wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 12:37 am BST

PDB ID	:	5E7K / pdb_00005e7k
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 (1)) were used in the production of this report:

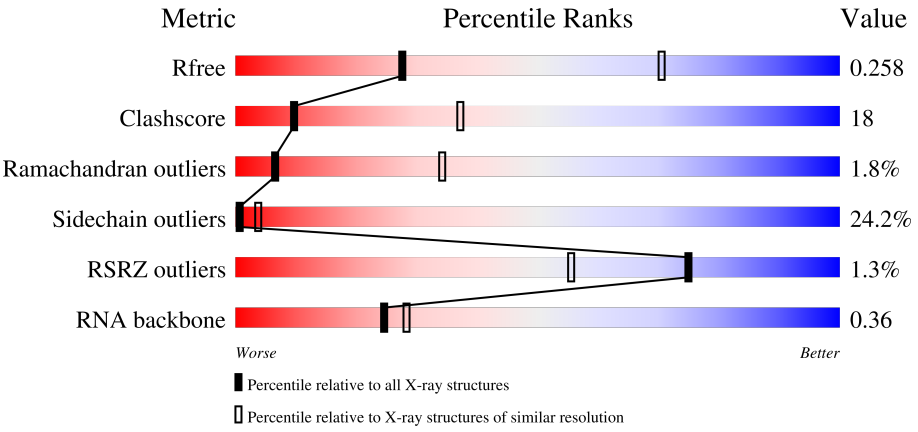
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (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	39% 45% 15% .
1	1G	1522	38% 46% 15% .
2	12	256	% 34% 34% 12% . 18%
2	1E	256	30% 41% 18% . 10%

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Mol	Chain	Length	Quality of chain
3	22	239	38% 37% 7% 18%
3	2E	239	44% 34% 8% 14%
4	32	209	31% 56% 12%
4	3E	209	44% 41% 12%
5	42	162	46% 38% 7% 9%
5	4E	162	45% 39% 8% 8%
6	52	101	54% 37% 9%
6	5E	101	47% 43% 9%
7	62	156	5% 40% 42% 7% 12%
7	6E	156	56% 32% 10%
8	72	138	53% 35% 12%
8	7E	138	38% 43% 18%
9	82	128	35% 44% 14% 5%
9	8E	128	43% 47% 8%
10	1A	105	34% 30% 12% 24%
10	1I	105	43% 31% 11% 13%
11	2A	129	4% 47% 31% 10% 12%
11	2I	129	31% 37% 16% 14%
12	3A	132	9% 39% 40% 13% 8%
12	3I	132	54% 27% 10% 8%
13	4A	126	32% 41% 13% 12%
13	4I	126	44% 37% 12% 6%
14	5A	61	3% 43% 41% 13%
14	5I	61	44% 34% 16%
15	6A	89	45% 47% 7%

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Mol	Chain	Length	Quality of chain
15	6I	89	45% 42% 10%
16	7A	88	45% 35% 14% 5%
16	7I	88	26% 56% 13% 6%
17	8A	105	52% 32% 10% 6%
17	8I	105	2% 45% 39% 11% 5%
18	9A	88	2% 36% 30% 10% 24%
18	9I	88	2% 33% 31% 13% 23%
19	AA	93	2% 25% 31% 11% 33%
19	AI	93	38% 34% 13% 13%
20	BA	106	50% 35% 7% 7%
20	BI	106	34% 45% 12% 8%
21	1B	27	37% 44% 19%
21	1F	27	52% 33% 15%
22	1K	75	% 23% 51% 21% 5%
23	2K	77	% 44% 32% 22%
23	2L	77	35% 43% 19%
24	3K	76	5% 17% 50% 33%
25	4K	27	4% 22% 22% 26% 30%
25	4L	27	26% 15% 26% 33%
26	14	2917	40% 44% 13%
26	1H	2917	41% 41% 14%
27	16	122	52% 34% 14%
27	1J	122	% 36% 43% 20%
28	71	229	2% 22% 24% 10% 42%
28	79	229	15% 7% 75%

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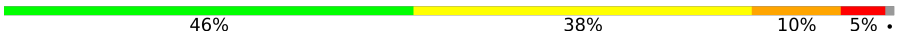
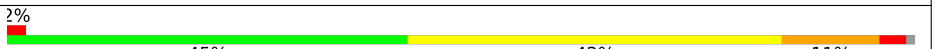
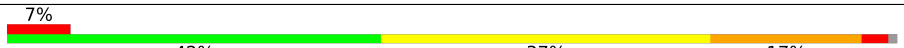
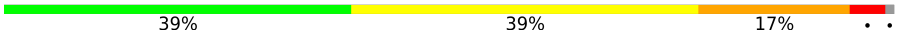
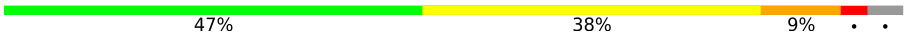
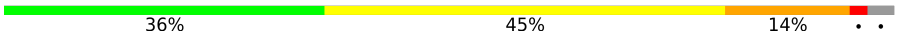
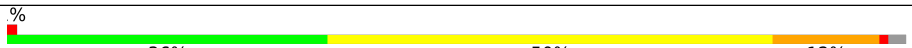
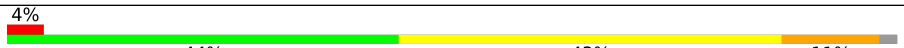
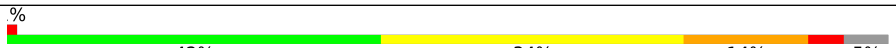
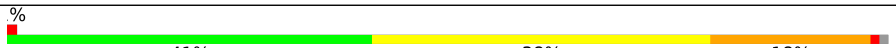
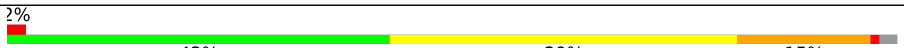
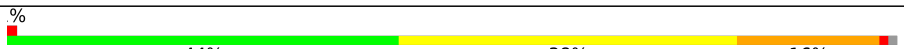
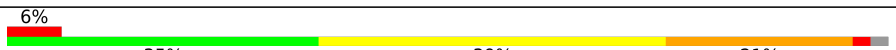
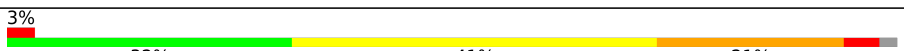
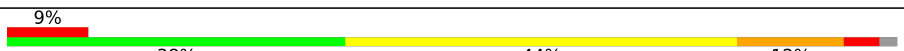
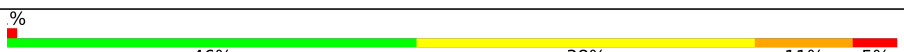
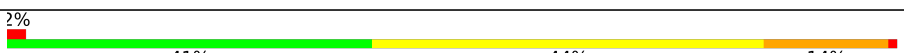
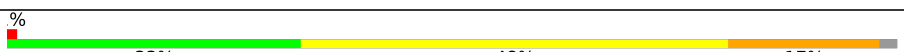
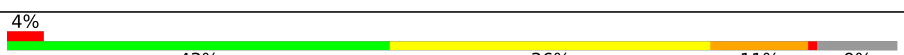
Mol	Chain	Length	Quality of chain
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	

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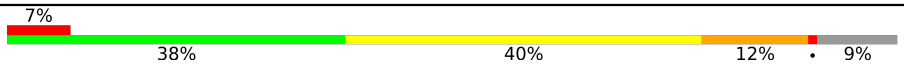
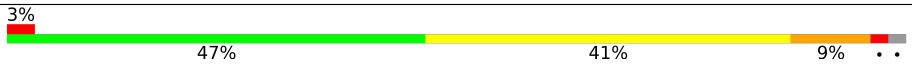
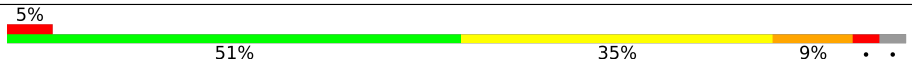
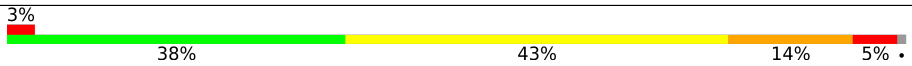
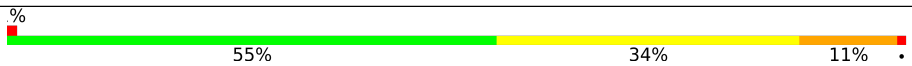
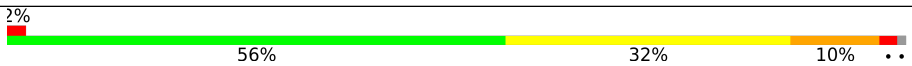
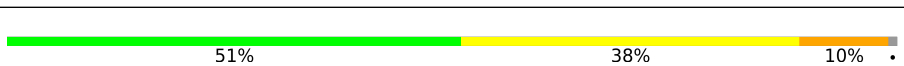
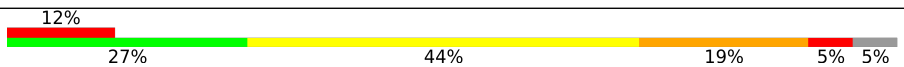
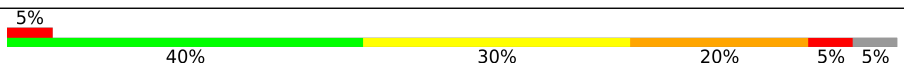
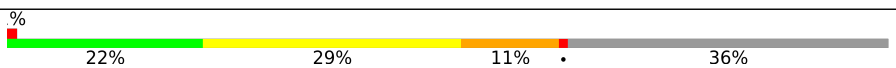
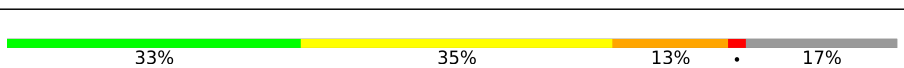
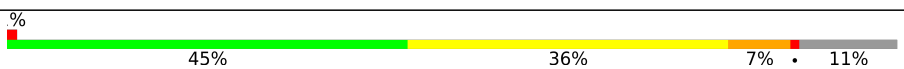
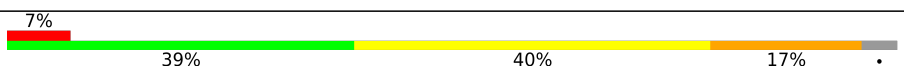
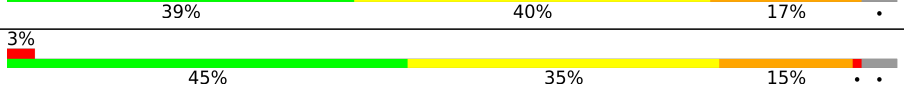
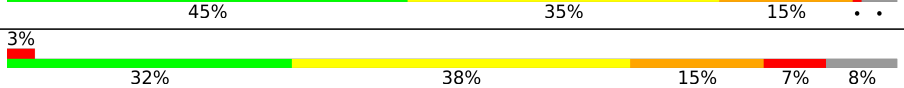
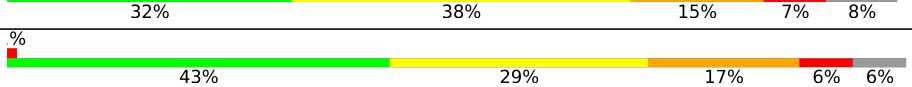
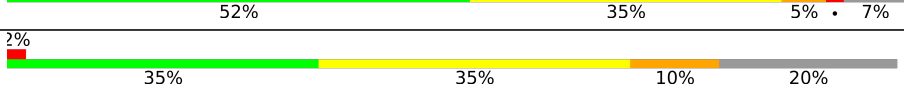
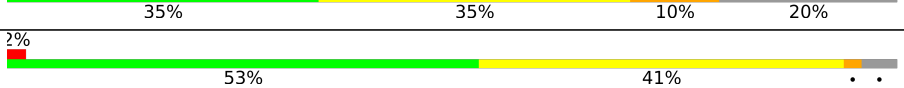
Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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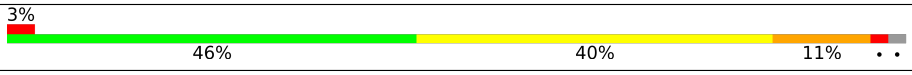
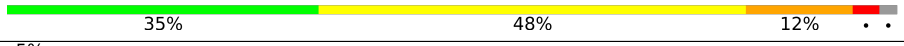
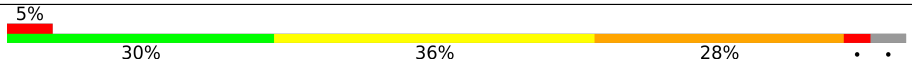
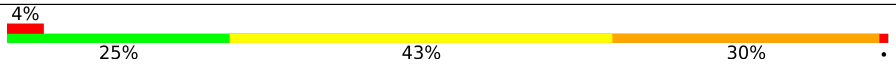
Mol	Chain	Length	Quality of chain
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3089	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1644	-	-	-	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
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

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

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
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			

- Molecule 24 is a RNA chain called tRNALys.

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

- Molecule 25 is a RNA chain called mRNA.

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

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	11	273	Total C N O S 2120 1338 421 358 3	0	0	0
29	19	274	Total C N O S 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
30	21	203	Total C N O S 1558 985 298 269 6	0	0	0
30	29	204	Total C N O S 1563 988 299 270 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	31	202	Total C N O S 1585 1011 297 275 2	0	0	0
31	39	204	Total C N O S 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
32	41	179	Total C N O S 1457 931 265 257 4	0	0	0
32	49	179	Total C N O S 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
33	51	171	Total C N O S 1312 832 246 233 1	0	0	0
33	59	73	Total C N O 568 356 116 96	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNALys.

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

- Molecule 57 is a RNA chain called tRNALys.

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

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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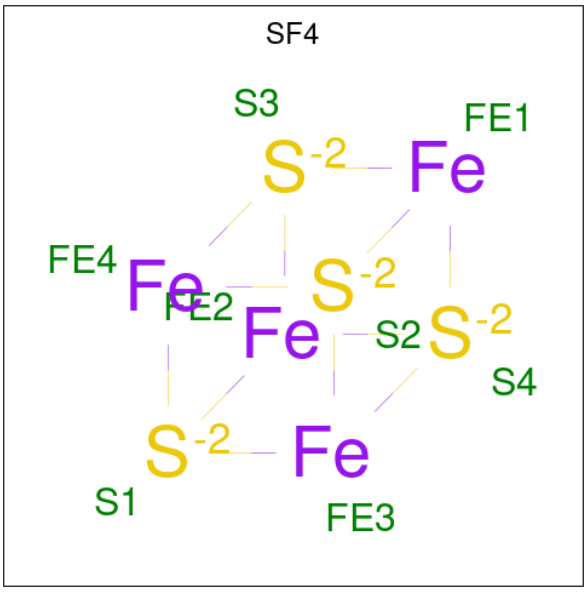
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	98	1	Total Mg 1 1	0	0
58	I8	3	Total Mg 3 3	0	0
58	J8	1	Total Mg 1 1	0	0
58	L8	1	Total Mg 1 1	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	90	Total Mg 90 90	0	0
58	6A	1	Total Mg 1 1	0	0
58	2L	2	Total Mg 2 2	0	0
58	14	399	Total Mg 399 399	0	0
58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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: 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

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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

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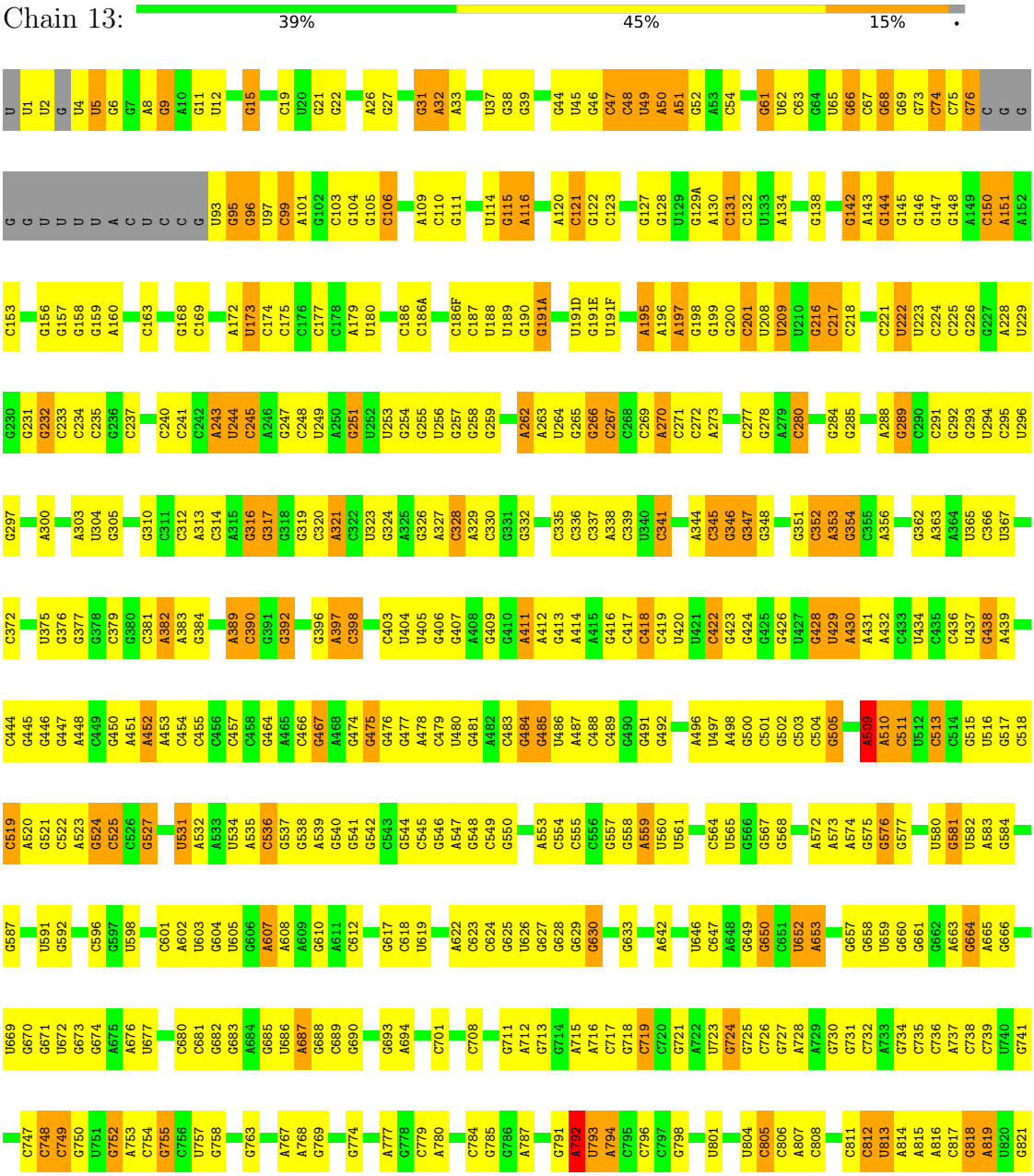
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1J	6	Total O 6 6	0	0
61	19	8	Total O 8 8	0	0
61	29	2	Total O 2 2	0	0
61	39	5	Total O 5 5	0	0
61	35	1	Total O 1 1	0	0
61	55	1	Total O 1 1	0	0
61	A5	1	Total O 1 1	0	0
61	H5	2	Total O 2 2	0	0

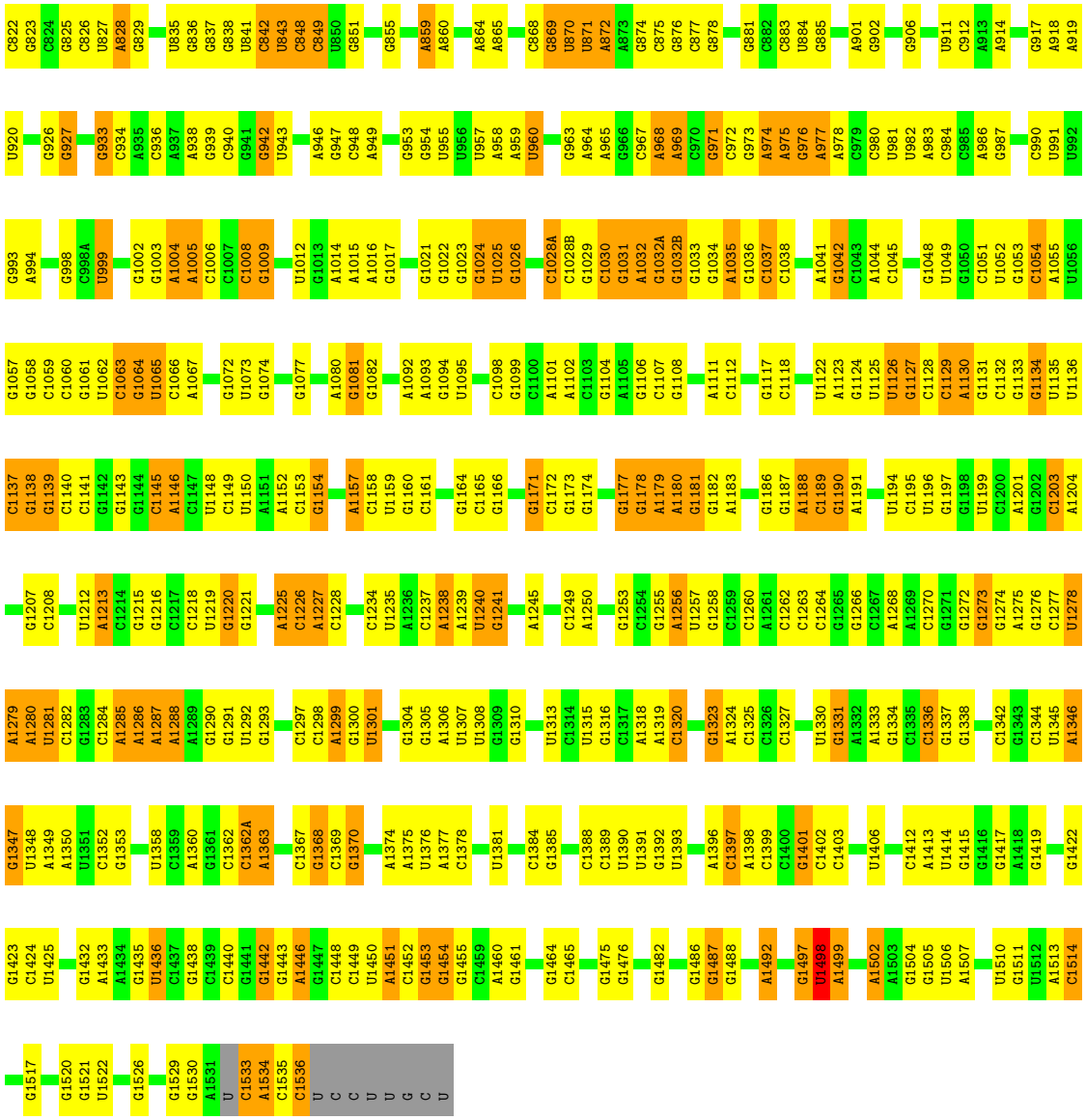
3 Residue-property plots (i)

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

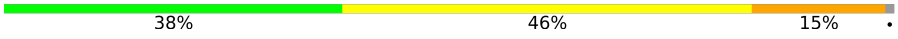
Chain 13:

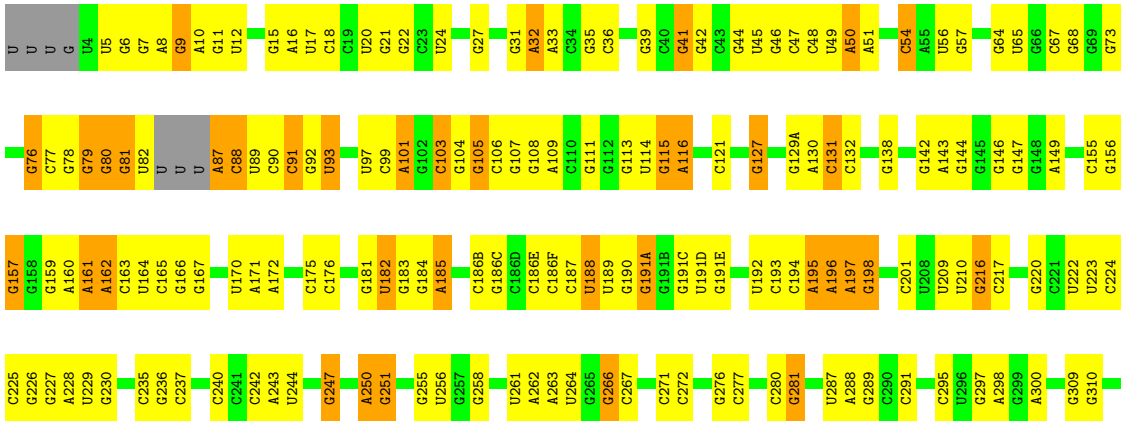


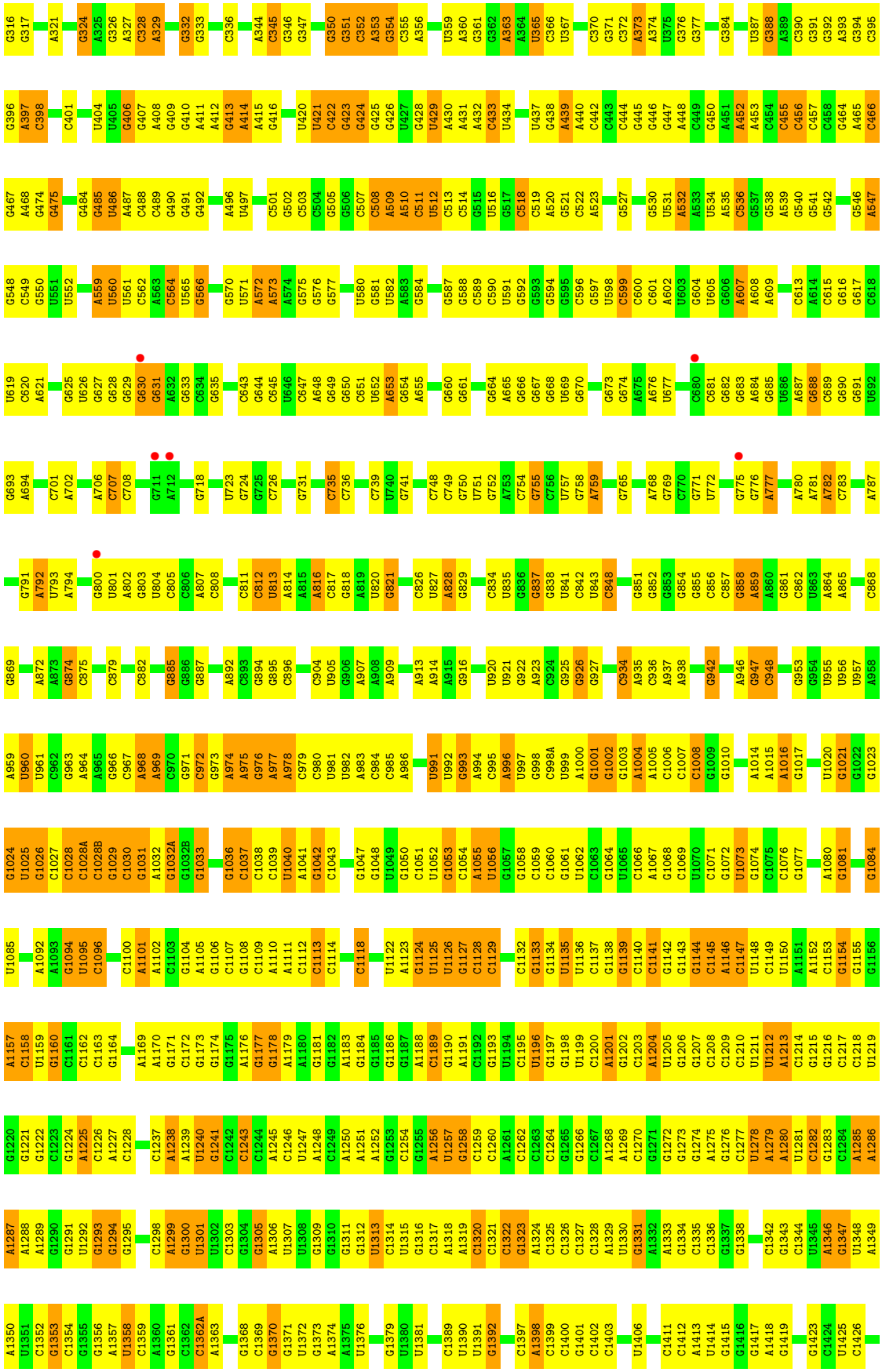


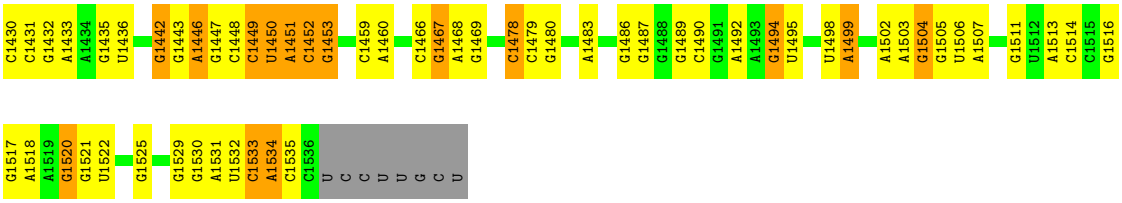
• Molecule 1: 16S rRNA

Chain 1G:



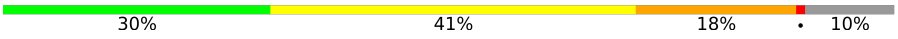


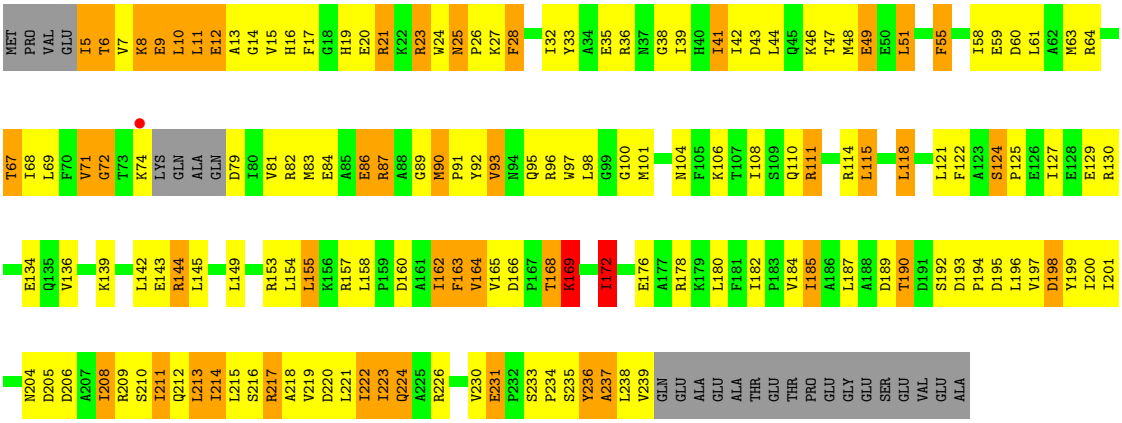




• Molecule 2: 30S ribosomal protein S2

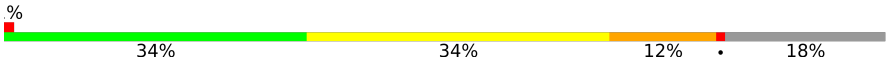
Chain 1E:

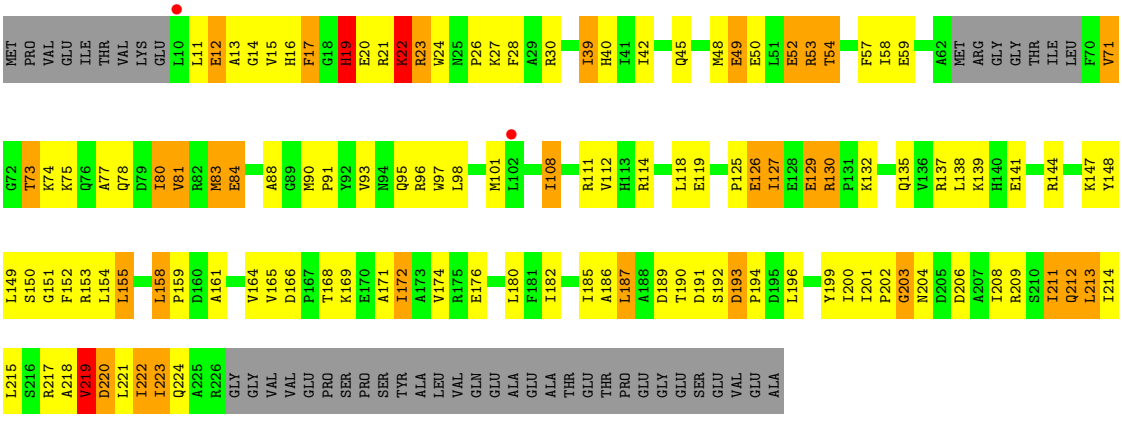




• Molecule 2: 30S ribosomal protein S2

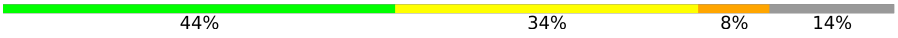
Chain 12:

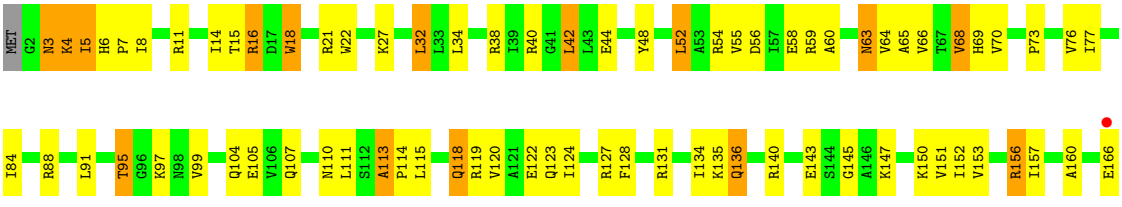


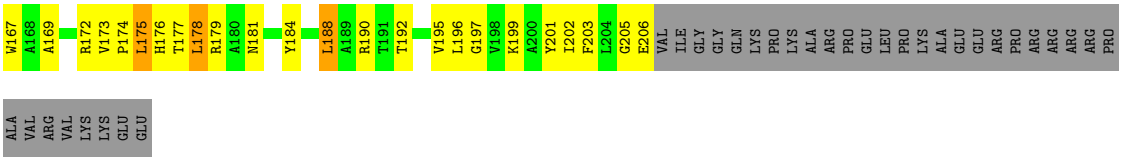


• Molecule 3: 30S ribosomal protein S3

Chain 2E:



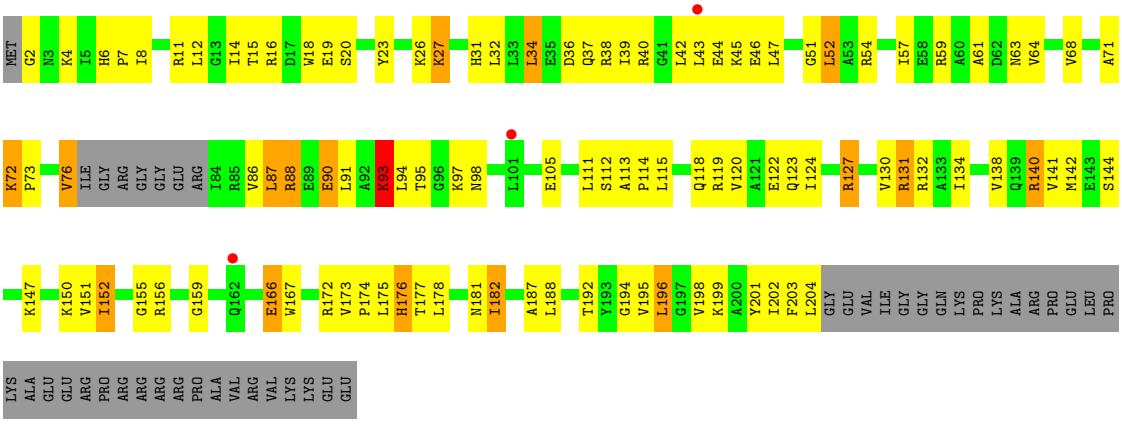




• Molecule 3: 30S ribosomal protein S3

Chain 22:

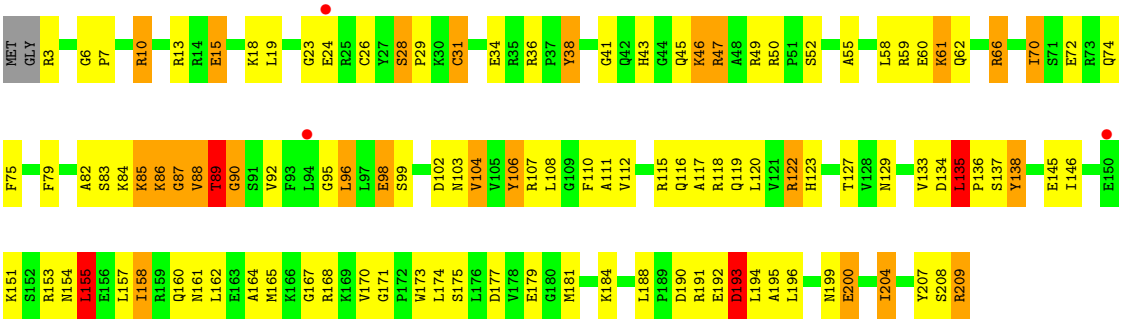




• Molecule 4: 30S ribosomal protein S4

Chain 3E:

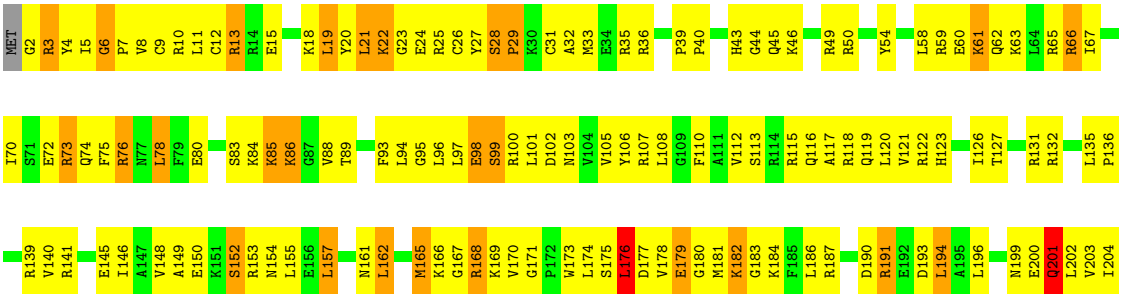




• Molecule 4: 30S ribosomal protein S4

Chain 32:



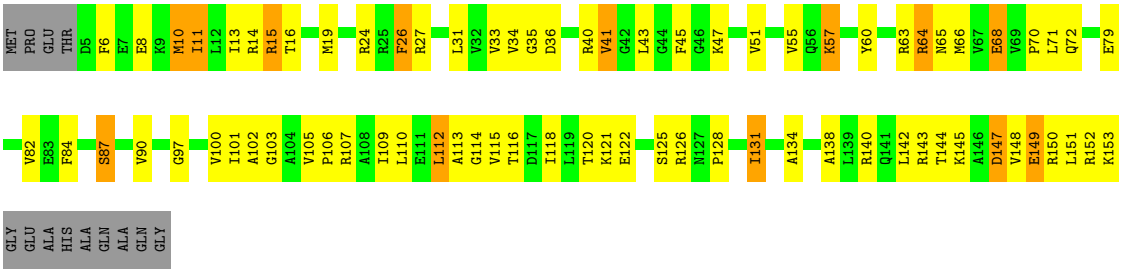




• Molecule 5: 30S ribosomal protein S5

Chain 4E:





• Molecule 5: 30S ribosomal protein S5

Chain 42:

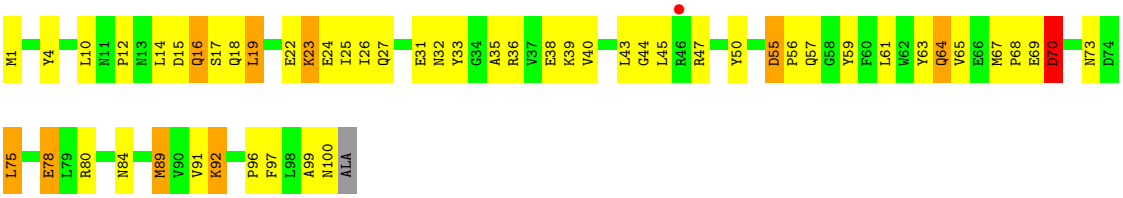




• Molecule 6: 30S ribosomal protein S6

Chain 5E:

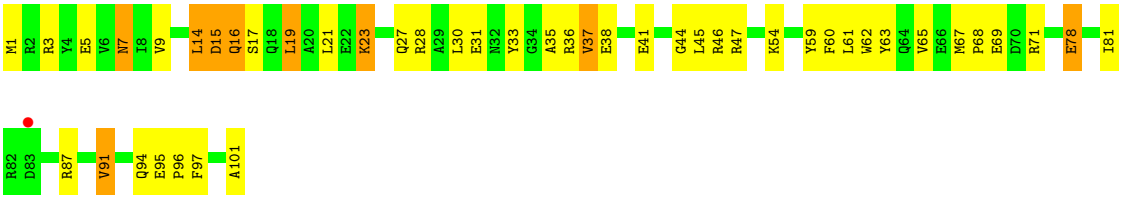




• Molecule 6: 30S ribosomal protein S6

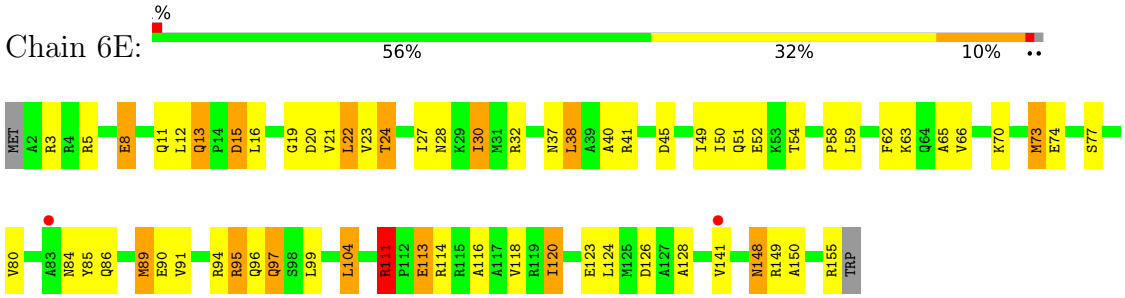
Chain 52:





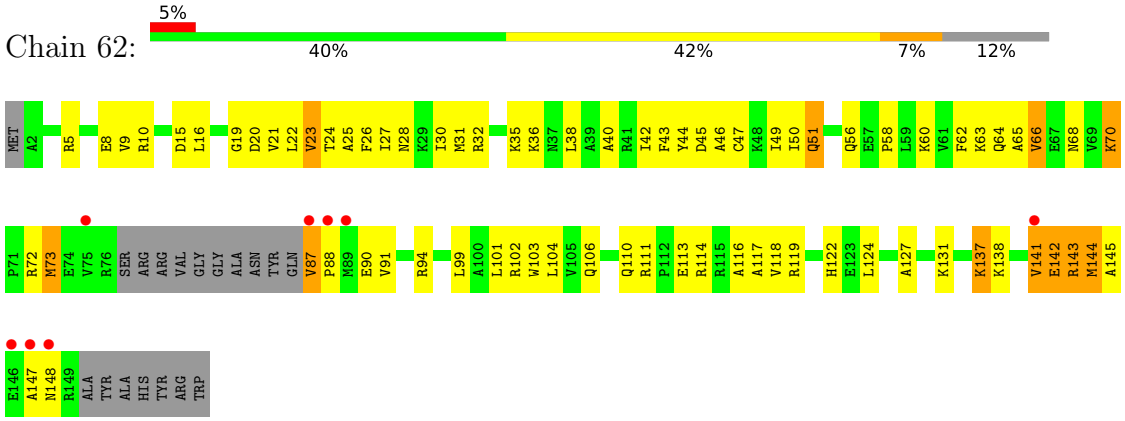
• Molecule 7: 30S ribosomal protein S7

Chain 6E:



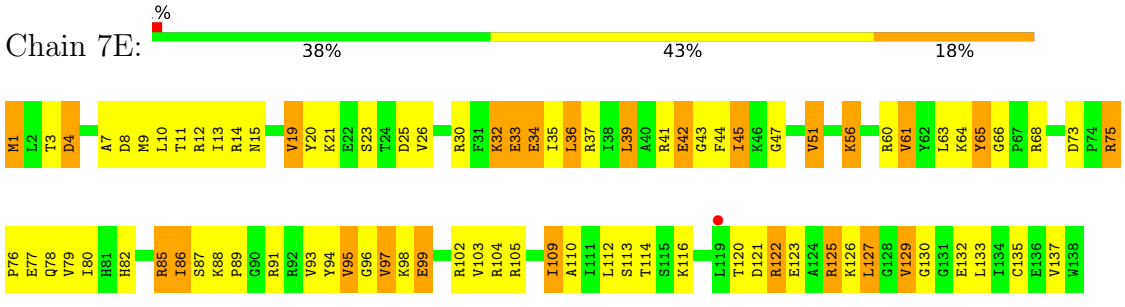
• Molecule 7: 30S ribosomal protein S7

Chain 62:



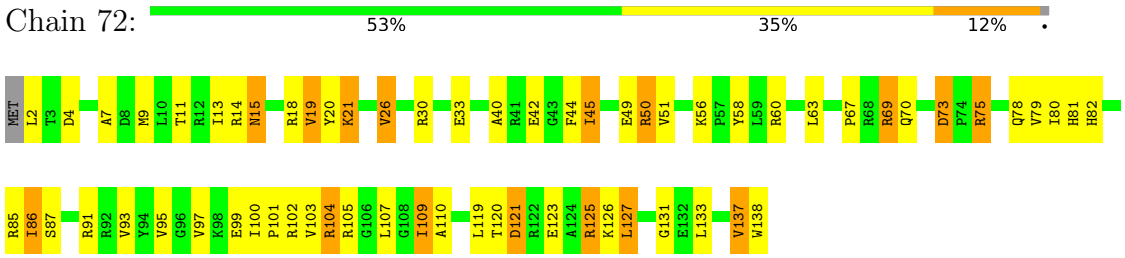
• Molecule 8: 30S ribosomal protein S8

Chain 7E:



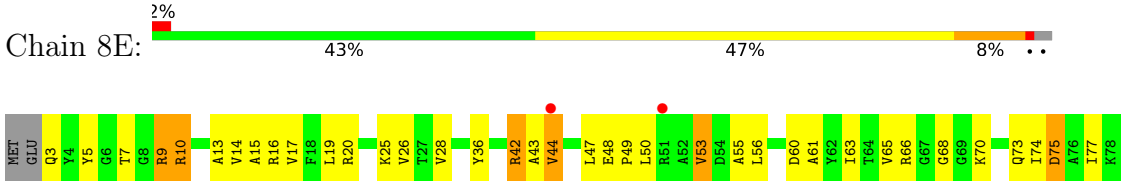
• Molecule 8: 30S ribosomal protein S8

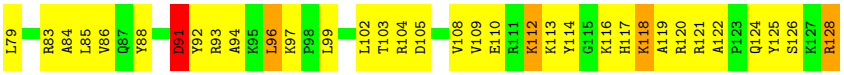
Chain 72:



• Molecule 9: 30S ribosomal protein S9

Chain 8E:

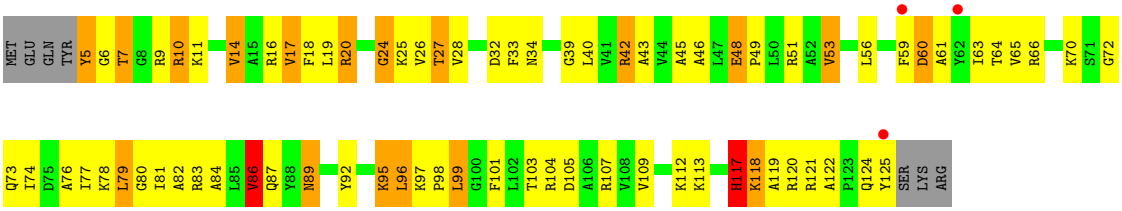




• Molecule 9: 30S ribosomal protein S9

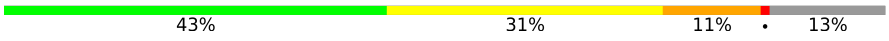
Chain 82:





• Molecule 10: 30S ribosomal protein S10

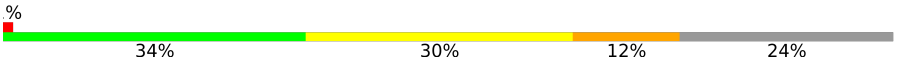
Chain 1I:

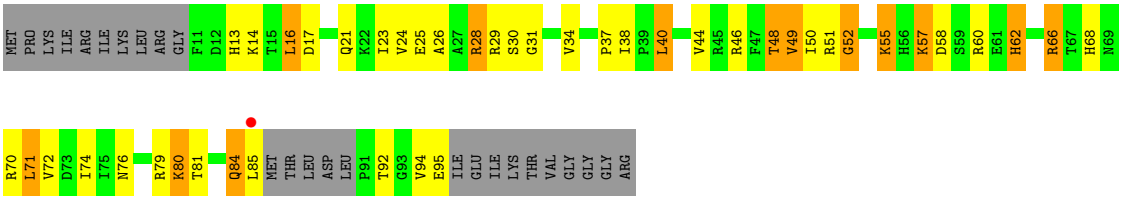




• Molecule 10: 30S ribosomal protein S10

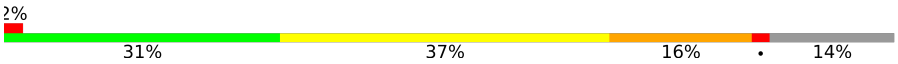
Chain 1A:

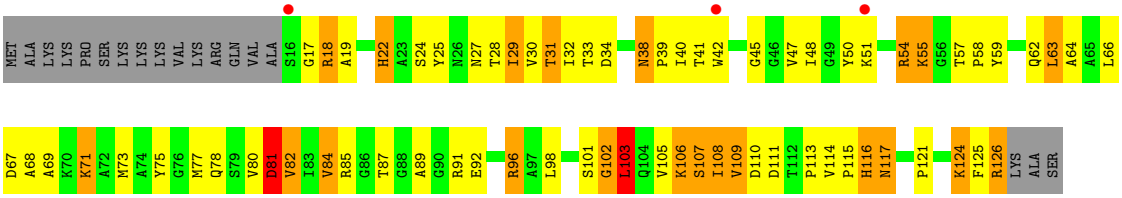




• Molecule 11: 30S ribosomal protein S11

Chain 2I:

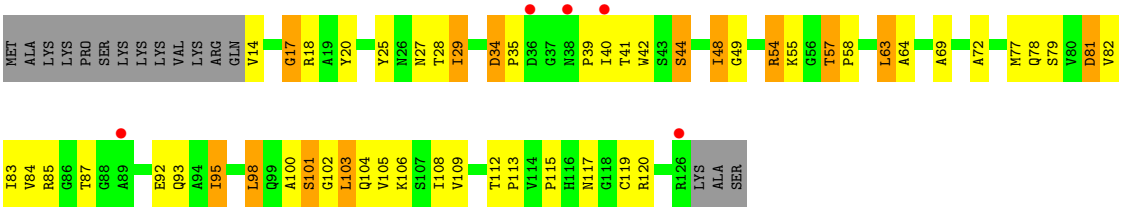




• Molecule 11: 30S ribosomal protein S11

Chain 2A:

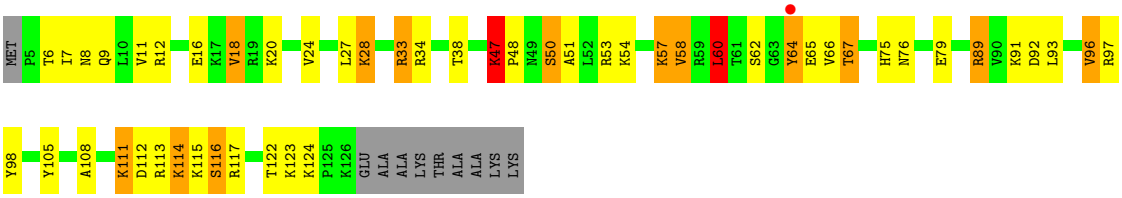




• Molecule 12: 30S ribosomal protein S12

Chain 3I:

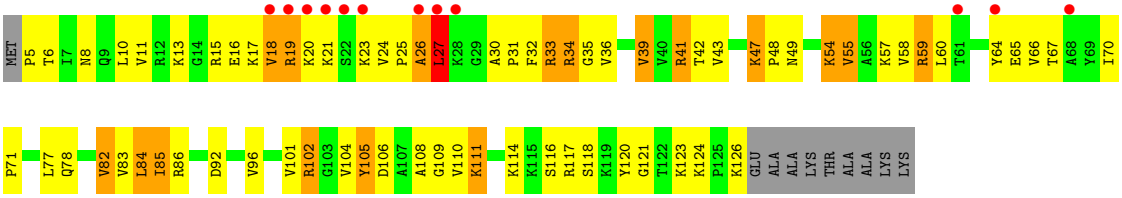




• Molecule 12: 30S ribosomal protein S12

Chain 3A:

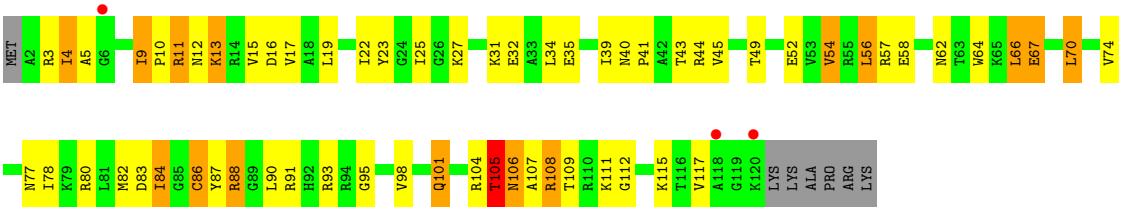




• Molecule 13: 30S ribosomal protein S13

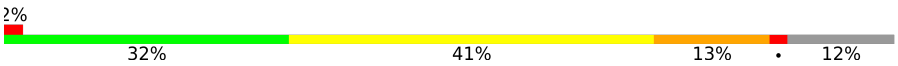
Chain 4I:

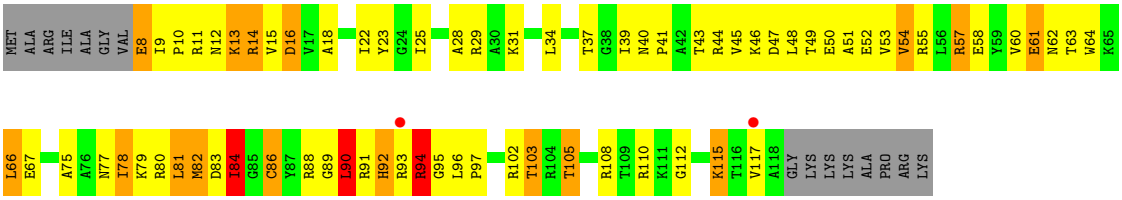




• Molecule 13: 30S ribosomal protein S13

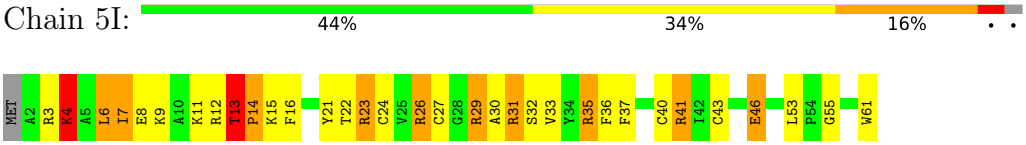
Chain 4A:





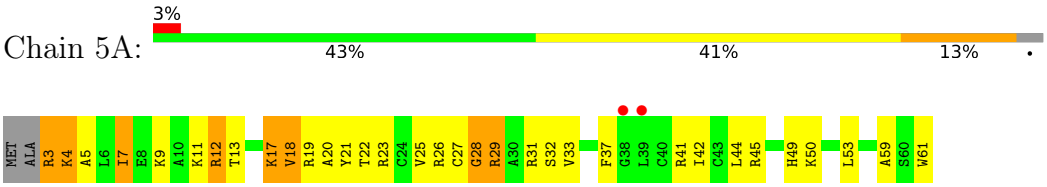
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



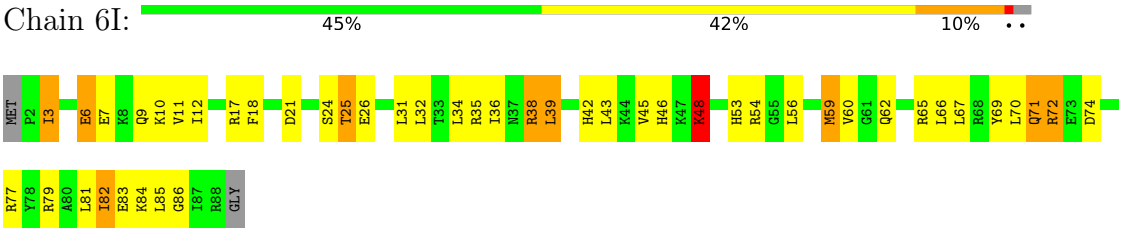
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



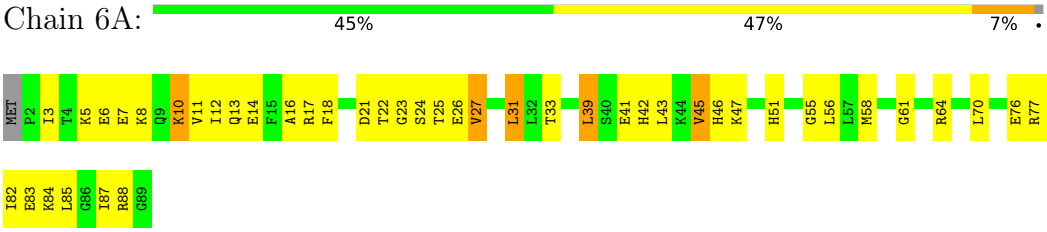
• Molecule 15: 30S ribosomal protein S15

Chain 6I:



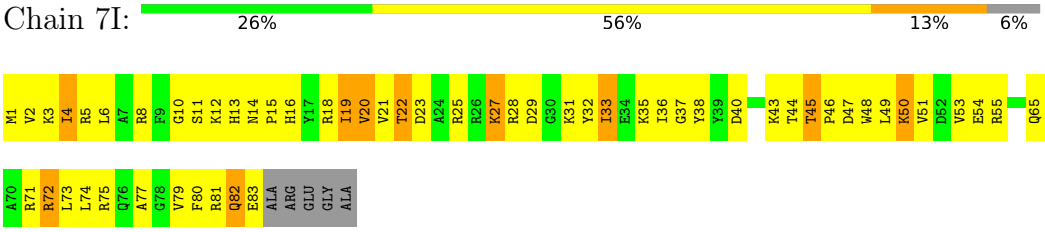
• Molecule 15: 30S ribosomal protein S15

Chain 6A:



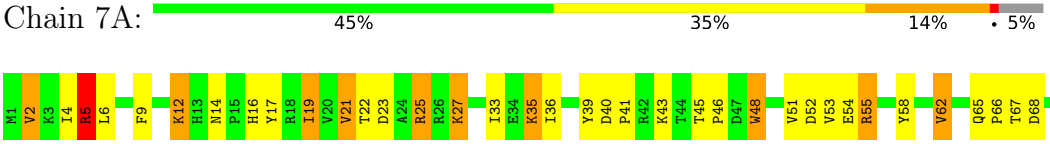
• Molecule 16: 30S ribosomal protein S16

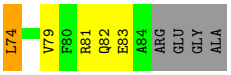
Chain 7I:



• Molecule 16: 30S ribosomal protein S16

Chain 7A:

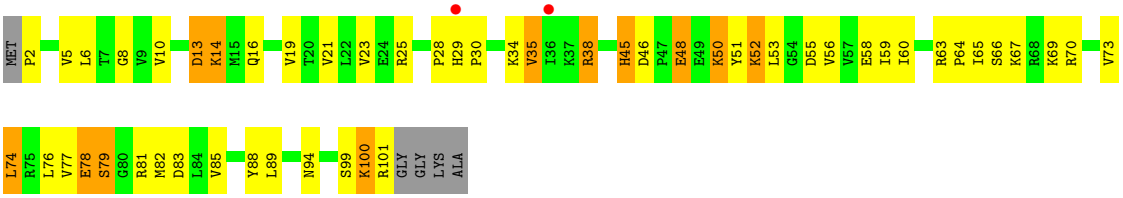




• Molecule 17: 30S ribosomal protein S17

Chain 8I:

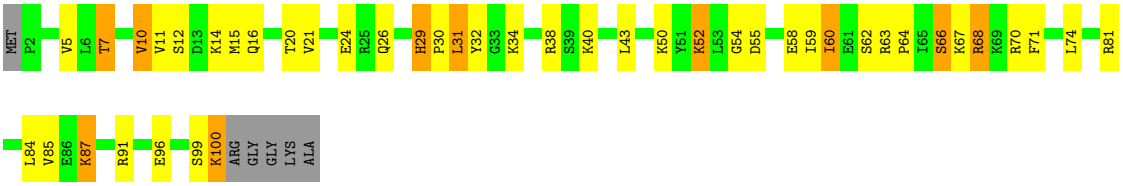




• Molecule 17: 30S ribosomal protein S17

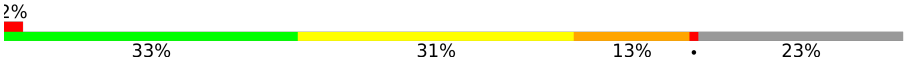
Chain 8A:

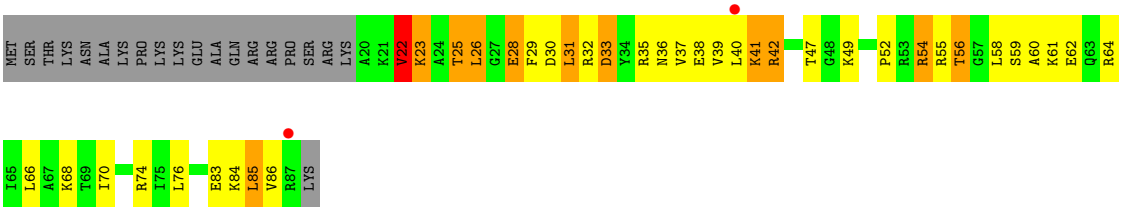




• Molecule 18: 30S ribosomal protein S18

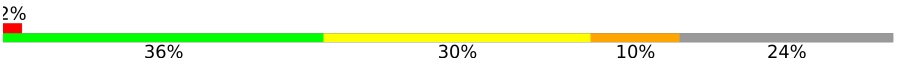
Chain 9I:

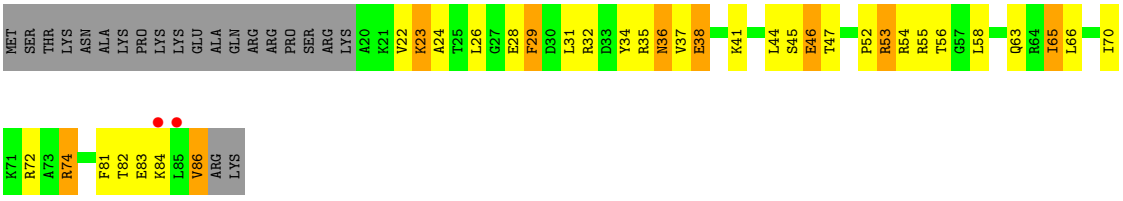




• Molecule 18: 30S ribosomal protein S18

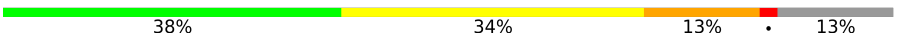
Chain 9A:

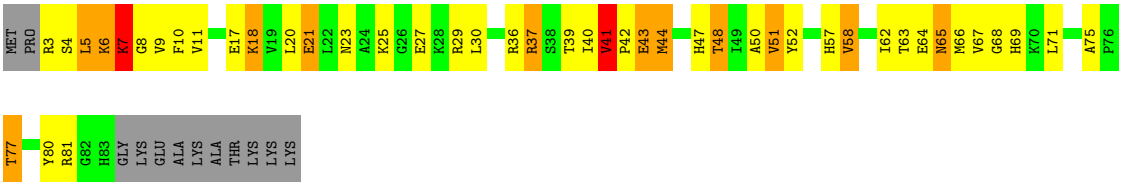




• Molecule 19: 30S ribosomal protein S19

Chain AI:

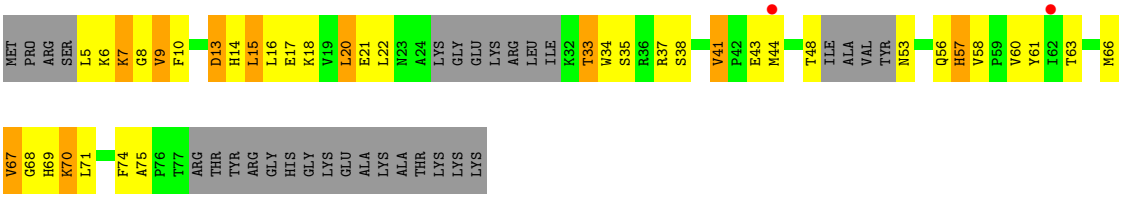




• Molecule 19: 30S ribosomal protein S19

Chain AA:

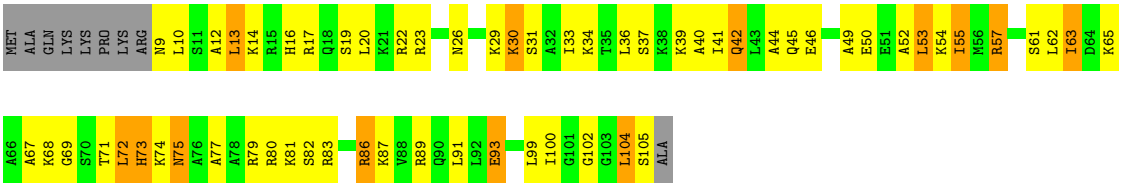




• Molecule 20: 30S ribosomal protein S20

Chain BI:

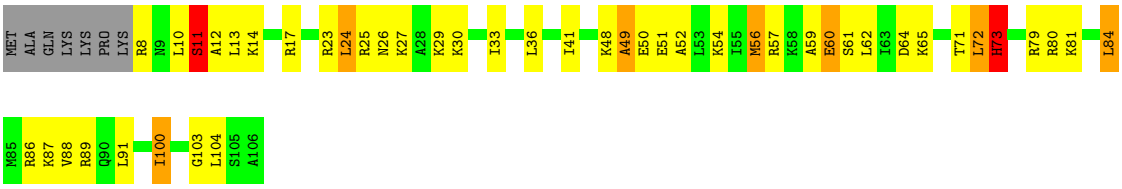




• Molecule 20: 30S ribosomal protein S20

Chain BA:

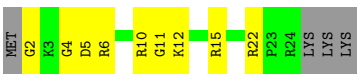




• Molecule 21: 30S ribosomal protein Thx

Chain 1F:





• Molecule 21: 30S ribosomal protein Thx

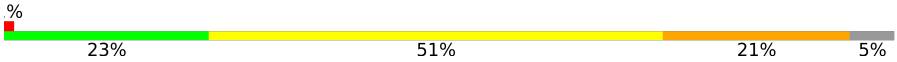
Chain 1B:

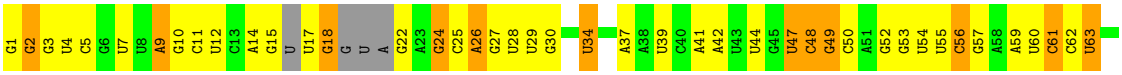




• Molecule 22: tRNALys

Chain 1K:



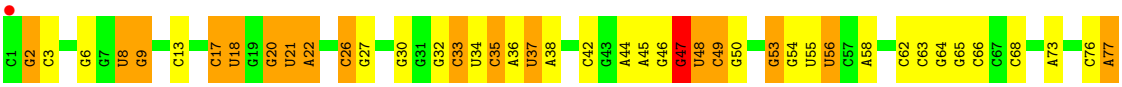




• Molecule 23: tRNAfMet

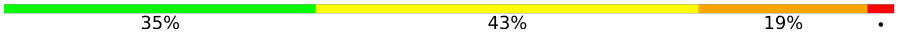
Chain 2K:

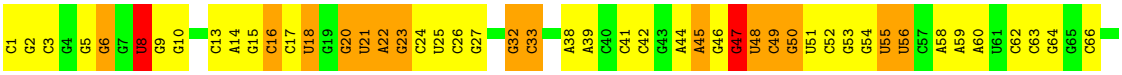




• Molecule 23: tRNAfMet

Chain 2L:



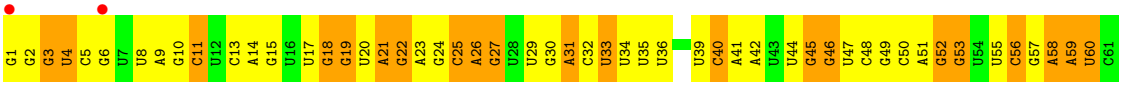


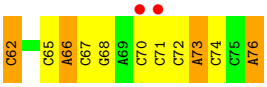


• Molecule 24: tRNALys

Chain 3K:



