



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 08:45 pm GMT

PDB ID : 5EL6  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA<sup>Lys</sup> 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

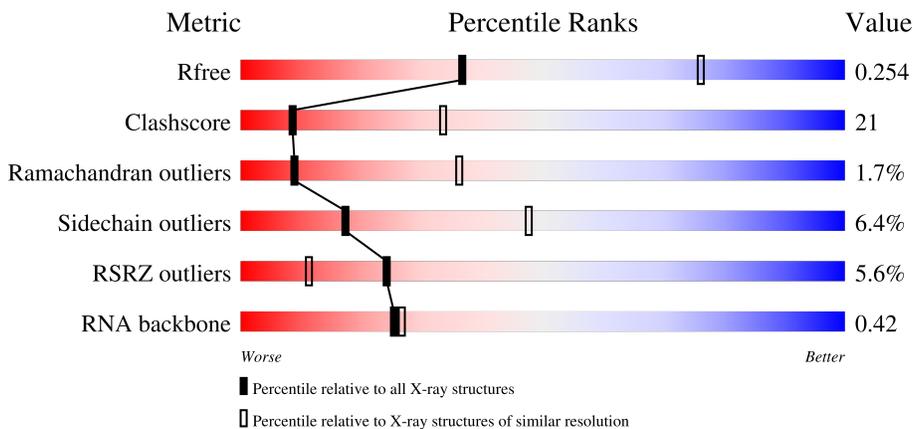
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	 5% 27% 42% 24%
1	1G	1522	 5% 23% 47% 26%
2	12	256	 5% 5% 43% 33% 18%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1E	256	38% 45% 8% 10%
3	22	239	12% 38% 41% 18%
3	2E	239	18% 48% 35% 14%
4	32	209	5% 37% 56% 7%
4	3E	209	4% 46% 45% 8%
5	42	162	3% 38% 49% 9%
5	4E	162	2% 47% 43% 8%
6	52	101	12% 63% 34%
6	5E	101	5% 55% 42% ...
7	62	156	15% 47% 39% 12%
7	6E	156	10% 58% 38% ..
8	72	138	7% 46% 49% ..
8	7E	138	4% 46% 50% ..
9	82	128	34% 51% 9% 5%
9	8E	128	% 41% 51% 6%
10	1A	105	2% 31% 38% 7% 24%
10	1I	105	7% 47% 35% 5% 13%
11	2A	129	50% 52% 34% 12%
11	2I	129	21% 46% 39% 14%
12	3A	132	15% 46% 39% 8% 8%
12	3I	132	14% 48% 39% 5% 8%
13	4A	126	% 31% 50% 7% 12%
13	4I	126	40% 50% 6%
14	5A	61	18% 38% 51% 7% ..
14	5I	61	57% 34% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6A	89	3% 54% 42% ..
15	6I	89	3% 46% 47% . .
16	7A	88	% 53% 41% . 5%
16	7I	88	47% 44% . 6%
17	8A	105	13% 53% 40% . 6%
17	8I	105	10% 48% 45% . 5%
18	9A	88	6% 49% 26% . 24%
18	9I	88	42% 33% . 23%
19	AA	93	2% 27% 32% 8% 33%
19	AI	93	41% 43% . 12%
20	BA	106	17% 48% 41% 5% 7%
20	BI	106	7% 36% 53% .. 8%
21	1B	27	33% 48% 19%
21	1F	27	22% 56% 7% 15%
22	1K	76	4% 16% 34% 30% 11% 9%
22	1L	76	3% 9% 53% 28% 7% .
23	2K	77	26% 47% 22% 5%
23	2L	77	% 25% 43% 23% 9%
24	3K	76	7% 11% 25% 53% 12%
24	3L	76	3% 20% 42% 32% 7%
25	4K	27	4% 15% 37% 19% . 26%
25	4L	27	15% 15% 33% . 33%
26	14	2912	% 21% 43% 27% 7% .
26	1H	2912	15% 40% 33% 8% .
27	16	122	31% 42% 21% 6%

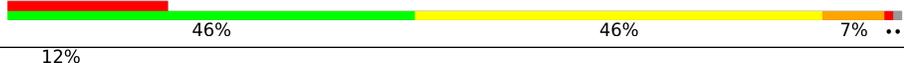
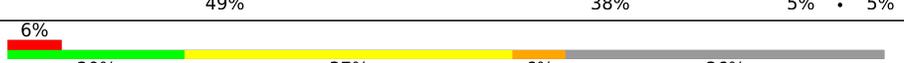
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	1J	122	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	65	112	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	J5	60	
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

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	16	207	-	-	-	X
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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
56	MG	3E	301	-	-	-	X
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
			Total	C	N	O	P			
1	13	1496	Total 32157	C 14313	N 5960	O 10388	P 1496	0	0	0
1	1G	1507	Total 32391	C 14418	N 6004	O 10463	P 1506	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	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<sup>Lys</sup>.

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<sup>fMet</sup>.

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<sup>Lys</sup>.

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
			Total	C	N	O	P			
26	14	2861	61630	27429	11535	19806	2860	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	71	133	1033	651	194	187	1	0	0	0
28	79	57	456	283	91	82		0	0	0

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

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

Continued on next page...

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	0
			1109	691	228	189	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
44	A5	111	Total	C	N	O	S	0	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	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
			Total	C	N	O			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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	13	131	Total	Mg	0	0
			131	131		

*Continued on next page...*

*Continued from previous page...*

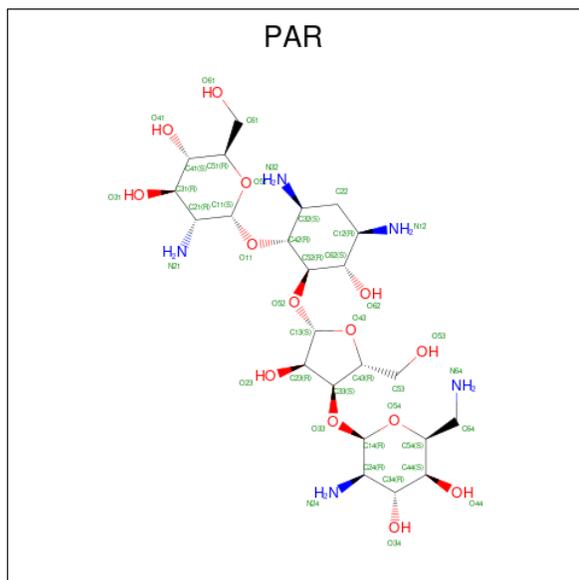
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	3E	1	Total Mg 1 1	0	0
56	5E	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	5I	1	Total Mg 1 1	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	3	Total Mg 3 3	0	0
56	3K	1	Total Mg 1 1	0	0
56	4K	1	Total Mg 1 1	0	0
56	1H	429	Total Mg 429 429	0	0
56	16	11	Total Mg 11 11	0	0
56	21	2	Total Mg 2 2	0	0
56	41	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	88	2	Total Mg 2 2	0	0
56	I8	3	Total Mg 3 3	0	0
56	L8	1	Total Mg 1 1	0	0
56	P8	1	Total Mg 1 1	0	0
56	Q8	1	Total Mg 1 1	0	0
56	1G	81	Total Mg 81 81	0	0
56	2L	3	Total Mg 3 3	0	0
56	14	382	Total Mg 382 382	0	0

*Continued on next page...*

Continued from previous page...

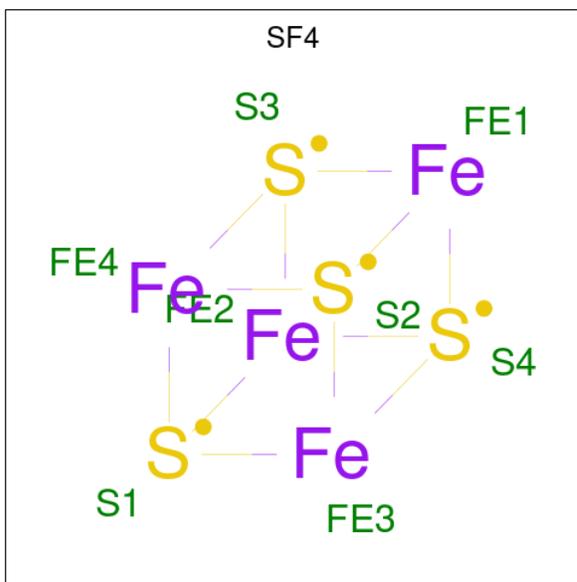
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1J	5	Total Mg 5 5	0	0
56	29	1	Total Mg 1 1	0	0
56	39	1	Total Mg 1 1	0	0
56	35	1	Total Mg 1 1	0	0
56	45	3	Total Mg 3 3	0	0
56	85	1	Total Mg 1 1	0	0
56	C5	1	Total Mg 1 1	0	0
56	E5	1	Total Mg 1 1	0	0

- 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 42 23 5 14	0	0
57	1G	1	Total C N O 42 23 5 14	0	0

- 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 8 4 4	0	0
58	32	1	Total Fe S 8 4 4	0	0

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

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

- Molecule 60 is water.

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

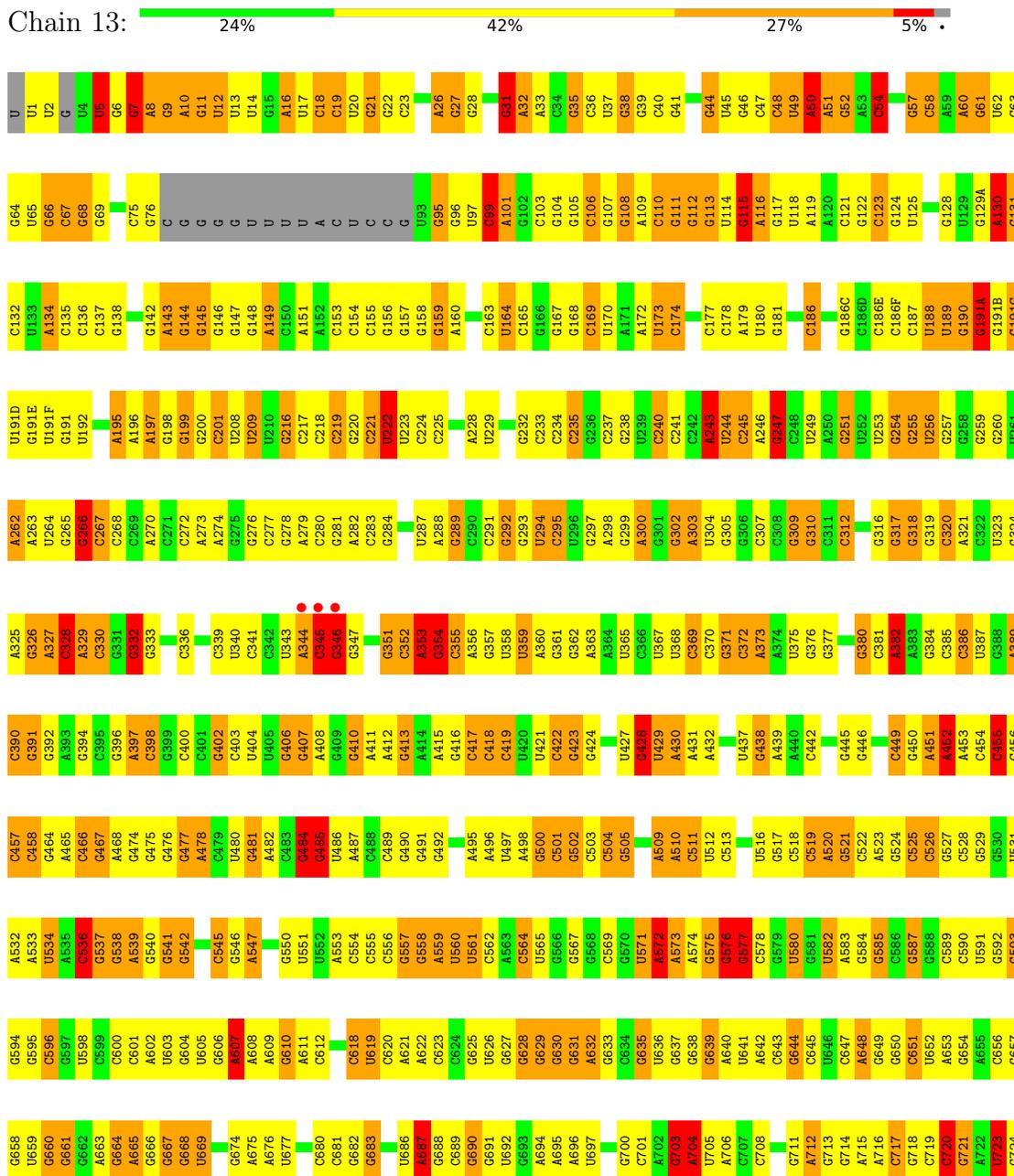
*Continued from previous page...*

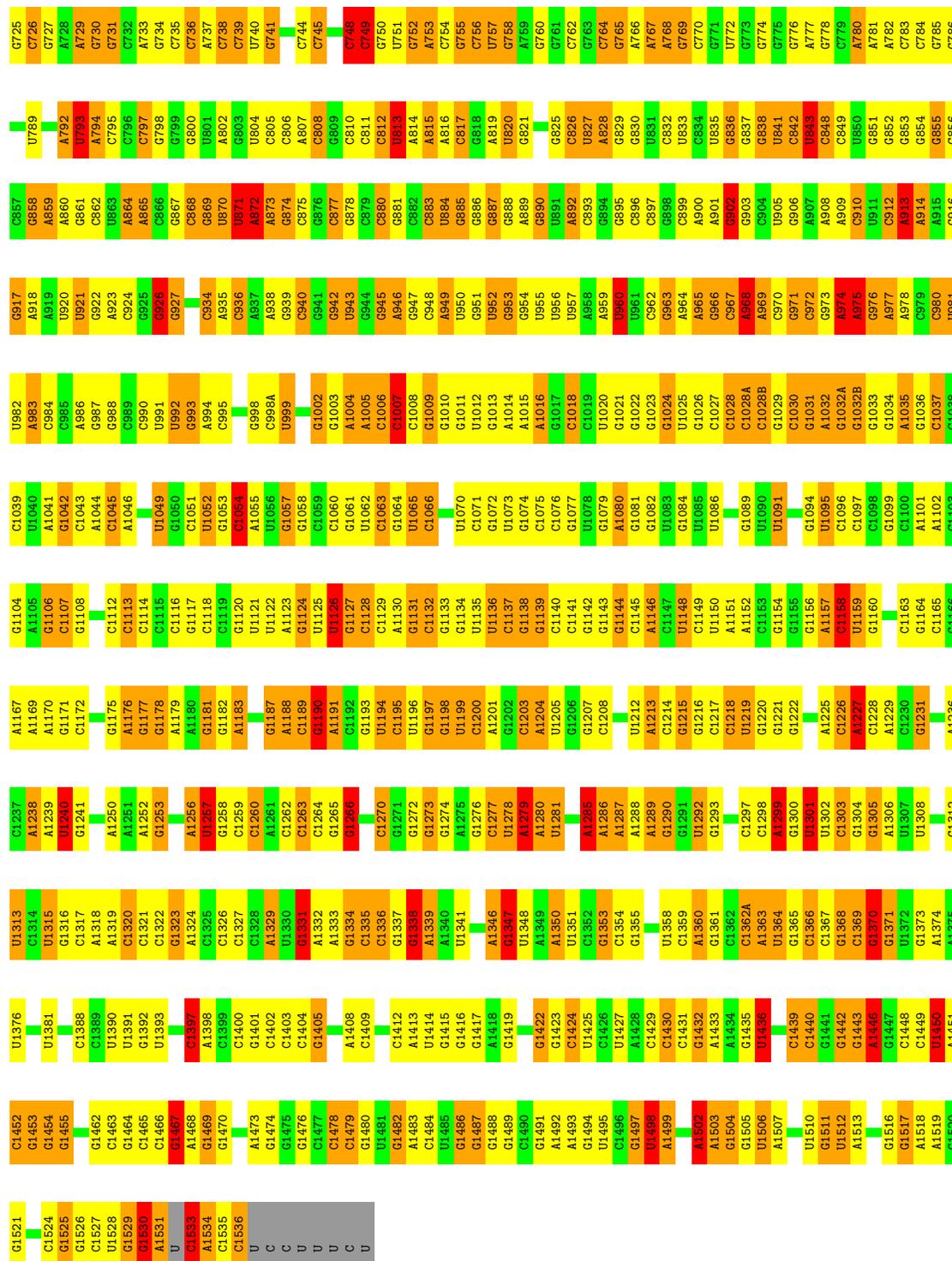
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
60	19	8	Total O 8 8	0	0
60	29	2	Total O 2 2	0	0
60	39	3	Total O 3 3	0	0
60	35	2	Total O 2 2	0	0
60	55	2	Total O 2 2	0	0
60	H5	1	Total O 1 1	0	0
60	L5	1	Total O 1 1	0	0

### 3 Residue-property plots

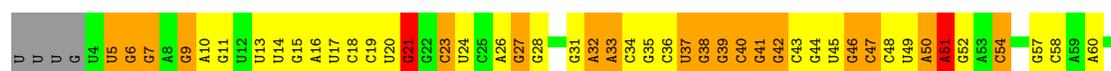
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

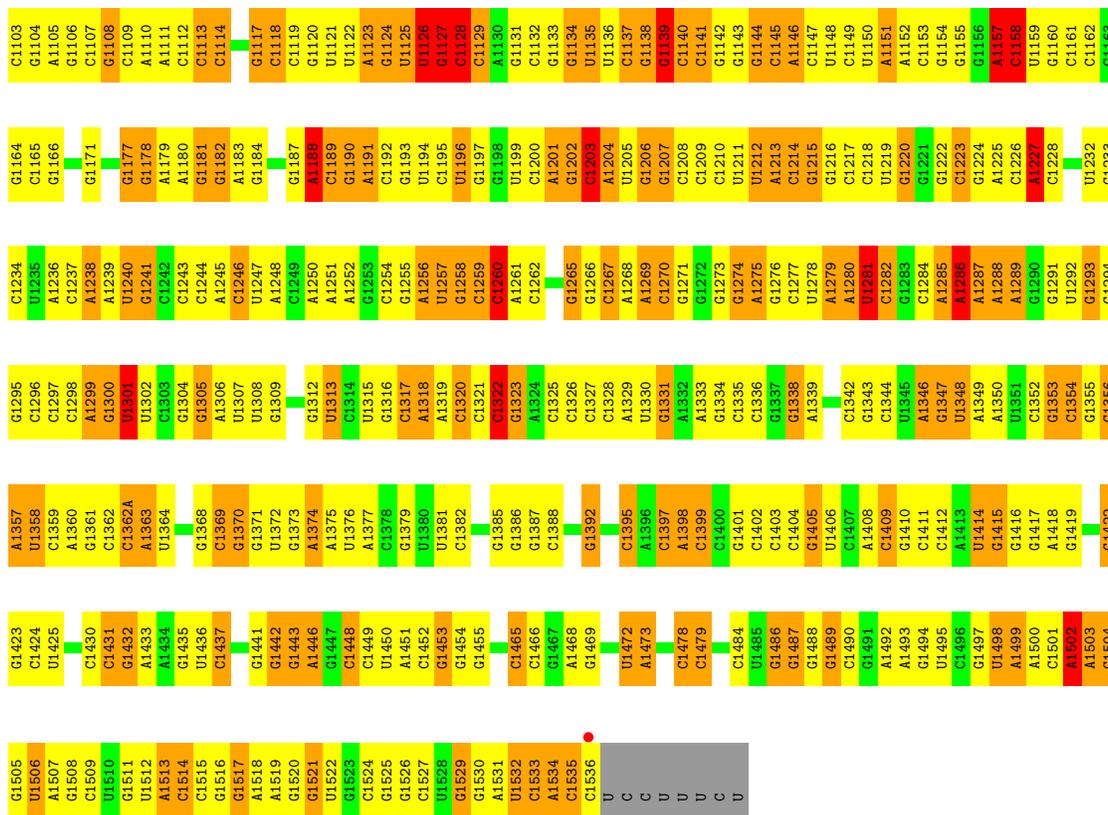




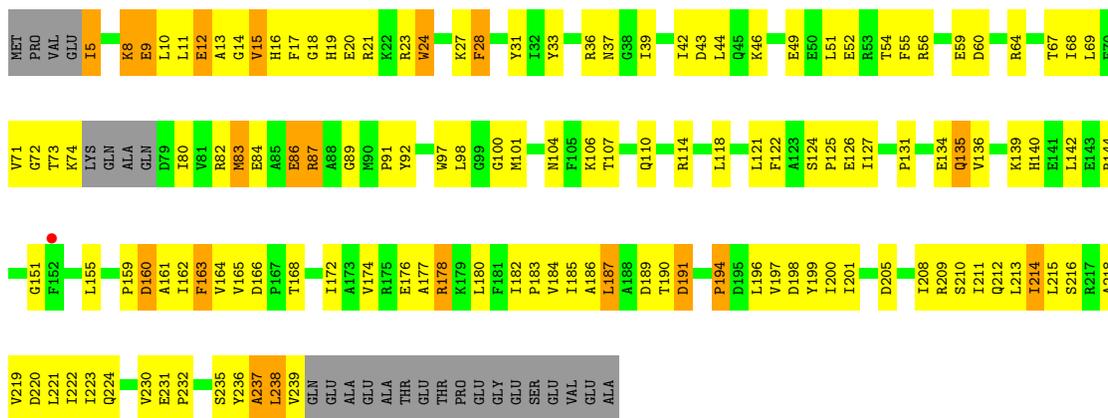
● Molecule 1: 16S rRNA



C1039	C1040	A1041	G1042	C1043	A1044	C1045	A1046	G1047	G1048	G1049	G1050	C1051	U1052	G1053	A1054	A1055	U1056	C1059	C1060	G1061	G1062	C1063	G1064	A1067	G1068	C1069	G1070	C1071	G1072	U1073	G1077	G1078	G1079	A1080	G1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	G1096	C1097	G1098	A1099	C1100	G1101	C1102	C1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	U1114	G1115	A1116	G1117	U1118	C1121	G1122	C1123	G1124	U1125	U1126	G1127	G1128	U1129	G1129A	G1129B	G1129C	U1191D
C979	C980	U991	U992	A983	C984	C985	A986	G987	U991	U992	U993	A994	C995	A996	U997	C998A	U999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	C1007	G1008	C1009	G1010	A1014	A1015	G1018	C1019	U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	G1028A	G1028B	G1029	C1030	G1031	A1032	G1032A	G1032B	C1033	G1034	A1035	G1036	C1037	C1038																														
C848	A914	A915	G916	G917	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	G928	G929	G930	G932	G933	G934	A935	A938	G939	C940	G941	G942	G945	A946	G947	C948	A949	G951	G952	G953	G954	U955	U956	U957	G958	G959	U960	U961	A964	A965	G966	C967	A968	A969	C970	G971	G972	G973	A974	A975	G976	A977	A978																												
G855	G856	A857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	A889	G890	U891	A892	C893	G894	G895	G896	G897	G898	G899	A900	A901	G902	G903	C904	U905	G906	U907	G908	A909	C910	U911	C912	A913																											
G617	C618	U619	C620	A621	G622	C623	G624	G625	U626	G627	G628	G629	G630	G631	A632	G633	C634	A635	G636	G637	G638	G639	A640	U641	A642	C643	G644	G645	U646	C647	A648	G649	G650	G651	U652	A653	G654	G655	C656	G657	G658	G659	U660	A661	A662	G663	G664	A665	G666	G667	G668	U669	G673	G674	G675	G676	U677	U678	U679	C680	G681	G682																							
C556	U559	A560	G561	U562	A563	C564	U565	G566	C567	G568	G569	G570	U571	A572	C573	A574	G575	G576	G577	G578	G579	U580	U581	U582	A583	C584	G585	U586	G587	A588	C589	U590	U591	G592	G593	G594	G595	C596	G597	U598	C599	C600	C601	A602	U603	G604	U605	G606	A607	A608	G609	G610	A611	U612	C613	A614	C615	G616																											
G491	G492	U493	U494	A495	C496	U497	U420	U421	C422	G423	G424	G425	G426	U427	A428	U429	A430	C433	C436	U437	G438	A439	C444	G445	G446	G447	A448	C449	G450	C451	A452	A453	C456	C457	C458	A464	A465	A466	G467	A468	G474	G475	G476	C477	U480	G481	A482	C483	U484	G485	G486	A487	A488	G489	C490	C491	C492	C493	C494	C495																									
C345	G346	G347	G348	A349	G350	C351	C352	G353	G354	C355	A356	U359	A360	G361	C362	A363	A364	U365	C366	U367	G371	C372	A373	A374	U375	G376	G377	A382	A383	C384	C385	C386	U387	G388	A389	C390	G391	G392	A393	G396	A397	C398	G399	C400	C401	G402	C403	U404	U405	G406	A408	G409	U410	A411																															
C269	A270	C271	C272	A273	G276	C277	G278	A279	C280	G281	A282	U287	G288	G289	U296	G297	A300	G303	U304	G305	G306	G307	G308	G309	G310	C311	C312	A315	G316	G317	G318	G319	C320	A321	A325	G326	A327	C328	A329	G332	G333	C334	C335	C336	G339	U340	U341	A403	C342	U343	A344																																		
C131	C132	A133	U134	C137	G142	A143	G144	G145	G146	G147	G148	A149	C150	C155	G156	G157	C221	U222	U223	C224	C225	A228	U229	G230	G231	G232	C235	G236	C237	G238	A243	U244	C245	A246	G247	C248	U249	A250	G251	G254	G255	G256	G257	G260	U261	A262	U263	U264	G265	G266	G267	U191D																																	
G63	G64	U65	G66	C67	G68	G69	G73	C74	C75	G76	C77	G79	G80	G81	U82	U83	U84	A87	C88	U89	C90	C91	G92	U93	G95	G96	U97	C99	A101	U101	G102	C103	G104	G105	G106	G107	G108	A109	G112	G113	U114	G115	A116	G117	U118	C121	G122	C123	G124	U125	G126	U127	G128	U129	G129A	A130																													

