



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 02:04 AM GMT

PDB ID : 5EL5  
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 second position  
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.  
Deposited on : 2015-11-04  
Resolution : 3.15 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

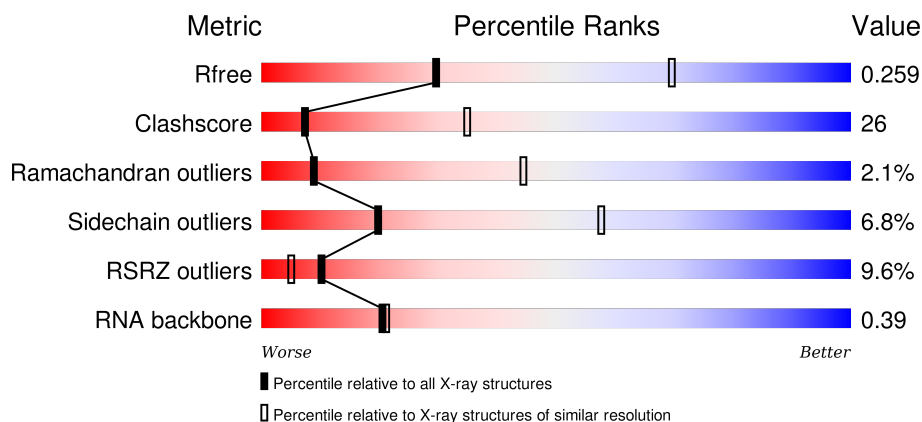
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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.



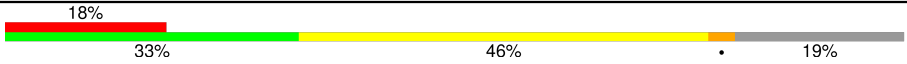
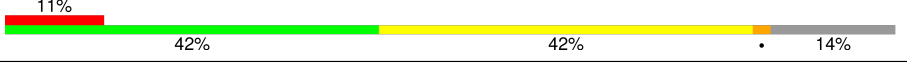
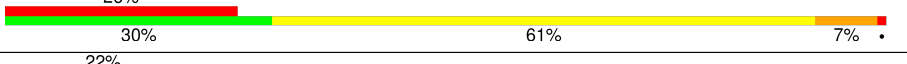
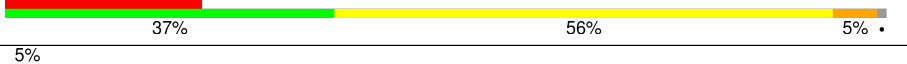
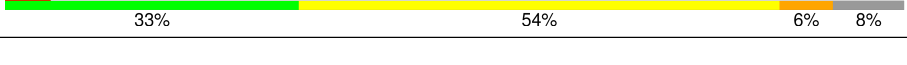
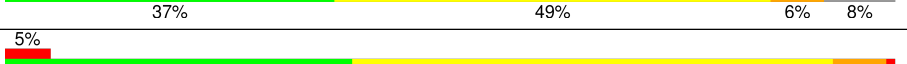

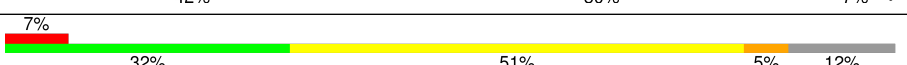


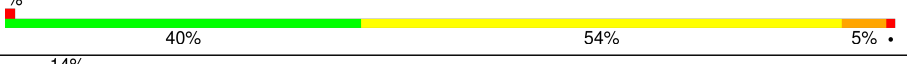
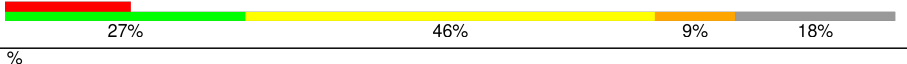
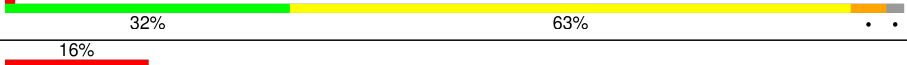

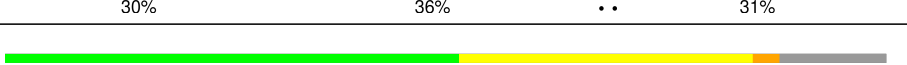
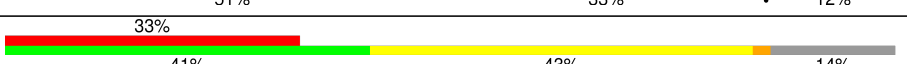
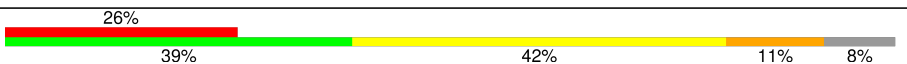

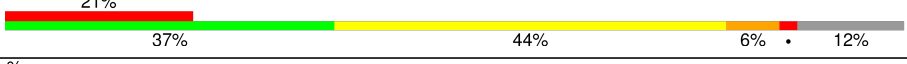

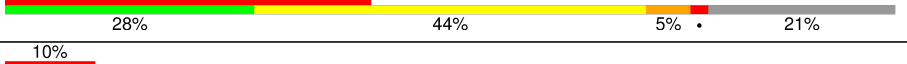




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

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

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>7%</div> <div>38%</div> <div>41%</div> <div>12%</div> <div>•</div> </div>
1	1G	1522	<div> <div>10%</div> <div>37%</div> <div>41%</div> <div>11%</div> <div>•</div> </div>
2	12	256	<div> <div>25%</div> <div>49%</div> <div>6%</div> <div>20%</div> <div>•</div> </div>
2	1E	256	<div> <div>17%</div> <div>32%</div> <div>52%</div> <div>7%</div> <div>10%</div> </div>

*Continued on next page...*

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	
27	1J	122	
28	7I	229	
29	11	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	
41	B8	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	

Continued on next page...

*Continued from previous page...*

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	13	1601	-	-	-	X
58	MG	13	1610	-	-	-	X
58	MG	13	1611	-	-	-	X
58	MG	13	1614	-	-	-	X
58	MG	13	1620	-	-	-	X
58	MG	13	1631	-	-	-	X
58	MG	13	1638	-	-	-	X
58	MG	13	1639	-	-	-	X
58	MG	13	1642	-	-	-	X
58	MG	13	1643	-	-	-	X
58	MG	13	1648	-	-	-	X
58	MG	13	1651	-	-	-	X
58	MG	13	1657	-	-	-	X
58	MG	13	1658	-	-	-	X
58	MG	13	1659	-	-	-	X
58	MG	13	1671	-	-	-	X
58	MG	13	1672	-	-	-	X
58	MG	13	1682	-	-	-	X
58	MG	13	1686	-	-	-	X
58	MG	14	3005	-	-	-	X
58	MG	14	3008	-	-	-	X
58	MG	14	3009	-	-	-	X
58	MG	14	3011	-	-	-	X
58	MG	14	3014	-	-	-	X
58	MG	14	3016	-	-	-	X
58	MG	14	3017	-	-	-	X
58	MG	14	3021	-	-	-	X
58	MG	14	3027	-	-	-	X
58	MG	14	3043	-	-	-	X
58	MG	14	3044	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3054	-	-	-	X
58	MG	14	3059	-	-	-	X
58	MG	14	3065	-	-	-	X
58	MG	14	3071	-	-	-	X
58	MG	14	3072	-	-	-	X
58	MG	14	3074	-	-	-	X
58	MG	14	3076	-	-	-	X
58	MG	14	3081	-	-	-	X
58	MG	14	3088	-	-	-	X
58	MG	14	3093	-	-	-	X
58	MG	14	3095	-	-	-	X
58	MG	14	3097	-	-	-	X
58	MG	14	3106	-	-	-	X
58	MG	14	3108	-	-	-	X
58	MG	14	3111	-	-	-	X
58	MG	14	3116	-	-	-	X
58	MG	14	3118	-	-	-	X
58	MG	14	3119	-	-	-	X
58	MG	14	3121	-	-	-	X
58	MG	14	3125	-	-	-	X
58	MG	14	3127	-	-	-	X
58	MG	14	3129	-	-	-	X
58	MG	14	3130	-	-	-	X
58	MG	14	3145	-	-	-	X
58	MG	14	3152	-	-	-	X
58	MG	14	3155	-	-	-	X
58	MG	14	3158	-	-	-	X
58	MG	14	3166	-	-	-	X
58	MG	14	3172	-	-	-	X
58	MG	14	3173	-	-	-	X
58	MG	14	3182	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3191	-	-	-	X
58	MG	14	3193	-	-	-	X
58	MG	14	3195	-	-	-	X
58	MG	14	3200	-	-	-	X
58	MG	14	3202	-	-	-	X
58	MG	14	3214	-	-	-	X
58	MG	14	3215	-	-	-	X
58	MG	14	3216	-	-	-	X
58	MG	14	3218	-	-	-	X
58	MG	14	3219	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3224	-	-	-	X
58	MG	14	3232	-	-	-	X
58	MG	14	3233	-	-	-	X
58	MG	14	3237	-	-	-	X
58	MG	14	3239	-	-	-	X
58	MG	14	3245	-	-	-	X
58	MG	14	3246	-	-	-	X
58	MG	14	3250	-	-	-	X
58	MG	14	3251	-	-	-	X
58	MG	14	3254	-	-	-	X
58	MG	14	3255	-	-	-	X
58	MG	14	3258	-	-	-	X
58	MG	14	3269	-	-	-	X
58	MG	14	3271	-	-	-	X
58	MG	14	3279	-	-	-	X
58	MG	14	3282	-	-	-	X
58	MG	14	3287	-	-	-	X
58	MG	14	3289	-	-	-	X
58	MG	14	3290	-	-	-	X
58	MG	14	3297	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	14	3316	-	-	-	X
58	MG	14	3317	-	-	-	X
58	MG	14	3321	-	-	-	X
58	MG	14	3332	-	-	-	X
58	MG	14	3334	-	-	-	X
58	MG	14	3335	-	-	-	X
58	MG	14	3341	-	-	-	X
58	MG	14	3363	-	-	-	X
58	MG	1G	1606	-	-	-	X
58	MG	1G	1613	-	-	-	X
58	MG	1G	1615	-	-	-	X
58	MG	1G	1616	-	-	-	X
58	MG	1G	1619	-	-	-	X
58	MG	1G	1625	-	-	-	X
58	MG	1G	1626	-	-	-	X
58	MG	1G	1627	-	-	-	X
58	MG	1G	1634	-	-	-	X
58	MG	1G	1640	-	-	-	X
58	MG	1G	1649	-	-	-	X
58	MG	1G	1667	-	-	-	X
58	MG	1G	1669	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1G	1673	-	-	-	X
58	MG	1G	1676	-	-	-	X
58	MG	1H	3001	-	-	-	X
58	MG	1H	3002	-	-	-	X
58	MG	1H	3006	-	-	-	X
58	MG	1H	3007	-	-	-	X
58	MG	1H	3008	-	-	-	X
58	MG	1H	3015	-	-	-	X
58	MG	1H	3018	-	-	-	X
58	MG	1H	3023	-	-	-	X
58	MG	1H	3028	-	-	-	X
58	MG	1H	3030	-	-	-	X
58	MG	1H	3034	-	-	-	X
58	MG	1H	3041	-	-	-	X
58	MG	1H	3045	-	-	-	X
58	MG	1H	3048	-	-	-	X
58	MG	1H	3053	-	-	-	X
58	MG	1H	3057	-	-	-	X
58	MG	1H	3064	-	-	-	X
58	MG	1H	3068	-	-	-	X
58	MG	1H	3069	-	-	-	X
58	MG	1H	3071	-	-	-	X
58	MG	1H	3075	-	-	-	X
58	MG	1H	3076	-	-	-	X
58	MG	1H	3078	-	-	-	X
58	MG	1H	3079	-	-	-	X
58	MG	1H	3083	-	-	-	X
58	MG	1H	3085	-	-	-	X
58	MG	1H	3088	-	-	-	X
58	MG	1H	3090	-	-	-	X
58	MG	1H	3091	-	-	-	X
58	MG	1H	3092	-	-	-	X
58	MG	1H	3097	-	-	-	X
58	MG	1H	3098	-	-	-	X
58	MG	1H	3101	-	-	-	X
58	MG	1H	3103	-	-	-	X
58	MG	1H	3104	-	-	-	X
58	MG	1H	3111	-	-	-	X
58	MG	1H	3117	-	-	-	X
58	MG	1H	3124	-	-	-	X
58	MG	1H	3126	-	-	-	X
58	MG	1H	3127	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3130	-	-	-	X
58	MG	1H	3136	-	-	-	X
58	MG	1H	3139	-	-	-	X
58	MG	1H	3143	-	-	-	X
58	MG	1H	3148	-	-	-	X
58	MG	1H	3150	-	-	-	X
58	MG	1H	3164	-	-	-	X
58	MG	1H	3165	-	-	-	X
58	MG	1H	3171	-	-	-	X
58	MG	1H	3175	-	-	-	X
58	MG	1H	3179	-	-	-	X
58	MG	1H	3185	-	-	-	X
58	MG	1H	3190	-	-	-	X
58	MG	1H	3194	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3202	-	-	-	X
58	MG	1H	3214	-	-	-	X
58	MG	1H	3221	-	-	-	X
58	MG	1H	3222	-	-	-	X
58	MG	1H	3225	-	-	-	X
58	MG	1H	3226	-	-	-	X
58	MG	1H	3227	-	-	-	X
58	MG	1H	3235	-	-	-	X
58	MG	1H	3236	-	-	-	X
58	MG	1H	3237	-	-	-	X
58	MG	1H	3239	-	-	-	X
58	MG	1H	3242	-	-	-	X
58	MG	1H	3244	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3255	-	-	-	X
58	MG	1H	3257	-	-	-	X
58	MG	1H	3261	-	-	-	X
58	MG	1H	3267	-	-	-	X
58	MG	1H	3282	-	-	-	X
58	MG	1H	3283	-	-	-	X
58	MG	1H	3284	-	-	-	X
58	MG	1H	3286	-	-	-	X
58	MG	1H	3290	-	-	-	X
58	MG	1H	3296	-	-	-	X
58	MG	1H	3308	-	-	-	X
58	MG	1H	3333	-	-	-	X
58	MG	1H	3340	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3398	-	-	-	X
58	MG	1H	3408	-	-	-	X
58	MG	1H	3433	-	-	-	X
58	MG	1H	3443	-	-	-	X
58	MG	1H	3457	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	29	303	-	-	-	X
58	MG	2K	101	-	-	-	X
58	MG	2L	101	-	-	-	X
58	MG	35	201	-	-	-	X
58	MG	45	201	-	-	-	X
58	MG	85	202	-	-	-	X
58	MG	C8	201	-	-	-	X
58	MG	E5	101	-	-	-	X
58	MG	Q8	101	-	-	-	X
59	SF4	32	302	-	-	X	-

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 292607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1493	Total	C	N	O	P	0	0	0
			32097	14286	5951	10367	1493			
1	1G	1496	Total	C	N	O	P	0	0	0
			32152	14311	5953	10392	1496			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	206	Total	C	N	O	S	0	0	0
			1695	1082	305	304	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	194	Total	C	N	O	S	0	0	0
			1529	967	296	265	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1696	1062	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1136	716	216	200	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	151	Total	C	N	O	S	0	0	0
			1229	763	247	213	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	105	Total	C	N	O		0	0	0
			820	523	158	139				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	72	Total	C	N	O	S	0	0	0
			593	373	115	104	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	60	Total	C	N	O	0	0	0
			474	298	91	85			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	0	0	0
			956	603	193	159			
12	3A	121	Total	C	N	O	0	0	0
			947	597	191	158			

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

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

- 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	0	0	0
			491	312	104	71			
14	5A	48	Total	C	N	O	0	0	0
			388	245	82	57			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	80	Total	C	N	O	S	0	0	0
			671	427	132	111	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	67	Total	C	N	O	0	0	0
			544	349	104	91			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	36	Total	C	N	O	S	0	0	0
			283	182	49	51	1			

- 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	98	Total	C	N	O	S	0	0	0
			757	467	161	127	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	23	Total	C	N	O	0	0	0
			204	126	49	29			

- 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			

- Molecule 23 is a RNA chain called 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			

- 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	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2830	Total	C	N	O	P	0	0	0
			60960	27129	11403	19598	2830			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	135	Total	C	N	O	S	0	0	0
			1050	662	197	190	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	29	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- 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	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	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	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
41	75	136	Total	C	N	O		0	0	0
			1133	705	233	195				

- 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	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
43	95	99	Total	C	N	O		0	0	0
			766	494	140	132				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	110	Total	C	N	O	S	0	0	0
			876	552	171	151	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	0	0	0
			740	480	134	126			
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	104	Total	C	N	O	S	0	0	0
			788	507	149	127	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	148	Total	C	N	O	S	0	0	0
			1218	779	220	217	2			
47	D5	130	Total	C	N	O	S	0	0	0
			1064	685	191	186	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	78	Total	C	N	O	S	0	0	0
			616	381	130	104	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	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

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

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

- Molecule 56 is a RNA chain called tRNA<sup>Lys</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	74	Total	C	N	O	P	0	0	0
			1570	702	271	523	74			

- Molecule 57 is a RNA chain called tRNA<sup>Lys</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	45	3	Total 3 Mg 3	0	0
58	P8	1	Total 1 Mg 1	0	0
58	85	2	Total 2 Mg 2	0	0
58	32	1	Total 1 Mg 1	0	0
58	C5	1	Total 1 Mg 1	0	0
58	13	141	Total 141 Mg 141	0	0
58	1J	6	Total 6 Mg 6	0	0
58	5I	1	Total 1 Mg 1	0	0
58	35	1	Total 1 Mg 1	0	0
58	C8	1	Total 1 Mg 1	0	0
58	16	12	Total 12 Mg 12	0	0
58	21	2	Total 2 Mg 2	0	0
58	2K	3	Total 3 Mg 3	0	0
58	Q8	1	Total 1 Mg 1	0	0
58	3I	1	Total 1 Mg 1	0	0
58	I8	1	Total 1 Mg 1	0	0
58	L5	1	Total 1 Mg 1	0	0
58	5E	2	Total 2 Mg 2	0	0
58	29	3	Total 3 Mg 3	0	0
58	7A	1	Total 1 Mg 1	0	0
58	78	1	Total 1 Mg 1	0	0
58	J8	2	Total 2 Mg 2	0	0

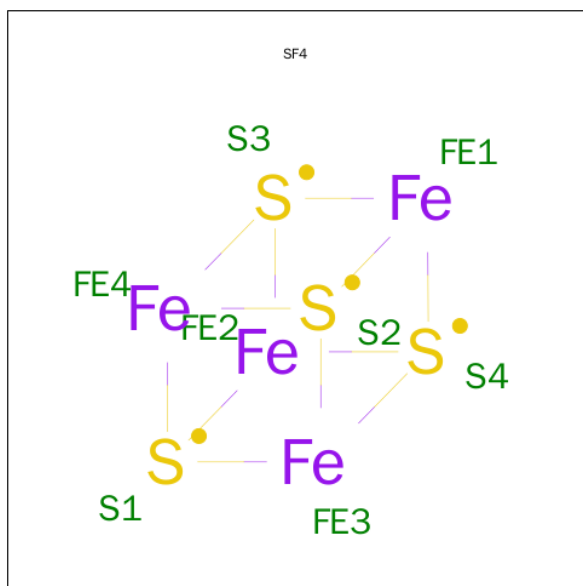
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1G	78	Total 78	Mg 78	0	0
58	11	1	Total 1	Mg 1	0	0
58	1H	488	Total 488	Mg 488	0	0
58	E5	1	Total 1	Mg 1	0	0
58	88	1	Total 1	Mg 1	0	0
58	14	420	Total 420	Mg 420	0	0
58	55	1	Total 1	Mg 1	0	0
58	41	1	Total 1	Mg 1	0	0
58	2L	3	Total 3	Mg 3	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	148	Total 148	O 148	0	0
61	3E	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	6I	1	Total 1	O 1	0	0
61	1K	1	Total 1	O 1	0	0
61	4K	6	Total 6	O 6	0	0
61	1H	670	Total 670	O 670	0	0
61	16	18	Total 18	O 18	0	0
61	11	9	Total 9	O 9	0	0
61	21	5	Total 5	O 5	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	78	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0

*Continued on next page...*

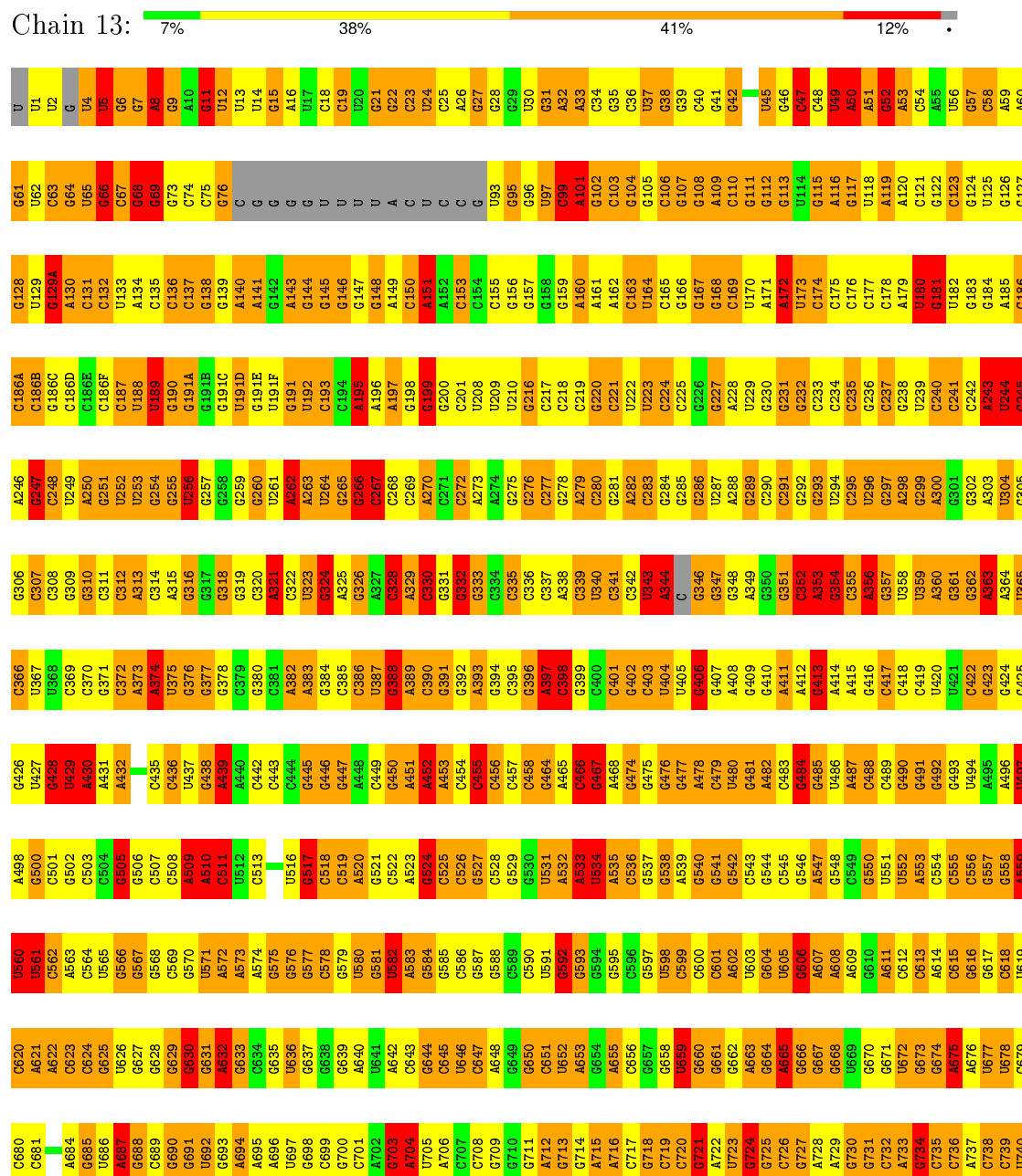
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	G8	1	Total 1	O 1	0	0
61	I8	1	Total 1	O 1	0	0
61	Q8	1	Total 1	O 1	0	0
61	1G	44	Total 44	O 44	0	0
61	5A	3	Total 3	O 3	0	0
61	BA	1	Total 1	O 1	0	0
61	14	411	Total 411	O 411	0	0
61	1J	11	Total 11	O 11	0	0
61	19	4	Total 4	O 4	0	0
61	29	3	Total 3	O 3	0	0
61	39	8	Total 8	O 8	0	0
61	35	2	Total 2	O 2	0	0
61	55	1	Total 1	O 1	0	0
61	E5	1	Total 1	O 1	0	0
61	F5	2	Total 2	O 2	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	2	Total 2	O 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S ribosomal RNA



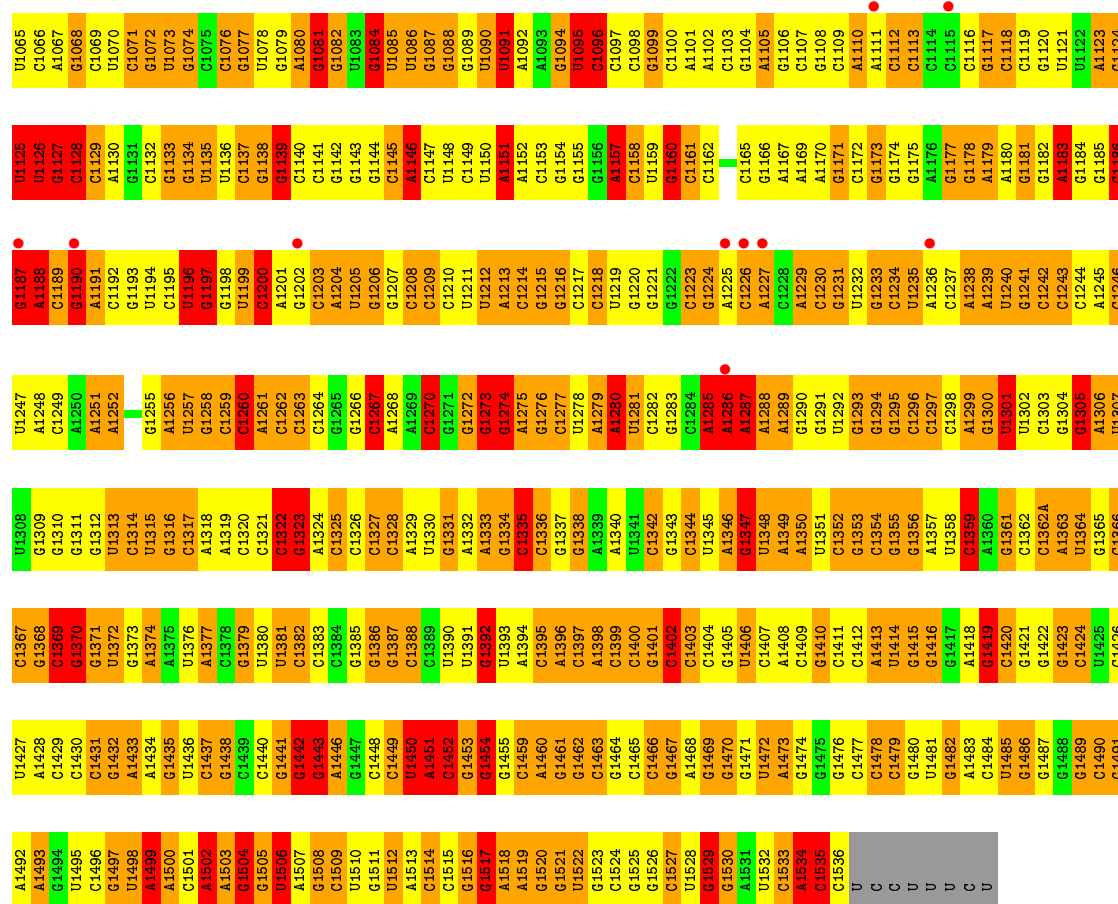
U	G1476	G1410	A1350	G1290	A1229	A1169	G1108	G1047	G988	G928	C868	U801	G741
C	C1477	C1411	U1351	G1291	C1230	A1170	G1109	G1048	C989	G929	G869	A802	G742
U	C1478	C1412	G1352	U1292	G1231	G1171	A1110	U1049	C990	C930	U870	A803	G743
C	C1479	A1413	G1353	G1293	U1232	C1172	A1111	G1050	U991	G931	U871	U804	C744
U	G1480	U1414	C1354	G1294	G1233	G1173	C1112	C1051	U992	G932	A872	C805	G745
U	U1481	U1415	G1355	G1295	C1234	G1174	C1113	U1052	G993	G933	A873	C806	G746
U	G1482	G1416	G1356	C1296	U1235	G1175	G1114	G1053	A994	G934	G874	A807	C747
C	A1483	G1417	A1357	C1297	U1236	G1176	C1115	G1054	A995	A935	C875	C808	C748
U	C1484	A1418	U1358	C1298	A1237	G1177	C1116	A1055	A996	G936	G876	C809	C749
U	U1485	G1419	A1359	A1299	A1238	G1178	C1117	U1056	U997	A937	C877	C810	G750
U	G1486	C1420	C1360	G1300	A1239	A1179	C1118	G1057	G998	A938	C878	C811	G751
U	G1487	G1421	G1361	U1301	U1240	A1180	C1119	G1058	G999	G939	C879	C812	G752
U	G1488	C1422	C1362	U1302	G1241	G1181	G1120	C1059	C880	C940	C880	U813	A753
U	G1489	G1423	A1362A	G1303	C1242	G1182	U1121	C1060	G881	G941	G881	A814	C754
U	C1490	U1424	A1363	G1304	C1243	A1183	U1122	G1061	C882	G942	C882	A815	G755
U	G1491	U1425	G1364	G1305	C1244	A1184	A1123	U1062	C883	U943	C883	A816	C756
U	A1492	C1426	G1365	A1306	A1245	G1185	C1124	C1063	U884	G944	U884	C817	U757
U	A1493	U1427	C1366	U1307	G1253	G1186	U1125	G1064	C1007	G945	G885	G818	G758
U	G1494	G1428	C1367	U1308	A1248	G1187	U1126	U1065	C1008	A946	G886	A819	A759
U	U1495	C1429	G1368	G1309	C1249	A1188	G1127	C1066	G887	G947	G887	U820	G760
U	C1496	C1430	C1369	G1310	A1250	C1189	C1128	A1067	G888	G948	C888	G821	G761
U	G1497	C1431	G1370	G1311	A1251	G1190	C1129	G1068	A889	A949	C889	C822	C762
U	U1498	G1432	G1371	G1312	A1252	A1191	A1130	C1069	U890	U950	C890	G823	G763
U	A1499	A1433	U1372	U1313	G1253	C1192	G1131	U1070	G951	G951	U891	C824	G764
U	A1500	G1434	G1373	C1314	C1254	G1193	C1132	C1071	A1013	U952	A892	G825	G765
U	C1501	G1435	A1374	U1315	G1255	U1194	G1133	G1072	A1015	G953	C893	C826	A766
U	A1502	U1436	A1375	C1316	A1256	C1195	G1134	U1073	A1016	G954	G894	U827	A767
U	A1503	C1437	G1376	G1317	U1257	U1196	U1135	G1074	G895	U955	A894	A828	A768
U	G1504	G1438	A1377	A1318	G1258	G1197	U1136	C1075	C896	U956	C896	G829	G769
U	G1505	C1439	C1378	A1319	C1259	G1198	C1137	C1076	C897	U957	C897	G830	C770
U	U1506	C1440	G1379	G1320	C1260	U1199	G1138	G1077	C898	A958	C898	U831	G771
U	A1507	G1441	U1380	C1321	A1261	C1200	G1139	U1078	C899	A959	C899	C832	U772
A	A52	G1442	U1381	C1322	C1262	A1201	C1140	G1079	A900	U960	A900	U833	G773
C	C53	G1443	G1382	G1323	C1263	C1202	C1141	A1080	G961	U961	G902	C834	G774
U	A510	A1446	A1324	C1324	C1264	C1203	G1142	U1081	U1025	G962	G903	U835	G775
U	G1511	G1447	G1385	G1325	G1265	A1204	G1143	G1082	G963	G963	G904	G836	G776
U	U1512	C1448	G1386	C1326	G1266	U1205	G1144	U1083	A964	A964	C904	G837	A777
U	A1513	C1449	G1387	C1327	C1267	G1206	C1145	G1084	A965	A965	U905	G838	G778
U	C1514	U1450	C1388	C1328	A1268	G1207	A1146	U1085	G966	G966	G906	U841	C779
U	G1515	A1451	C1389	A1329	A1269	C1208	C1147	U1086	C967	C967	A907	C842	A780
U	C1516	G1452	U1390	U1330	C1270	C1209	U1148	G1087	A968	A968	C908	U843	A781
U	G1517	G1453	U1391	G1331	G1271	C1210	G1149	G1088	C1030	A969	A909	C848	A782
U	A1518	G1454	A1392	A1332	C1272	U1211	U1150	G1089	G1031	C970	C910	C849	C783
U	U1519	U1455	U1393	A1333	G1273	U1212	A1151	U1090	A1032	G971	U911	U850	C784
U	G1520	A1394	G1334	G1334	G1274	A1213	A1152	U1091	G1032A	C972	C912	G851	G785
U	U1521	C1395	C1335	C1335	A1275	C1214	C1153	A1092	G1032B	G973	A913	G852	G786
U	G1522	A1396	G1336	G1336	G1276	G1215	G1154	A1093	G1033	A974	A914	G853	A787
U	G1523	C1397	G1337	G1337	C1277	G1216	G1155	G1094	G1034	A975	A915	U788	U788
U	C1524	G1464	A1398	G1338	U1278	C1217	G1156	U1095	A1035	G976	G916	U789	U789
U	G1525	C1399	A1339	A1339	A1279	U1218	A1157	C1096	G1036	A977	G917	C856	A790
U	A50	C1400	A1340	A1340	A1280	U1219	C1158	C1097	C1037	A978	A918	C857	A791
U	G1526	G1401	U1341	G1341	U1281	G1220	U1159	C1098	C1038	C979	A919	G858	A792
U	U1528	C1402	C1342	G1342	C1282	G1221	G1160	C1099	C1039	C980	U920	A860	U793
U	G1529	G1469	C1403	G1343	G1283	C1222	G1161	U1040	U1040	U981	U921	G861	A794
U	C1530	G1470	C1404	C1344	C1284	C1223	C1162	A1041	A1041	U982	G922	U862	C795
U	A1531	G1471	U1345	U1345	A1285	G1224	C1163	C1103	G1042	A983	A923	U863	C796
U	U1472	U1406	A1346	A1346	A1286	A1225	G1164	G1104	C1043	C984	C924	A864	C797
U	C1533	G1473	G1347	G1347	A1287	C1226	G1165	A1105	C1044	C985	G925	A865	G798
U	A1534	G1474	U1408	U1348	A1288	C1227	G1166	G1106	A1045	A986	G926	C866	G799
C	A59	G1475	C1409	A1349	A1289	C1228	A1167	C1107	A1046	G987	G927	G867	G800

• Molecule 1: 16S ribosomal RNA

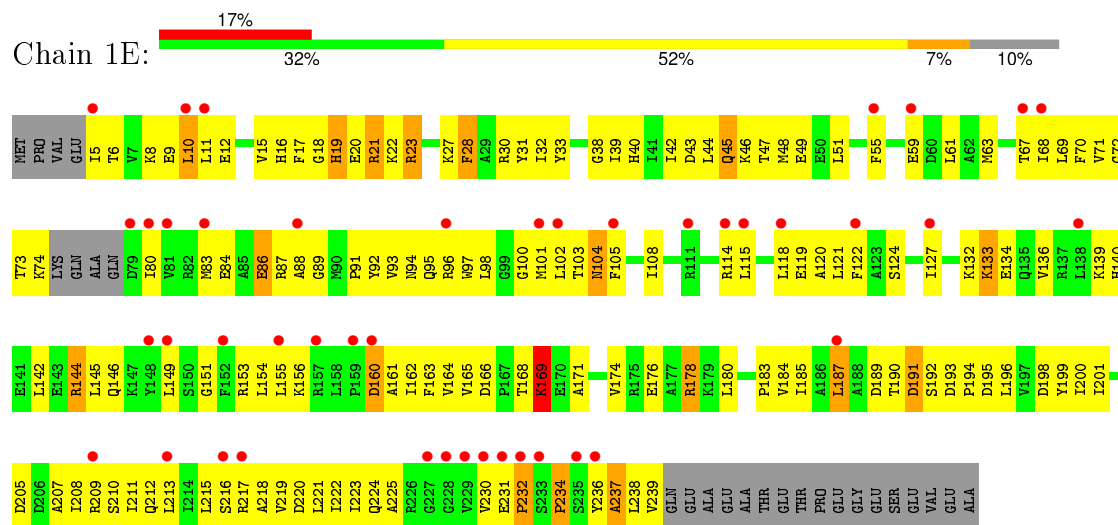


U	U1	U2	G	U4	U5	G6	G7	A8	G9	A10	G11	U12	U13	U14	G15	A16	U17	A19	U20	G21	G22	G23	C24	U25	C26	A26	A27	G28	G29	U30	G31	A32	A33	U34	G35	G36	U37	G38	G39	C40	G41	G42	C43	A44	U45	G46	C47	C48	U49	A50	G51	G52	A53	C54	A55	U56	C1533	G57	C58	A59
---	----	----	---	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-----	-----	-----

