



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 12:38 pm BST

PDB ID : 5OBM  
Title : Crystal structure of Gentamicin bound to the yeast 80S ribosome  
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2017-06-28  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

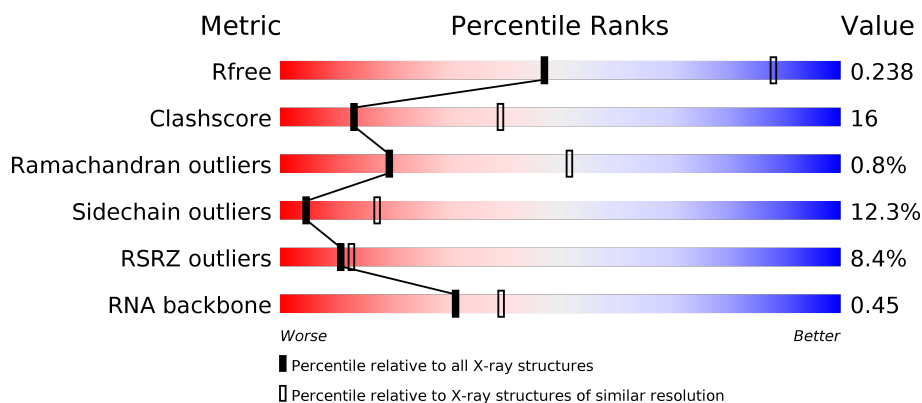
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.



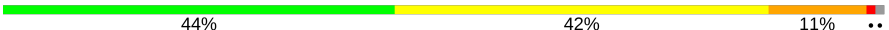

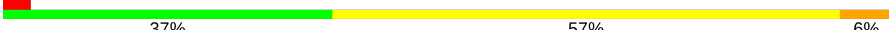

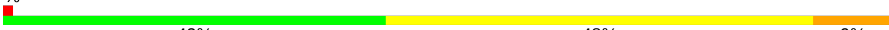




















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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

Mol	Chain	Length	Quality of chain
1	1	3396	<div> <div>37%</div> <div>38%</div> <div>13%</div> <div>9%</div> </div>
1	5	3396	<div> <div>34%</div> <div>41%</div> <div>15%</div> <div>8%</div> </div>
2	3	121	<div> <div>41%</div> <div>49%</div> <div>9%</div> </div>
2	7	121	<div> <div>34%</div> <div>50%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	4	158	
3	8	158	
4	L2	252	
4	l2	252	
5	L3	386	
5	l3	386	
6	L4	361	
6	l4	361	
7	L5	296	
7	l5	296	
8	L6	176	
8	l6	176	
9	L7	223	
9	l7	223	
10	L8	233	
10	l8	233	
11	L9	191	
11	l9	191	
12	M0	221	
12	m0	221	
13	M1	169	
13	m1	169	
14	M3	194	
14	m3	194	
15	M4	137	

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Mol	Chain	Length	Quality of chain
15	m4	137	
16	M5	203	
16	m5	203	
17	M6	197	
17	m6	197	
18	M7	184	
18	m7	184	
19	M8	185	
19	m8	185	
20	M9	188	
20	m9	188	
21	N0	172	
21	n0	172	
22	N1	159	
22	n1	159	
23	N2	100	
23	n2	100	
24	N3	136	
24	n3	136	
25	N4	155	
26	N5	121	
26	n5	121	
27	N6	126	
27	n6	126	
28	N7	135	

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Mol	Chain	Length	Quality of chain
28	n7	135	
29	N8	148	
29	n8	148	
30	N9	58	
30	n9	58	
31	O0	100	
31	o0	100	
32	O1	109	
32	o1	109	
33	O2	127	
33	o2	127	
34	O3	106	
34	o3	106	
35	O4	112	
35	o4	112	
36	O5	119	
36	o5	119	
37	O6	99	
37	o6	99	
38	O7	87	
38	o7	87	
39	O8	77	
39	o8	77	
40	O9	50	
40	o9	50	

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Mol	Chain	Length	Quality of chain
41	Q0	52	
41	q0	52	
42	Q1	25	
42	q1	25	
43	Q2	105	
43	q2	105	
44	Q3	91	
44	q3	91	
45	2	1800	
45	6	1800	
46	S0	206	
46	s0	206	
47	S1	216	
47	s1	216	
48	S2	217	
48	s2	217	
49	S3	223	
49	s3	223	
50	S4	260	
50	s4	260	
51	S5	206	
51	s5	206	
52	S6	236	
52	s6	236	
53	S7	186	

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Mol	Chain	Length	Quality of chain
53	s7	186	
54	S8	200	
54	s8	200	
55	S9	185	
55	s9	185	
56	C0	105	
56	c0	105	
57	C1	156	
57	c1	156	
58	C2	143	
58	c2	143	
59	C3	150	
59	c3	150	
60	C4	128	
60	c4	128	
61	C5	141	
61	c5	141	
62	C6	142	
62	c6	142	
63	C7	136	
63	c7	136	
64	C8	145	
64	c8	145	
65	C9	143	
65	c9	143	

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Mol	Chain	Length	Quality of chain
66	D0	110	
66	d0	110	
67	D1	87	
67	d1	87	
68	D2	129	
68	d2	129	
69	D3	144	
69	d3	144	
70	D4	134	
70	d4	134	
71	D5	70	
71	d5	70	
72	D6	97	
72	d6	97	
73	D7	81	
73	d7	81	
74	D8	63	
74	d8	63	
75	D9	53	
75	d9	53	
76	E0	62	
76	e0	62	
77	E1	72	
77	e1	72	
78	SR	318	

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Mol	Chain	Length	Quality of chain
78	sR	318	
79	SM	272	
79	sM	272	
80	m2	165	
81	n4	135	
82	p0	312	
83	p1	47	

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
84	MG	1	3444	-	-	-	X
84	MG	1	3447	-	-	-	X
84	MG	1	3461	-	-	-	X
84	MG	1	3481	-	-	-	X
84	MG	1	3483	-	-	-	X
84	MG	1	3493	-	-	-	X
84	MG	1	3495	-	-	-	X
84	MG	1	3499	-	-	-	X
84	MG	1	3508	-	-	-	X
84	MG	1	3510	-	-	-	X
84	MG	1	3514	-	-	-	X
84	MG	1	3515	-	-	-	X
84	MG	1	3521	-	-	-	X
84	MG	1	3545	-	-	-	X
84	MG	1	3627	-	-	-	X
84	MG	1	3628	-	-	-	X
84	MG	1	3667	-	-	-	X
84	MG	1	3726	-	-	-	X
84	MG	1	3738	-	-	-	X
84	MG	1	3742	-	-	-	X
84	MG	1	3758	-	-	-	X
84	MG	1	3759	-	-	-	X
84	MG	1	3763	-	-	-	X
84	MG	1	3764	-	-	-	X
84	MG	1	3769	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	1	3782	-	-	-	X
84	MG	1	3803	-	-	-	X
84	MG	1	3804	-	-	-	X
84	MG	1	3815	-	-	-	X
84	MG	1	3816	-	-	-	X
84	MG	1	3818	-	-	-	X
84	MG	1	3820	-	-	-	X
84	MG	1	3823	-	-	-	X
84	MG	1	3827	-	-	-	X
84	MG	1	3829	-	-	-	X
84	MG	1	3842	-	-	-	X
84	MG	1	3847	-	-	-	X
84	MG	1	3865	-	-	-	X
84	MG	1	3873	-	-	-	X
84	MG	1	3876	-	-	-	X
84	MG	1	3879	-	-	-	X
84	MG	1	3880	-	-	-	X
84	MG	1	3932	-	-	-	X
84	MG	1	3934	-	-	-	X
84	MG	1	3948	-	-	-	X
84	MG	1	3950	-	-	-	X
84	MG	1	3952	-	-	-	X
84	MG	1	3955	-	-	-	X
84	MG	1	3985	-	-	-	X
84	MG	2	1913	-	-	-	X
84	MG	2	1929	-	-	-	X
84	MG	2	1931	-	-	-	X
84	MG	2	1940	-	-	-	X
84	MG	2	1977	-	-	-	X
84	MG	2	1978	-	-	-	X
84	MG	2	1979	-	-	-	X
84	MG	2	1980	-	-	-	X
84	MG	2	1984	-	-	-	X
84	MG	2	2001	-	-	-	X
84	MG	2	2004	-	-	-	X
84	MG	2	2015	-	-	-	X
84	MG	2	2017	-	-	-	X
84	MG	3	206	-	-	-	X
84	MG	3	208	-	-	-	X
84	MG	4	206	-	-	-	X
84	MG	4	208	-	-	-	X
84	MG	4	221	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	5	3442	-	-	-	X
84	MG	5	3469	-	-	-	X
84	MG	5	3492	-	-	-	X
84	MG	5	3524	-	-	-	X
84	MG	5	3526	-	-	-	X
84	MG	5	3542	-	-	-	X
84	MG	5	3558	-	-	-	X
84	MG	5	3563	-	-	-	X
84	MG	5	3564	-	-	-	X
84	MG	5	3574	-	-	-	X
84	MG	5	3577	-	-	-	X
84	MG	5	3583	-	-	-	X
84	MG	5	3588	-	-	-	X
84	MG	5	3591	-	-	-	X
84	MG	5	3593	-	-	-	X
84	MG	5	3594	-	-	-	X
84	MG	5	3601	-	-	-	X
84	MG	5	3624	-	-	-	X
84	MG	5	3634	-	-	-	X
84	MG	5	3645	-	-	-	X
84	MG	5	3664	-	-	-	X
84	MG	5	3697	-	-	-	X
84	MG	5	3706	-	-	-	X
84	MG	5	3751	-	-	-	X
84	MG	5	3755	-	-	-	X
84	MG	5	3766	-	-	-	X
84	MG	5	3768	-	-	-	X
84	MG	5	3775	-	-	-	X
84	MG	5	3813	-	-	-	X
84	MG	5	3855	-	-	-	X
84	MG	5	3859	-	-	-	X
84	MG	5	3863	-	-	-	X
84	MG	5	3868	-	-	-	X
84	MG	5	3869	-	-	-	X
84	MG	5	3878	-	-	-	X
84	MG	5	3896	-	-	-	X
84	MG	5	3904	-	-	-	X
84	MG	5	3915	-	-	-	X
84	MG	5	3934	-	-	-	X
84	MG	5	3936	-	-	-	X
84	MG	5	3948	-	-	-	X
84	MG	5	3954	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	5	3958	-	-	-	X
84	MG	5	3965	-	-	-	X
84	MG	5	3966	-	-	-	X
84	MG	5	3970	-	-	-	X
84	MG	5	3974	-	-	-	X
84	MG	5	3975	-	-	-	X
84	MG	5	3984	-	-	-	X
84	MG	5	4007	-	-	-	X
84	MG	5	4030	-	-	-	X
84	MG	5	4046	-	-	-	X
84	MG	5	4052	-	-	-	X
84	MG	5	4097	-	-	-	X
84	MG	5	4129	-	-	-	X
84	MG	6	1901	-	-	-	X
84	MG	6	1903	-	-	-	X
84	MG	6	1933	-	-	-	X
84	MG	6	1940	-	-	-	X
84	MG	6	1944	-	-	-	X
84	MG	6	1945	-	-	-	X
84	MG	6	1960	-	-	-	X
84	MG	6	1967	-	-	-	X
84	MG	6	1968	-	-	-	X
84	MG	6	1989	-	-	-	X
84	MG	6	1991	-	-	-	X
84	MG	6	1992	-	-	-	X
84	MG	6	1993	-	-	-	X
84	MG	6	2090	-	-	-	X
84	MG	6	2106	-	-	-	X
84	MG	6	2107	-	-	-	X
84	MG	6	2121	-	-	-	X
84	MG	8	201	-	-	-	X
84	MG	8	213	-	-	-	X
84	MG	8	216	-	-	-	X
84	MG	D3	204	-	-	-	X
84	MG	S2	301	-	-	-	X
84	MG	c1	201	-	-	-	X
84	MG	c3	201	-	-	-	X
84	MG	d1	101	-	-	-	X
84	MG	d3	201	-	-	-	X
84	MG	l3	406	-	-	-	X
84	MG	l3	408	-	-	-	X
84	MG	l8	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	m6	208	-	-	-	X
84	MG	m7	207	-	-	-	X
84	MG	m8	202	-	-	-	X

## 2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 404238 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3100	Total	C	N	O	P	0	0	0
			66304	29617	11950	21637	3100			
1	5	3134	Total	C	N	O	P	0	0	0
			67039	29943	12089	21873	3134			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	156	Total	C	N	O	P	0	0	0
			3313	1482	582	1093	156			
3	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
4	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			
5	l3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			
6	l4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L8	233	Total	C	N	O	S	0	0	0
			1817	1159	326	329	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
11	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M0	212	Total	C	N	O	S	0	0	0
			1707	1084	323	295	5			
12	m0	211	Total	C	N	O	S	0	0	0
			1716	1090	324	296	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
13	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M3	193	Total	C	N	O	0	0	0
			1543	962	315	266			
14	m3	194	Total	C	N	O	0	0	0
			1548	965	316	267			

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M4	136	Total	C	N	O	0	0	0
			1053	675	199	177			
15	m4	137	Total	C	N	O	0	0	0
			1059	678	200	179			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	M7	183	Total	C	N	O	S	0	0	0
			1415	877	281	257				
18	m7	155	Total	C	N	O	S	0	0	0
			1227	764	238	225				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	M9	182	Total	C	N	O	S	0	0	0
			1474	905	319	250				
20	m9	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	N2	100	Total	C	N	O		0	0	0
			796	516	131	149				
23	n2	98	Total	C	N	O		0	0	0
			778	505	127	146				

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
26	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
27	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
28	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
29	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
30	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
31	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	O1	109	Total	C	N	O	S	0	0	0
			890	565	168	156	1			
32	o1	109	Total	C	N	O	S	0	0	0
			890	565	168	156	1			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
33	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
34	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	O4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			
35	o4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
36	o5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	o6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
38	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	O8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				
39	o8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
40	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
41	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
42	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
43	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
44	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 45 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	2	1712	Total	C	N	O	P	0	0	0
			36488	16313	6466	11997	1712			
45	6	1739	Total	C	N	O	P	0	0	0
			37060	16570	6568	12183	1739			

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	S0	206	Total	C	N	O	S	0	0	0
			1612	1034	285	291	2			
46	s0	206	Total	C	N	O	S	0	0	0
			1612	1034	285	291	2			

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
47	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 48 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
48	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
49	s3	223	Total	C	N	O	S	0	0	0
			1728	1098	310	314	6			

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
50	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 51 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
51	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	S6	226	Total	C	N	O	S	0	0	0
			1813	1137	350	323	3			
52	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
54	s8	186	Total	C	N	O	S	0	0	0
			1471	913	294	262	2			

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
55	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
56	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
57	c1	142	Total	C	N	O	S	0	0	0
			1138	729	217	189	3			

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
58	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 59 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
59	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 60 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
60	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
61	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
62	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	C7	120	Total	C	N	O	S	0	0	0
			965	603	183	177	2			
63	c7	117	Total	C	N	O	S	0	0	0
			917	569	175	171	2			

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
64	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
65	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 66 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
66	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
67	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
68	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	D4	134	Total	C	N	O		0	0	0
			1073	676	208	189				
70	d4	133	Total	C	N	O		0	0	0
			1065	672	207	186				

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	D5	70	Total	C	N	O		0	0	0
			563	360	104	99				
71	d5	69	Total	C	N	O		0	0	0
			558	357	103	98				

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
72	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
73	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
74	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	D9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			
75	d9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
76	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
77	e1	72	Total	C	N	O	S	0	0	0
			575	368	108	95	4			

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	SR	318	Total	C	N	O	S	0	0	0
			2441	1543	418	472	8			
78	sR	318	Total	C	N	O	S	0	0	0
			2441	1543	418	472	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011
sR	161	ALA	LYS	conflict	UNP P38011

- Molecule 79 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
79	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
79	sM	129	Total	C	N	O	0	0	0
			923	546	184	193			

- Molecule 80 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 81 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	n4	135	Total	C	N	O	S	0	0	0
			1044	654	209	180	1			

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 83 is a protein called Ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	s0	1	Total	Mg	0	0
			1	1		
84	n8	3	Total	Mg	0	0
			3	3		
84	N0	4	Total	Mg	0	0
			4	4		
84	S3	1	Total	Mg	0	0
			1	1		
84	N5	1	Total	Mg	0	0
			1	1		
84	d2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	s3	1	Total 1	Mg 1	0	0
84	n5	3	Total 3	Mg 3	0	0
84	q0	1	Total 1	Mg 1	0	0
84	c1	1	Total 1	Mg 1	0	0
84	o1	1	Total 1	Mg 1	0	0
84	L5	1	Total 1	Mg 1	0	0
84	O2	4	Total 4	Mg 4	0	0
84	m9	2	Total 2	Mg 2	0	0
84	M3	5	Total 5	Mg 5	0	0
84	S4	1	Total 1	Mg 1	0	0
84	l5	6	Total 6	Mg 6	0	0
84	o2	3	Total 3	Mg 3	0	0
84	d5	1	Total 1	Mg 1	0	0
84	d9	1	Total 1	Mg 1	0	0
84	m3	4	Total 4	Mg 4	0	0
84	2	142	Total 142	Mg 142	0	0
84	M6	1	Total 1	Mg 1	0	0
84	l6	2	Total 2	Mg 2	0	0
84	m6	8	Total 8	Mg 8	0	0
84	n9	1	Total 1	Mg 1	0	0
84	M5	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	S2	1	Total 1	Mg 1	0	0
84	m5	3	Total 3	Mg 3	0	0
84	s4	1	Total 1	Mg 1	0	0
84	s2	2	Total 2	Mg 2	0	0
84	M8	1	Total 1	Mg 1	0	0
84	q3	3	Total 3	Mg 3	0	0
84	N3	4	Total 4	Mg 4	0	0
84	4	23	Total 23	Mg 23	0	0
84	L2	5	Total 5	Mg 5	0	0
84	m8	4	Total 4	Mg 4	0	0
84	n3	2	Total 2	Mg 2	0	0
84	l2	5	Total 5	Mg 5	0	0
84	c3	6	Total 6	Mg 6	0	0
84	L7	1	Total 1	Mg 1	0	0
84	D3	5	Total 5	Mg 5	0	0
84	6	263	Total 263	Mg 263	0	0
84	d7	1	Total 1	Mg 1	0	0
84	O4	3	Total 3	Mg 3	0	0
84	C1	1	Total 1	Mg 1	0	0
84	n0	7	Total 7	Mg 7	0	0
84	l7	3	Total 3	Mg 3	0	0

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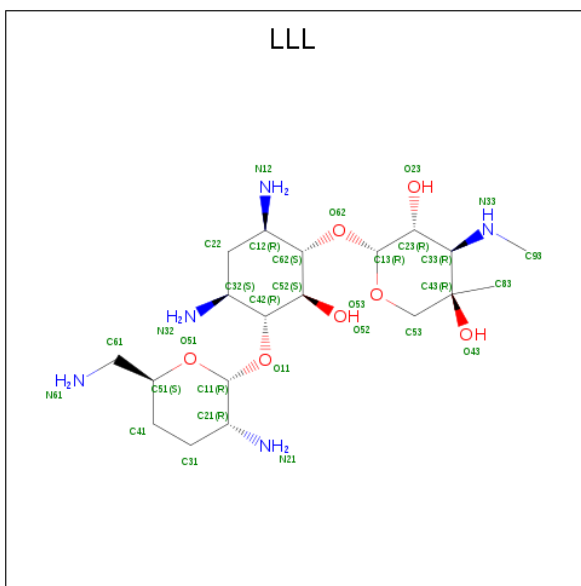
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	L8	1	Total 1	Mg 1	0	0
84	o4	2	Total 2	Mg 2	0	0
84	O7	3	Total 3	Mg 3	0	0
84	s6	1	Total 1	Mg 1	0	0
84	1	588	Total 588	Mg 588	0	0
84	S1	1	Total 1	Mg 1	0	0
84	c4	1	Total 1	Mg 1	0	0
84	l8	1	Total 1	Mg 1	0	0
84	Q2	4	Total 4	Mg 4	0	0
84	m4	6	Total 6	Mg 6	0	0
84	d6	3	Total 3	Mg 3	0	0
84	q2	7	Total 7	Mg 7	0	0
84	N4	1	Total 1	Mg 1	0	0
84	Q1	1	Total 1	Mg 1	0	0
84	L3	3	Total 3	Mg 3	0	0
84	8	20	Total 20	Mg 20	0	0
84	3	19	Total 19	Mg 19	0	0
84	d1	2	Total 2	Mg 2	0	0
84	q1	2	Total 2	Mg 2	0	0
84	l3	11	Total 11	Mg 11	0	0
84	N1	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	C8	1	Total 1	Mg 1	0	0
84	O3	1	Total 1	Mg 1	0	0
84	L4	6	Total 6	Mg 6	0	0
84	M0	4	Total 4	Mg 4	0	0
84	5	750	Total 750	Mg 750	0	0
84	n1	2	Total 2	Mg 2	0	0
84	c8	3	Total 3	Mg 3	0	0
84	l4	2	Total 2	Mg 2	0	0
84	L9	1	Total 1	Mg 1	0	0
84	d3	5	Total 5	Mg 5	0	0
84	o3	2	Total 2	Mg 2	0	0
84	m0	2	Total 2	Mg 2	0	0
84	O6	1	Total 1	Mg 1	0	0
84	s5	3	Total 3	Mg 3	0	0
84	C3	1	Total 1	Mg 1	0	0
84	M7	5	Total 5	Mg 5	0	0
84	N8	3	Total 3	Mg 3	0	0
84	l9	8	Total 8	Mg 8	0	0
84	sR	1	Total 1	Mg 1	0	0
84	7	30	Total 30	Mg 30	0	0
84	m7	7	Total 7	Mg 7	0	0

- Molecule 85 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C<sub>19</sub>H<sub>39</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	3	1	Total	C	N	O	0	0
			31	19	5	7		
85	4	1	Total	C	N	O	0	0
			31	19	5	7		
85	L3	1	Total	C	N	O	0	0
			31	19	5	7		
85	2	1	Total	C	N	O	0	0
			31	19	5	7		
85	2	1	Total	C	N	O	0	0
			31	19	5	7		
85	2	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	5	1	Total	C	N	O	0	0
			31	19	5	7		
85	7	1	Total	C	N	O	0	0
			31	19	5	7		
85	7	1	Total	C	N	O	0	0
			31	19	5	7		
85	7	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
85	8	1	Total	C	N	O	0	0
			31	19	5	7		
85	8	1	Total	C	N	O	0	0
			31	19	5	7		
85	l3	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		
85	6	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	o4	1	Total	Zn	0	0
			1	1		
86	O7	1	Total	Zn	0	0
			1	1		
86	q3	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	q0	1	Total 1	Zn 1	0	0
86	Q2	1	Total 1	Zn 1	0	0
86	e1	1	Total 1	Zn 1	0	0
86	Q3	1	Total 1	Zn 1	0	0
86	D9	1	Total 1	Zn 1	0	0
86	E1	1	Total 1	Zn 1	0	0
86	Q0	1	Total 1	Zn 1	0	0
86	d7	1	Total 1	Zn 1	0	0
86	O4	1	Total 1	Zn 1	0	0
86	d9	1	Total 1	Zn 1	0	0
86	D7	1	Total 1	Zn 1	0	0
86	d6	1	Total 1	Zn 1	0	0
86	o7	1	Total 1	Zn 1	0	0
86	D6	1	Total 1	Zn 1	0	0
86	q2	1	Total 1	Zn 1	0	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	1	473	Total 473	O 473	0	0
87	3	15	Total 15	O 15	0	0
87	4	5	Total 5	O 5	0	0
87	L2	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L3	7	Total 7	O 7	0	0
87	L4	2	Total 2	O 2	0	0
87	L5	2	Total 2	O 2	0	0
87	M0	1	Total 1	O 1	0	0
87	M3	2	Total 2	O 2	0	0
87	M5	3	Total 3	O 3	0	0
87	M6	6	Total 6	O 6	0	0
87	M7	5	Total 5	O 5	0	0
87	N0	4	Total 4	O 4	0	0
87	N1	3	Total 3	O 3	0	0
87	N3	5	Total 5	O 5	0	0
87	N4	2	Total 2	O 2	0	0
87	N5	2	Total 2	O 2	0	0
87	N8	3	Total 3	O 3	0	0
87	N9	2	Total 2	O 2	0	0
87	O2	2	Total 2	O 2	0	0
87	O4	1	Total 1	O 1	0	0
87	O7	1	Total 1	O 1	0	0
87	Q1	1	Total 1	O 1	0	0
87	Q2	1	Total 1	O 1	0	0
87	2	111	Total 111	O 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	S1	1	Total 1	O 1	0	0
87	S3	3	Total 3	O 3	0	0
87	S4	1	Total 1	O 1	0	0
87	S8	1	Total 1	O 1	0	0
87	C9	2	Total 2	O 2	0	0
87	D0	1	Total 1	O 1	0	0
87	D3	1	Total 1	O 1	0	0
87	SR	2	Total 2	O 2	0	0
87	5	514	Total 514	O 514	0	0
87	7	33	Total 33	O 33	0	0
87	8	11	Total 11	O 11	0	0
87	12	7	Total 7	O 7	0	0
87	13	6	Total 6	O 6	0	0
87	15	5	Total 5	O 5	0	0
87	19	3	Total 3	O 3	0	0
87	m0	1	Total 1	O 1	0	0
87	m4	1	Total 1	O 1	0	0
87	m5	2	Total 2	O 2	0	0
87	m6	8	Total 8	O 8	0	0
87	m7	4	Total 4	O 4	0	0
87	m9	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	n0	4	Total 4	O 4	0	0
87	n1	2	Total 2	O 2	0	0
87	n3	2	Total 2	O 2	0	0
87	n4	1	Total 1	O 1	0	0
87	n5	2	Total 2	O 2	0	0
87	n6	1	Total 1	O 1	0	0
87	n8	4	Total 4	O 4	0	0
87	n9	1	Total 1	O 1	0	0
87	o0	1	Total 1	O 1	0	0
87	o1	2	Total 2	O 2	0	0
87	o2	4	Total 4	O 4	0	0
87	o4	2	Total 2	O 2	0	0
87	q0	1	Total 1	O 1	0	0
87	q2	2	Total 2	O 2	0	0
87	q3	3	Total 3	O 3	0	0
87	6	224	Total 224	O 224	0	0
87	s4	1	Total 1	O 1	0	0
87	s5	1	Total 1	O 1	0	0
87	s7	1	Total 1	O 1	0	0
87	c3	5	Total 5	O 5	0	0
87	c6	1	Total 1	O 1	0	0

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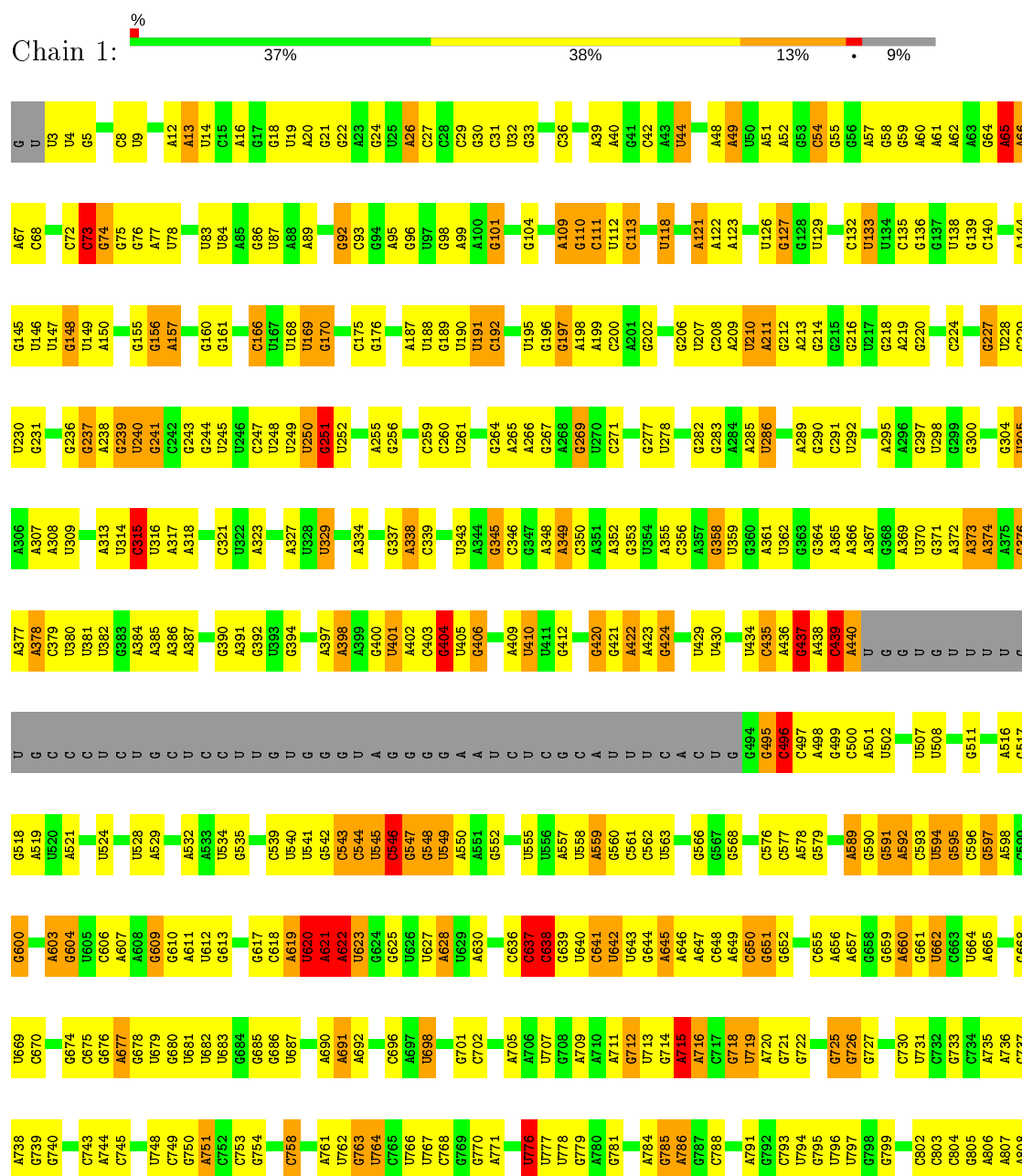
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	c8	3	Total 3	O 3	0	0
87	c9	5	Total 5	O 5	0	0
87	d3	5	Total 5	O 5	0	0
87	d5	3	Total 3	O 3	0	0
87	d6	3	Total 3	O 3	0	0
87	d9	2	Total 2	O 2	0	0
87	e1	1	Total 1	O 1	0	0
87	sR	1	Total 1	O 1	0	0

### 3 Residue-property plots

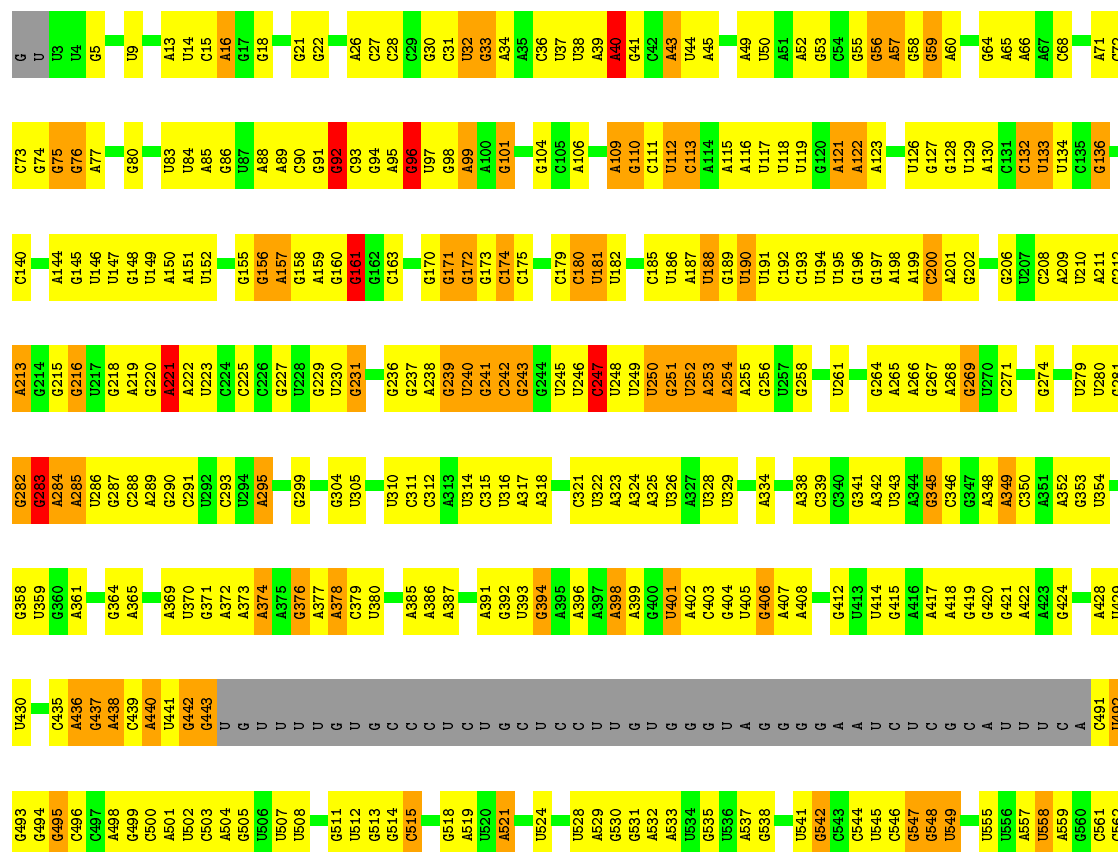
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 25S ribosomal RNA



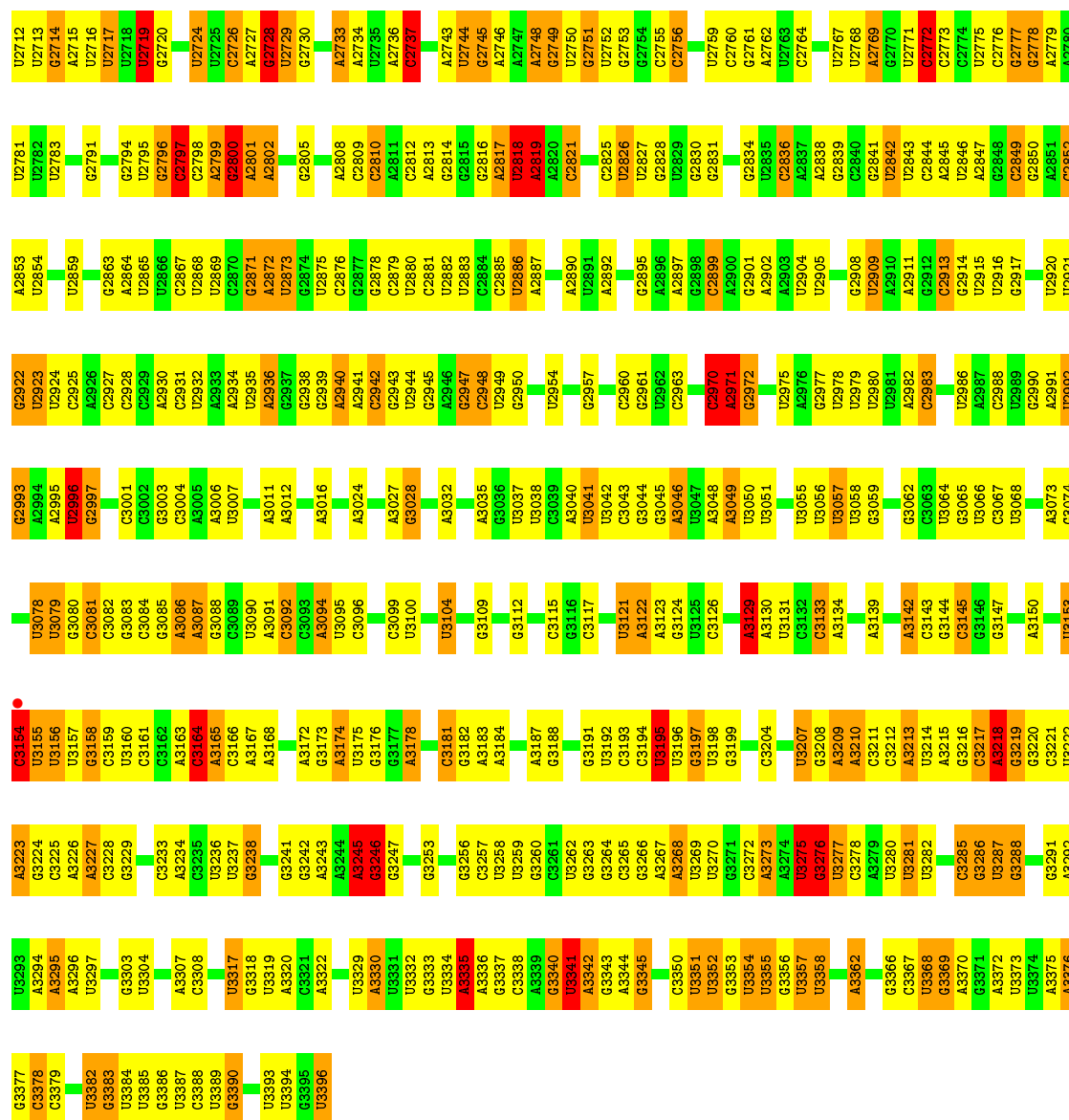
U1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1829	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850											
G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1666	G1667	G1668	G1669	G1679	G1680	G1681	G1682	G1683	G1686	G1687	G1688	G1689	G1693	G1700	G1701	G1702	G1703				
G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1611	G1612	G1613	G1614	G1615					
A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1514	A1517	A1522	A1523	A1524	A1525	A1526	A1527	A1536	A1537	A1538	A1539	A1546				
G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456			
U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1366	U1367	U1368	U1369	U1373	U1377	U1381	U1382	U1383	U1384	U1385	U1386	U1388							
A	A	U	C	C	G	G	C	C	U	A	A	G	G	G	G	G	G	G	U	U	A	A	C	A	A	A	C	A	A	C	C	U	C	A1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1292	C1293	C1294	C1295	C1296	C1297	C1298	A1301	A1302	A1303	A1304	U1305	G1306	G1307	G1308	A1309	G1313	C1314					
U1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1176	G1177	G1178	G1179	A1180	U1181	G1182	G1183	G1184	G1185	G1186
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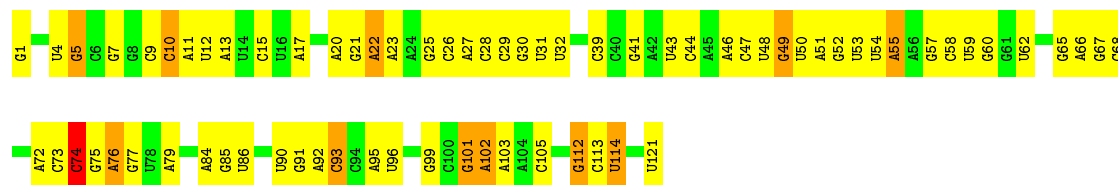
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U2514	C2393	C2393	U2318	G2249	A2167	U	G	U	U1833	C1762	U1686
A2515	C2394	C2394	U2319	G2250	A2168	C	G	U	U1834	U1764	U1687
G2519	G2395	G2395	G2320	G2251	G2169	C	C	U	G1838	U1765	U1688
A2520	G2396	G2396	A2324	A2252	U2170	U	U	U	A1839	G1766	U1689
G2521	A2397	A2397	G2325	G2253		C	C	U	U1840	G1767	C1690
A2522	A2398	A2398	A2326	U2254	U2173	C	A	U	A1841	U1768	U1691
C2523	A2399	A2399	U2327	G2255	G2174	C	U	U	C1842	U1769	U1692
A2524	G2400	G2400	G2328	A2256	U2175	C	C	U	A1843	G1770	A1696
U2525	G2401	G2401	U2329	G2257	U2176	U	G	U	G1844	C1771	
U2526	A2402	A2402	C2330	U2258	G2177	U	G	U	G1845	U1772	
C2527	G2403	G2403	G2331	A2259	A2178	U	C	U	C1846	A1699	
G2528	A2404	A2404	A2332	U2260	G2179	U	C	U	A1847	G1700	
A2529	C2405	C2405	G2333	G2261	G2180	G	U	U	G1848	G1776	
G2530	C2406	C2406	U2334	A2262	A2181	U	U	U	C1849	U1777	A1704
C2531	C2407	C2407	G2335	C2263	A2182	A	G	U	C1923	G1778	U1705
U2532	U2410	U2410	U2336	U2264	A2183	C	C	U	U1924	C1779	C1706
G2533	U2411	U2411	G2337	C2265		A	U	U	U1925	G1780	
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A2535	A2413	A2413	A2341	C2267	G2187	G	U	U	A1930	G1784	G1712
U2537	G2414	G2414	U2342	U2268	A2188	C	G	U	U1931	A1785	A1745
C2538	U2415	U2415	G2343	U2269	G2189	C	G	U	G1857	U1786	U1746
C2539	U2416	U2416	U2344	A2270	A2192	U	A	U	A1858	U1787	U1717
A2540	U2417	U2417	A2345	G2271	U2193	U	C	U	G1859	G1718	
U2541	G2418	G2418	G2346	G2272	G2194	G	U	U	G1860	C1793	
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C2546	U2421	U2421	U2349	C2276	A2198	U	U	U	G1939	G1796	U1724
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C2555	U2428	U2428	A2357	G2284	A2207	U	C	U	U1947	U1877	G1735
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C2557	U2433	U2433	C2360	C2290	U2209	U	U	U	G1949	U1880	U1737
U2634	U2434	U2434		A2291	G2210	A	U	U	U1950	A1810	C1738
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• Molecule 2: 5S Ribosomal RNA

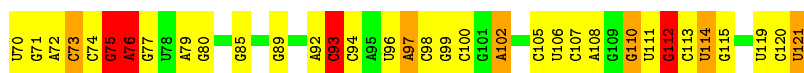
Chain 3: 41% 49% 9% .



• Molecule 2: 5S Ribosomal RNA

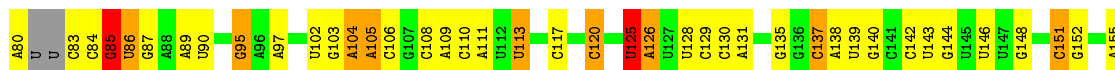
Chain 7: 34% 50% 12% .





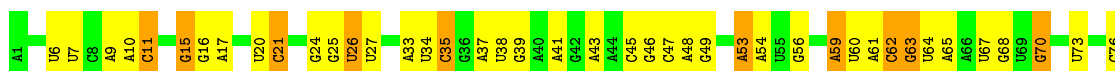
• Molecule 3: 5.8S ribosomal RNA

Chain 4: 44% 42% 11% ..



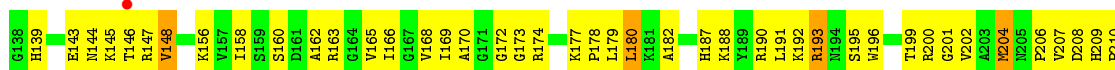
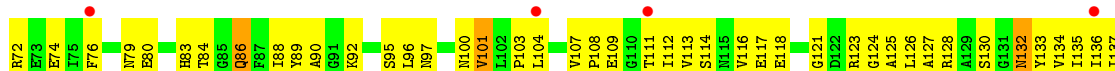
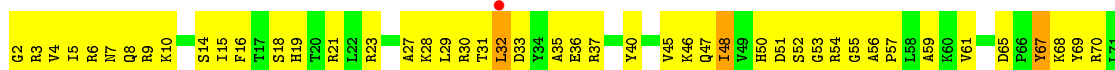
• Molecule 3: 5.8S ribosomal RNA

Chain 8: 36% 44% 18% .



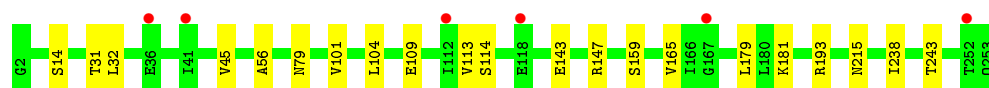
• Molecule 4: 60S ribosomal protein L2-A

Chain L2: 3% 37% 57% 6%

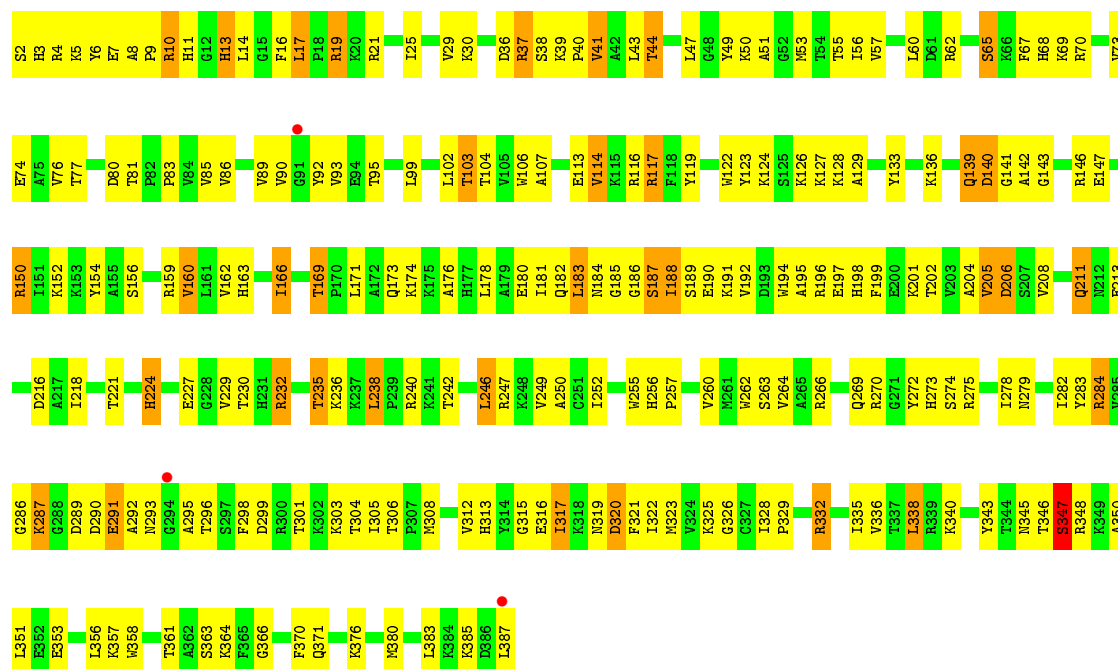
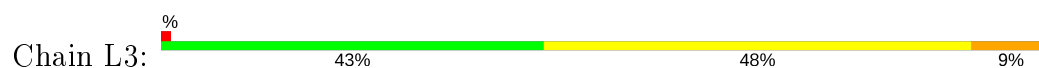


• Molecule 4: 60S ribosomal protein L2-A

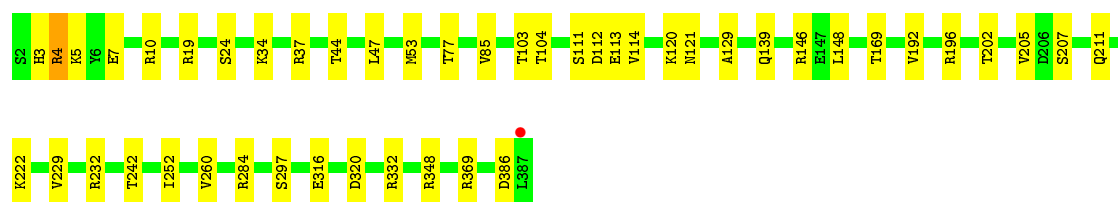
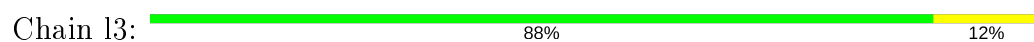
Chain l2: 2% 92% 8%



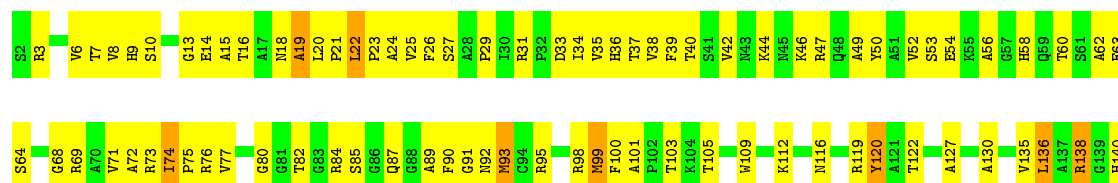
• Molecule 5: 60S ribosomal protein L3

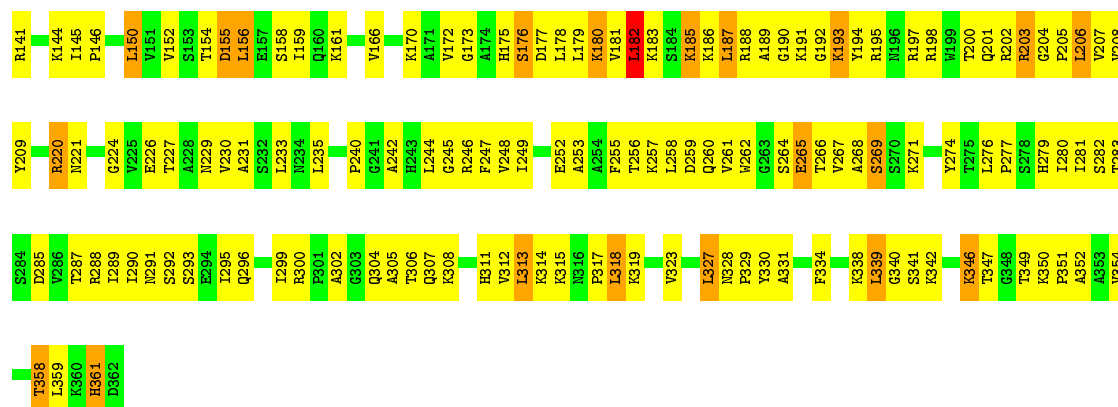


• Molecule 5: 60S ribosomal protein L3

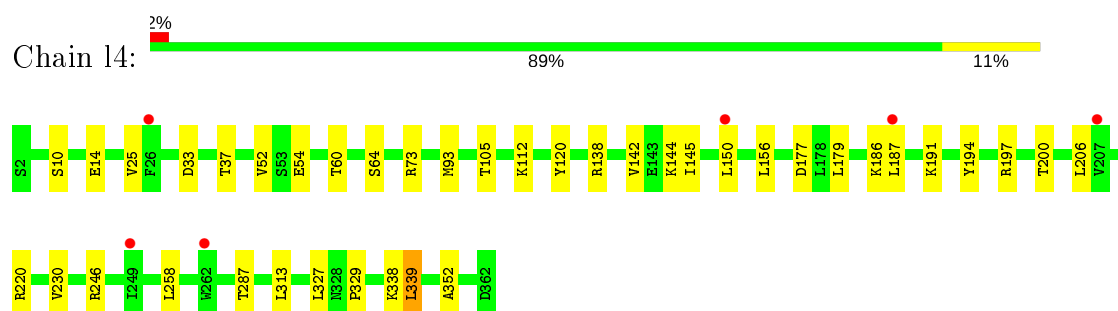


• Molecule 6: 60S ribosomal protein L4-A

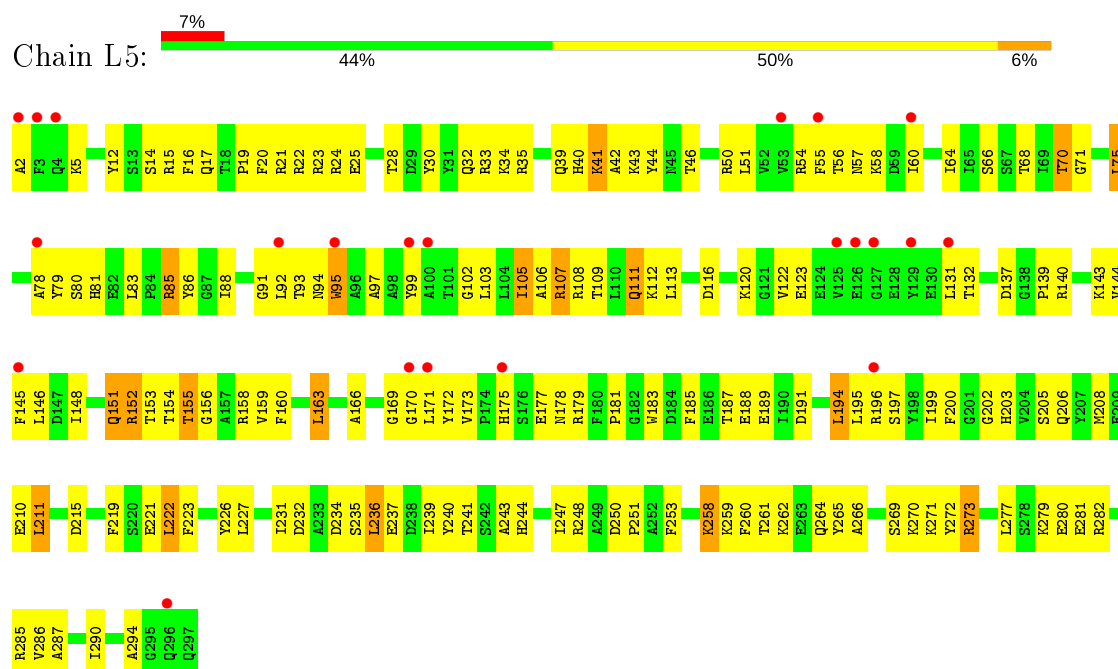




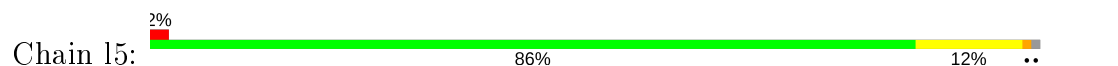
• Molecule 6: 60S ribosomal protein L4-A

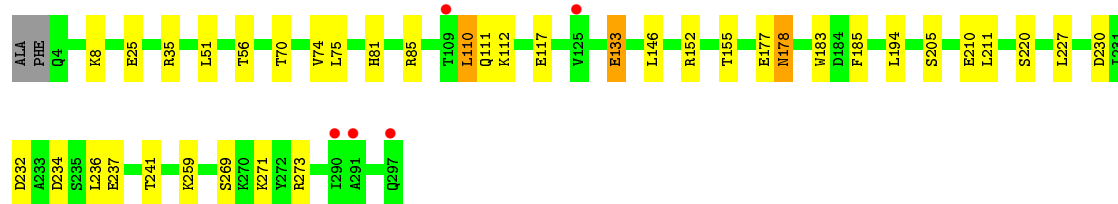


• Molecule 7: 60S ribosomal protein L5

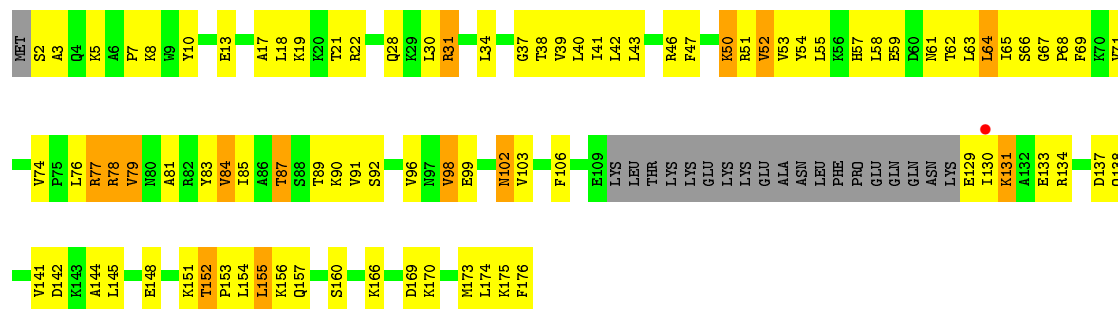


• Molecule 7: 60S ribosomal protein L5

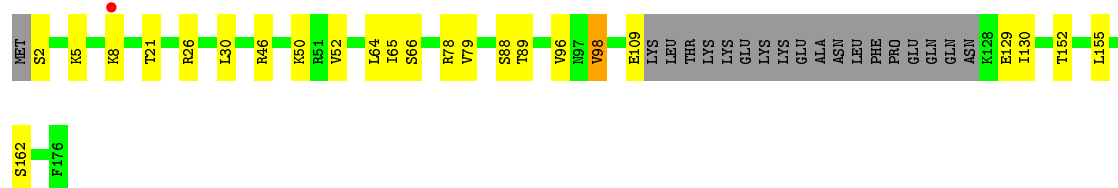
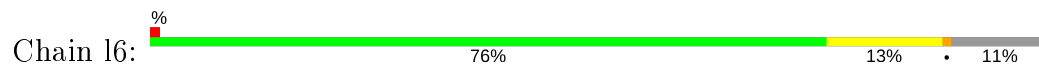




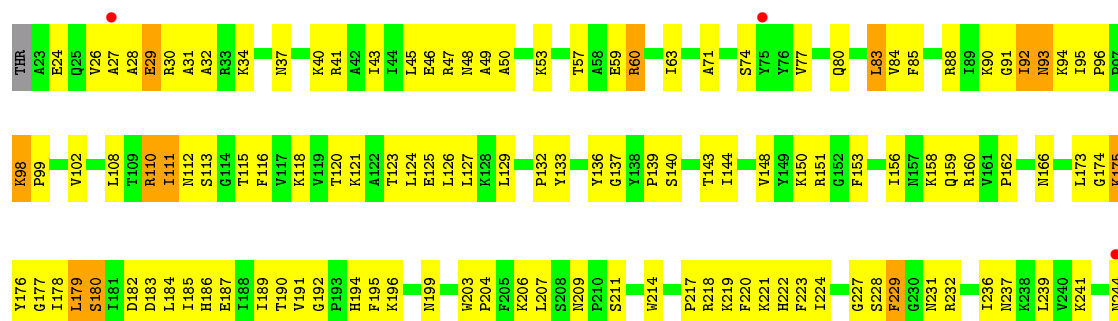
• Molecule 8: 60S ribosomal protein L6-A



• Molecule 8: 60S ribosomal protein L6-A



• Molecule 9: 60S ribosomal protein L7-A

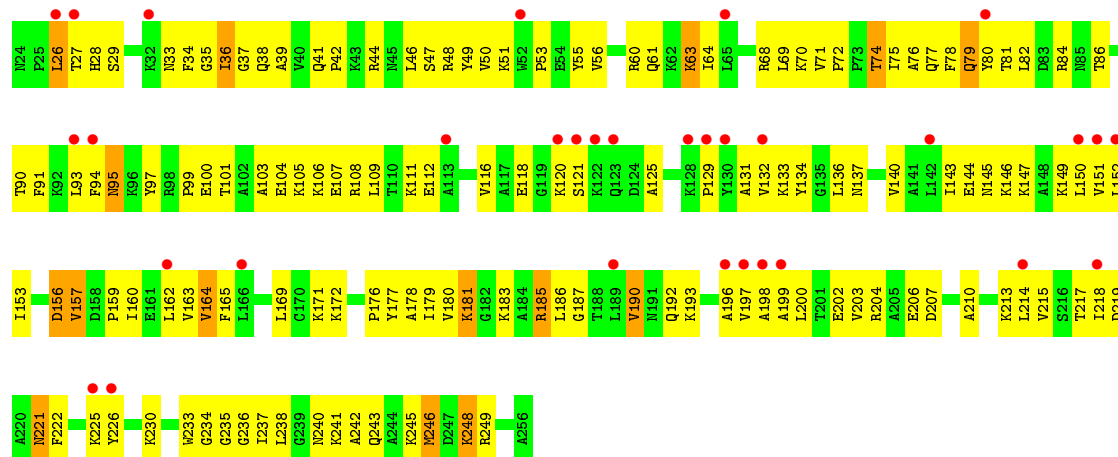


• Molecule 9: 60S ribosomal protein L7-A

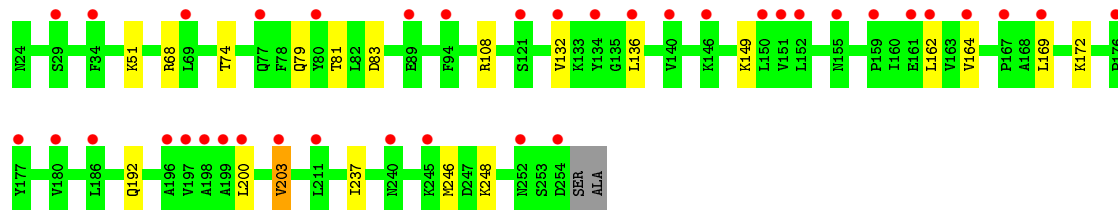




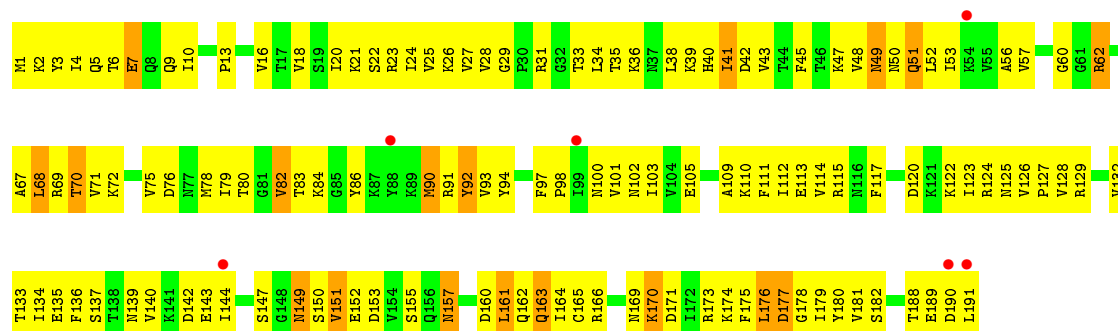
• Molecule 10: 60S ribosomal protein L8-A



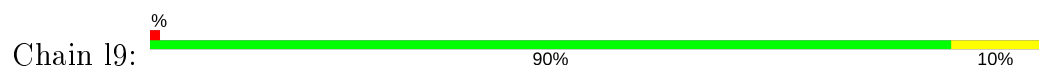
• Molecule 10: 60S ribosomal protein L8-A



• Molecule 11: 60S ribosomal protein L9-A

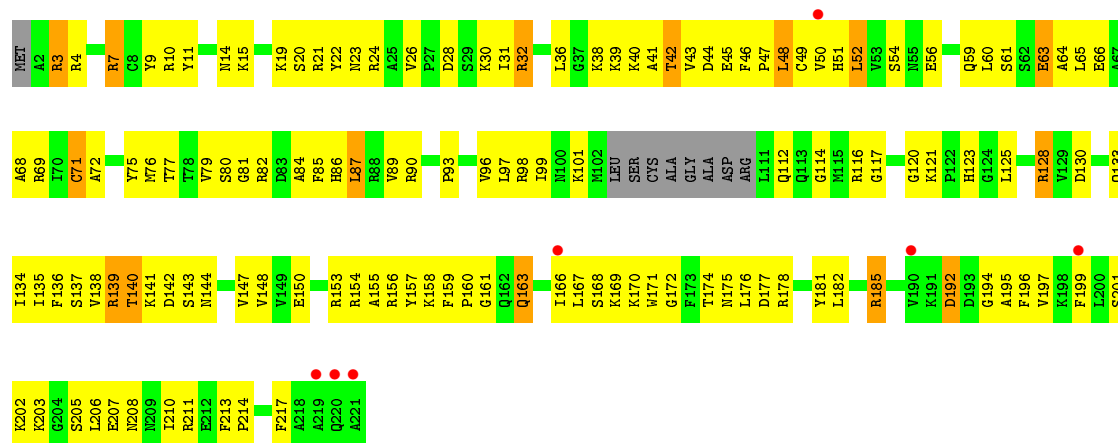


• Molecule 11: 60S ribosomal protein L9-A

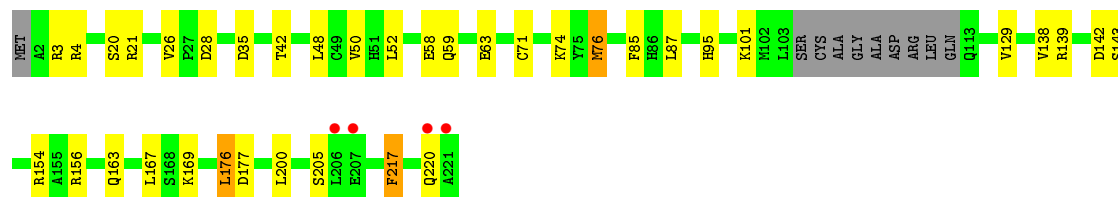
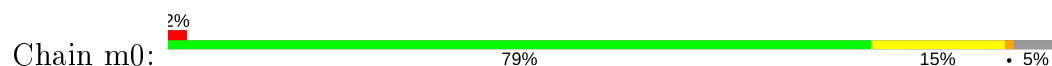




