



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:26 AM UTC

PDB ID : 5NDJ / pdb\_00005ndj  
Title : Crystal structure of aminoglycoside TC007 in complex with 70S ribosome from *Thermus thermophilus*, three tRNAs and mRNA (soaking)  
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2017-03-08  
Resolution : 3.15 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

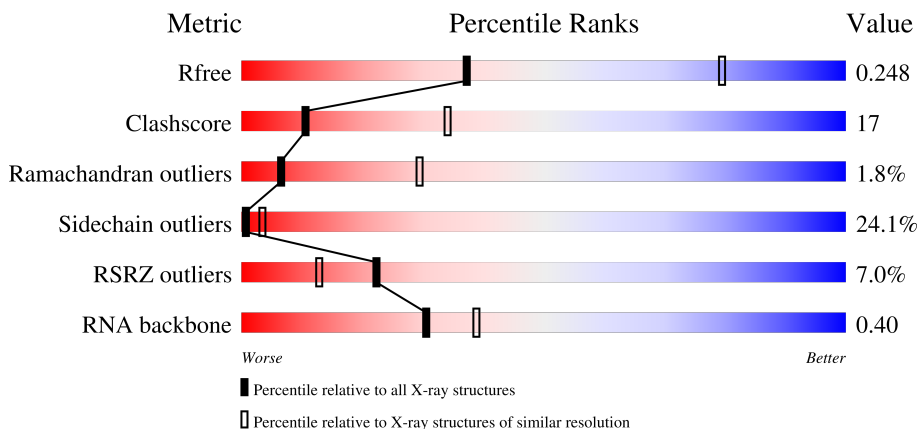
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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	7% (Poor fit) 42% (0 outliers), 45% (1 outlier), 11% (2 outliers)
1	1G	1522	9% (Poor fit) 44% (0 outliers), 44% (1 outlier), 11% (2 outliers)
2	65	112	3% (Poor fit) 34% (0 outliers), 46% (1 outlier), 16% (2 outliers)
2	A8	112	% (Poor fit) 37% (0 outliers), 40% (1 outlier), 21% (2 outliers)

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Mol	Chain	Length	Quality of chain
3	B5	96	4% 40% 45% 11% .
3	F8	96	4% 51% 34% 11% ..
4	11	276	% 50% 36% 12% ..
4	19	276	3% 51% 33% 12% ..
5	L5	49	41% 53% . .
5	P8	49	8% 57% 33% . . .
6	2A	129	10% 47% 33% 9% 10%
6	2I	129	4% 42% 34% 13% . 10%
7	8A	105	4% 50% 39% 5% . 6%
7	8I	105	7% 35% 47% 12% . 5%
8	22	239	18% 40% 36% 10% 14%
8	2E	239	15% 43% 34% 8% . 14%
9	82	128	35% 44% 43% 9% . .
9	8E	128	15% 37% 46% 16% .
10	15	140	11% 50% 37% 11% ..
10	58	140	9% 41% 39% 17% ..
11	C5	110	35% 30% 44% 19% . 5%
11	G8	110	3% 34% 33% 21% 6% 6%
12	M5	65	15% 35% 40% 15% 8% .
12	Q8	65	20% 6% 35% 31% 20% 8%
13	3A	132	10% 47% 35% 11% . 5%
13	3I	132	5% 50% 33% 9% 8%
14	32	209	12% 51% 35% 12% .
14	3E	209	8% 47% 40% 12%
15	14	2917	3% 45% 43% 12%

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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	
28	M8	71	
29	AA	93	
29	AI	93	
30	35	150	
30	78	150	
31	E5	85	
31	I8	85	
32	31	210	
32	39	210	
33	5A	61	
33	5I	61	
34	52	101	
34	5E	101	
35	95	101	
35	D8	101	
36	J5	60	
36	N8	60	
37	BA	106	
37	BI	106	
38	45	141	
38	88	141	
39	F5	98	
39	J8	98	
40	41	182	

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Mol	Chain	Length	Quality of chain
40	49	182	15% 43% 45% 10% ..
41	6A	89	4% 63% 27% 9% .
41	6I	89	% 52% 36% 11% .
42	62	156	13% 52% 33% 10% 6%
42	6E	156	8% 56% 29% 7% 8%
43	A5	113	49% 39% 12%
43	E8	113	55% 37% 7% .
44	12	256	8% 36% 42% 13% . 7%
44	1E	256	5% 42% 34% 16% . 7%
45	55	118	3% 46% 42% 10% ..
45	98	118	46% 37% 14% .
46	G5	72	3% 39% 36% 15% . 7%
46	K8	72	3% 36% 39% 14% 6% 6%
47	51	180	7% 44% 37% 13% . .
47	59	180	40% 35% 45% 14% . 6%
48	1A	105	25% 30% 51% 12% 6%
48	1I	105	29% 30% 50% 12% . 6%
49	7A	88	2% 51% 35% 9% 5%
49	7I	88	22% 36% 50% 8% . 5%
50	72	138	20% 53% 36% 9% .
50	7E	138	7% 44% 44% 12%
51	Y1	25	28% 48% 24% 28%
51	Y4	25	36% 32% 32% 36%
52	V1	76	20% 21% 42% 37%
52	V4	76	14% 32% 34% 34%

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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	2250	-	-	-	X
54	MG	13	2292	-	-	-	X
54	MG	13	2330	-	-	-	X
54	MG	14	3106	-	-	-	X
54	MG	14	3249	-	-	-	X
54	MG	14	3261	-	-	-	X
54	MG	14	3265	-	-	-	X
54	MG	14	3437	-	-	-	X
54	MG	14	3474	-	-	-	X
54	MG	14	3513	-	-	-	X
54	MG	1G	2225	-	-	-	X
54	MG	1G	2263	-	-	-	X
54	MG	1G	2264	-	-	-	X
54	MG	1G	2277	-	-	-	X
54	MG	1G	2311	-	-	-	X
54	MG	1G	2318	-	-	-	X
54	MG	1G	2326	-	-	-	X
54	MG	1G	2359	-	-	-	X
54	MG	1G	2360	-	-	-	X
54	MG	1G	2368	-	-	-	X
54	MG	1G	2377	-	-	-	X
54	MG	1G	2378	-	-	-	X
54	MG	1H	3236	-	-	-	X
54	MG	25	202	-	-	-	X
54	MG	51	201	-	-	-	X
54	MG	X1	101	-	-	-	X
54	MG	X1	102	-	-	-	X
54	MG	X1	105	-	-	-	X
54	MG	X4	101	-	-	-	X
54	MG	X4	103	-	-	-	X

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 300009 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	C	N	O	P	0	0	0
			32409	14425	6001	10475	1508			
1	1G	1513	Total	C	N	O	P	0	0	0
			32514	14473	6021	10508	1512			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	2165	G	U	conflict	GB 55771382
1G	2165	G	U	conflict	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	C	N	O	0	0	0
			881	556	176	149			
2	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- 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	C	N	O	0	0	0	
			725	471	131	123				
3	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
9	8E	127	Total 1009	C 639	N 197	O 173	0	0	0
9	82	124	Total 983	C 624	N 190	O 169	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
12	M5	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

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

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

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

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

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

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
16	B8	129	Total	C	N	O	S	0	0	0
			1081	674	223	183	1			
16	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

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

- 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	S	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			

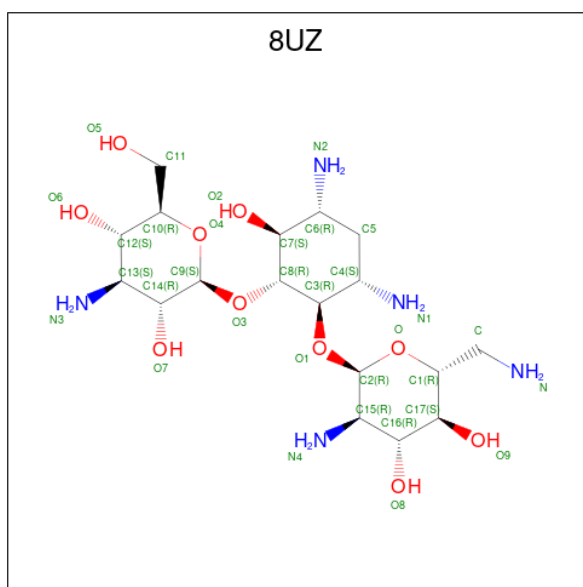
- Molecule 51 is a RNA chain called mRNA.

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 (CCD ID: 8UZ) (formula: C<sub>18</sub>H<sub>37</sub>N<sub>5</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
53	13	1	33	18	5	10	0	0
53	13	1	33	18	5	10	0	0
53	1G	1	33	18	5	10	0	0
53	1G	1	33	18	5	10	0	0
53	1H	1	33	18	5	10	0	0
53	1H	1	33	18	5	10	0	0
53	1H	1	33	18	5	10	0	0
53	1H	1	33	18	5	10	0	0
53	14	1	33	18	5	10	0	0
53	14	1	33	18	5	10	0	0
53	14	1	33	18	5	10	0	0
53	14	1	33	18	5	10	0	0
53	14	1	33	18	5	10	0	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	13	197	Total Mg 197 197	0	0
54	A8	1	Total Mg 1 1	0	0
54	B5	1	Total Mg 1 1	0	0
54	11	4	Total Mg 4 4	0	0
54	2A	1	Total Mg 1 1	0	0
54	8I	1	Total Mg 1 1	0	0
54	1G	189	Total Mg 189 189	0	0
54	58	1	Total Mg 1 1	0	0
54	G8	1	Total Mg 1 1	0	0
54	19	1	Total Mg 1 1	0	0
54	3I	1	Total Mg 1 1	0	0
54	8A	1	Total Mg 1 1	0	0
54	3E	2	Total Mg 2 2	0	0
54	1H	657	Total Mg 657 657	0	0
54	15	1	Total Mg 1 1	0	0
54	B8	1	Total Mg 1 1	0	0
54	C5	1	Total Mg 1 1	0	0
54	32	3	Total Mg 3 3	0	0
54	14	591	Total Mg 591 591	0	0
54	68	2	Total Mg 2 2	0	0
54	75	1	Total Mg 1 1	0	0
54	21	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	4I	1	Total Mg 1 1	0	0
54	4E	1	Total Mg 1 1	0	0
54	16	14	Total Mg 14 14	0	0
54	25	3	Total Mg 3 3	0	0
54	C8	1	Total Mg 1 1	0	0
54	29	6	Total Mg 6 6	0	0
54	42	1	Total Mg 1 1	0	0
54	1J	14	Total Mg 14 14	0	0
54	78	3	Total Mg 3 3	0	0
54	I8	3	Total Mg 3 3	0	0
54	31	4	Total Mg 4 4	0	0
54	5I	1	Total Mg 1 1	0	0
54	5E	1	Total Mg 1 1	0	0
54	35	2	Total Mg 2 2	0	0
54	D8	2	Total Mg 2 2	0	0
54	E5	2	Total Mg 2 2	0	0
54	N8	1	Total Mg 1 1	0	0
54	39	1	Total Mg 1 1	0	0
54	52	1	Total Mg 1 1	0	0
54	88	5	Total Mg 5 5	0	0
54	J8	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	41	2	Total Mg 2 2	0	0
54	BA	1	Total Mg 1 1	0	0
54	45	2	Total Mg 2 2	0	0
54	49	1	Total Mg 1 1	0	0
54	6A	1	Total Mg 1 1	0	0
54	98	3	Total Mg 3 3	0	0
54	K8	1	Total Mg 1 1	0	0
54	51	1	Total Mg 1 1	0	0
54	55	3	Total Mg 3 3	0	0
54	P8	1	Total Mg 1 1	0	0
54	7A	1	Total Mg 1 1	0	0
54	Y1	1	Total Mg 1 1	0	0
54	W1	3	Total Mg 3 3	0	0
54	X1	9	Total Mg 9 9	0	0
54	Y4	1	Total Mg 1 1	0	0
54	W4	4	Total Mg 4 4	0	0
54	X4	5	Total Mg 5 5	0	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	G8	1	Total Zn 1 1	0	0
55	3E	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	2	Total 2	O 2	0	0
56	1G	72	Total 72	O 72	0	0
56	19	8	Total 8	O 8	0	0
56	1H	532	Total 532	O 532	0	0
56	M5	2	Total 2	O 2	0	0
56	14	512	Total 512	O 512	0	0
56	21	2	Total 2	O 2	0	0
56	C8	2	Total 2	O 2	0	0
56	29	3	Total 3	O 3	0	0
56	78	2	Total 2	O 2	0	0
56	I8	3	Total 3	O 3	0	0
56	31	3	Total 3	O 3	0	0
56	35	1	Total 1	O 1	0	0

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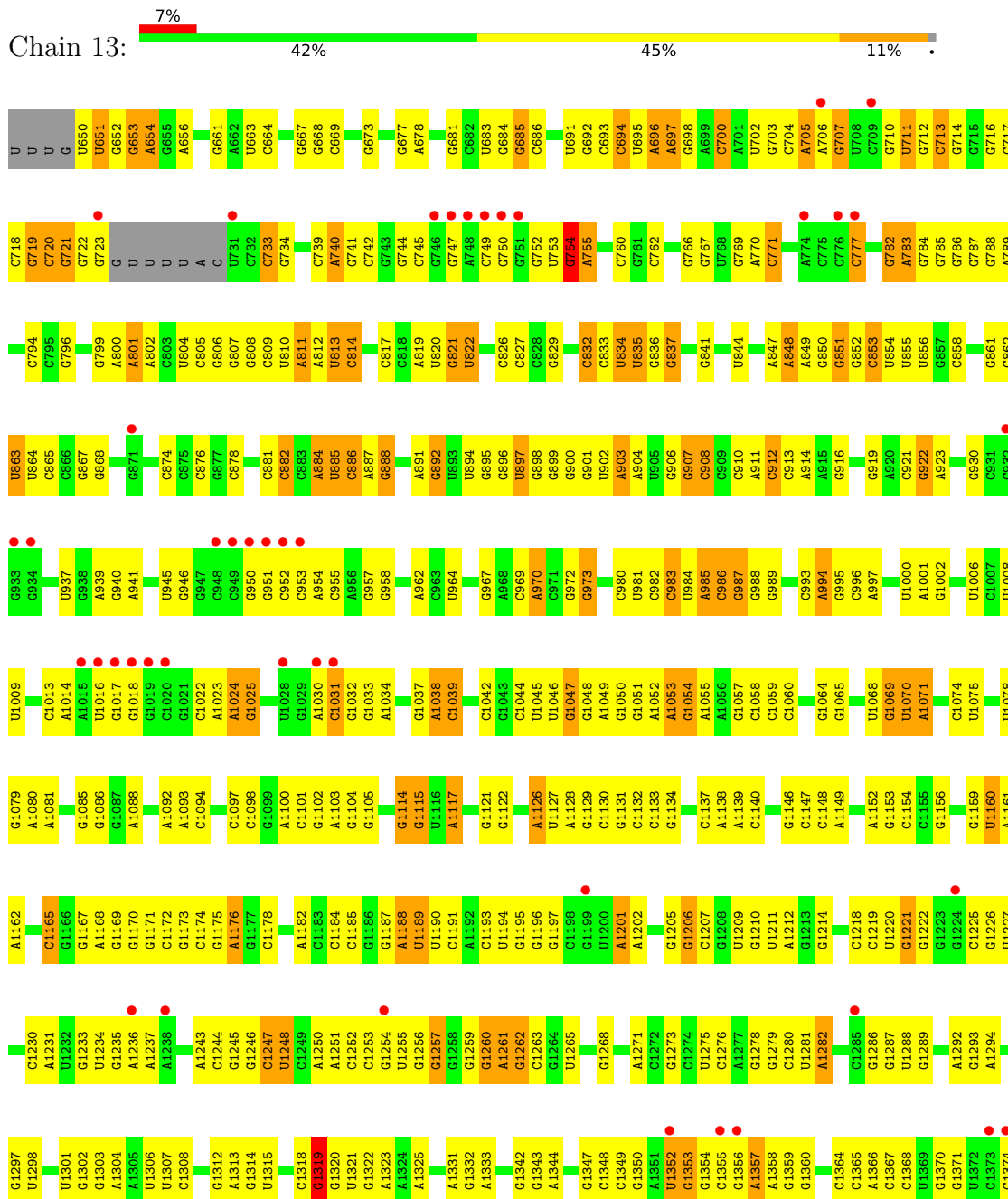
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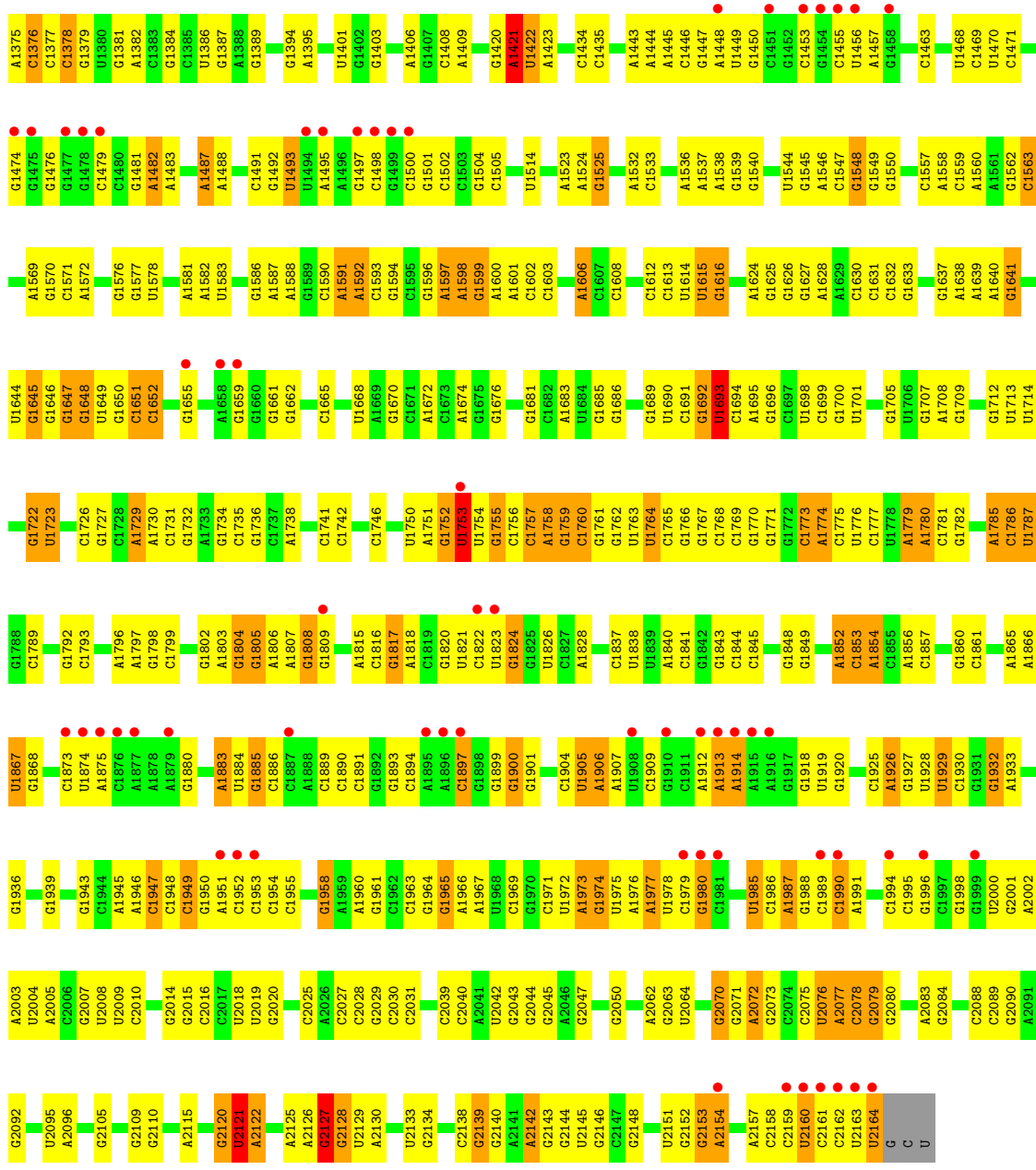
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	D8	1	Total O 1 1	0	0
56	39	3	Total O 3 3	0	0
56	5A	1	Total O 1 1	0	0
56	J8	2	Total O 2 2	0	0
56	6I	1	Total O 1 1	0	0
56	E8	1	Total O 1 1	0	0
56	F5	1	Total O 1 1	0	0
56	6A	2	Total O 2 2	0	0
56	A5	1	Total O 1 1	0	0
56	55	2	Total O 2 2	0	0
56	F8	1	Total O 1 1	0	0
56	P8	1	Total O 1 1	0	0
56	7A	1	Total O 1 1	0	0
56	Y4	2	Total O 2 2	0	0

### 3 Residue-property plots

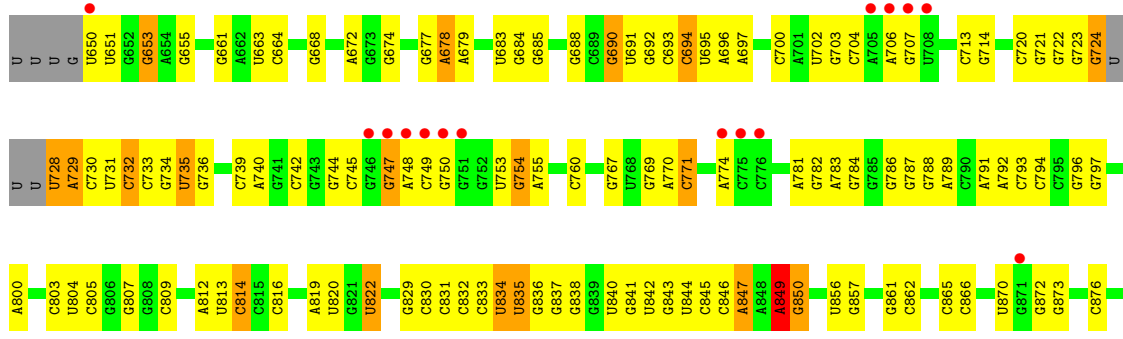
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

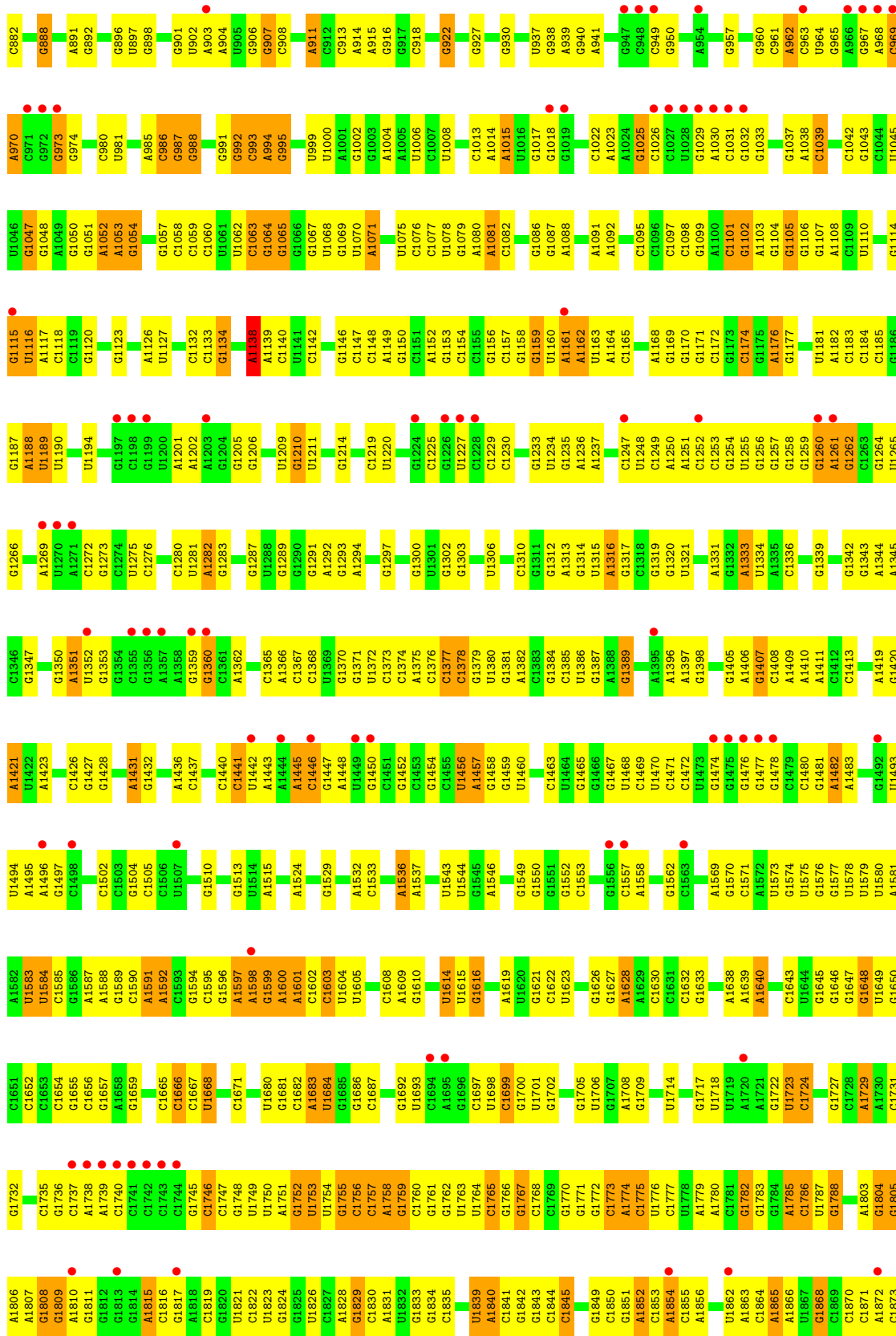
- Molecule 1: 16S ribosomal RNA

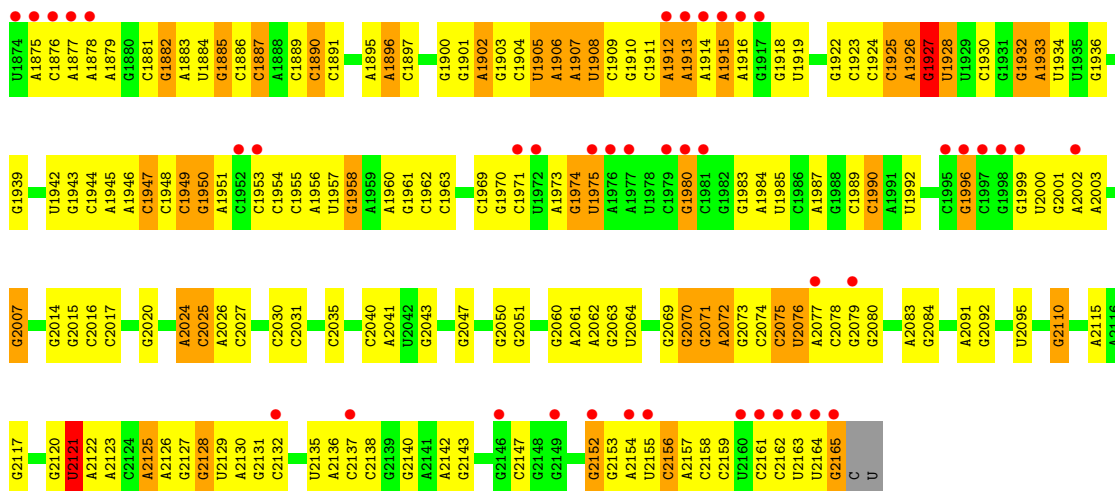




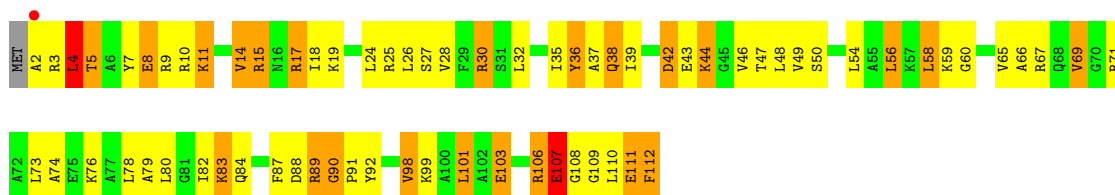
● Molecule 1: 16S ribosomal RNA



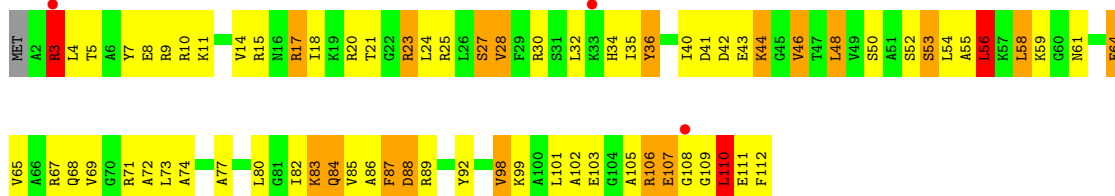




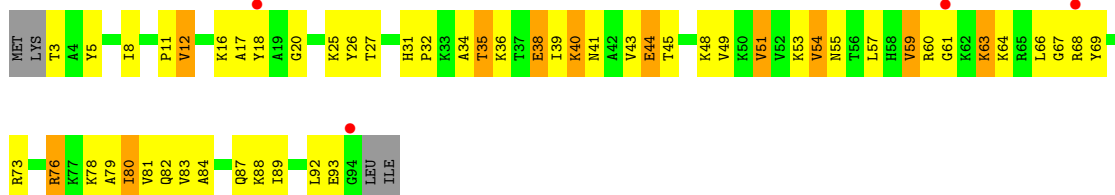
• Molecule 2: 50S ribosomal protein L18



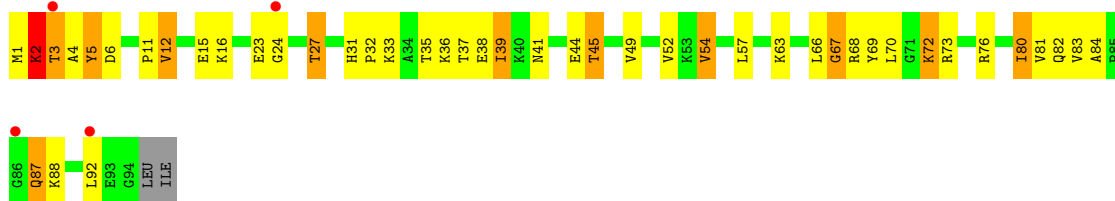
• Molecule 2: 50S ribosomal protein L18



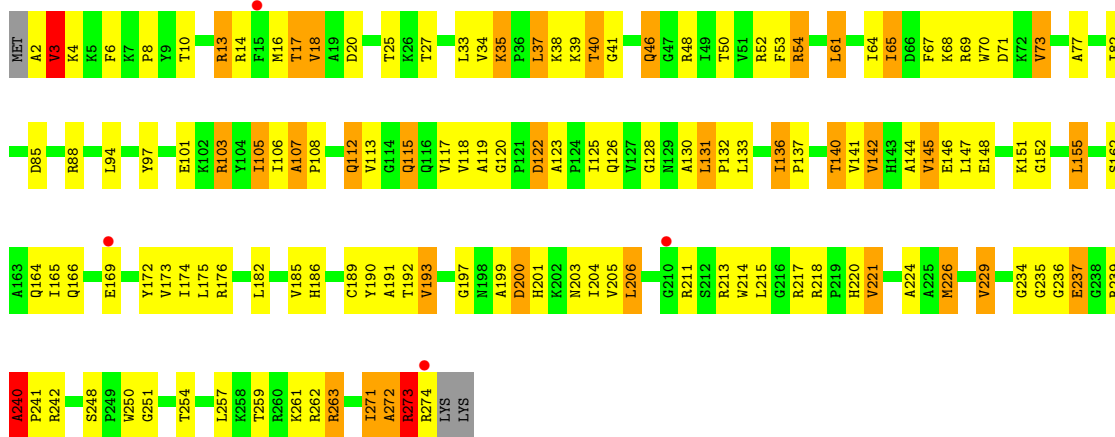
• Molecule 3: 50S ribosomal protein L23



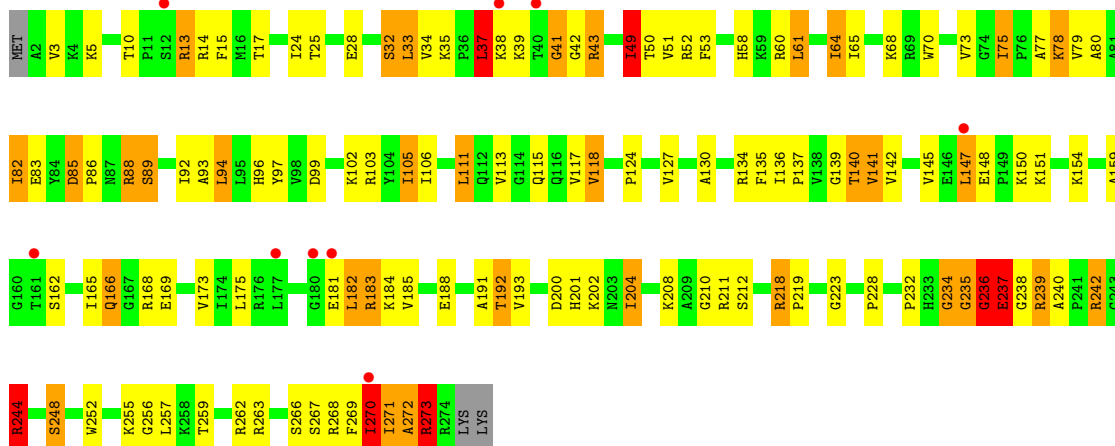
• Molecule 3: 50S ribosomal protein L23



• Molecule 4: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L2

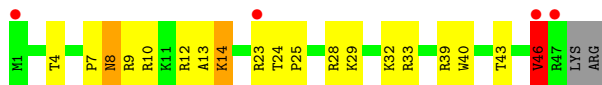


• Molecule 5: 50S ribosomal protein L34





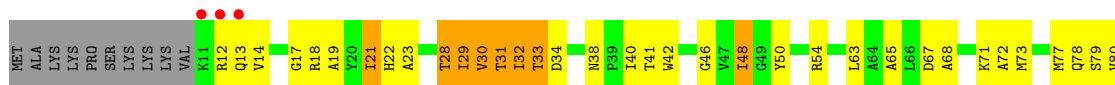
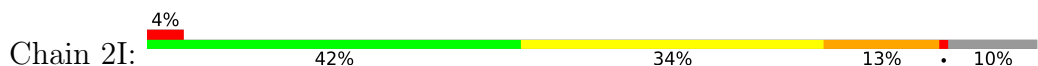
• Molecule 5: 50S ribosomal protein L34



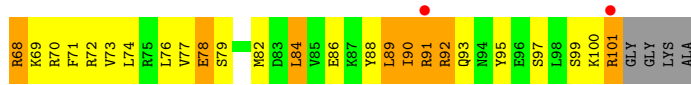
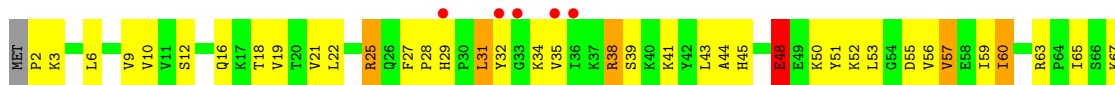
• Molecule 6: 30S ribosomal protein S11



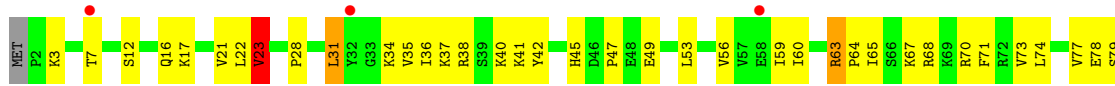
• Molecule 6: 30S ribosomal protein S11



• Molecule 7: 30S ribosomal protein S17

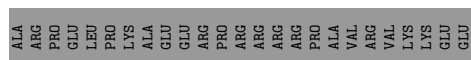
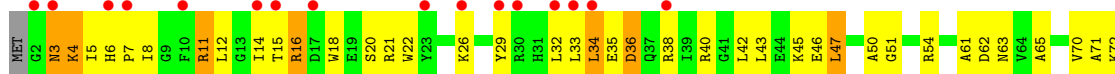


• Molecule 7: 30S ribosomal protein S17

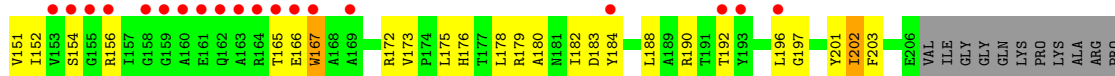
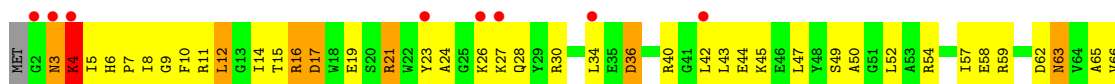
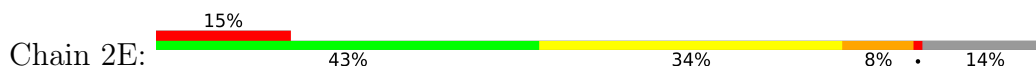




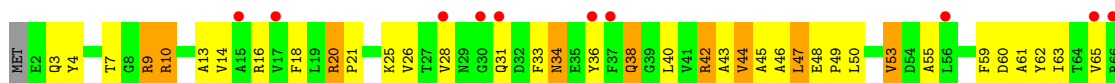
- Molecule 8: 30S ribosomal protein S3



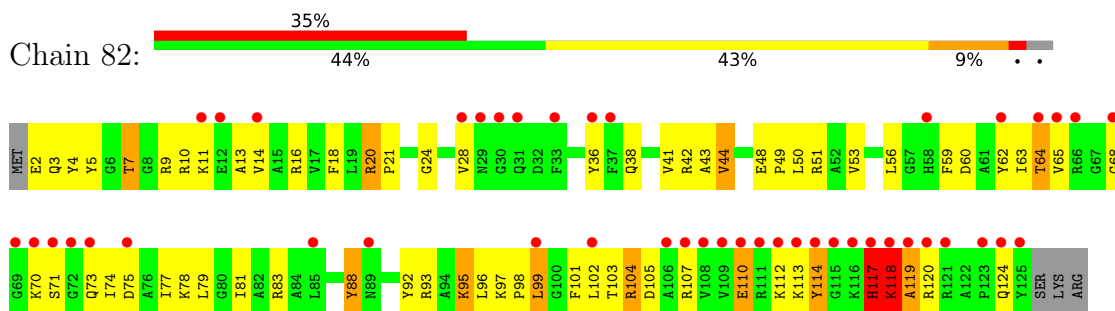
- Molecule 8: 30S ribosomal protein S3



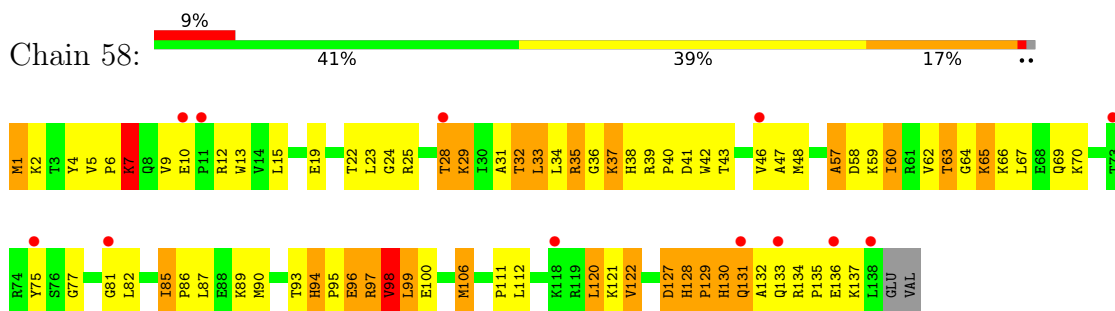
- Molecule 9: 30S ribosomal protein S9



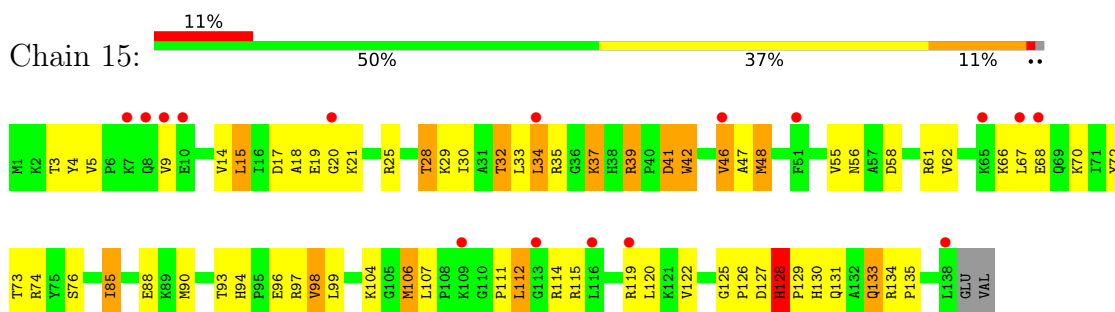
- Molecule 9: 30S ribosomal protein S9



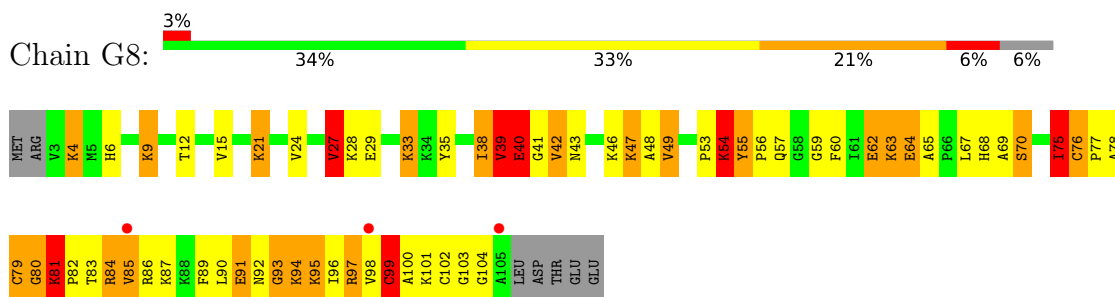
- Molecule 10: 50S ribosomal protein L13



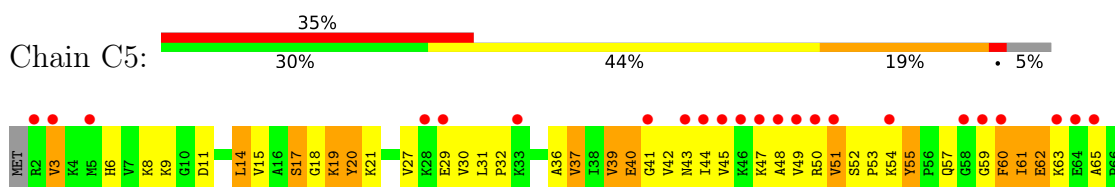
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L24

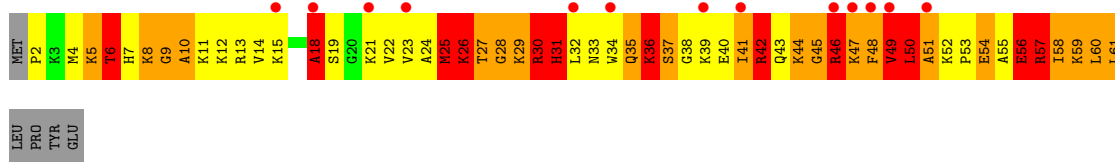


- Molecule 11: 50S ribosomal protein L24





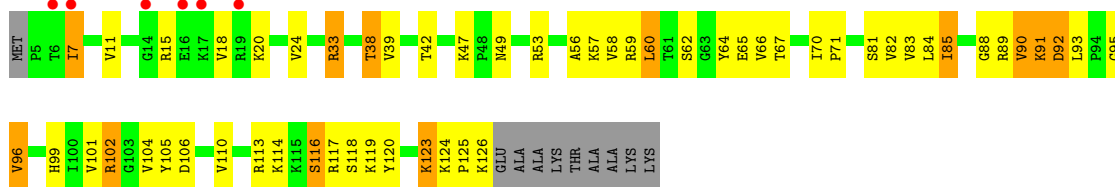
• Molecule 12: 50S ribosomal protein L35



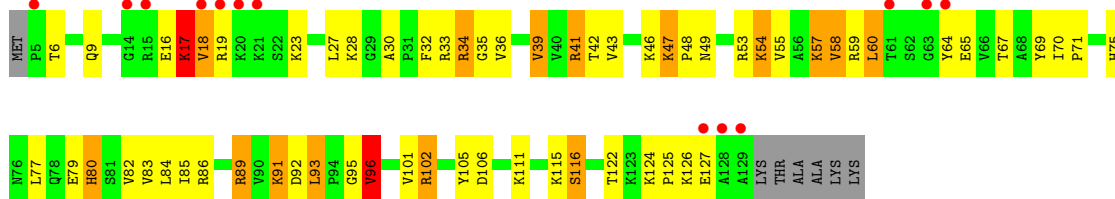
• Molecule 12: 50S ribosomal protein L35