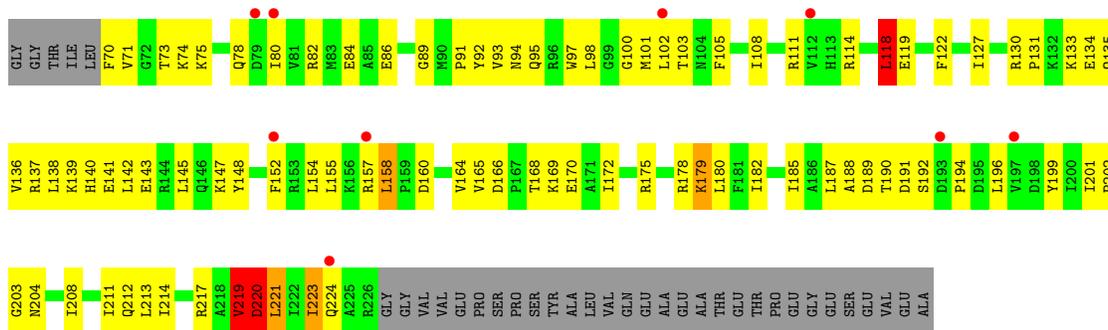


• Molecule 2: 30S ribosomal protein S2

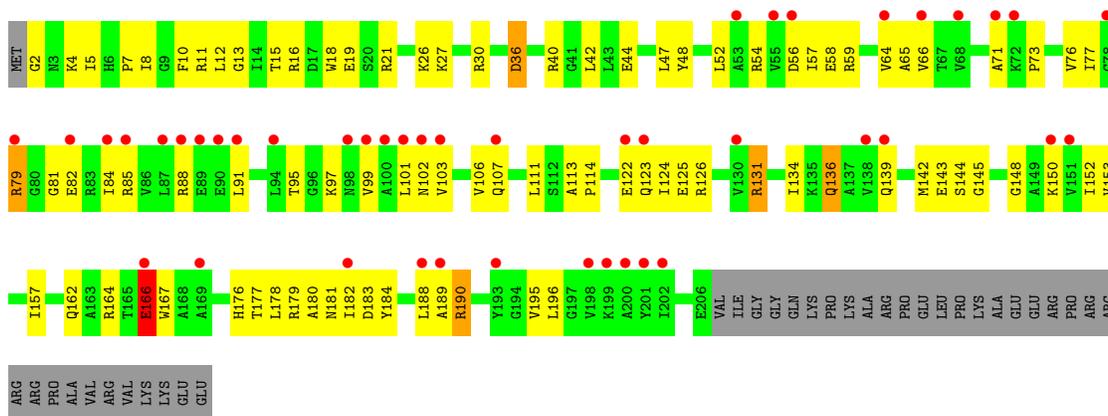


• Molecule 2: 30S ribosomal protein S2

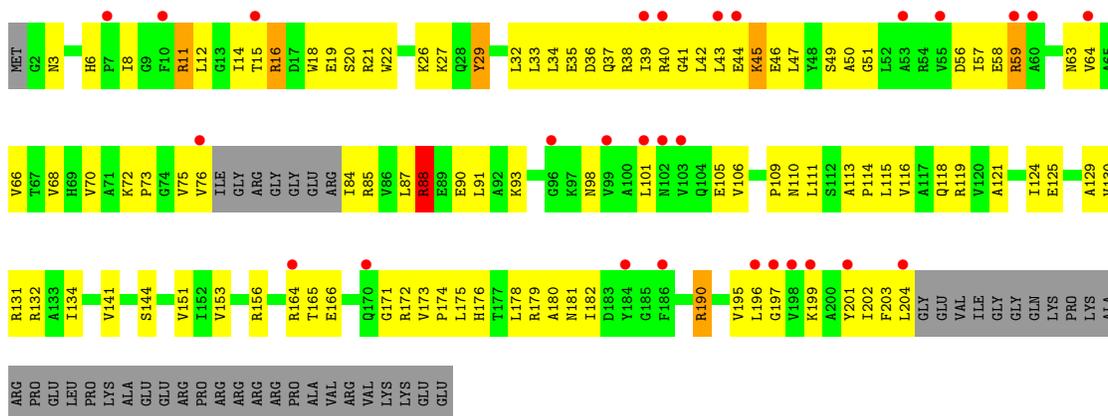




• Molecule 3: 30S ribosomal protein S3

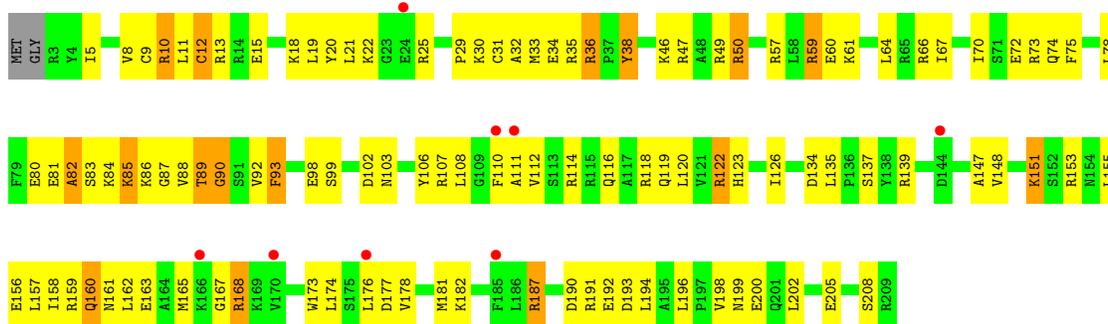


• Molecule 3: 30S ribosomal protein S3

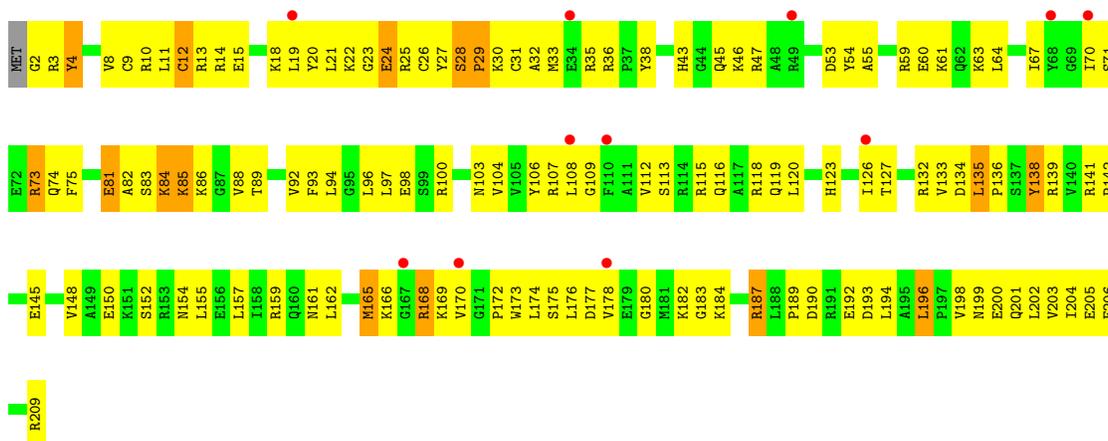


• Molecule 4: 30S ribosomal protein S4

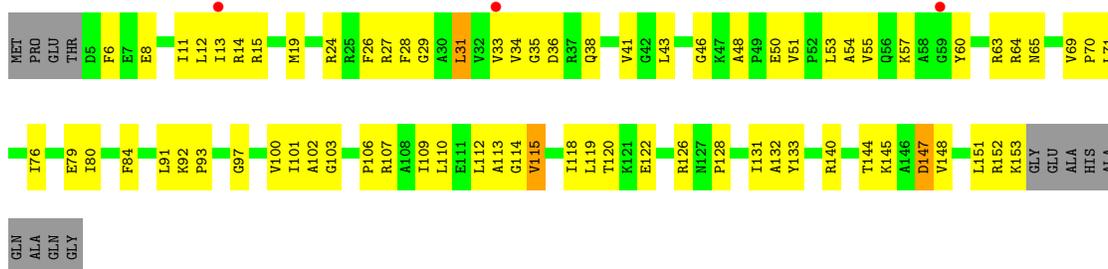




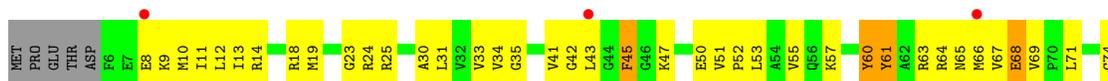
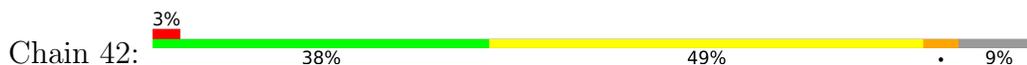
• Molecule 4: 30S ribosomal protein S4

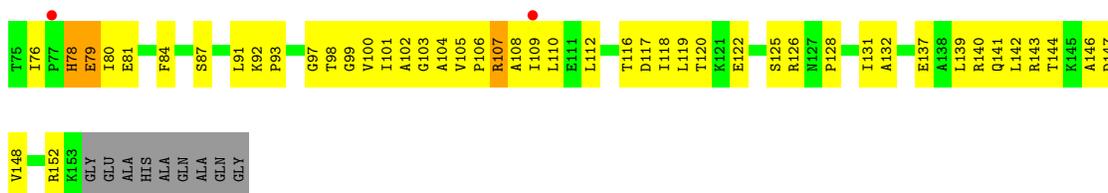


• Molecule 5: 30S ribosomal protein S5

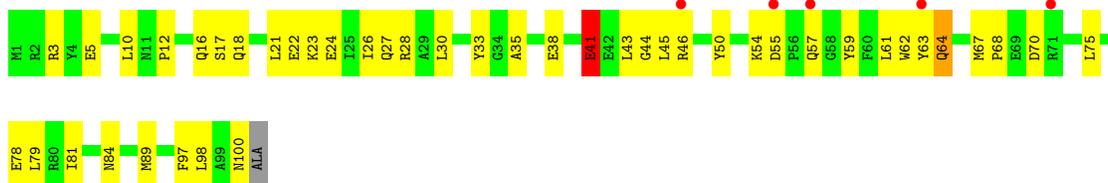


• Molecule 5: 30S ribosomal protein S5

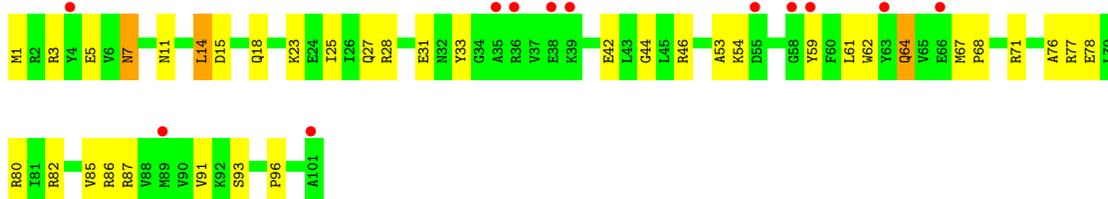




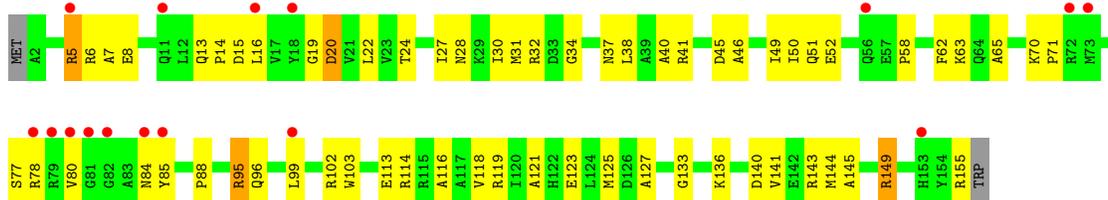
- Molecule 6: 30S ribosomal protein S6



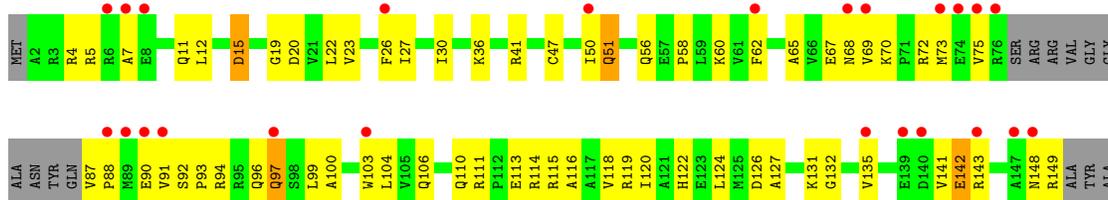
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

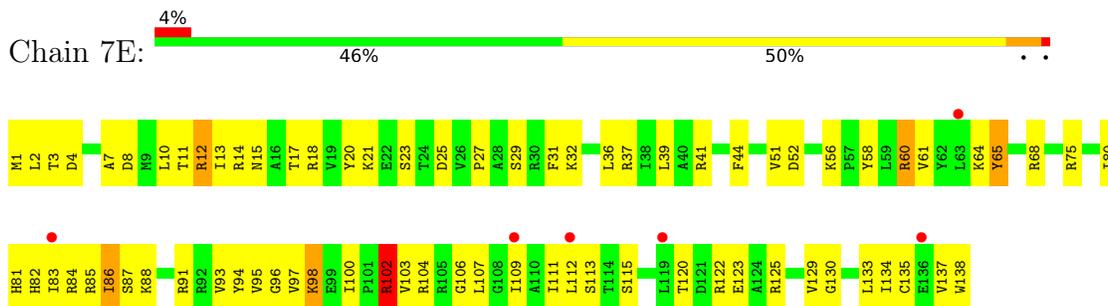


- Molecule 7: 30S ribosomal protein S7

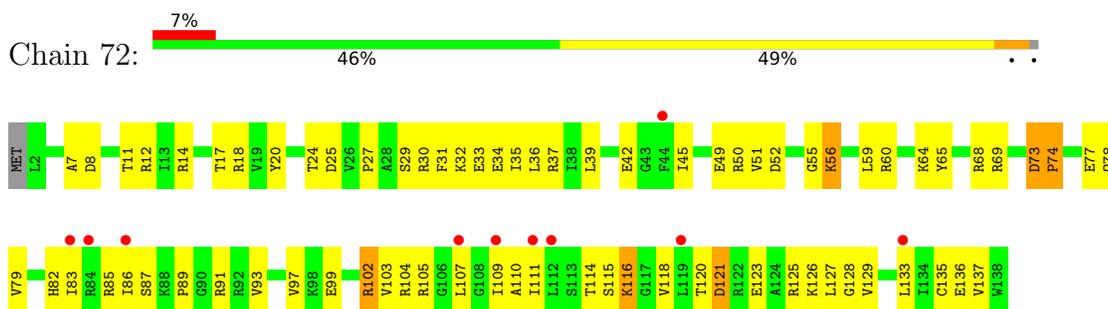


HIS  
TYR  
ARG  
TRP

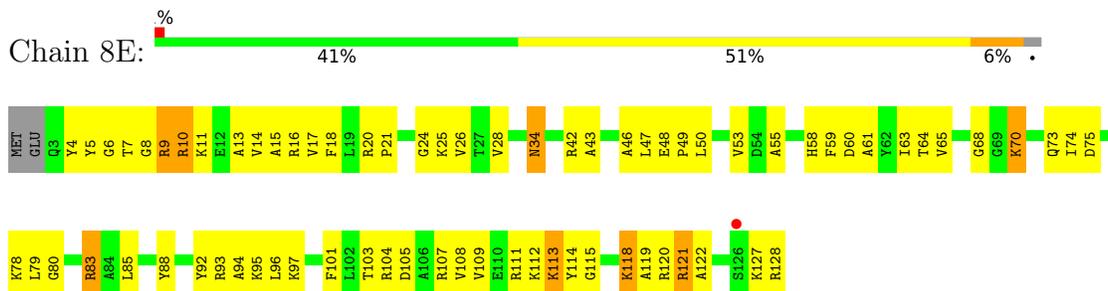
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9

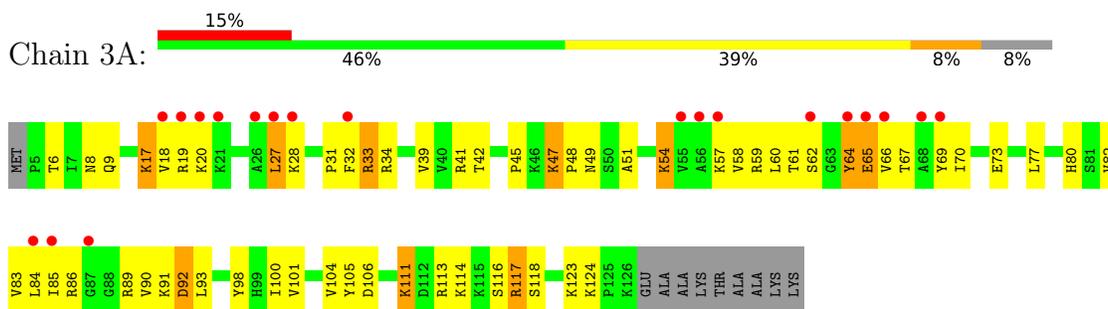


- Molecule 10: 30S ribosomal protein S10

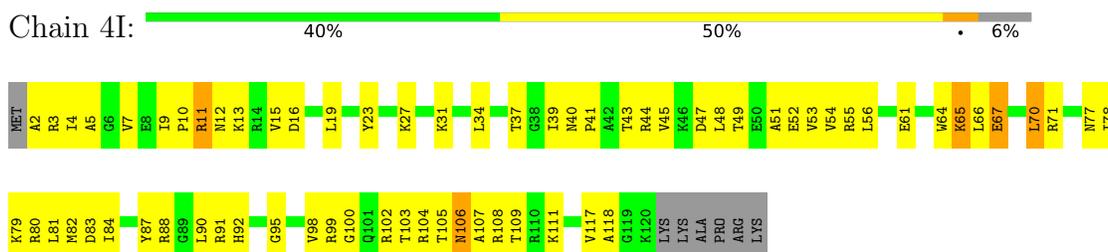




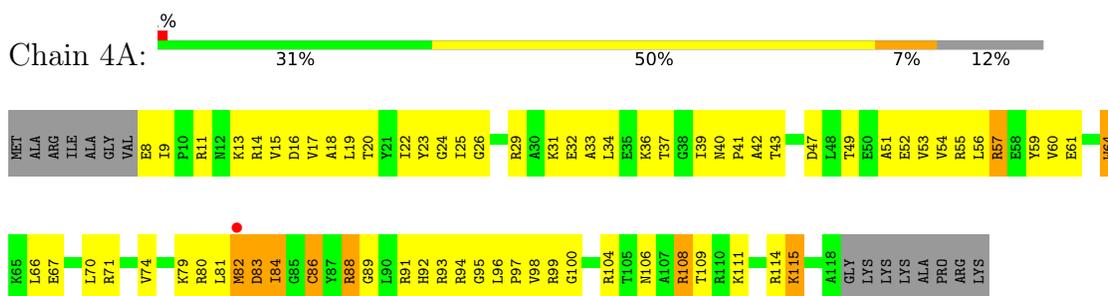
- Molecule 12: 30S ribosomal protein S12



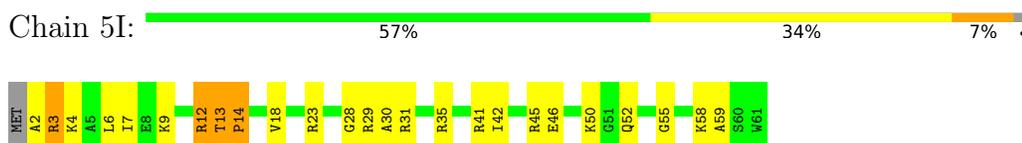
- Molecule 13: 30S ribosomal protein S13



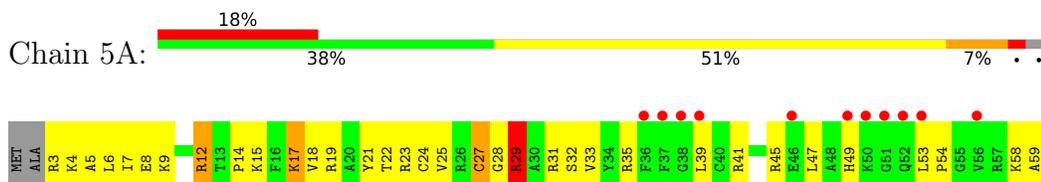
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

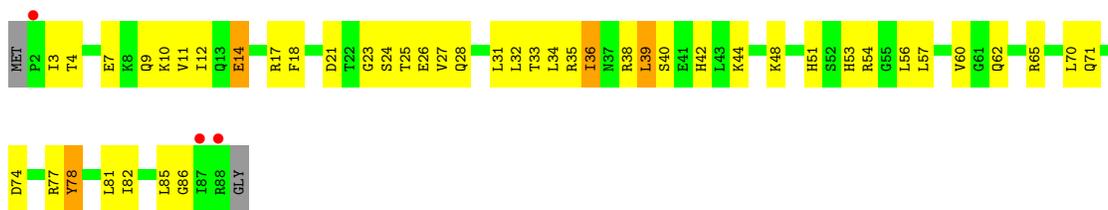


- Molecule 14: 30S ribosomal protein S14 type Z

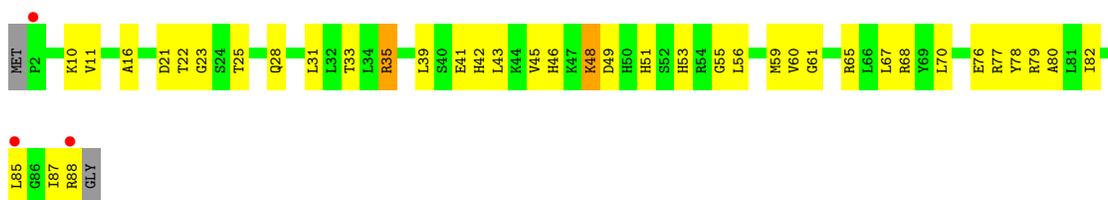


- Molecule 15: 30S ribosomal protein S15





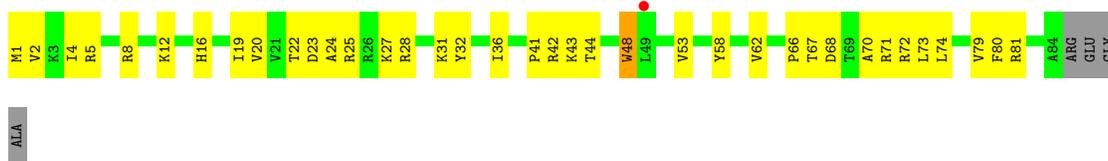
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

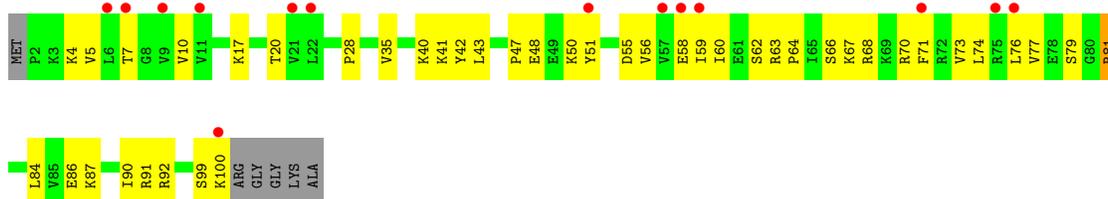


- Molecule 17: 30S ribosomal protein S17



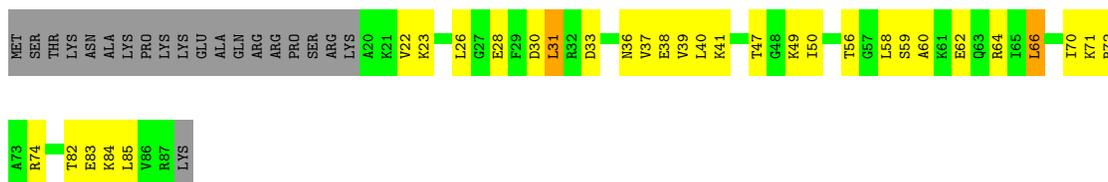
- Molecule 17: 30S ribosomal protein S17

Chain 8A: 



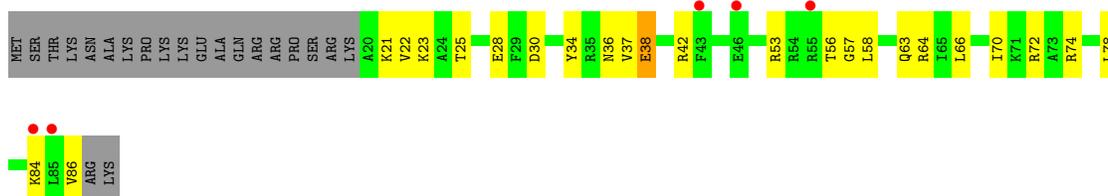
• Molecule 18: 30S ribosomal protein S18

Chain 9I: 



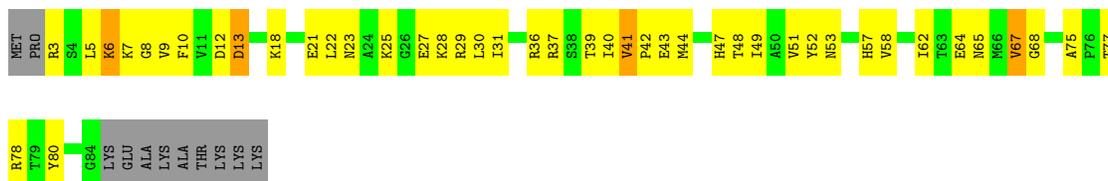
• Molecule 18: 30S ribosomal protein S18

Chain 9A: 



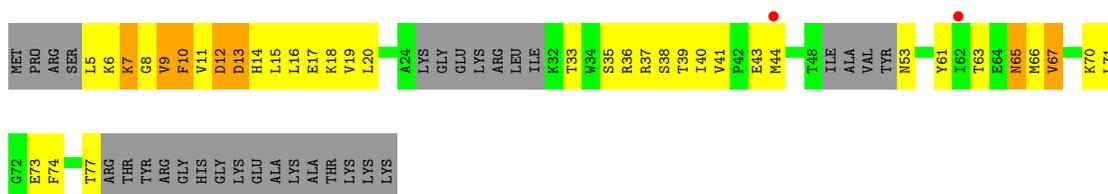
• Molecule 19: 30S ribosomal protein S19

Chain AI: 

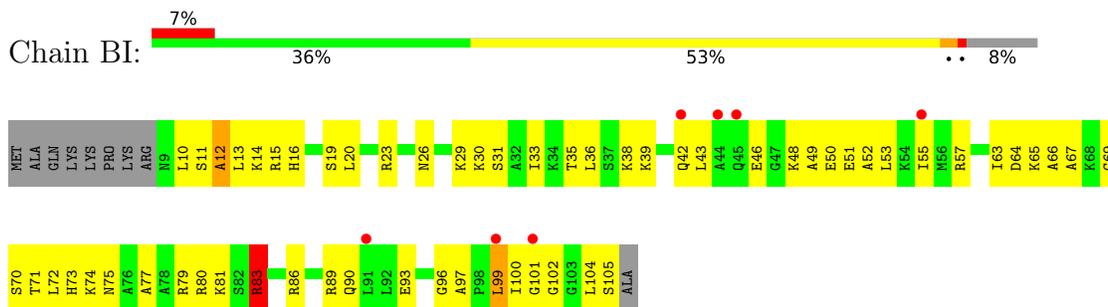


• Molecule 19: 30S ribosomal protein S19

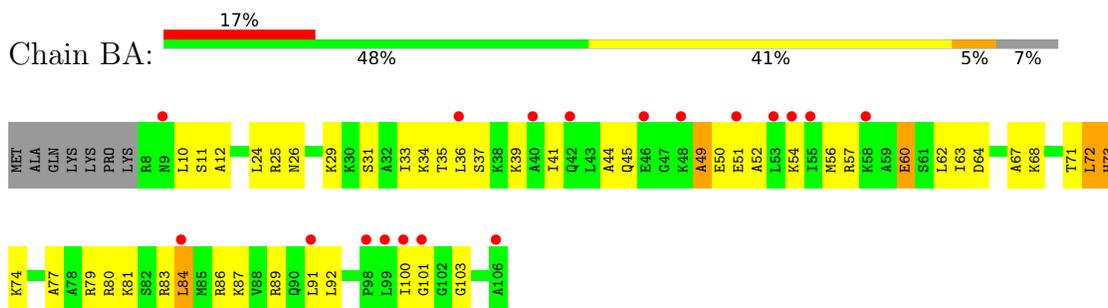
Chain AA: 



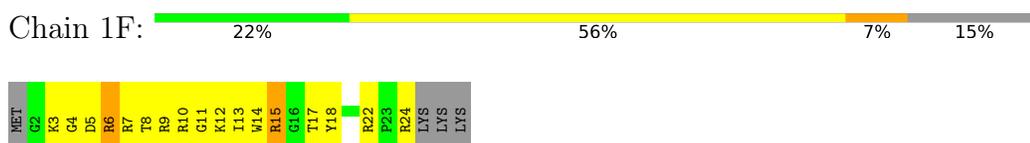
- Molecule 20: 30S ribosomal protein S20