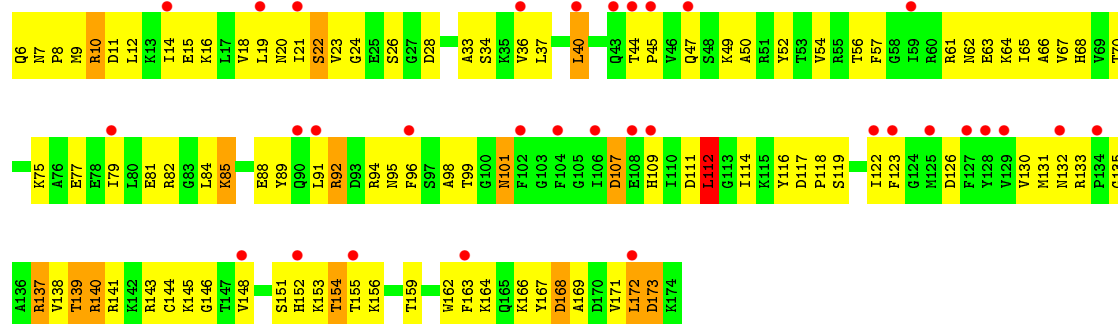
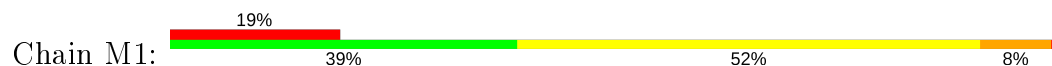
- Molecule 12: 60S ribosomal protein L10



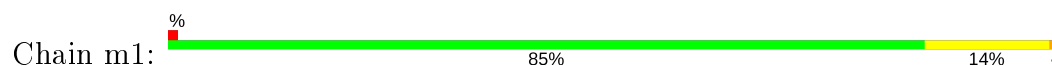
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-B

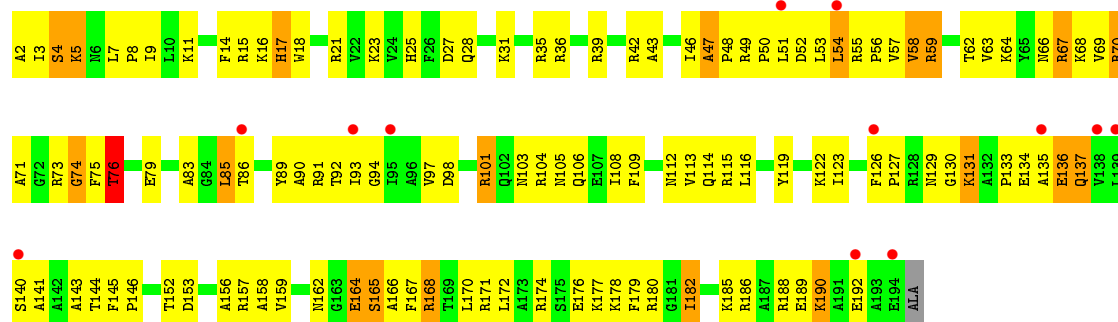


- Molecule 13: 60S ribosomal protein L11-B





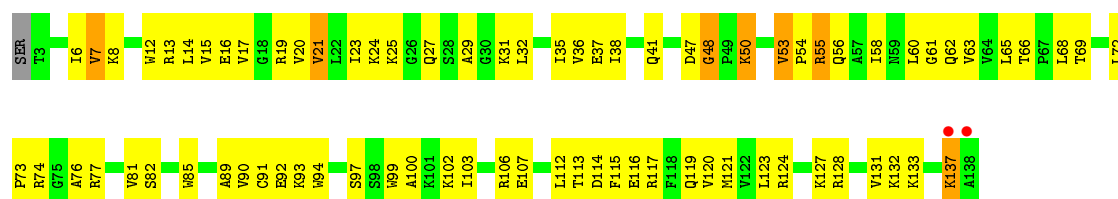
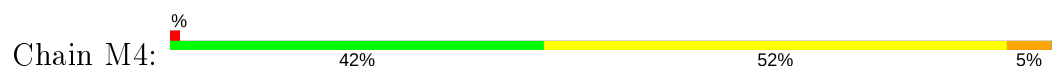
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A



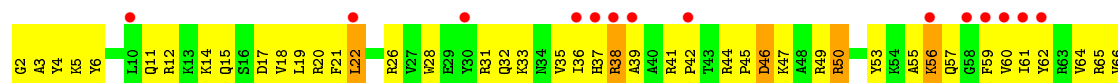
- Molecule 15: 60S ribosomal protein L14-A

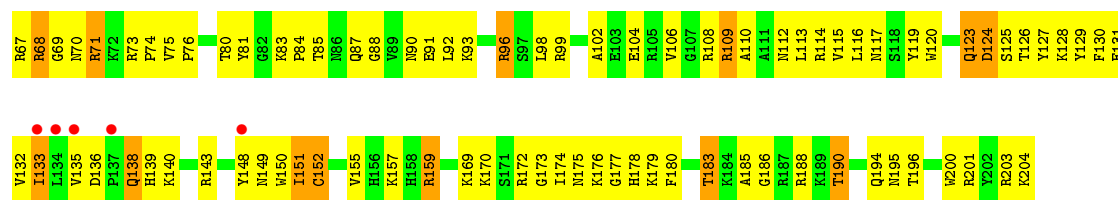


- Molecule 15: 60S ribosomal protein L14-A

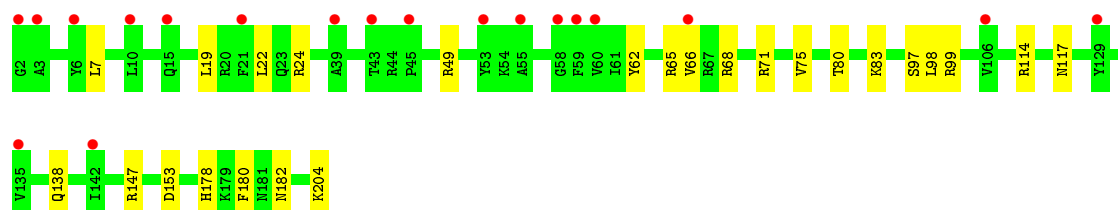
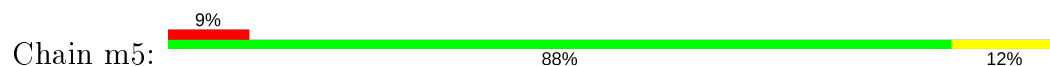


- Molecule 16: 60S ribosomal protein L15-A

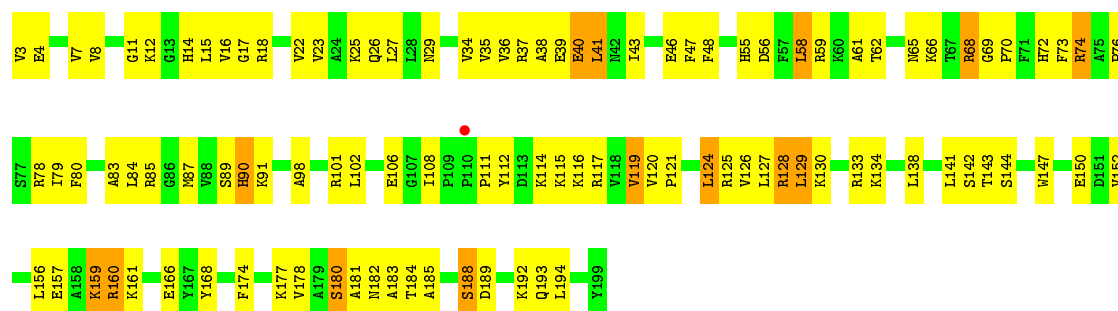




• Molecule 16: 60S ribosomal protein L15-A



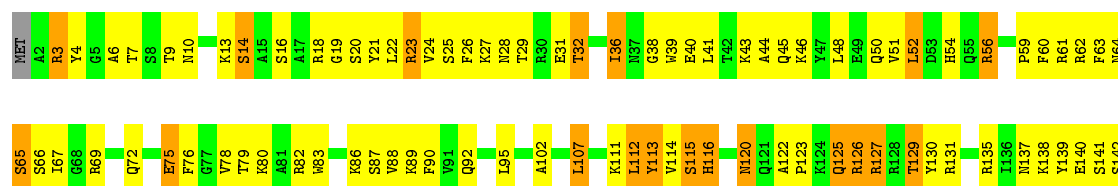
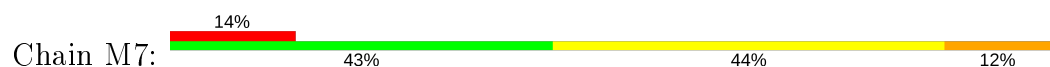
• Molecule 17: 60S ribosomal protein L16-A

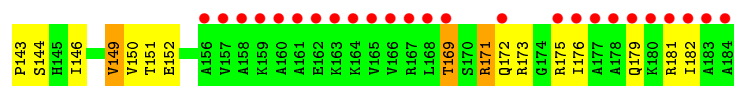


• Molecule 17: 60S ribosomal protein L16-A

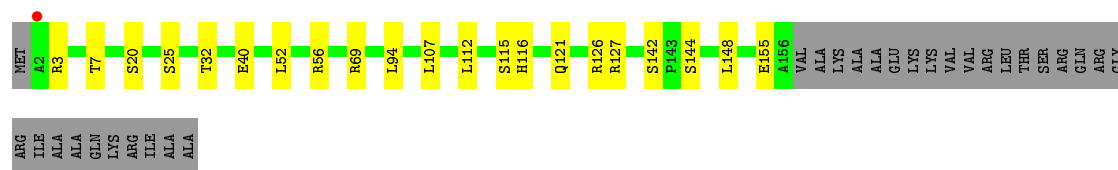
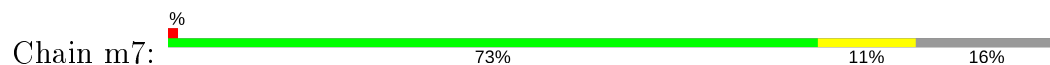


• Molecule 18: 60S ribosomal protein L17-A

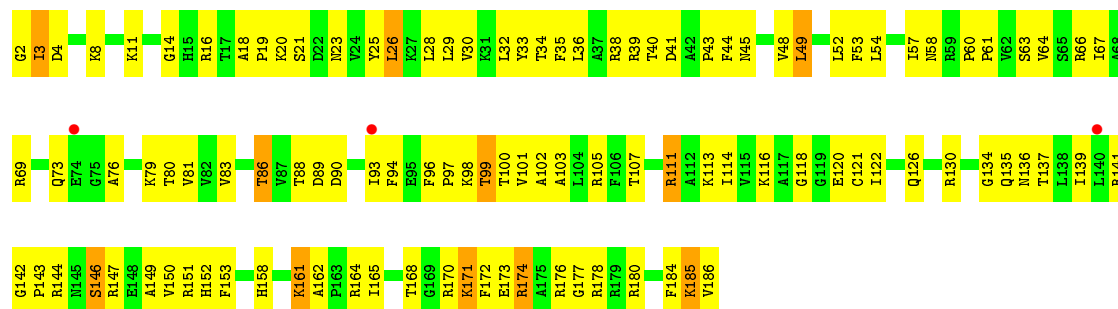
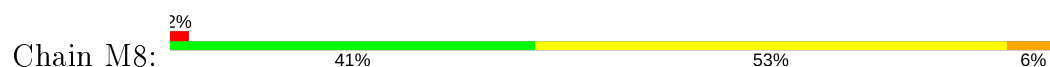




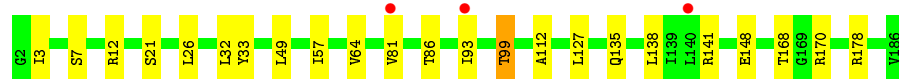
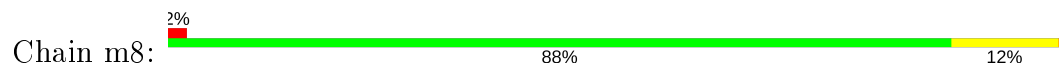
- Molecule 18: 60S ribosomal protein L17-A



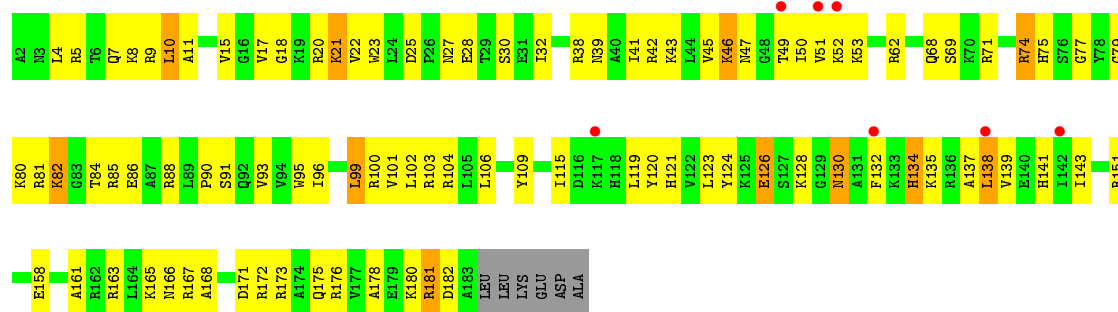
- Molecule 19: 60S ribosomal protein L18-A



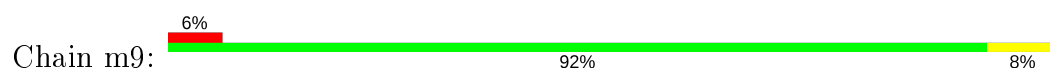
- Molecule 19: 60S ribosomal protein L18-A



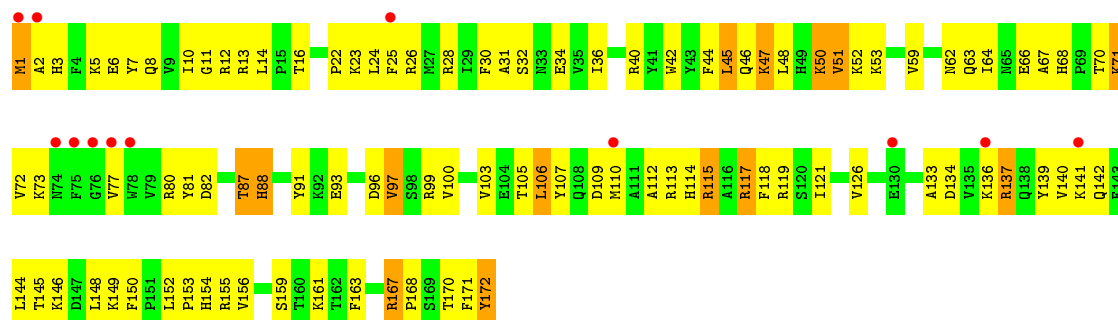
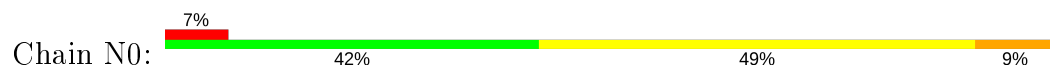
- Molecule 20: 60S ribosomal protein L19-A



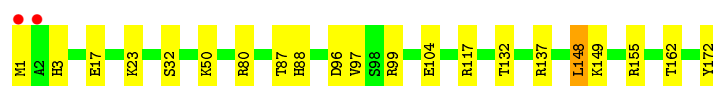
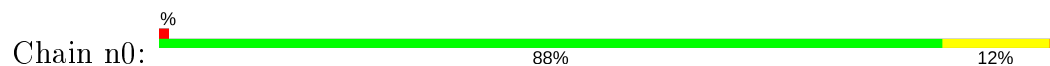
- Molecule 20: 60S ribosomal protein L19-A



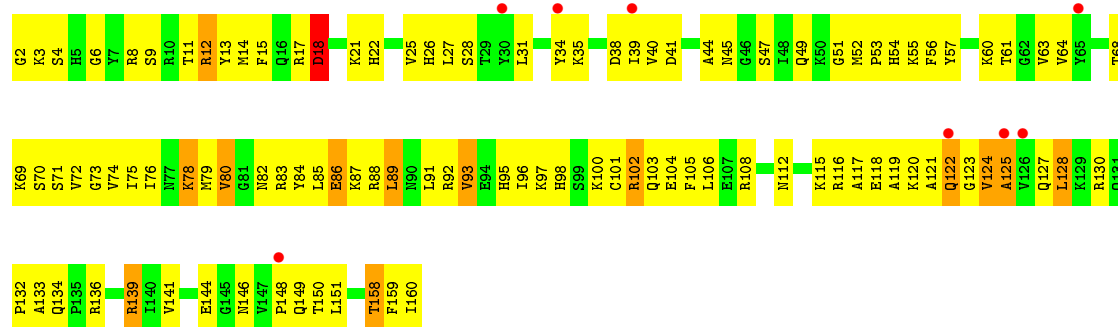
- Molecule 21: 60S ribosomal protein L20-A



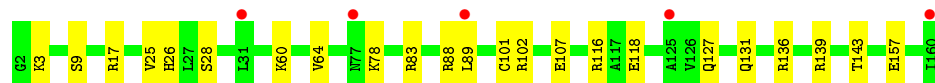
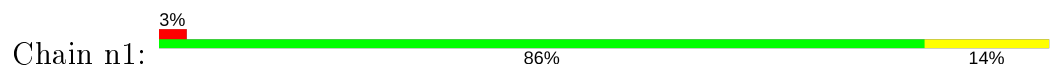
- Molecule 21: 60S ribosomal protein L20-A



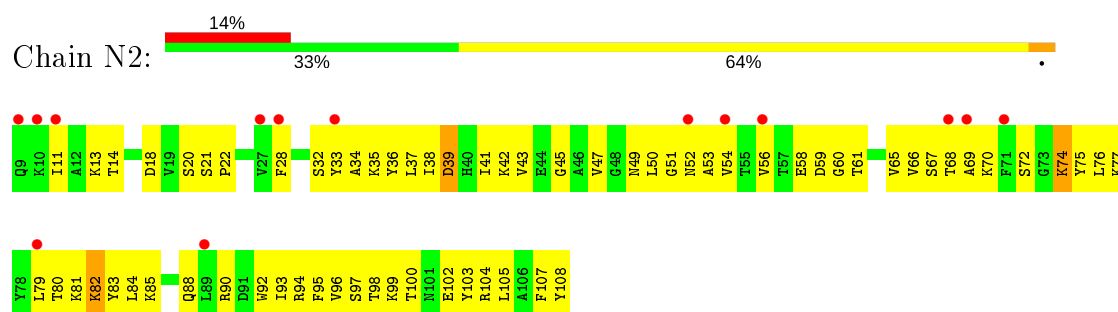
- Molecule 22: 60S ribosomal protein L21-A



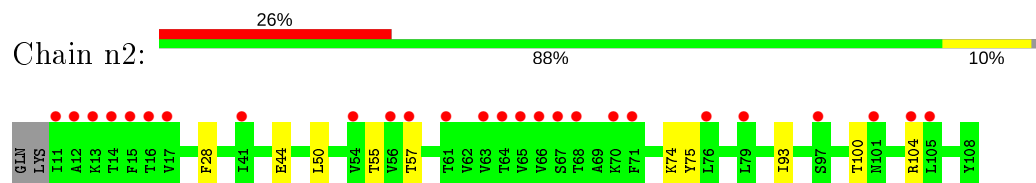
- Molecule 22: 60S ribosomal protein L21-A



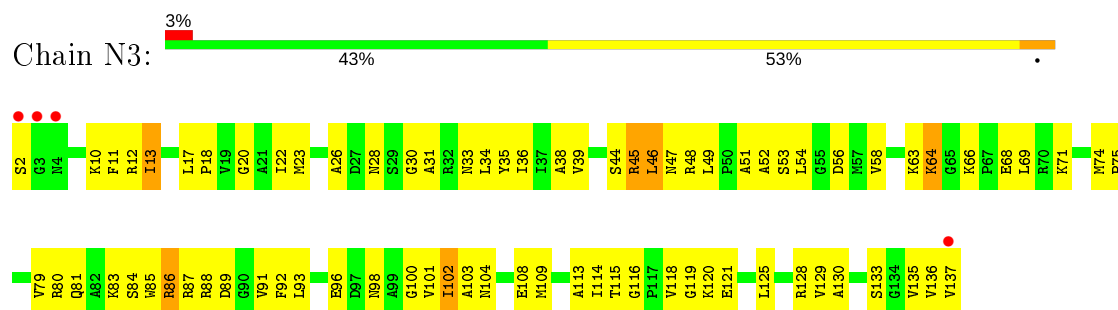
- Molecule 23: 60S ribosomal protein L22-A



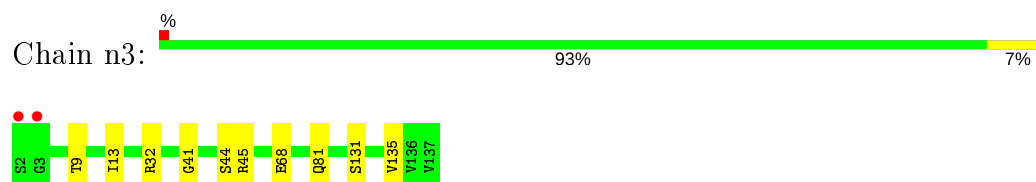
- Molecule 23: 60S ribosomal protein L22-A



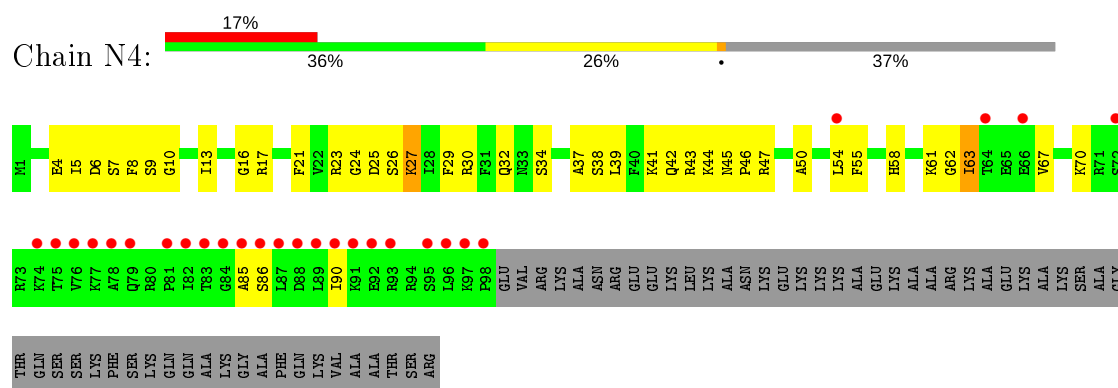
- Molecule 24: 60S ribosomal protein L23-A



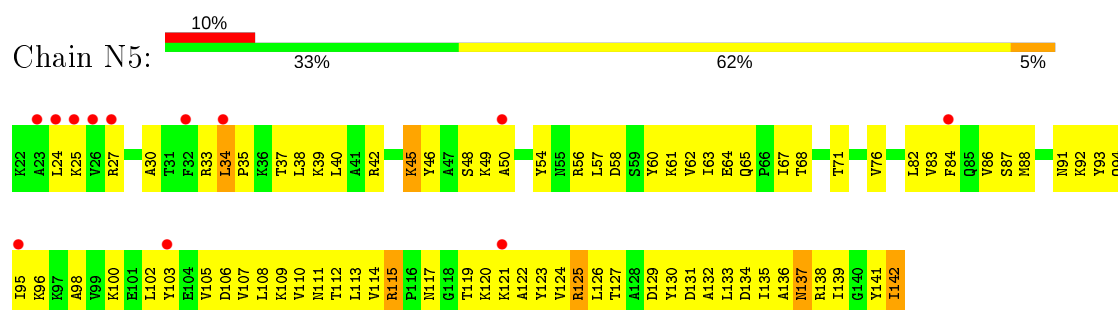
- Molecule 24: 60S ribosomal protein L23-A



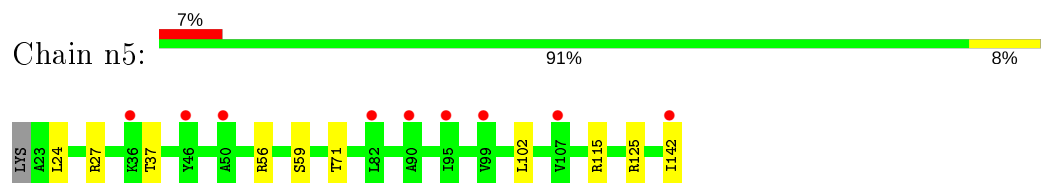
- Molecule 25: 60S ribosomal protein L24-A



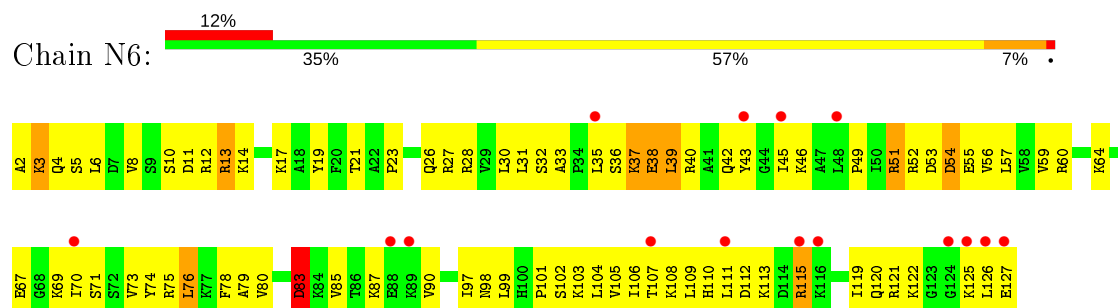
- Molecule 26: 60S ribosomal protein L25



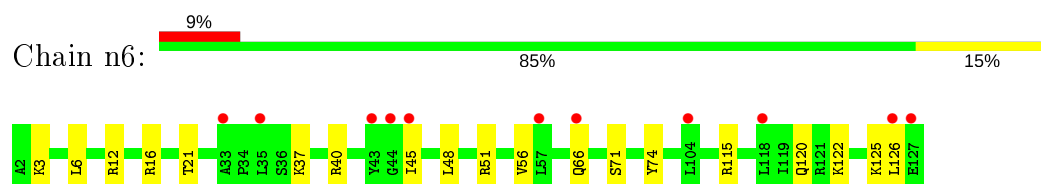
- Molecule 26: 60S ribosomal protein L25



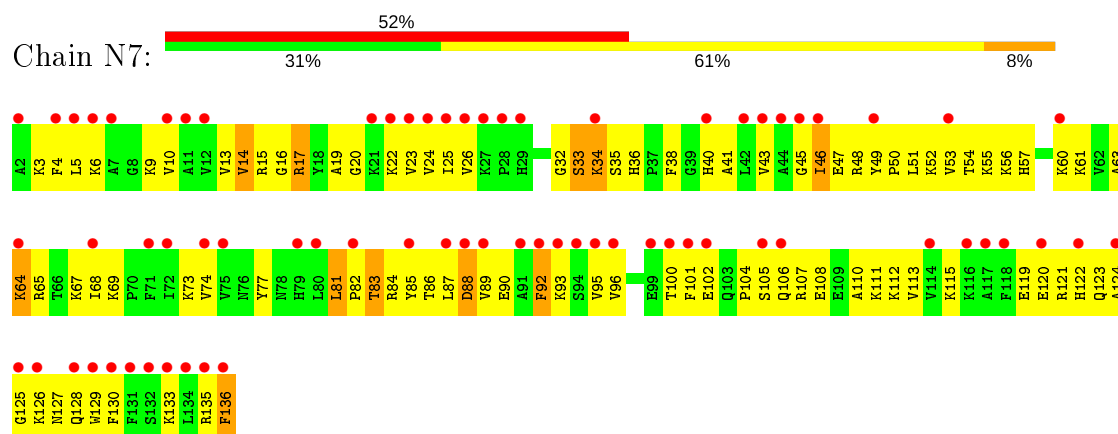
- Molecule 27: 60S ribosomal protein L26-A



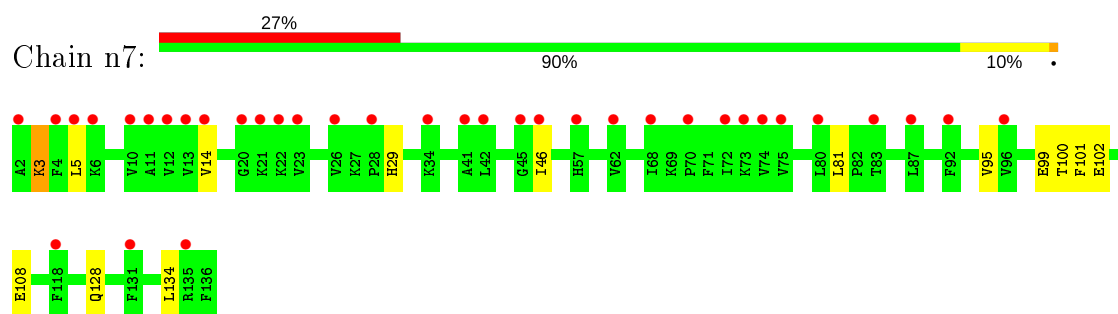
- Molecule 27: 60S ribosomal protein L26-A



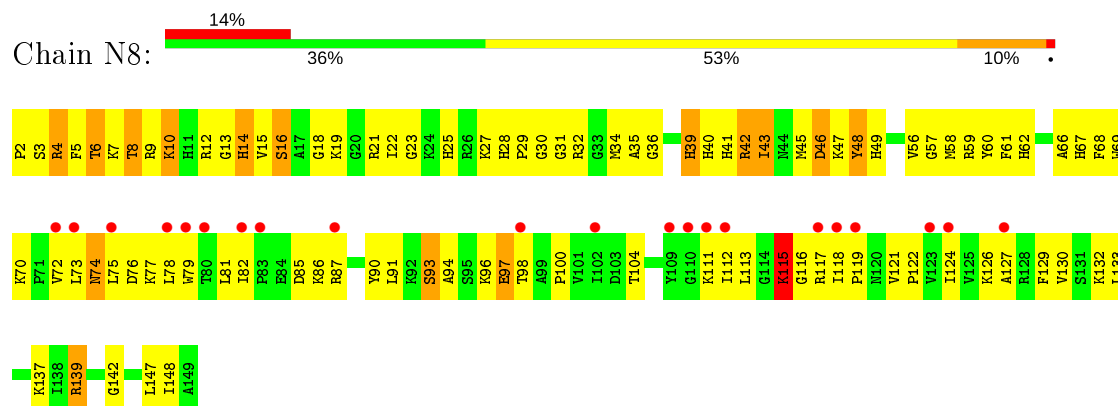
- Molecule 28: 60S ribosomal protein L27-A



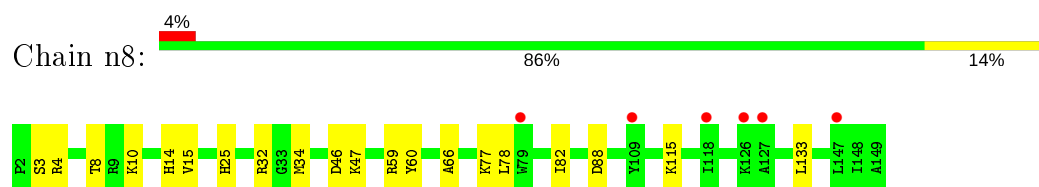
- Molecule 28: 60S ribosomal protein L27-A



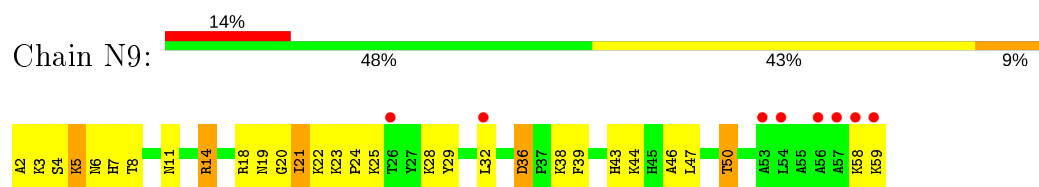
- Molecule 29: 60S ribosomal protein L28



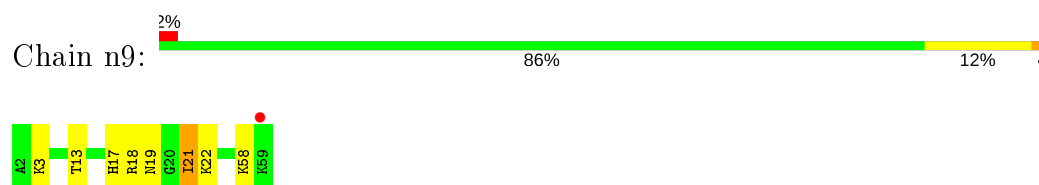
- Molecule 29: 60S ribosomal protein L28



- Molecule 30: 60S ribosomal protein L29

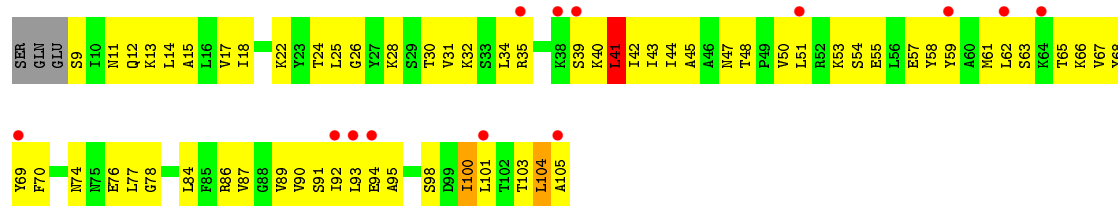


- Molecule 30: 60S ribosomal protein L29

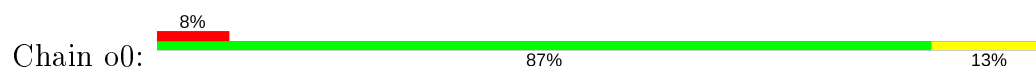


- Molecule 31: 60S ribosomal protein L30

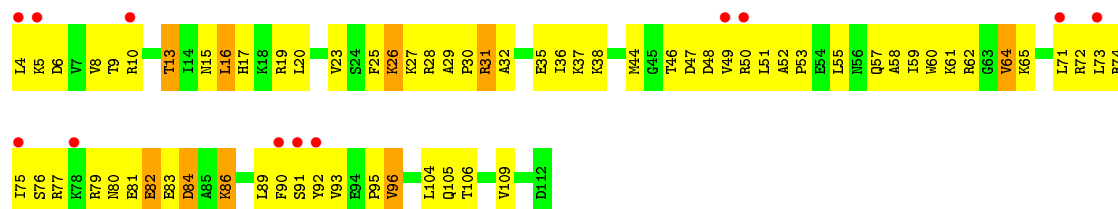




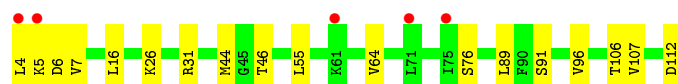
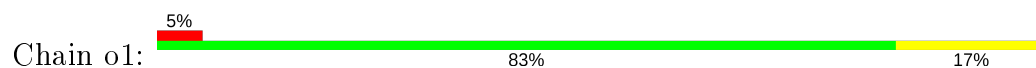
- Molecule 31: 60S ribosomal protein L30



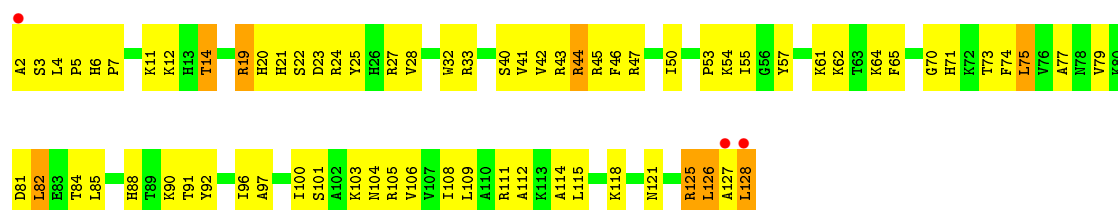
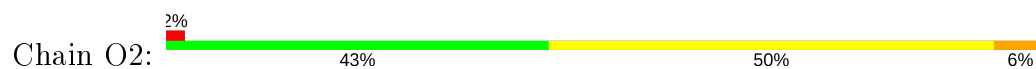
- Molecule 32: 60S ribosomal protein L31-A



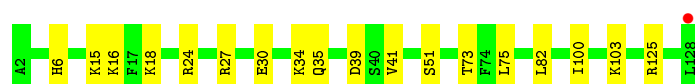
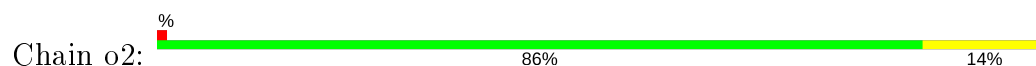
- Molecule 32: 60S ribosomal protein L31-A



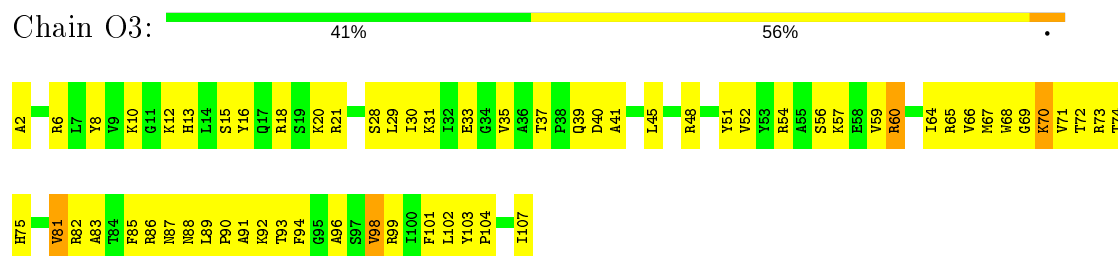
- Molecule 33: 60S ribosomal protein L32



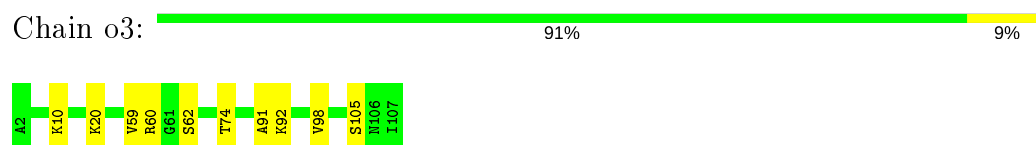
- Molecule 33: 60S ribosomal protein L32



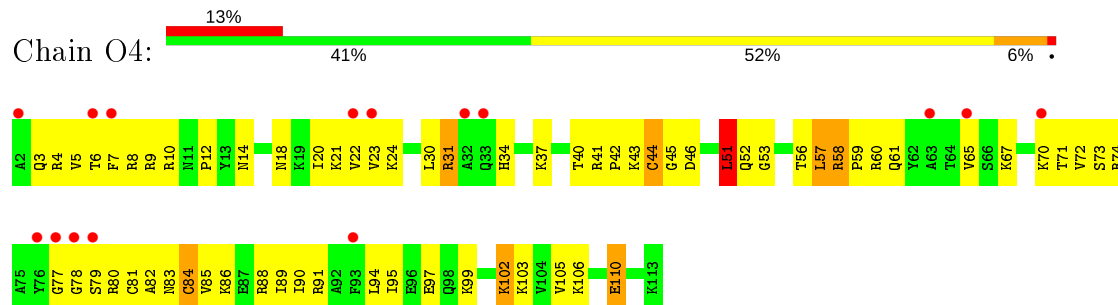
- Molecule 34: 60S ribosomal protein L33-A



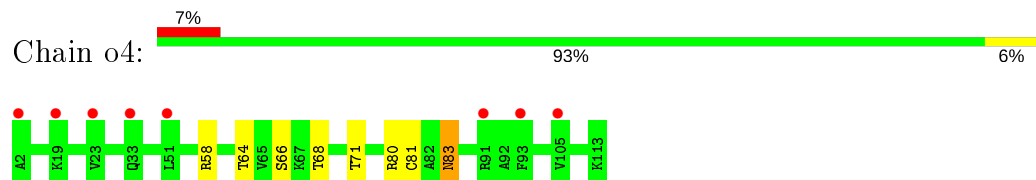
- Molecule 34: 60S ribosomal protein L33-A



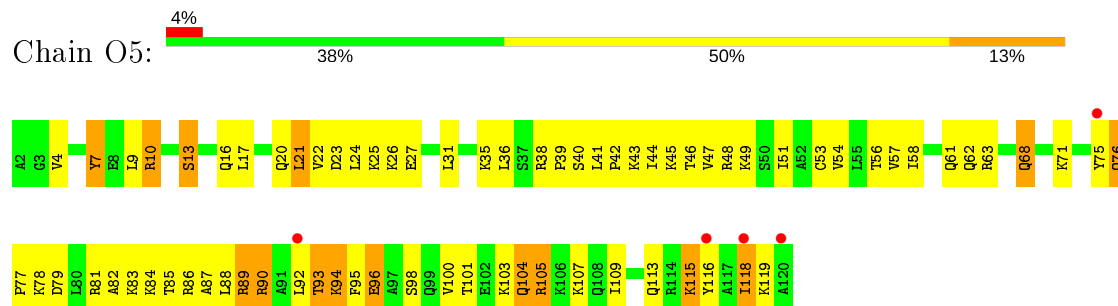
- Molecule 35: 60S ribosomal protein L34-A



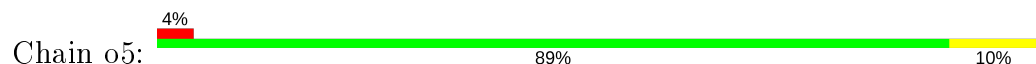
- Molecule 35: 60S ribosomal protein L34-A



- Molecule 36: 60S ribosomal protein L35-A



- Molecule 36: 60S ribosomal protein L35-A

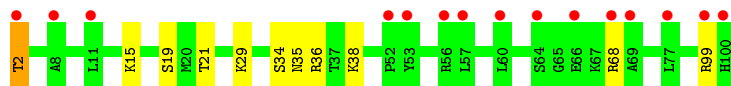
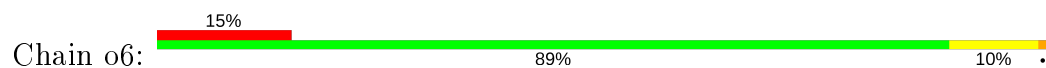




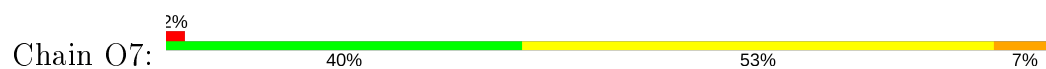
- Molecule 37: 60S ribosomal protein L36-A



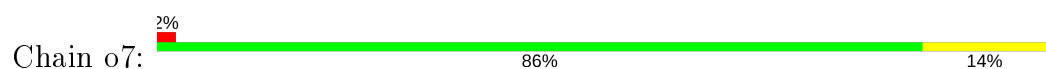
- Molecule 37: 60S ribosomal protein L36-A



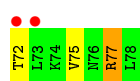
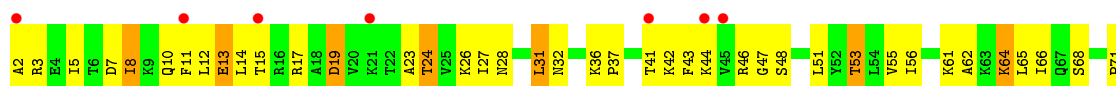
- Molecule 38: 60S ribosomal protein L37-A



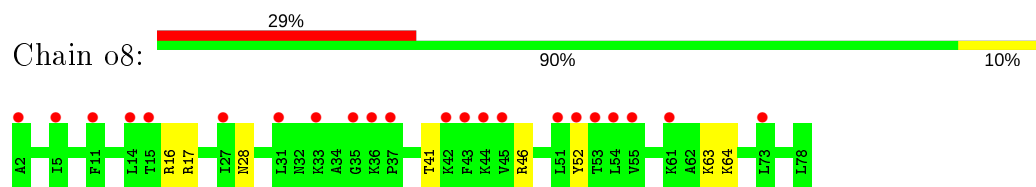
- Molecule 38: 60S ribosomal protein L37-A



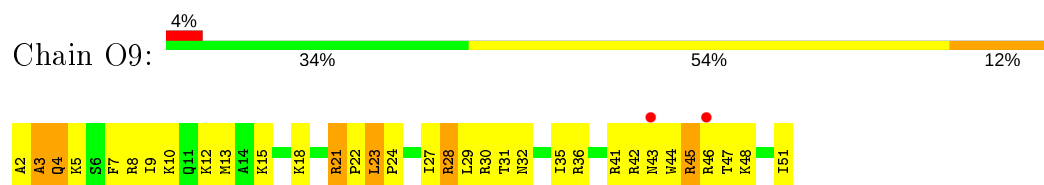
- Molecule 39: 60S ribosomal protein L38



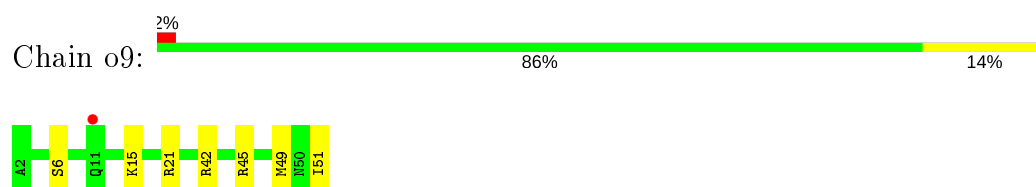
- Molecule 39: 60S ribosomal protein L38



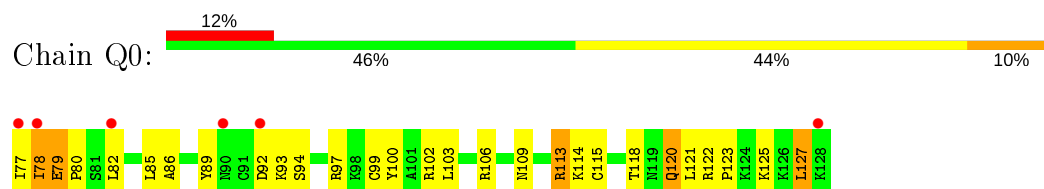
- Molecule 40: 60S ribosomal protein L39



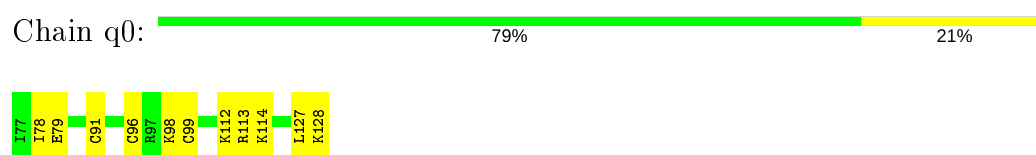
- Molecule 40: 60S ribosomal protein L39



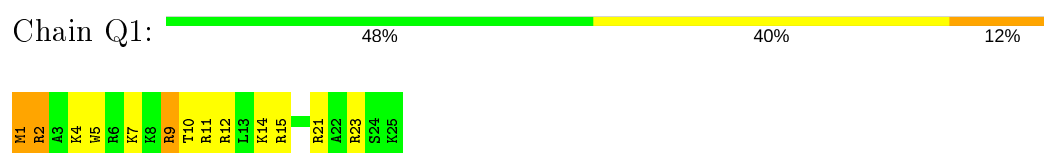
- Molecule 41: Ubiquitin-60S ribosomal protein L40



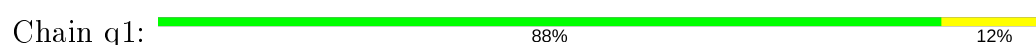
- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 42: 60S ribosomal protein L41-A

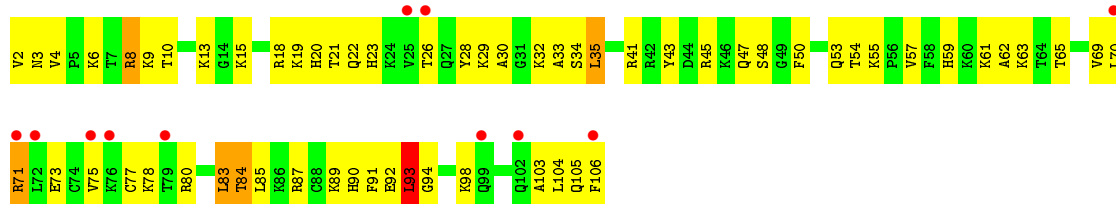


- Molecule 42: 60S ribosomal protein L41-A

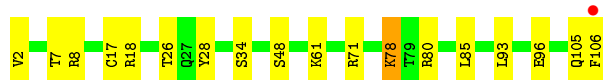
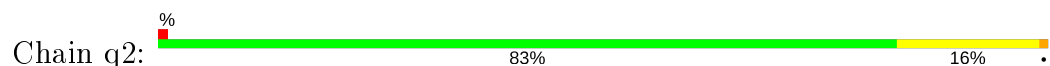




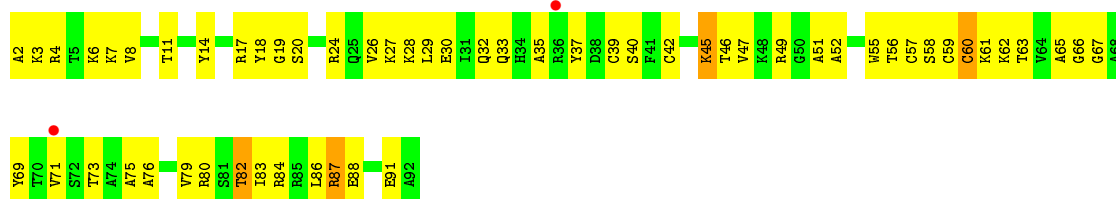
- Molecule 43: 60S ribosomal protein L42-A



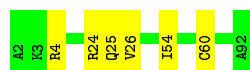
- Molecule 43: 60S ribosomal protein L42-A



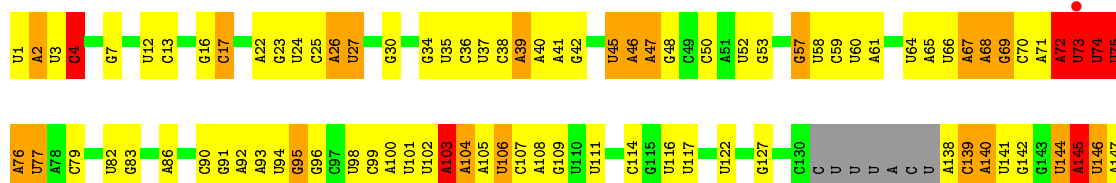
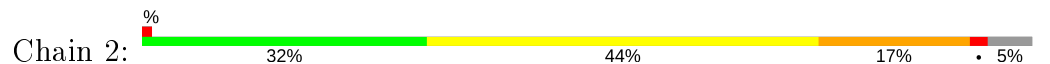
- Molecule 44: 60S ribosomal protein L43-A



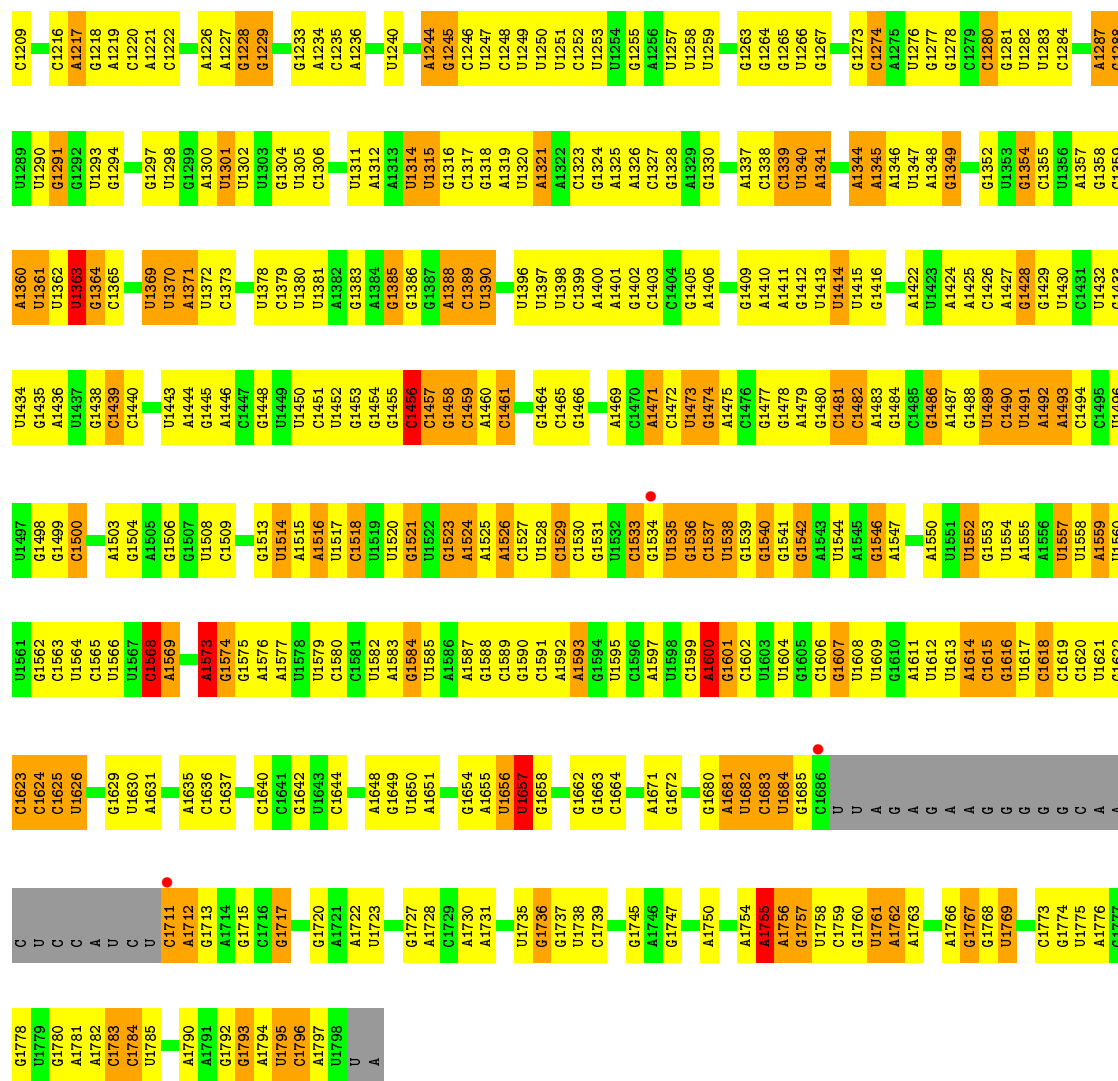
- Molecule 44: 60S ribosomal protein L43-A



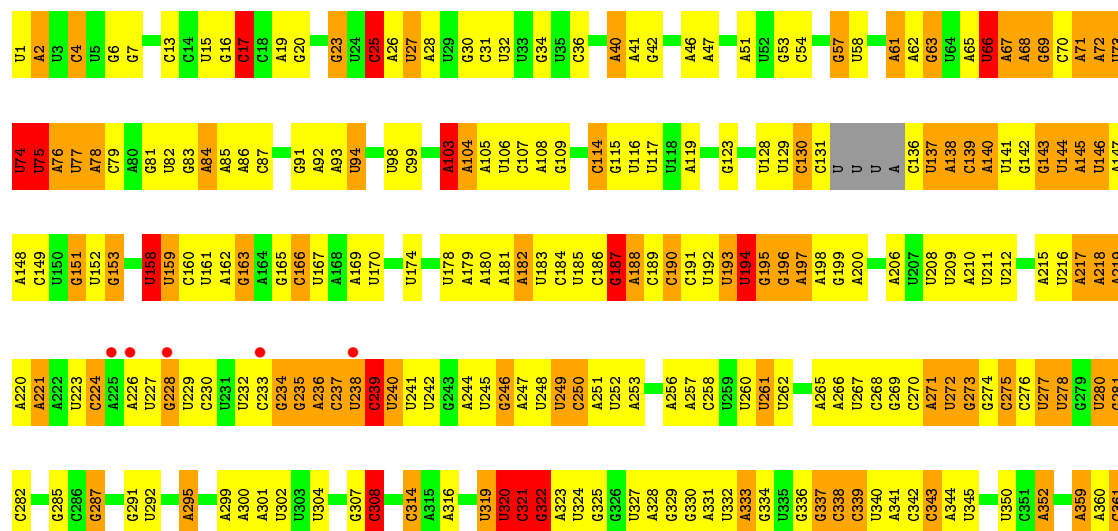
- Molecule 45: 18S ribosomal RNA



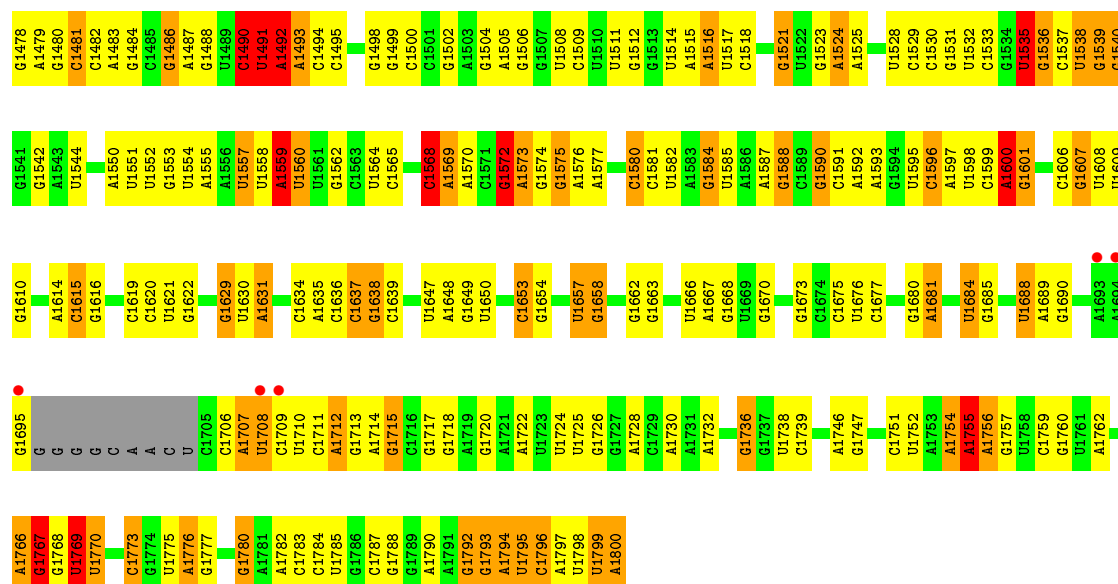




### • Molecule 45: 18S ribosomal RNA



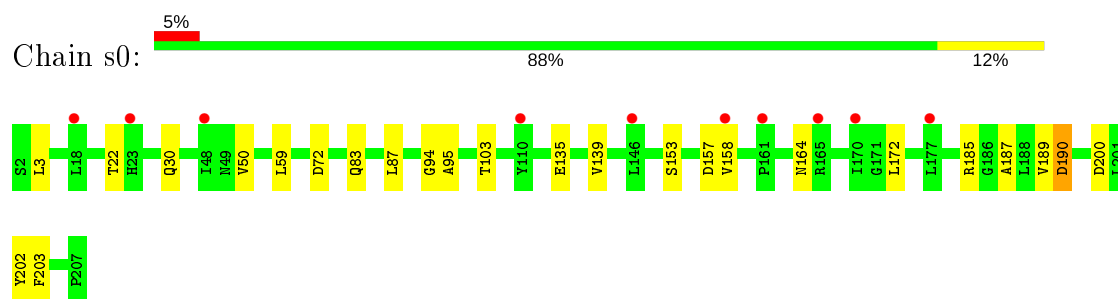
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



• Molecule 46: 40S ribosomal protein S0-A

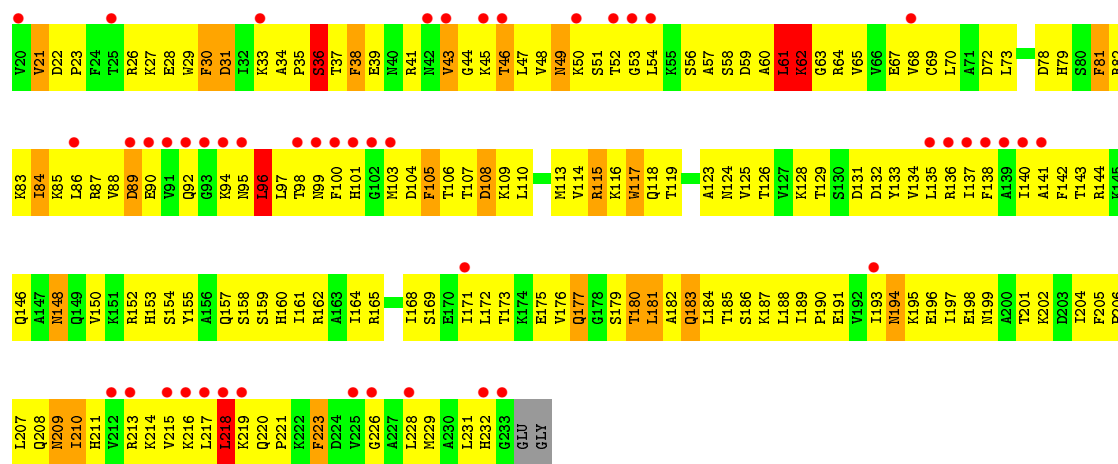


• Molecule 46: 40S ribosomal protein S0-A

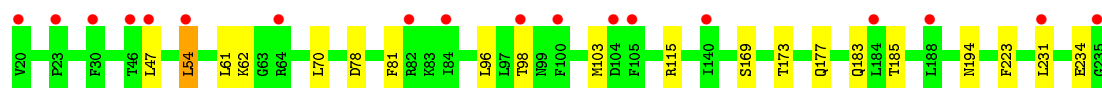


• Molecule 47: 40S ribosomal protein S1-A

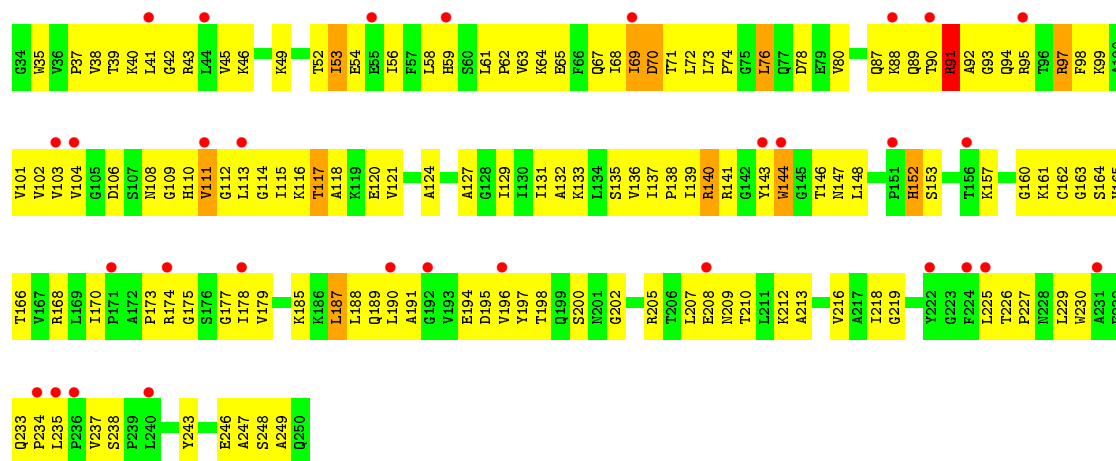




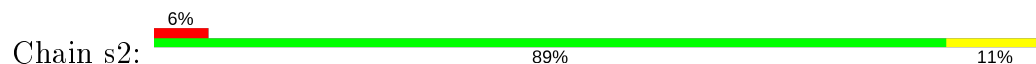
- Molecule 47: 40S ribosomal protein S1-A



