3160	1/1	0.94	0.40	86,86,86,86	0
55	MG	16	201	1/1	0.94	0.22	92,92,92,92	0
55	MG	1G	1719	1/1	0.94	0.10	123,123,123,123	0
55	MG	13	1649	1/1	0.94	0.54	127,127,127,127	0
55	MG	13	1725	1/1	0.94	0.15	119,119,119,119	0
55	MG	1H	3400	1/1	0.94	0.30	78,78,78,78	0
55	MG	1H	3053	1/1	0.94	0.17	77,77,77,77	0
55	MG	1H	3020	1/1	0.94	0.12	77,77,77,77	0
55	MG	1H	3094	1/1	0.94	0.15	95,95,95,95	0
55	MG	39	301	1/1	0.94	0.18	109,109,109,109	0
55	MG	14	3171	1/1	0.94	0.20	98,98,98,98	0
55	MG	14	3087	1/1	0.94	0.79	66,66,66,66	0
55	MG	14	3173	1/1	0.94	0.34	66,66,66,66	0
55	MG	14	3175	1/1	0.94	0.14	85,85,85,85	0
55	MG	1H	3095	1/1	0.94	0.35	63,63,63,63	0
55	MG	1H	3078	1/1	0.95	0.24	63,63,63,63	0
55	MG	13	1645	1/1	0.95	0.13	97,97,97,97	0
55	MG	13	1683	1/1	0.95	0.21	103,103,103,103	0
55	MG	14	3008	1/1	0.95	0.11	81,81,81,81	0
55	MG	1H	3046	1/1	0.95	0.19	69,69,69,69	0
55	MG	1H	3288	1/1	0.95	0.04	99,99,99,99	0
55	MG	1G	1677	1/1	0.95	0.23	110,110,110,110	0
55	MG	1G	1678	1/1	0.95	0.34	99,99,99,99	0
55	MG	1H	3086	1/1	0.95	0.26	79,79,79,79	0
55	MG	14	3196	1/1	0.95	0.10	85,85,85,85	0
55	MG	1H	3245	1/1	0.95	0.51	76,76,76,76	0
55	MG	14	3015	1/1	0.95	0.15	70,70,70,70	0
55	MG	1H	3047	1/1	0.95	0.22	66,66,66,66	0
55	MG	14	3017	1/1	0.95	0.15	83,83,83,83	0
55	MG	1H	3120	1/1	0.95	0.27	81,81,81,81	0
55	MG	1G	1625	1/1	0.95	0.30	118,118,118,118	0
55	MG	13	1684	1/1	0.95	0.12	89,89,89,89	0
55	MG	1H	3442	1/1	0.95	0.14	111,111,111,111	0
55	MG	13	1667	1/1	0.95	0.13	101,101,101,101	0
55	MG	1H	3298	1/1	0.95	0.30	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3299	1/1	0.95	0.10	84,84,84,84	0
55	MG	1H	3251	1/1	0.95	0.38	87,87,87,87	0
55	MG	13	1615	1/1	0.95	0.13	71,71,71,71	0
55	MG	14	3226	1/1	0.95	0.12	59,59,59,59	0
55	MG	14	3127	1/1	0.95	0.27	64,64,64,64	0
55	MG	14	3230	1/1	0.95	0.09	76,76,76,76	0
55	MG	14	3231	1/1	0.95	0.31	65,65,65,65	0
55	MG	1H	3008	1/1	0.95	0.21	82,82,82,82	0
55	MG	1G	1695	1/1	0.95	0.07	130,130,130,130	0
55	MG	1H	3355	1/1	0.95	0.09	83,83,83,83	0
55	MG	14	3238	1/1	0.95	0.07	83,83,83,83	0
55	MG	14	3240	1/1	0.95	0.09	135,135,135,135	0
55	MG	14	3033	1/1	0.95	0.11	76,76,76,76	0
55	MG	14	3034	1/1	0.95	0.19	77,77,77,77	0
55	MG	13	1659	1/1	0.95	0.18	105,105,105,105	0
