



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:26 am BST

PDB ID : 5EL7  
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 and antibiotic paromomycin  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

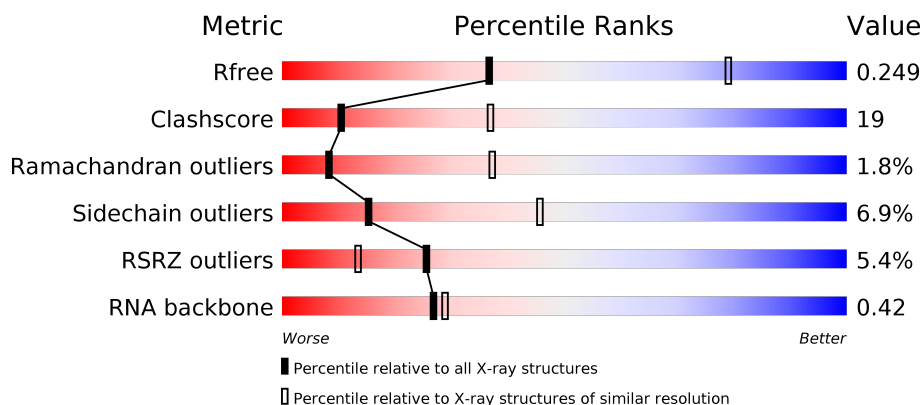
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>6%</div> <div>36% 44% 16%</div> <div>• •</div> </div>
1	1G	1522	<div> <div>37% 45% 15%</div> <div>• •</div> </div>
2	12	256	<div> <div>6%</div> <div>34% 42% 5% 18%</div> <div>•</div> </div>
2	1E	256	<div> <div>6%</div> <div>40% 44% 6% 10%</div> </div>

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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	

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

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Mol	Chain	Length	Quality of chain
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	

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Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	

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Mol	Chain	Length	Quality of chain
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	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
57	MG	11	303	-	-	-	X
57	MG	13	1655	-	-	-	X
57	MG	13	1656	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1665	-	-	-	X
57	MG	13	1667	-	-	-	X
57	MG	14	3016	-	-	-	X
57	MG	14	3075	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3190	-	-	-	X
57	MG	14	3191	-	-	-	X
57	MG	14	3206	-	-	-	X
57	MG	14	3223	-	-	-	X
57	MG	14	3237	-	-	-	X
57	MG	14	3243	-	-	-	X
57	MG	14	3257	-	-	-	X
57	MG	14	3265	-	-	-	X
57	MG	14	3268	-	-	-	X
57	MG	16	206	-	-	-	X
57	MG	1G	1620	-	-	-	X
57	MG	1H	3069	-	-	-	X
57	MG	1H	3103	-	-	-	X
57	MG	1H	3108	-	-	-	X
57	MG	1H	3121	-	-	-	X
57	MG	1H	3136	-	-	-	X
57	MG	1H	3144	-	-	-	X
57	MG	1H	3190	-	-	-	X
57	MG	1H	3220	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3244	-	-	-	X
57	MG	1H	3280	-	-	-	X
57	MG	1H	3284	-	-	-	X
57	MG	1H	3289	-	-	-	X
57	MG	29	301	-	-	-	X
57	MG	2L	103	-	-	-	X
57	MG	P8	101	-	-	-	X
59	SF4	32	301	-	-	X	-



## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32368	14408	5999	10456	1505			

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1690	1058	336	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	139	Total	C	N	O	S	0	0	0
			1115	692	222	195	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNA<sup>Lys</sup>.

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

- Molecule 23 is a RNA chain called E. coli tRNA<sup>fMet</sup>.

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

- Molecule 24 is a RNA chain called tRNA<sup>Lys</sup>.

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

- 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	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	74	Total	C	N	O	S	0	0	0
			573	359	117	97				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

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

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

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

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

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

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

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

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

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

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



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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			875	550	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
44	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			568	352	115	100	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
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	3L	75	Total	C	N	O	P	0	0	0
			1601	717	280	530	74			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

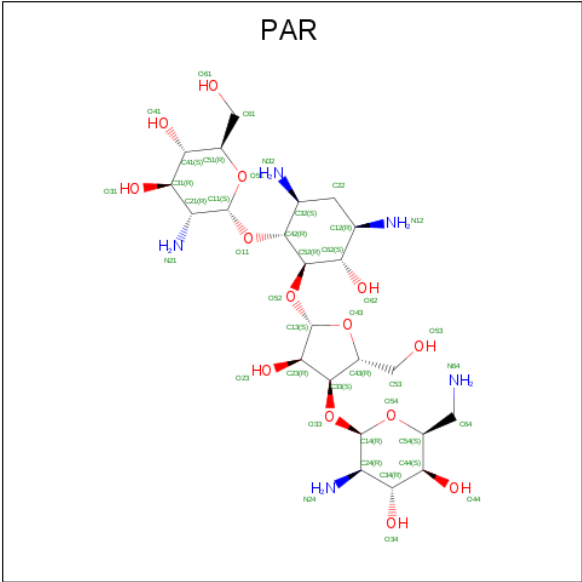
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	3	Total	Mg	0	0
			3	3		
57	P8	1	Total	Mg	0	0
			1	1		
57	85	1	Total	Mg	0	0
			1	1		
57	C5	1	Total	Mg	0	0
			1	1		
57	13	150	Total	Mg	0	0
			150	150		
57	1J	6	Total	Mg	0	0
			6	6		
57	5I	1	Total	Mg	0	0
			1	1		
57	35	2	Total	Mg	0	0
			2	2		
57	BI	1	Total	Mg	0	0
			1	1		
57	16	12	Total	Mg	0	0
			12	12		
57	M5	1	Total	Mg	0	0
			1	1		
57	21	3	Total	Mg	0	0
			3	3		
57	31	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		
57	L8	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		
57	I8	1	Total	Mg	0	0
			1	1		
57	5E	1	Total	Mg	0	0
			1	1		
57	29	4	Total	Mg	0	0
			4	4		

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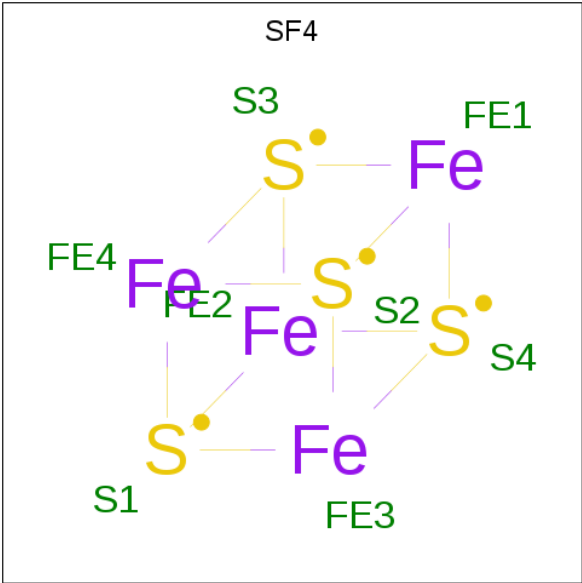
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7A	1	Total 1	Mg 1	0	0
57	2K	3	Total 3	Mg 3	0	0
57	39	2	Total 2	Mg 2	0	0
57	1G	93	Total 93	Mg 93	0	0
57	11	3	Total 3	Mg 3	0	0
57	1H	502	Total 502	Mg 502	0	0
57	E5	1	Total 1	Mg 1	0	0
57	88	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	14	454	Total 454	Mg 454	0	0
57	78	1	Total 1	Mg 1	0	0
57	55	1	Total 1	Mg 1	0	0
57	41	2	Total 2	Mg 2	0	0
57	2L	4	Total 4	Mg 4	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total	C	N	O	0	0
			42	23	5	14		
58	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- 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	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- 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	319	Total 319	O 319	0	0
61	3E	3	Total 3	O 3	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	3I	3	Total 3	O 3	0	0
61	5I	1	Total 1	O 1	0	0
61	6I	2	Total 2	O 2	0	0
61	8I	2	Total 2	O 2	0	0
61	BI	5	Total 5	O 5	0	0
61	1F	1	Total 1	O 1	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	7	Total 7	O 7	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	1158	Total 1158	O 1158	0	0
61	16	26	Total 26	O 26	0	0
61	11	12	Total 12	O 12	0	0
61	21	6	Total 6	O 6	0	0
61	31	9	Total 9	O 9	0	0
61	58	1	Total 1	O 1	0	0
61	78	6	Total 6	O 6	0	0
61	88	2	Total 2	O 2	0	0
61	C8	2	Total 2	O 2	0	0
61	E8	3	Total 3	O 3	0	0
61	F8	2	Total 2	O 2	0	0
61	G8	2	Total 2	O 2	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	3	Total 3	O 3	0	0
61	K8	2	Total 2	O 2	0	0
61	L8	2	Total 2	O 2	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	9	Total 9	O 9	0	0
61	1G	226	Total 226	O 226	0	0
61	32	3	Total 3	O 3	0	0
61	42	1	Total 1	O 1	0	0

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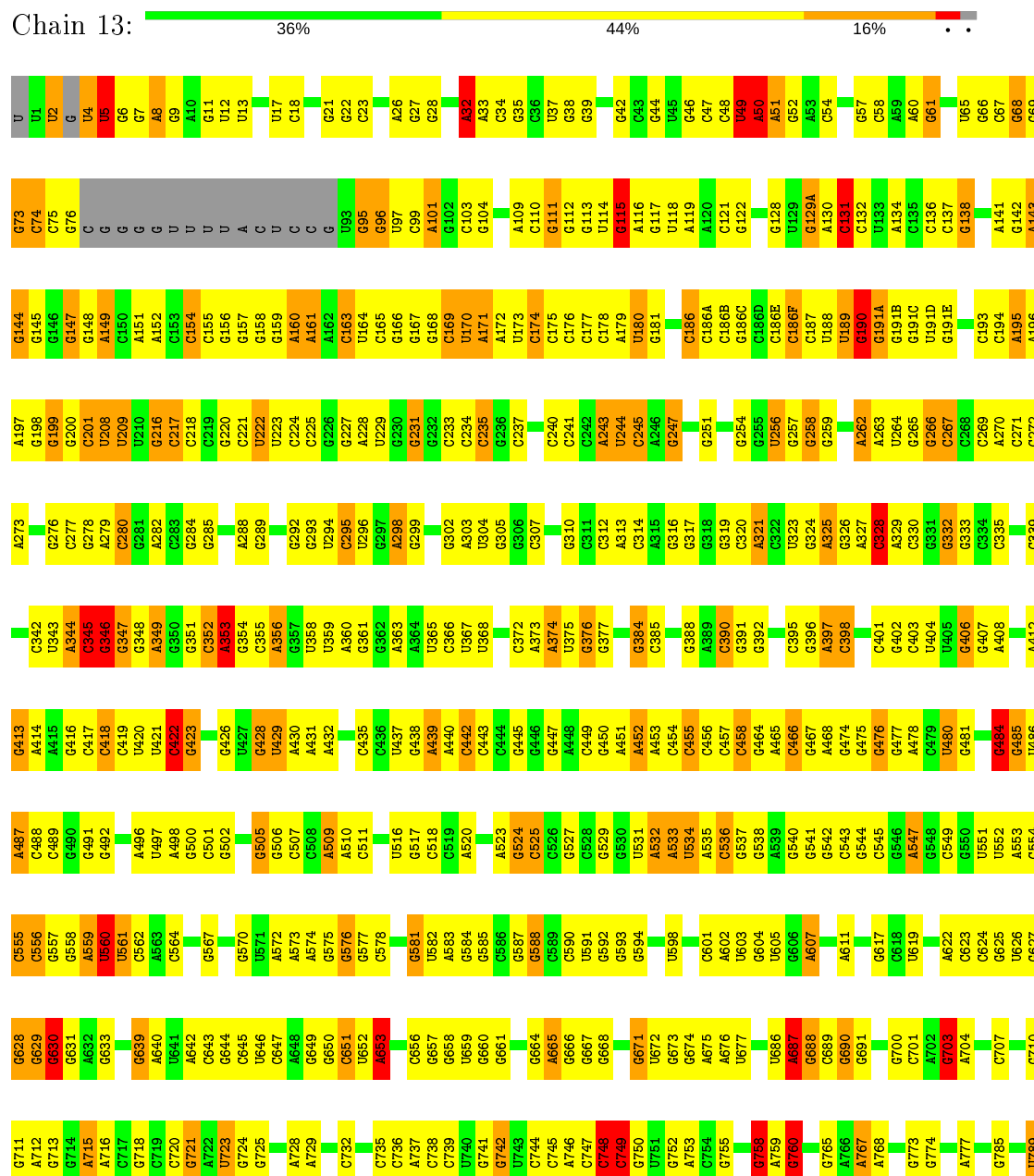
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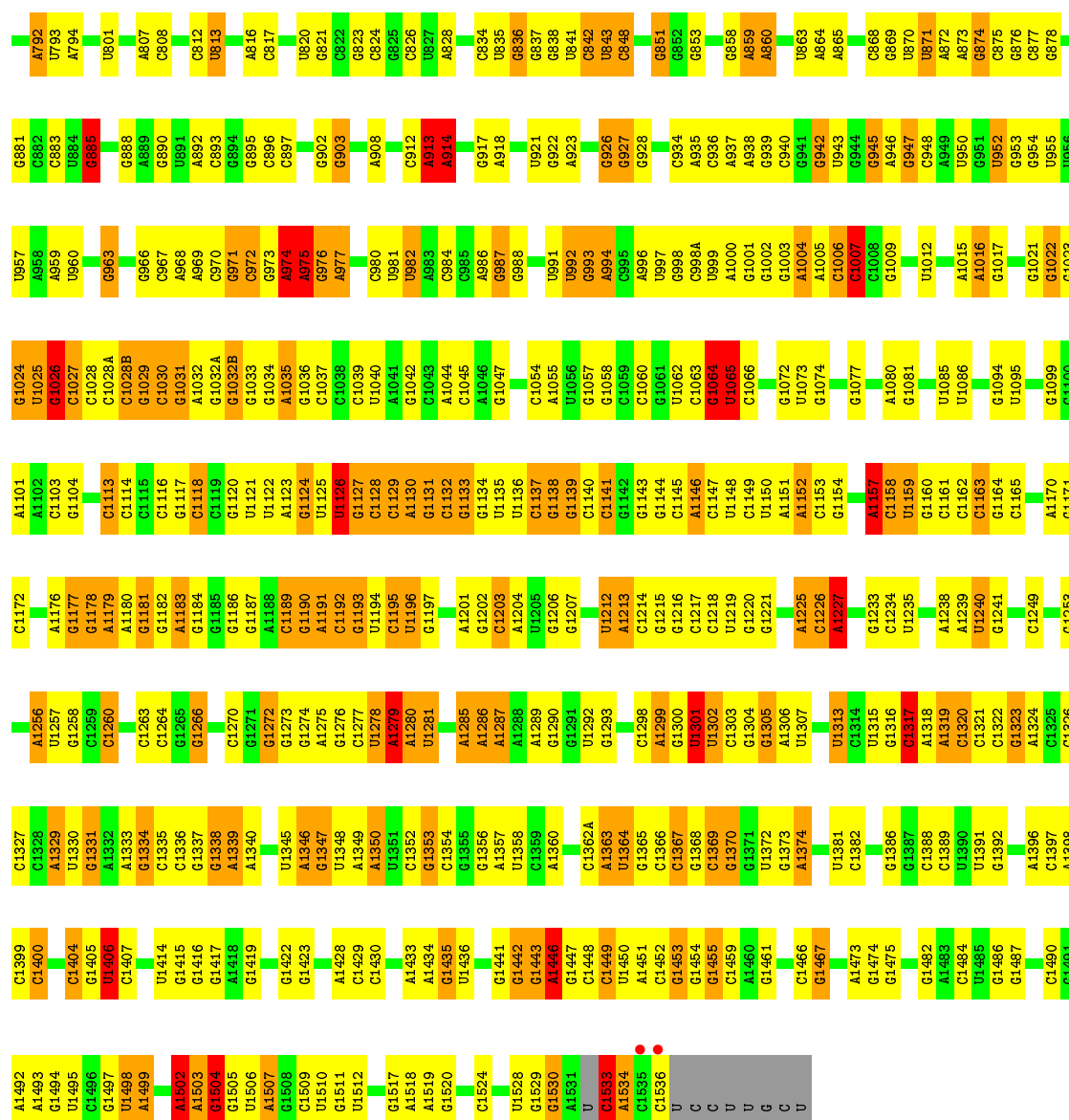
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3A	1	Total 1	O 1	0	0
61	6A	3	Total 3	O 3	0	0
61	8A	1	Total 1	O 1	0	0
61	BA	3	Total 3	O 3	0	0
61	2L	1	Total 1	O 1	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1015	Total 1015	O 1015	0	0
61	1J	18	Total 18	O 18	0	0
61	19	12	Total 12	O 12	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	35	5	Total 5	O 5	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	2	Total 2	O 2	0	0
61	A5	2	Total 2	O 2	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	4	Total 4	O 4	0	0
61	H5	3	Total 3	O 3	0	0
61	L5	2	Total 2	O 2	0	0
61	M5	10	Total 10	O 10	0	0

### 3 Residue-property plots

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

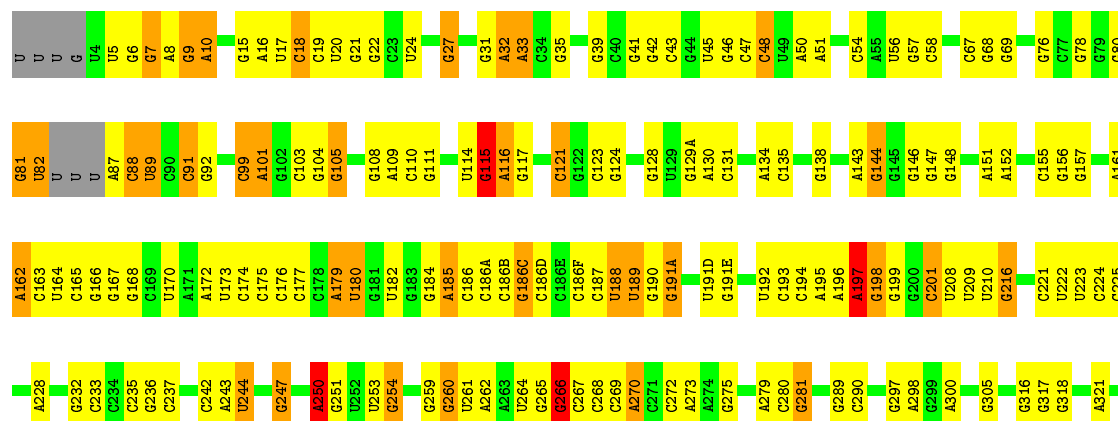
#### • Molecule 1: 16S rRNA



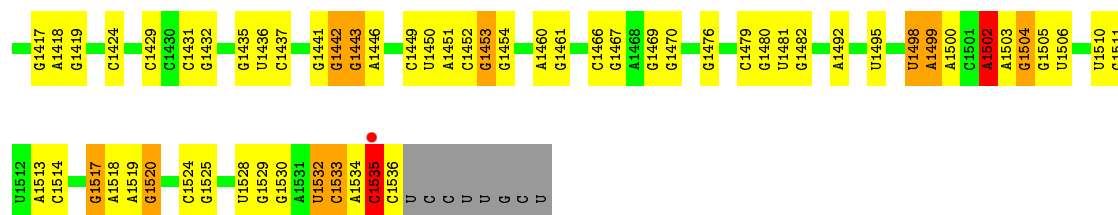


# • Molecule 1: 16S rRNA

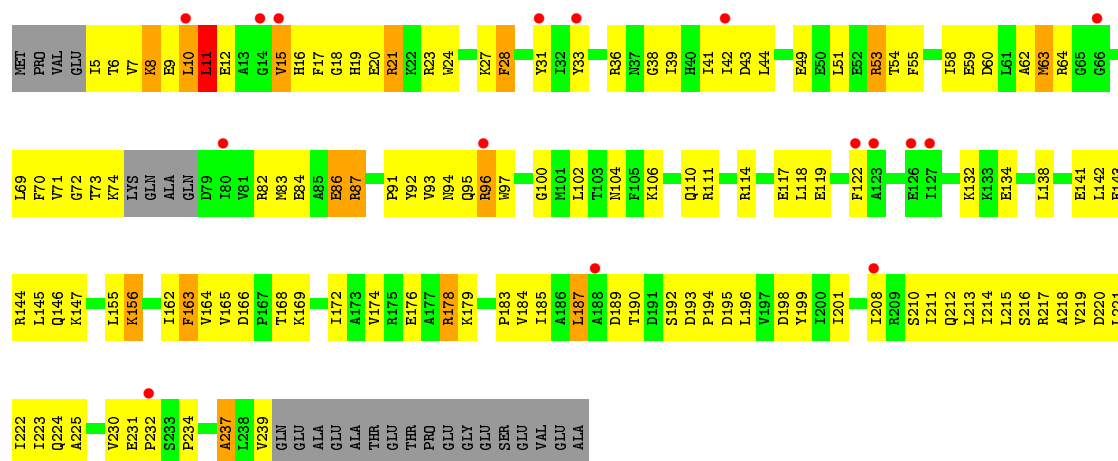
Chain 1G: 37% 45% 15% ..



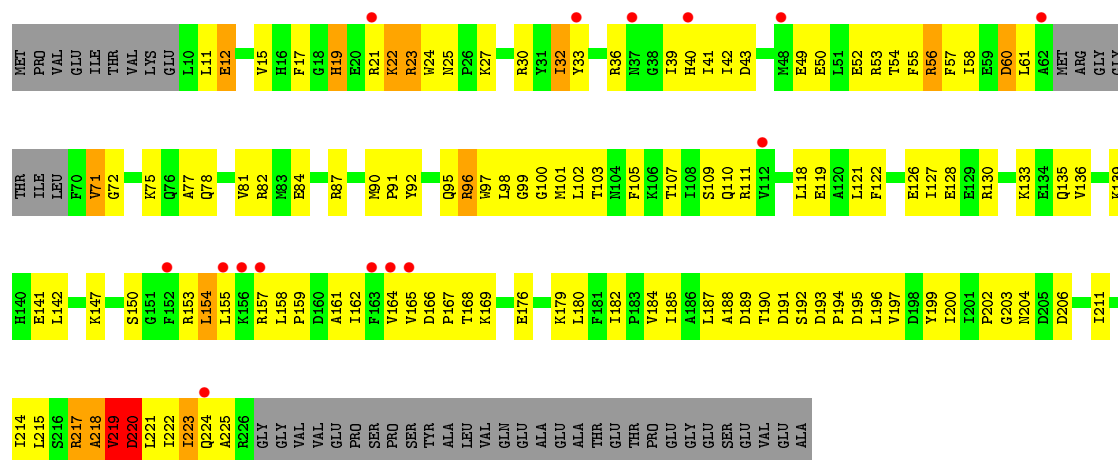
C1342	G1274	G1207	G1139	G1007	G942	C862	A768	C689	A609	G541	C466	G391	A325
G1343	A1275	C1208	C1140	C1008	G942	U863	G769	G690	G610	G542	G467	G392	G326
C1344	C1276	C1209	G1141	G1009	A946	A864	C770	G691	A614	G543	A468	A393	A327
U1345	C1277	C1210	G1142	G1010	A947	A865	G771	C699	G615	G544	G474	G394	C328
A1346	U1278	G1211	G1143	G1011	C948	C866	U772	G700	G616	A547	G481	A397	A329
A1280	A1279	U1212	G1144	A1014	C948	G867	G773	C701	G617	C331	C482	C398	C330
U1348	A1280	A1213	C1145	A1080	A949	C868	G774	A702	U618	G550	A483	C401	C335
A1349	U1281	G1214	A1146	G1081	A950	C869	G775	A706	U619	C554	G484	C403	C336
	C1282	G1215	C1147	A1015	G953	U870	A777	A707	A621	C555	G	C403	C337
C1352	A1285	C1216	U1148	G1017	G954	U871	A780	C708	G624	A559	U466	G406	A338
G1353	U1286	G1217	U1149	C1018	G955	A872	A781	A706	G625	U560	C488	G407	C339
C1354	A1287	C1218	U1150	G1085	U956	C876	A782	C707	U626	U561	G	A408	U340
G1355	A1287	U1219	U1151	C1019	U957	A873	A783	C708	G627	C562	U487	G409	C341
G1356	A1288	G1220	A1152	U1020	U957	C874	A784	G709	G628	C562	C488	A411	G410
A1357	A1289	G1221	G1153	G1088	A958	C875	C784	G710	G629	A563	U496	A412	A344
U1358	G1290	G1222	G1154	G1089	A959	C876	C785	G711	G630	C564	U497	G413	C345
C1359	G1291	C1223	G1155	U1091	U960	C877	U789	G713	U631	U565	A498	G416	G350
U1292	G1292	G1224	G1156	A1092	U961	C878	A790	G714	A632	G567	C489	C419	G351
A1293	A1293	A1225	A1157	U1093	C962	C882	A792	A715	G633	U571	U499	U427	C352
G1294	G1294	C1226	C1158	G1094	A963	C883	U793	C719	U645	A572	A496	G428	A360
G1295	A1227	C1228	U1159	U1095	A965	C884	A794	U723	U646	A573	U497	U429	A362
	C1298	C1161	C1162	C1096	C967	C885	C806	G725	C647	U574	C488	U434	A364
A1299	A1299	C1163	C1163	G1099	A968	C886	A807	G726	U652	G575	C511	C435	C366
G1300	G1300	A1169	A1170	C1100	A969	C887	C808	G727	U653	G577	U512	C436	U367
U1301	U1301	G1171	G1171	G1031	C970	C888	A816	U735	A653	C577	U513	U437	C370
U1302	U1302	A1170	A1170	A1032	G971	C889	A817	C736	A654	U580	C513	G438	G371
G1303	C1234	G1171	G1171	G1032A	C972	C890	C826	G741	U659	G581	C514	A439	C372
G1304	U1235	G1172	G1172	G1032B	G973	C891	U827	G742	G660	U582	U515	C440	A373
A1305	C1236	G1173	G1173	G1033	A974	C892	A818	G731	G661	A583	U516	G442	A374
A1306	C1237	G1174	G1174	G1034	A975	C893	A819	C735		G584	C518	C443	U375
U1307	A1238	G1175	G1175	G1035	A976	C894	U828	C745	G664	U591	C525	G446	G377
A1239	A1239	A1176	A1176	A1036	G977	C895	C829	G746	A665	G592	C526	G447	A448
U1240	U1240	G1177	G1177	G1036	A978	C896	G830	A747	A666	G594	G529	A449	G450
C1241	C1241	A1178	A1178	C1037	A979	C897	U833	C748	G667	G594	G530	C380	C361
C1243	C1243	A1180	A1180	C1038	C979	C898	U834	G749	G668	G594	U531	A382	A382
G1316	C1244	G1181	G1181	G1039	U981	C899	U835	G750	U669	G594	U532	A383	G384
C1317	A1245	G1182	G1182	U1040	U982	C900	C836	G751	G670	G594	U533	A453	A385
	U1246	A1183	A1183	A1041	U983	C901	G837	G752	G671	G594	C527	C456	C386
G1385	A1318	C1247	C1247	G1042	A983	C902	U838	A753	U672	G594	G529	G456	U387
G1386	A1319	U1247	U1247	C1043	C984	C910	U839	G754	G673	G594	G530	C457	C388
C1387	C1320	A1187	A1187	A1044	C985	C911	U841	C755	G674	G594	U531	C458	A389
C1388	C1321	G1189	G1189	G1047	A986	C912	U842	G756	A675	G594	U532	G459	A461
C1389	G1322	A1189	A1189	U1048	G987	C913	U843	C757	U675	G594	U533	C456	C386
U1390	A1324	A1191	A1191	U1049	U991	C914	U844	G758	A676	G594	U534	C457	C387
U1391	C1325	C1192	C1192	G1050	U992	C915	C842	G759	U677	G594	U535	C458	A388
	G1254	G1193	G1193	G1051	G993	C916	U845	G760	G678	G594	U536	C459	A462
A1396	C1326	G1194	G1194	G1052	G994	C917	U846	C761	G679	G594	U537	C456	C386
C1397	C1327	U1125	U1125	G1053	U995	C918	U847	G762	G680	G594	U538	C457	C387
C1398	U1257	U1126	U1126	C1054	U996	C919	U848	C763	G681	G594	U539	C458	A389
A1399	A1329	U1127	U1127	A1055	U997	C920	U849	G764	G682	G594	U540	C459	A463
	U1350	G1128	G1128	A1056	U998	C921	U850	G765	G683	G594	U541	C456	C386
C1399	C1260	C1129	C1129	C1060	G999	C922	U851	G766	A676	G594	U542	C457	C387
A1400	A1261	U1130	U1130	G1061	U999	C923	U852	G767	U677	G594	U543	C458	A388
C1401	C1332	G1131	G1131	G1062	U999	C924	U853	G768	G684	G594	U544	C459	A464
C1402	A1333	C1132	C1132	G1063	U999	C925	U854	G769	G685	G594	U545	C456	C386
C1403	G1334	G1133	G1133	G1064	U999	C926	U855	G770	G686	G594	U546	C457	C387
	C1335	A1201	A1201	G1065	U999	C927	U856	G771	G687	G594	U547	C458	A388
C1396	C1336	C1283	C1283	G1066	U999	C928	U857	G772	G688	G594	U548	C459	A465
C1412	A1413	U1204	U1204	C1067	U999	C929	U858	G773	G689	G594	U549	C456	C386
G1338	G1338	G1206	G1206	G1072	U999	C930	U859	G774	G690	G594	U550	C457	C387



• Molecule 2: 30S ribosomal protein S2

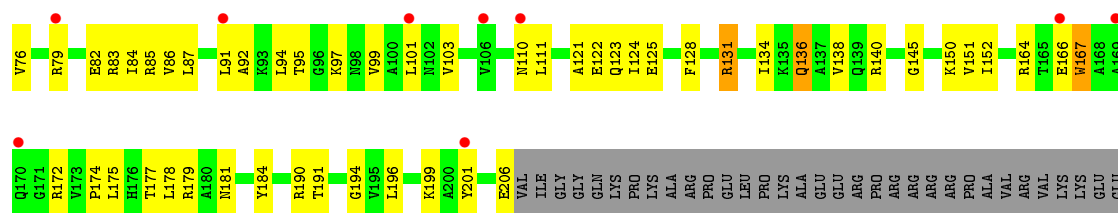


• Molecule 2: 30S ribosomal protein S2

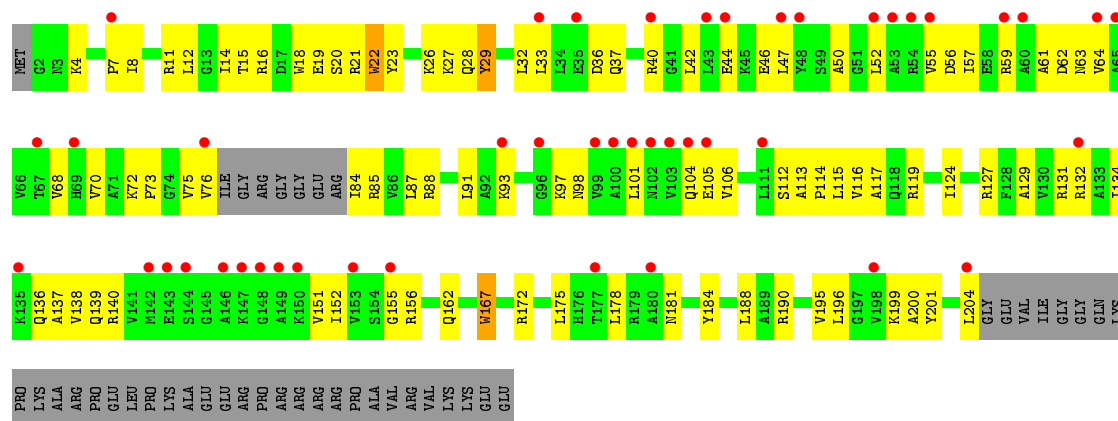
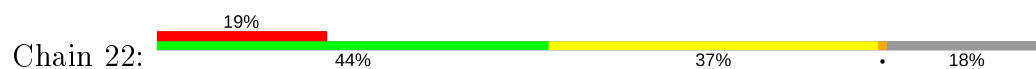