• Molecule 13: 30S ribosomal protein S12

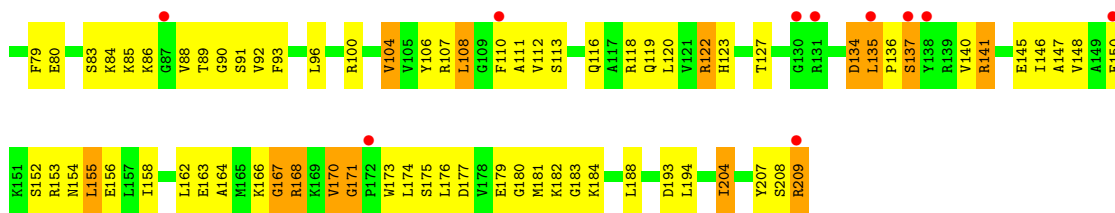


• Molecule 13: 30S ribosomal protein S12

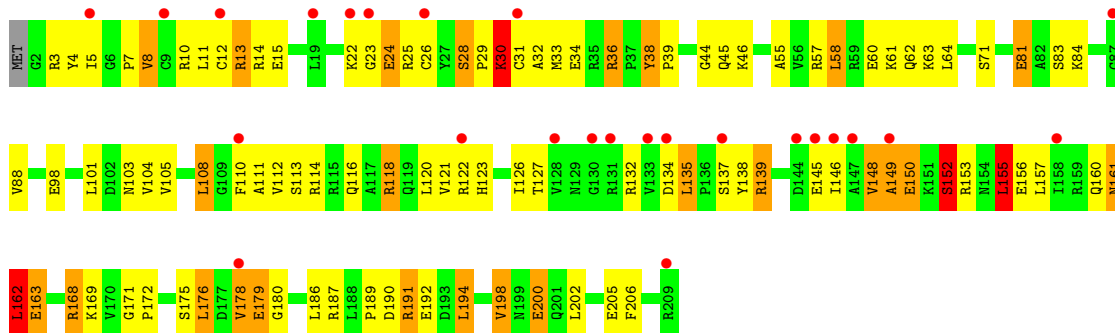


• Molecule 14: 30S ribosomal protein S4

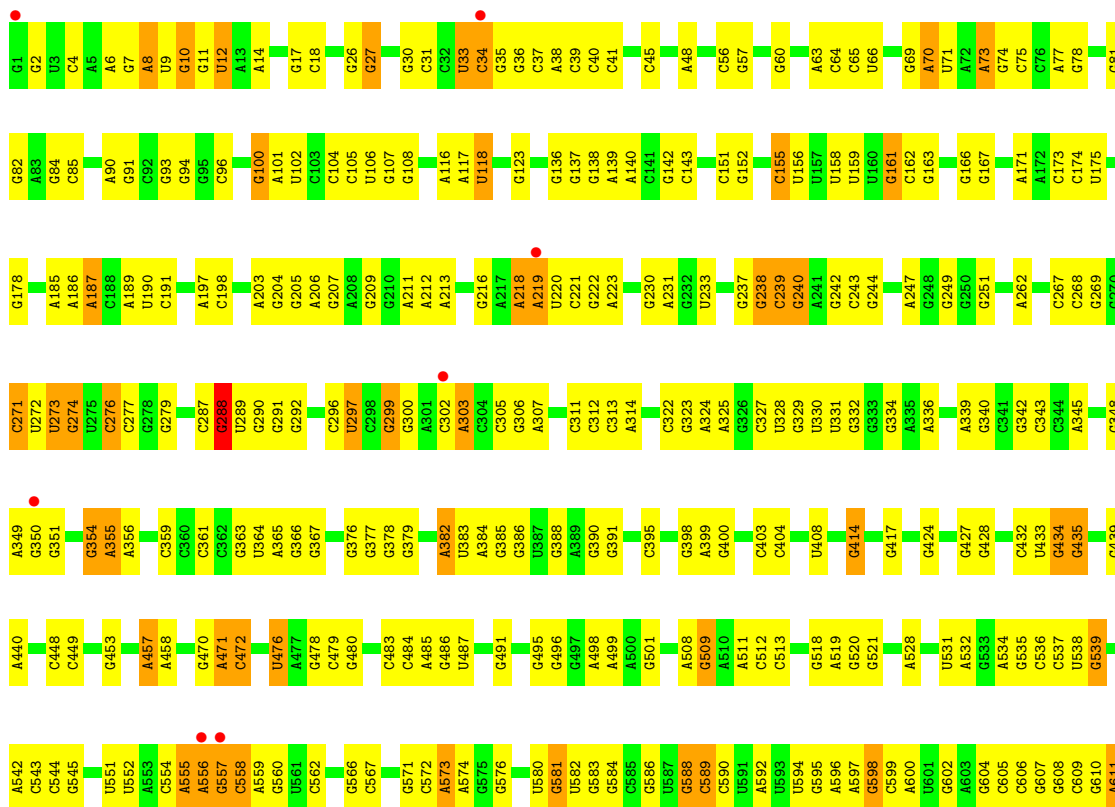


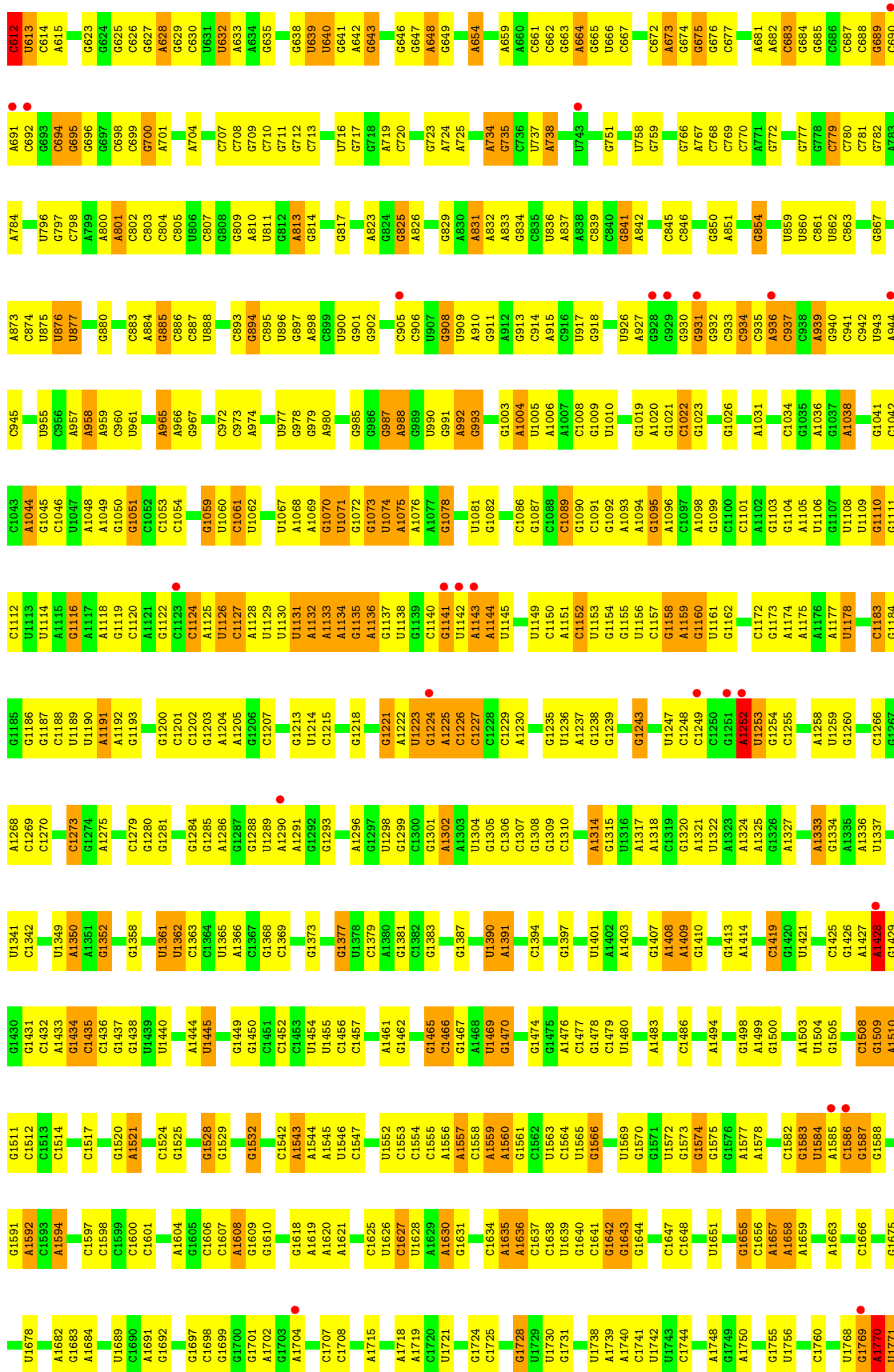


• Molecule 14: 30S ribosomal protein S4



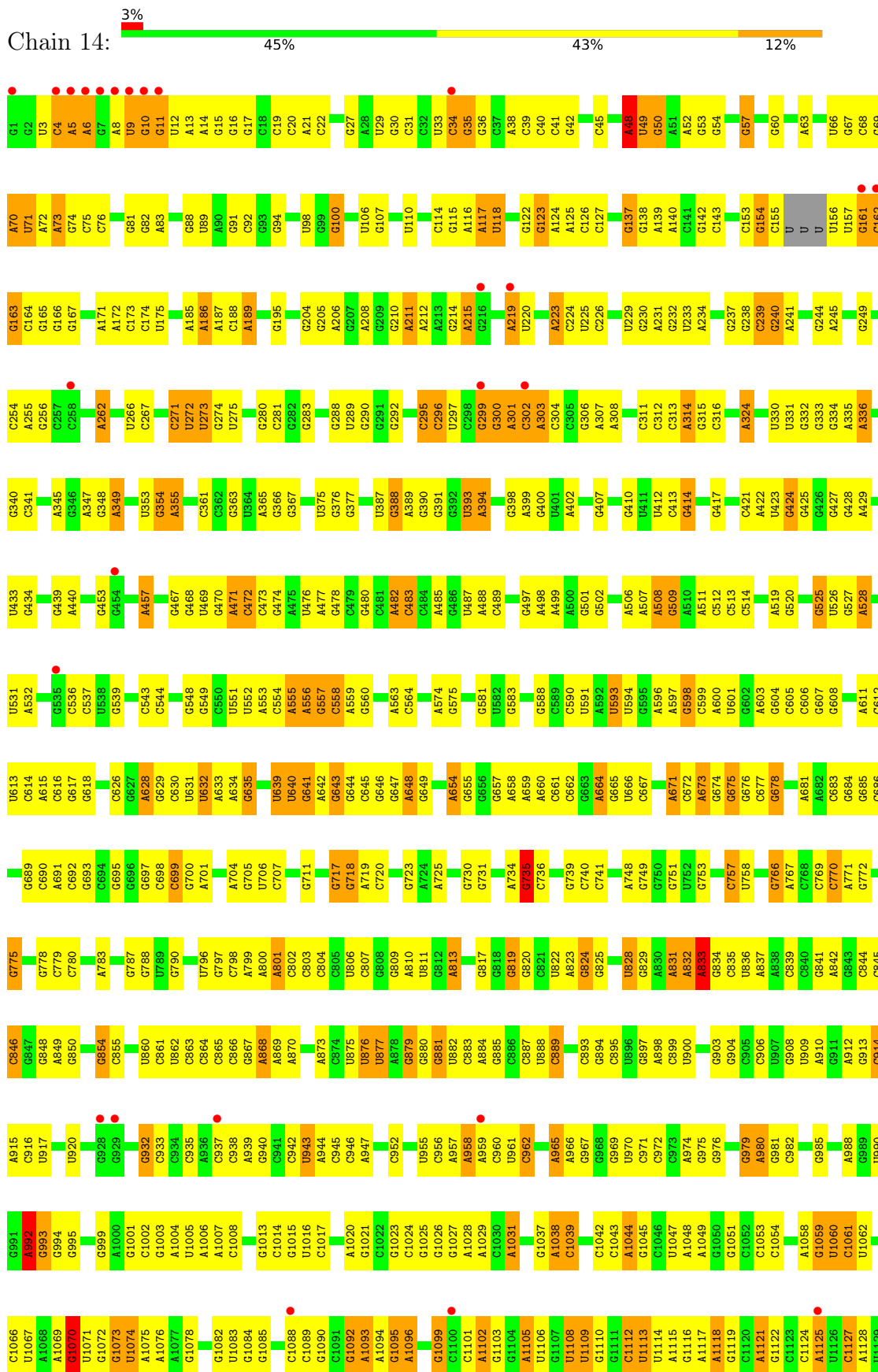
• Molecule 15: 23S ribosomal RNA



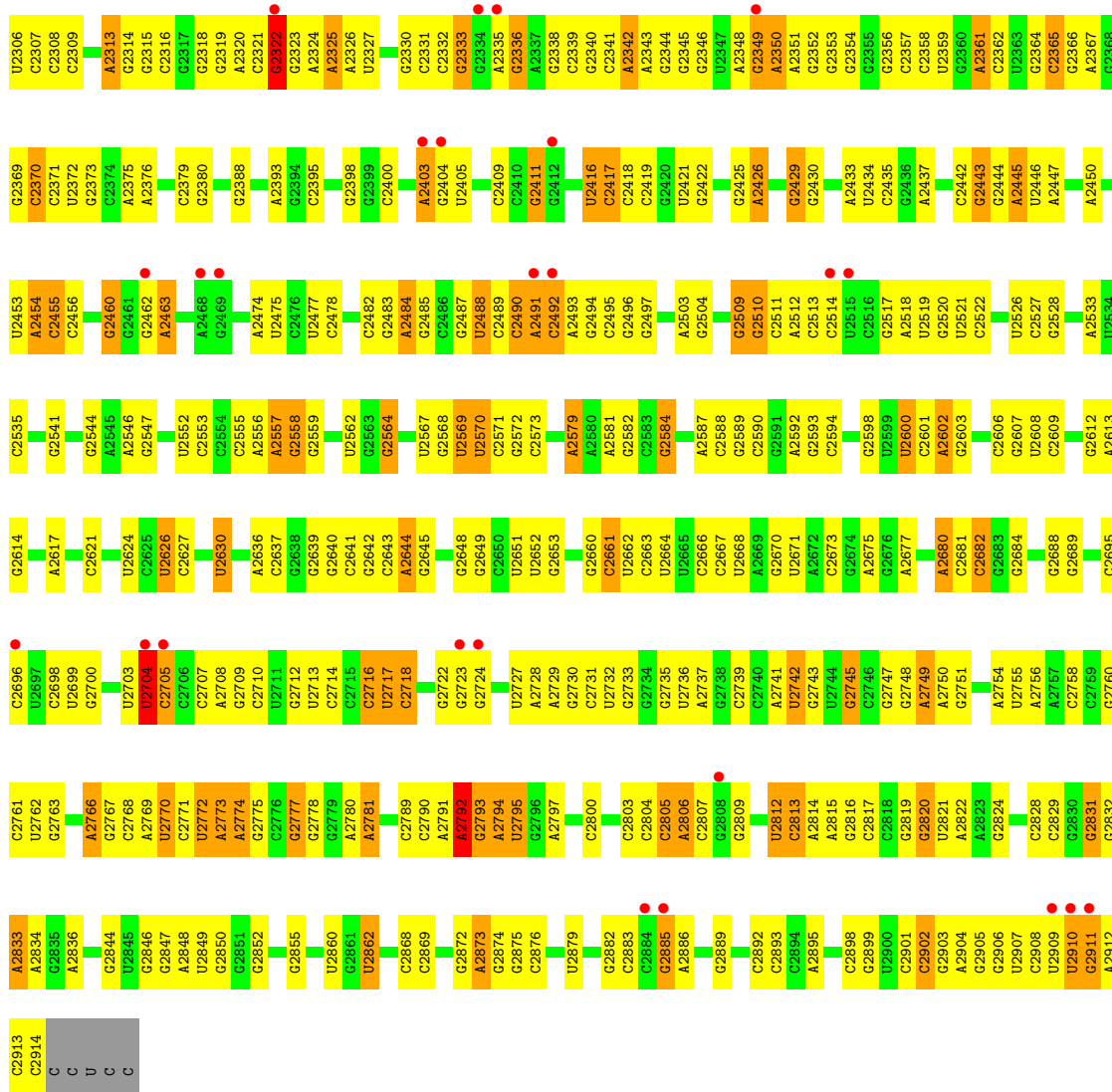




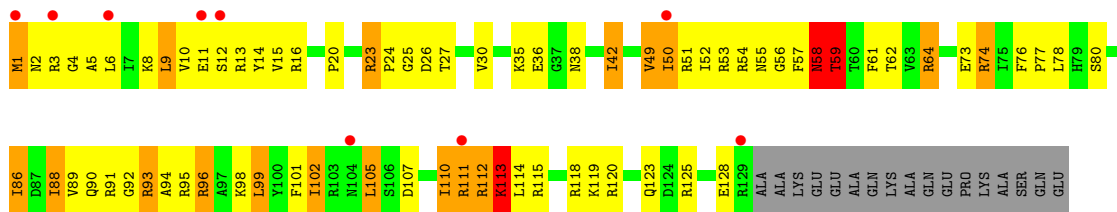
● Molecule 15: 23S ribosomal RNA



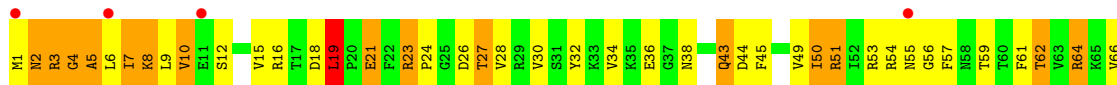
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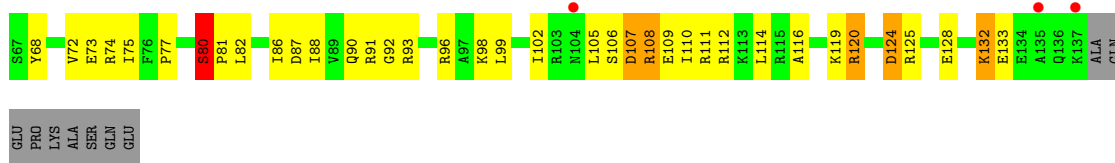


• Molecule 16: 50S ribosomal protein L19

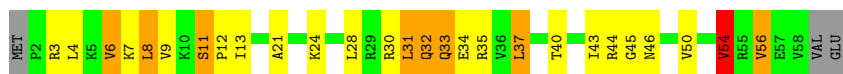


• Molecule 16: 50S ribosomal protein L19

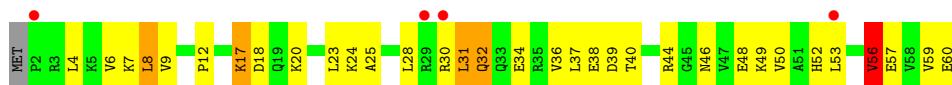




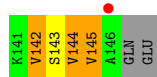
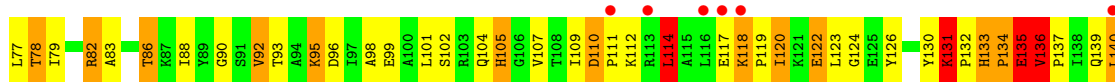
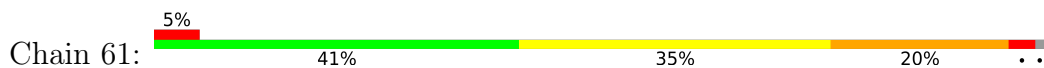
• Molecule 17: 50S ribosomal protein L30



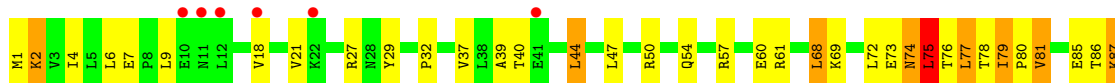
• Molecule 17: 50S ribosomal protein L30



• Molecule 18: 50S ribosomal protein L9



• Molecule 18: 50S ribosomal protein L9

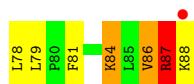
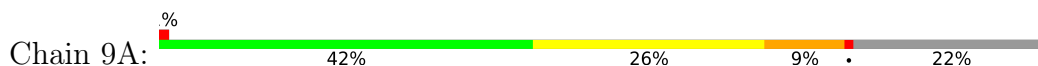


• Molecule 19: 30S ribosomal protein S18

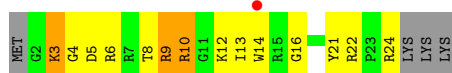




- Molecule 19: 30S ribosomal protein S18



- Molecule 20: 30S ribosomal protein Thx



- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: 50S ribosomal protein L14

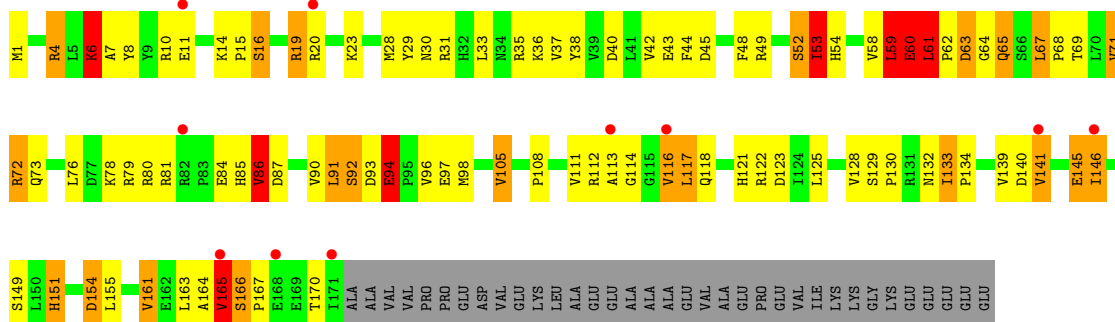


- Molecule 21: 50S ribosomal protein L14

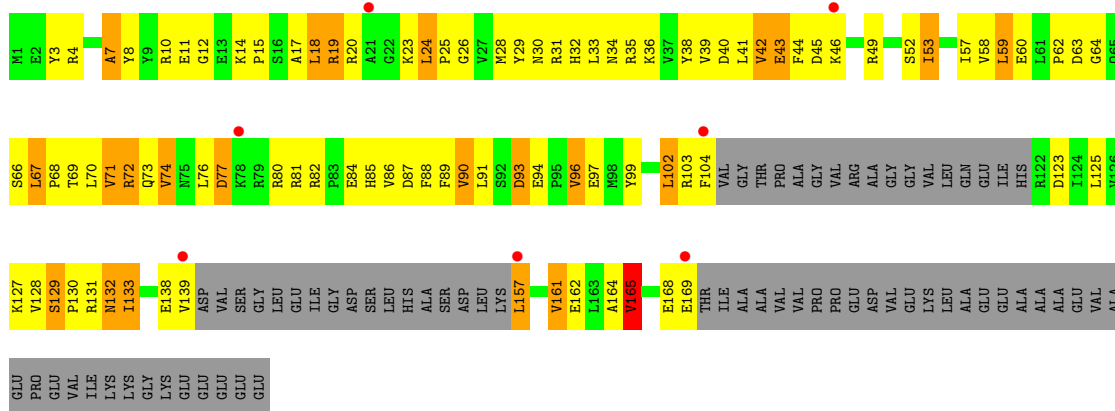
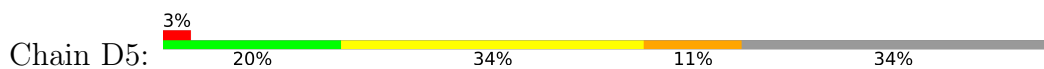




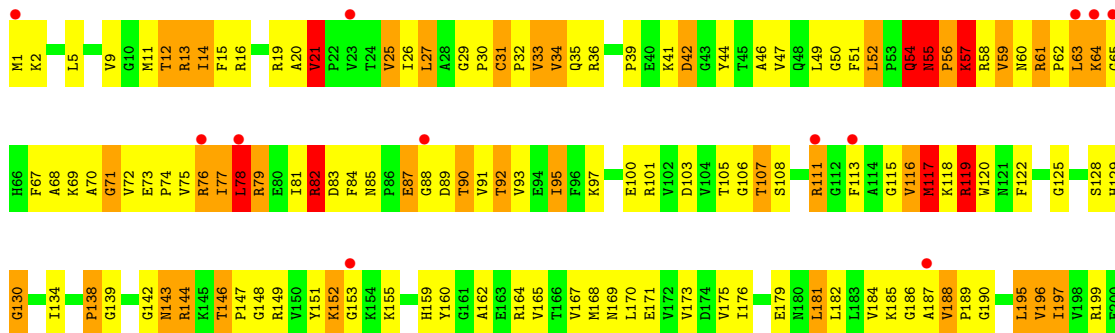
• Molecule 22: 50S ribosomal protein L25

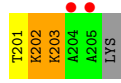


• Molecule 22: 50S ribosomal protein L25

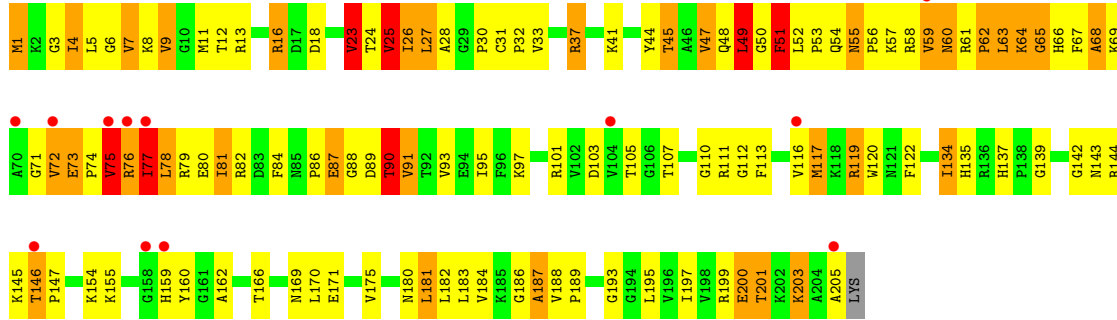


• Molecule 23: 50S ribosomal protein L3

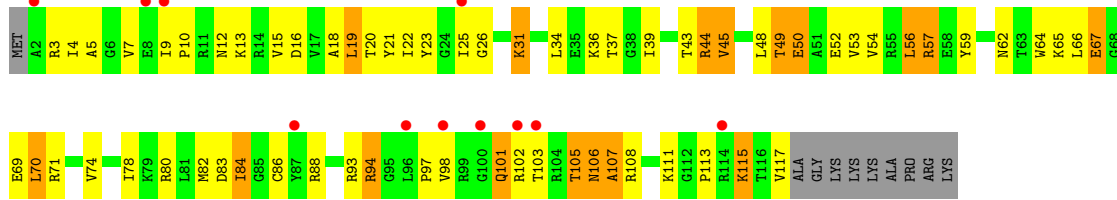




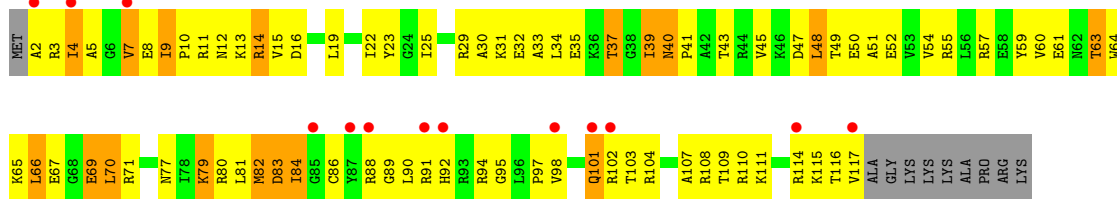
• Molecule 23: 50S ribosomal protein L3



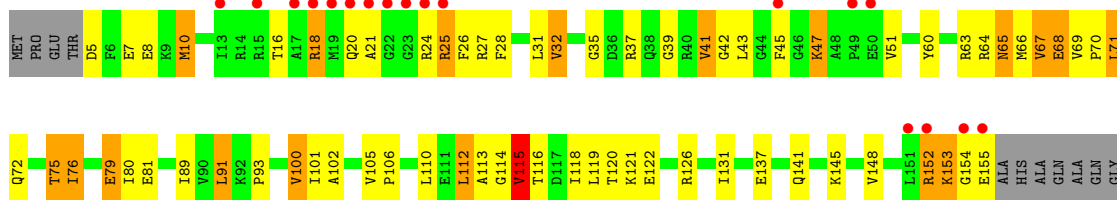
• Molecule 24: 30S ribosomal protein S13



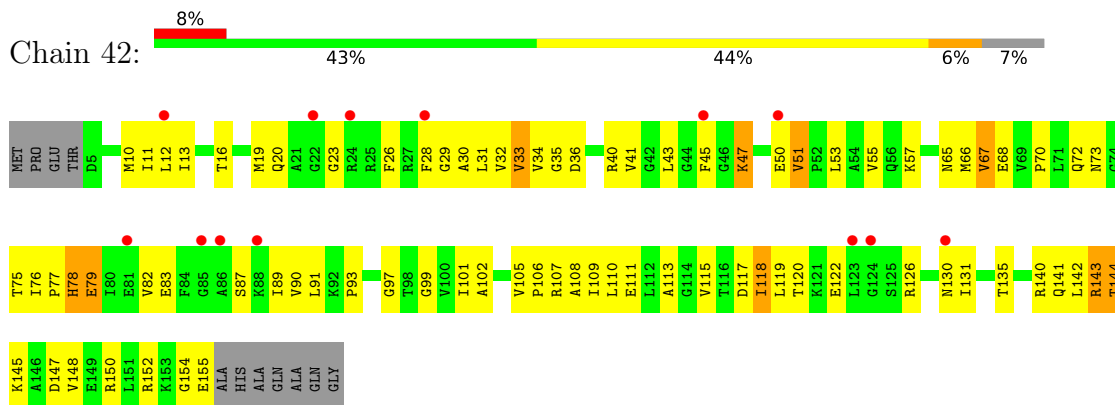
• Molecule 24: 30S ribosomal protein S13



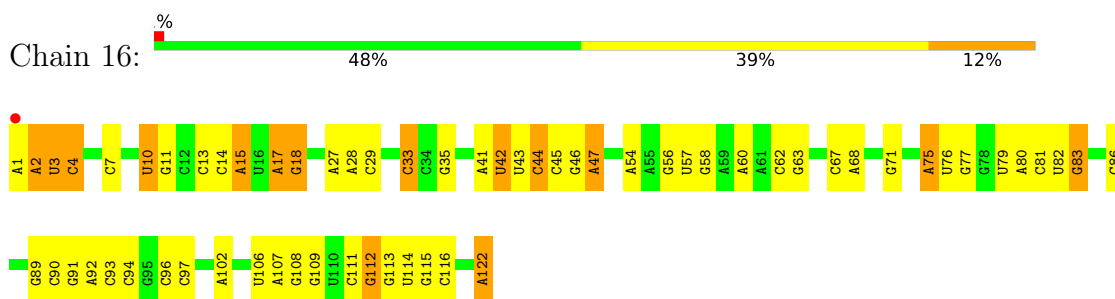
• Molecule 25: 30S ribosomal protein S5



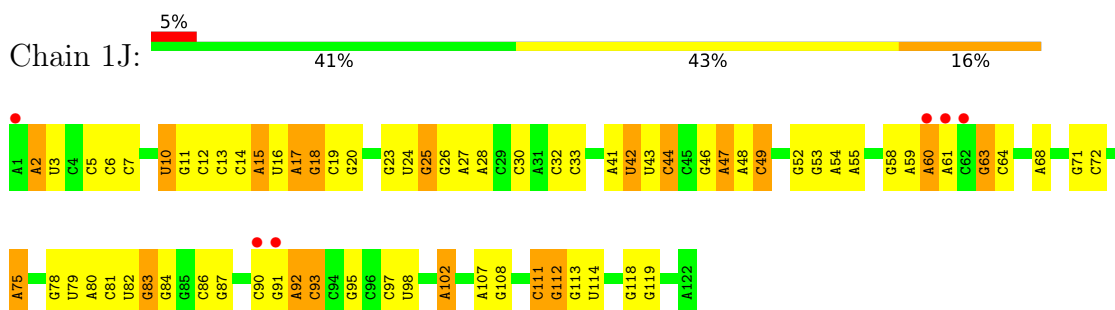
● Molecule 25: 30S ribosomal protein S5



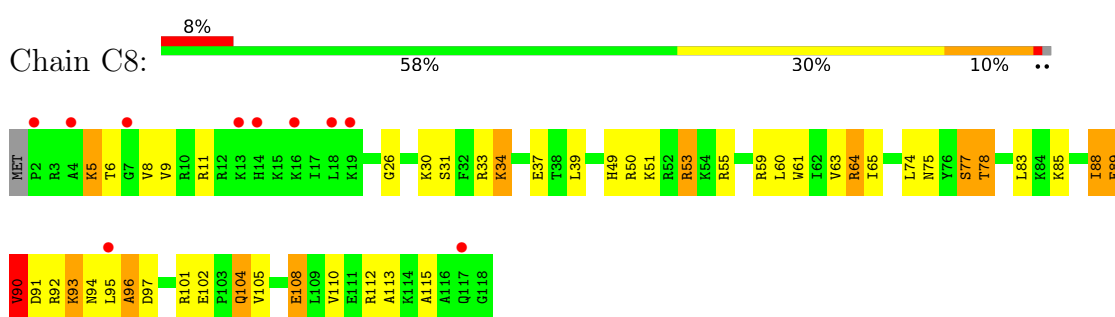
● Molecule 26: 5S ribosomal RNA



● Molecule 26: 5S ribosomal RNA

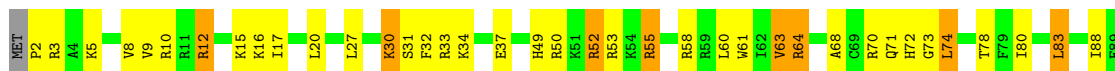


● Molecule 27: 50S ribosomal protein L20

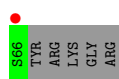


● Molecule 27: 50S ribosomal protein L20

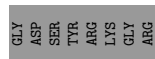
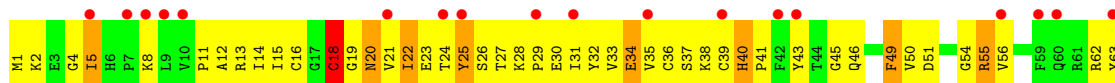




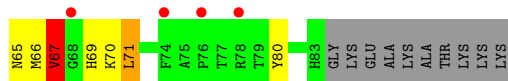
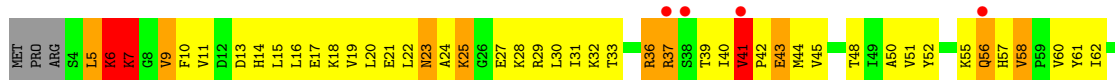
• Molecule 28: 50S ribosomal protein L31



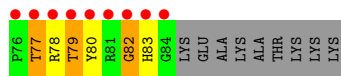
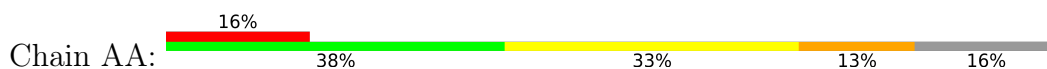
• Molecule 28: 50S ribosomal protein L31



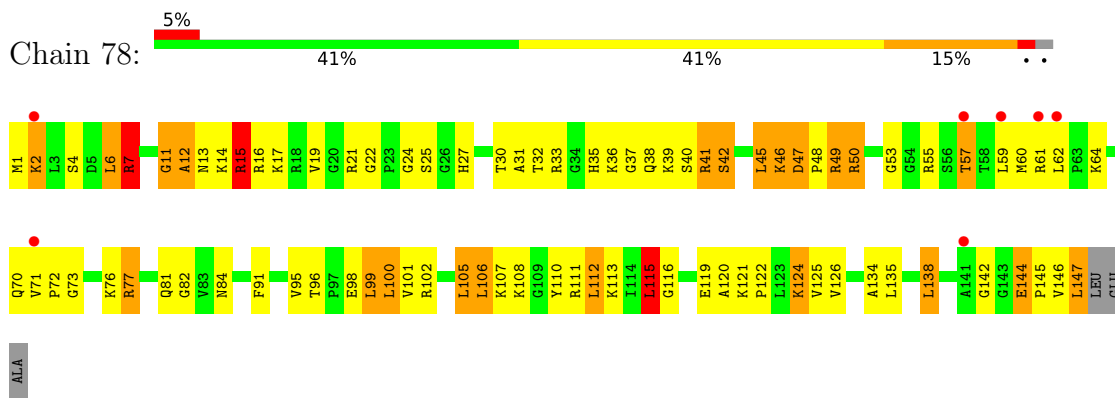
• Molecule 29: 30S ribosomal protein S19



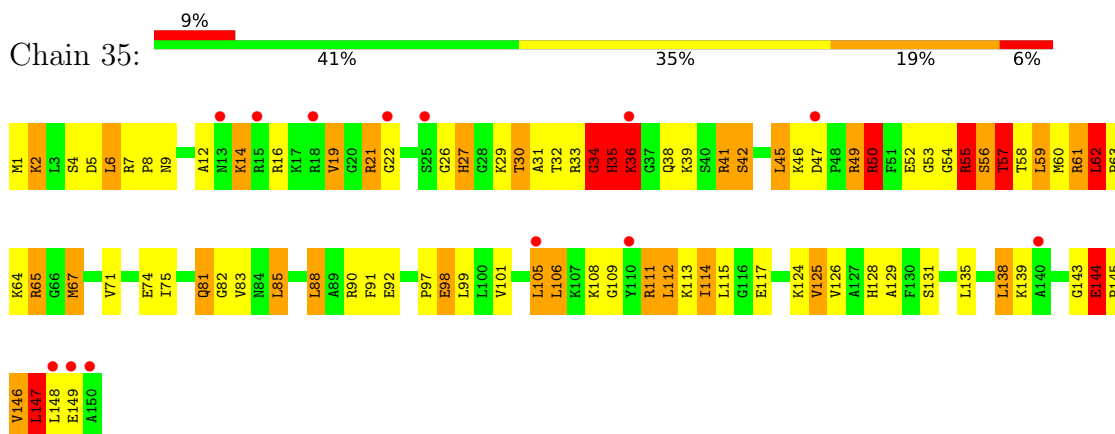
• Molecule 29: 30S ribosomal protein S19



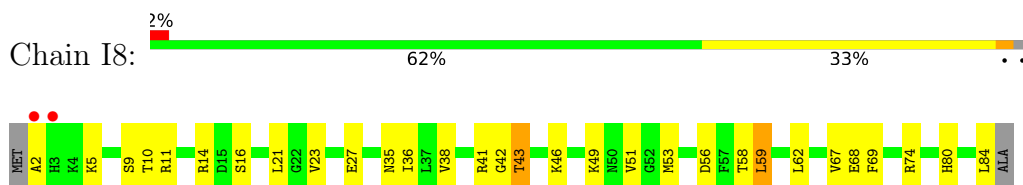
• Molecule 30: 50S ribosomal protein L15



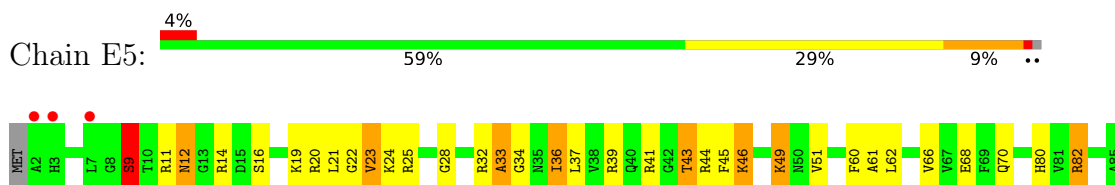
- Molecule 30: 50S ribosomal protein L15



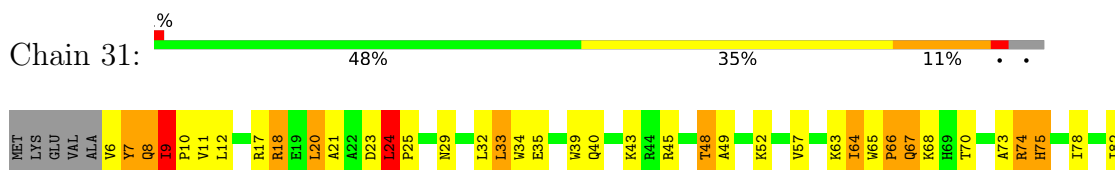
- Molecule 31: 50S ribosomal protein L27

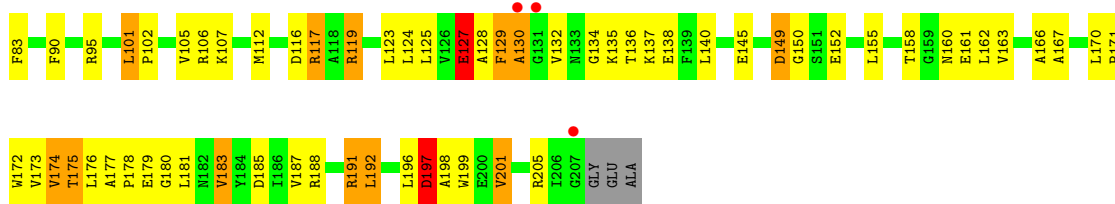


- Molecule 31: 50S ribosomal protein L27

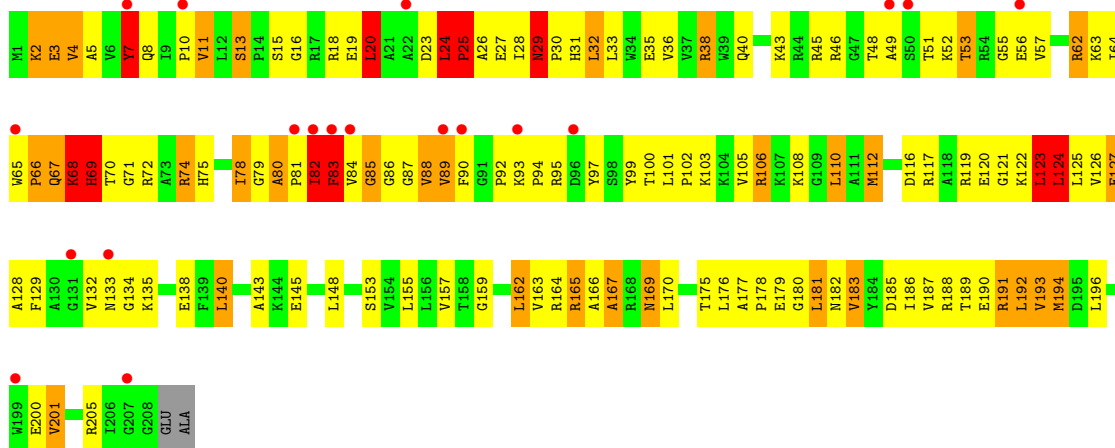


- Molecule 32: 50S ribosomal protein L4

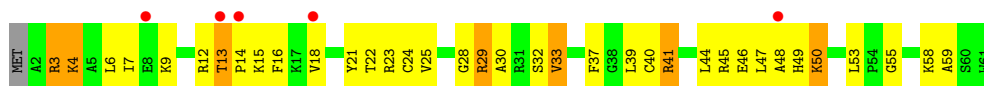




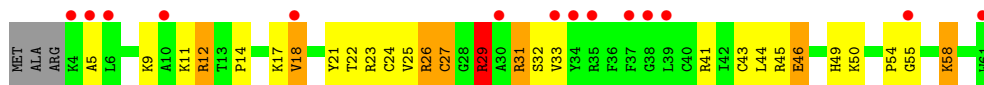
• Molecule 32: 50S ribosomal protein L4



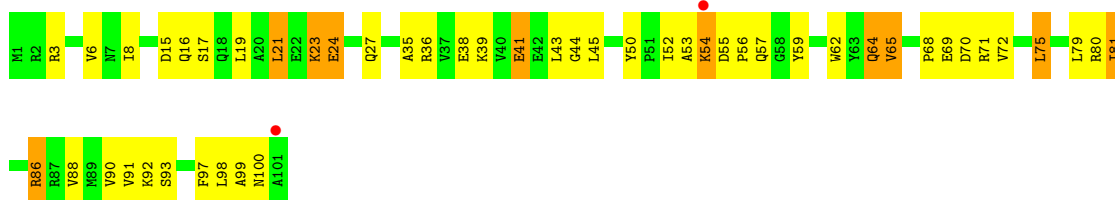
• Molecule 33: 30S ribosomal protein S14 type Z



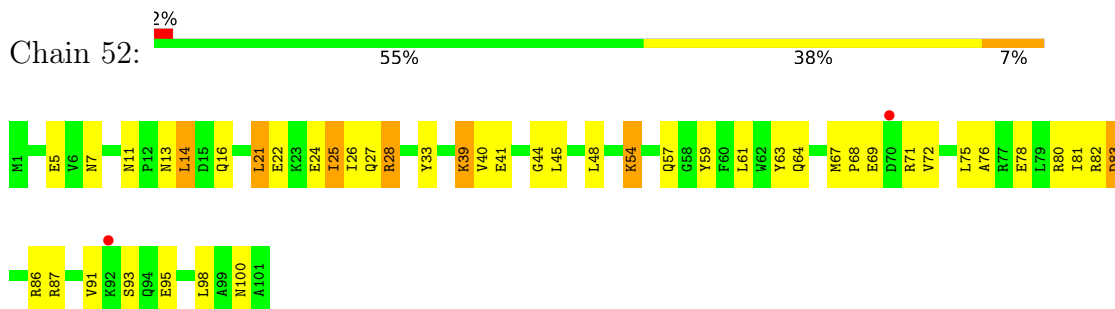
• Molecule 33: 30S ribosomal protein S14 type Z



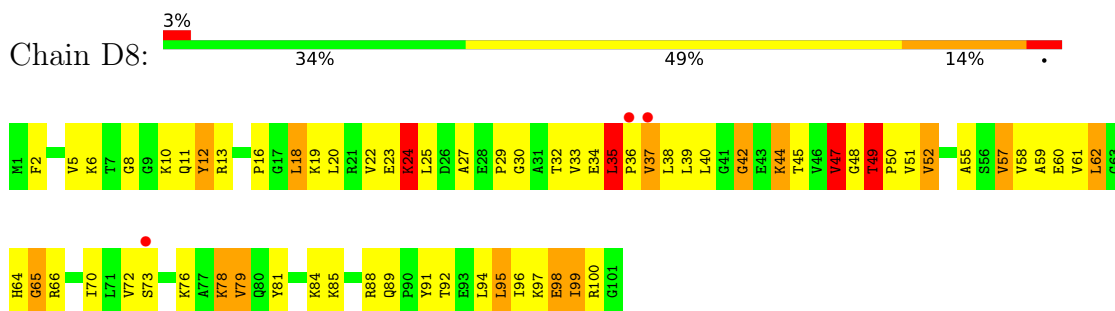
• Molecule 34: 30S ribosomal protein S6



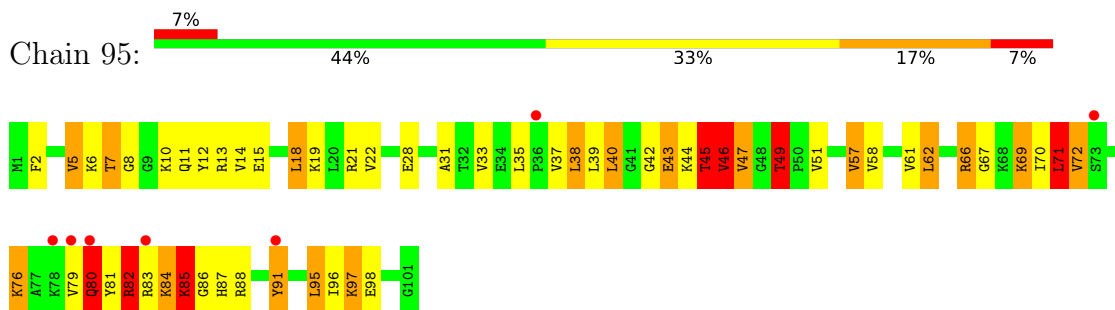
- Molecule 34: 30S ribosomal protein S6



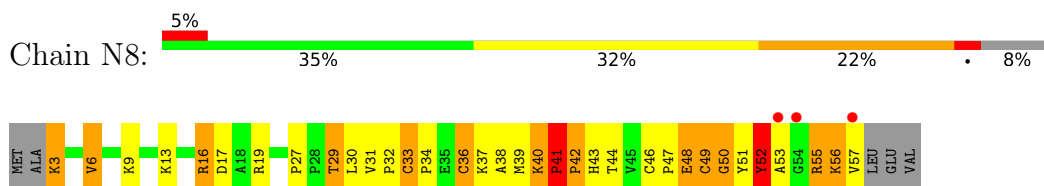
- Molecule 35: 50S ribosomal protein L21



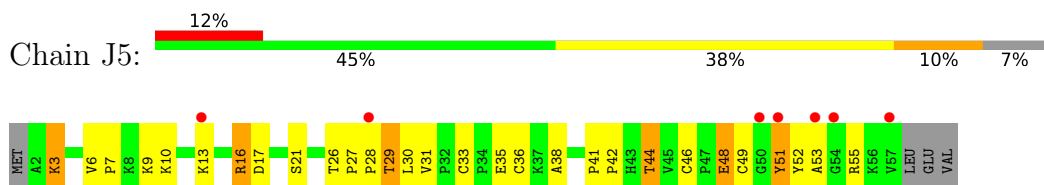
- Molecule 35: 50S ribosomal protein L21



