



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:03 pm BST

PDB ID : 5EL6
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the first position and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.10 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

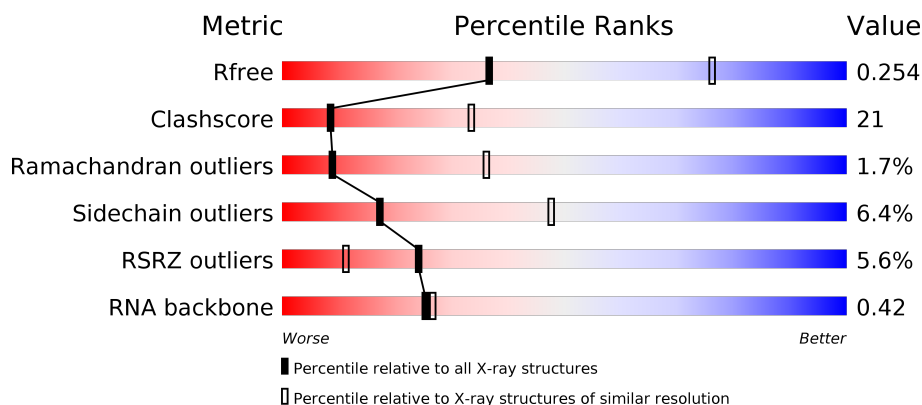
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



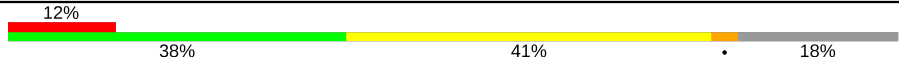

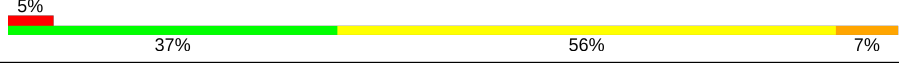

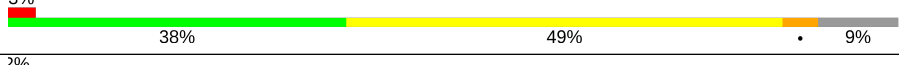
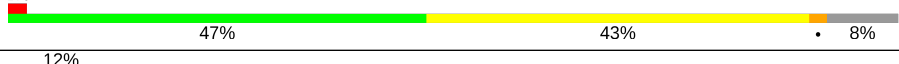
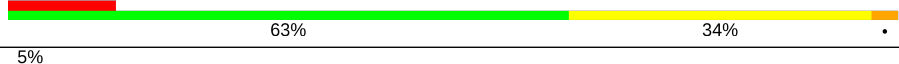




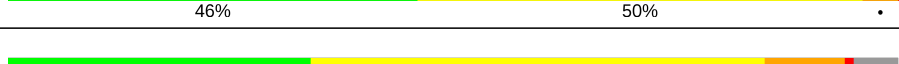
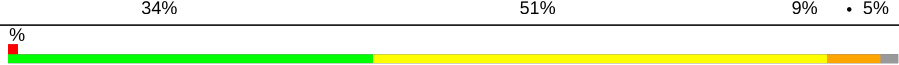
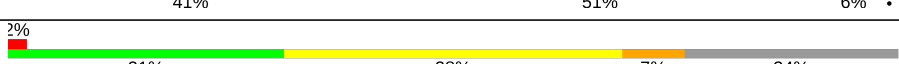
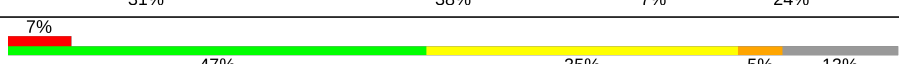
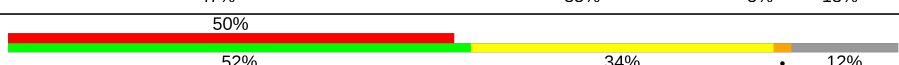
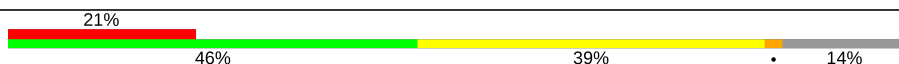
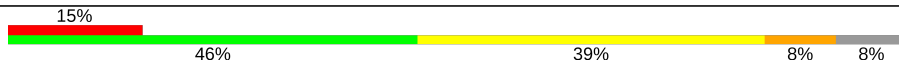



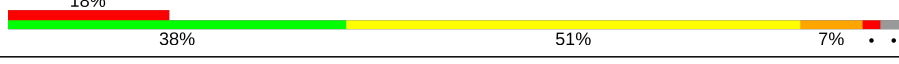
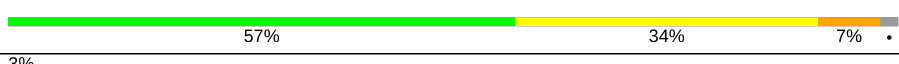


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	
27	1J	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	71	229	
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1629	-	-	-	X
56	MG	13	1646	-	-	-	X
56	MG	13	1648	-	-	-	X
56	MG	13	1674	-	-	-	X
56	MG	13	1690	-	-	-	X
56	MG	13	1693	-	-	-	X
56	MG	13	1695	-	-	-	X
56	MG	14	3032	-	-	-	X
56	MG	14	3055	-	-	-	X
56	MG	14	3091	-	-	-	X
56	MG	14	3110	-	-	-	X
56	MG	14	3126	-	-	-	X
56	MG	14	3156	-	-	-	X
56	MG	14	3162	-	-	-	X
56	MG	14	3177	-	-	-	X
56	MG	14	3205	-	-	-	X
56	MG	14	3222	-	-	-	X
56	MG	14	3224	-	-	-	X
56	MG	14	3229	-	-	-	X
56	MG	14	3233	-	-	-	X
56	MG	14	3254	-	-	-	X
56	MG	14	3261	-	-	-	X
56	MG	14	3262	-	-	-	X
56	MG	14	3291	-	-	-	X
56	MG	14	3302	-	-	-	X
56	MG	14	3303	-	-	-	X
56	MG	14	3304	-	-	-	X
56	MG	16	207	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1G	1602	-	-	-	X
56	MG	1G	1616	-	-	-	X
56	MG	1G	1622	-	-	-	X
56	MG	1G	1637	-	-	-	X
56	MG	1G	1638	-	-	-	X
56	MG	1G	1644	-	-	-	X
56	MG	1G	1651	-	-	-	X
56	MG	1G	1654	-	-	-	X
56	MG	1G	1666	-	-	-	X
56	MG	1G	1668	-	-	-	X
56	MG	1H	3015	-	-	-	X
56	MG	1H	3018	-	-	-	X
56	MG	1H	3028	-	-	-	X
56	MG	1H	3039	-	-	-	X
56	MG	1H	3046	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3099	-	-	-	X
56	MG	1H	3134	-	-	-	X
56	MG	1H	3189	-	-	-	X
56	MG	1H	3206	-	-	-	X
56	MG	1H	3213	-	-	-	X
56	MG	1H	3219	-	-	-	X
56	MG	1H	3224	-	-	-	X
56	MG	1H	3250	-	-	-	X
56	MG	1H	3270	-	-	-	X
56	MG	1H	3273	-	-	-	X
56	MG	1H	3274	-	-	-	X
56	MG	1H	3275	-	-	-	X
56	MG	1H	3291	-	-	-	X
56	MG	1H	3295	-	-	-	X
56	MG	1H	3299	-	-	-	X
56	MG	1H	3302	-	-	-	X
56	MG	1H	3308	-	-	-	X
56	MG	1H	3316	-	-	-	X
56	MG	1H	3317	-	-	-	X
56	MG	1J	203	-	-	-	X
56	MG	1K	101	-	-	-	X
56	MG	2K	101	-	-	-	X
56	MG	2K	102	-	-	-	X
56	MG	2L	102	-	-	-	X
56	MG	35	201	-	-	-	X
56	MG	3E	301	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	SF4	32	301	-	-	X	-
58	SF4	3E	302	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294257 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			

- 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				
9	82	121	Total	C	N	O		0	0	0
			953	605	186	162				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	80	Total	C	N	O	0	0	0
			646	403	129	114			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	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	82	Total	C	N	O	S	0	0	0
			658	419	123	114	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 tRNA^{Lys}.

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

- Molecule 23 is a RNA chain called E. coli tRNA^{fMet}.

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

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			
24	3L	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	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	18	Total	C	N	O	P	0	0	0
			395	177	81	119	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			

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	69	Total	C	N	O	S	0	0	0
			539	339	109	91				

- 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	132	Total	C	N	O	0	0	0
			1101	686	227	188			
41	75	133	Total	C	N	O	S	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
			950	603	199	147	1		
42	85	116	Total	C	N	O	S	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
			774	499	141	133	1		
43	95	100	Total	C	N	O	S	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
			890	560	175	153	2		
44	A5	111	Total	C	N	O	S	0	0
			886	558	174	152	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
			743	482	134	126	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	105	Total	C	N	O	S	0	0	0
			799	513	153	128	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	68	Total	C	N	O	S	0	0	0
			568	352	115	100	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			
55	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	45	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

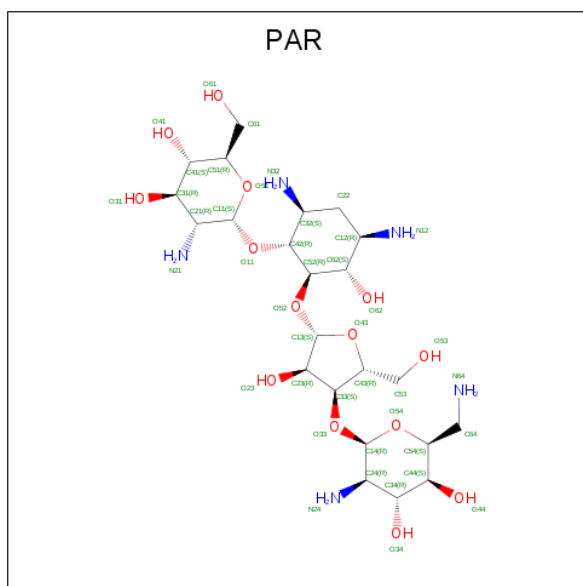
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	P8	1	Total 1	Mg 1	0	0
56	85	1	Total 1	Mg 1	0	0
56	C5	1	Total 1	Mg 1	0	0
56	13	131	Total 131	Mg 131	0	0
56	1J	5	Total 5	Mg 5	0	0
56	5I	1	Total 1	Mg 1	0	0
56	35	1	Total 1	Mg 1	0	0
56	16	11	Total 11	Mg 11	0	0
56	3K	1	Total 1	Mg 1	0	0
56	21	2	Total 2	Mg 2	0	0
56	2K	3	Total 3	Mg 3	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0
56	3I	1	Total 1	Mg 1	0	0
56	I8	3	Total 3	Mg 3	0	0
56	5E	1	Total 1	Mg 1	0	0
56	29	1	Total 1	Mg 1	0	0
56	78	1	Total 1	Mg 1	0	0
56	39	1	Total 1	Mg 1	0	0
56	1G	81	Total 81	Mg 81	0	0
56	1H	429	Total 429	Mg 429	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	E5	1	Total	Mg	0	0
			1	1		
56	88	2	Total	Mg	0	0
			2	2		
56	14	382	Total	Mg	0	0
			382	382		
56	3E	1	Total	Mg	0	0
			1	1		
56	4K	1	Total	Mg	0	0
			1	1		
56	1K	1	Total	Mg	0	0
			1	1		
56	41	1	Total	Mg	0	0
			1	1		
56	2L	3	Total	Mg	0	0
			3	3		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	13	1	Total	C	N	O	0	0
			42	23	5	14		
57	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C5	1	Total	Zn	0	0
			1	1		
59	5A	1	Total	Zn	0	0
			1	1		
59	G8	1	Total	Zn	0	0
			1	1		
59	5I	1	Total	Zn	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	144	Total	O	0	0
			144	144		
60	3E	2	Total	O	0	0
			2	2		
60	1I	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	5I	2	Total 2	O 2	0	0
60	6I	1	Total 1	O 1	0	0
60	7I	1	Total 1	O 1	0	0
60	BI	1	Total 1	O 1	0	0
60	3K	1	Total 1	O 1	0	0
60	4K	3	Total 3	O 3	0	0
60	1H	540	Total 540	O 540	0	0
60	16	22	Total 22	O 22	0	0
60	11	10	Total 10	O 10	0	0
60	31	7	Total 7	O 7	0	0
60	58	2	Total 2	O 2	0	0
60	78	4	Total 4	O 4	0	0
60	98	1	Total 1	O 1	0	0
60	G8	1	Total 1	O 1	0	0
60	I8	2	Total 2	O 2	0	0
60	L8	3	Total 3	O 3	0	0
60	P8	1	Total 1	O 1	0	0
60	1G	68	Total 68	O 68	0	0
60	32	2	Total 2	O 2	0	0
60	14	367	Total 367	O 367	0	0
60	1J	12	Total 12	O 12	0	0

Continued on next page...

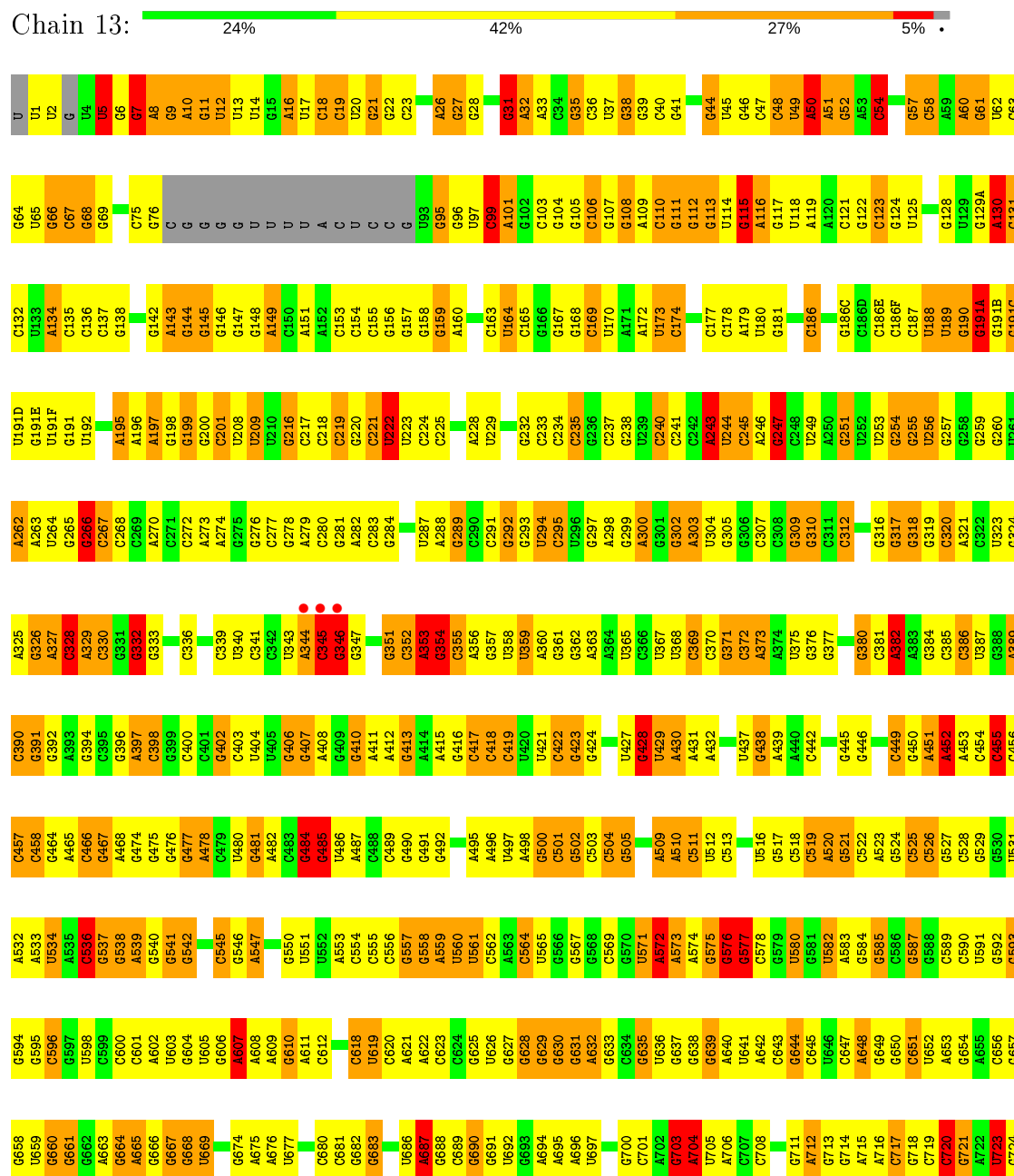
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	19	8	Total 8	O 8	0	0
60	29	2	Total 2	O 2	0	0
60	39	3	Total 3	O 3	0	0
60	35	2	Total 2	O 2	0	0
60	55	2	Total 2	O 2	0	0
60	H5	1	Total 1	O 1	0	0
60	L5	1	Total 1	O 1	0	0

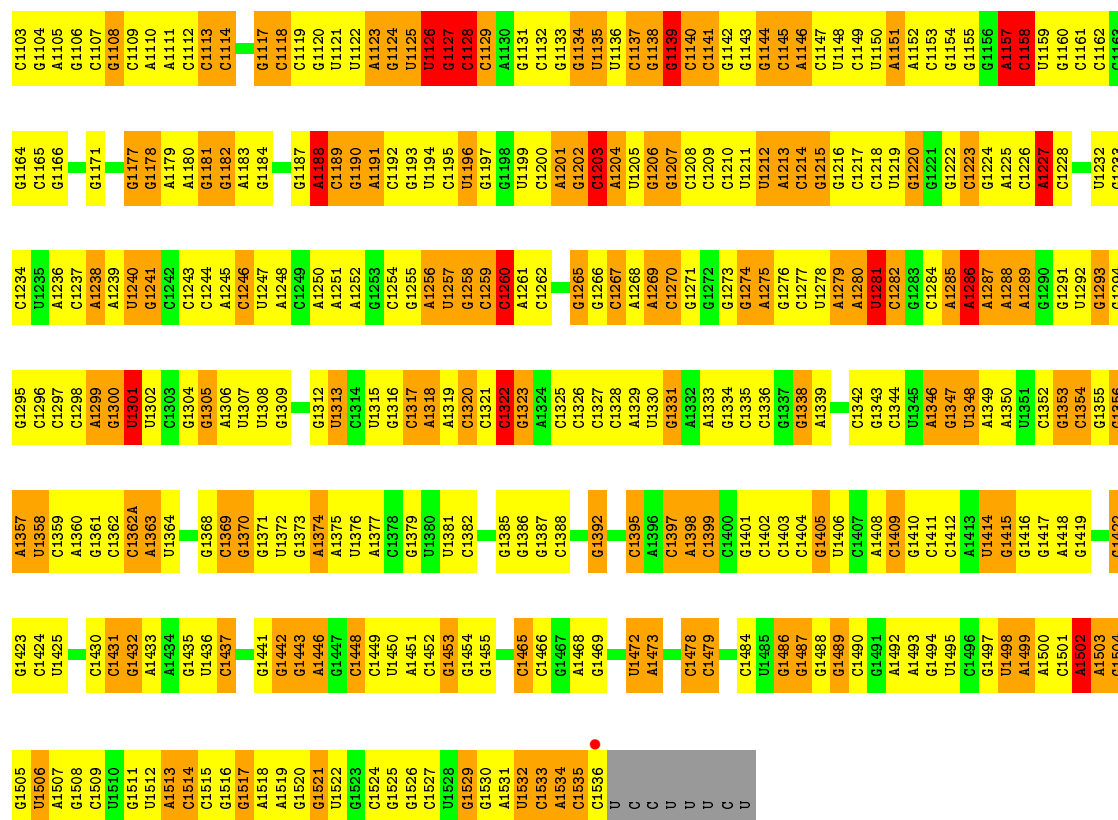
3 Residue-property plots

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

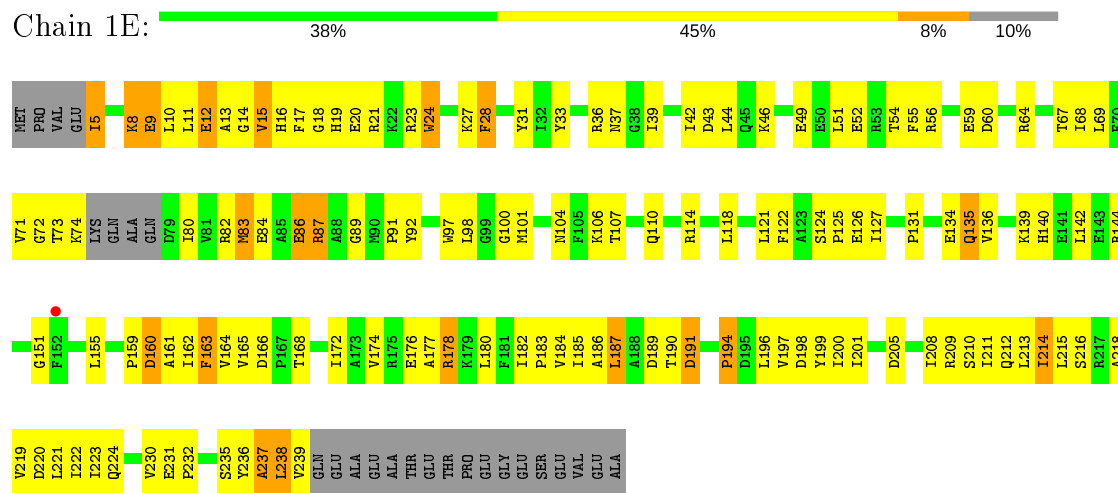
• Molecule 1: 16S rRNA



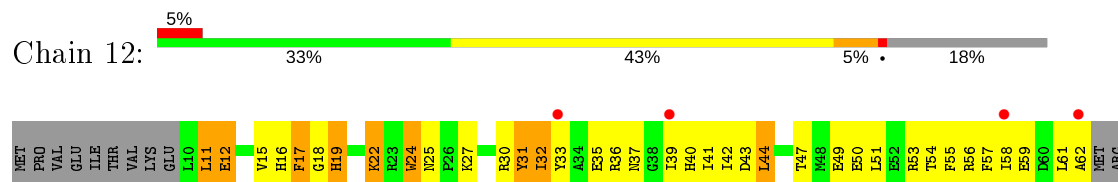


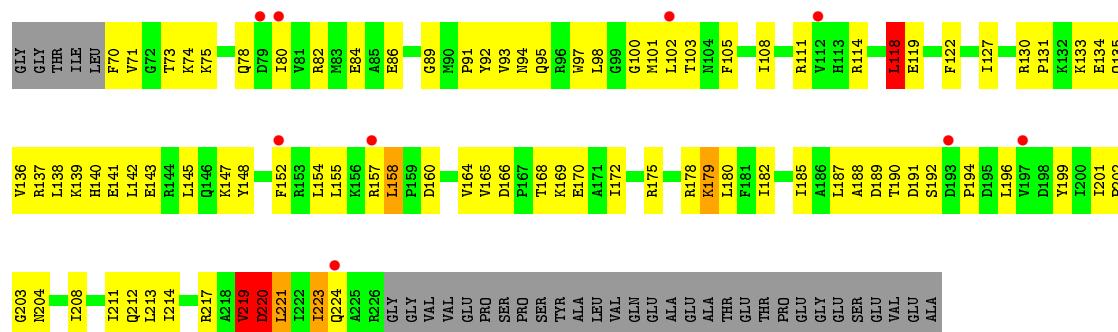


• Molecule 2: 30S ribosomal protein S2

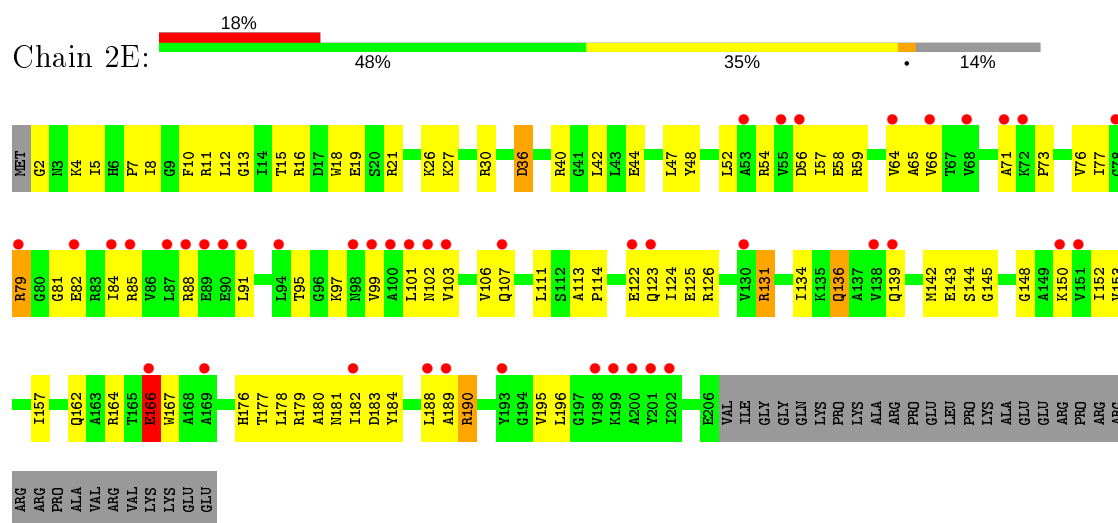


• Molecule 2: 30S ribosomal protein S2

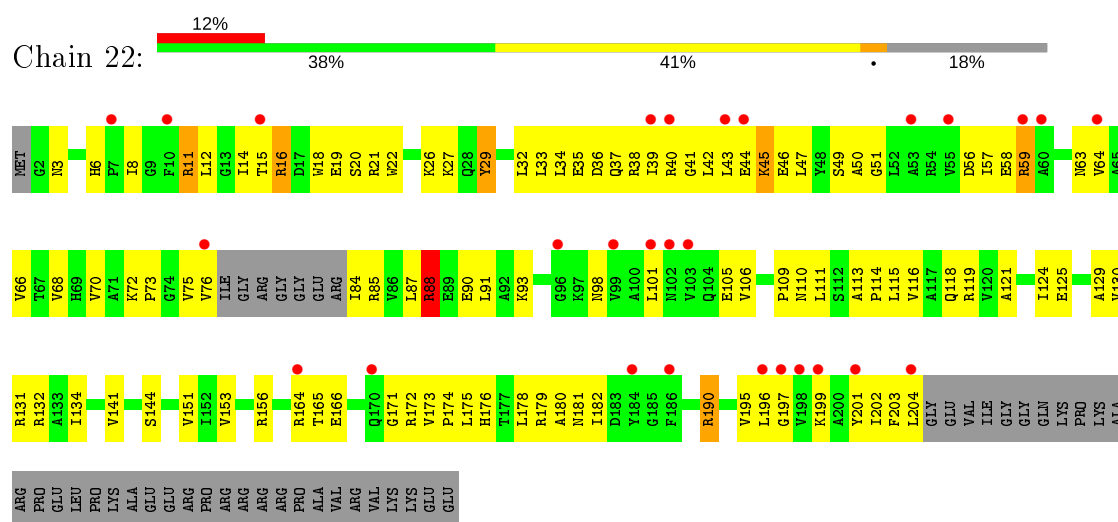




• Molecule 3: 30S ribosomal protein S3

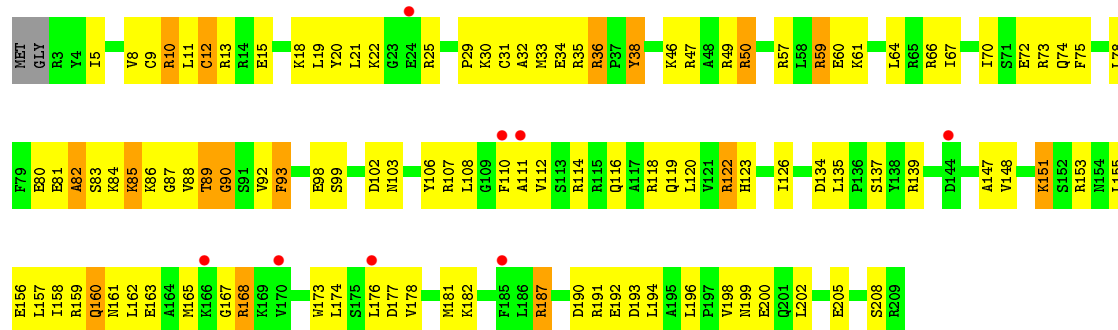


• Molecule 3: 30S ribosomal protein S3

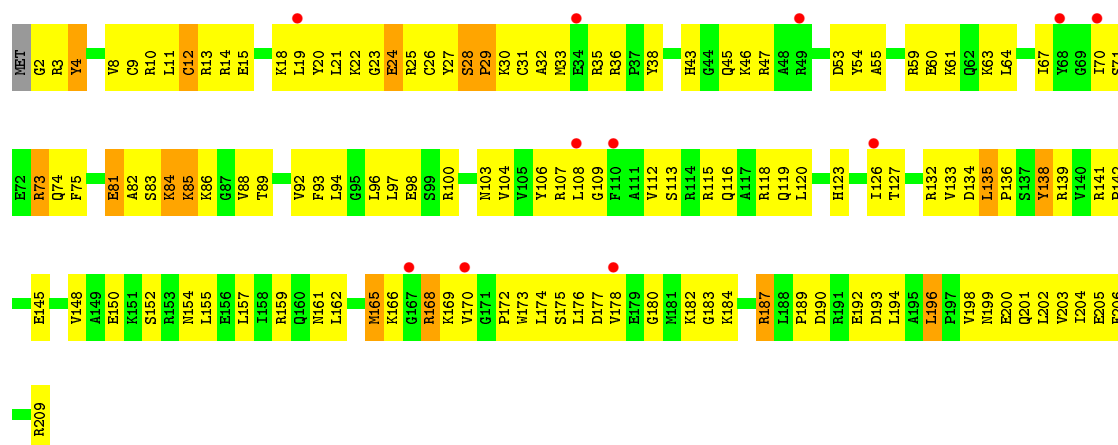


• Molecule 4: 30S ribosomal protein S4

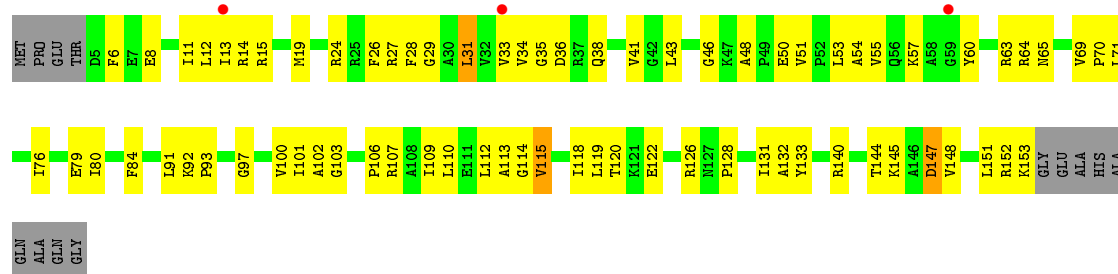




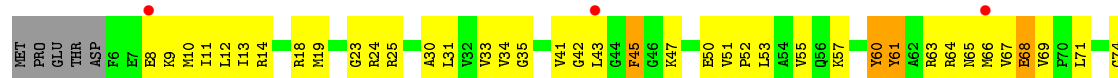
• Molecule 4: 30S ribosomal protein S4

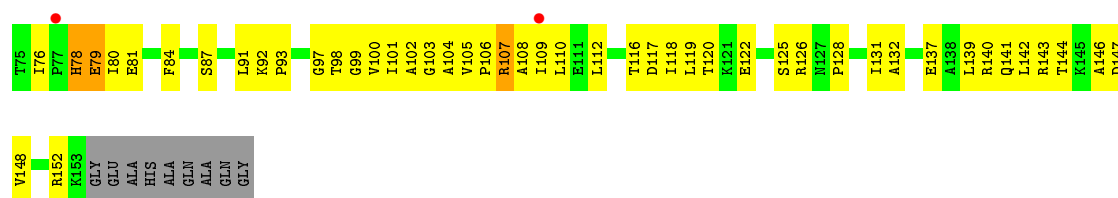


• Molecule 5: 30S ribosomal protein S5

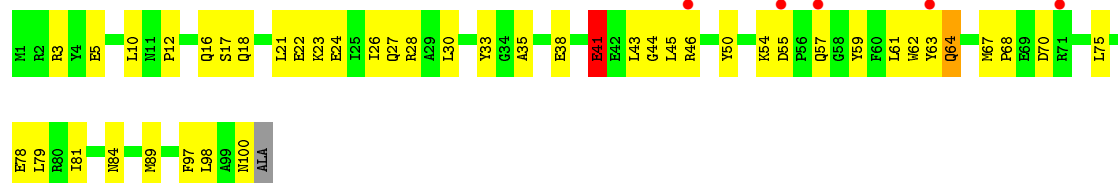


• Molecule 5: 30S ribosomal protein S5

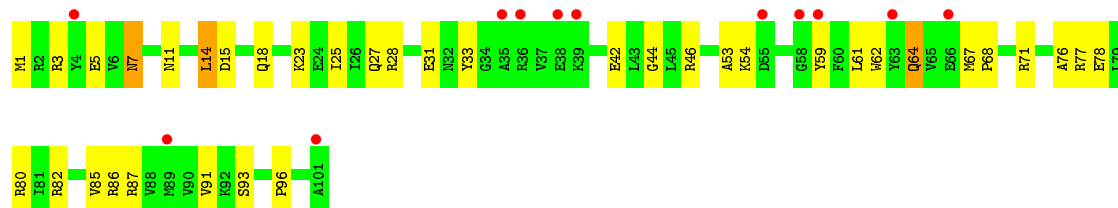




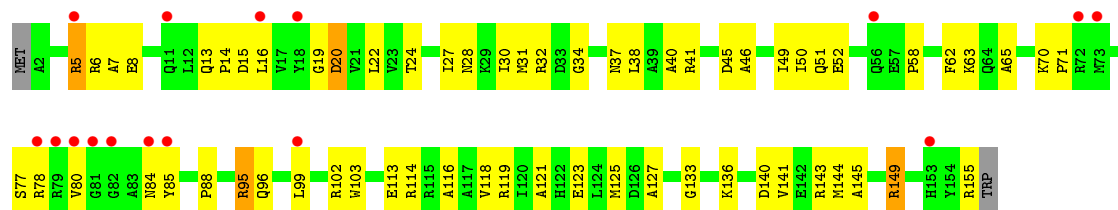
- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6