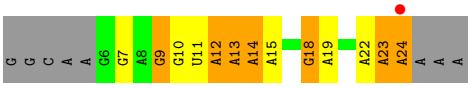




• Molecule 25: mRNA

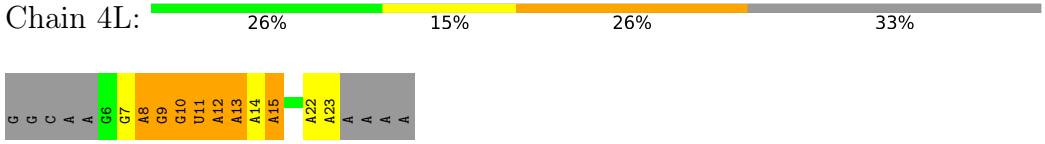
Chain 4K:





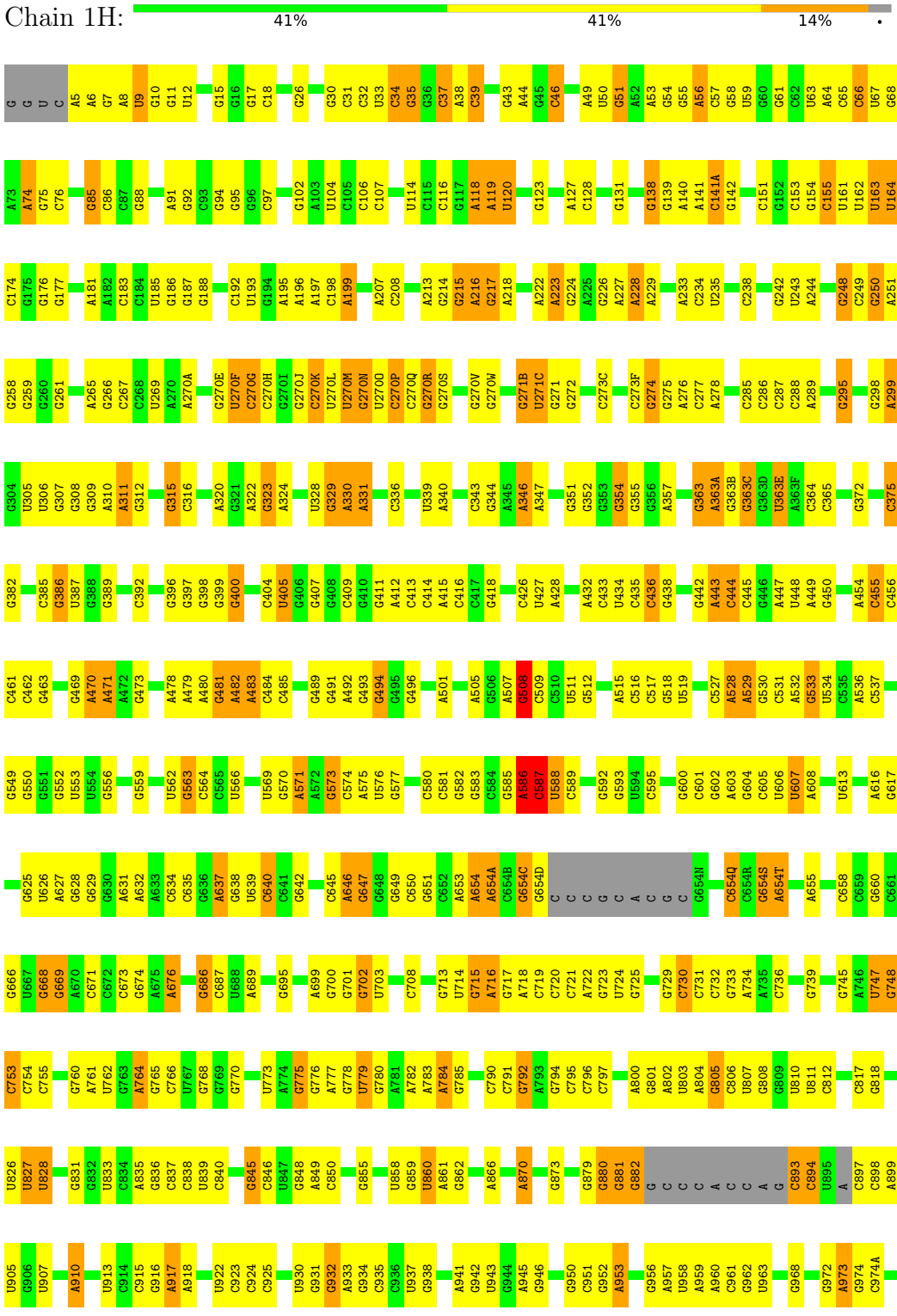
• Molecule 25: mRNA

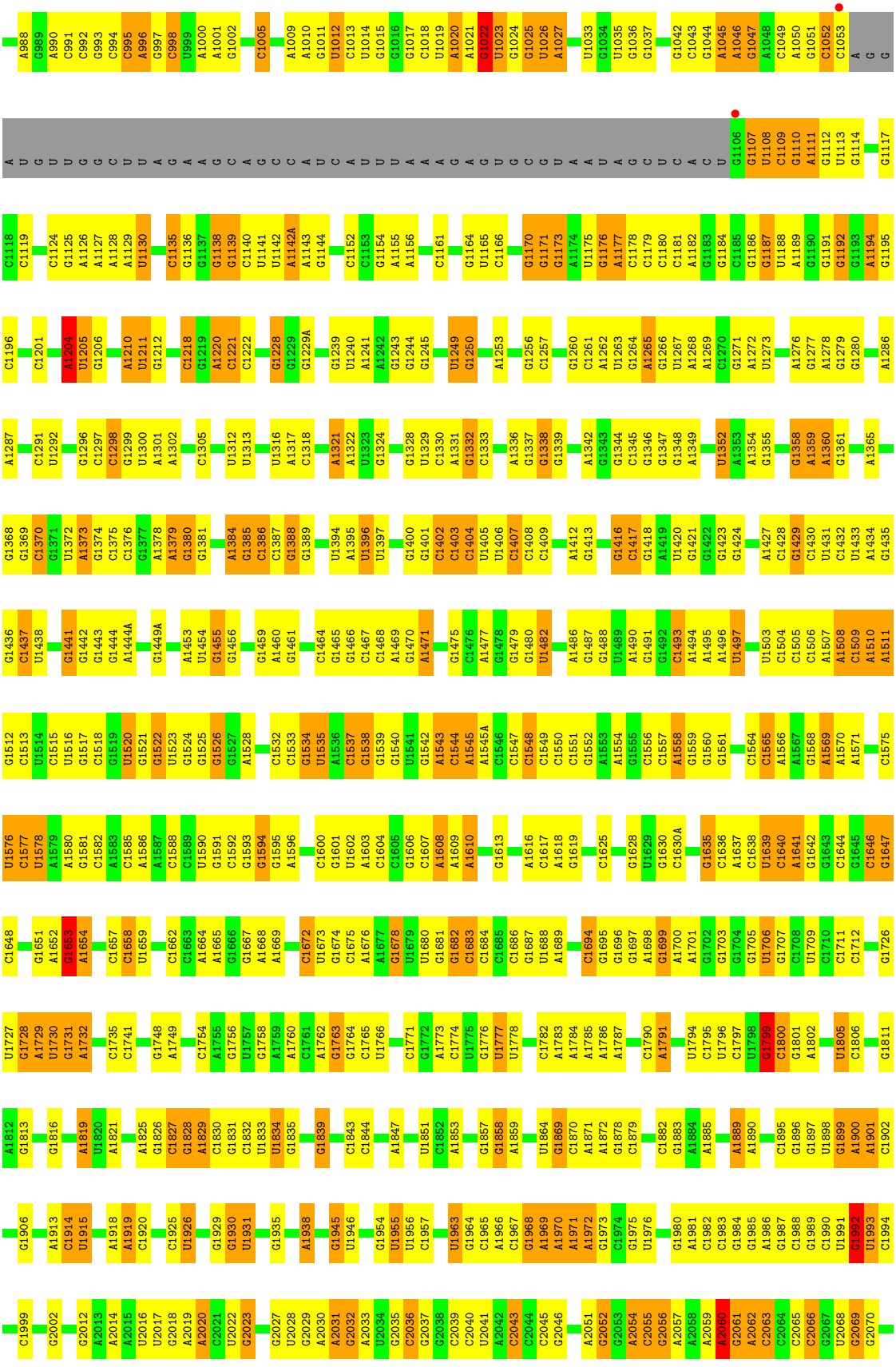
Chain 4L:



• Molecule 26: 23S rRNA

Chain 1H:

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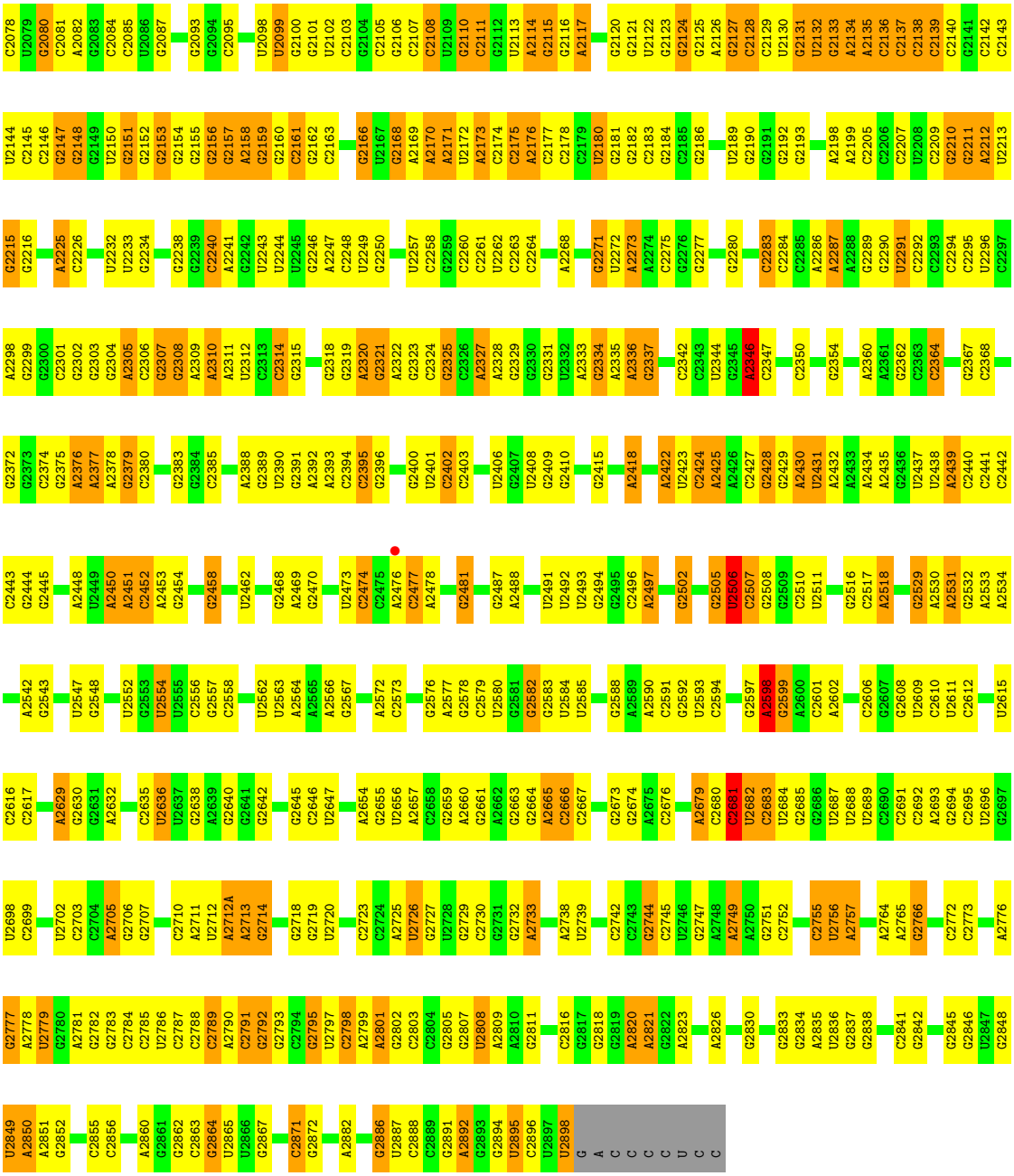
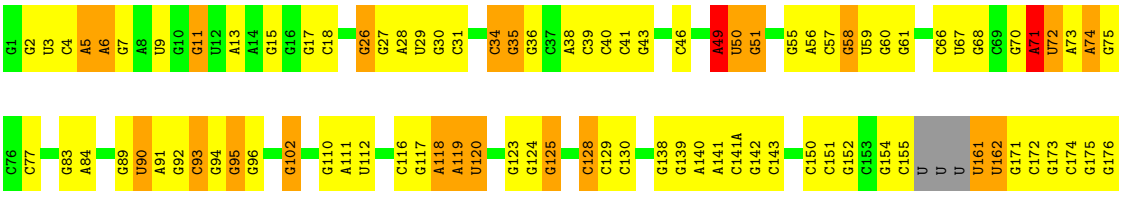
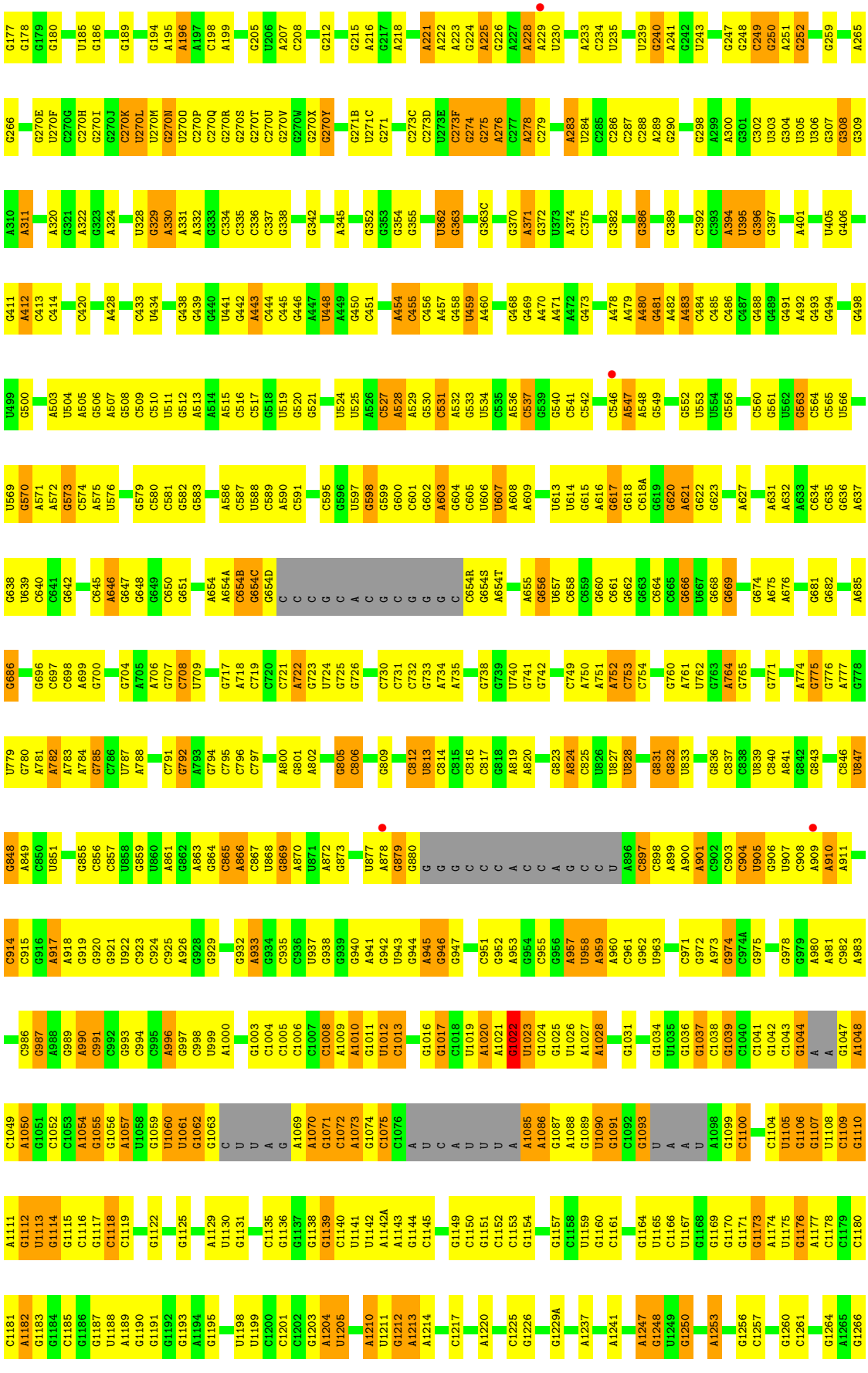


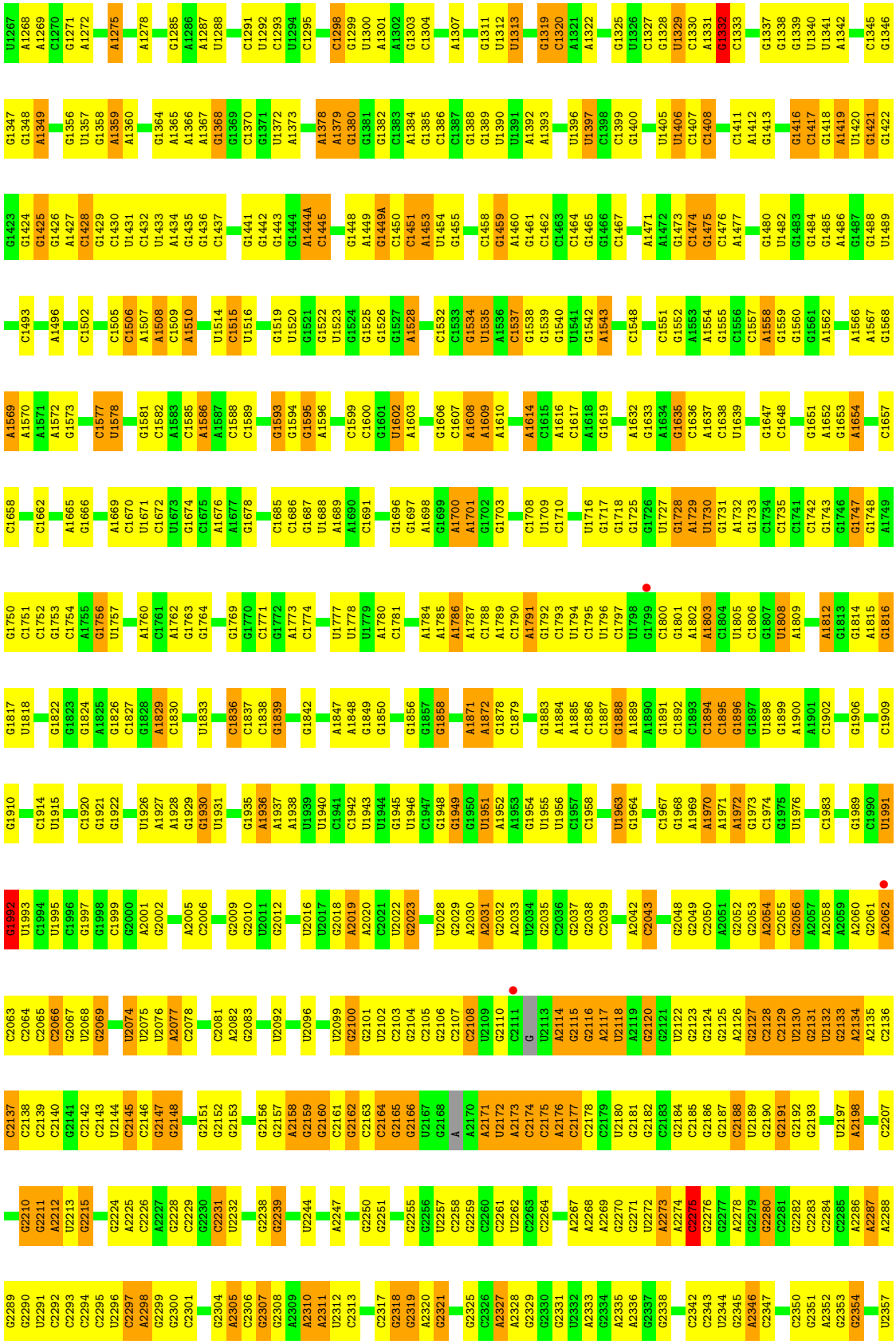
• Molecule 26: 23S rRNA

Chain 14:





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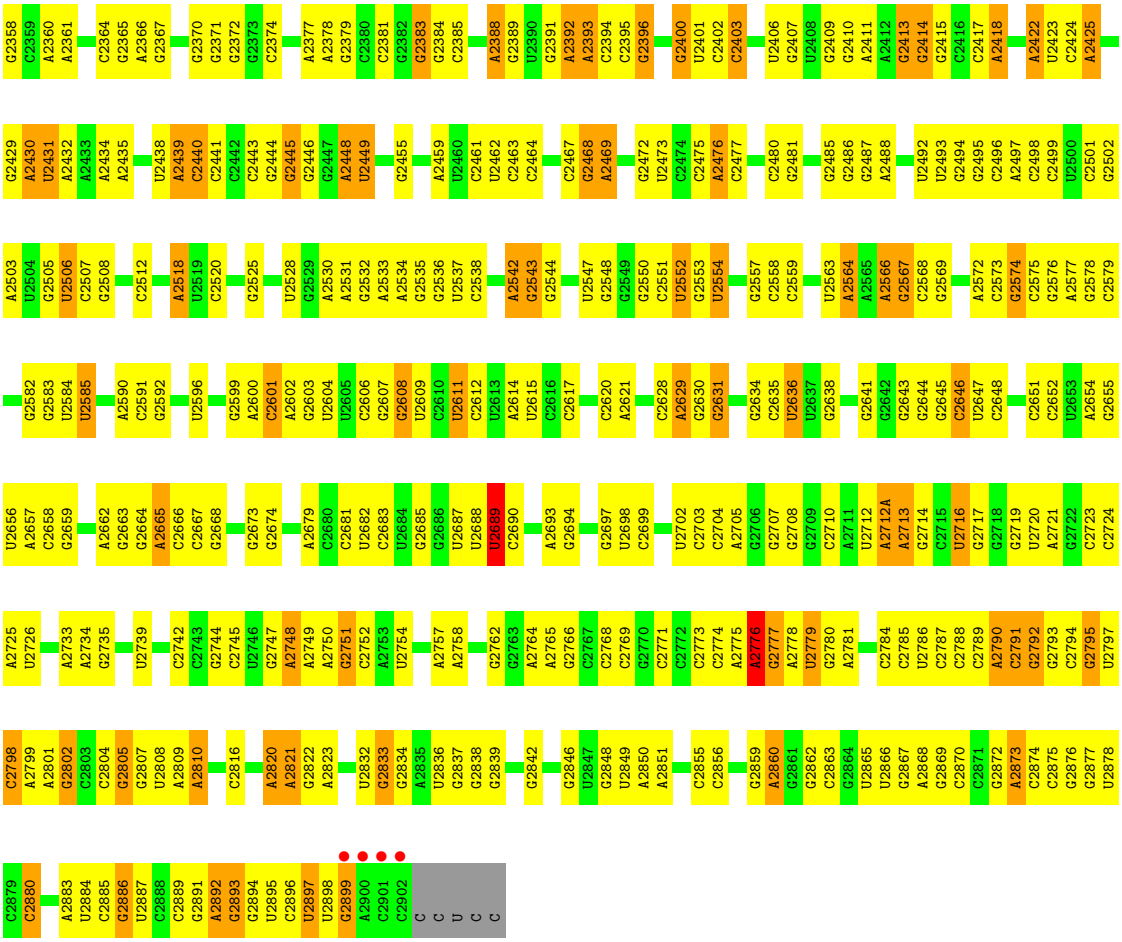
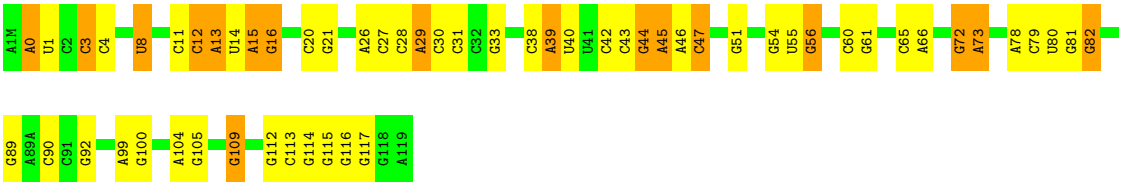


• Molecule 27: 5S rRNA

Chain 16:

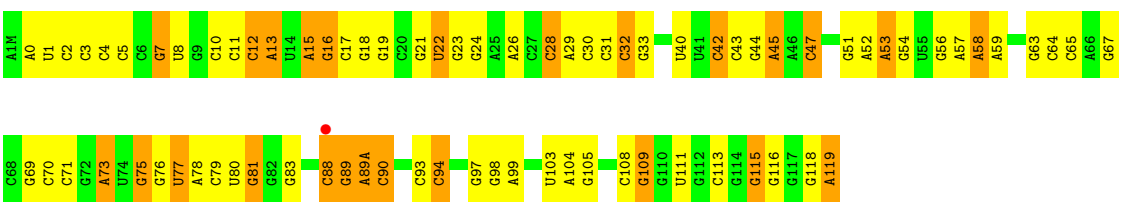




• Molecule 27: 5S rRNA

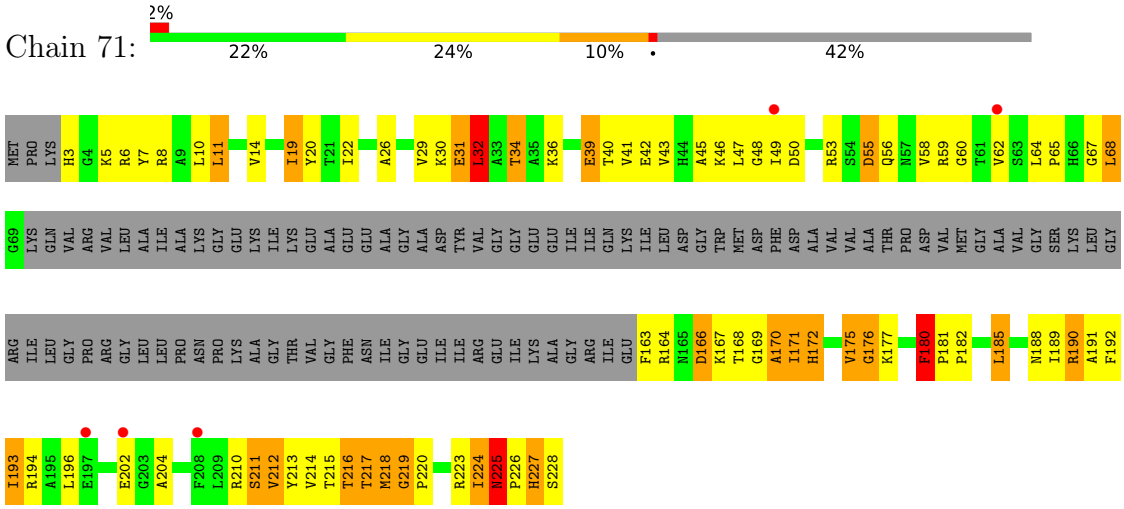
Chain 1J:





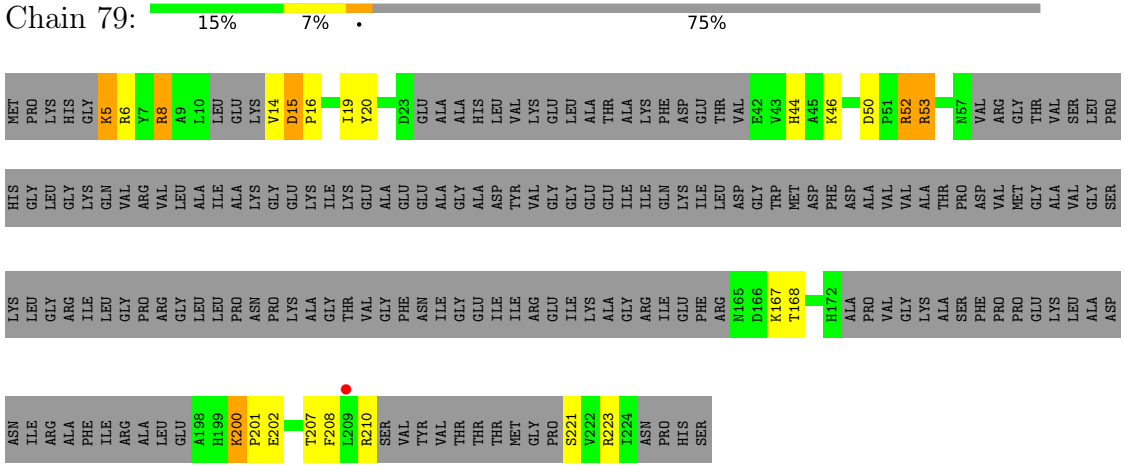
• Molecule 28: 50S ribosomal protein L1

Chain 71:



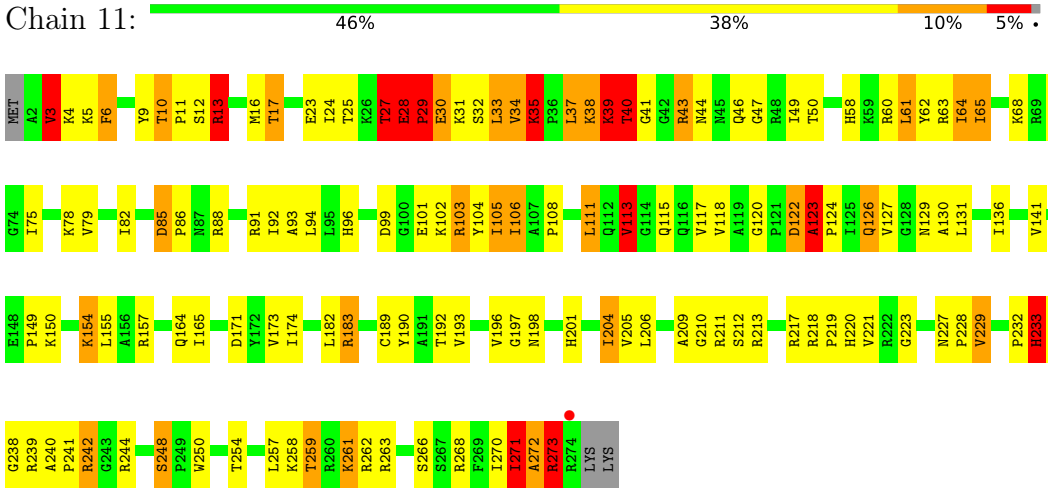
• Molecule 28: 50S ribosomal protein L1

Chain 79:



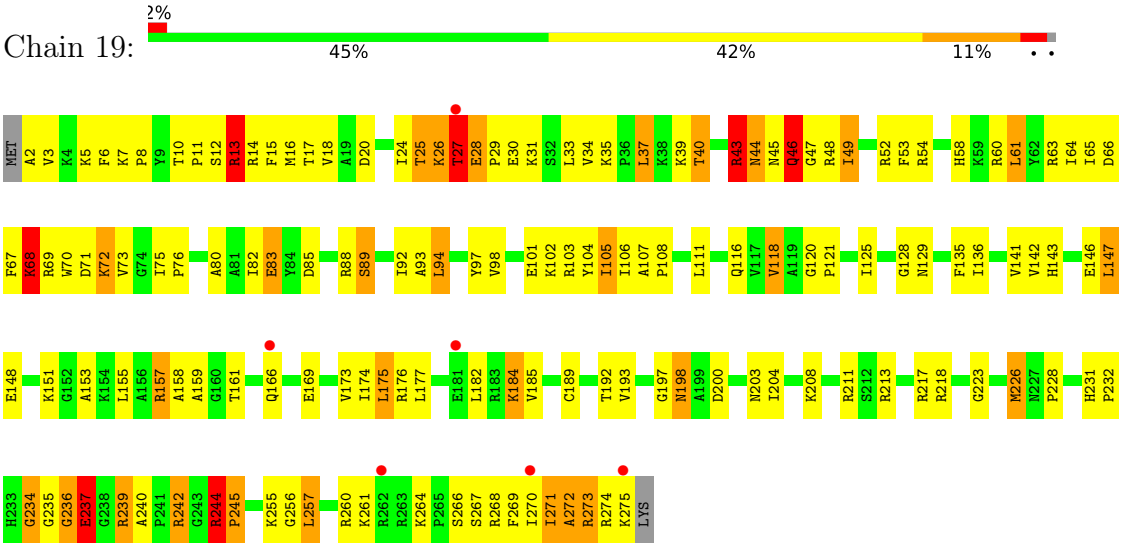
• Molecule 29: 50S ribosomal protein L2

Chain 11:



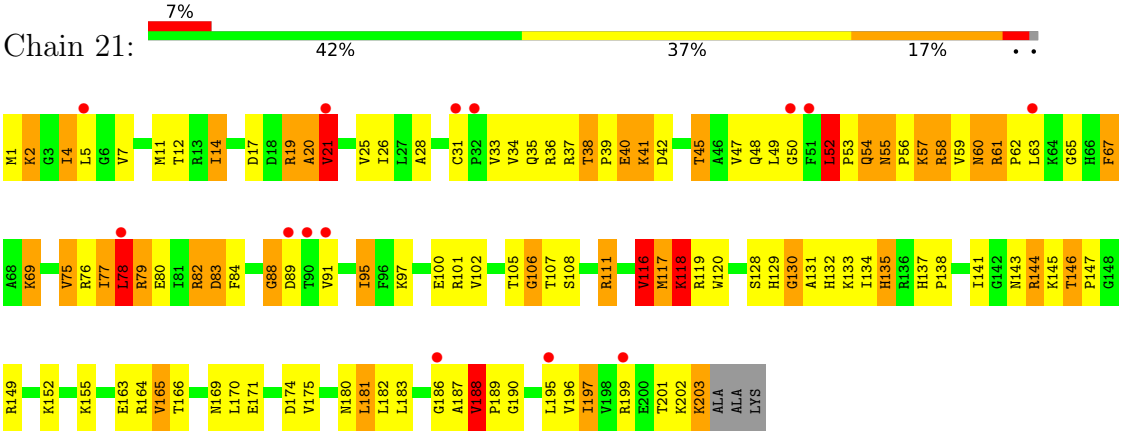
• Molecule 29: 50S ribosomal protein L2

Chain 19:



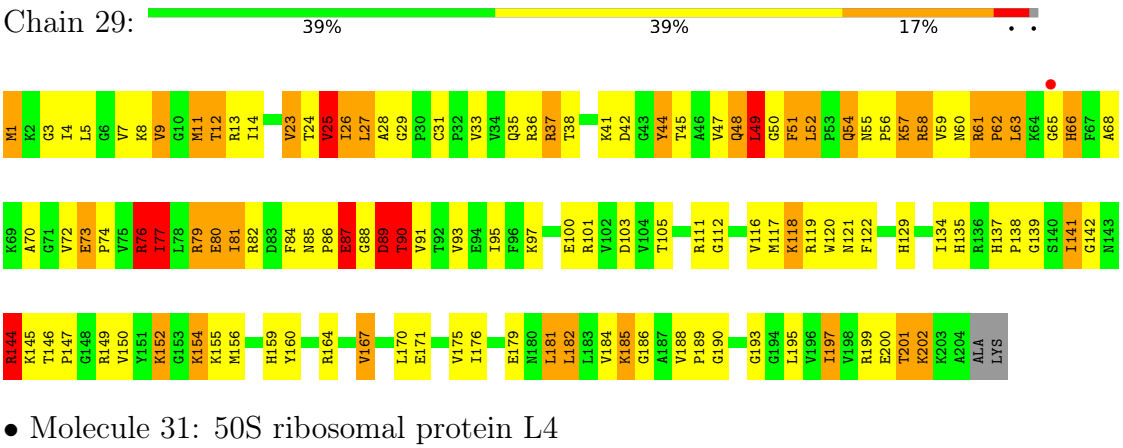
• Molecule 30: 50S ribosomal protein L3

Chain 21:



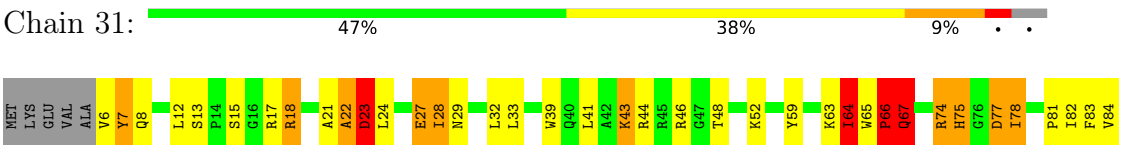
• Molecule 30: 50S ribosomal protein L3

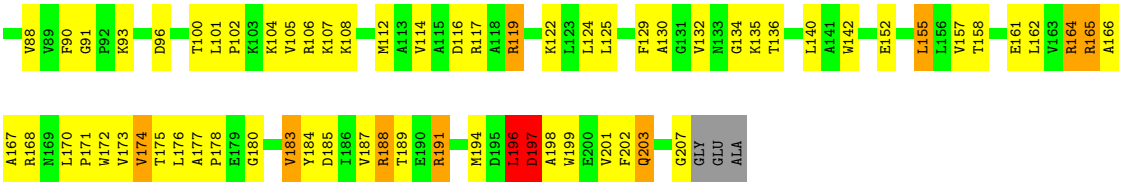
Chain 29:



• Molecule 31: 50S ribosomal protein L4

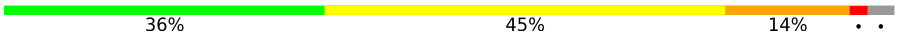
Chain 31:

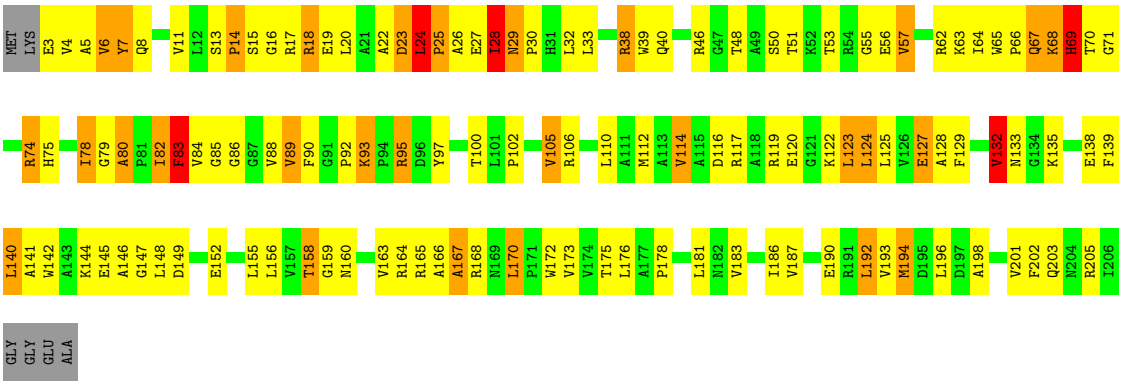




• Molecule 31: 50S ribosomal protein L4

Chain 39:

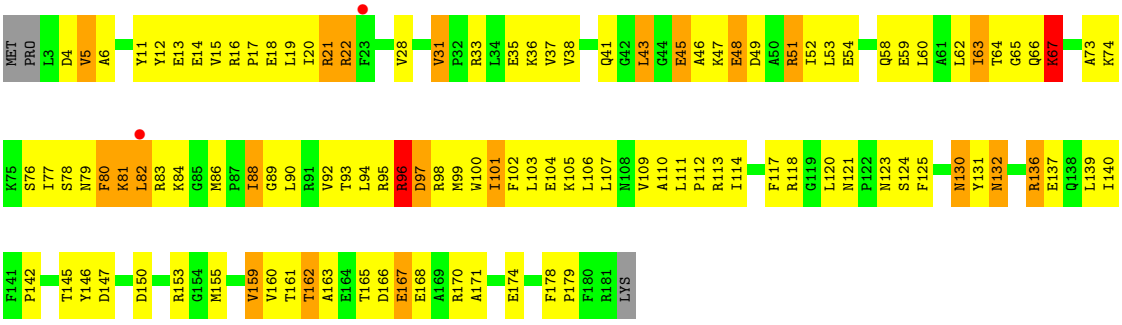




• Molecule 32: 50S ribosomal protein L5

Chain 41:

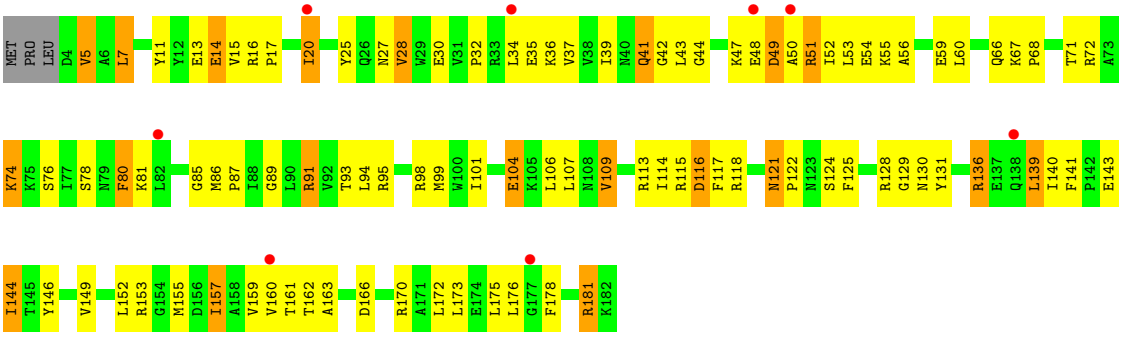




• Molecule 32: 50S ribosomal protein L5

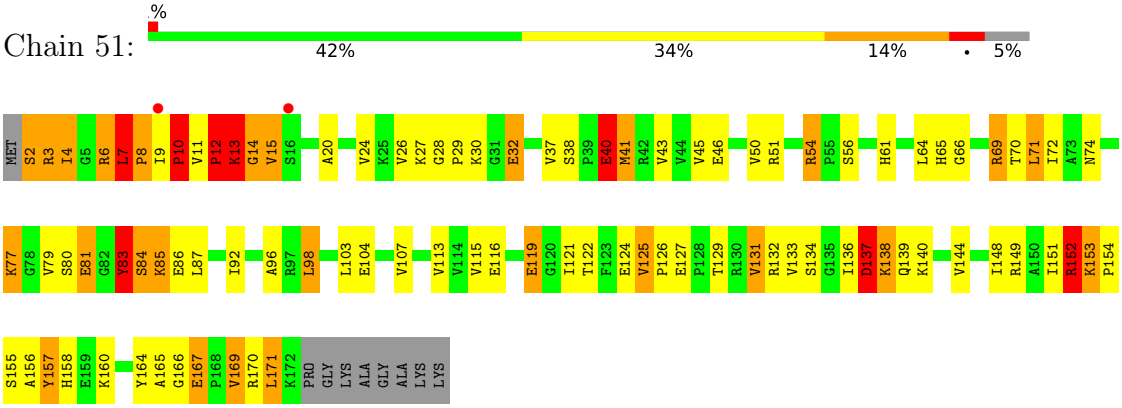
Chain 49:





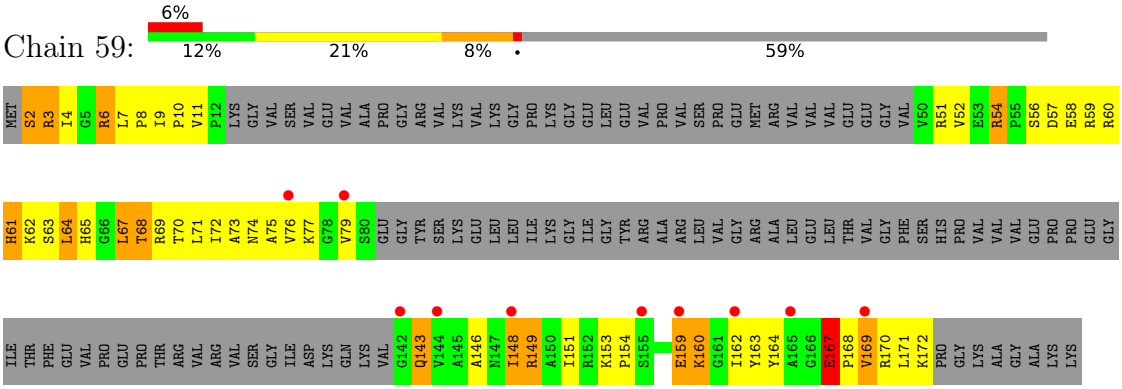
• Molecule 33: 50S ribosomal protein L6

Chain 51:



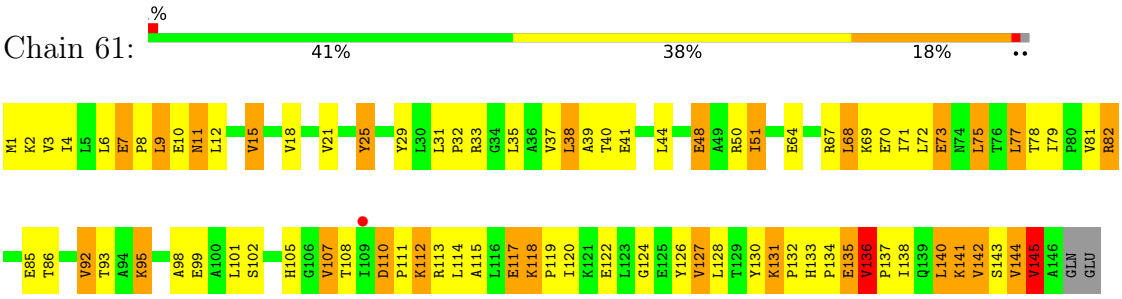
• Molecule 33: 50S ribosomal protein L6

Chain 59:



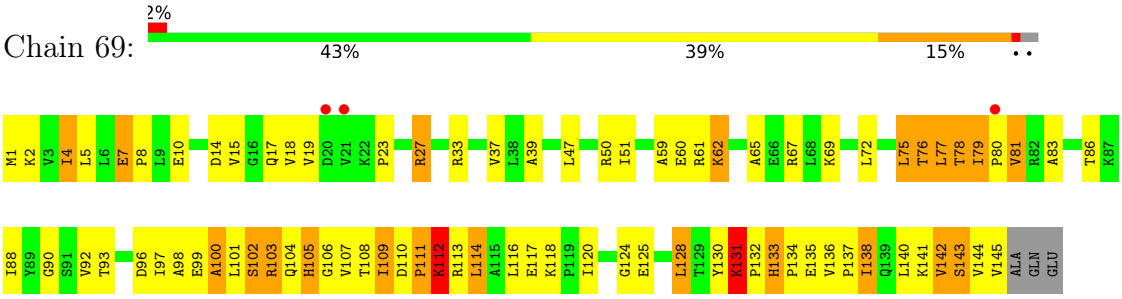
• Molecule 34: 50S ribosomal protein L9

Chain 61:



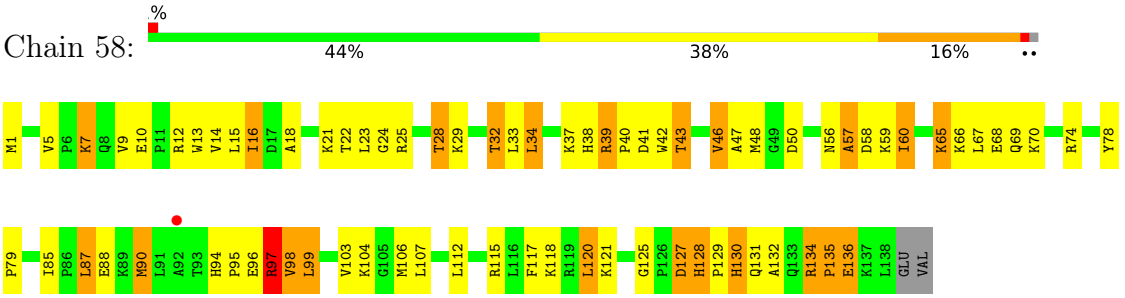
• Molecule 34: 50S ribosomal protein L9

Chain 69:



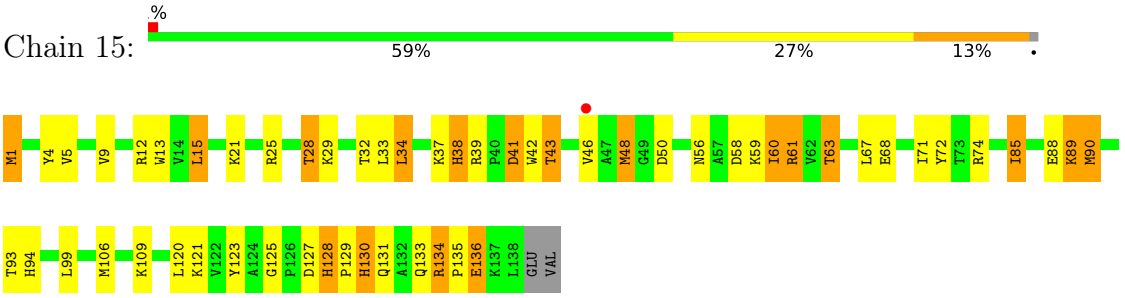
• Molecule 35: 50S ribosomal protein L13

Chain 58:



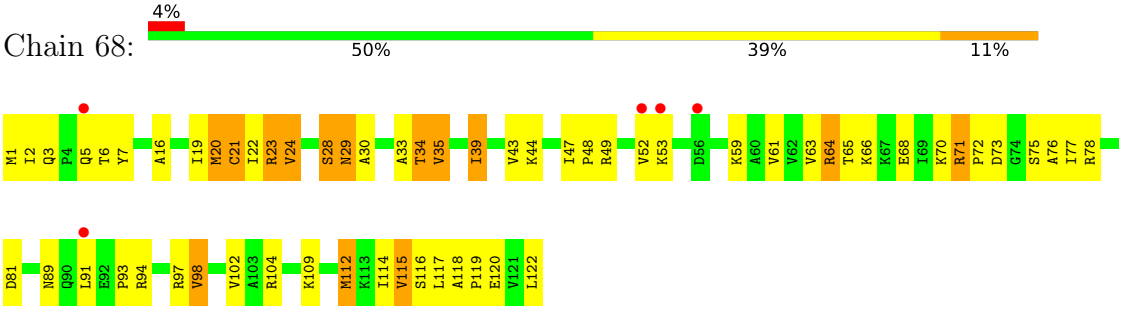
• Molecule 35: 50S ribosomal protein L13

Chain 15:



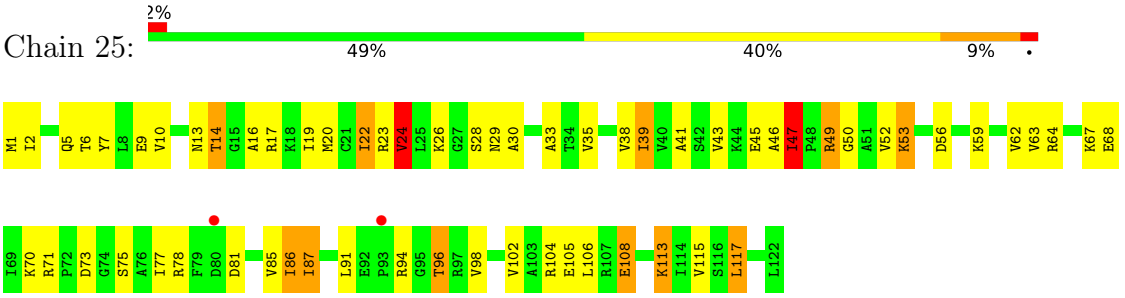
• Molecule 36: 50S ribosomal protein L14

Chain 68:



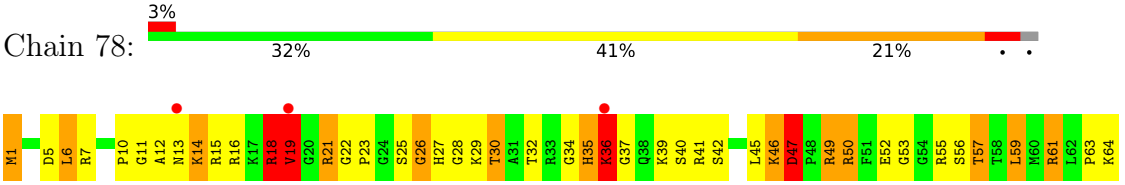
• Molecule 36: 50S ribosomal protein L14

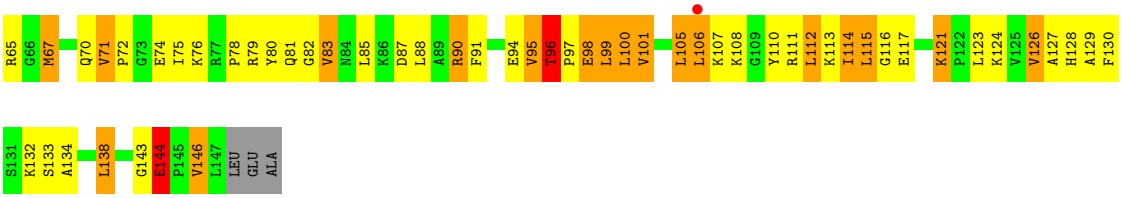
Chain 25:



• Molecule 37: 50S ribosomal protein L15

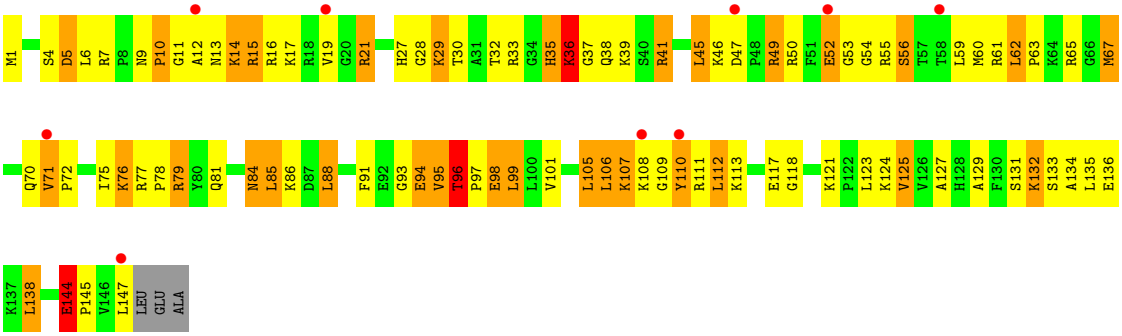
Chain 78:





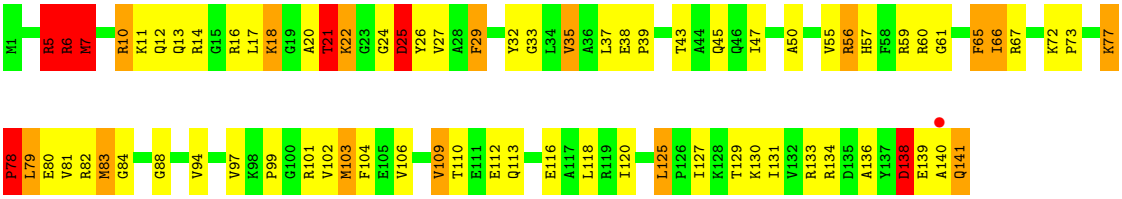
• Molecule 37: 50S ribosomal protein L15





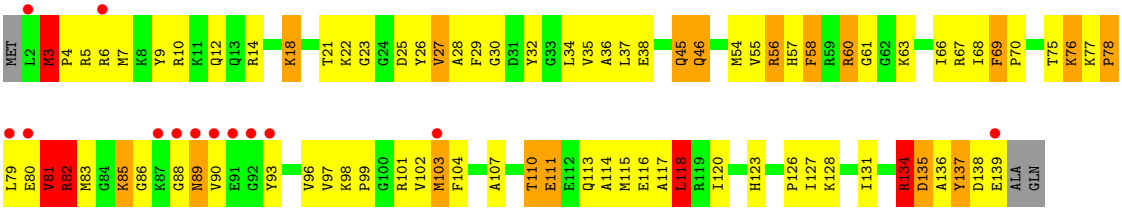
• Molecule 38: 50S ribosomal protein L16





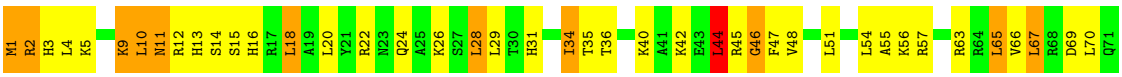
• Molecule 38: 50S ribosomal protein L16

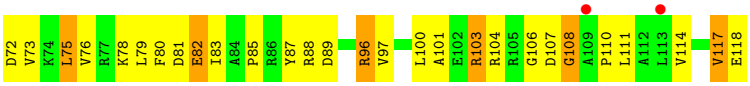




• Molecule 39: 50S ribosomal protein L17

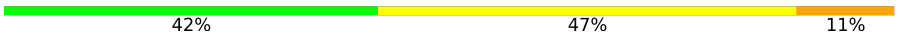


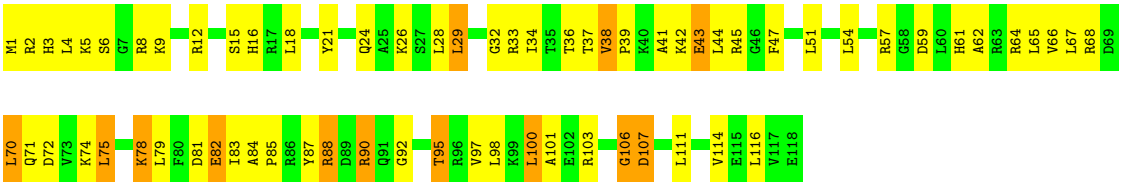




• Molecule 39: 50S ribosomal protein L17

Chain 55:

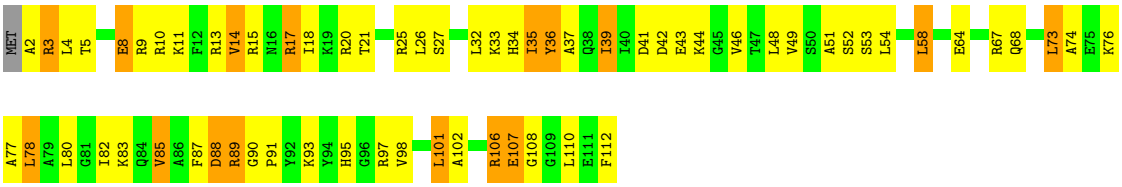




• Molecule 40: 50S ribosomal protein L18

Chain A8:

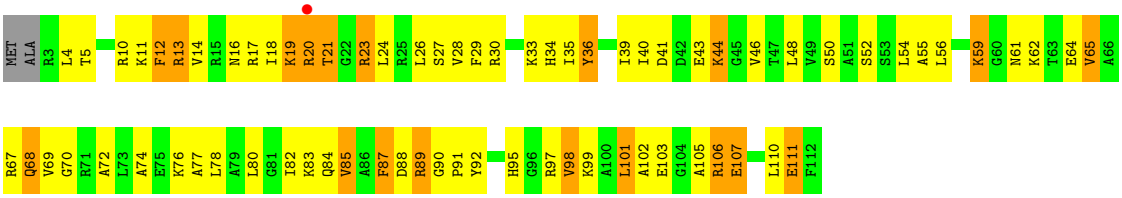




• Molecule 40: 50S ribosomal protein L18

Chain 65:

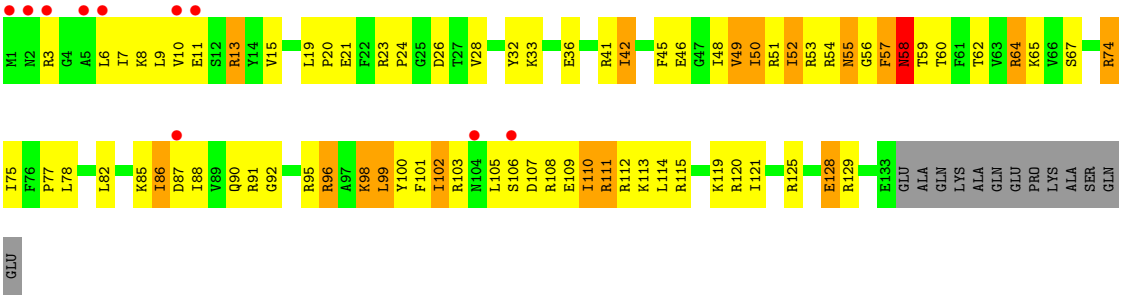




• Molecule 41: 50S ribosomal protein L19

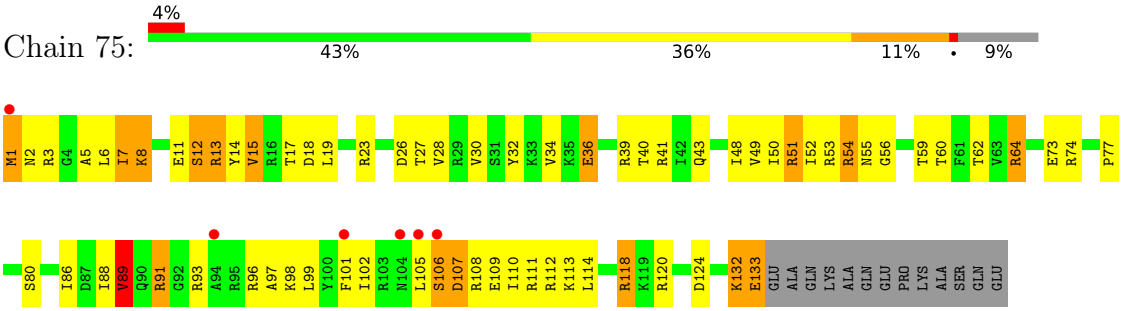
Chain B8:





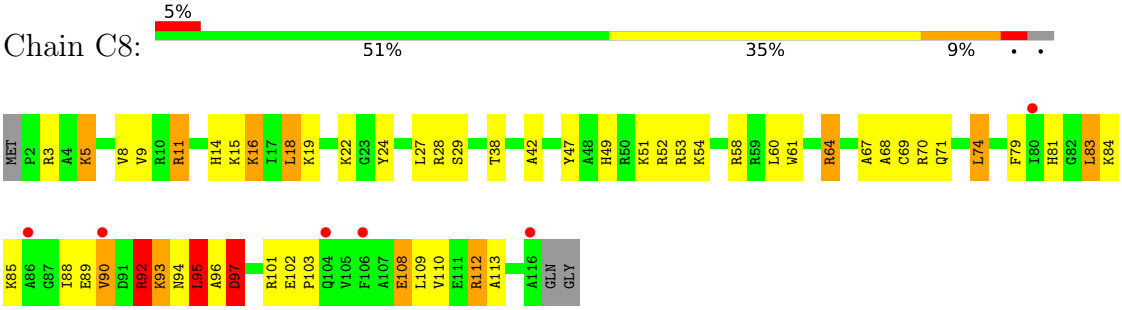
• Molecule 41: 50S ribosomal protein L19

Chain 75:



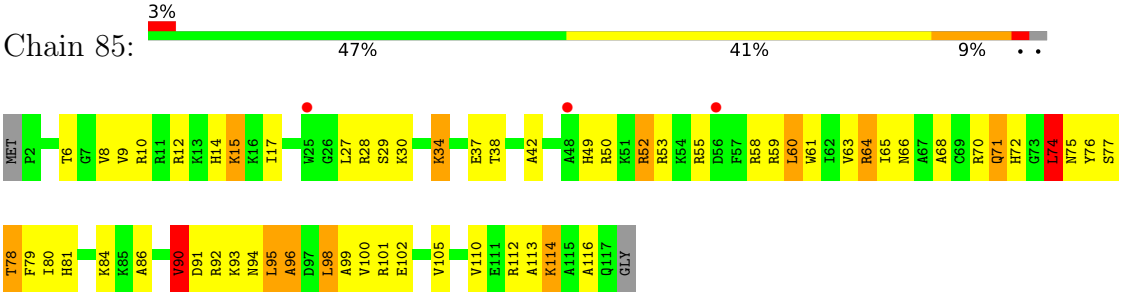
• Molecule 42: 50S ribosomal protein L20

Chain C8:



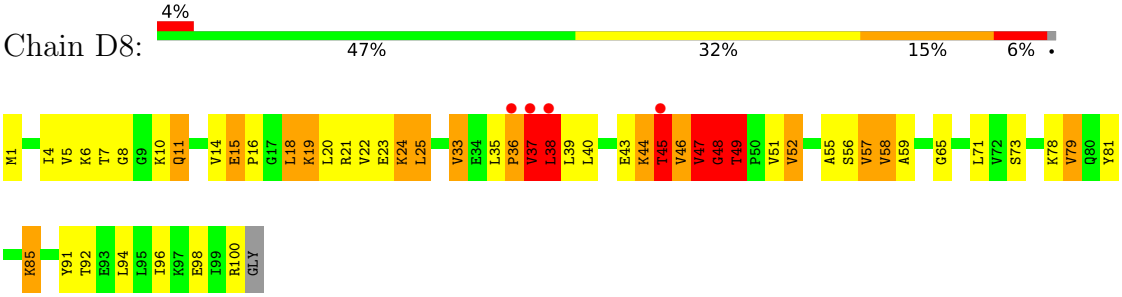
• Molecule 42: 50S ribosomal protein L20

Chain 85:



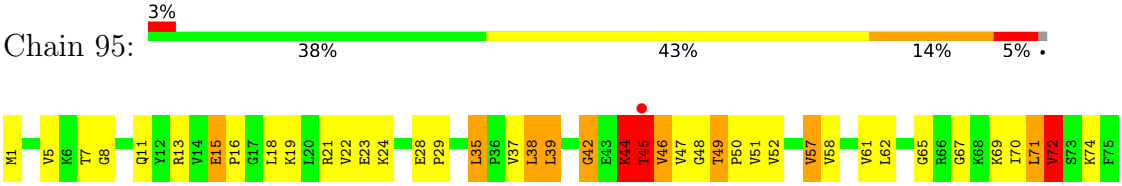
• Molecule 43: 50S ribosomal protein L21

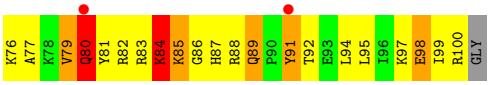
Chain D8:



• Molecule 43: 50S ribosomal protein L21

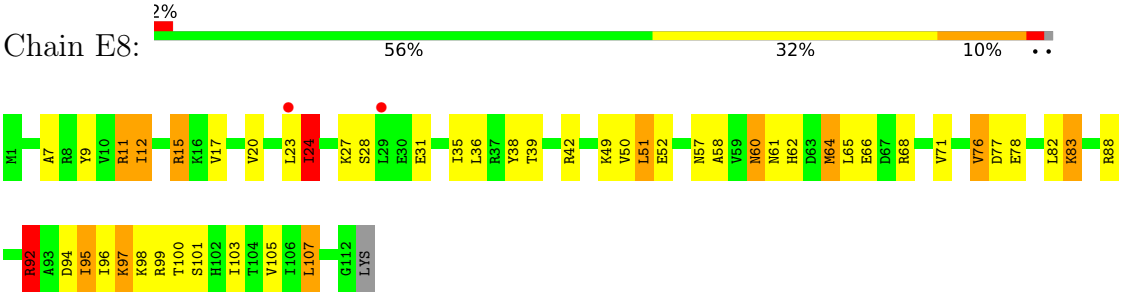
Chain 95:





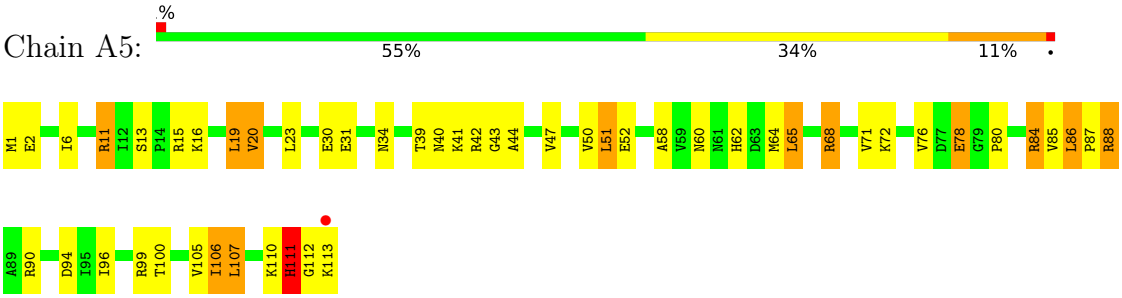
• Molecule 44: 50S ribosomal protein L22

Chain E8:



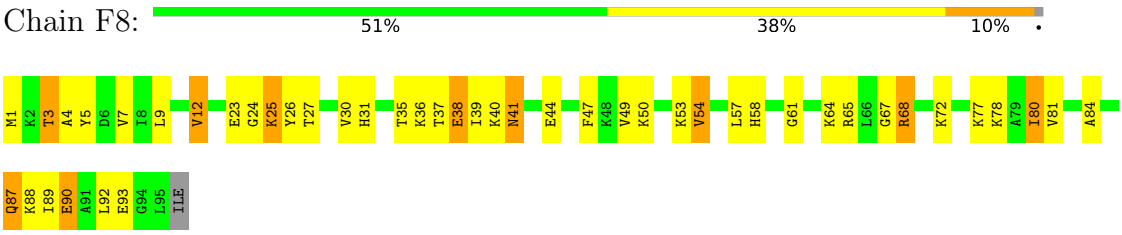
• Molecule 44: 50S ribosomal protein L22

Chain A5:



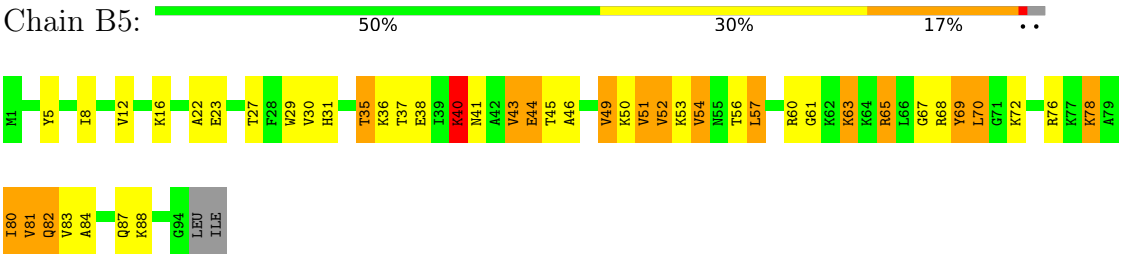
• Molecule 45: 50S ribosomal protein L23

Chain F8:



• Molecule 45: 50S ribosomal protein L23

Chain B5:



• Molecule 46: 50S ribosomal protein L24

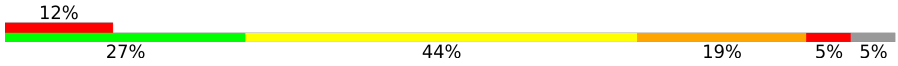
Chain G8:

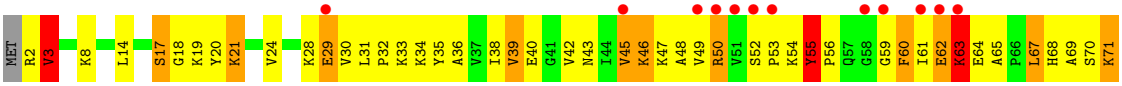




• Molecule 46: 50S ribosomal protein L24

Chain C5:

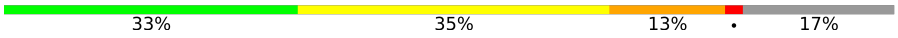


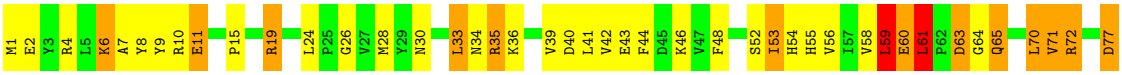




• Molecule 47: 50S ribosomal protein L25

Chain H8:





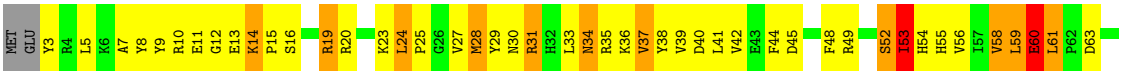


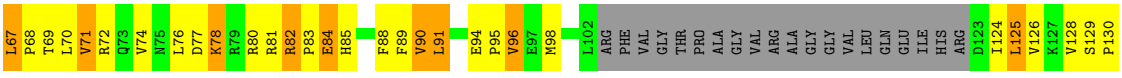


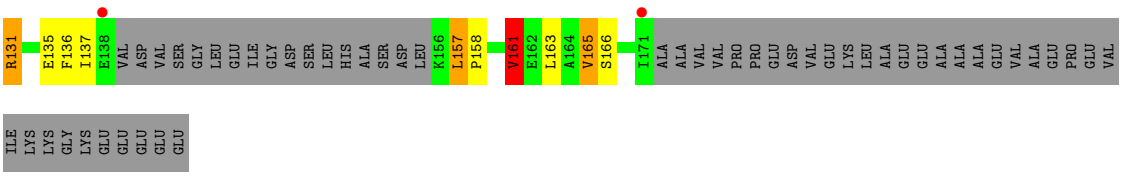
• Molecule 47: 50S ribosomal protein L25

Chain D5:





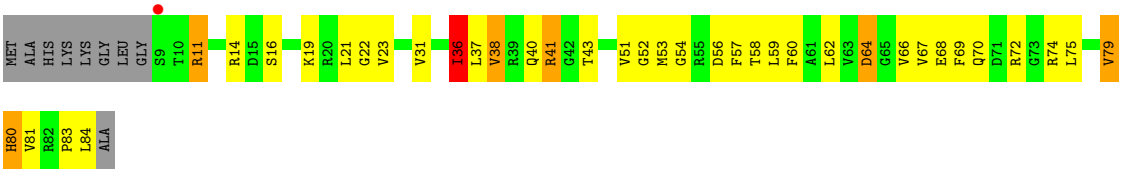




• Molecule 48: 50S ribosomal protein L27

Chain I8:

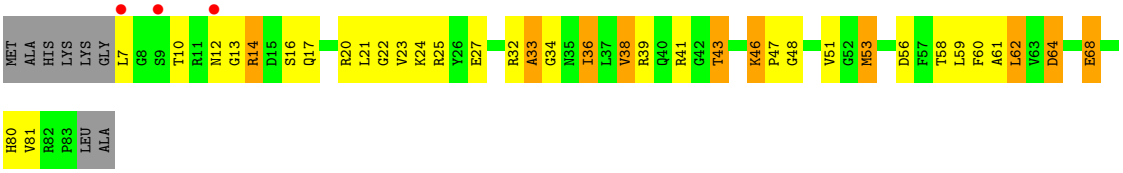




• Molecule 48: 50S ribosomal protein L27

Chain E5:

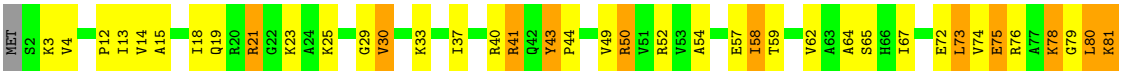


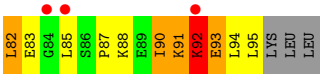


• Molecule 49: 50S ribosomal protein L28

Chain J8:





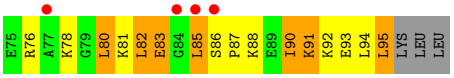


• Molecule 49: 50S ribosomal protein L28

Chain F5:



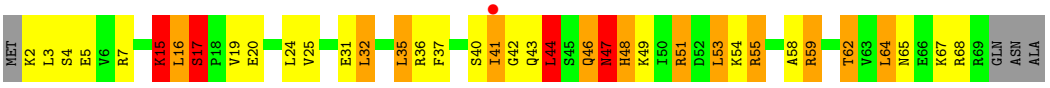




• Molecule 50: 50S ribosomal protein L29

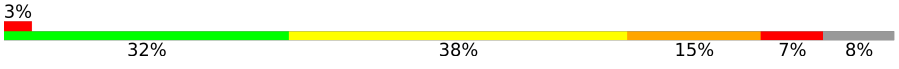
Chain K8:

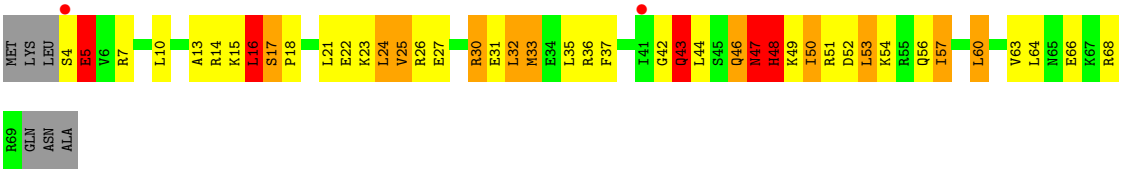




• Molecule 50: 50S ribosomal protein L29

Chain G5:

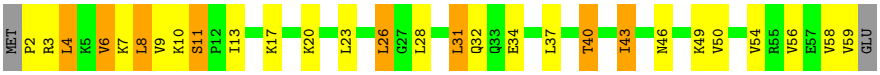




• Molecule 51: 50S ribosomal protein L30

Chain L8:

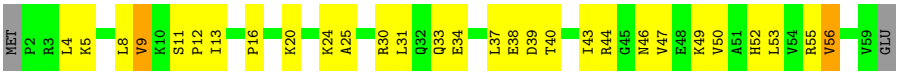




• Molecule 51: 50S ribosomal protein L30

Chain H5:

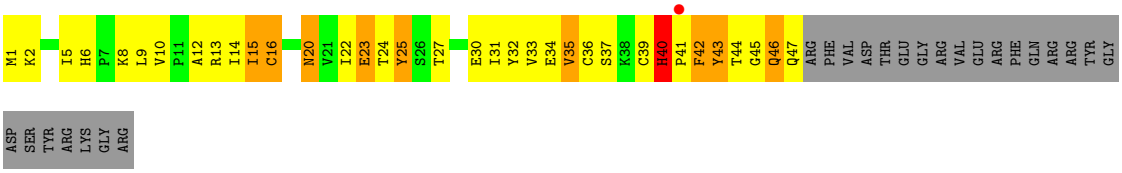




• Molecule 52: 50S ribosomal protein L31

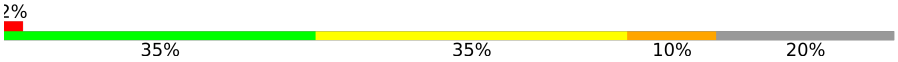
Chain M8:

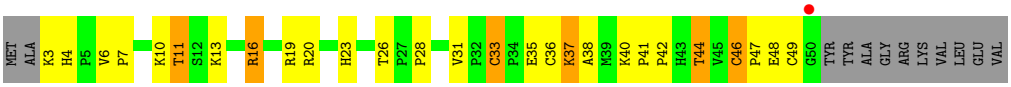




• Molecule 53: 50S ribosomal protein L32

Chain N8:





• Molecule 53: 50S ribosomal protein L32

Chain J5:

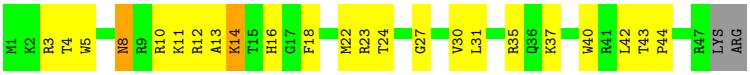




• Molecule 54: 50S ribosomal protein L34

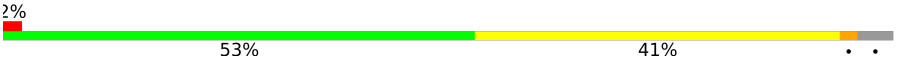
Chain P8:

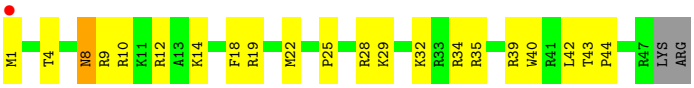




• Molecule 54: 50S ribosomal protein L34

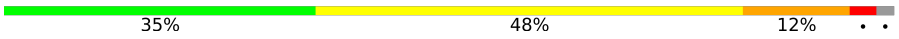
Chain L5:





• Molecule 55: 50S ribosomal protein L35

Chain Q8:

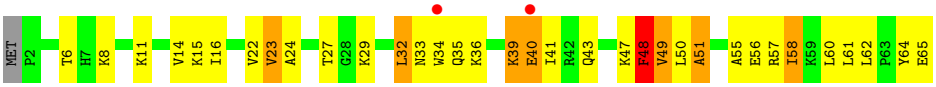




• Molecule 55: 50S ribosomal protein L35

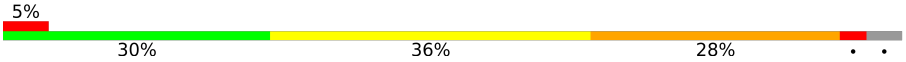
Chain M5:

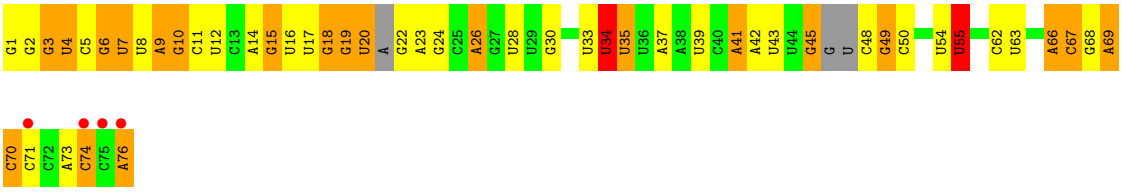




• Molecule 56: tRNALys

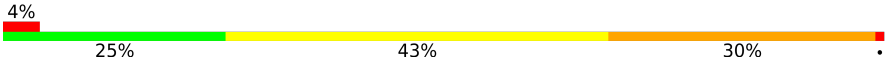
Chain 1L:

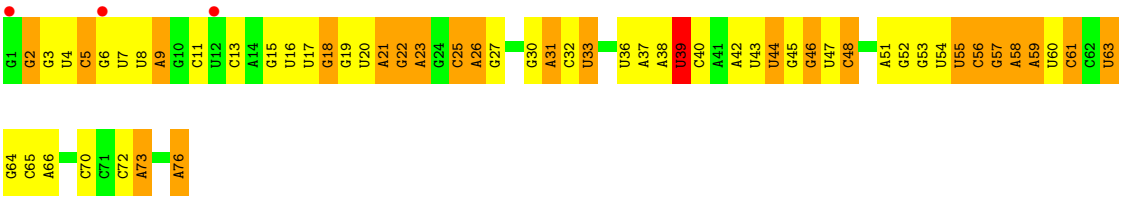




• Molecule 57: tRNALys

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 0.195 , 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)	0.26 , 42.3	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	0.95	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: ZN, G7M, 5MU, T6A, U8U, 4SU, SF4, MG, OMC, PSU

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	0.41	0/35994	0.66	8/56171 (0.0%)
1	1G	0.35	0/36258	0.59	2/56589 (0.0%)
2	12	0.57	0/1752	1.18	17/2360 (0.7%)
2	1E	0.61	0/1908	1.17	19/2573 (0.7%)
3	22	0.53	0/1564	1.03	4/2109 (0.2%)
3	2E	0.62	0/1629	0.98	5/2195 (0.2%)
4	32	0.60	0/1732	1.12	12/2318 (0.5%)
4	3E	0.64	0/1728	1.11	12/2313 (0.5%)
5	42	0.59	0/1150	1.04	4/1548 (0.3%)
5	4E	0.69	0/1158	1.04	1/1559 (0.1%)
6	52	0.63	0/855	1.01	0/1154
6	5E	0.67	0/850	1.02	2/1147 (0.2%)
7	62	0.55	0/1122	1.10	6/1500 (0.4%)
7	6E	0.56	0/1259	0.97	4/1686 (0.2%)
8	72	0.53	0/1127	1.08	8/1517 (0.5%)
8	7E	0.61	0/1135	1.17	8/1527 (0.5%)
9	82	0.54	0/971	1.10	6/1304 (0.5%)
9	8E	0.56	0/1019	1.02	3/1367 (0.2%)
10	1A	0.57	0/658	1.03	4/885 (0.5%)
10	1I	0.74	1/747 (0.1%)	1.10	6/1006 (0.6%)
11	2A	0.60	0/850	1.09	5/1150 (0.4%)
11	2I	0.69	0/838	1.11	7/1133 (0.6%)
12	3A	0.72	0/972	1.10	3/1301 (0.2%)
12	3I	0.93	1/972 (0.1%)	1.30	6/1301 (0.5%)
13	4A	0.58	0/903	1.12	8/1211 (0.7%)
13	4I	0.67	0/952	1.07	2/1277 (0.2%)
14	5A	0.58	0/495	1.11	3/657 (0.5%)
14	5I	0.75	1/500 (0.2%)	0.99	2/664 (0.3%)
15	6A	0.57	0/744	0.89	0/992
15	6I	0.65	0/740	1.06	1/987 (0.1%)
16	7A	0.62	0/721	1.15	5/970 (0.5%)
16	7I	0.63	0/716	1.14	3/963 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.56	0/836	1.01	2/1117 (0.2%)
17	8I	0.64	0/847	1.09	4/1131 (0.4%)
18	9A	0.57	0/549	0.99	0/732
18	9I	0.68	0/554	1.10	2/739 (0.3%)
19	AA	0.63	0/490	1.14	6/662 (0.9%)
19	AI	0.69	0/668	1.14	0/899
20	BA	0.62	0/764	1.09	1/1007 (0.1%)
20	BI	0.56	0/748	1.02	1/986 (0.1%)
21	1B	0.61	0/192	1.04	0/252
21	1F	0.58	0/203	0.88	0/266
22	1K	0.37	0/1565	0.57	0/2429
23	2K	0.49	1/1721 (0.1%)	0.69	0/2682
23	2L	0.40	1/1721 (0.1%)	0.60	0/2682
24	3K	0.38	0/1799	0.58	0/2801
25	4K	0.48	0/473	0.73	1/737 (0.1%)
25	4L	0.35	0/448	0.50	0/698
26	14	0.48	0/69023	0.73	14/107740 (0.0%)
26	1H	0.56	0/68351	0.82	30/106700 (0.0%)
27	16	0.46	0/2928	0.74	0/4568
27	1J	0.39	0/2928	0.66	0/4568
28	71	0.66	0/1055	1.23	15/1425 (1.1%)
28	79	0.58	0/459	1.19	6/608 (1.0%)
29	11	1.03	5/2170 (0.2%)	1.50	37/2926 (1.3%)
29	19	0.91	3/2175 (0.1%)	1.45	27/2933 (0.9%)
30	21	0.86	1/1591 (0.1%)	1.57	25/2146 (1.2%)
30	29	0.84	0/1596	1.34	18/2153 (0.8%)
31	31	0.86	0/1620	1.29	11/2194 (0.5%)
31	39	0.81	1/1637 (0.1%)	1.40	20/2218 (0.9%)
32	41	0.67	0/1481	1.11	7/1994 (0.4%)
32	49	0.55	0/1482	1.07	8/1994 (0.4%)
33	51	0.90	3/1337 (0.2%)	1.46	24/1809 (1.3%)
33	59	0.63	0/577	1.45	13/776 (1.7%)
34	61	0.70	0/1151	1.23	12/1558 (0.8%)
34	69	0.66	0/1146	1.18	13/1551 (0.8%)
35	15	0.59	0/1131	1.11	5/1525 (0.3%)
35	58	0.78	0/1131	1.25	11/1525 (0.7%)
36	25	0.75	1/942 (0.1%)	1.13	4/1269 (0.3%)
36	68	0.86	0/942	1.18	4/1269 (0.3%)
37	35	0.79	0/1139	1.51	23/1514 (1.5%)
37	78	0.94	4/1139 (0.4%)	1.46	18/1514 (1.2%)
38	45	0.95	4/1120 (0.4%)	1.39	13/1498 (0.9%)
38	88	0.98	1/1134 (0.1%)	1.43	22/1519 (1.4%)
39	55	0.87	1/981 (0.1%)	1.15	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	98	0.76	0/981	1.19	5/1312 (0.4%)
40	65	0.65	0/886	1.17	1/1180 (0.1%)
40	A8	0.76	0/891	1.15	1/1187 (0.1%)
41	75	0.70	0/1123	1.06	3/1500 (0.2%)
41	B8	0.83	0/1123	1.25	6/1500 (0.4%)
42	85	0.75	0/977	1.08	3/1301 (0.2%)
42	C8	0.83	1/968 (0.1%)	1.16	7/1289 (0.5%)
43	95	0.93	2/785 (0.3%)	1.26	6/1052 (0.6%)
43	D8	0.71	0/785	1.29	6/1052 (0.6%)
44	A5	0.83	0/910	1.17	3/1220 (0.2%)
44	E8	0.84	0/901	1.17	3/1209 (0.2%)
45	B5	0.84	0/749	1.16	3/1007 (0.3%)
45	F8	0.99	0/757	1.21	4/1017 (0.4%)
46	C5	0.85	1/807 (0.1%)	1.33	5/1076 (0.5%)
46	G8	1.06	2/809 (0.2%)	1.56	21/1080 (1.9%)
47	D5	0.69	0/1098	1.23	13/1487 (0.9%)
47	H8	0.69	2/1403 (0.1%)	1.16	8/1901 (0.4%)
48	E5	0.71	0/616	1.21	5/821 (0.6%)
48	I8	0.92	1/614 (0.2%)	1.30	2/819 (0.2%)
49	F5	0.81	0/744	1.25	7/989 (0.7%)
49	J8	0.91	0/744	1.29	4/989 (0.4%)
50	G5	0.65	0/560	1.27	5/741 (0.7%)
50	K8	0.82	0/570	1.29	4/755 (0.5%)
51	H5	0.66	0/464	1.12	3/623 (0.5%)
51	L8	0.78	0/464	1.21	3/623 (0.5%)
52	M8	0.75	0/375	1.37	9/507 (1.8%)
53	J5	0.81	1/448 (0.2%)	1.32	5/606 (0.8%)
53	N8	0.87	0/381	1.39	9/516 (1.7%)
54	L5	0.88	0/409	1.32	1/540 (0.2%)
54	P8	1.06	1/409 (0.2%)	1.26	0/540
55	M5	0.93	0/524	1.45	7/691 (1.0%)
55	Q8	1.02	0/524	1.61	7/691 (1.0%)
56	1L	0.35	0/1613	0.53	0/2504
57	3L	0.37	0/1733	0.57	0/2699
All	All	0.57	40/317108 (0.0%)	0.87	744/475084 (0.2%)

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

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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

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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 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	55	38	VAL	CA-CB	-9.58	1.49	1.54
38	45	82	ARG	CA-C	8.19	1.63	1.52
46	G8	83	THR	CA-C	7.96	1.57	1.52
43	95	80	GLN	CA-C	7.29	1.62	1.52
29	19	40	THR	CA-C	7.04	1.61	1.52

The worst 5 of 744 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	21	52	LEU	CA-C-N	19.38	139.13	119.56
30	21	52	LEU	C-N-CA	19.38	139.13	119.56
29	19	271	ILE	N-CA-C	16.79	127.87	112.43
29	19	235	GLY	N-CA-C	14.63	126.96	112.04
38	45	82	ARG	N-CA-C	13.21	133.43	113.61

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

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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	764	0
1	1G	32391	0	16353	746	0
2	12	1721	0	1758	106	0
2	1E	1874	0	1926	108	0
3	22	1541	0	1606	70	0
3	2E	1605	0	1668	61	0
4	32	1702	0	1765	118	0
4	3E	1698	0	1761	85	0
5	42	1134	0	1200	45	0
5	4E	1142	0	1204	63	0
6	52	842	0	857	31	0
6	5E	837	0	852	38	0
7	62	1110	0	1163	52	0
7	6E	1242	0	1286	45	0
8	72	1107	0	1165	39	0
8	7E	1115	0	1177	61	0
9	82	953	0	983	70	0
9	8E	1000	0	1031	59	0
10	1A	646	0	662	33	0
10	1I	734	0	761	44	0
11	2A	835	0	847	33	0
11	2I	823	0	833	51	0
12	3A	956	0	1046	57	0
12	3I	956	0	1046	33	0
13	4A	893	0	946	63	0
13	4I	942	0	997	54	0
14	5A	486	0	525	27	0
14	5I	491	0	529	30	0
15	6A	733	0	771	33	0

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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	49	0
17	8A	823	0	891	35	0
17	8I	834	0	904	44	0
18	9A	544	0	605	26	0
18	9I	549	0	607	36	0
19	AA	481	0	468	33	0
19	AI	654	0	675	45	0
20	BA	762	0	861	33	0
20	BI	746	0	843	50	0
21	1B	188	0	195	13	0
21	1F	199	0	208	6	0
22	1K	1520	0	778	39	0
23	2K	1646	0	843	30	0
23	2L	1646	0	843	39	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	1329	0
26	1H	61028	0	30763	1358	0
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	66	0
28	71	1033	0	1048	77	0
28	79	456	0	460	20	0
29	11	2120	0	2197	135	0
29	19	2125	0	2199	106	0
30	21	1558	0	1624	88	0
30	29	1563	0	1629	122	0
31	31	1585	0	1632	97	0
31	39	1602	0	1649	91	0
32	41	1457	0	1514	94	0
32	49	1458	0	1516	63	0
33	51	1312	0	1384	70	0
33	59	568	0	595	49	0
34	61	1136	0	1223	59	0
34	69	1131	0	1218	50	0
35	15	1104	0	1180	37	0
35	58	1104	0	1180	56	0
36	25	932	0	996	38	0
36	68	932	0	996	44	0
37	35	1122	0	1206	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	78	1122	0	1206	97	0
38	45	1099	0	1154	84	0
38	88	1113	0	1157	53	0
39	55	967	0	1033	50	0
39	98	967	0	1033	49	0
40	65	876	0	938	64	0
40	A8	881	0	943	53	0
41	75	1109	0	1170	56	0
41	B8	1109	0	1170	65	0
42	85	959	0	1019	55	0
42	C8	950	0	1011	55	0
43	95	774	0	849	65	0
43	D8	774	0	849	45	0
44	A5	899	0	964	30	0
44	E8	890	0	951	24	0
45	B5	735	0	785	35	0
45	F8	743	0	794	35	0
46	C5	794	0	886	72	0
46	G8	796	0	886	48	0
47	D5	1074	0	1086	55	0
47	H8	1373	0	1402	57	0
48	E5	608	0	622	26	0
48	I8	606	0	625	30	0
49	F5	737	0	813	33	0
49	J8	737	0	813	39	0
50	G5	558	0	610	33	0
50	K8	568	0	614	34	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	16	0
54	P8	401	0	436	16	0
55	M5	516	0	582	26	0
55	Q8	516	0	582	37	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

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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	102	0
61	1J	6	0	0	1	0
61	1K	8	0	0	0	0
61	21	4	0	0	2	0

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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	8390	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 18.

The worst 5 of 8390 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 20
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	9 40
3	22	192/239 (80%)	169 (88%)	22 (12%)	1 (0%)	24 59
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100 100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	24 59
4	3E	205/209 (98%)	188 (92%)	14 (7%)	3 (2%)	8 37
5	42	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	18 52
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	18 52
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%)	18 52
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100 100
8	72	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	18 52
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	18 52
9	82	119/128 (93%)	107 (90%)	11 (9%)	1 (1%)	16 50
9	8E	124/128 (97%)	104 (84%)	19 (15%)	1 (1%)	16 50
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%)	6 34
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	14 47
12	3A	120/132 (91%)	102 (85%)	13 (11%)	5 (4%)	2 16
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16 50
13	4A	109/126 (86%)	95 (87%)	13 (12%)	1 (1%)	14 47
13	4I	117/126 (93%)	97 (83%)	19 (16%)	1 (1%)	14 47
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3 20
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%)	8 37
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8 37
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	2 19
19	AI	79/93 (85%)	67 (85%)	10 (13%)	2 (2%)	4 27
20	BA	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	5 31
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%)	2 17
29	19	272/276 (99%)	241 (89%)	25 (9%)	6 (2%)	5 29
30	21	201/206 (98%)	157 (78%)	36 (18%)	8 (4%)	2 17
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	2 17
31	31	200/210 (95%)	175 (88%)	25 (12%)	0	100 100
31	39	202/210 (96%)	157 (78%)	36 (18%)	9 (4%)	2 15
32	41	177/182 (97%)	155 (88%)	19 (11%)	3 (2%)	7 35
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	11 43
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1 10
33	59	67/180 (37%)	50 (75%)	14 (21%)	3 (4%)	2 15
34	61	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	9 39
34	69	143/148 (97%)	116 (81%)	26 (18%)	1 (1%)	18 52
35	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	18 52
35	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	5 29

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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%)	9 39
37	78	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3 20
38	45	136/141 (96%)	112 (82%)	21 (15%)	3 (2%)	5 29
38	88	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2 19
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14 47
39	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	14 47
40	65	108/112 (96%)	86 (80%)	20 (18%)	2 (2%)	6 33
40	A8	109/112 (97%)	92 (84%)	14 (13%)	3 (3%)	4 25
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%)	6 34
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	4 25
43	95	98/101 (97%)	77 (79%)	14 (14%)	7 (7%)	1 6
43	D8	98/101 (97%)	87 (89%)	6 (6%)	5 (5%)	1 13
44	A5	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	14 47
44	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100 100
45	B5	92/96 (96%)	85 (92%)	4 (4%)	3 (3%)	3 21
45	F8	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	11 43
46	C5	102/110 (93%)	75 (74%)	17 (17%)	10 (10%)	0 2
46	G8	103/110 (94%)	86 (84%)	13 (13%)	4 (4%)	2 18
47	D5	126/206 (61%)	100 (79%)	21 (17%)	5 (4%)	2 17
47	H8	169/206 (82%)	136 (80%)	25 (15%)	8 (5%)	2 14
48	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	9 40
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100 100
49	F5	92/98 (94%)	85 (92%)	6 (6%)	1 (1%)	11 43
49	J8	92/98 (94%)	83 (90%)	8 (9%)	1 (1%)	11 43
50	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	3 22
50	K8	66/72 (92%)	58 (88%)	5 (8%)	3 (4%)	2 15
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100 100

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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%)	5 29
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%)	3 21
55	Q8	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2 14
All	All	10973/12333 (89%)	9576 (87%)	1201 (11%)	196 (2%)	6 34

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%)	151 (83%)	31 (17%)	2 11
2	1E	200/220 (91%)	138 (69%)	62 (31%)	0 1
3	22	154/188 (82%)	122 (79%)	32 (21%)	1 7
3	2E	159/188 (85%)	121 (76%)	38 (24%)	1 4
4	32	180/181 (99%)	138 (77%)	42 (23%)	1 5
4	3E	180/181 (99%)	133 (74%)	47 (26%)	0 3
5	42	114/123 (93%)	89 (78%)	25 (22%)	1 5
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	52	90/90 (100%)	71 (79%)	19 (21%)	1 6
6	5E	90/90 (100%)	70 (78%)	20 (22%)	1 5
7	62	114/127 (90%)	91 (80%)	23 (20%)	1 7
7	6E	125/127 (98%)	98 (78%)	27 (22%)	1 6
8	72	118/119 (99%)	93 (79%)	25 (21%)	1 6
8	7E	119/119 (100%)	86 (72%)	33 (28%)	0 2
9	82	92/99 (93%)	70 (76%)	22 (24%)	1 4
9	8E	97/99 (98%)	76 (78%)	21 (22%)	1 6
10	1A	71/92 (77%)	45 (63%)	26 (37%)	0 0
10	1I	81/92 (88%)	61 (75%)	20 (25%)	1 3
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2 10
11	2I	84/99 (85%)	56 (67%)	28 (33%)	0 1
12	3A	103/109 (94%)	78 (76%)	25 (24%)	1 4
12	3I	103/109 (94%)	83 (81%)	20 (19%)	1 8
13	4A	91/101 (90%)	66 (72%)	25 (28%)	0 2
13	4I	94/101 (93%)	73 (78%)	21 (22%)	1 5
14	5A	49/50 (98%)	39 (80%)	10 (20%)	1 7
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0 3
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2 12
15	6I	79/80 (99%)	58 (73%)	21 (27%)	0 3
16	7A	72/74 (97%)	51 (71%)	21 (29%)	0 1
16	7I	72/74 (97%)	50 (69%)	22 (31%)	0 1
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2 11
17	8I	95/97 (98%)	81 (85%)	14 (15%)	3 16
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0 2
18	9I	58/77 (75%)	42 (72%)	16 (28%)	0 2
19	AA	52/80 (65%)	38 (73%)	14 (27%)	0 2
19	AI	71/80 (89%)	52 (73%)	19 (27%)	0 2
20	BA	76/82 (93%)	60 (79%)	16 (21%)	1 6
20	BI	75/82 (92%)	55 (73%)	20 (27%)	0 3
21	1B	17/22 (77%)	17 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	1F	18/22 (82%)	17 (94%)	1 (6%)	19 52
28	71	109/181 (60%)	84 (77%)	25 (23%)	1 5
28	79	48/181 (26%)	39 (81%)	9 (19%)	1 9
29	11	214/218 (98%)	160 (75%)	54 (25%)	0 3
29	19	214/218 (98%)	166 (78%)	48 (22%)	1 5
30	21	165/166 (99%)	121 (73%)	44 (27%)	0 3
30	29	165/166 (99%)	121 (73%)	44 (27%)	0 3
31	31	161/166 (97%)	126 (78%)	35 (22%)	1 6
31	39	163/166 (98%)	125 (77%)	38 (23%)	1 5
32	41	153/156 (98%)	121 (79%)	32 (21%)	1 6
32	49	153/156 (98%)	127 (83%)	26 (17%)	2 11
33	51	142/148 (96%)	106 (75%)	36 (25%)	0 3
33	59	59/148 (40%)	47 (80%)	12 (20%)	1 7
34	61	122/124 (98%)	86 (70%)	36 (30%)	0 1
34	69	122/124 (98%)	85 (70%)	37 (30%)	0 1
35	15	117/119 (98%)	90 (77%)	27 (23%)	1 5
35	58	117/119 (98%)	86 (74%)	31 (26%)	0 3
36	25	100/100 (100%)	73 (73%)	27 (27%)	0 2
36	68	100/100 (100%)	80 (80%)	20 (20%)	1 7
37	35	114/116 (98%)	77 (68%)	37 (32%)	0 1
37	78	114/116 (98%)	74 (65%)	40 (35%)	0 0
38	45	109/111 (98%)	87 (80%)	22 (20%)	1 7
38	88	109/111 (98%)	86 (79%)	23 (21%)	1 6
39	55	101/101 (100%)	78 (77%)	23 (23%)	1 5
39	98	101/101 (100%)	76 (75%)	25 (25%)	1 3
40	65	87/88 (99%)	61 (70%)	26 (30%)	0 1
40	A8	87/88 (99%)	67 (77%)	20 (23%)	1 5
41	75	117/127 (92%)	83 (71%)	34 (29%)	0 1
41	B8	117/127 (92%)	87 (74%)	30 (26%)	0 3
42	85	93/94 (99%)	79 (85%)	14 (15%)	3 14
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	95	82/82 (100%)	64 (78%)	18 (22%)	1 6
43	D8	82/82 (100%)	56 (68%)	26 (32%)	0 1
44	A5	92/92 (100%)	71 (77%)	21 (23%)	1 5
44	E8	91/92 (99%)	65 (71%)	26 (29%)	0 2
45	B5	74/78 (95%)	49 (66%)	25 (34%)	0 1
45	F8	75/78 (96%)	62 (83%)	13 (17%)	2 10
46	C5	85/91 (93%)	57 (67%)	28 (33%)	0 1
46	G8	85/91 (93%)	62 (73%)	23 (27%)	0 2
47	D5	118/179 (66%)	89 (75%)	29 (25%)	1 3
47	H8	152/179 (85%)	106 (70%)	46 (30%)	0 1
48	E5	61/67 (91%)	49 (80%)	12 (20%)	1 8
48	I8	61/67 (91%)	49 (80%)	12 (20%)	1 8
49	F5	79/83 (95%)	52 (66%)	27 (34%)	0 0
49	J8	79/83 (95%)	57 (72%)	22 (28%)	0 2
50	G5	62/67 (92%)	44 (71%)	18 (29%)	0 1
50	K8	62/67 (92%)	40 (64%)	22 (36%)	0 0
51	H5	50/52 (96%)	37 (74%)	13 (26%)	0 3
51	L8	50/52 (96%)	37 (74%)	13 (26%)	0 3
52	M8	42/63 (67%)	30 (71%)	12 (29%)	0 2
53	J5	48/52 (92%)	40 (83%)	8 (17%)	2 11
53	N8	43/52 (83%)	35 (81%)	8 (19%)	1 9
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4 19
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2 13
55	M5	54/55 (98%)	45 (83%)	9 (17%)	2 11
55	Q8	54/55 (98%)	40 (74%)	14 (26%)	0 3
All	All	9277/10193 (91%)	7029 (76%)	2248 (24%)	1 4