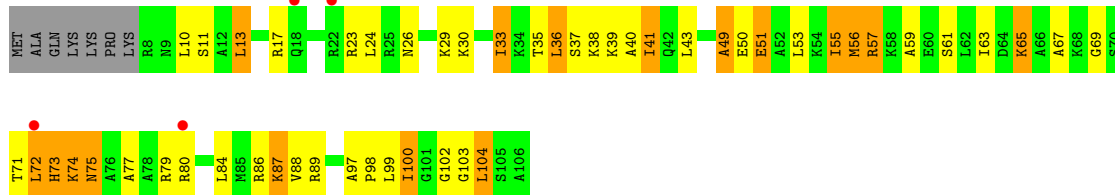
- Molecule 36: 50S ribosomal protein L32



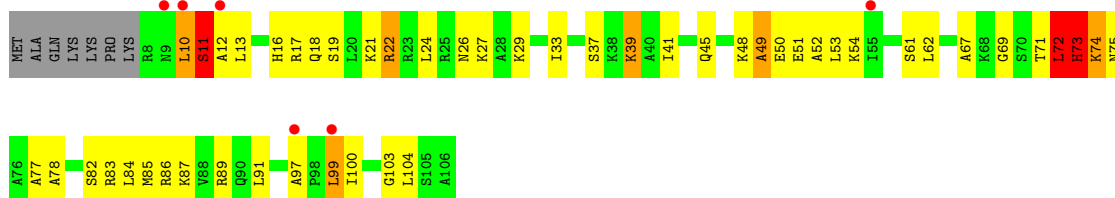
- Molecule 36: 50S ribosomal protein L32



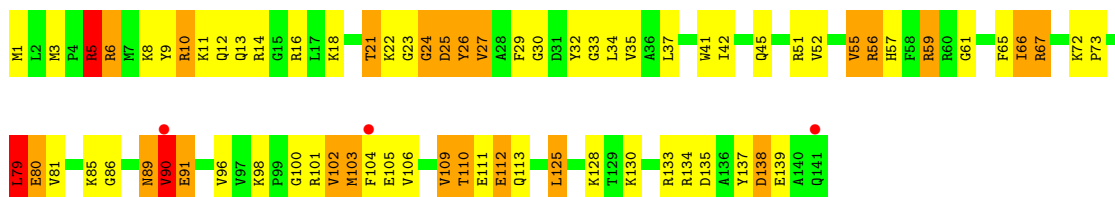
- Molecule 37: 30S ribosomal protein S20



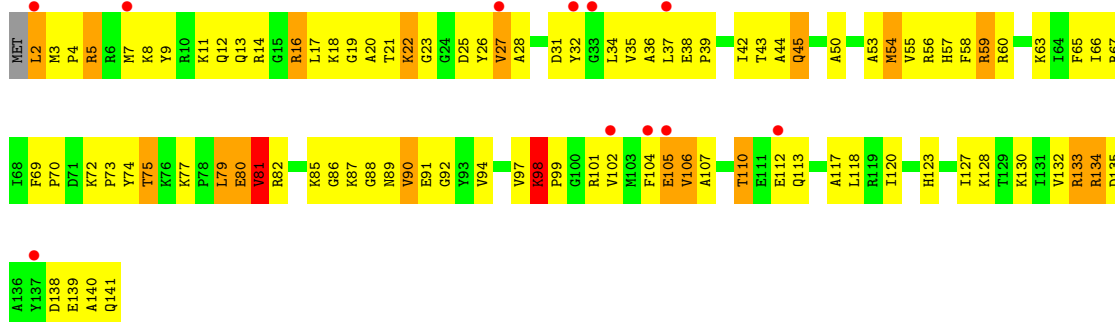
• Molecule 37: 30S ribosomal protein S20



• Molecule 38: 50S ribosomal protein L16

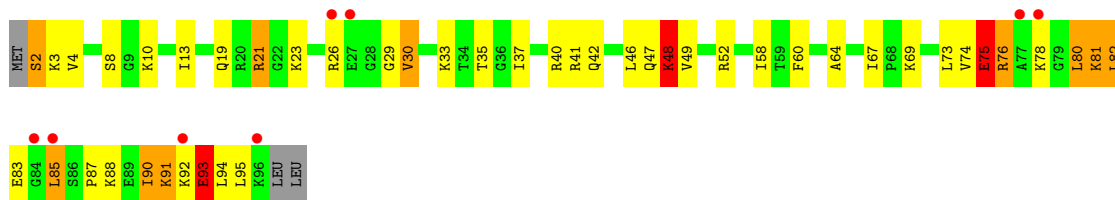


• Molecule 38: 50S ribosomal protein L16

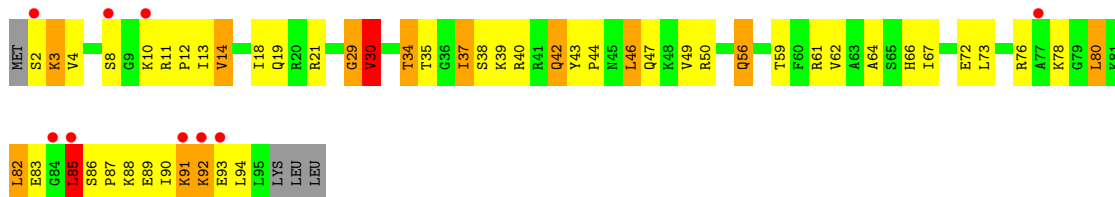
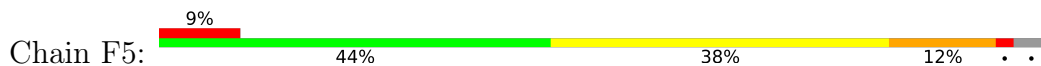


• Molecule 39: 50S ribosomal protein L28

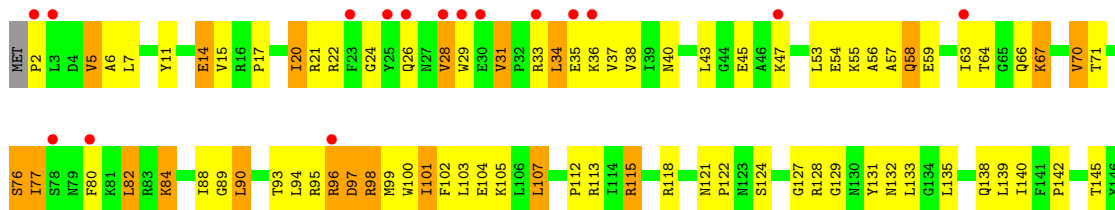




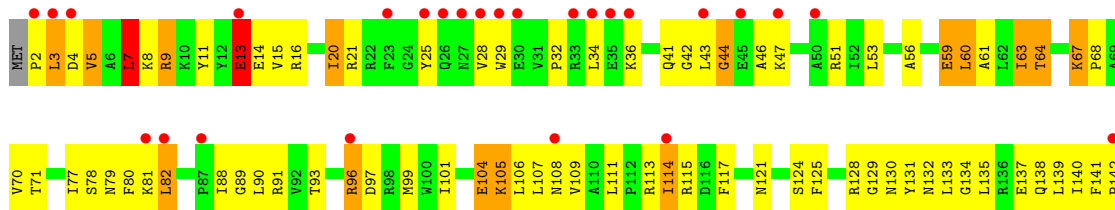
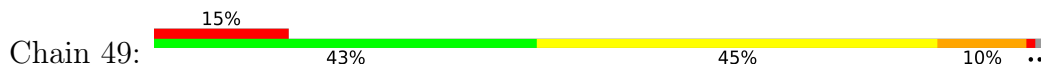
• Molecule 39: 50S ribosomal protein L28



• Molecule 40: 50S ribosomal protein L5

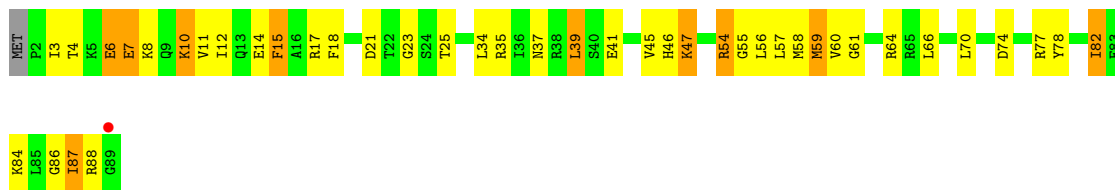


• Molecule 40: 50S ribosomal protein L5

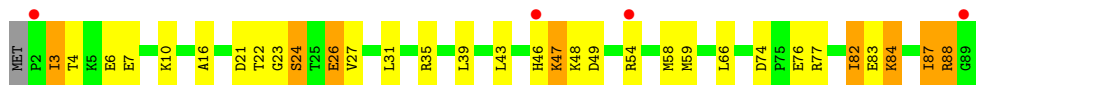


• Molecule 41: 30S ribosomal protein S15

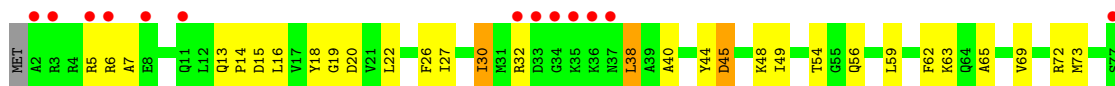




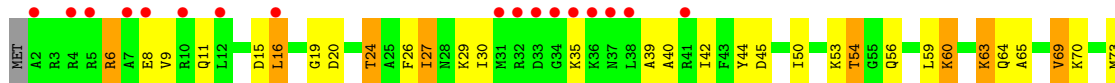
- Molecule 41: 30S ribosomal protein S15



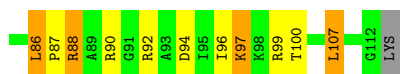
- Molecule 42: 30S ribosomal protein S7



- Molecule 42: 30S ribosomal protein S7



- Molecule 43: 50S ribosomal protein L22



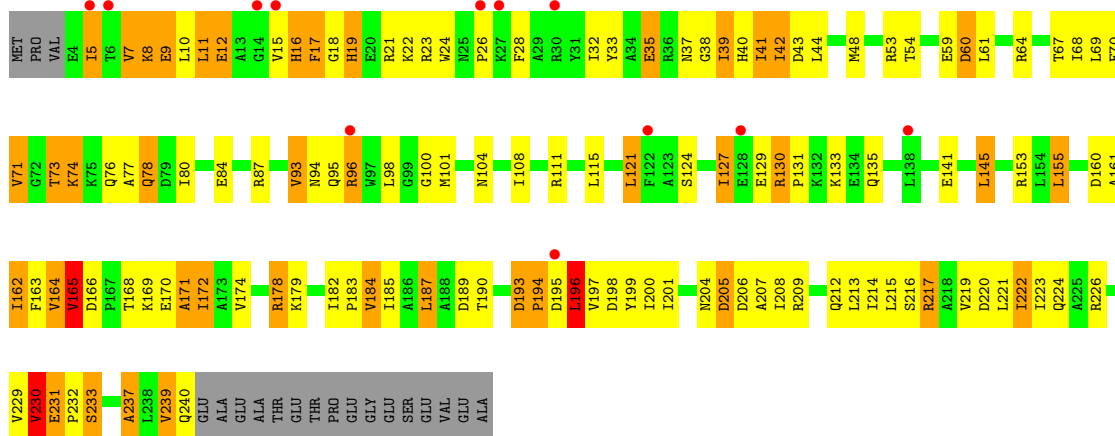
- Molecule 43: 50S ribosomal protein L22

Chain A5: 49% 39% 12%



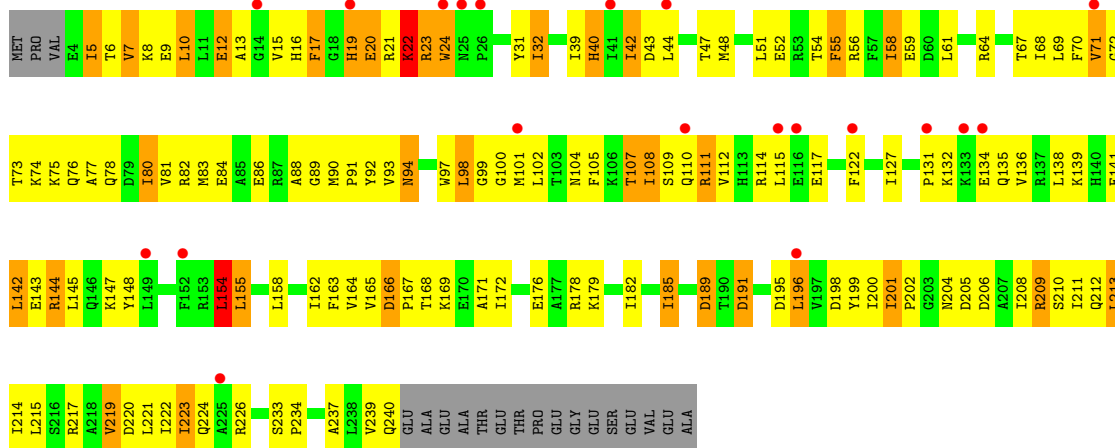
• Molecule 44: 30S ribosomal protein S2

Chain 1E: 5% 42% 34% 16% 7%



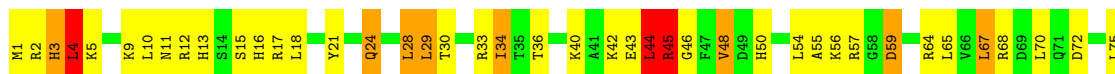
• Molecule 44: 30S ribosomal protein S2

Chain 12: 8% 36% 42% 13% 7%



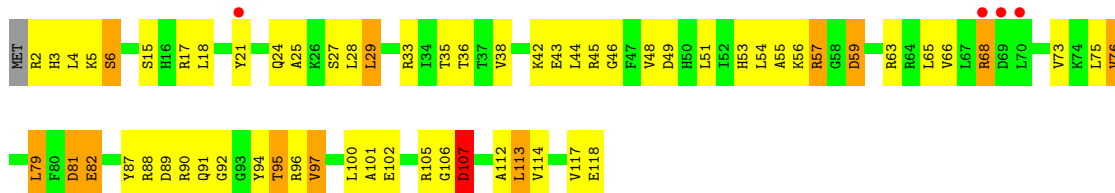
• Molecule 45: 50S ribosomal protein L17

Chain 98: 46% 37% 14%





- Molecule 45: 50S ribosomal protein L17



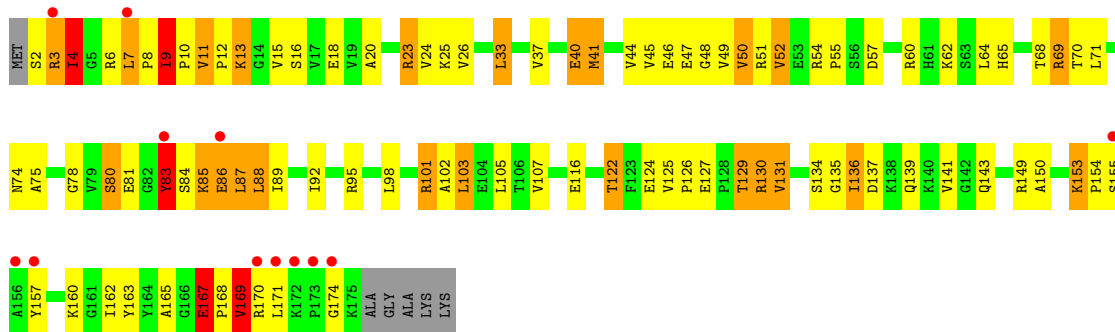
- Molecule 46: 50S ribosomal protein L29



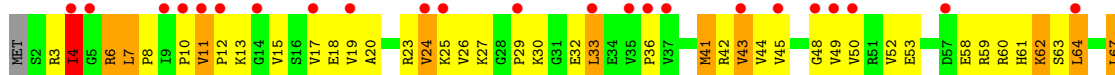
- Molecule 46: 50S ribosomal protein L29

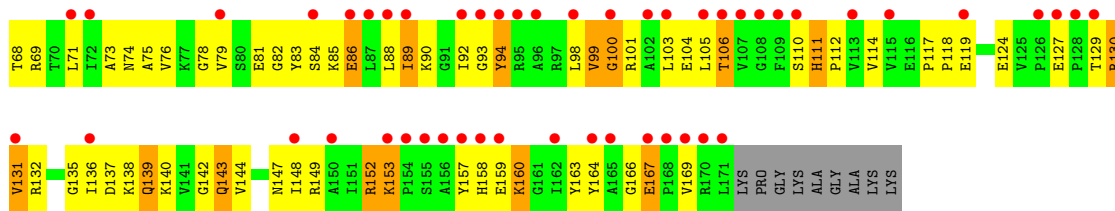


- Molecule 47: 50S ribosomal protein L6

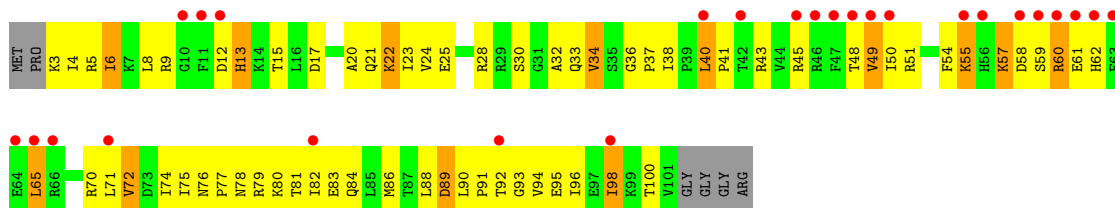


- Molecule 47: 50S ribosomal protein L6

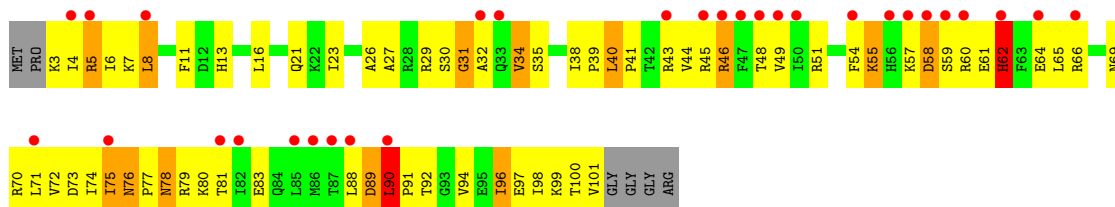




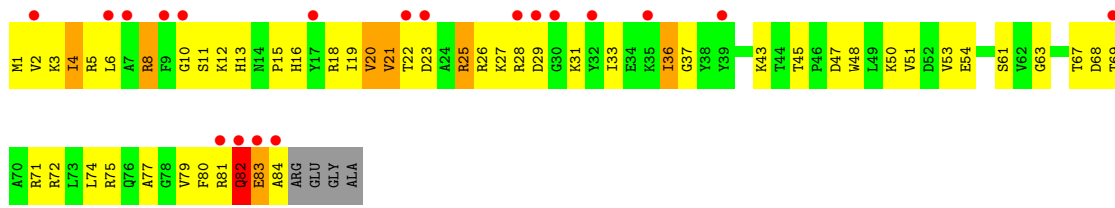
• Molecule 48: 30S ribosomal protein S10



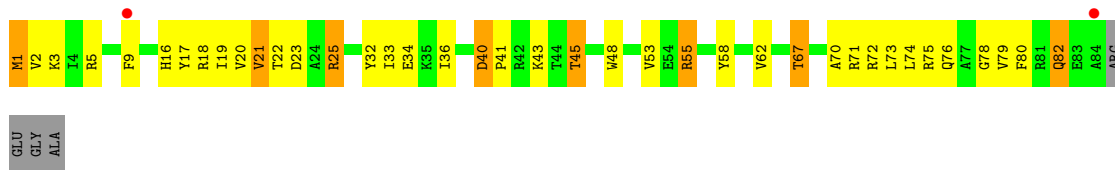
• Molecule 48: 30S ribosomal protein S10



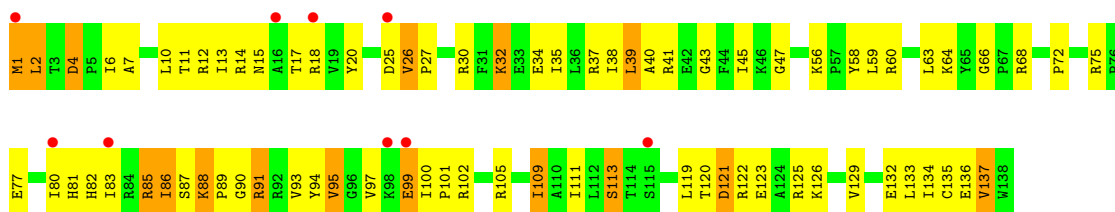
• Molecule 49: 30S ribosomal protein S16



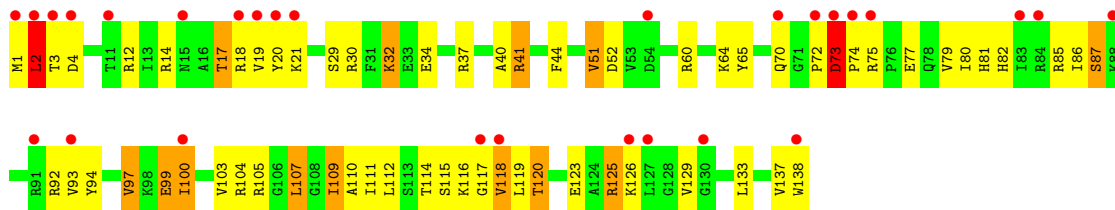
• Molecule 49: 30S ribosomal protein S16



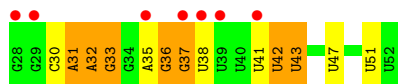
• Molecule 50: 30S ribosomal protein S8



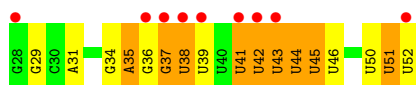
- Molecule 50: 30S ribosomal protein S8



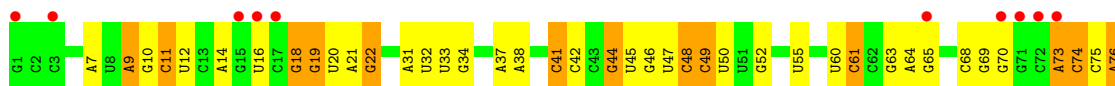
- Molecule 51: mRNA



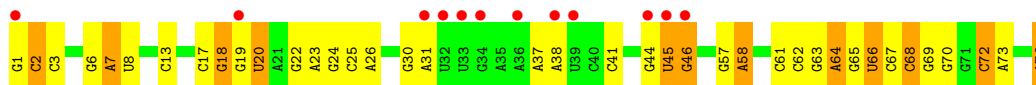
- Molecule 51: mRNA



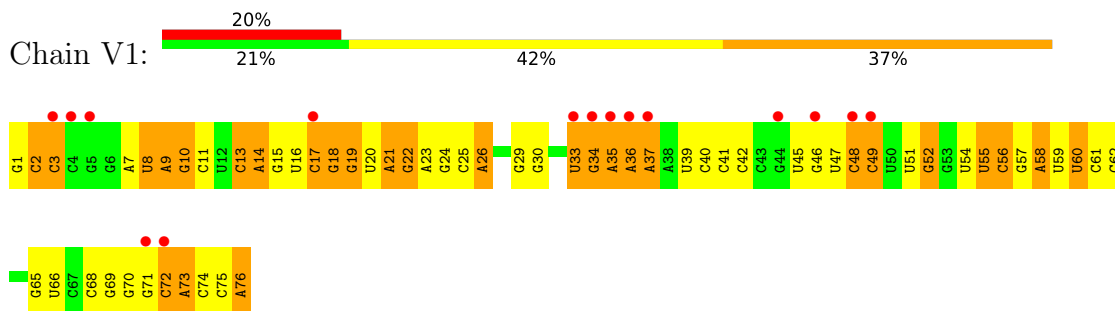
- Molecule 52: tRNA-Phe



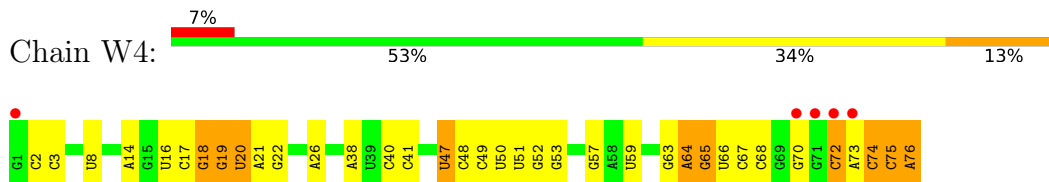
- Molecule 52: tRNA-Phe



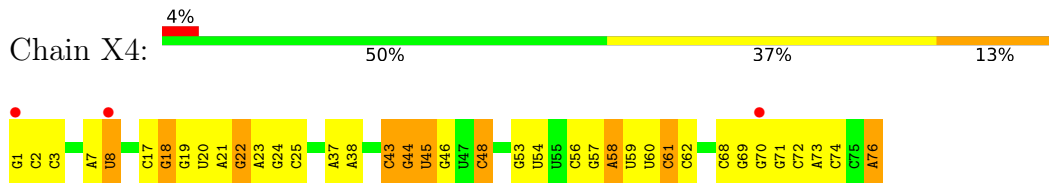
- Molecule 52: tRNA-Phe



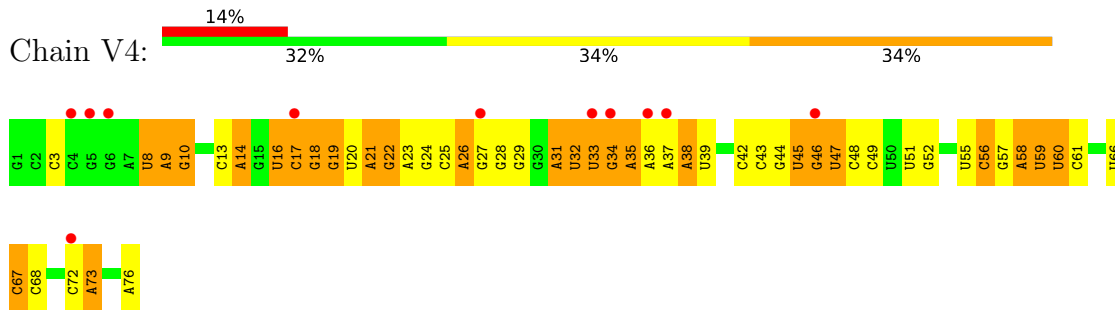
• Molecule 52: tRNA-Phe



• 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, $\alpha$ , $\beta$ , $\gamma$	209.21Å 447.98Å 620.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.61 – 3.15 104.61 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (104.61-3.15) 94.4 (104.61-3.15)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.89 (at 3.13Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.202 , 0.247 0.205 , 0.248	Depositor DCC
$R_{free}$ test set	19886 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 83.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	300009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	13	0.43	0/36276	0.65	10/56615 (0.0%)
1	1G	0.39	1/36394 (0.0%)	0.61	10/56800 (0.0%)
2	65	0.75	0/891	1.26	8/1187 (0.7%)
2	A8	0.78	0/891	1.15	3/1187 (0.3%)
3	B5	0.92	0/739	1.29	4/993 (0.4%)
3	F8	0.98	0/756	1.33	4/1014 (0.4%)
4	11	1.05	4/2176 (0.2%)	1.47	36/2933 (1.2%)
4	19	0.95	2/2170 (0.1%)	1.42	33/2926 (1.1%)
5	L5	1.09	0/417	1.25	3/550 (0.5%)
5	P8	1.15	1/417 (0.2%)	1.27	0/550
6	2A	0.62	0/879	1.09	5/1187 (0.4%)
6	2I	0.70	0/879	1.20	6/1187 (0.5%)
7	8A	0.64	0/836	1.02	1/1117 (0.1%)
7	8I	0.72	0/847	1.08	3/1131 (0.3%)
8	22	0.62	0/1636	1.05	4/2205 (0.2%)
8	2E	0.71	0/1629	1.03	3/2195 (0.1%)
9	82	0.53	1/1002 (0.1%)	0.96	4/1346 (0.3%)
9	8E	0.57	0/1028	1.02	3/1379 (0.2%)
10	15	0.70	0/1131	1.20	8/1525 (0.5%)
10	58	0.86	1/1131 (0.1%)	1.31	10/1525 (0.7%)
11	C5	1.00	2/807 (0.2%)	1.40	5/1076 (0.5%)
11	G8	1.02	1/796 (0.1%)	1.43	12/1062 (1.1%)
12	M5	1.16	3/525 (0.6%)	1.54	7/691 (1.0%)
12	Q8	1.71	8/486 (1.6%)	2.07	21/638 (3.3%)
13	3A	0.83	0/991	1.22	6/1327 (0.5%)
13	3I	0.93	0/972	1.29	7/1301 (0.5%)
14	32	0.64	0/1732	1.13	12/2318 (0.5%)
14	3E	0.79	0/1732	1.14	9/2318 (0.4%)
15	14	0.51	0/70167	0.72	20/109541 (0.0%)
15	1H	0.60	0/70233	0.77	23/109643 (0.0%)
16	75	0.85	0/1155	1.26	8/1542 (0.5%)
16	B8	0.93	0/1095	1.29	6/1463 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	H5	0.74	0/473	1.02	1/635 (0.2%)
17	L8	0.99	0/457	1.37	5/613 (0.8%)
18	61	0.78	0/1151	1.19	13/1558 (0.8%)
18	69	0.73	0/1151	1.22	14/1558 (0.9%)
19	9A	0.69	0/569	1.15	3/757 (0.4%)
19	9I	0.69	0/555	1.14	2/739 (0.3%)
20	1B	0.68	0/221	1.05	1/288 (0.3%)
20	1F	0.50	0/203	1.02	0/266
21	25	0.83	0/942	1.20	6/1269 (0.5%)
21	68	0.89	0/942	1.23	9/1269 (0.7%)
22	D5	0.65	0/1145	1.14	7/1547 (0.5%)
22	H8	0.75	1/1403 (0.1%)	1.27	16/1901 (0.8%)
23	21	0.98	0/1601	1.57	31/2160 (1.4%)
23	29	0.93	2/1601 (0.1%)	1.46	19/2160 (0.9%)
24	4A	0.52	0/938	0.94	3/1258 (0.2%)
24	4I	0.60	0/938	1.02	2/1258 (0.2%)
25	42	0.62	0/1171	1.06	3/1576 (0.2%)
25	4E	0.80	0/1171	1.13	4/1576 (0.3%)
26	16	0.51	0/2928	0.74	0/4568
26	1J	0.44	0/2928	0.73	0/4568
27	85	0.81	0/981	1.17	4/1306 (0.3%)
27	C8	0.96	0/981	1.18	5/1306 (0.4%)
28	I5	0.99	0/527	1.35	8/709 (1.1%)
28	M8	0.92	1/545 (0.2%)	1.17	2/733 (0.3%)
29	AA	0.61	0/638	1.15	8/860 (0.9%)
29	AI	0.69	1/657 (0.2%)	1.14	2/885 (0.2%)
30	35	0.88	0/1161	1.48	21/1544 (1.4%)
30	78	0.92	0/1139	1.43	16/1514 (1.1%)
31	E5	0.92	0/653	1.39	5/872 (0.6%)
31	I8	0.93	0/665	1.28	2/885 (0.2%)
32	31	1.01	1/1620 (0.1%)	1.27	10/2194 (0.5%)
32	39	0.86	0/1662	1.46	22/2249 (1.0%)
33	5A	0.56	0/484	1.06	1/643 (0.2%)
33	5I	0.70	1/500 (0.2%)	1.02	0/664
34	52	0.70	0/855	1.03	2/1154 (0.2%)
34	5E	0.69	0/855	1.03	2/1154 (0.2%)
35	95	0.88	2/789 (0.3%)	1.34	6/1057 (0.6%)
35	D8	0.96	1/789 (0.1%)	1.40	9/1057 (0.9%)
36	J5	0.90	0/448	1.27	4/606 (0.7%)
36	N8	1.07	0/443	2.06	13/599 (2.2%)
37	BA	0.63	0/764	1.20	7/1007 (0.7%)
37	BI	0.59	0/764	1.06	3/1007 (0.3%)
38	45	0.89	2/1134 (0.2%)	1.22	5/1517 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	88	1.00	1/1142 (0.1%)	1.40	15/1527 (1.0%)
39	F5	0.86	0/744	1.30	5/989 (0.5%)
39	J8	0.99	0/753	1.35	7/1000 (0.7%)
40	41	0.67	0/1498	1.10	4/2016 (0.2%)
40	49	0.54	0/1498	1.12	12/2016 (0.6%)
41	6A	0.67	0/744	0.89	1/992 (0.1%)
41	6I	0.75	0/744	1.11	2/992 (0.2%)
42	62	0.59	0/1218	0.95	0/1632
42	6E	0.59	0/1171	0.96	1/1567 (0.1%)
43	A5	0.93	0/910	1.24	5/1220 (0.4%)
43	E8	0.97	0/901	1.25	6/1209 (0.5%)
44	12	0.57	0/1959	1.02	7/2642 (0.3%)
44	1E	0.60	1/1959 (0.1%)	1.01	3/2642 (0.1%)
45	55	0.83	0/973	1.11	2/1302 (0.2%)
45	98	0.90	1/981 (0.1%)	1.16	6/1312 (0.5%)
46	G5	0.77	0/569	1.22	5/753 (0.7%)
46	K8	0.94	0/577	1.39	6/763 (0.8%)
47	51	0.79	0/1362	1.31	10/1841 (0.5%)
47	59	0.67	0/1332	1.26	15/1802 (0.8%)
48	1A	0.54	0/814	0.99	3/1095 (0.3%)
48	1I	0.63	0/814	1.12	9/1095 (0.8%)
49	7A	0.68	0/721	1.04	2/970 (0.2%)
49	7I	0.66	0/721	1.11	1/970 (0.1%)
50	72	0.61	0/1135	1.09	5/1527 (0.3%)
50	7E	0.69	0/1135	1.16	7/1527 (0.5%)
51	Y1	0.50	0/579	0.64	0/899
51	Y4	0.42	0/579	0.66	0/899
52	V1	0.41	0/1809	0.62	0/2819
52	V4	0.36	0/1809	0.57	0/2819
52	W1	0.38	0/1809	0.54	0/2819
52	W4	0.33	0/1809	0.47	0/2819
52	X1	0.48	0/1809	0.72	0/2819
52	X4	0.43	0/1809	0.70	0/2819
All	All	0.61	39/322745 (0.0%)	0.87	729/483631 (0.2%)

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
3	B5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	11	0	2
4	19	0	5
5	P8	0	1
6	2A	0	1
9	82	0	1
9	8E	0	1
10	15	0	1
11	C5	0	2
11	G8	0	4
12	M5	0	3
12	Q8	0	9
13	3A	0	2
14	32	0	3
16	75	0	2
16	B8	0	1
18	61	0	4
18	69	0	3
22	H8	0	3
23	21	0	5
23	29	0	1
24	4I	0	1
27	85	0	1
27	C8	0	1
28	M8	0	2
29	AI	0	1
30	35	0	6
30	78	0	6
31	I8	0	1
32	39	0	7
33	5A	0	1
35	D8	0	1
36	J5	0	1
36	N8	0	2
37	BA	0	2
37	BI	0	1
38	45	0	2
38	88	0	2
39	F5	0	1
39	J8	0	3
40	41	0	1
40	49	0	1
43	A5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	12	0	2
44	1E	0	2
45	98	0	2
46	G5	0	3
46	K8	0	2
48	1A	0	1
All	All	0	112

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	29	135	HIS	CA-C	-7.71	1.44	1.52
12	Q8	57	ARG	CA-C	7.32	1.60	1.52
38	45	27	VAL	CA-CB	7.10	1.64	1.54
12	M5	50	LEU	CA-C	6.86	1.60	1.52
35	95	79	VAL	CA-C	6.46	1.60	1.52

The worst 5 of 729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	N8	41	PRO	CA-C-N	19.11	143.73	119.84
36	N8	41	PRO	C-N-CA	19.11	143.73	119.84
4	19	235	GLY	N-CA-C	16.30	128.66	112.04
6	2I	102	GLY	N-CA-C	-14.31	89.81	111.42
11	C5	39	VAL	N-CA-C	13.85	126.20	112.90

There are no chirality outliers.

5 of 112 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	11	197	GLY	Peptide
4	11	273	ARG	Peptide
6	2A	49	GLY	Peptide
9	8E	110	GLU	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	16361	686	0
1	1G	32514	0	16416	653	0
2	65	881	0	943	62	0
2	A8	881	0	943	57	0
3	B5	725	0	778	41	0
3	F8	742	0	803	42	0
4	11	2126	0	2208	73	0
4	19	2120	0	2197	107	0
5	L5	409	0	454	15	0
5	P8	409	0	454	9	0
6	2A	864	0	881	31	0
6	2I	864	0	881	44	0
7	8A	823	0	891	28	0
7	8I	834	0	904	58	0
8	22	1612	0	1677	77	0
8	2E	1605	0	1668	73	0
9	82	983	0	1006	68	0
9	8E	1009	0	1037	72	0
10	15	1104	0	1180	45	0
10	58	1104	0	1180	68	0
11	C5	794	0	886	67	0
11	G8	783	0	873	62	0
12	M5	517	0	582	51	0
12	Q8	480	0	549	111	0
13	3A	975	0	1062	39	0
13	3I	956	0	1046	45	0
14	32	1702	0	1764	76	0
14	3E	1702	0	1763	80	0
15	14	62647	0	31583	1253	0
15	1H	62707	0	31614	1211	0
16	75	1141	0	1202	61	0
16	B8	1081	0	1141	61	0
17	H5	468	0	518	22	0
17	L8	452	0	503	15	0
18	61	1136	0	1223	62	0
18	69	1136	0	1223	44	0
19	9A	564	0	631	28	0
19	9I	550	0	613	31	0
20	1B	217	0	234	14	0
20	1F	199	0	208	14	0
21	25	932	0	996	42	0
21	68	932	0	996	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D5	1120	0	1146	65	0
22	H8	1373	0	1402	77	0
23	21	1568	0	1634	109	0
23	29	1568	0	1633	119	0
24	4A	928	0	987	68	0
24	4I	928	0	987	58	0
25	42	1155	0	1213	50	0
25	4E	1155	0	1213	50	0
26	16	2617	0	1328	56	0
26	1J	2617	0	1328	58	0
27	85	963	0	1022	57	0
27	C8	963	0	1022	44	0
28	I5	515	0	514	38	0
28	M8	533	0	526	50	0
29	AA	624	0	636	34	0
29	AI	643	0	662	41	0
30	35	1144	0	1228	84	0
30	78	1122	0	1206	82	0
31	E5	645	0	652	31	0
31	I8	656	0	683	23	0
32	31	1585	0	1632	85	0
32	39	1627	0	1680	100	0
33	5A	475	0	511	27	0
33	5I	491	0	529	28	0
34	52	842	0	857	27	0
34	5E	842	0	857	31	0
35	95	778	0	852	71	0
35	D8	778	0	852	49	0
36	J5	434	0	454	22	0
36	N8	429	0	449	40	0
37	BA	762	0	861	38	0
37	BI	762	0	861	44	0
38	45	1113	0	1167	92	0
38	88	1121	0	1179	67	0
39	F5	737	0	813	40	0
39	J8	746	0	826	41	0
40	41	1473	0	1535	86	0
40	49	1473	0	1535	77	0
41	6A	733	0	771	18	0
41	6I	733	0	771	30	0
42	62	1200	0	1238	44	0
42	6E	1157	0	1202	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	A5	899	0	964	36	0
43	E8	890	0	951	27	0
44	12	1924	0	1975	110	0
44	1E	1924	0	1975	92	0
45	55	959	0	1021	37	0
45	98	967	0	1033	58	0
46	G5	567	0	618	30	0
46	K8	575	0	634	31	0
47	51	1336	0	1418	76	0
47	59	1307	0	1382	73	0
48	1A	801	0	849	45	0
48	1I	801	0	849	48	0
49	7A	705	0	725	29	0
49	7I	705	0	725	47	0
50	72	1115	0	1177	50	0
50	7E	1115	0	1177	55	0
51	Y1	521	0	262	11	0
51	Y4	521	0	262	21	0
52	V1	1619	0	822	58	0
52	V4	1619	0	822	46	0
52	W1	1619	0	822	24	0
52	W4	1619	0	822	24	0
52	X1	1619	0	822	22	0
52	X4	1619	0	822	31	0
53	13	66	0	0	1	0
53	14	165	0	0	8	0
53	1G	66	0	0	3	0
53	1H	132	0	0	14	0
54	11	4	0	0	0	0
54	13	197	0	0	0	0
54	14	591	0	0	0	0
54	15	1	0	0	0	0
54	16	14	0	0	0	0
54	19	1	0	0	0	0
54	1G	189	0	0	0	0
54	1H	657	0	0	0	0
54	1J	14	0	0	0	0
54	21	4	0	0	0	0
54	25	3	0	0	0	0
54	29	6	0	0	0	0
54	2A	1	0	0	0	0
54	31	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	32	3	0	0	0	0
54	35	2	0	0	0	0
54	39	1	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	51	1	0	0	0	0
54	52	1	0	0	0	0
54	55	3	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	75	1	0	0	0	0
54	78	3	0	0	0	0
54	7A	1	0	0	0	0
54	88	5	0	0	0	0
54	8A	1	0	0	0	0
54	8I	1	0	0	0	0
54	98	3	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	BA	1	0	0	0	0
54	C5	1	0	0	0	0
54	C8	1	0	0	0	0
54	D8	2	0	0	0	0
54	E5	2	0	0	0	0
54	G8	1	0	0	0	0
54	I8	3	0	0	0	0
54	J8	1	0	0	0	0
54	K8	1	0	0	0	0
54	N8	1	0	0	0	0
54	P8	1	0	0	0	0
54	W1	3	0	0	0	0
54	W4	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	X1	9	0	0	0	0
54	X4	5	0	0	0	0
54	Y1	1	0	0	0	0
54	Y4	1	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	114	0
56	19	8	0	0	1	0
56	1G	72	0	0	6	0
56	1H	532	0	0	124	0
56	21	2	0	0	1	0
56	29	3	0	0	0	0
56	31	3	0	0	0	0
56	35	1	0	0	0	0
56	39	3	0	0	0	0
56	55	2	0	0	0	0
56	5A	1	0	0	1	0
56	6A	2	0	0	0	0
56	6I	1	0	0	0	0
56	78	2	0	0	0	0
56	7A	1	0	0	0	0
56	A5	1	0	0	0	0
56	C8	2	0	0	1	0
56	D8	1	0	0	0	0
56	E8	1	0	0	0	0
56	F5	1	0	0	0	0
56	F8	1	0	0	0	0
56	I8	3	0	0	0	0
56	J8	2	0	0	0	0
56	L5	2	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	300009	0	199455	8077	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 8077 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)
1:1G:2165:G:O6	51:Y4:29:G:N2	1.73	1.19
15:14:1697:G:OP2	56:14:3601:HOH:O	1.72	1.08
15:14:1808:C:OP1	56:14:3602:HOH:O	1.74	1.04
15:14:2463:A:OP1	56:14:3604:HOH:O	1.76	1.04
15:1H:1067:U:HO2'	15:1H:1069:A:H2	1.04	1.03

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%)	87 (80%)	19 (17%)	3 (3%)	4	20
2	A8	109/112 (97%)	94 (86%)	14 (13%)	1 (1%)	14	43
3	B5	90/96 (94%)	80 (89%)	7 (8%)	3 (3%)	3	17
3	F8	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	5	25
4	11	271/276 (98%)	255 (94%)	11 (4%)	5 (2%)	6	29
4	19	271/276 (98%)	252 (93%)	15 (6%)	4 (2%)	8	33
5	L5	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
5	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	5	25
6	2A	114/129 (88%)	103 (90%)	9 (8%)	2 (2%)	6	29
6	2I	114/129 (88%)	102 (90%)	10 (9%)	2 (2%)	6	29
7	8A	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
7	8I	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
8	22	204/239 (85%)	181 (89%)	22 (11%)	1 (0%)	24	55
8	2E	203/239 (85%)	184 (91%)	18 (9%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	82	122/128 (95%)	113 (93%)	8 (7%)	1 (1%)	16	46
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	15	136/140 (97%)	126 (93%)	9 (7%)	1 (1%)	18	49
10	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	3	20
11	C5	102/110 (93%)	75 (74%)	22 (22%)	5 (5%)	1	11
11	G8	101/110 (92%)	78 (77%)	18 (18%)	5 (5%)	1	10
12	M5	62/65 (95%)	53 (86%)	8 (13%)	1 (2%)	7	32
12	Q8	58/65 (89%)	39 (67%)	14 (24%)	5 (9%)	0	3
13	3A	123/132 (93%)	107 (87%)	13 (11%)	3 (2%)	4	23
13	3I	120/132 (91%)	103 (86%)	17 (14%)	0	100	100
14	32	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	12	41
14	3E	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	24	55
16	75	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	8	33
16	B8	127/146 (87%)	120 (94%)	7 (6%)	0	100	100
17	H5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
17	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	6	29
18	61	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	5	26
18	69	144/148 (97%)	113 (78%)	26 (18%)	5 (4%)	3	16
19	9A	67/88 (76%)	63 (94%)	4 (6%)	0	100	100
19	9I	65/88 (74%)	62 (95%)	2 (3%)	1 (2%)	8	33
20	1B	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
20	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
21	68	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	46
22	D5	129/206 (63%)	104 (81%)	22 (17%)	3 (2%)	5	24
22	H8	169/206 (82%)	139 (82%)	22 (13%)	8 (5%)	2	11
23	21	203/206 (98%)	163 (80%)	32 (16%)	8 (4%)	2	14
23	29	203/206 (98%)	161 (79%)	31 (15%)	11 (5%)	1	9
24	4A	114/126 (90%)	94 (82%)	17 (15%)	3 (3%)	4	21
24	4I	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	14	43
25	42	149/162 (92%)	143 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	4E	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	49
27	85	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
27	C8	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	16
28	I5	61/71 (86%)	42 (69%)	16 (26%)	3 (5%)	1	11
28	M8	64/71 (90%)	49 (77%)	14 (22%)	1 (2%)	7	32
29	AA	76/93 (82%)	62 (82%)	12 (16%)	2 (3%)	4	21
29	AI	78/93 (84%)	67 (86%)	6 (8%)	5 (6%)	1	6
30	35	148/150 (99%)	115 (78%)	27 (18%)	6 (4%)	2	14
30	78	145/150 (97%)	117 (81%)	23 (16%)	5 (3%)	3	16
31	E5	82/85 (96%)	74 (90%)	5 (6%)	3 (4%)	2	15
31	I8	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
32	31	200/210 (95%)	182 (91%)	16 (8%)	2 (1%)	12	41
32	39	206/210 (98%)	165 (80%)	33 (16%)	8 (4%)	2	14
33	5A	56/61 (92%)	47 (84%)	8 (14%)	1 (2%)	6	29
33	5I	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	16
34	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
34	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
35	95	99/101 (98%)	76 (77%)	20 (20%)	3 (3%)	3	19
35	D8	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	41
36	J5	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
36	N8	53/60 (88%)	42 (79%)	9 (17%)	2 (4%)	2	15
37	BA	97/106 (92%)	84 (87%)	11 (11%)	2 (2%)	5	26
37	BI	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
38	45	138/141 (98%)	111 (80%)	25 (18%)	2 (1%)	9	34
38	88	139/141 (99%)	120 (86%)	14 (10%)	5 (4%)	2	16
39	F5	92/98 (94%)	86 (94%)	5 (5%)	1 (1%)	11	39
39	J8	93/98 (95%)	84 (90%)	7 (8%)	2 (2%)	5	25
40	41	179/182 (98%)	162 (90%)	14 (8%)	3 (2%)	7	30
40	49	179/182 (98%)	156 (87%)	21 (12%)	2 (1%)	11	39
41	6A	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
41	6I	86/89 (97%)	82 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	62	143/156 (92%)	133 (93%)	10 (7%)	0	100	100
42	6E	140/156 (90%)	131 (94%)	8 (6%)	1 (1%)	18	49
43	A5	111/113 (98%)	103 (93%)	7 (6%)	1 (1%)	14	43
43	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
44	12	235/256 (92%)	197 (84%)	35 (15%)	3 (1%)	9	36
44	1E	235/256 (92%)	196 (83%)	36 (15%)	3 (1%)	9	36
45	55	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	7	30
45	98	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	4	21
46	G5	65/72 (90%)	59 (91%)	4 (6%)	2 (3%)	3	18
46	K8	66/72 (92%)	63 (96%)	1 (2%)	2 (3%)	3	19
47	51	172/180 (96%)	149 (87%)	17 (10%)	6 (4%)	3	16
47	59	168/180 (93%)	128 (76%)	36 (21%)	4 (2%)	4	23
48	1A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
49	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
50	72	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	33
50	7E	136/138 (99%)	127 (93%)	8 (6%)	1 (1%)	18	49
All	All	11147/11946 (93%)	9805 (88%)	1146 (10%)	196 (2%)	6	29