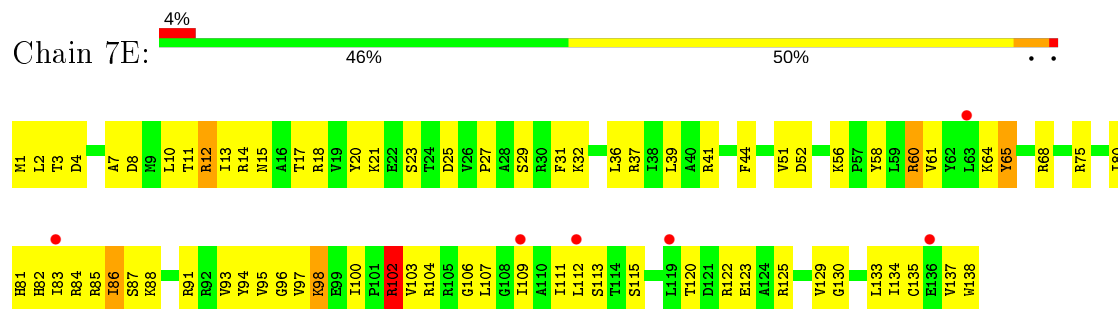


- Molecule 7: 30S ribosomal protein S7

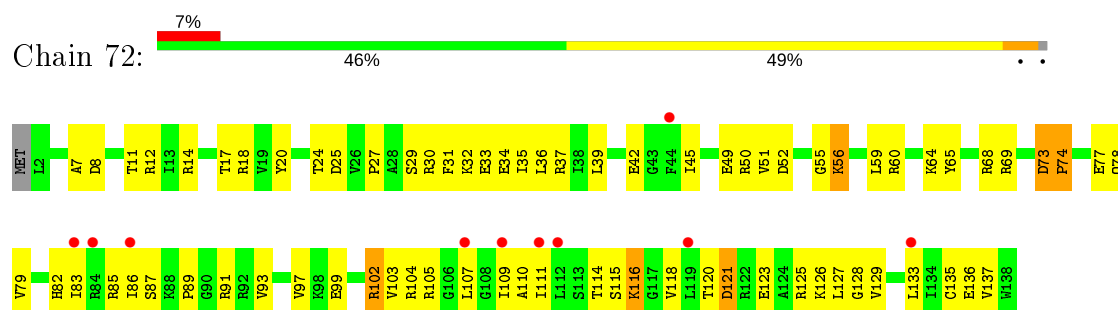


HIS
TYR
ARG
TRP

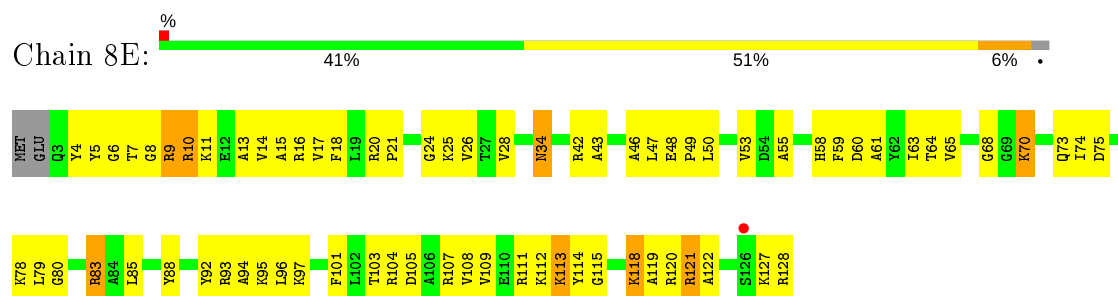
• Molecule 8: 30S ribosomal protein S8



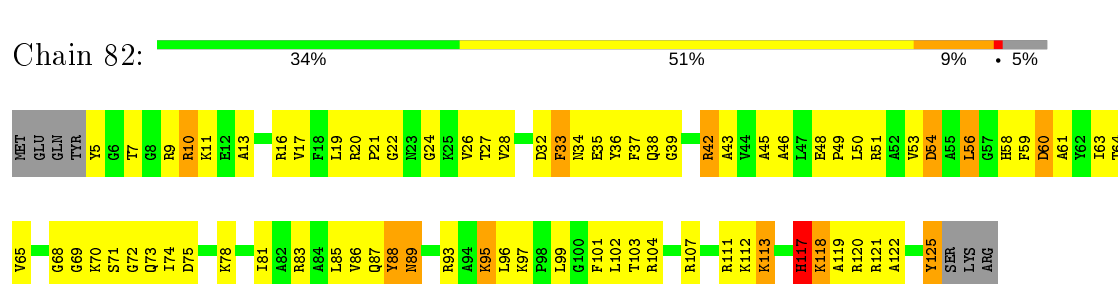
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

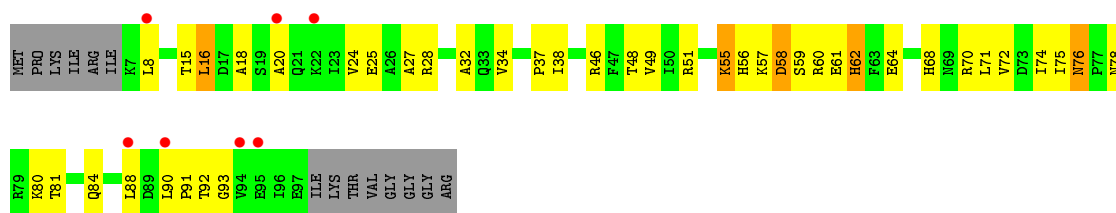


• Molecule 9: 30S ribosomal protein S9

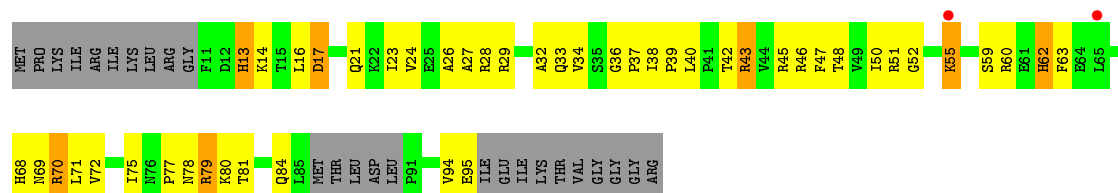


• Molecule 10: 30S ribosomal protein S10

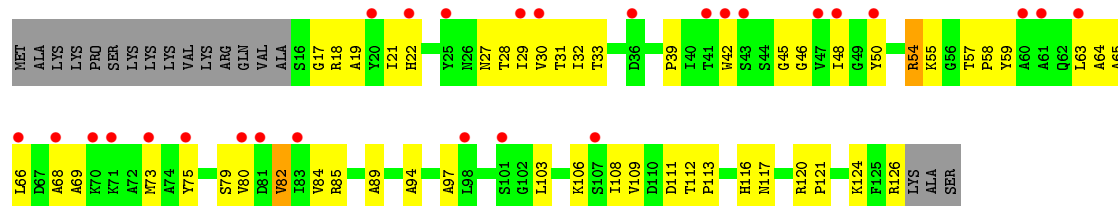




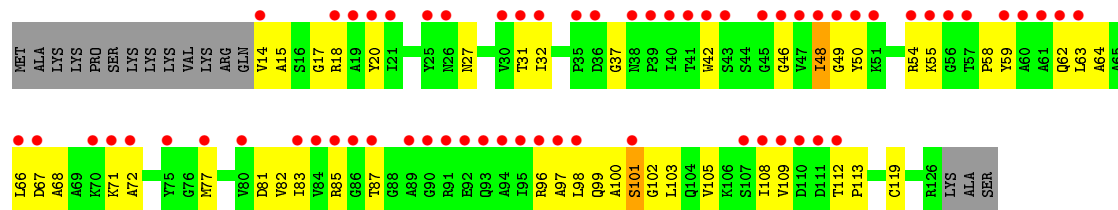
• Molecule 10: 30S ribosomal protein S10



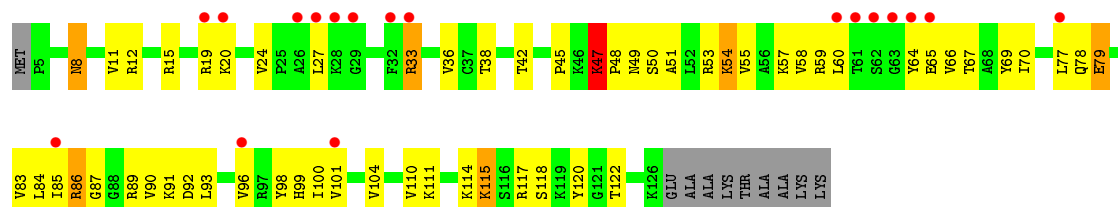
• Molecule 11: 30S ribosomal protein S11



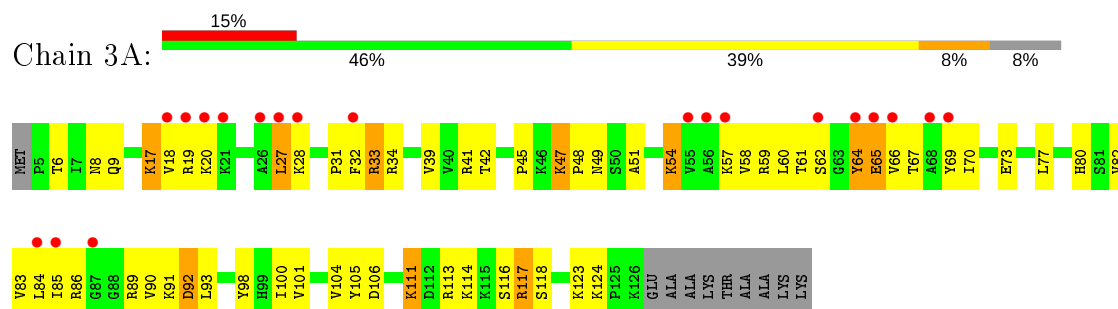
• Molecule 11: 30S ribosomal protein S11



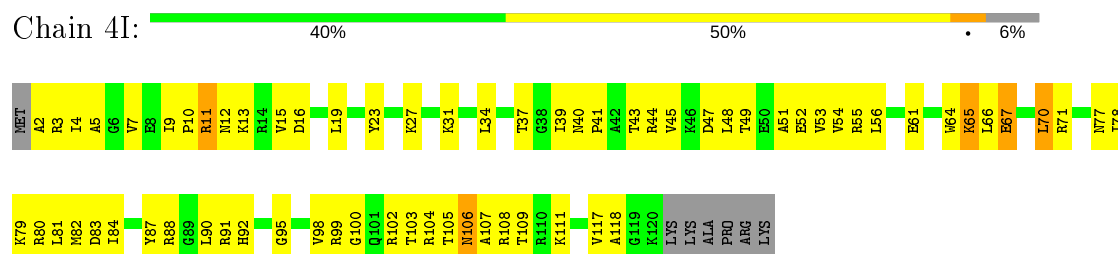
• Molecule 12: 30S ribosomal protein S12



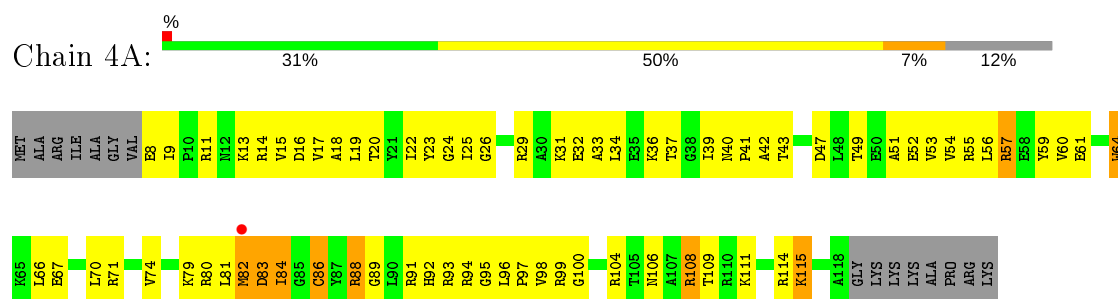
- Molecule 12: 30S ribosomal protein S12



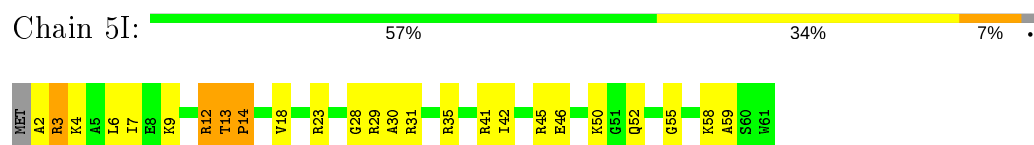
- Molecule 13: 30S ribosomal protein S13



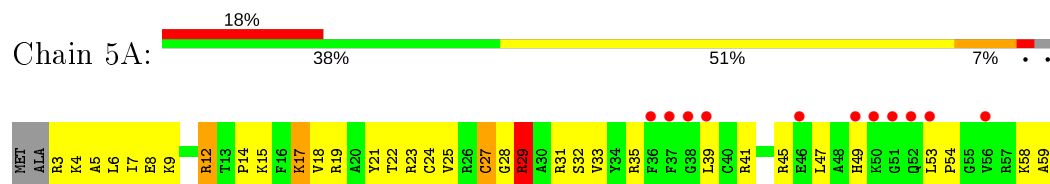
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

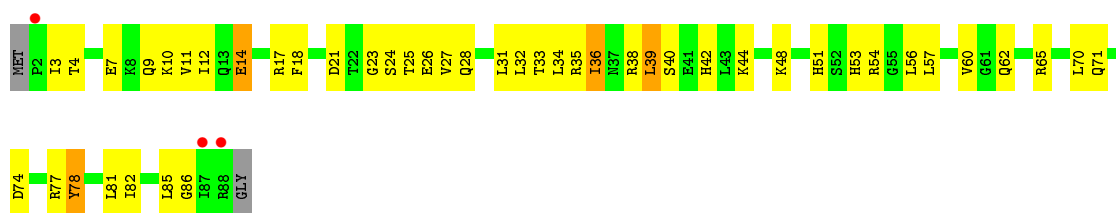


- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

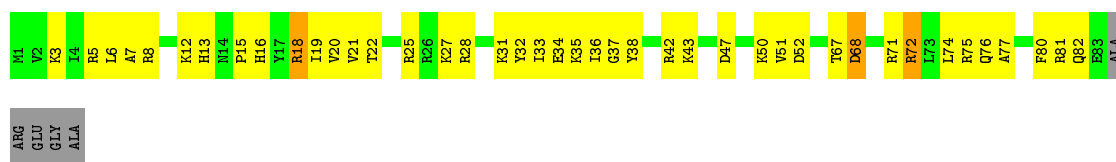




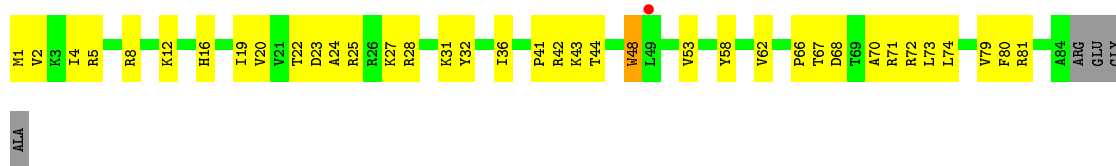
- Molecule 15: 30S ribosomal protein S15



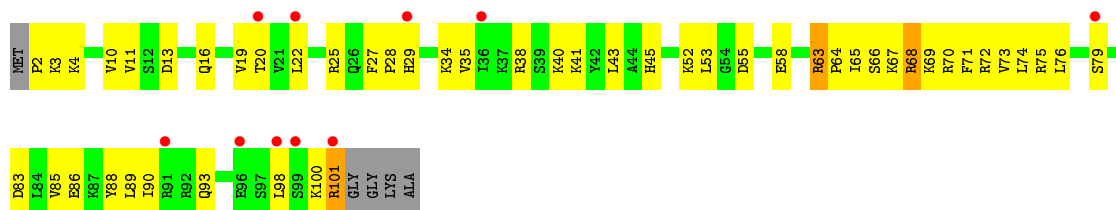
- Molecule 16: 30S ribosomal protein S16



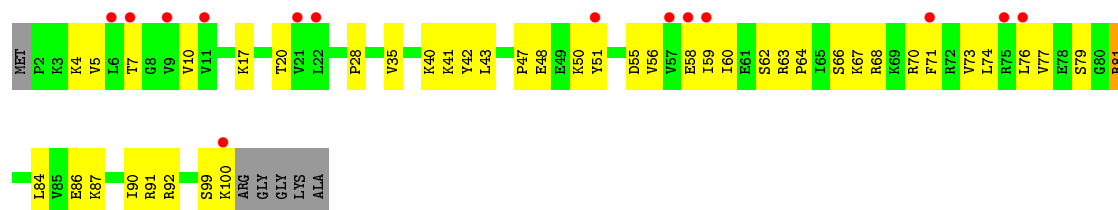
- Molecule 16: 30S ribosomal protein S16



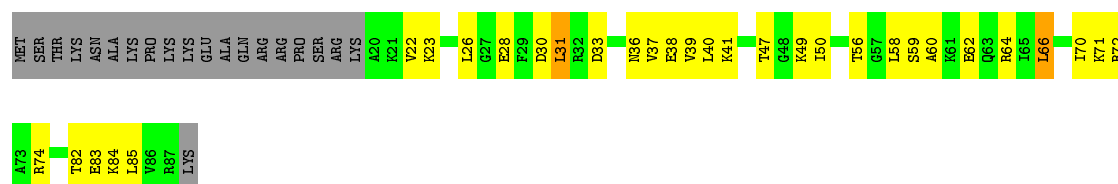
- Molecule 17: 30S ribosomal protein S17



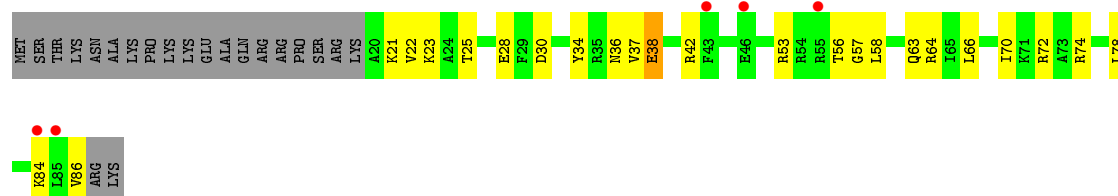
- Molecule 17: 30S ribosomal protein S17



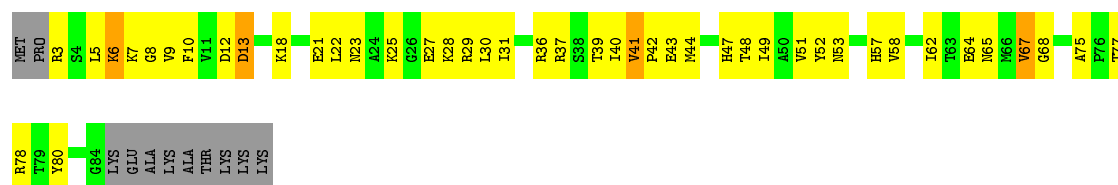
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

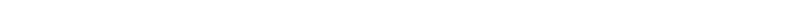


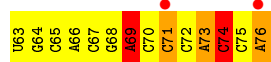
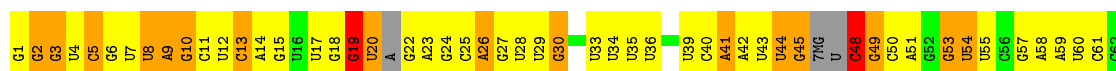
- Molecule 19: 30S ribosomal protein S19



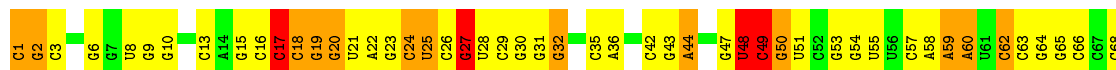
- Molecule 19: 30S ribosomal protein S19



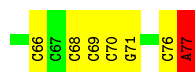
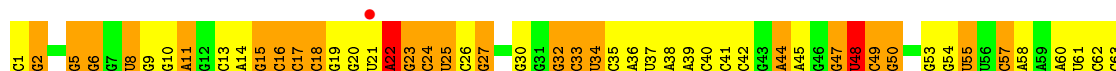
- Chain 1L: 



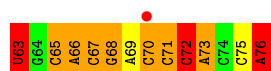
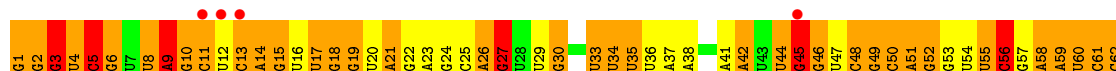
• Molecule 23: E. coli tRNA^{fMet}



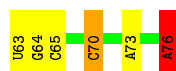
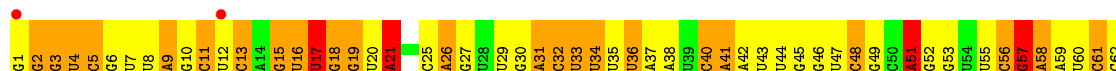
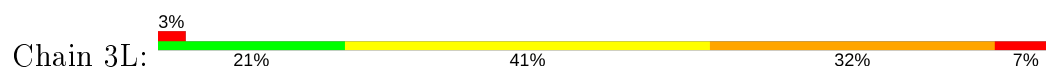
• Molecule 23: E. coli tRNA^{fMet}



• Molecule 24: tRNA^{Lys}

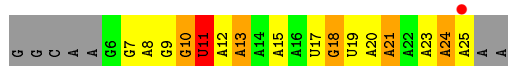


• Molecule 24: tRNA^{Lys}

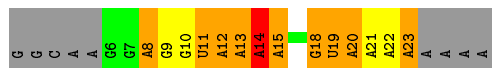


• Molecule 25: mRNA

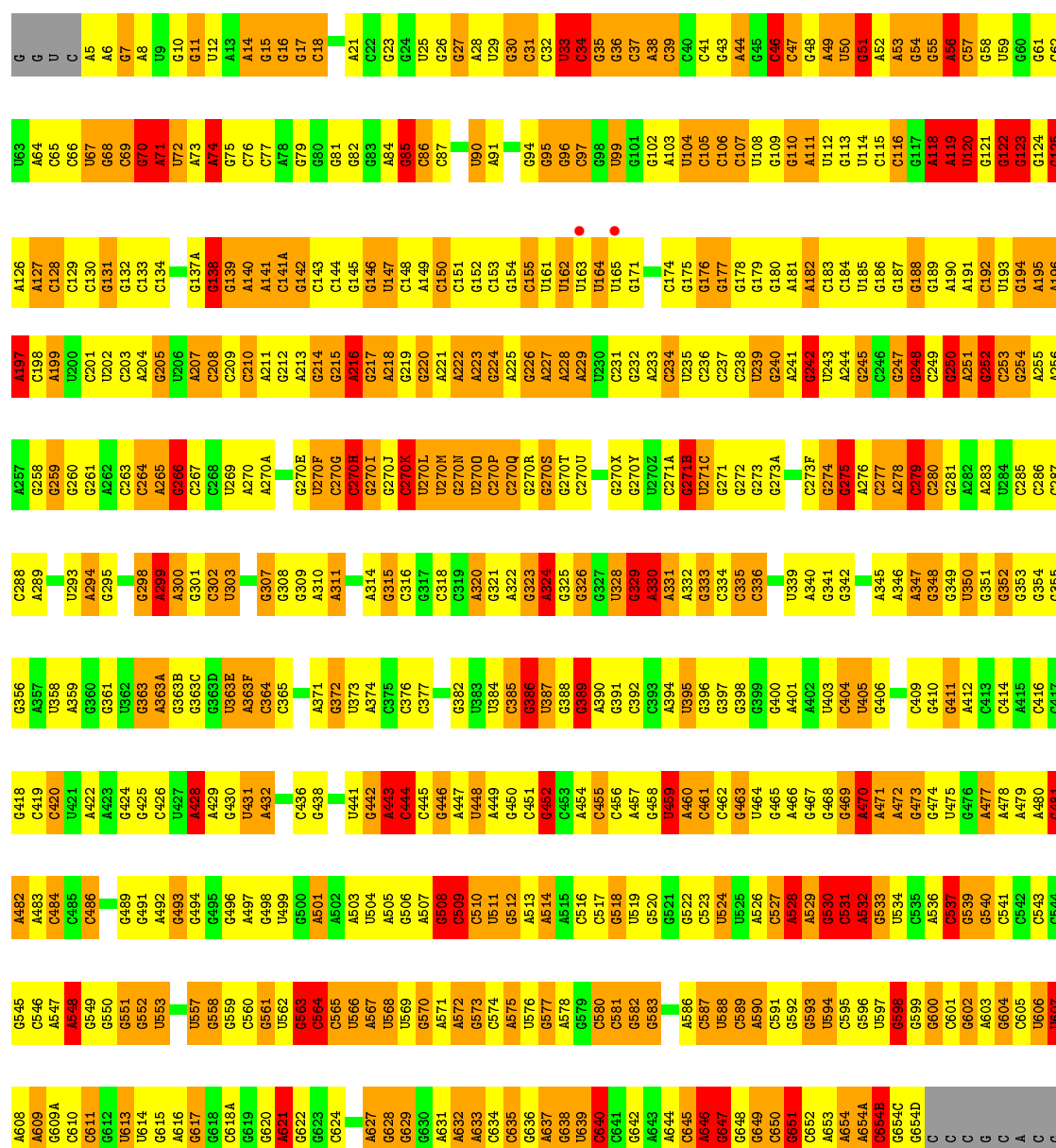




• Molecule 25: mRNA

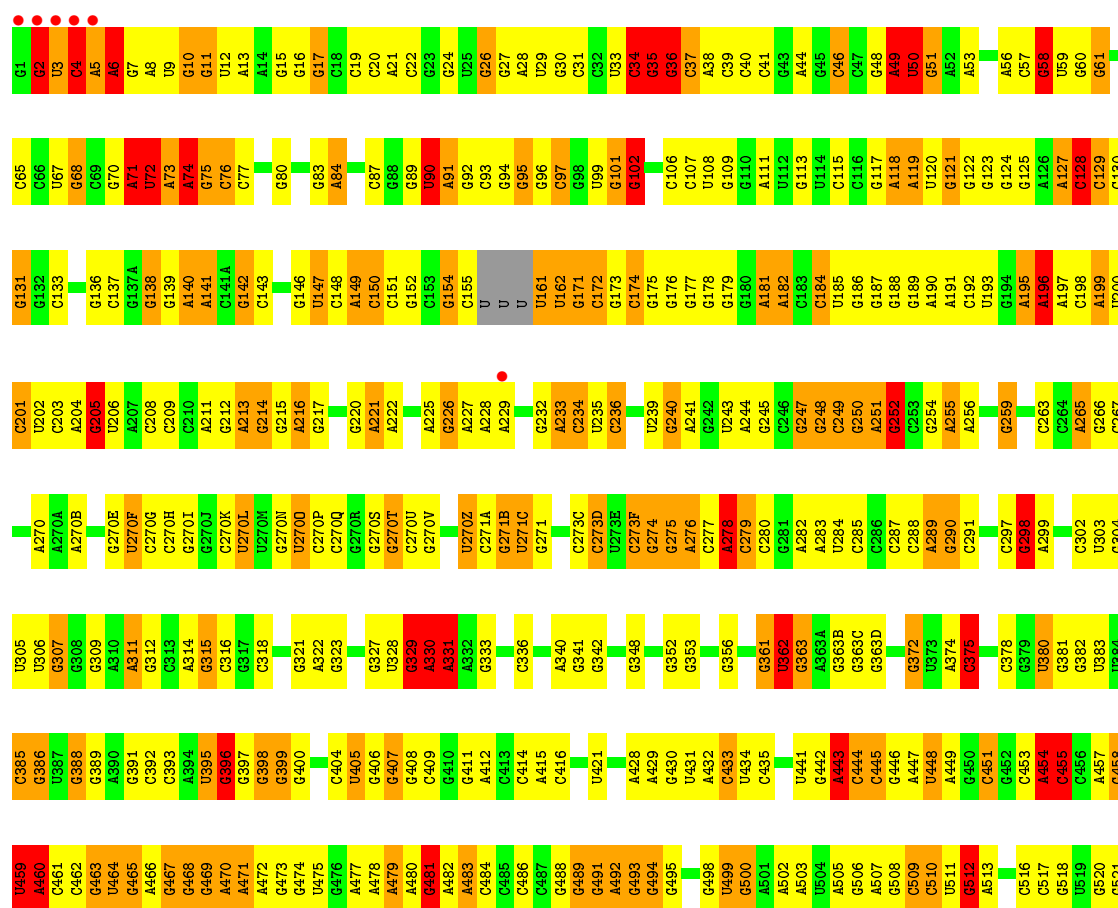


• Molecule 26: 23S rRNA



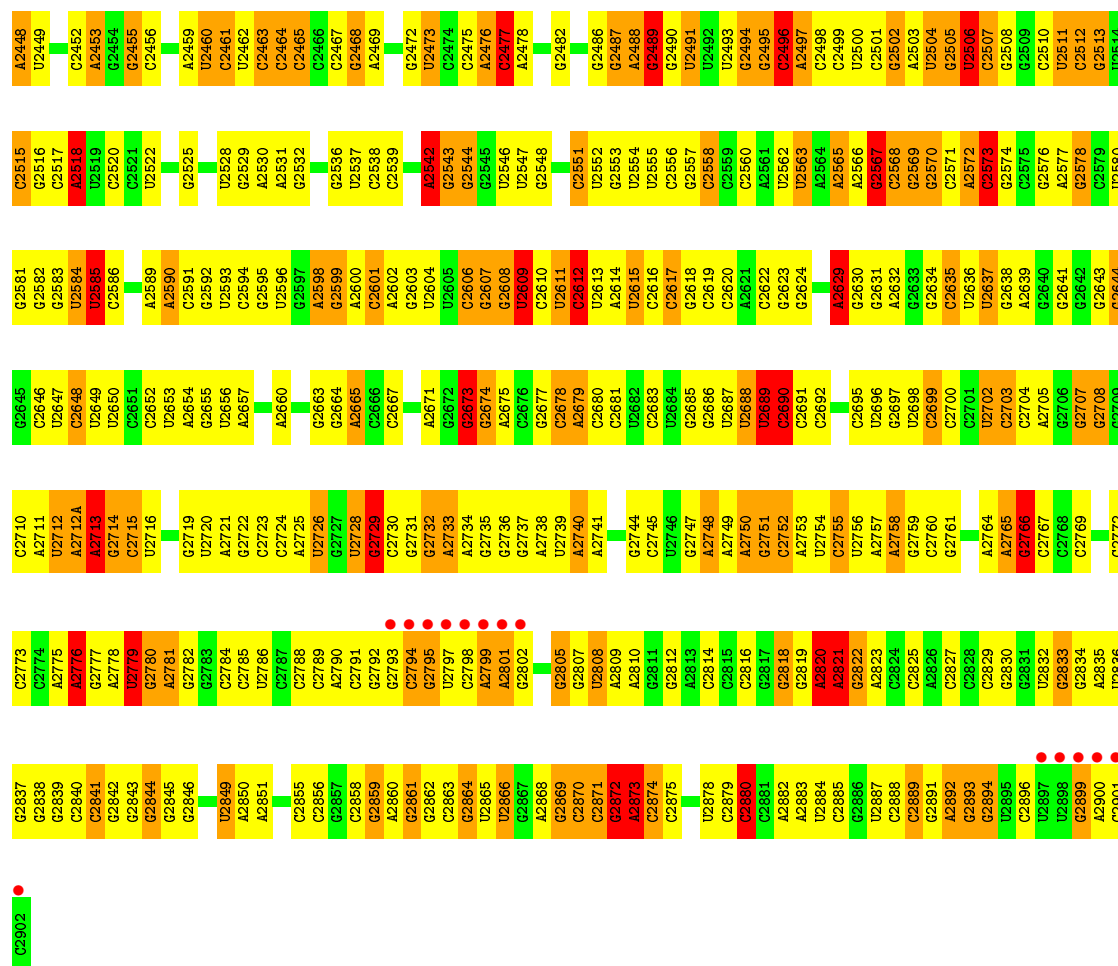
A1508	C1445	C1386	U1326	U1263	C1201	U1141	C	U1012	G950	C	U826	C766	A706	C
C1509	C1446	C1387	C1327	G1264	G1202	U1142	C	C1013	C951	C	U827	U767	G707	G654N
A1510	G1447	C1388	G1328	A1265	A1204	A1143	A	G1016	G952	A	U828	G768	C708	G654O
A1511	G1448	G1389	U1329	C1266	G1203	A1144	U		A953	G	A829	G769	U709	G654P
G1512	A1449	U1390	C1330	U1267	U1205	C1145	C		G954	C	G830	G770	G710	G654Q
C1513	G1450	U1391	A1331	A1268	G1206	C1146	A	U1019	C955	A	G831	G771	G711	G654R
U1514	G1451	A1392	G1332	A1269	C1207	C1147	U	A1020	G956	U	G832	C772	G712	G654S
C1515	A1453	A1393	G1333	C1270	C1208	C1148	U	G1021	A957	A	U833	U773	G713	A654T
U1516	U1454	G1394	G1334	G1271	G1209	A1148	U	A1022	U958	C	G834	A774	U714	
G1517	G1455	A1395	U1335	A1272	A1210	C1149	A	U1023	A959	C	A835	G775	A715	A655
C1518	G1456	U1396	A1336	U1273	G1211	C1150	A	G1024	A960	C	G836	G776	A716	G656
G1519	A1457	U1397	G1337	A1274	G1212	G1151	A	A1025	A961	C	C837	A777	G717	U657
U1520	C1458	C1398	G1338	A1275	A1213	G1152	G	U1026	G962	A	C838	G778	A718	C658
G1521	G1459	C1399	G1339	A1276	A1214	C1153	A	A1027	U963	C	U839	U779	C719	C659
G1522	A1460	G1400	U1340	G1277	G1215	G1154	U		G964	C	G840	G780	G720	G660
U1523	G1461	U1341	U1341	A1278		G1155	G	G1030	C965	C	A841	A781	C721	C661
G1524	C1462	C1402	A1342	G1279	G1218	A1156	G	G1031	G966	C	G842	A782	A722	G662
G1525	C1463	C1403	G1343	G1280	G1219	G1157	C	A1032	C967	C	G843	A783	G723	G663
G1526	G1464	G1404	G1344	G1281	A1220	C1158	G	U1033	G968	C	G844	A784	U724	C664
G1527	C1465	U1405	C1345	U1282	C1221	U1159	U	G1034	U969	C	G845	G785	G725	C665
A1528	G1466	U1406	G1346	G1283	C1222	G1160	A	U1035	C970	C	C846	G786	G726	G666
C1529	C1467	C1407	G1347	U1284	G1224	C1161	U	G1036	C971	C	U847	A787	A727	U667
	C1468	C1408	G1348	A1286	G1224	G1162	A	G1037	G972	C	G848	A788	G728	G668
	A1469	C1409	A1349	U1287	G1225	G1163	A	C1038	A973	C	G849	A789	G729	G669
C1532	G1470	C1350	C1350	A1288	G1226	G1164	G	G1039	G974	C	C850	A790	C730	A670
G1533	A1471	C1351	C1351	C1289	A1227	U1165	C	C1040	C974A	C	U851	C791	C731	G671
G1534	A1472	A1412	U1352	C1290	G1228	C1166	U	G1041	G975	C	G852	G792	G732	G672
A1535	G1473	C1353	A1353	C1291	G1229	U1167	C	G1042	C976	C	G853	A793	G733	G673
C1536	C1474	G1413	A1354	U1292	G1229A	G1168	A	C1043	G977	C	G854	G794	A734	G674
G1537	G1475	U1414	G1355	U1293	G1230	G1169	C	G1044	G978	C	G855	C795	A735	A675
C1538	G1476	G1415	G1356	G1296	G1231	G1170	U	A1045	G979	C	C856	C796	C736	A676
G1540	A1477	C1417	U1357	C1297		G1171	G	A1046		C	C857	C797	C737	A677
U1541	G1478	G1418	G1358	C1298	U1234	G1173	G	G1047	C982	C	U858	G798	G738	C678
G1542	G1479	A1419	A1359	G1299	G1235	A1174	U	A1048	A983	C	C859	G799	G739	C679
A1543	G1480	U1420	A1360	U1300	U1236	U1175	U	C1049	A984	C	U860	A800	U740	G680
C1544	U1482	G1421	G1361	A1301	A1237	G1176	G	A1050		C	A861	A801	G741	G681
G1545	G1483	G1422	C1362	A1302	G1238	A1177	G	G1051	G987	C	G862	A802	G742	G682
A1545A	G1484	G1423	C1363	G1303	G1239	C1178	G	C1052	A988	C	A863	U803	G743	C683
C1546	G1485	G1424	G1364	C1304	U1240	C1179	U	A	G989	C	G864	A804	G744	G684
U1547	A1486	G1425	A1365	C1305	A1241	C1180	G	C1053	A990	C	C865	C805	G745	A685
C1548	G1487	G1426	A1366	C1306		G1181	G	A	C991	C	A866	C806		
C1549	G1488	A1427	A1367	A1307	G1244	A1182	G	G	C992	C	C867	U807	U747	G687
C1550	U1489	G1428	G1368	A1308	G1245	G1183	G	G	C993	C	G868	G808	G748	U688
C1551	A1490	G1429	G1369	G1309	A1246	C1184	A	U	C994	C	U869	G809	C749	A689
G1552	G1491	C1430	C1370	G1310	A1247	C1185	U	G	C995	C	A870	U810	A750	G690
A1553	G1492	U1431	G1371	G1311	G1248	C1186	U	U	A996	C	U871	U811	A751	C691
C1554	C1493	C1432	U1372	U1312	U1249	G1187	U	G	C997	C	A872	C812	A752	C692
G1555	U1494	U1433	A1373	U1313	G1250	U1188	U	U	C998	C	G873	U813	C753	C693
C1556	A1495	A1434	G1374	C1314	G1251	A1189	C	G	U999	C		C814	C754	U694
C1557	U1496	G1435	C1375	C1315	G1252	G1190	U	C	A1000	C		C815	C755	G695
A1558	U1497	G1436	C1376	U1316	A1253		U	U	A1001	C	U877	C816	C756	G696
G1559	C1498	C1437	G1377	A1317	A1254	G1191	U	U	G940	C	A878	C817	U757	C697
G1560	U1499	U1438	A1378	C1318	U1255	G1192	U	A	A941	C	G879	C817	U757	C697
G1561	G1500	A1439	A1379	G1319	G1256	C1193	A	G	G1002	C	G880	G818	C758	C698
A1562	C1501	G1440	G1380	C1320	U1257	A1194	U	C	G1003	C	G881	A819	G759	A699
G1563	C1502	G1441	G1381	A1321	G1258	G1195	A	A	C1004	C	G882	A820	G760	G700
C1564		G1442	G1382	A1322	G1259	C1196	A	A	G1005	C	G	A821	A761	G701
A1565	C1503	C1443	C1383	U1323	G1260	G1197	G	G	C1006	C	C	U822	U762	G702
C1566	U1504	G1444	C1384	G1324	G1261	U1198	C	A	A1009	C	C	G823	G763	U703
A1567	A1507	A1444A	G1385	G1325	A1262	C1200	U	G	G1011	C	A	A824	A764	G704
												C825	G765	A705