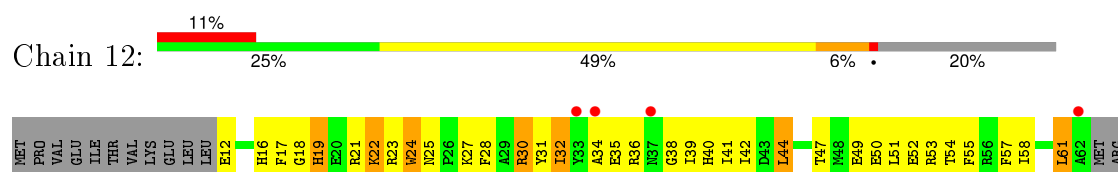
C1007	C948	G887	U820	G760	G629	C569	A509	C435	A373	C312	A250	C186E	G127	A60
C1008	A949	G888	G821	G761	G630	G670	A510	C436	A374	A313	G251	C186F	G128	A61
G1009	U950	A889	G822	G762	G631	U571	C511	U437	U375	C314	U252	C187	U129	G62
G1010	G951	G890	G823	G763	A632	A572	U512	U438	G376	C315	U253	U188	G129A	G63
G1011	U952	U891	C824	G764	G633	A573	C513	A439	G377	G316	G254	U189	A130	G64
U1012	G953	A892	G825	G765	G634	A574	C514	A440	G381	G317	G255	G190	C131	U65
G1013	G954	C893	C826	A766	G635	G575	U515	C462		G318	U256	G191A	C132	U66
A1014	U955	G894	U827	A767	U636	G576	U516	C443	A382	G319	G257	G191B	U133	C67
A1015	U956	A895	A828	A768	G637	G577	C517	C444	A383	C320	G258	G191C	A134	G68
C896	U957	G896	G829	A769	G638	C578	C518	C445	G384	A321	G259	G191D	C135	G69
G1017	A958	C897	G830	C770	G639	G579	C519	U446	G385	C322	G260	G191E	C136	G73
C1018	U959	G898	U831	G771	G644	U580	A520	U447	G386	U323	U261	U191F	C137	C74
U1019	U960	C899	G832	U772		G581	A521	A448	U387	G324	A262	G191	C138	C75
U1020	U961	A900	U833	G773	C645	U582	C522	C449	G388	A325	A263	U192	G76	G77
A901	G962	G902	G836	G774	U646	A583	A523	G450	A389	G326	U264	C193	G142	
G1022	G963	G903		G775	C647	A584	G524	A451	C390	A327	U265	C194	G78	G78
G1023	A964	G904	G837	G776	A648	G585	C525	A452	G391	C328	G266	A195	G144	G79
G1024	A965	C903	G838	A777	G649	G586	C526	A453	G392	A329	A196	G197	G145	G80
U1025	G966	U905	U841	G778	G650	G587	G527	C454	A393	C330	C267	A197	G146	G81
G906	C967	G906	G842	C779	C651	G588	C528	C455	G394	G331	A270	G198	G147	U82
C	A968	A907	U843	A780	U652	G589	C529	U456	C395	G332		G199	G148	U
C	A969	A908	C948	A781	A653	C590	G530	C457	G396	C333	C272	G200	G149	U
C	C970	A909	C949	A782	G654	U591	U531	C458	A397	C334	A273	G201	C150	U
C	G971	C910	U850	C783	G657	G592	A532	G464	G398	C335	A274	U208	C153	A87
C	G972	U911	G851	C784		G593	A533	A465	G399	C336	G275	U209		C88
C	G973	C912	G852	G785	G658	G594	U534	C466	C400	C337	G276	U210	C154	U89
G	A974	A913	G853	C726	U659	G595	A535	C467	C401	A338	C277	G216	C155	C90
A	A975	A914	G854	A727	U660	C596	C536	A468	G402	C339	G278	C217	G158	C91
G	G976	G915	G855	U788	G661	G597	G537	U475	C403	U340	A279	C218		G92
G	A977	G916	C856	A729	G662	U598	G538	G475	U404	C341	C280	C219	U93	U93
G	A978	G917	G857	A790	A663	C599	A539	G476	U405	C342	G281	G220	A160	G95
C	C979	A918	G858	G731	G664	C600	G540	G406	U406	C345	G284	C221	A161	G96
A	G980	A792	A859	C732	A665	C601	G541		G407		G285	U222	A162	U97
G1036	U981	U920	A860	G733	G666	A602	G542	U480	A408	C346	G286	U223	C163	C99
C1037	U982	U921	G861	G734	G667	U603	C543	A481	A409	G347	G287	U224	U170	A101
C1038	A983	G922	C862	C735	G668	G604	G544	A482	G409	A348	U287	C225	C165	G102
C1039	C984	A923	U863	G736	G669	U605	G545	C483	G410	A349	A288	G226	G166	C103
U1040	C985	C924	A864	A737	U669	G606	G546	G484	A411	G350	G289	G227	G167	G104
A1041	A986	G925	A865	C738		A607	G547	G485	A412	C351	C290	A228	A168	G105
G1042	G987	G926	C866	G739	G674	A608	G548	U486	G413	C352	C291	G229	G169	
C1043	U988	G927	G867	U740	A675	A609	C549	C488	A415	A353	G292	G230	U171	C106
A1044	C989	G928	C868	G741	A676	G610	G550	C489	G416	G354	G293	G231	A171	G108
G1045	C990	G929	G869	U742	U677	A611	U551	G490	C417	C355	U294	G232	A172	A109
A1046	U991	C930	U870	G743	U678	C612	U552	G491	C418	A356	C295	G233	U173	C110
G1047	U992	C931	U871	U744	C679	C613	A553	G492	C419	G357	U296	C234	C174	G111
G1048	G993	C932	A872	C745	C680	A614	C554	G493	U420	U358	G297	C235	C175	G112
U1049	A994	G933	A873	A746	G683	C615	C555	U494	U421	U359	A298	G236	C176	G113
G1050	C995	C934	G874	C747		G616	C556	U495	C422	A360	G299	G237	C177	U114
C1051	A996	A935	C875	G748	G684	G617	G557	A496	G423	G361	A300	G238	U180	G115
U1052	U997	G936	G876	C749		C618	G558	U497	G424	G362	G301	U239		A116
G1053	G998	A937	C877	G750	U686	U619	A559	A498	G425	A363	G302	C240	G181	G117
C1054	C998A	A938	G878	U751	A687	C620	U560	G500	G426	A364	G303	C241	U182	U118
A1055	U999	G939	C879	G752	G688	A621	U561	C501	U427	U365	U304	C242	G183	A119
U1056	A1000	C940	G880	A753	C689	A622	C562	G502	G428	C366	G305	A243	G184	A120
G1057	G1001	G941	G881	A814	G690	C623	A563	C503	U429	U367	G306	U244	A185	G121
G1058	G1002	G942	C882	A815	G691	C624	C564	C504	A430	U368	C307	C245	C186	G122
C1059	G1003	U943	C883	A816	U692	G625	U565	G505	A431	C369	C308	A246	C186A	G123
C1060	A1004	A946	U884	C817	G693	U626	G566	G506	A432	C370	G309	G247	C186B	U125
G1064	C1006		G886	A819	U697	G628	G568	C508	U434	C372	C311	U249	C186D	G126

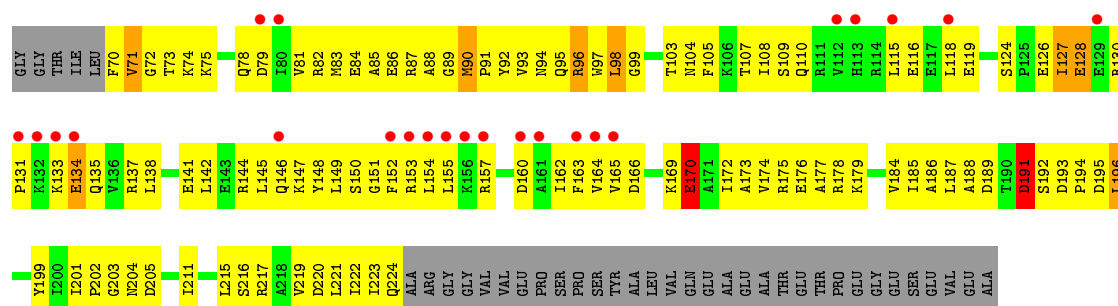


### • Molecule 2: 30S ribosomal protein S2

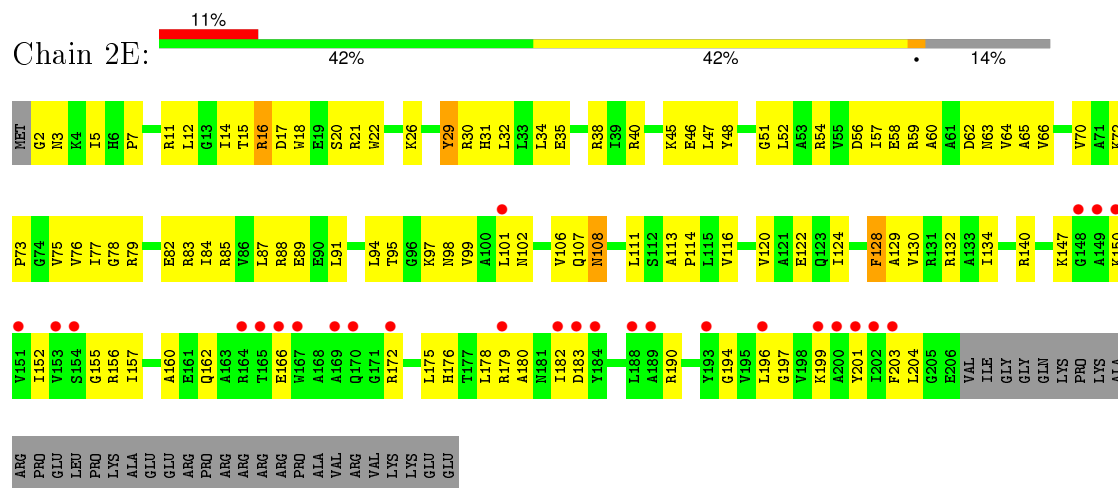


### • Molecule 2: 30S ribosomal protein S2

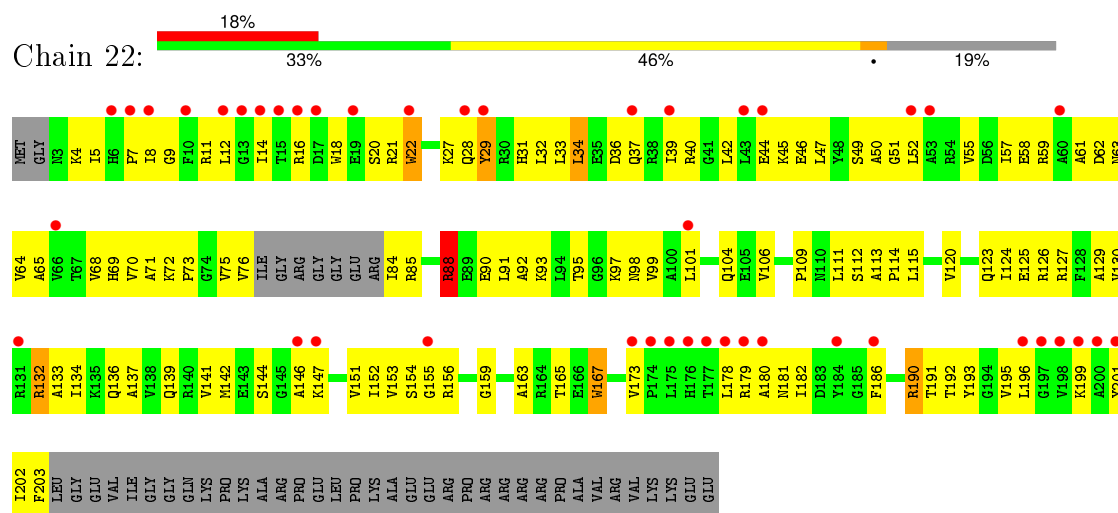




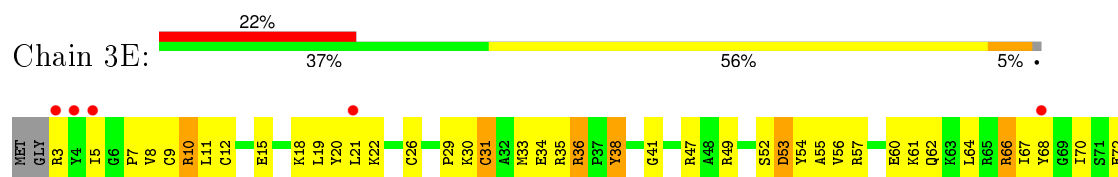
• Molecule 3: 30S ribosomal protein S3



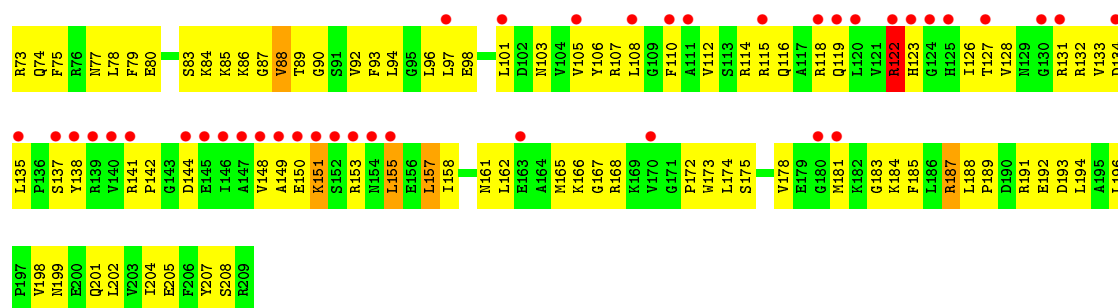
• Molecule 3: 30S ribosomal protein S3



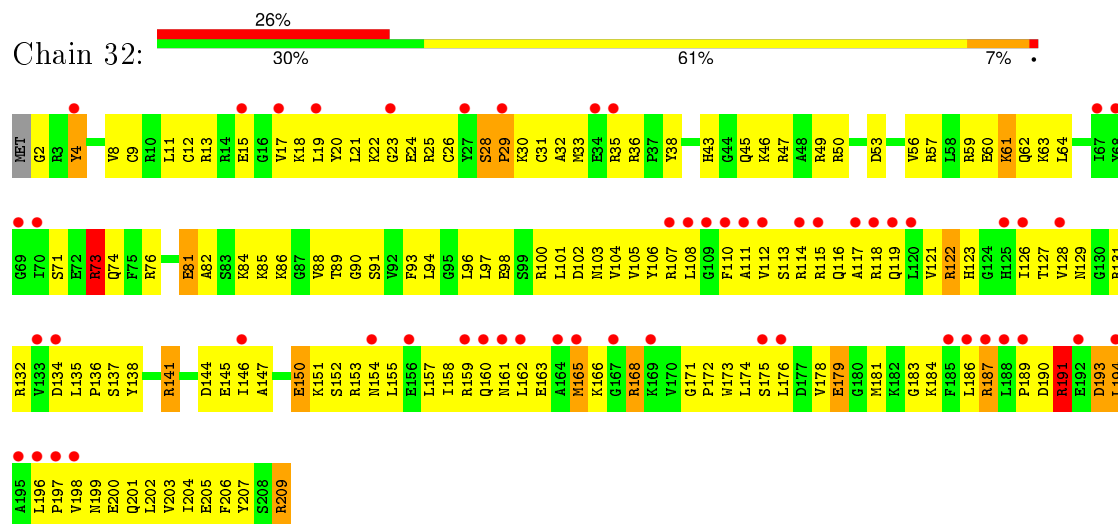
• Molecule 4: 30S ribosomal protein S4



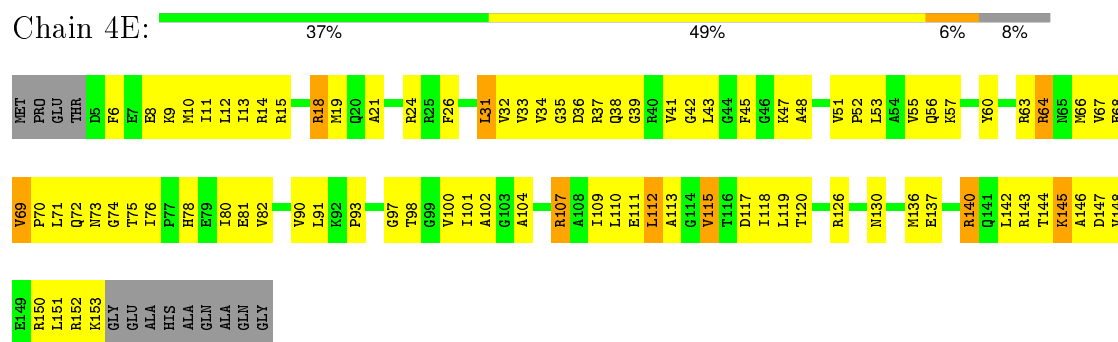




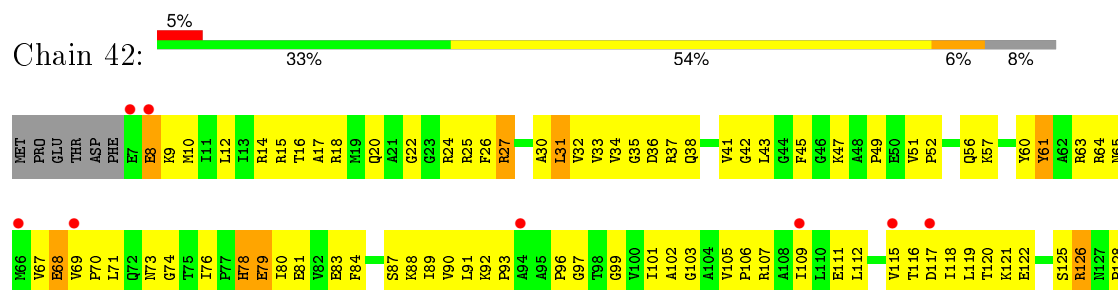
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

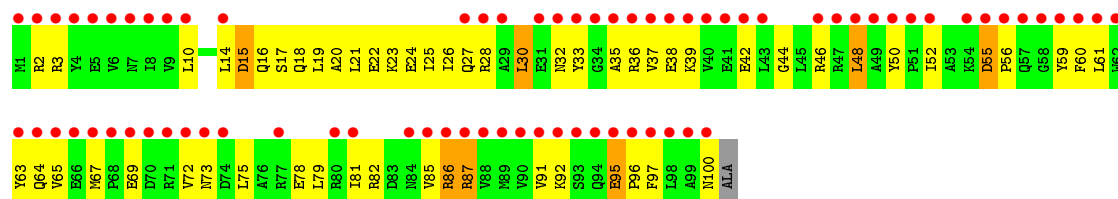
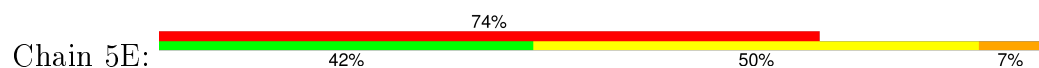


• Molecule 5: 30S ribosomal protein S5

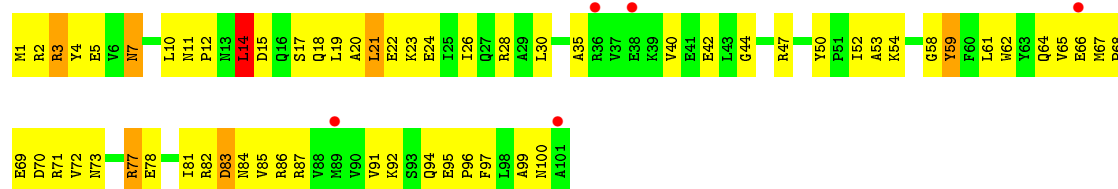




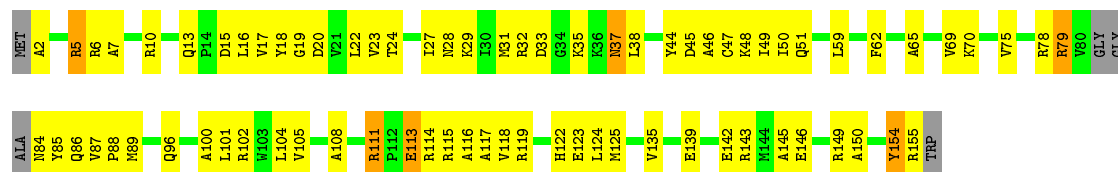
• Molecule 6: 30S ribosomal protein S6



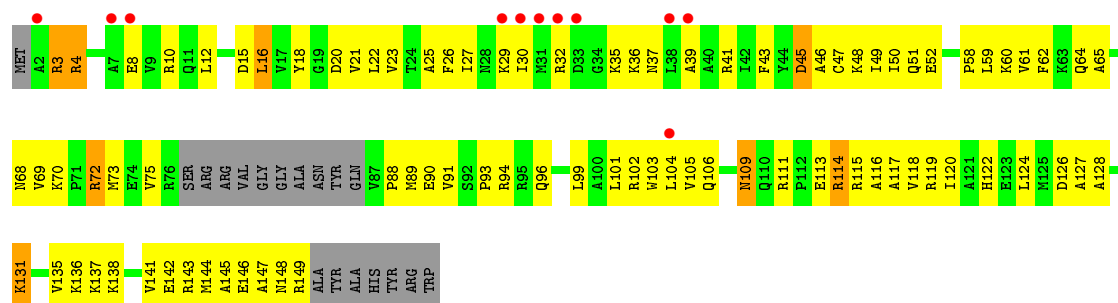
• Molecule 6: 30S ribosomal protein S6



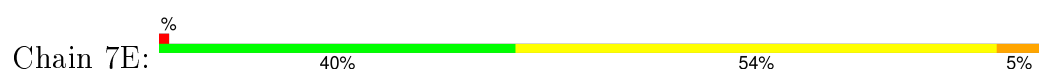
• Molecule 7: 30S ribosomal protein S7

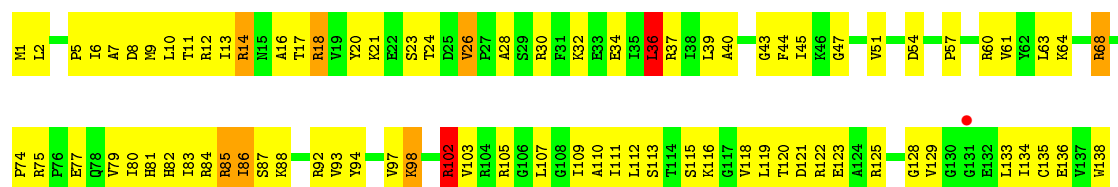


• Molecule 7: 30S ribosomal protein S7

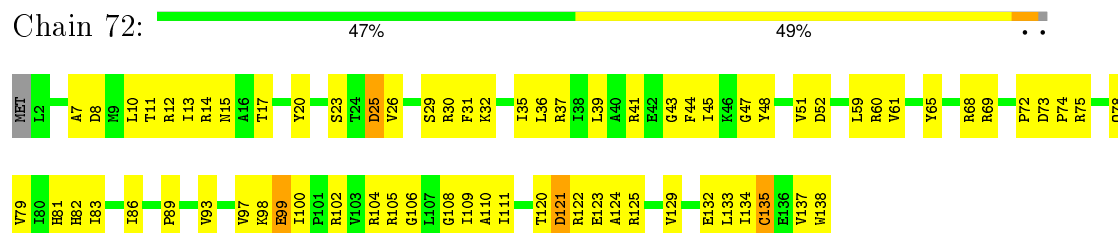


• Molecule 8: 30S ribosomal protein S8

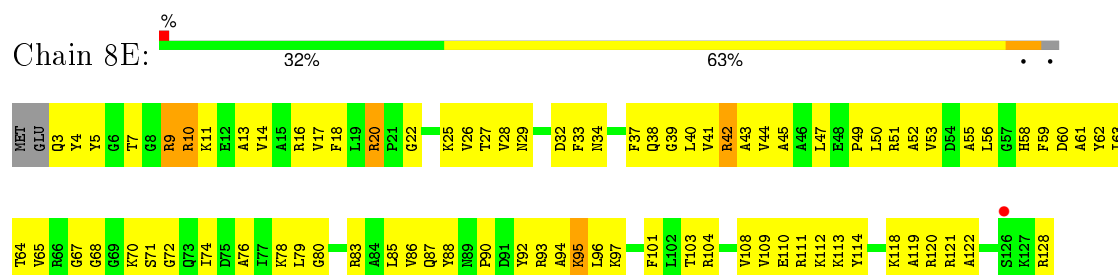




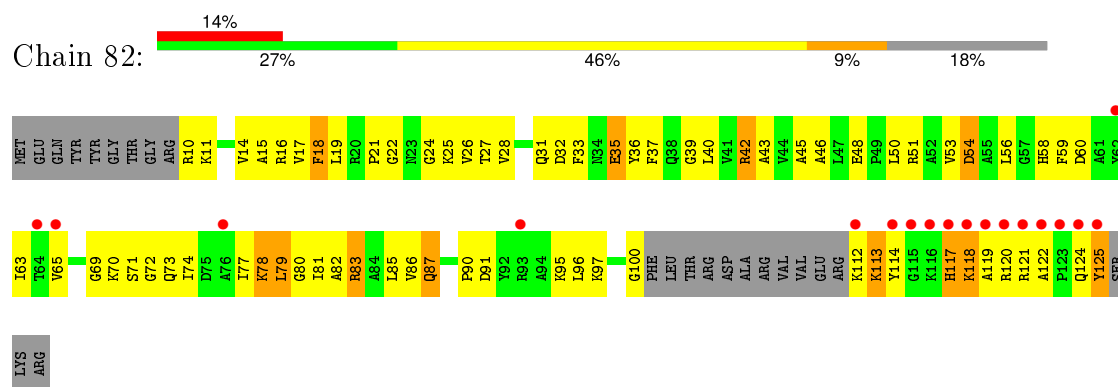
• Molecule 8: 30S ribosomal protein S8



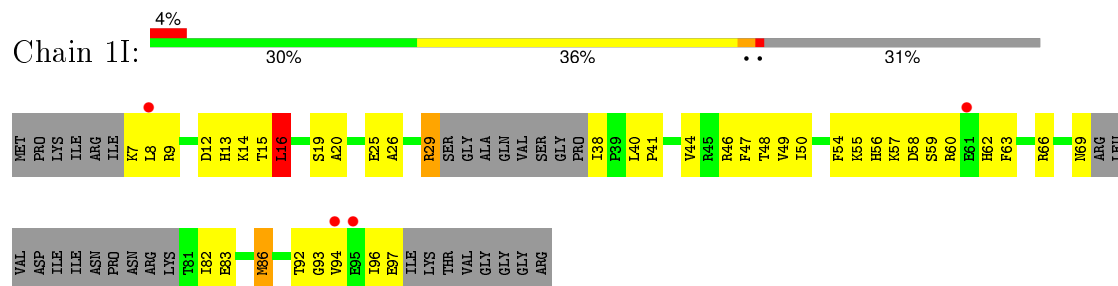
• Molecule 9: 30S ribosomal protein S9



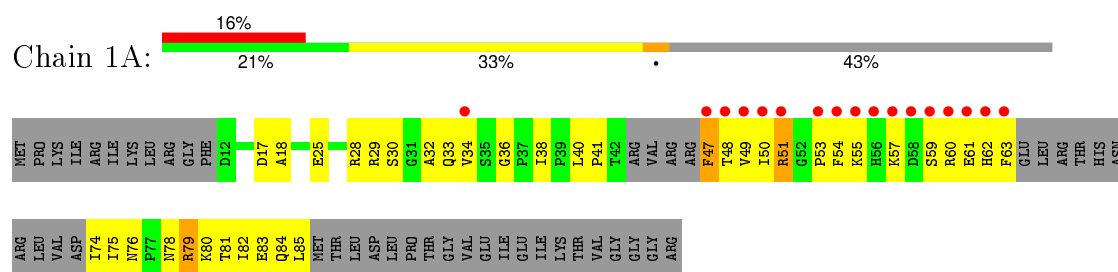
• Molecule 9: 30S ribosomal protein S9



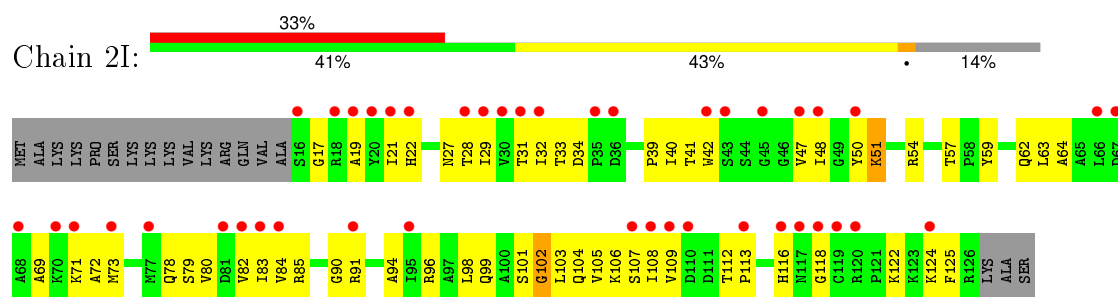
• Molecule 10: 30S ribosomal protein S10



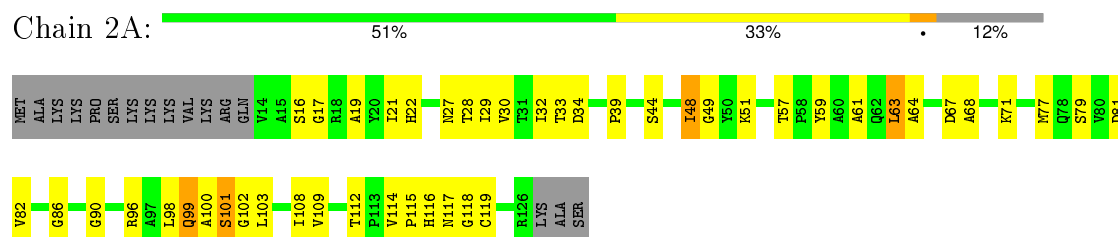
• Molecule 10: 30S ribosomal protein S10



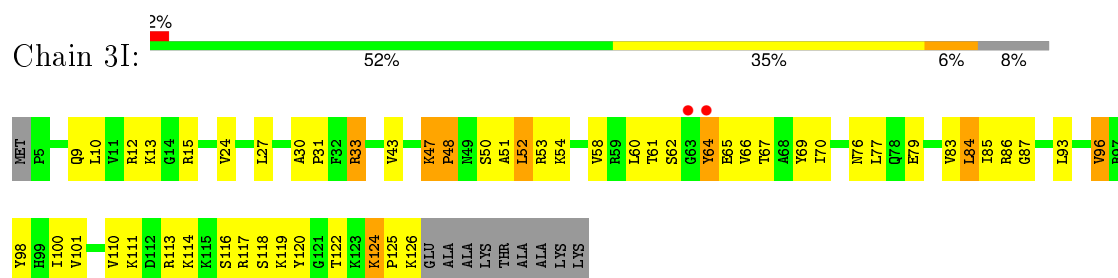
- Molecule 11: 30S ribosomal protein S11



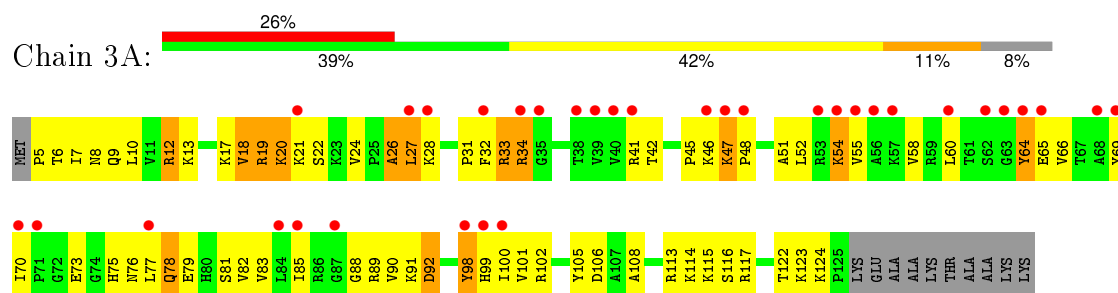
- Molecule 11: 30S ribosomal protein S11



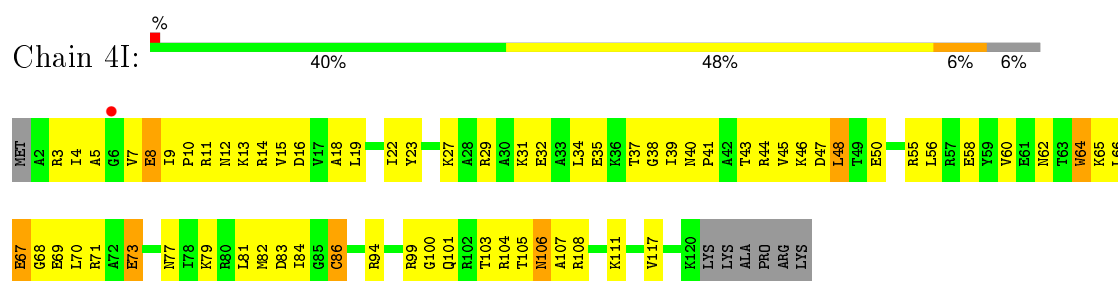
- Molecule 12: 30S ribosomal protein S12



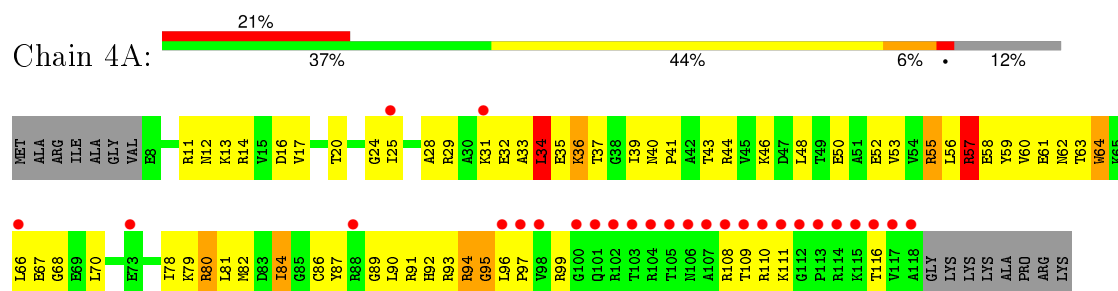
- Molecule 12: 30S ribosomal protein S12



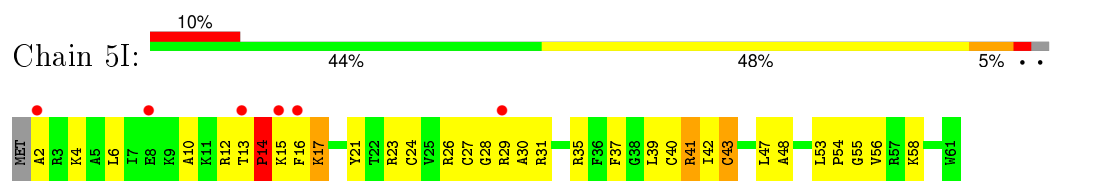
- Molecule 13: 30S ribosomal protein S13



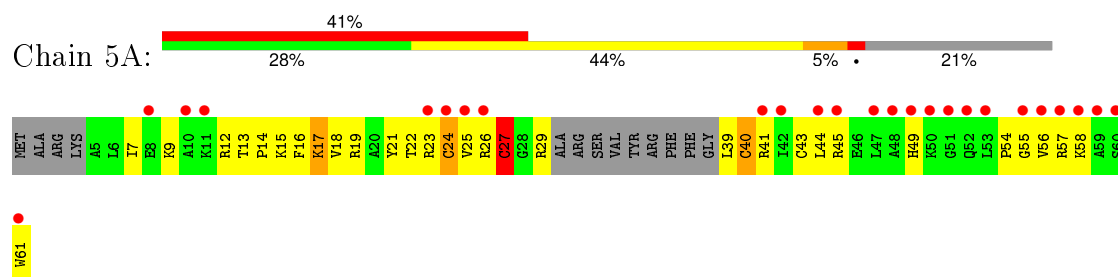
- Molecule 13: 30S ribosomal protein S13



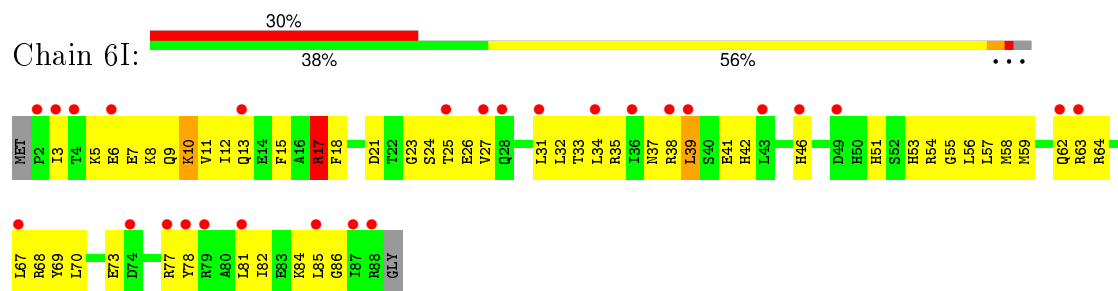
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