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	2A	48	ILE
12	Q8	31	HIS
14	3E	31	CYS
9	82	118	LYS
11	C5	29	GLU

### 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%)	62 (71%)	25 (29%)	0	1
2	A8	87/88 (99%)	53 (61%)	34 (39%)	0	0
3	B5	74/78 (95%)	60 (81%)	14 (19%)	1	8
3	F8	76/78 (97%)	57 (75%)	19 (25%)	0	3
4	11	215/218 (99%)	163 (76%)	52 (24%)	1	3
4	19	214/218 (98%)	169 (79%)	45 (21%)	1	6
5	L5	40/42 (95%)	33 (82%)	7 (18%)	2	9
5	P8	40/42 (95%)	30 (75%)	10 (25%)	0	3
6	2A	88/99 (89%)	67 (76%)	21 (24%)	1	3
6	2I	88/99 (89%)	69 (78%)	19 (22%)	1	5
7	8A	94/97 (97%)	77 (82%)	17 (18%)	2	8
7	8I	95/97 (98%)	74 (78%)	21 (22%)	1	5
8	22	160/188 (85%)	117 (73%)	43 (27%)	0	2
8	2E	159/188 (85%)	118 (74%)	41 (26%)	0	2
9	82	95/99 (96%)	81 (85%)	14 (15%)	3	14
9	8E	98/99 (99%)	71 (72%)	27 (28%)	0	2
10	15	117/119 (98%)	92 (79%)	25 (21%)	1	5
10	58	117/119 (98%)	84 (72%)	33 (28%)	0	1
11	C5	85/91 (93%)	64 (75%)	21 (25%)	1	3
11	G8	84/91 (92%)	54 (64%)	30 (36%)	0	0
12	M5	54/55 (98%)	36 (67%)	18 (33%)	0	1
12	Q8	50/55 (91%)	31 (62%)	19 (38%)	0	0
13	3A	104/109 (95%)	79 (76%)	25 (24%)	1	3
13	3I	103/109 (94%)	85 (82%)	18 (18%)	2	9
14	32	180/181 (99%)	143 (79%)	37 (21%)	1	6
14	3E	180/181 (99%)	145 (81%)	35 (19%)	1	7
16	75	120/127 (94%)	84 (70%)	36 (30%)	0	1
16	B8	115/127 (91%)	80 (70%)	35 (30%)	0	1
17	H5	51/52 (98%)	39 (76%)	12 (24%)	1	4
17	L8	49/52 (94%)	37 (76%)	12 (24%)	1	3
18	61	122/124 (98%)	85 (70%)	37 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	69	122/124 (98%)	92 (75%)	30 (25%)	1	3
19	9A	60/77 (78%)	47 (78%)	13 (22%)	1	5
19	9I	59/77 (77%)	42 (71%)	17 (29%)	0	1
20	1B	20/22 (91%)	18 (90%)	2 (10%)	7	27
20	1F	18/22 (82%)	14 (78%)	4 (22%)	1	5
21	25	100/100 (100%)	71 (71%)	29 (29%)	0	1
21	68	100/100 (100%)	76 (76%)	24 (24%)	1	3
22	D5	125/179 (70%)	92 (74%)	33 (26%)	0	2
22	H8	152/179 (85%)	119 (78%)	33 (22%)	1	5
23	21	165/166 (99%)	119 (72%)	46 (28%)	0	2
23	29	165/166 (99%)	121 (73%)	44 (27%)	0	2
24	4A	94/101 (93%)	73 (78%)	21 (22%)	1	4
24	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
25	42	116/123 (94%)	88 (76%)	28 (24%)	1	3
25	4E	116/123 (94%)	88 (76%)	28 (24%)	1	3
27	85	93/94 (99%)	73 (78%)	20 (22%)	1	5
27	C8	93/94 (99%)	79 (85%)	14 (15%)	3	13
28	I5	57/63 (90%)	44 (77%)	13 (23%)	1	4
28	M8	59/63 (94%)	45 (76%)	14 (24%)	1	4
29	AA	67/80 (84%)	54 (81%)	13 (19%)	1	7
29	AI	70/80 (88%)	48 (69%)	22 (31%)	0	1
30	35	116/116 (100%)	79 (68%)	37 (32%)	0	1
30	78	114/116 (98%)	87 (76%)	27 (24%)	1	4
31	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
31	I8	66/67 (98%)	55 (83%)	11 (17%)	2	10
32	31	161/166 (97%)	129 (80%)	32 (20%)	1	7
32	39	165/166 (99%)	114 (69%)	51 (31%)	0	1
33	5A	48/50 (96%)	35 (73%)	13 (27%)	0	2
33	5I	49/50 (98%)	37 (76%)	12 (24%)	1	3
34	52	90/90 (100%)	71 (79%)	19 (21%)	1	6
34	5E	90/90 (100%)	71 (79%)	19 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	95	82/82 (100%)	55 (67%)	27 (33%)	0	1
35	D8	82/82 (100%)	55 (67%)	27 (33%)	0	1
36	J5	48/52 (92%)	39 (81%)	9 (19%)	1	8
36	N8	48/52 (92%)	37 (77%)	11 (23%)	1	4
37	BA	76/82 (93%)	63 (83%)	13 (17%)	2	9
37	BI	76/82 (93%)	58 (76%)	18 (24%)	1	4
38	45	110/111 (99%)	85 (77%)	25 (23%)	1	4
38	88	111/111 (100%)	86 (78%)	25 (22%)	1	4
39	F5	79/83 (95%)	56 (71%)	23 (29%)	0	1
39	J8	80/83 (96%)	61 (76%)	19 (24%)	1	4
40	41	155/156 (99%)	127 (82%)	28 (18%)	2	8
40	49	155/156 (99%)	127 (82%)	28 (18%)	2	8
41	6A	79/80 (99%)	64 (81%)	15 (19%)	1	7
41	6I	79/80 (99%)	64 (81%)	15 (19%)	1	7
42	62	121/127 (95%)	92 (76%)	29 (24%)	1	3
42	6E	118/127 (93%)	98 (83%)	20 (17%)	2	9
43	A5	92/92 (100%)	70 (76%)	22 (24%)	1	3
43	E8	91/92 (99%)	70 (77%)	21 (23%)	1	4
44	12	205/220 (93%)	158 (77%)	47 (23%)	1	4
44	1E	205/220 (93%)	149 (73%)	56 (27%)	0	2
45	55	100/101 (99%)	73 (73%)	27 (27%)	0	2
45	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
46	G5	63/67 (94%)	46 (73%)	17 (27%)	0	2
46	K8	64/67 (96%)	45 (70%)	19 (30%)	0	1
47	51	145/148 (98%)	104 (72%)	41 (28%)	0	1
47	59	142/148 (96%)	105 (74%)	37 (26%)	0	2
48	1A	89/92 (97%)	68 (76%)	21 (24%)	1	4
48	1I	89/92 (97%)	59 (66%)	30 (34%)	0	0
49	7A	72/74 (97%)	62 (86%)	10 (14%)	3	15
49	7I	72/74 (97%)	54 (75%)	18 (25%)	0	3
50	72	119/119 (100%)	99 (83%)	20 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	7E	119/119 (100%)	94 (79%)	25 (21%)	1 6
All	All	9414/9894 (95%)	7147 (76%)	2267 (24%)	1 3

5 of 2267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	A5	59	VAL
47	51	86	GLU
43	A5	51	LEU
45	55	63	ARG
22	H8	161	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
42	62	11	GLN
6	2I	13	GLN
45	98	61	HIS
49	7I	82	GLN
8	2E	136	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1506/1522 (98%)	327 (21%)	33 (2%)
1	1G	1512/1522 (99%)	326 (21%)	34 (2%)
15	14	2908/2917 (99%)	662 (22%)	40 (1%)
15	1H	2911/2917 (99%)	619 (21%)	56 (1%)
26	16	121/122 (99%)	29 (23%)	3 (2%)
26	1J	121/122 (99%)	35 (28%)	3 (2%)
51	Y1	24/25 (96%)	10 (41%)	2 (8%)
51	Y4	24/25 (96%)	11 (45%)	0
52	V1	75/76 (98%)	35 (46%)	7 (9%)
52	V4	75/76 (98%)	36 (48%)	5 (6%)
52	W1	75/76 (98%)	20 (26%)	0
52	W4	75/76 (98%)	22 (29%)	0
52	X1	75/76 (98%)	22 (29%)	2 (2%)
52	X4	75/76 (98%)	19 (25%)	3 (4%)
All	All	9577/9628 (99%)	2173 (22%)	188 (1%)

5 of 2173 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	678	A

5 of 188 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	1H	2454	A
15	14	1608	A
15	1H	2581	A
15	14	335	A
15	14	2350	A

#### 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 oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 1789 ligands modelled in this entry, 1776 are monoatomic - leaving 13 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	14	3005	-	34,35,35	0.46	0	50,52,52	0.98	1 (2%)
53	8UZ	1H	3004	-	34,35,35	0.54	0	50,52,52	1.88	9 (18%)
53	8UZ	1G	2201	-	34,35,35	0.23	0	50,52,52	0.81	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	8UZ	1H	3002	-	34,35,35	0.21	0	50,52,52	0.89	2 (4%)
53	8UZ	1H	3003	-	34,35,35	0.30	0	50,52,52	0.80	2 (4%)
53	8UZ	1G	2202	54	34,35,35	0.17	0	50,52,52	0.71	1 (2%)
53	8UZ	14	3003	-	34,35,35	0.28	0	50,52,52	1.57	6 (12%)
53	8UZ	14	3004	-	34,35,35	0.21	0	50,52,52	0.75	2 (4%)
53	8UZ	13	2201	-	34,35,35	0.21	0	50,52,52	1.27	1 (2%)
53	8UZ	14	3002	-	34,35,35	0.24	0	50,52,52	0.97	2 (4%)
53	8UZ	14	3006	-	34,35,35	0.18	0	50,52,52	1.25	3 (6%)
53	8UZ	13	2202	54	34,35,35	0.21	0	50,52,52	1.03	3 (6%)
53	8UZ	1H	3005	-	34,35,35	0.32	0	50,52,52	1.98	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	8UZ	14	3005	-	-	3/12/72/72	0/3/3/3
53	8UZ	1H	3004	-	-	6/12/72/72	0/3/3/3
53	8UZ	1G	2201	-	-	5/12/72/72	0/3/3/3
53	8UZ	1H	3002	-	-	3/12/72/72	0/3/3/3
53	8UZ	1H	3003	-	-	6/12/72/72	0/3/3/3
53	8UZ	1G	2202	54	-	3/12/72/72	0/3/3/3
53	8UZ	14	3003	-	-	8/12/72/72	0/3/3/3
53	8UZ	14	3004	-	-	6/12/72/72	0/3/3/3
53	8UZ	13	2201	-	-	3/12/72/72	0/3/3/3
53	8UZ	14	3002	-	-	2/12/72/72	0/3/3/3
53	8UZ	14	3006	-	-	4/12/72/72	0/3/3/3
53	8UZ	13	2202	54	-	0/12/72/72	0/3/3/3
53	8UZ	1H	3005	-	-	7/12/72/72	0/3/3/3

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1H	3005	8UZ	C10-C12-C13	-9.95	99.66	110.67
53	1H	3004	8UZ	C10-C12-C13	7.42	118.88	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	13	2201	8UZ	C10-C12-C13	6.73	118.12	110.67
53	14	3003	8UZ	C14-C13-C12	-5.68	98.72	111.06
53	14	3006	8UZ	C10-C12-C13	5.66	116.93	110.67

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	13	2201	8UZ	N-C-C1-C17
53	13	2201	8UZ	N-C-C1-O
53	1G	2201	8UZ	N-C-C1-C17
53	1G	2201	8UZ	N-C-C1-O
53	1G	2202	8UZ	N-C-C1-C17

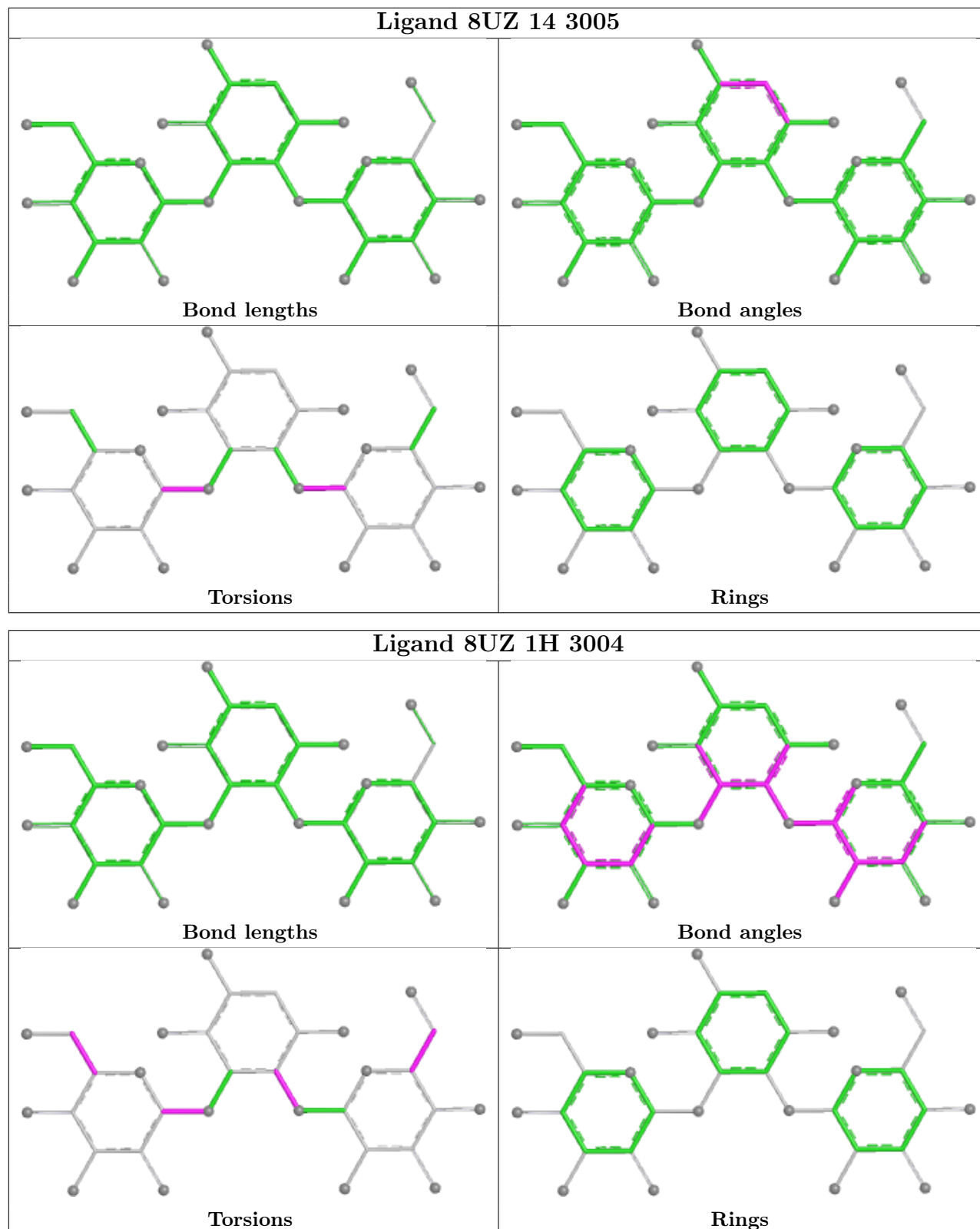
There are no ring outliers.

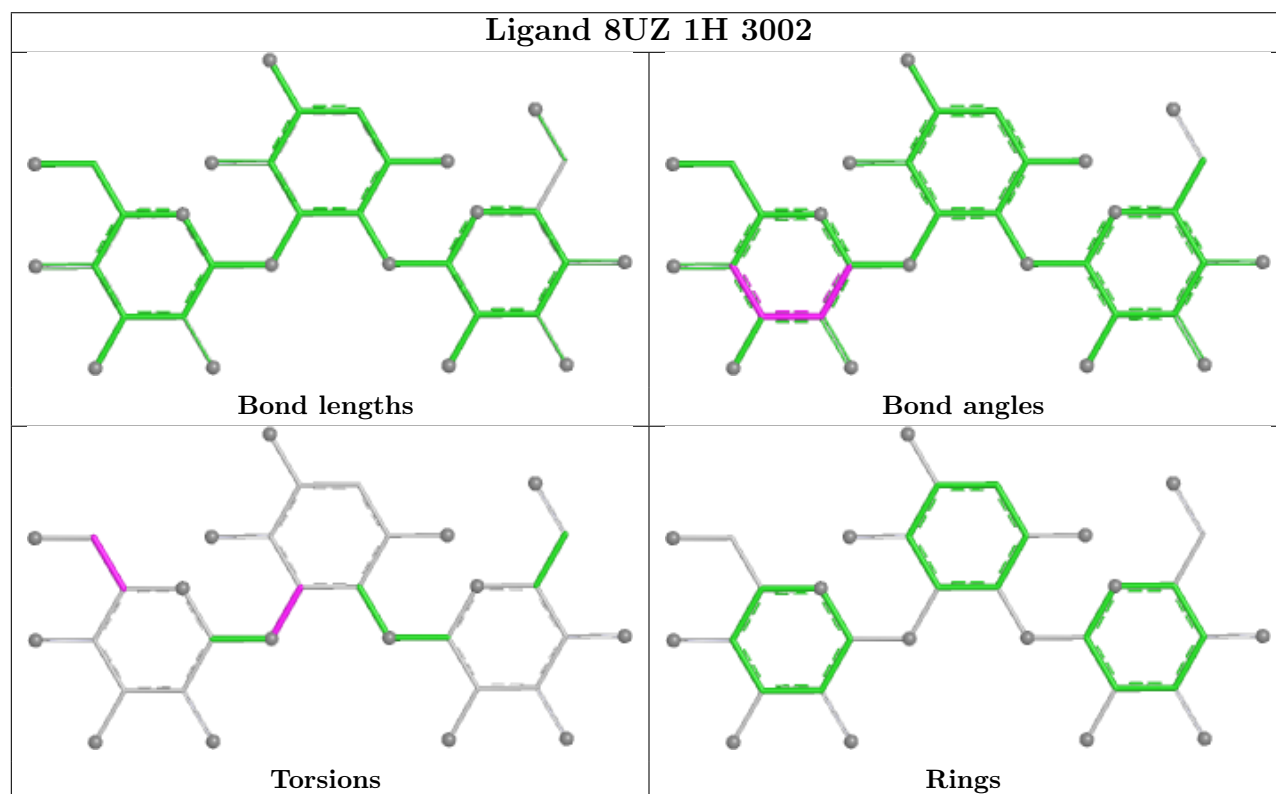
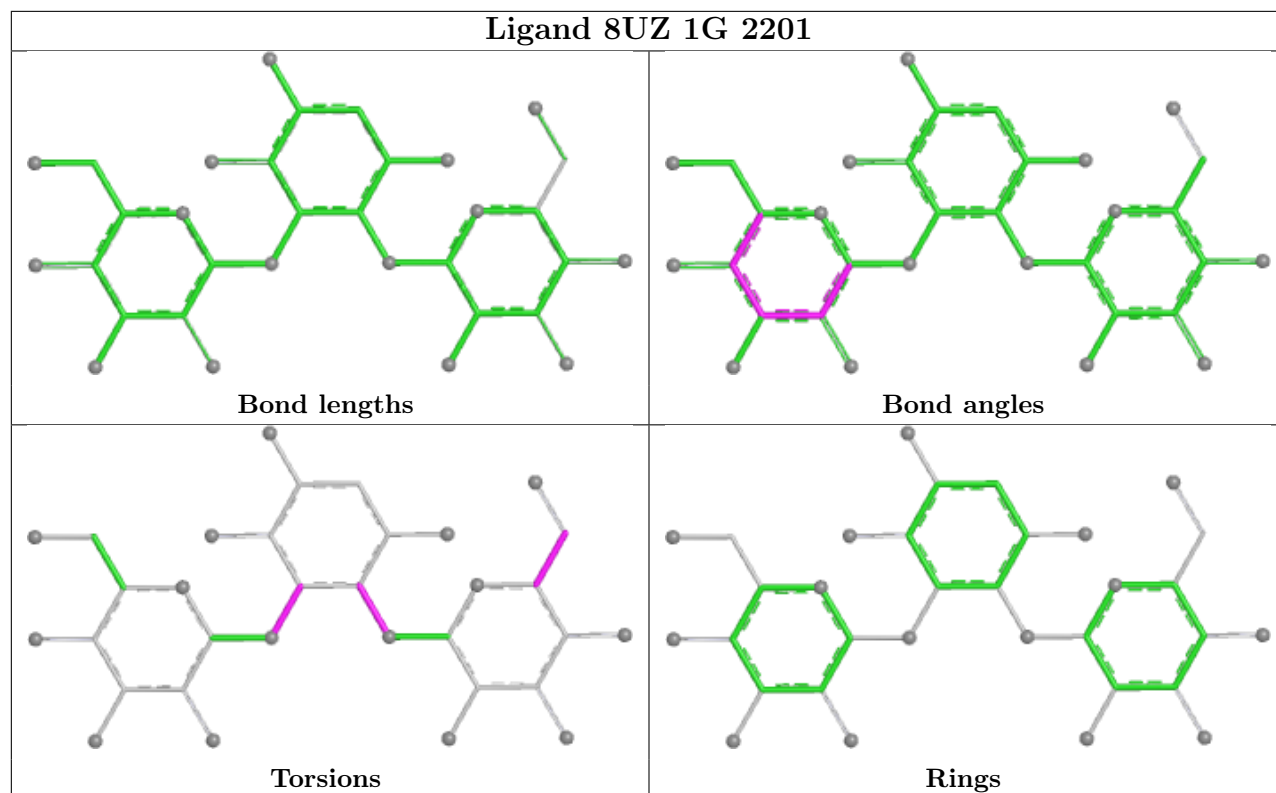
12 monomers are involved in 26 short contacts:

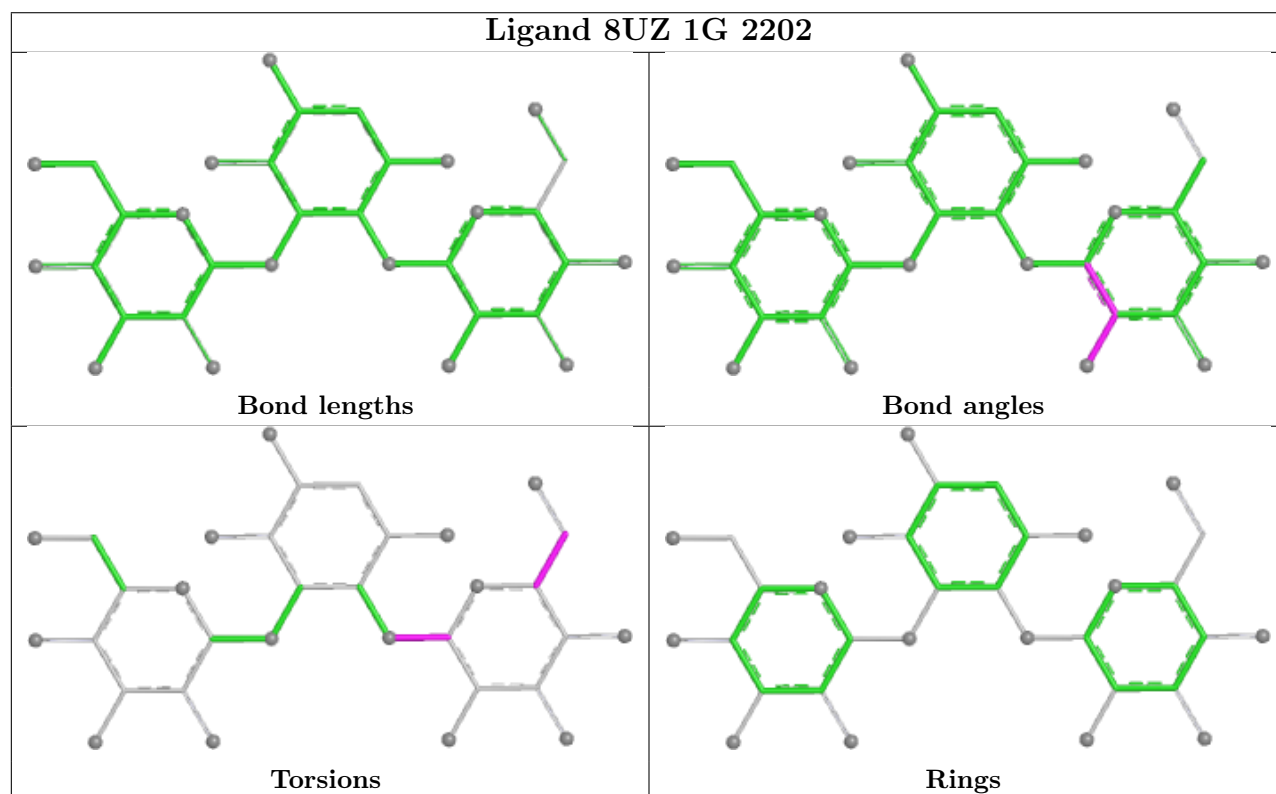
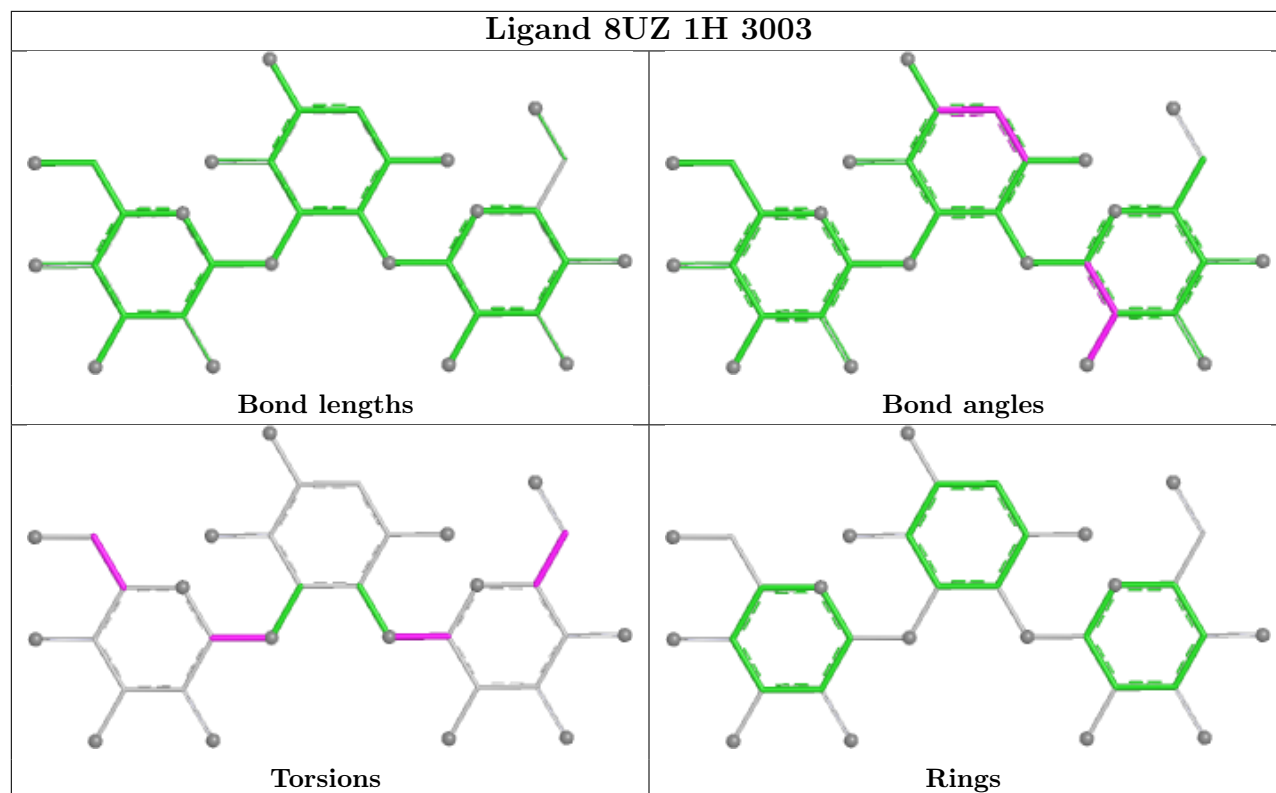
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	14	3005	8UZ	1	0
53	1H	3004	8UZ	7	0
53	1G	2201	8UZ	1	0
53	1H	3002	8UZ	2	0
53	1H	3003	8UZ	1	0
53	1G	2202	8UZ	2	0
53	14	3003	8UZ	1	0
53	14	3004	8UZ	2	0
53	14	3002	8UZ	2	0
53	14	3006	8UZ	2	0
53	13	2202	8UZ	1	0
53	1H	3005	8UZ	4	0

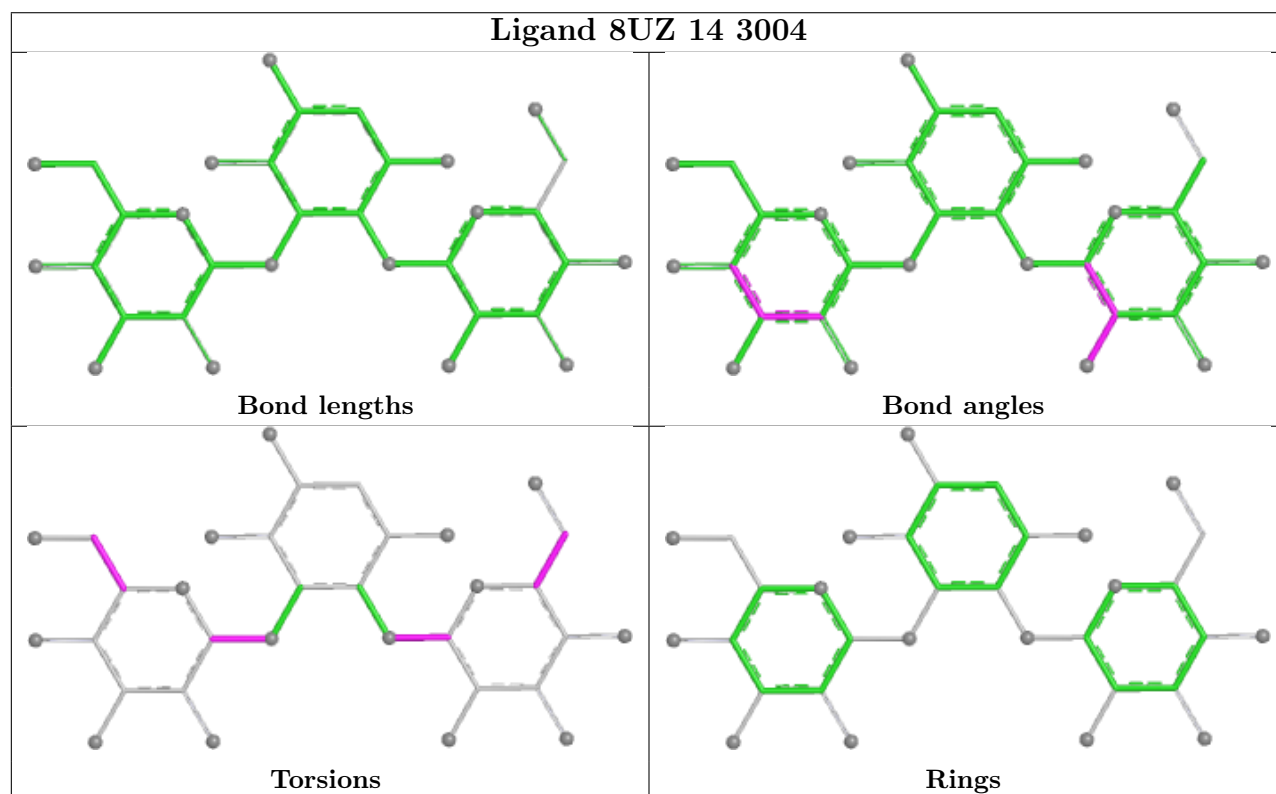
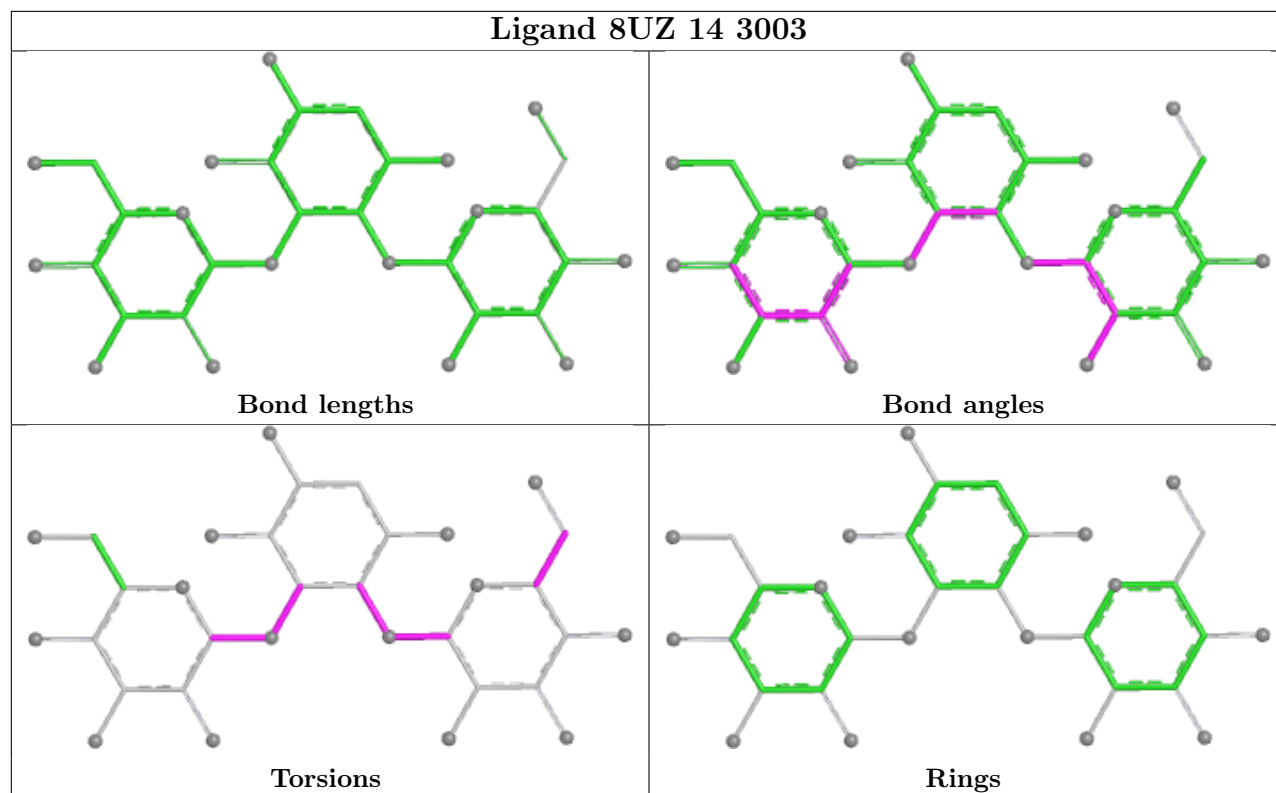
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

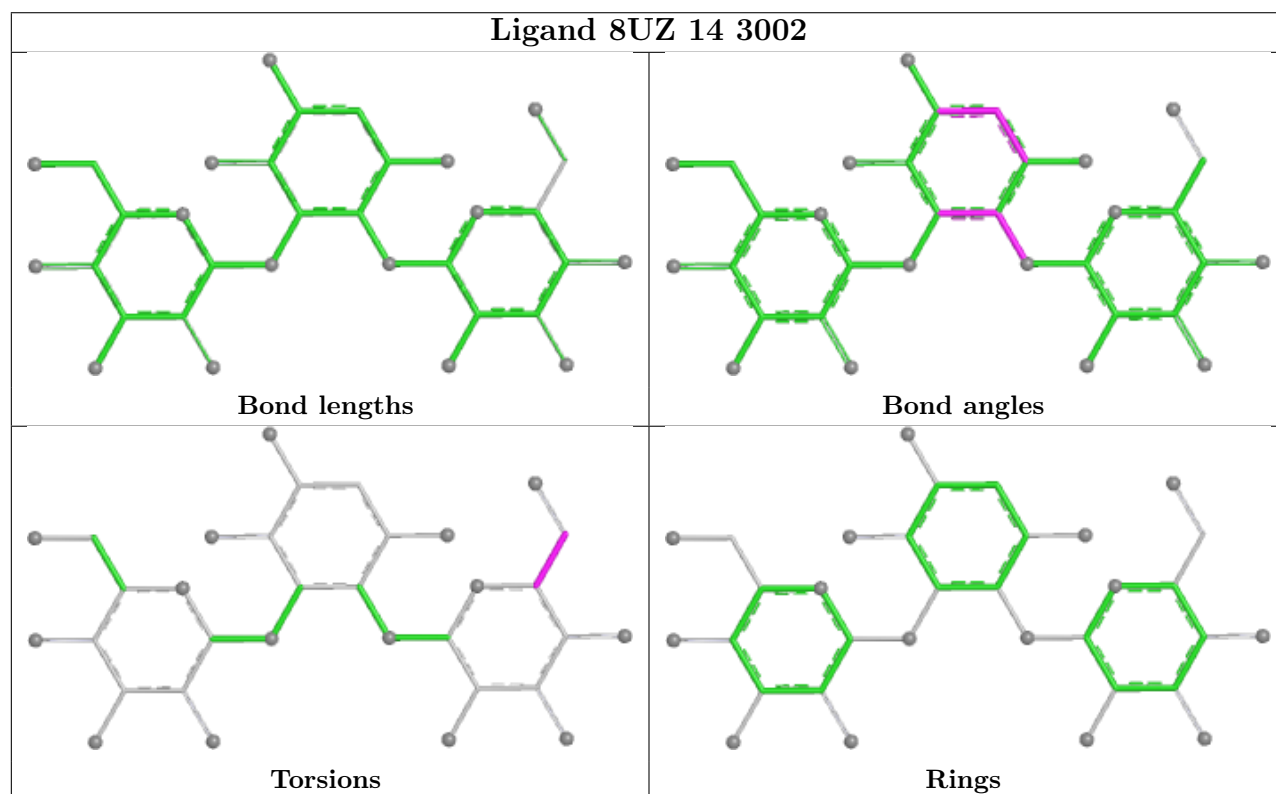
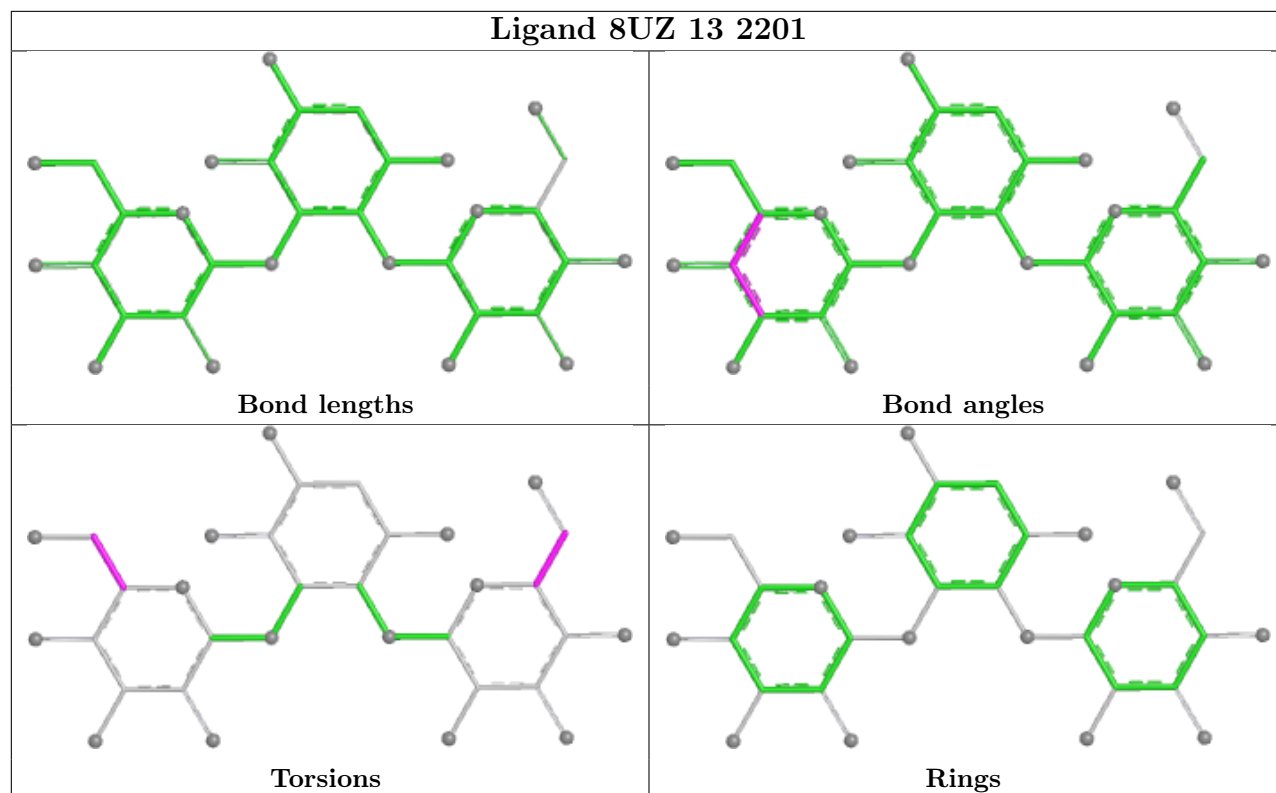
equivalents in the CSD to analyse the geometry.