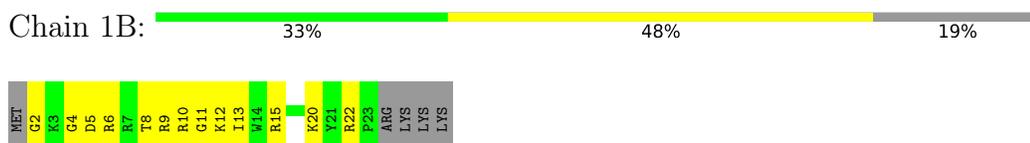
- Molecule 20: 30S ribosomal protein S20



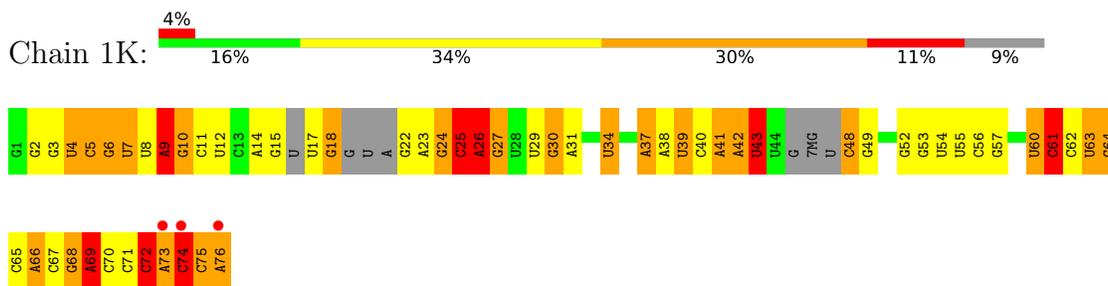
- Molecule 21: 30S ribosomal protein Thx



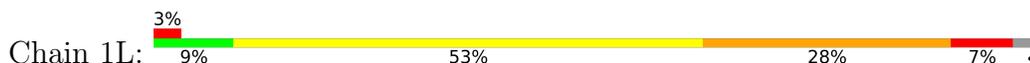
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA<sup>Lys</sup>



- Molecule 22: tRNA<sup>Lys</sup>





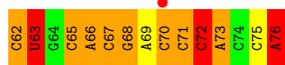
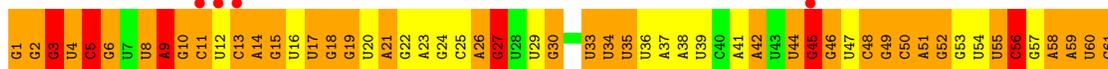
• Molecule 23: E. coli tRNA<sup>fMet</sup>



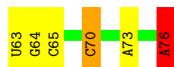
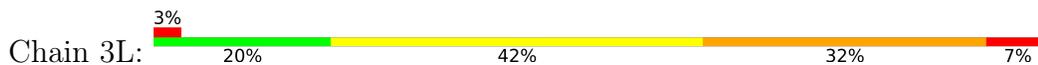
• Molecule 23: E. coli tRNA<sup>fMet</sup>



• Molecule 24: tRNA<sup>Lys</sup>



• Molecule 24: tRNA<sup>Lys</sup>



• Molecule 25: mRNA

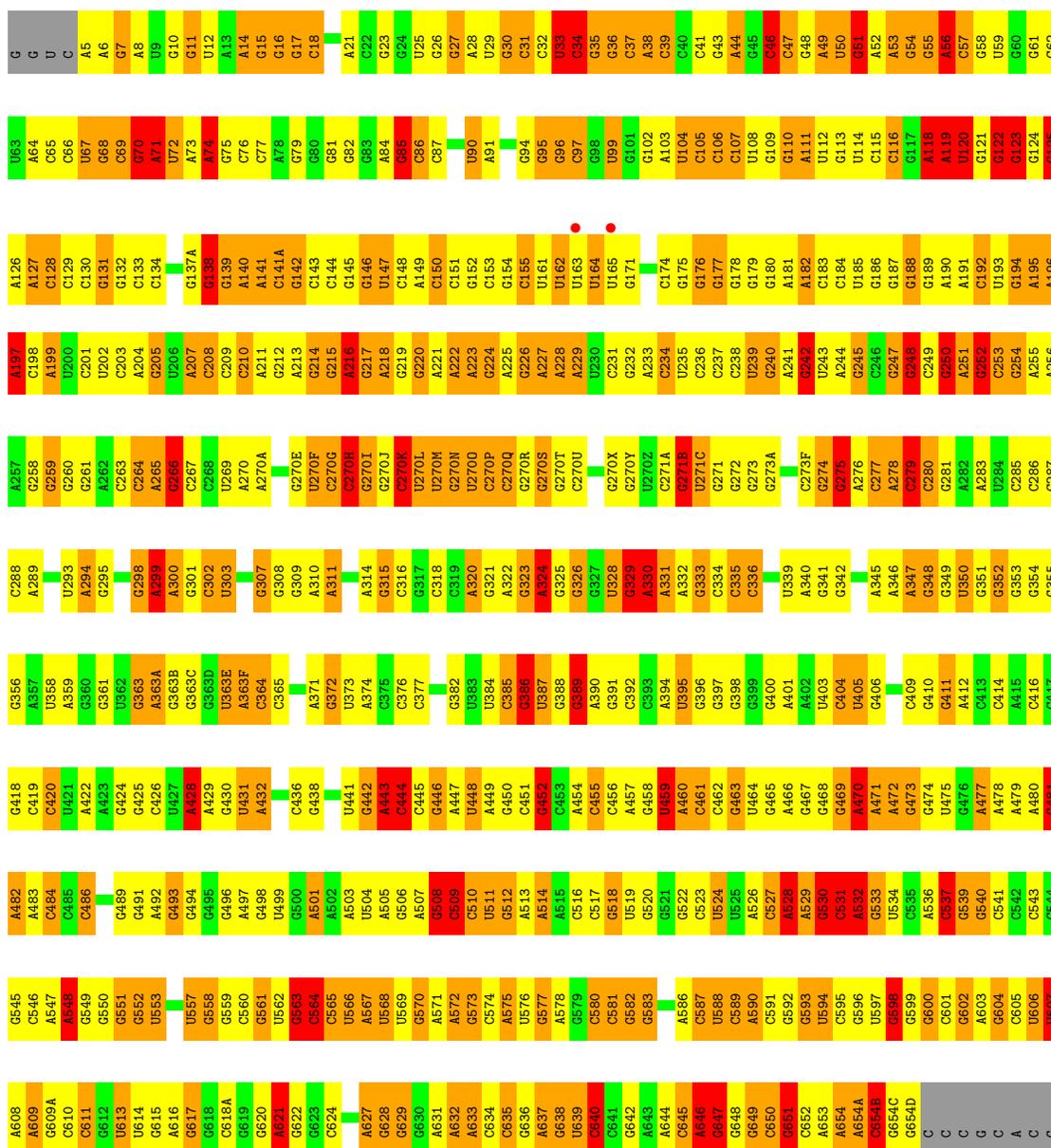




● Molecule 25: mRNA

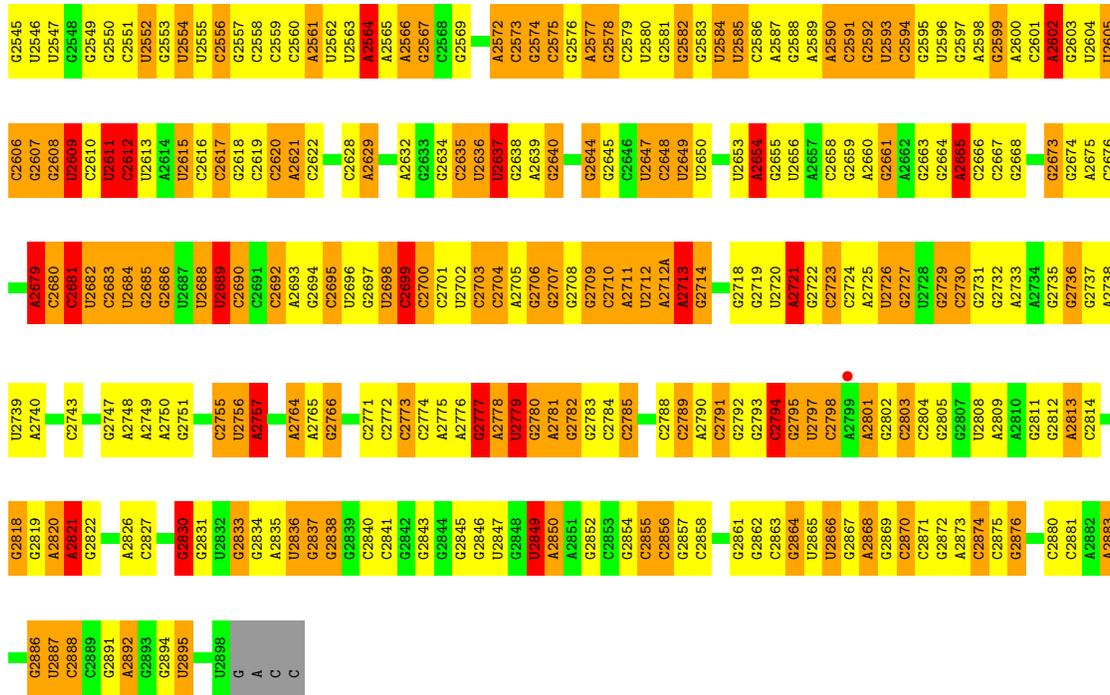


● Molecule 26: 23S rRNA

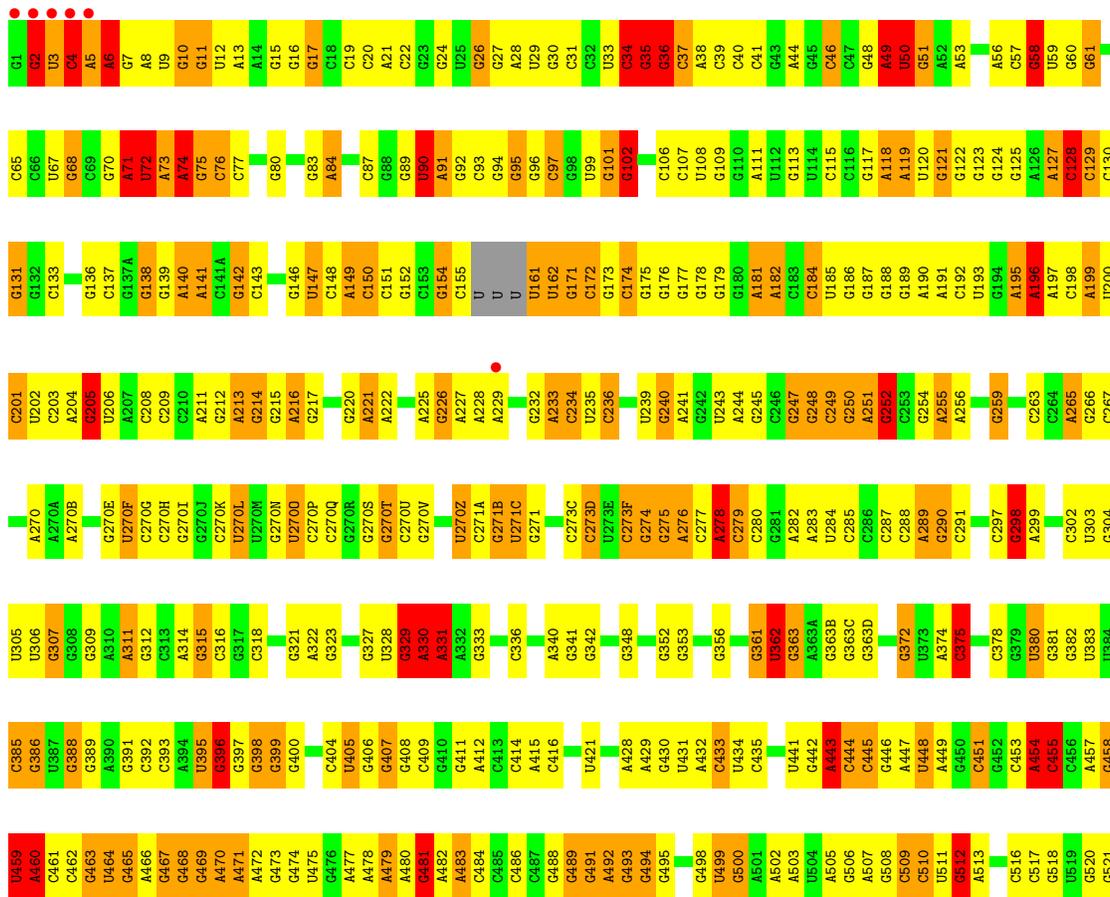
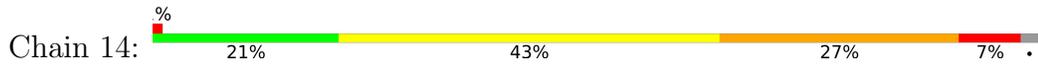


A1508	C1532	C1445	C1386	U1326	U1263	C1201	U1141	U1012	G950	C	U826	C766	A706	C	G654N
C1509	C1533	C1446	C1387	C1327	G1264	G1202	U1142	C1013	C951	C	U827	U767	G707	C	G654O
A1510	C1534	G1447	G1388	G1328	A1265	G1203	A1143A	A	G952	A	U828	G768	C708	G	G654P
A1511	G1448	G1448	G1389	U1329	G1266	A1204	A1143	G1016	A953	G	U829	G769	U709	A	G654Q
C1512	A1449	A1449	U1390	C1330	U1267	U1205	G1144	U1019	C954	C893	G830	G770	G710	C894	C654R
C1513	G1449A	A1449A	U1391	C1331	A1268	G1206	C1145	U1019	C955	C894	G831	G771	G711	C895	C654S
U1514	A1453	A1453	A1392	G1332	A1269	C1207	C1146	A1020	G956	U895	G832	C772	G712	A	G654S
C1515	U1454	U1454	A1393	G1333	C1270	C1208	C1147	A1021	A957	A	U833	U773	G713	G713	A654T
C1516	U1454	U1454	A1394	G1334	G1271	G1209	A1148	G1022	U858	C897	C834	U774	U714	U714	
C1517	G1455	G1455	A1395	U1335	A1272	A1210	A1150	U1023	A959	C898	A835	G775	G715	G715	A655
C1518	G1456	G1456	A1396	U1336	A1273	U1211	C1150	G1024	A960	C899	G836	G776	A716	A716	A656
C1519	U1457	U1457	G1337	G1337	A1274	G1212	G1151	G1025	G961	A900	C837	A777	G717	G717	U657
U1520	C1458	C1458	G1338	U1339	A1275	A1213	G1152	U1026	G962	A901	C838	G778	A718	A718	C658
G1521	G1459	G1459	C1339	G1339	A1276	A1214	C1153	A1027	U885	C902	U839	U779	C719	C719	C659
U1522	A1460	A1460	G1400	U1340	G1277	G1215	G1154	G	C964	C903	C840	G780	C720	C720	G660
U1523	G1461	G1461	U1341	U1341	A1278	G1218	A1155	G1030	C965	C904	A841	A781	C721	C721	G661
G1524	C1462	C1462	C1402	A1342	G1279	G1219	G1156	A1032	C966	U905	G842	A782	A722	A722	G662
G1526	C1464	C1464	C1403	G1343	G1280	G1220	G1158	U1033	C967	U906	G843	A783	G723	G723	G663
G1527	C1465	C1465	U1405	C1345	G1281	A1220	U1159	U1034	G968	U907	C844	A784	U724	U724	C664
A1528	G1466	G1466	U1406	G1346	U1282	G1221	U1159	G1035	U969	C908	G845	G785	G725	G725	C665
A1529	C1467	C1467	U1407	G1347	A1283	C1222	G1160	U1036	C970	A909	C846	G786	G726	G726	G666
C1532	A1469	A1469	C1409	A1349	A1286	G1223	G1161	G1037	C971	A910	U847	A727	A727	A727	U667
C1533	C1470	C1470	G1410	C1350	U1287	G1225	G1163	G1038	A973	C912	A849	A789	G729	G729	G668
G1534	A1471	A1471	C1411	C1351	C1288	A1227	U1165	C1040	C974A	U913	C850	G790	C730	A670	A670
U1535	A1472	A1472	A1412	U1352	C1290	G1228	C1166	C1041	G975	C914	U851	C791	C731	C731	G671
A1536	C1473	C1473	G1413	A1353	C1291	G1229	U1167	G1042	C976	C915	G852	G792	C732	C732	G672
C1537	C1474	C1474	U1414	A1354	U1292	G1230	G1168	A1043	G977	C916	G853	A793	U740	U740	G680
G1538	G1475	G1475	U1415	G1355	U1293	C1230	G1169	G1044	G978	A917	G854	G794	A734	A734	G682
C1539	C1476	C1476	G1416	G1356	G1286	G1231	G1170	A1045	G979	C918	G855	A735	A735	A735	G683
G1540	A1477	A1477	G1417	U1357	C1297	U1240	C1179	U1046	G987	C919	C856	G796	C736	C736	A676
U1541	G1478	G1478	G1418	U1358	C1298	U1241	C1180	A1047	G989	G920	C857	G797	C737	C737	A677
A1542	G1479	G1479	A1419	A1359	G1299	U1234	G1173	G1047	C982	G921	U858	G798	G738	G738	G678
G1543	G1480	G1480	U1420	A1360	U1300	G1235	A1174	A1048	A983	U922	C859	G799	G739	G739	G679
U1544	U1482	U1482	G1421	G1361	U1301	U1175	U1176	G1049	A984	C923	U860	A800	U740	U740	G680
A1545	G1483	G1483	G1422	C1362	A1302	G1237	A1177	A1050	G987	C924	A861	G801	G741	G741	G681
A1545A	G1484	G1484	G1423	C1363	G1303	U1239	C1178	G1051	A988	C925	G862	A802	G742	G742	G682
C1546	G1485	G1485	G1424	G1364	C1304	U1240	C1179	C1052	G989	A926	A863	U803	G743	G743	C683
C1547	A1486	A1486	G1425	A1365	C1305	A1241	C1180	A1053	A990	G929	G864	A804	G744	G744	G684
C1548	G1487	G1487	G1426	A1366	A1307	G1244	C1181	G	C991	U930	C865	C805	G745	G745	A685
C1549	U1489	U1489	A1427	A1367	G1308	G1245	A1182	G	C992	G931	A866	A746	A746	A746	G686
C1550	A1490	A1490	G1429	G1369	G1309	A1246	G1183	A	G993	G932	C867	U807	U747	U747	G687
C1551	G1491	G1491	C1430	C1370	G1310	A1247	C1185	U	C994	A933	U868	G808	G748	G748	U688
A1553	G1492	G1492	U1431	G1371	G1311	U1248	C1186	G	A996	G834	G869	G809	C749	C749	A689
C1554	C1493	C1493	U1433	U1372	U1312	G1249	G1187	U	U871	C935	U811	U811	A751	A751	G691
C1555	A1494	A1494	A1434	G1373	U1313	U1249	C1124	U	G997	C936	A872	C912	A752	A752	C692
C1556	A1495	A1495	A1434	G1374	C1314	G1250	G1125	G	U999	U937	G873	U813	C753	C753	C693
C1557	A1496	A1496	G1435	C1375	C1315	U1251	A1189	G	A1000	G938	U877	C814	C754	C754	U694
A1558	U1497	U1497	G1436	C1376	U1316	A1252	G1190	U	A1001	G939	U877	C815	C755	C755	G695
C1559	C1498	C1498	U1437	G1377	G1317	A1253	A1128	C	A1002	G940	A878	C816	C756	C756	G696
G1560	C1499	C1499	U1438	A1378	C1318	U1254	G1192	U	U1002	A941	G879	C817	U757	U757	C697
G1561	G1500	G1500	A1439	A1379	C1319	U1255	A1193	A	G1003	G942	G880	G818	C758	C758	C698
A1562	C1501	C1501	G1440	G1380	G1320	U1257	A1194	G	C1004	U943	G881	A819	G759	G759	A699
G1563	C1502	C1502	G1441	G1381	C1321	C1257	G1195	A	C1005	G944	A820	A820	G760	G760	G700
C1564	G1442	G1442	G1442	G1382	A1322	G1258	G1196	A	C1006	A845	A821	A821	A761	A761	G701
C1565	G1443	G1443	G1443	C1383	U1323	G1259	G1197	G	U1009	G946	U822	U822	U762	U762	G702
A1566	C1506	C1506	G1444	C1384	U1324	G1260	U1198	A	A1010	G947	G823	G823	A764	A764	G704
A1567	A1507	A1507	A1444A	G1385	A1262	A1262	C1200	G	G1011	C949	A	C825	G765	G765	A705

G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544																
G2421	A2422	U2423	G2424	A2425	G2426	G2427	G2428	G2429	A2430	G2431	G2432	A2433	A2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	A2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481																
C2359	A2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420															
G2299	G2300	G2301	G2302	G2303	G2304	A2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	A2320	G2321	A2322	G2323	G2324	G2325	G2326	A2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360															
G2238	G2239	G2240	U2241	U2242	U2243	U2244	U2245	G2246	G2247	G2248	U2249	G2250	G2251	G2252	G2253	G2254	G2255	U2257	G2258	G2259	G2260	G2261	U2262	G2263	G2264	U2265	G2266	G2267	G2268	G2269	G2270	G2271	U2272	A2273	A2274	G2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	A2286	A2287	A2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	U2296	G2297	A2298																	
C2184	G2185	G2186	U2187	G2188	G2189	A2190	A2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	A2225	G2226	A2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237																							
G2101	U2102	G2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	G2111	G2112	G2113	U2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	U2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	U2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163														
G2037	G2038	G2039	C2040	A2041	C2042	C2043	G2044	G2045	G2046	U2047	G2048	G2049	G2050	G2051	G2052	G2053	A2054	G2055	G2056	A2057	A2058	A2059	A2060	G2061	G2062	G2063	C2064	G2065	G2066	G2067	U2068	G2069	G2070	A2071	G2072	G2073	U2074	U2075	U2076	A2077	G2078	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	U2089	U2090	U2091	U2092	G2093	G2094	G2095	A2096	G2097	U2098	U2099	G2100													
A1912	A1913	C1914	C1915	G1916	U1917	U1918	A1919	C1920	C1921	C1922	C1923	C1924	C1925	U1926	A1927	A1928	G1929	G1930	U1931	A1932	G1933	G1934	G1935	G1936	G1937	A1938	U1939	U1940	G1941	G1942	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	U1951	U1952	A1953	G1954	U1955	U1956	C1957	C1958	G1959	A1960	G1961	G1962	G1963	G1964	G1965	A1966	G1967	G1968	A1969	G1970	A1971	A1972	G1973	G1974	G1975													
U1976	A1977	A1978	C1979	G1980	U1981	C1982	C1983	G1984	G1985	A1986	G1987	G2049	C2050	G1989	C1990	U1991	G1992	U1993	C1994	U1995	A2057	A2058	A2059	A2060	G2061	G2062	G2063	G2004	A2005	G2006	G2007	G2008	G2009	U2010	U2011	G2012	A2013	A2014	A2015	G1954	U1955	U1956	C1957	C1958	G1959	A1960	U1961	G1962	G1963	G1964	G1965	A1966	G1967	G1968	A1969	G1970	A1971	A1972	G1973	G1974	G1975															
C1832	U1833	G1834	C1835	U1836	C1837	G1838	G1839	G1840	U1841	G1842	G1843	C1844	G1845	G1846	G1847	U1848	G1849	G1850	U1851	C1852	A1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	A1861	G1862	G1863	G1864	A1865	G1866	G1867	G1868	G1869	A1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	A1884	C1885	C1886	G1887	G1888	A1889	G1890	G1891	U1892	G1893	G1894	G1895	G1896	G1897	U1898	G1899	A1900	A1901	C1902	G1903	G1904	U1905	G1906	G1907	U1911
G1772	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	C1781	G1782	A1783	A1784	G1785	G1786	A1787	G1788	U1789	G1790	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	U1799	G1799	G1800	G1801	G1802	A1803	C1804	U1805	G1806	G1807	U1808	A1809	A1810	G1811	A1812	G1813	G1814	G1815	G1816	G1817	U1818	U1819	U1820	A1821	G1822	G1823	G1824	A1825	G1826	U1827	G1828	A1829	G1830	G1831																
U1629	G1630	C1630A	A1631	G1632	G1633	A1634	G1635	C1636	A1637	C1638	U1639	C1640	A1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	A1654	A1655	G1656	G1657	C1658	U1659	G1660	G1661	G1662	C1663	A1664	A1665	G1666	G1667	A1668	A1669	A1670	A1671	G1672	G1673	A1674	A1675	A1676	A1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	U1689															
G1568	A1569	A1570	A1571	G1572	G1573	C1574	C1575	U1576	C1577	U1578	A1579	A1580	G1581	G1582	A1583	C1585	A1586	A1587	C1588	G1589	U1590	G1591	C1592	G1593	G1594	G1595	A1596	G1597	C1598	C1599	G1600	G1601	A1602	G1603	C1604	C1605	G1606	C1607	A1608	A1609	A1610	C1611	G1612	G1613	A1614	G1615	A1616	G1617	A1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628																	

