



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2024 – 03:46 am BST

PDB ID : 5NDK  
Title : Crystal structure of aminoglycoside TC007 co-crystallized with 70S ribosome from *Thermus thermophilus*, three tRNAs and mRNA  
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2017-03-08  
Resolution : 2.95 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

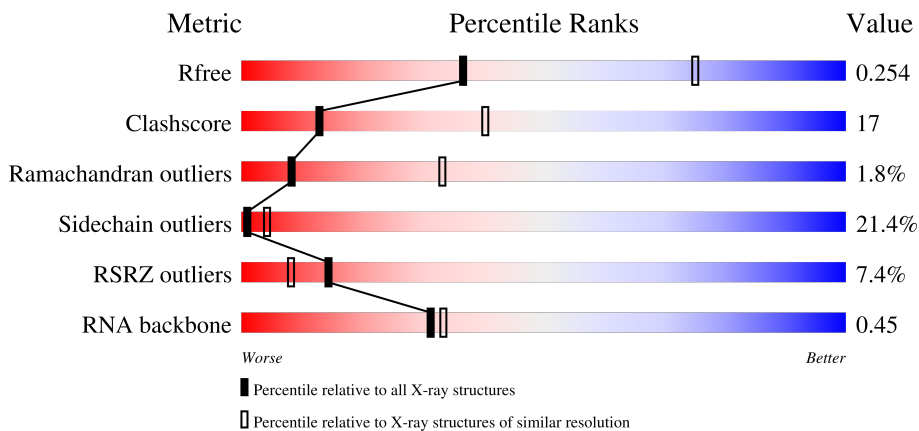
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	65	112	
2	A8	112	

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Mol	Chain	Length	Quality of chain
3	B5	96	11% 54% 33% 8%
3	F8	96	4% 54% 33% 8%
4	11	276	2% 64% 25% 8%
4	19	276	% 60% 29% 7%
5	L5	49	4% 57% 27% 12%
5	P8	49	4% 61% 24% 8%
6	2A	129	45% 51% 35% 10%
6	2I	129	16% 53% 31% 6% 10%
7	8A	105	32% 56% 32% 6% 6%
7	8I	105	6% 43% 40% 12% 5%
8	22	239	8% 43% 32% 11% 14%
8	2E	239	16% 46% 33% 6% 14%
9	82	128	14% 46% 42% 7%
9	8E	128	17% 38% 48% 11%
10	15	140	19% 55% 33% 11%
10	58	140	10% 45% 41% 13%
11	C5	110	39% 31% 50% 12% 5%
11	G8	110	9% 40% 32% 17% 5% 6%
12	M5	65	15% 45% 31% 15% 5% 5%
12	Q8	65	6% 12% 32% 32% 15% 8%
13	3A	132	24% 48% 35% 12% 5%
13	3I	132	10% 55% 27% 11% 8%
14	32	209	6% 50% 39% 10%
14	3E	209	4% 53% 40% 6%
15	14	2917	2% 23% 45% 27% 5%

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Mol	Chain	Length	Quality of chain
15	1H	2917	
16	75	146	
16	B8	146	
17	H5	60	
17	L8	60	
18	61	148	
18	69	148	
19	9A	88	
19	9I	88	
20	1B	27	
20	1F	27	
21	25	122	
21	68	122	
22	D5	206	
22	H8	206	
23	21	206	
23	29	206	
24	4A	126	
24	4I	126	
25	42	162	
25	4E	162	
26	16	122	
26	1J	122	
27	85	118	
27	C8	118	

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Mol	Chain	Length	Quality of chain
28	I5	71	87% 24% 51% 13% 11%
28	M8	71	86% 31% 44% 17% 7%
29	AA	93	10% 41% 33% 10% 16%
29	AI	93	13% 30% 40% 12% 14%
30	35	150	7% 38% 41% 17%
30	78	150	3% 37% 41% 19%
31	E5	85	11% 49% 41% 8%
31	I8	85	5% 71% 24%
32	31	210	3% 45% 41% 9%
32	39	210	5% 42% 39% 17%
33	5A	61	28% 38% 46% 10% 5%
33	5I	61	20% 44% 39% 15%
34	52	101	52% 37% 11%
34	5E	101	61% 32% 7%
35	95	101	24% 35% 49% 15%
35	D8	101	6% 34% 49% 14%
36	J5	60	7% 47% 33% 13% 7%
36	N8	60	13% 45% 28% 13% 5% 8%
37	BA	106	10% 49% 37% 7% 7%
37	BI	106	17% 45% 38% 10% 7%
38	45	141	9% 41% 44% 13%
38	88	141	% 46% 37% 15%
39	F5	98	7% 42% 45% 8%
39	J8	98	8% 46% 36% 12%
40	41	182	10% 47% 38% 14%

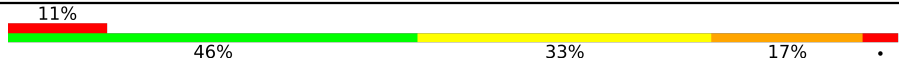

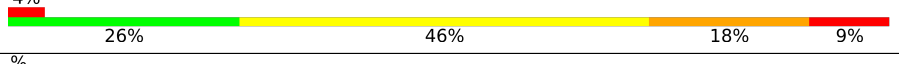
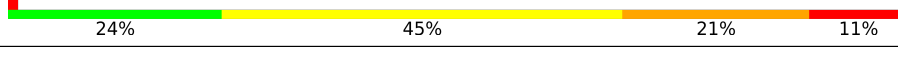
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Mol	Chain	Length	Quality of chain
40	49	182	
41	6A	89	
41	6I	89	
42	62	156	
42	6E	156	
43	A5	113	
43	E8	113	
44	12	256	
44	1E	256	
45	55	118	
45	98	118	
46	G5	72	
46	K8	72	
47	51	180	
47	59	180	
48	1A	105	
48	1I	105	
49	7A	88	
49	7I	88	
50	72	138	
50	7E	138	
51	Y1	25	
51	Y4	25	
52	V1	76	
52	V4	76	

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Mol	Chain	Length	Quality of chain
52	W1	76	
52	W4	76	
52	X1	76	
52	X4	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
54	MG	13	2287	-	-	-	X
54	MG	13	2307	-	-	-	X
54	MG	13	2335	-	-	-	X
54	MG	13	2372	-	-	-	X
54	MG	14	3169	-	-	-	X
54	MG	14	3222	-	-	-	X
54	MG	14	3231	-	-	-	X
54	MG	14	3251	-	-	-	X
54	MG	14	3263	-	-	-	X
54	MG	14	3276	-	-	-	X
54	MG	14	3308	-	-	-	X
54	MG	14	3364	-	-	-	X
54	MG	14	3367	-	-	-	X
54	MG	14	3460	-	-	-	X
54	MG	14	3485	-	-	-	X
54	MG	1G	2253	-	-	-	X
54	MG	1G	2269	-	-	-	X
54	MG	1G	2284	-	-	-	X
54	MG	1G	2288	-	-	-	X
54	MG	1H	3286	-	-	-	X
54	MG	1H	3346	-	-	-	X
54	MG	1H	3492	-	-	-	X
54	MG	1H	3561	-	-	-	X
54	MG	1H	3590	-	-	-	X
54	MG	58	201	-	-	-	X
54	MG	X1	105	-	-	-	X

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 299577 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	13	1508	Total 32409	C 14425	N 6001	O 10475	P 1508	0	0	0
1	1G	1513	Total 32514	C 14473	N 6021	O 10508	P 1512	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	2165	G	-	expression tag	GB 55771382
13	2166	C	-	expression tag	GB 55771382
13	2167	U	-	expression tag	GB 55771382
1G	2165	G	-	expression tag	GB 55771382
1G	2166	C	-	expression tag	GB 55771382
1G	2167	U	-	expression tag	GB 55771382

- Molecule 2 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A8	111	Total 881	C 556	N 176	O 149	0	0	0
2	65	111	Total 881	C 556	N 176	O 149	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B5	92	Total 725	C 471	N 131	O 123	0	0	0	
3	F8	94	Total 742	C 482	N 134	O 125	S 1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	11	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			
4	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 5 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L5	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
5	P8	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	2A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
6	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 7 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
7	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
8	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	82	124	983	624	190	169	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	58	138	1104	712	206	182	4	0	0	0
10	15	138	1104	712	206	182	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	G8	103	783	504	148	126	5	0	0	0
11	C5	104	794	510	152	127	5	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	Q8	60	480	306	98	74	2	0	0	0
12	M5	62	495	317	100	76	2	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	3I	122	956	603	193	159	1	0	0	0
13	3A	125	975	614	196	164	1	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	3E	208	1702	1066	339	290	7	0	0	0
14	32	208	1702	1066	339	290	7	0	0	0

- Molecule 15 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	1H	2912	62707	27911	11722	20163	2911	0	0	0
15	14	2909	62647	27884	11716	20139	2908	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	156	U	UNK	conflict	GB 55771382
1H	682	A	G	conflict	GB 55771382
1H	686	C	G	conflict	GB 55771382
1H	697	G	C	conflict	GB 55771382
1H	701	A	C	conflict	GB 55771382
1H	1106	U	G	conflict	GB 55771382
1H	1128	A	C	conflict	GB 55771382
14	155A	U	UNK	conflict	GB 55771382
14	682	A	G	conflict	GB 55771382
14	686	C	G	conflict	GB 55771382
14	697	G	C	conflict	GB 55771382
14	701	A	C	conflict	GB 55771382
14	1106	U	G	conflict	GB 55771382
14	1128	A	C	conflict	GB 55771382

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	B8	129	1081	674	223	183	1	0	0	0
16	75	137	1141	710	234	196	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	L8	57	452	288	88	76	0	0	0
17	H5	59	468	298	90	80	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
18	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	9I	67	Total	C	N	O	0	0	0
			550	352	107	91			
19	9A	69	Total	C	N	O	0	0	0
			564	361	110	93			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
20	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
21	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	H8	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
22	D5	135	Total	C	N	O	S	0	0	0
			1120	720	202	195	3			

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 24 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
24	4A	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			

- Molecule 25 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
25	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
27	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
28	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 29 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AI	80	Total	C	N	O	S	0	0	0
			643	411	118	112	2			
29	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
30	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I8	83	Total	C	N	O	S	0	0	0
			656	407	139	109	1			
31	E5	84	Total	C	N	O	S	0	0	0
			645	398	136	110	1			

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
32	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 33 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
33	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

- Molecule 34 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
34	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
35	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 36 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	N8	55	Total	C	N	O	S	0	0	0
			429	269	86	69	5			
36	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 37 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			
37	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- 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
			1121	715	212	187	7			
38	45	140	Total	C	N	O	S	0	0	0
			1113	710	211	186	6			

- Molecule 39 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	J8	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	41	181	1473	942	268	259	4	0	0	0
40	49	181	1473	942	268	259	4	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	6I	88	733	459	147	125	2	0	0	0
41	6A	88	733	459	147	125	2	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	6E	144	1157	718	230	203	6	0	0	0
42	62	147	1200	750	237	207	6	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1E	237	1924	1228	344	347	5	0	0	0
44	12	237	1924	1228	344	347	5	0	0	0



- Molecule 45 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
45	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
46	G5	67	Total	C	N	O	S	0	0	0
			567	351	115	100	1			

- Molecule 47 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
47	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 48 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
48	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
49	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 50 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
50	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

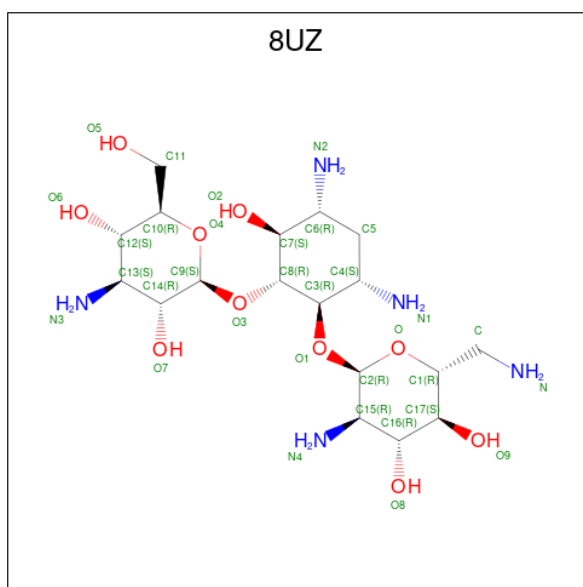
- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	Y1	25	Total	C	N	O	P	0	0	0
			521	234	78	185	24			
51	Y4	25	Total	C	N	O	P	0	0	0
			521	234	78	185	24			

- Molecule 52 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	W1	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
52	X1	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
52	V1	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
52	W4	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
52	X4	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
52	V4	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 53 is TC007 (three-letter code: 8UZ) (formula: C<sub>18</sub>H<sub>37</sub>N<sub>5</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
53	13	1	Total	C	N	O	0	0
			33	18	5	10		
53	13	1	Total	C	N	O	0	0
			33	18	5	10		
53	1G	1	Total	C	N	O	0	0
			33	18	5	10		
53	1G	1	Total	C	N	O	0	0
			33	18	5	10		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	13	182	Total	Mg	0	0
			182	182		
54	A8	1	Total	Mg	0	0
			1	1		
54	B5	1	Total	Mg	0	0
			1	1		
54	11	5	Total	Mg	0	0
			5	5		
54	2A	1	Total	Mg	0	0
			1	1		
54	1G	178	Total	Mg	0	0
			178	178		
54	58	1	Total	Mg	0	0
			1	1		
54	G8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	19	3	Total 3	Mg 3	0	0
54	3I	1	Total 1	Mg 1	0	0
54	3E	2	Total 2	Mg 2	0	0
54	1H	597	Total 597	Mg 597	0	0
54	B8	1	Total 1	Mg 1	0	0
54	C5	2	Total 2	Mg 2	0	0
54	L8	1	Total 1	Mg 1	0	0
54	14	568	Total 568	Mg 568	0	0
54	68	2	Total 2	Mg 2	0	0
54	21	3	Total 3	Mg 3	0	0
54	4I	1	Total 1	Mg 1	0	0
54	4E	1	Total 1	Mg 1	0	0
54	16	14	Total 14	Mg 14	0	0
54	25	2	Total 2	Mg 2	0	0
54	29	5	Total 5	Mg 5	0	0
54	42	1	Total 1	Mg 1	0	0
54	1J	14	Total 14	Mg 14	0	0
54	78	3	Total 3	Mg 3	0	0
54	85	1	Total 1	Mg 1	0	0
54	I8	2	Total 2	Mg 2	0	0
54	31	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	5I	1	Total 1	Mg 1	0	0
54	5E	1	Total 1	Mg 1	0	0
54	35	1	Total 1	Mg 1	0	0
54	E5	2	Total 2	Mg 2	0	0
54	39	2	Total 2	Mg 2	0	0
54	52	1	Total 1	Mg 1	0	0
54	88	5	Total 5	Mg 5	0	0
54	41	2	Total 2	Mg 2	0	0
54	45	2	Total 2	Mg 2	0	0
54	49	1	Total 1	Mg 1	0	0
54	6A	1	Total 1	Mg 1	0	0
54	98	1	Total 1	Mg 1	0	0
54	A5	1	Total 1	Mg 1	0	0
54	K8	1	Total 1	Mg 1	0	0
54	55	2	Total 2	Mg 2	0	0
54	P8	1	Total 1	Mg 1	0	0
54	7A	1	Total 1	Mg 1	0	0
54	W1	4	Total 4	Mg 4	0	0
54	X1	9	Total 9	Mg 9	0	0
54	W4	4	Total 4	Mg 4	0	0
54	X4	6	Total 6	Mg 6	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	G8	1	Total 1	Zn 1	0	0
55	3E	1	Total 1	Zn 1	0	0
55	C5	1	Total 1	Zn 1	0	0
55	32	1	Total 1	Zn 1	0	0
55	5I	1	Total 1	Zn 1	0	0
55	5A	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	76	Total 76	O 76	0	0
56	11	1	Total 1	O 1	0	0
56	L5	3	Total 3	O 3	0	0
56	1G	72	Total 72	O 72	0	0
56	19	8	Total 8	O 8	0	0
56	1H	533	Total 533	O 533	0	0
56	B8	1	Total 1	O 1	0	0
56	M5	2	Total 2	O 2	0	0
56	14	512	Total 512	O 512	0	0
56	21	1	Total 1	O 1	0	0
56	C8	3	Total 3	O 3	0	0
56	29	4	Total 4	O 4	0	0
56	78	4	Total 4	O 4	0	0

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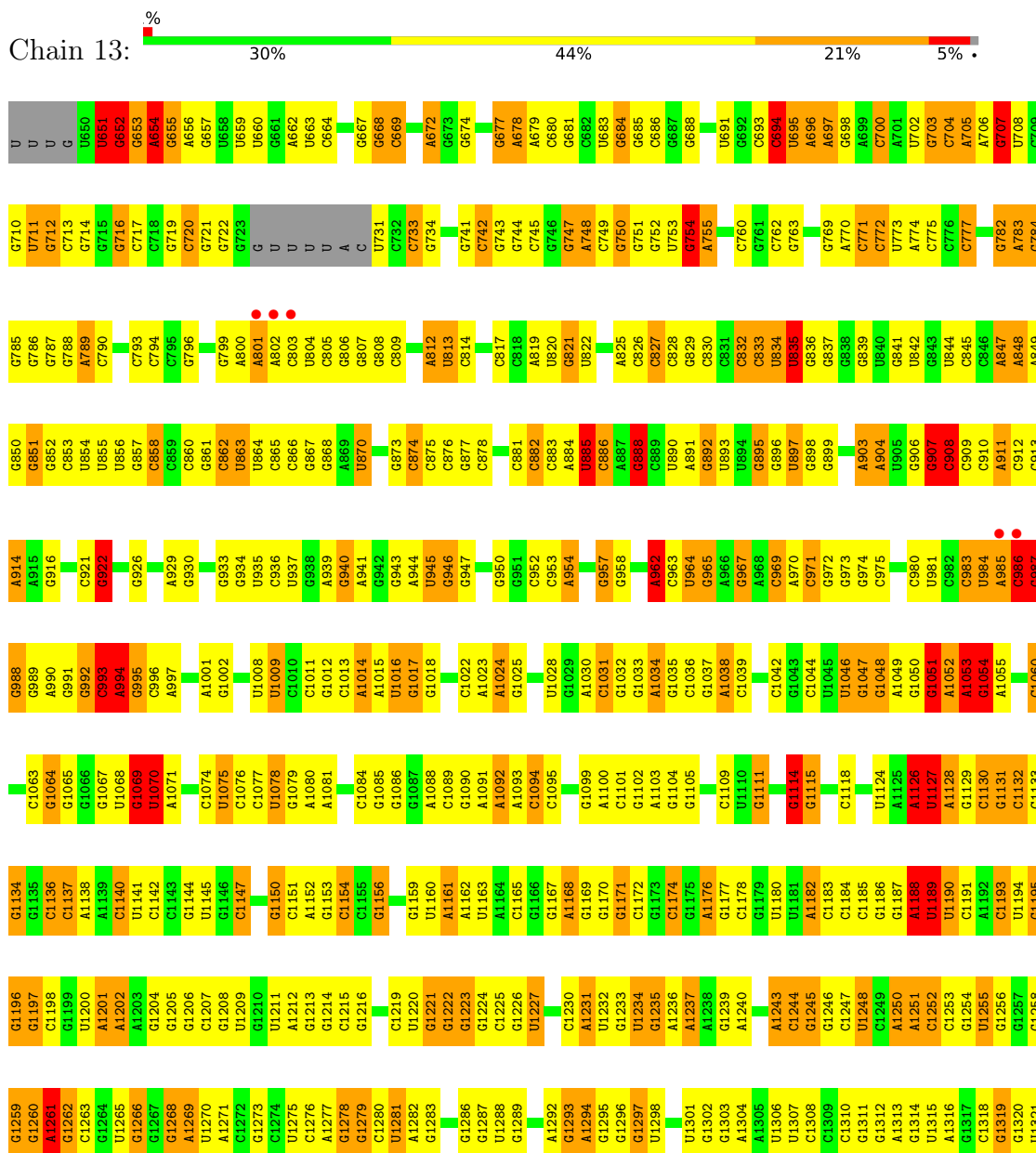
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	I8	5	Total 5	O 5	0	0
56	31	5	Total 5	O 5	0	0
56	35	1	Total 1	O 1	0	0
56	D8	1	Total 1	O 1	0	0
56	39	6	Total 6	O 6	0	0
56	5A	1	Total 1	O 1	0	0
56	J8	1	Total 1	O 1	0	0
56	J5	1	Total 1	O 1	0	0
56	6I	1	Total 1	O 1	0	0
56	E8	1	Total 1	O 1	0	0
56	6A	2	Total 2	O 2	0	0
56	A5	1	Total 1	O 1	0	0
56	55	1	Total 1	O 1	0	0
56	F8	1	Total 1	O 1	0	0
56	P8	1	Total 1	O 1	0	0
56	7A	1	Total 1	O 1	0	0
56	Y4	2	Total 2	O 2	0	0

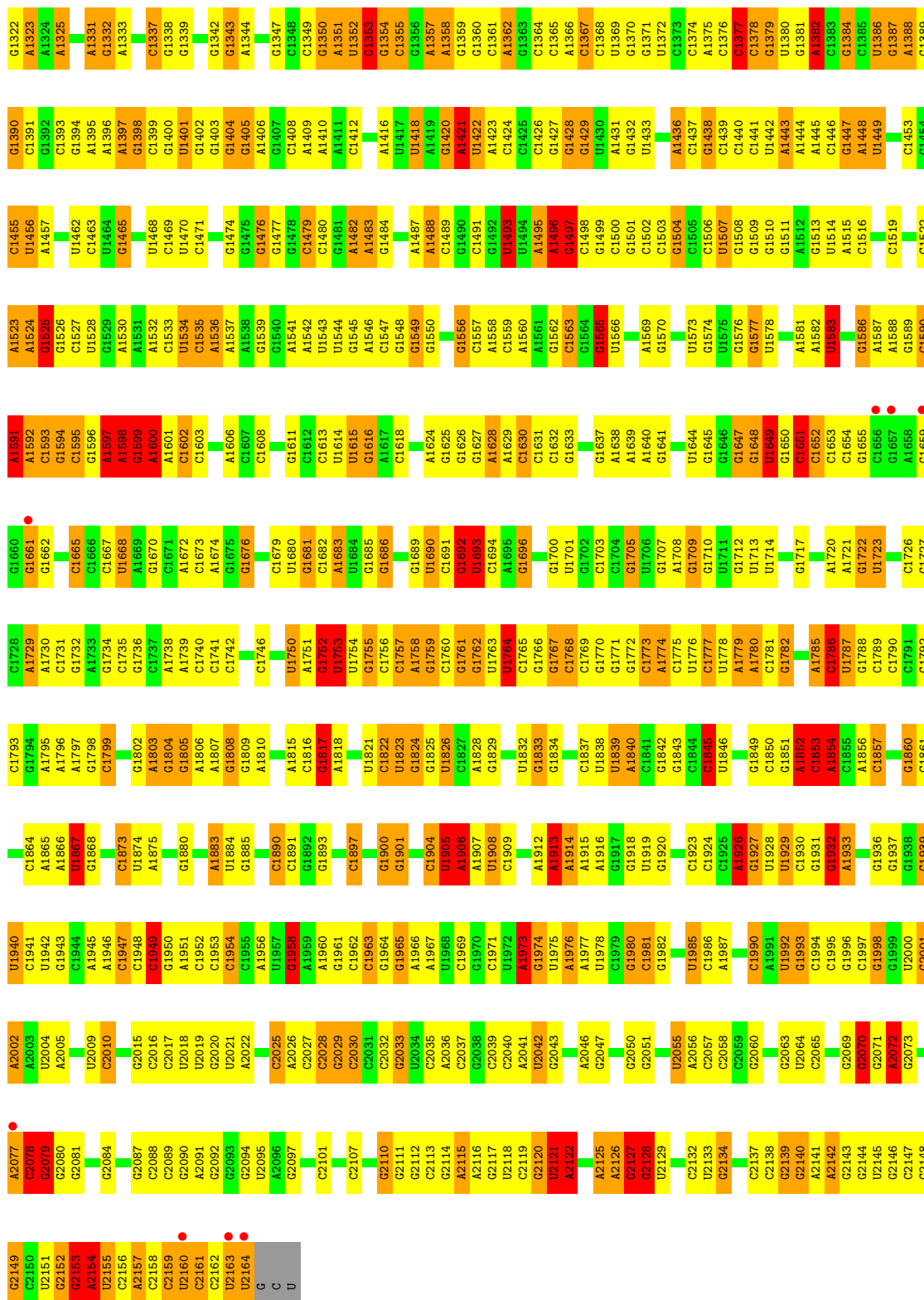
### 3 Residue-property plots [i](#)

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

- Molecule 1: 16S ribosomal RNA



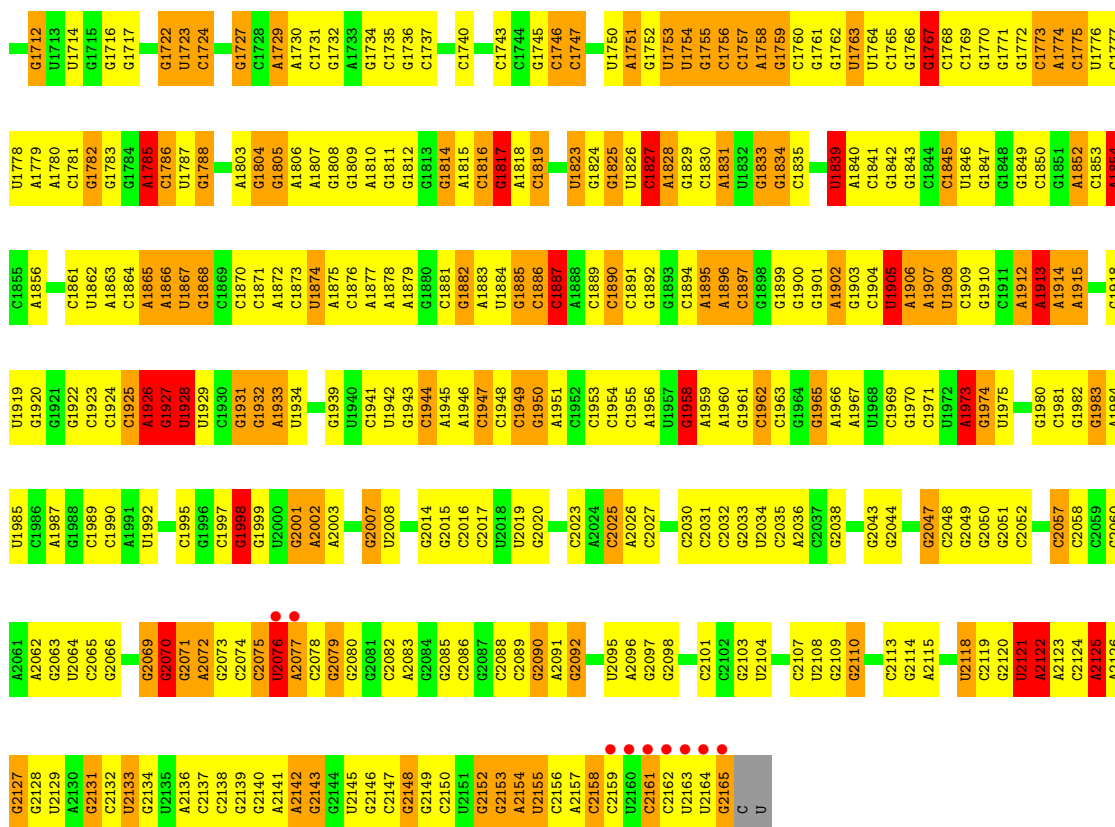




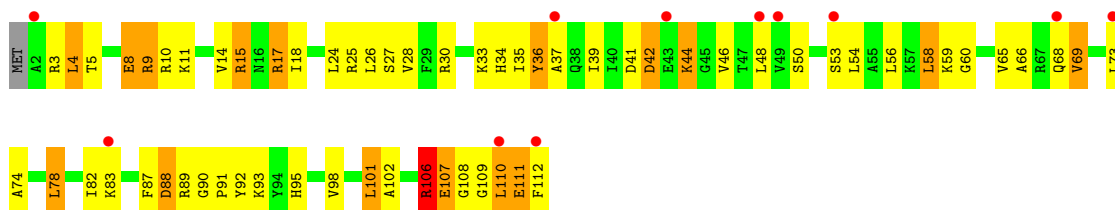
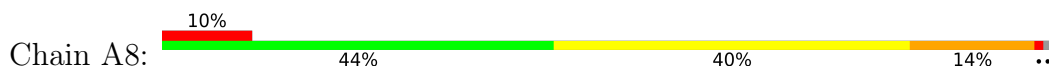
● Molecule 1: 16S ribosomal RNA



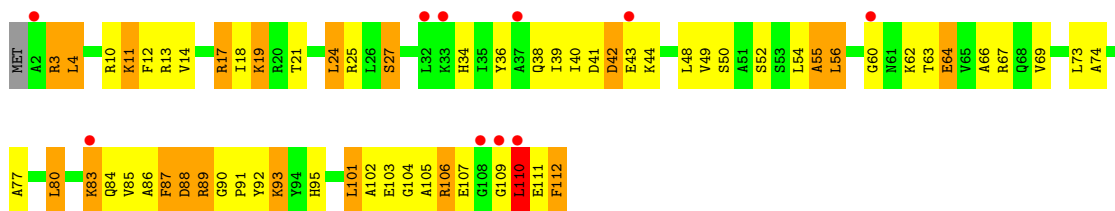
G1633	G1571	G1497	G1429	G1359	U1288	G1216	G1148	A1081	G1014	G943	C876	C805	G724	U	U
G1636	A1572	C1500	U1430	G1360	G1289	G1217	A1149	C1082	A1015	G946	G877	G806	U	U	U
G1637	U1573	C1501	G1432	C1361	G1290	G1217	G1150	G1087	U1016	G947	G877	G807	U	U	G
A1638	U1574	C1502	G1433	A1362	G1291	U1220	G1151	G1088	G1018	G950	C882	C809	A728	A729	U650
A1639	U1575	C1503	G1434	C1363	A1292	G1224	A1152	G1089	G1019	G951	C883	U810	C730	C730	U651
A1640	U1576	C1504	G1435	A1364	G1293	G1225	G1153	G1090	G1021	G952	C884	A811	C731	C731	G652
G1641	U1577	C1505	G1436	A1365	A1294	C1229	G1154	G1091	G1022	C955	U885	A812	U731	U731	G653
G1642	U1578	C1506	C1437	C1367	G1295	C1230	G1155	A1092	G1023	C956	C886	A813	C732	C732	A654
G1643	U1579	C1507	G1438	C1368	U1298	C1231	C1157	A1093	C1024	C957	A887	U814	C733	C733	G655
U1644	G1508	G1369	G1439	C1369	U1299	U1232	C1158	G1094	C1025	C958	G888	C815	G734	G734	A656
U1645	G1509	G1370	G1440	C1370	G1300	U1233	G1159	C1097	C1026	C959	G889	C816	G735	G735	G657
G1646	G1510	U1371	U1441	U1372	U1301	U1234	U1160	C1098	G1027	G958	U890	C817	G736	G736	U658
G1647	G1511	C1373	A1442	C1373	G1302	G1285	A1161	G1099	A1089	G959	A891	A819	G737	G737	U659
G1648	G1513	C1374	A1443	C1374	G1303	G1286	A1162	A1100	C1031	C960	G892	U820	U738	U738	G660
G1649	U1514	C1374	A1444	C1374	A1304	A1236	U1163	C1101	C1032	C961	G893	U821	U739	U739	G661
G1650	A1515	C1375	A1445	C1375	A1305	A1237	U1164	G1102	G1033	C962	U894	U822	A740	A740	G662
G1651	C1516	C1376	G1446	C1376	A1306	A1238	C1165	A1103	G1034	A962	G895	G823	G741	G741	U666
G1652	G1517	C1377	G1447	C1377	U1306	C1242	C1166	G1104	G1035	U964	G896	G824	G742	G742	G667
G1653	G1518	C1378	U1448	C1378	U1307	C1243	G1167	G1105	C1036	G965	U897	A825	A748	A748	G668
G1654	G1519	G1379	U1449	C1379	C1309	A1244	G1168	G1106	C1037	G966	G898	U826	C749	C749	G669
G1655	A1591	U1380	U1450	C1380	G1312	C1245	A1169	G1107	A1038	C967	G899	C830	G750	G750	G677
G1656	A1592	G1381	C1451	G1381	A1313	G1246	G1170	A1108	C1039	A968	U902	C832	U753	U753	A678
G1657	C1522	C1382	G1452	A1382	A1314	G1247	G1171	G1109	G1040	A970	A903	C833	G754	G754	A679
G1658	G1523	C1383	C1453	G1383	G1314	C1248	G1172	G1110	C1041	C971	A904	U834	A755	A755	C682
G1659	A1524	G1384	U1454	C1384	U1315	U1249	U1181	U1116	C1042	C972	U905	U835	A756	A756	C683
G1660	G1525	C1385	G1455	C1385	A1316	C1249	A1182	U1117	C1043	C973	G906	U836	A757	A757	G684
G1661	U1526	U1386	U1456	C1386	G1317	A1250	G1175	G1118	G1044	G974	G907	U837	A758	A758	G685
G1662	C1527	G1387	A1457	C1387	C1318	A1251	U1176	C1112	C1045	G975	G908	U838	C760	C760	G686
G1663	U1528	C1388	G1458	A1388	G1319	C1252	G1177	G1113	U1046	C976	C908	U839	G761	G761	G687
G1664	U1529	C1389	G1459	G1389	G1320	C1253	U1188	G1114	U1047	C977	C909	U840	G762	G762	G688
G1665	A1531	C1391	C1460	C1391	U1321	G1254	U1189	U1115	G1048	C978	C910	U841	G763	G763	G689
G1666	G1532	G1394	U1461	C1394	U1322	U1255	A1182	U1116	C1049	C979	C911	U842	G764	G764	G690
G1667	U1533	A1395	U1462	C1395	U1323	G1256	U1190	U1117	A1049	C980	C912	U843	G765	G765	G691
G1668	C1534	G1396	G1463	C1396	G1329	G1257	G1186	C1119	G1050	C981	C913	U844	G766	G766	G692
G1669	U1535	A1397	U1464	C1397	U1330	G1258	A1188	G1120	C1051	A985	C914	U845	A770	A770	U691
G1670	C1536	G1398	G1465	G1398	G1331	G1259	U1189	G1121	A1052	C986	C915	U846	C771	C771	G692
G1671	U1537	C1399	G1466	C1399	A1332	G1260	U1190	G1122	G1053	C987	C916	U847	C772	C772	G693
G1672	A1538	G1400	G1467	G1400	U1333	A1261	U1191	G1123	G1054	C988	C917	U848	A773	A773	C694
G1673	U1539	U1401	U1468	C1401	A1334	G1262	C1193	A1126	G1057	G989	C918	U849	A774	A774	C695
G1674	G1543	G1404	G1469	C1404	U1335	C1263	U1194	U1127	C1058	A990	C919	U850	C775	C775	U695
G1675	U1544	A1405	U1470	C1405	G1336	G1264	U1195	A1128	C1059	A991	C920	U851	A781	A781	A696
G1676	G1545	G1406	G1471	C1406	C1337	U1265	G1196	G1129	C1060	G992	C921	U852	A782	A782	A697
G1677	A1546	C1407	G1472	C1407	A1341	G1266	G1197	C1130	G1063	C993	G925	U854	G783	G783	G698
G1678	U1547	A1408	G1473	C1408	G1342	G1267	C1198	G1131	C1064	A994	G926	U855	G784	G784	C700
G1679	G1548	A1410	G1474	C1410	G1343	G1268	G1199	C1132	G1065	G995	G927	U856	G785	G785	U702
G1680	U1549	A1411	G1475	C1411	U1344	G1269	U1200	G1133	G1066	C996	G928	U857	G786	G786	G703
G1681	G1550	G1414	G1476	C1414	A1345	A1271	A1201	G1135	U1068	U999	G930	U858	G787	G787	G704
G1682	U1551	G1415	G1477	C1415	G1346	U1275	A1202	G1136	C1069	U1000	C931	U859	G788	G788	A705
G1683	G1552	A1416	U1482	C1416	C1349	C1276	A1203	C1137	G1070	A1001	C932	U860	A791	A791	A706
G1684	C1553	U1417	G1483	C1417	G1350	G1277	G1204	A1138	U1071	G1002	C933	U861	A792	A792	G712
G1685	U1554	A1418	G1484	C1418	G1351	A1278	G1205	A1139	G1003	G1003	C934	U862	A793	A793	G713
G1686	G1555	G1420	U1485	C1420	U1352	G1279	G1206	C1140	U1004	A1004	C935	U863	C794	C794	G714
G1687	U1556	A1488	G1486	C1421	G1353	U1280	U1209	U1141	A1005	A1005	C936	U864	C795	C795	G715
G1688	C1557	U1422	U1487	C1422	G1354	U1281	G1210	C1142	U1006	U937	C937	U865	C796	C796	G716
G1689	G1563	A1423	G1488	C1423	C1355	U1282	U1211	C1143	C1007	C938	C938	U866	A800	A800	G717
G1690	U1568	G1427	U1489	C1427	G1356	G1283	U1212	G1144	U1008	U939	C939	U867	A801	A801	C720
G1691	C1570	G1428	G1490	C1428	U1357	G1287	G1213	U1145	G1012	G940	C940	U868	A802	A802	G721
G1692	G1570	A1496	U1496	C1496	A1358	G1287	G1214	C1147	G1013	G941	C941	U869	U804	U804	G722



• Molecule 2: 50S ribosomal protein L18

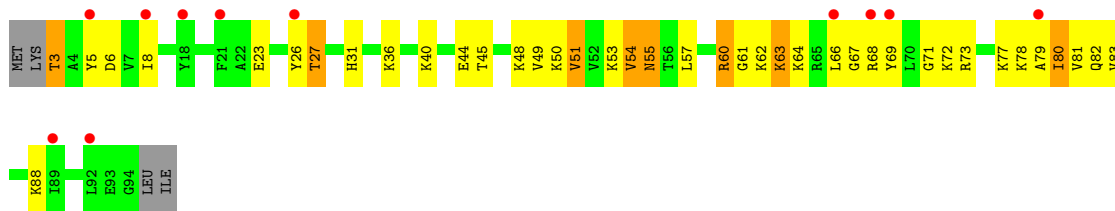


• Molecule 2: 50S ribosomal protein L18

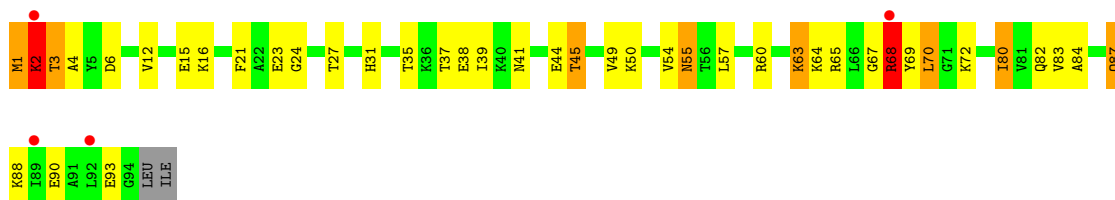


• Molecule 3: 50S ribosomal protein L23

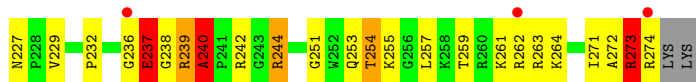
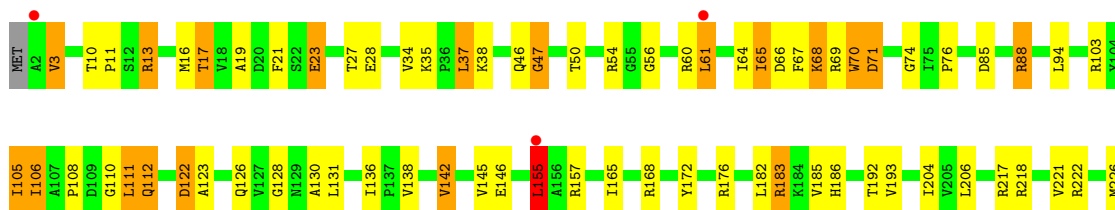




