wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 06:35 pm GMT

PDB ID	:	5E7K
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and cognate tRNALys in the A-site
Authors	:	Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on	:	2015-10-12
Resolution	:	3.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

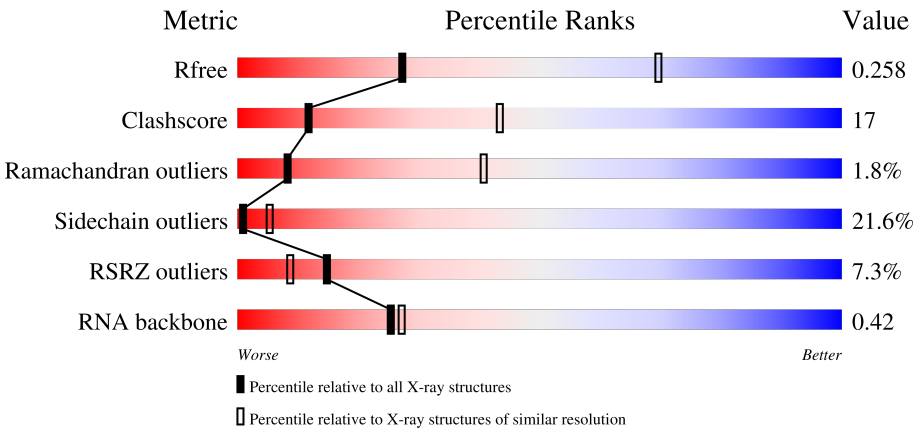
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	13	1522	34% 44% 17% • •
1	1G	1522	36% 43% 18% • •
2	12	256	9% 38% 35% 8% • 18%
2	1E	256	11% 34% 41% 15% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	22	239	20% 40% 36% 5% • 18%
3	2E	239	15% 46% 33% 7% 14%
4	32	209	22% 35% 53% 11%
4	3E	209	13% 47% 40% 11% ••
5	42	162	6% 49% 35% 7% 9%
5	4E	162	6% 48% 38% 7% 8%
6	52	101	21% 55% 36% 9%
6	5E	101	11% 50% 41% 8% •
7	62	156	44% 41% • 12%
7	6E	156	.% 58% 31% 9% •
8	72	138	3% 57% 33% 9% •
8	7E	138	.% 41% 47% 12%
9	82	128	2% 36% 45% 12% • 5%
9	8E	128	45% 47% 7% •
10	1A	105	2% 38% 30% 9% 24%
10	1I	105	7% 45% 34% 8% 13%
11	2A	129	10% 48% 31% 9% 12%
11	2I	129	4% 34% 39% 13% 14%
12	3A	132	21% 42% 36% 13% • 8%
12	3I	132	12% 56% 30% 6% • 8%
13	4A	126	9% 35% 40% 13% 12%
13	4I	126	3% 46% 38% 10% • 6%
14	5A	61	36% 43% 46% 7% • •
14	5I	61	48% 36% 15% •
15	6A	89	2% 46% 46% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6I	89	47% 42% 9% •
16	7A	88	2% 47% 38% 11% 5%
16	7I	88	8% 30% 53% 11% 6%
17	8A	105	3% 53% 32% 9% 6%
17	8I	105	% 48% 37% 10% 5%
18	9A	88	25% 36% 30% 10% 24%
18	9I	88	19% 34% 32% 10% • 23%
19	AA	93	15% 28% 31% 8% 33%
19	AI	93	6% 38% 40% 9% • 13%
20	BA	106	% 54% 32% 6% • 7%
20	BI	106	% 36% 45% 10% 8%
21	1B	27	19% 33% 48% 19%
21	1F	27	52% 33% 15%
22	1K	75	% 21% 49% 20% • 5%
23	2K	77	35% 31% 25% 9%
23	2L	77	32% 42% 21% 5%
24	3K	76	% 16% 47% 32% 5%
25	4K	27	4% 22% 22% 26% 30%
25	4L	27	26% 15% 26% 33%
26	14	2917	% 32% 41% 21% • •
26	1H	2917	27% 40% 24% 6% •
27	16	122	% 44% 33% 16% 7%
27	1J	122	31% 43% 23% •
28	71	229	15% 24% 26% 8% 42%
28	79	229	15% 7% • 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	11	276	50% 33% 11%
29	19	276	4% 49% 39% 11%
30	21	206	17% 47% 38% 11%
30	29	206	18% 44% 38% 16%
31	31	210	10% 47% 40% 9%
31	39	210	16% 42% 43% 11%
32	41	182	21% 38% 47% 13%
32	49	182	23% 48% 41% 10%
33	51	180	5% 44% 36% 12% 5%
33	59	180	4% 13% 22% 6% 59%
34	61	148	24% 45% 41% 10%
34	69	148	29% 45% 41% 10%
35	15	140	40% 57% 30% 11%
35	58	140	4% 50% 39% 9%
36	25	122	56% 38% 7%
36	68	122	2% 54% 38% 8%
37	35	150	5% 39% 43% 15%
37	78	150	2% 37% 39% 19%
38	45	141	49% 43% 40% 13%
38	88	141	22% 52% 36% 9%
39	55	118	% 44% 50% 5%
39	98	118	8% 42% 46% 11%
40	65	112	4% 35% 46% 16%
40	A8	112	58% 41% 46% 12%
41	75	146	2% 49% 33% 10% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	B8	146	%, 42%, 37%, 11%, 9%
42	85	118	28%, 49%, 41%, 7%
42	C8	118	3%, 56%, 28%, 12%
43	95	101	68%, 40%, 43%, 12%, 5%
43	D8	101	6%, 46%, 33%, 18%
44	A5	113	2%, 58%, 32%, 9%
44	E8	113	4%, 57%, 31%, 12%
45	B5	96	14%, 53%, 28%, 17%
45	F8	96	10%, 53%, 40%, 6%
46	C5	110	8%, 28%, 46%, 17%, 5%
46	G8	110	47%, 30%, 16%, 5%
47	D5	206	28%, 23%, 32%, 8%, 36%
47	H8	206	32%, 37%, 33%, 12%, 17%
48	E5	85	5%, 53%, 29%, 8%, 9%
48	I8	85	4%, 47%, 36%, 6%, 11%
49	F5	98	2%, 47%, 38%, 11%
49	J8	98	2%, 47%, 36%, 10%
50	G5	72	6%, 35%, 39%, 12%, 6%, 8%
50	K8	72	3%, 43%, 36%, 11%, 6%
51	H5	60	43%, 55%, 40%
51	L8	60	5%, 52%, 33%, 12%
52	M8	71	44%, 20%, 37%, 8%, 34%
53	J5	60	55%, 32%, 7%, 7%
53	N8	60	12%, 38%, 32%, 10%, 20%
54	L5	49	4%, 57%, 37%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	P8	49	55% 37%
55	M5	65	43% 43% 11%
55	Q8	65	37% 45% 15%
56	1L	76	20% 30% 36% 21% 9%
57	3L	76	24% 45% 25% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	13	1603	-	-	-	X
58	MG	13	1630	-	-	-	X
58	MG	13	1641	-	-	-	X
58	MG	13	1644	-	-	-	X
58	MG	13	1653	-	-	-	X
58	MG	13	1659	-	-	-	X
58	MG	13	1672	-	-	-	X
58	MG	13	1689	-	-	-	X
58	MG	13	1694	-	-	-	X
58	MG	13	1695	-	-	-	X
58	MG	13	1704	-	-	-	X
58	MG	14	3017	-	-	-	X
58	MG	14	3018	-	-	-	X
58	MG	14	3019	-	-	-	X
58	MG	14	3029	-	-	-	X
58	MG	14	3034	-	-	-	X
58	MG	14	3037	-	-	-	X
58	MG	14	3052	-	-	-	X
58	MG	14	3068	-	-	-	X
58	MG	14	3073	-	-	-	X
58	MG	14	3080	-	-	-	X
58	MG	14	3085	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3108	-	-	-	X
58	MG	14	3117	-	-	-	X
58	MG	14	3129	-	-	-	X
58	MG	14	3144	-	-	-	X
58	MG	14	3150	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3153	-	-	-	X
58	MG	14	3155	-	-	-	X
58	MG	14	3181	-	-	-	X
58	MG	14	3182	-	-	-	X
58	MG	14	3183	-	-	-	X
58	MG	14	3185	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3188	-	-	-	X
58	MG	14	3190	-	-	-	X
58	MG	14	3191	-	-	-	X
58	MG	14	3227	-	-	-	X
58	MG	14	3229	-	-	-	X
58	MG	14	3234	-	-	-	X
58	MG	14	3243	-	-	-	X
58	MG	14	3250	-	-	-	X
58	MG	14	3251	-	-	-	X
58	MG	14	3257	-	-	-	X
58	MG	14	3259	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3261	-	-	-	X
58	MG	14	3264	-	-	-	X
58	MG	14	3265	-	-	-	X
58	MG	14	3268	-	-	-	X
58	MG	14	3269	-	-	-	X
58	MG	14	3280	-	-	-	X
58	MG	14	3282	-	-	-	X
58	MG	14	3288	-	-	-	X
58	MG	14	3293	-	-	-	X
58	MG	14	3297	-	-	-	X
58	MG	14	3302	-	-	-	X
58	MG	14	3304	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	14	3313	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1604	-	-	-	X
58	MG	1G	1649	-	-	-	X
58	MG	1G	1666	-	-	-	X
58	MG	1G	1672	-	-	-	X
58	MG	1H	3016	-	-	-	X
58	MG	1H	3024	-	-	-	X
58	MG	1H	3031	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3032	-	-	-	X
58	MG	1H	3033	-	-	-	X
58	MG	1H	3035	-	-	-	X
58	MG	1H	3036	-	-	-	X
58	MG	1H	3043	-	-	-	X
58	MG	1H	3087	-	-	-	X
58	MG	1H	3122	-	-	-	X
58	MG	1H	3142	-	-	-	X
58	MG	1H	3154	-	-	-	X
58	MG	1H	3167	-	-	-	X
58	MG	1H	3171	-	-	-	X
58	MG	1H	3175	-	-	-	X
58	MG	1H	3180	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3201	-	-	-	X
58	MG	1H	3207	-	-	-	X
58	MG	1H	3224	-	-	-	X
58	MG	1H	3228	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3268	-	-	-	X
58	MG	1H	3278	-	-	-	X
58	MG	1H	3279	-	-	-	X
58	MG	1H	3282	-	-	-	X
58	MG	1H	3284	-	-	-	X
58	MG	1H	3285	-	-	-	X
58	MG	1H	3288	-	-	-	X
58	MG	1H	3301	-	-	-	X
58	MG	1H	3309	-	-	-	X
58	MG	1H	3315	-	-	-	X
58	MG	1H	3324	-	-	-	X
58	MG	1H	3327	-	-	-	X
58	MG	1H	3328	-	-	-	X
58	MG	1H	3331	-	-	-	X
58	MG	1H	3342	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	2K	102	-	-	-	X
58	MG	2K	103	-	-	-	X
58	MG	2L	102	-	-	-	X
58	MG	E5	101	-	-	-	X
59	SF4	32	301	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 294444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	13	1496	32157	14313	5960	10388	1496	0	0	0
1	1G	1507	32391	14418	6004	10463	1506	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3E	207	1698	1064	338	289	7	0	0	0
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	148	1134	718	215	197	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
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	91	734	459	144	130	1	0	0	0
			Total	C	N	O				
10	1A	80	646	403	129	114		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	823	512	154	154	3	0	0	0
			Total	C	N	O	S			
11	2A	113	835	520	156	156	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
22	1K	71	1520	681	264	503	71	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1K	?	-	G	deletion	GB 836716955

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

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

- Molecule 25 is a RNA chain called mRNA.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	4L	18	397	178	84	117	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	1H	2833	61028	27159	11418	19618	2833	0	0	0
			Total	C	N	O	P			
26	14	2861	61630	27429	11535	19806	2860	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	71	133	1033	651	194	187	1	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
28	79	57	456	283	91	82	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	51	171	1312	832	246	233	1	0	0	0
			Total	C	N	O				
33	59	73	568	356	116	96		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	61	146	1136	726	201	208	1	0	0	0
34	69	145	1131	723	200	207	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	E8	112	890	560	175	153	2	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	A5	113	899	566	177	154	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	K8	68	568	352	115	100	1	0	0	0
50	G5	66	558	346	113	98	1	0	0	0

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 56 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
56	1L	73	1563	700	271	518	73	1	0	0	0

- Molecule 57 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
57	3L	76	1612	722	281	534	75	0	0	0

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

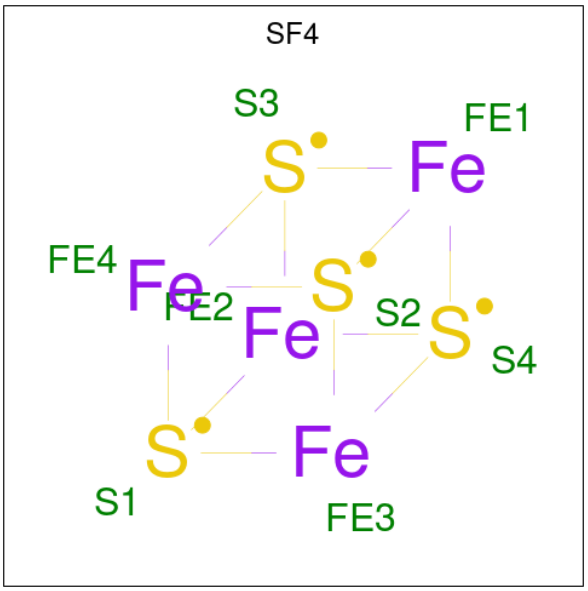
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	13	132	132	132	0	0
58	1E	1	1	1	0	0
58	5E	1	1	1	0	0
58	1K	1	1	1	0	0
58	2K	3	3	3	0	0
58	3K	1	1	1	0	0
58	1H	467	467	467	0	0
58	16	9	9	9	0	0
58	21	2	2	2	0	0
58	41	1	1	1	0	0
58	78	1	1	1	0	0
58	88	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	98	1	1	1	0	0
58	I8	3	3	3	0	0
58	J8	1	1	1	0	0
58	L8	1	1	1	0	0
58	P8	1	1	1	0	0
58	Q8	1	1	1	0	0
58	1G	90	90	90	0	0
58	6A	1	1	1	0	0
58	2L	2	2	2	0	0
58	14	399	399	399	0	0
58	1J	5	5	5	0	0
58	29	4	4	4	0	0
58	39	1	1	1	0	0
58	25	1	1	1	0	0
58	35	3	3	3	0	0
58	45	2	2	2	0	0
58	55	1	1	1	0	0
58	E5	1	1	1	0	0

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



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	126	Total O 126 126	0	0
61	3I	2	Total O 2 2	0	0
61	5I	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1K	8	Total O 8 8	0	0
61	3K	1	Total O 1 1	0	0
61	4K	2	Total O 2 2	0	0
61	1H	629	Total O 629 629	0	0
61	16	29	Total O 29 29	0	0
61	11	7	Total O 7 7	0	0
61	21	4	Total O 4 4	0	0
61	31	9	Total O 9 9	0	0
61	58	2	Total O 2 2	0	0
61	78	7	Total O 7 7	0	0
61	88	1	Total O 1 1	0	0
61	B8	1	Total O 1 1	0	0
61	E8	2	Total O 2 2	0	0
61	F8	1	Total O 1 1	0	0
61	G8	1	Total O 1 1	0	0
61	I8	3	Total O 3 3	0	0
61	L8	2	Total O 2 2	0	0
61	1G	78	Total O 78 78	0	0
61	32	1	Total O 1 1	0	0
61	5A	2	Total O 2 2	0	0
61	14	417	Total O 417 417	0	0

Continued on next page...

Continued from previous page...

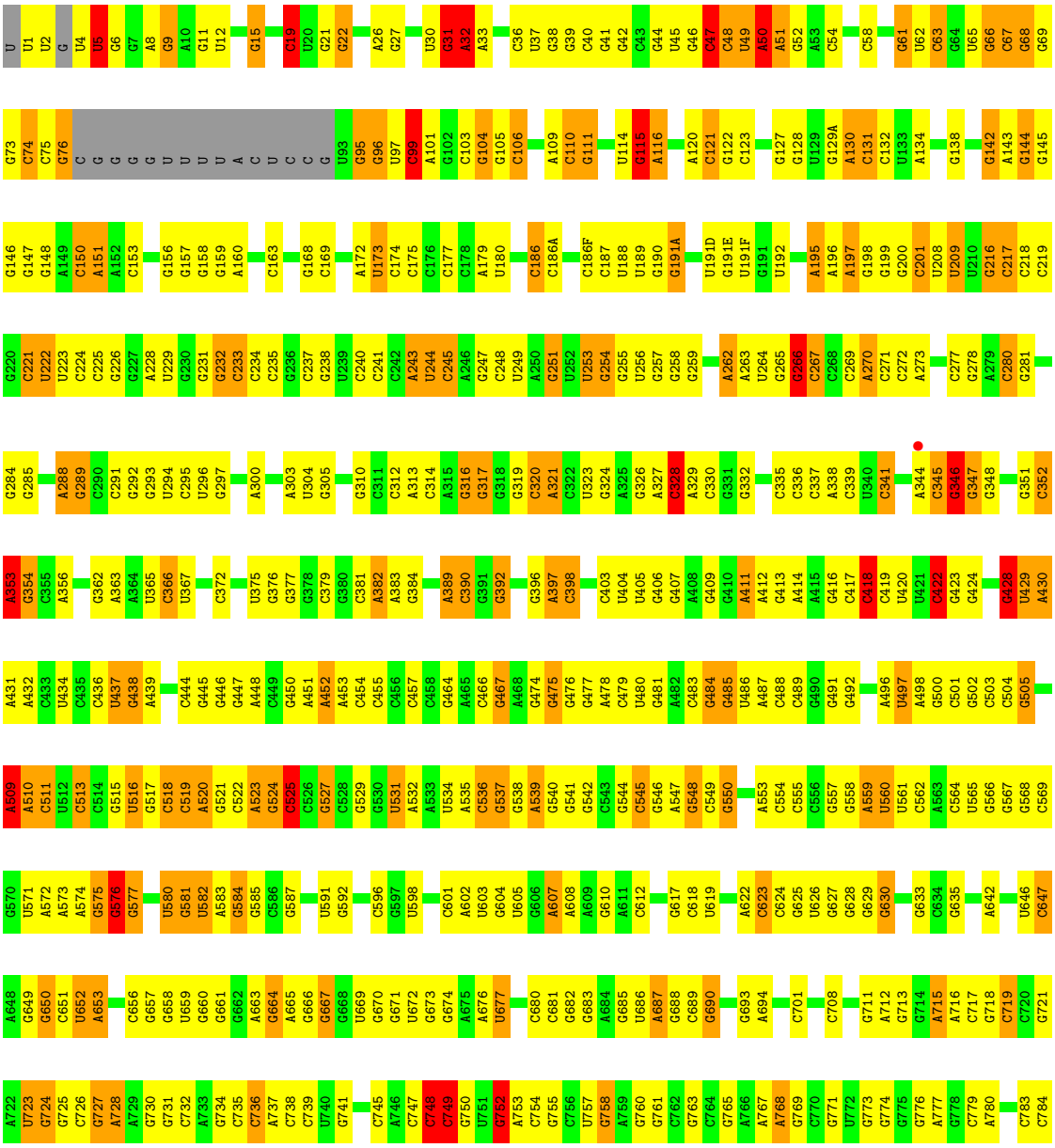
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1J	6	Total O 6 6	0	0
61	19	8	Total O 8 8	0	0
61	29	2	Total O 2 2	0	0
61	39	5	Total O 5 5	0	0
61	35	1	Total O 1 1	0	0
61	55	1	Total O 1 1	0	0
61	A5	1	Total O 1 1	0	0
61	H5	2	Total O 2 2	0	0

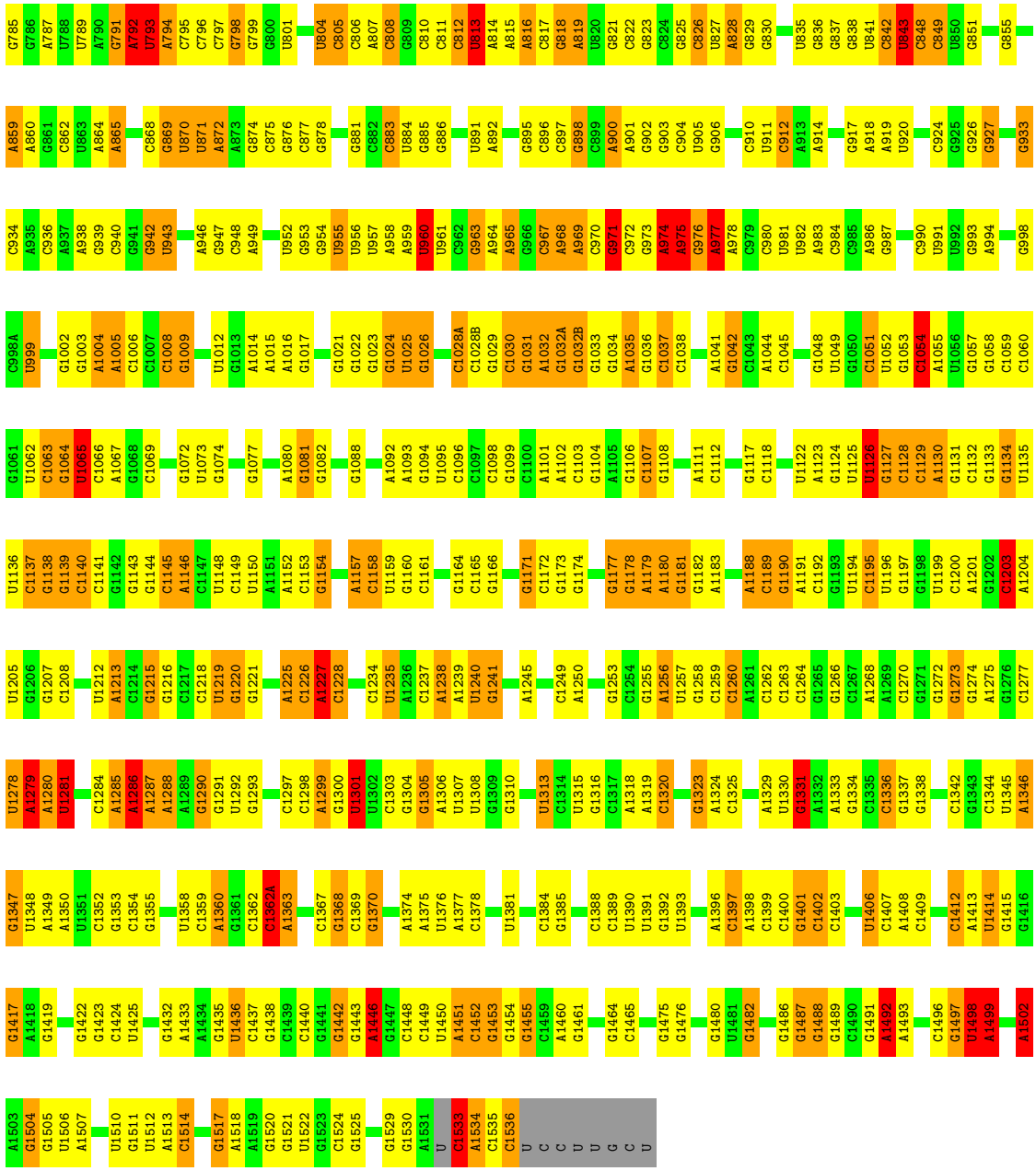
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

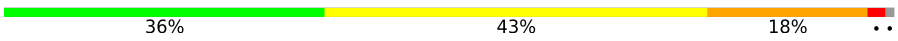
Chain 13: 34% 44% 17%

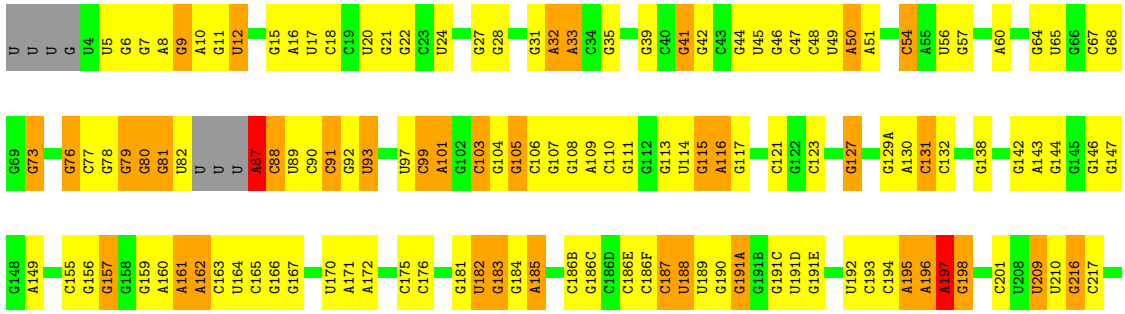




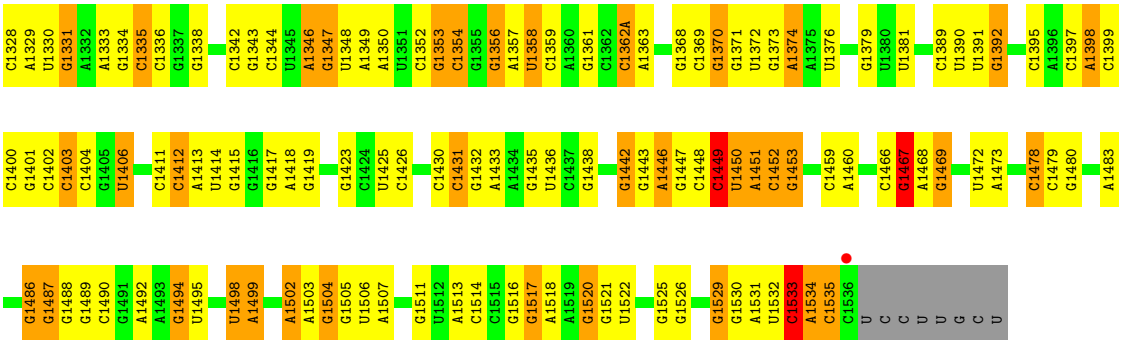
• Molecule 1: 16S rRNA

Chain 1G:



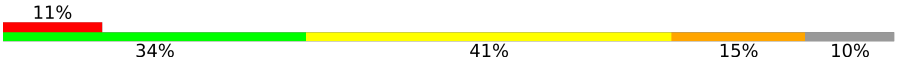


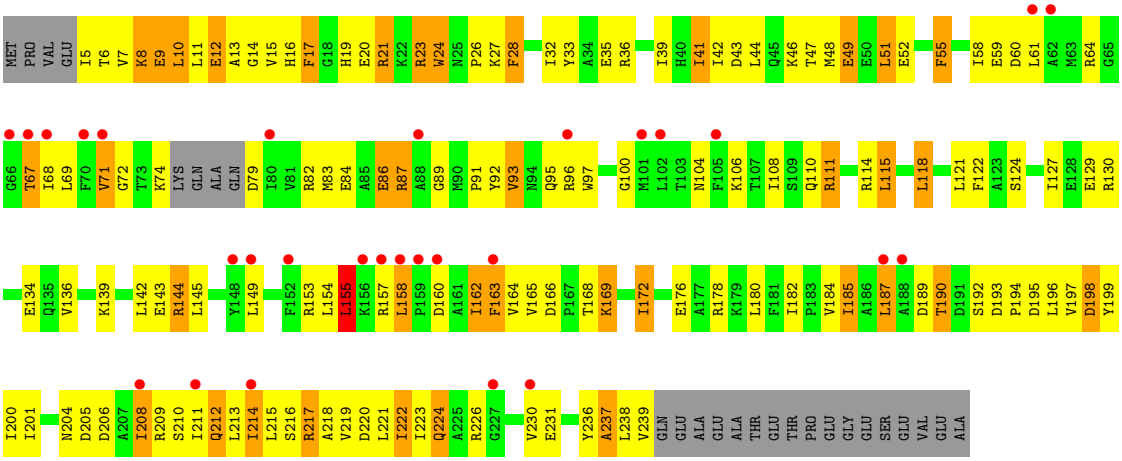
C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295
C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228
U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164
G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 C1076 G1077 A1080 G1081 G1084 U1085 A1092 A1093 G1094 U1095 C1096
U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 A1014 A1015 A1016 G1017 U1020 U1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060
C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1118 C1119 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 C1132 G1133 G1134
C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 G1263 C1264 G1265 G1266
C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327
G933 C934 A935 C936 A937 A938 G942 G945 A946 G947 C948 A949 U950 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 U991 U992 G993 A994 C995 A996 U997 G998 C998A
A768 G769 C770 G771 U772 G775 G776 A777 A780 A781 A782 C783 C784 A787 G791 A792 U793 A794 G800 U801 A802 G803 U804 C805 C806 A807 C808 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C826 U827 A828 G829 C834 U835 G836 G837 G838 U841 C842 U843 C848
G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C868 G869 A872 A873 G874 C875 C879 C882 G885 G886 G887 A892 C893 G894 G895 C896 C904 U905 G906 A907 A908 A909 A913 A914 A915 G916 U920 U921 G922 A923 C924 G925 G926 G927 C932
G674 A675 A676 U677 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 C701 A702 A706 C707 C708 G718 C719 C720 U723 G724 G725 C726 G731 C735 C736 C739 U740 G741 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G765
C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 G610 C613 A614 C615 G616 G617 C618 U619 C620 A621 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 G660 G661 G664 A665 G666 G667 G668 U669 G670 G673
A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 G546 A547 G548 G549 G550 U551 U552 C555 A559 U560 U561 C562 A563 C564 U565 G566 G570 U571 A572 A573 A574 G575 G576 G577 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 G593 G594 G596 C596 G597 U598 C599
C449 G450 A451 A452 A453 C454 C455 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G484 G485 U486 A487 C488 C489 G490 G491 G492 A496 U497 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G527 C528 G529 G530 U531
G377 G384 U387 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 C398 C401 U404 U405 G406 A407 A408 G409 G410 A411 A412 G413 A414 A415 G416 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 U437 G438 A439 A440 C442 C443 C444 G445 G446 G447 A448
G297 A298 G299 A300 G301 G309 G310 C311 C312 G316 G317 A321 G324 A325 G326 A327 C328 A329 G332 G333 C334 C335 C336 C337 A344 C345 G346 G347 G350 G351 C352 A353 G354 C355 A356 U359 A360 G361 G362 A363 A364 U365 C366 U367 C370 G371 C372 A373 A374 U375 G376
G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 C235 G236 C237 C240 C241 C242 A243 U244 C245 A246 G247 A250 G251 U252 U253 G254 G255 U256 G257 G258 U261 A262 A263 U264 G265 G266 C267 C271 C272 G276 C277 C280 G281 U287 A288 G289 C290 C291 C295 U296



• Molecule 2: 30S ribosomal protein S2

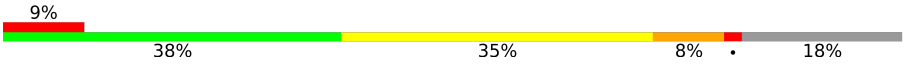
Chain 1E:

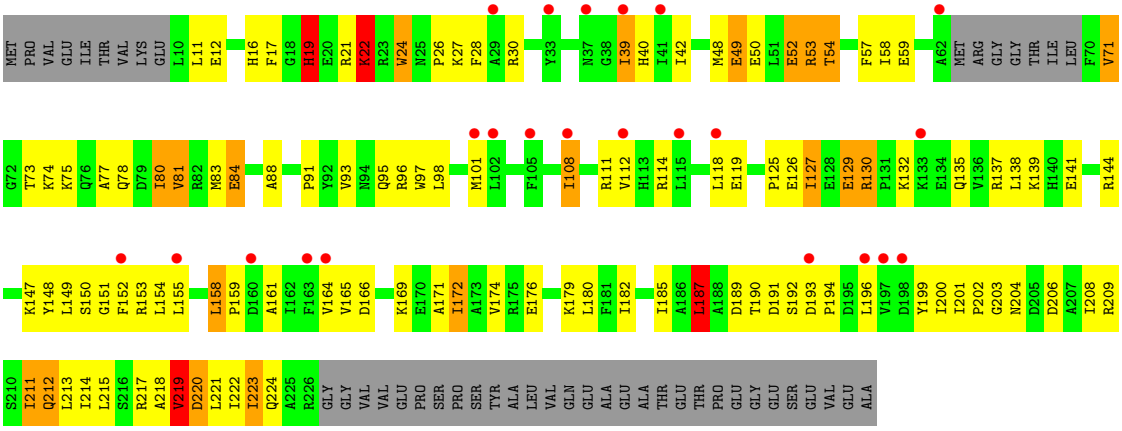




• Molecule 2: 30S ribosomal protein S2

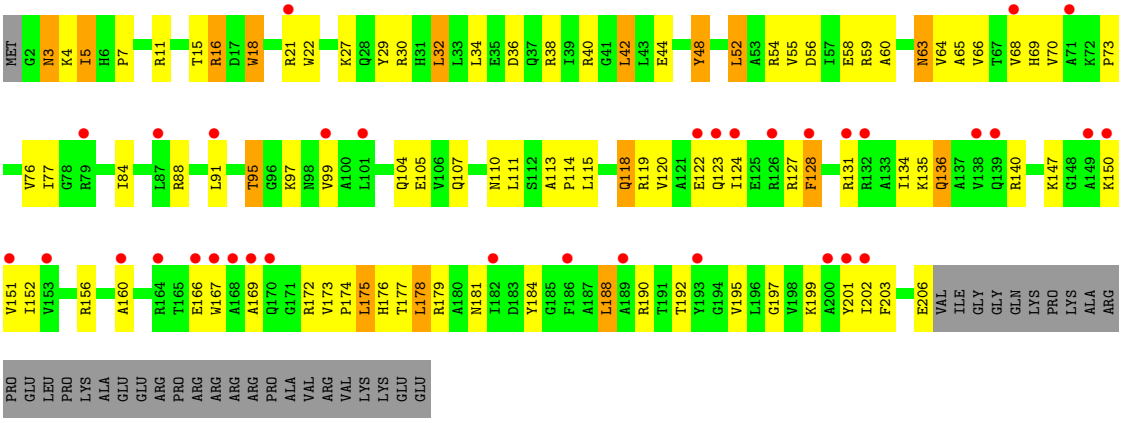
Chain 12:





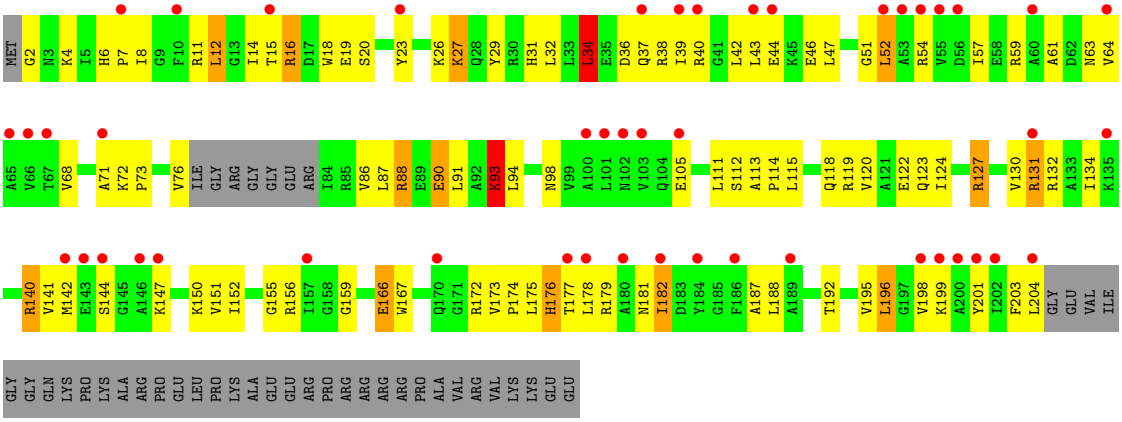
• Molecule 3: 30S ribosomal protein S3

Chain 2E:



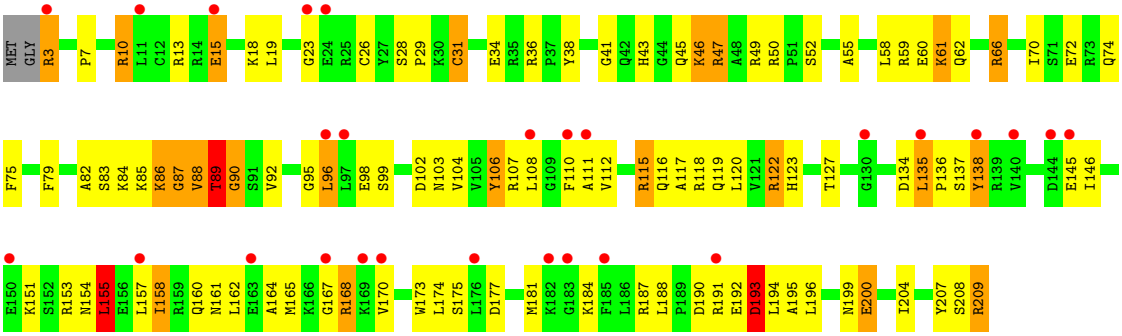
- Molecule 3: 30S ribosomal protein S3

Chain 22:



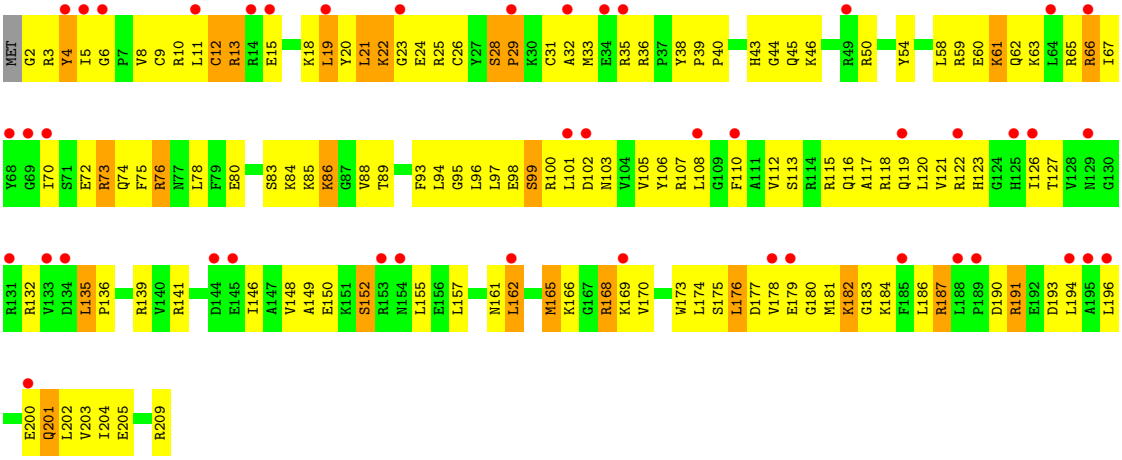
- Molecule 4: 30S ribosomal protein S4

Chain 3E:



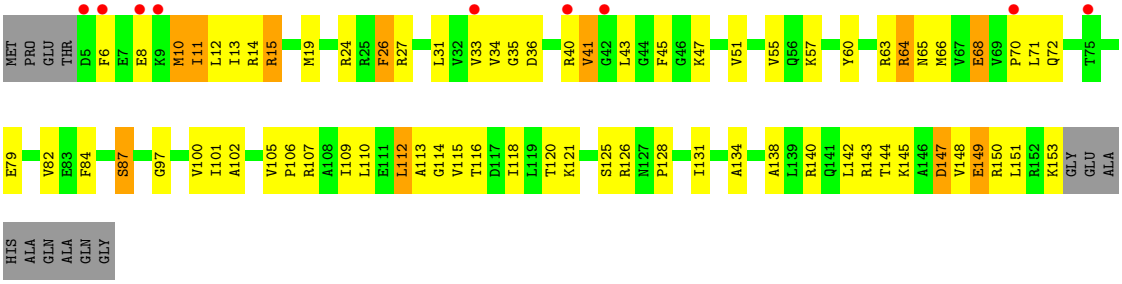
- Molecule 4: 30S ribosomal protein S4

Chain 32:



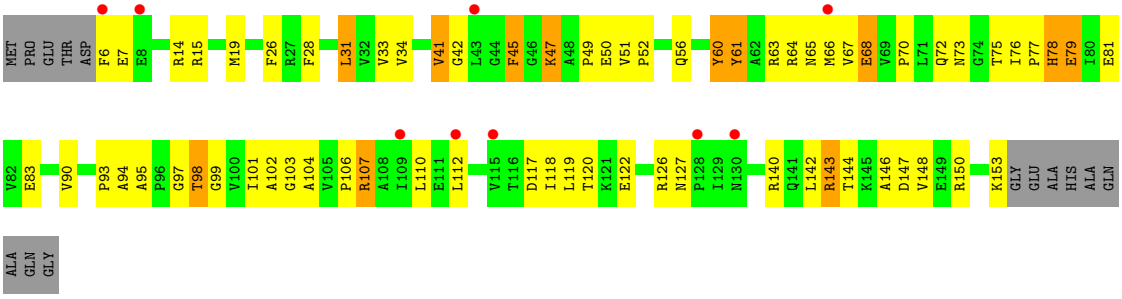
• Molecule 5: 30S ribosomal protein S5

Chain 4E:



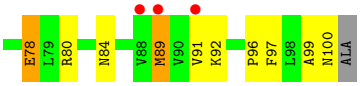
• Molecule 5: 30S ribosomal protein S5

Chain 42:



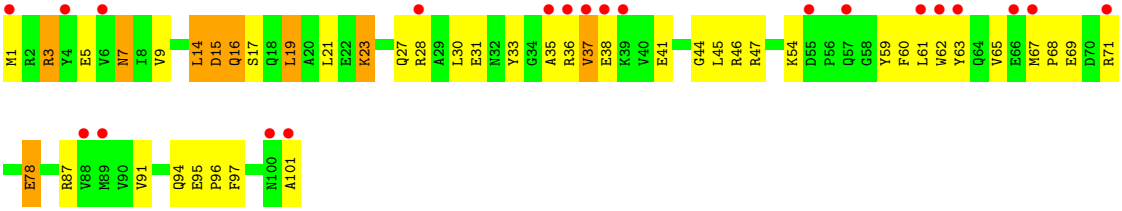
• Molecule 6: 30S ribosomal protein S6

Chain 5E:



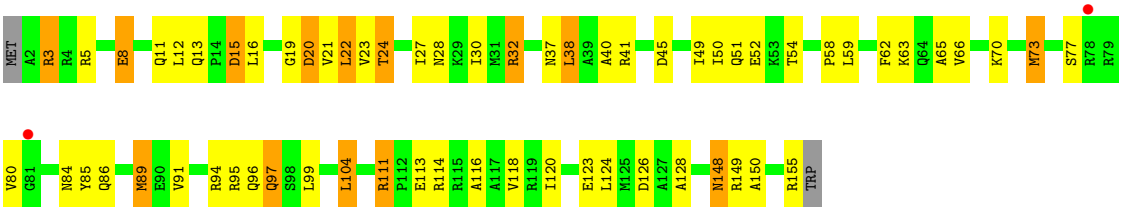
• Molecule 6: 30S ribosomal protein S6

Chain 52:



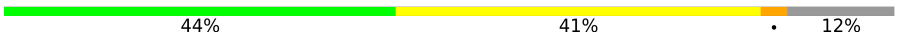
• Molecule 7: 30S ribosomal protein S7

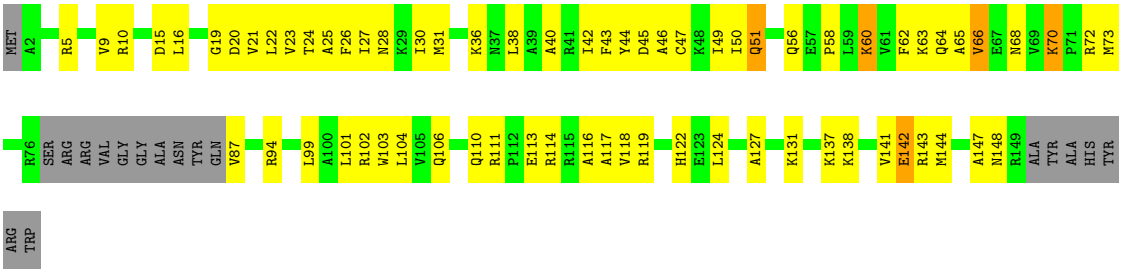
Chain 6E:



• Molecule 7: 30S ribosomal protein S7

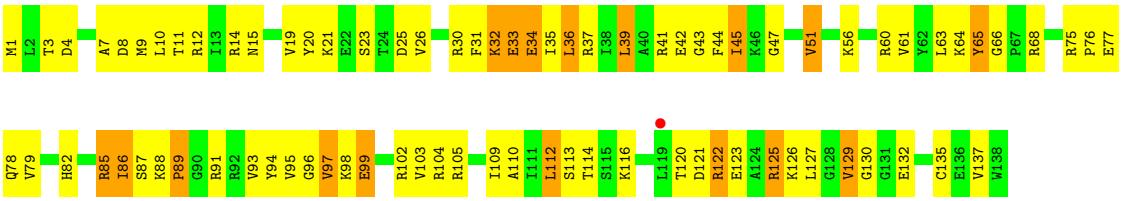
Chain 62:





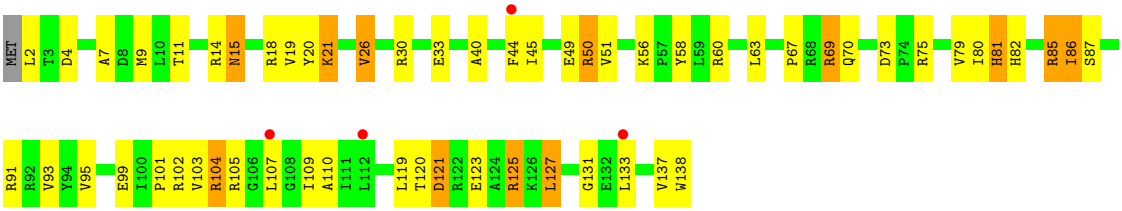
• Molecule 8: 30S ribosomal protein S8

Chain 7E:



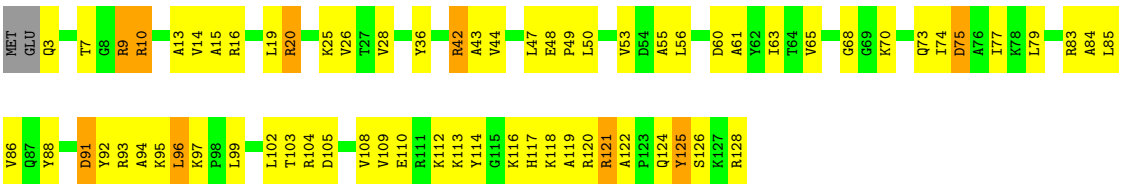
• Molecule 8: 30S ribosomal protein S8

Chain 72:



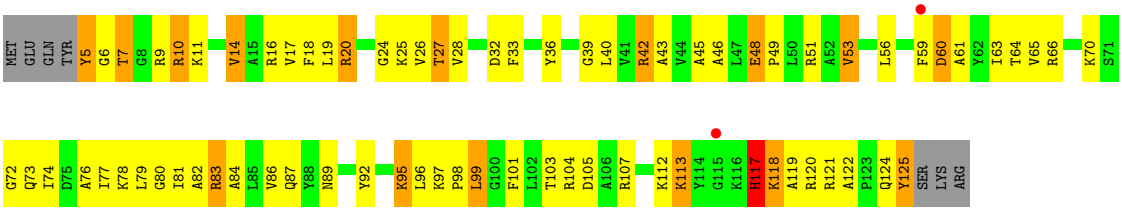
- Molecule 9: 30S ribosomal protein S9

Chain 8E:



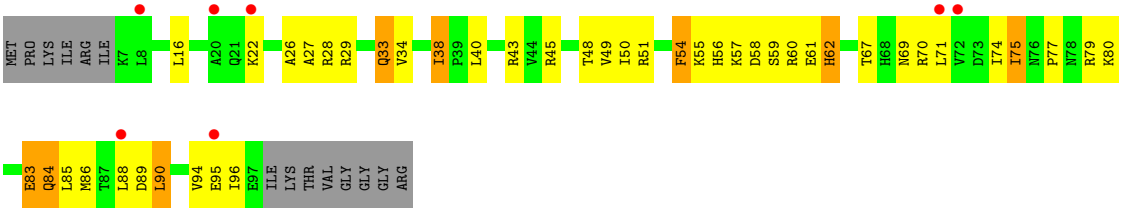
- Molecule 9: 30S ribosomal protein S9

Chain 82:



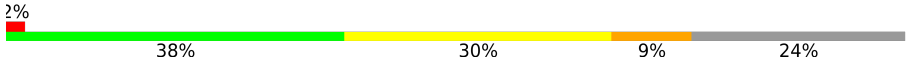
- Molecule 10: 30S ribosomal protein S10

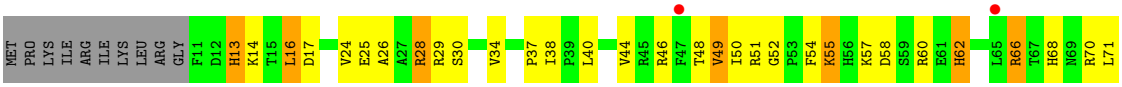
Chain 1I:



- Molecule 10: 30S ribosomal protein S10

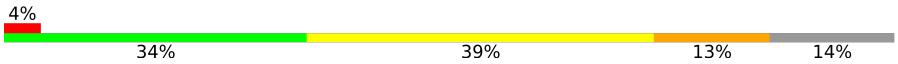
Chain 1A:

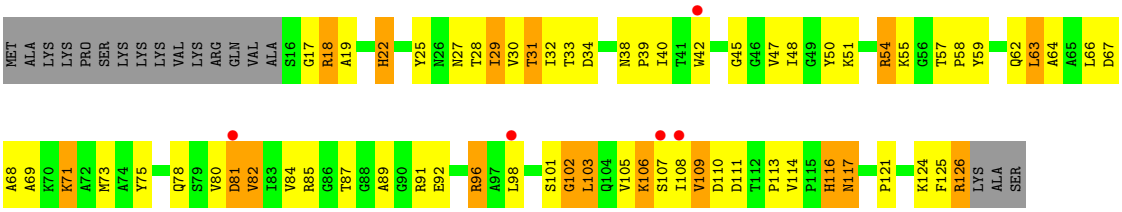




• Molecule 11: 30S ribosomal protein S11

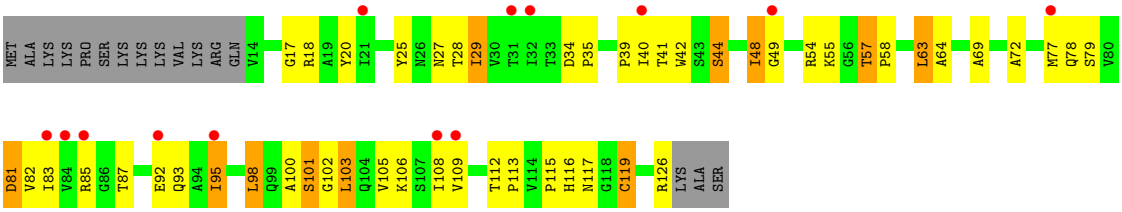
Chain 2I:





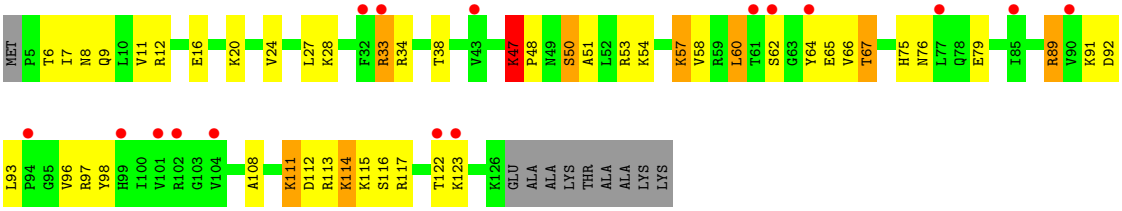
• Molecule 11: 30S ribosomal protein S11

Chain 2A:



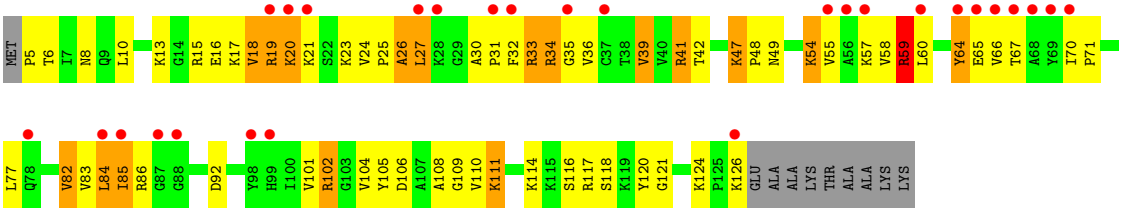
• Molecule 12: 30S ribosomal protein S12

Chain 3I:



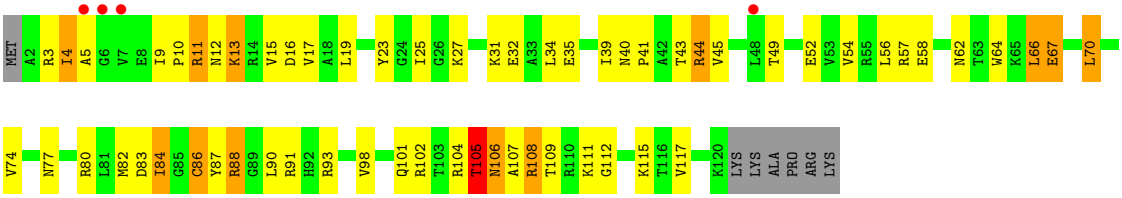
• Molecule 12: 30S ribosomal protein S12

Chain 3A:



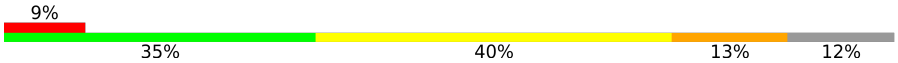
• Molecule 13: 30S ribosomal protein S13

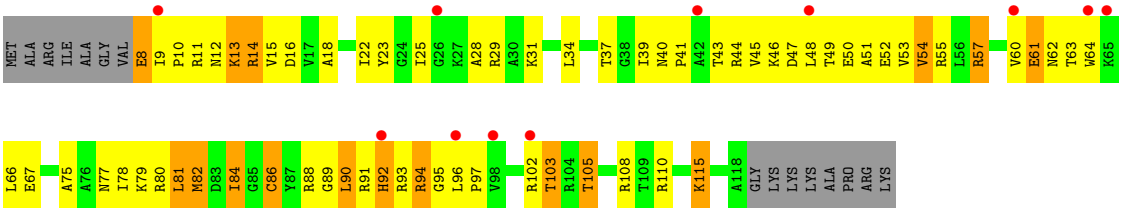
Chain 4I:



• Molecule 13: 30S ribosomal protein S13

Chain 4A:



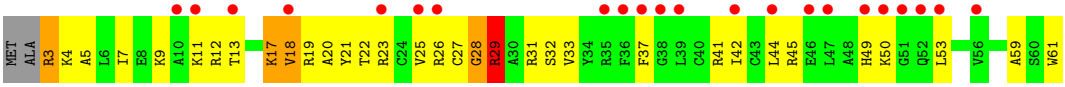


• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:

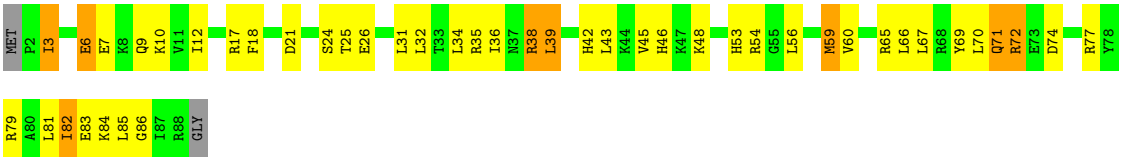
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



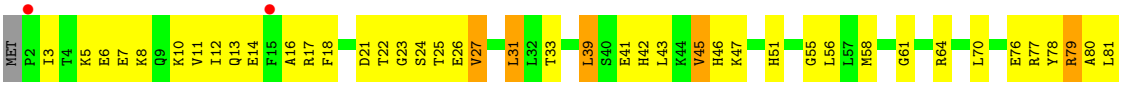
• Molecule 15: 30S ribosomal protein S15

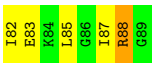
Chain 6I:



• Molecule 15: 30S ribosomal protein S15

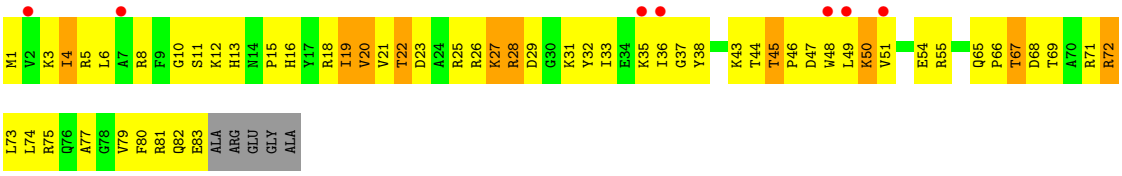
Chain 6A:





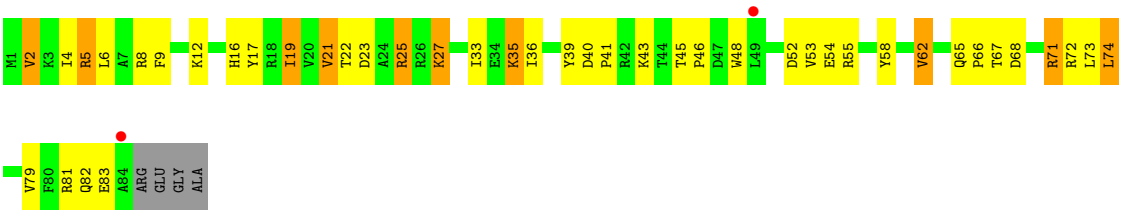
• Molecule 16: 30S ribosomal protein S16

Chain 7I:



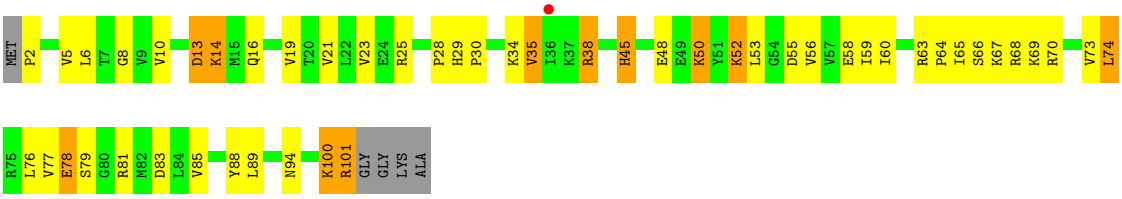
• Molecule 16: 30S ribosomal protein S16

Chain 7A:



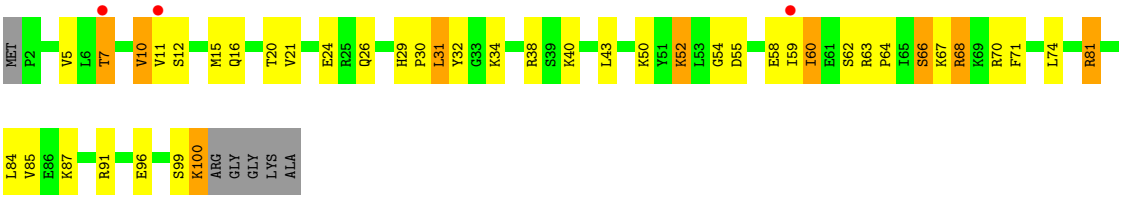
• Molecule 17: 30S ribosomal protein S17

Chain 8I:



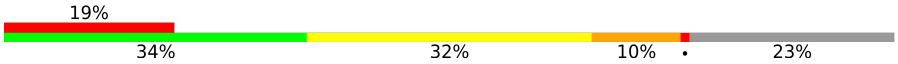
• Molecule 17: 30S ribosomal protein S17

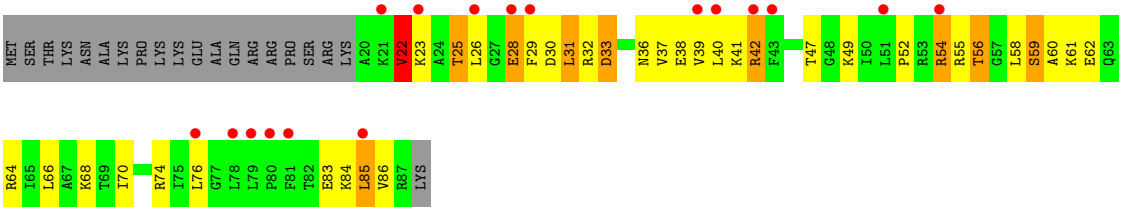
Chain 8A:



• Molecule 18: 30S ribosomal protein S18

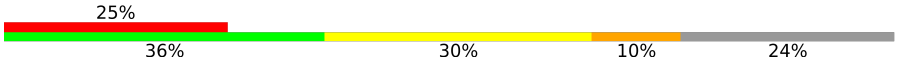
Chain 9I:

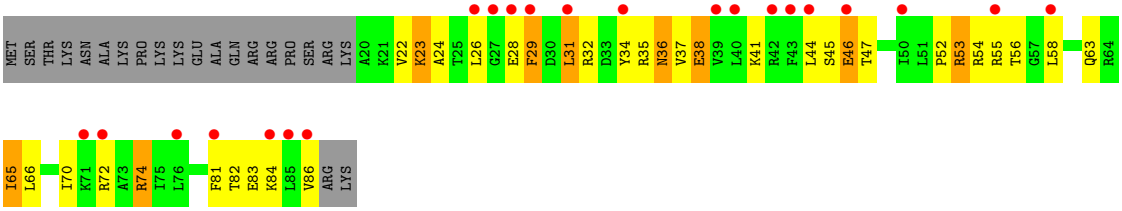




- Molecule 18: 30S ribosomal protein S18

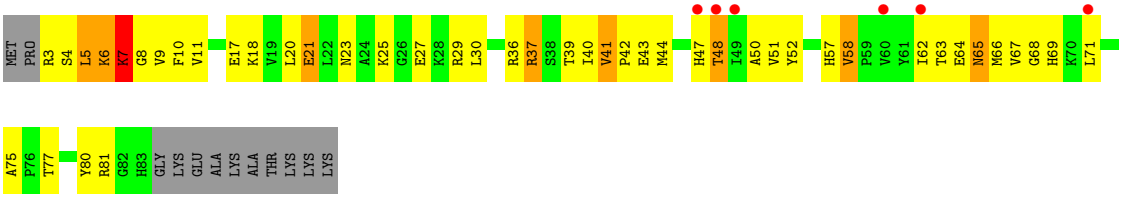
Chain 9A:





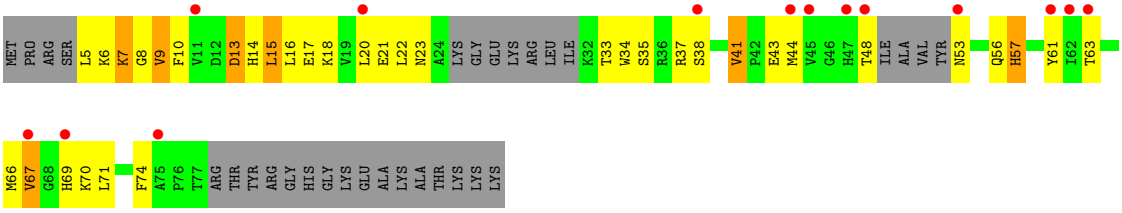
- Molecule 19: 30S ribosomal protein S19

Chain AI:



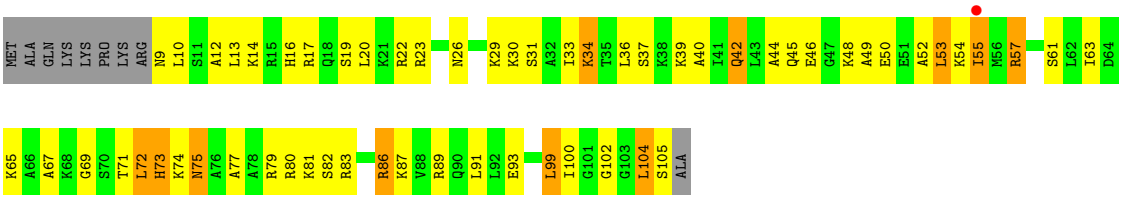
- Molecule 19: 30S ribosomal protein S19

Chain AA:



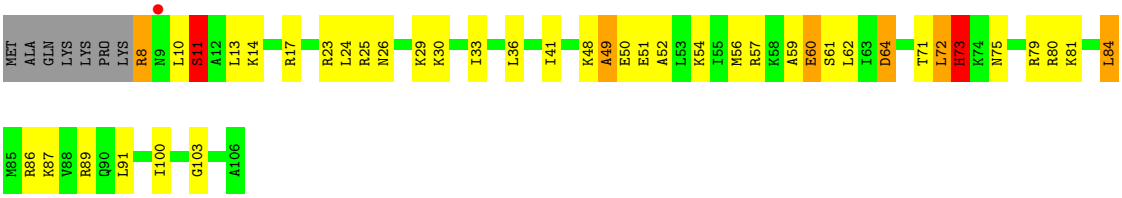
- Molecule 20: 30S ribosomal protein S20

Chain BI:



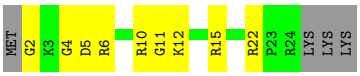
• Molecule 20: 30S ribosomal protein S20

Chain BA:



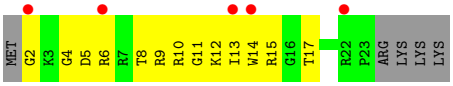
• Molecule 21: 30S ribosomal protein Thx

Chain 1F:



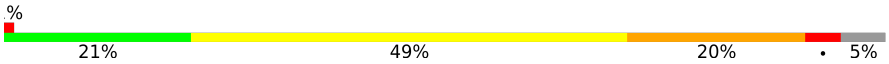
• Molecule 21: 30S ribosomal protein Thx

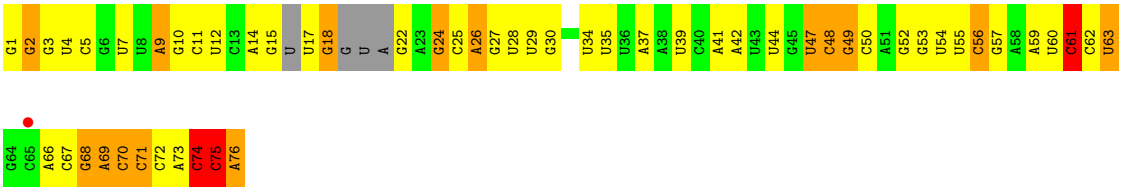
Chain 1B:



• Molecule 22: tRNALys

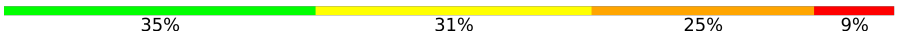
Chain 1K:

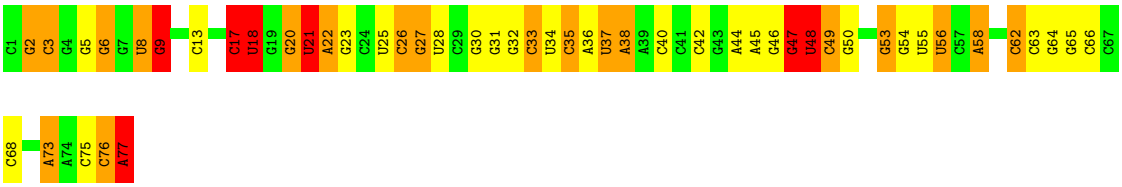




• Molecule 23: tRNAfMet

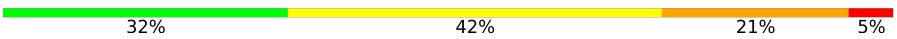
Chain 2K:

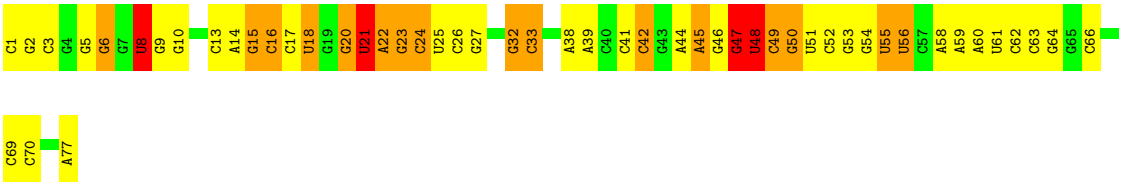




• Molecule 23: tRNAfMet

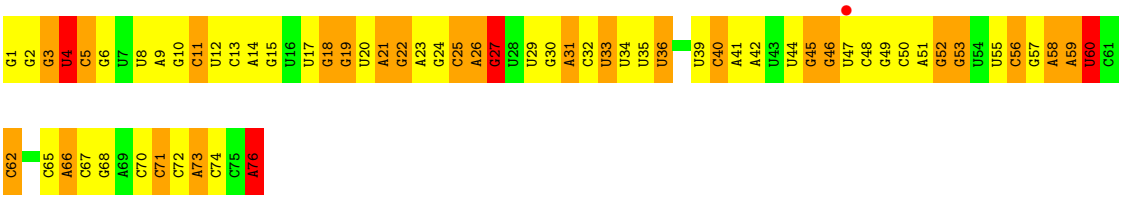
Chain 2L:





• Molecule 24: tRNALys

Chain 3K:

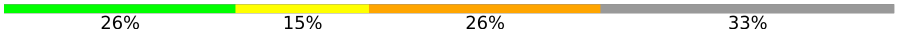


• Molecule 25: mRNA

Chain 4K:

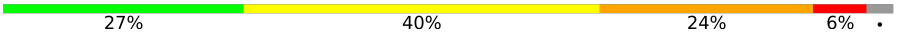
• Molecule 25: mRNA

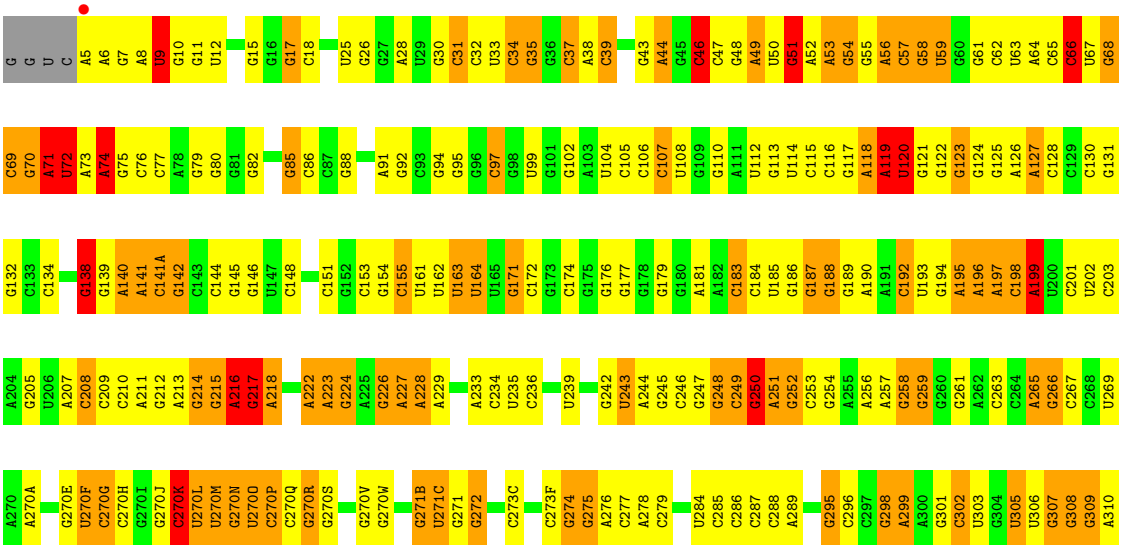
Chain 4L:

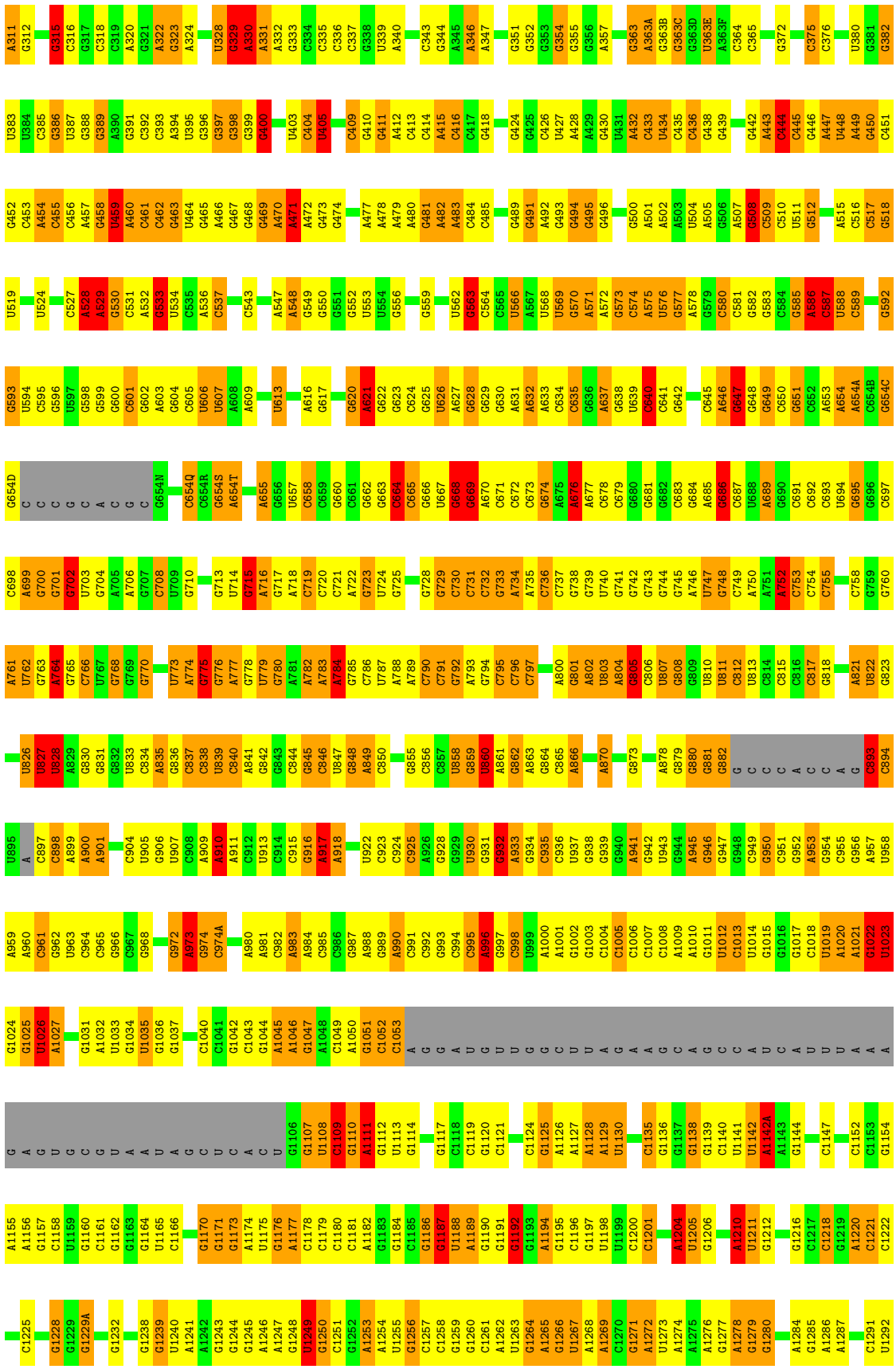


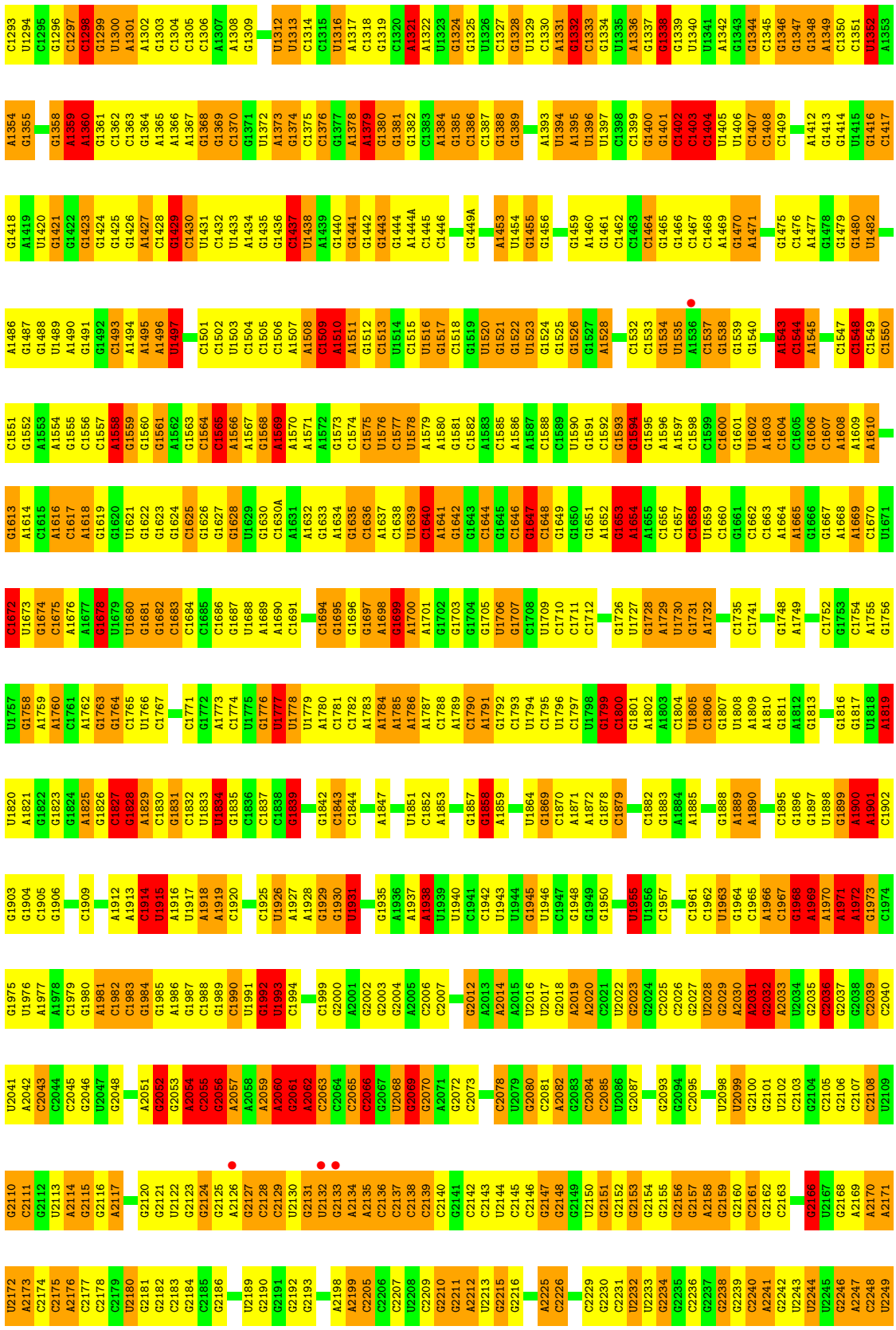
• Molecule 26: 23S rRNA

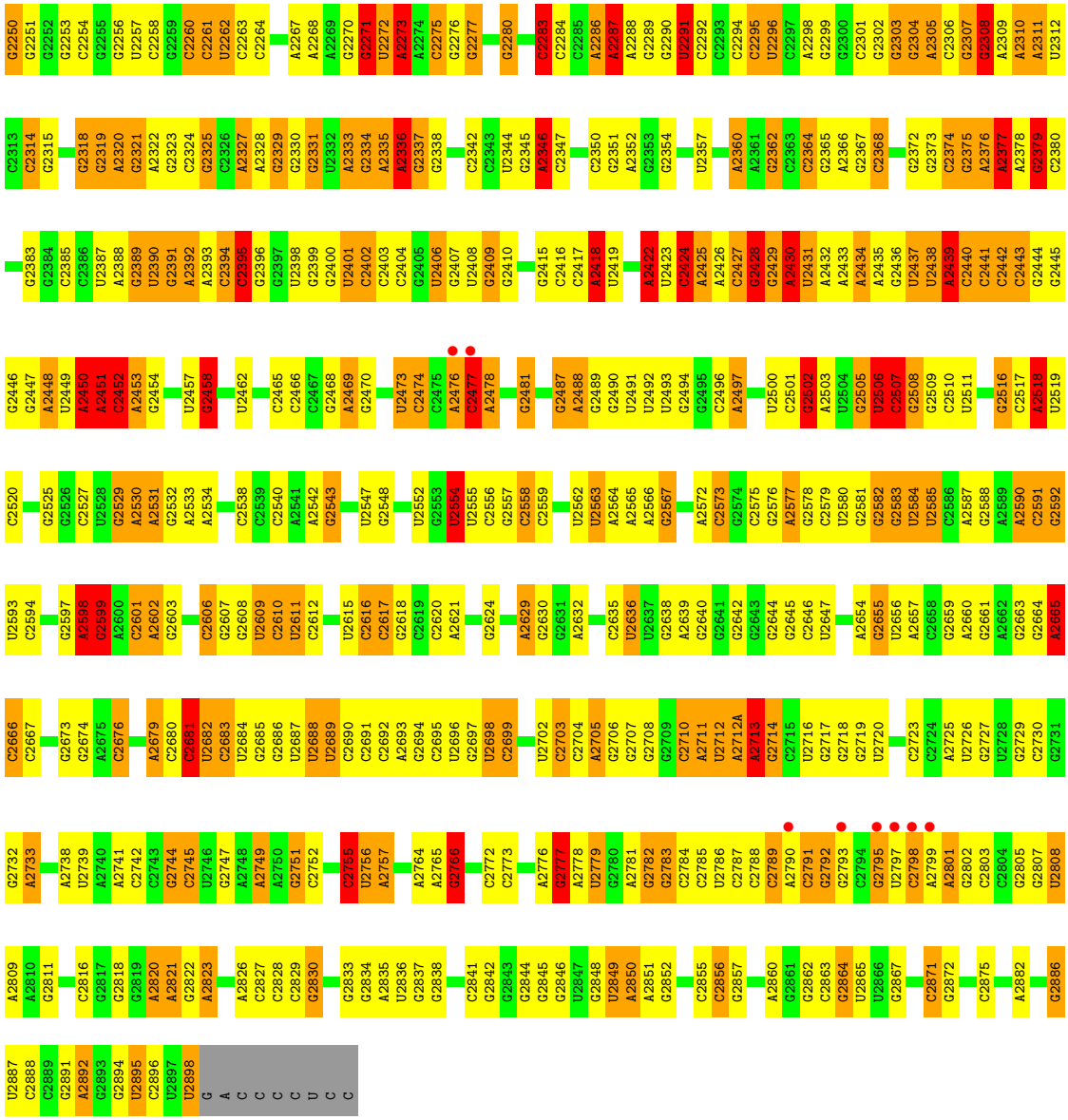
Chain 1H:





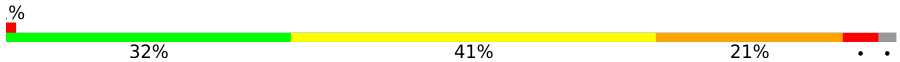

A311 G312 G315 C316 G317 C318 C319 A320 G321 A322 G323 A324 U328 G329 A330 A331 A332 G333 G334 C335 C336 C337 G338 U339 A340 C343 G344 A345 A346 A347 G351 G352 G353 G354 G355 G356 A357 G363 A363A G363B G363C G363D U363E A363F C364 C365 G372 C375 C376 U380 G381 G382
U383 U384 C385 G386 U387 G388 G389 A390 G391 C392 C393 A394 U395 G396 G397 G398 G399 G400 U403 C404 U405 C409 G410 G411 A412 C413 C414 A415 C416 C417 C418 G424 G425 C426 U427 A428 A429 G430 U431 A432 C433 U434 C435 C436 G438 G439 G442 A443 C444 C445 G446 A447 U448 A449 G450 C451
G452 C453 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 G473 G474 A477 A478 A479 A480 G481 A482 A483 C484 C485 G489 G491 A492 G493 G494 G495 G496 G500 A501 A502 A503 U504 A505 G506 A507 G508 G509 C510 U511 G512 A515 C516 C517 G518
U519 U524 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 C543 A547 A548 G549 G550 G551 G552 U553 U554 C556 C559 U562 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 G592
G593 U594 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 U613 A616 G617 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 C645 A646 G647 G648 G649 C650 G651 C652 A653 A654 A654A C654B G654C
G654D C C C G C A C G C G654N C654Q C654R G654S A654T A655 G656 U657 C658 C659 G660 C661 G662 G663 G664 C665 G666 U667 G668 G669 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G680 G681 G682 C683 G684 A685 G686 C687 U688 A689 G690 C691 C692 G693 U694 G695 G696 C697
C698 A699 G700 G701 G702 U703 G704 A705 A706 G707 C708 U709 G710 G713 U714 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 G728 G729 C730 C731 C732 G733 A734 A735 C736 C737 G738 G739 U740 G741 C742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 C755 C758 G759 G760
A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A821 U822 G823
U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 G842 G843 C844 C845 G846 U847 G848 A849 C850 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 A870 G873 A878 G879 G880 G881 G882 G C C C A C C A G C393 C394
U895 A C897 C898 A899 A900 A901 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 U922 C923 C924 C925 A926 G928 G929 U930 G931 G932 A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 A953 G954 C955 G956 A957 U958
A959 A960 C961 G962 U963 C964 C965 G966 C967 G968 G972 A973 G974 C974A A980 A981 C982 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 C1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 C1017 C1018 U1019 A1020 A1021 G1022 U1023
G1024 G1025 U1026 A1027 G1031 A1032 U1033 G1034 U1035 G1036 G1037 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A G G G A U G U C U U U G G C U U A A G A A G C A A C C C U U A A A
G C A G U C G C A A U A G C U C A G U G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1117 C1118 C1119 G1120 C1121 C1124 G1125 A1126 A1127 A1128 A1129 U1130 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1147 C1152 C1153 G1154
A1155 A1156 G1157 C1158 U1159 G1160 C1161 G1162 G1163 G1164 U1165 C1166 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 A1204 U1205 G1206 A1210 U1211 G1212 G1216 C1217 C1218 G1219 A1220 C1221 C1222
C1225 G1228 G1229 G1229A G1232 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1279 G1280 A1284 G1285 A1286 A1287 C1291 U1292

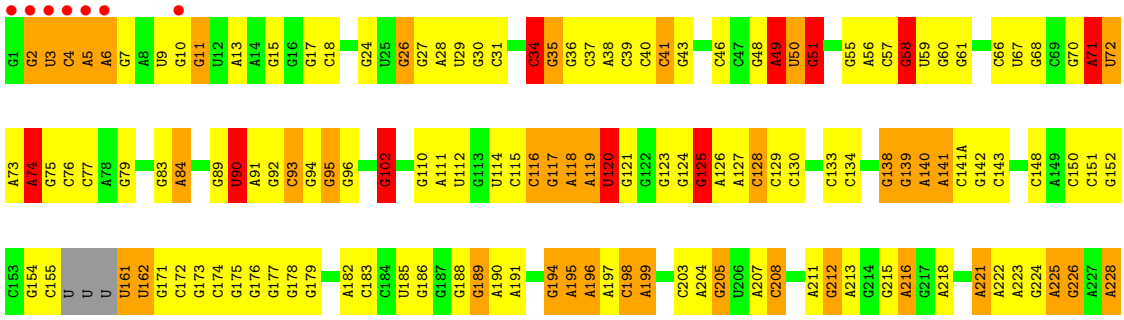


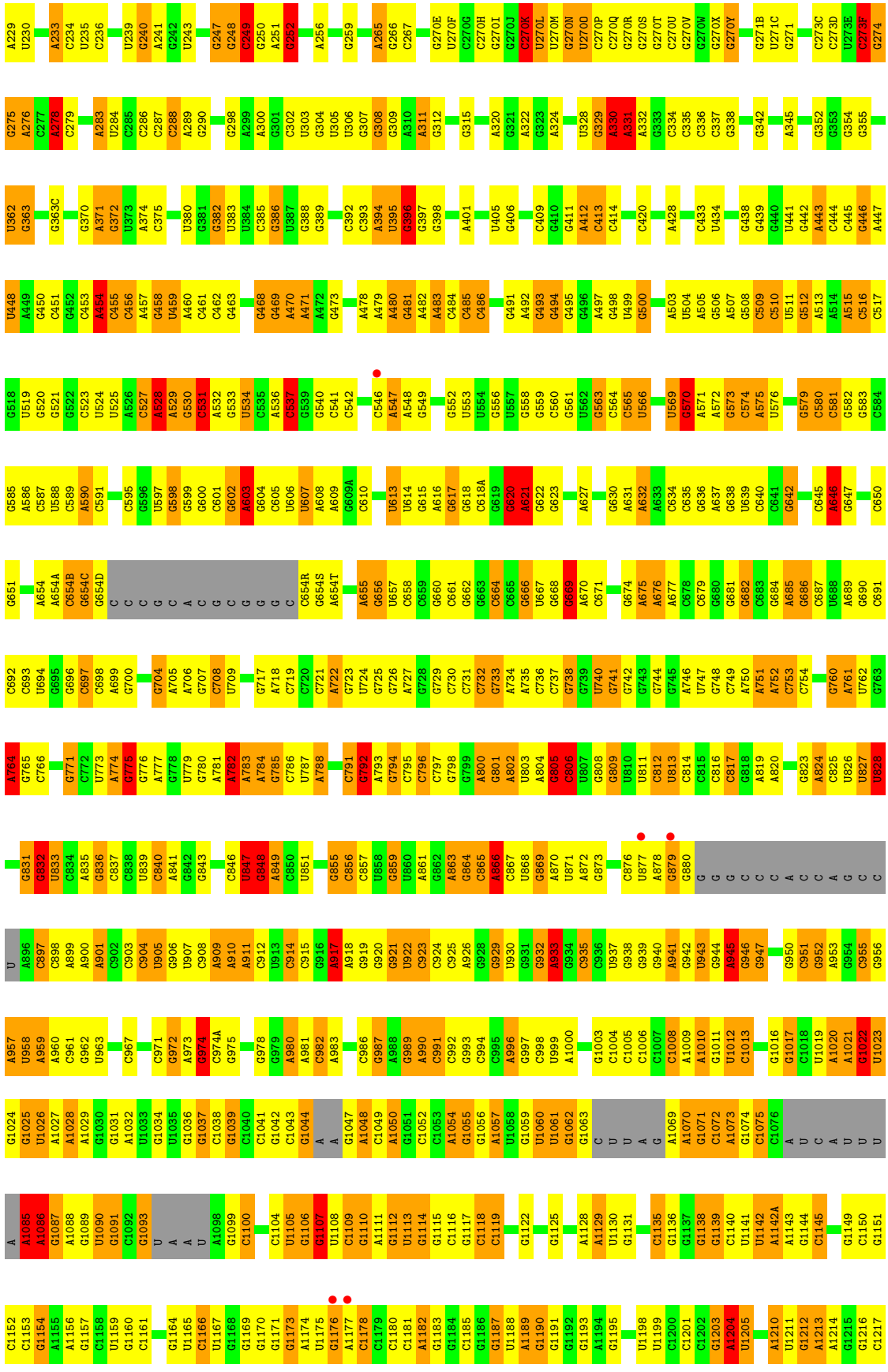


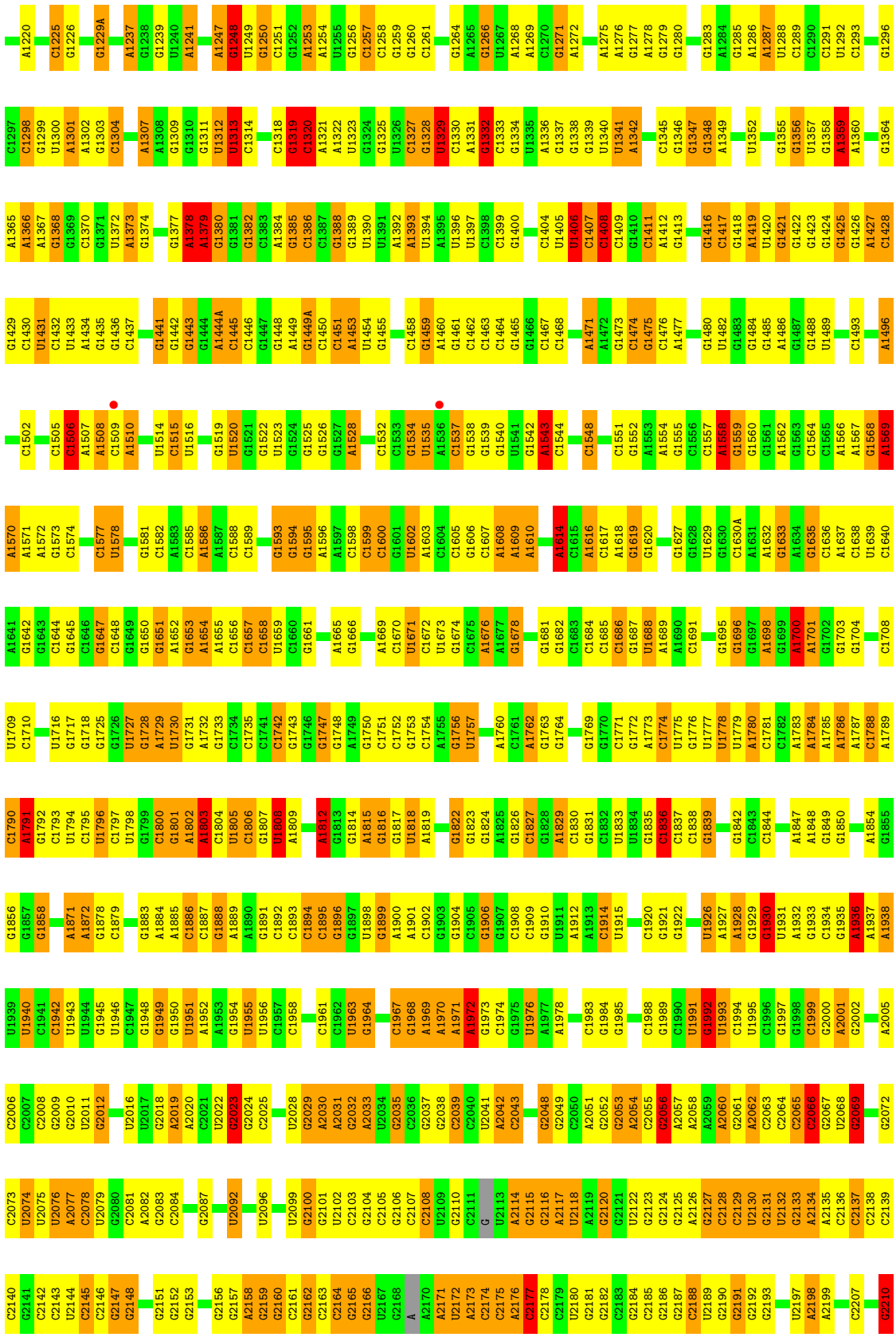
• Molecule 26: 23S rRNA

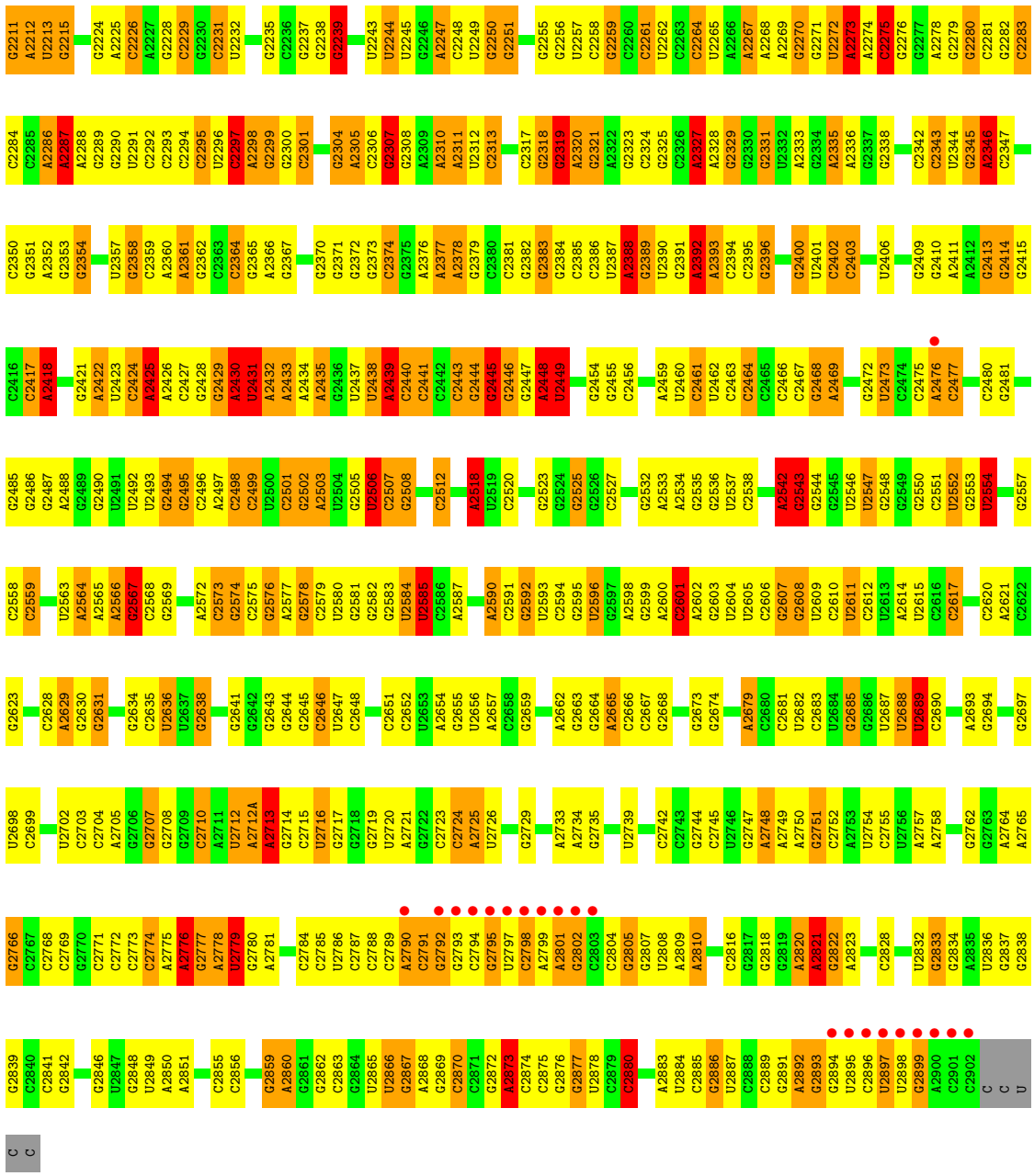
Chain 14:





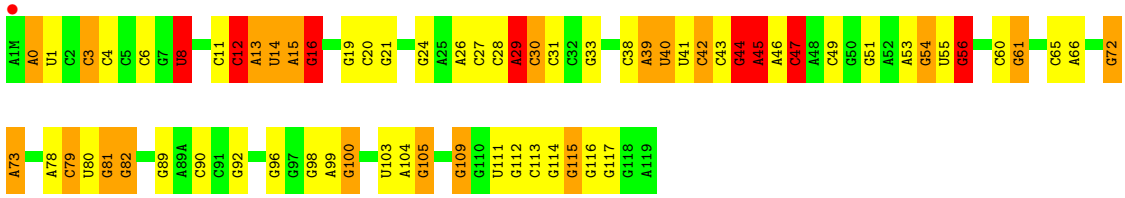

A229 U230 A233 C234 U235 C236 U239 G240 A241 G242 U243 G247 G248 C249 G250 A251 G252 A256 G259 A265 G266 C267 G270E U270F C270G C270H G270I G270J G270K U270L U270M G270N U270O C270P C270Q G270R G270S G270T C270U G270V G270W G270X G270Y G271B U271C G271 C273C C273D U273E C273F G274
G275 A276 C277 A278 C279 A283 U284 C285 C286 C287 C288 A289 G290 G298 A299 A300 G301 C302 U303 G304 U305 U306 G307 G308 G309 A310 A311 G312 G315 A320 G321 A322 G323 A324 U328 G329 A330 A331 A332 G333 C334 C335 C336 C337 G338 G342 A345 G352 G353 G354 G355
U362 G363 G363C G370 A371 G372 U373 A374 C375 U380 G381 G382 U383 U384 C385 G386 U387 G388 G389 C392 C393 A394 U395 G396 G397 G398 A401 U405 G406 C409 G410 G411 A412 C413 C414 C420 A428 C433 U434 G438 G439 G440 U441 G442 A443 C444 C445 G446 A447
U448 A449 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 G468 G469 A470 A471 A472 G473 A478 A479 A480 G481 A482 A483 C484 C485 C486 G491 A492 G493 G494 G495 G496 A497 G498 U499 G500 A503 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 A515 C516 C517
G518 U519 G520 G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G539 G540 C541 C542 C546 A547 A548 G549 G552 U553 U554 G556 U557 G558 G559 C560 G561 U562 G563 C564 C565 U566 U569 G570 A571 A572 G573 C574 A575 U576 G579 C580 C581 G582 G583 C584
G585 A586 C587 U588 C589 A590 C591 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G609A C610 U613 U614 G615 A616 G617 G618 C618A G619 G620 A621 G622 G623 A627 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 C645 A646 G647 C650
G651 A654 A654A C654B G654C G654D C C C G C A C G C G G G C C654R G654S A654T A655 G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666 U667 G668 G669 A670 C671 G674 A675 A676 A677 C678 C679 G680 G681 G682 C683 G684 A685 G686 C687 U688 A689 G690 C691
C692 C693 U694 G695 G696 C697 C698 A699 G700 G704 A705 A706 G707 C708 U709 G717 A718 C719 C720 C721 A722 G723 U724 G725 G726 A727 G728 G729 C730 C731 C732 G733 A734 A735 C736 C737 G738 G739 U740 G741 G742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 G760 A761 U762 G763
A764 G765 C766 G771 C772 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 C791 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 G823 A824 C825 U826 U827 U828
G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 G842 G843 C846 U847 G848 A849 C850 U851 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 U871 A872 G873 C876 U877 A878 G879 G880 G G G C C C A C C A G G C C
U A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 C925 A926 G928 G929 U930 G931 G932 A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G950 C951 G952 A953 G954 C955 G956
A957 U958 A959 A960 C961 G962 U963 C967 C971 G972 A973 G974 C974A G975 G978 G979 A980 A981 C982 A983 C986 G987 A988 G989 U990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023
G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A A G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C U U A G A1069 A1070 G1071 G1072 A1073 G1074 C1075 C1076 A U C A U U U


C2140 C2141 C2142 C2143 U2144 C2145 C2146 C2147 C2148 G2151 G2152 G2153 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 C2165 G2166 U2167 G2168 A A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 U2197 A2198 A2199 C2207 G2210
C2073 U2074 U2075 U2076 A2077 C2078 U2079 G2080 C2081 A2082 G2083 C2084 G2087 U2092 U2096 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139
C2006 C2007 C2008 G2009 G2010 U2011 G2012 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2048 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 C2067 U2068 G2069 G2072
U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 C1961 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976 A1977 A1978 C1983 G1984 G1985 C1988 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 C1997 G1998 C1999 G2000 A2001 G2002 A2005
G1856 G1857 G1858 A1871 A1872 G1878 C1879 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893 C1894 C1895 G1896 G1897 U1898 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 U1910 U1911 A1912 A1913 C1914 U1915 C1920 G1921 G1922 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938
C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 U1808 A1809 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1842 C1843 C1844 A1847 A1848 G1849 G1850 A1854 G1855
U1709 C1710 U1716 G1717 G1718 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 C1741 C1742 G1743 G1746 G1747 G1748 A1749 G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757 A1760 C1761 A1762 G1763 G1764 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789
A1641 G1642 G1643 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 A1665 G1666 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677 G1678 G1681 G1682 C1683 C1684 C1685 C1686 G1687 U1688 A1689 A1690 C1691 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1704 C1708
A1570 A1571 A1572 G1573 C1574 C1577 U1578 G1581 C1582 A1583 C1585 A1586 A1587 C1588 C1589 G1593 G1594 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610 A1614 C1615 A1616 C1617 A1618 G1619 G1620 G1627 G1628 U1629 G1630 C1630A A1631 A1632 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640
C1502 C1505 C1506 A1507 A1508 C1509 A1510 U1514 C1515 U1516 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 C1548 C1551 G1552 A1553 A1554 G1555 C1556 C1557 A1558 G1559 G1560 G1561 A1562 G1563 C1564 C1565 A1566 A1567 G1568 A1569
G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 G1441 G1442 G1443 G1444 A1444A C1445 C1446 G1447 G1448 A1449 G1449A C1450 C1451 A1453 U1454 G1455 C1458 G1459 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 C1468 A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1480 U1482 G1483 G1484 G1485 A1486 G1487 G1488 U1489 C1493 A1496
C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1304 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1318 G1319 C1320 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 C1345 G1346 G1347 G1348 A1349 U1352 G1355 G1356 U1357 G1358 A1359 A1360 G1364
A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 G1377 A1378 A1379 G1380 G1381 G1382 G1383 A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 G1400 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428
A1220 C1225 G1226 G1229A A1237 G1238 G1239 U1240 A1241 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 A1275 A1276 G1277 A1278 G1279 G1280 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1293 G1296



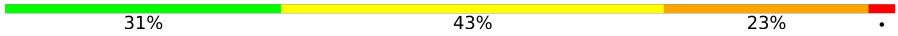
• Molecule 27: 5S rRNA

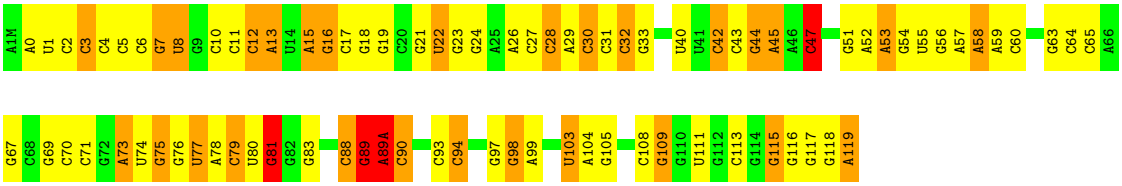
Chain 16:



• Molecule 27: 5S rRNA

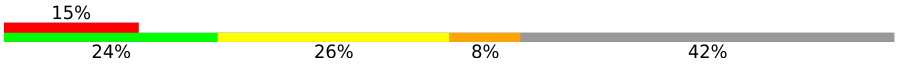
Chain 1J:

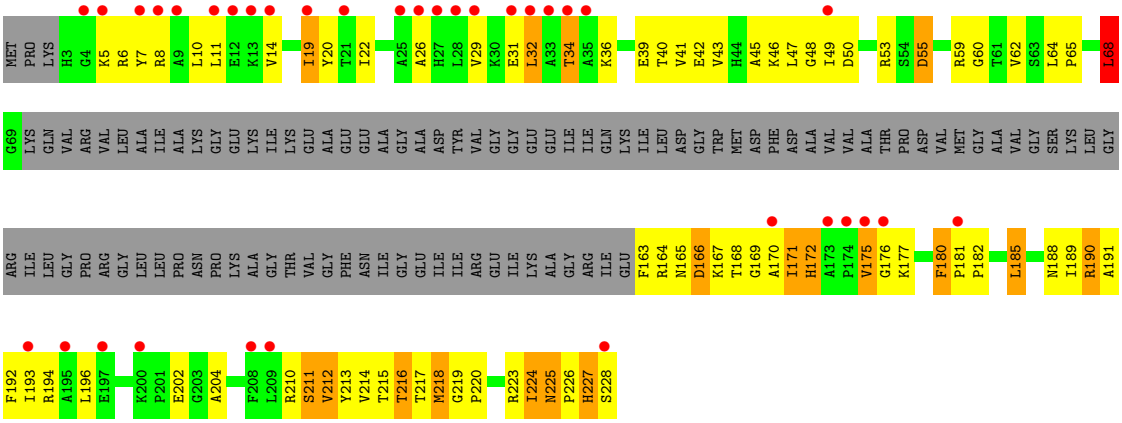




- Molecule 28: 50S ribosomal protein L1

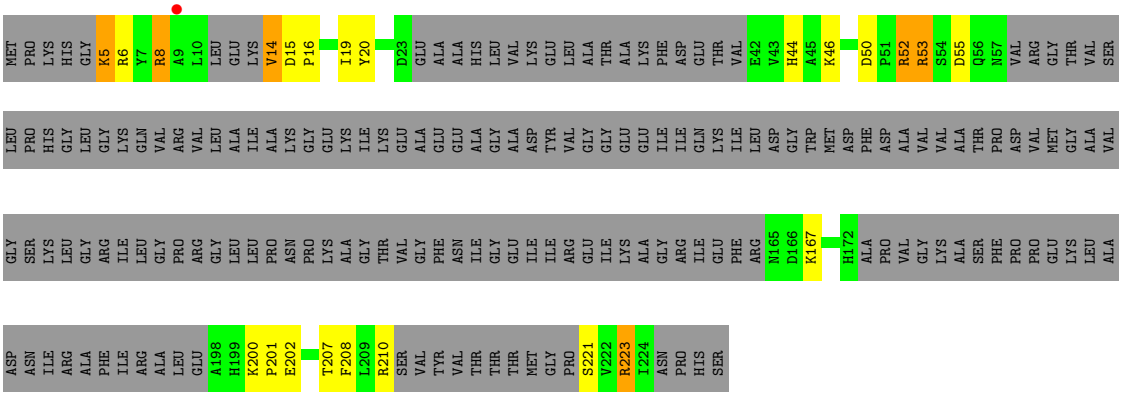
Chain 71:





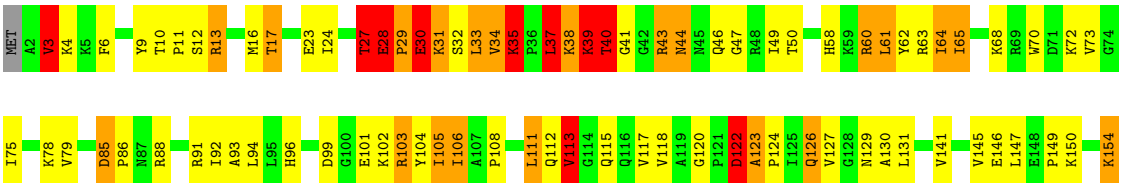
- Molecule 28: 50S ribosomal protein L1

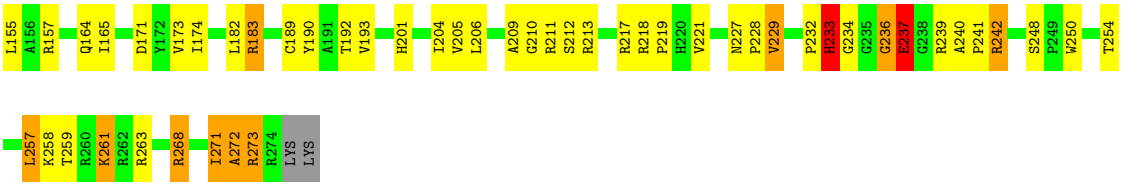
Chain 79:



- Molecule 29: 50S ribosomal protein L2

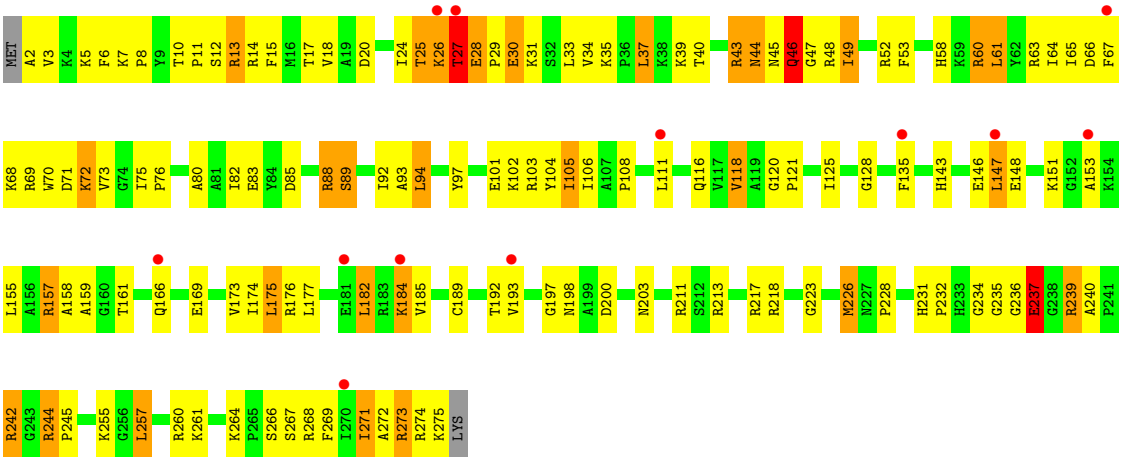
Chain 11:





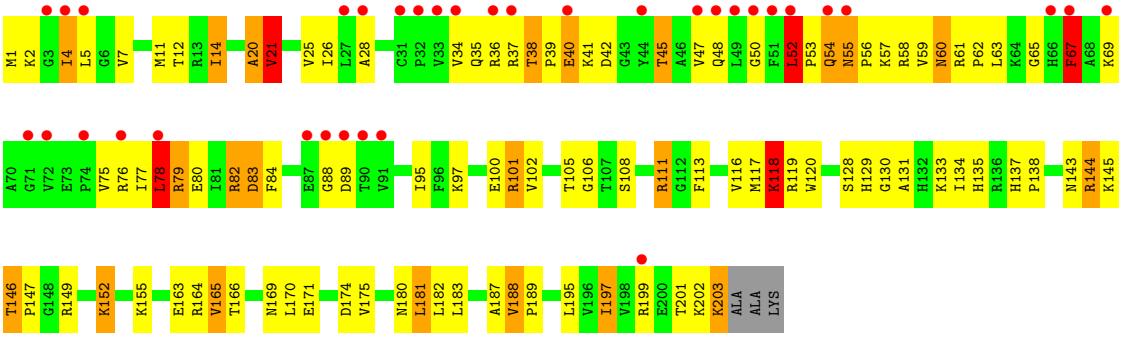
• Molecule 29: 50S ribosomal protein L2

Chain 19:



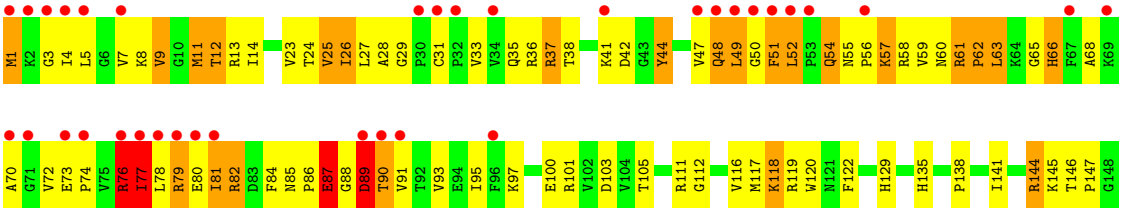
• Molecule 30: 50S ribosomal protein L3

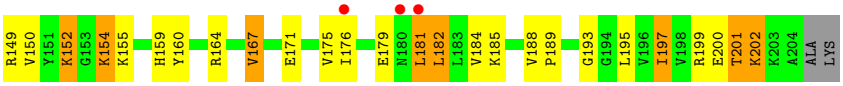
Chain 21:



• Molecule 30: 50S ribosomal protein L3

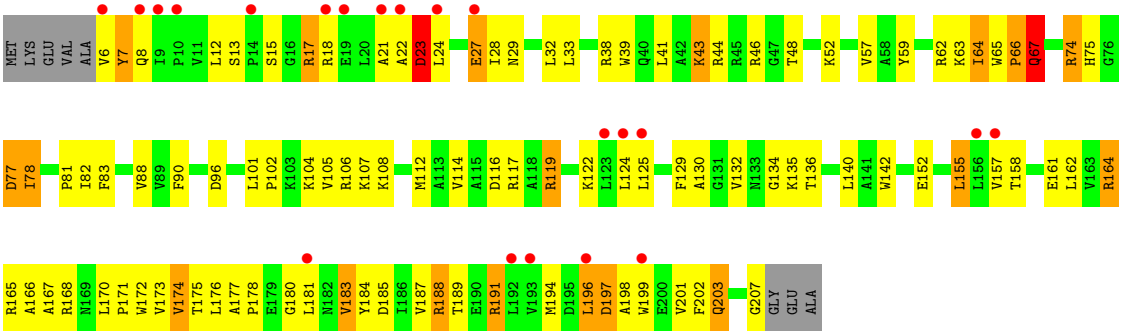
Chain 29:





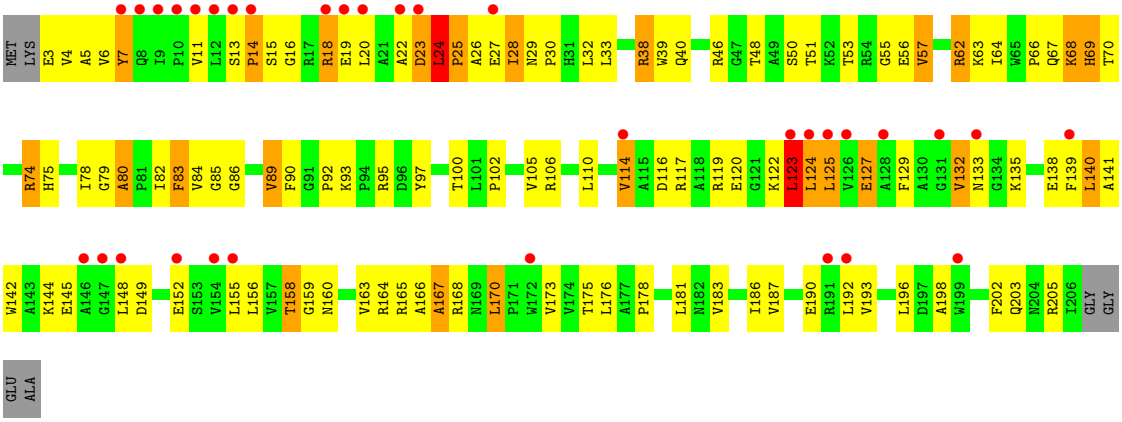
• Molecule 31: 50S ribosomal protein L4

Chain 31:



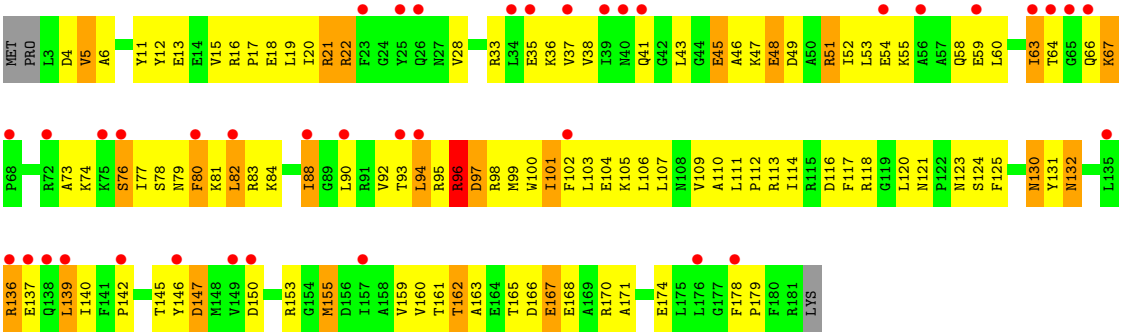
• Molecule 31: 50S ribosomal protein L4

Chain 39:



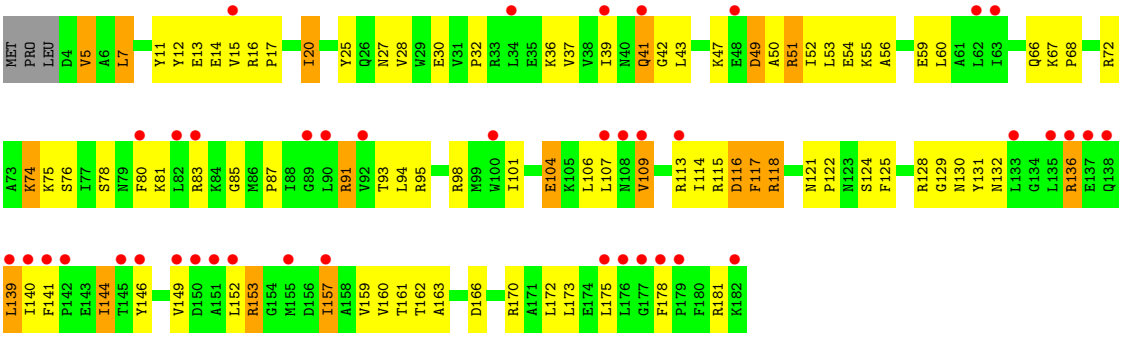
• Molecule 32: 50S ribosomal protein L5

Chain 41:



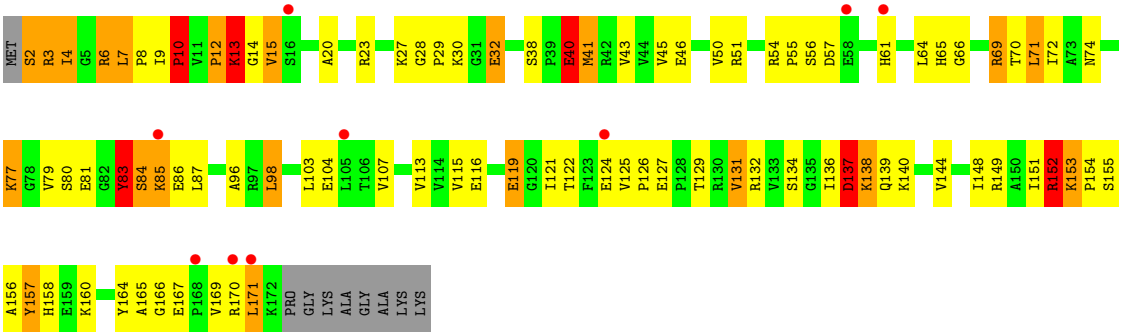
• Molecule 32: 50S ribosomal protein L5

Chain 49:



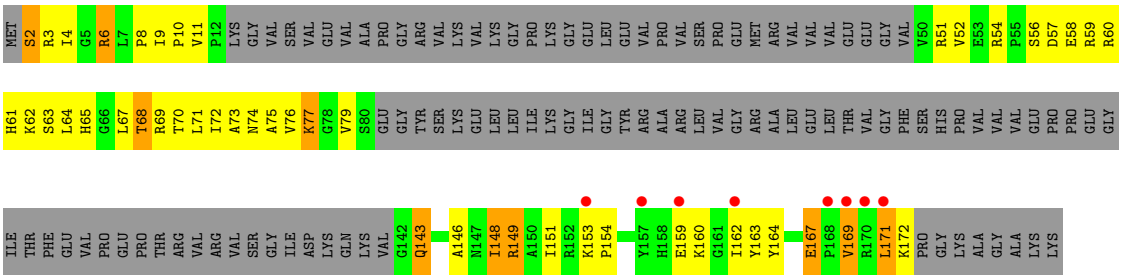
- Molecule 33: 50S ribosomal protein L6

Chain 51:



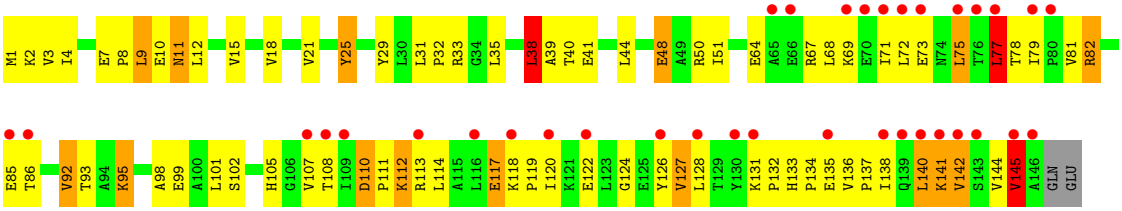
- Molecule 33: 50S ribosomal protein L6

Chain 59:



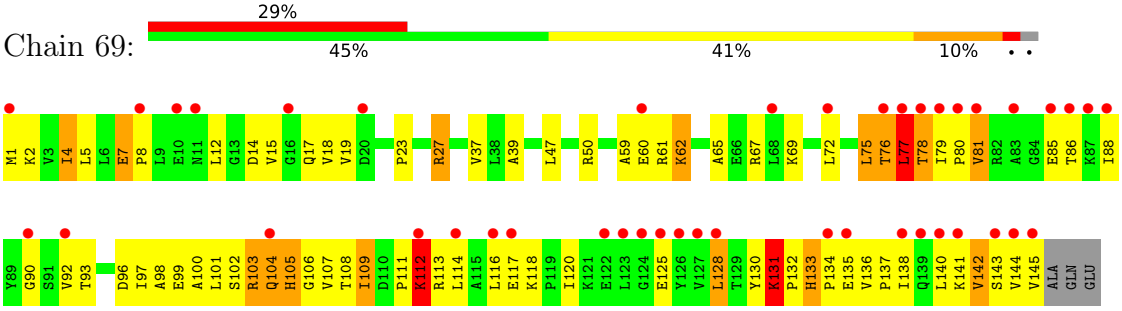
- Molecule 34: 50S ribosomal protein L9

Chain 61:



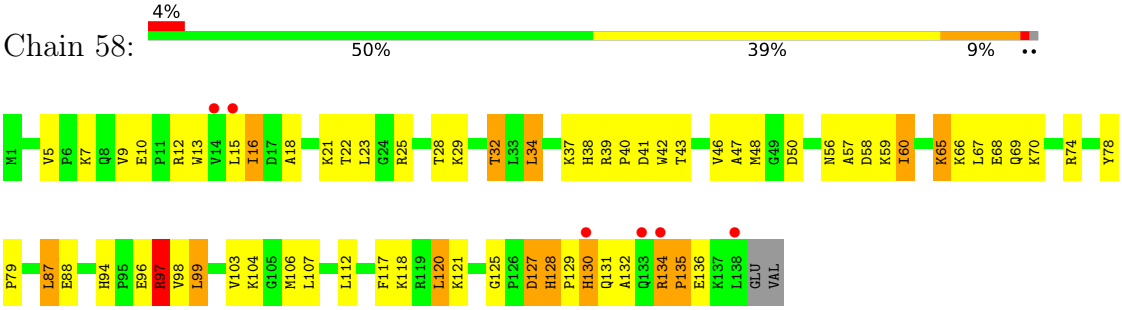
- Molecule 34: 50S ribosomal protein L9

Chain 69:



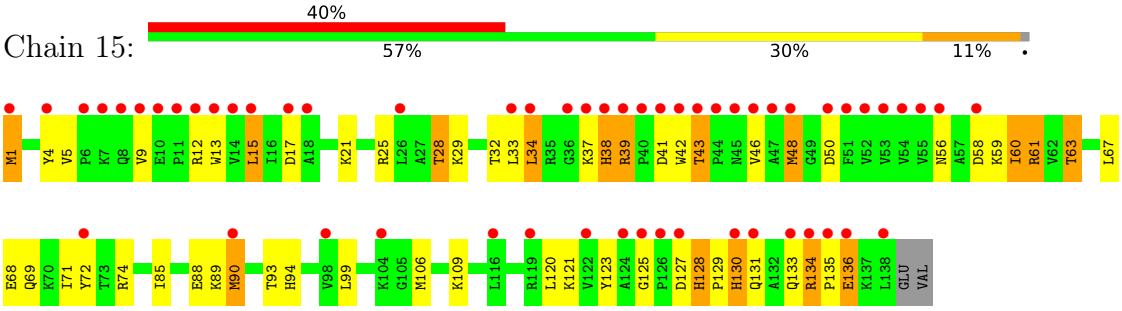
- Molecule 35: 50S ribosomal protein L13

Chain 58:



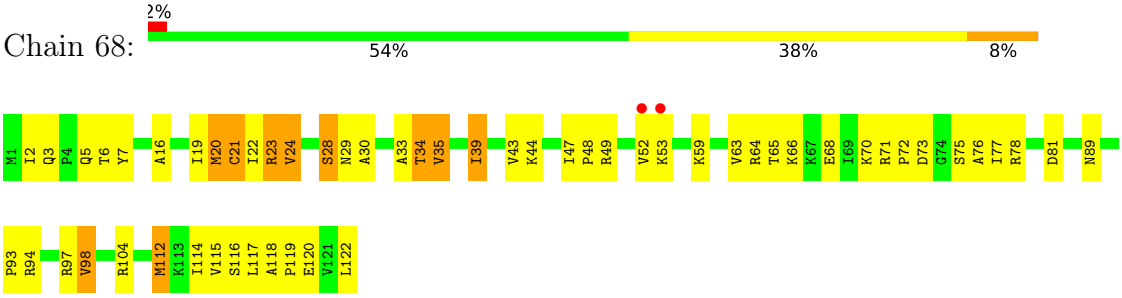
- Molecule 35: 50S ribosomal protein L13

Chain 15:



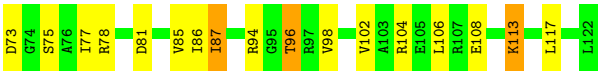
- Molecule 36: 50S ribosomal protein L14

Chain 68:



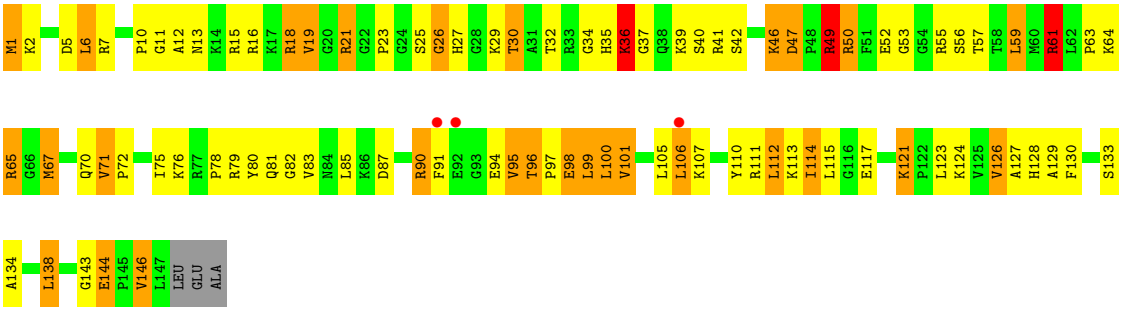
- Molecule 36: 50S ribosomal protein L14

Chain 25:



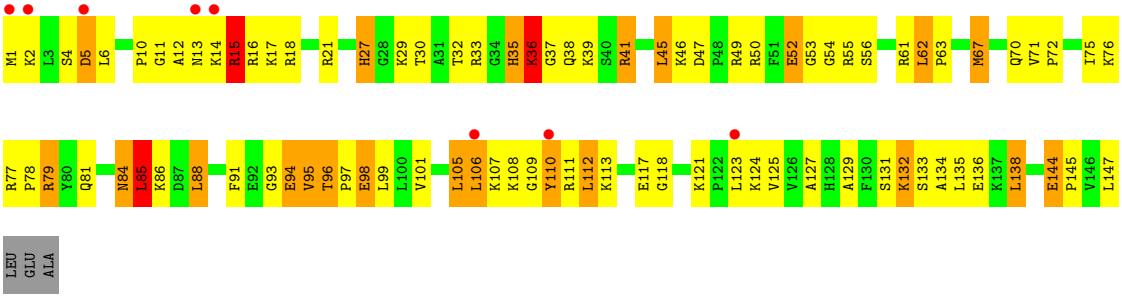
• Molecule 37: 50S ribosomal protein L15

Chain 78:



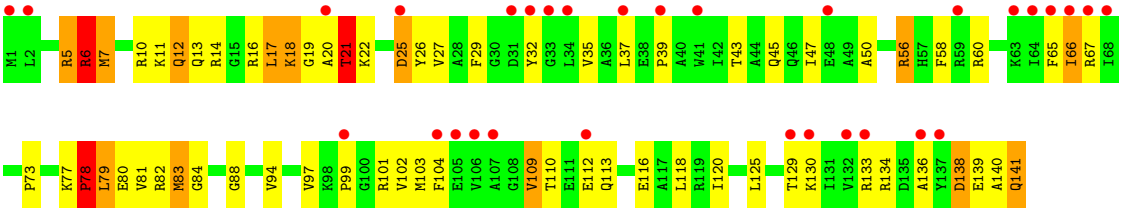
• Molecule 37: 50S ribosomal protein L15

Chain 35:



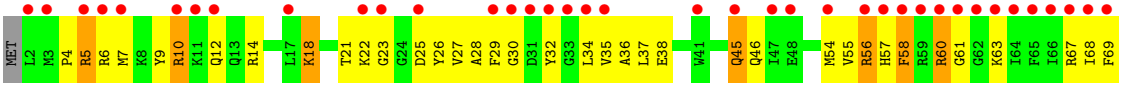
• Molecule 38: 50S ribosomal protein L16

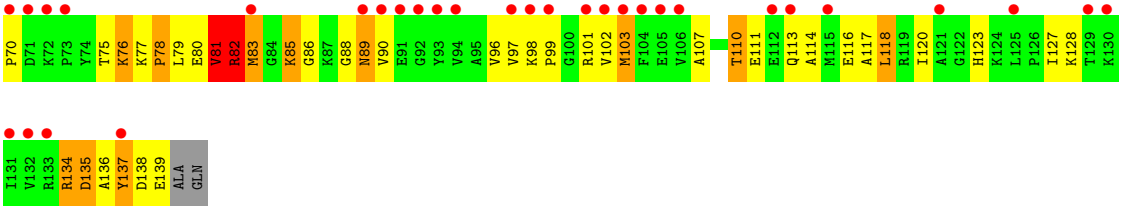
Chain 88:



• Molecule 38: 50S ribosomal protein L16

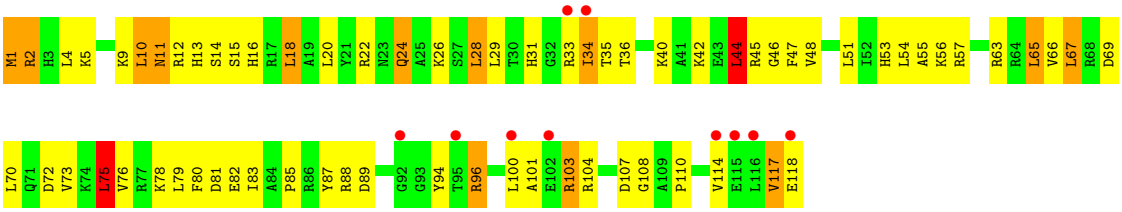
Chain 45:





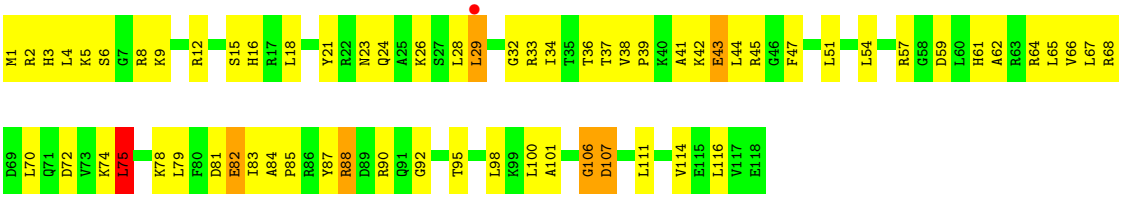
• Molecule 39: 50S ribosomal protein L17

Chain 98:



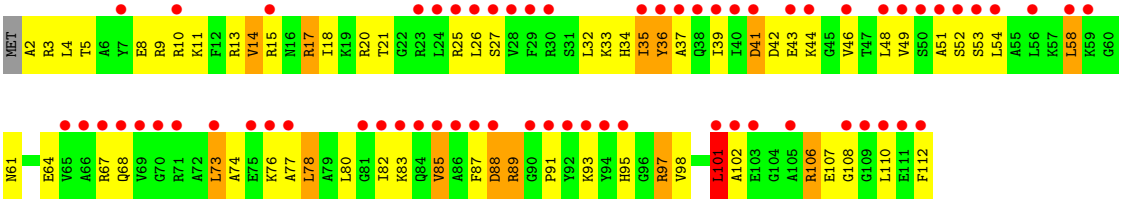
• Molecule 39: 50S ribosomal protein L17

Chain 55:



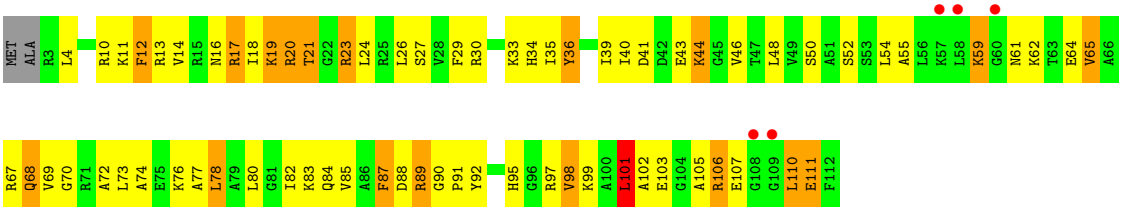
• Molecule 40: 50S ribosomal protein L18

Chain A8:



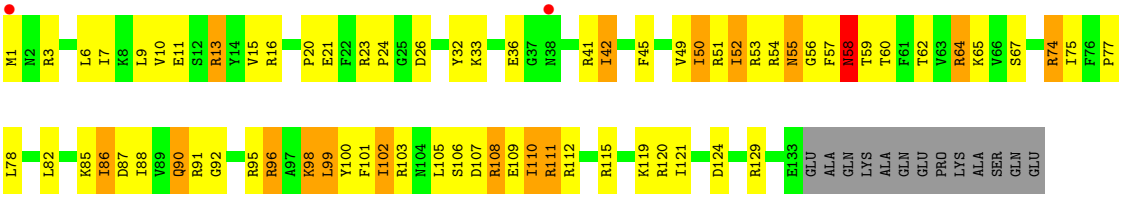
• Molecule 40: 50S ribosomal protein L18

Chain 65:



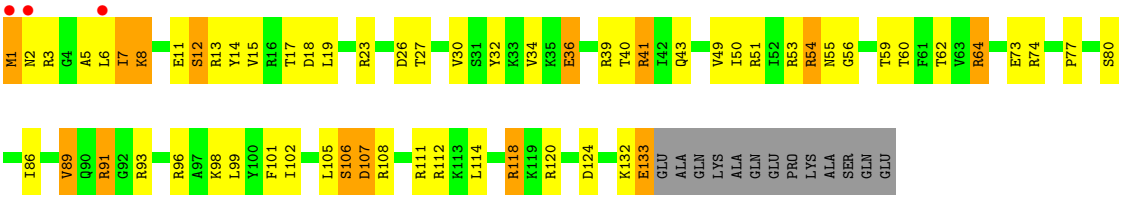
• Molecule 41: 50S ribosomal protein L19

Chain B8:



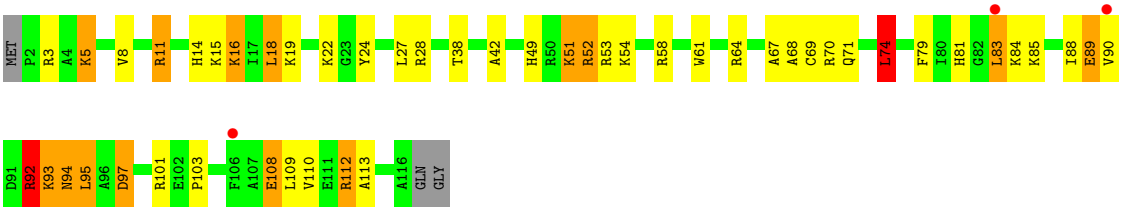
• Molecule 41: 50S ribosomal protein L19

Chain 75:



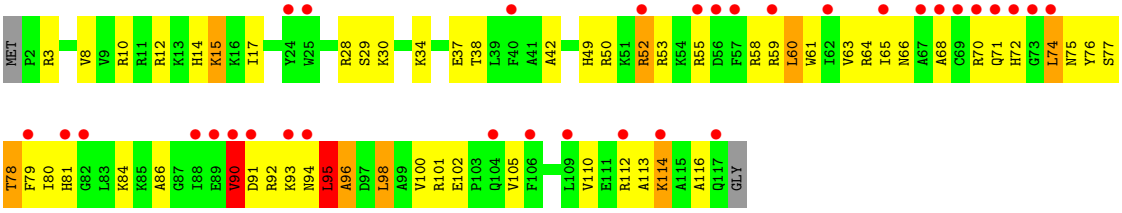
• Molecule 42: 50S ribosomal protein L20

Chain C8:



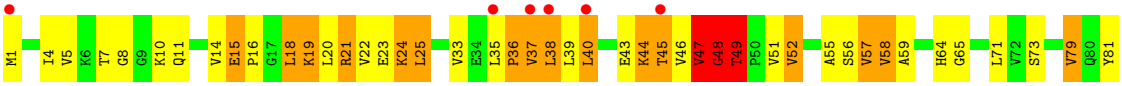
• Molecule 42: 50S ribosomal protein L20

Chain 85:



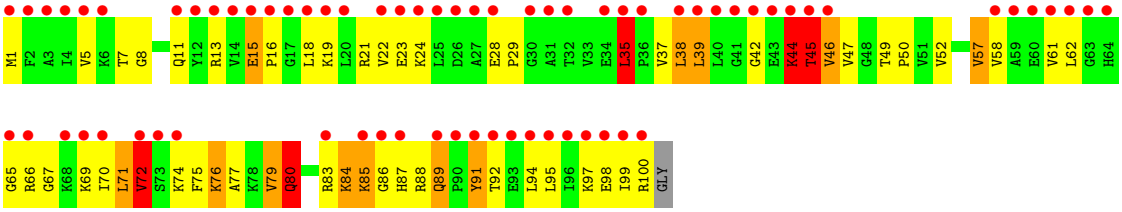
• Molecule 43: 50S ribosomal protein L21

Chain D8:



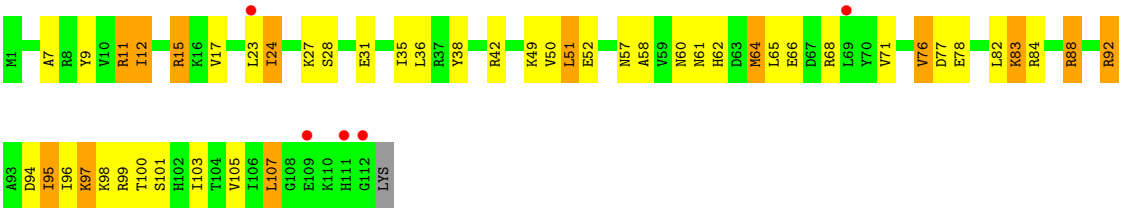
• Molecule 43: 50S ribosomal protein L21

Chain 95:



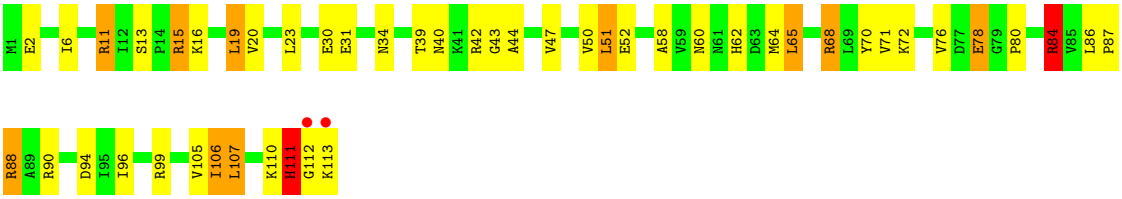
• Molecule 44: 50S ribosomal protein L22

Chain E8:



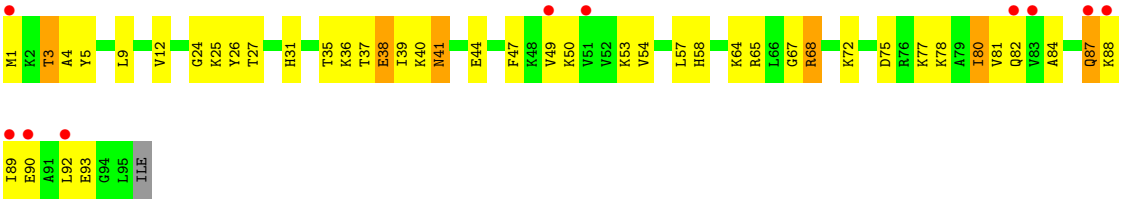
• Molecule 44: 50S ribosomal protein L22

Chain A5:



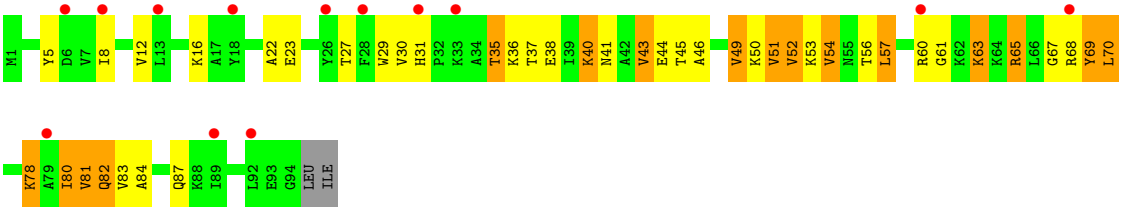
• Molecule 45: 50S ribosomal protein L23

Chain F8:



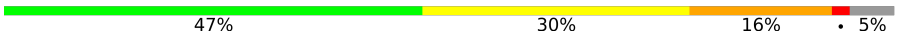
• Molecule 45: 50S ribosomal protein L23

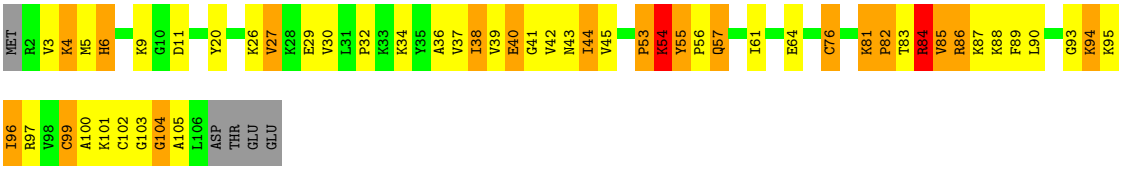
Chain B5:



• Molecule 46: 50S ribosomal protein L24

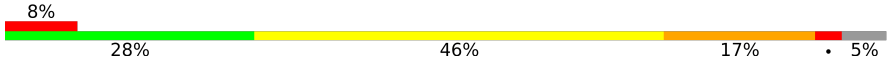
Chain G8:

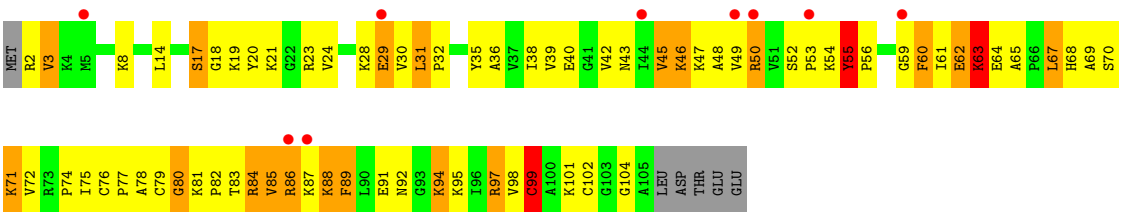




• Molecule 46: 50S ribosomal protein L24

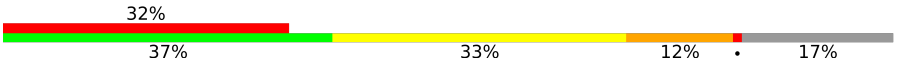
Chain C5:

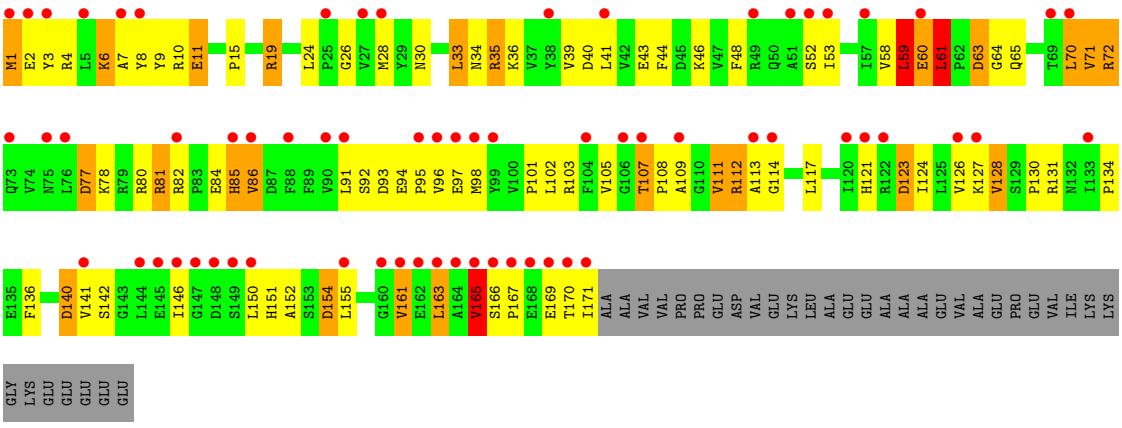




• Molecule 47: 50S ribosomal protein L25

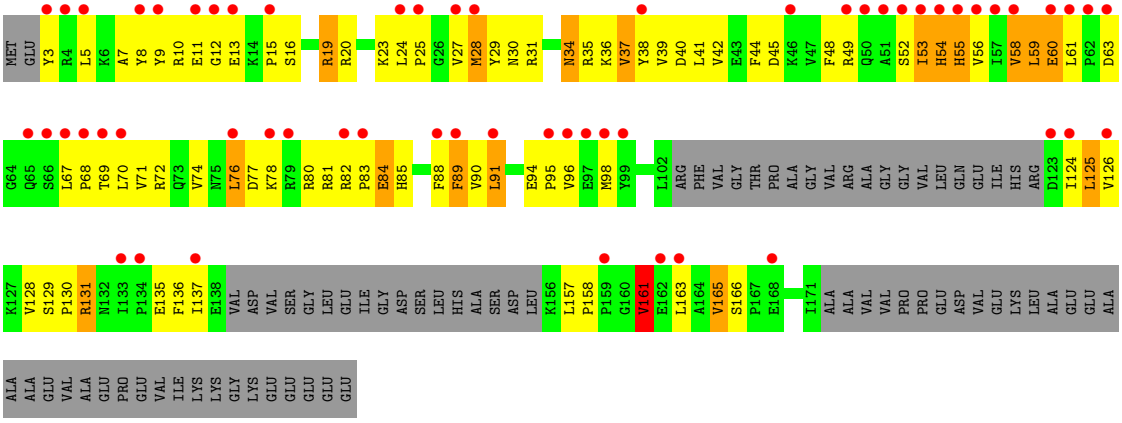
Chain H8:





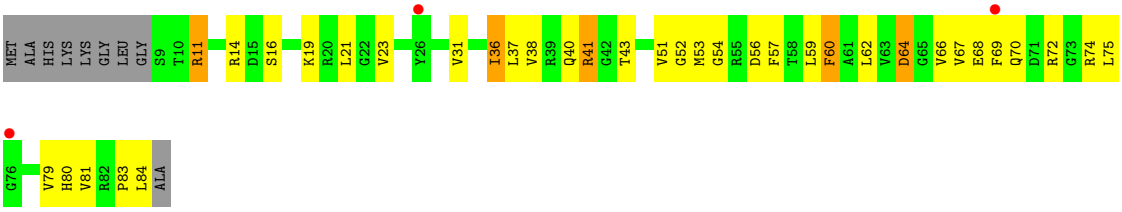
• Molecule 47: 50S ribosomal protein L25

Chain D5:



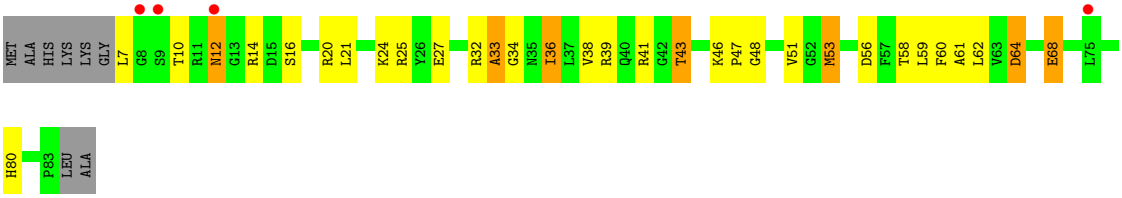
- Molecule 48: 50S ribosomal protein L27

Chain I8:



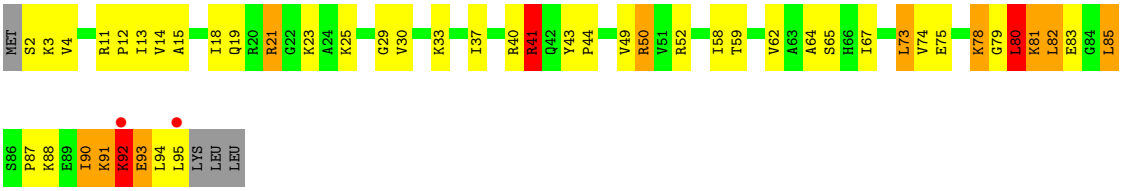
- Molecule 48: 50S ribosomal protein L27

Chain E5:



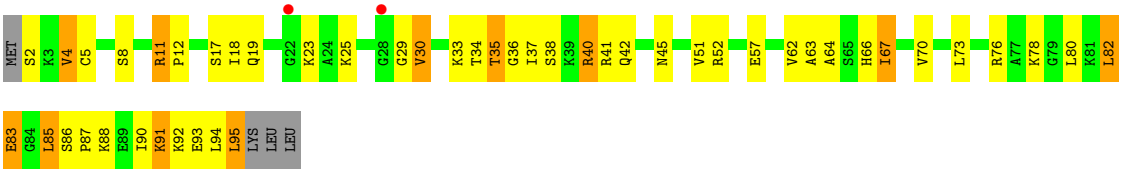
- Molecule 49: 50S ribosomal protein L28

Chain J8:



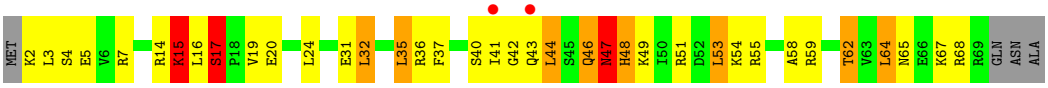
- Molecule 49: 50S ribosomal protein L28

Chain F5:



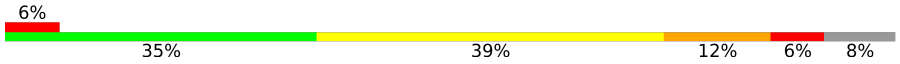
- Molecule 50: 50S ribosomal protein L29

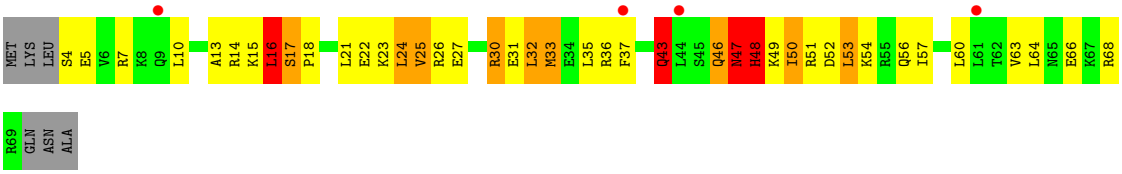
Chain K8:



- Molecule 50: 50S ribosomal protein L29

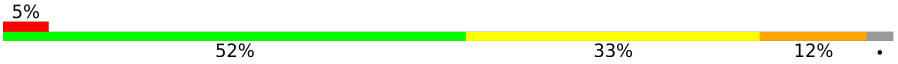
Chain G5:

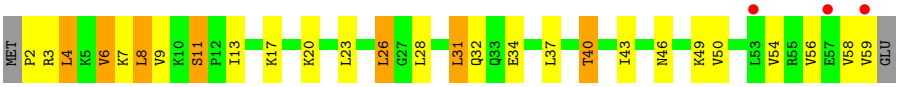




- Molecule 51: 50S ribosomal protein L30

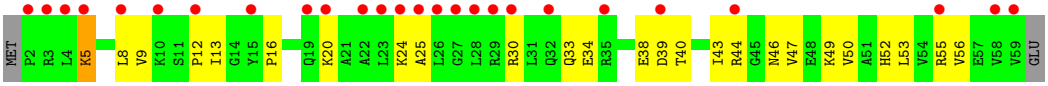
Chain L8:





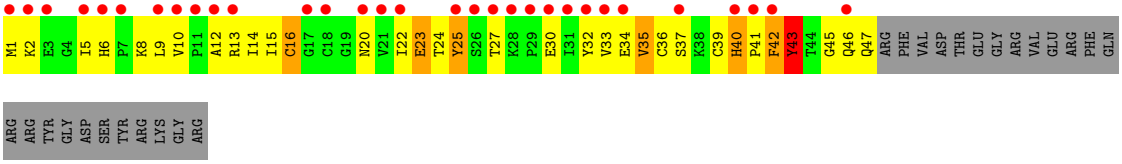
- Molecule 51: 50S ribosomal protein L30

Chain H5:



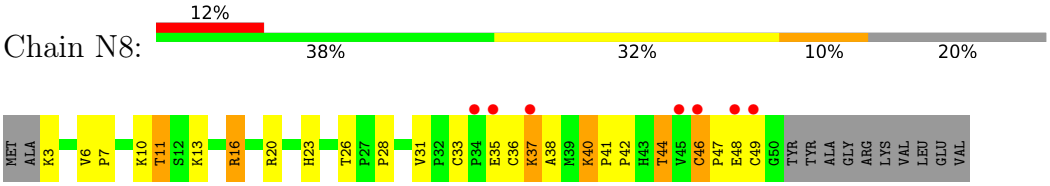
- Molecule 52: 50S ribosomal protein L31

Chain M8:



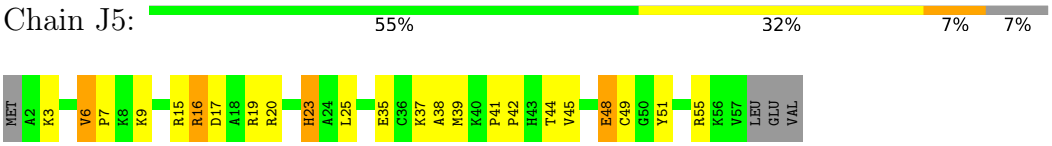
- Molecule 53: 50S ribosomal protein L32

Chain N8:



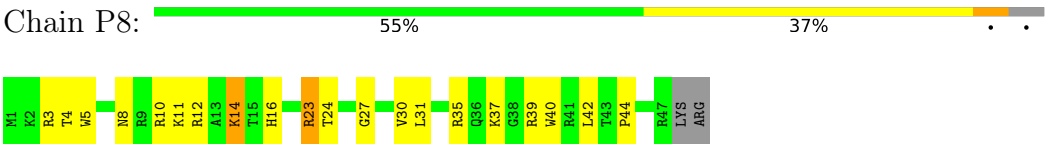
• Molecule 53: 50S ribosomal protein L32

Chain J5:



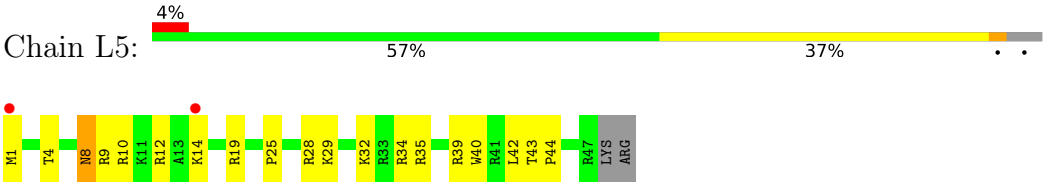
• Molecule 54: 50S ribosomal protein L34

Chain P8:



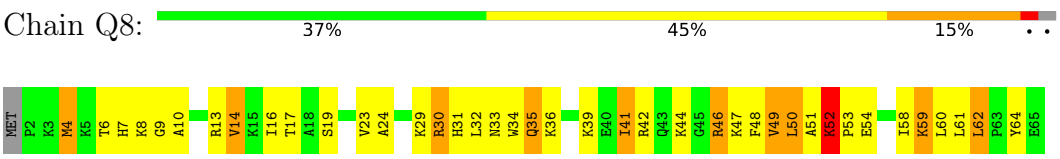
• Molecule 54: 50S ribosomal protein L34

Chain L5:



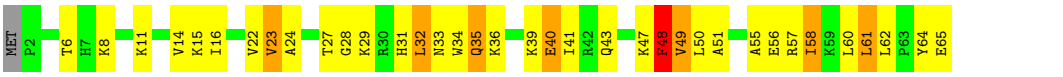
• Molecule 55: 50S ribosomal protein L35

Chain Q8:



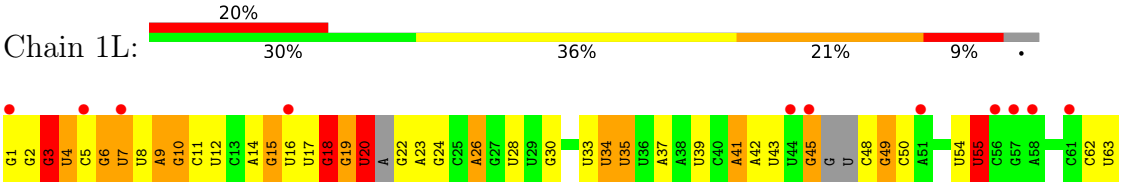
• Molecule 55: 50S ribosomal protein L35

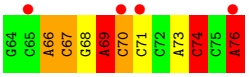
Chain M5:



• Molecule 56: tRNALys

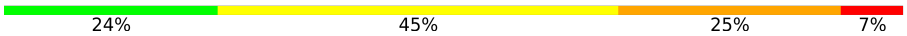
Chain 1L:

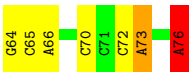




- Molecule 57: tRNALys

Chain 3L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.50Å 450.10Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.72 – 3.20 173.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.72-3.20) 93.8 (173.72-3.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.258 0.192 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 77.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	294444	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage'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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	13	0.75	5/35994 (0.0%)	1.39	368/56171 (0.7%)
1	1G	0.64	1/36258 (0.0%)	1.26	191/56589 (0.3%)
2	12	0.44	0/1752	0.74	1/2360 (0.0%)
2	1E	0.46	0/1908	0.74	4/2573 (0.2%)
3	22	0.40	0/1564	0.64	1/2109 (0.0%)
3	2E	0.49	0/1629	0.67	0/2195
4	32	0.48	0/1732	0.74	1/2318 (0.0%)
4	3E	0.52	0/1728	0.74	1/2313 (0.0%)
5	42	0.45	0/1150	0.69	0/1548
5	4E	0.53	0/1158	0.71	0/1559
6	52	0.51	0/855	0.68	0/1154
6	5E	0.57	0/850	0.72	0/1147
7	62	0.43	0/1122	0.65	0/1500
7	6E	0.43	0/1259	0.59	0/1686
8	72	0.41	0/1127	0.65	0/1517
8	7E	0.47	0/1135	0.74	1/1527 (0.1%)
9	82	0.42	0/971	0.71	0/1304
9	8E	0.44	0/1019	0.66	0/1367
10	1A	0.42	0/658	0.60	0/885
10	1I	0.51	0/747	0.75	1/1006 (0.1%)
11	2A	0.45	0/850	0.63	0/1150
11	2I	0.49	0/838	0.69	0/1133
12	3A	0.55	0/972	0.83	2/1301 (0.2%)
12	3I	0.72	0/972	0.87	0/1301
13	4A	0.42	0/903	0.72	1/1211 (0.1%)
13	4I	0.53	0/952	0.73	0/1277
14	5A	0.47	0/495	0.72	1/657 (0.2%)
14	5I	0.62	0/500	0.75	0/664
15	6A	0.44	0/744	0.59	0/992
15	6I	0.52	0/740	0.71	0/987
16	7A	0.49	0/721	0.74	0/970
16	7I	0.47	0/716	0.73	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.45	0/836	0.64	0/1117
17	8I	0.52	0/847	0.70	0/1131
18	9A	0.46	0/549	0.70	0/732
18	9I	0.53	0/554	0.77	0/739
19	AA	0.44	0/490	0.70	0/662
19	AI	0.53	0/668	0.79	0/899
20	BA	0.43	0/764	0.73	0/1007
20	BI	0.43	0/748	0.65	1/986 (0.1%)
21	1B	0.47	0/192	0.70	0/252
21	1F	0.52	0/203	0.68	0/266
22	1K	0.66	0/1565	1.29	14/2429 (0.6%)
23	2K	0.84	1/1721 (0.1%)	1.50	32/2682 (1.2%)
23	2L	0.66	1/1721 (0.1%)	1.24	10/2682 (0.4%)
24	3K	0.67	0/1799	1.31	17/2801 (0.6%)
25	4K	0.91	0/473	1.34	1/737 (0.1%)
25	4L	0.67	0/448	1.13	0/698
26	14	0.90	57/69023 (0.1%)	1.59	1407/107740 (1.3%)
26	1H	1.06	113/68351 (0.2%)	1.80	2304/106700 (2.2%)
27	16	0.84	0/2928	1.55	47/4568 (1.0%)
27	1J	0.70	0/2928	1.36	28/4568 (0.6%)
28	71	0.46	0/1055	0.72	1/1425 (0.1%)
28	79	0.43	0/459	0.90	3/608 (0.5%)
29	11	0.82	2/2170 (0.1%)	1.01	7/2926 (0.2%)
29	19	0.71	1/2175 (0.0%)	0.93	3/2933 (0.1%)
30	21	0.67	0/1591	0.96	2/2146 (0.1%)
30	29	0.63	0/1596	0.92	2/2153 (0.1%)
31	31	0.73	1/1620 (0.1%)	0.91	1/2194 (0.0%)
31	39	0.62	0/1637	0.90	3/2218 (0.1%)
32	41	0.52	0/1481	0.78	1/1994 (0.1%)
32	49	0.43	0/1482	0.68	0/1994
33	51	0.68	0/1337	1.00	9/1809 (0.5%)
33	59	0.46	0/577	0.88	2/776 (0.3%)
34	61	0.52	0/1151	0.80	2/1558 (0.1%)
34	69	0.46	0/1146	0.77	3/1551 (0.2%)
35	15	0.46	0/1131	0.68	0/1525
35	58	0.60	0/1131	0.82	0/1525
36	25	0.58	0/942	0.74	0/1269
36	68	0.67	0/942	0.81	0/1269
37	35	0.61	0/1139	0.98	2/1514 (0.1%)
37	78	0.70	0/1139	1.12	8/1514 (0.5%)
38	45	0.69	0/1120	0.97	4/1498 (0.3%)
38	88	0.78	0/1134	0.98	2/1519 (0.1%)
39	55	0.64	0/981	0.85	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	98	0.56	0/981	0.85	1/1312 (0.1%)
40	65	0.51	0/886	0.86	3/1180 (0.3%)
40	A8	0.63	0/891	0.85	1/1187 (0.1%)
41	75	0.56	0/1123	0.72	0/1500
41	B8	0.66	0/1123	0.82	0/1500
42	85	0.59	0/977	0.75	1/1301 (0.1%)
42	C8	0.67	0/968	0.82	1/1289 (0.1%)
43	95	0.70	0/785	0.87	1/1052 (0.1%)
43	D8	0.58	0/785	0.90	4/1052 (0.4%)
44	A5	0.62	0/910	0.84	1/1220 (0.1%)
44	E8	0.66	0/901	0.87	0/1209
45	B5	0.68	0/749	0.79	0/1007
45	F8	0.76	0/757	0.87	0/1017
46	C5	0.63	0/807	0.93	2/1076 (0.2%)
46	G8	0.82	1/809 (0.1%)	1.08	4/1080 (0.4%)
47	D5	0.51	0/1098	0.73	0/1487
47	H8	0.53	0/1403	0.81	1/1901 (0.1%)
48	E5	0.57	0/616	0.84	0/821
48	I8	0.76	0/614	0.94	0/819
49	F5	0.66	0/744	0.88	1/989 (0.1%)
49	J8	0.73	0/744	0.93	4/989 (0.4%)
50	G5	0.59	0/560	0.82	2/741 (0.3%)
50	K8	0.72	0/570	0.97	0/755
51	H5	0.49	0/464	0.66	0/623
51	L8	0.63	0/464	0.84	0/623
52	M8	0.53	0/375	0.95	2/507 (0.4%)
53	J5	0.61	0/448	0.81	0/606
53	N8	0.69	1/381 (0.3%)	0.86	0/516
54	L5	0.69	0/409	0.89	0/540
54	P8	0.85	0/409	1.07	2/540 (0.4%)
55	M5	0.75	0/524	1.00	3/691 (0.4%)
55	Q8	0.79	0/524	1.17	4/691 (0.6%)
56	1L	0.61	1/1613 (0.1%)	1.18	11/2504 (0.4%)
57	3L	0.65	0/1733	1.28	14/2699 (0.5%)
All	All	0.81	185/317108 (0.1%)	1.41	4553/475084 (1.0%)

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
1	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	4
2	1E	0	4
3	22	0	2
4	32	0	1
4	3E	0	1
9	82	0	1
9	8E	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	1
13	4A	0	2
13	4I	0	3
14	5A	0	1
18	9I	0	1
19	AI	0	2
20	BA	0	2
28	71	0	3
29	11	0	4
29	19	0	4
30	21	0	5
30	29	0	5
31	31	0	4
31	39	0	7
32	41	0	1
32	49	0	1
33	51	0	6
34	61	0	4
34	69	0	2
37	35	0	3
37	78	0	5
38	45	0	6
38	88	0	1
39	55	0	1
39	98	0	1
40	65	0	1
41	75	0	1
41	B8	0	1
42	85	0	4
42	C8	0	2
43	95	0	2
43	D8	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
44	A5	0	2
45	B5	0	1
45	F8	0	2
46	C5	0	3
46	G8	0	7
47	D5	0	2
47	H8	0	4
49	J8	0	2
50	G5	0	4
50	K8	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	1
All	All	1	141

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-11.99	1.30	1.37
26	1H	2430	A	N9-C4	-11.47	1.30	1.37
26	1H	783	A	N3-C4	-11.40	1.28	1.34
26	14	2430	A	N9-C4	-10.71	1.31	1.37
26	14	528	A	N9-C4	-10.24	1.31	1.37

The worst 5 of 4553 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-19.34	114.40	126.00
26	1H	783	A	C8-N9-C4	-17.08	98.97	105.80
26	14	2518	A	N1-C6-N6	17.07	128.84	118.60
26	1H	676	A	C2-N3-C4	-16.88	102.16	110.60
26	14	774	A	C2-N3-C4	-16.75	102.23	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	A	C1'

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	9	GLU	Peptide
4	3E	193	ASP	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	32157	0	16233	755	0
1	1G	32391	0	16353	749	0
2	12	1721	0	1758	101	0
2	1E	1874	0	1926	103	0
3	22	1541	0	1606	69	0
3	2E	1605	0	1668	58	0
4	32	1702	0	1765	110	0
4	3E	1698	0	1761	83	0
5	42	1134	0	1200	45	0
5	4E	1142	0	1204	62	0
6	52	842	0	857	30	0
6	5E	837	0	852	35	0
7	62	1110	0	1163	49	0
7	6E	1242	0	1286	44	0
8	72	1107	0	1165	39	0
8	7E	1115	0	1177	58	0
9	82	953	0	983	70	0
9	8E	1000	0	1031	58	0
10	1A	646	0	662	33	0
10	1I	734	0	761	43	0
11	2A	835	0	847	31	0
11	2I	823	0	833	49	0
12	3A	956	0	1046	56	0
12	3I	956	0	1046	33	0
13	4A	893	0	946	61	0
13	4I	942	0	997	53	0
14	5A	486	0	525	25	0
14	5I	491	0	529	26	0
15	6A	733	0	771	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	29	0
16	7A	705	0	725	29	0
16	7I	700	0	720	47	0
17	8A	823	0	891	35	0
17	8I	834	0	904	42	0
18	9A	544	0	605	26	0
18	9I	549	0	607	36	0
19	AA	481	0	468	32	0
19	AI	654	0	675	44	0
20	BA	762	0	861	32	0
20	BI	746	0	843	49	0
21	1B	188	0	195	13	0
21	1F	199	0	208	5	0
22	1K	1520	0	778	41	0
23	2K	1646	0	843	30	0
23	2L	1646	0	843	40	0
24	3K	1611	0	817	48	0
25	4K	419	0	208	6	0
25	4L	397	0	197	12	0
26	14	61630	0	31073	1315	0
26	1H	61028	0	30763	1351	0
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	65	0
28	71	1033	0	1048	77	0
28	79	456	0	460	22	0
29	11	2120	0	2197	131	0
29	19	2125	0	2199	104	0
30	21	1558	0	1624	83	0
30	29	1563	0	1629	117	0
31	31	1585	0	1632	89	0
31	39	1602	0	1649	80	0
32	41	1457	0	1514	94	0
32	49	1458	0	1516	59	0
33	51	1312	0	1384	66	0
33	59	568	0	595	48	0
34	61	1136	0	1223	57	0
34	69	1131	0	1218	48	0
35	15	1104	0	1180	38	0
35	58	1104	0	1180	54	0
36	25	932	0	996	36	0
36	68	932	0	996	42	0
37	35	1122	0	1206	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	78	1122	0	1206	94	0
38	45	1099	0	1154	79	0
38	88	1113	0	1157	51	0
39	55	967	0	1033	49	0
39	98	967	0	1033	49	0
40	65	876	0	938	65	0
40	A8	881	0	943	52	0
41	75	1109	0	1170	55	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	53	0
42	C8	950	0	1011	52	0
43	95	774	0	849	63	0
43	D8	774	0	849	43	0
44	A5	899	0	964	28	0
44	E8	890	0	951	25	0
45	B5	735	0	785	35	0
45	F8	743	0	794	36	0
46	C5	794	0	886	68	0
46	G8	796	0	886	45	0
47	D5	1074	0	1086	53	0
47	H8	1373	0	1402	59	0
48	E5	608	0	622	26	0
48	I8	606	0	625	30	0
49	F5	737	0	813	32	0
49	J8	737	0	813	39	0
50	G5	558	0	610	33	0
50	K8	568	0	614	36	0
51	H5	459	0	512	10	0
51	L8	459	0	512	18	0
52	M8	366	0	370	37	0
53	J5	434	0	454	22	0
53	N8	369	0	388	22	0
54	L5	401	0	436	14	0
54	P8	401	0	436	14	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1563	0	799	42	0
57	3L	1612	0	819	41	0
58	13	132	0	0	0	0
58	14	399	0	0	0	0
58	16	9	0	0	0	0
58	1E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1G	90	0	0	0	0
58	1H	467	0	0	0	0
58	1J	5	0	0	0	0
58	1K	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	4	0	0	0	0
58	2K	3	0	0	0	0
58	2L	2	0	0	0	0
58	35	3	0	0	0	0
58	39	1	0	0	0	0
58	3K	1	0	0	0	0
58	41	1	0	0	0	0
58	45	2	0	0	0	0
58	55	1	0	0	0	0
58	5E	1	0	0	0	0
58	6A	1	0	0	0	0
58	78	1	0	0	0	0
58	88	1	0	0	0	0
58	98	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	3	0	0	0	0
58	J8	1	0	0	0	0
58	L8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	2	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	7	0	0	5	0
61	13	126	0	0	21	0
61	14	417	0	0	73	0
61	16	29	0	0	6	0
61	19	8	0	0	1	0
61	1G	78	0	0	9	0
61	1H	629	0	0	101	0
61	1J	6	0	0	1	0
61	1K	8	0	0	0	0
61	21	4	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	2	0	0	0	0
61	31	9	0	0	0	0
61	32	1	0	0	0	0
61	35	1	0	0	0	0
61	39	5	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	4K	2	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	2	0	0	0	0
61	5I	2	0	0	0	0
61	78	7	0	0	2	0
61	88	1	0	0	0	0
61	A5	1	0	0	0	0
61	B8	1	0	0	0	0
61	E8	2	0	0	0	0
61	F8	1	0	0	0	0
61	G8	1	0	0	0	0
61	H5	2	0	0	1	0
61	I8	3	0	0	1	0
61	L8	2	0	0	1	0
All	All	294444	0	196318	8229	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 17.

The worst 5 of 8229 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:G8:100:ALA:HB1	46:G8:101:LYS:HG2	1.34	1.09
55:M5:48:PHE:HB2	55:M5:49:VAL:HG22	1.31	1.07
26:14:161:U:H5'	26:14:171:G:H21	1.18	1.06
26:1H:2711:A:OP2	61:1H:3501:HOH:O	1.73	1.05
26:14:2002:G:N7	61:14:3505:HOH:O	1.91	1.03

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	206/256 (80%)	168 (82%)	31 (15%)	7 (3%)	3 24
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12 47
3	22	192/239 (80%)	169 (88%)	22 (12%)	1 (0%)	29 67
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100 100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29 67
4	3E	205/209 (98%)	188 (92%)	14 (7%)	3 (2%)	10 44
5	42	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22 61
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	22 61
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100 100
6	5E	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22 61
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100 100
8	72	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	22 61
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22 61
9	82	119/128 (93%)	107 (90%)	11 (9%)	1 (1%)	19 58
9	8E	124/128 (97%)	104 (84%)	19 (15%)	1 (1%)	19 58
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100 100
10	1I	89/105 (85%)	83 (93%)	6 (7%)	0	100 100
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	8 41
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	17 56
12	3A	120/132 (91%)	102 (85%)	13 (11%)	5 (4%)	3 20
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19 58
13	4A	109/126 (86%)	95 (87%)	13 (12%)	1 (1%)	17 56
13	4I	117/126 (93%)	97 (83%)	19 (16%)	1 (1%)	17 56
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8 41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	24
15	6A	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	2 (3%)	1 (2%)	10	44
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	44
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	3	23
19	AI	79/93 (85%)	67 (85%)	10 (13%)	2 (2%)	5	32
20	BA	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	7	37
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	119 (92%)	10 (8%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	243 (90%)	17 (6%)	11 (4%)	3	21
29	19	272/276 (99%)	241 (89%)	25 (9%)	6 (2%)	6	35
30	21	201/206 (98%)	157 (78%)	36 (18%)	8 (4%)	3	21
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	21
31	31	200/210 (95%)	175 (88%)	25 (12%)	0	100	100
31	39	202/210 (96%)	157 (78%)	36 (18%)	9 (4%)	2	18
32	41	177/182 (97%)	155 (88%)	19 (11%)	3 (2%)	9	42
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	14	51
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	12
33	59	67/180 (37%)	50 (75%)	14 (21%)	3 (4%)	2	18
34	61	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	11	46
34	69	143/148 (97%)	116 (81%)	26 (18%)	1 (1%)	22	61
35	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	61
35	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	6	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
36	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	35	145/150 (97%)	114 (79%)	29 (20%)	2 (1%)	11	46
37	78	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3	24
38	45	136/141 (96%)	112 (82%)	21 (15%)	3 (2%)	6	35
38	88	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	23
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	56
39	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	17	56
40	65	108/112 (96%)	86 (80%)	20 (18%)	2 (2%)	8	39
40	A8	109/112 (97%)	92 (84%)	14 (13%)	3 (3%)	5	29
41	75	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
41	B8	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
42	85	114/118 (97%)	101 (89%)	11 (10%)	2 (2%)	8	41
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	30
43	95	98/101 (97%)	77 (79%)	14 (14%)	7 (7%)	1	8
43	D8	98/101 (97%)	87 (89%)	6 (6%)	5 (5%)	2	15
44	A5	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	17	56
44	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	4 (4%)	3 (3%)	4	25
45	F8	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	51
46	C5	102/110 (93%)	75 (74%)	17 (17%)	10 (10%)	0	3
46	G8	103/110 (94%)	86 (84%)	13 (13%)	4 (4%)	3	22
47	D5	126/206 (61%)	100 (79%)	21 (17%)	5 (4%)	3	21
47	H8	169/206 (82%)	136 (80%)	25 (15%)	8 (5%)	2	17
48	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	12	47
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	85 (92%)	6 (6%)	1 (1%)	14	51
49	J8	92/98 (94%)	83 (90%)	8 (9%)	1 (1%)	14	51
50	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	4	26
50	K8	66/72 (92%)	58 (88%)	5 (8%)	3 (4%)	2	18
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	M8	45/71 (63%)	29 (64%)	15 (33%)	1 (2%)	6	35
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	P8	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
55	M5	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	26
55	Q8	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	17
All	All	10973/12333 (89%)	9576 (87%)	1201 (11%)	196 (2%)	8	41

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	13	THR
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU

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	182/220 (83%)	154 (85%)	28 (15%)	2	13
2	1E	200/220 (91%)	143 (72%)	57 (28%)	0	1
3	22	154/188 (82%)	123 (80%)	31 (20%)	1	6
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	5
4	32	180/181 (99%)	143 (79%)	37 (21%)	1	6
4	3E	180/181 (99%)	137 (76%)	43 (24%)	0	3
5	42	114/123 (93%)	91 (80%)	23 (20%)	1	6
5	4E	115/123 (94%)	98 (85%)	17 (15%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	6
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1	8
7	62	114/127 (90%)	95 (83%)	19 (17%)	2	10
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1	8
8	72	118/119 (99%)	98 (83%)	20 (17%)	2	10
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	92/99 (93%)	71 (77%)	21 (23%)	1	4
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	6
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	1
10	1I	81/92 (88%)	65 (80%)	16 (20%)	1	7
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	9
11	2I	84/99 (85%)	61 (73%)	23 (27%)	0	1
12	3A	103/109 (94%)	81 (79%)	22 (21%)	1	5
12	3I	103/109 (94%)	87 (84%)	16 (16%)	2	12
13	4A	91/101 (90%)	70 (77%)	21 (23%)	1	3
13	4I	94/101 (93%)	75 (80%)	19 (20%)	1	6
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1	4
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	13
15	6I	79/80 (99%)	62 (78%)	17 (22%)	1	5
16	7A	72/74 (97%)	52 (72%)	20 (28%)	0	1
16	7I	72/74 (97%)	51 (71%)	21 (29%)	0	1
17	8A	94/97 (97%)	79 (84%)	15 (16%)	2	11
17	8I	95/97 (98%)	79 (83%)	16 (17%)	2	10
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0	1
18	9I	58/77 (75%)	44 (76%)	14 (24%)	0	3
19	AA	52/80 (65%)	40 (77%)	12 (23%)	1	3
19	AI	71/80 (89%)	58 (82%)	13 (18%)	1	8
20	BA	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	BI	75/82 (92%)	59 (79%)	16 (21%)	1	5
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1F	18/22 (82%)	17 (94%)	1 (6%)	21	57
28	71	109/181 (60%)	87 (80%)	22 (20%)	1	6
28	79	48/181 (26%)	38 (79%)	10 (21%)	1	6
29	11	214/218 (98%)	161 (75%)	53 (25%)	0	2
29	19	214/218 (98%)	169 (79%)	45 (21%)	1	6
30	21	165/166 (99%)	128 (78%)	37 (22%)	1	4
30	29	165/166 (99%)	126 (76%)	39 (24%)	1	3
31	31	161/166 (97%)	126 (78%)	35 (22%)	1	5
31	39	163/166 (98%)	130 (80%)	33 (20%)	1	6
32	41	153/156 (98%)	121 (79%)	32 (21%)	1	6
32	49	153/156 (98%)	125 (82%)	28 (18%)	1	8
33	51	142/148 (96%)	109 (77%)	33 (23%)	1	3
33	59	59/148 (40%)	50 (85%)	9 (15%)	2	13
34	61	122/124 (98%)	95 (78%)	27 (22%)	1	4
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	117/119 (98%)	87 (74%)	30 (26%)	0	2
35	58	117/119 (98%)	90 (77%)	27 (23%)	1	3
36	25	100/100 (100%)	82 (82%)	18 (18%)	1	9
36	68	100/100 (100%)	85 (85%)	15 (15%)	3	14
37	35	114/116 (98%)	78 (68%)	36 (32%)	0	0
37	78	114/116 (98%)	80 (70%)	34 (30%)	0	1
38	45	109/111 (98%)	89 (82%)	20 (18%)	1	8
38	88	109/111 (98%)	87 (80%)	22 (20%)	1	6
39	55	101/101 (100%)	83 (82%)	18 (18%)	2	9
39	98	101/101 (100%)	76 (75%)	25 (25%)	0	2
40	65	87/88 (99%)	64 (74%)	23 (26%)	0	2
40	A8	87/88 (99%)	67 (77%)	20 (23%)	1	3
41	75	117/127 (92%)	91 (78%)	26 (22%)	1	4
41	B8	117/127 (92%)	87 (74%)	30 (26%)	0	2
42	85	93/94 (99%)	83 (89%)	10 (11%)	6	27
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	95	82/82 (100%)	61 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	59 (72%)	23 (28%)	0	1
44	A5	92/92 (100%)	73 (79%)	19 (21%)	1	6
44	E8	91/92 (99%)	65 (71%)	26 (29%)	0	1
45	B5	74/78 (95%)	52 (70%)	22 (30%)	0	1
45	F8	75/78 (96%)	64 (85%)	11 (15%)	3	14
46	C5	85/91 (93%)	60 (71%)	25 (29%)	0	1
46	G8	85/91 (93%)	70 (82%)	15 (18%)	2	9
47	D5	118/179 (66%)	93 (79%)	25 (21%)	1	5
47	H8	152/179 (85%)	113 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	4	19
48	I8	61/67 (91%)	51 (84%)	10 (16%)	2	11
49	F5	79/83 (95%)	61 (77%)	18 (23%)	1	4
49	J8	79/83 (95%)	60 (76%)	19 (24%)	0	3
50	G5	62/67 (92%)	47 (76%)	15 (24%)	0	2
50	K8	62/67 (92%)	44 (71%)	18 (29%)	0	1
51	H5	50/52 (96%)	40 (80%)	10 (20%)	1	6
51	L8	50/52 (96%)	38 (76%)	12 (24%)	0	3
52	M8	42/63 (67%)	31 (74%)	11 (26%)	0	2
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	8
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	6
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4	19
54	P8	38/42 (90%)	34 (90%)	4 (10%)	7	28
55	M5	54/55 (98%)	44 (82%)	10 (18%)	1	8
55	Q8	54/55 (98%)	39 (72%)	15 (28%)	0	1
All	All	9277/10193 (91%)	7277 (78%)	2000 (22%)	1	5

5 of 2000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	2	GLU
40	65	89	ARG
4	32	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	65	4	LEU
46	C5	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
10	1A	84	GLN
18	9A	36	ASN
44	A5	60	ASN
14	5A	49	HIS
19	AA	57	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	361 (24%)	29 (1%)
1	1G	1506/1522 (98%)	367 (24%)	27 (1%)
22	1K	67/75 (89%)	27 (40%)	2 (2%)
23	2K	76/77 (98%)	22 (28%)	1 (1%)
23	2L	76/77 (98%)	14 (18%)	2 (2%)
24	3K	75/76 (98%)	42 (56%)	4 (5%)
25	4K	18/27 (66%)	12 (66%)	2 (11%)
25	4L	17/27 (62%)	9 (52%)	0
26	14	2853/2917 (97%)	731 (25%)	38 (1%)
26	1H	2829/2917 (96%)	722 (25%)	50 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	1 (0%)
56	1L	69/76 (90%)	27 (39%)	4 (5%)
57	3L	75/76 (98%)	35 (46%)	1 (1%)
All	All	9396/9633 (97%)	2428 (25%)	162 (1%)

5 of 2428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	9	G
1	13	15	G

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1533	C
26	14	1558	A
56	1L	69	A
26	14	528	A
26	14	2275	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PSU	3L	39	57	18,21,22	1.24	1 (5%)	22,30,33	1.46	4 (18%)
56	T6A	1L	37	56	27,34,35	2.48	6 (22%)	29,49,52	2.37	8 (27%)
57	5MU	3L	54	57	19,22,23	4.05	6 (31%)	28,32,35	2.95	10 (35%)
22	T6A	1K	37	22	27,34,35	2.37	7 (25%)	29,49,52	1.98	5 (17%)
56	U8U	1L	34	25,56	19,24,25	2.68	7 (36%)	23,34,37	0.94	1 (4%)
56	PSU	1L	55	56	18,21,22	1.09	1 (5%)	22,30,33	1.60	4 (18%)
22	PSU	1K	39	22	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
23	4SU	2K	8	23	18,21,22	1.82	4 (22%)	26,30,33	2.30	5 (19%)
23	5MU	2K	55	23	19,22,23	3.79	5 (26%)	28,32,35	3.53	9 (32%)
23	G7M	2L	47	23	20,26,27	4.82	5 (25%)	17,39,42	1.15	1 (5%)
56	PSU	1L	39	56	18,21,22	1.14	1 (5%)	22,30,33	1.57	3 (13%)
23	OMC	2L	33	23	19,22,23	1.71	3 (15%)	26,31,34	1.06	3 (11%)
57	PSU	3L	55	57	18,21,22	1.20	1 (5%)	22,30,33	1.73	5 (22%)
22	U8U	1K	34	22,25	19,24,25	2.42	6 (31%)	23,34,37	0.91	1 (4%)
23	PSU	2K	56	23	18,21,22	1.21	2 (11%)	22,30,33	1.91	3 (13%)
23	5MU	2L	55	23	19,22,23	3.80	5 (26%)	28,32,35	3.40	8 (28%)
22	5MU	1K	54	22	19,22,23	3.69	5 (26%)	28,32,35	3.13	6 (21%)
23	G7M	2K	47	23	20,26,27	4.75	6 (30%)	17,39,42	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	OMC	2K	33	23	19,22,23	1.72	4 (21%)	26,31,34	0.95	2 (7%)
56	5MU	1L	54	56	19,22,23	3.84	5 (26%)	28,32,35	3.25	8 (28%)
22	PSU	1K	55	22	18,21,22	1.08	1 (5%)	22,30,33	1.56	4 (18%)
23	PSU	2L	56	23	18,21,22	1.28	1 (5%)	22,30,33	1.73	4 (18%)
23	4SU	2L	8	23	18,21,22	1.76	3 (16%)	26,30,33	2.66	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	3L	39	57	-	2/7/25/26	0/2/2/2
56	T6A	1L	37	56	-	5/19/41/42	0/3/3/3
57	5MU	3L	54	57	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/19/41/42	0/3/3/3
56	U8U	1L	34	25,56	-	2/9/28/29	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
57	PSU	3L	55	57	-	4/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	2/9/28/29	0/2/2/2
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	3/3/25/26	0/3/3/3
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	17.70	1.65	1.33
23	2K	47	G7M	C8-N7	17.48	1.65	1.33
57	3L	54	5MU	C2-N1	12.59	1.58	1.38
56	1L	54	5MU	C2-N1	12.47	1.58	1.38
23	2L	55	5MU	C2-N1	12.19	1.58	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	11.30	124.95	115.31
22	1K	54	5MU	C5-C4-N3	10.92	124.63	115.31
23	2L	55	5MU	C5-C4-N3	10.89	124.61	115.31
56	1L	54	5MU	C5-C4-N3	10.30	124.10	115.31
57	3L	54	5MU	C5-C4-N3	8.97	122.97	115.31

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
56	1L	37	T6A	C13-C12-C14-C15
57	3L	55	PSU	C2'-C1'-C5-C4
56	1L	34	U8U	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	3L	39	PSU	1	0
56	1L	34	U8U	2	0
56	1L	55	PSU	1	0
23	2L	47	G7M	2	0
23	2L	33	OMC	1	0
57	3L	55	PSU	1	0
23	2K	56	PSU	1	0
23	2L	55	5MU	1	0
23	2K	47	G7M	1	0
23	2K	33	OMC	2	0
23	2L	56	PSU	1	0
23	2L	8	4SU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1144 ligands modelled in this entry, 1142 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	301	SF4	2	0
59	3E	301	SF4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13	1496/1522 (98%)	-0.66	1 (0%)	95	95	62, 109, 164, 193	0
1	1G	1507/1522 (99%)	-0.64	2 (0%)	95	95	80, 127, 170, 197	0
2	12	210/256 (82%)	0.46	23 (10%)	5	3	127, 152, 162, 177	0
2	1E	231/256 (90%)	0.62	29 (12%)	3	2	117, 141, 159, 166	0
3	22	196/239 (82%)	1.21	47 (23%)	0	0	129, 143, 156, 164	0
3	2E	205/239 (85%)	0.92	35 (17%)	1	1	94, 114, 136, 145	0
4	32	208/209 (99%)	1.20	45 (21%)	0	1	108, 128, 145, 152	0
4	3E	207/209 (99%)	0.82	27 (13%)	3	2	92, 114, 134, 139	0
5	42	148/162 (91%)	0.60	9 (6%)	21	12	114, 129, 143, 152	0
5	4E	149/162 (91%)	0.53	9 (6%)	21	12	89, 108, 124, 140	0
6	52	101/101 (100%)	1.28	21 (20%)	1	1	95, 111, 129, 137	0
6	5E	100/101 (99%)	0.77	11 (11%)	5	3	87, 107, 126, 136	0
7	62	138/156 (88%)	-0.42	0	100	100	121, 134, 144, 148	0
7	6E	154/156 (98%)	-0.23	2 (1%)	77	65	109, 125, 148, 166	0
8	72	137/138 (99%)	0.07	4 (2%)	51	36	111, 133, 142, 145	0
8	7E	138/138 (100%)	-0.05	1 (0%)	87	81	97, 117, 128, 138	0
9	82	121/128 (94%)	-0.34	2 (1%)	70	57	117, 149, 158, 163	0
9	8E	126/128 (98%)	-0.44	0	100	100	96, 135, 152, 157	0
10	1A	80/105 (76%)	0.04	2 (2%)	57	43	129, 146, 156, 161	0
10	1I	91/105 (86%)	0.47	7 (7%)	13	7	87, 128, 159, 165	0
11	2A	113/129 (87%)	0.76	13 (11%)	4	3	94, 117, 130, 138	0
11	2I	111/129 (86%)	0.35	5 (4%)	33	21	85, 113, 127, 142	0
12	3A	122/132 (92%)	1.10	28 (22%)	0	0	89, 107, 130, 146	0
12	3I	122/132 (92%)	1.08	16 (13%)	3	2	73, 82, 106, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	0.72	11 (9%) 7 4	125, 145, 156, 160	0
13	4I	119/126 (94%)	0.18	4 (3%) 45 29	93, 123, 136, 147	0
14	5A	59/61 (96%)	1.75	22 (37%) 0 0	134, 143, 153, 154	0
14	5I	60/61 (98%)	-0.16	0 100 100	92, 103, 118, 131	0
15	6A	88/89 (98%)	0.30	2 (2%) 60 47	96, 119, 135, 139	0
15	6I	87/89 (97%)	-0.07	0 100 100	88, 104, 122, 127	0
16	7A	84/88 (95%)	0.19	2 (2%) 59 44	102, 117, 135, 152	0
16	7I	83/88 (94%)	0.53	7 (8%) 11 6	110, 119, 143, 150	0
17	8A	99/105 (94%)	0.19	3 (3%) 50 34	105, 120, 132, 133	0
17	8I	100/105 (95%)	0.32	1 (1%) 82 72	98, 114, 124, 126	0
18	9A	67/88 (76%)	1.36	22 (32%) 0 0	106, 121, 135, 142	0
18	9I	68/88 (77%)	1.17	17 (25%) 0 0	94, 109, 133, 136	0
19	AA	62/93 (66%)	1.29	14 (22%) 0 0	134, 149, 156, 158	0
19	AI	81/93 (87%)	0.54	6 (7%) 14 8	102, 122, 138, 151	0
20	BA	99/106 (93%)	-0.19	1 (1%) 82 72	100, 118, 141, 152	0
20	BI	97/106 (91%)	-0.10	1 (1%) 82 72	112, 125, 148, 157	0
21	1B	22/27 (81%)	1.15	5 (22%) 0 0	129, 137, 145, 148	0
21	1F	23/27 (85%)	-0.33	0 100 100	94, 112, 118, 122	0
22	1K	66/75 (88%)	0.07	1 (1%) 73 61	85, 153, 177, 183	0
23	2K	72/77 (93%)	-0.44	0 100 100	77, 104, 132, 146	0
23	2L	72/77 (93%)	-0.30	0 100 100	85, 122, 151, 162	0
24	3K	76/76 (100%)	-0.28	1 (1%) 77 65	79, 178, 191, 196	0
25	4K	19/27 (70%)	-0.20	1 (5%) 26 14	79, 152, 184, 184	0
25	4L	18/27 (66%)	0.10	0 100 100	101, 161, 187, 187	0
26	14	2861/2917 (98%)	-0.36	35 (1%) 79 67	55, 92, 180, 204	0
26	1H	2833/2917 (97%)	-0.42	13 (0%) 91 86	49, 79, 168, 203	0
27	16	122/122 (100%)	-0.12	1 (0%) 86 78	74, 98, 119, 179	0
27	1J	122/122 (100%)	-0.73	0 100 100	93, 125, 145, 177	0
28	71	133/229 (58%)	1.28	35 (26%) 0 0	143, 174, 185, 189	0
28	79	57/229 (24%)	-0.24	1 (1%) 68 55	140, 165, 176, 179	0
29	11	273/276 (98%)	-0.20	0 100 100	48, 71, 89, 113	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
29	19	274/276 (99%)	0.53	12 (4%)	34	21	58, 82, 101, 117	0
30	21	203/206 (98%)	0.81	35 (17%)	1	1	55, 93, 139, 153	0
30	29	204/206 (99%)	0.63	38 (18%)	1	1	60, 99, 134, 144	0
31	31	202/210 (96%)	0.39	21 (10%)	6	4	54, 84, 118, 142	0
31	39	204/210 (97%)	0.79	33 (16%)	1	1	62, 111, 151, 168	0
32	41	179/182 (98%)	1.18	39 (21%)	0	0	85, 107, 140, 156	0
32	49	179/182 (98%)	0.97	41 (22%)	0	0	122, 139, 155, 171	0
33	51	171/180 (95%)	0.46	9 (5%)	26	14	89, 110, 127, 139	0
33	59	73/180 (40%)	0.25	8 (10%)	5	3	136, 154, 165, 177	0
34	61	146/148 (98%)	1.08	35 (23%)	0	0	83, 130, 143, 150	0
34	69	145/148 (97%)	1.35	43 (29%)	0	0	93, 129, 147, 152	0
35	15	138/140 (98%)	1.92	56 (40%)	0	0	86, 114, 139, 155	0
35	58	138/140 (98%)	0.27	6 (4%)	35	22	68, 97, 130, 145	0
36	25	122/122 (100%)	0.04	0	100	100	77, 94, 114, 120	0
36	68	122/122 (100%)	0.03	2 (1%)	72	59	64, 81, 99, 104	0
37	35	147/150 (98%)	0.31	8 (5%)	25	14	65, 111, 138, 144	0
37	78	147/150 (98%)	0.05	3 (2%)	65	51	53, 88, 113, 120	0
38	45	138/141 (97%)	2.27	69 (50%)	0	0	78, 108, 128, 142	0
38	88	141/141 (100%)	1.23	31 (21%)	0	0	63, 83, 108, 129	0
39	55	118/118 (100%)	-0.03	1 (0%)	86	78	69, 86, 108, 127	0
39	98	118/118 (100%)	0.49	10 (8%)	10	6	67, 90, 109, 122	0
40	65	110/112 (98%)	0.34	5 (4%)	33	21	92, 117, 135, 142	0
40	A8	111/112 (99%)	2.42	65 (58%)	0	0	71, 93, 115, 123	0
41	75	133/146 (91%)	-0.35	3 (2%)	60	47	87, 101, 129, 141	0
41	B8	133/146 (91%)	-0.43	2 (1%)	73	61	78, 98, 133, 149	0
42	85	116/118 (98%)	1.37	33 (28%)	0	0	73, 100, 132, 138	0
42	C8	115/118 (97%)	-0.16	3 (2%)	56	40	59, 86, 114, 118	0
43	95	100/101 (99%)	2.98	69 (69%)	0	0	69, 121, 139, 153	0
43	D8	100/101 (99%)	0.14	6 (6%)	21	12	62, 106, 126, 144	0
44	A5	113/113 (100%)	0.01	2 (1%)	68	55	68, 82, 112, 158	0
44	E8	112/113 (99%)	0.36	5 (4%)	33	21	63, 79, 106, 147	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
45	B5	94/96 (97%)	0.94	13 (13%)	2	2	77, 91, 118, 128	0
45	F8	95/96 (98%)	0.67	10 (10%)	6	3	60, 76, 104, 118	0
46	C5	104/110 (94%)	0.44	9 (8%)	10	5	91, 122, 149, 154	0
46	G8	105/110 (95%)	-0.23	0	100	100	75, 101, 131, 139	0
47	D5	132/206 (64%)	1.81	58 (43%)	0	0	115, 135, 150, 158	0
47	H8	171/206 (83%)	1.74	66 (38%)	0	0	90, 122, 167, 172	0
48	E5	77/85 (90%)	0.12	4 (5%)	27	15	72, 94, 111, 131	0
48	I8	76/85 (89%)	0.49	3 (3%)	39	25	61, 75, 90, 102	0
49	F5	94/98 (95%)	0.15	2 (2%)	63	49	67, 88, 121, 136	0
49	J8	94/98 (95%)	0.10	2 (2%)	63	49	62, 77, 120, 122	0
50	G5	66/72 (91%)	0.52	4 (6%)	21	12	87, 108, 126, 145	0
50	K8	68/72 (94%)	0.15	2 (2%)	51	36	68, 84, 102, 124	0
51	H5	58/60 (96%)	1.89	26 (44%)	0	0	81, 106, 128, 135	0
51	L8	58/60 (96%)	0.37	3 (5%)	27	15	63, 85, 115, 127	0
52	M8	47/71 (66%)	2.74	31 (65%)	0	0	109, 143, 158, 163	0
53	J5	56/60 (93%)	-0.11	0	100	100	66, 86, 141, 148	0
53	N8	48/60 (80%)	0.41	7 (14%)	2	1	56, 84, 140, 142	0
54	L5	47/49 (95%)	0.14	2 (4%)	35	22	58, 66, 85, 91	0
54	P8	47/49 (95%)	-0.44	0	100	100	52, 57, 77, 88	0
55	M5	64/65 (98%)	0.14	0	100	100	76, 85, 101, 117	0
55	Q8	64/65 (98%)	0.15	0	100	100	61, 71, 88, 99	0
56	1L	68/76 (89%)	1.09	15 (22%)	0	0	118, 173, 181, 188	0
57	3L	73/76 (96%)	-0.60	0	100	100	87, 172, 185, 190	0
All	All	20602/21966 (93%)	0.11	1495 (7%)	15	9	48, 107, 162, 204	0