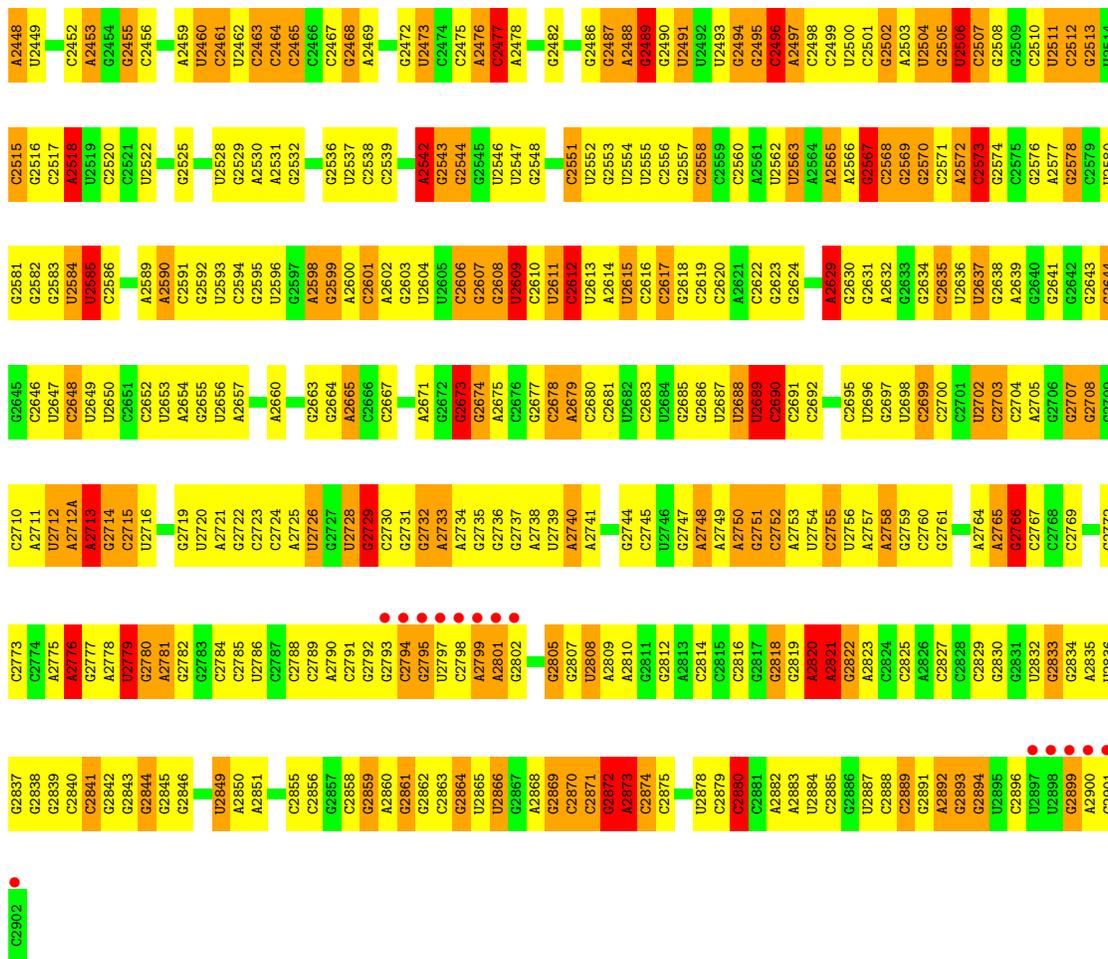


• Molecule 26: 23S rRNA





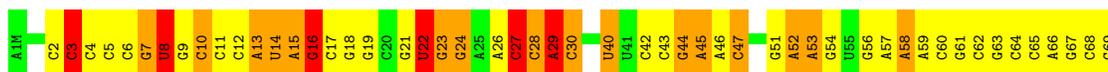
G2384	C2384	U2189	C2128	C2066	A2005	A1986	G1863	C1795	G1717	C1648	C1589	G1524	U1454
G2385	C2129	G2190	C2129	G2067	C2006	A1937	U1864	U1796	G1718	G1649	U1590	G1525	G1456
C2386	U2130	G2191	U2130	G2068	C2007	A1938	G1869	C1797	G1725	G1649	U1591	G1526	G1455
A2387	A2367	A2368	A2367	A2069	C2008	A1939	C1870	C1798	G1726	G1653	G1592	G1527	G1459
G2388	A2369	A2369	U2132	G2069	G2009	U1940	A1871	G1799	U1727	A1654	G1593	A1528	A1460
A2389	G2193	G2193	G2133	G2070	G2010	G1941	A1872	G1800	G1728	A1655	G1594	G1529	G1461
G2390	A2134	C2195	A2134	G2072	U2011	C1942	G1878	G1801	A1729	C1656	G1595	G1532	G1462
G2391	A2135	C2196	A2135	C2073	G2012	U1943	C1879	A1802	U1730	C1657	G1596	C1533	C1463
A2392	C2136	U2197	C2136	U2074	A2013	U1944	G1883	A1803	G1731	C1658	A1597	G1534	C1464
A2393	A2217	U2075	A2217	U2075	A2014	G1945	G1884	C1804	A1732	U1659	C1598	U1535	G1470
G2394	C2137	U2076	C2137	U2076	A2015	U1946	G1885	A1805	G1733	C1660	C1599	U1536	G1466
C2395	C2139	A2077	C2139	A2077	U2016	C1947	G1886	C1806	G1734	G1661	G1600	G1537	C1467
A2396	C2140	C2078	C2140	U2078	U2017	G1948	C1887	G1807	C1735	C1662	G1601	G1538	C1468
G2397	G2141	U2079	G2141	U2079	G2018	G1949	G1888	U1808	C1741	C1663	U1602	G1539	A1469
A2398	C2142	G2080	C2142	G2080	A2019	U1950	G1889	A1809	G1742	C1664	A1599	G1540	G1470
G2399	G2210	G2081	G2210	G2081	A2020	U1951	A1889	A1810	G1743	A1665	G1604	U1541	A1471
A2400	C2145	A2082	C2145	A2082	C2021	A1952	A1890	G1811	G1746	G1666	G1605	A1542	
G2401	G2146	G2083	G2146	G2083	U2022	A1953	G1891	A1812		G1667	G1606	A1543	
C2402	G2147	C2084	G2147	C2084	G2023	A1954	C1892	G1813	G1751	A1668	G1607	C1544	C1474
G2403	G2148	C2085	G2148	C2085	G2024	U1955	C1893	G1814	C1752	A1669	A1608	C1545	G1475
U2404	G2149	U2086	G2149	U2086	C2025	U1956	C1894	U1815	G1753	C1670	U1609	G1546	A1477
G2405	U2150	G2087	U2150	G2087	C2026		G1895	G1816	C1754	C1671	C1549	C1549	G1478
U2406	G2151	G2088	G2151	G2088	G2027	A1960	G1896	G1817	A1755	C1672	C1550	C1550	G1479
G2407	G2152	U2089	G2152	U2089	U2028	G1961	G1897	U1818	G1756	G1673	G1551	G1551	G1480
A2408	G2153	G2090	G2153	G2090	G2029	C1962	U1898	A1819	U1757	G1674	G1552	G1552	U1482
G2409	G2154	U2091	G2154	U2091	A2030	U1963	G1899	U1820	G1758	C1675	A1614	A1553	G1483
U2410	G2155	U2092	G2155	U2092	A2031	G1964	A1900	A1821	A1759	A1676	C1615	A1554	G1484
G2411	G2156	G2093	G2156	G2093	A2032	U1965	A1901	G1822	A1760	G1677	G1616	G1555	G1485
A2412	G2157	C2094	G2157	C2094	G2033	A1966	C1902	A1823	G1761	G1678	C1617	G1556	A1486
G2413	A2158	C2095	A2158	C2095	U2034	C1967	G1903	G1824	A1762	U1679	A1618	G1557	G1487
U2414	G2159	U2096	G2159	U2096	G2035	G1968	G1904	A1825	G1763	U1680	G1619	A1558	G1488
G2415	G2160	C2097	G2160	C2097	C2036	A1969	C1905	G1826	G1764	G1681	G1620	G1559	U1489
C2416	C2161	U2098	C2161	U2098	G2037	A1970	G1906	G1827	C1765	C1682	U1621	G1560	A1490
A2417	C2162	U2099	C2162	U2099	G2038	A1971	G1907	G1828		C1683	G1622	G1561	
G2418	C2163	G2100	C2163	G2100	C2039	A1972	C1908	A1829	G1769	C1684	G1623	A1562	C1493
C2419	C2164		C2164		G1973	G1973	C1909	G1830	G1770	C1685	G1624	G1563	
A2420	G2165	G2103	G2165	G2103	A2042	G1974	A1913	U1834	G1771	C1686	C1625	C1564	A1496
A2421	G2166	G2104	G2166	G2104	C2043	G1975	A1914	U1835	G1772	G1687	G1626	C1565	
A2422	U2167	C2105	U2167	C2105	C2044	U1976	C1914	G1836	A1773	U1688	G1627	A1566	G1500
A2423	C2168	G2106	C2168	G2106	C2045	A1977	U1915	C1836	C1774	A1689	G1628	A1567	C1504
A2424	A	C2107	A	C2107	G2046	A1978	U1916	G1839	G1775	G1690	G1629	A1568	C1505
A2425	U2170	C2108	U2170	C2108	U2047	C1979	A1917	G1840	G1776	G1691	G1630	A1569	C1506
G2426	A2171	G2109	A2171	G2109	G2048	G1980	U1917	G1839	U1777	U1693	C1630A	A1570	A1507
A2427	U2172	C2110	U2172	C2110	G2049	G1981	A1918	C1841	U1778	C1694	A1631	A1571	A1508
G2428	A2173	C2111	A2173	C2111	C2050	C1983	A1919	G1845	U1779	G1695	A1632	A1572	C1509
A2429	C2174	G	C2174	G	A2051	G1984	A1920	G1846	A1780	G1696	G1633	G1573	C1510
G2430	C2175	U2113	C2175	U2113	C2052	G1985	G1921	A1847	G1781	G1697	A1634	C1574	A1510
A2431	G2176	A2114	G2176	A2114	G2053		U1922	A1698	G1782	A1698	G1635	C1575	A1511
A2432	C2177	G2115	C2177	G2115	A2054	G1989	U1923	G1699	A1783	G1699	G1636	U1576	G1512
G2433	C2178	G2116	C2178	G2116	C2055	C1990	C1924	U1851	A1784	A1700	C1637	C1577	C1513
A2434	C2179	U2117	C2179	U2117	C2056	U1991	C1925	G1852	A1785	A1701	G1638	U1578	U1514
A2435	G2210	A2118	G2210	A2118	A2057	G1992	U1926	C1853	A1786	G1702	U1639	A1579	C1515
A2436	G2211	U2119	G2211	U2119	A2058	U1993	A1927	A1854	A1787	G1703	C1640	A1580	U1516
A2437	G2212	G	G2212	G	A2059	C1994	A1928	A1857	G1788	G1704	A1641	A1581	G1517
G2438	U2122	C2183	U2122	C2183	A2060	U1995	G1929	G1858	A1789	G1705	G1642	C1582	C1518
A2439	G2213	G2184	G2213	G2184	G2061	C1999	U1930	A1859	A1790	G1709	C1643	A1583	G1519
A2440	C2185	G2184	C2185	G2184	A2062	G2000	U1931	A1859	A1791	U1709	C1644	C1585	U1520
A2441	G2186	A2126	G2186	A2126	C2063	G2001	A1932	G1860	G1792	G1710	G1645	A1586	G1522
A2442	C2187	G2202	C2187	G2202	C2064	G2002	A1933	G1861	C1793	G1711	C1646	A1587	U1523
G2443	C2188	G2203	C2188	G2203	C2065		G1935	G1862	U1794	G1716	G1647	C1588	



• Molecule 27: 5S rRNA



• Molecule 27: 5S rRNA

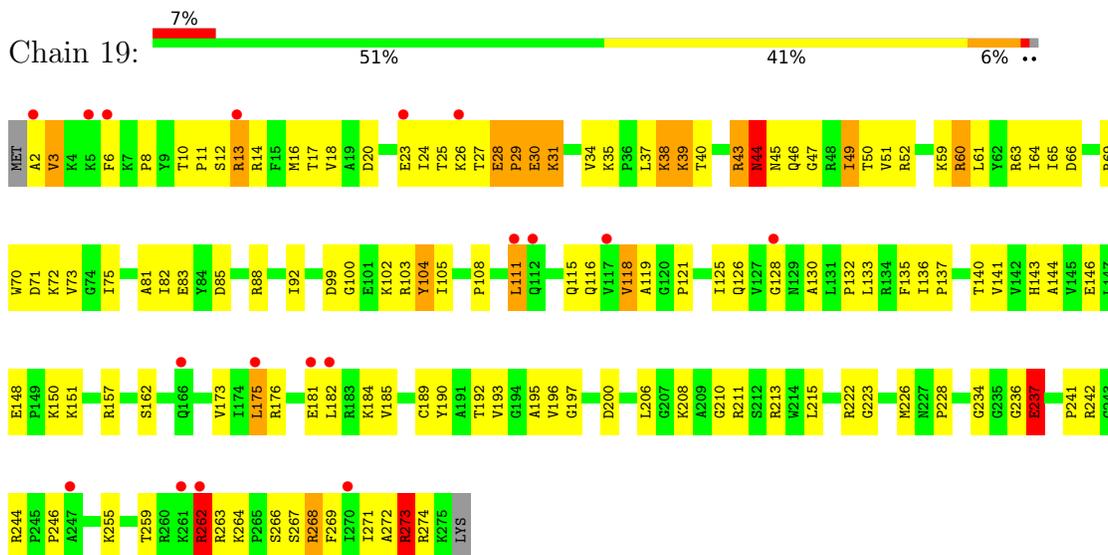


• Molecule 28: 50S ribosomal protein L1

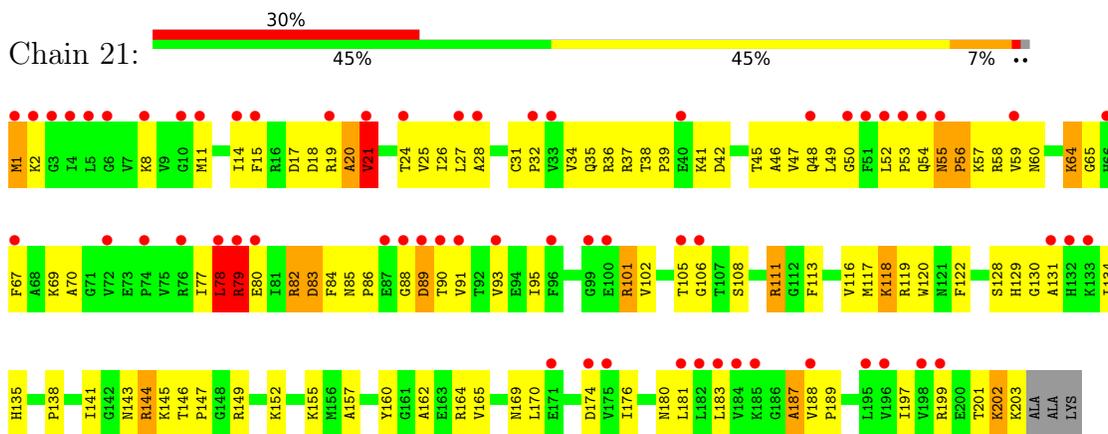




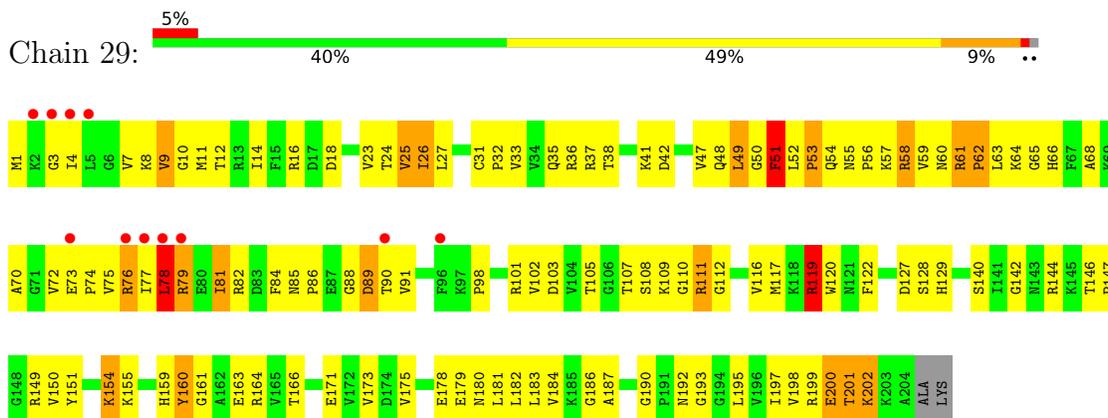
- Molecule 29: 50S ribosomal protein L2



- Molecule 30: 50S ribosomal protein L3

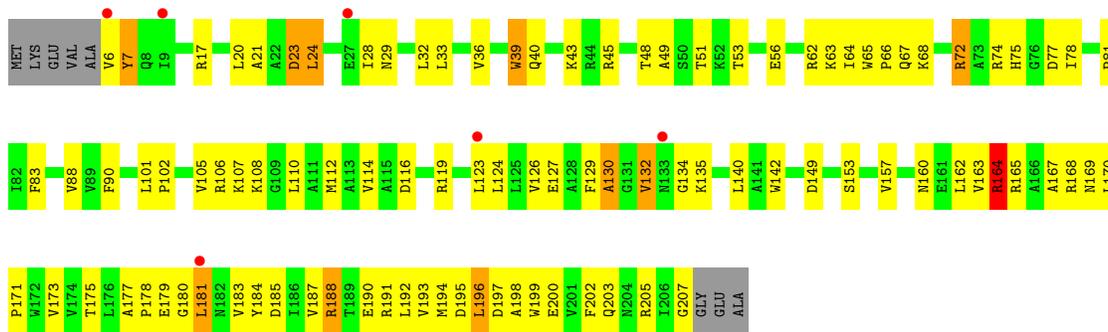


- Molecule 30: 50S ribosomal protein L3

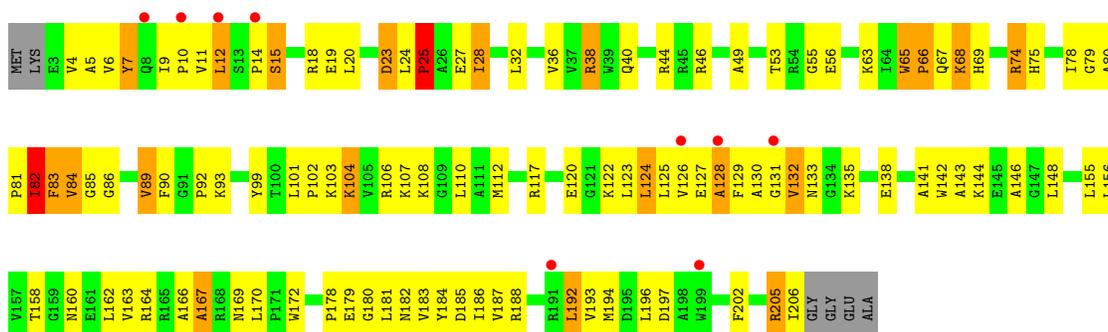


- Molecule 31: 50S ribosomal protein L4

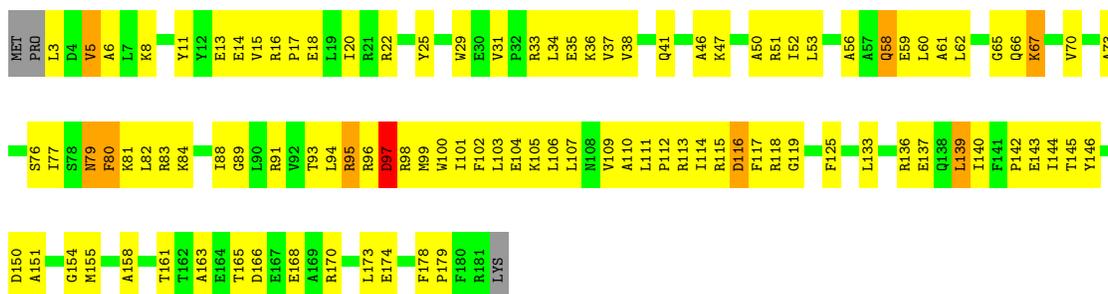




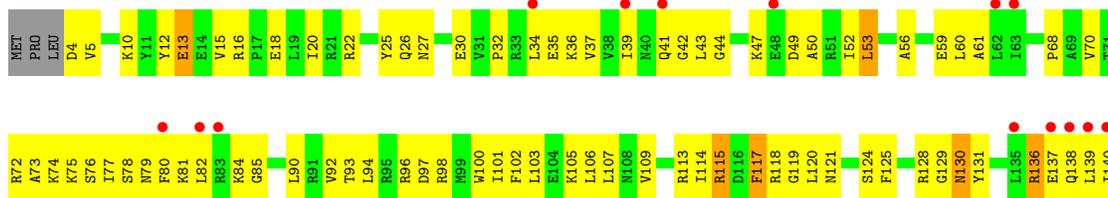
• Molecule 31: 50S ribosomal protein L4



• Molecule 32: 50S ribosomal protein L5

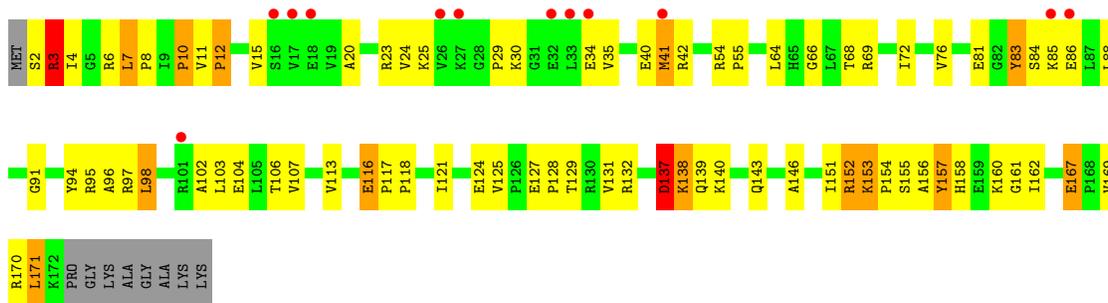


• Molecule 32: 50S ribosomal protein L5

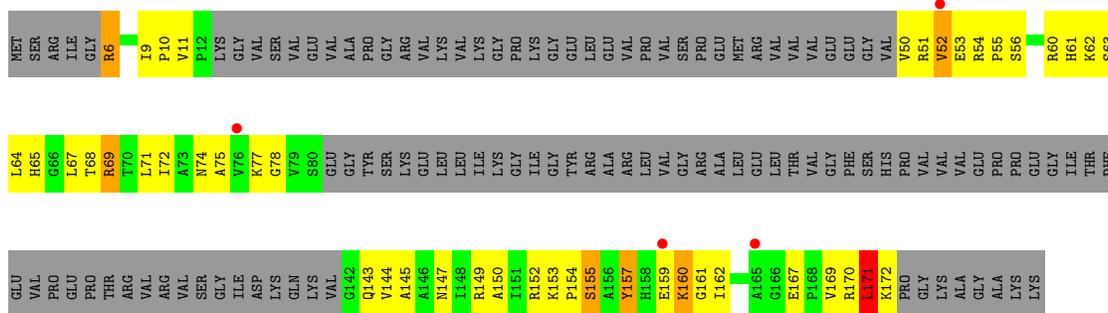




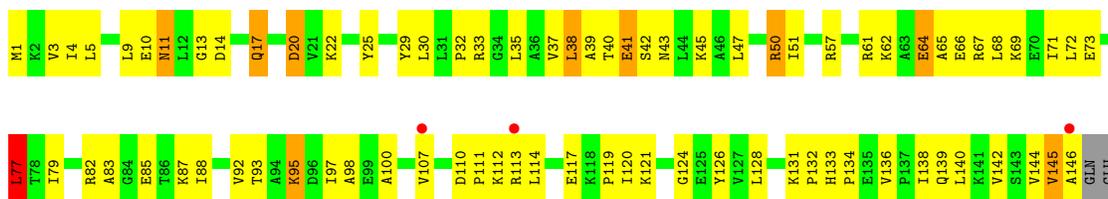
• Molecule 33: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L6



• Molecule 34: 50S ribosomal protein L9

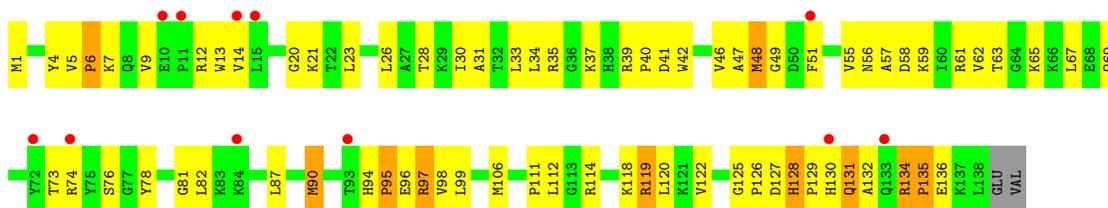


• Molecule 34: 50S ribosomal protein L9

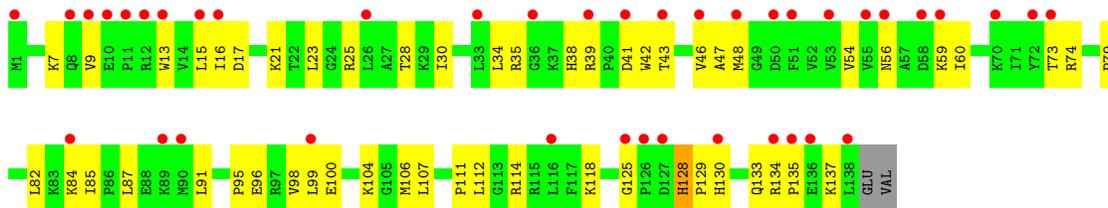




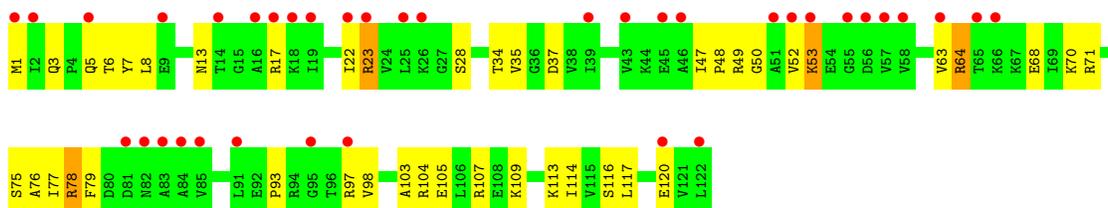
- Molecule 35: 50S ribosomal protein L13



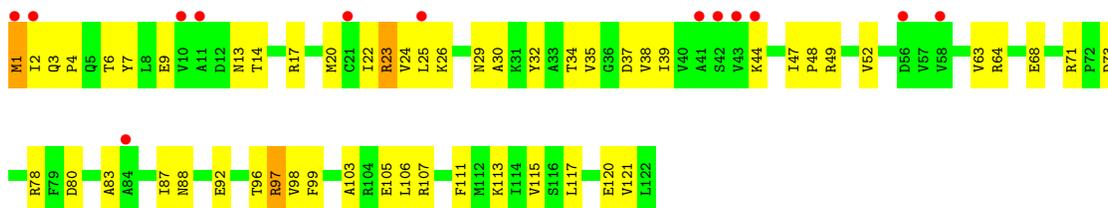
- Molecule 35: 50S ribosomal protein L13



- Molecule 36: 50S ribosomal protein L14

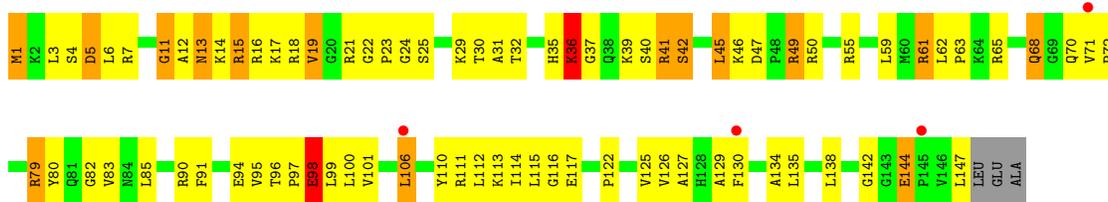


- Molecule 36: 50S ribosomal protein L14

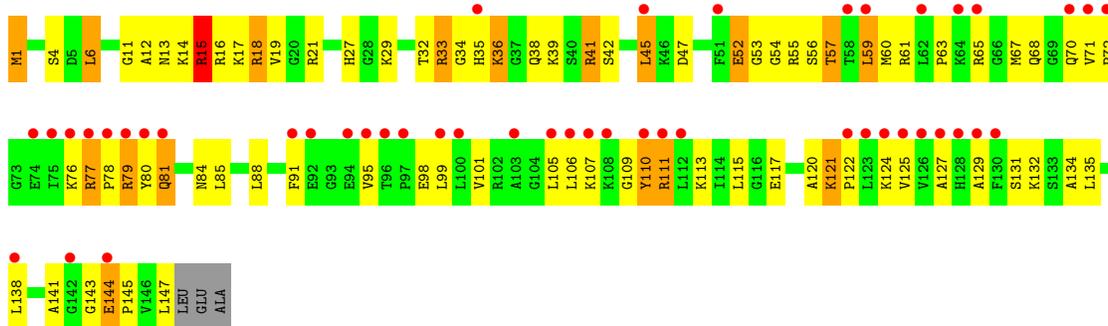


- Molecule 37: 50S ribosomal protein L15





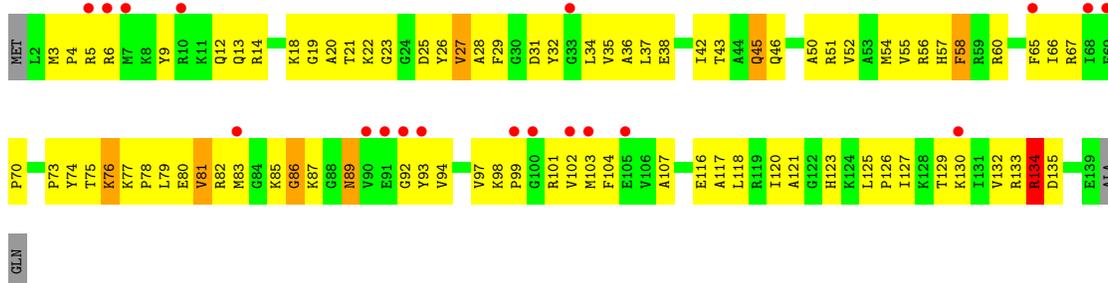
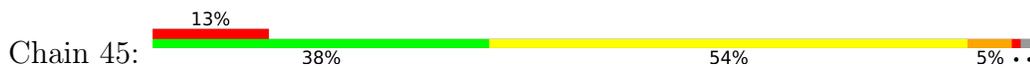
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16