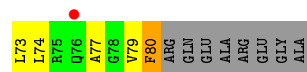
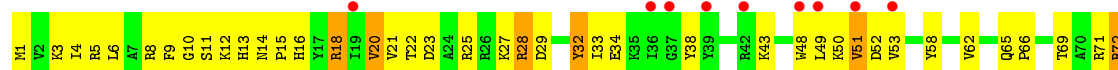


- Molecule 15: 30S ribosomal protein S15

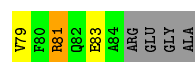
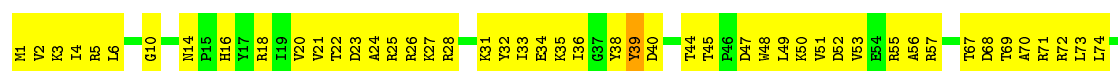




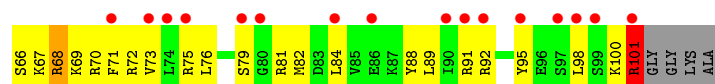
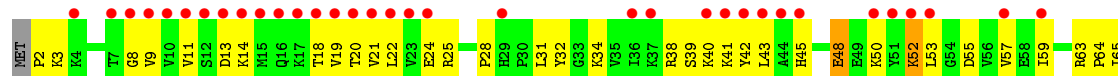
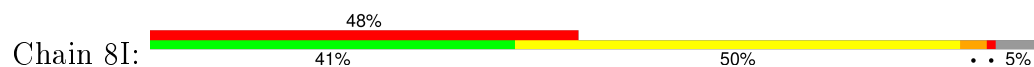
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



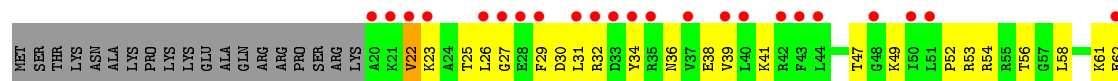
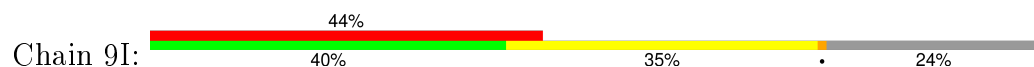
- Molecule 17: 30S ribosomal protein S17

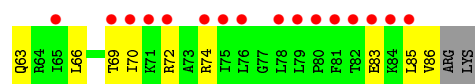


- Molecule 17: 30S ribosomal protein S17

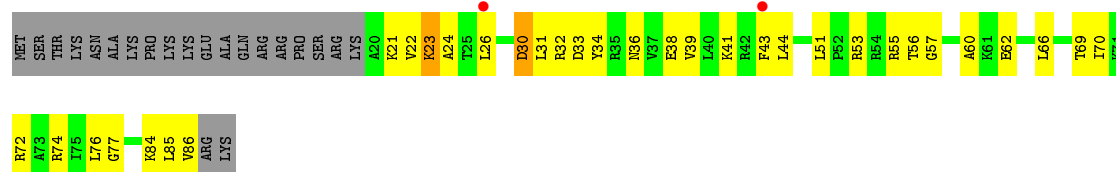


- Molecule 18: 30S ribosomal protein S18

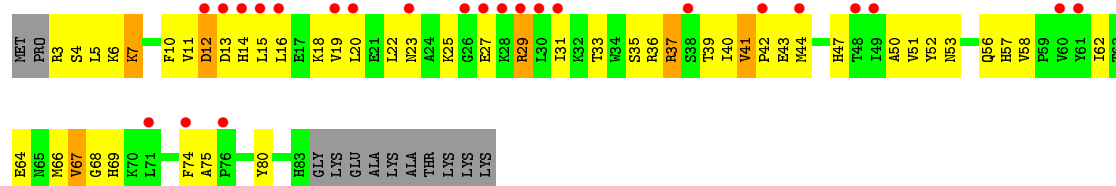




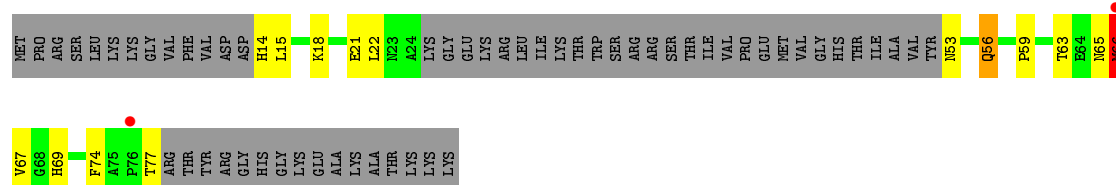
• Molecule 18: 30S ribosomal protein S18



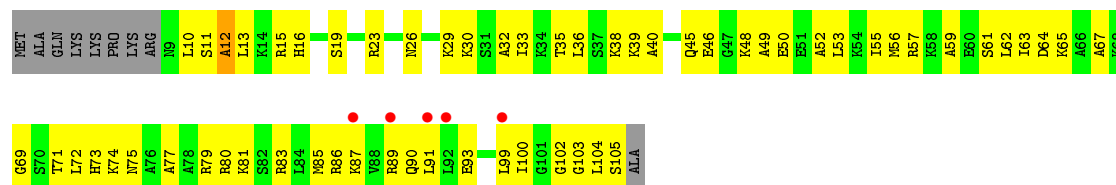
• Molecule 19: 30S ribosomal protein S19



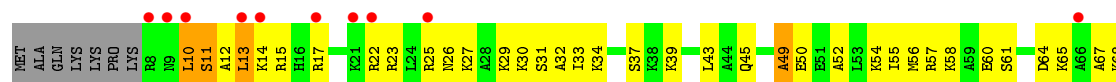
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

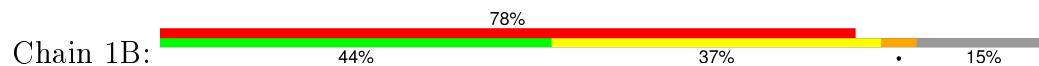




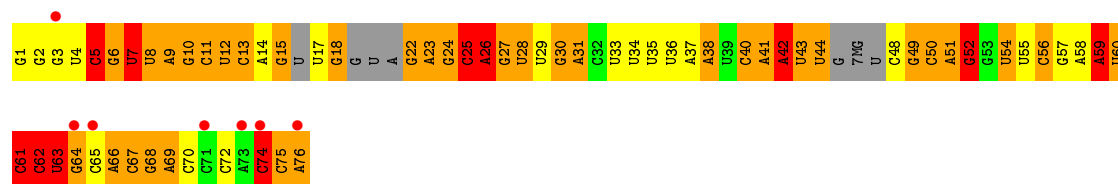
- Molecule 21: 30S ribosomal protein Thx



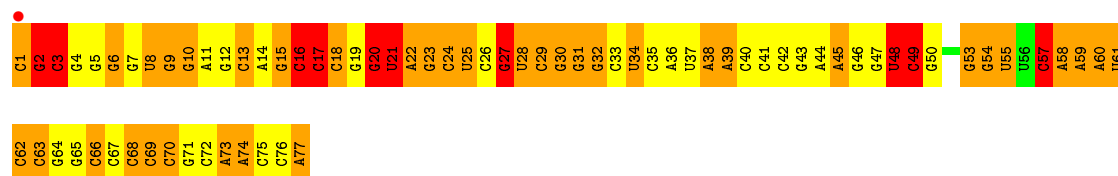
- Molecule 21: 30S ribosomal protein Thx



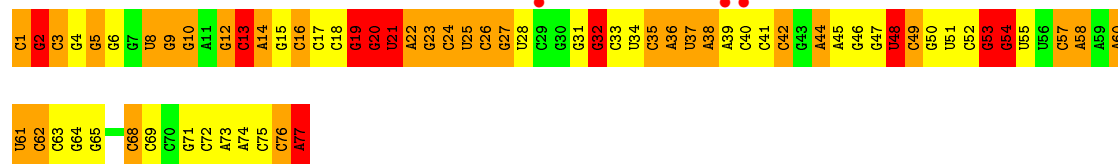
- Molecule 22: tRNA<sup>Lys</sup>



- Molecule 23: tRNA<sup>fMet</sup>



- Molecule 23: tRNA<sup>fMet</sup>

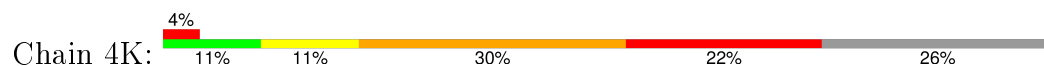


- Molecule 24: tRNA<sup>Lys</sup>

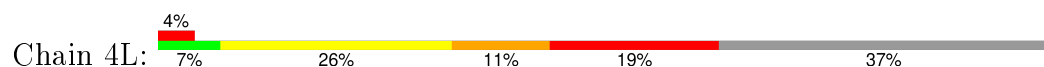




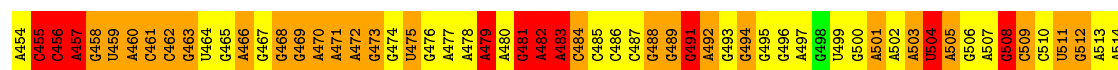
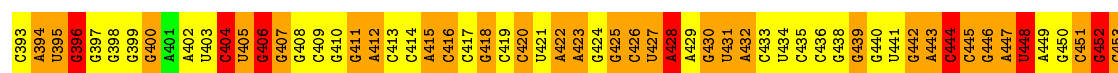
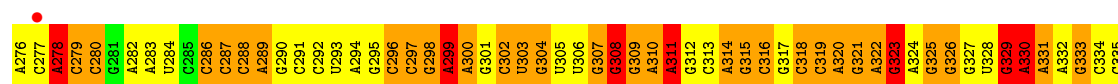
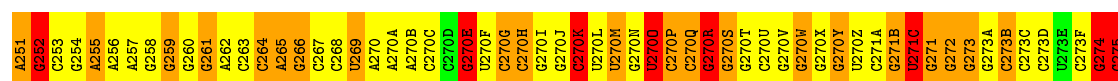
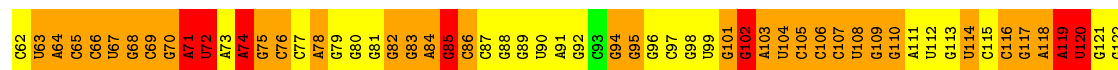
- Molecule 25: mRNA



- Molecule 25: mRNA

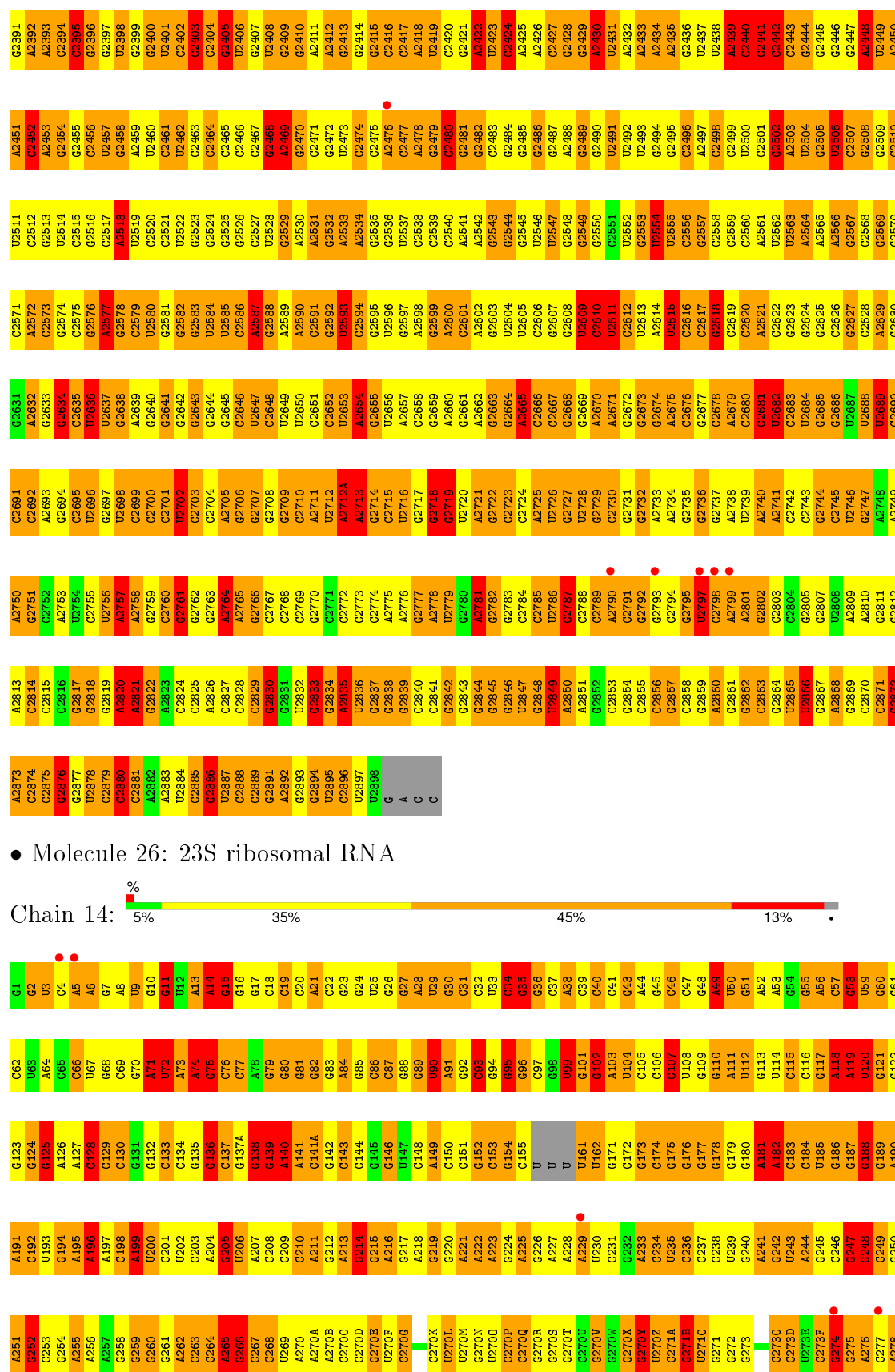


- Molecule 26: 23S ribosomal RNA



U1394	U1395	U1396	U1397	U1398	U1399	U1400	G1401	U1402	G1403	G1404	U1405	U1406	G1407	G1408	A1409	G1410	G1411	G1412	G1413	G1414	U1415	G1416	G1417	G1418	A1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	G1428	G1429	G1430	U1431	G1432	G1433	G1434	G1435	G1436	G1437	U1438	A1439	G1440	G1441	G1442	G1443	G1444	A1444A	G1445	G1446	G1447	G1448	A1449	G1449A	G1450	A1392	A1393																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1384	U1385	A1386	U1387	G1388	G1389	U1390	U1391	U1392	G1393	G1394	G1395	G1396	G1397	G1398	A1399	G13950	G1391	U1392	U1393	U1394	U1395	U1396	U1397	G1398	U1399	U1400	A1401	A1402	G1403	G1404	A1405	G1406	A1407	A1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	U1430	U1431	G1432	G1433	G1434	G1435	G1436	G1437	U1438	A1439	G1440	G1441	G1442	G1443	G1444	A1444A	G1445	G1446	G1447	G1448	A1449	G1449A	G1450	A1392	A1393																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1229A	G1230	G1231	G1232	G1233	U1234	G1235	G1236	U1237	G1238	G1239	U1240	A1241	A1242	G1243	G1244	G1245	A1246	G1247	G1248	U1249	G1250	G1251	G1252	A1253	G1254	U1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	A1263	U1264	G1265	G1266	G1267	G1268	G1269	A1270	U1271	G1272	U1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	A1301	A1302	G1303	G1304	G1305	G1306	A1307	A1308	G1309	G1310	G1311	G1312	U1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	A1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	U1330	U1331	A1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	U2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U23

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	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																															
G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330																															
C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270																										
G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140																															
G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A	G	G	G	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200																														
C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140																															
C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080																															
C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020																															
A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960																															
G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	A1900																						
G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831																															
G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	G1771															
C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695																															
C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635																													
U1514	C1515	U1516	G1517	G1518	G1519	U1520	G1521	G1522	U1523	U1524	G1525	G1526	G1527	A1528	A1529	C1468	A1469	G1470	A1471	C1533	G1534	U1541	G1542	A1543	C1544	A1545	A1546	A1547	C1548	C1549	C1550	C1551	G1552	A1553	A1554	G1555	C1556	C1557	A1558	C1559	G1560	C1561	C1562	U1563	C1564	C1565	C1566	A1567	C1568	A1569	A1570	A1571	A1572	G1573																																				
A1483	U1484	G1485	G1486	G1487	G1488	U1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	G1500	C1501	C1502	U1503	C1504	C1505	C1506	A1507	C1508	C1509	A1510	A1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	A1570	A1571	A1572	G1573



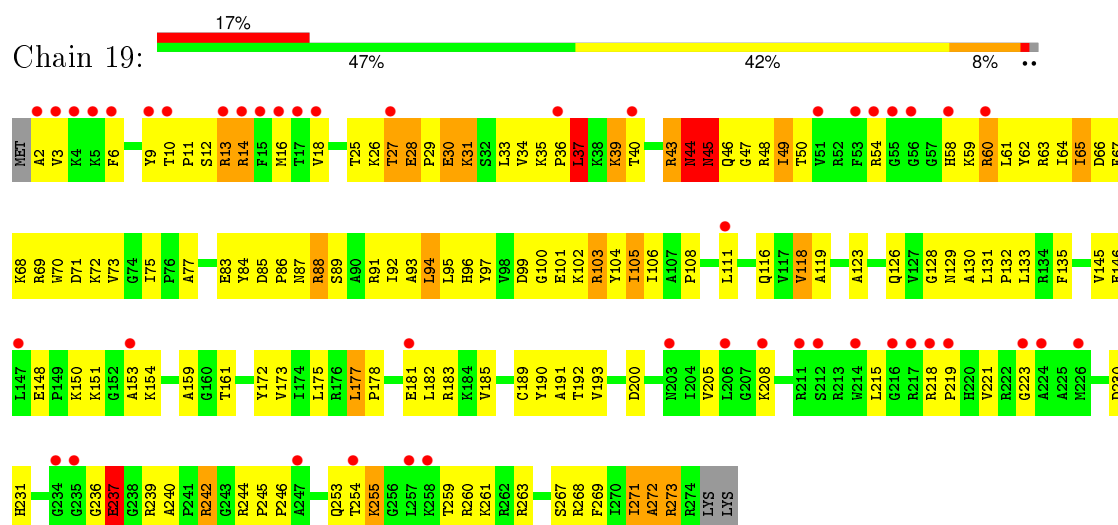
G1166	A1103	G1043	A983	U922	A861	G801	G741	G680	G642	C584	G522	C461	G398	A340	C279
U1167	C1104	G1044	A984	C923	G862	A802	G742	G681	A643	G585	G523	C462	G399	G341	
G1168	U1105	A	C985	C924	A863	U803	G743	G682	A644	A586	U824	G463	G400	G342	A282
G1169	G1106	A	C986	C925	A864	A804	G744	G683	G645	C587	U825	U464	A401	C343	A283
G1170	G1107	G1047	A988	A926	C865	G805	G745	G684	A646	U588	A526	G465	U402	G344	U284
G1171	U1108	A1048	A989	G928	A866	C806	A746	A685	G647	C589	G527	A466	U403	A345	C285
G1173	G1109	G1049	G989	G929	C867	U807	U747	G686	G648	A590	A528	G467	C404	A346	C286
A1174	G1110	A1050	A990	U930	U868	G808	G748	G687	G649	C591	A529	G468	U405	A347	C287
U1175	A1111	G1051	C991	G931	G869	G809	C749	G688	G650	G592	G530	G469	G406	G348	C288
G1176	G1112	A1052	C992	G932	A870	U810	A750	A689	G651	G593	A470	A470	G407	G349	A289
A1177	U1113	C1053	G993	A933	U871	U811	A751	G690	G652	U594	A532	A471	G408	U350	G290
G1178	G1114	A1054	C994	G934	A872	G812	A752	C691	A653	G595	G533	A472	G409	G351	C291
G1179	G1115	A1055	C995	C935	G873	U813	G753	C692	A654	G596	U534	A473	G410	G352	C292
C1180	C1116	G1056	A996	C936	G874	C814	C754	C693	A654A	U597	C535	G474	G411	G353	U293
G1181	G1117	A1057	G997	U937	G875	C815	C755	U694	G654B	G598	A536	U475	A412	G354	A294
A1182		U1058	C998	G938	C876	C816	C756	G695	G654C	G599	C537	A476	C413	G355	G295
G1183	G1120	G1059	U999	G939	U877	G817	U757	G696	G654D	G600	G539	A477	C414	G356	C296
G1184	G1121	U1060	A1000	G940	A878	G818	C758	C697	C	C601	G540	A478	C415		C297
C1185	G1122	U1061	A1001	A941	G879	A819	G759	C698	C	G602	C541	A479	C416	A359	G298
G1186		G1062	G1002	G942	G880	A820	G760	A699	C	A603	C542	A480	C417	G360	A299
G1187	G1125	G1063	U943	U943	G	A821	A761	G700	C	G604	C543	G481		G361	A300
U1188	A1126	C	C1004	G944	G	U822	U762	G701	C	C605	C544	U482	U421	G362	G301
A1189	A1127	U	C1005	A945	G	G823	G763	G702	A	U606	G545	A483	A422	G363	C302
G1190	A1128	U	C1006	G946	C	A824	A764	U703	C	U607	C546	A484	A423	A363A	U303
G1191	A1129	A	C1007	G947	C	G825	G765	G704	G	A567	C485	A485	G424	G363B	G304
G1192	U1130	G	C1008	G948	C	U826	C766	A705	C	A609	A548	C486	G425	G363C	U305
G1193	G1131	A1069	A1009	C949	A	A827	U767	A706	G	G609A	G549	C487	A426	G363D	U306
A1194	A1132	A1070	A1010	G950	C	U828	G768	G707	G	C610	G550	G488	U427	G363E	G307
G1195	U1133	G1071	G1011	C951	G	A829	G769	C708	A	C611	G551	G489	A428	A363F	G308
C1196	G1135	C1072	U1012	G952	A	G830	G770	U709	C	G612	G552	A491	A429	C364	G309
G1197	G1136	A1073	A953	A953	G	G831	G771	G710	C	U613	U553	A492	G430	C365	A310
U1198	G1137	G1074	U1014	G954	C	G832	C772	G711	G654R	U614	U554	G493	U431	G366	A311
U1199	G1138	C1075	C955	G955	C	U833	U773	G712	A654I	G615	G556	G494	A432	G370	G312
C1200	G1139	G1076	U1016	G956	U	G834	A774	G715	A654U	A616	U557	G495	C433	A371	C313
G1201	C1140	A	G1017	A957	C	A835	G775	A716	A654V	G617	G558	G496	U434	G372	A314
C1202	U1141	U	U1018	U958	C897	G836	G776	A717	A655	G618	G559	A497	C435	U373	G315
G1203	U1142	C	U1019	A959	C898	C837	A777	G717	G656	C618A	C560	G498	C436	A374	C316
A1204	A1142A	A	A1020	A960	A899	C838	G778	A718	U857	G619	G561	U499	G438	G375	G317
U1205	A1143	U	A1021	C961	A900	U839	U779	C719	C688	G620	U562	G500	G439	C376	C318
G1206	G1144	U	G1022	G962	A901	C840	G780	C720	C659	A621	G563	A501	G440	C377	C319
C1207	C1145	U	U1023	U963	C902	A841	A781	C721	G660	G622	C564	A502	U441	G378	A320
G1208		A	G1024	C964	C903	G842	A782	A722	C661	G623	C565	A503	G442	C379	G321
G1209	A1148	A1085	G1025	C965	C904	G843	A783	G723	G662	G624	U566	U504	A443	U380	A322
A1210	G1149	A1086	U1026	G966	U905	C844	A784	U724	G663	G625	A567	A505	C444	C381	G323
U1211	C1150	G1087	A1027	C967	G906	G845	G785	G725	C664	U626	U568	G506	C445	G382	A324
G1212	G1151	A1088	A1028	G968	U907	C846	C786	G726	G665	A627	U569	A507	G446	U383	G325
A1213	C1152	G1089	U1029	G969	C908	U847	U787	A727	G666	G628	G570	G508	A447	U384	G326
G1214	G1153	U1090	G1030	C970	A909	G848	A788	G728	U667	G629	A571	C509	U448	C385	G327
G1215	G1154	G1091	A910	C971	A910	A849	A789	G729	G668	G630	A572	C510	A449	G386	U328
G1216	A1155	C1092	A1032	G972	A911	C850	C790	C730	G669	A631	G573	U511	G450	U387	G329
G1217	A1156	G1093	U1033	A973	C912	U851	C791	C731	A670	A632	C574	G512	C451	G388	A330
G1218	G1157	U	G1034	G974	U913	G852	G792	C732	C671	A633	A575	A513	G452	G389	A331
G1219	C1158	A	U1035	C974A	C914	G853	A793	G733	C672	C634	U576	A514	C453	A390	A332
A1220	U1159	A	G1036		C915	G854	G794	A734	C673	G635	G577	A515	A454	G391	G333
G1221	G1160	U	G1037	G977	G916	G855	C795	A735	G674	G636	A578	C516	C455	C392	C334
C1222	C1161	A1098	C1038	G978	A917	C856	C796	C736	A675	A637	G579	C517	C456	C393	C335
C1223	G1162	G1099	G1039	G979	A918	C857	C797	C737	A676	G638	C580	G518	A457	A394	G336
G1224	G1163	A1100	A980	G980	G919	U858	G798	G738	A677	G639	C581	U519	G458	U395	C337
C1225	G1164	U1101	C1041	A981	G920	G859	G799	G739	C678	C640	G582	G520	U459	G396	G338
G1226	U1165	C1102	G1042	C982	G921	U860	A800	U740	C679	C641	G583	G521	A460	G397	U339

U2096	C2036	U1976	A1916	A1847	A1787	U1706	C1646	A1587	G1527	G1466	U1406	G1346	A1286	A1227
G2037	A1848	A1977	U1917	A1848	C1788	G1647	G1647	C1588	A1528	C1467	C1407	G1347	A1287	G1228
G2038	A1918	A1978	A1918	G1849	A1789	C1710	C1648	C1589	A1529	C1468	C1408	A1348	A1288	G1229
G2039	G1850	C1979	G1850	G1850	U1790	C1711	G1649	U1590	G1530	A1469	C1409	A1349	C1289	G1229A
C2040	G2010	G1851	C1920	U1851	A1791	C1712	G1650	G1591	C1531	G1470	G1410	C1350	C1290	C1230
U2041	G1921	C1852	G1921	C1852	G1792	U1716	G1651	C1592	C1532	A1471	C1411	C1351	C1291	G1231
A2042	C1853	C1822	G1922	A1853	C1793	C1717	A1652	G1593	C1533	A1472	G1412	U1352	U1292	G1232
C2043	C1983	C1983	C1923	A1854	U1794	G1718	G1653	C1594	C1534	G1473	G1413	A1353	C1293	G1233
G2044	G1955	G1955	C1924	G1854	C1795	G1725	A1654	G1595	U1535	C1474	G1414	A1354	U1294	U1234
C2045	G1856	G1856	G1925	A1856	U1796	G1726	A1655	A1596	A1536	G1475	U1415	G1355	C1295	G1235
C2107	G1926	A1886	U1926	G1857	C1797	U1727	C1656	A1597	C1537	C1476	G1416	G1356	G1296	G1236
U2047	G1987	G1987	G1927	G1858	U1798	G1728	C1657	C1598	G1538	A1477	G1417	U1357	C1297	A1237
C2108	A1928	A1928	A1928	A1859	U1799	A1729	C1658	C1599	G1539	G1478	G1418	G1358	C1298	G1238
U2109	G1860	G1860	G1928	G1860	C1800	A1729	C1659	C1600	G1540	G1479	A1419	A1359	G1299	G1239
G2049	G1861	G1861	G1929	G1861	G1801	U1730	U1659	C1601	U1541	G1480	U1420	A1360	U1300	U1240
C2050	C1930	C1930	G1930	G1862	A1802	G1731	C1660	G1602	G1542	G1482	G1421	G1361	A1301	A1241
A2051	G1863	G1863	U1931	G1862	G1803	A1732	G1661	U1602	G1543	G1483	G1422	C1362	A1302	A1242
G2052	G1933	G1933	A1932	G1863	A1804	C1733	C1662	A1603	A1543	G1484	G1423	G1363	G1303	G1243
G2053	U1864	U1864	G1934	G1864	C1804	C1734	C1663	C1604	C1544	G1485	G1424	G1364	C1304	G1244
A2054	G1869	G1869	C1934	G1869	U1805	C1735	A1664	C1605	A1545	G1486	G1425	A1365	C1305	G1245
C2055	C1870	C1870	G1935	A1870	C1806	C1741	A1665	C1606	A1545A	A1486	C1426	A1366	C1306	G1246
G2056	A1871	A1871	A1936	C1871	C1807	C1742	G1666	C1607	C1546	G1487	G1427	A1367	A1307	A1247
A2057	A1872	A1872	A1937	A1872	U1808	G1743	C1667	A1608	C1547	G1488	A1428	G1368	A1308	G1248
A2058	G1878	G1878	A1938	G1878	A1809	G1746	A1668	A1609	C1548	G1489	C1429	G1369	G1309	U1249
A2059	C1879	C1879	U1939	A1879	A1810	G1751	A1669	C1610	C1549	A1490	G1429	G1370	G1310	U1250
G2060	G1880	G1880	U1940	C1880	G1811	C1751	C1670	C1611	G1549	G1491	G1430	G1370	G1310	G1250
G2061	C1881	C1881	C1941	C1881	A1812	C1752	U1671	C1612	C1551	G1492	U1431	G1371	G1311	C1251
A2062	G1882	G1882	G1942	C1882	G1813	G1753	C1672	C1613	G1552	C1493	G1432	U1372	U1312	G1252
C2063	C1883	C1883	U1943	G1883	G1814	C1754	U1673	A1614	A1553	A1494	C1433	A1373	U1313	A1253
G2064	A1884	A1884	U1944	A1884	A1815	A1755	G1674	C1615	A1554	A1495	A1434	G1374	C1314	A1254
A2005	A1885	A1885	G1945	A1885	G1816	G1756	C1675	A1616	G1555	A1496	G1435	C1375	C1315	U1255
C2066	C1886	C1886	U1946	C1886	G1817	U1757	A1676	C1617	C1556	U1497	G1436	C1376	G1256	U1256
G2067	G1887	G1887	C1947	G1887	U1818	G1758	A1677	A1618	C1557	C1498	G1437	G1377	A1317	C1257
U2068	C1888	C1888	C1948	C1888	A1819	A1759	G1678	G1619	A1558	C1499	U1438	A1378	C1318	C1258
C2069	A1889	A1889	G1949	A1889	U1820	A1760	U1679	G1620	G1559	G1500	A1439	A1379	G1319	G1259
G2070	A1890	A1890	G1950	A1890	U1821	C1761	U1680	U1621	G1560	C1501	G1440	G1380	G1320	G1260
U2011	G1891	G1891	U1951	G1891	G1822	A1762	G1681	G1622	G1561	G1502	G1441	G1381	A1321	C1261
G2012	C1892	C1892	A1952	C1892	G1823	G1763	G1682	G1623	A1562	U1503	G1442	G1382	A1322	U1262
A2013	C1893	C1893	A1953	C1893	G1824	G1764	C1683	G1624	G1563	C1504	G1443	C1383	U1323	U1263
A2014	C1894	C1894	C1954	C1894	A1825	C1765	C1684	C1625	G1564	C1505	G1444	A1384	G1324	U1264
U2075	G1895	G1895	U1955	G1895	G1826	U1766	C1685	C1626	C1565	A1507	C1445	G1385	G1325	A1265
U2076	G1896	G1896	U1956	G1896	C1827	C1767	C1686	G1627	A1566	C1508	G1446	C1386	G1326	U1266
A2077	G1897	G1897	C1957	G1897	G1828	U1768	G1687	G1628	A1567	A1509	G1447	C1387	C1327	U1267
C2078	U1898	U1898	G1958	U1898	A1829	G1769	U1688	U1629	G1568	C1509	G1448	G1388	G1328	A1268
A2019	G1899	G1899	G1959	U1899	C1830	G1770	A1689	G1630	A1569	A1510	G1449	G1389	U1329	A1269
G2080	A1900	A1900	U1960	A1900	G1831	C1771	A1690	C1630A	A1570	A1511	A1449	U1390	C1330	C1270
C2021	C1901	C1901	C1961	C1901	C1832	G1772	C1691	A1631	A1571	G1449A	G1449	U1391	A1331	G1271
U2022	C1902	C1902	C1962	C1902	U1833	A1773	U1692	A1632	A1572	C1513	C1450	A1392	G1332	A1272
G2023	G1903	G1903	C1963	G1903	U1834	C1774	U1693	G1633	U1514	C1451	C1450	A1393	C1333	U1273
G2024	G1904	G1904	G1964	G1904	G1835	U1775	C1694	A1634	C1574	A1453	U1394	U1394	A1274	A1274
C2025	C1905	C1905	C1965	C1905	G1836	G1776	G1695	G1635	C1575	U1516	U1454	A1395	U1335	A1275
G2026	G1906	G1906	A1966	G1906	C1837	U1777	G1696	C1636	U1576	G1517	G1455	U1396	A1336	A1276
G2027	G1907	G1907	G1967	G1907	C1838	U1778	G1697	A1637	U1577	C1518	G1456	U1397	G1337	G1277
U2028	C1908	C1908	G1968	C1908	G1839	U1779	A1698	C1638	U1578	G1519	G1457	C1398	G1338	A1278
G2029	U1909	U1909	A1969	G1909	G1840	A1780	G1699	U1639	A1579	U1520	G1459	C1399	G1339	G1279
A2030	G1910	G1910	A1970	G1910	U1841	C1781	A1700	C1640	A1580	G1521	A1460	G1401	U1340	G1280
U2031	U1911	U1911	A1971	U1911	G1842	C1782	A1701	C1641	A1581	G1522	G1461	G1402	U1341	G1281
G2032	A1912	A1912	A1972	A1912	C1843	A1783	G1702	G1642	G1582	U1523	C1462	C1402	A1342	U1282
A2033	C1913	C1913	G1973	A1913	G1844	A1784	G1703	G1643	C1583	G1524	C1463	C1403	G1343	G1283
U2034	C1914	C1914	C1974	A1914	G1845	A1785	G1704	G1644	C1585	G1525	C1464	C1404	A1284	A1284
G2035	U1915	U1915	G1975	U1915	G1846	A1786	G1705	G1645	A1586	G1526	G1465	U1405	C1345	G1285