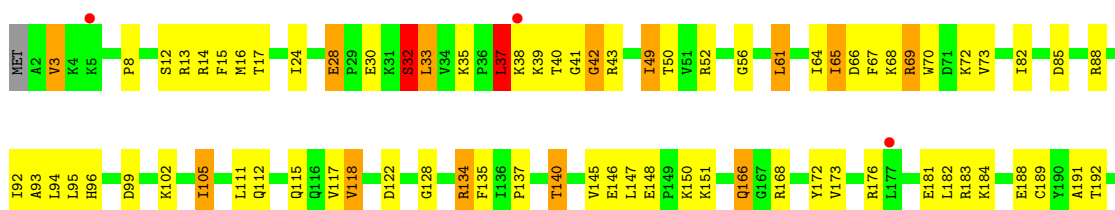
• Molecule 3: 50S ribosomal protein L23



• Molecule 4: 50S ribosomal protein L2

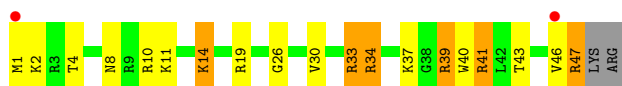


• Molecule 4: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L34

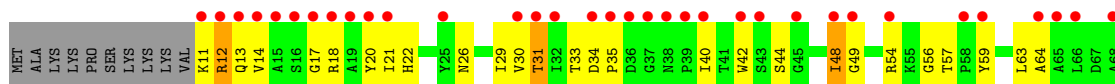




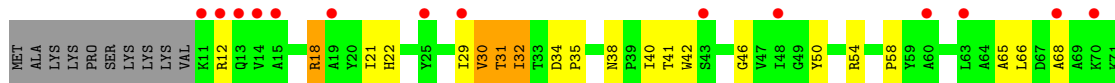
- Molecule 5: 50S ribosomal protein L34



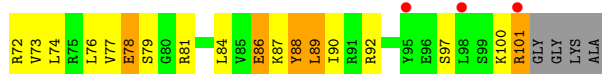
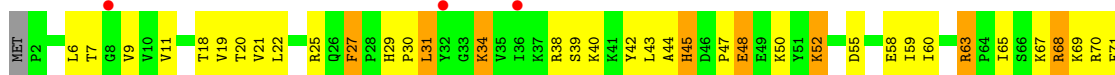
- Molecule 6: 30S ribosomal protein S11



- Molecule 6: 30S ribosomal protein S11

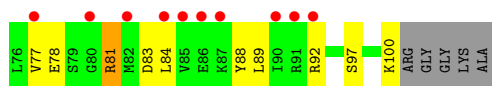


- Molecule 7: 30S ribosomal protein S17

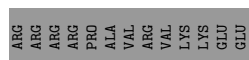
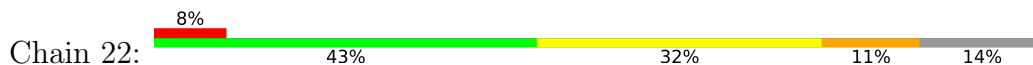


- Molecule 7: 30S ribosomal protein S17

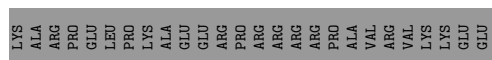
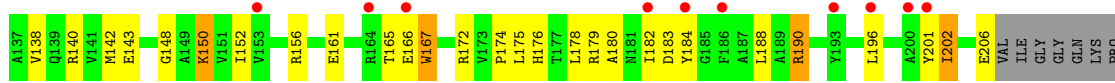
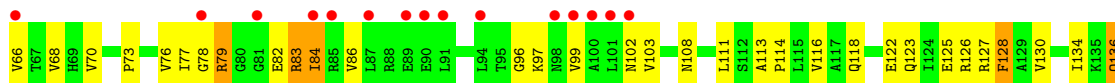
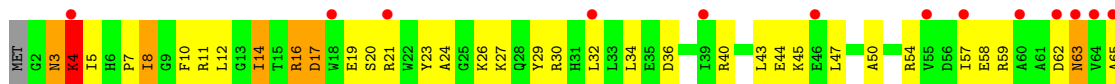




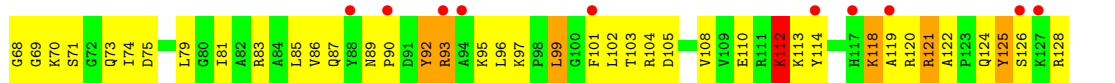
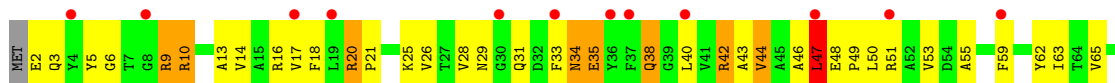
• Molecule 8: 30S ribosomal protein S3



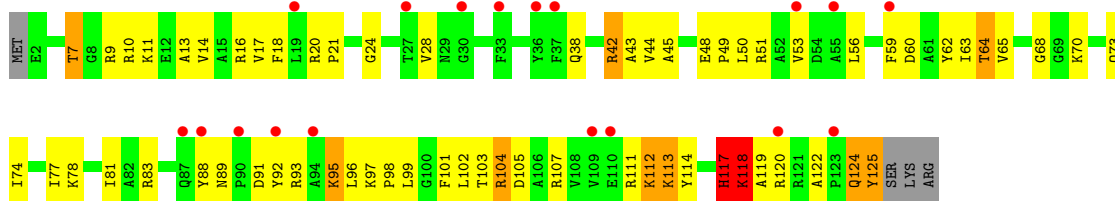
• Molecule 8: 30S ribosomal protein S3



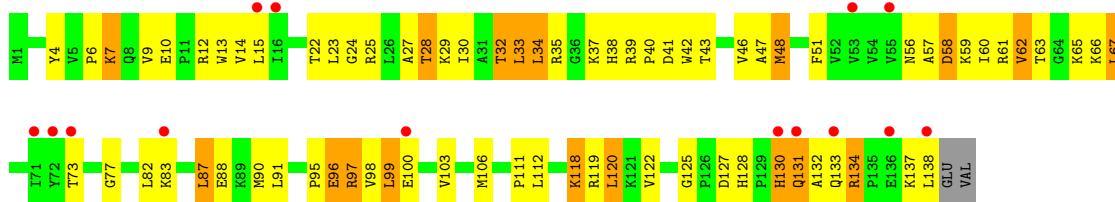
• Molecule 9: 30S ribosomal protein S9



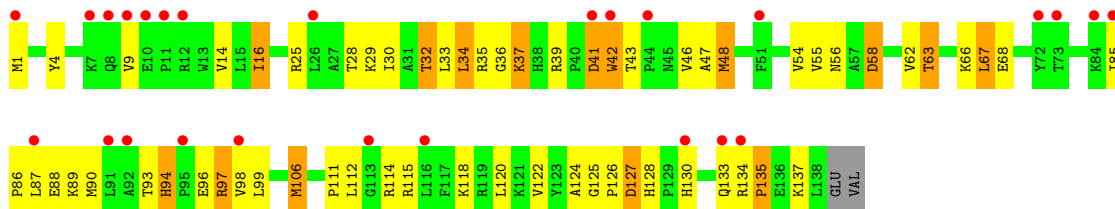
• Molecule 9: 30S ribosomal protein S9



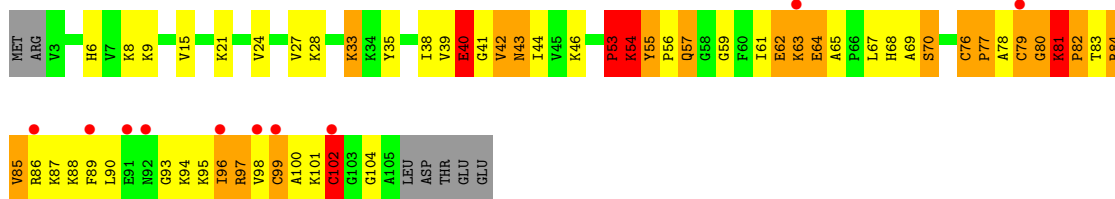
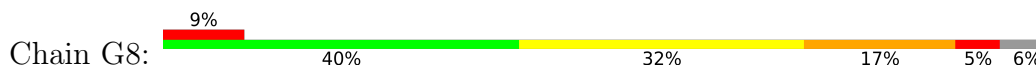
- Molecule 10: 50S ribosomal protein L13



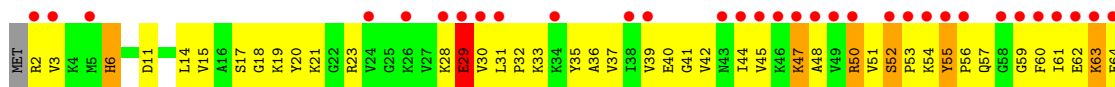
- Molecule 10: 50S ribosomal protein L13

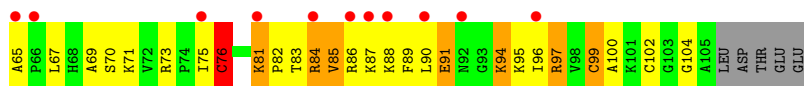


- Molecule 11: 50S ribosomal protein L24

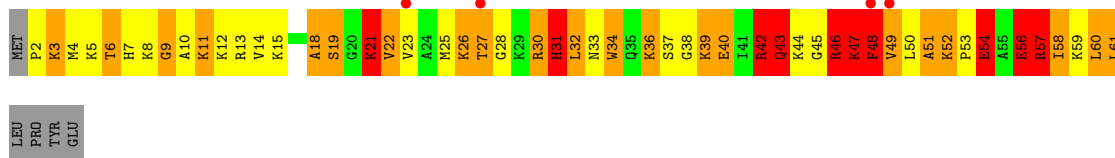


- Molecule 11: 50S ribosomal protein L24

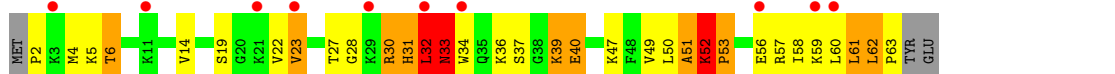




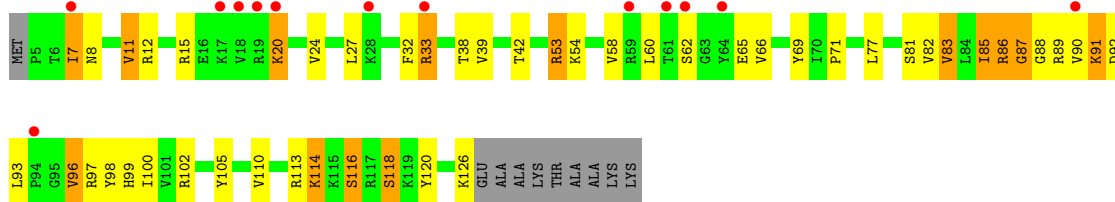
• Molecule 12: 50S ribosomal protein L35



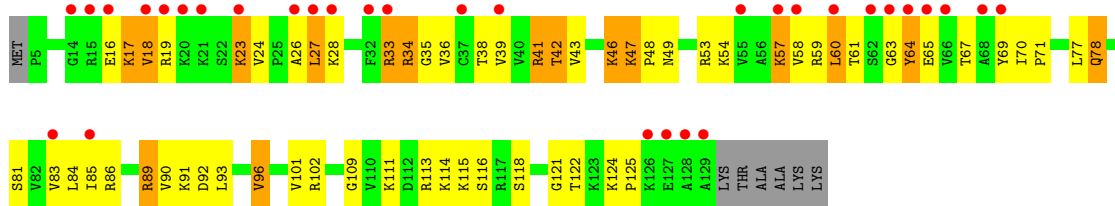
• Molecule 12: 50S ribosomal protein L35



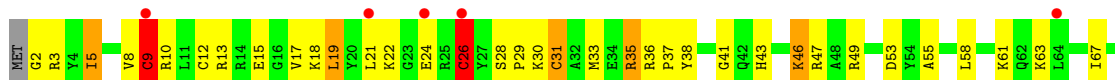
• Molecule 13: 30S ribosomal protein S12



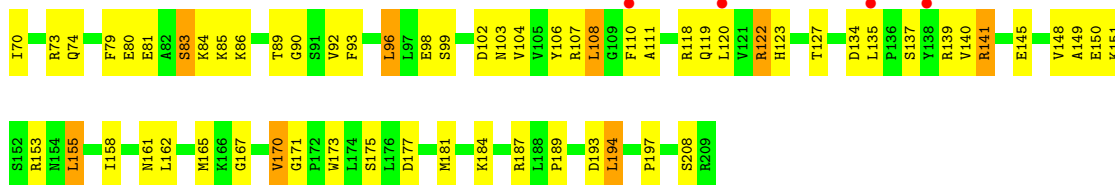
• Molecule 13: 30S ribosomal protein S12



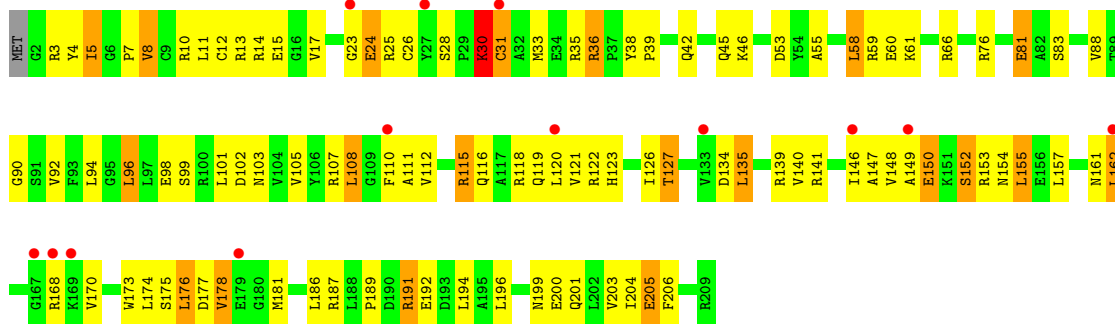
• Molecule 14: 30S ribosomal protein S4



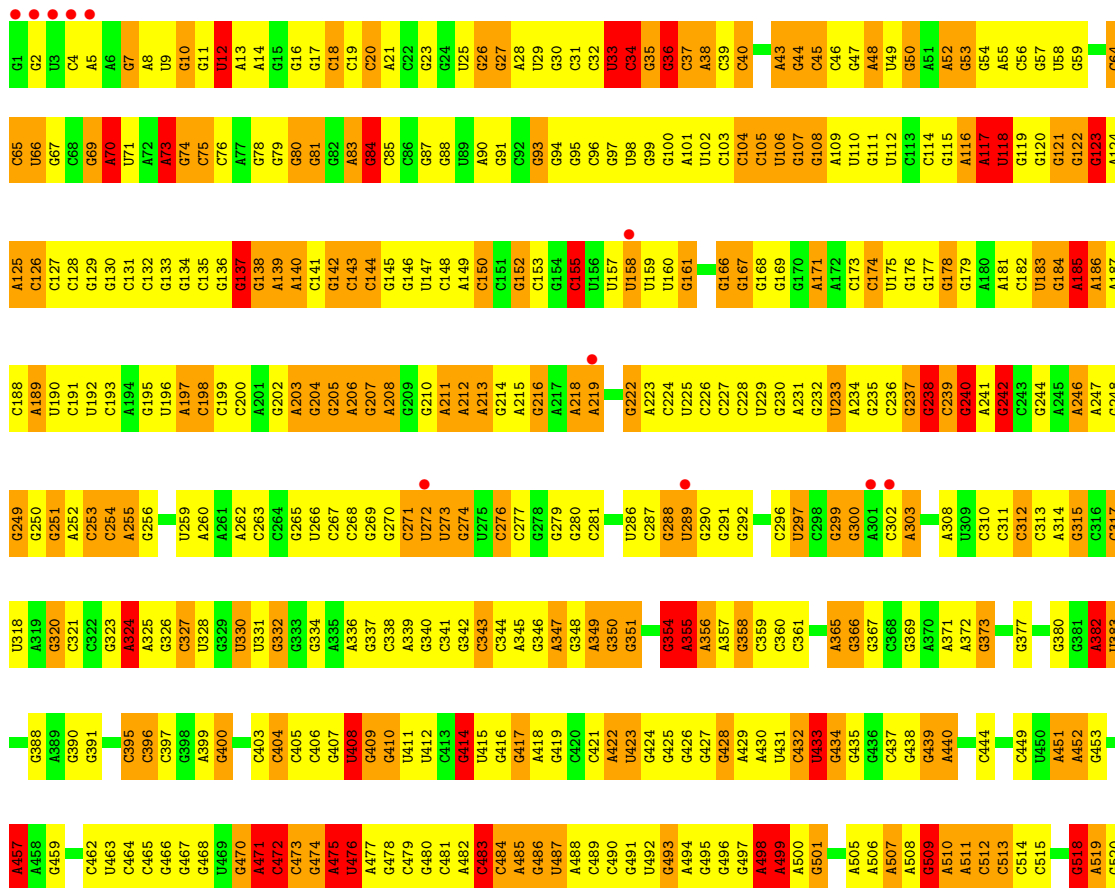
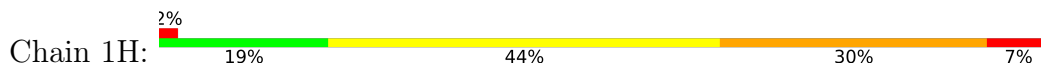




• Molecule 14: 30S ribosomal protein S4

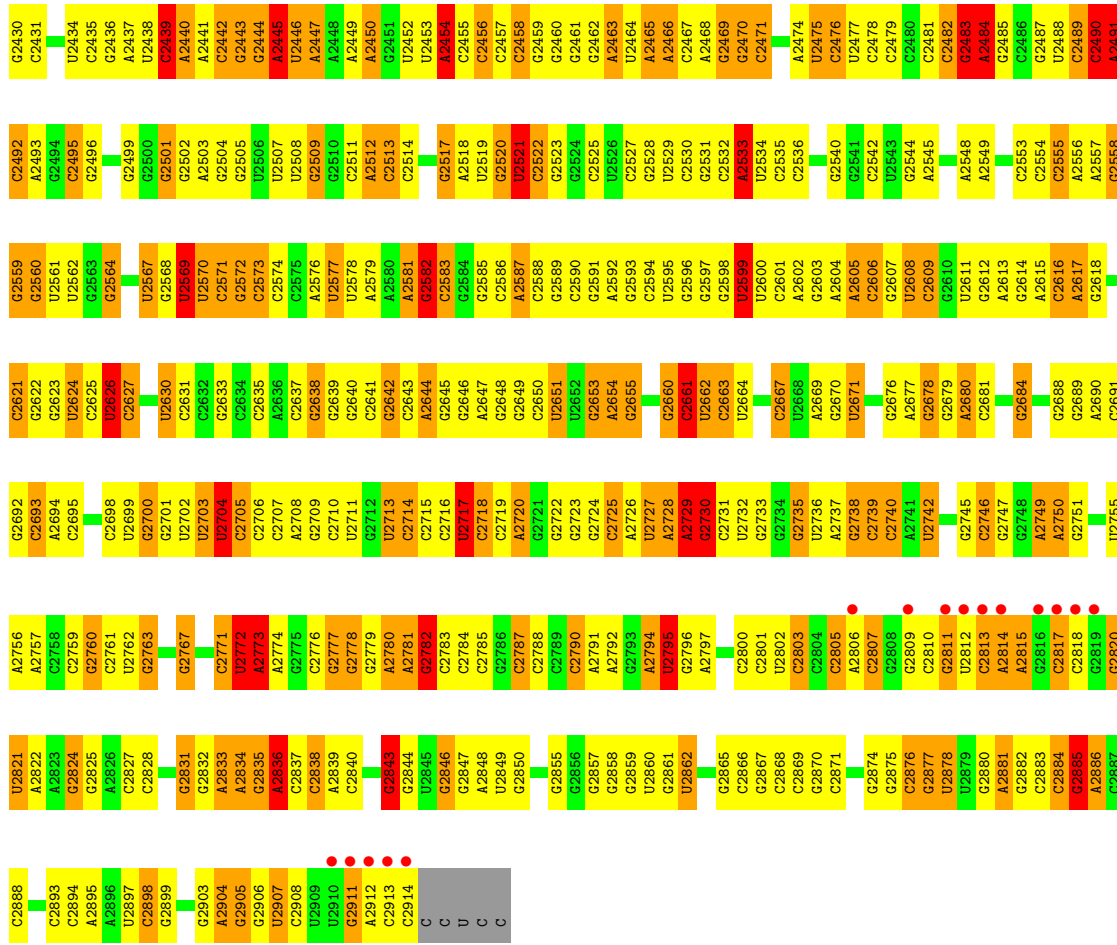


• Molecule 15: 23S ribosomal RNA

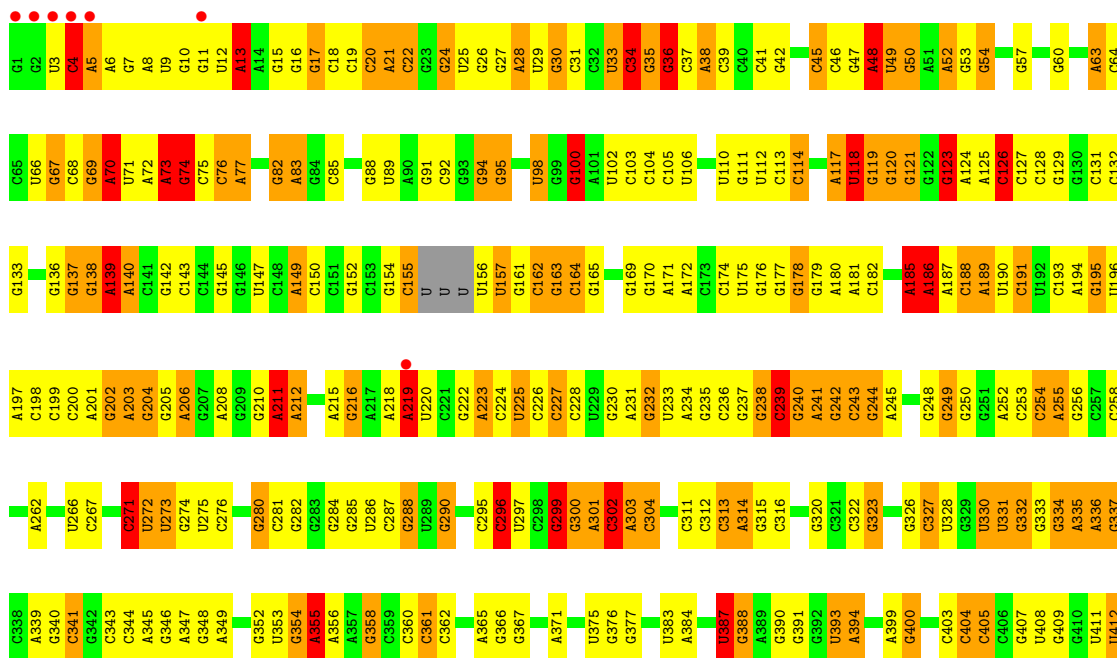
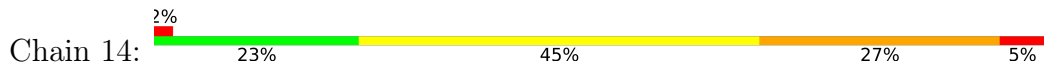




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U2250	G2250
C2251	G2251
C2252	G2252
G2253	G2253
G2254	G2254
C2255	G2255
A2256	G2256
G2257	G2257
U2258	G2258
U2259	G2259
U2260	G2260
U2261	G2261
A2262	G2262
C2263	G2263
U2264	G2264
G2265	G2

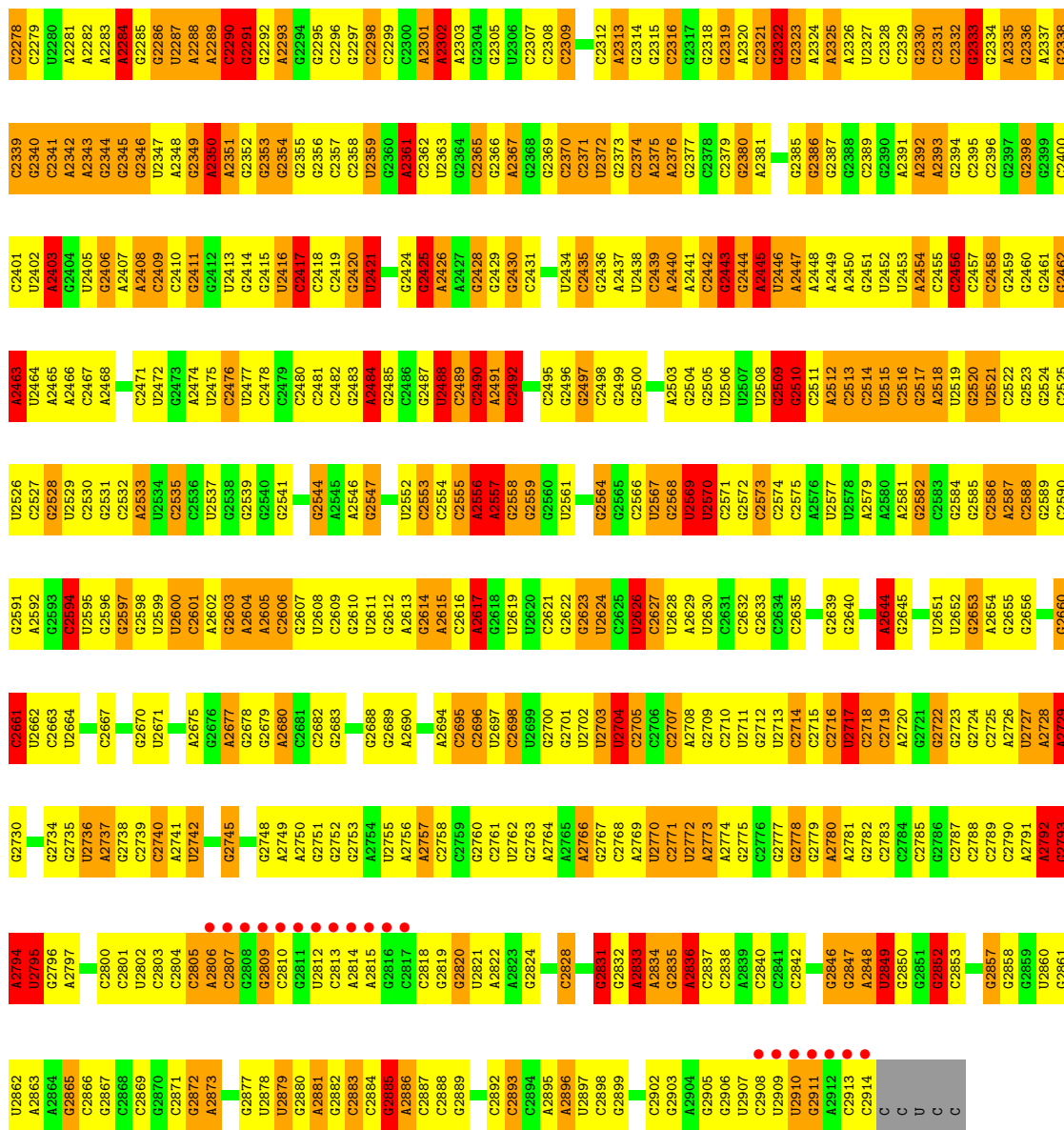


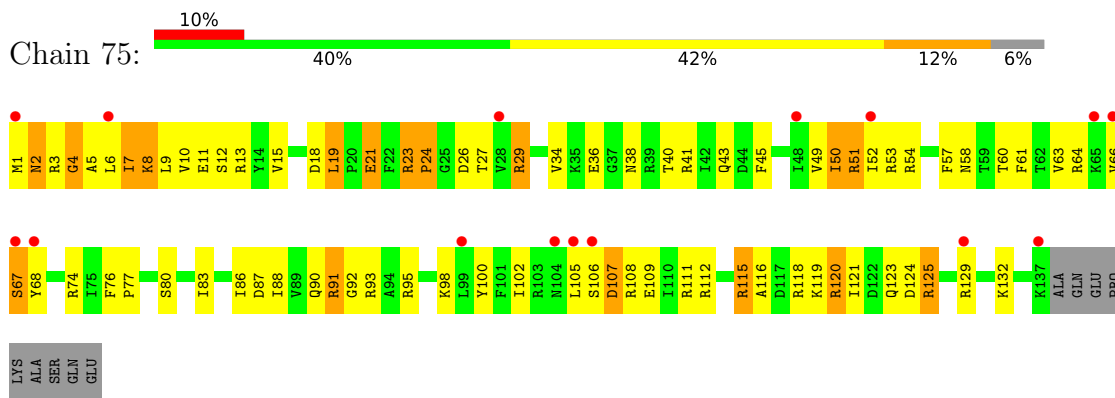
● Molecule 15: 23S ribosomal RNA



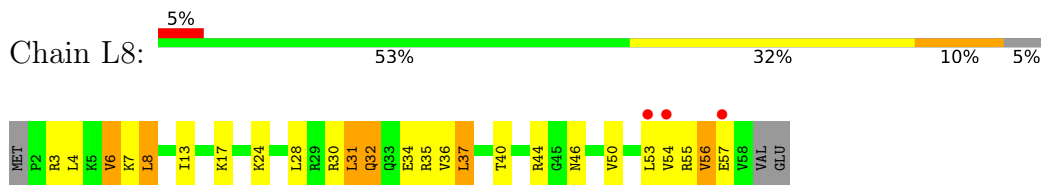




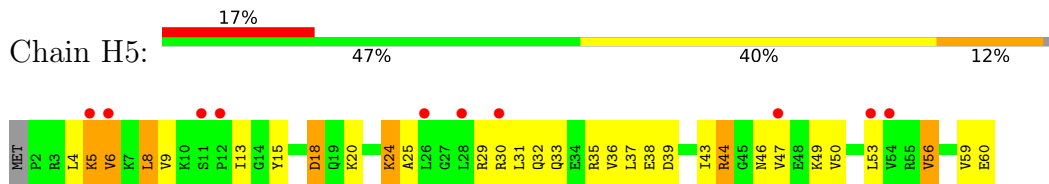




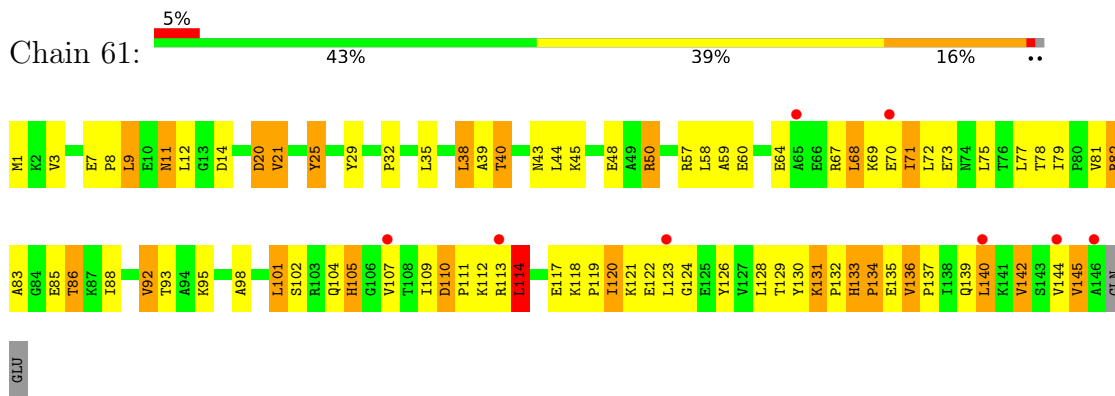
• Molecule 17: 50S ribosomal protein L30



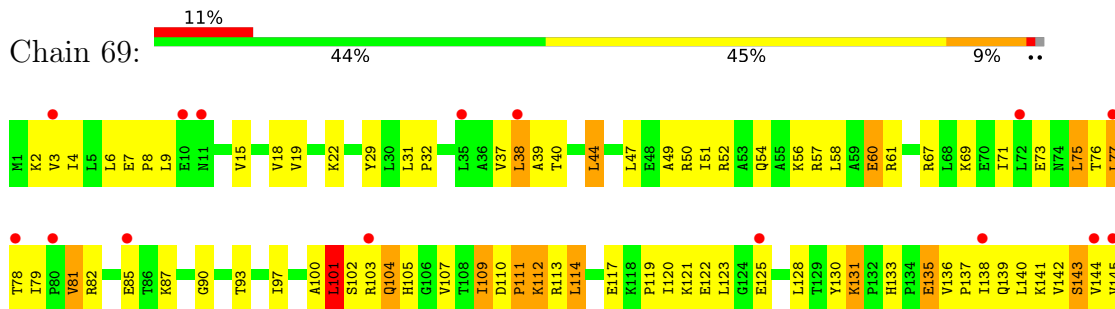
• Molecule 17: 50S ribosomal protein L30



• Molecule 18: 50S ribosomal protein L9



• Molecule 18: 50S ribosomal protein L9

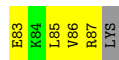
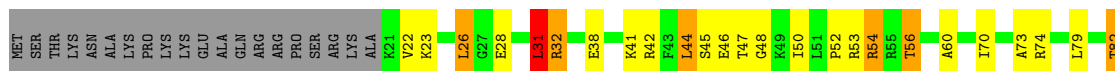






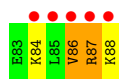
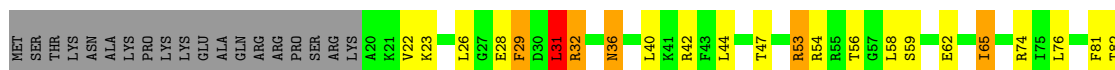
- Molecule 19: 30S ribosomal protein S18

Chain 9I: 43% 25% 7% 24%



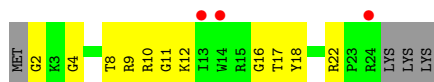
- Molecule 19: 30S ribosomal protein S18

Chain 9A: 6% 48% 22% 8% 22%



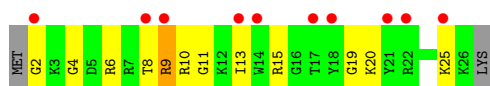
- Molecule 20: 30S ribosomal protein Thx

Chain 1F: 11% 44% 41% 15%



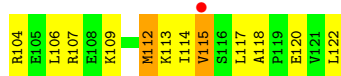
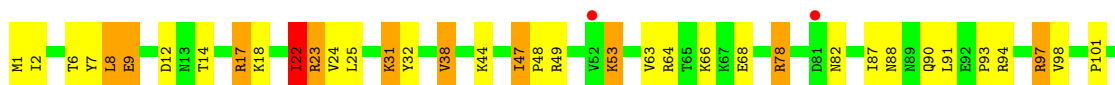
- Molecule 20: 30S ribosomal protein Thx

Chain 1B: 37% 48% 41% 7%

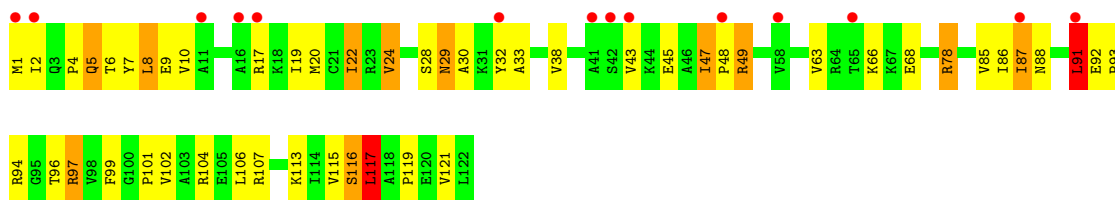


- Molecule 21: 50S ribosomal protein L14

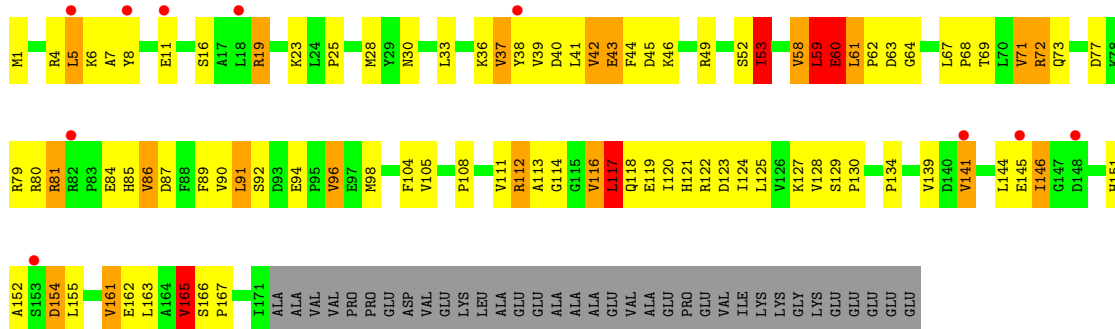
Chain 68: 2% 60% 30% 10%



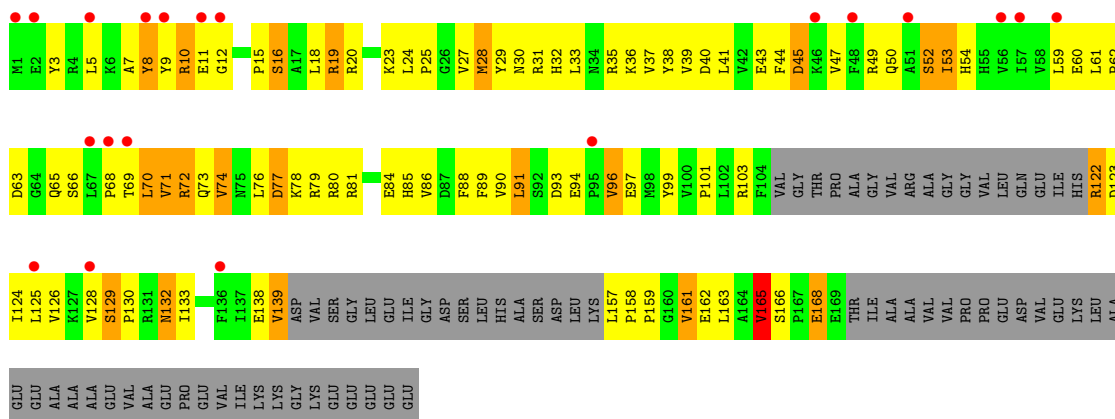
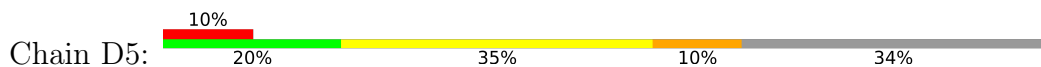
- Molecule 21: 50S ribosomal protein L14



• Molecule 22: 50S ribosomal protein L25

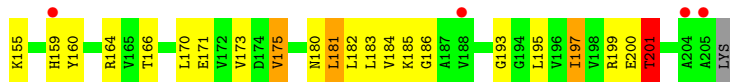


• Molecule 22: 50S ribosomal protein L25





• Molecule 23: 50S ribosomal protein L3



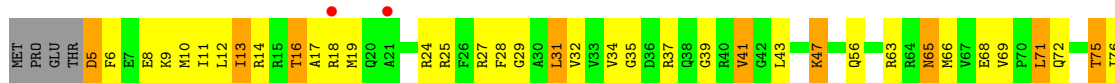
• Molecule 24: 30S ribosomal protein S13



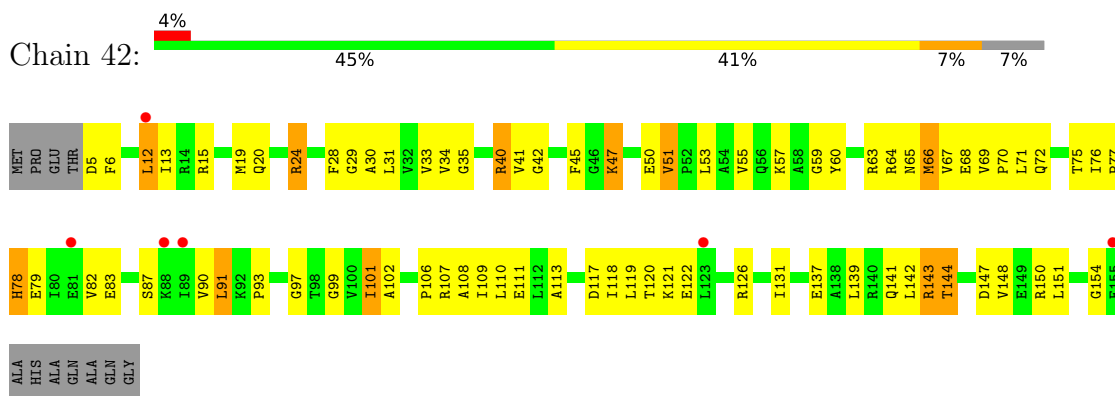
• Molecule 24: 30S ribosomal protein S13