G2484	G2485	A2486	A2487	A2488	G2489	G2490	G2491	G2492	A2493	A2494	G2495	G2496	A2497	C2498	C2499	G2500	G2501	G2502	G2503	U2504	G2505	U2506	G2507	G2508	G2509	G2510	U2511	G2512	U2513	U2514	G2515	A2516	G2517	G2518	U2519	G2520	G2521	U2522	G2523	G2524	G2525	G2526	G2527	U2528	G2529	A2530	G2531	G2532	A2533	A2534	G2535	G2536	U2537	C2538	C2539	U2540	A2541	A2542	G2543	G2544																						
G2421	A2422	U2423	C2424	A2425	A2426	A2427	G2428	G2429	U2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	U2438	A2439	C2440	C2441	C2442	C2443	C2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	C2452	A2453	A2454	C2455	U2456	U2457	G2458	C2459	U2460	A2461	U2462	C2463	C2464	C2465	G2466	G2467	G2468	A2469	G2470	C2471	G2472	U2473	C2474	C2475	C2476	C2477	A2478	G2479	G2480	G2481																						
C2359	A2360	C2361	G2362	C2363	C2364	G2365	A2366	G2367	A2368	C2369	G2370	G2371	G2372	G2373	C2374	G2375	A2376	A2377	G2378	A2379	C2380	C2381	G2382	C2383	G2384	C2385	C2386	C2387	A2388	G2389	U2390	G2391	C2392	A2393	C2394	C2395	G2396	G2397	U2398	G2399	G2400	U2401	C2402	C2403	C2404	G2405	U2406	G2407	U2408	G2409	G2410	A2411	A2412	G2413	G2414	C2415	C2416	C2417	A2418	G2419	G2420																					
G2299	G2300	C2301	G2302	G2303	G2304	A2305	C2306	G2307	G2308	A2309	G2310	A2311	U2312	C2313	C2314	G2315	G2316	C2317	G2318	G2319	C2320	G2321	A2322	C2323	G2324	G2325	C2326	A2327	C2328	G2329	G2330	G2331	U2332	C2333	G2334	C2335	A2336	G2337	G2338	G2339	G2340	G2341	G2342	C2343	G2344	G2345	A2346	G2347	U2348	G2349	G2350	G2351	A2352	C2353	C2354	G2355	C2356	U2357	G2358																							
G2238	G2239	G2240	U2241	U2242	U2243	U2244	U2245	G2246	A2247	U2248	G2249	A2250	G2251	U2252	G2253	G2254	G2255	U2256	G2257	G2258	G2259	C2260	G2261	U2262	C2263	C2264	U2265	A2266	A2267	A2268	A2269	G2270	G2271	U2272	A2273	A2274	G2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	C2283	G2284	G2285	A2286	A2287	A2288	G2289	G2290	U2291	A2292	C2293	G2294	C2295	U2296	G2297	A2298																						
C2184	G2185	C2186	U2187	G2188	G2189	A2190	A2191	U2192	A2193	A2194	G2195	C2196	C2197	U2198	G2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240																										
U2101	U2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	C2116	A2117	U2118	U2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	C2135	C2136	C2137	C2138	C2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163																				
G2037	G2038	C2039	G2040	U2041	A2042	C2043	G2044	U2045	G2046	U2047	G2048	G2049	A2050	A2051	G2052	G2053	A2054	C2055	G2056	A2057	U2058	A2059	A2060	G2061	A2062	C2063	G2064	C2065	C2066	G2067	U2068	G2069	G2070	U2071	G2072	C2073	U2074	U2075	U2076	A2077	G2078	C2079	U2080	U2081	A2082	G2083	C2084	U2085	U2086	G2087	G2088	U2089	U2090	U2091	U2092	G2093	G2094	A2095	G2096	A2097	U2098	U2099	G2100																			
U1976	A1977	A1978	C1979	U1980	A1981	C1982	C1983	U1984	G1985	G1986	G1987	G1988	G1989	C1990	U1991	G1992	U1993	C1994	U1995	C1996	G1997	G1998	C1999	G2000	G2001	G2002	G2003	A2004	A2005	C2006	G2007	C2008	G2009	U2010	U2011	G2012	A2013	A2014	U2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	G2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036																						
A1912	A1913	C1914	U1915	U1916	U1917	A1918	A1919	C1920	U1921	G1922	A1923	U1924	U1925	U1926	A1927	U1928	G1929	U1930	A1931	U1932	G1933	C1934	G1935	A1936	A1937	U1938	U1939	U1940	C1941	U1942	U1943	U1944	G1945	U1946	G1947	U1948	U1949	A1950	U1951	U1952	A1953	U1954	U1955	U1956	U1957	C1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	A1972	G1973	U1974	U1975																			
G1832	U1833	A1834	G1835	C1836	U1837	C1838	A1839	G1840	U1841	G1842	C1843	A1844	G1845	A1846	U1847	G1848	U1849	U1850	A1851	C1852	A1853	G1854	U1855	G1856	G1857	U1858	A1859	G1860	U1861	G1862	A1863	C1864	U1865	A1866	U1867	G1868	U1869	A1870	U1871	G1872	A1873	U1874	G1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	A1884	U1885	C1886	U1887	U1888	A1889	G1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	A1901	C1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910				
G1772	A1773	C1774	U1775	U1776	U1777	U1778	U1779	A1780	C1781	G1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	C1791	G1792	U1793	U1794	C1795	U1796	C1797	U1798	U1799	A1800	U1801	A1802	A1803	C1804	U1805	C1806	G1807	U1808	U1809	A1810	U1811	A1812	G1813	G1814	U1815	A1816	G1817	U1818	U1819	U1820	A1821	U1822	U1823	G1824	U1825	U1826	C1827	U1828	A1829	C1830	U1831																							
A1689	A1690	C1691	A1692	U1693	U1694	G1695	G1696	C1697	A1698	C1699	A1700	A1701	G1702	G1703	A1704	U1705	U1706	G1707	C1708	U1709	C1710	U1711	G1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	A1730	A1731	A1732	G1733	C1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771
U1629	G1630	A1631	A1632	G1633	U1634	G1635	C1636	A1637	C1638	A1639	U1640	A1641	G1642	G1643	U1644	G1645	G1646	C1647	U1648	G1649	U1650	U1651	G1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	C1660	G1661	G1662	C1663	A1664	A1665	U1666	G1667	A1668	A1669	U1670	G1671	U1672	C1673	A1674	U1675	G1676	A1677	U1678	U1679	U1680	U1681	G1682	U1683	U1684	U1685	U1686	U1687	U1688																							
G1568	A1569	A1570	A1571	G1572	U1573	C1574	U1575	U1576	C1577	U1578	A1579	U1580	G1581	C1582	U1583	A1584	U1585	A1586	U1587	C1588	U1589	U1590	U1591	C1592	U1593	G1594	U1595	A1596	U1597	C1598	U1599	C1600	G1601	A1602	C1603	C1604	A1605	U1606	C1607	A1608	U1609	U1610	C1611	G1612	U1613	A1614	U1615	A1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629																					

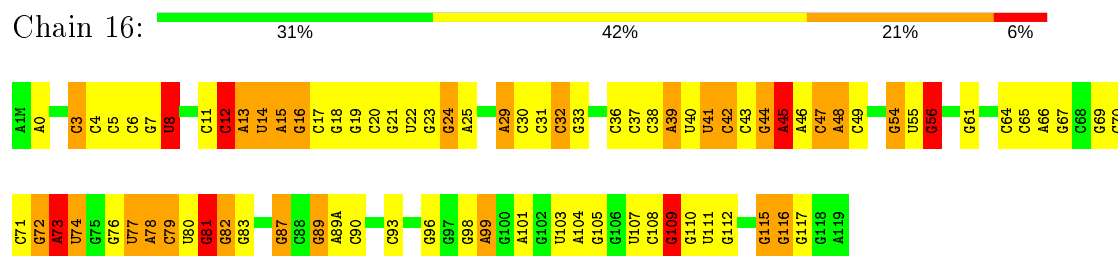




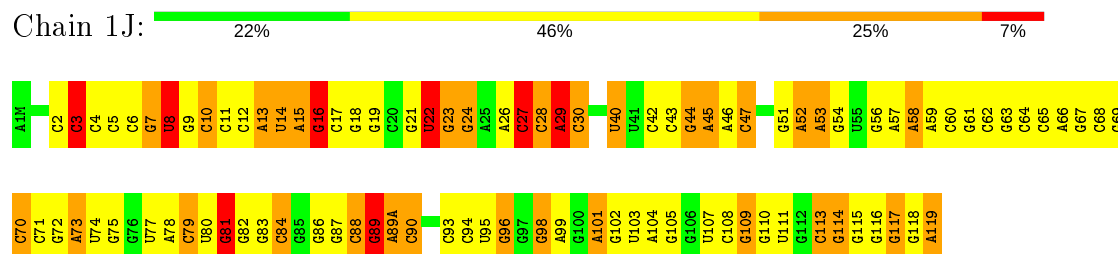
G2384	C2324	U2189	C2128	C2066	A2005	A1936	G1863	G1795	G1717	G1648	C1589	G1524	U1454
C2385	U2265	G2190	C2129	G2067	C2006	A1937	U1864	U1796	G1718	G1649	U1590	G1525	G1485
C2386	C2266	G2191	U2130	U2068	C2007	A1938	G1869	U1797	G1725		C1591	G1526	
A2327	A2267	G2192	A2327	C2069	C2008	U1939	C1870	U1798	G1726	G1653	C1592	G1527	G1459
A2328	A2268	G2193	U2132	G2070	G2009	U1940	A1871	G1799	U1727	A1654	G1593	A1528	A1460
A2389	G2269	G2194	G2133	A2071	G2010	U1941	A1872	C1800	G1728	C1655	G1594	G1461	
U2390	C2320	C2195	A2134	G2072	U2011	C1942	G1878	G1801	A1729	C1656	G1595	C1462	
C2391	C2196	C2196	A2136	C2073	A2012	U1943	C1879	A1802	U1730	C1657	C1596	C1463	
U2392	U2197	U2197	C2136	U2074	A2013	U1944		A1803	G1731	C1658	A1597	C1464	
C2393	A2273	A2198	C2137	U2075	A2014	U1945	A1884	C1804	A1732	C1659	C1598	G1465	
C2394	A2274	A2199	C2138	U2076	U2076	U1946	A1885	U1805	G1733	C1660	C1599	G1466	
C2395	C2275		C2139	A2077	U2016	G1947	A1886	C1806	G1734	G1661	C1600	G1467	
A2396	G2276	U2208	C2140	C2078	U2017	G1948	C1886	G1807	G1735	C1662	G1601	C1468	
G2397	G2277	C2209	G2141	U2079	G2018	G1949	C1887	U1808	C1741	C1663	U1602	G1538	
G2398	A2278	G2210	C2142	G2080	A2019	U1950	A1888	A1809	G1742	A1664	A1603	G1539	A1469
G2399	G2279	G2211		G2081	A2020	U1951	A1889	A1810	G1743	A1665	G1604	G1540	G1470
G2400	A2280	A2212	C2145	A2082	C2021	U1952	A1890	G1811	G1744	G1666	C1605	U1541	A1471
C2401	G2281	U2213	C2146	G2083	U2022	A1953	G1891	A1812		G1667	G1606	A1542	
C2402	G2282	G2215	G2147	C2084	G2023	A1954	C1892	G1813	G1751	A1668	C1607	C1544	G1474
C2403	C2283	G2216	C2148	C2085	G2024	U1955	C1893	G1814	G1752	A1669	A1608	G1475	
G2404	G2284	G2217	U2149	U2086	C2025	U1956	C1894	A1815	G1753	C1670	A1609	C1476	
G2405			C2150	G2087	C2026		C1895	G1816	U1754	U1671	A1610	G1478	
G2406	G2285		G2151	G2088	G2027		G1896	G1817	A1755	C1672	C1611	G1479	
U2408	A2286	G2226	U2152	U2089	U2028	G1961	G1897	U1818	G1756	U1673	G1612	G1480	
G2409	A2287	C2227	G2153	G2090	G2029	C1962	U1898	A1819	U1757	G1674	G1613	U1482	
	C2288	G2228	C2154	U2091	A2030	U1963	C1899	U1820	G1758	C1675	A1614	A1553	
G2413	G2289	G2229	G2155	U2092	A2031	G1964	A1900	G1822	A1759	A1676	C1615	A1554	
G2414	U2290	C2230	G2156	G2093	C2032	U1965	A1901	G1823	A1760	U1677	A1616	G1555	
G2415	U2291	G2231	C2157	G2094	C2033	A1966	C1902	G1824	C1761	C1617	C1618	C1556	
C2417	C2292	C2232	A2158	C2095	U2034	G1967	G1903	G1825	A1762	U1679	G1619	G1557	
C2418	G2293	U2233	G2159	U2096	G2035	G1968	G1904	G1826	U1680	U1679	G1620	A1558	
U2419	C2294	G2234	C2160	C2097	C2036	A1969	G1905	G1827	G1764	G1681	C1621	G1559	
C2420	C2161	U2296	C2162	U2098	G2037	A1970	G1906	C1827	G1765	G1682	U1621	G1560	
G2421	G2297	G2237	C2163	U2099	G2038	A1971	C1907	G1828		C1683	G1622	G1561	
C2422	C2298	G2238	C2164	C2100	C2039	G1972	C1908	A1829	C1684	G1685	G1623	G1562	
C2423	C2299	G2239	G2165		A2042	G1973	G1910	G1830	G1770	C1686	G1624	G1564	
C2424	G2300	C2240	C2166	G2104	C2043	G1974	A1913	G1831	G1771	G1687	C1625	C1565	A1486
A2425	C2301	A2241	C2167	C2105	C2044	U1976	A1914	U1834	G1772	U1688	G1626	G1566	
C2426	G2302	G2242	U2167	G2106	C2045	A1977	C1914	G1835	A1773	U1689	G1627	A1567	
C2427	G2303	U2243	C2168	C2107	G2046	A1978	U1915	C1836	C1774	A1690	G1628	G1568	
G2428	G2304	U2244	A	C2108	U2047	G1979	A1916		G1775		G1629	G1569	
G2429	A2305	U2245	A2170	C2109	G2048	G1980	U1917	G1839	U1777	U1693	G1630	A1570	
C2430	C2306	G2246	A2171	G2110	G2049		A1918		U1778	C1694	A1631	C1506	
U2431	G2307	C2247	U2172	C2111	C2050	C1983	A1919	G1845	U1779	G1695	A1632	A1507	
A2432	G2308	C2248	A2173	G	A2051	G1984	C1920	G1846	A1780	C1696	G1633	A1508	
A2433	A2309	U2249	C2174	U2113	G2052	G1984	G1921	A1847	G1697	C1698	A1634	C1509	
A2434	A2310	G2250	C2175	A2114	G2053	G1985	G1922	A1847	C1781	A1699	C1635	C1510	
A2435	A2311	G2251	A2176	C2115	C2054		U1923	G1850	G1782	G1699	C1636	A1511	
G2436	U2312	G2252	C2177	G2116	C2055	G1989	C1924	U1851	A1783	A1700	G1637	U1576	
G2437	C2313	G2253	C2178	A2117	C2056	C1990	U1925	G1852	A1784	A1637	C1638	C1577	
U2438	C2314	C2254	C2179	U2118	A2057	U1991	C1926	A1854	A1785	A1701	G1639	U1578	
A2439	G2315	G2255	U2180	G	A2058	G1992	U1927	A1853	A1786	G1702	U1639	A1579	
C2440	C2316	G2256	G2181	U2121	A2059	U1993	A1928	A1854	A1787	G1703	C1640	C1515	
C2441	U2257	U2257	C2182	C2122	A2060	C1994	G1929		G1704	C1705	A1641	G1517	
A2442	G2318	G2258	C2183	U2123	G2061		G1857	G1858	A1789		G1642	C1518	
C2443	G2319	G2259	C2184	G2123	A2062	C1989	G1930	A1859	G1790		C1644	A1583	
G2444	C2260	C2260	C2185	G2124	A2063	G2000	U1931	A1860	A1791	U1709	G1645	C1585	
G2445	G2261	U2262	C2186	G2125	C2064	A2001	A1932	G1861	G1792	G1710	G1646	A1586	
G2446	U2262	A2126	G2187	C2126	C2065	G2002		G1793			C1647	G1522	
G2447	G2263		C2188	G2127	C2065		G1935	G1882	U1794	U1716	G1647	U1523	



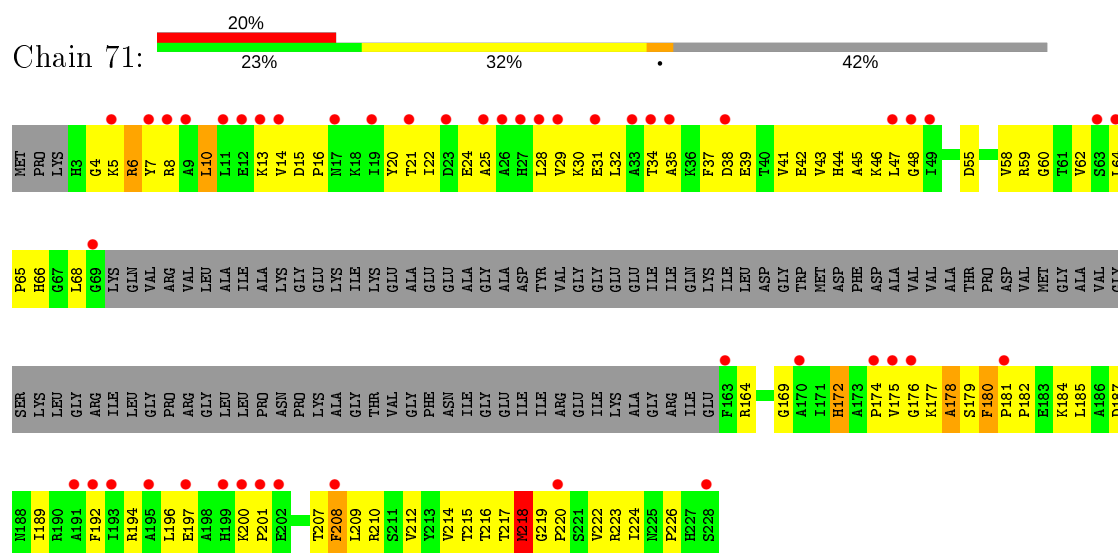
- Molecule 27: 5S rRNA



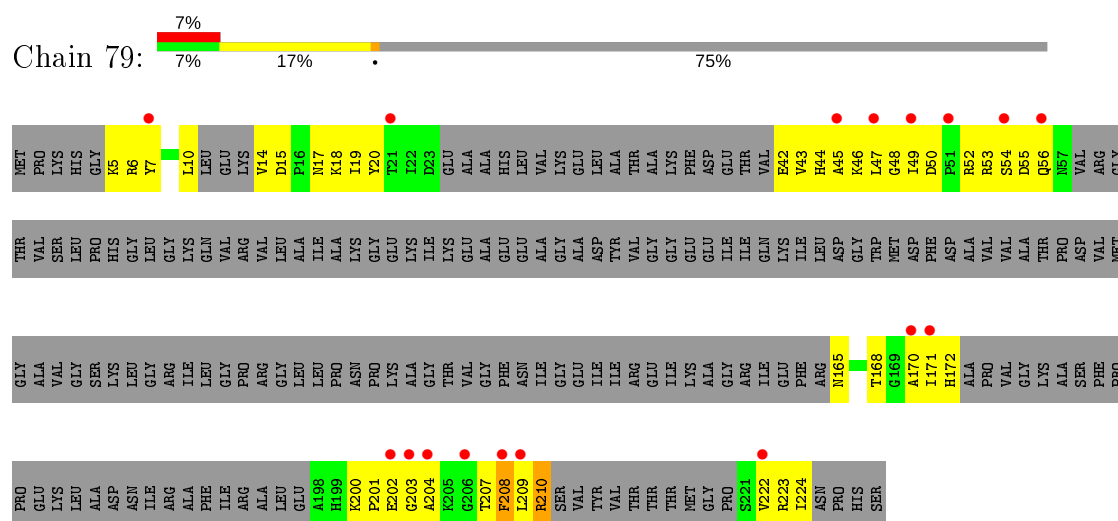
- Molecule 27: 5S rRNA



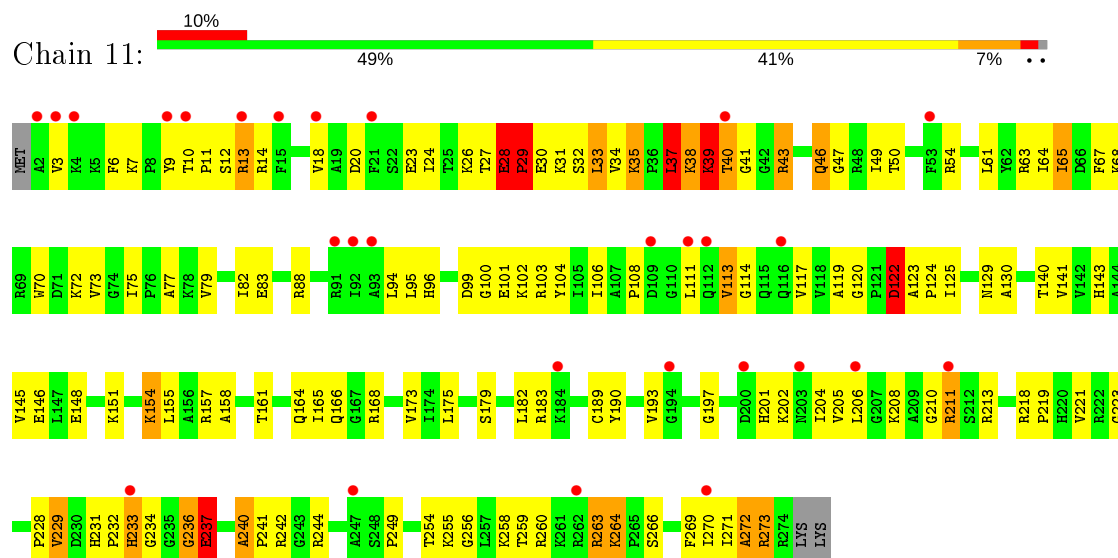
- Molecule 28: 50S ribosomal protein L1



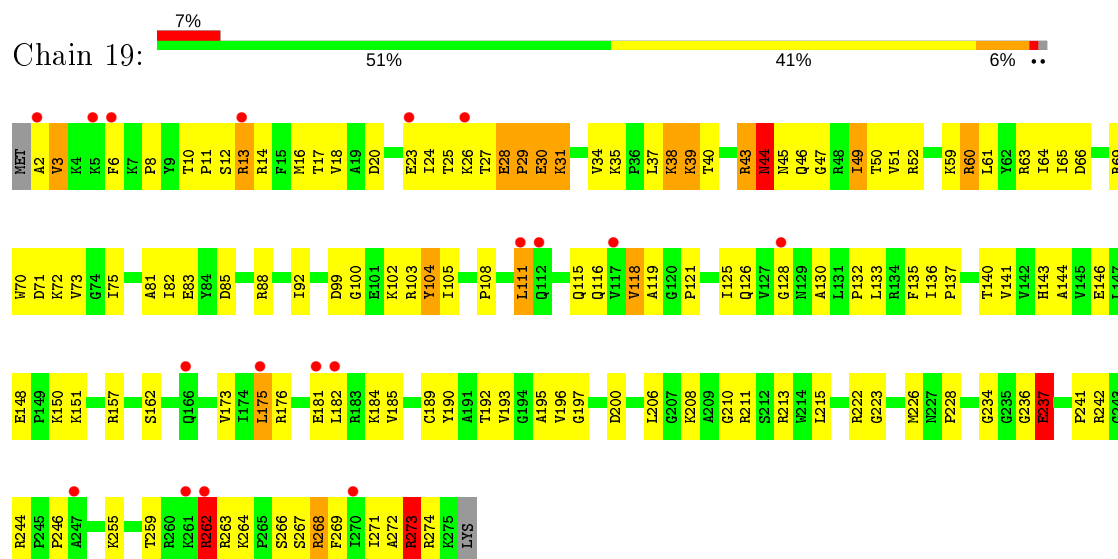
- Molecule 28: 50S ribosomal protein L1



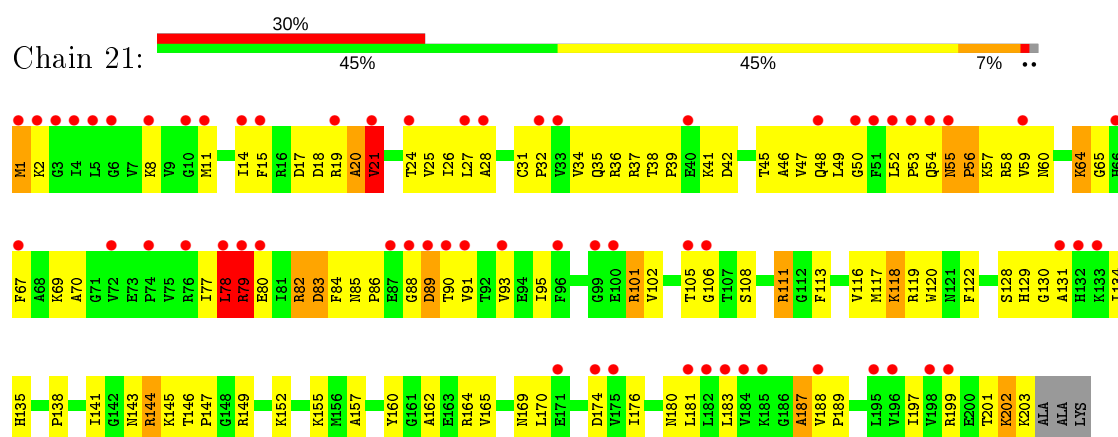
- Molecule 29: 50S ribosomal protein L2



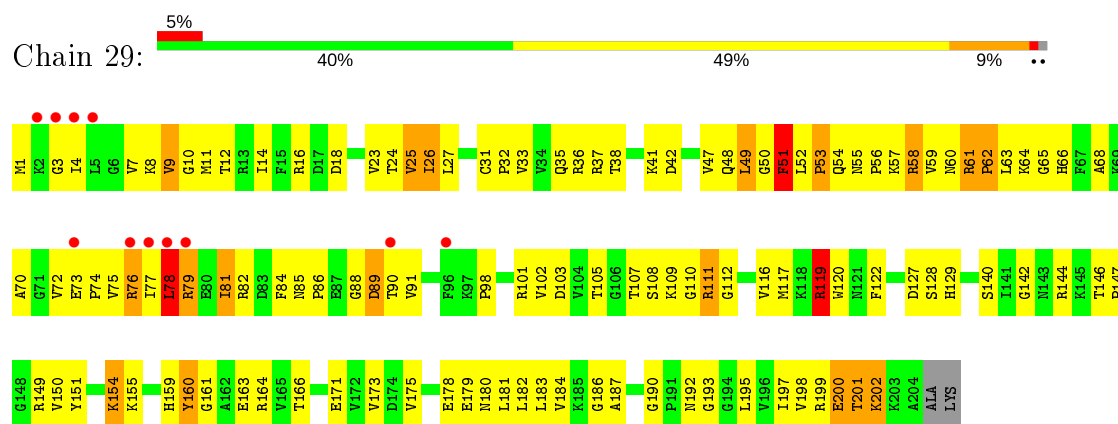
- Molecule 29: 50S ribosomal protein L2



- Molecule 30: 50S ribosomal protein L3

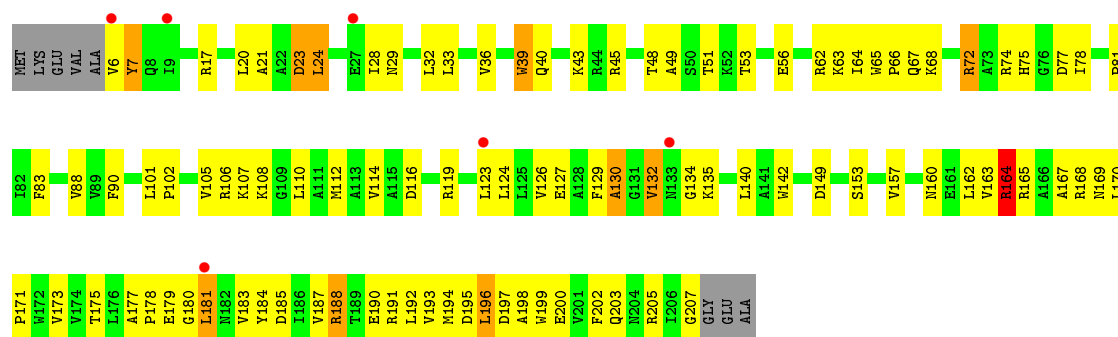


- Molecule 30: 50S ribosomal protein L3

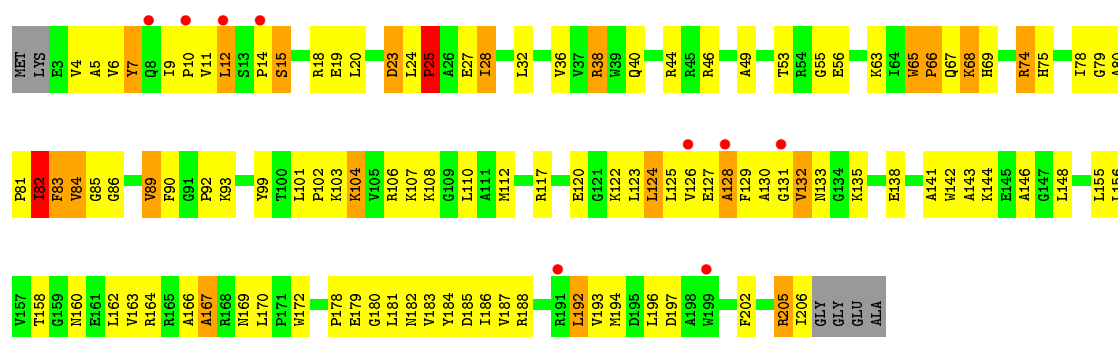
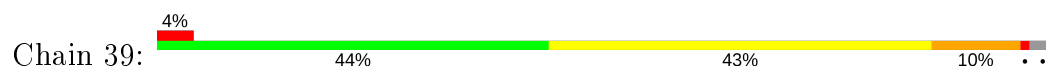