5 of 2248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	25	1	MET
37	35	106	LEU
35	15	131	GLN

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Mol	Chain	Res	Type
45	B5	40	LYS
35	58	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
37	35	128	HIS
39	55	3	HIS
53	J5	4	HIS
43	D8	80	GLN
39	98	24	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	364 (24%)	29 (1%)
1	1G	1506/1522 (98%)	367 (24%)	27 (1%)
22	1K	68/75 (90%)	28 (41%)	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%)	13 (72%)	2 (11%)
25	4L	17/27 (62%)	9 (52%)	0
26	14	2853/2917 (97%)	734 (25%)	38 (1%)
26	1H	2829/2917 (96%)	723 (25%)	50 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	1 (0%)
56	1L	70/76 (92%)	28 (40%)	4 (5%)
57	3L	75/76 (98%)	35 (46%)	1 (1%)
All	All	9398/9633 (97%)	2438 (25%)	162 (1%)

5 of 2438 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%)
23	OMC	2L	33	23	19,22,23	1.71	3 (15%)	26,31,34	1.06	3 (11%)
23	4SU	2K	8	23	18,21,22	1.82	4 (22%)	26,30,33	2.30	5 (19%)
23	G7M	2L	47	23	23,26,27	4.52	7 (30%)	35,39,42	3.24	13 (37%)
22	PSU	1K	39	22	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
57	5MU	3L	54	57	19,22,23	4.05	6 (31%)	28,32,35	2.95	10 (35%)
57	PSU	3L	55	57	18,21,22	1.20	1 (5%)	22,30,33	1.73	5 (22%)
23	5MU	2L	55	23	19,22,23	3.80	5 (26%)	28,32,35	3.40	8 (28%)
56	T6A	1L	37	56	31,34,35	2.15	7 (22%)	44,49,52	2.29	14 (31%)
56	PSU	1L	39	56	18,21,22	1.14	1 (5%)	22,30,33	1.57	3 (13%)
56	U8U	1L	34	56,25	19,24,25	2.68	7 (36%)	23,34,37	0.94	1 (4%)
22	PSU	1K	55	22	18,21,22	1.08	1 (5%)	22,30,33	1.56	4 (18%)
23	G7M	2K	47	23	23,26,27	4.43	8 (34%)	35,39,42	3.33	13 (37%)
22	5MU	1K	54	22	19,22,23	3.69	5 (26%)	28,32,35	3.13	6 (21%)
22	T6A	1K	37	22	31,34,35	2.11	10 (32%)	44,49,52	2.06	10 (22%)
23	4SU	2L	8	23	18,21,22	1.76	3 (16%)	26,30,33	2.66	4 (15%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	2L	56	23	18,21,22	1.28	1 (5%)	22,30,33	1.73	4 (18%)
56	5MU	1L	54	56	19,22,23	3.84	5 (26%)	28,32,35	3.25	8 (28%)
23	5MU	2K	55	23	19,22,23	3.79	5 (26%)	28,32,35	3.53	9 (32%)
23	OMC	2K	33	23	19,22,23	1.72	4 (21%)	26,31,34	0.95	2 (7%)
56	PSU	1L	55	56	18,21,22	1.09	1 (5%)	22,30,33	1.60	4 (18%)

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

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	18.01	1.65	1.33
23	2K	47	G7M	C8-N7	17.79	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 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	47	G7M	CN7-N7-C5	11.56	141.13	126.77
23	2L	47	G7M	CN7-N7-C5	11.34	140.86	126.77
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

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
23	2L	33	OMC	1	0
23	2L	47	G7M	2	0
57	3L	55	PSU	1	0
23	2L	55	5MU	1	0
56	1L	34	U8U	2	0
23	2K	47	G7M	1	0
23	2L	8	4SU	2	0
23	2K	56	PSU	1	0
23	2L	56	PSU	1	0
23	2K	33	OMC	2	0
56	1L	55	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	13	1496/1522 (98%)	-0.80	0 100 100	62, 109, 164, 193	0
1	1G	1507/1522 (99%)	-0.77	6 (0%) 88 79	80, 127, 170, 197	0
2	12	210/256 (82%)	-0.11	2 (0%) 79 63	127, 152, 162, 177	0
2	1E	231/256 (90%)	-0.18	1 (0%) 88 79	117, 141, 159, 166	0
3	22	196/239 (82%)	-0.16	3 (1%) 72 52	129, 143, 156, 164	0
3	2E	205/239 (85%)	-0.28	1 (0%) 87 76	94, 114, 136, 145	0
4	32	208/209 (99%)	0.12	0 100 100	108, 128, 145, 152	0
4	3E	207/209 (99%)	0.04	3 (1%) 73 54	92, 114, 134, 139	0
5	42	148/162 (91%)	0.04	0 100 100	114, 129, 143, 152	0
5	4E	149/162 (91%)	-0.05	0 100 100	89, 108, 124, 140	0
6	52	101/101 (100%)	-0.14	1 (0%) 79 63	95, 111, 129, 137	0
6	5E	100/101 (99%)	-0.22	1 (1%) 79 63	87, 107, 126, 136	0
7	62	138/156 (88%)	0.21	8 (5%) 29 18	121, 134, 144, 148	0
7	6E	154/156 (98%)	0.25	2 (1%) 75 55	109, 125, 148, 166	0
8	72	137/138 (99%)	-0.27	0 100 100	111, 133, 142, 145	0
8	7E	138/138 (100%)	0.15	1 (0%) 84 69	97, 117, 128, 138	0
9	82	121/128 (94%)	-0.08	3 (2%) 58 39	117, 149, 158, 163	0
9	8E	126/128 (98%)	0.10	2 (1%) 70 51	96, 135, 152, 157	0
10	1A	80/105 (76%)	-0.12	1 (1%) 75 55	129, 146, 156, 161	0
10	1I	91/105 (86%)	-0.18	0 100 100	87, 128, 159, 165	0
11	2A	113/129 (87%)	0.42	5 (4%) 39 24	94, 117, 130, 138	0
11	2I	111/129 (86%)	0.26	3 (2%) 56 36	85, 113, 127, 142	0
12	3A	122/132 (92%)	0.45	12 (9%) 13 9	89, 107, 130, 146	0
12	3I	122/132 (92%)	-0.18	1 (0%) 82 67	73, 82, 106, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	-0.22	2 (1%) 67 48	125, 145, 156, 160	0
13	4I	119/126 (94%)	-0.20	3 (2%) 58 39	93, 123, 136, 147	0
14	5A	59/61 (96%)	-0.07	2 (3%) 48 30	134, 143, 153, 154	0
14	5I	60/61 (98%)	-0.46	0 100 100	92, 103, 118, 131	0
15	6A	88/89 (98%)	-0.53	0 100 100	96, 119, 135, 139	0
15	6I	87/89 (97%)	-0.36	0 100 100	88, 104, 122, 127	0
16	7A	84/88 (95%)	-0.18	0 100 100	102, 117, 135, 152	0
16	7I	83/88 (94%)	-0.10	0 100 100	110, 119, 143, 150	0
17	8A	99/105 (94%)	-0.40	0 100 100	105, 120, 132, 133	0
17	8I	100/105 (95%)	-0.18	2 (2%) 65 45	98, 114, 124, 126	0
18	9A	67/88 (76%)	-0.18	2 (2%) 52 33	106, 121, 135, 142	0
18	9I	68/88 (77%)	-0.09	2 (2%) 53 35	94, 109, 133, 136	0
19	AA	62/93 (66%)	-0.03	2 (3%) 50 31	134, 149, 156, 158	0
19	AI	81/93 (87%)	-0.18	0 100 100	102, 122, 138, 151	0
20	BA	99/106 (93%)	-0.30	0 100 100	100, 118, 141, 152	0
20	BI	97/106 (91%)	-0.02	0 100 100	112, 125, 148, 157	0
21	1B	22/27 (81%)	-0.15	0 100 100	129, 137, 145, 148	0
21	1F	23/27 (85%)	-0.62	0 100 100	94, 112, 118, 122	0
22	1K	66/75 (88%)	-0.00	1 (1%) 72 52	85, 153, 177, 183	0
23	2K	72/77 (93%)	-0.52	1 (1%) 73 54	77, 104, 132, 146	0
23	2L	72/77 (93%)	-0.40	0 100 100	85, 122, 151, 162	0
24	3K	76/76 (100%)	0.50	4 (5%) 32 20	79, 178, 191, 196	0
25	4K	19/27 (70%)	0.41	1 (5%) 32 20	79, 152, 184, 184	0
25	4L	18/27 (66%)	0.05	0 100 100	101, 161, 187, 187	0
26	14	2861/2917 (98%)	-0.79	11 (0%) 88 79	55, 92, 180, 204	0
26	1H	2833/2917 (97%)	-0.94	3 (0%) 92 89	49, 79, 168, 203	0
27	16	122/122 (100%)	-1.10	0 100 100	74, 98, 119, 179	0
27	1J	122/122 (100%)	-0.74	1 (0%) 82 67	93, 125, 145, 177	0
28	71	133/229 (58%)	0.30	5 (3%) 44 27	143, 174, 185, 189	0
28	79	57/229 (24%)	0.16	1 (1%) 67 48	140, 165, 176, 179	0
29	11	273/276 (98%)	-0.14	1 (0%) 88 79	48, 71, 89, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	19	274/276 (99%)	0.14	6 (2%) 62 42	58, 82, 101, 117	0
30	21	203/206 (98%)	0.38	14 (6%) 23 14	55, 93, 139, 153	0
30	29	204/206 (99%)	-0.15	1 (0%) 87 76	60, 99, 134, 144	0
31	31	202/210 (96%)	-0.40	0 100 100	54, 84, 118, 142	0
31	39	204/210 (97%)	-0.10	0 100 100	62, 111, 151, 168	0
32	41	179/182 (98%)	-0.43	2 (1%) 78 61	85, 107, 140, 156	0
32	49	179/182 (98%)	0.32	8 (4%) 38 24	122, 139, 155, 171	0
33	51	171/180 (95%)	-0.04	2 (1%) 76 58	89, 110, 127, 139	0
33	59	73/180 (40%)	0.83	10 (13%) 6 5	136, 154, 165, 177	0
34	61	146/148 (98%)	-0.39	1 (0%) 84 69	83, 130, 143, 150	0
34	69	145/148 (97%)	-0.06	3 (2%) 63 43	93, 129, 147, 152	0
35	15	138/140 (98%)	0.25	1 (0%) 84 69	86, 114, 139, 155	0
35	58	138/140 (98%)	0.19	1 (0%) 84 69	68, 97, 130, 145	0
36	25	122/122 (100%)	0.16	2 (1%) 70 51	77, 94, 114, 120	0
36	68	122/122 (100%)	0.18	5 (4%) 41 25	64, 81, 99, 104	0
37	35	147/150 (98%)	0.15	9 (6%) 27 17	65, 111, 138, 144	0
37	78	147/150 (98%)	-0.09	4 (2%) 56 36	53, 88, 113, 120	0
38	45	138/141 (97%)	0.24	13 (9%) 14 9	78, 108, 128, 142	0
38	88	141/141 (100%)	-0.41	1 (0%) 84 69	63, 83, 108, 129	0
39	55	118/118 (100%)	-0.48	0 100 100	69, 86, 108, 127	0
39	98	118/118 (100%)	-0.07	2 (1%) 69 49	67, 90, 109, 122	0
40	65	110/112 (98%)	-0.38	1 (0%) 81 64	92, 117, 135, 142	0
40	A8	111/112 (99%)	-0.51	0 100 100	71, 93, 115, 123	0
41	75	133/146 (91%)	-0.01	6 (4%) 38 24	87, 101, 129, 141	0
41	B8	133/146 (91%)	0.27	10 (7%) 20 13	78, 98, 133, 149	0
42	85	116/118 (98%)	0.12	3 (2%) 57 37	73, 100, 132, 138	0
42	C8	115/118 (97%)	0.12	6 (5%) 33 21	59, 86, 114, 118	0
43	95	100/101 (99%)	0.33	3 (3%) 52 33	69, 121, 139, 153	0
43	D8	100/101 (99%)	0.35	4 (4%) 42 26	62, 106, 126, 144	0
44	A5	113/113 (100%)	-0.07	1 (0%) 81 64	68, 82, 112, 158	0
44	E8	112/113 (99%)	-0.22	2 (1%) 67 48	63, 79, 106, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	B5	94/96 (97%)	-0.27	0 100 100	77, 91, 118, 128	0
45	F8	95/96 (98%)	-0.23	0 100 100	60, 76, 104, 118	0
46	C5	104/110 (94%)	0.79	13 (12%) 8 6	91, 122, 149, 154	0
46	G8	105/110 (95%)	0.19	5 (4%) 35 22	75, 101, 131, 139	0
47	D5	132/206 (64%)	-0.27	2 (1%) 72 52	115, 135, 150, 158	0
47	H8	171/206 (83%)	-0.39	0 100 100	90, 122, 167, 172	0
48	E5	77/85 (90%)	0.02	3 (3%) 43 27	72, 94, 111, 131	0
48	I8	76/85 (89%)	-0.36	1 (1%) 75 55	61, 75, 90, 102	0
49	F5	94/98 (95%)	0.40	7 (7%) 20 13	67, 88, 121, 136	0
49	J8	94/98 (95%)	-0.06	3 (3%) 50 31	62, 77, 120, 122	0
50	G5	66/72 (91%)	-0.17	2 (3%) 52 33	87, 108, 126, 145	0
50	K8	68/72 (94%)	-0.14	1 (1%) 72 52	68, 84, 102, 124	0
51	H5	58/60 (96%)	-0.22	0 100 100	81, 106, 128, 135	0
51	L8	58/60 (96%)	-0.12	0 100 100	63, 85, 115, 127	0
52	M8	47/71 (66%)	-0.10	1 (2%) 63 43	109, 143, 158, 163	0
53	J5	56/60 (93%)	-0.19	0 100 100	66, 86, 141, 148	0
53	N8	48/60 (80%)	0.16	1 (2%) 63 43	56, 84, 140, 142	0
54	L5	47/49 (95%)	-0.38	1 (2%) 63 43	58, 66, 85, 91	0
54	P8	47/49 (95%)	-0.54	0 100 100	52, 57, 77, 88	0
55	M5	64/65 (98%)	0.11	2 (3%) 51 32	76, 85, 101, 117	0
55	Q8	64/65 (98%)	-0.29	0 100 100	61, 71, 88, 99	0
56	1L	68/76 (89%)	-0.16	4 (5%) 28 18	118, 173, 181, 188	0
57	3L	73/76 (96%)	0.21	3 (4%) 41 25	87, 172, 185, 190	0
All	All	20602/21966 (93%)	-0.39	270 (1%) 75 55	48, 107, 162, 204	0

The worst 5 of 270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	1	MET	8.5
12	3A	19	ARG	7.5
43	D8	37	VAL	7.0
41	75	104	ASN	6.5
41	75	106	SER	6.5