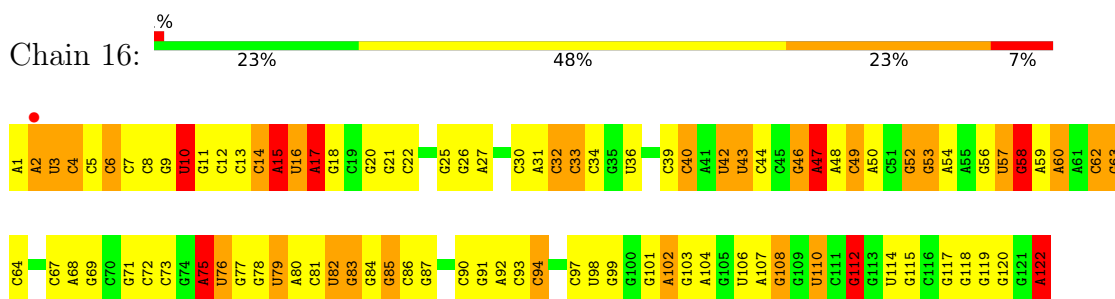
• Molecule 25: 30S ribosomal protein S5



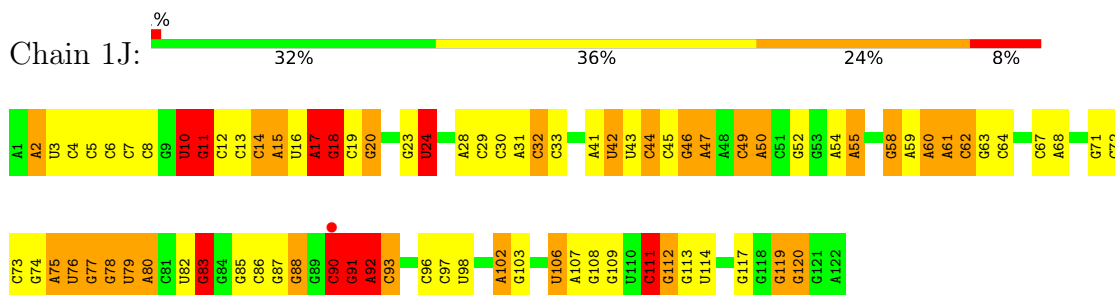
- Molecule 25: 30S ribosomal protein S5



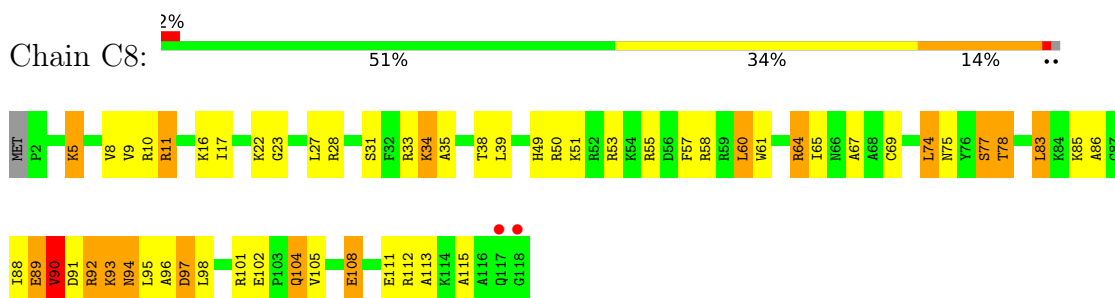
- Molecule 26: 5S ribosomal RNA



- Molecule 26: 5S ribosomal RNA

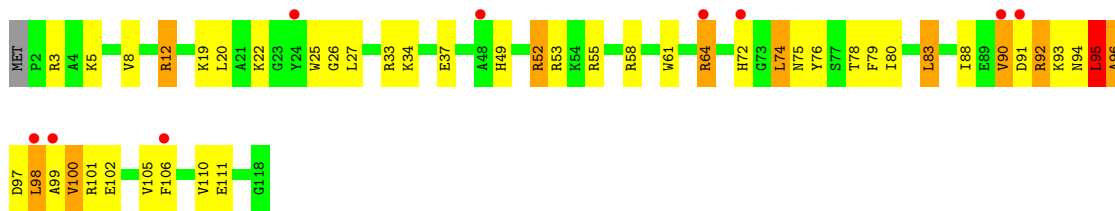


- Molecule 27: 50S ribosomal protein L20

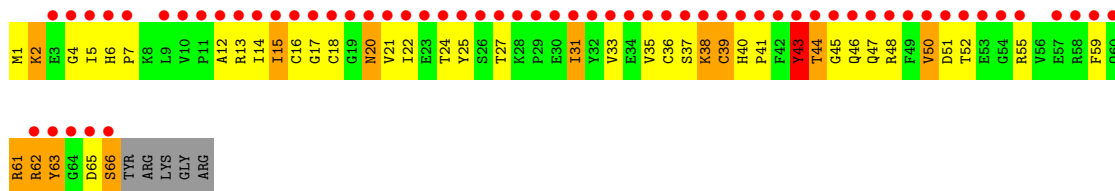
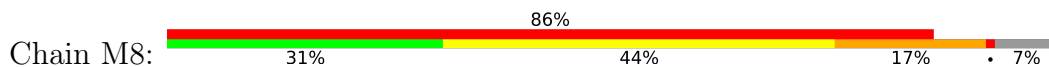


- Molecule 27: 50S ribosomal protein L20

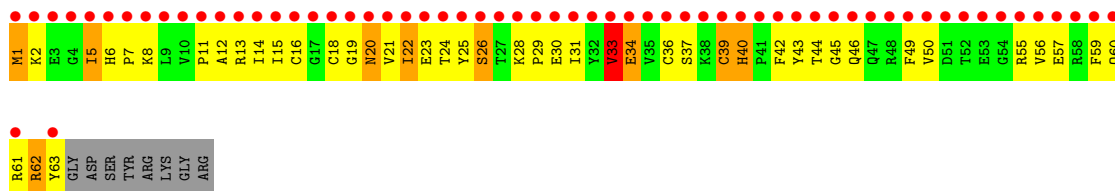
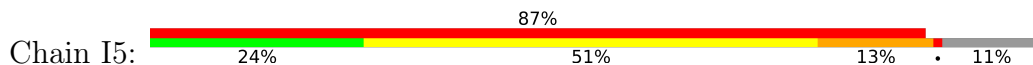




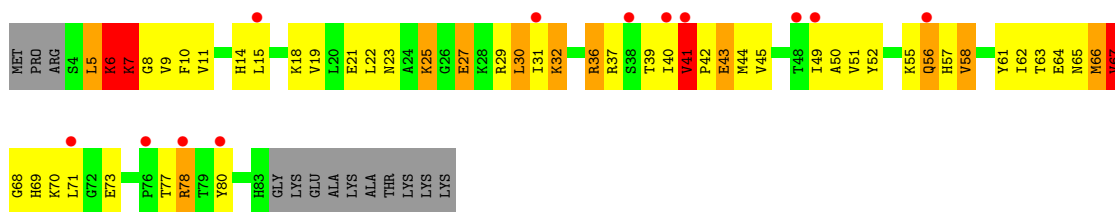
• Molecule 28: 50S ribosomal protein L31



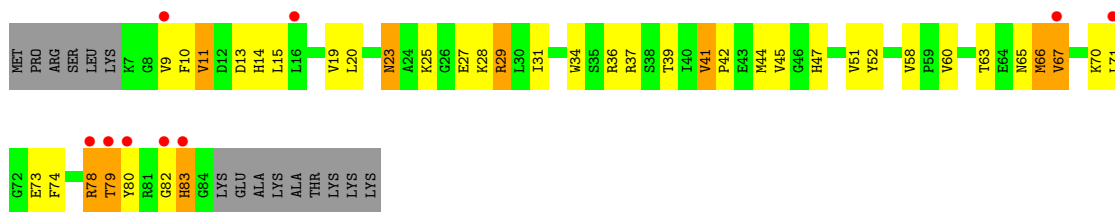
• Molecule 28: 50S ribosomal protein L31



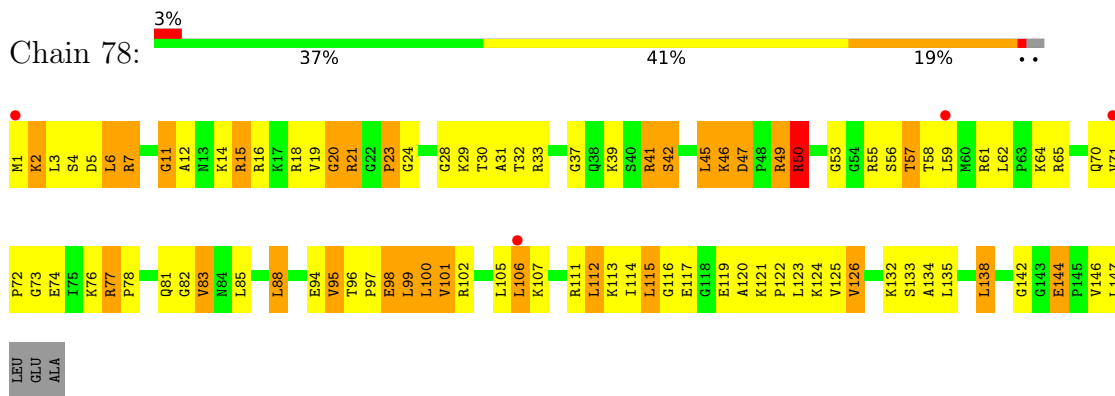
• Molecule 29: 30S ribosomal protein S19



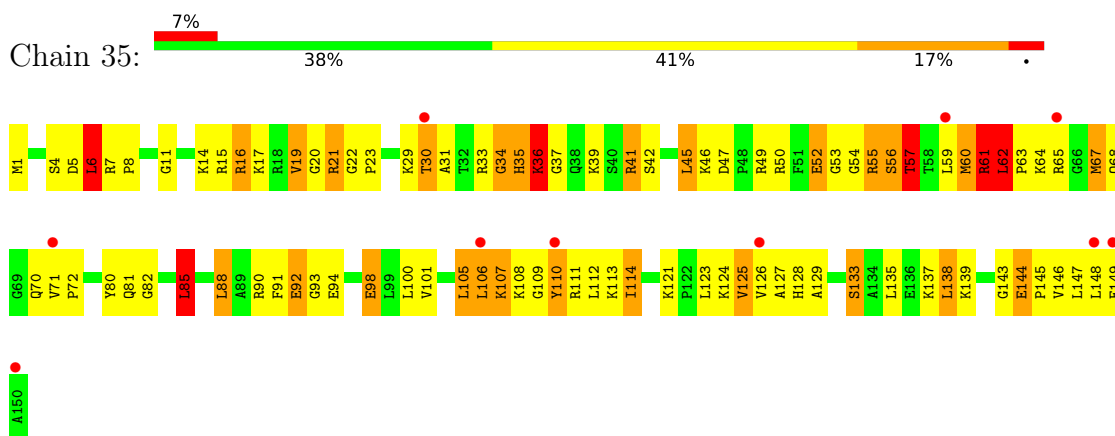
• Molecule 29: 30S ribosomal protein S19



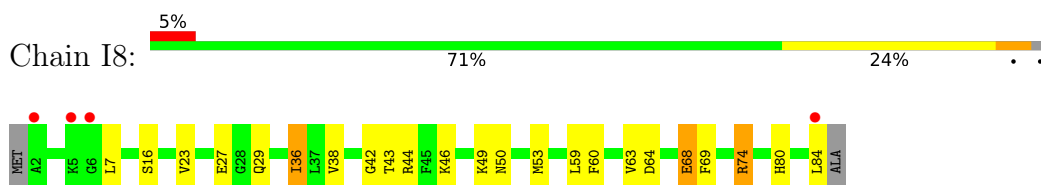
- Molecule 30: 50S ribosomal protein L15



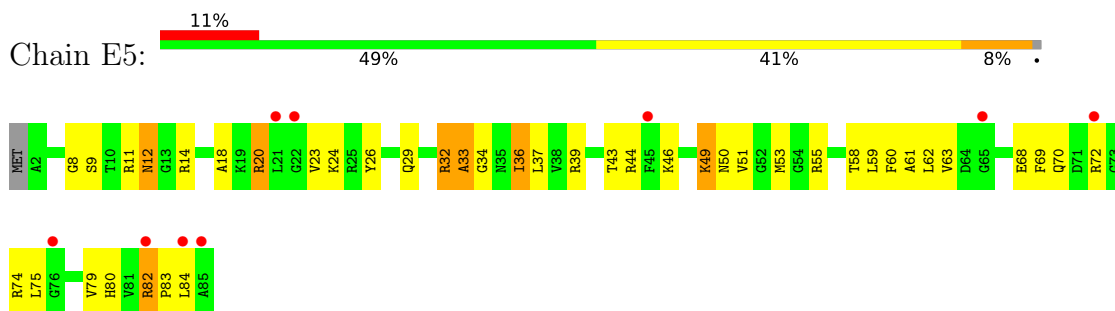
- Molecule 30: 50S ribosomal protein L15



- Molecule 31: 50S ribosomal protein L27

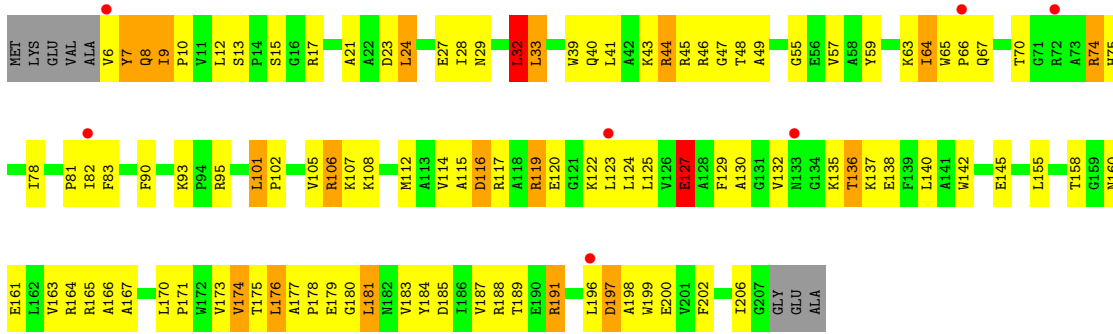


- Molecule 31: 50S ribosomal protein L27

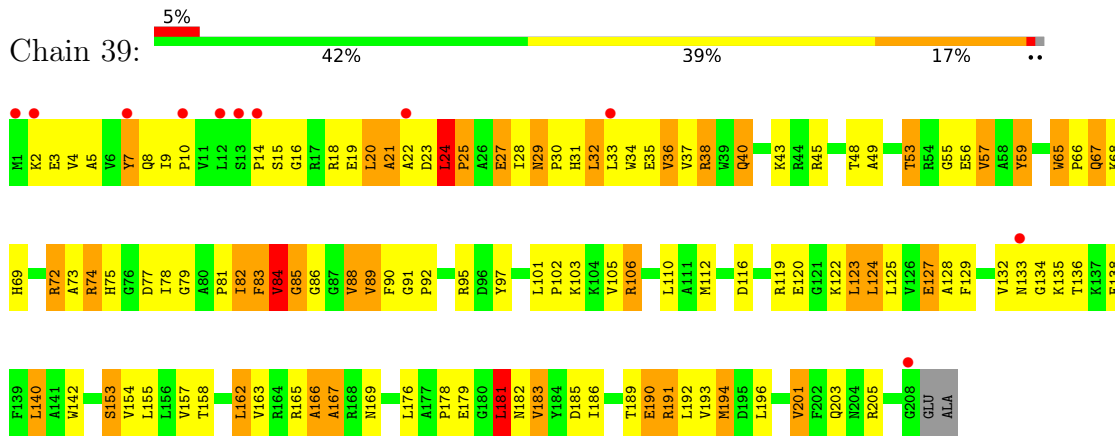


- Molecule 32: 50S ribosomal protein L4

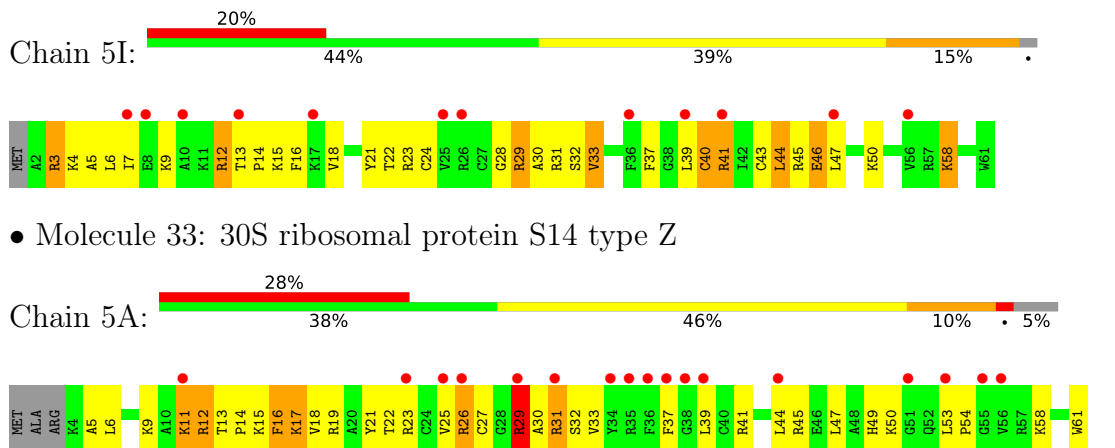




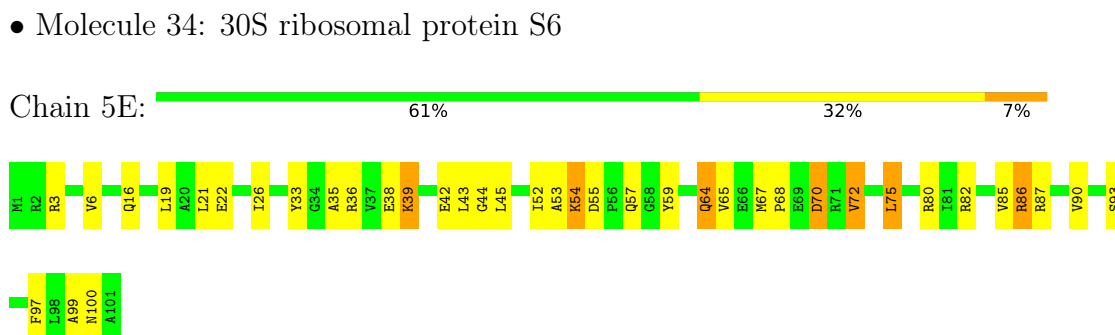
- Molecule 32: 50S ribosomal protein L4



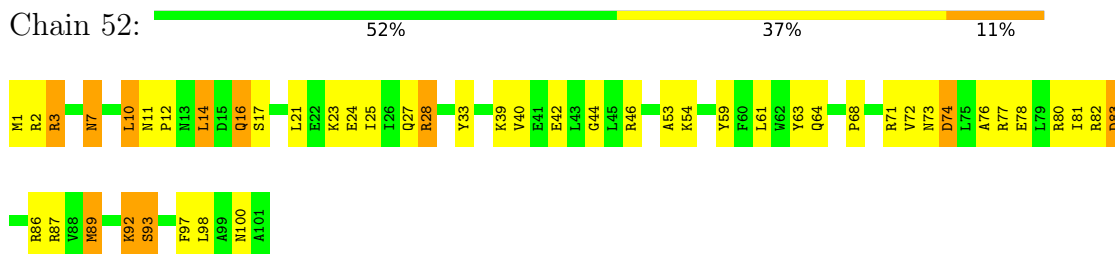
- Molecule 33: 30S ribosomal protein S14 type Z



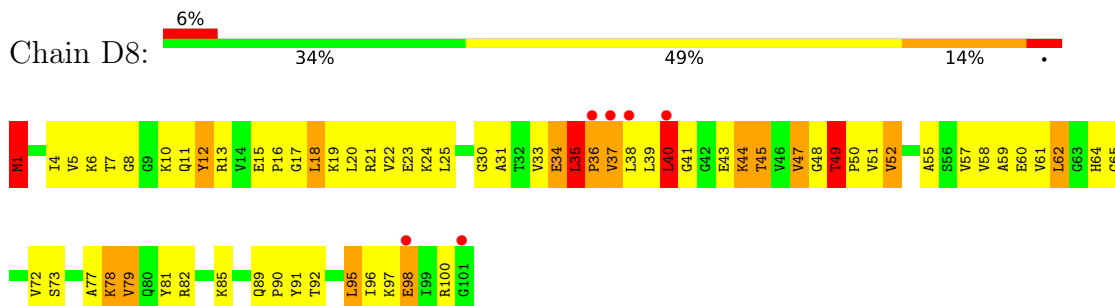
- Molecule 33: 30S ribosomal protein S14 type Z



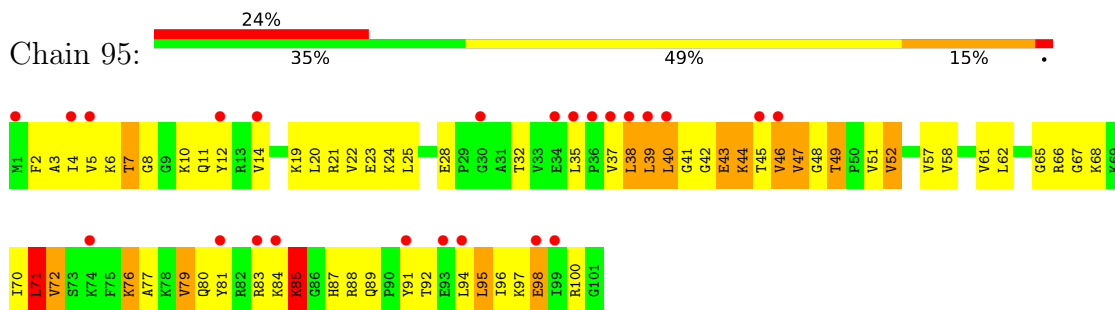
- Molecule 34: 30S ribosomal protein S6



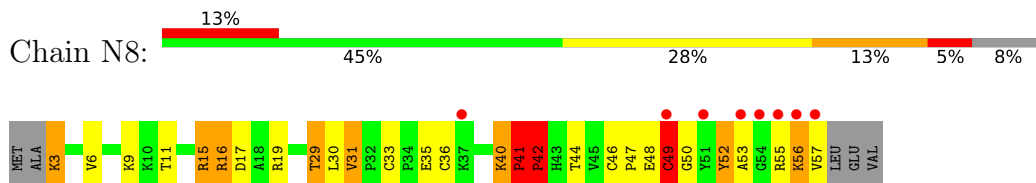
- Molecule 35: 50S ribosomal protein L21



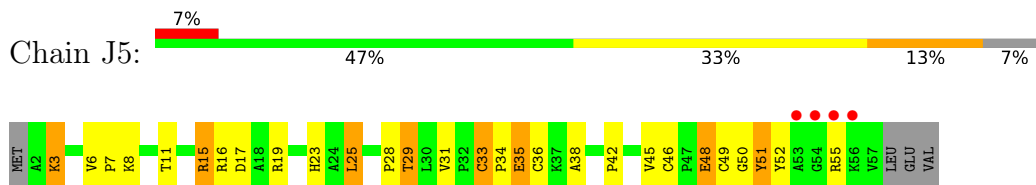
- Molecule 35: 50S ribosomal protein L21



- Molecule 36: 50S ribosomal protein L32



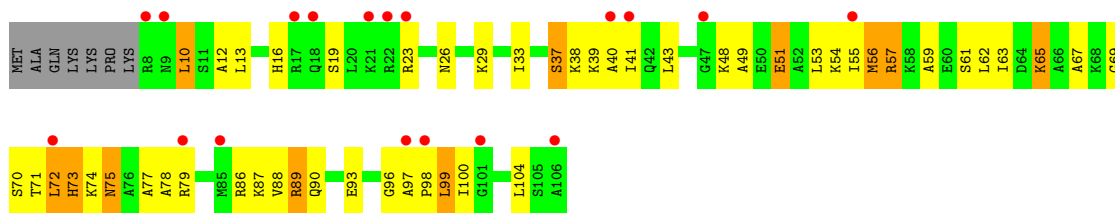
- Molecule 36: 50S ribosomal protein L32



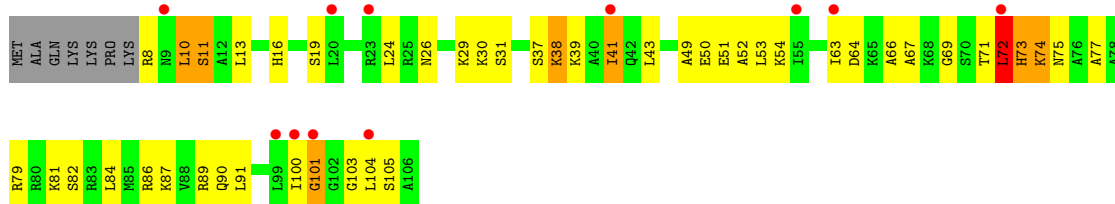
- Molecule 37: 30S ribosomal protein S20



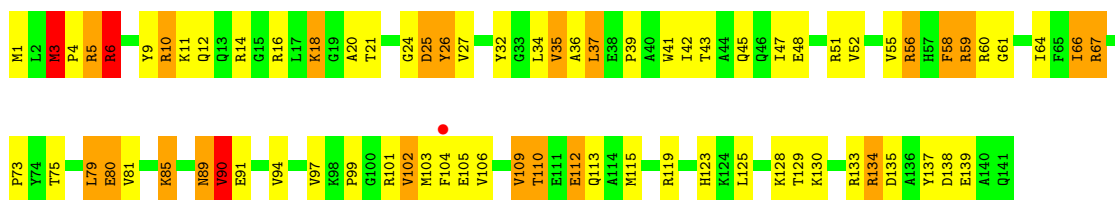




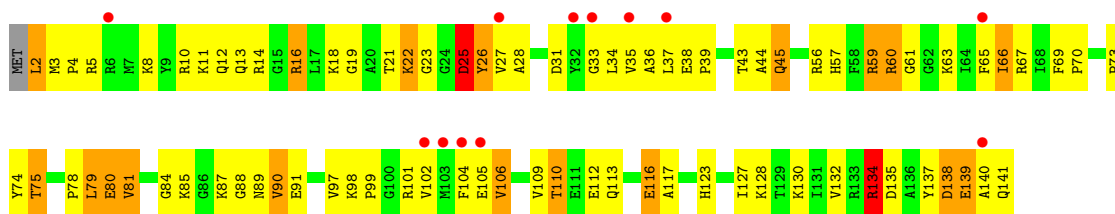
• Molecule 37: 30S ribosomal protein S20



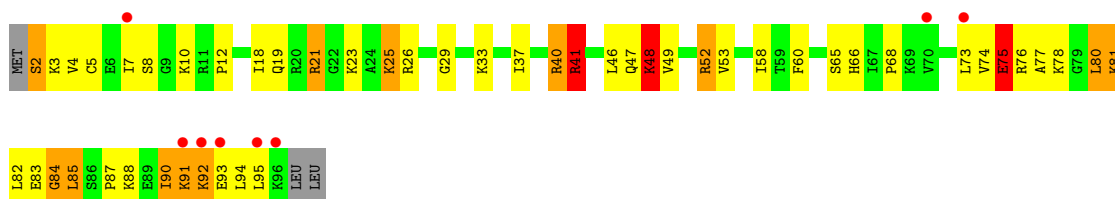
• Molecule 38: 50S ribosomal protein L16



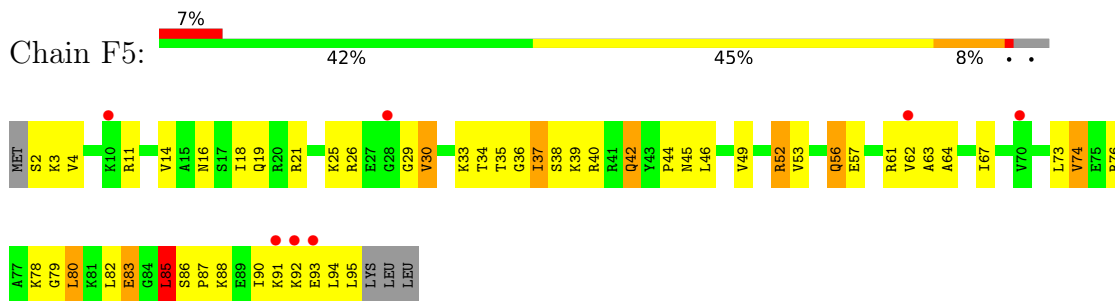
• Molecule 38: 50S ribosomal protein L16



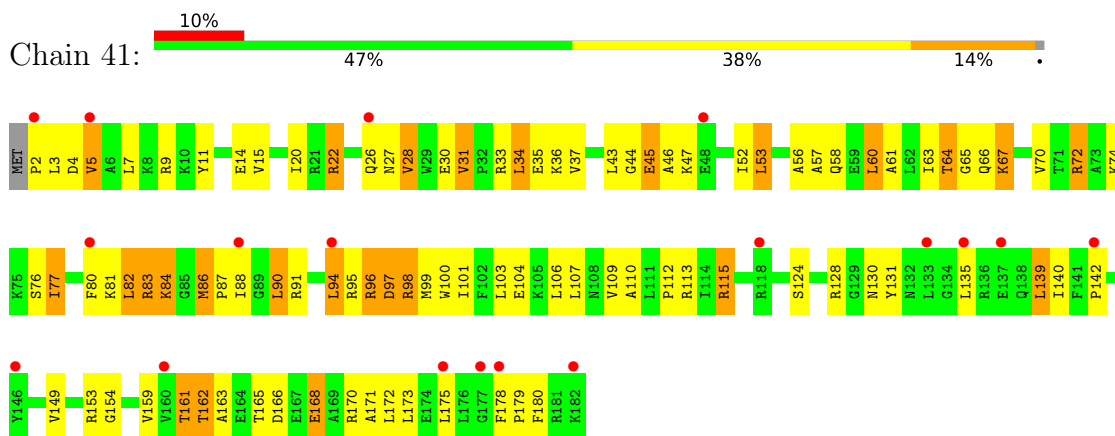
• Molecule 39: 50S ribosomal protein L28



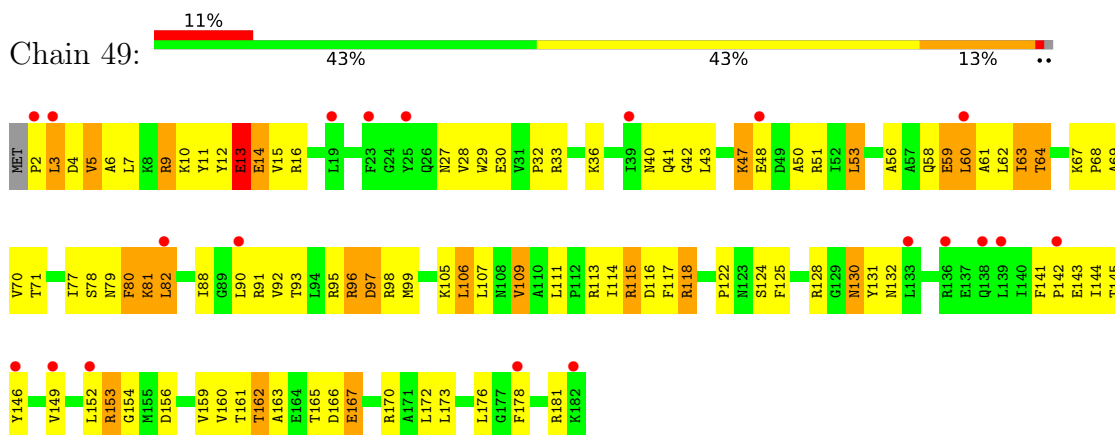
- Molecule 39: 50S ribosomal protein L28



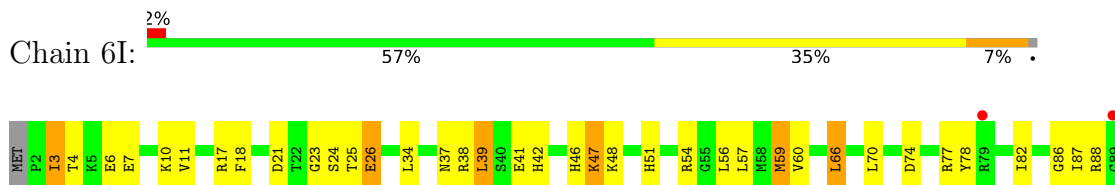
- Molecule 40: 50S ribosomal protein L5



- Molecule 40: 50S ribosomal protein L5

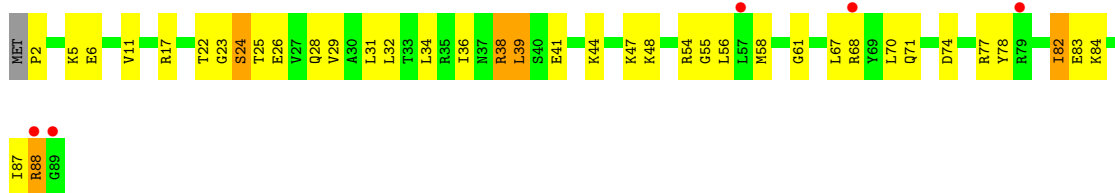


- Molecule 41: 30S ribosomal protein S15

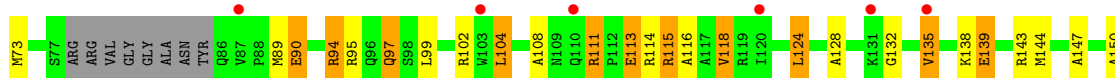
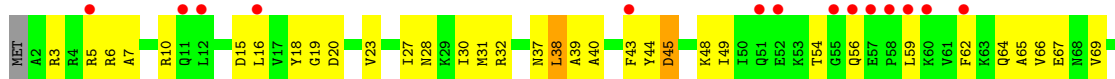


- Molecule 41: 30S ribosomal protein S15





- Molecule 42: 30S ribosomal protein S7



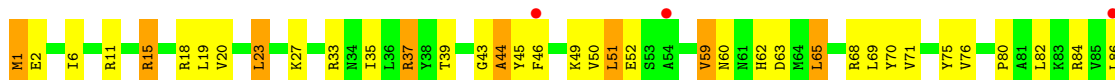
- Molecule 42: 30S ribosomal protein S7

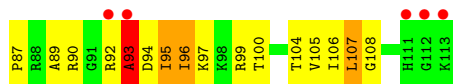


- Molecule 43: 50S ribosomal protein L22

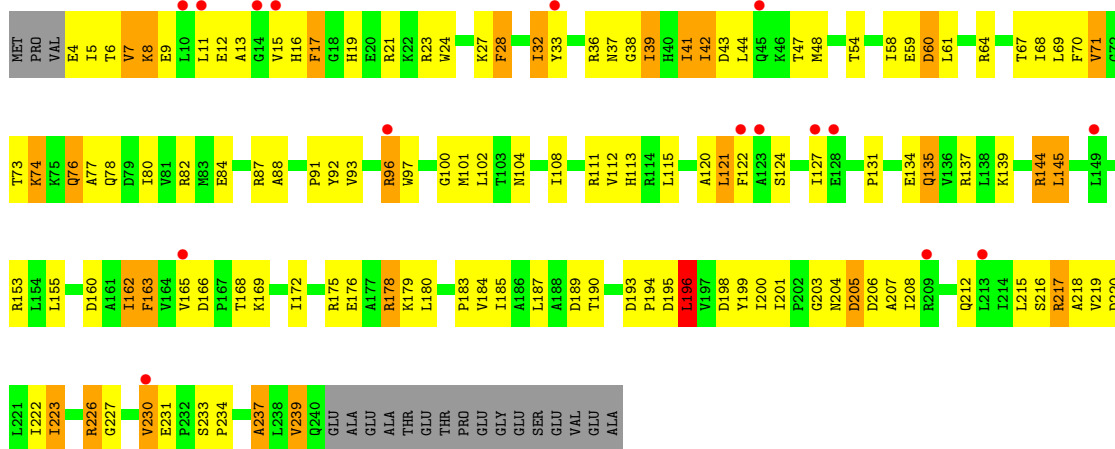


- Molecule 43: 50S ribosomal protein L22

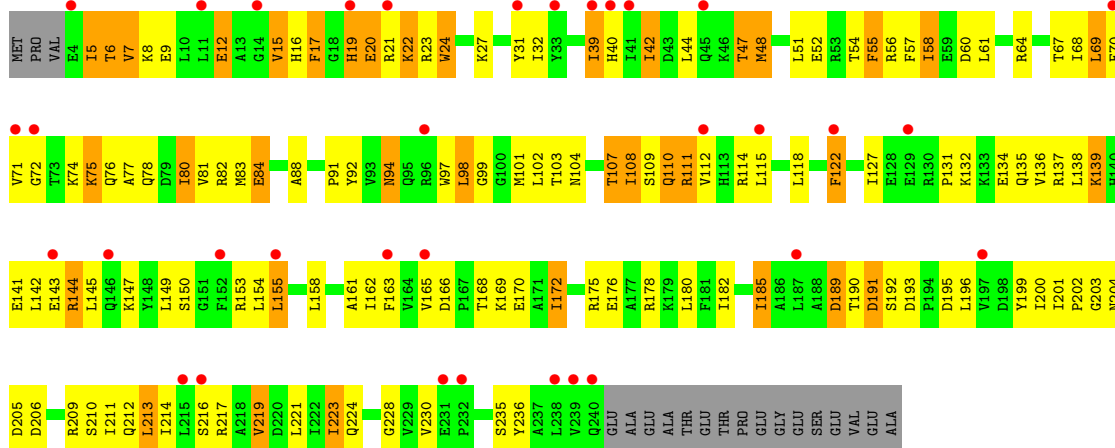




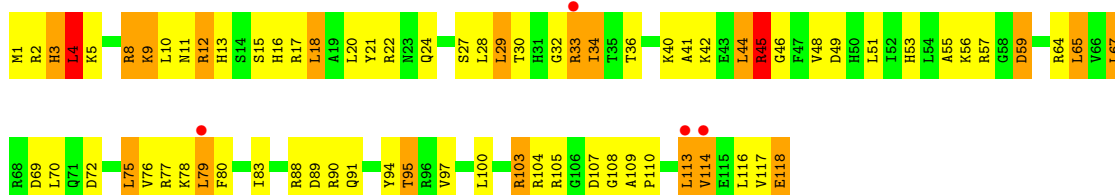
• Molecule 44: 30S ribosomal protein S2



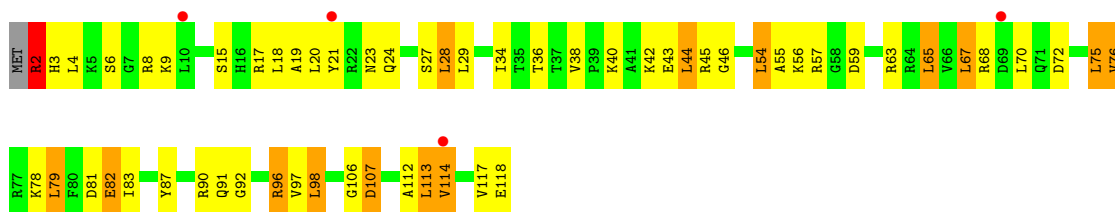
• Molecule 44: 30S ribosomal protein S2



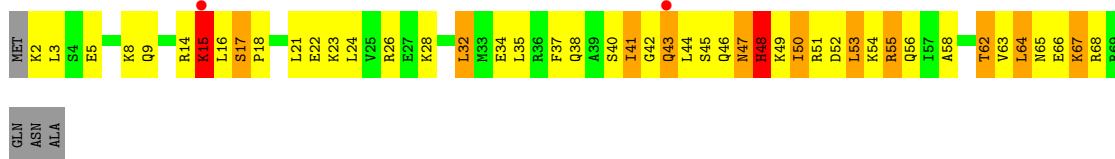
• Molecule 45: 50S ribosomal protein L17



• Molecule 45: 50S ribosomal protein L17



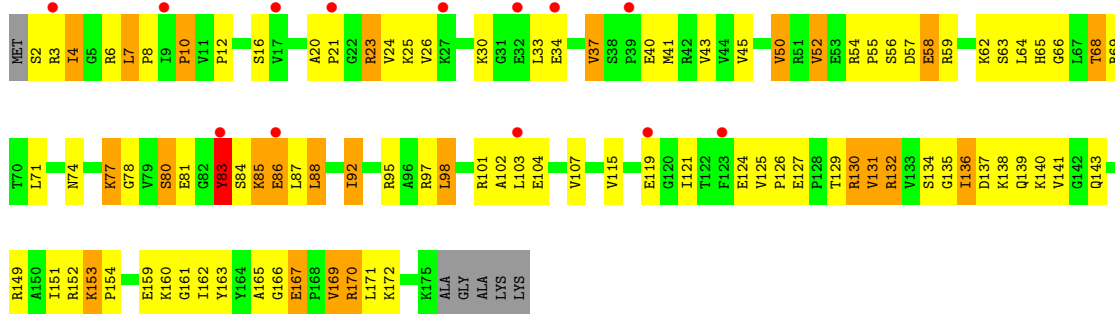
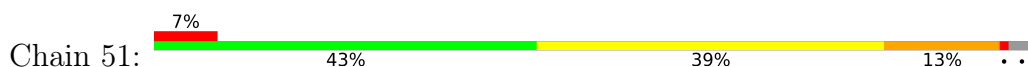
• Molecule 46: 50S ribosomal protein L29



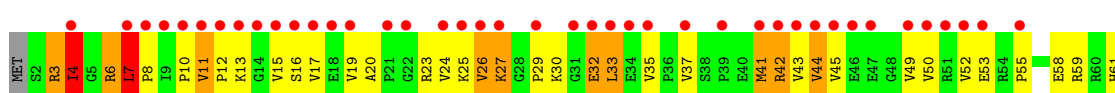
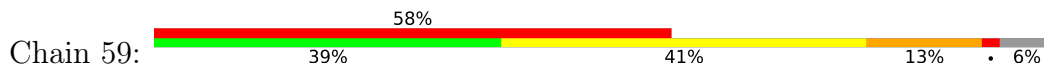
• Molecule 46: 50S ribosomal protein L29