- Molecule 31: 50S ribosomal protein L4

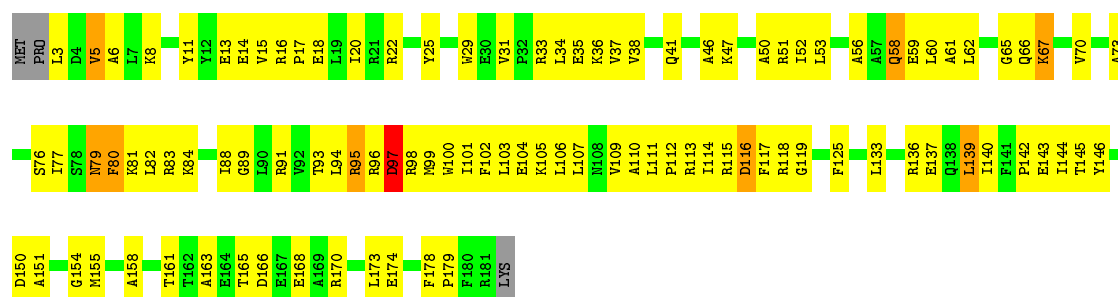




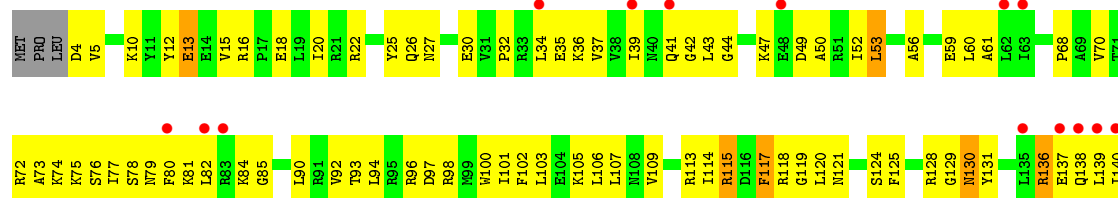
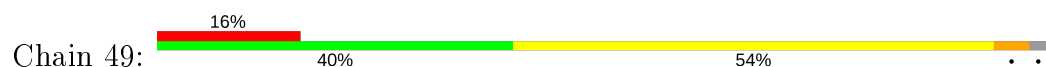
• Molecule 31: 50S ribosomal protein L4



• Molecule 32: 50S ribosomal protein L5

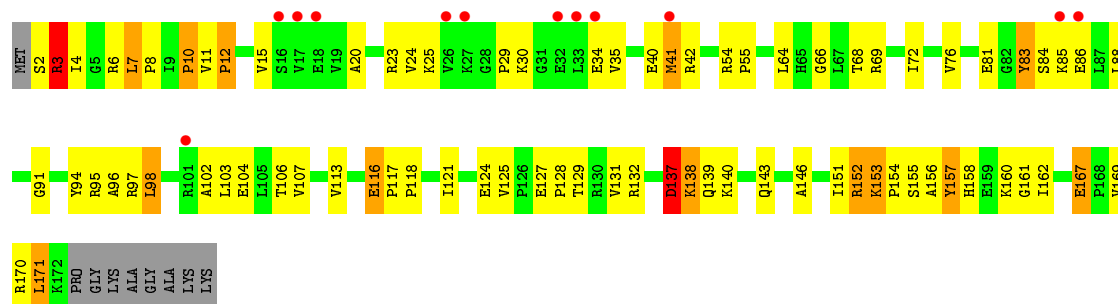


• Molecule 32: 50S ribosomal protein L5

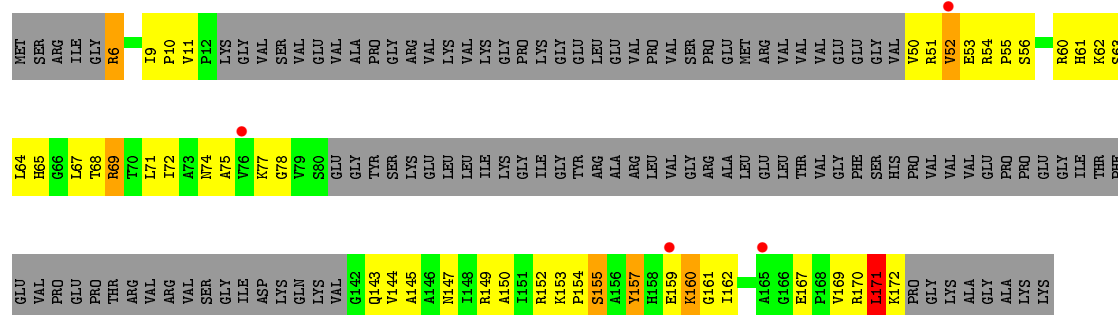




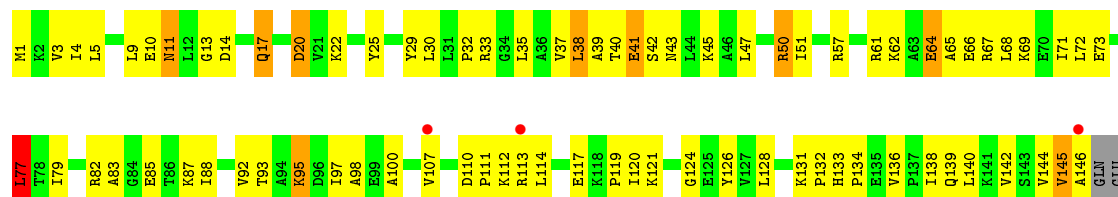
• Molecule 33: 50S ribosomal protein L6



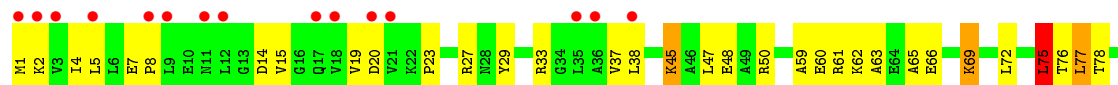
• Molecule 33: 50S ribosomal protein L6

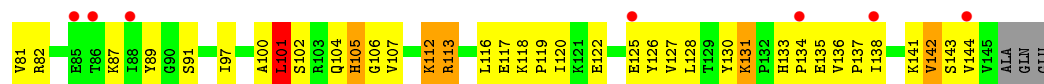


• Molecule 34: 50S ribosomal protein L9

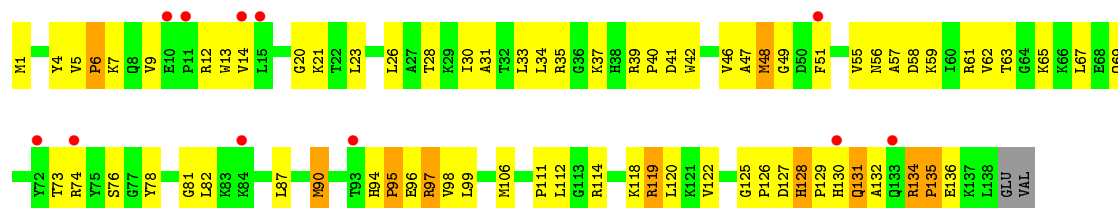


• Molecule 34: 50S ribosomal protein L9

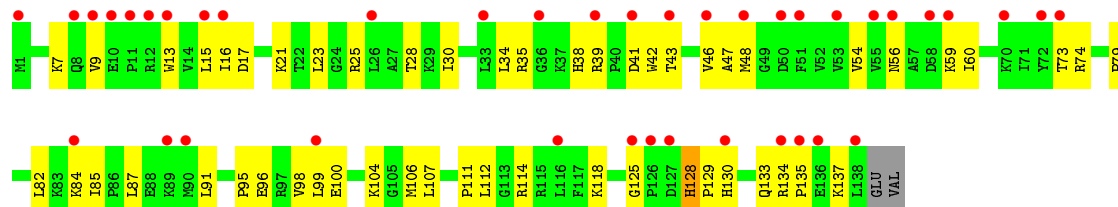




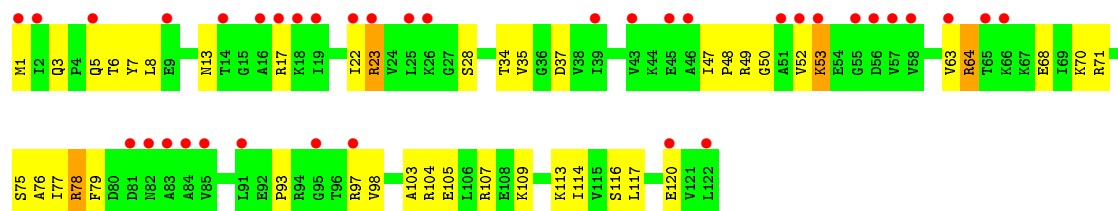
- Molecule 35: 50S ribosomal protein L13



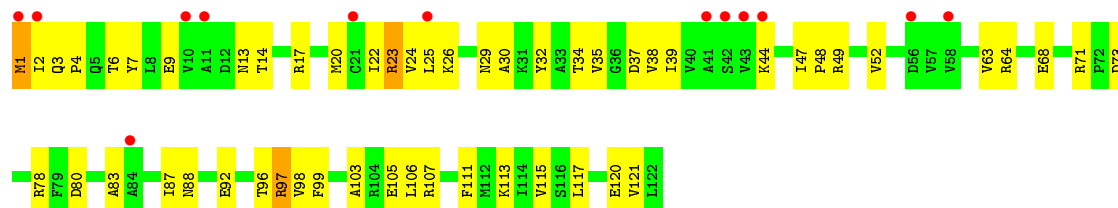
- Molecule 35: 50S ribosomal protein L13



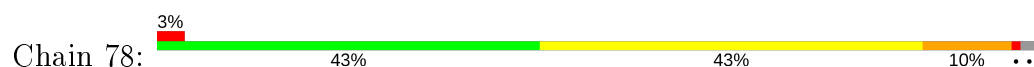
- Molecule 36: 50S ribosomal protein L14

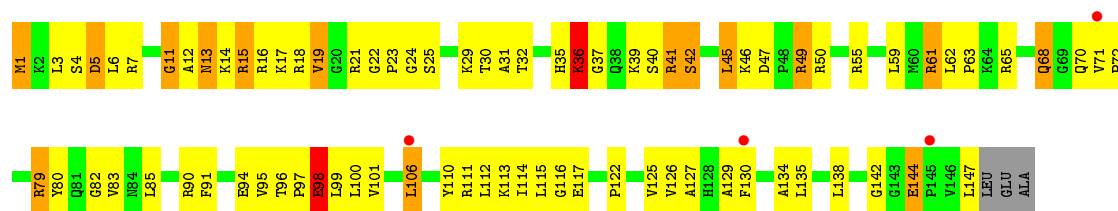


- Molecule 36: 50S ribosomal protein L14

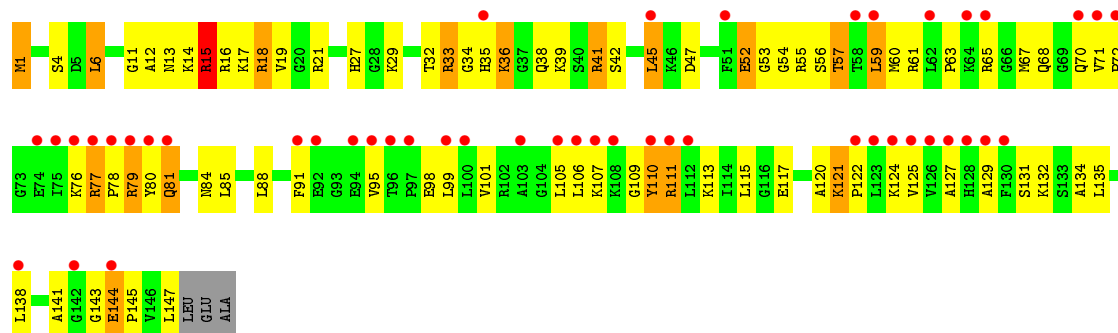
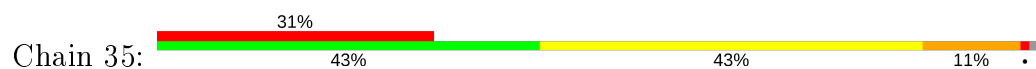


- Molecule 37: 50S ribosomal protein L15

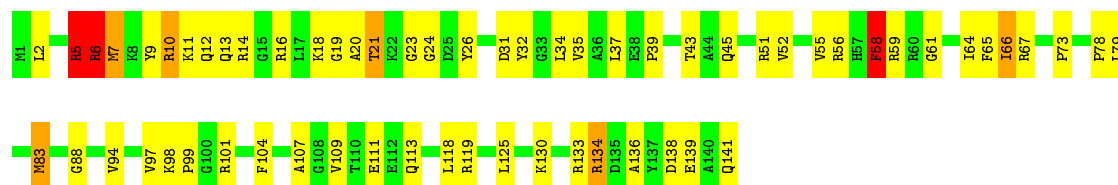




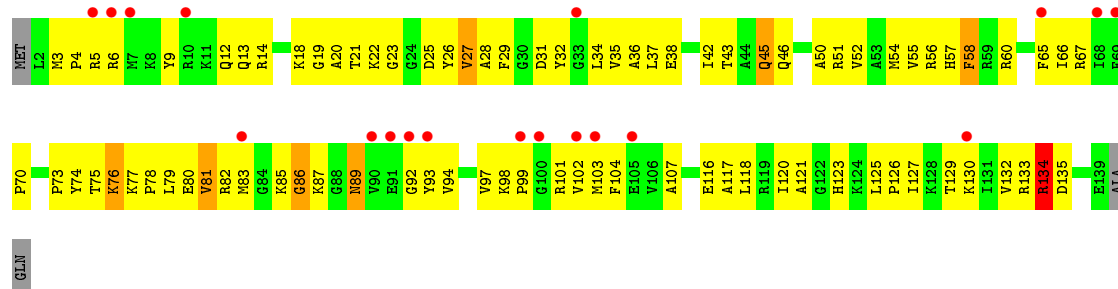
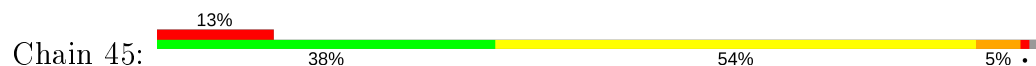
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16

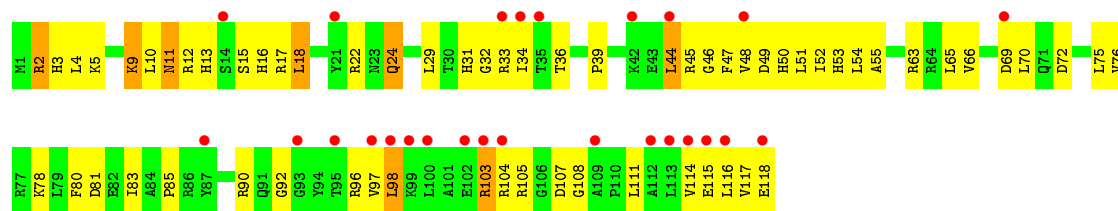


• Molecule 38: 50S ribosomal protein L16



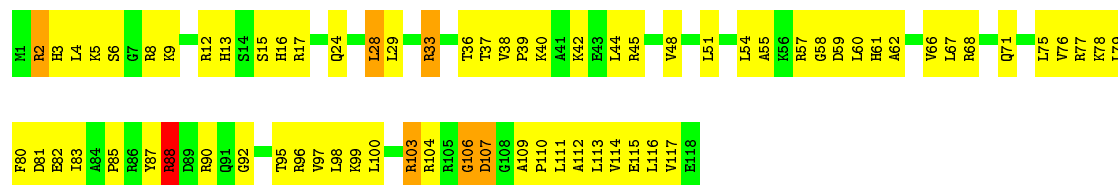
• Molecule 39: 50S ribosomal protein L17





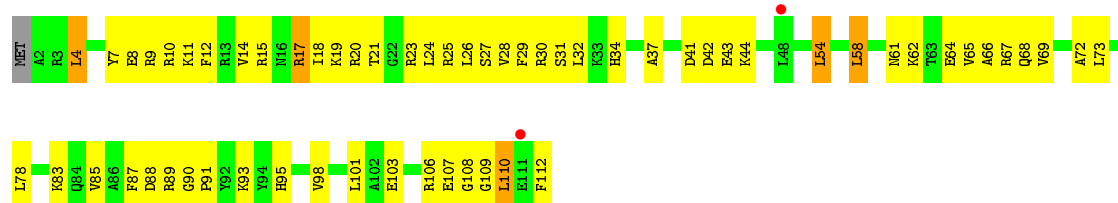
• Molecule 39: 50S ribosomal protein L17

Chain 55: 40% 54% 5% •



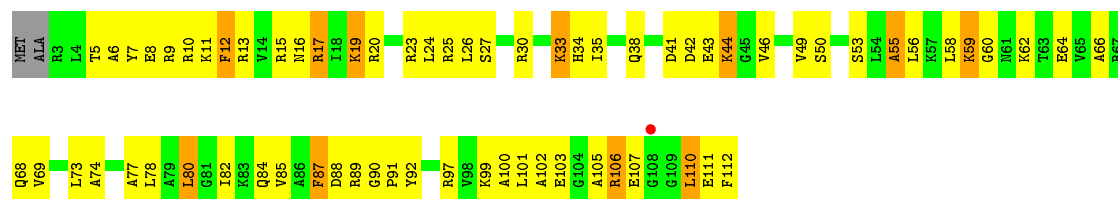
• Molecule 40: 50S ribosomal protein L18

Chain A8: 45% 50% 2% •



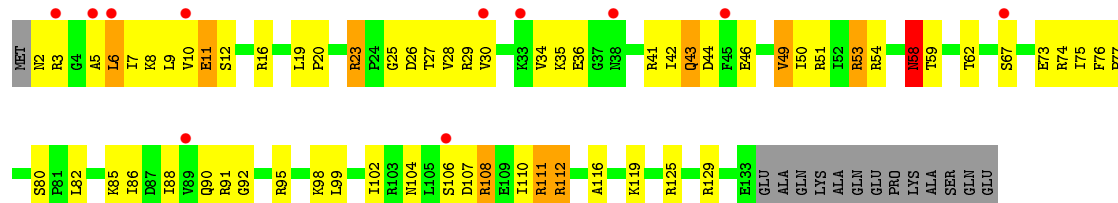
• Molecule 40: 50S ribosomal protein L18

Chain 65: 38% 51% 10% •

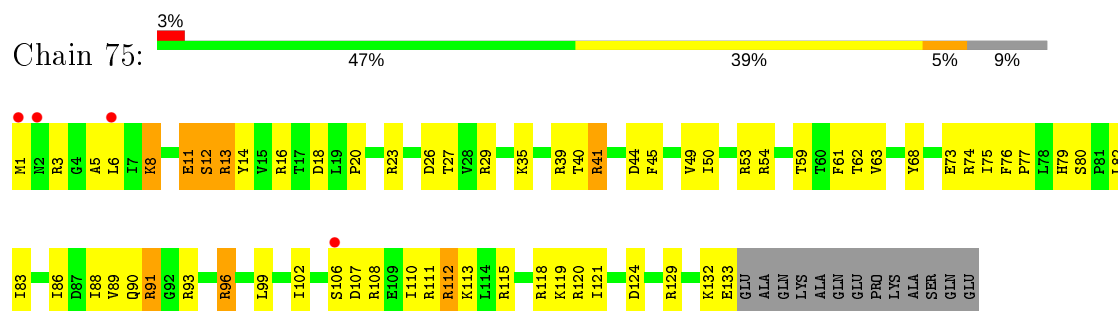


• Molecule 41: 50S ribosomal protein L19

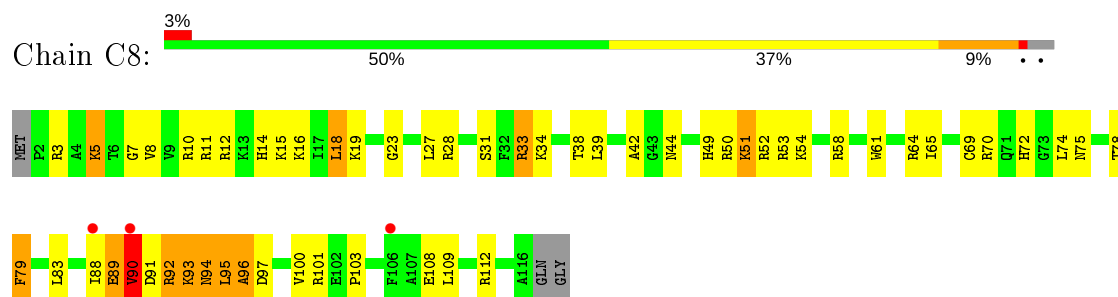
Chain B8: 46% 38% 6% 10% •



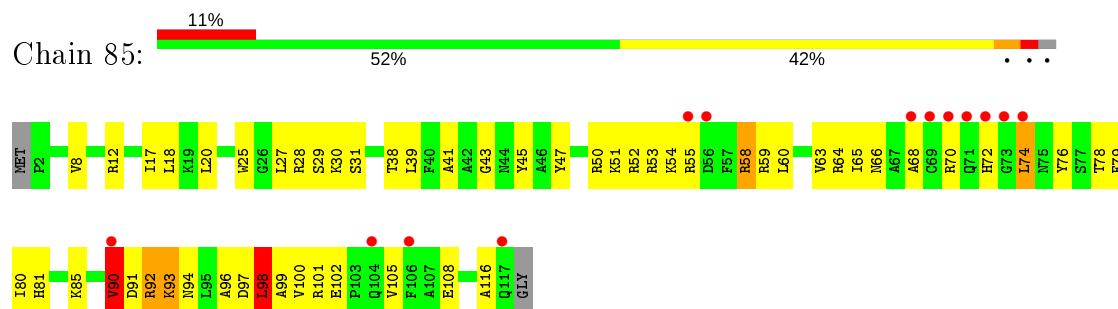
- Molecule 41: 50S ribosomal protein L19



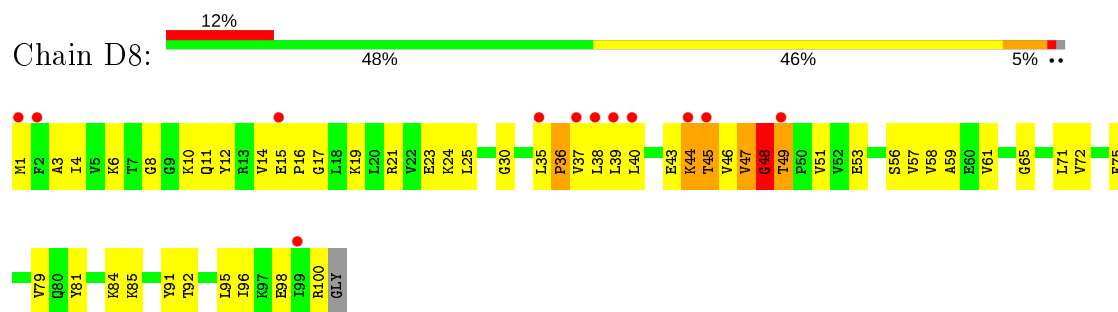
- Molecule 42: 50S ribosomal protein L20



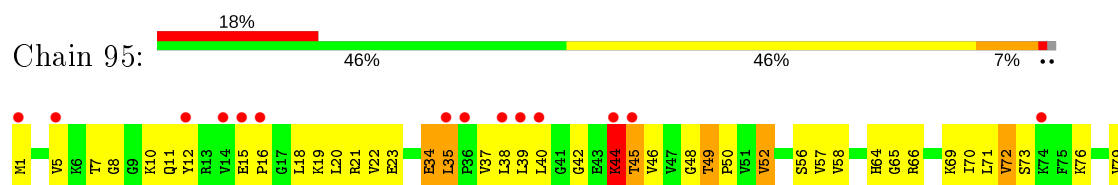
- Molecule 42: 50S ribosomal protein L20

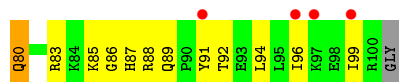


- Molecule 43: 50S ribosomal protein L21

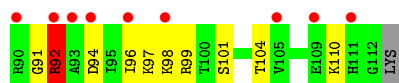


- Molecule 43: 50S ribosomal protein L21

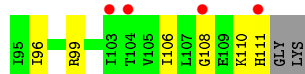
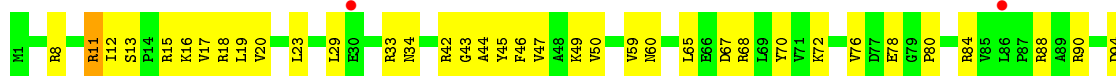




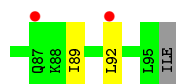
- Molecule 44: 50S ribosomal protein L22



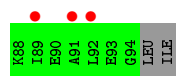
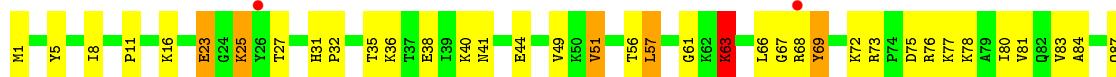
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23

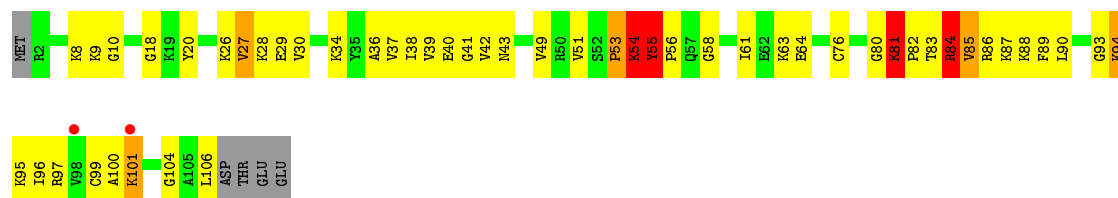


- Molecule 45: 50S ribosomal protein L23

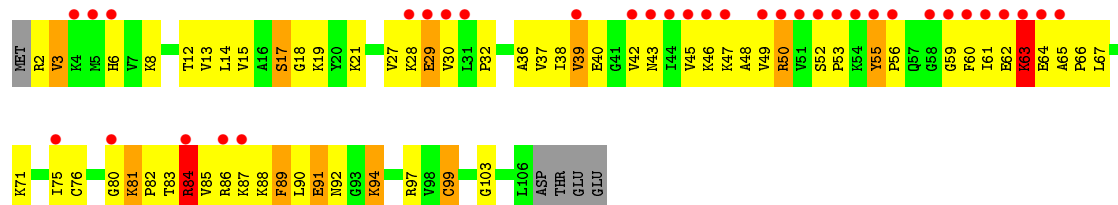


- Molecule 46: 50S ribosomal protein L24

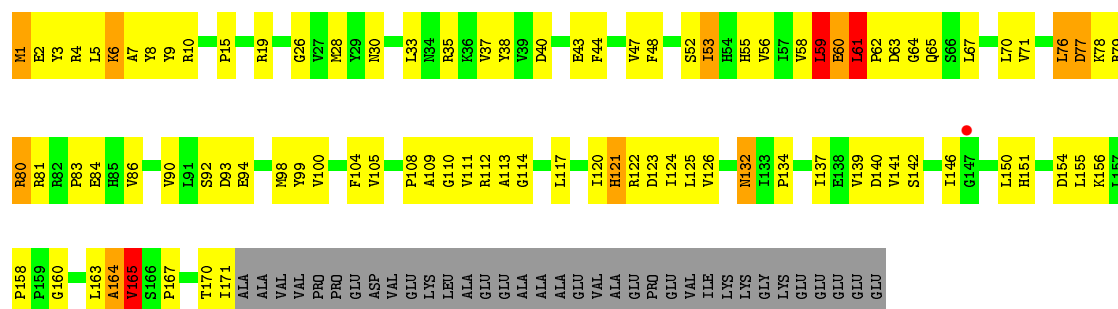




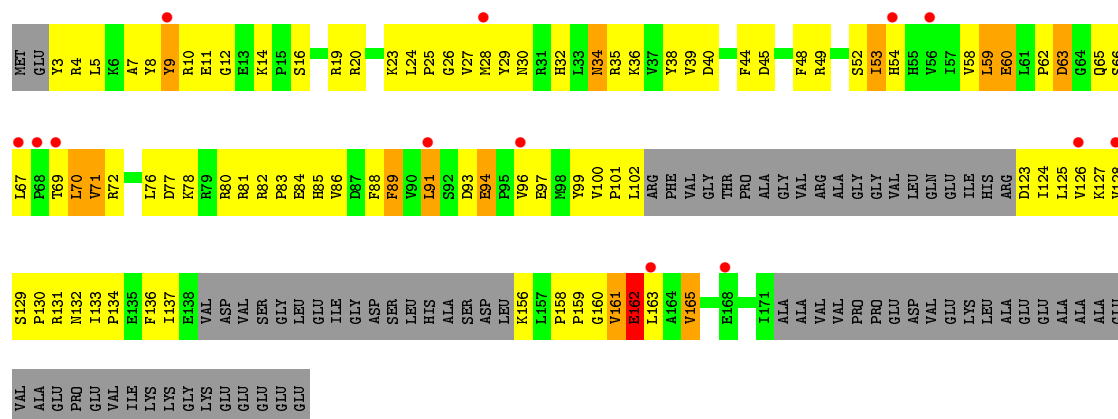
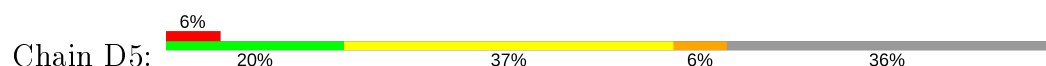
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L25

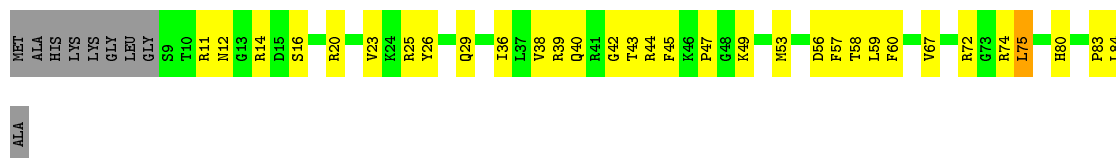


• Molecule 47: 50S ribosomal protein L25



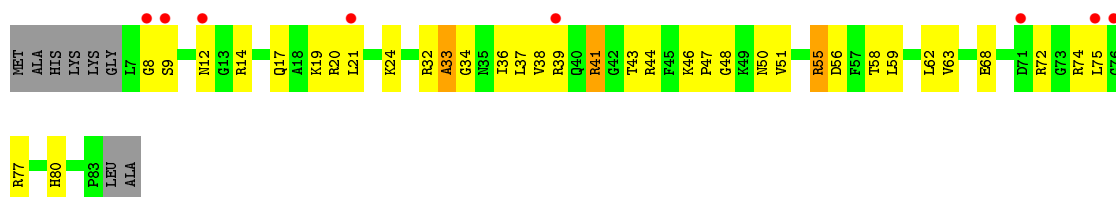
• Molecule 48: 50S ribosomal protein L27

Chain I8: 



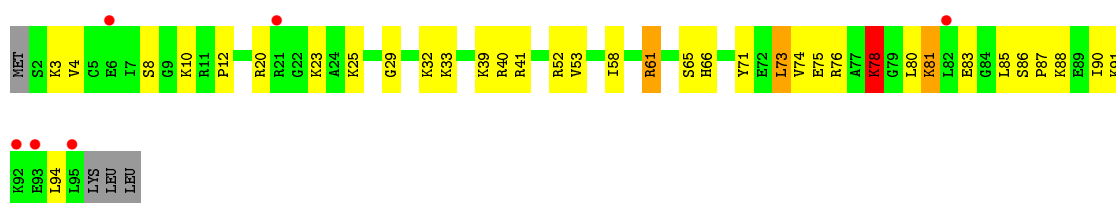
- Molecule 48: 50S ribosomal protein L27

Chain E5: 



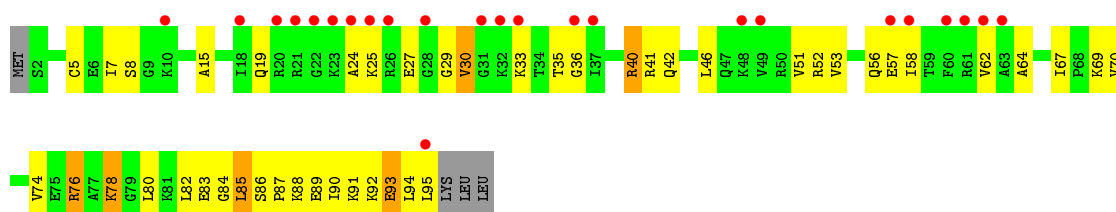
- Molecule 49: 50S ribosomal protein L28

Chain J8: 



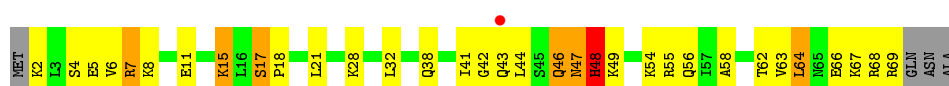
- Molecule 49: 50S ribosomal protein L28

Chain F5: 




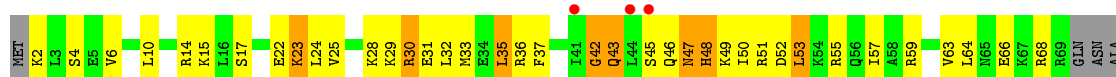
- Molecule 50: 50S ribosomal protein L29

Chain K8: 

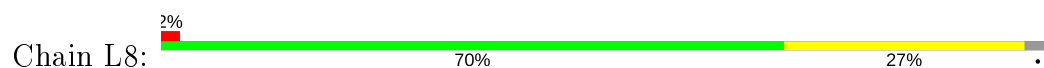


- Molecule 50: 50S ribosomal protein L29

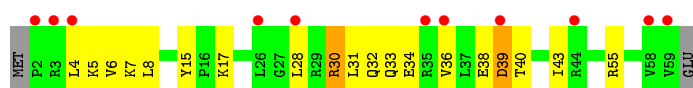
Chain G5: 



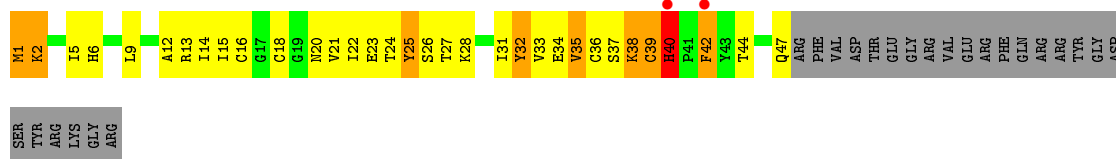
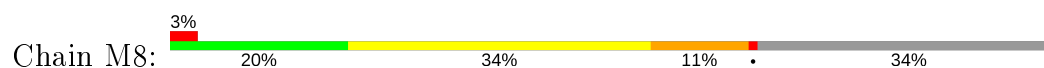
- Molecule 51: 50S ribosomal protein L30



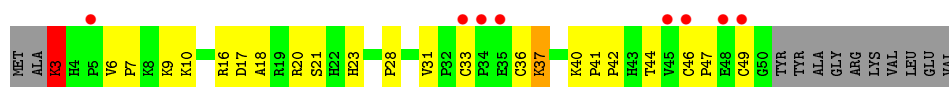
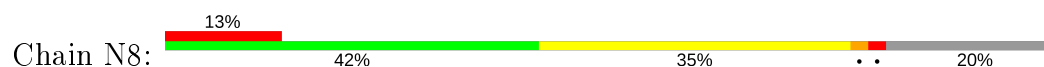
- Molecule 51: 50S ribosomal protein L30



