



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:30 am BST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

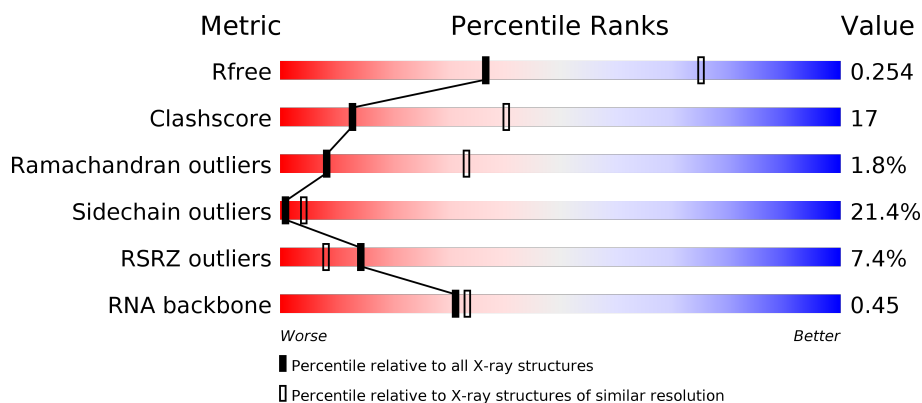
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>9%</div> <div>30% 44% 21% 5%</div> </div>
1	1G	1522	<div> <div>33% 45% 18%</div> </div>
2	65	112	<div> <div>9%</div> <div>42% 38% 18%</div> </div>
2	A8	112	<div> <div>10%</div> <div>44% 40% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	B5	96	
3	F8	96	
4	11	276	
4	19	276	
5	L5	49	
5	P8	49	
6	2A	129	
6	2I	129	
7	8A	105	
7	8I	105	
8	22	239	
8	2E	239	
9	82	128	
9	8E	128	
10	15	140	
10	58	140	
11	C5	110	
11	G8	110	
12	M5	65	
12	Q8	65	
13	3A	132	
13	3I	132	
14	32	209	
14	3E	209	
15	14	2917	

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

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Mol	Chain	Length	Quality of chain
52	W1	76	
52	W4	76	
52	X1	76	
52	X4	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	13	2287	-	-	-	X
54	MG	13	2307	-	-	-	X
54	MG	13	2335	-	-	-	X
54	MG	13	2372	-	-	-	X
54	MG	14	3169	-	-	-	X
54	MG	14	3222	-	-	-	X
54	MG	14	3231	-	-	-	X
54	MG	14	3251	-	-	-	X
54	MG	14	3263	-	-	-	X
54	MG	14	3276	-	-	-	X
54	MG	14	3308	-	-	-	X
54	MG	14	3364	-	-	-	X
54	MG	14	3367	-	-	-	X
54	MG	14	3460	-	-	-	X
54	MG	14	3485	-	-	-	X
54	MG	1G	2253	-	-	-	X
54	MG	1G	2269	-	-	-	X
54	MG	1G	2284	-	-	-	X
54	MG	1G	2288	-	-	-	X
54	MG	1H	3286	-	-	-	X
54	MG	1H	3346	-	-	-	X
54	MG	1H	3492	-	-	-	X
54	MG	1H	3561	-	-	-	X
54	MG	1H	3590	-	-	-	X
54	MG	58	201	-	-	-	X
54	MG	X1	105	-	-	-	X

2 Entry composition [i](#)

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	124	Total	C	N	O			
			983	624	190	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			
			1104	712	206	182	4	0	0	0
10	15	138	Total	C	N	O	S			
			1104	712	206	182	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

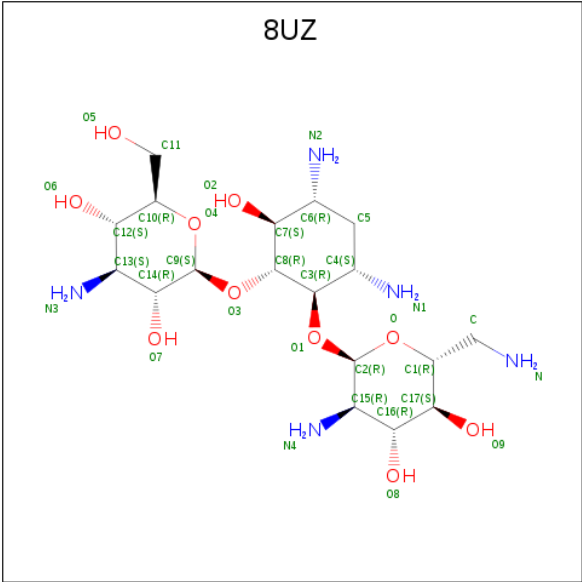
- Molecule 51 is a RNA chain called mRNA.

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

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

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

- Molecule 53 is TC007 (three-letter code: 8UZ) (formula: C₁₈H₃₇N₅O₁₀).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	98	1	Total	Mg	0	0
			1	1		
54	45	2	Total	Mg	0	0
			2	2		
54	55	2	Total	Mg	0	0
			2	2		
54	P8	1	Total	Mg	0	0
			1	1		
54	85	1	Total	Mg	0	0
			1	1		
54	C5	2	Total	Mg	0	0
			2	2		
54	13	182	Total	Mg	0	0
			182	182		
54	B8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1J	14	Total 14	Mg 14	0	0
54	5I	1	Total 1	Mg 1	0	0
54	X4	6	Total 6	Mg 6	0	0
54	35	1	Total 1	Mg 1	0	0
54	16	14	Total 14	Mg 14	0	0
54	42	1	Total 1	Mg 1	0	0
54	B5	1	Total 1	Mg 1	0	0
54	I8	2	Total 2	Mg 2	0	0
54	21	3	Total 3	Mg 3	0	0
54	31	3	Total 3	Mg 3	0	0
54	L8	1	Total 1	Mg 1	0	0
54	4I	1	Total 1	Mg 1	0	0
54	88	5	Total 5	Mg 5	0	0
54	25	2	Total 2	Mg 2	0	0
54	W1	4	Total 4	Mg 4	0	0
54	X1	9	Total 9	Mg 9	0	0
54	52	1	Total 1	Mg 1	0	0
54	A5	1	Total 1	Mg 1	0	0
54	68	2	Total 2	Mg 2	0	0
54	29	5	Total 5	Mg 5	0	0
54	7A	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	41	2	Total 2	Mg 2	0	0
54	78	3	Total 3	Mg 3	0	0
54	39	2	Total 2	Mg 2	0	0
54	1G	178	Total 178	Mg 178	0	0
54	4E	1	Total 1	Mg 1	0	0
54	11	5	Total 5	Mg 5	0	0
54	1H	597	Total 597	Mg 597	0	0
54	14	568	Total 568	Mg 568	0	0
54	W4	4	Total 4	Mg 4	0	0
54	E5	2	Total 2	Mg 2	0	0
54	3I	1	Total 1	Mg 1	0	0
54	49	1	Total 1	Mg 1	0	0
54	5E	1	Total 1	Mg 1	0	0
54	58	1	Total 1	Mg 1	0	0
54	3E	2	Total 2	Mg 2	0	0
54	19	3	Total 3	Mg 3	0	0
54	K8	1	Total 1	Mg 1	0	0
54	6A	1	Total 1	Mg 1	0	0
54	2A	1	Total 1	Mg 1	0	0
54	G8	1	Total 1	Mg 1	0	0
54	A8	1	Total 1	Mg 1	0	0

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

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

- Molecule 56 is water.

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

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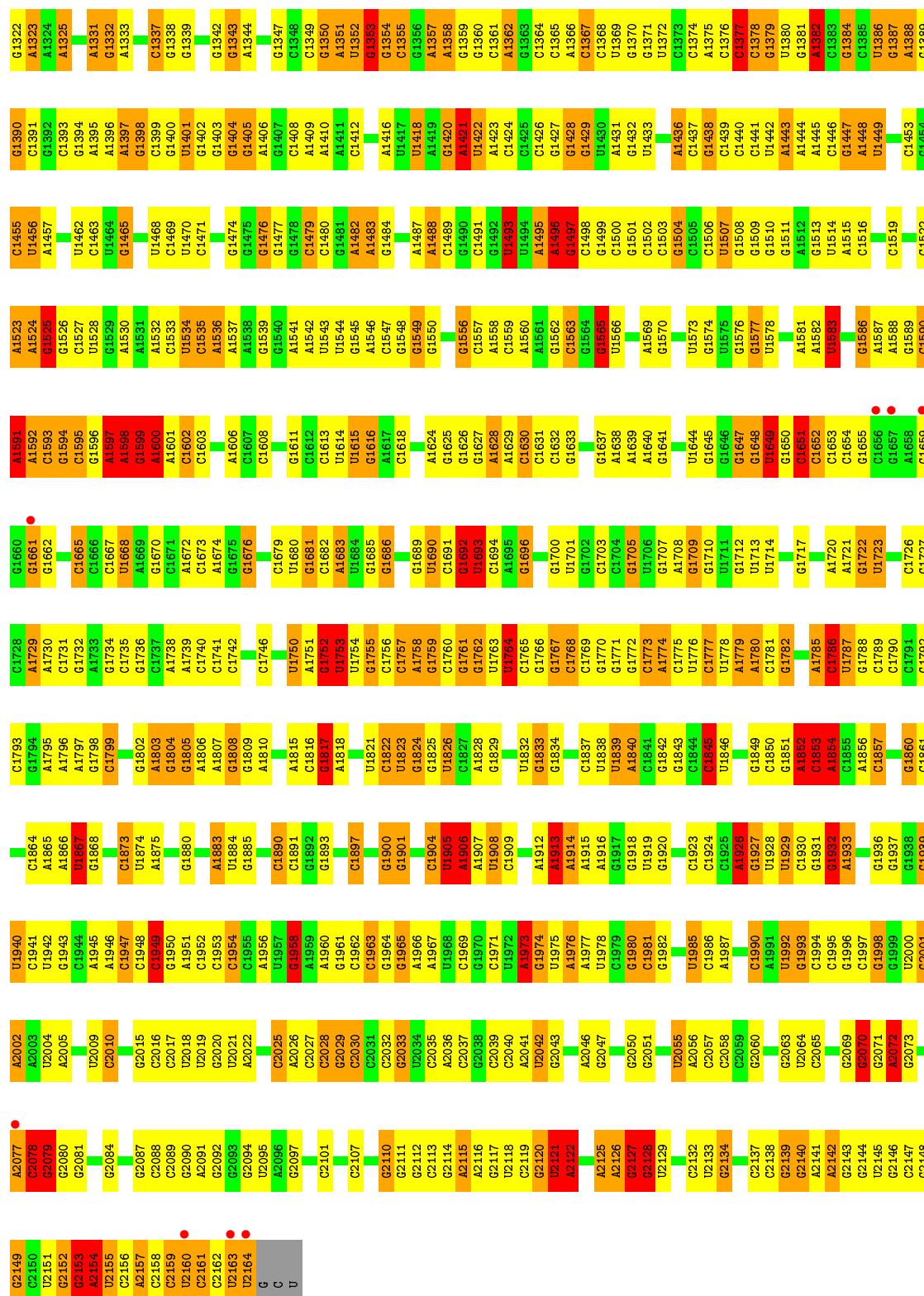
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	I8	5	Total 5	O 5	0	0
56	31	5	Total 5	O 5	0	0
56	35	1	Total 1	O 1	0	0
56	D8	1	Total 1	O 1	0	0
56	39	6	Total 6	O 6	0	0
56	5A	1	Total 1	O 1	0	0
56	J8	1	Total 1	O 1	0	0
56	J5	1	Total 1	O 1	0	0
56	6I	1	Total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

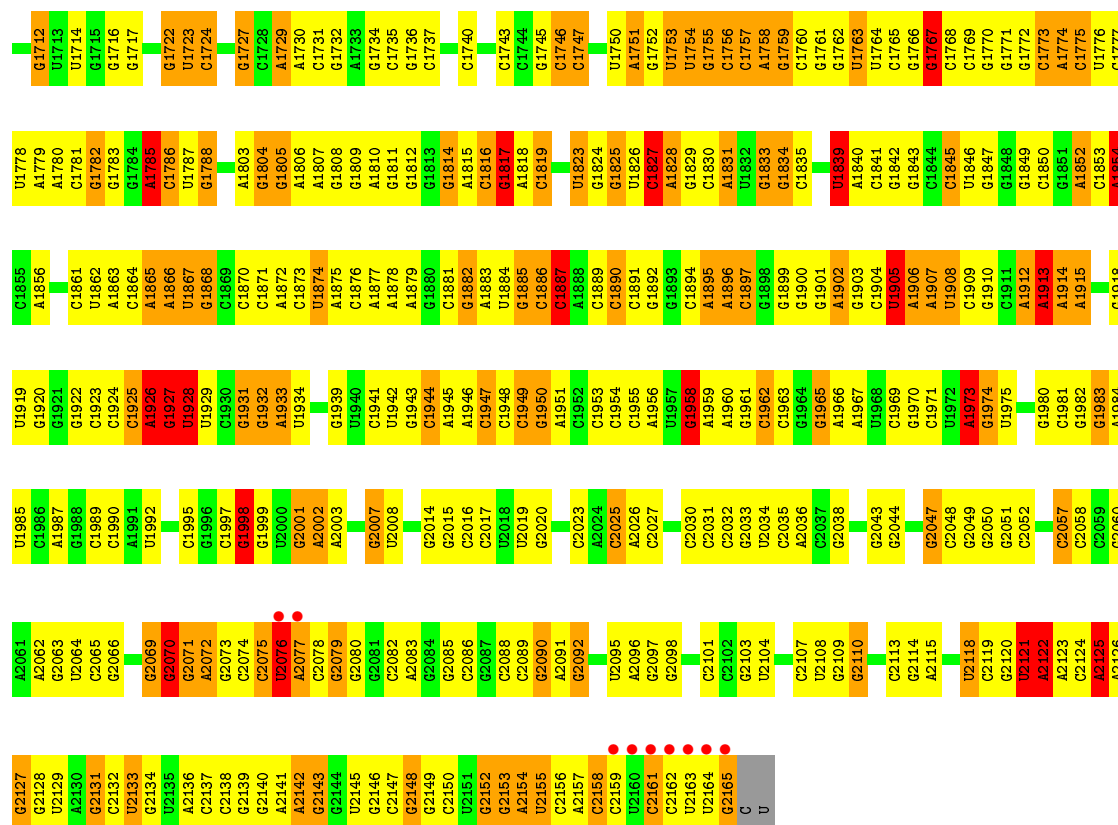
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

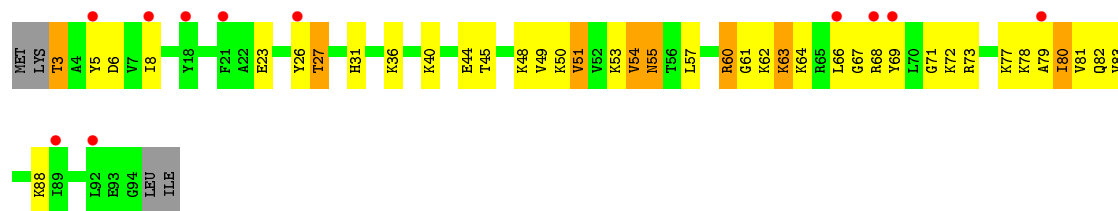
- Chain 13:

Category	Item Count
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B	100
C	100
D	100
E	100
F	100
G	100
H	100
I	100
J	100
K	100
L	100
M	100
N	100
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Q	100
R	100
S	100
T	100
U	100
V	100

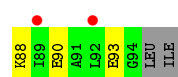








• Molecule 3: 50S ribosomal protein L23



• Molecule 4: 50S ribosomal protein L2

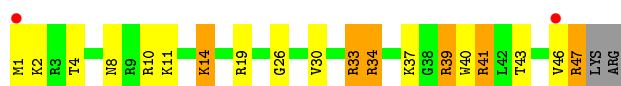


• Molecule 4: 50S ribosomal protein L2

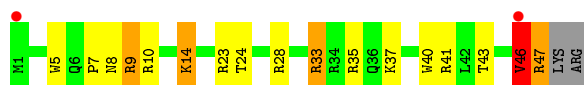


• Molecule 5: 50S ribosomal protein L34

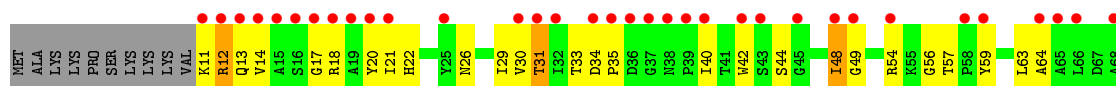




- Molecule 5: 50S ribosomal protein L34



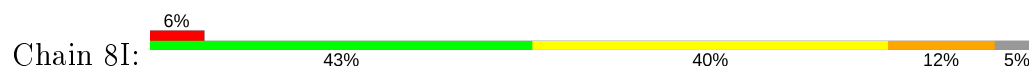
- Molecule 6: 30S ribosomal protein S11



- Molecule 6: 30S ribosomal protein S11

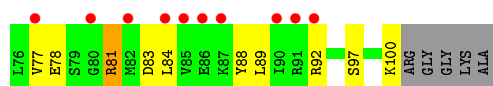


- Molecule 7: 30S ribosomal protein S17

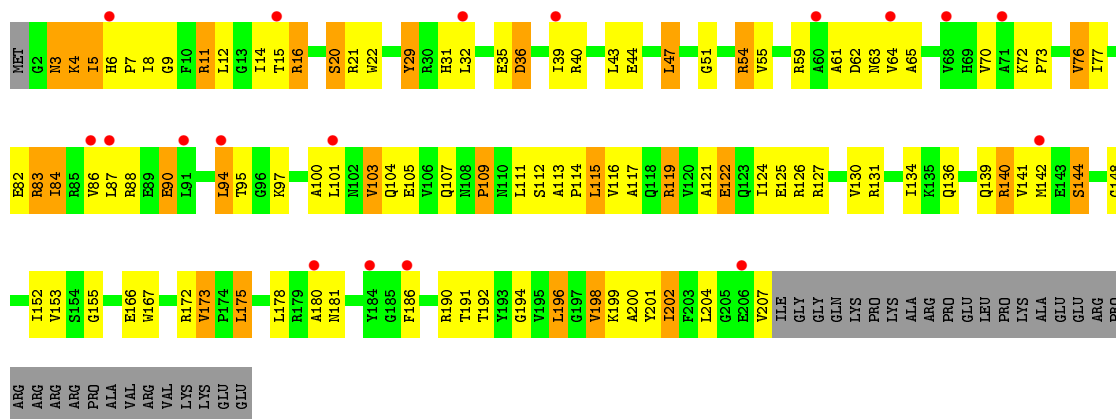
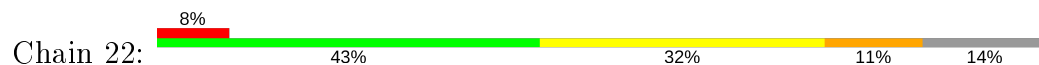


- Molecule 7: 30S ribosomal protein S17

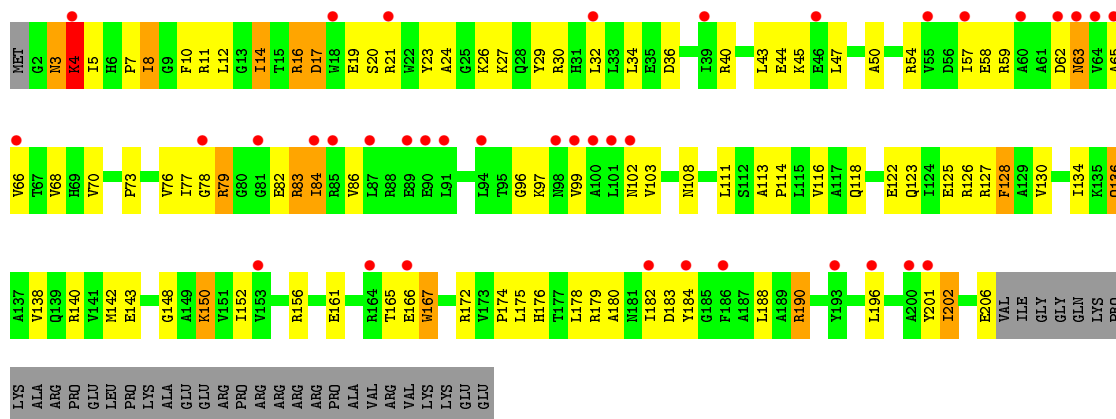




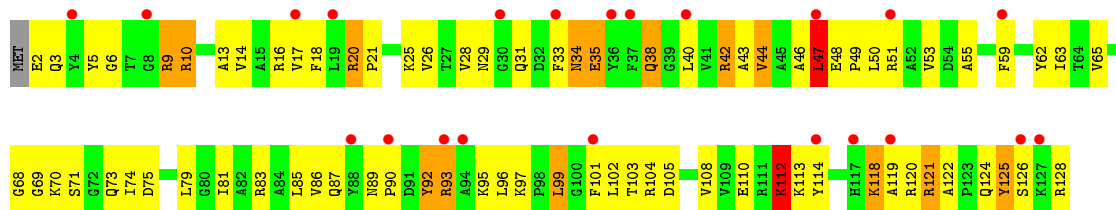
- Molecule 8: 30S ribosomal protein S3



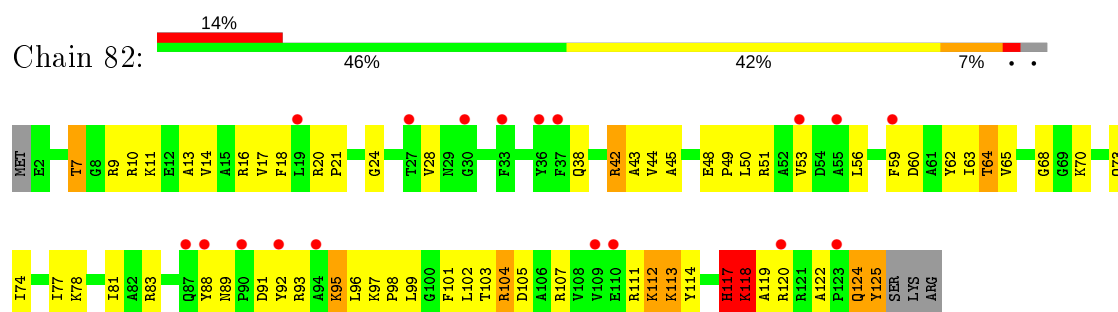
- Molecule 8: 30S ribosomal protein S3



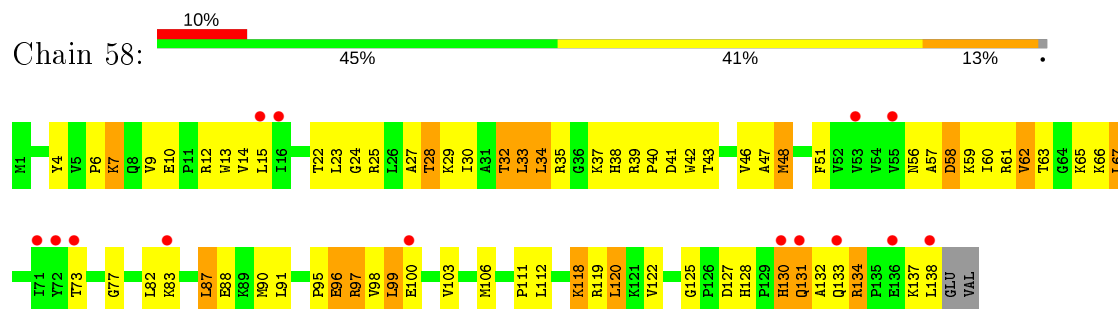
- Molecule 9: 30S ribosomal protein S9



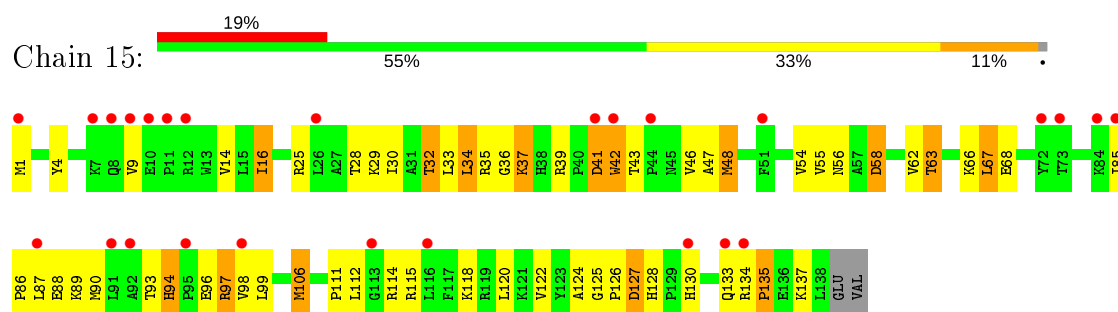
- Molecule 9: 30S ribosomal protein S9



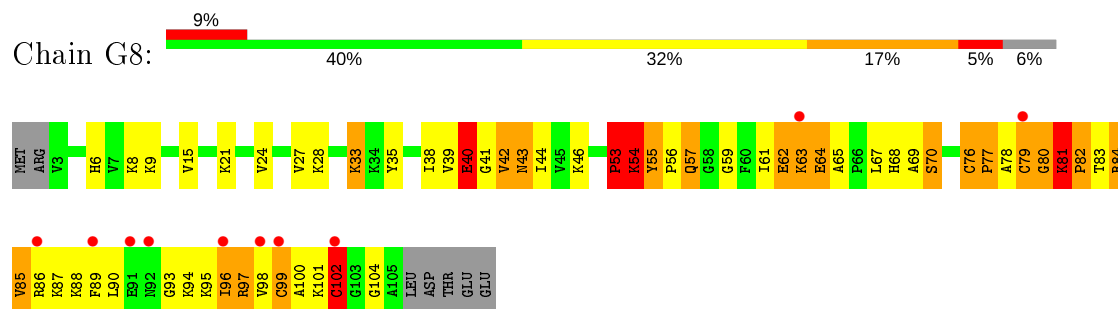
• Molecule 10: 50S ribosomal protein L13



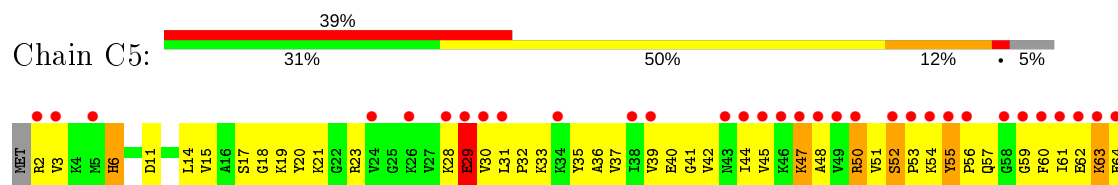
• Molecule 10: 50S ribosomal protein L13

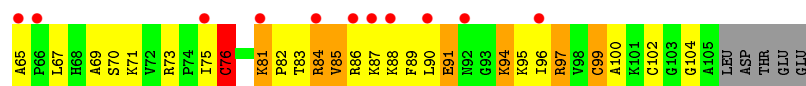


• Molecule 11: 50S ribosomal protein L24

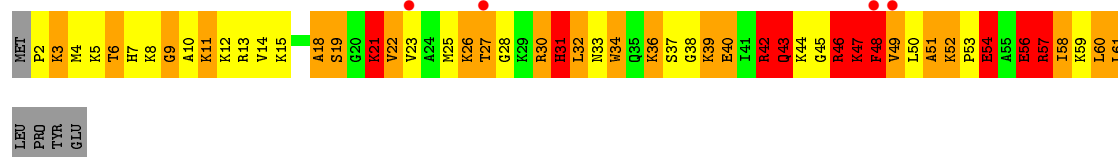


• Molecule 11: 50S ribosomal protein L24

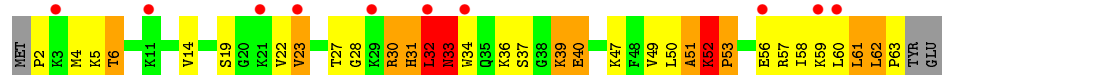




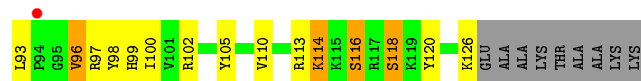
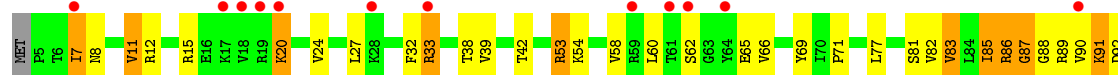
- Molecule 12: 50S ribosomal protein L35



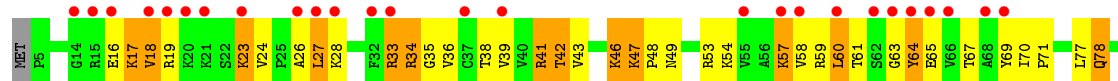
- Molecule 12: 50S ribosomal protein L35



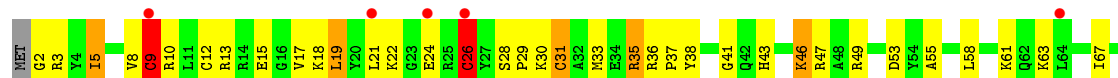
- Molecule 13: 30S ribosomal protein S12

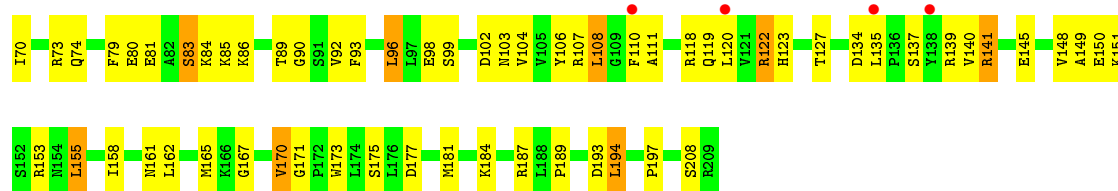


- Molecule 13: 30S ribosomal protein S12

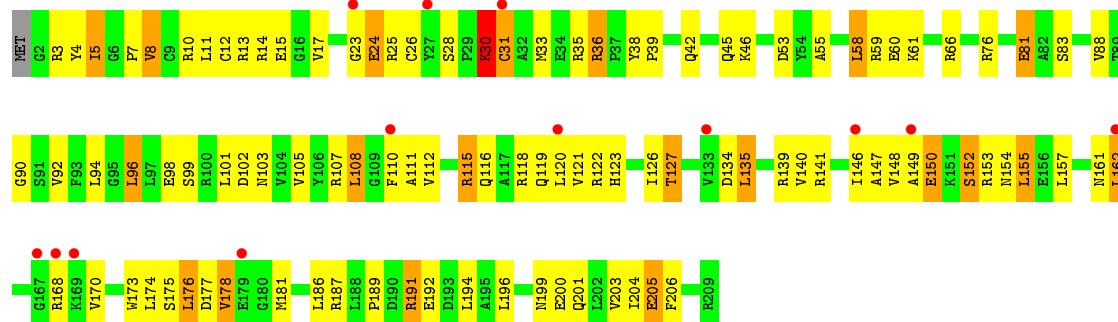


- Molecule 14: 30S ribosomal protein S4

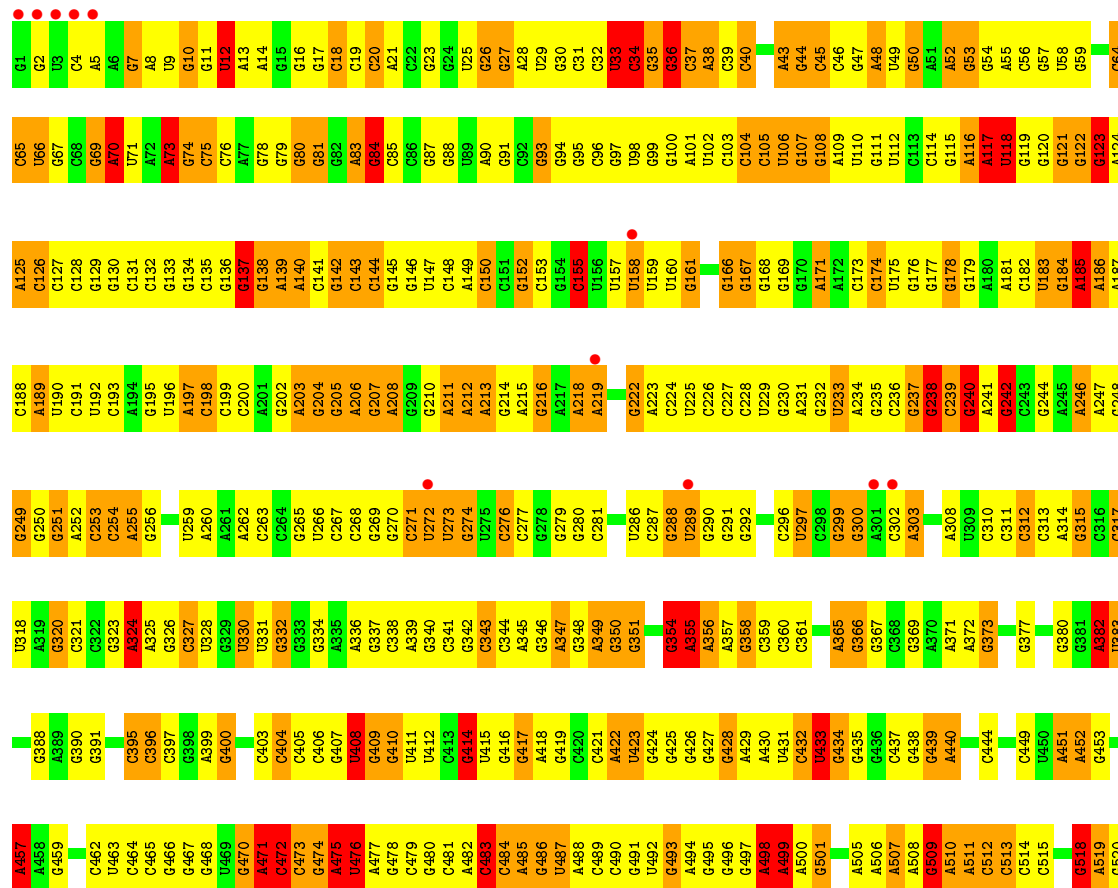
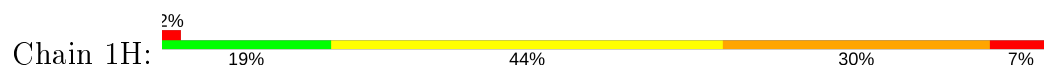