- Molecule 48: 40S ribosomal protein S2

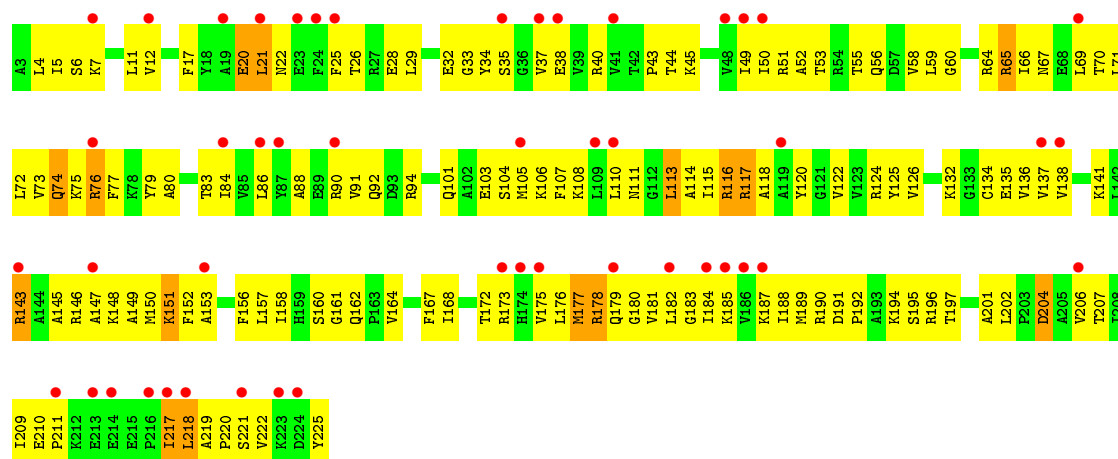


- Molecule 48: 40S ribosomal protein S2

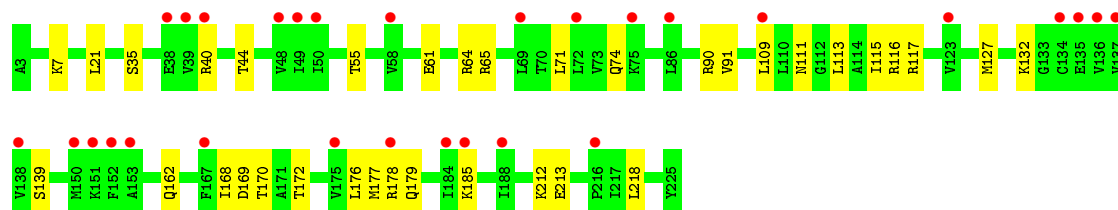
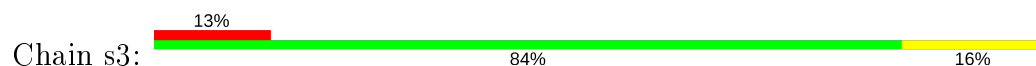


- Molecule 49: 40S ribosomal protein S3

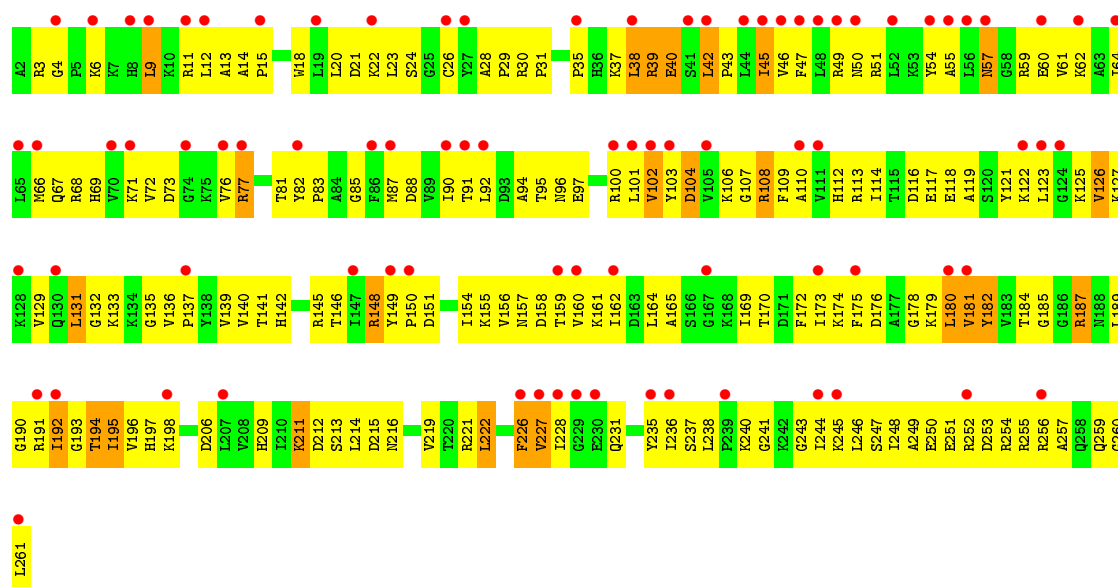




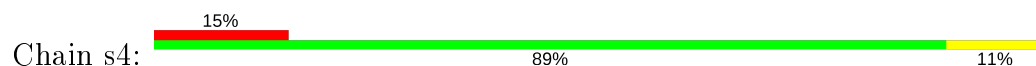
- Molecule 49: 40S ribosomal protein S3

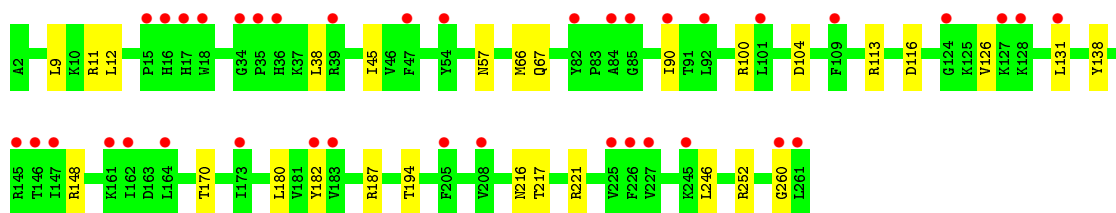


- Molecule 50: 40S ribosomal protein S4-A

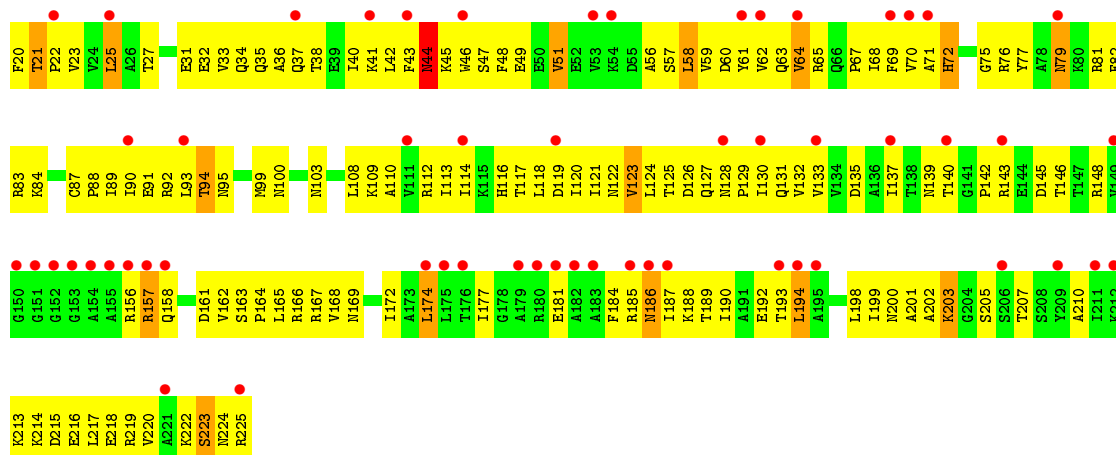


- Molecule 50: 40S ribosomal protein S4-A

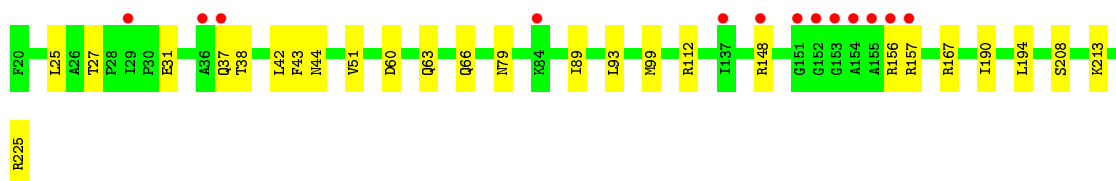
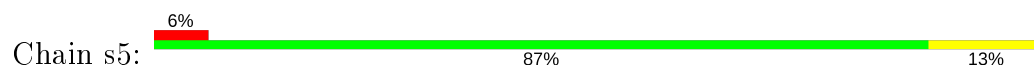




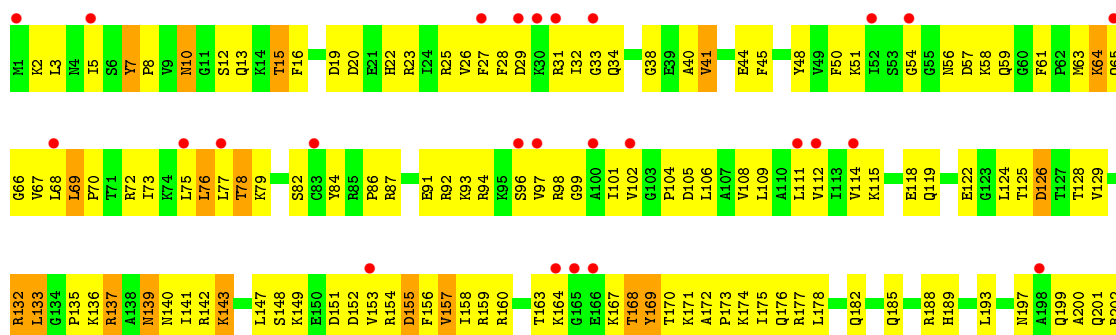
• Molecule 51: 40S ribosomal protein S5



• Molecule 51: 40S ribosomal protein S5

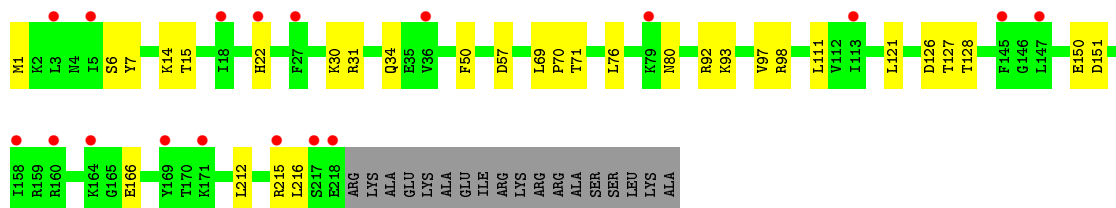
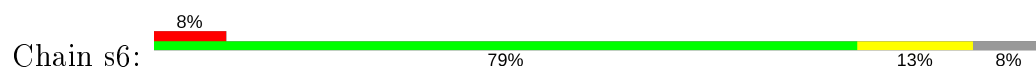


• Molecule 52: 40S ribosomal protein S6-A

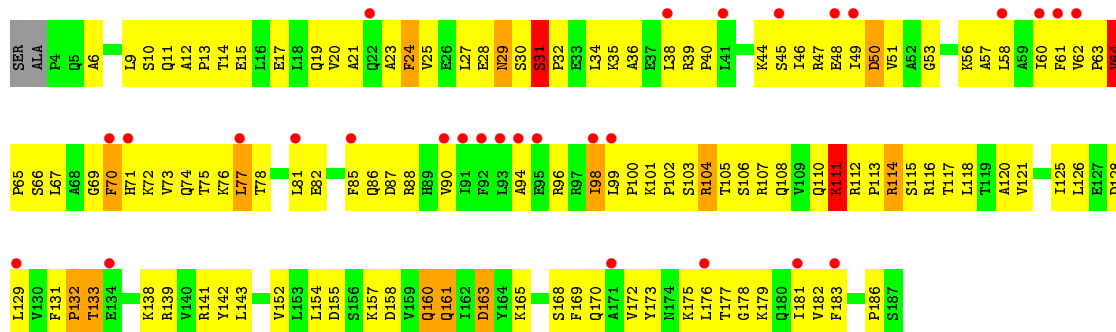




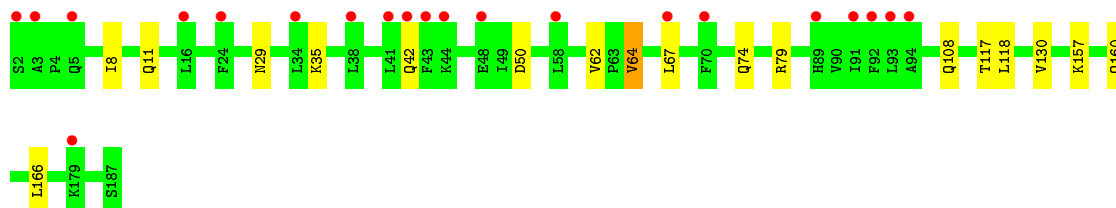
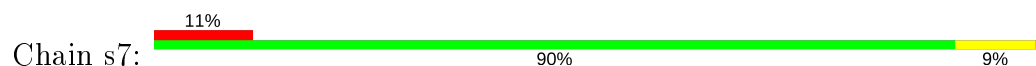
- Molecule 52: 40S ribosomal protein S6-A



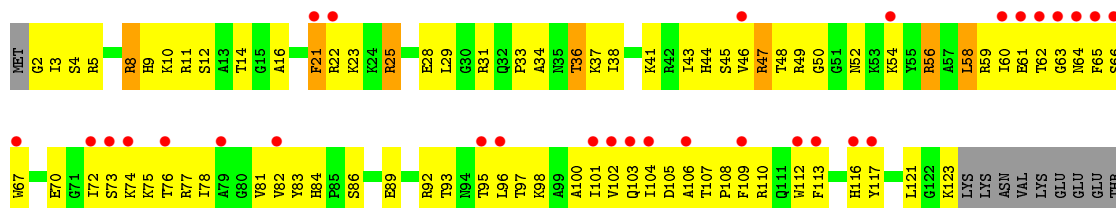
- Molecule 53: 40S ribosomal protein S7-A

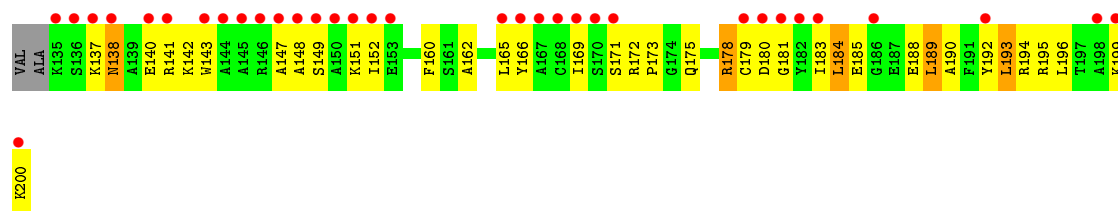


- Molecule 53: 40S ribosomal protein S7-A

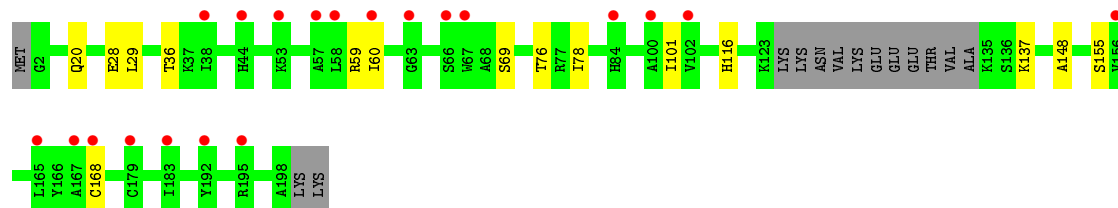
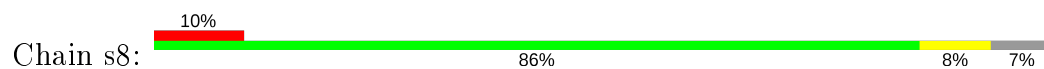


- Molecule 54: 40S ribosomal protein S8-A

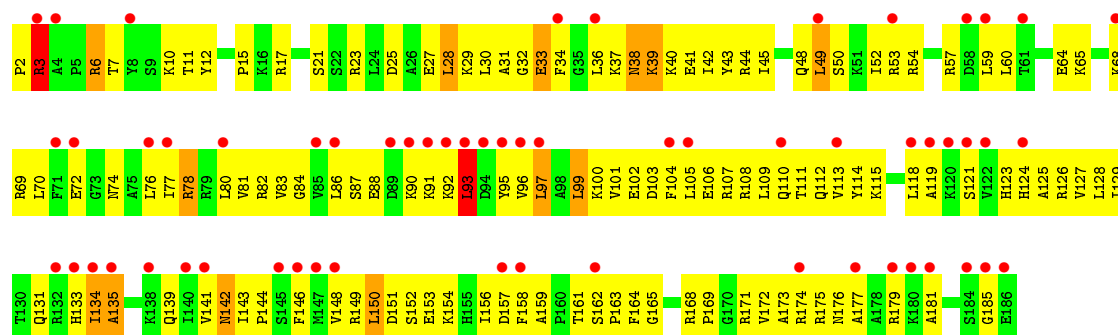




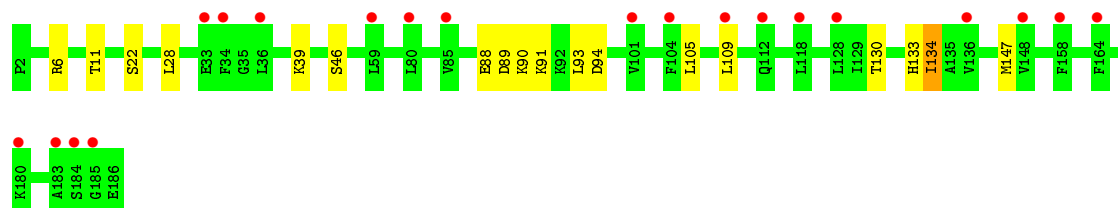
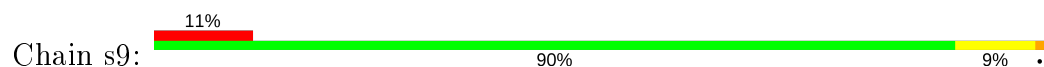
- Molecule 54: 40S ribosomal protein S8-A



- Molecule 55: 40S ribosomal protein S9-A

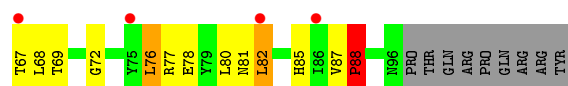


- Molecule 55: 40S ribosomal protein S9-A

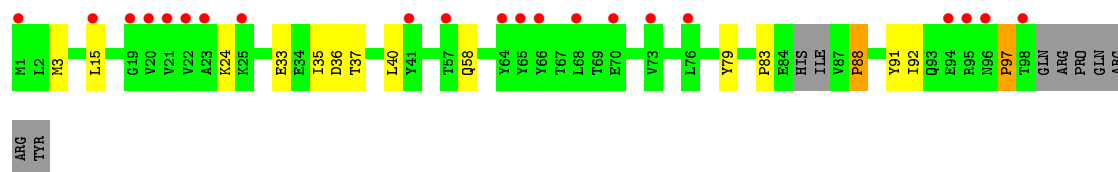
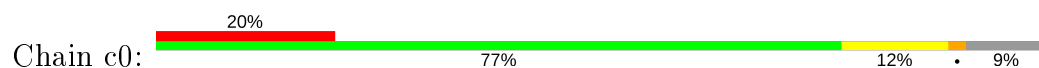


- Molecule 56: 40S ribosomal protein S10-A

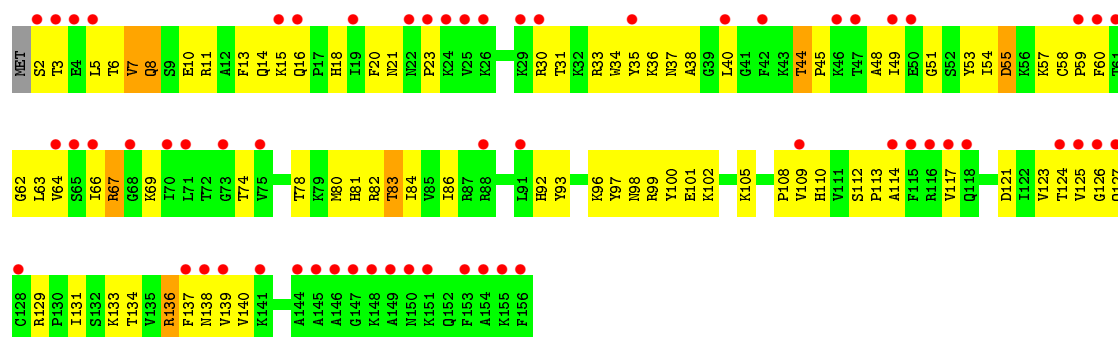
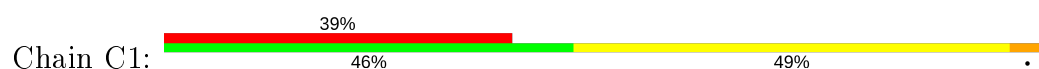




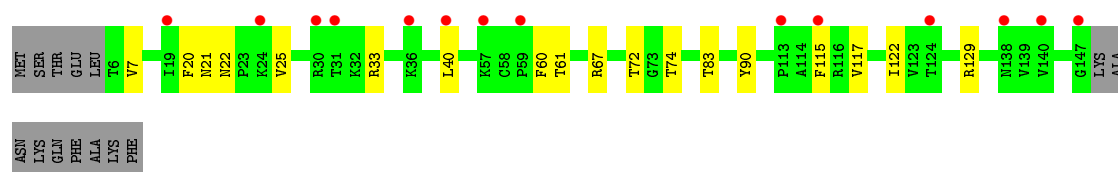
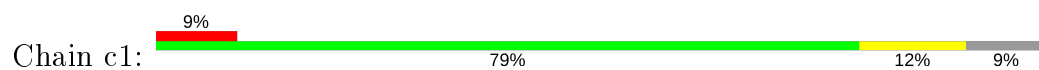
- Molecule 56: 40S ribosomal protein S10-A



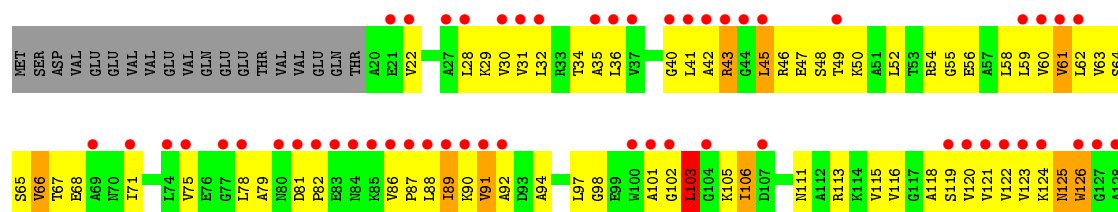
- Molecule 57: 40S ribosomal protein S11-A

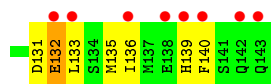


- Molecule 57: 40S ribosomal protein S11-A

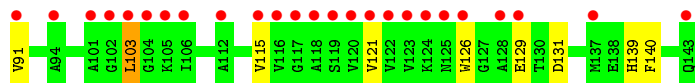
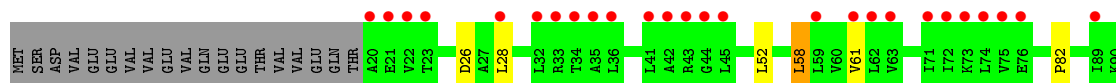
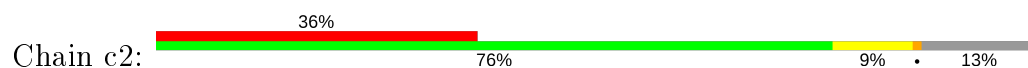


- Molecule 58: 40S ribosomal protein S12

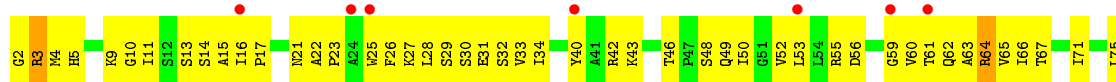
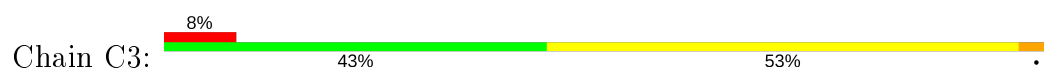




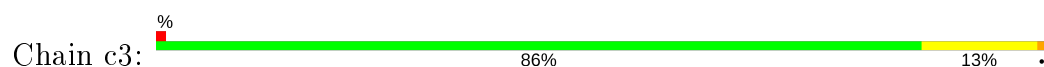
- Molecule 58: 40S ribosomal protein S12



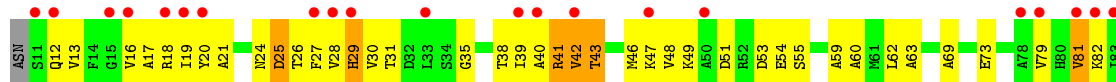
- Molecule 59: 40S ribosomal protein S13



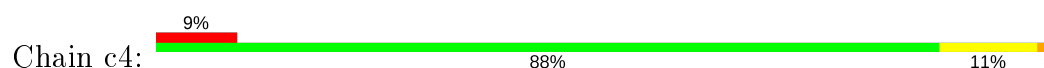
- Molecule 59: 40S ribosomal protein S13



- Molecule 60: 40S ribosomal protein S14-B

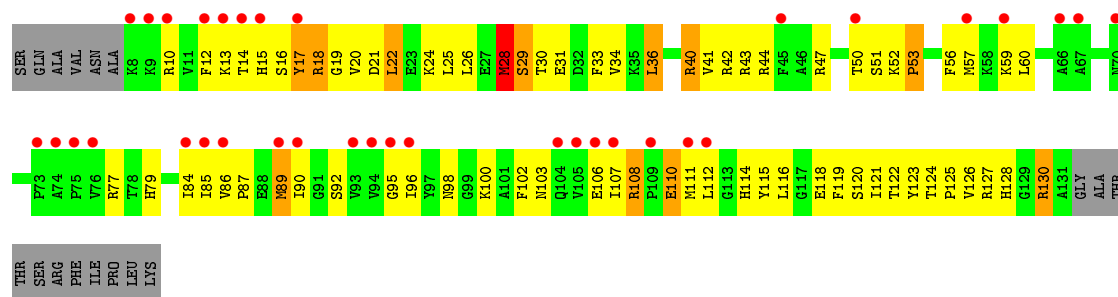


- Molecule 60: 40S ribosomal protein S14-B

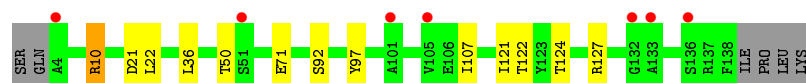
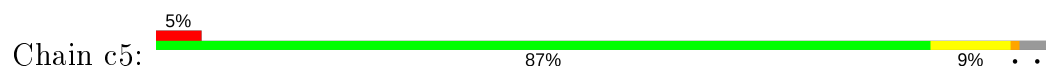




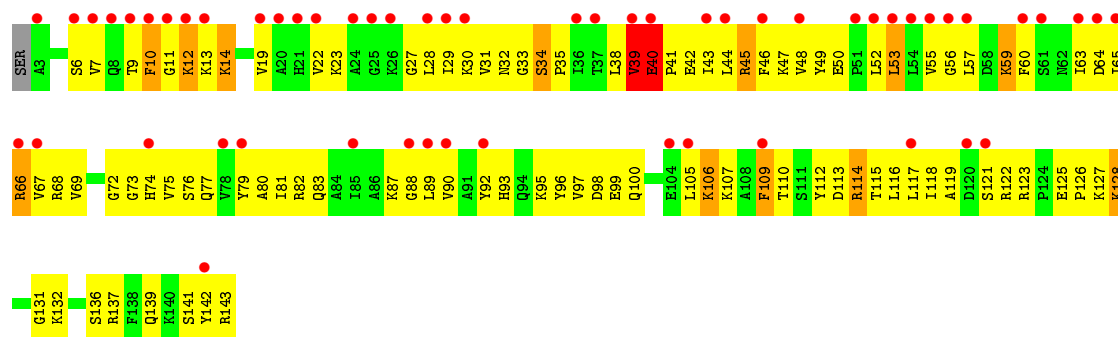
- Molecule 61: 40S ribosomal protein S15



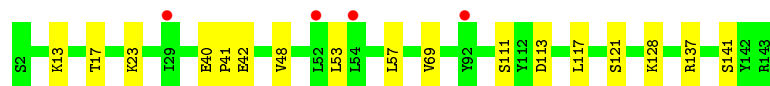
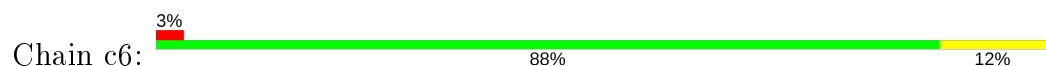
- Molecule 61: 40S ribosomal protein S15



- Molecule 62: 40S ribosomal protein S16-A



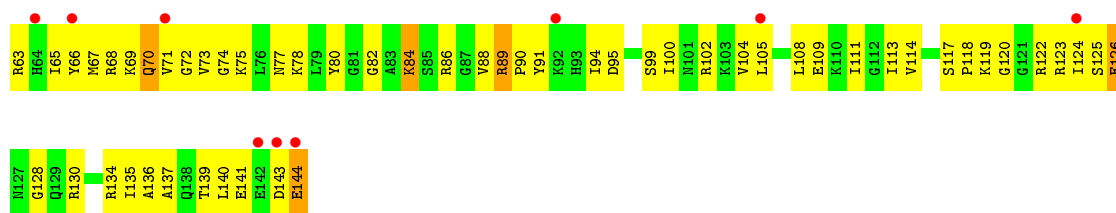
- Molecule 62: 40S ribosomal protein S16-A



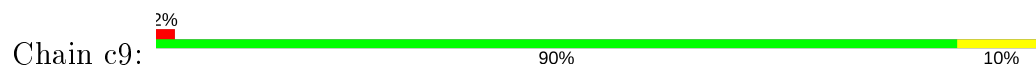
- Molecule 63: 40S ribosomal protein S17-A



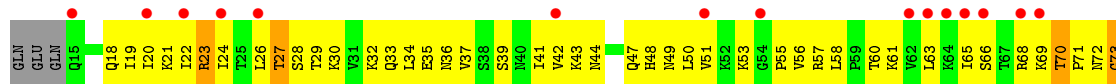




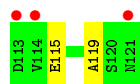
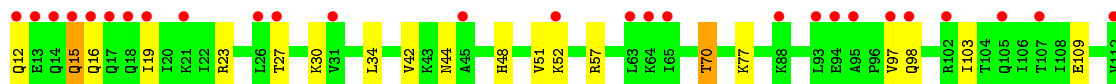
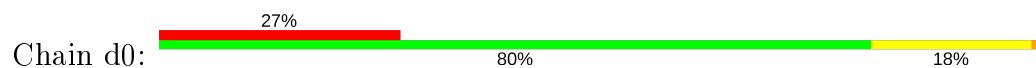
- Molecule 65: 40S ribosomal protein S19-A



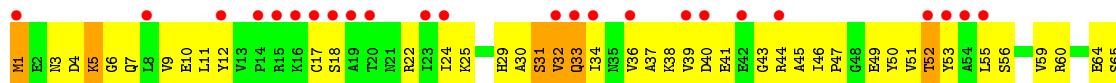
- Molecule 66: 40S ribosomal protein S20



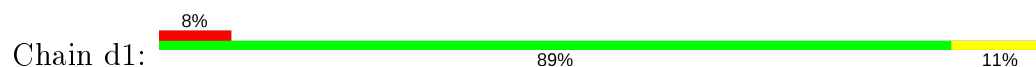
- Molecule 66: 40S ribosomal protein S20

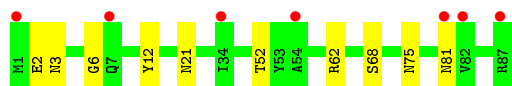


- Molecule 67: 40S ribosomal protein S21-A

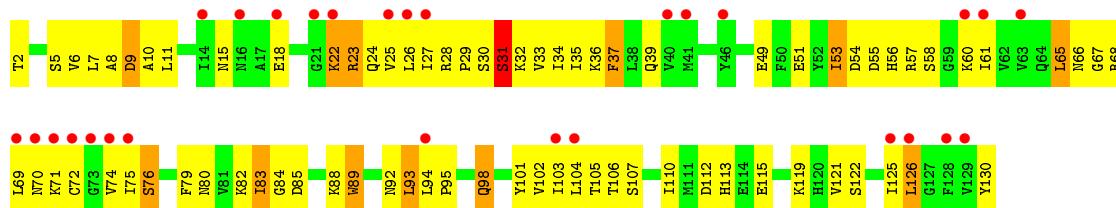


- Molecule 67: 40S ribosomal protein S21-A

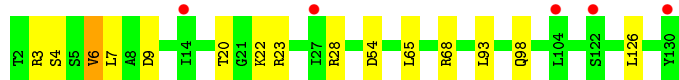
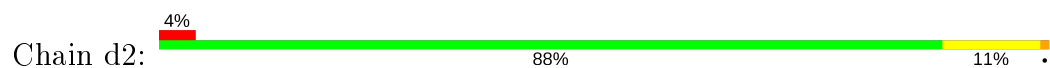




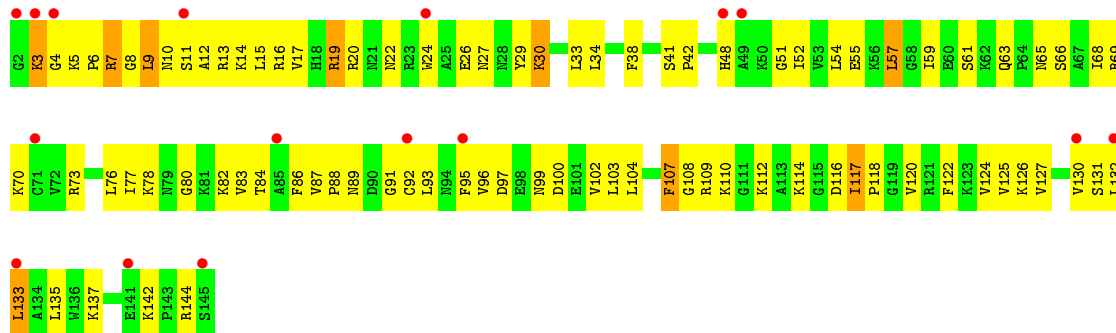
- Molecule 68: 40S ribosomal protein S22-A



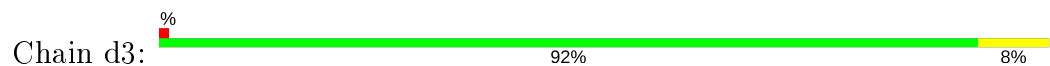
- Molecule 68: 40S ribosomal protein S22-A



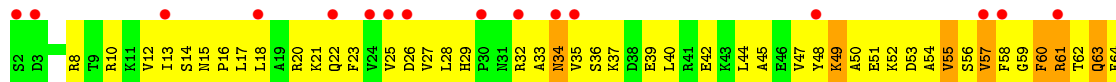
- Molecule 69: 40S ribosomal protein S23-A

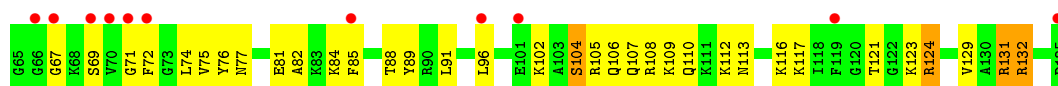


- Molecule 69: 40S ribosomal protein S23-A

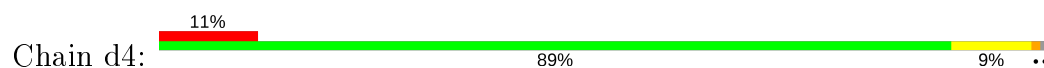


- Molecule 70: 40S ribosomal protein S24-A

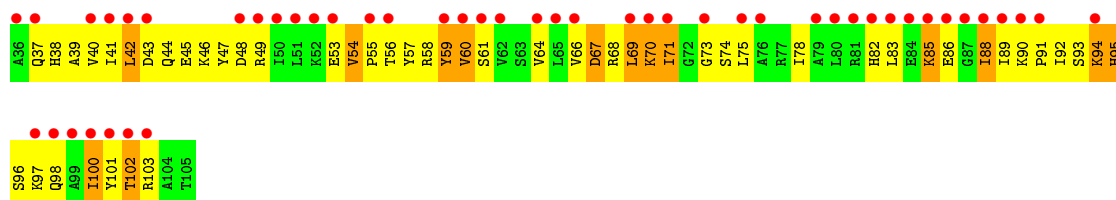




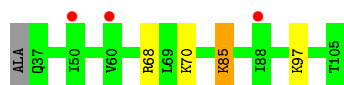
- Molecule 70: 40S ribosomal protein S24-A



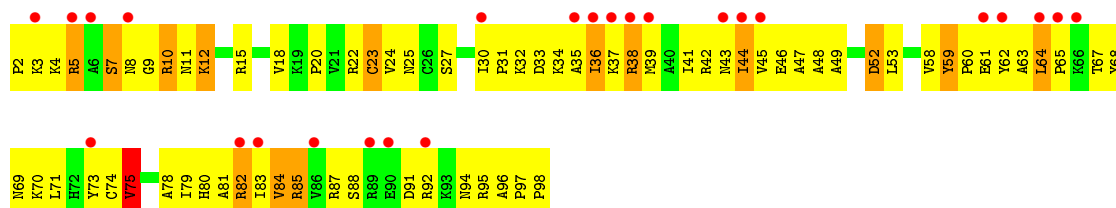
- Molecule 71: 40S ribosomal protein S25-A



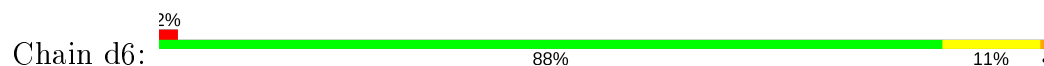
- Molecule 71: 40S ribosomal protein S25-A



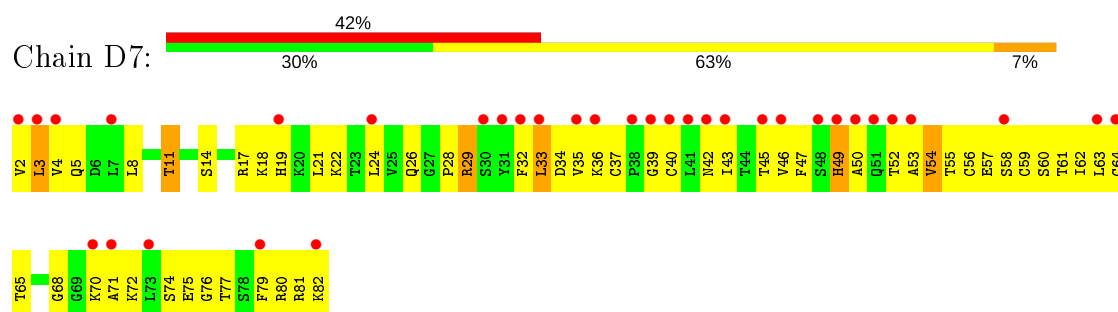
- Molecule 72: 40S ribosomal protein S26-B



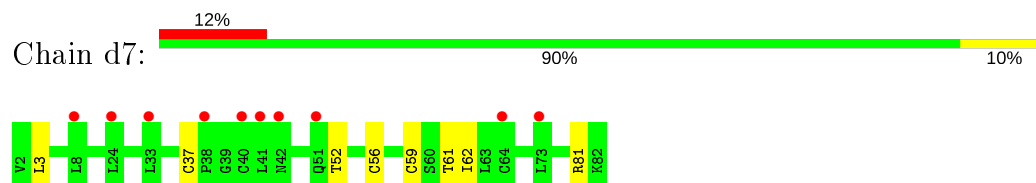
- Molecule 72: 40S ribosomal protein S26-B



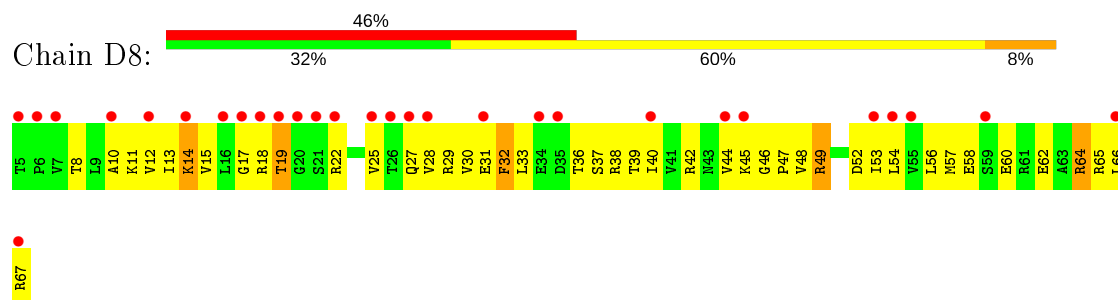
- Molecule 73: 40S ribosomal protein S27-A



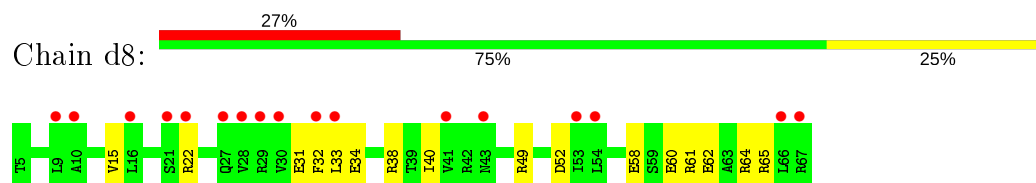
- Molecule 73: 40S ribosomal protein S27-A



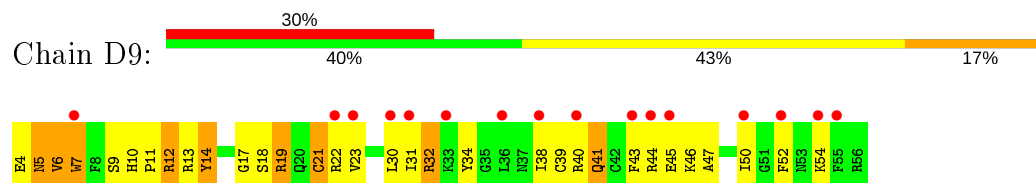
- Molecule 74: 40S ribosomal protein S28-A



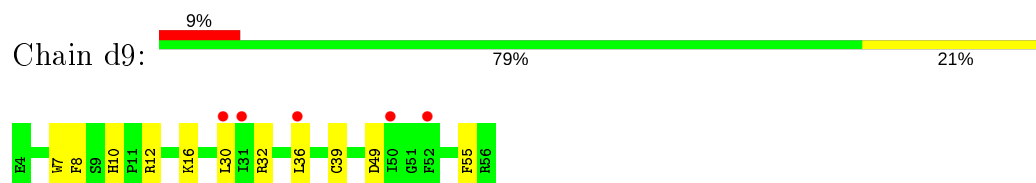
- Molecule 74: 40S ribosomal protein S28-A



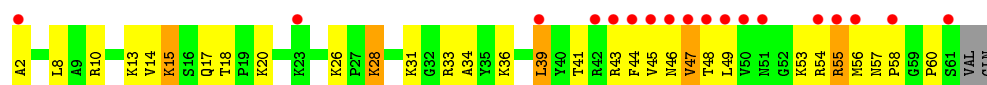
- Molecule 75: 40S ribosomal protein S29-A



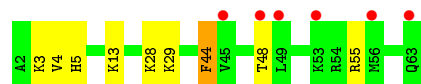
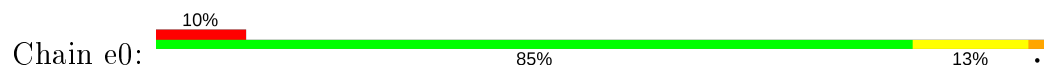
- Molecule 75: 40S ribosomal protein S29-A



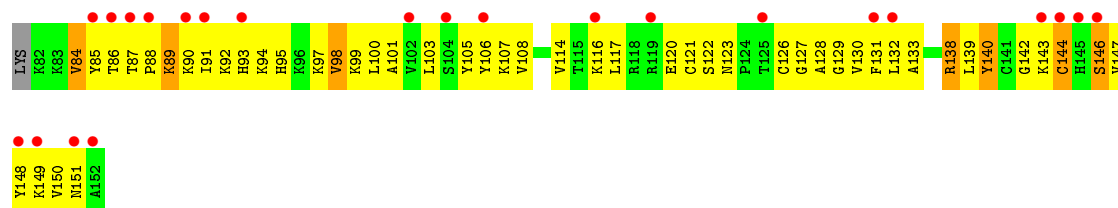
- Molecule 76: 40S ribosomal protein S30-A



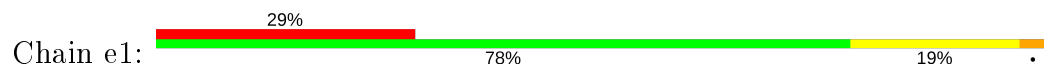
- Molecule 76: 40S ribosomal protein S30-A



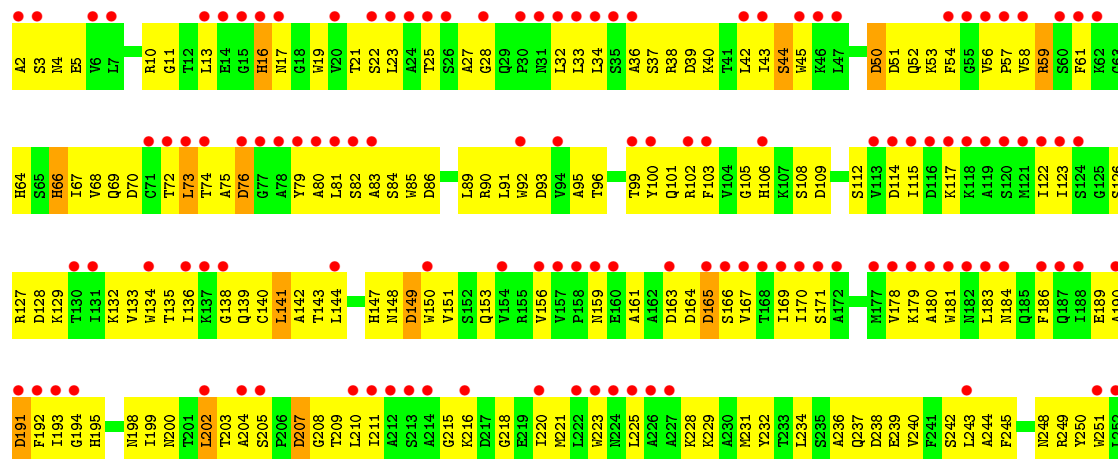
- Molecule 77: Ubiquitin-40S ribosomal protein S31

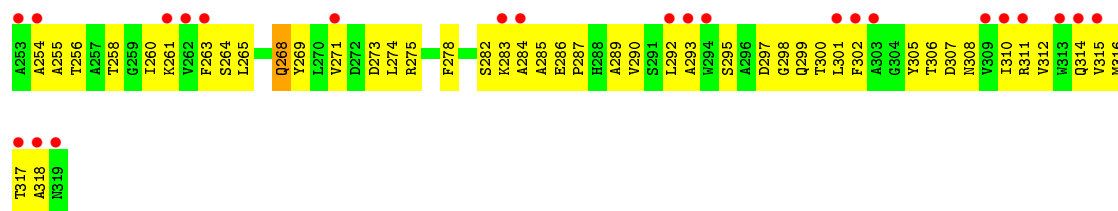


- Molecule 77: Ubiquitin-40S ribosomal protein S31

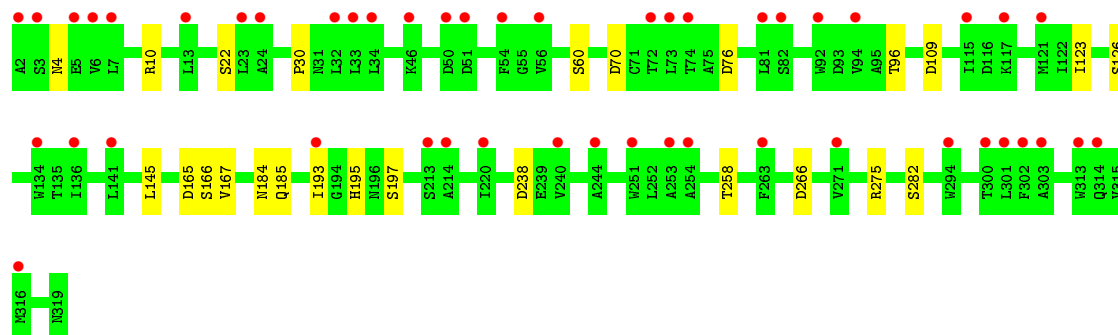


- Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein

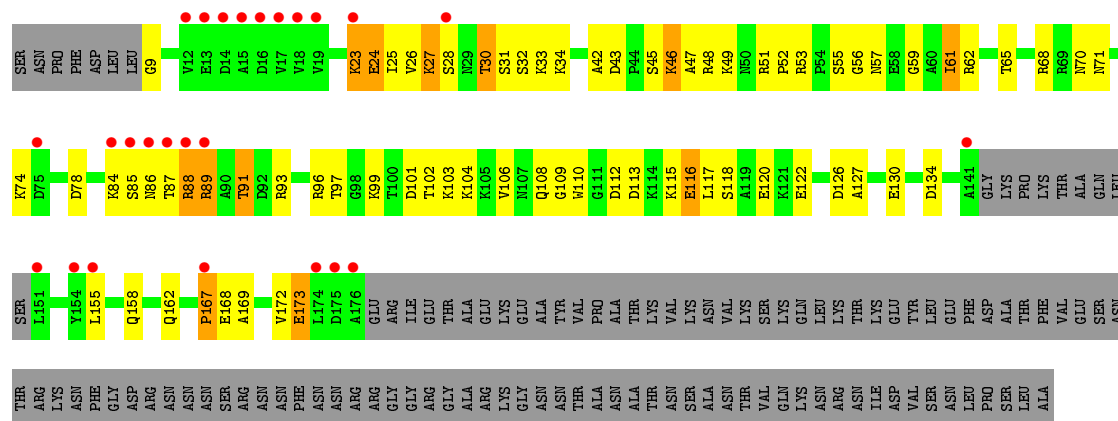




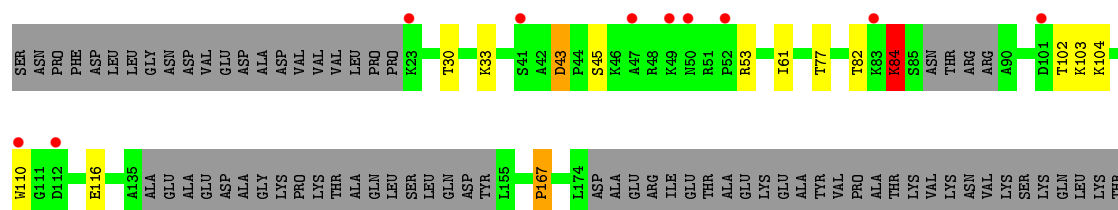
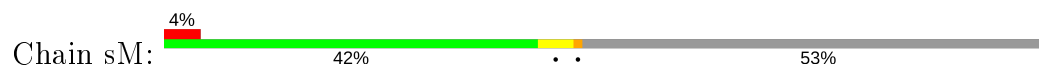
• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 79: Suppressor protein STM1

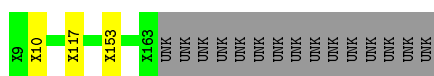


• Molecule 79: Suppressor protein STM1



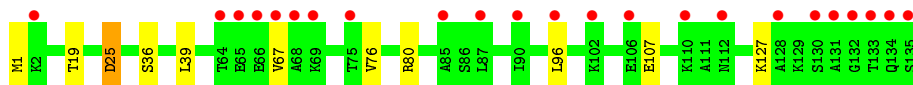
- Molecule 80: 60S ribosomal protein L12

Chain m2:  89% • 9%

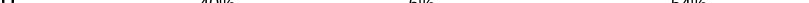


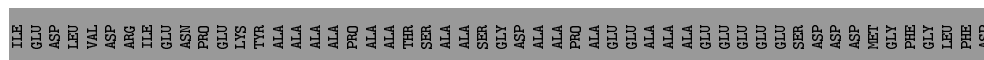
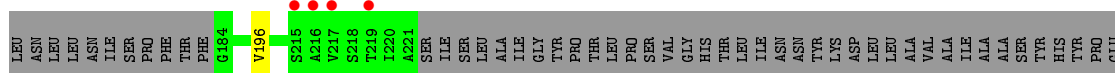
- Molecule 81: 60S ribosomal protein L24-A

Chain n4:  17% 92% 7%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 



- Molecule 83: Ribosomal protein P1 alpha

Chain p1:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	436.63Å 287.00Å 304.73Å 90.00° 99.08° 90.00°	Depositor
Resolution (Å)	143.72 – 3.40 143.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (143.72-3.40) 92.9 (143.72-3.40)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.189 , 0.238 0.189 , 0.238	Depositor DCC
$R_{free}$ test set	20266 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 85.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	404238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, LLL

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	1	0.73	10/74216 (0.0%)	1.29	499/115705 (0.4%)
1	5	0.83	19/75037 (0.0%)	1.37	668/116983 (0.6%)
2	3	0.62	0/2883	1.14	5/4491 (0.1%)
2	7	0.81	0/2883	1.33	18/4491 (0.4%)
3	4	0.66	0/3701	1.20	14/5760 (0.2%)
3	8	0.63	0/3746	1.18	14/5832 (0.2%)
4	L2	0.42	0/1948	0.66	0/2617
4	l2	0.44	0/1946	0.71	0/2614
5	L3	0.49	0/3152	0.67	1/4239 (0.0%)
5	l3	0.56	0/3152	0.71	1/4239 (0.0%)
6	L4	0.49	1/2801 (0.0%)	0.72	3/3792 (0.1%)
6	l4	0.47	0/2801	0.68	1/3792 (0.0%)
7	L5	0.41	0/2425	0.60	0/3271
7	l5	0.53	0/2408	0.67	1/3248 (0.0%)
8	L6	0.49	0/1260	0.63	0/1694
8	l6	0.53	0/1269	0.67	0/1705
9	L7	0.45	0/1821	0.64	0/2451
9	l7	0.54	0/1828	0.69	1/2461 (0.0%)
10	L8	0.38	0/1849	0.55	0/2495
10	l8	0.43	1/1795 (0.1%)	0.61	0/2429
11	L9	0.46	0/1539	0.64	0/2073
11	l9	0.60	0/1539	0.68	0/2073
12	M0	0.52	0/1743	0.64	0/2339
12	m0	0.63	0/1752	0.76	2/2349 (0.1%)
13	M1	0.40	0/1374	0.63	2/1842 (0.1%)
13	m1	0.54	0/1374	0.69	1/1842 (0.1%)
14	M3	0.47	0/1568	0.67	0/2106
14	m3	0.45	0/1573	0.66	0/2113
15	M4	0.48	0/1068	0.60	0/1438
15	m4	0.55	0/1074	0.67	0/1446
16	M5	0.43	0/1757	0.63	0/2354
16	m5	0.44	0/1757	0.63	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	M6	0.58	1/1585 (0.1%)	0.69	0/2128
17	m6	0.67	0/1585	0.74	3/2128 (0.1%)
18	M7	0.49	0/1438	0.65	0/1937
18	m7	0.51	0/1250	0.69	0/1683
19	M8	0.45	0/1465	0.67	0/1965
19	m8	0.49	0/1465	0.68	0/1965
20	M9	0.36	0/1491	0.57	0/1987
20	m9	0.39	0/1538	0.54	0/2050
21	N0	0.44	0/1481	0.61	0/1990
21	n0	0.58	0/1481	0.68	2/1990 (0.1%)
22	N1	0.48	0/1300	0.64	0/1743
22	n1	0.59	0/1300	0.66	0/1743
23	N2	0.34	0/812	0.53	0/1099
23	n2	0.39	0/794	0.56	0/1076
24	N3	0.51	0/1018	0.65	0/1369
24	n3	0.59	0/1018	0.74	0/1369
25	N4	0.40	0/712	0.58	0/958
26	N5	0.39	0/979	0.60	1/1321 (0.1%)
26	n5	0.41	0/974	0.64	0/1314
27	N6	0.45	0/1004	0.69	0/1341
27	n6	0.41	0/1004	0.65	0/1341
28	N7	0.37	0/1118	0.58	0/1497
28	n7	0.38	0/1118	0.55	0/1497
29	N8	0.47	0/1204	0.68	0/1612
29	n8	0.50	0/1204	0.70	0/1612
30	N9	0.50	0/473	0.68	0/629
30	n9	0.54	0/473	0.74	0/629
31	O0	0.34	0/751	0.56	1/1008 (0.1%)
31	o0	0.36	0/775	0.56	0/1040
32	O1	0.43	0/904	0.60	0/1213
32	o1	0.51	0/904	0.65	0/1213
33	O2	0.53	0/1041	0.67	0/1394
33	o2	0.49	0/1041	0.66	0/1394
34	O3	0.55	0/868	0.66	0/1168
34	o3	0.64	0/868	0.69	0/1168
35	O4	0.39	0/891	0.57	1/1191 (0.1%)
35	o4	0.39	0/891	0.61	0/1191
36	O5	0.43	0/978	0.62	0/1301
36	o5	0.39	0/978	0.58	1/1301 (0.1%)
37	O6	0.41	0/778	0.66	0/1034
37	o6	0.41	0/778	0.57	0/1034
38	O7	0.46	0/696	0.72	0/923
38	o7	0.50	0/696	0.71	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	O8	0.35	0/618	0.55	0/826
39	o8	0.36	0/618	0.60	0/826
40	O9	0.49	0/443	0.66	0/588
40	o9	0.48	0/443	0.67	0/588
41	Q0	0.55	0/423	0.74	0/562
41	q0	0.77	2/423 (0.5%)	0.80	0/562
42	Q1	0.42	0/234	0.57	0/300
42	q1	0.56	0/234	0.77	0/300
43	Q2	0.50	0/860	0.72	1/1136 (0.1%)
43	q2	0.59	0/860	0.74	0/1136
44	Q3	0.40	0/701	0.61	0/934
44	q3	0.47	0/701	0.65	0/934
45	2	0.50	0/40811	1.07	126/63585 (0.2%)
45	6	0.66	4/41451 (0.0%)	1.23	234/64581 (0.4%)
46	S0	0.35	1/1653 (0.1%)	0.56	0/2261
46	s0	0.37	0/1653	0.61	0/2261
47	S1	0.33	0/1735	0.63	3/2335 (0.1%)
47	s1	0.37	0/1748	0.63	2/2352 (0.1%)
48	S2	0.37	0/1665	0.59	0/2263
48	s2	0.41	0/1665	0.67	1/2263 (0.0%)
49	S3	0.34	0/1759	0.53	0/2368
49	s3	0.40	0/1753	0.59	0/2361
50	S4	0.36	0/2109	0.63	1/2839 (0.0%)
50	s4	0.39	0/2109	0.66	1/2839 (0.0%)
51	S5	0.59	1/1629 (0.1%)	0.52	0/2202
51	s5	0.42	0/1629	0.67	0/2202
52	S6	0.37	0/1837	0.55	0/2455
52	s6	0.40	0/1779	0.59	1/2379 (0.0%)
53	S7	0.34	0/1506	0.59	0/2028
53	s7	0.36	0/1516	0.61	1/2043 (0.0%)
54	S8	0.36	0/1514	0.58	1/2021 (0.0%)
54	s8	0.40	0/1496	0.61	0/1999
55	S9	0.34	0/1519	0.59	2/2035 (0.1%)
55	s9	0.38	0/1519	0.62	0/2035
56	C0	0.34	0/789	0.62	1/1067 (0.1%)
56	c0	0.36	0/776	0.76	4/1047 (0.4%)
57	C1	0.38	0/1239	0.54	0/1673
57	c1	0.43	0/1164	0.60	0/1569
58	C2	0.31	0/898	0.66	1/1220 (0.1%)
58	c2	0.33	0/898	0.65	2/1220 (0.2%)
59	C3	0.33	0/1215	0.52	0/1638
59	c3	0.41	0/1215	0.62	1/1638 (0.1%)
60	C4	0.30	0/901	0.60	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	c4	0.39	0/960	0.70	0/1290
61	C5	0.37	0/998	0.59	0/1341
61	c5	0.45	0/1060	0.69	1/1426 (0.1%)
62	C6	0.32	0/1125	0.57	1/1510 (0.1%)
62	c6	0.46	0/1131	0.63	0/1518
63	C7	0.35	0/975	0.61	1/1307 (0.1%)
63	c7	0.38	0/925	0.63	0/1239
64	C8	0.32	0/1211	0.54	0/1628
64	c8	0.48	0/1211	0.67	1/1628 (0.1%)
65	C9	0.33	0/1130	0.54	1/1517 (0.1%)
65	c9	0.46	0/1130	0.60	0/1517
66	D0	0.36	0/865	0.56	0/1169
66	d0	0.43	0/892	0.65	0/1205
67	D1	0.31	0/693	0.60	0/935
67	d1	0.37	0/693	0.60	0/935
68	D2	0.35	0/1038	0.61	0/1395
68	d2	0.40	0/1038	0.64	1/1395 (0.1%)
69	D3	0.43	0/1139	0.63	1/1518 (0.1%)
69	d3	0.52	1/1139 (0.1%)	0.68	0/1518
70	D4	0.38	0/1087	0.57	0/1449
70	d4	0.39	0/1079	0.60	0/1438
71	D5	0.29	0/571	0.58	0/768
71	d5	0.43	0/566	0.55	0/761
72	D6	0.48	1/782 (0.1%)	0.66	1/1047 (0.1%)
72	d6	0.52	0/782	0.72	0/1047
73	D7	0.32	0/620	0.59	0/838
73	d7	0.37	0/620	0.69	1/838 (0.1%)
74	D8	0.30	0/499	0.52	0/670
74	d8	0.40	0/499	0.60	0/670
75	D9	0.46	0/453	0.69	0/602
75	d9	0.44	0/453	0.68	0/602
76	E0	0.36	0/483	0.57	0/643
76	e0	0.40	0/499	0.67	0/665
77	E1	0.34	0/577	0.66	0/770
77	e1	0.39	0/586	0.78	0/781
78	SR	0.30	0/2494	0.55	0/3394
78	sR	0.34	0/2494	0.59	0/3394
79	SM	0.34	0/1113	0.64	1/1502 (0.1%)
79	sM	0.41	0/929	0.68	3/1246 (0.2%)
81	n4	0.42	0/1058	0.62	0/1405
82	p0	0.36	0/1092	0.56	0/1474
All	All	0.61	42/426558 (0.0%)	1.06	1636/625790 (0.3%)

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
4	L2	0	1
4	l2	0	2
5	l3	0	1
6	L4	0	1
6	l4	0	2
7	L5	0	1
7	l5	0	2
9	L7	0	1
9	l7	0	2
11	L9	0	1
12	M0	0	1
12	m0	0	1
13	M1	0	1
13	m1	0	1
14	M3	0	1
15	M4	0	1
16	m5	0	1
18	M7	0	1
19	M8	0	1
21	N0	0	2
23	n2	0	1
24	n3	0	1
25	N4	0	2
27	N6	0	1
28	N7	0	1
28	n7	0	2
29	N8	0	3
29	n8	0	1
30	N9	0	1
32	o1	0	1
33	o2	0	2
34	o3	0	1
35	o4	0	1
37	o6	0	1
40	O9	0	1
46	s0	0	3
47	S1	0	1
48	S2	0	2
49	s3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
50	S4	0	3
51	S5	0	1
51	s5	0	2
52	S6	0	1
52	s6	0	1
53	S7	0	5
53	s7	0	3
54	s8	0	2
55	s9	0	2
58	c2	0	1
59	c3	0	1
60	C4	0	2
60	c4	0	4
61	C5	0	2
61	c5	0	2
62	C6	0	1
63	C7	0	2
63	c7	0	2
64	C8	0	1
66	D0	0	2
66	d0	0	5
67	D1	0	1
68	D2	0	1
68	d2	0	1
69	d3	0	1
70	D4	0	1
70	d4	0	2
71	D5	0	3
71	d5	0	1
72	D6	0	2
72	d6	0	1
73	D7	0	1
76	e0	0	1
77	E1	0	3
77	e1	0	2
78	sR	0	4
79	SM	0	2
79	sM	0	2
80	m2	0	3
82	p0	0	1
All	All	0	130

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S5	21	THR	C-N	20.19	1.72	1.34
1	5	2971	A	N9-C4	12.79	1.45	1.37
1	5	1152	G	N9-C4	-9.61	1.30	1.38
6	L4	19	ALA	C-N	8.69	1.54	1.34
72	D6	59	TYR	C-N	8.53	1.50	1.34

The worst 5 of 1636 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-N9	-18.77	114.74	126.00
1	5	1152	G	N3-C4-C5	17.59	137.39	128.60
1	1	1201	C	C6-N1-C2	-14.35	114.56	120.30
6	L4	182	LEU	CA-CB-CG	12.68	144.47	115.30
1	5	420	G	C5-C6-O6	-12.32	121.21	128.60

There are no chirality outliers.