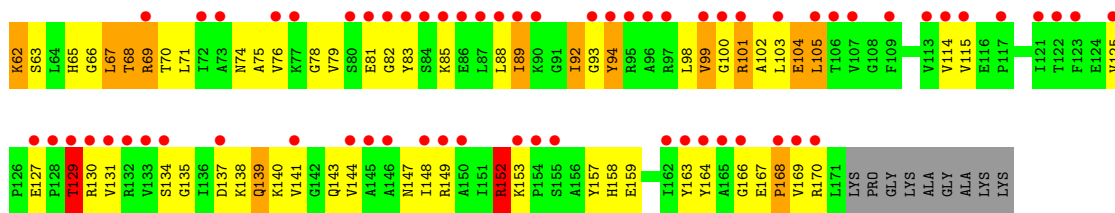


• Molecule 47: 50S ribosomal protein L6

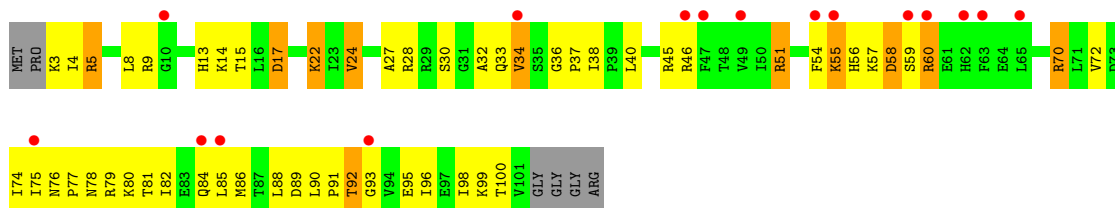


• Molecule 47: 50S ribosomal protein L6

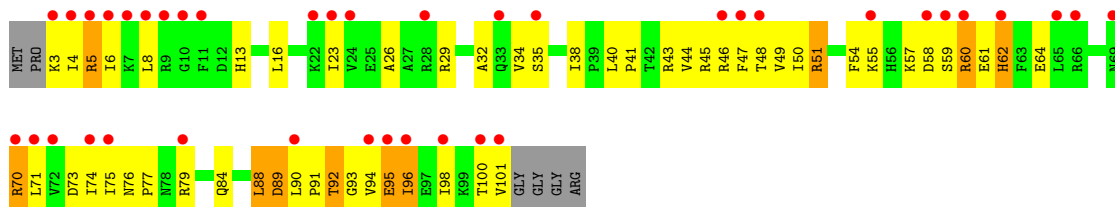




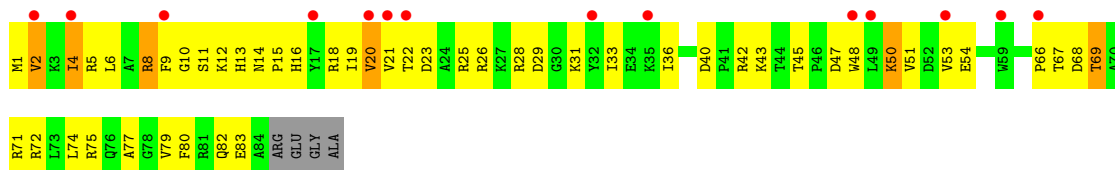
● Molecule 48: 30S ribosomal protein S10



● Molecule 48: 30S ribosomal protein S10



● Molecule 49: 30S ribosomal protein S16

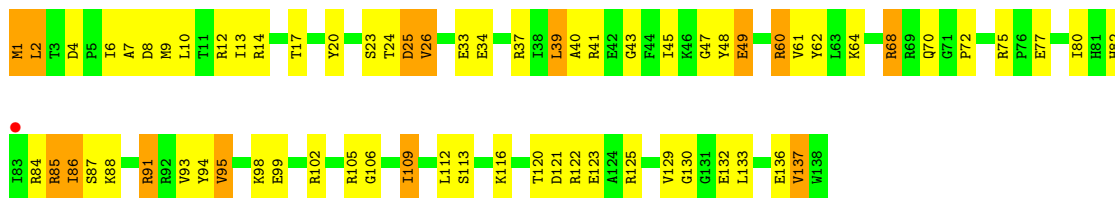


● Molecule 49: 30S ribosomal protein S16

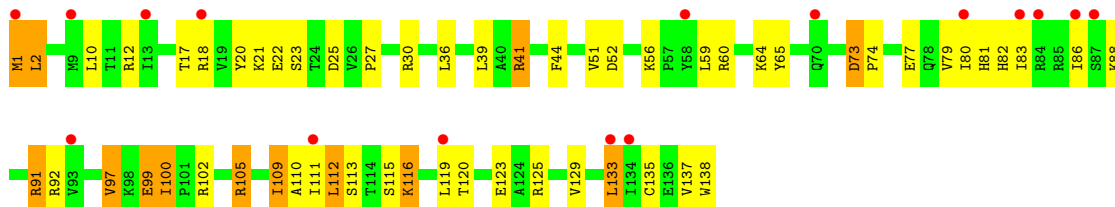


● Molecule 50: 30S ribosomal protein S8

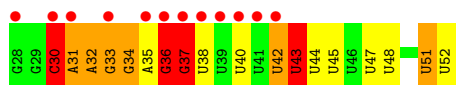
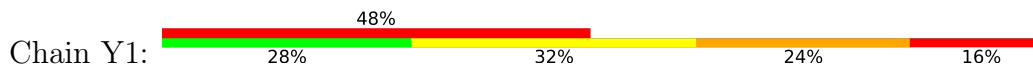




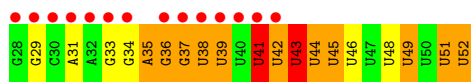
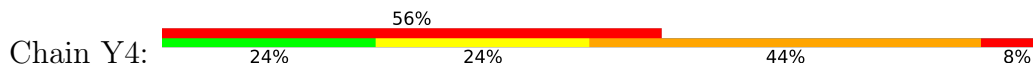
• Molecule 50: 30S ribosomal protein S8



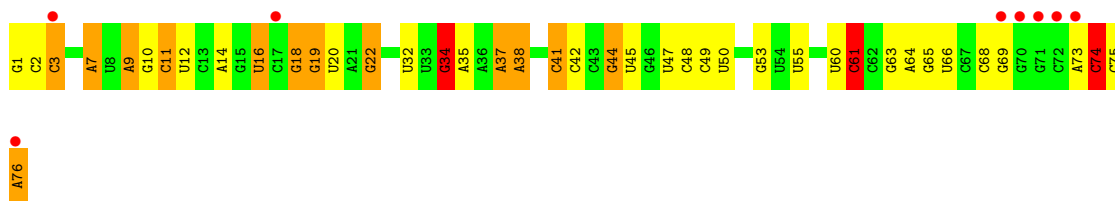
• Molecule 51: mRNA



• Molecule 51: mRNA



• Molecule 52: tRNA-Phe

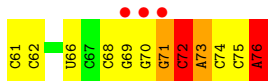
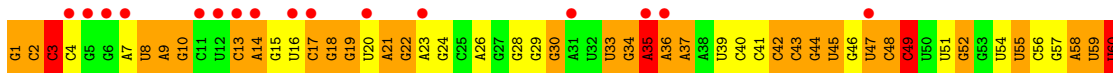
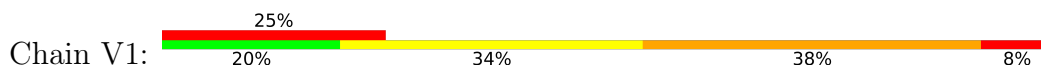


• Molecule 52: tRNA-Phe

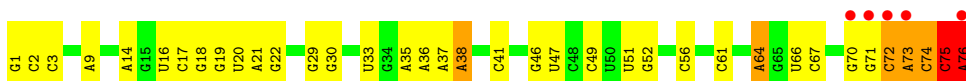




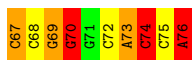
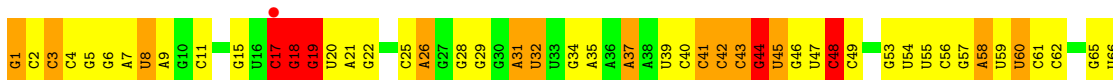
- Molecule 52: tRNA-Phe



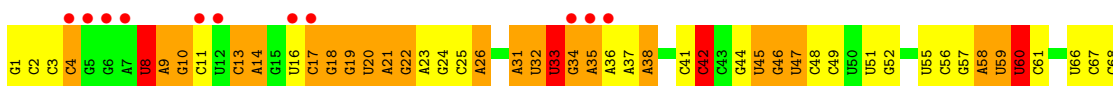
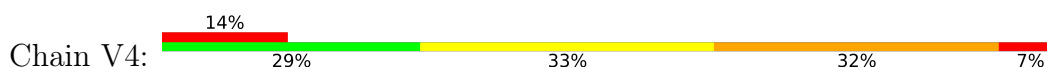
- Molecule 52: tRNA-Phe



- Molecule 52: tRNA-Phe



- Molecule 52: tRNA-Phe





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.07Å 447.36Å 619.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.74 – 2.95 187.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (152.74-2.95) 94.2 (187.49-2.95)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.96Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.213 , 0.253 0.214 , 0.254	Depositor DCC
$R_{free}$ test set	24081 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.3	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	299577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 8UZ, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	13	1.05	64/36276 (0.2%)	1.71	947/56615 (1.7%)
1	1G	0.94	22/36394 (0.1%)	1.56	681/56800 (1.2%)
2	65	0.75	0/891	1.00	3/1187 (0.3%)
2	A8	0.83	1/891 (0.1%)	0.99	2/1187 (0.2%)
3	B5	0.91	1/739 (0.1%)	0.91	1/993 (0.1%)
3	F8	1.01	2/756 (0.3%)	1.02	5/1014 (0.5%)
4	11	1.02	7/2176 (0.3%)	1.10	14/2933 (0.5%)
4	19	0.86	1/2170 (0.0%)	1.03	10/2926 (0.3%)
5	L5	1.03	0/417	1.04	1/550 (0.2%)
5	P8	1.09	0/417	1.19	4/550 (0.7%)
6	2A	0.56	0/879	0.68	0/1187
6	2I	0.60	0/879	0.77	0/1187
7	8A	0.70	1/836 (0.1%)	0.74	0/1117
7	8I	0.65	0/847	0.75	0/1131
8	22	0.60	1/1636 (0.1%)	0.65	0/2205
8	2E	0.65	0/1629	0.73	0/2195
9	82	0.46	0/1002	0.64	0/1346
9	8E	0.51	0/1028	0.69	0/1379
10	15	0.61	0/1131	0.76	1/1525 (0.1%)
10	58	0.73	0/1131	0.86	0/1525
11	C5	0.88	1/807 (0.1%)	0.95	1/1076 (0.1%)
11	G8	0.98	2/796 (0.3%)	1.10	4/1062 (0.4%)
12	M5	1.09	2/502 (0.4%)	1.21	3/661 (0.5%)
12	Q8	1.54	8/486 (1.6%)	1.71	14/638 (2.2%)
13	3A	0.84	3/991 (0.3%)	0.90	0/1327
13	3I	0.82	1/972 (0.1%)	0.98	2/1301 (0.2%)
14	32	0.61	1/1732 (0.1%)	0.76	2/2318 (0.1%)
14	3E	0.88	6/1732 (0.3%)	0.83	3/2318 (0.1%)
15	14	1.29	390/70167 (0.6%)	2.01	3453/109541 (3.2%)
15	1H	1.51	711/70233 (1.0%)	2.23	4800/109643 (4.4%)
16	75	0.76	0/1155	0.87	1/1542 (0.1%)
16	B8	0.84	0/1095	0.99	1/1463 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	H5	0.64	0/473	0.81	0/635
17	L8	1.01	2/457 (0.4%)	0.96	0/613
18	61	0.64	0/1151	0.82	2/1558 (0.1%)
18	69	0.57	0/1151	0.76	1/1558 (0.1%)
19	9A	0.62	0/569	0.81	1/757 (0.1%)
19	9I	0.71	0/555	0.80	1/739 (0.1%)
20	1B	0.54	0/221	0.67	0/288
20	1F	0.55	0/203	0.70	0/266
21	25	0.80	2/942 (0.2%)	0.86	1/1269 (0.1%)
21	68	0.80	0/942	0.89	2/1269 (0.2%)
22	D5	0.62	0/1145	0.73	1/1547 (0.1%)
22	H8	0.64	0/1403	0.82	1/1901 (0.1%)
23	21	0.89	3/1601 (0.2%)	1.00	7/2160 (0.3%)
23	29	0.79	2/1601 (0.1%)	1.04	6/2160 (0.3%)
24	4A	0.48	0/938	0.66	0/1258
24	4I	0.56	0/938	0.75	0/1258
25	42	0.62	0/1171	0.73	0/1576
25	4E	0.68	0/1171	0.79	1/1576 (0.1%)
26	16	1.20	10/2928 (0.3%)	2.01	140/4568 (3.1%)
26	1J	1.05	6/2928 (0.2%)	1.80	103/4568 (2.3%)
27	85	0.69	0/981	0.83	2/1306 (0.2%)
27	C8	0.88	1/981 (0.1%)	1.00	4/1306 (0.3%)
28	I5	0.66	0/527	0.78	0/709
28	M8	0.76	0/545	0.84	1/733 (0.1%)
29	AA	0.52	0/638	0.70	0/860
29	AI	0.63	1/657 (0.2%)	0.76	0/885
30	35	0.81	0/1161	1.08	3/1544 (0.2%)
30	78	0.82	0/1139	1.13	5/1514 (0.3%)
31	E5	0.80	0/653	0.95	0/872
31	I8	0.94	1/665 (0.2%)	1.02	0/885
32	31	1.00	5/1620 (0.3%)	0.99	4/2194 (0.2%)
32	39	0.79	2/1662 (0.1%)	0.97	4/2249 (0.2%)
33	5A	0.53	0/484	0.76	0/643
33	5I	0.54	0/500	0.78	2/664 (0.3%)
34	52	0.70	0/855	0.77	0/1154
34	5E	0.62	0/855	0.76	0/1154
35	95	0.83	0/789	0.97	2/1057 (0.2%)
35	D8	0.78	1/789 (0.1%)	0.95	4/1057 (0.4%)
36	J5	0.81	0/448	0.93	2/606 (0.3%)
36	N8	0.93	1/443 (0.2%)	1.02	2/599 (0.3%)
37	BA	0.54	0/764	0.76	0/1007
37	BI	0.48	0/764	0.70	0/1007
38	45	0.75	0/1134	0.91	1/1517 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	88	0.94	1/1142 (0.1%)	1.05	1/1527 (0.1%)
39	F5	0.83	0/744	0.94	2/989 (0.2%)
39	J8	0.96	1/753 (0.1%)	1.15	6/1000 (0.6%)
40	41	0.67	0/1498	0.77	0/2016
40	49	0.52	0/1498	0.69	0/2016
41	6A	0.65	0/744	0.69	0/992
41	6I	0.66	0/744	0.80	1/992 (0.1%)
42	62	0.52	0/1218	0.60	0/1632
42	6E	0.53	0/1171	0.60	0/1567
43	A5	0.78	0/910	0.94	2/1220 (0.2%)
43	E8	0.81	0/901	1.01	3/1209 (0.2%)
44	12	0.47	0/1959	0.64	0/2642
44	1E	0.49	0/1959	0.67	2/2642 (0.1%)
45	55	0.79	2/973 (0.2%)	1.02	2/1302 (0.2%)
45	98	0.71	0/981	0.94	2/1312 (0.2%)
46	G5	0.83	2/569 (0.4%)	0.91	0/753
46	K8	0.97	0/577	1.04	0/763
47	51	0.74	2/1362 (0.1%)	0.85	1/1841 (0.1%)
47	59	0.45	0/1332	0.71	5/1802 (0.3%)
48	1A	0.49	0/814	0.66	0/1095
48	1I	0.52	0/814	0.70	0/1095
49	7A	0.58	0/721	0.75	1/970 (0.1%)
49	7I	0.59	0/721	0.82	0/970
50	72	0.54	1/1135 (0.1%)	0.67	1/1527 (0.1%)
50	7E	0.59	0/1135	0.75	0/1527
51	Y1	1.24	2/579 (0.3%)	1.63	13/899 (1.4%)
51	Y4	1.00	0/579	1.44	6/899 (0.7%)
52	V1	0.96	7/1809 (0.4%)	1.47	24/2819 (0.9%)
52	V4	0.83	1/1809 (0.1%)	1.36	25/2819 (0.9%)
52	W1	0.92	4/1809 (0.2%)	1.34	17/2819 (0.6%)
52	W4	0.89	4/1809 (0.2%)	1.30	21/2819 (0.7%)
52	X1	1.25	7/1809 (0.4%)	2.02	91/2819 (3.2%)
52	X4	1.10	5/1809 (0.3%)	1.83	68/2819 (2.4%)
All	All	1.14	1301/322722 (0.4%)	1.74	10550/483601 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	65	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	A8	0	1
3	B5	0	1
4	11	0	3
4	19	0	8
5	P8	0	1
6	2A	0	1
6	2I	0	1
8	22	0	2
9	82	0	1
9	8E	0	2
10	15	0	4
11	C5	0	5
11	G8	0	4
12	M5	0	2
12	Q8	0	9
13	3A	0	3
13	3I	0	2
14	32	0	5
14	3E	0	1
16	75	0	2
16	B8	0	2
18	61	0	4
18	69	0	4
22	H8	0	3
23	21	0	7
23	29	0	3
24	4A	0	1
27	85	0	5
27	C8	0	2
28	I5	0	1
28	M8	0	2
29	AI	0	2
30	35	0	11
30	78	0	7
31	E5	0	2
31	I8	0	1
32	31	0	2
32	39	0	6
33	5A	0	2
35	95	0	2
35	D8	0	1
36	J5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	N8	0	2
37	BA	0	3
37	BI	0	3
38	45	0	3
38	88	0	4
39	F5	0	1
39	J8	0	3
40	41	0	1
40	49	0	1
43	A5	0	2
44	12	0	1
44	1E	0	3
45	98	0	2
46	G5	0	3
46	K8	0	3
47	59	0	1
48	1A	0	2
All	All	0	168

The worst 5 of 1301 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1H	2445	A	N9-C4	-21.99	1.24	1.37
15	1H	725	A	N9-C8	15.20	1.50	1.37
15	1H	823	A	N9-C4	-14.86	1.28	1.37
15	1H	832	A	N3-C4	-14.69	1.26	1.34
15	14	2445	A	N9-C4	-14.61	1.29	1.37

The worst 5 of 10550 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1H	1924	G	N3-C4-N9	-30.57	107.66	126.00
15	1H	1924	G	N3-C4-C5	25.42	141.31	128.60
15	1H	992	A	N1-C6-N6	24.66	133.40	118.60
15	1H	992	A	C6-C5-N7	-24.47	115.17	132.30
15	1H	832	A	C2-N3-C4	-24.00	98.60	110.60

There are no chirality outliers.

5 of 168 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	11	239	ARG	Mainchain
4	11	273	ARG	Peptide
4	11	47	GLY	Peptide
2	A8	106	ARG	Peptide
3	B5	61	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32409	0	16360	705	0
1	1G	32514	0	16415	698	0
2	65	881	0	943	59	0
2	A8	881	0	943	51	0
3	B5	725	0	778	28	0
3	F8	742	0	803	39	0
4	11	2126	0	2208	61	0
4	19	2120	0	2197	80	0
5	L5	409	0	454	12	0
5	P8	409	0	454	13	0
6	2A	864	0	881	33	0
6	2I	864	0	881	31	0
7	8A	823	0	891	29	0
7	8I	834	0	904	48	0
8	22	1612	0	1677	74	0
8	2E	1605	0	1668	70	0
9	82	983	0	1006	68	0
9	8E	1009	0	1037	68	0
10	15	1104	0	1180	40	0
10	58	1104	0	1180	68	0
11	C5	794	0	886	60	0
11	G8	783	0	873	60	0
12	M5	495	0	567	54	0
12	Q8	480	0	549	91	0
13	3A	975	0	1062	41	0
13	3I	956	0	1046	36	0
14	32	1702	0	1764	83	0
14	3E	1702	0	1762	84	0
15	14	62647	0	31575	1194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	1H	62707	0	31583	1236	0
16	75	1141	0	1202	55	0
16	B8	1081	0	1141	61	0
17	H5	468	0	518	21	0
17	L8	452	0	503	12	0
18	61	1136	0	1223	51	0
18	69	1136	0	1223	61	0
19	9A	564	0	631	20	0
19	9I	550	0	613	18	0
20	1B	217	0	234	13	0
20	1F	199	0	208	11	0
21	25	932	0	996	41	0
21	68	932	0	996	38	0
22	D5	1120	0	1146	68	0
22	H8	1373	0	1402	71	0
23	21	1568	0	1634	98	0
23	29	1568	0	1633	100	0
24	4A	928	0	987	49	0
24	4I	928	0	987	52	0
25	42	1155	0	1213	49	0
25	4E	1155	0	1213	51	0
26	16	2617	0	1328	47	0
26	1J	2617	0	1328	70	0
27	85	963	0	1022	54	0
27	C8	963	0	1022	53	0
28	I5	515	0	514	45	0
28	M8	533	0	526	47	0
29	AA	624	0	636	38	0
29	AI	643	0	662	54	0
30	35	1144	0	1228	91	0
30	78	1122	0	1206	92	0
31	E5	645	0	652	28	0
31	I8	656	0	683	23	0
32	31	1585	0	1632	91	0
32	39	1627	0	1680	92	0
33	5A	475	0	511	26	0
33	5I	491	0	529	27	0
34	52	842	0	857	36	0
34	5E	842	0	857	25	0
35	95	778	0	852	70	0
35	D8	778	0	852	45	0
36	J5	434	0	454	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	N8	429	0	449	31	0
37	BA	762	0	861	37	0
37	BI	762	0	861	37	0
38	45	1113	0	1167	81	0
38	88	1121	0	1179	77	0
39	F5	737	0	813	41	0
39	J8	746	0	826	54	0
40	41	1473	0	1535	81	0
40	49	1473	0	1535	77	0
41	6A	733	0	771	21	0
41	6I	733	0	771	31	0
42	62	1200	0	1238	36	0
42	6E	1157	0	1202	47	0
43	A5	899	0	964	42	0
43	E8	890	0	951	29	0
44	12	1924	0	1975	108	0
44	1E	1924	0	1975	94	0
45	55	959	0	1021	37	0
45	98	967	0	1033	71	0
46	G5	567	0	618	25	0
46	K8	575	0	634	38	0
47	51	1336	0	1418	80	0
47	59	1307	0	1382	74	0
48	1A	801	0	849	55	0
48	1I	801	0	849	54	0
49	7A	705	0	725	24	0
49	7I	705	0	725	44	0
50	72	1115	0	1177	39	0
50	7E	1115	0	1177	49	0
51	Y1	521	0	262	13	0
51	Y4	521	0	262	26	0
52	V1	1619	0	822	65	0
52	V4	1619	0	822	50	0
52	W1	1619	0	822	23	0
52	W4	1619	0	822	30	0
52	X1	1619	0	822	25	0
52	X4	1619	0	822	37	0
53	13	66	0	0	0	0
53	1G	66	0	0	4	0
54	11	5	0	0	0	0
54	13	182	0	0	0	0
54	14	568	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	16	14	0	0	0	0
54	19	3	0	0	0	0
54	1G	178	0	0	0	0
54	1H	597	0	0	0	0
54	1J	14	0	0	0	0
54	21	3	0	0	0	0
54	25	2	0	0	0	0
54	29	5	0	0	0	0
54	2A	1	0	0	0	0
54	31	3	0	0	0	0
54	35	1	0	0	0	0
54	39	2	0	0	0	0
54	3E	2	0	0	0	0
54	3I	1	0	0	0	0
54	41	2	0	0	0	0
54	42	1	0	0	0	0
54	45	2	0	0	0	0
54	49	1	0	0	0	0
54	4E	1	0	0	0	0
54	4I	1	0	0	0	0
54	52	1	0	0	0	0
54	55	2	0	0	0	0
54	58	1	0	0	0	0
54	5E	1	0	0	0	0
54	5I	1	0	0	0	0
54	68	2	0	0	0	0
54	6A	1	0	0	0	0
54	78	3	0	0	0	0
54	7A	1	0	0	0	0
54	85	1	0	0	0	0
54	88	5	0	0	0	0
54	98	1	0	0	0	0
54	A5	1	0	0	0	0
54	A8	1	0	0	0	0
54	B5	1	0	0	0	0
54	B8	1	0	0	0	0
54	C5	2	0	0	0	0
54	E5	2	0	0	0	0
54	G8	1	0	0	0	0
54	I8	2	0	0	0	0
54	K8	1	0	0	0	0
54	L8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	P8	1	0	0	0	0
54	W1	4	0	0	0	0
54	W4	4	0	0	0	0
54	X1	9	0	0	0	0
54	X4	6	0	0	0	0
55	32	1	0	0	0	0
55	3E	1	0	0	0	0
55	5A	1	0	0	0	0
55	5I	1	0	0	0	0
55	C5	1	0	0	0	0
55	G8	1	0	0	0	0
56	11	1	0	0	0	0
56	13	76	0	0	7	0
56	14	512	0	0	62	0
56	19	8	0	0	0	0
56	1G	72	0	0	10	0
56	1H	533	0	0	61	0
56	21	1	0	0	0	0
56	29	4	0	0	0	0
56	31	5	0	0	0	0
56	35	1	0	0	0	0
56	39	6	0	0	0	0
56	55	1	0	0	0	0
56	5A	1	0	0	0	0
56	6A	2	0	0	0	0
56	6I	1	0	0	0	0
56	78	4	0	0	0	0
56	7A	1	0	0	0	0
56	A5	1	0	0	0	0
56	B8	1	0	0	0	0
56	C8	3	0	0	0	0
56	D8	1	0	0	0	0
56	E8	1	0	0	0	0
56	F8	1	0	0	0	0
56	I8	5	0	0	1	0
56	J5	1	0	0	0	0
56	J8	1	0	0	0	0
56	L5	3	0	0	0	0
56	M5	2	0	0	0	0
56	P8	1	0	0	0	0
56	Y4	2	0	0	0	0
All	All	299577	0	199398	7944	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 7944 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)
4:11:105:ILE:CD1	4:11:105:ILE:CG1	1.76	1.54
14:3E:9:CYS:CB	14:3E:9:CYS:SG	2.01	1.48
12:Q8:46:ARG:HH11	12:Q8:46:ARG:HB2	1.09	1.16
12:Q8:46:ARG:HB2	12:Q8:46:ARG:NH1	1.67	1.10
30:78:15:ARG:HB2	30:78:16:ARG:HB2	1.29	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	65	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	5	22
2	A8	109/112 (97%)	92 (84%)	15 (14%)	2 (2%)	8	33
3	B5	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	28
3	F8	92/96 (96%)	87 (95%)	3 (3%)	2 (2%)	6	28
4	11	271/276 (98%)	255 (94%)	12 (4%)	4 (2%)	10	38
4	19	271/276 (98%)	252 (93%)	13 (5%)	6 (2%)	6	28
5	L5	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
5	P8	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	6	28
6	2A	114/129 (88%)	104 (91%)	8 (7%)	2 (2%)	8	33
6	2I	114/129 (88%)	102 (90%)	10 (9%)	2 (2%)	8	33
7	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
7	8I	98/105 (93%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	22	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
8	2E	203/239 (85%)	182 (90%)	20 (10%)	1 (0%)	29	64
9	82	122/128 (95%)	112 (92%)	9 (7%)	1 (1%)	19	53
9	8E	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	53
10	15	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	22	56
10	58	136/140 (97%)	116 (85%)	17 (12%)	3 (2%)	6	28
11	C5	102/110 (93%)	72 (71%)	28 (28%)	2 (2%)	7	30
11	G8	101/110 (92%)	79 (78%)	16 (16%)	6 (6%)	1	7
12	M5	60/65 (92%)	50 (83%)	6 (10%)	4 (7%)	1	5
12	Q8	58/65 (89%)	37 (64%)	16 (28%)	5 (9%)	1	3
13	3A	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	6	26
13	3I	120/132 (91%)	105 (88%)	15 (12%)	0	100	100
14	32	206/209 (99%)	180 (87%)	26 (13%)	0	100	100
14	3E	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	64
16	75	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	38
16	B8	127/146 (87%)	118 (93%)	9 (7%)	0	100	100
17	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
17	L8	55/60 (92%)	48 (87%)	5 (9%)	2 (4%)	3	16
18	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	7	29
18	69	144/148 (97%)	111 (77%)	29 (20%)	4 (3%)	5	22
19	9A	67/88 (76%)	63 (94%)	4 (6%)	0	100	100
19	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	10	38
20	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
20	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	25	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
21	68	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	53
22	D5	129/206 (63%)	106 (82%)	19 (15%)	4 (3%)	4	19
22	H8	169/206 (82%)	137 (81%)	24 (14%)	8 (5%)	2	11
23	21	203/206 (98%)	161 (79%)	33 (16%)	9 (4%)	2	12
23	29	203/206 (98%)	157 (77%)	34 (17%)	12 (6%)	1	7
24	4A	114/126 (90%)	94 (82%)	19 (17%)	1 (1%)	17	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	4I	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	17	51
25	42	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
25	4E	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22	56
27	85	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
27	C8	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5	24
28	I5	61/71 (86%)	31 (51%)	28 (46%)	2 (3%)	4	18
28	M8	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	4	19
29	AA	76/93 (82%)	62 (82%)	12 (16%)	2 (3%)	5	24
29	AI	78/93 (84%)	67 (86%)	7 (9%)	4 (5%)	2	9
30	35	148/150 (99%)	112 (76%)	28 (19%)	8 (5%)	2	9
30	78	145/150 (97%)	117 (81%)	22 (15%)	6 (4%)	3	13
31	E5	82/85 (96%)	75 (92%)	5 (6%)	2 (2%)	6	26
31	I8	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
32	31	200/210 (95%)	181 (90%)	16 (8%)	3 (2%)	10	38
32	39	206/210 (98%)	164 (80%)	33 (16%)	9 (4%)	2	12
33	5A	56/61 (92%)	48 (86%)	7 (12%)	1 (2%)	8	33
33	5I	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	17
34	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
34	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
35	95	99/101 (98%)	77 (78%)	18 (18%)	4 (4%)	3	14
35	D8	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	30
36	J5	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
36	N8	53/60 (88%)	44 (83%)	7 (13%)	2 (4%)	3	15
37	BA	97/106 (92%)	84 (87%)	11 (11%)	2 (2%)	7	29
37	BI	97/106 (92%)	85 (88%)	12 (12%)	0	100	100
38	45	138/141 (98%)	111 (80%)	25 (18%)	2 (1%)	11	39
38	88	139/141 (99%)	120 (86%)	13 (9%)	6 (4%)	2	12
39	F5	92/98 (94%)	85 (92%)	6 (6%)	1 (1%)	14	46
39	J8	93/98 (95%)	82 (88%)	8 (9%)	3 (3%)	4	19
40	41	179/182 (98%)	161 (90%)	15 (8%)	3 (2%)	9	34
40	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	14	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
41	6I	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
42	62	143/156 (92%)	135 (94%)	8 (6%)	0	100	100
42	6E	140/156 (90%)	133 (95%)	6 (4%)	1 (1%)	22	56
43	A5	111/113 (98%)	104 (94%)	5 (4%)	2 (2%)	8	33
43	E8	110/113 (97%)	102 (93%)	8 (7%)	0	100	100
44	12	235/256 (92%)	199 (85%)	33 (14%)	3 (1%)	12	41
44	1E	235/256 (92%)	195 (83%)	38 (16%)	2 (1%)	17	51
45	55	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	5	24
45	98	116/118 (98%)	101 (87%)	12 (10%)	3 (3%)	5	24
46	G5	65/72 (90%)	59 (91%)	4 (6%)	2 (3%)	4	19
46	K8	66/72 (92%)	62 (94%)	1 (2%)	3 (4%)	2	12
47	51	172/180 (96%)	150 (87%)	16 (9%)	6 (4%)	3	17
47	59	168/180 (93%)	131 (78%)	32 (19%)	5 (3%)	4	20
48	1A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
49	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
50	72	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	56
50	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	56
All	All	11145/11946 (93%)	9763 (88%)	1178 (11%)	204 (2%)	8	33

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	11	240	ALA
6	2A	48	ILE
4	19	237	GLU
12	Q8	51	ALA
14	3E	31	CYS

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	65	87/88 (99%)	60 (69%)	27 (31%)	0	1
2	A8	87/88 (99%)	65 (75%)	22 (25%)	0	2
3	B5	74/78 (95%)	60 (81%)	14 (19%)	1	7
3	F8	76/78 (97%)	64 (84%)	12 (16%)	2	10
4	11	215/218 (99%)	178 (83%)	37 (17%)	2	8
4	19	214/218 (98%)	174 (81%)	40 (19%)	1	7
5	L5	40/42 (95%)	29 (72%)	11 (28%)	0	1
5	P8	40/42 (95%)	33 (82%)	7 (18%)	2	8
6	2A	88/99 (89%)	77 (88%)	11 (12%)	4	17
6	2I	88/99 (89%)	73 (83%)	15 (17%)	2	9
7	8A	94/97 (97%)	80 (85%)	14 (15%)	3	12
7	8I	95/97 (98%)	75 (79%)	20 (21%)	1	4
8	22	160/188 (85%)	121 (76%)	39 (24%)	0	2
8	2E	159/188 (85%)	122 (77%)	37 (23%)	1	3
9	82	95/99 (96%)	80 (84%)	15 (16%)	2	10
9	8E	98/99 (99%)	72 (74%)	26 (26%)	0	2
10	15	117/119 (98%)	91 (78%)	26 (22%)	1	3
10	58	117/119 (98%)	90 (77%)	27 (23%)	1	3
11	C5	85/91 (93%)	62 (73%)	23 (27%)	0	1
11	G8	84/91 (92%)	59 (70%)	25 (30%)	0	1
12	M5	52/55 (94%)	42 (81%)	10 (19%)	1	6
12	Q8	50/55 (91%)	34 (68%)	16 (32%)	0	1
13	3A	104/109 (95%)	80 (77%)	24 (23%)	1	3
13	3I	103/109 (94%)	87 (84%)	16 (16%)	2	11
14	32	180/181 (99%)	146 (81%)	34 (19%)	1	7
14	3E	180/181 (99%)	151 (84%)	29 (16%)	2	10
16	75	120/127 (94%)	86 (72%)	34 (28%)	0	1
16	B8	115/127 (91%)	81 (70%)	34 (30%)	0	1
17	H5	51/52 (98%)	41 (80%)	10 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L8	49/52 (94%)	38 (78%)	11 (22%)	1	3
18	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
18	69	122/124 (98%)	99 (81%)	23 (19%)	1	7
19	9A	60/77 (78%)	44 (73%)	16 (27%)	0	2
19	9I	59/77 (77%)	47 (80%)	12 (20%)	1	5
20	1B	20/22 (91%)	19 (95%)	1 (5%)	24	57
20	1F	18/22 (82%)	18 (100%)	0	100	100
21	25	100/100 (100%)	80 (80%)	20 (20%)	1	5
21	68	100/100 (100%)	83 (83%)	17 (17%)	2	9
22	D5	125/179 (70%)	93 (74%)	32 (26%)	0	2
22	H8	152/179 (85%)	122 (80%)	30 (20%)	1	6
23	21	165/166 (99%)	129 (78%)	36 (22%)	1	4
23	29	165/166 (99%)	128 (78%)	37 (22%)	1	3
24	4A	94/101 (93%)	78 (83%)	16 (17%)	2	9
24	4I	94/101 (93%)	77 (82%)	17 (18%)	1	7
25	42	116/123 (94%)	92 (79%)	24 (21%)	1	4
25	4E	116/123 (94%)	90 (78%)	26 (22%)	1	3
27	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
27	C8	93/94 (99%)	75 (81%)	18 (19%)	1	6
28	I5	57/63 (90%)	42 (74%)	15 (26%)	0	2
28	M8	59/63 (94%)	43 (73%)	16 (27%)	0	1
29	AA	67/80 (84%)	50 (75%)	17 (25%)	0	2
29	AI	70/80 (88%)	49 (70%)	21 (30%)	0	1
30	35	116/116 (100%)	82 (71%)	34 (29%)	0	1
30	78	114/116 (98%)	82 (72%)	32 (28%)	0	1
31	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
31	I8	66/67 (98%)	63 (96%)	3 (4%)	27	61
32	31	161/166 (97%)	133 (83%)	28 (17%)	2	8
32	39	165/166 (99%)	123 (74%)	42 (26%)	0	2
33	5A	48/50 (96%)	36 (75%)	12 (25%)	0	2
33	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	52	90/90 (100%)	69 (77%)	21 (23%)	1	3
34	5E	90/90 (100%)	78 (87%)	12 (13%)	4	15
35	95	82/82 (100%)	59 (72%)	23 (28%)	0	1
35	D8	82/82 (100%)	55 (67%)	27 (33%)	0	1
36	J5	48/52 (92%)	41 (85%)	7 (15%)	3	13
36	N8	48/52 (92%)	38 (79%)	10 (21%)	1	4
37	BA	76/82 (93%)	63 (83%)	13 (17%)	2	8
37	BI	76/82 (93%)	62 (82%)	14 (18%)	1	7
38	45	110/111 (99%)	85 (77%)	25 (23%)	1	3
38	88	111/111 (100%)	87 (78%)	24 (22%)	1	4
39	F5	79/83 (95%)	61 (77%)	18 (23%)	1	3
39	J8	80/83 (96%)	63 (79%)	17 (21%)	1	4
40	41	155/156 (99%)	118 (76%)	37 (24%)	0	2
40	49	155/156 (99%)	123 (79%)	32 (21%)	1	4
41	6A	79/80 (99%)	65 (82%)	14 (18%)	2	8
41	6I	79/80 (99%)	70 (89%)	9 (11%)	5	21
42	62	121/127 (95%)	98 (81%)	23 (19%)	1	6
42	6E	118/127 (93%)	97 (82%)	21 (18%)	2	8
43	A5	92/92 (100%)	75 (82%)	17 (18%)	1	7
43	E8	91/92 (99%)	73 (80%)	18 (20%)	1	6
44	12	205/220 (93%)	158 (77%)	47 (23%)	1	3
44	1E	205/220 (93%)	162 (79%)	43 (21%)	1	4
45	55	100/101 (99%)	77 (77%)	23 (23%)	1	3
45	98	101/101 (100%)	79 (78%)	22 (22%)	1	4
46	G5	63/67 (94%)	46 (73%)	17 (27%)	0	2
46	K8	64/67 (96%)	43 (67%)	21 (33%)	0	1
47	51	145/148 (98%)	108 (74%)	37 (26%)	0	2
47	59	142/148 (96%)	105 (74%)	37 (26%)	0	2
48	1A	89/92 (97%)	72 (81%)	17 (19%)	1	6
48	1I	89/92 (97%)	73 (82%)	16 (18%)	1	7
49	7A	72/74 (97%)	62 (86%)	10 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	7I	72/74 (97%)	57 (79%)	15 (21%)	1	4
50	72	119/119 (100%)	98 (82%)	21 (18%)	2	8
50	7E	119/119 (100%)	97 (82%)	22 (18%)	1	7
All	All	9412/9894 (95%)	7396 (79%)	2016 (21%)	1	4

5 of 2016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	29	170	LEU
44	12	22	LYS
30	35	90	ARG
49	7I	2	VAL
5	P8	24	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
42	6E	13	GLN
44	1E	16	HIS
3	F8	31	HIS
40	49	132	ASN
45	98	13	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1506/1522 (98%)	313 (20%)	31 (2%)
1	1G	1512/1522 (99%)	323 (21%)	36 (2%)
15	14	2908/2917 (99%)	646 (22%)	49 (1%)
15	1H	2911/2917 (99%)	614 (21%)	54 (1%)
26	16	121/122 (99%)	19 (15%)	0
26	1J	121/122 (99%)	29 (23%)	2 (1%)
51	Y1	24/25 (96%)	8 (33%)	3 (12%)
51	Y4	24/25 (96%)	13 (54%)	1 (4%)
52	V1	75/76 (98%)	38 (50%)	6 (8%)
52	V4	75/76 (98%)	35 (46%)	4 (5%)
52	W1	75/76 (98%)	18 (24%)	0
52	W4	75/76 (98%)	19 (25%)	0
52	X1	75/76 (98%)	20 (26%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	X4	75/76 (98%)	20 (26%)	3 (4%)
All	All	9577/9628 (99%)	2115 (22%)	190 (1%)

5 of 2115 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	651	U
1	13	652	G
1	13	653	G
1	13	654	A
1	13	667	G

5 of 190 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	1H	2454	A
15	14	1608	A
15	1H	2704	U
15	14	498	A
15	14	2182	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1656 ligands modelled in this entry, 1652 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
53	8UZ	13	2201	-	35,35,35	0.44	0	49,52,52	1.25	4 (8%)
53	8UZ	1G	2201	-	35,35,35	0.33	0	49,52,52	0.90	1 (2%)
53	8UZ	13	2202	54	35,35,35	0.34	0	49,52,52	0.90	2 (4%)
53	8UZ	1G	2202	54	35,35,35	0.17	0	49,52,52	0.77	2 (4%)