• Molecule 14: 30S ribosomal protein S4



• Molecule 15: 23S ribosomal RNA



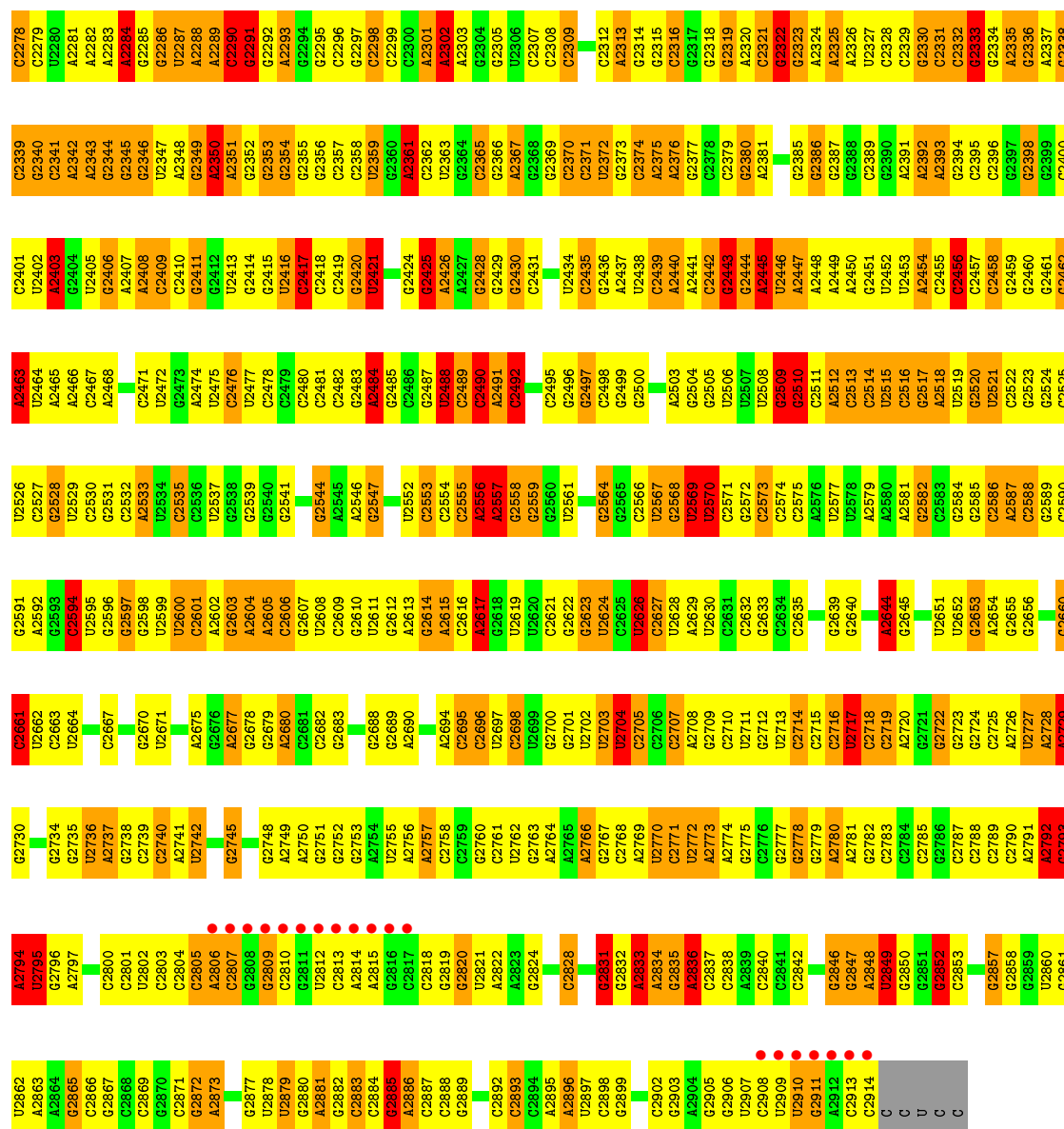
C1400	U1401	C1339	A1275	U1149	G1085	G1023	C963	G892	A832	G772	G708	G521
U1402	C1340	C1340	G1276	C1150	C1086	G1026	G964	C893	A833	U773	G709	G522
A1403	U1341	U1341	G1277	A1151	G1087	G1026	A985	G894	C834	G774	G710	U526
G1404	C1342	C1342	G1278	C1152	C1088	G1027	C985	C895	G835	G775	G711	U527
G1405	U1343	U1343	G1279	U1153	G1089	A1028	G967	U896	U836	A776	G712	A528
U1406	G1344	G1344	C1280	G1154	G1090	A1029	G968	G897	U837	G777	G713	G529
G1345	U1345	U1345	G1281	G1155	C1091	C1030	G969	A898	A838	G778	G714	A529
C1346	C1346	C1346	G1282	U1156	C1092	A1031	U970	A899	C839	G779	G715	A530
A1408	U1347	U1347	G1283	C1157	A1093	A1032	C971	U900	C840	G780	U716	U531
G1409	G1348	G1348	G1284	A1158	G1094	C1033	C972	G901	A841	C781	G717	A532
C1410	U1349	U1349	G1285	G1159	G1095	C1034	C973	G902	A842	G782	G718	G533
C1411	A1350	A1350	U1289	G1160	A1096	G1035	A974	G903	G843	A783	A719	A534
C1412	G1351	G1351	A1290	U1161	C1097	A1036	G975	G904	C844	A784	C720	G535
G1413	G1352	G1352	A1291	G1162	A1098	G1037	G976	C905	C845	G785	C721	C536
A1414	C1353	C1353	G1292	C1163	G1099	A1038	U977	C906	C846	G786	G722	C537
A1415	G1354	G1354	G1293	C1164	C1100	C1039	G978	U907	G847	G787	G723	U538
G1416	G1355	G1355	G1294	C1165	C1101	G1040	G979	U908	C848	G788	G724	G539
G1417	A1356	A1356	A1295	C1167	A1102	C1041	G981	U909	A849	U789	A725	G605
G1418	A1357	A1357	A1296	G1168	G1103	C1042	G982	A910	G850	G790	A726	G606
C1419	G1358	G1358	G1297	C1169	G1104	C1043	C983	G911	A851	G791	C727	G607
G1420	U1359	U1359	U1298	G1170	A1105	A1044	G984	A912	U852	G792	C728	G608
U1421	C1360	C1360	G1299	C1171	U1106	G1045	U984	G913	A853	G793	G729	C609
A1422	U1361	U1361	C1300	C1172	G1107	C1046	G985	C914	A854	G794	G730	G610
G1423	U1362	U1362	G1301	G1173	U1108	U1047	G986	A915	C855	A795	G731	A611
C1424	A1363	A1363	A1302	A1174	U1109	A1048	G987	C916	U856	U796	C732	G612
C1425	C1364	C1364	A1303	A1175	G1110	A1049	A988	U917	G857	G797	G733	G546
G1426	U1365	U1365	U1304	A1176	C1111	G1050	G989	G918	U858	G798	A734	G548
A1427	A1366	A1366	G1305	A1177	G1112	C1051	U990	A919	U859	A799	G735	G549
A1428	C1367	C1367	C1306	U1178	U1113	C1052	G991	U920	U860	A800	C736	C550
G1429	G1368	G1368	C1307	G1179	U1114	G1053	A992	U921	C861	A801	U737	G616
G1430	C1369	C1369	G1308	A1180	A1115	C1054	G993	A927	U862	C802	A738	U551
C1431	A1370	A1370	G1309	U1181	G1116	G1057	G994	G928	C863	C803	G739	A553
A1432	C1371	C1371	C1310	C1183	A1117	A1057	G995	G929	C864	G804	C740	C554
G1433	G1372	G1372	U1311	G1184	A1118	A1058	C996	G930	C865	C805	C741	A555
C1434	C1373	C1373	G1312	G1185	G1119	G1059	G997	G931	C866	U806	C742	A556
A1435	U1374	U1374	A1314	G1186	C1120	U1060	C998	G932	G867	C807	U743	C557
C1436	U1375	U1375	G1315	G1187	A1121	U1061	G999	C933	A868	G808	G744	C558
G1437	C1376	C1376	U1316	C1188	G1122	U1062	A1000	C934	A869	G809	G745	G560
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A1440	C1379	C1379	G1319	G1185	G1125	G1065	G1003	C937	A872	A812	A748	A563
A1441	A1380	A1380	G1320	A1191	U1126	C1066	A1004	C938	C873	A813	G749	C564
A1442	G1381	G1381	A1321	A1192	U1127	U1067	U1005	A939	C874	G814	G750	C565
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U1445	U1384	U1384	A1324	C1195	U1129	U1068	C1008	C942	U877	G817	G753	C568
U1446	A1385	A1385	A1325	A1197	U1130	G1070	G1009	C943	A878	G818	A754	C569
C1447	G1386	G1386	G1326	G1198	A1132	U1071	U1010	A944	G879	G819	G754	G571
C1448	U1387	U1387	A1327	C1199	A1133	G1072	U1011	C945	G880	G820	G755	C572
G1449	G1388	G1388	G1328	G1200	A1134	U1074	C1012	A948	G881	G821	G756	A573
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U1455	U1394	U1394	A1334	A1205	U1140	A1080	C1018	A958	C887	G827	A767	G583
C1456	G1395	G1395	G1334	G1206	U1142	U1081	G1019	A959	U888	U828	C768	G584
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G1459	A1398	A1398	C1273	C1209	U1145	U1084	C1022	C962	G891	A831	A771	U587

G2369	G2370	C2371	G2372	G2373	G2374	A2375	A2313	A2314	G2315	C2376	G2377	C2378	G2379	G2380	A2381	G2382	G2383	G2384	A2385	A2326	A2327	C2328	G2329	C2330	C2331	C2332	G2333	A2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	A2402	A2403	G2404	G2405	G2406	A2407	A2408	G2409	G2410	G2411																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										</
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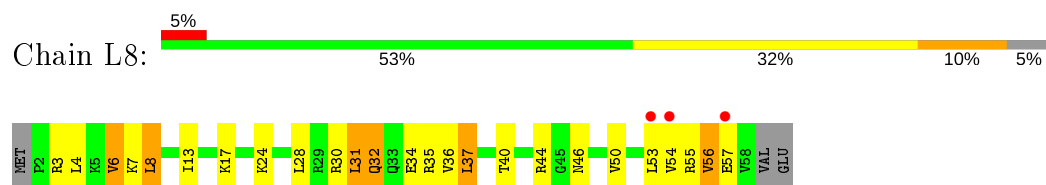


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G1269	A1204	G1135	G1072	G1010	U944	U876	C815	G751	G689	C626	A563	G497	G419
A1326	A1205	A1136	G1073	U1010	C945	U877	U816	U752	G690	A627	C564	A498	C420
G1270	G1206	G1137	U1074	G1013	C946	U878	G817	G753	C691	A628	C565	A499	C421
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G1273	G1211	U1142	G1079	G1019	U956	C883	U822	U758	G695	A633	A574	G504	G426
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G1277	G1214	U1145	G1082	G1021	A958	C886	G826	G764	C699	C636	G577	G509	U431
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C1346	U1222	G1155	G1090	C1030	A964	C893	A832	G772	C706	G644	G584	G518	A440
G1347	G1223	G1156	G1091	C1031	A965	C894	A833	C773	G707	C645	C585	A519	C441
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U1289	A1225	G1158	A1093	A1032	C967	G896	C835	C775	G709	U647	U587	G521	A443
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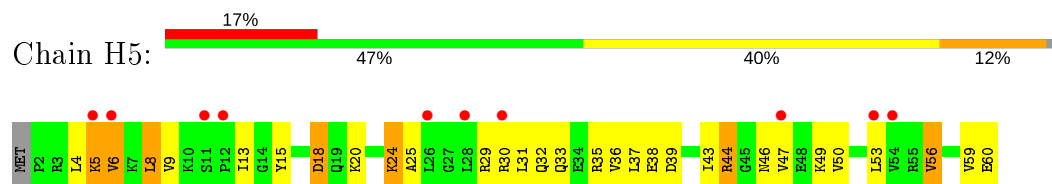
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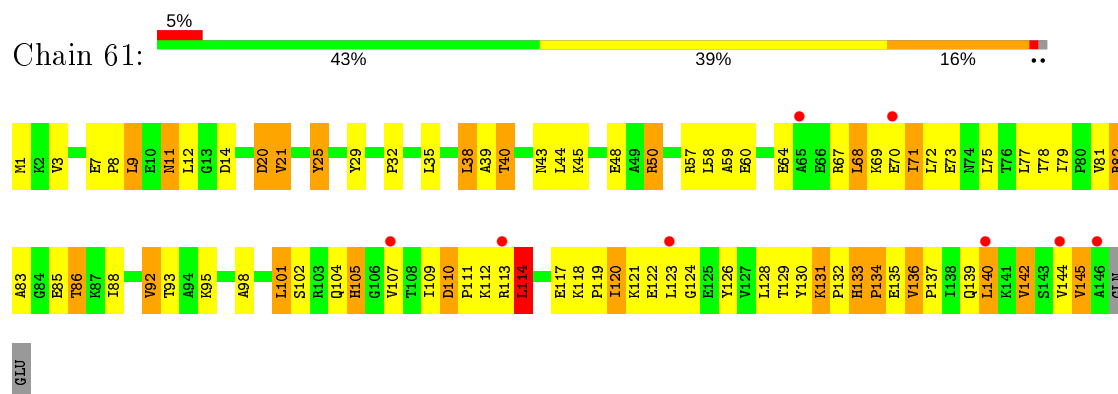
- Molecule 17: 50S ribosomal protein L30



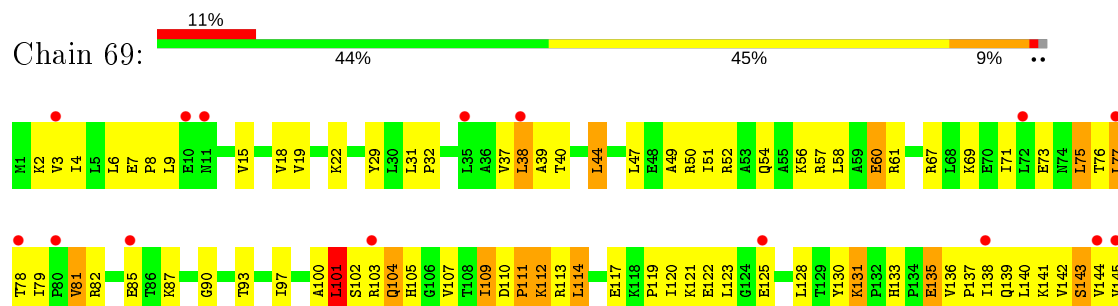
- Molecule 17: 50S ribosomal protein L30

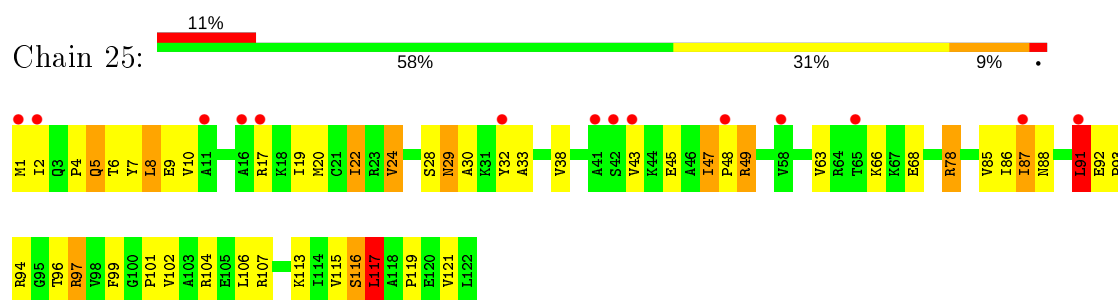


- Molecule 18: 50S ribosomal protein L9

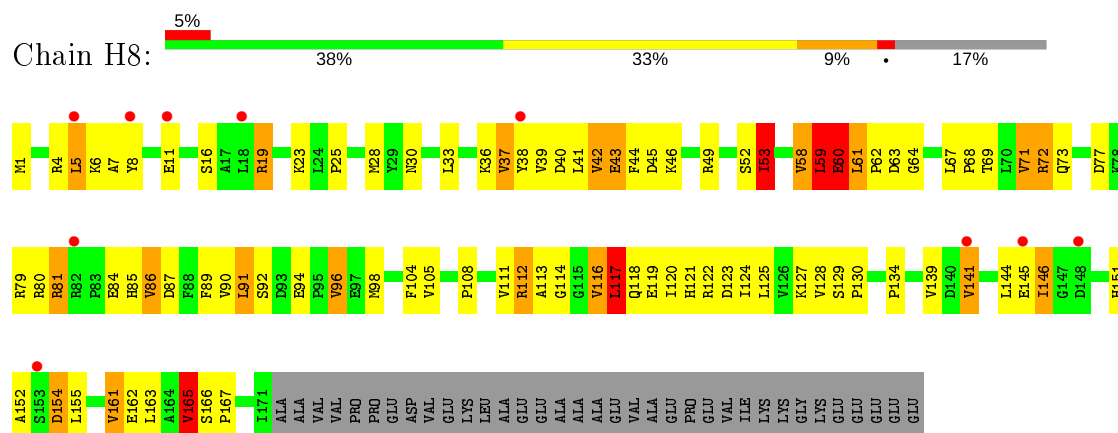


- Molecule 18: 50S ribosomal protein L9

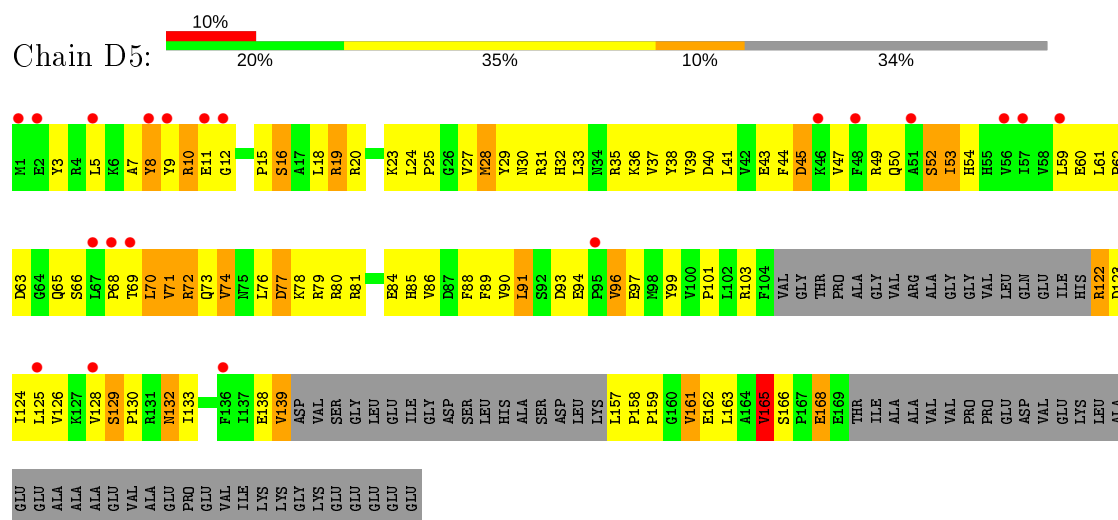




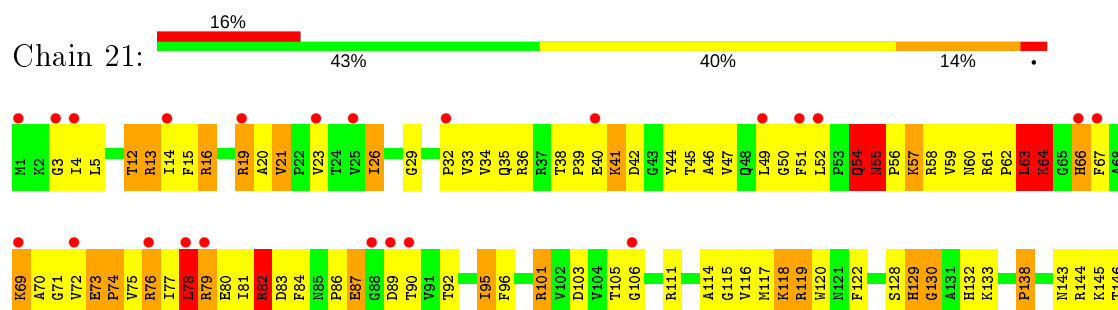
• Molecule 22: 50S ribosomal protein L25

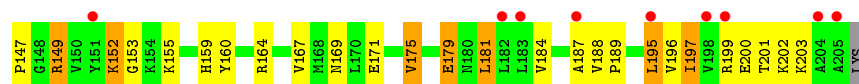


• Molecule 22: 50S ribosomal protein L25

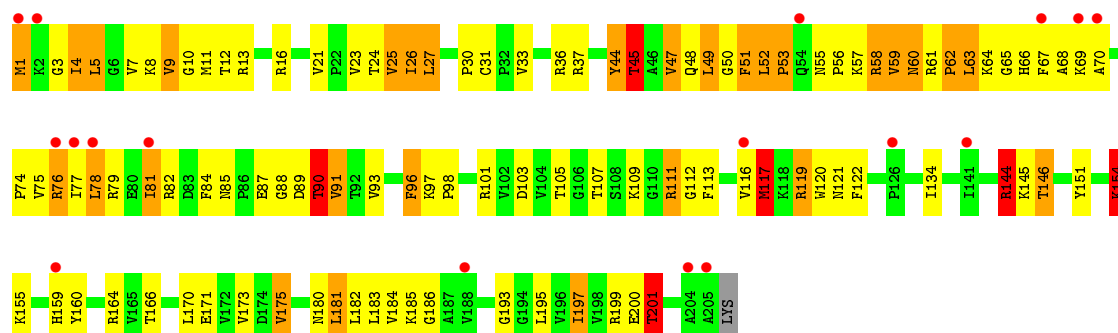


• Molecule 23: 50S ribosomal protein L3

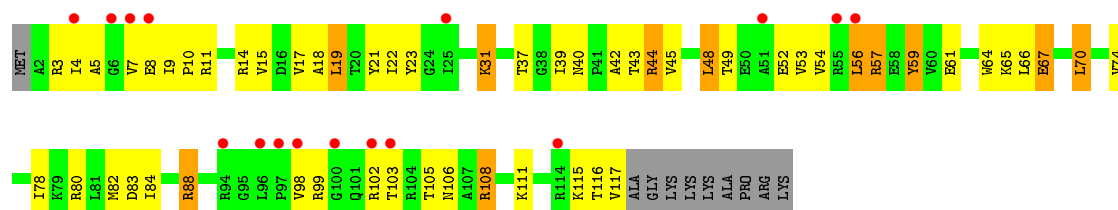




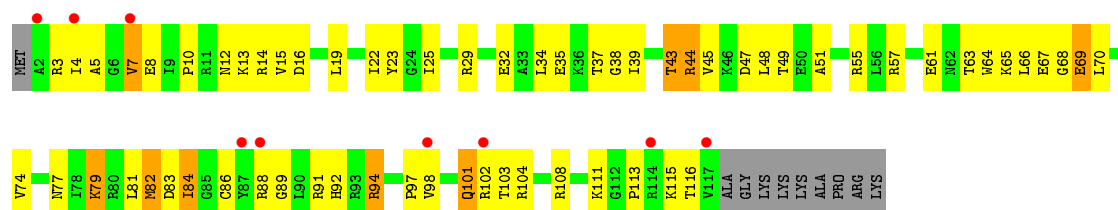
- Molecule 23: 50S ribosomal protein L3



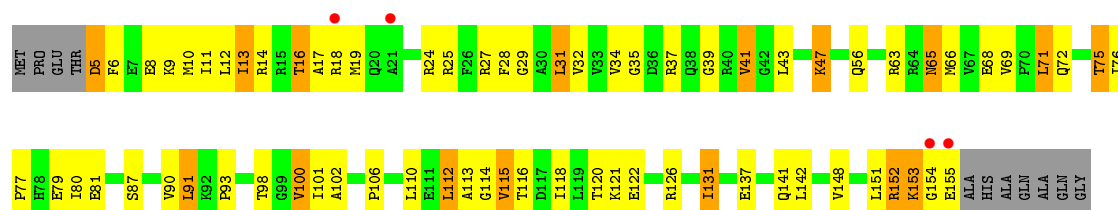
- Molecule 24: 30S ribosomal protein S13



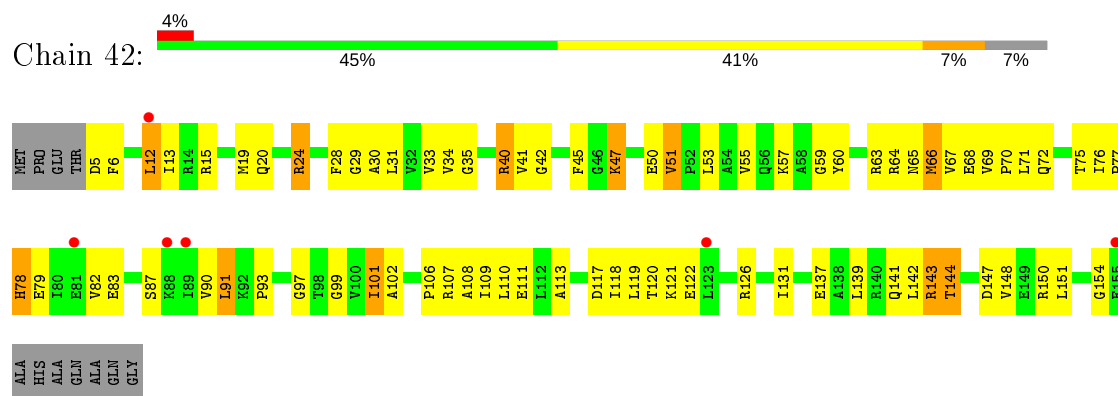
- Molecule 24: 30S ribosomal protein S13

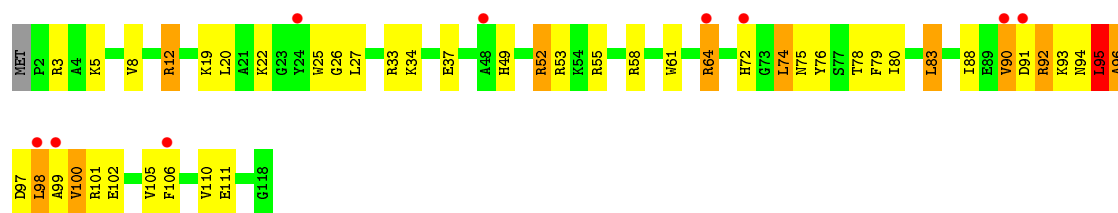


- Molecule 25: 30S ribosomal protein S5

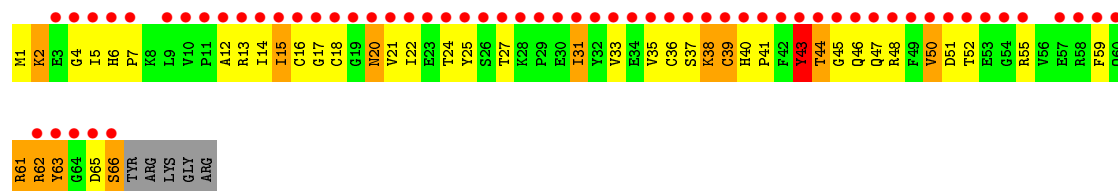
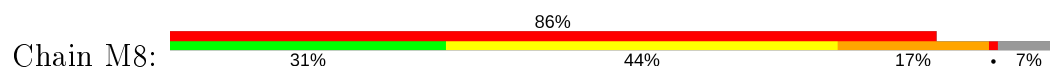


- Molecule 25: 30S ribosomal protein S5

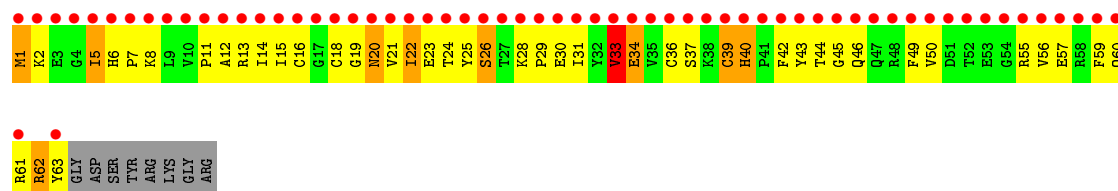
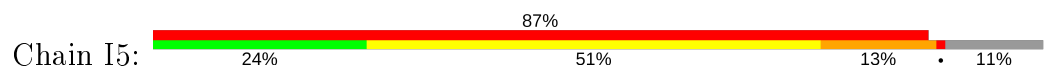




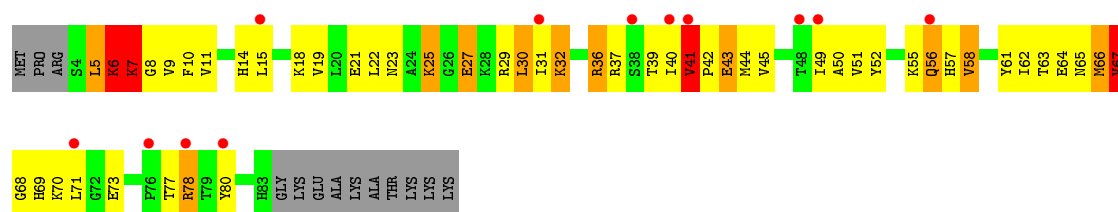
• Molecule 28: 50S ribosomal protein L31



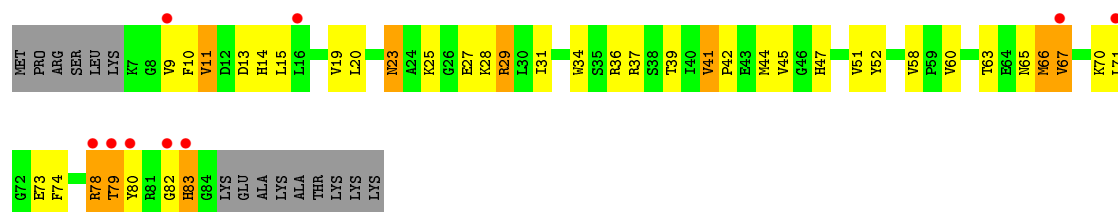
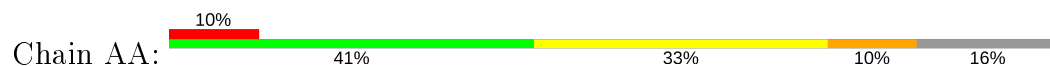
• Molecule 28: 50S ribosomal protein L31