• Molecule 3: 30S ribosomal protein S3

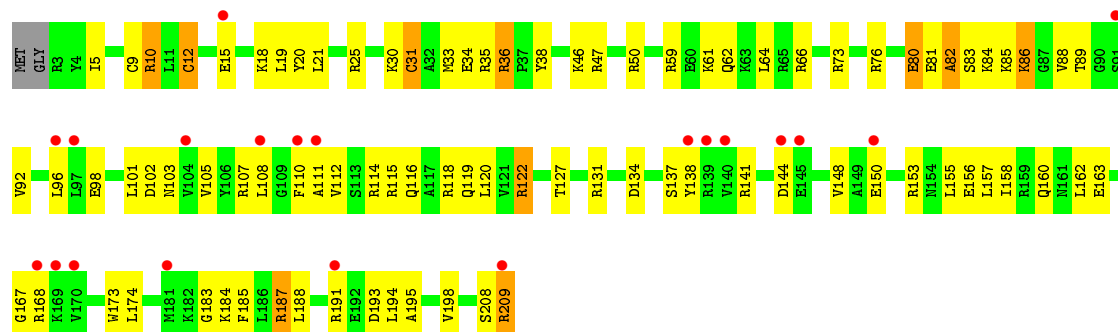




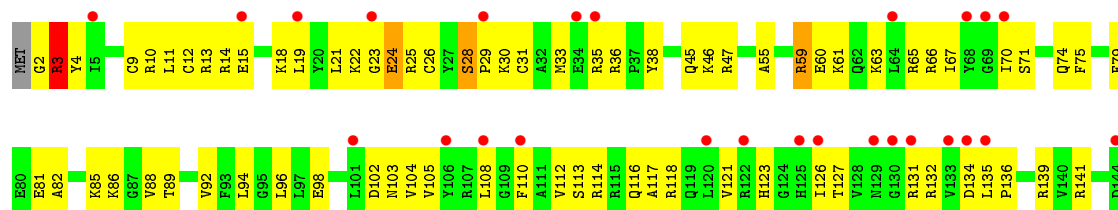
• Molecule 3: 30S ribosomal protein S3

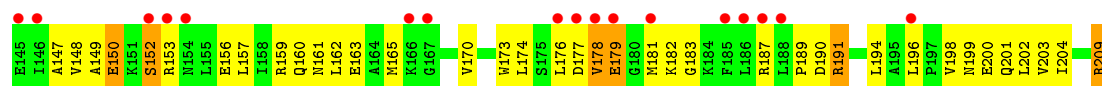


• Molecule 4: 30S ribosomal protein S4

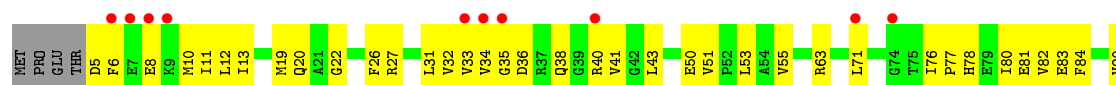


• Molecule 4: 30S ribosomal protein S4

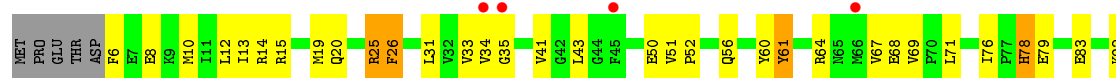




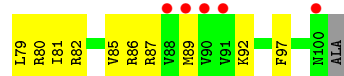
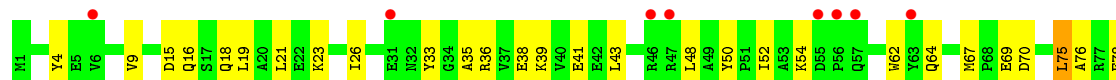
- Molecule 5: 30S ribosomal protein S5



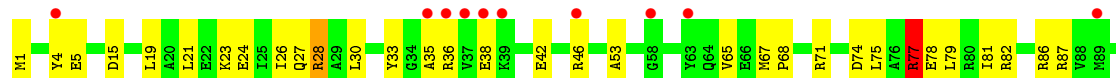
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

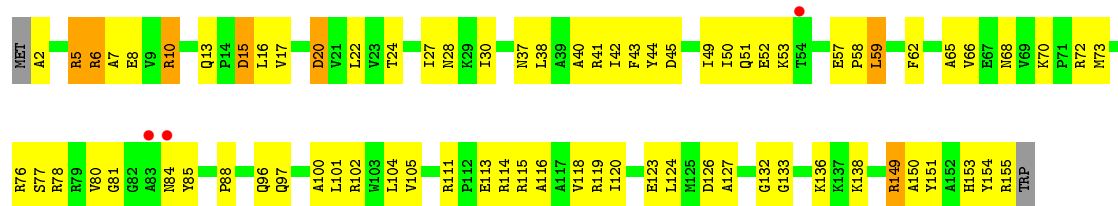


- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

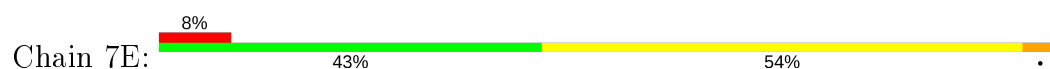




• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

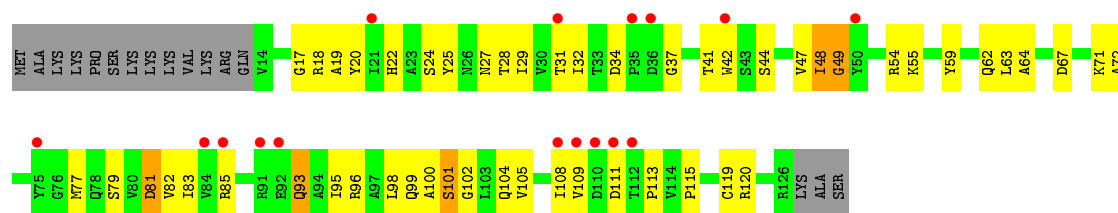


• Molecule 9: 30S ribosomal protein S9

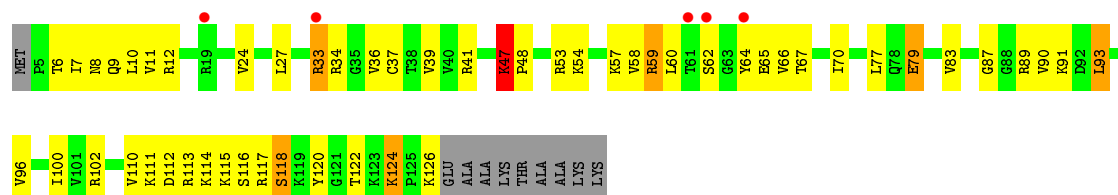




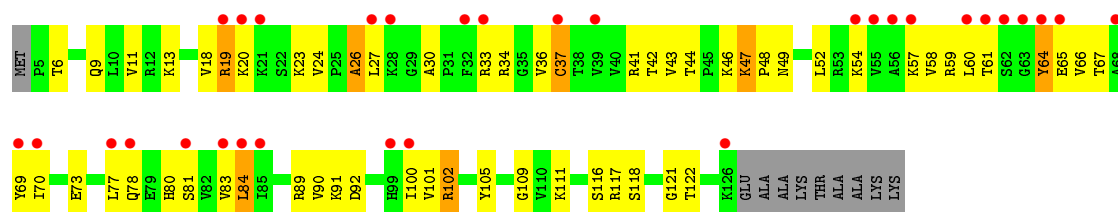




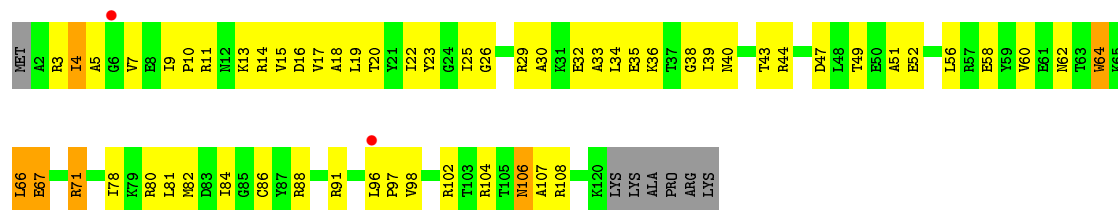
• Molecule 12: 30S ribosomal protein S12



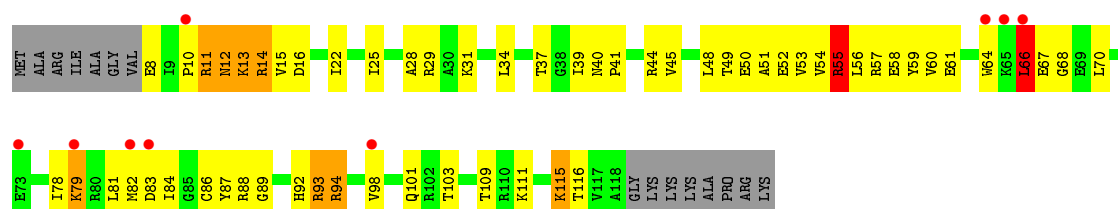
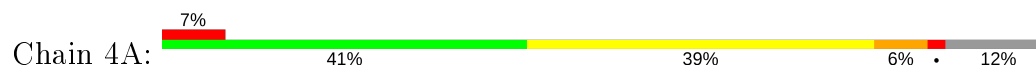
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



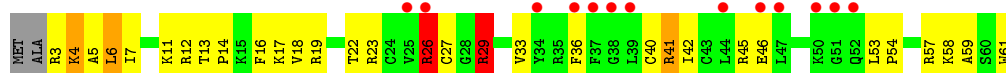
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I: 



- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A: 



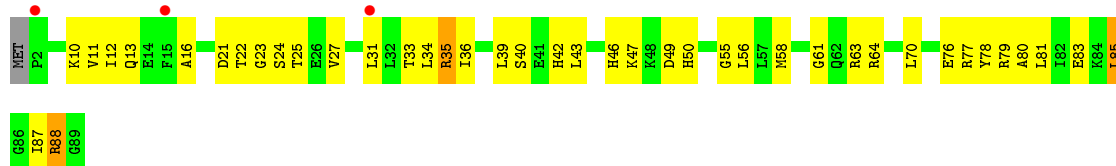
- Molecule 15: 30S ribosomal protein S15

Chain 6I: 



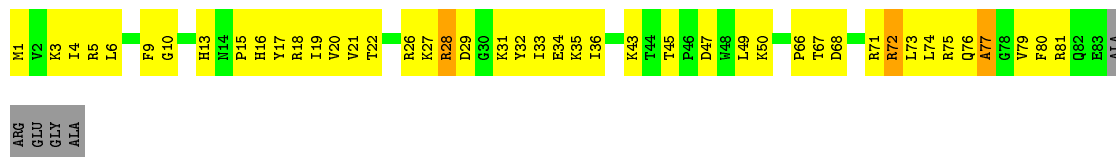
- Molecule 15: 30S ribosomal protein S15

Chain 6A: 



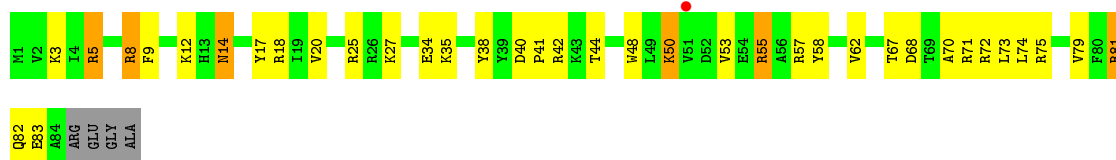
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 

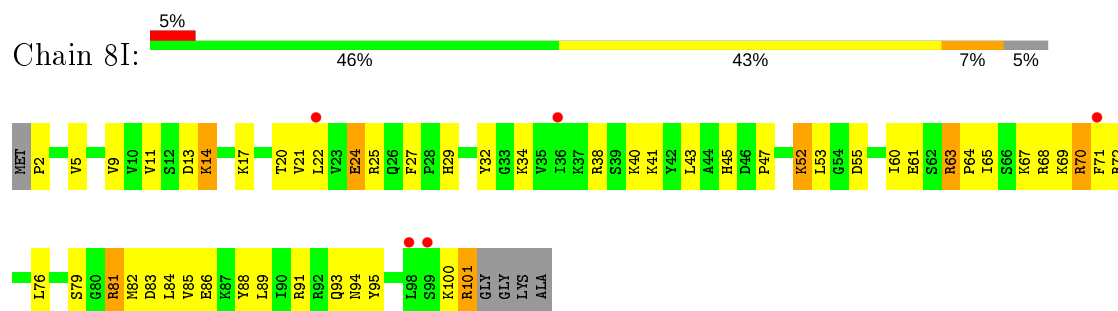


- Molecule 16: 30S ribosomal protein S16

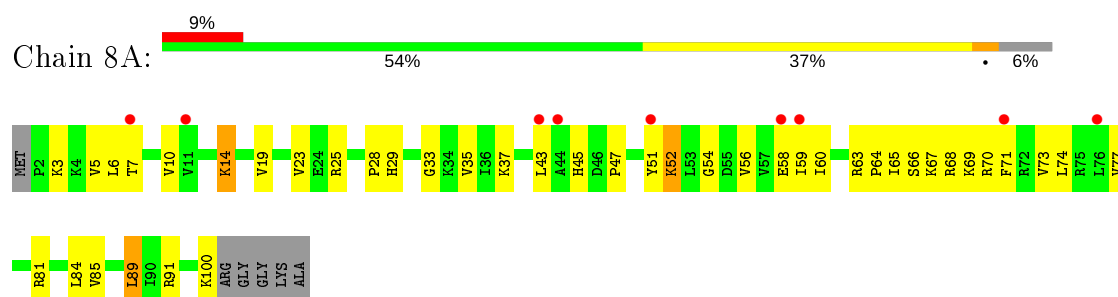
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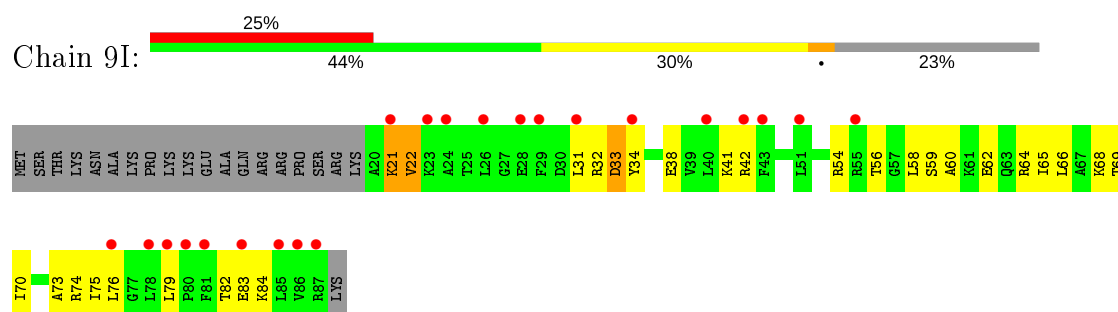
- Molecule 17: 30S ribosomal protein S17



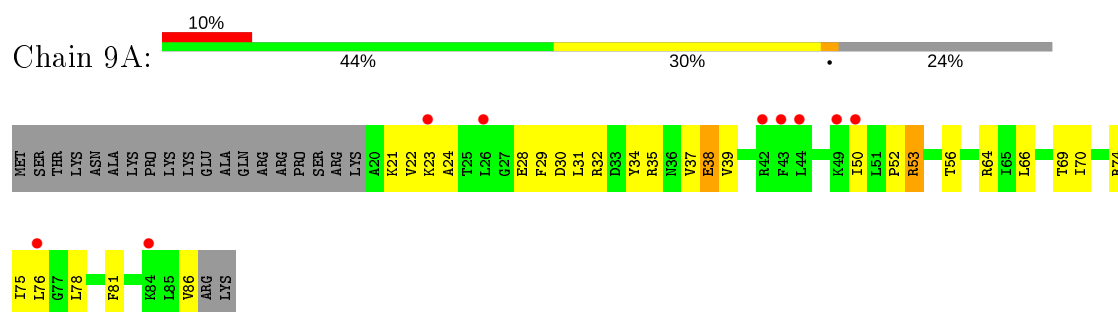
- Molecule 17: 30S ribosomal protein S17



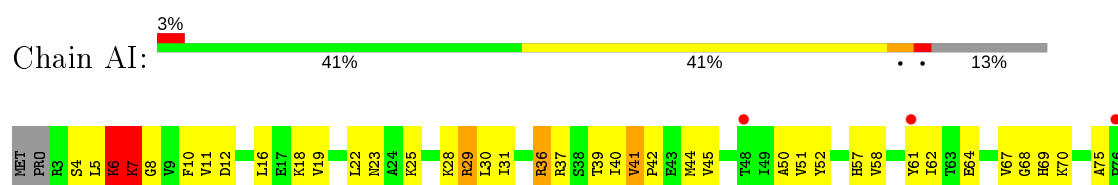
- Molecule 18: 30S ribosomal protein S18



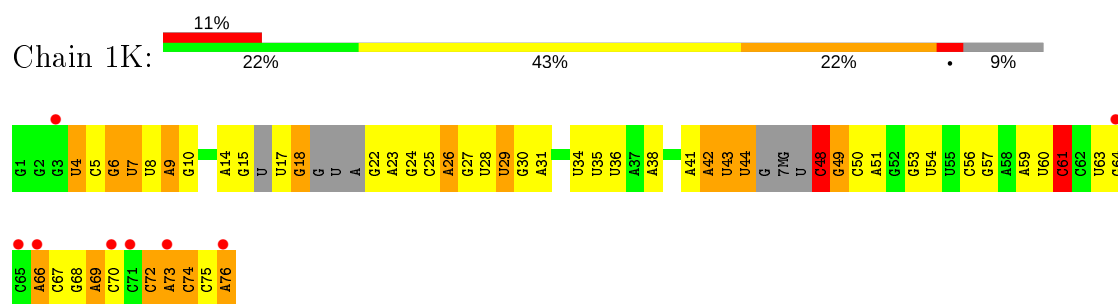
- Molecule 18: 30S ribosomal protein S18



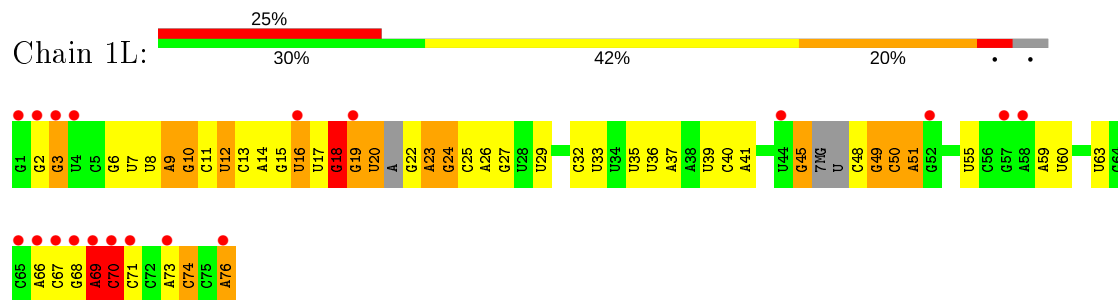
- Molecule 19: 30S ribosomal protein S19



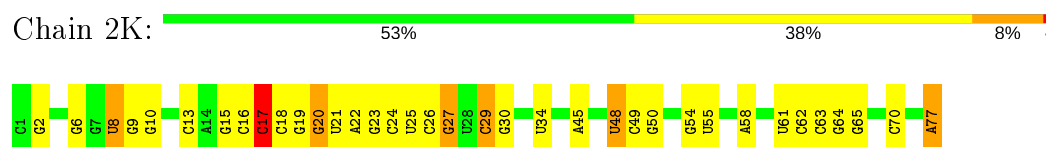




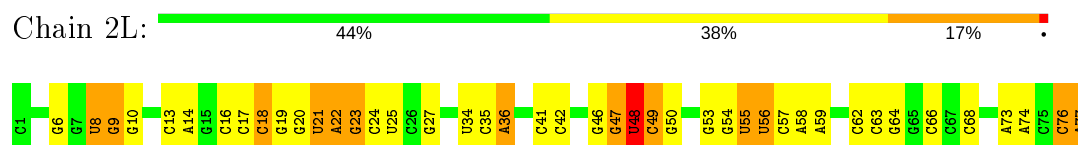
- Molecule 22: tRNA<sup>Lys</sup>



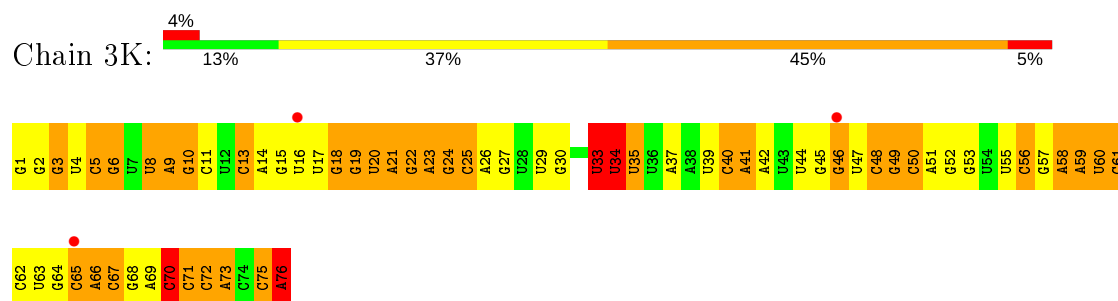
- Molecule 23: E. coli tRNA<sup>fMet</sup>



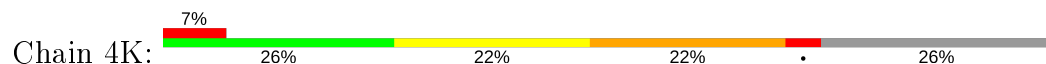
- Molecule 23: E. coli tRNA<sup>fMet</sup>



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



- Molecule 25: mRNA

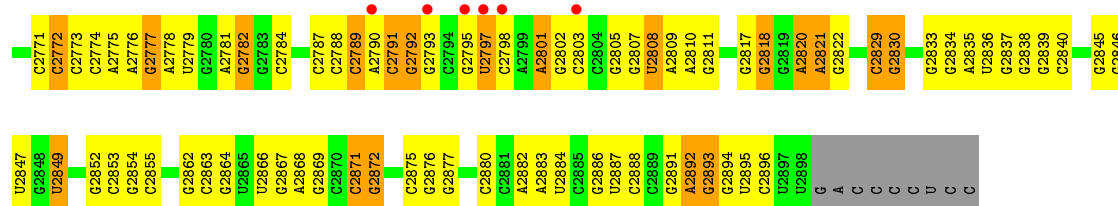




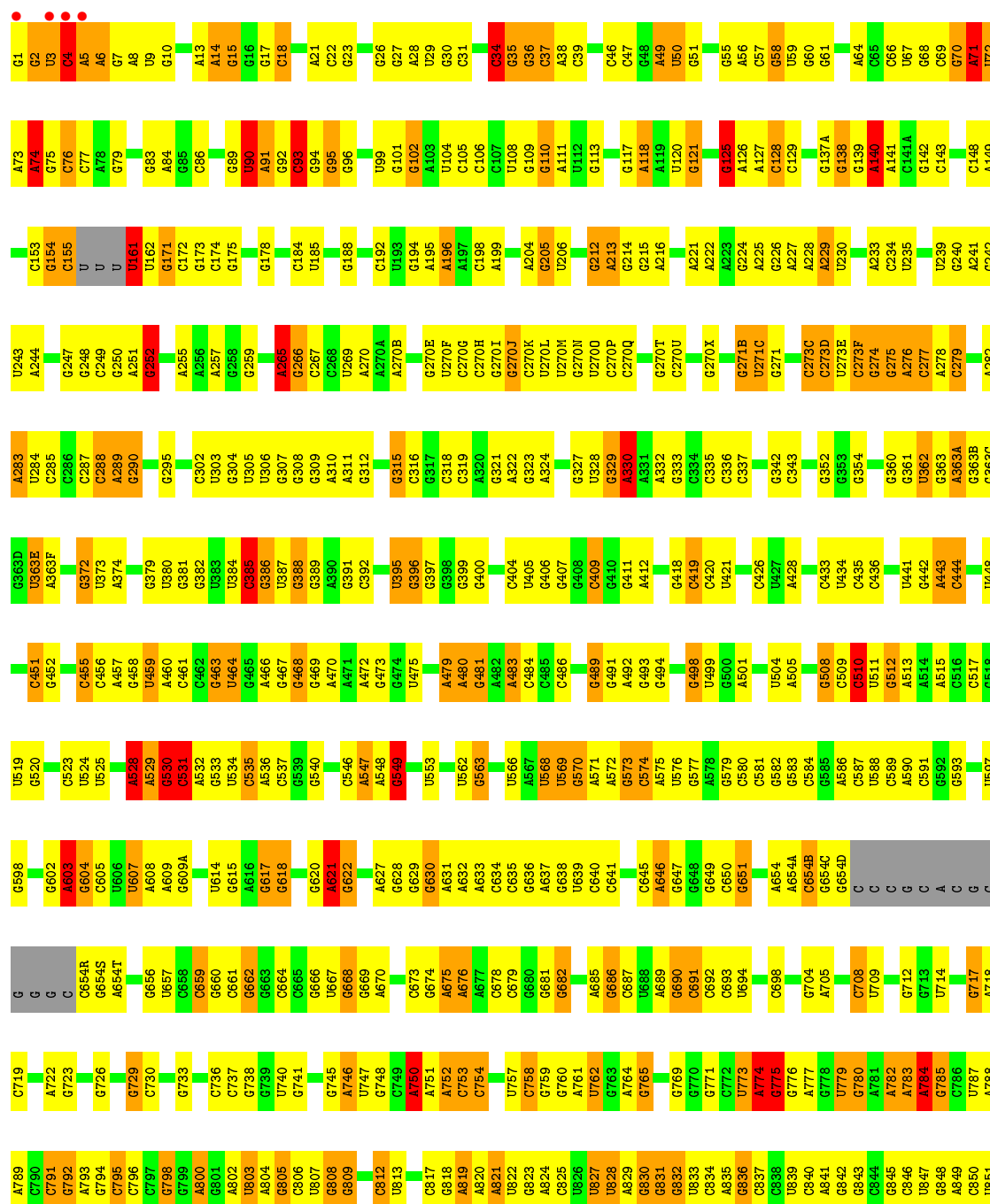
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U2739	U2679	C2590	G2506	G2360	C2301	G2231	C2160	C2087	C1870	G1944	U1796	
A2740	C2680	G2591	U2507	G2361	G2302	U2232	G2161	C2088	A1871	U1945	U1797	
U2741	U2681	U2592	G2508	G2362	G2303	G2233	C2162	U2089	G1872	C1946	U1798	
G2742	G2682	C2593	C2511	U2363	G2304	G2234	C2163	U2090	G1799	G1947	A1872	
U2743	U2683	U2594	C2512	G2364	A2305	G2235	G2164	G2091	G1878	G1948	G1799	
G2744	C2684	A2598	G2513	G2365	C2306	G2236	G2165	G2092	C1879	G1949	C1800	
U2745	U2685	G2599	G2514	G2366	G2307	G2237	G2166	U2102	G1880	G1950	G1801	
G2746	G2686	A2600	G2515	U2367	G2308	U2238	U2167	C2103	A1802	U1951	A1802	
U2747	U2687	C2601	U2516	G2368	A2309	G2239	G2168	G2104	G1883	A1952	G1803	
G2748	C2688	A2602	G2517	G2369	G2310	A2240	A2169	C2105	G1884	C1953	C1804	
U2749	U2689	U2603	U2518	A2370	A2311	G2241	A2170	G2106	U1885	U1954	U1805	
G2750	G2690	G2607	G2519	A2371	U2312	G2242	A2171	C2107	A1886	U1955	A1806	
U2751	U2691	U2608	G2520	A2372	C2313	G2243	U2172	C2108	G1887	U1956	G1807	
G2752	C2692	A2609	G2521	G2373	C2314	G2244	A2173	U2109	G1888	C1957	U1808	
U2753	U2693	G2610	G2522	G2374	G2315	U2245	G2174	C2110	A1889	U1958	G1811	
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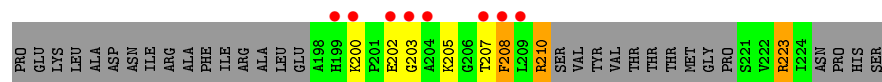
• Molecule 26: 23S rRNA



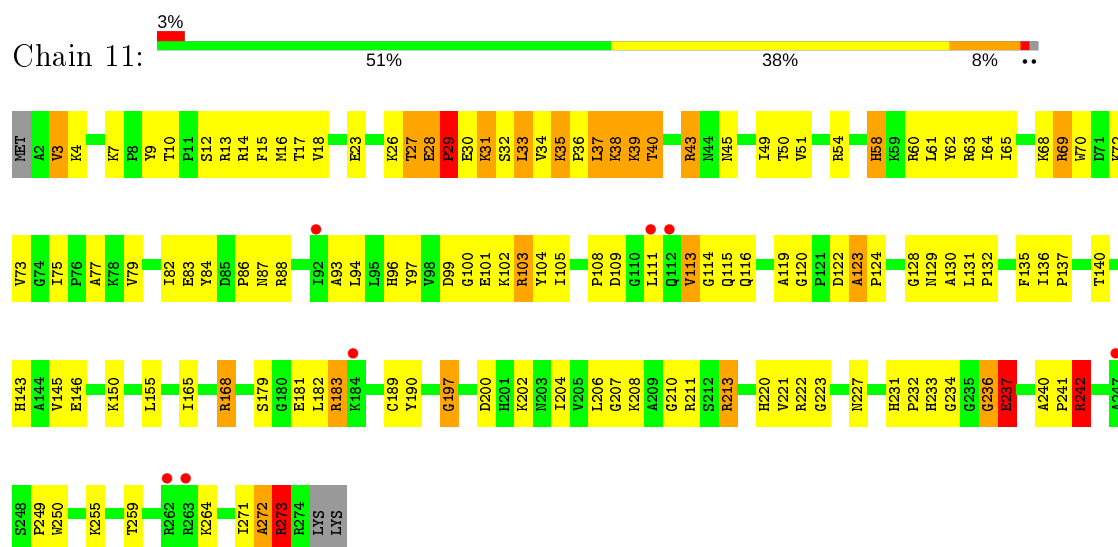
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U1778	U1778	C1615	G1542	A1471	G1404	C1330	A1257	U1175	U1108	U1048	A980	G916	G854
G1857	U1779	A1616	A1543	A1472	A1405	A1331	C1257	G1176	C1109	C1049		A917	G855
G1858	A1780	C1617	G1544	U1406	U1405	C1332	C1258	A1177	G1110	G1050	A983	G918	G856
A1859	G1781		G1545	G1475	U1406	C1333	C1259	G1178	A1111	G1051		G919	C957
G1860	C1782	G1622	A1545A	G1476	C1407	G1334	G1260	C1179	G1112	C1052	G987	G920	U858
	A1783		G1546	G1477	C1408	U1335	C1261	C1180	U1113	C1053	A988	G921	U859
G1869	A1784	C1625	C1547	U1480	C1409	A1336	A1262	C1181	G1114	G1054	G989	U922	G862
A1870	C1548	G1626	C1548	U1482		G1337	U1263	A1182		G1055	A990	G923	A861
A1871	G1555	G1627	U1482	G1483	A1412	G1338	G1264		C1118	G1056		G924	G862
A1872	G1556	G1628	U1483	G1486	G1413	G1339	A1265	U1187	C1119	A1057	G953	G925	A863
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C1788	A1558	G1630A	G1487		U1415	U1341	U1267	A1189	G1122	G1059	C995	G928	C885
A1789	G1559		G1488	A1486	G1416	A1342	A1268	U1190	C1123	U1060	A996	G929	A866
C1882	A1791	G1633	U1560	G1489	G1417		A1269	G1191	C1124	U1061			C867
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A1884	G1703	G1635	U1566	A1491	U1420	G1346	G1271	G1193	A1126	G1063	G999	A933	U869
A1885	G1704		A1567	G1492	A1419	G1347	A1272	G1194	A1127	C	A1000	G934	A870
A1886	G1705		A1567	G1492	G1421	G1348	A1275	G1195	A1128	U	A1001	G935	U871
C1887	U1709	U1639	A1568	G1493	G1422	A1349	A1275		A1129	U	G1002	C936	A872
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A1889	U1798		A1570	A1495	G1424	U1352		U1199		G	C1004	G938	G874
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C1893	G1725	G1647		C1499	C1428	U1358		G1203	G1138	A1072	C1008	U943	A878
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	G1811	A1655	C1583	A1510	G1435	A1367	C1293	G1151	C1144	C	G1015	G950	C
C1905	G1812	G1656	C1585	A1511	G1436	G1368		C1218	G1145	U	G1016	G951	C
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	A1815	G1658	U1587		U1438	G1369	G1298	G1219	C1147	U	C1018	A953	C
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U1915	U1820	A1664	C1592	G1519	G1443	C1376		A1227	G1152	G1087	U1023	U958	C
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G1922	C1753	G1667	G1595	G1522	C1445	G1380	U1312		A1155	U1090	U1026	C961	C897
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C1925	U1757	C1670	G1600	G1525	G1448	C1383	C1315	G1236	G1158	G1093	G1039	C971	G906
	G1758	U1671	G1601	G1526	A1449	A1384	U1316	A1237	U1159	U1093	C1040	A973	U907
G1929	A1829	C1672	G1602	G1530	G1449A	G1385	A1317		G1160	U	A1029	G972	A901
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A1932	G1835	G1674	A1603	C1532		C1387	G1319	A1242	C1162	A		G966	C903
C1933	C1836	C1675	C1604	C1533	G1455		C1320	G1243	G1163	U	U1035	G968	C904
C1934		A1676		G1534	G1459	A1392	A1321	G1243	G1164	A1098	G1036	U969	C905
A1935	G1839	G1677	A1608	U1535	G1460	U1393	A1322	U1247	G1165	G1099	C1037	C970	U905
A1936	G1770	A1678	A1609	G1536	A1460	U1394	U1323	G1248	U1166	C1100	G1038	A973	G906
A1937	U1679	U1679	A1609	A1586		A1395	G1324	U1249	C1166	U1101	C1040	G974	U907
A1938	G1772	U1680	A1610	A1587	G1466	U1396	G1325	U1250		G1102	C1041	G974	A910
U1939	A1849	G1681	C1611	C1538	G1467	U1397	U1326	G1251	G1169	A1103		C974A	A911
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- Molecule 27: 5S rRNA