55	MG	14	3038	1/1	0.95	0.18	91,91,91,91	0
55	MG	1H	3371	1/1	0.95	0.18	85,85,85,85	0
55	MG	1H	3054	1/1	0.95	0.08	77,77,77,77	0
55	MG	1H	3010	1/1	0.95	0.39	70,70,70,70	0
55	MG	1H	3381	1/1	0.95	0.18	68,68,68,68	0
55	MG	14	3050	1/1	0.95	0.23	54,54,54,54	0
55	MG	14	3053	1/1	0.95	0.22	91,91,91,91	0
55	MG	14	3056	1/1	0.95	0.22	60,60,60,60	0
55	MG	1H	3213	1/1	0.95	0.17	100,100,100,100	0
55	MG	1H	3011	1/1	0.95	0.17	48,48,48,48	0
55	MG	14	3259	1/1	0.95	0.10	75,75,75,75	0
55	MG	14	3261	1/1	0.95	0.20	92,92,92,92	0
55	MG	14	3262	1/1	0.95	0.07	60,60,60,60	0
55	MG	14	3263	1/1	0.95	0.17	76,76,76,76	0
55	MG	1H	3159	1/1	0.95	0.27	79,79,79,79	0
55	MG	1G	1710	1/1	0.95	0.07	125,125,125,125	0
55	MG	1H	3217	1/1	0.95	0.24	43,43,43,43	0
55	MG	1H	3393	1/1	0.95	0.09	79,79,79,79	0
55	MG	14	3274	1/1	0.95	0.09	110,110,110,110	0
55	MG	14	3153	1/1	0.95	0.20	59,59,59,59	0
55	MG	1H	3058	1/1	0.95	0.23	58,58,58,58	0
55	MG	14	3280	1/1	0.95	0.12	101,101,101,101	0
55	MG	14	3281	1/1	0.95	0.16	92,92,92,92	0
55	MG	1H	3469	1/1	0.95	0.20	110,110,110,110	0
55	MG	1H	3063	1/1	0.95	0.24	63,63,63,63	0
55	MG	1H	3012	1/1	0.95	0.13	47,47,47,47	0
55	MG	1H	3316	1/1	0.95	0.05	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3225	1/1	0.95	0.21	109,109,109,109	0
55	MG	13	1728	1/1	0.95	0.09	114,114,114,114	0
55	MG	1H	3228	1/1	0.95	0.43	86,86,86,86	0
55	MG	1G	1658	1/1	0.95	0.19	114,114,114,114	0
55	MG	13	1732	1/1	0.95	0.22	108,108,108,108	0
55	MG	1H	3409	1/1	0.95	0.13	63,63,63,63	0
55	MG	1H	3276	1/1	0.95	0.21	74,74,74,74	0
55	MG	1G	1726	1/1	0.95	0.09	136,136,136,136	0
55	MG	1H	3411	1/1	0.95	0.12	81,81,81,81	0
55	MG	P8	101	1/1	0.95	0.27	61,61,61,61	0
55	MG	13	1717	1/1	0.95	0.13	109,109,109,109	0
55	MG	13	1613	1/1	0.95	0.22	129,129,129,129	0
55	MG	14	3180	1/1	0.95	0.25	81,81,81,81	0
55	MG	1H	3235	1/1	0.95	0.25	57,57,57,57	0
55	MG	7A	101	1/1	0.95	0.12	116,116,116,116	0
55	MG	1H	3236	1/1	0.95	0.15	72,72,72,72	0
55	MG	13	1699	1/1	0.95	0.12	116,116,116,116	0
55	MG	1H	3002	1/1	0.95	0.20	55,55,55,55	0
55	MG	1H	3157	1/1	0.96	0.38	73,73,73,73	0
55	MG	14	3005	1/1	0.96	0.28	85,85,85,85	0
55	MG	14	3100	1/1	0.96	0.10	91,91,91,91	0
55	MG	14	3101	1/1	0.96	0.17	88,88,88,88	0