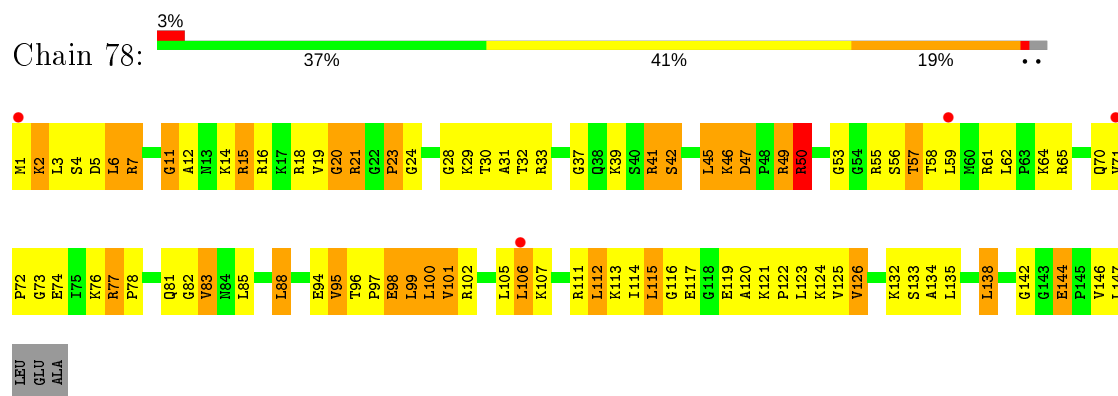
• Molecule 29: 30S ribosomal protein S19



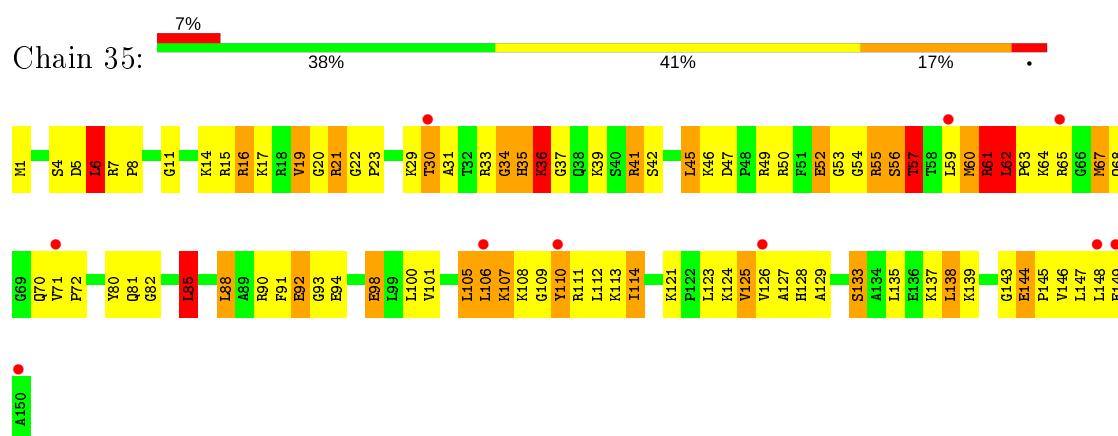
• Molecule 29: 30S ribosomal protein S19



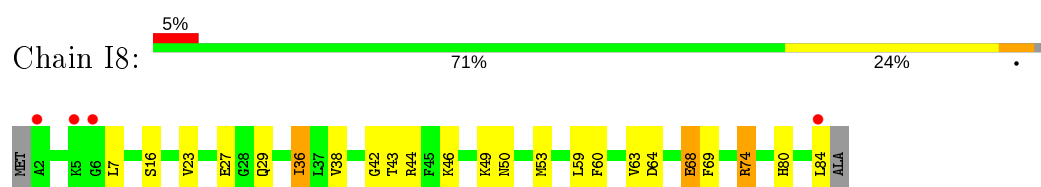
- Molecule 30: 50S ribosomal protein L15



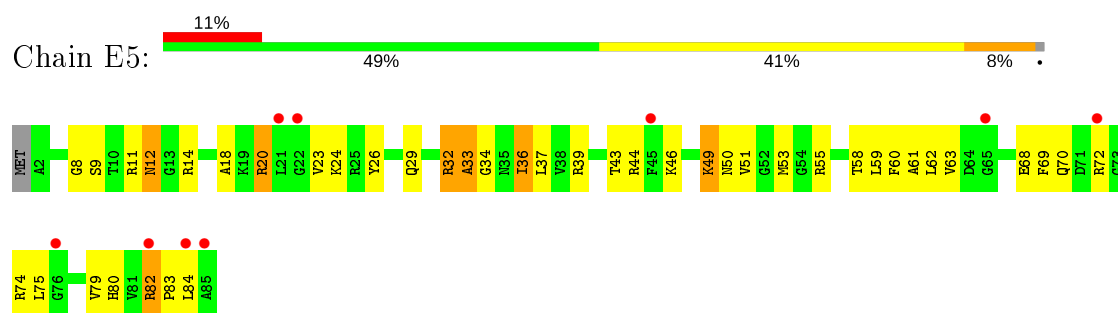
- Molecule 30: 50S ribosomal protein L15



- Molecule 31: 50S ribosomal protein L27

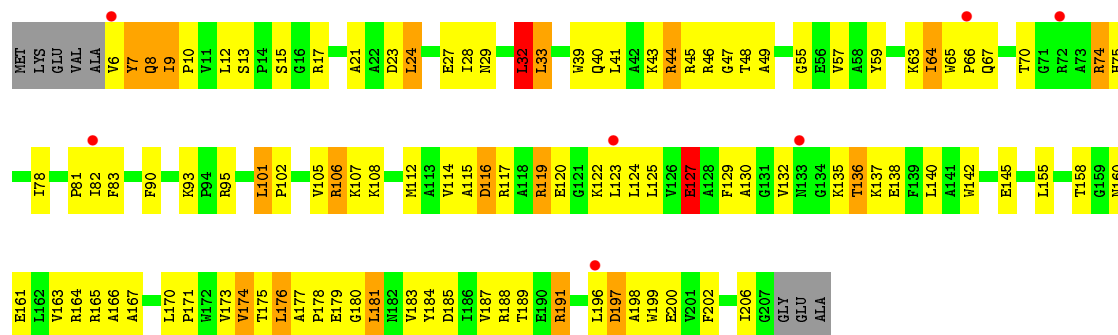


- Molecule 31: 50S ribosomal protein L27

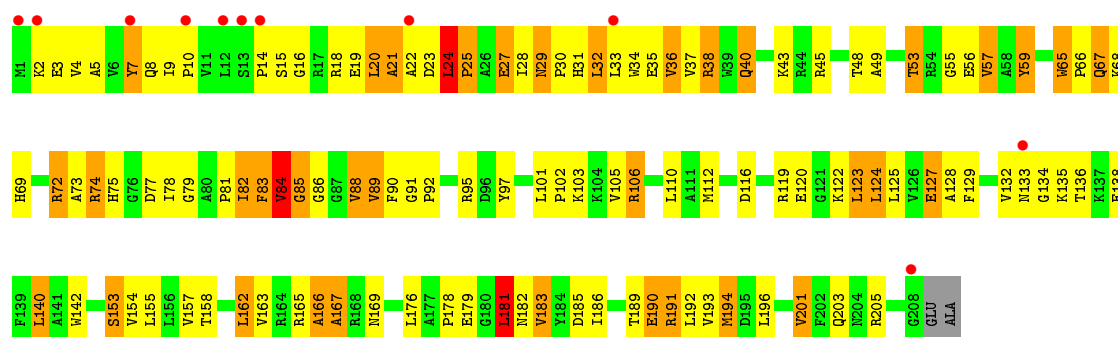
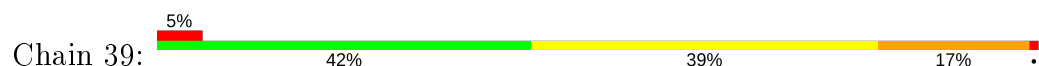


- Molecule 32: 50S ribosomal protein L4

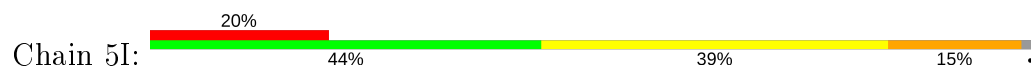




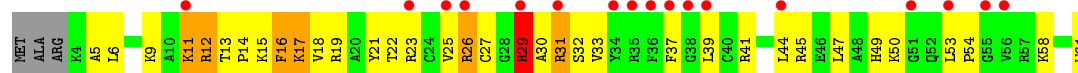
• Molecule 32: 50S ribosomal protein L4



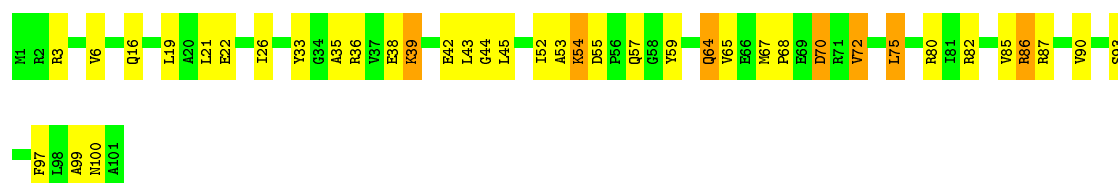
• Molecule 33: 30S ribosomal protein S14 type Z



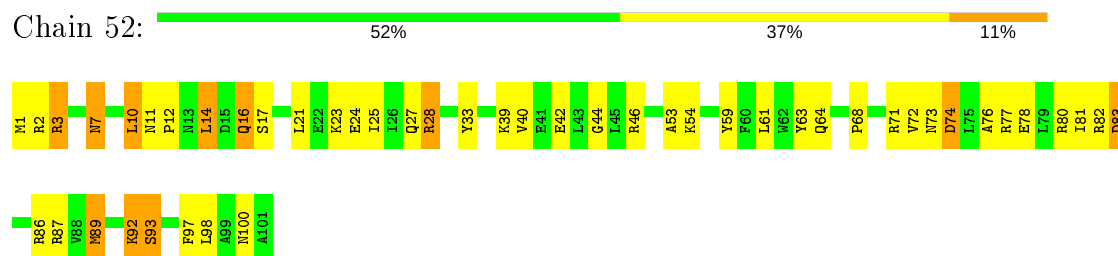
• Molecule 33: 30S ribosomal protein S14 type Z



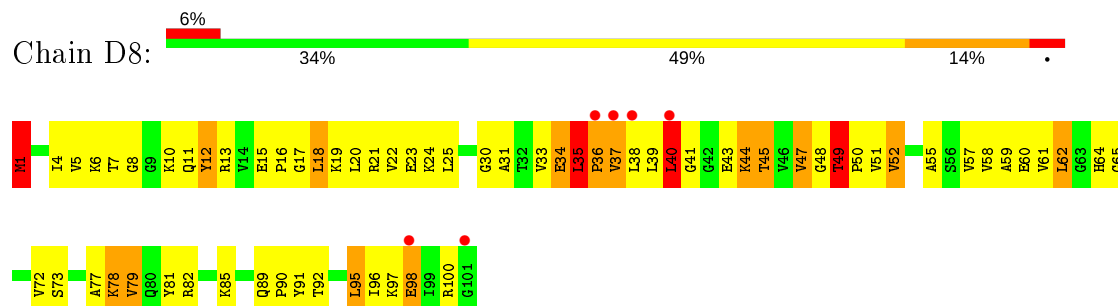
• Molecule 34: 30S ribosomal protein S6



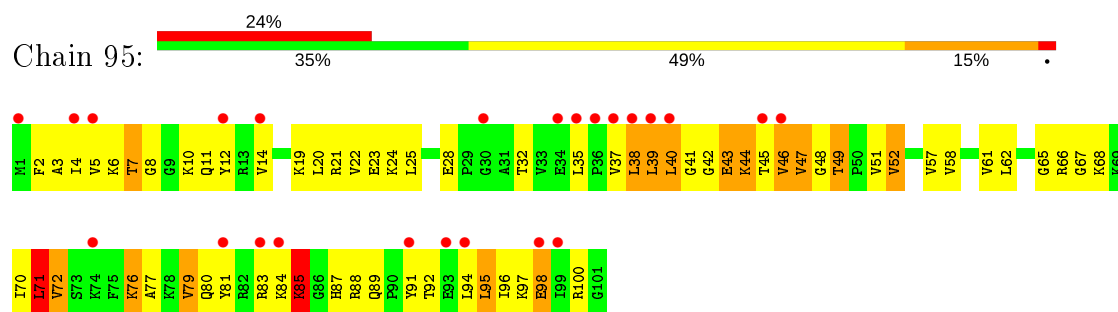
- Molecule 34: 30S ribosomal protein S6



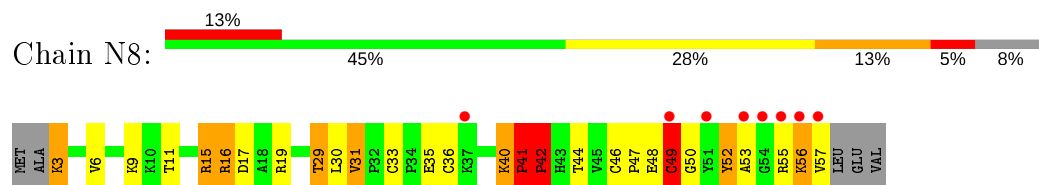
- Molecule 35: 50S ribosomal protein L21



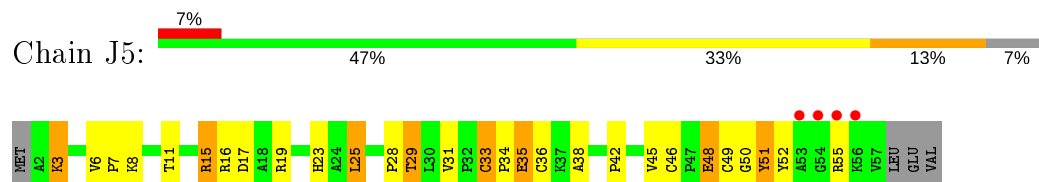
- Molecule 35: 50S ribosomal protein L21



- Molecule 36: 50S ribosomal protein L32

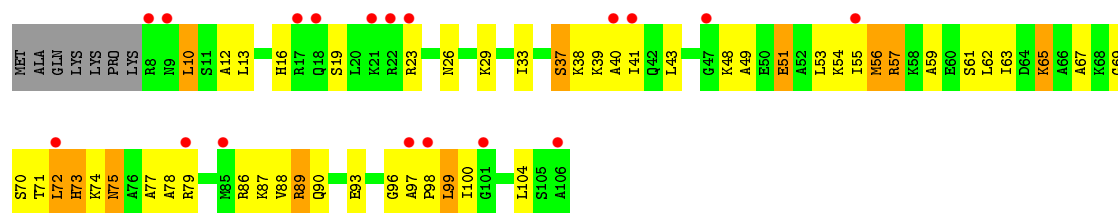


- Molecule 36: 50S ribosomal protein L32

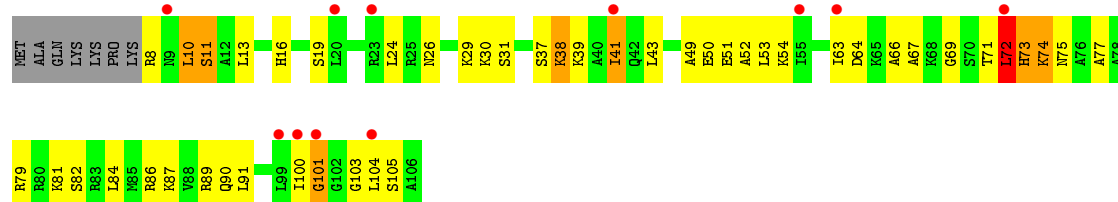


- Molecule 37: 30S ribosomal protein S20

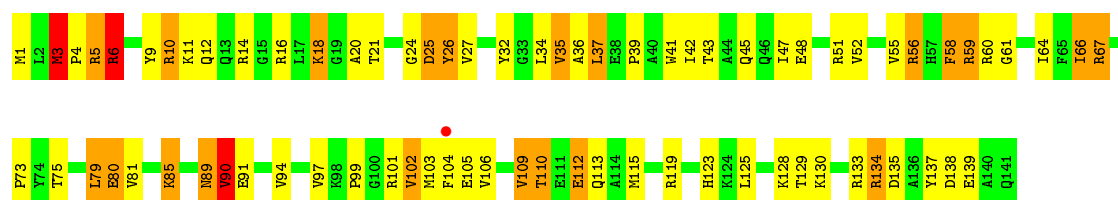




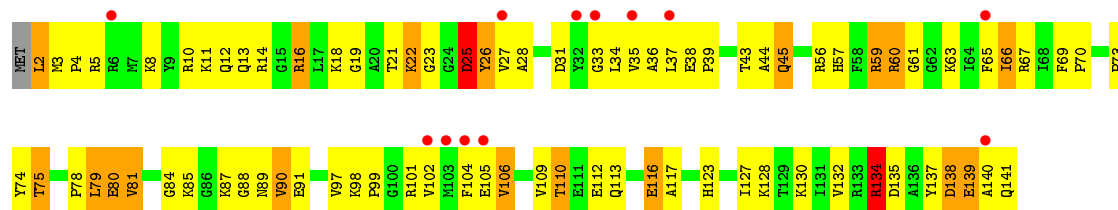
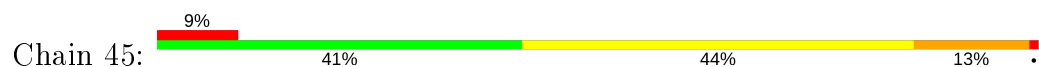
• Molecule 37: 30S ribosomal protein S20



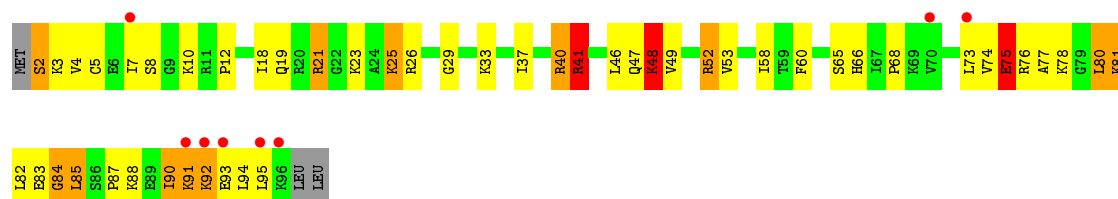
• Molecule 38: 50S ribosomal protein L16



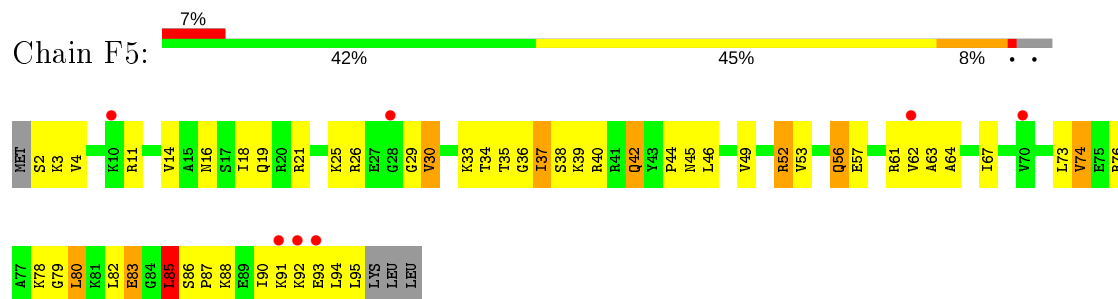
• Molecule 38: 50S ribosomal protein L16



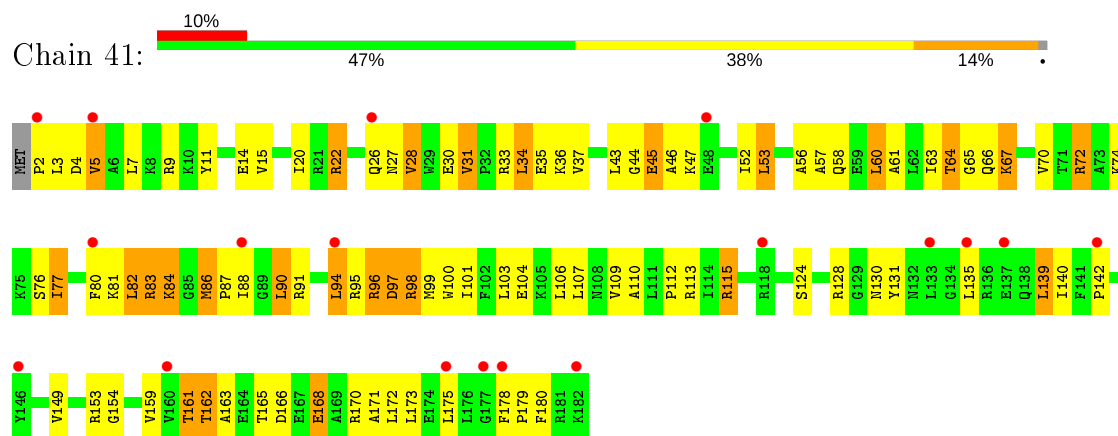
• Molecule 39: 50S ribosomal protein L28



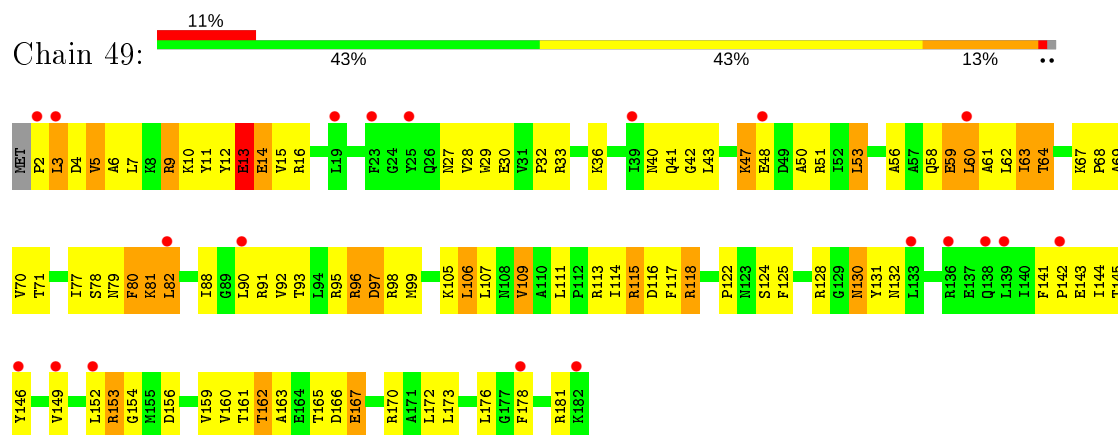
- Molecule 39: 50S ribosomal protein L28



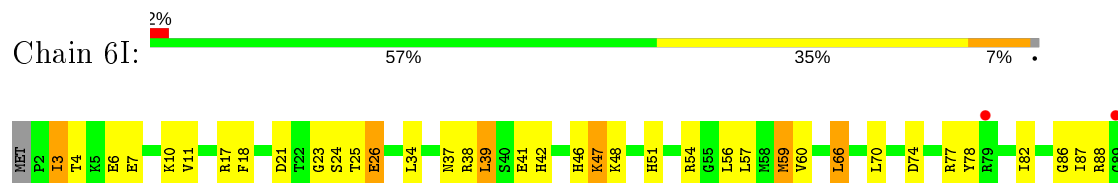
- Molecule 40: 50S ribosomal protein L5



- Molecule 40: 50S ribosomal protein L5

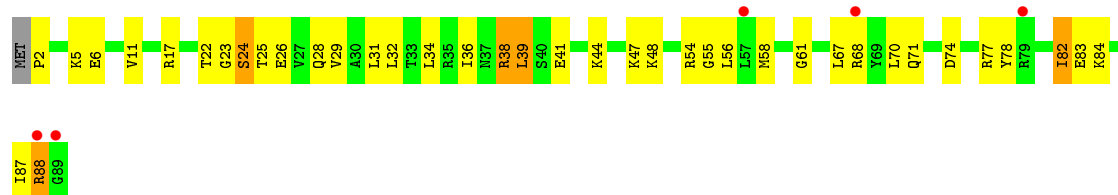


- Molecule 41: 30S ribosomal protein S15

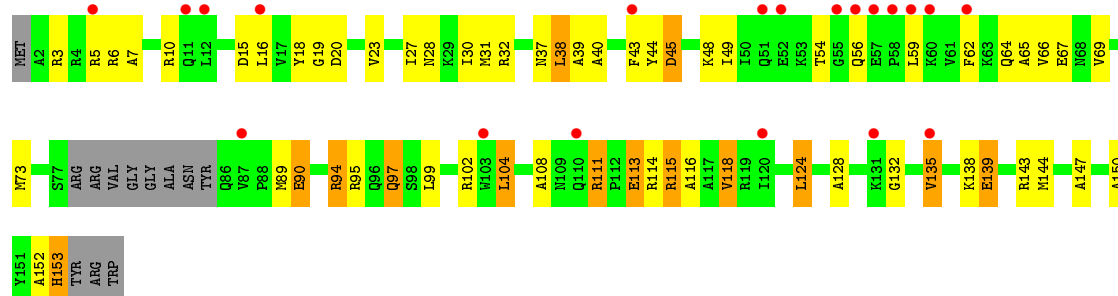


- Molecule 41: 30S ribosomal protein S15

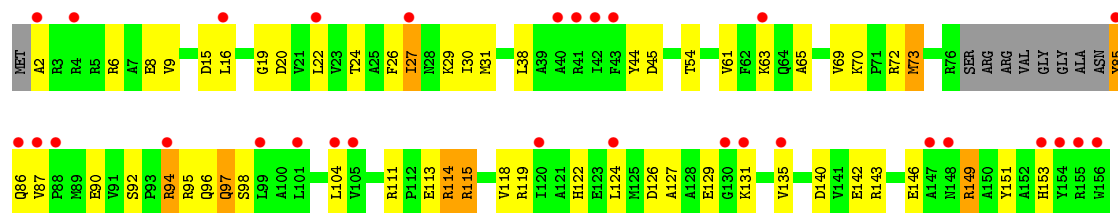




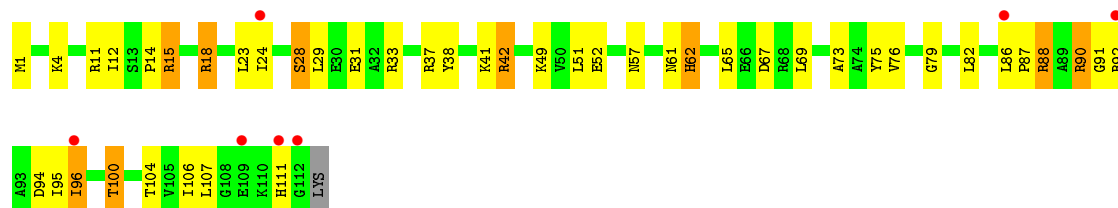
- Molecule 42: 30S ribosomal protein S7



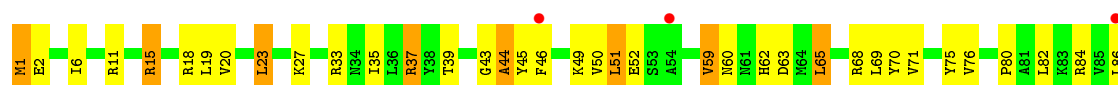
- Molecule 42: 30S ribosomal protein S7

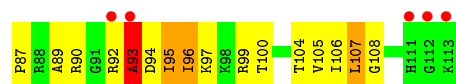


- Molecule 43: 50S ribosomal protein L22

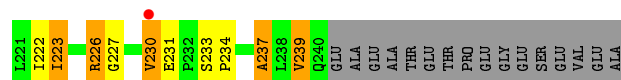
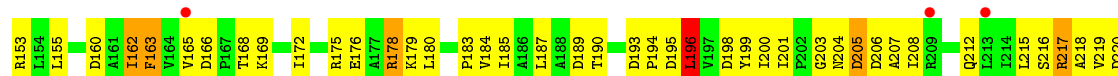
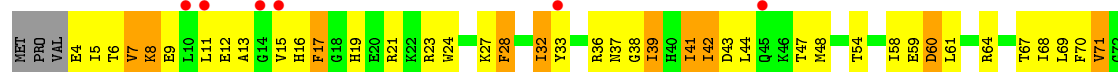
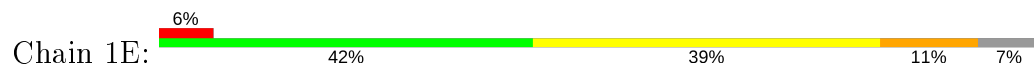


- Molecule 43: 50S ribosomal protein L22

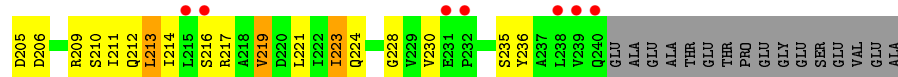
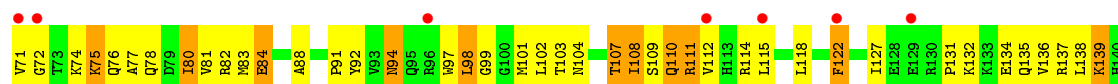




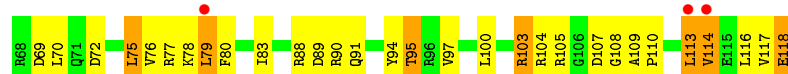
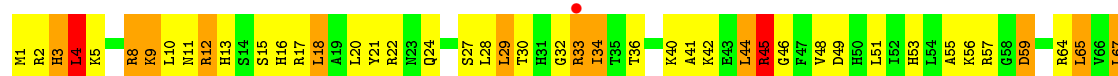
• Molecule 44: 30S ribosomal protein S2



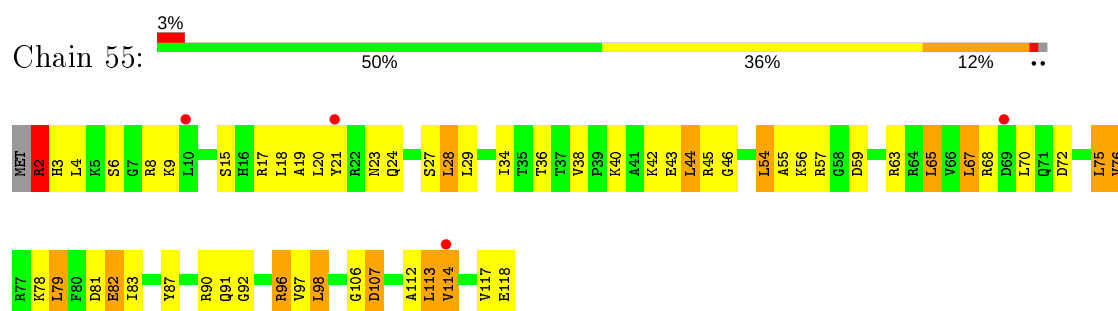
• Molecule 44: 30S ribosomal protein S2



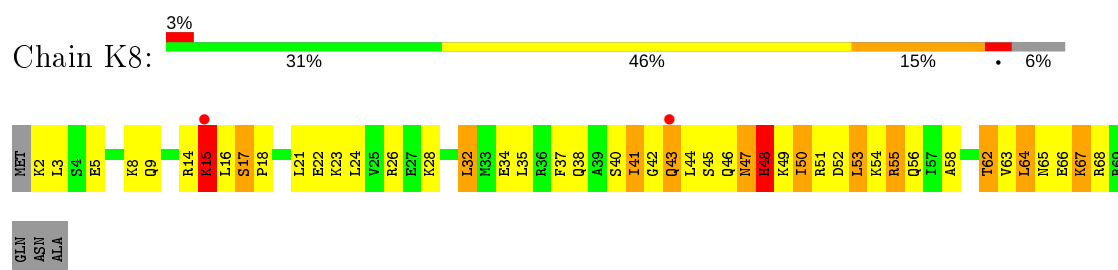
• Molecule 45: 50S ribosomal protein L17



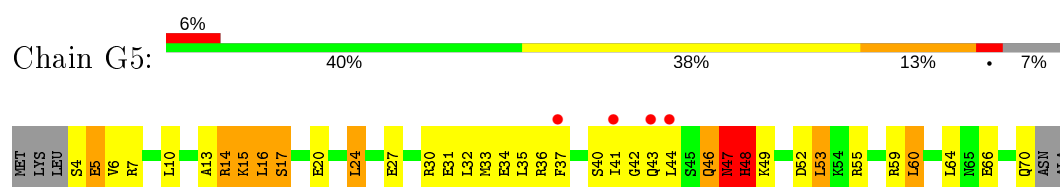
- Molecule 45: 50S ribosomal protein L17