5 of 130 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L2	48	ILE	Peptide
6	L4	318	LEU	Peptide
7	L5	251	PRO	Peptide
9	L7	29	GLU	Peptide
11	L9	21	LYS	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	66304	0	33321	1403	0
1	5	67039	0	33693	1455	0
2	3	2579	0	1304	53	0
2	7	2579	0	1304	78	0
3	4	3313	0	1676	58	0
3	8	3353	0	1695	89	0
4	L2	1914	0	1981	181	0
4	12	1912	0	1976	0	0
5	L3	3081	0	3165	231	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	l3	3081	0	3165	0	0
6	L4	2749	0	2863	255	0
6	l4	2749	0	2863	0	0
7	L5	2375	0	2325	184	0
7	l5	2359	0	2311	0	0
8	L6	1239	0	1326	101	0
8	l6	1248	0	1339	0	0
9	L7	1784	0	1862	129	0
9	l7	1791	0	1869	0	0
10	L8	1817	0	1908	148	0
10	l8	1763	0	1818	0	0
11	L9	1518	0	1587	153	0
11	l9	1518	0	1587	0	0
12	M0	1707	0	1731	144	0
12	m0	1716	0	1757	0	0
13	M1	1353	0	1383	104	0
13	m1	1353	0	1383	0	0
14	M3	1543	0	1608	153	0
14	m3	1548	0	1613	0	0
15	M4	1053	0	1149	90	0
15	m4	1059	0	1154	0	0
16	M5	1720	0	1779	161	0
16	m5	1720	0	1779	0	0
17	M6	1555	0	1659	101	0
17	m6	1555	0	1659	0	0
18	M7	1415	0	1421	109	0
18	m7	1227	0	1236	0	0
19	M8	1441	0	1543	129	0
19	m8	1441	0	1543	0	0
20	M9	1474	0	1567	101	0
20	m9	1521	0	1617	0	0
21	N0	1445	0	1487	99	0
21	n0	1445	0	1487	0	0
22	N1	1276	0	1323	133	0
22	n1	1276	0	1323	0	0
23	N2	796	0	812	56	0
23	n2	778	0	791	0	0
24	N3	1003	0	1048	78	0
24	n3	1003	0	1048	0	0
25	N4	699	0	640	35	0
26	N5	964	0	1025	83	0
26	n5	959	0	1023	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	N6	993	0	1081	84	0
27	n6	993	0	1081	0	0
28	N7	1092	0	1155	105	0
28	n7	1092	0	1155	0	0
29	N8	1173	0	1215	117	0
29	n8	1173	0	1215	0	0
30	N9	462	0	491	35	0
30	n9	462	0	491	0	0
31	O0	743	0	797	58	0
31	o0	767	0	816	0	0
32	O1	890	0	938	59	0
32	o1	890	0	938	0	0
33	O2	1020	0	1090	78	0
33	o2	1020	0	1090	0	0
34	O3	850	0	880	53	0
34	o3	850	0	880	0	0
35	O4	881	0	947	76	0
35	o4	881	0	947	0	0
36	O5	969	0	1078	98	0
36	o5	969	0	1078	0	0
37	O6	771	0	849	73	0
37	o6	771	0	849	0	0
38	O7	681	0	683	68	0
38	o7	681	0	684	0	0
39	O8	612	0	682	40	0
39	o8	612	0	682	0	0
40	O9	436	0	475	55	0
40	o9	436	0	475	0	0
41	Q0	417	0	456	32	0
41	q0	417	0	455	0	0
42	Q1	233	0	284	16	0
42	q1	233	0	284	0	0
43	Q2	847	0	915	64	0
43	q2	847	0	914	0	0
44	Q3	694	0	734	61	0
44	q3	694	0	734	0	0
45	2	36488	0	18357	1002	1
45	6	37060	0	18648	922	0
46	S0	1612	0	1623	180	0
46	s0	1612	0	1623	0	0
47	S1	1709	0	1784	210	0
47	s1	1722	0	1793	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	S2	1635	0	1723	151	0
48	s2	1635	0	1723	0	0
49	S3	1734	0	1817	150	0
49	s3	1728	0	1806	0	0
50	S4	2068	0	2154	184	0
50	s4	2068	0	2154	0	0
51	S5	1609	0	1675	191	0
51	s5	1609	0	1675	0	0
52	S6	1813	0	1905	141	0
52	s6	1755	0	1846	0	0
53	S7	1481	0	1572	131	0
53	s7	1491	0	1578	0	0
54	S8	1489	0	1525	146	0
54	s8	1471	0	1499	0	0
55	S9	1494	0	1573	163	0
55	s9	1494	0	1573	0	0
56	C0	772	0	727	70	0
56	c0	761	0	697	0	0
57	C1	1213	0	1257	105	0
57	c1	1138	0	1204	0	0
58	C2	890	0	887	82	0
58	c2	890	0	887	0	0
59	C3	1192	0	1255	85	0
59	c3	1192	0	1255	0	0
60	C4	891	0	883	84	0
60	c4	949	0	985	0	0
61	C5	977	0	1002	95	0
61	c5	1039	0	1050	0	0
62	C6	1105	0	1166	116	0
62	c6	1111	0	1171	0	0
63	C7	965	0	1027	115	0
63	c7	917	0	932	0	0
64	C8	1192	0	1222	132	0
64	c8	1192	0	1222	0	0
65	C9	1112	0	1124	98	0
65	c9	1112	0	1124	0	0
66	D0	855	0	917	100	0
66	d0	882	0	939	0	1
67	D1	684	0	672	70	0
67	d1	684	0	672	0	0
68	D2	1021	0	1060	102	0
68	d2	1021	0	1060	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	D3	1121	0	1196	98	0
69	d3	1121	0	1196	0	0
70	D4	1073	0	1132	88	0
70	d4	1065	0	1128	0	0
71	D5	563	0	603	78	0
71	d5	558	0	598	0	0
72	D6	769	0	815	110	0
72	d6	769	0	814	0	0
73	D7	610	0	633	55	0
73	d7	610	0	633	0	0
74	D8	497	0	535	59	0
74	d8	497	0	535	0	0
75	D9	443	0	433	55	0
75	d9	443	0	431	0	0
76	E0	475	0	525	53	0
76	e0	491	0	542	0	0
77	E1	566	0	604	60	0
77	e1	575	0	617	0	0
78	SR	2441	0	2393	195	0
78	sR	2441	0	2393	0	0
79	SM	1104	0	996	93	0
79	sM	923	0	868	0	0
80	m2	750	0	167	0	0
81	n4	1044	0	1082	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	1	588	0	0	0	0
84	2	142	0	0	0	0
84	3	19	0	0	0	0
84	4	23	0	0	0	0
84	5	750	0	0	0	0
84	6	263	0	0	0	0
84	7	30	0	0	0	0
84	8	20	0	0	0	0
84	C1	1	0	0	0	0
84	C3	1	0	0	0	0
84	C8	1	0	0	0	0
84	D3	5	0	0	0	0
84	L2	5	0	0	0	0
84	L3	3	0	0	0	0
84	L4	6	0	0	0	0
84	L5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	L7	1	0	0	0	0
84	L8	1	0	0	0	0
84	L9	1	0	0	0	0
84	M0	4	0	0	0	0
84	M3	5	0	0	0	0
84	M5	5	0	0	0	0
84	M6	1	0	0	0	0
84	M7	5	0	0	0	0
84	M8	1	0	0	0	0
84	N0	4	0	0	0	0
84	N1	2	0	0	0	0
84	N3	4	0	0	0	0
84	N4	1	0	0	0	0
84	N5	1	0	0	0	0
84	N8	3	0	0	0	0
84	O2	4	0	0	0	0
84	O3	1	0	0	0	0
84	O4	3	0	0	0	0
84	O6	1	0	0	0	0
84	O7	3	0	0	0	0
84	Q1	1	0	0	0	0
84	Q2	4	0	0	0	0
84	S1	1	0	0	0	0
84	S2	1	0	0	0	0
84	S3	1	0	0	0	0
84	S4	1	0	0	0	0
84	c1	1	0	0	0	0
84	c3	6	0	0	0	0
84	c4	1	0	0	0	0
84	c8	3	0	0	0	0
84	d1	2	0	0	0	0
84	d2	1	0	0	0	0
84	d3	5	0	0	0	0
84	d5	1	0	0	0	0
84	d6	3	0	0	0	0
84	d7	1	0	0	0	0
84	d9	1	0	0	0	0
84	l2	5	0	0	0	0
84	l3	11	0	0	0	0
84	l4	2	0	0	0	0
84	l5	6	0	0	0	0
84	l6	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	l7	3	0	0	0	0
84	l8	1	0	0	0	0
84	l9	8	0	0	0	0
84	m0	2	0	0	0	0
84	m3	4	0	0	0	0
84	m4	6	0	0	0	0
84	m5	3	0	0	0	0
84	m6	8	0	0	0	0
84	m7	7	0	0	0	0
84	m8	4	0	0	0	0
84	m9	2	0	0	0	0
84	n0	7	0	0	0	0
84	n1	2	0	0	0	0
84	n3	2	0	0	0	0
84	n5	3	0	0	0	0
84	n8	3	0	0	0	0
84	n9	1	0	0	0	0
84	o1	1	0	0	0	0
84	o2	3	0	0	0	0
84	o3	2	0	0	0	0
84	o4	2	0	0	0	0
84	q0	1	0	0	0	0
84	q1	2	0	0	0	0
84	q2	7	0	0	0	0
84	q3	3	0	0	0	0
84	s0	1	0	0	0	0
84	s2	2	0	0	0	0
84	s3	1	0	0	0	0
84	s4	1	0	0	0	0
84	s5	3	0	0	0	0
84	s6	1	0	0	0	0
84	sR	1	0	0	0	0
85	1	496	0	624	28	0
85	2	93	0	117	9	0
85	3	31	0	39	2	0
85	4	31	0	39	9	0
85	5	868	0	1092	53	0
85	6	403	0	507	27	0
85	7	93	0	117	11	0
85	8	62	0	78	16	0
85	L3	31	0	39	2	0
85	l3	31	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	D6	1	0	0	0	0
86	D7	1	0	0	0	0
86	D9	1	0	0	0	0
86	E1	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
86	d6	1	0	0	0	0
86	d7	1	0	0	0	0
86	d9	1	0	0	0	0
86	e1	1	0	0	0	0
86	o4	1	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q2	1	0	0	0	0
86	q3	1	0	0	0	0
87	1	473	0	0	38	0
87	2	111	0	0	2	0
87	3	15	0	0	0	0
87	4	5	0	0	0	0
87	5	514	0	0	34	0
87	6	224	0	0	8	0
87	7	33	0	0	2	0
87	8	11	0	0	1	0
87	C9	2	0	0	0	0
87	D0	1	0	0	0	0
87	D3	1	0	0	0	0
87	L2	1	0	0	0	0
87	L3	7	0	0	2	0
87	L4	2	0	0	0	0
87	L5	2	0	0	1	0
87	M0	1	0	0	1	0
87	M3	2	0	0	0	0
87	M5	3	0	0	0	0
87	M6	6	0	0	0	0
87	M7	5	0	0	1	0
87	N0	4	0	0	1	0
87	N1	3	0	0	1	0
87	N3	5	0	0	3	0
87	N4	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	N5	2	0	0	1	0
87	N8	3	0	0	0	0
87	N9	2	0	0	0	0
87	O2	2	0	0	0	0
87	O4	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q1	1	0	0	2	0
87	Q2	1	0	0	0	0
87	S1	1	0	0	0	0
87	S3	3	0	0	0	0
87	S4	1	0	0	0	0
87	S8	1	0	0	0	0
87	SR	2	0	0	0	0
87	c3	5	0	0	0	0
87	c6	1	0	0	0	0
87	c8	3	0	0	0	0
87	c9	5	0	0	0	0
87	d3	5	0	0	0	0
87	d5	3	0	0	0	0
87	d6	3	0	0	0	0
87	d9	2	0	0	0	0
87	e1	1	0	0	0	0
87	l2	7	0	0	0	0
87	l3	6	0	0	0	0
87	l5	5	0	0	0	0
87	l9	3	0	0	0	0
87	m0	1	0	0	0	0
87	m4	1	0	0	0	0
87	m5	2	0	0	0	0
87	m6	8	0	0	0	0
87	m7	4	0	0	0	0
87	m9	3	0	0	0	0
87	n0	4	0	0	0	0
87	n1	2	0	0	0	0
87	n3	2	0	0	0	0
87	n4	1	0	0	0	0
87	n5	2	0	0	0	0
87	n6	1	0	0	0	0
87	n8	4	0	0	0	0
87	n9	1	0	0	0	0
87	o0	1	0	0	0	0
87	o1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	o2	4	0	0	0	0
87	o4	2	0	0	0	0
87	q0	1	0	0	0	0
87	q2	2	0	0	0	0
87	q3	3	0	0	0	0
87	s4	1	0	0	0	0
87	s5	1	0	0	0	0
87	s7	1	0	0	0	0
87	sR	1	0	0	0	0
All	All	404238	0	298719	11005	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 11005 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)
51:S5:21:THR:C	51:S5:22:PRO:N	1.72	1.42
45:2:1755:A:C2'	45:2:1756:A:H5'	1.74	1.17
45:2:1755:A:H2'	45:2:1756:A:C5'	1.76	1.16
54:S8:83:TYR:H	54:S8:101:ILE:HG21	4.57	1.11
45:2:74:U:H1'	45:2:75:U:H5'	1.33	1.09

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2:1491:U:O2'	66:d0:12:GLN:OE1[1_454]	2.11	0.09

## 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	
4	L2	250/252 (99%)	233 (93%)	17 (7%)	0	100	100
4	l2	250/252 (99%)	227 (91%)	21 (8%)	2 (1%)	19	51
5	L3	384/386 (100%)	349 (91%)	32 (8%)	3 (1%)	19	51
5	l3	384/386 (100%)	354 (92%)	29 (8%)	1 (0%)	41	72
6	L4	359/361 (99%)	323 (90%)	34 (10%)	2 (1%)	25	57
6	l4	359/361 (99%)	313 (87%)	43 (12%)	3 (1%)	19	51
7	L5	294/296 (99%)	266 (90%)	28 (10%)	0	100	100
7	l5	292/296 (99%)	266 (91%)	24 (8%)	2 (1%)	22	55
8	L6	152/176 (86%)	141 (93%)	10 (7%)	1 (1%)	22	55
8	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	12	39
9	L7	220/223 (99%)	204 (93%)	16 (7%)	0	100	100
9	l7	221/223 (99%)	206 (93%)	13 (6%)	2 (1%)	17	49
10	L8	231/233 (99%)	199 (86%)	30 (13%)	2 (1%)	17	49
10	l8	229/233 (98%)	194 (85%)	33 (14%)	2 (1%)	17	49
11	L9	189/191 (99%)	169 (89%)	20 (11%)	0	100	100
11	l9	189/191 (99%)	176 (93%)	11 (6%)	2 (1%)	14	44
12	M0	208/221 (94%)	188 (90%)	19 (9%)	1 (0%)	29	61
12	m0	207/221 (94%)	184 (89%)	23 (11%)	0	100	100
13	M1	167/169 (99%)	142 (85%)	25 (15%)	0	100	100
13	m1	167/169 (99%)	146 (87%)	19 (11%)	2 (1%)	13	41
14	M3	191/194 (98%)	170 (89%)	19 (10%)	2 (1%)	15	46
14	m3	192/194 (99%)	164 (85%)	26 (14%)	2 (1%)	15	46
15	M4	134/137 (98%)	120 (90%)	14 (10%)	0	100	100
15	m4	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
16	M5	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
16	m5	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
17	M6	195/197 (99%)	187 (96%)	7 (4%)	1 (0%)	29	61
17	m6	195/197 (99%)	190 (97%)	5 (3%)	0	100	100
18	M7	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
18	m7	153/184 (83%)	140 (92%)	13 (8%)	0	100	100
19	M8	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
19	m8	183/185 (99%)	167 (91%)	14 (8%)	2 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	M9	180/188 (96%)	169 (94%)	11 (6%)	0	100	100
20	m9	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
21	N0	170/172 (99%)	157 (92%)	13 (8%)	0	100	100
21	n0	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	N1	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	31
22	n1	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
23	N2	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	46
23	n2	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
24	N3	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
24	n3	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
25	N4	96/155 (62%)	83 (86%)	12 (12%)	1 (1%)	15	46
26	N5	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
26	n5	118/121 (98%)	108 (92%)	10 (8%)	0	100	100
27	N6	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
27	n6	124/126 (98%)	117 (94%)	5 (4%)	2 (2%)	9	34
28	N7	133/135 (98%)	114 (86%)	19 (14%)	0	100	100
28	n7	133/135 (98%)	116 (87%)	16 (12%)	1 (1%)	19	51
29	N8	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	22	55
29	n8	146/148 (99%)	132 (90%)	13 (9%)	1 (1%)	22	55
30	N9	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	32
30	n9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	3	21
31	O0	95/100 (95%)	89 (94%)	5 (5%)	1 (1%)	14	44
31	o0	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
32	O1	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
32	o1	107/109 (98%)	96 (90%)	10 (9%)	1 (1%)	17	49
33	O2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
33	o2	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
34	O3	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
34	o3	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	O4	110/112 (98%)	100 (91%)	10 (9%)	0	100	100
35	o4	110/112 (98%)	99 (90%)	10 (9%)	1 (1%)	17	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	O5	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
36	o5	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
37	O6	97/99 (98%)	80 (82%)	15 (16%)	2 (2%)	7	30
37	o6	97/99 (98%)	86 (89%)	11 (11%)	0	100	100
38	O7	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
38	o7	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	O8	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
39	o8	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
40	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
40	o9	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Q0	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
41	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	7	30
42	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
43	Q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
43	q2	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	15	46
44	Q3	89/91 (98%)	77 (86%)	12 (14%)	0	100	100
44	q3	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
46	S0	204/206 (99%)	176 (86%)	27 (13%)	1 (0%)	29	61
46	s0	204/206 (99%)	170 (83%)	30 (15%)	4 (2%)	7	30
47	S1	212/216 (98%)	175 (82%)	35 (16%)	2 (1%)	17	49
47	s1	214/216 (99%)	188 (88%)	25 (12%)	1 (0%)	29	61
48	S2	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	29	61
48	s2	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	29	61
49	S3	221/223 (99%)	201 (91%)	19 (9%)	1 (0%)	29	61
49	s3	221/223 (99%)	194 (88%)	25 (11%)	2 (1%)	17	49
50	S4	258/260 (99%)	230 (89%)	27 (10%)	1 (0%)	34	67
50	s4	258/260 (99%)	225 (87%)	32 (12%)	1 (0%)	34	67
51	S5	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	36
51	s5	204/206 (99%)	182 (89%)	21 (10%)	1 (0%)	29	61
52	S6	224/236 (95%)	207 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	s6	216/236 (92%)	198 (92%)	16 (7%)	2 (1%)	17	49
53	S7	182/186 (98%)	156 (86%)	22 (12%)	4 (2%)	6	29
53	s7	184/186 (99%)	159 (86%)	23 (12%)	2 (1%)	14	44
54	S8	184/200 (92%)	158 (86%)	24 (13%)	2 (1%)	14	44
54	s8	182/200 (91%)	164 (90%)	16 (9%)	2 (1%)	14	44
55	S9	183/185 (99%)	153 (84%)	28 (15%)	2 (1%)	14	44
55	s9	183/185 (99%)	158 (86%)	23 (13%)	2 (1%)	14	44
56	C0	94/105 (90%)	73 (78%)	17 (18%)	4 (4%)	2	17
56	c0	92/105 (88%)	74 (80%)	13 (14%)	5 (5%)	2	13
57	C1	153/156 (98%)	138 (90%)	14 (9%)	1 (1%)	22	55
57	c1	140/156 (90%)	124 (89%)	15 (11%)	1 (1%)	22	55
58	C2	122/143 (85%)	91 (75%)	26 (21%)	5 (4%)	3	18
58	c2	122/143 (85%)	88 (72%)	32 (26%)	2 (2%)	9	34
59	C3	148/150 (99%)	136 (92%)	12 (8%)	0	100	100
59	c3	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	26
60	C4	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	9	34
60	c4	126/128 (98%)	107 (85%)	18 (14%)	1 (1%)	19	51
61	C5	122/141 (86%)	104 (85%)	15 (12%)	3 (2%)	5	26
61	c5	133/141 (94%)	109 (82%)	23 (17%)	1 (1%)	19	51
62	C6	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	22	55
62	c6	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	37
63	C7	118/136 (87%)	100 (85%)	15 (13%)	3 (2%)	5	26
63	c7	113/136 (83%)	97 (86%)	12 (11%)	4 (4%)	3	21
64	C8	143/145 (99%)	120 (84%)	21 (15%)	2 (1%)	11	37
64	c8	143/145 (99%)	125 (87%)	15 (10%)	3 (2%)	7	30
65	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
65	c9	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
66	D0	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	15	46
66	d0	108/110 (98%)	87 (81%)	17 (16%)	4 (4%)	3	20
67	D1	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	13	41
67	d1	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	13	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	D2	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	34
68	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	51
69	D3	142/144 (99%)	119 (84%)	23 (16%)	0	100	100
69	d3	142/144 (99%)	128 (90%)	14 (10%)	0	100	100
70	D4	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
70	d4	131/134 (98%)	110 (84%)	18 (14%)	3 (2%)	6	28
71	D5	68/70 (97%)	53 (78%)	12 (18%)	3 (4%)	2	16
71	d5	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
72	D6	95/97 (98%)	75 (79%)	17 (18%)	3 (3%)	4	22
72	d6	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	14	44
73	D7	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
73	d7	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5	26
74	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
74	d8	61/63 (97%)	51 (84%)	9 (15%)	1 (2%)	9	34
75	D9	51/53 (96%)	44 (86%)	5 (10%)	2 (4%)	3	19
75	d9	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
76	E0	58/62 (94%)	46 (79%)	10 (17%)	2 (3%)	3	21
76	e0	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
77	E1	69/72 (96%)	53 (77%)	15 (22%)	1 (1%)	11	37
77	e1	70/72 (97%)	44 (63%)	22 (31%)	4 (6%)	1	12
78	SR	316/318 (99%)	283 (90%)	33 (10%)	0	100	100
78	sR	316/318 (99%)	293 (93%)	21 (7%)	2 (1%)	25	57
79	SM	155/272 (57%)	127 (82%)	26 (17%)	2 (1%)	12	39
79	sM	123/272 (45%)	105 (85%)	15 (12%)	3 (2%)	6	28
81	n4	133/135 (98%)	116 (87%)	14 (10%)	3 (2%)	6	28
82	p0	139/312 (45%)	124 (89%)	13 (9%)	2 (1%)	11	37
All	All	22342/23454 (95%)	19892 (89%)	2273 (10%)	177 (1%)	19	51

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L4	339	LEU
8	L6	98	VAL

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Mol	Chain	Res	Type
25	N4	63	ILE
51	S5	64	VAL
56	C0	88	PRO

### 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	
4	L2	193/194 (100%)	172 (89%)	21 (11%)	6	23
4	l2	192/194 (99%)	175 (91%)	17 (9%)	9	33
5	L3	322/322 (100%)	273 (85%)	49 (15%)	3	11
5	l3	322/322 (100%)	277 (86%)	45 (14%)	3	13
6	L4	288/288 (100%)	254 (88%)	34 (12%)	5	19
6	l4	288/288 (100%)	253 (88%)	35 (12%)	5	18
7	L5	244/244 (100%)	219 (90%)	25 (10%)	7	26
7	l5	243/244 (100%)	207 (85%)	36 (15%)	3	12
8	L6	134/153 (88%)	115 (86%)	19 (14%)	3	13
8	l6	135/153 (88%)	112 (83%)	23 (17%)	2	8
9	L7	186/187 (100%)	168 (90%)	18 (10%)	8	28
9	l7	187/187 (100%)	168 (90%)	19 (10%)	7	26
10	L8	191/191 (100%)	171 (90%)	20 (10%)	7	25
10	l8	177/191 (93%)	159 (90%)	18 (10%)	7	26
11	L9	171/171 (100%)	143 (84%)	28 (16%)	2	9
11	l9	171/171 (100%)	153 (90%)	18 (10%)	7	25
12	M0	176/187 (94%)	151 (86%)	25 (14%)	3	13
12	m0	180/187 (96%)	143 (79%)	37 (21%)	1	3
13	M1	147/147 (100%)	127 (86%)	20 (14%)	3	14
13	m1	147/147 (100%)	125 (85%)	22 (15%)	3	12
14	M3	154/154 (100%)	127 (82%)	27 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	m3	154/154 (100%)	137 (89%)	17 (11%)	6	23
15	M4	107/108 (99%)	96 (90%)	11 (10%)	7	26
15	m4	108/108 (100%)	96 (89%)	12 (11%)	6	22
16	M5	175/175 (100%)	151 (86%)	24 (14%)	3	14
16	m5	175/175 (100%)	151 (86%)	24 (14%)	3	14
17	M6	160/160 (100%)	144 (90%)	16 (10%)	7	27
17	m6	160/160 (100%)	141 (88%)	19 (12%)	5	19
18	M7	138/146 (94%)	110 (80%)	28 (20%)	1	3
18	m7	125/146 (86%)	104 (83%)	21 (17%)	2	8
19	M8	150/150 (100%)	134 (89%)	16 (11%)	6	24
19	m8	150/150 (100%)	128 (85%)	22 (15%)	3	12
20	M9	148/153 (97%)	133 (90%)	15 (10%)	7	27
20	m9	153/153 (100%)	138 (90%)	15 (10%)	8	28
21	N0	156/156 (100%)	127 (81%)	29 (19%)	1	5
21	n0	156/156 (100%)	136 (87%)	20 (13%)	4	16
22	N1	136/136 (100%)	118 (87%)	18 (13%)	4	15
22	n1	136/136 (100%)	113 (83%)	23 (17%)	2	8
23	N2	87/87 (100%)	80 (92%)	7 (8%)	12	38
23	n2	85/87 (98%)	76 (89%)	9 (11%)	6	24
24	N3	104/104 (100%)	96 (92%)	8 (8%)	13	40
24	n3	104/104 (100%)	95 (91%)	9 (9%)	10	34
25	N4	57/129 (44%)	53 (93%)	4 (7%)	15	44
26	N5	104/105 (99%)	94 (90%)	10 (10%)	8	29
26	n5	104/105 (99%)	94 (90%)	10 (10%)	8	29
27	N6	109/109 (100%)	95 (87%)	14 (13%)	4	16
27	n6	109/109 (100%)	92 (84%)	17 (16%)	2	11
28	N7	115/115 (100%)	101 (88%)	14 (12%)	5	18
28	n7	115/115 (100%)	103 (90%)	12 (10%)	7	25
29	N8	118/118 (100%)	101 (86%)	17 (14%)	3	13
29	n8	118/118 (100%)	100 (85%)	18 (15%)	2	11
30	N9	46/46 (100%)	41 (89%)	5 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	n9	46/46 (100%)	39 (85%)	7 (15%)	3	11
31	O0	81/84 (96%)	75 (93%)	6 (7%)	13	42
31	o0	84/84 (100%)	71 (84%)	13 (16%)	2	11
32	O1	96/96 (100%)	82 (85%)	14 (15%)	3	12
32	o1	96/96 (100%)	80 (83%)	16 (17%)	2	8
33	O2	109/109 (100%)	97 (89%)	12 (11%)	6	23
33	o2	109/109 (100%)	93 (85%)	16 (15%)	3	12
34	O3	90/90 (100%)	84 (93%)	6 (7%)	16	46
34	o3	90/90 (100%)	81 (90%)	9 (10%)	7	27
35	O4	95/95 (100%)	84 (88%)	11 (12%)	5	20
35	o4	95/95 (100%)	88 (93%)	7 (7%)	13	42
36	O5	104/104 (100%)	88 (85%)	16 (15%)	2	11
36	o5	104/104 (100%)	91 (88%)	13 (12%)	4	17
37	O6	81/81 (100%)	71 (88%)	10 (12%)	4	17
37	o6	81/81 (100%)	70 (86%)	11 (14%)	3	14
38	O7	70/70 (100%)	62 (89%)	8 (11%)	5	21
38	o7	70/70 (100%)	58 (83%)	12 (17%)	2	8
39	O8	68/68 (100%)	58 (85%)	10 (15%)	3	12
39	o8	68/68 (100%)	60 (88%)	8 (12%)	5	19
40	O9	45/45 (100%)	39 (87%)	6 (13%)	4	15
40	o9	45/45 (100%)	38 (84%)	7 (16%)	2	11
41	Q0	47/47 (100%)	42 (89%)	5 (11%)	6	24
41	q0	47/47 (100%)	39 (83%)	8 (17%)	2	8
42	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	7
42	q1	23/23 (100%)	20 (87%)	3 (13%)	4	16
43	Q2	90/90 (100%)	81 (90%)	9 (10%)	7	27
43	q2	90/90 (100%)	72 (80%)	18 (20%)	1	3
44	Q3	71/71 (100%)	65 (92%)	6 (8%)	10	35
44	q3	71/71 (100%)	65 (92%)	6 (8%)	10	35
46	S0	173/173 (100%)	153 (88%)	20 (12%)	5	20
46	s0	173/173 (100%)	154 (89%)	19 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	S1	191/192 (100%)	161 (84%)	30 (16%)	2	10
47	s1	192/192 (100%)	174 (91%)	18 (9%)	8	30
48	S2	176/176 (100%)	163 (93%)	13 (7%)	13	42
48	s2	176/176 (100%)	154 (88%)	22 (12%)	4	17
49	S3	182/182 (100%)	162 (89%)	20 (11%)	6	23
49	s3	181/182 (100%)	149 (82%)	32 (18%)	2	6
50	S4	221/221 (100%)	195 (88%)	26 (12%)	5	19
50	s4	221/221 (100%)	195 (88%)	26 (12%)	5	19
51	S5	173/173 (100%)	158 (91%)	15 (9%)	10	34
51	s5	173/173 (100%)	150 (87%)	23 (13%)	4	15
52	S6	191/201 (95%)	167 (87%)	24 (13%)	4	17
52	s6	187/201 (93%)	160 (86%)	27 (14%)	3	13
53	S7	165/166 (99%)	151 (92%)	14 (8%)	10	35
53	s7	165/166 (99%)	152 (92%)	13 (8%)	12	39
54	S8	150/161 (93%)	132 (88%)	18 (12%)	5	19
54	s8	148/161 (92%)	137 (93%)	11 (7%)	13	42
55	S9	158/158 (100%)	140 (89%)	18 (11%)	5	21
55	s9	158/158 (100%)	143 (90%)	15 (10%)	8	29
56	C0	77/98 (79%)	66 (86%)	11 (14%)	3	13
56	c0	73/98 (74%)	65 (89%)	8 (11%)	6	23
57	C1	129/137 (94%)	119 (92%)	10 (8%)	12	39
57	c1	125/137 (91%)	108 (86%)	17 (14%)	3	14
58	C2	88/119 (74%)	80 (91%)	8 (9%)	9	32
58	c2	88/119 (74%)	76 (86%)	12 (14%)	3	14
59	C3	127/127 (100%)	117 (92%)	10 (8%)	12	39
59	c3	127/127 (100%)	110 (87%)	17 (13%)	4	15
60	C4	81/97 (84%)	70 (86%)	11 (14%)	3	14
60	c4	97/97 (100%)	84 (87%)	13 (13%)	4	15
61	C5	101/117 (86%)	91 (90%)	10 (10%)	8	27
61	c5	103/117 (88%)	93 (90%)	10 (10%)	8	28
62	C6	117/118 (99%)	101 (86%)	16 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	c6	118/118 (100%)	103 (87%)	15 (13%)	4	16
63	C7	109/124 (88%)	91 (84%)	18 (16%)	2	9
63	c7	97/124 (78%)	87 (90%)	10 (10%)	7	26
64	C8	128/128 (100%)	114 (89%)	14 (11%)	6	23
64	c8	128/128 (100%)	108 (84%)	20 (16%)	2	11
65	C9	115/115 (100%)	102 (89%)	13 (11%)	6	21
65	c9	115/115 (100%)	100 (87%)	15 (13%)	4	16
66	D0	100/103 (97%)	89 (89%)	11 (11%)	6	23
66	d0	103/103 (100%)	89 (86%)	14 (14%)	3	14
67	D1	74/74 (100%)	65 (88%)	9 (12%)	5	18
67	d1	74/74 (100%)	65 (88%)	9 (12%)	5	18
68	D2	110/110 (100%)	97 (88%)	13 (12%)	5	19
68	d2	110/110 (100%)	97 (88%)	13 (12%)	5	19
69	D3	119/119 (100%)	107 (90%)	12 (10%)	7	27
69	d3	119/119 (100%)	109 (92%)	10 (8%)	11	36
70	D4	112/112 (100%)	99 (88%)	13 (12%)	5	20
70	d4	111/112 (99%)	100 (90%)	11 (10%)	8	27
71	D5	61/61 (100%)	51 (84%)	10 (16%)	2	9
71	d5	61/61 (100%)	57 (93%)	4 (7%)	16	46
72	D6	83/83 (100%)	71 (86%)	12 (14%)	3	12
72	d6	83/83 (100%)	72 (87%)	11 (13%)	4	15
73	D7	70/70 (100%)	62 (89%)	8 (11%)	5	21
73	d7	70/70 (100%)	65 (93%)	5 (7%)	14	44
74	D8	56/56 (100%)	50 (89%)	6 (11%)	6	24
74	d8	56/56 (100%)	41 (73%)	15 (27%)	0	1
75	D9	47/47 (100%)	39 (83%)	8 (17%)	2	8
75	d9	47/47 (100%)	36 (77%)	11 (23%)	1	2
76	E0	51/53 (96%)	46 (90%)	5 (10%)	8	28
76	e0	53/53 (100%)	44 (83%)	9 (17%)	2	8
77	E1	62/63 (98%)	56 (90%)	6 (10%)	8	28
77	e1	63/63 (100%)	51 (81%)	12 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	SR	260/260 (100%)	239 (92%)	21 (8%)	11	38
78	sR	260/260 (100%)	241 (93%)	19 (7%)	14	43
79	SM	97/227 (43%)	81 (84%)	16 (16%)	2	9
79	sM	88/227 (39%)	77 (88%)	11 (12%)	4	17
81	n4	101/114 (89%)	92 (91%)	9 (9%)	9	33
82	p0	105/254 (41%)	90 (86%)	15 (14%)	3	13
All	All	18802/19697 (96%)	16495 (88%)	2307 (12%)	4	17

5 of 2307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	D6	85	ARG
10	l8	79	GLN
64	c8	101	LEU
77	E1	144	CYS
5	l3	316	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
70	D4	63	GLN
7	l5	81	HIS
67	d1	3	ASN
71	D5	95	HIS
5	l3	211	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3095/3396 (91%)	696 (22%)	86 (2%)
1	5	3129/3396 (92%)	752 (24%)	83 (2%)
2	3	120/121 (99%)	22 (18%)	1 (0%)
2	7	120/121 (99%)	24 (20%)	1 (0%)
3	4	154/158 (97%)	36 (23%)	2 (1%)
3	8	157/158 (99%)	43 (27%)	1 (0%)
45	2	1708/1800 (94%)	481 (28%)	59 (3%)
45	6	1733/1800 (96%)	485 (27%)	62 (3%)
All	All	10216/10950 (93%)	2539 (24%)	295 (2%)

5 of 2539 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	14	U
1	1	16	A
1	1	26	A
1	1	30	G

5 of 295 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	2	1226	A
1	5	1160	C
45	6	832	U
45	2	1344	A
1	5	242	C

## 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 2153 ligands modelled in this entry, 2084 are monoatomic - leaving 69 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	$\# Z  > 2$
85	LLL	2	2043	-	29,33,33	0.17	0	34,49,49	0.79	3 (8%)
85	LLL	5	4178	-	29,33,33	0.20	0	34,49,49	0.86	1 (2%)
85	LLL	5	4160	-	29,33,33	0.24	0	34,49,49	1.86	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	LLL	1	3992	-	29,33,33	0.21	0	34,49,49	1.23	2 (5%)
85	LLL	5	4152	-	29,33,33	0.18	0	34,49,49	1.48	2 (5%)
85	LLL	1	3990	-	29,33,33	0.25	0	34,49,49	1.82	1 (2%)
85	LLL	4	224	-	29,33,33	0.20	0	34,49,49	1.46	2 (5%)
85	LLL	6	2174	-	29,33,33	0.27	0	34,49,49	1.27	3 (8%)
85	LLL	5	4163	-	29,33,33	0.15	0	34,49,49	1.06	3 (8%)
85	LLL	5	4153	-	29,33,33	0.25	0	34,49,49	1.79	2 (5%)
85	LLL	6	2173	-	29,33,33	0.19	0	34,49,49	1.11	3 (8%)
85	LLL	2	2045	-	29,33,33	0.19	0	34,49,49	1.53	4 (11%)
85	LLL	5	4173	-	29,33,33	0.17	0	34,49,49	1.12	3 (8%)
85	LLL	1	4002	-	29,33,33	0.20	0	34,49,49	2.11	3 (8%)
85	LLL	5	4176	-	29,33,33	0.22	0	34,49,49	1.26	3 (8%)
85	LLL	1	3996	-	29,33,33	0.21	0	34,49,49	0.89	2 (5%)
85	LLL	6	2176	-	29,33,33	0.22	0	34,49,49	1.29	3 (8%)
85	LLL	5	4161	-	29,33,33	0.19	0	34,49,49	1.25	3 (8%)
85	LLL	6	2165	-	29,33,33	0.21	0	34,49,49	1.14	2 (5%)
85	LLL	L3	404	-	29,33,33	0.22	0	34,49,49	1.33	3 (8%)
85	LLL	6	2175	-	29,33,33	0.19	0	34,49,49	1.37	2 (5%)
85	LLL	1	4003	-	29,33,33	0.18	0	34,49,49	1.37	3 (8%)
85	LLL	1	3995	-	29,33,33	0.16	0	34,49,49	2.08	2 (5%)
85	LLL	5	4174	-	29,33,33	0.24	0	34,49,49	1.58	4 (11%)
85	LLL	8	221	-	29,33,33	0.21	0	34,49,49	1.73	2 (5%)
85	LLL	7	233	-	29,33,33	0.22	0	34,49,49	0.93	2 (5%)
85	LLL	1	3994	-	29,33,33	0.20	0	34,49,49	1.14	3 (8%)
85	LLL	1	3998	-	29,33,33	0.15	0	34,49,49	0.76	1 (2%)
85	LLL	5	4172	-	29,33,33	0.22	0	34,49,49	1.36	3 (8%)
85	LLL	5	4157	-	29,33,33	0.25	0	34,49,49	1.13	2 (5%)
85	LLL	5	4169	-	29,33,33	0.20	0	34,49,49	1.46	4 (11%)
85	LLL	1	4001	-	29,33,33	0.17	0	34,49,49	1.08	2 (5%)
85	LLL	2	2044	-	29,33,33	0.20	0	34,49,49	1.50	4 (11%)
85	LLL	7	231	-	29,33,33	0.17	0	34,49,49	2.01	7 (20%)
85	LLL	5	4170	-	29,33,33	0.24	0	34,49,49	1.52	2 (5%)
85	LLL	5	4177	-	29,33,33	0.26	0	34,49,49	1.79	6 (17%)
85	LLL	7	232	-	29,33,33	0.17	0	34,49,49	0.90	2 (5%)
85	LLL	5	4155	-	29,33,33	0.24	0	34,49,49	1.00	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	LLL	5	4167	-	29,33,33	0.15	0	34,49,49	1.00	2 (5%)
85	LLL	1	3999	-	29,33,33	0.17	0	34,49,49	0.97	2 (5%)
85	LLL	5	4156	-	29,33,33	0.22	0	34,49,49	1.29	3 (8%)
85	LLL	13	412	-	29,33,33	0.25	0	34,49,49	1.88	3 (8%)
85	LLL	1	4000	-	29,33,33	0.18	0	34,49,49	2.11	5 (14%)
85	LLL	1	3993	-	29,33,33	0.24	0	34,49,49	1.47	5 (14%)
85	LLL	6	2168	-	29,33,33	0.21	0	34,49,49	1.28	3 (8%)
85	LLL	5	4159	-	29,33,33	0.21	0	34,49,49	1.06	3 (8%)
85	LLL	5	4165	-	29,33,33	0.16	0	34,49,49	1.04	2 (5%)
85	LLL	6	2171	-	29,33,33	0.14	0	34,49,49	1.14	1 (2%)
85	LLL	6	2169	-	29,33,33	0.14	0	34,49,49	0.89	2 (5%)
85	LLL	5	4154	-	29,33,33	0.25	0	34,49,49	0.68	0
85	LLL	6	2167	-	29,33,33	0.21	0	34,49,49	1.96	5 (14%)
85	LLL	3	220	-	29,33,33	0.21	0	34,49,49	1.50	3 (8%)
85	LLL	1	3991	-	29,33,33	0.20	0	34,49,49	0.82	3 (8%)
85	LLL	5	4168	-	29,33,33	0.20	0	34,49,49	1.67	3 (8%)
85	LLL	6	2166	-	29,33,33	0.20	0	34,49,49	1.11	3 (8%)
85	LLL	5	4171	-	29,33,33	0.19	0	34,49,49	0.97	1 (2%)
85	LLL	1	3989	-	29,33,33	0.21	0	34,49,49	1.43	3 (8%)
85	LLL	8	222	-	29,33,33	0.16	0	34,49,49	0.79	1 (2%)
85	LLL	5	4166	-	29,33,33	0.15	0	34,49,49	1.16	2 (5%)
85	LLL	5	4158	-	29,33,33	0.21	0	34,49,49	1.99	5 (14%)
85	LLL	5	4162	-	29,33,33	0.18	0	34,49,49	0.86	1 (2%)
85	LLL	1	3997	-	29,33,33	0.19	0	34,49,49	1.22	3 (8%)
85	LLL	6	2170	-	29,33,33	0.23	0	34,49,49	1.25	2 (5%)
85	LLL	6	2172	-	29,33,33	0.19	0	34,49,49	1.12	2 (5%)
85	LLL	6	2164	-	29,33,33	0.18	0	34,49,49	1.82	2 (5%)
85	LLL	5	4151	-	29,33,33	0.32	0	34,49,49	1.46	2 (5%)
85	LLL	5	4175	-	29,33,33	0.23	0	34,49,49	1.44	3 (8%)
85	LLL	1	4004	-	29,33,33	0.19	0	34,49,49	1.08	1 (2%)
85	LLL	5	4164	-	29,33,33	0.21	0	34,49,49	1.93	3 (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
85	LLL	2	2043	-	-	3/11/65/65	1/3/3/3
85	LLL	5	4178	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4160	-	-	3/11/65/65	0/3/3/3
85	LLL	1	3992	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4152	-	-	5/11/65/65	0/3/3/3
85	LLL	1	3990	-	-	2/11/65/65	0/3/3/3
85	LLL	4	224	-	-	2/11/65/65	0/3/3/3
85	LLL	6	2174	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4163	-	-	6/11/65/65	2/3/3/3
85	LLL	5	4153	-	-	4/11/65/65	0/3/3/3
85	LLL	6	2173	-	-	5/11/65/65	1/3/3/3
85	LLL	2	2045	-	-	7/11/65/65	0/3/3/3
85	LLL	5	4173	-	-	2/11/65/65	1/3/3/3
85	LLL	1	4002	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4176	-	-	2/11/65/65	0/3/3/3
85	LLL	1	3996	-	-	3/11/65/65	0/3/3/3
85	LLL	6	2176	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4161	-	-	2/11/65/65	1/3/3/3
85	LLL	6	2165	-	-	3/11/65/65	0/3/3/3
85	LLL	L3	404	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2175	-	-	4/11/65/65	1/3/3/3
85	LLL	1	4003	-	-	4/11/65/65	2/3/3/3
85	LLL	1	3995	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4174	-	-	2/11/65/65	0/3/3/3
85	LLL	8	221	-	-	6/11/65/65	0/3/3/3
85	LLL	7	233	-	-	3/11/65/65	2/3/3/3
85	LLL	1	3994	-	-	1/11/65/65	0/3/3/3
85	LLL	1	3998	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4172	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4157	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4169	-	-	1/11/65/65	0/3/3/3
85	LLL	1	4001	-	-	2/11/65/65	0/3/3/3
85	LLL	2	2044	-	-	3/11/65/65	1/3/3/3
85	LLL	7	231	-	-	4/11/65/65	0/3/3/3
85	LLL	5	4170	-	-	1/11/65/65	1/3/3/3
85	LLL	5	4177	-	-	4/11/65/65	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	LLL	7	232	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4155	-	-	5/11/65/65	1/3/3/3
85	LLL	5	4167	-	-	2/11/65/65	0/3/3/3
85	LLL	1	3999	-	-	4/11/65/65	0/3/3/3
85	LLL	5	4156	-	-	4/11/65/65	0/3/3/3
85	LLL	13	412	-	-	1/11/65/65	0/3/3/3
85	LLL	1	4000	-	-	2/11/65/65	0/3/3/3
85	LLL	1	3993	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2168	-	-	5/11/65/65	1/3/3/3
85	LLL	5	4159	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4165	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2171	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2169	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4154	-	-	2/11/65/65	0/3/3/3
85	LLL	6	2167	-	-	4/11/65/65	0/3/3/3
85	LLL	3	220	-	-	3/11/65/65	0/3/3/3
85	LLL	1	3991	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4168	-	-	0/11/65/65	0/3/3/3
85	LLL	6	2166	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4171	-	-	4/11/65/65	0/3/3/3
85	LLL	1	3989	-	-	2/11/65/65	0/3/3/3
85	LLL	8	222	-	-	3/11/65/65	2/3/3/3
85	LLL	5	4166	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4158	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4162	-	-	3/11/65/65	1/3/3/3
85	LLL	1	3997	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2170	-	-	2/11/65/65	0/3/3/3
85	LLL	6	2172	-	-	3/11/65/65	1/3/3/3
85	LLL	6	2164	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4151	-	-	8/11/65/65	0/3/3/3
85	LLL	5	4175	-	-	1/11/65/65	0/3/3/3
85	LLL	1	4004	-	-	3/11/65/65	1/3/3/3
85	LLL	5	4164	-	-	4/11/65/65	0/3/3/3

There are no bond length outliers.

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	1	4002	LLL	C11-O51-C51	11.16	125.50	113.13
85	1	3995	LLL	C11-O51-C51	11.05	125.37	113.13
85	1	4000	LLL	C11-O51-C51	10.82	125.12	113.13
85	1	3990	LLL	C11-O51-C51	9.69	123.86	113.13
85	6	2164	LLL	C11-O51-C51	9.60	123.77	113.13

There are no chirality outliers.

5 of 195 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	6	2167	LLL	C41-C51-C61-N61
85	6	2167	LLL	C23-C33-N33-C93
85	1	3999	LLL	O51-C51-C61-N61
85	1	3999	LLL	C23-C33-N33-C93
85	1	3998	LLL	C23-C33-N33-C93

5 of 20 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	6	2172	LLL	C12-C22-C32-C42-C52-C62
85	5	4155	LLL	C11-C21-C31-C41-C51-O51
85	1	4004	LLL	C11-C21-C31-C41-C51-O51
85	5	4170	LLL	C11-C21-C31-C41-C51-O51
85	6	2168	LLL	C11-C21-C31-C41-C51-O51

60 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	2043	LLL	5	0
85	5	4178	LLL	4	0
85	5	4160	LLL	2	0
85	1	3992	LLL	3	0
85	5	4152	LLL	2	0
85	1	3990	LLL	1	0
85	4	224	LLL	9	0
85	5	4163	LLL	2	0
85	5	4153	LLL	1	0
85	6	2173	LLL	3	0
85	2	2045	LLL	2	0
85	5	4173	LLL	2	0
85	1	4002	LLL	4	0
85	5	4176	LLL	1	0
85	1	3996	LLL	2	0

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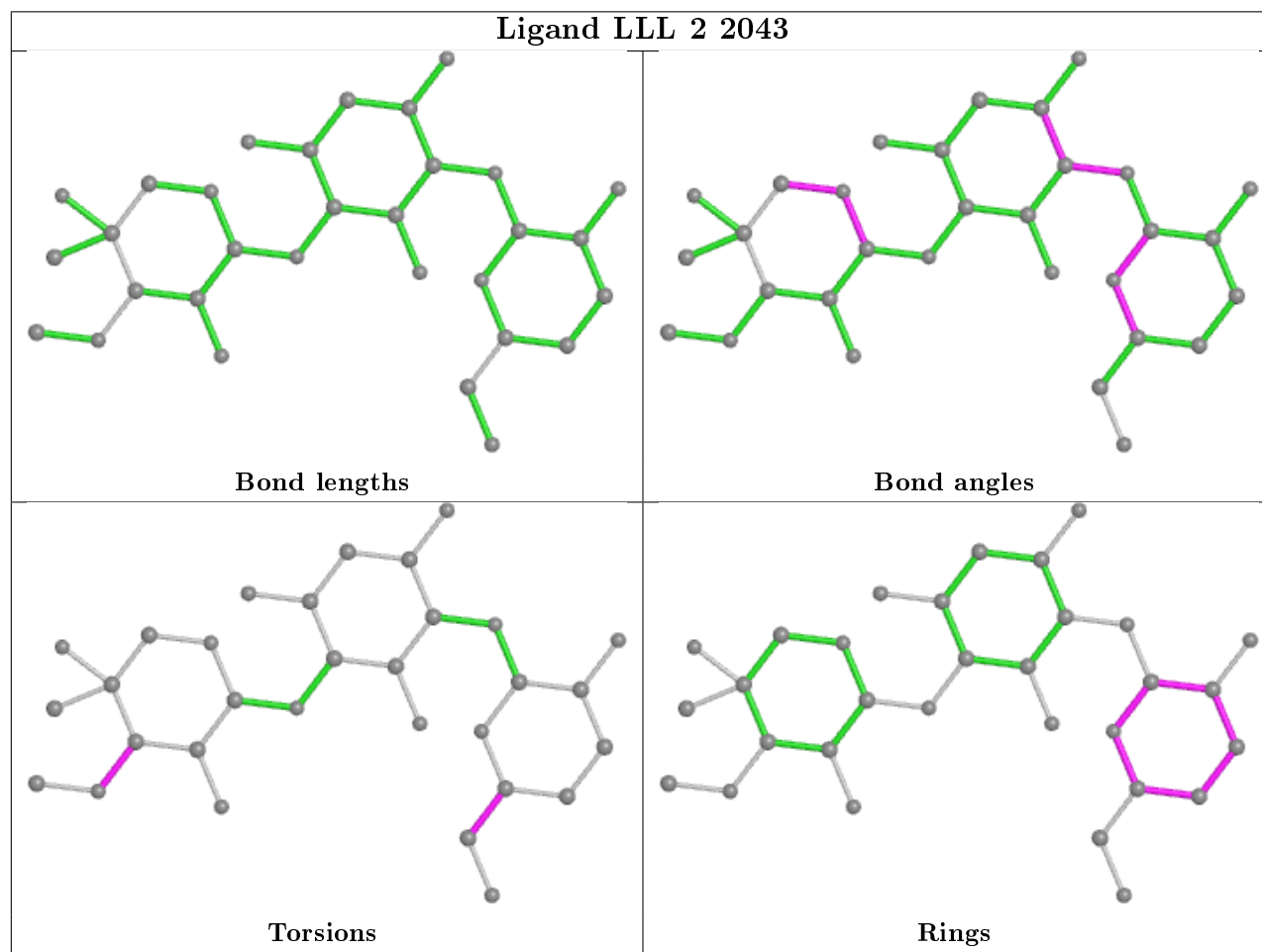
Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	6	2176	LLL	1	0
85	L3	404	LLL	2	0
85	6	2175	LLL	2	0
85	1	4003	LLL	1	0
85	5	4174	LLL	3	0
85	8	221	LLL	6	0
85	7	233	LLL	3	0
85	1	3994	LLL	1	0
85	1	3998	LLL	1	0
85	5	4172	LLL	3	0
85	5	4157	LLL	1	0
85	5	4169	LLL	1	0
85	1	4001	LLL	1	0
85	2	2044	LLL	2	0
85	7	231	LLL	4	0
85	5	4170	LLL	1	0
85	5	4177	LLL	3	0
85	7	232	LLL	4	0
85	5	4155	LLL	2	0
85	1	3999	LLL	3	0
85	5	4156	LLL	2	0
85	1	4000	LLL	3	0
85	1	3993	LLL	1	0
85	6	2168	LLL	4	0
85	5	4159	LLL	1	0
85	6	2171	LLL	2	0
85	6	2169	LLL	3	0
85	5	4154	LLL	3	0
85	6	2167	LLL	6	0
85	3	220	LLL	2	0
85	1	3991	LLL	3	0
85	5	4168	LLL	4	0
85	6	2166	LLL	3	0
85	5	4171	LLL	3	0
85	1	3989	LLL	2	0
85	8	222	LLL	10	0
85	5	4166	LLL	1	0
85	5	4158	LLL	2	0
85	5	4162	LLL	4	0
85	1	3997	LLL	2	0
85	6	2170	LLL	1	0
85	6	2172	LLL	2	0

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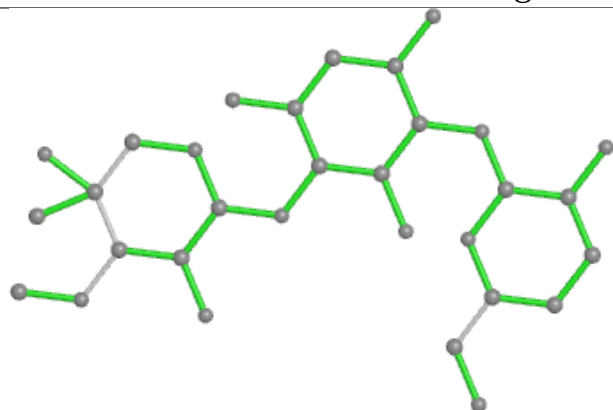
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	4151	LLL	2	0
85	5	4175	LLL	2	0
85	5	4164	LLL	1	0

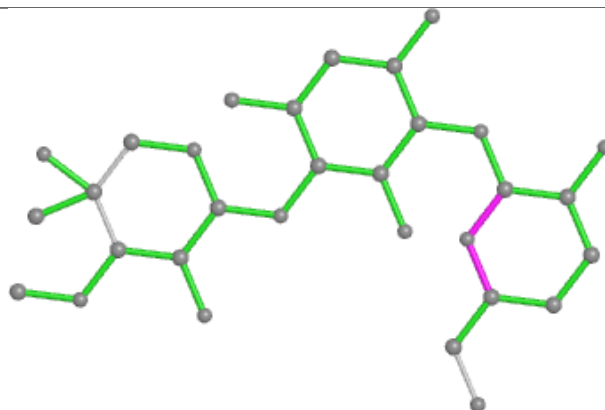
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



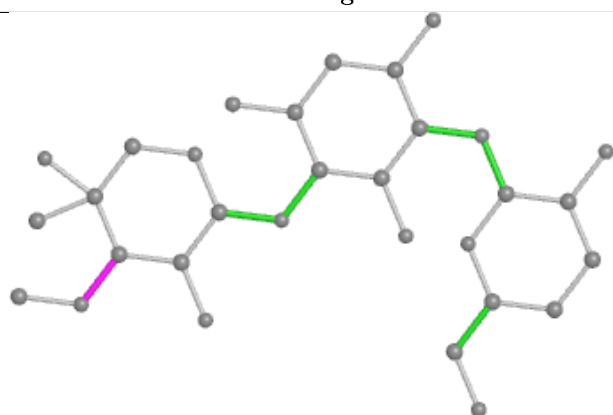
## Ligand LLL 5 4178



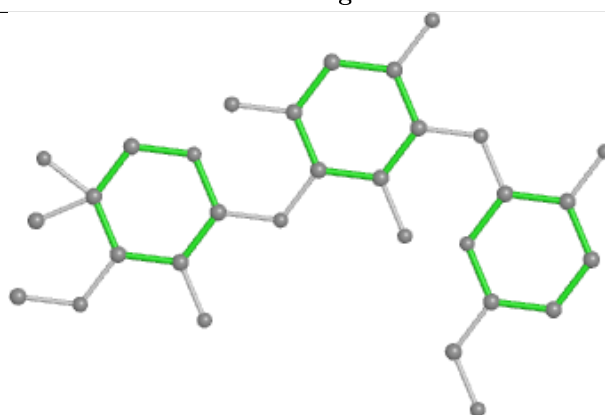
Bond lengths



Bond angles

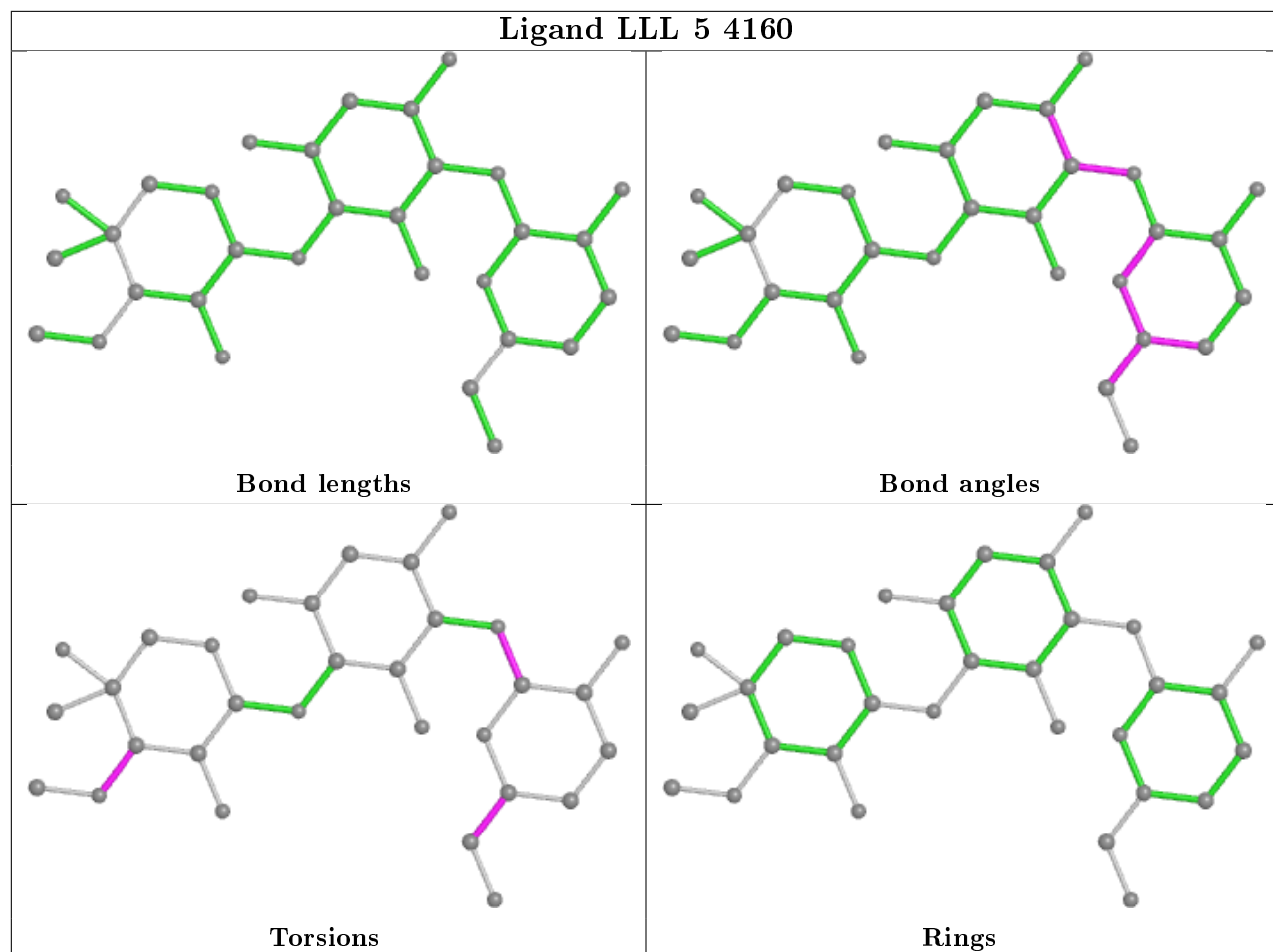


Torsions

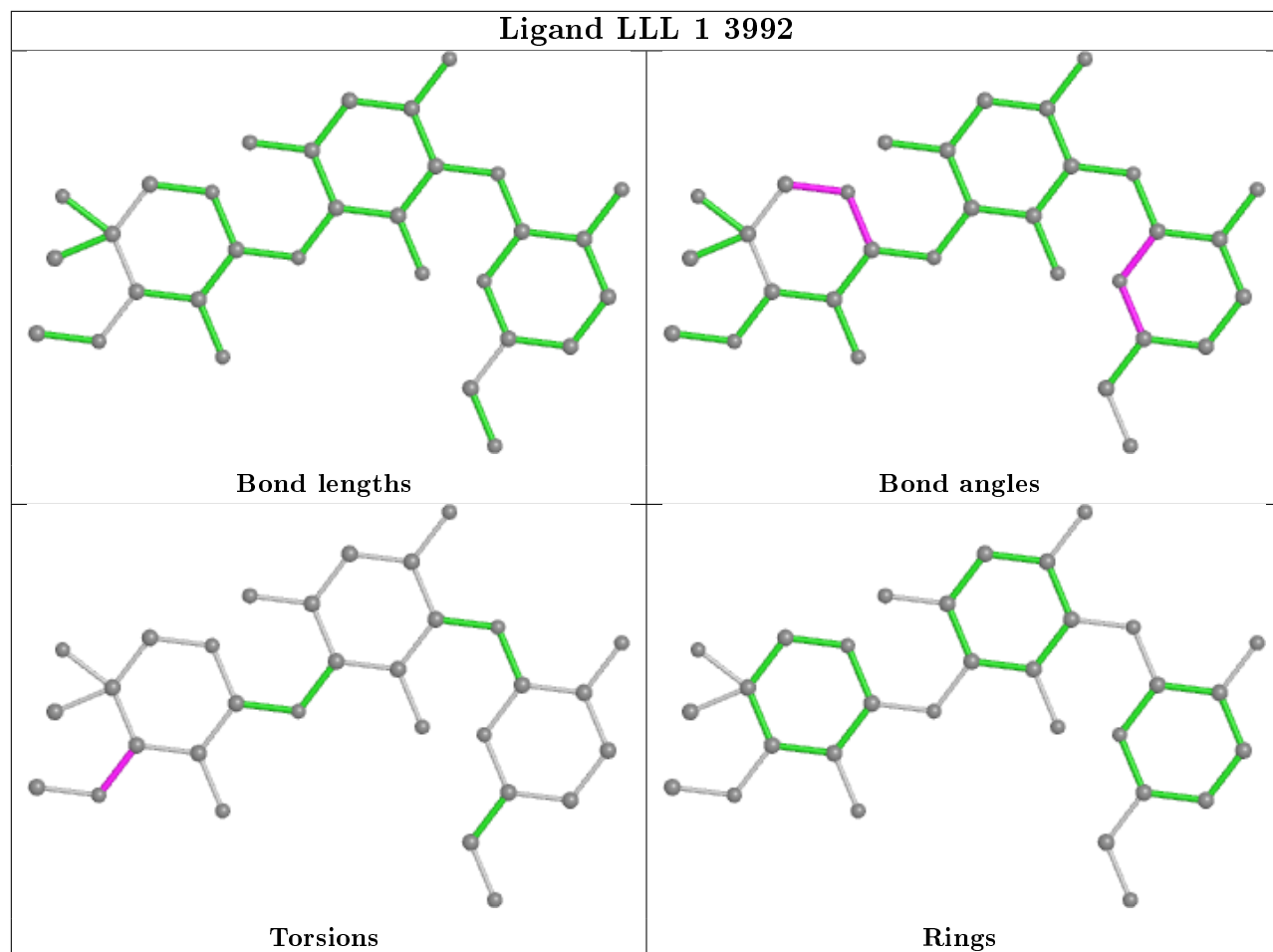


Rings

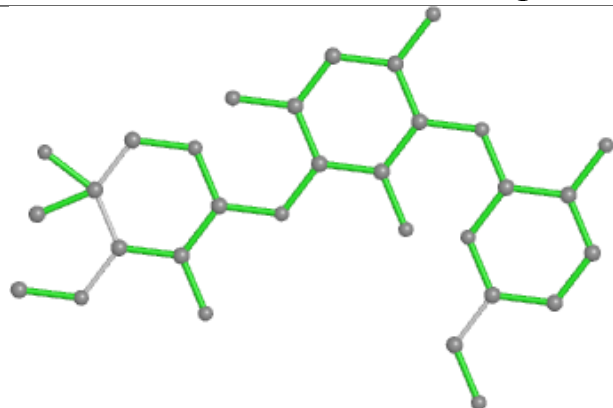
## Ligand LLL 5 4160



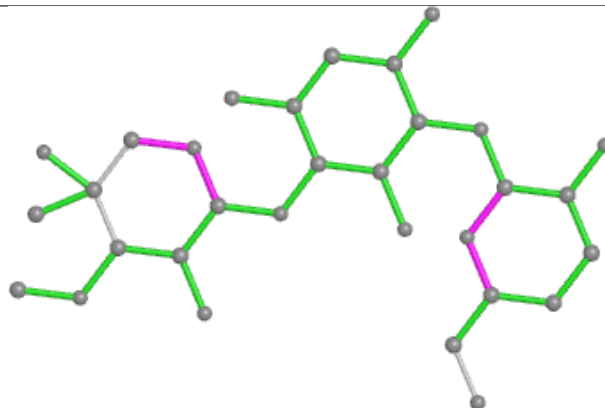
## Ligand LLL 1 3992



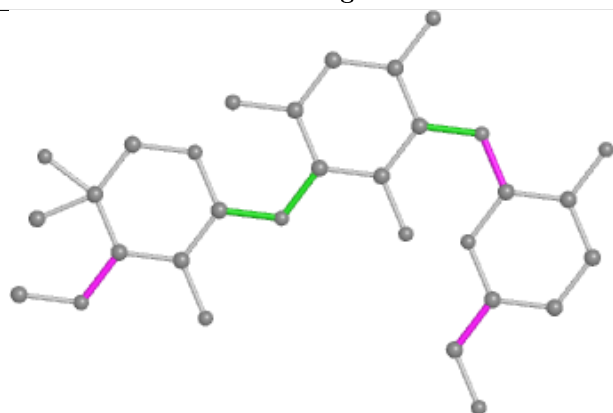
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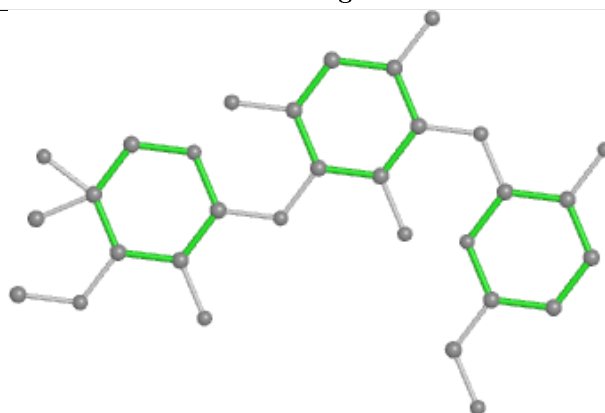
Bond lengths