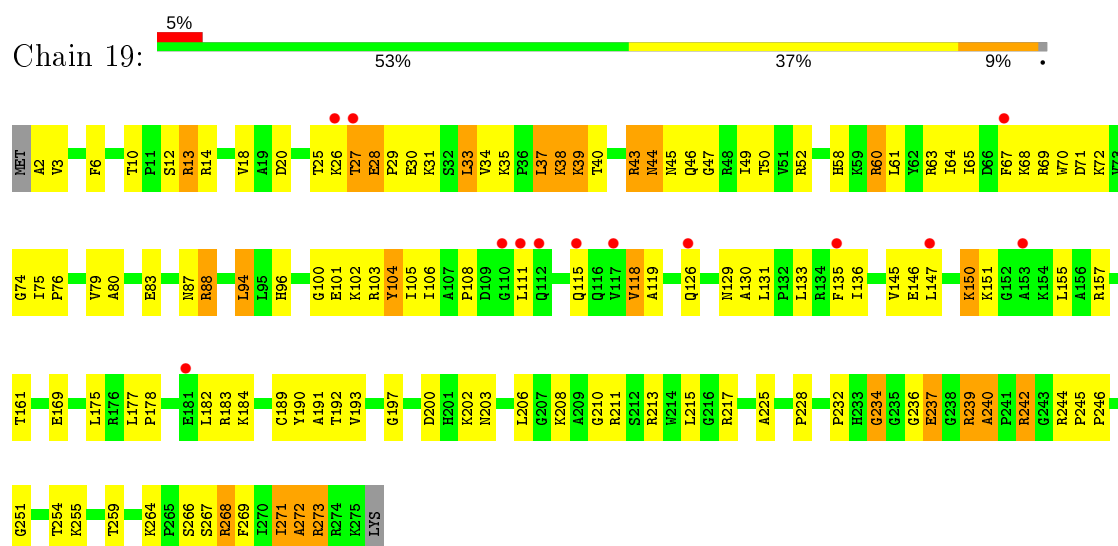




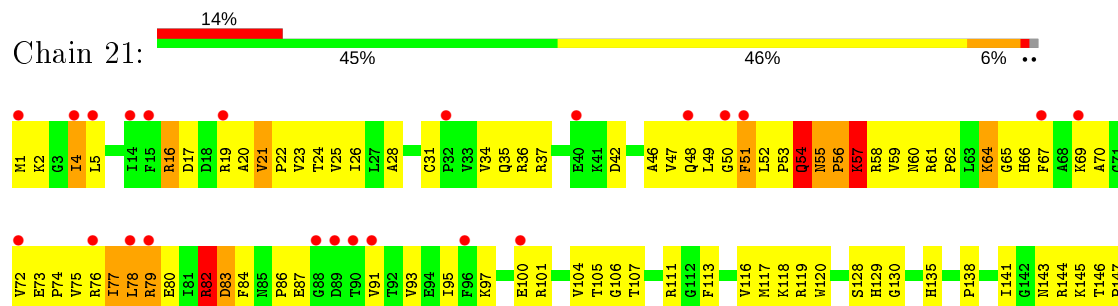
• Molecule 29: 50S ribosomal protein L2



• Molecule 29: 50S ribosomal protein L2

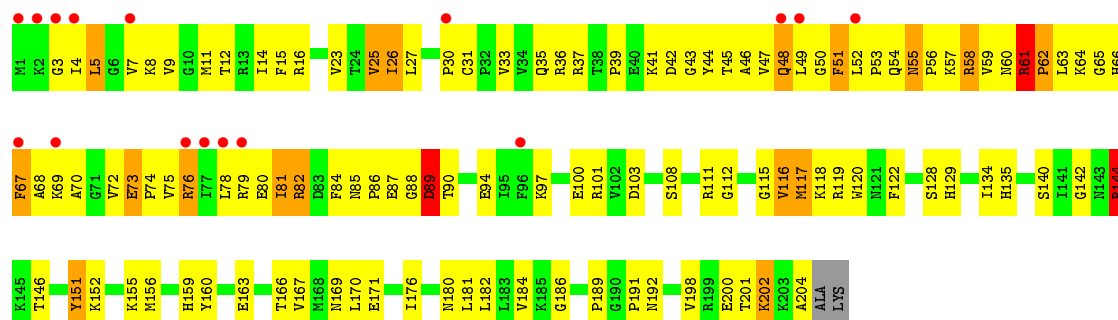
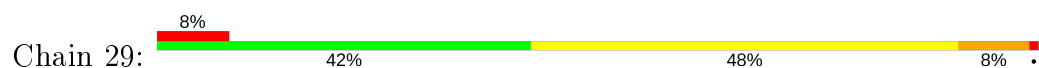


• Molecule 30: 50S ribosomal protein L3

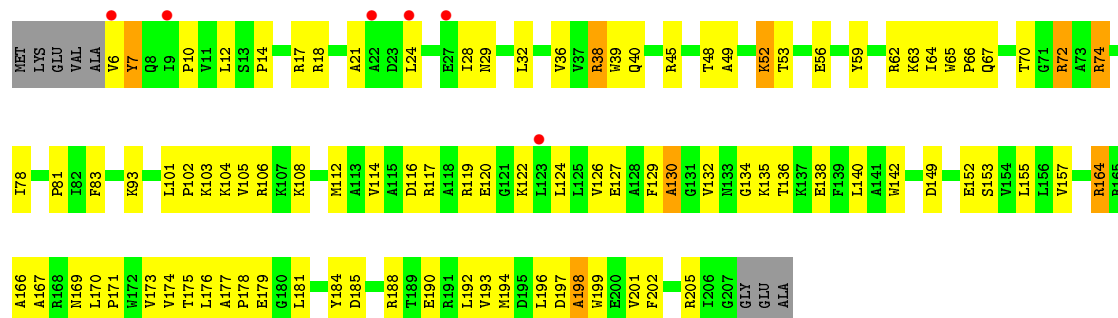




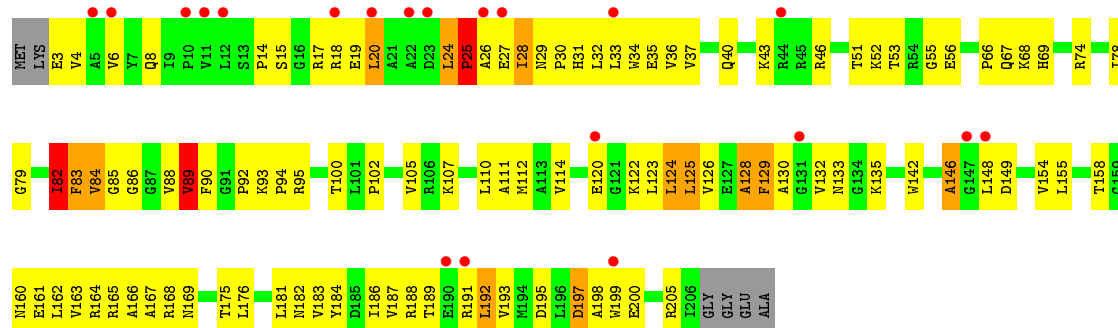
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4

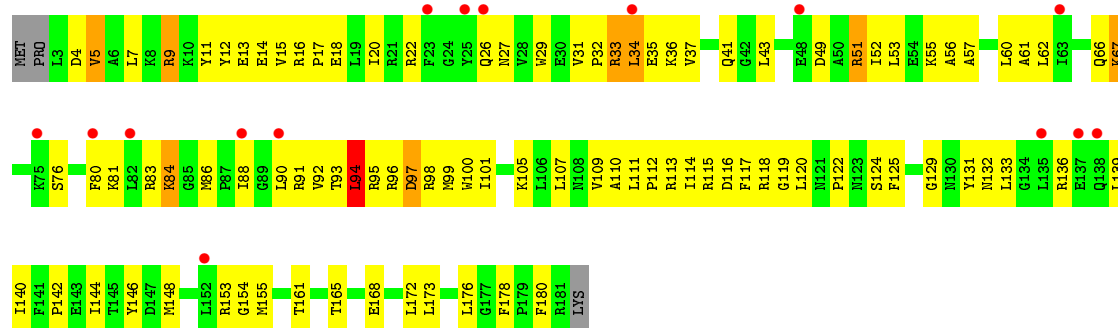


• Molecule 31: 50S ribosomal protein L4

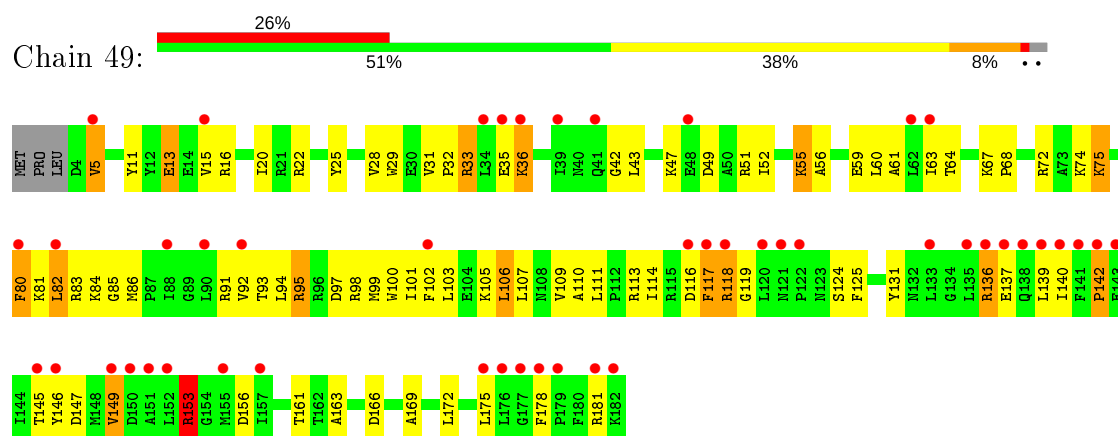


• Molecule 32: 50S ribosomal protein L5

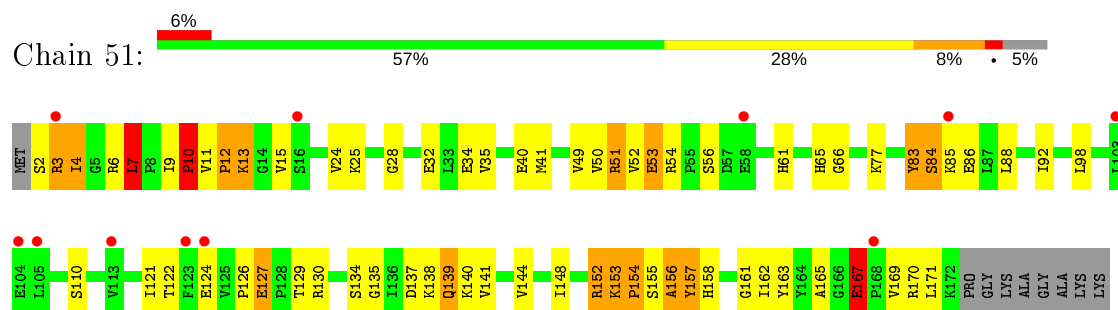




- Molecule 32: 50S ribosomal protein L5



- Molecule 33: 50S ribosomal protein L6

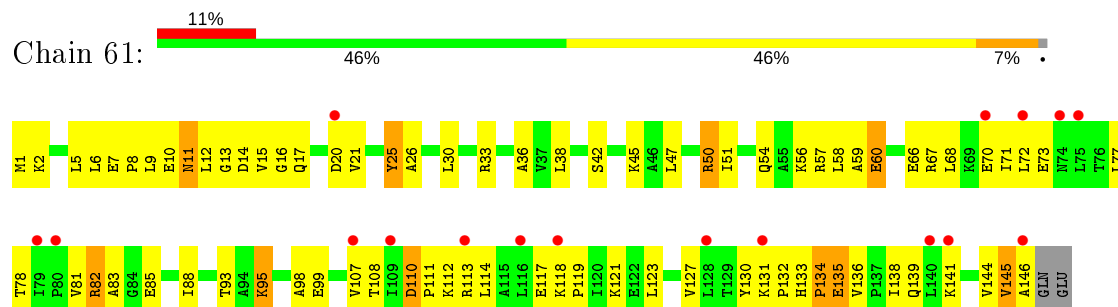


- Molecule 33: 50S ribosomal protein L6

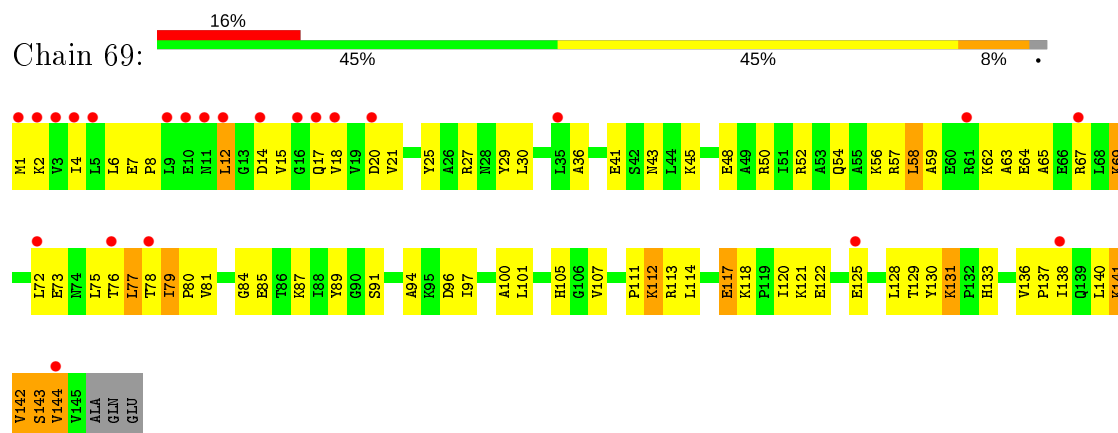




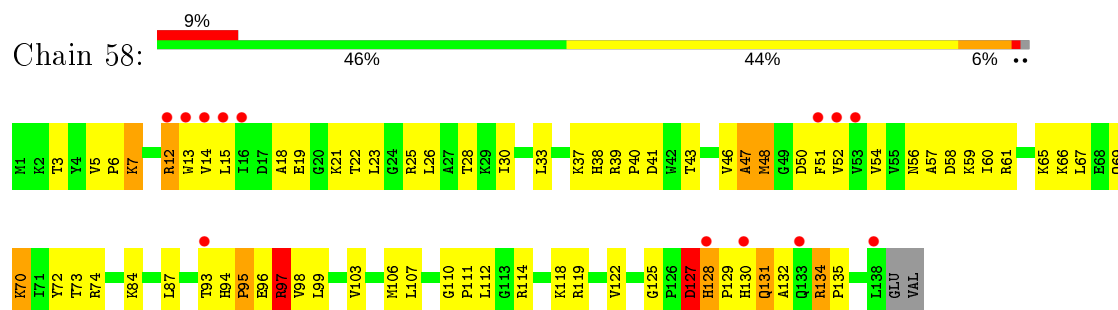
- Molecule 34: 50S ribosomal protein L9



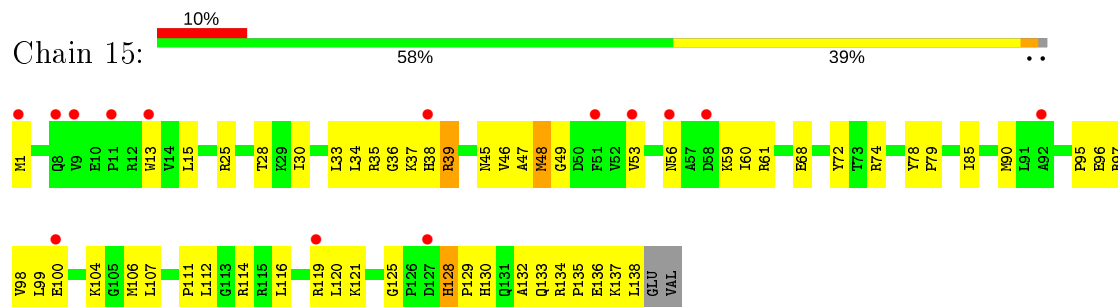
- Molecule 34: 50S ribosomal protein L9



- Molecule 35: 50S ribosomal protein L13

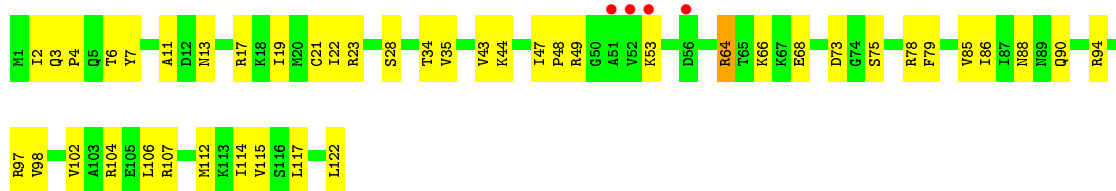


- Molecule 35: 50S ribosomal protein L13

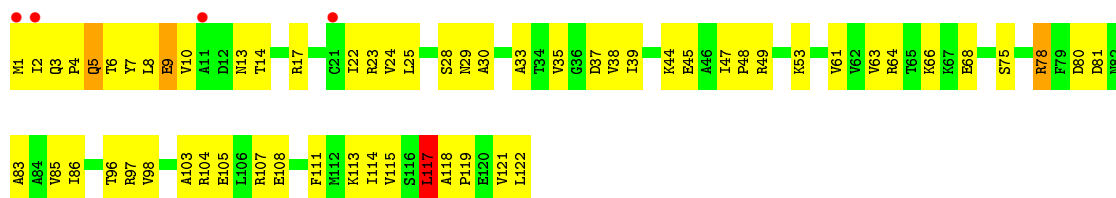


- Molecule 36: 50S ribosomal protein L14

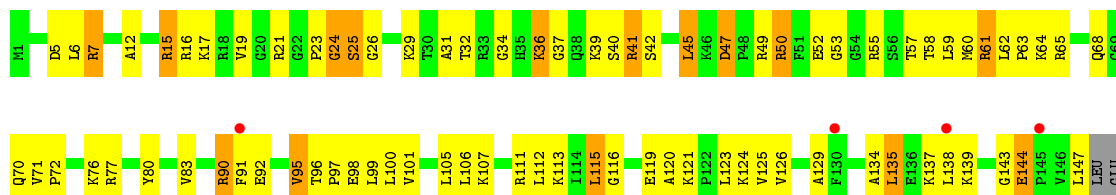
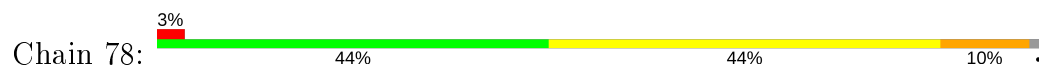




- Molecule 36: 50S ribosomal protein L14

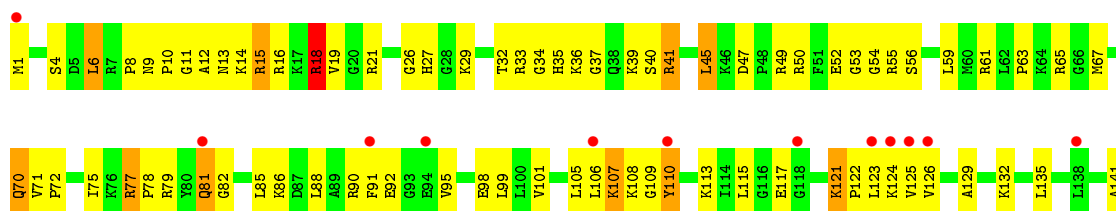
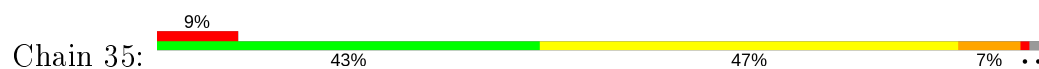


- Molecule 37: 50S ribosomal protein L15



ALA

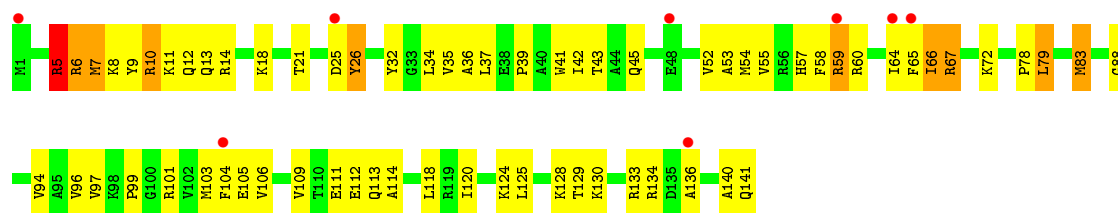
- Molecule 37: 50S ribosomal protein L15



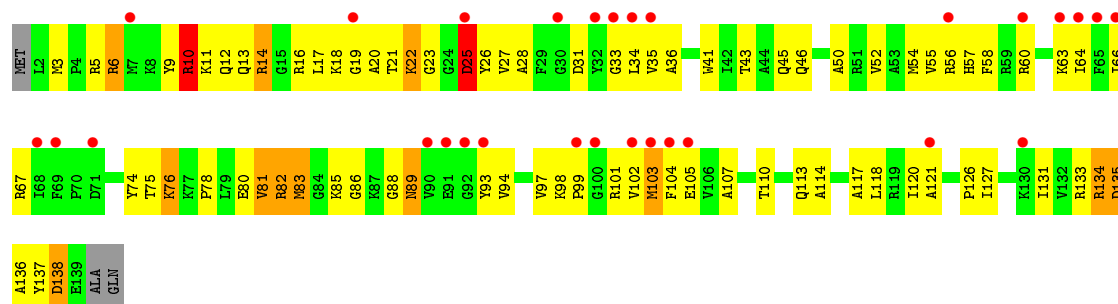
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G143  
E144  
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V146  
L147  
LEU  
GLU  
ALA

- Molecule 38: 50S ribosomal protein L16

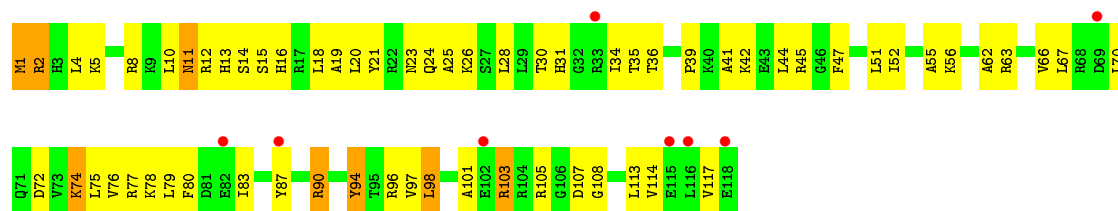




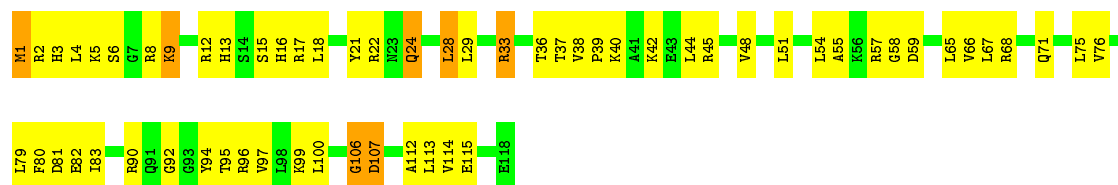
• Molecule 38: 50S ribosomal protein L16



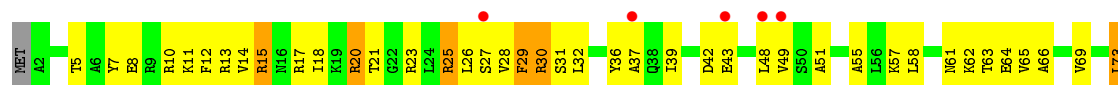
• Molecule 39: 50S ribosomal protein L17

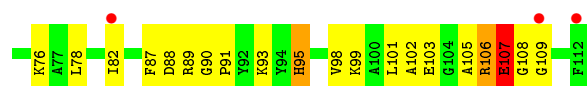


• Molecule 39: 50S ribosomal protein L17

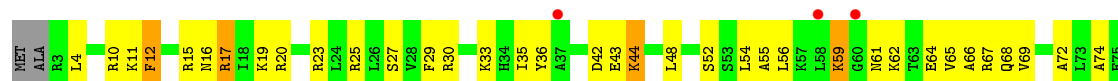


• Molecule 40: 50S ribosomal protein L18

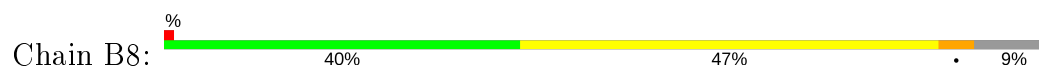




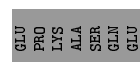
- Molecule 40: 50S ribosomal protein L18



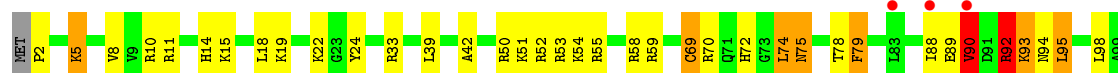
- Molecule 41: 50S ribosomal protein L19



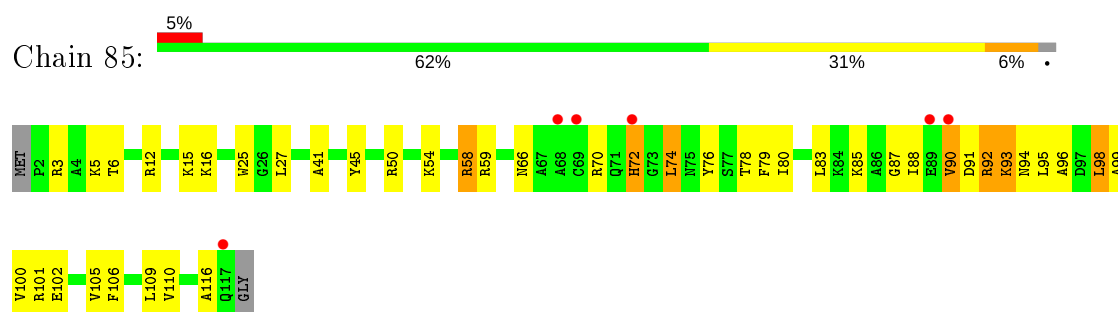
- Molecule 41: 50S ribosomal protein L19



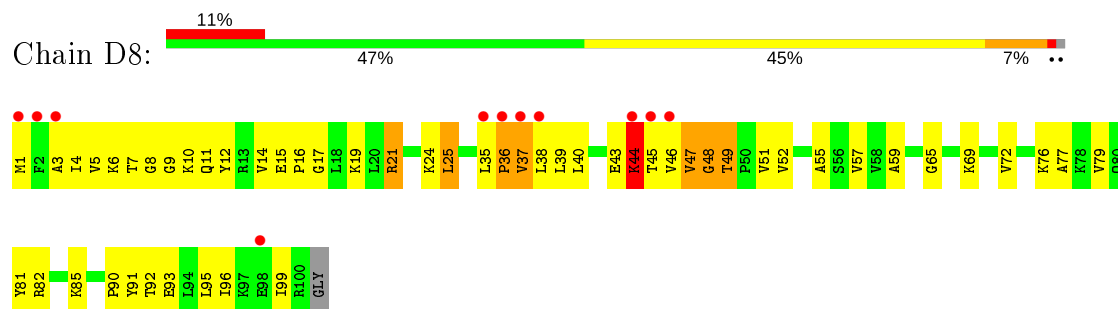
- Molecule 42: 50S ribosomal protein L20



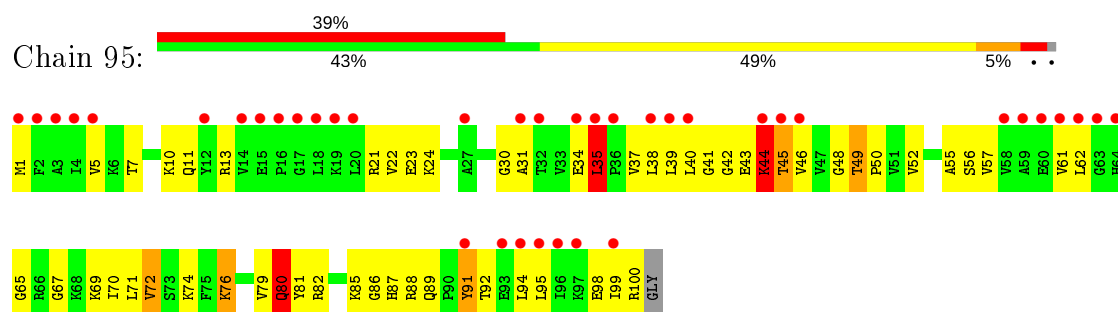
- Molecule 42: 50S ribosomal protein L20



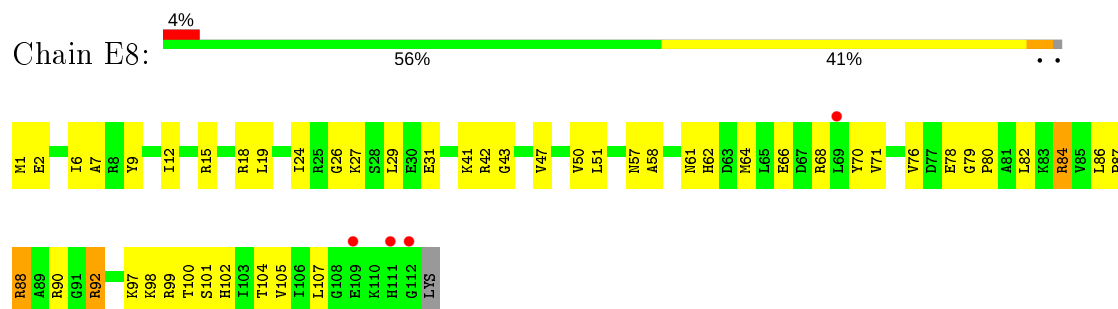
- Molecule 43: 50S ribosomal protein L21



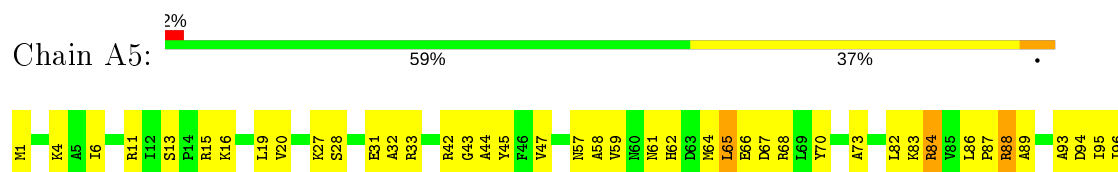
- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22

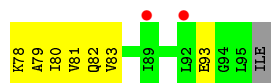


- Molecule 44: 50S ribosomal protein L22

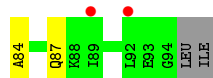
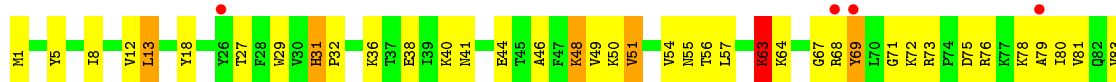