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	0.66	0.08	166,169,175,175	0
57	5MU	3L	54	21/22	0.68	0.09	162,169,172,173	0
56	T6A	1L	37	32/33	0.82	0.09	102,120,127,130	0
22	PSU	1K	55	20/21	0.84	0.08	109,120,133,134	0
56	PSU	1L	55	20/21	0.85	0.07	134,150,156,159	0
23	5MU	2L	55	21/22	0.87	0.10	128,133,141,143	0
56	U8U	1L	34	23/24	0.87	0.10	110,126,134,138	0
23	G7M	2L	47	24/25	0.87	0.10	129,137,150,151	0
57	PSU	3L	39	20/21	0.89	0.08	153,162,166,168	0
23	PSU	2K	56	20/21	0.89	0.07	104,113,121,127	0
23	5MU	2K	55	21/22	0.89	0.08	112,118,125,127	0
23	PSU	2L	56	20/21	0.90	0.08	116,129,133,137	0
56	5MU	1L	54	21/22	0.90	0.06	138,147,154,155	0
23	4SU	2K	8	20/21	0.91	0.08	93,98,102,106	0
23	4SU	2L	8	20/21	0.91	0.08	112,125,130,135	0
56	PSU	1L	39	20/21	0.92	0.07	105,127,133,134	0
22	5MU	1K	54	21/22	0.92	0.06	114,122,134,142	0
23	OMC	2L	33	21/22	0.94	0.09	109,114,117,125	0
23	G7M	2K	47	24/25	0.95	0.07	104,115,129,135	0
22	PSU	1K	39	20/21	0.95	0.06	79,98,105,108	0
22	U8U	1K	34	23/24	0.96	0.06	78,88,93,105	0
22	T6A	1K	37	32/33	0.96	0.07	76,86,103,106	0
23	OMC	2K	33	21/22	0.97	0.07	82,87,92,96	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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	3K	101	1/1	0.14	0.24	162,162,162,162	0
58	MG	1G	1668	1/1	0.41	0.33	116,116,116,116	0
58	MG	1G	1665	1/1	0.42	0.25	113,113,113,113	0
58	MG	14	3129	1/1	0.47	0.36	73,73,73,73	0
58	MG	14	3052	1/1	0.50	0.34	113,113,113,113	0
58	MG	14	3034	1/1	0.51	0.27	88,88,88,88	0
58	MG	1H	3287	1/1	0.52	0.28	104,104,104,104	0
58	MG	14	3316	1/1	0.53	0.28	122,122,122,122	0
58	MG	2K	103	1/1	0.55	0.26	114,114,114,114	0
58	MG	14	3293	1/1	0.56	0.37	91,91,91,91	0
58	MG	14	3310	1/1	0.56	0.23	114,114,114,114	0
58	MG	1H	3336	1/1	0.56	0.30	104,104,104,104	0
58	MG	14	3282	1/1	0.57	0.26	109,109,109,109	0
58	MG	14	3300	1/1	0.58	0.27	117,117,117,117	0
58	MG	14	3174	1/1	0.58	0.29	101,101,101,101	0
58	MG	14	3252	1/1	0.58	0.32	84,84,84,84	0
58	MG	1J	203	1/1	0.58	0.27	103,103,103,103	0
58	MG	14	3012	1/1	0.60	0.34	80,80,80,80	0
58	MG	13	1685	1/1	0.60	0.18	121,121,121,121	0
58	MG	1G	1664	1/1	0.61	0.26	100,100,100,100	0
58	MG	1H	3037	1/1	0.61	0.29	121,121,121,121	0
58	MG	1H	3342	1/1	0.61	0.37	92,92,92,92	0
58	MG	1G	1641	1/1	0.61	0.26	113,113,113,113	0
58	MG	14	3317	1/1	0.61	0.35	89,89,89,89	0
58	MG	1G	1644	1/1	0.61	0.41	92,92,92,92	0
58	MG	13	1657	1/1	0.62	0.24	103,103,103,103	0
58	MG	14	3184	1/1	0.62	0.24	98,98,98,98	0
58	MG	14	3288	1/1	0.62	0.31	86,86,86,86	0
58	MG	14	3238	1/1	0.63	0.22	99,99,99,99	0
58	MG	14	3108	1/1	0.63	0.30	92,92,92,92	0
58	MG	1H	3251	1/1	0.63	0.20	71,71,71,71	0
58	MG	1G	1634	1/1	0.63	0.24	112,112,112,112	0
58	MG	1G	1659	1/1	0.63	0.16	142,142,142,142	0
58	MG	14	3221	1/1	0.64	0.16	69,69,69,69	0
58	MG	14	3222	1/1	0.64	0.22	97,97,97,97	0
58	MG	1G	1635	1/1	0.64	0.26	107,107,107,107	0
58	MG	1H	3249	1/1	0.64	0.22	80,80,80,80	0
58	MG	1G	1661	1/1	0.64	0.26	123,123,123,123	0
58	MG	14	3057	1/1	0.64	0.28	101,101,101,101	0
58	MG	14	3303	1/1	0.65	0.22	106,106,106,106	0
58	MG	14	3308	1/1	0.65	0.28	106,106,106,106	0
58	MG	14	3017	1/1	0.65	0.28	90,90,90,90	0
58	MG	13	1688	1/1	0.65	0.28	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1602	1/1	0.65	0.32	79,79,79,79	0
58	MG	1H	3194	1/1	0.65	0.26	84,84,84,84	0
58	MG	14	3171	1/1	0.66	0.23	99,99,99,99	0
58	MG	1H	3308	1/1	0.66	0.32	90,90,90,90	0
58	MG	1H	3122	1/1	0.66	0.27	79,79,79,79	0
58	MG	1H	3255	1/1	0.66	0.34	73,73,73,73	0
58	MG	14	3290	1/1	0.66	0.22	92,92,92,92	0
58	MG	1H	3139	1/1	0.66	0.25	71,71,71,71	0
58	MG	14	3294	1/1	0.66	0.26	87,87,87,87	0
58	MG	1G	1611	1/1	0.67	0.27	104,104,104,104	0
58	MG	1H	3309	1/1	0.67	0.29	90,90,90,90	0
58	MG	14	3399	1/1	0.67	0.24	107,107,107,107	0
58	MG	13	1659	1/1	0.67	0.33	97,97,97,97	0
58	MG	13	1607	1/1	0.68	0.39	116,116,116,116	0
58	MG	14	3309	1/1	0.68	0.30	110,110,110,110	0
58	MG	1H	3222	1/1	0.68	0.25	98,98,98,98	0
58	MG	2K	102	1/1	0.68	0.39	94,94,94,94	0
58	MG	1G	1604	1/1	0.68	0.25	87,87,87,87	0
58	MG	1H	3016	1/1	0.68	0.36	75,75,75,75	0
58	MG	1G	1628	1/1	0.68	0.25	95,95,95,95	0
58	MG	13	1698	1/1	0.69	0.21	138,138,138,138	0
58	MG	14	3243	1/1	0.69	0.24	81,81,81,81	0
58	MG	1H	3279	1/1	0.69	0.20	67,67,67,67	0
58	MG	14	3255	1/1	0.69	0.22	78,78,78,78	0
58	MG	13	1623	1/1	0.69	0.28	108,108,108,108	0
58	MG	13	1672	1/1	0.69	0.20	109,109,109,109	0
58	MG	13	1699	1/1	0.70	0.30	94,94,94,94	0
58	MG	1H	3132	1/1	0.70	0.32	85,85,85,85	0
58	MG	14	3053	1/1	0.70	0.17	61,61,61,61	0
58	MG	14	3193	1/1	0.70	0.29	77,77,77,77	0
58	MG	13	1692	1/1	0.70	0.18	122,122,122,122	0
58	MG	1H	3171	1/1	0.70	0.30	83,83,83,83	0
58	MG	14	3292	1/1	0.70	0.11	113,113,113,113	0
58	MG	14	3231	1/1	0.70	0.28	86,86,86,86	0
58	MG	13	1678	1/1	0.70	0.26	93,93,93,93	0
58	MG	1H	3118	1/1	0.71	0.37	77,77,77,77	0
58	MG	1G	1674	1/1	0.71	0.22	102,102,102,102	0
58	MG	14	3242	1/1	0.71	0.27	67,67,67,67	0
58	MG	14	3168	1/1	0.71	0.32	106,106,106,106	0
58	MG	13	1615	1/1	0.71	0.32	77,77,77,77	0
58	MG	1H	3313	1/1	0.71	0.24	98,98,98,98	0
58	MG	14	3258	1/1	0.71	0.36	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3330	1/1	0.71	0.20	102,102,102,102	0
58	MG	1G	1614	1/1	0.71	0.27	107,107,107,107	0
58	MG	1H	3201	1/1	0.71	0.31	92,92,92,92	0
58	MG	1H	3341	1/1	0.71	0.20	79,79,79,79	0
58	MG	1G	1675	1/1	0.72	0.30	91,91,91,91	0
58	MG	14	3185	1/1	0.72	0.33	82,82,82,82	0
58	MG	2L	102	1/1	0.72	0.27	83,83,83,83	0
58	MG	14	3089	1/1	0.72	0.41	79,79,79,79	0
58	MG	1H	3236	1/1	0.72	0.19	99,99,99,99	0
58	MG	1G	1654	1/1	0.72	0.36	83,83,83,83	0
58	MG	14	3023	1/1	0.72	0.24	83,83,83,83	0
58	MG	13	1689	1/1	0.72	0.28	107,107,107,107	0
58	MG	1H	3292	1/1	0.72	0.21	77,77,77,77	0
58	MG	45	201	1/1	0.72	0.22	108,108,108,108	0
58	MG	13	1704	1/1	0.73	0.26	82,82,82,82	0
58	MG	14	3068	1/1	0.73	0.34	100,100,100,100	0
58	MG	1H	3286	1/1	0.73	0.26	94,94,94,94	0
58	MG	13	1604	1/1	0.73	0.28	87,87,87,87	0
58	MG	1H	3021	1/1	0.73	0.19	83,83,83,83	0
58	MG	14	3223	1/1	0.73	0.19	86,86,86,86	0
58	MG	14	3227	1/1	0.73	0.27	76,76,76,76	0
58	MG	13	1695	1/1	0.73	0.30	83,83,83,83	0
58	MG	1H	3265	1/1	0.73	0.26	78,78,78,78	0
58	MG	1H	3278	1/1	0.73	0.31	95,95,95,95	0
58	MG	14	3133	1/1	0.74	0.22	107,107,107,107	0
58	MG	14	3143	1/1	0.74	0.23	102,102,102,102	0
58	MG	13	1631	1/1	0.74	0.28	93,93,93,93	0
58	MG	1G	1638	1/1	0.74	0.28	93,93,93,93	0
58	MG	13	1632	1/1	0.74	0.28	107,107,107,107	0
58	MG	1G	1673	1/1	0.74	0.25	93,93,93,93	0
58	MG	13	1624	1/1	0.74	0.27	103,103,103,103	0
58	MG	1G	1629	1/1	0.74	0.35	104,104,104,104	0
58	MG	14	3211	1/1	0.74	0.26	91,91,91,91	0
58	MG	1G	1633	1/1	0.74	0.23	98,98,98,98	0
58	MG	1H	3217	1/1	0.74	0.28	71,71,71,71	0
58	MG	1J	204	1/1	0.74	0.26	101,101,101,101	0
58	MG	1G	1663	1/1	0.74	0.26	94,94,94,94	0
58	MG	1G	1660	1/1	0.75	0.23	85,85,85,85	0
58	MG	1H	3160	1/1	0.75	0.12	72,72,72,72	0
58	MG	1H	3167	1/1	0.75	0.31	93,93,93,93	0
58	MG	14	3217	1/1	0.75	0.19	83,83,83,83	0
58	MG	1H	3319	1/1	0.75	0.32	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1681	1/1	0.75	0.18	116,116,116,116	0
58	MG	14	3301	1/1	0.75	0.20	109,109,109,109	0
58	MG	1H	3334	1/1	0.75	0.23	76,76,76,76	0
58	MG	13	1653	1/1	0.75	0.28	72,72,72,72	0
58	MG	1H	3044	1/1	0.75	0.20	82,82,82,82	0
58	MG	13	1696	1/1	0.75	0.29	92,92,92,92	0
58	MG	14	3135	1/1	0.75	0.23	95,95,95,95	0
58	MG	1G	1642	1/1	0.75	0.23	91,91,91,91	0
58	MG	13	1670	1/1	0.75	0.19	97,97,97,97	0
58	MG	1H	3013	1/1	0.75	0.27	82,82,82,82	0
58	MG	14	3020	1/1	0.75	0.29	75,75,75,75	0
58	MG	13	1680	1/1	0.75	0.23	96,96,96,96	0
58	MG	1H	3033	1/1	0.76	0.28	88,88,88,88	0
58	MG	1G	1605	1/1	0.76	0.27	101,101,101,101	0
58	MG	14	3283	1/1	0.76	0.11	69,69,69,69	0
58	MG	1H	3185	1/1	0.76	0.27	95,95,95,95	0
58	MG	13	1679	1/1	0.76	0.24	100,100,100,100	0
58	MG	14	3191	1/1	0.76	0.28	96,96,96,96	0
58	MG	1H	3316	1/1	0.76	0.38	92,92,92,92	0
58	MG	1H	3043	1/1	0.76	0.35	81,81,81,81	0
58	MG	14	3059	1/1	0.76	0.35	86,86,86,86	0
58	MG	1H	3321	1/1	0.76	0.19	67,67,67,67	0
58	MG	14	3302	1/1	0.76	0.29	66,66,66,66	0
58	MG	14	3080	1/1	0.76	0.33	82,82,82,82	0
58	MG	1H	3154	1/1	0.76	0.27	84,84,84,84	0
58	MG	14	3096	1/1	0.76	0.27	73,73,73,73	0
58	MG	13	1701	1/1	0.76	0.18	114,114,114,114	0
58	MG	14	3311	1/1	0.76	0.33	100,100,100,100	0
58	MG	14	3235	1/1	0.76	0.35	72,72,72,72	0
58	MG	13	1662	1/1	0.76	0.21	118,118,118,118	0
58	MG	1H	3170	1/1	0.76	0.18	65,65,65,65	0
58	MG	1H	3300	1/1	0.76	0.26	87,87,87,87	0
58	MG	1H	3306	1/1	0.76	0.20	91,91,91,91	0
58	MG	35	201	1/1	0.76	0.21	74,74,74,74	0
58	MG	1G	1653	1/1	0.76	0.26	97,97,97,97	0
58	MG	1H	3331	1/1	0.77	0.28	73,73,73,73	0
58	MG	14	3058	1/1	0.77	0.19	84,84,84,84	0
58	MG	13	1687	1/1	0.77	0.29	99,99,99,99	0
58	MG	1E	301	1/1	0.77	0.26	106,106,106,106	0
58	MG	1G	1655	1/1	0.77	0.20	100,100,100,100	0
58	MG	1G	1630	1/1	0.77	0.25	103,103,103,103	0
58	MG	14	3197	1/1	0.77	0.21	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3265	1/1	0.77	0.27	98,98,98,98	0
58	MG	14	3313	1/1	0.77	0.19	92,92,92,92	0
58	MG	14	3315	1/1	0.77	0.28	93,93,93,93	0
58	MG	1H	3196	1/1	0.77	0.30	83,83,83,83	0
58	MG	1H	3027	1/1	0.77	0.20	81,81,81,81	0
58	MG	14	3022	1/1	0.77	0.20	64,64,64,64	0
58	MG	13	1702	1/1	0.77	0.34	98,98,98,98	0
58	MG	1H	3293	1/1	0.77	0.20	84,84,84,84	0
58	MG	1H	3220	1/1	0.77	0.15	82,82,82,82	0
58	MG	1H	3305	1/1	0.77	0.19	67,67,67,67	0
58	MG	1G	1603	1/1	0.78	0.41	102,102,102,102	0
58	MG	1H	3328	1/1	0.78	0.25	80,80,80,80	0
58	MG	1H	3152	1/1	0.78	0.30	100,100,100,100	0
58	MG	14	3099	1/1	0.78	0.27	87,87,87,87	0
58	MG	14	3295	1/1	0.78	0.20	85,85,85,85	0
58	MG	14	3299	1/1	0.78	0.22	98,98,98,98	0
58	MG	1G	1650	1/1	0.78	0.24	114,114,114,114	0
58	MG	1H	3219	1/1	0.78	0.17	103,103,103,103	0
58	MG	1H	3333	1/1	0.78	0.29	100,100,100,100	0
58	MG	1G	1615	1/1	0.78	0.26	125,125,125,125	0
58	MG	1H	3314	1/1	0.78	0.25	85,85,85,85	0
58	MG	14	3146	1/1	0.78	0.29	57,57,57,57	0
58	MG	14	3152	1/1	0.78	0.24	92,92,92,92	0
58	MG	14	3155	1/1	0.78	0.28	64,64,64,64	0
58	MG	14	3250	1/1	0.78	0.30	78,78,78,78	0
58	MG	14	3314	1/1	0.78	0.20	94,94,94,94	0
58	MG	1H	3335	1/1	0.78	0.31	74,74,74,74	0
58	MG	14	3254	1/1	0.78	0.18	111,111,111,111	0
58	MG	1H	3199	1/1	0.78	0.21	69,69,69,69	0
58	MG	13	1660	1/1	0.78	0.20	103,103,103,103	0
58	MG	1H	3224	1/1	0.78	0.32	73,73,73,73	0
58	MG	16	203	1/1	0.78	0.12	90,90,90,90	0
58	MG	1H	3324	1/1	0.78	0.34	89,89,89,89	0
58	MG	1G	1640	1/1	0.78	0.30	87,87,87,87	0
58	MG	14	3204	1/1	0.79	0.16	77,77,77,77	0
58	MG	14	3150	1/1	0.79	0.20	87,87,87,87	0
58	MG	14	3304	1/1	0.79	0.36	92,92,92,92	0
58	MG	1G	1617	1/1	0.79	0.15	135,135,135,135	0
58	MG	1H	3073	1/1	0.79	0.26	81,81,81,81	0
58	MG	14	3267	1/1	0.79	0.18	92,92,92,92	0
58	MG	1G	1646	1/1	0.79	0.23	100,100,100,100	0
58	MG	1G	1637	1/1	0.79	0.29	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3224	1/1	0.79	0.26	90,90,90,90	0
58	MG	1H	3237	1/1	0.79	0.19	84,84,84,84	0
58	MG	1H	3327	1/1	0.79	0.35	82,82,82,82	0
58	MG	1H	3144	1/1	0.79	0.30	77,77,77,77	0
58	MG	14	3190	1/1	0.79	0.25	86,86,86,86	0
58	MG	14	3079	1/1	0.79	0.28	70,70,70,70	0
58	MG	1G	1657	1/1	0.79	0.29	92,92,92,92	0
58	MG	14	3147	1/1	0.79	0.20	95,95,95,95	0
58	MG	14	3203	1/1	0.79	0.22	56,56,56,56	0
58	MG	1H	3268	1/1	0.80	0.31	85,85,85,85	0
58	MG	1H	3107	1/1	0.80	0.22	71,71,71,71	0
58	MG	14	3251	1/1	0.80	0.29	69,69,69,69	0
58	MG	1H	3232	1/1	0.80	0.15	52,52,52,52	0
58	MG	1G	1662	1/1	0.80	0.24	72,72,72,72	0
58	MG	1H	3233	1/1	0.80	0.37	62,62,62,62	0
58	MG	1H	3028	1/1	0.80	0.19	68,68,68,68	0
58	MG	14	3262	1/1	0.80	0.29	96,96,96,96	0
58	MG	1G	1618	1/1	0.80	0.26	109,109,109,109	0
58	MG	14	3312	1/1	0.80	0.23	80,80,80,80	0
58	MG	13	1697	1/1	0.80	0.19	92,92,92,92	0
58	MG	1H	3071	1/1	0.80	0.33	61,61,61,61	0
58	MG	14	3067	1/1	0.80	0.19	87,87,87,87	0
58	MG	1H	3298	1/1	0.80	0.21	74,74,74,74	0
58	MG	1H	3072	1/1	0.80	0.24	77,77,77,77	0
58	MG	13	1706	1/1	0.80	0.26	109,109,109,109	0
58	MG	1H	3090	1/1	0.80	0.21	71,71,71,71	0
58	MG	14	3236	1/1	0.80	0.23	89,89,89,89	0
58	MG	39	301	1/1	0.80	0.17	96,96,96,96	0
58	MG	1G	1658	1/1	0.80	0.24	92,92,92,92	0
58	MG	14	3019	1/1	0.80	0.32	90,90,90,90	0
58	MG	14	3276	1/1	0.81	0.26	92,92,92,92	0
58	MG	1H	3239	1/1	0.81	0.19	75,75,75,75	0
58	MG	13	1605	1/1	0.81	0.24	76,76,76,76	0
58	MG	1H	3020	1/1	0.81	0.19	66,66,66,66	0
58	MG	1H	3254	1/1	0.81	0.29	99,99,99,99	0
58	MG	14	3291	1/1	0.81	0.27	87,87,87,87	0
58	MG	1H	3045	1/1	0.81	0.25	82,82,82,82	0
58	MG	13	1656	1/1	0.81	0.14	103,103,103,103	0
58	MG	1H	3204	1/1	0.81	0.28	69,69,69,69	0
58	MG	1H	3269	1/1	0.81	0.16	65,65,65,65	0
58	MG	1H	3211	1/1	0.81	0.18	83,83,83,83	0
58	MG	1H	3216	1/1	0.81	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3283	1/1	0.81	0.24	92,92,92,92	0
58	MG	1H	3024	1/1	0.81	0.44	82,82,82,82	0
58	MG	13	1700	1/1	0.81	0.18	94,94,94,94	0
58	MG	1H	3089	1/1	0.81	0.22	59,59,59,59	0
58	MG	13	1677	1/1	0.81	0.21	104,104,104,104	0
58	MG	14	3144	1/1	0.81	0.36	71,71,71,71	0
58	MG	14	3009	1/1	0.81	0.26	52,52,52,52	0
58	MG	1H	3337	1/1	0.81	0.19	89,89,89,89	0
58	MG	14	3247	1/1	0.81	0.20	67,67,67,67	0
58	MG	1H	3340	1/1	0.81	0.32	78,78,78,78	0
58	MG	13	1661	1/1	0.81	0.27	103,103,103,103	0
58	MG	1H	3116	1/1	0.81	0.26	55,55,55,55	0
58	MG	1H	3176	1/1	0.81	0.30	76,76,76,76	0
58	MG	1G	1647	1/1	0.81	0.27	83,83,83,83	0
58	MG	78	201	1/1	0.81	0.29	70,70,70,70	0
58	MG	14	3260	1/1	0.81	0.24	72,72,72,72	0
58	MG	14	3035	1/1	0.81	0.16	93,93,93,93	0
58	MG	13	1625	1/1	0.81	0.29	86,86,86,86	0
58	MG	1H	3187	1/1	0.81	0.20	69,69,69,69	0
58	MG	35	202	1/1	0.81	0.15	87,87,87,87	0
58	MG	35	203	1/1	0.81	0.38	75,75,75,75	0
58	MG	14	3271	1/1	0.81	0.16	81,81,81,81	0
58	MG	14	3192	1/1	0.82	0.30	63,63,63,63	0
58	MG	14	3279	1/1	0.82	0.17	104,104,104,104	0
58	MG	14	3280	1/1	0.82	0.25	86,86,86,86	0
58	MG	1G	1672	1/1	0.82	0.30	99,99,99,99	0
58	MG	1G	1607	1/1	0.82	0.19	73,73,73,73	0
58	MG	13	1629	1/1	0.82	0.21	96,96,96,96	0
58	MG	13	1705	1/1	0.82	0.28	90,90,90,90	0
58	MG	1H	3172	1/1	0.82	0.23	87,87,87,87	0
58	MG	14	3214	1/1	0.82	0.24	88,88,88,88	0
58	MG	14	3100	1/1	0.82	0.25	76,76,76,76	0
58	MG	14	3106	1/1	0.82	0.23	61,61,61,61	0
58	MG	14	3004	1/1	0.82	0.18	67,67,67,67	0
58	MG	14	3111	1/1	0.82	0.15	81,81,81,81	0
58	MG	14	3117	1/1	0.82	0.30	81,81,81,81	0
58	MG	1G	1616	1/1	0.82	0.28	87,87,87,87	0
58	MG	14	3229	1/1	0.82	0.51	88,88,88,88	0
58	MG	1G	1652	1/1	0.82	0.28	71,71,71,71	0
58	MG	1H	3079	1/1	0.82	0.20	79,79,79,79	0
58	MG	1H	3262	1/1	0.82	0.26	94,94,94,94	0
58	MG	1H	3184	1/1	0.82	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1656	1/1	0.82	0.31	78,78,78,78	0
58	MG	13	1648	1/1	0.82	0.21	95,95,95,95	0
58	MG	1H	3050	1/1	0.82	0.28	60,60,60,60	0
58	MG	1H	3190	1/1	0.82	0.20	73,73,73,73	0
58	MG	14	3153	1/1	0.82	0.29	89,89,89,89	0
58	MG	1H	3191	1/1	0.82	0.26	90,90,90,90	0
58	MG	14	3253	1/1	0.82	0.18	94,94,94,94	0
58	MG	1H	3101	1/1	0.82	0.18	59,59,59,59	0
58	MG	1G	1636	1/1	0.82	0.23	101,101,101,101	0
58	MG	1J	202	1/1	0.82	0.22	95,95,95,95	0
58	MG	1H	3056	1/1	0.82	0.27	56,56,56,56	0
58	MG	14	3179	1/1	0.82	0.21	60,60,60,60	0
58	MG	1H	3108	1/1	0.82	0.24	74,74,74,74	0
58	MG	13	1652	1/1	0.82	0.19	99,99,99,99	0
58	MG	1H	3247	1/1	0.82	0.20	81,81,81,81	0
58	MG	14	3269	1/1	0.82	0.41	88,88,88,88	0
58	MG	14	3074	1/1	0.82	0.41	79,79,79,79	0
58	MG	14	3029	1/1	0.83	0.24	78,78,78,78	0
58	MG	14	3139	1/1	0.83	0.14	99,99,99,99	0
58	MG	13	1676	1/1	0.83	0.23	76,76,76,76	0
58	MG	13	1646	1/1	0.83	0.24	75,75,75,75	0
58	MG	14	3044	1/1	0.83	0.28	64,64,64,64	0
58	MG	14	3048	1/1	0.83	0.19	90,90,90,90	0
58	MG	14	3050	1/1	0.83	0.37	59,59,59,59	0
58	MG	13	1658	1/1	0.83	0.17	83,83,83,83	0
58	MG	1H	3036	1/1	0.83	0.46	100,100,100,100	0
58	MG	1H	3297	1/1	0.83	0.14	99,99,99,99	0
58	MG	14	3165	1/1	0.83	0.27	77,77,77,77	0
58	MG	1H	3230	1/1	0.83	0.28	43,43,43,43	0
58	MG	14	3305	1/1	0.83	0.18	75,75,75,75	0
58	MG	1H	3264	1/1	0.83	0.16	76,76,76,76	0
58	MG	1H	3304	1/1	0.83	0.20	86,86,86,86	0
58	MG	1H	3019	1/1	0.83	0.39	92,92,92,92	0
58	MG	14	3181	1/1	0.83	0.25	89,89,89,89	0
58	MG	5E	201	1/1	0.83	0.17	89,89,89,89	0
58	MG	2L	101	1/1	0.83	0.30	73,73,73,73	0
58	MG	14	3259	1/1	0.83	0.66	98,98,98,98	0
58	MG	1H	3182	1/1	0.83	0.13	78,78,78,78	0
58	MG	1G	1625	1/1	0.83	0.20	93,93,93,93	0
58	MG	13	1647	1/1	0.83	0.21	89,89,89,89	0
58	MG	13	1602	1/1	0.83	0.16	86,86,86,86	0
58	MG	1J	201	1/1	0.83	0.22	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3013	1/1	0.83	0.25	78,78,78,78	0
58	MG	14	3015	1/1	0.83	0.43	49,49,49,49	0
58	MG	1H	3282	1/1	0.83	0.39	88,88,88,88	0
58	MG	1G	1631	1/1	0.83	0.17	96,96,96,96	0
58	MG	14	3113	1/1	0.83	0.27	73,73,73,73	0
58	MG	16	202	1/1	0.83	0.11	64,64,64,64	0
58	MG	1H	3025	1/1	0.83	0.28	64,64,64,64	0
58	MG	1H	3284	1/1	0.83	0.29	81,81,81,81	0
58	MG	1H	3010	1/1	0.84	0.30	63,63,63,63	0
58	MG	1G	1606	1/1	0.84	0.24	88,88,88,88	0
58	MG	1H	3242	1/1	0.84	0.25	52,52,52,52	0
58	MG	14	3296	1/1	0.84	0.17	84,84,84,84	0
58	MG	14	3297	1/1	0.84	0.36	70,70,70,70	0
58	MG	14	3244	1/1	0.84	0.28	70,70,70,70	0
58	MG	14	3245	1/1	0.84	0.28	77,77,77,77	0
58	MG	14	3175	1/1	0.84	0.16	92,92,92,92	0
58	MG	1H	3011	1/1	0.84	0.28	51,51,51,51	0
58	MG	1G	1612	1/1	0.84	0.25	81,81,81,81	0
58	MG	13	1640	1/1	0.84	0.29	74,74,74,74	0
58	MG	1G	1667	1/1	0.84	0.23	109,109,109,109	0
58	MG	13	1671	1/1	0.84	0.18	87,87,87,87	0
58	MG	14	3038	1/1	0.84	0.19	71,71,71,71	0
58	MG	14	3121	1/1	0.84	0.28	78,78,78,78	0
58	MG	1G	1670	1/1	0.84	0.33	86,86,86,86	0
58	MG	14	3131	1/1	0.84	0.23	95,95,95,95	0
58	MG	14	3132	1/1	0.84	0.23	68,68,68,68	0
58	MG	1H	3205	1/1	0.84	0.13	81,81,81,81	0
58	MG	1H	3209	1/1	0.84	0.30	90,90,90,90	0
58	MG	1H	3258	1/1	0.84	0.19	59,59,59,59	0
58	MG	1H	3259	1/1	0.84	0.28	79,79,79,79	0
58	MG	14	3397	1/1	0.84	0.41	73,73,73,73	0
58	MG	14	3275	1/1	0.84	0.23	91,91,91,91	0
58	MG	1H	3376	1/1	0.84	0.14	76,76,76,76	0
58	MG	1H	3290	1/1	0.84	0.15	70,70,70,70	0
58	MG	1H	3291	1/1	0.84	0.10	73,73,73,73	0
58	MG	14	3007	1/1	0.84	0.20	54,54,54,54	0
58	MG	13	1669	1/1	0.84	0.27	68,68,68,68	0
58	MG	1H	3263	1/1	0.84	0.12	76,76,76,76	0
58	MG	1H	3007	1/1	0.84	0.20	54,54,54,54	0
58	MG	14	3163	1/1	0.84	0.21	90,90,90,90	0
58	MG	1H	3009	1/1	0.84	0.17	62,62,62,62	0
58	MG	14	3126	1/1	0.85	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3031	1/1	0.85	0.28	76,76,76,76	0
58	MG	14	3249	1/1	0.85	0.24	80,80,80,80	0
58	MG	14	3187	1/1	0.85	0.28	80,80,80,80	0
58	MG	14	3189	1/1	0.85	0.13	82,82,82,82	0
58	MG	14	3130	1/1	0.85	0.23	86,86,86,86	0
58	MG	98	201	1/1	0.85	0.23	72,72,72,72	0
58	MG	14	3065	1/1	0.85	0.26	67,67,67,67	0
58	MG	I8	101	1/1	0.85	0.34	73,73,73,73	0
58	MG	Q8	101	1/1	0.85	0.26	70,70,70,70	0
58	MG	1G	1601	1/1	0.85	0.21	91,91,91,91	0
58	MG	1H	3081	1/1	0.85	0.20	87,87,87,87	0
58	MG	13	1606	1/1	0.85	0.29	94,94,94,94	0
58	MG	14	3081	1/1	0.85	0.23	76,76,76,76	0
58	MG	14	3266	1/1	0.85	0.28	85,85,85,85	0
58	MG	13	1618	1/1	0.85	0.26	80,80,80,80	0
58	MG	14	3148	1/1	0.85	0.29	77,77,77,77	0
58	MG	14	3095	1/1	0.85	0.24	71,71,71,71	0
58	MG	1H	3174	1/1	0.85	0.24	88,88,88,88	0
58	MG	1H	3197	1/1	0.85	0.29	80,80,80,80	0
58	MG	1H	3065	1/1	0.85	0.24	61,61,61,61	0
58	MG	1H	3271	1/1	0.85	0.22	76,76,76,76	0
58	MG	14	3281	1/1	0.85	0.20	86,86,86,86	0
58	MG	13	1603	1/1	0.85	0.21	92,92,92,92	0
58	MG	1H	3226	1/1	0.85	0.26	85,85,85,85	0
58	MG	14	3112	1/1	0.85	0.26	65,65,65,65	0
58	MG	13	1608	1/1	0.85	0.31	90,90,90,90	0
58	MG	14	3239	1/1	0.85	0.14	80,80,80,80	0
58	MG	14	3054	1/1	0.85	0.24	70,70,70,70	0
58	MG	14	3120	1/1	0.85	0.23	82,82,82,82	0
58	MG	13	1609	1/1	0.85	0.18	75,75,75,75	0
58	MG	1H	3223	1/1	0.86	0.26	78,78,78,78	0
58	MG	14	3180	1/1	0.86	0.26	88,88,88,88	0
58	MG	13	1691	1/1	0.86	0.20	90,90,90,90	0
58	MG	1H	3307	1/1	0.86	0.28	94,94,94,94	0
58	MG	1H	3252	1/1	0.86	0.31	66,66,66,66	0
58	MG	1H	3225	1/1	0.86	0.22	78,78,78,78	0
58	MG	1H	3207	1/1	0.86	0.28	84,84,84,84	0
58	MG	1H	3227	1/1	0.86	0.40	85,85,85,85	0
58	MG	13	1654	1/1	0.86	0.19	74,74,74,74	0
58	MG	14	3060	1/1	0.86	0.16	73,73,73,73	0
58	MG	14	3008	1/1	0.86	0.23	65,65,65,65	0
58	MG	14	3194	1/1	0.86	0.21	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3260	1/1	0.86	0.26	72,72,72,72	0
58	MG	14	3201	1/1	0.86	0.14	59,59,59,59	0
58	MG	1G	1626	1/1	0.86	0.24	82,82,82,82	0
58	MG	14	3142	1/1	0.86	0.25	76,76,76,76	0
58	MG	16	204	1/1	0.86	0.15	73,73,73,73	0
58	MG	1H	3130	1/1	0.86	0.24	74,74,74,74	0
58	MG	1H	3323	1/1	0.86	0.28	80,80,80,80	0
58	MG	14	3018	1/1	0.86	0.25	72,72,72,72	0
58	MG	1H	3213	1/1	0.86	0.18	74,74,74,74	0
58	MG	14	3094	1/1	0.86	0.30	60,60,60,60	0
58	MG	I8	102	1/1	0.86	0.15	70,70,70,70	0
58	MG	1H	3162	1/1	0.86	0.23	88,88,88,88	0
58	MG	14	3098	1/1	0.86	0.13	93,93,93,93	0
58	MG	14	3230	1/1	0.86	0.16	64,64,64,64	0
58	MG	1H	3294	1/1	0.86	0.15	57,57,57,57	0
58	MG	1H	3060	1/1	0.86	0.21	61,61,61,61	0
58	MG	13	1667	1/1	0.86	0.22	71,71,71,71	0
58	MG	1H	3332	1/1	0.86	0.20	74,74,74,74	0
58	MG	1H	3003	1/1	0.86	0.19	64,64,64,64	0
58	MG	1H	3188	1/1	0.86	0.25	73,73,73,73	0
58	MG	14	3037	1/1	0.87	0.26	106,106,106,106	0
58	MG	1G	1666	1/1	0.87	0.32	84,84,84,84	0
58	MG	1H	3322	1/1	0.87	0.27	81,81,81,81	0
58	MG	1H	3093	1/1	0.87	0.24	72,72,72,72	0
58	MG	14	3049	1/1	0.87	0.16	70,70,70,70	0
58	MG	14	3278	1/1	0.87	0.28	75,75,75,75	0
58	MG	14	3196	1/1	0.87	0.31	75,75,75,75	0
58	MG	1H	3100	1/1	0.87	0.14	61,61,61,61	0
58	MG	1G	1639	1/1	0.87	0.17	74,74,74,74	0
58	MG	14	3122	1/1	0.87	0.18	88,88,88,88	0
58	MG	1H	3069	1/1	0.87	0.19	90,90,90,90	0
58	MG	14	3205	1/1	0.87	0.27	96,96,96,96	0
58	MG	14	3289	1/1	0.87	0.30	83,83,83,83	0
58	MG	1H	3256	1/1	0.87	0.11	61,61,61,61	0
58	MG	13	1668	1/1	0.87	0.14	90,90,90,90	0
58	MG	1H	3164	1/1	0.87	0.19	64,64,64,64	0
58	MG	1H	3004	1/1	0.87	0.20	57,57,57,57	0
58	MG	1H	3296	1/1	0.87	0.14	57,57,57,57	0
58	MG	14	3134	1/1	0.87	0.20	74,74,74,74	0
58	MG	13	1621	1/1	0.87	0.19	90,90,90,90	0
58	MG	1H	3075	1/1	0.87	0.18	43,43,43,43	0
58	MG	14	3140	1/1	0.87	0.23	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3203	1/1	0.87	0.29	79,79,79,79	0
58	MG	14	3070	1/1	0.87	0.23	60,60,60,60	0
58	MG	14	3232	1/1	0.87	0.17	81,81,81,81	0
58	MG	14	3234	1/1	0.87	0.27	70,70,70,70	0
58	MG	14	3071	1/1	0.87	0.21	68,68,68,68	0
58	MG	14	3073	1/1	0.87	0.44	83,83,83,83	0
58	MG	1H	3303	1/1	0.87	0.36	78,78,78,78	0
58	MG	14	3076	1/1	0.87	0.20	62,62,62,62	0
58	MG	14	3077	1/1	0.87	0.23	68,68,68,68	0
58	MG	1H	3058	1/1	0.87	0.24	46,46,46,46	0
58	MG	1H	3125	1/1	0.87	0.29	69,69,69,69	0
58	MG	1H	3206	1/1	0.87	0.31	77,77,77,77	0
58	MG	14	3082	1/1	0.87	0.30	61,61,61,61	0
58	MG	14	3248	1/1	0.87	0.15	79,79,79,79	0
58	MG	14	3083	1/1	0.87	0.28	72,72,72,72	0
58	MG	14	3084	1/1	0.87	0.28	80,80,80,80	0
58	MG	1H	3080	1/1	0.87	0.17	65,65,65,65	0
58	MG	14	3091	1/1	0.87	0.24	86,86,86,86	0
58	MG	1H	3275	1/1	0.87	0.24	75,75,75,75	0
58	MG	14	3177	1/1	0.87	0.26	72,72,72,72	0
58	MG	1H	3179	1/1	0.87	0.18	83,83,83,83	0
58	MG	1H	3059	1/1	0.87	0.19	49,49,49,49	0
58	MG	29	301	1/1	0.87	0.23	77,77,77,77	0
58	MG	13	1686	1/1	0.87	0.20	76,76,76,76	0
58	MG	1H	3032	1/1	0.87	0.28	79,79,79,79	0
58	MG	1H	3149	1/1	0.87	0.33	60,60,60,60	0
58	MG	1H	3285	1/1	0.87	0.28	68,68,68,68	0
58	MG	14	3107	1/1	0.87	0.30	77,77,77,77	0
58	MG	14	3285	1/1	0.88	0.10	68,68,68,68	0
58	MG	14	3287	1/1	0.88	0.13	82,82,82,82	0
58	MG	14	3055	1/1	0.88	0.16	81,81,81,81	0
58	MG	1H	3165	1/1	0.88	0.32	78,78,78,78	0
58	MG	1G	1627	1/1	0.88	0.16	94,94,94,94	0
58	MG	14	3233	1/1	0.88	0.13	86,86,86,86	0
58	MG	1H	3318	1/1	0.88	0.26	79,79,79,79	0
58	MG	13	1635	1/1	0.88	0.33	74,74,74,74	0
58	MG	1H	3168	1/1	0.88	0.21	69,69,69,69	0
58	MG	14	3118	1/1	0.88	0.27	69,69,69,69	0
58	MG	13	1703	1/1	0.88	0.34	77,77,77,77	0
58	MG	1H	3137	1/1	0.88	0.24	88,88,88,88	0
58	MG	14	3069	1/1	0.88	0.17	70,70,70,70	0
58	MG	14	3186	1/1	0.88	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3218	1/1	0.88	0.19	56,56,56,56	0
58	MG	14	3188	1/1	0.88	0.27	88,88,88,88	0
58	MG	1H	3295	1/1	0.88	0.27	93,93,93,93	0
58	MG	1H	3266	1/1	0.88	0.13	81,81,81,81	0
58	MG	13	1639	1/1	0.88	0.32	82,82,82,82	0
58	MG	14	3026	1/1	0.88	0.23	89,89,89,89	0
58	MG	14	3027	1/1	0.88	0.28	96,96,96,96	0
58	MG	1H	3243	1/1	0.88	0.24	65,65,65,65	0
58	MG	14	3030	1/1	0.88	0.23	86,86,86,86	0
58	MG	1H	3049	1/1	0.88	0.29	52,52,52,52	0
58	MG	1H	3302	1/1	0.88	0.19	92,92,92,92	0
58	MG	13	1627	1/1	0.88	0.30	69,69,69,69	0
58	MG	1H	3277	1/1	0.88	0.15	68,68,68,68	0
58	MG	14	3085	1/1	0.88	0.12	67,67,67,67	0
58	MG	14	3210	1/1	0.88	0.15	80,80,80,80	0
58	MG	14	3042	1/1	0.88	0.32	70,70,70,70	0
58	MG	13	1651	1/1	0.88	0.31	88,88,88,88	0
58	MG	14	3215	1/1	0.88	0.22	72,72,72,72	0
58	MG	14	3045	1/1	0.88	0.15	58,58,58,58	0
58	MG	1H	3038	1/1	0.88	0.18	92,92,92,92	0
58	MG	1H	3253	1/1	0.88	0.11	66,66,66,66	0
58	MG	1H	3094	1/1	0.88	0.21	64,64,64,64	0
58	MG	1H	3128	1/1	0.88	0.08	62,62,62,62	0
58	MG	14	3226	1/1	0.88	0.19	73,73,73,73	0
58	MG	1H	3129	1/1	0.88	0.30	85,85,85,85	0
58	MG	14	3228	1/1	0.88	0.12	101,101,101,101	0
58	MG	1H	3228	1/1	0.88	0.32	83,83,83,83	0
58	MG	13	1690	1/1	0.89	0.10	74,74,74,74	0
58	MG	1H	3023	1/1	0.89	0.28	56,56,56,56	0
58	MG	1H	3082	1/1	0.89	0.18	78,78,78,78	0
58	MG	1G	1609	1/1	0.89	0.20	94,94,94,94	0
58	MG	1G	1610	1/1	0.89	0.17	98,98,98,98	0
58	MG	1H	3133	1/1	0.89	0.22	71,71,71,71	0
58	MG	1H	3135	1/1	0.89	0.15	65,65,65,65	0
58	MG	1G	1613	1/1	0.89	0.11	98,98,98,98	0
58	MG	14	3125	1/1	0.89	0.27	72,72,72,72	0
58	MG	13	1675	1/1	0.89	0.22	73,73,73,73	0
58	MG	1H	3005	1/1	0.89	0.24	54,54,54,54	0
58	MG	1H	3141	1/1	0.89	0.24	61,61,61,61	0
58	MG	14	3286	1/1	0.89	0.27	80,80,80,80	0
58	MG	1H	3091	1/1	0.89	0.32	65,65,65,65	0
58	MG	1H	3146	1/1	0.89	0.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	1619	1/1	0.89	0.21	101,101,101,101	0
58	MG	1G	1671	1/1	0.89	0.32	88,88,88,88	0
58	MG	1H	3198	1/1	0.89	0.20	69,69,69,69	0
58	MG	1H	3026	1/1	0.89	0.26	56,56,56,56	0
58	MG	1H	3200	1/1	0.89	0.36	81,81,81,81	0
58	MG	1H	3150	1/1	0.89	0.16	72,72,72,72	0
58	MG	1H	3248	1/1	0.89	0.26	74,74,74,74	0
58	MG	13	1682	1/1	0.89	0.35	88,88,88,88	0
58	MG	1H	3338	1/1	0.89	0.20	65,65,65,65	0
58	MG	1H	3096	1/1	0.89	0.19	60,60,60,60	0
58	MG	1H	3158	1/1	0.89	0.24	74,74,74,74	0