55	MG	13	1626	1/1	0.96	0.16	123,123,123,123	0
55	MG	1H	3349	1/1	0.96	0.10	67,67,67,67	0
55	MG	1H	3079	1/1	0.96	0.34	71,71,71,71	0
55	MG	1H	3425	1/1	0.96	0.16	102,102,102,102	0
55	MG	1H	3351	1/1	0.96	0.14	70,70,70,70	0
55	MG	1G	1613	1/1	0.96	0.19	94,94,94,94	0
55	MG	14	3199	1/1	0.96	0.09	97,97,97,97	0
55	MG	1H	3056	1/1	0.96	0.22	46,46,46,46	0
55	MG	14	3203	1/1	0.96	0.08	95,95,95,95	0
55	MG	1H	3016	1/1	0.96	0.09	62,62,62,62	0
55	MG	1G	1617	1/1	0.96	0.18	91,91,91,91	0
55	MG	1H	3432	1/1	0.96	0.07	71,71,71,71	0
55	MG	1G	1619	1/1	0.96	0.17	98,98,98,98	0
55	MG	14	3208	1/1	0.96	0.15	70,70,70,70	0
55	MG	14	3209	1/1	0.96	0.13	65,65,65,65	0
55	MG	14	3211	1/1	0.96	0.08	84,84,84,84	0
55	MG	14	3212	1/1	0.96	0.09	67,67,67,67	0
55	MG	1H	3433	1/1	0.96	0.09	87,87,87,87	0
55	MG	1H	3434	1/1	0.96	0.09	59,59,59,59	0
55	MG	1H	3109	1/1	0.96	0.11	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3357	1/1	0.96	0.08	89,89,89,89	0
55	MG	1G	1688	1/1	0.96	0.11	94,94,94,94	0
55	MG	14	3222	1/1	0.96	0.09	67,67,67,67	0
55	MG	13	1660	1/1	0.96	0.12	120,120,120,120	0
55	MG	1H	3364	1/1	0.96	0.10	74,74,74,74	0
55	MG	14	3025	1/1	0.96	0.13	90,90,90,90	0
55	MG	14	3229	1/1	0.96	0.12	74,74,74,74	0
55	MG	1H	3365	1/1	0.96	0.11	82,82,82,82	0
55	MG	1G	1628	1/1	0.96	0.21	118,118,118,118	0
55	MG	1H	3443	1/1	0.96	0.09	73,73,73,73	0
55	MG	1H	3060	1/1	0.96	0.32	68,68,68,68	0
55	MG	1H	3061	1/1	0.96	0.18	66,66,66,66	0
55	MG	1H	3374	1/1	0.96	0.11	47,47,47,47	0
55	MG	14	3239	1/1	0.96	0.13	106,106,106,106	0
55	MG	1H	3062	1/1	0.96	0.21	85,85,85,85	0
55	MG	1H	3377	1/1	0.96	0.11	58,58,58,58	0
55	MG	1H	3380	1/1	0.96	0.07	83,83,83,83	0
55	MG	1H	3089	1/1	0.96	0.28	82,82,82,82	0
55	MG	14	3040	1/1	0.96	0.23	62,62,62,62	0
55	MG	1G	1704	1/1	0.96	0.16	130,130,130,130	0
55	MG	14	3043	1/1	0.96	0.28	54,54,54,54	0
55	MG	1G	1705	1/1	0.96	0.10	102,102,102,102	0
55	MG	1H	3290	1/1	0.96	0.17	79,79,79,79	0
55	MG	1H	3323	1/1	0.96	0.20	100,100,100,100	0
55	MG	1H	3116	1/1	0.96	0.12	91,91,91,91	0
55	MG	1G	1709	1/1	0.96	0.06	127,127,127,127	0
55	MG	5I	102	1/1	0.96	0.43	119,119,119,119	0
55	MG	1H	3386	1/1	0.96	0.10	56,56,56,56	0
55	MG	1H	3390	1/1	0.96	0.09	74,74,74,74	0
55	MG	14	3260	1/1	0.96	0.20	110,110,110,110	0