- Molecule 45: 50S ribosomal protein L23



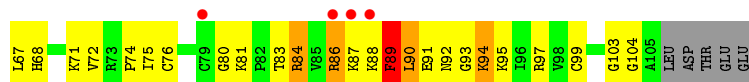
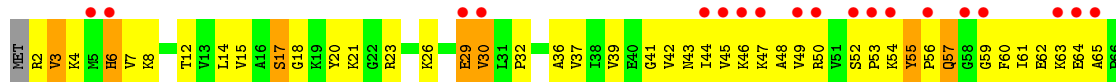
- Molecule 45: 50S ribosomal protein L23



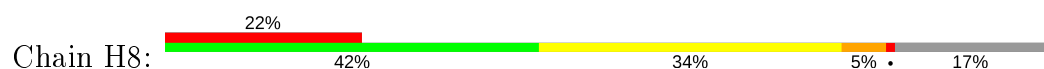
- Molecule 46: 50S ribosomal protein L24



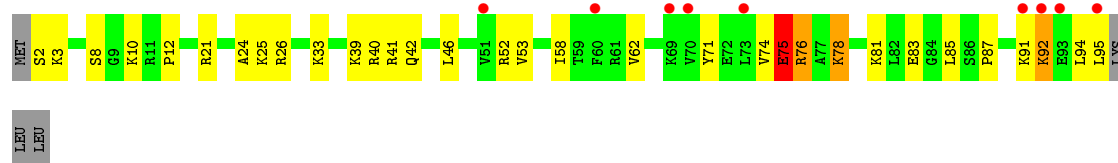
- Molecule 46: 50S ribosomal protein L24



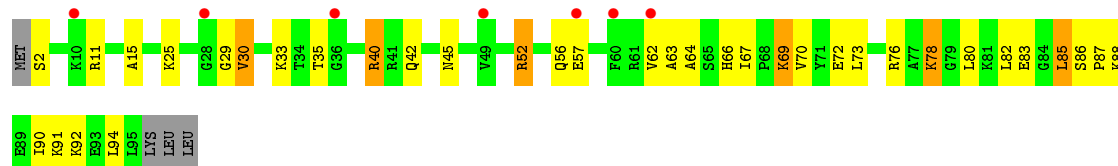
- Molecule 47: 50S ribosomal protein L25



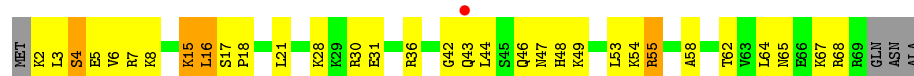




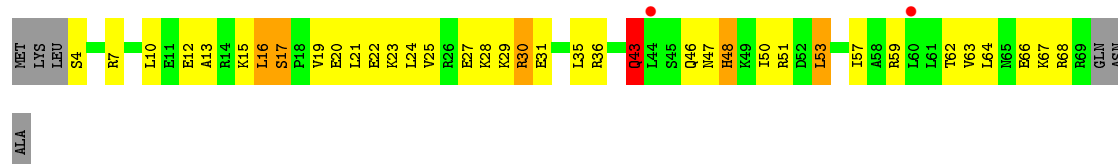
- Molecule 49: 50S ribosomal protein L28



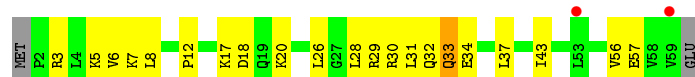
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30

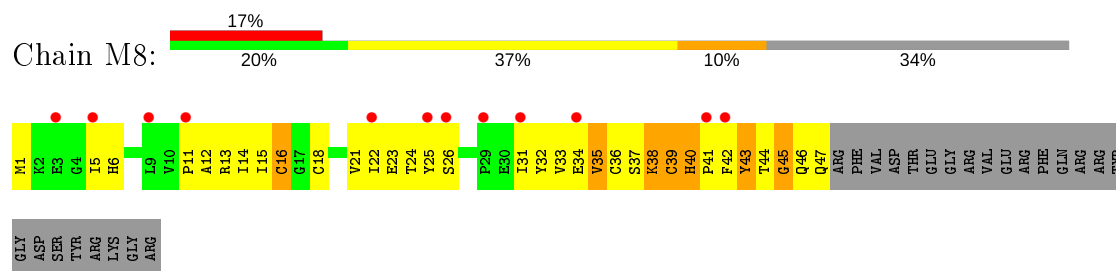


- Molecule 51: 50S ribosomal protein L30

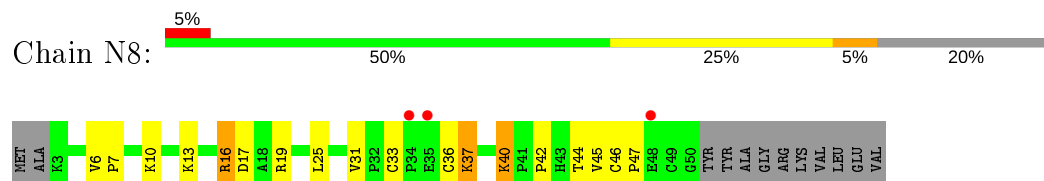




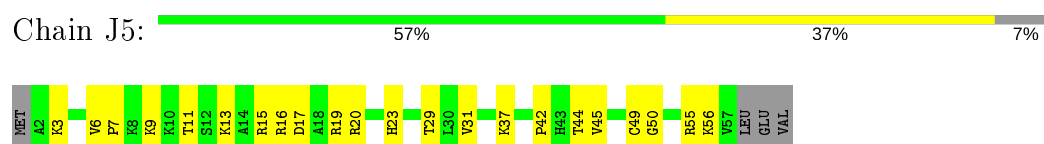
- Molecule 52: 50S ribosomal protein L31



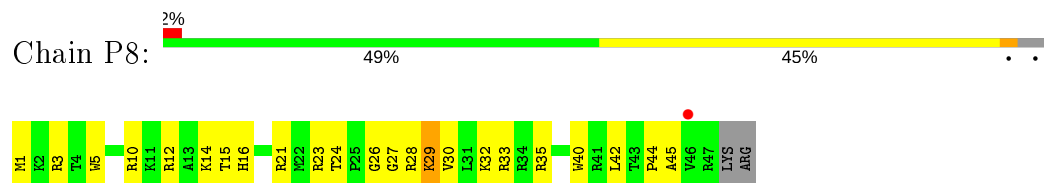
- Molecule 53: 50S ribosomal protein L32



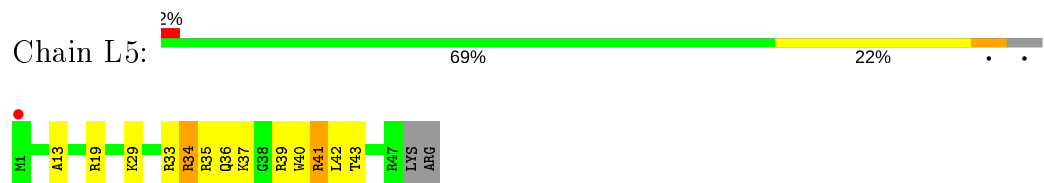
- Molecule 53: 50S ribosomal protein L32



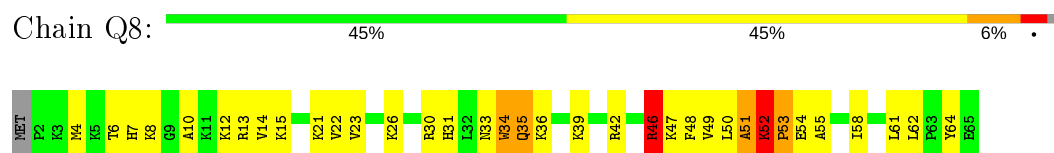
- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34

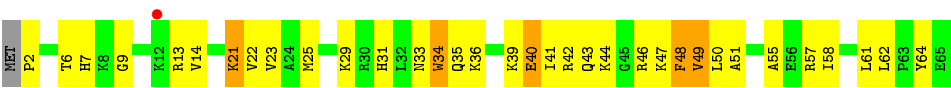


- Molecule 55: 50S ribosomal protein L35

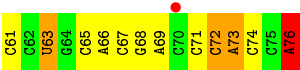
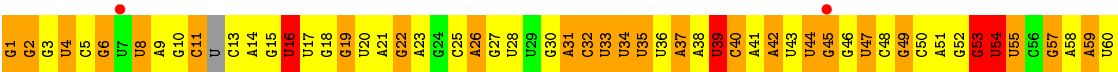


- Molecule 55: 50S ribosomal protein L35





● Molecule 56: tRNA<sup>Lys</sup>



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.70 Å   449.50 Å   620.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	152.17 – 3.15 152.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.17-3.15) 91.9 (152.17-3.15)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 3.13 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.192   ,   0.247 0.194   ,   0.249	Depositor DCC
$R_{free}$ test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	296184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	13	0.67	2/35994 (0.0%)	1.31	276/56171 (0.5%)
1	1G	0.58	0/36231	1.17	128/56544 (0.2%)
2	12	0.39	0/1752	0.71	0/2360
2	1E	0.46	1/1908 (0.1%)	0.69	3/2573 (0.1%)
3	22	0.39	0/1564	0.62	0/2109
3	2E	0.51	2/1629 (0.1%)	0.64	1/2195 (0.0%)
4	32	0.50	1/1732 (0.1%)	0.70	3/2318 (0.1%)
4	3E	0.54	2/1720 (0.1%)	0.69	0/2305
5	42	0.44	0/1150	0.66	1/1548 (0.1%)
5	4E	0.47	0/1158	0.68	1/1559 (0.1%)
6	52	0.52	0/855	0.66	1/1154 (0.1%)
6	5E	0.48	0/850	0.68	1/1147 (0.1%)
7	62	0.50	0/1127	0.67	0/1507
7	6E	0.39	0/1259	0.57	0/1686
8	72	0.36	0/1127	0.57	0/1517
8	7E	0.45	0/1135	0.72	2/1527 (0.1%)
9	82	0.37	0/971	0.71	0/1304
9	8E	0.42	0/1019	0.66	0/1367
10	1A	0.66	1/658 (0.2%)	0.63	0/885
10	1I	0.47	0/747	0.68	1/1006 (0.1%)
11	2A	0.38	0/850	0.58	0/1150
11	2I	0.40	0/838	0.62	0/1133
12	3A	0.44	0/972	0.70	0/1301
12	3I	0.55	0/972	0.78	1/1301 (0.1%)
13	4A	0.40	0/903	0.68	1/1211 (0.1%)
13	4I	0.49	0/952	0.67	0/1277
14	5A	0.40	0/495	0.71	1/657 (0.2%)
14	5I	0.45	0/500	0.73	1/664 (0.2%)
15	6A	0.42	0/744	0.58	0/992
15	6I	0.41	0/740	0.60	0/987
16	7A	0.48	1/721 (0.1%)	0.66	0/970
16	7I	0.44	0/716	0.69	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.41	0/836	0.59	0/1117
17	8I	0.48	2/847 (0.2%)	0.68	1/1131 (0.1%)
18	9A	0.44	0/549	0.63	0/732
18	9I	0.42	0/554	0.69	1/739 (0.1%)
19	AA	0.43	0/490	0.69	0/662
19	AI	0.49	0/668	0.73	0/899
20	BA	0.37	0/764	0.69	1/1007 (0.1%)
20	BI	0.40	0/748	0.76	1/986 (0.1%)
21	1B	0.44	0/192	0.63	0/252
21	1F	0.45	0/203	0.66	0/266
22	1K	0.58	0/1516	1.24	17/2350 (0.7%)
22	1L	0.48	0/1613	1.08	10/2504 (0.4%)
23	2K	0.74	0/1721	1.38	13/2682 (0.5%)
23	2L	0.63	0/1721	1.22	8/2682 (0.3%)
24	3K	0.49	0/1777	1.21	15/2767 (0.5%)
25	4K	0.77	0/495	1.38	6/771 (0.8%)
25	4L	0.69	0/470	1.27	2/732 (0.3%)
26	14	0.79	24/69023 (0.0%)	1.44	778/107740 (0.7%)
26	1H	0.88	50/68351 (0.1%)	1.58	1425/106700 (1.3%)
27	16	0.72	0/2928	1.46	42/4568 (0.9%)
27	1J	0.63	0/2928	1.30	18/4568 (0.4%)
28	71	0.34	0/1055	0.63	0/1425
28	79	0.31	0/459	0.57	0/608
29	11	0.75	6/2170 (0.3%)	0.93	4/2926 (0.1%)
29	19	0.58	0/2175	0.84	4/2933 (0.1%)
30	21	0.54	0/1591	0.86	2/2146 (0.1%)
30	29	0.68	5/1596 (0.3%)	1.00	7/2153 (0.3%)
31	31	0.55	0/1620	0.79	0/2194
31	39	0.48	0/1637	0.78	2/2218 (0.1%)
32	41	0.43	0/1481	0.74	1/1994 (0.1%)
32	49	0.53	3/1482 (0.2%)	0.72	1/1994 (0.1%)
33	51	0.56	1/1337 (0.1%)	0.85	4/1809 (0.2%)
33	59	0.50	1/582 (0.2%)	0.77	1/783 (0.1%)
34	61	0.42	0/1151	0.77	2/1558 (0.1%)
34	69	0.49	1/1146 (0.1%)	0.76	3/1551 (0.2%)
35	15	0.40	0/1131	0.65	1/1525 (0.1%)
35	58	0.49	1/1131 (0.1%)	0.73	1/1525 (0.1%)
36	25	0.56	2/942 (0.2%)	0.72	1/1269 (0.1%)
36	68	0.48	0/942	0.72	0/1269
37	35	0.61	1/1139 (0.1%)	0.90	1/1514 (0.1%)
37	78	0.54	0/1139	0.89	4/1514 (0.3%)
38	45	0.72	4/1120 (0.4%)	0.84	1/1498 (0.1%)
38	88	0.72	2/1134 (0.2%)	0.90	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	55	0.50	0/981	0.80	1/1312 (0.1%)
39	98	0.45	0/981	0.80	1/1312 (0.1%)
40	65	0.49	0/886	0.83	2/1180 (0.2%)
40	A8	0.56	0/884	0.76	0/1178
41	75	0.61	3/1123 (0.3%)	0.72	0/1500
41	B8	0.62	2/1123 (0.2%)	0.76	1/1500 (0.1%)
42	85	0.49	0/977	0.70	0/1301
42	C8	0.55	1/968 (0.1%)	0.76	1/1289 (0.1%)
43	95	0.57	0/785	0.85	2/1052 (0.2%)
43	D8	0.52	0/785	0.81	2/1052 (0.2%)
44	A5	0.56	0/910	0.73	0/1220
44	E8	0.51	0/901	0.77	0/1209
45	B5	0.55	0/749	0.77	1/1007 (0.1%)
45	F8	0.60	0/757	0.81	2/1017 (0.2%)
46	C5	0.51	0/807	0.89	2/1076 (0.2%)
46	G8	0.68	2/809 (0.2%)	1.05	4/1080 (0.4%)
47	D5	0.49	0/1098	0.75	0/1487
47	H8	0.46	0/1403	0.75	2/1901 (0.1%)
48	E5	0.50	0/616	0.77	0/821
48	I8	0.75	2/614 (0.3%)	0.86	1/819 (0.1%)
49	F5	0.52	0/744	0.81	0/989
49	J8	0.59	0/744	0.83	1/989 (0.1%)
50	G5	0.52	0/560	0.75	0/741
50	K8	0.84	4/570 (0.7%)	0.86	0/755
51	H5	0.42	0/464	0.65	1/623 (0.2%)
51	L8	0.53	0/464	0.73	0/623
52	M8	0.41	0/375	0.86	2/507 (0.4%)
53	J5	0.49	0/448	0.70	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.54	0/409	0.84	1/540 (0.2%)
54	P8	0.62	0/409	0.88	0/540
55	M5	0.66	1/524 (0.2%)	0.81	1/691 (0.1%)
55	Q8	0.56	0/524	1.02	2/691 (0.3%)
56	3L	0.54	0/1729	1.28	17/2690 (0.6%)
All	All	0.70	128/317045 (0.0%)	1.28	2847/474982 (0.6%)

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	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	3
4	3E	0	1
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	4
13	4A	0	3
13	4I	0	2
14	5A	0	3
14	5I	0	1
16	7I	0	2
18	9I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	3
20	BI	0	1
29	11	0	7
29	19	0	5
30	21	0	8
30	29	0	7
31	31	0	2
31	39	0	8
32	41	0	1
32	49	0	6
33	51	0	5
33	59	0	5
34	61	0	4
34	69	0	3
35	58	0	2
37	35	0	4
37	78	0	4
38	45	0	4
39	55	0	1
40	65	0	1
40	A8	0	1
41	75	0	1
42	85	0	4
42	C8	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	95	0	3
43	D8	0	3
44	A5	0	1
45	F8	0	1
46	C5	0	3
46	G8	0	4
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	4
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	169

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	2572	A	N7-C5	24.38	1.53	1.39
26	14	2572	A	N9-C8	-21.02	1.21	1.37
26	14	2572	A	C5-C4	-18.45	1.25	1.38
26	14	2572	A	C5-C6	-15.84	1.26	1.41
26	1H	774	A	N9-C4	-12.29	1.30	1.37

The worst 5 of 2847 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2572	A	N9-C4-C5	28.35	117.14	105.80
26	14	2572	A	C4-C5-C6	24.01	129.00	117.00
26	14	2572	A	C4-C5-N7	-20.90	100.25	110.70
26	1H	1899	G	N3-C4-N9	-19.20	114.48	126.00
26	14	2572	A	N7-C8-N9	18.60	123.10	113.80

There are no chirality outliers.

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
4	3E	82	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	754	0
1	1G	32368	0	16343	752	1
2	12	1721	0	1758	119	0
2	1E	1874	0	1926	112	0
3	22	1541	0	1606	76	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1765	101	0
4	3E	1690	0	1738	92	0
5	42	1134	0	1200	69	0
5	4E	1142	0	1204	51	0
6	52	842	0	857	28	0
6	5E	837	0	852	29	0
7	62	1115	0	1165	57	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	54	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	72	0
9	8E	1000	0	1031	69	0
10	1A	646	0	662	48	0
10	1I	734	0	761	53	0
11	2A	835	0	847	47	0
11	2I	823	0	833	37	0
12	3A	956	0	1046	54	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	55	0
13	4I	942	0	997	48	0
14	5A	486	0	524	28	0
14	5I	491	0	530	36	0
15	6A	733	0	771	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	26	0
16	7A	705	0	725	37	0
16	7I	700	0	720	51	0
17	8A	823	0	891	41	0
17	8I	834	0	904	59	0
18	9A	544	0	605	25	0
18	9I	549	0	607	22	0
19	AA	481	0	468	19	0
19	AI	654	0	675	52	0
20	BA	762	0	861	39	0
20	BI	746	0	843	50	0
21	1B	188	0	195	17	0
21	1F	199	0	208	15	0
22	1K	1477	0	758	30	0
22	1L	1563	0	799	31	0
23	2K	1646	0	844	19	0
23	2L	1646	0	844	33	0
24	3K	1611	0	817	74	0
25	4K	439	0	218	10	0
25	4L	417	0	207	11	0
26	14	61630	0	31072	1406	1
26	1H	61028	0	30762	1443	0
27	16	2617	0	1328	70	0
27	1J	2617	0	1328	79	0
28	7I	1033	0	1048	71	0
28	79	456	0	460	31	0
29	11	2120	0	2197	151	0
29	19	2125	0	2199	133	0
30	21	1558	0	1624	96	0
30	29	1563	0	1629	134	0
31	31	1585	0	1632	94	0
31	39	1602	0	1649	96	0
32	41	1457	0	1514	91	0
32	49	1458	0	1516	72	0
33	51	1312	0	1384	64	0
33	59	573	0	597	43	0
34	61	1136	0	1223	60	0
34	69	1131	0	1218	73	0
35	15	1104	0	1180	51	0
35	58	1104	0	1180	58	0
36	25	932	0	996	55	0
36	68	932	0	996	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	35	1122	0	1206	93	0
37	78	1122	0	1206	109	0
38	45	1099	0	1154	94	0
38	88	1113	0	1157	56	0
39	55	967	0	1033	56	0
39	98	967	0	1033	64	0
40	65	876	0	938	57	0
40	A8	875	0	936	54	0
41	75	1109	0	1169	74	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	54	0
42	C8	950	0	1011	53	0
43	95	774	0	849	82	0
43	D8	774	0	849	58	0
44	A5	899	0	964	34	0
44	E8	890	0	951	33	0
45	B5	735	0	785	43	0
45	F8	743	0	794	39	0
46	C5	794	0	886	74	0
46	G8	796	0	886	53	0
47	D5	1074	0	1086	63	0
47	H8	1373	0	1402	81	0
48	E5	608	0	622	37	0
48	I8	606	0	625	31	0
49	F5	737	0	813	41	0
49	J8	737	0	813	28	0
50	G5	558	0	610	33	0
50	K8	568	0	614	31	0
51	H5	459	0	512	15	0
51	L8	459	0	512	18	0
52	M8	366	0	370	31	0
53	J5	434	0	454	24	0
53	N8	369	0	388	22	0
54	L5	401	0	436	13	0
54	P8	401	0	436	17	0
55	M5	516	0	582	34	0
55	Q8	516	0	582	49	0
56	3L	1601	0	814	69	0
57	11	3	0	0	0	0
57	13	150	0	0	0	0
57	14	454	0	0	0	0
57	16	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	93	0	0	0	0
57	1H	502	0	0	0	0
57	1I	1	0	0	0	0
57	1J	6	0	0	0	0
57	2I	3	0	0	0	0
57	29	4	0	0	0	0
57	2K	3	0	0	0	0
57	2L	4	0	0	0	0
57	3I	1	0	0	0	0
57	31	1	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	4I	2	0	0	0	0
57	45	3	0	0	0	0
57	55	1	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	88	1	0	0	0	0
57	BI	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	45	3	0
58	1G	42	0	45	2	0
59	32	8	0	0	2	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	12	0	0	1	0
61	13	319	0	0	23	0
61	14	1015	0	0	117	0
61	16	26	0	0	6	0
61	19	12	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1F	1	0	0	0	0
61	1G	226	0	0	16	0
61	1H	1158	0	0	132	0
61	1I	1	0	0	0	0
61	1J	18	0	0	2	0
61	1K	1	0	0	0	0
61	2I	6	0	0	1	0
61	29	6	0	0	0	0
61	2K	7	0	0	0	0
61	2L	1	0	0	0	0
61	3I	9	0	0	0	0
61	32	3	0	0	0	0
61	35	5	0	0	1	0
61	39	8	0	0	1	0
61	3A	1	0	0	0	0
61	3E	3	0	0	0	0
61	3I	3	0	0	1	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4E	3	0	0	1	0
61	4K	4	0	0	0	0
61	4L	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	1	0	0	1	0
61	6A	3	0	0	0	0
61	6I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	6	0	0	1	0
61	85	2	0	0	0	0
61	88	2	0	0	0	0
61	8A	1	0	0	0	0
61	8E	1	0	0	0	0
61	8I	2	0	0	0	0
61	A5	2	0	0	0	0
61	B5	1	0	0	0	0
61	BA	3	0	0	1	0
61	BI	5	0	0	0	0
61	C5	4	0	0	0	0
61	C8	2	0	0	0	0
61	E8	3	0	0	0	0
61	F8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	G8	2	0	0	0	0
61	H5	3	0	0	0	0
61	I8	5	0	0	1	0
61	J8	3	0	0	0	0
61	K8	2	0	0	0	0
61	L5	2	0	0	0	0
61	L8	2	0	0	0	0
61	M5	10	0	0	0	0
61	P8	1	0	0	0	0
61	Q8	9	0	0	2	0
All	All	296184	0	196367	8846	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 8846 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)
37:35:81:GLN:NE2	37:35:106:LEU:HA	1.45	1.29
15:6A:27:VAL:O	15:6A:31:LEU:HD13	1.26	1.27
26:14:2572:A:C5	30:29:144:ARG:NH1	2.04	1.25
37:35:81:GLN:CD	37:35:106:LEU:HA	1.58	1.24
29:19:69:ARG:NH2	29:19:130:ALA:H	1.33	1.21

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	206/256 (80%)	175 (85%)	24 (12%)	7 (3%)	3	21
2	1E	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	17	53
3	22	192/239 (80%)	169 (88%)	23 (12%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	15	51
4	3E	205/209 (98%)	188 (92%)	16 (8%)	1 (0%)	29	65
5	42	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	22	59
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	135/156 (86%)	122 (90%)	12 (9%)	1 (1%)	22	59
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	10	41
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	59
9	82	119/128 (93%)	108 (91%)	9 (8%)	2 (2%)	9	38
9	8E	124/128 (97%)	105 (85%)	18 (14%)	1 (1%)	19	55
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	89/105 (85%)	82 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	98 (88%)	11 (10%)	2 (2%)	8	37
11	2I	109/129 (84%)	95 (87%)	12 (11%)	2 (2%)	8	37
12	3A	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	4	22
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	55
13	4A	109/126 (86%)	92 (84%)	15 (14%)	2 (2%)	8	37
13	4I	117/126 (93%)	98 (84%)	18 (15%)	1 (1%)	17	53
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	8	37
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	21
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10	41
19	AA	56/93 (60%)	49 (88%)	4 (7%)	3 (5%)	2	12
19	AI	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	5	29
20	BA	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	7	33
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	244 (90%)	17 (6%)	10 (4%)	3	19
29	19	272/276 (99%)	245 (90%)	21 (8%)	6 (2%)	6	32
30	21	201/206 (98%)	156 (78%)	36 (18%)	9 (4%)	2	16
30	29	202/206 (98%)	154 (76%)	39 (19%)	9 (4%)	2	16
31	31	200/210 (95%)	179 (90%)	20 (10%)	1 (0%)	29	65
31	39	202/210 (96%)	161 (80%)	31 (15%)	10 (5%)	2	14
32	41	177/182 (97%)	153 (86%)	21 (12%)	3 (2%)	9	38
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	14	48
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	11
33	59	68/180 (38%)	49 (72%)	14 (21%)	5 (7%)	1	6
34	61	144/148 (97%)	116 (81%)	26 (18%)	2 (1%)	11	43
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	7	33
35	15	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	22	59
35	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	4	25
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	55
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	116 (80%)	25 (17%)	4 (3%)	5	26
37	78	145/150 (97%)	115 (79%)	26 (18%)	4 (3%)	5	26
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	4	25
38	88	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	20
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	102 (88%)	13 (11%)	1 (1%)	17	53
40	65	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	8	36
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	116 (88%)	15 (12%)	0	100	100
41	B8	131/146 (90%)	118 (90%)	12 (9%)	1 (1%)	19	55
42	85	114/118 (97%)	101 (89%)	12 (10%)	1 (1%)	17	53
42	C8	113/118 (96%)	100 (88%)	10 (9%)	3 (3%)	5	27
43	95	98/101 (97%)	75 (76%)	19 (19%)	4 (4%)	3	18
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	3	18
44	A5	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	17	53
44	E8	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
45	B5	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	32
45	F8	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	14	48
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	7
46	G8	103/110 (94%)	85 (82%)	13 (13%)	5 (5%)	2	14
47	D5	126/206 (61%)	99 (79%)	20 (16%)	7 (6%)	2	12
47	H8	169/206 (82%)	132 (78%)	31 (18%)	6 (4%)	3	20
48	E5	75/85 (88%)	64 (85%)	9 (12%)	2 (3%)	5	27
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	14	48
49	J8	92/98 (94%)	85 (92%)	4 (4%)	3 (3%)	4	22
50	G5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	9	40
50	K8	66/72 (92%)	58 (88%)	6 (9%)	2 (3%)	4	24
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
52	M8	45/71 (63%)	30 (67%)	14 (31%)	1 (2%)	6	32
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	15
All	All	10975/12333 (89%)	9578 (87%)	1200 (11%)	197 (2%)	8	37

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU
29	11	273	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	172 (94%)	10 (6%)	21	54
2	1E	200/220 (91%)	183 (92%)	17 (8%)	10	36
3	22	154/188 (82%)	147 (96%)	7 (4%)	27	61
3	2E	159/188 (85%)	151 (95%)	8 (5%)	24	57
4	32	180/181 (99%)	167 (93%)	13 (7%)	14	43
4	3E	178/181 (98%)	166 (93%)	12 (7%)	16	47
5	42	114/123 (93%)	104 (91%)	10 (9%)	10	34
5	4E	115/123 (94%)	112 (97%)	3 (3%)	46	74
6	52	90/90 (100%)	86 (96%)	4 (4%)	28	61
6	5E	90/90 (100%)	85 (94%)	5 (6%)	21	53
7	62	114/127 (90%)	105 (92%)	9 (8%)	12	40
7	6E	125/127 (98%)	109 (87%)	16 (13%)	4	18
8	72	118/119 (99%)	107 (91%)	11 (9%)	9	31
8	7E	119/119 (100%)	111 (93%)	8 (7%)	16	47
9	82	92/99 (93%)	80 (87%)	12 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	91 (94%)	6 (6%)	18	50
10	1A	71/92 (77%)	63 (89%)	8 (11%)	6	23
10	1I	81/92 (88%)	79 (98%)	2 (2%)	47	75
11	2A	85/99 (86%)	82 (96%)	3 (4%)	36	67
11	2I	84/99 (85%)	82 (98%)	2 (2%)	49	76
12	3A	103/109 (94%)	92 (89%)	11 (11%)	6	25
12	3I	103/109 (94%)	97 (94%)	6 (6%)	20	52
13	4A	91/101 (90%)	81 (89%)	10 (11%)	6	24
13	4I	94/101 (93%)	85 (90%)	9 (10%)	8	29
14	5A	49/50 (98%)	43 (88%)	6 (12%)	5	20
14	5I	49/50 (98%)	47 (96%)	2 (4%)	30	63
15	6A	79/80 (99%)	74 (94%)	5 (6%)	18	49
15	6I	79/80 (99%)	75 (95%)	4 (5%)	24	56
16	7A	72/74 (97%)	66 (92%)	6 (8%)	11	37
16	7I	72/74 (97%)	69 (96%)	3 (4%)	30	62
17	8A	94/97 (97%)	89 (95%)	5 (5%)	22	55
17	8I	95/97 (98%)	87 (92%)	8 (8%)	11	37
18	9A	58/77 (75%)	56 (97%)	2 (3%)	37	68
18	9I	58/77 (75%)	55 (95%)	3 (5%)	23	55
19	AA	52/80 (65%)	49 (94%)	3 (6%)	20	52
19	AI	71/80 (89%)	64 (90%)	7 (10%)	8	28
20	BA	76/82 (93%)	72 (95%)	4 (5%)	22	55
20	BI	75/82 (92%)	72 (96%)	3 (4%)	31	64
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	51
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	71	109/181 (60%)	104 (95%)	5 (5%)	27	60
28	79	48/181 (26%)	41 (85%)	7 (15%)	3	14
29	11	214/218 (98%)	194 (91%)	20 (9%)	9	31
29	19	214/218 (98%)	198 (92%)	16 (8%)	13	42
30	21	165/166 (99%)	158 (96%)	7 (4%)	30	62
30	29	165/166 (99%)	155 (94%)	10 (6%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	151 (94%)	10 (6%)	18	50
31	39	163/166 (98%)	159 (98%)	4 (2%)	47	75
32	41	153/156 (98%)	142 (93%)	11 (7%)	14	43
32	49	153/156 (98%)	141 (92%)	12 (8%)	12	40
33	51	142/148 (96%)	134 (94%)	8 (6%)	21	53
33	59	59/148 (40%)	54 (92%)	5 (8%)	10	36
34	61	122/124 (98%)	114 (93%)	8 (7%)	16	47
34	69	122/124 (98%)	115 (94%)	7 (6%)	20	53
35	15	117/119 (98%)	112 (96%)	5 (4%)	29	62
35	58	117/119 (98%)	107 (92%)	10 (8%)	10	36
36	25	100/100 (100%)	96 (96%)	4 (4%)	31	64
36	68	100/100 (100%)	98 (98%)	2 (2%)	55	79
37	35	114/116 (98%)	106 (93%)	8 (7%)	15	45
37	78	114/116 (98%)	109 (96%)	5 (4%)	28	61
38	45	109/111 (98%)	98 (90%)	11 (10%)	7	27
38	88	109/111 (98%)	99 (91%)	10 (9%)	9	31
39	55	101/101 (100%)	96 (95%)	5 (5%)	24	57
39	98	101/101 (100%)	93 (92%)	8 (8%)	12	40
40	65	87/88 (99%)	79 (91%)	8 (9%)	9	31
40	A8	86/88 (98%)	75 (87%)	11 (13%)	4	18
41	75	117/127 (92%)	104 (89%)	13 (11%)	6	24
41	B8	117/127 (92%)	105 (90%)	12 (10%)	7	26
42	85	93/94 (99%)	86 (92%)	7 (8%)	13	42
42	C8	92/94 (98%)	83 (90%)	9 (10%)	8	28
43	95	82/82 (100%)	75 (92%)	7 (8%)	10	36
43	D8	82/82 (100%)	79 (96%)	3 (4%)	34	66
44	A5	92/92 (100%)	84 (91%)	8 (9%)	10	34
44	E8	91/92 (99%)	81 (89%)	10 (11%)	6	24
45	B5	74/78 (95%)	69 (93%)	5 (7%)	16	46
45	F8	75/78 (96%)	72 (96%)	3 (4%)	31	64
46	C5	85/91 (93%)	77 (91%)	8 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	85/91 (93%)	77 (91%)	8 (9%)	8	30
47	D5	118/179 (66%)	111 (94%)	7 (6%)	19	51
47	H8	152/179 (85%)	143 (94%)	9 (6%)	19	51
48	E5	61/67 (91%)	59 (97%)	2 (3%)	38	69
48	I8	61/67 (91%)	60 (98%)	1 (2%)	62	83
49	F5	79/83 (95%)	74 (94%)	5 (6%)	18	49
49	J8	79/83 (95%)	76 (96%)	3 (4%)	33	65
50	G5	62/67 (92%)	57 (92%)	5 (8%)	11	39
50	K8	62/67 (92%)	58 (94%)	4 (6%)	17	48
51	H5	50/52 (96%)	45 (90%)	5 (10%)	7	28
51	L8	50/52 (96%)	47 (94%)	3 (6%)	19	51
52	M8	42/63 (67%)	38 (90%)	4 (10%)	8	30
53	J5	48/52 (92%)	46 (96%)	2 (4%)	30	62
53	N8	43/52 (83%)	40 (93%)	3 (7%)	15	45
54	L5	38/42 (90%)	35 (92%)	3 (8%)	12	40
54	P8	38/42 (90%)	34 (90%)	4 (10%)	7	26
55	M5	54/55 (98%)	52 (96%)	2 (4%)	34	66
55	Q8	54/55 (98%)	52 (96%)	2 (4%)	34	66
All	All	9274/10193 (91%)	8636 (93%)	638 (7%)	15	46