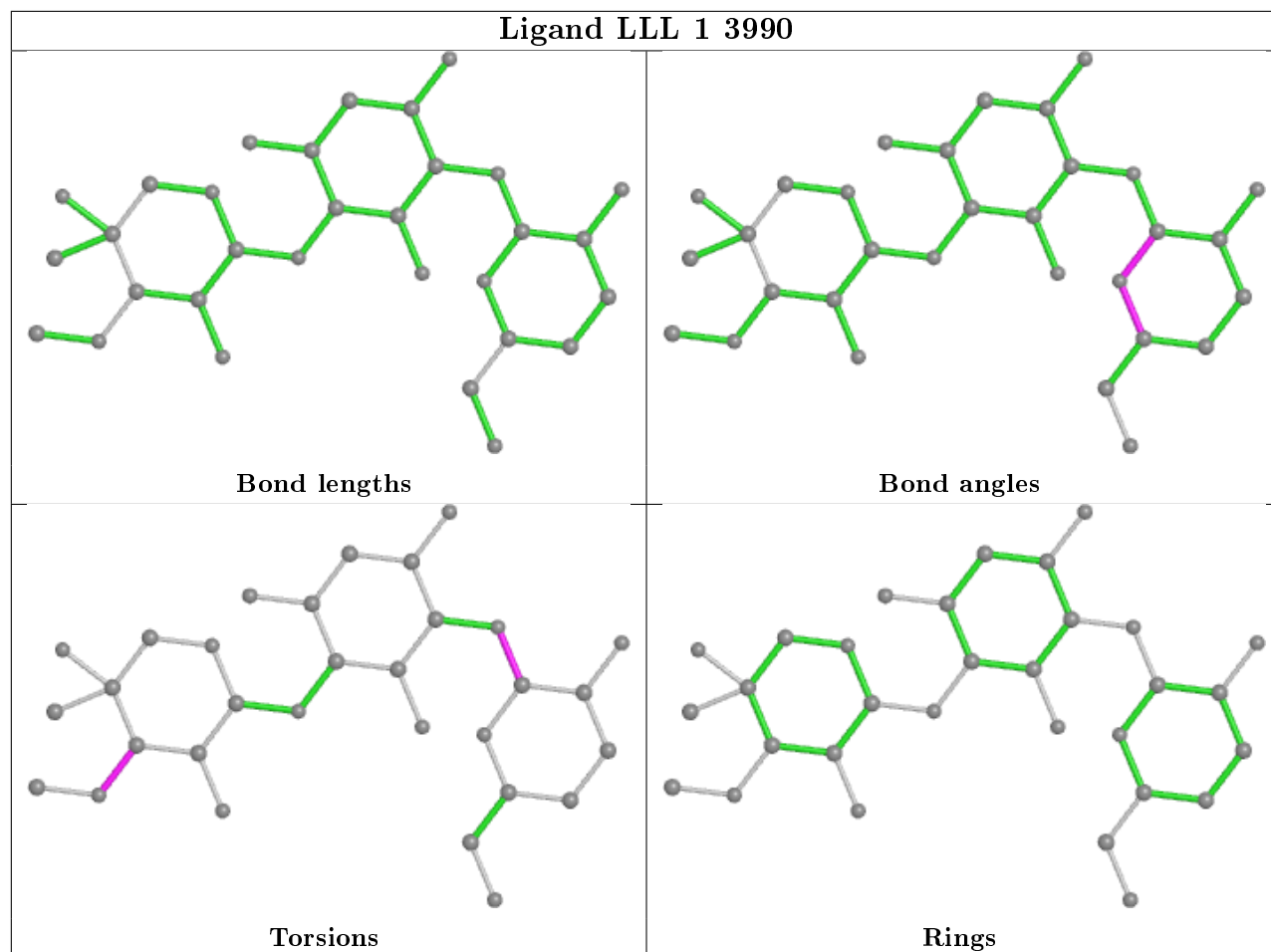
Bond angles

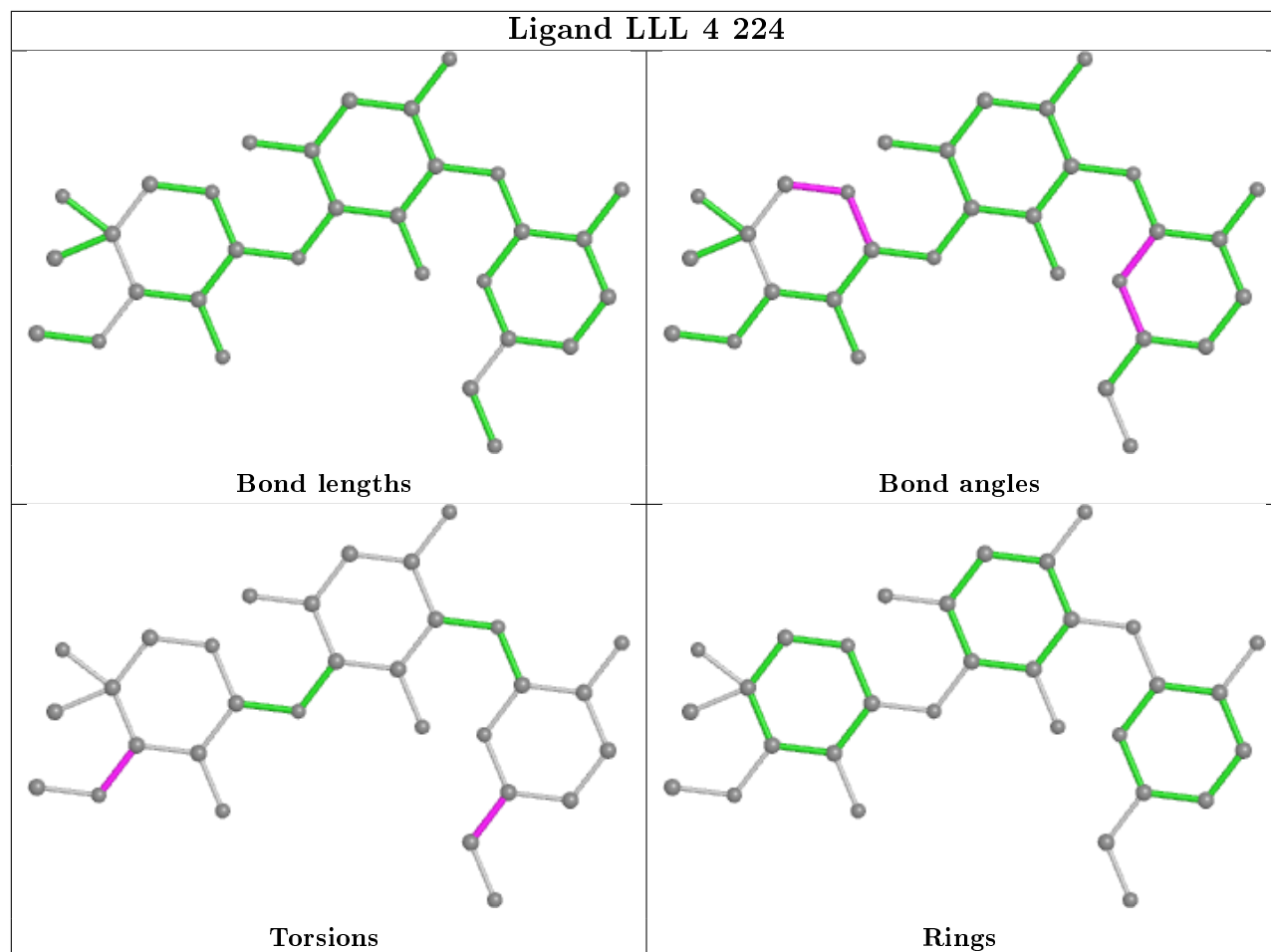


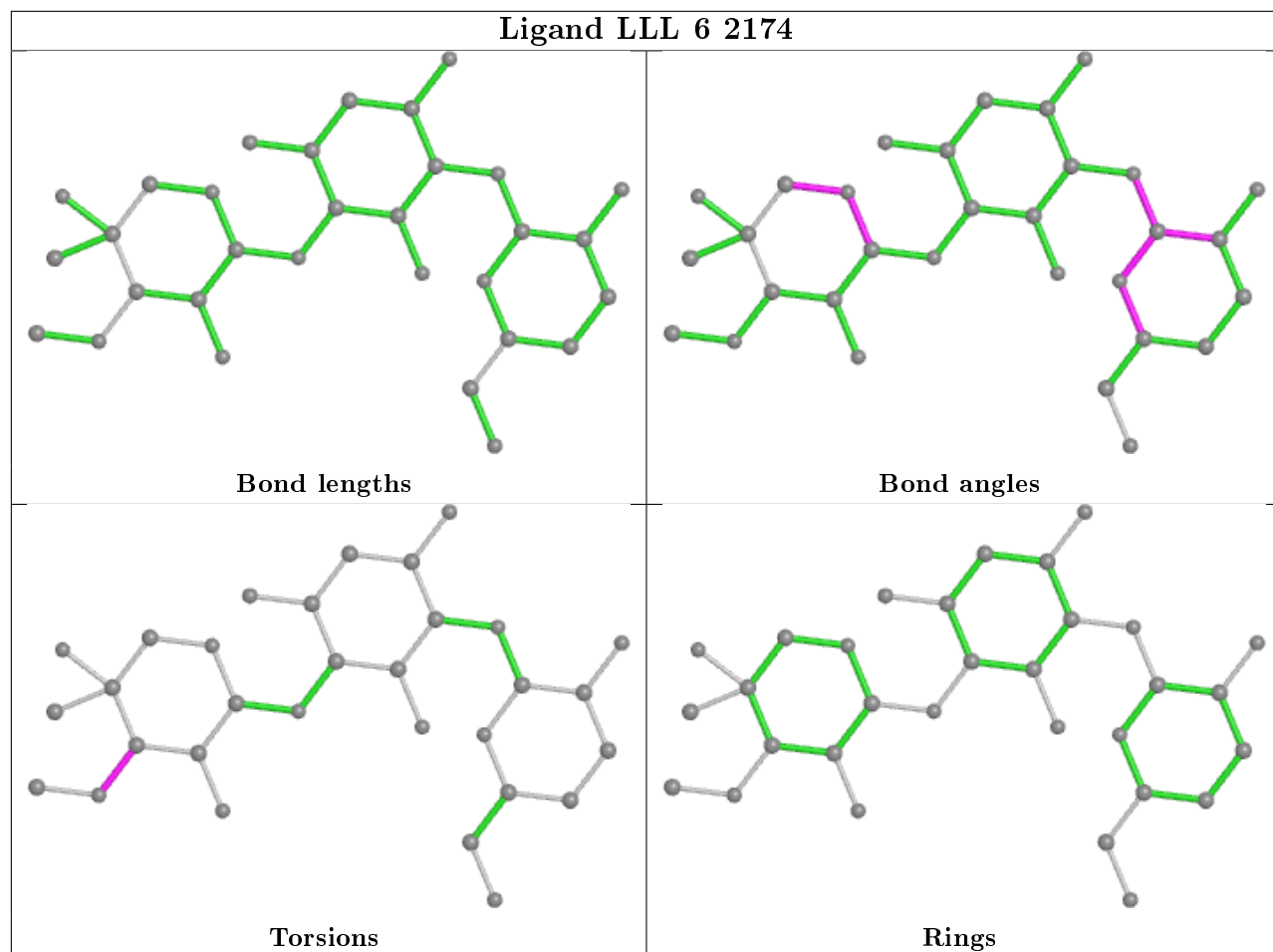
Torsions



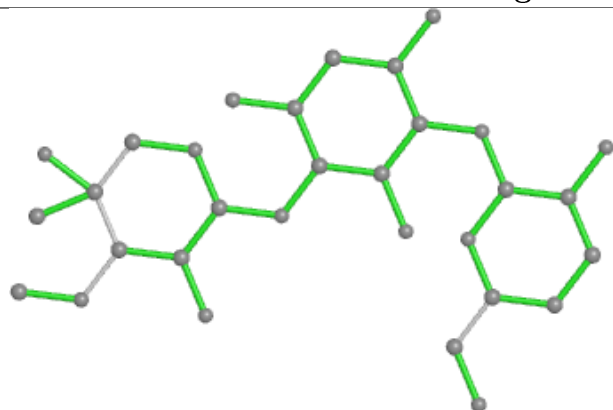
Rings



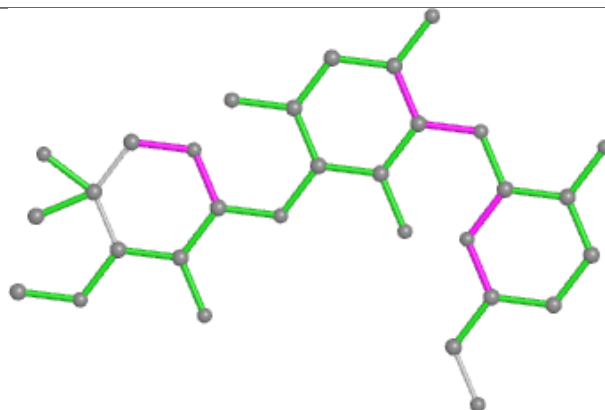




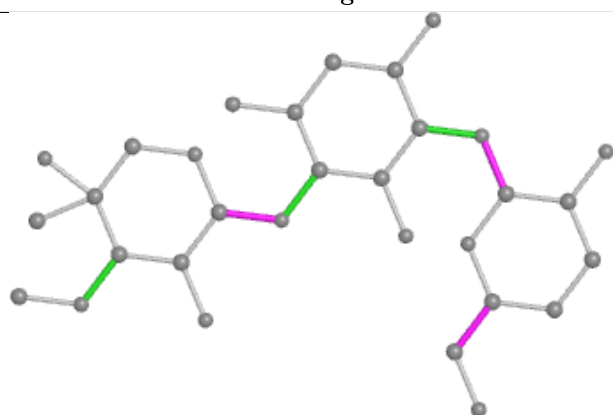
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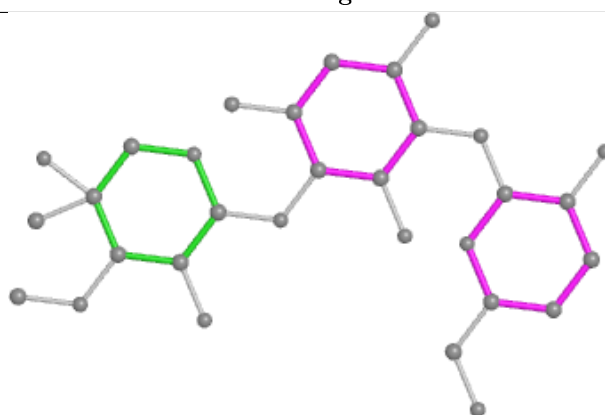
Bond lengths



Bond angles

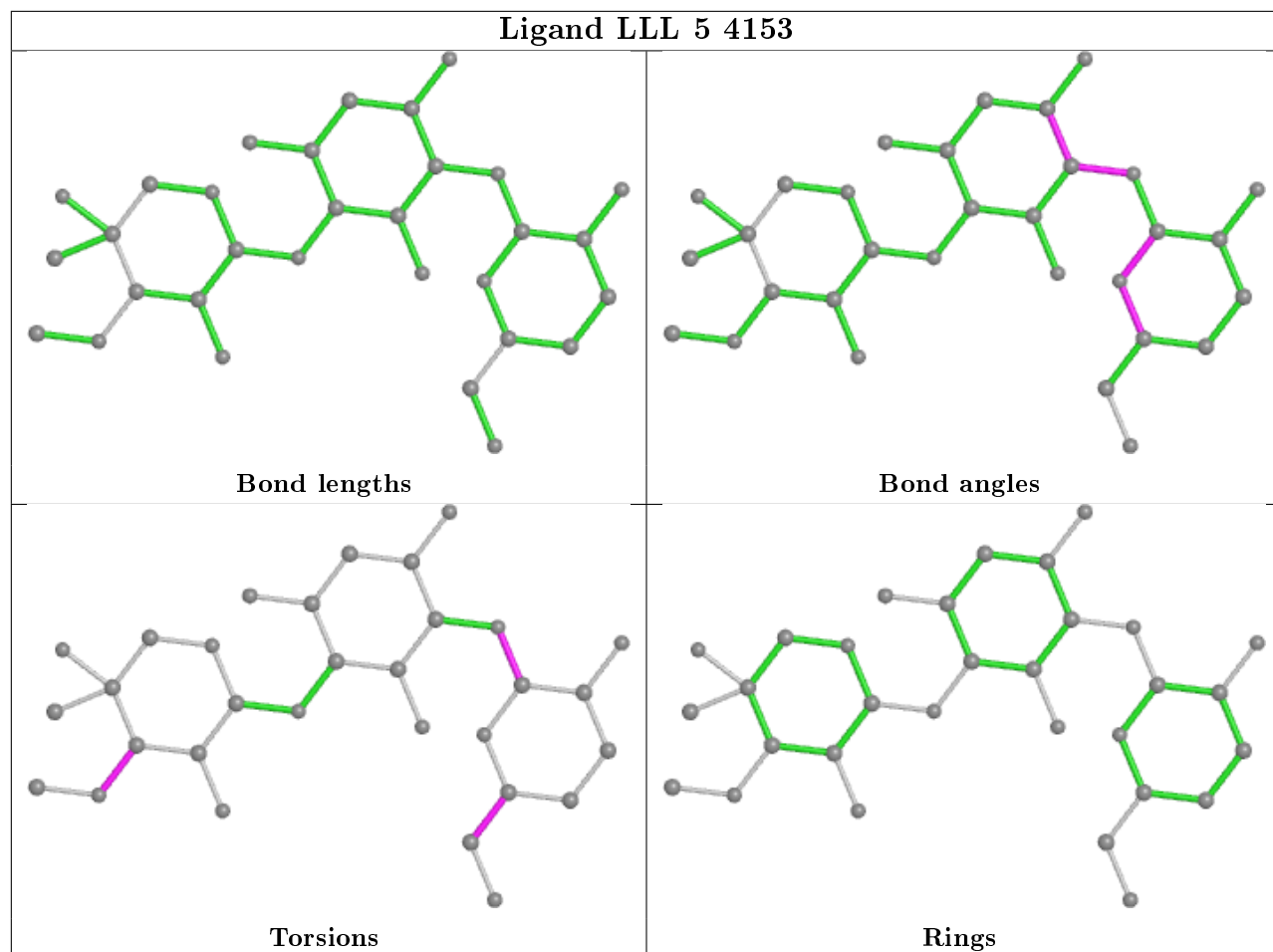


Torsions

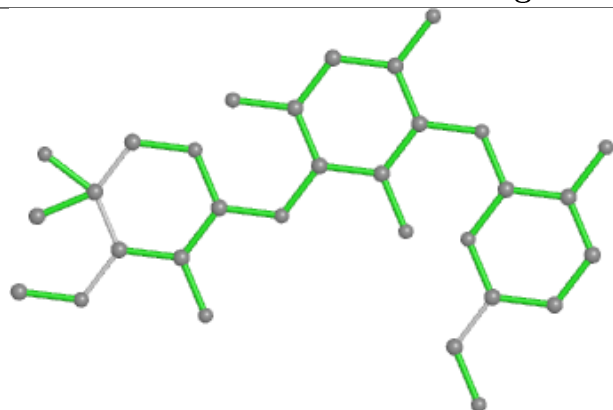


Rings

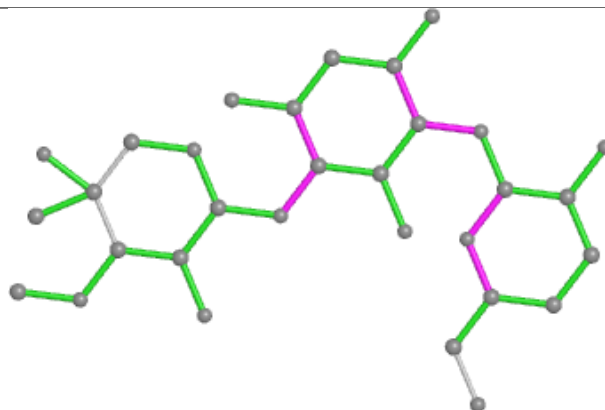
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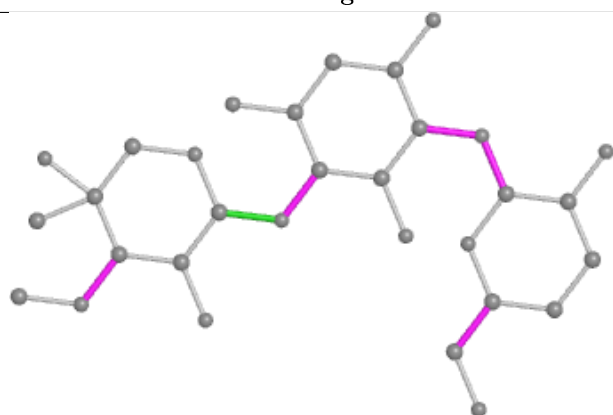
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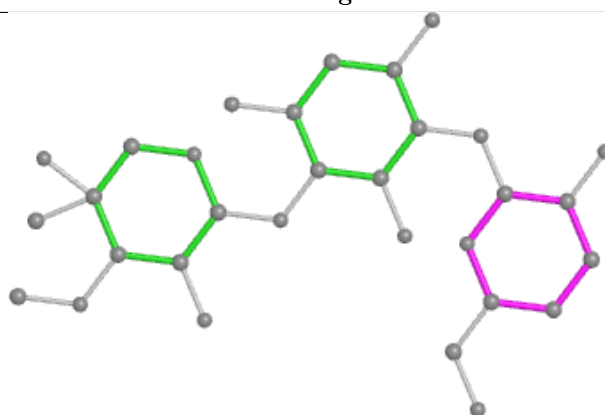
Bond lengths



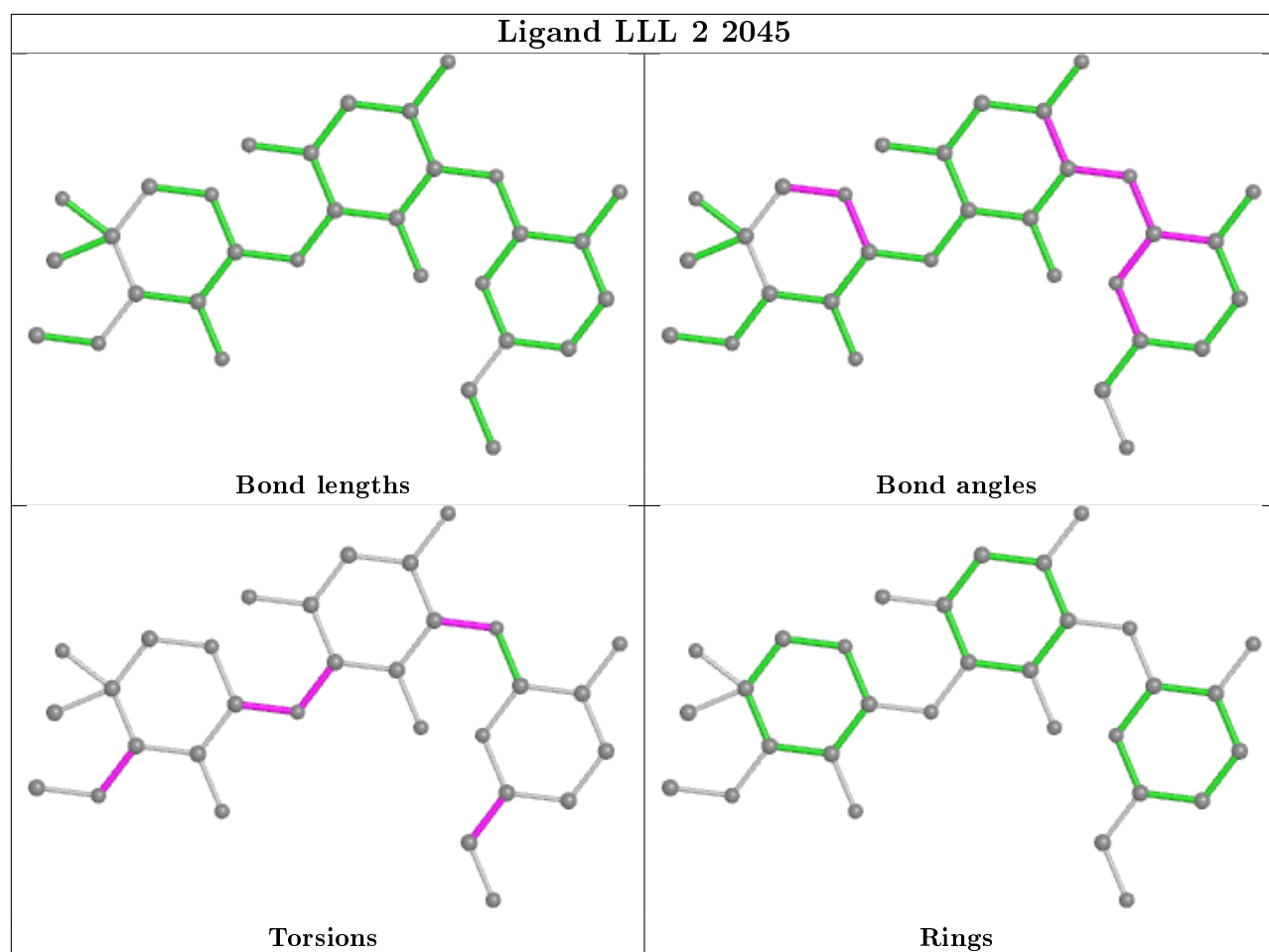
Bond angles



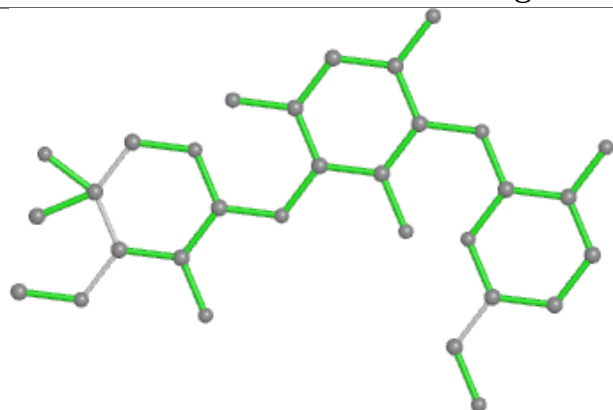
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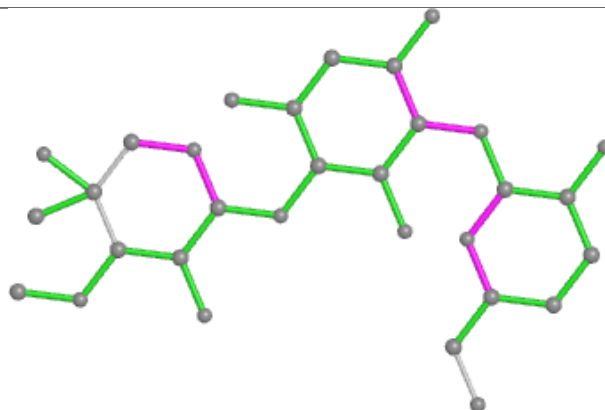
Rings



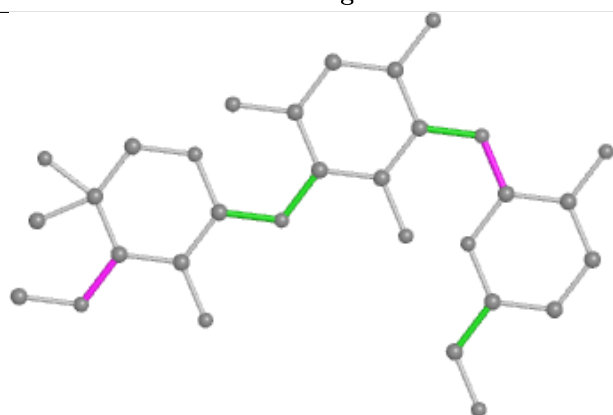
## Ligand LLL 5 4173



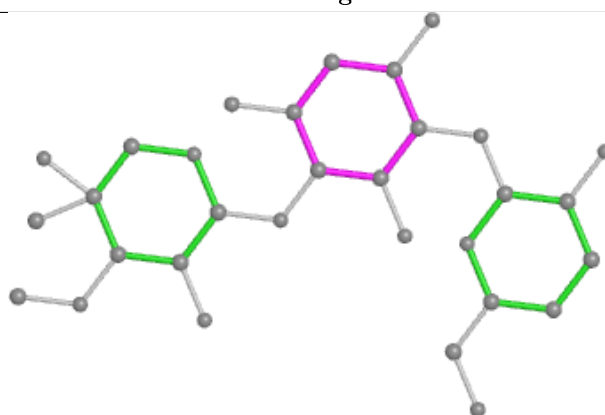
Bond lengths



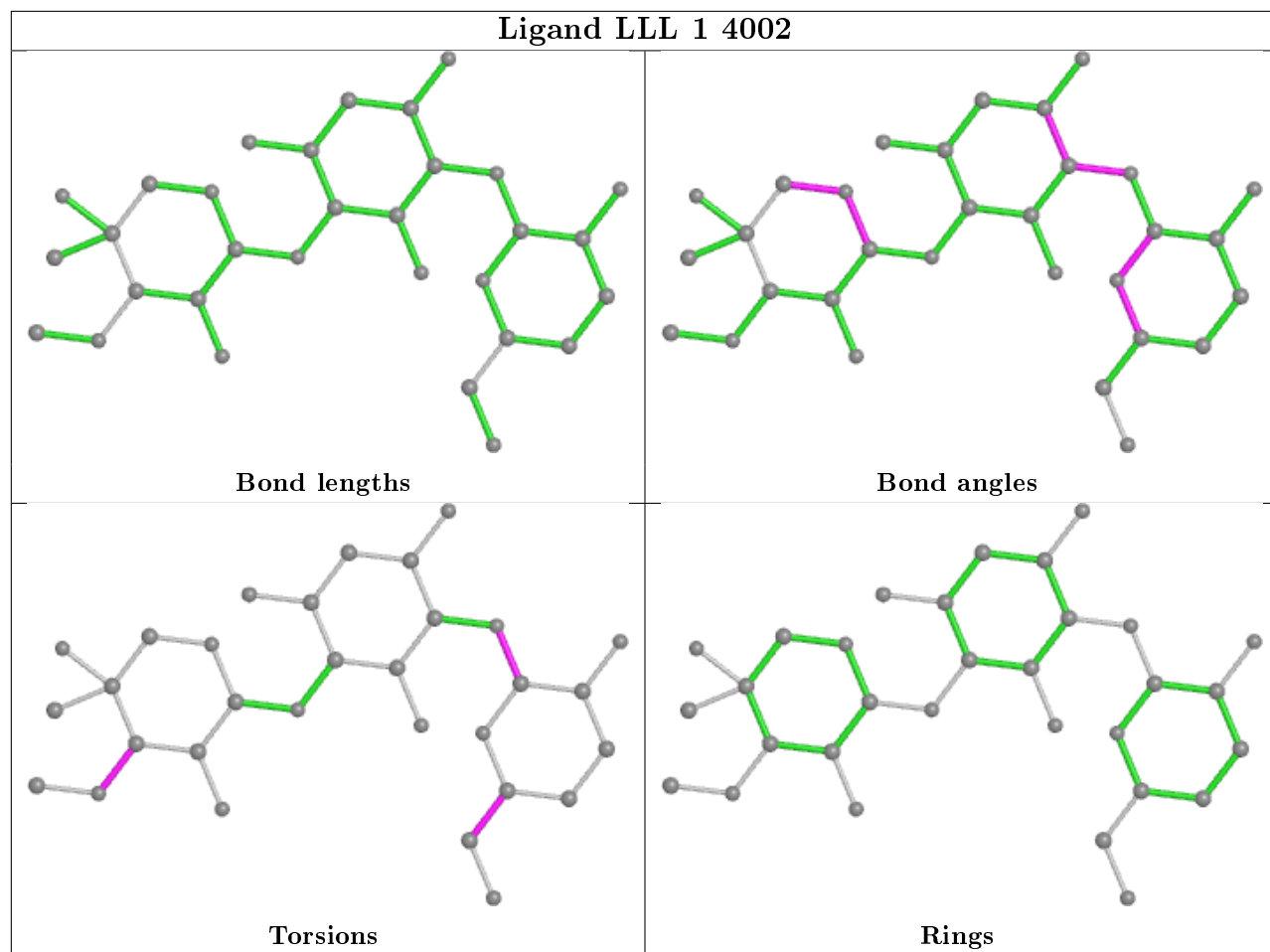
Bond angles



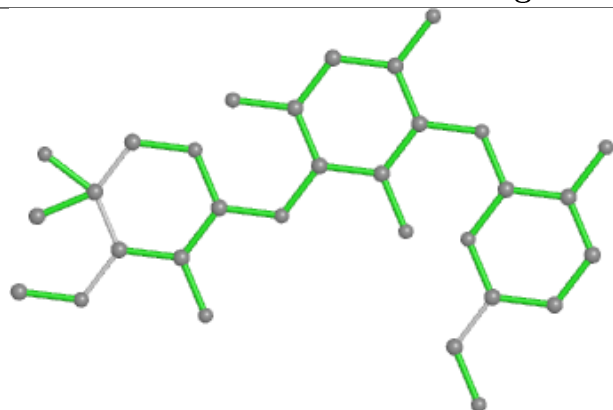
Torsions



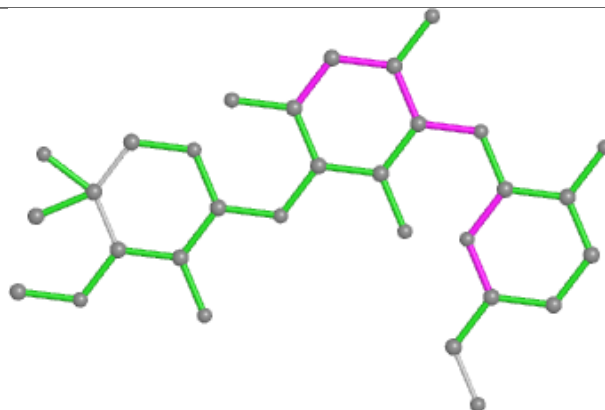
Rings



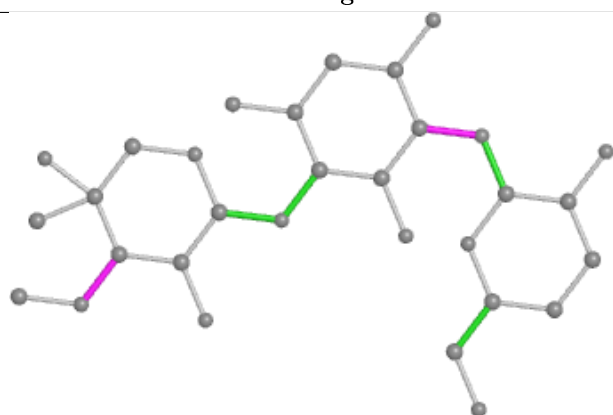
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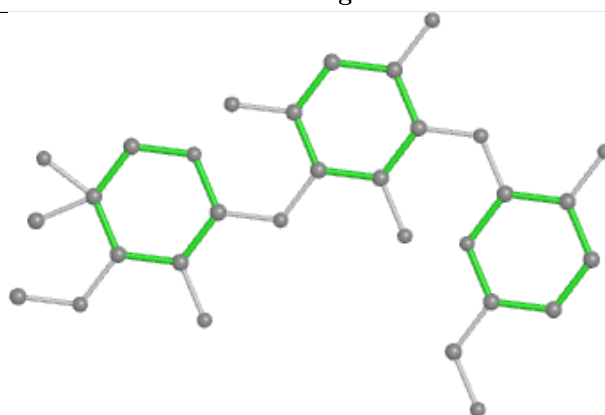
Bond lengths



Bond angles

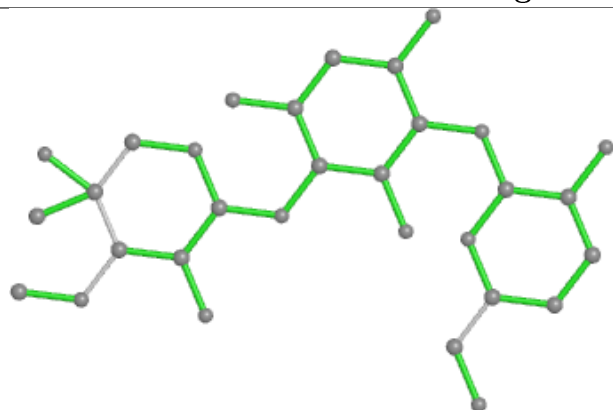


Torsions

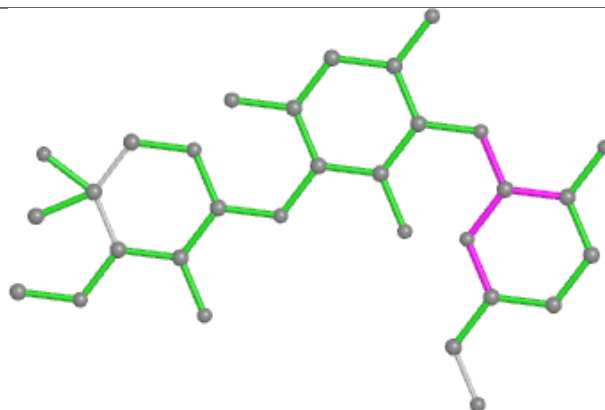


Rings

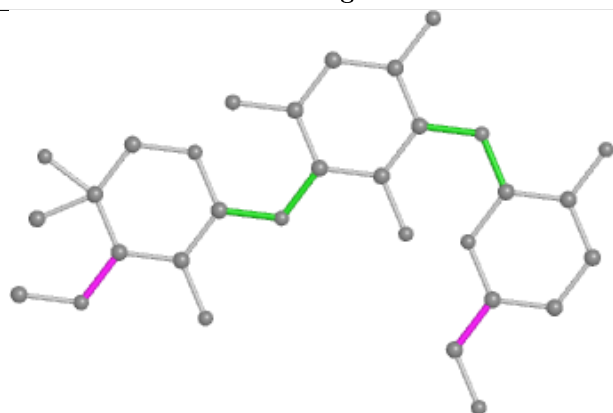
## Ligand LLL 1 3996



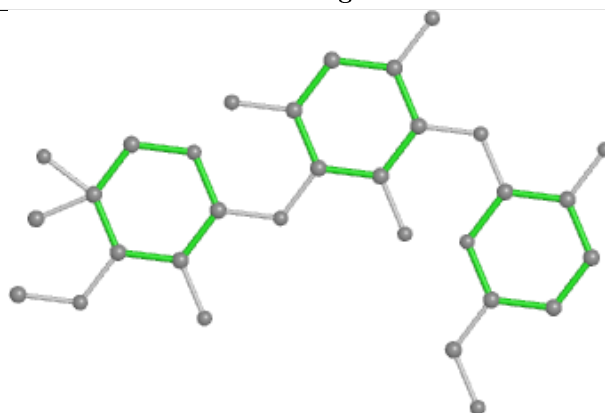
Bond lengths



Bond angles

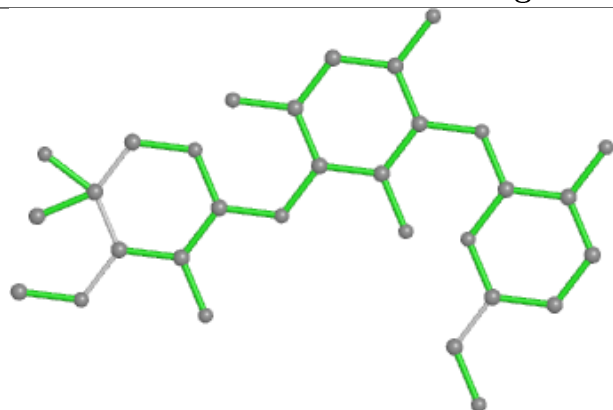


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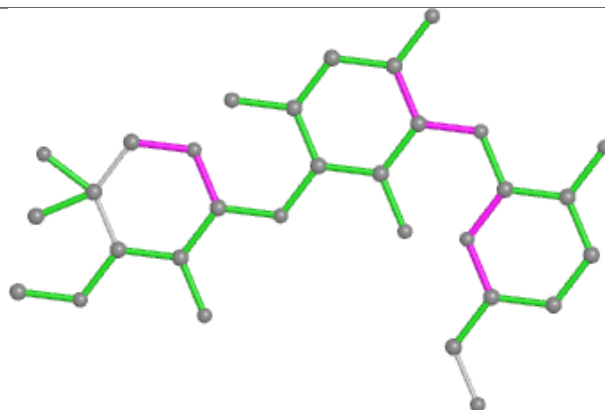


Rings

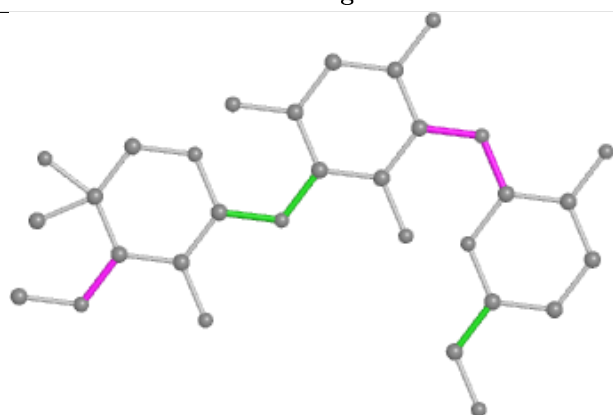
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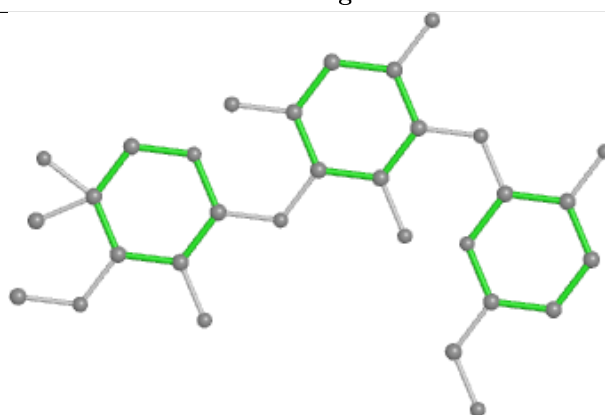
Bond lengths



Bond angles

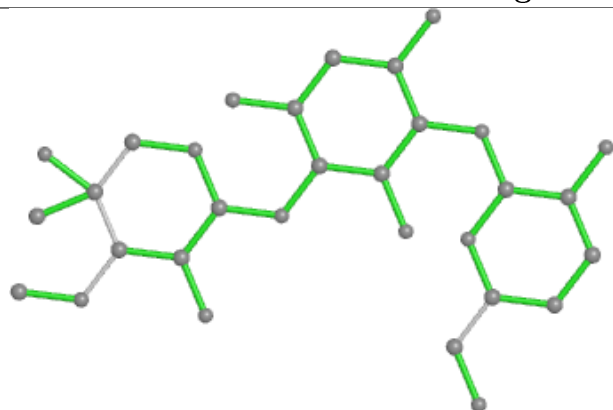


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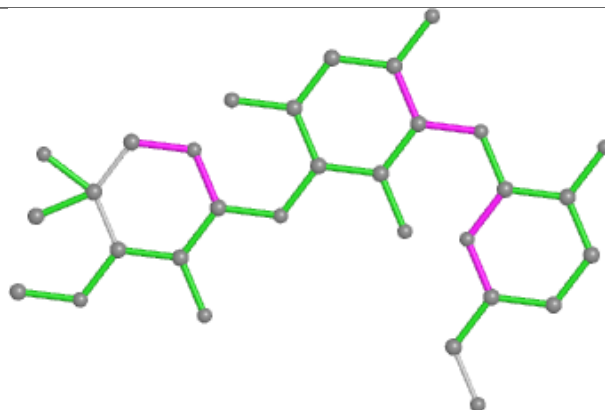


Rings

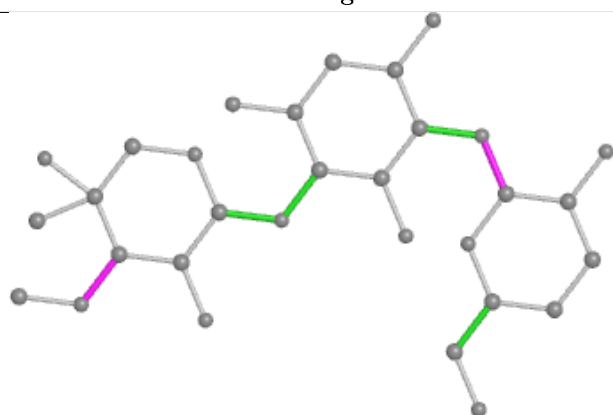
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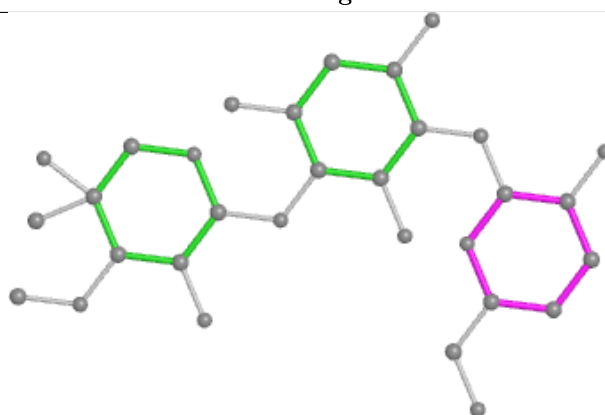
Bond lengths



Bond angles

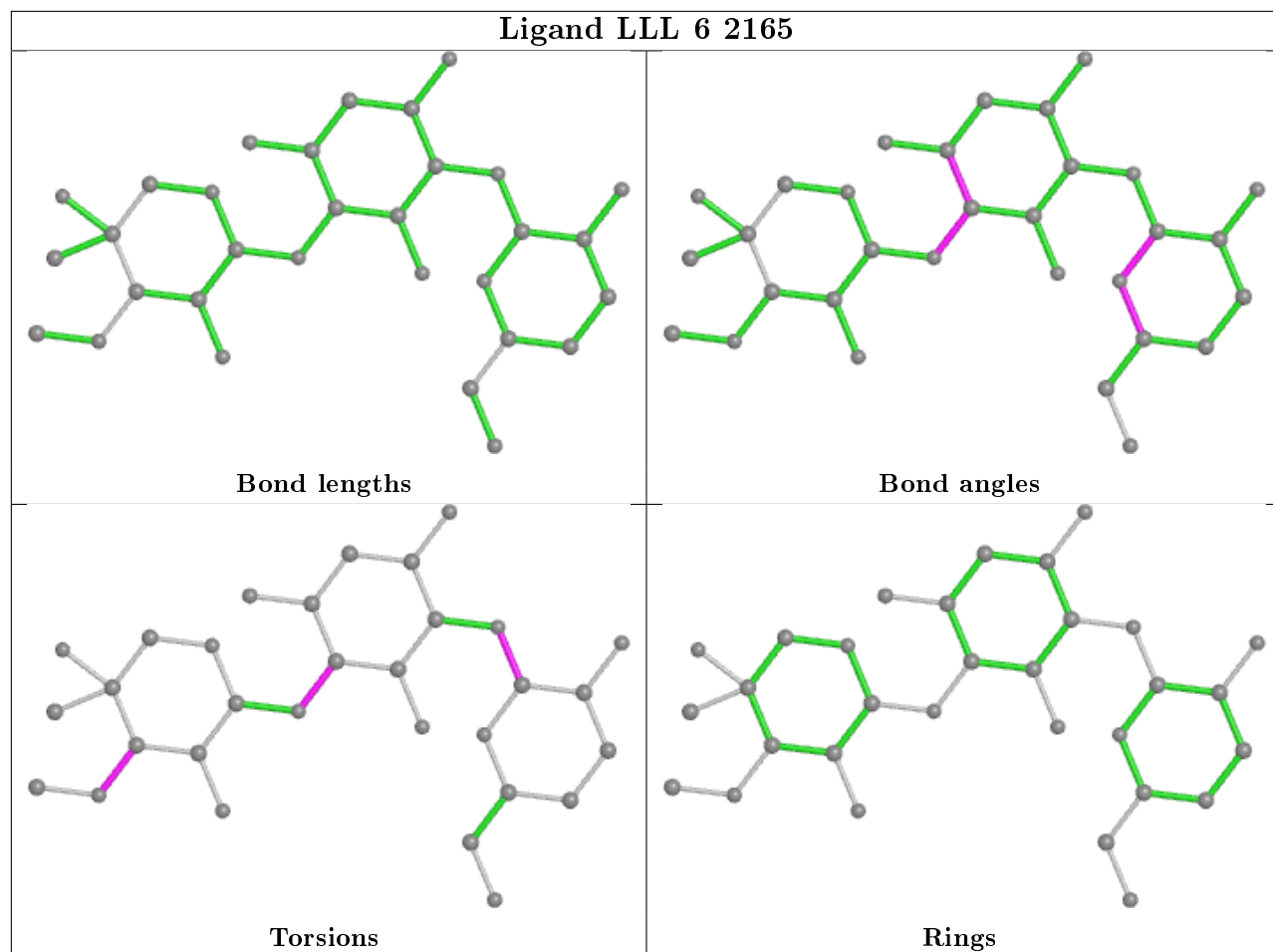


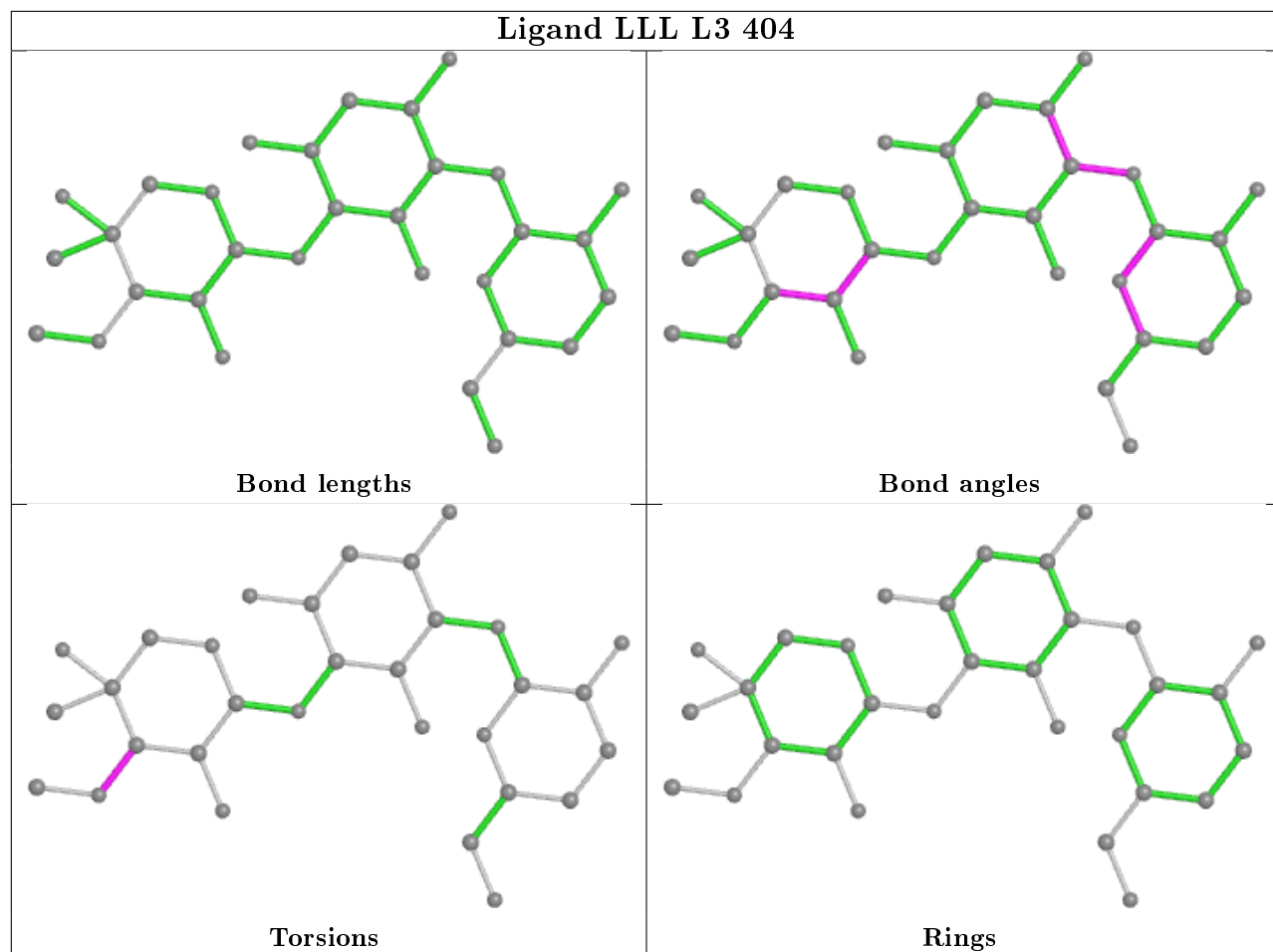
Torsions

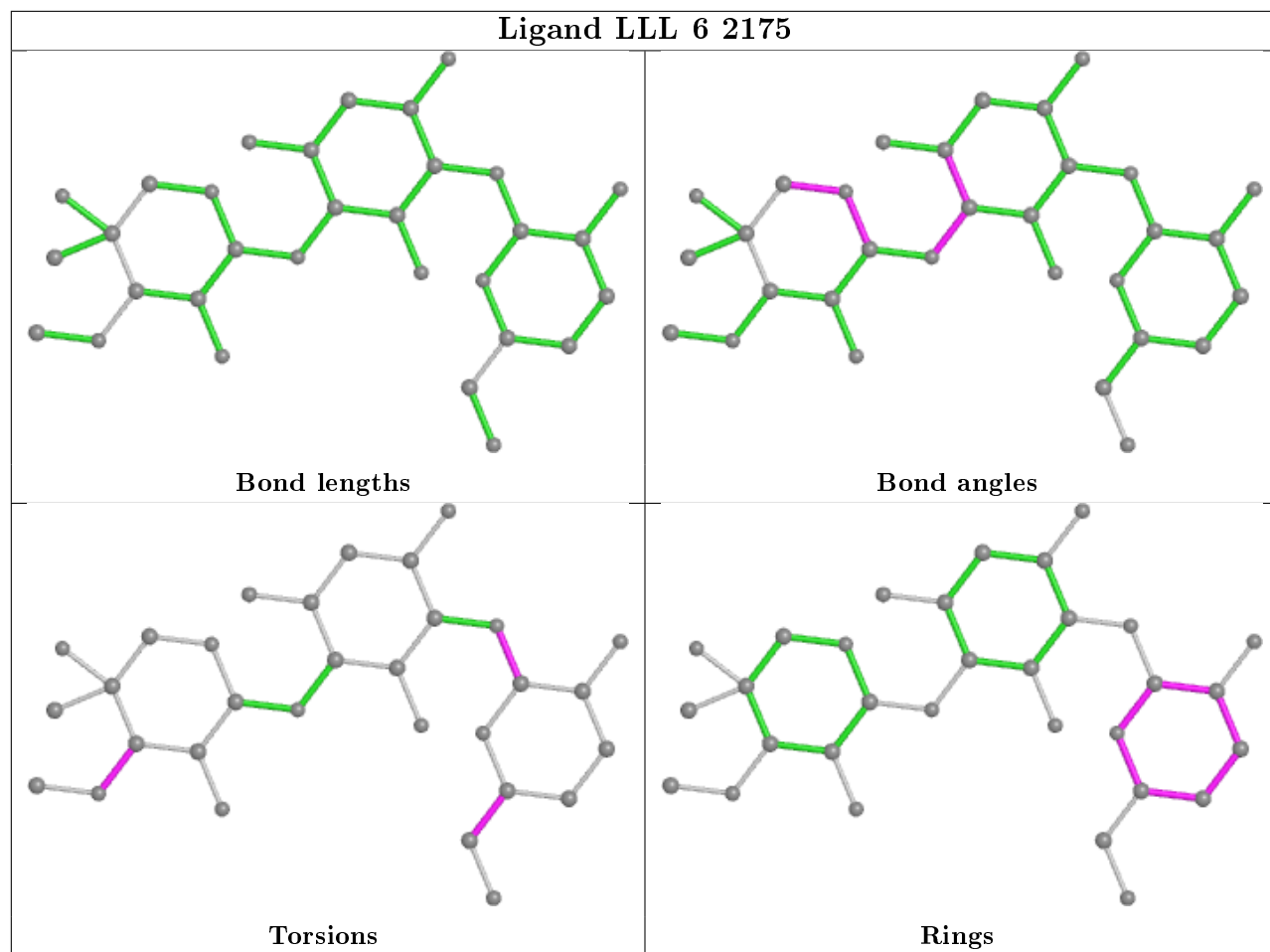


Rings

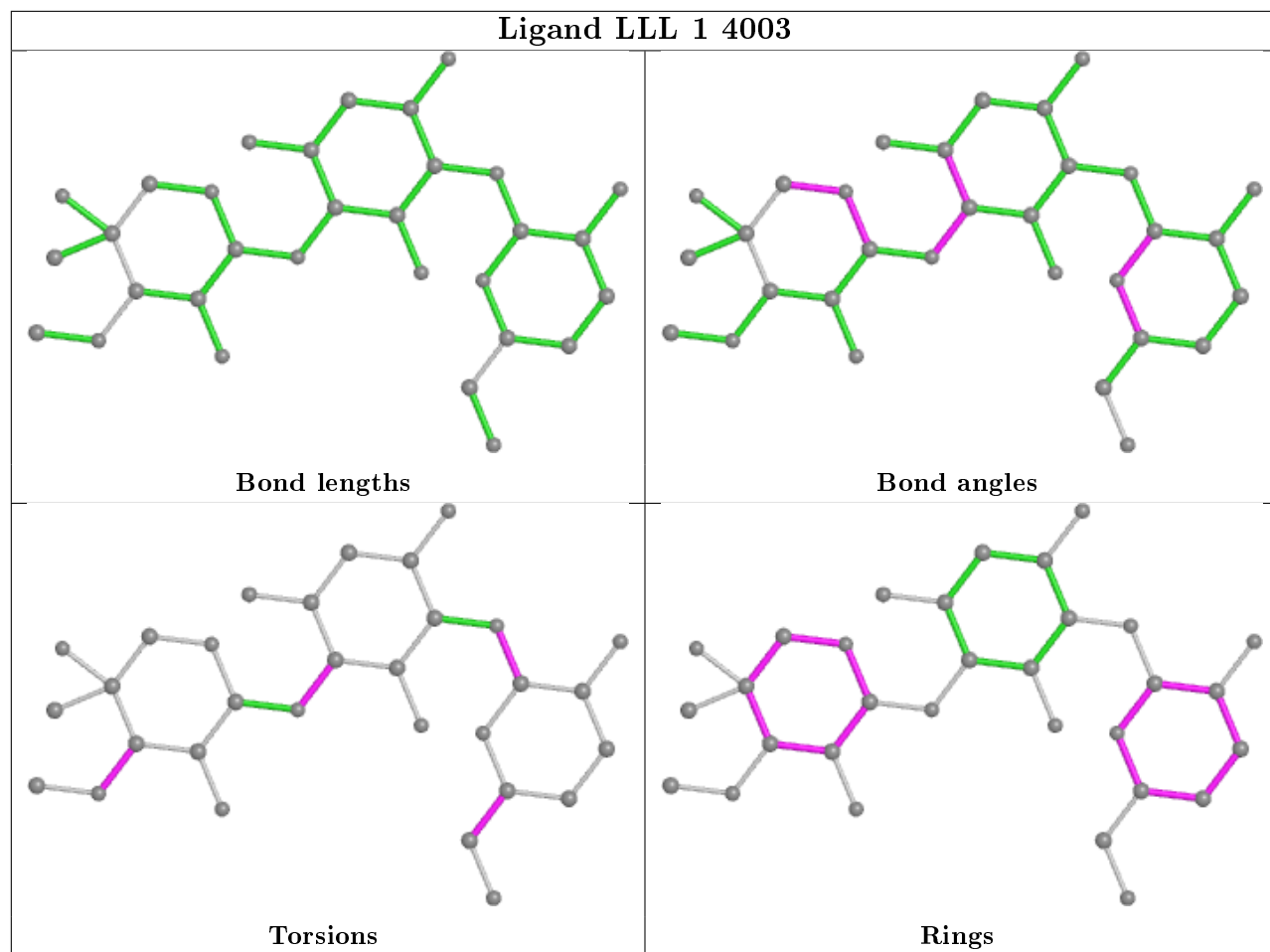
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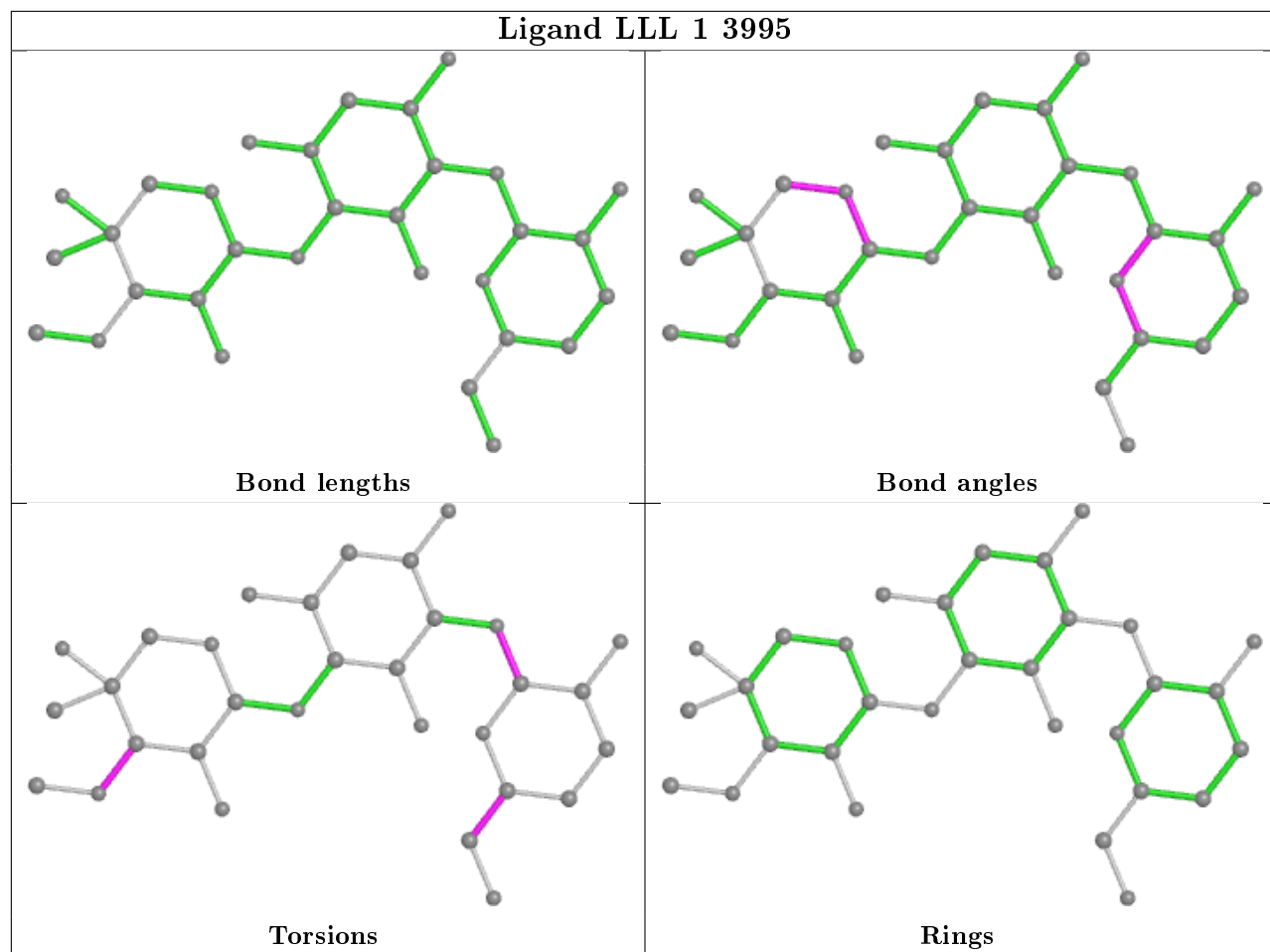