55	MG	14	3147	1/1	0.96	0.17	63,63,63,63	0
55	MG	1H	3326	1/1	0.96	0.09	109,109,109,109	0
55	MG	1H	3327	1/1	0.96	0.08	121,121,121,121	0
55	MG	1H	3259	1/1	0.96	0.30	53,53,53,53	0
55	MG	13	1646	1/1	0.96	0.17	122,122,122,122	0
55	MG	14	3156	1/1	0.96	0.28	80,80,80,80	0
55	MG	14	3158	1/1	0.96	0.22	51,51,51,51	0
55	MG	14	3065	1/1	0.96	0.19	68,68,68,68	0
55	MG	14	3276	1/1	0.96	0.10	109,109,109,109	0
55	MG	14	3067	1/1	0.96	0.17	97,97,97,97	0
55	MG	1H	3398	1/1	0.96	0.07	84,84,84,84	0
55	MG	1H	3468	1/1	0.96	0.51	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3262	1/1	0.96	0.27	74,74,74,74	0
55	MG	14	3283	1/1	0.96	0.05	106,106,106,106	0
55	MG	14	3073	1/1	0.96	0.18	69,69,69,69	0
55	MG	14	3167	1/1	0.96	0.17	100,100,100,100	0
55	MG	1H	3092	1/1	0.96	0.18	92,92,92,92	0
55	MG	1G	1721	1/1	0.96	0.09	123,123,123,123	0
55	MG	13	1716	1/1	0.96	0.05	103,103,103,103	0
55	MG	1H	3333	1/1	0.96	0.08	80,80,80,80	0
55	MG	13	1703	1/1	0.96	0.17	110,110,110,110	0
55	MG	21	303	1/1	0.96	0.13	63,63,63,63	0
55	MG	14	3174	1/1	0.96	0.39	60,60,60,60	0
55	MG	13	1632	1/1	0.96	0.47	109,109,109,109	0
55	MG	1H	3270	1/1	0.96	0.35	62,62,62,62	0
55	MG	2K	101	1/1	0.96	0.31	71,71,71,71	0
55	MG	14	3297	1/1	0.96	0.11	115,115,115,115	0
55	MG	1H	3070	1/1	0.96	0.20	55,55,55,55	0
55	MG	14	3299	1/1	0.96	0.21	89,89,89,89	0
55	MG	14	3086	1/1	0.96	0.51	97,97,97,97	0
55	MG	1H	3413	1/1	0.96	0.17	93,93,93,93	0
55	MG	13	1693	1/1	0.96	0.28	100,100,100,100	0
55	MG	29	301	1/1	0.96	0.14	64,64,64,64	0
55	MG	1H	3101	1/1	0.96	0.20	89,89,89,89	0
55	MG	BA	201	1/1	0.96	0.11	127,127,127,127	0
55	MG	1H	3073	1/1	0.96	0.22	74,74,74,74	0
55	MG	1G	1602	1/1	0.96	0.09	109,109,109,109	0
55	MG	85	201	1/1	0.96	0.40	72,72,72,72	0
55	MG	13	1730	1/1	0.96	0.18	125,125,125,125	0
55	MG	14	3095	1/1	0.96	0.31	88,88,88,88	0
55	MG	1H	3369	1/1	0.97	0.15	63,63,63,63	0
55	MG	1H	3370	1/1	0.97	0.13	59,59,59,59	0
55	MG	14	3218	1/1	0.97	0.12	69,69,69,69	0
55	MG	1H	3424	1/1	0.97	0.07	68,68,68,68	0
55	MG	14	3221	1/1	0.97	0.11	67,67,67,67	0
55	MG	1H	3230	1/1	0.97	0.24	73,73,73,73	0
55	MG	14	3223	1/1	0.97	0.09	81,81,81,81	0
55	MG	13	1611	1/1	0.97	0.14	81,81,81,81	0
55	MG	J8	101	1/1	0.97	0.43	74,74,74,74	0
55	MG	1H	3152	1/1	0.97	0.29	49,49,49,49	0