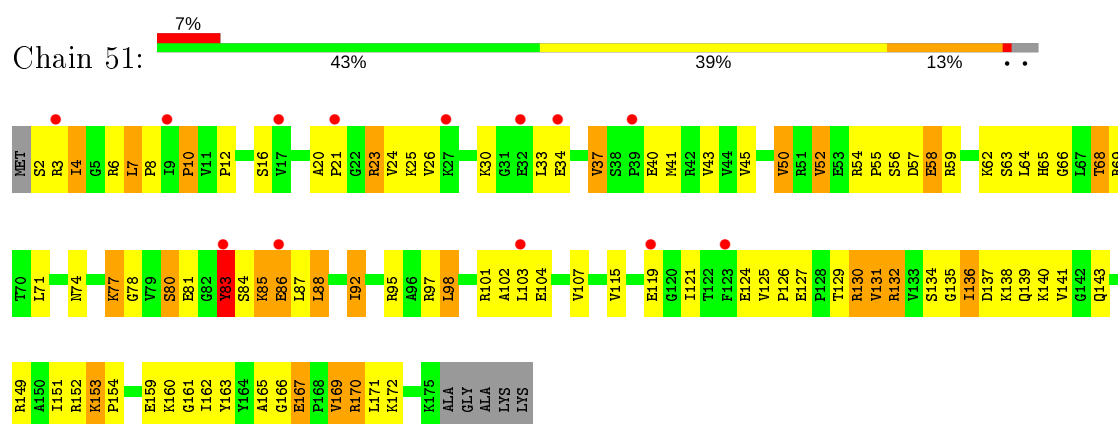
- Molecule 46: 50S ribosomal protein L29



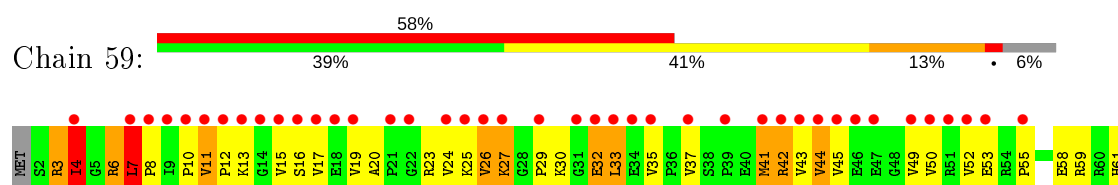
- Molecule 46: 50S ribosomal protein L29

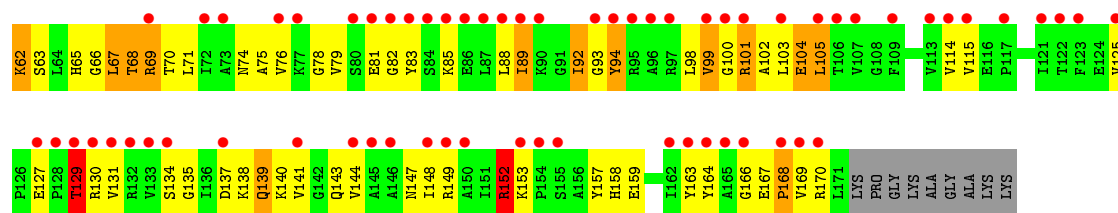


- Molecule 47: 50S ribosomal protein L6

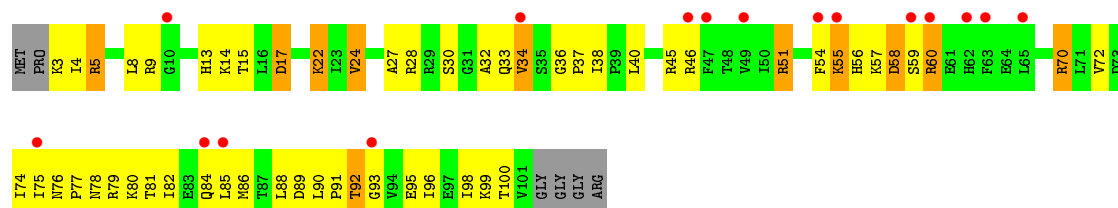


- Molecule 47: 50S ribosomal protein L6

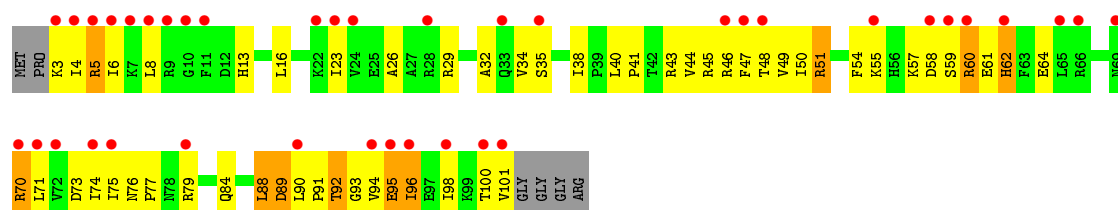




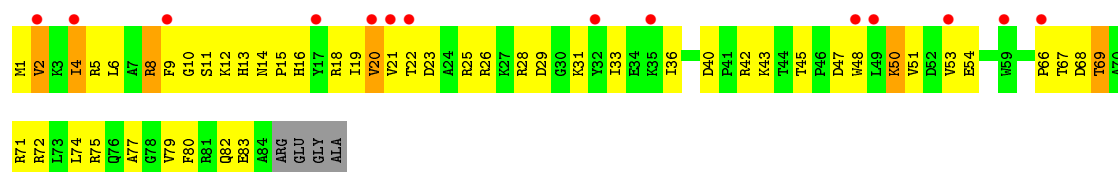
• Molecule 48: 30S ribosomal protein S10



• Molecule 48: 30S ribosomal protein S10



• Molecule 49: 30S ribosomal protein S16

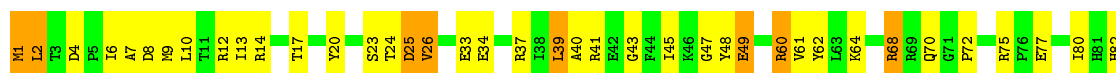


• Molecule 49: 30S ribosomal protein S16



• Molecule 50: 30S ribosomal protein S8

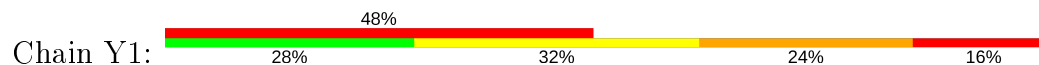




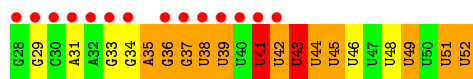
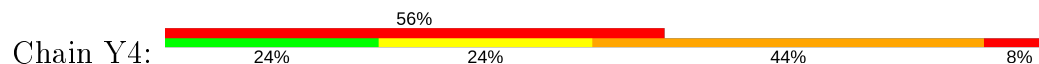
- Molecule 50: 30S ribosomal protein S8



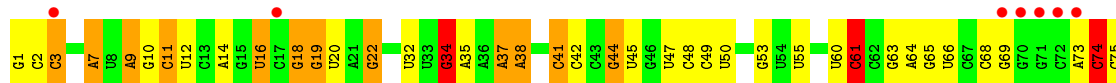
- Molecule 51: mRNA



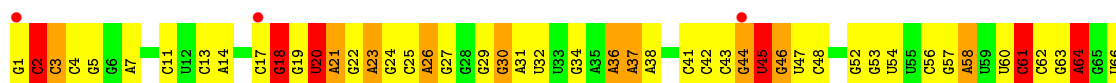
- Molecule 51: mRNA



- Molecule 52: tRNA-Phe

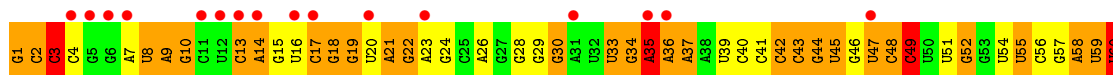
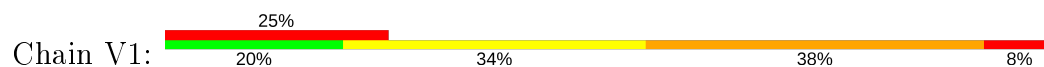


- Molecule 52: tRNA-Phe

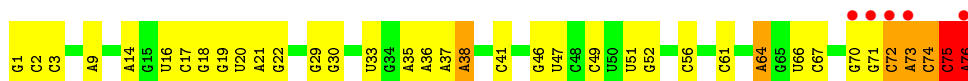




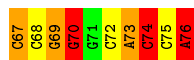
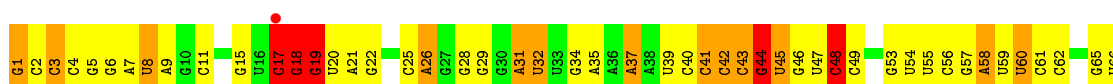
- Molecule 52: tRNA-Phe



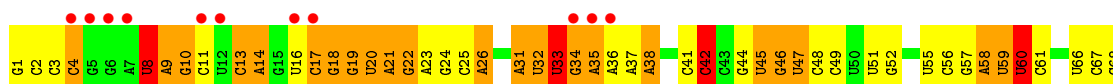
- Molecule 52: tRNA-Phe



- Molecule 52: tRNA-Phe



- Molecule 52: tRNA-Phe



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

²Theoretical 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, MG, 8UZ

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 168 planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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

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

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

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

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

The worst 5 of 7944 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:11:105:ILE:CD1	4:11:105:ILE:CG1	1.76	1.54
14:3E:9:CYS:CB	14:3E:9:CYS:SG	2.01	1.48
12:Q8:46:ARG:HH11	12:Q8:46:ARG:HB2	1.09	1.16
12:Q8:46:ARG:HB2	12:Q8:46:ARG:NH1	1.67	1.10
30:78:15:ARG:HB2	30:78:16:ARG:HB2	1.29	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

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

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

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1I	240	ALA
6	2A	48	ILE
4	19	237	GLU
12	Q8	51	ALA
14	3E	31	CYS

5.3.2 Protein sidechains ⓘ

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

resolution.

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

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

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

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

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

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

Mol	Chain	Res	Type
23	29	76	ARG
30	35	4	SER
3	F8	49	VAL
24	4A	66	LEU
30	78	147	LEU

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

Mol	Chain	Res	Type
35	D8	80	GLN
38	45	57	HIS
3	F8	31	HIS
32	39	203	GLN
14	32	161	ASN

5.3.3 RNA ⓘ

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

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

5 of 2115 RNA backbone outliers are listed below:

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

5 of 190 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	1H	1070	G
15	1H	1925	A
52	X1	45	U
15	1H	1109	U
15	1H	1445	U

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1656 ligands modelled in this entry, 1652 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	8UZ	13	2202	54	35,35,35	0.34	0	49,52,52	0.90	2 (4%)
53	8UZ	1G	2201	-	35,35,35	0.33	0	49,52,52	0.90	1 (2%)
53	8UZ	1G	2202	54	35,35,35	0.17	0	49,52,52	0.77	2 (4%)
53	8UZ	13	2201	-	35,35,35	0.44	0	49,52,52	1.25	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	8UZ	13	2202	54	-	2/12/72/72	0/3/3/3
53	8UZ	1G	2201	-	-	3/12/72/72	0/3/3/3
53	8UZ	1G	2202	54	-	3/12/72/72	0/3/3/3
53	8UZ	13	2201	-	-	0/12/72/72	0/3/3/3

There are no bond length outliers.

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

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

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

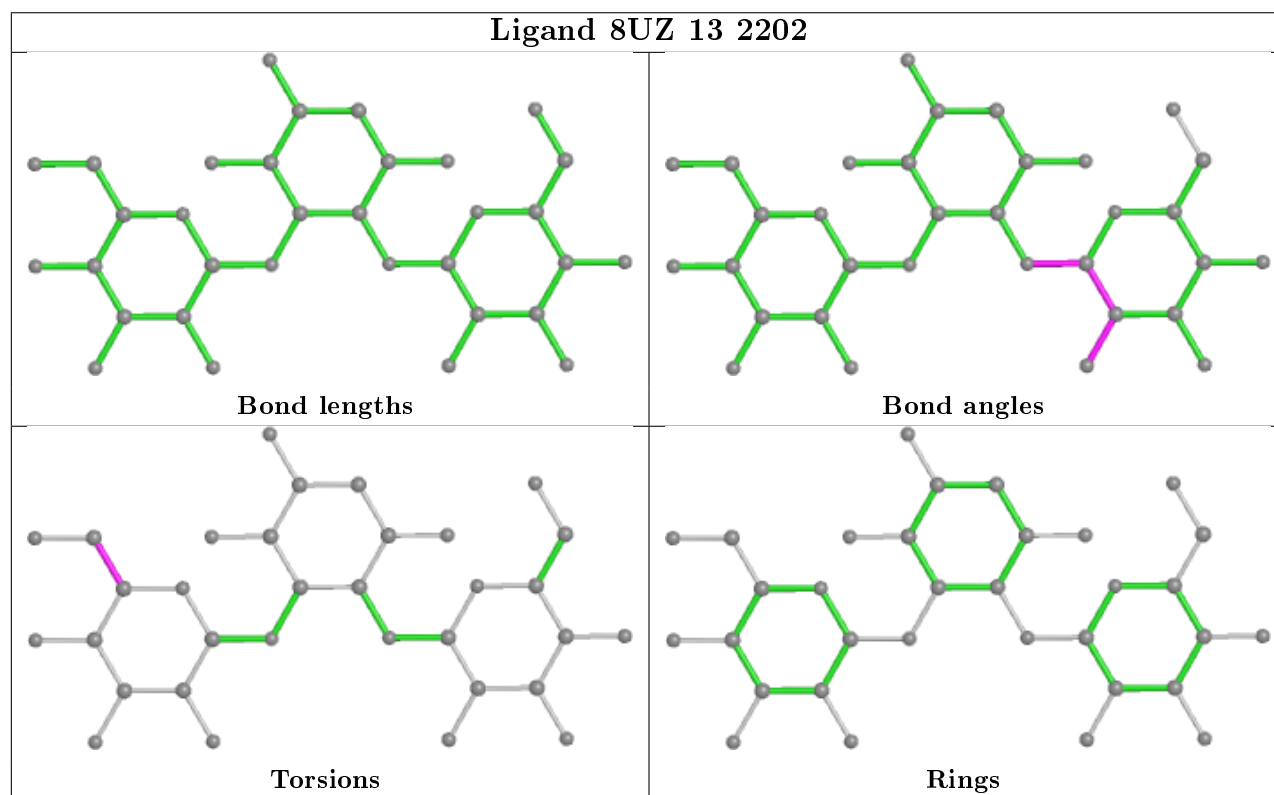
Mol	Chain	Res	Type	Atoms
53	1G	2202	8UZ	N-C-C1-C17
53	1G	2202	8UZ	N-C-C1-O
53	13	2202	8UZ	C12-C10-C11-O5
53	13	2202	8UZ	O4-C10-C11-O5
53	1G	2201	8UZ	N-C-C1-O

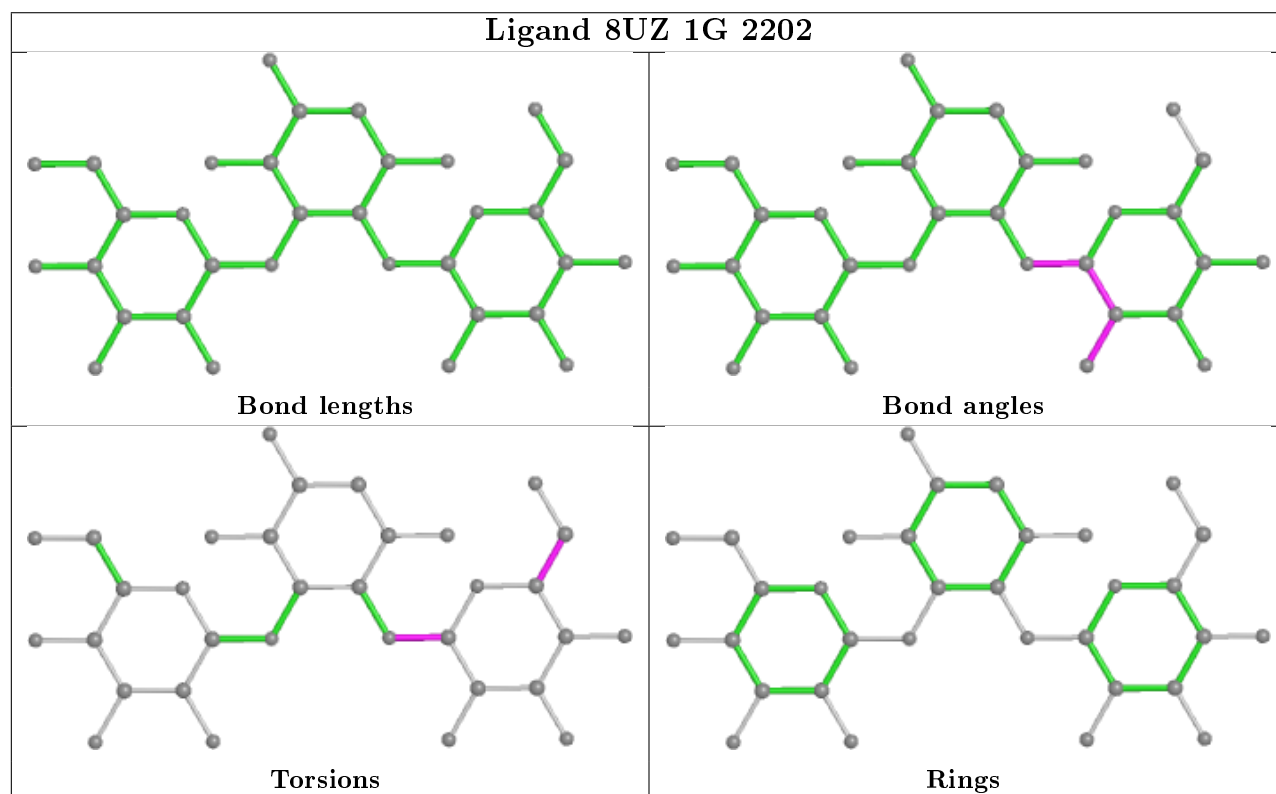
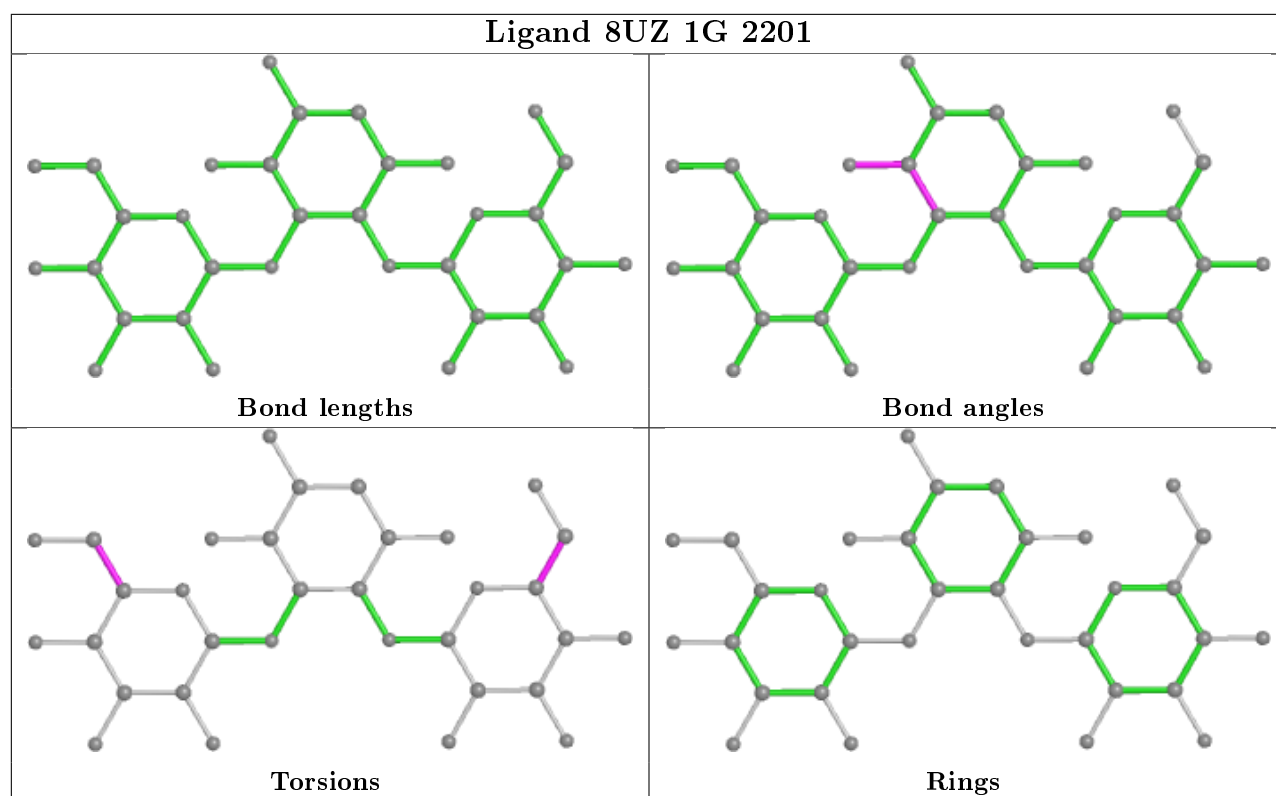
There are no ring outliers.

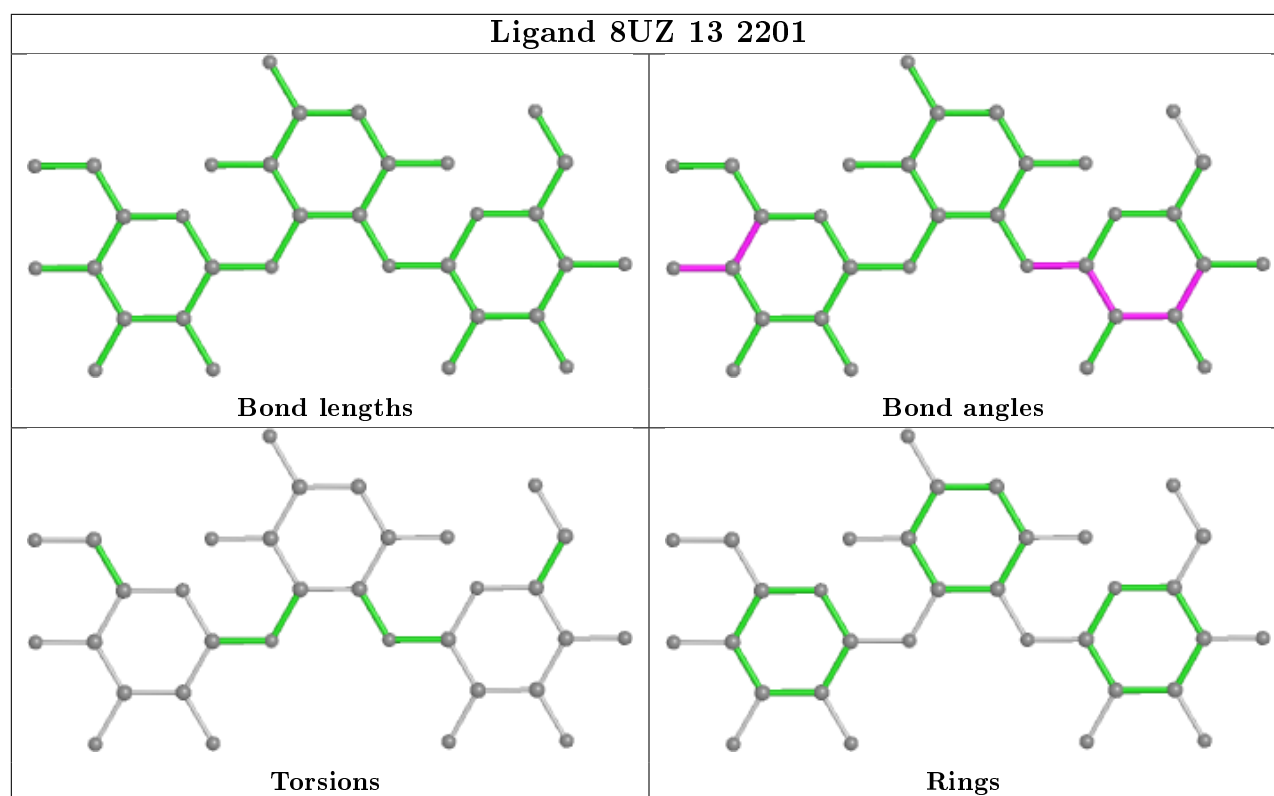
2 monomers are involved in 4 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