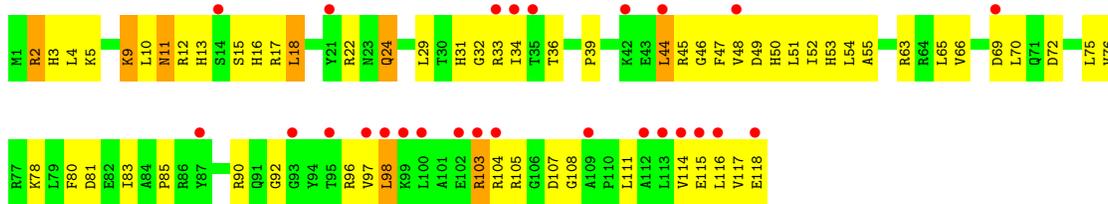


• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L17





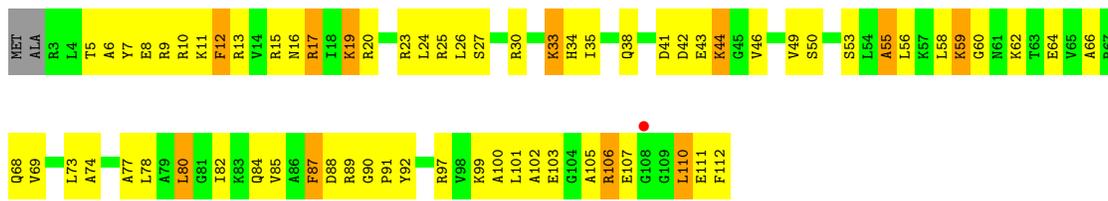
• Molecule 39: 50S ribosomal protein L17



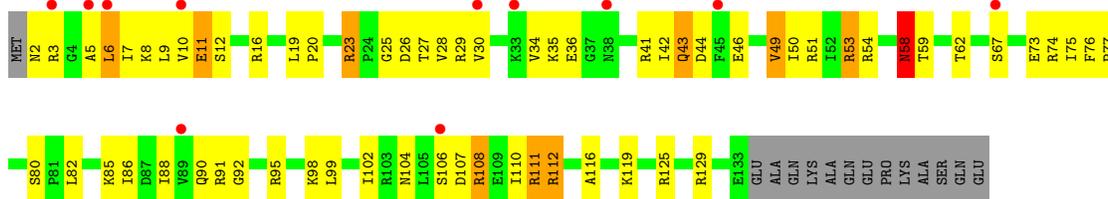
• Molecule 40: 50S ribosomal protein L18



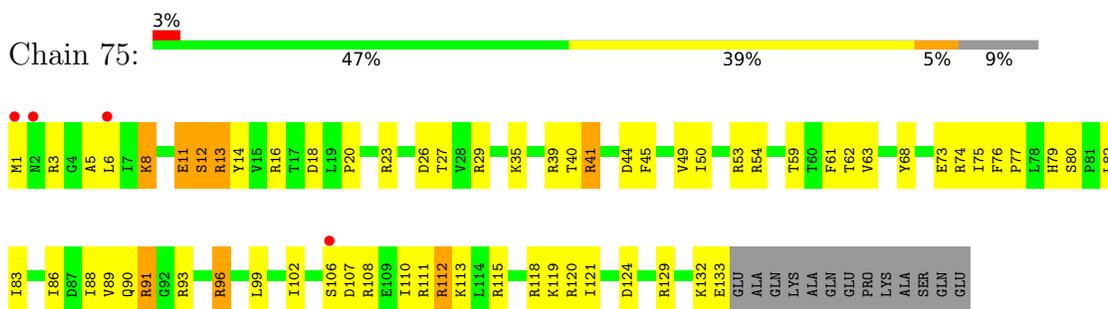
• Molecule 40: 50S ribosomal protein L18



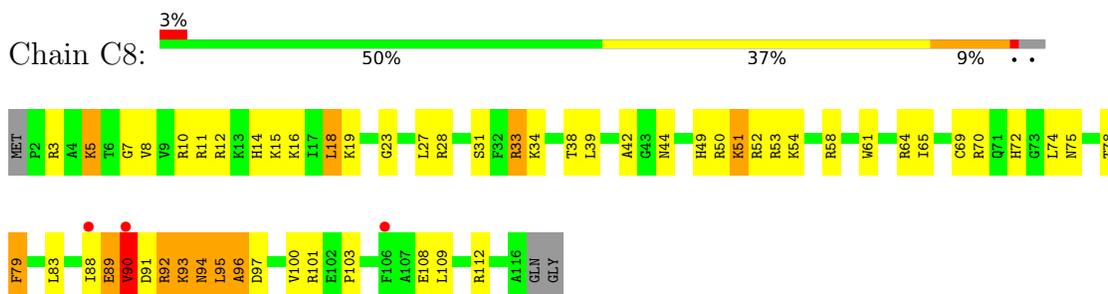
• Molecule 41: 50S ribosomal protein L19



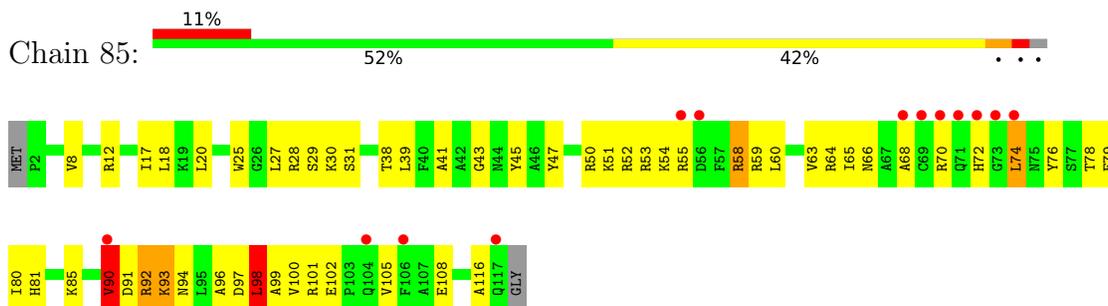
- Molecule 41: 50S ribosomal protein L19



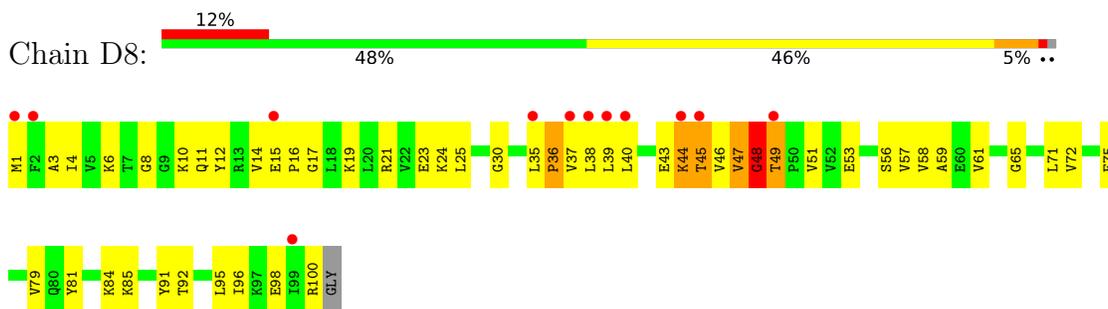
- Molecule 42: 50S ribosomal protein L20



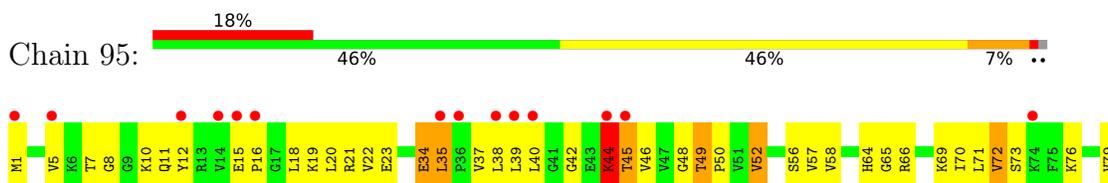
- Molecule 42: 50S ribosomal protein L20



- Molecule 43: 50S ribosomal protein L21

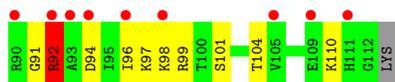


- Molecule 43: 50S ribosomal protein L21





- Molecule 44: 50S ribosomal protein L22



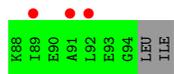
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23

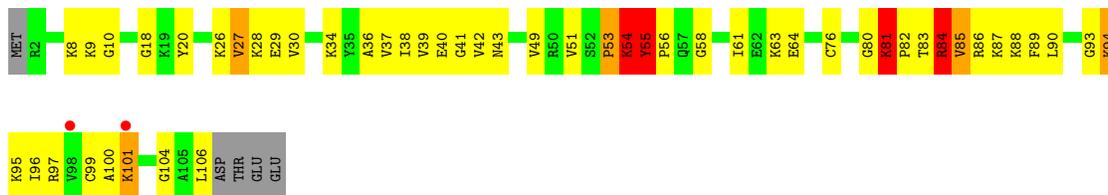


- Molecule 45: 50S ribosomal protein L23

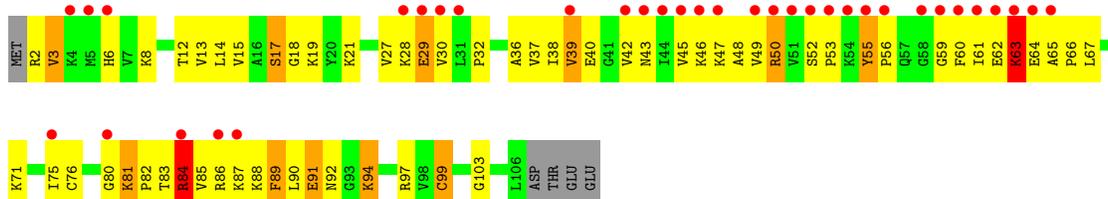


- Molecule 46: 50S ribosomal protein L24

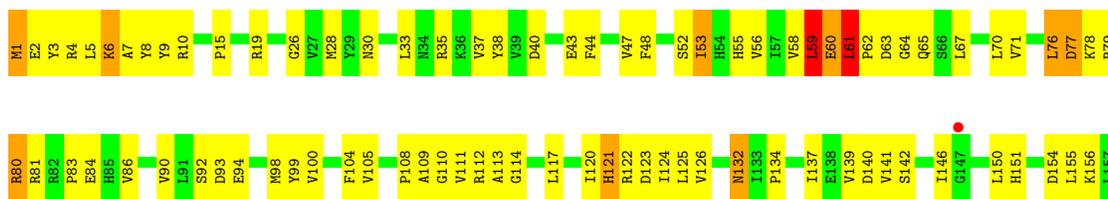




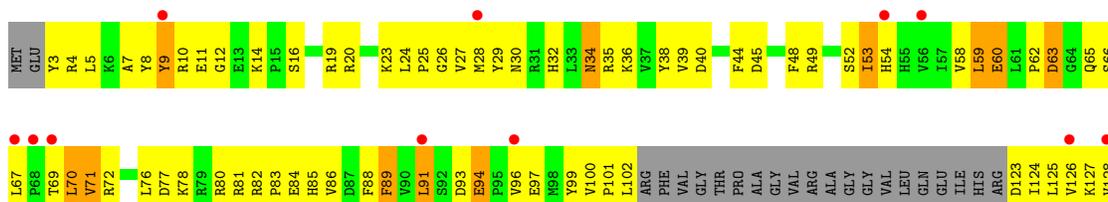
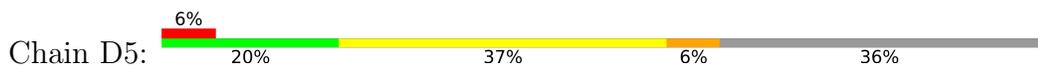
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L25



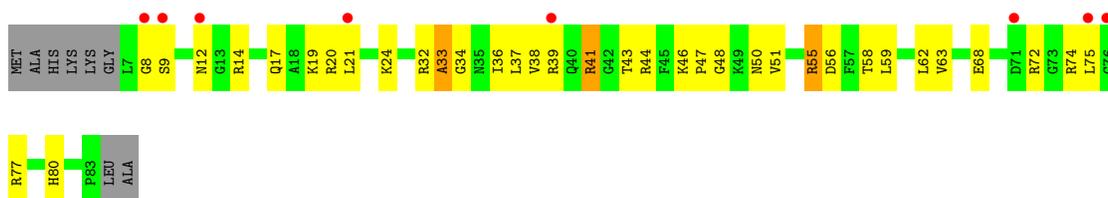
• Molecule 48: 50S ribosomal protein L27

Chain I8:  52% 36% 11%



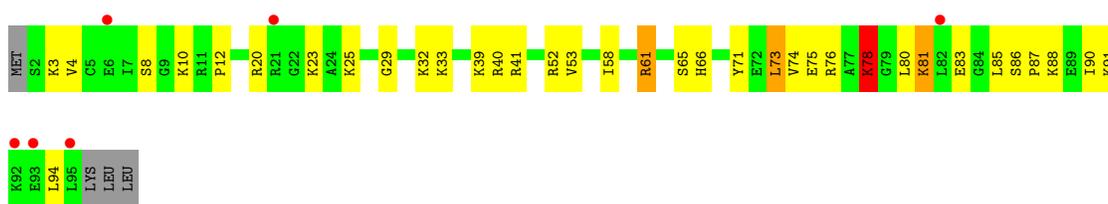
• Molecule 48: 50S ribosomal protein L27

Chain E5:  9% 48% 39% 9%



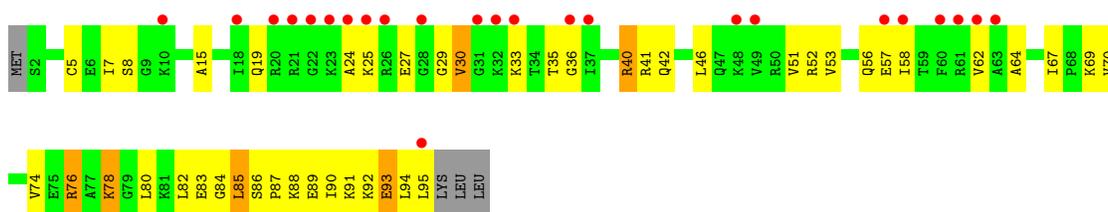
• Molecule 49: 50S ribosomal protein L28

Chain J8:  6% 59% 33%



• Molecule 49: 50S ribosomal protein L28

Chain F5:  24% 49% 41% 6%



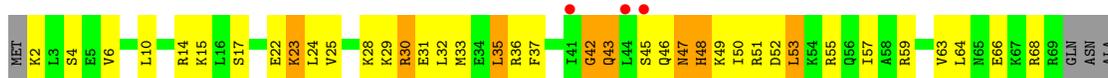
• Molecule 50: 50S ribosomal protein L29

Chain K8:  49% 36% 8% 6%

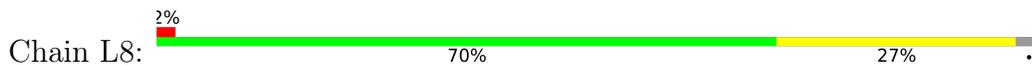


• Molecule 50: 50S ribosomal protein L29

Chain G5:  4% 42% 42% 11% 6%



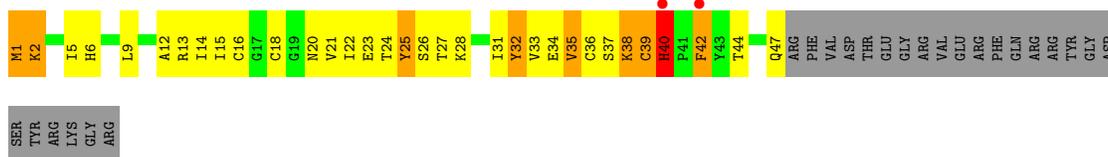
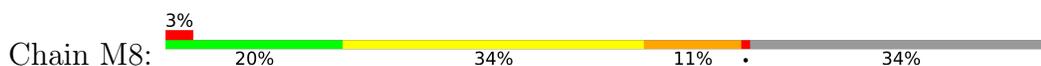
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



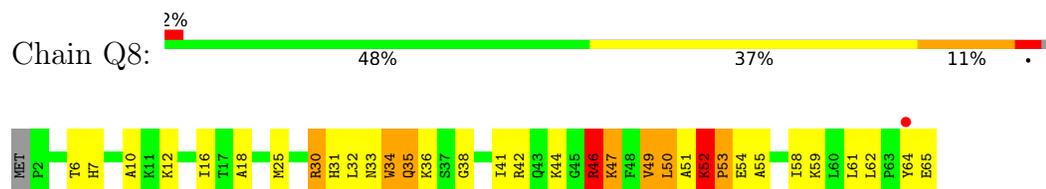
- Molecule 54: 50S ribosomal protein L34



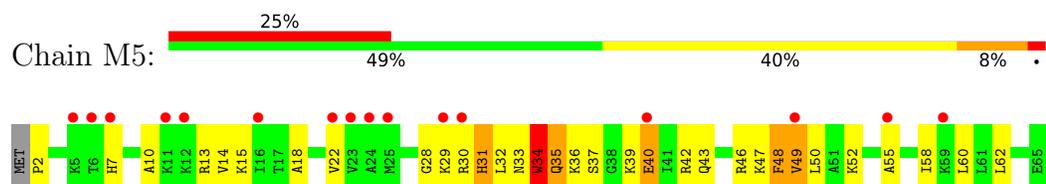
- Molecule 54: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	208.40Å 446.00Å 617.40Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 3.07Å)	Xtrriage
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 <sup>2</sup> )	91.6	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	294257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

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

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	13	0.93	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	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	29	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)
26:1H:943:U:OP2	37:78:36:LYS:NZ	1.64	1.30
31:39:38:ARG:NH2	31:39:99:TYR:CE1	1.96	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	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
31	39	197	ASP
49	F5	40	ARG
32	49	136	ARG
31	39	192	LEU
39	55	81	ASP

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

Mol	Chain	Res	Type
31	31	67	GLN
47	D5	65	GLN
3	22	181	ASN
50	G5	47	ASN
18	9A	63	GLN

### 5.3.3 RNA [i](#)

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
1	1G	1139	G
26	14	791	C
1	1G	1300	G
26	14	34	C
26	14	1396	U

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

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
22	PSU	1L	55	22	18,21,22	1.13	1 (5%)	22,30,33	1.57	4 (18%)
23	PSU	2K	56	23	18,21,22	1.23	2 (11%)	22,30,33	1.73	3 (13%)
22	PSU	1K	39	22	18,21,22	0.92	1 (5%)	22,30,33	1.54	3 (13%)
22	PSU	1K	55	22	18,21,22	1.15	1 (5%)	22,30,33	1.50	4 (18%)
24	PSU	3L	39	24	18,21,22	1.16	1 (5%)	22,30,33	1.43	2 (9%)
23	5MU	2K	55	23	19,22,23	3.69	5 (26%)	28,32,35	3.41	7 (25%)
23	4SU	2K	8	23	18,21,22	1.90	5 (27%)	26,30,33	2.73	8 (30%)
22	T6A	1K	37	22	27,34,35	2.55	5 (18%)	29,49,52	2.69	5 (17%)
22	U8U	1K	34	22	19,24,25	2.55	7 (36%)	23,34,37	1.05	2 (8%)
22	5MU	1K	54	22	19,22,23	3.70	5 (26%)	28,32,35	2.98	6 (21%)
23	OMC	2L	33	23	19,22,23	1.82	4 (21%)	26,31,34	1.27	2 (7%)
23	G7M	2K	47	23	20,26,27	2.36	6 (30%)	17,39,42	0.92	1 (5%)
23	PSU	2L	56	23	18,21,22	1.21	1 (5%)	22,30,33	1.83	4 (18%)
23	5MU	2L	55	23	19,22,23	3.86	5 (26%)	28,32,35	3.46	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	2L	8	23	18,21,22	1.78	3 (16%)	26,30,33	2.60	4 (15%)
24	PSU	3K	39	24	18,21,22	1.26	1 (5%)	22,30,33	1.82	7 (31%)
23	G7M	2L	47	23	20,26,27	2.47	7 (35%)	17,39,42	1.06	1 (5%)
22	5MU	1L	54	22	19,22,23	3.96	5 (26%)	28,32,35	3.36	9 (32%)
23	OMC	2K	33	23	19,22,23	1.73	3 (15%)	26,31,34	1.14	2 (7%)
22	T6A	1L	37	22	27,34,35	2.58	6 (22%)	29,49,52	2.36	9 (31%)
22	PSU	1L	39	22	18,21,22	1.10	1 (5%)	22,30,33	1.61	3 (13%)
22	U8U	1L	34	22,25	19,24,25	2.57	7 (36%)	23,34,37	0.91	2 (8%)

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
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/19/41/42	0/3/3/3
22	U8U	1K	34	22	-	0/9/28/29	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	3/9/27/28	0/2/2/2
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	1/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	2/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
22	5MU	1L	54	22	-	3/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	T6A	1L	37	22	-	5/19/41/42	0/3/3/3
22	PSU	1L	39	22	-	1/7/25/26	0/2/2/2
22	U8U	1L	34	22,25	-	4/9/28/29	0/2/2/2

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	12.96	1.59	1.38
23	2L	55	5MU	C2-N1	12.45	1.58	1.38
22	1K	54	5MU	C2-N1	11.70	1.57	1.38
23	2K	55	5MU	C2-N1	11.53	1.56	1.38
22	1L	37	T6A	C6-N6	7.58	1.49	1.36

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	11.33	124.98	115.31
23	2L	55	5MU	C5-C4-N3	10.65	124.40	115.31
22	1K	54	5MU	C5-C4-N3	10.44	124.22	115.31
22	1L	54	5MU	C5-C4-N3	10.32	124.12	115.31
22	1K	37	T6A	C2-N1-C6	9.05	124.35	116.59

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	34	U8U	N-C-C5-C4
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10
22	1L	54	5MU	O4'-C4'-C5'-O5'
23	2L	47	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 27 short contacts:

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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1L	39	PSU	2	0
22	1L	34	USU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	3E	302	4	0,12,12	-	-	-		
58	SF4	32	301	4	0,12,12	-	-	-		
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%)

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	3E	302	4	-	-	0/6/5/5
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

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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:

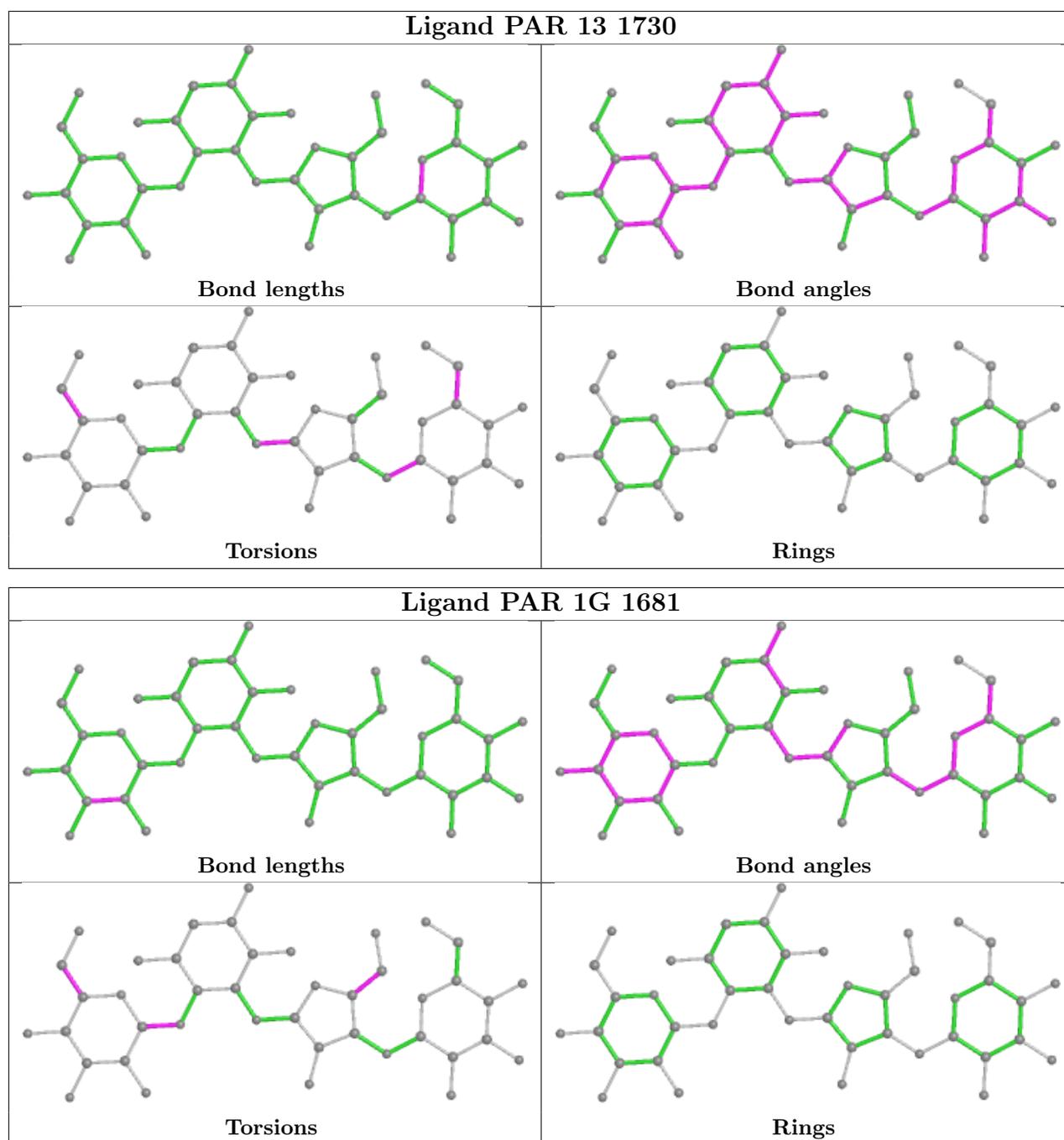
Mol	Chain	Res	Type	Atoms
57	13	1730	PAR	O54-C54-C64-N64
57	1G	1681	PAR	O51-C51-C61-O61
57	1G	1681	PAR	C41-C51-C61-O61
57	13	1730	PAR	C41-C51-C61-O61
57	1G	1681	PAR	O51-C11-O11-C42