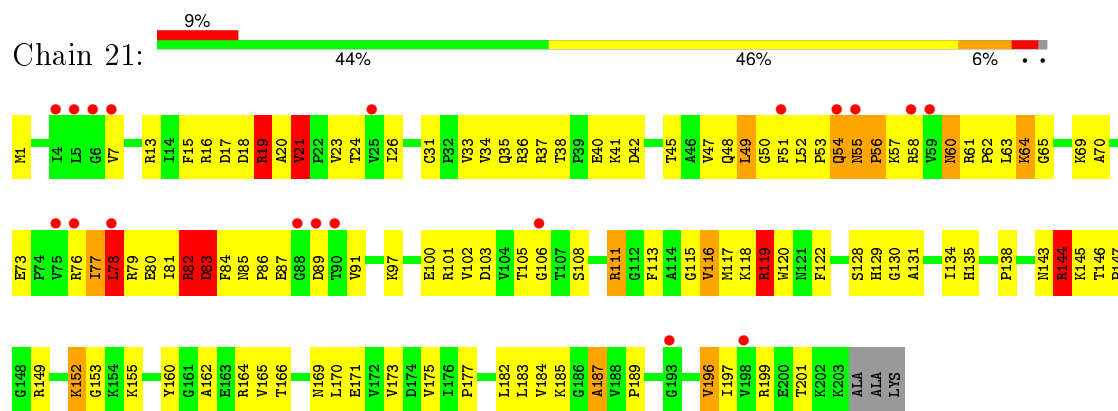




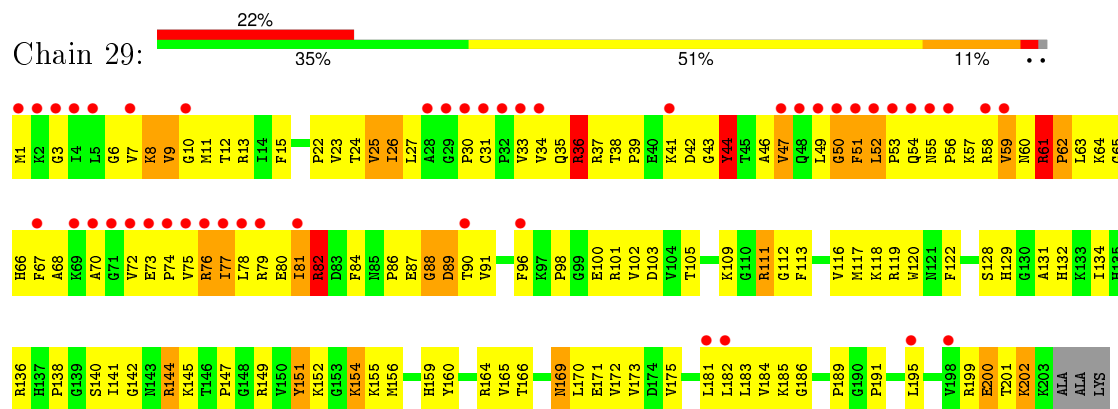




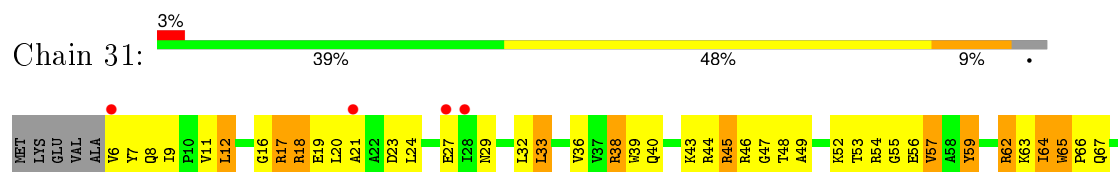
- Molecule 30: 50S ribosomal protein L3

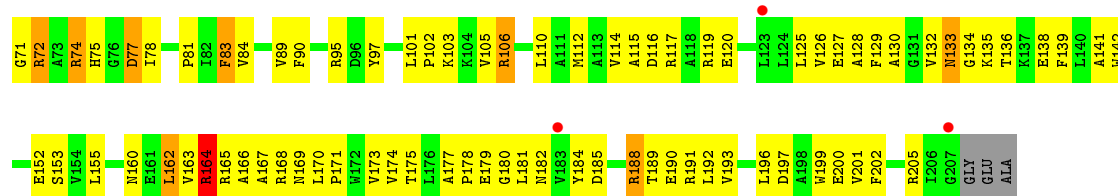


- Molecule 30: 50S ribosomal protein L3

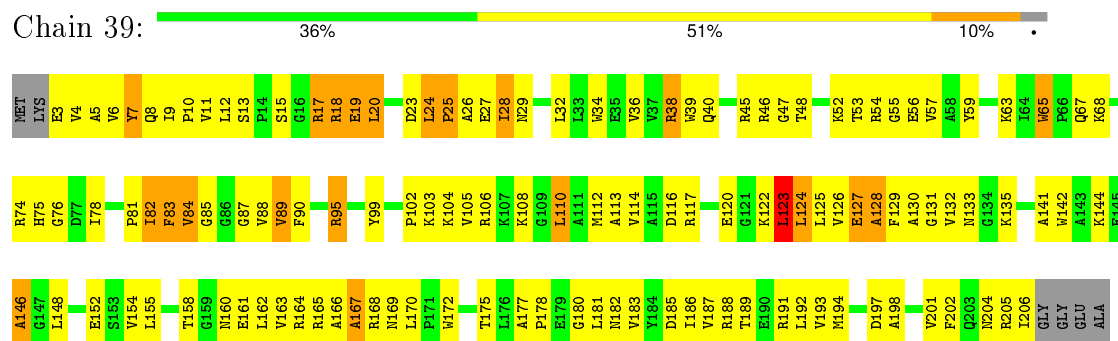


- Molecule 31: 50S ribosomal protein L4

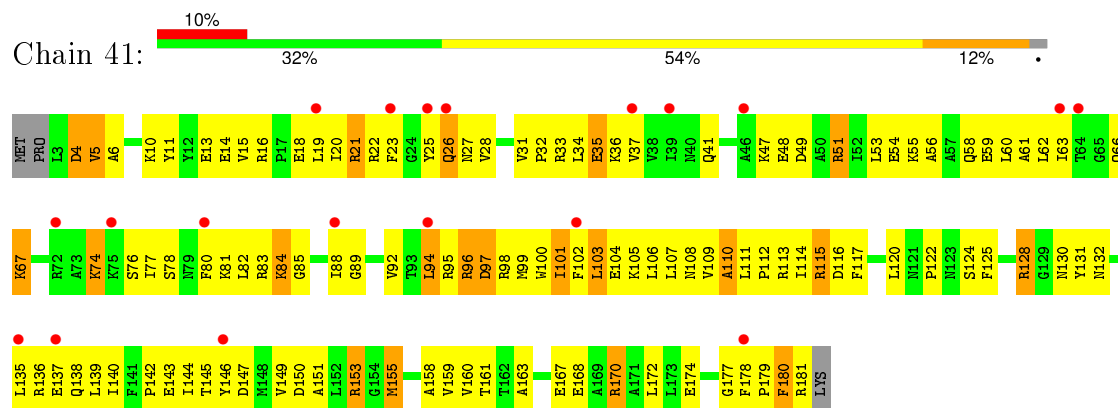




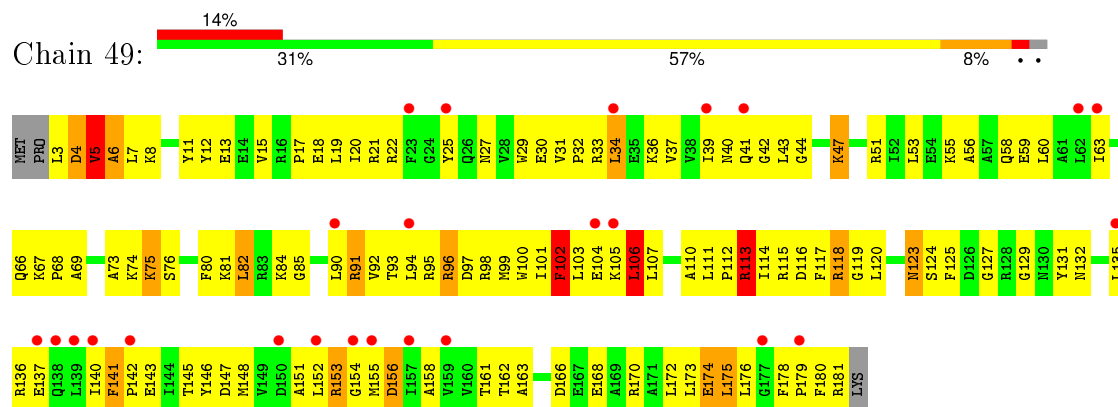
• Molecule 31: 50S ribosomal protein L4



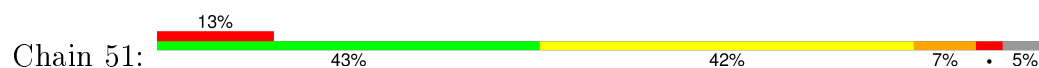
• Molecule 32: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L5

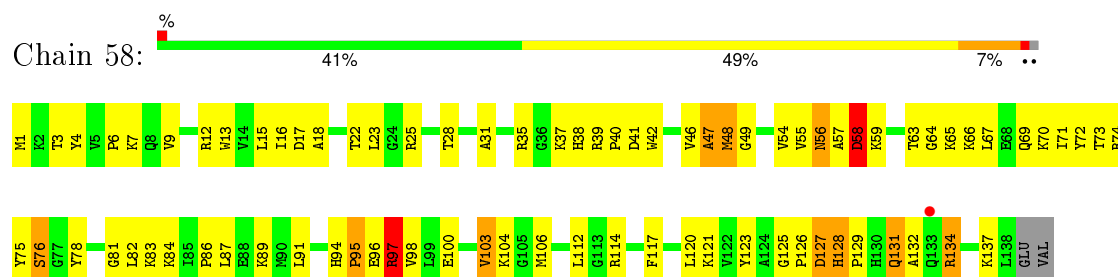


• Molecule 33: 50S ribosomal protein L6

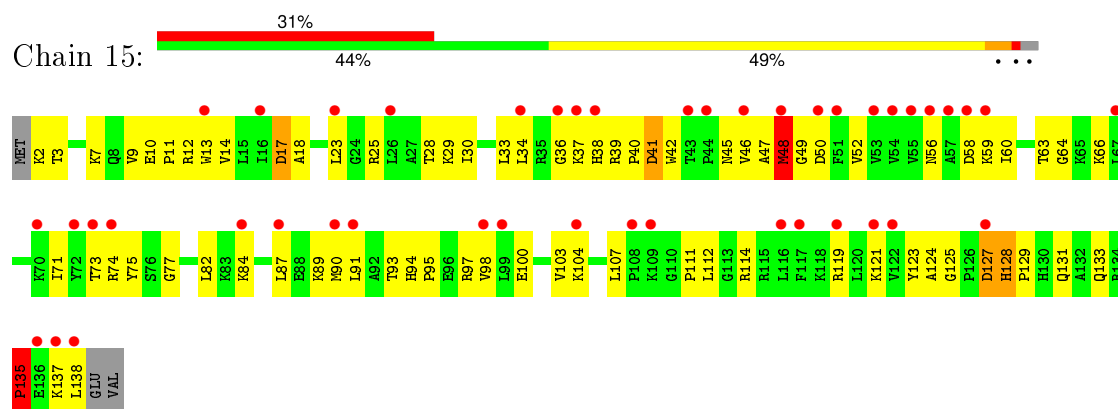




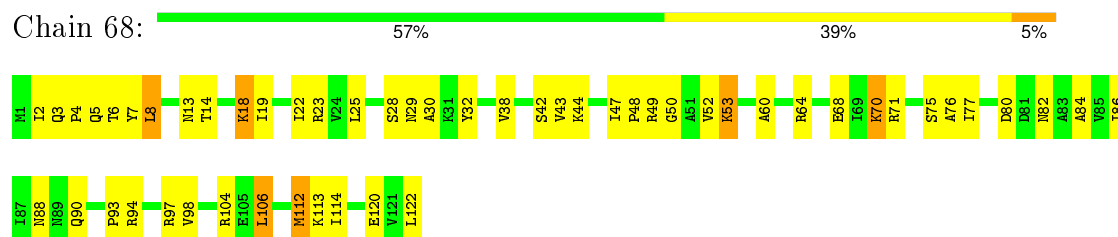
- Molecule 35: 50S ribosomal protein L13



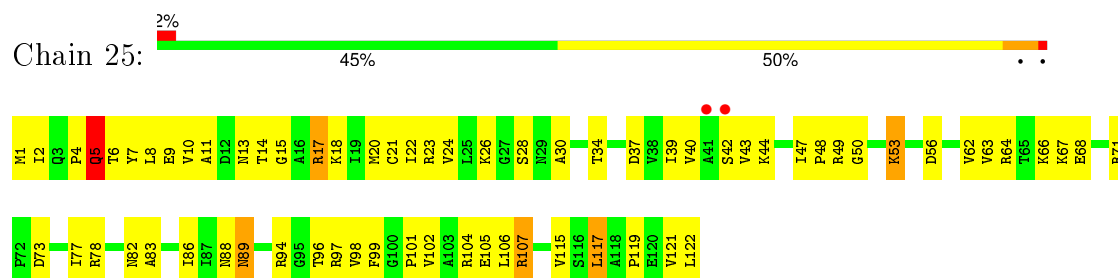
- Molecule 35: 50S ribosomal protein L13



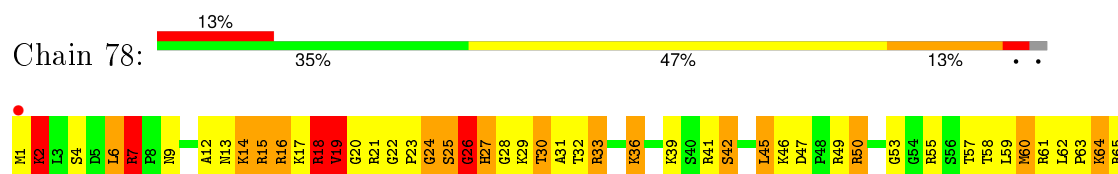
- Molecule 36: 50S ribosomal protein L14

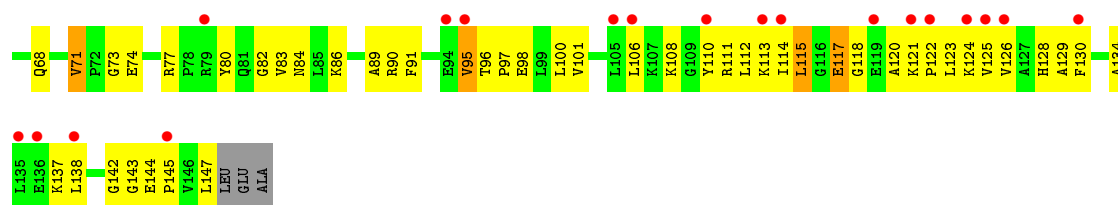


- Molecule 36: 50S ribosomal protein L14



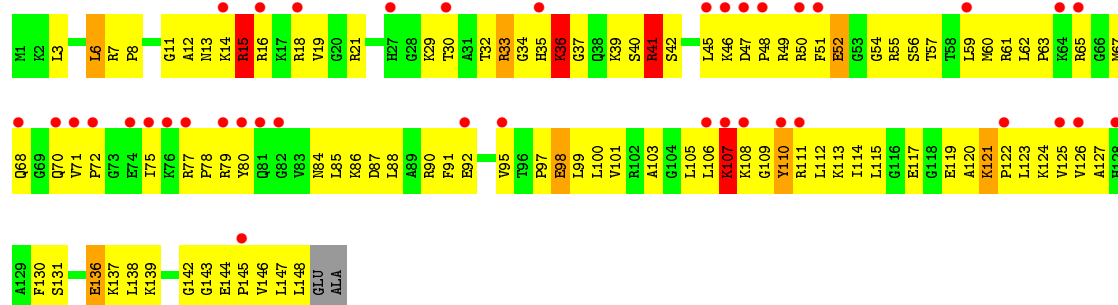
- Molecule 37: 50S ribosomal protein L15





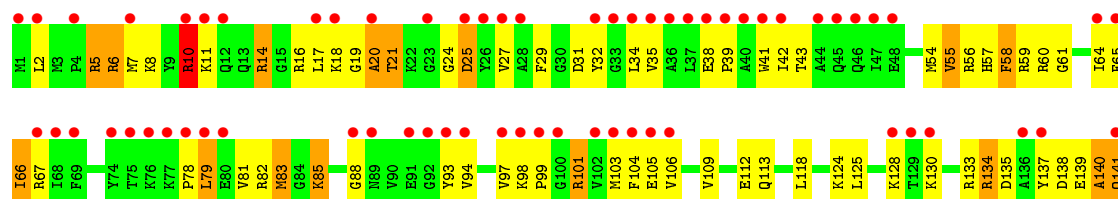
• Molecule 37: 50S ribosomal protein L15

Chain 35: 26% 31% 61% 5%



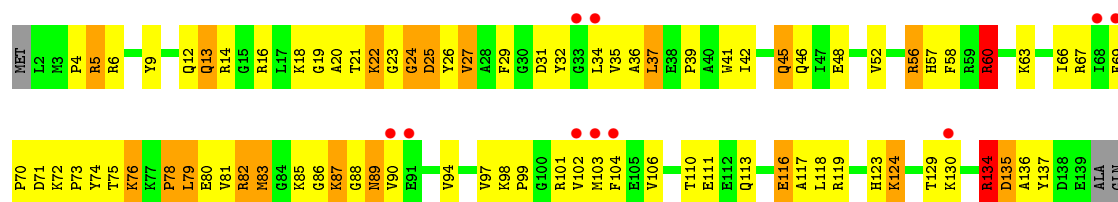
• Molecule 38: 50S ribosomal protein L16

Chain 88: 45% 49% 39% 11%



• Molecule 38: 50S ribosomal protein L16

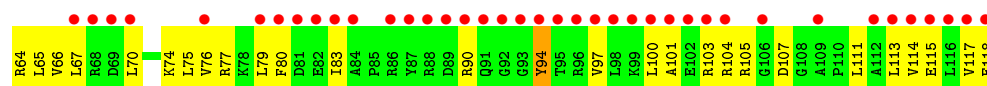
Chain 45: 7% 39% 44% 13%



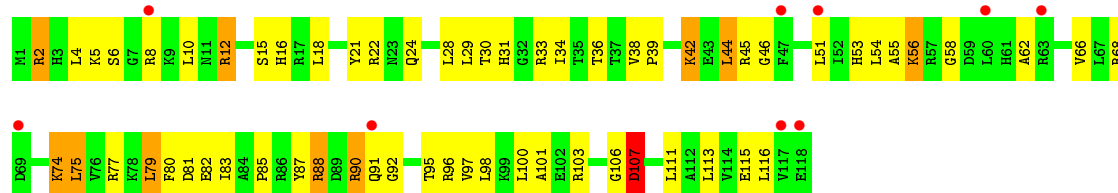
• Molecule 39: 50S ribosomal protein L17

Chain 98: 62% 42% 55%

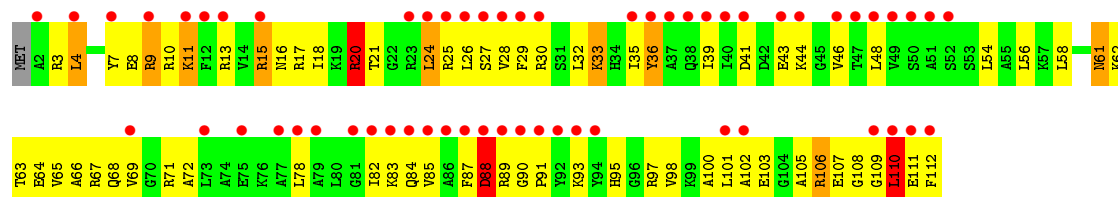




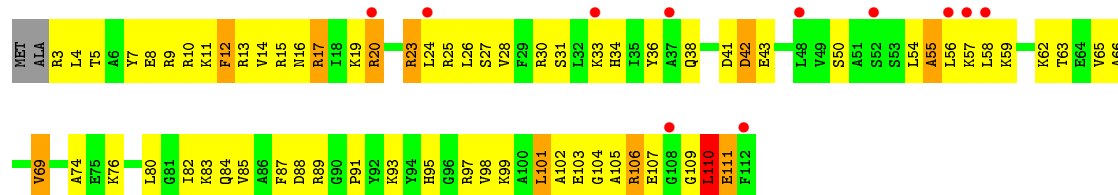
- Molecule 39: 50S ribosomal protein L17



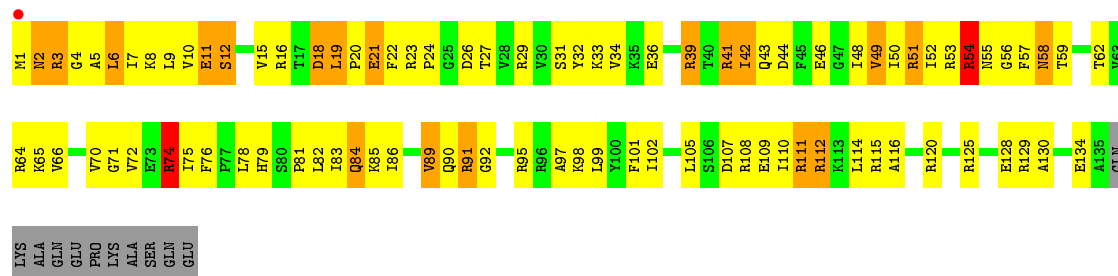
- Molecule 40: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L18

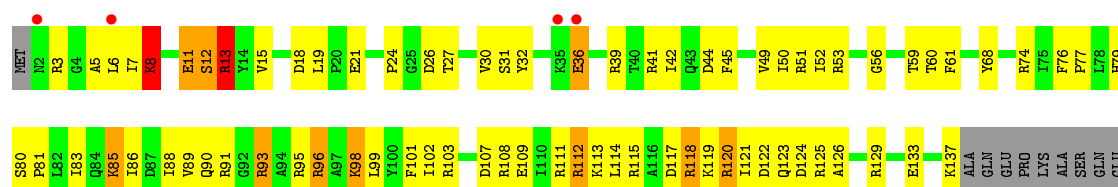


- Molecule 41: 50S ribosomal protein L19

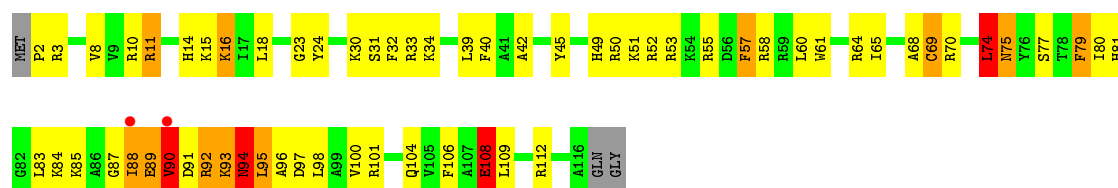


- Molecule 41: 50S ribosomal protein L19

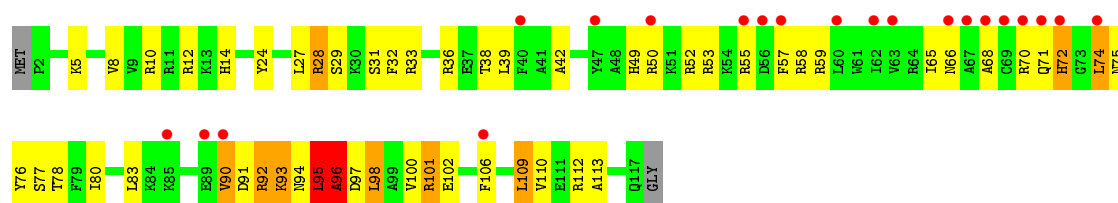




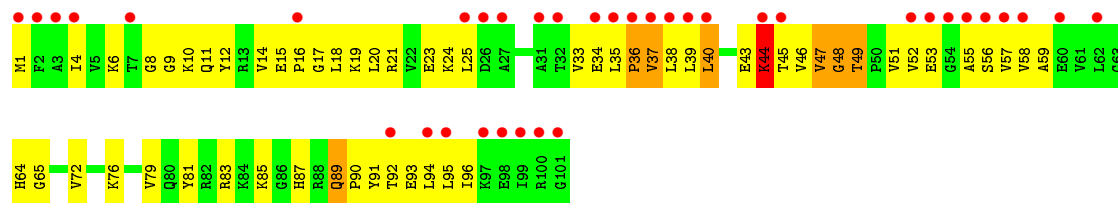
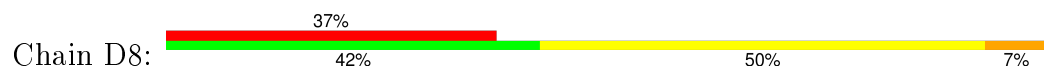
• Molecule 42: 50S ribosomal protein L20



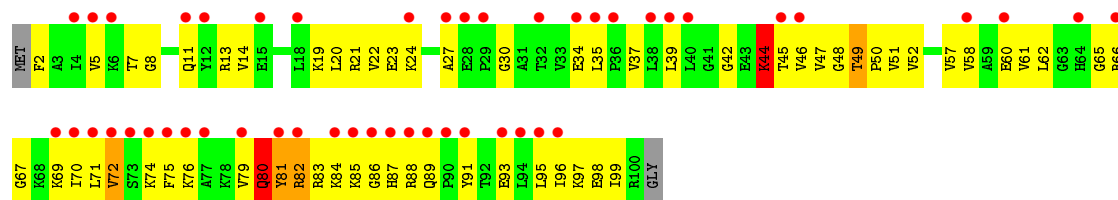
• Molecule 42: 50S ribosomal protein L20



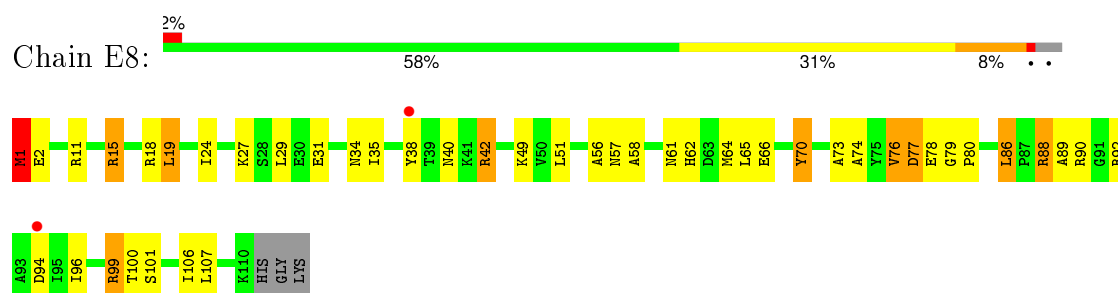
• Molecule 43: 50S ribosomal protein L21



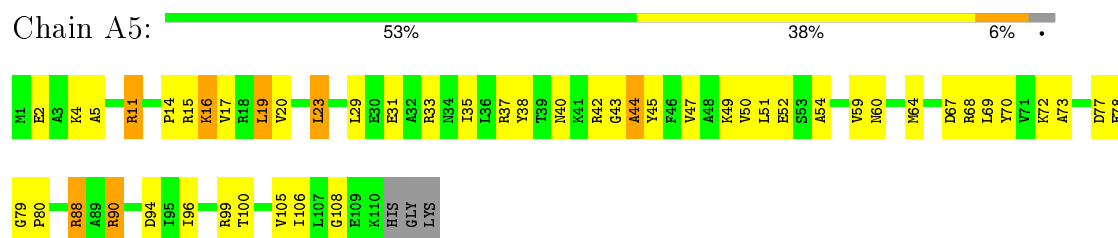
• Molecule 43: 50S ribosomal protein L21



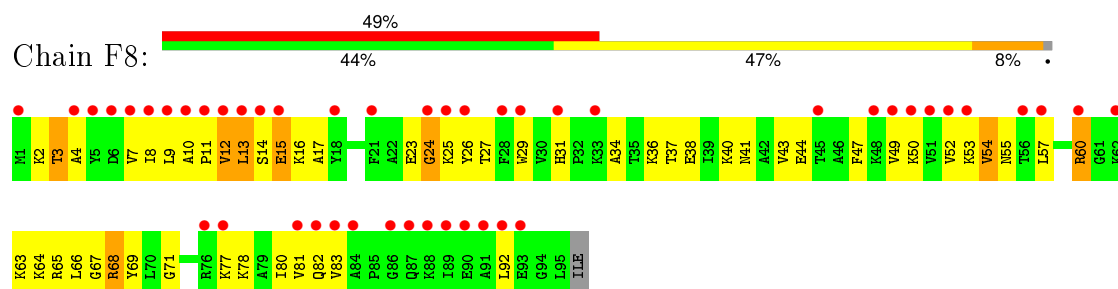
• Molecule 44: 50S ribosomal protein L22



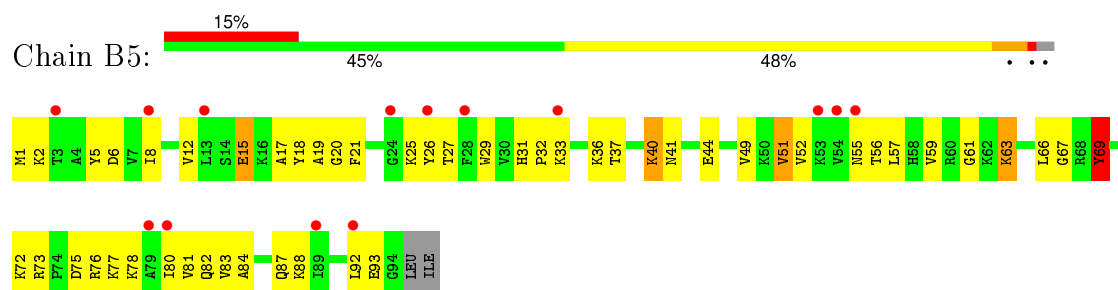
- Molecule 44: 50S ribosomal protein L22



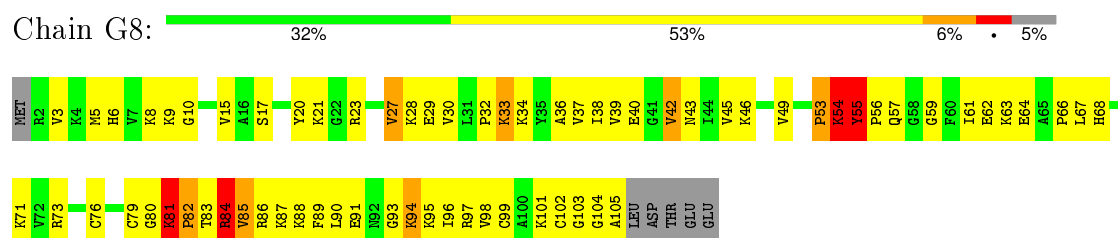
- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23

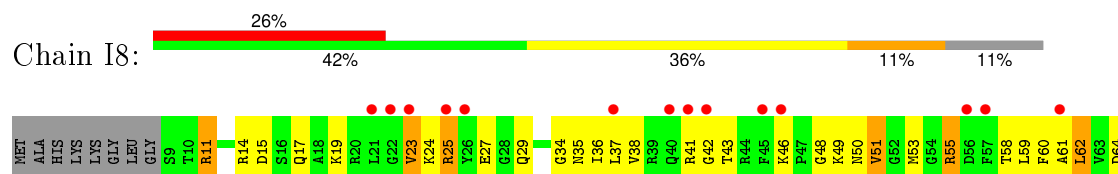
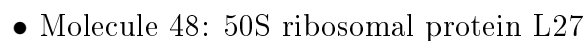
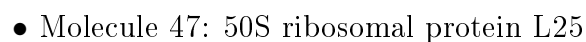


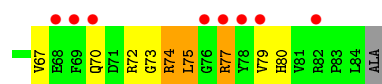
- Molecule 46: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L24



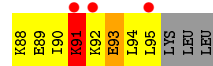




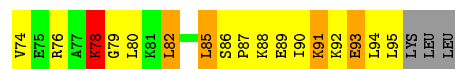
- Molecule 48: 50S ribosomal protein L27



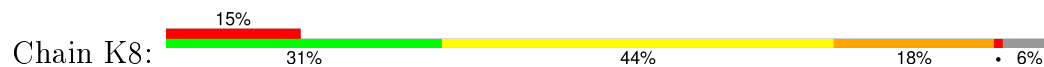
- Molecule 49: 50S ribosomal protein L28



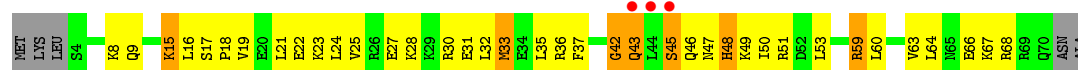
- Molecule 49: 50S ribosomal protein L28



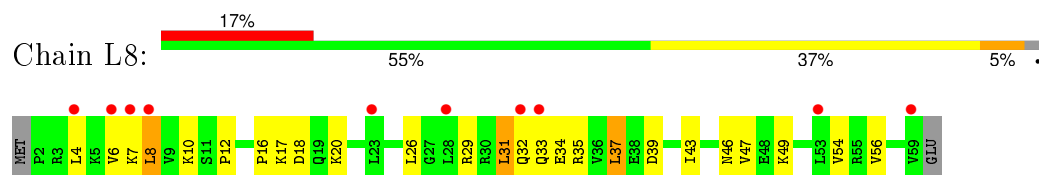
- Molecule 50: 50S ribosomal protein L29



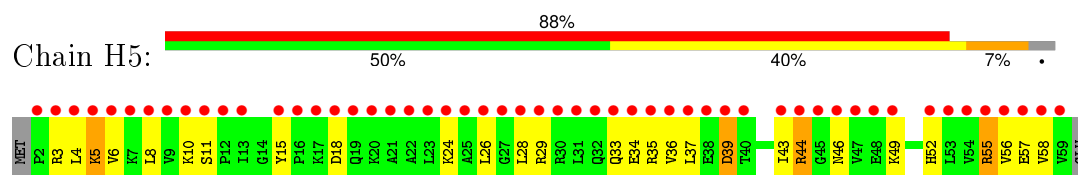
- Molecule 50: 50S ribosomal protein L29



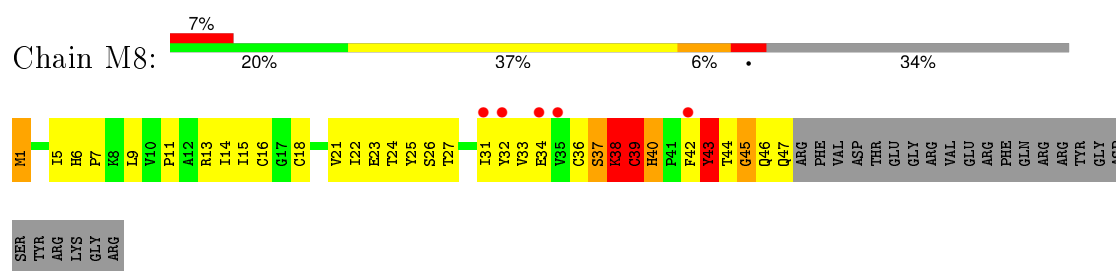
## • Molecule 51: 50S ribosomal protein L30



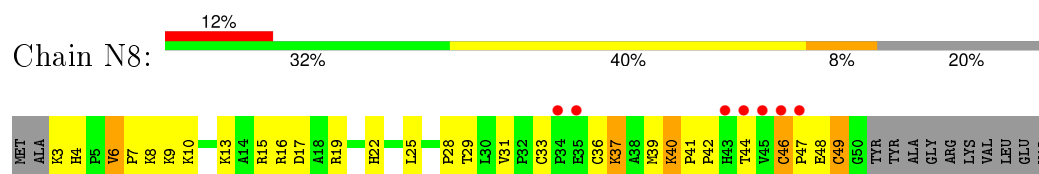
## • Molecule 51: 50S ribosomal protein L30



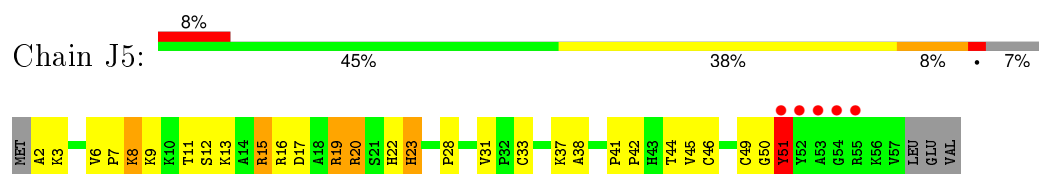
## • Molecule 52: 50S ribosomal protein L31



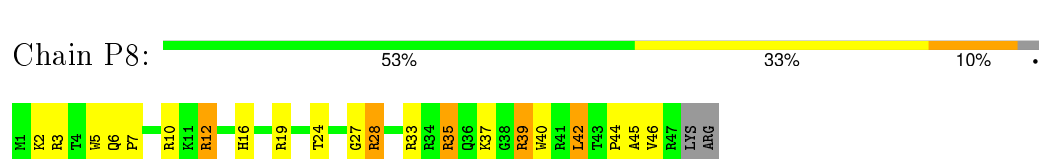
## • Molecule 53: 50S ribosomal protein L32



## • Molecule 53: 50S ribosomal protein L32

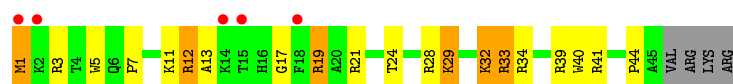


## • Molecule 54: 50S ribosomal protein L34



## • Molecule 54: 50S ribosomal protein L34

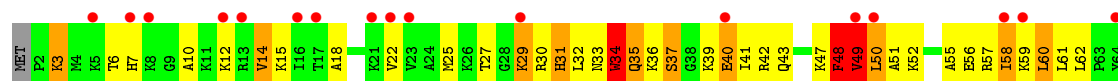




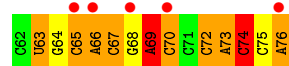
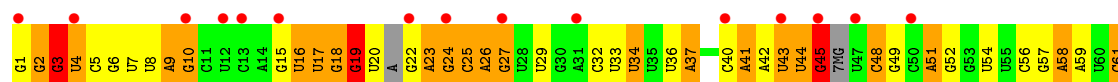
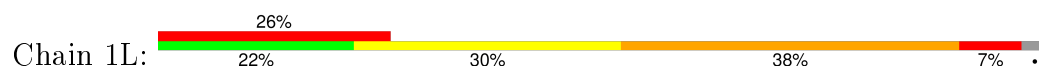
- Molecule 55: 50S ribosomal protein L35



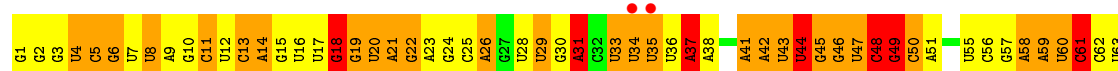
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA<sup>Lys</sup>