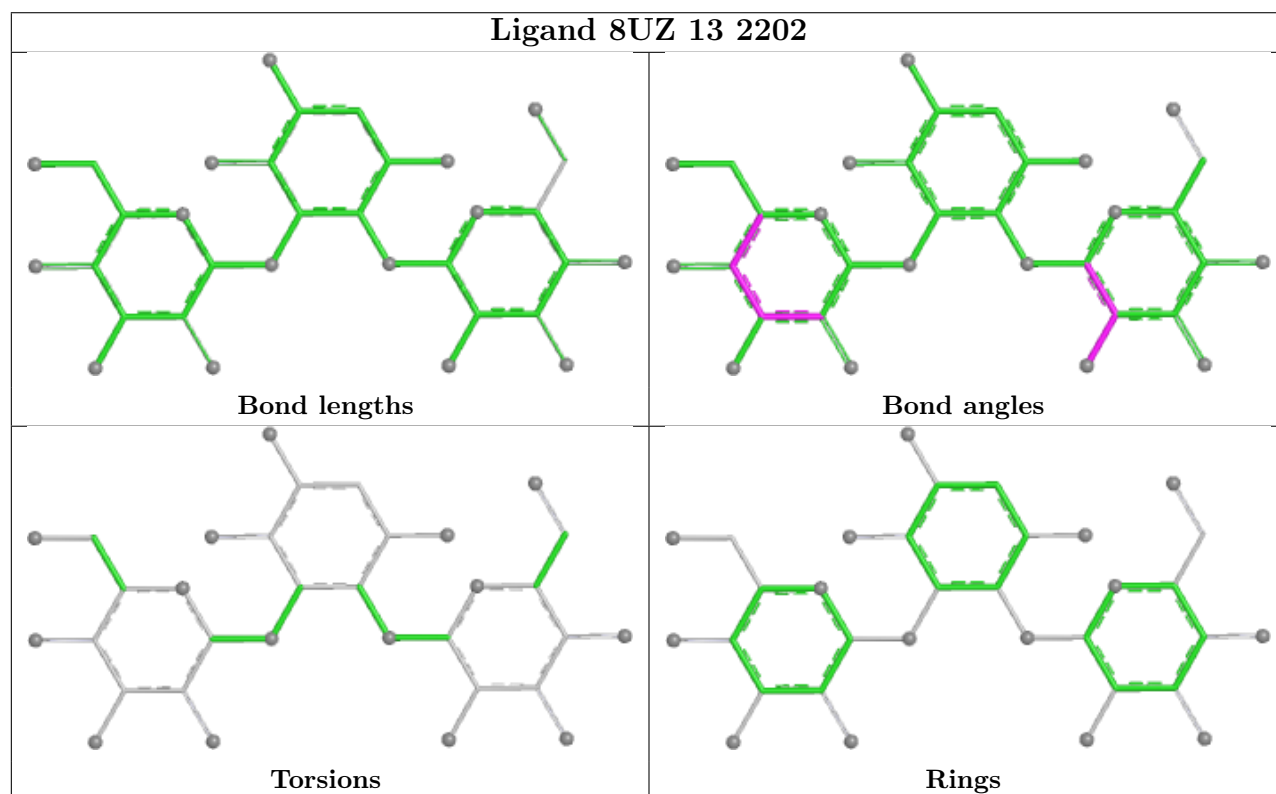
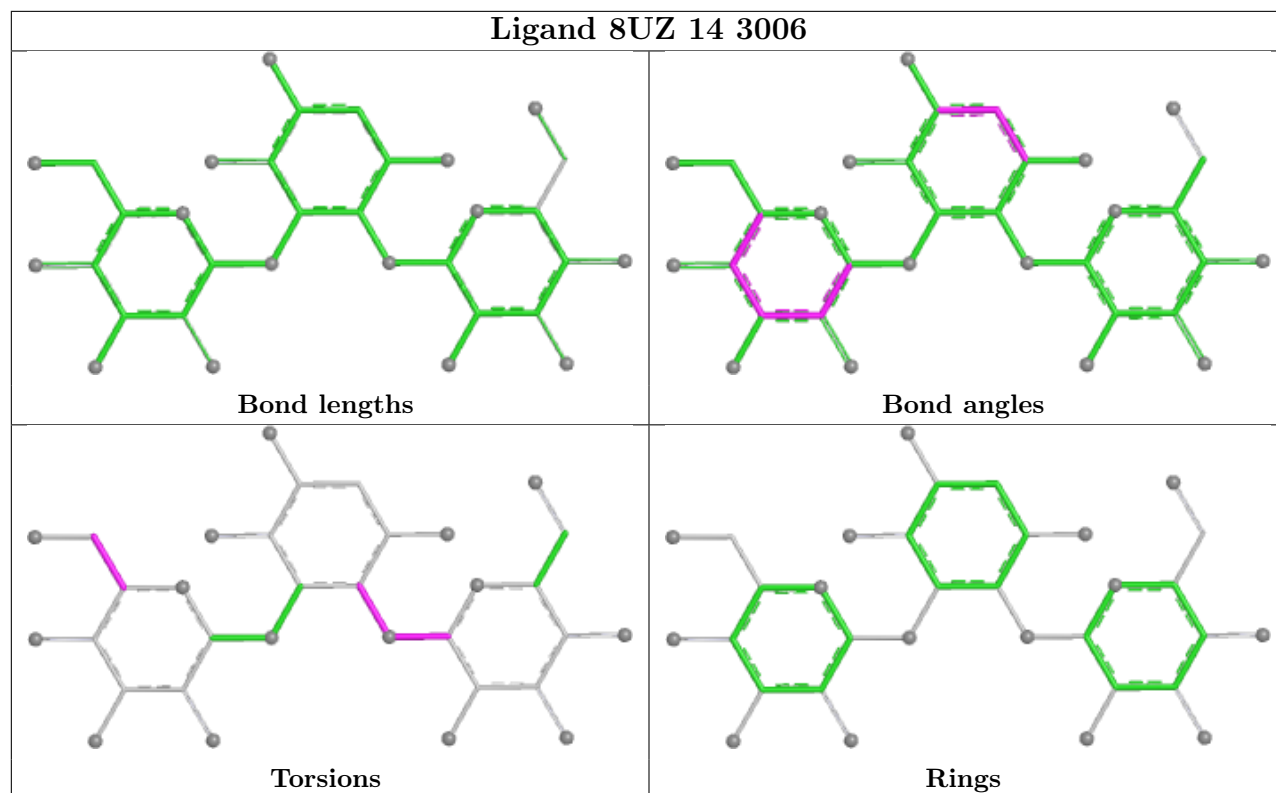


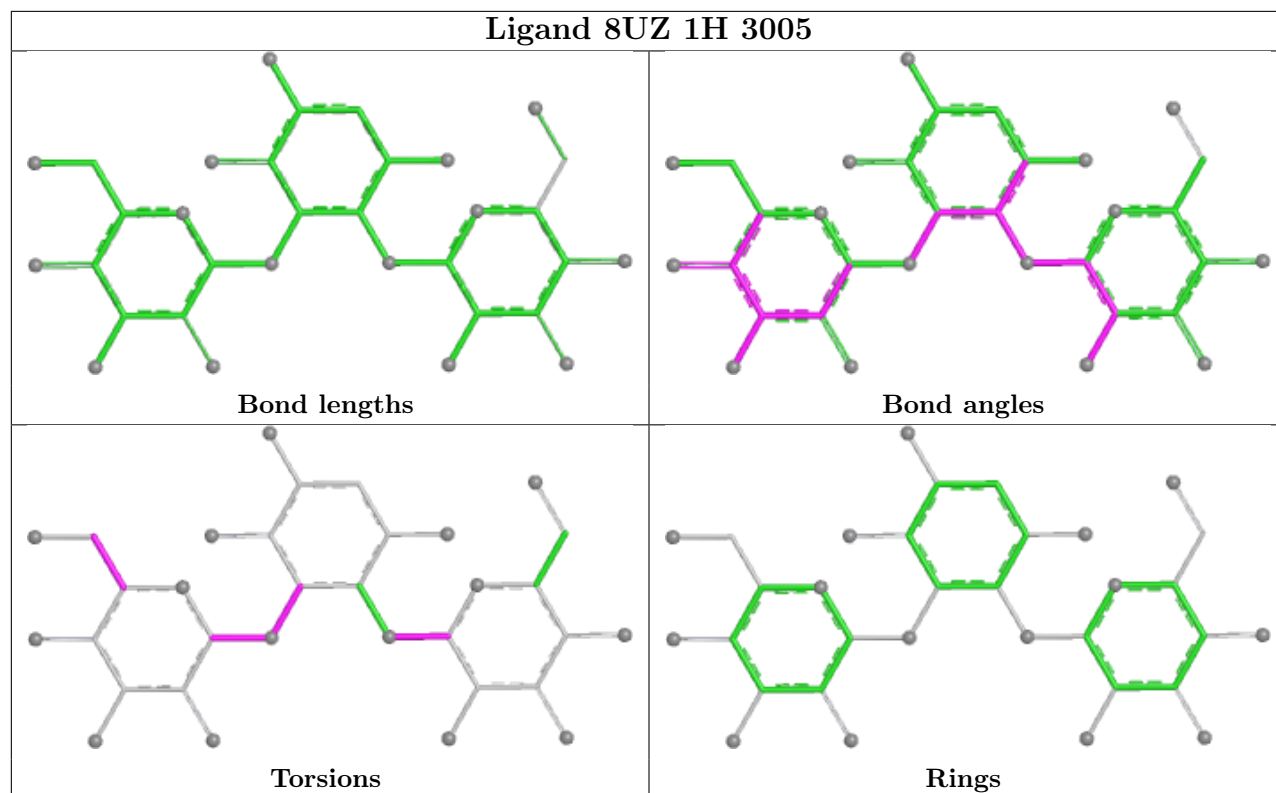












## 5.7 Other polymers [i](#)

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%)	0.30	103 (6%) 23 13	50, 86, 147, 226	0
1	1G	1513/1522 (99%)	0.46	138 (9%) 15 8	59, 93, 138, 228	0
2	65	111/112 (99%)	0.30	3 (2%) 56 35	76, 84, 90, 93	0
2	A8	111/112 (99%)	-0.10	1 (0%) 81 64	63, 71, 78, 80	0
3	B5	92/96 (95%)	0.35	4 (4%) 40 23	61, 70, 80, 82	0
3	F8	94/96 (97%)	0.32	4 (4%) 40 23	48, 54, 63, 64	0
4	11	273/276 (98%)	0.03	4 (1%) 72 52	39, 52, 59, 65	0
4	19	273/276 (98%)	0.34	9 (3%) 49 29	46, 60, 67, 73	0
5	L5	47/49 (95%)	0.05	0 100 100	48, 51, 56, 61	0
5	P8	47/49 (95%)	-0.02	4 (8%) 16 9	40, 42, 47, 52	0
6	2A	116/129 (89%)	0.80	13 (11%) 10 6	72, 92, 102, 113	0
6	2I	116/129 (89%)	0.46	5 (4%) 40 23	61, 87, 97, 117	0
7	8A	99/105 (94%)	0.41	4 (4%) 42 24	78, 86, 93, 95	0
7	8I	100/105 (95%)	0.71	7 (7%) 22 13	72, 87, 91, 93	0
8	22	206/239 (86%)	1.25	44 (21%) 2 2	102, 114, 136, 139	0
8	2E	205/239 (85%)	1.09	35 (17%) 4 2	78, 92, 115, 119	0
9	82	124/128 (96%)	2.24	45 (36%) 1 1	92, 130, 138, 140	0
9	8E	127/128 (99%)	1.03	19 (14%) 5 3	72, 121, 129, 131	0
10	15	138/140 (98%)	0.73	16 (11%) 9 6	61, 83, 99, 115	0
10	58	138/140 (98%)	0.61	12 (8%) 16 9	51, 65, 91, 102	0
11	C5	104/110 (94%)	1.73	39 (37%) 1 1	76, 85, 104, 111	0
11	G8	103/110 (93%)	0.35	3 (2%) 53 34	63, 71, 88, 90	0
12	M5	64/65 (98%)	0.80	10 (15%) 5 3	58, 65, 77, 84	0
12	Q8	60/65 (92%)	1.21	13 (21%) 2 2	45, 53, 65, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	3A	125/132 (94%)	0.82	13 (10%) 11 7	74, 77, 88, 119	0
13	3I	122/132 (92%)	0.18	6 (4%) 35 20	60, 64, 71, 83	0
14	32	208/209 (99%)	0.88	25 (12%) 9 5	84, 93, 103, 107	0
14	3E	208/209 (99%)	0.73	16 (7%) 19 11	76, 87, 97, 103	0
15	14	2909/2917 (99%)	-0.03	78 (2%) 56 35	46, 70, 190, 252	0
15	1H	2912/2917 (99%)	-0.20	55 (1%) 66 45	36, 58, 166, 235	0
16	75	137/146 (93%)	0.43	7 (5%) 33 19	67, 76, 115, 139	0
16	B8	129/146 (88%)	0.28	9 (6%) 22 13	61, 69, 87, 97	0
17	H5	59/60 (98%)	0.56	4 (6%) 23 13	68, 80, 110, 116	0
17	L8	57/60 (95%)	-0.01	0 100 100	52, 59, 67, 73	0
18	61	146/148 (98%)	0.51	7 (4%) 35 20	66, 101, 117, 119	0
18	69	146/148 (98%)	0.53	6 (4%) 41 24	74, 101, 123, 125	0
19	9A	69/88 (78%)	0.30	1 (1%) 73 53	80, 89, 98, 109	0
19	9I	67/88 (76%)	0.25	0 100 100	76, 83, 91, 97	0
20	1B	25/27 (92%)	1.38	4 (16%) 5 3	106, 115, 120, 123	0
20	1F	23/27 (85%)	0.32	1 (4%) 40 23	95, 99, 101, 101	0
21	25	122/122 (100%)	0.27	4 (3%) 49 29	58, 69, 78, 80	0
21	68	122/122 (100%)	-0.08	1 (0%) 82 66	49, 59, 68, 73	0
22	D5	135/206 (65%)	0.57	7 (5%) 33 19	86, 106, 122, 123	0
22	H8	171/206 (83%)	0.49	10 (5%) 29 16	70, 90, 145, 150	0
23	21	205/206 (99%)	0.39	14 (6%) 23 13	44, 66, 87, 92	0
23	29	205/206 (99%)	0.42	12 (5%) 28 16	52, 74, 99, 106	0
24	4A	116/126 (92%)	0.82	13 (11%) 10 6	96, 122, 128, 130	0
24	4I	116/126 (92%)	0.78	11 (9%) 14 8	80, 111, 116, 120	0
25	42	151/162 (93%)	0.77	13 (8%) 16 9	85, 95, 104, 115	0
25	4E	151/162 (93%)	0.71	18 (11%) 9 5	70, 79, 90, 106	0
26	16	122/122 (100%)	-0.29	1 (0%) 82 66	57, 73, 87, 127	0
26	1J	122/122 (100%)	0.17	6 (4%) 35 20	76, 89, 103, 127	0
27	85	117/118 (99%)	0.37	0 100 100	57, 80, 98, 105	0
27	C8	117/118 (99%)	0.48	10 (8%) 16 9	44, 59, 73, 79	0
28	I5	63/71 (88%)	1.51	18 (28%) 1 1	106, 139, 146, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	M8	66/71 (92%)	1.17	13 (19%) 3 2	92, 123, 130, 132	0
29	AA	78/93 (83%)	1.40	15 (19%) 3 2	103, 130, 142, 143	0
29	AI	80/93 (86%)	0.90	8 (10%) 12 7	84, 107, 117, 119	0
30	35	150/150 (100%)	0.79	13 (8%) 16 9	52, 78, 101, 114	0
30	78	147/150 (98%)	0.34	7 (4%) 35 20	39, 63, 77, 81	0
31	E5	84/85 (98%)	0.67	3 (3%) 46 27	61, 70, 80, 86	0
31	I8	83/85 (97%)	-0.06	2 (2%) 59 39	48, 56, 63, 70	0
32	31	202/210 (96%)	0.11	3 (1%) 72 52	39, 62, 78, 88	0
32	39	208/210 (99%)	0.71	19 (9%) 15 8	49, 81, 107, 117	0
33	5A	58/61 (95%)	1.49	14 (24%) 2 2	104, 111, 124, 125	0
33	5I	60/61 (98%)	0.66	5 (8%) 17 10	82, 90, 97, 99	0
34	52	101/101 (100%)	0.23	2 (1%) 65 44	76, 82, 92, 102	0
34	5E	101/101 (100%)	0.13	2 (1%) 65 44	75, 81, 90, 95	0
35	95	101/101 (100%)	0.57	7 (6%) 23 13	54, 93, 98, 100	0
35	D8	101/101 (100%)	0.40	3 (2%) 52 32	44, 73, 80, 83	0
36	J5	56/60 (93%)	0.51	7 (12%) 8 5	51, 73, 89, 90	0
36	N8	55/60 (91%)	0.46	3 (5%) 30 17	42, 69, 89, 92	0
37	BA	99/106 (93%)	0.60	6 (6%) 27 15	80, 93, 104, 110	0
37	BI	99/106 (93%)	0.75	4 (4%) 42 24	92, 104, 114, 117	0
38	45	140/141 (99%)	0.64	11 (7%) 18 10	59, 82, 98, 109	0
38	88	141/141 (100%)	0.19	3 (2%) 63 42	46, 65, 80, 96	0
39	F5	94/98 (95%)	0.59	9 (9%) 13 8	52, 67, 93, 96	0
39	J8	95/98 (96%)	0.42	8 (8%) 17 10	43, 59, 84, 89	0
40	41	181/182 (99%)	0.92	20 (11%) 10 6	74, 93, 111, 117	0
40	49	181/182 (99%)	1.03	28 (15%) 5 3	95, 112, 126, 130	0
41	6A	88/89 (98%)	0.18	4 (4%) 38 22	75, 88, 95, 96	0
41	6I	88/89 (98%)	0.00	1 (1%) 78 60	68, 82, 88, 89	0
42	62	147/156 (94%)	0.91	21 (14%) 6 4	101, 108, 114, 118	0
42	6E	144/156 (92%)	0.76	13 (9%) 15 9	93, 103, 111, 115	0
43	A5	113/113 (100%)	0.09	0 100 100	51, 62, 80, 107	0
43	E8	112/113 (99%)	-0.25	0 100 100	45, 56, 69, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	12	237/256 (92%)	0.77	20 (8%) 17 10	112, 130, 142, 146	0
44	1E	237/256 (92%)	0.72	12 (5%) 33 19	94, 115, 131, 137	0
45	55	117/118 (99%)	0.43	4 (3%) 48 28	56, 66, 73, 79	0
45	98	118/118 (100%)	0.01	0 100 100	52, 62, 70, 73	0
46	G5	67/72 (93%)	0.39	2 (2%) 52 32	74, 81, 87, 89	0
46	K8	68/72 (94%)	0.19	2 (2%) 53 34	55, 61, 65, 70	0
47	51	174/180 (96%)	0.64	12 (6%) 23 13	76, 88, 95, 107	0
47	59	170/180 (94%)	2.07	72 (42%) 0 1	128, 154, 172, 179	0
48	1A	99/105 (94%)	1.56	26 (26%) 1 1	97, 130, 139, 140	0
48	1I	99/105 (94%)	1.59	30 (30%) 1 1	77, 118, 132, 133	0
49	7A	84/88 (95%)	0.60	2 (2%) 59 39	79, 86, 98, 121	0
49	7I	84/88 (95%)	1.35	19 (22%) 2 2	83, 94, 109, 127	0
50	72	138/138 (100%)	1.05	28 (20%) 3 2	82, 97, 108, 114	0
50	7E	138/138 (100%)	0.76	9 (6%) 25 14	74, 87, 92, 97	0
51	Y1	25/25 (100%)	1.24	7 (28%) 1 1	63, 122, 175, 182	0
51	Y4	25/25 (100%)	1.75	9 (36%) 1 1	77, 133, 170, 175	0
52	V1	76/76 (100%)	1.34	15 (19%) 3 2	55, 173, 208, 211	0
52	V4	76/76 (100%)	1.21	11 (14%) 6 4	63, 178, 211, 214	0
52	W1	76/76 (100%)	0.68	10 (13%) 7 5	54, 144, 162, 164	0
52	W4	76/76 (100%)	0.53	5 (6%) 24 14	67, 155, 168, 170	0
52	X1	76/76 (100%)	1.07	12 (15%) 5 3	51, 92, 105, 112	0
52	X4	76/76 (100%)	0.60	3 (3%) 43 25	59, 103, 119, 125	0
All	All	20935/21574 (97%)	0.39	1469 (7%) 22 13	36, 80, 140, 252	0

The worst 5 of 1469 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
47	59	155	SER	12.1
9	82	110	GLU	12.0
47	59	168	PRO	10.9
1	1G	1913	A	10.8
47	59	169	VAL	10.6