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

The worst 5 of 1557 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
54	MG	14	3092	1/1	0.18	0.28	44,44,44,44	0
54	MG	1J	208	1/1	0.32	0.18	71,71,71,71	0
54	MG	14	3460	1/1	0.44	0.51	91,91,91,91	0
54	MG	14	3068	1/1	0.47	0.14	77,77,77,77	0
54	MG	13	2317	1/1	0.48	0.24	69,69,69,69	0
54	MG	13	2338	1/1	0.49	0.37	69,69,69,69	0
54	MG	1G	2315	1/1	0.49	0.20	93,93,93,93	0
54	MG	E5	202	1/1	0.51	0.22	60,60,60,60	0
54	MG	14	3053	1/1	0.52	0.13	67,67,67,67	0
54	MG	14	3328	1/1	0.53	0.22	84,84,84,84	0
54	MG	14	3465	1/1	0.54	0.34	92,92,92,92	0
54	MG	11	303	1/1	0.55	0.29	79,79,79,79	0
54	MG	14	3320	1/1	0.56	0.30	59,59,59,59	0
54	MG	13	2356	1/1	0.56	0.20	67,67,67,67	0
54	MG	14	3075	1/1	0.56	0.13	63,63,63,63	0
54	MG	14	3091	1/1	0.56	0.08	82,82,82,82	0
54	MG	14	3333	1/1	0.57	0.24	61,61,61,61	0
54	MG	1H	3424	1/1	0.58	0.17	59,59,59,59	0
54	MG	14	3088	1/1	0.58	0.27	59,59,59,59	0
54	MG	1H	3042	1/1	0.58	0.11	33,33,33,33	0
54	MG	13	2234	1/1	0.59	0.28	84,84,84,84	0
54	MG	14	3192	1/1	0.59	0.24	66,66,66,66	0
54	MG	1G	2347	1/1	0.60	0.17	74,74,74,74	0
54	MG	1H	3495	1/1	0.60	0.21	59,59,59,59	0
54	MG	14	3314	1/1	0.60	0.28	104,104,104,104	0
54	MG	1H	3280	1/1	0.60	0.35	46,46,46,46	0
54	MG	14	3221	1/1	0.60	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3367	1/1	0.61	0.64	51,51,51,51	0
54	MG	14	3393	1/1	0.61	0.23	71,71,71,71	0
54	MG	1H	3082	1/1	0.61	0.34	57,57,57,57	0
54	MG	13	2376	1/1	0.62	0.23	75,75,75,75	0
54	MG	14	3543	1/1	0.63	0.31	59,59,59,59	0
54	MG	1H	3463	1/1	0.63	0.32	60,60,60,60	0
54	MG	1H	3365	1/1	0.63	0.23	63,63,63,63	0
54	MG	1G	2372	1/1	0.63	0.19	67,67,67,67	0
54	MG	13	2281	1/1	0.64	0.23	61,61,61,61	0
54	MG	1G	2309	1/1	0.64	0.17	75,75,75,75	0
54	MG	1G	2338	1/1	0.64	0.14	72,72,72,72	0
54	MG	X1	105	1/1	0.64	0.43	79,79,79,79	0
54	MG	14	3265	1/1	0.65	0.34	64,64,64,64	0
54	MG	13	2314	1/1	0.65	0.22	67,67,67,67	0
54	MG	14	3548	1/1	0.65	0.28	53,53,53,53	0
54	MG	X1	104	1/1	0.66	0.14	79,79,79,79	0
54	MG	X4	105	1/1	0.66	0.30	83,83,83,83	0
54	MG	13	2333	1/1	0.67	0.17	86,86,86,86	0
54	MG	13	2227	1/1	0.67	0.26	55,55,55,55	0
54	MG	1H	3478	1/1	0.67	0.16	52,52,52,52	0
54	MG	1H	3066	1/1	0.67	0.07	64,64,64,64	0
54	MG	1G	2273	1/1	0.67	0.20	69,69,69,69	0
54	MG	W4	104	1/1	0.68	0.37	124,124,124,124	0
54	MG	58	201	1/1	0.68	0.46	88,88,88,88	0
54	MG	1H	3254	1/1	0.68	0.22	47,47,47,47	0
54	MG	1H	3345	1/1	0.68	0.29	45,45,45,45	0
54	MG	1H	3516	1/1	0.68	0.22	62,62,62,62	0
54	MG	1H	3027	1/1	0.68	0.21	51,51,51,51	0
54	MG	85	201	1/1	0.68	0.34	90,90,90,90	0
54	MG	1H	3572	1/1	0.69	0.17	60,60,60,60	0
54	MG	1H	3576	1/1	0.69	0.24	64,64,64,64	0
54	MG	14	3014	1/1	0.69	0.17	41,41,41,41	0
54	MG	14	3447	1/1	0.69	0.19	59,59,59,59	0
54	MG	14	3539	1/1	0.69	0.38	72,72,72,72	0
54	MG	14	3060	1/1	0.69	0.14	57,57,57,57	0
54	MG	14	3383	1/1	0.69	0.38	66,66,66,66	0
54	MG	1G	2272	1/1	0.69	0.22	66,66,66,66	0
54	MG	1H	3319	1/1	0.69	0.23	62,62,62,62	0
54	MG	1H	3061	1/1	0.69	0.10	68,68,68,68	0
54	MG	14	3409	1/1	0.69	0.23	51,51,51,51	0
54	MG	1H	3579	1/1	0.70	0.21	72,72,72,72	0
54	MG	14	3070	1/1	0.70	0.32	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3231	1/1	0.70	0.49	77,77,77,77	0
54	MG	1H	3057	1/1	0.70	0.15	46,46,46,46	0
54	MG	1H	3197	1/1	0.70	0.22	46,46,46,46	0
54	MG	1G	2346	1/1	0.71	0.12	69,69,69,69	0
54	MG	14	3482	1/1	0.71	0.17	58,58,58,58	0
54	MG	14	3423	1/1	0.71	0.21	68,68,68,68	0
54	MG	14	3483	1/1	0.71	0.23	55,55,55,55	0
54	MG	14	3549	1/1	0.71	0.26	72,72,72,72	0
54	MG	5I	102	1/1	0.71	0.15	72,72,72,72	0
54	MG	14	3038	1/1	0.71	0.12	54,54,54,54	0
54	MG	1H	3304	1/1	0.71	0.28	77,77,77,77	0
54	MG	25	201	1/1	0.71	0.22	79,79,79,79	0
54	MG	13	2367	1/1	0.71	0.18	58,58,58,58	0
54	MG	1H	3567	1/1	0.71	0.26	65,65,65,65	0
54	MG	1H	3490	1/1	0.72	0.21	45,45,45,45	0
54	MG	1H	3368	1/1	0.72	0.21	57,57,57,57	0
54	MG	16	214	1/1	0.72	0.38	66,66,66,66	0
54	MG	1H	3318	1/1	0.72	0.39	58,58,58,58	0
54	MG	1H	3553	1/1	0.72	0.20	46,46,46,46	0
54	MG	7A	101	1/1	0.72	0.21	70,70,70,70	0
54	MG	1H	3052	1/1	0.72	0.10	36,36,36,36	0
54	MG	14	3118	1/1	0.72	0.18	62,62,62,62	0
54	MG	1H	3071	1/1	0.72	0.10	102,102,102,102	0
54	MG	14	3417	1/1	0.72	0.32	51,51,51,51	0
54	MG	1H	3010	1/1	0.72	0.09	58,58,58,58	0
54	MG	16	204	1/1	0.72	0.22	63,63,63,63	0
54	MG	13	2287	1/1	0.72	0.45	89,89,89,89	0
54	MG	14	3308	1/1	0.72	0.43	93,93,93,93	0
54	MG	1H	3354	1/1	0.72	0.25	71,71,71,71	0
54	MG	1H	3491	1/1	0.73	0.25	55,55,55,55	0
54	MG	14	3414	1/1	0.73	0.27	67,67,67,67	0
54	MG	1H	3286	1/1	0.73	0.52	79,79,79,79	0
54	MG	14	3291	1/1	0.73	0.18	49,49,49,49	0
54	MG	1H	3413	1/1	0.73	0.25	77,77,77,77	0
54	MG	14	3364	1/1	0.73	0.43	67,67,67,67	0
54	MG	1H	3093	1/1	0.73	0.21	54,54,54,54	0
54	MG	14	3083	1/1	0.73	0.10	66,66,66,66	0
54	MG	13	2342	1/1	0.73	0.19	73,73,73,73	0
54	MG	X1	103	1/1	0.73	0.11	76,76,76,76	0
54	MG	14	3220	1/1	0.73	0.25	70,70,70,70	0
54	MG	1H	3167	1/1	0.73	0.27	40,40,40,40	0
54	MG	1H	3544	1/1	0.73	0.19	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3040	1/1	0.73	0.13	49,49,49,49	0
54	MG	13	2372	1/1	0.73	0.45	87,87,87,87	0
54	MG	14	3397	1/1	0.73	0.34	57,57,57,57	0
54	MG	1G	2303	1/1	0.73	0.33	72,72,72,72	0
54	MG	88	305	1/1	0.73	0.23	76,76,76,76	0
54	MG	1G	2379	1/1	0.73	0.22	85,85,85,85	0
54	MG	13	2235	1/1	0.73	0.27	81,81,81,81	0
54	MG	1H	3029	1/1	0.73	0.13	52,52,52,52	0
54	MG	1G	2370	1/1	0.74	0.25	59,59,59,59	0
54	MG	29	304	1/1	0.74	0.31	67,67,67,67	0
54	MG	1H	3064	1/1	0.74	0.20	47,47,47,47	0
54	MG	14	3342	1/1	0.74	0.18	66,66,66,66	0
54	MG	1H	3591	1/1	0.74	0.26	62,62,62,62	0
54	MG	1G	2210	1/1	0.74	0.21	67,67,67,67	0
54	MG	1H	3059	1/1	0.74	0.15	51,51,51,51	0
54	MG	1G	2287	1/1	0.74	0.18	77,77,77,77	0
54	MG	1H	3428	1/1	0.74	0.22	40,40,40,40	0
54	MG	1H	3346	1/1	0.74	0.64	61,61,61,61	0
54	MG	14	3353	1/1	0.74	0.13	82,82,82,82	0
54	MG	14	3451	1/1	0.74	0.20	52,52,52,52	0
54	MG	14	3046	1/1	0.74	0.05	71,71,71,71	0
54	MG	1H	3376	1/1	0.74	0.25	44,44,44,44	0
54	MG	14	3403	1/1	0.74	0.36	63,63,63,63	0
54	MG	14	3051	1/1	0.74	0.17	71,71,71,71	0
54	MG	14	3411	1/1	0.75	0.29	66,66,66,66	0
54	MG	14	3223	1/1	0.75	0.28	58,58,58,58	0
54	MG	1H	3011	1/1	0.75	0.17	46,46,46,46	0
54	MG	14	3306	1/1	0.75	0.21	68,68,68,68	0
54	MG	1G	2269	1/1	0.75	0.54	103,103,103,103	0
54	MG	1H	3561	1/1	0.75	0.46	72,72,72,72	0
54	MG	1G	2212	1/1	0.75	0.08	104,104,104,104	0
54	MG	1H	3068	1/1	0.75	0.09	64,64,64,64	0
54	MG	1H	3396	1/1	0.75	0.31	75,75,75,75	0
54	MG	14	3406	1/1	0.75	0.16	79,79,79,79	0
54	MG	14	3448	1/1	0.75	0.21	60,60,60,60	0
54	MG	14	3090	1/1	0.75	0.14	51,51,51,51	0
54	MG	1G	2288	1/1	0.75	0.45	84,84,84,84	0
54	MG	1H	3355	1/1	0.75	0.14	57,57,57,57	0
54	MG	1H	3415	1/1	0.76	0.16	61,61,61,61	0
54	MG	1H	3142	1/1	0.76	0.21	64,64,64,64	0
54	MG	14	3325	1/1	0.76	0.28	65,65,65,65	0
54	MG	1H	3521	1/1	0.76	0.30	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3040	1/1	0.76	0.16	70,70,70,70	0
54	MG	16	201	1/1	0.76	0.15	69,69,69,69	0
54	MG	14	3386	1/1	0.76	0.17	47,47,47,47	0
54	MG	1H	3379	1/1	0.76	0.13	64,64,64,64	0
54	MG	1H	3060	1/1	0.76	0.12	45,45,45,45	0
54	MG	14	3225	1/1	0.76	0.26	57,57,57,57	0
54	MG	1H	3331	1/1	0.76	0.33	50,50,50,50	0
54	MG	14	3522	1/1	0.76	0.15	54,54,54,54	0
54	MG	13	2377	1/1	0.76	0.21	81,81,81,81	0
54	MG	14	3433	1/1	0.76	0.26	67,67,67,67	0
54	MG	1G	2253	1/1	0.76	0.51	87,87,87,87	0
54	MG	14	3400	1/1	0.76	0.18	71,71,71,71	0
54	MG	1G	2326	1/1	0.76	0.33	84,84,84,84	0
54	MG	1H	3540	1/1	0.76	0.30	82,82,82,82	0
54	MG	1G	2214	1/1	0.77	0.14	74,74,74,74	0
54	MG	14	3479	1/1	0.77	0.23	56,56,56,56	0
54	MG	13	2350	1/1	0.77	0.20	53,53,53,53	0
54	MG	14	3251	1/1	0.77	0.52	88,88,88,88	0
54	MG	1G	2228	1/1	0.77	0.22	71,71,71,71	0
54	MG	13	2335	1/1	0.77	0.43	75,75,75,75	0
54	MG	1H	3085	1/1	0.77	0.16	45,45,45,45	0
54	MG	14	3123	1/1	0.77	0.34	45,45,45,45	0
54	MG	14	3276	1/1	0.77	0.45	45,45,45,45	0
54	MG	14	3485	1/1	0.77	0.49	73,73,73,73	0
54	MG	1H	3388	1/1	0.77	0.29	62,62,62,62	0
54	MG	1H	3081	1/1	0.77	0.33	49,49,49,49	0
54	MG	1H	3393	1/1	0.77	0.24	51,51,51,51	0
54	MG	1H	3492	1/1	0.77	0.53	84,84,84,84	0
54	MG	1H	3300	1/1	0.77	0.37	79,79,79,79	0
54	MG	13	2375	1/1	0.77	0.27	83,83,83,83	0
54	MG	14	3385	1/1	0.77	0.25	50,50,50,50	0
54	MG	1H	3358	1/1	0.77	0.24	49,49,49,49	0
54	MG	1G	2286	1/1	0.77	0.22	68,68,68,68	0
54	MG	14	3258	1/1	0.77	0.32	39,39,39,39	0
54	MG	13	2381	1/1	0.78	0.29	87,87,87,87	0
54	MG	13	2323	1/1	0.78	0.12	85,85,85,85	0
54	MG	1G	2262	1/1	0.78	0.22	87,87,87,87	0
54	MG	1G	2351	1/1	0.78	0.21	66,66,66,66	0
54	MG	P8	101	1/1	0.78	0.32	51,51,51,51	0
54	MG	14	3405	1/1	0.78	0.09	65,65,65,65	0
54	MG	13	2299	1/1	0.78	0.29	85,85,85,85	0
54	MG	35	201	1/1	0.78	0.21	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3584	1/1	0.78	0.25	54,54,54,54	0
54	MG	1H	3434	1/1	0.78	0.31	59,59,59,59	0
54	MG	X1	101	1/1	0.78	0.17	84,84,84,84	0
54	MG	1J	204	1/1	0.78	0.24	67,67,67,67	0
54	MG	13	2301	1/1	0.78	0.11	72,72,72,72	0
54	MG	1H	3590	1/1	0.78	0.46	67,67,67,67	0
54	MG	13	2307	1/1	0.78	0.45	77,77,77,77	0
54	MG	14	3542	1/1	0.78	0.14	65,65,65,65	0
54	MG	14	3481	1/1	0.78	0.20	82,82,82,82	0
54	MG	14	3517	1/1	0.78	0.26	65,65,65,65	0
54	MG	1H	3507	1/1	0.78	0.17	68,68,68,68	0
54	MG	1H	3440	1/1	0.78	0.18	39,39,39,39	0
54	MG	1H	3164	1/1	0.78	0.34	45,45,45,45	0
54	MG	13	2293	1/1	0.78	0.28	109,109,109,109	0
54	MG	1H	3438	1/1	0.78	0.18	54,54,54,54	0
54	MG	1J	205	1/1	0.78	0.36	64,64,64,64	0
54	MG	14	3368	1/1	0.78	0.21	50,50,50,50	0
54	MG	1H	3079	1/1	0.78	0.27	59,59,59,59	0
54	MG	14	3499	1/1	0.78	0.15	80,80,80,80	0
54	MG	14	3062	1/1	0.78	0.10	51,51,51,51	0
54	MG	14	3462	1/1	0.78	0.28	55,55,55,55	0
54	MG	1J	214	1/1	0.78	0.24	71,71,71,71	0
54	MG	14	3263	1/1	0.78	0.59	77,77,77,77	0
54	MG	1H	3287	1/1	0.79	0.15	59,59,59,59	0
54	MG	5E	201	1/1	0.79	0.20	66,66,66,66	0
54	MG	1G	2284	1/1	0.79	0.49	90,90,90,90	0
54	MG	14	3472	1/1	0.79	0.25	58,58,58,58	0
54	MG	13	2294	1/1	0.79	0.19	57,57,57,57	0
54	MG	14	3296	1/1	0.79	0.16	59,59,59,59	0
54	MG	88	303	1/1	0.79	0.19	56,56,56,56	0
54	MG	13	2364	1/1	0.79	0.15	69,69,69,69	0
54	MG	1H	3342	1/1	0.79	0.36	62,62,62,62	0
54	MG	14	3399	1/1	0.79	0.29	70,70,70,70	0
54	MG	13	2320	1/1	0.79	0.38	75,75,75,75	0
54	MG	1J	203	1/1	0.79	0.39	67,67,67,67	0
54	MG	13	2278	1/1	0.79	0.37	62,62,62,62	0
54	MG	14	3169	1/1	0.79	0.49	57,57,57,57	0
54	MG	14	3565	1/1	0.79	0.22	69,69,69,69	0
54	MG	1H	3067	1/1	0.79	0.19	42,42,42,42	0
54	MG	14	3346	1/1	0.79	0.16	83,83,83,83	0
54	MG	1H	3442	1/1	0.79	0.19	55,55,55,55	0
54	MG	14	3525	1/1	0.79	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3322	1/1	0.79	0.19	51,51,51,51	0
54	MG	14	3032	1/1	0.79	0.09	46,46,46,46	0
54	MG	14	3056	1/1	0.79	0.09	48,48,48,48	0
54	MG	1H	3211	1/1	0.79	0.14	50,50,50,50	0
54	MG	1H	3479	1/1	0.80	0.19	67,67,67,67	0
54	MG	14	3302	1/1	0.80	0.32	52,52,52,52	0
54	MG	1G	2330	1/1	0.80	0.17	93,93,93,93	0
54	MG	14	3504	1/1	0.80	0.24	71,71,71,71	0
54	MG	1G	2380	1/1	0.80	0.12	70,70,70,70	0
54	MG	1H	3383	1/1	0.80	0.38	88,88,88,88	0
54	MG	C5	202	1/1	0.80	0.55	70,70,70,70	0
54	MG	14	3008	1/1	0.80	0.10	53,53,53,53	0
54	MG	14	3279	1/1	0.80	0.23	66,66,66,66	0
54	MG	1G	2311	1/1	0.80	0.26	87,87,87,87	0
54	MG	1G	2356	1/1	0.80	0.10	74,74,74,74	0
54	MG	14	3521	1/1	0.80	0.10	58,58,58,58	0
54	MG	1G	2313	1/1	0.80	0.36	62,62,62,62	0
54	MG	14	3410	1/1	0.80	0.20	59,59,59,59	0
54	MG	14	3529	1/1	0.80	0.14	63,63,63,63	0
54	MG	13	2211	1/1	0.80	0.10	67,67,67,67	0
54	MG	1H	3058	1/1	0.80	0.08	39,39,39,39	0
54	MG	1H	3549	1/1	0.80	0.18	61,61,61,61	0
54	MG	1G	2341	1/1	0.80	0.22	86,86,86,86	0
54	MG	1H	3529	1/1	0.80	0.18	42,42,42,42	0
54	MG	13	2297	1/1	0.80	0.32	62,62,62,62	0
54	MG	X4	106	1/1	0.80	0.23	73,73,73,73	0
54	MG	14	3501	1/1	0.80	0.14	47,47,47,47	0
54	MG	14	3394	1/1	0.80	0.57	54,54,54,54	0
54	MG	14	3357	1/1	0.80	0.17	53,53,53,53	0
54	MG	14	3222	1/1	0.80	0.41	70,70,70,70	0
54	MG	1H	3144	1/1	0.80	0.26	47,47,47,47	0
54	MG	1G	2355	1/1	0.80	0.23	76,76,76,76	0
54	MG	1G	2319	1/1	0.80	0.22	77,77,77,77	0
54	MG	14	3269	1/1	0.81	0.11	55,55,55,55	0
54	MG	1G	2366	1/1	0.81	0.21	100,100,100,100	0
54	MG	14	3241	1/1	0.81	0.19	72,72,72,72	0
54	MG	1H	3054	1/1	0.81	0.11	46,46,46,46	0
54	MG	1H	3447	1/1	0.81	0.15	59,59,59,59	0
54	MG	1H	3378	1/1	0.81	0.23	51,51,51,51	0
54	MG	1H	3140	1/1	0.81	0.19	42,42,42,42	0
54	MG	1H	3153	1/1	0.81	0.43	45,45,45,45	0
54	MG	14	3247	1/1	0.81	0.41	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2292	1/1	0.81	0.17	67,67,67,67	0
54	MG	13	2288	1/1	0.81	0.11	80,80,80,80	0
54	MG	14	3177	1/1	0.81	0.43	67,67,67,67	0
54	MG	14	3059	1/1	0.81	0.07	58,58,58,58	0
54	MG	1G	2295	1/1	0.81	0.23	75,75,75,75	0
54	MG	13	2339	1/1	0.81	0.16	79,79,79,79	0
54	MG	14	3453	1/1	0.81	0.21	44,44,44,44	0
54	MG	14	3315	1/1	0.81	0.21	62,62,62,62	0
54	MG	1H	3460	1/1	0.81	0.33	61,61,61,61	0
54	MG	14	3250	1/1	0.81	0.57	83,83,83,83	0
54	MG	14	3512	1/1	0.81	0.39	57,57,57,57	0
54	MG	14	3204	1/1	0.81	0.39	59,59,59,59	0
54	MG	1G	2293	1/1	0.81	0.23	83,83,83,83	0
54	MG	1H	3307	1/1	0.81	0.23	31,31,31,31	0
54	MG	1H	3226	1/1	0.81	0.29	43,43,43,43	0
54	MG	14	3057	1/1	0.81	0.19	48,48,48,48	0
54	MG	13	2321	1/1	0.81	0.30	81,81,81,81	0
54	MG	13	2316	1/1	0.81	0.37	74,74,74,74	0
54	MG	14	3343	1/1	0.81	0.19	62,62,62,62	0
54	MG	14	3151	1/1	0.81	0.34	56,56,56,56	0
54	MG	13	2327	1/1	0.81	0.25	81,81,81,81	0
54	MG	14	3554	1/1	0.81	0.23	62,62,62,62	0
54	MG	14	3541	1/1	0.81	0.24	71,71,71,71	0
54	MG	14	3331	1/1	0.81	0.21	54,54,54,54	0
54	MG	14	3473	1/1	0.81	0.22	77,77,77,77	0
54	MG	13	2374	1/1	0.81	0.08	79,79,79,79	0
54	MG	1H	3403	1/1	0.81	0.19	46,46,46,46	0
54	MG	1H	3518	1/1	0.81	0.31	41,41,41,41	0
54	MG	1J	213	1/1	0.81	0.19	78,78,78,78	0
54	MG	14	3146	1/1	0.81	0.29	54,54,54,54	0
54	MG	14	3335	1/1	0.81	0.18	57,57,57,57	0
54	MG	1H	3078	1/1	0.82	0.19	64,64,64,64	0
54	MG	14	3404	1/1	0.82	0.21	60,60,60,60	0
54	MG	14	3388	1/1	0.82	0.57	70,70,70,70	0
54	MG	13	2359	1/1	0.82	0.16	78,78,78,78	0
54	MG	1H	3159	1/1	0.82	0.30	52,52,52,52	0
54	MG	14	3361	1/1	0.82	0.24	64,64,64,64	0
54	MG	31	301	1/1	0.82	0.14	37,37,37,37	0
54	MG	14	3049	1/1	0.82	0.18	52,52,52,52	0
54	MG	X1	107	1/1	0.82	0.24	78,78,78,78	0
54	MG	14	3516	1/1	0.82	0.24	61,61,61,61	0
54	MG	1H	3488	1/1	0.82	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3290	1/1	0.82	0.34	73,73,73,73	0
54	MG	13	2290	1/1	0.82	0.29	67,67,67,67	0
54	MG	1H	3340	1/1	0.82	0.27	59,59,59,59	0
54	MG	1H	3328	1/1	0.82	0.26	49,49,49,49	0
54	MG	19	301	1/1	0.82	0.25	54,54,54,54	0
54	MG	13	2328	1/1	0.82	0.31	76,76,76,76	0
54	MG	14	3126	1/1	0.82	0.32	63,63,63,63	0
54	MG	W1	104	1/1	0.82	0.20	120,120,120,120	0
54	MG	13	2226	1/1	0.82	0.13	82,82,82,82	0
54	MG	14	3558	1/1	0.82	0.26	88,88,88,88	0
54	MG	14	3509	1/1	0.82	0.20	62,62,62,62	0
54	MG	13	2263	1/1	0.82	0.19	77,77,77,77	0
54	MG	13	2284	1/1	0.82	0.25	73,73,73,73	0
54	MG	14	3496	1/1	0.82	0.13	58,58,58,58	0
54	MG	1H	3542	1/1	0.82	0.16	48,48,48,48	0
54	MG	1H	3090	1/1	0.82	0.24	49,49,49,49	0
54	MG	78	202	1/1	0.82	0.23	54,54,54,54	0
54	MG	1H	3468	1/1	0.82	0.10	51,51,51,51	0
54	MG	14	3139	1/1	0.83	0.18	46,46,46,46	0
54	MG	1J	210	1/1	0.83	0.19	70,70,70,70	0
54	MG	1H	3015	1/1	0.83	0.09	41,41,41,41	0
54	MG	1H	3577	1/1	0.83	0.14	51,51,51,51	0
54	MG	1G	2350	1/1	0.83	0.17	80,80,80,80	0
54	MG	14	3377	1/1	0.83	0.23	49,49,49,49	0
54	MG	1H	3041	1/1	0.83	0.14	40,40,40,40	0
54	MG	14	3469	1/1	0.83	0.12	78,78,78,78	0
54	MG	13	2207	1/1	0.83	0.08	69,69,69,69	0
54	MG	14	3490	1/1	0.83	0.37	52,52,52,52	0
54	MG	14	3009	1/1	0.83	0.21	53,53,53,53	0
54	MG	14	3217	1/1	0.83	0.15	58,58,58,58	0
54	MG	1H	3392	1/1	0.83	0.19	50,50,50,50	0
54	MG	14	3341	1/1	0.83	0.18	65,65,65,65	0
54	MG	1H	3554	1/1	0.83	0.20	53,53,53,53	0
54	MG	1G	2263	1/1	0.83	0.33	61,61,61,61	0
54	MG	14	3257	1/1	0.83	0.26	42,42,42,42	0
54	MG	1H	3257	1/1	0.83	0.34	46,46,46,46	0
54	MG	14	3381	1/1	0.83	0.23	65,65,65,65	0
54	MG	1H	3545	1/1	0.83	0.31	66,66,66,66	0
54	MG	1H	3063	1/1	0.83	0.07	71,71,71,71	0
54	MG	1H	3397	1/1	0.83	0.43	60,60,60,60	0
54	MG	14	3407	1/1	0.83	0.23	68,68,68,68	0
54	MG	13	2360	1/1	0.83	0.24	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3562	1/1	0.83	0.14	61,61,61,61	0
54	MG	1H	3493	1/1	0.83	0.26	62,62,62,62	0
54	MG	1G	2247	1/1	0.83	0.41	74,74,74,74	0
54	MG	A8	201	1/1	0.83	0.28	60,60,60,60	0
54	MG	1G	2310	1/1	0.83	0.27	75,75,75,75	0
54	MG	1H	3074	1/1	0.83	0.18	43,43,43,43	0
54	MG	1H	3163	1/1	0.83	0.27	43,43,43,43	0
54	MG	1H	3588	1/1	0.83	0.21	51,51,51,51	0
54	MG	1H	3364	1/1	0.83	0.42	57,57,57,57	0
54	MG	1H	3391	1/1	0.83	0.26	56,56,56,56	0
54	MG	1G	2343	1/1	0.83	0.37	75,75,75,75	0
54	MG	1H	3427	1/1	0.83	0.20	43,43,43,43	0
54	MG	14	3442	1/1	0.84	0.61	73,73,73,73	0
54	MG	1H	3037	1/1	0.84	0.27	44,44,44,44	0
54	MG	14	3491	1/1	0.84	0.31	52,52,52,52	0
54	MG	14	3537	1/1	0.84	0.26	70,70,70,70	0
54	MG	14	3337	1/1	0.84	0.43	69,69,69,69	0
54	MG	14	3304	1/1	0.84	0.21	46,46,46,46	0
54	MG	14	3334	1/1	0.84	0.22	75,75,75,75	0
54	MG	1H	3225	1/1	0.84	0.17	51,51,51,51	0
54	MG	1H	3268	1/1	0.84	0.28	65,65,65,65	0
54	MG	1G	2223	1/1	0.84	0.21	66,66,66,66	0
54	MG	1H	3135	1/1	0.84	0.20	49,49,49,49	0
54	MG	1H	3174	1/1	0.84	0.39	50,50,50,50	0
54	MG	1H	3217	1/1	0.84	0.21	36,36,36,36	0
54	MG	1H	3303	1/1	0.84	0.42	59,59,59,59	0
54	MG	14	3390	1/1	0.84	0.33	44,44,44,44	0
54	MG	14	3567	1/1	0.84	0.09	73,73,73,73	0
54	MG	14	3209	1/1	0.84	0.19	47,47,47,47	0
54	MG	1G	2339	1/1	0.84	0.20	76,76,76,76	0
54	MG	W4	103	1/1	0.84	0.23	81,81,81,81	0
54	MG	1G	2246	1/1	0.84	0.21	68,68,68,68	0
54	MG	1H	3091	1/1	0.84	0.14	37,37,37,37	0
54	MG	1H	3222	1/1	0.84	0.24	40,40,40,40	0
54	MG	14	3513	1/1	0.84	0.46	66,66,66,66	0
54	MG	14	3234	1/1	0.84	0.42	57,57,57,57	0
54	MG	14	3443	1/1	0.84	0.17	52,52,52,52	0
54	MG	1H	3475	1/1	0.84	0.23	49,49,49,49	0
54	MG	1H	3575	1/1	0.84	0.13	59,59,59,59	0
54	MG	1H	3292	1/1	0.84	0.17	45,45,45,45	0
54	MG	1G	2259	1/1	0.84	0.32	80,80,80,80	0
54	MG	1H	3527	1/1	0.84	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3242	1/1	0.84	0.19	51,51,51,51	0
54	MG	13	2352	1/1	0.84	0.15	52,52,52,52	0
54	MG	14	3166	1/1	0.84	0.15	52,52,52,52	0
54	MG	1H	3281	1/1	0.84	0.19	61,61,61,61	0
54	MG	13	2228	1/1	0.84	0.26	50,50,50,50	0
54	MG	1H	3262	1/1	0.84	0.40	68,68,68,68	0
54	MG	14	3359	1/1	0.84	0.37	62,62,62,62	0
54	MG	1H	3471	1/1	0.84	0.17	71,71,71,71	0
54	MG	1G	2249	1/1	0.84	0.31	66,66,66,66	0
54	MG	13	2378	1/1	0.84	0.24	73,73,73,73	0
54	MG	13	2345	1/1	0.85	0.13	47,47,47,47	0
54	MG	13	2292	1/1	0.85	0.23	54,54,54,54	0
54	MG	1H	3534	1/1	0.85	0.15	43,43,43,43	0
54	MG	1H	3161	1/1	0.85	0.29	32,32,32,32	0
54	MG	14	3280	1/1	0.85	0.18	56,56,56,56	0
54	MG	1H	3312	1/1	0.85	0.19	41,41,41,41	0
54	MG	13	2233	1/1	0.85	0.34	84,84,84,84	0
54	MG	14	3203	1/1	0.85	0.30	75,75,75,75	0
54	MG	39	302	1/1	0.85	0.18	49,49,49,49	0
54	MG	14	3396	1/1	0.85	0.56	77,77,77,77	0
54	MG	14	3556	1/1	0.85	0.19	59,59,59,59	0
54	MG	1H	3132	1/1	0.85	0.17	65,65,65,65	0
54	MG	1H	3586	1/1	0.85	0.32	62,62,62,62	0
54	MG	13	2358	1/1	0.85	0.11	74,74,74,74	0
54	MG	1G	2374	1/1	0.85	0.49	86,86,86,86	0
55	ZN	G8	201	1/1	0.85	0.17	95,95,95,95	0
54	MG	1H	3528	1/1	0.85	0.22	58,58,58,58	0
54	MG	1H	3404	1/1	0.85	0.30	68,68,68,68	0
54	MG	13	2368	1/1	0.85	0.11	84,84,84,84	0
54	MG	14	3085	1/1	0.85	0.08	49,49,49,49	0
54	MG	1H	3520	1/1	0.85	0.18	51,51,51,51	0
54	MG	14	3232	1/1	0.85	0.77	74,74,74,74	0
54	MG	14	3464	1/1	0.85	0.30	53,53,53,53	0
54	MG	14	3022	1/1	0.85	0.15	45,45,45,45	0
54	MG	14	3307	1/1	0.85	0.29	71,71,71,71	0
54	MG	1H	3188	1/1	0.85	0.14	35,35,35,35	0
54	MG	14	3058	1/1	0.85	0.10	50,50,50,50	0
54	MG	1H	3326	1/1	0.85	0.49	68,68,68,68	0
54	MG	14	3018	1/1	0.85	0.09	58,58,58,58	0
54	MG	1H	3022	1/1	0.85	0.11	45,45,45,45	0
54	MG	14	3445	1/1	0.85	0.20	58,58,58,58	0
54	MG	14	3530	1/1	0.85	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3313	1/1	0.85	0.40	51,51,51,51	0
54	MG	13	2243	1/1	0.85	0.30	48,48,48,48	0
54	MG	1G	2294	1/1	0.85	0.41	75,75,75,75	0
54	MG	14	3295	1/1	0.85	0.32	56,56,56,56	0
54	MG	13	2344	1/1	0.85	0.16	66,66,66,66	0
54	MG	14	3434	1/1	0.85	0.25	57,57,57,57	0
54	MG	1G	2242	1/1	0.85	0.62	81,81,81,81	0
54	MG	1H	3448	1/1	0.85	0.17	50,50,50,50	0
54	MG	11	301	1/1	0.85	0.25	34,34,34,34	0
54	MG	14	3238	1/1	0.85	0.34	60,60,60,60	0
54	MG	29	301	1/1	0.85	0.12	52,52,52,52	0
54	MG	1H	3387	1/1	0.85	0.40	55,55,55,55	0
54	MG	13	2322	1/1	0.85	0.43	81,81,81,81	0
54	MG	14	3362	1/1	0.85	0.15	59,59,59,59	0
54	MG	16	203	1/1	0.85	0.21	62,62,62,62	0
54	MG	14	3259	1/1	0.85	0.38	46,46,46,46	0
54	MG	14	3520	1/1	0.85	0.13	77,77,77,77	0
54	MG	13	2341	1/1	0.85	0.09	89,89,89,89	0
54	MG	14	3015	1/1	0.85	0.16	40,40,40,40	0
54	MG	1G	2323	1/1	0.85	0.36	67,67,67,67	0
54	MG	1G	2348	1/1	0.85	0.29	71,71,71,71	0
54	MG	16	209	1/1	0.85	0.12	54,54,54,54	0
54	MG	1G	2240	1/1	0.85	0.40	81,81,81,81	0
54	MG	1H	3508	1/1	0.85	0.32	36,36,36,36	0
54	MG	13	2302	1/1	0.85	0.30	69,69,69,69	0
54	MG	1H	3536	1/1	0.85	0.14	43,43,43,43	0
54	MG	13	2273	1/1	0.85	0.24	62,62,62,62	0
54	MG	1H	3504	1/1	0.86	0.11	55,55,55,55	0
54	MG	16	210	1/1	0.86	0.20	58,58,58,58	0
54	MG	13	2365	1/1	0.86	0.27	75,75,75,75	0
54	MG	13	2222	1/1	0.86	0.25	75,75,75,75	0
54	MG	13	2275	1/1	0.86	0.19	75,75,75,75	0
54	MG	X1	109	1/1	0.86	0.09	71,71,71,71	0
54	MG	14	3260	1/1	0.86	0.14	41,41,41,41	0
54	MG	13	2212	1/1	0.86	0.08	89,89,89,89	0
54	MG	14	3084	1/1	0.86	0.14	54,54,54,54	0
54	MG	13	2325	1/1	0.86	0.43	77,77,77,77	0
54	MG	14	3205	1/1	0.86	0.53	61,61,61,61	0
54	MG	1H	3232	1/1	0.86	0.17	34,34,34,34	0
54	MG	1H	3343	1/1	0.86	0.28	50,50,50,50	0
54	MG	1H	3500	1/1	0.86	0.21	71,71,71,71	0
54	MG	1H	3535	1/1	0.86	0.29	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3370	1/1	0.86	0.35	62,62,62,62	0
54	MG	14	3043	1/1	0.86	0.11	47,47,47,47	0
54	MG	1H	3008	1/1	0.86	0.07	40,40,40,40	0
54	MG	14	3079	1/1	0.86	0.06	54,54,54,54	0
54	MG	13	2330	1/1	0.86	0.22	55,55,55,55	0
54	MG	1H	3317	1/1	0.86	0.24	56,56,56,56	0
54	MG	16	211	1/1	0.86	0.20	59,59,59,59	0
54	MG	1H	3477	1/1	0.86	0.28	51,51,51,51	0
54	MG	68	202	1/1	0.86	0.20	63,63,63,63	0
54	MG	14	3452	1/1	0.86	0.18	59,59,59,59	0
54	MG	1H	3369	1/1	0.86	0.30	71,71,71,71	0
54	MG	13	2244	1/1	0.86	0.21	45,45,45,45	0
54	MG	14	3066	1/1	0.86	0.07	86,86,86,86	0
54	MG	W1	103	1/1	0.86	0.22	73,73,73,73	0
54	MG	1H	3278	1/1	0.86	0.28	48,48,48,48	0
54	MG	14	3254	1/1	0.86	0.45	66,66,66,66	0
54	MG	14	3074	1/1	0.86	0.12	52,52,52,52	0
54	MG	78	201	1/1	0.86	0.13	47,47,47,47	0
54	MG	14	3413	1/1	0.86	0.21	79,79,79,79	0
54	MG	41	201	1/1	0.86	0.16	68,68,68,68	0
54	MG	13	2279	1/1	0.86	0.24	55,55,55,55	0
54	MG	1H	3486	1/1	0.86	0.28	40,40,40,40	0
54	MG	13	2382	1/1	0.86	0.17	60,60,60,60	0
54	MG	49	201	1/1	0.86	0.18	86,86,86,86	0
54	MG	14	3389	1/1	0.86	0.17	63,63,63,63	0
54	MG	14	3534	1/1	0.86	0.18	70,70,70,70	0
54	MG	1H	3299	1/1	0.86	0.26	53,53,53,53	0
54	MG	13	2282	1/1	0.86	0.30	57,57,57,57	0
54	MG	13	2324	1/1	0.86	0.14	63,63,63,63	0
54	MG	1H	3465	1/1	0.86	0.35	47,47,47,47	0
54	MG	14	3326	1/1	0.86	0.22	70,70,70,70	0
54	MG	14	3243	1/1	0.86	0.55	76,76,76,76	0
54	MG	13	2366	1/1	0.87	0.25	65,65,65,65	0
54	MG	13	2210	1/1	0.87	0.13	82,82,82,82	0
54	MG	1G	2363	1/1	0.87	0.28	92,92,92,92	0
54	MG	A5	201	1/1	0.87	0.45	45,45,45,45	0
54	MG	16	205	1/1	0.87	0.44	58,58,58,58	0
54	MG	1H	3411	1/1	0.87	0.21	50,50,50,50	0
54	MG	1H	3080	1/1	0.87	0.08	58,58,58,58	0
54	MG	13	2240	1/1	0.87	0.55	74,74,74,74	0
54	MG	6A	101	1/1	0.87	0.51	86,86,86,86	0
54	MG	14	3207	1/1	0.87	0.41	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3464	1/1	0.87	0.23	53,53,53,53	0
54	MG	1H	3334	1/1	0.87	0.30	50,50,50,50	0
54	MG	1H	3350	1/1	0.87	0.26	57,57,57,57	0
54	MG	1G	2373	1/1	0.87	0.12	94,94,94,94	0
54	MG	E5	201	1/1	0.87	0.13	55,55,55,55	0
54	MG	1H	3574	1/1	0.87	0.33	58,58,58,58	0
54	MG	1H	3367	1/1	0.87	0.20	57,57,57,57	0
54	MG	1G	2264	1/1	0.87	0.36	94,94,94,94	0
54	MG	14	3210	1/1	0.87	0.22	50,50,50,50	0
54	MG	1H	3297	1/1	0.87	0.16	51,51,51,51	0
54	MG	14	3310	1/1	0.87	0.13	59,59,59,59	0
54	MG	14	3412	1/1	0.87	0.35	73,73,73,73	0
54	MG	1H	3473	1/1	0.87	0.09	48,48,48,48	0
54	MG	1H	3419	1/1	0.87	0.16	63,63,63,63	0
54	MG	45	202	1/1	0.87	0.23	65,65,65,65	0
54	MG	I8	102	1/1	0.87	0.31	61,61,61,61	0
54	MG	1G	2331	1/1	0.87	0.43	72,72,72,72	0
54	MG	14	3478	1/1	0.87	0.26	60,60,60,60	0
54	MG	14	3233	1/1	0.87	0.13	58,58,58,58	0
54	MG	1H	3429	1/1	0.87	0.14	41,41,41,41	0
54	MG	1H	3127	1/1	0.87	0.17	60,60,60,60	0
54	MG	1H	3076	1/1	0.87	0.12	62,62,62,62	0
54	MG	14	3262	1/1	0.87	0.15	53,53,53,53	0
54	MG	1G	2299	1/1	0.87	0.17	60,60,60,60	0
54	MG	14	3495	1/1	0.87	0.45	64,64,64,64	0
54	MG	3E	302	1/1	0.87	0.47	84,84,84,84	0
54	MG	1H	3295	1/1	0.87	0.26	49,49,49,49	0
54	MG	1G	2376	1/1	0.87	0.25	99,99,99,99	0
54	MG	14	3402	1/1	0.87	0.22	70,70,70,70	0
54	MG	1G	2367	1/1	0.87	0.29	92,92,92,92	0
54	MG	1H	3031	1/1	0.87	0.12	49,49,49,49	0
54	MG	14	3036	1/1	0.87	0.10	53,53,53,53	0
54	MG	14	3344	1/1	0.87	0.14	81,81,81,81	0
54	MG	21	303	1/1	0.87	0.23	72,72,72,72	0
54	MG	14	3477	1/1	0.88	0.56	64,64,64,64	0
54	MG	1H	3410	1/1	0.88	0.12	57,57,57,57	0
54	MG	14	3117	1/1	0.88	0.15	64,64,64,64	0
54	MG	1H	3177	1/1	0.88	0.38	46,46,46,46	0
54	MG	14	3078	1/1	0.88	0.13	46,46,46,46	0
54	MG	14	3494	1/1	0.88	0.59	62,62,62,62	0
54	MG	13	2262	1/1	0.88	0.13	70,70,70,70	0
54	MG	14	3454	1/1	0.88	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3525	1/1	0.88	0.16	43,43,43,43	0
54	MG	14	3183	1/1	0.88	0.40	57,57,57,57	0
54	MG	1J	209	1/1	0.88	0.05	69,69,69,69	0
54	MG	14	3421	1/1	0.88	0.40	42,42,42,42	0
54	MG	14	3305	1/1	0.88	0.15	52,52,52,52	0
54	MG	1H	3291	1/1	0.88	0.32	68,68,68,68	0
54	MG	14	3321	1/1	0.88	0.16	68,68,68,68	0
54	MG	1G	2360	1/1	0.88	0.11	68,68,68,68	0
54	MG	55	202	1/1	0.88	0.13	57,57,57,57	0
54	MG	13	2343	1/1	0.88	0.14	62,62,62,62	0
54	MG	14	3355	1/1	0.88	0.16	61,61,61,61	0
54	MG	13	2272	1/1	0.88	0.15	54,54,54,54	0
54	MG	W4	101	1/1	0.88	0.22	88,88,88,88	0
54	MG	1G	2337	1/1	0.88	0.13	70,70,70,70	0
54	MG	14	3444	1/1	0.88	0.25	62,62,62,62	0
54	MG	41	202	1/1	0.88	0.25	73,73,73,73	0
54	MG	14	3253	1/1	0.88	0.49	55,55,55,55	0
54	MG	14	3228	1/1	0.88	0.52	65,65,65,65	0
54	MG	14	3324	1/1	0.88	0.23	67,67,67,67	0
54	MG	14	3398	1/1	0.88	0.30	75,75,75,75	0
54	MG	1H	3407	1/1	0.88	0.32	65,65,65,65	0
54	MG	1G	2344	1/1	0.88	0.20	76,76,76,76	0
54	MG	3I	201	1/1	0.88	0.25	52,52,52,52	0
54	MG	16	207	1/1	0.88	0.39	53,53,53,53	0
54	MG	25	202	1/1	0.88	0.12	67,67,67,67	0
54	MG	1H	3035	1/1	0.88	0.14	60,60,60,60	0
54	MG	14	3467	1/1	0.88	0.26	66,66,66,66	0
54	MG	1G	2321	1/1	0.88	0.38	75,75,75,75	0
54	MG	1H	3338	1/1	0.88	0.10	48,48,48,48	0
54	MG	14	3161	1/1	0.88	0.23	45,45,45,45	0
54	MG	14	3566	1/1	0.88	0.09	68,68,68,68	0
54	MG	14	3073	1/1	0.88	0.27	53,53,53,53	0
54	MG	14	3489	1/1	0.88	0.21	49,49,49,49	0
54	MG	1H	3004	1/1	0.88	0.10	40,40,40,40	0
54	MG	1G	2305	1/1	0.88	0.10	77,77,77,77	0
54	MG	1H	3353	1/1	0.88	0.44	57,57,57,57	0
54	MG	39	301	1/1	0.88	0.32	74,74,74,74	0
54	MG	14	3401	1/1	0.88	0.51	73,73,73,73	0
54	MG	1H	3220	1/1	0.88	0.28	44,44,44,44	0
54	MG	14	3432	1/1	0.88	0.10	55,55,55,55	0
54	MG	14	3431	1/1	0.88	0.33	57,57,57,57	0
54	MG	1H	3414	1/1	0.88	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3137	1/1	0.88	0.21	42,42,42,42	0
54	MG	1H	3272	1/1	0.88	0.13	47,47,47,47	0
54	MG	1H	3157	1/1	0.88	0.30	61,61,61,61	0
54	MG	1H	3583	1/1	0.88	0.28	53,53,53,53	0
54	MG	1H	3236	1/1	0.88	0.11	62,62,62,62	0
54	MG	14	3369	1/1	0.88	0.33	62,62,62,62	0
54	MG	14	3245	1/1	0.88	0.28	64,64,64,64	0
54	MG	1H	3209	1/1	0.88	0.23	52,52,52,52	0
54	MG	13	2340	1/1	0.88	0.16	52,52,52,52	0
54	MG	1G	2320	1/1	0.88	0.22	70,70,70,70	0
54	MG	1H	3551	1/1	0.88	0.19	57,57,57,57	0
54	MG	1G	2365	1/1	0.88	0.47	84,84,84,84	0
54	MG	1G	2342	1/1	0.88	0.24	73,73,73,73	0
54	MG	1G	2236	1/1	0.88	0.30	70,70,70,70	0
54	MG	1H	3020	1/1	0.88	0.16	39,39,39,39	0
54	MG	1G	2225	1/1	0.88	0.40	72,72,72,72	0
54	MG	1H	3445	1/1	0.88	0.22	73,73,73,73	0
54	MG	1H	3470	1/1	0.88	0.30	43,43,43,43	0
54	MG	1G	2340	1/1	0.89	0.42	81,81,81,81	0
54	MG	1H	3506	1/1	0.89	0.31	59,59,59,59	0
54	MG	1H	3036	1/1	0.89	0.06	48,48,48,48	0
54	MG	1J	212	1/1	0.89	0.08	81,81,81,81	0
54	MG	14	3560	1/1	0.89	0.22	51,51,51,51	0
54	MG	88	301	1/1	0.89	0.12	59,59,59,59	0
54	MG	13	2289	1/1	0.89	0.39	71,71,71,71	0
54	MG	1G	2298	1/1	0.89	0.21	71,71,71,71	0
54	MG	1H	3563	1/1	0.89	0.47	57,57,57,57	0
54	MG	14	3395	1/1	0.89	0.24	67,67,67,67	0
54	MG	1H	3400	1/1	0.89	0.38	66,66,66,66	0
54	MG	14	3005	1/1	0.89	0.24	51,51,51,51	0
54	MG	13	2311	1/1	0.89	0.32	71,71,71,71	0
54	MG	14	3047	1/1	0.89	0.08	64,64,64,64	0
54	MG	14	3375	1/1	0.89	0.15	71,71,71,71	0
54	MG	13	2326	1/1	0.89	0.31	59,59,59,59	0
54	MG	14	3459	1/1	0.89	0.17	49,49,49,49	0
54	MG	13	2300	1/1	0.89	0.26	76,76,76,76	0
54	MG	1H	3336	1/1	0.89	0.13	45,45,45,45	0
54	MG	1H	3320	1/1	0.89	0.33	46,46,46,46	0
54	MG	1H	3481	1/1	0.89	0.27	57,57,57,57	0
54	MG	1G	2244	1/1	0.89	0.30	72,72,72,72	0
54	MG	1H	3499	1/1	0.89	0.30	49,49,49,49	0
54	MG	1H	3578	1/1	0.89	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3230	1/1	0.89	0.16	67,67,67,67	0
54	MG	14	3408	1/1	0.89	0.26	52,52,52,52	0
54	MG	1H	3541	1/1	0.89	0.14	52,52,52,52	0
54	MG	1H	3371	1/1	0.89	0.17	60,60,60,60	0
54	MG	14	3439	1/1	0.89	0.47	77,77,77,77	0
54	MG	14	3463	1/1	0.89	0.23	65,65,65,65	0
54	MG	1J	207	1/1	0.89	0.10	80,80,80,80	0
54	MG	1H	3212	1/1	0.89	0.20	35,35,35,35	0
54	MG	1H	3051	1/1	0.89	0.08	59,59,59,59	0
54	MG	1H	3094	1/1	0.89	0.48	36,36,36,36	0
54	MG	14	3218	1/1	0.89	0.24	50,50,50,50	0
54	MG	1G	2268	1/1	0.89	0.12	77,77,77,77	0
54	MG	1H	3487	1/1	0.89	0.13	54,54,54,54	0
54	MG	1G	2251	1/1	0.89	0.24	67,67,67,67	0
54	MG	1H	3260	1/1	0.89	0.27	37,37,37,37	0
54	MG	B8	201	1/1	0.89	0.13	60,60,60,60	0
54	MG	1H	3276	1/1	0.89	0.34	57,57,57,57	0
54	MG	1H	3406	1/1	0.89	0.45	63,63,63,63	0
54	MG	1H	3546	1/1	0.89	0.35	69,69,69,69	0
54	MG	14	3551	1/1	0.89	0.17	47,47,47,47	0
54	MG	13	2214	1/1	0.89	0.15	88,88,88,88	0
54	MG	X4	104	1/1	0.89	0.23	91,91,91,91	0
54	MG	13	2223	1/1	0.89	0.36	48,48,48,48	0
54	MG	1G	2203	1/1	0.89	0.43	68,68,68,68	0
54	MG	14	3351	1/1	0.89	0.29	61,61,61,61	0
54	MG	14	3120	1/1	0.89	0.19	45,45,45,45	0
54	MG	14	3552	1/1	0.89	0.12	49,49,49,49	0
54	MG	1H	3524	1/1	0.89	0.20	45,45,45,45	0
54	MG	1H	3229	1/1	0.89	0.14	52,52,52,52	0
54	MG	14	3089	1/1	0.89	0.11	56,56,56,56	0
54	MG	13	2334	1/1	0.89	0.24	85,85,85,85	0
54	MG	1H	3430	1/1	0.89	0.32	56,56,56,56	0
54	MG	C5	203	1/1	0.89	0.36	86,86,86,86	0
54	MG	13	2298	1/1	0.89	0.52	87,87,87,87	0
54	MG	13	2250	1/1	0.89	0.31	70,70,70,70	0
54	MG	1H	3375	1/1	0.89	0.39	53,53,53,53	0
54	MG	1H	3517	1/1	0.89	0.18	53,53,53,53	0
54	MG	13	2353	1/1	0.89	0.22	60,60,60,60	0
54	MG	1H	3165	1/1	0.89	0.32	46,46,46,46	0
54	MG	1J	202	1/1	0.89	0.10	79,79,79,79	0
54	MG	14	3061	1/1	0.89	0.11	48,48,48,48	0
54	MG	13	2237	1/1	0.89	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3530	1/1	0.89	0.25	48,48,48,48	0
54	MG	1G	2209	1/1	0.89	0.10	68,68,68,68	0
54	MG	14	3106	1/1	0.90	0.29	52,52,52,52	0
54	MG	1G	2297	1/1	0.90	0.15	90,90,90,90	0
54	MG	1G	2378	1/1	0.90	0.33	81,81,81,81	0
54	MG	1H	3513	1/1	0.90	0.43	63,63,63,63	0
54	MG	1G	2304	1/1	0.90	0.59	85,85,85,85	0
54	MG	1H	3587	1/1	0.90	0.14	47,47,47,47	0
54	MG	1H	3069	1/1	0.90	0.22	45,45,45,45	0
54	MG	14	3319	1/1	0.90	0.11	67,67,67,67	0
54	MG	4I	201	1/1	0.90	0.06	75,75,75,75	0
54	MG	14	3508	1/1	0.90	0.09	57,57,57,57	0
54	MG	1G	2248	1/1	0.90	0.44	61,61,61,61	0
54	MG	1H	3243	1/1	0.90	0.23	59,59,59,59	0
54	MG	14	3044	1/1	0.90	0.07	75,75,75,75	0
54	MG	1H	3289	1/1	0.90	0.40	56,56,56,56	0
54	MG	1H	3433	1/1	0.90	0.29	45,45,45,45	0
54	MG	1H	3146	1/1	0.90	0.39	55,55,55,55	0
54	MG	13	2329	1/1	0.90	0.32	73,73,73,73	0
54	MG	1H	3497	1/1	0.90	0.23	50,50,50,50	0
54	MG	14	3514	1/1	0.90	0.11	60,60,60,60	0
54	MG	13	2312	1/1	0.90	0.41	52,52,52,52	0
54	MG	1H	3282	1/1	0.90	0.44	61,61,61,61	0
54	MG	1G	2333	1/1	0.90	0.32	85,85,85,85	0
54	MG	14	3356	1/1	0.90	0.30	51,51,51,51	0
54	MG	1H	3408	1/1	0.90	0.26	51,51,51,51	0
54	MG	1H	3241	1/1	0.90	0.25	48,48,48,48	0
54	MG	1H	3055	1/1	0.90	0.19	56,56,56,56	0
54	MG	14	3518	1/1	0.90	0.29	86,86,86,86	0
54	MG	13	2373	1/1	0.90	0.16	88,88,88,88	0
54	MG	13	2354	1/1	0.90	0.11	70,70,70,70	0
54	MG	14	3215	1/1	0.90	0.23	49,49,49,49	0
54	MG	14	3440	1/1	0.90	0.33	61,61,61,61	0
54	MG	1H	3556	1/1	0.90	0.16	59,59,59,59	0
54	MG	13	2285	1/1	0.90	0.07	72,72,72,72	0
54	MG	14	3345	1/1	0.90	0.09	60,60,60,60	0
54	MG	1H	3432	1/1	0.90	0.15	43,43,43,43	0
54	MG	13	2283	1/1	0.90	0.17	63,63,63,63	0
54	MG	1G	2349	1/1	0.90	0.12	83,83,83,83	0
54	MG	14	3039	1/1	0.90	0.08	43,43,43,43	0
54	MG	1H	3172	1/1	0.90	0.35	36,36,36,36	0
54	MG	14	3422	1/1	0.90	0.26	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3469	1/1	0.90	0.29	47,47,47,47	0
54	MG	1H	3399	1/1	0.90	0.21	55,55,55,55	0
54	MG	1H	3310	1/1	0.90	0.15	30,30,30,30	0
54	MG	13	2303	1/1	0.90	0.09	70,70,70,70	0
54	MG	13	2265	1/1	0.90	0.27	51,51,51,51	0
54	MG	13	2271	1/1	0.90	0.29	65,65,65,65	0
54	MG	14	3077	1/1	0.90	0.05	59,59,59,59	0
54	MG	14	3050	1/1	0.90	0.07	61,61,61,61	0
54	MG	14	3275	1/1	0.90	0.13	46,46,46,46	0
54	MG	1H	3089	1/1	0.90	0.20	38,38,38,38	0
54	MG	1G	2282	1/1	0.90	0.41	75,75,75,75	0
54	MG	14	3318	1/1	0.90	0.10	78,78,78,78	0
54	MG	1H	3421	1/1	0.90	0.26	62,62,62,62	0
54	MG	13	2308	1/1	0.90	0.21	78,78,78,78	0
54	MG	13	2257	1/1	0.90	0.27	82,82,82,82	0
54	MG	13	2363	1/1	0.90	0.08	76,76,76,76	0
54	MG	14	3284	1/1	0.90	0.38	82,82,82,82	0
54	MG	13	2268	1/1	0.90	0.25	55,55,55,55	0
54	MG	1H	3570	1/1	0.90	0.16	51,51,51,51	0
54	MG	16	213	1/1	0.90	0.30	66,66,66,66	0
54	MG	1H	3537	1/1	0.90	0.35	60,60,60,60	0
54	MG	1H	3088	1/1	0.90	0.09	37,37,37,37	0
54	MG	14	3330	1/1	0.90	0.08	76,76,76,76	0
54	MG	13	2225	1/1	0.90	0.24	67,67,67,67	0
54	MG	14	3546	1/1	0.90	0.22	42,42,42,42	0
54	MG	1H	3233	1/1	0.90	0.16	36,36,36,36	0
54	MG	14	3441	1/1	0.90	0.11	76,76,76,76	0
54	MG	14	3515	1/1	0.90	0.17	60,60,60,60	0
54	MG	1H	3496	1/1	0.90	0.17	52,52,52,52	0
54	MG	1H	3462	1/1	0.90	0.16	53,53,53,53	0
54	MG	14	3384	1/1	0.90	0.24	47,47,47,47	0
54	MG	1H	3017	1/1	0.90	0.19	41,41,41,41	0
54	MG	14	3527	1/1	0.90	0.15	52,52,52,52	0
54	MG	21	301	1/1	0.90	0.28	40,40,40,40	0
54	MG	14	3006	1/1	0.90	0.10	46,46,46,46	0
54	MG	X4	101	1/1	0.90	0.20	91,91,91,91	0
54	MG	14	3480	1/1	0.90	0.20	58,58,58,58	0
54	MG	1H	3585	1/1	0.90	0.26	39,39,39,39	0
54	MG	1H	3418	1/1	0.90	0.29	54,54,54,54	0
54	MG	1H	3007	1/1	0.91	0.08	72,72,72,72	0
54	MG	14	3292	1/1	0.91	0.15	39,39,39,39	0
54	MG	1G	2277	1/1	0.91	0.33	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3128	1/1	0.91	0.30	39,39,39,39	0
54	MG	13	2348	1/1	0.91	0.22	58,58,58,58	0
54	MG	14	3474	1/1	0.91	0.47	50,50,50,50	0
54	MG	13	2332	1/1	0.91	0.19	58,58,58,58	0
54	MG	1G	2229	1/1	0.91	0.30	84,84,84,84	0
54	MG	1H	3409	1/1	0.91	0.14	30,30,30,30	0
54	MG	14	3206	1/1	0.91	0.52	57,57,57,57	0
54	MG	1H	3194	1/1	0.91	0.47	46,46,46,46	0
54	MG	13	2362	1/1	0.91	0.15	77,77,77,77	0
54	MG	1H	3494	1/1	0.91	0.35	62,62,62,62	0
54	MG	1H	3210	1/1	0.91	0.22	44,44,44,44	0
54	MG	13	2355	1/1	0.91	0.31	65,65,65,65	0
54	MG	14	3498	1/1	0.91	0.34	44,44,44,44	0
54	MG	14	3289	1/1	0.91	0.31	63,63,63,63	0
54	MG	11	305	1/1	0.91	0.25	31,31,31,31	0
54	MG	13	2245	1/1	0.91	0.14	49,49,49,49	0
54	MG	1H	3305	1/1	0.91	0.24	46,46,46,46	0
54	MG	1H	3531	1/1	0.91	0.18	52,52,52,52	0
54	MG	1H	3335	1/1	0.91	0.54	75,75,75,75	0
54	MG	14	3252	1/1	0.91	0.25	62,62,62,62	0
54	MG	1H	3459	1/1	0.91	0.13	44,44,44,44	0
54	MG	1G	2250	1/1	0.91	0.33	66,66,66,66	0
54	MG	1H	3489	1/1	0.91	0.21	53,53,53,53	0
54	MG	1H	3270	1/1	0.91	0.17	55,55,55,55	0
54	MG	14	3564	1/1	0.91	0.10	50,50,50,50	0
54	MG	1H	3344	1/1	0.91	0.14	42,42,42,42	0
54	MG	1G	2291	1/1	0.91	0.52	79,79,79,79	0