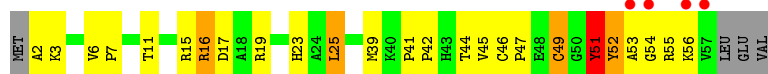
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



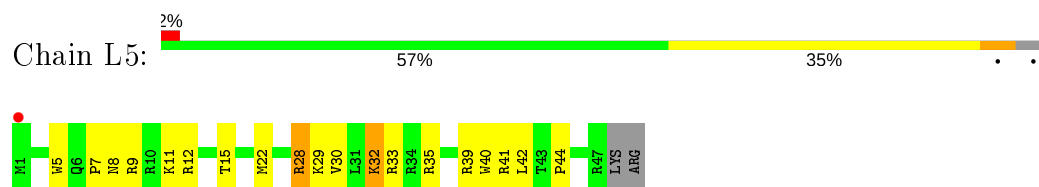
- Molecule 53: 50S ribosomal protein L32



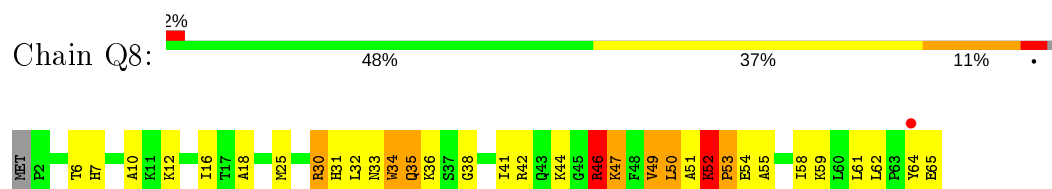
- Molecule 54: 50S ribosomal protein L34



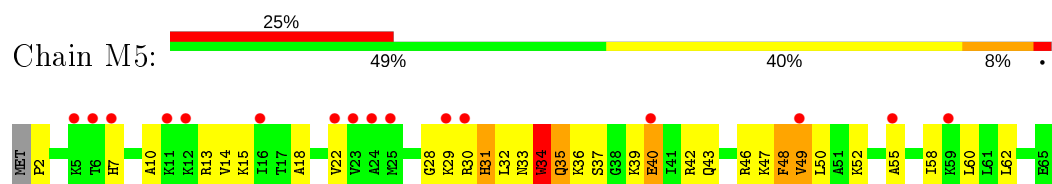
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40 Å 446.00 Å 617.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.24 – 3.10 161.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.24-3.10) 93.3 (161.07-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.249 0.196 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294257	wwPDB-VP
Average B, all atoms (Å ²)	106.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, PAR, U8U, 4SU, G7M, SF4, MG, ZN, T6A, 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	0.93	18/35994 (0.1%)	1.69	967/56171 (1.7%)
1	1G	0.78	4/36258 (0.0%)	1.46	463/56589 (0.8%)
2	12	0.53	0/1752	0.74	3/2360 (0.1%)
2	1E	0.46	0/1908	0.72	2/2573 (0.1%)
3	22	0.61	5/1564 (0.3%)	0.65	0/2109
3	2E	0.61	2/1629 (0.1%)	0.71	0/2195
4	32	0.55	0/1732	0.73	2/2318 (0.1%)
4	3E	0.63	0/1728	0.78	2/2313 (0.1%)
5	42	0.49	0/1150	0.73	0/1548
5	4E	0.58	0/1158	0.76	0/1559
6	52	0.56	0/855	0.75	2/1154 (0.2%)
6	5E	0.71	2/850 (0.2%)	0.77	1/1147 (0.1%)
7	62	0.46	0/1122	0.65	0/1500
7	6E	0.48	0/1259	0.63	0/1686
8	72	0.43	0/1127	0.65	1/1517 (0.1%)
8	7E	0.71	4/1135 (0.4%)	0.76	0/1527
9	82	0.46	0/971	0.66	0/1304
9	8E	0.46	0/1019	0.69	0/1367
10	1A	0.51	0/658	0.65	0/885
10	1I	0.47	0/747	0.73	0/1006
11	2A	0.46	0/850	0.66	0/1150
11	2I	0.51	0/838	0.71	1/1133 (0.1%)
12	3A	0.55	0/972	0.79	2/1301 (0.2%)
12	3I	0.73	0/972	0.88	1/1301 (0.1%)
13	4A	0.52	0/903	0.76	1/1211 (0.1%)
13	4I	0.66	2/952 (0.2%)	0.72	0/1277
14	5A	0.51	0/495	0.76	0/657
14	5I	0.56	0/500	0.79	1/664 (0.2%)
15	6A	0.47	0/740	0.66	0/987
15	6I	0.56	0/740	0.69	0/987
16	7A	0.52	0/721	0.71	0/970
16	7I	0.53	0/716	0.75	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.48	0/836	0.66	0/1117
17	8I	0.53	0/847	0.74	0/1131
18	9A	0.52	0/549	0.68	0/732
18	9I	0.63	0/554	0.77	1/739 (0.1%)
19	AA	0.50	0/490	0.73	0/662
19	AI	0.55	0/672	0.77	0/904
20	BA	0.44	0/764	0.72	1/1007 (0.1%)
20	BI	0.55	1/748 (0.1%)	0.75	2/986 (0.2%)
21	1B	0.40	0/192	0.61	0/252
21	1F	0.54	0/203	0.64	0/266
22	1K	0.91	2/1516 (0.1%)	1.53	28/2350 (1.2%)
22	1L	0.76	1/1613 (0.1%)	1.29	18/2504 (0.7%)
23	2K	0.97	2/1721 (0.1%)	1.63	38/2682 (1.4%)
23	2L	0.78	1/1721 (0.1%)	1.51	26/2682 (1.0%)
24	3K	0.85	1/1777 (0.1%)	1.52	32/2767 (1.2%)
24	3L	0.81	4/1777 (0.2%)	1.46	28/2767 (1.0%)
25	4K	1.19	0/494	1.43	7/767 (0.9%)
25	4L	0.84	0/445	1.23	4/693 (0.6%)
26	14	1.06	133/69023 (0.2%)	1.87	2721/107740 (2.5%)
26	1H	1.24	276/68351 (0.4%)	2.12	4205/106700 (3.9%)
27	16	0.97	2/2928 (0.1%)	1.82	99/4568 (2.2%)
27	1J	0.85	0/2928	1.58	53/4568 (1.2%)
28	71	0.41	0/1055	0.67	1/1425 (0.1%)
28	79	0.44	0/459	0.66	0/608
29	11	0.90	6/2170 (0.3%)	1.13	16/2926 (0.5%)
29	19	0.82	5/2175 (0.2%)	0.97	9/2933 (0.3%)
30	21	0.68	0/1591	0.92	2/2146 (0.1%)
30	29	0.76	3/1596 (0.2%)	0.96	3/2153 (0.1%)
31	31	0.78	1/1620 (0.1%)	0.89	1/2194 (0.0%)
31	39	0.83	2/1637 (0.1%)	0.88	1/2218 (0.0%)
32	41	0.54	0/1481	0.76	0/1994
32	49	0.45	0/1482	0.67	0/1994
33	51	0.64	0/1337	0.91	5/1809 (0.3%)
33	59	0.63	1/548 (0.2%)	1.13	6/738 (0.8%)
34	61	0.53	0/1151	0.79	1/1558 (0.1%)
34	69	0.52	0/1146	0.78	2/1551 (0.1%)
35	15	0.53	0/1131	0.73	0/1525
35	58	0.59	0/1131	0.81	2/1525 (0.1%)
36	25	0.69	1/942 (0.1%)	0.76	0/1269
36	68	0.66	0/942	0.83	1/1269 (0.1%)
37	35	0.79	2/1139 (0.2%)	0.99	3/1514 (0.2%)
37	78	0.84	4/1139 (0.4%)	1.08	7/1514 (0.5%)
38	45	0.64	1/1120 (0.1%)	0.87	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	88	0.81	0/1134	1.02	3/1519 (0.2%)
39	55	0.71	2/981 (0.2%)	0.89	1/1312 (0.1%)
39	98	0.54	0/981	0.87	1/1312 (0.1%)
40	65	0.57	0/886	0.87	1/1180 (0.1%)
40	A8	0.64	0/891	0.89	3/1187 (0.3%)
41	75	0.72	3/1123 (0.3%)	0.79	1/1500 (0.1%)
41	B8	0.75	3/1115 (0.3%)	0.88	0/1490
42	85	0.57	0/977	0.77	1/1301 (0.1%)
42	C8	0.67	0/968	0.86	2/1289 (0.2%)
43	95	0.65	0/785	0.92	1/1052 (0.1%)
43	D8	0.62	0/785	0.88	1/1052 (0.1%)
44	A5	0.67	0/897	0.83	0/1204
44	E8	0.66	0/901	0.91	3/1209 (0.2%)
45	B5	0.69	0/749	0.87	3/1007 (0.3%)
45	F8	0.72	0/757	0.96	2/1017 (0.2%)
46	C5	0.89	4/812 (0.5%)	0.96	1/1083 (0.1%)
46	G8	0.93	6/809 (0.7%)	1.07	3/1080 (0.3%)
47	D5	0.58	3/1099 (0.3%)	0.77	1/1490 (0.1%)
47	H8	0.52	0/1403	0.79	3/1901 (0.2%)
48	E5	0.62	0/616	0.86	0/821
48	I8	0.81	0/614	0.91	1/819 (0.1%)
49	F5	0.63	0/744	0.86	1/989 (0.1%)
49	J8	0.73	1/744 (0.1%)	0.88	1/989 (0.1%)
50	G5	0.61	0/570	0.76	0/755
50	K8	0.73	0/570	0.99	1/755 (0.1%)
51	H5	0.48	0/464	0.68	0/623
51	L8	0.63	0/464	0.82	0/623
52	M8	0.54	0/375	0.94	1/507 (0.2%)
53	J5	0.64	0/448	0.85	2/606 (0.3%)
53	N8	0.90	1/381 (0.3%)	0.86	0/516
54	L5	0.69	0/409	0.97	1/540 (0.2%)
54	P8	0.84	0/409	1.05	0/540
55	M5	0.79	1/524 (0.2%)	1.01	2/691 (0.3%)
55	Q8	0.72	0/524	1.18	4/691 (0.6%)
All	All	0.95	510/317065 (0.2%)	1.64	8817/475024 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	5
4	32	0	6
4	3E	0	2
5	42	0	1
7	62	0	1
8	72	0	1
9	82	0	1
10	1A	0	2
11	2A	0	1
12	3I	0	2
13	4A	0	5
13	4I	0	2
14	5A	0	1
14	5I	0	1
19	AA	0	2
19	AI	0	2
20	BA	0	3
20	BI	0	2
28	71	0	3
29	11	0	8
29	19	0	4
30	21	0	10
30	29	0	6
31	31	0	2
31	39	0	9
32	49	0	3
33	51	0	6
33	59	0	5
34	61	0	4
34	69	0	4
35	58	0	1
37	35	0	4
37	78	0	7
38	45	0	6
38	88	0	3
39	55	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	1
41	B8	0	2
42	85	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
42	C8	0	4
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	3
46	C5	0	4
46	G8	0	7
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	3
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	191

The worst 5 of 510 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	39	66	PRO	N-CD	-23.13	1.15	1.47
26	1H	774	A	N9-C4	-14.86	1.28	1.37
37	35	121	LYS	C-N	14.12	1.61	1.34
26	1H	783	A	N9-C4	-12.71	1.30	1.37
26	14	783	A	N9-C4	-12.47	1.30	1.37

The worst 5 of 8817 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	945	A	N1-C6-N6	20.77	131.06	118.60
26	1H	676	A	C2-N3-C4	-19.63	100.78	110.60
26	1H	783	A	C5-N7-C8	-19.52	94.14	103.90
26	1H	1332	G	C5-N7-C8	-18.53	95.04	104.30
26	1H	945	A	C6-C5-N7	-18.52	119.34	132.30

There are no chirality outliers.

5 of 191 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
2	1E	9	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	901	0
1	1G	32391	0	16353	955	1
2	12	1721	0	1758	123	0
2	1E	1874	0	1926	124	0
3	22	1541	0	1606	89	0
3	2E	1605	0	1668	68	0
4	32	1702	0	1765	145	0
4	3E	1698	0	1760	124	0
5	42	1134	0	1200	78	0
5	4E	1142	0	1204	67	0
6	52	842	0	857	29	0
6	5E	837	0	852	43	0
7	62	1110	0	1163	63	0
7	6E	1242	0	1286	49	0
8	72	1107	0	1165	63	0
8	7E	1115	0	1177	71	0
9	82	953	0	983	91	0
9	8E	1000	0	1031	64	0
10	1A	646	0	662	42	0
10	1I	734	0	761	48	0
11	2A	835	0	847	36	0
11	2I	823	0	833	42	0
12	3A	956	0	1046	70	0
12	3I	956	0	1046	49	0
13	4A	893	0	946	71	0
13	4I	942	0	997	66	0
14	5A	486	0	525	50	0
14	5I	491	0	529	31	0
15	6A	729	0	768	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	40	0
16	7A	705	0	725	44	0
16	7I	700	0	720	53	0
17	8A	823	0	891	39	0
17	8I	834	0	904	55	0
18	9A	544	0	605	22	0
18	9I	549	0	607	29	0
19	AA	481	0	468	45	0
19	AI	658	0	678	51	0
20	BA	762	0	861	44	0
20	BI	746	0	843	60	0
21	1B	188	0	195	11	0
21	1F	199	0	208	15	0
22	1K	1477	0	758	51	0
22	1L	1563	0	799	55	0
23	2K	1646	0	844	33	0
23	2L	1646	0	844	58	0
24	3K	1611	0	817	79	0
24	3L	1611	0	817	54	0
25	4K	439	0	219	11	0
25	4L	395	0	196	12	0
26	14	61630	0	31073	1520	1
26	1H	61028	0	30758	1551	0
27	16	2617	0	1328	65	0
27	1J	2617	0	1328	87	0
28	71	1033	0	1048	76	0
28	79	456	0	460	51	0
29	11	2120	0	2197	142	0
29	19	2125	0	2199	130	0
30	21	1558	0	1623	113	0
30	29	1563	0	1629	130	0
31	31	1585	0	1632	103	0
31	39	1602	0	1649	134	0
32	41	1457	0	1514	106	0
32	49	1458	0	1515	81	0
33	51	1312	0	1384	72	0
33	59	539	0	563	38	0
34	61	1136	0	1223	58	0
34	69	1131	0	1218	60	0
35	15	1104	0	1180	40	0
35	58	1104	0	1180	69	0
36	25	932	0	996	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	68	932	0	996	42	0
37	35	1122	0	1206	96	0
37	78	1122	0	1206	105	0
38	45	1099	0	1154	88	0
38	88	1113	0	1157	60	0
39	55	967	0	1033	65	0
39	98	967	0	1033	54	0
40	65	876	0	938	76	0
40	A8	881	0	943	58	0
41	75	1109	0	1170	64	0
41	B8	1101	0	1158	61	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	65	0
43	95	774	0	849	64	0
43	D8	774	0	849	56	0
44	A5	886	0	948	31	0
44	E8	890	0	951	30	0
45	B5	735	0	785	37	0
45	F8	743	0	794	32	0
46	C5	799	0	888	67	0
46	G8	796	0	886	60	0
47	D5	1074	0	1087	75	0
47	H8	1373	0	1402	79	0
48	E5	608	0	622	33	0
48	I8	606	0	625	29	0
49	F5	737	0	813	52	0
49	J8	737	0	813	29	0
50	G5	568	0	614	43	0
50	K8	568	0	614	39	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	366	0	370	51	0
53	J5	434	0	454	23	0
53	N8	369	0	388	24	0
54	L5	401	0	436	21	0
54	P8	401	0	436	21	0
55	M5	516	0	582	35	0
55	Q8	516	0	582	39	0
56	13	131	0	0	0	0
56	14	382	0	0	0	0
56	16	11	0	0	0	0
56	1G	81	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	429	0	0	0	0
56	1J	5	0	0	0	0
56	1K	1	0	0	0	0
56	2I	2	0	0	0	0
56	2J	1	0	0	0	0
56	2K	3	0	0	0	0
56	2L	3	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	3K	1	0	0	0	0
56	4I	1	0	0	0	0
56	45	3	0	0	0	0
56	4K	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	C5	1	0	0	0	0
56	E5	1	0	0	0	0
56	I8	3	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	13	42	0	45	3	0
57	1G	42	0	45	2	0
58	32	8	0	0	3	0
58	3E	8	0	0	3	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	11	10	0	0	3	0
60	13	144	0	0	15	0
60	14	367	0	0	32	0
60	16	22	0	0	1	0
60	19	8	0	0	0	0
60	1G	68	0	0	4	0
60	1H	540	0	0	71	0
60	1I	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1J	12	0	0	3	0
60	29	2	0	0	1	0
60	31	7	0	0	0	0
60	32	2	0	0	0	0
60	35	2	0	0	0	0
60	39	3	0	0	1	0
60	3E	2	0	0	1	0
60	3K	1	0	0	0	0
60	4K	3	0	0	1	0
60	55	2	0	0	2	0
60	58	2	0	0	0	0
60	5I	2	0	0	0	0
60	6I	1	0	0	0	0
60	78	4	0	0	1	0
60	7I	1	0	0	0	0
60	98	1	0	0	1	0
60	BI	1	0	0	0	0
60	G8	1	0	0	0	0
60	H5	1	0	0	0	0
60	I8	2	0	0	0	0
60	L5	1	0	0	0	0
60	L8	3	0	0	1	0
60	P8	1	0	0	0	0
All	All	294257	0	196338	9801	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 9801 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)
31:39:38:ARG:NH2	31:39:99:TYR:CE1	1.96	1.30
26:1H:943:U:OP2	37:78:36:LYS:NZ	1.64	1.30
44:E8:92:ARG:NH1	44:E8:94:ASP:OD1	1.71	1.22
35:58:49:GLY:O	35:58:119:ARG:NH1	1.77	1.16
29:11:183:ARG:NH1	29:11:269:PHE:HB2	1.61	1.15

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.16	0.04

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%)	171 (83%)	30 (15%)	5 (2%)	6	27
2	1E	227/256 (89%)	188 (83%)	36 (16%)	3 (1%)	12	42
3	22	192/239 (80%)	172 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	175 (85%)	29 (14%)	2 (1%)	15	49
4	3E	205/209 (98%)	188 (92%)	15 (7%)	2 (1%)	15	49
5	42	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	22	57
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	22	57
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	122 (91%)	12 (9%)	0	100	100
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	57
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	57
9	82	119/128 (93%)	111 (93%)	7 (6%)	1 (1%)	19	54
9	8E	124/128 (97%)	106 (86%)	16 (13%)	2 (2%)	9	37
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	89/105 (85%)	80 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	100 (90%)	9 (8%)	2 (2%)	8	34
11	2I	109/129 (84%)	98 (90%)	9 (8%)	2 (2%)	8	34
12	3A	120/132 (91%)	98 (82%)	19 (16%)	3 (2%)	5	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3I	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	19	54
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	17	52
13	4I	117/126 (93%)	95 (81%)	22 (19%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	34
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	21
15	6A	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	13	44
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	2 (3%)	2 (3%)	4	23
19	AA	56/93 (60%)	47 (84%)	7 (12%)	2 (4%)	3	20
19	AI	80/93 (86%)	67 (84%)	10 (12%)	3 (4%)	3	19
20	BA	97/106 (92%)	86 (89%)	9 (9%)	2 (2%)	7	30
20	BI	95/106 (90%)	84 (88%)	11 (12%)	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	7I	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%)	19 (7%)	9 (3%)	4	21
29	19	272/276 (99%)	242 (89%)	23 (8%)	7 (3%)	5	26
30	21	201/206 (98%)	158 (79%)	35 (17%)	8 (4%)	3	17
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	17
31	31	200/210 (95%)	183 (92%)	14 (7%)	3 (2%)	10	39
31	39	202/210 (96%)	155 (77%)	40 (20%)	7 (4%)	3	20
32	41	177/182 (97%)	154 (87%)	21 (12%)	2 (1%)	14	46
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	14	46
33	51	169/180 (94%)	135 (80%)	25 (15%)	9 (5%)	2	12
33	59	63/180 (35%)	48 (76%)	13 (21%)	2 (3%)	4	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	61	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	11	40
34	69	143/148 (97%)	114 (80%)	28 (20%)	1 (1%)	22	57
35	15	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	57
35	58	136/140 (97%)	114 (84%)	18 (13%)	4 (3%)	4	24
36	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
37	35	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3	21
37	78	145/150 (97%)	117 (81%)	24 (17%)	4 (3%)	5	25
38	45	136/141 (96%)	115 (85%)	18 (13%)	3 (2%)	6	29
38	88	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	4	24
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	52
39	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	52
40	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	17	52
40	A8	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
41	75	131/146 (90%)	121 (92%)	10 (8%)	0	100	100
41	B8	130/146 (89%)	115 (88%)	14 (11%)	1 (1%)	19	54
42	85	114/118 (97%)	105 (92%)	7 (6%)	2 (2%)	8	34
42	C8	113/118 (96%)	103 (91%)	7 (6%)	3 (3%)	5	25
43	95	98/101 (97%)	73 (74%)	20 (20%)	5 (5%)	2	13
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	3	16
44	A5	109/113 (96%)	103 (94%)	4 (4%)	2 (2%)	8	34
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	6	29
45	F8	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
46	C5	103/110 (94%)	72 (70%)	24 (23%)	7 (7%)	1	7
46	G8	103/110 (94%)	87 (84%)	13 (13%)	3 (3%)	4	24
47	D5	128/206 (62%)	104 (81%)	20 (16%)	4 (3%)	4	23
47	H8	169/206 (82%)	136 (80%)	26 (15%)	7 (4%)	3	16
48	E5	75/85 (88%)	67 (89%)	5 (7%)	3 (4%)	3	17
48	I8	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
49	F5	92/98 (94%)	85 (92%)	5 (5%)	2 (2%)	6	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	J8	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	14	46
50	G5	66/72 (92%)	62 (94%)	2 (3%)	2 (3%)	4	23
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	2	15
51	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	45/71 (63%)	31 (69%)	13 (29%)	1 (2%)	6	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%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	14
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	14
All	All	10971/12333 (89%)	9586 (87%)	1202 (11%)	183 (2%)	9	36

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	127	LYS
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
30	21	83	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	170 (93%)	12 (7%)	16	47
2	1E	200/220 (91%)	186 (93%)	14 (7%)	15	45
3	22	154/188 (82%)	143 (93%)	11 (7%)	14	44
3	2E	159/188 (85%)	150 (94%)	9 (6%)	20	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	168 (93%)	12 (7%)	16	46
4	3E	180/181 (99%)	166 (92%)	14 (8%)	12	40
5	42	114/123 (93%)	105 (92%)	9 (8%)	12	40
5	4E	115/123 (94%)	112 (97%)	3 (3%)	46	74
6	52	90/90 (100%)	85 (94%)	5 (6%)	21	52
6	5E	90/90 (100%)	87 (97%)	3 (3%)	38	69
7	62	114/127 (90%)	107 (94%)	7 (6%)	18	49
7	6E	125/127 (98%)	117 (94%)	8 (6%)	17	48
8	72	118/119 (99%)	109 (92%)	9 (8%)	13	41
8	7E	119/119 (100%)	109 (92%)	10 (8%)	11	38
9	82	92/99 (93%)	78 (85%)	14 (15%)	3	12
9	8E	97/99 (98%)	87 (90%)	10 (10%)	7	27
10	1A	71/92 (77%)	61 (86%)	10 (14%)	3	15
10	1I	81/92 (88%)	75 (93%)	6 (7%)	13	42
11	2A	85/99 (86%)	83 (98%)	2 (2%)	49	76
11	2I	84/99 (85%)	80 (95%)	4 (5%)	25	58
12	3A	103/109 (94%)	93 (90%)	10 (10%)	8	30
12	3I	103/109 (94%)	95 (92%)	8 (8%)	12	40
13	4A	91/101 (90%)	82 (90%)	9 (10%)	8	29
13	4I	94/101 (93%)	87 (93%)	7 (7%)	13	42
14	5A	49/50 (98%)	44 (90%)	5 (10%)	7	27
14	5I	49/50 (98%)	49 (100%)	0	100	100
15	6A	79/80 (99%)	76 (96%)	3 (4%)	33	66
15	6I	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	7A	72/74 (97%)	69 (96%)	3 (4%)	30	62
16	7I	72/74 (97%)	66 (92%)	6 (8%)	11	38
17	8A	94/97 (97%)	93 (99%)	1 (1%)	73	89
17	8I	95/97 (98%)	90 (95%)	5 (5%)	22	54
18	9A	58/77 (75%)	55 (95%)	3 (5%)	23	55
18	9I	58/77 (75%)	55 (95%)	3 (5%)	23	55
19	AA	52/80 (65%)	48 (92%)	4 (8%)	13	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	71/80 (89%)	70 (99%)	1 (1%)	67	86
20	BA	76/82 (93%)	74 (97%)	2 (3%)	46	74
20	BI	75/82 (92%)	72 (96%)	3 (4%)	31	65
21	1B	17/22 (77%)	17 (100%)	0	100	100
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	9
28	71	109/181 (60%)	102 (94%)	7 (6%)	17	48
28	79	48/181 (26%)	44 (92%)	4 (8%)	11	38
29	11	214/218 (98%)	199 (93%)	15 (7%)	15	45
29	19	214/218 (98%)	201 (94%)	13 (6%)	18	49
30	21	165/166 (99%)	158 (96%)	7 (4%)	30	62
30	29	165/166 (99%)	154 (93%)	11 (7%)	16	46
31	31	161/166 (97%)	155 (96%)	6 (4%)	34	66
31	39	163/166 (98%)	152 (93%)	11 (7%)	16	46
32	41	153/156 (98%)	140 (92%)	13 (8%)	10	37
32	49	153/156 (98%)	139 (91%)	14 (9%)	9	33
33	51	142/148 (96%)	134 (94%)	8 (6%)	21	52
33	59	56/148 (38%)	52 (93%)	4 (7%)	14	44
34	61	122/124 (98%)	111 (91%)	11 (9%)	9	34
34	69	122/124 (98%)	115 (94%)	7 (6%)	20	52
35	15	117/119 (98%)	113 (97%)	4 (3%)	37	69
35	58	117/119 (98%)	109 (93%)	8 (7%)	16	45
36	25	100/100 (100%)	93 (93%)	7 (7%)	15	45
36	68	100/100 (100%)	95 (95%)	5 (5%)	24	57
37	35	114/116 (98%)	105 (92%)	9 (8%)	12	40
37	78	114/116 (98%)	102 (90%)	12 (10%)	7	26
38	45	109/111 (98%)	103 (94%)	6 (6%)	21	53
38	88	109/111 (98%)	103 (94%)	6 (6%)	21	53
39	55	101/101 (100%)	95 (94%)	6 (6%)	19	50
39	98	101/101 (100%)	96 (95%)	5 (5%)	24	57
40	65	87/88 (99%)	79 (91%)	8 (9%)	9	33
40	A8	87/88 (99%)	83 (95%)	4 (5%)	27	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	75	117/127 (92%)	110 (94%)	7 (6%)	19	49
41	B8	116/127 (91%)	105 (90%)	11 (10%)	8	31
42	85	93/94 (99%)	89 (96%)	4 (4%)	29	62
42	C8	92/94 (98%)	82 (89%)	10 (11%)	6	25
43	95	82/82 (100%)	77 (94%)	5 (6%)	18	49
43	D8	82/82 (100%)	79 (96%)	3 (4%)	34	66
44	A5	91/92 (99%)	88 (97%)	3 (3%)	38	69
44	E8	91/92 (99%)	86 (94%)	5 (6%)	21	53
45	B5	74/78 (95%)	70 (95%)	4 (5%)	22	53
45	F8	75/78 (96%)	72 (96%)	3 (4%)	31	65
46	C5	85/91 (93%)	79 (93%)	6 (7%)	14	44
46	G8	85/91 (93%)	83 (98%)	2 (2%)	49	76
47	D5	118/179 (66%)	109 (92%)	9 (8%)	13	41
47	H8	152/179 (85%)	142 (93%)	10 (7%)	16	47
48	E5	61/67 (91%)	57 (93%)	4 (7%)	16	47
48	I8	61/67 (91%)	61 (100%)	0	100	100
49	F5	79/83 (95%)	76 (96%)	3 (4%)	33	66
49	J8	79/83 (95%)	74 (94%)	5 (6%)	18	48
50	G5	62/67 (92%)	57 (92%)	5 (8%)	11	39
50	K8	62/67 (92%)	60 (97%)	2 (3%)	39	69
51	H5	50/52 (96%)	45 (90%)	5 (10%)	7	28
51	L8	50/52 (96%)	50 (100%)	0	100	100
52	M8	42/63 (67%)	36 (86%)	6 (14%)	3	14
53	J5	48/52 (92%)	41 (85%)	7 (15%)	3	13
53	N8	43/52 (83%)	40 (93%)	3 (7%)	15	45
54	L5	38/42 (90%)	37 (97%)	1 (3%)	46	74
54	P8	38/42 (90%)	36 (95%)	2 (5%)	22	54
55	M5	54/55 (98%)	51 (94%)	3 (6%)	21	52
55	Q8	54/55 (98%)	50 (93%)	4 (7%)	13	42
All	All	9272/10193 (91%)	8675 (94%)	597 (6%)	17	48

5 of 597 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	121	HIS
5	42	50	GLU
45	B5	57	LEU
49	J8	78	LYS
2	12	122	PHE

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

Mol	Chain	Res	Type
29	11	231	HIS
52	M8	47	GLN
47	D5	65	GLN
38	88	12	GLN
3	22	181	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	348 (23%)	32 (2%)
1	1G	1505/1522 (98%)	383 (25%)	30 (1%)
22	1K	65/76 (85%)	31 (47%)	3 (4%)
22	1L	70/76 (92%)	30 (42%)	5 (7%)
23	2K	76/77 (98%)	23 (30%)	1 (1%)
23	2L	76/77 (98%)	19 (25%)	2 (2%)
24	3K	75/76 (98%)	45 (60%)	3 (4%)
24	3L	75/76 (98%)	33 (44%)	0
25	4K	18/27 (66%)	10 (55%)	1 (5%)
25	4L	17/27 (62%)	10 (58%)	0
26	14	2852/2912 (97%)	735 (25%)	51 (1%)
26	1H	2828/2912 (97%)	733 (25%)	51 (1%)
27	16	121/122 (99%)	17 (14%)	2 (1%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
All	All	9392/9624 (97%)	2450 (26%)	183 (1%)

5 of 2450 RNA backbone outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	8	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2422	A
1	1G	345	C
26	14	2335	A
26	1H	2448	A
27	16	108	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	OMC	2L	33	23	15,22,23	2.37	4 (26%)	17,31,34	2.03	4 (23%)
22	U8U	1L	34	25,22	17,24,25	2.61	5 (29%)	19,34,37	1.69	3 (15%)
22	T6A	1K	37	22	24,34,35	2.63	4 (16%)	24,49,52	3.20	5 (20%)
22	PSU	1K	39	22	17,21,22	0.90	1 (5%)	20,30,33	3.33	5 (25%)
23	4SU	2K	8	23	14,21,22	3.17	2 (14%)	15,30,33	1.36	2 (13%)
22	U8U	1K	34	22	17,24,25	2.59	5 (29%)	19,34,37	1.47	3 (15%)
23	G7M	2L	47	23	20,26,27	3.49	8 (40%)	20,39,42	1.79	4 (20%)
24	PSU	3L	39	24	17,21,22	1.10	1 (5%)	20,30,33	3.46	5 (25%)
23	PSU	2L	56	23	17,21,22	1.05	1 (5%)	20,30,33	2.93	5 (25%)
23	4SU	2L	8	23	14,21,22	3.37	2 (14%)	15,30,33	0.91	1 (6%)
22	5MU	1K	54	22	15,22,23	2.11	3 (20%)	16,32,35	2.01	2 (12%)
24	PSU	3K	39	24	17,21,22	1.38	3 (17%)	20,30,33	3.29	7 (35%)
22	5MU	1L	54	22	15,22,23	2.21	3 (20%)	16,32,35	1.79	2 (12%)
23	PSU	2K	56	23	17,21,22	1.06	1 (5%)	20,30,33	3.05	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	1K	55	22	17,21,22	1.02	1 (5%)	20,30,33	3.70	5 (25%)
23	5MU	2L	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.85	2 (12%)
23	G7M	2K	47	23	20,26,27	3.47	7 (35%)	20,39,42	1.96	4 (20%)
22	PSU	1L	55	22	17,21,22	1.18	3 (17%)	20,30,33	3.47	7 (35%)
23	OMC	2K	33	23	15,22,23	2.19	4 (26%)	17,31,34	1.81	2 (11%)
22	PSU	1L	39	22	17,21,22	1.01	1 (5%)	20,30,33	3.31	5 (25%)
23	5MU	2K	55	23	15,22,23	2.18	3 (20%)	16,32,35	1.78	2 (12%)
22	T6A	1L	37	22	24,34,35	2.65	5 (20%)	24,49,52	2.45	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2L	33	23	-	3/7/27/28	0/2/2/2
22	U8U	1L	34	25,22	-	4/7/28/29	0/2/2/2
22	T6A	1K	37	22	-	1/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/5/25/26	0/2/2/2
22	U8U	1K	34	22	-	0/7/28/29	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	1/5/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	3/5/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/5/25/26	0/2/2/2
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
22	PSU	1L	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
22	T6A	1L	37	22	-	4/15/41/42	0/3/3/3

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	8	4SU	C5-C4	9.70	1.49	1.38
23	2K	8	4SU	C5-C4	9.57	1.49	1.38
23	2K	47	G7M	C4-N3	8.70	1.49	1.35
23	2L	47	G7M	C4-N3	8.38	1.48	1.35
23	2L	8	4SU	C6-N1	7.71	1.45	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3L	39	PSU	N1-C2-N3	-12.11	118.81	128.43
22	1K	55	PSU	N1-C2-N3	-11.88	118.99	128.43
22	1K	39	PSU	N1-C2-N3	-11.79	119.06	128.43
22	1L	55	PSU	N1-C2-N3	-11.77	119.08	128.43
22	1L	39	PSU	N1-C2-N3	-11.38	119.38	128.43

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2L	33	OMC	C2'-C1'-N1-C6
23	2L	33	OMC	O4'-C1'-N1-C6
23	2L	47	G7M	O4'-C4'-C5'-O5'
22	1L	54	5MU	O4'-C4'-C5'-O5'
22	1L	37	T6A	C5-C6-N6-C10

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	33	OMC	3	0
22	1L	34	U8U	1	0
22	1K	37	T6A	2	0
22	1K	39	PSU	1	0
22	1K	34	U8U	1	0
23	2L	47	G7M	1	0
23	2L	8	4SU	4	0
22	1L	54	5MU	2	0
23	2L	55	5MU	4	0
23	2K	47	G7M	1	0
22	1L	55	PSU	2	0
22	1L	39	PSU	2	0
23	2K	55	5MU	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1081 ligands modelled in this entry, 1077 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	SF4	32	301	4	0,12,12	0.00	-	-		
57	PAR	13	1730	-	45,45,45	0.87	1 (2%)	64,67,67	2.10	21 (32%)
57	PAR	1G	1681	-	45,45,45	0.82	1 (2%)	64,67,67	1.71	11 (17%)
58	SF4	3E	302	4	0,12,12	0.00	-	-		