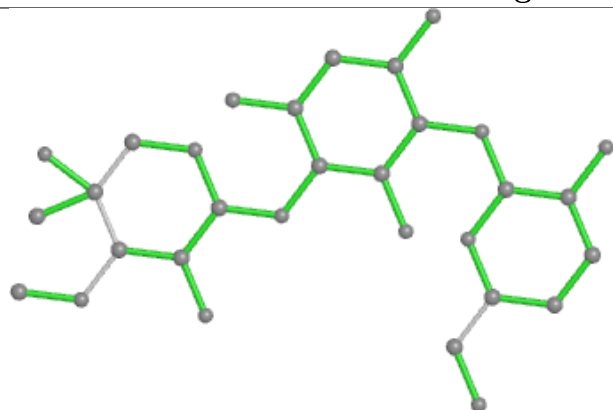


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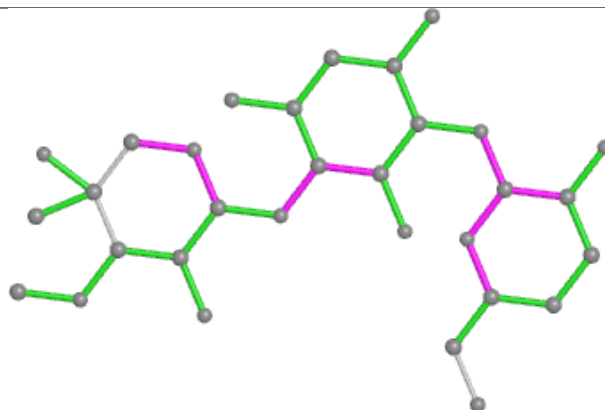




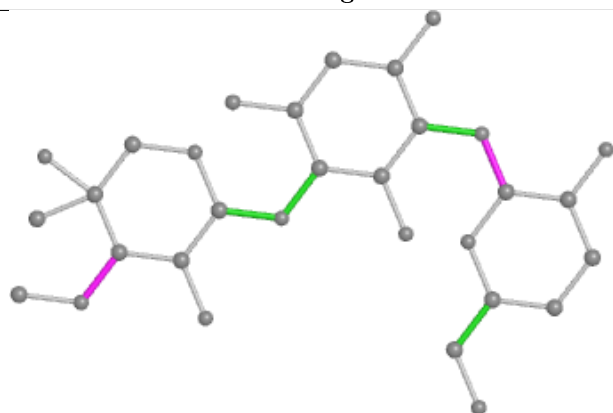
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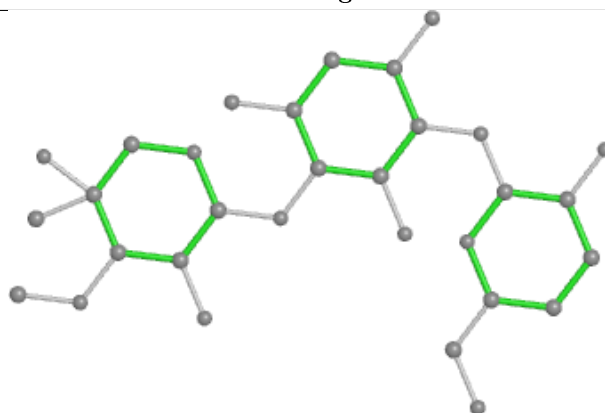
Bond lengths



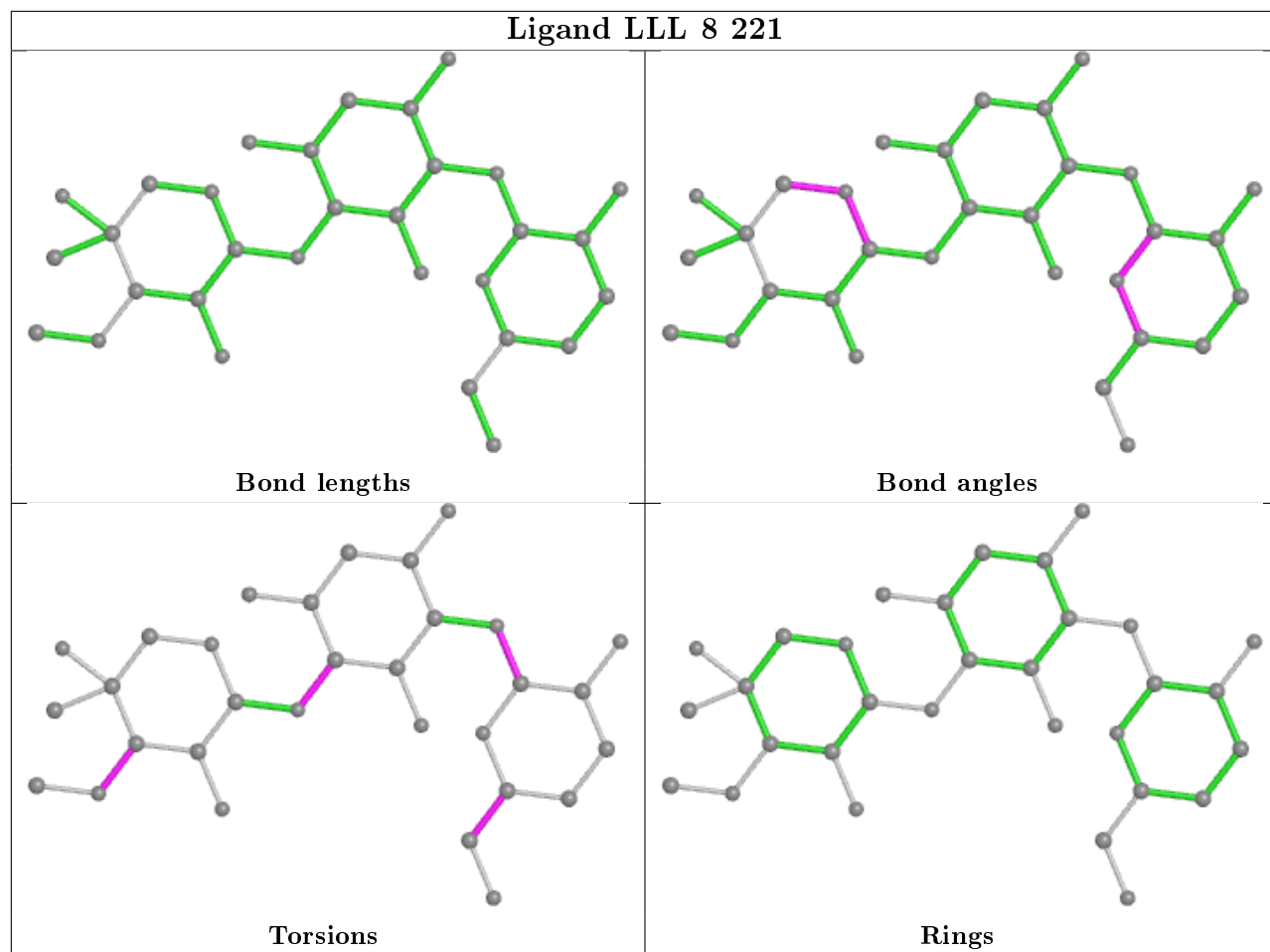
Bond angles



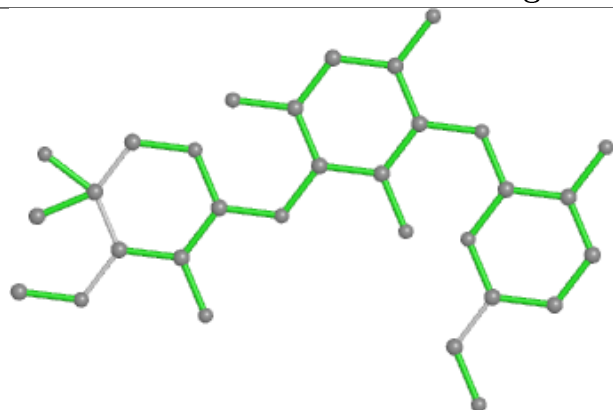
Torsions



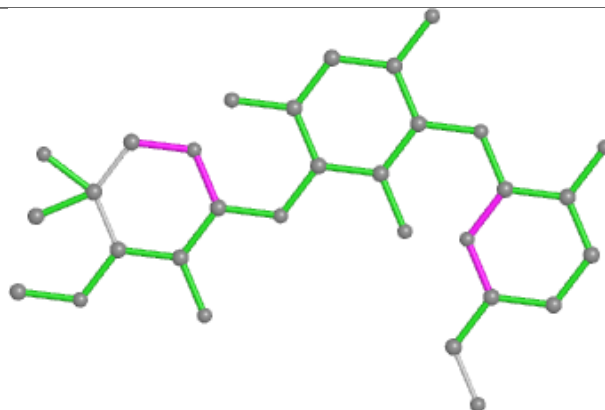
Rings



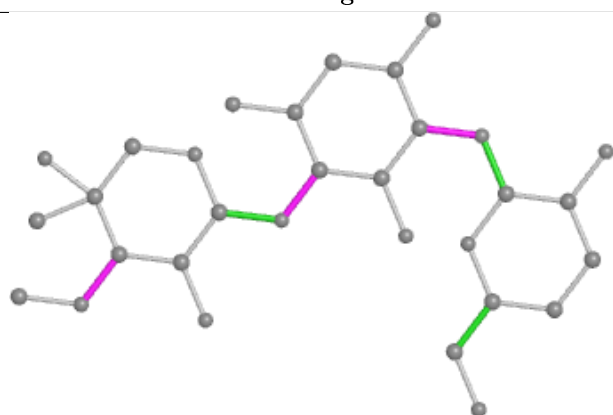
## Ligand LLL 7 233



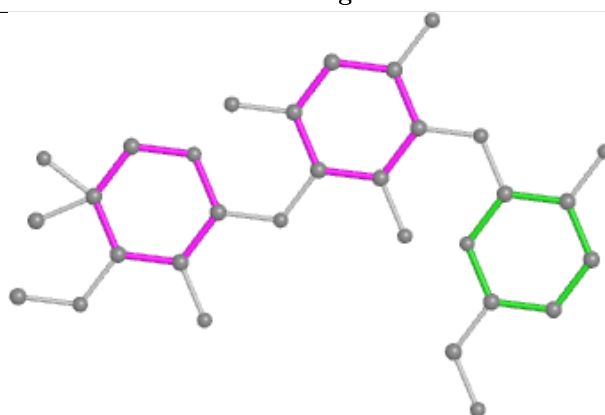
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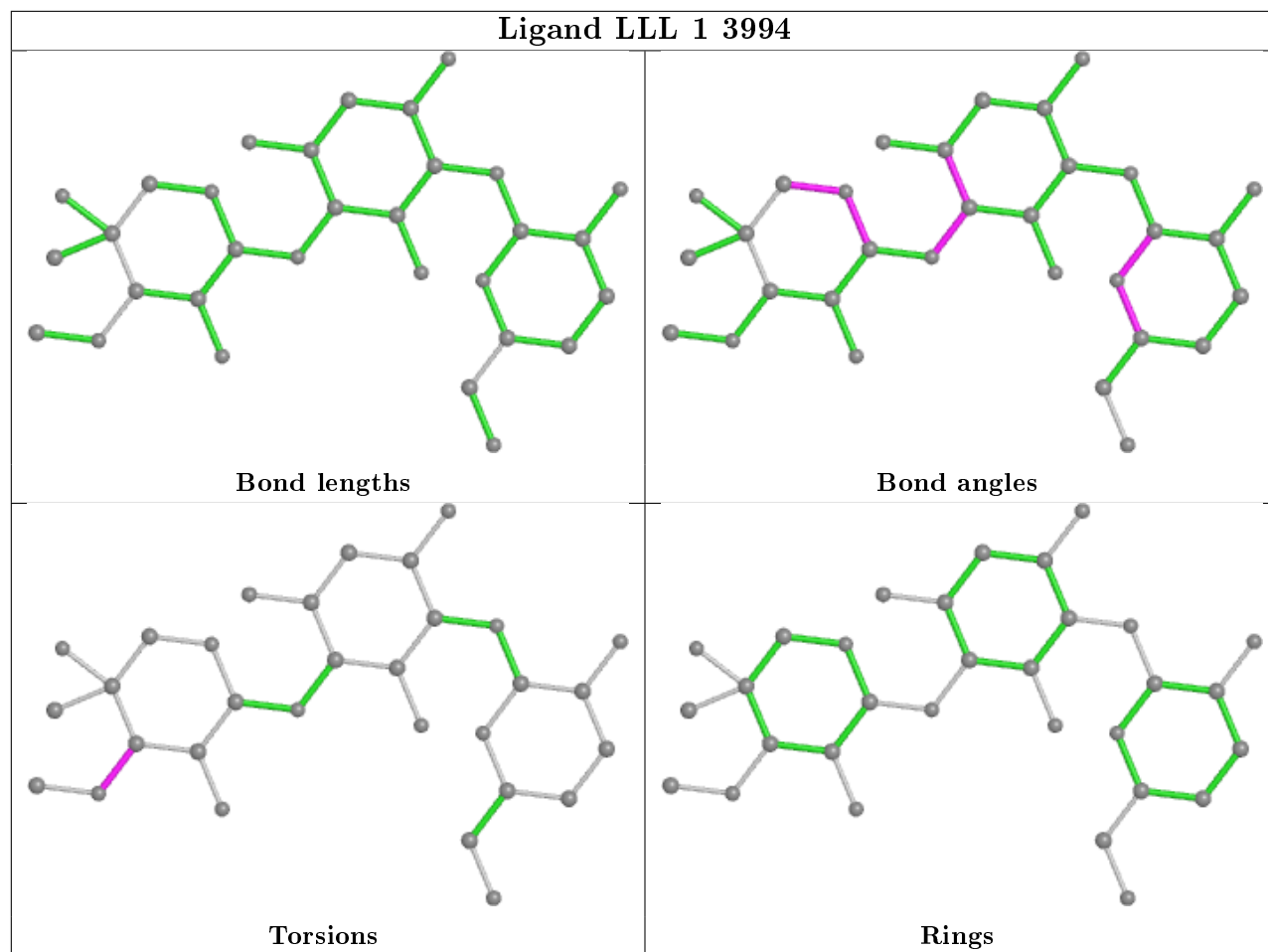
Bond angles