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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
25	4K	1
37	35	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	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, 158	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 <sup>2</sup> )	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 <sup>2</sup> )	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, 138	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, 128, 134	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	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	4SU	2L	8	20/21	0.90	0.16	114,124,129,130	0
23	OMC	2L	33	21/22	0.90	0.15	105,114,118,121	0
22	PSU	1K	55	20/21	0.91	0.15	102,113,120,131	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
24	PSU	3K	39	20/21	0.92	0.17	141,151,156,159	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
22	T6A	1K	37	32/33	0.92	0.21	79,94,121,123	0
23	G7M	2L	47	24/25	0.93	0.12	126,133,141,145	0
22	PSU	1K	39	20/21	0.93	0.14	98,115,125,127	0
23	PSU	2L	56	20/21	0.93	0.11	115,126,131,135	0
23	4SU	2K	8	20/21	0.94	0.14	91,98,107,109	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
24	PSU	3L	39	20/21	0.94	0.23	145,155,159,162	0
22	U8U	1K	34	23/24	0.95	0.15	84,92,100,108	0
23	G7M	2K	47	24/25	0.95	0.13	102,114,127,133	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2K	102	1/1	0.28	0.72	126,126,126,126	0
56	MG	1H	3317	1/1	0.28	0.63	105,105,105,105	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	1H	3298	1/1	0.47	0.35	93,93,93,93	0
56	MG	13	1655	1/1	0.47	0.33	103,103,103,103	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	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	14	3298	1/1	0.58	0.28	94,94,94,94	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	3295	1/1	0.60	0.41	85,85,85,85	0
56	MG	1H	3250	1/1	0.60	0.45	87,87,87,87	0
56	MG	1H	3206	1/1	0.61	0.51	94,94,94,94	0
56	MG	13	1701	1/1	0.61	0.23	121,121,121,121	0
56	MG	1H	3274	1/1	0.61	0.46	85,85,85,85	0
56	MG	1H	3028	1/1	0.61	0.60	72,72,72,72	0
56	MG	1H	3319	1/1	0.61	0.26	102,102,102,102	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	14	3289	1/1	0.63	0.29	91,91,91,91	0
56	MG	1H	3264	1/1	0.63	0.18	84,84,84,84	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	3018	1/1	0.64	0.59	78,78,78,78	0
56	MG	1H	3308	1/1	0.64	0.57	99,99,99,99	0
56	MG	13	1642	1/1	0.64	0.19	73,73,73,73	0
56	MG	1H	3110	1/1	0.64	0.28	65,65,65,65	0
56	MG	E5	101	1/1	0.64	0.32	83,83,83,83	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
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	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	3181	1/1	0.65	0.18	98,98,98,98	0
56	MG	14	3262	1/1	0.65	0.44	91,91,91,91	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	14	3153	1/1	0.66	0.38	78,78,78,78	0
56	MG	1H	3189	1/1	0.67	0.42	84,84,84,84	0
56	MG	1H	3213	1/1	0.67	0.61	84,84,84,84	0
56	MG	14	3162	1/1	0.67	0.51	83,83,83,83	0
56	MG	1G	1643	1/1	0.67	0.33	91,91,91,91	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	14	3169	1/1	0.69	0.10	104,104,104,104	0
56	MG	1H	3052	1/1	0.69	0.84	99,99,99,99	0
56	MG	14	3140	1/1	0.69	0.18	87,87,87,87	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	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	3200	1/1	0.70	0.33	87,87,87,87	0
56	MG	1H	3423	1/1	0.70	0.06	147,147,147,147	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	14	3261	1/1	0.71	0.59	83,83,83,83	0
56	MG	13	1674	1/1	0.71	0.50	92,92,92,92	0
56	MG	45	202	1/1	0.71	0.20	103,103,103,103	0
56	MG	1H	3275	1/1	0.71	0.42	74,74,74,74	0
56	MG	14	3126	1/1	0.72	1.12	83,83,83,83	0
56	MG	14	3220	1/1	0.72	0.37	107,107,107,107	0
56	MG	14	3296	1/1	0.72	0.26	91,91,91,91	0
56	MG	1H	3193	1/1	0.72	0.40	72,72,72,72	0
56	MG	1H	3301	1/1	0.72	0.29	128,128,128,128	0
56	MG	14	3301	1/1	0.72	0.39	99,99,99,99	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	13	1695	1/1	0.72	0.42	103,103,103,103	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3091	1/1	0.72	0.92	87,87,87,87	0
56	MG	1H	3214	1/1	0.72	0.25	68,68,68,68	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	3252	1/1	0.73	0.09	73,73,73,73	0
56	MG	14	3249	1/1	0.73	0.15	78,78,78,78	0
56	MG	1H	3302	1/1	0.74	0.51	89,89,89,89	0
56	MG	1H	3015	1/1	0.74	0.41	77,77,77,77	0
56	MG	14	3272	1/1	0.74	0.40	93,93,93,93	0
56	MG	16	207	1/1	0.74	0.42	76,76,76,76	0
56	MG	1H	3284	1/1	0.74	0.18	88,88,88,88	0
56	MG	1H	3160	1/1	0.74	0.40	69,69,69,69	0
56	MG	1H	3185	1/1	0.74	0.24	78,78,78,78	0
56	MG	13	1693	1/1	0.74	0.41	88,88,88,88	0
56	MG	1H	3277	1/1	0.75	0.30	100,100,100,100	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	1H	3032	1/1	0.75	0.21	80,80,80,80	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	3273	1/1	0.75	0.33	94,94,94,94	0
56	MG	1H	3198	1/1	0.75	0.20	67,67,67,67	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	3110	1/1	0.75	0.76	88,88,88,88	0
56	MG	1H	3042	1/1	0.76	0.26	93,93,93,93	0
56	MG	14	3254	1/1	0.76	0.73	78,78,78,78	0
56	MG	14	3198	1/1	0.76	0.30	80,80,80,80	0
56	MG	1H	3299	1/1	0.76	0.45	86,86,86,86	0
56	MG	1G	1638	1/1	0.76	0.54	81,81,81,81	0
56	MG	1H	3258	1/1	0.76	0.37	72,72,72,72	0
56	MG	1H	3125	1/1	0.76	0.23	87,87,87,87	0
56	MG	1H	3041	1/1	0.76	0.32	77,77,77,77	0
56	MG	14	3233	1/1	0.76	0.76	80,80,80,80	0
56	MG	1H	3315	1/1	0.76	0.13	91,91,91,91	0
56	MG	1H	3099	1/1	0.76	0.45	75,75,75,75	0
56	MG	1G	1616	1/1	0.77	0.49	96,96,96,96	0
56	MG	14	3197	1/1	0.77	0.36	84,84,84,84	0
56	MG	13	1623	1/1	0.77	0.33	105,105,105,105	0
56	MG	14	3255	1/1	0.77	0.25	87,87,87,87	0
56	MG	1H	3039	1/1	0.77	0.55	80,80,80,80	0
56	MG	1H	3273	1/1	0.77	0.64	84,84,84,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3046	1/1	0.78	0.47	87,87,87,87	0
56	MG	14	3278	1/1	0.78	0.35	96,96,96,96	0
56	MG	1G	1654	1/1	0.78	0.45	86,86,86,86	0
56	MG	14	3284	1/1	0.78	0.23	84,84,84,84	0
56	MG	1G	1666	1/1	0.78	0.51	85,85,85,85	0
56	MG	14	3146	1/1	0.78	0.37	61,61,61,61	0
56	MG	14	3291	1/1	0.78	0.66	94,94,94,94	0
56	MG	1K	101	1/1	0.78	0.54	138,138,138,138	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	14	3299	1/1	0.78	0.19	96,96,96,96	0
56	MG	1H	3269	1/1	0.78	0.35	97,97,97,97	0
56	MG	14	3177	1/1	0.78	0.45	87,87,87,87	0
56	MG	1H	3075	1/1	0.78	0.11	79,79,79,79	0
56	MG	14	3191	1/1	0.78	0.18	76,76,76,76	0
56	MG	1H	3291	1/1	0.78	0.46	99,99,99,99	0
56	MG	13	1690	1/1	0.78	0.44	81,81,81,81	0
56	MG	Q8	101	1/1	0.78	0.29	83,83,83,83	0
56	MG	14	3120	1/1	0.78	0.34	71,71,71,71	0
56	MG	1G	1637	1/1	0.79	0.46	97,97,97,97	0
56	MG	1H	3316	1/1	0.79	0.47	87,87,87,87	0
56	MG	13	1676	1/1	0.79	0.20	127,127,127,127	0
56	MG	14	3202	1/1	0.79	0.18	79,79,79,79	0
56	MG	41	201	1/1	0.79	0.27	71,71,71,71	0
56	MG	1H	3134	1/1	0.79	0.41	90,90,90,90	0
56	MG	14	3222	1/1	0.79	0.42	80,80,80,80	0
56	MG	14	3156	1/1	0.79	0.40	62,62,62,62	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	1H	3093	1/1	0.79	0.22	72,72,72,72	0
56	MG	1G	1651	1/1	0.79	0.58	93,93,93,93	0
56	MG	1H	3034	1/1	0.79	0.35	78,78,78,78	0
56	MG	1H	3038	1/1	0.79	0.35	81,81,81,81	0
56	MG	1H	3155	1/1	0.80	0.36	86,86,86,86	0
56	MG	14	3227	1/1	0.80	0.28	81,81,81,81	0
56	MG	1H	3278	1/1	0.80	0.75	92,92,92,92	0
56	MG	I8	102	1/1	0.80	0.45	83,83,83,83	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	13	1629	1/1	0.80	0.41	90,90,90,90	0
56	MG	1H	3289	1/1	0.80	0.33	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1608	1/1	0.80	0.30	91,91,91,91	0
56	MG	14	3214	1/1	0.80	0.51	87,87,87,87	0
56	MG	1G	1622	1/1	0.80	0.68	99,99,99,99	0
56	MG	13	1698	1/1	0.80	0.22	81,81,81,81	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	3045	1/1	0.81	0.39	116,116,116,116	0
56	MG	14	3003	1/1	0.81	0.28	69,69,69,69	0
56	MG	14	3130	1/1	0.81	0.68	78,78,78,78	0
56	MG	1H	3297	1/1	0.81	0.11	101,101,101,101	0
56	MG	14	3143	1/1	0.81	0.29	70,70,70,70	0
56	MG	14	3024	1/1	0.81	0.37	74,74,74,74	0
56	MG	13	1627	1/1	0.81	0.45	81,81,81,81	0
56	MG	1H	3205	1/1	0.81	0.41	83,83,83,83	0
56	MG	14	3221	1/1	0.81	0.17	91,91,91,91	0
56	MG	14	3308	1/1	0.81	0.27	82,82,82,82	0
56	MG	1H	3280	1/1	0.81	0.22	88,88,88,88	0
56	MG	1J	202	1/1	0.81	0.25	104,104,104,104	0
56	MG	1H	3220	1/1	0.81	0.37	87,87,87,87	0
56	MG	1H	3019	1/1	0.81	0.38	89,89,89,89	0
56	MG	1H	3138	1/1	0.81	0.37	61,61,61,61	0
56	MG	14	3180	1/1	0.81	0.25	79,79,79,79	0
56	MG	1H	3011	1/1	0.82	0.49	71,71,71,71	0
56	MG	1H	3123	1/1	0.82	0.43	77,77,77,77	0
56	MG	14	3114	1/1	0.82	0.25	81,81,81,81	0
56	MG	14	3117	1/1	0.82	0.55	77,77,77,77	0
56	MG	13	1604	1/1	0.82	0.29	93,93,93,93	0
56	MG	1G	1630	1/1	0.82	0.72	108,108,108,108	0
56	MG	1H	3096	1/1	0.82	0.34	78,78,78,78	0
56	MG	1H	3044	1/1	0.82	0.49	89,89,89,89	0
56	MG	1H	3201	1/1	0.82	0.43	70,70,70,70	0
56	MG	14	3023	1/1	0.82	0.34	55,55,55,55	0
56	MG	78	201	1/1	0.82	0.21	75,75,75,75	0
56	MG	14	3031	1/1	0.82	0.43	76,76,76,76	0
56	MG	1H	3236	1/1	0.82	0.32	91,91,91,91	0
56	MG	1H	3161	1/1	0.82	0.21	84,84,84,84	0
56	MG	14	3062	1/1	0.82	0.11	81,81,81,81	0
56	MG	1H	3182	1/1	0.82	0.28	77,77,77,77	0
56	MG	1G	1609	1/1	0.82	0.19	94,94,94,94	0
56	MG	14	3203	1/1	0.83	0.16	68,68,68,68	0
56	MG	1H	3241	1/1	0.83	0.29	73,73,73,73	0
56	MG	14	3211	1/1	0.83	0.28	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3277	1/1	0.83	0.52	92,92,92,92	0
56	MG	1H	3013	1/1	0.83	0.39	89,89,89,89	0
56	MG	1H	3141	1/1	0.83	0.17	69,69,69,69	0
56	MG	13	1696	1/1	0.83	0.43	111,111,111,111	0
56	MG	14	3035	1/1	0.83	0.41	84,84,84,84	0
56	MG	1H	3107	1/1	0.83	0.36	73,73,73,73	0
56	MG	1H	3202	1/1	0.83	0.32	75,75,75,75	0
56	MG	14	3168	1/1	0.83	0.45	66,66,66,66	0
56	MG	1H	3029	1/1	0.83	0.36	69,69,69,69	0
56	MG	1H	3053	1/1	0.83	0.54	82,82,82,82	0
56	MG	14	3240	1/1	0.83	0.38	87,87,87,87	0
56	MG	1H	3124	1/1	0.83	0.24	59,59,59,59	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	14	3186	1/1	0.83	0.79	83,83,83,83	0
56	MG	13	1700	1/1	0.83	0.12	111,111,111,111	0
56	MG	14	3259	1/1	0.83	0.23	84,84,84,84	0
56	MG	1H	3083	1/1	0.83	0.17	75,75,75,75	0
56	MG	1H	3186	1/1	0.83	0.17	71,71,71,71	0
56	MG	13	1694	1/1	0.83	0.15	96,96,96,96	0
56	MG	14	3019	1/1	0.83	0.43	84,84,84,84	0
56	MG	85	201	1/1	0.83	0.49	88,88,88,88	0
56	MG	14	3269	1/1	0.83	0.38	75,75,75,75	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	14	3075	1/1	0.84	1.26	90,90,90,90	0
56	MG	14	3279	1/1	0.84	0.25	73,73,73,73	0
56	MG	1H	3135	1/1	0.84	0.29	81,81,81,81	0
56	MG	13	1605	1/1	0.84	0.19	75,75,75,75	0
56	MG	1H	3211	1/1	0.84	0.36	71,71,71,71	0
56	MG	13	1636	1/1	0.84	0.55	85,85,85,85	0
56	MG	14	3239	1/1	0.84	0.26	79,79,79,79	0
56	MG	1H	3040	1/1	0.84	0.66	72,72,72,72	0
56	MG	14	3245	1/1	0.84	0.23	88,88,88,88	0
56	MG	1H	3296	1/1	0.84	0.53	92,92,92,92	0
56	MG	14	3187	1/1	0.84	0.42	75,75,75,75	0
56	MG	1H	3112	1/1	0.84	0.24	66,66,66,66	0
56	MG	1H	3271	1/1	0.84	0.46	94,94,94,94	0
56	MG	14	3196	1/1	0.84	0.33	69,69,69,69	0
56	MG	14	3257	1/1	0.84	0.38	68,68,68,68	0
56	MG	14	3026	1/1	0.84	0.51	68,68,68,68	0
56	MG	1H	3147	1/1	0.84	0.14	72,72,72,72	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3151	1/1	0.84	0.10	52,52,52,52	0
56	MG	13	1702	1/1	0.84	0.60	103,103,103,103	0
56	MG	39	301	1/1	0.84	0.12	80,80,80,80	0
56	MG	13	1689	1/1	0.84	0.21	92,92,92,92	0
56	MG	14	3060	1/1	0.84	0.25	92,92,92,92	0
56	MG	13	1637	1/1	0.84	0.50	68,68,68,68	0
56	MG	13	1664	1/1	0.84	0.34	99,99,99,99	0
56	MG	1H	3321	1/1	0.85	0.22	85,85,85,85	0
56	MG	2L	103	1/1	0.85	0.39	79,79,79,79	0
56	MG	14	3111	1/1	0.85	0.42	69,69,69,69	0
56	MG	1G	1627	1/1	0.85	0.28	85,85,85,85	0
56	MG	14	3012	1/1	0.85	0.67	82,82,82,82	0
56	MG	13	1677	1/1	0.85	0.33	91,91,91,91	0
56	MG	14	3188	1/1	0.85	0.44	92,92,92,92	0
56	MG	13	1692	1/1	0.85	0.36	100,100,100,100	0
56	MG	1H	3084	1/1	0.85	0.22	82,82,82,82	0
56	MG	1H	3257	1/1	0.85	0.34	94,94,94,94	0
56	MG	13	1681	1/1	0.85	0.25	106,106,106,106	0
56	MG	1H	3162	1/1	0.85	0.38	87,87,87,87	0
56	MG	14	3144	1/1	0.85	0.54	58,58,58,58	0
56	MG	1H	3304	1/1	0.85	0.40	73,73,73,73	0
56	MG	1G	1645	1/1	0.85	0.63	88,88,88,88	0
56	MG	1H	3282	1/1	0.85	0.15	78,78,78,78	0
56	MG	1H	3192	1/1	0.85	0.24	81,81,81,81	0
56	MG	14	3216	1/1	0.85	0.22	70,70,70,70	0
56	MG	1H	3287	1/1	0.85	0.65	86,86,86,86	0
56	MG	1H	3207	1/1	0.85	0.40	81,81,81,81	0
56	MG	14	3070	1/1	0.85	0.39	71,71,71,71	0
56	MG	1H	3240	1/1	0.85	0.21	56,56,56,56	0
56	MG	13	1603	1/1	0.85	0.56	92,92,92,92	0
56	MG	13	1672	1/1	0.86	0.19	81,81,81,81	0
56	MG	1H	3314	1/1	0.86	0.66	92,92,92,92	0
56	MG	14	3271	1/1	0.86	0.23	74,74,74,74	0
56	MG	1H	3043	1/1	0.86	0.51	87,87,87,87	0
56	MG	14	3210	1/1	0.86	0.38	96,96,96,96	0
56	MG	1H	3061	1/1	0.86	0.29	62,62,62,62	0
56	MG	14	3149	1/1	0.86	0.53	92,92,92,92	0
56	MG	14	3033	1/1	0.86	0.16	84,84,84,84	0
56	MG	1H	3128	1/1	0.86	0.27	83,83,83,83	0
56	MG	1H	3276	1/1	0.86	0.34	85,85,85,85	0
56	MG	1H	3173	1/1	0.86	0.47	79,79,79,79	0
56	MG	1G	1613	1/1	0.86	0.19	100,100,100,100	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1659	1/1	0.86	0.82	85,85,85,85	0
56	MG	1H	3149	1/1	0.86	0.26	65,65,65,65	0
56	MG	14	3292	1/1	0.86	0.22	86,86,86,86	0
56	MG	1G	1619	1/1	0.86	0.29	89,89,89,89	0
56	MG	14	3170	1/1	0.86	0.82	81,81,81,81	0
56	MG	14	3079	1/1	0.86	0.42	72,72,72,72	0
56	MG	1G	1679	1/1	0.86	0.05	138,138,138,138	0
56	MG	14	3244	1/1	0.86	0.32	74,74,74,74	0
56	MG	1H	3322	1/1	0.86	0.14	68,68,68,68	0
56	MG	14	3247	1/1	0.86	0.36	73,73,73,73	0
56	MG	4K	101	1/1	0.86	0.22	156,156,156,156	0
56	MG	1H	3348	1/1	0.86	0.10	100,100,100,100	0
56	MG	14	3309	1/1	0.86	0.25	90,90,90,90	0
56	MG	13	1654	1/1	0.86	0.34	88,88,88,88	0
56	MG	14	3015	1/1	0.86	0.42	63,63,63,63	0
56	MG	16	202	1/1	0.86	0.46	86,86,86,86	0
56	MG	14	3018	1/1	0.86	0.41	73,73,73,73	0
56	MG	14	3193	1/1	0.86	0.36	78,78,78,78	0
56	MG	45	201	1/1	0.86	0.20	96,96,96,96	0
56	MG	1H	3232	1/1	0.86	0.10	71,71,71,71	0
56	MG	13	1666	1/1	0.86	0.12	89,89,89,89	0
56	MG	14	3133	1/1	0.86	0.38	97,97,97,97	0
56	MG	1G	1649	1/1	0.87	0.49	96,96,96,96	0
56	MG	14	3235	1/1	0.87	0.43	104,104,104,104	0
56	MG	14	3280	1/1	0.87	0.23	99,99,99,99	0
56	MG	13	1638	1/1	0.87	0.47	87,87,87,87	0
56	MG	1H	3047	1/1	0.87	0.38	92,92,92,92	0
56	MG	14	3288	1/1	0.87	0.34	109,109,109,109	0
56	MG	1H	3230	1/1	0.87	0.17	73,73,73,73	0
56	MG	1G	1663	1/1	0.87	0.18	97,97,97,97	0
56	MG	14	3058	1/1	0.87	0.07	80,80,80,80	0
56	MG	1H	3300	1/1	0.87	0.30	77,77,77,77	0
56	MG	14	3148	1/1	0.87	0.20	72,72,72,72	0
56	MG	1H	3268	1/1	0.87	0.39	79,79,79,79	0
56	MG	1H	3164	1/1	0.87	0.23	73,73,73,73	0
56	MG	1H	3190	1/1	0.87	0.48	67,67,67,67	0
56	MG	1H	3307	1/1	0.87	0.20	82,82,82,82	0
56	MG	14	3258	1/1	0.87	0.62	99,99,99,99	0
56	MG	13	1649	1/1	0.87	0.15	75,75,75,75	0
56	MG	14	3088	1/1	0.87	0.40	73,73,73,73	0
56	MG	1H	3309	1/1	0.87	0.27	79,79,79,79	0
56	MG	13	1620	1/1	0.87	0.24	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3265	1/1	0.87	0.45	89,89,89,89	0
56	MG	1H	3290	1/1	0.87	0.32	80,80,80,80	0
56	MG	14	3268	1/1	0.87	0.15	86,86,86,86	0
56	MG	1H	3092	1/1	0.87	0.39	67,67,67,67	0
56	MG	L8	101	1/1	0.87	0.66	88,88,88,88	0
56	MG	14	3178	1/1	0.87	0.85	90,90,90,90	0
56	MG	1H	3178	1/1	0.87	0.35	74,74,74,74	0
56	MG	1H	3129	1/1	0.87	0.10	56,56,56,56	0
56	MG	1G	1606	1/1	0.87	0.20	82,82,82,82	0
56	MG	1H	3303	1/1	0.88	0.25	73,73,73,73	0
56	MG	14	3238	1/1	0.88	0.36	78,78,78,78	0
56	MG	1G	1642	1/1	0.88	0.30	123,123,123,123	0
56	MG	1H	3252	1/1	0.88	0.29	72,72,72,72	0
56	MG	14	3241	1/1	0.88	0.39	68,68,68,68	0
56	MG	14	3068	1/1	0.88	0.34	89,89,89,89	0
56	MG	1H	3216	1/1	0.88	0.37	80,80,80,80	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	13	1658	1/1	0.88	0.09	82,82,82,82	0
56	MG	1H	3311	1/1	0.88	0.48	96,96,96,96	0
56	MG	1H	3152	1/1	0.88	0.56	99,99,99,99	0
56	MG	1H	3242	1/1	0.88	0.33	64,64,64,64	0
56	MG	1G	1626	1/1	0.88	0.23	95,95,95,95	0
56	MG	1H	3244	1/1	0.88	0.19	84,84,84,84	0
56	MG	14	3212	1/1	0.88	0.31	69,69,69,69	0
56	MG	1G	1661	1/1	0.88	0.23	150,150,150,150	0
56	MG	1H	3247	1/1	0.88	0.23	73,73,73,73	0
56	MG	14	3176	1/1	0.88	0.43	88,88,88,88	0
56	MG	14	3305	1/1	0.88	0.32	86,86,86,86	0
56	MG	14	3263	1/1	0.88	0.31	82,82,82,82	0
56	MG	13	1641	1/1	0.88	0.45	75,75,75,75	0
56	MG	13	1680	1/1	0.88	0.56	87,87,87,87	0
56	MG	14	3382	1/1	0.88	0.16	100,100,100,100	0
56	MG	14	3179	1/1	0.88	0.85	84,84,84,84	0
56	MG	14	3037	1/1	0.88	0.33	70,70,70,70	0
56	MG	14	3270	1/1	0.88	0.24	84,84,84,84	0
56	MG	1G	1675	1/1	0.88	0.10	116,116,116,116	0
56	MG	14	3231	1/1	0.88	0.23	84,84,84,84	0
56	MG	14	3056	1/1	0.88	0.14	62,62,62,62	0
56	MG	14	3274	1/1	0.88	0.27	99,99,99,99	0
56	MG	13	1616	1/1	0.88	0.43	77,77,77,77	0
59	ZN	G8	201	1/1	0.88	0.15	144,144,144,144	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3132	1/1	0.89	0.52	78,78,78,78	0
56	MG	14	3208	1/1	0.89	0.16	67,67,67,67	0
56	MG	14	3253	1/1	0.89	0.39	76,76,76,76	0
56	MG	1H	3225	1/1	0.89	0.37	74,74,74,74	0
56	MG	1H	3209	1/1	0.89	0.35	82,82,82,82	0
56	MG	1H	3254	1/1	0.89	0.45	95,95,95,95	0
56	MG	13	1685	1/1	0.89	0.49	95,95,95,95	0
56	MG	14	3025	1/1	0.89	0.26	69,69,69,69	0
56	MG	1H	3327	1/1	0.89	0.23	95,95,95,95	0
56	MG	1H	3142	1/1	0.89	0.18	68,68,68,68	0
56	MG	1H	3263	1/1	0.89	0.47	94,94,94,94	0
56	MG	1H	3154	1/1	0.89	0.39	69,69,69,69	0
56	MG	1G	1664	1/1	0.89	0.39	119,119,119,119	0
56	MG	1H	3266	1/1	0.89	0.09	60,60,60,60	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	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	13	1686	1/1	0.89	0.50	73,73,73,73	0
56	MG	1H	3203	1/1	0.89	0.53	75,75,75,75	0
56	MG	1H	3218	1/1	0.89	0.22	76,76,76,76	0
56	MG	13	1691	1/1	0.89	0.27	109,109,109,109	0
56	MG	14	3007	1/1	0.89	0.64	63,63,63,63	0
56	MG	1H	3272	1/1	0.89	0.14	89,89,89,89	0
56	MG	14	3154	1/1	0.89	0.28	90,90,90,90	0
56	MG	1H	3159	1/1	0.89	0.43	83,83,83,83	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	1H	3286	1/1	0.90	0.13	64,64,64,64	0
56	MG	1H	3050	1/1	0.90	0.36	78,78,78,78	0
56	MG	14	3199	1/1	0.90	0.33	59,59,59,59	0
56	MG	1H	3188	1/1	0.90	0.47	76,76,76,76	0
56	MG	13	1728	1/1	0.90	0.09	127,127,127,127	0
56	MG	13	1684	1/1	0.90	0.27	114,114,114,114	0
56	MG	1H	3163	1/1	0.90	0.35	48,48,48,48	0
56	MG	14	3293	1/1	0.90	0.06	99,99,99,99	0
56	MG	14	3161	1/1	0.90	0.46	73,73,73,73	0
56	MG	I8	103	1/1	0.90	0.46	86,86,86,86	0
56	MG	1H	3102	1/1	0.90	0.33	55,55,55,55	0
56	MG	14	3165	1/1	0.90	0.29	60,60,60,60	0
56	MG	14	3102	1/1	0.90	0.27	76,76,76,76	0
56	MG	1H	3169	1/1	0.90	0.36	95,95,95,95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
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	3137	1/1	0.90	0.15	73,73,73,73	0
56	MG	14	3119	1/1	0.90	0.26	86,86,86,86	0
56	MG	1H	3325	1/1	0.90	0.30	76,76,76,76	0
56	MG	14	3310	1/1	0.90	0.25	120,120,120,120	0
56	MG	13	1628	1/1	0.90	0.34	95,95,95,95	0
56	MG	1G	1618	1/1	0.90	0.13	101,101,101,101	0
56	MG	1H	3204	1/1	0.90	0.16	100,100,100,100	0
56	MG	1H	3180	1/1	0.90	0.39	76,76,76,76	0
56	MG	14	3041	1/1	0.90	0.21	49,49,49,49	0
56	MG	13	1639	1/1	0.90	0.33	85,85,85,85	0
56	MG	1H	3283	1/1	0.90	0.24	85,85,85,85	0
56	MG	14	3145	1/1	0.90	0.24	67,67,67,67	0
56	MG	1H	3049	1/1	0.90	0.17	65,65,65,65	0
56	MG	C5	201	1/1	0.90	0.27	109,109,109,109	0
56	MG	16	204	1/1	0.90	0.40	98,98,98,98	0
56	MG	16	205	1/1	0.90	0.47	84,84,84,84	0
56	MG	P8	101	1/1	0.91	0.08	78,78,78,78	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	14	3039	1/1	0.91	1.32	103,103,103,103	0
56	MG	1G	1652	1/1	0.91	0.15	88,88,88,88	0
56	MG	1G	1603	1/1	0.91	0.36	101,101,101,101	0
56	MG	1H	3231	1/1	0.91	0.31	56,56,56,56	0
56	MG	14	3057	1/1	0.91	0.36	63,63,63,63	0
56	MG	13	1625	1/1	0.91	0.55	82,82,82,82	0
56	MG	1G	1611	1/1	0.91	0.45	108,108,108,108	0
56	MG	14	3281	1/1	0.91	1.28	89,89,89,89	0
56	MG	14	3228	1/1	0.91	0.33	93,93,93,93	0
56	MG	14	3159	1/1	0.91	0.44	81,81,81,81	0
56	MG	14	3061	1/1	0.91	0.18	97,97,97,97	0
56	MG	1H	3035	1/1	0.91	0.37	76,76,76,76	0
56	MG	1G	1665	1/1	0.91	0.28	93,93,93,93	0
56	MG	1H	3238	1/1	0.91	0.12	82,82,82,82	0
56	MG	14	3069	1/1	0.91	0.74	91,91,91,91	0
56	MG	13	1656	1/1	0.91	0.30	88,88,88,88	0
56	MG	14	3071	1/1	0.91	0.16	84,84,84,84	0
56	MG	1H	3183	1/1	0.91	0.41	90,90,90,90	0
56	MG	14	3076	1/1	0.91	0.43	89,89,89,89	0
56	MG	1H	3184	1/1	0.91	0.42	96,96,96,96	0
56	MG	14	3087	1/1	0.91	0.34	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3246	1/1	0.91	0.31	72,72,72,72	0
56	MG	13	1673	1/1	0.91	0.12	102,102,102,102	0
56	MG	1G	1625	1/1	0.91	0.60	76,76,76,76	0
56	MG	14	3092	1/1	0.91	0.17	75,75,75,75	0
56	MG	13	1607	1/1	0.91	0.65	85,85,85,85	0
56	MG	1H	3187	1/1	0.91	0.38	95,95,95,95	0
56	MG	13	1697	1/1	0.91	0.45	96,96,96,96	0
56	MG	1G	1632	1/1	0.91	0.49	102,102,102,102	0
56	MG	14	3256	1/1	0.91	0.60	76,76,76,76	0
56	MG	13	1644	1/1	0.91	0.28	84,84,84,84	0
56	MG	13	1663	1/1	0.91	0.18	75,75,75,75	0
56	MG	16	211	1/1	0.91	0.11	85,85,85,85	0
56	MG	1G	1639	1/1	0.91	0.74	80,80,80,80	0
56	MG	14	3022	1/1	0.91	0.43	83,83,83,83	0
56	MG	1H	3121	1/1	0.91	0.51	53,53,53,53	0
56	MG	1H	3076	1/1	0.91	0.14	65,65,65,65	0
56	MG	1H	3079	1/1	0.91	0.18	61,61,61,61	0
56	MG	1H	3259	1/1	0.91	0.14	80,80,80,80	0
56	MG	1H	3221	1/1	0.91	0.41	78,78,78,78	0
56	MG	1H	3148	1/1	0.91	0.17	49,49,49,49	0
56	MG	1H	3098	1/1	0.92	0.20	69,69,69,69	0
56	MG	1H	3153	1/1	0.92	0.16	60,60,60,60	0
56	MG	1H	3293	1/1	0.92	0.43	98,98,98,98	0
56	MG	1G	1656	1/1	0.92	0.30	138,138,138,138	0
56	MG	13	1643	1/1	0.92	0.30	79,79,79,79	0
56	MG	1H	3054	1/1	0.92	0.20	87,87,87,87	0
56	MG	1G	1662	1/1	0.92	0.24	133,133,133,133	0
56	MG	1H	3156	1/1	0.92	0.36	77,77,77,77	0
56	MG	1G	1614	1/1	0.92	0.28	93,93,93,93	0
56	MG	14	3155	1/1	0.92	0.22	71,71,71,71	0
56	MG	1H	3027	1/1	0.92	0.35	48,48,48,48	0
56	MG	1H	3373	1/1	0.92	0.04	82,82,82,82	0
56	MG	1H	3415	1/1	0.92	0.11	94,94,94,94	0
56	MG	14	3230	1/1	0.92	0.36	72,72,72,72	0
56	MG	1H	3418	1/1	0.92	0.07	88,88,88,88	0
56	MG	1G	1672	1/1	0.92	0.11	121,121,121,121	0
56	MG	14	3285	1/1	0.92	0.56	72,72,72,72	0
56	MG	13	1633	1/1	0.92	0.20	65,65,65,65	0
56	MG	1G	1677	1/1	0.92	0.12	119,119,119,119	0
56	MG	16	201	1/1	0.92	0.21	92,92,92,92	0
56	MG	1G	1682	1/1	0.92	0.14	91,91,91,91	0
56	MG	13	1650	1/1	0.92	0.34	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3083	1/1	0.92	0.37	87,87,87,87	0
56	MG	14	3295	1/1	0.92	0.21	114,114,114,114	0
56	MG	14	3175	1/1	0.92	0.46	96,96,96,96	0
56	MG	14	3242	1/1	0.92	0.32	70,70,70,70	0
56	MG	5E	201	1/1	0.92	0.26	84,84,84,84	0
56	MG	1G	1629	1/1	0.92	0.52	104,104,104,104	0
56	MG	14	3004	1/1	0.92	0.18	83,83,83,83	0
56	MG	3I	201	1/1	0.92	0.19	62,62,62,62	0
56	MG	14	3095	1/1	0.92	0.47	56,56,56,56	0
56	MG	13	1651	1/1	0.92	0.19	86,86,86,86	0
56	MG	14	3251	1/1	0.92	0.23	106,106,106,106	0
56	MG	14	3013	1/1	0.92	0.20	83,83,83,83	0
56	MG	13	1688	1/1	0.92	0.25	94,94,94,94	0
56	MG	1H	3166	1/1	0.92	0.13	68,68,68,68	0
56	MG	14	3338	1/1	0.92	0.12	111,111,111,111	0
56	MG	14	3374	1/1	0.92	0.08	129,129,129,129	0
56	MG	14	3380	1/1	0.92	0.07	83,83,83,83	0
56	MG	14	3113	1/1	0.92	0.16	78,78,78,78	0
56	MG	1H	3126	1/1	0.92	0.34	72,72,72,72	0
56	MG	1J	201	1/1	0.92	0.30	90,90,90,90	0
56	MG	21	301	1/1	0.92	0.19	57,57,57,57	0