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
58	SF4	32	301	4	-	-	0/6/5/5
57	PAR	13	1730	-	-	6/18/94/94	0/4/4/4
57	PAR	1G	1681	-	-	4/18/94/94	0/4/4/4
58	SF4	3E	302	4	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1681	PAR	C31-C21	-2.75	1.50	1.53
57	13	1730	PAR	O54-C14	2.13	1.47	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1G	1681	PAR	O52-C13-O43	-6.13	104.79	111.43
57	13	1730	PAR	O52-C13-O43	-5.61	105.35	111.43
57	13	1730	PAR	C32-C22-C12	-4.88	101.16	111.18
57	1G	1681	PAR	C14-O54-C54	4.67	122.86	113.69
57	1G	1681	PAR	C13-O52-C52	-4.49	106.84	117.96

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

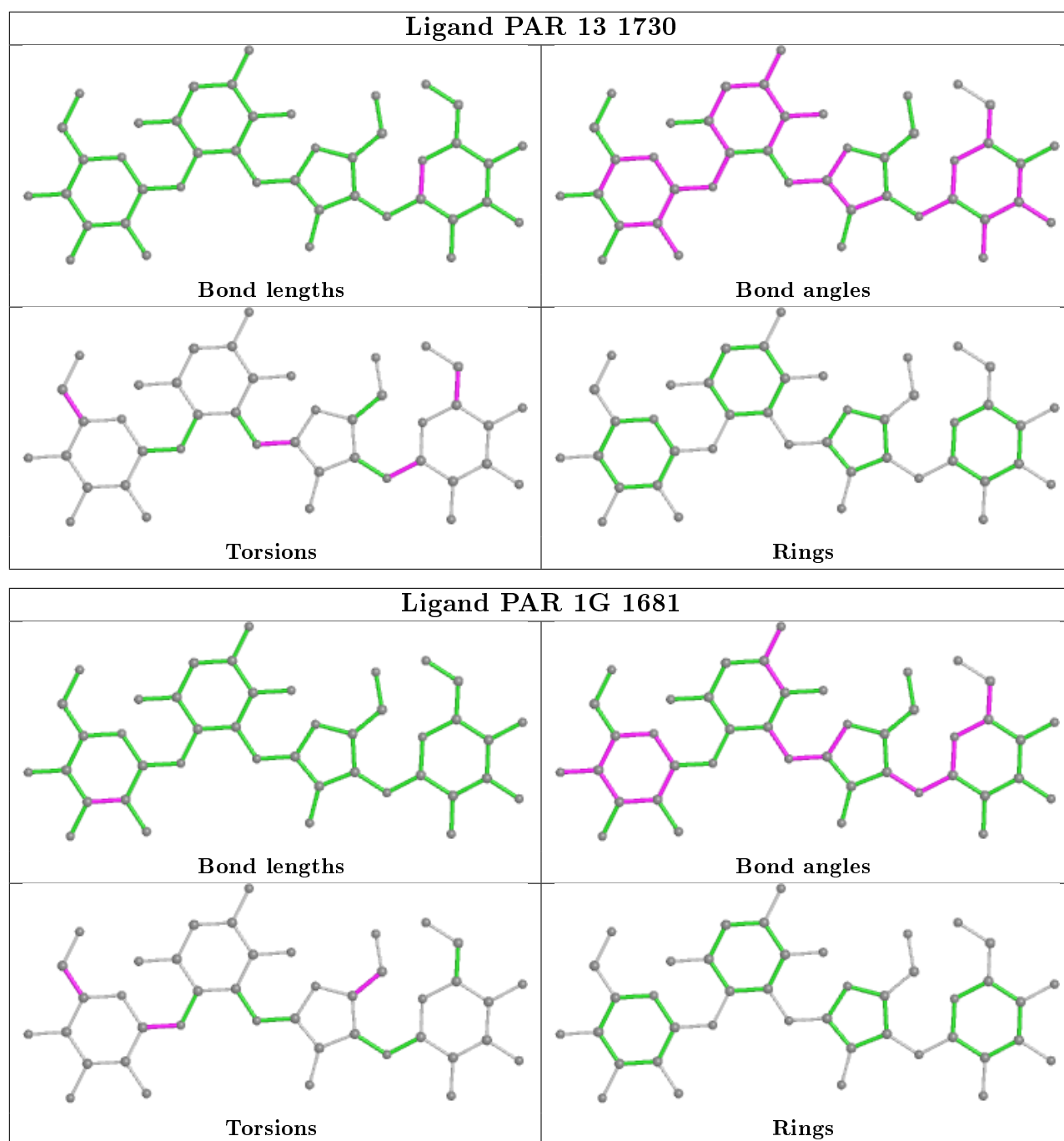
Mol	Chain	Res	Type	Atoms
57	13	1730	PAR	O54-C54-C64-N64
57	1G	1681	PAR	O51-C51-C61-O61
57	1G	1681	PAR	C41-C51-C61-O61
57	13	1730	PAR	C41-C51-C61-O61
57	1G	1681	PAR	O51-C11-O11-C42

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	32	301	SF4	3	0
57	13	1730	PAR	3	0
57	1G	1681	PAR	2	0
58	3E	302	SF4	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	35	1
25	4K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3'	25:A	P	4.27
1	35	121:LYS	C	122:PRO	N	1.61

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.70	3 (0%)	95	90	64, 104, 160, 189	0
1	1G	1507/1522 (99%)	-0.75	2 (0%)	95	92	78, 123, 164, 193	0
2	12	210/256 (82%)	0.27	13 (6%)	20	9	121, 148, 157, 163	0
2	1E	231/256 (90%)	-0.08	1 (0%)	92	84	112, 136, 153, 161	0
3	22	196/239 (82%)	0.85	28 (14%)	2	1	128, 141, 155, 161	0
3	2E	205/239 (85%)	1.04	44 (21%)	0	0	90, 109, 133, 144	0
4	32	208/209 (99%)	0.28	11 (5%)	26	12	101, 123, 139, 150	0
4	3E	207/209 (99%)	0.13	8 (3%)	39	20	88, 106, 126, 133	0
5	42	148/162 (91%)	0.32	5 (3%)	45	24	110, 128, 140, 145	0
5	4E	149/162 (91%)	0.30	3 (2%)	65	44	80, 101, 118, 130	0
6	52	101/101 (100%)	0.65	12 (11%)	4	2	96, 111, 126, 136	0
6	5E	100/101 (99%)	0.43	5 (5%)	28	13	84, 102, 119, 129	0
7	62	138/156 (88%)	0.89	24 (17%)	1	0	120, 131, 141, 145	0
7	6E	154/156 (98%)	0.63	16 (10%)	6	2	105, 124, 144, 159	0
8	72	137/138 (99%)	0.47	10 (7%)	15	6	111, 131, 141, 147	0
8	7E	138/138 (100%)	0.29	6 (4%)	35	17	92, 110, 121, 130	0
9	82	121/128 (94%)	-0.21	0	100	100	115, 146, 155, 160	0
9	8E	126/128 (98%)	-0.13	1 (0%)	86	72	93, 132, 149, 152	0
10	1A	80/105 (76%)	-0.28	2 (2%)	57	34	125, 141, 153, 156	0
10	1I	91/105 (86%)	0.50	7 (7%)	13	5	84, 125, 153, 159	0
11	2A	113/129 (87%)	2.19	64 (56%)	0	0	90, 119, 128, 133	0
11	2I	111/129 (86%)	1.24	27 (24%)	0	0	82, 112, 129, 144	0
12	3A	122/132 (92%)	0.73	20 (16%)	1	1	88, 112, 132, 146	0
12	3I	122/132 (92%)	0.95	18 (14%)	2	1	73, 82, 106, 139	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	-0.19	1 (0%) 84 69	124, 141, 150, 165	0
13	4I	119/126 (94%)	-0.54	0 100 100	94, 120, 135, 146	0
14	5A	59/61 (96%)	0.66	11 (18%) 1 0	130, 140, 148, 150	0
14	5I	60/61 (98%)	-0.37	0 100 100	88, 100, 112, 125	0
15	6A	87/89 (97%)	0.17	3 (3%) 45 24	93, 117, 132, 135	0
15	6I	87/89 (97%)	0.21	3 (3%) 45 24	84, 103, 120, 126	0
16	7A	84/88 (95%)	-0.16	1 (1%) 79 61	93, 111, 130, 141	0
16	7I	83/88 (94%)	-0.34	0 100 100	102, 112, 135, 147	0
17	8A	99/105 (94%)	0.92	14 (14%) 2 1	108, 120, 133, 138	0
17	8I	100/105 (95%)	0.74	10 (10%) 7 2	89, 111, 126, 131	0
18	9A	67/88 (76%)	0.47	5 (7%) 14 5	106, 117, 135, 139	0
18	9I	68/88 (77%)	0.12	0 100 100	89, 105, 124, 127	0
19	AA	62/93 (66%)	0.03	2 (3%) 47 25	123, 149, 157, 163	0
19	AI	82/93 (88%)	-0.45	0 100 100	99, 118, 134, 142	0
20	BA	99/106 (93%)	0.85	18 (18%) 1 0	94, 116, 141, 150	0
20	BI	97/106 (91%)	0.52	7 (7%) 15 6	114, 126, 144, 148	0
21	1B	22/27 (81%)	-0.30	0 100 100	124, 136, 143, 147	0
21	1F	23/27 (85%)	-1.05	0 100 100	99, 109, 116, 120	0
22	1K	64/76 (84%)	-0.05	3 (4%) 31 15	93, 158, 171, 173	0
22	1L	68/76 (89%)	-0.37	2 (2%) 51 28	125, 171, 178, 184	0
23	2K	72/77 (93%)	-0.43	0 100 100	77, 104, 130, 146	0
23	2L	72/77 (93%)	-0.28	1 (1%) 75 56	84, 122, 150, 165	0
24	3K	75/76 (98%)	0.36	5 (6%) 17 7	81, 170, 184, 189	0
24	3L	75/76 (98%)	0.28	2 (2%) 54 31	89, 167, 182, 188	0
25	4K	20/27 (74%)	-0.04	1 (5%) 28 13	76, 144, 177, 178	0
25	4L	18/27 (66%)	0.03	0 100 100	103, 157, 182, 183	0
26	14	2861/2912 (98%)	-0.48	20 (0%) 87 75	58, 92, 173, 197	0
26	1H	2833/2912 (97%)	-0.43	6 (0%) 95 90	50, 80, 164, 199	0
27	16	122/122 (100%)	-0.57	0 100 100	75, 98, 119, 170	0
27	1J	122/122 (100%)	-0.99	0 100 100	93, 123, 141, 174	0
28	7I	133/229 (58%)	1.46	46 (34%) 0 0	137, 169, 179, 181	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	79	57/229 (24%)	1.40	17 (29%) 0 0	139, 160, 169, 174	0
29	11	273/276 (98%)	0.93	28 (10%) 6 2	48, 74, 92, 101	0
29	19	274/276 (99%)	0.64	18 (6%) 18 7	60, 82, 99, 116	0
30	21	203/206 (98%)	1.47	62 (30%) 0 0	58, 95, 135, 146	0
30	29	204/206 (99%)	0.16	11 (5%) 25 12	67, 99, 134, 144	0
31	31	202/210 (96%)	0.33	6 (2%) 50 27	54, 85, 119, 138	0
31	39	204/210 (97%)	0.22	9 (4%) 34 17	64, 112, 147, 163	0
32	41	179/182 (98%)	-0.52	0 100 100	87, 107, 136, 148	0
32	49	179/182 (98%)	0.76	30 (16%) 1 0	121, 137, 156, 168	0
33	51	171/180 (95%)	0.35	12 (7%) 16 7	89, 110, 125, 137	0
33	59	69/180 (38%)	0.47	4 (5%) 23 10	131, 151, 162, 166	0
34	61	146/148 (98%)	-0.24	3 (2%) 63 43	85, 129, 142, 149	0
34	69	145/148 (97%)	0.49	22 (15%) 2 1	91, 126, 142, 151	0
35	15	138/140 (98%)	1.33	40 (28%) 0 0	87, 114, 138, 154	0
35	58	138/140 (98%)	0.63	11 (7%) 12 5	69, 97, 124, 140	0
36	25	122/122 (100%)	0.71	13 (10%) 6 2	76, 96, 112, 118	0
36	68	122/122 (100%)	1.44	37 (30%) 0 0	63, 84, 101, 110	0
37	35	147/150 (98%)	1.26	47 (31%) 0 0	65, 110, 135, 148	0
37	78	147/150 (98%)	0.22	4 (2%) 54 31	50, 89, 113, 128	0
38	45	138/141 (97%)	0.77	19 (13%) 2 1	84, 111, 129, 137	0
38	88	141/141 (100%)	-0.38	0 100 100	58, 84, 107, 125	0
39	55	118/118 (100%)	0.26	0 100 100	70, 86, 108, 121	0
39	98	118/118 (100%)	1.15	26 (22%) 0 0	71, 92, 112, 126	0
40	65	110/112 (98%)	-0.13	1 (0%) 84 69	91, 116, 132, 137	0
40	A8	111/112 (99%)	-0.20	2 (1%) 68 47	76, 94, 117, 123	0
41	75	133/146 (91%)	-0.09	4 (3%) 50 27	86, 102, 130, 142	0
41	B8	132/146 (90%)	0.59	11 (8%) 11 4	78, 99, 128, 139	0
42	85	116/118 (98%)	0.74	13 (11%) 5 2	76, 101, 130, 139	0
42	C8	115/118 (97%)	0.25	3 (2%) 56 33	65, 83, 114, 118	0
43	95	100/101 (99%)	1.06	18 (18%) 1 0	76, 123, 139, 141	0
43	D8	100/101 (99%)	0.78	12 (12%) 4 2	64, 105, 129, 134	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	A5	111/113 (98%)	0.67	6 (5%) 25 12	68, 84, 114, 141	0
44	E8	112/113 (99%)	1.04	19 (16%) 1 0	64, 82, 112, 142	0
45	B5	94/96 (97%)	0.24	5 (5%) 26 12	75, 91, 115, 123	0
45	F8	95/96 (98%)	0.65	6 (6%) 20 8	62, 79, 111, 125	0
46	C5	105/110 (95%)	1.70	35 (33%) 0 0	91, 124, 146, 152	0
46	G8	105/110 (95%)	0.12	2 (1%) 66 46	79, 101, 127, 132	0
47	D5	132/206 (64%)	0.70	13 (9%) 7 2	115, 136, 152, 155	0
47	H8	171/206 (83%)	-0.31	1 (0%) 89 78	90, 124, 164, 168	0
48	E5	77/85 (90%)	0.62	8 (10%) 6 2	75, 96, 113, 135	0
48	I8	76/85 (89%)	-0.48	0 100 100	65, 78, 91, 107	0
49	F5	94/98 (95%)	1.21	24 (25%) 0 0	70, 90, 123, 133	0
49	J8	94/98 (95%)	0.74	6 (6%) 19 8	61, 81, 120, 128	0
50	G5	68/72 (94%)	-0.16	3 (4%) 34 17	88, 109, 129, 150	0
50	K8	68/72 (94%)	0.36	1 (1%) 73 54	66, 84, 104, 128	0
51	H5	58/60 (96%)	1.32	11 (18%) 1 0	85, 106, 134, 140	0
51	L8	58/60 (96%)	0.06	1 (1%) 70 49	65, 87, 115, 132	0
52	M8	47/71 (66%)	-0.03	2 (4%) 35 17	111, 137, 156, 163	0
53	J5	56/60 (93%)	0.63	4 (7%) 16 6	67, 92, 137, 147	0
53	N8	48/60 (80%)	0.93	8 (16%) 1 1	61, 87, 134, 141	0
54	L5	47/49 (95%)	-0.19	1 (2%) 63 43	57, 68, 85, 103	0
54	P8	47/49 (95%)	0.57	4 (8%) 10 4	53, 60, 79, 88	0
55	M5	64/65 (98%)	1.24	16 (25%) 0 0	75, 86, 103, 126	0
55	Q8	64/65 (98%)	0.36	1 (1%) 72 51	64, 74, 92, 108	0
All	All	20598/21957 (93%)	0.02	1151 (5%) 24 11	48, 105, 159, 199	0