55	MG	14	3068	1/1	0.97	0.10	71,71,71,71	0
55	MG	1H	3430	1/1	0.97	0.12	54,54,54,54	0
55	MG	1G	1664	1/1	0.97	0.10	105,105,105,105	0
55	MG	1H	3306	1/1	0.97	0.06	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	14	3235	1/1	0.97	0.21	73,73,73,73	0
55	MG	1H	3307	1/1	0.97	0.07	100,100,100,100	0
55	MG	1H	3048	1/1	0.97	0.34	93,93,93,93	0
55	MG	1G	1605	1/1	0.97	0.17	98,98,98,98	0
55	MG	1H	3209	1/1	0.97	0.37	84,84,84,84	0
55	MG	14	3155	1/1	0.97	0.38	92,92,92,92	0
55	MG	1H	3435	1/1	0.97	0.06	80,80,80,80	0
55	MG	1H	3039	1/1	0.97	0.20	73,73,73,73	0
55	MG	1G	1672	1/1	0.97	0.18	102,102,102,102	0
55	MG	1H	3023	1/1	0.97	0.21	85,85,85,85	0
55	MG	1H	3338	1/1	0.97	0.30	105,105,105,105	0
55	MG	1H	3439	1/1	0.97	0.09	69,69,69,69	0
55	MG	13	1689	1/1	0.97	0.43	85,85,85,85	0
55	MG	14	3249	1/1	0.97	0.07	110,110,110,110	0
55	MG	1H	3441	1/1	0.97	0.09	64,64,64,64	0
55	MG	14	3166	1/1	0.97	0.24	82,82,82,82	0
55	MG	1H	3266	1/1	0.97	0.19	64,64,64,64	0
55	MG	1H	3388	1/1	0.97	0.15	56,56,56,56	0
55	MG	14	3255	1/1	0.97	0.15	80,80,80,80	0
55	MG	14	3089	1/1	0.97	0.16	79,79,79,79	0
55	MG	1H	3444	1/1	0.97	0.10	50,50,50,50	0
55	MG	1H	3389	1/1	0.97	0.09	68,68,68,68	0
55	MG	1H	3314	1/1	0.97	0.07	113,113,113,113	0
55	MG	1H	3289	1/1	0.97	0.20	102,102,102,102	0
55	MG	1H	3075	1/1	0.97	0.23	72,72,72,72	0
55	MG	1H	3395	1/1	0.97	0.07	67,67,67,67	0
55	MG	1H	3077	1/1	0.97	0.18	60,60,60,60	0
55	MG	14	3267	1/1	0.97	0.11	88,88,88,88	0
55	MG	1H	3108	1/1	0.97	0.42	58,58,58,58	0
55	MG	14	3269	1/1	0.97	0.18	104,104,104,104	0
55	MG	1H	3453	1/1	0.97	0.13	99,99,99,99	0
55	MG	1H	3032	1/1	0.97	0.24	66,66,66,66	0
55	MG	14	3273	1/1	0.97	0.09	89,89,89,89	0
55	MG	1G	1691	1/1	0.97	0.19	115,115,115,115	0
55	MG	14	3275	1/1	0.97	0.16	94,94,94,94	0
55	MG	1H	3294	1/1	0.97	0.59	83,83,83,83	0
55	MG	1G	1631	1/1	0.97	0.09	95,95,95,95	0
55	MG	1H	3013	1/1	0.97	0.22	63,63,63,63	0
55	MG	14	3023	1/1	0.97	0.05	99,99,99,99	0
55	MG	1H	3080	1/1	0.97	0.24	64,64,64,64	0
55	MG	14	3282	1/1	0.97	0.09	117,117,117,117	0
55	MG	13	1612	1/1	0.97	0.24	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3187	1/1	0.97	0.14	74,74,74,74	0
55	MG	1H	3459	1/1	0.97	0.21	112,112,112,112	0
55	MG	1H	3146	1/1	0.97	0.10	80,80,80,80	0