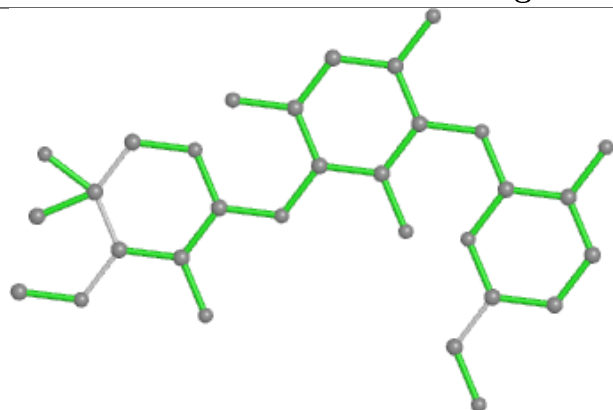
Torsions



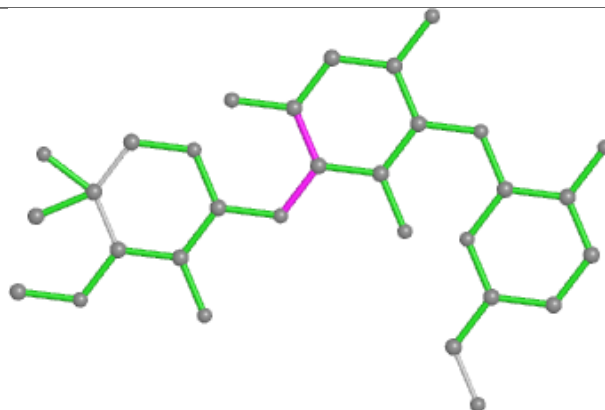
Rings



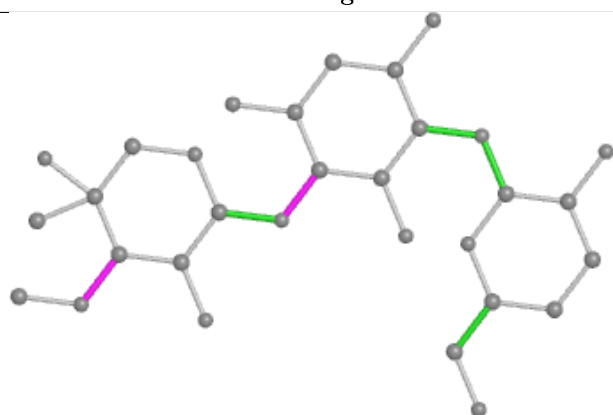
## Ligand LLL 1 3998



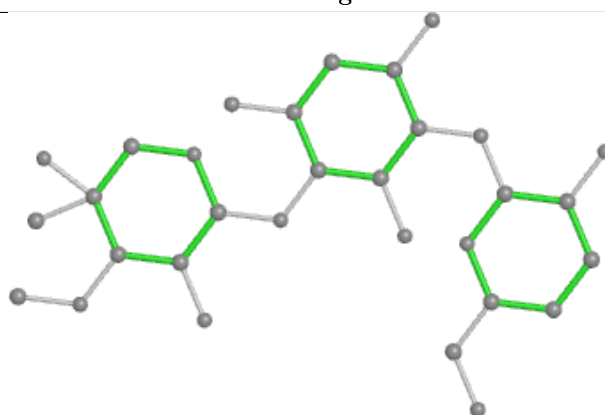
Bond lengths



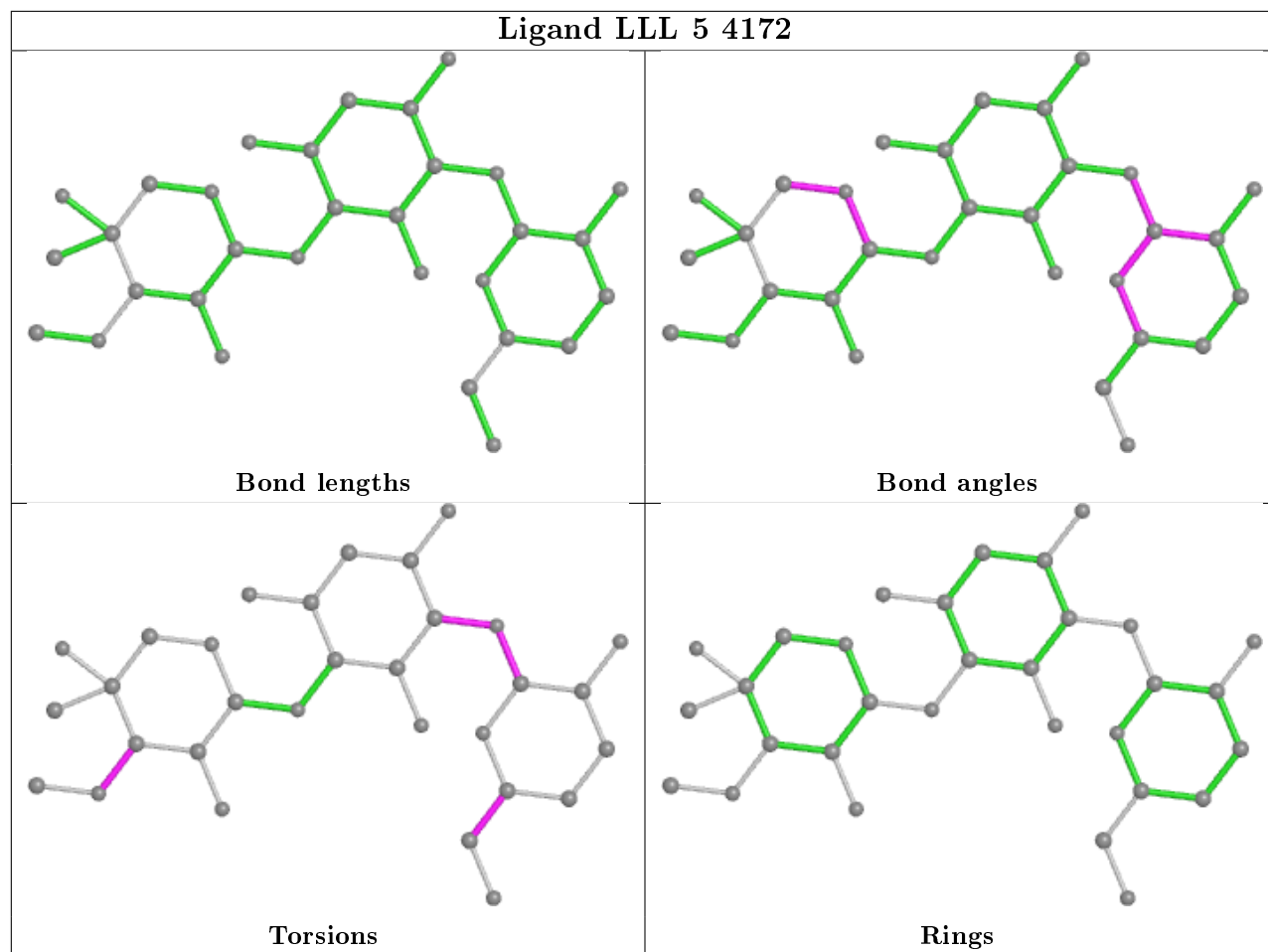
Bond angles

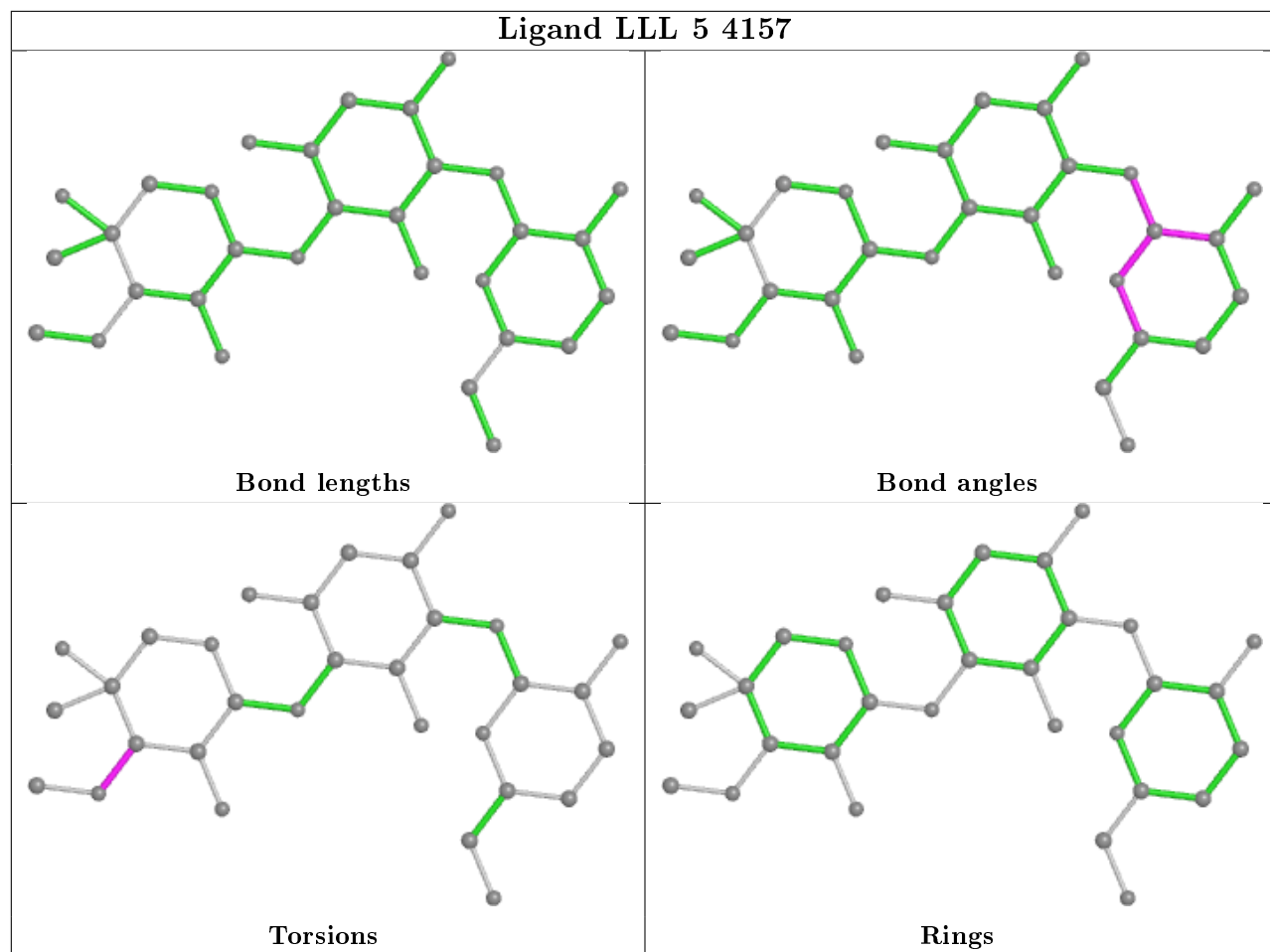


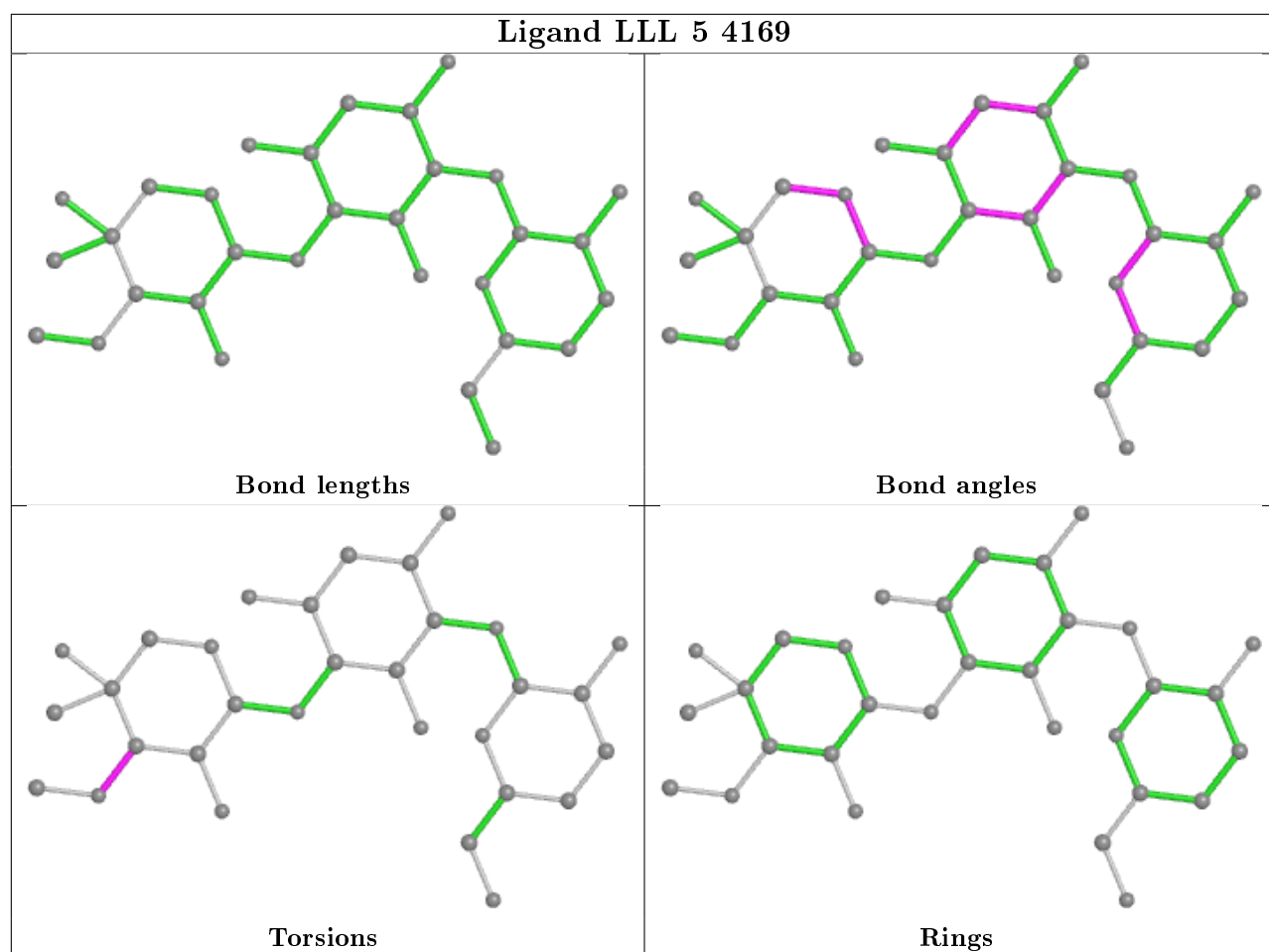
Torsions

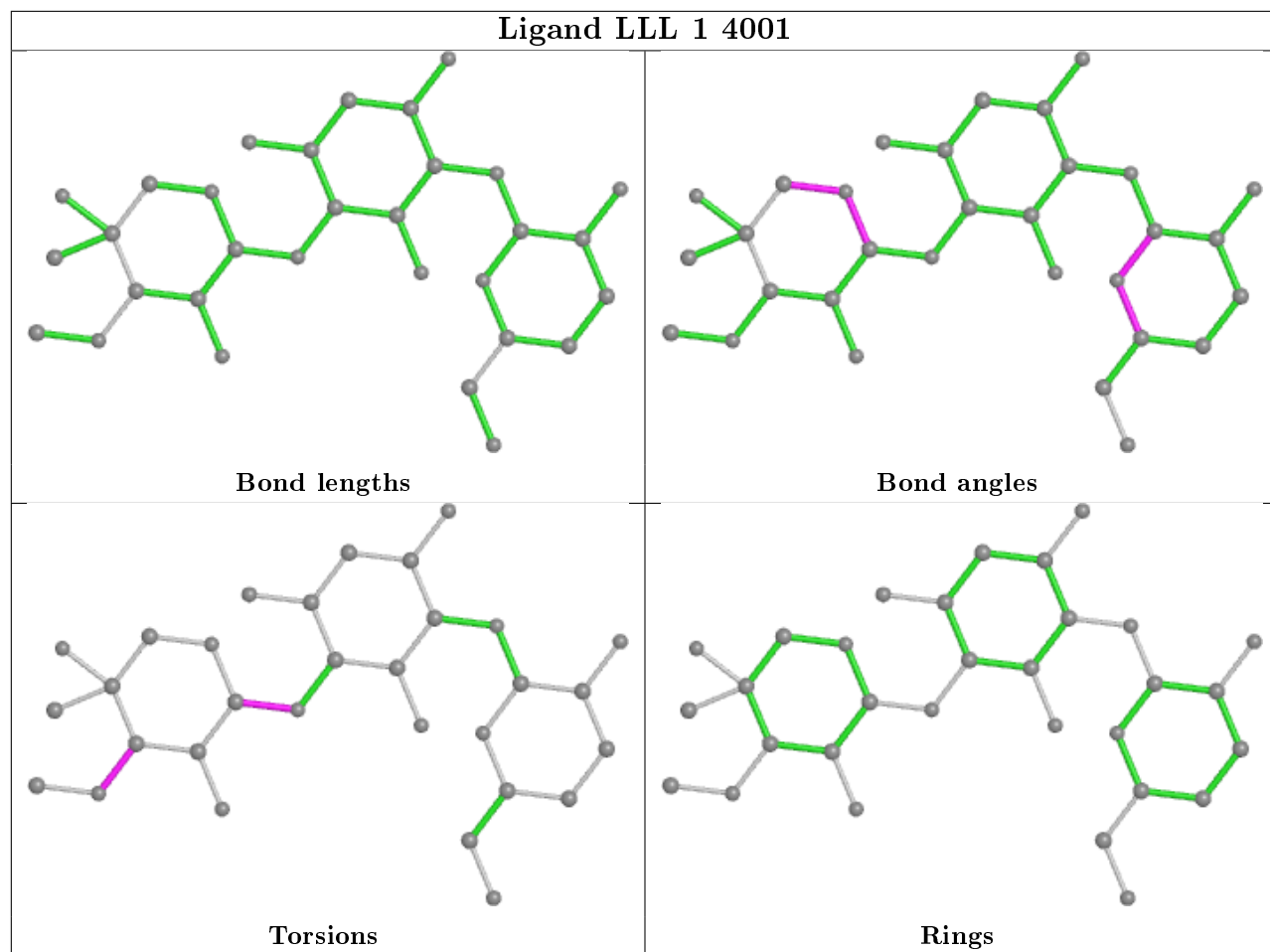


Rings

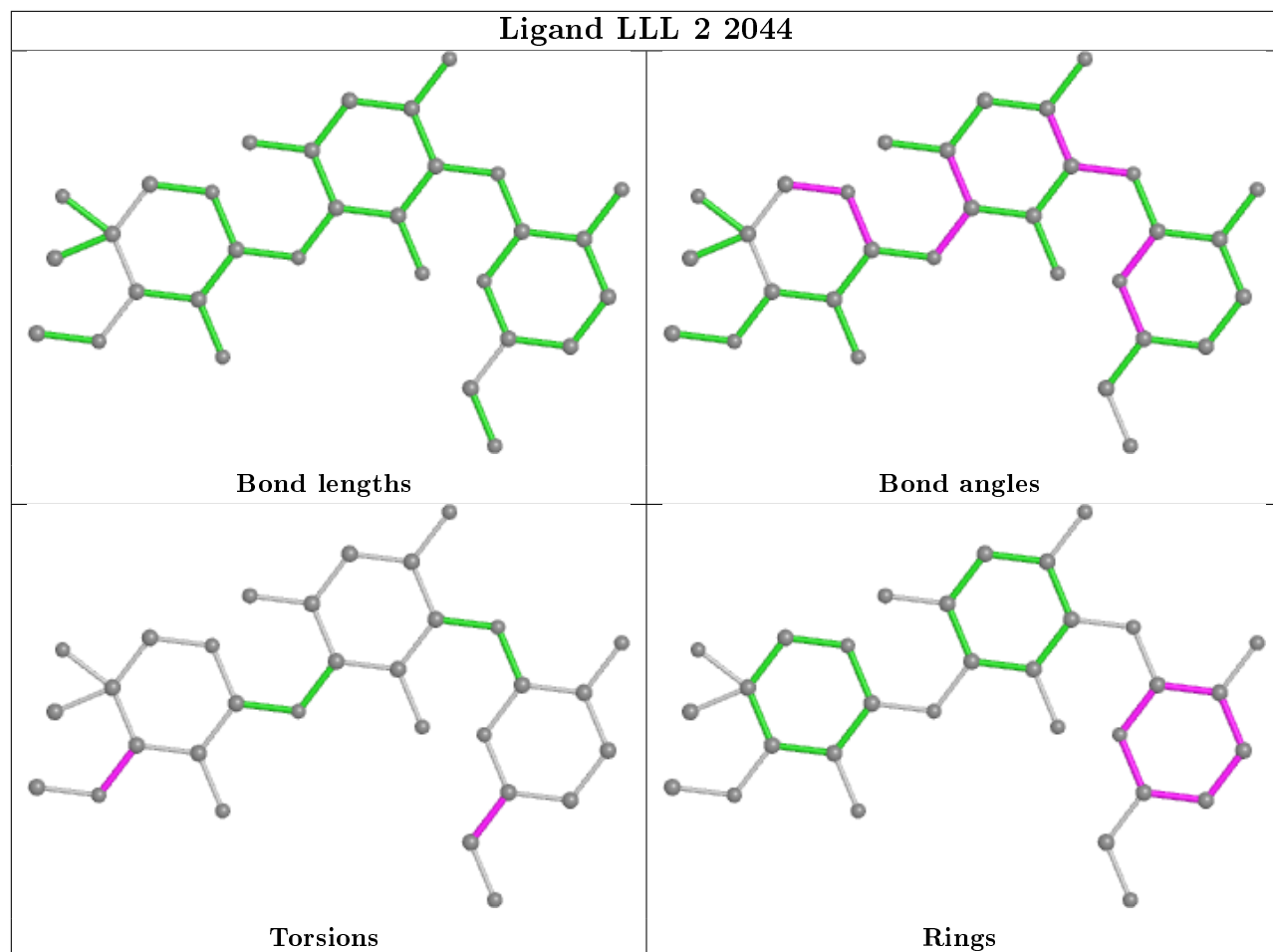




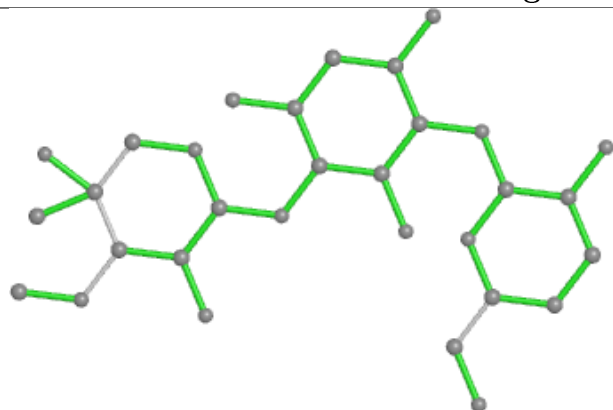




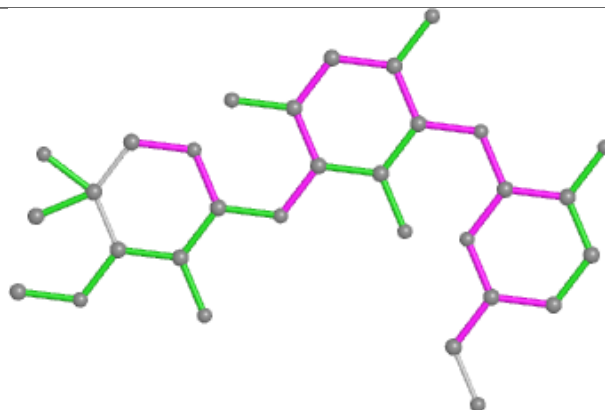
## Ligand LLL 2 2044



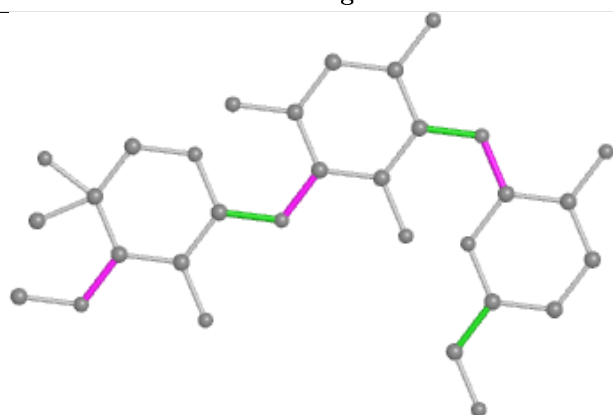
## Ligand LLL 7 231



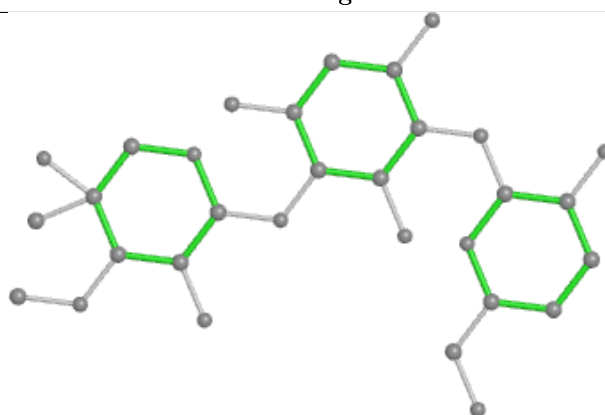
Bond lengths



Bond angles

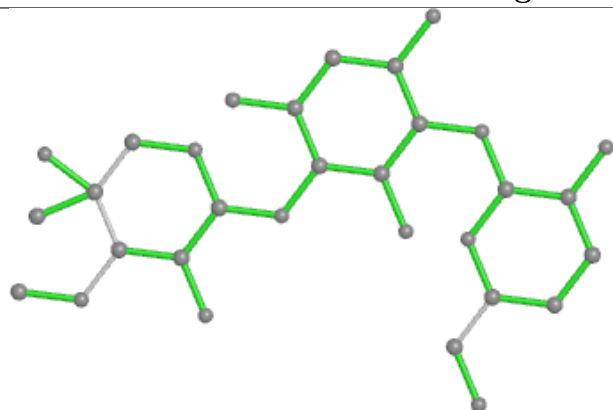


Torsions

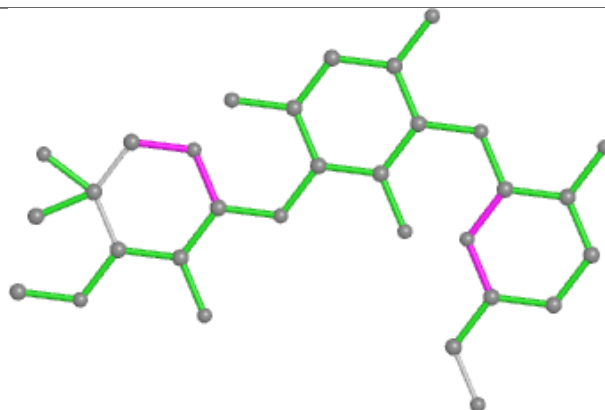


Rings

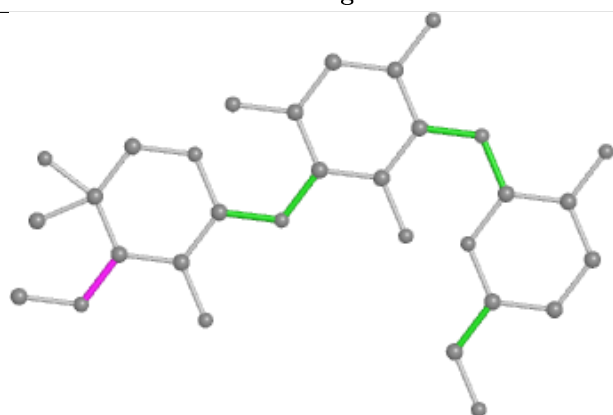
## Ligand LLL 5 4170



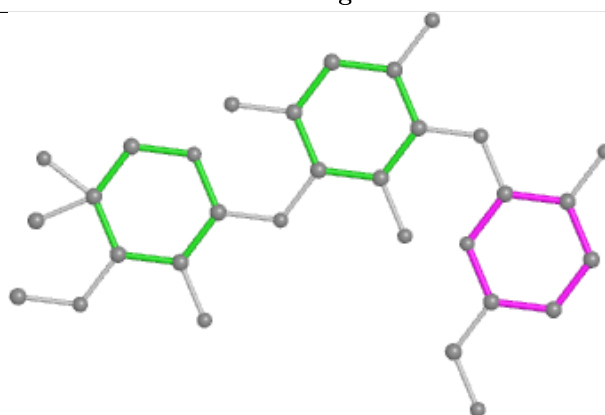
Bond lengths



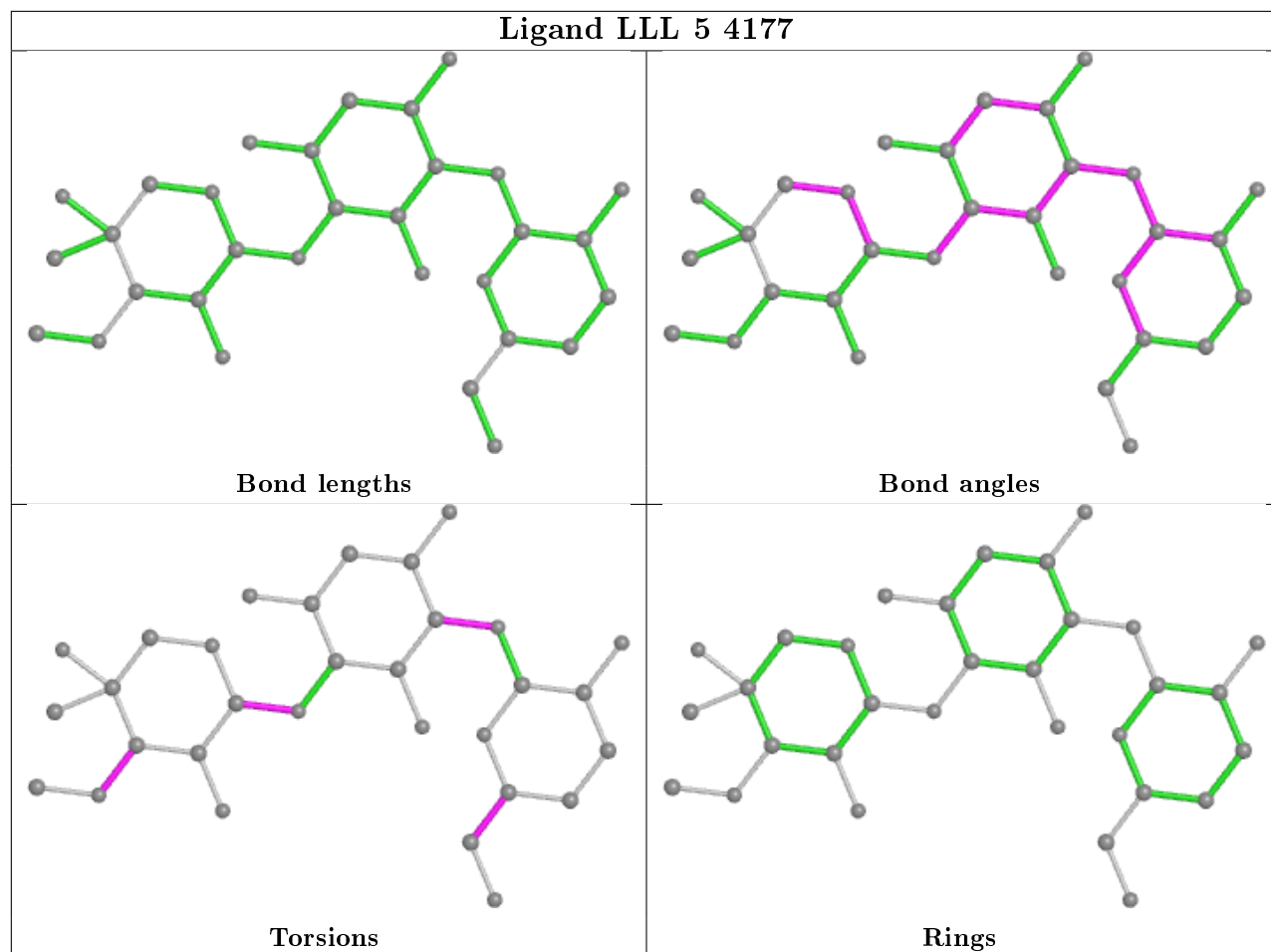
Bond angles



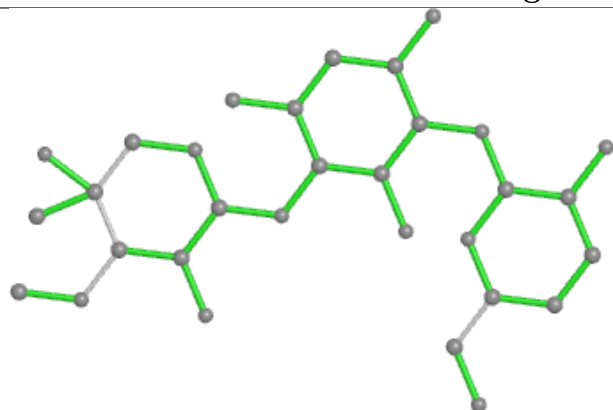
Torsions



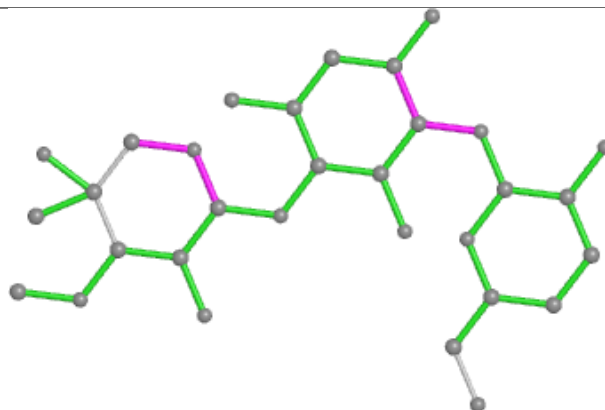
Rings



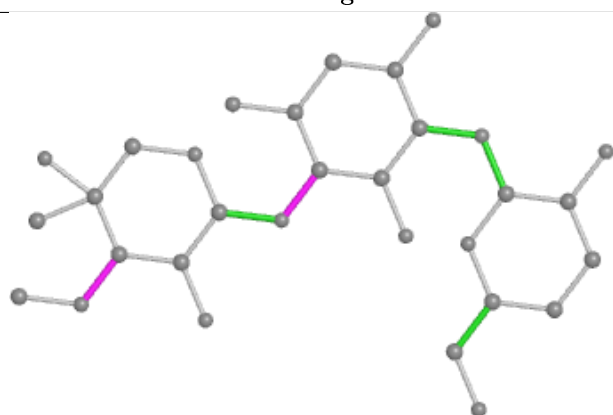
## Ligand LLL 7 232



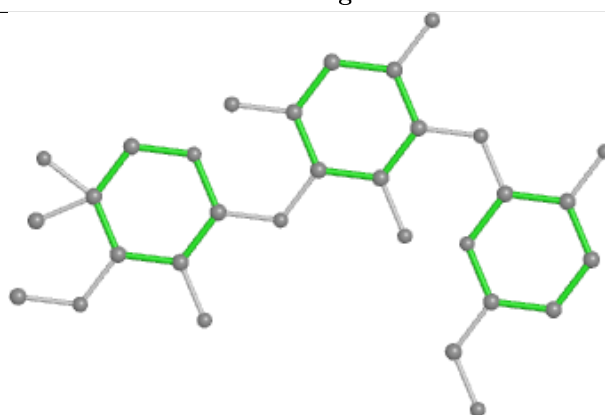
Bond lengths



Bond angles

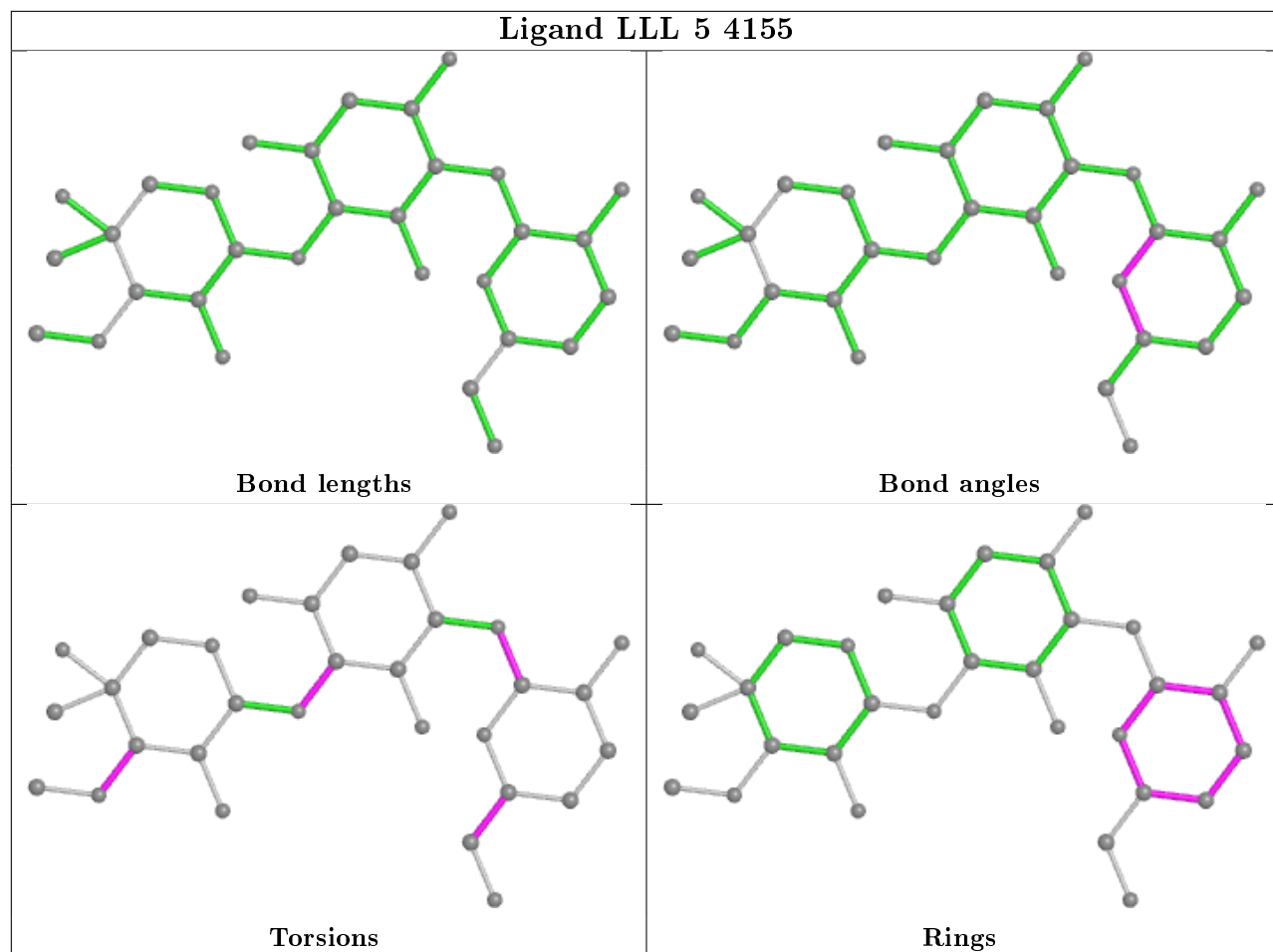


Torsions

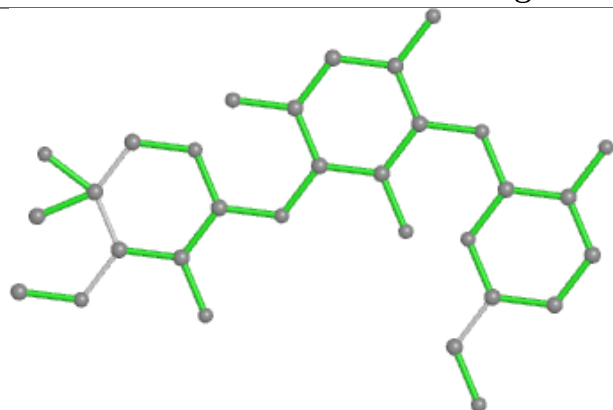


Rings

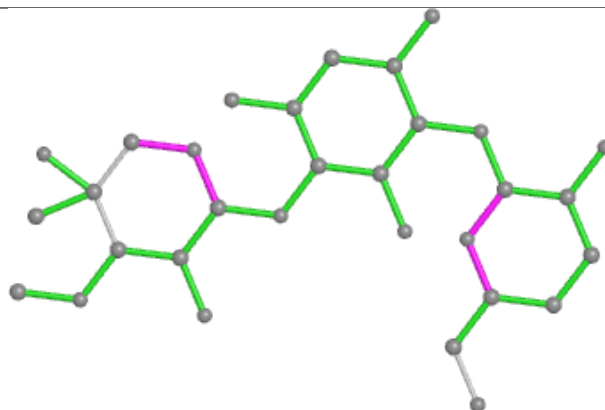
## Ligand LLL 5 4155



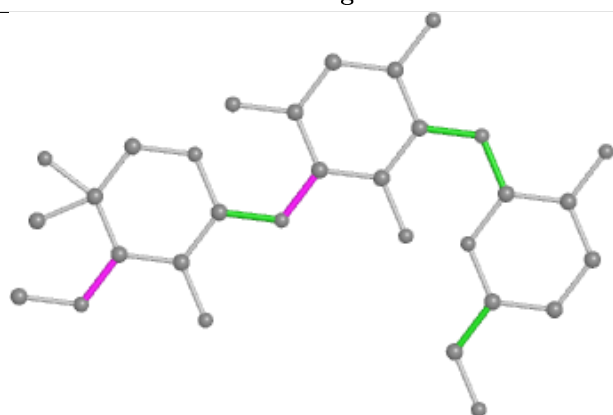
## Ligand LLL 5 4167



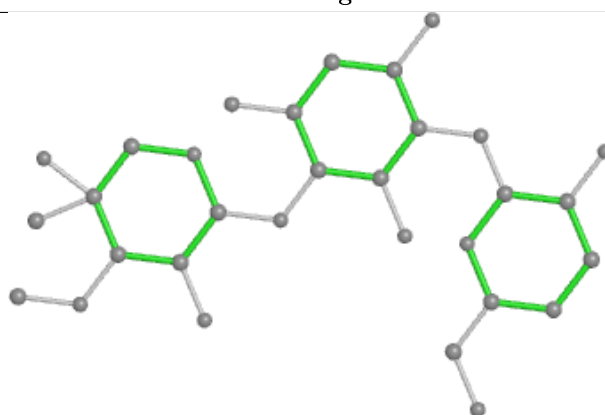
Bond lengths



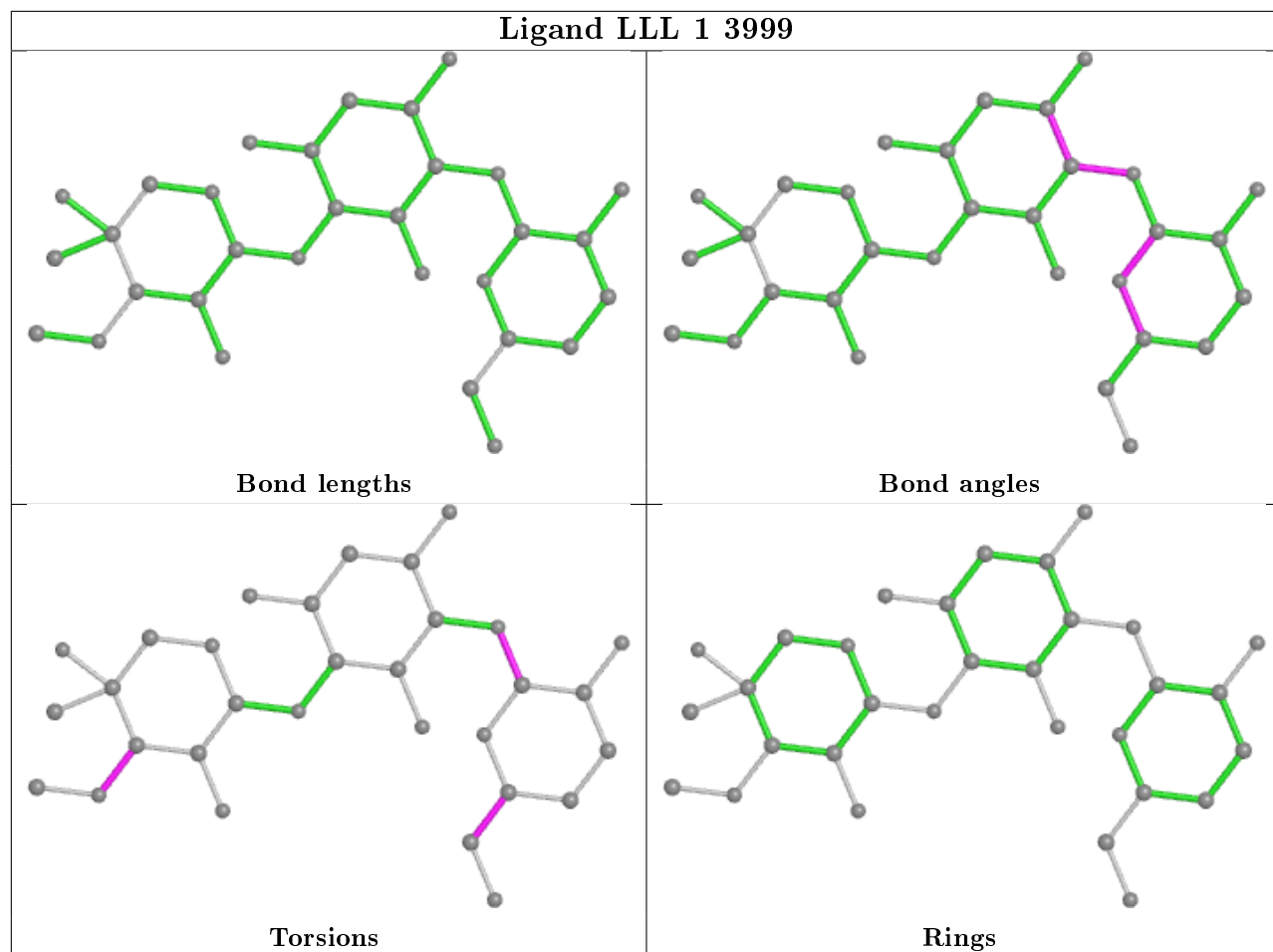
Bond angles



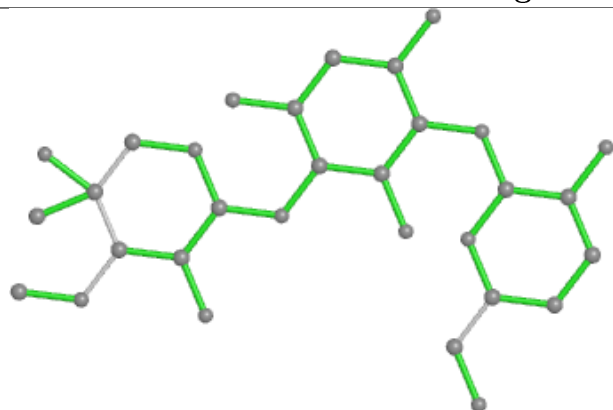
Torsions



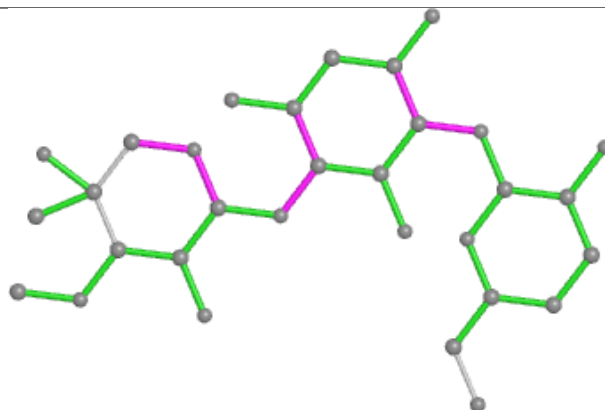
Rings



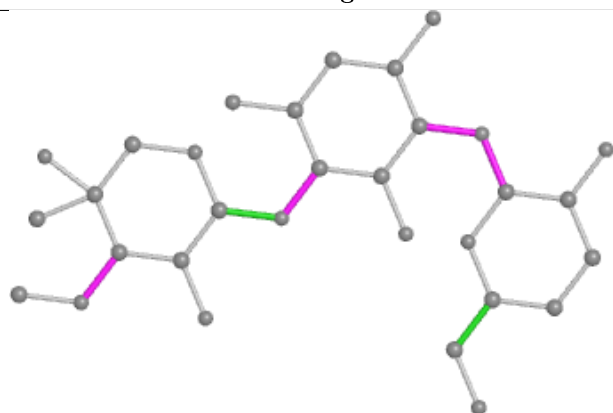
## Ligand LLL 5 4156



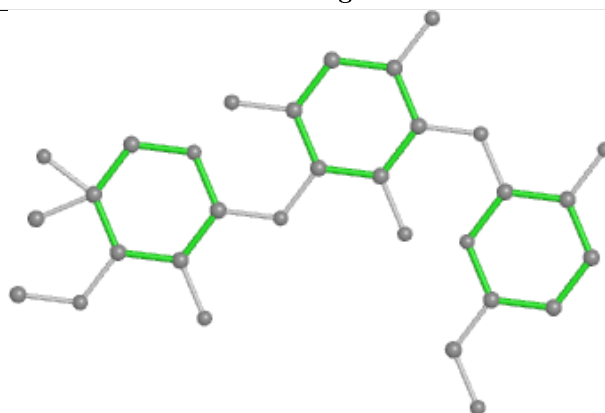
Bond lengths



Bond angles

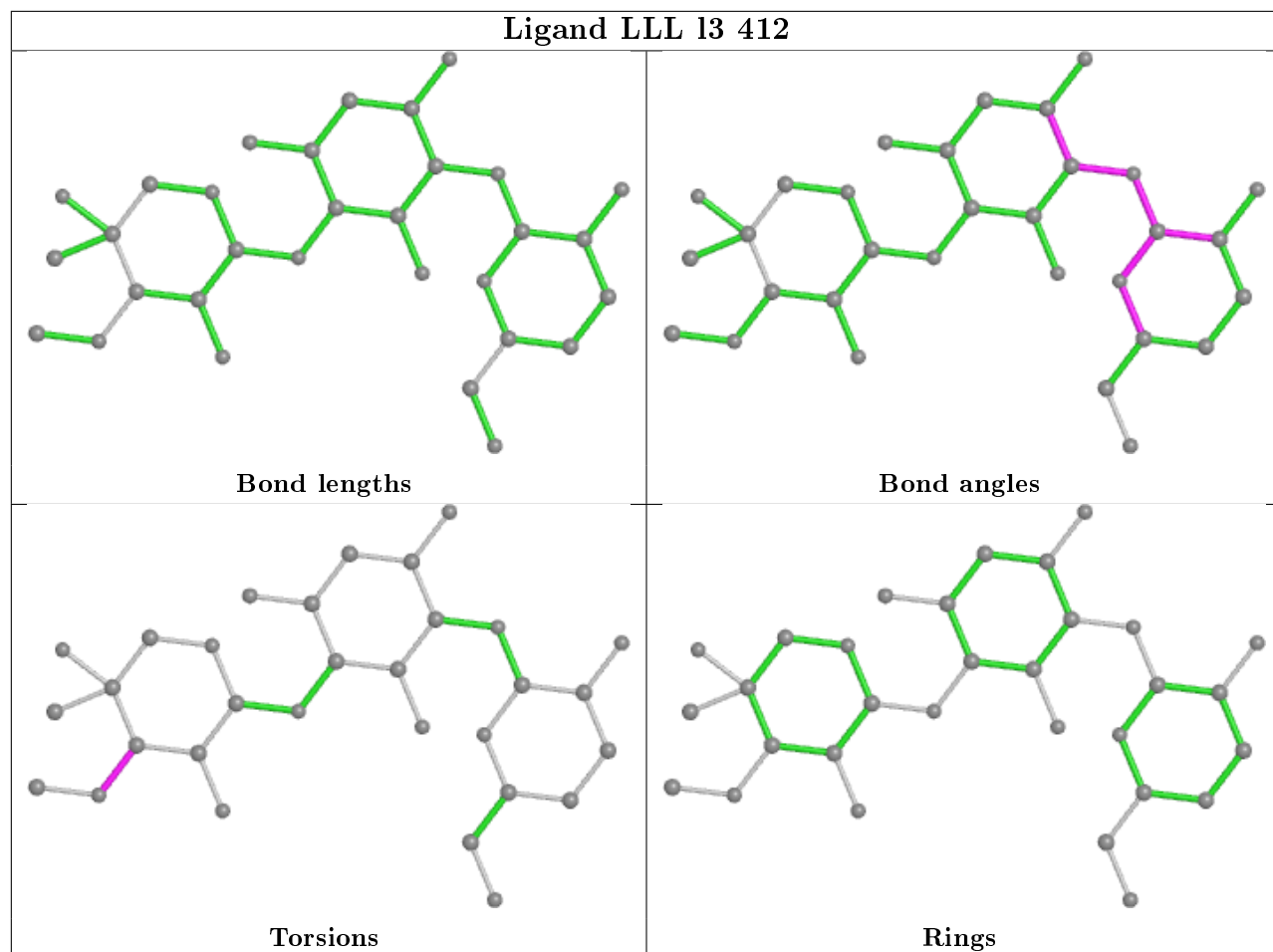


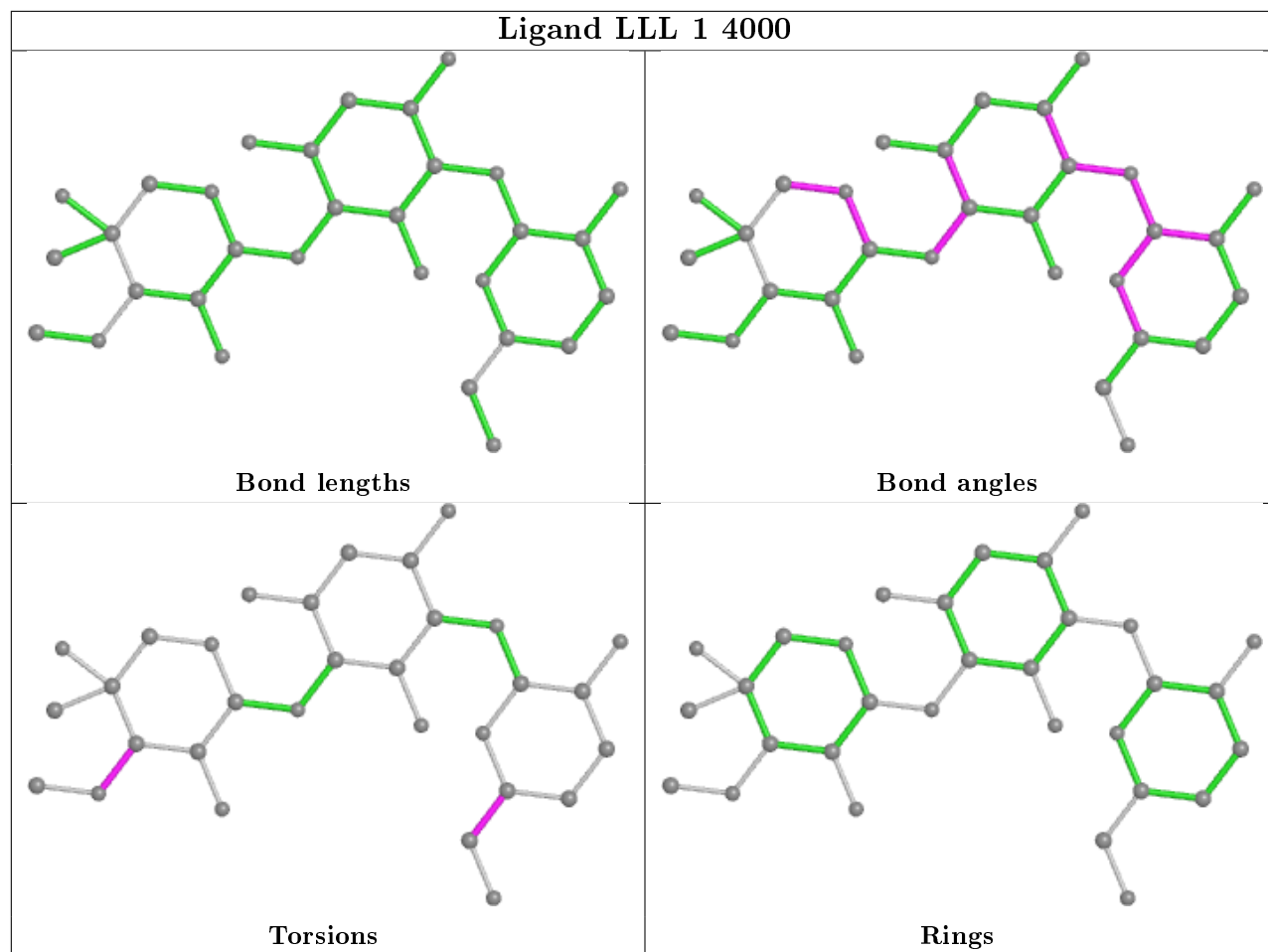
Torsions



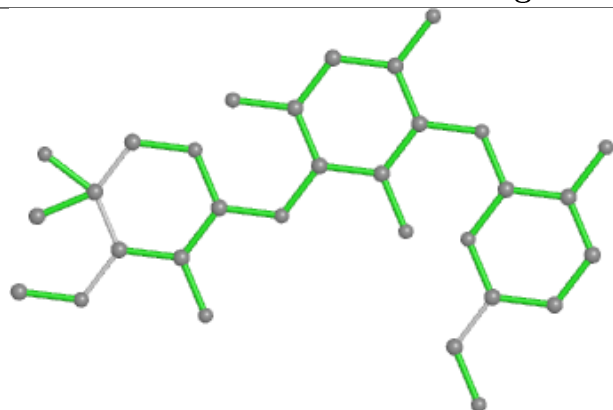
Rings

## Ligand LLL 13 412

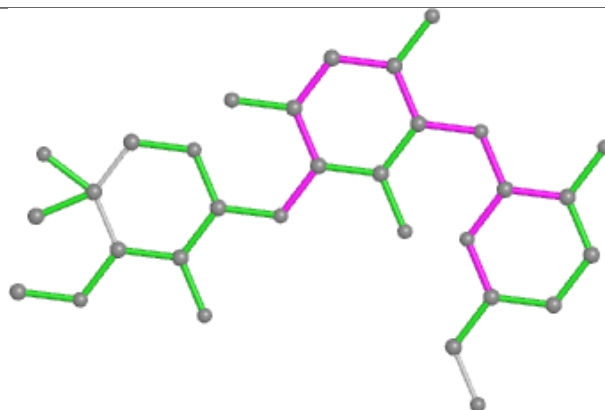




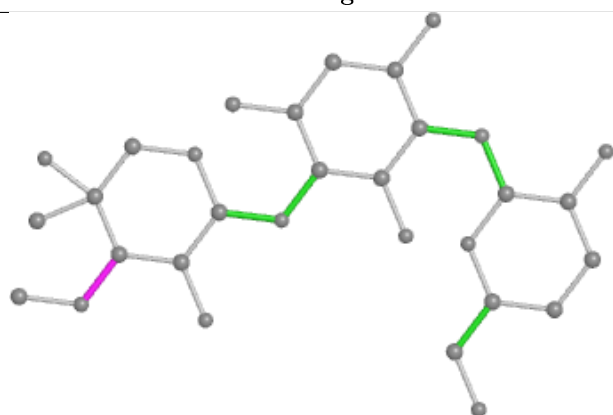
## Ligand LLL 1 3993



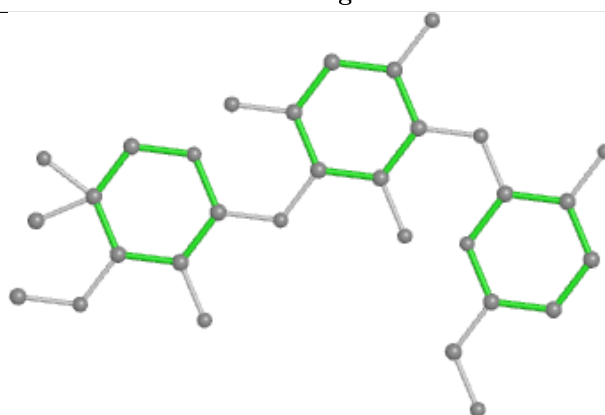
Bond lengths



Bond angles

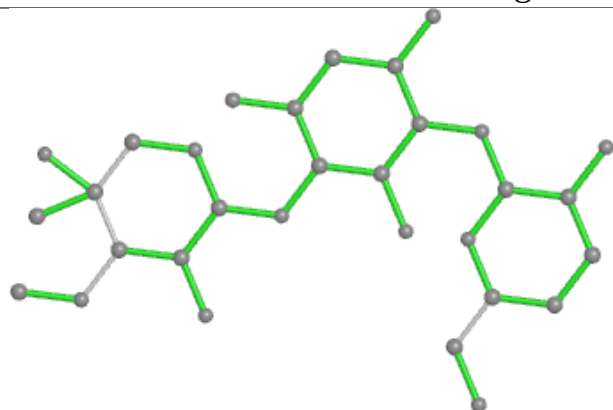


Torsions

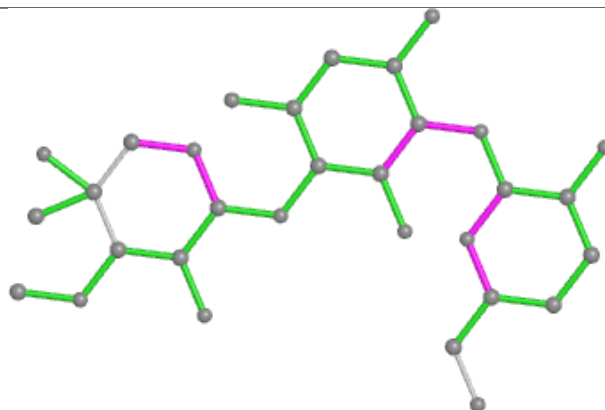


Rings

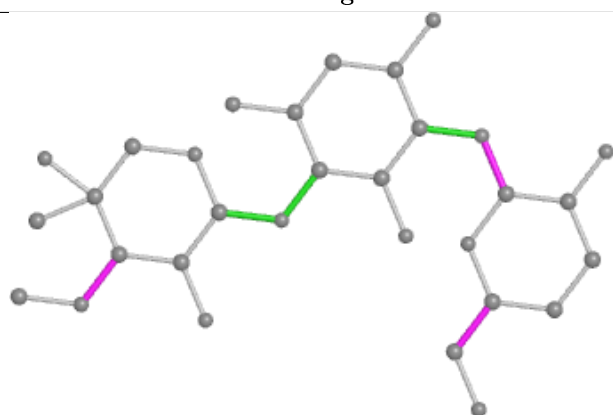
## Ligand LLL 6 2168



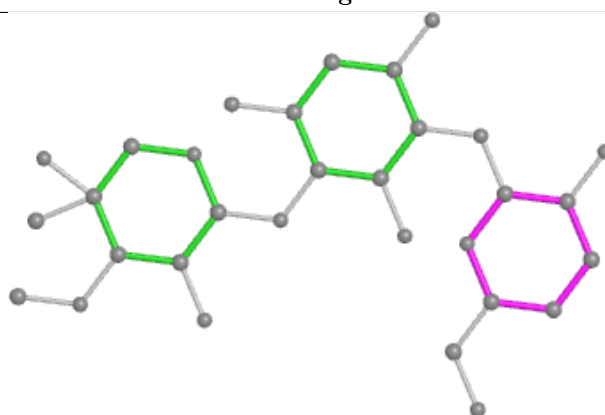
Bond lengths



Bond angles

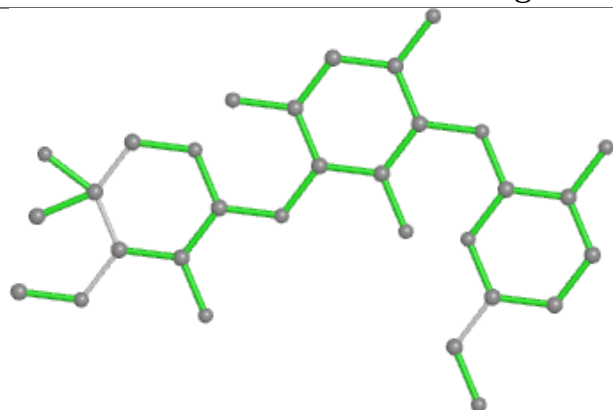


Torsions

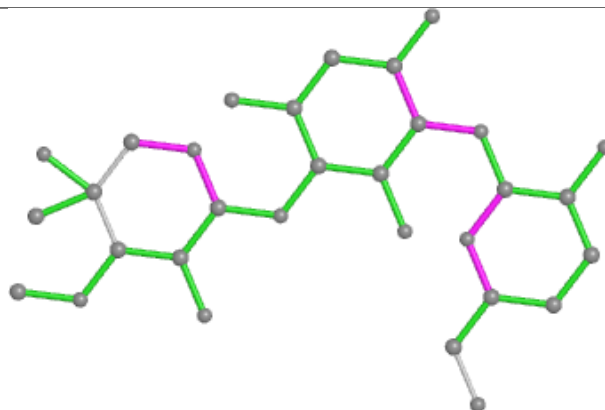


Rings

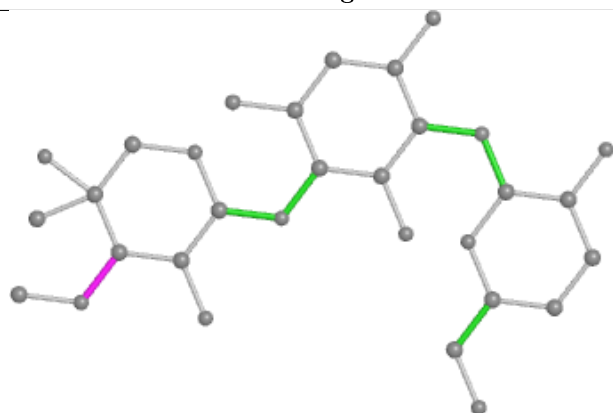
## Ligand LLL 5 4159



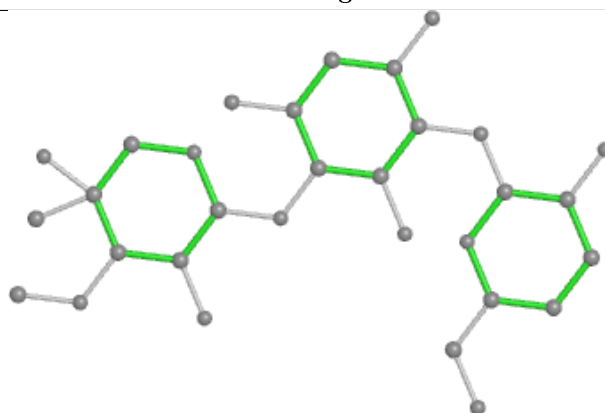
Bond lengths



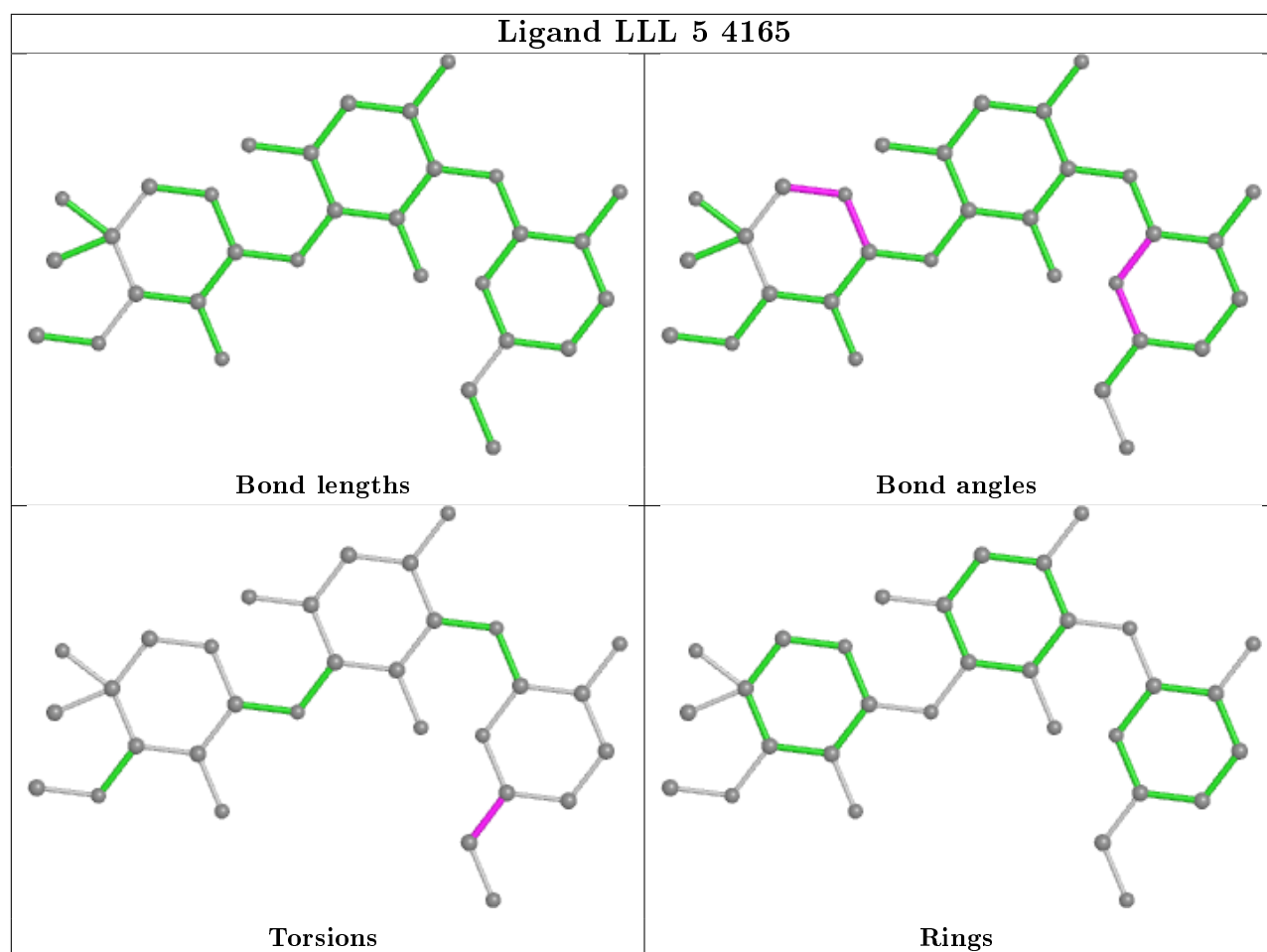
Bond angles

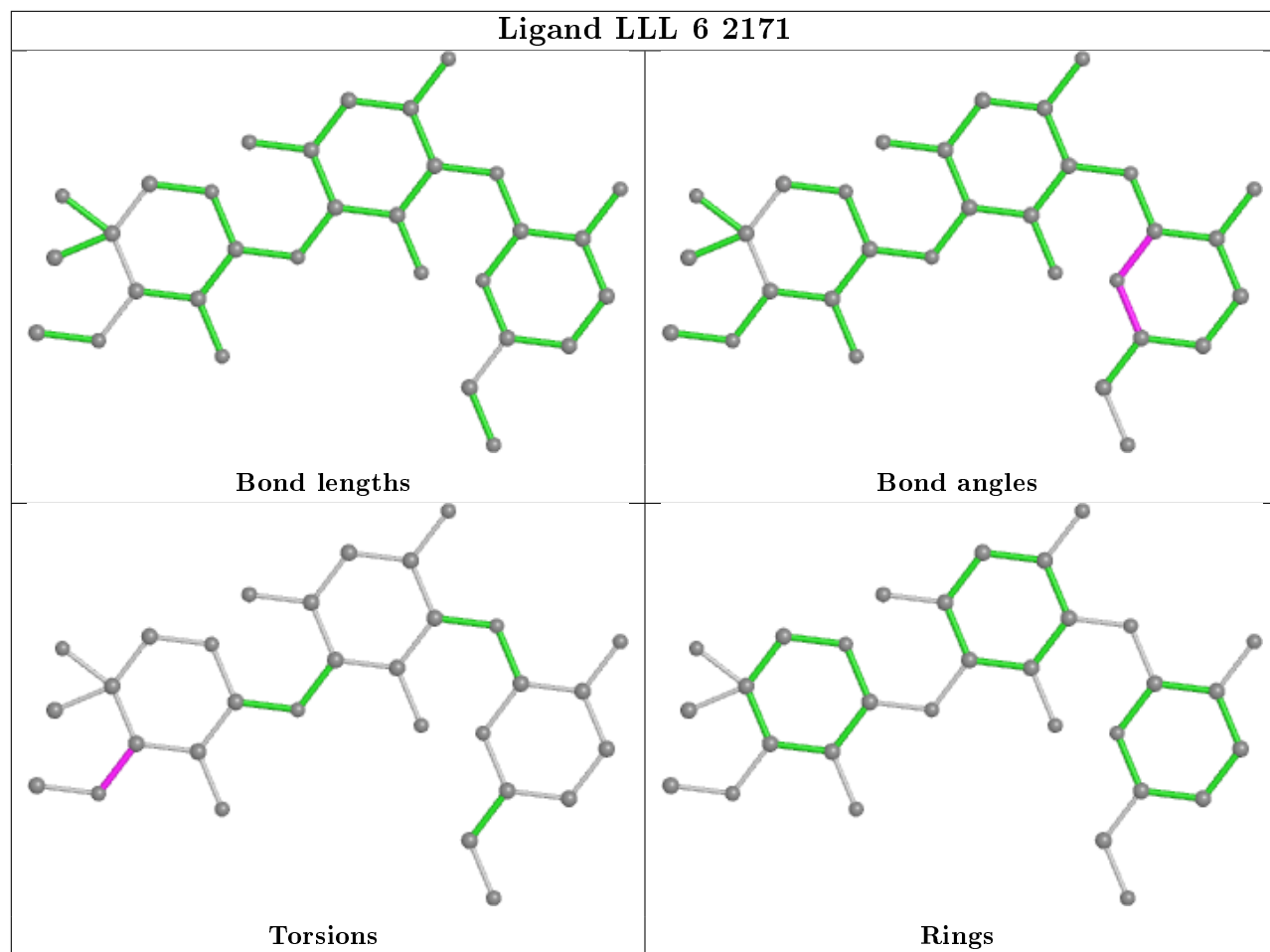


Torsions

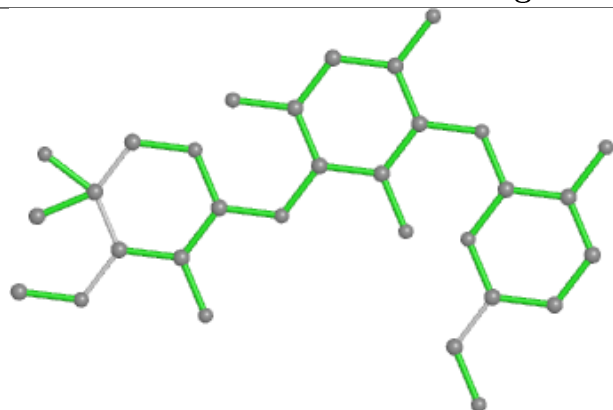


Rings

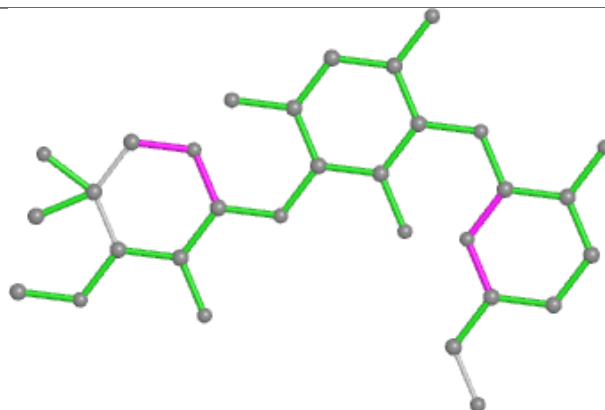




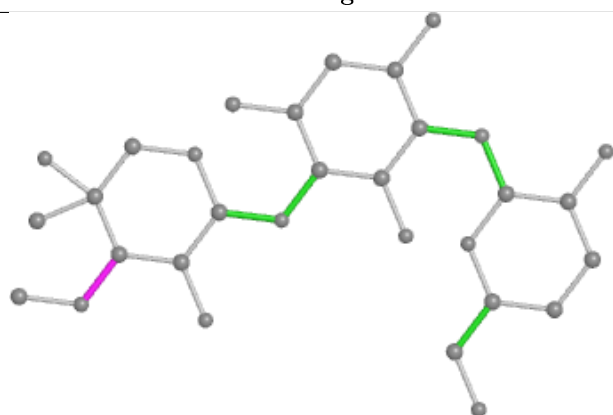
## Ligand LLL 6 2169



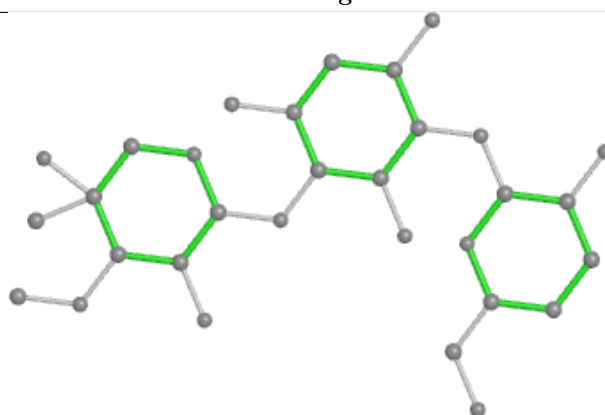
Bond lengths



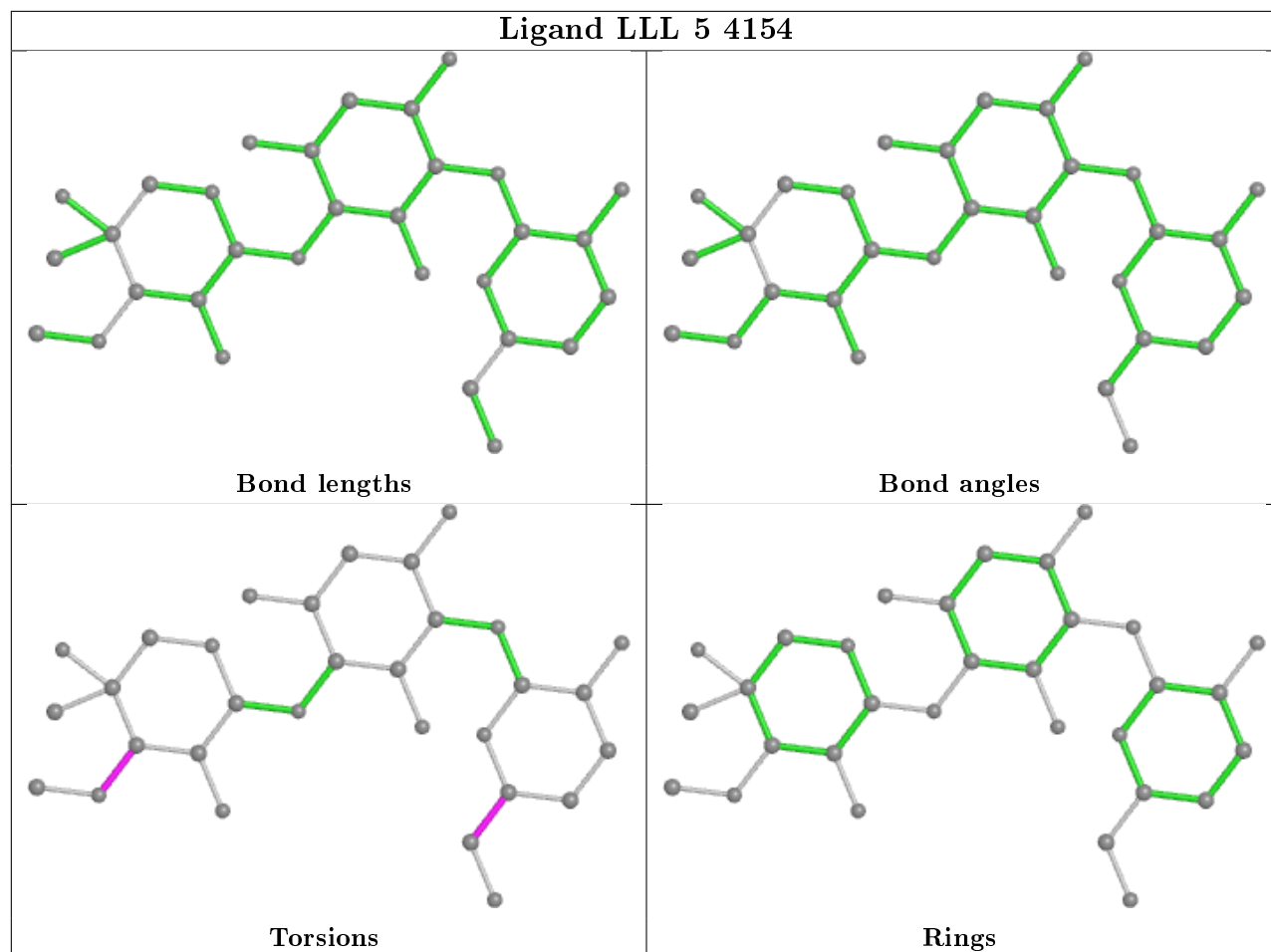
Bond angles



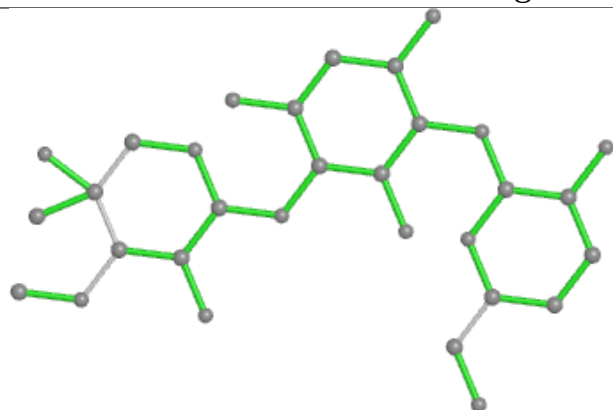
Torsions



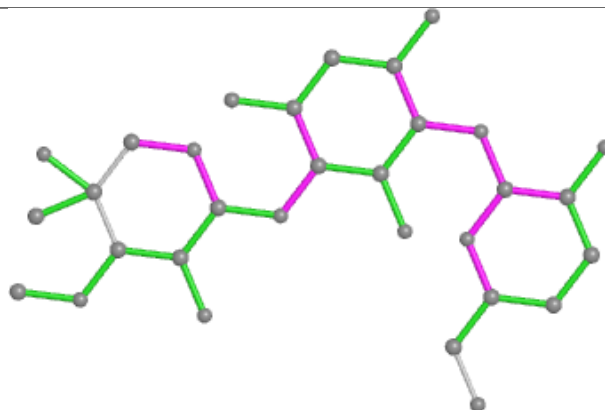
Rings



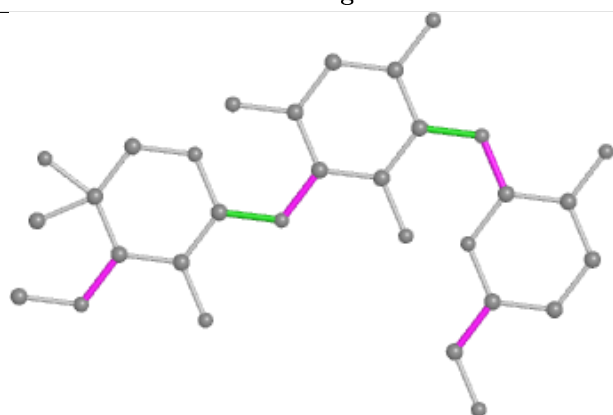
## Ligand LLL 6 2167



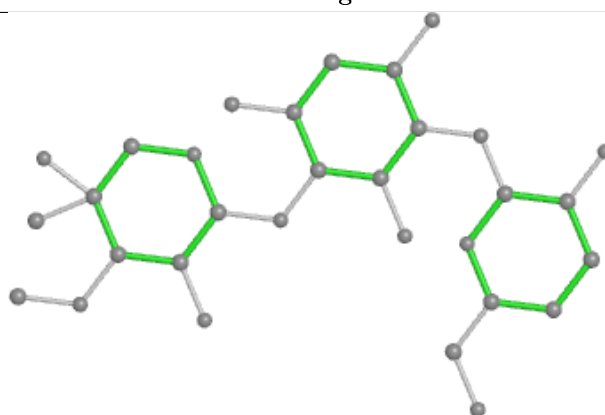
Bond lengths



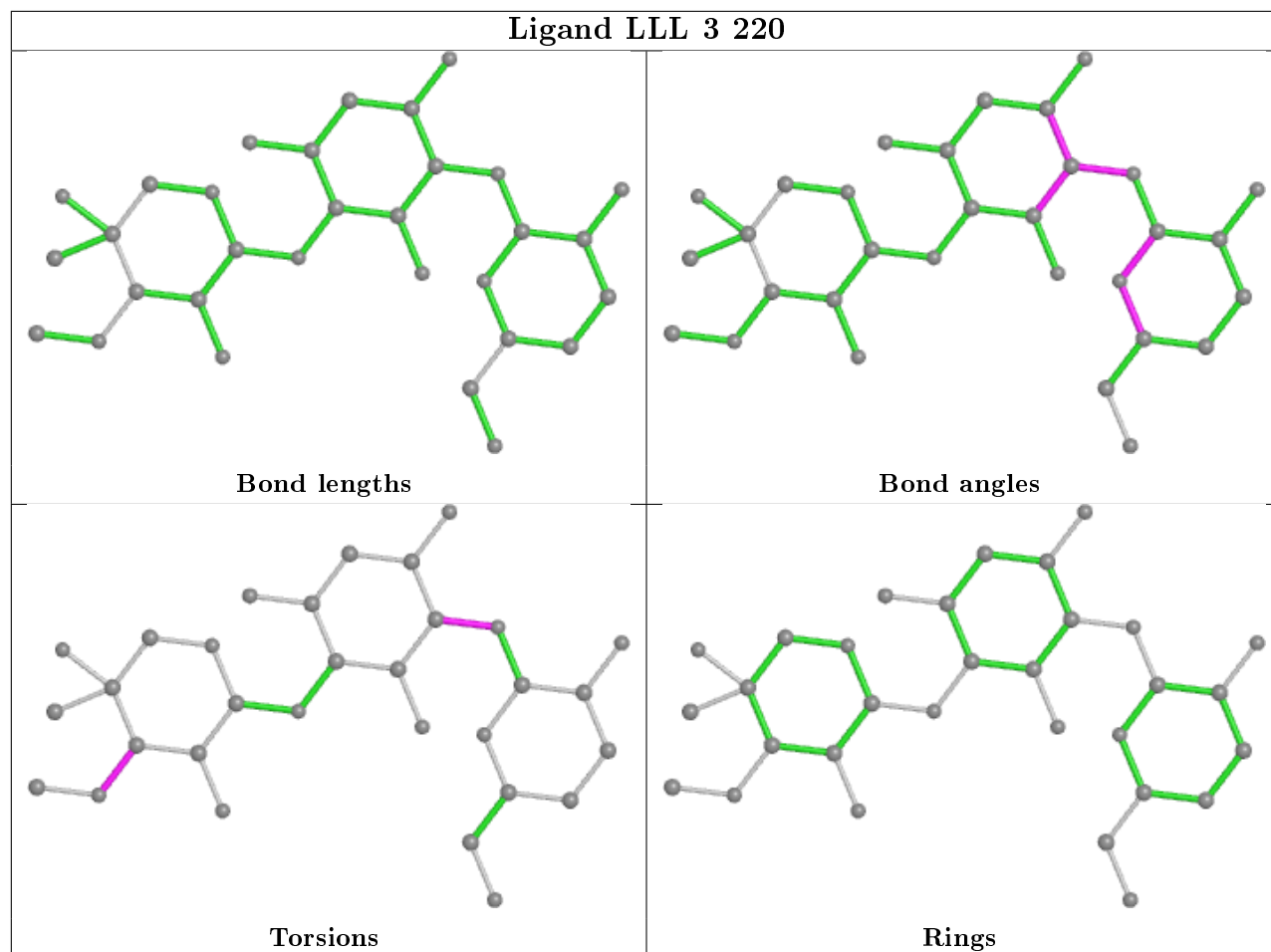
Bond angles

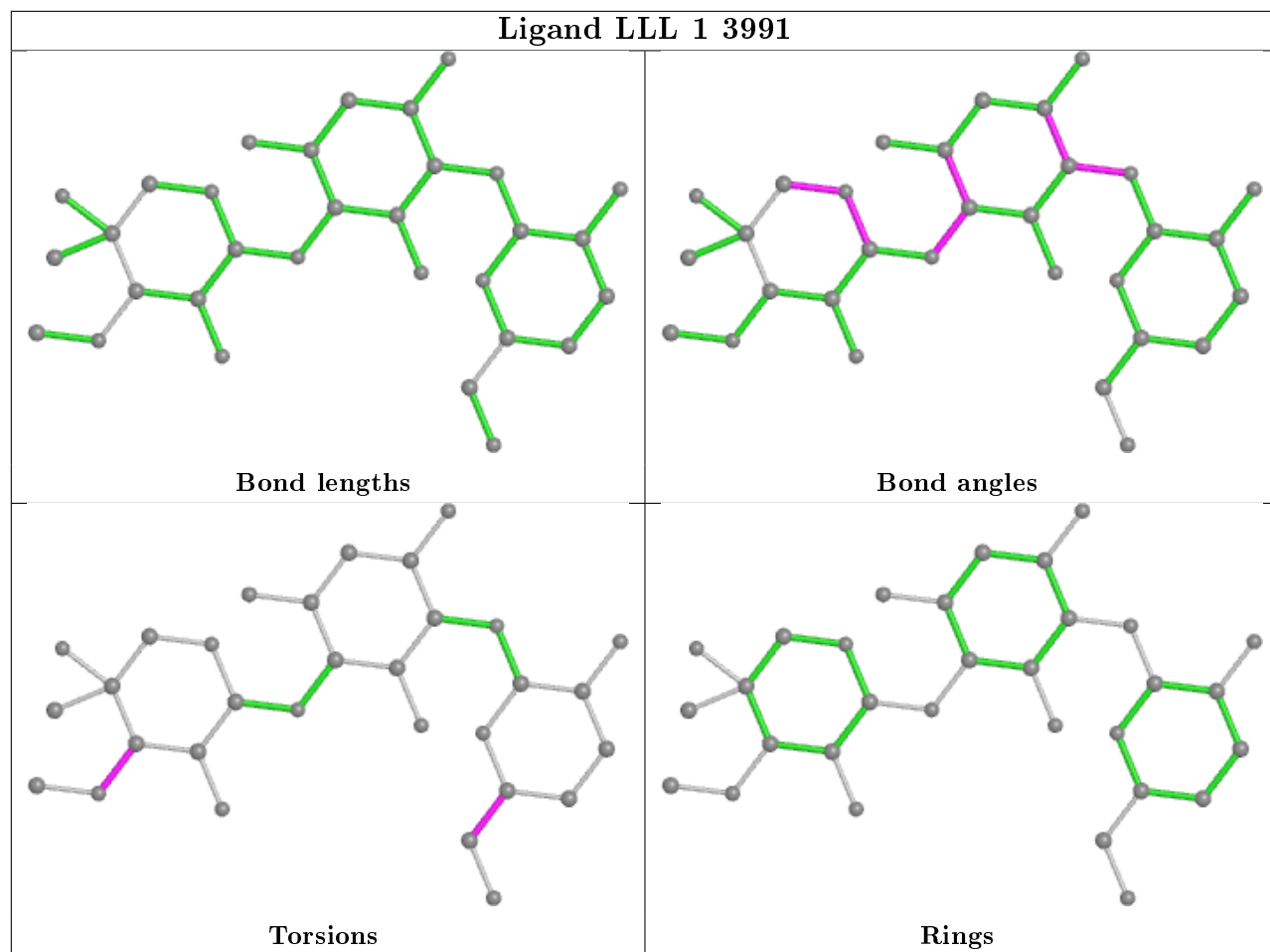


Torsions

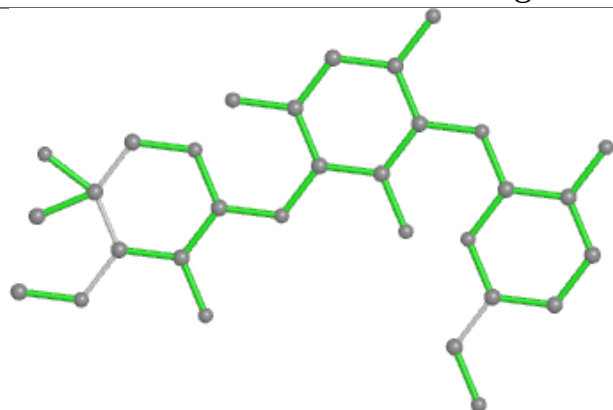


Rings

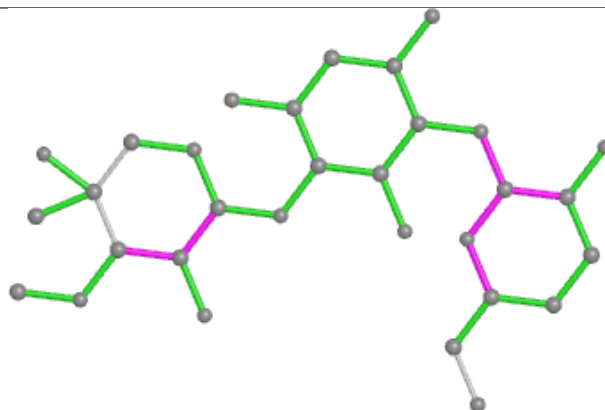




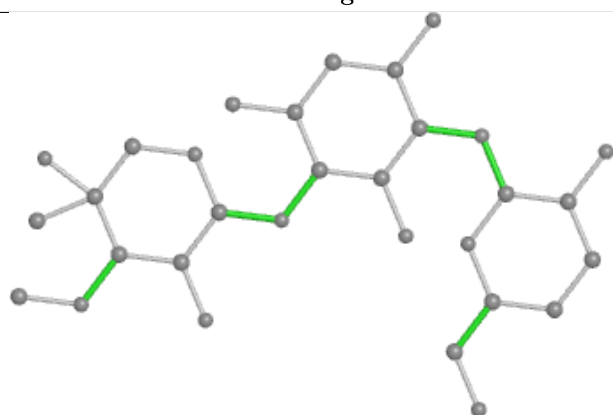
## Ligand LLL 5 4168



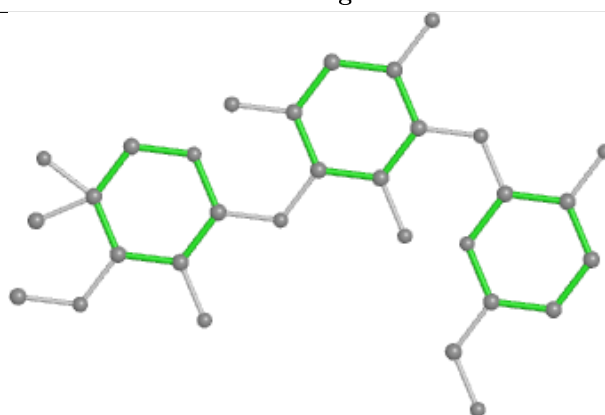
Bond lengths



Bond angles

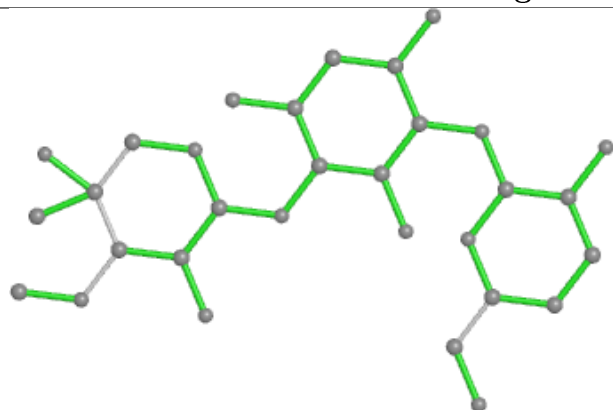


Torsions

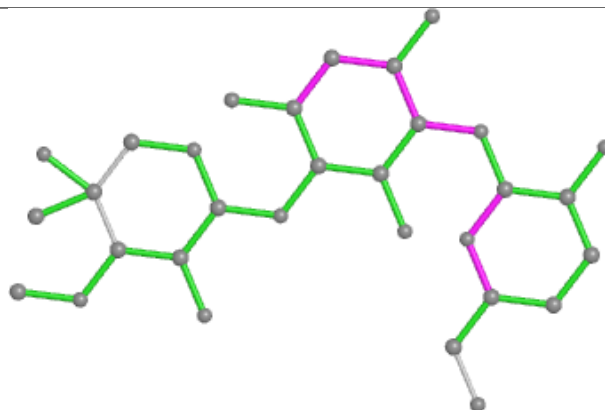


Rings

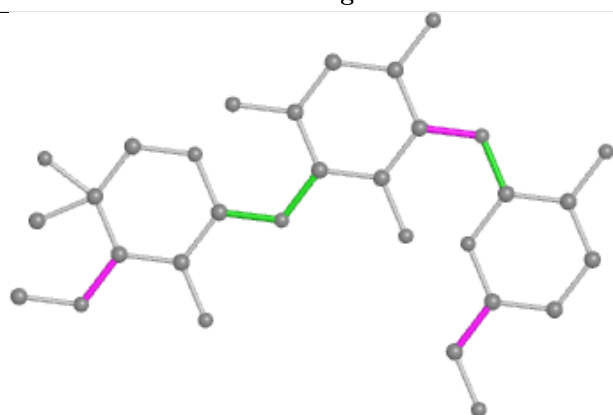
## Ligand LLL 6 2166



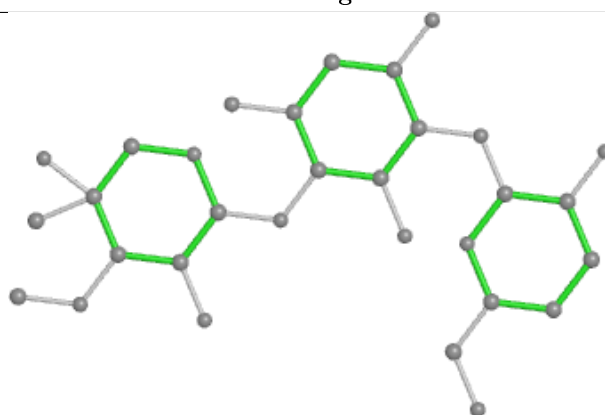
Bond lengths



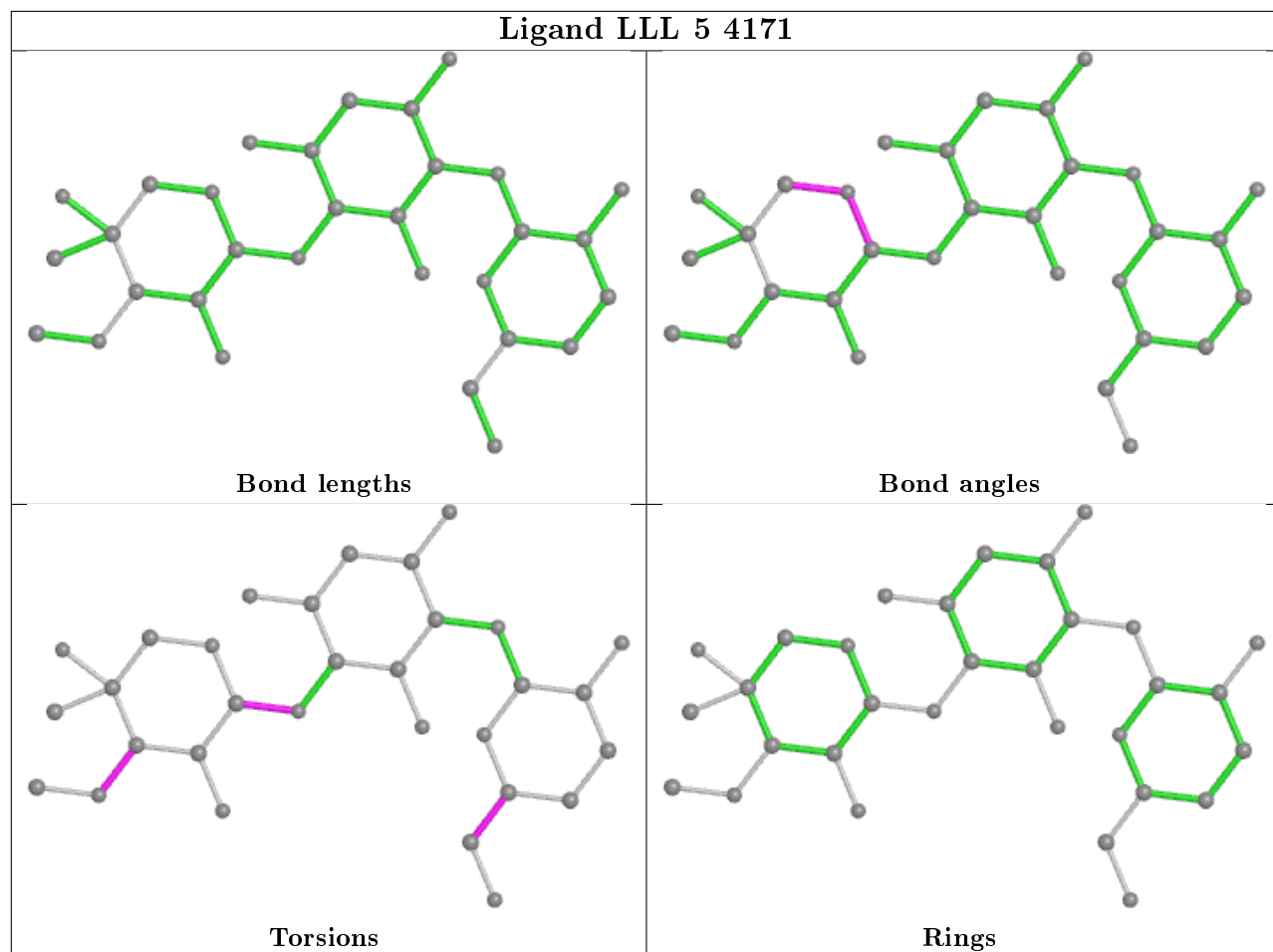
Bond angles



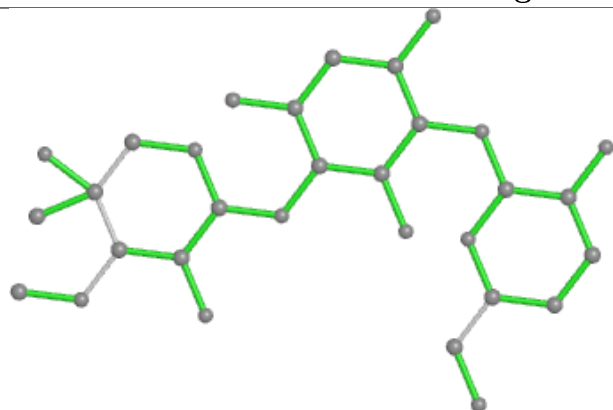
Torsions



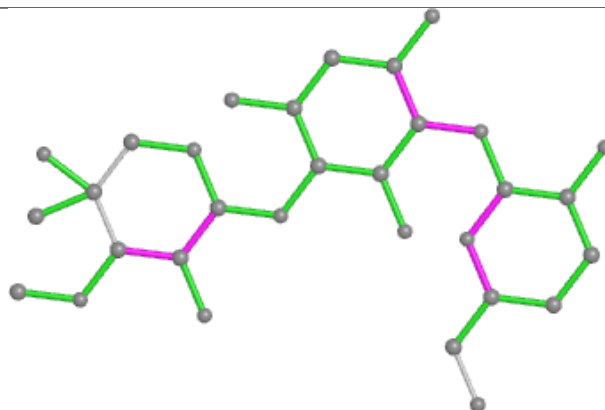
Rings



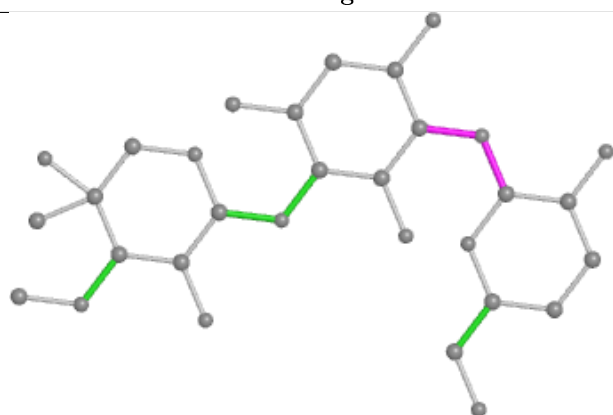
## Ligand LLL 1 3989



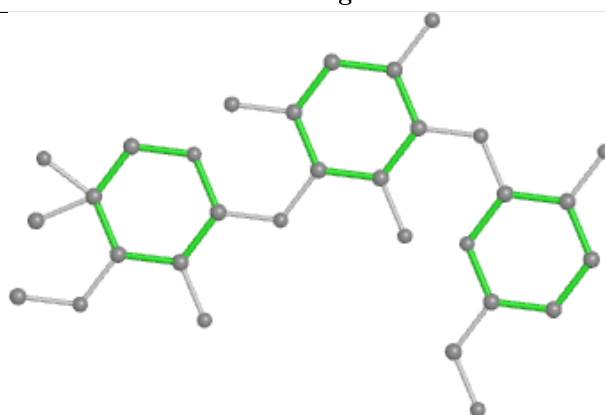
Bond lengths



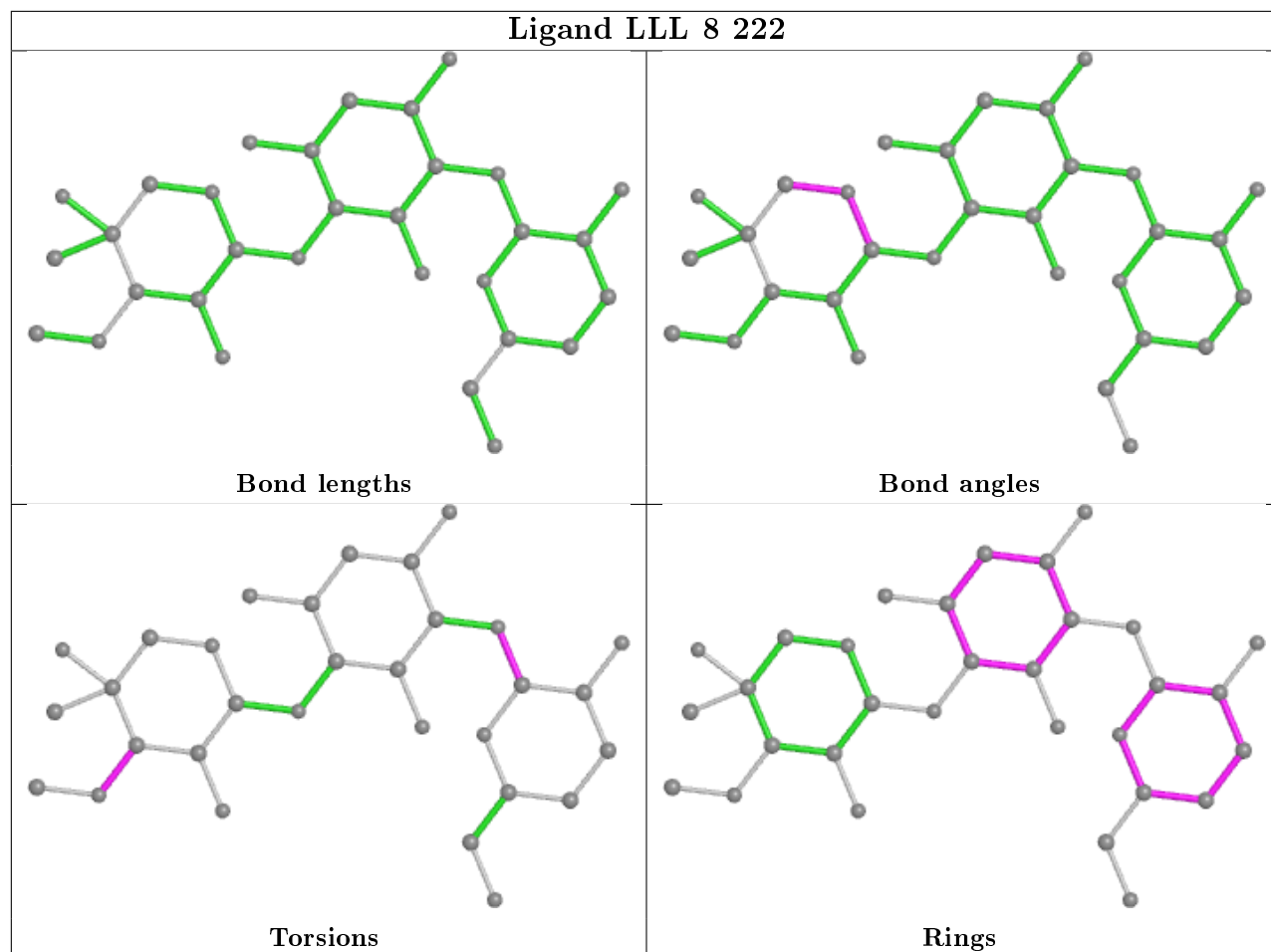
Bond angles



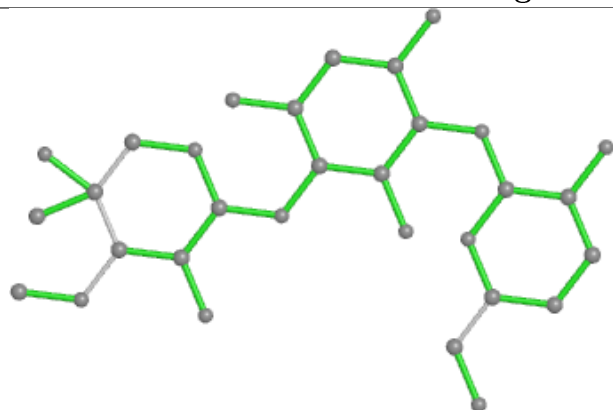
Torsions



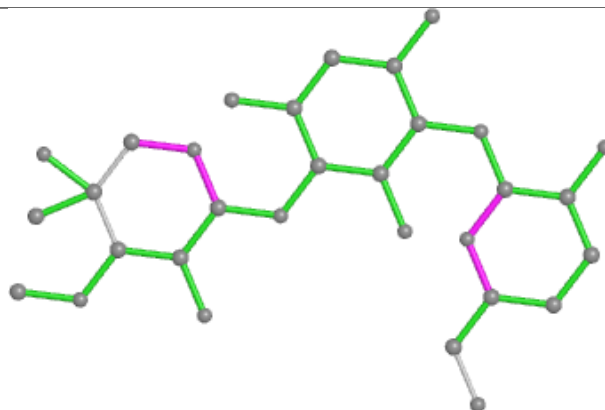
Rings



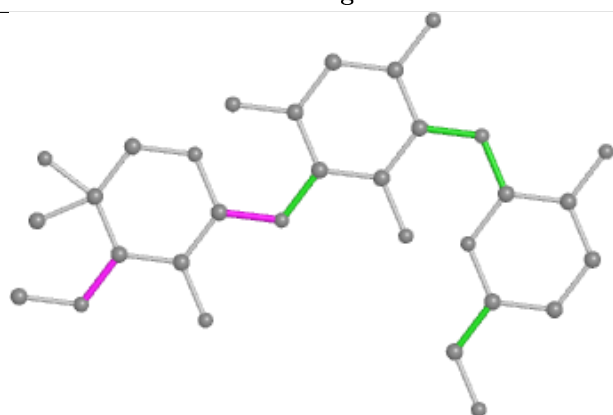
## Ligand LLL 5 4166



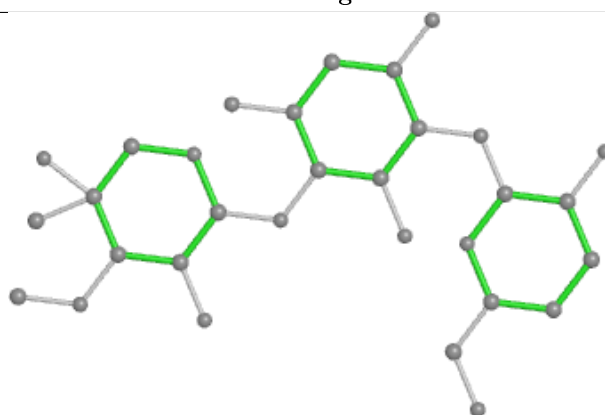
Bond lengths



Bond angles

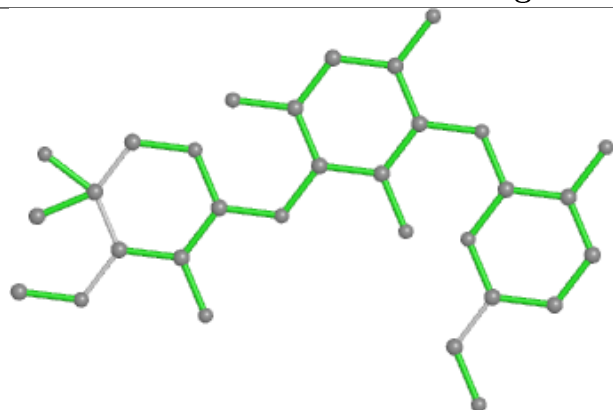


Torsions

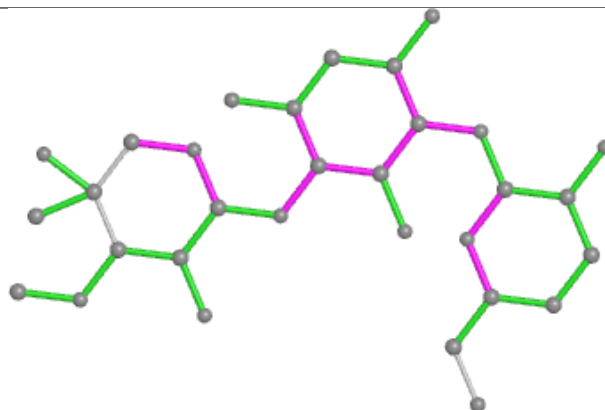


Rings

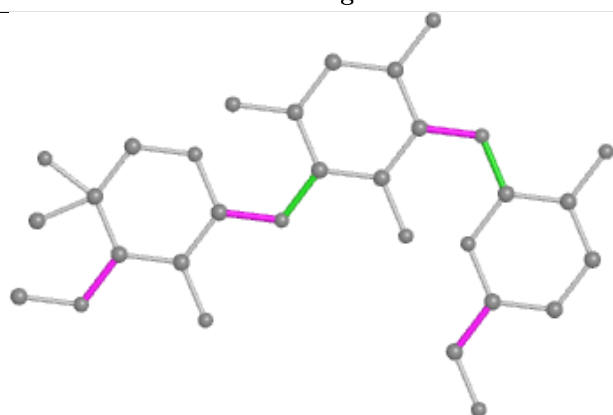
## Ligand LLL 5 4158



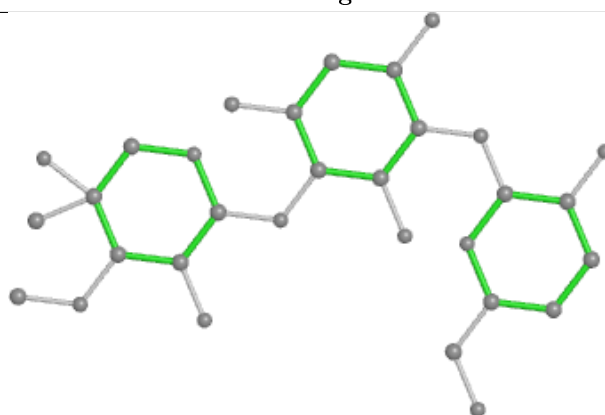
Bond lengths



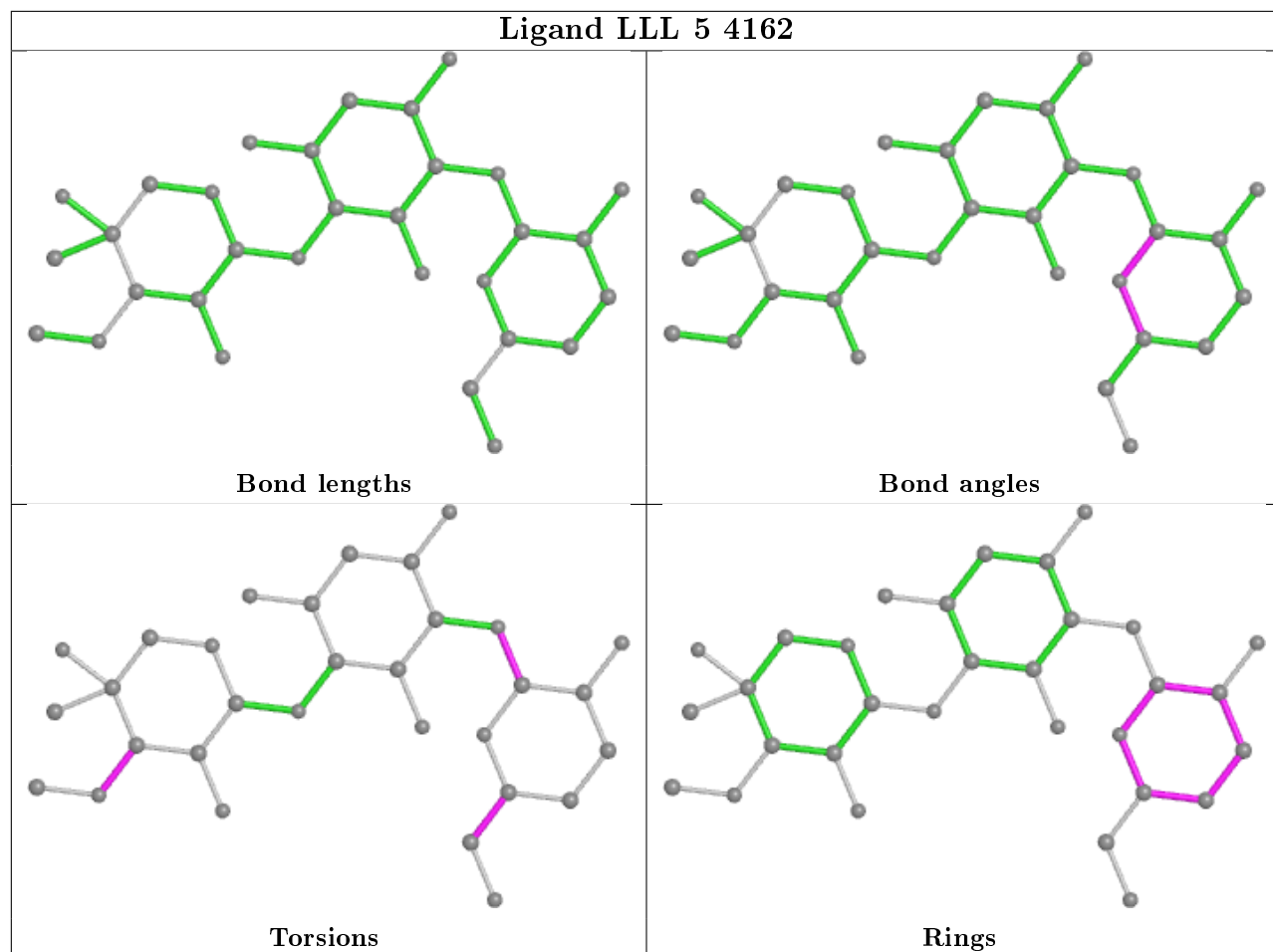
Bond angles

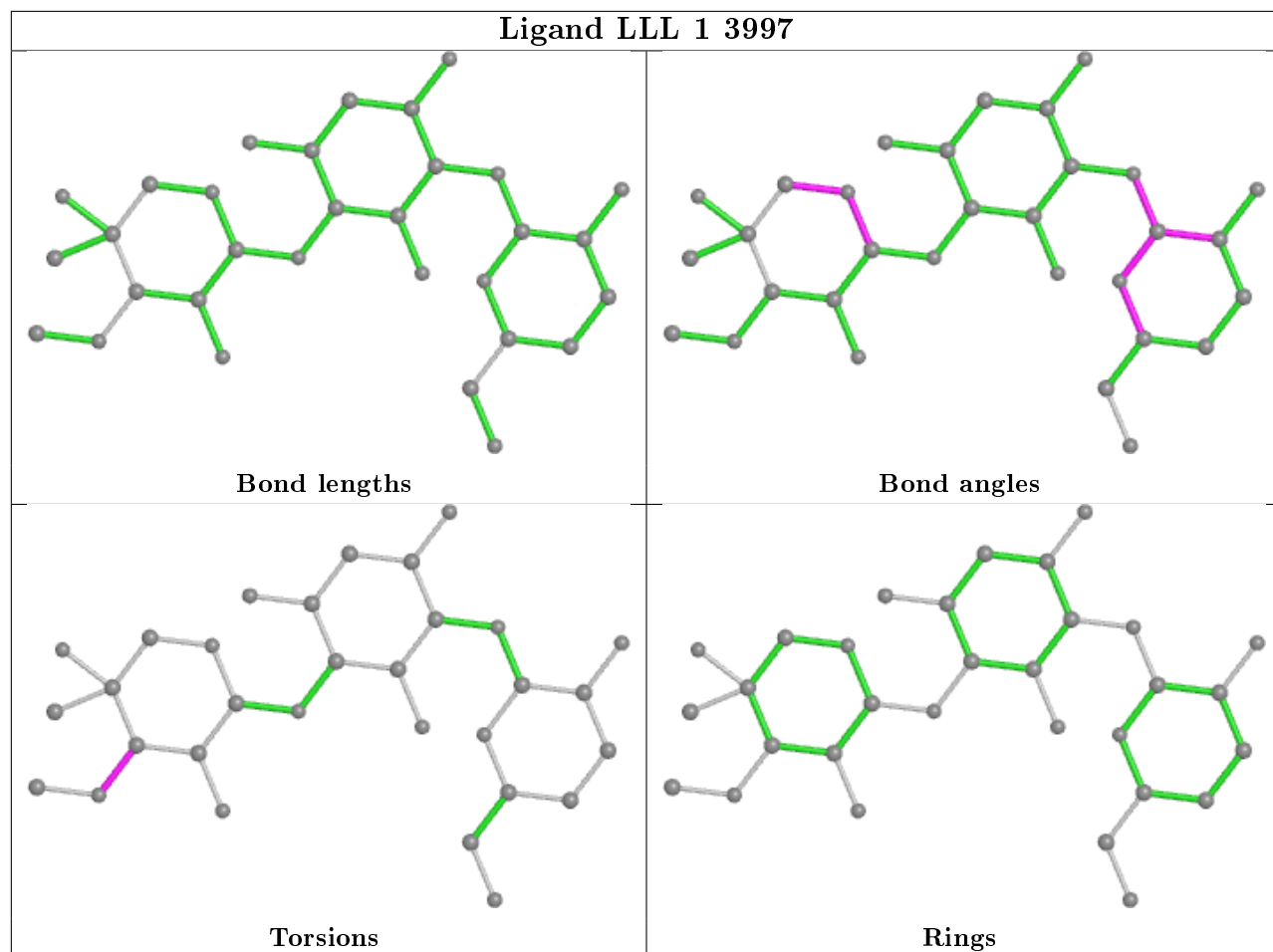


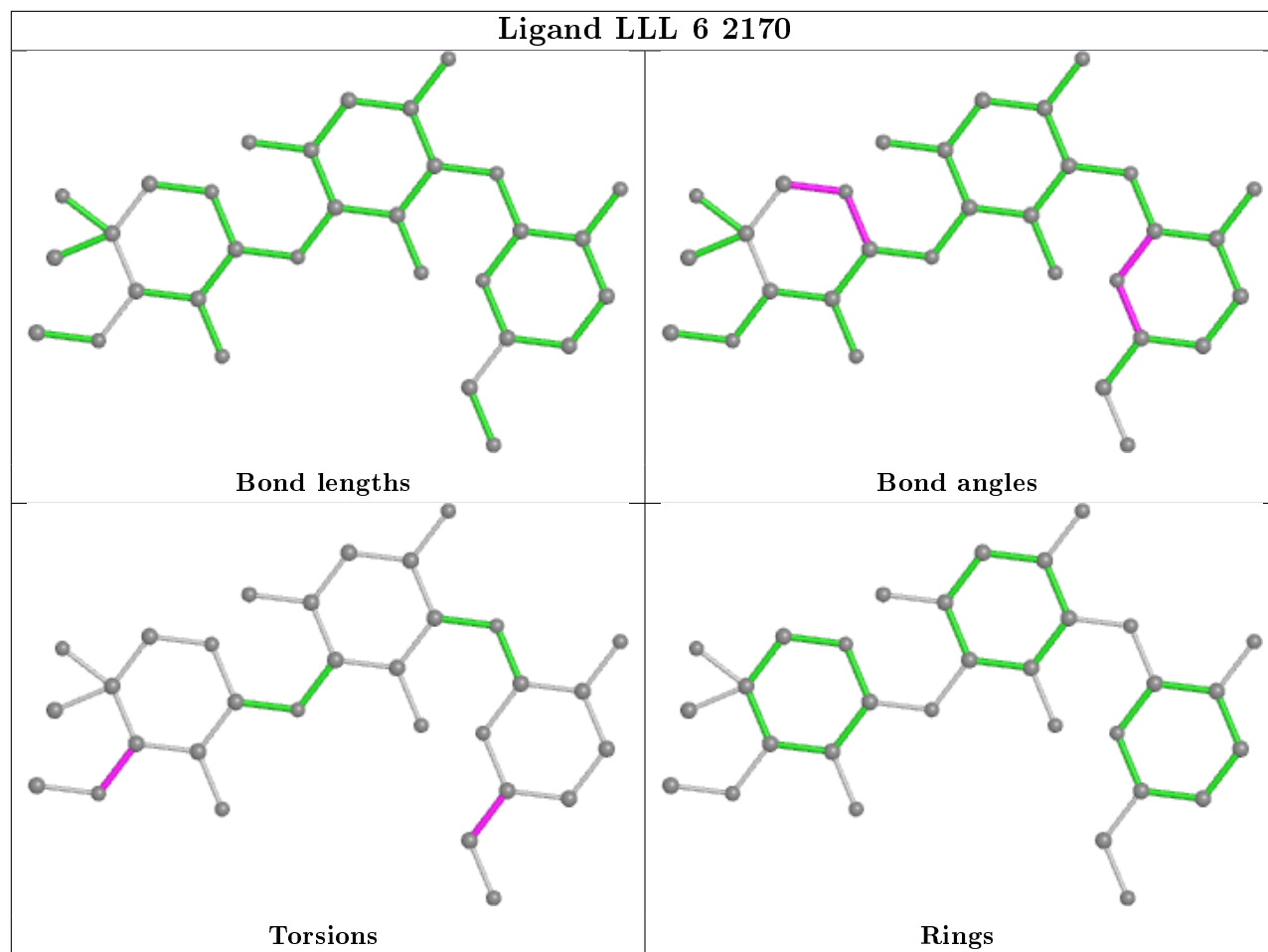
Torsions



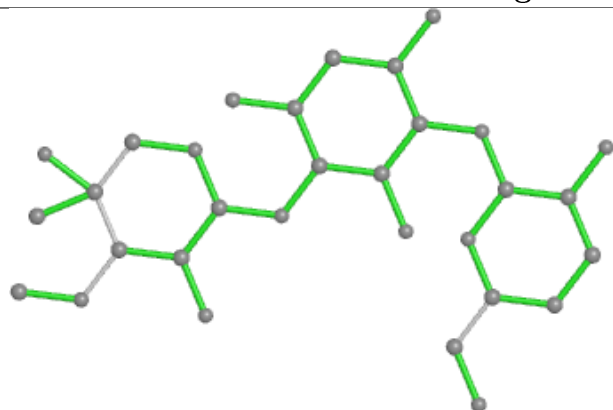
Rings



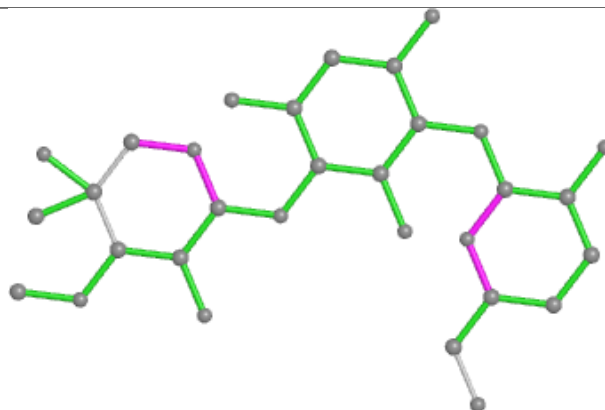




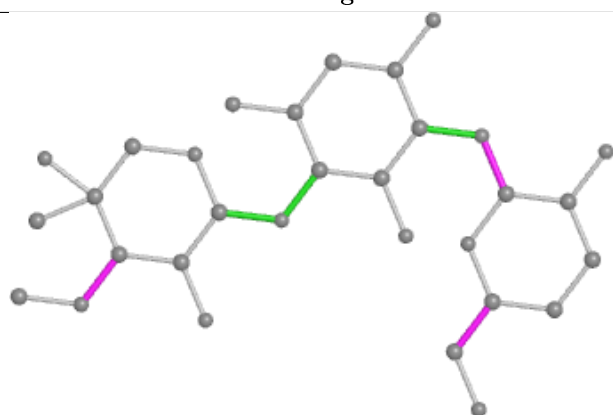
## Ligand LLL 6 2172



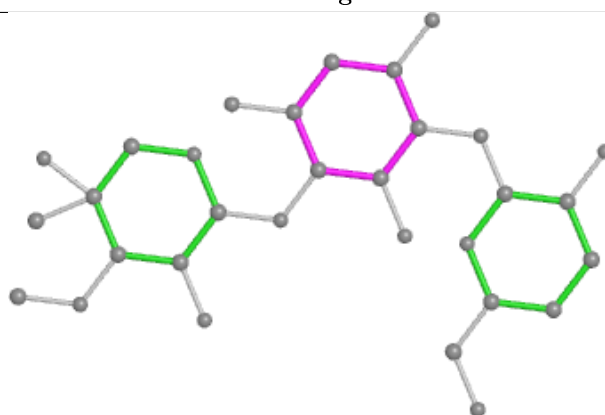
Bond lengths



Bond angles

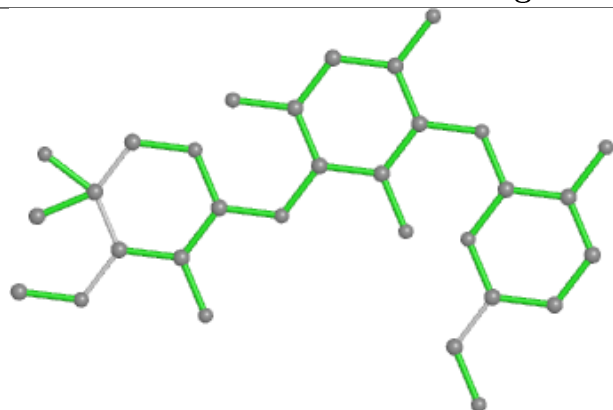


Torsions

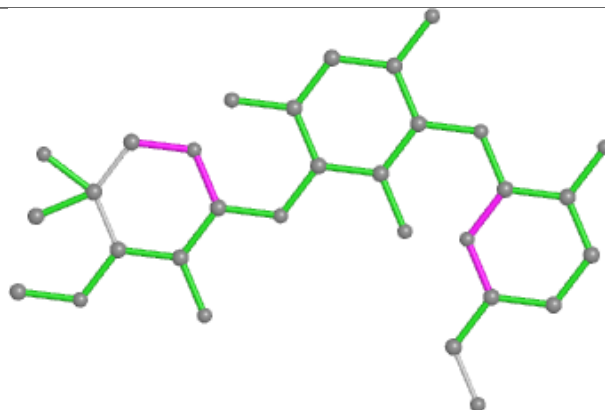


Rings

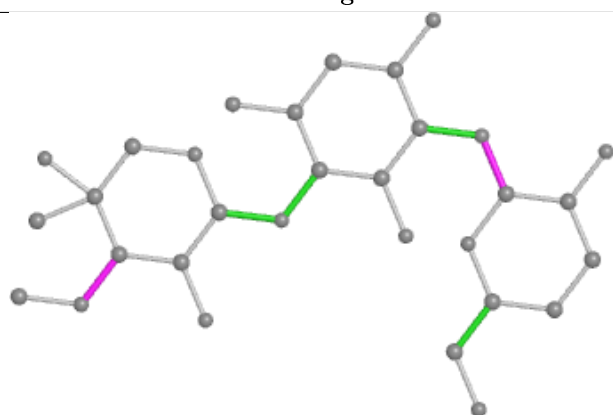
## Ligand LLL 6 2164



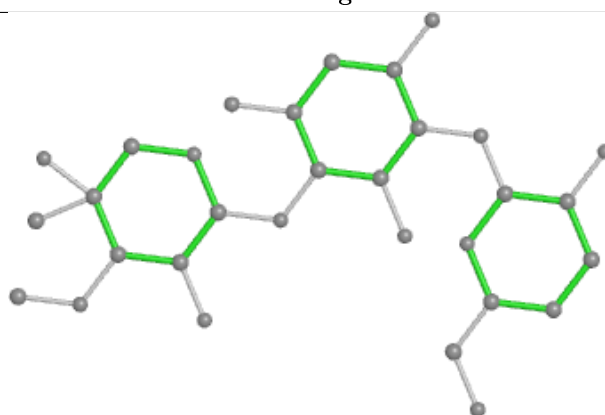
Bond lengths



Bond angles

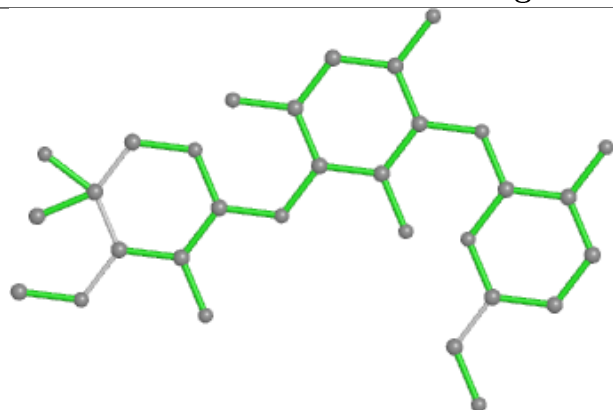


Torsions

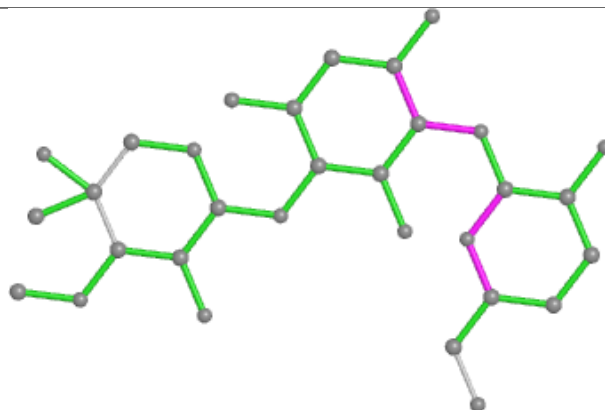


Rings

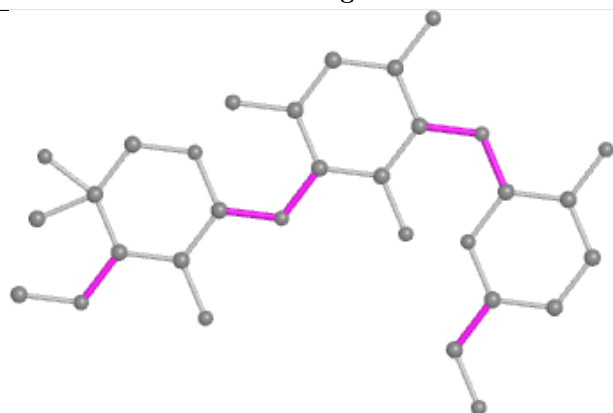
## Ligand LLL 5 4151



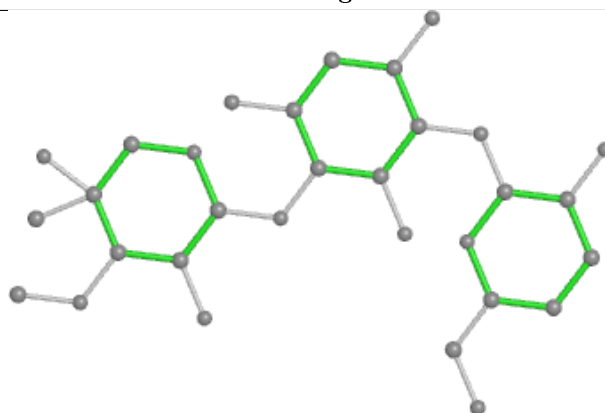
Bond lengths



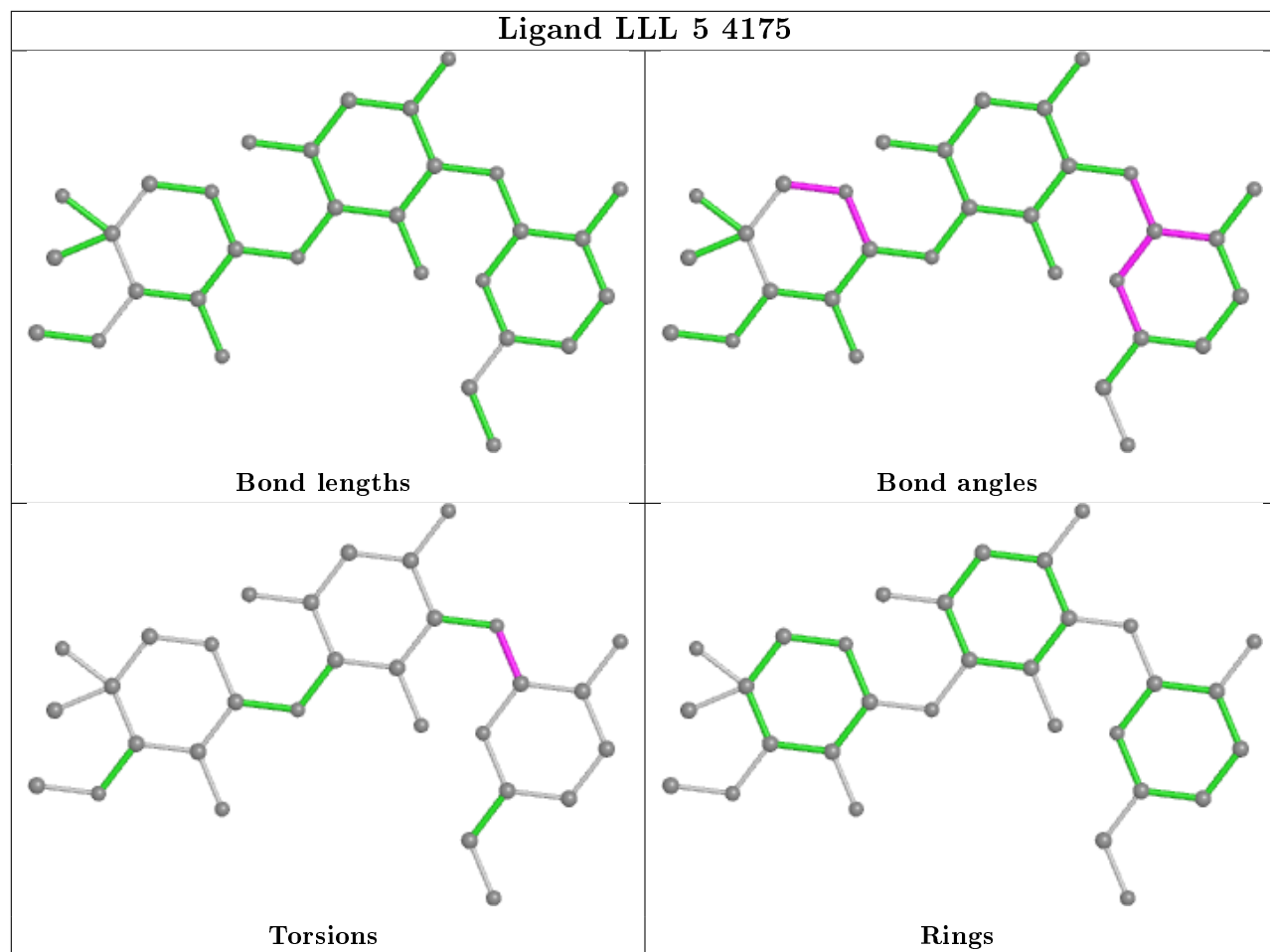
Bond angles

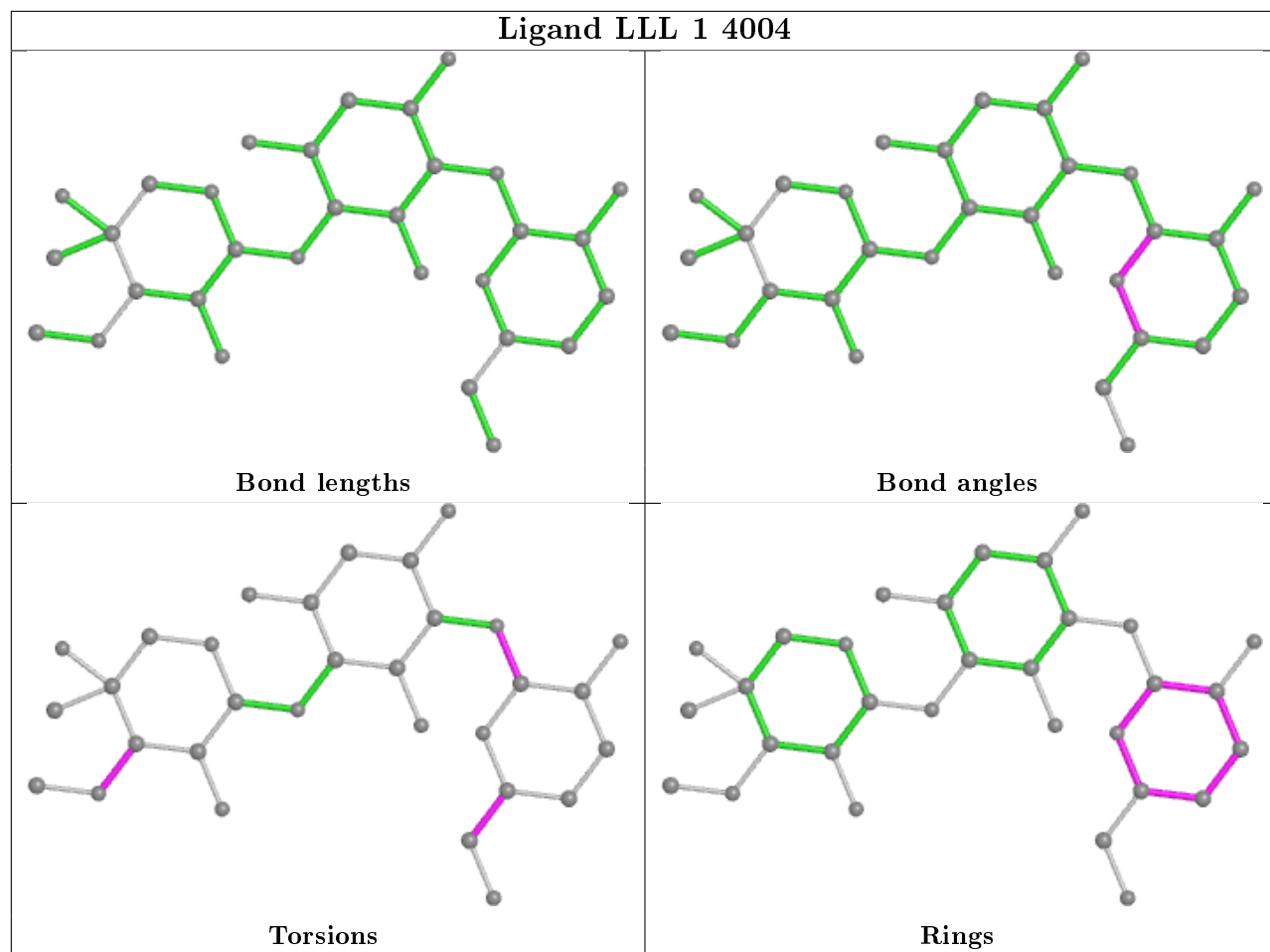


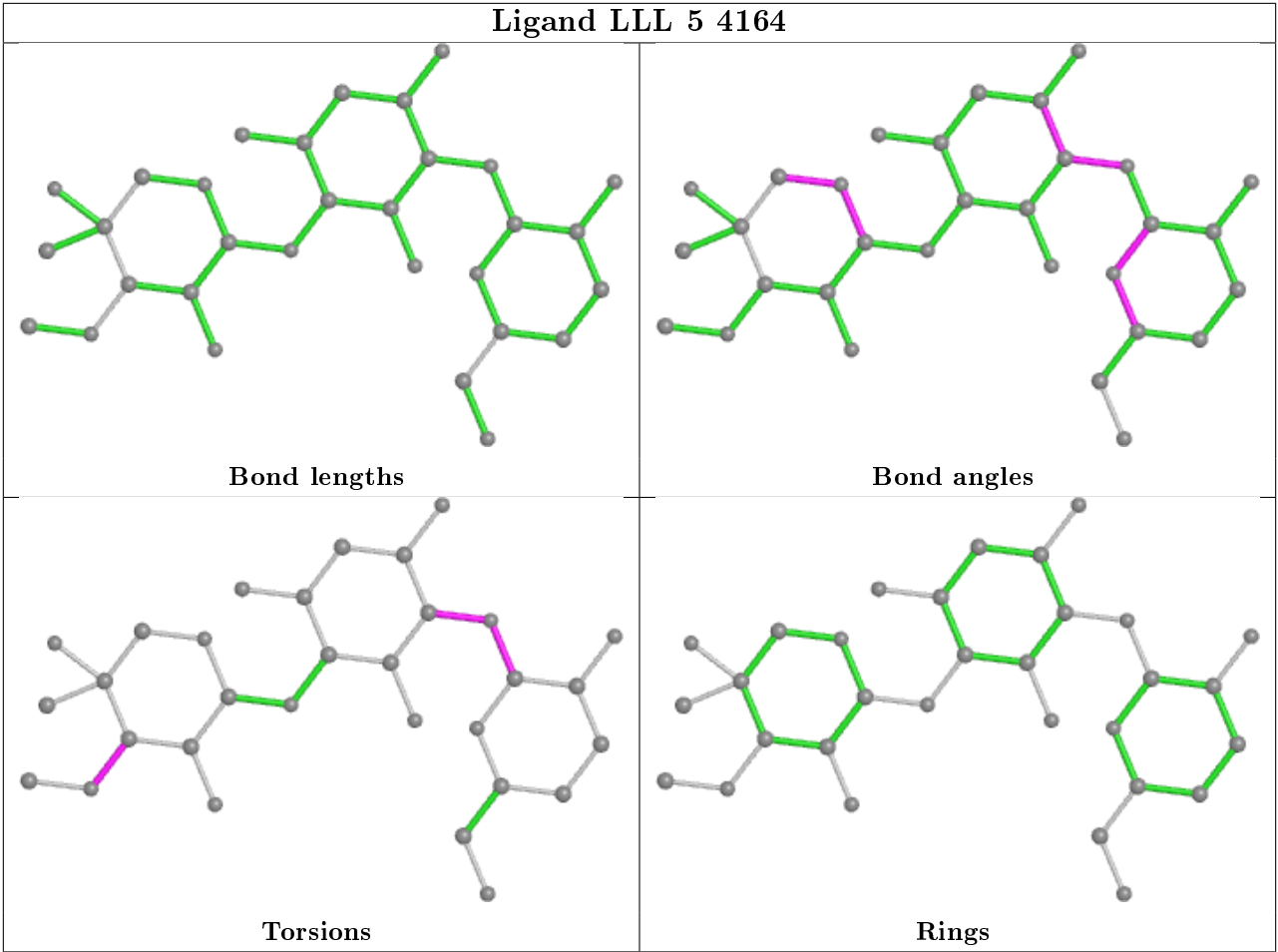
Torsions



Rings







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	m2	2
51	S5	1
10	l8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m2	23:UNK	C	28:UNK	N	6.26
1	m2	52:UNK	C	54:UNK	N	3.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S5	21:THR	C	22:PRO	N	1.72
1	l8	51:LYS	C	52:TRP	N	1.16

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	3100/3396 (91%)	0.02	23 (0%) 87 87	47, 83, 190, 354	0
1	5	3134/3396 (92%)	0.06	13 (0%) 92 92	37, 76, 173, 292	0
2	3	121/121 (100%)	-0.29	0 100 100	58, 107, 135, 155	0
2	7	121/121 (100%)	-0.24	0 100 100	45, 72, 94, 160	0
3	4	156/158 (98%)	-0.02	0 100 100	54, 94, 152, 260	0
3	8	158/158 (100%)	0.02	0 100 100	61, 102, 164, 234	0
4	L2	252/252 (100%)	0.40	7 (2%) 53 51	51, 88, 124, 174	0
4	12	252/252 (100%)	0.48	6 (2%) 59 57	51, 84, 121, 177	0
5	L3	386/386 (100%)	0.22	3 (0%) 86 85	41, 77, 104, 170	0
5	13	386/386 (100%)	0.08	1 (0%) 94 93	34, 60, 91, 165	0
6	L4	361/361 (100%)	0.19	0 100 100	45, 85, 119, 142	0
6	14	361/361 (100%)	0.23	6 (1%) 70 68	44, 90, 128, 167	0
7	L5	296/296 (100%)	0.59	22 (7%) 14 16	74, 120, 162, 214	0
7	15	294/296 (99%)	0.21	5 (1%) 70 68	51, 80, 124, 155	0
8	L6	156/176 (88%)	0.14	1 (0%) 89 89	61, 84, 119, 149	0
8	16	157/176 (89%)	0.18	1 (0%) 89 89	53, 81, 129, 204	0
9	L7	222/223 (99%)	0.14	3 (1%) 75 74	47, 76, 119, 219	0
9	17	223/223 (100%)	0.03	0 100 100	39, 66, 123, 205	0
10	L8	233/233 (100%)	0.96	32 (13%) 3 3	96, 131, 183, 250	0
10	18	231/233 (99%)	0.95	38 (16%) 1 2	96, 137, 184, 229	0
11	L9	191/191 (100%)	0.35	6 (3%) 49 48	60, 91, 121, 162	0
11	19	191/191 (100%)	0.00	1 (0%) 91 90	41, 60, 92, 148	0
12	M0	212/221 (95%)	0.34	7 (3%) 46 45	52, 84, 129, 242	0
12	m0	211/221 (95%)	0.24	4 (1%) 66 65	32, 65, 120, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M1	169/169 (100%)	1.06	32 (18%) 1 1	88, 124, 153, 166	0
13	m1	169/169 (100%)	0.16	1 (0%) 89 89	51, 77, 104, 125	0
14	M3	193/194 (99%)	0.55	12 (6%) 20 21	55, 102, 161, 213	0
14	m3	194/194 (100%)	0.59	16 (8%) 11 13	53, 113, 167, 220	0
15	M4	136/137 (99%)	0.25	2 (1%) 73 72	61, 88, 115, 151	0
15	m4	137/137 (100%)	-0.10	1 (0%) 87 87	45, 67, 96, 170	0
16	M5	203/203 (100%)	0.79	19 (9%) 8 10	52, 88, 116, 130	0
16	m5	203/203 (100%)	0.88	19 (9%) 8 10	58, 97, 120, 136	0
17	M6	197/197 (100%)	0.14	1 (0%) 91 90	45, 64, 104, 140	0
17	m6	197/197 (100%)	-0.08	0 100 100	34, 50, 93, 123	0
18	M7	183/184 (99%)	0.91	25 (13%) 3 3	50, 70, 209, 262	0
18	m7	155/184 (84%)	0.12	1 (0%) 89 89	49, 67, 96, 136	0
19	M8	185/185 (100%)	0.48	3 (1%) 72 70	62, 83, 102, 160	0
19	m8	185/185 (100%)	0.42	3 (1%) 72 70	47, 83, 108, 135	0
20	M9	182/188 (96%)	0.42	7 (3%) 40 39	77, 106, 198, 250	0
20	m9	188/188 (100%)	0.46	11 (5%) 22 23	63, 95, 190, 264	0
21	N0	172/172 (100%)	0.56	12 (6%) 16 18	59, 80, 108, 150	0
21	n0	172/172 (100%)	0.08	2 (1%) 79 77	40, 57, 88, 123	0
22	N1	159/159 (100%)	0.53	8 (5%) 28 29	56, 84, 149, 195	0
22	n1	159/159 (100%)	0.32	5 (3%) 49 48	43, 68, 130, 165	0
23	N2	100/100 (100%)	0.79	14 (14%) 2 3	115, 150, 198, 212	0
23	n2	98/100 (98%)	1.42	26 (26%) 0 0	92, 136, 165, 200	0
24	N3	136/136 (100%)	0.41	4 (2%) 51 50	47, 75, 111, 159	0
24	n3	136/136 (100%)	0.44	2 (1%) 73 72	34, 55, 87, 130	0
25	N4	98/155 (63%)	1.76	27 (27%) 0 0	67, 97, 245, 294	0
26	N5	121/121 (100%)	0.92	12 (9%) 7 8	76, 107, 137, 228	0
26	n5	120/121 (99%)	0.69	9 (7%) 14 16	73, 116, 150, 171	0
27	N6	126/126 (100%)	0.98	15 (11%) 4 5	60, 96, 132, 163	0
27	n6	126/126 (100%)	0.73	11 (8%) 10 12	75, 110, 146, 183	0
28	N7	135/135 (100%)	2.24	70 (51%) 0 0	114, 145, 176, 223	0
28	n7	135/135 (100%)	1.48	36 (26%) 0 0	106, 144, 172, 207	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	N8	148/148 (100%)	0.74	21 (14%) 2 3	46, 84, 125, 154	0
29	n8	148/148 (100%)	0.40	6 (4%) 37 36	46, 85, 128, 156	0
30	N9	58/58 (100%)	0.75	8 (13%) 2 3	50, 90, 159, 165	0
30	n9	58/58 (100%)	0.36	1 (1%) 70 68	43, 87, 136, 176	0
31	O0	97/100 (97%)	0.79	13 (13%) 3 4	96, 132, 178, 188	0
31	o0	100/100 (100%)	0.61	8 (8%) 12 13	93, 124, 178, 229	0
32	O1	109/109 (100%)	1.04	12 (11%) 5 6	65, 92, 156, 210	0
32	o1	109/109 (100%)	0.58	5 (4%) 32 32	57, 80, 146, 186	0
33	O2	127/127 (100%)	0.14	3 (2%) 59 57	42, 67, 95, 128	0
33	o2	127/127 (100%)	0.13	1 (0%) 86 85	42, 76, 105, 157	0
34	O3	106/106 (100%)	0.11	0 100 100	51, 68, 106, 147	0