58	MG	1H	3008	1/1	0.89	0.23	81,81,81,81	0
58	MG	14	3011	1/1	0.89	0.28	48,48,48,48	0
58	MG	13	1683	1/1	0.89	0.17	94,94,94,94	0
58	MG	1H	3467	1/1	0.89	0.15	84,84,84,84	0
58	MG	14	3156	1/1	0.89	0.25	63,63,63,63	0
58	MG	14	3014	1/1	0.89	0.26	57,57,57,57	0
58	MG	13	1684	1/1	0.89	0.12	128,128,128,128	0
58	MG	14	3166	1/1	0.89	0.15	60,60,60,60	0
58	MG	13	1641	1/1	0.89	0.24	93,93,93,93	0
58	MG	1H	3111	1/1	0.89	0.31	74,74,74,74	0
58	MG	14	3173	1/1	0.89	0.16	66,66,66,66	0
58	MG	14	3086	1/1	0.89	0.28	83,83,83,83	0
58	MG	14	3088	1/1	0.89	0.20	52,52,52,52	0
58	MG	21	302	1/1	0.89	0.25	77,77,77,77	0
58	MG	14	3090	1/1	0.89	0.14	74,74,74,74	0
58	MG	1H	3215	1/1	0.89	0.24	63,63,63,63	0
58	MG	1H	3035	1/1	0.89	0.32	83,83,83,83	0
58	MG	1G	1645	1/1	0.89	0.25	74,74,74,74	0
58	MG	13	1636	1/1	0.89	0.11	64,64,64,64	0
58	MG	14	3257	1/1	0.89	0.45	86,86,86,86	0
58	MG	13	1634	1/1	0.89	0.37	93,93,93,93	0
58	MG	13	1663	1/1	0.89	0.20	82,82,82,82	0
58	MG	1H	3126	1/1	0.89	0.13	58,58,58,58	0
58	MG	1H	3221	1/1	0.89	0.24	89,89,89,89	0
58	MG	14	3264	1/1	0.89	0.33	85,85,85,85	0
58	MG	1H	3127	1/1	0.89	0.09	59,59,59,59	0
58	MG	13	1633	1/1	0.89	0.28	62,62,62,62	0
58	MG	1H	3241	1/1	0.90	0.23	66,66,66,66	0
58	MG	13	1628	1/1	0.90	0.28	65,65,65,65	0
58	MG	1H	3267	1/1	0.90	0.28	73,73,73,73	0
58	MG	1H	3051	1/1	0.90	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2K	101	1/1	0.90	0.27	68,68,68,68	0
58	MG	13	1611	1/1	0.90	0.14	72,72,72,72	0
58	MG	1H	3273	1/1	0.90	0.18	68,68,68,68	0
58	MG	1H	3166	1/1	0.90	0.20	71,71,71,71	0
58	MG	1H	3276	1/1	0.90	0.23	75,75,75,75	0
58	MG	14	3195	1/1	0.90	0.29	68,68,68,68	0
58	MG	13	1664	1/1	0.90	0.13	89,89,89,89	0
58	MG	13	1630	1/1	0.90	0.24	80,80,80,80	0
58	MG	1H	3210	1/1	0.90	0.26	71,71,71,71	0
58	MG	1H	3192	1/1	0.90	0.16	80,80,80,80	0
58	MG	13	1730	1/1	0.90	0.16	86,86,86,86	0
58	MG	1H	3310	1/1	0.90	0.06	75,75,75,75	0
58	MG	14	3154	1/1	0.90	0.17	69,69,69,69	0
58	MG	1H	3311	1/1	0.90	0.20	75,75,75,75	0
58	MG	1G	1620	1/1	0.90	0.13	82,82,82,82	0
58	MG	14	3159	1/1	0.90	0.26	63,63,63,63	0
58	MG	14	3216	1/1	0.90	0.25	77,77,77,77	0
58	MG	14	3064	1/1	0.90	0.15	78,78,78,78	0
58	MG	14	3016	1/1	0.90	0.26	61,61,61,61	0
58	MG	1H	3231	1/1	0.90	0.24	58,58,58,58	0
58	MG	14	3167	1/1	0.90	0.26	87,87,87,87	0
58	MG	1H	3257	1/1	0.90	0.20	70,70,70,70	0
58	MG	14	3273	1/1	0.90	0.30	101,101,101,101	0
58	MG	14	3274	1/1	0.90	0.08	76,76,76,76	0
58	MG	1H	3066	1/1	0.90	0.22	59,59,59,59	0
58	MG	1H	3131	1/1	0.90	0.33	73,73,73,73	0
58	MG	1H	3288	1/1	0.90	0.37	93,93,93,93	0
58	MG	1H	3153	1/1	0.90	0.12	62,62,62,62	0
58	MG	14	3176	1/1	0.90	0.33	79,79,79,79	0
58	MG	1H	3068	1/1	0.90	0.20	86,86,86,86	0
58	MG	13	1637	1/1	0.90	0.17	56,56,56,56	0
58	MG	1H	3240	1/1	0.90	0.14	74,74,74,74	0
58	MG	1H	3325	1/1	0.90	0.24	71,71,71,71	0
58	MG	14	3033	1/1	0.90	0.16	77,77,77,77	0
58	MG	1H	3326	1/1	0.90	0.28	83,83,83,83	0
60	ZN	G8	201	1/1	0.90	0.14	149,149,149,149	0
58	MG	14	3002	1/1	0.91	0.20	57,57,57,57	0
58	MG	14	3092	1/1	0.91	0.15	76,76,76,76	0
58	MG	14	3003	1/1	0.91	0.16	62,62,62,62	0
58	MG	1G	1648	1/1	0.91	0.23	117,117,117,117	0
58	MG	14	3158	1/1	0.91	0.23	75,75,75,75	0
58	MG	14	3051	1/1	0.91	0.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3120	1/1	0.91	0.18	74,74,74,74	0
58	MG	1G	1651	1/1	0.91	0.15	104,104,104,104	0
58	MG	13	1666	1/1	0.91	0.10	78,78,78,78	0
58	MG	14	3101	1/1	0.91	0.20	64,64,64,64	0
58	MG	14	3104	1/1	0.91	0.19	86,86,86,86	0
58	MG	1H	3053	1/1	0.91	0.18	50,50,50,50	0
58	MG	14	3056	1/1	0.91	0.20	55,55,55,55	0
58	MG	1H	3173	1/1	0.91	0.33	84,84,84,84	0
58	MG	1H	3054	1/1	0.91	0.17	52,52,52,52	0
58	MG	1H	3202	1/1	0.91	0.28	70,70,70,70	0
58	MG	1H	3029	1/1	0.91	0.24	42,42,42,42	0
58	MG	14	3062	1/1	0.91	0.18	68,68,68,68	0
58	MG	1H	3074	1/1	0.91	0.16	64,64,64,64	0
58	MG	1H	3042	1/1	0.91	0.43	90,90,90,90	0
58	MG	14	3183	1/1	0.91	0.35	79,79,79,79	0
58	MG	1H	3183	1/1	0.91	0.24	67,67,67,67	0
58	MG	1H	3155	1/1	0.91	0.22	74,74,74,74	0
58	MG	1H	3208	1/1	0.91	0.31	88,88,88,88	0
58	MG	14	3021	1/1	0.91	0.22	52,52,52,52	0
58	MG	14	3306	1/1	0.91	0.22	88,88,88,88	0
58	MG	1H	3076	1/1	0.91	0.21	65,65,65,65	0
58	MG	1H	3186	1/1	0.91	0.22	75,75,75,75	0
58	MG	14	3024	1/1	0.91	0.28	77,77,77,77	0
58	MG	1H	3103	1/1	0.91	0.14	54,54,54,54	0
58	MG	1H	3015	1/1	0.91	0.27	63,63,63,63	0
58	MG	14	3078	1/1	0.91	0.21	64,64,64,64	0
58	MG	14	3028	1/1	0.91	0.24	69,69,69,69	0
58	MG	1H	3299	1/1	0.91	0.12	74,74,74,74	0
58	MG	1H	3214	1/1	0.91	0.45	76,76,76,76	0
58	MG	14	3141	1/1	0.91	0.14	93,93,93,93	0
58	MG	14	3261	1/1	0.91	0.17	77,77,77,77	0
58	MG	14	3198	1/1	0.91	0.09	107,107,107,107	0
58	MG	1H	3189	1/1	0.91	0.34	67,67,67,67	0
58	MG	14	3202	1/1	0.91	0.20	63,63,63,63	0
58	MG	13	1622	1/1	0.91	0.28	74,74,74,74	0
58	MG	1H	3246	1/1	0.91	0.13	54,54,54,54	0
58	MG	1H	3017	1/1	0.91	0.24	71,71,71,71	0
58	MG	29	303	1/1	0.91	0.25	52,52,52,52	0
58	MG	13	1650	1/1	0.91	0.27	94,94,94,94	0
58	MG	25	201	1/1	0.91	0.32	102,102,102,102	0
58	MG	1H	3117	1/1	0.91	0.18	48,48,48,48	0
58	MG	14	3213	1/1	0.91	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3149	1/1	0.91	0.31	73,73,73,73	0
58	MG	13	1620	1/1	0.91	0.19	73,73,73,73	0
58	MG	E5	101	1/1	0.91	0.32	89,89,89,89	0
58	MG	1H	3280	1/1	0.91	0.20	77,77,77,77	0
58	MG	14	3043	1/1	0.92	0.20	57,57,57,57	0
58	MG	1H	3178	1/1	0.92	0.16	71,71,71,71	0
58	MG	1H	3061	1/1	0.92	0.22	48,48,48,48	0
58	MG	14	3047	1/1	0.92	0.10	74,74,74,74	0
58	MG	1H	3317	1/1	0.92	0.26	68,68,68,68	0
58	MG	14	3241	1/1	0.92	0.12	56,56,56,56	0
58	MG	1H	3180	1/1	0.92	0.29	75,75,75,75	0
58	MG	1H	3422	1/1	0.92	0.06	112,112,112,112	0
58	MG	1H	3438	1/1	0.92	0.08	83,83,83,83	0
58	MG	1H	3136	1/1	0.92	0.23	49,49,49,49	0
58	MG	16	201	1/1	0.92	0.11	85,85,85,85	0
58	MG	1H	3320	1/1	0.92	0.27	77,77,77,77	0
58	MG	13	1601	1/1	0.92	0.17	68,68,68,68	0
58	MG	1H	3250	1/1	0.92	0.23	74,74,74,74	0
58	MG	13	1612	1/1	0.92	0.18	63,63,63,63	0
58	MG	41	201	1/1	0.92	0.14	78,78,78,78	0
58	MG	14	3200	1/1	0.92	0.52	74,74,74,74	0
58	MG	1H	3163	1/1	0.92	0.30	50,50,50,50	0
58	MG	1H	3140	1/1	0.92	0.13	58,58,58,58	0
58	MG	1H	3018	1/1	0.92	0.30	71,71,71,71	0
58	MG	14	3307	1/1	0.92	0.28	101,101,101,101	0
58	MG	14	3105	1/1	0.92	0.16	67,67,67,67	0
58	MG	13	1732	1/1	0.92	0.16	65,65,65,65	0
58	MG	14	3209	1/1	0.92	0.14	66,66,66,66	0
58	MG	J8	101	1/1	0.92	0.19	66,66,66,66	0
58	MG	1H	3145	1/1	0.92	0.16	73,73,73,73	0
58	MG	14	3025	1/1	0.92	0.28	84,84,84,84	0
58	MG	1H	3329	1/1	0.92	0.32	81,81,81,81	0
58	MG	1H	3281	1/1	0.92	0.14	88,88,88,88	0
58	MG	14	3114	1/1	0.92	0.18	58,58,58,58	0
58	MG	14	3268	1/1	0.92	0.27	94,94,94,94	0
58	MG	1H	3039	1/1	0.92	0.15	68,68,68,68	0
58	MG	14	3169	1/1	0.92	0.18	58,58,58,58	0
58	MG	14	3272	1/1	0.92	0.25	76,76,76,76	0
58	MG	1H	3147	1/1	0.92	0.19	64,64,64,64	0
58	MG	14	3119	1/1	0.92	0.22	62,62,62,62	0
58	MG	13	1610	1/1	0.92	0.18	80,80,80,80	0
58	MG	14	3075	1/1	0.92	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3277	1/1	0.92	0.21	85,85,85,85	0
58	MG	13	1694	1/1	0.92	0.30	64,64,64,64	0
58	MG	13	1617	1/1	0.92	0.12	83,83,83,83	0
58	MG	14	3178	1/1	0.92	0.20	84,84,84,84	0
58	MG	1G	1643	1/1	0.92	0.18	132,132,132,132	0
58	MG	1H	3006	1/1	0.92	0.21	46,46,46,46	0
58	MG	1H	3175	1/1	0.92	0.26	65,65,65,65	0
58	MG	14	3284	1/1	0.92	0.32	78,78,78,78	0
58	MG	1H	3119	1/1	0.92	0.13	69,69,69,69	0
58	MG	14	3207	1/1	0.93	0.16	80,80,80,80	0
58	MG	1H	3085	1/1	0.93	0.17	63,63,63,63	0
58	MG	1H	3159	1/1	0.93	0.24	67,67,67,67	0
58	MG	1H	3086	1/1	0.93	0.18	70,70,70,70	0
58	MG	14	3036	1/1	0.93	0.33	96,96,96,96	0
58	MG	1H	3161	1/1	0.93	0.21	84,84,84,84	0
58	MG	1H	3088	1/1	0.93	0.24	68,68,68,68	0
58	MG	1G	1669	1/1	0.93	0.19	107,107,107,107	0
58	MG	13	1642	1/1	0.93	0.17	74,74,74,74	0
58	MG	14	3219	1/1	0.93	0.12	48,48,48,48	0
58	MG	14	3220	1/1	0.93	0.39	76,76,76,76	0
58	MG	1H	3063	1/1	0.93	0.06	78,78,78,78	0
58	MG	1G	1632	1/1	0.93	0.23	75,75,75,75	0
58	MG	14	3046	1/1	0.93	0.12	66,66,66,66	0
58	MG	14	3097	1/1	0.93	0.14	65,65,65,65	0
58	MG	14	3161	1/1	0.93	0.21	70,70,70,70	0
58	MG	14	3162	1/1	0.93	0.31	70,70,70,70	0
58	MG	1H	3064	1/1	0.93	0.11	65,65,65,65	0
58	MG	21	301	1/1	0.93	0.33	54,54,54,54	0
58	MG	13	1731	1/1	0.93	0.18	84,84,84,84	0
58	MG	1G	1690	1/1	0.93	0.12	93,93,93,93	0
58	MG	1H	3030	1/1	0.93	0.11	67,67,67,67	0
58	MG	1H	3095	1/1	0.93	0.20	65,65,65,65	0
58	MG	1H	3169	1/1	0.93	0.18	85,85,85,85	0
58	MG	13	1645	1/1	0.93	0.30	64,64,64,64	0
58	MG	1H	3097	1/1	0.93	0.27	71,71,71,71	0
58	MG	14	3237	1/1	0.93	0.15	83,83,83,83	0
58	MG	1H	3048	1/1	0.93	0.17	56,56,56,56	0
58	MG	1H	3138	1/1	0.93	0.22	58,58,58,58	0
58	MG	14	3240	1/1	0.93	0.10	83,83,83,83	0
58	MG	1H	3001	1/1	0.93	0.16	43,43,43,43	0
58	MG	1H	3022	1/1	0.93	0.21	62,62,62,62	0
58	MG	14	3115	1/1	0.93	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3105	1/1	0.93	0.22	66,66,66,66	0
58	MG	14	3061	1/1	0.93	0.14	81,81,81,81	0
58	MG	14	3246	1/1	0.93	0.07	69,69,69,69	0
58	MG	1H	3177	1/1	0.93	0.17	74,74,74,74	0
58	MG	1H	3142	1/1	0.93	0.27	68,68,68,68	0
58	MG	1H	3106	1/1	0.93	0.21	63,63,63,63	0
58	MG	1G	1649	1/1	0.93	0.29	83,83,83,83	0
58	MG	14	3124	1/1	0.93	0.26	54,54,54,54	0
58	MG	1H	3002	1/1	0.93	0.13	38,38,38,38	0
58	MG	13	1655	1/1	0.93	0.29	87,87,87,87	0
58	MG	14	3127	1/1	0.93	0.19	69,69,69,69	0
58	MG	13	1616	1/1	0.93	0.04	88,88,88,88	0
58	MG	14	3398	1/1	0.93	0.06	108,108,108,108	0
58	MG	1H	3148	1/1	0.93	0.16	50,50,50,50	0
58	MG	1H	3055	1/1	0.93	0.21	49,49,49,49	0
58	MG	1K	101	1/1	0.93	0.06	145,145,145,145	0
58	MG	1H	3151	1/1	0.93	0.12	55,55,55,55	0
58	MG	1H	3301	1/1	0.93	0.35	84,84,84,84	0
58	MG	13	1619	1/1	0.93	0.14	91,91,91,91	0
58	MG	29	302	1/1	0.93	0.22	65,65,65,65	0
58	MG	1H	3040	1/1	0.93	0.28	70,70,70,70	0
58	MG	1H	3041	1/1	0.93	0.16	76,76,76,76	0
58	MG	1H	3083	1/1	0.93	0.23	67,67,67,67	0
58	MG	1H	3357	1/1	0.93	0.11	71,71,71,71	0
58	MG	1G	1621	1/1	0.93	0.10	92,92,92,92	0
58	MG	14	3031	1/1	0.93	0.27	68,68,68,68	0
58	MG	14	3270	1/1	0.93	0.19	63,63,63,63	0
58	MG	55	201	1/1	0.93	0.27	74,74,74,74	0
58	MG	14	3145	1/1	0.93	0.16	65,65,65,65	0
58	MG	14	3206	1/1	0.93	0.12	80,80,80,80	0
58	MG	1H	3375	1/1	0.94	0.15	60,60,60,60	0
58	MG	14	3006	1/1	0.94	0.32	56,56,56,56	0
58	MG	14	3109	1/1	0.94	0.24	73,73,73,73	0
58	MG	1H	3181	1/1	0.94	0.10	61,61,61,61	0
58	MG	14	3208	1/1	0.94	0.10	91,91,91,91	0
58	MG	1H	3312	1/1	0.94	0.15	67,67,67,67	0
58	MG	14	3032	1/1	0.94	0.29	75,75,75,75	0
58	MG	1H	3193	1/1	0.94	0.38	73,73,73,73	0
58	MG	1H	3441	1/1	0.94	0.06	89,89,89,89	0
58	MG	14	3087	1/1	0.94	0.18	40,40,40,40	0
58	MG	1H	3067	1/1	0.94	0.20	55,55,55,55	0
58	MG	1H	3315	1/1	0.94	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3052	1/1	0.94	0.12	53,53,53,53	0
58	MG	14	3358	1/1	0.94	0.13	91,91,91,91	0
58	MG	14	3396	1/1	0.94	0.08	108,108,108,108	0
58	MG	13	1614	1/1	0.94	0.16	78,78,78,78	0
58	MG	13	1644	1/1	0.94	0.25	96,96,96,96	0
58	MG	14	3093	1/1	0.94	0.18	42,42,42,42	0
58	MG	13	1719	1/1	0.94	0.06	71,71,71,71	0
58	MG	14	3157	1/1	0.94	0.10	57,57,57,57	0
58	MG	1H	3212	1/1	0.94	0.19	76,76,76,76	0
58	MG	14	3225	1/1	0.94	0.27	82,82,82,82	0
58	MG	13	1649	1/1	0.94	0.18	72,72,72,72	0
58	MG	14	3128	1/1	0.94	0.22	58,58,58,58	0
58	MG	1H	3244	1/1	0.94	0.17	62,62,62,62	0
58	MG	1G	1689	1/1	0.94	0.07	121,121,121,121	0
58	MG	1H	3057	1/1	0.94	0.22	66,66,66,66	0
58	MG	6A	101	1/1	0.94	0.24	93,93,93,93	0
58	MG	1H	3124	1/1	0.94	0.16	46,46,46,46	0
58	MG	14	3199	1/1	0.94	0.23	69,69,69,69	0
58	MG	1H	3012	1/1	0.94	0.37	83,83,83,83	0
58	MG	1H	3110	1/1	0.94	0.30	55,55,55,55	0
58	MG	1H	3364	1/1	0.94	0.06	98,98,98,98	0
58	MG	14	3172	1/1	0.94	0.37	70,70,70,70	0
58	MG	1H	3235	1/1	0.95	0.08	53,53,53,53	0
58	MG	13	1708	1/1	0.95	0.07	89,89,89,89	0
58	MG	14	3039	1/1	0.95	0.10	50,50,50,50	0
58	MG	L8	101	1/1	0.95	0.31	84,84,84,84	0
58	MG	1H	3134	1/1	0.95	0.08	69,69,69,69	0
58	MG	14	3110	1/1	0.95	0.19	57,57,57,57	0
58	MG	1H	3238	1/1	0.95	0.12	65,65,65,65	0
58	MG	1H	3034	1/1	0.95	0.28	80,80,80,80	0
58	MG	1H	3368	1/1	0.95	0.10	74,74,74,74	0
58	MG	1H	3014	1/1	0.95	0.23	70,70,70,70	0
58	MG	1H	3047	1/1	0.95	0.17	47,47,47,47	0
58	MG	1H	3084	1/1	0.95	0.14	94,94,94,94	0
58	MG	1H	3426	1/1	0.95	0.09	58,58,58,58	0
58	MG	1H	3261	1/1	0.95	0.15	69,69,69,69	0
58	MG	1H	3109	1/1	0.95	0.12	47,47,47,47	0
58	MG	1H	3446	1/1	0.95	0.10	84,84,84,84	0
58	MG	1H	3457	1/1	0.95	0.07	141,141,141,141	0
58	MG	14	3324	1/1	0.95	0.06	99,99,99,99	0
58	MG	14	3123	1/1	0.95	0.16	64,64,64,64	0
58	MG	14	3380	1/1	0.95	0.06	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3391	1/1	0.95	0.13	104,104,104,104	0
58	MG	14	3392	1/1	0.95	0.05	128,128,128,128	0
58	MG	1H	3466	1/1	0.95	0.17	56,56,56,56	0
58	MG	14	3164	1/1	0.95	0.28	74,74,74,74	0
58	MG	13	1693	1/1	0.95	0.15	55,55,55,55	0
58	MG	1H	3245	1/1	0.95	0.34	62,62,62,62	0
58	MG	13	1613	1/1	0.95	0.08	81,81,81,81	0
58	MG	1G	1680	1/1	0.95	0.05	140,140,140,140	0
58	MG	1H	3156	1/1	0.95	0.25	67,67,67,67	0
58	MG	14	3170	1/1	0.95	0.14	83,83,83,83	0
58	MG	1H	3229	1/1	0.95	0.17	48,48,48,48	0
58	MG	16	205	1/1	0.95	0.08	81,81,81,81	0
58	MG	1H	3112	1/1	0.95	0.20	56,56,56,56	0
58	MG	14	3212	1/1	0.95	0.34	70,70,70,70	0
58	MG	1H	3098	1/1	0.95	0.14	53,53,53,53	0
58	MG	14	3066	1/1	0.95	0.28	62,62,62,62	0
58	MG	1H	3077	1/1	0.95	0.12	60,60,60,60	0
58	MG	14	3137	1/1	0.95	0.05	57,57,57,57	0
58	MG	1H	3272	1/1	0.95	0.13	64,64,64,64	0
58	MG	1H	3062	1/1	0.95	0.17	64,64,64,64	0
58	MG	14	3103	1/1	0.95	0.13	51,51,51,51	0
58	MG	1H	3274	1/1	0.95	0.17	59,59,59,59	0
58	MG	1H	3465	1/1	0.96	0.09	71,71,71,71	0
58	MG	1H	3121	1/1	0.96	0.20	62,62,62,62	0
58	MG	14	3063	1/1	0.96	0.12	58,58,58,58	0
58	MG	13	1720	1/1	0.96	0.06	90,90,90,90	0
58	MG	1H	3123	1/1	0.96	0.10	69,69,69,69	0
58	MG	13	1727	1/1	0.96	0.05	112,112,112,112	0
58	MG	1G	1608	1/1	0.96	0.09	89,89,89,89	0
58	MG	13	1729	1/1	0.96	0.05	113,113,113,113	0
58	MG	13	1707	1/1	0.96	0.07	76,76,76,76	0
58	MG	1H	3370	1/1	0.96	0.11	71,71,71,71	0
58	MG	14	3136	1/1	0.96	0.09	62,62,62,62	0
58	MG	14	3040	1/1	0.96	0.19	59,59,59,59	0
58	MG	14	3041	1/1	0.96	0.15	54,54,54,54	0
58	MG	14	3353	1/1	0.96	0.04	118,118,118,118	0
58	MG	14	3357	1/1	0.96	0.11	76,76,76,76	0
58	MG	16	209	1/1	0.96	0.08	100,100,100,100	0
58	MG	14	3363	1/1	0.96	0.06	72,72,72,72	0
58	MG	1H	3114	1/1	0.96	0.30	74,74,74,74	0
58	MG	14	3389	1/1	0.96	0.07	102,102,102,102	0
58	MG	1H	3104	1/1	0.96	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3381	1/1	0.96	0.06	63,63,63,63	0
58	MG	14	3393	1/1	0.96	0.06	127,127,127,127	0
58	MG	14	3395	1/1	0.96	0.05	103,103,103,103	0
58	MG	1H	3413	1/1	0.96	0.05	102,102,102,102	0
58	MG	1H	3078	1/1	0.96	0.24	67,67,67,67	0
58	MG	1H	3234	1/1	0.96	0.05	66,66,66,66	0
58	MG	13	1626	1/1	0.96	0.17	69,69,69,69	0
58	MG	1H	3087	1/1	0.96	0.31	70,70,70,70	0
58	MG	14	3218	1/1	0.96	0.28	62,62,62,62	0
58	MG	1H	3445	1/1	0.96	0.05	110,110,110,110	0
58	MG	1G	1622	1/1	0.96	0.38	92,92,92,92	0
58	MG	14	3256	1/1	0.96	0.28	83,83,83,83	0
58	MG	14	3151	1/1	0.96	0.27	79,79,79,79	0
58	MG	1G	1623	1/1	0.96	0.21	62,62,62,62	0
58	MG	1G	1678	1/1	0.96	0.06	128,128,128,128	0
58	MG	1G	1624	1/1	0.96	0.23	65,65,65,65	0
58	MG	1G	1681	1/1	0.96	0.06	78,78,78,78	0
58	MG	P8	101	1/1	0.96	0.31	77,77,77,77	0
58	MG	14	3263	1/1	0.96	0.17	75,75,75,75	0
58	MG	1H	3157	1/1	0.96	0.28	73,73,73,73	0
58	MG	13	1673	1/1	0.96	0.33	70,70,70,70	0
58	MG	1H	3463	1/1	0.96	0.05	112,112,112,112	0
58	MG	14	3160	1/1	0.96	0.17	72,72,72,72	0
58	MG	14	3182	1/1	0.97	0.30	75,75,75,75	0
58	MG	1G	1682	1/1	0.97	0.05	97,97,97,97	0
58	MG	1G	1686	1/1	0.97	0.07	125,125,125,125	0
58	MG	1G	1687	1/1	0.97	0.07	139,139,139,139	0
58	MG	1H	3339	1/1	0.97	0.17	48,48,48,48	0
58	MG	1H	3383	1/1	0.97	0.07	60,60,60,60	0
58	MG	1H	3399	1/1	0.97	0.07	62,62,62,62	0
58	MG	13	1665	1/1	0.97	0.04	82,82,82,82	0
58	MG	14	3364	1/1	0.97	0.08	85,85,85,85	0
58	MG	14	3376	1/1	0.97	0.04	94,94,94,94	0
58	MG	1H	3417	1/1	0.97	0.08	94,94,94,94	0
58	MG	14	3385	1/1	0.97	0.04	116,116,116,116	0
58	MG	1H	3113	1/1	0.97	0.23	51,51,51,51	0
58	MG	1H	3425	1/1	0.97	0.05	63,63,63,63	0
58	MG	1H	3195	1/1	0.97	0.27	62,62,62,62	0
58	MG	14	3005	1/1	0.97	0.24	48,48,48,48	0
58	MG	1H	3433	1/1	0.97	0.12	87,87,87,87	0
58	MG	1H	3343	1/1	0.97	0.06	54,54,54,54	0
58	MG	88	201	1/1	0.97	0.17	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1674	1/1	0.97	0.06	91,91,91,91	0
58	MG	14	3298	1/1	0.97	0.37	64,64,64,64	0
58	MG	14	3010	1/1	0.97	0.23	41,41,41,41	0
58	MG	14	3102	1/1	0.97	0.07	61,61,61,61	0
58	MG	1H	3443	1/1	0.97	0.11	76,76,76,76	0
58	MG	1H	3115	1/1	0.97	0.13	43,43,43,43	0
58	MG	1H	3367	1/1	0.97	0.05	71,71,71,71	0
58	MG	1H	3447	1/1	0.97	0.07	86,86,86,86	0
58	MG	1H	3452	1/1	0.97	0.06	104,104,104,104	0
58	MG	29	304	1/1	0.97	0.26	81,81,81,81	0
58	MG	13	1725	1/1	0.97	0.05	94,94,94,94	0
58	MG	1H	3459	1/1	0.97	0.05	106,106,106,106	0
58	MG	1H	3070	1/1	0.97	0.21	58,58,58,58	0
58	MG	1H	3464	1/1	0.97	0.04	107,107,107,107	0
58	MG	13	1710	1/1	0.97	0.04	97,97,97,97	0
58	MG	1G	1679	1/1	0.97	0.08	119,119,119,119	0
58	MG	45	202	1/1	0.97	0.19	72,72,72,72	0
58	MG	1H	3046	1/1	0.97	0.17	47,47,47,47	0
58	MG	1H	3379	1/1	0.97	0.07	73,73,73,73	0
58	MG	14	3116	1/1	0.97	0.11	64,64,64,64	0
60	ZN	C5	201	1/1	0.97	0.07	165,165,165,165	0
58	MG	1H	3361	1/1	0.98	0.05	63,63,63,63	0
58	MG	1H	3442	1/1	0.98	0.05	69,69,69,69	0
58	MG	13	1715	1/1	0.98	0.07	109,109,109,109	0
58	MG	1H	3365	1/1	0.98	0.09	74,74,74,74	0
58	MG	1G	1676	1/1	0.98	0.05	90,90,90,90	0
58	MG	14	3319	1/1	0.98	0.09	59,59,59,59	0
58	MG	14	3321	1/1	0.98	0.04	78,78,78,78	0
58	MG	14	3322	1/1	0.98	0.05	65,65,65,65	0
58	MG	13	1638	1/1	0.98	0.08	59,59,59,59	0
58	MG	14	3325	1/1	0.98	0.04	63,63,63,63	0
58	MG	14	3326	1/1	0.98	0.05	90,90,90,90	0
58	MG	14	3327	1/1	0.98	0.04	59,59,59,59	0
58	MG	14	3333	1/1	0.98	0.06	74,74,74,74	0
58	MG	14	3335	1/1	0.98	0.04	61,61,61,61	0
58	MG	14	3336	1/1	0.98	0.04	62,62,62,62	0
58	MG	14	3345	1/1	0.98	0.04	90,90,90,90	0
58	MG	14	3347	1/1	0.98	0.03	108,108,108,108	0
58	MG	14	3349	1/1	0.98	0.04	83,83,83,83	0
58	MG	14	3352	1/1	0.98	0.08	97,97,97,97	0
58	MG	1H	3270	1/1	0.98	0.54	80,80,80,80	0
58	MG	14	3355	1/1	0.98	0.04	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3451	1/1	0.98	0.04	114,114,114,114	0
58	MG	13	1643	1/1	0.98	0.09	99,99,99,99	0
58	MG	14	3362	1/1	0.98	0.03	77,77,77,77	0
58	MG	1H	3454	1/1	0.98	0.04	96,96,96,96	0
58	MG	14	3072	1/1	0.98	0.10	45,45,45,45	0
58	MG	14	3365	1/1	0.98	0.06	94,94,94,94	0
58	MG	14	3369	1/1	0.98	0.06	59,59,59,59	0
58	MG	14	3372	1/1	0.98	0.04	70,70,70,70	0
58	MG	14	3374	1/1	0.98	0.09	76,76,76,76	0
58	MG	14	3375	1/1	0.98	0.05	97,97,97,97	0
58	MG	1G	1683	1/1	0.98	0.04	89,89,89,89	0
58	MG	14	3378	1/1	0.98	0.06	100,100,100,100	0
58	MG	1G	1685	1/1	0.98	0.05	87,87,87,87	0
58	MG	14	3381	1/1	0.98	0.04	81,81,81,81	0
58	MG	14	3382	1/1	0.98	0.06	87,87,87,87	0
58	MG	14	3383	1/1	0.98	0.05	86,86,86,86	0
58	MG	14	3384	1/1	0.98	0.06	83,83,83,83	0
58	MG	1H	3456	1/1	0.98	0.06	97,97,97,97	0
58	MG	14	3386	1/1	0.98	0.04	90,90,90,90	0
58	MG	14	3387	1/1	0.98	0.04	96,96,96,96	0
58	MG	1H	3099	1/1	0.98	0.06	55,55,55,55	0
58	MG	1G	1688	1/1	0.98	0.03	138,138,138,138	0
58	MG	13	1722	1/1	0.98	0.05	103,103,103,103	0
58	MG	1H	3461	1/1	0.98	0.11	92,92,92,92	0
58	MG	14	3394	1/1	0.98	0.07	109,109,109,109	0
58	MG	1H	3462	1/1	0.98	0.04	97,97,97,97	0
58	MG	1H	3092	1/1	0.98	0.07	49,49,49,49	0
58	MG	1H	3102	1/1	0.98	0.19	35,35,35,35	0
58	MG	1H	3143	1/1	0.98	0.06	56,56,56,56	0
58	MG	1H	3387	1/1	0.98	0.04	80,80,80,80	0
58	MG	1H	3393	1/1	0.98	0.10	54,54,54,54	0
58	MG	1H	3289	1/1	0.98	0.07	49,49,49,49	0
58	MG	1H	3403	1/1	0.98	0.04	76,76,76,76	0
58	MG	1H	3406	1/1	0.98	0.07	76,76,76,76	0
58	MG	1J	205	1/1	0.98	0.04	101,101,101,101	0
58	MG	1H	3412	1/1	0.98	0.05	78,78,78,78	0
58	MG	13	1711	1/1	0.98	0.04	97,97,97,97	0
58	MG	13	1712	1/1	0.98	0.05	83,83,83,83	0
58	MG	1H	3418	1/1	0.98	0.05	92,92,92,92	0
58	MG	1H	3345	1/1	0.98	0.06	61,61,61,61	0
58	MG	1H	3347	1/1	0.98	0.13	51,51,51,51	0
58	MG	1H	3354	1/1	0.98	0.04	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3429	1/1	0.98	0.04	71,71,71,71	0
58	MG	14	3138	1/1	0.98	0.16	45,45,45,45	0
58	MG	13	1728	1/1	0.98	0.03	118,118,118,118	0
58	MG	1H	3435	1/1	0.98	0.04	56,56,56,56	0
58	MG	1H	3436	1/1	0.98	0.10	73,73,73,73	0
58	MG	1H	3437	1/1	0.98	0.07	58,58,58,58	0
59	SF4	3E	301	8/8	0.98	0.03	86,99,103,105	0
58	MG	1H	3360	1/1	0.98	0.04	61,61,61,61	0
60	ZN	5A	101	1/1	0.98	0.04	142,142,142,142	0
58	MG	1H	3439	1/1	0.98	0.05	99,99,99,99	0
58	MG	1H	3371	1/1	0.99	0.04	59,59,59,59	0
58	MG	14	3320	1/1	0.99	0.06	64,64,64,64	0
58	MG	1G	1677	1/1	0.99	0.09	96,96,96,96	0
58	MG	1H	3372	1/1	0.99	0.03	62,62,62,62	0
58	MG	14	3323	1/1	0.99	0.04	64,64,64,64	0
58	MG	1H	3373	1/1	0.99	0.04	51,51,51,51	0
58	MG	13	1724	1/1	0.99	0.06	102,102,102,102	0
58	MG	1H	3348	1/1	0.99	0.05	50,50,50,50	0
58	MG	1H	3377	1/1	0.99	0.06	70,70,70,70	0
58	MG	14	3328	1/1	0.99	0.03	74,74,74,74	0
58	MG	14	3329	1/1	0.99	0.03	56,56,56,56	0
58	MG	14	3330	1/1	0.99	0.03	77,77,77,77	0
58	MG	14	3332	1/1	0.99	0.03	53,53,53,53	0
58	MG	1H	3349	1/1	0.99	0.05	64,64,64,64	0
58	MG	1G	1684	1/1	0.99	0.03	109,109,109,109	0
58	MG	1H	3380	1/1	0.99	0.03	59,59,59,59	0
58	MG	14	3337	1/1	0.99	0.03	66,66,66,66	0
58	MG	14	3338	1/1	0.99	0.10	60,60,60,60	0
58	MG	14	3340	1/1	0.99	0.03	79,79,79,79	0
58	MG	14	3341	1/1	0.99	0.08	68,68,68,68	0
58	MG	14	3342	1/1	0.99	0.05	80,80,80,80	0
58	MG	14	3343	1/1	0.99	0.07	82,82,82,82	0
58	MG	14	3344	1/1	0.99	0.08	81,81,81,81	0
58	MG	1H	3444	1/1	0.99	0.04	69,69,69,69	0
58	MG	14	3346	1/1	0.99	0.07	85,85,85,85	0
58	MG	1H	3350	1/1	0.99	0.03	48,48,48,48	0
58	MG	14	3348	1/1	0.99	0.06	70,70,70,70	0
58	MG	1H	3353	1/1	0.99	0.06	57,57,57,57	0
58	MG	14	3350	1/1	0.99	0.03	85,85,85,85	0
58	MG	14	3351	1/1	0.99	0.04	85,85,85,85	0
58	MG	1H	3384	1/1	0.99	0.04	58,58,58,58	0
58	MG	1H	3448	1/1	0.99	0.03	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1H	3449	1/1	0.99	0.07	106,106,106,106	0
58	MG	14	3356	1/1	0.99	0.04	58,58,58,58	0
58	MG	1H	3450	1/1	0.99	0.02	54,54,54,54	0
58	MG	1H	3385	1/1	0.99	0.07	47,47,47,47	0
58	MG	14	3359	1/1	0.99	0.03	79,79,79,79	0
58	MG	14	3360	1/1	0.99	0.04	83,83,83,83	0
58	MG	14	3361	1/1	0.99	0.03	64,64,64,64	0
58	MG	14	3001	1/1	0.99	0.04	46,46,46,46	0
58	MG	13	1717	1/1	0.99	0.05	92,92,92,92	0
58	MG	1H	3453	1/1	0.99	0.03	84,84,84,84	0
58	MG	1H	3388	1/1	0.99	0.03	77,77,77,77	0
58	MG	14	3366	1/1	0.99	0.02	86,86,86,86	0
58	MG	14	3367	1/1	0.99	0.05	65,65,65,65	0
58	MG	14	3368	1/1	0.99	0.06	62,62,62,62	0
58	MG	1H	3455	1/1	0.99	0.05	59,59,59,59	0
58	MG	14	3370	1/1	0.99	0.04	64,64,64,64	0
58	MG	14	3371	1/1	0.99	0.04	53,53,53,53	0
58	MG	1H	3389	1/1	0.99	0.03	38,38,38,38	0
58	MG	14	3373	1/1	0.99	0.05	61,61,61,61	0
58	MG	1H	3391	1/1	0.99	0.03	61,61,61,61	0
58	MG	1H	3458	1/1	0.99	0.09	73,73,73,73	0
58	MG	1H	3392	1/1	0.99	0.03	68,68,68,68	0
58	MG	1H	3460	1/1	0.99	0.03	104,104,104,104	0
58	MG	1H	3355	1/1	0.99	0.06	48,48,48,48	0
58	MG	1H	3394	1/1	0.99	0.08	53,53,53,53	0
58	MG	1H	3395	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3397	1/1	0.99	0.04	71,71,71,71	0
58	MG	13	1726	1/1	0.99	0.03	126,126,126,126	0
58	MG	1H	3400	1/1	0.99	0.03	72,72,72,72	0
58	MG	1H	3402	1/1	0.99	0.03	51,51,51,51	0
58	MG	1H	3358	1/1	0.99	0.04	45,45,45,45	0
58	MG	14	3388	1/1	0.99	0.10	68,68,68,68	0
58	MG	1H	3405	1/1	0.99	0.03	63,63,63,63	0
58	MG	14	3390	1/1	0.99	0.03	89,89,89,89	0
58	MG	1H	3359	1/1	0.99	0.06	59,59,59,59	0
58	MG	1H	3407	1/1	0.99	0.07	116,116,116,116	0
58	MG	1H	3408	1/1	0.99	0.07	82,82,82,82	0
58	MG	16	207	1/1	0.99	0.03	80,80,80,80	0
58	MG	16	208	1/1	0.99	0.04	86,86,86,86	0
58	MG	1H	3409	1/1	0.99	0.02	85,85,85,85	0
58	MG	1H	3410	1/1	0.99	0.03	58,58,58,58	0
58	MG	1H	3411	1/1	0.99	0.04	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	1718	1/1	0.99	0.07	83,83,83,83	0
58	MG	13	1714	1/1	0.99	0.03	73,73,73,73	0
58	MG	1H	3414	1/1	0.99	0.04	80,80,80,80	0
58	MG	1H	3415	1/1	0.99	0.05	73,73,73,73	0
58	MG	1H	3362	1/1	0.99	0.04	53,53,53,53	0
58	MG	13	1709	1/1	0.99	0.08	92,92,92,92	0
58	MG	I8	103	1/1	0.99	0.07	73,73,73,73	0
58	MG	1H	3419	1/1	0.99	0.04	101,101,101,101	0
58	MG	1H	3420	1/1	0.99	0.04	92,92,92,92	0
58	MG	1H	3421	1/1	0.99	0.03	64,64,64,64	0
58	MG	13	1716	1/1	0.99	0.03	76,76,76,76	0
58	MG	1H	3423	1/1	0.99	0.03	66,66,66,66	0
58	MG	1H	3424	1/1	0.99	0.04	48,48,48,48	0
58	MG	1H	3344	1/1	0.99	0.02	58,58,58,58	0
58	MG	13	1723	1/1	0.99	0.03	87,87,87,87	0
58	MG	1H	3428	1/1	0.99	0.06	51,51,51,51	0
58	MG	1H	3369	1/1	0.99	0.06	49,49,49,49	0
58	MG	1H	3430	1/1	0.99	0.08	49,49,49,49	0
58	MG	1H	3431	1/1	0.99	0.04	70,70,70,70	0
58	MG	1H	3432	1/1	0.99	0.03	50,50,50,50	0
59	SF4	32	301	8/8	0.99	0.03	115,123,133,136	0
58	MG	1H	3346	1/1	0.99	0.03	45,45,45,45	0
58	MG	1H	3434	1/1	0.99	0.05	51,51,51,51	0
58	MG	14	3318	1/1	0.99	0.10	64,64,64,64	0
58	MG	1H	3382	1/1	1.00	0.03	77,77,77,77	0
58	MG	1H	3366	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3396	1/1	1.00	0.02	78,78,78,78	0
58	MG	1H	3374	1/1	1.00	0.04	53,53,53,53	0
58	MG	1H	3398	1/1	1.00	0.08	66,66,66,66	0
58	MG	1H	3351	1/1	1.00	0.03	46,46,46,46	0
58	MG	14	3377	1/1	1.00	0.03	52,52,52,52	0
58	MG	1H	3416	1/1	1.00	0.03	69,69,69,69	0
58	MG	14	3379	1/1	1.00	0.02	60,60,60,60	0
58	MG	14	3354	1/1	1.00	0.03	70,70,70,70	0
58	MG	14	3331	1/1	1.00	0.02	63,63,63,63	0
58	MG	16	206	1/1	1.00	0.01	73,73,73,73	0
58	MG	1H	3386	1/1	1.00	0.02	57,57,57,57	0
58	MG	14	3334	1/1	1.00	0.06	64,64,64,64	0
58	MG	1H	3401	1/1	1.00	0.03	69,69,69,69	0
58	MG	1H	3356	1/1	1.00	0.05	42,42,42,42	0
58	MG	1H	3352	1/1	1.00	0.02	61,61,61,61	0
58	MG	1H	3404	1/1	1.00	0.03	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	14	3339	1/1	1.00	0.03	82,82,82,82	0
58	MG	1H	3440	1/1	1.00	0.04	58,58,58,58	0
58	MG	1H	3378	1/1	1.00	0.04	53,53,53,53	0
58	MG	1H	3390	1/1	1.00	0.06	50,50,50,50	0
58	MG	1H	3363	1/1	1.00	0.02	68,68,68,68	0
60	ZN	5I	101	1/1	1.00	0.03	102,102,102,102	0
58	MG	13	1713	1/1	1.00	0.03	101,101,101,101	0
58	MG	13	1721	1/1	1.00	0.02	66,66,66,66	0
58	MG	1H	3427	1/1	1.00	0.02	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.