## 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
54	MG	13	2390	1/1	0.30	0.30	117,117,117,117	0
54	MG	X4	103	1/1	0.36	0.43	109,109,109,109	0
54	MG	88	205	1/1	0.37	0.20	124,124,124,124	0
54	MG	13	2367	1/1	0.37	0.26	92,92,92,92	0
54	MG	14	3316	1/1	0.38	0.23	116,116,116,116	0
54	MG	1G	2327	1/1	0.39	0.25	100,100,100,100	0
54	MG	Y4	101	1/1	0.43	0.38	83,83,83,83	0
54	MG	1G	2356	1/1	0.44	0.32	99,99,99,99	0
54	MG	14	3437	1/1	0.45	0.44	87,87,87,87	0
54	MG	X1	105	1/1	0.49	0.46	97,97,97,97	0
54	MG	1G	2298	1/1	0.50	0.34	92,92,92,92	0
54	MG	13	2370	1/1	0.53	0.38	92,92,92,92	0
54	MG	1G	2382	1/1	0.55	0.32	75,75,75,75	0
54	MG	1G	2358	1/1	0.55	0.29	94,94,94,94	0
54	MG	X1	101	1/1	0.55	0.42	95,95,95,95	0
54	MG	14	3471	1/1	0.56	0.17	57,57,57,57	0
54	MG	1G	2369	1/1	0.56	0.29	87,87,87,87	0
54	MG	13	2322	1/1	0.57	0.24	91,91,91,91	0
54	MG	1G	2372	1/1	0.57	0.28	85,85,85,85	0
54	MG	13	2292	1/1	0.57	0.66	116,116,116,116	0
54	MG	14	3180	1/1	0.57	0.33	75,75,75,75	0
54	MG	14	3234	1/1	0.58	0.39	85,85,85,85	0
54	MG	1G	2313	1/1	0.58	0.22	66,66,66,66	0
54	MG	16	204	1/1	0.58	0.15	72,72,72,72	0
54	MG	14	3329	1/1	0.58	0.37	90,90,90,90	0
54	MG	1H	3265	1/1	0.59	0.23	62,62,62,62	0
54	MG	14	3490	1/1	0.59	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	25	202	1/1	0.60	0.41	74,74,74,74	0
54	MG	X1	108	1/1	0.60	0.33	77,77,77,77	0
54	MG	13	2396	1/1	0.60	0.31	120,120,120,120	0
54	MG	W4	104	1/1	0.60	0.33	124,124,124,124	0
54	MG	1G	2368	1/1	0.60	0.42	88,88,88,88	0
54	MG	13	2326	1/1	0.62	0.29	86,86,86,86	0
54	MG	1H	3631	1/1	0.62	0.29	88,88,88,88	0
54	MG	1G	2307	1/1	0.62	0.18	82,82,82,82	0
54	MG	1G	2311	1/1	0.63	0.41	62,62,62,62	0
54	MG	14	3475	1/1	0.63	0.40	66,66,66,66	0
54	MG	13	2318	1/1	0.63	0.25	86,86,86,86	0
54	MG	14	3533	1/1	0.63	0.27	78,78,78,78	0
54	MG	14	3561	1/1	0.63	0.23	74,74,74,74	0
54	MG	1G	2295	1/1	0.63	0.31	91,91,91,91	0
54	MG	14	3233	1/1	0.63	0.28	72,72,72,72	0
54	MG	41	202	1/1	0.64	0.30	83,83,83,83	0
54	MG	13	2256	1/1	0.64	0.29	59,59,59,59	0
54	MG	1G	2239	1/1	0.64	0.31	89,89,89,89	0
54	MG	14	3401	1/1	0.64	0.35	73,73,73,73	0
54	MG	1J	213	1/1	0.64	0.31	86,86,86,86	0
54	MG	E5	202	1/1	0.64	0.21	77,77,77,77	0
54	MG	1G	2362	1/1	0.64	0.30	97,97,97,97	0
54	MG	14	3458	1/1	0.65	0.33	94,94,94,94	0
54	MG	1G	2277	1/1	0.66	0.43	87,87,87,87	0
54	MG	14	3549	1/1	0.66	0.18	70,70,70,70	0
54	MG	1G	2359	1/1	0.66	0.52	102,102,102,102	0
54	MG	14	3438	1/1	0.67	0.25	67,67,67,67	0
54	MG	1G	2261	1/1	0.67	0.28	99,99,99,99	0
54	MG	14	3346	1/1	0.67	0.17	92,92,92,92	0
54	MG	1G	2268	1/1	0.67	0.37	109,109,109,109	0
54	MG	1G	2326	1/1	0.67	0.57	91,91,91,91	0
54	MG	1G	2350	1/1	0.68	0.30	81,81,81,81	0
54	MG	14	3514	1/1	0.68	0.34	97,97,97,97	0
54	MG	14	3519	1/1	0.68	0.10	64,64,64,64	0
54	MG	13	2374	1/1	0.68	0.33	86,86,86,86	0
54	MG	14	3240	1/1	0.68	0.28	66,66,66,66	0
54	MG	X4	102	1/1	0.68	0.30	107,107,107,107	0
54	MG	13	2233	1/1	0.68	0.36	94,94,94,94	0
54	MG	14	3462	1/1	0.69	0.28	92,92,92,92	0
54	MG	14	3443	1/1	0.69	0.22	65,65,65,65	0
54	MG	X1	106	1/1	0.69	0.30	88,88,88,88	0
54	MG	1G	2283	1/1	0.69	0.32	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	13	2312	1/1	0.70	0.30	86,86,86,86	0
54	MG	14	3404	1/1	0.70	0.24	71,71,71,71	0
54	MG	1G	2262	1/1	0.70	0.28	89,89,89,89	0
54	MG	14	3192	1/1	0.70	0.33	82,82,82,82	0
54	MG	16	214	1/1	0.70	0.25	68,68,68,68	0
54	MG	49	201	1/1	0.70	0.20	95,95,95,95	0
54	MG	6A	101	1/1	0.70	0.40	89,89,89,89	0
54	MG	51	201	1/1	0.70	0.49	74,74,74,74	0
54	MG	1G	2285	1/1	0.71	0.27	80,80,80,80	0
54	MG	1G	2355	1/1	0.71	0.22	76,76,76,76	0
54	MG	1G	2288	1/1	0.71	0.27	79,79,79,79	0
54	MG	13	2297	1/1	0.71	0.27	95,95,95,95	0
54	MG	13	2307	1/1	0.71	0.17	89,89,89,89	0
54	MG	13	2239	1/1	0.71	0.37	77,77,77,77	0
54	MG	14	3491	1/1	0.71	0.27	62,62,62,62	0
54	MG	1G	2264	1/1	0.71	0.47	95,95,95,95	0
54	MG	X1	103	1/1	0.71	0.29	91,91,91,91	0
54	MG	13	2228	1/1	0.71	0.29	56,56,56,56	0
54	MG	14	3341	1/1	0.71	0.25	71,71,71,71	0
54	MG	13	2221	1/1	0.71	0.24	72,72,72,72	0
54	MG	1G	2378	1/1	0.71	0.44	96,96,96,96	0
54	MG	13	2324	1/1	0.71	0.26	78,78,78,78	0
54	MG	1G	2345	1/1	0.71	0.14	84,84,84,84	0
54	MG	1H	3334	1/1	0.71	0.34	78,78,78,78	0
54	MG	1G	2373	1/1	0.72	0.28	89,89,89,89	0
54	MG	13	2373	1/1	0.72	0.21	88,88,88,88	0
54	MG	1H	3607	1/1	0.72	0.19	66,66,66,66	0
54	MG	13	2363	1/1	0.72	0.24	74,74,74,74	0
54	MG	X4	104	1/1	0.72	0.32	86,86,86,86	0
54	MG	13	2308	1/1	0.73	0.25	62,62,62,62	0
54	MG	1G	2225	1/1	0.73	0.41	77,77,77,77	0
54	MG	1G	2229	1/1	0.73	0.26	89,89,89,89	0
54	MG	13	2222	1/1	0.73	0.39	79,79,79,79	0
54	MG	14	3554	1/1	0.73	0.31	91,91,91,91	0
54	MG	14	3440	1/1	0.73	0.22	78,78,78,78	0
54	MG	3E	303	1/1	0.73	0.32	87,87,87,87	0
54	MG	14	3236	1/1	0.73	0.20	59,59,59,59	0
54	MG	13	2333	1/1	0.73	0.20	89,89,89,89	0
54	MG	1H	3291	1/1	0.73	0.24	76,76,76,76	0
54	MG	13	2341	1/1	0.73	0.23	80,80,80,80	0
54	MG	1H	3454	1/1	0.73	0.27	69,69,69,69	0
54	MG	13	2323	1/1	0.73	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3370	1/1	0.74	0.17	58,58,58,58	0
54	MG	1H	3340	1/1	0.74	0.12	61,61,61,61	0
54	MG	1G	2314	1/1	0.74	0.30	96,96,96,96	0
54	MG	1H	3503	1/1	0.74	0.32	73,73,73,73	0
54	MG	13	2302	1/1	0.74	0.27	75,75,75,75	0
54	MG	1G	2287	1/1	0.74	0.28	86,86,86,86	0
54	MG	1H	3639	1/1	0.74	0.23	72,72,72,72	0
54	MG	C5	202	1/1	0.74	0.37	90,90,90,90	0
54	MG	1G	2263	1/1	0.74	0.43	65,65,65,65	0
54	MG	13	2330	1/1	0.74	0.41	78,78,78,78	0
54	MG	1G	2267	1/1	0.74	0.35	87,87,87,87	0
54	MG	1G	2299	1/1	0.74	0.35	96,96,96,96	0
54	MG	1H	3168	1/1	0.74	0.31	39,39,39,39	0
54	MG	14	3512	1/1	0.74	0.32	69,69,69,69	0
54	MG	1H	3236	1/1	0.74	0.50	79,79,79,79	0
54	MG	14	3254	1/1	0.74	0.35	92,92,92,92	0
54	MG	1G	2240	1/1	0.74	0.35	86,86,86,86	0
54	MG	1G	2259	1/1	0.74	0.37	87,87,87,87	0
54	MG	1H	3300	1/1	0.74	0.35	84,84,84,84	0
54	MG	13	2300	1/1	0.74	0.26	81,81,81,81	0
54	MG	1H	3400	1/1	0.75	0.31	73,73,73,73	0
54	MG	1J	209	1/1	0.75	0.24	77,77,77,77	0
54	MG	1H	3412	1/1	0.75	0.17	86,86,86,86	0
53	8UZ	14	3005	33/33	0.75	0.14	82,82,82,82	0
54	MG	1G	2351	1/1	0.75	0.24	78,78,78,78	0
54	MG	1H	3549	1/1	0.75	0.20	57,57,57,57	0
54	MG	1H	3606	1/1	0.75	0.11	63,63,63,63	0
54	MG	14	3323	1/1	0.75	0.14	84,84,84,84	0
54	MG	1G	2217	1/1	0.75	0.27	73,73,73,73	0
54	MG	13	2261	1/1	0.75	0.30	66,66,66,66	0
54	MG	13	2263	1/1	0.75	0.28	81,81,81,81	0
54	MG	1G	2234	1/1	0.75	0.29	72,72,72,72	0
54	MG	14	3538	1/1	0.75	0.12	78,78,78,78	0
54	MG	32	304	1/1	0.75	0.29	86,86,86,86	0
54	MG	14	3145	1/1	0.75	0.32	54,54,54,54	0
54	MG	14	3559	1/1	0.75	0.19	75,75,75,75	0
54	MG	1G	2237	1/1	0.75	0.24	78,78,78,78	0
54	MG	1H	3363	1/1	0.75	0.30	67,67,67,67	0
54	MG	14	3195	1/1	0.75	0.26	71,71,71,71	0
54	MG	42	201	1/1	0.76	0.23	99,99,99,99	0
54	MG	1J	208	1/1	0.76	0.28	75,75,75,75	0
54	MG	14	3464	1/1	0.76	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3157	1/1	0.76	0.28	57,57,57,57	0
54	MG	31	302	1/1	0.76	0.21	68,68,68,68	0
54	MG	1H	3581	1/1	0.76	0.25	63,63,63,63	0
54	MG	1G	2289	1/1	0.76	0.30	90,90,90,90	0
54	MG	1G	2309	1/1	0.76	0.21	92,92,92,92	0
54	MG	13	2250	1/1	0.76	0.44	74,74,74,74	0
54	MG	14	3387	1/1	0.76	0.12	73,73,73,73	0
54	MG	14	3399	1/1	0.76	0.17	79,79,79,79	0
54	MG	1H	3315	1/1	0.76	0.34	73,73,73,73	0
54	MG	1G	2366	1/1	0.76	0.20	71,71,71,71	0
54	MG	14	3546	1/1	0.76	0.19	71,71,71,71	0
54	MG	14	3435	1/1	0.76	0.32	72,72,72,72	0
54	MG	1H	3538	1/1	0.76	0.24	81,81,81,81	0
54	MG	14	3249	1/1	0.76	0.41	66,66,66,66	0
54	MG	14	3131	1/1	0.76	0.29	70,70,70,70	0
54	MG	14	3261	1/1	0.76	0.45	45,45,45,45	0
54	MG	14	3265	1/1	0.76	0.44	85,85,85,85	0
54	MG	1G	2377	1/1	0.76	0.48	92,92,92,92	0
54	MG	1H	3133	1/1	0.77	0.28	65,65,65,65	0
54	MG	14	3106	1/1	0.77	0.46	49,49,49,49	0
54	MG	13	2249	1/1	0.77	0.34	66,66,66,66	0
54	MG	1H	3573	1/1	0.77	0.36	78,78,78,78	0
54	MG	14	3156	1/1	0.77	0.27	63,63,63,63	0
54	MG	13	2372	1/1	0.77	0.23	93,93,93,93	0
54	MG	1G	2312	1/1	0.77	0.12	101,101,101,101	0
54	MG	14	3187	1/1	0.77	0.26	53,53,53,53	0
54	MG	14	3558	1/1	0.77	0.18	71,71,71,71	0
54	MG	13	2342	1/1	0.77	0.22	69,69,69,69	0
54	MG	1H	3611	1/1	0.77	0.10	47,47,47,47	0
54	MG	14	3574	1/1	0.77	0.37	73,73,73,73	0
54	MG	1H	3436	1/1	0.77	0.29	78,78,78,78	0
54	MG	1G	2233	1/1	0.77	0.38	67,67,67,67	0
54	MG	14	3388	1/1	0.77	0.30	70,70,70,70	0
54	MG	13	2397	1/1	0.77	0.20	77,77,77,77	0
54	MG	14	3493	1/1	0.77	0.29	50,50,50,50	0
54	MG	14	3503	1/1	0.77	0.14	62,62,62,62	0
54	MG	1G	2389	1/1	0.78	0.31	105,105,105,105	0
54	MG	1H	3427	1/1	0.78	0.11	46,46,46,46	0
54	MG	14	3167	1/1	0.78	0.33	54,54,54,54	0
54	MG	1G	2318	1/1	0.78	0.52	76,76,76,76	0
54	MG	16	203	1/1	0.78	0.13	69,69,69,69	0
54	MG	1G	2361	1/1	0.78	0.24	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2223	1/1	0.78	0.31	51,51,51,51	0
54	MG	1H	3516	1/1	0.78	0.16	52,52,52,52	0
54	MG	14	3198	1/1	0.78	0.38	74,74,74,74	0
54	MG	1J	204	1/1	0.78	0.33	67,67,67,67	0
54	MG	1H	3214	1/1	0.78	0.39	37,37,37,37	0
54	MG	1G	2258	1/1	0.78	0.34	86,86,86,86	0
54	MG	1H	3249	1/1	0.78	0.27	65,65,65,65	0
54	MG	1J	214	1/1	0.78	0.23	80,80,80,80	0
54	MG	1H	3262	1/1	0.78	0.36	75,75,75,75	0
54	MG	1G	2339	1/1	0.78	0.25	78,78,78,78	0
54	MG	1H	3270	1/1	0.78	0.21	65,65,65,65	0
54	MG	14	3487	1/1	0.78	0.24	45,45,45,45	0
54	MG	1G	2228	1/1	0.78	0.38	75,75,75,75	0
54	MG	13	2375	1/1	0.78	0.31	78,78,78,78	0
54	MG	14	3274	1/1	0.78	0.26	71,71,71,71	0
54	MG	14	3291	1/1	0.78	0.23	69,69,69,69	0
54	MG	14	3504	1/1	0.78	0.40	75,75,75,75	0
54	MG	14	3309	1/1	0.78	0.29	70,70,70,70	0
54	MG	13	2232	1/1	0.78	0.35	75,75,75,75	0
54	MG	13	2295	1/1	0.78	0.34	113,113,113,113	0
54	MG	32	302	1/1	0.78	0.33	95,95,95,95	0
54	MG	W4	102	1/1	0.78	0.22	88,88,88,88	0
54	MG	13	2316	1/1	0.78	0.22	72,72,72,72	0
54	MG	X4	101	1/1	0.78	0.48	91,91,91,91	0
54	MG	1G	2379	1/1	0.78	0.23	78,78,78,78	0
54	MG	1H	3383	1/1	0.78	0.15	62,62,62,62	0
54	MG	13	2325	1/1	0.78	0.21	64,64,64,64	0
54	MG	14	3563	1/1	0.79	0.30	70,70,70,70	0
54	MG	14	3152	1/1	0.79	0.34	49,49,49,49	0
54	MG	14	3586	1/1	0.79	0.29	77,77,77,77	0
54	MG	4I	201	1/1	0.79	0.15	84,84,84,84	0
54	MG	1G	2244	1/1	0.79	0.32	80,80,80,80	0
54	MG	14	3282	1/1	0.79	0.23	64,64,64,64	0
54	MG	14	3461	1/1	0.79	0.30	61,61,61,61	0
54	MG	13	2360	1/1	0.79	0.18	82,82,82,82	0
54	MG	14	3463	1/1	0.79	0.11	71,71,71,71	0
54	MG	14	3300	1/1	0.79	0.38	73,73,73,73	0
54	MG	14	3465	1/1	0.79	0.22	76,76,76,76	0
54	MG	13	2306	1/1	0.79	0.34	81,81,81,81	0
54	MG	1H	3138	1/1	0.79	0.22	54,54,54,54	0
54	MG	13	2364	1/1	0.79	0.14	75,75,75,75	0
54	MG	14	3325	1/1	0.79	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	35	201	1/1	0.79	0.25	64,64,64,64	0
54	MG	1H	3210	1/1	0.79	0.24	52,52,52,52	0
54	MG	13	2246	1/1	0.79	0.36	64,64,64,64	0
54	MG	13	2234	1/1	0.79	0.33	89,89,89,89	0
54	MG	14	3352	1/1	0.79	0.35	87,87,87,87	0
54	MG	14	3511	1/1	0.79	0.29	68,68,68,68	0
54	MG	13	2266	1/1	0.79	0.19	87,87,87,87	0
54	MG	14	3513	1/1	0.79	0.46	71,71,71,71	0
54	MG	X1	102	1/1	0.79	0.46	79,79,79,79	0
54	MG	14	3374	1/1	0.79	0.16	78,78,78,78	0
54	MG	1G	2293	1/1	0.79	0.20	85,85,85,85	0
54	MG	1G	2357	1/1	0.79	0.23	96,96,96,96	0
54	MG	14	3392	1/1	0.79	0.24	78,78,78,78	0
54	MG	14	3239	1/1	0.79	0.29	62,62,62,62	0
54	MG	1H	3490	1/1	0.79	0.28	91,91,91,91	0
54	MG	14	3551	1/1	0.79	0.23	78,78,78,78	0
54	MG	14	3245	1/1	0.79	0.40	65,65,65,65	0
54	MG	1G	2317	1/1	0.79	0.35	78,78,78,78	0
54	MG	1H	3512	1/1	0.79	0.19	55,55,55,55	0
54	MG	13	2259	1/1	0.79	0.24	80,80,80,80	0
54	MG	1H	3297	1/1	0.80	0.19	57,57,57,57	0
54	MG	14	3118	1/1	0.80	0.35	44,44,44,44	0
54	MG	13	2244	1/1	0.80	0.19	53,53,53,53	0
54	MG	14	3132	1/1	0.80	0.28	47,47,47,47	0
54	MG	1H	3301	1/1	0.80	0.28	74,74,74,74	0
54	MG	1H	3304	1/1	0.80	0.33	82,82,82,82	0
54	MG	14	3286	1/1	0.80	0.29	90,90,90,90	0
54	MG	1G	2276	1/1	0.80	0.33	67,67,67,67	0
54	MG	1H	3326	1/1	0.80	0.35	73,73,73,73	0
54	MG	13	2398	1/1	0.80	0.26	76,76,76,76	0
54	MG	13	2238	1/1	0.80	0.21	80,80,80,80	0
54	MG	13	2219	1/1	0.80	0.25	71,71,71,71	0
54	MG	1H	3382	1/1	0.80	0.27	94,94,94,94	0
54	MG	55	203	1/1	0.80	0.12	56,56,56,56	0
54	MG	1G	2360	1/1	0.80	0.41	83,83,83,83	0
54	MG	1G	2286	1/1	0.80	0.21	85,85,85,85	0
54	MG	1H	3634	1/1	0.80	0.30	66,66,66,66	0
54	MG	14	3474	1/1	0.80	0.45	63,63,63,63	0
54	MG	13	2298	1/1	0.80	0.35	86,86,86,86	0
54	MG	14	3363	1/1	0.80	0.12	75,75,75,75	0
54	MG	16	201	1/1	0.80	0.11	72,72,72,72	0
54	MG	15	201	1/1	0.80	0.08	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2321	1/1	0.80	0.23	84,84,84,84	0
54	MG	1H	3280	1/1	0.80	0.19	50,50,50,50	0
54	MG	25	201	1/1	0.80	0.31	83,83,83,83	0
54	MG	14	3499	1/1	0.80	0.30	69,69,69,69	0
54	MG	1G	2255	1/1	0.80	0.32	68,68,68,68	0
54	MG	13	2344	1/1	0.81	0.18	50,50,50,50	0
54	MG	14	3308	1/1	0.81	0.30	66,66,66,66	0
54	MG	1H	3643	1/1	0.81	0.32	68,68,68,68	0
54	MG	1G	2241	1/1	0.81	0.31	75,75,75,75	0
54	MG	1G	2367	1/1	0.81	0.21	101,101,101,101	0
54	MG	1H	3142	1/1	0.81	0.45	72,72,72,72	0
54	MG	14	3208	1/1	0.81	0.30	68,68,68,68	0
54	MG	14	3334	1/1	0.81	0.24	83,83,83,83	0
54	MG	14	3224	1/1	0.81	0.25	66,66,66,66	0
54	MG	14	3342	1/1	0.81	0.19	75,75,75,75	0
54	MG	14	3345	1/1	0.81	0.09	66,66,66,66	0
54	MG	1H	3341	1/1	0.81	0.32	55,55,55,55	0
54	MG	14	3494	1/1	0.81	0.18	91,91,91,91	0
54	MG	14	3348	1/1	0.81	0.22	68,68,68,68	0
54	MG	14	3105	1/1	0.81	0.34	48,48,48,48	0
54	MG	14	3360	1/1	0.81	0.15	70,70,70,70	0
54	MG	88	204	1/1	0.81	0.39	81,81,81,81	0
54	MG	1H	3352	1/1	0.81	0.22	70,70,70,70	0
54	MG	1H	3353	1/1	0.81	0.20	58,58,58,58	0
54	MG	1H	3162	1/1	0.81	0.32	39,39,39,39	0
54	MG	14	3244	1/1	0.81	0.16	83,83,83,83	0
54	MG	1H	3288	1/1	0.81	0.22	62,62,62,62	0
54	MG	1G	2242	1/1	0.81	0.43	79,79,79,79	0
54	MG	14	3395	1/1	0.81	0.43	80,80,80,80	0
54	MG	13	2362	1/1	0.81	0.17	81,81,81,81	0
54	MG	1G	2385	1/1	0.81	0.16	88,88,88,88	0
54	MG	1H	3219	1/1	0.81	0.28	48,48,48,48	0
54	MG	14	3273	1/1	0.81	0.29	72,72,72,72	0
54	MG	14	3163	1/1	0.81	0.26	57,57,57,57	0
54	MG	14	3164	1/1	0.81	0.30	52,52,52,52	0
54	MG	14	3285	1/1	0.81	0.26	49,49,49,49	0
54	MG	1G	2342	1/1	0.81	0.19	76,76,76,76	0
54	MG	14	3456	1/1	0.81	0.08	78,78,78,78	0
54	MG	14	3582	1/1	0.81	0.19	77,77,77,77	0
54	MG	14	3169	1/1	0.81	0.25	64,64,64,64	0
54	MG	14	3592	1/1	0.81	0.28	77,77,77,77	0
54	MG	X4	105	1/1	0.81	0.27	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2248	1/1	0.82	0.46	62,62,62,62	0
54	MG	14	3371	1/1	0.82	0.22	68,68,68,68	0
54	MG	1H	3562	1/1	0.82	0.35	73,73,73,73	0
54	MG	8I	201	1/1	0.82	0.30	77,77,77,77	0
54	MG	13	2216	1/1	0.82	0.32	59,59,59,59	0
54	MG	1H	3591	1/1	0.82	0.25	68,68,68,68	0
54	MG	1H	3592	1/1	0.82	0.16	63,63,63,63	0
54	MG	1H	3307	1/1	0.82	0.31	36,36,36,36	0
54	MG	1H	3135	1/1	0.82	0.40	51,51,51,51	0
54	MG	13	2268	1/1	0.82	0.27	58,58,58,58	0
54	MG	14	3417	1/1	0.82	0.34	66,66,66,66	0
54	MG	1H	3621	1/1	0.82	0.15	50,50,50,50	0
54	MG	1H	3627	1/1	0.82	0.10	65,65,65,65	0
54	MG	1H	3630	1/1	0.82	0.24	76,76,76,76	0
54	MG	1G	2315	1/1	0.82	0.32	76,76,76,76	0
54	MG	1H	3144	1/1	0.82	0.25	65,65,65,65	0
54	MG	14	3253	1/1	0.82	0.30	89,89,89,89	0
54	MG	1H	3636	1/1	0.82	0.30	72,72,72,72	0
54	MG	14	3260	1/1	0.82	0.36	48,48,48,48	0
54	MG	1H	3148	1/1	0.82	0.17	61,61,61,61	0
54	MG	1H	3156	1/1	0.82	0.26	63,63,63,63	0
54	MG	1H	3661	1/1	0.82	0.30	48,48,48,48	0
54	MG	1G	2316	1/1	0.82	0.22	82,82,82,82	0
54	MG	14	3470	1/1	0.82	0.18	85,85,85,85	0
54	MG	D8	202	1/1	0.82	0.27	72,72,72,72	0
54	MG	1H	3360	1/1	0.82	0.26	65,65,65,65	0
54	MG	13	2376	1/1	0.82	0.25	84,84,84,84	0
54	MG	1H	3371	1/1	0.82	0.16	59,59,59,59	0
54	MG	14	3478	1/1	0.82	0.22	89,89,89,89	0
54	MG	14	3097	1/1	0.82	0.38	45,45,45,45	0
54	MG	13	2377	1/1	0.82	0.43	78,78,78,78	0
54	MG	13	2383	1/1	0.82	0.25	77,77,77,77	0
54	MG	55	201	1/1	0.82	0.24	58,58,58,58	0
54	MG	1H	3395	1/1	0.82	0.27	79,79,79,79	0
54	MG	14	3122	1/1	0.82	0.22	66,66,66,66	0
54	MG	14	3321	1/1	0.82	0.15	73,73,73,73	0
54	MG	1H	3396	1/1	0.82	0.23	78,78,78,78	0
54	MG	X1	104	1/1	0.82	0.47	82,82,82,82	0
54	MG	13	2284	1/1	0.82	0.23	69,69,69,69	0
54	MG	1G	2236	1/1	0.82	0.26	77,77,77,77	0
54	MG	13	2392	1/1	0.82	0.28	64,64,64,64	0
54	MG	14	3155	1/1	0.82	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1G	2344	1/1	0.82	0.28	82,82,82,82	0
54	MG	13	2351	1/1	0.82	0.23	58,58,58,58	0
54	MG	1G	2346	1/1	0.82	0.26	73,73,73,73	0
54	MG	13	2299	1/1	0.82	0.39	83,83,83,83	0
54	MG	1G	2272	1/1	0.82	0.27	72,72,72,72	0
54	MG	1G	2383	1/1	0.82	0.27	78,78,78,78	0
54	MG	1G	2273	1/1	0.82	0.25	70,70,70,70	0
54	MG	14	3402	1/1	0.83	0.24	72,72,72,72	0
54	MG	14	3262	1/1	0.83	0.38	49,49,49,49	0
54	MG	14	3405	1/1	0.83	0.23	78,78,78,78	0
54	MG	14	3566	1/1	0.83	0.20	66,66,66,66	0
54	MG	14	3407	1/1	0.83	0.14	62,62,62,62	0
54	MG	1H	3576	1/1	0.83	0.19	55,55,55,55	0
54	MG	14	3271	1/1	0.83	0.18	60,60,60,60	0
54	MG	14	3591	1/1	0.83	0.29	51,51,51,51	0
54	MG	1H	3578	1/1	0.83	0.26	59,59,59,59	0
54	MG	1H	3358	1/1	0.83	0.20	52,52,52,52	0
54	MG	1H	3143	1/1	0.83	0.27	66,66,66,66	0
54	MG	14	3283	1/1	0.83	0.26	67,67,67,67	0
54	MG	1G	2253	1/1	0.83	0.39	85,85,85,85	0
54	MG	16	212	1/1	0.83	0.10	73,73,73,73	0
54	MG	1G	2343	1/1	0.83	0.24	79,79,79,79	0
54	MG	13	2226	1/1	0.83	0.24	89,89,89,89	0
54	MG	14	3159	1/1	0.83	0.43	46,46,46,46	0
54	MG	1H	3608	1/1	0.83	0.20	66,66,66,66	0
54	MG	1J	201	1/1	0.83	0.12	90,90,90,90	0
54	MG	1G	2291	1/1	0.83	0.18	91,91,91,91	0
54	MG	1H	3612	1/1	0.83	0.18	56,56,56,56	0
54	MG	13	2275	1/1	0.83	0.16	81,81,81,81	0
54	MG	13	2282	1/1	0.83	0.40	64,64,64,64	0
54	MG	13	2247	1/1	0.83	0.31	68,68,68,68	0
54	MG	1H	3407	1/1	0.83	0.37	58,58,58,58	0
54	MG	1G	2203	1/1	0.83	0.31	73,73,73,73	0
54	MG	14	3481	1/1	0.83	0.25	78,78,78,78	0
54	MG	1H	3227	1/1	0.83	0.46	46,46,46,46	0
54	MG	1H	3230	1/1	0.83	0.40	61,61,61,61	0
54	MG	14	3343	1/1	0.83	0.17	56,56,56,56	0
54	MG	14	3211	1/1	0.83	0.32	56,56,56,56	0
54	MG	1H	3640	1/1	0.83	0.22	73,73,73,73	0
54	MG	1H	3318	1/1	0.83	0.27	52,52,52,52	0
54	MG	1H	3319	1/1	0.83	0.25	69,69,69,69	0
54	MG	1H	3492	1/1	0.83	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3510	1/1	0.83	0.21	65,65,65,65	0
54	MG	14	3361	1/1	0.83	0.17	66,66,66,66	0
54	MG	13	2394	1/1	0.83	0.42	87,87,87,87	0
54	MG	1H	3241	1/1	0.83	0.38	54,54,54,54	0
54	MG	1H	3246	1/1	0.83	0.28	51,51,51,51	0
54	MG	1H	3527	1/1	0.83	0.12	50,50,50,50	0
54	MG	14	3530	1/1	0.83	0.16	76,76,76,76	0
54	MG	14	3382	1/1	0.83	0.37	70,70,70,70	0
54	MG	14	3534	1/1	0.83	0.31	71,71,71,71	0
54	MG	14	3246	1/1	0.83	0.31	80,80,80,80	0
54	MG	14	3545	1/1	0.83	0.28	83,83,83,83	0
54	MG	1H	3248	1/1	0.83	0.17	53,53,53,53	0
54	MG	1H	3349	1/1	0.83	0.27	74,74,74,74	0
54	MG	1G	2249	1/1	0.83	0.33	69,69,69,69	0
54	MG	1G	2252	1/1	0.83	0.28	84,84,84,84	0
54	MG	14	3126	1/1	0.83	0.44	53,53,53,53	0
54	MG	1H	3099	1/1	0.84	0.27	40,40,40,40	0
54	MG	14	3305	1/1	0.84	0.19	68,68,68,68	0
54	MG	14	3579	1/1	0.84	0.24	51,51,51,51	0
54	MG	1H	3105	1/1	0.84	0.24	46,46,46,46	0
54	MG	14	3452	1/1	0.84	0.29	76,76,76,76	0
54	MG	14	3455	1/1	0.84	0.37	86,86,86,86	0
54	MG	1H	3215	1/1	0.84	0.22	49,49,49,49	0
54	MG	1H	3111	1/1	0.84	0.40	34,34,34,34	0
54	MG	14	3190	1/1	0.84	0.50	53,53,53,53	0
54	MG	14	3322	1/1	0.84	0.36	64,64,64,64	0
54	MG	1H	3220	1/1	0.84	0.23	44,44,44,44	0
54	MG	1H	3439	1/1	0.84	0.20	43,43,43,43	0
54	MG	1H	3448	1/1	0.84	0.26	56,56,56,56	0
54	MG	14	3468	1/1	0.84	0.11	71,71,71,71	0
54	MG	1H	3114	1/1	0.84	0.17	49,49,49,49	0
54	MG	13	2264	1/1	0.84	0.21	76,76,76,76	0
54	MG	1G	2256	1/1	0.84	0.30	74,74,74,74	0
54	MG	1H	3493	1/1	0.84	0.18	55,55,55,55	0
54	MG	1H	3239	1/1	0.84	0.31	54,54,54,54	0
54	MG	1H	3505	1/1	0.84	0.26	70,70,70,70	0
54	MG	1J	210	1/1	0.84	0.21	77,77,77,77	0
54	MG	1H	3511	1/1	0.84	0.15	64,64,64,64	0
54	MG	14	3489	1/1	0.84	0.40	71,71,71,71	0
54	MG	1G	2330	1/1	0.84	0.20	95,95,95,95	0
54	MG	14	3358	1/1	0.84	0.24	71,71,71,71	0
54	MG	1H	3245	1/1	0.84	0.43	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1G	2363	1/1	0.84	0.11	85,85,85,85	0
54	MG	39	301	1/1	0.84	0.10	59,59,59,59	0
54	MG	1H	3247	1/1	0.84	0.24	55,55,55,55	0
54	MG	14	3369	1/1	0.84	0.42	49,49,49,49	0
54	MG	1G	2224	1/1	0.84	0.36	78,78,78,78	0
53	8UZ	1H	3005	33/33	0.84	0.11	70,70,70,70	0
54	MG	14	3125	1/1	0.84	0.26	63,63,63,63	0
54	MG	14	3379	1/1	0.84	0.42	56,56,56,56	0
54	MG	14	3259	1/1	0.84	0.34	47,47,47,47	0
54	MG	14	3386	1/1	0.84	0.21	75,75,75,75	0
54	MG	P8	101	1/1	0.84	0.24	52,52,52,52	0
54	MG	1H	3563	1/1	0.84	0.14	71,71,71,71	0
54	MG	1H	3260	1/1	0.84	0.24	42,42,42,42	0
54	MG	1G	2226	1/1	0.84	0.14	104,104,104,104	0
54	MG	14	3263	1/1	0.84	0.30	49,49,49,49	0
54	MG	14	3143	1/1	0.84	0.23	52,52,52,52	0
54	MG	13	2335	1/1	0.84	0.28	59,59,59,59	0
54	MG	1H	3159	1/1	0.84	0.22	65,65,65,65	0
54	MG	1H	3380	1/1	0.84	0.06	62,62,62,62	0
54	MG	1H	3273	1/1	0.84	0.29	63,63,63,63	0
54	MG	58	201	1/1	0.84	0.57	82,82,82,82	0
54	MG	14	3411	1/1	0.84	0.15	77,77,77,77	0
54	MG	13	2277	1/1	0.84	0.12	73,73,73,73	0
54	MG	1H	3170	1/1	0.84	0.24	40,40,40,40	0
54	MG	1H	3399	1/1	0.84	0.24	59,59,59,59	0
54	MG	14	3565	1/1	0.84	0.25	68,68,68,68	0
54	MG	14	3247	1/1	0.85	0.26	55,55,55,55	0
54	MG	14	3547	1/1	0.85	0.13	52,52,52,52	0
54	MG	1G	2340	1/1	0.85	0.10	79,79,79,79	0
54	MG	1G	2278	1/1	0.85	0.10	79,79,79,79	0
54	MG	1H	3174	1/1	0.85	0.27	51,51,51,51	0
54	MG	14	3109	1/1	0.85	0.22	70,70,70,70	0
54	MG	14	3113	1/1	0.85	0.38	50,50,50,50	0
54	MG	1H	3355	1/1	0.85	0.13	66,66,66,66	0
54	MG	1H	3207	1/1	0.85	0.38	47,47,47,47	0
54	MG	1G	2281	1/1	0.85	0.30	78,78,78,78	0
54	MG	13	2289	1/1	0.85	0.37	71,71,71,71	0
54	MG	14	3408	1/1	0.85	0.09	57,57,57,57	0
54	MG	14	3575	1/1	0.85	0.24	65,65,65,65	0
54	MG	14	3130	1/1	0.85	0.29	64,64,64,64	0
54	MG	1H	3365	1/1	0.85	0.11	58,58,58,58	0
54	MG	14	3418	1/1	0.85	0.47	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	14	3587	1/1	0.85	0.27	65,65,65,65	0
54	MG	14	3590	1/1	0.85	0.18	80,80,80,80	0
54	MG	14	3421	1/1	0.85	0.34	73,73,73,73	0
54	MG	1H	3569	1/1	0.85	0.29	60,60,60,60	0
54	MG	14	3281	1/1	0.85	0.29	70,70,70,70	0
54	MG	14	3135	1/1	0.85	0.35	47,47,47,47	0
54	MG	1H	3281	1/1	0.85	0.23	66,66,66,66	0
54	MG	1H	3374	1/1	0.85	0.30	48,48,48,48	0
54	MG	14	3448	1/1	0.85	0.20	63,63,63,63	0
54	MG	1H	3377	1/1	0.85	0.15	63,63,63,63	0
54	MG	1H	3286	1/1	0.85	0.47	84,84,84,84	0
54	MG	14	3292	1/1	0.85	0.30	77,77,77,77	0
53	8UZ	14	3003	33/33	0.85	0.23	64,64,64,64	33
54	MG	14	3301	1/1	0.85	0.38	62,62,62,62	0
54	MG	13	2399	1/1	0.85	0.27	75,75,75,75	0
54	MG	14	3307	1/1	0.85	0.24	58,58,58,58	0
54	MG	1H	3605	1/1	0.85	0.09	66,66,66,66	0
54	MG	1H	3296	1/1	0.85	0.30	82,82,82,82	0
54	MG	14	3310	1/1	0.85	0.29	91,91,91,91	0
54	MG	1H	3125	1/1	0.85	0.30	43,43,43,43	0
54	MG	14	3166	1/1	0.85	0.71	49,49,49,49	0
54	MG	1G	2370	1/1	0.85	0.16	102,102,102,102	0
54	MG	1G	2250	1/1	0.85	0.26	71,71,71,71	0
54	MG	14	3172	1/1	0.85	0.48	63,63,63,63	0
54	MG	14	3479	1/1	0.85	0.10	65,65,65,65	0
54	MG	1H	3404	1/1	0.85	0.34	68,68,68,68	0
54	MG	13	2224	1/1	0.85	0.31	65,65,65,65	0
54	MG	13	2353	1/1	0.85	0.14	76,76,76,76	0
54	MG	1H	3416	1/1	0.85	0.28	36,36,36,36	0
54	MG	1H	3312	1/1	0.85	0.13	45,45,45,45	0
54	MG	1G	2290	1/1	0.85	0.23	73,73,73,73	0
54	MG	14	3199	1/1	0.85	0.21	75,75,75,75	0
54	MG	1H	3243	1/1	0.85	0.12	57,57,57,57	0
54	MG	14	3500	1/1	0.85	0.35	67,67,67,67	0
54	MG	W1	103	1/1	0.85	0.27	80,80,80,80	0
54	MG	13	2235	1/1	0.85	0.23	82,82,82,82	0
54	MG	14	3216	1/1	0.85	0.27	55,55,55,55	0
54	MG	13	2225	1/1	0.85	0.26	72,72,72,72	0
54	MG	1H	3327	1/1	0.85	0.18	60,60,60,60	0
54	MG	1H	3653	1/1	0.85	0.29	86,86,86,86	0
54	MG	1H	3655	1/1	0.85	0.13	66,66,66,66	0
54	MG	1H	3333	1/1	0.85	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	14	3515	1/1	0.85	0.14	76,76,76,76	0
54	MG	W4	101	1/1	0.85	0.24	89,89,89,89	0
54	MG	14	3518	1/1	0.85	0.17	61,61,61,61	0
54	MG	1G	2275	1/1	0.85	0.14	87,87,87,87	0
54	MG	14	3242	1/1	0.85	0.47	62,62,62,62	0
54	MG	14	3377	1/1	0.85	0.17	55,55,55,55	0
54	MG	1H	3501	1/1	0.85	0.08	52,52,52,52	0
54	MG	13	2395	1/1	0.85	0.28	89,89,89,89	0
54	MG	13	2257	1/1	0.85	0.36	68,68,68,68	0
54	MG	13	2368	1/1	0.86	0.22	59,59,59,59	0
54	MG	1H	3161	1/1	0.86	0.19	56,56,56,56	0
54	MG	14	3415	1/1	0.86	0.13	52,52,52,52	0
54	MG	14	3555	1/1	0.86	0.21	79,79,79,79	0
54	MG	1G	2300	1/1	0.86	0.22	91,91,91,91	0
54	MG	1G	2301	1/1	0.86	0.23	77,77,77,77	0
54	MG	14	3420	1/1	0.86	0.49	46,46,46,46	0
54	MG	1H	3387	1/1	0.86	0.16	66,66,66,66	0
54	MG	14	3428	1/1	0.86	0.19	52,52,52,52	0
54	MG	14	3297	1/1	0.86	0.19	61,61,61,61	0
54	MG	14	3568	1/1	0.86	0.17	71,71,71,71	0
54	MG	14	3436	1/1	0.86	0.34	72,72,72,72	0
54	MG	13	2245	1/1	0.86	0.11	56,56,56,56	0
54	MG	1G	2308	1/1	0.86	0.22	79,79,79,79	0
54	MG	13	2371	1/1	0.86	0.48	89,89,89,89	0
54	MG	1G	2349	1/1	0.86	0.33	67,67,67,67	0
54	MG	14	3445	1/1	0.86	0.25	63,63,63,63	0
53	8UZ	1H	3004	33/33	0.86	0.14	75,75,75,75	0
54	MG	14	3449	1/1	0.86	0.23	52,52,52,52	0
54	MG	14	3451	1/1	0.86	0.41	51,51,51,51	0
54	MG	14	3596	1/1	0.86	0.24	58,58,58,58	0
54	MG	1H	3405	1/1	0.86	0.18	63,63,63,63	0
54	MG	13	2293	1/1	0.86	0.22	63,63,63,63	0
54	MG	14	3312	1/1	0.86	0.20	66,66,66,66	0
54	MG	14	3457	1/1	0.86	0.28	52,52,52,52	0
54	MG	14	3313	1/1	0.86	0.19	77,77,77,77	0
54	MG	1G	2352	1/1	0.86	0.21	79,79,79,79	0
54	MG	14	3318	1/1	0.86	0.25	63,63,63,63	0
54	MG	8A	201	1/1	0.86	0.14	88,88,88,88	0
54	MG	14	3189	1/1	0.86	0.34	51,51,51,51	0
54	MG	1H	3223	1/1	0.86	0.36	52,52,52,52	0
54	MG	1J	202	1/1	0.86	0.15	86,86,86,86	0
54	MG	13	2218	1/1	0.86	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2310	1/1	0.86	0.40	80,80,80,80	0
54	MG	13	2361	1/1	0.86	0.18	81,81,81,81	0
54	MG	14	3472	1/1	0.86	0.14	61,61,61,61	0
54	MG	1H	3450	1/1	0.86	0.25	60,60,60,60	0
54	MG	1H	3329	1/1	0.86	0.30	57,57,57,57	0
54	MG	1H	3652	1/1	0.86	0.26	90,90,90,90	0
54	MG	5I	102	1/1	0.86	0.17	81,81,81,81	0
54	MG	1H	3468	1/1	0.86	0.13	47,47,47,47	0
54	MG	1H	3109	1/1	0.86	0.42	36,36,36,36	0
54	MG	13	2276	1/1	0.86	0.25	69,69,69,69	0
54	MG	1G	2265	1/1	0.86	0.17	86,86,86,86	0
54	MG	13	2231	1/1	0.86	0.24	74,74,74,74	0
54	MG	1H	3346	1/1	0.86	0.15	52,52,52,52	0
54	MG	14	3492	1/1	0.86	0.27	63,63,63,63	0
54	MG	32	303	1/1	0.86	0.31	77,77,77,77	0
54	MG	1H	3131	1/1	0.86	0.29	53,53,53,53	0
54	MG	14	3367	1/1	0.86	0.20	55,55,55,55	0
54	MG	1G	2322	1/1	0.86	0.35	75,75,75,75	0
54	MG	1G	2325	1/1	0.86	0.23	76,76,76,76	0
53	8UZ	1H	3003	33/33	0.86	0.22	54,54,54,54	33
54	MG	1H	3357	1/1	0.86	0.21	56,56,56,56	0
54	MG	14	3111	1/1	0.86	0.36	61,61,61,61	0
54	MG	14	3112	1/1	0.86	0.30	53,53,53,53	0
54	MG	1H	3139	1/1	0.86	0.21	46,46,46,46	0
54	MG	1H	3541	1/1	0.86	0.24	49,49,49,49	0
54	MG	1H	3543	1/1	0.86	0.13	56,56,56,56	0
54	MG	13	2391	1/1	0.86	0.17	78,78,78,78	0
54	MG	1G	2328	1/1	0.86	0.13	74,74,74,74	0
54	MG	14	3520	1/1	0.86	0.20	72,72,72,72	0
54	MG	1G	2251	1/1	0.86	0.19	71,71,71,71	0
54	MG	1G	2337	1/1	0.86	0.23	91,91,91,91	0
54	MG	1H	3570	1/1	0.86	0.10	57,57,57,57	0
54	MG	14	3535	1/1	0.86	0.34	77,77,77,77	0
54	MG	1H	3571	1/1	0.86	0.14	67,67,67,67	0
54	MG	14	3138	1/1	0.86	0.30	56,56,56,56	0
54	MG	14	3141	1/1	0.86	0.26	55,55,55,55	0
53	8UZ	14	3006	33/33	0.86	0.21	68,68,68,68	33
54	MG	1H	3393	1/1	0.87	0.22	54,54,54,54	0
54	MG	14	3268	1/1	0.87	0.18	49,49,49,49	0
54	MG	14	3406	1/1	0.87	0.28	72,72,72,72	0
53	8UZ	14	3004	33/33	0.87	0.12	87,87,87,87	0
54	MG	1G	2297	1/1	0.87	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	14	3409	1/1	0.87	0.12	65,65,65,65	0
54	MG	1H	3397	1/1	0.87	0.37	62,62,62,62	0
54	MG	1H	3225	1/1	0.87	0.18	58,58,58,58	0
54	MG	13	2236	1/1	0.87	0.15	64,64,64,64	0
54	MG	1G	2254	1/1	0.87	0.37	65,65,65,65	0
54	MG	13	2328	1/1	0.87	0.21	74,74,74,74	0
54	MG	3E	302	1/1	0.87	0.36	92,92,92,92	0
54	MG	14	3425	1/1	0.87	0.34	55,55,55,55	0
54	MG	14	3287	1/1	0.87	0.23	64,64,64,64	0
54	MG	14	3432	1/1	0.87	0.21	58,58,58,58	0
54	MG	1H	3152	1/1	0.87	0.35	46,46,46,46	0
54	MG	1H	3155	1/1	0.87	0.27	39,39,39,39	0
54	MG	14	3577	1/1	0.87	0.18	54,54,54,54	0
54	MG	1H	3423	1/1	0.87	0.27	55,55,55,55	0
54	MG	1H	3425	1/1	0.87	0.28	64,64,64,64	0
54	MG	14	3583	1/1	0.87	0.26	69,69,69,69	0
54	MG	14	3585	1/1	0.87	0.26	57,57,57,57	0
54	MG	14	3439	1/1	0.87	0.15	78,78,78,78	0
54	MG	13	2317	1/1	0.87	0.25	71,71,71,71	0
54	MG	1H	3624	1/1	0.87	0.09	61,61,61,61	0
54	MG	1H	3331	1/1	0.87	0.19	84,84,84,84	0
54	MG	14	3446	1/1	0.87	0.21	69,69,69,69	0
54	MG	1H	3438	1/1	0.87	0.14	60,60,60,60	0
54	MG	21	301	1/1	0.87	0.30	41,41,41,41	0
54	MG	1G	2319	1/1	0.87	0.20	68,68,68,68	0
54	MG	14	3450	1/1	0.87	0.36	61,61,61,61	0
54	MG	14	3181	1/1	0.87	0.28	68,68,68,68	0
54	MG	1G	2302	1/1	0.87	0.27	85,85,85,85	0
54	MG	16	209	1/1	0.87	0.19	58,58,58,58	0
54	MG	16	211	1/1	0.87	0.30	64,64,64,64	0
54	MG	1H	3339	1/1	0.87	0.18	72,72,72,72	0
54	MG	1H	3106	1/1	0.87	0.33	37,37,37,37	0
54	MG	1H	3461	1/1	0.87	0.33	61,61,61,61	0
54	MG	1H	3463	1/1	0.87	0.23	48,48,48,48	0
54	MG	29	303	1/1	0.87	0.10	57,57,57,57	0
54	MG	14	3196	1/1	0.87	0.23	54,54,54,54	0
54	MG	1G	2304	1/1	0.87	0.19	82,82,82,82	0
54	MG	1H	3475	1/1	0.87	0.16	60,60,60,60	0
54	MG	14	3204	1/1	0.87	0.30	51,51,51,51	0
54	MG	1J	206	1/1	0.87	0.17	82,82,82,82	0
54	MG	1H	3654	1/1	0.87	0.14	51,51,51,51	0
54	MG	14	3209	1/1	0.87	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3342	1/1	0.87	0.09	45,45,45,45	0
54	MG	14	3212	1/1	0.87	0.19	53,53,53,53	0
54	MG	14	3344	1/1	0.87	0.11	81,81,81,81	0
54	MG	14	3215	1/1	0.87	0.36	65,65,65,65	0
54	MG	1G	2305	1/1	0.87	0.29	85,85,85,85	0
54	MG	14	3222	1/1	0.87	0.12	58,58,58,58	0
54	MG	14	3223	1/1	0.87	0.18	74,74,74,74	0
54	MG	14	3354	1/1	0.87	0.30	66,66,66,66	0
54	MG	14	3486	1/1	0.87	0.25	51,51,51,51	0
54	MG	1H	3173	1/1	0.87	0.39	42,42,42,42	0
54	MG	14	3231	1/1	0.87	0.35	67,67,67,67	0
54	MG	1H	3496	1/1	0.87	0.38	55,55,55,55	0
54	MG	45	202	1/1	0.87	0.17	62,62,62,62	0
54	MG	14	3362	1/1	0.87	0.35	63,63,63,63	0
54	MG	1G	2231	1/1	0.87	0.30	61,61,61,61	0
54	MG	98	202	1/1	0.87	0.32	60,60,60,60	0
54	MG	1H	3178	1/1	0.87	0.23	48,48,48,48	0
54	MG	1H	3271	1/1	0.87	0.26	58,58,58,58	0
54	MG	1H	3272	1/1	0.87	0.19	54,54,54,54	0
54	MG	1H	3188	1/1	0.87	0.13	41,41,41,41	0
54	MG	Y1	101	1/1	0.87	0.24	69,69,69,69	0
54	MG	1H	3276	1/1	0.87	0.19	61,61,61,61	0
54	MG	1H	3193	1/1	0.87	0.34	42,42,42,42	0
54	MG	14	3509	1/1	0.87	0.14	72,72,72,72	0
54	MG	1H	3534	1/1	0.87	0.25	45,45,45,45	0
54	MG	14	3381	1/1	0.87	0.24	62,62,62,62	0
54	MG	1H	3206	1/1	0.87	0.23	52,52,52,52	0
54	MG	1H	3283	1/1	0.87	0.35	77,77,77,77	0
54	MG	14	3115	1/1	0.87	0.27	47,47,47,47	0
54	MG	13	2345	1/1	0.87	0.14	66,66,66,66	0
54	MG	14	3517	1/1	0.87	0.19	59,59,59,59	0
54	MG	1G	2223	1/1	0.87	0.20	72,72,72,72	0
54	MG	1G	2235	1/1	0.87	0.36	70,70,70,70	0
54	MG	14	3397	1/1	0.87	0.18	78,78,78,78	0
54	MG	13	2281	1/1	0.87	0.39	70,70,70,70	0
54	MG	14	3400	1/1	0.87	0.36	79,79,79,79	0
54	MG	1H	3217	1/1	0.87	0.27	52,52,52,52	0
54	MG	1H	3137	1/1	0.87	0.25	53,53,53,53	0
54	MG	14	3567	1/1	0.88	0.15	60,60,60,60	0
54	MG	13	2346	1/1	0.88	0.12	59,59,59,59	0
54	MG	1H	3537	1/1	0.88	0.36	85,85,85,85	0
54	MG	13	2334	1/1	0.88	0.33	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3096	1/1	0.88	0.18	51,51,51,51	0
54	MG	14	3213	1/1	0.88	0.14	52,52,52,52	0
54	MG	1G	2374	1/1	0.88	0.25	70,70,70,70	0
54	MG	13	2320	1/1	0.88	0.59	86,86,86,86	0
54	MG	1H	3321	1/1	0.88	0.15	51,51,51,51	0
54	MG	14	3107	1/1	0.88	0.39	46,46,46,46	0
54	MG	1H	3121	1/1	0.88	0.26	38,38,38,38	0
54	MG	13	2267	1/1	0.88	0.21	87,87,87,87	0
54	MG	1H	3256	1/1	0.88	0.30	77,77,77,77	0
54	MG	13	2381	1/1	0.88	0.27	82,82,82,82	0
54	MG	1H	3204	1/1	0.88	0.28	42,42,42,42	0
54	MG	1H	3263	1/1	0.88	0.36	62,62,62,62	0
54	MG	1H	3424	1/1	0.88	0.13	50,50,50,50	0
54	MG	1H	3577	1/1	0.88	0.22	71,71,71,71	0
54	MG	1H	3264	1/1	0.88	0.26	62,62,62,62	0
54	MG	14	3128	1/1	0.88	0.17	74,74,74,74	0
54	MG	1H	3205	1/1	0.88	0.21	45,45,45,45	0
54	MG	1H	3586	1/1	0.88	0.22	69,69,69,69	0
54	MG	14	3248	1/1	0.88	0.37	66,66,66,66	0
54	MG	1G	2381	1/1	0.88	0.14	75,75,75,75	0
54	MG	14	3133	1/1	0.88	0.36	46,46,46,46	0
54	MG	14	3375	1/1	0.88	0.25	58,58,58,58	0
54	MG	13	2253	1/1	0.88	0.19	57,57,57,57	0
54	MG	1G	2320	1/1	0.88	0.38	71,71,71,71	0
54	MG	1H	3213	1/1	0.88	0.27	40,40,40,40	0
54	MG	13	2387	1/1	0.88	0.12	64,64,64,64	0
54	MG	14	3385	1/1	0.88	0.27	49,49,49,49	0
54	MG	14	3144	1/1	0.88	0.23	54,54,54,54	0
54	MG	1G	2388	1/1	0.88	0.14	106,106,106,106	0
54	MG	1H	3457	1/1	0.88	0.13	49,49,49,49	0
54	MG	1G	2323	1/1	0.88	0.30	80,80,80,80	0
54	MG	1H	3616	1/1	0.88	0.11	60,60,60,60	0
54	MG	14	3502	1/1	0.88	0.14	50,50,50,50	0
54	MG	14	3272	1/1	0.88	0.22	82,82,82,82	0
54	MG	14	3398	1/1	0.88	0.23	72,72,72,72	0
54	MG	1H	3218	1/1	0.88	0.20	40,40,40,40	0
54	MG	1H	3285	1/1	0.88	0.26	74,74,74,74	0
54	MG	14	3276	1/1	0.88	0.30	63,63,63,63	0
54	MG	1H	3626	1/1	0.88	0.11	59,59,59,59	0
54	MG	1G	2390	1/1	0.88	0.12	70,70,70,70	0
54	MG	1H	3483	1/1	0.88	0.15	53,53,53,53	0
54	MG	1H	3489	1/1	0.88	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3168	1/1	0.88	0.38	57,57,57,57	0
54	MG	1H	3633	1/1	0.88	0.18	74,74,74,74	0
54	MG	1G	2364	1/1	0.88	0.07	88,88,88,88	0
54	MG	14	3176	1/1	0.88	0.31	63,63,63,63	0
54	MG	14	3526	1/1	0.88	0.24	52,52,52,52	0
54	MG	14	3413	1/1	0.88	0.19	71,71,71,71	0
54	MG	55	202	1/1	0.88	0.12	65,65,65,65	0
54	MG	1G	2348	1/1	0.88	0.46	67,67,67,67	0
54	MG	14	3299	1/1	0.88	0.21	69,69,69,69	0
54	MG	1H	3368	1/1	0.88	0.14	64,64,64,64	0
54	MG	W1	102	1/1	0.88	0.23	75,75,75,75	0
54	MG	1H	3294	1/1	0.88	0.24	45,45,45,45	0
54	MG	14	3544	1/1	0.88	0.15	61,61,61,61	0
54	MG	11	303	1/1	0.88	0.21	48,48,48,48	0
54	MG	14	3422	1/1	0.88	0.29	50,50,50,50	0
54	MG	14	3306	1/1	0.88	0.36	53,53,53,53	0
54	MG	2A	201	1/1	0.88	0.22	80,80,80,80	0
54	MG	14	3431	1/1	0.88	0.31	67,67,67,67	0
54	MG	14	3552	1/1	0.88	0.09	58,58,58,58	0
54	MG	1H	3095	1/1	0.88	0.16	58,58,58,58	0
54	MG	1H	3097	1/1	0.88	0.28	42,42,42,42	0
54	MG	13	2301	1/1	0.88	0.24	75,75,75,75	0
54	MG	1H	3305	1/1	0.88	0.24	51,51,51,51	0
54	MG	14	3560	1/1	0.88	0.09	56,56,56,56	0
54	MG	1H	3520	1/1	0.88	0.20	53,53,53,53	0
54	MG	13	2319	1/1	0.88	0.22	68,68,68,68	0
54	MG	14	3205	1/1	0.88	0.36	51,51,51,51	0
54	MG	14	3206	1/1	0.88	0.28	65,65,65,65	0
54	MG	14	3314	1/1	0.89	0.24	67,67,67,67	0
54	MG	14	3202	1/1	0.89	0.20	52,52,52,52	0
54	MG	13	2332	1/1	0.89	0.14	85,85,85,85	0
54	MG	14	3320	1/1	0.89	0.37	79,79,79,79	0
54	MG	13	2271	1/1	0.89	0.33	69,69,69,69	0
54	MG	1G	2212	1/1	0.89	0.09	112,112,112,112	0
54	MG	14	3572	1/1	0.89	0.31	63,63,63,63	0
54	MG	13	2382	1/1	0.89	0.20	71,71,71,71	0
54	MG	14	3032	1/1	0.89	0.13	47,47,47,47	0
54	MG	14	3576	1/1	0.89	0.29	65,65,65,65	0
54	MG	14	3328	1/1	0.89	0.30	67,67,67,67	0
54	MG	14	3210	1/1	0.89	0.31	66,66,66,66	0
54	MG	14	3066	1/1	0.89	0.19	55,55,55,55	0
54	MG	1H	3544	1/1	0.89	0.25	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3454	1/1	0.89	0.34	64,64,64,64	0
54	MG	1H	3548	1/1	0.89	0.12	51,51,51,51	0
54	MG	14	3103	1/1	0.89	0.27	49,49,49,49	0
54	MG	1G	2218	1/1	0.89	0.27	59,59,59,59	0
54	MG	1H	3558	1/1	0.89	0.22	57,57,57,57	0
54	MG	1H	3560	1/1	0.89	0.19	66,66,66,66	0
54	MG	13	2296	1/1	0.89	0.35	64,64,64,64	0
54	MG	68	202	1/1	0.89	0.10	62,62,62,62	0
54	MG	13	2283	1/1	0.89	0.33	61,61,61,61	0
54	MG	14	3353	1/1	0.89	0.19	74,74,74,74	0
54	MG	13	2336	1/1	0.89	0.30	57,57,57,57	0
54	MG	14	3466	1/1	0.89	0.25	80,80,80,80	0
54	MG	14	3356	1/1	0.89	0.17	62,62,62,62	0
54	MG	13	2337	1/1	0.89	0.12	75,75,75,75	0
54	MG	1H	3343	1/1	0.89	0.24	46,46,46,46	0
54	MG	13	2339	1/1	0.89	0.16	58,58,58,58	0
54	MG	14	3120	1/1	0.89	0.23	73,73,73,73	0
54	MG	1H	3347	1/1	0.89	0.26	45,45,45,45	0
54	MG	14	3124	1/1	0.89	0.21	50,50,50,50	0
54	MG	13	2340	1/1	0.89	0.06	92,92,92,92	0
54	MG	14	3480	1/1	0.89	0.17	65,65,65,65	0
54	MG	13	2213	1/1	0.89	0.31	68,68,68,68	0
54	MG	14	3127	1/1	0.89	0.24	49,49,49,49	0
54	MG	1H	3222	1/1	0.89	0.32	43,43,43,43	0
54	MG	1H	3158	1/1	0.89	0.14	59,59,59,59	0
54	MG	1J	207	1/1	0.89	0.12	86,86,86,86	0
54	MG	1H	3589	1/1	0.89	0.32	62,62,62,62	0
54	MG	1H	3453	1/1	0.89	0.35	39,39,39,39	0
54	MG	1G	2232	1/1	0.89	0.21	60,60,60,60	0
54	MG	1H	3455	1/1	0.89	0.35	40,40,40,40	0
54	MG	13	2287	1/1	0.89	0.24	91,91,91,91	0
54	MG	14	3495	1/1	0.89	0.14	38,38,38,38	0
54	MG	1H	3359	1/1	0.89	0.30	53,53,53,53	0
54	MG	1H	3293	1/1	0.89	0.13	38,38,38,38	0
54	MG	1H	3228	1/1	0.89	0.29	45,45,45,45	0
54	MG	1H	3472	1/1	0.89	0.32	56,56,56,56	0
54	MG	N8	101	1/1	0.89	0.11	55,55,55,55	0
54	MG	13	2230	1/1	0.89	0.24	79,79,79,79	0
54	MG	88	201	1/1	0.89	0.15	63,63,63,63	0
54	MG	14	3505	1/1	0.89	0.10	65,65,65,65	0
54	MG	1H	3479	1/1	0.89	0.22	63,63,63,63	0
54	MG	41	201	1/1	0.89	0.14	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1H	3623	1/1	0.89	0.18	51,51,51,51	0
54	MG	1H	3232	1/1	0.89	0.19	42,42,42,42	0
54	MG	1H	3487	1/1	0.89	0.17	59,59,59,59	0
54	MG	14	3161	1/1	0.89	0.36	61,61,61,61	0
54	MG	14	3162	1/1	0.89	0.44	49,49,49,49	0
53	8UZ	1G	2202	33/33	0.89	0.10	83,83,83,83	0
54	MG	1H	3372	1/1	0.89	0.26	40,40,40,40	0
54	MG	1G	2375	1/1	0.89	0.12	79,79,79,79	0
54	MG	1H	3632	1/1	0.89	0.27	74,74,74,74	0
54	MG	1H	3171	1/1	0.89	0.30	38,38,38,38	0
54	MG	7A	101	1/1	0.89	0.18	72,72,72,72	0
54	MG	13	2270	1/1	0.89	0.23	66,66,66,66	0
54	MG	14	3296	1/1	0.89	0.24	57,57,57,57	0
54	MG	14	3412	1/1	0.89	0.24	81,81,81,81	0
54	MG	A8	201	1/1	0.89	0.09	57,57,57,57	0
54	MG	1H	3175	1/1	0.89	0.27	53,53,53,53	0
54	MG	14	3536	1/1	0.89	0.39	82,82,82,82	0
54	MG	1H	3123	1/1	0.89	0.22	47,47,47,47	0
54	MG	1H	3390	1/1	0.89	0.16	58,58,58,58	0
54	MG	1H	3644	1/1	0.89	0.16	59,59,59,59	0
54	MG	X1	107	1/1	0.89	0.28	89,89,89,89	0
54	MG	1H	3647	1/1	0.89	0.12	56,56,56,56	0
54	MG	1H	3186	1/1	0.89	0.29	43,43,43,43	0
54	MG	14	3423	1/1	0.89	0.21	64,64,64,64	0
54	MG	13	2305	1/1	0.89	0.34	49,49,49,49	0
54	MG	14	3426	1/1	0.89	0.20	53,53,53,53	0
54	MG	13	2352	1/1	0.89	0.40	63,63,63,63	0
54	MG	1H	3201	1/1	0.89	0.34	42,42,42,42	0
54	MG	14	3311	1/1	0.89	0.40	43,43,43,43	0
54	MG	1H	3533	1/1	0.89	0.10	43,43,43,43	0
54	MG	1H	3398	1/1	0.89	0.16	61,61,61,61	0
54	MG	1H	3471	1/1	0.90	0.09	55,55,55,55	0
54	MG	1G	2338	1/1	0.90	0.38	80,80,80,80	0
54	MG	1H	3208	1/1	0.90	0.23	54,54,54,54	0
54	MG	1H	3478	1/1	0.90	0.32	49,49,49,49	0
54	MG	1G	2384	1/1	0.90	0.23	66,66,66,66	0
54	MG	13	2269	1/1	0.90	0.40	70,70,70,70	0
54	MG	1H	3485	1/1	0.90	0.09	57,57,57,57	0
54	MG	1H	3486	1/1	0.90	0.15	59,59,59,59	0
54	MG	14	3525	1/1	0.90	0.15	68,68,68,68	0
54	MG	14	3365	1/1	0.90	0.20	62,62,62,62	0
54	MG	1H	3637	1/1	0.90	0.14	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	1G	2386	1/1	0.90	0.32	72,72,72,72	0
54	MG	1H	3488	1/1	0.90	0.21	50,50,50,50	0
54	MG	1H	3642	1/1	0.90	0.27	61,61,61,61	0
53	8UZ	1H	3002	33/33	0.90	0.11	68,68,68,68	0
54	MG	14	3537	1/1	0.90	0.18	71,71,71,71	0
54	MG	1H	3367	1/1	0.90	0.38	83,83,83,83	0
54	MG	14	3541	1/1	0.90	0.19	48,48,48,48	0
54	MG	13	2258	1/1	0.90	0.21	89,89,89,89	0
54	MG	13	2311	1/1	0.90	0.35	54,54,54,54	0
54	MG	14	3380	1/1	0.90	0.12	71,71,71,71	0
54	MG	B5	101	1/1	0.90	0.35	68,68,68,68	0
54	MG	1H	3151	1/1	0.90	0.34	51,51,51,51	0
54	MG	14	3218	1/1	0.90	0.20	56,56,56,56	0
54	MG	14	3220	1/1	0.90	0.23	63,63,63,63	0
54	MG	1H	3375	1/1	0.90	0.26	53,53,53,53	0
54	MG	1H	3656	1/1	0.90	0.34	44,44,44,44	0
54	MG	14	3389	1/1	0.90	0.36	51,51,51,51	0
54	MG	1H	3658	1/1	0.90	0.12	43,43,43,43	0
54	MG	14	3394	1/1	0.90	0.31	58,58,58,58	0
54	MG	14	3228	1/1	0.90	0.10	65,65,65,65	0
54	MG	1H	3504	1/1	0.90	0.15	58,58,58,58	0
54	MG	1G	2243	1/1	0.90	0.29	78,78,78,78	0
54	MG	1H	3153	1/1	0.90	0.17	46,46,46,46	0
54	MG	14	3235	1/1	0.90	0.36	68,68,68,68	0
54	MG	1H	3154	1/1	0.90	0.34	47,47,47,47	0
54	MG	1H	3513	1/1	0.90	0.16	45,45,45,45	0
54	MG	14	3573	1/1	0.90	0.21	59,59,59,59	0
54	MG	14	3403	1/1	0.90	0.27	62,62,62,62	0
54	MG	13	2288	1/1	0.90	0.28	73,73,73,73	0
54	MG	14	3007	1/1	0.90	0.35	63,63,63,63	0
54	MG	1H	3385	1/1	0.90	0.15	74,74,74,74	0
54	MG	1H	3522	1/1	0.90	0.33	49,49,49,49	0
54	MG	14	3077	1/1	0.90	0.26	60,60,60,60	0
54	MG	14	3080	1/1	0.90	0.14	70,70,70,70	0
54	MG	1G	2347	1/1	0.90	0.30	65,65,65,65	0
54	MG	1H	3528	1/1	0.90	0.31	51,51,51,51	0
54	MG	1H	3001	1/1	0.90	0.33	35,35,35,35	0
54	MG	1G	2247	1/1	0.90	0.31	76,76,76,76	0
54	MG	14	3255	1/1	0.90	0.35	63,63,63,63	0
54	MG	14	3256	1/1	0.90	0.35	58,58,58,58	0
54	MG	14	3593	1/1	0.90	0.10	80,80,80,80	0
54	MG	14	3419	1/1	0.90	0.41	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	68	201	1/1	0.90	0.23	65,65,65,65	0
54	MG	14	3257	1/1	0.90	0.26	72,72,72,72	0
54	MG	75	201	1/1	0.90	0.13	57,57,57,57	0
54	MG	1H	3535	1/1	0.90	0.28	63,63,63,63	0
54	MG	21	303	1/1	0.90	0.22	76,76,76,76	0
54	MG	1H	3235	1/1	0.90	0.12	44,44,44,44	0
54	MG	13	2313	1/1	0.90	0.37	74,74,74,74	0
54	MG	1H	3316	1/1	0.90	0.21	44,44,44,44	0
54	MG	13	2304	1/1	0.90	0.38	56,56,56,56	0
54	MG	16	205	1/1	0.90	0.32	60,60,60,60	0
54	MG	14	3427	1/1	0.90	0.19	57,57,57,57	0
54	MG	1H	3100	1/1	0.90	0.24	39,39,39,39	0
54	MG	13	2359	1/1	0.90	0.10	81,81,81,81	0
54	MG	16	213	1/1	0.90	0.12	68,68,68,68	0
54	MG	14	3116	1/1	0.90	0.26	52,52,52,52	0
54	MG	1G	2310	1/1	0.90	0.22	71,71,71,71	0
54	MG	1H	3550	1/1	0.90	0.19	58,58,58,58	0
54	MG	1H	3557	1/1	0.90	0.13	56,56,56,56	0
54	MG	1G	2353	1/1	0.90	0.24	73,73,73,73	0
54	MG	1G	2376	1/1	0.90	0.10	92,92,92,92	0
54	MG	1G	2354	1/1	0.90	0.42	74,74,74,74	0
54	MG	1J	203	1/1	0.90	0.38	75,75,75,75	0
54	MG	1H	3414	1/1	0.90	0.11	60,60,60,60	0
54	MG	1H	3566	1/1	0.90	0.08	66,66,66,66	0
54	MG	1H	3120	1/1	0.90	0.32	40,40,40,40	0
54	MG	1H	3419	1/1	0.90	0.26	48,48,48,48	0
54	MG	1H	3421	1/1	0.90	0.20	47,47,47,47	0
54	MG	1H	3572	1/1	0.90	0.13	57,57,57,57	0
54	MG	14	3293	1/1	0.90	0.46	52,52,52,52	0
54	MG	14	3134	1/1	0.90	0.36	52,52,52,52	0
54	MG	1H	3182	1/1	0.90	0.38	33,33,33,33	0
54	MG	1H	3574	1/1	0.90	0.31	74,74,74,74	0
54	MG	14	3139	1/1	0.90	0.24	49,49,49,49	0
54	MG	14	3140	1/1	0.90	0.28	53,53,53,53	0
54	MG	1H	3335	1/1	0.90	0.23	51,51,51,51	0
54	MG	14	3459	1/1	0.90	0.07	59,59,59,59	0
54	MG	1H	3336	1/1	0.90	0.21	60,60,60,60	0
54	MG	1H	3338	1/1	0.90	0.22	57,57,57,57	0
54	MG	1H	3431	1/1	0.90	0.23	48,48,48,48	0
54	MG	14	3148	1/1	0.90	0.29	62,62,62,62	0
54	MG	1H	3585	1/1	0.90	0.32	65,65,65,65	0
54	MG	1H	3258	1/1	0.90	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	13	2251	1/1	0.90	0.15	67,67,67,67	0
54	MG	13	2327	1/1	0.90	0.17	78,78,78,78	0
54	MG	1H	3442	1/1	0.90	0.15	53,53,53,53	0
54	MG	1H	3596	1/1	0.90	0.19	45,45,45,45	0
54	MG	14	3473	1/1	0.90	0.36	65,65,65,65	0
54	MG	1H	3600	1/1	0.90	0.22	59,59,59,59	0
54	MG	14	3319	1/1	0.90	0.18	65,65,65,65	0
54	MG	1H	3190	1/1	0.90	0.13	37,37,37,37	0
54	MG	1G	2380	1/1	0.90	0.13	77,77,77,77	0
54	MG	1H	3345	1/1	0.90	0.20	42,42,42,42	0
54	MG	1H	3127	1/1	0.90	0.28	43,43,43,43	0
54	MG	W1	101	1/1	0.90	0.34	72,72,72,72	0
54	MG	1H	3610	1/1	0.90	0.33	48,48,48,48	0
54	MG	14	3326	1/1	0.90	0.44	68,68,68,68	0
54	MG	1H	3266	1/1	0.90	0.35	51,51,51,51	0
54	MG	1H	3203	1/1	0.90	0.35	43,43,43,43	0
54	MG	14	3333	1/1	0.90	0.14	67,67,67,67	0
54	MG	14	3174	1/1	0.90	0.30	46,46,46,46	0
54	MG	14	3337	1/1	0.90	0.40	76,76,76,76	0
54	MG	14	3338	1/1	0.90	0.18	65,65,65,65	0
54	MG	14	3339	1/1	0.90	0.17	53,53,53,53	0
54	MG	14	3340	1/1	0.90	0.28	59,59,59,59	0
54	MG	14	3175	1/1	0.90	0.38	58,58,58,58	0
54	MG	1H	3615	1/1	0.90	0.16	64,64,64,64	0
54	MG	14	3178	1/1	0.90	0.47	77,77,77,77	0
54	MG	1H	3128	1/1	0.90	0.20	53,53,53,53	0
54	MG	1G	2331	1/1	0.90	0.24	92,92,92,92	0
54	MG	14	3507	1/1	0.90	0.29	53,53,53,53	0
54	MG	14	3184	1/1	0.90	0.34	43,43,43,43	0
54	MG	13	2290	1/1	0.90	0.32	63,63,63,63	0
54	MG	1H	3469	1/1	0.90	0.08	73,73,73,73	0
54	MG	1H	3555	1/1	0.91	0.17	73,73,73,73	0
54	MG	1H	3417	1/1	0.91	0.21	57,57,57,57	0
54	MG	14	3114	1/1	0.91	0.23	63,63,63,63	0
54	MG	1H	3418	1/1	0.91	0.07	56,56,56,56	0
54	MG	13	2347	1/1	0.91	0.18	62,62,62,62	0
54	MG	14	3117	1/1	0.91	0.17	69,69,69,69	0
54	MG	14	3258	1/1	0.91	0.11	60,60,60,60	0
54	MG	14	3550	1/1	0.91	0.17	69,69,69,69	0
54	MG	1H	3420	1/1	0.91	0.13	61,61,61,61	0
54	MG	13	2348	1/1	0.91	0.22	63,63,63,63	0
54	MG	1H	3422	1/1	0.91	0.23	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	3244	1/1	0.91	0.36	63,63,63,63	0
54	MG	13	2217	1/1	0.91	0.23	69,69,69,69	0
54	MG	1G	2329	1/1	0.91	0.11	67,67,67,67	0
54	MG	14	3266	1/1	0.91	0.25	51,51,51,51	0
54	MG	14	3410	1/1	0.91	0.17	71,71,71,71	0
54	MG	13	2274	1/1	0.91	0.21	52,52,52,52	0
54	MG	13	2229	1/1	0.91	0.24	78,78,78,78	0
54	MG	1H	3435	1/1	0.91	0.15	51,51,51,51	0
54	MG	1H	3575	1/1	0.91	0.29	60,60,60,60	0
54	MG	1H	3177	1/1	0.91	0.23	41,41,41,41	0
54	MG	1H	3251	1/1	0.91	0.26	52,52,52,52	0
54	MG	14	3277	1/1	0.91	0.25	54,54,54,54	0
54	MG	1G	2332	1/1	0.91	0.17	74,74,74,74	0
54	MG	1H	3440	1/1	0.91	0.32	62,62,62,62	0
54	MG	14	3137	1/1	0.91	0.33	53,53,53,53	0
54	MG	14	3284	1/1	0.91	0.30	50,50,50,50	0
54	MG	1G	2333	1/1	0.91	0.33	76,76,76,76	0
54	MG	1G	2334	1/1	0.91	0.18	76,76,76,76	0
54	MG	1H	3587	1/1	0.91	0.15	61,61,61,61	0
54	MG	1H	3118	1/1	0.91	0.26	48,48,48,48	0
54	MG	14	3430	1/1	0.91	0.08	60,60,60,60	0
54	MG	1H	3344	1/1	0.91	0.28	67,67,67,67	0
54	MG	1H	3189	1/1	0.91	0.26	40,40,40,40	0
54	MG	14	3294	1/1	0.91	0.17	48,48,48,48	0
54	MG	1H	3595	1/1	0.91	0.20	49,49,49,49	0
54	MG	13	2354	1/1	0.91	0.32	62,62,62,62	0
54	MG	14	3150	1/1	0.91	0.39	55,55,55,55	0
54	MG	1G	2266	1/1	0.91	0.13	76,76,76,76	0
54	MG	1H	3459	1/1	0.91	0.15	57,57,57,57	0
54	MG	14	3303	1/1	0.91	0.25	68,68,68,68	0
54	MG	1H	3348	1/1	0.91	0.22	56,56,56,56	0
54	MG	1H	3194	1/1	0.91	0.16	53,53,53,53	0
54	MG	21	304	1/1	0.91	0.15	63,63,63,63	0
54	MG	1H	3467	1/1	0.91	0.14	51,51,51,51	0
54	MG	1H	3199	1/1	0.91	0.32	37,37,37,37	0
54	MG	1G	2303	1/1	0.91	0.14	80,80,80,80	0
54	MG	13	2356	1/1	0.91	0.16	64,64,64,64	0
54	MG	13	2357	1/1	0.91	0.13	86,86,86,86	0
54	MG	13	2338	1/1	0.91	0.26	82,82,82,82	0
54	MG	16	210	1/1	0.91	0.17	61,61,61,61	0
54	MG	1H	3277	1/1	0.91	0.28	53,53,53,53	0
54	MG	13	2286	1/1	0.91	0.37	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	3361	1/1	0.91	0.13	61,61,61,61	0
54	MG	14	3317	1/1	0.91	0.41	68,68,68,68	0
54	MG	14	3170	1/1	0.91	0.36	42,42,42,42	0
54	MG	1H	3625	1/1	0.91	0.09	64,64,64,64	0
54	MG	13	2329	1/1	0.91	0.25	59,59,59,59	0
54	MG	29	305	1/1	0.91	0.25	67,67,67,67	0
54	MG	1H	3282	1/1	0.91	0.26	61,61,61,61	0
54	MG	13	2389	1/1	0.91	0.20	75,75,75,75	0
54	MG	1G	2245	1/1	0.91	0.27	73,73,73,73	0
54	MG	14	3324	1/1	0.91	0.09	56,56,56,56	0
54	MG	14	3179	1/1	0.91	0.39	56,56,56,56	0
54	MG	1G	2246	1/1	0.91	0.36	70,70,70,70	0
54	MG	1G	2221	1/1	0.91	0.13	74,74,74,74	0
53	8UZ	13	2202	33/33	0.91	0.09	74,74,74,74	0
54	MG	1H	3216	1/1	0.91	0.20	52,52,52,52	0
54	MG	1G	2284	1/1	0.91	0.11	75,75,75,75	0
54	MG	1H	3638	1/1	0.91	0.34	78,78,78,78	0
54	MG	14	3191	1/1	0.91	0.24	57,57,57,57	0
54	MG	78	203	1/1	0.91	0.22	51,51,51,51	0
54	MG	31	301	1/1	0.91	0.10	42,42,42,42	0
54	MG	1H	3500	1/1	0.91	0.10	54,54,54,54	0
54	MG	13	2331	1/1	0.91	0.19	65,65,65,65	0
54	MG	1H	3641	1/1	0.91	0.17	52,52,52,52	0
54	MG	13	2343	1/1	0.91	0.13	72,72,72,72	0
54	MG	E5	201	1/1	0.91	0.18	51,51,51,51	0
54	MG	1H	3298	1/1	0.91	0.28	46,46,46,46	0
54	MG	13	2393	1/1	0.91	0.17	63,63,63,63	0
54	MG	1H	3506	1/1	0.91	0.33	38,38,38,38	0
54	MG	1G	2227	1/1	0.91	0.09	74,74,74,74	0
54	MG	1H	3302	1/1	0.91	0.36	44,44,44,44	0
54	MG	14	3349	1/1	0.91	0.13	82,82,82,82	0
54	MG	J8	101	1/1	0.91	0.17	52,52,52,52	0
54	MG	1H	3303	1/1	0.91	0.34	60,60,60,60	0
54	MG	1H	3514	1/1	0.91	0.15	62,62,62,62	0
54	MG	1H	3515	1/1	0.91	0.14	59,59,59,59	0
54	MG	13	2241	1/1	0.91	0.31	48,48,48,48	0
54	MG	3I	201	1/1	0.91	0.11	66,66,66,66	0
54	MG	1G	2321	1/1	0.91	0.23	70,70,70,70	0
54	MG	1H	3526	1/1	0.91	0.22	57,57,57,57	0
54	MG	13	2314	1/1	0.91	0.37	75,75,75,75	0
54	MG	14	3506	1/1	0.91	0.15	57,57,57,57	0
54	MG	1G	2230	1/1	0.91	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	8UZ	14	3002	33/33	0.91	0.10	77,77,77,77	0
54	MG	1H	3401	1/1	0.91	0.29	33,33,33,33	0
54	MG	14	3023	1/1	0.91	0.20	65,65,65,65	0
54	MG	1H	3403	1/1	0.91	0.12	54,54,54,54	0
54	MG	14	3226	1/1	0.91	0.31	67,67,67,67	0
54	MG	1H	3317	1/1	0.91	0.16	61,61,61,61	0
54	MG	1H	3234	1/1	0.91	0.17	40,40,40,40	0
54	MG	1H	3539	1/1	0.91	0.10	55,55,55,55	0
54	MG	1H	3406	1/1	0.91	0.10	67,67,67,67	0
54	MG	1H	3013	1/1	0.91	0.20	55,55,55,55	0
54	MG	14	3100	1/1	0.91	0.28	51,51,51,51	0
54	MG	14	3521	1/1	0.91	0.29	57,57,57,57	0
54	MG	14	3524	1/1	0.91	0.13	68,68,68,68	0
54	MG	14	3101	1/1	0.91	0.23	49,49,49,49	0
54	MG	1H	3409	1/1	0.91	0.17	67,67,67,67	0
54	MG	14	3528	1/1	0.91	0.17	61,61,61,61	0
54	MG	1H	3545	1/1	0.91	0.24	54,54,54,54	0
54	MG	14	3532	1/1	0.91	0.11	63,63,63,63	0
54	MG	1H	3546	1/1	0.91	0.18	59,59,59,59	0
54	MG	1H	3060	1/1	0.91	0.12	49,49,49,49	0
54	MG	14	3108	1/1	0.91	0.10	52,52,52,52	0
54	MG	1H	3324	1/1	0.91	0.17	56,56,56,56	0
54	MG	1H	3166	1/1	0.91	0.36	46,46,46,46	0
54	MG	14	3075	1/1	0.92	0.24	56,56,56,56	0
54	MG	13	2214	1/1	0.92	0.11	98,98,98,98	0
54	MG	14	3194	1/1	0.92	0.25	65,65,65,65	0
54	MG	14	3562	1/1	0.92	0.20	69,69,69,69	0
54	MG	1H	3129	1/1	0.92	0.11	60,60,60,60	0
54	MG	14	3092	1/1	0.92	0.25	66,66,66,66	0
54	MG	14	3433	1/1	0.92	0.13	65,65,65,65	0
54	MG	14	3095	1/1	0.92	0.07	93,93,93,93	0
54	MG	1H	3130	1/1	0.92	0.24	36,36,36,36	0
54	MG	14	3569	1/1	0.92	0.26	74,74,74,74	0
54	MG	13	2294	1/1	0.92	0.10	72,72,72,72	0
54	MG	14	3098	1/1	0.92	0.19	56,56,56,56	0
54	MG	14	3099	1/1	0.92	0.20	52,52,52,52	0
54	MG	1H	3278	1/1	0.92	0.17	52,52,52,52	0
54	MG	1H	3579	1/1	0.92	0.13	51,51,51,51	0
54	MG	1H	3041	1/1	0.92	0.20	47,47,47,47	0
54	MG	14	3578	1/1	0.92	0.20	46,46,46,46	0
54	MG	1H	3176	1/1	0.92	0.36	53,53,53,53	0
54	MG	14	3580	1/1	0.92	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3447	1/1	0.92	0.18	58,58,58,58	0
54	MG	1G	2282	1/1	0.92	0.11	71,71,71,71	0
54	MG	1H	3082	1/1	0.92	0.23	61,61,61,61	0
54	MG	1H	3181	1/1	0.92	0.12	55,55,55,55	0
54	MG	1H	3408	1/1	0.92	0.17	38,38,38,38	0
54	MG	14	3332	1/1	0.92	0.29	57,57,57,57	0
54	MG	13	2366	1/1	0.92	0.23	62,62,62,62	0
54	MG	11	304	1/1	0.92	0.26	35,35,35,35	0
54	MG	1H	3413	1/1	0.92	0.10	59,59,59,59	0
54	MG	13	2280	1/1	0.92	0.26	58,58,58,58	0
54	MG	1H	3601	1/1	0.92	0.31	56,56,56,56	0
54	MG	1H	3604	1/1	0.92	0.14	65,65,65,65	0
54	MG	14	3460	1/1	0.92	0.29	69,69,69,69	0
54	MG	1H	3292	1/1	0.92	0.14	47,47,47,47	0
54	MG	1G	2324	1/1	0.92	0.13	79,79,79,79	0
54	MG	1H	3510	1/1	0.92	0.17	56,56,56,56	0
54	MG	14	3121	1/1	0.92	0.21	68,68,68,68	0
54	MG	1H	3350	1/1	0.92	0.26	56,56,56,56	0
54	MG	1H	3238	1/1	0.92	0.35	59,59,59,59	0
54	MG	14	3467	1/1	0.92	0.24	63,63,63,63	0
54	MG	13	2272	1/1	0.92	0.26	61,61,61,61	0
54	MG	14	3237	1/1	0.92	0.36	58,58,58,58	0
54	MG	14	3350	1/1	0.92	0.35	61,61,61,61	0
54	MG	14	3351	1/1	0.92	0.17	80,80,80,80	0
54	MG	14	3238	1/1	0.92	0.24	53,53,53,53	0
54	MG	1H	3192	1/1	0.92	0.28	34,34,34,34	0
54	MG	13	2379	1/1	0.92	0.07	56,56,56,56	0
54	MG	1H	3149	1/1	0.92	0.30	33,33,33,33	0
54	MG	14	3243	1/1	0.92	0.23	67,67,67,67	0
54	MG	25	203	1/1	0.92	0.13	66,66,66,66	0
54	MG	29	301	1/1	0.92	0.23	58,58,58,58	0
54	MG	1G	2209	1/1	0.92	0.12	75,75,75,75	0
53	8UZ	1G	2201	33/33	0.92	0.13	74,74,74,74	0
54	MG	14	3482	1/1	0.92	0.09	61,61,61,61	0
54	MG	1H	3202	1/1	0.92	0.32	34,34,34,34	0
54	MG	1H	3362	1/1	0.92	0.33	60,60,60,60	0
54	MG	13	2237	1/1	0.92	0.23	65,65,65,65	0
54	MG	1H	3115	1/1	0.92	0.41	35,35,35,35	0
54	MG	1H	3306	1/1	0.92	0.20	40,40,40,40	0
54	MG	1H	3116	1/1	0.92	0.20	40,40,40,40	0
54	MG	1H	3536	1/1	0.92	0.16	50,50,50,50	0
54	MG	14	3372	1/1	0.92	0.12	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	3252	1/1	0.92	0.07	50,50,50,50	0
54	MG	14	3496	1/1	0.92	0.13	53,53,53,53	0
54	MG	14	3497	1/1	0.92	0.32	55,55,55,55	0
54	MG	78	201	1/1	0.92	0.23	44,44,44,44	0
54	MG	1H	3255	1/1	0.92	0.28	56,56,56,56	0
54	MG	I8	102	1/1	0.92	0.20	45,45,45,45	0
54	MG	14	3142	1/1	0.92	0.26	55,55,55,55	0
54	MG	1H	3447	1/1	0.92	0.24	55,55,55,55	0
54	MG	1H	3540	1/1	0.92	0.25	56,56,56,56	0
54	MG	1G	2271	1/1	0.92	0.15	64,64,64,64	0
54	MG	D8	201	1/1	0.92	0.13	48,48,48,48	0
54	MG	14	3146	1/1	0.92	0.20	58,58,58,58	0
54	MG	14	3383	1/1	0.92	0.28	52,52,52,52	0
54	MG	1H	3257	1/1	0.92	0.27	49,49,49,49	0
54	MG	14	3149	1/1	0.92	0.28	56,56,56,56	0
54	MG	1H	3452	1/1	0.92	0.22	42,42,42,42	0
54	MG	14	3267	1/1	0.92	0.23	65,65,65,65	0
54	MG	13	2254	1/1	0.92	0.24	59,59,59,59	0
54	MG	13	2384	1/1	0.92	0.34	75,75,75,75	0
54	MG	1H	3160	1/1	0.92	0.24	54,54,54,54	0
54	MG	1H	3323	1/1	0.92	0.29	66,66,66,66	0
54	MG	14	3396	1/1	0.92	0.25	63,63,63,63	0
54	MG	1H	3645	1/1	0.92	0.28	64,64,64,64	0
54	MG	14	3160	1/1	0.92	0.19	49,49,49,49	0
54	MG	1H	3384	1/1	0.92	0.09	62,62,62,62	0
54	MG	14	3280	1/1	0.92	0.24	49,49,49,49	0
54	MG	1H	3648	1/1	0.92	0.25	61,61,61,61	0
54	MG	1H	3651	1/1	0.92	0.17	57,57,57,57	0
54	MG	1H	3553	1/1	0.92	0.12	52,52,52,52	0
54	MG	14	3527	1/1	0.92	0.12	66,66,66,66	0
54	MG	1H	3554	1/1	0.92	0.08	64,64,64,64	0
54	MG	1H	3460	1/1	0.92	0.23	57,57,57,57	0
54	MG	1H	3556	1/1	0.92	0.17	71,71,71,71	0
54	MG	1H	3212	1/1	0.92	0.16	55,55,55,55	0
54	MG	1H	3122	1/1	0.92	0.22	38,38,38,38	0
54	MG	1H	3559	1/1	0.92	0.15	55,55,55,55	0
54	MG	14	3173	1/1	0.92	0.37	45,45,45,45	0
54	MG	1H	3464	1/1	0.92	0.34	62,62,62,62	0
54	MG	B8	201	1/1	0.92	0.18	69,69,69,69	0
54	MG	14	3539	1/1	0.92	0.56	64,64,64,64	0
54	MG	1H	3389	1/1	0.92	0.21	47,47,47,47	0
54	MG	14	3414	1/1	0.92	0.42	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	1G	2222	1/1	0.92	0.12	74,74,74,74	0
54	MG	1H	3392	1/1	0.92	0.22	60,60,60,60	0
54	MG	X1	109	1/1	0.92	0.32	79,79,79,79	0
54	MG	13	2385	1/1	0.92	0.20	75,75,75,75	0
54	MG	14	3302	1/1	0.92	0.17	74,74,74,74	0
54	MG	1H	3394	1/1	0.92	0.18	54,54,54,54	0
54	MG	W4	103	1/1	0.92	0.44	90,90,90,90	0
54	MG	14	3183	1/1	0.92	0.21	69,69,69,69	0
54	MG	1H	3474	1/1	0.92	0.27	63,63,63,63	0
54	MG	1H	3167	1/1	0.92	0.39	34,34,34,34	0
54	MG	14	3054	1/1	0.92	0.14	60,60,60,60	0
54	MG	14	3557	1/1	0.92	0.14	65,65,65,65	0
54	MG	13	2386	1/1	0.92	0.12	75,75,75,75	0
54	MG	14	3366	1/1	0.93	0.30	57,57,57,57	0
54	MG	14	3104	1/1	0.93	0.25	48,48,48,48	0
54	MG	13	2285	1/1	0.93	0.09	82,82,82,82	0
54	MG	14	3469	1/1	0.93	0.16	66,66,66,66	0
54	MG	13	2355	1/1	0.93	0.38	72,72,72,72	0
54	MG	1H	3618	1/1	0.93	0.14	54,54,54,54	0
54	MG	1H	3542	1/1	0.93	0.16	46,46,46,46	0
54	MG	14	3279	1/1	0.93	0.08	55,55,55,55	0
54	MG	14	3185	1/1	0.93	0.44	44,44,44,44	0
54	MG	14	3376	1/1	0.93	0.22	53,53,53,53	0
54	MG	14	3477	1/1	0.93	0.10	62,62,62,62	0
54	MG	13	2291	1/1	0.93	0.17	60,60,60,60	0
54	MG	14	3378	1/1	0.93	0.10	73,73,73,73	0
54	MG	1H	3411	1/1	0.93	0.28	52,52,52,52	0
54	MG	1H	3309	1/1	0.93	0.30	38,38,38,38	0
54	MG	1G	2391	1/1	0.93	0.10	61,61,61,61	0
54	MG	14	3483	1/1	0.93	0.17	52,52,52,52	0
54	MG	14	3484	1/1	0.93	0.17	59,59,59,59	0
54	MG	14	3485	1/1	0.93	0.16	50,50,50,50	0
54	MG	4E	201	1/1	0.93	0.17	81,81,81,81	0
54	MG	1H	3107	1/1	0.93	0.21	44,44,44,44	0
54	MG	16	202	1/1	0.93	0.20	66,66,66,66	0
54	MG	1H	3629	1/1	0.93	0.35	80,80,80,80	0
54	MG	14	3488	1/1	0.93	0.28	64,64,64,64	0
54	MG	1H	3108	1/1	0.93	0.11	53,53,53,53	0
54	MG	16	207	1/1	0.93	0.36	52,52,52,52	0
54	MG	14	3288	1/1	0.93	0.25	47,47,47,47	0
54	MG	14	3290	1/1	0.93	0.27	48,48,48,48	0
54	MG	13	2210	1/1	0.93	0.09	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3197	1/1	0.93	0.16	58,58,58,58	0
54	MG	1H	3551	1/1	0.93	0.12	62,62,62,62	0
54	MG	1G	2260	1/1	0.93	0.08	81,81,81,81	0
54	MG	1H	3113	1/1	0.93	0.23	51,51,51,51	0
54	MG	1H	3224	1/1	0.93	0.26	47,47,47,47	0
54	MG	1G	2296	1/1	0.93	0.08	78,78,78,78	0
54	MG	1H	3226	1/1	0.93	0.14	48,48,48,48	0
54	MG	29	302	1/1	0.93	0.23	49,49,49,49	0
54	MG	14	3207	1/1	0.93	0.33	56,56,56,56	0
54	MG	1G	2215	1/1	0.93	0.15	78,78,78,78	0
54	MG	29	306	1/1	0.93	0.17	69,69,69,69	0
54	MG	1H	3376	1/1	0.93	0.12	52,52,52,52	0
54	MG	1H	3274	1/1	0.93	0.30	57,57,57,57	0
54	MG	1H	3499	1/1	0.93	0.10	49,49,49,49	0
54	MG	1H	3379	1/1	0.93	0.34	56,56,56,56	0
54	MG	1H	3430	1/1	0.93	0.09	52,52,52,52	0
54	MG	1J	205	1/1	0.93	0.37	72,72,72,72	0
54	MG	1H	3568	1/1	0.93	0.10	48,48,48,48	0
54	MG	1H	3502	1/1	0.93	0.14	59,59,59,59	0
53	8UZ	13	2201	33/33	0.93	0.10	63,63,63,63	0
54	MG	14	3136	1/1	0.93	0.37	45,45,45,45	0
54	MG	14	3221	1/1	0.93	0.29	53,53,53,53	0
54	MG	1J	211	1/1	0.93	0.27	81,81,81,81	0
54	MG	13	2388	1/1	0.93	0.14	63,63,63,63	0
54	MG	1H	3231	1/1	0.93	0.20	50,50,50,50	0
54	MG	13	2378	1/1	0.93	0.31	66,66,66,66	0
54	MG	78	202	1/1	0.93	0.19	47,47,47,47	0
54	MG	1H	3508	1/1	0.93	0.34	45,45,45,45	0
54	MG	1H	3233	1/1	0.93	0.28	42,42,42,42	0
54	MG	1H	3035	1/1	0.93	0.12	55,55,55,55	0
54	MG	14	3523	1/1	0.93	0.14	62,62,62,62	0
54	MG	14	3232	1/1	0.93	0.31	67,67,67,67	0
54	MG	5E	201	1/1	0.93	0.18	69,69,69,69	0
54	MG	1H	3197	1/1	0.93	0.35	39,39,39,39	0
54	MG	35	202	1/1	0.93	0.28	61,61,61,61	0
54	MG	1H	3198	1/1	0.93	0.11	48,48,48,48	0
54	MG	1H	3237	1/1	0.93	0.12	62,62,62,62	0
54	MG	13	2278	1/1	0.93	0.34	68,68,68,68	0
54	MG	1H	3582	1/1	0.93	0.11	50,50,50,50	0
54	MG	14	3424	1/1	0.93	0.30	55,55,55,55	0
54	MG	14	3327	1/1	0.93	0.22	71,71,71,71	0
54	MG	1H	3200	1/1	0.93	0.28	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	3519	1/1	0.93	0.19	50,50,50,50	0
54	MG	1H	3050	1/1	0.93	0.08	42,42,42,42	0
54	MG	14	3153	1/1	0.93	0.23	47,47,47,47	0
54	MG	1H	3588	1/1	0.93	0.23	52,52,52,52	0
54	MG	14	3335	1/1	0.93	0.18	64,64,64,64	0
54	MG	BA	201	1/1	0.93	0.28	85,85,85,85	0
54	MG	14	3540	1/1	0.93	0.17	61,61,61,61	0
54	MG	11	302	1/1	0.93	0.22	51,51,51,51	0
54	MG	14	3542	1/1	0.93	0.11	47,47,47,47	0
54	MG	1H	3523	1/1	0.93	0.14	45,45,45,45	0
54	MG	14	3158	1/1	0.93	0.39	42,42,42,42	0
54	MG	1H	3525	1/1	0.93	0.07	51,51,51,51	0
54	MG	14	3056	1/1	0.93	0.20	74,74,74,74	0
54	MG	14	3061	1/1	0.93	0.12	54,54,54,54	0
54	MG	14	3250	1/1	0.93	0.25	74,74,74,74	0
54	MG	14	3441	1/1	0.93	0.31	58,58,58,58	0
54	MG	1H	3126	1/1	0.93	0.19	40,40,40,40	0
54	MG	1H	3456	1/1	0.93	0.12	55,55,55,55	0
54	MG	1H	3062	1/1	0.93	0.22	57,57,57,57	0
54	MG	14	3347	1/1	0.93	0.15	64,64,64,64	0
54	MG	1H	3531	1/1	0.93	0.32	45,45,45,45	0
54	MG	14	3085	1/1	0.93	0.19	57,57,57,57	0
54	MG	1H	3532	1/1	0.93	0.09	51,51,51,51	0
54	MG	1H	3164	1/1	0.93	0.21	45,45,45,45	0
54	MG	1H	3071	1/1	0.93	0.11	71,71,71,71	0
54	MG	14	3453	1/1	0.93	0.45	64,64,64,64	0
54	MG	14	3171	1/1	0.93	0.22	49,49,49,49	0
54	MG	1H	3072	1/1	0.93	0.23	48,48,48,48	0
54	MG	14	3355	1/1	0.93	0.28	55,55,55,55	0
54	MG	13	2380	1/1	0.93	0.24	65,65,65,65	0
54	MG	14	3357	1/1	0.93	0.11	50,50,50,50	0
54	MG	14	3571	1/1	0.93	0.30	63,63,63,63	0
54	MG	14	3264	1/1	0.93	0.27	56,56,56,56	0
54	MG	1H	3169	1/1	0.93	0.29	36,36,36,36	0
54	MG	13	2315	1/1	0.93	0.23	73,73,73,73	0
54	MG	13	2260	1/1	0.93	0.39	58,58,58,58	0
54	MG	14	3177	1/1	0.93	0.28	52,52,52,52	0
54	MG	14	3364	1/1	0.93	0.17	55,55,55,55	0
54	MG	1H	3613	1/1	0.93	0.33	68,68,68,68	0
55	ZN	G8	201	1/1	0.93	0.17	105,105,105,105	0
54	MG	14	3269	1/1	0.94	0.30	50,50,50,50	0
54	MG	14	3119	1/1	0.94	0.28	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3058	1/1	0.94	0.17	62,62,62,62	0
54	MG	14	3434	1/1	0.94	0.17	46,46,46,46	0
54	MG	1H	3287	1/1	0.94	0.21	64,64,64,64	0
54	MG	14	3193	1/1	0.94	0.23	46,46,46,46	0
54	MG	1H	3325	1/1	0.94	0.21	65,65,65,65	0
54	MG	14	3522	1/1	0.94	0.24	58,58,58,58	0
54	MG	1H	3517	1/1	0.94	0.08	41,41,41,41	0
54	MG	13	2242	1/1	0.94	0.33	61,61,61,61	0
54	MG	1H	3290	1/1	0.94	0.31	38,38,38,38	0
54	MG	C8	201	1/1	0.94	0.20	50,50,50,50	0
54	MG	1H	3364	1/1	0.94	0.10	72,72,72,72	0
54	MG	13	2365	1/1	0.94	0.12	68,68,68,68	0
54	MG	14	3444	1/1	0.94	0.20	51,51,51,51	0
54	MG	1H	3524	1/1	0.94	0.25	57,57,57,57	0
54	MG	1H	3330	1/1	0.94	0.26	51,51,51,51	0
54	MG	1H	3583	1/1	0.94	0.26	49,49,49,49	0
54	MG	1H	3259	1/1	0.94	0.24	54,54,54,54	0
54	MG	1H	3070	1/1	0.94	0.12	46,46,46,46	0
54	MG	1H	3209	1/1	0.94	0.28	39,39,39,39	0
54	MG	14	3368	1/1	0.94	0.32	60,60,60,60	0
54	MG	1H	3657	1/1	0.94	0.42	47,47,47,47	0
54	MG	1G	2341	1/1	0.94	0.38	65,65,65,65	0
54	MG	1G	2257	1/1	0.94	0.15	73,73,73,73	0
54	MG	1H	3337	1/1	0.94	0.16	45,45,45,45	0
54	MG	14	3373	1/1	0.94	0.28	72,72,72,72	0
54	MG	1G	2294	1/1	0.94	0.09	71,71,71,71	0
54	MG	14	3295	1/1	0.94	0.24	63,63,63,63	0
54	MG	14	3214	1/1	0.94	0.19	51,51,51,51	0
54	MG	1H	3593	1/1	0.94	0.09	55,55,55,55	0
54	MG	1H	3476	1/1	0.94	0.12	57,57,57,57	0
54	MG	1H	3087	1/1	0.94	0.20	45,45,45,45	0
54	MG	1H	3597	1/1	0.94	0.09	42,42,42,42	0
54	MG	1H	3598	1/1	0.94	0.20	50,50,50,50	0
54	MG	14	3020	1/1	0.94	0.08	49,49,49,49	0
54	MG	1H	3119	1/1	0.94	0.32	44,44,44,44	0
54	MG	14	3384	1/1	0.94	0.21	56,56,56,56	0
54	MG	1H	3381	1/1	0.94	0.23	53,53,53,53	0
54	MG	1H	3602	1/1	0.94	0.13	55,55,55,55	0
54	MG	14	3151	1/1	0.94	0.33	45,45,45,45	0
54	MG	1H	3484	1/1	0.94	0.08	42,42,42,42	0
54	MG	1H	3141	1/1	0.94	0.18	45,45,45,45	0
54	MG	1H	3165	1/1	0.94	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3564	1/1	0.94	0.19	62,62,62,62	0
54	MG	14	3068	1/1	0.94	0.08	53,53,53,53	0
54	MG	13	2303	1/1	0.94	0.07	62,62,62,62	0
54	MG	1H	3426	1/1	0.94	0.11	49,49,49,49	0
54	MG	88	202	1/1	0.94	0.16	59,59,59,59	0
54	MG	14	3078	1/1	0.94	0.35	61,61,61,61	0
54	MG	1G	2269	1/1	0.94	0.44	65,65,65,65	0
54	MG	14	3570	1/1	0.94	0.21	59,59,59,59	0
54	MG	1G	2270	1/1	0.94	0.30	83,83,83,83	0
54	MG	1H	3491	1/1	0.94	0.22	66,66,66,66	0
54	MG	14	3094	1/1	0.94	0.20	58,58,58,58	0
54	MG	1H	3388	1/1	0.94	0.12	57,57,57,57	0
54	MG	1H	3614	1/1	0.94	0.28	77,77,77,77	0
54	MG	1H	3432	1/1	0.94	0.10	51,51,51,51	0
54	MG	1H	3494	1/1	0.94	0.24	53,53,53,53	0
54	MG	1H	3434	1/1	0.94	0.05	45,45,45,45	0
54	MG	1H	3620	1/1	0.94	0.16	60,60,60,60	0
54	MG	1H	3497	1/1	0.94	0.34	55,55,55,55	0
54	MG	1H	3221	1/1	0.94	0.24	47,47,47,47	0
54	MG	14	3251	1/1	0.94	0.24	61,61,61,61	0
54	MG	14	3584	1/1	0.94	0.14	59,59,59,59	0
54	MG	14	3252	1/1	0.94	0.24	56,56,56,56	0
54	MG	1H	3145	1/1	0.94	0.12	50,50,50,50	0
54	MG	1H	3311	1/1	0.94	0.19	42,42,42,42	0
54	MG	14	3589	1/1	0.94	0.25	57,57,57,57	0
54	MG	1H	3279	1/1	0.94	0.22	46,46,46,46	0
54	MG	14	3336	1/1	0.94	0.24	53,53,53,53	0
54	MG	1H	3147	1/1	0.94	0.22	57,57,57,57	0
54	MG	1H	3351	1/1	0.94	0.27	55,55,55,55	0
54	MG	14	3594	1/1	0.94	0.19	51,51,51,51	0
54	MG	14	3595	1/1	0.94	0.20	68,68,68,68	0
54	MG	1H	3444	1/1	0.94	0.23	79,79,79,79	0
54	MG	1G	2335	1/1	0.94	0.15	78,78,78,78	0
54	MG	1G	2336	1/1	0.94	0.16	76,76,76,76	0
54	MG	1H	3564	1/1	0.94	0.17	46,46,46,46	0
54	MG	14	3182	1/1	0.94	0.18	56,56,56,56	0
54	MG	21	302	1/1	0.94	0.09	50,50,50,50	0
54	MG	1H	3509	1/1	0.94	0.19	56,56,56,56	0
54	MG	1H	3354	1/1	0.94	0.22	46,46,46,46	0
54	MG	14	3508	1/1	0.94	0.09	58,58,58,58	0
54	MG	1G	2279	1/1	0.94	0.28	67,67,67,67	0
54	MG	1H	3284	1/1	0.94	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3188	1/1	0.94	0.21	53,53,53,53	0
54	MG	14	3429	1/1	0.94	0.42	61,61,61,61	0
54	MG	1G	2219	1/1	0.94	0.20	65,65,65,65	0
54	MG	1H	3320	1/1	0.95	0.21	42,42,42,42	0
54	MG	13	2350	1/1	0.95	0.25	55,55,55,55	0
54	MG	13	2309	1/1	0.95	0.44	55,55,55,55	0
54	MG	14	3241	1/1	0.95	0.30	65,65,65,65	0
54	MG	14	3331	1/1	0.95	0.14	62,62,62,62	0
54	MG	16	206	1/1	0.95	0.43	57,57,57,57	0
54	MG	14	3034	1/1	0.95	0.14	55,55,55,55	0
54	MG	14	3038	1/1	0.95	0.10	57,57,57,57	0
54	MG	1H	3599	1/1	0.95	0.20	53,53,53,53	0
54	MG	14	3516	1/1	0.95	0.20	78,78,78,78	0
54	MG	1H	3366	1/1	0.95	0.19	53,53,53,53	0
54	MG	1H	3473	1/1	0.95	0.17	55,55,55,55	0
54	MG	14	3062	1/1	0.95	0.17	55,55,55,55	0
54	MG	14	3064	1/1	0.95	0.11	63,63,63,63	0
54	MG	1H	3415	1/1	0.95	0.28	62,62,62,62	0
54	MG	1H	3603	1/1	0.95	0.31	49,49,49,49	0
54	MG	14	3165	1/1	0.95	0.54	47,47,47,47	0
54	MG	14	3071	1/1	0.95	0.07	93,93,93,93	0
54	MG	1H	3085	1/1	0.95	0.33	65,65,65,65	0
54	MG	1G	2220	1/1	0.95	0.10	72,72,72,72	0
54	MG	1H	3477	1/1	0.95	0.12	66,66,66,66	0
54	MG	14	3079	1/1	0.95	0.16	59,59,59,59	0
54	MG	1H	3369	1/1	0.95	0.23	63,63,63,63	0
54	MG	1H	3150	1/1	0.95	0.20	53,53,53,53	0
54	MG	1H	3481	1/1	0.95	0.31	47,47,47,47	0
54	MG	1H	3482	1/1	0.95	0.30	50,50,50,50	0
54	MG	1H	3211	1/1	0.95	0.20	47,47,47,47	0
54	MG	1H	3088	1/1	0.95	0.19	52,52,52,52	0
54	MG	1H	3179	1/1	0.95	0.16	49,49,49,49	0
54	MG	1H	3547	1/1	0.95	0.20	54,54,54,54	0
54	MG	1H	3180	1/1	0.95	0.15	56,56,56,56	0
54	MG	1H	3617	1/1	0.95	0.17	46,46,46,46	0
54	MG	1G	2371	1/1	0.95	0.05	86,86,86,86	0
54	MG	14	3102	1/1	0.95	0.27	51,51,51,51	0
54	MG	14	3543	1/1	0.95	0.10	52,52,52,52	0
54	MG	1H	3619	1/1	0.95	0.08	50,50,50,50	0
54	MG	13	2255	1/1	0.95	0.17	70,70,70,70	0
54	MG	1H	3250	1/1	0.95	0.36	42,42,42,42	0
54	MG	1H	3622	1/1	0.95	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3548	1/1	0.95	0.27	55,55,55,55	0
54	MG	I8	103	1/1	0.95	0.17	52,52,52,52	0
54	MG	1H	3552	1/1	0.95	0.16	49,49,49,49	0
54	MG	14	3275	1/1	0.95	0.08	55,55,55,55	0
54	MG	1H	3184	1/1	0.95	0.26	46,46,46,46	0
54	MG	1H	3429	1/1	0.95	0.28	54,54,54,54	0
54	MG	14	3278	1/1	0.95	0.27	46,46,46,46	0
54	MG	1H	3098	1/1	0.95	0.27	39,39,39,39	0
54	MG	14	3556	1/1	0.95	0.08	56,56,56,56	0
54	MG	1H	3254	1/1	0.95	0.19	52,52,52,52	0
54	MG	1H	3628	1/1	0.95	0.22	68,68,68,68	0
54	MG	1H	3187	1/1	0.95	0.14	42,42,42,42	0
54	MG	1G	2238	1/1	0.95	0.20	72,72,72,72	0
54	MG	1H	3386	1/1	0.95	0.32	61,61,61,61	0
54	MG	52	201	1/1	0.95	0.16	71,71,71,71	0
54	MG	1H	3498	1/1	0.95	0.13	64,64,64,64	0
54	MG	1H	3295	1/1	0.95	0.30	49,49,49,49	0
54	MG	88	203	1/1	0.95	0.13	48,48,48,48	0
54	MG	1H	3437	1/1	0.95	0.07	53,53,53,53	0
54	MG	14	3200	1/1	0.95	0.32	53,53,53,53	0
54	MG	1H	3635	1/1	0.95	0.20	54,54,54,54	0
54	MG	14	3203	1/1	0.95	0.17	57,57,57,57	0
54	MG	1G	2248	1/1	0.95	0.42	61,61,61,61	0
54	MG	1H	3101	1/1	0.95	0.38	38,38,38,38	0
54	MG	1H	3039	1/1	0.95	0.13	62,62,62,62	0
54	MG	1H	3441	1/1	0.95	0.23	60,60,60,60	0
54	MG	1G	2387	1/1	0.95	0.25	58,58,58,58	0
54	MG	1H	3132	1/1	0.95	0.35	68,68,68,68	0
54	MG	14	3298	1/1	0.95	0.19	63,63,63,63	0
54	MG	1H	3446	1/1	0.95	0.18	61,61,61,61	0
54	MG	1H	3195	1/1	0.95	0.33	47,47,47,47	0
54	MG	14	3390	1/1	0.95	0.17	53,53,53,53	0
54	MG	14	3391	1/1	0.95	0.20	56,56,56,56	0
54	MG	1H	3046	1/1	0.95	0.14	39,39,39,39	0
54	MG	1H	3449	1/1	0.95	0.33	37,37,37,37	0
54	MG	1G	2210	1/1	0.95	0.15	72,72,72,72	0
54	MG	1H	3051	1/1	0.95	0.07	42,42,42,42	0
54	MG	1H	3267	1/1	0.95	0.13	49,49,49,49	0
54	MG	14	3217	1/1	0.95	0.24	64,64,64,64	0
54	MG	1H	3268	1/1	0.95	0.20	77,77,77,77	0
54	MG	1H	3580	1/1	0.95	0.10	43,43,43,43	0
54	MG	1H	3308	1/1	0.95	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3269	1/1	0.95	0.25	48,48,48,48	0
54	MG	13	2273	1/1	0.95	0.30	63,63,63,63	0
54	MG	1H	3458	1/1	0.95	0.12	60,60,60,60	0
54	MG	1H	3521	1/1	0.95	0.17	44,44,44,44	0
54	MG	1H	3112	1/1	0.95	0.26	40,40,40,40	0
54	MG	14	3229	1/1	0.95	0.28	67,67,67,67	0
54	MG	14	3498	1/1	0.95	0.12	51,51,51,51	0
54	MG	14	3230	1/1	0.95	0.28	54,54,54,54	0
54	MG	1G	2365	1/1	0.95	0.23	62,62,62,62	0
54	MG	14	3501	1/1	0.95	0.08	101,101,101,101	0
54	MG	13	2220	1/1	0.95	0.16	66,66,66,66	0
54	MG	13	2252	1/1	0.95	0.43	72,72,72,72	0
54	MG	1H	3275	1/1	0.95	0.42	54,54,54,54	0
54	MG	1H	3466	1/1	0.95	0.14	54,54,54,54	0
54	MG	1H	3594	1/1	0.95	0.08	51,51,51,51	0
54	MG	19	301	1/1	0.95	0.28	43,43,43,43	0
55	ZN	3E	301	1/1	0.95	0.30	86,86,86,86	0
54	MG	1H	3410	1/1	0.96	0.05	48,48,48,48	0
54	MG	1H	3650	1/1	0.96	0.09	56,56,56,56	0
54	MG	1H	3163	1/1	0.96	0.22	57,57,57,57	0
54	MG	14	3393	1/1	0.96	0.12	57,57,57,57	0
54	MG	1H	3370	1/1	0.96	0.16	56,56,56,56	0
54	MG	13	2211	1/1	0.96	0.05	69,69,69,69	0
54	MG	1H	3196	1/1	0.96	0.16	39,39,39,39	0
54	MG	14	3110	1/1	0.96	0.19	58,58,58,58	0
54	MG	1H	3373	1/1	0.96	0.14	57,57,57,57	0
54	MG	1H	3057	1/1	0.96	0.07	48,48,48,48	0
54	MG	14	3476	1/1	0.96	0.13	62,62,62,62	0
54	MG	1H	3462	1/1	0.96	0.20	55,55,55,55	0
54	MG	1H	3136	1/1	0.96	0.12	48,48,48,48	0
54	MG	1H	3660	1/1	0.96	0.09	59,59,59,59	0
54	MG	1H	3609	1/1	0.96	0.28	45,45,45,45	0
54	MG	1J	212	1/1	0.96	0.07	91,91,91,91	0
54	MG	1H	3261	1/1	0.96	0.22	43,43,43,43	0
54	MG	1H	3561	1/1	0.96	0.14	51,51,51,51	0
54	MG	14	3186	1/1	0.96	0.40	55,55,55,55	0
54	MG	G8	202	1/1	0.96	0.35	52,52,52,52	0
54	MG	1H	3378	1/1	0.96	0.26	50,50,50,50	0
54	MG	1H	3229	1/1	0.96	0.15	53,53,53,53	0
54	MG	1H	3565	1/1	0.96	0.21	49,49,49,49	0
54	MG	14	3123	1/1	0.96	0.37	45,45,45,45	0
54	MG	1H	3110	1/1	0.96	0.35	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	31	304	1/1	0.96	0.09	41,41,41,41	0
54	MG	14	3014	1/1	0.96	0.08	60,60,60,60	0
54	MG	14	3015	1/1	0.96	0.23	60,60,60,60	0
54	MG	14	3019	1/1	0.96	0.07	48,48,48,48	0
54	MG	14	3416	1/1	0.96	0.14	57,57,57,57	0
54	MG	13	2265	1/1	0.96	0.33	57,57,57,57	0
54	MG	14	3129	1/1	0.96	0.31	49,49,49,49	0
54	MG	1G	2280	1/1	0.96	0.08	76,76,76,76	0
54	MG	14	3270	1/1	0.96	0.48	53,53,53,53	0
54	MG	14	3024	1/1	0.96	0.08	57,57,57,57	0
54	MG	14	3027	1/1	0.96	0.08	51,51,51,51	0
54	MG	14	3201	1/1	0.96	0.41	45,45,45,45	0
54	MG	1G	2292	1/1	0.96	0.27	73,73,73,73	0
54	MG	13	2227	1/1	0.96	0.29	57,57,57,57	0
54	MG	1G	2306	1/1	0.96	0.12	61,61,61,61	0
54	MG	14	3043	1/1	0.96	0.12	60,60,60,60	0
54	MG	1H	3428	1/1	0.96	0.11	50,50,50,50	0
54	MG	13	2349	1/1	0.96	0.10	57,57,57,57	0
54	MG	14	3058	1/1	0.96	0.12	75,75,75,75	0
54	MG	14	3588	1/1	0.96	0.35	63,63,63,63	0
54	MG	1H	3117	1/1	0.96	0.21	36,36,36,36	0
54	MG	45	201	1/1	0.96	0.29	63,63,63,63	0
54	MG	1H	3084	1/1	0.96	0.23	54,54,54,54	0
54	MG	1H	3009	1/1	0.96	0.08	46,46,46,46	0
54	MG	14	3359	1/1	0.96	0.42	63,63,63,63	0
54	MG	98	201	1/1	0.96	0.13	52,52,52,52	0
54	MG	1H	3310	1/1	0.96	0.17	37,37,37,37	0
54	MG	98	203	1/1	0.96	0.24	57,57,57,57	0
54	MG	K8	101	1/1	0.96	0.12	60,60,60,60	0
54	MG	14	3067	1/1	0.96	0.15	60,60,60,60	0
54	MG	1H	3240	1/1	0.96	0.31	57,57,57,57	0
54	MG	14	3070	1/1	0.96	0.20	74,74,74,74	0
54	MG	14	3147	1/1	0.96	0.43	63,63,63,63	0
54	MG	1H	3010	1/1	0.96	0.09	51,51,51,51	0
54	MG	14	3074	1/1	0.96	0.08	77,77,77,77	0
54	MG	14	3219	1/1	0.96	0.21	57,57,57,57	0
54	MG	1H	3242	1/1	0.96	0.27	38,38,38,38	0
54	MG	14	3076	1/1	0.96	0.21	61,61,61,61	0
54	MG	13	2240	1/1	0.96	0.36	74,74,74,74	0
54	MG	1H	3014	1/1	0.96	0.08	63,63,63,63	0
54	MG	11	301	1/1	0.96	0.29	38,38,38,38	0
54	MG	14	3225	1/1	0.96	0.34	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3183	1/1	0.96	0.14	43,43,43,43	0
54	MG	14	3081	1/1	0.96	0.20	61,61,61,61	0
54	MG	1H	3037	1/1	0.96	0.09	51,51,51,51	0
54	MG	14	3529	1/1	0.96	0.24	61,61,61,61	0
54	MG	14	3087	1/1	0.96	0.06	73,73,73,73	0
54	MG	14	3531	1/1	0.96	0.04	66,66,66,66	0
54	MG	13	2212	1/1	0.96	0.05	91,91,91,91	0
54	MG	1H	3445	1/1	0.96	0.12	45,45,45,45	0
54	MG	1H	3322	1/1	0.96	0.34	57,57,57,57	0
54	MG	1G	2214	1/1	0.96	0.07	81,81,81,81	0
54	MG	1H	3045	1/1	0.96	0.09	46,46,46,46	0
54	MG	1H	3102	1/1	0.96	0.15	49,49,49,49	0
54	MG	1H	3104	1/1	0.96	0.20	50,50,50,50	0
54	MG	1H	3451	1/1	0.96	0.15	46,46,46,46	0
54	MG	1H	3253	1/1	0.96	0.15	51,51,51,51	0
54	MG	13	2279	1/1	0.96	0.24	58,58,58,58	0
54	MG	1G	2216	1/1	0.96	0.06	80,80,80,80	0
54	MG	14	3315	1/1	0.96	0.14	55,55,55,55	0
54	MG	14	3042	1/1	0.97	0.09	65,65,65,65	0
54	MG	1H	3590	1/1	0.97	0.26	61,61,61,61	0
54	MG	14	3053	1/1	0.97	0.08	51,51,51,51	0
54	MG	31	303	1/1	0.97	0.06	47,47,47,47	0
54	MG	14	3289	1/1	0.97	0.34	57,57,57,57	0
54	MG	1H	3103	1/1	0.97	0.30	44,44,44,44	0
54	MG	14	3055	1/1	0.97	0.06	67,67,67,67	0
54	MG	1H	3172	1/1	0.97	0.10	41,41,41,41	0
54	MG	1H	3124	1/1	0.97	0.24	35,35,35,35	0
54	MG	1H	3470	1/1	0.97	0.24	50,50,50,50	0
54	MG	1H	3063	1/1	0.97	0.07	51,51,51,51	0
54	MG	1H	3402	1/1	0.97	0.05	45,45,45,45	0
54	MG	14	3065	1/1	0.97	0.15	65,65,65,65	0
54	MG	1H	3064	1/1	0.97	0.06	68,68,68,68	0
54	MG	13	2205	1/1	0.97	0.06	70,70,70,70	0
54	MG	1G	2213	1/1	0.97	0.15	68,68,68,68	0
54	MG	14	3069	1/1	0.97	0.08	76,76,76,76	0
54	MG	13	2209	1/1	0.97	0.08	75,75,75,75	0
54	MG	13	2243	1/1	0.97	0.20	51,51,51,51	0
54	MG	14	3304	1/1	0.97	0.22	48,48,48,48	0
54	MG	1H	3314	1/1	0.97	0.33	42,42,42,42	0
54	MG	1H	3518	1/1	0.97	0.09	56,56,56,56	0
54	MG	1H	3443	1/1	0.97	0.12	53,53,53,53	0
54	MG	1H	3649	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3480	1/1	0.97	0.16	56,56,56,56	0
54	MG	1H	3042	1/1	0.97	0.07	55,55,55,55	0
54	MG	1H	3044	1/1	0.97	0.08	54,54,54,54	0
54	MG	1H	3157	1/1	0.97	0.32	43,43,43,43	0
54	MG	16	208	1/1	0.97	0.34	59,59,59,59	0
54	MG	1H	3086	1/1	0.97	0.24	55,55,55,55	0
54	MG	1H	3289	1/1	0.97	0.21	52,52,52,52	0
54	MG	14	3553	1/1	0.97	0.12	75,75,75,75	0
54	MG	14	3091	1/1	0.97	0.07	56,56,56,56	0
54	MG	1H	3134	1/1	0.97	0.10	69,69,69,69	0
54	MG	1H	3185	1/1	0.97	0.24	37,37,37,37	0
54	MG	1G	2207	1/1	0.97	0.08	78,78,78,78	0
54	MG	1H	3529	1/1	0.97	0.10	54,54,54,54	0
54	MG	1H	3530	1/1	0.97	0.05	45,45,45,45	0
54	MG	13	2358	1/1	0.97	0.06	85,85,85,85	0
54	MG	1H	3091	1/1	0.97	0.07	43,43,43,43	0
54	MG	14	3154	1/1	0.97	0.32	54,54,54,54	0
54	MG	14	3442	1/1	0.97	0.24	64,64,64,64	0
54	MG	29	304	1/1	0.97	0.10	55,55,55,55	0
54	MG	1H	3011	1/1	0.97	0.06	76,76,76,76	0
54	MG	1H	3356	1/1	0.97	0.16	53,53,53,53	0
54	MG	1G	2274	1/1	0.97	0.15	56,56,56,56	0
54	MG	1H	3054	1/1	0.97	0.06	50,50,50,50	0
54	MG	1H	3495	1/1	0.97	0.17	55,55,55,55	0
54	MG	14	3011	1/1	0.97	0.08	55,55,55,55	0
54	MG	14	3330	1/1	0.97	0.15	49,49,49,49	0
54	MG	14	3012	1/1	0.97	0.08	53,53,53,53	0
54	MG	1H	3328	1/1	0.97	0.29	52,52,52,52	0
54	MG	1H	3391	1/1	0.97	0.22	51,51,51,51	0
54	MG	13	2262	1/1	0.97	0.34	56,56,56,56	0
54	MG	1H	3021	1/1	0.97	0.07	44,44,44,44	0
54	MG	1H	3584	1/1	0.97	0.10	49,49,49,49	0
54	MG	1H	3024	1/1	0.97	0.08	43,43,43,43	0
54	MG	1H	3332	1/1	0.97	0.19	52,52,52,52	0
54	MG	14	3030	1/1	0.97	0.07	53,53,53,53	0
54	MG	1H	3031	1/1	0.97	0.24	56,56,56,56	0
54	MG	1H	3465	1/1	0.97	0.17	43,43,43,43	0
54	MG	14	3227	1/1	0.97	0.40	55,55,55,55	0
54	MG	14	3035	1/1	0.97	0.05	49,49,49,49	0
54	MG	1H	3146	1/1	0.97	0.28	45,45,45,45	0
55	ZN	C5	201	1/1	0.97	0.06	116,116,116,116	0
55	ZN	32	301	1/1	0.97	0.26	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1H	3313	1/1	0.98	0.28	45,45,45,45	0
54	MG	13	2369	1/1	0.98	0.04	96,96,96,96	0
54	MG	1H	3038	1/1	0.98	0.10	52,52,52,52	0
54	MG	1H	3066	1/1	0.98	0.05	77,77,77,77	0
54	MG	1H	3069	1/1	0.98	0.07	65,65,65,65	0
54	MG	13	2208	1/1	0.98	0.07	84,84,84,84	0
54	MG	13	2204	1/1	0.98	0.04	66,66,66,66	0
54	MG	1H	3012	1/1	0.98	0.08	44,44,44,44	0
54	MG	1H	3074	1/1	0.98	0.09	105,105,105,105	0
54	MG	1H	3077	1/1	0.98	0.17	47,47,47,47	0
54	MG	14	3009	1/1	0.98	0.04	51,51,51,51	0
54	MG	14	3072	1/1	0.98	0.13	51,51,51,51	0
54	MG	14	3073	1/1	0.98	0.05	86,86,86,86	0
54	MG	14	3010	1/1	0.98	0.07	55,55,55,55	0
54	MG	1H	3078	1/1	0.98	0.26	54,54,54,54	0
54	MG	1H	3080	1/1	0.98	0.08	49,49,49,49	0
54	MG	13	2203	1/1	0.98	0.05	90,90,90,90	0
54	MG	1G	2206	1/1	0.98	0.07	84,84,84,84	0
54	MG	14	3016	1/1	0.98	0.05	50,50,50,50	0
54	MG	1H	3015	1/1	0.98	0.07	48,48,48,48	0
54	MG	1H	3191	1/1	0.98	0.39	35,35,35,35	0
54	MG	14	3083	1/1	0.98	0.05	54,54,54,54	0
54	MG	14	3084	1/1	0.98	0.08	60,60,60,60	0
54	MG	14	3021	1/1	0.98	0.07	54,54,54,54	0
54	MG	13	2206	1/1	0.98	0.03	86,86,86,86	0
54	MG	14	3089	1/1	0.98	0.06	56,56,56,56	0
54	MG	14	3090	1/1	0.98	0.06	56,56,56,56	0
54	MG	1H	3140	1/1	0.98	0.17	43,43,43,43	0
54	MG	14	3026	1/1	0.98	0.10	54,54,54,54	0
54	MG	1H	3646	1/1	0.98	0.21	47,47,47,47	0
54	MG	14	3028	1/1	0.98	0.05	53,53,53,53	0
54	MG	13	2207	1/1	0.98	0.07	75,75,75,75	0
54	MG	1H	3025	1/1	0.98	0.06	48,48,48,48	0
54	MG	14	3033	1/1	0.98	0.07	65,65,65,65	0
54	MG	1H	3089	1/1	0.98	0.08	46,46,46,46	0
54	MG	1H	3056	1/1	0.98	0.10	41,41,41,41	0
54	MG	14	3037	1/1	0.98	0.08	53,53,53,53	0
54	MG	1H	3093	1/1	0.98	0.10	40,40,40,40	0
54	MG	14	3039	1/1	0.98	0.07	53,53,53,53	0
54	MG	14	3040	1/1	0.98	0.07	54,54,54,54	0
54	MG	14	3041	1/1	0.98	0.06	60,60,60,60	0
54	MG	1H	3006	1/1	0.98	0.05	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	I8	101	1/1	0.98	0.10	50,50,50,50	0
54	MG	1H	3096	1/1	0.98	0.14	52,52,52,52	0
54	MG	14	3044	1/1	0.98	0.07	51,51,51,51	0
54	MG	14	3047	1/1	0.98	0.04	58,58,58,58	0
54	MG	14	3048	1/1	0.98	0.15	53,53,53,53	0
54	MG	14	3049	1/1	0.98	0.08	83,83,83,83	0
54	MG	14	3050	1/1	0.98	0.06	70,70,70,70	0
54	MG	14	3051	1/1	0.98	0.05	75,75,75,75	0
54	MG	14	3052	1/1	0.98	0.04	70,70,70,70	0
54	MG	1H	3507	1/1	0.98	0.28	40,40,40,40	0
54	MG	1H	3033	1/1	0.98	0.05	55,55,55,55	0
54	MG	1H	3034	1/1	0.98	0.09	54,54,54,54	0
54	MG	1H	3008	1/1	0.98	0.05	44,44,44,44	0
54	MG	13	2215	1/1	0.99	0.04	69,69,69,69	0
54	MG	14	3008	1/1	0.99	0.07	49,49,49,49	0
54	MG	1H	3079	1/1	0.99	0.09	65,65,65,65	0
54	MG	1H	3026	1/1	0.99	0.04	49,49,49,49	0
54	MG	1H	3081	1/1	0.99	0.17	70,70,70,70	0
54	MG	1H	3048	1/1	0.99	0.06	42,42,42,42	0
54	MG	14	3013	1/1	0.99	0.05	49,49,49,49	0
54	MG	1H	3083	1/1	0.99	0.16	62,62,62,62	0
54	MG	1H	3049	1/1	0.99	0.05	45,45,45,45	0
54	MG	1H	3028	1/1	0.99	0.03	43,43,43,43	0
54	MG	14	3017	1/1	0.99	0.04	50,50,50,50	0
54	MG	1H	3029	1/1	0.99	0.06	43,43,43,43	0
54	MG	1H	3433	1/1	0.99	0.38	57,57,57,57	0
54	MG	1H	3052	1/1	0.99	0.07	46,46,46,46	0
54	MG	14	3022	1/1	0.99	0.04	57,57,57,57	0
54	MG	1H	3053	1/1	0.99	0.08	40,40,40,40	0
54	MG	1H	3030	1/1	0.99	0.03	44,44,44,44	0
54	MG	1H	3090	1/1	0.99	0.05	42,42,42,42	0
54	MG	14	3082	1/1	0.99	0.07	68,68,68,68	0
54	MG	1H	3055	1/1	0.99	0.10	59,59,59,59	0
54	MG	1H	3092	1/1	0.99	0.06	54,54,54,54	0
54	MG	14	3029	1/1	0.99	0.11	56,56,56,56	0
54	MG	14	3086	1/1	0.99	0.04	55,55,55,55	0
54	MG	1H	3007	1/1	0.99	0.06	46,46,46,46	0
54	MG	14	3088	1/1	0.99	0.06	59,59,59,59	0
54	MG	14	3031	1/1	0.99	0.09	48,48,48,48	0
54	MG	1H	3094	1/1	0.99	0.03	59,59,59,59	0
54	MG	1H	3032	1/1	0.99	0.04	53,53,53,53	0
54	MG	1G	2211	1/1	0.99	0.03	69,69,69,69	0