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
53	8UZ	13	2201	-	-	0/12/72/72	0/3/3/3
53	8UZ	1G	2201	-	-	3/12/72/72	0/3/3/3
53	8UZ	13	2202	54	-	2/12/72/72	0/3/3/3
53	8UZ	1G	2202	54	-	3/12/72/72	0/3/3/3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	13	2201	8UZ	O1-C2-C15	-4.32	100.78	108.22
53	13	2202	8UZ	O1-C2-C15	-3.46	102.26	108.22
53	1G	2202	8UZ	C2-C15-N4	2.88	115.40	110.20
53	13	2202	8UZ	C2-C15-N4	2.59	114.87	110.20
53	13	2201	8UZ	C17-C16-C15	2.25	114.93	111.07

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

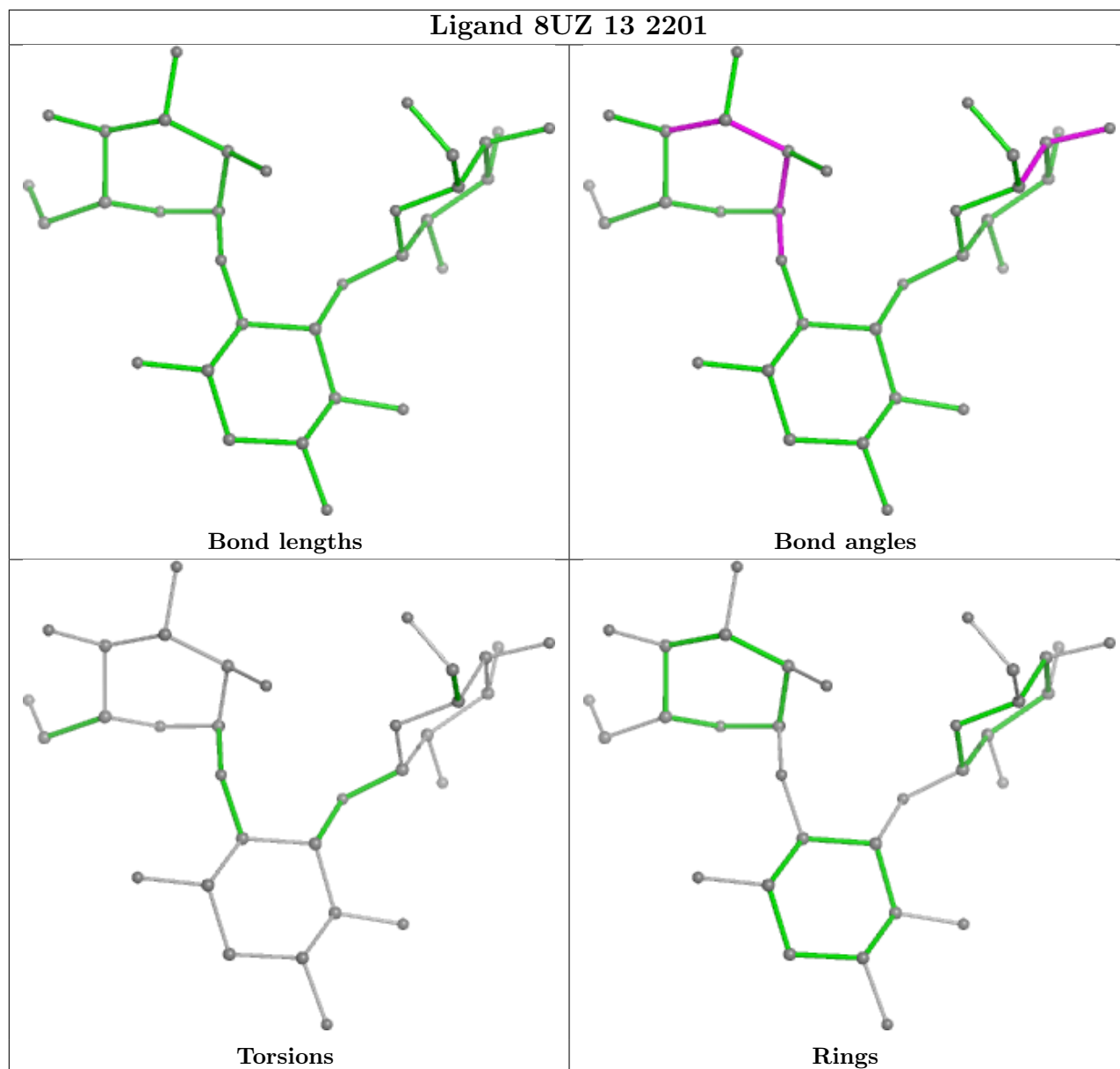
Mol	Chain	Res	Type	Atoms
53	1G	2202	8UZ	N-C-C1-C17
53	1G	2202	8UZ	N-C-C1-O
53	13	2202	8UZ	C12-C10-C11-O5
53	13	2202	8UZ	O4-C10-C11-O5
53	1G	2201	8UZ	N-C-C1-O

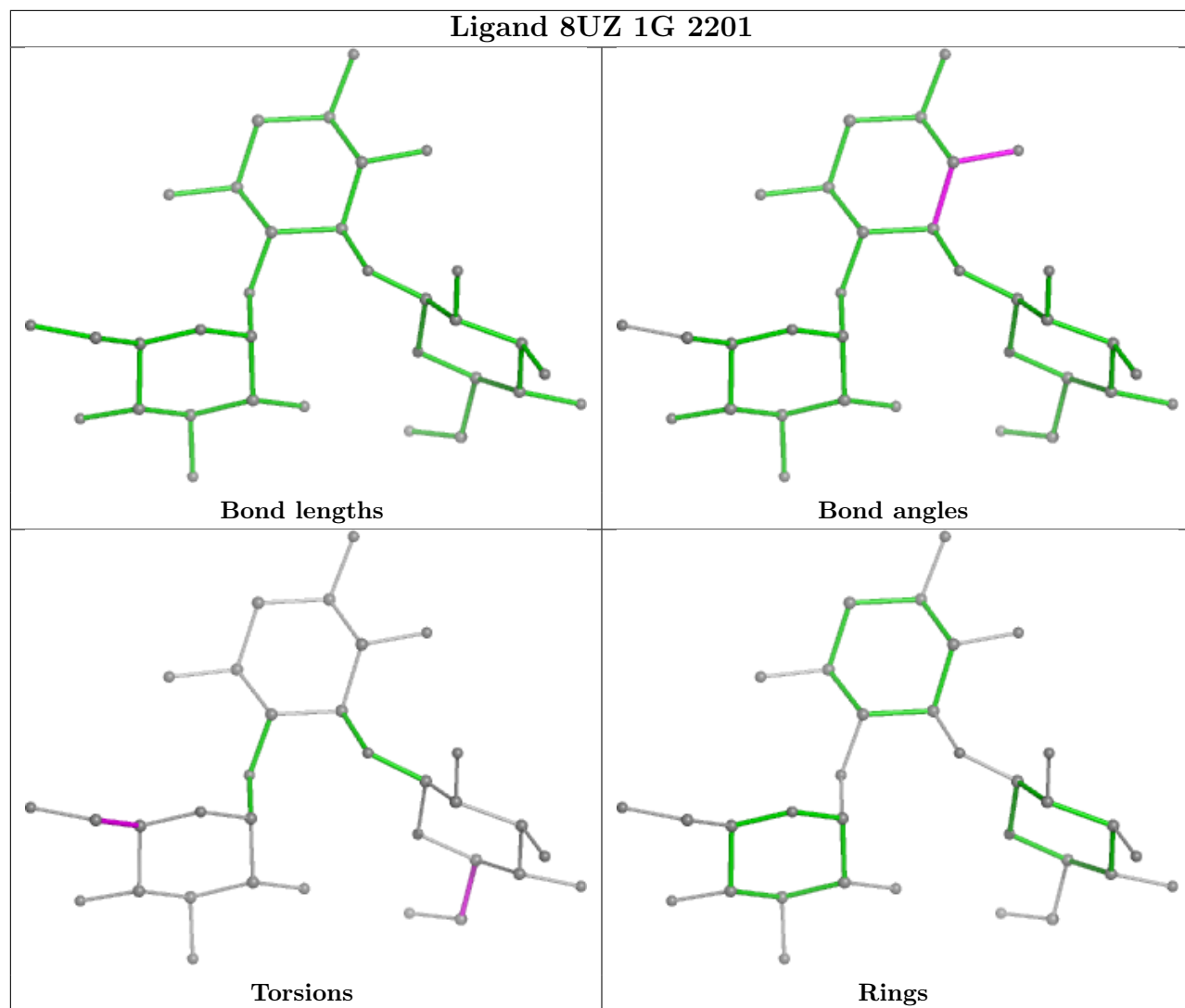
There are no ring outliers.

2 monomers are involved in 4 short contacts:

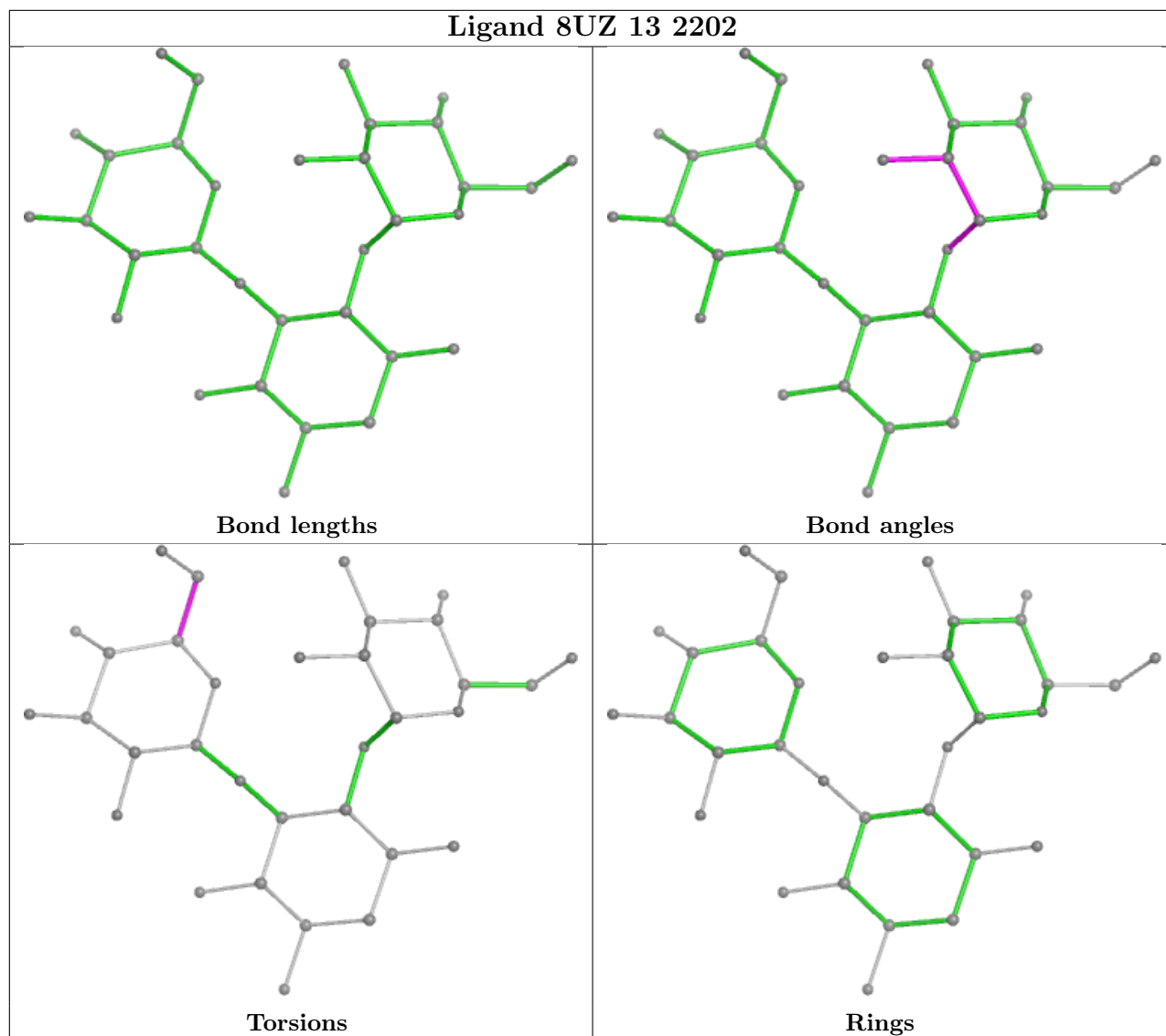
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1G	2201	8UZ	1	0
53	1G	2202	8UZ	3	0

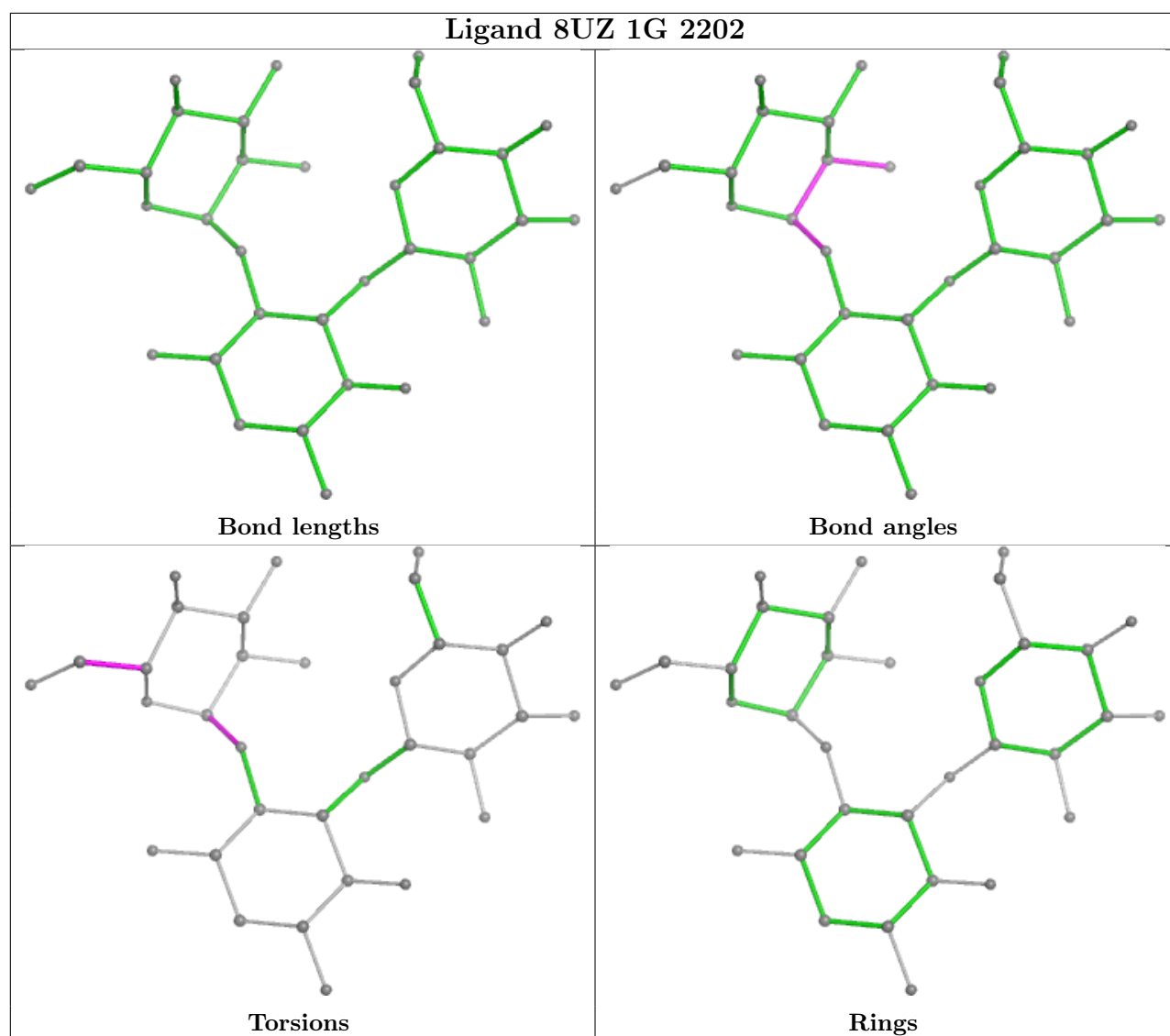
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1508/1522 (99%)	-0.16	13 (0%) 84 71	44, 79, 139, 211	0
1	1G	1513/1522 (99%)	-0.17	15 (0%) 82 68	52, 86, 129, 216	0
2	65	111/112 (99%)	0.63	10 (9%) 9 5	69, 76, 82, 83	0
2	A8	111/112 (99%)	0.69	11 (9%) 7 4	58, 64, 72, 74	0
3	B5	92/96 (95%)	0.71	11 (11%) 4 2	54, 63, 71, 74	0
3	F8	94/96 (97%)	0.44	4 (4%) 35 22	44, 51, 59, 62	0
4	11	273/276 (98%)	0.17	6 (2%) 62 45	33, 48, 55, 60	0
4	19	273/276 (98%)	0.20	3 (1%) 80 65	39, 53, 61, 65	0
5	L5	47/49 (95%)	0.36	2 (4%) 35 22	40, 45, 49, 55	0
5	P8	47/49 (95%)	0.19	2 (4%) 35 22	34, 37, 43, 47	0
6	2A	116/129 (89%)	2.09	58 (50%) 0 0	64, 86, 97, 108	0
6	2I	116/129 (89%)	1.01	20 (17%) 1 1	56, 83, 93, 111	0
7	8A	99/105 (94%)	1.48	34 (34%) 0 0	71, 80, 87, 88	0
7	8I	100/105 (95%)	0.53	6 (6%) 21 13	67, 82, 87, 89	0
8	22	206/239 (86%)	0.55	18 (8%) 10 6	94, 108, 130, 132	0
8	2E	205/239 (85%)	1.12	38 (18%) 1 0	70, 85, 108, 111	0
9	82	124/128 (96%)	0.93	18 (14%) 2 1	86, 123, 131, 133	0
9	8E	127/128 (99%)	0.86	22 (17%) 1 1	64, 114, 123, 126	0
10	15	138/140 (98%)	1.11	26 (18%) 1 0	55, 76, 95, 107	0
10	58	138/140 (98%)	0.79	14 (10%) 7 4	48, 64, 91, 100	0
11	C5	104/110 (94%)	2.49	43 (41%) 0 0	70, 81, 97, 101	0
11	G8	103/110 (93%)	0.72	10 (9%) 7 4	59, 67, 81, 84	0
12	M5	62/65 (95%)	1.12	10 (16%) 1 1	52, 58, 69, 79	0
12	Q8	60/65 (92%)	0.73	4 (6%) 17 10	40, 49, 60, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	3A	125/132 (94%)	1.37	32 (25%) 0 0	68, 71, 81, 108	0
13	3I	122/132 (92%)	0.50	13 (10%) 6 3	53, 57, 65, 78	0
14	32	208/209 (99%)	0.43	13 (6%) 20 11	78, 88, 100, 103	0
14	3E	208/209 (99%)	0.23	9 (4%) 35 22	67, 79, 88, 94	0
15	14	2909/2917 (99%)	-0.00	49 (1%) 70 53	39, 63, 177, 242	0
15	1H	2912/2917 (99%)	0.03	48 (1%) 72 55	31, 53, 154, 220	0
16	75	137/146 (93%)	0.74	15 (10%) 5 3	61, 71, 110, 130	0
16	B8	129/146 (88%)	0.66	12 (9%) 8 5	57, 66, 82, 90	0
17	H5	59/60 (98%)	1.00	10 (16%) 1 1	62, 72, 95, 103	0
17	L8	57/60 (95%)	0.44	3 (5%) 26 16	47, 56, 64, 69	0
18	61	146/148 (98%)	0.33	8 (5%) 25 15	61, 94, 112, 114	0
18	69	146/148 (98%)	0.69	16 (10%) 5 3	67, 97, 119, 121	0
19	9A	69/88 (78%)	0.53	5 (7%) 15 8	73, 82, 90, 98	0
19	9I	67/88 (76%)	0.01	0 100 100	72, 81, 90, 93	0
20	1B	25/27 (92%)	1.87	10 (40%) 0 0	98, 108, 114, 118	0
20	1F	23/27 (85%)	0.90	3 (13%) 3 2	85, 89, 91, 92	0
21	25	122/122 (100%)	0.92	14 (11%) 4 3	52, 63, 72, 73	0
21	68	122/122 (100%)	0.69	3 (2%) 57 40	44, 56, 66, 70	0
22	D5	135/206 (65%)	0.85	20 (14%) 2 1	80, 98, 117, 120	0
22	H8	171/206 (83%)	0.45	10 (5%) 23 14	64, 86, 138, 142	0
23	21	205/206 (99%)	0.99	32 (15%) 2 1	39, 64, 85, 92	0
23	29	205/206 (99%)	0.66	17 (8%) 11 6	46, 69, 90, 98	0
24	4A	116/126 (92%)	0.47	9 (7%) 13 7	88, 115, 121, 122	0
24	4I	116/126 (92%)	0.68	16 (13%) 2 1	73, 103, 110, 112	0
25	42	151/162 (93%)	0.19	6 (3%) 38 25	77, 88, 97, 106	0
25	4E	151/162 (93%)	0.20	4 (2%) 56 39	65, 74, 85, 97	0
26	16	122/122 (100%)	-0.33	1 (0%) 86 73	52, 67, 78, 116	0
26	1J	122/122 (100%)	-0.42	1 (0%) 86 73	67, 80, 93, 118	0
27	85	117/118 (99%)	0.69	9 (7%) 13 7	50, 72, 92, 99	0
27	C8	117/118 (99%)	0.40	2 (1%) 70 53	40, 58, 73, 76	0
28	I5	63/71 (88%)	5.40	62 (98%) 0 0	96, 130, 139, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	M8	66/71 (92%)	4.48	61 (92%) 0 0	83, 114, 122, 123	0
29	AA	78/93 (83%)	0.60	9 (11%) 4 3	96, 123, 136, 137	0
29	AI	80/93 (86%)	0.74	12 (15%) 2 1	76, 98, 106, 108	0
30	35	150/150 (100%)	0.52	10 (6%) 17 10	45, 72, 95, 103	0
30	78	147/150 (98%)	0.23	4 (2%) 54 38	34, 57, 71, 74	0
31	E5	84/85 (98%)	0.92	9 (10%) 6 3	54, 63, 71, 80	0
31	I8	83/85 (97%)	0.29	4 (4%) 30 19	44, 51, 58, 64	0
32	31	202/210 (96%)	0.46	7 (3%) 44 29	35, 58, 73, 83	0
32	39	208/210 (99%)	0.42	11 (5%) 26 16	42, 77, 103, 110	0
33	5A	58/61 (95%)	1.33	17 (29%) 0 0	98, 104, 118, 119	0
33	5I	60/61 (98%)	1.35	12 (20%) 1 0	72, 80, 89, 89	0
34	52	101/101 (100%)	0.06	0 100 100	69, 76, 84, 93	0
34	5E	101/101 (100%)	0.20	0 100 100	71, 77, 86, 92	0
35	95	101/101 (100%)	1.28	24 (23%) 0 0	49, 86, 93, 97	0
35	D8	101/101 (100%)	0.57	6 (5%) 22 13	39, 74, 82, 84	0
36	J5	56/60 (93%)	0.59	4 (7%) 16 9	43, 65, 81, 83	0
36	N8	55/60 (91%)	0.86	8 (14%) 2 1	39, 69, 89, 91	0
37	BA	99/106 (93%)	0.74	11 (11%) 5 3	74, 87, 99, 105	0
37	BI	99/106 (93%)	1.08	18 (18%) 1 1	86, 101, 112, 116	0
38	45	140/141 (99%)	0.60	12 (8%) 10 6	52, 74, 90, 100	0
38	88	141/141 (100%)	0.23	1 (0%) 87 76	42, 59, 75, 91	0
39	F5	94/98 (95%)	0.80	7 (7%) 14 8	45, 60, 90, 97	0
39	J8	95/98 (96%)	0.98	8 (8%) 11 6	37, 53, 81, 86	0
40	41	181/182 (99%)	0.69	18 (9%) 7 4	69, 84, 102, 106	0
40	49	181/182 (99%)	0.77	20 (11%) 5 3	86, 100, 117, 122	0
41	6A	88/89 (98%)	0.51	5 (5%) 23 14	67, 81, 88, 88	0
41	6I	88/89 (98%)	-0.03	2 (2%) 60 43	63, 77, 82, 84	0
42	62	147/156 (94%)	1.04	30 (20%) 1 0	95, 103, 110, 113	0
42	6E	144/156 (92%)	1.03	20 (13%) 2 1	86, 96, 105, 109	0
43	A5	113/113 (100%)	0.92	8 (7%) 16 9	44, 55, 72, 102	0
43	E8	112/113 (99%)	0.58	7 (6%) 20 11	40, 54, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	12	237/256 (92%)	0.89	34 (14%) 2 1	104, 124, 135, 141	0
44	1E	237/256 (92%)	0.44	16 (6%) 17 10	90, 112, 129, 135	0
45	55	117/118 (99%)	0.52	4 (3%) 45 29	49, 58, 66, 72	0
45	98	118/118 (100%)	0.39	4 (3%) 45 29	47, 60, 68, 70	0
46	G5	67/72 (93%)	0.70	4 (5%) 21 13	67, 74, 81, 84	0
46	K8	68/72 (94%)	0.39	2 (2%) 51 35	51, 56, 61, 67	0
47	51	174/180 (96%)	0.54	13 (7%) 14 8	70, 81, 86, 100	0
47	59	170/180 (94%)	2.92	105 (61%) 0 0	116, 145, 162, 170	0
48	1A	99/105 (94%)	0.55	16 (16%) 1 1	92, 124, 132, 133	0
48	1I	99/105 (94%)	1.94	39 (39%) 0 0	68, 111, 126, 127	0
49	7A	84/88 (95%)	0.17	1 (1%) 79 63	71, 81, 94, 117	0
49	7I	84/88 (95%)	0.85	14 (16%) 1 1	76, 88, 103, 123	0
50	72	138/138 (100%)	0.67	16 (11%) 4 2	75, 91, 101, 107	0
50	7E	138/138 (100%)	0.26	1 (0%) 87 76	68, 82, 87, 92	0
51	Y1	25/25 (100%)	1.70	12 (48%) 0 0	55, 111, 161, 168	0
51	Y4	25/25 (100%)	2.28	14 (56%) 0 0	70, 122, 156, 160	0
52	V1	76/76 (100%)	1.33	19 (25%) 0 0	50, 161, 195, 197	0
52	V4	76/76 (100%)	1.19	11 (14%) 2 1	57, 168, 201, 204	0
52	W1	76/76 (100%)	0.40	8 (10%) 6 4	52, 137, 156, 158	0
52	W4	76/76 (100%)	0.16	5 (6%) 18 10	67, 149, 162, 163	0
52	X1	76/76 (100%)	-0.03	3 (3%) 39 25	46, 76, 90, 99	0
52	X4	76/76 (100%)	-0.16	1 (1%) 77 61	54, 85, 102, 108	0
All	All	20933/21574 (97%)	0.40	1557 (7%) 14 8	31, 74, 132, 242	0