The worst 5 of 1495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2899	G	12.6
26	14	2901	C	10.8
26	14	2799	A	10.4
26	14	2902	C	9.9
43	95	45	THR	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	PSU	3L	55	20/21	0.83	0.08	166,169,175,175	0
57	5MU	3L	54	21/22	0.87	0.09	162,169,172,173	0
56	PSU	1L	55	20/21	0.87	0.30	134,150,156,159	0
56	PSU	1L	39	20/21	0.88	0.18	105,127,133,134	0
23	PSU	2L	56	20/21	0.88	0.12	116,129,133,137	0
22	PSU	1K	55	20/21	0.90	0.17	109,120,133,134	0
57	PSU	3L	39	20/21	0.91	0.13	153,162,166,168	0
23	4SU	2L	8	20/21	0.91	0.17	112,125,130,135	0
56	U8U	1L	34	23/24	0.91	0.18	110,126,134,138	0
23	4SU	2K	8	20/21	0.92	0.17	93,98,102,106	0
56	T6A	1L	37	32/33	0.93	0.18	102,120,127,130	0
23	G7M	2L	47	24/25	0.93	0.12	129,137,150,151	0
22	5MU	1K	54	21/22	0.94	0.22	114,122,134,142	0
23	G7M	2K	47	24/25	0.94	0.12	104,115,129,135	0
23	PSU	2K	56	20/21	0.94	0.14	104,113,121,127	0
23	5MU	2L	55	21/22	0.94	0.13	128,133,141,143	0
22	PSU	1K	39	20/21	0.95	0.15	79,98,105,108	0
56	5MU	1L	54	21/22	0.95	0.25	138,147,154,155	0
22	T6A	1K	37	32/33	0.96	0.16	76,86,103,106	0
23	OMC	2L	33	21/22	0.96	0.15	109,114,117,125	0
22	U8U	1K	34	23/24	0.96	0.15	78,88,93,105	0
23	5MU	2K	55	21/22	0.96	0.12	112,118,125,127	0
23	OMC	2K	33	21/22	0.97	0.14	82,87,92,96	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1698	1/1	0.08	0.21	138,138,138,138	0
58	MG	13	1699	1/1	0.28	0.31	94,94,94,94	0
58	MG	14	3282	1/1	0.32	0.42	109,109,109,109	0
58	MG	14	3303	1/1	0.32	0.18	106,106,106,106	0
58	MG	13	1603	1/1	0.33	0.47	92,92,92,92	0
58	MG	1H	3016	1/1	0.34	0.56	75,75,75,75	0
58	MG	1H	3297	1/1	0.39	0.24	99,99,99,99	0
58	MG	14	3258	1/1	0.41	0.38	92,92,92,92	0
58	MG	14	3311	1/1	0.42	0.36	100,100,100,100	0
58	MG	1H	3219	1/1	0.43	0.37	103,103,103,103	0
58	MG	1G	1638	1/1	0.44	0.30	93,93,93,93	0
58	MG	14	3108	1/1	0.46	0.73	92,92,92,92	0
58	MG	1H	3283	1/1	0.48	0.24	92,92,92,92	0
58	MG	13	1697	1/1	0.49	0.22	92,92,92,92	0
58	MG	1H	3152	1/1	0.51	0.34	100,100,100,100	0
58	MG	14	3224	1/1	0.51	0.38	90,90,90,90	0
58	MG	1G	1664	1/1	0.51	0.30	100,100,100,100	0
58	MG	2K	102	1/1	0.52	0.69	94,94,94,94	0
58	MG	13	1700	1/1	0.52	0.33	94,94,94,94	0
58	MG	14	3034	1/1	0.52	0.97	88,88,88,88	0
58	MG	39	301	1/1	0.52	0.21	96,96,96,96	0
58	MG	14	3399	1/1	0.53	0.28	107,107,107,107	0
58	MG	13	1672	1/1	0.54	0.45	109,109,109,109	0
58	MG	1H	3249	1/1	0.54	0.37	80,80,80,80	0
58	MG	13	1653	1/1	0.54	0.41	72,72,72,72	0
58	MG	13	1696	1/1	0.55	0.32	92,92,92,92	0
58	MG	1H	3171	1/1	0.56	0.43	83,83,83,83	0
58	MG	14	3037	1/1	0.56	0.46	106,106,106,106	0
58	MG	1H	3309	1/1	0.56	0.51	90,90,90,90	0
58	MG	1H	3036	1/1	0.56	0.74	100,100,100,100	0
58	MG	1H	3284	1/1	0.56	0.48	81,81,81,81	0
58	MG	14	3294	1/1	0.57	0.26	87,87,87,87	0
58	MG	14	3304	1/1	0.58	0.71	92,92,92,92	0
58	MG	13	1688	1/1	0.58	0.34	101,101,101,101	0
58	MG	1H	3035	1/1	0.59	0.45	83,83,83,83	0
58	MG	1H	3279	1/1	0.59	0.49	67,67,67,67	0
58	MG	25	201	1/1	0.59	0.34	102,102,102,102	0
58	MG	14	3316	1/1	0.60	0.35	122,122,122,122	0
58	MG	1H	3336	1/1	0.60	0.24	104,104,104,104	0
58	MG	14	3283	1/1	0.60	0.32	69,69,69,69	0
58	MG	14	3184	1/1	0.60	0.24	98,98,98,98	0
58	MG	14	3197	1/1	0.61	0.34	116,116,116,116	0
58	MG	14	3180	1/1	0.61	0.30	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3229	1/1	0.61	0.76	88,88,88,88	0
58	MG	1H	3164	1/1	0.61	0.21	64,64,64,64	0
58	MG	14	3185	1/1	0.61	0.51	82,82,82,82	0
58	MG	14	3190	1/1	0.61	0.58	86,86,86,86	0
58	MG	14	3191	1/1	0.61	0.58	96,96,96,96	0
58	MG	1H	3264	1/1	0.62	0.18	76,76,76,76	0
58	MG	1H	3278	1/1	0.62	0.48	95,95,95,95	0
58	MG	14	3017	1/1	0.62	0.51	90,90,90,90	0
58	MG	1H	3024	1/1	0.62	0.69	82,82,82,82	0
58	MG	1H	3331	1/1	0.62	0.62	73,73,73,73	0
58	MG	13	1605	1/1	0.62	0.24	76,76,76,76	0
58	MG	14	3129	1/1	0.62	0.69	73,73,73,73	0
58	MG	14	3140	1/1	0.62	0.33	82,82,82,82	0
58	MG	1G	1603	1/1	0.62	0.59	102,102,102,102	0
58	MG	1G	1635	1/1	0.63	0.28	107,107,107,107	0
58	MG	14	3269	1/1	0.63	0.50	88,88,88,88	0
58	MG	1H	3160	1/1	0.63	0.28	72,72,72,72	0
58	MG	1G	1646	1/1	0.63	0.24	100,100,100,100	0
58	MG	14	3068	1/1	0.63	0.65	100,100,100,100	0
58	MG	1G	1616	1/1	0.63	0.31	87,87,87,87	0
58	MG	14	3302	1/1	0.64	0.46	66,66,66,66	0
58	MG	14	3085	1/1	0.64	0.47	67,67,67,67	0
58	MG	14	3089	1/1	0.64	0.88	79,79,79,79	0
58	MG	13	1630	1/1	0.64	0.48	80,80,80,80	0
58	MG	1H	3285	1/1	0.65	0.47	68,68,68,68	0
58	MG	14	3261	1/1	0.65	0.49	77,77,77,77	0
58	MG	14	3026	1/1	0.66	0.34	89,89,89,89	0
58	MG	1J	203	1/1	0.66	0.23	103,103,103,103	0
58	MG	14	3153	1/1	0.66	0.44	89,89,89,89	0
58	MG	1E	301	1/1	0.66	0.20	106,106,106,106	0
58	MG	1H	3194	1/1	0.67	0.40	84,84,84,84	0
58	MG	1H	3207	1/1	0.67	0.48	84,84,84,84	0
58	MG	14	3264	1/1	0.67	0.57	85,85,85,85	0
58	MG	1H	3167	1/1	0.67	0.54	93,93,93,93	0
58	MG	14	3275	1/1	0.67	0.37	91,91,91,91	0
58	MG	14	3277	1/1	0.67	0.34	85,85,85,85	0
58	MG	35	202	1/1	0.67	0.24	87,87,87,87	0
58	MG	14	3262	1/1	0.68	0.34	96,96,96,96	0
58	MG	1H	3122	1/1	0.68	0.63	79,79,79,79	0
58	MG	14	3135	1/1	0.68	0.24	95,95,95,95	0
58	MG	13	1695	1/1	0.68	0.43	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3392	1/1	0.68	0.06	128,128,128,128	0
58	MG	1H	3292	1/1	0.68	0.30	77,77,77,77	0
58	MG	14	3227	1/1	0.68	0.44	76,76,76,76	0
58	MG	2L	102	1/1	0.68	0.64	83,83,83,83	0
58	MG	1H	3253	1/1	0.68	0.37	66,66,66,66	0
58	MG	1H	3254	1/1	0.68	0.57	99,99,99,99	0
58	MG	1H	3459	1/1	0.69	0.06	106,106,106,106	0
58	MG	13	1632	1/1	0.69	0.40	107,107,107,107	0
58	MG	1H	3293	1/1	0.69	0.35	84,84,84,84	0
58	MG	14	3308	1/1	0.69	0.70	106,106,106,106	0
58	MG	14	3186	1/1	0.69	0.45	82,82,82,82	0
58	MG	1H	3079	1/1	0.69	0.38	79,79,79,79	0
58	MG	1H	3277	1/1	0.70	0.32	68,68,68,68	0
58	MG	1H	3314	1/1	0.70	0.30	85,85,85,85	0
58	MG	1H	3178	1/1	0.70	0.38	71,71,71,71	0
58	MG	1G	1648	1/1	0.70	0.32	117,117,117,117	0
58	MG	1G	1649	1/1	0.70	0.41	83,83,83,83	0
58	MG	13	1646	1/1	0.70	0.29	75,75,75,75	0
58	MG	1H	3301	1/1	0.70	0.44	84,84,84,84	0
58	MG	1H	3305	1/1	0.70	0.39	67,67,67,67	0
58	MG	1H	3306	1/1	0.70	0.31	91,91,91,91	0
58	MG	14	3030	1/1	0.70	0.39	86,86,86,86	0
58	MG	14	3257	1/1	0.70	1.14	86,86,86,86	0
58	MG	1H	3315	1/1	0.71	0.53	76,76,76,76	0
58	MG	1H	3328	1/1	0.71	0.58	80,80,80,80	0
58	MG	1H	3302	1/1	0.71	0.22	92,92,92,92	0
58	MG	13	1705	1/1	0.71	0.35	90,90,90,90	0
58	MG	14	3313	1/1	0.71	0.49	92,92,92,92	0
58	MG	13	1728	1/1	0.71	0.11	118,118,118,118	0
58	MG	16	204	1/1	0.71	0.32	73,73,73,73	0
58	MG	14	3255	1/1	0.71	0.25	78,78,78,78	0
58	MG	1H	3251	1/1	0.71	0.39	71,71,71,71	0
58	MG	1H	3217	1/1	0.71	0.34	71,71,71,71	0
58	MG	14	3295	1/1	0.71	0.20	85,85,85,85	0
58	MG	14	3259	1/1	0.71	0.75	98,98,98,98	0
58	MG	14	3231	1/1	0.72	0.34	86,86,86,86	0
58	MG	13	1656	1/1	0.72	0.15	103,103,103,103	0
58	MG	13	1659	1/1	0.72	0.62	97,97,97,97	0
58	MG	1J	201	1/1	0.72	0.30	94,94,94,94	0
58	MG	1H	3224	1/1	0.72	0.58	73,73,73,73	0
58	MG	1H	3368	1/1	0.72	0.24	74,74,74,74	0
58	MG	1H	3324	1/1	0.72	0.57	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3058	1/1	0.72	0.18	84,84,84,84	0
58	MG	E5	101	1/1	0.72	0.47	89,89,89,89	0
58	MG	1H	3139	1/1	0.73	0.36	71,71,71,71	0
58	MG	13	1641	1/1	0.73	0.44	93,93,93,93	0
58	MG	1H	3101	1/1	0.73	0.26	59,59,59,59	0
58	MG	1H	3180	1/1	0.73	0.43	75,75,75,75	0
58	MG	1H	3032	1/1	0.73	0.49	79,79,79,79	0
58	MG	14	3234	1/1	0.73	0.89	70,70,70,70	0
58	MG	14	3155	1/1	0.73	0.71	64,64,64,64	0
58	MG	14	3251	1/1	0.74	0.50	69,69,69,69	0
58	MG	1H	3288	1/1	0.74	0.87	93,93,93,93	0
58	MG	14	3194	1/1	0.74	0.34	81,81,81,81	0
58	MG	14	3019	1/1	0.74	0.67	90,90,90,90	0
58	MG	14	3181	1/1	0.74	0.41	89,89,89,89	0
58	MG	14	3260	1/1	0.74	0.78	72,72,72,72	0
58	MG	14	3300	1/1	0.74	0.24	117,117,117,117	0
58	MG	29	301	1/1	0.74	0.34	77,77,77,77	0
58	MG	13	1689	1/1	0.74	0.52	107,107,107,107	0
58	MG	1H	3222	1/1	0.74	0.33	98,98,98,98	0
58	MG	14	3143	1/1	0.74	0.30	102,102,102,102	0
58	MG	1H	3342	1/1	0.74	0.63	92,92,92,92	0
58	MG	1H	3031	1/1	0.75	0.53	76,76,76,76	0
58	MG	1H	3080	1/1	0.75	0.21	65,65,65,65	0
58	MG	I8	101	1/1	0.75	0.32	73,73,73,73	0
58	MG	14	3144	1/1	0.75	0.41	71,71,71,71	0
58	MG	2K	103	1/1	0.75	0.42	114,114,114,114	0
58	MG	1H	3228	1/1	0.75	0.45	83,83,83,83	0
58	MG	14	3250	1/1	0.75	0.41	78,78,78,78	0
58	MG	1H	3457	1/1	0.75	0.06	141,141,141,141	0
58	MG	1H	3313	1/1	0.76	0.26	98,98,98,98	0
58	MG	14	3147	1/1	0.76	0.23	95,95,95,95	0
58	MG	14	3310	1/1	0.76	0.23	114,114,114,114	0
58	MG	14	3052	1/1	0.76	0.50	113,113,113,113	0
58	MG	1H	3199	1/1	0.76	0.25	69,69,69,69	0
58	MG	1H	3247	1/1	0.76	0.21	81,81,81,81	0
58	MG	1G	1666	1/1	0.76	0.50	84,84,84,84	0
58	MG	1H	3154	1/1	0.76	0.54	84,84,84,84	0
58	MG	13	1681	1/1	0.76	0.19	116,116,116,116	0
58	MG	14	3288	1/1	0.76	0.74	86,86,86,86	0
58	MG	13	1662	1/1	0.76	0.36	118,118,118,118	0
58	MG	14	3188	1/1	0.76	0.56	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3043	1/1	0.76	0.76	81,81,81,81	0
58	MG	1H	3197	1/1	0.76	0.63	80,80,80,80	0
58	MG	35	203	1/1	0.76	0.24	75,75,75,75	0
58	MG	1H	3291	1/1	0.76	0.31	73,73,73,73	0
58	MG	14	3291	1/1	0.77	0.35	87,87,87,87	0
58	MG	14	3293	1/1	0.77	0.51	91,91,91,91	0
58	MG	14	3345	1/1	0.77	0.10	90,90,90,90	0
58	MG	1G	1672	1/1	0.77	0.43	99,99,99,99	0
58	MG	14	3268	1/1	0.77	0.41	94,94,94,94	0
58	MG	1H	3087	1/1	0.77	0.57	70,70,70,70	0
58	MG	14	3301	1/1	0.77	0.21	109,109,109,109	0
58	MG	14	3117	1/1	0.77	0.44	81,81,81,81	0
58	MG	29	302	1/1	0.77	0.45	65,65,65,65	0
58	MG	1H	3296	1/1	0.77	0.22	57,57,57,57	0
58	MG	1H	3136	1/1	0.77	0.34	49,49,49,49	0
58	MG	13	1621	1/1	0.77	0.21	90,90,90,90	0
58	MG	1H	3142	1/1	0.77	0.45	68,68,68,68	0
58	MG	14	3290	1/1	0.77	0.22	92,92,92,92	0
58	MG	14	3306	1/1	0.78	0.29	88,88,88,88	0
58	MG	1G	1643	1/1	0.78	0.24	132,132,132,132	0
58	MG	1H	3263	1/1	0.78	0.25	76,76,76,76	0
58	MG	1H	3439	1/1	0.78	0.07	99,99,99,99	0
58	MG	13	1644	1/1	0.78	0.43	96,96,96,96	0
58	MG	1H	3271	1/1	0.78	0.39	76,76,76,76	0
58	MG	14	3247	1/1	0.78	0.28	67,67,67,67	0
58	MG	14	3073	1/1	0.78	1.32	83,83,83,83	0
58	MG	14	3183	1/1	0.78	0.77	79,79,79,79	0
58	MG	1H	3327	1/1	0.78	0.79	82,82,82,82	0
58	MG	1H	3175	1/1	0.78	0.53	65,65,65,65	0
58	MG	1H	3022	1/1	0.78	0.39	62,62,62,62	0
58	MG	1G	1604	1/1	0.78	0.44	87,87,87,87	0
58	MG	1H	3201	1/1	0.78	0.69	92,92,92,92	0
58	MG	13	1706	1/1	0.78	0.39	109,109,109,109	0
58	MG	35	201	1/1	0.78	0.26	74,74,74,74	0
58	MG	14	3029	1/1	0.78	0.72	78,78,78,78	0
58	MG	1H	3364	1/1	0.78	0.10	98,98,98,98	0
58	MG	14	3265	1/1	0.78	0.52	98,98,98,98	0
58	MG	13	1694	1/1	0.79	0.55	64,64,64,64	0
58	MG	14	3018	1/1	0.79	0.61	72,72,72,72	0
58	MG	14	3353	1/1	0.79	0.09	118,118,118,118	0
58	MG	1G	1606	1/1	0.79	0.22	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3243	1/1	0.79	0.47	81,81,81,81	0
58	MG	1H	3414	1/1	0.79	0.19	80,80,80,80	0
58	MG	1G	1618	1/1	0.79	0.33	109,109,109,109	0
58	MG	16	209	1/1	0.79	0.10	100,100,100,100	0
58	MG	14	3252	1/1	0.79	0.39	84,84,84,84	0
58	MG	14	3253	1/1	0.79	0.26	94,94,94,94	0
58	MG	14	3280	1/1	0.79	0.91	86,86,86,86	0
58	MG	1H	3045	1/1	0.79	0.33	82,82,82,82	0
58	MG	1G	1680	1/1	0.79	0.06	140,140,140,140	0
58	MG	14	3182	1/1	0.79	0.74	75,75,75,75	0
58	MG	1H	3083	1/1	0.79	0.33	67,67,67,67	0
58	MG	14	3023	1/1	0.80	0.29	83,83,83,83	0
58	MG	13	1675	1/1	0.80	0.30	73,73,73,73	0
58	MG	1H	3268	1/1	0.80	0.42	85,85,85,85	0
58	MG	14	3221	1/1	0.80	0.20	69,69,69,69	0
58	MG	1H	3196	1/1	0.80	0.44	83,83,83,83	0
58	MG	1H	3033	1/1	0.80	0.58	88,88,88,88	0
58	MG	14	3150	1/1	0.80	0.40	87,87,87,87	0
58	MG	1H	3021	1/1	0.80	0.30	83,83,83,83	0
58	MG	1H	3298	1/1	0.80	0.35	74,74,74,74	0
58	MG	14	3179	1/1	0.80	0.24	60,60,60,60	0
58	MG	14	3391	1/1	0.80	0.13	104,104,104,104	0
58	MG	1G	1667	1/1	0.80	0.28	109,109,109,109	0
58	MG	1H	3173	1/1	0.80	0.47	84,84,84,84	0
58	MG	1G	1678	1/1	0.80	0.06	128,128,128,128	0
58	MG	14	3080	1/1	0.80	0.46	82,82,82,82	0
58	MG	1J	204	1/1	0.80	0.27	101,101,101,101	0
58	MG	14	3292	1/1	0.80	0.14	113,113,113,113	0
58	MG	1H	3282	1/1	0.80	0.60	88,88,88,88	0
58	MG	1H	3205	1/1	0.80	0.19	81,81,81,81	0
58	MG	13	1704	1/1	0.80	0.41	82,82,82,82	0
58	MG	14	3297	1/1	0.80	0.69	70,70,70,70	0
58	MG	14	3187	1/1	0.80	0.45	80,80,80,80	0
58	MG	13	1678	1/1	0.80	0.27	93,93,93,93	0
58	MG	13	1679	1/1	0.80	0.28	100,100,100,100	0
58	MG	1G	1663	1/1	0.81	0.10	94,94,94,94	0
58	MG	1H	3307	1/1	0.81	0.52	94,94,94,94	0
58	MG	98	201	1/1	0.81	0.41	72,72,72,72	0
58	MG	1H	3337	1/1	0.81	0.22	89,89,89,89	0
58	MG	P8	101	1/1	0.81	0.58	77,77,77,77	0
58	MG	13	1637	1/1	0.81	0.38	56,56,56,56	0
58	MG	1G	1679	1/1	0.81	0.11	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1670	1/1	0.81	0.19	97,97,97,97	0
58	MG	1G	1686	1/1	0.81	0.08	125,125,125,125	0
58	MG	1H	3179	1/1	0.81	0.35	83,83,83,83	0
58	MG	1H	3097	1/1	0.81	0.44	71,71,71,71	0
58	MG	14	3271	1/1	0.81	0.21	81,81,81,81	0
58	MG	1H	3246	1/1	0.81	0.23	54,54,54,54	0
58	MG	1H	3441	1/1	0.81	0.13	89,89,89,89	0
58	MG	14	3395	1/1	0.81	0.10	103,103,103,103	0
58	MG	14	3146	1/1	0.81	0.43	57,57,57,57	0
58	MG	14	3228	1/1	0.81	0.17	101,101,101,101	0
58	MG	13	1661	1/1	0.81	0.48	103,103,103,103	0
58	MG	1H	3209	1/1	0.81	0.42	90,90,90,90	0
58	MG	16	203	1/1	0.81	0.14	90,90,90,90	0
58	MG	1H	3019	1/1	0.81	0.49	92,92,92,92	0
58	MG	14	3245	1/1	0.81	0.47	77,77,77,77	0
58	MG	14	3170	1/1	0.81	0.37	83,83,83,83	0
58	MG	14	3177	1/1	0.81	0.46	72,72,72,72	0
58	MG	16	205	1/1	0.81	0.11	81,81,81,81	0
58	MG	1G	1657	1/1	0.81	0.36	92,92,92,92	0
58	MG	1G	1659	1/1	0.81	0.18	142,142,142,142	0
58	MG	14	3109	1/1	0.82	0.38	73,73,73,73	0
58	MG	1G	1636	1/1	0.82	0.32	101,101,101,101	0
58	MG	14	3125	1/1	0.82	0.75	72,72,72,72	0
58	MG	1G	1668	1/1	0.82	0.36	116,116,116,116	0
58	MG	3K	101	1/1	0.82	0.34	162,162,162,162	0
58	MG	13	1682	1/1	0.82	0.45	88,88,88,88	0
58	MG	1H	3151	1/1	0.82	0.20	55,55,55,55	0
58	MG	14	3393	1/1	0.82	0.06	127,127,127,127	0
58	MG	1H	3128	1/1	0.82	0.22	62,62,62,62	0
58	MG	1G	1684	1/1	0.82	0.11	109,109,109,109	0
58	MG	14	3193	1/1	0.82	0.40	77,77,77,77	0
58	MG	1J	202	1/1	0.82	0.27	95,95,95,95	0
58	MG	14	3059	1/1	0.82	0.32	86,86,86,86	0
58	MG	14	3060	1/1	0.82	0.23	73,73,73,73	0
58	MG	13	1685	1/1	0.82	0.24	121,121,121,121	0
58	MG	14	3222	1/1	0.82	0.23	97,97,97,97	0
58	MG	1H	3413	1/1	0.82	0.08	102,102,102,102	0
58	MG	14	3074	1/1	0.82	0.81	79,79,79,79	0
58	MG	1G	1615	1/1	0.82	0.23	125,125,125,125	0
58	MG	1H	3280	1/1	0.82	0.33	77,77,77,77	0
58	MG	1H	3438	1/1	0.82	0.11	83,83,83,83	0
58	MG	78	201	1/1	0.82	0.36	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3287	1/1	0.83	0.29	104,104,104,104	0
58	MG	1H	3018	1/1	0.83	0.55	71,71,71,71	0
58	MG	1G	1609	1/1	0.83	0.18	94,94,94,94	0
58	MG	13	1715	1/1	0.83	0.10	109,109,109,109	0
58	MG	1H	3190	1/1	0.83	0.32	73,73,73,73	0
58	MG	1H	3159	1/1	0.83	0.42	67,67,67,67	0
58	MG	1G	1620	1/1	0.83	0.31	82,82,82,82	0
58	MG	14	3107	1/1	0.83	0.51	77,77,77,77	0
58	MG	1G	1630	1/1	0.83	0.41	103,103,103,103	0
58	MG	6A	101	1/1	0.83	0.26	93,93,93,93	0
58	MG	13	1650	1/1	0.83	0.30	94,94,94,94	0
58	MG	14	3012	1/1	0.83	0.81	80,80,80,80	0
58	MG	13	1604	1/1	0.83	0.27	87,87,87,87	0
58	MG	13	1634	1/1	0.83	1.02	93,93,93,93	0
58	MG	14	3201	1/1	0.83	0.27	59,59,59,59	0
58	MG	1H	3335	1/1	0.83	0.68	74,74,74,74	0
58	MG	14	3273	1/1	0.83	0.46	101,101,101,101	0
58	MG	14	3022	1/1	0.83	0.38	64,64,64,64	0
58	MG	1H	3137	1/1	0.83	0.61	88,88,88,88	0
58	MG	13	1668	1/1	0.83	0.09	90,90,90,90	0
58	MG	21	302	1/1	0.83	0.33	77,77,77,77	0
58	MG	1G	1650	1/1	0.83	0.30	114,114,114,114	0
58	MG	14	3230	1/1	0.83	0.41	64,64,64,64	0
58	MG	1H	3338	1/1	0.83	0.37	65,65,65,65	0
58	MG	1H	3341	1/1	0.83	0.21	79,79,79,79	0
58	MG	14	3236	1/1	0.83	0.51	89,89,89,89	0
58	MG	14	3238	1/1	0.83	0.33	99,99,99,99	0
58	MG	13	1669	1/1	0.83	0.30	68,68,68,68	0
58	MG	13	1708	1/1	0.83	0.13	89,89,89,89	0
58	MG	1H	3262	1/1	0.83	0.37	94,94,94,94	0
58	MG	1H	3184	1/1	0.84	0.26	82,82,82,82	0
58	MG	14	3248	1/1	0.84	0.21	79,79,79,79	0
58	MG	1H	3233	1/1	0.84	0.59	62,62,62,62	0
58	MG	1H	3187	1/1	0.84	0.25	69,69,69,69	0
58	MG	1H	3316	1/1	0.84	0.88	92,92,92,92	0
58	MG	1H	3089	1/1	0.84	0.44	59,59,59,59	0
58	MG	14	3021	1/1	0.84	0.45	52,52,52,52	0
58	MG	14	3278	1/1	0.84	0.34	75,75,75,75	0
58	MG	14	3256	1/1	0.84	0.54	83,83,83,83	0
58	MG	5E	201	1/1	0.84	0.26	89,89,89,89	0
58	MG	14	3067	1/1	0.84	0.31	87,87,87,87	0
58	MG	29	304	1/1	0.84	0.22	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3125	1/1	0.84	0.50	69,69,69,69	0
58	MG	14	3237	1/1	0.84	0.37	83,83,83,83	0
58	MG	1H	3308	1/1	0.84	0.51	90,90,90,90	0
58	MG	14	3027	1/1	0.84	0.39	96,96,96,96	0
58	MG	1H	3226	1/1	0.84	0.38	85,85,85,85	0
58	MG	14	3363	1/1	0.84	0.19	72,72,72,72	0
58	MG	1G	1633	1/1	0.85	0.31	98,98,98,98	0
58	MG	1H	3252	1/1	0.85	0.50	66,66,66,66	0
58	MG	1H	3071	1/1	0.85	0.38	61,61,61,61	0
58	MG	1G	1637	1/1	0.85	0.55	87,87,87,87	0
58	MG	41	201	1/1	0.85	0.07	78,78,78,78	0
58	MG	14	3061	1/1	0.85	0.12	81,81,81,81	0
58	MG	14	3205	1/1	0.85	0.34	96,96,96,96	0
58	MG	1H	3322	1/1	0.85	0.65	81,81,81,81	0
58	MG	1H	3108	1/1	0.85	0.33	74,74,74,74	0
58	MG	1H	3072	1/1	0.85	0.30	77,77,77,77	0
58	MG	1H	3422	1/1	0.85	0.16	112,112,112,112	0
58	MG	1H	3227	1/1	0.85	0.68	85,85,85,85	0
58	MG	13	1703	1/1	0.85	0.78	77,77,77,77	0
58	MG	1H	3332	1/1	0.85	0.32	74,74,74,74	0
58	MG	1H	3096	1/1	0.85	0.33	60,60,60,60	0
58	MG	1H	3193	1/1	0.85	0.50	73,73,73,73	0
58	MG	14	3266	1/1	0.85	0.53	85,85,85,85	0
58	MG	1G	1665	1/1	0.85	0.26	113,113,113,113	0
58	MG	1H	3463	1/1	0.85	0.08	112,112,112,112	0
58	MG	1H	3213	1/1	0.85	0.38	74,74,74,74	0
58	MG	14	3309	1/1	0.85	0.44	110,110,110,110	0
58	MG	1H	3130	1/1	0.85	0.32	74,74,74,74	0
58	MG	1H	3020	1/1	0.85	0.32	66,66,66,66	0
58	MG	1H	3290	1/1	0.86	0.22	70,70,70,70	0
58	MG	1G	1619	1/1	0.86	0.21	101,101,101,101	0
58	MG	1H	3321	1/1	0.86	0.25	67,67,67,67	0
58	MG	1H	3157	1/1	0.86	0.47	73,73,73,73	0
58	MG	13	1692	1/1	0.86	0.16	122,122,122,122	0
58	MG	1G	1634	1/1	0.86	0.29	112,112,112,112	0
58	MG	13	1606	1/1	0.86	0.46	94,94,94,94	0
58	MG	1H	3141	1/1	0.86	0.40	61,61,61,61	0
58	MG	14	3013	1/1	0.86	0.23	78,78,78,78	0
58	MG	14	3199	1/1	0.86	0.50	69,69,69,69	0
58	MG	14	3118	1/1	0.86	0.45	69,69,69,69	0
58	MG	1H	3329	1/1	0.86	0.77	81,81,81,81	0
58	MG	1H	3203	1/1	0.86	0.37	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1641	1/1	0.86	0.34	113,113,113,113	0
58	MG	1H	3276	1/1	0.86	0.68	75,75,75,75	0
58	MG	1H	3185	1/1	0.86	0.40	95,95,95,95	0
58	MG	1H	3234	1/1	0.86	0.08	66,66,66,66	0
58	MG	1H	3303	1/1	0.86	0.77	78,78,78,78	0
58	MG	1H	3242	1/1	0.86	0.36	52,52,52,52	0
58	MG	1G	1654	1/1	0.86	0.53	83,83,83,83	0
58	MG	1H	3340	1/1	0.86	0.50	78,78,78,78	0
58	MG	1H	3206	1/1	0.86	0.35	77,77,77,77	0
58	MG	14	3163	1/1	0.86	0.27	90,90,90,90	0
58	MG	1H	3126	1/1	0.86	0.23	58,58,58,58	0
58	MG	1H	3188	1/1	0.86	0.38	73,73,73,73	0
58	MG	13	1647	1/1	0.86	0.23	89,89,89,89	0
58	MG	1H	3216	1/1	0.86	0.40	67,67,67,67	0
58	MG	13	1707	1/1	0.86	0.15	76,76,76,76	0
58	MG	1H	3015	1/1	0.86	0.27	63,63,63,63	0
58	MG	14	3296	1/1	0.86	0.41	84,84,84,84	0
58	MG	1G	1671	1/1	0.86	0.38	88,88,88,88	0
58	MG	55	201	1/1	0.86	0.30	74,74,74,74	0
58	MG	1H	3426	1/1	0.86	0.13	58,58,58,58	0
58	MG	1H	3452	1/1	0.87	0.13	104,104,104,104	0
58	MG	14	3263	1/1	0.87	0.24	75,75,75,75	0
58	MG	14	3169	1/1	0.87	0.40	58,58,58,58	0
58	MG	1H	3168	1/1	0.87	0.38	69,69,69,69	0
58	MG	14	3084	1/1	0.87	0.56	80,80,80,80	0
58	MG	1G	1662	1/1	0.87	0.68	72,72,72,72	0
58	MG	13	1686	1/1	0.87	0.50	76,76,76,76	0
58	MG	1H	3156	1/1	0.87	0.31	67,67,67,67	0
58	MG	14	3272	1/1	0.87	0.38	76,76,76,76	0
58	MG	16	202	1/1	0.87	0.25	64,64,64,64	0
58	MG	14	3274	1/1	0.87	0.15	76,76,76,76	0
58	MG	13	1680	1/1	0.87	0.28	96,96,96,96	0
58	MG	1H	3176	1/1	0.87	0.46	76,76,76,76	0
58	MG	1H	3158	1/1	0.87	0.49	74,74,74,74	0
58	MG	1H	3066	1/1	0.87	0.33	59,59,59,59	0
58	MG	14	3281	1/1	0.87	0.38	86,86,86,86	0
58	MG	14	3246	1/1	0.87	0.22	69,69,69,69	0
58	MG	1H	3281	1/1	0.87	0.20	88,88,88,88	0
58	MG	14	3284	1/1	0.87	0.78	78,78,78,78	0
58	MG	14	3131	1/1	0.87	0.33	95,95,95,95	0
58	MG	1H	3376	1/1	0.87	0.23	76,76,76,76	0
58	MG	1J	205	1/1	0.87	0.09	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3326	1/1	0.87	0.56	83,83,83,83	0
58	MG	13	1639	1/1	0.87	0.56	82,82,82,82	0
58	MG	1H	3182	1/1	0.87	0.20	78,78,78,78	0
58	MG	1H	3258	1/1	0.87	0.27	59,59,59,59	0
58	MG	1H	3135	1/1	0.87	0.12	65,65,65,65	0
58	MG	1K	101	1/1	0.87	0.09	145,145,145,145	0
58	MG	1H	3186	1/1	0.87	0.34	75,75,75,75	0
58	MG	14	3211	1/1	0.87	0.37	91,91,91,91	0
58	MG	14	3154	1/1	0.87	0.25	69,69,69,69	0
58	MG	1H	3445	1/1	0.87	0.07	110,110,110,110	0
58	MG	13	1608	1/1	0.88	0.75	90,90,90,90	0
58	MG	13	1624	1/1	0.88	0.23	103,103,103,103	0
58	MG	1H	3286	1/1	0.88	0.32	94,94,94,94	0
58	MG	I8	102	1/1	0.88	0.24	70,70,70,70	0
58	MG	14	3286	1/1	0.88	0.38	80,80,80,80	0
58	MG	14	3364	1/1	0.88	0.16	85,85,85,85	0
58	MG	14	3386	1/1	0.88	0.16	90,90,90,90	0
58	MG	14	3100	1/1	0.88	0.38	76,76,76,76	0
58	MG	L8	101	1/1	0.88	0.62	84,84,84,84	0
58	MG	1H	3140	1/1	0.88	0.27	58,58,58,58	0
58	MG	Q8	101	1/1	0.88	0.33	70,70,70,70	0
58	MG	1G	1677	1/1	0.88	0.12	96,96,96,96	0
58	MG	14	3032	1/1	0.88	0.45	75,75,75,75	0
58	MG	14	3232	1/1	0.88	0.21	81,81,81,81	0
58	MG	1H	3041	1/1	0.88	0.22	76,76,76,76	0
58	MG	1H	3467	1/1	0.88	0.10	84,84,84,84	0
58	MG	14	3299	1/1	0.88	0.20	98,98,98,98	0
58	MG	13	1677	1/1	0.88	0.16	104,104,104,104	0
58	MG	14	3055	1/1	0.88	0.10	81,81,81,81	0
58	MG	1H	3333	1/1	0.88	0.34	100,100,100,100	0
58	MG	1G	1613	1/1	0.88	0.21	98,98,98,98	0
58	MG	1H	3320	1/1	0.88	0.46	77,77,77,77	0
58	MG	1H	3170	1/1	0.88	0.46	65,65,65,65	0
58	MG	1H	3269	1/1	0.88	0.32	65,65,65,65	0
58	MG	1H	3323	1/1	0.88	0.45	80,80,80,80	0
58	MG	1H	3144	1/1	0.88	0.40	77,77,77,77	0
58	MG	1G	1628	1/1	0.88	0.44	95,95,95,95	0
58	MG	1G	1689	1/1	0.89	0.17	121,121,121,121	0
58	MG	14	3126	1/1	0.89	0.39	67,67,67,67	0
58	MG	13	1652	1/1	0.89	0.24	99,99,99,99	0
58	MG	1H	3334	1/1	0.89	0.30	76,76,76,76	0
58	MG	14	3244	1/1	0.89	0.59	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3007	1/1	0.89	0.48	54,54,54,54	0
58	MG	14	3324	1/1	0.89	0.06	99,99,99,99	0
58	MG	1G	1631	1/1	0.89	0.25	96,96,96,96	0
58	MG	1H	3388	1/1	0.89	0.07	77,77,77,77	0
58	MG	13	1691	1/1	0.89	0.48	90,90,90,90	0
58	MG	1H	3325	1/1	0.89	0.44	71,71,71,71	0
58	MG	14	3195	1/1	0.89	0.37	68,68,68,68	0
58	MG	14	3285	1/1	0.89	0.25	68,68,68,68	0
58	MG	1H	3417	1/1	0.89	0.22	94,94,94,94	0
58	MG	14	3287	1/1	0.89	0.22	82,82,82,82	0
58	MG	1H	3419	1/1	0.89	0.06	101,101,101,101	0
58	MG	1H	3131	1/1	0.89	0.56	73,73,73,73	0
58	MG	14	3203	1/1	0.89	0.34	56,56,56,56	0
58	MG	1H	3232	1/1	0.89	0.17	52,52,52,52	0
58	MG	14	3024	1/1	0.89	0.57	77,77,77,77	0
58	MG	14	3220	1/1	0.89	0.43	76,76,76,76	0
58	MG	14	3160	1/1	0.89	0.37	72,72,72,72	0
58	MG	1H	3042	1/1	0.89	0.85	90,90,90,90	0
58	MG	14	3090	1/1	0.89	0.29	74,74,74,74	0
58	MG	1H	3221	1/1	0.89	0.40	89,89,89,89	0
58	MG	14	3104	1/1	0.89	0.65	86,86,86,86	0
58	MG	1G	1647	1/1	0.89	0.80	83,83,83,83	0
58	MG	13	1687	1/1	0.89	0.27	99,99,99,99	0
58	MG	1H	3353	1/1	0.89	0.16	57,57,57,57	0
58	MG	13	1620	1/1	0.89	0.28	73,73,73,73	0
58	MG	1G	1622	1/1	0.89	1.19	92,92,92,92	0
58	MG	14	3307	1/1	0.89	0.48	101,101,101,101	0
58	MG	13	1655	1/1	0.90	0.46	87,87,87,87	0
58	MG	1H	3034	1/1	0.90	0.45	80,80,80,80	0
58	MG	1H	3446	1/1	0.90	0.09	84,84,84,84	0
58	MG	14	3033	1/1	0.90	0.26	77,77,77,77	0
58	MG	14	3149	1/1	0.90	0.54	73,73,73,73	0
58	MG	1H	3238	1/1	0.90	0.14	65,65,65,65	0
58	MG	14	3035	1/1	0.90	0.22	93,93,93,93	0
58	MG	13	1651	1/1	0.90	0.41	88,88,88,88	0
58	MG	14	3049	1/1	0.90	0.21	70,70,70,70	0
58	MG	14	3157	1/1	0.90	0.25	57,57,57,57	0
58	MG	1H	3155	1/1	0.90	0.34	74,74,74,74	0
58	MG	1H	3003	1/1	0.90	0.26	64,64,64,64	0
58	MG	14	3165	1/1	0.90	0.51	77,77,77,77	0
58	MG	14	3168	1/1	0.90	0.53	106,106,106,106	0
58	MG	1H	3464	1/1	0.90	0.14	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3249	1/1	0.90	0.24	80,80,80,80	0
58	MG	1H	3039	1/1	0.90	0.32	68,68,68,68	0
58	MG	14	3172	1/1	0.90	0.70	70,70,70,70	0
58	MG	14	3176	1/1	0.90	0.47	79,79,79,79	0
58	MG	1H	3085	1/1	0.90	0.42	63,63,63,63	0
58	MG	1H	3215	1/1	0.90	0.28	63,63,63,63	0
58	MG	14	3312	1/1	0.90	0.54	80,80,80,80	0
58	MG	1H	3132	1/1	0.90	0.65	85,85,85,85	0
58	MG	1H	3318	1/1	0.90	0.42	79,79,79,79	0
58	MG	16	207	1/1	0.90	0.07	80,80,80,80	0
58	MG	14	3325	1/1	0.90	0.14	63,63,63,63	0
58	MG	14	3333	1/1	0.90	0.17	74,74,74,74	0
58	MG	1H	3362	1/1	0.90	0.11	53,53,53,53	0
58	MG	1G	1687	1/1	0.90	0.06	139,139,139,139	0
58	MG	1H	3319	1/1	0.90	0.52	110,110,110,110	0
58	MG	1H	3009	1/1	0.90	0.27	62,62,62,62	0
58	MG	14	3378	1/1	0.90	0.07	100,100,100,100	0
58	MG	1G	1639	1/1	0.90	0.51	74,74,74,74	0
58	MG	14	3389	1/1	0.90	0.09	102,102,102,102	0
58	MG	1G	1640	1/1	0.90	0.48	87,87,87,87	0
58	MG	14	3096	1/1	0.90	0.34	73,73,73,73	0
58	MG	1H	3088	1/1	0.90	0.34	68,68,68,68	0
58	MG	13	1702	1/1	0.90	0.27	98,98,98,98	0
58	MG	1H	3027	1/1	0.90	0.32	81,81,81,81	0
58	MG	13	1631	1/1	0.90	0.37	93,93,93,93	0
58	MG	1H	3267	1/1	0.90	0.49	73,73,73,73	0
58	MG	14	3111	1/1	0.90	0.14	81,81,81,81	0
58	MG	14	3200	1/1	0.90	0.46	74,74,74,74	0
58	MG	14	3115	1/1	0.90	0.40	80,80,80,80	0
58	MG	1H	3063	1/1	0.90	0.13	78,78,78,78	0
58	MG	14	3204	1/1	0.90	0.19	77,77,77,77	0
58	MG	13	1629	1/1	0.90	0.39	96,96,96,96	0
58	MG	1H	3119	1/1	0.90	0.20	69,69,69,69	0
58	MG	14	3212	1/1	0.90	0.39	70,70,70,70	0
58	MG	1H	3272	1/1	0.90	0.18	64,64,64,64	0
58	MG	14	3025	1/1	0.90	0.62	84,84,84,84	0
58	MG	1H	3200	1/1	0.90	0.49	81,81,81,81	0
58	MG	45	201	1/1	0.90	0.16	108,108,108,108	0
58	MG	1G	1661	1/1	0.90	0.23	123,123,123,123	0
58	MG	14	3028	1/1	0.90	0.25	69,69,69,69	0
58	MG	1H	3460	1/1	0.91	0.09	104,104,104,104	0
58	MG	14	3305	1/1	0.91	0.49	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3047	1/1	0.91	0.32	47,47,47,47	0
58	MG	1G	1614	1/1	0.91	0.30	107,107,107,107	0
58	MG	1H	3002	1/1	0.91	0.25	38,38,38,38	0
58	MG	1H	3367	1/1	0.91	0.09	71,71,71,71	0
58	MG	13	1654	1/1	0.91	0.38	74,74,74,74	0
58	MG	14	3215	1/1	0.91	0.22	72,72,72,72	0
58	MG	14	3217	1/1	0.91	0.43	83,83,83,83	0
58	MG	1H	3095	1/1	0.91	0.33	65,65,65,65	0
58	MG	1H	3220	1/1	0.91	0.27	82,82,82,82	0
58	MG	1H	3004	1/1	0.91	0.32	57,57,57,57	0
58	MG	14	3223	1/1	0.91	0.35	86,86,86,86	0