- Molecule 57: tRNA<sup>Lys</sup>



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.40 Å   447.10 Å   616.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	152.44 – 3.15 152.44 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (152.44-3.15) 92.0 (152.44-3.15)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.13 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.198   ,   0.254 0.200   ,   0.259	Depositor DCC
$R_{free}$ test set	2000 reflections (0.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 87.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 982379 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	292607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	13	1.35	176/35927 (0.5%)	2.42	3309/56065 (5.9%)
1	1G	1.15	83/35987 (0.2%)	2.10	2179/56159 (3.9%)
2	12	0.54	2/1726 (0.1%)	0.74	0/2324
2	1E	0.60	0/1908	0.80	2/2573 (0.1%)
3	22	0.50	1/1552 (0.1%)	0.72	2/2093 (0.1%)
3	2E	0.80	0/1629	0.87	2/2195 (0.1%)
4	32	0.72	1/1732 (0.1%)	0.89	3/2318 (0.1%)
4	3E	0.86	2/1726 (0.1%)	0.90	3/2310 (0.1%)
5	42	0.75	3/1151 (0.3%)	0.76	1/1549 (0.1%)
5	4E	0.85	1/1158 (0.1%)	0.91	1/1559 (0.1%)
6	52	0.75	0/855	0.85	2/1154 (0.2%)
6	5E	0.77	1/850 (0.1%)	0.97	4/1147 (0.3%)
7	62	0.66	1/1122 (0.1%)	0.78	1/1500 (0.1%)
7	6E	0.64	0/1245	0.72	0/1666
8	72	0.57	1/1127 (0.1%)	0.74	1/1517 (0.1%)
8	7E	0.94	4/1135 (0.4%)	0.93	3/1527 (0.2%)
9	82	0.64	1/835 (0.1%)	0.84	1/1120 (0.1%)
9	8E	0.61	0/1019	0.77	0/1367
10	1A	0.56	0/482	0.73	0/647
10	1I	0.73	0/602	0.84	1/806 (0.1%)
11	2A	0.70	1/850 (0.1%)	0.80	1/1150 (0.1%)
11	2I	0.71	0/838	0.88	0/1133
12	3A	0.69	0/963	0.95	3/1290 (0.2%)
12	3I	0.99	2/972 (0.2%)	1.12	2/1301 (0.2%)
13	4A	0.61	0/903	0.87	2/1211 (0.2%)
13	4I	0.79	2/952 (0.2%)	0.89	2/1277 (0.2%)
14	5A	0.63	1/393 (0.3%)	0.91	1/521 (0.2%)
14	5I	0.83	1/500 (0.2%)	0.98	1/664 (0.2%)
15	6A	0.75	2/740 (0.3%)	0.81	0/987
15	6I	0.81	1/740 (0.1%)	0.87	0/987
16	7A	0.77	0/721	0.90	0/970
16	7I	0.74	1/687 (0.1%)	0.86	0/925

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.65	0/836	0.75	0/1117
17	8I	0.85	3/847 (0.4%)	0.89	0/1131
18	9A	0.80	0/549	0.81	1/732 (0.1%)
18	9I	0.68	0/549	0.88	0/732
19	AA	0.54	0/288	0.90	1/388 (0.3%)
19	AI	0.80	0/668	0.93	0/899
20	BA	0.64	0/759	0.86	1/1000 (0.1%)
20	BI	0.57	0/748	0.80	0/986
21	1B	0.57	0/208	0.76	0/272
21	1F	0.56	0/203	0.79	0/266
22	1K	1.14	11/1516 (0.7%)	1.96	70/2350 (3.0%)
23	2K	1.63	25/1721 (1.5%)	2.75	223/2682 (8.3%)
23	2L	1.15	2/1721 (0.1%)	2.03	86/2682 (3.2%)
24	3K	1.13	5/1799 (0.3%)	1.94	76/2801 (2.7%)
25	4K	1.74	7/494 (1.4%)	2.28	40/767 (5.2%)
25	4L	1.44	3/420 (0.7%)	2.11	26/654 (4.0%)
26	14	1.58	825/69023 (1.2%)	2.76	8688/107740 (8.1%)
26	1H	1.84	1510/68273 (2.2%)	3.14	11225/106575 (10.5%)
27	16	1.49	22/2928 (0.8%)	2.87	390/4568 (8.5%)
27	1J	1.26	10/2928 (0.3%)	2.37	253/4568 (5.5%)
28	71	0.68	0/1073	0.78	0/1447
29	11	1.14	8/2170 (0.4%)	1.34	30/2926 (1.0%)
29	19	1.05	3/2170 (0.1%)	1.24	22/2926 (0.8%)
30	21	1.06	9/1591 (0.6%)	1.16	8/2146 (0.4%)
30	29	0.99	5/1591 (0.3%)	1.13	5/2146 (0.2%)
31	31	1.11	8/1620 (0.5%)	1.23	15/2194 (0.7%)
31	39	0.88	2/1637 (0.1%)	1.08	6/2218 (0.3%)
32	41	0.85	4/1481 (0.3%)	1.01	3/1994 (0.2%)
32	49	0.63	0/1481	0.91	4/1994 (0.2%)
33	51	0.96	2/1337 (0.1%)	1.17	6/1809 (0.3%)
33	59	0.67	1/548 (0.2%)	0.82	0/738
34	61	0.70	0/1146	0.89	0/1551
34	69	0.70	2/1146 (0.2%)	0.89	3/1551 (0.2%)
35	15	0.78	0/1123	0.93	2/1515 (0.1%)
35	58	0.90	1/1131 (0.1%)	1.00	3/1525 (0.2%)
36	25	0.90	0/942	1.00	1/1269 (0.1%)
36	68	0.97	0/942	1.11	4/1269 (0.3%)
37	35	1.11	1/1147 (0.1%)	1.16	6/1525 (0.4%)
37	78	1.08	3/1139 (0.3%)	1.33	14/1514 (0.9%)
38	45	0.98	4/1120 (0.4%)	1.06	2/1498 (0.1%)
38	88	1.13	6/1134 (0.5%)	1.22	7/1519 (0.5%)
39	55	0.89	1/981 (0.1%)	1.20	10/1312 (0.8%)
39	98	0.81	0/981	1.13	4/1312 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	65	0.76	1/886 (0.1%)	1.04	4/1180 (0.3%)
40	A8	0.95	1/891 (0.1%)	1.26	6/1187 (0.5%)
41	75	0.98	4/1147 (0.3%)	1.10	3/1532 (0.2%)
41	B8	1.10	7/1137 (0.6%)	1.11	5/1519 (0.3%)
42	85	0.83	0/977	1.01	4/1301 (0.3%)
42	C8	1.02	4/968 (0.4%)	1.08	2/1289 (0.2%)
43	95	1.01	4/777 (0.5%)	1.02	0/1042
43	D8	0.93	1/789 (0.1%)	1.08	1/1057 (0.1%)
44	A5	1.05	1/886 (0.1%)	1.15	6/1189 (0.5%)
44	E8	1.03	1/886 (0.1%)	1.21	8/1189 (0.7%)
45	B5	1.08	2/749 (0.3%)	1.09	2/1007 (0.2%)
45	F8	1.17	5/754 (0.7%)	1.27	6/1014 (0.6%)
46	C5	1.09	5/812 (0.6%)	1.08	4/1083 (0.4%)
46	G8	1.33	8/801 (1.0%)	1.34	6/1069 (0.6%)
47	D5	0.84	4/1088 (0.4%)	0.85	2/1473 (0.1%)
47	H8	0.78	1/1244 (0.1%)	0.96	3/1683 (0.2%)
48	E5	0.87	0/624	1.08	1/832 (0.1%)
48	I8	1.12	1/614 (0.2%)	1.28	8/819 (1.0%)
49	F5	0.94	2/744 (0.3%)	1.09	3/989 (0.3%)
49	J8	1.09	4/744 (0.5%)	1.18	5/989 (0.5%)
50	G5	0.80	0/565	0.99	1/748 (0.1%)
50	K8	1.09	0/570	1.43	11/755 (1.5%)
51	H5	0.80	0/464	0.90	0/623
51	L8	0.92	1/464 (0.2%)	1.13	1/623 (0.2%)
52	M8	0.77	0/375	1.08	3/507 (0.6%)
53	J5	0.92	2/448 (0.4%)	1.08	4/606 (0.7%)
53	N8	1.02	1/381 (0.3%)	1.08	0/516
54	L5	0.99	0/399	1.23	3/526 (0.6%)
54	P8	1.17	0/409	1.62	9/540 (1.7%)
55	M5	1.10	5/524 (1.0%)	1.18	4/691 (0.6%)
55	Q8	1.13	1/524 (0.2%)	1.41	9/691 (1.3%)
56	1L	0.76	1/1683 (0.1%)	1.38	20/2615 (0.8%)
57	3L	0.96	7/1777 (0.4%)	1.72	50/2767 (1.8%)
All	All	1.39	2845/315237 (0.9%)	2.39	26956/472471 (5.7%)

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	3
3	22	0	2
3	2E	0	2
4	32	0	4
4	3E	0	1
5	4E	0	1
7	6E	0	1
9	82	0	1
9	8E	0	1
11	2A	0	1
11	2I	0	1
12	3A	0	1
12	3I	0	5
13	4A	0	2
13	4I	0	3
14	5A	0	1
14	5I	0	1
15	6A	0	1
16	7I	0	1
17	8I	0	1
19	AA	0	1
19	AI	0	2
20	BA	0	4
20	BI	0	1
26	14	0	1
28	71	0	1
29	11	0	6
29	19	0	6
30	21	0	11
30	29	0	6
31	31	0	3
31	39	0	11
32	41	0	3
32	49	0	6
33	51	0	3
33	59	0	3
34	61	0	4
34	69	0	6
35	15	0	4
35	58	0	3
37	35	0	4
37	78	0	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
38	45	0	7
38	88	0	3
40	A8	0	2
41	75	0	2
41	B8	0	4
42	85	0	5
42	C8	0	3
43	95	0	3
43	D8	0	4
44	A5	0	1
45	B5	0	2
45	F8	0	2
46	C5	0	1
46	G8	0	6
47	D5	0	1
47	H8	0	2
48	E5	0	1
49	F5	0	3
49	J8	0	2
50	G5	0	4
50	K8	0	4
52	M8	0	5
54	P8	0	1
55	M5	0	3
55	Q8	0	2
All	All	0	209

The worst 5 of 2845 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	35	121	LYS	C-N	22.50	1.76	1.34
26	1H	783	A	N3-C4	-21.39	1.22	1.34
26	1H	676	A	N9-C4	-19.81	1.25	1.37
26	14	783	A	N9-C4	-18.75	1.26	1.37
26	1H	2346	A	N3-C4	-16.77	1.24	1.34

The worst 5 of 26956 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	783	A	C2-N3-C4	-38.22	91.49	110.60
26	1H	783	A	C2-N3-C4	-32.53	94.33	110.60
26	1H	1899	G	C2-N3-C4	-29.93	96.93	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	676	A	C2-N3-C4	-28.68	96.26	110.60
26	14	929	G	N1-C6-O6	25.84	135.40	119.90

There are no chirality outliers.

5 of 209 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
2	1E	9	GLU	Peptide
3	2E	128	PHE	Peptide
3	2E	166	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	32097	0	16197	1109	0
1	1G	32152	0	16231	1228	2
2	12	1695	0	1729	133	0
2	1E	1874	0	1926	143	0
3	22	1529	0	1592	134	0
3	2E	1605	0	1668	83	0
4	32	1702	0	1764	160	0
4	3E	1696	0	1752	134	0
5	42	1136	0	1200	105	0
5	4E	1142	0	1204	90	0
6	52	842	0	857	50	0
6	5E	837	0	852	48	0
7	62	1110	0	1163	82	0
7	6E	1229	0	1274	76	0
8	72	1107	0	1165	73	0
8	7E	1115	0	1177	78	0
9	82	820	0	848	83	0
9	8E	1000	0	1031	93	0
10	1A	474	0	484	43	0
10	1I	593	0	610	46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	2A	835	0	847	31	0
11	2I	823	0	833	53	0
12	3A	947	0	1033	81	0
12	3I	956	0	1046	47	0
13	4A	893	0	946	85	0
13	4I	942	0	997	66	0
14	5A	388	0	424	47	0
14	5I	491	0	530	37	0
15	6A	729	0	768	35	0
15	6I	729	0	768	52	0
16	7A	705	0	725	55	0
16	7I	671	0	693	60	0
17	8A	823	0	891	37	0
17	8I	834	0	904	56	0
18	9A	544	0	605	35	0
18	9I	544	0	605	33	0
19	AA	283	0	284	22	0
19	AI	654	0	675	55	0
20	BA	757	0	856	56	0
20	BI	746	0	843	56	0
21	1B	204	0	218	18	0
21	1F	199	0	208	10	0
22	1K	1477	0	758	66	0
23	2K	1646	0	844	42	0
23	2L	1646	0	844	59	0
24	3K	1611	0	817	93	0
25	4K	439	0	219	17	0
25	4L	373	0	185	10	0
26	14	61630	0	31047	1916	1
26	1H	60960	0	30668	1946	0
27	16	2617	0	1328	91	0
27	1J	2617	0	1328	133	0
28	7I	1050	0	1071	88	0
29	11	2120	0	2197	169	0
29	19	2120	0	2197	169	0
30	21	1558	0	1624	120	0
30	29	1558	0	1622	186	0
31	31	1585	0	1632	121	0
31	39	1602	0	1649	122	0
32	41	1457	0	1514	130	0
32	49	1457	0	1514	161	0
33	51	1312	0	1384	87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	59	539	0	563	41	0
34	61	1131	0	1218	80	1
34	69	1131	0	1218	86	0
35	15	1096	0	1168	60	0
35	58	1104	0	1180	75	0
36	25	932	0	996	65	0
36	68	932	0	996	50	0
37	35	1130	0	1217	140	0
37	78	1122	0	1206	122	0
38	45	1099	0	1153	112	0
38	88	1113	0	1156	82	0
39	55	967	0	1033	57	0
39	98	967	0	1033	62	0
40	65	876	0	938	85	0
40	A8	881	0	943	86	0
41	75	1133	0	1190	80	0
41	B8	1123	0	1181	105	0
42	85	959	0	1019	68	0
42	C8	950	0	1011	82	0
43	95	766	0	837	77	0
43	D8	778	0	851	80	0
44	A5	876	0	941	41	0
44	E8	876	0	941	46	0
45	B5	735	0	785	54	0
45	F8	740	0	787	50	0
46	C5	799	0	888	79	0
46	G8	788	0	875	88	0
47	D5	1064	0	1082	88	0
47	H8	1218	0	1241	75	0
48	E5	616	0	633	49	0
48	I8	606	0	625	40	0
49	F5	737	0	813	60	0
49	J8	737	0	813	50	0
50	G5	563	0	612	35	0
50	K8	568	0	614	47	0
51	H5	459	0	512	19	0
51	L8	459	0	512	20	0
52	M8	366	0	370	49	0
53	J5	434	0	454	33	0
53	N8	369	0	388	44	0
54	L5	391	0	432	22	0
54	P8	401	0	436	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	M5	516	0	582	50	0
55	Q8	516	0	582	54	0
56	1L	1570	0	798	39	0
57	3L	1611	0	817	69	0
58	11	1	0	0	0	0
58	13	141	0	0	0	0
58	14	420	0	0	0	0
58	16	12	0	0	0	0
58	1G	78	0	0	0	0
58	1H	488	0	0	0	0
58	1J	6	0	0	0	0
58	21	2	0	0	0	0
58	29	3	0	0	0	0
58	2K	3	0	0	0	0
58	2L	3	0	0	0	0
58	32	1	0	0	0	0
58	35	1	0	0	0	0
58	3I	1	0	0	0	0
58	41	1	0	0	0	0
58	45	3	0	0	0	0
58	55	1	0	0	0	0
58	5E	2	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7A	1	0	0	0	0
58	85	2	0	0	0	0
58	88	1	0	0	0	0
58	C5	1	0	0	0	0
58	C8	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	2	0	0	0	0
58	L5	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	4	0
59	3E	8	0	0	0	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	9	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	13	148	0	0	21	0
61	14	411	0	0	57	0
61	16	18	0	0	4	0
61	19	4	0	0	2	0
61	1G	44	0	0	6	0
61	1H	670	0	0	78	0
61	1J	11	0	0	2	0
61	1K	1	0	0	0	0
61	21	5	0	0	2	0
61	29	3	0	0	0	0
61	31	6	0	0	0	0
61	35	2	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	1	0
61	3I	2	0	0	0	0
61	4K	6	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	3	0	0	2	0
61	5I	1	0	0	0	0
61	6I	1	0	0	0	0
61	78	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	D8	1	0	0	0	0
61	E5	1	0	0	0	0
61	E8	1	0	0	0	0
61	F5	2	0	0	0	0
61	G8	1	0	0	0	0
61	I8	1	0	0	0	0
61	L5	1	0	0	0	0
61	M5	2	0	0	0	0
61	Q8	1	0	0	0	0
All	All	292607	0	194505	12060	2

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 26.

The worst 5 of 12060 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:G8:84:ARG:CB	46:G8:84:ARG:CG	1.75	1.63
46:G8:84:ARG:CG	46:G8:84:ARG:CD	1.76	1.61
29:19:246:PRO:N	29:19:255:LYS:HZ1	1.10	1.44
3:22:29:TYR:CE1	3:22:33:LEU:HD22	1.61	1.35
37:35:121:LYS:C	37:35:122:PRO:N	1.77	1.35

All (2) 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]	1.99	0.21
34:61:89:TYR:O	1:1G:357:G:O2'[4_555]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	202/256 (79%)	170 (84%)	26 (13%)	6 (3%)	5	34
2	1E	227/256 (89%)	194 (86%)	28 (12%)	5 (2%)	8	43
3	22	190/239 (80%)	167 (88%)	22 (12%)	1 (0%)	34	76
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	181 (88%)	22 (11%)	3 (2%)	13	53
4	3E	205/209 (98%)	189 (92%)	14 (7%)	2 (1%)	19	63
5	42	147/162 (91%)	136 (92%)	11 (8%)	0	100	100
5	4E	147/162 (91%)	137 (93%)	9 (6%)	1 (1%)	26	71
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	121 (90%)	13 (10%)	0	100	100
7	6E	147/156 (94%)	141 (96%)	6 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	26	71
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	71
9	82	101/128 (79%)	88 (87%)	11 (11%)	2 (2%)	9	46
9	8E	124/128 (97%)	103 (83%)	20 (16%)	1 (1%)	24	67
10	1A	54/105 (51%)	46 (85%)	8 (15%)	0	100	100
10	1I	66/105 (63%)	58 (88%)	6 (9%)	2 (3%)	5	34
11	2A	111/129 (86%)	97 (87%)	12 (11%)	2 (2%)	11	49
11	2I	109/129 (84%)	94 (86%)	13 (12%)	2 (2%)	11	49
12	3A	119/132 (90%)	97 (82%)	17 (14%)	5 (4%)	3	24
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	24	67
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	21	65
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	44/61 (72%)	37 (84%)	7 (16%)	0	100	100
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	5	29
15	6A	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
15	6I	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	78/88 (89%)	73 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	13	53
19	AA	32/93 (34%)	25 (78%)	6 (19%)	1 (3%)	5	32
19	AI	79/93 (85%)	66 (84%)	11 (14%)	2 (2%)	7	39
20	BA	96/106 (91%)	81 (84%)	12 (12%)	3 (3%)	5	32
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	21/27 (78%)	21 (100%)	0	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	7I	131/229 (57%)	121 (92%)	9 (7%)	1 (1%)	24	67
29	11	271/276 (98%)	233 (86%)	26 (10%)	12 (4%)	3	22
29	19	271/276 (98%)	245 (90%)	19 (7%)	7 (3%)	7	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	21	201/206 (98%)	158 (79%)	34 (17%)	9 (4%)	3	22
30	29	201/206 (98%)	153 (76%)	37 (18%)	11 (6%)	2	17
31	31	200/210 (95%)	176 (88%)	22 (11%)	2 (1%)	19	63
31	39	202/210 (96%)	158 (78%)	36 (18%)	8 (4%)	4	25
32	41	177/182 (97%)	154 (87%)	18 (10%)	5 (3%)	6	36
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	17	61
33	51	169/180 (94%)	135 (80%)	20 (12%)	14 (8%)	1	6
33	59	63/180 (35%)	44 (70%)	13 (21%)	6 (10%)	1	4
34	61	143/148 (97%)	118 (82%)	24 (17%)	1 (1%)	26	71
34	69	143/148 (97%)	111 (78%)	27 (19%)	5 (4%)	4	29
35	15	135/140 (96%)	119 (88%)	13 (10%)	3 (2%)	8	43
35	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	6	35
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	24	67
36	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
37	35	146/150 (97%)	111 (76%)	31 (21%)	4 (3%)	6	37
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	2	17
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	6	35
38	88	139/141 (99%)	115 (83%)	17 (12%)	7 (5%)	3	19
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	65
39	98	116/118 (98%)	93 (80%)	22 (19%)	1 (1%)	21	65
40	65	108/112 (96%)	87 (81%)	18 (17%)	3 (3%)	6	36
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	65
41	75	134/146 (92%)	121 (90%)	13 (10%)	0	100	100
41	B8	133/146 (91%)	117 (88%)	14 (10%)	2 (2%)	13	53
42	85	114/118 (97%)	99 (87%)	13 (11%)	2 (2%)	11	49
42	C8	113/118 (96%)	104 (92%)	5 (4%)	4 (4%)	4	29
43	95	97/101 (96%)	77 (79%)	16 (16%)	4 (4%)	3	25
43	D8	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	5	34
44	A5	108/113 (96%)	100 (93%)	7 (6%)	1 (1%)	21	65
44	E8	108/113 (96%)	97 (90%)	11 (10%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	5 (5%)	2 (2%)	8	43

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	F8	93/96 (97%)	82 (88%)	10 (11%)	1 (1%)	17	61
46	C5	103/110 (94%)	70 (68%)	26 (25%)	7 (7%)	1	10
46	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	2	15
47	D5	124/206 (60%)	96 (77%)	25 (20%)	3 (2%)	7	41
47	H8	142/206 (69%)	112 (79%)	22 (16%)	8 (6%)	2	17
48	E5	76/85 (89%)	66 (87%)	8 (10%)	2 (3%)	7	38
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	8	43
49	J8	92/98 (94%)	84 (91%)	6 (6%)	2 (2%)	8	43
50	G5	65/72 (90%)	61 (94%)	3 (5%)	1 (2%)	13	53
50	K8	66/72 (92%)	55 (83%)	7 (11%)	4 (6%)	2	14
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
52	M8	45/71 (63%)	28 (62%)	15 (33%)	2 (4%)	3	22
53	J5	54/60 (90%)	46 (85%)	8 (15%)	0	100	100
53	N8	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
54	L5	43/49 (88%)	39 (91%)	4 (9%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	8	43
55	M5	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	3	20
55	Q8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	12
All	All	10778/12104 (89%)	9303 (86%)	1246 (12%)	229 (2%)	9	44

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	91	ARG
18	9I	22	VAL
19	AI	67	VAL
29	11	28	GLU
29	11	40	THR

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	180/220 (82%)	164 (91%)	16 (9%)	12	42
2	1E	200/220 (91%)	181 (90%)	19 (10%)	11	38
3	22	153/188 (81%)	143 (94%)	10 (6%)	21	60
3	2E	159/188 (85%)	148 (93%)	11 (7%)	19	57
4	32	180/181 (99%)	165 (92%)	15 (8%)	14	48
4	3E	179/181 (99%)	167 (93%)	12 (7%)	20	58
5	42	114/123 (93%)	106 (93%)	8 (7%)	19	57
5	4E	115/123 (94%)	106 (92%)	9 (8%)	16	51
6	52	90/90 (100%)	81 (90%)	9 (10%)	9	36
6	5E	90/90 (100%)	87 (97%)	3 (3%)	45	80
7	62	114/127 (90%)	101 (89%)	13 (11%)	7	30
7	6E	125/127 (98%)	118 (94%)	7 (6%)	26	66
8	72	118/119 (99%)	112 (95%)	6 (5%)	29	69
8	7E	119/119 (100%)	111 (93%)	8 (7%)	20	58
9	82	79/99 (80%)	69 (87%)	10 (13%)	5	24
9	8E	97/99 (98%)	90 (93%)	7 (7%)	18	55
10	1A	52/92 (56%)	48 (92%)	4 (8%)	16	52
10	1I	65/92 (71%)	62 (95%)	3 (5%)	33	73
11	2A	85/99 (86%)	82 (96%)	3 (4%)	43	79
11	2I	84/99 (85%)	81 (96%)	3 (4%)	42	78
12	3A	102/109 (94%)	95 (93%)	7 (7%)	19	57
12	3I	103/109 (94%)	95 (92%)	8 (8%)	16	51
13	4A	91/101 (90%)	85 (93%)	6 (7%)	21	59
13	4I	94/101 (93%)	87 (93%)	7 (7%)	17	54
14	5A	40/50 (80%)	36 (90%)	4 (10%)	9	36
14	5I	49/50 (98%)	48 (98%)	1 (2%)	63	88
15	6A	79/80 (99%)	75 (95%)	4 (5%)	29	69
15	6I	79/80 (99%)	75 (95%)	4 (5%)	29	69
16	7A	72/74 (97%)	70 (97%)	2 (3%)	51	83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	7I	69/74 (93%)	63 (91%)	6 (9%)	13	44
17	8A	94/97 (97%)	90 (96%)	4 (4%)	35	74
17	8I	95/97 (98%)	91 (96%)	4 (4%)	36	74
18	9A	58/77 (75%)	56 (97%)	2 (3%)	44	80
18	9I	58/77 (75%)	57 (98%)	1 (2%)	68	90
19	AA	31/80 (39%)	28 (90%)	3 (10%)	10	37
19	AI	71/80 (89%)	66 (93%)	5 (7%)	19	57
20	BA	76/82 (93%)	74 (97%)	2 (3%)	54	85
20	BI	75/82 (92%)	72 (96%)	3 (4%)	38	76
21	1B	19/22 (86%)	18 (95%)	1 (5%)	28	67
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	7I	111/181 (61%)	106 (96%)	5 (4%)	34	73
29	11	214/218 (98%)	205 (96%)	9 (4%)	36	74
29	19	214/218 (98%)	204 (95%)	10 (5%)	32	72
30	21	165/166 (99%)	159 (96%)	6 (4%)	42	78
30	29	165/166 (99%)	155 (94%)	10 (6%)	23	62
31	31	161/166 (97%)	153 (95%)	8 (5%)	30	70
31	39	163/166 (98%)	153 (94%)	10 (6%)	23	62
32	41	153/156 (98%)	136 (89%)	17 (11%)	8	31
32	49	153/156 (98%)	134 (88%)	19 (12%)	6	26
33	51	142/148 (96%)	134 (94%)	8 (6%)	26	66
33	59	56/148 (38%)	53 (95%)	3 (5%)	27	67
34	61	122/124 (98%)	112 (92%)	10 (8%)	14	48
34	69	122/124 (98%)	114 (93%)	8 (7%)	21	59
35	15	116/119 (98%)	112 (97%)	4 (3%)	44	80
35	58	117/119 (98%)	109 (93%)	8 (7%)	20	57
36	25	100/100 (100%)	92 (92%)	8 (8%)	15	50
36	68	100/100 (100%)	96 (96%)	4 (4%)	38	76
37	35	115/116 (99%)	110 (96%)	5 (4%)	35	74
37	78	114/116 (98%)	107 (94%)	7 (6%)	23	62
38	45	109/111 (98%)	96 (88%)	13 (12%)	6	27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	88	109/111 (98%)	104 (95%)	5 (5%)	33	73
39	55	101/101 (100%)	94 (93%)	7 (7%)	19	57
39	98	101/101 (100%)	98 (97%)	3 (3%)	48	82
40	65	87/88 (99%)	81 (93%)	6 (7%)	19	57
40	A8	87/88 (99%)	78 (90%)	9 (10%)	9	34
41	75	119/127 (94%)	105 (88%)	14 (12%)	6	28
41	B8	118/127 (93%)	106 (90%)	12 (10%)	9	35
42	85	93/94 (99%)	85 (91%)	8 (9%)	13	45
42	C8	92/94 (98%)	82 (89%)	10 (11%)	8	31
43	95	81/82 (99%)	76 (94%)	5 (6%)	23	62
43	D8	82/82 (100%)	76 (93%)	6 (7%)	17	55
44	A5	90/92 (98%)	84 (93%)	6 (7%)	20	58
44	E8	90/92 (98%)	84 (93%)	6 (7%)	20	58
45	B5	74/78 (95%)	72 (97%)	2 (3%)	52	84
45	F8	74/78 (95%)	70 (95%)	4 (5%)	27	67
46	C5	85/91 (93%)	72 (85%)	13 (15%)	3	16
46	G8	84/91 (92%)	79 (94%)	5 (6%)	24	63
47	D5	118/179 (66%)	107 (91%)	11 (9%)	11	40
47	H8	137/179 (76%)	133 (97%)	4 (3%)	50	83
48	E5	62/67 (92%)	56 (90%)	6 (10%)	10	37
48	I8	61/67 (91%)	58 (95%)	3 (5%)	31	71
49	F5	79/83 (95%)	76 (96%)	3 (4%)	40	77
49	J8	79/83 (95%)	75 (95%)	4 (5%)	29	69
50	G5	62/67 (92%)	60 (97%)	2 (3%)	46	81
50	K8	62/67 (92%)	56 (90%)	6 (10%)	10	37
51	H5	50/52 (96%)	44 (88%)	6 (12%)	6	27
51	L8	50/52 (96%)	48 (96%)	2 (4%)	38	76
52	M8	42/63 (67%)	40 (95%)	2 (5%)	31	71
53	J5	48/52 (92%)	44 (92%)	4 (8%)	14	48
53	N8	43/52 (83%)	38 (88%)	5 (12%)	7	29
54	L5	38/42 (90%)	32 (84%)	6 (16%)	3	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	P8	38/42 (90%)	38 (100%)	0	100	100
55	M5	54/55 (98%)	49 (91%)	5 (9%)	11	40
55	Q8	54/55 (98%)	49 (91%)	5 (9%)	11	40
All	All	9127/10012 (91%)	8510 (93%)	617 (7%)	20	57

5 of 617 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	K8	66	GLU
6	52	14	LEU
46	C5	84	ARG
53	N8	46	CYS
3	22	88	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	16	HIS
19	AA	65	ASN
50	G5	47	ASN
2	12	78	GLN
2	12	135	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1488/1522 (97%)	386 (25%)	35 (2%)
1	1G	1492/1522 (98%)	427 (28%)	39 (2%)
22	1K	64/76 (84%)	41 (64%)	2 (3%)
23	2K	76/77 (98%)	23 (30%)	2 (2%)
23	2L	76/77 (98%)	21 (27%)	2 (2%)
24	3K	75/76 (98%)	40 (53%)	4 (5%)
25	4K	18/27 (66%)	9 (50%)	2 (11%)
25	4L	16/27 (59%)	9 (56%)	1 (6%)
26	14	2852/2912 (97%)	788 (27%)	58 (2%)
26	1H	2824/2912 (96%)	736 (26%)	78 (2%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	40 (56%)	5 (7%)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	3L	75/76 (98%)	40 (53%)	1 (1%)
All	All	9369/9624 (97%)	2628 (28%)	232 (2%)

5 of 2628 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2035	G
1	1G	210	U
26	14	2238	G
26	1H	2172	U
26	1H	2611	U

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

19 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	U8U	1K	34	25,22	15,24,25	2.58	3 (20%)	17,34,37	2.16	3 (17%)
22	T6A	1K	37	22	23,34,35	2.76	7 (30%)	26,49,52	5.18	8 (30%)
22	PSU	1K	39	22	15,21,22	1.56	4 (26%)	16,30,33	1.84	4 (25%)
22	5MU	1K	54	22	13,22,23	1.72	2 (15%)	16,32,35	1.88	2 (12%)
22	PSU	1K	55	22	15,21,22	1.01	1 (6%)	16,30,33	2.34	3 (18%)
56	PSU	1L	39	56	15,21,22	1.05	1 (6%)	16,30,33	2.03	3 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	5MU	1L	54	56	13,22,23	1.62	2 (15%)	16,32,35	1.31	1 (6%)
56	PSU	1L	55	56	15,21,22	1.10	1 (6%)	16,30,33	2.05	3 (18%)
23	OMC	2K	33	23	15,22,23	1.93	4 (26%)	20,31,34	1.79	3 (15%)
23	G7M	2K	47	23	18,26,27	3.43	6 (33%)	21,39,42	1.96	4 (19%)
23	5MU	2K	55	23	13,22,23	1.75	1 (7%)	16,32,35	1.44	2 (12%)
23	PSU	2K	56	23	15,21,22	1.22	1 (6%)	16,30,33	2.14	2 (12%)
23	4SU	2K	8	23	12,21,22	3.25	2 (16%)	15,30,33	1.42	1 (6%)
23	OMC	2L	33	23	15,22,23	2.29	4 (26%)	20,31,34	2.46	5 (25%)
23	G7M	2L	47	23	18,26,27	3.29	6 (33%)	21,39,42	2.26	4 (19%)
23	5MU	2L	55	23	13,22,23	1.72	2 (15%)	16,32,35	1.71	2 (12%)
23	PSU	2L	56	23	15,21,22	1.38	2 (13%)	16,30,33	1.98	4 (25%)
23	4SU	2L	8	23	12,21,22	3.18	2 (16%)	15,30,33	0.53	0
57	PSU	3L	39	57	15,21,22	1.10	1 (6%)	16,30,33	2.08	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/3/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	G7M	2K	47	23	-	0/3/25/26	0/3/3/3
23	5MU	2K	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	G7M	2L	47	23	-	0/3/25/26	0/3/3/3
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/3/25/26	0/2/2/2
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	34	U8U	C2-S2	-3.96	1.58	1.66
22	1K	39	PSU	C5-C1'	-3.70	1.49	1.52
23	2L	56	PSU	C5-C1'	-3.19	1.49	1.52
56	1L	54	5MU	C4-N3	-2.99	1.27	1.33
22	1K	37	T6A	C5-C4	-2.67	1.34	1.40

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	T6A	N3-C2-N1	-19.86	113.27	128.87
23	2L	47	G7M	C1'-N9-C4	-7.19	118.78	126.81
22	1K	34	U8U	C5-C4-N3	-6.86	119.03	125.19
23	2K	47	G7M	C5-C6-N1	-6.31	115.28	123.52
22	1K	37	T6A	O10-C10-N6	-5.57	115.07	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	34	U8U	3	0
22	1K	37	T6A	1	0
22	1K	54	5MU	1	0
22	1K	55	PSU	1	0
56	1L	54	5MU	2	0
23	2K	33	OMC	3	0
23	2K	47	G7M	2	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	1	0
23	2L	47	G7M	3	0
23	2L	55	5MU	4	0
23	2L	8	4SU	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1188 ligands modelled in this entry, 1186 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	SF4	32	302	4	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	3E	301	4	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	32	302	4	-	0/0/48/48	0/6/5/5
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	302	SF4	4	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	45	1
4	3E	1
5	4E	1
25	4K	1
37	35	1
38	88	1

The worst 5 of 6 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	4.44
1	35	121:LYS	C	122:PRO	N	1.77
1	45	124:LYS	C	125:LEU	N	1.15
1	4E	69:VAL	C	70:PRO	N	1.12
1	88	124:LYS	C	125:LEU	N	1.12