The worst 5 of 1557 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	C5	59	GLY	17.6
15	14	2914	C	15.3
15	14	2812	U	14.8
15	14	2912	A	11.5
28	I5	18	CYS	10.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3092	1/1	0.18	0.28	44,44,44,44	0
54	MG	1J	208	1/1	0.32	0.18	71,71,71,71	0
54	MG	14	3460	1/1	0.44	0.51	91,91,91,91	0
54	MG	14	3068	1/1	0.47	0.14	77,77,77,77	0
54	MG	13	2317	1/1	0.48	0.24	69,69,69,69	0
54	MG	13	2338	1/1	0.49	0.37	69,69,69,69	0
54	MG	1G	2315	1/1	0.49	0.20	93,93,93,93	0
54	MG	E5	202	1/1	0.51	0.22	60,60,60,60	0
54	MG	14	3053	1/1	0.52	0.13	67,67,67,67	0
54	MG	14	3328	1/1	0.53	0.22	84,84,84,84	0
54	MG	14	3465	1/1	0.54	0.34	92,92,92,92	0
54	MG	11	303	1/1	0.55	0.29	79,79,79,79	0
54	MG	14	3091	1/1	0.56	0.08	82,82,82,82	0
54	MG	13	2356	1/1	0.56	0.20	67,67,67,67	0
54	MG	14	3320	1/1	0.56	0.30	59,59,59,59	0
54	MG	14	3075	1/1	0.56	0.13	63,63,63,63	0
54	MG	14	3333	1/1	0.57	0.24	61,61,61,61	0
54	MG	1H	3424	1/1	0.58	0.17	59,59,59,59	0
54	MG	1H	3042	1/1	0.58	0.11	33,33,33,33	0
54	MG	14	3088	1/1	0.58	0.27	59,59,59,59	0
54	MG	14	3192	1/1	0.59	0.24	66,66,66,66	0
54	MG	13	2234	1/1	0.59	0.28	84,84,84,84	0
54	MG	1H	3280	1/1	0.60	0.35	46,46,46,46	0
54	MG	14	3221	1/1	0.60	0.32	61,61,61,61	0
54	MG	14	3314	1/1	0.60	0.28	104,104,104,104	0
54	MG	1G	2347	1/1	0.60	0.17	74,74,74,74	0
54	MG	1H	3495	1/1	0.60	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3367	1/1	0.61	0.64	51,51,51,51	0
54	MG	14	3393	1/1	0.61	0.23	71,71,71,71	0
54	MG	1H	3082	1/1	0.61	0.34	57,57,57,57	0
54	MG	13	2376	1/1	0.62	0.23	75,75,75,75	0
54	MG	1G	2372	1/1	0.63	0.19	67,67,67,67	0
54	MG	14	3543	1/1	0.63	0.31	59,59,59,59	0
54	MG	1H	3463	1/1	0.63	0.32	60,60,60,60	0
54	MG	1H	3365	1/1	0.63	0.23	63,63,63,63	0
54	MG	13	2281	1/1	0.64	0.23	61,61,61,61	0
54	MG	1G	2338	1/1	0.64	0.14	72,72,72,72	0
54	MG	1G	2309	1/1	0.64	0.17	75,75,75,75	0
54	MG	X1	105	1/1	0.64	0.43	79,79,79,79	0
54	MG	14	3265	1/1	0.65	0.34	64,64,64,64	0
54	MG	13	2314	1/1	0.65	0.22	67,67,67,67	0
54	MG	14	3548	1/1	0.65	0.28	53,53,53,53	0
54	MG	X1	104	1/1	0.66	0.14	79,79,79,79	0
54	MG	X4	105	1/1	0.66	0.30	83,83,83,83	0
54	MG	13	2333	1/1	0.67	0.17	86,86,86,86	0
54	MG	1G	2273	1/1	0.67	0.20	69,69,69,69	0
54	MG	1H	3066	1/1	0.67	0.07	64,64,64,64	0
54	MG	13	2227	1/1	0.67	0.26	55,55,55,55	0
54	MG	1H	3478	1/1	0.67	0.16	52,52,52,52	0
54	MG	1H	3516	1/1	0.68	0.22	62,62,62,62	0
54	MG	85	201	1/1	0.68	0.34	90,90,90,90	0
54	MG	1H	3254	1/1	0.68	0.22	47,47,47,47	0
54	MG	1H	3027	1/1	0.68	0.21	51,51,51,51	0
54	MG	1H	3345	1/1	0.68	0.29	45,45,45,45	0
54	MG	W4	104	1/1	0.68	0.37	124,124,124,124	0
54	MG	58	201	1/1	0.68	0.46	88,88,88,88	0
54	MG	1G	2272	1/1	0.69	0.22	66,66,66,66	0
54	MG	14	3539	1/1	0.69	0.38	72,72,72,72	0
54	MG	1H	3572	1/1	0.69	0.17	60,60,60,60	0
54	MG	1H	3576	1/1	0.69	0.24	64,64,64,64	0
54	MG	14	3014	1/1	0.69	0.17	41,41,41,41	0
54	MG	1H	3061	1/1	0.69	0.10	68,68,68,68	0
54	MG	14	3383	1/1	0.69	0.38	66,66,66,66	0
54	MG	14	3060	1/1	0.69	0.14	57,57,57,57	0
54	MG	14	3409	1/1	0.69	0.23	51,51,51,51	0
54	MG	14	3447	1/1	0.69	0.19	59,59,59,59	0
54	MG	1H	3319	1/1	0.69	0.23	62,62,62,62	0
54	MG	1H	3197	1/1	0.70	0.22	46,46,46,46	0
54	MG	1H	3579	1/1	0.70	0.21	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3231	1/1	0.70	0.49	77,77,77,77	0
54	MG	1H	3057	1/1	0.70	0.15	46,46,46,46	0
54	MG	14	3070	1/1	0.70	0.32	49,49,49,49	0
54	MG	14	3423	1/1	0.71	0.21	68,68,68,68	0
54	MG	14	3549	1/1	0.71	0.26	72,72,72,72	0
54	MG	25	201	1/1	0.71	0.22	79,79,79,79	0
54	MG	1H	3304	1/1	0.71	0.28	77,77,77,77	0
54	MG	13	2367	1/1	0.71	0.18	58,58,58,58	0
54	MG	5I	102	1/1	0.71	0.15	72,72,72,72	0
54	MG	1G	2346	1/1	0.71	0.12	69,69,69,69	0
54	MG	14	3482	1/1	0.71	0.17	58,58,58,58	0
54	MG	14	3483	1/1	0.71	0.23	55,55,55,55	0
54	MG	1H	3567	1/1	0.71	0.26	65,65,65,65	0
54	MG	14	3038	1/1	0.71	0.12	54,54,54,54	0
54	MG	1H	3010	1/1	0.72	0.09	58,58,58,58	0
54	MG	14	3118	1/1	0.72	0.18	62,62,62,62	0
54	MG	1H	3490	1/1	0.72	0.21	45,45,45,45	0
54	MG	16	204	1/1	0.72	0.22	63,63,63,63	0
54	MG	16	214	1/1	0.72	0.38	66,66,66,66	0
54	MG	1H	3052	1/1	0.72	0.10	36,36,36,36	0
54	MG	14	3417	1/1	0.72	0.32	51,51,51,51	0
54	MG	1H	3354	1/1	0.72	0.25	71,71,71,71	0
54	MG	1H	3553	1/1	0.72	0.20	46,46,46,46	0
54	MG	14	3308	1/1	0.72	0.43	93,93,93,93	0
54	MG	7A	101	1/1	0.72	0.21	70,70,70,70	0
54	MG	1H	3071	1/1	0.72	0.10	102,102,102,102	0
54	MG	1H	3368	1/1	0.72	0.21	57,57,57,57	0
54	MG	13	2287	1/1	0.72	0.45	89,89,89,89	0
54	MG	1H	3318	1/1	0.72	0.39	58,58,58,58	0
54	MG	1G	2379	1/1	0.73	0.22	85,85,85,85	0
54	MG	13	2235	1/1	0.73	0.27	81,81,81,81	0
54	MG	14	3291	1/1	0.73	0.18	49,49,49,49	0
54	MG	1H	3286	1/1	0.73	0.52	79,79,79,79	0
54	MG	1G	2303	1/1	0.73	0.33	72,72,72,72	0
54	MG	1H	3491	1/1	0.73	0.25	55,55,55,55	0
54	MG	13	2342	1/1	0.73	0.19	73,73,73,73	0
54	MG	1H	3029	1/1	0.73	0.13	52,52,52,52	0
54	MG	14	3364	1/1	0.73	0.43	67,67,67,67	0
54	MG	14	3083	1/1	0.73	0.10	66,66,66,66	0
54	MG	1H	3544	1/1	0.73	0.19	57,57,57,57	0
54	MG	1H	3040	1/1	0.73	0.13	49,49,49,49	0
54	MG	14	3397	1/1	0.73	0.34	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3093	1/1	0.73	0.21	54,54,54,54	0
54	MG	88	305	1/1	0.73	0.23	76,76,76,76	0
54	MG	14	3414	1/1	0.73	0.27	67,67,67,67	0
54	MG	X1	103	1/1	0.73	0.11	76,76,76,76	0
54	MG	1H	3167	1/1	0.73	0.27	40,40,40,40	0
54	MG	13	2372	1/1	0.73	0.45	87,87,87,87	0
54	MG	14	3220	1/1	0.73	0.25	70,70,70,70	0
54	MG	1H	3413	1/1	0.73	0.25	77,77,77,77	0
54	MG	1G	2287	1/1	0.74	0.18	77,77,77,77	0
54	MG	14	3403	1/1	0.74	0.36	63,63,63,63	0
54	MG	1H	3064	1/1	0.74	0.20	47,47,47,47	0
54	MG	1G	2370	1/1	0.74	0.25	59,59,59,59	0
54	MG	29	304	1/1	0.74	0.31	67,67,67,67	0
54	MG	1H	3591	1/1	0.74	0.26	62,62,62,62	0
54	MG	1H	3376	1/1	0.74	0.25	44,44,44,44	0
54	MG	1G	2210	1/1	0.74	0.21	67,67,67,67	0
54	MG	14	3451	1/1	0.74	0.20	52,52,52,52	0
54	MG	14	3046	1/1	0.74	0.05	71,71,71,71	0
54	MG	14	3342	1/1	0.74	0.18	66,66,66,66	0
54	MG	14	3353	1/1	0.74	0.13	82,82,82,82	0
54	MG	14	3051	1/1	0.74	0.17	71,71,71,71	0
54	MG	1H	3059	1/1	0.74	0.15	51,51,51,51	0
54	MG	1H	3428	1/1	0.74	0.22	40,40,40,40	0
54	MG	1H	3346	1/1	0.74	0.64	61,61,61,61	0
54	MG	1G	2269	1/1	0.75	0.54	103,103,103,103	0
54	MG	1H	3355	1/1	0.75	0.14	57,57,57,57	0
54	MG	14	3223	1/1	0.75	0.28	58,58,58,58	0
54	MG	14	3448	1/1	0.75	0.21	60,60,60,60	0
54	MG	1H	3068	1/1	0.75	0.09	64,64,64,64	0
54	MG	1H	3561	1/1	0.75	0.46	72,72,72,72	0
54	MG	14	3090	1/1	0.75	0.14	51,51,51,51	0
54	MG	14	3306	1/1	0.75	0.21	68,68,68,68	0
54	MG	1G	2212	1/1	0.75	0.08	104,104,104,104	0
54	MG	1H	3011	1/1	0.75	0.17	46,46,46,46	0
54	MG	14	3406	1/1	0.75	0.16	79,79,79,79	0
54	MG	1H	3396	1/1	0.75	0.31	75,75,75,75	0
54	MG	14	3411	1/1	0.75	0.29	66,66,66,66	0
54	MG	1G	2288	1/1	0.75	0.45	84,84,84,84	0
54	MG	1G	2253	1/1	0.76	0.51	87,87,87,87	0
54	MG	1G	2326	1/1	0.76	0.33	84,84,84,84	0
54	MG	16	201	1/1	0.76	0.15	69,69,69,69	0
54	MG	14	3325	1/1	0.76	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3331	1/1	0.76	0.33	50,50,50,50	0
54	MG	13	2377	1/1	0.76	0.21	81,81,81,81	0
54	MG	1H	3379	1/1	0.76	0.13	64,64,64,64	0
54	MG	14	3433	1/1	0.76	0.26	67,67,67,67	0
54	MG	1H	3142	1/1	0.76	0.21	64,64,64,64	0
54	MG	14	3225	1/1	0.76	0.26	57,57,57,57	0
54	MG	1H	3060	1/1	0.76	0.12	45,45,45,45	0
54	MG	1H	3415	1/1	0.76	0.16	61,61,61,61	0
54	MG	14	3386	1/1	0.76	0.17	47,47,47,47	0
54	MG	1H	3521	1/1	0.76	0.30	43,43,43,43	0
54	MG	1H	3540	1/1	0.76	0.30	82,82,82,82	0
54	MG	14	3522	1/1	0.76	0.15	54,54,54,54	0
54	MG	14	3400	1/1	0.76	0.18	71,71,71,71	0
54	MG	14	3040	1/1	0.76	0.16	70,70,70,70	0
54	MG	1H	3358	1/1	0.77	0.24	49,49,49,49	0
54	MG	14	3276	1/1	0.77	0.45	45,45,45,45	0
54	MG	1H	3300	1/1	0.77	0.37	79,79,79,79	0
54	MG	1H	3085	1/1	0.77	0.16	45,45,45,45	0
54	MG	1G	2286	1/1	0.77	0.22	68,68,68,68	0
54	MG	1H	3492	1/1	0.77	0.53	84,84,84,84	0
54	MG	1G	2228	1/1	0.77	0.22	71,71,71,71	0
54	MG	1H	3388	1/1	0.77	0.29	62,62,62,62	0
54	MG	14	3123	1/1	0.77	0.34	45,45,45,45	0
54	MG	1H	3393	1/1	0.77	0.24	51,51,51,51	0
54	MG	13	2375	1/1	0.77	0.27	83,83,83,83	0
54	MG	13	2350	1/1	0.77	0.20	53,53,53,53	0
54	MG	13	2335	1/1	0.77	0.43	75,75,75,75	0
54	MG	1H	3081	1/1	0.77	0.33	49,49,49,49	0
54	MG	1G	2214	1/1	0.77	0.14	74,74,74,74	0
54	MG	14	3479	1/1	0.77	0.23	56,56,56,56	0
54	MG	14	3385	1/1	0.77	0.25	50,50,50,50	0
54	MG	14	3251	1/1	0.77	0.52	88,88,88,88	0
54	MG	14	3485	1/1	0.77	0.49	73,73,73,73	0
54	MG	14	3258	1/1	0.77	0.32	39,39,39,39	0
54	MG	14	3263	1/1	0.78	0.59	77,77,77,77	0
54	MG	14	3499	1/1	0.78	0.15	80,80,80,80	0
54	MG	14	3517	1/1	0.78	0.26	65,65,65,65	0
54	MG	1H	3438	1/1	0.78	0.18	54,54,54,54	0
54	MG	1H	3440	1/1	0.78	0.18	39,39,39,39	0
54	MG	14	3542	1/1	0.78	0.14	65,65,65,65	0
54	MG	13	2301	1/1	0.78	0.11	72,72,72,72	0
54	MG	14	3405	1/1	0.78	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2381	1/1	0.78	0.29	87,87,87,87	0
54	MG	1G	2351	1/1	0.78	0.21	66,66,66,66	0
54	MG	1H	3584	1/1	0.78	0.25	54,54,54,54	0
54	MG	1H	3590	1/1	0.78	0.46	67,67,67,67	0
54	MG	1H	3164	1/1	0.78	0.34	45,45,45,45	0
54	MG	1G	2262	1/1	0.78	0.22	87,87,87,87	0
54	MG	1J	204	1/1	0.78	0.24	67,67,67,67	0
54	MG	1J	205	1/1	0.78	0.36	64,64,64,64	0
54	MG	13	2307	1/1	0.78	0.45	77,77,77,77	0
54	MG	1J	214	1/1	0.78	0.24	71,71,71,71	0
54	MG	1H	3507	1/1	0.78	0.17	68,68,68,68	0
54	MG	13	2293	1/1	0.78	0.28	109,109,109,109	0
54	MG	35	201	1/1	0.78	0.21	60,60,60,60	0
54	MG	1H	3079	1/1	0.78	0.27	59,59,59,59	0
54	MG	13	2299	1/1	0.78	0.29	85,85,85,85	0
54	MG	P8	101	1/1	0.78	0.32	51,51,51,51	0
54	MG	14	3462	1/1	0.78	0.28	55,55,55,55	0
54	MG	X1	101	1/1	0.78	0.17	84,84,84,84	0
54	MG	14	3368	1/1	0.78	0.21	50,50,50,50	0
54	MG	13	2323	1/1	0.78	0.12	85,85,85,85	0
54	MG	14	3481	1/1	0.78	0.20	82,82,82,82	0
54	MG	14	3062	1/1	0.78	0.10	51,51,51,51	0
54	MG	1H	3434	1/1	0.78	0.31	59,59,59,59	0
54	MG	1H	3067	1/1	0.79	0.19	42,42,42,42	0
54	MG	1H	3342	1/1	0.79	0.36	62,62,62,62	0
54	MG	14	3472	1/1	0.79	0.25	58,58,58,58	0
54	MG	1J	203	1/1	0.79	0.39	67,67,67,67	0
54	MG	14	3399	1/1	0.79	0.29	70,70,70,70	0
54	MG	13	2364	1/1	0.79	0.15	69,69,69,69	0
54	MG	14	3322	1/1	0.79	0.19	51,51,51,51	0
54	MG	1H	3442	1/1	0.79	0.19	55,55,55,55	0
54	MG	1G	2284	1/1	0.79	0.49	90,90,90,90	0
54	MG	14	3032	1/1	0.79	0.09	46,46,46,46	0
54	MG	5E	201	1/1	0.79	0.20	66,66,66,66	0
54	MG	1H	3287	1/1	0.79	0.15	59,59,59,59	0
54	MG	14	3346	1/1	0.79	0.16	83,83,83,83	0
54	MG	88	303	1/1	0.79	0.19	56,56,56,56	0
54	MG	14	3525	1/1	0.79	0.11	51,51,51,51	0
54	MG	13	2278	1/1	0.79	0.37	62,62,62,62	0
54	MG	13	2320	1/1	0.79	0.38	75,75,75,75	0
54	MG	13	2294	1/1	0.79	0.19	57,57,57,57	0
54	MG	1H	3211	1/1	0.79	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3056	1/1	0.79	0.09	48,48,48,48	0
54	MG	14	3565	1/1	0.79	0.22	69,69,69,69	0
54	MG	14	3296	1/1	0.79	0.16	59,59,59,59	0
54	MG	14	3169	1/1	0.79	0.49	57,57,57,57	0
54	MG	1G	2330	1/1	0.80	0.17	93,93,93,93	0
54	MG	1H	3529	1/1	0.80	0.18	42,42,42,42	0
54	MG	1G	2311	1/1	0.80	0.26	87,87,87,87	0
54	MG	1H	3058	1/1	0.80	0.08	39,39,39,39	0
54	MG	14	3222	1/1	0.80	0.41	70,70,70,70	0
54	MG	1H	3549	1/1	0.80	0.18	61,61,61,61	0
54	MG	1G	2380	1/1	0.80	0.12	70,70,70,70	0
54	MG	14	3357	1/1	0.80	0.17	53,53,53,53	0
54	MG	1G	2341	1/1	0.80	0.22	86,86,86,86	0
54	MG	1G	2313	1/1	0.80	0.36	62,62,62,62	0
54	MG	1H	3383	1/1	0.80	0.38	88,88,88,88	0
54	MG	1H	3479	1/1	0.80	0.19	67,67,67,67	0
54	MG	1H	3144	1/1	0.80	0.26	47,47,47,47	0
54	MG	13	2211	1/1	0.80	0.10	67,67,67,67	0
54	MG	14	3279	1/1	0.80	0.23	66,66,66,66	0
54	MG	14	3394	1/1	0.80	0.57	54,54,54,54	0
54	MG	1G	2319	1/1	0.80	0.22	77,77,77,77	0
54	MG	1G	2355	1/1	0.80	0.23	76,76,76,76	0
54	MG	14	3501	1/1	0.80	0.14	47,47,47,47	0
54	MG	14	3504	1/1	0.80	0.24	71,71,71,71	0
54	MG	14	3302	1/1	0.80	0.32	52,52,52,52	0
54	MG	14	3521	1/1	0.80	0.10	58,58,58,58	0
54	MG	C5	202	1/1	0.80	0.55	70,70,70,70	0
54	MG	14	3008	1/1	0.80	0.10	53,53,53,53	0
54	MG	14	3529	1/1	0.80	0.14	63,63,63,63	0
54	MG	1G	2356	1/1	0.80	0.10	74,74,74,74	0
54	MG	13	2297	1/1	0.80	0.32	62,62,62,62	0
54	MG	14	3410	1/1	0.80	0.20	59,59,59,59	0
54	MG	X4	106	1/1	0.80	0.23	73,73,73,73	0
54	MG	13	2374	1/1	0.81	0.08	79,79,79,79	0
54	MG	1G	2366	1/1	0.81	0.21	100,100,100,100	0
54	MG	1G	2292	1/1	0.81	0.17	67,67,67,67	0
54	MG	14	3241	1/1	0.81	0.19	72,72,72,72	0
54	MG	14	3247	1/1	0.81	0.41	68,68,68,68	0
54	MG	14	3250	1/1	0.81	0.57	83,83,83,83	0
54	MG	14	3541	1/1	0.81	0.24	71,71,71,71	0
54	MG	14	3057	1/1	0.81	0.19	48,48,48,48	0
54	MG	14	3059	1/1	0.81	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1G	2293	1/1	0.81	0.23	83,83,83,83	0
54	MG	1H	3226	1/1	0.81	0.29	43,43,43,43	0
54	MG	14	3554	1/1	0.81	0.23	62,62,62,62	0
54	MG	14	3269	1/1	0.81	0.11	55,55,55,55	0
54	MG	1H	3054	1/1	0.81	0.11	46,46,46,46	0
54	MG	1G	2295	1/1	0.81	0.23	75,75,75,75	0
54	MG	1H	3447	1/1	0.81	0.15	59,59,59,59	0
54	MG	1H	3460	1/1	0.81	0.33	61,61,61,61	0
54	MG	13	2316	1/1	0.81	0.37	74,74,74,74	0
54	MG	13	2321	1/1	0.81	0.30	81,81,81,81	0
54	MG	1H	3378	1/1	0.81	0.23	51,51,51,51	0
54	MG	13	2288	1/1	0.81	0.11	80,80,80,80	0
54	MG	14	3315	1/1	0.81	0.21	62,62,62,62	0
54	MG	1J	213	1/1	0.81	0.19	78,78,78,78	0
54	MG	1H	3140	1/1	0.81	0.19	42,42,42,42	0
54	MG	1H	3307	1/1	0.81	0.23	31,31,31,31	0
54	MG	14	3453	1/1	0.81	0.21	44,44,44,44	0
54	MG	14	3146	1/1	0.81	0.29	54,54,54,54	0
54	MG	14	3151	1/1	0.81	0.34	56,56,56,56	0
54	MG	14	3331	1/1	0.81	0.21	54,54,54,54	0
54	MG	13	2339	1/1	0.81	0.16	79,79,79,79	0
54	MG	14	3473	1/1	0.81	0.22	77,77,77,77	0
54	MG	14	3335	1/1	0.81	0.18	57,57,57,57	0
54	MG	14	3177	1/1	0.81	0.43	67,67,67,67	0
54	MG	14	3343	1/1	0.81	0.19	62,62,62,62	0
54	MG	13	2327	1/1	0.81	0.25	81,81,81,81	0
54	MG	14	3204	1/1	0.81	0.39	59,59,59,59	0
54	MG	1H	3403	1/1	0.81	0.19	46,46,46,46	0
54	MG	1H	3518	1/1	0.81	0.31	41,41,41,41	0
54	MG	1H	3153	1/1	0.81	0.43	45,45,45,45	0
54	MG	14	3512	1/1	0.81	0.39	57,57,57,57	0
54	MG	19	301	1/1	0.82	0.25	54,54,54,54	0
54	MG	13	2263	1/1	0.82	0.19	77,77,77,77	0
54	MG	14	3496	1/1	0.82	0.13	58,58,58,58	0
54	MG	1H	3090	1/1	0.82	0.24	49,49,49,49	0
54	MG	1H	3328	1/1	0.82	0.26	49,49,49,49	0
54	MG	14	3290	1/1	0.82	0.34	73,73,73,73	0
54	MG	14	3509	1/1	0.82	0.20	62,62,62,62	0
54	MG	13	2359	1/1	0.82	0.16	78,78,78,78	0
54	MG	14	3516	1/1	0.82	0.24	61,61,61,61	0
54	MG	78	202	1/1	0.82	0.23	54,54,54,54	0
54	MG	14	3361	1/1	0.82	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	3I	301	1/1	0.82	0.14	37,37,37,37	0
54	MG	1H	3340	1/1	0.82	0.27	59,59,59,59	0
54	MG	13	2290	1/1	0.82	0.29	67,67,67,67	0
54	MG	13	2284	1/1	0.82	0.25	73,73,73,73	0
54	MG	1H	3078	1/1	0.82	0.19	64,64,64,64	0
54	MG	1H	3542	1/1	0.82	0.16	48,48,48,48	0
54	MG	1H	3468	1/1	0.82	0.10	51,51,51,51	0
54	MG	14	3388	1/1	0.82	0.57	70,70,70,70	0
54	MG	13	2328	1/1	0.82	0.31	76,76,76,76	0
54	MG	W1	104	1/1	0.82	0.20	120,120,120,120	0
54	MG	1H	3159	1/1	0.82	0.30	52,52,52,52	0
54	MG	14	3049	1/1	0.82	0.18	52,52,52,52	0
54	MG	1H	3488	1/1	0.82	0.16	54,54,54,54	0
54	MG	14	3558	1/1	0.82	0.26	88,88,88,88	0
54	MG	X1	107	1/1	0.82	0.24	78,78,78,78	0
54	MG	14	3126	1/1	0.82	0.32	63,63,63,63	0
54	MG	13	2226	1/1	0.82	0.13	82,82,82,82	0
54	MG	14	3404	1/1	0.82	0.21	60,60,60,60	0
54	MG	1H	3163	1/1	0.83	0.27	43,43,43,43	0
54	MG	A8	201	1/1	0.83	0.28	60,60,60,60	0
54	MG	14	3562	1/1	0.83	0.14	61,61,61,61	0
54	MG	1H	3554	1/1	0.83	0.20	53,53,53,53	0
54	MG	13	2207	1/1	0.83	0.08	69,69,69,69	0
54	MG	1H	3015	1/1	0.83	0.09	41,41,41,41	0
54	MG	1H	3391	1/1	0.83	0.26	56,56,56,56	0
54	MG	14	3257	1/1	0.83	0.26	42,42,42,42	0
54	MG	14	3469	1/1	0.83	0.12	78,78,78,78	0
54	MG	1H	3392	1/1	0.83	0.19	50,50,50,50	0
54	MG	1H	3577	1/1	0.83	0.14	51,51,51,51	0
54	MG	14	3377	1/1	0.83	0.23	49,49,49,49	0
54	MG	14	3381	1/1	0.83	0.23	65,65,65,65	0
54	MG	1J	210	1/1	0.83	0.19	70,70,70,70	0
54	MG	1G	2343	1/1	0.83	0.37	75,75,75,75	0
54	MG	1G	2263	1/1	0.83	0.33	61,61,61,61	0
54	MG	1H	3588	1/1	0.83	0.21	51,51,51,51	0
54	MG	14	3490	1/1	0.83	0.37	52,52,52,52	0
54	MG	1H	3397	1/1	0.83	0.43	60,60,60,60	0
54	MG	1H	3063	1/1	0.83	0.07	71,71,71,71	0
54	MG	1H	3493	1/1	0.83	0.26	62,62,62,62	0
54	MG	1H	3257	1/1	0.83	0.34	46,46,46,46	0
54	MG	14	3139	1/1	0.83	0.18	46,46,46,46	0
54	MG	14	3009	1/1	0.83	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2360	1/1	0.83	0.24	71,71,71,71	0
54	MG	1H	3041	1/1	0.83	0.14	40,40,40,40	0
54	MG	1H	3427	1/1	0.83	0.20	43,43,43,43	0
54	MG	1G	2350	1/1	0.83	0.17	80,80,80,80	0
54	MG	14	3407	1/1	0.83	0.23	68,68,68,68	0
54	MG	1H	3364	1/1	0.83	0.42	57,57,57,57	0
54	MG	14	3217	1/1	0.83	0.15	58,58,58,58	0
54	MG	1G	2247	1/1	0.83	0.41	74,74,74,74	0
54	MG	1G	2310	1/1	0.83	0.27	75,75,75,75	0
54	MG	1H	3074	1/1	0.83	0.18	43,43,43,43	0
54	MG	1H	3545	1/1	0.83	0.31	66,66,66,66	0
54	MG	14	3341	1/1	0.83	0.18	65,65,65,65	0
54	MG	14	3234	1/1	0.84	0.42	57,57,57,57	0
54	MG	14	3442	1/1	0.84	0.61	73,73,73,73	0
54	MG	14	3443	1/1	0.84	0.17	52,52,52,52	0
54	MG	1H	3475	1/1	0.84	0.23	49,49,49,49	0
54	MG	1H	3575	1/1	0.84	0.13	59,59,59,59	0
54	MG	1G	2223	1/1	0.84	0.21	66,66,66,66	0
54	MG	14	3567	1/1	0.84	0.09	73,73,73,73	0
54	MG	1H	3303	1/1	0.84	0.42	59,59,59,59	0
54	MG	14	3359	1/1	0.84	0.37	62,62,62,62	0
54	MG	1G	2339	1/1	0.84	0.20	76,76,76,76	0
54	MG	13	2228	1/1	0.84	0.26	50,50,50,50	0
54	MG	1H	3174	1/1	0.84	0.39	50,50,50,50	0
54	MG	1H	3091	1/1	0.84	0.14	37,37,37,37	0
54	MG	1G	2246	1/1	0.84	0.21	68,68,68,68	0
54	MG	1H	3217	1/1	0.84	0.21	36,36,36,36	0
54	MG	1H	3222	1/1	0.84	0.24	40,40,40,40	0
54	MG	1H	3225	1/1	0.84	0.17	51,51,51,51	0
54	MG	1H	3135	1/1	0.84	0.20	49,49,49,49	0
54	MG	1H	3242	1/1	0.84	0.19	51,51,51,51	0
54	MG	14	3390	1/1	0.84	0.33	44,44,44,44	0
54	MG	14	3491	1/1	0.84	0.31	52,52,52,52	0
54	MG	14	3166	1/1	0.84	0.15	52,52,52,52	0
54	MG	14	3304	1/1	0.84	0.21	46,46,46,46	0
54	MG	1H	3527	1/1	0.84	0.14	45,45,45,45	0
54	MG	13	2352	1/1	0.84	0.15	52,52,52,52	0
54	MG	1G	2249	1/1	0.84	0.31	66,66,66,66	0
54	MG	1H	3262	1/1	0.84	0.40	68,68,68,68	0
54	MG	14	3513	1/1	0.84	0.46	66,66,66,66	0
54	MG	14	3209	1/1	0.84	0.19	47,47,47,47	0
54	MG	1H	3268	1/1	0.84	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3037	1/1	0.84	0.27	44,44,44,44	0
54	MG	1H	3281	1/1	0.84	0.19	61,61,61,61	0
54	MG	13	2378	1/1	0.84	0.24	73,73,73,73	0
54	MG	1G	2259	1/1	0.84	0.32	80,80,80,80	0
54	MG	14	3537	1/1	0.84	0.26	70,70,70,70	0
54	MG	14	3334	1/1	0.84	0.22	75,75,75,75	0
54	MG	W4	103	1/1	0.84	0.23	81,81,81,81	0
54	MG	1H	3292	1/1	0.84	0.17	45,45,45,45	0
54	MG	14	3337	1/1	0.84	0.43	69,69,69,69	0
54	MG	1H	3471	1/1	0.84	0.17	71,71,71,71	0
54	MG	1H	3520	1/1	0.85	0.18	51,51,51,51	0
54	MG	1H	3404	1/1	0.85	0.30	68,68,68,68	0
54	MG	14	3520	1/1	0.85	0.13	77,77,77,77	0
54	MG	1H	3188	1/1	0.85	0.14	35,35,35,35	0
54	MG	1H	3528	1/1	0.85	0.22	58,58,58,58	0
54	MG	1H	3326	1/1	0.85	0.49	68,68,68,68	0
54	MG	14	3259	1/1	0.85	0.38	46,46,46,46	0
54	MG	14	3530	1/1	0.85	0.19	49,49,49,49	0
54	MG	14	3396	1/1	0.85	0.56	77,77,77,77	0
54	MG	14	3058	1/1	0.85	0.10	50,50,50,50	0
54	MG	1H	3534	1/1	0.85	0.15	43,43,43,43	0
54	MG	1H	3536	1/1	0.85	0.14	43,43,43,43	0
54	MG	1G	2294	1/1	0.85	0.41	75,75,75,75	0
54	MG	13	2358	1/1	0.85	0.11	74,74,74,74	0
54	MG	14	3280	1/1	0.85	0.18	56,56,56,56	0
54	MG	1G	2348	1/1	0.85	0.29	71,71,71,71	0
54	MG	14	3556	1/1	0.85	0.19	59,59,59,59	0
54	MG	13	2322	1/1	0.85	0.43	81,81,81,81	0
54	MG	14	3295	1/1	0.85	0.32	56,56,56,56	0
54	MG	13	2273	1/1	0.85	0.24	62,62,62,62	0
54	MG	14	3085	1/1	0.85	0.08	49,49,49,49	0
54	MG	11	301	1/1	0.85	0.25	34,34,34,34	0
54	MG	16	203	1/1	0.85	0.21	62,62,62,62	0
54	MG	13	2341	1/1	0.85	0.09	89,89,89,89	0
54	MG	16	209	1/1	0.85	0.12	54,54,54,54	0
54	MG	14	3307	1/1	0.85	0.29	71,71,71,71	0
54	MG	13	2292	1/1	0.85	0.23	54,54,54,54	0
54	MG	29	301	1/1	0.85	0.12	52,52,52,52	0
54	MG	14	3434	1/1	0.85	0.25	57,57,57,57	0
54	MG	1H	3448	1/1	0.85	0.17	50,50,50,50	0
54	MG	13	2368	1/1	0.85	0.11	84,84,84,84	0
54	MG	14	3445	1/1	0.85	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3132	1/1	0.85	0.17	65,65,65,65	0
54	MG	13	2344	1/1	0.85	0.16	66,66,66,66	0
54	MG	1G	2374	1/1	0.85	0.49	86,86,86,86	0
54	MG	1G	2323	1/1	0.85	0.36	67,67,67,67	0
54	MG	13	2345	1/1	0.85	0.13	47,47,47,47	0
54	MG	1H	3586	1/1	0.85	0.32	62,62,62,62	0
54	MG	14	3464	1/1	0.85	0.30	53,53,53,53	0
54	MG	13	2243	1/1	0.85	0.30	48,48,48,48	0
54	MG	1G	2240	1/1	0.85	0.40	81,81,81,81	0
54	MG	1H	3387	1/1	0.85	0.40	55,55,55,55	0
54	MG	14	3203	1/1	0.85	0.30	75,75,75,75	0
54	MG	39	302	1/1	0.85	0.18	49,49,49,49	0
54	MG	1H	3161	1/1	0.85	0.29	32,32,32,32	0
54	MG	1G	2242	1/1	0.85	0.62	81,81,81,81	0
54	MG	13	2302	1/1	0.85	0.30	69,69,69,69	0
54	MG	13	2233	1/1	0.85	0.34	84,84,84,84	0
54	MG	14	3015	1/1	0.85	0.16	40,40,40,40	0
54	MG	14	3018	1/1	0.85	0.09	58,58,58,58	0
54	MG	14	3022	1/1	0.85	0.15	45,45,45,45	0
54	MG	14	3362	1/1	0.85	0.15	59,59,59,59	0
54	MG	1H	3312	1/1	0.85	0.19	41,41,41,41	0
54	MG	1H	3508	1/1	0.85	0.32	36,36,36,36	0
54	MG	14	3232	1/1	0.85	0.77	74,74,74,74	0
54	MG	1H	3313	1/1	0.85	0.40	51,51,51,51	0
54	MG	14	3238	1/1	0.85	0.34	60,60,60,60	0
54	MG	1H	3022	1/1	0.85	0.11	45,45,45,45	0
55	ZN	G8	201	1/1	0.85	0.17	95,95,95,95	0
54	MG	13	2330	1/1	0.86	0.22	55,55,55,55	0
54	MG	68	202	1/1	0.86	0.20	63,63,63,63	0
54	MG	14	3043	1/1	0.86	0.11	47,47,47,47	0
54	MG	1H	3486	1/1	0.86	0.28	40,40,40,40	0
54	MG	13	2279	1/1	0.86	0.24	55,55,55,55	0
54	MG	1H	3232	1/1	0.86	0.17	34,34,34,34	0
54	MG	16	210	1/1	0.86	0.20	58,58,58,58	0
54	MG	16	211	1/1	0.86	0.20	59,59,59,59	0
54	MG	14	3389	1/1	0.86	0.17	63,63,63,63	0
54	MG	13	2222	1/1	0.86	0.25	75,75,75,75	0
54	MG	13	2282	1/1	0.86	0.30	57,57,57,57	0
54	MG	14	3205	1/1	0.86	0.53	61,61,61,61	0
54	MG	13	2212	1/1	0.86	0.08	89,89,89,89	0
54	MG	1H	3369	1/1	0.86	0.30	71,71,71,71	0
54	MG	1H	3500	1/1	0.86	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3504	1/1	0.86	0.11	55,55,55,55	0
54	MG	1H	3370	1/1	0.86	0.35	62,62,62,62	0
54	MG	14	3066	1/1	0.86	0.07	86,86,86,86	0
54	MG	1H	3317	1/1	0.86	0.24	56,56,56,56	0
54	MG	78	201	1/1	0.86	0.13	47,47,47,47	0
54	MG	14	3326	1/1	0.86	0.22	70,70,70,70	0
54	MG	13	2324	1/1	0.86	0.14	63,63,63,63	0
54	MG	14	3074	1/1	0.86	0.12	52,52,52,52	0
54	MG	13	2325	1/1	0.86	0.43	77,77,77,77	0
54	MG	14	3079	1/1	0.86	0.06	54,54,54,54	0
54	MG	14	3413	1/1	0.86	0.21	79,79,79,79	0
54	MG	1H	3278	1/1	0.86	0.28	48,48,48,48	0
54	MG	14	3243	1/1	0.86	0.55	76,76,76,76	0
54	MG	14	3084	1/1	0.86	0.14	54,54,54,54	0
54	MG	13	2382	1/1	0.86	0.17	60,60,60,60	0
54	MG	41	201	1/1	0.86	0.16	68,68,68,68	0
54	MG	49	201	1/1	0.86	0.18	86,86,86,86	0
54	MG	14	3534	1/1	0.86	0.18	70,70,70,70	0
54	MG	13	2365	1/1	0.86	0.27	75,75,75,75	0
54	MG	W1	103	1/1	0.86	0.22	73,73,73,73	0
54	MG	14	3254	1/1	0.86	0.45	66,66,66,66	0
54	MG	13	2275	1/1	0.86	0.19	75,75,75,75	0
54	MG	1H	3465	1/1	0.86	0.35	47,47,47,47	0
54	MG	1H	3008	1/1	0.86	0.07	40,40,40,40	0
54	MG	14	3260	1/1	0.86	0.14	41,41,41,41	0
54	MG	1H	3535	1/1	0.86	0.29	39,39,39,39	0
54	MG	X1	109	1/1	0.86	0.09	71,71,71,71	0
54	MG	14	3452	1/1	0.86	0.18	59,59,59,59	0
54	MG	1H	3343	1/1	0.86	0.28	50,50,50,50	0
54	MG	13	2244	1/1	0.86	0.21	45,45,45,45	0
54	MG	1H	3477	1/1	0.86	0.28	51,51,51,51	0
54	MG	1H	3299	1/1	0.86	0.26	53,53,53,53	0
54	MG	14	3495	1/1	0.87	0.45	64,64,64,64	0
54	MG	14	3036	1/1	0.87	0.10	53,53,53,53	0
54	MG	1G	2367	1/1	0.87	0.29	92,92,92,92	0
54	MG	1G	2264	1/1	0.87	0.36	94,94,94,94	0
54	MG	1H	3411	1/1	0.87	0.21	50,50,50,50	0
54	MG	1H	3076	1/1	0.87	0.12	62,62,62,62	0
54	MG	13	2240	1/1	0.87	0.55	74,74,74,74	0
54	MG	14	3412	1/1	0.87	0.35	73,73,73,73	0
54	MG	1H	3419	1/1	0.87	0.16	63,63,63,63	0
54	MG	14	3344	1/1	0.87	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3262	1/1	0.87	0.15	53,53,53,53	0
54	MG	1G	2373	1/1	0.87	0.12	94,94,94,94	0
54	MG	1H	3367	1/1	0.87	0.20	57,57,57,57	0
54	MG	1H	3574	1/1	0.87	0.33	58,58,58,58	0
54	MG	I8	102	1/1	0.87	0.31	61,61,61,61	0
54	MG	1H	3080	1/1	0.87	0.08	58,58,58,58	0
54	MG	1H	3429	1/1	0.87	0.14	41,41,41,41	0
54	MG	13	2210	1/1	0.87	0.13	82,82,82,82	0
54	MG	14	3207	1/1	0.87	0.41	63,63,63,63	0
54	MG	E5	201	1/1	0.87	0.13	55,55,55,55	0
54	MG	1G	2376	1/1	0.87	0.25	99,99,99,99	0
54	MG	14	3210	1/1	0.87	0.22	50,50,50,50	0
54	MG	13	2366	1/1	0.87	0.25	65,65,65,65	0
54	MG	1H	3031	1/1	0.87	0.12	49,49,49,49	0
54	MG	1G	2299	1/1	0.87	0.17	60,60,60,60	0
54	MG	45	202	1/1	0.87	0.23	65,65,65,65	0
54	MG	1G	2363	1/1	0.87	0.28	92,92,92,92	0
54	MG	6A	101	1/1	0.87	0.51	86,86,86,86	0
54	MG	A5	201	1/1	0.87	0.45	45,45,45,45	0
54	MG	1H	3334	1/1	0.87	0.30	50,50,50,50	0
54	MG	1H	3127	1/1	0.87	0.17	60,60,60,60	0
54	MG	14	3310	1/1	0.87	0.13	59,59,59,59	0
54	MG	1H	3464	1/1	0.87	0.23	53,53,53,53	0
54	MG	1G	2331	1/1	0.87	0.43	72,72,72,72	0
54	MG	14	3478	1/1	0.87	0.26	60,60,60,60	0
54	MG	14	3233	1/1	0.87	0.13	58,58,58,58	0
54	MG	21	303	1/1	0.87	0.23	72,72,72,72	0
54	MG	1H	3295	1/1	0.87	0.26	49,49,49,49	0
54	MG	1H	3297	1/1	0.87	0.16	51,51,51,51	0
54	MG	1H	3473	1/1	0.87	0.09	48,48,48,48	0
54	MG	16	205	1/1	0.87	0.44	58,58,58,58	0
54	MG	14	3402	1/1	0.87	0.22	70,70,70,70	0
54	MG	3E	302	1/1	0.87	0.47	84,84,84,84	0
54	MG	1H	3350	1/1	0.87	0.26	57,57,57,57	0
54	MG	14	3324	1/1	0.88	0.23	67,67,67,67	0
54	MG	1G	2225	1/1	0.88	0.40	72,72,72,72	0
54	MG	14	3421	1/1	0.88	0.40	42,42,42,42	0
54	MG	1H	3220	1/1	0.88	0.28	44,44,44,44	0
54	MG	14	3431	1/1	0.88	0.33	57,57,57,57	0
54	MG	14	3432	1/1	0.88	0.10	55,55,55,55	0
54	MG	14	3566	1/1	0.88	0.09	68,68,68,68	0
54	MG	1G	2365	1/1	0.88	0.47	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3551	1/1	0.88	0.19	57,57,57,57	0
54	MG	1H	3470	1/1	0.88	0.30	43,43,43,43	0
54	MG	14	3228	1/1	0.88	0.52	65,65,65,65	0
54	MG	14	3444	1/1	0.88	0.25	62,62,62,62	0
54	MG	13	2340	1/1	0.88	0.16	52,52,52,52	0
54	MG	1G	2342	1/1	0.88	0.24	73,73,73,73	0
54	MG	16	207	1/1	0.88	0.39	53,53,53,53	0
54	MG	1H	3020	1/1	0.88	0.16	39,39,39,39	0
54	MG	1H	3236	1/1	0.88	0.11	62,62,62,62	0
54	MG	14	3073	1/1	0.88	0.27	53,53,53,53	0
54	MG	1H	3137	1/1	0.88	0.21	42,42,42,42	0
54	MG	14	3454	1/1	0.88	0.23	72,72,72,72	0
54	MG	25	202	1/1	0.88	0.12	67,67,67,67	0
54	MG	1G	2320	1/1	0.88	0.22	70,70,70,70	0
54	MG	14	3245	1/1	0.88	0.28	64,64,64,64	0
54	MG	14	3355	1/1	0.88	0.16	61,61,61,61	0
54	MG	14	3078	1/1	0.88	0.13	46,46,46,46	0
54	MG	14	3467	1/1	0.88	0.26	66,66,66,66	0
54	MG	1G	2344	1/1	0.88	0.20	76,76,76,76	0
54	MG	1J	209	1/1	0.88	0.05	69,69,69,69	0
54	MG	1H	3338	1/1	0.88	0.10	48,48,48,48	0
54	MG	14	3253	1/1	0.88	0.49	55,55,55,55	0
54	MG	14	3477	1/1	0.88	0.56	64,64,64,64	0
54	MG	1G	2321	1/1	0.88	0.38	75,75,75,75	0
54	MG	1H	3583	1/1	0.88	0.28	53,53,53,53	0
54	MG	1H	3407	1/1	0.88	0.32	65,65,65,65	0
54	MG	14	3369	1/1	0.88	0.33	62,62,62,62	0
54	MG	1H	3410	1/1	0.88	0.12	57,57,57,57	0
54	MG	1G	2305	1/1	0.88	0.10	77,77,77,77	0
54	MG	14	3489	1/1	0.88	0.21	49,49,49,49	0
54	MG	1H	3272	1/1	0.88	0.13	47,47,47,47	0
54	MG	14	3117	1/1	0.88	0.15	64,64,64,64	0
54	MG	14	3494	1/1	0.88	0.59	62,62,62,62	0
54	MG	39	301	1/1	0.88	0.32	74,74,74,74	0
54	MG	1H	3414	1/1	0.88	0.24	62,62,62,62	0
54	MG	1H	3157	1/1	0.88	0.30	61,61,61,61	0
54	MG	1H	3035	1/1	0.88	0.14	60,60,60,60	0
54	MG	1G	2236	1/1	0.88	0.30	70,70,70,70	0
54	MG	41	202	1/1	0.88	0.25	73,73,73,73	0
54	MG	1H	3353	1/1	0.88	0.44	57,57,57,57	0
54	MG	13	2262	1/1	0.88	0.13	70,70,70,70	0
54	MG	14	3161	1/1	0.88	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2272	1/1	0.88	0.15	54,54,54,54	0
54	MG	55	202	1/1	0.88	0.13	57,57,57,57	0
54	MG	14	3398	1/1	0.88	0.30	75,75,75,75	0
54	MG	1H	3291	1/1	0.88	0.32	68,68,68,68	0
54	MG	1H	3525	1/1	0.88	0.16	43,43,43,43	0
54	MG	14	3401	1/1	0.88	0.51	73,73,73,73	0
54	MG	14	3183	1/1	0.88	0.40	57,57,57,57	0
54	MG	14	3305	1/1	0.88	0.15	52,52,52,52	0
54	MG	1G	2337	1/1	0.88	0.13	70,70,70,70	0
54	MG	13	2343	1/1	0.88	0.14	62,62,62,62	0
54	MG	1H	3177	1/1	0.88	0.38	46,46,46,46	0
54	MG	1H	3445	1/1	0.88	0.22	73,73,73,73	0
54	MG	W4	101	1/1	0.88	0.22	88,88,88,88	0
54	MG	3I	201	1/1	0.88	0.25	52,52,52,52	0
54	MG	1G	2360	1/1	0.88	0.11	68,68,68,68	0
54	MG	1H	3209	1/1	0.88	0.23	52,52,52,52	0
54	MG	14	3321	1/1	0.88	0.16	68,68,68,68	0
54	MG	1H	3004	1/1	0.88	0.10	40,40,40,40	0
54	MG	14	3439	1/1	0.89	0.47	77,77,77,77	0
54	MG	13	2223	1/1	0.89	0.36	48,48,48,48	0
54	MG	13	2334	1/1	0.89	0.24	85,85,85,85	0
54	MG	1G	2203	1/1	0.89	0.43	68,68,68,68	0
54	MG	14	3047	1/1	0.89	0.08	64,64,64,64	0
54	MG	1H	3371	1/1	0.89	0.17	60,60,60,60	0
54	MG	1H	3530	1/1	0.89	0.25	48,48,48,48	0
54	MG	14	3230	1/1	0.89	0.16	67,67,67,67	0
54	MG	1H	3375	1/1	0.89	0.39	53,53,53,53	0
54	MG	14	3351	1/1	0.89	0.29	61,61,61,61	0
54	MG	1G	2251	1/1	0.89	0.24	67,67,67,67	0
54	MG	14	3459	1/1	0.89	0.17	49,49,49,49	0
54	MG	1H	3229	1/1	0.89	0.14	52,52,52,52	0
54	MG	1G	2209	1/1	0.89	0.10	68,68,68,68	0
54	MG	14	3463	1/1	0.89	0.23	65,65,65,65	0
54	MG	1H	3541	1/1	0.89	0.14	52,52,52,52	0
54	MG	1G	2298	1/1	0.89	0.21	71,71,71,71	0
54	MG	14	3061	1/1	0.89	0.11	48,48,48,48	0
54	MG	1J	202	1/1	0.89	0.10	79,79,79,79	0
54	MG	13	2237	1/1	0.89	0.19	61,61,61,61	0
54	MG	1H	3320	1/1	0.89	0.33	46,46,46,46	0
54	MG	1H	3546	1/1	0.89	0.35	69,69,69,69	0
54	MG	1J	207	1/1	0.89	0.10	80,80,80,80	0
54	MG	1G	2340	1/1	0.89	0.42	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3375	1/1	0.89	0.15	71,71,71,71	0
54	MG	13	2353	1/1	0.89	0.22	60,60,60,60	0
54	MG	1J	212	1/1	0.89	0.08	81,81,81,81	0
54	MG	1H	3260	1/1	0.89	0.27	37,37,37,37	0
54	MG	13	2250	1/1	0.89	0.31	70,70,70,70	0
54	MG	1H	3336	1/1	0.89	0.13	45,45,45,45	0
54	MG	1H	3563	1/1	0.89	0.47	57,57,57,57	0
54	MG	1H	3400	1/1	0.89	0.38	66,66,66,66	0
54	MG	1H	3036	1/1	0.89	0.06	48,48,48,48	0
54	MG	1H	3481	1/1	0.89	0.27	57,57,57,57	0
54	MG	13	2311	1/1	0.89	0.32	71,71,71,71	0
54	MG	14	3089	1/1	0.89	0.11	56,56,56,56	0
54	MG	14	3395	1/1	0.89	0.24	67,67,67,67	0
54	MG	1H	3487	1/1	0.89	0.13	54,54,54,54	0
54	MG	1H	3406	1/1	0.89	0.45	63,63,63,63	0
54	MG	1H	3578	1/1	0.89	0.36	75,75,75,75	0
54	MG	1H	3276	1/1	0.89	0.34	57,57,57,57	0
54	MG	88	301	1/1	0.89	0.12	59,59,59,59	0
54	MG	1G	2268	1/1	0.89	0.12	77,77,77,77	0
54	MG	14	3120	1/1	0.89	0.19	45,45,45,45	0
54	MG	1H	3165	1/1	0.89	0.32	46,46,46,46	0
54	MG	13	2289	1/1	0.89	0.39	71,71,71,71	0
54	MG	13	2326	1/1	0.89	0.31	59,59,59,59	0
54	MG	1H	3499	1/1	0.89	0.30	49,49,49,49	0
54	MG	1H	3051	1/1	0.89	0.08	59,59,59,59	0
54	MG	B8	201	1/1	0.89	0.13	60,60,60,60	0
54	MG	14	3408	1/1	0.89	0.26	52,52,52,52	0
54	MG	13	2298	1/1	0.89	0.52	87,87,87,87	0
54	MG	C5	203	1/1	0.89	0.36	86,86,86,86	0
54	MG	14	3005	1/1	0.89	0.24	51,51,51,51	0
54	MG	1H	3506	1/1	0.89	0.31	59,59,59,59	0
54	MG	13	2214	1/1	0.89	0.15	88,88,88,88	0
54	MG	13	2300	1/1	0.89	0.26	76,76,76,76	0
54	MG	1G	2244	1/1	0.89	0.30	72,72,72,72	0
54	MG	1H	3517	1/1	0.89	0.18	53,53,53,53	0
54	MG	1H	3212	1/1	0.89	0.20	35,35,35,35	0
54	MG	14	3551	1/1	0.89	0.17	47,47,47,47	0
54	MG	14	3552	1/1	0.89	0.12	49,49,49,49	0
54	MG	1H	3430	1/1	0.89	0.32	56,56,56,56	0
54	MG	1H	3094	1/1	0.89	0.48	36,36,36,36	0
54	MG	X4	104	1/1	0.89	0.23	91,91,91,91	0
54	MG	1H	3524	1/1	0.89	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3560	1/1	0.89	0.22	51,51,51,51	0
54	MG	14	3218	1/1	0.89	0.24	50,50,50,50	0
54	MG	1G	2333	1/1	0.90	0.32	85,85,85,85	0
54	MG	1H	3421	1/1	0.90	0.26	62,62,62,62	0
54	MG	14	3318	1/1	0.90	0.10	78,78,78,78	0
54	MG	14	3319	1/1	0.90	0.11	67,67,67,67	0
54	MG	14	3422	1/1	0.90	0.26	66,66,66,66	0
54	MG	1G	2297	1/1	0.90	0.15	90,90,90,90	0
54	MG	14	3006	1/1	0.90	0.10	46,46,46,46	0
54	MG	1H	3513	1/1	0.90	0.43	63,63,63,63	0
54	MG	13	2303	1/1	0.90	0.09	70,70,70,70	0
54	MG	1H	3282	1/1	0.90	0.44	61,61,61,61	0
54	MG	13	2354	1/1	0.90	0.11	70,70,70,70	0
54	MG	21	301	1/1	0.90	0.28	40,40,40,40	0
54	MG	14	3440	1/1	0.90	0.33	61,61,61,61	0
54	MG	4I	201	1/1	0.90	0.06	75,75,75,75	0
54	MG	14	3441	1/1	0.90	0.11	76,76,76,76	0
54	MG	1H	3172	1/1	0.90	0.35	36,36,36,36	0
54	MG	14	3330	1/1	0.90	0.08	76,76,76,76	0
54	MG	1H	3432	1/1	0.90	0.15	43,43,43,43	0
54	MG	1H	3433	1/1	0.90	0.29	45,45,45,45	0
54	MG	1H	3289	1/1	0.90	0.40	56,56,56,56	0
54	MG	14	3215	1/1	0.90	0.23	49,49,49,49	0
54	MG	13	2285	1/1	0.90	0.07	72,72,72,72	0
54	MG	16	213	1/1	0.90	0.30	66,66,66,66	0
54	MG	14	3039	1/1	0.90	0.08	43,43,43,43	0
54	MG	1G	2304	1/1	0.90	0.59	85,85,85,85	0
54	MG	13	2308	1/1	0.90	0.21	78,78,78,78	0
54	MG	14	3044	1/1	0.90	0.07	75,75,75,75	0
54	MG	14	3345	1/1	0.90	0.09	60,60,60,60	0
54	MG	1G	2378	1/1	0.90	0.33	81,81,81,81	0
54	MG	13	2268	1/1	0.90	0.25	55,55,55,55	0
54	MG	1H	3088	1/1	0.90	0.09	37,37,37,37	0
54	MG	14	3050	1/1	0.90	0.07	61,61,61,61	0
54	MG	14	3356	1/1	0.90	0.30	51,51,51,51	0
54	MG	1H	3089	1/1	0.90	0.20	38,38,38,38	0
54	MG	1H	3537	1/1	0.90	0.35	60,60,60,60	0
54	MG	1H	3462	1/1	0.90	0.16	53,53,53,53	0
54	MG	13	2312	1/1	0.90	0.41	52,52,52,52	0
54	MG	13	2363	1/1	0.90	0.08	76,76,76,76	0
54	MG	1H	3310	1/1	0.90	0.15	30,30,30,30	0
54	MG	14	3480	1/1	0.90	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1G	2282	1/1	0.90	0.41	75,75,75,75	0
54	MG	1H	3469	1/1	0.90	0.29	47,47,47,47	0
54	MG	1H	3055	1/1	0.90	0.19	56,56,56,56	0
54	MG	13	2271	1/1	0.90	0.29	65,65,65,65	0
54	MG	1G	2349	1/1	0.90	0.12	83,83,83,83	0
54	MG	13	2225	1/1	0.90	0.24	67,67,67,67	0
54	MG	14	3384	1/1	0.90	0.24	47,47,47,47	0
54	MG	1H	3556	1/1	0.90	0.16	59,59,59,59	0
54	MG	1H	3233	1/1	0.90	0.16	36,36,36,36	0
54	MG	13	2329	1/1	0.90	0.32	73,73,73,73	0
54	MG	14	3077	1/1	0.90	0.05	59,59,59,59	0
54	MG	1H	3399	1/1	0.90	0.21	55,55,55,55	0
54	MG	1H	3570	1/1	0.90	0.16	51,51,51,51	0
54	MG	14	3508	1/1	0.90	0.09	57,57,57,57	0
54	MG	1H	3241	1/1	0.90	0.25	48,48,48,48	0
54	MG	1G	2248	1/1	0.90	0.44	61,61,61,61	0
54	MG	1H	3243	1/1	0.90	0.23	59,59,59,59	0
54	MG	14	3514	1/1	0.90	0.11	60,60,60,60	0
54	MG	14	3515	1/1	0.90	0.17	60,60,60,60	0
54	MG	14	3275	1/1	0.90	0.13	46,46,46,46	0
54	MG	13	2257	1/1	0.90	0.27	82,82,82,82	0
54	MG	14	3518	1/1	0.90	0.29	86,86,86,86	0
54	MG	13	2283	1/1	0.90	0.17	63,63,63,63	0
54	MG	1H	3408	1/1	0.90	0.26	51,51,51,51	0
54	MG	14	3284	1/1	0.90	0.38	82,82,82,82	0
54	MG	1H	3146	1/1	0.90	0.39	55,55,55,55	0
54	MG	14	3527	1/1	0.90	0.15	52,52,52,52	0
54	MG	1H	3017	1/1	0.90	0.19	41,41,41,41	0
54	MG	14	3106	1/1	0.90	0.29	52,52,52,52	0
54	MG	13	2265	1/1	0.90	0.27	51,51,51,51	0
54	MG	1H	3585	1/1	0.90	0.26	39,39,39,39	0
54	MG	1H	3496	1/1	0.90	0.17	52,52,52,52	0
54	MG	1H	3587	1/1	0.90	0.14	47,47,47,47	0
54	MG	1H	3497	1/1	0.90	0.23	50,50,50,50	0
54	MG	X4	101	1/1	0.90	0.20	91,91,91,91	0
54	MG	13	2373	1/1	0.90	0.16	88,88,88,88	0
54	MG	14	3546	1/1	0.90	0.22	42,42,42,42	0
54	MG	1H	3069	1/1	0.90	0.22	45,45,45,45	0
54	MG	1H	3418	1/1	0.90	0.29	54,54,54,54	0
54	MG	11	305	1/1	0.91	0.25	31,31,31,31	0
54	MG	14	3559	1/1	0.91	0.27	70,70,70,70	0
54	MG	14	3437	1/1	0.91	0.60	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3001	1/1	0.91	0.47	57,57,57,57	0
54	MG	14	3564	1/1	0.91	0.10	50,50,50,50	0
54	MG	1G	2322	1/1	0.91	0.34	63,63,63,63	0
54	MG	1H	3416	1/1	0.91	0.48	72,72,72,72	0
54	MG	13	2221	1/1	0.91	0.23	63,63,63,63	0
54	MG	1H	3261	1/1	0.91	0.19	39,39,39,39	0
54	MG	1H	3344	1/1	0.91	0.14	42,42,42,42	0
54	MG	14	3206	1/1	0.91	0.52	57,57,57,57	0
54	MG	1G	2361	1/1	0.91	0.19	92,92,92,92	0
54	MG	14	3208	1/1	0.91	0.31	50,50,50,50	0
54	MG	1H	3158	1/1	0.91	0.23	61,61,61,61	0
54	MG	1H	3270	1/1	0.91	0.17	55,55,55,55	0
54	MG	1G	2291	1/1	0.91	0.52	79,79,79,79	0
54	MG	1H	3021	1/1	0.91	0.11	46,46,46,46	0
54	MG	13	2269	1/1	0.91	0.26	57,57,57,57	0
54	MG	1G	2250	1/1	0.91	0.33	66,66,66,66	0
54	MG	1H	3359	1/1	0.91	0.41	54,54,54,54	0
54	MG	13	2348	1/1	0.91	0.22	58,58,58,58	0
54	MG	1H	3531	1/1	0.91	0.18	52,52,52,52	0
54	MG	13	2362	1/1	0.91	0.15	77,77,77,77	0
54	MG	13	2256	1/1	0.91	0.37	64,64,64,64	0
54	MG	14	3048	1/1	0.91	0.25	43,43,43,43	0
54	MG	14	3470	1/1	0.91	0.12	51,51,51,51	0
54	MG	13	2245	1/1	0.91	0.14	49,49,49,49	0
54	MG	13	2332	1/1	0.91	0.19	58,58,58,58	0
54	MG	14	3474	1/1	0.91	0.47	50,50,50,50	0
54	MG	1H	3038	1/1	0.91	0.06	51,51,51,51	0
54	MG	1H	3459	1/1	0.91	0.13	44,44,44,44	0
54	MG	1H	3194	1/1	0.91	0.47	46,46,46,46	0
54	MG	14	3365	1/1	0.91	0.17	56,56,56,56	0
54	MG	1G	2375	1/1	0.91	0.16	85,85,85,85	0
54	MG	13	2319	1/1	0.91	0.35	77,77,77,77	0
54	MG	1H	3210	1/1	0.91	0.22	44,44,44,44	0
54	MG	1H	3547	1/1	0.91	0.12	41,41,41,41	0
54	MG	14	3488	1/1	0.91	0.18	55,55,55,55	0
54	MG	1G	2266	1/1	0.91	0.11	71,71,71,71	0
54	MG	1H	3381	1/1	0.91	0.45	58,58,58,58	0
54	MG	14	3252	1/1	0.91	0.25	62,62,62,62	0
54	MG	1H	3552	1/1	0.91	0.14	52,52,52,52	0
54	MG	1H	3046	1/1	0.91	0.24	38,38,38,38	0
54	MG	1H	3384	1/1	0.91	0.23	57,57,57,57	0
54	MG	14	3498	1/1	0.91	0.34	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1G	2229	1/1	0.91	0.30	84,84,84,84	0
54	MG	1H	3557	1/1	0.91	0.19	45,45,45,45	0
54	MG	1H	3305	1/1	0.91	0.24	46,46,46,46	0
54	MG	14	3076	1/1	0.91	0.21	55,55,55,55	0
54	MG	1H	3306	1/1	0.91	0.24	36,36,36,36	0
54	MG	1H	3565	1/1	0.91	0.19	67,67,67,67	0
54	MG	13	2355	1/1	0.91	0.31	65,65,65,65	0
54	MG	1G	2237	1/1	0.91	0.20	70,70,70,70	0
54	MG	1H	3394	1/1	0.91	0.23	55,55,55,55	0
54	MG	1H	3097	1/1	0.91	0.28	38,38,38,38	0
54	MG	1H	3102	1/1	0.91	0.24	41,41,41,41	0
54	MG	13	2384	1/1	0.91	0.13	70,70,70,70	0
54	MG	14	3289	1/1	0.91	0.31	63,63,63,63	0
54	MG	55	201	1/1	0.91	0.25	53,53,53,53	0
54	MG	1H	3130	1/1	0.91	0.53	71,71,71,71	0
54	MG	1H	3489	1/1	0.91	0.21	53,53,53,53	0
54	MG	14	3292	1/1	0.91	0.15	39,39,39,39	0
54	MG	14	3293	1/1	0.91	0.28	57,57,57,57	0
54	MG	1G	2277	1/1	0.91	0.33	56,56,56,56	0
54	MG	1H	3234	1/1	0.91	0.17	39,39,39,39	0
54	MG	14	3111	1/1	0.91	0.17	41,41,41,41	0
54	MG	1H	3405	1/1	0.91	0.12	62,62,62,62	0
54	MG	13	2296	1/1	0.91	0.37	110,110,110,110	0
54	MG	1H	3494	1/1	0.91	0.35	62,62,62,62	0
54	MG	13	2369	1/1	0.91	0.19	51,51,51,51	0
54	MG	1H	3007	1/1	0.91	0.08	72,72,72,72	0
54	MG	14	3128	1/1	0.91	0.30	39,39,39,39	0
54	MG	1H	3409	1/1	0.91	0.14	30,30,30,30	0
54	MG	13	2371	1/1	0.91	0.26	92,92,92,92	0
54	MG	14	3317	1/1	0.91	0.41	79,79,79,79	0
54	MG	1H	3597	1/1	0.91	0.20	45,45,45,45	0
54	MG	1H	3335	1/1	0.91	0.54	75,75,75,75	0
54	MG	1H	3246	1/1	0.91	0.48	58,58,58,58	0
54	MG	1H	3048	1/1	0.92	0.05	42,42,42,42	0
54	MG	1G	2332	1/1	0.92	0.28	64,64,64,64	0
54	MG	1H	3533	1/1	0.92	0.23	46,46,46,46	0
54	MG	1H	3349	1/1	0.92	0.22	39,39,39,39	0
54	MG	14	3239	1/1	0.92	0.30	58,58,58,58	0
54	MG	13	2379	1/1	0.92	0.28	68,68,68,68	0
54	MG	14	3242	1/1	0.92	0.31	59,59,59,59	0
54	MG	1H	3351	1/1	0.92	0.29	71,71,71,71	0
54	MG	1G	2335	1/1	0.92	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3437	1/1	0.92	0.38	73,73,73,73	0
54	MG	14	3248	1/1	0.92	0.22	54,54,54,54	0
54	MG	1G	2256	1/1	0.92	0.25	67,67,67,67	0
54	MG	14	3545	1/1	0.92	0.30	47,47,47,47	0
54	MG	13	2218	1/1	0.92	0.19	58,58,58,58	0
54	MG	1H	3145	1/1	0.92	0.30	45,45,45,45	0
54	MG	1G	2224	1/1	0.92	0.41	72,72,72,72	0
54	MG	1H	3361	1/1	0.92	0.16	51,51,51,51	0
54	MG	1H	3273	1/1	0.92	0.37	60,60,60,60	0
54	MG	14	3553	1/1	0.92	0.17	60,60,60,60	0
54	MG	1H	3548	1/1	0.92	0.07	51,51,51,51	0
54	MG	14	3067	1/1	0.92	0.12	43,43,43,43	0
54	MG	1H	3150	1/1	0.92	0.29	51,51,51,51	0
54	MG	14	3069	1/1	0.92	0.04	70,70,70,70	0
54	MG	13	2286	1/1	0.92	0.35	59,59,59,59	0
54	MG	14	3071	1/1	0.92	0.19	54,54,54,54	0
54	MG	14	3072	1/1	0.92	0.18	52,52,52,52	0
54	MG	14	3272	1/1	0.92	0.26	67,67,67,67	0
54	MG	14	3274	1/1	0.92	0.55	59,59,59,59	0
54	MG	1H	3279	1/1	0.92	0.17	40,40,40,40	0
54	MG	1H	3154	1/1	0.92	0.25	37,37,37,37	0
54	MG	13	2383	1/1	0.92	0.24	70,70,70,70	0
54	MG	1H	3555	1/1	0.92	0.37	53,53,53,53	0
54	MG	13	2315	1/1	0.92	0.34	67,67,67,67	0
54	MG	13	2264	1/1	0.92	0.47	74,74,74,74	0
54	MG	13	2220	1/1	0.92	0.24	60,60,60,60	0
54	MG	14	3430	1/1	0.92	0.28	46,46,46,46	0
54	MG	1H	3562	1/1	0.92	0.23	56,56,56,56	0
54	MG	1H	3065	1/1	0.92	0.10	70,70,70,70	0
54	MG	3E	303	1/1	0.92	0.20	81,81,81,81	0
54	MG	14	3294	1/1	0.92	0.32	62,62,62,62	0
54	MG	14	3087	1/1	0.92	0.13	49,49,49,49	0
54	MG	1H	3380	1/1	0.92	0.38	55,55,55,55	0
54	MG	14	3299	1/1	0.92	0.27	57,57,57,57	0
54	MG	13	2266	1/1	0.92	0.14	77,77,77,77	0
54	MG	13	2280	1/1	0.92	0.44	63,63,63,63	0
54	MG	1H	3170	1/1	0.92	0.35	32,32,32,32	0
54	MG	13	2236	1/1	0.92	0.17	54,54,54,54	0
54	MG	42	201	1/1	0.92	0.12	92,92,92,92	0
54	MG	14	3094	1/1	0.92	0.31	50,50,50,50	0
54	MG	1G	2280	1/1	0.92	0.24	62,62,62,62	0
54	MG	1H	3390	1/1	0.92	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1G	2314	1/1	0.92	0.35	74,74,74,74	0
54	MG	1G	2281	1/1	0.92	0.16	70,70,70,70	0
54	MG	1H	3580	1/1	0.92	0.44	58,58,58,58	0
54	MG	1G	2352	1/1	0.92	0.36	65,65,65,65	0
54	MG	1G	2353	1/1	0.92	0.48	65,65,65,65	0
54	MG	1H	3395	1/1	0.92	0.47	72,72,72,72	0
54	MG	14	3134	1/1	0.92	0.35	53,53,53,53	0
54	MG	1G	2354	1/1	0.92	0.37	62,62,62,62	0
54	MG	1G	2317	1/1	0.92	0.33	91,91,91,91	0
54	MG	1G	2205	1/1	0.92	0.19	71,71,71,71	0
54	MG	14	3466	1/1	0.92	0.10	68,68,68,68	0
54	MG	1H	3084	1/1	0.92	0.07	41,41,41,41	0
54	MG	1G	2206	1/1	0.92	0.09	80,80,80,80	0
54	MG	1H	3218	1/1	0.92	0.41	48,48,48,48	0
54	MG	1H	3030	1/1	0.92	0.07	48,48,48,48	0
54	MG	14	3180	1/1	0.92	0.51	65,65,65,65	0
54	MG	1G	2207	1/1	0.92	0.10	70,70,70,70	0
54	MG	14	3190	1/1	0.92	0.19	38,38,38,38	0
54	MG	1H	3503	1/1	0.92	0.23	52,52,52,52	0
54	MG	14	3339	1/1	0.92	0.22	46,46,46,46	0
54	MG	14	3340	1/1	0.92	0.14	54,54,54,54	0
54	MG	14	3193	1/1	0.92	0.31	49,49,49,49	0
54	MG	14	3201	1/1	0.92	0.24	42,42,42,42	0
54	MG	L8	101	1/1	0.92	0.34	54,54,54,54	0
54	MG	1H	3322	1/1	0.92	0.34	58,58,58,58	0
54	MG	14	3487	1/1	0.92	0.23	45,45,45,45	0
54	MG	13	2206	1/1	0.92	0.06	79,79,79,79	0
54	MG	1H	3327	1/1	0.92	0.20	54,54,54,54	0
54	MG	14	3348	1/1	0.92	0.28	59,59,59,59	0
54	MG	13	2213	1/1	0.92	0.18	62,62,62,62	0
54	MG	1H	3512	1/1	0.92	0.43	56,56,56,56	0
54	MG	14	3354	1/1	0.92	0.46	68,68,68,68	0
54	MG	1G	2289	1/1	0.92	0.22	80,80,80,80	0
54	MG	1H	3412	1/1	0.92	0.20	49,49,49,49	0
54	MG	14	3211	1/1	0.92	0.30	44,44,44,44	0
54	MG	1H	3333	1/1	0.92	0.21	46,46,46,46	0
54	MG	14	3502	1/1	0.92	0.23	51,51,51,51	0
54	MG	1G	2329	1/1	0.92	0.24	87,87,87,87	0
54	MG	1G	2369	1/1	0.92	0.12	82,82,82,82	0
54	MG	14	3363	1/1	0.92	0.35	63,63,63,63	0
54	MG	X1	108	1/1	0.92	0.17	77,77,77,77	0
54	MG	14	3510	1/1	0.92	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2209	1/1	0.92	0.07	67,67,67,67	0
54	MG	1H	3111	1/1	0.92	0.33	45,45,45,45	0
54	MG	1H	3114	1/1	0.92	0.34	43,43,43,43	0
54	MG	1H	3118	1/1	0.92	0.34	38,38,38,38	0
54	MG	14	3041	1/1	0.92	0.13	44,44,44,44	0
54	MG	14	3042	1/1	0.92	0.11	51,51,51,51	0
54	MG	1G	2371	1/1	0.92	0.14	58,58,58,58	0
54	MG	1G	2252	1/1	0.92	0.54	78,78,78,78	0
54	MG	1H	3248	1/1	0.93	0.40	56,56,56,56	0
54	MG	1H	3075	1/1	0.93	0.30	48,48,48,48	0
54	MG	1H	3422	1/1	0.93	0.14	45,45,45,45	0
53	8UZ	13	2202	33/33	0.93	0.14	70,70,70,70	0
54	MG	1H	3259	1/1	0.93	0.31	49,49,49,49	0
54	MG	14	3366	1/1	0.93	0.14	53,53,53,53	0
54	MG	1H	3156	1/1	0.93	0.32	42,42,42,42	0
54	MG	2A	201	1/1	0.93	0.15	74,74,74,74	0
54	MG	13	2254	1/1	0.93	0.12	64,64,64,64	0
54	MG	14	3373	1/1	0.93	0.23	46,46,46,46	0
54	MG	14	3374	1/1	0.93	0.21	70,70,70,70	0
54	MG	1H	3265	1/1	0.93	0.30	58,58,58,58	0
54	MG	14	3052	1/1	0.93	0.08	50,50,50,50	0
54	MG	14	3378	1/1	0.93	0.25	59,59,59,59	0
54	MG	1H	3267	1/1	0.93	0.10	44,44,44,44	0
54	MG	14	3533	1/1	0.93	0.32	58,58,58,58	0
54	MG	14	3054	1/1	0.93	0.08	48,48,48,48	0
54	MG	13	2295	1/1	0.93	0.14	65,65,65,65	0
54	MG	14	3538	1/1	0.93	0.40	74,74,74,74	0
54	MG	14	3240	1/1	0.93	0.27	59,59,59,59	0
54	MG	14	3540	1/1	0.93	0.35	81,81,81,81	0
54	MG	1H	3269	1/1	0.93	0.55	46,46,46,46	0
54	MG	1G	2258	1/1	0.93	0.21	82,82,82,82	0
54	MG	1H	3356	1/1	0.93	0.25	45,45,45,45	0
54	MG	13	2276	1/1	0.93	0.31	62,62,62,62	0
54	MG	1H	3443	1/1	0.93	0.30	52,52,52,52	0
54	MG	1G	2238	1/1	0.93	0.24	69,69,69,69	0
54	MG	1H	3275	1/1	0.93	0.40	51,51,51,51	0
54	MG	1G	2239	1/1	0.93	0.27	82,82,82,82	0
54	MG	1H	3450	1/1	0.93	0.18	50,50,50,50	0
54	MG	1H	3453	1/1	0.93	0.25	43,43,43,43	0
54	MG	1H	3457	1/1	0.93	0.37	35,35,35,35	0
54	MG	14	3555	1/1	0.93	0.35	71,71,71,71	0
54	MG	1H	3086	1/1	0.93	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3169	1/1	0.93	0.23	36,36,36,36	0
54	MG	1H	3087	1/1	0.93	0.06	45,45,45,45	0
54	MG	19	302	1/1	0.93	0.34	55,55,55,55	0
54	MG	14	3561	1/1	0.93	0.20	60,60,60,60	0
54	MG	1H	3047	1/1	0.93	0.09	37,37,37,37	0
54	MG	1H	3284	1/1	0.93	0.15	44,44,44,44	0
54	MG	1H	3175	1/1	0.93	0.45	57,57,57,57	0
54	MG	1H	3566	1/1	0.93	0.14	48,48,48,48	0
54	MG	13	2304	1/1	0.93	0.24	55,55,55,55	0
54	MG	68	201	1/1	0.93	0.19	62,62,62,62	0
54	MG	13	2347	1/1	0.93	0.17	57,57,57,57	0
54	MG	1G	2267	1/1	0.93	0.17	81,81,81,81	0
54	MG	13	2336	1/1	0.93	0.45	54,54,54,54	0
54	MG	1H	3200	1/1	0.93	0.35	37,37,37,37	0
54	MG	1H	3296	1/1	0.93	0.49	77,77,77,77	0
54	MG	1H	3202	1/1	0.93	0.21	38,38,38,38	0
54	MG	1H	3385	1/1	0.93	0.22	61,61,61,61	0
54	MG	1H	3386	1/1	0.93	0.18	65,65,65,65	0
54	MG	1H	3205	1/1	0.93	0.28	45,45,45,45	0
54	MG	13	2277	1/1	0.93	0.14	66,66,66,66	0
54	MG	14	3425	1/1	0.93	0.28	54,54,54,54	0
54	MG	14	3099	1/1	0.93	0.32	45,45,45,45	0
54	MG	14	3105	1/1	0.93	0.31	63,63,63,63	0
54	MG	1H	3100	1/1	0.93	0.24	43,43,43,43	0
54	MG	1G	2270	1/1	0.93	0.45	67,67,67,67	0
54	MG	14	3297	1/1	0.93	0.12	61,61,61,61	0
54	MG	14	3298	1/1	0.93	0.57	69,69,69,69	0
54	MG	13	2258	1/1	0.93	0.21	76,76,76,76	0
54	MG	1G	2301	1/1	0.93	0.27	88,88,88,88	0
54	MG	14	3303	1/1	0.93	0.34	62,62,62,62	0
54	MG	1H	3013	1/1	0.93	0.12	52,52,52,52	0
54	MG	1H	3589	1/1	0.93	0.18	45,45,45,45	0
54	MG	14	3124	1/1	0.93	0.24	67,67,67,67	0
54	MG	1G	2302	1/1	0.93	0.17	86,86,86,86	0
54	MG	1H	3311	1/1	0.93	0.14	34,34,34,34	0
54	MG	14	3309	1/1	0.93	0.43	39,39,39,39	0
54	MG	1H	3016	1/1	0.93	0.09	40,40,40,40	0
54	MG	1H	3398	1/1	0.93	0.11	55,55,55,55	0
54	MG	1G	2336	1/1	0.93	0.30	72,72,72,72	0
54	MG	14	3316	1/1	0.93	0.20	59,59,59,59	0
54	MG	14	3456	1/1	0.93	0.15	56,56,56,56	0
54	MG	14	3457	1/1	0.93	0.49	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3147	1/1	0.93	0.43	53,53,53,53	0
54	MG	1G	2218	1/1	0.93	0.38	54,54,54,54	0
54	MG	14	3156	1/1	0.93	0.41	41,41,41,41	0
54	MG	1G	2274	1/1	0.93	0.23	63,63,63,63	0
54	MG	14	3163	1/1	0.93	0.38	44,44,44,44	0
54	MG	14	3165	1/1	0.93	0.30	52,52,52,52	0
54	MG	11	302	1/1	0.93	0.24	46,46,46,46	0
54	MG	1H	3141	1/1	0.93	0.52	67,67,67,67	0
54	MG	14	3468	1/1	0.93	0.20	66,66,66,66	0
54	MG	14	3171	1/1	0.93	0.29	40,40,40,40	0
54	MG	14	3327	1/1	0.93	0.58	66,66,66,66	0
54	MG	14	3471	1/1	0.93	0.25	62,62,62,62	0
54	MG	1H	3023	1/1	0.93	0.10	39,39,39,39	0
54	MG	14	3178	1/1	0.93	0.45	61,61,61,61	0
54	MG	1H	3323	1/1	0.93	0.34	62,62,62,62	0
54	MG	14	3475	1/1	0.93	0.25	64,64,64,64	0
54	MG	14	3476	1/1	0.93	0.17	57,57,57,57	0
54	MG	1H	3235	1/1	0.93	0.66	76,76,76,76	0
54	MG	14	3184	1/1	0.93	0.21	45,45,45,45	0
54	MG	14	3012	1/1	0.93	0.18	43,43,43,43	0
54	MG	14	3336	1/1	0.93	0.30	51,51,51,51	0
54	MG	14	3013	1/1	0.93	0.15	41,41,41,41	0
54	MG	14	3338	1/1	0.93	0.24	63,63,63,63	0
54	MG	W1	101	1/1	0.93	0.32	64,64,64,64	0
54	MG	1G	2306	1/1	0.93	0.12	76,76,76,76	0
54	MG	1H	3237	1/1	0.93	0.51	50,50,50,50	0
54	MG	1H	3329	1/1	0.93	0.14	46,46,46,46	0
54	MG	14	3021	1/1	0.93	0.11	45,45,45,45	0
54	MG	1H	3239	1/1	0.93	0.45	59,59,59,59	0
54	MG	14	3025	1/1	0.93	0.10	45,45,45,45	0
54	MG	14	3028	1/1	0.93	0.07	59,59,59,59	0
54	MG	14	3030	1/1	0.93	0.10	42,42,42,42	0
54	MG	1H	3070	1/1	0.93	0.15	36,36,36,36	0
54	MG	1G	2279	1/1	0.93	0.22	76,76,76,76	0
54	MG	14	3352	1/1	0.93	0.26	74,74,74,74	0
54	MG	1H	3148	1/1	0.93	0.45	30,30,30,30	0
54	MG	13	2255	1/1	0.93	0.34	53,53,53,53	0
54	MG	14	3216	1/1	0.93	0.29	56,56,56,56	0
54	MG	1H	3417	1/1	0.93	0.33	38,38,38,38	0
54	MG	1H	3247	1/1	0.93	0.21	46,46,46,46	0
54	MG	14	3219	1/1	0.93	0.70	53,53,53,53	0
54	MG	1H	3594	1/1	0.94	0.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2247	1/1	0.94	0.27	61,61,61,61	0
54	MG	1G	2271	1/1	0.94	0.28	81,81,81,81	0
54	MG	14	3167	1/1	0.94	0.33	39,39,39,39	0
54	MG	1G	2368	1/1	0.94	0.22	82,82,82,82	0
54	MG	1G	2334	1/1	0.94	0.21	86,86,86,86	0
54	MG	14	3173	1/1	0.94	0.52	60,60,60,60	0
54	MG	14	3503	1/1	0.94	0.12	45,45,45,45	0
54	MG	1H	3230	1/1	0.94	0.50	62,62,62,62	0
54	MG	13	2349	1/1	0.94	0.30	53,53,53,53	0
54	MG	1H	3309	1/1	0.94	0.24	37,37,37,37	0
54	MG	14	3181	1/1	0.94	0.37	41,41,41,41	0
54	MG	1G	2300	1/1	0.94	0.26	86,86,86,86	0
54	MG	13	2208	1/1	0.94	0.17	78,78,78,78	0
54	MG	14	3187	1/1	0.94	0.23	47,47,47,47	0
54	MG	1H	3152	1/1	0.94	0.20	41,41,41,41	0
54	MG	14	3010	1/1	0.94	0.08	42,42,42,42	0
54	MG	13	2351	1/1	0.94	0.33	59,59,59,59	0
54	MG	14	3194	1/1	0.94	0.24	52,52,52,52	0
54	MG	14	3519	1/1	0.94	0.11	71,71,71,71	0
54	MG	14	3198	1/1	0.94	0.49	40,40,40,40	0
54	MG	1G	2275	1/1	0.94	0.27	52,52,52,52	0
54	MG	1G	2276	1/1	0.94	0.25	82,82,82,82	0
54	MG	14	3523	1/1	0.94	0.21	52,52,52,52	0
54	MG	14	3524	1/1	0.94	0.17	65,65,65,65	0
54	MG	1H	3505	1/1	0.94	0.37	66,66,66,66	0
54	MG	1H	3402	1/1	0.94	0.17	40,40,40,40	0
54	MG	13	2270	1/1	0.94	0.19	59,59,59,59	0
54	MG	1G	2278	1/1	0.94	0.44	81,81,81,81	0
54	MG	14	3531	1/1	0.94	0.09	59,59,59,59	0
54	MG	1H	3511	1/1	0.94	0.36	56,56,56,56	0
54	MG	14	3026	1/1	0.94	0.20	41,41,41,41	0
54	MG	13	2313	1/1	0.94	0.20	78,78,78,78	0
54	MG	1H	3245	1/1	0.94	0.43	49,49,49,49	0
54	MG	1H	3514	1/1	0.94	0.32	57,57,57,57	0
54	MG	1H	3515	1/1	0.94	0.38	38,38,38,38	0
54	MG	14	3371	1/1	0.94	0.15	50,50,50,50	0
54	MG	1H	3160	1/1	0.94	0.34	53,53,53,53	0
54	MG	13	2260	1/1	0.94	0.27	63,63,63,63	0
54	MG	1H	3162	1/1	0.94	0.42	55,55,55,55	0
54	MG	1H	3519	1/1	0.94	0.13	34,34,34,34	0
54	MG	14	3547	1/1	0.94	0.13	48,48,48,48	0
54	MG	1H	3250	1/1	0.94	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1H	3330	1/1	0.94	0.22	51,51,51,51	0
54	MG	1H	3523	1/1	0.94	0.09	42,42,42,42	0
54	MG	14	3224	1/1	0.94	0.43	55,55,55,55	0
54	MG	1H	3252	1/1	0.94	0.25	47,47,47,47	0
54	MG	14	3226	1/1	0.94	0.34	64,64,64,64	0
54	MG	14	3227	1/1	0.94	0.31	51,51,51,51	0
54	MG	1H	3332	1/1	0.94	0.35	75,75,75,75	0
54	MG	1G	2227	1/1	0.94	0.06	67,67,67,67	0
54	MG	1G	2312	1/1	0.94	0.11	63,63,63,63	0
54	MG	1H	3258	1/1	0.94	0.39	55,55,55,55	0
54	MG	13	2251	1/1	0.94	0.21	62,62,62,62	0
54	MG	19	303	1/1	0.94	0.30	37,37,37,37	0
54	MG	14	3237	1/1	0.94	0.30	56,56,56,56	0
54	MG	1H	3339	1/1	0.94	0.40	62,62,62,62	0
54	MG	1H	3168	1/1	0.94	0.17	34,34,34,34	0
54	MG	1G	2283	1/1	0.94	0.13	68,68,68,68	0
54	MG	1H	3263	1/1	0.94	0.50	65,65,65,65	0
54	MG	1H	3426	1/1	0.94	0.37	56,56,56,56	0
54	MG	1H	3538	1/1	0.94	0.10	45,45,45,45	0
54	MG	13	2252	1/1	0.94	0.48	68,68,68,68	0
54	MG	1H	3266	1/1	0.94	0.30	46,46,46,46	0
54	MG	1G	2231	1/1	0.94	0.39	57,57,57,57	0
54	MG	14	3064	1/1	0.94	0.15	68,68,68,68	0
54	MG	1H	3347	1/1	0.94	0.23	36,36,36,36	0
54	MG	1G	2233	1/1	0.94	0.42	59,59,59,59	0
54	MG	13	2217	1/1	0.94	0.20	66,66,66,66	0
54	MG	1H	3103	1/1	0.94	0.30	42,42,42,42	0
54	MG	14	3255	1/1	0.94	0.27	57,57,57,57	0
54	MG	1H	3271	1/1	0.94	0.41	57,57,57,57	0
54	MG	1H	3178	1/1	0.94	0.26	46,46,46,46	0
54	MG	1H	3181	1/1	0.94	0.51	37,37,37,37	0
54	MG	1H	3182	1/1	0.94	0.12	39,39,39,39	0
54	MG	1H	3357	1/1	0.94	0.14	58,58,58,58	0
54	MG	1H	3183	1/1	0.94	0.29	43,43,43,43	0
54	MG	1H	3277	1/1	0.94	0.33	51,51,51,51	0
54	MG	1H	3186	1/1	0.94	0.19	38,38,38,38	0
54	MG	14	3270	1/1	0.94	0.23	78,78,78,78	0
54	MG	1H	3363	1/1	0.94	0.12	57,57,57,57	0
54	MG	1H	3452	1/1	0.94	0.29	52,52,52,52	0
54	MG	1H	3107	1/1	0.94	0.36	33,33,33,33	0
54	MG	14	3436	1/1	0.94	0.14	39,39,39,39	0
54	MG	13	2229	1/1	0.94	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3564	1/1	0.94	0.28	47,47,47,47	0
54	MG	14	3086	1/1	0.94	0.10	49,49,49,49	0
54	MG	14	3281	1/1	0.94	0.28	61,61,61,61	0
54	MG	13	2331	1/1	0.94	0.15	69,69,69,69	0
54	MG	14	3285	1/1	0.94	0.22	59,59,59,59	0
54	MG	14	3286	1/1	0.94	0.13	40,40,40,40	0
54	MG	14	3288	1/1	0.94	0.26	43,43,43,43	0
54	MG	13	2361	1/1	0.94	0.27	81,81,81,81	0
54	MG	I8	101	1/1	0.94	0.29	43,43,43,43	0
54	MG	1H	3283	1/1	0.94	0.36	76,76,76,76	0
54	MG	14	3449	1/1	0.94	0.11	53,53,53,53	0
54	MG	31	303	1/1	0.94	0.12	63,63,63,63	0
54	MG	1H	3568	1/1	0.94	0.09	61,61,61,61	0
54	MG	1H	3569	1/1	0.94	0.13	47,47,47,47	0
54	MG	1G	2357	1/1	0.94	0.12	74,74,74,74	0
54	MG	1H	3285	1/1	0.94	0.47	69,69,69,69	0
54	MG	14	3098	1/1	0.94	0.28	46,46,46,46	0
54	MG	1H	3372	1/1	0.94	0.17	54,54,54,54	0
54	MG	14	3102	1/1	0.94	0.35	45,45,45,45	0
54	MG	52	201	1/1	0.94	0.20	63,63,63,63	0
54	MG	1H	3466	1/1	0.94	0.35	65,65,65,65	0
54	MG	88	302	1/1	0.94	0.10	58,58,58,58	0
54	MG	14	3461	1/1	0.94	0.30	70,70,70,70	0
54	MG	1H	3373	1/1	0.94	0.15	55,55,55,55	0
54	MG	14	3107	1/1	0.94	0.39	55,55,55,55	0
54	MG	14	3108	1/1	0.94	0.23	47,47,47,47	0
54	MG	1H	3374	1/1	0.94	0.26	36,36,36,36	0
54	MG	14	3112	1/1	0.94	0.29	47,47,47,47	0
54	MG	14	3116	1/1	0.94	0.31	70,70,70,70	0
54	MG	1H	3129	1/1	0.94	0.29	49,49,49,49	0
54	MG	1G	2359	1/1	0.94	0.48	62,62,62,62	0
54	MG	14	3119	1/1	0.94	0.39	39,39,39,39	0
54	MG	1H	3377	1/1	0.94	0.30	51,51,51,51	0
54	MG	14	3313	1/1	0.94	0.16	50,50,50,50	0
54	MG	1H	3581	1/1	0.94	0.27	54,54,54,54	0
54	MG	13	2306	1/1	0.94	0.38	46,46,46,46	0
54	MG	1H	3134	1/1	0.94	0.12	43,43,43,43	0
53	8UZ	1G	2202	33/33	0.94	0.14	78,78,78,78	0
54	MG	14	3130	1/1	0.94	0.34	48,48,48,48	0
54	MG	1H	3293	1/1	0.94	0.11	37,37,37,37	0
54	MG	14	3136	1/1	0.94	0.21	44,44,44,44	0
54	MG	X1	106	1/1	0.94	0.29	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3138	1/1	0.94	0.28	47,47,47,47	0
54	MG	1H	3480	1/1	0.94	0.18	46,46,46,46	0
54	MG	1H	3214	1/1	0.94	0.23	44,44,44,44	0
54	MG	1G	2243	1/1	0.94	0.51	76,76,76,76	0
54	MG	14	3484	1/1	0.94	0.13	62,62,62,62	0
54	MG	1H	3139	1/1	0.94	0.19	37,37,37,37	0
54	MG	14	3152	1/1	0.94	0.28	53,53,53,53	0
54	MG	14	3155	1/1	0.94	0.41	39,39,39,39	0
54	MG	1G	2296	1/1	0.94	0.14	69,69,69,69	0
54	MG	14	3157	1/1	0.94	0.25	45,45,45,45	0
54	MG	1H	3593	1/1	0.94	0.36	46,46,46,46	0
55	ZN	C5	201	1/1	0.94	0.19	110,110,110,110	0
54	MG	1H	3467	1/1	0.95	0.21	37,37,37,37	0
54	MG	1G	2257	1/1	0.95	0.29	66,66,66,66	0
54	MG	1H	3155	1/1	0.95	0.28	56,56,56,56	0
54	MG	14	3358	1/1	0.95	0.13	46,46,46,46	0
54	MG	1G	2325	1/1	0.95	0.33	71,71,71,71	0
54	MG	14	3360	1/1	0.95	0.46	59,59,59,59	0
54	MG	1H	3039	1/1	0.95	0.09	41,41,41,41	0
54	MG	13	2249	1/1	0.95	0.34	56,56,56,56	0
54	MG	14	3229	1/1	0.95	0.30	64,64,64,64	0
54	MG	1H	3474	1/1	0.95	0.17	51,51,51,51	0
54	MG	14	3080	1/1	0.95	0.13	60,60,60,60	0
54	MG	1G	2327	1/1	0.95	0.10	69,69,69,69	0
54	MG	1H	3571	1/1	0.95	0.09	57,57,57,57	0
54	MG	13	2357	1/1	0.95	0.20	59,59,59,59	0
54	MG	14	3236	1/1	0.95	0.24	56,56,56,56	0
54	MG	1H	3316	1/1	0.95	0.14	40,40,40,40	0
54	MG	14	3372	1/1	0.95	0.33	62,62,62,62	0
54	MG	1H	3044	1/1	0.95	0.12	38,38,38,38	0
54	MG	1G	2260	1/1	0.95	0.31	77,77,77,77	0
54	MG	14	3526	1/1	0.95	0.26	50,50,50,50	0
54	MG	1G	2219	1/1	0.95	0.26	59,59,59,59	0
54	MG	1H	3092	1/1	0.95	0.09	54,54,54,54	0
54	MG	1H	3321	1/1	0.95	0.14	44,44,44,44	0
54	MG	1G	2358	1/1	0.95	0.11	68,68,68,68	0
54	MG	14	3532	1/1	0.95	0.27	59,59,59,59	0
54	MG	14	3093	1/1	0.95	0.38	40,40,40,40	0
54	MG	1H	3249	1/1	0.95	0.36	44,44,44,44	0
54	MG	1H	3324	1/1	0.95	0.12	59,59,59,59	0
54	MG	1H	3049	1/1	0.95	0.08	35,35,35,35	0
54	MG	1H	3095	1/1	0.95	0.34	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3253	1/1	0.95	0.40	63,63,63,63	0
54	MG	1H	3096	1/1	0.95	0.30	37,37,37,37	0
54	MG	14	3391	1/1	0.95	0.26	47,47,47,47	0
54	MG	1G	2222	1/1	0.95	0.08	66,66,66,66	0
54	MG	1H	3005	1/1	0.95	0.15	41,41,41,41	0
54	MG	14	3256	1/1	0.95	0.20	38,38,38,38	0
54	MG	14	3109	1/1	0.95	0.29	44,44,44,44	0
54	MG	14	3110	1/1	0.95	0.27	56,56,56,56	0
54	MG	13	2205	1/1	0.95	0.13	64,64,64,64	0
53	8UZ	1G	2201	33/33	0.95	0.18	65,65,65,65	0
54	MG	14	3113	1/1	0.95	0.14	63,63,63,63	0
54	MG	14	3115	1/1	0.95	0.19	54,54,54,54	0
54	MG	1H	3592	1/1	0.95	0.19	57,57,57,57	0
54	MG	14	3266	1/1	0.95	0.28	46,46,46,46	0
54	MG	14	3267	1/1	0.95	0.23	53,53,53,53	0
54	MG	1H	3009	1/1	0.95	0.12	50,50,50,50	0
54	MG	1H	3502	1/1	0.95	0.17	52,52,52,52	0
54	MG	1H	3109	1/1	0.95	0.29	38,38,38,38	0
54	MG	1H	3179	1/1	0.95	0.35	55,55,55,55	0
54	MG	1H	3337	1/1	0.95	0.30	55,55,55,55	0
54	MG	1G	2362	1/1	0.95	0.31	91,91,91,91	0
54	MG	14	3277	1/1	0.95	0.24	46,46,46,46	0
54	MG	1H	3112	1/1	0.95	0.41	36,36,36,36	0
54	MG	14	3127	1/1	0.95	0.30	66,66,66,66	0
54	MG	1H	3113	1/1	0.95	0.36	34,34,34,34	0
54	MG	14	3416	1/1	0.95	0.17	46,46,46,46	0
54	MG	1H	3510	1/1	0.95	0.61	48,48,48,48	0
54	MG	14	3419	1/1	0.95	0.45	41,41,41,41	0
54	MG	14	3131	1/1	0.95	0.44	44,44,44,44	0
54	MG	14	3133	1/1	0.95	0.34	49,49,49,49	0
54	MG	16	202	1/1	0.95	0.34	64,64,64,64	0
54	MG	1G	2307	1/1	0.95	0.51	70,70,70,70	0
54	MG	14	3424	1/1	0.95	0.36	44,44,44,44	0
54	MG	1H	3187	1/1	0.95	0.14	35,35,35,35	0
54	MG	16	206	1/1	0.95	0.52	52,52,52,52	0
54	MG	14	3426	1/1	0.95	0.42	56,56,56,56	0
54	MG	14	3429	1/1	0.95	0.24	50,50,50,50	0
54	MG	1H	3012	1/1	0.95	0.12	36,36,36,36	0
54	MG	1H	3190	1/1	0.95	0.42	38,38,38,38	0
54	MG	1H	3192	1/1	0.95	0.38	38,38,38,38	0
53	8UZ	13	2201	33/33	0.95	0.23	55,55,55,55	0
54	MG	1H	3420	1/1	0.95	0.33	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3435	1/1	0.95	0.26	58,58,58,58	0
54	MG	1H	3348	1/1	0.95	0.22	47,47,47,47	0
54	MG	29	303	1/1	0.95	0.10	51,51,51,51	0
54	MG	1H	3274	1/1	0.95	0.45	56,56,56,56	0
54	MG	14	3019	1/1	0.95	0.12	50,50,50,50	0
54	MG	1H	3423	1/1	0.95	0.23	55,55,55,55	0
54	MG	14	3159	1/1	0.95	0.38	43,43,43,43	0
54	MG	14	3300	1/1	0.95	0.23	67,67,67,67	0
54	MG	14	3301	1/1	0.95	0.23	65,65,65,65	0
54	MG	1J	206	1/1	0.95	0.21	75,75,75,75	0
54	MG	1H	3195	1/1	0.95	0.18	34,34,34,34	0
54	MG	1H	3196	1/1	0.95	0.36	35,35,35,35	0
54	MG	14	3164	1/1	0.95	0.30	49,49,49,49	0
54	MG	1H	3352	1/1	0.95	0.37	61,61,61,61	0
54	MG	13	2259	1/1	0.95	0.37	55,55,55,55	0
54	MG	14	3450	1/1	0.95	0.16	57,57,57,57	0
54	MG	1H	3526	1/1	0.95	0.20	56,56,56,56	0
54	MG	13	2274	1/1	0.95	0.17	50,50,50,50	0
54	MG	14	3170	1/1	0.95	0.40	42,42,42,42	0
54	MG	1G	2290	1/1	0.95	0.27	70,70,70,70	0
54	MG	14	3455	1/1	0.95	0.18	60,60,60,60	0
54	MG	14	3312	1/1	0.95	0.40	64,64,64,64	0
54	MG	1H	3431	1/1	0.95	0.15	45,45,45,45	0
54	MG	31	302	1/1	0.95	0.12	56,56,56,56	0
54	MG	14	3458	1/1	0.95	0.22	70,70,70,70	0
54	MG	1H	3204	1/1	0.95	0.24	40,40,40,40	0
54	MG	13	2242	1/1	0.95	0.33	59,59,59,59	0
54	MG	1H	3532	1/1	0.95	0.23	41,41,41,41	0
54	MG	1G	2230	1/1	0.95	0.15	57,57,57,57	0
54	MG	1H	3435	1/1	0.95	0.10	40,40,40,40	0
54	MG	13	2337	1/1	0.95	0.37	56,56,56,56	0
54	MG	1G	2316	1/1	0.95	0.10	58,58,58,58	0
54	MG	1H	3025	1/1	0.95	0.14	39,39,39,39	0
54	MG	14	3191	1/1	0.95	0.22	60,60,60,60	0
54	MG	14	3323	1/1	0.95	0.15	46,46,46,46	0
54	MG	1H	3213	1/1	0.95	0.47	34,34,34,34	0
54	MG	1H	3539	1/1	0.95	0.25	76,76,76,76	0
54	MG	1G	2232	1/1	0.95	0.29	52,52,52,52	0
54	MG	14	3196	1/1	0.95	0.24	68,68,68,68	0
54	MG	45	201	1/1	0.95	0.20	53,53,53,53	0
54	MG	14	3197	1/1	0.95	0.26	45,45,45,45	0
54	MG	14	3329	1/1	0.95	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3366	1/1	0.95	0.22	68,68,68,68	0
54	MG	1H	3216	1/1	0.95	0.20	48,48,48,48	0
54	MG	K8	101	1/1	0.95	0.17	57,57,57,57	0
54	MG	14	3332	1/1	0.95	0.19	52,52,52,52	0
54	MG	1H	3543	1/1	0.95	0.17	44,44,44,44	0
54	MG	1G	2318	1/1	0.95	0.21	73,73,73,73	0
54	MG	1H	3143	1/1	0.95	0.38	64,64,64,64	0
54	MG	1H	3451	1/1	0.95	0.40	37,37,37,37	0
54	MG	13	2346	1/1	0.95	0.18	56,56,56,56	0
54	MG	1G	2234	1/1	0.95	0.25	66,66,66,66	0
54	MG	1H	3454	1/1	0.95	0.35	41,41,41,41	0
54	MG	1H	3077	1/1	0.95	0.09	43,43,43,43	0
54	MG	14	3486	1/1	0.95	0.10	55,55,55,55	0
54	MG	1H	3147	1/1	0.95	0.27	54,54,54,54	0
54	MG	14	3212	1/1	0.95	0.49	59,59,59,59	0
54	MG	14	3213	1/1	0.95	0.32	52,52,52,52	0
54	MG	1H	3032	1/1	0.95	0.14	43,43,43,43	0
54	MG	1H	3461	1/1	0.95	0.12	51,51,51,51	0
54	MG	14	3492	1/1	0.95	0.20	42,42,42,42	0
54	MG	1H	3033	1/1	0.95	0.06	46,46,46,46	0
54	MG	1H	3301	1/1	0.95	0.45	69,69,69,69	0
54	MG	14	3349	1/1	0.95	0.26	63,63,63,63	0
54	MG	X4	102	1/1	0.95	0.43	79,79,79,79	0
54	MG	14	3497	1/1	0.95	0.13	59,59,59,59	0
54	MG	1H	3231	1/1	0.95	0.16	35,35,35,35	0
54	MG	1H	3558	1/1	0.95	0.26	56,56,56,56	0
54	MG	1G	2254	1/1	0.95	0.43	62,62,62,62	0
54	MG	1G	2213	1/1	0.95	0.05	60,60,60,60	0
54	MG	14	3544	1/1	0.96	0.17	57,57,57,57	0
54	MG	13	2318	1/1	0.96	0.43	68,68,68,68	0
54	MG	1H	3302	1/1	0.96	0.42	44,44,44,44	0
54	MG	1H	3073	1/1	0.96	0.15	44,44,44,44	0
54	MG	1H	3256	1/1	0.96	0.33	69,69,69,69	0
54	MG	1H	3043	1/1	0.96	0.08	45,45,45,45	0
54	MG	14	3438	1/1	0.96	0.18	64,64,64,64	0
54	MG	14	3114	1/1	0.96	0.27	36,36,36,36	0
54	MG	13	2309	1/1	0.96	0.23	54,54,54,54	0
54	MG	13	2215	1/1	0.96	0.10	63,63,63,63	0
54	MG	14	3027	1/1	0.96	0.14	40,40,40,40	0
54	MG	1H	3484	1/1	0.96	0.18	52,52,52,52	0
54	MG	14	3557	1/1	0.96	0.08	68,68,68,68	0
54	MG	14	3029	1/1	0.96	0.04	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3550	1/1	0.96	0.27	58,58,58,58	0
54	MG	14	3121	1/1	0.96	0.24	57,57,57,57	0
54	MG	14	3031	1/1	0.96	0.12	52,52,52,52	0
54	MG	1H	3485	1/1	0.96	0.20	52,52,52,52	0
54	MG	14	3563	1/1	0.96	0.15	65,65,65,65	0
54	MG	1H	3362	1/1	0.96	0.30	59,59,59,59	0
54	MG	1G	2324	1/1	0.96	0.17	60,60,60,60	0
54	MG	1G	2208	1/1	0.96	0.07	70,70,70,70	0
54	MG	B5	101	1/1	0.96	0.49	63,63,63,63	0
54	MG	1G	2261	1/1	0.96	0.40	95,95,95,95	0
54	MG	1H	3264	1/1	0.96	0.35	52,52,52,52	0
54	MG	1H	3314	1/1	0.96	0.33	44,44,44,44	0
54	MG	21	302	1/1	0.96	0.18	47,47,47,47	0
54	MG	14	3350	1/1	0.96	0.13	77,77,77,77	0
54	MG	14	3135	1/1	0.96	0.29	45,45,45,45	0
54	MG	1H	3559	1/1	0.96	0.08	61,61,61,61	0
54	MG	14	3045	1/1	0.96	0.12	64,64,64,64	0
54	MG	1H	3560	1/1	0.96	0.36	69,69,69,69	0
54	MG	14	3142	1/1	0.96	0.37	51,51,51,51	0
54	MG	14	3145	1/1	0.96	0.35	60,60,60,60	0
54	MG	1H	3315	1/1	0.96	0.36	68,68,68,68	0
54	MG	1H	3425	1/1	0.96	0.13	46,46,46,46	0
54	MG	14	3148	1/1	0.96	0.45	45,45,45,45	0
54	MG	1H	3024	1/1	0.96	0.12	40,40,40,40	0
54	MG	1H	3053	1/1	0.96	0.10	36,36,36,36	0
54	MG	16	212	1/1	0.96	0.13	67,67,67,67	0
54	MG	1H	3083	1/1	0.96	0.23	50,50,50,50	0
54	MG	1H	3498	1/1	0.96	0.32	52,52,52,52	0
54	MG	1H	3219	1/1	0.96	0.35	44,44,44,44	0
54	MG	1G	2328	1/1	0.96	0.45	69,69,69,69	0
54	MG	14	3160	1/1	0.96	0.25	54,54,54,54	0
54	MG	29	302	1/1	0.96	0.33	47,47,47,47	0
54	MG	13	2203	1/1	0.96	0.06	80,80,80,80	0
54	MG	1H	3223	1/1	0.96	0.40	48,48,48,48	0
54	MG	13	2267	1/1	0.96	0.40	82,82,82,82	0
54	MG	1J	201	1/1	0.96	0.20	78,78,78,78	0
54	MG	14	3370	1/1	0.96	0.25	43,43,43,43	0
54	MG	14	3273	1/1	0.96	0.13	46,46,46,46	0
54	MG	1H	3001	1/1	0.96	0.39	33,33,33,33	0
54	MG	1H	3227	1/1	0.96	0.38	44,44,44,44	0
54	MG	1H	3228	1/1	0.96	0.40	45,45,45,45	0
54	MG	13	2305	1/1	0.96	0.40	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3376	1/1	0.96	0.12	51,51,51,51	0
54	MG	11	304	1/1	0.96	0.29	48,48,48,48	0
54	MG	1H	3006	1/1	0.96	0.06	45,45,45,45	0
54	MG	1J	211	1/1	0.96	0.19	73,73,73,73	0
54	MG	14	3379	1/1	0.96	0.09	67,67,67,67	0
54	MG	14	3380	1/1	0.96	0.28	57,57,57,57	0
54	MG	14	3172	1/1	0.96	0.30	48,48,48,48	0
54	MG	1H	3180	1/1	0.96	0.21	52,52,52,52	0
54	MG	14	3175	1/1	0.96	0.71	72,72,72,72	0
54	MG	78	203	1/1	0.96	0.65	40,40,40,40	0
54	MG	1H	3444	1/1	0.96	0.12	50,50,50,50	0
54	MG	14	3287	1/1	0.96	0.24	56,56,56,56	0
54	MG	14	3387	1/1	0.96	0.11	64,64,64,64	0
54	MG	1H	3062	1/1	0.96	0.07	51,51,51,51	0
54	MG	14	3179	1/1	0.96	0.39	53,53,53,53	0
54	MG	1H	3582	1/1	0.96	0.29	71,71,71,71	0
54	MG	1H	3034	1/1	0.96	0.04	47,47,47,47	0
54	MG	1G	2215	1/1	0.96	0.15	71,71,71,71	0
54	MG	14	3500	1/1	0.96	0.20	42,42,42,42	0
54	MG	1H	3449	1/1	0.96	0.18	48,48,48,48	0
54	MG	1H	3389	1/1	0.96	0.34	55,55,55,55	0
54	MG	14	3188	1/1	0.96	0.31	53,53,53,53	0
54	MG	1G	2217	1/1	0.96	0.24	66,66,66,66	0
54	MG	14	3505	1/1	0.96	0.13	64,64,64,64	0
54	MG	14	3506	1/1	0.96	0.15	91,91,91,91	0
54	MG	14	3507	1/1	0.96	0.14	50,50,50,50	0
54	MG	13	2231	1/1	0.96	0.18	64,64,64,64	0
54	MG	1G	2285	1/1	0.96	0.30	67,67,67,67	0
54	MG	1H	3189	1/1	0.96	0.14	32,32,32,32	0
54	MG	1H	3455	1/1	0.96	0.39	36,36,36,36	0
54	MG	1H	3456	1/1	0.96	0.34	62,62,62,62	0
54	MG	14	3082	1/1	0.96	0.15	47,47,47,47	0
54	MG	13	2241	1/1	0.96	0.33	45,45,45,45	0
54	MG	14	3199	1/1	0.96	0.25	47,47,47,47	0
54	MG	1H	3288	1/1	0.96	0.33	55,55,55,55	0
54	MG	1H	3341	1/1	0.96	0.54	61,61,61,61	0
54	MG	1H	3151	1/1	0.96	0.26	42,42,42,42	0
54	MG	1H	3290	1/1	0.96	0.42	39,39,39,39	0
54	MG	1H	3244	1/1	0.96	0.37	33,33,33,33	0
54	MG	1H	3193	1/1	0.96	0.33	46,46,46,46	0
54	MG	14	3311	1/1	0.96	0.35	71,71,71,71	0
54	MG	1H	3098	1/1	0.96	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3002	1/1	0.96	0.15	41,41,41,41	0
54	MG	14	3415	1/1	0.96	0.25	59,59,59,59	0
54	MG	14	3004	1/1	0.96	0.11	48,48,48,48	0
54	MG	14	3528	1/1	0.96	0.21	66,66,66,66	0
54	MG	1H	3294	1/1	0.96	0.17	37,37,37,37	0
54	MG	1H	3099	1/1	0.96	0.30	36,36,36,36	0
54	MG	14	3097	1/1	0.96	0.28	41,41,41,41	0
54	MG	14	3007	1/1	0.96	0.11	43,43,43,43	0
54	MG	13	2246	1/1	0.96	0.36	62,62,62,62	0
54	MG	14	3101	1/1	0.96	0.27	40,40,40,40	0
54	MG	W4	102	1/1	0.96	0.07	83,83,83,83	0
54	MG	14	3535	1/1	0.96	0.07	60,60,60,60	0
54	MG	14	3536	1/1	0.96	0.27	62,62,62,62	0
54	MG	1H	3101	1/1	0.96	0.42	43,43,43,43	0
54	MG	14	3103	1/1	0.96	0.37	43,43,43,43	0
54	MG	X4	103	1/1	0.96	0.12	92,92,92,92	0
54	MG	14	3427	1/1	0.96	0.28	52,52,52,52	0
54	MG	1H	3298	1/1	0.96	0.27	45,45,45,45	0
54	MG	1H	3199	1/1	0.96	0.35	38,38,38,38	0
54	MG	1H	3472	1/1	0.96	0.17	57,57,57,57	0
55	ZN	3E	301	1/1	0.96	0.41	81,81,81,81	0
54	MG	1G	2377	1/1	0.96	0.05	78,78,78,78	0
54	MG	14	3185	1/1	0.97	0.20	48,48,48,48	0
54	MG	1H	3224	1/1	0.97	0.23	42,42,42,42	0
54	MG	1H	3002	1/1	0.97	0.11	36,36,36,36	0
54	MG	14	3189	1/1	0.97	0.54	76,76,76,76	0
54	MG	1H	3173	1/1	0.97	0.31	50,50,50,50	0
54	MG	1H	3003	1/1	0.97	0.11	43,43,43,43	0
54	MG	14	3104	1/1	0.97	0.14	47,47,47,47	0
54	MG	13	2219	1/1	0.97	0.24	60,60,60,60	0
54	MG	14	3382	1/1	0.97	0.30	54,54,54,54	0
54	MG	14	3034	1/1	0.97	0.09	46,46,46,46	0
54	MG	14	3195	1/1	0.97	0.37	63,63,63,63	0
54	MG	13	2238	1/1	0.97	0.46	75,75,75,75	0
54	MG	13	2239	1/1	0.97	0.47	70,70,70,70	0
54	MG	16	208	1/1	0.97	0.48	58,58,58,58	0
54	MG	1H	3509	1/1	0.97	0.22	34,34,34,34	0
54	MG	1H	3136	1/1	0.97	0.38	47,47,47,47	0
54	MG	14	3200	1/1	0.97	0.17	50,50,50,50	0
54	MG	1G	2226	1/1	0.97	0.17	97,97,97,97	0
54	MG	14	3202	1/1	0.97	0.24	42,42,42,42	0
54	MG	1H	3138	1/1	0.97	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1G	2245	1/1	0.97	0.30	67,67,67,67	0
54	MG	1H	3573	1/1	0.97	0.19	47,47,47,47	0
54	MG	13	2261	1/1	0.97	0.40	53,53,53,53	0
54	MG	14	3493	1/1	0.97	0.23	57,57,57,57	0
54	MG	1H	3184	1/1	0.97	0.34	35,35,35,35	0
54	MG	1H	3185	1/1	0.97	0.26	39,39,39,39	0
54	MG	29	305	1/1	0.97	0.14	64,64,64,64	0
54	MG	1G	2211	1/1	0.97	0.08	63,63,63,63	0
54	MG	1H	3458	1/1	0.97	0.14	51,51,51,51	0
54	MG	1H	3240	1/1	0.97	0.44	56,56,56,56	0
54	MG	1H	3401	1/1	0.97	0.30	31,31,31,31	0
54	MG	14	3122	1/1	0.97	0.35	52,52,52,52	0
54	MG	14	3214	1/1	0.97	0.49	62,62,62,62	0
54	MG	13	2253	1/1	0.97	0.21	49,49,49,49	0
54	MG	13	2310	1/1	0.97	0.46	54,54,54,54	0
54	MG	14	3125	1/1	0.97	0.54	48,48,48,48	0
54	MG	13	2230	1/1	0.97	0.17	71,71,71,71	0
54	MG	1H	3014	1/1	0.97	0.08	42,42,42,42	0
54	MG	1H	3191	1/1	0.97	0.37	29,29,29,29	0
54	MG	13	2291	1/1	0.97	0.36	59,59,59,59	0
54	MG	G8	202	1/1	0.97	0.55	53,53,53,53	0
54	MG	1G	2216	1/1	0.97	0.09	73,73,73,73	0
54	MG	14	3511	1/1	0.97	0.26	48,48,48,48	0
54	MG	1H	3072	1/1	0.97	0.04	55,55,55,55	0
54	MG	1H	3018	1/1	0.97	0.11	36,36,36,36	0
54	MG	14	3063	1/1	0.97	0.06	46,46,46,46	0
54	MG	1H	3251	1/1	0.97	0.15	47,47,47,47	0
54	MG	14	3418	1/1	0.97	0.25	59,59,59,59	0
54	MG	14	3065	1/1	0.97	0.09	68,68,68,68	0
54	MG	14	3140	1/1	0.97	0.28	44,44,44,44	0
54	MG	14	3141	1/1	0.97	0.30	51,51,51,51	0
54	MG	1H	3045	1/1	0.97	0.08	41,41,41,41	0
54	MG	14	3143	1/1	0.97	0.34	56,56,56,56	0
54	MG	14	3144	1/1	0.97	0.47	63,63,63,63	0
54	MG	1H	3198	1/1	0.97	0.40	36,36,36,36	0
54	MG	14	3235	1/1	0.97	0.21	45,45,45,45	0
54	MG	1H	3360	1/1	0.97	0.11	46,46,46,46	0
54	MG	1H	3019	1/1	0.97	0.12	38,38,38,38	0
54	MG	1H	3255	1/1	0.97	0.35	51,51,51,51	0
54	MG	14	3149	1/1	0.97	0.46	42,42,42,42	0
54	MG	14	3150	1/1	0.97	0.28	46,46,46,46	0
54	MG	13	2380	1/1	0.97	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3108	1/1	0.97	0.39	30,30,30,30	0
54	MG	14	3153	1/1	0.97	0.41	60,60,60,60	0
54	MG	14	3244	1/1	0.97	0.30	48,48,48,48	0
54	MG	14	3154	1/1	0.97	0.27	53,53,53,53	0
54	MG	1H	3203	1/1	0.97	0.24	40,40,40,40	0
54	MG	13	2224	1/1	0.97	0.37	59,59,59,59	0
54	MG	1H	3483	1/1	0.97	0.21	42,42,42,42	0
54	MG	98	201	1/1	0.97	0.16	56,56,56,56	0
54	MG	14	3158	1/1	0.97	0.45	56,56,56,56	0
54	MG	14	3347	1/1	0.97	0.21	65,65,65,65	0
54	MG	14	3003	1/1	0.97	0.09	44,44,44,44	0
54	MG	1G	2255	1/1	0.97	0.27	67,67,67,67	0
54	MG	14	3446	1/1	0.97	0.21	48,48,48,48	0
54	MG	1H	3207	1/1	0.97	0.25	56,56,56,56	0
54	MG	14	3162	1/1	0.97	0.45	44,44,44,44	0
54	MG	1H	3208	1/1	0.97	0.23	32,32,32,32	0
54	MG	1H	3050	1/1	0.97	0.15	42,42,42,42	0
54	MG	13	2248	1/1	0.97	0.50	57,57,57,57	0
54	MG	X1	102	1/1	0.97	0.32	66,66,66,66	0
54	MG	1G	2221	1/1	0.97	0.17	68,68,68,68	0
54	MG	1H	3116	1/1	0.97	0.27	43,43,43,43	0
54	MG	14	3550	1/1	0.97	0.13	63,63,63,63	0
54	MG	14	3168	1/1	0.97	0.37	47,47,47,47	0
54	MG	1H	3117	1/1	0.97	0.46	42,42,42,42	0
54	MG	14	3264	1/1	0.97	0.21	44,44,44,44	0
54	MG	13	2232	1/1	0.97	0.22	64,64,64,64	0
54	MG	1H	3119	1/1	0.97	0.22	36,36,36,36	0
54	MG	1H	3124	1/1	0.97	0.15	38,38,38,38	0
54	MG	1H	3166	1/1	0.97	0.36	34,34,34,34	0
54	MG	14	3174	1/1	0.97	0.43	53,53,53,53	0
54	MG	1H	3125	1/1	0.97	0.23	40,40,40,40	0
54	MG	1H	3126	1/1	0.97	0.41	52,52,52,52	0
54	MG	1H	3221	1/1	0.97	0.35	42,42,42,42	0
54	MG	14	3024	1/1	0.97	0.14	48,48,48,48	0
54	MG	1H	3026	1/1	0.97	0.09	40,40,40,40	0
54	MG	14	3096	1/1	0.97	0.28	44,44,44,44	0
54	MG	14	3278	1/1	0.97	0.19	39,39,39,39	0
54	MG	1H	3128	1/1	0.97	0.23	29,29,29,29	0
54	MG	1H	3501	1/1	0.97	0.21	44,44,44,44	0
55	ZN	5A	101	1/1	0.97	0.11	99,99,99,99	0
54	MG	1H	3171	1/1	0.98	0.18	39,39,39,39	0
54	MG	1H	3105	1/1	0.98	0.36	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3106	1/1	0.98	0.21	44,44,44,44	0
54	MG	14	3568	1/1	0.98	0.23	53,53,53,53	0
54	MG	1H	3120	1/1	0.98	0.19	33,33,33,33	0
54	MG	14	3081	1/1	0.98	0.06	48,48,48,48	0
54	MG	14	3261	1/1	0.98	0.23	51,51,51,51	0
54	MG	1H	3482	1/1	0.98	0.11	48,48,48,48	0
54	MG	1H	3121	1/1	0.98	0.29	44,44,44,44	0
54	MG	1H	3382	1/1	0.98	0.30	53,53,53,53	0
54	MG	1H	3123	1/1	0.98	0.29	40,40,40,40	0
54	MG	1G	2235	1/1	0.98	0.36	64,64,64,64	0
54	MG	14	3129	1/1	0.98	0.48	45,45,45,45	0
54	MG	88	304	1/1	0.98	0.24	48,48,48,48	0
54	MG	1G	2220	1/1	0.98	0.08	66,66,66,66	0
54	MG	1H	3238	1/1	0.98	0.50	57,57,57,57	0
54	MG	14	3271	1/1	0.98	0.30	68,68,68,68	0
54	MG	14	3176	1/1	0.98	0.70	60,60,60,60	0
54	MG	1H	3028	1/1	0.98	0.15	49,49,49,49	0
54	MG	1H	3110	1/1	0.98	0.31	47,47,47,47	0
54	MG	13	2204	1/1	0.98	0.07	61,61,61,61	0
54	MG	14	3428	1/1	0.98	0.37	47,47,47,47	0
54	MG	1H	3436	1/1	0.98	0.25	47,47,47,47	0
54	MG	14	3137	1/1	0.98	0.24	46,46,46,46	0
54	MG	1H	3522	1/1	0.98	0.30	50,50,50,50	0
54	MG	1G	2308	1/1	0.98	0.31	56,56,56,56	0
54	MG	14	3095	1/1	0.98	0.31	44,44,44,44	0
54	MG	14	3186	1/1	0.98	0.22	45,45,45,45	0
54	MG	14	3282	1/1	0.98	0.35	47,47,47,47	0
54	MG	W1	102	1/1	0.98	0.21	67,67,67,67	0
54	MG	14	3283	1/1	0.98	0.21	44,44,44,44	0
54	MG	14	3055	1/1	0.98	0.12	54,54,54,54	0
54	MG	14	3016	1/1	0.98	0.09	47,47,47,47	0
54	MG	14	3017	1/1	0.98	0.08	51,51,51,51	0
54	MG	13	2370	1/1	0.98	0.08	86,86,86,86	0
54	MG	1H	3439	1/1	0.98	0.17	53,53,53,53	0
54	MG	1H	3325	1/1	0.98	0.22	60,60,60,60	0
54	MG	1H	3441	1/1	0.98	0.25	59,59,59,59	0
54	MG	14	3023	1/1	0.98	0.07	46,46,46,46	0
54	MG	14	3392	1/1	0.98	0.27	49,49,49,49	0
54	MG	1H	3131	1/1	0.98	0.30	62,62,62,62	0
54	MG	1H	3056	1/1	0.98	0.07	45,45,45,45	0
54	MG	1H	3206	1/1	0.98	0.39	44,44,44,44	0
54	MG	1H	3133	1/1	0.98	0.41	47,47,47,47	0