58	MG	14	3099	1/1	0.91	0.56	87,87,87,87	0
58	MG	13	1710	1/1	0.91	0.09	97,97,97,97	0
58	MG	14	3352	1/1	0.91	0.07	97,97,97,97	0
58	MG	14	3171	1/1	0.91	0.32	99,99,99,99	0
58	MG	1H	3100	1/1	0.91	0.24	61,61,61,61	0
58	MG	1H	3418	1/1	0.91	0.08	92,92,92,92	0
58	MG	14	3365	1/1	0.91	0.05	94,94,94,94	0
58	MG	13	1657	1/1	0.91	0.28	103,103,103,103	0
58	MG	14	3384	1/1	0.91	0.14	83,83,83,83	0
58	MG	14	3279	1/1	0.91	0.09	104,104,104,104	0
58	MG	14	3178	1/1	0.91	0.50	84,84,84,84	0
58	MG	1G	1670	1/1	0.91	0.43	86,86,86,86	0
58	MG	1H	3104	1/1	0.91	0.58	69,69,69,69	0
58	MG	14	3031	1/1	0.91	0.42	68,68,68,68	0
58	MG	1H	3204	1/1	0.91	0.42	69,69,69,69	0
58	MG	14	3397	1/1	0.91	0.50	73,73,73,73	0
58	MG	14	3239	1/1	0.91	0.17	80,80,80,80	0
58	MG	14	3241	1/1	0.91	0.35	56,56,56,56	0
58	MG	14	3242	1/1	0.91	0.52	67,67,67,67	0
58	MG	1G	1674	1/1	0.91	0.44	102,102,102,102	0
58	MG	14	3122	1/1	0.91	0.28	88,88,88,88	0
58	MG	1H	3265	1/1	0.91	0.40	78,78,78,78	0
58	MG	13	1720	1/1	0.91	0.10	90,90,90,90	0
58	MG	J8	101	1/1	0.91	0.19	66,66,66,66	0
58	MG	1H	3162	1/1	0.91	0.39	88,88,88,88	0
58	MG	1H	3118	1/1	0.91	0.84	77,77,77,77	0
58	MG	1H	3270	1/1	0.91	0.86	80,80,80,80	0
58	MG	1G	1602	1/1	0.91	0.42	79,79,79,79	0
58	MG	1G	1645	1/1	0.91	0.52	74,74,74,74	0
58	MG	13	1627	1/1	0.91	0.55	69,69,69,69	0
58	MG	1H	3294	1/1	0.91	0.34	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3148	1/1	0.91	0.31	77,77,77,77	0
58	MG	13	1731	1/1	0.91	0.14	84,84,84,84	0
60	ZN	G8	201	1/1	0.91	0.11	149,149,149,149	0
58	MG	14	3056	1/1	0.92	0.34	55,55,55,55	0
58	MG	1H	3038	1/1	0.92	0.34	92,92,92,92	0
58	MG	1H	3304	1/1	0.92	0.33	86,86,86,86	0
58	MG	1G	1681	1/1	0.92	0.10	78,78,78,78	0
58	MG	13	1625	1/1	0.92	0.33	86,86,86,86	0
58	MG	13	1626	1/1	0.92	0.37	69,69,69,69	0
58	MG	14	3314	1/1	0.92	0.32	94,94,94,94	0
58	MG	14	3267	1/1	0.92	0.25	92,92,92,92	0
58	MG	13	1636	1/1	0.92	0.28	64,64,64,64	0
58	MG	1H	3198	1/1	0.92	0.43	69,69,69,69	0
58	MG	1H	3177	1/1	0.92	0.23	74,74,74,74	0
58	MG	14	3340	1/1	0.92	0.09	79,79,79,79	0
58	MG	14	3343	1/1	0.92	0.08	82,82,82,82	0
58	MG	14	3076	1/1	0.92	0.34	62,62,62,62	0
58	MG	14	3347	1/1	0.92	0.06	108,108,108,108	0
58	MG	1H	3078	1/1	0.92	0.51	67,67,67,67	0
58	MG	13	1623	1/1	0.92	0.23	108,108,108,108	0
58	MG	14	3355	1/1	0.92	0.10	102,102,102,102	0
58	MG	14	3362	1/1	0.92	0.12	77,77,77,77	0
58	MG	1H	3044	1/1	0.92	0.27	82,82,82,82	0
58	MG	14	3086	1/1	0.92	0.43	83,83,83,83	0
58	MG	1H	3161	1/1	0.92	0.30	84,84,84,84	0
58	MG	14	3374	1/1	0.92	0.07	76,76,76,76	0
58	MG	14	3175	1/1	0.92	0.16	92,92,92,92	0
58	MG	14	3381	1/1	0.92	0.14	81,81,81,81	0
58	MG	14	3233	1/1	0.92	0.15	86,86,86,86	0
58	MG	1H	3317	1/1	0.92	0.38	68,68,68,68	0
58	MG	1G	1653	1/1	0.92	0.15	97,97,97,97	0
58	MG	13	1729	1/1	0.92	0.07	113,113,113,113	0
58	MG	1G	1655	1/1	0.92	0.25	100,100,100,100	0
58	MG	1G	1656	1/1	0.92	0.41	78,78,78,78	0
58	MG	14	3394	1/1	0.92	0.05	109,109,109,109	0
58	MG	14	3240	1/1	0.92	0.21	83,83,83,83	0
58	MG	1H	3149	1/1	0.92	0.34	60,60,60,60	0
58	MG	1H	3355	1/1	0.92	0.20	48,48,48,48	0
58	MG	1H	3166	1/1	0.92	0.27	71,71,71,71	0
58	MG	1H	3150	1/1	0.92	0.23	72,72,72,72	0
58	MG	16	201	1/1	0.92	0.11	85,85,85,85	0
58	MG	1H	3239	1/1	0.92	0.21	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3028	1/1	0.92	0.28	68,68,68,68	0
58	MG	14	3119	1/1	0.92	0.37	62,62,62,62	0
58	MG	1H	3371	1/1	0.92	0.12	59,59,59,59	0
58	MG	1G	1629	1/1	0.92	0.63	104,104,104,104	0
58	MG	1H	3273	1/1	0.92	0.22	68,68,68,68	0
58	MG	1H	3387	1/1	0.92	0.07	80,80,80,80	0
58	MG	1G	1632	1/1	0.92	0.43	75,75,75,75	0
58	MG	1H	3244	1/1	0.92	0.28	62,62,62,62	0
58	MG	1G	1673	1/1	0.92	0.33	93,93,93,93	0
58	MG	14	3047	1/1	0.92	0.18	74,74,74,74	0
58	MG	45	202	1/1	0.92	0.41	72,72,72,72	0
58	MG	1H	3392	1/1	0.92	0.11	68,68,68,68	0
58	MG	1H	3214	1/1	0.92	0.63	76,76,76,76	0
58	MG	1H	3105	1/1	0.92	0.33	66,66,66,66	0
58	MG	1G	1688	1/1	0.93	0.07	138,138,138,138	0
58	MG	13	1660	1/1	0.93	0.24	103,103,103,103	0
58	MG	1H	3070	1/1	0.93	0.47	58,58,58,58	0
58	MG	1G	1644	1/1	0.93	0.67	92,92,92,92	0
58	MG	1H	3395	1/1	0.93	0.07	77,77,77,77	0
58	MG	1H	3407	1/1	0.93	0.12	116,116,116,116	0
58	MG	1H	3410	1/1	0.93	0.10	58,58,58,58	0
58	MG	13	1645	1/1	0.93	0.42	64,64,64,64	0
58	MG	13	1693	1/1	0.93	0.21	55,55,55,55	0
58	MG	14	3105	1/1	0.93	0.31	67,67,67,67	0
58	MG	14	3106	1/1	0.93	0.40	61,61,61,61	0
58	MG	1H	3225	1/1	0.93	0.35	78,78,78,78	0
58	MG	1G	1651	1/1	0.93	0.20	104,104,104,104	0
58	MG	1H	3107	1/1	0.93	0.28	71,71,71,71	0
58	MG	14	3326	1/1	0.93	0.09	90,90,90,90	0
58	MG	1H	3040	1/1	0.93	0.44	70,70,70,70	0
58	MG	1H	3111	1/1	0.93	0.53	74,74,74,74	0
58	MG	1H	3172	1/1	0.93	0.41	87,87,87,87	0
58	MG	1H	3145	1/1	0.93	0.14	73,73,73,73	0
58	MG	1G	1658	1/1	0.93	0.23	92,92,92,92	0
58	MG	1H	3116	1/1	0.93	0.44	55,55,55,55	0
58	MG	1G	1660	1/1	0.93	0.45	85,85,85,85	0
58	MG	1H	3274	1/1	0.93	0.18	59,59,59,59	0
58	MG	13	1713	1/1	0.93	0.05	101,101,101,101	0
58	MG	1H	3012	1/1	0.93	0.80	83,83,83,83	0
58	MG	1H	3447	1/1	0.93	0.04	86,86,86,86	0
58	MG	13	1607	1/1	0.93	0.19	116,116,116,116	0
58	MG	14	3208	1/1	0.93	0.15	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3141	1/1	0.93	0.21	93,93,93,93	0
58	MG	14	3142	1/1	0.93	0.41	76,76,76,76	0
58	MG	14	3383	1/1	0.93	0.12	86,86,86,86	0
58	MG	1H	3456	1/1	0.93	0.07	97,97,97,97	0
58	MG	14	3276	1/1	0.93	0.37	92,92,92,92	0
58	MG	14	3387	1/1	0.93	0.10	96,96,96,96	0
58	MG	14	3216	1/1	0.93	0.31	77,77,77,77	0
58	MG	1H	3243	1/1	0.93	0.50	65,65,65,65	0
58	MG	14	3219	1/1	0.93	0.31	48,48,48,48	0
58	MG	1H	3311	1/1	0.93	0.29	75,75,75,75	0
58	MG	13	1665	1/1	0.93	0.09	82,82,82,82	0
58	MG	1H	3343	1/1	0.93	0.15	54,54,54,54	0
58	MG	14	3396	1/1	0.93	0.06	108,108,108,108	0
58	MG	14	3054	1/1	0.93	0.37	70,70,70,70	0
58	MG	13	1724	1/1	0.93	0.09	102,102,102,102	0
58	MG	14	3225	1/1	0.93	0.41	82,82,82,82	0
58	MG	1H	3466	1/1	0.93	0.30	56,56,56,56	0
58	MG	1H	3211	1/1	0.93	0.24	83,83,83,83	0
58	MG	1G	1676	1/1	0.93	0.11	90,90,90,90	0
58	MG	14	3289	1/1	0.93	0.76	83,83,83,83	0
58	MG	14	3156	1/1	0.93	0.61	63,63,63,63	0
58	MG	1H	3127	1/1	0.93	0.14	59,59,59,59	0
58	MG	13	1725	1/1	0.93	0.08	94,94,94,94	0
58	MG	14	3162	1/1	0.93	0.54	70,70,70,70	0
58	MG	1H	3050	1/1	0.93	0.39	60,60,60,60	0
58	MG	14	3164	1/1	0.93	0.79	74,74,74,74	0
58	MG	1H	3056	1/1	0.93	0.50	56,56,56,56	0
58	MG	14	3166	1/1	0.93	0.21	60,60,60,60	0
58	MG	1H	3370	1/1	0.93	0.16	71,71,71,71	0
58	MG	13	1726	1/1	0.93	0.05	126,126,126,126	0
58	MG	1H	3064	1/1	0.93	0.32	65,65,65,65	0
58	MG	14	3077	1/1	0.93	0.45	68,68,68,68	0
58	MG	1H	3261	1/1	0.93	0.19	69,69,69,69	0
58	MG	1G	1624	1/1	0.94	0.62	65,65,65,65	0
58	MG	1G	1626	1/1	0.94	0.29	82,82,82,82	0
58	MG	14	3112	1/1	0.94	0.48	65,65,65,65	0
58	MG	14	3114	1/1	0.94	0.42	58,58,58,58	0
58	MG	1H	3098	1/1	0.94	0.24	53,53,53,53	0
58	MG	1H	3065	1/1	0.94	0.35	61,61,61,61	0
58	MG	14	3002	1/1	0.94	0.37	57,57,57,57	0
58	MG	14	3003	1/1	0.94	0.24	62,62,62,62	0
58	MG	13	1712	1/1	0.94	0.12	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3443	1/1	0.94	0.19	76,76,76,76	0
58	MG	13	1663	1/1	0.94	0.26	82,82,82,82	0
58	MG	14	3014	1/1	0.94	0.47	57,57,57,57	0
58	MG	1H	3208	1/1	0.94	0.51	88,88,88,88	0
58	MG	14	3132	1/1	0.94	0.27	68,68,68,68	0
58	MG	1H	3023	1/1	0.94	0.46	56,56,56,56	0
58	MG	14	3136	1/1	0.94	0.17	62,62,62,62	0
58	MG	1H	3449	1/1	0.94	0.12	106,106,106,106	0
58	MG	14	3020	1/1	0.94	0.47	75,75,75,75	0
58	MG	1H	3451	1/1	0.94	0.13	114,114,114,114	0
58	MG	1H	3106	1/1	0.94	0.41	63,63,63,63	0
58	MG	13	1664	1/1	0.94	0.12	89,89,89,89	0
58	MG	1H	3073	1/1	0.94	0.50	81,81,81,81	0
58	MG	1H	3458	1/1	0.94	0.07	73,73,73,73	0
58	MG	14	3315	1/1	0.94	1.07	93,93,93,93	0
58	MG	1H	3299	1/1	0.94	0.17	74,74,74,74	0
58	MG	14	3322	1/1	0.94	0.22	65,65,65,65	0
58	MG	14	3323	1/1	0.94	0.14	64,64,64,64	0
58	MG	1H	3300	1/1	0.94	0.42	87,87,87,87	0
58	MG	1H	3461	1/1	0.94	0.04	92,92,92,92	0
58	MG	14	3151	1/1	0.94	0.77	79,79,79,79	0
58	MG	1H	3110	1/1	0.94	0.51	55,55,55,55	0
58	MG	1H	3146	1/1	0.94	0.39	72,72,72,72	0
58	MG	13	1719	1/1	0.94	0.13	71,71,71,71	0
58	MG	1H	3266	1/1	0.94	0.25	81,81,81,81	0
58	MG	1H	3181	1/1	0.94	0.25	61,61,61,61	0
58	MG	14	3348	1/1	0.94	0.17	70,70,70,70	0
58	MG	14	3350	1/1	0.94	0.11	85,85,85,85	0
58	MG	14	3159	1/1	0.94	0.47	63,63,63,63	0
58	MG	1H	3361	1/1	0.94	0.13	63,63,63,63	0
58	MG	1H	3112	1/1	0.94	0.41	56,56,56,56	0
58	MG	1G	1652	1/1	0.94	0.54	71,71,71,71	0
58	MG	1H	3115	1/1	0.94	0.26	43,43,43,43	0
58	MG	1H	3014	1/1	0.94	0.33	70,70,70,70	0
58	MG	1H	3117	1/1	0.94	0.23	48,48,48,48	0
58	MG	14	3053	1/1	0.94	0.23	61,61,61,61	0
58	MG	13	1640	1/1	0.94	0.35	74,74,74,74	0
58	MG	13	1676	1/1	0.94	0.51	76,76,76,76	0
58	MG	1H	3189	1/1	0.94	0.57	67,67,67,67	0
58	MG	14	3057	1/1	0.94	0.27	101,101,101,101	0
58	MG	14	3385	1/1	0.94	0.07	116,116,116,116	0
58	MG	1H	3379	1/1	0.94	0.11	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3381	1/1	0.94	0.14	63,63,63,63	0
58	MG	1H	3275	1/1	0.94	0.37	75,75,75,75	0
58	MG	14	3390	1/1	0.94	0.10	89,89,89,89	0
58	MG	1H	3017	1/1	0.94	0.44	71,71,71,71	0
58	MG	14	3063	1/1	0.94	0.28	58,58,58,58	0
58	MG	1H	3229	1/1	0.94	0.27	48,48,48,48	0
58	MG	1H	3393	1/1	0.94	0.20	54,54,54,54	0
58	MG	14	3069	1/1	0.94	0.38	70,70,70,70	0
58	MG	1H	3123	1/1	0.94	0.39	69,69,69,69	0
58	MG	13	1683	1/1	0.94	0.23	94,94,94,94	0
58	MG	1H	3055	1/1	0.94	0.34	49,49,49,49	0
58	MG	13	1619	1/1	0.94	0.13	91,91,91,91	0
58	MG	1H	3091	1/1	0.94	0.46	65,65,65,65	0
58	MG	14	3082	1/1	0.94	0.47	61,61,61,61	0
58	MG	14	3189	1/1	0.94	0.33	82,82,82,82	0
58	MG	1H	3415	1/1	0.94	0.06	73,73,73,73	0
58	MG	1G	1607	1/1	0.94	0.34	73,73,73,73	0
58	MG	1H	3240	1/1	0.94	0.30	74,74,74,74	0
58	MG	1G	1611	1/1	0.94	0.38	104,104,104,104	0
58	MG	1G	1612	1/1	0.94	0.36	81,81,81,81	0
58	MG	1H	3061	1/1	0.94	0.30	48,48,48,48	0
58	MG	14	3198	1/1	0.94	0.18	107,107,107,107	0
58	MG	1H	3165	1/1	0.94	0.52	78,78,78,78	0
58	MG	1H	3420	1/1	0.94	0.06	92,92,92,92	0
58	MG	1H	3421	1/1	0.94	0.06	64,64,64,64	0
58	MG	13	1601	1/1	0.94	0.34	68,68,68,68	0
58	MG	1H	3037	1/1	0.94	0.46	121,121,121,121	0
58	MG	1H	3431	1/1	0.94	0.13	70,70,70,70	0
58	MG	1H	3436	1/1	0.94	0.17	73,73,73,73	0
58	MG	1H	3455	1/1	0.95	0.08	59,59,59,59	0
58	MG	13	1616	1/1	0.95	0.04	88,88,88,88	0
58	MG	1H	3223	1/1	0.95	0.52	78,78,78,78	0
58	MG	14	3016	1/1	0.95	0.40	61,61,61,61	0
58	MG	1H	3250	1/1	0.95	0.27	74,74,74,74	0
58	MG	14	3336	1/1	0.95	0.17	62,62,62,62	0
58	MG	14	3338	1/1	0.95	0.23	60,60,60,60	0
58	MG	1H	3048	1/1	0.95	0.30	56,56,56,56	0
58	MG	1H	3113	1/1	0.95	0.44	51,51,51,51	0
58	MG	1H	3394	1/1	0.95	0.20	53,53,53,53	0
58	MG	14	3346	1/1	0.95	0.09	85,85,85,85	0
58	MG	1H	3153	1/1	0.95	0.20	62,62,62,62	0
58	MG	1H	3049	1/1	0.95	0.50	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3256	1/1	0.95	0.17	61,61,61,61	0
58	MG	14	3351	1/1	0.95	0.12	85,85,85,85	0
58	MG	14	3087	1/1	0.95	0.35	40,40,40,40	0
58	MG	1H	3310	1/1	0.95	0.17	75,75,75,75	0
58	MG	14	3158	1/1	0.95	0.42	75,75,75,75	0
58	MG	14	3358	1/1	0.95	0.09	91,91,91,91	0
58	MG	13	1628	1/1	0.95	0.41	65,65,65,65	0
58	MG	14	3094	1/1	0.95	0.64	60,60,60,60	0
58	MG	14	3095	1/1	0.95	0.41	71,71,71,71	0
58	MG	13	1671	1/1	0.95	0.31	87,87,87,87	0
58	MG	14	3371	1/1	0.95	0.12	53,53,53,53	0
58	MG	1H	3230	1/1	0.95	0.41	43,43,43,43	0
58	MG	1H	3192	1/1	0.95	0.23	80,80,80,80	0
58	MG	14	3380	1/1	0.95	0.10	96,96,96,96	0
58	MG	1H	3005	1/1	0.95	0.34	54,54,54,54	0
58	MG	1H	3345	1/1	0.95	0.18	61,61,61,61	0
58	MG	16	208	1/1	0.95	0.16	86,86,86,86	0
58	MG	1H	3346	1/1	0.95	0.14	45,45,45,45	0
58	MG	1H	3058	1/1	0.95	0.43	46,46,46,46	0
58	MG	1G	1675	1/1	0.95	0.33	91,91,91,91	0
58	MG	14	3388	1/1	0.95	0.10	68,68,68,68	0
58	MG	14	3173	1/1	0.95	0.30	66,66,66,66	0
58	MG	14	3174	1/1	0.95	0.27	101,101,101,101	0
58	MG	14	3110	1/1	0.95	0.37	57,57,57,57	0
58	MG	1H	3235	1/1	0.95	0.16	53,53,53,53	0
58	MG	1H	3428	1/1	0.95	0.19	51,51,51,51	0
58	MG	1H	3357	1/1	0.95	0.23	71,71,71,71	0
58	MG	1H	3432	1/1	0.95	0.11	50,50,50,50	0
58	MG	14	3051	1/1	0.95	0.11	81,81,81,81	0
58	MG	1H	3236	1/1	0.95	0.18	99,99,99,99	0
58	MG	1H	3237	1/1	0.95	0.28	84,84,84,84	0
58	MG	14	3121	1/1	0.95	0.48	78,78,78,78	0
58	MG	1H	3007	1/1	0.95	0.34	54,54,54,54	0
58	MG	14	3124	1/1	0.95	0.40	54,54,54,54	0
58	MG	1H	3084	1/1	0.95	0.20	94,94,94,94	0
58	MG	13	1633	1/1	0.95	0.63	62,62,62,62	0
58	MG	1H	3444	1/1	0.95	0.16	69,69,69,69	0
58	MG	1H	3218	1/1	0.95	0.25	56,56,56,56	0
58	MG	1H	3011	1/1	0.95	0.38	51,51,51,51	0
58	MG	14	3133	1/1	0.95	0.19	107,107,107,107	0
58	MG	14	3134	1/1	0.95	0.28	74,74,74,74	0
58	MG	1H	3375	1/1	0.95	0.29	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1673	1/1	0.95	0.53	70,70,70,70	0
58	MG	14	3137	1/1	0.95	0.09	57,57,57,57	0
58	MG	1H	3377	1/1	0.95	0.13	70,70,70,70	0
58	MG	14	3066	1/1	0.95	0.41	62,62,62,62	0
58	MG	14	3317	1/1	0.95	0.70	89,89,89,89	0
58	MG	14	3319	1/1	0.95	0.10	59,59,59,59	0
58	MG	13	1643	1/1	0.95	0.11	99,99,99,99	0
60	ZN	C5	201	1/1	0.95	0.07	165,165,165,165	0
58	MG	1H	3183	1/1	0.96	0.52	67,67,67,67	0
58	MG	1G	1617	1/1	0.96	0.14	135,135,135,135	0
58	MG	1H	3121	1/1	0.96	0.38	62,62,62,62	0
58	MG	1H	3090	1/1	0.96	0.36	71,71,71,71	0
58	MG	13	1714	1/1	0.96	0.10	73,73,73,73	0
58	MG	13	1658	1/1	0.96	0.24	83,83,83,83	0
58	MG	14	3078	1/1	0.96	0.38	64,64,64,64	0
58	MG	1G	1683	1/1	0.96	0.13	89,89,89,89	0
58	MG	14	3321	1/1	0.96	0.09	78,78,78,78	0
58	MG	2K	101	1/1	0.96	0.36	68,68,68,68	0
58	MG	14	3083	1/1	0.96	0.63	72,72,72,72	0
58	MG	14	3167	1/1	0.96	0.29	87,87,87,87	0
58	MG	1G	1625	1/1	0.96	0.32	93,93,93,93	0
58	MG	13	1666	1/1	0.96	0.13	78,78,78,78	0
58	MG	14	3328	1/1	0.96	0.06	74,74,74,74	0
58	MG	14	3330	1/1	0.96	0.14	77,77,77,77	0
58	MG	1G	1627	1/1	0.96	0.22	94,94,94,94	0
58	MG	13	1615	1/1	0.96	0.40	77,77,77,77	0
58	MG	1H	3454	1/1	0.96	0.07	96,96,96,96	0
58	MG	1H	3260	1/1	0.96	0.37	72,72,72,72	0
58	MG	14	3093	1/1	0.96	0.42	42,42,42,42	0
58	MG	1H	3382	1/1	0.96	0.06	77,77,77,77	0
58	MG	1H	3129	1/1	0.96	0.52	85,85,85,85	0
58	MG	1H	3067	1/1	0.96	0.32	55,55,55,55	0
58	MG	14	3008	1/1	0.96	0.36	65,65,65,65	0
58	MG	14	3349	1/1	0.96	0.15	83,83,83,83	0
58	MG	1H	3389	1/1	0.96	0.10	38,38,38,38	0
58	MG	14	3101	1/1	0.96	0.43	64,64,64,64	0
58	MG	1H	3391	1/1	0.96	0.09	61,61,61,61	0
58	MG	1H	3295	1/1	0.96	0.46	93,93,93,93	0
58	MG	14	3015	1/1	0.96	0.44	49,49,49,49	0
58	MG	13	1722	1/1	0.96	0.08	103,103,103,103	0
58	MG	14	3360	1/1	0.96	0.06	83,83,83,83	0
58	MG	13	1723	1/1	0.96	0.10	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1610	1/1	0.96	0.25	80,80,80,80	0
58	MG	1H	3397	1/1	0.96	0.07	71,71,71,71	0
58	MG	1H	3399	1/1	0.96	0.15	62,62,62,62	0
58	MG	14	3366	1/1	0.96	0.04	86,86,86,86	0
58	MG	14	3368	1/1	0.96	0.21	62,62,62,62	0
58	MG	14	3369	1/1	0.96	0.12	59,59,59,59	0
58	MG	1H	3405	1/1	0.96	0.09	63,63,63,63	0
58	MG	1H	3406	1/1	0.96	0.07	76,76,76,76	0
58	MG	14	3376	1/1	0.96	0.07	94,94,94,94	0
58	MG	14	3377	1/1	0.96	0.20	52,52,52,52	0
58	MG	13	1618	1/1	0.96	0.36	80,80,80,80	0
58	MG	1H	3025	1/1	0.96	0.40	64,64,64,64	0
58	MG	1H	3412	1/1	0.96	0.10	78,78,78,78	0
58	MG	14	3382	1/1	0.96	0.07	87,87,87,87	0
58	MG	1H	3231	1/1	0.96	0.20	58,58,58,58	0
58	MG	14	3120	1/1	0.96	0.38	82,82,82,82	0
58	MG	1H	3046	1/1	0.96	0.32	47,47,47,47	0
58	MG	21	301	1/1	0.96	0.38	54,54,54,54	0
58	MG	14	3123	1/1	0.96	0.30	64,64,64,64	0
58	MG	13	1649	1/1	0.96	0.37	72,72,72,72	0
58	MG	1H	3081	1/1	0.96	0.39	87,87,87,87	0
58	MG	1H	3082	1/1	0.96	0.26	78,78,78,78	0
58	MG	1H	3174	1/1	0.96	0.36	88,88,88,88	0
58	MG	14	3206	1/1	0.96	0.09	80,80,80,80	0
58	MG	13	1727	1/1	0.96	0.08	112,112,112,112	0
58	MG	14	3209	1/1	0.96	0.24	66,66,66,66	0
58	MG	1H	3114	1/1	0.96	0.54	74,74,74,74	0
58	MG	I8	103	1/1	0.96	0.04	73,73,73,73	0
58	MG	14	3213	1/1	0.96	0.36	64,64,64,64	0
58	MG	14	3214	1/1	0.96	0.34	88,88,88,88	0
58	MG	13	1690	1/1	0.96	0.13	74,74,74,74	0
58	MG	14	3039	1/1	0.96	0.23	50,50,50,50	0
58	MG	1H	3423	1/1	0.96	0.10	66,66,66,66	0
58	MG	13	1711	1/1	0.96	0.11	97,97,97,97	0
58	MG	13	1730	1/1	0.96	0.17	86,86,86,86	0
58	MG	1H	3429	1/1	0.96	0.12	71,71,71,71	0
58	MG	1H	3430	1/1	0.96	0.17	49,49,49,49	0
58	MG	1H	3354	1/1	0.96	0.13	49,49,49,49	0
58	MG	1G	1605	1/1	0.96	0.38	101,101,101,101	0
58	MG	1H	3312	1/1	0.96	0.24	67,67,67,67	0
58	MG	1H	3433	1/1	0.96	0.17	87,87,87,87	0
58	MG	1H	3434	1/1	0.96	0.08	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1610	1/1	0.96	0.31	98,98,98,98	0
58	MG	1H	3212	1/1	0.96	0.43	76,76,76,76	0
58	MG	13	1612	1/1	0.96	0.33	63,63,63,63	0
58	MG	13	1614	1/1	0.96	0.20	78,78,78,78	0
58	MG	1H	3120	1/1	0.96	0.34	74,74,74,74	0
58	MG	1H	3442	1/1	0.96	0.08	69,69,69,69	0
58	MG	14	3235	1/1	0.96	0.66	72,72,72,72	0
58	MG	14	3038	1/1	0.97	0.33	71,71,71,71	0
58	MG	13	1701	1/1	0.97	0.14	114,114,114,114	0
58	MG	1G	1601	1/1	0.97	0.29	91,91,91,91	0
58	MG	14	3226	1/1	0.97	0.41	73,73,73,73	0
58	MG	13	1613	1/1	0.97	0.22	81,81,81,81	0
58	MG	1H	3257	1/1	0.97	0.30	70,70,70,70	0
58	MG	1H	3195	1/1	0.97	0.50	62,62,62,62	0
58	MG	1H	3259	1/1	0.97	0.48	79,79,79,79	0
58	MG	1H	3057	1/1	0.97	0.41	66,66,66,66	0
58	MG	14	3318	1/1	0.97	0.24	64,64,64,64	0
58	MG	13	1684	1/1	0.97	0.14	128,128,128,128	0
58	MG	1H	3440	1/1	0.97	0.05	58,58,58,58	0
58	MG	1H	3380	1/1	0.97	0.11	59,59,59,59	0
58	MG	13	1667	1/1	0.97	0.47	71,71,71,71	0
58	MG	1H	3086	1/1	0.97	0.37	70,70,70,70	0
58	MG	1H	3384	1/1	0.97	0.06	58,58,58,58	0
58	MG	14	3152	1/1	0.97	0.33	92,92,92,92	0
58	MG	1H	3062	1/1	0.97	0.20	64,64,64,64	0
58	MG	14	3062	1/1	0.97	0.17	68,68,68,68	0
58	MG	14	3332	1/1	0.97	0.10	53,53,53,53	0
58	MG	1H	3330	1/1	0.97	0.34	102,102,102,102	0
58	MG	14	3334	1/1	0.97	0.05	64,64,64,64	0
58	MG	14	3335	1/1	0.97	0.09	61,61,61,61	0
58	MG	14	3064	1/1	0.97	0.19	78,78,78,78	0
58	MG	14	3065	1/1	0.97	0.32	67,67,67,67	0
58	MG	13	1717	1/1	0.97	0.08	92,92,92,92	0
58	MG	14	3341	1/1	0.97	0.08	68,68,68,68	0
58	MG	1H	3448	1/1	0.97	0.08	82,82,82,82	0
58	MG	14	3344	1/1	0.97	0.15	81,81,81,81	0
58	MG	1H	3202	1/1	0.97	0.82	70,70,70,70	0
58	MG	14	3161	1/1	0.97	0.52	70,70,70,70	0
58	MG	1H	3450	1/1	0.97	0.10	54,54,54,54	0
58	MG	14	3070	1/1	0.97	0.51	60,60,60,60	0
58	MG	14	3072	1/1	0.97	0.22	45,45,45,45	0
58	MG	13	1718	1/1	0.97	0.04	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1621	1/1	0.97	0.12	92,92,92,92	0
58	MG	14	3075	1/1	0.97	0.29	68,68,68,68	0
58	MG	14	3254	1/1	0.97	0.19	111,111,111,111	0
58	MG	1G	1682	1/1	0.97	0.13	97,97,97,97	0
58	MG	1H	3148	1/1	0.97	0.24	50,50,50,50	0
58	MG	14	3359	1/1	0.97	0.06	79,79,79,79	0
58	MG	13	1732	1/1	0.97	0.20	65,65,65,65	0
58	MG	1G	1685	1/1	0.97	0.09	87,87,87,87	0
58	MG	1H	3010	1/1	0.97	0.36	63,63,63,63	0
58	MG	1H	3396	1/1	0.97	0.10	78,78,78,78	0
58	MG	1H	3026	1/1	0.97	0.47	56,56,56,56	0
58	MG	1H	3398	1/1	0.97	0.16	66,66,66,66	0
58	MG	14	3367	1/1	0.97	0.09	65,65,65,65	0
58	MG	1G	1690	1/1	0.97	0.16	93,93,93,93	0
58	MG	1H	3068	1/1	0.97	0.28	86,86,86,86	0
58	MG	14	3370	1/1	0.97	0.10	64,64,64,64	0
58	MG	14	3088	1/1	0.97	0.45	52,52,52,52	0
58	MG	1H	3401	1/1	0.97	0.18	69,69,69,69	0
58	MG	14	3001	1/1	0.97	0.16	46,46,46,46	0
58	MG	1H	3403	1/1	0.97	0.14	76,76,76,76	0
58	MG	1H	3462	1/1	0.97	0.04	97,97,97,97	0
58	MG	14	3379	1/1	0.97	0.12	60,60,60,60	0
58	MG	14	3270	1/1	0.97	0.30	63,63,63,63	0
58	MG	14	3004	1/1	0.97	0.37	67,67,67,67	0
58	MG	14	3005	1/1	0.97	0.45	48,48,48,48	0
58	MG	14	3098	1/1	0.97	0.17	93,93,93,93	0
58	MG	14	3006	1/1	0.97	0.63	56,56,56,56	0
58	MG	1H	3404	1/1	0.97	0.13	48,48,48,48	0
58	MG	1H	3069	1/1	0.97	0.42	90,90,90,90	0
58	MG	14	3103	1/1	0.97	0.28	51,51,51,51	0
58	MG	1H	3465	1/1	0.97	0.15	71,71,71,71	0
58	MG	1H	3210	1/1	0.97	0.47	71,71,71,71	0
58	MG	14	3192	1/1	0.97	0.51	63,63,63,63	0
58	MG	13	1622	1/1	0.97	0.37	74,74,74,74	0
58	MG	1H	3408	1/1	0.97	0.12	82,82,82,82	0
58	MG	1H	3409	1/1	0.97	0.07	85,85,85,85	0
58	MG	14	3196	1/1	0.97	0.55	75,75,75,75	0
58	MG	13	1635	1/1	0.97	0.52	74,74,74,74	0
58	MG	1H	3030	1/1	0.97	0.22	67,67,67,67	0
58	MG	1G	1642	1/1	0.97	0.48	91,91,91,91	0
58	MG	14	3398	1/1	0.97	0.07	108,108,108,108	0
58	MG	1H	3103	1/1	0.97	0.28	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16	206	1/1	0.97	0.05	73,73,73,73	0
58	MG	1H	3347	1/1	0.97	0.28	51,51,51,51	0
58	MG	14	3116	1/1	0.97	0.20	64,64,64,64	0
58	MG	1H	3350	1/1	0.97	0.12	48,48,48,48	0
58	MG	1H	3416	1/1	0.97	0.08	69,69,69,69	0
58	MG	1H	3245	1/1	0.97	0.70	62,62,62,62	0
58	MG	13	1648	1/1	0.97	0.50	95,95,95,95	0
58	MG	14	3210	1/1	0.97	0.17	80,80,80,80	0
58	MG	1H	3075	1/1	0.97	0.48	43,43,43,43	0
58	MG	1H	3356	1/1	0.97	0.17	42,42,42,42	0
58	MG	88	201	1/1	0.97	0.21	81,81,81,81	0
58	MG	13	1642	1/1	0.97	0.27	74,74,74,74	0
58	MG	1H	3358	1/1	0.97	0.14	45,45,45,45	0
58	MG	1H	3359	1/1	0.97	0.12	59,59,59,59	0
58	MG	13	1609	1/1	0.97	0.37	75,75,75,75	0
58	MG	1H	3133	1/1	0.97	0.34	71,71,71,71	0
58	MG	1H	3163	1/1	0.97	0.35	50,50,50,50	0
58	MG	14	3036	1/1	0.97	0.74	96,96,96,96	0
58	MG	13	1617	1/1	0.97	0.24	83,83,83,83	0
58	MG	1H	3077	1/1	0.98	0.23	60,60,60,60	0
58	MG	14	3337	1/1	0.98	0.06	66,66,66,66	0
58	MG	1H	3008	1/1	0.98	0.26	81,81,81,81	0
58	MG	1H	3385	1/1	0.98	0.20	47,47,47,47	0
58	MG	1H	3386	1/1	0.98	0.11	57,57,57,57	0
58	MG	14	3342	1/1	0.98	0.07	80,80,80,80	0
58	MG	1H	3001	1/1	0.98	0.32	43,43,43,43	0
58	MG	13	1716	1/1	0.98	0.07	76,76,76,76	0
58	MG	1H	3344	1/1	0.98	0.13	58,58,58,58	0
58	MG	1H	3437	1/1	0.98	0.09	58,58,58,58	0
58	MG	14	3127	1/1	0.98	0.27	69,69,69,69	0
58	MG	1H	3390	1/1	0.98	0.09	50,50,50,50	0
58	MG	14	3130	1/1	0.98	0.53	86,86,86,86	0
58	MG	1H	3289	1/1	0.98	0.17	49,49,49,49	0
58	MG	1H	3029	1/1	0.98	0.35	42,42,42,42	0
58	MG	14	3202	1/1	0.98	0.31	63,63,63,63	0
58	MG	1H	3143	1/1	0.98	0.14	56,56,56,56	0
58	MG	1H	3348	1/1	0.98	0.19	50,50,50,50	0
58	MG	14	3356	1/1	0.98	0.17	58,58,58,58	0
58	MG	1H	3349	1/1	0.98	0.18	64,64,64,64	0
58	MG	1H	3102	1/1	0.98	0.39	35,35,35,35	0
58	MG	14	3207	1/1	0.98	0.37	80,80,80,80	0
58	MG	14	3361	1/1	0.98	0.15	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3191	1/1	0.98	0.50	90,90,90,90	0
58	MG	14	3139	1/1	0.98	0.34	99,99,99,99	0
58	MG	14	3009	1/1	0.98	0.46	52,52,52,52	0
58	MG	14	3010	1/1	0.98	0.48	41,41,41,41	0
58	MG	14	3071	1/1	0.98	0.58	68,68,68,68	0
58	MG	14	3011	1/1	0.98	0.59	48,48,48,48	0
58	MG	13	1721	1/1	0.98	0.12	66,66,66,66	0
58	MG	14	3145	1/1	0.98	0.32	65,65,65,65	0
58	MG	1H	3241	1/1	0.98	0.35	66,66,66,66	0
58	MG	1H	3400	1/1	0.98	0.11	72,72,72,72	0
58	MG	14	3372	1/1	0.98	0.09	70,70,70,70	0
58	MG	14	3373	1/1	0.98	0.19	61,61,61,61	0
58	MG	14	3218	1/1	0.98	0.56	62,62,62,62	0
58	MG	14	3375	1/1	0.98	0.07	97,97,97,97	0
58	MG	1H	3169	1/1	0.98	0.21	85,85,85,85	0
58	MG	1H	3402	1/1	0.98	0.15	51,51,51,51	0
58	MG	1H	3051	1/1	0.98	0.35	45,45,45,45	0
58	MG	14	3079	1/1	0.98	0.46	70,70,70,70	0
58	MG	1H	3124	1/1	0.98	0.36	46,46,46,46	0
58	MG	14	3081	1/1	0.98	0.32	76,76,76,76	0
58	MG	1H	3453	1/1	0.98	0.10	84,84,84,84	0
58	MG	1H	3052	1/1	0.98	0.33	53,53,53,53	0
58	MG	1H	3360	1/1	0.98	0.10	61,61,61,61	0
58	MG	13	1602	1/1	0.98	0.28	86,86,86,86	0
58	MG	1H	3013	1/1	0.98	0.29	82,82,82,82	0
58	MG	13	1674	1/1	0.98	0.09	91,91,91,91	0
58	MG	1H	3365	1/1	0.98	0.14	74,74,74,74	0
58	MG	1H	3366	1/1	0.98	0.14	76,76,76,76	0
58	MG	1H	3109	1/1	0.98	0.30	47,47,47,47	0
58	MG	14	3092	1/1	0.98	0.32	76,76,76,76	0
58	MG	1G	1669	1/1	0.98	0.36	107,107,107,107	0
58	MG	1H	3006	1/1	0.98	0.36	46,46,46,46	0
58	MG	1H	3369	1/1	0.98	0.18	49,49,49,49	0
58	MG	1H	3060	1/1	0.98	0.40	61,61,61,61	0
58	MG	1H	3074	1/1	0.98	0.29	64,64,64,64	0
58	MG	1H	3373	1/1	0.98	0.12	51,51,51,51	0
58	MG	1H	3374	1/1	0.98	0.16	53,53,53,53	0
58	MG	13	1611	1/1	0.98	0.24	72,72,72,72	0
58	MG	14	3102	1/1	0.98	0.26	61,61,61,61	0
58	MG	1H	3255	1/1	0.98	0.39	73,73,73,73	0
58	MG	1H	3134	1/1	0.98	0.08	69,69,69,69	0
58	MG	1H	3093	1/1	0.98	0.36	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3424	1/1	0.98	0.10	48,48,48,48	0
58	MG	14	3040	1/1	0.98	0.35	59,59,59,59	0
58	MG	14	3041	1/1	0.98	0.35	54,54,54,54	0
58	MG	29	303	1/1	0.98	0.40	52,52,52,52	0
58	MG	14	3043	1/1	0.98	0.38	57,57,57,57	0
58	MG	14	3044	1/1	0.98	0.51	64,64,64,64	0
58	MG	14	3046	1/1	0.98	0.28	66,66,66,66	0
58	MG	1H	3425	1/1	0.98	0.12	63,63,63,63	0
58	MG	14	3327	1/1	0.98	0.16	59,59,59,59	0
58	MG	14	3113	1/1	0.98	0.41	73,73,73,73	0
58	MG	14	3048	1/1	0.98	0.29	90,90,90,90	0
58	MG	14	3331	1/1	0.98	0.14	63,63,63,63	0
58	MG	1H	3076	1/1	0.98	0.41	65,65,65,65	0
58	MG	14	3050	1/1	0.98	0.51	59,59,59,59	0
59	SF4	3E	301	8/8	0.98	0.17	86,99,103,105	0
58	MG	1H	3427	1/1	0.98	0.07	72,72,72,72	0
60	ZN	5A	101	1/1	0.98	0.08	142,142,142,142	0
58	MG	1H	3339	1/1	0.98	0.43	48,48,48,48	0
58	MG	14	3354	1/1	0.99	0.10	70,70,70,70	0
58	MG	1H	3054	1/1	0.99	0.24	52,52,52,52	0
58	MG	1H	3059	1/1	0.99	0.24	49,49,49,49	0
58	MG	14	3357	1/1	0.99	0.22	76,76,76,76	0
58	MG	1H	3372	1/1	0.99	0.11	62,62,62,62	0
58	MG	13	1638	1/1	0.99	0.26	59,59,59,59	0
58	MG	14	3128	1/1	0.99	0.45	58,58,58,58	0
58	MG	1H	3147	1/1	0.99	0.31	64,64,64,64	0
58	MG	14	3298	1/1	0.99	0.90	64,64,64,64	0
58	MG	14	3329	1/1	0.99	0.17	56,56,56,56	0
58	MG	1H	3248	1/1	0.99	0.50	74,74,74,74	0
58	MG	1H	3138	1/1	0.99	0.41	58,58,58,58	0
58	MG	1H	3411	1/1	0.99	0.12	69,69,69,69	0
58	MG	13	1709	1/1	0.99	0.07	92,92,92,92	0
58	MG	1H	3378	1/1	0.99	0.16	53,53,53,53	0
58	MG	1H	3363	1/1	0.99	0.06	68,68,68,68	0
58	MG	1H	3099	1/1	0.99	0.20	55,55,55,55	0
58	MG	1H	3351	1/1	0.99	0.08	46,46,46,46	0
58	MG	14	3138	1/1	0.99	0.32	45,45,45,45	0
58	MG	14	3339	1/1	0.99	0.11	82,82,82,82	0
58	MG	1G	1623	1/1	0.99	0.50	62,62,62,62	0
58	MG	1H	3435	1/1	0.99	0.13	56,56,56,56	0
58	MG	1H	3352	1/1	0.99	0.12	61,61,61,61	0
58	MG	1H	3383	1/1	0.99	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3092	1/1	0.99	0.26	49,49,49,49	0
58	MG	14	3042	1/1	0.99	0.54	70,70,70,70	0
58	MG	14	3091	1/1	0.99	0.43	86,86,86,86	0
58	MG	1H	3053	1/1	0.99	0.34	50,50,50,50	0
58	MG	2L	101	1/1	0.99	0.56	73,73,73,73	0
58	MG	14	3045	1/1	0.99	0.33	58,58,58,58	0
58	MG	1G	1608	1/1	0.99	0.18	89,89,89,89	0
59	SF4	32	301	8/8	0.99	0.15	115,123,133,136	0
60	ZN	5I	101	1/1	0.99	0.13	102,102,102,102	0
58	MG	1H	3094	1/1	0.99	0.37	64,64,64,64	0
58	MG	14	3320	1/1	0.99	0.18	64,64,64,64	0
58	MG	14	3097	1/1	0.99	0.22	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.