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1493/1522 (98%)	-0.64	0 100 100	83, 129, 202, 287	0
1	1G	1496/1522 (98%)	-0.44	11 (0%) 89 82	100, 152, 223, 279	0
2	12	206/256 (80%)	0.22	27 (13%) 5 2	173, 206, 218, 228	0
2	1E	231/256 (90%)	0.83	44 (19%) 2 1	140, 173, 197, 207	0
3	22	194/239 (81%)	0.97	43 (22%) 1 1	172, 196, 209, 214	0
3	2E	205/239 (85%)	0.57	27 (13%) 4 2	115, 136, 165, 176	0
4	32	208/209 (99%)	1.16	54 (25%) 1 0	129, 152, 173, 183	0
4	3E	207/209 (99%)	0.76	45 (21%) 1 1	104, 131, 154, 164	0
5	42	149/162 (91%)	0.17	8 (5%) 29 15	138, 160, 177, 190	0
5	4E	149/162 (91%)	-0.20	0 100 100	104, 125, 147, 155	0
6	52	101/101 (100%)	0.19	5 (4%) 32 17	119, 135, 156, 163	0
6	5E	100/101 (99%)	3.70	75 (75%) 0 0	103, 129, 149, 159	0
7	62	138/156 (88%)	0.02	11 (7%) 15 7	150, 164, 173, 181	0
7	6E	151/156 (96%)	-0.84	0 100 100	134, 150, 170, 179	0
8	72	137/138 (99%)	-0.75	0 100 100	136, 164, 180, 190	0
8	7E	138/138 (100%)	-0.49	1 (0%) 89 82	112, 138, 152, 161	0
9	82	105/128 (82%)	0.72	18 (17%) 2 1	149, 196, 209, 221	0
9	8E	126/128 (98%)	-0.63	1 (0%) 87 79	111, 170, 192, 200	0
10	1A	60/105 (57%)	1.65	17 (28%) 1 0	166, 193, 204, 205	0
10	1I	72/105 (68%)	0.13	4 (5%) 28 14	112, 150, 193, 204	0
11	2A	113/129 (87%)	-0.40	0 100 100	118, 143, 157, 167	0
11	2I	111/129 (86%)	1.71	43 (38%) 0 0	102, 136, 151, 164	0
12	3A	121/132 (91%)	1.11	34 (28%) 1 0	119, 142, 165, 179	0
12	3I	122/132 (92%)	0.13	2 (1%) 74 61	91, 102, 126, 160	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%)	1.07	27 (24%) 1 1	162, 187, 202, 212	0
13	4I	119/126 (94%)	-0.38	1 (0%) 87 79	111, 146, 162, 173	0
14	5A	48/61 (78%)	2.62	25 (52%) 0 0	170, 191, 208, 218	0
14	5I	60/61 (98%)	0.65	6 (10%) 9 4	107, 124, 141, 155	0
15	6A	87/89 (97%)	-0.17	2 (2%) 64 47	123, 148, 167, 174	0
15	6I	87/89 (97%)	1.59	27 (31%) 1 0	106, 127, 148, 153	0
16	7A	84/88 (95%)	-0.33	0 100 100	120, 139, 161, 184	0
16	7I	80/88 (90%)	0.56	10 (12%) 5 3	127, 140, 169, 180	0
17	8A	99/105 (94%)	-0.82	0 100 100	121, 143, 156, 159	0
17	8I	100/105 (95%)	2.18	50 (50%) 0 0	117, 136, 148, 154	0
18	9A	67/88 (76%)	0.09	2 (2%) 54 37	128, 145, 163, 171	0
18	9I	67/88 (76%)	2.73	39 (58%) 0 0	115, 134, 159, 164	0
19	AA	36/93 (38%)	-0.14	2 (5%) 28 14	191, 209, 217, 223	0
19	AI	81/93 (87%)	1.19	24 (29%) 1 0	125, 148, 173, 183	0
20	BA	98/106 (92%)	0.52	12 (12%) 5 3	107, 139, 163, 176	0
20	BI	97/106 (91%)	-0.13	5 (5%) 31 16	135, 152, 181, 193	0
21	1B	23/27 (85%)	3.96	21 (91%) 0 0	157, 179, 187, 189	0
21	1F	23/27 (85%)	-0.89	0 100 100	119, 134, 143, 145	0
22	1K	64/76 (84%)	0.39	7 (10%) 7 3	112, 226, 251, 253	0
23	2K	72/77 (93%)	-0.38	1 (1%) 78 64	94, 125, 153, 169	0
23	2L	72/77 (93%)	0.10	3 (4%) 40 24	100, 151, 178, 198	0
24	3K	76/76 (100%)	-0.22	3 (3%) 43 26	96, 189, 207, 218	0
25	4K	20/27 (74%)	0.13	1 (5%) 32 17	96, 156, 196, 199	0
25	4L	17/27 (62%)	0.42	1 (5%) 26 13	131, 170, 208, 211	0
26	14	2861/2912 (98%)	-0.35	27 (0%) 85 77	72, 111, 235, 276	0
26	1H	2830/2912 (97%)	-0.37	24 (0%) 87 79	65, 97, 204, 287	0
27	16	122/122 (100%)	-0.18	3 (2%) 61 45	92, 117, 143, 228	0
27	1J	122/122 (100%)	-0.74	0 100 100	117, 155, 179, 225	0
28	7I	135/229 (58%)	1.84	56 (41%) 0 0	149, 167, 190, 202	0
29	11	273/276 (98%)	0.08	8 (2%) 55 39	65, 90, 111, 122	0
29	19	273/276 (98%)	0.91	46 (16%) 2 1	74, 100, 121, 136	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	21	203/206 (98%)	0.50	19 (9%) 11 5	73, 112, 157, 172	0
30	29	203/206 (98%)	1.04	46 (22%) 1 1	79, 116, 162, 178	0
31	31	202/210 (96%)	0.16	7 (3%) 48 30	70, 102, 136, 155	0
31	39	204/210 (97%)	-0.32	0 100 100	83, 128, 181, 201	0
32	41	179/182 (98%)	0.48	19 (10%) 8 4	107, 128, 164, 174	0
32	49	179/182 (98%)	0.63	25 (13%) 4 2	151, 171, 195, 204	0
33	51	171/180 (95%)	0.31	23 (13%) 4 2	102, 128, 146, 157	0
33	59	69/180 (38%)	0.75	12 (17%) 2 1	170, 198, 213, 220	0
34	61	145/148 (97%)	1.24	40 (27%) 1 0	102, 163, 188, 199	0
34	69	145/148 (97%)	1.03	37 (25%) 1 0	111, 152, 176, 189	0
35	15	137/140 (97%)	1.46	44 (32%) 1 0	106, 134, 162, 179	0
35	58	138/140 (98%)	-0.27	1 (0%) 89 82	86, 112, 154, 172	0
36	25	122/122 (100%)	0.42	2 (1%) 74 61	92, 113, 132, 142	0
36	68	122/122 (100%)	-0.19	0 100 100	81, 98, 118, 131	0
37	35	148/150 (98%)	1.16	39 (26%) 1 0	84, 135, 174, 190	0
37	78	147/150 (98%)	0.42	20 (13%) 4 2	72, 104, 136, 144	0
38	45	138/141 (97%)	0.20	10 (7%) 18 9	99, 131, 151, 168	0
38	88	141/141 (100%)	1.77	64 (45%) 0 0	76, 101, 123, 153	0
39	55	118/118 (100%)	0.58	9 (7%) 17 8	87, 102, 118, 138	0
39	98	118/118 (100%)	2.87	73 (61%) 0 0	87, 109, 131, 147	0
40	65	110/112 (98%)	0.57	11 (10%) 9 4	116, 145, 164, 173	0
40	A8	111/112 (99%)	2.28	58 (52%) 0 0	93, 112, 135, 144	0
41	75	136/146 (93%)	-0.40	4 (2%) 55 39	102, 120, 169, 198	0
41	B8	135/146 (92%)	-0.50	1 (0%) 89 82	92, 116, 166, 185	0
42	85	116/118 (98%)	0.99	21 (18%) 2 1	90, 121, 154, 166	0
42	C8	115/118 (97%)	-0.12	2 (1%) 73 59	77, 102, 130, 141	0
43	95	99/101 (98%)	1.93	48 (48%) 0 0	91, 152, 166, 174	0
43	D8	101/101 (100%)	1.67	37 (36%) 0 0	78, 124, 149, 160	0
44	A5	110/113 (97%)	-0.36	0 100 100	84, 96, 127, 133	0
44	E8	110/113 (97%)	0.03	2 (1%) 71 56	79, 95, 125, 140	0
45	B5	94/96 (97%)	0.75	14 (14%) 3 2	94, 110, 134, 144	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	F8	95/96 (98%)	2.15	47 (49%) 0 0	78, 93, 120, 133	0
46	C5	105/110 (95%)	1.17	22 (20%) 1 1	110, 143, 175, 185	0
46	G8	104/110 (94%)	-0.66	0 100 100	88, 116, 148, 161	0
47	D5	130/206 (63%)	1.16	35 (26%) 1 0	138, 163, 188, 194	0
47	H8	148/206 (71%)	1.96	68 (45%) 0 0	106, 140, 195, 207	0
48	E5	78/85 (91%)	0.59	5 (6%) 23 11	99, 116, 136, 149	0
48	I8	76/85 (89%)	1.41	22 (28%) 1 0	79, 95, 111, 130	0
49	F5	94/98 (95%)	0.72	12 (12%) 5 2	86, 109, 144, 159	0
49	J8	94/98 (95%)	0.40	8 (8%) 13 6	79, 96, 143, 153	0
50	G5	67/72 (93%)	0.23	3 (4%) 37 21	113, 134, 152, 171	0
50	K8	68/72 (94%)	1.03	11 (16%) 3 1	82, 105, 124, 151	0
51	H5	58/60 (96%)	3.98	53 (91%) 0 0	103, 128, 155, 180	0
51	L8	58/60 (96%)	0.96	10 (17%) 2 1	83, 104, 140, 152	0
52	M8	47/71 (66%)	0.56	5 (10%) 8 4	131, 172, 183, 188	0
53	J5	56/60 (93%)	-0.19	5 (8%) 12 6	82, 108, 155, 165	0
53	N8	48/60 (80%)	0.59	7 (14%) 3 2	72, 108, 153, 164	0
54	L5	45/49 (91%)	0.55	5 (11%) 7 3	75, 83, 95, 107	0
54	P8	47/49 (95%)	-0.23	0 100 100	68, 74, 98, 108	0
55	M5	64/65 (98%)	1.41	17 (26%) 1 0	90, 105, 123, 143	0
55	Q8	64/65 (98%)	0.18	1 (1%) 74 61	80, 91, 108, 123	0
56	1L	71/76 (93%)	1.63	20 (28%) 1 0	140, 257, 274, 277	0
57	3L	75/76 (98%)	-0.08	2 (2%) 58 42	107, 259, 277, 285	0
All	All	20395/21728 (93%)	0.17	1949 (9%) 10 5	65, 127, 204, 287	0

The worst 5 of 1949 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	71	1	PRO	15.3
43	D8	101	GLY	10.4
10	1A	59	SER	10.2
21	1B	14	TRP	9.9
32	49	137	GLU	9.6