54	MG	1H	3547	1/1	0.91	0.12	41,41,41,41	0
54	MG	14	3001	1/1	0.91	0.47	57,57,57,57	0
54	MG	13	2256	1/1	0.91	0.37	64,64,64,64	0
54	MG	1H	3384	1/1	0.91	0.23	57,57,57,57	0
54	MG	1H	3552	1/1	0.91	0.14	52,52,52,52	0
54	MG	1G	2375	1/1	0.91	0.16	85,85,85,85	0
54	MG	14	3365	1/1	0.91	0.17	56,56,56,56	0
54	MG	1H	3405	1/1	0.91	0.12	62,62,62,62	0
54	MG	14	3317	1/1	0.91	0.41	79,79,79,79	0
54	MG	1H	3261	1/1	0.91	0.19	39,39,39,39	0
54	MG	13	2384	1/1	0.91	0.13	70,70,70,70	0
54	MG	14	3559	1/1	0.91	0.27	70,70,70,70	0
54	MG	1H	3246	1/1	0.91	0.48	58,58,58,58	0
54	MG	13	2296	1/1	0.91	0.37	110,110,110,110	0
54	MG	14	3048	1/1	0.91	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3097	1/1	0.91	0.28	38,38,38,38	0
54	MG	14	3293	1/1	0.91	0.28	57,57,57,57	0
54	MG	1H	3046	1/1	0.91	0.24	38,38,38,38	0
54	MG	1H	3102	1/1	0.91	0.24	41,41,41,41	0
54	MG	1H	3394	1/1	0.91	0.23	55,55,55,55	0
54	MG	13	2369	1/1	0.91	0.19	51,51,51,51	0
54	MG	13	2269	1/1	0.91	0.26	57,57,57,57	0
54	MG	14	3111	1/1	0.91	0.17	41,41,41,41	0
54	MG	1G	2322	1/1	0.91	0.34	63,63,63,63	0
54	MG	13	2319	1/1	0.91	0.35	77,77,77,77	0
54	MG	55	201	1/1	0.91	0.25	53,53,53,53	0
54	MG	1H	3381	1/1	0.91	0.45	58,58,58,58	0
54	MG	1H	3234	1/1	0.91	0.17	39,39,39,39	0
54	MG	14	3470	1/1	0.91	0.12	51,51,51,51	0
54	MG	1H	3038	1/1	0.91	0.06	51,51,51,51	0
54	MG	1G	2237	1/1	0.91	0.20	70,70,70,70	0
54	MG	1H	3130	1/1	0.91	0.53	71,71,71,71	0
54	MG	1G	2361	1/1	0.91	0.19	92,92,92,92	0
54	MG	1H	3597	1/1	0.91	0.20	45,45,45,45	0
54	MG	14	3437	1/1	0.91	0.60	69,69,69,69	0
54	MG	1G	2266	1/1	0.91	0.11	71,71,71,71	0
54	MG	1H	3021	1/1	0.91	0.11	46,46,46,46	0
54	MG	13	2221	1/1	0.91	0.23	63,63,63,63	0
54	MG	13	2371	1/1	0.91	0.26	92,92,92,92	0
54	MG	1H	3416	1/1	0.91	0.48	72,72,72,72	0
54	MG	14	3076	1/1	0.91	0.21	55,55,55,55	0
54	MG	1H	3359	1/1	0.91	0.41	54,54,54,54	0
54	MG	14	3208	1/1	0.91	0.31	50,50,50,50	0
54	MG	1H	3158	1/1	0.91	0.23	61,61,61,61	0
54	MG	1H	3557	1/1	0.91	0.19	45,45,45,45	0
54	MG	1H	3306	1/1	0.91	0.24	36,36,36,36	0
54	MG	1H	3565	1/1	0.91	0.19	67,67,67,67	0
54	MG	14	3488	1/1	0.91	0.18	55,55,55,55	0
54	MG	13	2236	1/1	0.92	0.17	54,54,54,54	0
54	MG	13	2286	1/1	0.92	0.35	59,59,59,59	0
54	MG	14	3211	1/1	0.92	0.30	44,44,44,44	0
54	MG	1H	3118	1/1	0.92	0.34	38,38,38,38	0
54	MG	14	3339	1/1	0.92	0.22	46,46,46,46	0
54	MG	13	2206	1/1	0.92	0.06	79,79,79,79	0
54	MG	1H	3412	1/1	0.92	0.20	49,49,49,49	0
54	MG	13	2379	1/1	0.92	0.28	68,68,68,68	0
54	MG	1G	2205	1/1	0.92	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3190	1/1	0.92	0.19	38,38,38,38	0
54	MG	1H	3333	1/1	0.92	0.21	46,46,46,46	0
54	MG	1G	2280	1/1	0.92	0.24	62,62,62,62	0
54	MG	1G	2369	1/1	0.92	0.12	82,82,82,82	0
54	MG	1H	3154	1/1	0.92	0.25	37,37,37,37	0
54	MG	1H	3580	1/1	0.92	0.44	58,58,58,58	0
54	MG	1H	3380	1/1	0.92	0.38	55,55,55,55	0
54	MG	1H	3533	1/1	0.92	0.23	46,46,46,46	0
54	MG	14	3487	1/1	0.92	0.23	45,45,45,45	0
54	MG	1H	3111	1/1	0.92	0.33	45,45,45,45	0
54	MG	1H	3145	1/1	0.92	0.30	45,45,45,45	0
54	MG	13	2209	1/1	0.92	0.07	67,67,67,67	0
54	MG	1G	2252	1/1	0.92	0.54	78,78,78,78	0
54	MG	1H	3327	1/1	0.92	0.20	54,54,54,54	0
54	MG	1G	2354	1/1	0.92	0.37	62,62,62,62	0
54	MG	1G	2329	1/1	0.92	0.24	87,87,87,87	0
54	MG	1H	3395	1/1	0.92	0.47	72,72,72,72	0
54	MG	1G	2371	1/1	0.92	0.14	58,58,58,58	0
54	MG	1G	2207	1/1	0.92	0.10	70,70,70,70	0
54	MG	14	3041	1/1	0.92	0.13	44,44,44,44	0
54	MG	1G	2281	1/1	0.92	0.16	70,70,70,70	0
54	MG	13	2383	1/1	0.92	0.24	70,70,70,70	0
54	MG	14	3348	1/1	0.92	0.28	59,59,59,59	0
54	MG	1H	3322	1/1	0.92	0.34	58,58,58,58	0
54	MG	14	3553	1/1	0.92	0.17	60,60,60,60	0
54	MG	1H	3030	1/1	0.92	0.07	48,48,48,48	0
54	MG	14	3201	1/1	0.92	0.24	42,42,42,42	0
54	MG	14	3071	1/1	0.92	0.19	54,54,54,54	0
54	MG	1H	3437	1/1	0.92	0.38	73,73,73,73	0
54	MG	1G	2353	1/1	0.92	0.48	65,65,65,65	0
54	MG	1H	3218	1/1	0.92	0.41	48,48,48,48	0
54	MG	14	3069	1/1	0.92	0.04	70,70,70,70	0
54	MG	14	3299	1/1	0.92	0.27	57,57,57,57	0
54	MG	1H	3361	1/1	0.92	0.16	51,51,51,51	0
54	MG	14	3242	1/1	0.92	0.31	59,59,59,59	0
54	MG	14	3087	1/1	0.92	0.13	49,49,49,49	0
54	MG	14	3274	1/1	0.92	0.55	59,59,59,59	0
54	MG	1H	3150	1/1	0.92	0.29	51,51,51,51	0
54	MG	42	201	1/1	0.92	0.12	92,92,92,92	0
54	MG	1H	3390	1/1	0.92	0.12	39,39,39,39	0
54	MG	14	3354	1/1	0.92	0.46	68,68,68,68	0
54	MG	1H	3170	1/1	0.92	0.35	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2317	1/1	0.92	0.33	91,91,91,91	0
54	MG	L8	101	1/1	0.92	0.34	54,54,54,54	0
54	MG	1H	3555	1/1	0.92	0.37	53,53,53,53	0
54	MG	1G	2289	1/1	0.92	0.22	80,80,80,80	0
54	MG	14	3430	1/1	0.92	0.28	46,46,46,46	0
54	MG	1H	3562	1/1	0.92	0.23	56,56,56,56	0
54	MG	3E	303	1/1	0.92	0.20	81,81,81,81	0
54	MG	14	3510	1/1	0.92	0.16	50,50,50,50	0
54	MG	14	3134	1/1	0.92	0.35	53,53,53,53	0
54	MG	14	3248	1/1	0.92	0.22	54,54,54,54	0
54	MG	14	3193	1/1	0.92	0.31	49,49,49,49	0
54	MG	1H	3084	1/1	0.92	0.07	41,41,41,41	0
54	MG	14	3502	1/1	0.92	0.23	51,51,51,51	0
54	MG	13	2218	1/1	0.92	0.19	58,58,58,58	0
54	MG	14	3294	1/1	0.92	0.32	62,62,62,62	0
54	MG	1H	3503	1/1	0.92	0.23	52,52,52,52	0
54	MG	14	3239	1/1	0.92	0.30	58,58,58,58	0
54	MG	1H	3065	1/1	0.92	0.10	70,70,70,70	0
54	MG	14	3180	1/1	0.92	0.51	65,65,65,65	0
54	MG	1H	3548	1/1	0.92	0.07	51,51,51,51	0
54	MG	1H	3048	1/1	0.92	0.05	42,42,42,42	0
54	MG	14	3272	1/1	0.92	0.26	67,67,67,67	0
54	MG	1H	3349	1/1	0.92	0.22	39,39,39,39	0
54	MG	1G	2206	1/1	0.92	0.09	80,80,80,80	0
54	MG	1G	2224	1/1	0.92	0.41	72,72,72,72	0
54	MG	1H	3114	1/1	0.92	0.34	43,43,43,43	0
54	MG	1G	2332	1/1	0.92	0.28	64,64,64,64	0
54	MG	14	3340	1/1	0.92	0.14	54,54,54,54	0
54	MG	13	2213	1/1	0.92	0.18	62,62,62,62	0
54	MG	13	2315	1/1	0.92	0.34	67,67,67,67	0
54	MG	1G	2314	1/1	0.92	0.35	74,74,74,74	0
54	MG	14	3072	1/1	0.92	0.18	52,52,52,52	0
54	MG	1H	3279	1/1	0.92	0.17	40,40,40,40	0
54	MG	1H	3512	1/1	0.92	0.43	56,56,56,56	0
54	MG	13	2264	1/1	0.92	0.47	74,74,74,74	0
54	MG	14	3466	1/1	0.92	0.10	68,68,68,68	0
54	MG	14	3042	1/1	0.92	0.11	51,51,51,51	0
54	MG	1G	2335	1/1	0.92	0.12	71,71,71,71	0
54	MG	13	2266	1/1	0.92	0.14	77,77,77,77	0
54	MG	14	3067	1/1	0.92	0.12	43,43,43,43	0
54	MG	13	2280	1/1	0.92	0.44	63,63,63,63	0
54	MG	1H	3273	1/1	0.92	0.37	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2352	1/1	0.92	0.36	65,65,65,65	0
54	MG	14	3363	1/1	0.92	0.35	63,63,63,63	0
54	MG	14	3545	1/1	0.92	0.30	47,47,47,47	0
54	MG	14	3094	1/1	0.92	0.31	50,50,50,50	0
54	MG	1G	2256	1/1	0.92	0.25	67,67,67,67	0
54	MG	1H	3351	1/1	0.92	0.29	71,71,71,71	0
54	MG	13	2220	1/1	0.92	0.24	60,60,60,60	0
54	MG	X1	108	1/1	0.92	0.17	77,77,77,77	0
54	MG	1H	3265	1/1	0.93	0.30	58,58,58,58	0
54	MG	14	3147	1/1	0.93	0.43	53,53,53,53	0
54	MG	1H	3016	1/1	0.93	0.09	40,40,40,40	0
54	MG	1H	3417	1/1	0.93	0.33	38,38,38,38	0
54	MG	14	3468	1/1	0.93	0.20	66,66,66,66	0
54	MG	14	3374	1/1	0.93	0.21	70,70,70,70	0
54	MG	14	3378	1/1	0.93	0.25	59,59,59,59	0
54	MG	1H	3323	1/1	0.93	0.34	62,62,62,62	0
54	MG	14	3298	1/1	0.93	0.57	69,69,69,69	0
54	MG	13	2254	1/1	0.93	0.12	64,64,64,64	0
54	MG	1H	3311	1/1	0.93	0.14	34,34,34,34	0
54	MG	14	3475	1/1	0.93	0.25	64,64,64,64	0
54	MG	14	3165	1/1	0.93	0.30	52,52,52,52	0
54	MG	1G	2279	1/1	0.93	0.22	76,76,76,76	0
54	MG	14	3555	1/1	0.93	0.35	71,71,71,71	0
54	MG	1H	3259	1/1	0.93	0.31	49,49,49,49	0
54	MG	14	3540	1/1	0.93	0.35	81,81,81,81	0
54	MG	14	3025	1/1	0.93	0.10	45,45,45,45	0
54	MG	14	3309	1/1	0.93	0.43	39,39,39,39	0
54	MG	1G	2270	1/1	0.93	0.45	67,67,67,67	0
54	MG	14	3030	1/1	0.93	0.10	42,42,42,42	0
54	MG	1H	3175	1/1	0.93	0.45	57,57,57,57	0
54	MG	14	3012	1/1	0.93	0.18	43,43,43,43	0
54	MG	1H	3275	1/1	0.93	0.40	51,51,51,51	0
54	MG	1H	3589	1/1	0.93	0.18	45,45,45,45	0
54	MG	1H	3237	1/1	0.93	0.51	50,50,50,50	0
54	MG	1H	3457	1/1	0.93	0.37	35,35,35,35	0
54	MG	1H	3205	1/1	0.93	0.28	45,45,45,45	0
54	MG	14	3219	1/1	0.93	0.70	53,53,53,53	0
54	MG	14	3021	1/1	0.93	0.11	45,45,45,45	0
54	MG	13	2336	1/1	0.93	0.45	54,54,54,54	0
54	MG	1H	3075	1/1	0.93	0.30	48,48,48,48	0
54	MG	13	2255	1/1	0.93	0.34	53,53,53,53	0
54	MG	1H	3248	1/1	0.93	0.40	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3373	1/1	0.93	0.23	46,46,46,46	0
54	MG	14	3216	1/1	0.93	0.29	56,56,56,56	0
54	MG	1H	3100	1/1	0.93	0.24	43,43,43,43	0
54	MG	14	3184	1/1	0.93	0.21	45,45,45,45	0
54	MG	1H	3070	1/1	0.93	0.15	36,36,36,36	0
54	MG	1H	3086	1/1	0.93	0.16	42,42,42,42	0
54	MG	13	2258	1/1	0.93	0.21	76,76,76,76	0
54	MG	1H	3087	1/1	0.93	0.06	45,45,45,45	0
53	8UZ	13	2202	33/33	0.93	0.14	70,70,70,70	0
54	MG	1H	3453	1/1	0.93	0.25	43,43,43,43	0
54	MG	14	3425	1/1	0.93	0.28	54,54,54,54	0
54	MG	14	3297	1/1	0.93	0.12	61,61,61,61	0
54	MG	14	3178	1/1	0.93	0.45	61,61,61,61	0
54	MG	14	3124	1/1	0.93	0.24	67,67,67,67	0
54	MG	1H	3450	1/1	0.93	0.18	50,50,50,50	0
54	MG	68	201	1/1	0.93	0.19	62,62,62,62	0
54	MG	1H	3013	1/1	0.93	0.12	52,52,52,52	0
54	MG	13	2277	1/1	0.93	0.14	66,66,66,66	0
54	MG	1H	3296	1/1	0.93	0.49	77,77,77,77	0
54	MG	14	3099	1/1	0.93	0.32	45,45,45,45	0
54	MG	1G	2301	1/1	0.93	0.27	88,88,88,88	0
54	MG	14	3533	1/1	0.93	0.32	58,58,58,58	0
54	MG	14	3561	1/1	0.93	0.20	60,60,60,60	0
54	MG	1H	3386	1/1	0.93	0.18	65,65,65,65	0
54	MG	1H	3398	1/1	0.93	0.11	55,55,55,55	0
54	MG	13	2276	1/1	0.93	0.31	62,62,62,62	0
54	MG	14	3352	1/1	0.93	0.26	74,74,74,74	0
54	MG	14	3366	1/1	0.93	0.14	53,53,53,53	0
54	MG	1H	3269	1/1	0.93	0.55	46,46,46,46	0
54	MG	1H	3235	1/1	0.93	0.66	76,76,76,76	0
54	MG	14	3171	1/1	0.93	0.29	40,40,40,40	0
54	MG	1H	3202	1/1	0.93	0.21	38,38,38,38	0
54	MG	13	2295	1/1	0.93	0.14	65,65,65,65	0
54	MG	1H	3156	1/1	0.93	0.32	42,42,42,42	0
54	MG	2A	201	1/1	0.93	0.15	74,74,74,74	0
54	MG	14	3471	1/1	0.93	0.25	62,62,62,62	0
54	MG	14	3316	1/1	0.93	0.20	59,59,59,59	0
54	MG	14	3457	1/1	0.93	0.49	84,84,84,84	0
54	MG	14	3013	1/1	0.93	0.15	41,41,41,41	0
54	MG	13	2304	1/1	0.93	0.24	55,55,55,55	0
54	MG	1G	2336	1/1	0.93	0.30	72,72,72,72	0
54	MG	14	3456	1/1	0.93	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2267	1/1	0.93	0.17	81,81,81,81	0
54	MG	14	3303	1/1	0.93	0.34	62,62,62,62	0
54	MG	1H	3141	1/1	0.93	0.52	67,67,67,67	0
54	MG	14	3338	1/1	0.93	0.24	63,63,63,63	0
54	MG	14	3476	1/1	0.93	0.17	57,57,57,57	0
54	MG	11	302	1/1	0.93	0.24	46,46,46,46	0
54	MG	1H	3247	1/1	0.93	0.21	46,46,46,46	0
54	MG	1H	3329	1/1	0.93	0.14	46,46,46,46	0
54	MG	1G	2238	1/1	0.93	0.24	69,69,69,69	0
54	MG	1H	3385	1/1	0.93	0.22	61,61,61,61	0
54	MG	1G	2274	1/1	0.93	0.23	63,63,63,63	0
54	MG	1H	3239	1/1	0.93	0.45	59,59,59,59	0
54	MG	1H	3169	1/1	0.93	0.23	36,36,36,36	0
54	MG	1H	3422	1/1	0.93	0.14	45,45,45,45	0
54	MG	1H	3148	1/1	0.93	0.45	30,30,30,30	0
54	MG	14	3028	1/1	0.93	0.07	59,59,59,59	0
54	MG	1H	3356	1/1	0.93	0.25	45,45,45,45	0
54	MG	1G	2258	1/1	0.93	0.21	82,82,82,82	0
54	MG	1G	2218	1/1	0.93	0.38	54,54,54,54	0
54	MG	1G	2306	1/1	0.93	0.12	76,76,76,76	0
54	MG	14	3156	1/1	0.93	0.41	41,41,41,41	0
54	MG	13	2347	1/1	0.93	0.17	57,57,57,57	0
54	MG	14	3163	1/1	0.93	0.38	44,44,44,44	0
54	MG	14	3327	1/1	0.93	0.58	66,66,66,66	0
54	MG	1H	3047	1/1	0.93	0.09	37,37,37,37	0
54	MG	14	3052	1/1	0.93	0.08	50,50,50,50	0
54	MG	1H	3023	1/1	0.93	0.10	39,39,39,39	0
54	MG	1G	2239	1/1	0.93	0.27	82,82,82,82	0
54	MG	14	3054	1/1	0.93	0.08	48,48,48,48	0
54	MG	1H	3200	1/1	0.93	0.35	37,37,37,37	0
54	MG	14	3105	1/1	0.93	0.31	63,63,63,63	0
54	MG	14	3336	1/1	0.93	0.30	51,51,51,51	0
54	MG	1H	3284	1/1	0.93	0.15	44,44,44,44	0
54	MG	19	302	1/1	0.93	0.34	55,55,55,55	0
54	MG	1G	2302	1/1	0.93	0.17	86,86,86,86	0
54	MG	1H	3443	1/1	0.93	0.30	52,52,52,52	0
54	MG	1H	3267	1/1	0.93	0.10	44,44,44,44	0
54	MG	14	3240	1/1	0.93	0.27	59,59,59,59	0
54	MG	14	3538	1/1	0.93	0.40	74,74,74,74	0
54	MG	1H	3566	1/1	0.93	0.14	48,48,48,48	0
54	MG	W1	101	1/1	0.93	0.32	64,64,64,64	0
54	MG	1H	3250	1/1	0.94	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3167	1/1	0.94	0.33	39,39,39,39	0
54	MG	14	3547	1/1	0.94	0.13	48,48,48,48	0
54	MG	1H	3594	1/1	0.94	0.26	41,41,41,41	0
54	MG	1H	3466	1/1	0.94	0.35	65,65,65,65	0
54	MG	14	3285	1/1	0.94	0.22	59,59,59,59	0
54	MG	14	3237	1/1	0.94	0.30	56,56,56,56	0
54	MG	1G	2271	1/1	0.94	0.28	81,81,81,81	0
54	MG	14	3152	1/1	0.94	0.28	53,53,53,53	0
54	MG	14	3086	1/1	0.94	0.10	49,49,49,49	0
54	MG	1H	3285	1/1	0.94	0.47	69,69,69,69	0
54	MG	14	3524	1/1	0.94	0.17	65,65,65,65	0
54	MG	14	3519	1/1	0.94	0.11	71,71,71,71	0
54	MG	1G	2233	1/1	0.94	0.42	59,59,59,59	0
54	MG	52	201	1/1	0.94	0.20	63,63,63,63	0
54	MG	13	2252	1/1	0.94	0.48	68,68,68,68	0
54	MG	14	3288	1/1	0.94	0.26	43,43,43,43	0
54	MG	1G	2312	1/1	0.94	0.11	63,63,63,63	0
54	MG	18	101	1/1	0.94	0.29	43,43,43,43	0
54	MG	88	302	1/1	0.94	0.10	58,58,58,58	0
54	MG	13	2270	1/1	0.94	0.19	59,59,59,59	0
54	MG	19	303	1/1	0.94	0.30	37,37,37,37	0
54	MG	1H	3452	1/1	0.94	0.29	52,52,52,52	0
54	MG	1H	3271	1/1	0.94	0.41	57,57,57,57	0
54	MG	14	3010	1/1	0.94	0.08	42,42,42,42	0
54	MG	14	3313	1/1	0.94	0.16	50,50,50,50	0
54	MG	1H	3107	1/1	0.94	0.36	33,33,33,33	0
54	MG	14	3181	1/1	0.94	0.37	41,41,41,41	0
54	MG	14	3371	1/1	0.94	0.15	50,50,50,50	0
54	MG	1H	3183	1/1	0.94	0.29	43,43,43,43	0
54	MG	1H	3263	1/1	0.94	0.50	65,65,65,65	0
54	MG	14	3107	1/1	0.94	0.39	55,55,55,55	0
54	MG	14	3484	1/1	0.94	0.13	62,62,62,62	0
54	MG	1H	3258	1/1	0.94	0.39	55,55,55,55	0
54	MG	1H	3181	1/1	0.94	0.51	37,37,37,37	0
54	MG	1H	3515	1/1	0.94	0.38	38,38,38,38	0
54	MG	1H	3162	1/1	0.94	0.42	55,55,55,55	0
54	MG	13	2361	1/1	0.94	0.27	81,81,81,81	0
54	MG	1G	2283	1/1	0.94	0.13	68,68,68,68	0
54	MG	1H	3332	1/1	0.94	0.35	75,75,75,75	0
54	MG	1H	3377	1/1	0.94	0.30	51,51,51,51	0
54	MG	1H	3252	1/1	0.94	0.25	47,47,47,47	0
54	MG	13	2247	1/1	0.94	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3186	1/1	0.94	0.19	38,38,38,38	0
54	MG	1H	3363	1/1	0.94	0.12	57,57,57,57	0
54	MG	14	3116	1/1	0.94	0.31	70,70,70,70	0
54	MG	14	3281	1/1	0.94	0.28	61,61,61,61	0
54	MG	1H	3182	1/1	0.94	0.12	39,39,39,39	0
54	MG	14	3157	1/1	0.94	0.25	45,45,45,45	0
54	MG	14	3523	1/1	0.94	0.21	52,52,52,52	0
54	MG	14	3108	1/1	0.94	0.23	47,47,47,47	0
54	MG	13	2251	1/1	0.94	0.21	62,62,62,62	0
54	MG	14	3461	1/1	0.94	0.30	70,70,70,70	0
54	MG	14	3270	1/1	0.94	0.23	78,78,78,78	0
54	MG	1H	3564	1/1	0.94	0.28	47,47,47,47	0
54	MG	14	3136	1/1	0.94	0.21	44,44,44,44	0
54	MG	1H	3581	1/1	0.94	0.27	54,54,54,54	0
54	MG	1H	3277	1/1	0.94	0.33	51,51,51,51	0
54	MG	1H	3309	1/1	0.94	0.24	37,37,37,37	0
54	MG	1H	3372	1/1	0.94	0.17	54,54,54,54	0
54	MG	1G	2275	1/1	0.94	0.27	52,52,52,52	0
54	MG	1H	3511	1/1	0.94	0.36	56,56,56,56	0
54	MG	1H	3134	1/1	0.94	0.12	43,43,43,43	0
54	MG	14	3226	1/1	0.94	0.34	64,64,64,64	0
54	MG	13	2351	1/1	0.94	0.33	59,59,59,59	0
54	MG	14	3173	1/1	0.94	0.52	60,60,60,60	0
54	MG	1H	3330	1/1	0.94	0.22	51,51,51,51	0
54	MG	1H	3160	1/1	0.94	0.34	53,53,53,53	0
54	MG	1G	2357	1/1	0.94	0.12	74,74,74,74	0
54	MG	14	3026	1/1	0.94	0.20	41,41,41,41	0
54	MG	1H	3293	1/1	0.94	0.11	37,37,37,37	0
54	MG	1H	3245	1/1	0.94	0.43	49,49,49,49	0
54	MG	1H	3214	1/1	0.94	0.23	44,44,44,44	0
54	MG	1H	3402	1/1	0.94	0.17	40,40,40,40	0
54	MG	13	2331	1/1	0.94	0.15	69,69,69,69	0
54	MG	1H	3373	1/1	0.94	0.15	55,55,55,55	0
54	MG	1G	2276	1/1	0.94	0.25	82,82,82,82	0
54	MG	31	303	1/1	0.94	0.12	63,63,63,63	0
54	MG	1H	3283	1/1	0.94	0.36	76,76,76,76	0
54	MG	13	2260	1/1	0.94	0.27	63,63,63,63	0
54	MG	1G	2300	1/1	0.94	0.26	86,86,86,86	0
54	MG	1H	3139	1/1	0.94	0.19	37,37,37,37	0
54	MG	13	2306	1/1	0.94	0.38	46,46,46,46	0
54	MG	1G	2359	1/1	0.94	0.48	62,62,62,62	0
54	MG	1H	3230	1/1	0.94	0.50	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3224	1/1	0.94	0.43	55,55,55,55	0
54	MG	14	3130	1/1	0.94	0.34	48,48,48,48	0
54	MG	1G	2243	1/1	0.94	0.51	76,76,76,76	0
54	MG	14	3255	1/1	0.94	0.27	57,57,57,57	0
54	MG	1H	3103	1/1	0.94	0.30	42,42,42,42	0
54	MG	1H	3519	1/1	0.94	0.13	34,34,34,34	0
54	MG	1H	3426	1/1	0.94	0.37	56,56,56,56	0
54	MG	14	3119	1/1	0.94	0.39	39,39,39,39	0
54	MG	14	3227	1/1	0.94	0.31	51,51,51,51	0
54	MG	1H	3569	1/1	0.94	0.13	47,47,47,47	0
54	MG	1H	3152	1/1	0.94	0.20	41,41,41,41	0
54	MG	14	3503	1/1	0.94	0.12	45,45,45,45	0
54	MG	14	3449	1/1	0.94	0.11	53,53,53,53	0
54	MG	1H	3523	1/1	0.94	0.09	42,42,42,42	0
54	MG	1H	3374	1/1	0.94	0.26	36,36,36,36	0
54	MG	1H	3538	1/1	0.94	0.10	45,45,45,45	0
54	MG	1H	3347	1/1	0.94	0.23	36,36,36,36	0
54	MG	13	2313	1/1	0.94	0.20	78,78,78,78	0
54	MG	1G	2231	1/1	0.94	0.39	57,57,57,57	0
54	MG	14	3198	1/1	0.94	0.49	40,40,40,40	0
54	MG	14	3138	1/1	0.94	0.28	47,47,47,47	0
54	MG	14	3098	1/1	0.94	0.28	46,46,46,46	0
54	MG	1H	3480	1/1	0.94	0.18	46,46,46,46	0
54	MG	14	3531	1/1	0.94	0.09	59,59,59,59	0
54	MG	13	2208	1/1	0.94	0.17	78,78,78,78	0
54	MG	14	3286	1/1	0.94	0.13	40,40,40,40	0
54	MG	1G	2227	1/1	0.94	0.06	67,67,67,67	0
54	MG	1G	2368	1/1	0.94	0.22	82,82,82,82	0
54	MG	X1	106	1/1	0.94	0.29	84,84,84,84	0
54	MG	13	2229	1/1	0.94	0.21	68,68,68,68	0
54	MG	1H	3178	1/1	0.94	0.26	46,46,46,46	0
53	8UZ	1G	2202	33/33	0.94	0.14	78,78,78,78	0
54	MG	14	3064	1/1	0.94	0.15	68,68,68,68	0
54	MG	14	3155	1/1	0.94	0.41	39,39,39,39	0
54	MG	1H	3505	1/1	0.94	0.37	66,66,66,66	0
54	MG	1H	3514	1/1	0.94	0.32	57,57,57,57	0
54	MG	1H	3266	1/1	0.94	0.30	46,46,46,46	0
54	MG	1G	2334	1/1	0.94	0.21	86,86,86,86	0
54	MG	14	3194	1/1	0.94	0.24	52,52,52,52	0
55	ZN	C5	201	1/1	0.94	0.19	110,110,110,110	0
54	MG	1G	2296	1/1	0.94	0.14	69,69,69,69	0
54	MG	1H	3339	1/1	0.94	0.40	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3436	1/1	0.94	0.14	39,39,39,39	0
54	MG	14	3112	1/1	0.94	0.29	47,47,47,47	0
54	MG	1G	2278	1/1	0.94	0.44	81,81,81,81	0
54	MG	1H	3593	1/1	0.94	0.36	46,46,46,46	0
54	MG	1H	3129	1/1	0.94	0.29	49,49,49,49	0
54	MG	1H	3168	1/1	0.94	0.17	34,34,34,34	0
54	MG	1H	3357	1/1	0.94	0.14	58,58,58,58	0
54	MG	1H	3568	1/1	0.94	0.09	61,61,61,61	0
54	MG	13	2349	1/1	0.94	0.30	53,53,53,53	0
54	MG	14	3187	1/1	0.94	0.23	47,47,47,47	0
54	MG	13	2217	1/1	0.94	0.20	66,66,66,66	0
54	MG	14	3102	1/1	0.94	0.35	45,45,45,45	0
54	MG	13	2249	1/1	0.95	0.34	56,56,56,56	0
54	MG	14	3349	1/1	0.95	0.26	63,63,63,63	0
54	MG	1H	3049	1/1	0.95	0.08	35,35,35,35	0
54	MG	1H	3539	1/1	0.95	0.25	76,76,76,76	0
54	MG	1H	3196	1/1	0.95	0.36	35,35,35,35	0
54	MG	14	3019	1/1	0.95	0.12	50,50,50,50	0
54	MG	1H	3526	1/1	0.95	0.20	56,56,56,56	0
54	MG	1H	3109	1/1	0.95	0.29	38,38,38,38	0
54	MG	16	206	1/1	0.95	0.52	52,52,52,52	0
54	MG	1G	2260	1/1	0.95	0.31	77,77,77,77	0
54	MG	1G	2358	1/1	0.95	0.11	68,68,68,68	0
54	MG	1H	3451	1/1	0.95	0.40	37,37,37,37	0
54	MG	13	2357	1/1	0.95	0.20	59,59,59,59	0
53	8UZ	13	2201	33/33	0.95	0.23	55,55,55,55	0
54	MG	1H	3092	1/1	0.95	0.09	54,54,54,54	0
54	MG	13	2337	1/1	0.95	0.37	56,56,56,56	0
54	MG	14	3159	1/1	0.95	0.38	43,43,43,43	0
54	MG	1H	3216	1/1	0.95	0.20	48,48,48,48	0
54	MG	1H	3366	1/1	0.95	0.22	68,68,68,68	0
54	MG	13	2346	1/1	0.95	0.18	56,56,56,56	0
54	MG	1H	3301	1/1	0.95	0.45	69,69,69,69	0
54	MG	1G	2327	1/1	0.95	0.10	69,69,69,69	0
54	MG	14	3115	1/1	0.95	0.19	54,54,54,54	0
54	MG	1H	3454	1/1	0.95	0.35	41,41,41,41	0
54	MG	14	3419	1/1	0.95	0.45	41,41,41,41	0
54	MG	14	3372	1/1	0.95	0.33	62,62,62,62	0
53	8UZ	1G	2201	33/33	0.95	0.18	65,65,65,65	0
54	MG	1H	3195	1/1	0.95	0.18	34,34,34,34	0
54	MG	1H	3032	1/1	0.95	0.14	43,43,43,43	0
54	MG	14	3256	1/1	0.95	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3113	1/1	0.95	0.14	63,63,63,63	0
54	MG	1H	3112	1/1	0.95	0.41	36,36,36,36	0
54	MG	1H	3077	1/1	0.95	0.09	43,43,43,43	0
54	MG	1G	2318	1/1	0.95	0.21	73,73,73,73	0
54	MG	1H	3324	1/1	0.95	0.12	59,59,59,59	0
54	MG	13	2259	1/1	0.95	0.37	55,55,55,55	0
54	MG	1G	2219	1/1	0.95	0.26	59,59,59,59	0
54	MG	14	3426	1/1	0.95	0.42	56,56,56,56	0
54	MG	1H	3113	1/1	0.95	0.36	34,34,34,34	0
54	MG	1H	3143	1/1	0.95	0.38	64,64,64,64	0
54	MG	1H	3147	1/1	0.95	0.27	54,54,54,54	0
54	MG	14	3164	1/1	0.95	0.30	49,49,49,49	0
54	MG	14	3229	1/1	0.95	0.30	64,64,64,64	0
54	MG	1J	206	1/1	0.95	0.21	75,75,75,75	0
54	MG	1H	3435	1/1	0.95	0.10	40,40,40,40	0
54	MG	45	201	1/1	0.95	0.20	53,53,53,53	0
54	MG	1H	3420	1/1	0.95	0.33	46,46,46,46	0
54	MG	14	3450	1/1	0.95	0.16	57,57,57,57	0
54	MG	14	3170	1/1	0.95	0.40	42,42,42,42	0
54	MG	14	3191	1/1	0.95	0.22	60,60,60,60	0
54	MG	14	3312	1/1	0.95	0.40	64,64,64,64	0
54	MG	1G	2230	1/1	0.95	0.15	57,57,57,57	0
54	MG	14	3093	1/1	0.95	0.38	40,40,40,40	0
54	MG	1H	3467	1/1	0.95	0.21	37,37,37,37	0
54	MG	14	3300	1/1	0.95	0.23	67,67,67,67	0
54	MG	14	3266	1/1	0.95	0.28	46,46,46,46	0
54	MG	1H	3190	1/1	0.95	0.42	38,38,38,38	0
54	MG	14	3329	1/1	0.95	0.15	46,46,46,46	0
54	MG	14	3301	1/1	0.95	0.23	65,65,65,65	0
54	MG	14	3358	1/1	0.95	0.13	46,46,46,46	0
54	MG	14	3196	1/1	0.95	0.24	68,68,68,68	0
54	MG	1G	2213	1/1	0.95	0.05	60,60,60,60	0
54	MG	1H	3005	1/1	0.95	0.15	41,41,41,41	0
54	MG	1H	3461	1/1	0.95	0.12	51,51,51,51	0
54	MG	1H	3502	1/1	0.95	0.17	52,52,52,52	0
54	MG	1H	3274	1/1	0.95	0.45	56,56,56,56	0
54	MG	14	3486	1/1	0.95	0.10	55,55,55,55	0
54	MG	14	3416	1/1	0.95	0.17	46,46,46,46	0
54	MG	1H	3179	1/1	0.95	0.35	55,55,55,55	0
54	MG	1H	3423	1/1	0.95	0.23	55,55,55,55	0
54	MG	K8	101	1/1	0.95	0.17	57,57,57,57	0
54	MG	1G	2254	1/1	0.95	0.43	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3458	1/1	0.95	0.22	70,70,70,70	0
54	MG	14	3212	1/1	0.95	0.49	59,59,59,59	0
54	MG	31	302	1/1	0.95	0.12	56,56,56,56	0
54	MG	1H	3321	1/1	0.95	0.14	44,44,44,44	0
54	MG	1H	3558	1/1	0.95	0.26	56,56,56,56	0
54	MG	1G	2222	1/1	0.95	0.08	66,66,66,66	0
54	MG	14	3197	1/1	0.95	0.26	45,45,45,45	0
54	MG	14	3435	1/1	0.95	0.26	58,58,58,58	0
54	MG	14	3110	1/1	0.95	0.27	56,56,56,56	0
54	MG	14	3127	1/1	0.95	0.30	66,66,66,66	0
54	MG	14	3080	1/1	0.95	0.13	60,60,60,60	0
54	MG	14	3213	1/1	0.95	0.32	52,52,52,52	0
54	MG	1H	3253	1/1	0.95	0.40	63,63,63,63	0
54	MG	14	3492	1/1	0.95	0.20	42,42,42,42	0
54	MG	1H	3474	1/1	0.95	0.17	51,51,51,51	0
54	MG	14	3133	1/1	0.95	0.34	49,49,49,49	0
54	MG	1H	3431	1/1	0.95	0.15	45,45,45,45	0
54	MG	1G	2290	1/1	0.95	0.27	70,70,70,70	0
54	MG	14	3109	1/1	0.95	0.29	44,44,44,44	0
54	MG	1H	3249	1/1	0.95	0.36	44,44,44,44	0
54	MG	1G	2325	1/1	0.95	0.33	71,71,71,71	0
54	MG	1H	3543	1/1	0.95	0.17	44,44,44,44	0
54	MG	13	2205	1/1	0.95	0.13	64,64,64,64	0
54	MG	29	303	1/1	0.95	0.10	51,51,51,51	0
54	MG	16	202	1/1	0.95	0.34	64,64,64,64	0
54	MG	1H	3316	1/1	0.95	0.14	40,40,40,40	0
54	MG	1H	3204	1/1	0.95	0.24	40,40,40,40	0
54	MG	1H	3231	1/1	0.95	0.16	35,35,35,35	0
54	MG	14	3323	1/1	0.95	0.15	46,46,46,46	0
54	MG	14	3455	1/1	0.95	0.18	60,60,60,60	0
54	MG	1H	3352	1/1	0.95	0.37	61,61,61,61	0
54	MG	1H	3213	1/1	0.95	0.47	34,34,34,34	0
54	MG	14	3429	1/1	0.95	0.24	50,50,50,50	0
54	MG	1H	3096	1/1	0.95	0.30	37,37,37,37	0
54	MG	14	3277	1/1	0.95	0.24	46,46,46,46	0
54	MG	1G	2307	1/1	0.95	0.51	70,70,70,70	0
54	MG	14	3497	1/1	0.95	0.13	59,59,59,59	0
54	MG	1H	3012	1/1	0.95	0.12	36,36,36,36	0
54	MG	14	3424	1/1	0.95	0.36	44,44,44,44	0
54	MG	14	3526	1/1	0.95	0.26	50,50,50,50	0
54	MG	1H	3155	1/1	0.95	0.28	56,56,56,56	0
54	MG	1H	3025	1/1	0.95	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2362	1/1	0.95	0.31	91,91,91,91	0
54	MG	13	2274	1/1	0.95	0.17	50,50,50,50	0
54	MG	14	3236	1/1	0.95	0.24	56,56,56,56	0
54	MG	14	3360	1/1	0.95	0.46	59,59,59,59	0
54	MG	13	2242	1/1	0.95	0.33	59,59,59,59	0
54	MG	1H	3187	1/1	0.95	0.14	35,35,35,35	0
54	MG	1H	3095	1/1	0.95	0.34	46,46,46,46	0
54	MG	1H	3009	1/1	0.95	0.12	50,50,50,50	0
54	MG	1H	3033	1/1	0.95	0.06	46,46,46,46	0
54	MG	1G	2316	1/1	0.95	0.10	58,58,58,58	0
54	MG	1H	3337	1/1	0.95	0.30	55,55,55,55	0
54	MG	14	3391	1/1	0.95	0.26	47,47,47,47	0
54	MG	1H	3044	1/1	0.95	0.12	38,38,38,38	0
54	MG	1H	3571	1/1	0.95	0.09	57,57,57,57	0
54	MG	1H	3532	1/1	0.95	0.23	41,41,41,41	0
54	MG	1G	2234	1/1	0.95	0.25	66,66,66,66	0
54	MG	14	3267	1/1	0.95	0.23	53,53,53,53	0
54	MG	14	3131	1/1	0.95	0.44	44,44,44,44	0
54	MG	14	3332	1/1	0.95	0.19	52,52,52,52	0
54	MG	14	3532	1/1	0.95	0.27	59,59,59,59	0
54	MG	1H	3348	1/1	0.95	0.22	47,47,47,47	0
54	MG	1G	2257	1/1	0.95	0.29	66,66,66,66	0
54	MG	1H	3192	1/1	0.95	0.38	38,38,38,38	0
54	MG	1H	3039	1/1	0.95	0.09	41,41,41,41	0
54	MG	X4	102	1/1	0.95	0.43	79,79,79,79	0
54	MG	1H	3592	1/1	0.95	0.19	57,57,57,57	0
54	MG	1G	2232	1/1	0.95	0.29	52,52,52,52	0
54	MG	1H	3510	1/1	0.95	0.61	48,48,48,48	0
54	MG	1H	3389	1/1	0.96	0.34	55,55,55,55	0
54	MG	13	2203	1/1	0.96	0.06	80,80,80,80	0
54	MG	14	3376	1/1	0.96	0.12	51,51,51,51	0
54	MG	1H	3425	1/1	0.96	0.13	46,46,46,46	0
54	MG	14	3544	1/1	0.96	0.17	57,57,57,57	0
54	MG	14	3415	1/1	0.96	0.25	59,59,59,59	0
54	MG	1H	3199	1/1	0.96	0.35	38,38,38,38	0
54	MG	14	3172	1/1	0.96	0.30	48,48,48,48	0
54	MG	14	3004	1/1	0.96	0.11	48,48,48,48	0
54	MG	14	3379	1/1	0.96	0.09	67,67,67,67	0
54	MG	1H	3043	1/1	0.96	0.08	45,45,45,45	0
54	MG	14	3380	1/1	0.96	0.28	57,57,57,57	0
54	MG	1H	3083	1/1	0.96	0.23	50,50,50,50	0
54	MG	14	3350	1/1	0.96	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3098	1/1	0.96	0.23	35,35,35,35	0
54	MG	1H	3034	1/1	0.96	0.04	47,47,47,47	0
54	MG	1H	3001	1/1	0.96	0.39	33,33,33,33	0
54	MG	14	3097	1/1	0.96	0.28	41,41,41,41	0
54	MG	13	2231	1/1	0.96	0.18	64,64,64,64	0
54	MG	1H	3550	1/1	0.96	0.27	58,58,58,58	0
54	MG	1H	3298	1/1	0.96	0.27	45,45,45,45	0
54	MG	1H	3219	1/1	0.96	0.35	44,44,44,44	0
54	MG	1H	3294	1/1	0.96	0.17	37,37,37,37	0
54	MG	14	3175	1/1	0.96	0.71	72,72,72,72	0
54	MG	1H	3341	1/1	0.96	0.54	61,61,61,61	0
54	MG	1H	3455	1/1	0.96	0.39	36,36,36,36	0
54	MG	1H	3456	1/1	0.96	0.34	62,62,62,62	0
54	MG	1H	3099	1/1	0.96	0.30	36,36,36,36	0
54	MG	1G	2261	1/1	0.96	0.40	95,95,95,95	0
54	MG	1H	3484	1/1	0.96	0.18	52,52,52,52	0
54	MG	1H	3582	1/1	0.96	0.29	71,71,71,71	0
54	MG	1G	2217	1/1	0.96	0.24	66,66,66,66	0
54	MG	14	3103	1/1	0.96	0.37	43,43,43,43	0
54	MG	14	3438	1/1	0.96	0.18	64,64,64,64	0
54	MG	13	2267	1/1	0.96	0.40	82,82,82,82	0
54	MG	14	3121	1/1	0.96	0.24	57,57,57,57	0
54	MG	14	3045	1/1	0.96	0.12	64,64,64,64	0
54	MG	1G	2285	1/1	0.96	0.30	67,67,67,67	0
54	MG	1J	201	1/1	0.96	0.20	78,78,78,78	0
54	MG	14	3142	1/1	0.96	0.37	51,51,51,51	0
54	MG	1H	3315	1/1	0.96	0.36	68,68,68,68	0
54	MG	14	3002	1/1	0.96	0.15	41,41,41,41	0
54	MG	1H	3151	1/1	0.96	0.26	42,42,42,42	0
54	MG	14	3007	1/1	0.96	0.11	43,43,43,43	0
54	MG	14	3199	1/1	0.96	0.25	47,47,47,47	0
54	MG	11	304	1/1	0.96	0.29	48,48,48,48	0
54	MG	1H	3101	1/1	0.96	0.42	43,43,43,43	0
54	MG	14	3536	1/1	0.96	0.27	62,62,62,62	0
54	MG	14	3031	1/1	0.96	0.12	52,52,52,52	0
54	MG	14	3505	1/1	0.96	0.13	64,64,64,64	0
54	MG	14	3528	1/1	0.96	0.21	66,66,66,66	0
54	MG	1G	2377	1/1	0.96	0.05	78,78,78,78	0
54	MG	13	2309	1/1	0.96	0.23	54,54,54,54	0
54	MG	14	3506	1/1	0.96	0.15	91,91,91,91	0
54	MG	14	3311	1/1	0.96	0.35	71,71,71,71	0
54	MG	14	3563	1/1	0.96	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3227	1/1	0.96	0.38	44,44,44,44	0
54	MG	14	3427	1/1	0.96	0.28	52,52,52,52	0
54	MG	1H	3024	1/1	0.96	0.12	40,40,40,40	0
54	MG	1H	3228	1/1	0.96	0.40	45,45,45,45	0
54	MG	14	3500	1/1	0.96	0.20	42,42,42,42	0
54	MG	14	3029	1/1	0.96	0.04	50,50,50,50	0
54	MG	1H	3290	1/1	0.96	0.42	39,39,39,39	0
54	MG	1H	3472	1/1	0.96	0.17	57,57,57,57	0
54	MG	29	302	1/1	0.96	0.33	47,47,47,47	0
54	MG	1H	3264	1/1	0.96	0.35	52,52,52,52	0
54	MG	X4	103	1/1	0.96	0.12	92,92,92,92	0
54	MG	14	3101	1/1	0.96	0.27	40,40,40,40	0
54	MG	1H	3560	1/1	0.96	0.36	69,69,69,69	0
54	MG	W4	102	1/1	0.96	0.07	83,83,83,83	0
54	MG	14	3179	1/1	0.96	0.39	53,53,53,53	0
54	MG	14	3507	1/1	0.96	0.14	50,50,50,50	0
54	MG	1H	3180	1/1	0.96	0.21	52,52,52,52	0
54	MG	14	3145	1/1	0.96	0.35	60,60,60,60	0
54	MG	1H	3053	1/1	0.96	0.10	36,36,36,36	0
54	MG	14	3160	1/1	0.96	0.25	54,54,54,54	0
54	MG	16	212	1/1	0.96	0.13	67,67,67,67	0
54	MG	78	203	1/1	0.96	0.65	40,40,40,40	0
54	MG	1H	3223	1/1	0.96	0.40	48,48,48,48	0
54	MG	1H	3062	1/1	0.96	0.07	51,51,51,51	0
54	MG	1H	3314	1/1	0.96	0.33	44,44,44,44	0
54	MG	14	3082	1/1	0.96	0.15	47,47,47,47	0
54	MG	13	2215	1/1	0.96	0.10	63,63,63,63	0
54	MG	1H	3362	1/1	0.96	0.30	59,59,59,59	0
54	MG	1H	3498	1/1	0.96	0.32	52,52,52,52	0
54	MG	14	3273	1/1	0.96	0.13	46,46,46,46	0
55	ZN	3E	301	1/1	0.96	0.41	81,81,81,81	0
54	MG	14	3135	1/1	0.96	0.29	45,45,45,45	0
54	MG	1G	2215	1/1	0.96	0.15	71,71,71,71	0
54	MG	13	2305	1/1	0.96	0.40	53,53,53,53	0
54	MG	1H	3302	1/1	0.96	0.42	44,44,44,44	0
54	MG	1J	211	1/1	0.96	0.19	73,73,73,73	0
54	MG	14	3535	1/1	0.96	0.07	60,60,60,60	0
54	MG	13	2246	1/1	0.96	0.36	62,62,62,62	0
54	MG	1H	3189	1/1	0.96	0.14	32,32,32,32	0
54	MG	1G	2208	1/1	0.96	0.07	70,70,70,70	0
54	MG	1H	3288	1/1	0.96	0.33	55,55,55,55	0
54	MG	14	3114	1/1	0.96	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2I	302	1/1	0.96	0.18	47,47,47,47	0
54	MG	1H	3559	1/1	0.96	0.08	61,61,61,61	0
54	MG	1H	3485	1/1	0.96	0.20	52,52,52,52	0
54	MG	B5	101	1/1	0.96	0.49	63,63,63,63	0
54	MG	1G	2324	1/1	0.96	0.17	60,60,60,60	0
54	MG	1H	3073	1/1	0.96	0.15	44,44,44,44	0
54	MG	1H	3444	1/1	0.96	0.12	50,50,50,50	0
54	MG	14	3287	1/1	0.96	0.24	56,56,56,56	0
54	MG	14	3557	1/1	0.96	0.08	68,68,68,68	0
54	MG	13	2318	1/1	0.96	0.43	68,68,68,68	0
54	MG	14	3188	1/1	0.96	0.31	53,53,53,53	0
54	MG	1H	3006	1/1	0.96	0.06	45,45,45,45	0
54	MG	13	2241	1/1	0.96	0.33	45,45,45,45	0
54	MG	14	3387	1/1	0.96	0.11	64,64,64,64	0
54	MG	14	3370	1/1	0.96	0.25	43,43,43,43	0
54	MG	1H	3244	1/1	0.96	0.37	33,33,33,33	0
54	MG	14	3027	1/1	0.96	0.14	40,40,40,40	0
54	MG	1H	3449	1/1	0.96	0.18	48,48,48,48	0
54	MG	1H	3256	1/1	0.96	0.33	69,69,69,69	0
54	MG	1H	3193	1/1	0.96	0.33	46,46,46,46	0
54	MG	14	3148	1/1	0.96	0.45	45,45,45,45	0
54	MG	1G	2328	1/1	0.96	0.45	69,69,69,69	0
54	MG	14	3168	1/1	0.97	0.37	47,47,47,47	0
54	MG	13	2239	1/1	0.97	0.47	70,70,70,70	0
54	MG	1H	3019	1/1	0.97	0.12	38,38,38,38	0
54	MG	1H	3119	1/1	0.97	0.22	36,36,36,36	0
54	MG	1H	3203	1/1	0.97	0.24	40,40,40,40	0
54	MG	1H	3509	1/1	0.97	0.22	34,34,34,34	0
54	MG	14	3493	1/1	0.97	0.23	57,57,57,57	0
54	MG	14	3185	1/1	0.97	0.20	48,48,48,48	0
54	MG	14	3125	1/1	0.97	0.54	48,48,48,48	0
54	MG	14	3149	1/1	0.97	0.46	42,42,42,42	0
54	MG	1H	3483	1/1	0.97	0.21	42,42,42,42	0
55	ZN	5A	101	1/1	0.97	0.11	99,99,99,99	0
54	MG	14	3104	1/1	0.97	0.14	47,47,47,47	0
54	MG	13	2219	1/1	0.97	0.24	60,60,60,60	0
54	MG	14	3382	1/1	0.97	0.30	54,54,54,54	0
54	MG	X1	102	1/1	0.97	0.32	66,66,66,66	0
54	MG	1H	3045	1/1	0.97	0.08	41,41,41,41	0
54	MG	14	3153	1/1	0.97	0.41	60,60,60,60	0
54	MG	1G	2226	1/1	0.97	0.17	97,97,97,97	0
54	MG	1H	3116	1/1	0.97	0.27	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	14	3244	1/1	0.97	0.30	48,48,48,48	0
54	MG	14	3174	1/1	0.97	0.43	53,53,53,53	0
54	MG	1H	3198	1/1	0.97	0.40	36,36,36,36	0
54	MG	14	3264	1/1	0.97	0.21	44,44,44,44	0
54	MG	1H	3018	1/1	0.97	0.11	36,36,36,36	0
54	MG	1H	3138	1/1	0.97	0.11	38,38,38,38	0
54	MG	14	3063	1/1	0.97	0.06	46,46,46,46	0
54	MG	1H	3026	1/1	0.97	0.09	40,40,40,40	0
54	MG	14	3003	1/1	0.97	0.09	44,44,44,44	0
54	MG	14	3446	1/1	0.97	0.21	48,48,48,48	0
54	MG	13	2380	1/1	0.97	0.11	50,50,50,50	0
54	MG	14	3200	1/1	0.97	0.17	50,50,50,50	0
54	MG	1H	3191	1/1	0.97	0.37	29,29,29,29	0
54	MG	13	2310	1/1	0.97	0.46	54,54,54,54	0
54	MG	1H	3166	1/1	0.97	0.36	34,34,34,34	0
54	MG	14	3150	1/1	0.97	0.28	46,46,46,46	0
54	MG	1H	3240	1/1	0.97	0.44	56,56,56,56	0
54	MG	1H	3255	1/1	0.97	0.35	51,51,51,51	0
54	MG	13	2248	1/1	0.97	0.50	57,57,57,57	0
54	MG	14	3154	1/1	0.97	0.27	53,53,53,53	0
54	MG	1H	3573	1/1	0.97	0.19	47,47,47,47	0
54	MG	1H	3124	1/1	0.97	0.15	38,38,38,38	0
54	MG	13	2224	1/1	0.97	0.37	59,59,59,59	0
54	MG	G8	202	1/1	0.97	0.55	53,53,53,53	0
54	MG	13	2238	1/1	0.97	0.46	75,75,75,75	0
54	MG	16	208	1/1	0.97	0.48	58,58,58,58	0
54	MG	1G	2221	1/1	0.97	0.17	68,68,68,68	0
54	MG	14	3418	1/1	0.97	0.25	59,59,59,59	0
54	MG	14	3162	1/1	0.97	0.45	44,44,44,44	0
54	MG	13	2232	1/1	0.97	0.22	64,64,64,64	0
54	MG	14	3189	1/1	0.97	0.54	76,76,76,76	0
54	MG	14	3158	1/1	0.97	0.45	56,56,56,56	0
54	MG	1H	3014	1/1	0.97	0.08	42,42,42,42	0
54	MG	1H	3003	1/1	0.97	0.11	43,43,43,43	0
54	MG	14	3122	1/1	0.97	0.35	52,52,52,52	0
54	MG	1H	3207	1/1	0.97	0.25	56,56,56,56	0
54	MG	1H	3108	1/1	0.97	0.39	30,30,30,30	0
54	MG	1H	3251	1/1	0.97	0.15	47,47,47,47	0
54	MG	14	3065	1/1	0.97	0.09	68,68,68,68	0
54	MG	14	3140	1/1	0.97	0.28	44,44,44,44	0
54	MG	14	3144	1/1	0.97	0.47	63,63,63,63	0
54	MG	1H	3185	1/1	0.97	0.26	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3401	1/1	0.97	0.30	31,31,31,31	0
54	MG	29	305	1/1	0.97	0.14	64,64,64,64	0
54	MG	1H	3072	1/1	0.97	0.04	55,55,55,55	0
54	MG	1H	3128	1/1	0.97	0.23	29,29,29,29	0
54	MG	1H	3136	1/1	0.97	0.38	47,47,47,47	0
54	MG	13	2253	1/1	0.97	0.21	49,49,49,49	0
54	MG	14	3202	1/1	0.97	0.24	42,42,42,42	0
54	MG	1H	3360	1/1	0.97	0.11	46,46,46,46	0
54	MG	1G	2255	1/1	0.97	0.27	67,67,67,67	0
54	MG	14	3195	1/1	0.97	0.37	63,63,63,63	0
54	MG	1H	3126	1/1	0.97	0.41	52,52,52,52	0
54	MG	1H	3224	1/1	0.97	0.23	42,42,42,42	0
54	MG	13	2261	1/1	0.97	0.40	53,53,53,53	0
54	MG	1H	3221	1/1	0.97	0.35	42,42,42,42	0
54	MG	13	2230	1/1	0.97	0.17	71,71,71,71	0
54	MG	14	3143	1/1	0.97	0.34	56,56,56,56	0
54	MG	14	3511	1/1	0.97	0.26	48,48,48,48	0
54	MG	1H	3002	1/1	0.97	0.11	36,36,36,36	0
54	MG	1H	3458	1/1	0.97	0.14	51,51,51,51	0
54	MG	1H	3117	1/1	0.97	0.46	42,42,42,42	0
54	MG	1G	2216	1/1	0.97	0.09	73,73,73,73	0
54	MG	1G	2211	1/1	0.97	0.08	63,63,63,63	0
54	MG	14	3096	1/1	0.97	0.28	44,44,44,44	0
54	MG	1H	3125	1/1	0.97	0.23	40,40,40,40	0
54	MG	1H	3208	1/1	0.97	0.23	32,32,32,32	0
54	MG	14	3278	1/1	0.97	0.19	39,39,39,39	0
54	MG	1H	3501	1/1	0.97	0.21	44,44,44,44	0
54	MG	14	3214	1/1	0.97	0.49	62,62,62,62	0
54	MG	14	3034	1/1	0.97	0.09	46,46,46,46	0
54	MG	14	3141	1/1	0.97	0.30	51,51,51,51	0
54	MG	14	3024	1/1	0.97	0.14	48,48,48,48	0
54	MG	13	2291	1/1	0.97	0.36	59,59,59,59	0
54	MG	98	201	1/1	0.97	0.16	56,56,56,56	0
54	MG	1G	2245	1/1	0.97	0.30	67,67,67,67	0
54	MG	1H	3184	1/1	0.97	0.34	35,35,35,35	0
54	MG	1H	3050	1/1	0.97	0.15	42,42,42,42	0
54	MG	14	3550	1/1	0.97	0.13	63,63,63,63	0
54	MG	14	3347	1/1	0.97	0.21	65,65,65,65	0
54	MG	1H	3173	1/1	0.97	0.31	50,50,50,50	0
54	MG	14	3235	1/1	0.97	0.21	45,45,45,45	0
54	MG	1H	3436	1/1	0.98	0.25	47,47,47,47	0
54	MG	1H	3522	1/1	0.98	0.30	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1H	3382	1/1	0.98	0.30	53,53,53,53	0
54	MG	1G	2308	1/1	0.98	0.31	56,56,56,56	0
54	MG	1H	3056	1/1	0.98	0.07	45,45,45,45	0
54	MG	14	3249	1/1	0.98	0.15	55,55,55,55	0
54	MG	14	3282	1/1	0.98	0.35	47,47,47,47	0
54	MG	1H	3121	1/1	0.98	0.29	44,44,44,44	0
55	ZN	32	301	1/1	0.98	0.37	90,90,90,90	0
54	MG	1H	3131	1/1	0.98	0.30	62,62,62,62	0
54	MG	14	3081	1/1	0.98	0.06	48,48,48,48	0
54	MG	14	3033	1/1	0.98	0.06	52,52,52,52	0
54	MG	W1	102	1/1	0.98	0.21	67,67,67,67	0
55	ZN	5I	101	1/1	0.98	0.12	74,74,74,74	0
54	MG	13	2204	1/1	0.98	0.07	61,61,61,61	0
54	MG	1H	3439	1/1	0.98	0.17	53,53,53,53	0
54	MG	1H	3110	1/1	0.98	0.31	47,47,47,47	0
54	MG	1H	3133	1/1	0.98	0.41	47,47,47,47	0
54	MG	1H	3206	1/1	0.98	0.39	44,44,44,44	0
54	MG	1H	3123	1/1	0.98	0.29	40,40,40,40	0
54	MG	14	3095	1/1	0.98	0.31	44,44,44,44	0
54	MG	1H	3238	1/1	0.98	0.50	57,57,57,57	0
54	MG	1H	3120	1/1	0.98	0.19	33,33,33,33	0
54	MG	14	3055	1/1	0.98	0.12	54,54,54,54	0
54	MG	14	3037	1/1	0.98	0.12	59,59,59,59	0
54	MG	14	3016	1/1	0.98	0.09	47,47,47,47	0
54	MG	1H	3106	1/1	0.98	0.21	44,44,44,44	0
54	MG	14	3283	1/1	0.98	0.21	44,44,44,44	0
54	MG	13	2370	1/1	0.98	0.08	86,86,86,86	0
54	MG	14	3035	1/1	0.98	0.12	46,46,46,46	0
54	MG	14	3392	1/1	0.98	0.27	49,49,49,49	0
54	MG	14	3176	1/1	0.98	0.70	60,60,60,60	0
54	MG	1H	3482	1/1	0.98	0.11	48,48,48,48	0
54	MG	1H	3476	1/1	0.98	0.26	52,52,52,52	0
54	MG	1H	3596	1/1	0.98	0.26	49,49,49,49	0
54	MG	14	3261	1/1	0.98	0.23	51,51,51,51	0
54	MG	14	3023	1/1	0.98	0.07	46,46,46,46	0
54	MG	14	3137	1/1	0.98	0.24	46,46,46,46	0
54	MG	88	304	1/1	0.98	0.24	48,48,48,48	0
54	MG	1H	3595	1/1	0.98	0.33	43,43,43,43	0
54	MG	1H	3105	1/1	0.98	0.36	41,41,41,41	0
54	MG	14	3129	1/1	0.98	0.48	45,45,45,45	0
54	MG	14	3568	1/1	0.98	0.23	53,53,53,53	0
54	MG	1H	3171	1/1	0.98	0.18	39,39,39,39	0