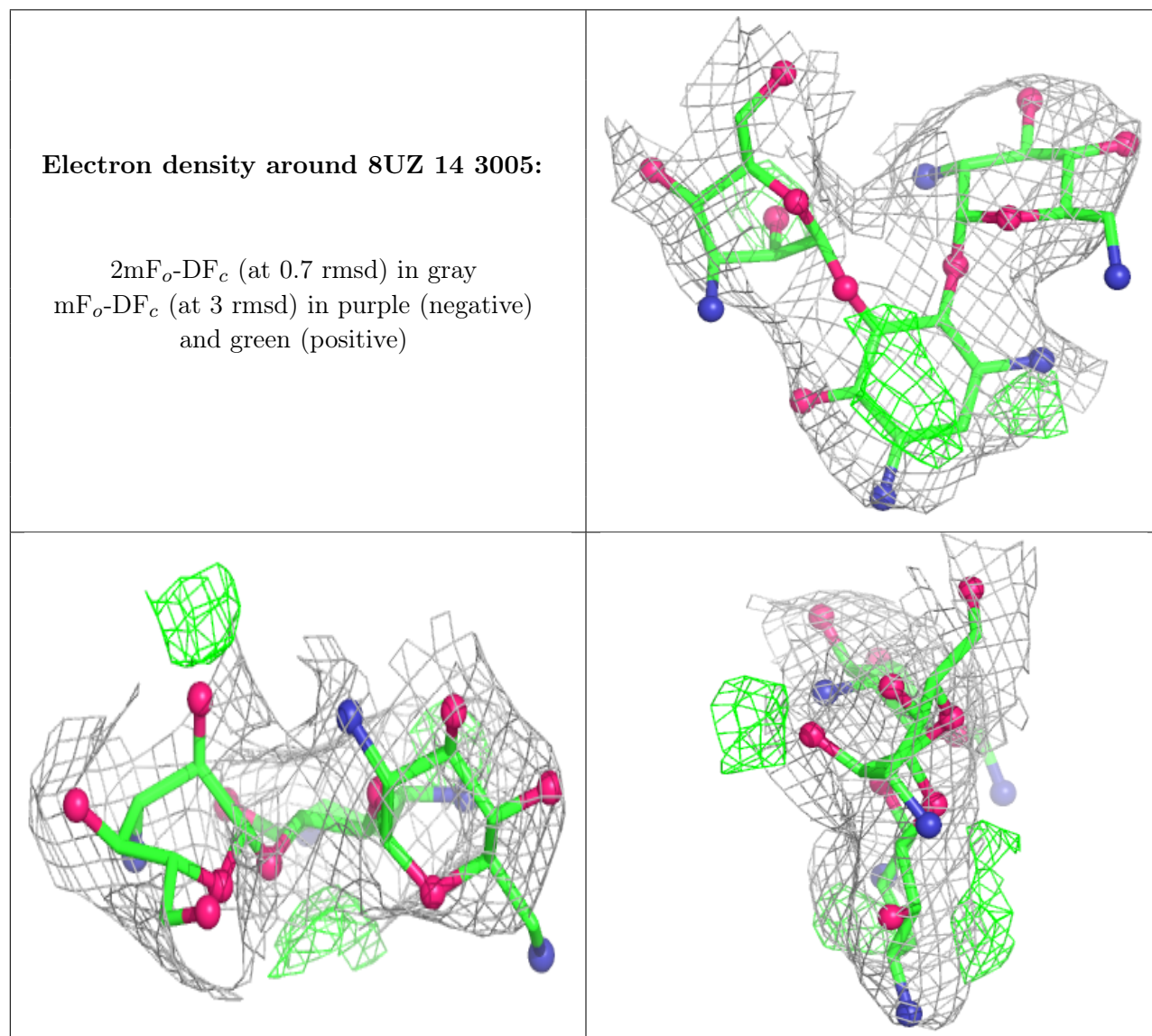
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	14	3093	1/1	0.99	0.08	63,63,63,63	0
54	MG	1H	3059	1/1	0.99	0.03	50,50,50,50	0
54	MG	14	3036	1/1	0.99	0.06	59,59,59,59	0
54	MG	1G	2204	1/1	0.99	0.04	64,64,64,64	0
54	MG	1H	3061	1/1	0.99	0.04	43,43,43,43	0
54	MG	1H	3567	1/1	0.99	0.07	57,57,57,57	0
54	MG	1H	3016	1/1	0.99	0.04	41,41,41,41	0
54	MG	1H	3036	1/1	0.99	0.05	47,47,47,47	0
54	MG	1H	3017	1/1	0.99	0.07	54,54,54,54	0
54	MG	1H	3065	1/1	0.99	0.05	56,56,56,56	0
54	MG	1H	3019	1/1	0.99	0.15	46,46,46,46	0
54	MG	14	3045	1/1	0.99	0.09	76,76,76,76	0
54	MG	14	3046	1/1	0.99	0.04	51,51,51,51	0
54	MG	1H	3067	1/1	0.99	0.10	53,53,53,53	0
54	MG	1H	3068	1/1	0.99	0.07	72,72,72,72	0
54	MG	1H	3020	1/1	0.99	0.14	44,44,44,44	0
54	MG	14	3581	1/1	0.99	0.29	55,55,55,55	0
54	MG	1H	3040	1/1	0.99	0.03	53,53,53,53	0
54	MG	1H	3299	1/1	0.99	0.05	56,56,56,56	0
54	MG	1G	2208	1/1	0.99	0.04	78,78,78,78	0
54	MG	1H	3023	1/1	0.99	0.09	43,43,43,43	0
54	MG	1H	3073	1/1	0.99	0.08	40,40,40,40	0
54	MG	1H	3043	1/1	0.99	0.07	44,44,44,44	0
54	MG	1H	3075	1/1	0.99	0.08	58,58,58,58	0
54	MG	14	3057	1/1	0.99	0.08	55,55,55,55	0
54	MG	1H	3076	1/1	0.99	0.05	49,49,49,49	0
54	MG	14	3059	1/1	0.99	0.07	55,55,55,55	0
54	MG	14	3060	1/1	0.99	0.04	59,59,59,59	0
54	MG	1G	2205	1/1	0.99	0.13	79,79,79,79	0
54	MG	14	3001	1/1	0.99	0.06	48,48,48,48	0
54	MG	14	3063	1/1	0.99	0.11	55,55,55,55	0
55	ZN	5I	101	1/1	0.99	0.02	84,84,84,84	0
55	ZN	5A	101	1/1	0.99	0.02	103,103,103,103	0
54	MG	14	3025	1/1	1.00	0.02	52,52,52,52	0
54	MG	1H	3047	1/1	1.00	0.03	48,48,48,48	0
54	MG	1H	3022	1/1	1.00	0.09	41,41,41,41	0
54	MG	1H	3027	1/1	1.00	0.04	43,43,43,43	0
54	MG	1H	3018	1/1	1.00	0.17	46,46,46,46	0
54	MG	1H	3659	1/1	1.00	0.07	41,41,41,41	0
54	MG	14	3018	1/1	1.00	0.13	51,51,51,51	0