The worst 5 of 1151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2901	C	10.5
26	14	2902	C	9.9
46	C5	59	GLY	9.1
41	75	1	MET	8.0
43	D8	37	VAL	8.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	1L	39	20/21	0.87	0.14	135,144,149,150	0
22	T6A	1L	37	32/33	0.88	0.21	132,140,153,154	0
23	OMC	2L	33	21/22	0.90	0.15	105,114,118,121	0
23	4SU	2L	8	20/21	0.90	0.16	114,124,129,130	0
22	PSU	1L	55	20/21	0.91	0.09	129,139,149,150	0
23	PSU	2K	56	20/21	0.91	0.16	99,110,121,122	0
22	PSU	1K	55	20/21	0.91	0.15	102,113,120,131	0
22	U8U	1L	34	23/24	0.92	0.17	123,133,138,150	0
22	5MU	1K	54	21/22	0.92	0.15	110,117,132,137	0
24	PSU	3K	39	20/21	0.92	0.17	141,151,156,159	0
22	T6A	1K	37	32/33	0.92	0.21	79,94,121,123	0
23	PSU	2L	56	20/21	0.93	0.11	115,126,131,135	0
22	PSU	1K	39	20/21	0.93	0.14	98,115,125,127	0
23	G7M	2L	47	24/25	0.93	0.12	126,133,141,145	0
23	5MU	2L	55	21/22	0.94	0.13	119,131,141,145	0
22	5MU	1L	54	21/22	0.94	0.12	133,141,146,152	0
23	4SU	2K	8	20/21	0.94	0.14	91,98,107,109	0
24	PSU	3L	39	20/21	0.94	0.23	145,155,159,162	0
23	G7M	2K	47	24/25	0.95	0.13	102,114,127,133	0
22	U8U	1K	34	23/24	0.95	0.15	84,92,100,108	0
23	5MU	2K	55	21/22	0.96	0.18	106,117,125,127	0
23	OMC	2K	33	21/22	0.96	0.17	77,83,91,93	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3317	1/1	0.28	0.63	105,105,105,105	0
56	MG	2K	102	1/1	0.28	0.72	126,126,126,126	0
56	MG	1H	3318	1/1	0.30	0.34	96,96,96,96	0
56	MG	14	3229	1/1	0.30	0.52	86,86,86,86	0
56	MG	13	1648	1/1	0.37	0.42	82,82,82,82	0
56	MG	2L	102	1/1	0.42	0.58	98,98,98,98	0
56	MG	14	3302	1/1	0.42	0.51	110,110,110,110	0
56	MG	1H	3281	1/1	0.43	0.36	81,81,81,81	0
56	MG	1G	1647	1/1	0.44	0.28	102,102,102,102	0
56	MG	1G	1633	1/1	0.45	0.35	83,83,83,83	0
56	MG	13	1655	1/1	0.47	0.33	103,103,103,103	0
56	MG	1H	3298	1/1	0.47	0.35	93,93,93,93	0
56	MG	1G	1602	1/1	0.51	0.59	105,105,105,105	0
56	MG	14	3232	1/1	0.55	0.33	127,127,127,127	0
56	MG	1H	3326	1/1	0.55	0.15	91,91,91,91	0
56	MG	14	3224	1/1	0.57	0.57	75,75,75,75	0
56	MG	14	3298	1/1	0.58	0.28	94,94,94,94	0
56	MG	13	1646	1/1	0.58	0.48	95,95,95,95	0
56	MG	1H	3140	1/1	0.58	0.14	69,69,69,69	0
56	MG	3E	301	1/1	0.58	0.48	94,94,94,94	0
56	MG	5I	101	1/1	0.59	0.17	88,88,88,88	0
56	MG	1H	3157	1/1	0.59	0.34	83,83,83,83	0
56	MG	1H	3250	1/1	0.60	0.45	87,87,87,87	0
56	MG	1H	3295	1/1	0.60	0.41	85,85,85,85	0
56	MG	1H	3028	1/1	0.61	0.60	72,72,72,72	0
56	MG	13	1701	1/1	0.61	0.23	121,121,121,121	0
56	MG	1H	3319	1/1	0.61	0.26	102,102,102,102	0
56	MG	1H	3274	1/1	0.61	0.46	85,85,85,85	0
56	MG	1H	3206	1/1	0.61	0.51	94,94,94,94	0
56	MG	1H	3224	1/1	0.62	0.54	88,88,88,88	0
56	MG	14	3381	1/1	0.62	0.15	102,102,102,102	0
56	MG	13	1647	1/1	0.63	0.34	95,95,95,95	0
56	MG	14	3250	1/1	0.63	0.31	99,99,99,99	0
56	MG	1G	1640	1/1	0.63	0.14	108,108,108,108	0
56	MG	1G	1646	1/1	0.63	0.32	86,86,86,86	0
56	MG	1H	3264	1/1	0.63	0.18	84,84,84,84	0
56	MG	14	3289	1/1	0.63	0.29	91,91,91,91	0
56	MG	E5	101	1/1	0.64	0.32	83,83,83,83	0
56	MG	1H	3018	1/1	0.64	0.59	78,78,78,78	0
56	MG	13	1642	1/1	0.64	0.19	73,73,73,73	0
56	MG	1H	3308	1/1	0.64	0.57	99,99,99,99	0
56	MG	1H	3110	1/1	0.64	0.28	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3262	1/1	0.65	0.44	91,91,91,91	0
56	MG	14	3266	1/1	0.65	0.26	90,90,90,90	0
56	MG	1H	3270	1/1	0.65	0.47	70,70,70,70	0
56	MG	14	3181	1/1	0.65	0.18	98,98,98,98	0
56	MG	1H	3248	1/1	0.65	0.32	83,83,83,83	0
56	MG	21	302	1/1	0.65	0.20	78,78,78,78	0
56	MG	14	3153	1/1	0.66	0.38	78,78,78,78	0
56	MG	14	3101	1/1	0.66	0.28	91,91,91,91	0
56	MG	1J	203	1/1	0.66	0.75	113,113,113,113	0
56	MG	1H	3213	1/1	0.67	0.61	84,84,84,84	0
56	MG	1H	3189	1/1	0.67	0.42	84,84,84,84	0
56	MG	1G	1643	1/1	0.67	0.33	91,91,91,91	0
56	MG	14	3162	1/1	0.67	0.51	83,83,83,83	0
56	MG	14	3304	1/1	0.68	0.50	90,90,90,90	0
56	MG	1G	1668	1/1	0.68	0.48	106,106,106,106	0
56	MG	14	3064	1/1	0.68	0.10	84,84,84,84	0
56	MG	14	3192	1/1	0.68	0.23	80,80,80,80	0
56	MG	1H	3052	1/1	0.69	0.84	99,99,99,99	0
56	MG	14	3290	1/1	0.69	0.36	90,90,90,90	0
56	MG	14	3205	1/1	0.69	0.49	80,80,80,80	0
56	MG	14	3169	1/1	0.69	0.10	104,104,104,104	0
56	MG	14	3140	1/1	0.69	0.18	87,87,87,87	0
56	MG	16	203	1/1	0.70	0.27	91,91,91,91	0
56	MG	14	3297	1/1	0.70	0.30	124,124,124,124	0
56	MG	1H	3200	1/1	0.70	0.33	87,87,87,87	0
56	MG	14	3150	1/1	0.70	0.35	91,91,91,91	0
56	MG	14	3032	1/1	0.70	0.52	88,88,88,88	0
56	MG	1H	3423	1/1	0.70	0.06	147,147,147,147	0
56	MG	14	3261	1/1	0.71	0.59	83,83,83,83	0
56	MG	45	202	1/1	0.71	0.20	103,103,103,103	0
56	MG	13	1674	1/1	0.71	0.50	92,92,92,92	0
56	MG	1H	3275	1/1	0.71	0.42	74,74,74,74	0
56	MG	1G	1644	1/1	0.72	0.70	86,86,86,86	0
56	MG	14	3055	1/1	0.72	0.51	112,112,112,112	0
56	MG	1H	3193	1/1	0.72	0.40	72,72,72,72	0
56	MG	14	3091	1/1	0.72	0.92	87,87,87,87	0
56	MG	14	3220	1/1	0.72	0.37	107,107,107,107	0
56	MG	14	3126	1/1	0.72	1.12	83,83,83,83	0
56	MG	14	3296	1/1	0.72	0.26	91,91,91,91	0
56	MG	13	1695	1/1	0.72	0.42	103,103,103,103	0
56	MG	1H	3214	1/1	0.72	0.25	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3301	1/1	0.72	0.39	99,99,99,99	0
56	MG	1H	3301	1/1	0.72	0.29	128,128,128,128	0
56	MG	14	3283	1/1	0.72	0.29	80,80,80,80	0
56	MG	13	1661	1/1	0.73	0.09	93,93,93,93	0
56	MG	14	3249	1/1	0.73	0.15	78,78,78,78	0
56	MG	14	3252	1/1	0.73	0.09	73,73,73,73	0
56	MG	1H	3185	1/1	0.74	0.24	78,78,78,78	0
56	MG	1H	3015	1/1	0.74	0.41	77,77,77,77	0
56	MG	1H	3160	1/1	0.74	0.40	69,69,69,69	0
56	MG	13	1693	1/1	0.74	0.41	88,88,88,88	0
56	MG	1H	3284	1/1	0.74	0.18	88,88,88,88	0
56	MG	16	207	1/1	0.74	0.42	76,76,76,76	0
56	MG	14	3272	1/1	0.74	0.40	93,93,93,93	0
56	MG	1H	3302	1/1	0.74	0.51	89,89,89,89	0
56	MG	1H	3032	1/1	0.75	0.21	80,80,80,80	0
56	MG	1H	3198	1/1	0.75	0.20	67,67,67,67	0
56	MG	1H	3277	1/1	0.75	0.30	100,100,100,100	0
56	MG	35	201	1/1	0.75	0.41	76,76,76,76	0
56	MG	13	1699	1/1	0.75	0.31	81,81,81,81	0
56	MG	14	3273	1/1	0.75	0.33	94,94,94,94	0
56	MG	1H	3143	1/1	0.75	0.37	77,77,77,77	0
56	MG	1H	3025	1/1	0.75	0.40	77,77,77,77	0
56	MG	14	3260	1/1	0.75	0.27	90,90,90,90	0
56	MG	14	3127	1/1	0.75	0.27	71,71,71,71	0
56	MG	14	3110	1/1	0.75	0.76	88,88,88,88	0
56	MG	1H	3315	1/1	0.76	0.13	91,91,91,91	0
56	MG	14	3233	1/1	0.76	0.76	80,80,80,80	0
56	MG	1H	3258	1/1	0.76	0.37	72,72,72,72	0
56	MG	1H	3041	1/1	0.76	0.32	77,77,77,77	0
56	MG	1H	3299	1/1	0.76	0.45	86,86,86,86	0
56	MG	14	3254	1/1	0.76	0.73	78,78,78,78	0
56	MG	1G	1638	1/1	0.76	0.54	81,81,81,81	0
56	MG	1H	3099	1/1	0.76	0.45	75,75,75,75	0
56	MG	1H	3042	1/1	0.76	0.26	93,93,93,93	0
56	MG	14	3198	1/1	0.76	0.30	80,80,80,80	0
56	MG	1H	3125	1/1	0.76	0.23	87,87,87,87	0
56	MG	1G	1616	1/1	0.77	0.49	96,96,96,96	0
56	MG	1H	3273	1/1	0.77	0.64	84,84,84,84	0
56	MG	14	3197	1/1	0.77	0.36	84,84,84,84	0
56	MG	14	3255	1/1	0.77	0.25	87,87,87,87	0
56	MG	13	1623	1/1	0.77	0.33	105,105,105,105	0
56	MG	1H	3039	1/1	0.77	0.55	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3299	1/1	0.78	0.19	96,96,96,96	0
56	MG	13	1690	1/1	0.78	0.44	81,81,81,81	0
56	MG	14	3278	1/1	0.78	0.35	96,96,96,96	0
56	MG	14	3284	1/1	0.78	0.23	84,84,84,84	0
56	MG	1H	3291	1/1	0.78	0.46	99,99,99,99	0
56	MG	14	3191	1/1	0.78	0.18	76,76,76,76	0
56	MG	Q8	101	1/1	0.78	0.29	83,83,83,83	0
56	MG	1H	3046	1/1	0.78	0.47	87,87,87,87	0
56	MG	1G	1654	1/1	0.78	0.45	86,86,86,86	0
56	MG	1K	101	1/1	0.78	0.54	138,138,138,138	0
56	MG	14	3177	1/1	0.78	0.45	87,87,87,87	0
56	MG	14	3146	1/1	0.78	0.37	61,61,61,61	0
56	MG	1G	1666	1/1	0.78	0.51	85,85,85,85	0
56	MG	1H	3075	1/1	0.78	0.11	79,79,79,79	0
56	MG	1H	3269	1/1	0.78	0.35	97,97,97,97	0
56	MG	14	3291	1/1	0.78	0.66	94,94,94,94	0
56	MG	14	3120	1/1	0.78	0.34	71,71,71,71	0
56	MG	1G	1620	1/1	0.78	0.25	94,94,94,94	0
56	MG	1H	3219	1/1	0.78	0.44	89,89,89,89	0
56	MG	1H	3134	1/1	0.79	0.41	90,90,90,90	0
56	MG	14	3303	1/1	0.79	0.46	98,98,98,98	0
56	MG	2K	101	1/1	0.79	0.55	86,86,86,86	0
56	MG	14	3275	1/1	0.79	0.34	68,68,68,68	0
56	MG	1G	1651	1/1	0.79	0.58	93,93,93,93	0
56	MG	1H	3038	1/1	0.79	0.35	81,81,81,81	0
56	MG	41	201	1/1	0.79	0.27	71,71,71,71	0
56	MG	13	1676	1/1	0.79	0.20	127,127,127,127	0
56	MG	14	3156	1/1	0.79	0.40	62,62,62,62	0
56	MG	14	3222	1/1	0.79	0.42	80,80,80,80	0
56	MG	1H	3316	1/1	0.79	0.47	87,87,87,87	0
56	MG	1G	1637	1/1	0.79	0.46	97,97,97,97	0
56	MG	1H	3093	1/1	0.79	0.22	72,72,72,72	0
56	MG	14	3202	1/1	0.79	0.18	79,79,79,79	0
56	MG	1H	3034	1/1	0.79	0.35	78,78,78,78	0
56	MG	1H	3278	1/1	0.80	0.75	92,92,92,92	0
56	MG	1G	1622	1/1	0.80	0.68	99,99,99,99	0
56	MG	14	3017	1/1	0.80	0.52	92,92,92,92	0
56	MG	1H	3212	1/1	0.80	0.57	89,89,89,89	0
56	MG	14	3227	1/1	0.80	0.28	81,81,81,81	0
56	MG	13	1608	1/1	0.80	0.30	91,91,91,91	0
56	MG	1H	3155	1/1	0.80	0.36	86,86,86,86	0
56	MG	13	1698	1/1	0.80	0.22	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1629	1/1	0.80	0.41	90,90,90,90	0
56	MG	I8	102	1/1	0.80	0.45	83,83,83,83	0
56	MG	14	3214	1/1	0.80	0.51	87,87,87,87	0
56	MG	1H	3289	1/1	0.80	0.33	82,82,82,82	0
56	MG	1H	3297	1/1	0.81	0.11	101,101,101,101	0
56	MG	13	1627	1/1	0.81	0.45	81,81,81,81	0
56	MG	14	3143	1/1	0.81	0.29	70,70,70,70	0
56	MG	1H	3045	1/1	0.81	0.39	116,116,116,116	0
56	MG	1H	3249	1/1	0.81	0.79	86,86,86,86	0
56	MG	14	3183	1/1	0.81	0.30	89,89,89,89	0
56	MG	1H	3138	1/1	0.81	0.37	61,61,61,61	0
56	MG	14	3003	1/1	0.81	0.28	69,69,69,69	0
56	MG	1H	3280	1/1	0.81	0.22	88,88,88,88	0
56	MG	14	3221	1/1	0.81	0.17	91,91,91,91	0
56	MG	14	3130	1/1	0.81	0.68	78,78,78,78	0
56	MG	14	3180	1/1	0.81	0.25	79,79,79,79	0
56	MG	1H	3220	1/1	0.81	0.37	87,87,87,87	0
56	MG	1J	202	1/1	0.81	0.25	104,104,104,104	0
56	MG	14	3308	1/1	0.81	0.27	82,82,82,82	0
56	MG	14	3024	1/1	0.81	0.37	74,74,74,74	0
56	MG	1H	3205	1/1	0.81	0.41	83,83,83,83	0
56	MG	1H	3019	1/1	0.81	0.38	89,89,89,89	0
56	MG	13	1604	1/1	0.82	0.29	93,93,93,93	0
56	MG	14	3023	1/1	0.82	0.34	55,55,55,55	0
56	MG	14	3062	1/1	0.82	0.11	81,81,81,81	0
56	MG	1H	3161	1/1	0.82	0.21	84,84,84,84	0
56	MG	14	3031	1/1	0.82	0.43	76,76,76,76	0
56	MG	1H	3096	1/1	0.82	0.34	78,78,78,78	0
56	MG	78	201	1/1	0.82	0.21	75,75,75,75	0
56	MG	1H	3182	1/1	0.82	0.28	77,77,77,77	0
56	MG	14	3114	1/1	0.82	0.25	81,81,81,81	0
56	MG	1G	1630	1/1	0.82	0.72	108,108,108,108	0
56	MG	1G	1609	1/1	0.82	0.19	94,94,94,94	0
56	MG	1H	3236	1/1	0.82	0.32	91,91,91,91	0
56	MG	1H	3123	1/1	0.82	0.43	77,77,77,77	0
56	MG	1H	3044	1/1	0.82	0.49	89,89,89,89	0
56	MG	1H	3011	1/1	0.82	0.49	71,71,71,71	0
56	MG	1H	3201	1/1	0.82	0.43	70,70,70,70	0
56	MG	14	3117	1/1	0.82	0.55	77,77,77,77	0
56	MG	1H	3107	1/1	0.83	0.36	73,73,73,73	0
56	MG	14	3019	1/1	0.83	0.43	84,84,84,84	0
56	MG	1H	3013	1/1	0.83	0.39	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3035	1/1	0.83	0.41	84,84,84,84	0
56	MG	1H	3186	1/1	0.83	0.17	71,71,71,71	0
56	MG	1H	3170	1/1	0.83	0.32	81,81,81,81	0
56	MG	1H	3175	1/1	0.83	0.47	70,70,70,70	0
56	MG	1H	3029	1/1	0.83	0.36	69,69,69,69	0
56	MG	13	1694	1/1	0.83	0.15	96,96,96,96	0
56	MG	14	3259	1/1	0.83	0.23	84,84,84,84	0
56	MG	1H	3241	1/1	0.83	0.29	73,73,73,73	0
56	MG	13	1696	1/1	0.83	0.43	111,111,111,111	0
56	MG	14	3186	1/1	0.83	0.79	83,83,83,83	0
56	MG	14	3211	1/1	0.83	0.28	74,74,74,74	0
56	MG	13	1700	1/1	0.83	0.12	111,111,111,111	0
56	MG	85	201	1/1	0.83	0.49	88,88,88,88	0
56	MG	1H	3124	1/1	0.83	0.24	59,59,59,59	0
56	MG	1H	3202	1/1	0.83	0.32	75,75,75,75	0
56	MG	14	3240	1/1	0.83	0.38	87,87,87,87	0
56	MG	14	3168	1/1	0.83	0.45	66,66,66,66	0
56	MG	1H	3141	1/1	0.83	0.17	69,69,69,69	0
56	MG	1H	3083	1/1	0.83	0.17	75,75,75,75	0
56	MG	1H	3053	1/1	0.83	0.54	82,82,82,82	0
56	MG	14	3203	1/1	0.83	0.16	68,68,68,68	0
56	MG	14	3269	1/1	0.83	0.38	75,75,75,75	0
56	MG	14	3277	1/1	0.83	0.52	92,92,92,92	0
56	MG	1H	3135	1/1	0.84	0.29	81,81,81,81	0
56	MG	14	3060	1/1	0.84	0.25	92,92,92,92	0
56	MG	13	1664	1/1	0.84	0.34	99,99,99,99	0
56	MG	14	3245	1/1	0.84	0.23	88,88,88,88	0
56	MG	13	1636	1/1	0.84	0.55	85,85,85,85	0
56	MG	14	3163	1/1	0.84	0.89	76,76,76,76	0
56	MG	14	3166	1/1	0.84	0.32	85,85,85,85	0
56	MG	1H	3271	1/1	0.84	0.46	94,94,94,94	0
56	MG	14	3279	1/1	0.84	0.25	73,73,73,73	0
56	MG	14	3257	1/1	0.84	0.38	68,68,68,68	0
56	MG	1H	3112	1/1	0.84	0.24	66,66,66,66	0
56	MG	14	3075	1/1	0.84	1.26	90,90,90,90	0
56	MG	14	3187	1/1	0.84	0.42	75,75,75,75	0
56	MG	1H	3211	1/1	0.84	0.36	71,71,71,71	0
56	MG	13	1637	1/1	0.84	0.50	68,68,68,68	0
56	MG	13	1702	1/1	0.84	0.60	103,103,103,103	0
56	MG	14	3026	1/1	0.84	0.51	68,68,68,68	0
56	MG	13	1689	1/1	0.84	0.21	92,92,92,92	0
56	MG	1H	3040	1/1	0.84	0.66	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3239	1/1	0.84	0.26	79,79,79,79	0
56	MG	1H	3296	1/1	0.84	0.53	92,92,92,92	0
56	MG	39	301	1/1	0.84	0.12	80,80,80,80	0
56	MG	1H	3151	1/1	0.84	0.10	52,52,52,52	0
56	MG	14	3196	1/1	0.84	0.33	69,69,69,69	0
56	MG	1H	3147	1/1	0.84	0.14	72,72,72,72	0
56	MG	13	1605	1/1	0.84	0.19	75,75,75,75	0
56	MG	14	3216	1/1	0.85	0.22	70,70,70,70	0
56	MG	13	1681	1/1	0.85	0.25	106,106,106,106	0
56	MG	1H	3257	1/1	0.85	0.34	94,94,94,94	0
56	MG	13	1692	1/1	0.85	0.36	100,100,100,100	0
56	MG	1H	3304	1/1	0.85	0.40	73,73,73,73	0
56	MG	1H	3240	1/1	0.85	0.21	56,56,56,56	0
56	MG	13	1677	1/1	0.85	0.33	91,91,91,91	0
56	MG	1H	3192	1/1	0.85	0.24	81,81,81,81	0
56	MG	1H	3162	1/1	0.85	0.38	87,87,87,87	0
56	MG	1H	3287	1/1	0.85	0.65	86,86,86,86	0
56	MG	13	1603	1/1	0.85	0.56	92,92,92,92	0
56	MG	1H	3084	1/1	0.85	0.22	82,82,82,82	0
56	MG	14	3111	1/1	0.85	0.42	69,69,69,69	0
56	MG	1H	3321	1/1	0.85	0.22	85,85,85,85	0
56	MG	1G	1627	1/1	0.85	0.28	85,85,85,85	0
56	MG	1G	1645	1/1	0.85	0.63	88,88,88,88	0
56	MG	2L	103	1/1	0.85	0.39	79,79,79,79	0
56	MG	14	3188	1/1	0.85	0.44	92,92,92,92	0
56	MG	14	3144	1/1	0.85	0.54	58,58,58,58	0
56	MG	14	3070	1/1	0.85	0.39	71,71,71,71	0
56	MG	14	3012	1/1	0.85	0.67	82,82,82,82	0
56	MG	1H	3207	1/1	0.85	0.40	81,81,81,81	0
56	MG	1H	3282	1/1	0.85	0.15	78,78,78,78	0
56	MG	14	3018	1/1	0.86	0.41	73,73,73,73	0
56	MG	1H	3276	1/1	0.86	0.34	85,85,85,85	0
56	MG	14	3170	1/1	0.86	0.82	81,81,81,81	0
56	MG	4K	101	1/1	0.86	0.22	156,156,156,156	0
56	MG	14	3015	1/1	0.86	0.42	63,63,63,63	0
56	MG	14	3292	1/1	0.86	0.22	86,86,86,86	0
56	MG	14	3247	1/1	0.86	0.36	73,73,73,73	0
56	MG	1G	1679	1/1	0.86	0.05	138,138,138,138	0
56	MG	13	1672	1/1	0.86	0.19	81,81,81,81	0
56	MG	14	3149	1/1	0.86	0.53	92,92,92,92	0
56	MG	16	202	1/1	0.86	0.46	86,86,86,86	0
56	MG	14	3193	1/1	0.86	0.36	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3149	1/1	0.86	0.26	65,65,65,65	0
56	MG	14	3133	1/1	0.86	0.38	97,97,97,97	0
56	MG	13	1666	1/1	0.86	0.12	89,89,89,89	0
56	MG	13	1654	1/1	0.86	0.34	88,88,88,88	0
56	MG	1G	1619	1/1	0.86	0.29	89,89,89,89	0
56	MG	45	201	1/1	0.86	0.20	96,96,96,96	0
56	MG	1H	3314	1/1	0.86	0.66	92,92,92,92	0
56	MG	14	3244	1/1	0.86	0.32	74,74,74,74	0
56	MG	1H	3128	1/1	0.86	0.27	83,83,83,83	0
56	MG	14	3079	1/1	0.86	0.42	72,72,72,72	0
56	MG	1H	3043	1/1	0.86	0.51	87,87,87,87	0
56	MG	14	3309	1/1	0.86	0.25	90,90,90,90	0
56	MG	1H	3322	1/1	0.86	0.14	68,68,68,68	0
56	MG	1H	3348	1/1	0.86	0.10	100,100,100,100	0
56	MG	1H	3232	1/1	0.86	0.10	71,71,71,71	0
56	MG	14	3271	1/1	0.86	0.23	74,74,74,74	0
56	MG	1G	1613	1/1	0.86	0.19	100,100,100,100	0
56	MG	1H	3173	1/1	0.86	0.47	79,79,79,79	0
56	MG	14	3210	1/1	0.86	0.38	96,96,96,96	0
56	MG	1G	1659	1/1	0.86	0.82	85,85,85,85	0
56	MG	14	3033	1/1	0.86	0.16	84,84,84,84	0
56	MG	1H	3061	1/1	0.86	0.29	62,62,62,62	0
56	MG	1H	3129	1/1	0.87	0.10	56,56,56,56	0
56	MG	1H	3309	1/1	0.87	0.27	79,79,79,79	0
56	MG	1G	1649	1/1	0.87	0.49	96,96,96,96	0
56	MG	14	3258	1/1	0.87	0.62	99,99,99,99	0
56	MG	L8	101	1/1	0.87	0.66	88,88,88,88	0
56	MG	1G	1663	1/1	0.87	0.18	97,97,97,97	0
56	MG	1H	3190	1/1	0.87	0.48	67,67,67,67	0
56	MG	14	3268	1/1	0.87	0.15	86,86,86,86	0
56	MG	14	3265	1/1	0.87	0.45	89,89,89,89	0
56	MG	14	3178	1/1	0.87	0.85	90,90,90,90	0
56	MG	14	3280	1/1	0.87	0.23	99,99,99,99	0
56	MG	1H	3307	1/1	0.87	0.20	82,82,82,82	0
56	MG	14	3088	1/1	0.87	0.40	73,73,73,73	0
56	MG	14	3288	1/1	0.87	0.34	109,109,109,109	0
56	MG	14	3058	1/1	0.87	0.07	80,80,80,80	0
56	MG	1H	3268	1/1	0.87	0.39	79,79,79,79	0
56	MG	1H	3092	1/1	0.87	0.39	67,67,67,67	0
56	MG	1H	3047	1/1	0.87	0.38	92,92,92,92	0
56	MG	14	3148	1/1	0.87	0.20	72,72,72,72	0
56	MG	13	1638	1/1	0.87	0.47	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1606	1/1	0.87	0.20	82,82,82,82	0
56	MG	1H	3164	1/1	0.87	0.23	73,73,73,73	0
56	MG	14	3235	1/1	0.87	0.43	104,104,104,104	0
56	MG	13	1620	1/1	0.87	0.24	82,82,82,82	0
56	MG	1H	3300	1/1	0.87	0.30	77,77,77,77	0
56	MG	1H	3290	1/1	0.87	0.32	80,80,80,80	0
56	MG	13	1649	1/1	0.87	0.15	75,75,75,75	0
56	MG	1H	3230	1/1	0.87	0.17	73,73,73,73	0
56	MG	1H	3178	1/1	0.87	0.35	74,74,74,74	0
56	MG	1H	3247	1/1	0.88	0.23	73,73,73,73	0
56	MG	1G	1675	1/1	0.88	0.10	116,116,116,116	0
56	MG	14	3274	1/1	0.88	0.27	99,99,99,99	0
56	MG	1H	3303	1/1	0.88	0.25	73,73,73,73	0
56	MG	1G	1626	1/1	0.88	0.23	95,95,95,95	0
56	MG	14	3176	1/1	0.88	0.43	88,88,88,88	0
56	MG	14	3382	1/1	0.88	0.16	100,100,100,100	0
56	MG	14	3037	1/1	0.88	0.33	70,70,70,70	0
56	MG	14	3212	1/1	0.88	0.31	69,69,69,69	0
56	MG	1H	3244	1/1	0.88	0.19	84,84,84,84	0
56	MG	14	3263	1/1	0.88	0.31	82,82,82,82	0
56	MG	1H	3216	1/1	0.88	0.37	80,80,80,80	0
56	MG	14	3179	1/1	0.88	0.85	84,84,84,84	0
56	MG	13	1641	1/1	0.88	0.45	75,75,75,75	0
59	ZN	G8	201	1/1	0.88	0.15	144,144,144,144	0
56	MG	1H	3242	1/1	0.88	0.33	64,64,64,64	0
56	MG	13	1680	1/1	0.88	0.56	87,87,87,87	0
56	MG	1H	3292	1/1	0.88	0.37	61,61,61,61	0
56	MG	14	3151	1/1	0.88	0.72	81,81,81,81	0
56	MG	1H	3152	1/1	0.88	0.56	99,99,99,99	0
56	MG	14	3305	1/1	0.88	0.32	86,86,86,86	0
56	MG	14	3056	1/1	0.88	0.14	62,62,62,62	0
56	MG	13	1658	1/1	0.88	0.09	82,82,82,82	0
56	MG	1G	1661	1/1	0.88	0.23	150,150,150,150	0
56	MG	13	1616	1/1	0.88	0.43	77,77,77,77	0
56	MG	1H	3252	1/1	0.88	0.29	72,72,72,72	0
56	MG	14	3231	1/1	0.88	0.23	84,84,84,84	0
56	MG	14	3238	1/1	0.88	0.36	78,78,78,78	0
56	MG	14	3241	1/1	0.88	0.39	68,68,68,68	0
56	MG	14	3270	1/1	0.88	0.24	84,84,84,84	0
56	MG	1H	3311	1/1	0.88	0.48	96,96,96,96	0
56	MG	14	3068	1/1	0.88	0.34	89,89,89,89	0
56	MG	1G	1642	1/1	0.88	0.30	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3132	1/1	0.89	0.52	78,78,78,78	0
56	MG	1H	3327	1/1	0.89	0.23	95,95,95,95	0
56	MG	1G	1664	1/1	0.89	0.39	119,119,119,119	0
56	MG	1H	3209	1/1	0.89	0.35	82,82,82,82	0
56	MG	16	206	1/1	0.89	0.25	84,84,84,84	0
56	MG	1G	1671	1/1	0.89	0.10	90,90,90,90	0
56	MG	13	1691	1/1	0.89	0.27	109,109,109,109	0
56	MG	14	3253	1/1	0.89	0.39	76,76,76,76	0
56	MG	1H	3142	1/1	0.89	0.18	68,68,68,68	0
56	MG	1H	3225	1/1	0.89	0.37	74,74,74,74	0
56	MG	1H	3159	1/1	0.89	0.43	83,83,83,83	0
56	MG	1H	3266	1/1	0.89	0.09	60,60,60,60	0
56	MG	1H	3267	1/1	0.89	0.20	69,69,69,69	0
56	MG	14	3234	1/1	0.89	0.49	89,89,89,89	0
56	MG	1H	3203	1/1	0.89	0.53	75,75,75,75	0
56	MG	14	3282	1/1	0.89	0.51	84,84,84,84	0
56	MG	14	3158	1/1	0.89	0.18	71,71,71,71	0
56	MG	14	3025	1/1	0.89	0.26	69,69,69,69	0
56	MG	1H	3263	1/1	0.89	0.47	94,94,94,94	0
56	MG	1H	3254	1/1	0.89	0.45	95,95,95,95	0
56	MG	14	3154	1/1	0.89	0.28	90,90,90,90	0
56	MG	1H	3154	1/1	0.89	0.39	69,69,69,69	0
56	MG	14	3007	1/1	0.89	0.64	63,63,63,63	0
56	MG	13	1685	1/1	0.89	0.49	95,95,95,95	0
56	MG	13	1686	1/1	0.89	0.50	73,73,73,73	0
56	MG	14	3208	1/1	0.89	0.16	67,67,67,67	0
56	MG	1H	3272	1/1	0.89	0.14	89,89,89,89	0
56	MG	1H	3218	1/1	0.89	0.22	76,76,76,76	0
56	MG	13	1728	1/1	0.90	0.09	127,127,127,127	0
56	MG	1H	3169	1/1	0.90	0.36	95,95,95,95	0
56	MG	1H	3286	1/1	0.90	0.13	64,64,64,64	0
56	MG	14	3102	1/1	0.90	0.27	76,76,76,76	0
56	MG	1H	3204	1/1	0.90	0.16	100,100,100,100	0
56	MG	1H	3188	1/1	0.90	0.47	76,76,76,76	0
56	MG	14	3119	1/1	0.90	0.26	86,86,86,86	0
56	MG	1H	3137	1/1	0.90	0.15	73,73,73,73	0
56	MG	1H	3325	1/1	0.90	0.30	76,76,76,76	0
56	MG	16	204	1/1	0.90	0.40	98,98,98,98	0
56	MG	13	1628	1/1	0.90	0.34	95,95,95,95	0
56	MG	1H	3050	1/1	0.90	0.36	78,78,78,78	0
56	MG	14	3310	1/1	0.90	0.25	120,120,120,120	0
56	MG	1G	1618	1/1	0.90	0.13	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3102	1/1	0.90	0.33	55,55,55,55	0
56	MG	16	205	1/1	0.90	0.47	84,84,84,84	0
56	MG	1H	3049	1/1	0.90	0.17	65,65,65,65	0
56	MG	14	3161	1/1	0.90	0.46	73,73,73,73	0
56	MG	14	3293	1/1	0.90	0.06	99,99,99,99	0
56	MG	13	1684	1/1	0.90	0.27	114,114,114,114	0
56	MG	C5	201	1/1	0.90	0.27	109,109,109,109	0
56	MG	13	1639	1/1	0.90	0.33	85,85,85,85	0
56	MG	14	3145	1/1	0.90	0.24	67,67,67,67	0
56	MG	1H	3022	1/1	0.90	0.21	52,52,52,52	0
56	MG	13	1632	1/1	0.90	0.50	73,73,73,73	0
56	MG	1H	3283	1/1	0.90	0.24	85,85,85,85	0
56	MG	I8	103	1/1	0.90	0.46	86,86,86,86	0
56	MG	1H	3180	1/1	0.90	0.39	76,76,76,76	0
56	MG	1H	3163	1/1	0.90	0.35	48,48,48,48	0
56	MG	14	3041	1/1	0.90	0.21	49,49,49,49	0
56	MG	14	3199	1/1	0.90	0.33	59,59,59,59	0
56	MG	14	3165	1/1	0.90	0.29	60,60,60,60	0
56	MG	13	1656	1/1	0.91	0.30	88,88,88,88	0
56	MG	14	3039	1/1	0.91	1.32	103,103,103,103	0
56	MG	1G	1625	1/1	0.91	0.60	76,76,76,76	0
56	MG	13	1678	1/1	0.91	0.24	83,83,83,83	0
56	MG	13	1618	1/1	0.91	0.14	97,97,97,97	0
56	MG	13	1673	1/1	0.91	0.12	102,102,102,102	0
56	MG	14	3092	1/1	0.91	0.17	75,75,75,75	0
56	MG	1H	3221	1/1	0.91	0.41	78,78,78,78	0
56	MG	1H	3076	1/1	0.91	0.14	65,65,65,65	0
56	MG	1G	1603	1/1	0.91	0.36	101,101,101,101	0
56	MG	1H	3148	1/1	0.91	0.17	49,49,49,49	0
56	MG	1G	1639	1/1	0.91	0.74	80,80,80,80	0
56	MG	13	1663	1/1	0.91	0.18	75,75,75,75	0
56	MG	13	1644	1/1	0.91	0.28	84,84,84,84	0
56	MG	1G	1632	1/1	0.91	0.49	102,102,102,102	0
56	MG	14	3022	1/1	0.91	0.43	83,83,83,83	0
56	MG	1H	3184	1/1	0.91	0.42	96,96,96,96	0
56	MG	1H	3238	1/1	0.91	0.12	82,82,82,82	0
56	MG	1H	3183	1/1	0.91	0.41	90,90,90,90	0
56	MG	1H	3079	1/1	0.91	0.18	61,61,61,61	0
56	MG	1G	1665	1/1	0.91	0.28	93,93,93,93	0
56	MG	1H	3121	1/1	0.91	0.51	53,53,53,53	0
56	MG	P8	101	1/1	0.91	0.08	78,78,78,78	0
56	MG	13	1697	1/1	0.91	0.45	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3246	1/1	0.91	0.31	72,72,72,72	0
56	MG	1H	3035	1/1	0.91	0.37	76,76,76,76	0
56	MG	14	3069	1/1	0.91	0.74	91,91,91,91	0
56	MG	16	211	1/1	0.91	0.11	85,85,85,85	0
56	MG	14	3076	1/1	0.91	0.43	89,89,89,89	0
56	MG	1H	3187	1/1	0.91	0.38	95,95,95,95	0
56	MG	1H	3231	1/1	0.91	0.31	56,56,56,56	0
56	MG	1G	1652	1/1	0.91	0.15	88,88,88,88	0
56	MG	14	3228	1/1	0.91	0.33	93,93,93,93	0
56	MG	13	1607	1/1	0.91	0.65	85,85,85,85	0
56	MG	14	3256	1/1	0.91	0.60	76,76,76,76	0
56	MG	14	3057	1/1	0.91	0.36	63,63,63,63	0
56	MG	1G	1611	1/1	0.91	0.45	108,108,108,108	0
56	MG	1H	3259	1/1	0.91	0.14	80,80,80,80	0
56	MG	14	3071	1/1	0.91	0.16	84,84,84,84	0
56	MG	14	3087	1/1	0.91	0.34	79,79,79,79	0
56	MG	14	3061	1/1	0.91	0.18	97,97,97,97	0
56	MG	14	3281	1/1	0.91	1.28	89,89,89,89	0
56	MG	14	3159	1/1	0.91	0.44	81,81,81,81	0
56	MG	13	1625	1/1	0.91	0.55	82,82,82,82	0
56	MG	1H	3223	1/1	0.92	0.44	88,88,88,88	0
56	MG	14	3380	1/1	0.92	0.07	83,83,83,83	0
56	MG	1H	3373	1/1	0.92	0.04	82,82,82,82	0
56	MG	14	3013	1/1	0.92	0.20	83,83,83,83	0
56	MG	14	3004	1/1	0.92	0.18	83,83,83,83	0
56	MG	1G	1677	1/1	0.92	0.12	119,119,119,119	0
56	MG	14	3338	1/1	0.92	0.12	111,111,111,111	0
56	MG	1H	3293	1/1	0.92	0.43	98,98,98,98	0
56	MG	1G	1629	1/1	0.92	0.52	104,104,104,104	0
56	MG	14	3083	1/1	0.92	0.37	87,87,87,87	0
56	MG	1H	3098	1/1	0.92	0.20	69,69,69,69	0
56	MG	1G	1682	1/1	0.92	0.14	91,91,91,91	0
56	MG	13	1652	1/1	0.92	0.26	74,74,74,74	0
56	MG	3I	201	1/1	0.92	0.19	62,62,62,62	0
56	MG	1G	1672	1/1	0.92	0.11	121,121,121,121	0
56	MG	1J	201	1/1	0.92	0.30	90,90,90,90	0
56	MG	14	3230	1/1	0.92	0.36	72,72,72,72	0
56	MG	14	3264	1/1	0.92	0.16	92,92,92,92	0
56	MG	14	3295	1/1	0.92	0.21	114,114,114,114	0
56	MG	1H	3054	1/1	0.92	0.20	87,87,87,87	0
56	MG	14	3374	1/1	0.92	0.08	129,129,129,129	0
56	MG	13	1651	1/1	0.92	0.19	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3415	1/1	0.92	0.11	94,94,94,94	0
56	MG	1H	3126	1/1	0.92	0.34	72,72,72,72	0
56	MG	1H	3171	1/1	0.92	0.25	74,74,74,74	0
56	MG	16	201	1/1	0.92	0.21	92,92,92,92	0
56	MG	13	1688	1/1	0.92	0.25	94,94,94,94	0
56	MG	1H	3312	1/1	0.92	0.21	67,67,67,67	0
56	MG	1H	3199	1/1	0.92	0.54	74,74,74,74	0
56	MG	14	3251	1/1	0.92	0.23	106,106,106,106	0
56	MG	13	1650	1/1	0.92	0.34	79,79,79,79	0
56	MG	1H	3024	1/1	0.92	0.46	70,70,70,70	0
56	MG	1G	1614	1/1	0.92	0.28	93,93,93,93	0
56	MG	1H	3027	1/1	0.92	0.35	48,48,48,48	0
56	MG	21	301	1/1	0.92	0.19	57,57,57,57	0
56	MG	1H	3166	1/1	0.92	0.13	68,68,68,68	0
56	MG	1H	3418	1/1	0.92	0.07	88,88,88,88	0
56	MG	1H	3222	1/1	0.92	0.50	79,79,79,79	0
56	MG	1H	3156	1/1	0.92	0.36	77,77,77,77	0
56	MG	14	3285	1/1	0.92	0.56	72,72,72,72	0
56	MG	14	3155	1/1	0.92	0.22	71,71,71,71	0
56	MG	14	3175	1/1	0.92	0.46	96,96,96,96	0
56	MG	1G	1656	1/1	0.92	0.30	138,138,138,138	0
56	MG	1G	1662	1/1	0.92	0.24	133,133,133,133	0
56	MG	1H	3227	1/1	0.92	0.17	50,50,50,50	0
56	MG	13	1643	1/1	0.92	0.30	79,79,79,79	0
56	MG	14	3095	1/1	0.92	0.47	56,56,56,56	0
56	MG	14	3113	1/1	0.92	0.16	78,78,78,78	0
56	MG	14	3242	1/1	0.92	0.32	70,70,70,70	0
56	MG	1H	3153	1/1	0.92	0.16	60,60,60,60	0
56	MG	13	1633	1/1	0.92	0.20	65,65,65,65	0
56	MG	5E	201	1/1	0.92	0.26	84,84,84,84	0
56	MG	14	3020	1/1	0.93	0.48	76,76,76,76	0
56	MG	13	1706	1/1	0.93	0.04	87,87,87,87	0
56	MG	14	3040	1/1	0.93	0.49	84,84,84,84	0
56	MG	13	1720	1/1	0.93	0.16	115,115,115,115	0
56	MG	1H	3077	1/1	0.93	0.11	63,63,63,63	0
56	MG	14	3173	1/1	0.93	0.19	82,82,82,82	0
56	MG	14	3317	1/1	0.93	0.16	64,64,64,64	0
56	MG	1H	3057	1/1	0.93	0.26	52,52,52,52	0
56	MG	88	202	1/1	0.93	0.30	87,87,87,87	0
56	MG	1H	3243	1/1	0.93	0.13	56,56,56,56	0
56	MG	14	3164	1/1	0.93	0.44	83,83,83,83	0
56	MG	1H	3009	1/1	0.93	0.24	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3014	1/1	0.93	0.26	69,69,69,69	0
56	MG	1H	3226	1/1	0.93	0.29	55,55,55,55	0
56	MG	1H	3037	1/1	0.93	0.48	63,63,63,63	0
56	MG	14	3215	1/1	0.93	0.16	83,83,83,83	0
56	MG	1H	3262	1/1	0.93	0.40	77,77,77,77	0
56	MG	14	3106	1/1	0.93	0.81	69,69,69,69	0
56	MG	14	3219	1/1	0.93	0.55	78,78,78,78	0
56	MG	14	3027	1/1	0.93	0.61	71,71,71,71	0
56	MG	14	3218	1/1	0.93	0.35	60,60,60,60	0
56	MG	1H	3313	1/1	0.93	0.32	66,66,66,66	0
56	MG	14	3107	1/1	0.93	0.45	87,87,87,87	0
56	MG	14	3276	1/1	0.93	0.11	102,102,102,102	0
56	MG	13	1683	1/1	0.93	0.28	91,91,91,91	0
56	MG	14	3073	1/1	0.93	0.53	81,81,81,81	0
56	MG	14	3134	1/1	0.93	0.24	74,74,74,74	0
56	MG	1H	3119	1/1	0.93	0.35	78,78,78,78	0
56	MG	14	3029	1/1	0.93	0.15	83,83,83,83	0
56	MG	14	3036	1/1	0.93	0.17	73,73,73,73	0
56	MG	1H	3008	1/1	0.93	0.32	74,74,74,74	0
56	MG	1H	3055	1/1	0.93	0.41	88,88,88,88	0
56	MG	14	3344	1/1	0.93	0.04	95,95,95,95	0
56	MG	1H	3120	1/1	0.93	0.12	41,41,41,41	0
56	MG	14	3300	1/1	0.93	0.58	89,89,89,89	0
56	MG	1H	3005	1/1	0.93	0.22	62,62,62,62	0
56	MG	1H	3251	1/1	0.93	0.24	63,63,63,63	0
56	MG	1H	3106	1/1	0.93	0.41	77,77,77,77	0
56	MG	13	1671	1/1	0.93	0.44	102,102,102,102	0
56	MG	1G	1674	1/1	0.93	0.06	123,123,123,123	0
56	MG	13	1630	1/1	0.94	0.56	71,71,71,71	0
56	MG	1G	1635	1/1	0.94	0.14	93,93,93,93	0
56	MG	14	3341	1/1	0.94	0.10	94,94,94,94	0
56	MG	14	3243	1/1	0.94	0.18	89,89,89,89	0
56	MG	1H	3088	1/1	0.94	0.28	54,54,54,54	0
56	MG	14	3377	1/1	0.94	0.05	60,60,60,60	0
56	MG	1H	3067	1/1	0.94	0.33	63,63,63,63	0
56	MG	14	3081	1/1	0.94	0.39	62,62,62,62	0
56	MG	1H	3323	1/1	0.94	0.50	91,91,91,91	0
56	MG	14	3142	1/1	0.94	0.12	111,111,111,111	0
56	MG	1H	3089	1/1	0.94	0.36	74,74,74,74	0
56	MG	1H	3197	1/1	0.94	0.27	80,80,80,80	0
56	MG	1H	3265	1/1	0.94	0.21	74,74,74,74	0
56	MG	14	3237	1/1	0.94	0.29	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3176	1/1	0.94	0.31	68,68,68,68	0
56	MG	14	3137	1/1	0.94	0.18	62,62,62,62	0
56	MG	1H	3414	1/1	0.94	0.11	83,83,83,83	0
56	MG	13	1731	1/1	0.94	0.12	94,94,94,94	0
56	MG	14	3379	1/1	0.94	0.07	107,107,107,107	0
56	MG	14	3362	1/1	0.94	0.09	77,77,77,77	0
56	MG	1H	3016	1/1	0.94	0.41	48,48,48,48	0
56	MG	1H	3094	1/1	0.94	0.26	91,91,91,91	0
56	MG	14	3189	1/1	0.94	0.41	73,73,73,73	0
56	MG	1G	1680	1/1	0.94	0.06	120,120,120,120	0
56	MG	1H	3113	1/1	0.94	0.20	67,67,67,67	0
56	MG	1G	1623	1/1	0.94	0.48	83,83,83,83	0
56	MG	1G	1655	1/1	0.94	0.07	94,94,94,94	0
56	MG	14	3006	1/1	0.94	0.54	58,58,58,58	0
56	MG	14	3167	1/1	0.94	0.40	99,99,99,99	0
56	MG	1H	3412	1/1	0.94	0.11	68,68,68,68	0
56	MG	1H	3425	1/1	0.94	0.12	92,92,92,92	0
56	MG	14	3201	1/1	0.94	0.28	60,60,60,60	0
56	MG	1H	3376	1/1	0.94	0.07	60,60,60,60	0
56	MG	14	3124	1/1	0.94	0.27	70,70,70,70	0
56	MG	14	3294	1/1	0.94	0.38	74,74,74,74	0
56	MG	1H	3210	1/1	0.94	0.28	73,73,73,73	0
56	MG	1H	3369	1/1	0.94	0.17	69,69,69,69	0
56	MG	14	3125	1/1	0.94	0.37	54,54,54,54	0
56	MG	1H	3115	1/1	0.94	0.34	76,76,76,76	0
56	MG	1H	3191	1/1	0.94	0.29	90,90,90,90	0
56	MG	1H	3310	1/1	0.94	0.22	72,72,72,72	0
56	MG	13	1662	1/1	0.94	0.33	82,82,82,82	0
56	MG	1G	1676	1/1	0.94	0.07	111,111,111,111	0
56	MG	1G	1636	1/1	0.94	0.33	101,101,101,101	0
56	MG	1H	3195	1/1	0.94	0.58	78,78,78,78	0
56	MG	14	3109	1/1	0.94	0.38	72,72,72,72	0
56	MG	14	3184	1/1	0.94	0.46	86,86,86,86	0
56	MG	13	1621	1/1	0.94	0.27	95,95,95,95	0
56	MG	1H	3239	1/1	0.94	0.28	81,81,81,81	0
56	MG	14	3248	1/1	0.94	0.24	94,94,94,94	0
56	MG	14	3185	1/1	0.94	0.20	74,74,74,74	0
56	MG	13	1613	1/1	0.94	0.29	77,77,77,77	0
56	MG	45	203	1/1	0.94	0.35	73,73,73,73	0
56	MG	14	3063	1/1	0.94	0.07	77,77,77,77	0
56	MG	1H	3017	1/1	0.94	0.36	77,77,77,77	0
56	MG	1H	3150	1/1	0.94	0.14	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1622	1/1	0.94	0.34	94,94,94,94	0
56	MG	1H	3179	1/1	0.94	0.23	93,93,93,93	0
56	MG	1H	3306	1/1	0.94	0.43	84,84,84,84	0
56	MG	1H	3411	1/1	0.94	0.05	100,100,100,100	0
56	MG	14	3147	1/1	0.94	0.14	93,93,93,93	0
56	MG	14	3132	1/1	0.94	0.40	91,91,91,91	0
56	MG	1H	3391	1/1	0.94	0.08	107,107,107,107	0
56	MG	1H	3352	1/1	0.94	0.12	71,71,71,71	0
56	MG	1H	3167	1/1	0.95	0.28	81,81,81,81	0
56	MG	1H	3145	1/1	0.95	0.30	77,77,77,77	0
56	MG	1H	3246	1/1	0.95	0.53	88,88,88,88	0
56	MG	14	3225	1/1	0.95	0.14	71,71,71,71	0
56	MG	14	3157	1/1	0.95	0.60	66,66,66,66	0
56	MG	14	3236	1/1	0.95	0.11	79,79,79,79	0
56	MG	13	1713	1/1	0.95	0.09	88,88,88,88	0
56	MG	1H	3133	1/1	0.95	0.32	69,69,69,69	0
56	MG	1H	3023	1/1	0.95	0.40	57,57,57,57	0
56	MG	1G	1634	1/1	0.95	0.39	109,109,109,109	0
56	MG	14	3051	1/1	0.95	0.31	90,90,90,90	0
56	MG	1G	1628	1/1	0.95	0.19	98,98,98,98	0
56	MG	1H	3215	1/1	0.95	0.27	81,81,81,81	0
56	MG	1H	3082	1/1	0.95	0.27	65,65,65,65	0
56	MG	14	3367	1/1	0.95	0.09	94,94,94,94	0
56	MG	1H	3111	1/1	0.95	0.18	60,60,60,60	0
56	MG	1H	3217	1/1	0.95	0.20	67,67,67,67	0
56	MG	14	3360	1/1	0.95	0.13	75,75,75,75	0
56	MG	13	1669	1/1	0.95	0.39	72,72,72,72	0
56	MG	13	1624	1/1	0.95	0.14	71,71,71,71	0
56	MG	13	1682	1/1	0.95	0.14	73,73,73,73	0
56	MG	14	3005	1/1	0.95	0.33	44,44,44,44	0
56	MG	14	3370	1/1	0.95	0.06	99,99,99,99	0
56	MG	1G	1615	1/1	0.95	0.17	119,119,119,119	0
56	MG	14	3287	1/1	0.95	0.63	105,105,105,105	0
56	MG	14	3207	1/1	0.95	0.19	89,89,89,89	0
56	MG	1G	1641	1/1	0.95	0.47	92,92,92,92	0
56	MG	1H	3194	1/1	0.95	0.38	73,73,73,73	0
56	MG	14	3122	1/1	0.95	0.43	91,91,91,91	0
56	MG	14	3038	1/1	0.95	0.23	86,86,86,86	0
56	MG	14	3123	1/1	0.95	0.26	82,82,82,82	0
56	MG	1H	3237	1/1	0.95	0.08	77,77,77,77	0
56	MG	1H	3389	1/1	0.95	0.15	64,64,64,64	0
56	MG	13	1614	1/1	0.95	0.04	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1605	1/1	0.95	0.31	85,85,85,85	0
56	MG	14	3059	1/1	0.95	0.32	55,55,55,55	0
56	MG	1H	3429	1/1	0.95	0.20	66,66,66,66	0
56	MG	1H	3305	1/1	0.95	0.30	68,68,68,68	0
56	MG	1H	3288	1/1	0.95	0.08	94,94,94,94	0
56	MG	1H	3064	1/1	0.95	0.24	54,54,54,54	0
56	MG	13	1617	1/1	0.95	0.33	77,77,77,77	0
56	MG	14	3096	1/1	0.95	0.53	60,60,60,60	0
56	MG	1H	3235	1/1	0.95	0.19	85,85,85,85	0
56	MG	14	3141	1/1	0.95	0.22	90,90,90,90	0
56	MG	1H	3260	1/1	0.95	0.42	88,88,88,88	0
56	MG	14	3002	1/1	0.95	0.38	62,62,62,62	0
56	MG	14	3072	1/1	0.95	0.40	55,55,55,55	0
56	MG	13	1714	1/1	0.95	0.06	104,104,104,104	0
56	MG	13	1710	1/1	0.95	0.09	72,72,72,72	0
56	MG	14	3116	1/1	0.95	0.46	63,63,63,63	0
56	MG	13	1687	1/1	0.95	0.33	76,76,76,76	0
56	MG	1H	3320	1/1	0.95	0.20	68,68,68,68	0
56	MG	3K	101	1/1	0.95	0.13	162,162,162,162	0
56	MG	14	3028	1/1	0.95	0.64	79,79,79,79	0
56	MG	1H	3196	1/1	0.95	0.52	80,80,80,80	0
56	MG	14	3348	1/1	0.95	0.07	83,83,83,83	0
56	MG	14	3009	1/1	0.95	0.37	52,52,52,52	0
56	MG	1G	1678	1/1	0.95	0.09	92,92,92,92	0
56	MG	1H	3172	1/1	0.95	0.27	82,82,82,82	0
56	MG	14	3108	1/1	0.95	0.32	75,75,75,75	0
56	MG	13	1631	1/1	0.95	0.60	93,93,93,93	0
56	MG	14	3021	1/1	0.95	0.36	78,78,78,78	0
56	MG	13	1668	1/1	0.95	0.19	80,80,80,80	0
56	MG	1H	3406	1/1	0.95	0.14	65,65,65,65	0
56	MG	1H	3070	1/1	0.95	0.34	50,50,50,50	0
56	MG	1H	3334	1/1	0.95	0.08	51,51,51,51	0
56	MG	13	1659	1/1	0.96	0.11	87,87,87,87	0
57	PAR	1G	1681	42/42	0.96	0.16	79,90,98,101	0
56	MG	14	3226	1/1	0.96	0.17	72,72,72,72	0
56	MG	1H	3177	1/1	0.96	0.23	82,82,82,82	0
56	MG	1H	3021	1/1	0.96	0.24	57,57,57,57	0
56	MG	14	3136	1/1	0.96	0.26	62,62,62,62	0
56	MG	1G	1660	1/1	0.96	0.46	97,97,97,97	0
56	MG	14	3103	1/1	0.96	0.33	66,66,66,66	0
56	MG	1H	3058	1/1	0.96	0.20	62,62,62,62	0
56	MG	1H	3398	1/1	0.96	0.09	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1665	1/1	0.96	0.30	64,64,64,64	0
56	MG	1H	3131	1/1	0.96	0.21	62,62,62,62	0
56	MG	1H	3233	1/1	0.96	0.11	50,50,50,50	0
56	MG	1H	3091	1/1	0.96	0.10	61,61,61,61	0
56	MG	1H	3130	1/1	0.96	0.17	60,60,60,60	0
56	MG	14	3340	1/1	0.96	0.10	83,83,83,83	0
56	MG	1J	205	1/1	0.96	0.07	109,109,109,109	0
56	MG	1H	3059	1/1	0.96	0.29	48,48,48,48	0
56	MG	14	3086	1/1	0.96	0.64	82,82,82,82	0
59	ZN	C5	202	1/1	0.96	0.10	165,165,165,165	0
56	MG	1H	3116	1/1	0.96	0.17	56,56,56,56	0
56	MG	14	3355	1/1	0.96	0.05	92,92,92,92	0
56	MG	1H	3080	1/1	0.96	0.18	86,86,86,86	0
56	MG	14	3054	1/1	0.96	0.17	83,83,83,83	0
56	MG	14	3316	1/1	0.96	0.07	67,67,67,67	0
56	MG	14	3152	1/1	0.96	0.15	91,91,91,91	0
56	MG	14	3195	1/1	0.96	0.10	107,107,107,107	0
56	MG	1H	3165	1/1	0.96	0.42	79,79,79,79	0
56	MG	1H	3285	1/1	0.96	0.33	72,72,72,72	0
56	MG	13	1640	1/1	0.96	0.15	91,91,91,91	0
56	MG	1H	3118	1/1	0.96	0.14	61,61,61,61	0
56	MG	13	1612	1/1	0.96	0.24	79,79,79,79	0
56	MG	1H	3228	1/1	0.96	0.16	57,57,57,57	0
56	MG	13	1667	1/1	0.96	0.09	85,85,85,85	0
56	MG	1H	3328	1/1	0.96	0.10	52,52,52,52	0
56	MG	1H	3065	1/1	0.96	0.33	55,55,55,55	0
56	MG	1H	3069	1/1	0.96	0.20	60,60,60,60	0
56	MG	1G	1631	1/1	0.96	0.36	91,91,91,91	0
56	MG	14	3121	1/1	0.96	0.32	84,84,84,84	0
56	MG	14	3376	1/1	0.96	0.13	90,90,90,90	0
56	MG	1G	1612	1/1	0.96	0.41	93,93,93,93	0
56	MG	1H	3036	1/1	0.96	0.38	77,77,77,77	0
56	MG	1H	3379	1/1	0.96	0.10	61,61,61,61	0
56	MG	14	3307	1/1	0.96	0.30	108,108,108,108	0
56	MG	1H	3351	1/1	0.96	0.09	73,73,73,73	0
56	MG	1H	3294	1/1	0.96	0.51	71,71,71,71	0
56	MG	13	1723	1/1	0.96	0.10	73,73,73,73	0
56	MG	1H	3012	1/1	0.96	0.31	79,79,79,79	0
56	MG	1H	3068	1/1	0.96	0.30	56,56,56,56	0
56	MG	14	3342	1/1	0.96	0.08	94,94,94,94	0
56	MG	14	3172	1/1	0.96	0.14	98,98,98,98	0
56	MG	14	3174	1/1	0.96	0.35	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3361	1/1	0.96	0.13	82,82,82,82	0
56	MG	1H	3122	1/1	0.96	0.20	50,50,50,50	0
56	MG	14	3085	1/1	0.96	0.39	51,51,51,51	0
56	MG	1H	3144	1/1	0.96	0.18	54,54,54,54	0
56	MG	13	1611	1/1	0.96	0.34	61,61,61,61	0
56	MG	14	3213	1/1	0.96	0.26	89,89,89,89	0
56	MG	1G	1650	1/1	0.96	0.20	91,91,91,91	0
56	MG	13	1670	1/1	0.96	0.23	95,95,95,95	0
56	MG	1H	3234	1/1	0.96	0.22	99,99,99,99	0
56	MG	1H	3086	1/1	0.96	0.40	41,41,41,41	0
56	MG	1H	3087	1/1	0.96	0.17	65,65,65,65	0
56	MG	1H	3136	1/1	0.96	0.10	68,68,68,68	0
56	MG	1G	1657	1/1	0.96	0.58	90,90,90,90	0
56	MG	14	3332	1/1	0.96	0.15	64,64,64,64	0
56	MG	1H	3146	1/1	0.96	0.27	59,59,59,59	0
56	MG	14	3267	1/1	0.96	0.21	66,66,66,66	0
56	MG	14	3034	1/1	0.96	0.62	74,74,74,74	0
56	MG	13	1609	1/1	0.96	0.22	73,73,73,73	0
56	MG	14	3336	1/1	0.96	0.06	77,77,77,77	0
56	MG	14	3194	1/1	0.96	0.51	86,86,86,86	0
56	MG	1H	3033	1/1	0.96	0.18	68,68,68,68	0
56	MG	1H	3101	1/1	0.96	0.27	64,64,64,64	0
56	MG	14	3356	1/1	0.96	0.04	98,98,98,98	0
56	MG	13	1711	1/1	0.96	0.12	92,92,92,92	0
56	MG	1H	3117	1/1	0.96	0.17	82,82,82,82	0
56	MG	14	3190	1/1	0.96	0.28	95,95,95,95	0
56	MG	1H	3208	1/1	0.96	0.36	63,63,63,63	0
56	MG	1H	3026	1/1	0.96	0.59	50,50,50,50	0
56	MG	14	3052	1/1	0.96	0.27	71,71,71,71	0
56	MG	14	3204	1/1	0.96	0.36	82,82,82,82	0
56	MG	1G	1617	1/1	0.96	0.15	125,125,125,125	0
56	MG	16	208	1/1	0.96	0.27	82,82,82,82	0
56	MG	1H	3168	1/1	0.96	0.17	65,65,65,65	0
56	MG	1H	3020	1/1	0.96	0.24	60,60,60,60	0
56	MG	1H	3408	1/1	0.96	0.06	80,80,80,80	0
56	MG	13	1675	1/1	0.96	0.22	124,124,124,124	0
56	MG	14	3371	1/1	0.96	0.08	72,72,72,72	0
56	MG	1G	1610	1/1	0.96	0.28	102,102,102,102	0
56	MG	14	3286	1/1	0.96	0.39	83,83,83,83	0
56	MG	1H	3409	1/1	0.96	0.05	86,86,86,86	0
56	MG	14	3118	1/1	0.96	0.11	66,66,66,66	0
56	MG	1H	3056	1/1	0.96	0.14	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1635	1/1	0.96	0.18	54,54,54,54	0
56	MG	14	3369	1/1	0.97	0.06	84,84,84,84	0
56	MG	1H	3363	1/1	0.97	0.04	69,69,69,69	0
56	MG	14	3365	1/1	0.97	0.07	88,88,88,88	0
56	MG	1H	3103	1/1	0.97	0.24	51,51,51,51	0
56	MG	1H	3335	1/1	0.97	0.07	50,50,50,50	0
56	MG	13	1703	1/1	0.97	0.15	70,70,70,70	0
56	MG	1H	3387	1/1	0.97	0.10	72,72,72,72	0
56	MG	1H	3081	1/1	0.97	0.42	85,85,85,85	0
56	MG	14	3375	1/1	0.97	0.07	111,111,111,111	0
56	MG	14	3171	1/1	0.97	0.27	56,56,56,56	0
56	MG	1G	1658	1/1	0.97	0.11	124,124,124,124	0
56	MG	14	3366	1/1	0.97	0.11	92,92,92,92	0
56	MG	1H	3114	1/1	0.97	0.26	67,67,67,67	0
56	MG	1G	1653	1/1	0.97	0.27	85,85,85,85	0
56	MG	14	3182	1/1	0.97	0.40	73,73,73,73	0
56	MG	14	3314	1/1	0.97	0.07	73,73,73,73	0
56	MG	1H	3051	1/1	0.97	0.24	84,84,84,84	0
56	MG	14	3078	1/1	0.97	0.25	64,64,64,64	0
56	MG	1H	3085	1/1	0.97	0.40	82,82,82,82	0
56	MG	1H	3100	1/1	0.97	0.22	56,56,56,56	0
56	MG	14	3049	1/1	0.97	0.21	58,58,58,58	0
56	MG	13	1727	1/1	0.97	0.07	115,115,115,115	0
56	MG	14	3359	1/1	0.97	0.10	55,55,55,55	0
56	MG	13	1724	1/1	0.97	0.05	108,108,108,108	0
56	MG	14	3217	1/1	0.97	0.29	87,87,87,87	0
56	MG	13	1729	1/1	0.97	0.11	103,103,103,103	0
56	MG	1H	3104	1/1	0.97	0.30	71,71,71,71	0
56	MG	14	3139	1/1	0.97	0.33	93,93,93,93	0
56	MG	14	3319	1/1	0.97	0.06	62,62,62,62	0
56	MG	1G	1648	1/1	0.97	0.48	78,78,78,78	0
56	MG	13	1725	1/1	0.97	0.10	102,102,102,102	0
56	MG	14	3345	1/1	0.97	0.12	118,118,118,118	0
56	MG	14	3200	1/1	0.97	0.26	67,67,67,67	0
56	MG	1H	3405	1/1	0.97	0.09	52,52,52,52	0
56	MG	14	3131	1/1	0.97	0.46	76,76,76,76	0
56	MG	1H	3229	1/1	0.97	0.12	45,45,45,45	0
56	MG	13	1610	1/1	0.97	0.19	72,72,72,72	0
56	MG	13	1615	1/1	0.97	0.18	85,85,85,85	0
56	MG	1H	3006	1/1	0.97	0.18	61,61,61,61	0
56	MG	1H	3390	1/1	0.97	0.05	88,88,88,88	0
56	MG	14	3223	1/1	0.97	0.20	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3279	1/1	0.97	0.09	51,51,51,51	0
56	MG	1H	3002	1/1	0.97	0.32	49,49,49,49	0
56	MG	1H	3420	1/1	0.97	0.09	76,76,76,76	0
56	MG	1H	3397	1/1	0.97	0.07	71,71,71,71	0
56	MG	14	3084	1/1	0.97	0.26	73,73,73,73	0
56	MG	1H	3181	1/1	0.97	0.10	74,74,74,74	0
56	MG	14	3128	1/1	0.97	0.18	73,73,73,73	0
56	MG	14	3097	1/1	0.97	0.28	74,74,74,74	0
56	MG	1H	3421	1/1	0.97	0.09	83,83,83,83	0
56	MG	13	1721	1/1	0.97	0.07	79,79,79,79	0
57	PAR	13	1730	42/42	0.97	0.19	67,77,86,91	0
56	MG	14	3030	1/1	0.97	0.49	87,87,87,87	0
56	MG	1H	3424	1/1	0.97	0.07	89,89,89,89	0
56	MG	14	3050	1/1	0.97	0.30	73,73,73,73	0
56	MG	1H	3003	1/1	0.97	0.22	54,54,54,54	0
56	MG	13	1645	1/1	0.97	0.28	66,66,66,66	0
56	MG	I8	101	1/1	0.97	0.05	59,59,59,59	0
56	MG	14	3115	1/1	0.97	0.34	66,66,66,66	0
56	MG	13	1709	1/1	0.97	0.10	94,94,94,94	0
56	MG	14	3008	1/1	0.97	0.57	65,65,65,65	0
56	MG	1H	3384	1/1	0.97	0.11	109,109,109,109	0
56	MG	1G	1601	1/1	0.97	0.28	96,96,96,96	0
56	MG	14	3339	1/1	0.97	0.12	64,64,64,64	0
56	MG	14	3011	1/1	0.97	0.55	58,58,58,58	0
56	MG	1H	3380	1/1	0.97	0.13	70,70,70,70	0
56	MG	13	1679	1/1	0.97	0.24	107,107,107,107	0
56	MG	13	1606	1/1	0.97	0.22	115,115,115,115	0
56	MG	1H	3428	1/1	0.97	0.19	54,54,54,54	0
56	MG	1H	3074	1/1	0.97	0.20	69,69,69,69	0
56	MG	13	1653	1/1	0.97	0.17	89,89,89,89	0
56	MG	14	3093	1/1	0.97	0.43	85,85,85,85	0
56	MG	14	3046	1/1	0.97	0.33	66,66,66,66	0
56	MG	1H	3378	1/1	0.97	0.10	68,68,68,68	0
56	MG	14	3077	1/1	0.97	0.18	60,60,60,60	0
56	MG	1H	3386	1/1	0.97	0.08	52,52,52,52	0
59	ZN	5A	101	1/1	0.97	0.12	139,139,139,139	0
56	MG	14	3373	1/1	0.97	0.08	87,87,87,87	0
56	MG	1H	3095	1/1	0.97	0.18	73,73,73,73	0
56	MG	16	209	1/1	0.97	0.14	64,64,64,64	0
56	MG	1G	1604	1/1	0.97	0.36	97,97,97,97	0
56	MG	1H	3073	1/1	0.97	0.19	47,47,47,47	0
56	MG	1H	3030	1/1	0.97	0.33	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1657	1/1	0.97	0.13	80,80,80,80	0
56	MG	1J	204	1/1	0.97	0.09	99,99,99,99	0
56	MG	14	3099	1/1	0.97	0.31	62,62,62,62	0
56	MG	1H	3255	1/1	0.97	0.10	81,81,81,81	0
56	MG	14	3206	1/1	0.97	0.39	82,82,82,82	0
56	MG	1H	3350	1/1	0.97	0.17	72,72,72,72	0
56	MG	1H	3078	1/1	0.97	0.19	57,57,57,57	0
56	MG	14	3082	1/1	0.97	0.44	63,63,63,63	0
56	MG	1H	3413	1/1	0.97	0.05	107,107,107,107	0
56	MG	1H	3324	1/1	0.97	0.32	69,69,69,69	0
56	MG	13	1708	1/1	0.97	0.12	85,85,85,85	0
56	MG	1H	3097	1/1	0.97	0.16	103,103,103,103	0
56	MG	1H	3422	1/1	0.97	0.09	100,100,100,100	0
56	MG	1H	3343	1/1	0.97	0.07	65,65,65,65	0
56	MG	14	3105	1/1	0.97	0.24	52,52,52,52	0
56	MG	14	3067	1/1	0.97	0.21	74,74,74,74	0
56	MG	14	3306	1/1	0.97	0.20	110,110,110,110	0
56	MG	1H	3048	1/1	0.97	0.43	92,92,92,92	0
56	MG	14	3138	1/1	0.97	0.31	55,55,55,55	0
56	MG	1H	3329	1/1	0.97	0.06	59,59,59,59	0
56	MG	14	3135	1/1	0.98	0.19	78,78,78,78	0
56	MG	14	3066	1/1	0.98	0.13	72,72,72,72	0
56	MG	1H	3063	1/1	0.98	0.24	55,55,55,55	0
56	MG	13	1717	1/1	0.98	0.10	74,74,74,74	0
56	MG	1G	1624	1/1	0.98	0.43	76,76,76,76	0
56	MG	14	3325	1/1	0.98	0.11	76,76,76,76	0
56	MG	1H	3404	1/1	0.98	0.07	64,64,64,64	0
56	MG	14	3089	1/1	0.98	0.47	54,54,54,54	0
56	MG	14	3318	1/1	0.98	0.19	71,71,71,71	0
56	MG	1H	3261	1/1	0.98	0.23	90,90,90,90	0
56	MG	1G	1669	1/1	0.98	0.10	82,82,82,82	0
56	MG	1G	1621	1/1	0.98	0.55	61,61,61,61	0
56	MG	1H	3394	1/1	0.98	0.05	60,60,60,60	0
56	MG	1H	3383	1/1	0.98	0.08	65,65,65,65	0
56	MG	14	3337	1/1	0.98	0.13	79,79,79,79	0
59	ZN	5I	102	1/1	0.98	0.13	99,99,99,99	0
56	MG	14	3320	1/1	0.98	0.07	84,84,84,84	0
56	MG	1H	3416	1/1	0.98	0.17	104,104,104,104	0
56	MG	14	3361	1/1	0.98	0.07	60,60,60,60	0
56	MG	1H	3337	1/1	0.98	0.13	55,55,55,55	0
56	MG	14	3333	1/1	0.98	0.12	79,79,79,79	0
56	MG	1H	3388	1/1	0.98	0.11	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3044	1/1	0.98	0.45	68,68,68,68	0
56	MG	1H	3071	1/1	0.98	0.16	56,56,56,56	0
56	MG	14	3364	1/1	0.98	0.06	73,73,73,73	0
56	MG	14	3074	1/1	0.98	0.26	45,45,45,45	0
56	MG	14	3315	1/1	0.98	0.04	71,71,71,71	0
56	MG	14	3080	1/1	0.98	0.29	67,67,67,67	0
56	MG	1H	3396	1/1	0.98	0.09	58,58,58,58	0
56	MG	14	3350	1/1	0.98	0.12	76,76,76,76	0
56	MG	13	1707	1/1	0.98	0.11	85,85,85,85	0
56	MG	1H	3331	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3357	1/1	0.98	0.12	58,58,58,58	0
56	MG	1H	3367	1/1	0.98	0.07	71,71,71,71	0
56	MG	1H	3407	1/1	0.98	0.11	86,86,86,86	0
56	MG	1H	3419	1/1	0.98	0.07	73,73,73,73	0
56	MG	1H	3256	1/1	0.98	0.24	76,76,76,76	0
56	MG	1H	3427	1/1	0.98	0.10	84,84,84,84	0
56	MG	14	3129	1/1	0.98	0.39	58,58,58,58	0
56	MG	29	301	1/1	0.98	0.27	63,63,63,63	0
56	MG	1H	3345	1/1	0.98	0.10	58,58,58,58	0
56	MG	1H	3174	1/1	0.98	0.35	85,85,85,85	0
56	MG	14	3335	1/1	0.98	0.07	63,63,63,63	0
56	MG	1H	3400	1/1	0.98	0.06	52,52,52,52	0
56	MG	1H	3365	1/1	0.98	0.05	54,54,54,54	0
56	MG	1H	3060	1/1	0.98	0.34	52,52,52,52	0
56	MG	1H	3395	1/1	0.98	0.04	74,74,74,74	0
56	MG	14	3010	1/1	0.98	0.44	54,54,54,54	0
56	MG	14	3349	1/1	0.98	0.04	90,90,90,90	0
56	MG	1G	1667	1/1	0.98	0.39	100,100,100,100	0
56	MG	14	3104	1/1	0.98	0.26	64,64,64,64	0
56	MG	1H	3382	1/1	0.98	0.10	60,60,60,60	0
56	MG	1H	3354	1/1	0.98	0.17	65,65,65,65	0
56	MG	1H	3001	1/1	0.98	0.32	53,53,53,53	0
56	MG	1H	3127	1/1	0.98	0.28	53,53,53,53	0
56	MG	14	3001	1/1	0.98	0.15	51,51,51,51	0
56	MG	14	3354	1/1	0.98	0.14	87,87,87,87	0
56	MG	1H	3158	1/1	0.98	0.41	68,68,68,68	0
56	MG	1H	3399	1/1	0.98	0.05	91,91,91,91	0
56	MG	1H	3072	1/1	0.98	0.47	72,72,72,72	0
56	MG	14	3014	1/1	0.98	0.43	49,49,49,49	0
56	MG	1H	3370	1/1	0.98	0.09	76,76,76,76	0
56	MG	14	3343	1/1	0.98	0.09	71,71,71,71	0
56	MG	1H	3344	1/1	0.98	0.13	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3330	1/1	0.98	0.10	60,60,60,60	0
56	MG	1H	3253	1/1	0.98	0.16	60,60,60,60	0
56	MG	14	3100	1/1	0.98	0.24	91,91,91,91	0
56	MG	14	3322	1/1	0.98	0.03	72,72,72,72	0
56	MG	1H	3368	1/1	0.98	0.08	57,57,57,57	0
56	MG	13	1722	1/1	0.98	0.05	93,93,93,93	0
56	MG	13	1705	1/1	0.98	0.09	94,94,94,94	0
56	MG	14	3334	1/1	0.98	0.06	85,85,85,85	0
56	MG	1H	3004	1/1	0.98	0.26	41,41,41,41	0
56	MG	1H	3360	1/1	0.98	0.09	57,57,57,57	0
56	MG	13	1626	1/1	0.98	0.35	87,87,87,87	0
56	MG	1H	3341	1/1	0.98	0.10	57,57,57,57	0
56	MG	1H	3007	1/1	0.98	0.21	80,80,80,80	0
56	MG	14	3372	1/1	0.98	0.09	87,87,87,87	0
56	MG	1H	3338	1/1	0.98	0.11	59,59,59,59	0
56	MG	13	1660	1/1	0.98	0.51	81,81,81,81	0
56	MG	1H	3010	1/1	0.98	0.35	57,57,57,57	0
56	MG	13	1704	1/1	0.98	0.07	85,85,85,85	0
56	MG	13	1732	1/1	0.98	0.14	65,65,65,65	0
56	MG	13	1715	1/1	0.98	0.07	100,100,100,100	0
56	MG	1H	3347	1/1	0.98	0.07	78,78,78,78	0
56	MG	14	3053	1/1	0.98	0.36	61,61,61,61	0
56	MG	14	3016	1/1	0.98	0.30	60,60,60,60	0
56	MG	13	1634	1/1	0.98	0.26	53,53,53,53	0
56	MG	14	3098	1/1	0.98	0.33	68,68,68,68	0
56	MG	1H	3392	1/1	0.98	0.14	71,71,71,71	0
56	MG	1H	3374	1/1	0.98	0.09	88,88,88,88	0
56	MG	1G	1673	1/1	0.98	0.12	85,85,85,85	0
56	MG	14	3352	1/1	0.98	0.11	78,78,78,78	0
56	MG	14	3065	1/1	0.98	0.13	68,68,68,68	0
56	MG	14	3313	1/1	0.98	0.16	64,64,64,64	0
56	MG	2L	101	1/1	0.98	0.41	72,72,72,72	0
56	MG	14	3048	1/1	0.99	0.48	55,55,55,55	0
56	MG	14	3329	1/1	0.99	0.08	55,55,55,55	0
56	MG	1H	3385	1/1	0.99	0.12	78,78,78,78	0
56	MG	1H	3090	1/1	0.99	0.41	72,72,72,72	0
56	MG	1H	3358	1/1	0.99	0.17	68,68,68,68	0
56	MG	1H	3105	1/1	0.99	0.26	64,64,64,64	0
56	MG	13	1719	1/1	0.99	0.13	86,86,86,86	0
56	MG	14	3363	1/1	0.99	0.11	51,51,51,51	0
56	MG	1H	3372	1/1	0.99	0.13	53,53,53,53	0
56	MG	14	3209	1/1	0.99	0.20	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3402	1/1	0.99	0.08	60,60,60,60	0
56	MG	14	3321	1/1	0.99	0.07	73,73,73,73	0
56	MG	1H	3356	1/1	0.99	0.08	61,61,61,61	0
56	MG	1H	3031	1/1	0.99	0.29	65,65,65,65	0
56	MG	14	3045	1/1	0.99	0.30	64,64,64,64	0
56	MG	13	1716	1/1	0.99	0.09	88,88,88,88	0
56	MG	14	3347	1/1	0.99	0.13	77,77,77,77	0
56	MG	1H	3377	1/1	0.99	0.11	77,77,77,77	0
56	MG	14	3378	1/1	0.99	0.07	62,62,62,62	0
56	MG	1H	3364	1/1	0.99	0.15	56,56,56,56	0
56	MG	14	3330	1/1	0.99	0.11	65,65,65,65	0
58	SF4	3E	302	8/8	0.99	0.18	76,86,96,96	0
56	MG	14	3358	1/1	0.99	0.12	64,64,64,64	0
56	MG	14	3328	1/1	0.99	0.07	64,64,64,64	0
56	MG	14	3323	1/1	0.99	0.14	66,66,66,66	0
56	MG	14	3326	1/1	0.99	0.13	61,61,61,61	0
56	MG	1H	3108	1/1	0.99	0.28	62,62,62,62	0
56	MG	1H	3342	1/1	0.99	0.06	59,59,59,59	0
56	MG	14	3112	1/1	0.99	0.20	61,61,61,61	0
56	MG	14	3094	1/1	0.99	0.32	82,82,82,82	0
56	MG	1H	3410	1/1	0.99	0.12	53,53,53,53	0
56	MG	14	3346	1/1	0.99	0.10	64,64,64,64	0
56	MG	1H	3403	1/1	0.99	0.06	61,61,61,61	0
56	MG	14	3368	1/1	0.99	0.17	49,49,49,49	0
56	MG	1H	3139	1/1	0.99	0.32	64,64,64,64	0
56	MG	14	3311	1/1	0.99	0.22	83,83,83,83	0
56	MG	14	3043	1/1	0.99	0.36	52,52,52,52	0
56	MG	2K	103	1/1	0.99	0.28	71,71,71,71	0
56	MG	13	1726	1/1	0.99	0.04	82,82,82,82	0
56	MG	1G	1608	1/1	0.99	0.11	101,101,101,101	0
56	MG	1H	3062	1/1	0.99	0.19	54,54,54,54	0
56	MG	14	3357	1/1	0.99	0.06	77,77,77,77	0
56	MG	13	1601	1/1	0.99	0.25	59,59,59,59	0
56	MG	14	3090	1/1	0.99	0.31	70,70,70,70	0
56	MG	1H	3332	1/1	0.99	0.13	66,66,66,66	0
56	MG	1G	1607	1/1	0.99	0.27	77,77,77,77	0
56	MG	1H	3359	1/1	0.99	0.22	66,66,66,66	0
56	MG	13	1718	1/1	0.99	0.05	67,67,67,67	0
56	MG	1H	3375	1/1	0.99	0.10	67,67,67,67	0
56	MG	1H	3340	1/1	0.99	0.10	58,58,58,58	0
56	MG	1H	3381	1/1	0.99	0.12	59,59,59,59	0
56	MG	1H	3353	1/1	0.99	0.10	53,53,53,53	0