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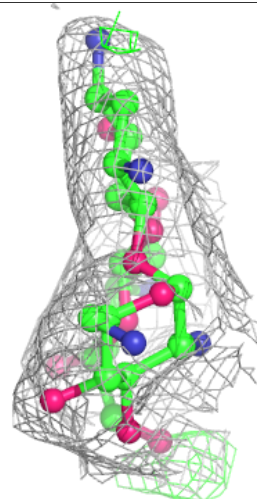
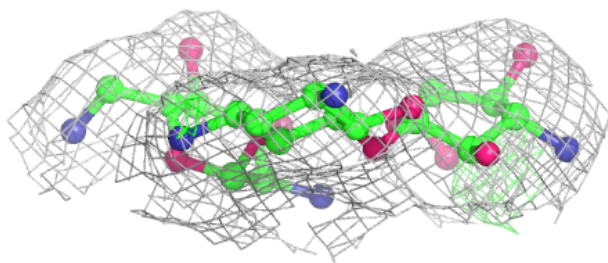
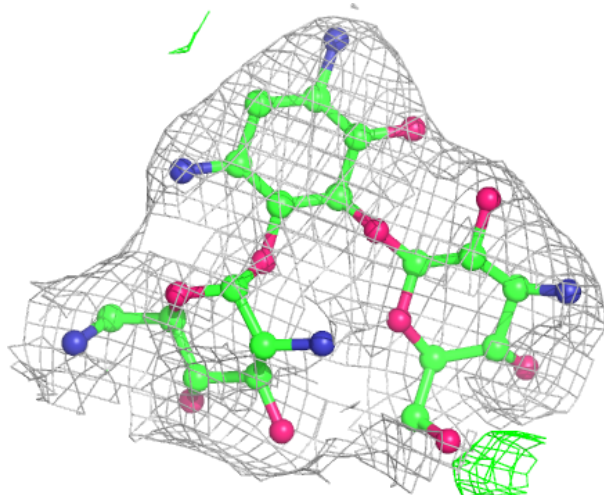
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1H	3446	1/1	0.98	0.20	39,39,39,39	0
54	MG	1H	3308	1/1	0.98	0.14	32,32,32,32	0
54	MG	1G	2345	1/1	0.98	0.25	55,55,55,55	0
54	MG	1H	3595	1/1	0.98	0.33	43,43,43,43	0
54	MG	14	3249	1/1	0.98	0.15	55,55,55,55	0
54	MG	1H	3596	1/1	0.98	0.26	49,49,49,49	0
54	MG	14	3033	1/1	0.98	0.06	52,52,52,52	0
54	MG	1H	3476	1/1	0.98	0.26	52,52,52,52	0
54	MG	14	3035	1/1	0.98	0.12	46,46,46,46	0
54	MG	1G	2364	1/1	0.98	0.18	93,93,93,93	0
55	ZN	32	301	1/1	0.98	0.37	90,90,90,90	0
55	ZN	5I	101	1/1	0.98	0.12	74,74,74,74	0
54	MG	14	3037	1/1	0.98	0.12	59,59,59,59	0
54	MG	1G	2265	1/1	0.99	0.18	81,81,81,81	0
54	MG	1G	2241	1/1	0.99	0.37	71,71,71,71	0
54	MG	13	2216	1/1	0.99	0.30	53,53,53,53	0
54	MG	14	3246	1/1	0.99	0.43	64,64,64,64	0
54	MG	14	3182	1/1	0.99	0.43	44,44,44,44	0
54	MG	1H	3104	1/1	0.99	0.32	30,30,30,30	0
54	MG	1H	3149	1/1	0.99	0.34	53,53,53,53	0
54	MG	1H	3201	1/1	0.99	0.43	33,33,33,33	0
54	MG	14	3268	1/1	0.99	0.43	51,51,51,51	0
54	MG	1H	3115	1/1	0.99	0.32	30,30,30,30	0
54	MG	14	3020	1/1	0.99	0.09	45,45,45,45	0
54	MG	1H	3122	1/1	0.99	0.31	30,30,30,30	0
54	MG	14	3100	1/1	0.99	0.31	45,45,45,45	0
54	MG	1H	3176	1/1	0.99	0.40	40,40,40,40	0
54	MG	1H	3215	1/1	0.99	0.31	45,45,45,45	0
54	MG	14	3011	1/1	0.99	0.10	42,42,42,42	0
54	MG	14	3420	1/1	0.99	0.46	44,44,44,44	0
54	MG	14	3132	1/1	0.99	0.37	38,38,38,38	0
54	MG	1G	2204	1/1	0.99	0.12	58,58,58,58	0
54	MG	4E	201	1/1	0.99	0.24	78,78,78,78	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.