5 of 638 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	121	HIS
6	52	28	ARG
44	A5	67	ASP
50	K8	4	SER
2	12	191	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	40	HIS
5	42	127	ASN
47	D5	75	ASN

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Mol	Chain	Res	Type
2	12	224	GLN
5	42	78	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	362 (24%)	32 (2%)
1	1G	1503/1522 (98%)	365 (24%)	35 (2%)
22	1K	65/76 (85%)	32 (49%)	3 (4%)
22	1L	69/76 (90%)	37 (53%)	3 (4%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	75/76 (98%)	49 (65%)	3 (4%)
25	4K	19/27 (70%)	10 (52%)	1 (5%)
25	4L	18/27 (66%)	10 (55%)	1 (5%)
26	14	2852/2917 (97%)	745 (26%)	45 (1%)
26	1H	2828/2917 (96%)	684 (24%)	52 (1%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
56	3L	73/76 (96%)	44 (60%)	5 (6%)
All	All	9389/9634 (97%)	2432 (25%)	189 (2%)

5 of 2432 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	28	G

5 of 189 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2225	A
1	1G	429	U
26	14	1992	G
26	1H	2476	A
27	16	108	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	U8U	1K	34	25,22	17,24,25	2.52	5 (29%)	19,34,37	1.63	3 (15%)
22	T6A	1K	37	22	24,34,35	2.86	5 (20%)	24,49,52	2.79	7 (29%)
22	PSU	1K	55	22	17,21,22	1.02	1 (5%)	20,30,33	3.38	6 (30%)
22	T6A	1L	37	22	24,34,35	2.66	5 (20%)	24,49,52	2.72	8 (33%)
23	OMC	2K	33	23	15,22,23	2.26	4 (26%)	17,31,34	1.43	3 (17%)
23	4SU	2L	8	23	14,21,22	3.45	2 (14%)	15,30,33	0.86	1 (6%)
24	PSU	3K	39	24	17,21,22	1.15	2 (11%)	20,30,33	3.48	6 (30%)
23	PSU	2K	56	23	17,21,22	1.09	1 (5%)	20,30,33	2.98	5 (25%)
22	5MU	1K	54	22	15,22,23	2.17	3 (20%)	16,32,35	1.81	2 (12%)
23	OMC	2L	33	23	15,22,23	2.61	4 (26%)	17,31,34	1.67	3 (17%)
22	PSU	1L	55	22	17,21,22	1.06	1 (5%)	20,30,33	3.35	6 (30%)
56	PSU	3L	39	56	17,21,22	1.26	3 (17%)	20,30,33	4.91	9 (45%)
23	5MU	2K	55	23	15,22,23	2.11	3 (20%)	16,32,35	1.80	2 (12%)
22	PSU	1L	39	22	17,21,22	1.02	1 (5%)	20,30,33	3.18	6 (30%)
23	PSU	2L	56	23	17,21,22	1.10	1 (5%)	20,30,33	3.51	5 (25%)
22	5MU	1L	54	22	15,22,23	2.17	3 (20%)	16,32,35	1.78	2 (12%)
22	PSU	1K	39	22	17,21,22	1.04	2 (11%)	20,30,33	3.11	6 (30%)
56	T6A	3L	37	56	24,34,35	2.69	4 (16%)	24,49,52	2.37	9 (37%)
23	G7M	2L	47	23	20,26,27	3.44	7 (35%)	20,39,42	2.29	6 (30%)
23	G7M	2K	47	23	20,26,27	3.44	6 (30%)	20,39,42	1.82	4 (20%)
23	4SU	2K	8	23	14,21,22	3.37	2 (14%)	15,30,33	1.21	2 (13%)
23	5MU	2L	55	23	15,22,23	2.23	3 (20%)	16,32,35	1.72	2 (12%)
22	U8U	1L	34	25,22	17,24,25	2.60	5 (29%)	19,34,37	1.51	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	U8U	1K	34	25,22	-	2/7/28/29	0/2/2/2
22	T6A	1K	37	22	-	2/15/41/42	0/3/3/3
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	6/15/41/42	0/3/3/3
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
23	4SU	2L	8	23	-	0/5/25/26	0/2/2/2
24	PSU	3K	39	24	-	4/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/7/27/28	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
56	PSU	3L	39	56	-	2/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/5/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
56	T6A	3L	37	56	-	8/15/41/42	0/3/3/3
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/5/25/26	0/2/2/2
22	U8U	1L	34	25,22	-	1/7/28/29	0/2/2/2

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	8	4SU	C5-C4	9.99	1.49	1.38
23	2K	8	4SU	C5-C4	9.93	1.49	1.38
23	2K	47	G7M	C4-N3	8.42	1.48	1.35
56	3L	37	T6A	C6-N6	8.37	1.51	1.36
23	2L	47	G7M	C4-N3	8.23	1.48	1.35

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	3L	39	PSU	C5-C1'-C2'	-15.88	86.99	115.32
23	2L	56	PSU	N1-C2-N3	-11.86	119.00	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	39	PSU	N1-C2-N3	-11.06	119.64	128.43
22	1K	39	PSU	N1-C2-N3	-11.02	119.67	128.43
22	1L	55	PSU	N1-C2-N3	-10.85	119.81	128.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10
22	1L	37	T6A	C14-C12-N11-C10
22	1L	37	T6A	C13-C12-C14-O14
24	3K	39	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	34	U8U	1	0
22	1L	37	T6A	2	0
23	2L	8	4SU	2	0
22	1K	54	5MU	1	0
56	3L	39	PSU	1	0
23	2K	55	5MU	2	0
23	2L	56	PSU	3	0
56	3L	37	T6A	2	0
23	2L	47	G7M	4	0
23	2K	8	4SU	1	0
23	2L	55	5MU	3	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1269 ligands modelled in this entry, 1265 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	SF4	3E	301	4	0,12,12	0.00	-	-		
59	SF4	32	301	-	0,12,12	0.00	-	-		
58	PAR	13	1749	-	45,45,45	0.85	0	64,67,67	2.01	16 (25%)
58	PAR	1G	1691	-	45,45,45	0.71	0	64,67,67	1.73	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	13	1749	-	-	4/18/94/94	0/4/4/4
59	SF4	3E	301	4	-	-	0/6/5/5
58	PAR	1G	1691	-	-	6/18/94/94	0/4/4/4
59	SF4	32	301	-	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	C22-C12-C62	-4.86	102.69	110.04
58	13	1749	PAR	C14-O33-C33	-4.70	106.32	117.96
58	1G	1691	PAR	O11-C11-C21	-4.60	100.30	108.22
58	13	1749	PAR	C11-O51-C51	4.53	122.58	113.69
58	13	1749	PAR	C14-O54-C54	4.32	122.17	113.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

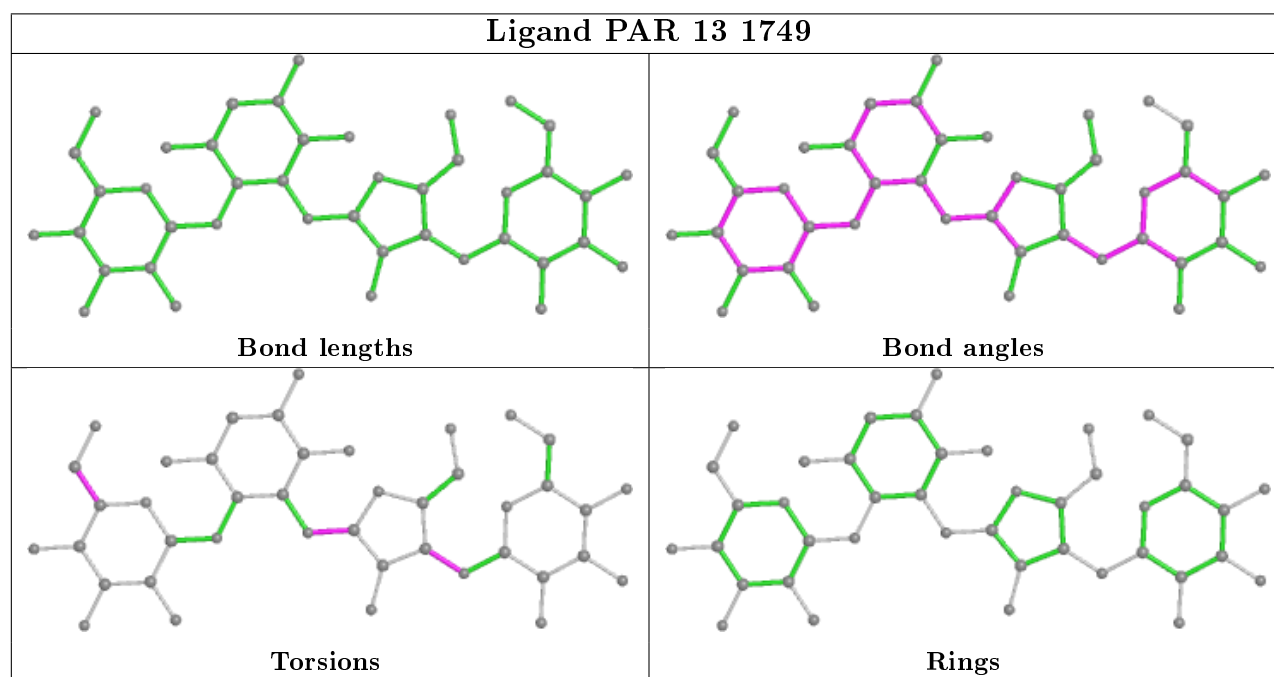
Mol	Chain	Res	Type	Atoms
58	13	1749	PAR	C41-C51-C61-O61
58	1G	1691	PAR	C33-C43-C53-O53
58	1G	1691	PAR	O43-C43-C53-O53
58	13	1749	PAR	O51-C51-C61-O61
58	1G	1691	PAR	O43-C13-O52-C52

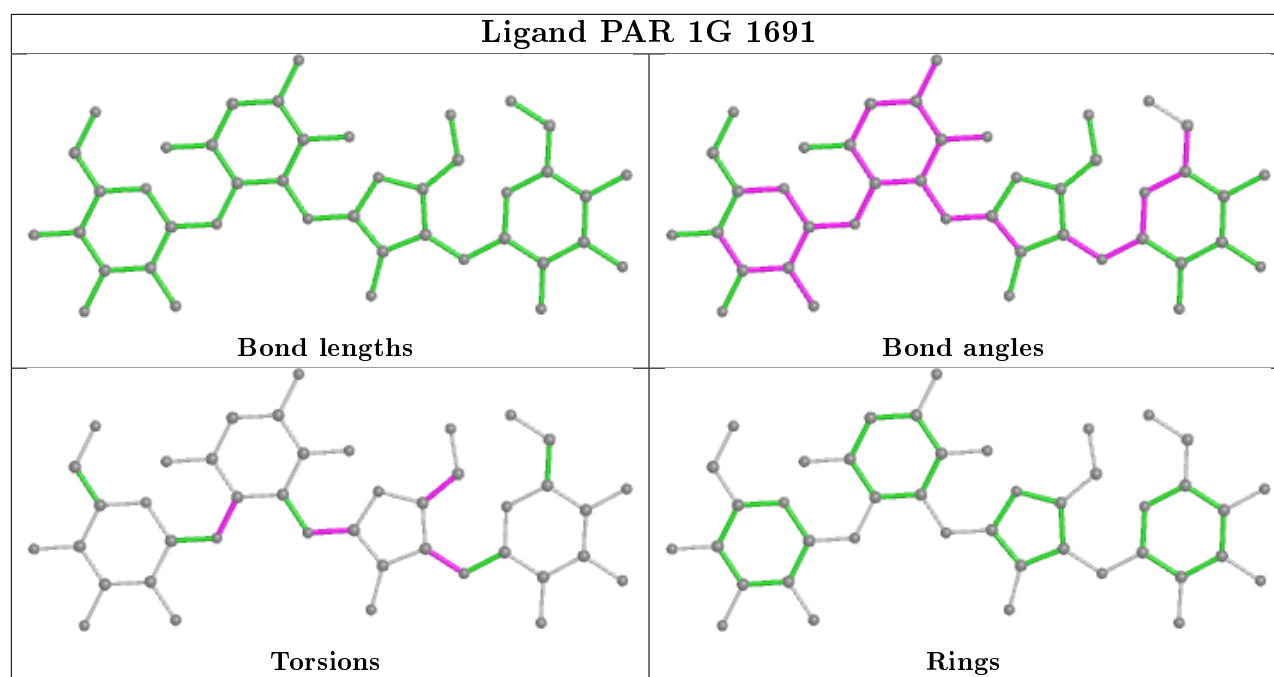
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	301	SF4	2	0
58	13	1749	PAR	3	0
58	1G	1691	PAR	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	69	1
4	3E	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3E	36:ARG	C	37:PRO	N	1.17
1	69	79:ILE	C	80:PRO	N	1.16
1	1A	76:ASN	C	77:PRO	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(Å²)	Q<0.9
1	13	1496/1522 (98%)	-0.82	2 (0%)	95	95	58, 99, 162, 246	0
1	1G	1506/1522 (98%)	-0.86	1 (0%)	95	95	73, 114, 168, 253	0
2	12	210/256 (82%)	0.45	15 (7%)	16	8	127, 152, 169, 182	0
2	1E	231/256 (90%)	0.44	16 (6%)	16	9	105, 136, 157, 168	0
3	22	196/239 (82%)	1.11	45 (22%)	0	0	122, 138, 165, 170	0
3	2E	205/239 (85%)	0.46	11 (5%)	25	13	81, 103, 128, 138	0
4	32	208/209 (99%)	0.99	43 (20%)	1	0	98, 118, 136, 144	0
4	3E	207/209 (99%)	0.54	20 (9%)	7	4	80, 101, 121, 129	0
5	42	148/162 (91%)	0.40	6 (4%)	37	22	104, 121, 137, 147	0
5	4E	149/162 (91%)	0.55	13 (8%)	10	5	79, 96, 112, 121	0
6	52	101/101 (100%)	0.58	10 (9%)	7	4	83, 101, 118, 131	0
6	5E	100/101 (99%)	0.88	13 (13%)	3	2	83, 100, 115, 121	0
7	62	139/156 (89%)	0.17	4 (2%)	51	35	111, 124, 135, 141	0
7	6E	154/156 (98%)	-0.07	3 (1%)	66	53	101, 115, 132, 141	0
8	72	137/138 (99%)	0.41	8 (5%)	23	12	104, 124, 136, 142	0
8	7E	138/138 (100%)	0.57	11 (7%)	12	6	91, 106, 118, 127	0
9	82	121/128 (94%)	0.20	3 (2%)	57	42	110, 151, 165, 175	0
9	8E	126/128 (98%)	-0.18	0	100	100	89, 128, 147, 153	0
10	1A	80/105 (76%)	-0.01	1 (1%)	77	66	116, 145, 154, 156	0
10	1I	91/105 (86%)	0.24	7 (7%)	13	6	80, 121, 156, 161	0
11	2A	113/129 (87%)	0.82	16 (14%)	2	1	86, 110, 123, 130	0
11	2I	111/129 (86%)	0.91	15 (13%)	3	2	77, 102, 118, 125	0
12	3A	122/132 (92%)	1.17	31 (25%)	0	0	84, 102, 126, 145	0
12	3I	122/132 (92%)	0.40	5 (4%)	37	22	67, 77, 99, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	111/126 (88%)	0.61	9 (8%) 12 6	109, 138, 154, 162	0
13	4I	119/126 (94%)	0.12	2 (1%) 70 57	84, 113, 128, 142	0
14	5A	59/61 (96%)	0.79	13 (22%) 0 0	122, 135, 145, 150	0
14	5I	60/61 (98%)	-0.33	0 100 100	82, 92, 108, 112	0
15	6A	88/89 (98%)	0.07	3 (3%) 45 28	89, 109, 128, 132	0
15	6I	87/89 (97%)	0.29	1 (1%) 80 70	83, 99, 116, 124	0
16	7A	84/88 (95%)	0.07	1 (1%) 79 68	92, 107, 125, 140	0
16	7I	83/88 (94%)	-0.26	0 100 100	97, 106, 136, 155	0
17	8A	99/105 (94%)	0.48	9 (9%) 9 5	95, 114, 127, 134	0
17	8I	100/105 (95%)	0.32	5 (5%) 28 15	88, 104, 115, 121	0
18	9A	67/88 (76%)	0.90	9 (13%) 3 2	93, 111, 130, 132	0
18	9I	68/88 (77%)	1.64	22 (32%) 0 0	87, 102, 124, 127	0
19	AA	62/93 (66%)	0.43	5 (8%) 12 6	123, 142, 153, 156	0
19	AI	81/93 (87%)	0.41	3 (3%) 41 25	91, 110, 132, 138	0
20	BA	99/106 (93%)	-0.06	2 (2%) 65 50	90, 110, 133, 142	0
20	BI	97/106 (91%)	-0.12	1 (1%) 82 73	104, 121, 147, 152	0
21	1B	22/27 (81%)	0.04	2 (9%) 9 5	119, 130, 141, 145	0
21	1F	23/27 (85%)	-0.35	0 100 100	89, 102, 110, 112	0
22	1K	64/76 (84%)	0.37	8 (12%) 3 2	84, 173, 191, 198	0
22	1L	68/76 (89%)	1.45	19 (27%) 0 0	115, 198, 216, 220	0
23	2K	72/77 (93%)	-0.54	0 100 100	74, 96, 123, 139	0
23	2L	72/77 (93%)	-0.48	0 100 100	81, 109, 138, 153	0
24	3K	75/76 (98%)	-0.33	3 (4%) 38 23	76, 207, 224, 234	0
25	4K	20/27 (74%)	0.14	2 (10%) 7 4	73, 133, 219, 222	0
25	4L	19/27 (70%)	0.29	2 (10%) 6 3	92, 146, 215, 217	0
26	14	2861/2917 (98%)	-0.59	18 (0%) 89 84	54, 86, 192, 250	0
26	1H	2833/2917 (97%)	-0.61	12 (0%) 92 89	44, 76, 171, 250	0
27	16	122/122 (100%)	-0.83	1 (0%) 86 78	69, 93, 114, 188	0
27	1J	122/122 (100%)	-0.87	0 100 100	87, 113, 134, 182	0
28	71	133/229 (58%)	1.48	45 (33%) 0 0	135, 198, 223, 231	0
28	79	57/229 (24%)	1.56	22 (38%) 0 0	141, 174, 199, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	11	273/276 (98%)	0.32	7 (2%) 56 40	43, 68, 86, 96	0
29	19	274/276 (99%)	0.45	13 (4%) 31 17	52, 75, 91, 115	0
30	21	203/206 (98%)	0.66	29 (14%) 2 1	55, 93, 129, 137	0
30	29	204/206 (99%)	0.40	16 (7%) 13 6	63, 94, 125, 142	0
31	31	202/210 (96%)	0.11	6 (2%) 50 33	49, 80, 114, 128	0
31	39	204/210 (97%)	0.52	20 (9%) 7 4	60, 101, 144, 170	0
32	41	179/182 (98%)	0.45	15 (8%) 11 5	80, 101, 132, 143	0
32	49	179/182 (98%)	1.36	47 (26%) 0 0	107, 123, 144, 167	0
33	51	171/180 (95%)	0.34	11 (6%) 19 10	84, 103, 118, 126	0
33	59	74/180 (41%)	0.50	10 (13%) 3 2	127, 155, 176, 191	0
34	61	146/148 (98%)	0.68	17 (11%) 4 2	80, 125, 142, 155	0
34	69	145/148 (97%)	0.86	23 (15%) 1 1	86, 121, 142, 152	0
35	15	138/140 (98%)	0.74	14 (10%) 7 3	80, 104, 132, 141	0
35	58	138/140 (98%)	0.65	13 (9%) 8 4	67, 94, 126, 137	0
36	25	122/122 (100%)	0.37	4 (3%) 46 29	69, 87, 103, 112	0
36	68	122/122 (100%)	0.25	4 (3%) 46 29	61, 79, 95, 103	0
37	35	147/150 (98%)	0.52	13 (8%) 10 5	60, 102, 129, 139	0
37	78	147/150 (98%)	0.03	4 (2%) 54 38	50, 84, 111, 117	0
38	45	138/141 (97%)	1.28	29 (21%) 1 0	74, 100, 118, 130	0
38	88	141/141 (100%)	0.47	8 (5%) 23 12	61, 80, 100, 123	0
39	55	118/118 (100%)	-0.11	0 100 100	64, 80, 96, 107	0
39	98	118/118 (100%)	0.51	8 (6%) 17 9	66, 89, 106, 118	0
40	65	110/112 (98%)	0.55	6 (5%) 25 13	84, 106, 121, 127	0
40	A8	111/112 (99%)	0.58	8 (7%) 15 8	76, 88, 107, 116	0
41	75	133/146 (91%)	0.03	4 (3%) 50 33	76, 95, 122, 143	0
41	B8	133/146 (91%)	-0.17	1 (0%) 86 78	71, 94, 126, 141	0
42	85	116/118 (98%)	0.27	6 (5%) 27 14	67, 90, 121, 132	0
42	C8	115/118 (97%)	0.19	5 (4%) 35 21	60, 84, 111, 120	0
43	95	100/101 (99%)	1.72	39 (39%) 0 0	68, 117, 131, 142	0
43	D8	100/101 (99%)	0.82	11 (11%) 5 3	62, 103, 123, 129	0
44	A5	113/113 (100%)	0.18	2 (1%) 68 55	61, 75, 104, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	E8	112/113 (99%)	0.44	4 (3%) 42 26	60, 76, 104, 136	0
45	B5	94/96 (97%)	0.35	6 (6%) 19 10	72, 83, 104, 119	0
45	F8	95/96 (98%)	0.21	3 (3%) 47 30	59, 74, 97, 107	0
46	C5	104/110 (94%)	1.12	23 (22%) 0 0	89, 114, 147, 154	0
46	G8	105/110 (95%)	0.11	2 (1%) 66 53	72, 94, 124, 135	0
47	D5	132/206 (64%)	1.65	54 (40%) 0 0	104, 132, 155, 163	0
47	H8	171/206 (83%)	1.27	45 (26%) 0 0	87, 118, 188, 193	0
48	E5	77/85 (90%)	0.66	4 (5%) 27 14	69, 87, 102, 123	0
48	I8	76/85 (89%)	-0.12	1 (1%) 77 66	59, 72, 85, 100	0
49	F5	94/98 (95%)	0.57	7 (7%) 14 8	66, 84, 115, 128	0
49	J8	94/98 (95%)	0.41	9 (9%) 8 4	54, 77, 114, 120	0
50	G5	66/72 (91%)	0.25	2 (3%) 50 33	81, 101, 121, 132	0
50	K8	68/72 (94%)	0.29	1 (1%) 73 61	67, 84, 98, 115	0
51	H5	58/60 (96%)	0.94	9 (15%) 2 1	77, 98, 128, 136	0
51	L8	58/60 (96%)	0.33	2 (3%) 45 28	65, 83, 107, 123	0
52	M8	47/71 (66%)	1.16	12 (25%) 0 0	102, 135, 150, 157	0
53	J5	56/60 (93%)	-0.10	0 100 100	59, 87, 127, 134	0
53	N8	48/60 (80%)	0.21	3 (6%) 20 10	55, 86, 128, 132	0
54	L5	47/49 (95%)	-0.19	1 (2%) 63 49	54, 62, 83, 88	0
54	P8	47/49 (95%)	-0.39	1 (2%) 63 49	49, 55, 72, 81	0
55	M5	64/65 (98%)	0.18	1 (1%) 72 59	68, 78, 93, 111	0
55	Q8	64/65 (98%)	-0.14	0 100 100	62, 70, 84, 97	0
56	3L	73/76 (96%)	0.11	3 (4%) 37 22	84, 205, 228, 235	0
All	All	20602/21967 (93%)	-0.02	1104 (5%) 25 13	43, 99, 165, 253	0

The worst 5 of 1104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	12.8
26	14	2901	C	9.8
32	49	138	GLN	8.4
44	A5	113	LYS	8.2
22	1L	71	C	8.2