55	MG	1H	3356	1/1	0.97	0.11	59,59,59,59	0
55	MG	1H	3097	1/1	0.97	0.29	66,66,66,66	0
55	MG	1H	3464	1/1	0.97	0.12	67,67,67,67	0
55	MG	1G	1702	1/1	0.97	0.13	83,83,83,83	0
55	MG	1H	3359	1/1	0.97	0.12	51,51,51,51	0
55	MG	1H	3227	1/1	0.97	0.14	61,61,61,61	0
55	MG	1H	3361	1/1	0.97	0.07	53,53,53,53	0
55	MG	14	3037	1/1	0.97	0.10	54,54,54,54	0
55	MG	1H	3414	1/1	0.97	0.08	82,82,82,82	0
55	MG	1H	3415	1/1	0.97	0.06	88,88,88,88	0
55	MG	1H	3471	1/1	0.97	0.11	79,79,79,79	0
55	MG	1H	3362	1/1	0.97	0.11	69,69,69,69	0
55	MG	1H	3363	1/1	0.97	0.11	61,61,61,61	0
55	MG	1H	3035	1/1	0.97	0.17	71,71,71,71	0
55	MG	11	301	1/1	0.97	0.23	52,52,52,52	0
55	MG	13	1623	1/1	0.97	0.35	112,112,112,112	0
55	MG	14	3131	1/1	0.97	0.59	88,88,88,88	0
55	MG	14	3051	1/1	0.97	0.21	67,67,67,67	0
55	MG	1H	3366	1/1	0.97	0.14	75,75,75,75	0
55	MG	14	3054	1/1	0.97	0.07	113,113,113,113	0
55	MG	14	3213	1/1	0.97	0.12	77,77,77,77	0
55	MG	1G	1653	1/1	0.97	0.17	103,103,103,103	0
55	MG	1H	3367	1/1	0.97	0.11	92,92,92,92	0
57	ZN	5A	101	1/1	0.97	0.07	159,159,159,159	0
55	MG	14	3219	1/1	0.98	0.10	63,63,63,63	0
55	MG	14	3055	1/1	0.98	0.12	80,80,80,80	0
55	MG	1H	3125	1/1	0.98	0.09	125,125,125,125	0
55	MG	14	3058	1/1	0.98	0.15	95,95,95,95	0
55	MG	1H	3250	1/1	0.98	0.32	53,53,53,53	0
55	MG	1H	3391	1/1	0.98	0.08	81,81,81,81	0
55	MG	14	3225	1/1	0.98	0.09	63,63,63,63	0
55	MG	1H	3222	1/1	0.98	0.11	101,101,101,101	0
55	MG	1H	3177	1/1	0.98	0.13	82,82,82,82	0
55	MG	14	3228	1/1	0.98	0.14	72,72,72,72	0
55	MG	13	1625	1/1	0.98	0.26	101,101,101,101	0
55	MG	1H	3098	1/1	0.98	0.17	54,54,54,54	0
55	MG	1G	1608	1/1	0.98	0.07	114,114,114,114	0
55	MG	14	3066	1/1	0.98	0.31	82,82,82,82	0
55	MG	14	3234	1/1	0.98	0.21	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3112	1/1	0.98	0.21	68,68,68,68	0
55	MG	1G	1610	1/1	0.98	0.13	100,100,100,100	0
55	MG	1H	3025	1/1	0.98	0.16	55,55,55,55	0
55	MG	14	3070	1/1	0.98	0.21	72,72,72,72	0
55	MG	1H	3446	1/1	0.98	0.10	88,88,88,88	0
55	MG	1H	3399	1/1	0.98	0.13	86,86,86,86	0
55	MG	14	3154	1/1	0.98	0.35	65,65,65,65	0
55	MG	14	3242	1/1	0.98	0.05	89,89,89,89	0
55	MG	13	1729	1/1	0.98	0.09	86,86,86,86	0
55	MG	14	3075	1/1	0.98	0.17	99,99,99,99	0
55	MG	14	3157	1/1	0.98	0.19	61,61,61,61	0