56	MG	13	1652	1/1	0.92	0.26	74,74,74,74	0
56	MG	1H	3199	1/1	0.92	0.54	74,74,74,74	0
56	MG	1H	3312	1/1	0.92	0.21	67,67,67,67	0
56	MG	1H	3222	1/1	0.92	0.50	79,79,79,79	0
56	MG	1H	3223	1/1	0.92	0.44	88,88,88,88	0
56	MG	1H	3171	1/1	0.92	0.25	74,74,74,74	0
56	MG	14	3264	1/1	0.92	0.16	92,92,92,92	0
56	MG	1H	3024	1/1	0.92	0.46	70,70,70,70	0
56	MG	1H	3227	1/1	0.92	0.17	50,50,50,50	0
56	MG	14	3073	1/1	0.93	0.53	81,81,81,81	0
56	MG	1H	3226	1/1	0.93	0.29	55,55,55,55	0
56	MG	1H	3009	1/1	0.93	0.24	66,66,66,66	0
56	MG	13	1683	1/1	0.93	0.28	91,91,91,91	0
56	MG	13	1706	1/1	0.93	0.04	87,87,87,87	0
56	MG	14	3027	1/1	0.93	0.61	71,71,71,71	0
56	MG	14	3029	1/1	0.93	0.15	83,83,83,83	0
56	MG	1H	3262	1/1	0.93	0.40	77,77,77,77	0
56	MG	1G	1674	1/1	0.93	0.06	123,123,123,123	0
56	MG	1H	3014	1/1	0.93	0.26	69,69,69,69	0
56	MG	13	1720	1/1	0.93	0.16	115,115,115,115	0
56	MG	14	3036	1/1	0.93	0.17	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3106	1/1	0.93	0.81	69,69,69,69	0
56	MG	14	3300	1/1	0.93	0.58	89,89,89,89	0
56	MG	14	3215	1/1	0.93	0.16	83,83,83,83	0
56	MG	14	3164	1/1	0.93	0.44	83,83,83,83	0
56	MG	14	3218	1/1	0.93	0.35	60,60,60,60	0
56	MG	14	3219	1/1	0.93	0.55	78,78,78,78	0
56	MG	14	3107	1/1	0.93	0.45	87,87,87,87	0
56	MG	13	1671	1/1	0.93	0.44	102,102,102,102	0
56	MG	1H	3055	1/1	0.93	0.41	88,88,88,88	0
56	MG	14	3040	1/1	0.93	0.49	84,84,84,84	0
56	MG	14	3317	1/1	0.93	0.16	64,64,64,64	0
56	MG	1H	3313	1/1	0.93	0.32	66,66,66,66	0
56	MG	14	3344	1/1	0.93	0.04	95,95,95,95	0
56	MG	14	3173	1/1	0.93	0.19	82,82,82,82	0
56	MG	1H	3057	1/1	0.93	0.26	52,52,52,52	0
56	MG	1H	3005	1/1	0.93	0.22	62,62,62,62	0
56	MG	1H	3243	1/1	0.93	0.13	56,56,56,56	0
56	MG	1H	3106	1/1	0.93	0.41	77,77,77,77	0
56	MG	1H	3008	1/1	0.93	0.32	74,74,74,74	0
56	MG	1H	3037	1/1	0.93	0.48	63,63,63,63	0
56	MG	14	3276	1/1	0.93	0.11	102,102,102,102	0
56	MG	1H	3077	1/1	0.93	0.11	63,63,63,63	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	88	202	1/1	0.93	0.30	87,87,87,87	0
56	MG	1H	3251	1/1	0.93	0.24	63,63,63,63	0
56	MG	14	3020	1/1	0.93	0.48	76,76,76,76	0
56	MG	1H	3120	1/1	0.93	0.12	41,41,41,41	0
56	MG	14	3124	1/1	0.94	0.27	70,70,70,70	0
56	MG	14	3125	1/1	0.94	0.37	54,54,54,54	0
56	MG	1H	3094	1/1	0.94	0.26	91,91,91,91	0
56	MG	1G	1655	1/1	0.94	0.07	94,94,94,94	0
56	MG	14	3201	1/1	0.94	0.28	60,60,60,60	0
56	MG	1H	3323	1/1	0.94	0.50	91,91,91,91	0
56	MG	14	3132	1/1	0.94	0.40	91,91,91,91	0
56	MG	1H	3239	1/1	0.94	0.28	81,81,81,81	0
56	MG	1H	3210	1/1	0.94	0.28	73,73,73,73	0
56	MG	14	3137	1/1	0.94	0.18	62,62,62,62	0
56	MG	1H	3067	1/1	0.94	0.33	63,63,63,63	0
56	MG	14	3142	1/1	0.94	0.12	111,111,111,111	0
56	MG	1H	3016	1/1	0.94	0.41	48,48,48,48	0
56	MG	1H	3352	1/1	0.94	0.12	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3369	1/1	0.94	0.17	69,69,69,69	0
56	MG	1H	3017	1/1	0.94	0.36	77,77,77,77	0
56	MG	14	3147	1/1	0.94	0.14	93,93,93,93	0
56	MG	1H	3376	1/1	0.94	0.07	60,60,60,60	0
56	MG	1H	3391	1/1	0.94	0.08	107,107,107,107	0
56	MG	1H	3411	1/1	0.94	0.05	100,100,100,100	0
56	MG	1H	3412	1/1	0.94	0.11	68,68,68,68	0
56	MG	1H	3414	1/1	0.94	0.11	83,83,83,83	0
56	MG	14	3063	1/1	0.94	0.07	77,77,77,77	0
56	MG	1G	1676	1/1	0.94	0.07	111,111,111,111	0
56	MG	1G	1623	1/1	0.94	0.48	83,83,83,83	0
56	MG	1H	3150	1/1	0.94	0.14	70,70,70,70	0
56	MG	14	3294	1/1	0.94	0.38	74,74,74,74	0
56	MG	1G	1680	1/1	0.94	0.06	120,120,120,120	0
56	MG	1H	3191	1/1	0.94	0.29	90,90,90,90	0
56	MG	13	1622	1/1	0.94	0.34	94,94,94,94	0
56	MG	1H	3425	1/1	0.94	0.12	92,92,92,92	0
56	MG	14	3237	1/1	0.94	0.29	62,62,62,62	0
56	MG	13	1613	1/1	0.94	0.29	77,77,77,77	0
56	MG	1H	3306	1/1	0.94	0.43	84,84,84,84	0
56	MG	14	3081	1/1	0.94	0.39	62,62,62,62	0
56	MG	14	3167	1/1	0.94	0.40	99,99,99,99	0
56	MG	14	3006	1/1	0.94	0.54	58,58,58,58	0
56	MG	14	3243	1/1	0.94	0.18	89,89,89,89	0
56	MG	1H	3195	1/1	0.94	0.58	78,78,78,78	0
56	MG	1G	1635	1/1	0.94	0.14	93,93,93,93	0
56	MG	1G	1636	1/1	0.94	0.33	101,101,101,101	0
56	MG	1H	3197	1/1	0.94	0.27	80,80,80,80	0
56	MG	14	3248	1/1	0.94	0.24	94,94,94,94	0
56	MG	14	3341	1/1	0.94	0.10	94,94,94,94	0
56	MG	13	1731	1/1	0.94	0.12	94,94,94,94	0
56	MG	14	3362	1/1	0.94	0.09	77,77,77,77	0
56	MG	1H	3310	1/1	0.94	0.22	72,72,72,72	0
56	MG	14	3377	1/1	0.94	0.05	60,60,60,60	0
56	MG	14	3379	1/1	0.94	0.07	107,107,107,107	0
56	MG	13	1662	1/1	0.94	0.33	82,82,82,82	0
56	MG	1H	3176	1/1	0.94	0.31	68,68,68,68	0
56	MG	1H	3088	1/1	0.94	0.28	54,54,54,54	0
56	MG	14	3109	1/1	0.94	0.38	72,72,72,72	0
56	MG	1H	3179	1/1	0.94	0.23	93,93,93,93	0
56	MG	14	3184	1/1	0.94	0.46	86,86,86,86	0
56	MG	14	3185	1/1	0.94	0.20	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3113	1/1	0.94	0.20	67,67,67,67	0
56	MG	1H	3115	1/1	0.94	0.34	76,76,76,76	0
56	MG	1H	3089	1/1	0.94	0.36	74,74,74,74	0
56	MG	45	203	1/1	0.94	0.35	73,73,73,73	0
56	MG	14	3189	1/1	0.94	0.41	73,73,73,73	0
56	MG	1H	3265	1/1	0.94	0.21	74,74,74,74	0
56	MG	13	1621	1/1	0.94	0.27	95,95,95,95	0
56	MG	13	1630	1/1	0.94	0.56	71,71,71,71	0
56	MG	13	1710	1/1	0.95	0.09	72,72,72,72	0
56	MG	1H	3196	1/1	0.95	0.52	80,80,80,80	0
56	MG	13	1713	1/1	0.95	0.09	88,88,88,88	0
56	MG	1H	3260	1/1	0.95	0.42	88,88,88,88	0
56	MG	1H	3334	1/1	0.95	0.08	51,51,51,51	0
56	MG	14	3207	1/1	0.95	0.19	89,89,89,89	0
56	MG	1G	1605	1/1	0.95	0.31	85,85,85,85	0
56	MG	1H	3172	1/1	0.95	0.27	82,82,82,82	0
56	MG	14	3038	1/1	0.95	0.23	86,86,86,86	0
56	MG	3K	101	1/1	0.95	0.13	162,162,162,162	0
56	MG	14	3141	1/1	0.95	0.22	90,90,90,90	0
56	MG	13	1714	1/1	0.95	0.06	104,104,104,104	0
56	MG	1H	3023	1/1	0.95	0.40	57,57,57,57	0
56	MG	14	3051	1/1	0.95	0.31	90,90,90,90	0
56	MG	13	1631	1/1	0.95	0.60	93,93,93,93	0
56	MG	1G	1615	1/1	0.95	0.17	119,119,119,119	0
56	MG	1H	3389	1/1	0.95	0.15	64,64,64,64	0
56	MG	14	3287	1/1	0.95	0.63	105,105,105,105	0
56	MG	1H	3064	1/1	0.95	0.24	54,54,54,54	0
56	MG	14	3059	1/1	0.95	0.32	55,55,55,55	0
56	MG	14	3225	1/1	0.95	0.14	71,71,71,71	0
56	MG	1H	3406	1/1	0.95	0.14	65,65,65,65	0
56	MG	13	1624	1/1	0.95	0.14	71,71,71,71	0
56	MG	1H	3235	1/1	0.95	0.19	85,85,85,85	0
56	MG	1H	3070	1/1	0.95	0.34	50,50,50,50	0
56	MG	1H	3237	1/1	0.95	0.08	77,77,77,77	0
56	MG	1G	1678	1/1	0.95	0.09	92,92,92,92	0
56	MG	14	3157	1/1	0.95	0.60	66,66,66,66	0
56	MG	1H	3305	1/1	0.95	0.30	68,68,68,68	0
56	MG	1H	3133	1/1	0.95	0.32	69,69,69,69	0
56	MG	14	3236	1/1	0.95	0.11	79,79,79,79	0
56	MG	1G	1628	1/1	0.95	0.19	98,98,98,98	0
56	MG	14	3072	1/1	0.95	0.40	55,55,55,55	0
56	MG	13	1682	1/1	0.95	0.14	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3429	1/1	0.95	0.20	66,66,66,66	0
56	MG	14	3002	1/1	0.95	0.38	62,62,62,62	0
56	MG	13	1617	1/1	0.95	0.33	77,77,77,77	0
56	MG	13	1668	1/1	0.95	0.19	80,80,80,80	0
56	MG	14	3005	1/1	0.95	0.33	44,44,44,44	0
56	MG	1G	1634	1/1	0.95	0.39	109,109,109,109	0
56	MG	1H	3111	1/1	0.95	0.18	60,60,60,60	0
56	MG	14	3009	1/1	0.95	0.37	52,52,52,52	0
56	MG	13	1669	1/1	0.95	0.39	72,72,72,72	0
56	MG	14	3348	1/1	0.95	0.07	83,83,83,83	0
56	MG	14	3360	1/1	0.95	0.13	75,75,75,75	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	14	3370	1/1	0.95	0.06	99,99,99,99	0
56	MG	14	3096	1/1	0.95	0.53	60,60,60,60	0
56	MG	1H	3246	1/1	0.95	0.53	88,88,88,88	0
56	MG	13	1614	1/1	0.95	0.04	81,81,81,81	0
56	MG	1H	3215	1/1	0.95	0.27	81,81,81,81	0
56	MG	1G	1641	1/1	0.95	0.47	92,92,92,92	0
56	MG	14	3108	1/1	0.95	0.32	75,75,75,75	0
56	MG	13	1687	1/1	0.95	0.33	76,76,76,76	0
56	MG	14	3021	1/1	0.95	0.36	78,78,78,78	0
56	MG	1H	3217	1/1	0.95	0.20	67,67,67,67	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	14	3116	1/1	0.95	0.46	63,63,63,63	0
56	MG	1H	3320	1/1	0.95	0.20	68,68,68,68	0
56	MG	1H	3288	1/1	0.95	0.08	94,94,94,94	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	3123	1/1	0.95	0.26	82,82,82,82	0
56	MG	14	3028	1/1	0.95	0.64	79,79,79,79	0
56	MG	1H	3208	1/1	0.96	0.36	63,63,63,63	0
56	MG	1H	3165	1/1	0.96	0.42	79,79,79,79	0
56	MG	13	1667	1/1	0.96	0.09	85,85,85,85	0
56	MG	1H	3080	1/1	0.96	0.18	86,86,86,86	0
56	MG	14	3172	1/1	0.96	0.14	98,98,98,98	0
56	MG	1H	3168	1/1	0.96	0.17	65,65,65,65	0
56	MG	14	3174	1/1	0.96	0.35	81,81,81,81	0
56	MG	13	1659	1/1	0.96	0.11	87,87,87,87	0
56	MG	1H	3026	1/1	0.96	0.59	50,50,50,50	0
56	MG	13	1609	1/1	0.96	0.22	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3130	1/1	0.96	0.17	60,60,60,60	0
56	MG	14	3085	1/1	0.96	0.39	51,51,51,51	0
56	MG	14	3086	1/1	0.96	0.64	82,82,82,82	0
56	MG	14	3267	1/1	0.96	0.21	66,66,66,66	0
56	MG	1H	3131	1/1	0.96	0.21	62,62,62,62	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	3177	1/1	0.96	0.23	82,82,82,82	0
56	MG	1G	1610	1/1	0.96	0.28	102,102,102,102	0
56	MG	1H	3012	1/1	0.96	0.31	79,79,79,79	0
56	MG	1G	1612	1/1	0.96	0.41	93,93,93,93	0
56	MG	13	1670	1/1	0.96	0.23	95,95,95,95	0
56	MG	14	3190	1/1	0.96	0.28	95,95,95,95	0
56	MG	14	3103	1/1	0.96	0.33	66,66,66,66	0
56	MG	1H	3136	1/1	0.96	0.10	68,68,68,68	0
56	MG	1H	3091	1/1	0.96	0.10	61,61,61,61	0
56	MG	14	3194	1/1	0.96	0.51	86,86,86,86	0
56	MG	14	3195	1/1	0.96	0.10	107,107,107,107	0
56	MG	13	1611	1/1	0.96	0.34	61,61,61,61	0
56	MG	1G	1617	1/1	0.96	0.15	125,125,125,125	0
56	MG	1H	3033	1/1	0.96	0.18	68,68,68,68	0
56	MG	13	1612	1/1	0.96	0.24	79,79,79,79	0
56	MG	14	3286	1/1	0.96	0.39	83,83,83,83	0
56	MG	1H	3328	1/1	0.96	0.10	52,52,52,52	0
56	MG	1H	3228	1/1	0.96	0.16	57,57,57,57	0
56	MG	13	1635	1/1	0.96	0.18	54,54,54,54	0
56	MG	14	3204	1/1	0.96	0.36	82,82,82,82	0
56	MG	1H	3351	1/1	0.96	0.09	73,73,73,73	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
56	MG	1H	3361	1/1	0.96	0.13	82,82,82,82	0
56	MG	14	3121	1/1	0.96	0.32	84,84,84,84	0
56	MG	1H	3144	1/1	0.96	0.18	54,54,54,54	0
56	MG	14	3213	1/1	0.96	0.26	89,89,89,89	0
56	MG	1H	3233	1/1	0.96	0.11	50,50,50,50	0
56	MG	1H	3285	1/1	0.96	0.33	72,72,72,72	0
56	MG	1G	1631	1/1	0.96	0.36	91,91,91,91	0
56	MG	1H	3379	1/1	0.96	0.10	61,61,61,61	0
56	MG	1H	3234	1/1	0.96	0.22	99,99,99,99	0
56	MG	1H	3036	1/1	0.96	0.38	77,77,77,77	0
56	MG	1H	3398	1/1	0.96	0.09	83,83,83,83	0
56	MG	1H	3146	1/1	0.96	0.27	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3307	1/1	0.96	0.30	108,108,108,108	0
56	MG	1H	3408	1/1	0.96	0.06	80,80,80,80	0
56	MG	14	3136	1/1	0.96	0.26	62,62,62,62	0
56	MG	14	3226	1/1	0.96	0.17	72,72,72,72	0
56	MG	14	3316	1/1	0.96	0.07	67,67,67,67	0
56	MG	1H	3409	1/1	0.96	0.05	86,86,86,86	0
56	MG	14	3332	1/1	0.96	0.15	64,64,64,64	0
56	MG	14	3336	1/1	0.96	0.06	77,77,77,77	0
56	MG	1H	3101	1/1	0.96	0.27	64,64,64,64	0
56	MG	14	3340	1/1	0.96	0.10	83,83,83,83	0
56	MG	1H	3058	1/1	0.96	0.20	62,62,62,62	0
56	MG	14	3342	1/1	0.96	0.08	94,94,94,94	0
56	MG	14	3034	1/1	0.96	0.62	74,74,74,74	0
56	MG	1H	3059	1/1	0.96	0.29	48,48,48,48	0
56	MG	14	3355	1/1	0.96	0.05	92,92,92,92	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	13	1665	1/1	0.96	0.30	64,64,64,64	0
56	MG	1H	3294	1/1	0.96	0.51	71,71,71,71	0
56	MG	1H	3065	1/1	0.96	0.33	55,55,55,55	0
56	MG	14	3371	1/1	0.96	0.08	72,72,72,72	0
56	MG	13	1675	1/1	0.96	0.22	124,124,124,124	0
56	MG	14	3376	1/1	0.96	0.13	90,90,90,90	0
56	MG	1H	3068	1/1	0.96	0.30	56,56,56,56	0
56	MG	1H	3069	1/1	0.96	0.20	60,60,60,60	0
56	MG	14	3052	1/1	0.96	0.27	71,71,71,71	0
56	MG	14	3152	1/1	0.96	0.15	91,91,91,91	0
56	MG	14	3054	1/1	0.96	0.17	83,83,83,83	0
56	MG	1G	1650	1/1	0.96	0.20	91,91,91,91	0
56	MG	1H	3116	1/1	0.96	0.17	56,56,56,56	0
56	MG	1H	3117	1/1	0.96	0.17	82,82,82,82	0
56	MG	1J	205	1/1	0.96	0.07	109,109,109,109	0
56	MG	1H	3118	1/1	0.96	0.14	61,61,61,61	0
56	MG	1H	3020	1/1	0.96	0.24	60,60,60,60	0
56	MG	1H	3021	1/1	0.96	0.24	57,57,57,57	0
56	MG	1G	1657	1/1	0.96	0.58	90,90,90,90	0
56	MG	16	208	1/1	0.96	0.27	82,82,82,82	0
56	MG	1G	1660	1/1	0.96	0.46	97,97,97,97	0
56	MG	13	1640	1/1	0.96	0.15	91,91,91,91	0
56	MG	1H	3122	1/1	0.96	0.20	50,50,50,50	0
57	PAR	1G	1681	42/42	0.96	0.16	79,90,98,101	0
56	MG	13	1723	1/1	0.96	0.10	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	C5	202	1/1	0.96	0.10	165,165,165,165	0
56	MG	1G	1604	1/1	0.97	0.36	97,97,97,97	0
56	MG	14	3171	1/1	0.97	0.27	56,56,56,56	0
56	MG	14	3077	1/1	0.97	0.18	60,60,60,60	0
56	MG	14	3078	1/1	0.97	0.25	64,64,64,64	0
56	MG	1H	3051	1/1	0.97	0.24	84,84,84,84	0
56	MG	1H	3030	1/1	0.97	0.33	69,69,69,69	0
56	MG	14	3082	1/1	0.97	0.44	63,63,63,63	0
56	MG	1H	3363	1/1	0.97	0.04	69,69,69,69	0
56	MG	14	3084	1/1	0.97	0.26	73,73,73,73	0
56	MG	13	1729	1/1	0.97	0.11	103,103,103,103	0
56	MG	1H	3085	1/1	0.97	0.40	82,82,82,82	0
56	MG	13	1606	1/1	0.97	0.22	115,115,115,115	0
56	MG	14	3182	1/1	0.97	0.40	73,73,73,73	0
56	MG	1H	3378	1/1	0.97	0.10	68,68,68,68	0
56	MG	13	1708	1/1	0.97	0.12	85,85,85,85	0
56	MG	1H	3380	1/1	0.97	0.13	70,70,70,70	0
56	MG	14	3093	1/1	0.97	0.43	85,85,85,85	0
56	MG	1H	3384	1/1	0.97	0.11	109,109,109,109	0
56	MG	1H	3386	1/1	0.97	0.08	52,52,52,52	0
56	MG	14	3097	1/1	0.97	0.28	74,74,74,74	0
56	MG	14	3099	1/1	0.97	0.31	62,62,62,62	0
56	MG	1H	3387	1/1	0.97	0.10	72,72,72,72	0
56	MG	13	1709	1/1	0.97	0.10	94,94,94,94	0
56	MG	1H	3390	1/1	0.97	0.05	88,88,88,88	0
56	MG	14	3105	1/1	0.97	0.24	52,52,52,52	0
56	MG	14	3008	1/1	0.97	0.57	65,65,65,65	0
56	MG	13	1657	1/1	0.97	0.13	80,80,80,80	0
56	MG	14	3011	1/1	0.97	0.55	58,58,58,58	0
56	MG	1H	3397	1/1	0.97	0.07	71,71,71,71	0
56	MG	13	1610	1/1	0.97	0.19	72,72,72,72	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	1H	3229	1/1	0.97	0.12	45,45,45,45	0
56	MG	13	1653	1/1	0.97	0.17	89,89,89,89	0
56	MG	14	3115	1/1	0.97	0.34	66,66,66,66	0
56	MG	13	1679	1/1	0.97	0.24	107,107,107,107	0
56	MG	14	3206	1/1	0.97	0.39	82,82,82,82	0
56	MG	13	1645	1/1	0.97	0.28	66,66,66,66	0
56	MG	1H	3095	1/1	0.97	0.18	73,73,73,73	0
56	MG	1H	3413	1/1	0.97	0.05	107,107,107,107	0
56	MG	13	1721	1/1	0.97	0.07	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3097	1/1	0.97	0.16	103,103,103,103	0
56	MG	13	1615	1/1	0.97	0.18	85,85,85,85	0
56	MG	1H	3420	1/1	0.97	0.09	76,76,76,76	0
56	MG	1H	3421	1/1	0.97	0.09	83,83,83,83	0
56	MG	1H	3422	1/1	0.97	0.09	100,100,100,100	0
56	MG	14	3306	1/1	0.97	0.20	110,110,110,110	0
56	MG	14	3217	1/1	0.97	0.29	87,87,87,87	0
56	MG	1H	3002	1/1	0.97	0.32	49,49,49,49	0
56	MG	14	3030	1/1	0.97	0.49	87,87,87,87	0
56	MG	14	3128	1/1	0.97	0.18	73,73,73,73	0
56	MG	14	3314	1/1	0.97	0.07	73,73,73,73	0
56	MG	1H	3424	1/1	0.97	0.07	89,89,89,89	0
56	MG	14	3131	1/1	0.97	0.46	76,76,76,76	0
56	MG	14	3319	1/1	0.97	0.06	62,62,62,62	0
56	MG	14	3223	1/1	0.97	0.20	83,83,83,83	0
56	MG	1H	3100	1/1	0.97	0.22	56,56,56,56	0
56	MG	1H	3428	1/1	0.97	0.19	54,54,54,54	0
56	MG	14	3339	1/1	0.97	0.12	64,64,64,64	0
56	MG	1H	3003	1/1	0.97	0.22	54,54,54,54	0
56	MG	1H	3279	1/1	0.97	0.09	51,51,51,51	0
56	MG	13	1724	1/1	0.97	0.05	108,108,108,108	0
56	MG	14	3138	1/1	0.97	0.31	55,55,55,55	0
56	MG	14	3345	1/1	0.97	0.12	118,118,118,118	0
56	MG	14	3139	1/1	0.97	0.33	93,93,93,93	0
56	MG	1H	3103	1/1	0.97	0.24	51,51,51,51	0
56	MG	1H	3104	1/1	0.97	0.30	71,71,71,71	0
56	MG	14	3359	1/1	0.97	0.10	55,55,55,55	0
56	MG	1G	1648	1/1	0.97	0.48	78,78,78,78	0
56	MG	1H	3073	1/1	0.97	0.19	47,47,47,47	0
56	MG	14	3365	1/1	0.97	0.07	88,88,88,88	0
56	MG	14	3366	1/1	0.97	0.11	92,92,92,92	0
56	MG	1H	3074	1/1	0.97	0.20	69,69,69,69	0
56	MG	14	3369	1/1	0.97	0.06	84,84,84,84	0
56	MG	14	3046	1/1	0.97	0.33	66,66,66,66	0
56	MG	14	3049	1/1	0.97	0.21	58,58,58,58	0
56	MG	14	3373	1/1	0.97	0.08	87,87,87,87	0
56	MG	14	3050	1/1	0.97	0.30	73,73,73,73	0
56	MG	14	3375	1/1	0.97	0.07	111,111,111,111	0
56	MG	1H	3006	1/1	0.97	0.18	61,61,61,61	0
56	MG	13	1725	1/1	0.97	0.10	102,102,102,102	0
56	MG	1G	1653	1/1	0.97	0.27	85,85,85,85	0
56	MG	16	209	1/1	0.97	0.14	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3048	1/1	0.97	0.43	92,92,92,92	0
56	MG	1H	3324	1/1	0.97	0.32	69,69,69,69	0
56	MG	1H	3181	1/1	0.97	0.10	74,74,74,74	0
56	MG	1G	1658	1/1	0.97	0.11	124,124,124,124	0
56	MG	1H	3078	1/1	0.97	0.19	57,57,57,57	0
56	MG	1J	204	1/1	0.97	0.09	99,99,99,99	0
56	MG	1H	3114	1/1	0.97	0.26	67,67,67,67	0
56	MG	13	1727	1/1	0.97	0.07	115,115,115,115	0
56	MG	18	101	1/1	0.97	0.05	59,59,59,59	0
56	MG	1H	3329	1/1	0.97	0.06	59,59,59,59	0
56	MG	14	3067	1/1	0.97	0.21	74,74,74,74	0
56	MG	13	1703	1/1	0.97	0.15	70,70,70,70	0
56	MG	1H	3335	1/1	0.97	0.07	50,50,50,50	0
56	MG	1H	3343	1/1	0.97	0.07	65,65,65,65	0
56	MG	1H	3255	1/1	0.97	0.10	81,81,81,81	0
57	PAR	13	1730	42/42	0.97	0.19	67,77,86,91	0
56	MG	1G	1601	1/1	0.97	0.28	96,96,96,96	0
56	MG	1H	3350	1/1	0.97	0.17	72,72,72,72	0
59	ZN	5A	101	1/1	0.97	0.12	139,139,139,139	0
56	MG	1H	3081	1/1	0.97	0.42	85,85,85,85	0
56	MG	1G	1667	1/1	0.98	0.39	100,100,100,100	0
56	MG	1H	3399	1/1	0.98	0.05	91,91,91,91	0
56	MG	14	3135	1/1	0.98	0.19	78,78,78,78	0
56	MG	1G	1669	1/1	0.98	0.10	82,82,82,82	0
56	MG	1H	3400	1/1	0.98	0.06	52,52,52,52	0
56	MG	1H	3404	1/1	0.98	0.07	64,64,64,64	0
56	MG	1G	1673	1/1	0.98	0.12	85,85,85,85	0
56	MG	1H	3071	1/1	0.98	0.16	56,56,56,56	0
56	MG	1H	3330	1/1	0.98	0.10	60,60,60,60	0
56	MG	1H	3407	1/1	0.98	0.11	86,86,86,86	0
56	MG	1H	3331	1/1	0.98	0.09	51,51,51,51	0
56	MG	14	3065	1/1	0.98	0.13	68,68,68,68	0
56	MG	14	3066	1/1	0.98	0.13	72,72,72,72	0
56	MG	1H	3072	1/1	0.98	0.47	72,72,72,72	0
56	MG	1H	3010	1/1	0.98	0.35	57,57,57,57	0
56	MG	1H	3337	1/1	0.98	0.13	55,55,55,55	0
56	MG	1G	1621	1/1	0.98	0.55	61,61,61,61	0
56	MG	2L	101	1/1	0.98	0.41	72,72,72,72	0
56	MG	1H	3338	1/1	0.98	0.11	59,59,59,59	0
56	MG	1H	3341	1/1	0.98	0.10	57,57,57,57	0
56	MG	14	3074	1/1	0.98	0.26	45,45,45,45	0
56	MG	14	3001	1/1	0.98	0.15	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1624	1/1	0.98	0.43	76,76,76,76	0
56	MG	13	1707	1/1	0.98	0.11	85,85,85,85	0
56	MG	14	3313	1/1	0.98	0.16	64,64,64,64	0
56	MG	1H	3416	1/1	0.98	0.17	104,104,104,104	0
56	MG	14	3315	1/1	0.98	0.04	71,71,71,71	0
56	MG	1H	3344	1/1	0.98	0.13	75,75,75,75	0
56	MG	14	3080	1/1	0.98	0.29	67,67,67,67	0
56	MG	14	3318	1/1	0.98	0.19	71,71,71,71	0
56	MG	1H	3419	1/1	0.98	0.07	73,73,73,73	0
56	MG	14	3320	1/1	0.98	0.07	84,84,84,84	0
56	MG	14	3322	1/1	0.98	0.03	72,72,72,72	0
56	MG	14	3325	1/1	0.98	0.11	76,76,76,76	0
56	MG	1H	3345	1/1	0.98	0.10	58,58,58,58	0
56	MG	14	3333	1/1	0.98	0.12	79,79,79,79	0
56	MG	14	3334	1/1	0.98	0.06	85,85,85,85	0
56	MG	14	3335	1/1	0.98	0.07	63,63,63,63	0
56	MG	1H	3347	1/1	0.98	0.07	78,78,78,78	0
56	MG	14	3337	1/1	0.98	0.13	79,79,79,79	0
56	MG	1H	3261	1/1	0.98	0.23	90,90,90,90	0
56	MG	14	3010	1/1	0.98	0.44	54,54,54,54	0
56	MG	1H	3174	1/1	0.98	0.35	85,85,85,85	0
56	MG	13	1715	1/1	0.98	0.07	100,100,100,100	0
56	MG	13	1717	1/1	0.98	0.10	74,74,74,74	0
56	MG	14	3343	1/1	0.98	0.09	71,71,71,71	0
56	MG	14	3089	1/1	0.98	0.47	54,54,54,54	0
56	MG	14	3014	1/1	0.98	0.43	49,49,49,49	0
56	MG	1H	3427	1/1	0.98	0.10	84,84,84,84	0
56	MG	14	3349	1/1	0.98	0.04	90,90,90,90	0
56	MG	14	3350	1/1	0.98	0.12	76,76,76,76	0
56	MG	14	3352	1/1	0.98	0.11	78,78,78,78	0
56	MG	14	3354	1/1	0.98	0.14	87,87,87,87	0
56	MG	14	3016	1/1	0.98	0.30	60,60,60,60	0
56	MG	1H	3354	1/1	0.98	0.17	65,65,65,65	0
56	MG	1H	3357	1/1	0.98	0.12	58,58,58,58	0
56	MG	1H	3360	1/1	0.98	0.09	57,57,57,57	0
56	MG	14	3361	1/1	0.98	0.07	60,60,60,60	0
56	MG	14	3098	1/1	0.98	0.33	68,68,68,68	0
56	MG	14	3364	1/1	0.98	0.06	73,73,73,73	0
56	MG	13	1660	1/1	0.98	0.51	81,81,81,81	0
56	MG	14	3100	1/1	0.98	0.24	91,91,91,91	0
56	MG	1H	3001	1/1	0.98	0.32	53,53,53,53	0
56	MG	1H	3365	1/1	0.98	0.05	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3367	1/1	0.98	0.07	71,71,71,71	0
56	MG	14	3104	1/1	0.98	0.26	64,64,64,64	0
56	MG	14	3372	1/1	0.98	0.09	87,87,87,87	0
56	MG	1H	3368	1/1	0.98	0.08	57,57,57,57	0
56	MG	1H	3158	1/1	0.98	0.41	68,68,68,68	0
56	MG	1H	3370	1/1	0.98	0.09	76,76,76,76	0
56	MG	13	1732	1/1	0.98	0.14	65,65,65,65	0
56	MG	1H	3374	1/1	0.98	0.09	88,88,88,88	0
56	MG	1H	3060	1/1	0.98	0.34	52,52,52,52	0
56	MG	13	1634	1/1	0.98	0.26	53,53,53,53	0
56	MG	1H	3063	1/1	0.98	0.24	55,55,55,55	0
56	MG	1H	3004	1/1	0.98	0.26	41,41,41,41	0
56	MG	1H	3382	1/1	0.98	0.10	60,60,60,60	0
56	MG	1H	3383	1/1	0.98	0.08	65,65,65,65	0
56	MG	13	1722	1/1	0.98	0.05	93,93,93,93	0
56	MG	13	1704	1/1	0.98	0.07	85,85,85,85	0
56	MG	1H	3007	1/1	0.98	0.21	80,80,80,80	0
56	MG	29	301	1/1	0.98	0.27	63,63,63,63	0
56	MG	1H	3388	1/1	0.98	0.11	63,63,63,63	0
56	MG	1H	3127	1/1	0.98	0.28	53,53,53,53	0
56	MG	1H	3253	1/1	0.98	0.16	60,60,60,60	0
56	MG	13	1705	1/1	0.98	0.09	94,94,94,94	0
56	MG	14	3044	1/1	0.98	0.45	68,68,68,68	0
56	MG	1H	3392	1/1	0.98	0.14	71,71,71,71	0
56	MG	1H	3394	1/1	0.98	0.05	60,60,60,60	0
56	MG	1H	3395	1/1	0.98	0.04	74,74,74,74	0
56	MG	1H	3396	1/1	0.98	0.09	58,58,58,58	0
56	MG	14	3129	1/1	0.98	0.39	58,58,58,58	0
59	ZN	5I	102	1/1	0.98	0.13	99,99,99,99	0
56	MG	13	1626	1/1	0.98	0.35	87,87,87,87	0
56	MG	14	3053	1/1	0.98	0.36	61,61,61,61	0
56	MG	1H	3256	1/1	0.98	0.24	76,76,76,76	0
56	MG	14	3327	1/1	0.99	0.11	84,84,84,84	0
56	MG	14	3328	1/1	0.99	0.07	64,64,64,64	0
56	MG	14	3329	1/1	0.99	0.08	55,55,55,55	0
56	MG	14	3330	1/1	0.99	0.11	65,65,65,65	0
56	MG	14	3331	1/1	0.99	0.06	63,63,63,63	0
56	MG	14	3042	1/1	0.99	0.28	58,58,58,58	0
56	MG	14	3043	1/1	0.99	0.36	52,52,52,52	0
56	MG	14	3209	1/1	0.99	0.20	67,67,67,67	0
56	MG	1H	3393	1/1	0.99	0.07	70,70,70,70	0
56	MG	14	3045	1/1	0.99	0.30	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3356	1/1	0.99	0.08	61,61,61,61	0
56	MG	14	3047	1/1	0.99	0.25	57,57,57,57	0
56	MG	14	3048	1/1	0.99	0.48	55,55,55,55	0
56	MG	1H	3090	1/1	0.99	0.41	72,72,72,72	0
56	MG	16	210	1/1	0.99	0.17	81,81,81,81	0
56	MG	14	3160	1/1	0.99	0.44	57,57,57,57	0
56	MG	1H	3358	1/1	0.99	0.17	68,68,68,68	0
56	MG	1H	3359	1/1	0.99	0.22	66,66,66,66	0
56	MG	1H	3245	1/1	0.99	0.29	74,74,74,74	0
56	MG	14	3346	1/1	0.99	0.10	64,64,64,64	0
56	MG	14	3347	1/1	0.99	0.13	77,77,77,77	0
56	MG	13	1716	1/1	0.99	0.09	88,88,88,88	0
56	MG	1H	3362	1/1	0.99	0.10	64,64,64,64	0
56	MG	88	201	1/1	0.99	0.19	81,81,81,81	0
56	MG	14	3351	1/1	0.99	0.14	65,65,65,65	0
56	MG	1H	3401	1/1	0.99	0.05	55,55,55,55	0
56	MG	14	3112	1/1	0.99	0.20	61,61,61,61	0
56	MG	1H	3402	1/1	0.99	0.08	60,60,60,60	0
56	MG	1H	3403	1/1	0.99	0.06	61,61,61,61	0
56	MG	14	3357	1/1	0.99	0.06	77,77,77,77	0
56	MG	14	3358	1/1	0.99	0.12	64,64,64,64	0
56	MG	1H	3332	1/1	0.99	0.13	66,66,66,66	0
56	MG	1H	3364	1/1	0.99	0.15	56,56,56,56	0
56	MG	1H	3333	1/1	0.99	0.09	63,63,63,63	0
56	MG	13	1712	1/1	0.99	0.11	78,78,78,78	0
56	MG	14	3363	1/1	0.99	0.11	51,51,51,51	0
56	MG	1H	3105	1/1	0.99	0.26	64,64,64,64	0
56	MG	1H	3336	1/1	0.99	0.07	49,49,49,49	0
56	MG	1H	3410	1/1	0.99	0.12	53,53,53,53	0
56	MG	13	1718	1/1	0.99	0.05	67,67,67,67	0
56	MG	14	3368	1/1	0.99	0.17	49,49,49,49	0
56	MG	1H	3371	1/1	0.99	0.09	63,63,63,63	0
56	MG	1H	3372	1/1	0.99	0.13	53,53,53,53	0
56	MG	1G	1607	1/1	0.99	0.27	77,77,77,77	0
56	MG	1G	1608	1/1	0.99	0.11	101,101,101,101	0
56	MG	13	1726	1/1	0.99	0.04	82,82,82,82	0
56	MG	1H	3339	1/1	0.99	0.05	70,70,70,70	0
56	MG	1H	3375	1/1	0.99	0.10	67,67,67,67	0
56	MG	1H	3417	1/1	0.99	0.07	62,62,62,62	0
56	MG	1H	3340	1/1	0.99	0.10	58,58,58,58	0
56	MG	14	3378	1/1	0.99	0.07	62,62,62,62	0
56	MG	1H	3377	1/1	0.99	0.11	77,77,77,77	0