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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	PSU	3L	39	20/21	0.85	0.17	118,132,140,141	0
22	T6A	1K	37	32/33	0.87	0.28	66,85,127,129	0
22	PSU	1L	55	20/21	0.88	0.21	126,149,158,158	0
22	T6A	1L	37	32/33	0.88	0.23	104,115,143,144	0
56	T6A	3L	37	32/33	0.89	0.19	121,132,147,147	0
22	5MU	1K	54	21/22	0.91	0.18	118,126,140,143	0
22	U8U	1L	34	23/24	0.91	0.17	115,123,131,134	0
22	PSU	1K	55	20/21	0.92	0.14	107,132,143,147	0
23	PSU	2L	56	20/21	0.92	0.10	106,110,116,120	0
22	PSU	1L	39	20/21	0.93	0.13	104,123,128,130	0
23	G7M	2K	47	24/25	0.93	0.12	90,101,110,116	0
23	4SU	2L	8	20/21	0.93	0.14	100,111,114,121	0
23	5MU	2L	55	21/22	0.94	0.10	105,114,119,125	0
23	OMC	2L	33	21/22	0.94	0.15	96,100,104,113	0
23	5MU	2K	55	21/22	0.95	0.09	90,103,110,112	0
22	U8U	1K	34	23/24	0.95	0.14	81,89,100,107	0
23	4SU	2K	8	20/21	0.95	0.13	87,92,97,98	0
24	PSU	3K	39	20/21	0.95	0.09	109,116,128,137	0
22	5MU	1L	54	21/22	0.95	0.20	131,141,157,158	0
23	PSU	2K	56	20/21	0.96	0.08	95,100,104,111	0
22	PSU	1K	39	20/21	0.96	0.11	79,97,103,106	0
23	OMC	2K	33	21/22	0.96	0.14	73,80,83,87	0
23	G7M	2L	47	24/25	0.96	0.12	114,121,128,132	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3031	1/1	0.32	0.26	105,105,105,105	0
57	MG	13	1646	1/1	0.44	0.17	109,109,109,109	0
57	MG	1H	3282	1/1	0.45	0.25	96,96,96,96	0
57	MG	1H	3183	1/1	0.46	0.35	92,92,92,92	0
57	MG	14	3266	1/1	0.53	0.24	84,84,84,84	0
57	MG	13	1643	1/1	0.57	0.21	89,89,89,89	0
57	MG	13	1689	1/1	0.59	0.40	99,99,99,99	0
57	MG	1H	3277	1/1	0.59	0.18	77,77,77,77	0
57	MG	55	201	1/1	0.59	0.33	83,83,83,83	0
57	MG	13	1635	1/1	0.62	0.07	85,85,85,85	0
57	MG	35	202	1/1	0.62	0.22	75,75,75,75	0
57	MG	13	1661	1/1	0.62	0.11	102,102,102,102	0
57	MG	14	3116	1/1	0.63	0.39	87,87,87,87	0
57	MG	14	3206	1/1	0.64	0.55	95,95,95,95	0
57	MG	1G	1620	1/1	0.64	0.77	79,79,79,79	0
57	MG	14	3162	1/1	0.65	0.30	67,67,67,67	0
57	MG	1G	1621	1/1	0.65	0.18	103,103,103,103	0
57	MG	1H	3210	1/1	0.65	0.32	74,74,74,74	0
57	MG	14	3237	1/1	0.66	0.50	72,72,72,72	0
57	MG	14	3272	1/1	0.66	0.30	77,77,77,77	0
57	MG	14	3267	1/1	0.66	0.15	83,83,83,83	0
57	MG	1H	3496	1/1	0.66	0.06	94,94,94,94	0
57	MG	14	3016	1/1	0.67	0.56	73,73,73,73	0
57	MG	1H	3180	1/1	0.67	0.38	76,76,76,76	0
57	MG	14	3268	1/1	0.67	0.44	60,60,60,60	0
57	MG	14	3120	1/1	0.67	0.35	67,67,67,67	0
57	MG	14	3179	1/1	0.68	0.35	74,74,74,74	0
57	MG	2L	103	1/1	0.68	0.57	80,80,80,80	0
57	MG	16	206	1/1	0.68	0.41	81,81,81,81	0
57	MG	14	3155	1/1	0.68	0.26	66,66,66,66	0
57	MG	14	3157	1/1	0.68	0.32	99,99,99,99	0
57	MG	13	1667	1/1	0.68	0.43	97,97,97,97	0
57	MG	14	3243	1/1	0.69	0.41	86,86,86,86	0
57	MG	29	304	1/1	0.69	0.23	71,71,71,71	0
57	MG	1H	3129	1/1	0.69	0.31	76,76,76,76	0
57	MG	14	3224	1/1	0.69	0.38	80,80,80,80	0
57	MG	14	3265	1/1	0.69	0.51	79,79,79,79	0
57	MG	13	1628	1/1	0.69	0.37	96,96,96,96	0
57	MG	1H	3207	1/1	0.70	0.16	56,56,56,56	0
57	MG	13	1665	1/1	0.70	0.46	82,82,82,82	0
57	MG	14	3248	1/1	0.70	0.35	75,75,75,75	0
57	MG	14	3013	1/1	0.70	0.24	74,74,74,74	0
57	MG	13	1650	1/1	0.71	0.38	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3063	1/1	0.71	0.31	76,76,76,76	0
57	MG	14	3202	1/1	0.72	0.23	90,90,90,90	0
57	MG	16	203	1/1	0.72	0.16	79,79,79,79	0
57	MG	13	1625	1/1	0.72	0.27	96,96,96,96	0
57	MG	13	1655	1/1	0.72	0.46	71,71,71,71	0
57	MG	16	205	1/1	0.72	0.20	81,81,81,81	0
57	MG	1H	3493	1/1	0.72	0.19	94,94,94,94	0
57	MG	1H	3190	1/1	0.73	0.47	74,74,74,74	0
57	MG	14	3171	1/1	0.73	0.22	73,73,73,73	0
57	MG	1H	3205	1/1	0.73	0.17	77,77,77,77	0
57	MG	1H	3284	1/1	0.73	0.62	75,75,75,75	0
57	MG	1H	3020	1/1	0.74	0.19	107,107,107,107	0
57	MG	1H	3278	1/1	0.74	0.20	82,82,82,82	0
57	MG	14	3223	1/1	0.74	0.42	75,75,75,75	0
57	MG	1H	3019	1/1	0.74	0.27	78,78,78,78	0
57	MG	1H	3289	1/1	0.74	0.40	82,82,82,82	0
57	MG	14	3374	1/1	0.74	0.07	96,96,96,96	0
57	MG	29	301	1/1	0.74	0.44	80,80,80,80	0
57	MG	1H	3198	1/1	0.75	0.26	76,76,76,76	0
57	MG	13	1684	1/1	0.75	0.22	85,85,85,85	0
57	MG	14	3190	1/1	0.75	0.88	82,82,82,82	0
57	MG	1H	3121	1/1	0.75	0.42	79,79,79,79	0
57	MG	14	3357	1/1	0.75	0.11	84,84,84,84	0
57	MG	14	3257	1/1	0.75	0.58	87,87,87,87	0
57	MG	7A	101	1/1	0.75	0.23	89,89,89,89	0
57	MG	11	303	1/1	0.75	0.51	65,65,65,65	0
57	MG	1H	3069	1/1	0.75	0.46	65,65,65,65	0
57	MG	5I	101	1/1	0.75	0.08	88,88,88,88	0
57	MG	1J	203	1/1	0.75	0.30	93,93,93,93	0
57	MG	14	3075	1/1	0.75	0.46	70,70,70,70	0
57	MG	14	3236	1/1	0.76	0.21	88,88,88,88	0
57	MG	1G	1641	1/1	0.76	0.34	78,78,78,78	0
57	MG	1H	3287	1/1	0.76	0.37	80,80,80,80	0
57	MG	1H	3233	1/1	0.76	0.34	70,70,70,70	0
57	MG	1H	3220	1/1	0.76	0.40	73,73,73,73	0
57	MG	1H	3244	1/1	0.77	0.41	84,84,84,84	0
57	MG	16	207	1/1	0.77	0.26	77,77,77,77	0
57	MG	14	3241	1/1	0.77	0.33	84,84,84,84	0
57	MG	14	3037	1/1	0.77	0.21	63,63,63,63	0
57	MG	1H	3128	1/1	0.77	0.22	64,64,64,64	0
57	MG	13	1659	1/1	0.78	0.42	75,75,75,75	0
57	MG	1H	3249	1/1	0.78	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3143	1/1	0.78	0.24	73,73,73,73	0
57	MG	2K	101	1/1	0.78	0.29	95,95,95,95	0
57	MG	13	1656	1/1	0.78	0.50	62,62,62,62	0
57	MG	14	3443	1/1	0.78	0.07	108,108,108,108	0
57	MG	14	3005	1/1	0.78	0.37	70,70,70,70	0
57	MG	1H	3125	1/1	0.78	0.34	61,61,61,61	0
57	MG	14	3097	1/1	0.78	0.51	65,65,65,65	0
57	MG	1G	1626	1/1	0.78	0.29	73,73,73,73	0
57	MG	1H	3103	1/1	0.79	0.43	82,82,82,82	0
57	MG	1H	3108	1/1	0.79	0.41	82,82,82,82	0
57	MG	14	3423	1/1	0.79	0.06	144,144,144,144	0
57	MG	1H	3280	1/1	0.79	0.42	80,80,80,80	0
57	MG	1H	3107	1/1	0.79	0.19	64,64,64,64	0
57	MG	1G	1657	1/1	0.79	0.13	105,105,105,105	0
57	MG	1H	3054	1/1	0.79	0.34	59,59,59,59	0
57	MG	1H	3136	1/1	0.79	0.84	73,73,73,73	0
57	MG	14	3226	1/1	0.79	0.27	78,78,78,78	0
57	MG	1I	201	1/1	0.79	0.12	100,100,100,100	0
57	MG	P8	101	1/1	0.80	0.44	66,66,66,66	0
57	MG	1G	1609	1/1	0.80	0.19	108,108,108,108	0
57	MG	1H	3199	1/1	0.80	0.38	75,75,75,75	0
57	MG	35	201	1/1	0.80	0.33	71,71,71,71	0
57	MG	14	3232	1/1	0.80	0.26	130,130,130,130	0
57	MG	1H	3139	1/1	0.80	0.35	71,71,71,71	0
57	MG	1H	3144	1/1	0.80	0.48	75,75,75,75	0
57	MG	14	3191	1/1	0.80	0.44	73,73,73,73	0
57	MG	13	1603	1/1	0.81	0.36	76,76,76,76	0
57	MG	1H	3066	1/1	0.81	0.21	57,57,57,57	0
57	MG	1H	3208	1/1	0.81	0.23	76,76,76,76	0
57	MG	14	3036	1/1	0.81	0.24	76,76,76,76	0
57	MG	29	303	1/1	0.81	0.16	67,67,67,67	0
57	MG	1G	1692	1/1	0.81	0.36	105,105,105,105	0
57	MG	1H	3242	1/1	0.81	0.27	80,80,80,80	0
57	MG	14	3180	1/1	0.81	0.31	69,69,69,69	0
57	MG	1G	1618	1/1	0.81	0.19	86,86,86,86	0
57	MG	13	1618	1/1	0.82	0.33	64,64,64,64	0
57	MG	14	3144	1/1	0.82	0.52	80,80,80,80	0
57	MG	14	3108	1/1	0.82	0.11	90,90,90,90	0
57	MG	1G	1623	1/1	0.82	0.31	77,77,77,77	0
57	MG	1G	1631	1/1	0.82	0.29	107,107,107,107	0
57	MG	1G	1616	1/1	0.82	0.23	86,86,86,86	0
57	MG	14	3427	1/1	0.82	0.08	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1648	1/1	0.82	0.30	90,90,90,90	0
57	MG	14	3192	1/1	0.82	0.36	100,100,100,100	0
57	MG	14	3258	1/1	0.82	0.77	83,83,83,83	0
57	MG	1H	3192	1/1	0.82	0.32	82,82,82,82	0
57	MG	1G	1613	1/1	0.82	0.52	73,73,73,73	0
57	MG	14	3154	1/1	0.82	0.69	74,74,74,74	0
57	MG	14	3454	1/1	0.82	0.20	79,79,79,79	0
57	MG	13	1645	1/1	0.82	0.23	93,93,93,93	0
57	MG	1H	3036	1/1	0.82	0.20	78,78,78,78	0
57	MG	1H	3018	1/1	0.82	0.45	80,80,80,80	0
57	MG	1H	3200	1/1	0.82	0.35	73,73,73,73	0
57	MG	21	303	1/1	0.82	0.22	69,69,69,69	0
57	MG	1G	1639	1/1	0.83	0.18	97,97,97,97	0
57	MG	14	3212	1/1	0.83	0.43	80,80,80,80	0
57	MG	1H	3291	1/1	0.83	0.46	88,88,88,88	0
57	MG	13	1663	1/1	0.83	0.35	71,71,71,71	0
57	MG	1H	3188	1/1	0.83	0.38	74,74,74,74	0
57	MG	1H	3246	1/1	0.83	0.38	85,85,85,85	0
57	MG	1H	3093	1/1	0.83	0.63	71,71,71,71	0
57	MG	1H	3471	1/1	0.83	0.12	82,82,82,82	0
57	MG	14	3421	1/1	0.83	0.15	75,75,75,75	0
57	MG	1H	3115	1/1	0.83	0.29	82,82,82,82	0
57	MG	14	3129	1/1	0.83	0.16	69,69,69,69	0
57	MG	1H	3177	1/1	0.83	0.25	81,81,81,81	0
57	MG	14	3213	1/1	0.83	0.46	87,87,87,87	0
57	MG	16	204	1/1	0.83	0.27	90,90,90,90	0
57	MG	14	3204	1/1	0.83	0.19	90,90,90,90	0
57	MG	1H	3023	1/1	0.83	0.39	81,81,81,81	0
57	MG	1H	3120	1/1	0.83	0.16	63,63,63,63	0
57	MG	1H	3241	1/1	0.83	0.55	71,71,71,71	0
57	MG	14	3229	1/1	0.84	0.29	74,74,74,74	0
57	MG	14	3135	1/1	0.84	0.37	71,71,71,71	0
57	MG	1H	3083	1/1	0.84	0.21	74,74,74,74	0
57	MG	1H	3275	1/1	0.84	0.21	95,95,95,95	0
57	MG	14	3199	1/1	0.84	0.38	84,84,84,84	0
57	MG	1G	1688	1/1	0.84	0.06	100,100,100,100	0
57	MG	14	3264	1/1	0.84	0.32	90,90,90,90	0
57	MG	1H	3269	1/1	0.84	0.22	73,73,73,73	0
57	MG	13	1682	1/1	0.84	0.68	90,90,90,90	0
57	MG	14	3244	1/1	0.84	0.68	77,77,77,77	0
57	MG	14	3435	1/1	0.84	0.08	103,103,103,103	0
57	MG	14	3185	1/1	0.84	0.28	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3087	1/1	0.85	0.16	68,68,68,68	0
57	MG	14	3173	1/1	0.85	0.28	69,69,69,69	0
57	MG	14	3211	1/1	0.85	0.38	78,78,78,78	0
57	MG	14	3259	1/1	0.85	0.19	97,97,97,97	0
57	MG	1H	3092	1/1	0.85	0.34	57,57,57,57	0
57	MG	13	1649	1/1	0.85	0.37	78,78,78,78	0
57	MG	1H	3455	1/1	0.85	0.06	103,103,103,103	0
57	MG	14	3044	1/1	0.85	0.81	76,76,76,76	0
57	MG	1G	1627	1/1	0.85	0.25	86,86,86,86	0
57	MG	1H	3194	1/1	0.85	0.45	66,66,66,66	0
57	MG	1G	1655	1/1	0.85	0.07	120,120,120,120	0
57	MG	13	1670	1/1	0.85	0.33	78,78,78,78	0
57	MG	16	211	1/1	0.85	0.08	84,84,84,84	0
57	MG	41	202	1/1	0.85	0.26	82,82,82,82	0
57	MG	1H	3238	1/1	0.85	0.34	78,78,78,78	0
57	MG	1H	3209	1/1	0.85	0.23	78,78,78,78	0
57	MG	1G	1638	1/1	0.85	0.58	88,88,88,88	0
57	MG	1H	3279	1/1	0.85	0.99	71,71,71,71	0
57	MG	1H	3133	1/1	0.85	0.42	80,80,80,80	0
57	MG	1H	3086	1/1	0.85	0.07	71,71,71,71	0
57	MG	1H	3229	1/1	0.86	0.34	73,73,73,73	0
57	MG	14	3164	1/1	0.86	0.33	65,65,65,65	0
57	MG	1H	3281	1/1	0.86	0.52	69,69,69,69	0
57	MG	1H	3059	1/1	0.86	0.21	66,66,66,66	0
57	MG	14	3242	1/1	0.86	0.11	95,95,95,95	0
57	MG	1H	3077	1/1	0.86	0.55	74,74,74,74	0
57	MG	14	3152	1/1	0.86	0.32	67,67,67,67	0
57	MG	1H	3131	1/1	0.86	0.52	67,67,67,67	0
57	MG	14	3168	1/1	0.86	0.21	89,89,89,89	0
57	MG	1G	1646	1/1	0.86	0.67	84,84,84,84	0
57	MG	1H	3255	1/1	0.86	0.14	88,88,88,88	0
57	MG	1H	3286	1/1	0.86	0.23	82,82,82,82	0
57	MG	1G	1604	1/1	0.86	0.17	87,87,87,87	0
57	MG	14	3260	1/1	0.86	0.13	117,117,117,117	0
57	MG	1H	3487	1/1	0.86	0.08	91,91,91,91	0
57	MG	14	3238	1/1	0.86	0.55	69,69,69,69	0
57	MG	1H	3138	1/1	0.86	0.41	55,55,55,55	0
57	MG	13	1741	1/1	0.86	0.14	79,79,79,79	0
57	MG	1H	3428	1/1	0.86	0.08	87,87,87,87	0
57	MG	1H	3411	1/1	0.86	0.07	81,81,81,81	0
57	MG	1H	3195	1/1	0.86	0.28	73,73,73,73	0
57	MG	14	3113	1/1	0.86	0.41	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3212	1/1	0.86	0.35	77,77,77,77	0
57	MG	14	3188	1/1	0.86	0.40	66,66,66,66	0
57	MG	13	1668	1/1	0.86	0.23	95,95,95,95	0
57	MG	13	1626	1/1	0.86	0.14	87,87,87,87	0
57	MG	14	3107	1/1	0.86	0.42	81,81,81,81	0
57	MG	1H	3119	1/1	0.86	0.20	71,71,71,71	0
57	MG	1H	3226	1/1	0.86	0.15	64,64,64,64	0
57	MG	1H	3259	1/1	0.86	0.36	74,74,74,74	0
57	MG	14	3163	1/1	0.86	0.64	72,72,72,72	0
57	MG	14	3069	1/1	0.87	0.42	67,67,67,67	0
57	MG	1H	3285	1/1	0.87	0.55	87,87,87,87	0
57	MG	1H	3272	1/1	0.87	0.73	95,95,95,95	0
57	MG	14	3053	1/1	0.87	0.30	77,77,77,77	0
57	MG	14	3121	1/1	0.87	0.31	77,77,77,77	0
57	MG	1H	3452	1/1	0.87	0.09	89,89,89,89	0
57	MG	1H	3014	1/1	0.87	0.50	75,75,75,75	0
57	MG	13	1748	1/1	0.87	0.09	115,115,115,115	0
57	MG	14	3444	1/1	0.87	0.12	87,87,87,87	0
57	MG	14	3366	1/1	0.87	0.12	76,76,76,76	0
57	MG	13	1679	1/1	0.87	0.22	86,86,86,86	0
57	MG	1H	3007	1/1	0.87	0.29	68,68,68,68	0
57	MG	1H	3501	1/1	0.87	0.05	72,72,72,72	0
57	MG	1G	1628	1/1	0.87	0.24	124,124,124,124	0
57	MG	1H	3011	1/1	0.87	0.68	72,72,72,72	0
57	MG	14	3010	1/1	0.88	0.31	69,69,69,69	0
57	MG	13	1677	1/1	0.88	0.22	76,76,76,76	0
57	MG	14	3216	1/1	0.88	0.23	74,74,74,74	0
57	MG	39	301	1/1	0.88	0.14	95,95,95,95	0
57	MG	14	3146	1/1	0.88	0.44	76,76,76,76	0
57	MG	13	1620	1/1	0.88	0.35	58,58,58,58	0
57	MG	1G	1636	1/1	0.88	0.22	89,89,89,89	0
57	MG	13	1713	1/1	0.88	0.08	89,89,89,89	0
57	MG	13	1622	1/1	0.88	0.21	81,81,81,81	0
57	MG	1H	3466	1/1	0.88	0.05	83,83,83,83	0
57	MG	1H	3271	1/1	0.88	0.20	74,74,74,74	0
57	MG	1H	3193	1/1	0.88	0.61	84,84,84,84	0
57	MG	L8	101	1/1	0.88	0.39	72,72,72,72	0
57	MG	1H	3247	1/1	0.88	0.61	77,77,77,77	0
57	MG	1G	1624	1/1	0.88	0.19	87,87,87,87	0
57	MG	1G	1633	1/1	0.88	0.41	100,100,100,100	0
57	MG	13	1674	1/1	0.88	0.36	78,78,78,78	0
57	MG	13	1636	1/1	0.88	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3096	1/1	0.88	0.34	65,65,65,65	0
57	MG	14	3198	1/1	0.88	0.21	81,81,81,81	0
57	MG	1H	3015	1/1	0.88	0.24	72,72,72,72	0
57	MG	14	3324	1/1	0.88	0.09	107,107,107,107	0
57	MG	14	3054	1/1	0.88	0.40	67,67,67,67	0
57	MG	1H	3273	1/1	0.88	0.26	57,57,57,57	0
57	MG	1H	3134	1/1	0.88	0.31	76,76,76,76	0
57	MG	1H	3047	1/1	0.88	0.28	61,61,61,61	0
57	MG	1J	201	1/1	0.88	0.20	85,85,85,85	0
57	MG	1H	3243	1/1	0.88	0.24	62,62,62,62	0
57	MG	1H	3263	1/1	0.88	1.00	93,93,93,93	0
57	MG	1H	3186	1/1	0.88	0.24	57,57,57,57	0
57	MG	1H	3098	1/1	0.88	0.33	63,63,63,63	0
57	MG	13	1666	1/1	0.88	0.41	77,77,77,77	0
57	MG	13	1660	1/1	0.88	0.55	83,83,83,83	0
57	MG	1H	3489	1/1	0.88	0.08	125,125,125,125	0
57	MG	14	3147	1/1	0.88	0.29	72,72,72,72	0
57	MG	13	1642	1/1	0.88	0.26	107,107,107,107	0
57	MG	14	3441	1/1	0.88	0.08	72,72,72,72	0
57	MG	1H	3439	1/1	0.88	0.14	81,81,81,81	0
57	MG	1H	3495	1/1	0.88	0.07	98,98,98,98	0
57	MG	13	1739	1/1	0.88	0.06	104,104,104,104	0
57	MG	1H	3122	1/1	0.88	0.52	73,73,73,73	0
57	MG	14	3165	1/1	0.89	0.11	78,78,78,78	0
57	MG	1H	3148	1/1	0.89	0.23	65,65,65,65	0
57	MG	1H	3006	1/1	0.89	0.14	86,86,86,86	0
57	MG	14	3308	1/1	0.89	0.08	96,96,96,96	0
57	MG	1H	3075	1/1	0.89	0.12	60,60,60,60	0
57	MG	14	3058	1/1	0.89	0.25	66,66,66,66	0
57	MG	1G	1637	1/1	0.89	0.20	77,77,77,77	0
57	MG	14	3416	1/1	0.89	0.07	66,66,66,66	0
57	MG	14	3055	1/1	0.89	0.35	57,57,57,57	0
57	MG	1G	1619	1/1	0.89	0.21	92,92,92,92	0
57	MG	1H	3021	1/1	0.89	0.16	90,90,90,90	0
57	MG	1H	3178	1/1	0.89	0.12	93,93,93,93	0
57	MG	1H	3213	1/1	0.89	0.14	92,92,92,92	0
57	MG	14	3310	1/1	0.89	0.09	68,68,68,68	0
57	MG	1H	3171	1/1	0.89	0.43	68,68,68,68	0
57	MG	14	3380	1/1	0.89	0.12	93,93,93,93	0
57	MG	14	3303	1/1	0.89	0.13	63,63,63,63	0
57	MG	14	3123	1/1	0.89	0.49	70,70,70,70	0
57	MG	14	3215	1/1	0.89	0.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3269	1/1	0.89	0.30	102,102,102,102	0
57	MG	1H	3084	1/1	0.89	0.14	82,82,82,82	0
57	MG	14	3227	1/1	0.89	0.34	83,83,83,83	0
57	MG	13	1735	1/1	0.89	0.07	118,118,118,118	0
57	MG	1G	1683	1/1	0.89	0.09	96,96,96,96	0
57	MG	1H	3116	1/1	0.89	0.30	63,63,63,63	0
57	MG	1H	3114	1/1	0.89	0.41	78,78,78,78	0
57	MG	1H	3176	1/1	0.89	0.33	67,67,67,67	0
57	MG	78	201	1/1	0.89	0.24	75,75,75,75	0
57	MG	1G	1686	1/1	0.90	0.07	92,92,92,92	0
57	MG	13	1722	1/1	0.90	0.05	92,92,92,92	0
57	MG	1G	1642	1/1	0.90	0.30	82,82,82,82	0
57	MG	1H	3476	1/1	0.90	0.07	93,93,93,93	0
57	MG	14	3326	1/1	0.90	0.09	74,74,74,74	0
57	MG	1H	3097	1/1	0.90	0.16	51,51,51,51	0
57	MG	14	3194	1/1	0.90	0.21	68,68,68,68	0
57	MG	14	3057	1/1	0.90	0.36	41,41,41,41	0
57	MG	14	3448	1/1	0.90	0.06	92,92,92,92	0
57	MG	14	3233	1/1	0.90	0.26	79,79,79,79	0
57	MG	14	3261	1/1	0.90	0.21	102,102,102,102	0
57	MG	14	3001	1/1	0.90	0.05	103,103,103,103	0
57	MG	1G	1643	1/1	0.90	0.39	67,67,67,67	0
57	MG	14	3225	1/1	0.90	0.36	80,80,80,80	0
57	MG	1G	1617	1/1	0.90	0.22	61,61,61,61	0
57	MG	14	3027	1/1	0.90	0.31	83,83,83,83	0
57	MG	14	3009	1/1	0.90	0.20	68,68,68,68	0
57	MG	1G	1607	1/1	0.90	0.22	91,91,91,91	0
57	MG	1H	3211	1/1	0.90	0.34	80,80,80,80	0
57	MG	1H	3434	1/1	0.90	0.10	73,73,73,73	0
57	MG	41	201	1/1	0.90	0.14	75,75,75,75	0
57	MG	39	302	1/1	0.90	0.10	63,63,63,63	0
57	MG	13	1612	1/1	0.90	0.26	85,85,85,85	0
57	MG	14	3149	1/1	0.90	0.29	96,96,96,96	0
57	MG	14	3318	1/1	0.90	0.15	67,67,67,67	0
57	MG	14	3183	1/1	0.90	0.59	74,74,74,74	0
57	MG	13	1658	1/1	0.90	0.12	88,88,88,88	0
57	MG	1H	3488	1/1	0.90	0.05	113,113,113,113	0
57	MG	1H	3484	1/1	0.90	0.07	90,90,90,90	0
57	MG	1H	3091	1/1	0.90	0.26	57,57,57,57	0
57	MG	1H	3376	1/1	0.90	0.06	88,88,88,88	0
57	MG	14	3424	1/1	0.90	0.05	107,107,107,107	0
57	MG	14	3271	1/1	0.90	0.45	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3330	1/1	0.90	0.06	113,113,113,113	0
57	MG	14	3098	1/1	0.90	0.22	67,67,67,67	0
57	MG	1H	3262	1/1	0.90	0.17	68,68,68,68	0
57	MG	13	1631	1/1	0.90	0.10	73,73,73,73	0
57	MG	1H	3254	1/1	0.90	0.62	82,82,82,82	0
57	MG	1H	3470	1/1	0.90	0.08	100,100,100,100	0
57	MG	1H	3231	1/1	0.90	0.42	65,65,65,65	0
57	MG	1H	3196	1/1	0.90	0.56	88,88,88,88	0
57	MG	1H	3221	1/1	0.90	0.21	60,60,60,60	0
57	MG	14	3139	1/1	0.90	0.22	58,58,58,58	0
57	MG	14	3219	1/1	0.90	0.29	64,64,64,64	0
57	MG	14	3102	1/1	0.90	0.20	86,86,86,86	0
57	MG	1H	3267	1/1	0.90	0.17	67,67,67,67	0
57	MG	16	212	1/1	0.90	0.08	88,88,88,88	0
57	MG	1G	1666	1/1	0.90	0.05	106,106,106,106	0
57	MG	1H	3498	1/1	0.90	0.12	85,85,85,85	0
57	MG	1H	3149	1/1	0.90	0.15	61,61,61,61	0
57	MG	1H	3157	1/1	0.90	0.28	64,64,64,64	0
57	MG	14	3182	1/1	0.90	0.57	67,67,67,67	0
57	MG	13	1738	1/1	0.90	0.09	97,97,97,97	0
57	MG	1H	3105	1/1	0.90	0.24	79,79,79,79	0
57	MG	1H	3159	1/1	0.90	0.37	56,56,56,56	0
57	MG	14	3176	1/1	0.90	0.08	88,88,88,88	0
57	MG	14	3142	1/1	0.90	0.31	82,82,82,82	0
57	MG	1H	3143	1/1	0.90	0.45	89,89,89,89	0
57	MG	1G	1635	1/1	0.90	0.45	97,97,97,97	0
57	MG	14	3221	1/1	0.90	0.51	73,73,73,73	0
57	MG	14	3038	1/1	0.90	0.08	76,76,76,76	0
57	MG	1H	3189	1/1	0.91	0.31	87,87,87,87	0
57	MG	1H	3022	1/1	0.91	0.18	81,81,81,81	0
57	MG	14	3015	1/1	0.91	0.27	77,77,77,77	0
57	MG	14	3222	1/1	0.91	0.41	64,64,64,64	0
57	MG	13	1652	1/1	0.91	0.48	89,89,89,89	0
57	MG	13	1664	1/1	0.91	0.30	81,81,81,81	0
57	MG	88	201	1/1	0.91	0.18	82,82,82,82	0
57	MG	14	3024	1/1	0.91	0.26	58,58,58,58	0
57	MG	1H	3265	1/1	0.91	0.12	89,89,89,89	0
57	MG	1H	3053	1/1	0.91	0.47	56,56,56,56	0
57	MG	14	3193	1/1	0.91	0.15	70,70,70,70	0
57	MG	13	1736	1/1	0.91	0.06	95,95,95,95	0
57	MG	13	1672	1/1	0.91	0.11	96,96,96,96	0
57	MG	13	1637	1/1	0.91	0.26	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3334	1/1	0.91	0.10	82,82,82,82	0
57	MG	14	3017	1/1	0.91	0.23	97,97,97,97	0
57	MG	1H	3482	1/1	0.91	0.06	72,72,72,72	0
57	MG	1G	1610	1/1	0.91	0.13	114,114,114,114	0
57	MG	14	3208	1/1	0.91	0.31	75,75,75,75	0
57	MG	1H	3126	1/1	0.91	0.45	70,70,70,70	0
57	MG	14	3436	1/1	0.91	0.07	108,108,108,108	0
57	MG	1H	3371	1/1	0.91	0.05	85,85,85,85	0
57	MG	1H	3283	1/1	0.91	0.47	82,82,82,82	0
57	MG	E5	101	1/1	0.91	0.43	72,72,72,72	0
57	MG	45	202	1/1	0.91	0.10	102,102,102,102	0
57	MG	1H	3230	1/1	0.91	0.37	78,78,78,78	0
57	MG	1H	3008	1/1	0.91	0.26	57,57,57,57	0
57	MG	14	3111	1/1	0.91	0.15	79,79,79,79	0
57	MG	1H	3110	1/1	0.91	0.15	84,84,84,84	0
57	MG	1H	3290	1/1	0.91	0.23	62,62,62,62	0
57	MG	14	3425	1/1	0.91	0.06	122,122,122,122	0
57	MG	13	1662	1/1	0.91	0.21	119,119,119,119	0
57	MG	1G	1689	1/1	0.91	0.06	126,126,126,126	0
57	MG	13	1750	1/1	0.91	0.18	76,76,76,76	0
57	MG	14	3178	1/1	0.91	0.09	71,71,71,71	0
57	MG	14	3089	1/1	0.91	0.22	56,56,56,56	0
57	MG	1H	3109	1/1	0.91	0.33	65,65,65,65	0
57	MG	BI	201	1/1	0.91	0.03	103,103,103,103	0
57	MG	14	3442	1/1	0.91	0.07	95,95,95,95	0
57	MG	14	3175	1/1	0.91	0.24	90,90,90,90	0
57	MG	14	3428	1/1	0.91	0.09	104,104,104,104	0
57	MG	M5	101	1/1	0.91	0.17	77,77,77,77	0
57	MG	14	3086	1/1	0.91	0.22	61,61,61,61	0
57	MG	14	3124	1/1	0.91	0.27	64,64,64,64	0
57	MG	1H	3228	1/1	0.91	0.49	69,69,69,69	0
57	MG	1H	3010	1/1	0.91	0.47	59,59,59,59	0
57	MG	1H	3057	1/1	0.91	0.40	53,53,53,53	0
57	MG	1H	3090	1/1	0.91	0.48	57,57,57,57	0
57	MG	14	3207	1/1	0.91	0.10	71,71,71,71	0
57	MG	14	3234	1/1	0.91	0.16	64,64,64,64	0
57	MG	14	3200	1/1	0.91	0.21	69,69,69,69	0
57	MG	14	3452	1/1	0.91	0.09	113,113,113,113	0
57	MG	14	3239	1/1	0.91	0.36	87,87,87,87	0
57	MG	1H	3112	1/1	0.91	0.39	66,66,66,66	0
57	MG	14	3045	1/1	0.91	0.23	64,64,64,64	0
57	MG	14	3296	1/1	0.91	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3181	1/1	0.92	0.20	63,63,63,63	0
57	MG	1H	3174	1/1	0.92	0.28	59,59,59,59	0
57	MG	14	3263	1/1	0.92	0.44	80,80,80,80	0
57	MG	1H	3096	1/1	0.92	0.15	67,67,67,67	0
57	MG	14	3105	1/1	0.92	0.26	55,55,55,55	0
57	MG	14	3033	1/1	0.92	0.14	74,74,74,74	0
57	MG	1H	3222	1/1	0.92	0.11	68,68,68,68	0
57	MG	1G	1674	1/1	0.92	0.06	107,107,107,107	0
57	MG	1H	3481	1/1	0.92	0.06	92,92,92,92	0
57	MG	1H	3181	1/1	0.92	0.53	77,77,77,77	0
57	MG	1H	3101	1/1	0.92	0.18	58,58,58,58	0
57	MG	14	3270	1/1	0.92	0.28	83,83,83,83	0
57	MG	1H	3459	1/1	0.92	0.10	91,91,91,91	0
57	MG	13	1678	1/1	0.92	0.21	83,83,83,83	0
57	MG	14	3315	1/1	0.92	0.05	81,81,81,81	0
57	MG	14	3351	1/1	0.92	0.06	72,72,72,72	0
57	MG	1H	3162	1/1	0.92	0.15	61,61,61,61	0
57	MG	16	201	1/1	0.92	0.17	87,87,87,87	0
57	MG	14	3383	1/1	0.92	0.07	101,101,101,101	0
57	MG	14	3169	1/1	0.92	0.18	65,65,65,65	0
57	MG	1H	3245	1/1	0.92	0.57	69,69,69,69	0
57	MG	13	1704	1/1	0.92	0.13	105,105,105,105	0
57	MG	14	3228	1/1	0.92	0.15	81,81,81,81	0
57	MG	14	3400	1/1	0.92	0.06	86,86,86,86	0
57	MG	1H	3170	1/1	0.92	0.73	72,72,72,72	0
57	MG	1H	3035	1/1	0.92	0.24	57,57,57,57	0
57	MG	1H	3182	1/1	0.92	0.44	72,72,72,72	0
57	MG	1H	3052	1/1	0.92	0.32	57,57,57,57	0
57	MG	14	3422	1/1	0.92	0.09	84,84,84,84	0
57	MG	1H	3206	1/1	0.92	0.21	56,56,56,56	0
57	MG	14	3255	1/1	0.92	0.13	87,87,87,87	0
57	MG	13	1686	1/1	0.92	0.21	96,96,96,96	0
57	MG	1G	1668	1/1	0.92	0.07	111,111,111,111	0
57	MG	13	1724	1/1	0.92	0.08	114,114,114,114	0
57	MG	1H	3467	1/1	0.92	0.08	77,77,77,77	0
57	MG	1H	3258	1/1	0.92	0.21	79,79,79,79	0
57	MG	1G	1653	1/1	0.92	0.08	110,110,110,110	0
57	MG	1H	3236	1/1	0.92	0.32	75,75,75,75	0
57	MG	1G	1679	1/1	0.92	0.05	91,91,91,91	0
57	MG	14	3407	1/1	0.92	0.10	74,74,74,74	0
57	MG	14	3158	1/1	0.92	0.12	70,70,70,70	0
57	MG	14	3429	1/1	0.92	0.05	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3195	1/1	0.92	0.23	105,105,105,105	0
57	MG	1H	3140	1/1	0.92	0.22	62,62,62,62	0
57	MG	1H	3185	1/1	0.93	0.36	90,90,90,90	0
57	MG	1G	1648	1/1	0.93	0.23	86,86,86,86	0
57	MG	14	3074	1/1	0.93	0.27	62,62,62,62	0
57	MG	1H	3203	1/1	0.93	0.28	64,64,64,64	0
57	MG	1H	3385	1/1	0.93	0.08	57,57,57,57	0
57	MG	14	3240	1/1	0.93	0.30	85,85,85,85	0
57	MG	14	3007	1/1	0.93	0.29	50,50,50,50	0
57	MG	1H	3435	1/1	0.93	0.05	94,94,94,94	0
57	MG	14	3004	1/1	0.93	0.88	77,77,77,77	0
57	MG	14	3220	1/1	0.93	0.53	88,88,88,88	0
57	MG	1H	3235	1/1	0.93	0.14	65,65,65,65	0
57	MG	14	3439	1/1	0.93	0.06	96,96,96,96	0
57	MG	1H	3076	1/1	0.93	0.25	76,76,76,76	0
57	MG	1H	3288	1/1	0.93	0.38	80,80,80,80	0
57	MG	1G	1622	1/1	0.93	0.35	76,76,76,76	0
57	MG	1H	3046	1/1	0.93	0.56	73,73,73,73	0
57	MG	1H	3218	1/1	0.93	0.74	70,70,70,70	0
57	MG	14	3112	1/1	0.93	0.37	88,88,88,88	0
57	MG	1H	3380	1/1	0.93	0.14	55,55,55,55	0
57	MG	1H	3130	1/1	0.93	0.23	67,67,67,67	0
57	MG	14	3151	1/1	0.93	0.23	72,72,72,72	0
57	MG	1H	3431	1/1	0.93	0.16	52,52,52,52	0
57	MG	14	3049	1/1	0.93	0.27	63,63,63,63	0
57	MG	14	3082	1/1	0.93	0.40	55,55,55,55	0
57	MG	1H	3451	1/1	0.93	0.04	95,95,95,95	0
57	MG	14	3104	1/1	0.93	0.36	81,81,81,81	0
57	MG	14	3434	1/1	0.93	0.06	82,82,82,82	0
57	MG	1H	3325	1/1	0.93	0.11	69,69,69,69	0
57	MG	1G	1670	1/1	0.93	0.08	108,108,108,108	0
57	MG	1H	3163	1/1	0.93	0.28	59,59,59,59	0
57	MG	14	3387	1/1	0.93	0.05	97,97,97,97	0
57	MG	1H	3123	1/1	0.93	0.21	71,71,71,71	0
57	MG	16	202	1/1	0.93	0.28	73,73,73,73	0
57	MG	14	3235	1/1	0.93	0.50	69,69,69,69	0
57	MG	13	1671	1/1	0.93	0.32	71,71,71,71	0
57	MG	13	1621	1/1	0.93	0.23	67,67,67,67	0
57	MG	13	1630	1/1	0.93	0.28	92,92,92,92	0
57	MG	1H	3274	1/1	0.93	0.29	70,70,70,70	0
57	MG	1H	3215	1/1	0.93	0.27	65,65,65,65	0
57	MG	1H	3073	1/1	0.93	0.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3099	1/1	0.93	0.13	60,60,60,60	0
57	MG	14	3184	1/1	0.93	0.33	60,60,60,60	0
57	MG	1H	3395	1/1	0.93	0.11	59,59,59,59	0
57	MG	2L	102	1/1	0.93	0.36	96,96,96,96	0
57	MG	1H	3266	1/1	0.93	0.15	75,75,75,75	0
57	MG	1G	1678	1/1	0.93	0.03	115,115,115,115	0
57	MG	14	3166	1/1	0.93	0.24	61,61,61,61	0
57	MG	14	3230	1/1	0.93	0.23	70,70,70,70	0
57	MG	14	3210	1/1	0.93	0.34	80,80,80,80	0
57	MG	14	3110	1/1	0.93	0.18	86,86,86,86	0
57	MG	13	1714	1/1	0.93	0.10	93,93,93,93	0
57	MG	C5	201	1/1	0.93	0.04	110,110,110,110	0
57	MG	1H	3248	1/1	0.93	0.14	79,79,79,79	0
57	MG	14	3067	1/1	0.93	0.34	68,68,68,68	0
57	MG	1H	3168	1/1	0.93	0.27	80,80,80,80	0
57	MG	1H	3187	1/1	0.93	0.08	88,88,88,88	0
57	MG	1H	3438	1/1	0.93	0.05	75,75,75,75	0
57	MG	14	3150	1/1	0.93	0.46	68,68,68,68	0
57	MG	1H	3065	1/1	0.93	0.17	56,56,56,56	0
57	MG	1H	3480	1/1	0.93	0.08	78,78,78,78	0
57	MG	1H	3500	1/1	0.93	0.06	71,71,71,71	0
57	MG	14	3280	1/1	0.93	0.12	54,54,54,54	0
57	MG	14	3370	1/1	0.93	0.08	81,81,81,81	0
57	MG	2K	102	1/1	0.94	0.06	92,92,92,92	0
57	MG	14	3309	1/1	0.94	0.14	73,73,73,73	0
57	MG	1H	3472	1/1	0.94	0.07	93,93,93,93	0
57	MG	14	3131	1/1	0.94	0.22	78,78,78,78	0
57	MG	13	1669	1/1	0.94	0.46	74,74,74,74	0
57	MG	21	302	1/1	0.94	0.32	50,50,50,50	0
57	MG	13	1676	1/1	0.94	0.26	101,101,101,101	0
57	MG	14	3159	1/1	0.94	0.18	71,71,71,71	0
57	MG	14	3134	1/1	0.94	0.26	98,98,98,98	0
57	MG	14	3048	1/1	0.94	0.75	75,75,75,75	0
57	MG	1H	3326	1/1	0.94	0.07	49,49,49,49	0
57	MG	1H	3048	1/1	0.94	0.06	80,80,80,80	0
57	MG	1J	205	1/1	0.94	0.05	95,95,95,95	0
57	MG	13	1744	1/1	0.94	0.16	94,94,94,94	0
57	MG	1H	3111	1/1	0.94	0.31	80,80,80,80	0
57	MG	14	3071	1/1	0.94	0.15	73,73,73,73	0
57	MG	1H	3227	1/1	0.94	0.11	70,70,70,70	0
57	MG	1G	1671	1/1	0.94	0.07	117,117,117,117	0
57	MG	1H	3062	1/1	0.94	0.42	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3319	1/1	0.94	0.11	91,91,91,91	0
57	MG	1G	1601	1/1	0.94	0.46	86,86,86,86	0
57	MG	14	3321	1/1	0.94	0.06	89,89,89,89	0
57	MG	1H	3393	1/1	0.94	0.09	56,56,56,56	0
57	MG	14	3438	1/1	0.94	0.07	93,93,93,93	0
57	MG	1H	3323	1/1	0.94	0.06	61,61,61,61	0
57	MG	1G	1690	1/1	0.94	0.07	118,118,118,118	0
57	MG	13	1708	1/1	0.94	0.07	76,76,76,76	0
57	MG	14	3449	1/1	0.94	0.09	95,95,95,95	0
57	MG	14	3106	1/1	0.94	0.49	82,82,82,82	0
57	MG	1H	3478	1/1	0.94	0.06	85,85,85,85	0
57	MG	1H	3372	1/1	0.94	0.07	89,89,89,89	0
57	MG	1H	3224	1/1	0.94	0.28	63,63,63,63	0
57	MG	1H	3017	1/1	0.94	0.18	55,55,55,55	0
57	MG	1H	3252	1/1	0.94	0.32	80,80,80,80	0
57	MG	1G	1665	1/1	0.94	0.13	97,97,97,97	0
57	MG	2L	104	1/1	0.94	0.40	72,72,72,72	0
57	MG	13	1688	1/1	0.94	0.25	90,90,90,90	0
57	MG	1H	3369	1/1	0.94	0.16	74,74,74,74	0
57	MG	13	1719	1/1	0.94	0.15	72,72,72,72	0
57	MG	14	3076	1/1	0.94	0.20	77,77,77,77	0
57	MG	13	1617	1/1	0.94	0.23	53,53,53,53	0
57	MG	13	1651	1/1	0.94	0.21	68,68,68,68	0
57	MG	14	3056	1/1	0.94	0.67	82,82,82,82	0
57	MG	14	3128	1/1	0.94	0.12	60,60,60,60	0
57	MG	1H	3450	1/1	0.94	0.04	87,87,87,87	0
57	MG	13	1742	1/1	0.94	0.08	100,100,100,100	0
57	MG	13	1616	1/1	0.94	0.31	48,48,48,48	0
57	MG	1H	3104	1/1	0.94	0.20	62,62,62,62	0
57	MG	14	3372	1/1	0.94	0.09	73,73,73,73	0
57	MG	13	1640	1/1	0.94	0.24	71,71,71,71	0
57	MG	21	301	1/1	0.94	0.36	66,66,66,66	0
57	MG	1H	3049	1/1	0.94	0.28	68,68,68,68	0
57	MG	1H	3403	1/1	0.94	0.18	89,89,89,89	0
57	MG	13	1737	1/1	0.94	0.10	147,147,147,147	0
57	MG	1H	3366	1/1	0.94	0.08	65,65,65,65	0
57	MG	1G	1647	1/1	0.94	0.25	115,115,115,115	0
57	MG	1G	1634	1/1	0.94	0.18	93,93,93,93	0
57	MG	1G	1667	1/1	0.94	0.06	100,100,100,100	0
57	MG	14	3174	1/1	0.94	0.16	71,71,71,71	0
57	MG	1H	3436	1/1	0.94	0.10	65,65,65,65	0
57	MG	1H	3068	1/1	0.94	0.61	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3406	1/1	0.94	0.15	76,76,76,76	0
57	MG	13	1734	1/1	0.94	0.06	86,86,86,86	0
57	MG	14	3132	1/1	0.94	0.17	58,58,58,58	0
57	MG	1H	3191	1/1	0.94	0.13	95,95,95,95	0
57	MG	1H	3135	1/1	0.94	0.34	81,81,81,81	0
57	MG	1H	3142	1/1	0.94	0.52	85,85,85,85	0
57	MG	1H	3058	1/1	0.94	0.28	53,53,53,53	0
57	MG	1H	3165	1/1	0.94	0.32	72,72,72,72	0
57	MG	1G	1687	1/1	0.94	0.06	95,95,95,95	0
57	MG	1G	1614	1/1	0.94	0.27	99,99,99,99	0
57	MG	1H	3386	1/1	0.94	0.06	84,84,84,84	0
57	MG	14	3052	1/1	0.94	0.32	62,62,62,62	0
57	MG	14	3088	1/1	0.94	0.29	65,65,65,65	0
57	MG	14	3254	1/1	0.94	0.21	81,81,81,81	0
57	MG	14	3405	1/1	0.94	0.04	83,83,83,83	0
57	MG	14	3253	1/1	0.94	0.18	63,63,63,63	0
57	MG	13	1733	1/1	0.94	0.06	73,73,73,73	0
57	MG	14	3034	1/1	0.94	0.36	57,57,57,57	0
57	MG	14	3068	1/1	0.94	0.32	67,67,67,67	0
57	MG	14	3043	1/1	0.94	0.27	75,75,75,75	0
57	MG	13	1710	1/1	0.94	0.12	108,108,108,108	0
57	MG	1G	1649	1/1	0.94	0.12	115,115,115,115	0
57	MG	14	3095	1/1	0.94	0.22	85,85,85,85	0
57	MG	14	3030	1/1	0.94	0.22	68,68,68,68	0
57	MG	1H	3270	1/1	0.94	0.10	71,71,71,71	0
57	MG	14	3090	1/1	0.94	0.13	60,60,60,60	0
57	MG	13	1619	1/1	0.94	0.12	90,90,90,90	0
57	MG	1H	3202	1/1	0.94	0.39	58,58,58,58	0
57	MG	14	3446	1/1	0.94	0.04	109,109,109,109	0
57	MG	14	3325	1/1	0.94	0.05	78,78,78,78	0
57	MG	1H	3483	1/1	0.94	0.05	106,106,106,106	0
57	MG	1G	1640	1/1	0.94	0.18	100,100,100,100	0
57	MG	14	3390	1/1	0.94	0.06	82,82,82,82	0
57	MG	14	3136	1/1	0.94	0.37	59,59,59,59	0
57	MG	1H	3055	1/1	0.94	0.33	72,72,72,72	0
57	MG	1H	3360	1/1	0.94	0.09	60,60,60,60	0
57	MG	1H	3225	1/1	0.94	0.40	67,67,67,67	0
57	MG	1G	1606	1/1	0.94	0.27	67,67,67,67	0
57	MG	13	1680	1/1	0.94	0.36	75,75,75,75	0
57	MG	14	3217	1/1	0.94	0.30	76,76,76,76	0
57	MG	1H	3154	1/1	0.94	0.18	75,75,75,75	0
57	MG	1G	1644	1/1	0.94	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3397	1/1	0.94	0.07	85,85,85,85	0
57	MG	14	3245	1/1	0.94	0.36	79,79,79,79	0
57	MG	1H	3337	1/1	0.94	0.07	73,73,73,73	0
57	MG	1H	3454	1/1	0.95	0.08	62,62,62,62	0
57	MG	14	3138	1/1	0.95	0.08	68,68,68,68	0
57	MG	1H	3457	1/1	0.95	0.10	82,82,82,82	0
57	MG	1G	1694	1/1	0.95	0.48	98,98,98,98	0
57	MG	14	3316	1/1	0.95	0.07	102,102,102,102	0
57	MG	1H	3124	1/1	0.95	0.24	74,74,74,74	0
57	MG	1G	1632	1/1	0.95	0.15	132,132,132,132	0
57	MG	14	3378	1/1	0.95	0.04	93,93,93,93	0
57	MG	1H	3433	1/1	0.95	0.11	86,86,86,86	0
57	MG	1H	3173	1/1	0.95	0.15	63,63,63,63	0
57	MG	14	3371	1/1	0.95	0.05	83,83,83,83	0
57	MG	1H	3088	1/1	0.95	0.34	53,53,53,53	0
57	MG	14	3081	1/1	0.95	0.74	74,74,74,74	0
57	MG	1H	3080	1/1	0.95	0.72	82,82,82,82	0
57	MG	1H	3359	1/1	0.95	0.12	52,52,52,52	0
57	MG	13	1698	1/1	0.95	0.04	93,93,93,93	0
57	MG	14	3338	1/1	0.95	0.06	72,72,72,72	0
57	MG	14	3365	1/1	0.95	0.09	88,88,88,88	0
57	MG	14	3041	1/1	0.95	0.20	64,64,64,64	0
57	MG	14	3256	1/1	0.95	0.12	91,91,91,91	0
57	MG	1H	3156	1/1	0.95	0.33	61,61,61,61	0
57	MG	1H	3400	1/1	0.95	0.21	67,67,67,67	0
57	MG	1H	3448	1/1	0.95	0.09	62,62,62,62	0
57	MG	14	3353	1/1	0.95	0.10	67,67,67,67	0
57	MG	1H	3201	1/1	0.95	0.37	65,65,65,65	0
57	MG	1H	3260	1/1	0.95	0.25	65,65,65,65	0
57	MG	13	1699	1/1	0.95	0.06	73,73,73,73	0
57	MG	14	3114	1/1	0.95	0.39	63,63,63,63	0
57	MG	1H	3038	1/1	0.95	0.23	53,53,53,53	0
57	MG	14	3312	1/1	0.95	0.06	77,77,77,77	0
57	MG	14	3118	1/1	0.95	0.30	66,66,66,66	0
57	MG	14	3115	1/1	0.95	0.39	71,71,71,71	0
57	MG	14	3431	1/1	0.95	0.06	90,90,90,90	0
57	MG	14	3091	1/1	0.95	0.23	85,85,85,85	0
57	MG	1H	3374	1/1	0.95	0.07	55,55,55,55	0
57	MG	14	3156	1/1	0.95	0.41	75,75,75,75	0
57	MG	14	3231	1/1	0.95	0.44	76,76,76,76	0
57	MG	1H	3072	1/1	0.95	0.69	73,73,73,73	0
57	MG	1H	3442	1/1	0.95	0.11	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3262	1/1	0.95	0.14	72,72,72,72	0
57	MG	1J	206	1/1	0.95	0.05	94,94,94,94	0
57	MG	1G	1675	1/1	0.95	0.07	88,88,88,88	0
57	MG	13	1729	1/1	0.95	0.05	91,91,91,91	0
57	MG	1H	3141	1/1	0.95	0.21	67,67,67,67	0
57	MG	1G	1612	1/1	0.95	0.34	67,67,67,67	0
57	MG	13	1681	1/1	0.95	0.40	86,86,86,86	0
57	MG	16	210	1/1	0.95	0.09	88,88,88,88	0
57	MG	14	3177	1/1	0.95	0.35	79,79,79,79	0
57	MG	1H	3004	1/1	0.95	0.23	54,54,54,54	0
57	MG	1H	3082	1/1	0.95	0.23	49,49,49,49	0
57	MG	1G	1608	1/1	0.95	0.23	91,91,91,91	0
57	MG	1G	1611	1/1	0.95	0.39	74,74,74,74	0
57	MG	14	3336	1/1	0.95	0.05	83,83,83,83	0
57	MG	1H	3106	1/1	0.95	0.43	74,74,74,74	0
57	MG	14	3328	1/1	0.95	0.07	93,93,93,93	0
57	MG	1H	3067	1/1	0.95	0.33	52,52,52,52	0
57	MG	14	3313	1/1	0.95	0.07	72,72,72,72	0
57	MG	1H	3042	1/1	0.95	0.17	79,79,79,79	0
57	MG	13	1712	1/1	0.95	0.08	75,75,75,75	0
57	MG	13	1624	1/1	0.95	0.12	81,81,81,81	0
57	MG	14	3099	1/1	0.95	0.17	57,57,57,57	0
57	MG	14	3412	1/1	0.95	0.04	120,120,120,120	0
57	MG	1H	3197	1/1	0.95	0.34	67,67,67,67	0
57	MG	1G	1615	1/1	0.95	0.20	92,92,92,92	0
57	MG	1H	3427	1/1	0.95	0.04	88,88,88,88	0
57	MG	1H	3232	1/1	0.95	0.31	65,65,65,65	0
57	MG	13	1743	1/1	0.95	0.05	87,87,87,87	0
57	MG	13	1632	1/1	0.95	0.13	77,77,77,77	0
57	MG	14	3170	1/1	0.95	0.31	86,86,86,86	0
57	MG	1H	3251	1/1	0.95	0.22	78,78,78,78	0
57	MG	1H	3102	1/1	0.95	0.46	70,70,70,70	0
57	MG	1H	3061	1/1	0.95	0.29	68,68,68,68	0
57	MG	1H	3348	1/1	0.95	0.11	65,65,65,65	0
57	MG	1H	3037	1/1	0.95	0.17	55,55,55,55	0
57	MG	14	3209	1/1	0.95	0.79	64,64,64,64	0
57	MG	13	1673	1/1	0.95	0.14	90,90,90,90	0
57	MG	14	3408	1/1	0.95	0.08	78,78,78,78	0
57	MG	1G	1663	1/1	0.95	0.07	87,87,87,87	0
57	MG	1H	3463	1/1	0.95	0.07	82,82,82,82	0
57	MG	1G	1677	1/1	0.95	0.05	105,105,105,105	0
57	MG	13	1692	1/1	0.95	0.07	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3095	1/1	0.95	0.36	65,65,65,65	0
57	MG	14	3039	1/1	0.95	0.19	73,73,73,73	0
57	MG	1H	3045	1/1	0.95	0.29	54,54,54,54	0
57	MG	1H	3033	1/1	0.95	0.26	62,62,62,62	0
57	MG	13	1609	1/1	0.95	0.25	58,58,58,58	0
57	MG	13	1721	1/1	0.95	0.07	70,70,70,70	0
57	MG	1G	1684	1/1	0.95	0.08	121,121,121,121	0
57	MG	1H	3179	1/1	0.95	0.25	49,49,49,49	0
57	MG	2L	101	1/1	0.95	0.36	70,70,70,70	0
57	MG	1H	3078	1/1	0.95	0.35	60,60,60,60	0
57	MG	13	1687	1/1	0.95	0.23	70,70,70,70	0
57	MG	1G	1605	1/1	0.95	0.29	92,92,92,92	0
57	MG	13	1657	1/1	0.95	0.43	73,73,73,73	0
57	MG	1H	3409	1/1	0.95	0.08	69,69,69,69	0
57	MG	14	3251	1/1	0.95	0.23	82,82,82,82	0
57	MG	45	201	1/1	0.95	0.15	72,72,72,72	0
57	MG	14	3311	1/1	0.95	0.07	66,66,66,66	0
57	MG	14	3403	1/1	0.95	0.08	76,76,76,76	0
57	MG	14	3092	1/1	0.96	0.27	56,56,56,56	0
57	MG	14	3012	1/1	0.96	0.20	68,68,68,68	0
57	MG	1H	3005	1/1	0.96	0.34	74,74,74,74	0
57	MG	1H	3440	1/1	0.96	0.04	87,87,87,87	0
57	MG	1G	1645	1/1	0.96	0.55	88,88,88,88	0
58	PAR	13	1749	42/42	0.96	0.20	64,70,78,81	0
57	MG	13	1605	1/1	0.96	0.31	68,68,68,68	0
57	MG	1H	3146	1/1	0.96	0.25	51,51,51,51	0
57	MG	13	1711	1/1	0.96	0.05	99,99,99,99	0
57	MG	1H	3315	1/1	0.96	0.10	73,73,73,73	0
57	MG	13	1627	1/1	0.96	0.29	64,64,64,64	0
57	MG	1H	3377	1/1	0.96	0.11	76,76,76,76	0
57	MG	1H	3234	1/1	0.96	0.19	72,72,72,72	0
57	MG	1H	3458	1/1	0.96	0.11	87,87,87,87	0
57	MG	1H	3422	1/1	0.96	0.07	79,79,79,79	0
57	MG	14	3430	1/1	0.96	0.04	90,90,90,90	0
57	MG	14	3172	1/1	0.96	0.19	63,63,63,63	0
57	MG	1H	3137	1/1	0.96	0.09	72,72,72,72	0
57	MG	1H	3034	1/1	0.96	0.19	54,54,54,54	0
57	MG	14	3205	1/1	0.96	0.17	77,77,77,77	0
57	MG	1H	3485	1/1	0.96	0.05	76,76,76,76	0
57	MG	1H	3164	1/1	0.96	0.22	47,47,47,47	0
57	MG	14	3391	1/1	0.96	0.09	86,86,86,86	0
57	MG	1H	3474	1/1	0.96	0.09	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	Q8	101	1/1	0.96	0.15	73,73,73,73	0
57	MG	1H	3044	1/1	0.96	0.28	62,62,62,62	0
57	MG	31	301	1/1	0.96	0.06	61,61,61,61	0
57	MG	1H	3127	1/1	0.96	0.34	56,56,56,56	0
57	MG	1H	3316	1/1	0.96	0.14	63,63,63,63	0
57	MG	14	3014	1/1	0.96	0.17	72,72,72,72	0
57	MG	13	1720	1/1	0.96	0.07	86,86,86,86	0
57	MG	13	1685	1/1	0.96	0.12	101,101,101,101	0
57	MG	1H	3147	1/1	0.96	0.16	51,51,51,51	0
57	MG	14	3411	1/1	0.96	0.05	74,74,74,74	0
57	MG	1H	3264	1/1	0.96	0.18	74,74,74,74	0
57	MG	1H	3132	1/1	0.96	0.23	75,75,75,75	0
57	MG	1H	3003	1/1	0.96	0.19	57,57,57,57	0
57	MG	14	3388	1/1	0.96	0.07	82,82,82,82	0
57	MG	16	209	1/1	0.96	0.10	73,73,73,73	0
57	MG	1J	202	1/1	0.96	0.22	94,94,94,94	0
57	MG	1H	3040	1/1	0.96	0.15	60,60,60,60	0
57	MG	14	3426	1/1	0.96	0.04	80,80,80,80	0
57	MG	14	3402	1/1	0.96	0.08	88,88,88,88	0
57	MG	13	1654	1/1	0.96	0.32	75,75,75,75	0
57	MG	1H	3379	1/1	0.96	0.11	86,86,86,86	0
57	MG	13	1641	1/1	0.96	0.43	69,69,69,69	0
57	MG	14	3011	1/1	0.96	0.47	72,72,72,72	0
57	MG	13	1696	1/1	0.96	0.03	86,86,86,86	0
57	MG	14	3003	1/1	0.96	0.19	65,65,65,65	0
57	MG	1G	1669	1/1	0.96	0.08	114,114,114,114	0
57	MG	14	3344	1/1	0.96	0.09	72,72,72,72	0
57	MG	1H	3276	1/1	0.96	0.12	98,98,98,98	0
57	MG	14	3062	1/1	0.96	0.25	85,85,85,85	0
57	MG	1H	3335	1/1	0.96	0.09	61,61,61,61	0
57	MG	1H	3074	1/1	0.96	0.21	48,48,48,48	0
57	MG	13	1701	1/1	0.96	0.07	70,70,70,70	0
57	MG	1H	3345	1/1	0.96	0.15	56,56,56,56	0
57	MG	14	3101	1/1	0.96	0.47	64,64,64,64	0
58	PAR	1G	1691	42/42	0.96	0.16	70,82,88,95	0
57	MG	1H	3100	1/1	0.96	0.19	44,44,44,44	0
57	MG	1H	3013	1/1	0.96	0.34	60,60,60,60	0
57	MG	14	3026	1/1	0.96	0.32	72,72,72,72	0
57	MG	13	1629	1/1	0.96	0.29	98,98,98,98	0
57	MG	14	3354	1/1	0.96	0.15	78,78,78,78	0
57	MG	1H	3161	1/1	0.96	0.29	72,72,72,72	0
57	MG	14	3317	1/1	0.96	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3322	1/1	0.96	0.04	82,82,82,82	0
57	MG	1H	3421	1/1	0.96	0.05	78,78,78,78	0
57	MG	1H	3418	1/1	0.96	0.05	69,69,69,69	0
57	MG	13	1613	1/1	0.96	0.28	65,65,65,65	0
57	MG	13	1691	1/1	0.96	0.12	79,79,79,79	0
57	MG	1H	3363	1/1	0.96	0.09	61,61,61,61	0
57	MG	1H	3166	1/1	0.96	0.12	70,70,70,70	0
57	MG	1G	1630	1/1	0.96	0.22	113,113,113,113	0
57	MG	45	203	1/1	0.96	0.48	71,71,71,71	0
57	MG	14	3276	1/1	0.96	0.11	62,62,62,62	0
57	MG	13	1653	1/1	0.96	0.15	66,66,66,66	0
57	MG	1G	1693	1/1	0.96	0.09	92,92,92,92	0
57	MG	14	3130	1/1	0.96	0.32	71,71,71,71	0
57	MG	1H	3184	1/1	0.96	0.41	67,67,67,67	0
57	MG	14	3361	1/1	0.96	0.09	69,69,69,69	0
57	MG	13	1751	1/1	0.96	0.14	87,87,87,87	0
57	MG	13	1730	1/1	0.96	0.15	82,82,82,82	0
57	MG	1G	1682	1/1	0.96	0.10	127,127,127,127	0
57	MG	1H	3479	1/1	0.96	0.04	89,89,89,89	0
57	MG	1H	3378	1/1	0.96	0.06	84,84,84,84	0
57	MG	14	3447	1/1	0.96	0.06	101,101,101,101	0
57	MG	1H	3240	1/1	0.96	0.25	72,72,72,72	0
57	MG	1H	3425	1/1	0.96	0.07	83,83,83,83	0
57	MG	14	3145	1/1	0.96	0.44	74,74,74,74	0
57	MG	1H	3313	1/1	0.96	0.11	72,72,72,72	0
57	MG	14	3094	1/1	0.96	0.28	85,85,85,85	0
57	MG	14	3348	1/1	0.96	0.05	88,88,88,88	0
57	MG	1H	3012	1/1	0.96	0.41	42,42,42,42	0
57	MG	1H	3214	1/1	0.96	0.43	92,92,92,92	0
57	MG	1H	3175	1/1	0.96	0.31	65,65,65,65	0
57	MG	13	1633	1/1	0.96	0.13	85,85,85,85	0
57	MG	1H	3158	1/1	0.96	0.58	68,68,68,68	0
57	MG	1H	3406	1/1	0.96	0.05	87,87,87,87	0
57	MG	1H	3410	1/1	0.96	0.10	56,56,56,56	0
57	MG	1H	3113	1/1	0.96	0.36	82,82,82,82	0
57	MG	1H	3301	1/1	0.96	0.15	49,49,49,49	0
57	MG	14	3100	1/1	0.96	0.32	43,43,43,43	0
57	MG	1G	1650	1/1	0.96	0.21	87,87,87,87	0
57	MG	14	3117	1/1	0.96	0.36	66,66,66,66	0
57	MG	1H	3444	1/1	0.96	0.07	77,77,77,77	0
57	MG	1H	3447	1/1	0.96	0.12	97,97,97,97	0
60	ZN	C5	202	1/1	0.96	0.15	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3148	1/1	0.96	0.37	69,69,69,69	0
57	MG	14	3203	1/1	0.96	0.18	89,89,89,89	0
57	MG	14	3186	1/1	0.96	0.24	84,84,84,84	0
57	MG	14	3072	1/1	0.97	0.25	69,69,69,69	0
57	MG	13	1604	1/1	0.97	0.14	112,112,112,112	0
57	MG	14	3035	1/1	0.97	0.39	83,83,83,83	0
57	MG	14	3329	1/1	0.97	0.06	90,90,90,90	0
57	MG	14	3320	1/1	0.97	0.09	83,83,83,83	0
57	MG	14	3141	1/1	0.97	0.36	50,50,50,50	0
57	MG	1H	3432	1/1	0.97	0.09	75,75,75,75	0
57	MG	1H	3387	1/1	0.97	0.10	64,64,64,64	0
57	MG	14	3314	1/1	0.97	0.06	75,75,75,75	0
60	ZN	G8	201	1/1	0.97	0.18	146,146,146,146	0
57	MG	1H	3153	1/1	0.97	0.18	59,59,59,59	0
57	MG	13	1644	1/1	0.97	0.20	80,80,80,80	0
57	MG	13	1723	1/1	0.97	0.06	84,84,84,84	0
57	MG	14	3070	1/1	0.97	0.38	52,52,52,52	0
57	MG	13	1727	1/1	0.97	0.07	110,110,110,110	0
57	MG	13	1638	1/1	0.97	0.46	58,58,58,58	0
57	MG	14	3340	1/1	0.97	0.11	73,73,73,73	0
57	MG	1H	3321	1/1	0.97	0.09	77,77,77,77	0
57	MG	1H	3350	1/1	0.97	0.12	69,69,69,69	0
57	MG	1H	3375	1/1	0.97	0.18	57,57,57,57	0
57	MG	14	3384	1/1	0.97	0.06	95,95,95,95	0
57	MG	1H	3354	1/1	0.97	0.10	62,62,62,62	0
57	MG	1H	3094	1/1	0.97	0.12	52,52,52,52	0
57	MG	1H	3461	1/1	0.97	0.05	85,85,85,85	0
57	MG	13	1740	1/1	0.97	0.04	92,92,92,92	0
57	MG	14	3022	1/1	0.97	0.41	60,60,60,60	0
57	MG	I8	101	1/1	0.97	0.04	65,65,65,65	0
57	MG	14	3342	1/1	0.97	0.09	58,58,58,58	0
57	MG	1H	3001	1/1	0.97	0.16	53,53,53,53	0
57	MG	14	3394	1/1	0.97	0.05	78,78,78,78	0
57	MG	1H	3204	1/1	0.97	0.22	86,86,86,86	0
57	MG	14	3032	1/1	0.97	0.18	47,47,47,47	0
57	MG	1H	3352	1/1	0.97	0.15	72,72,72,72	0
57	MG	1H	3050	1/1	0.97	0.32	66,66,66,66	0
57	MG	14	3323	1/1	0.97	0.08	72,72,72,72	0
57	MG	1H	3041	1/1	0.97	0.28	72,72,72,72	0
57	MG	1H	3070	1/1	0.97	0.29	45,45,45,45	0
57	MG	13	1639	1/1	0.97	0.10	84,84,84,84	0
57	MG	1H	3056	1/1	0.97	0.28	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3433	1/1	0.97	0.05	71,71,71,71	0
57	MG	14	3247	1/1	0.97	0.25	67,67,67,67	0
57	MG	13	1747	1/1	0.97	0.13	72,72,72,72	0
57	MG	1H	3362	1/1	0.97	0.07	60,60,60,60	0
57	MG	1H	3253	1/1	0.97	0.69	76,76,76,76	0
57	MG	13	1647	1/1	0.97	0.21	104,104,104,104	0
57	MG	14	3279	1/1	0.97	0.09	62,62,62,62	0
57	MG	14	3006	1/1	0.97	0.24	66,66,66,66	0
57	MG	1H	3441	1/1	0.97	0.10	94,94,94,94	0
57	MG	14	3201	1/1	0.97	0.47	58,58,58,58	0
57	MG	13	1675	1/1	0.97	0.41	79,79,79,79	0
57	MG	1H	3416	1/1	0.97	0.16	48,48,48,48	0
57	MG	14	3047	1/1	0.97	0.33	42,42,42,42	0
57	MG	1H	3145	1/1	0.97	0.24	46,46,46,46	0
57	MG	1H	3437	1/1	0.97	0.04	57,57,57,57	0
57	MG	13	1615	1/1	0.97	0.24	91,91,91,91	0
57	MG	1H	3477	1/1	0.97	0.10	65,65,65,65	0
57	MG	14	3377	1/1	0.97	0.16	67,67,67,67	0
57	MG	1H	3367	1/1	0.97	0.09	54,54,54,54	0
57	MG	14	3018	1/1	0.97	0.26	49,49,49,49	0
57	MG	14	3021	1/1	0.97	0.32	53,53,53,53	0
57	MG	1H	3347	1/1	0.97	0.10	69,69,69,69	0
57	MG	1H	3150	1/1	0.97	0.09	50,50,50,50	0
57	MG	1H	3382	1/1	0.97	0.04	70,70,70,70	0
57	MG	1H	3368	1/1	0.97	0.15	60,60,60,60	0
57	MG	1G	1672	1/1	0.97	0.03	91,91,91,91	0
57	MG	3I	201	1/1	0.97	0.16	57,57,57,57	0
57	MG	14	3025	1/1	0.97	0.19	58,58,58,58	0
57	MG	14	3445	1/1	0.97	0.03	87,87,87,87	0
57	MG	14	3161	1/1	0.97	0.30	73,73,73,73	0
57	MG	1H	3340	1/1	0.97	0.11	54,54,54,54	0
57	MG	1H	3333	1/1	0.97	0.16	75,75,75,75	0
57	MG	14	3413	1/1	0.97	0.10	97,97,97,97	0
57	MG	14	3363	1/1	0.97	0.11	68,68,68,68	0
57	MG	14	3187	1/1	0.97	0.15	80,80,80,80	0
57	MG	14	3073	1/1	0.97	0.23	57,57,57,57	0
57	MG	14	3410	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3217	1/1	0.97	0.16	59,59,59,59	0
57	MG	13	1693	1/1	0.97	0.13	72,72,72,72	0
57	MG	1H	3118	1/1	0.97	0.12	60,60,60,60	0
57	MG	14	3398	1/1	0.97	0.13	83,83,83,83	0
57	MG	14	3087	1/1	0.97	0.09	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1614	1/1	0.97	0.59	64,64,64,64	0
57	MG	1H	3453	1/1	0.97	0.04	83,83,83,83	0
57	MG	14	3189	1/1	0.97	0.48	69,69,69,69	0
57	MG	1H	3357	1/1	0.97	0.09	68,68,68,68	0
57	MG	13	1601	1/1	0.97	0.21	68,68,68,68	0
57	MG	1H	3494	1/1	0.97	0.03	126,126,126,126	0
57	MG	14	3350	1/1	0.97	0.11	56,56,56,56	0
57	MG	1H	3344	1/1	0.97	0.08	49,49,49,49	0
57	MG	1H	3373	1/1	0.97	0.14	66,66,66,66	0
57	MG	1G	1685	1/1	0.97	0.06	109,109,109,109	0
57	MG	14	3077	1/1	0.97	0.41	80,80,80,80	0
57	MG	14	3109	1/1	0.97	0.32	60,60,60,60	0
57	MG	14	3066	1/1	0.97	0.18	53,53,53,53	0
57	MG	14	3393	1/1	0.97	0.09	79,79,79,79	0
57	MG	1G	1662	1/1	0.97	0.11	76,76,76,76	0
57	MG	1H	3028	1/1	0.97	0.26	51,51,51,51	0
57	MG	1H	3216	1/1	0.97	0.21	57,57,57,57	0
57	MG	1H	3364	1/1	0.97	0.03	106,106,106,106	0
57	MG	1H	3469	1/1	0.97	0.04	100,100,100,100	0
57	MG	13	1707	1/1	0.97	0.04	90,90,90,90	0
57	MG	1H	3430	1/1	0.97	0.06	85,85,85,85	0
57	MG	14	3250	1/1	0.97	0.18	65,65,65,65	0
57	MG	1H	3081	1/1	0.97	0.19	47,47,47,47	0
57	MG	14	3415	1/1	0.97	0.06	77,77,77,77	0
57	MG	13	1745	1/1	0.97	0.05	117,117,117,117	0
57	MG	1H	3237	1/1	0.97	0.18	61,61,61,61	0
57	MG	1H	3330	1/1	0.97	0.12	57,57,57,57	0
57	MG	1H	3413	1/1	0.97	0.08	78,78,78,78	0
57	MG	14	3196	1/1	0.97	0.17	90,90,90,90	0
57	MG	14	3078	1/1	0.97	0.28	86,86,86,86	0
57	MG	1H	3464	1/1	0.97	0.08	62,62,62,62	0
57	MG	1G	1652	1/1	0.97	0.11	82,82,82,82	0
57	MG	1H	3486	1/1	0.97	0.18	61,61,61,61	0
57	MG	14	3167	1/1	0.97	0.14	65,65,65,65	0
57	MG	14	3376	1/1	0.97	0.11	52,52,52,52	0
57	MG	13	1731	1/1	0.97	0.05	86,86,86,86	0
57	MG	14	3093	1/1	0.97	0.39	51,51,51,51	0
57	MG	13	1606	1/1	0.97	0.28	52,52,52,52	0
57	MG	1H	3465	1/1	0.97	0.26	53,53,53,53	0
57	MG	5E	201	1/1	0.97	0.20	81,81,81,81	0
57	MG	1H	3490	1/1	0.97	0.07	83,83,83,83	0
57	MG	14	3304	1/1	0.97	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3083	1/1	0.97	0.21	61,61,61,61	0
57	MG	14	3392	1/1	0.97	0.06	87,87,87,87	0
57	MG	14	3399	1/1	0.97	0.09	78,78,78,78	0
57	MG	14	3197	1/1	0.97	0.14	56,56,56,56	0
57	MG	1H	3475	1/1	0.97	0.13	88,88,88,88	0
57	MG	14	3404	1/1	0.97	0.09	94,94,94,94	0
57	MG	1H	3151	1/1	0.97	0.18	91,91,91,91	0
57	MG	14	3414	1/1	0.97	0.06	85,85,85,85	0
57	MG	14	3343	1/1	0.97	0.09	63,63,63,63	0
57	MG	1H	3250	1/1	0.97	0.19	67,67,67,67	0
57	MG	14	3218	1/1	0.97	0.28	54,54,54,54	0
57	MG	1H	3502	1/1	0.97	0.32	59,59,59,59	0
57	MG	13	1608	1/1	0.97	0.23	75,75,75,75	0
57	MG	14	3008	1/1	0.97	0.11	72,72,72,72	0
57	MG	13	1611	1/1	0.97	0.24	79,79,79,79	0
57	MG	1H	3429	1/1	0.97	0.11	75,75,75,75	0
57	MG	1H	3473	1/1	0.97	0.07	85,85,85,85	0
57	MG	14	3396	1/1	0.97	0.08	62,62,62,62	0
57	MG	1H	3414	1/1	0.97	0.13	53,53,53,53	0
57	MG	1G	1680	1/1	0.97	0.03	103,103,103,103	0
57	MG	1H	3303	1/1	0.97	0.11	63,63,63,63	0
57	MG	14	3440	1/1	0.97	0.04	94,94,94,94	0
57	MG	14	3153	1/1	0.98	0.09	79,79,79,79	0
57	MG	13	1610	1/1	0.98	0.15	79,79,79,79	0
57	MG	14	3285	1/1	0.98	0.05	59,59,59,59	0
57	MG	13	1700	1/1	0.98	0.07	93,93,93,93	0
57	MG	1H	3424	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3152	1/1	0.98	0.19	87,87,87,87	0
57	MG	14	3029	1/1	0.98	0.26	59,59,59,59	0
57	MG	14	3290	1/1	0.98	0.09	64,64,64,64	0
57	MG	1H	3328	1/1	0.98	0.08	52,52,52,52	0
57	MG	1H	3117	1/1	0.98	0.51	72,72,72,72	0
57	MG	1H	3002	1/1	0.98	0.31	39,39,39,39	0
57	MG	1H	3449	1/1	0.98	0.12	69,69,69,69	0
57	MG	11	302	1/1	0.98	0.11	57,57,57,57	0
57	MG	1H	3370	1/1	0.98	0.11	70,70,70,70	0
57	MG	14	3286	1/1	0.98	0.05	63,63,63,63	0
57	MG	14	3084	1/1	0.98	0.34	56,56,56,56	0
57	MG	1G	1661	1/1	0.98	0.05	111,111,111,111	0
57	MG	14	3359	1/1	0.98	0.11	67,67,67,67	0
57	MG	14	3283	1/1	0.98	0.09	74,74,74,74	0
57	MG	1H	3384	1/1	0.98	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1664	1/1	0.98	0.05	91,91,91,91	0
57	MG	1H	3446	1/1	0.98	0.04	93,93,93,93	0
57	MG	1H	3412	1/1	0.98	0.13	66,66,66,66	0
57	MG	1H	3426	1/1	0.98	0.08	57,57,57,57	0
57	MG	14	3368	1/1	0.98	0.07	72,72,72,72	0
57	MG	14	3080	1/1	0.98	0.38	46,46,46,46	0
57	MG	14	3020	1/1	0.98	0.38	51,51,51,51	0
57	MG	1H	3456	1/1	0.98	0.05	72,72,72,72	0
57	MG	13	1634	1/1	0.98	0.70	71,71,71,71	0
57	MG	14	3345	1/1	0.98	0.08	68,68,68,68	0
57	MG	14	3375	1/1	0.98	0.05	91,91,91,91	0
57	MG	1H	3071	1/1	0.98	0.43	54,54,54,54	0
57	MG	1H	3336	1/1	0.98	0.13	61,61,61,61	0
57	MG	14	3451	1/1	0.98	0.14	77,77,77,77	0
57	MG	1G	1654	1/1	0.98	0.09	93,93,93,93	0
57	MG	14	3050	1/1	0.98	0.29	59,59,59,59	0
57	MG	13	1706	1/1	0.98	0.12	71,71,71,71	0
57	MG	13	1607	1/1	0.98	0.27	74,74,74,74	0
57	MG	14	3103	1/1	0.98	0.52	68,68,68,68	0
57	MG	1H	3261	1/1	0.98	0.22	67,67,67,67	0
57	MG	14	3042	1/1	0.98	0.24	58,58,58,58	0
57	MG	14	3246	1/1	0.98	0.23	76,76,76,76	0
57	MG	14	3335	1/1	0.98	0.07	87,87,87,87	0
57	MG	14	3214	1/1	0.98	0.15	73,73,73,73	0
57	MG	14	3119	1/1	0.98	0.50	63,63,63,63	0
57	MG	1H	3293	1/1	0.98	0.06	63,63,63,63	0
57	MG	14	3292	1/1	0.98	0.13	61,61,61,61	0
57	MG	14	3419	1/1	0.98	0.05	70,70,70,70	0
57	MG	14	3385	1/1	0.98	0.07	70,70,70,70	0
57	MG	11	301	1/1	0.98	0.10	46,46,46,46	0
57	MG	1H	3402	1/1	0.98	0.09	73,73,73,73	0
57	MG	13	1709	1/1	0.98	0.09	75,75,75,75	0
57	MG	1G	1629	1/1	0.98	0.67	83,83,83,83	0
57	MG	1H	3497	1/1	0.98	0.07	97,97,97,97	0
57	MG	1H	3392	1/1	0.98	0.06	69,69,69,69	0
57	MG	14	3300	1/1	0.98	0.14	57,57,57,57	0
57	MG	14	3349	1/1	0.98	0.08	81,81,81,81	0
57	MG	14	3160	1/1	0.98	0.30	51,51,51,51	0
57	MG	14	3126	1/1	0.98	0.43	64,64,64,64	0
57	MG	1H	3032	1/1	0.98	0.14	61,61,61,61	0
57	MG	14	3079	1/1	0.98	0.30	64,64,64,64	0
57	MG	14	3360	1/1	0.98	0.06	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3079	1/1	0.98	0.30	47,47,47,47	0
57	MG	14	3334	1/1	0.98	0.11	61,61,61,61	0
57	MG	1H	3405	1/1	0.98	0.11	69,69,69,69	0
57	MG	13	1746	1/1	0.98	0.08	83,83,83,83	0
57	MG	13	1718	1/1	0.98	0.09	78,78,78,78	0
57	MG	1H	3404	1/1	0.98	0.09	76,76,76,76	0
57	MG	1G	1659	1/1	0.98	0.13	79,79,79,79	0
57	MG	14	3346	1/1	0.98	0.11	75,75,75,75	0
57	MG	14	3051	1/1	0.98	0.39	62,62,62,62	0
57	MG	13	1716	1/1	0.98	0.08	66,66,66,66	0
57	MG	14	3085	1/1	0.98	0.31	65,65,65,65	0
57	MG	1H	3341	1/1	0.98	0.09	57,57,57,57	0
57	MG	14	3347	1/1	0.98	0.13	67,67,67,67	0
57	MG	14	3302	1/1	0.98	0.10	68,68,68,68	0
57	MG	14	3122	1/1	0.98	0.07	104,104,104,104	0
57	MG	1H	3063	1/1	0.98	0.27	52,52,52,52	0
57	MG	1H	3025	1/1	0.98	0.32	56,56,56,56	0
57	MG	1G	1673	1/1	0.98	0.09	84,84,84,84	0
57	MG	14	3040	1/1	0.98	0.33	64,64,64,64	0
57	MG	1H	3332	1/1	0.98	0.07	63,63,63,63	0
57	MG	14	3397	1/1	0.98	0.14	64,64,64,64	0
57	MG	1H	3381	1/1	0.98	0.11	95,95,95,95	0
57	MG	14	3333	1/1	0.98	0.14	59,59,59,59	0
57	MG	13	1703	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3268	1/1	0.98	0.25	81,81,81,81	0
57	MG	14	3450	1/1	0.98	0.10	63,63,63,63	0
57	MG	14	3381	1/1	0.98	0.05	52,52,52,52	0
57	MG	1H	3492	1/1	0.98	0.06	105,105,105,105	0
57	MG	1H	3031	1/1	0.98	0.38	53,53,53,53	0
57	MG	1H	3299	1/1	0.98	0.06	50,50,50,50	0
57	MG	14	3389	1/1	0.98	0.07	81,81,81,81	0
57	MG	1G	1651	1/1	0.98	0.08	81,81,81,81	0
57	MG	13	1728	1/1	0.98	0.08	91,91,91,91	0
57	MG	1H	3085	1/1	0.98	0.29	71,71,71,71	0
57	MG	14	3437	1/1	0.98	0.03	93,93,93,93	0
57	MG	14	3395	1/1	0.98	0.04	78,78,78,78	0
57	MG	14	3379	1/1	0.98	0.10	94,94,94,94	0
57	MG	14	3061	1/1	0.98	0.34	61,61,61,61	0
57	MG	14	3337	1/1	0.98	0.05	76,76,76,76	0
57	MG	14	3386	1/1	0.98	0.07	56,56,56,56	0
57	MG	14	3125	1/1	0.98	0.17	54,54,54,54	0
57	MG	1H	3324	1/1	0.98	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3257	1/1	0.98	0.25	84,84,84,84	0
57	MG	1H	3398	1/1	0.98	0.12	50,50,50,50	0
57	MG	1H	3320	1/1	0.98	0.05	67,67,67,67	0
57	MG	13	1725	1/1	0.98	0.06	71,71,71,71	0
57	MG	14	3332	1/1	0.98	0.07	63,63,63,63	0
57	MG	14	3373	1/1	0.98	0.06	93,93,93,93	0
57	MG	1G	1625	1/1	0.98	0.20	89,89,89,89	0
57	MG	1H	3169	1/1	0.98	0.20	85,85,85,85	0
57	MG	1H	3256	1/1	0.98	0.34	71,71,71,71	0
57	MG	1H	3160	1/1	0.98	0.46	67,67,67,67	0
57	MG	14	3277	1/1	0.98	0.08	67,67,67,67	0
57	MG	1H	3026	1/1	0.98	0.44	40,40,40,40	0
57	MG	1H	3024	1/1	0.98	0.31	45,45,45,45	0
57	MG	1H	3329	1/1	0.98	0.13	55,55,55,55	0
57	MG	14	3364	1/1	0.98	0.05	73,73,73,73	0
57	MG	13	1726	1/1	0.98	0.08	85,85,85,85	0
57	MG	14	3369	1/1	0.98	0.19	56,56,56,56	0
57	MG	14	3278	1/1	0.98	0.05	65,65,65,65	0
57	MG	1H	3407	1/1	0.98	0.06	50,50,50,50	0
57	MG	1J	204	1/1	0.98	0.06	82,82,82,82	0
57	MG	1H	3468	1/1	0.98	0.11	71,71,71,71	0
57	MG	1H	3356	1/1	0.98	0.10	58,58,58,58	0
57	MG	1H	3009	1/1	0.98	0.25	54,54,54,54	0
57	MG	14	3064	1/1	0.98	0.36	58,58,58,58	0
57	MG	14	3282	1/1	0.98	0.09	58,58,58,58	0
57	MG	1H	3342	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3298	1/1	0.98	0.10	61,61,61,61	0
57	MG	1G	1676	1/1	0.98	0.04	86,86,86,86	0
57	MG	13	1623	1/1	0.98	0.35	61,61,61,61	0
57	MG	14	3140	1/1	0.98	0.31	81,81,81,81	0
57	MG	1H	3462	1/1	0.98	0.07	54,54,54,54	0
57	MG	1H	3399	1/1	0.98	0.13	61,61,61,61	0
57	MG	1H	3460	1/1	0.98	0.14	62,62,62,62	0
57	MG	14	3352	1/1	0.98	0.06	65,65,65,65	0
57	MG	1G	1603	1/1	0.98	0.20	81,81,81,81	0
57	MG	14	3273	1/1	0.98	0.19	58,58,58,58	0
57	MG	13	1705	1/1	0.98	0.07	76,76,76,76	0
57	MG	14	3382	1/1	0.98	0.09	91,91,91,91	0
57	MG	1H	3219	1/1	0.98	0.14	62,62,62,62	0
60	ZN	5A	101	1/1	0.98	0.09	128,128,128,128	0
57	MG	14	3358	1/1	0.98	0.12	54,54,54,54	0
57	MG	1H	3292	1/1	0.98	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3155	1/1	0.98	0.18	75,75,75,75	0
57	MG	13	1715	1/1	0.98	0.09	110,110,110,110	0
57	MG	14	3137	1/1	0.98	0.22	72,72,72,72	0
57	MG	13	1702	1/1	0.98	0.12	76,76,76,76	0
57	MG	1G	1658	1/1	0.98	0.05	94,94,94,94	0
57	MG	14	3065	1/1	0.98	0.28	54,54,54,54	0
57	MG	1H	3394	1/1	0.98	0.14	70,70,70,70	0
57	MG	1H	3314	1/1	0.98	0.13	75,75,75,75	0
57	MG	1H	3420	1/1	0.98	0.07	64,64,64,64	0
57	MG	1H	3223	1/1	0.98	0.18	64,64,64,64	0
57	MG	14	3060	1/1	0.98	0.30	74,74,74,74	0
57	MG	1H	3310	1/1	0.98	0.10	58,58,58,58	0
57	MG	14	3356	1/1	0.98	0.13	61,61,61,61	0
57	MG	1G	1602	1/1	0.98	0.28	72,72,72,72	0
57	MG	1H	3445	1/1	0.98	0.03	97,97,97,97	0
57	MG	14	3289	1/1	0.98	0.12	58,58,58,58	0
57	MG	1H	3391	1/1	0.98	0.13	49,49,49,49	0
57	MG	2K	103	1/1	0.98	0.36	61,61,61,61	0
57	MG	14	3046	1/1	0.99	0.41	58,58,58,58	0
57	MG	14	3288	1/1	0.99	0.14	50,50,50,50	0
57	MG	13	1602	1/1	0.99	0.41	88,88,88,88	0
57	MG	14	3127	1/1	0.99	0.34	48,48,48,48	0
60	ZN	5I	102	1/1	0.99	0.13	88,88,88,88	0
57	MG	1H	3443	1/1	0.99	0.08	67,67,67,67	0
57	MG	1H	3408	1/1	0.99	0.11	50,50,50,50	0
57	MG	1H	3349	1/1	0.99	0.17	53,53,53,53	0
57	MG	1H	3016	1/1	0.99	0.40	49,49,49,49	0
57	MG	14	3299	1/1	0.99	0.06	60,60,60,60	0
57	MG	13	1690	1/1	0.99	0.14	68,68,68,68	0
57	MG	14	3409	1/1	0.99	0.14	80,80,80,80	0
57	MG	1H	3419	1/1	0.99	0.06	63,63,63,63	0
57	MG	1G	1660	1/1	0.99	0.03	96,96,96,96	0
57	MG	14	3322	1/1	0.99	0.14	74,74,74,74	0
57	MG	14	3019	1/1	0.99	0.33	58,58,58,58	0
57	MG	1H	3311	1/1	0.99	0.10	53,53,53,53	0
57	MG	1H	3304	1/1	0.99	0.11	55,55,55,55	0
57	MG	1H	3317	1/1	0.99	0.20	45,45,45,45	0
57	MG	14	3291	1/1	0.99	0.12	66,66,66,66	0
57	MG	14	3297	1/1	0.99	0.08	74,74,74,74	0
57	MG	13	1732	1/1	0.99	0.08	108,108,108,108	0
57	MG	13	1717	1/1	0.99	0.10	66,66,66,66	0
57	MG	14	3059	1/1	0.99	0.41	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3499	1/1	0.99	0.26	67,67,67,67	0
57	MG	14	3401	1/1	0.99	0.10	66,66,66,66	0
57	MG	1H	3307	1/1	0.99	0.06	57,57,57,57	0
57	MG	1H	3296	1/1	0.99	0.18	49,49,49,49	0
57	MG	85	201	1/1	0.99	0.20	72,72,72,72	0
57	MG	1H	3365	1/1	0.99	0.10	70,70,70,70	0
57	MG	1H	3300	1/1	0.99	0.11	54,54,54,54	0
57	MG	14	3341	1/1	0.99	0.07	62,62,62,62	0
57	MG	1H	3346	1/1	0.99	0.11	58,58,58,58	0
57	MG	1G	1681	1/1	0.99	0.04	85,85,85,85	0
57	MG	1H	3361	1/1	0.99	0.08	53,53,53,53	0
57	MG	1H	3353	1/1	0.99	0.09	57,57,57,57	0
57	MG	1H	3309	1/1	0.99	0.12	48,48,48,48	0
59	SF4	32	301	8/8	0.99	0.17	100,111,117,118	0
57	MG	1H	3389	1/1	0.99	0.16	59,59,59,59	0
57	MG	1H	3295	1/1	0.99	0.11	52,52,52,52	0
59	SF4	3E	301	8/8	0.99	0.19	71,78,87,91	0
57	MG	1H	3027	1/1	0.99	0.40	63,63,63,63	0
57	MG	1H	3030	1/1	0.99	0.23	45,45,45,45	0
57	MG	14	3133	1/1	0.99	0.33	71,71,71,71	0
57	MG	1H	3338	1/1	0.99	0.18	53,53,53,53	0
57	MG	1H	3305	1/1	0.99	0.09	53,53,53,53	0
57	MG	14	3275	1/1	0.99	0.09	61,61,61,61	0
57	MG	14	3249	1/1	0.99	0.28	60,60,60,60	0
57	MG	14	3432	1/1	0.99	0.10	83,83,83,83	0
57	MG	1H	3396	1/1	0.99	0.08	60,60,60,60	0
57	MG	1H	3051	1/1	0.99	0.16	93,93,93,93	0
57	MG	14	3331	1/1	0.99	0.09	66,66,66,66	0
57	MG	1H	3351	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3302	1/1	0.99	0.07	47,47,47,47	0
57	MG	14	3023	1/1	0.99	0.30	54,54,54,54	0
57	MG	1H	3339	1/1	0.99	0.09	50,50,50,50	0
57	MG	1H	3060	1/1	0.99	0.37	55,55,55,55	0
57	MG	29	302	1/1	0.99	0.29	40,40,40,40	0
57	MG	1H	3172	1/1	0.99	0.14	73,73,73,73	0
57	MG	1G	1656	1/1	0.99	0.19	105,105,105,105	0
57	MG	14	3420	1/1	0.99	0.12	65,65,65,65	0
57	MG	13	1695	1/1	0.99	0.11	76,76,76,76	0
57	MG	1H	3417	1/1	0.99	0.11	56,56,56,56	0
57	MG	14	3367	1/1	0.99	0.05	60,60,60,60	0
57	MG	14	3298	1/1	0.99	0.03	79,79,79,79	0
57	MG	14	3287	1/1	0.99	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3339	1/1	0.99	0.07	86,86,86,86	0
57	MG	1H	3327	1/1	0.99	0.05	55,55,55,55	0
57	MG	1H	3239	1/1	0.99	0.09	67,67,67,67	0
57	MG	1H	3089	1/1	0.99	0.44	51,51,51,51	0
57	MG	14	3252	1/1	0.99	0.19	67,67,67,67	0
57	MG	14	3306	1/1	0.99	0.10	55,55,55,55	0
57	MG	1H	3039	1/1	0.99	0.12	90,90,90,90	0
57	MG	1H	3294	1/1	0.99	0.13	56,56,56,56	0
57	MG	14	3295	1/1	0.99	0.11	58,58,58,58	0
57	MG	14	3305	1/1	0.99	0.17	57,57,57,57	0
57	MG	14	3307	1/1	0.99	0.12	79,79,79,79	0
57	MG	1H	3297	1/1	0.99	0.14	49,49,49,49	0
57	MG	13	1683	1/1	0.99	0.21	67,67,67,67	0
57	MG	1H	3401	1/1	0.99	0.10	52,52,52,52	0
57	MG	13	1697	1/1	0.99	0.10	90,90,90,90	0
57	MG	14	3327	1/1	0.99	0.06	67,67,67,67	0
57	MG	1H	3306	1/1	0.99	0.09	60,60,60,60	0
57	MG	1H	3383	1/1	0.99	0.05	78,78,78,78	0
57	MG	1H	3029	1/1	0.99	0.35	49,49,49,49	0
57	MG	14	3274	1/1	0.99	0.13	62,62,62,62	0
57	MG	14	3301	1/1	0.99	0.15	56,56,56,56	0
57	MG	1H	3319	1/1	0.99	0.13	67,67,67,67	0
57	MG	14	3355	1/1	0.99	0.12	59,59,59,59	0
57	MG	14	3281	1/1	0.99	0.16	66,66,66,66	0
57	MG	1H	3043	1/1	0.99	0.28	70,70,70,70	0
57	MG	1H	3167	1/1	0.99	0.16	63,63,63,63	0
57	MG	1H	3491	1/1	0.99	0.13	75,75,75,75	0
57	MG	14	3002	1/1	0.99	0.12	49,49,49,49	0
57	MG	14	3028	1/1	0.99	0.21	60,60,60,60	0
57	MG	14	3453	1/1	0.99	0.04	88,88,88,88	0
57	MG	1H	3318	1/1	0.99	0.15	54,54,54,54	0
57	MG	16	208	1/1	0.99	0.05	67,67,67,67	0
57	MG	1H	3331	1/1	0.99	0.07	66,66,66,66	0
57	MG	14	3284	1/1	0.99	0.07	57,57,57,57	0
57	MG	1H	3355	1/1	0.99	0.10	68,68,68,68	0
57	MG	1H	3343	1/1	0.99	0.07	74,74,74,74	0
57	MG	1H	3388	1/1	0.99	0.14	57,57,57,57	0
57	MG	14	3417	1/1	0.99	0.07	87,87,87,87	0
57	MG	14	3362	1/1	0.99	0.05	62,62,62,62	0
57	MG	13	1694	1/1	0.99	0.17	79,79,79,79	0
57	MG	1H	3064	1/1	0.99	0.23	54,54,54,54	0
57	MG	14	3418	1/1	0.99	0.05	75,75,75,75	0