55	MG	13	1715	1/1	0.98	0.10	99,99,99,99	0
55	MG	14	3159	1/1	0.98	0.13	83,83,83,83	0
55	MG	1G	1616	1/1	0.98	0.16	93,93,93,93	0
55	MG	14	3002	1/1	0.98	0.15	53,53,53,53	0
55	MG	1H	3402	1/1	0.98	0.13	66,66,66,66	0
55	MG	1H	3358	1/1	0.98	0.10	60,60,60,60	0
55	MG	14	3252	1/1	0.98	0.16	66,66,66,66	0
55	MG	1H	3076	1/1	0.98	0.23	70,70,70,70	0
55	MG	1H	3261	1/1	0.98	0.17	70,70,70,70	0
55	MG	1G	1680	1/1	0.98	0.26	138,138,138,138	0
55	MG	1H	3406	1/1	0.98	0.08	70,70,70,70	0
55	MG	1H	3407	1/1	0.98	0.06	76,76,76,76	0
55	MG	1H	3408	1/1	0.98	0.13	58,58,58,58	0
55	MG	1H	3036	1/1	0.98	0.13	74,74,74,74	0
55	MG	1H	3263	1/1	0.98	0.23	53,53,53,53	0
55	MG	1H	3186	1/1	0.98	0.30	80,80,80,80	0
55	MG	1H	3460	1/1	0.98	0.07	64,64,64,64	0
55	MG	14	3264	1/1	0.98	0.17	88,88,88,88	0
55	MG	1H	3265	1/1	0.98	0.36	63,63,63,63	0
55	MG	14	3266	1/1	0.98	0.07	83,83,83,83	0
55	MG	1H	3233	1/1	0.98	0.29	102,102,102,102	0
55	MG	1H	3234	1/1	0.98	0.29	92,92,92,92	0
55	MG	1H	3150	1/1	0.98	0.24	79,79,79,79	0
55	MG	1H	3368	1/1	0.98	0.10	83,83,83,83	0
55	MG	14	3271	1/1	0.98	0.07	56,56,56,56	0
55	MG	14	3096	1/1	0.98	0.29	55,55,55,55	0
55	MG	13	1731	1/1	0.98	0.25	79,79,79,79	0
55	MG	13	1694	1/1	0.98	0.43	117,117,117,117	0
55	MG	13	1682	1/1	0.98	0.18	118,118,118,118	0
55	MG	1H	3171	1/1	0.98	0.14	91,91,91,91	0
55	MG	14	3277	1/1	0.98	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3470	1/1	0.98	0.13	69,69,69,69	0
55	MG	13	1727	1/1	0.98	0.26	100,100,100,100	0
55	MG	1H	3472	1/1	0.98	0.19	64,64,64,64	0
55	MG	1H	3059	1/1	0.98	0.15	78,78,78,78	0
55	MG	1H	3215	1/1	0.98	0.25	78,78,78,78	0
55	MG	1G	1643	1/1	0.98	0.31	105,105,105,105	0
55	MG	1G	1703	1/1	0.98	0.10	94,94,94,94	0
55	MG	14	3031	1/1	0.98	0.31	77,77,77,77	0
55	MG	1H	3378	1/1	0.98	0.12	75,75,75,75	0
55	MG	1H	3379	1/1	0.98	0.10	76,76,76,76	0
55	MG	1H	3339	1/1	0.98	0.11	78,78,78,78	0
55	MG	1H	3084	1/1	0.98	0.19	71,71,71,71	0
55	MG	1H	3429	1/1	0.98	0.07	92,92,92,92	0
55	MG	78	201	1/1	0.98	0.37	90,90,90,90	0
55	MG	14	3039	1/1	0.98	0.18	75,75,75,75	0
55	MG	1H	3124	1/1	0.98	0.39	69,69,69,69	0
55	MG	14	3201	1/1	0.98	0.08	101,101,101,101	0
55	MG	14	3295	1/1	0.98	0.11	104,104,104,104	0
55	MG	1H	3342	1/1	0.98	0.12	60,60,60,60	0