*Continued on next page...*

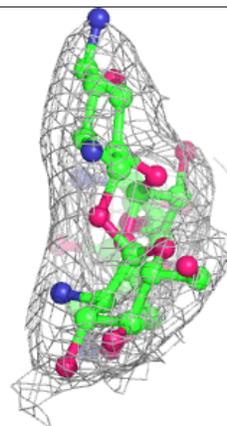
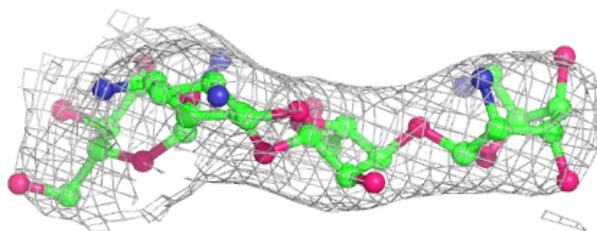
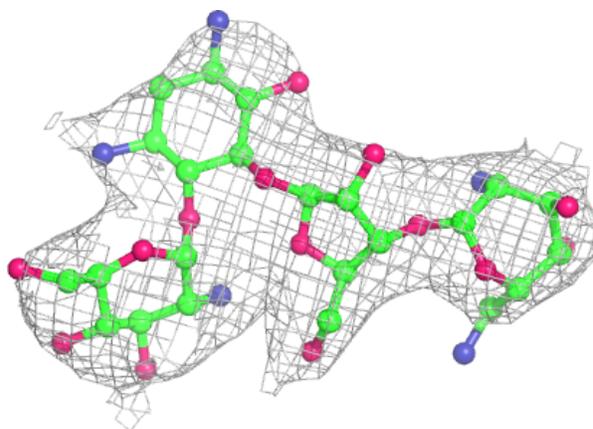
*Continued from previous page...*

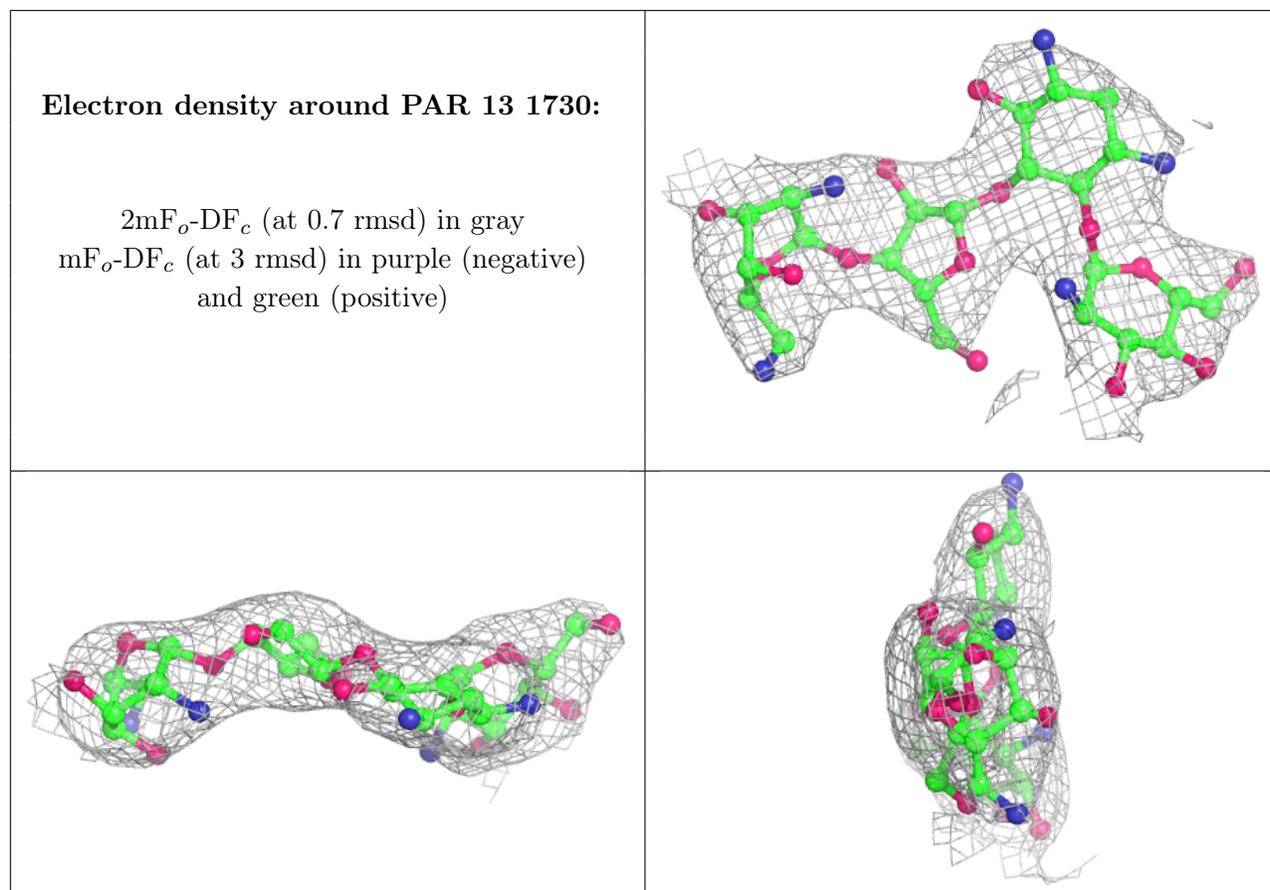
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3108	1/1	0.99	0.28	62,62,62,62	0
56	MG	1H	3342	1/1	0.99	0.06	59,59,59,59	0
56	MG	1H	3139	1/1	0.99	0.32	64,64,64,64	0
56	MG	1H	3381	1/1	0.99	0.12	59,59,59,59	0
56	MG	1H	3109	1/1	0.99	0.18	59,59,59,59	0
56	MG	13	1719	1/1	0.99	0.13	86,86,86,86	0
56	MG	1H	3426	1/1	0.99	0.07	54,54,54,54	0
56	MG	1H	3031	1/1	0.99	0.29	65,65,65,65	0
56	MG	14	3311	1/1	0.99	0.22	83,83,83,83	0
56	MG	14	3312	1/1	0.99	0.18	70,70,70,70	0
56	MG	1H	3385	1/1	0.99	0.12	78,78,78,78	0
56	MG	1H	3062	1/1	0.99	0.19	54,54,54,54	0
56	MG	13	1619	1/1	0.99	0.32	69,69,69,69	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	13	1602	1/1	0.99	0.38	89,89,89,89	0
56	MG	1H	3353	1/1	0.99	0.10	53,53,53,53	0
56	MG	2K	103	1/1	0.99	0.28	71,71,71,71	0
56	MG	14	3321	1/1	0.99	0.07	73,73,73,73	0
58	SF4	3E	302	8/8	0.99	0.18	76,86,96,96	0
58	SF4	32	301	8/8	0.99	0.18	92,113,120,129	0
56	MG	14	3094	1/1	0.99	0.32	82,82,82,82	0
56	MG	14	3323	1/1	0.99	0.14	66,66,66,66	0
56	MG	1H	3355	1/1	0.99	0.10	58,58,58,58	0
56	MG	14	3326	1/1	0.99	0.13	61,61,61,61	0
56	MG	1H	3349	1/1	1.00	0.09	74,74,74,74	0
56	MG	1H	3066	1/1	1.00	0.16	48,48,48,48	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	14	3353	1/1	1.00	0.15	69,69,69,69	0
56	MG	1H	3346	1/1	1.00	0.07	63,63,63,63	0
56	MG	14	3324	1/1	1.00	0.14	77,77,77,77	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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.