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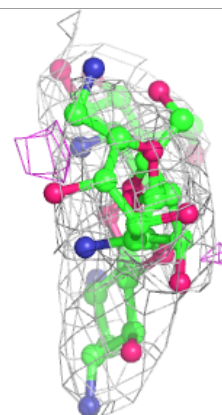
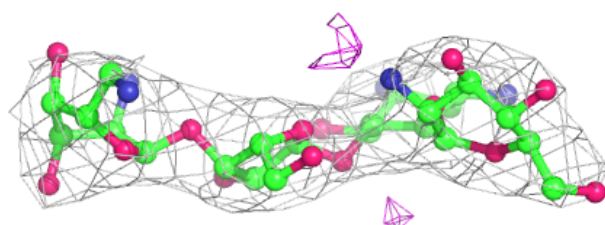
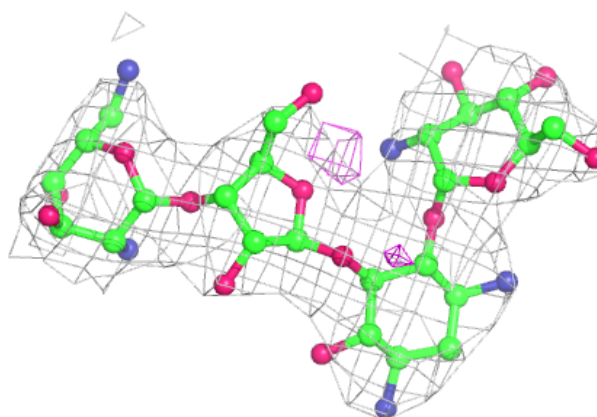
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3358	1/1	0.99	0.12	67,67,67,67	0
57	MG	1H	3415	1/1	0.99	0.10	52,52,52,52	0
57	MG	1H	3390	1/1	1.00	0.08	57,57,57,57	0
57	MG	1H	3308	1/1	1.00	0.08	61,61,61,61	0
57	MG	1H	3312	1/1	1.00	0.05	76,76,76,76	0
57	MG	14	3294	1/1	1.00	0.11	54,54,54,54	0
57	MG	1H	3423	1/1	1.00	0.10	55,55,55,55	0
57	MG	14	3293	1/1	1.00	0.09	51,51,51,51	0