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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	5MU	1K	54	21/22	0.88	0.21	-	155,171,185,188	0
23	PSU	2L	56	20/21	0.87	0.15	-	143,152,158,162	0
56	PSU	1L	55	20/21	0.88	0.12	-	176,201,207,207	0
22	PSU	1K	55	20/21	0.86	0.16	-	143,175,183,183	0
23	5MU	2K	55	21/22	0.94	0.15	-	122,135,144,159	0
23	G7M	2K	47	24/25	0.95	0.10	-	124,132,139,146	0
23	OMC	2K	33	21/22	0.96	0.12	-	95,105,111,117	0
56	PSU	1L	39	20/21	0.90	0.32	-	155,179,185,187	0
23	PSU	2K	56	20/21	0.94	0.12	-	122,127,139,140	0
22	U8U	1K	34	23/24	0.96	0.12	-	116,123,130,131	0
22	PSU	1K	39	20/21	0.95	0.17	-	98,124,139,139	0
23	4SU	2K	8	20/21	0.92	0.15	-	111,120,124,128	0
57	PSU	3L	39	20/21	0.93	0.12	-	160,164,169,170	0
23	5MU	2L	55	21/22	0.91	0.15	-	146,159,164,166	0
23	OMC	2L	33	21/22	0.93	0.23	-	132,140,144,151	0
23	4SU	2L	8	20/21	0.88	0.16	-	131,155,165,169	0
22	T6A	1K	37	32/33	0.89	0.25	-	100,113,152,156	0
23	G7M	2L	47	24/25	0.92	0.13	-	161,169,178,179	0
56	5MU	1L	54	21/22	0.92	0.16	-	184,194,212,217	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1638	1/1	0.81	0.54	96.04	82,82,82,82	0
58	MG	1H	3283	1/1	0.96	1.29	73.76	95,95,95,95	0
58	MG	13	1648	1/1	0.90	0.59	57.74	108,108,108,108	0
58	MG	1H	3257	1/1	0.69	1.56	56.76	97,97,97,97	0
58	MG	1H	3015	1/1	0.97	0.96	51.46	77,77,77,77	0
58	MG	14	3233	1/1	0.64	0.63	51.44	108,108,108,108	0
58	MG	1H	3254	1/1	0.84	1.18	43.62	91,91,91,91	0
58	MG	14	3239	1/1	0.96	0.67	42.94	90,90,90,90	0
58	MG	1H	3255	1/1	0.93	0.78	41.88	94,94,94,94	0
58	MG	1H	3171	1/1	0.95	0.79	40.89	83,83,83,83	0
58	MG	1H	3235	1/1	0.72	0.68	38.23	112,112,112,112	0
58	MG	14	3193	1/1	0.96	0.58	36.77	79,79,79,79	0
58	MG	1H	3290	1/1	0.87	0.51	36.68	103,103,103,103	0
58	MG	14	3308	1/1	0.77	0.55	36.20	104,104,104,104	0
58	MG	14	3255	1/1	0.89	0.39	32.04	105,105,105,105	0
58	MG	1H	3286	1/1	0.65	0.41	30.34	109,109,109,109	0
58	MG	13	1642	1/1	0.95	0.47	28.88	104,104,104,104	0
58	MG	1H	3018	1/1	0.98	0.58	28.53	66,66,66,66	0
58	MG	1H	3124	1/1	0.88	0.42	27.55	77,77,77,77	0
58	MG	14	3014	1/1	0.99	0.58	27.40	82,82,82,82	0
58	MG	1H	3296	1/1	0.96	0.89	26.90	86,86,86,86	0
58	MG	14	3152	1/1	0.88	0.58	26.83	102,102,102,102	0
58	MG	1H	3045	1/1	0.99	0.37	26.68	68,68,68,68	0
58	MG	14	3289	1/1	0.94	0.34	26.06	116,116,116,116	0
58	MG	14	3095	1/1	0.97	0.71	25.13	75,75,75,75	0
58	MG	14	3111	1/1	0.93	0.55	24.86	82,82,82,82	0
58	MG	1H	3079	1/1	0.97	0.45	24.27	68,68,68,68	0
58	MG	1H	3197	1/1	0.93	0.49	24.15	68,68,68,68	0
58	MG	1H	3075	1/1	0.85	0.93	24.08	82,82,82,82	0
58	MG	1H	3333	1/1	0.79	0.34	23.18	93,93,93,93	0
58	MG	14	3016	1/1	0.97	0.44	22.69	68,68,68,68	0
58	MG	14	3224	1/1	0.76	0.35	22.47	105,105,105,105	0
58	MG	14	3088	1/1	0.95	0.41	22.41	78,78,78,78	0
58	MG	1H	3030	1/1	0.68	0.67	20.92	85,85,85,85	0
58	MG	14	3254	1/1	0.85	0.45	20.90	83,83,83,83	0
58	MG	1H	3028	1/1	0.92	0.44	20.59	82,82,82,82	0
58	MG	1H	3034	1/1	0.91	0.33	20.53	145,145,145,145	0
58	MG	14	3200	1/1	0.81	0.55	20.07	94,94,94,94	0
58	MG	14	3258	1/1	0.85	0.27	19.75	93,93,93,93	0
58	MG	14	3009	1/1	0.96	0.51	19.48	74,74,74,74	0
58	MG	13	1658	1/1	0.95	0.58	19.02	89,89,89,89	0
58	MG	1H	3340	1/1	0.35	0.60	19.00	101,101,101,101	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3093	1/1	0.97	0.64	18.77	71,71,71,71	0
58	MG	14	3116	1/1	0.96	0.45	18.31	75,75,75,75	0
58	MG	1H	3267	1/1	0.88	0.48	18.22	85,85,85,85	0
58	MG	1H	3244	1/1	0.93	0.47	18.13	103,103,103,103	0
58	MG	1G	1606	1/1	0.97	0.53	18.05	93,93,93,93	0
58	MG	14	3081	1/1	0.98	0.27	17.29	89,89,89,89	0
58	MG	E5	101	1/1	0.75	0.65	16.89	100,100,100,100	0
58	MG	1H	3078	1/1	0.97	0.28	16.78	80,80,80,80	0
58	MG	1H	3023	1/1	0.90	0.44	16.61	92,92,92,92	0
58	MG	1H	3098	1/1	0.98	0.66	16.58	70,70,70,70	0
58	MG	14	3297	1/1	0.84	0.55	16.45	91,91,91,91	0
58	MG	1H	3085	1/1	0.82	0.47	16.04	92,92,92,92	0
58	MG	14	3341	1/1	0.85	0.36	16.03	105,105,105,105	0
58	MG	14	3129	1/1	0.91	0.40	15.90	84,84,84,84	0
58	MG	1H	3261	1/1	0.84	0.52	15.59	115,115,115,115	0
58	MG	14	3187	1/1	0.95	0.30	15.29	96,96,96,96	0
58	MG	1G	1613	1/1	0.95	0.28	15.16	114,114,114,114	0
58	MG	1H	3117	1/1	0.85	0.30	14.86	75,75,75,75	0
58	MG	1H	3225	1/1	0.93	0.33	14.73	70,70,70,70	0
58	MG	1H	3226	1/1	0.85	0.32	14.66	88,88,88,88	0
58	MG	14	3215	1/1	0.97	0.38	14.66	89,89,89,89	0
58	MG	1H	3068	1/1	0.94	0.45	14.37	70,70,70,70	0
58	MG	14	3250	1/1	0.86	0.47	14.29	79,79,79,79	0
58	MG	1H	3103	1/1	0.96	0.57	13.98	72,72,72,72	0
58	MG	1H	3090	1/1	0.93	0.43	13.90	76,76,76,76	0
58	MG	1H	3143	1/1	0.90	0.35	13.86	101,101,101,101	0
58	MG	14	3195	1/1	0.74	0.54	13.56	107,107,107,107	0
58	MG	1H	3164	1/1	0.89	0.24	13.44	86,86,86,86	0
58	MG	1G	1640	1/1	0.47	0.42	13.43	115,115,115,115	0
58	MG	2L	101	1/1	0.99	0.52	13.36	97,97,97,97	0
58	MG	1G	1616	1/1	0.90	0.34	13.21	118,118,118,118	0
58	MG	1H	3282	1/1	0.83	0.47	13.13	106,106,106,106	0
58	MG	14	3027	1/1	0.97	0.45	12.63	79,79,79,79	0
58	MG	14	3011	1/1	0.96	0.56	12.61	85,85,85,85	0
58	MG	1H	3242	1/1	0.90	0.41	12.55	90,90,90,90	0
58	MG	13	1620	1/1	0.93	0.24	12.32	117,117,117,117	0
58	MG	14	3334	1/1	0.88	0.74	12.21	92,92,92,92	0
58	MG	14	3335	1/1	0.85	0.23	12.18	124,124,124,124	0
58	MG	1H	3091	1/1	0.99	0.49	12.17	58,58,58,58	0
58	MG	1H	3002	1/1	0.97	0.45	12.07	64,64,64,64	0
58	MG	1H	3165	1/1	0.96	0.42	12.03	99,99,99,99	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3216	1/1	0.97	0.28	11.96	101,101,101,101	0
58	MG	14	3158	1/1	0.94	0.36	11.87	92,92,92,92	0
58	MG	14	3108	1/1	0.74	0.35	11.69	88,88,88,88	0
58	MG	1H	3136	1/1	0.91	0.25	11.40	80,80,80,80	0
58	MG	14	3017	1/1	0.97	0.42	11.13	68,68,68,68	0
58	MG	1G	1649	1/1	0.99	0.37	11.00	128,128,128,128	0
58	MG	14	3125	1/1	0.99	0.30	10.99	102,102,102,102	0
58	MG	14	3290	1/1	0.99	0.28	10.81	113,113,113,113	0
58	MG	14	3245	1/1	0.92	0.43	10.77	97,97,97,97	0
58	MG	1H	3006	1/1	0.94	0.27	10.76	71,71,71,71	0
58	MG	1H	3001	1/1	0.95	0.43	10.69	66,66,66,66	0
58	MG	1G	1627	1/1	0.80	0.49	10.55	142,142,142,142	0
58	MG	1G	1667	1/1	0.83	0.30	10.34	111,111,111,111	0
58	MG	1H	3127	1/1	0.92	0.34	10.26	79,79,79,79	0
58	MG	14	3279	1/1	0.51	0.59	10.21	103,103,103,103	0
58	MG	1H	3083	1/1	0.93	0.27	10.16	74,74,74,74	0
58	MG	1H	3048	1/1	0.93	0.36	10.10	80,80,80,80	0
58	MG	14	3202	1/1	0.82	0.33	10.05	79,79,79,79	0
58	MG	14	3232	1/1	0.84	0.41	10.05	89,89,89,89	0
58	MG	14	3005	1/1	0.89	0.34	9.96	101,101,101,101	0
58	MG	14	3106	1/1	0.96	0.36	9.70	85,85,85,85	0
58	MG	14	3043	1/1	0.95	0.38	9.63	69,69,69,69	0
58	MG	1H	3041	1/1	0.97	0.29	9.56	73,73,73,73	0
58	MG	14	3074	1/1	0.97	0.50	9.49	70,70,70,70	0
58	MG	1H	3179	1/1	0.95	0.37	9.41	101,101,101,101	0
58	MG	13	1639	1/1	0.96	0.24	9.19	87,87,87,87	0
58	MG	14	3021	1/1	0.88	0.40	8.97	73,73,73,73	0
58	MG	13	1651	1/1	0.95	0.31	8.96	96,96,96,96	0
58	MG	1H	3007	1/1	0.96	0.31	8.92	65,65,65,65	0
58	MG	14	3191	1/1	0.91	0.53	8.91	93,93,93,93	0
58	MG	1H	3221	1/1	0.98	0.27	8.90	81,81,81,81	0
58	MG	1H	3008	1/1	0.97	0.36	8.88	99,99,99,99	0
58	MG	1H	3214	1/1	0.95	0.28	8.75	65,65,65,65	0
58	MG	1H	3202	1/1	0.84	0.33	8.65	95,95,95,95	0
58	MG	1H	3071	1/1	0.98	0.41	8.61	94,94,94,94	0
58	MG	2K	101	1/1	0.99	0.43	8.55	84,84,84,84	0
58	MG	14	3072	1/1	0.93	0.34	8.52	84,84,84,84	0
58	MG	1H	3097	1/1	0.96	0.43	8.44	72,72,72,72	0
58	MG	1H	3150	1/1	0.94	0.40	8.40	63,63,63,63	0
58	MG	1H	3190	1/1	0.94	0.24	8.25	108,108,108,108	0
58	MG	14	3130	1/1	0.97	0.29	8.19	93,93,93,93	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3182	1/1	0.70	0.21	7.88	105,105,105,105	0
58	MG	14	3008	1/1	0.96	0.39	7.79	77,77,77,77	0
58	MG	14	3166	1/1	0.87	0.58	7.79	79,79,79,79	0
58	MG	14	3065	1/1	0.97	0.27	7.77	80,80,80,80	0
58	MG	1H	3092	1/1	0.92	0.36	7.67	76,76,76,76	0
58	MG	14	3044	1/1	0.93	0.28	7.29	88,88,88,88	0
58	MG	1H	3130	1/1	0.94	0.36	7.29	79,79,79,79	0
58	MG	1H	3104	1/1	0.96	0.31	7.20	66,66,66,66	0
58	MG	14	3251	1/1	0.86	0.17	7.20	90,90,90,90	0
58	MG	14	3214	1/1	0.90	0.31	6.96	94,94,94,94	0
58	MG	1H	3433	1/1	0.93	0.28	6.91	113,113,113,113	0
58	MG	14	3097	1/1	0.99	0.29	6.68	83,83,83,83	0
58	MG	1H	3148	1/1	0.89	0.21	6.58	92,92,92,92	0
58	MG	14	3246	1/1	0.77	0.36	6.37	95,95,95,95	0
58	MG	1H	3185	1/1	0.86	0.22	6.27	68,68,68,68	0
58	MG	1G	1634	1/1	0.98	0.34	6.20	127,127,127,127	0
58	MG	13	1610	1/1	0.96	0.30	6.07	92,92,92,92	0
58	MG	1H	3101	1/1	0.89	0.33	6.01	59,59,59,59	0
58	MG	13	1601	1/1	0.98	0.27	5.83	86,86,86,86	0
58	MG	13	1643	1/1	0.97	0.35	5.72	80,80,80,80	0
58	MG	1H	3126	1/1	0.68	0.26	5.71	83,83,83,83	0
58	MG	14	3321	1/1	0.72	0.43	5.66	109,109,109,109	0
58	MG	14	3287	1/1	0.87	0.20	5.52	101,101,101,101	0
58	MG	1H	3239	1/1	0.95	0.25	5.45	71,71,71,71	0
58	MG	1H	3284	1/1	0.89	0.20	5.43	97,97,97,97	0
58	MG	85	202	1/1	0.62	0.65	5.43	100,100,100,100	0
58	MG	14	3219	1/1	0.94	0.22	5.39	83,83,83,83	0
58	MG	14	3145	1/1	0.96	0.25	5.36	76,76,76,76	0
58	MG	1H	3236	1/1	0.95	0.19	5.34	89,89,89,89	0
58	MG	14	3271	1/1	0.83	0.27	5.31	101,101,101,101	0
58	MG	14	3121	1/1	0.97	0.39	5.24	69,69,69,69	0
58	MG	1G	1626	1/1	0.98	0.27	5.15	118,118,118,118	0
58	MG	1H	3111	1/1	0.95	0.28	4.96	64,64,64,64	0
58	MG	13	1659	1/1	0.69	0.28	4.94	116,116,116,116	0
58	MG	13	1631	1/1	0.93	0.27	4.80	82,82,82,82	0
58	MG	13	1614	1/1	0.89	0.20	4.77	97,97,97,97	0
58	MG	14	3332	1/1	0.88	0.25	4.73	98,98,98,98	0
58	MG	14	3316	1/1	0.59	0.29	4.62	111,111,111,111	0
58	MG	1H	3222	1/1	0.93	0.25	4.48	94,94,94,94	0
58	MG	1H	3443	1/1	0.98	0.24	4.47	80,80,80,80	0
58	MG	14	3071	1/1	0.97	0.34	4.38	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3127	1/1	0.98	0.27	4.31	67,67,67,67	0
58	MG	14	3155	1/1	0.82	0.35	4.26	101,101,101,101	0
58	MG	14	3076	1/1	0.97	0.30	4.23	83,83,83,83	0
58	MG	1H	3057	1/1	0.95	0.27	4.20	75,75,75,75	0
58	MG	1H	3076	1/1	0.80	0.36	4.01	78,78,78,78	0
58	MG	1H	3227	1/1	0.85	0.52	4.00	92,92,92,92	0
58	MG	C8	201	1/1	0.96	0.20	3.99	74,74,74,74	0
58	MG	1G	1625	1/1	0.95	0.25	3.91	136,136,136,136	0
58	MG	1H	3194	1/1	0.94	0.24	3.88	91,91,91,91	0
58	MG	1H	3175	1/1	0.70	0.15	3.84	92,92,92,92	0
58	MG	1H	3408	1/1	0.99	0.23	3.82	72,72,72,72	0
58	MG	14	3237	1/1	0.94	0.21	3.75	181,181,181,181	0
58	MG	1H	3088	1/1	0.97	0.22	3.57	81,81,81,81	0
58	MG	14	3269	1/1	0.89	0.29	3.57	115,115,115,115	0
58	MG	14	3218	1/1	0.93	0.15	3.39	97,97,97,97	0
58	MG	13	1657	1/1	0.98	0.17	3.38	103,103,103,103	0
58	MG	14	3172	1/1	0.97	0.23	3.32	75,75,75,75	0
58	MG	13	1672	1/1	0.90	0.15	3.24	133,133,133,133	0
58	MG	29	303	1/1	0.33	0.24	3.22	106,106,106,106	0
58	MG	1H	3064	1/1	0.97	0.26	3.07	82,82,82,82	0
58	MG	1G	1619	1/1	0.98	0.27	3.06	109,109,109,109	0
58	MG	14	3054	1/1	0.88	0.26	3.02	99,99,99,99	0
58	MG	14	3282	1/1	0.82	0.33	3.01	96,96,96,96	0
58	MG	1H	3139	1/1	0.88	0.18	2.97	75,75,75,75	0
58	MG	1H	3237	1/1	0.90	0.16	2.96	88,88,88,88	0
58	MG	1H	3053	1/1	0.95	0.17	2.92	81,81,81,81	0
58	MG	1H	3308	1/1	0.91	0.24	2.91	81,81,81,81	0
58	MG	29	302	1/1	0.88	0.54	2.67	94,94,94,94	0
58	MG	1G	1669	1/1	0.92	0.14	2.57	151,151,151,151	0
58	MG	1G	1615	1/1	0.95	0.22	2.57	142,142,142,142	0
58	MG	13	1671	1/1	0.94	0.20	2.49	107,107,107,107	0
58	MG	1G	1676	1/1	0.98	0.21	2.46	134,134,134,134	0
58	MG	13	1682	1/1	0.98	0.17	2.37	93,93,93,93	0
58	MG	13	1611	1/1	0.93	0.22	2.37	91,91,91,91	0
58	MG	1H	3069	1/1	0.77	0.16	2.35	101,101,101,101	0
58	MG	14	3317	1/1	0.91	0.16	2.34	122,122,122,122	0
58	MG	1H	3457	1/1	0.91	0.29	2.32	89,89,89,89	0
58	MG	1H	3398	1/1	0.91	0.19	2.22	76,76,76,76	0
58	MG	14	3363	1/1	1.00	0.23	2.20	80,80,80,80	0
58	MG	14	3059	1/1	0.67	0.17	2.19	92,92,92,92	0
58	MG	14	3173	1/1	0.89	0.14	2.17	96,96,96,96	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1673	1/1	0.92	0.17	2.17	145,145,145,145	0
58	MG	14	3118	1/1	0.97	0.26	2.16	73,73,73,73	0
58	MG	13	1686	1/1	0.81	0.17	2.15	79,79,79,79	0
58	MG	Q8	101	1/1	0.88	0.38	2.12	89,89,89,89	0
58	MG	45	201	1/1	0.92	0.27	2.06	101,101,101,101	0
58	MG	14	3119	1/1	0.95	0.27	2.03	83,83,83,83	0
58	MG	1H	3215	1/1	0.90	0.25	1.90	69,69,69,69	0
58	MG	14	3211	1/1	0.95	0.21	1.88	78,78,78,78	0
58	MG	14	3096	1/1	0.98	0.40	1.86	57,57,57,57	0
58	MG	1H	3364	1/1	0.98	0.20	1.77	74,74,74,74	0
58	MG	1H	3442	1/1	0.97	0.26	1.72	63,63,63,63	0
58	MG	1H	3428	1/1	0.97	0.20	1.56	89,89,89,89	0
58	MG	1H	3252	1/1	0.88	0.26	1.51	75,75,75,75	0
58	MG	1H	3173	1/1	0.80	0.24	1.47	108,108,108,108	0
58	MG	1H	3382	1/1	0.98	0.22	1.30	71,71,71,71	0
58	MG	1G	1601	1/1	0.99	0.20	1.29	115,115,115,115	0
58	MG	1H	3399	1/1	0.99	0.18	1.27	75,75,75,75	0
58	MG	1G	1668	1/1	0.51	0.28	1.16	138,138,138,138	0
58	MG	14	3203	1/1	0.95	0.28	1.09	84,84,84,84	0
58	MG	14	3045	1/1	0.92	0.20	1.07	89,89,89,89	0
58	MG	14	3048	1/1	0.95	0.21	1.05	90,90,90,90	0
58	MG	1H	3067	1/1	0.99	0.22	1.04	74,74,74,74	0
58	MG	1H	3486	1/1	0.77	0.31	1.02	106,106,106,106	0
58	MG	14	3138	1/1	0.98	0.18	0.99	96,96,96,96	0
58	MG	14	3273	1/1	0.88	0.15	0.99	110,110,110,110	0
58	MG	14	3306	1/1	0.96	0.20	0.97	129,129,129,129	0
58	MG	14	3066	1/1	0.98	0.32	0.93	95,95,95,95	0
58	MG	14	3265	1/1	0.96	0.14	0.90	110,110,110,110	0
58	MG	1H	3400	1/1	0.99	0.19	0.90	86,86,86,86	0
58	MG	14	3252	1/1	0.85	0.18	0.86	106,106,106,106	0
58	MG	13	1718	1/1	0.98	0.12	0.78	110,110,110,110	0
58	MG	14	3213	1/1	0.93	0.27	0.69	114,114,114,114	0
58	MG	13	1694	1/1	0.84	0.18	0.65	114,114,114,114	0
58	MG	1H	3461	1/1	0.99	0.20	0.63	97,97,97,97	0
58	MG	3I	201	1/1	0.92	0.19	0.61	87,87,87,87	0
58	MG	1H	3251	1/1	0.82	0.13	0.60	75,75,75,75	0
58	MG	1H	3140	1/1	0.76	0.30	0.57	89,89,89,89	0
58	MG	14	3364	1/1	0.98	0.16	0.52	105,105,105,105	0
58	MG	1H	3416	1/1	0.99	0.18	0.51	83,83,83,83	0
58	MG	1H	3115	1/1	0.92	0.26	0.50	70,70,70,70	0
58	MG	1H	3055	1/1	0.94	0.18	0.50	74,74,74,74	0
58	MG	13	1649	1/1	0.72	0.15	0.49	118,118,118,118	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3208	1/1	0.86	0.22	0.48	93,93,93,93	0
58	MG	1H	3368	1/1	0.99	0.21	0.47	76,76,76,76	0
58	MG	1H	3180	1/1	0.97	0.13	0.45	97,97,97,97	0
58	MG	13	1711	1/1	0.99	0.18	0.40	85,85,85,85	0
58	MG	J8	101	1/1	0.84	0.29	0.38	89,89,89,89	0
58	MG	1H	3330	1/1	0.76	0.14	0.37	105,105,105,105	0
58	MG	14	3010	1/1	0.98	0.30	0.30	73,73,73,73	0
58	MG	35	201	1/1	0.81	0.51	0.28	90,90,90,90	0
58	MG	1H	3153	1/1	0.91	0.13	0.28	86,86,86,86	0
58	MG	55	201	1/1	0.92	0.28	0.28	96,96,96,96	0
58	MG	13	1741	1/1	0.97	0.17	0.26	88,88,88,88	0
58	MG	1H	3122	1/1	0.92	0.14	0.25	83,83,83,83	0
58	MG	1H	3423	1/1	0.97	0.20	0.23	92,92,92,92	0
58	MG	14	3394	1/1	0.97	0.20	0.22	88,88,88,88	0
58	MG	14	3340	1/1	0.94	0.22	0.10	91,91,91,91	0
58	MG	14	3157	1/1	0.85	0.15	0.08	81,81,81,81	0
58	MG	1G	1641	1/1	0.56	0.17	0.05	131,131,131,131	0
58	MG	14	3154	1/1	0.85	0.17	0.04	84,84,84,84	0
58	MG	14	3099	1/1	0.96	0.25	0.03	91,91,91,91	0
58	MG	1H	3054	1/1	0.75	0.13	0.02	110,110,110,110	0
58	MG	1H	3230	1/1	0.70	0.12	-0.03	104,104,104,104	0
58	MG	1H	3381	1/1	0.97	0.15	-0.05	80,80,80,80	0
58	MG	1H	3250	1/1	0.84	0.13	-0.08	94,94,94,94	0
58	MG	85	201	1/1	0.85	0.20	-0.10	85,85,85,85	0
58	MG	14	3243	1/1	0.97	0.24	-0.11	102,102,102,102	0
58	MG	1G	1678	1/1	0.94	0.14	-0.20	119,119,119,119	0
58	MG	1G	1671	1/1	0.98	0.15	-0.32	121,121,121,121	0
58	MG	1H	3056	1/1	0.96	0.22	-0.33	89,89,89,89	0
58	MG	14	3226	1/1	0.97	0.28	-0.35	88,88,88,88	0
58	MG	1H	3397	1/1	0.98	0.14	-0.36	82,82,82,82	0
58	MG	14	3343	1/1	0.99	0.20	-0.42	87,87,87,87	0
58	MG	14	3212	1/1	0.94	0.17	-0.45	105,105,105,105	0
58	MG	45	202	1/1	0.71	0.15	-0.46	122,122,122,122	0
58	MG	14	3285	1/1	0.94	0.21	-0.47	77,77,77,77	0
58	MG	1H	3375	1/1	0.95	0.16	-0.47	81,81,81,81	0
58	MG	1H	3151	1/1	0.90	0.13	-0.55	90,90,90,90	0
58	MG	14	3205	1/1	0.92	0.16	-0.67	97,97,97,97	0
59	SF4	3E	301	8/8	0.99	0.18	-0.69	95,111,117,118	0
60	ZN	5I	102	1/1	0.98	0.14	-0.72	114,114,114,114	0
58	MG	1H	3367	1/1	0.98	0.18	-0.72	84,84,84,84	0
58	MG	13	1730	1/1	0.95	0.10	-0.73	108,108,108,108	0
58	MG	1H	3484	1/1	0.99	0.18	-0.75	81,81,81,81	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3114	1/1	0.94	0.15	-0.77	77,77,77,77	0
58	MG	5I	101	1/1	0.90	0.14	-0.78	110,110,110,110	0
58	MG	16	203	1/1	0.56	0.16	-0.80	112,112,112,112	0
58	MG	14	3139	1/1	0.92	0.12	-0.80	75,75,75,75	0
58	MG	1H	3387	1/1	1.00	0.18	-0.83	60,60,60,60	0
58	MG	13	1669	1/1	0.89	0.12	-0.83	120,120,120,120	0
58	MG	1H	3407	1/1	0.99	0.15	-0.86	83,83,83,83	0
58	MG	14	3393	1/1	0.98	0.15	-0.86	89,89,89,89	0
58	MG	1H	3113	1/1	0.94	0.15	-0.92	59,59,59,59	0
58	MG	13	1717	1/1	0.91	0.06	-0.98	123,123,123,123	0
58	MG	1H	3487	1/1	0.91	0.13	-1.01	96,96,96,96	0
58	MG	14	3070	1/1	0.95	0.16	-1.03	94,94,94,94	0
58	MG	1H	3441	1/1	0.99	0.13	-1.05	92,92,92,92	0
59	SF4	32	302	8/8	0.99	0.14	-1.06	127,146,153,155	0
58	MG	1H	3218	1/1	0.94	0.17	-1.08	68,68,68,68	0
58	MG	14	3349	1/1	1.00	0.18	-1.09	95,95,95,95	0
58	MG	14	3373	1/1	0.97	0.14	-1.09	86,86,86,86	0
58	MG	14	3037	1/1	0.99	0.18	-1.18	80,80,80,80	0
58	MG	1H	3380	1/1	0.97	0.10	-1.20	89,89,89,89	0
58	MG	1H	3424	1/1	0.99	0.12	-1.21	81,81,81,81	0
58	MG	41	201	1/1	0.82	0.10	-1.23	102,102,102,102	0
58	MG	14	3230	1/1	0.95	0.15	-1.24	122,122,122,122	0
58	MG	1G	1607	1/1	0.97	0.19	-1.25	109,109,109,109	0
58	MG	14	3345	1/1	0.99	0.16	-1.31	80,80,80,80	0
58	MG	13	1655	1/1	0.93	0.08	-1.32	106,106,106,106	0
58	MG	1H	3014	1/1	0.91	0.15	-1.34	65,65,65,65	0
58	MG	1H	3473	1/1	0.98	0.11	-1.34	89,89,89,89	0
58	MG	13	1665	1/1	0.94	0.10	-1.35	105,105,105,105	0
60	ZN	5A	101	1/1	0.97	0.06	-1.39	164,164,164,164	0
58	MG	14	3064	1/1	0.99	0.13	-1.40	86,86,86,86	0
58	MG	14	3077	1/1	0.98	0.15	-1.41	83,83,83,83	0
58	MG	1H	3356	1/1	0.98	0.16	-1.43	67,67,67,67	0
58	MG	14	3384	1/1	0.98	0.10	-1.45	96,96,96,96	0
58	MG	14	3073	1/1	0.99	0.15	-1.46	67,67,67,67	0
58	MG	14	3236	1/1	0.96	0.10	-1.46	121,121,121,121	0
58	MG	1G	1677	1/1	0.81	0.06	-1.48	185,185,185,185	0
58	MG	14	3407	1/1	0.95	0.07	-1.50	121,121,121,121	0
58	MG	1G	1617	1/1	0.96	0.05	-1.52	159,159,159,159	0
58	MG	13	1713	1/1	0.95	0.05	-1.54	117,117,117,117	0
58	MG	21	302	1/1	0.90	0.12	-1.58	91,91,91,91	0
58	MG	1H	3401	1/1	0.97	0.15	-1.66	71,71,71,71	0
58	MG	14	3419	1/1	0.99	0.09	-1.71	90,90,90,90	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3403	1/1	0.99	0.13	-1.72	81,81,81,81	0
58	MG	14	3142	1/1	0.98	0.14	-1.77	99,99,99,99	0
58	MG	1H	3372	1/1	0.96	0.07	-1.82	73,73,73,73	0
58	MG	13	1714	1/1	0.98	0.11	-1.87	98,98,98,98	0
58	MG	14	3357	1/1	0.99	0.07	-1.89	76,76,76,76	0
58	MG	1H	3106	1/1	0.97	0.10	-1.90	82,82,82,82	0
58	MG	1H	3425	1/1	0.97	0.12	-1.94	77,77,77,77	0
60	ZN	C5	202	1/1	0.81	0.13	-2.00	183,183,183,183	0
58	MG	16	201	1/1	0.96	0.11	-2.05	114,114,114,114	0
58	MG	1H	3294	1/1	0.97	0.09	-2.12	103,103,103,103	0
58	MG	14	3060	1/1	0.94	0.07	-2.12	103,103,103,103	0
58	MG	14	3061	1/1	0.92	0.12	-2.14	102,102,102,102	0
58	MG	1H	3133	1/1	0.83	0.11	-2.17	83,83,83,83	0
58	MG	14	3206	1/1	0.93	0.09	-2.17	88,88,88,88	0
58	MG	1H	3446	1/1	0.97	0.10	-2.18	94,94,94,94	0
58	MG	13	1700	1/1	0.95	0.08	-2.19	123,123,123,123	0
58	MG	1G	1609	1/1	0.89	0.09	-2.22	113,113,113,113	0
58	MG	1H	3378	1/1	0.96	0.10	-2.23	90,90,90,90	0
58	MG	1G	1657	1/1	0.96	0.16	-2.26	163,163,163,163	0
58	MG	14	3050	1/1	0.94	0.12	-2.36	87,87,87,87	0
58	MG	13	1630	1/1	0.92	0.14	-2.38	74,74,74,74	0
58	MG	13	1721	1/1	0.96	0.05	-2.41	100,100,100,100	0
58	MG	14	3408	1/1	0.98	0.07	-2.42	130,130,130,130	0
58	MG	13	1664	1/1	0.97	0.08	-2.42	105,105,105,105	0
58	MG	1H	3388	1/1	0.99	0.12	-2.43	78,78,78,78	0
58	MG	14	3411	1/1	0.89	0.05	-2.45	134,134,134,134	0
58	MG	14	3140	1/1	0.80	0.09	-2.46	79,79,79,79	0
58	MG	16	204	1/1	0.91	0.10	-2.49	106,106,106,106	0
58	MG	14	3351	1/1	0.93	0.06	-2.57	80,80,80,80	0
58	MG	1H	3362	1/1	0.98	0.13	-2.62	71,71,71,71	0
58	MG	14	3362	1/1	0.99	0.08	-2.63	86,86,86,86	0
58	MG	1H	3417	1/1	0.97	0.10	-2.71	77,77,77,77	0
58	MG	1J	204	1/1	0.81	0.07	-2.71	119,119,119,119	0
58	MG	14	3385	1/1	0.97	0.05	-2.74	92,92,92,92	0
58	MG	1H	3123	1/1	0.83	0.09	-2.80	85,85,85,85	0
58	MG	1H	3420	1/1	0.93	0.11	-2.81	81,81,81,81	0
58	MG	14	3112	1/1	0.95	0.10	-2.82	108,108,108,108	0
58	MG	14	3052	1/1	0.95	0.13	-2.85	83,83,83,83	0
58	MG	5E	202	1/1	0.76	0.18	-2.86	111,111,111,111	0
58	MG	14	3348	1/1	0.95	0.11	-2.87	86,86,86,86	0
58	MG	14	3420	1/1	0.87	0.08	-2.89	118,118,118,118	0
58	MG	88	201	1/1	0.99	0.23	-2.93	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3488	1/1	0.89	0.09	-2.97	92,92,92,92	0
58	MG	1H	3058	1/1	0.94	0.15	-2.99	76,76,76,76	0
58	MG	13	1725	1/1	0.98	0.10	-3.00	101,101,101,101	0
58	MG	14	3353	1/1	0.94	0.11	-3.01	73,73,73,73	0
58	MG	13	1616	1/1	0.98	0.05	-3.01	121,121,121,121	0
58	MG	1G	1651	1/1	0.85	0.14	-3.02	128,128,128,128	0
58	MG	14	3387	1/1	0.98	0.08	-3.04	88,88,88,88	0
58	MG	1H	3241	1/1	0.97	0.08	-3.12	100,100,100,100	0
58	MG	1H	3243	1/1	0.77	0.09	-3.23	96,96,96,96	0
58	MG	1H	3389	1/1	1.00	0.12	-3.23	71,71,71,71	0
58	MG	14	3391	1/1	0.98	0.09	-3.40	87,87,87,87	0
58	MG	1H	3453	1/1	0.95	0.08	-3.46	93,93,93,93	0
58	MG	1H	3386	1/1	0.97	0.06	-3.50	109,109,109,109	0
58	MG	1H	3359	1/1	0.99	0.15	-3.58	71,71,71,71	0
58	MG	14	3367	1/1	0.96	0.07	-3.68	86,86,86,86	0
58	MG	1H	3430	1/1	0.95	0.08	-3.82	81,81,81,81	0
58	MG	16	206	1/1	0.87	0.06	-3.96	89,89,89,89	0
58	MG	1H	3357	1/1	0.98	0.11	-3.97	79,79,79,79	0
58	MG	14	3307	1/1	0.96	0.10	-4.01	80,80,80,80	0
58	MG	1H	3390	1/1	0.96	0.12	-4.01	74,74,74,74	0
58	MG	14	3355	1/1	0.96	0.07	-4.04	92,92,92,92	0
58	MG	14	3242	1/1	0.92	0.10	-4.10	92,92,92,92	0
58	MG	14	3346	1/1	0.98	0.09	-4.14	81,81,81,81	0
58	MG	1H	3394	1/1	0.97	0.07	-4.22	89,89,89,89	0
58	MG	1G	1672	1/1	0.96	0.05	-4.38	115,115,115,115	0
58	MG	1H	3370	1/1	0.98	0.09	-4.43	68,68,68,68	0
58	MG	1H	3402	1/1	0.99	0.10	-4.51	76,76,76,76	0
58	MG	1H	3435	1/1	0.99	0.07	-4.56	85,85,85,85	0
58	MG	13	1727	1/1	0.98	0.08	-5.04	87,87,87,87	0
58	MG	14	3380	1/1	0.96	0.08	-5.66	94,94,94,94	0
58	MG	14	3347	1/1	0.95	0.05	-5.73	87,87,87,87	0
58	MG	14	3359	1/1	0.98	0.10	-6.02	94,94,94,94	0
58	MG	14	3395	1/1	0.95	0.06	-6.21	85,85,85,85	0
58	MG	14	3377	1/1	0.95	0.05	-6.37	106,106,106,106	0
58	MG	1H	3478	1/1	0.97	0.06	-11.36	95,95,95,95	0
58	MG	1G	1670	1/1	0.97	0.05	-14.06	112,112,112,112	0
58	MG	1H	3376	1/1	0.98	0.05	-20.22	106,106,106,106	0
58	MG	1H	3309	1/1	0.78	0.49	-	126,126,126,126	0
58	MG	1H	3365	1/1	0.97	0.17	-	64,64,64,64	0
58	MG	14	3131	1/1	0.98	0.33	-	79,79,79,79	0
58	MG	14	3107	1/1	0.98	0.41	-	80,80,80,80	0
58	MG	14	3323	1/1	0.89	0.07	-	159,159,159,159	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3299	1/1	0.56	0.36	-	118,118,118,118	0
58	MG	14	3092	1/1	0.99	0.34	-	91,91,91,91	0
58	MG	13	1703	1/1	0.49	0.38	-	128,128,128,128	0
58	MG	1G	1662	1/1	0.74	0.14	-	118,118,118,118	0
58	MG	14	3165	1/1	0.81	0.45	-	102,102,102,102	0
58	MG	1H	3451	1/1	0.94	0.20	-	85,85,85,85	0
58	MG	14	3102	1/1	0.95	0.25	-	92,92,92,92	0
58	MG	1G	1655	1/1	0.91	0.04	-	176,176,176,176	0
58	MG	13	1692	1/1	0.76	0.40	-	99,99,99,99	0
58	MG	14	3038	1/1	0.97	0.35	-	67,67,67,67	0
58	MG	1H	3246	1/1	0.88	0.33	-	87,87,87,87	0
58	MG	13	1635	1/1	0.89	0.36	-	111,111,111,111	0
58	MG	1H	3049	1/1	0.99	0.47	-	82,82,82,82	0
58	MG	1H	3232	1/1	0.88	0.44	-	98,98,98,98	0
58	MG	1H	3421	1/1	0.97	0.04	-	129,129,129,129	0
58	MG	1H	3120	1/1	0.90	0.57	-	107,107,107,107	0
58	MG	1H	3211	1/1	0.84	0.54	-	90,90,90,90	0
58	MG	14	3055	1/1	0.87	0.32	-	77,77,77,77	0
58	MG	13	1707	1/1	0.73	0.43	-	114,114,114,114	0
58	MG	13	1676	1/1	0.91	0.29	-	130,130,130,130	0
58	MG	14	3378	1/1	0.95	0.09	-	83,83,83,83	0
58	MG	1H	3234	1/1	0.89	1.04	-	90,90,90,90	0
58	MG	14	3329	1/1	0.95	1.17	-	91,91,91,91	0
58	MG	14	3133	1/1	0.98	0.39	-	98,98,98,98	0
58	MG	14	3309	1/1	0.87	0.20	-	109,109,109,109	0
58	MG	14	3324	1/1	0.61	0.27	-	104,104,104,104	0
58	MG	1H	3196	1/1	0.79	0.45	-	102,102,102,102	0
58	MG	1H	3289	1/1	0.65	1.03	-	86,86,86,86	0
58	MG	13	1656	1/1	0.92	0.10	-	105,105,105,105	0
58	MG	1H	3178	1/1	0.82	0.53	-	93,93,93,93	0
58	MG	14	3414	1/1	0.97	0.15	-	108,108,108,108	0
58	MG	14	3358	1/1	0.94	0.17	-	107,107,107,107	0
58	MG	1H	3032	1/1	0.55	0.35	-	110,110,110,110	0
58	MG	13	1627	1/1	0.37	0.42	-	105,105,105,105	0
58	MG	14	3041	1/1	0.94	0.39	-	80,80,80,80	0
58	MG	13	1731	1/1	0.98	0.08	-	108,108,108,108	0
58	MG	14	3185	1/1	0.82	0.71	-	113,113,113,113	0
58	MG	1H	3161	1/1	0.85	0.46	-	115,115,115,115	0
58	MG	1H	3094	1/1	0.97	0.35	-	77,77,77,77	0
58	MG	14	3372	1/1	0.90	0.08	-	134,134,134,134	0
58	MG	14	3012	1/1	0.99	0.38	-	67,67,67,67	0
58	MG	1H	3464	1/1	0.97	0.10	-	95,95,95,95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1644	1/1	0.74	0.38	-	120,120,120,120	0
58	MG	14	3062	1/1	0.60	0.56	-	129,129,129,129	0
58	MG	14	3209	1/1	0.96	0.31	-	90,90,90,90	0
58	MG	1G	1623	1/1	0.88	0.65	-	100,100,100,100	0
58	MG	1H	3052	1/1	0.97	0.27	-	69,69,69,69	0
58	MG	1G	1642	1/1	0.93	0.43	-	114,114,114,114	0
58	MG	13	1705	1/1	0.17	0.29	-	150,150,150,150	0
58	MG	14	3114	1/1	0.96	0.56	-	66,66,66,66	0
58	MG	1G	1643	1/1	0.63	0.57	-	102,102,102,102	0
58	MG	14	3389	1/1	0.98	0.11	-	92,92,92,92	0
58	MG	1G	1646	1/1	0.79	0.18	-	126,126,126,126	0
58	MG	1H	3199	1/1	0.59	0.69	-	87,87,87,87	0
58	MG	1H	3329	1/1	0.94	0.10	-	105,105,105,105	0
58	MG	14	3085	1/1	0.81	0.44	-	85,85,85,85	0
58	MG	1H	3429	1/1	0.94	0.13	-	82,82,82,82	0
58	MG	14	3261	1/1	0.69	0.43	-	101,101,101,101	0
58	MG	1G	1602	1/1	0.64	0.75	-	133,133,133,133	0
58	MG	1G	1656	1/1	0.98	0.57	-	102,102,102,102	0
58	MG	1H	3219	1/1	0.96	0.16	-	120,120,120,120	0
58	MG	1H	3379	1/1	0.98	0.17	-	103,103,103,103	0
58	MG	14	3094	1/1	0.94	0.55	-	82,82,82,82	0
58	MG	14	3146	1/1	0.78	0.36	-	77,77,77,77	0
58	MG	1H	3004	1/1	0.97	0.26	-	60,60,60,60	0
58	MG	13	1619	1/1	0.92	0.26	-	81,81,81,81	0
58	MG	1H	3144	1/1	0.70	0.27	-	89,89,89,89	0
58	MG	1H	3299	1/1	0.86	0.31	-	94,94,94,94	0
58	MG	1H	3040	1/1	0.96	0.41	-	71,71,71,71	0
58	MG	14	3262	1/1	0.73	0.16	-	109,109,109,109	0
58	MG	13	1696	1/1	0.89	0.43	-	95,95,95,95	0
58	MG	1H	3181	1/1	0.80	0.20	-	92,92,92,92	0
58	MG	1J	205	1/1	0.90	0.26	-	122,122,122,122	0
58	MG	14	3084	1/1	0.85	0.48	-	92,92,92,92	0
58	MG	1J	206	1/1	0.90	0.05	-	130,130,130,130	0
58	MG	1H	3348	1/1	0.87	0.36	-	111,111,111,111	0
58	MG	13	1673	1/1	0.71	0.40	-	106,106,106,106	0
58	MG	13	1708	1/1	0.66	0.82	-	102,102,102,102	0
58	MG	13	1685	1/1	0.95	0.39	-	107,107,107,107	0
58	MG	14	3371	1/1	0.99	0.06	-	95,95,95,95	0
58	MG	13	1603	1/1	0.55	0.40	-	102,102,102,102	0
58	MG	1H	3405	1/1	0.96	0.19	-	75,75,75,75	0
58	MG	1H	3024	1/1	0.85	0.28	-	99,99,99,99	0
58	MG	13	1738	1/1	0.84	0.05	-	106,106,106,106	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3287	1/1	0.76	0.31	-	96,96,96,96	0
58	MG	1H	3275	1/1	0.84	0.12	-	83,83,83,83	0
58	MG	1G	1661	1/1	0.87	0.06	-	169,169,169,169	0
58	MG	13	1733	1/1	0.99	0.03	-	102,102,102,102	0
58	MG	14	3002	1/1	0.99	0.12	-	65,65,65,65	0
58	MG	13	1604	1/1	0.91	0.47	-	90,90,90,90	0
58	MG	14	3381	1/1	0.84	0.12	-	116,116,116,116	0
58	MG	1H	3109	1/1	0.81	0.69	-	102,102,102,102	0
58	MG	13	1723	1/1	0.88	0.14	-	134,134,134,134	0
58	MG	1H	3383	1/1	0.98	0.14	-	75,75,75,75	0
58	MG	13	1661	1/1	0.75	0.49	-	90,90,90,90	0
58	MG	14	3023	1/1	0.71	0.47	-	103,103,103,103	0
58	MG	14	3319	1/1	0.39	0.17	-	128,128,128,128	0
58	MG	14	3418	1/1	0.92	0.09	-	88,88,88,88	0
58	MG	14	3415	1/1	0.92	0.07	-	126,126,126,126	0
58	MG	1H	3256	1/1	0.47	0.38	-	104,104,104,104	0
58	MG	14	3376	1/1	0.98	0.02	-	124,124,124,124	0
58	MG	14	3036	1/1	0.98	0.23	-	70,70,70,70	0
58	MG	14	3134	1/1	0.93	0.39	-	100,100,100,100	0
58	MG	14	3311	1/1	0.81	0.34	-	105,105,105,105	0
58	MG	13	1606	1/1	0.66	1.05	-	119,119,119,119	0
58	MG	14	3034	1/1	0.71	0.28	-	96,96,96,96	0
58	MG	1H	3406	1/1	0.97	0.08	-	82,82,82,82	0
58	MG	45	203	1/1	0.69	0.78	-	104,104,104,104	0
58	MG	13	1670	1/1	0.86	0.26	-	119,119,119,119	0
58	MG	1G	1650	1/1	0.87	0.32	-	98,98,98,98	0
58	MG	14	3302	1/1	0.77	0.83	-	95,95,95,95	0
58	MG	1H	3292	1/1	0.73	0.27	-	82,82,82,82	0
58	MG	1H	3377	1/1	0.98	0.04	-	119,119,119,119	0
58	MG	1H	3183	1/1	0.88	0.93	-	94,94,94,94	0
58	MG	1G	1637	1/1	0.80	0.42	-	101,101,101,101	0
58	MG	14	3199	1/1	0.78	0.61	-	91,91,91,91	0
58	MG	1H	3341	1/1	0.64	0.61	-	110,110,110,110	0
58	MG	1H	3229	1/1	0.90	0.76	-	89,89,89,89	0
58	MG	1H	3444	1/1	0.96	0.13	-	85,85,85,85	0
58	MG	13	1653	1/1	0.75	0.29	-	144,144,144,144	0
58	MG	1G	1639	1/1	0.69	0.81	-	93,93,93,93	0
58	MG	1H	3437	1/1	0.97	0.06	-	85,85,85,85	0
58	MG	14	3123	1/1	0.89	0.21	-	109,109,109,109	0
58	MG	1H	3274	1/1	0.90	0.54	-	105,105,105,105	0
58	MG	1H	3253	1/1	0.92	0.44	-	84,84,84,84	0
58	MG	13	1737	1/1	0.95	0.04	-	116,116,116,116	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3086	1/1	0.89	0.58	-	89,89,89,89	0
58	MG	1H	3051	1/1	0.99	0.32	-	90,90,90,90	0
58	MG	14	3058	1/1	0.81	0.26	-	107,107,107,107	0
58	MG	1H	3415	1/1	0.97	0.17	-	90,90,90,90	0
58	MG	14	3101	1/1	0.86	0.27	-	108,108,108,108	0
58	MG	1H	3026	1/1	0.91	0.40	-	80,80,80,80	0
58	MG	1G	1628	1/1	0.44	0.40	-	120,120,120,120	0
58	MG	1H	3385	1/1	0.94	0.07	-	91,91,91,91	0
58	MG	1H	3102	1/1	0.97	0.71	-	73,73,73,73	0
58	MG	1H	3145	1/1	0.79	0.56	-	117,117,117,117	0
58	MG	14	3120	1/1	0.92	0.25	-	94,94,94,94	0
58	MG	L5	101	1/1	0.87	0.88	-	96,96,96,96	0
58	MG	14	3122	1/1	0.91	0.44	-	95,95,95,95	0
58	MG	1H	3025	1/1	0.99	0.36	-	55,55,55,55	0
58	MG	13	1647	1/1	0.93	0.27	-	108,108,108,108	0
58	MG	1H	3125	1/1	0.97	0.38	-	75,75,75,75	0
58	MG	1H	3313	1/1	0.33	0.68	-	114,114,114,114	0
58	MG	1H	3259	1/1	0.87	0.12	-	106,106,106,106	0
58	MG	1H	3203	1/1	0.94	0.22	-	91,91,91,91	0
58	MG	14	3350	1/1	0.96	0.04	-	116,116,116,116	0
58	MG	1H	3263	1/1	0.62	0.68	-	92,92,92,92	0
58	MG	1H	3450	1/1	0.93	0.17	-	75,75,75,75	0
58	MG	13	1699	1/1	0.67	0.49	-	97,97,97,97	0
58	MG	13	1674	1/1	0.76	0.26	-	121,121,121,121	0
58	MG	1H	3280	1/1	0.84	0.14	-	114,114,114,114	0
58	MG	14	3079	1/1	0.96	0.25	-	87,87,87,87	0
58	MG	13	1716	1/1	0.95	0.10	-	108,108,108,108	0
58	MG	1H	3351	1/1	0.64	0.33	-	122,122,122,122	0