Continued on next page...

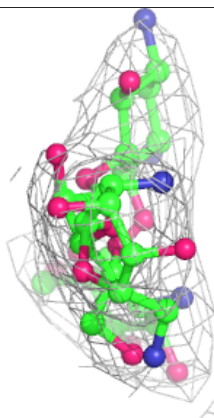
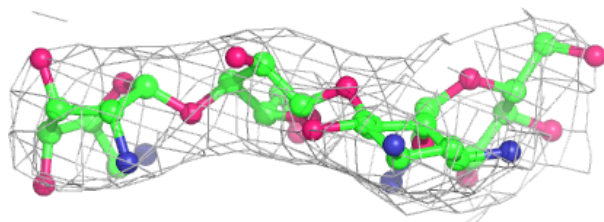
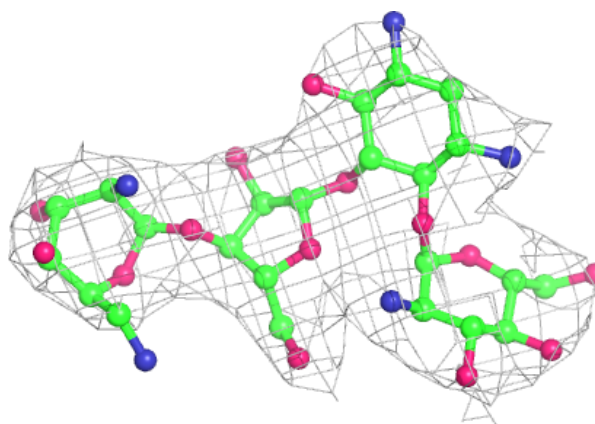
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1712	1/1	0.99	0.11	78,78,78,78	0
56	MG	1H	3245	1/1	0.99	0.29	74,74,74,74	0
56	MG	1H	3393	1/1	0.99	0.07	70,70,70,70	0
56	MG	88	201	1/1	0.99	0.19	81,81,81,81	0
56	MG	1H	3355	1/1	0.99	0.10	58,58,58,58	0
56	MG	14	3047	1/1	0.99	0.25	57,57,57,57	0
56	MG	1H	3339	1/1	0.99	0.05	70,70,70,70	0
56	MG	1H	3401	1/1	0.99	0.05	55,55,55,55	0
58	SF4	32	301	8/8	0.99	0.18	92,113,120,129	0
56	MG	1H	3333	1/1	0.99	0.09	63,63,63,63	0
56	MG	1H	3426	1/1	0.99	0.07	54,54,54,54	0
56	MG	1H	3109	1/1	0.99	0.18	59,59,59,59	0
56	MG	16	210	1/1	0.99	0.17	81,81,81,81	0
56	MG	1H	3336	1/1	0.99	0.07	49,49,49,49	0
56	MG	1H	3371	1/1	0.99	0.09	63,63,63,63	0
56	MG	14	3312	1/1	0.99	0.18	70,70,70,70	0
56	MG	13	1602	1/1	0.99	0.38	89,89,89,89	0
56	MG	1H	3362	1/1	0.99	0.10	64,64,64,64	0
56	MG	14	3351	1/1	0.99	0.14	65,65,65,65	0
56	MG	14	3327	1/1	0.99	0.11	84,84,84,84	0
56	MG	14	3331	1/1	0.99	0.06	63,63,63,63	0
56	MG	1H	3417	1/1	0.99	0.07	62,62,62,62	0
56	MG	13	1619	1/1	0.99	0.32	69,69,69,69	0
56	MG	14	3160	1/1	0.99	0.44	57,57,57,57	0
56	MG	14	3042	1/1	0.99	0.28	58,58,58,58	0
56	MG	1H	3066	1/1	1.00	0.16	48,48,48,48	0
56	MG	1H	3346	1/1	1.00	0.07	63,63,63,63	0
56	MG	14	3353	1/1	1.00	0.15	69,69,69,69	0
56	MG	14	3324	1/1	1.00	0.14	77,77,77,77	0
56	MG	1G	1670	1/1	1.00	0.11	88,88,88,88	0
56	MG	1H	3366	1/1	1.00	0.08	59,59,59,59	0
56	MG	1H	3349	1/1	1.00	0.09	74,74,74,74	0

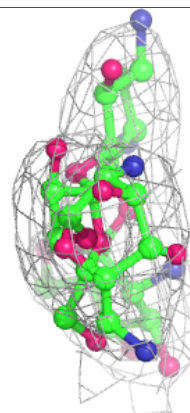
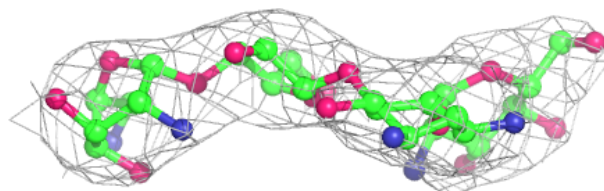
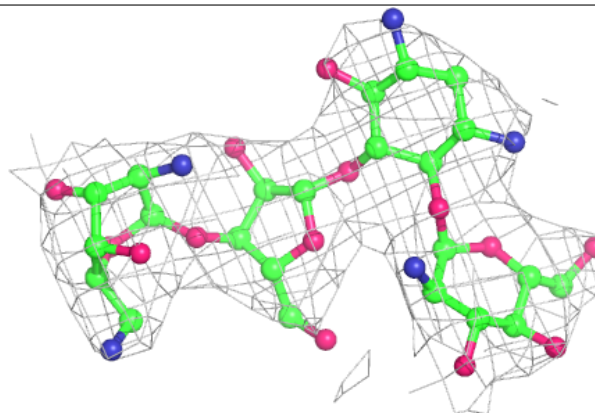
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR 1G 1681:

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

**Electron density around PAR 13 1730:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.