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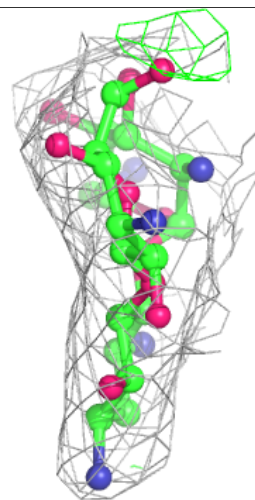
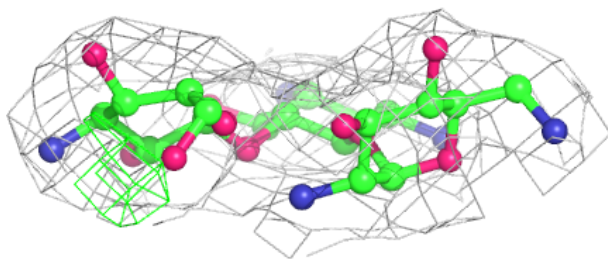
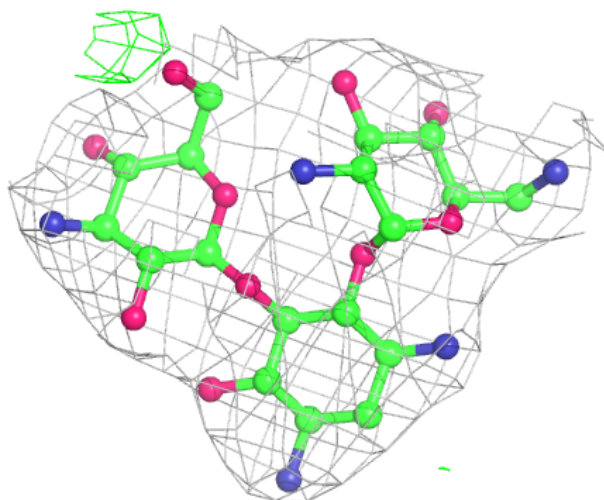
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1G	2364	1/1	0.98	0.18	93,93,93,93	0
54	MG	1G	2345	1/1	0.98	0.25	55,55,55,55	0
54	MG	1H	3028	1/1	0.98	0.15	49,49,49,49	0
54	MG	1H	3446	1/1	0.98	0.20	39,39,39,39	0
54	MG	14	3017	1/1	0.98	0.08	51,51,51,51	0
54	MG	1H	3325	1/1	0.98	0.22	60,60,60,60	0
54	MG	14	3271	1/1	0.98	0.30	68,68,68,68	0
54	MG	14	3428	1/1	0.98	0.37	47,47,47,47	0
54	MG	1G	2235	1/1	0.98	0.36	64,64,64,64	0
54	MG	1H	3441	1/1	0.98	0.25	59,59,59,59	0
54	MG	14	3186	1/1	0.98	0.22	45,45,45,45	0
54	MG	1G	2220	1/1	0.98	0.08	66,66,66,66	0
54	MG	1H	3308	1/1	0.98	0.14	32,32,32,32	0
54	MG	1H	3115	1/1	0.99	0.32	30,30,30,30	0
54	MG	14	3182	1/1	0.99	0.43	44,44,44,44	0
54	MG	4E	201	1/1	0.99	0.24	78,78,78,78	0
54	MG	1H	3149	1/1	0.99	0.34	53,53,53,53	0
54	MG	1H	3104	1/1	0.99	0.32	30,30,30,30	0
54	MG	14	3020	1/1	0.99	0.09	45,45,45,45	0
54	MG	1H	3176	1/1	0.99	0.40	40,40,40,40	0
54	MG	1H	3215	1/1	0.99	0.31	45,45,45,45	0
54	MG	14	3268	1/1	0.99	0.43	51,51,51,51	0
54	MG	1G	2265	1/1	0.99	0.18	81,81,81,81	0
54	MG	1H	3122	1/1	0.99	0.31	30,30,30,30	0
54	MG	1H	3201	1/1	0.99	0.43	33,33,33,33	0
54	MG	14	3420	1/1	0.99	0.46	44,44,44,44	0
54	MG	1G	2241	1/1	0.99	0.37	71,71,71,71	0
54	MG	13	2216	1/1	0.99	0.30	53,53,53,53	0
54	MG	14	3100	1/1	0.99	0.31	45,45,45,45	0
54	MG	14	3011	1/1	0.99	0.10	42,42,42,42	0
54	MG	14	3246	1/1	0.99	0.43	64,64,64,64	0
54	MG	1G	2204	1/1	0.99	0.12	58,58,58,58	0
54	MG	14	3132	1/1	0.99	0.37	38,38,38,38	0