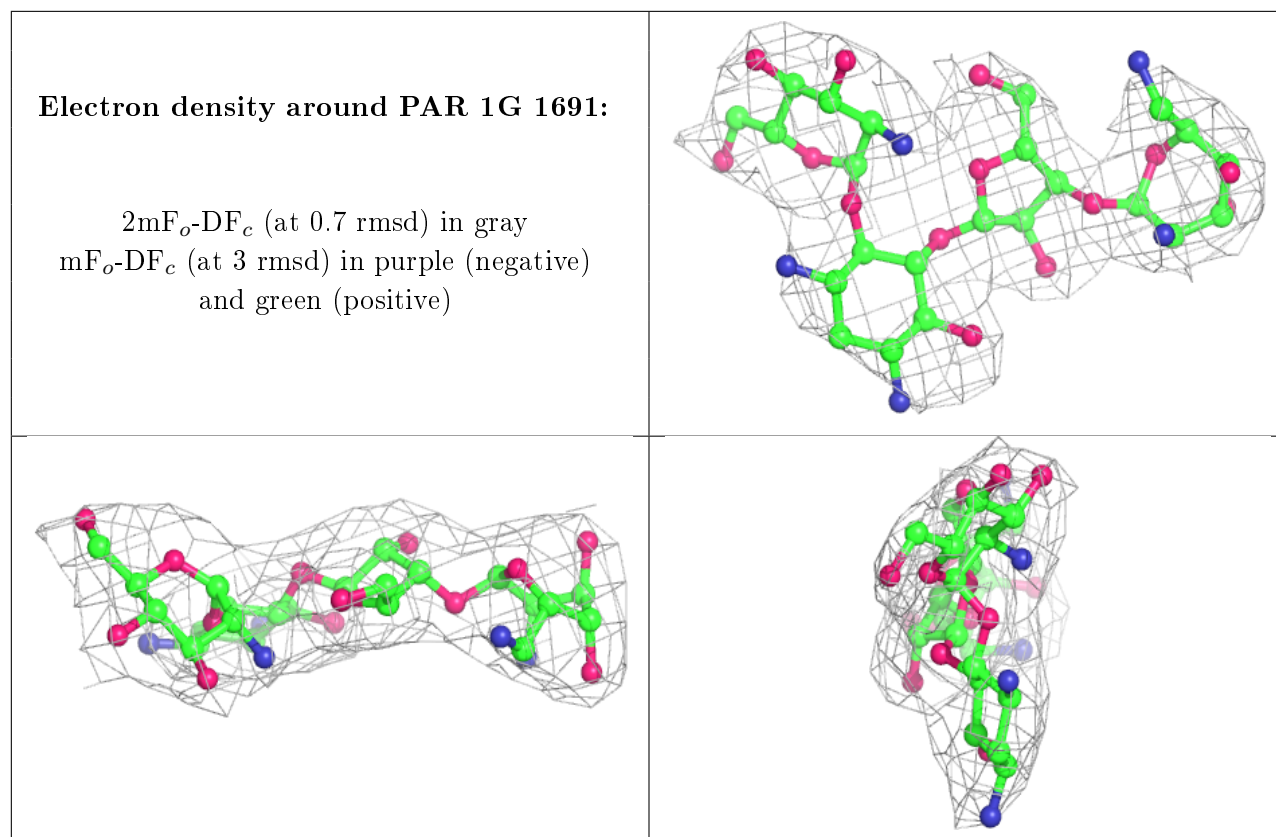
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PAR 13 1749:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.