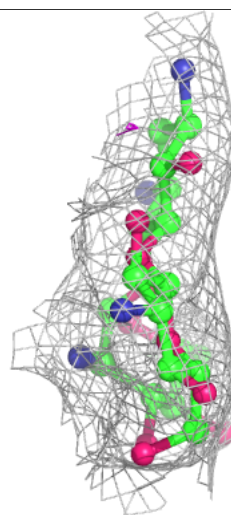
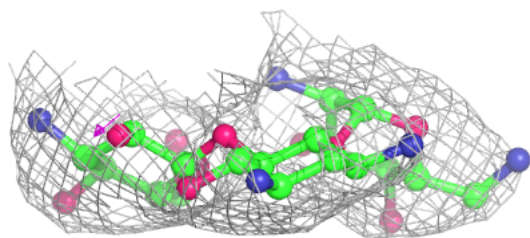
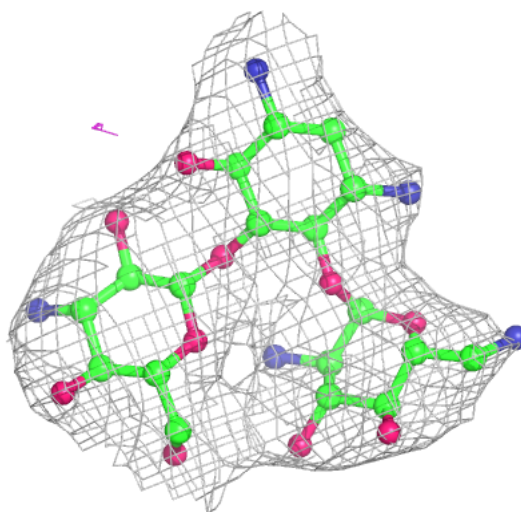
**Electron density around 8UZ 13 2202:**

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



**Electron density around 8UZ 1G 2202:**

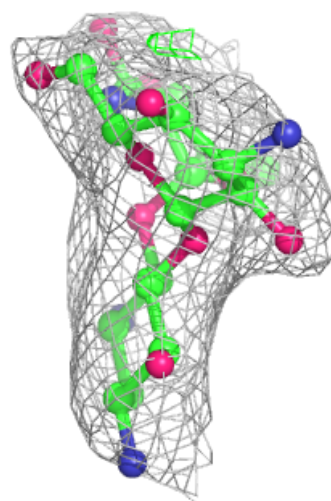
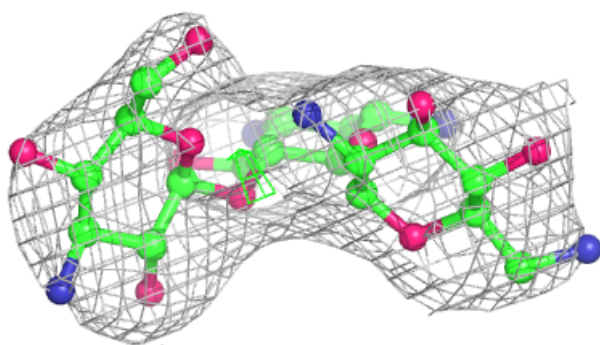
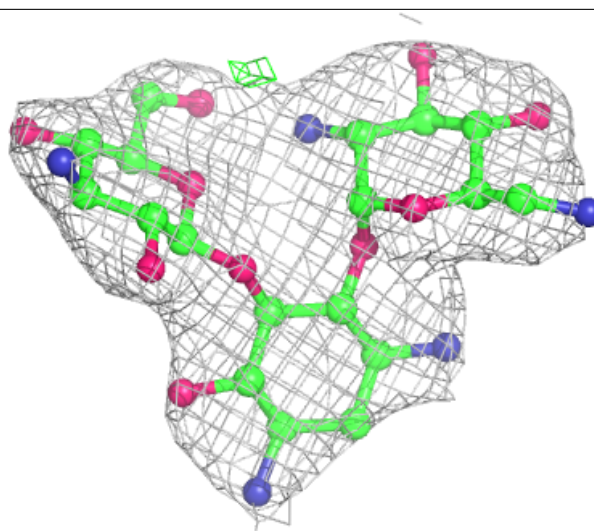
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

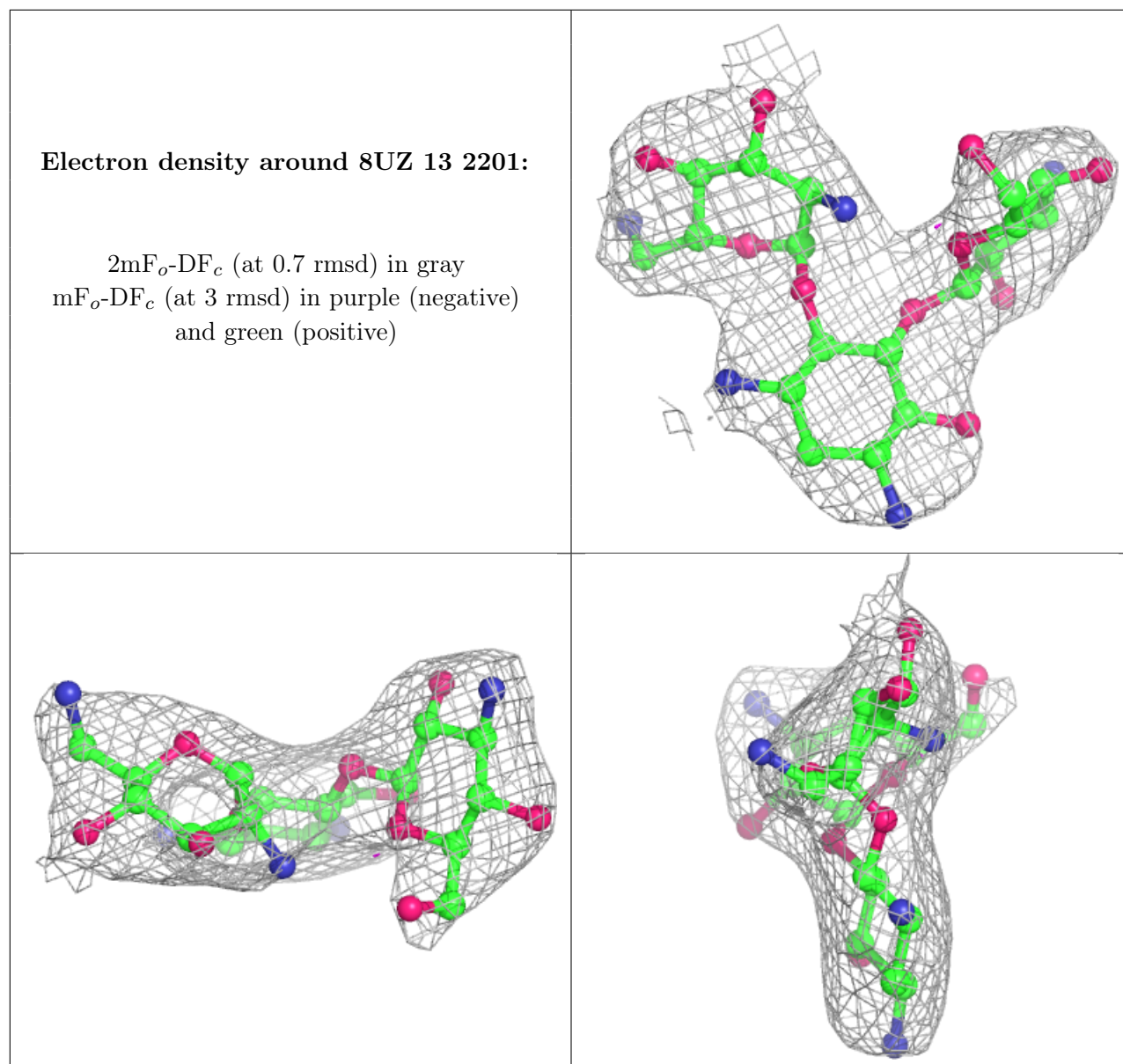




**Electron density around 8UZ 1G 2201:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.