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

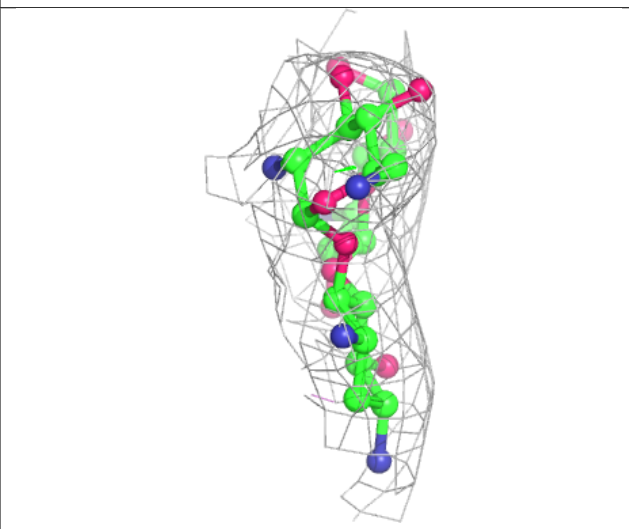
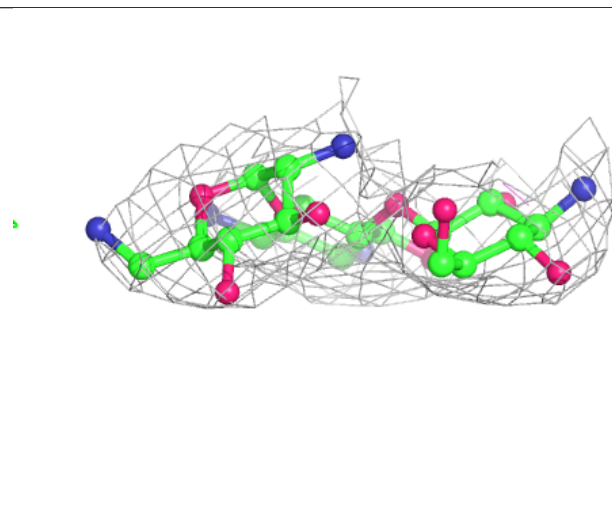
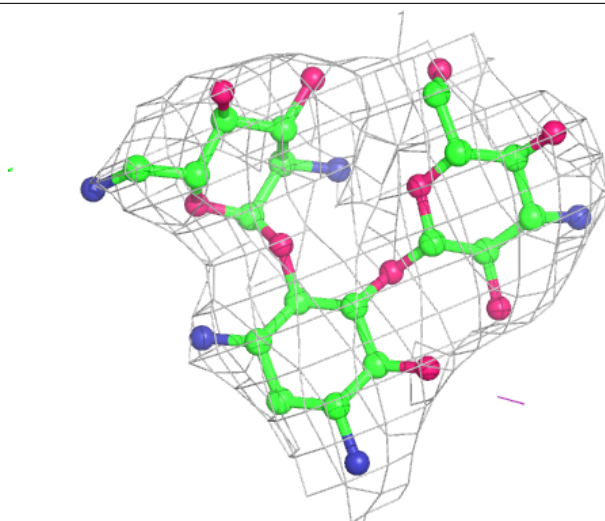
Electron density around 8UZ 13 2202:

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



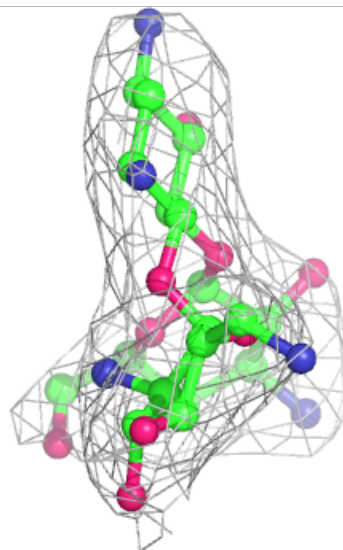
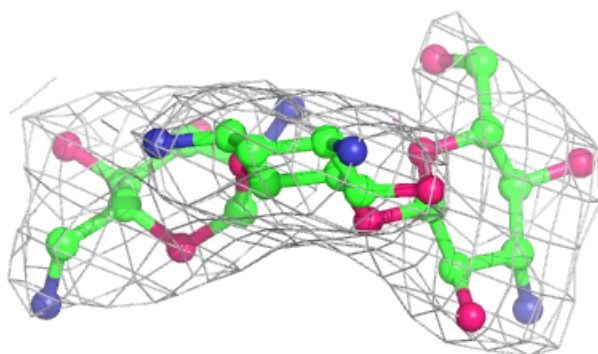
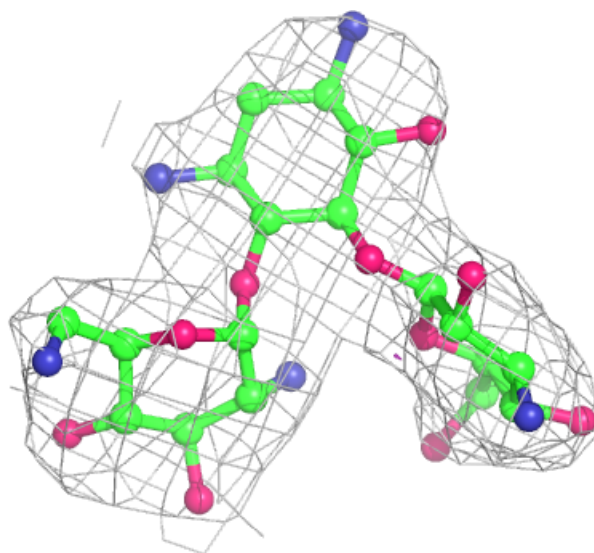
Electron density around 8UZ 1G 2202:

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



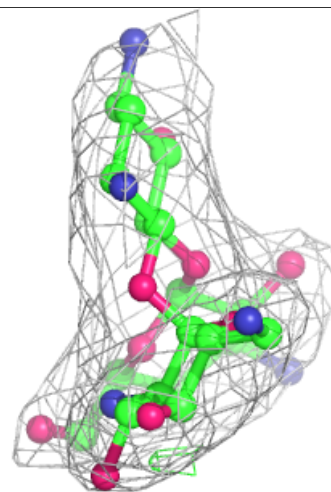
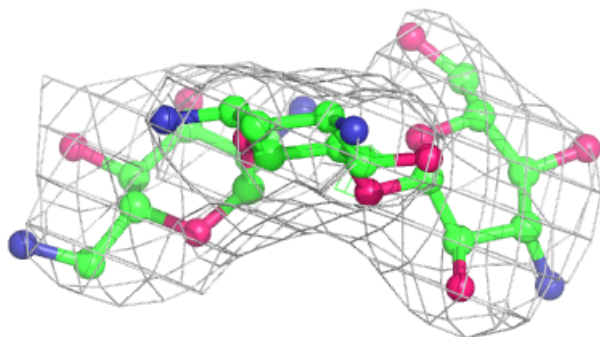
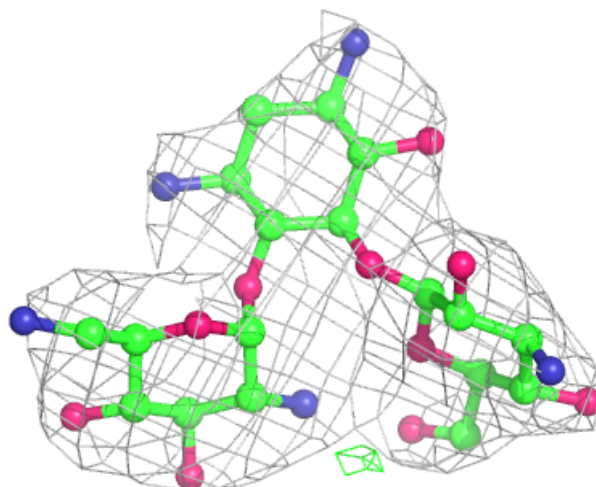
Electron density around 8UZ 13 2201:

$2mF_o-DF_c$ (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.