58	MG	1H	3189	1/1	0.82	0.79	-	93,93,93,93	0
58	MG	14	3234	1/1	0.49	0.49	-	85,85,85,85	0
58	MG	1H	3269	1/1	0.68	0.71	-	99,99,99,99	0
58	MG	14	3304	1/1	0.90	0.66	-	87,87,87,87	0
58	MG	1H	3268	1/1	0.95	0.55	-	104,104,104,104	0
58	MG	14	3078	1/1	0.97	0.44	-	82,82,82,82	0
58	MG	16	202	1/1	0.94	0.18	-	102,102,102,102	0
58	MG	14	3388	1/1	0.99	0.22	-	88,88,88,88	0
58	MG	1H	3262	1/1	0.39	0.26	-	100,100,100,100	0
58	MG	14	3217	1/1	0.74	0.74	-	89,89,89,89	0
58	MG	14	3024	1/1	0.63	1.13	-	106,106,106,106	0
58	MG	1H	3035	1/1	0.86	0.64	-	123,123,123,123	0
58	MG	1H	3321	1/1	0.90	0.43	-	84,84,84,84	0
58	MG	13	1684	1/1	0.70	0.26	-	141,141,141,141	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1687	1/1	0.58	1.49	-	100,100,100,100	0
58	MG	1H	3082	1/1	0.99	0.49	-	79,79,79,79	0
58	MG	13	1666	1/1	0.82	0.18	-	99,99,99,99	0
58	MG	14	3169	1/1	0.86	0.42	-	69,69,69,69	0
58	MG	1H	3288	1/1	0.66	0.32	-	99,99,99,99	0
58	MG	1H	3013	1/1	0.99	0.42	-	71,71,71,71	0
58	MG	1H	3207	1/1	0.92	0.46	-	93,93,93,93	0
58	MG	13	1628	1/1	0.74	0.68	-	94,94,94,94	0
58	MG	14	3086	1/1	0.94	0.70	-	95,95,95,95	0
58	MG	14	3201	1/1	0.69	0.49	-	91,91,91,91	0
58	MG	1H	3482	1/1	0.93	0.05	-	119,119,119,119	0
58	MG	14	3402	1/1	0.97	0.14	-	83,83,83,83	0
58	MG	14	3300	1/1	0.91	0.10	-	118,118,118,118	0
58	MG	1H	3393	1/1	0.99	0.08	-	95,95,95,95	0
58	MG	1H	3454	1/1	0.97	0.26	-	96,96,96,96	0
58	MG	13	1668	1/1	0.88	0.22	-	117,117,117,117	0
58	MG	14	3175	1/1	0.79	0.19	-	93,93,93,93	0
58	MG	1H	3300	1/1	0.94	0.86	-	99,99,99,99	0
58	MG	1H	3112	1/1	0.91	0.72	-	101,101,101,101	0
58	MG	14	3144	1/1	0.93	0.17	-	112,112,112,112	0
58	MG	14	3398	1/1	0.98	0.07	-	111,111,111,111	0
58	MG	13	1697	1/1	0.92	0.50	-	98,98,98,98	0
58	MG	14	3221	1/1	0.90	0.67	-	80,80,80,80	0
58	MG	1H	3100	1/1	0.88	0.86	-	82,82,82,82	0
58	MG	1H	3167	1/1	0.91	0.62	-	96,96,96,96	0
58	MG	J8	102	1/1	0.93	0.46	-	77,77,77,77	0
58	MG	11	301	1/1	0.90	0.31	-	73,73,73,73	0
58	MG	14	3225	1/1	0.93	0.46	-	95,95,95,95	0
58	MG	1H	3223	1/1	0.95	0.23	-	96,96,96,96	0
58	MG	14	3098	1/1	0.96	0.34	-	86,86,86,86	0
58	MG	1H	3350	1/1	0.51	0.61	-	113,113,113,113	0
58	MG	13	1626	1/1	0.89	0.34	-	113,113,113,113	0
58	MG	14	3410	1/1	0.97	0.09	-	91,91,91,91	0
58	MG	1H	3195	1/1	0.91	0.74	-	96,96,96,96	0
58	MG	13	1701	1/1	0.91	0.45	-	103,103,103,103	0
58	MG	14	3162	1/1	0.91	0.67	-	90,90,90,90	0
58	MG	1H	3060	1/1	0.96	0.57	-	111,111,111,111	0
58	MG	14	3416	1/1	0.93	0.04	-	124,124,124,124	0
58	MG	1H	3462	1/1	0.97	0.15	-	90,90,90,90	0
58	MG	1G	1611	1/1	0.85	0.33	-	129,129,129,129	0
58	MG	1H	3208	1/1	0.81	0.92	-	99,99,99,99	0
58	MG	14	3032	1/1	0.83	0.18	-	109,109,109,109	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1679	1/1	0.69	0.25	-	122,122,122,122	0
58	MG	14	3310	1/1	0.75	0.38	-	124,124,124,124	0
58	MG	13	1662	1/1	0.86	0.29	-	116,116,116,116	0
58	MG	14	3115	1/1	0.93	0.33	-	88,88,88,88	0
58	MG	1G	1621	1/1	0.60	0.75	-	110,110,110,110	0
58	MG	1H	3295	1/1	0.82	0.53	-	110,110,110,110	0
58	MG	1H	3188	1/1	0.87	0.40	-	84,84,84,84	0
58	MG	14	3397	1/1	0.93	0.09	-	103,103,103,103	0
58	MG	1H	3326	1/1	0.87	0.41	-	97,97,97,97	0
58	MG	1H	3314	1/1	0.90	0.23	-	107,107,107,107	0
58	MG	14	3001	1/1	0.95	0.94	-	97,97,97,97	0
58	MG	1H	3345	1/1	0.85	0.18	-	79,79,79,79	0
58	MG	1H	3395	1/1	0.98	0.17	-	103,103,103,103	0
58	MG	14	3160	1/1	0.82	0.37	-	98,98,98,98	0
58	MG	1H	3177	1/1	0.92	0.67	-	93,93,93,93	0
58	MG	1H	3480	1/1	0.91	0.07	-	114,114,114,114	0
58	MG	1H	3384	1/1	0.99	0.20	-	87,87,87,87	0
58	MG	1H	3247	1/1	0.78	0.43	-	101,101,101,101	0
58	MG	1G	1631	1/1	0.78	0.40	-	97,97,97,97	0
58	MG	1H	3184	1/1	0.92	0.76	-	94,94,94,94	0
58	MG	1H	3316	1/1	0.40	0.38	-	91,91,91,91	0
58	MG	14	3170	1/1	0.94	0.28	-	119,119,119,119	0
58	MG	14	3022	1/1	0.85	0.57	-	101,101,101,101	0
58	MG	1H	3074	1/1	0.90	0.40	-	94,94,94,94	0
58	MG	1H	3349	1/1	0.81	0.17	-	119,119,119,119	0
58	MG	14	3174	1/1	0.62	0.38	-	98,98,98,98	0
58	MG	1H	3200	1/1	0.96	0.29	-	79,79,79,79	0
58	MG	14	3049	1/1	0.98	0.50	-	74,74,74,74	0
58	MG	1G	1665	1/1	0.93	0.33	-	122,122,122,122	0
58	MG	1H	3426	1/1	0.98	0.25	-	109,109,109,109	0
58	MG	1H	3336	1/1	0.65	0.12	-	93,93,93,93	0
58	MG	13	1633	1/1	0.93	0.57	-	88,88,88,88	0
58	MG	1H	3279	1/1	0.83	0.30	-	106,106,106,106	0
58	MG	1H	3334	1/1	0.77	0.29	-	77,77,77,77	0
58	MG	13	1650	1/1	0.66	0.30	-	134,134,134,134	0
58	MG	14	3314	1/1	0.84	1.13	-	99,99,99,99	0
58	MG	1H	3017	1/1	0.91	0.50	-	79,79,79,79	0
58	MG	16	205	1/1	0.83	0.36	-	106,106,106,106	0
58	MG	1H	3141	1/1	0.74	0.93	-	83,83,83,83	0
58	MG	14	3337	1/1	0.90	0.50	-	125,125,125,125	0
58	MG	1H	3469	1/1	0.93	0.24	-	124,124,124,124	0
58	MG	1G	1663	1/1	0.97	0.44	-	133,133,133,133	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3412	1/1	0.96	0.06	-	84,84,84,84	0
58	MG	1G	1632	1/1	0.68	0.40	-	130,130,130,130	0
58	MG	1H	3248	1/1	0.89	1.58	-	93,93,93,93	0
58	MG	1H	3033	1/1	0.15	0.55	-	109,109,109,109	0
58	MG	14	3338	1/1	0.94	0.07	-	114,114,114,114	0
58	MG	14	3198	1/1	0.97	0.16	-	109,109,109,109	0
58	MG	14	3186	1/1	0.88	0.69	-	100,100,100,100	0
58	MG	13	1629	1/1	0.98	0.50	-	79,79,79,79	0
58	MG	14	3117	1/1	0.86	0.67	-	91,91,91,91	0
58	MG	1H	3249	1/1	0.95	0.15	-	83,83,83,83	0
58	MG	14	3132	1/1	0.73	0.69	-	86,86,86,86	0
58	MG	14	3047	1/1	0.97	0.17	-	102,102,102,102	0
58	MG	1H	3427	1/1	0.97	0.03	-	106,106,106,106	0
58	MG	1J	201	1/1	0.85	0.31	-	100,100,100,100	0
58	MG	1H	3062	1/1	0.92	0.44	-	103,103,103,103	0
58	MG	14	3328	1/1	0.79	1.41	-	107,107,107,107	0
58	MG	1H	3410	1/1	0.94	0.08	-	97,97,97,97	0
58	MG	13	1625	1/1	0.48	0.55	-	102,102,102,102	0
58	MG	14	3301	1/1	0.58	0.17	-	115,115,115,115	0
58	MG	1H	3448	1/1	0.98	0.21	-	88,88,88,88	0
58	MG	14	3374	1/1	0.99	0.16	-	107,107,107,107	0
58	MG	14	3113	1/1	0.93	0.49	-	102,102,102,102	0
58	MG	14	3264	1/1	0.87	0.50	-	106,106,106,106	0
58	MG	1H	3391	1/1	0.99	0.19	-	79,79,79,79	0
58	MG	1G	1638	1/1	0.78	0.43	-	102,102,102,102	0
58	MG	1G	1620	1/1	0.93	0.58	-	91,91,91,91	0
58	MG	14	3259	1/1	0.78	0.54	-	111,111,111,111	0
58	MG	13	1734	1/1	0.87	0.08	-	131,131,131,131	0
58	MG	14	3109	1/1	0.75	0.57	-	94,94,94,94	0
58	MG	1H	3105	1/1	0.60	0.90	-	86,86,86,86	0
58	MG	1H	3022	1/1	0.95	0.34	-	69,69,69,69	0
58	MG	14	3105	1/1	0.93	0.84	-	110,110,110,110	0
58	MG	13	1735	1/1	0.82	0.09	-	146,146,146,146	0
58	MG	13	1617	1/1	0.91	0.29	-	97,97,97,97	0
58	MG	13	1637	1/1	0.82	0.44	-	123,123,123,123	0
58	MG	14	3361	1/1	0.98	0.11	-	79,79,79,79	0
58	MG	14	3151	1/1	0.92	0.30	-	109,109,109,109	0
58	MG	1H	3081	1/1	0.97	0.21	-	88,88,88,88	0
58	MG	14	3190	1/1	0.96	0.22	-	91,91,91,91	0
58	MG	1H	3065	1/1	0.97	0.34	-	77,77,77,77	0
58	MG	1H	3138	1/1	0.98	0.17	-	67,67,67,67	0
58	MG	1H	3436	1/1	0.97	0.09	-	96,96,96,96	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3295	1/1	0.57	0.77	-	96,96,96,96	0
58	MG	14	3167	1/1	0.93	0.20	-	105,105,105,105	0
58	MG	14	3179	1/1	0.58	0.45	-	102,102,102,102	0
58	MG	1G	1645	1/1	0.43	0.56	-	122,122,122,122	0
58	MG	1H	3128	1/1	0.69	0.42	-	90,90,90,90	0
58	MG	1G	1675	1/1	0.85	0.11	-	150,150,150,150	0
58	MG	7A	101	1/1	0.77	0.23	-	104,104,104,104	0
58	MG	13	1726	1/1	0.99	0.07	-	91,91,91,91	0
58	MG	1H	3192	1/1	0.78	0.45	-	85,85,85,85	0
58	MG	1H	3134	1/1	0.83	0.23	-	103,103,103,103	0
58	MG	1H	3265	1/1	0.88	1.01	-	100,100,100,100	0
58	MG	14	3280	1/1	0.76	0.61	-	98,98,98,98	0
58	MG	13	1715	1/1	0.99	0.20	-	113,113,113,113	0
58	MG	1H	3460	1/1	0.96	0.18	-	86,86,86,86	0
58	MG	14	3305	1/1	0.98	0.24	-	127,127,127,127	0
58	MG	1H	3009	1/1	0.96	0.27	-	98,98,98,98	0
58	MG	14	3056	1/1	0.98	0.21	-	109,109,109,109	0
58	MG	1G	1604	1/1	0.86	0.28	-	119,119,119,119	0
58	MG	1H	3438	1/1	0.93	0.10	-	110,110,110,110	0
58	MG	1H	3087	1/1	0.99	0.28	-	69,69,69,69	0
58	MG	1H	3146	1/1	0.46	0.46	-	103,103,103,103	0
58	MG	14	3405	1/1	0.90	0.17	-	89,89,89,89	0
58	MG	1H	3059	1/1	0.94	0.12	-	110,110,110,110	0
58	MG	13	1740	1/1	0.90	0.20	-	107,107,107,107	0
58	MG	1H	3162	1/1	0.84	0.39	-	106,106,106,106	0
58	MG	16	209	1/1	0.84	0.14	-	106,106,106,106	0
58	MG	1H	3031	1/1	0.78	0.71	-	115,115,115,115	0
58	MG	1H	3159	1/1	0.90	0.38	-	89,89,89,89	0
58	MG	14	3220	1/1	0.98	0.40	-	97,97,97,97	0
58	MG	1H	3050	1/1	0.99	0.23	-	74,74,74,74	0
58	MG	13	1702	1/1	0.64	0.45	-	114,114,114,114	0
58	MG	1H	3445	1/1	0.93	0.17	-	71,71,71,71	0
58	MG	1H	3245	1/1	0.98	0.21	-	100,100,100,100	0
58	MG	14	3291	1/1	0.85	0.26	-	96,96,96,96	0
58	MG	1G	1630	1/1	0.90	0.42	-	120,120,120,120	0
58	MG	1H	3186	1/1	0.80	0.40	-	96,96,96,96	0
58	MG	1H	3193	1/1	0.94	0.40	-	104,104,104,104	0
58	MG	14	3366	1/1	0.87	0.12	-	114,114,114,114	0
58	MG	1H	3044	1/1	0.97	0.36	-	68,68,68,68	0
58	MG	1H	3110	1/1	0.89	0.35	-	83,83,83,83	0
58	MG	1H	3216	1/1	0.98	0.15	-	65,65,65,65	0
58	MG	14	3409	1/1	0.98	0.32	-	85,85,85,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3189	1/1	0.85	0.46	-	87,87,87,87	0
58	MG	14	3153	1/1	0.92	0.52	-	102,102,102,102	0
58	MG	14	3333	1/1	0.88	0.68	-	102,102,102,102	0
58	MG	1G	1644	1/1	0.66	0.70	-	110,110,110,110	0
58	MG	14	3035	1/1	0.99	0.28	-	89,89,89,89	0
58	MG	1H	3272	1/1	0.72	0.63	-	118,118,118,118	0
58	MG	13	1728	1/1	0.99	0.07	-	105,105,105,105	0
58	MG	14	3315	1/1	0.69	0.49	-	114,114,114,114	0
58	MG	1H	3016	1/1	0.83	0.44	-	105,105,105,105	0
58	MG	1H	3455	1/1	0.98	0.12	-	87,87,87,87	0
58	MG	14	3396	1/1	0.98	0.29	-	96,96,96,96	0
58	MG	1H	3354	1/1	0.87	0.33	-	98,98,98,98	0
58	MG	14	3288	1/1	0.78	0.80	-	120,120,120,120	0
58	MG	1H	3304	1/1	0.76	0.49	-	94,94,94,94	0
58	MG	1H	3483	1/1	0.75	0.11	-	119,119,119,119	0
58	MG	1H	3228	1/1	0.96	0.80	-	74,74,74,74	0
58	MG	14	3180	1/1	0.94	0.34	-	81,81,81,81	0
58	MG	1H	3439	1/1	0.96	0.14	-	72,72,72,72	0
58	MG	14	3083	1/1	0.94	0.28	-	94,94,94,94	0
58	MG	14	3019	1/1	0.84	0.39	-	87,87,87,87	0
58	MG	1H	3369	1/1	0.99	0.16	-	90,90,90,90	0
58	MG	1H	3319	1/1	0.76	0.62	-	102,102,102,102	0
58	MG	1H	3198	1/1	0.84	0.35	-	119,119,119,119	0
58	MG	1H	3010	1/1	0.84	0.21	-	98,98,98,98	0
58	MG	1H	3096	1/1	0.92	0.32	-	76,76,76,76	0
58	MG	I8	101	1/1	0.92	0.43	-	70,70,70,70	0
58	MG	14	3342	1/1	0.88	0.35	-	120,120,120,120	0
58	MG	13	1618	1/1	0.92	0.22	-	108,108,108,108	0
58	MG	1H	3352	1/1	0.96	0.26	-	75,75,75,75	0
58	MG	1H	3311	1/1	0.84	0.18	-	77,77,77,77	0
58	MG	1H	3168	1/1	0.84	0.41	-	82,82,82,82	0
58	MG	14	3069	1/1	0.95	0.32	-	106,106,106,106	0
58	MG	1H	3020	1/1	0.88	0.38	-	84,84,84,84	0
58	MG	1H	3475	1/1	0.98	0.10	-	89,89,89,89	0
58	MG	1H	3342	1/1	0.78	0.47	-	105,105,105,105	0
58	MG	1H	3467	1/1	0.97	0.13	-	115,115,115,115	0
58	MG	1H	3011	1/1	0.82	0.48	-	71,71,71,71	0
58	MG	14	3318	1/1	0.93	0.30	-	102,102,102,102	0
58	MG	14	3196	1/1	0.74	0.29	-	98,98,98,98	0
58	MG	1G	1652	1/1	0.72	0.32	-	110,110,110,110	0
58	MG	1H	3297	1/1	0.69	0.21	-	133,133,133,133	0
58	MG	1H	3131	1/1	0.86	0.32	-	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3477	1/1	0.94	0.05	-	114,114,114,114	0
58	MG	14	3053	1/1	0.98	0.56	-	82,82,82,82	0
58	MG	14	3368	1/1	0.94	0.14	-	87,87,87,87	0
58	MG	1H	3463	1/1	0.96	0.19	-	103,103,103,103	0
58	MG	14	3400	1/1	0.99	0.11	-	113,113,113,113	0
58	MG	1H	3374	1/1	0.92	0.13	-	77,77,77,77	0
58	MG	13	1720	1/1	0.96	0.05	-	126,126,126,126	0
58	MG	1H	3452	1/1	0.97	0.21	-	102,102,102,102	0
58	MG	1G	1633	1/1	0.72	0.25	-	137,137,137,137	0
58	MG	1H	3320	1/1	0.91	0.47	-	107,107,107,107	0
58	MG	1H	3077	1/1	0.79	0.46	-	65,65,65,65	0
58	MG	1H	3485	1/1	0.96	0.15	-	83,83,83,83	0
58	MG	1H	3305	1/1	0.84	0.57	-	96,96,96,96	0
58	MG	1H	3220	1/1	0.97	0.27	-	115,115,115,115	0
58	MG	1H	3063	1/1	0.93	0.44	-	57,57,57,57	0
58	MG	13	1722	1/1	0.98	0.06	-	99,99,99,99	0
58	MG	1H	3238	1/1	0.93	0.24	-	83,83,83,83	0
58	MG	14	3126	1/1	0.98	0.24	-	95,95,95,95	0
58	MG	1H	3281	1/1	0.98	0.68	-	108,108,108,108	0
58	MG	1G	1658	1/1	0.87	0.75	-	99,99,99,99	0
58	MG	13	1602	1/1	0.97	0.35	-	98,98,98,98	0
58	MG	1G	1612	1/1	0.86	0.36	-	105,105,105,105	0
58	MG	14	3025	1/1	0.91	0.79	-	87,87,87,87	0
58	MG	1H	3266	1/1	0.96	0.29	-	65,65,65,65	0
58	MG	14	3006	1/1	0.94	0.29	-	72,72,72,72	0
58	MG	1H	3472	1/1	0.88	0.08	-	108,108,108,108	0
58	MG	1H	3206	1/1	0.71	0.58	-	100,100,100,100	0
58	MG	14	3298	1/1	0.90	0.29	-	104,104,104,104	0
58	MG	14	3322	1/1	0.81	0.96	-	117,117,117,117	0
58	MG	1H	3205	1/1	0.87	0.65	-	114,114,114,114	0
58	MG	14	3135	1/1	0.97	0.28	-	115,115,115,115	0
58	MG	14	3004	1/1	0.88	0.70	-	76,76,76,76	0
58	MG	14	3326	1/1	0.96	0.65	-	104,104,104,104	0
58	MG	1H	3277	1/1	0.91	0.18	-	122,122,122,122	0
58	MG	1H	3324	1/1	0.84	0.11	-	97,97,97,97	0
58	MG	14	3046	1/1	0.97	0.26	-	86,86,86,86	0
58	MG	14	3110	1/1	0.66	0.32	-	94,94,94,94	0
58	MG	13	1621	1/1	0.69	0.33	-	99,99,99,99	0
58	MG	14	3033	1/1	0.95	0.79	-	95,95,95,95	0
58	MG	14	3156	1/1	0.91	0.70	-	88,88,88,88	0
58	MG	1H	3172	1/1	0.95	0.30	-	89,89,89,89	0
58	MG	1H	3119	1/1	0.87	0.59	-	81,81,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3479	1/1	0.77	0.20	-	91,91,91,91	0
58	MG	13	1624	1/1	0.98	0.55	-	118,118,118,118	0
58	MG	14	3067	1/1	0.93	0.27	-	100,100,100,100	0
58	MG	1H	3036	1/1	0.54	0.15	-	118,118,118,118	0
58	MG	14	3238	1/1	0.92	0.70	-	83,83,83,83	0
58	MG	1H	3344	1/1	0.78	0.31	-	81,81,81,81	0
58	MG	14	3013	1/1	0.87	0.20	-	98,98,98,98	0
58	MG	14	3030	1/1	0.65	0.34	-	104,104,104,104	0
58	MG	1H	3169	1/1	0.87	0.21	-	95,95,95,95	0
58	MG	1H	3209	1/1	0.76	0.53	-	99,99,99,99	0
58	MG	1H	3270	1/1	0.78	0.25	-	87,87,87,87	0
58	MG	14	3188	1/1	0.94	1.22	-	93,93,93,93	0
58	MG	14	3136	1/1	0.96	0.42	-	93,93,93,93	0
58	MG	14	3051	1/1	0.89	0.37	-	158,158,158,158	0
58	MG	1H	3449	1/1	0.99	0.13	-	89,89,89,89	0
58	MG	13	1739	1/1	0.85	0.17	-	113,113,113,113	0
58	MG	1G	1653	1/1	0.80	0.14	-	118,118,118,118	0
58	MG	13	1608	1/1	0.98	0.19	-	90,90,90,90	0
58	MG	14	3281	1/1	0.93	0.91	-	103,103,103,103	0
58	MG	2L	102	1/1	0.88	1.72	-	95,95,95,95	0
60	ZN	G8	201	1/1	0.96	0.05	-	171,171,171,171	0
58	MG	21	301	1/1	0.98	0.43	-	69,69,69,69	0
58	MG	14	3312	1/1	0.91	0.39	-	97,97,97,97	0
58	MG	14	3293	1/1	0.92	0.69	-	109,109,109,109	0
58	MG	14	3417	1/1	0.56	0.08	-	140,140,140,140	0
58	MG	14	3392	1/1	0.99	0.05	-	89,89,89,89	0
58	MG	14	3382	1/1	0.88	0.14	-	112,112,112,112	0
58	MG	1H	3118	1/1	0.95	0.60	-	104,104,104,104	0
58	MG	1H	3137	1/1	0.92	0.35	-	93,93,93,93	0
58	MG	13	1719	1/1	0.97	0.14	-	94,94,94,94	0
58	MG	14	3057	1/1	0.93	0.22	-	119,119,119,119	0
58	MG	14	3260	1/1	0.66	1.01	-	115,115,115,115	0
58	MG	1H	3474	1/1	0.97	0.05	-	110,110,110,110	0
58	MG	1H	3335	1/1	0.93	0.16	-	100,100,100,100	0
58	MG	14	3020	1/1	0.87	0.31	-	93,93,93,93	0
58	MG	14	3176	1/1	0.92	0.37	-	96,96,96,96	0
58	MG	1H	3154	1/1	0.80	0.49	-	106,106,106,106	0
58	MG	16	211	1/1	0.97	0.12	-	92,92,92,92	0
58	MG	1H	3029	1/1	0.80	0.42	-	92,92,92,92	0
58	MG	1H	3005	1/1	0.96	0.33	-	79,79,79,79	0
58	MG	2L	103	1/1	0.95	0.51	-	128,128,128,128	0
58	MG	1H	3163	1/1	0.70	0.49	-	84,84,84,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3327	1/1	0.90	0.46	-	83,83,83,83	0
58	MG	14	3275	1/1	0.76	0.47	-	90,90,90,90	0
58	MG	14	3007	1/1	0.91	0.50	-	81,81,81,81	0
58	MG	14	3365	1/1	0.97	0.09	-	96,96,96,96	0
58	MG	1H	3466	1/1	0.99	0.07	-	94,94,94,94	0
58	MG	1H	3170	1/1	0.89	0.07	-	92,92,92,92	0
58	MG	14	3031	1/1	0.77	0.47	-	89,89,89,89	0
58	MG	1H	3291	1/1	0.93	0.64	-	116,116,116,116	0
58	MG	14	3104	1/1	0.94	0.38	-	78,78,78,78	0
58	MG	14	3143	1/1	0.81	0.41	-	110,110,110,110	0
58	MG	14	3222	1/1	0.96	0.82	-	95,95,95,95	0
58	MG	1H	3210	1/1	0.97	0.47	-	101,101,101,101	0
58	MG	1H	3278	1/1	0.87	0.42	-	90,90,90,90	0
58	MG	1H	3012	1/1	0.81	0.40	-	93,93,93,93	0
58	MG	13	1704	1/1	0.79	0.08	-	134,134,134,134	0
58	MG	1H	3465	1/1	0.91	0.07	-	112,112,112,112	0
58	MG	1H	3346	1/1	0.81	0.33	-	113,113,113,113	0
58	MG	1G	1608	1/1	0.96	0.20	-	119,119,119,119	0
58	MG	1G	1647	1/1	0.68	0.27	-	101,101,101,101	0
58	MG	13	1710	1/1	0.79	0.33	-	118,118,118,118	0
58	MG	1H	3419	1/1	0.97	0.09	-	76,76,76,76	0
58	MG	1H	3306	1/1	0.93	0.42	-	77,77,77,77	0
58	MG	1H	3414	1/1	0.99	0.21	-	79,79,79,79	0
58	MG	14	3386	1/1	0.96	0.13	-	83,83,83,83	0
58	MG	1H	3107	1/1	0.97	0.35	-	95,95,95,95	0
58	MG	14	3296	1/1	0.58	0.32	-	110,110,110,110	0
58	MG	14	3244	1/1	0.93	0.12	-	79,79,79,79	0
58	MG	14	3149	1/1	0.76	0.58	-	94,94,94,94	0
58	MG	1H	3271	1/1	0.93	0.58	-	87,87,87,87	0
58	MG	1H	3481	1/1	0.89	0.15	-	133,133,133,133	0
58	MG	14	3240	1/1	0.78	0.21	-	111,111,111,111	0
58	MG	14	3028	1/1	0.39	0.40	-	124,124,124,124	0
58	MG	14	3164	1/1	0.93	0.31	-	93,93,93,93	0
58	MG	1H	3476	1/1	0.97	0.03	-	122,122,122,122	0
58	MG	14	3100	1/1	0.99	0.10	-	107,107,107,107	0
58	MG	13	1612	1/1	0.83	0.35	-	108,108,108,108	0
58	MG	5E	201	1/1	0.24	0.82	-	107,107,107,107	0
58	MG	1H	3093	1/1	0.85	0.87	-	88,88,88,88	0
58	MG	14	3210	1/1	0.98	0.13	-	113,113,113,113	0
58	MG	1H	3434	1/1	0.96	0.13	-	82,82,82,82	0
58	MG	14	3159	1/1	0.80	0.43	-	81,81,81,81	0
58	MG	1H	3325	1/1	0.87	0.23	-	100,100,100,100	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1615	1/1	0.98	0.20	-	90,90,90,90	0
58	MG	1G	1614	1/1	0.85	0.26	-	127,127,127,127	0
58	MG	1H	3046	1/1	0.99	0.29	-	61,61,61,61	0
58	MG	14	3356	1/1	0.98	0.18	-	85,85,85,85	0
58	MG	1H	3233	1/1	0.92	0.19	-	93,93,93,93	0
58	MG	13	1691	1/1	0.98	0.80	-	94,94,94,94	0
58	MG	1G	1674	1/1	0.98	0.06	-	124,124,124,124	0
58	MG	1H	3338	1/1	0.65	0.21	-	112,112,112,112	0
58	MG	1H	3363	1/1	0.95	0.21	-	81,81,81,81	0
58	MG	1H	3347	1/1	0.57	0.17	-	102,102,102,102	0
58	MG	14	3330	1/1	0.81	0.67	-	104,104,104,104	0
58	MG	14	3360	1/1	0.99	0.07	-	78,78,78,78	0
58	MG	14	3292	1/1	0.85	0.98	-	83,83,83,83	0
58	MG	16	208	1/1	0.69	0.42	-	111,111,111,111	0
58	MG	14	3029	1/1	0.85	0.96	-	90,90,90,90	0
58	MG	1H	3322	1/1	0.60	0.30	-	121,121,121,121	0
58	MG	1H	3152	1/1	0.92	0.59	-	108,108,108,108	0
58	MG	1H	3231	1/1	0.97	0.69	-	85,85,85,85	0
58	MG	1H	3315	1/1	0.85	0.22	-	99,99,99,99	0
58	MG	13	1636	1/1	0.93	0.10	-	123,123,123,123	0
58	MG	1H	3409	1/1	0.94	0.12	-	85,85,85,85	0
58	MG	13	1678	1/1	0.58	0.19	-	121,121,121,121	0
58	MG	14	3268	1/1	0.97	0.30	-	84,84,84,84	0
58	MG	1H	3240	1/1	0.89	0.49	-	96,96,96,96	0
58	MG	14	3277	1/1	0.62	0.50	-	111,111,111,111	0
58	MG	1H	3258	1/1	0.93	0.33	-	99,99,99,99	0
58	MG	13	1675	1/1	0.97	0.29	-	149,149,149,149	0
58	MG	13	1632	1/1	0.98	0.21	-	83,83,83,83	0
58	MG	14	3263	1/1	0.50	0.49	-	102,102,102,102	0
58	MG	1H	3116	1/1	0.91	0.39	-	88,88,88,88	0
58	MG	13	1698	1/1	0.82	0.46	-	96,96,96,96	0
58	MG	13	1613	1/1	0.98	0.09	-	109,109,109,109	0
58	MG	13	1605	1/1	0.96	0.20	-	134,134,134,134	0
58	MG	13	1688	1/1	0.62	0.51	-	96,96,96,96	0
58	MG	13	1690	1/1	0.84	0.69	-	113,113,113,113	0
58	MG	1H	3147	1/1	0.86	0.75	-	93,93,93,93	0
58	MG	1G	1635	1/1	0.68	0.81	-	111,111,111,111	0
58	MG	1H	3156	1/1	0.89	0.05	-	121,121,121,121	0
58	MG	13	1622	1/1	0.97	0.30	-	99,99,99,99	0
58	MG	1H	3310	1/1	0.93	0.53	-	95,95,95,95	0
58	MG	13	1736	1/1	0.98	0.09	-	126,126,126,126	0
58	MG	13	1729	1/1	0.97	0.13	-	96,96,96,96	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1712	1/1	0.99	0.14	-	98,98,98,98	0
58	MG	1H	3303	1/1	0.72	0.24	-	102,102,102,102	0
58	MG	1H	3307	1/1	0.91	0.56	-	97,97,97,97	0
58	MG	13	1645	1/1	0.92	0.38	-	113,113,113,113	0
58	MG	1H	3418	1/1	0.97	0.10	-	86,86,86,86	0
58	MG	16	210	1/1	0.97	0.09	-	87,87,87,87	0
58	MG	14	3274	1/1	0.87	0.14	-	97,97,97,97	0
58	MG	1H	3312	1/1	0.86	0.38	-	103,103,103,103	0
58	MG	14	3276	1/1	0.85	0.10	-	130,130,130,130	0
58	MG	1G	1622	1/1	0.97	0.46	-	103,103,103,103	0
58	MG	14	3401	1/1	0.98	0.10	-	127,127,127,127	0
58	MG	14	3171	1/1	0.62	0.95	-	91,91,91,91	0
58	MG	1H	3201	1/1	0.96	0.73	-	97,97,97,97	0
58	MG	14	3227	1/1	0.49	1.19	-	104,104,104,104	0
58	MG	1H	3204	1/1	0.91	0.25	-	87,87,87,87	0
58	MG	1H	3355	1/1	0.91	0.54	-	88,88,88,88	0
58	MG	1H	3213	1/1	0.89	0.17	-	81,81,81,81	0
58	MG	14	3223	1/1	0.91	0.19	-	116,116,116,116	0
58	MG	14	3147	1/1	0.94	0.34	-	110,110,110,110	0
58	MG	1H	3459	1/1	0.94	0.25	-	102,102,102,102	0
58	MG	1H	3182	1/1	0.96	0.52	-	91,91,91,91	0
58	MG	13	1695	1/1	0.89	0.29	-	122,122,122,122	0
58	MG	1J	203	1/1	0.95	0.33	-	124,124,124,124	0
58	MG	14	3080	1/1	0.86	0.41	-	105,105,105,105	0
58	MG	14	3370	1/1	0.98	0.04	-	94,94,94,94	0
58	MG	1H	3039	1/1	0.81	0.53	-	100,100,100,100	0
58	MG	1G	1603	1/1	0.95	0.56	-	132,132,132,132	0
58	MG	1H	3411	1/1	0.93	0.16	-	94,94,94,94	0
58	MG	1H	3343	1/1	0.75	0.12	-	137,137,137,137	0
58	MG	1H	3413	1/1	0.98	0.11	-	90,90,90,90	0
58	MG	13	1693	1/1	0.88	0.54	-	108,108,108,108	0
58	MG	78	201	1/1	0.93	0.26	-	92,92,92,92	0
58	MG	14	3183	1/1	0.66	0.34	-	89,89,89,89	0
58	MG	14	3320	1/1	0.86	0.21	-	119,119,119,119	0
58	MG	1H	3066	1/1	0.90	0.53	-	86,86,86,86	0
58	MG	1H	3353	1/1	0.93	0.52	-	96,96,96,96	0
58	MG	1H	3149	1/1	0.91	0.42	-	102,102,102,102	0
58	MG	13	1646	1/1	0.96	0.24	-	129,129,129,129	0
58	MG	14	3068	1/1	0.89	0.78	-	108,108,108,108	0
58	MG	1H	3129	1/1	0.88	0.60	-	85,85,85,85	0
58	MG	1H	3038	1/1	0.90	0.23	-	102,102,102,102	0
58	MG	14	3075	1/1	0.98	0.97	-	96,96,96,96	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3399	1/1	0.98	0.03	-	116,116,116,116	0
58	MG	14	3390	1/1	0.95	0.08	-	114,114,114,114	0
58	MG	1H	3317	1/1	0.50	0.44	-	106,106,106,106	0
58	MG	1H	3332	1/1	0.66	0.81	-	93,93,93,93	0
58	MG	1H	3339	1/1	0.89	0.38	-	104,104,104,104	0
58	MG	1H	3392	1/1	0.96	0.17	-	81,81,81,81	0
58	MG	14	3253	1/1	0.87	0.27	-	90,90,90,90	0
58	MG	14	3148	1/1	0.85	0.40	-	94,94,94,94	0
58	MG	14	3178	1/1	0.87	0.25	-	94,94,94,94	0
58	MG	1H	3422	1/1	0.99	0.15	-	102,102,102,102	0
58	MG	1H	3361	1/1	0.97	0.18	-	72,72,72,72	0
58	MG	14	3352	1/1	0.98	0.05	-	84,84,84,84	0
58	MG	14	3124	1/1	0.96	0.47	-	90,90,90,90	0
58	MG	13	1709	1/1	0.80	0.37	-	112,112,112,112	0
58	MG	14	3103	1/1	0.98	0.32	-	81,81,81,81	0
58	MG	14	3286	1/1	0.75	0.63	-	117,117,117,117	0
58	MG	14	3249	1/1	0.96	0.06	-	102,102,102,102	0
58	MG	1H	3027	1/1	0.89	0.17	-	95,95,95,95	0
58	MG	1H	3095	1/1	0.69	0.87	-	95,95,95,95	0
58	MG	13	1680	1/1	0.52	0.59	-	125,125,125,125	0
58	MG	14	3192	1/1	0.69	0.45	-	104,104,104,104	0
58	MG	1H	3089	1/1	0.91	0.33	-	83,83,83,83	0
58	MG	1H	3404	1/1	0.99	0.06	-	84,84,84,84	0
58	MG	1H	3260	1/1	0.93	1.54	-	95,95,95,95	0
58	MG	14	3228	1/1	0.93	0.29	-	96,96,96,96	0
58	MG	14	3313	1/1	0.80	0.35	-	107,107,107,107	0
58	MG	14	3331	1/1	0.78	0.52	-	108,108,108,108	0
58	MG	14	3241	1/1	0.95	0.48	-	115,115,115,115	0
58	MG	1G	1610	1/1	0.97	0.31	-	118,118,118,118	0
58	MG	14	3090	1/1	0.84	0.24	-	83,83,83,83	0
58	MG	1H	3360	1/1	0.99	0.16	-	86,86,86,86	0
58	MG	14	3247	1/1	0.85	0.90	-	104,104,104,104	0
58	MG	1H	3293	1/1	0.95	0.29	-	94,94,94,94	0
58	MG	14	3336	1/1	0.88	0.31	-	120,120,120,120	0
58	MG	1H	3019	1/1	0.98	0.56	-	65,65,65,65	0
58	MG	14	3229	1/1	0.90	0.46	-	93,93,93,93	0
58	MG	14	3344	1/1	0.99	0.08	-	91,91,91,91	0
58	MG	13	1724	1/1	0.98	0.11	-	99,99,99,99	0
58	MG	1H	3037	1/1	0.84	0.25	-	87,87,87,87	0
58	MG	13	1689	1/1	0.52	0.24	-	182,182,182,182	0
58	MG	13	1607	1/1	0.97	0.23	-	101,101,101,101	0
58	MG	14	3204	1/1	0.95	0.25	-	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3015	1/1	0.91	0.66	-	82,82,82,82	0
58	MG	14	3194	1/1	0.73	0.30	-	93,93,93,93	0
58	MG	14	3235	1/1	0.69	0.36	-	102,102,102,102	0
58	MG	13	1634	1/1	0.65	0.52	-	104,104,104,104	0
58	MG	14	3197	1/1	0.86	0.51	-	124,124,124,124	0
58	MG	1G	1629	1/1	0.95	0.34	-	121,121,121,121	0
58	MG	14	3270	1/1	0.80	0.50	-	97,97,97,97	0
58	MG	14	3137	1/1	0.84	0.27	-	119,119,119,119	0
58	MG	14	3413	1/1	0.93	0.04	-	92,92,92,92	0
58	MG	1H	3003	1/1	0.98	0.59	-	72,72,72,72	0
58	MG	14	3207	1/1	0.88	0.15	-	107,107,107,107	0
58	MG	14	3278	1/1	0.77	0.45	-	86,86,86,86	0
58	MG	14	3375	1/1	0.91	0.11	-	117,117,117,117	0
58	MG	1H	3358	1/1	0.99	0.12	-	70,70,70,70	0
58	MG	14	3150	1/1	0.51	0.86	-	102,102,102,102	0
58	MG	1H	3285	1/1	0.53	0.23	-	115,115,115,115	0
58	MG	13	1683	1/1	0.88	0.77	-	119,119,119,119	0
58	MG	14	3128	1/1	0.97	0.59	-	80,80,80,80	0
58	MG	14	3325	1/1	0.79	0.53	-	110,110,110,110	0
58	MG	1H	3132	1/1	0.98	0.52	-	87,87,87,87	0
58	MG	14	3026	1/1	0.56	0.36	-	115,115,115,115	0
58	MG	1H	3224	1/1	0.98	0.55	-	76,76,76,76	0
58	MG	1H	3373	1/1	0.98	0.15	-	86,86,86,86	0
58	MG	14	3087	1/1	0.96	0.42	-	68,68,68,68	0
58	MG	1H	3157	1/1	0.91	0.94	-	88,88,88,88	0
58	MG	1H	3337	1/1	0.63	0.52	-	140,140,140,140	0
58	MG	13	1681	1/1	0.90	0.49	-	124,124,124,124	0
58	MG	14	3339	1/1	0.81	0.64	-	120,120,120,120	0
58	MG	14	3141	1/1	0.99	0.29	-	76,76,76,76	0
58	MG	14	3042	1/1	0.99	0.26	-	74,74,74,74	0
58	MG	14	3406	1/1	0.96	0.06	-	121,121,121,121	0
58	MG	1H	3276	1/1	0.59	0.28	-	91,91,91,91	0
58	MG	1H	3302	1/1	0.85	0.42	-	89,89,89,89	0
58	MG	1H	3440	1/1	0.99	0.12	-	70,70,70,70	0
58	MG	14	3283	1/1	0.88	0.67	-	98,98,98,98	0
58	MG	1H	3217	1/1	0.83	0.22	-	81,81,81,81	0
58	MG	14	3403	1/1	0.97	0.18	-	114,114,114,114	0
58	MG	1H	3073	1/1	0.91	0.60	-	84,84,84,84	0
58	MG	1H	3471	1/1	0.91	0.04	-	128,128,128,128	0
58	MG	14	3063	1/1	0.97	0.42	-	79,79,79,79	0
58	MG	14	3266	1/1	0.82	0.47	-	99,99,99,99	0
58	MG	14	3163	1/1	0.85	0.57	-	104,104,104,104	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1660	1/1	0.73	0.92	-	111,111,111,111	0
58	MG	1H	3264	1/1	0.42	0.23	-	122,122,122,122	0
58	MG	1H	3212	1/1	0.72	0.40	-	93,93,93,93	0
58	MG	13	1654	1/1	0.98	0.21	-	111,111,111,111	0
58	MG	1H	3366	1/1	0.99	0.10	-	73,73,73,73	0
58	MG	1H	3432	1/1	0.93	0.12	-	111,111,111,111	0
58	MG	14	3267	1/1	0.62	0.59	-	104,104,104,104	0
58	MG	16	207	1/1	0.68	0.28	-	92,92,92,92	0
58	MG	1H	3447	1/1	0.98	0.11	-	115,115,115,115	0
58	MG	14	3383	1/1	0.98	0.11	-	137,137,137,137	0
58	MG	1G	1654	1/1	0.94	0.25	-	110,110,110,110	0
58	MG	1H	3155	1/1	0.36	0.21	-	86,86,86,86	0
58	MG	14	3248	1/1	0.83	0.52	-	89,89,89,89	0
58	MG	1H	3043	1/1	0.93	0.31	-	75,75,75,75	0
58	MG	1H	3396	1/1	0.93	0.06	-	99,99,99,99	0
58	MG	1H	3108	1/1	0.83	0.74	-	92,92,92,92	0
58	MG	13	1609	1/1	0.91	0.24	-	99,99,99,99	0
58	MG	1H	3160	1/1	0.94	0.40	-	88,88,88,88	0
58	MG	1G	1624	1/1	0.96	0.58	-	92,92,92,92	0
58	MG	13	1677	1/1	0.90	0.53	-	113,113,113,113	0
58	MG	13	1641	1/1	0.80	0.14	-	112,112,112,112	0
58	MG	14	3177	1/1	0.88	0.53	-	87,87,87,87	0
58	MG	14	3379	1/1	0.96	0.04	-	110,110,110,110	0
58	MG	1H	3301	1/1	0.92	0.54	-	99,99,99,99	0
58	MG	1G	1648	1/1	0.75	0.41	-	128,128,128,128	0
58	MG	1H	3470	1/1	0.98	0.13	-	85,85,85,85	0
58	MG	13	1706	1/1	0.91	0.24	-	91,91,91,91	0
58	MG	1H	3166	1/1	0.72	0.41	-	95,95,95,95	0
58	MG	1H	3142	1/1	0.82	0.45	-	89,89,89,89	0
58	MG	14	3257	1/1	0.84	0.16	-	143,143,143,143	0
58	MG	1H	3121	1/1	0.91	0.37	-	93,93,93,93	0
58	MG	1G	1636	1/1	0.69	0.35	-	111,111,111,111	0
58	MG	1H	3323	1/1	0.68	0.31	-	122,122,122,122	0
58	MG	1H	3187	1/1	0.65	0.53	-	105,105,105,105	0
58	MG	14	3089	1/1	0.71	1.15	-	104,104,104,104	0
58	MG	1H	3047	1/1	0.96	0.57	-	71,71,71,71	0
58	MG	14	3231	1/1	0.77	0.79	-	107,107,107,107	0
58	MG	1H	3072	1/1	0.99	0.17	-	120,120,120,120	0
58	MG	14	3040	1/1	0.96	0.41	-	72,72,72,72	0
58	MG	1H	3135	1/1	0.97	0.12	-	69,69,69,69	0
58	MG	16	212	1/1	0.96	0.11	-	104,104,104,104	0
58	MG	1J	202	1/1	0.71	0.33	-	110,110,110,110	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1660	1/1	0.79	0.12	-	104,104,104,104	0
58	MG	1H	3273	1/1	0.94	0.19	-	85,85,85,85	0
58	MG	1H	3099	1/1	0.96	0.44	-	74,74,74,74	0
58	MG	1H	3318	1/1	0.88	0.36	-	116,116,116,116	0
58	MG	1G	1605	1/1	0.99	0.37	-	125,125,125,125	0
58	MG	1H	3174	1/1	0.83	0.54	-	99,99,99,99	0
58	MG	P8	101	1/1	0.97	0.12	-	101,101,101,101	0
58	MG	1H	3298	1/1	0.87	0.49	-	95,95,95,95	0
58	MG	14	3161	1/1	0.95	0.54	-	80,80,80,80	0
58	MG	1G	1618	1/1	0.81	0.14	-	131,131,131,131	0
58	MG	14	3284	1/1	0.72	0.67	-	112,112,112,112	0
58	MG	1H	3061	1/1	0.96	0.84	-	79,79,79,79	0
58	MG	1H	3468	1/1	0.83	0.15	-	122,122,122,122	0
58	MG	1H	3084	1/1	0.98	0.59	-	57,57,57,57	0
58	MG	13	1652	1/1	0.85	0.32	-	138,138,138,138	0
58	MG	1H	3176	1/1	0.51	0.29	-	110,110,110,110	0
58	MG	C5	201	1/1	0.68	0.35	-	137,137,137,137	0
58	MG	1G	1659	1/1	0.88	0.31	-	142,142,142,142	0
58	MG	2K	102	1/1	0.38	0.63	-	109,109,109,109	0
58	MG	13	1667	1/1	0.93	0.59	-	91,91,91,91	0
58	MG	1G	1664	1/1	0.80	0.34	-	122,122,122,122	0
58	MG	1H	3331	1/1	0.23	0.23	-	120,120,120,120	0
58	MG	13	1640	1/1	0.95	0.70	-	73,73,73,73	0
58	MG	14	3369	1/1	0.92	0.10	-	105,105,105,105	0
58	MG	1H	3080	1/1	0.98	0.27	-	73,73,73,73	0
58	MG	14	3256	1/1	0.94	0.27	-	110,110,110,110	0
58	MG	1H	3327	1/1	0.70	0.76	-	120,120,120,120	0
58	MG	1H	3431	1/1	0.94	0.10	-	111,111,111,111	0
58	MG	2K	103	1/1	0.62	0.21	-	134,134,134,134	0
58	MG	14	3039	1/1	0.99	0.58	-	86,86,86,86	0
58	MG	14	3018	1/1	0.76	0.39	-	111,111,111,111	0
58	MG	14	3354	1/1	0.99	0.11	-	87,87,87,87	0
58	MG	14	3184	1/1	0.96	0.26	-	92,92,92,92	0
58	MG	1H	3042	1/1	0.95	0.34	-	59,59,59,59	0
58	MG	1H	3328	1/1	0.83	0.46	-	119,119,119,119	0
58	MG	1H	3070	1/1	0.92	0.45	-	100,100,100,100	0
58	MG	14	3003	1/1	0.97	0.34	-	76,76,76,76	0
58	MG	14	3168	1/1	0.84	0.30	-	122,122,122,122	0
58	MG	1H	3458	1/1	0.98	0.13	-	88,88,88,88	0
58	MG	14	3082	1/1	0.82	0.34	-	92,92,92,92	0
58	MG	1H	3371	1/1	0.98	0.06	-	77,77,77,77	0
58	MG	14	3404	1/1	0.73	0.28	-	101,101,101,101	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3191	1/1	0.93	0.36	-	95,95,95,95	0
58	MG	1H	3158	1/1	0.84	0.34	-	105,105,105,105	0
58	MG	32	301	1/1	0.49	0.61	-	128,128,128,128	0
58	MG	1G	1666	1/1	0.71	0.77	-	121,121,121,121	0
58	MG	13	1732	1/1	0.92	0.14	-	127,127,127,127	0
58	MG	29	301	1/1	0.98	0.42	-	69,69,69,69	0
58	MG	14	3303	1/1	0.55	0.54	-	115,115,115,115	0
58	MG	13	1663	1/1	0.90	0.66	-	86,86,86,86	0
58	MG	14	3294	1/1	0.87	0.80	-	100,100,100,100	0
58	MG	1H	3456	1/1	0.99	0.23	-	68,68,68,68	0
58	MG	13	1623	1/1	0.76	0.71	-	88,88,88,88	0
58	MG	14	3412	1/1	0.88	0.12	-	128,128,128,128	0
58	MG	14	3181	1/1	0.91	1.18	-	91,91,91,91	0
58	MG	14	3272	1/1	0.71	0.48	-	96,96,96,96	0
58	MG	1H	3021	1/1	0.96	0.36	-	86,86,86,86	0
58	MG	14	3091	1/1	0.99	0.37	-	92,92,92,92	0

## 6.5 Other polymers

There are no such residues in this entry.