55	MG	14	3042	1/1	0.98	0.17	80,80,80,80	0
55	MG	1H	3343	1/1	0.98	0.14	56,56,56,56	0
55	MG	1H	3218	1/1	0.98	0.16	95,95,95,95	0
55	MG	14	3046	1/1	0.98	0.12	76,76,76,76	0
55	MG	14	3124	1/1	0.98	0.13	95,95,95,95	0
55	MG	1G	1654	1/1	0.98	0.12	107,107,107,107	0
55	MG	14	3126	1/1	0.98	0.24	48,48,48,48	0
55	MG	C8	201	1/1	0.98	0.37	76,76,76,76	0
55	MG	14	3128	1/1	0.98	0.19	54,54,54,54	0
55	MG	14	3049	1/1	0.98	0.20	80,80,80,80	0
55	MG	1H	3219	1/1	0.98	0.15	91,91,91,91	0
55	MG	I8	101	1/1	0.98	0.19	87,87,87,87	0
55	MG	14	3052	1/1	0.98	0.15	64,64,64,64	0
55	MG	1H	3387	1/1	0.98	0.11	67,67,67,67	0
55	MG	1H	3220	1/1	0.98	0.18	85,85,85,85	0
55	MG	13	1650	1/1	0.99	0.19	106,106,106,106	0
55	MG	14	3074	1/1	0.99	0.16	92,92,92,92	0
55	MG	14	3097	1/1	0.99	0.25	55,55,55,55	0
55	MG	1H	3354	1/1	0.99	0.08	61,61,61,61	0
55	MG	14	3256	1/1	0.99	0.13	87,87,87,87	0
55	MG	1G	1624	1/1	0.99	0.14	94,94,94,94	0
55	MG	14	3200	1/1	0.99	0.07	70,70,70,70	0
55	MG	14	3148	1/1	0.99	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3035	1/1	0.99	0.17	68,68,68,68	0
55	MG	14	3150	1/1	0.99	0.15	89,89,89,89	0
55	MG	14	3232	1/1	0.99	0.11	59,59,59,59	0
55	MG	1H	3392	1/1	0.99	0.10	47,47,47,47	0
55	MG	14	3102	1/1	0.99	0.14	83,83,83,83	0
55	MG	14	3057	1/1	0.99	0.24	90,90,90,90	0
55	MG	1H	3072	1/1	0.99	0.26	53,53,53,53	0
55	MG	1H	3239	1/1	0.99	0.24	103,103,103,103	0
55	MG	1H	3015	1/1	0.99	0.16	93,93,93,93	0
55	MG	14	3210	1/1	0.99	0.14	60,60,60,60	0
55	MG	1H	3287	1/1	0.99	0.18	58,58,58,58	0
55	MG	1H	3068	1/1	0.99	0.14	53,53,53,53	0
55	MG	C8	202	1/1	0.99	0.39	70,70,70,70	0
55	MG	13	1658	1/1	0.99	0.11	114,114,114,114	0
55	MG	1H	3372	1/1	0.99	0.19	94,94,94,94	0
55	MG	14	3045	1/1	0.99	0.14	89,89,89,89	0
55	MG	1H	3428	1/1	0.99	0.14	66,66,66,66	0
55	MG	1H	3194	1/1	0.99	0.20	113,113,113,113	0
55	MG	1H	3082	1/1	0.99	0.22	77,77,77,77	0
55	MG	13	1721	1/1	0.99	0.08	87,87,87,87	0
55	MG	1H	3376	1/1	0.99	0.09	58,58,58,58	0
56	SF4	3E	301	8/8	0.99	0.20	96,110,122,122	0
56	SF4	32	302	8/8	0.99	0.20	112,135,144,151	0
57	ZN	5I	103	1/1	0.99	0.12	109,109,109,109	0
55	MG	21	302	1/1	0.99	0.17	50,50,50,50	0
55	MG	1H	3257	1/1	1.00	0.22	53,53,53,53	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.