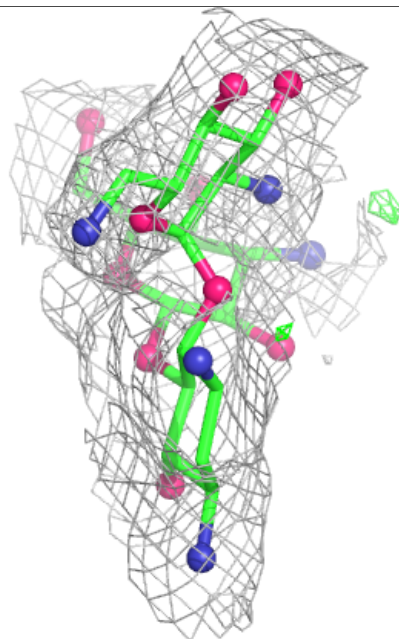
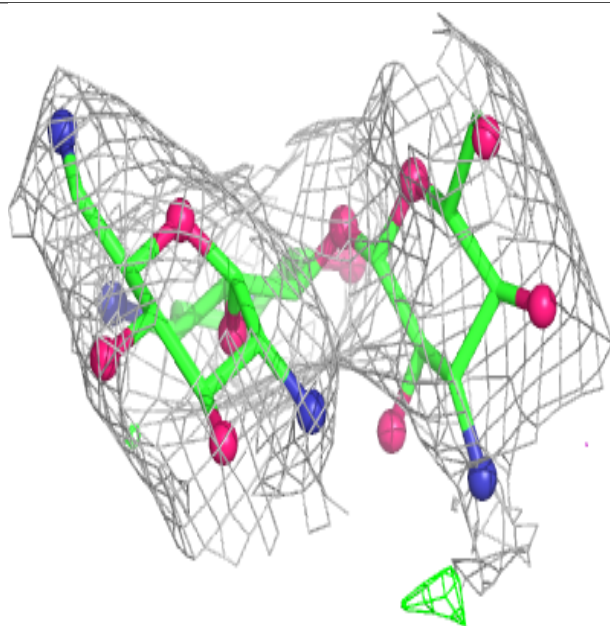
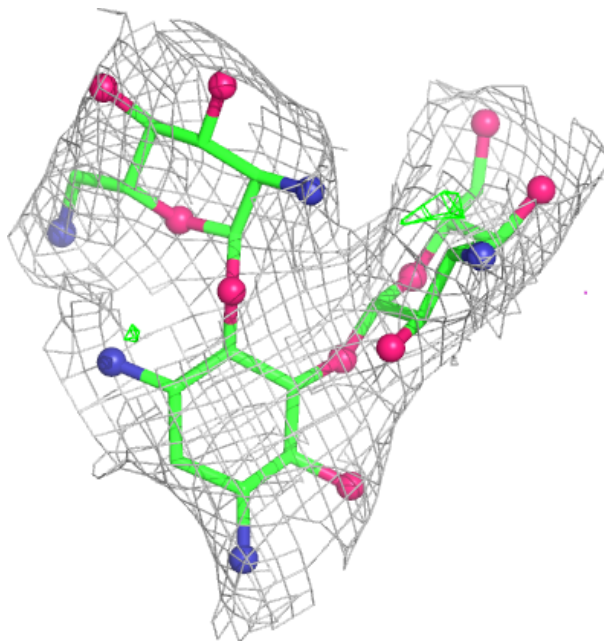
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



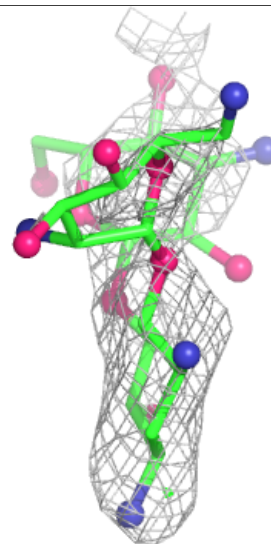
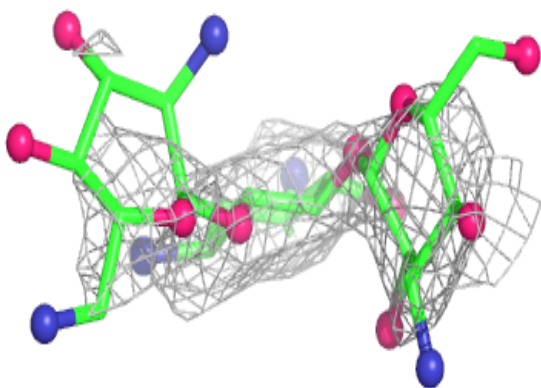
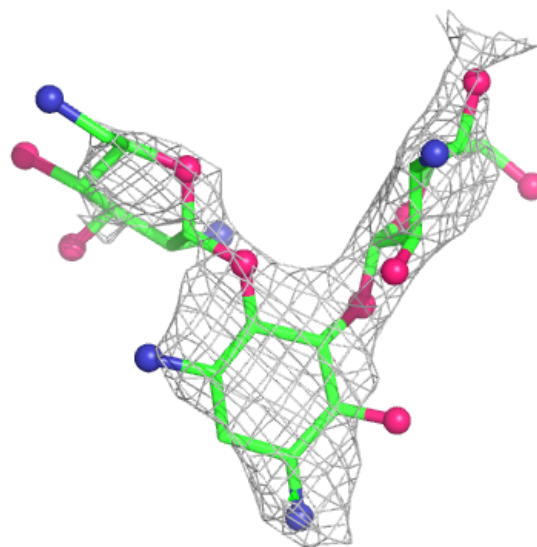
**Electron density around 8UZ 1H 3005:**

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



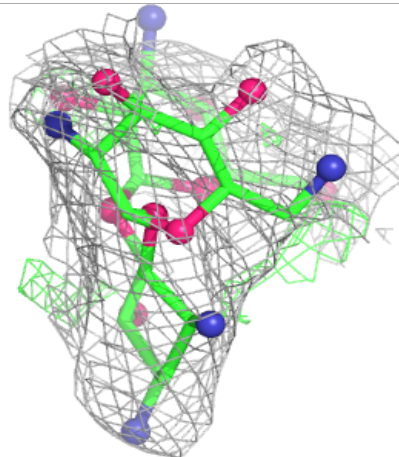
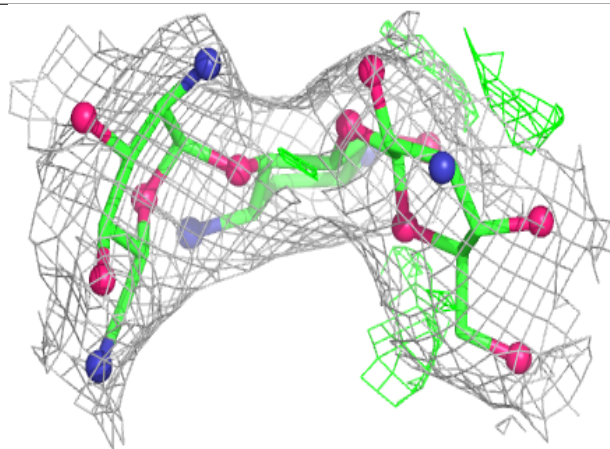
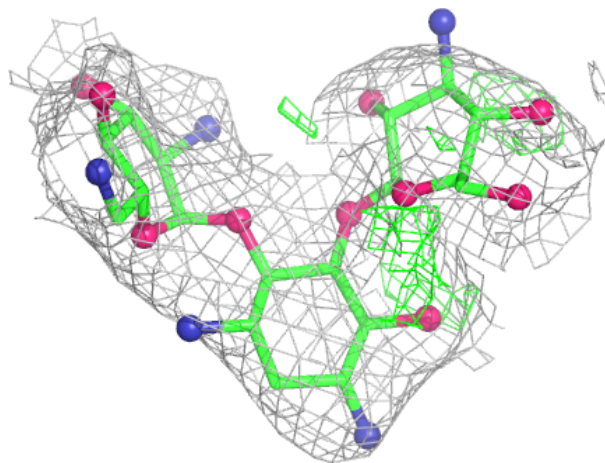
**Electron density around 8UZ 14 3003:**

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



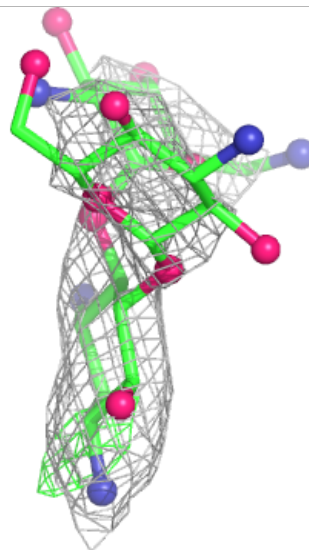
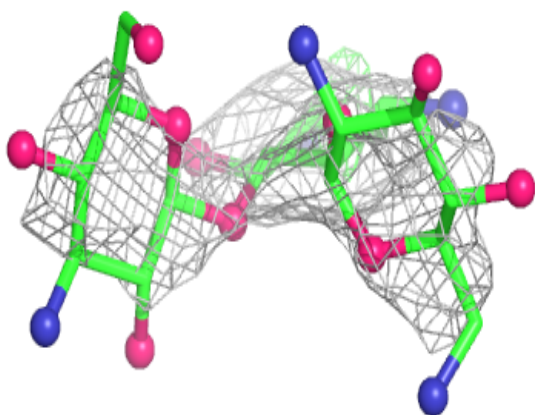
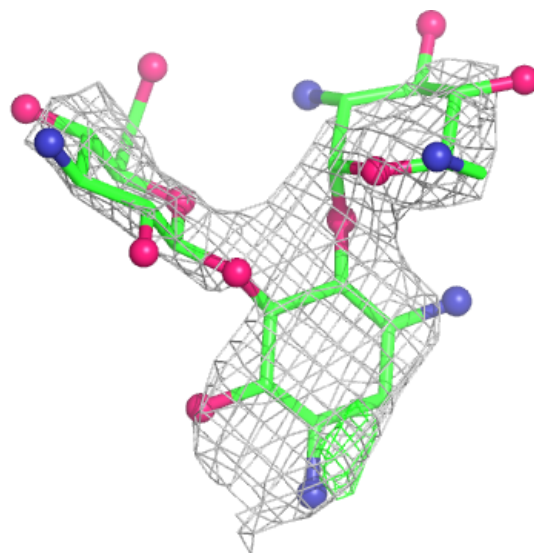
**Electron density around 8UZ 1H 3004:**

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



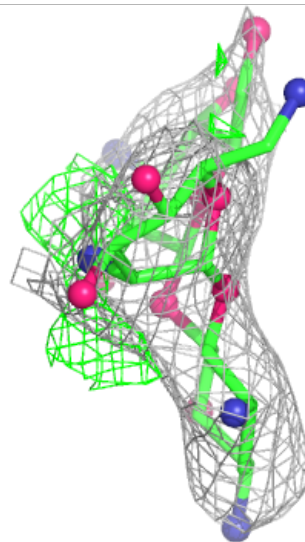
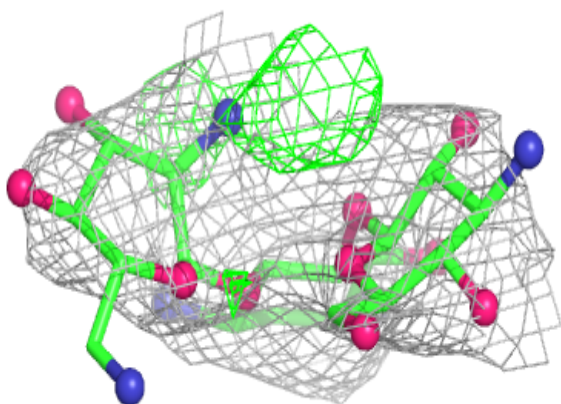
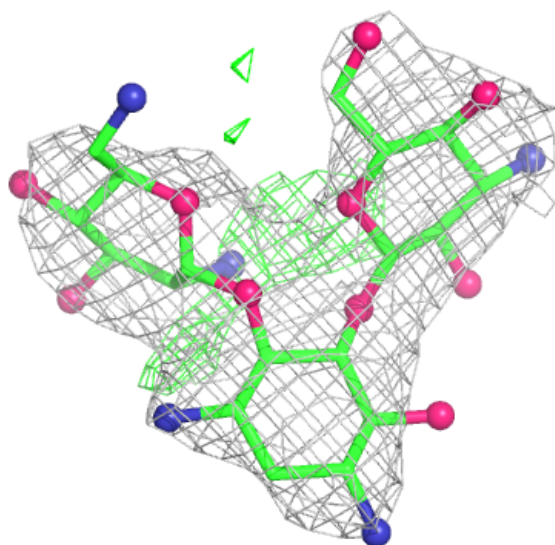
**Electron density around 8UZ 1H 3003:**

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



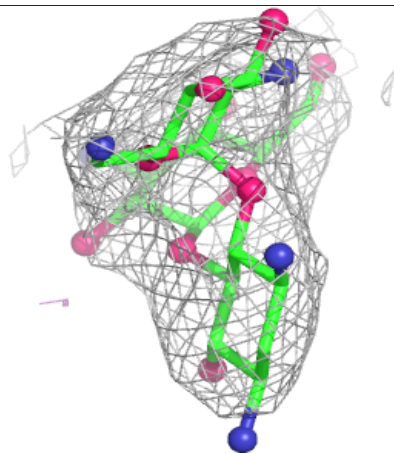
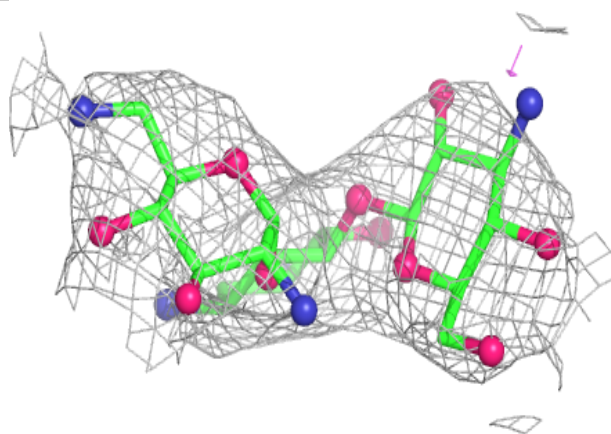
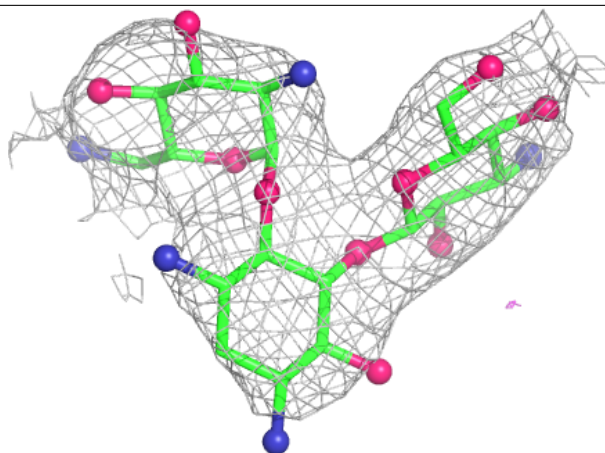
**Electron density around 8UZ 14 3006:**

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



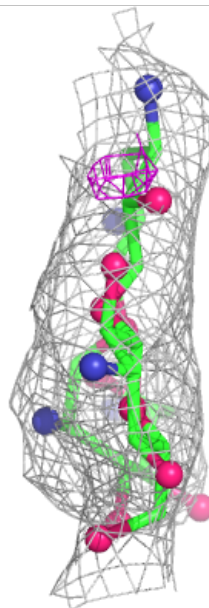
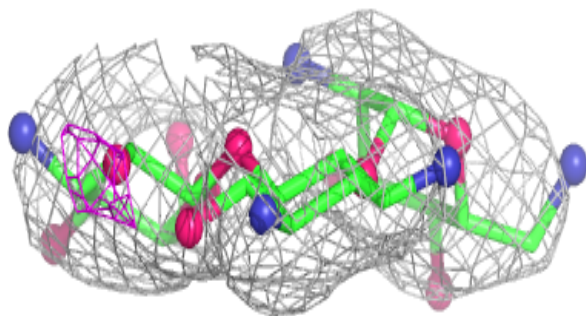
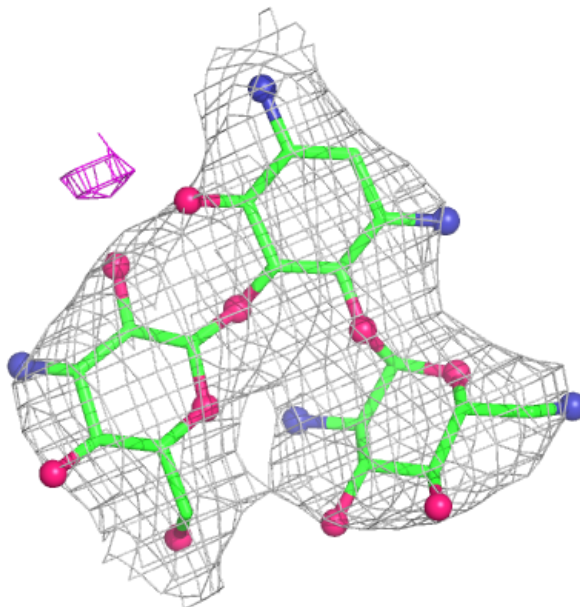
**Electron density around 8UZ 14 3004:**

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



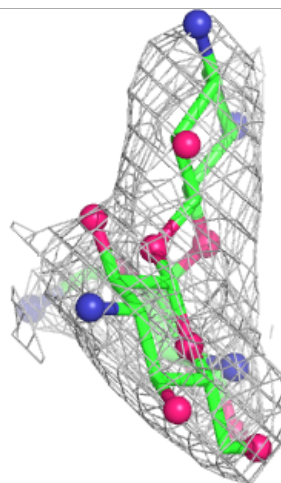
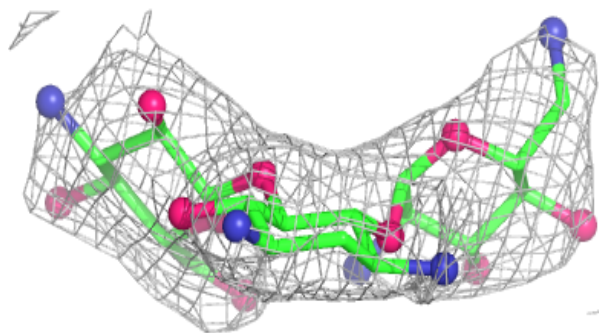
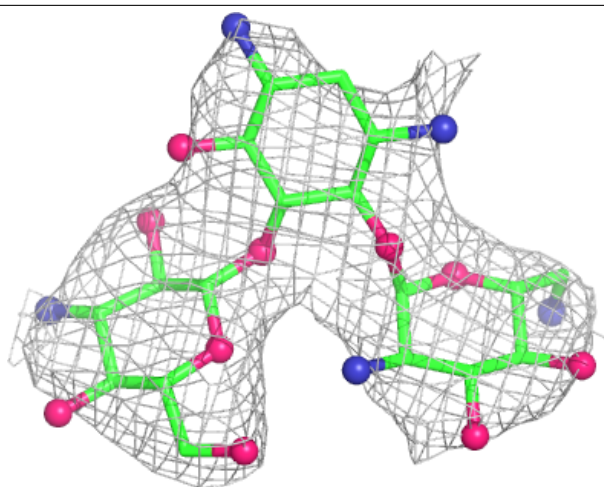
**Electron density around 8UZ 1G 2202:**

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



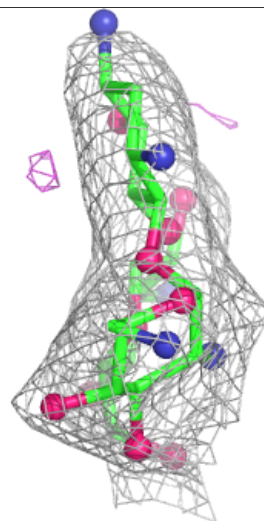
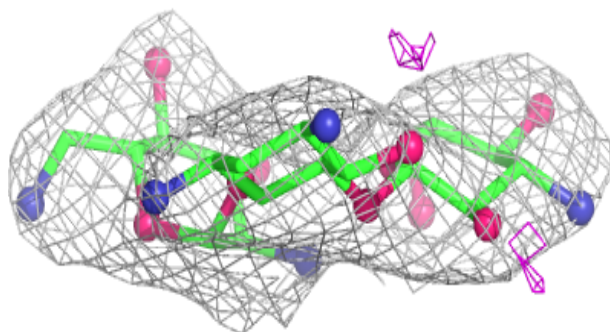
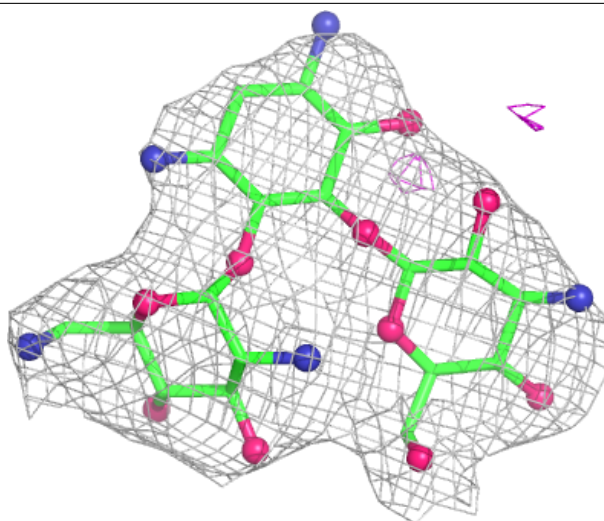
**Electron density around 8UZ 1H 3002:**

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



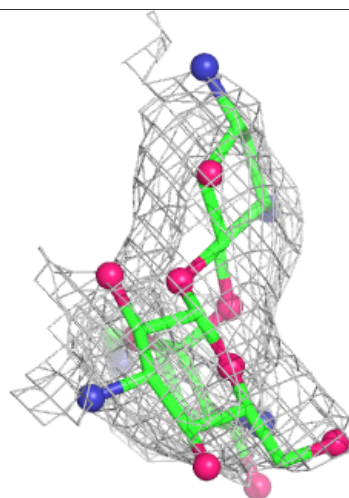
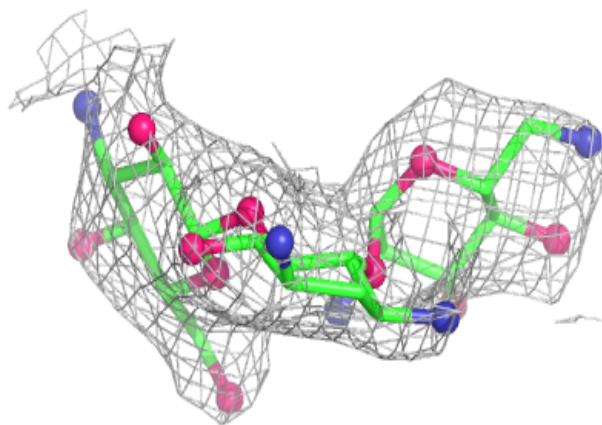
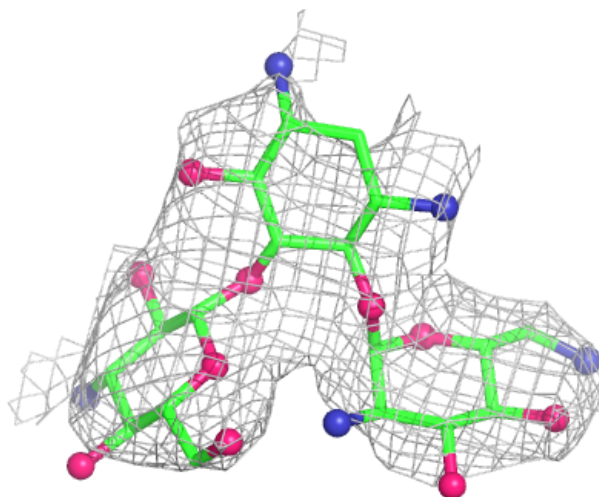
**Electron density around 8UZ 13 2202:**

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



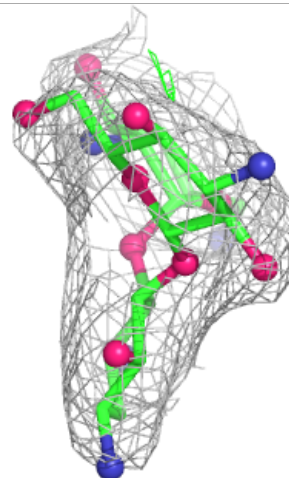
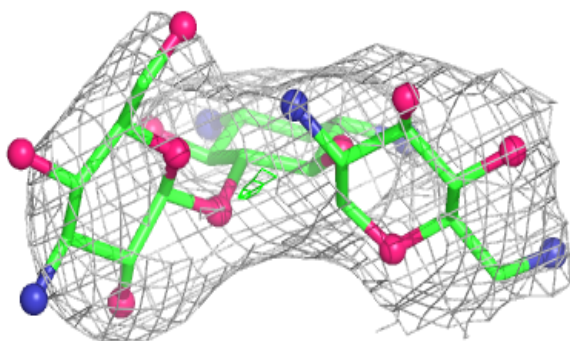
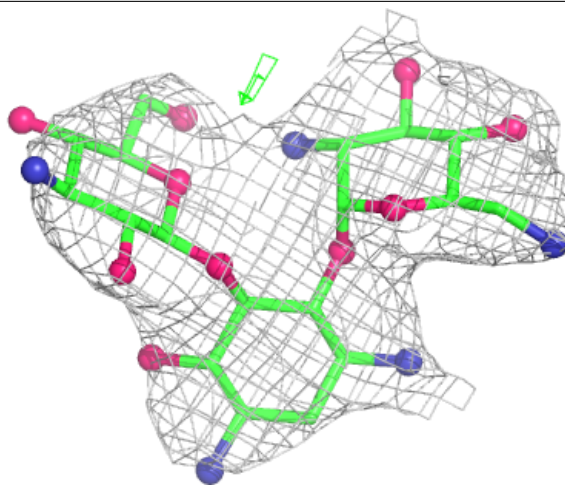
**Electron density around 8UZ 14 3002:**

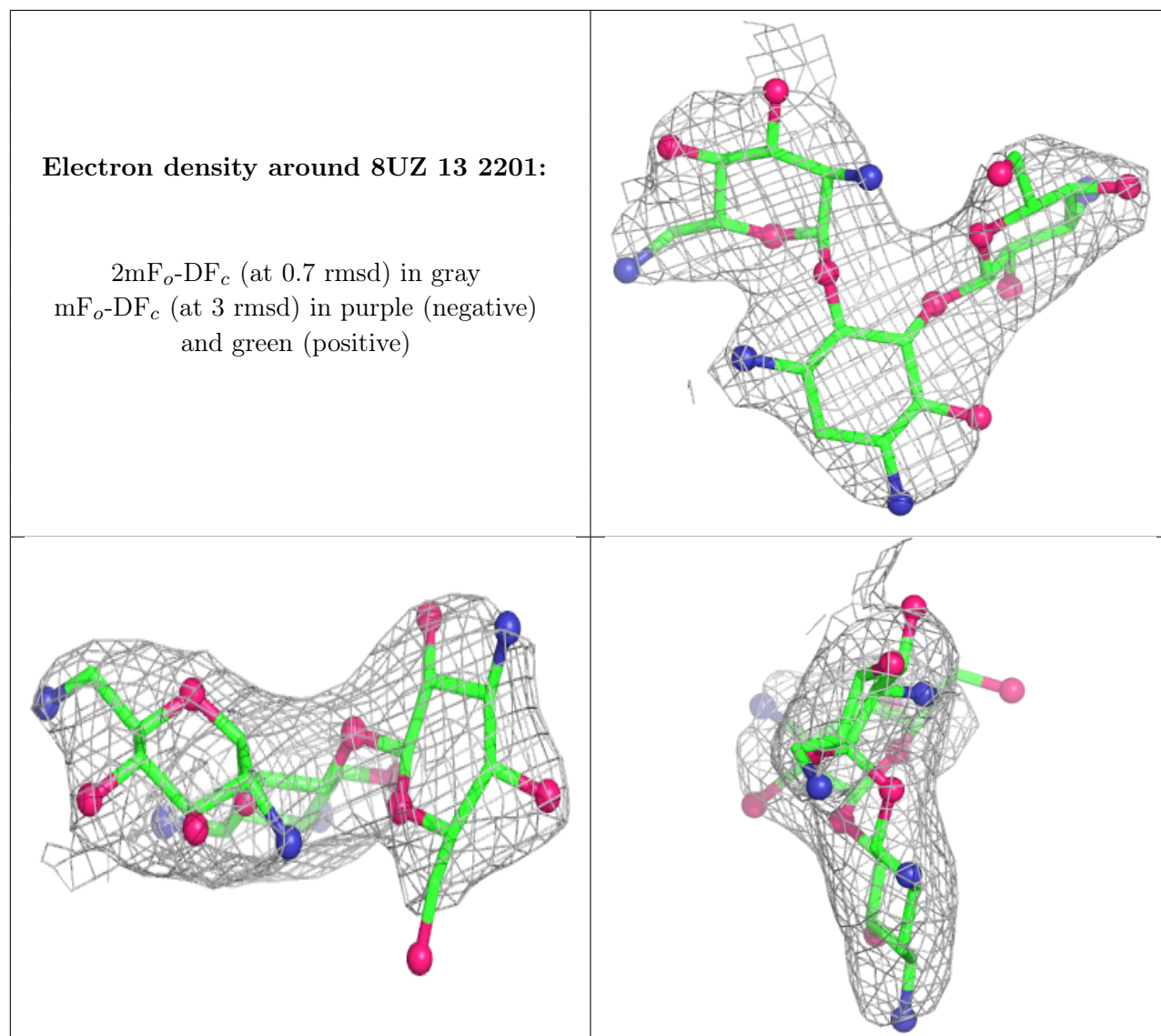
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.