34	o3	106/106 (100%)	0.07	0 100 100	41, 60, 94, 133	0
35	O4	112/112 (100%)	0.85	15 (13%) 3 4	73, 114, 163, 223	0
35	o4	112/112 (100%)	0.60	8 (7%) 16 18	69, 104, 163, 198	0
36	O5	119/119 (100%)	0.61	5 (4%) 36 35	81, 111, 140, 163	0
36	o5	119/119 (100%)	0.60	5 (4%) 36 35	78, 123, 152, 162	0
37	O6	99/99 (100%)	0.44	7 (7%) 16 18	85, 111, 160, 197	0
37	o6	99/99 (100%)	0.88	15 (15%) 2 2	89, 117, 162, 193	0
38	O7	87/87 (100%)	0.32	2 (2%) 60 59	56, 76, 125, 211	0
38	o7	87/87 (100%)	0.47	2 (2%) 60 59	54, 82, 153, 163	0
39	O8	77/77 (100%)	0.79	9 (11%) 4 5	114, 147, 172, 230	0
39	o8	77/77 (100%)	1.37	22 (28%) 0 0	106, 136, 170, 181	0
40	O9	50/50 (100%)	0.50	2 (4%) 38 37	63, 84, 106, 116	0
40	o9	50/50 (100%)	0.48	1 (2%) 65 64	70, 91, 106, 108	0
41	Q0	52/52 (100%)	0.81	6 (11%) 4 5	61, 79, 108, 126	0
41	q0	52/52 (100%)	0.14	0 100 100	37, 51, 72, 118	0
42	Q1	25/25 (100%)	0.49	0 100 100	71, 84, 103, 104	0
42	q1	25/25 (100%)	-0.03	0 100 100	55, 70, 90, 100	0
43	Q2	105/105 (100%)	0.72	11 (10%) 6 7	59, 84, 123, 165	0
43	q2	105/105 (100%)	0.19	1 (0%) 82 81	45, 74, 105, 179	0
44	Q3	91/91 (100%)	0.26	2 (2%) 62 60	54, 96, 128, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	q3	91/91 (100%)	0.25	0	100	100	44, 85, 112, 130	0
45	2	1712/1800 (95%)	-0.02	23 (1%)	77	76	70, 132, 242, 320	0
45	6	1739/1800 (96%)	-0.05	22 (1%)	77	76	49, 95, 249, 344	0
46	S0	206/206 (100%)	1.38	57 (27%)	0	0	109, 161, 224, 271	0
46	s0	206/206 (100%)	0.54	10 (4%)	29	29	81, 124, 166, 215	0
47	S1	214/216 (99%)	1.07	47 (21%)	0	1	114, 173, 227, 252	0
47	s1	216/216 (100%)	0.59	18 (8%)	11	13	81, 117, 159, 193	0
48	S2	217/217 (100%)	0.89	31 (14%)	2	3	84, 131, 171, 200	0
48	s2	217/217 (100%)	0.49	12 (5%)	25	25	71, 104, 138, 174	0
49	S3	223/223 (100%)	1.21	48 (21%)	0	1	82, 139, 193, 260	0
49	s3	223/223 (100%)	0.89	29 (13%)	3	4	78, 116, 163, 223	0
50	S4	260/260 (100%)	1.46	84 (32%)	0	0	97, 142, 169, 225	0
50	s4	260/260 (100%)	0.86	38 (14%)	2	3	72, 127, 165, 189	0
51	S5	206/206 (100%)	1.64	56 (27%)	0	0	131, 172, 213, 237	0
51	s5	206/206 (100%)	0.49	13 (6%)	20	21	64, 97, 147, 197	0
52	S6	226/236 (95%)	0.88	30 (13%)	3	4	82, 145, 214, 373	0
52	s6	218/236 (92%)	0.69	18 (8%)	11	13	73, 120, 168, 213	0
53	S7	184/186 (98%)	0.96	29 (15%)	2	2	115, 179, 224, 251	0
53	s7	186/186 (100%)	0.77	21 (11%)	5	6	99, 157, 207, 271	0
54	S8	188/200 (94%)	1.59	64 (34%)	0	0	84, 125, 176, 199	0
54	s8	186/200 (93%)	0.73	20 (10%)	5	7	70, 113, 164, 198	0
55	S9	185/185 (100%)	1.51	59 (31%)	0	0	111, 152, 192, 244	0
55	s9	185/185 (100%)	0.83	20 (10%)	5	7	87, 134, 188, 215	0
56	C0	96/105 (91%)	1.32	25 (26%)	0	0	127, 170, 212, 235	0
56	c0	96/105 (91%)	1.22	21 (21%)	0	1	93, 137, 193, 217	0
57	C1	155/156 (99%)	1.90	61 (39%)	0	0	84, 122, 201, 267	0
57	c1	142/156 (91%)	0.98	14 (9%)	7	8	69, 111, 169, 198	0
58	C2	124/143 (86%)	2.47	62 (50%)	0	0	175, 223, 267, 294	0
58	c2	124/143 (86%)	1.74	51 (41%)	0	0	132, 190, 233, 259	0
59	C3	150/150 (100%)	0.72	12 (8%)	12	13	95, 139, 177, 206	0
59	c3	150/150 (100%)	0.10	2 (1%)	77	76	67, 111, 148, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	C4	127/128 (99%)	1.16	37 (29%) 0 0	93, 164, 207, 215	0
60	c4	128/128 (100%)	0.81	11 (8%) 10 12	63, 103, 135, 156	0
61	C5	124/141 (87%)	1.25	35 (28%) 0 0	108, 165, 211, 236	0
61	c5	135/141 (95%)	0.40	7 (5%) 27 27	61, 96, 162, 201	0
62	C6	141/142 (99%)	1.94	56 (39%) 0 0	105, 157, 196, 212	0
62	c6	142/142 (100%)	0.38	4 (2%) 53 51	59, 91, 128, 197	0
63	C7	120/136 (88%)	1.34	31 (25%) 0 0	110, 161, 290, 384	0
63	c7	117/136 (86%)	0.58	8 (6%) 17 19	81, 123, 194, 239	0
64	C8	145/145 (100%)	1.46	51 (35%) 0 0	102, 165, 211, 235	0
64	c8	145/145 (100%)	0.02	2 (1%) 75 74	64, 82, 128, 184	0
65	C9	143/143 (100%)	1.17	31 (21%) 0 1	128, 159, 204, 232	0
65	c9	143/143 (100%)	0.18	3 (2%) 63 62	61, 84, 117, 154	0
66	D0	107/110 (97%)	1.38	29 (27%) 0 0	101, 156, 232, 270	0
66	d0	110/110 (100%)	1.31	30 (27%) 0 0	68, 121, 203, 223	0
67	D1	87/87 (100%)	1.47	26 (29%) 0 0	112, 151, 183, 198	0
67	d1	87/87 (100%)	0.48	7 (8%) 12 13	87, 117, 158, 188	0
68	D2	129/129 (100%)	1.09	28 (21%) 0 1	99, 127, 155, 176	0
68	d2	129/129 (100%)	0.64	5 (3%) 39 38	74, 99, 120, 137	0
69	D3	144/144 (100%)	0.77	16 (11%) 5 6	76, 102, 127, 174	0
69	d3	144/144 (100%)	0.08	1 (0%) 87 87	51, 73, 99, 157	0
70	D4	134/134 (100%)	1.13	27 (20%) 1 1	106, 152, 191, 215	0
70	d4	133/134 (99%)	0.61	15 (11%) 5 6	80, 134, 173, 195	0
71	D5	70/70 (100%)	2.72	48 (68%) 0 0	151, 189, 233, 266	0
71	d5	69/70 (98%)	0.48	3 (4%) 35 35	77, 108, 142, 162	0
72	D6	97/97 (100%)	1.20	25 (25%) 0 0	86, 126, 189, 239	0
72	d6	97/97 (100%)	0.31	2 (2%) 63 62	63, 88, 136, 238	0
73	D7	81/81 (100%)	1.67	34 (41%) 0 0	117, 161, 215, 267	0
73	d7	81/81 (100%)	0.69	10 (12%) 4 5	92, 124, 199, 227	0
74	D8	63/63 (100%)	1.96	29 (46%) 0 0	136, 175, 215, 257	0
74	d8	63/63 (100%)	1.33	17 (26%) 0 0	81, 117, 146, 165	0
75	D9	53/53 (100%)	1.31	16 (30%) 0 0	104, 128, 154, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	d9	53/53 (100%)	0.57	5 (9%) 8 10	64, 86, 109, 148	0
76	E0	60/62 (96%)	1.42	18 (30%) 0 0	98, 144, 215, 237	0
76	e0	62/62 (100%)	0.65	6 (9%) 7 9	64, 118, 179, 202	0
77	E1	71/72 (98%)	1.71	23 (32%) 0 0	143, 199, 243, 257	0
77	e1	72/72 (100%)	1.32	21 (29%) 0 0	125, 174, 212, 236	0
78	SR	318/318 (100%)	2.13	148 (46%) 0 0	131, 175, 225, 269	0
78	sR	318/318 (100%)	0.88	48 (15%) 2 2	88, 125, 174, 226	0
79	SM	159/272 (58%)	0.84	25 (15%) 2 2	88, 153, 237, 268	0
79	sM	129/272 (47%)	0.53	10 (7%) 13 14	76, 118, 187, 220	0
80	m2	0/165	-	-	-	-
81	n4	135/135 (100%)	1.00	23 (17%) 1 2	42, 139, 211, 238	0
82	p0	143/312 (45%)	0.94	22 (15%) 2 2	84, 138, 215, 261	0
83	p1	0/47	-	-	-	-
All	All	32909/34616 (95%)	0.50	2766 (8%) 11 13	32, 103, 196, 384	0

The worst 5 of 2766 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	N4	75	THR	15.5
25	N4	76	VAL	12.9
57	C1	146	ALA	12.4
18	M7	167	ARG	12.3
57	C1	145	ALA	11.4

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	5	3634	1/1	-0.07	1.24	57,57,57,57	0
84	MG	1	3950	1/1	0.03	0.55	85,85,85,85	0
84	MG	6	2162	1/1	0.22	0.21	96,96,96,96	0
84	MG	1	3628	1/1	0.42	0.69	80,80,80,80	0
84	MG	1	3917	1/1	0.42	0.35	74,74,74,74	0
84	MG	6	2072	1/1	0.43	0.26	77,77,77,77	0
84	MG	1	3759	1/1	0.43	0.82	73,73,73,73	0
84	MG	1	3637	1/1	0.43	0.37	91,91,91,91	0
84	MG	2	1961	1/1	0.44	0.17	109,109,109,109	0
84	MG	S2	301	1/1	0.44	0.55	107,107,107,107	0
84	MG	1	3842	1/1	0.45	0.98	92,92,92,92	0
84	MG	1	3493	1/1	0.46	0.65	76,76,76,76	0
84	MG	2	1980	1/1	0.46	0.54	77,77,77,77	0
84	MG	M3	203	1/1	0.47	0.24	92,92,92,92	0
84	MG	5	3611	1/1	0.47	0.38	104,104,104,104	0
84	MG	N3	204	1/1	0.49	0.39	87,87,87,87	0
84	MG	5	3970	1/1	0.49	0.72	75,75,75,75	0
84	MG	5	4097	1/1	0.49	0.48	68,68,68,68	0
84	MG	1	3510	1/1	0.50	0.51	57,57,57,57	0
84	MG	6	2090	1/1	0.50	0.40	91,91,91,91	0
84	MG	d6	102	1/1	0.50	0.28	76,76,76,76	0
84	MG	5	3695	1/1	0.50	0.35	93,93,93,93	0
84	MG	5	3654	1/1	0.50	0.39	79,79,79,79	0
84	MG	1	3636	1/1	0.51	0.22	104,104,104,104	0
84	MG	2	1940	1/1	0.51	0.64	82,82,82,82	0
84	MG	6	2120	1/1	0.52	0.14	110,110,110,110	0
84	MG	6	1924	1/1	0.52	0.29	70,70,70,70	0
84	MG	4	221	1/1	0.52	0.45	75,75,75,75	0
84	MG	8	213	1/1	0.52	0.58	68,68,68,68	0
84	MG	1	3902	1/1	0.52	0.19	77,77,77,77	0
84	MG	5	4057	1/1	0.53	0.15	99,99,99,99	1
84	MG	6	2121	1/1	0.53	0.61	97,97,97,97	0
84	MG	6	2141	1/1	0.53	0.32	99,99,99,99	0
84	MG	6	1944	1/1	0.53	0.86	71,71,71,71	0
84	MG	1	3876	1/1	0.53	0.67	76,76,76,76	0
84	MG	3	202	1/1	0.54	0.24	89,89,89,89	0
84	MG	O6	201	1/1	0.54	0.26	78,78,78,78	0
84	MG	6	1901	1/1	0.54	0.72	55,55,55,55	0
84	MG	6	1991	1/1	0.55	0.54	71,71,71,71	0
84	MG	s2	302	1/1	0.55	0.34	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3667	1/1	0.55	0.53	73,73,73,73	0
84	MG	2	1931	1/1	0.55	0.47	90,90,90,90	0
84	MG	1	3483	1/1	0.56	0.59	68,68,68,68	0
84	MG	6	2106	1/1	0.56	0.58	91,91,91,91	0
84	MG	4	212	1/1	0.56	0.38	84,84,84,84	0
84	MG	5	3751	1/1	0.56	0.59	61,61,61,61	0
84	MG	5	4031	1/1	0.56	0.37	65,65,65,65	0
84	MG	6	2129	1/1	0.56	0.36	88,88,88,88	0
84	MG	2	2023	1/1	0.57	0.15	132,132,132,132	0
84	MG	5	3645	1/1	0.57	0.55	59,59,59,59	0
84	MG	6	1967	1/1	0.57	0.85	74,74,74,74	0
86	ZN	D7	101	1/1	0.57	0.22	264,264,264,264	0
84	MG	3	206	1/1	0.58	0.50	72,72,72,72	0
84	MG	2	1929	1/1	0.59	0.60	88,88,88,88	0
84	MG	n5	201	1/1	0.59	0.13	96,96,96,96	0
84	MG	q2	506	1/1	0.59	0.33	68,68,68,68	0
84	MG	1	3927	1/1	0.60	0.17	77,77,77,77	1
84	MG	5	4030	1/1	0.60	0.50	99,99,99,99	0
84	MG	1	3490	1/1	0.60	0.16	80,80,80,80	0
84	MG	5	3886	1/1	0.60	0.36	77,77,77,77	0
84	MG	1	3744	1/1	0.60	0.17	82,82,82,82	0
84	MG	5	4080	1/1	0.60	0.16	67,67,67,67	0
84	MG	1	3980	1/1	0.60	0.14	91,91,91,91	0
84	MG	4	206	1/1	0.60	0.53	60,60,60,60	0
84	MG	1	3726	1/1	0.61	0.47	69,69,69,69	0
84	MG	6	2119	1/1	0.61	0.35	91,91,91,91	0
84	MG	6	2024	1/1	0.61	0.23	80,80,80,80	0
84	MG	5	3966	1/1	0.61	0.63	95,95,95,95	0
84	MG	1	3803	1/1	0.61	0.45	76,76,76,76	0
84	MG	6	2030	1/1	0.61	0.30	82,82,82,82	0
84	MG	1	3442	1/1	0.61	0.39	83,83,83,83	0
84	MG	6	2107	1/1	0.62	0.45	90,90,90,90	0
84	MG	1	3630	1/1	0.62	0.12	106,106,106,106	0
84	MG	2	1965	1/1	0.62	0.32	91,91,91,91	0
84	MG	1	3758	1/1	0.62	0.59	74,74,74,74	0
84	MG	1	3888	1/1	0.63	0.38	68,68,68,68	0
84	MG	1	3521	1/1	0.63	0.43	69,69,69,69	0
84	MG	1	3816	1/1	0.63	0.46	78,78,78,78	0
84	MG	5	3984	1/1	0.63	0.49	62,62,62,62	0
84	MG	5	3836	1/1	0.64	0.29	79,79,79,79	0
84	MG	c3	204	1/1	0.64	0.14	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1933	1/1	0.64	0.57	74,74,74,74	0
84	MG	1	3952	1/1	0.64	1.00	88,88,88,88	0
84	MG	5	3813	1/1	0.64	0.55	58,58,58,58	0
84	MG	5	4106	1/1	0.64	0.32	49,49,49,49	0
84	MG	M5	305	1/1	0.64	0.33	72,72,72,72	0
84	MG	1	3985	1/1	0.64	0.40	77,77,77,77	0
84	MG	2	2015	1/1	0.64	0.59	84,84,84,84	0
84	MG	5	4049	1/1	0.64	0.20	79,79,79,79	0
84	MG	1	3650	1/1	0.64	0.40	53,53,53,53	0
84	MG	d7	102	1/1	0.64	0.40	78,78,78,78	0
84	MG	5	3904	1/1	0.64	0.62	59,59,59,59	0
84	MG	2	1966	1/1	0.64	0.28	106,106,106,106	0
84	MG	1	3639	1/1	0.64	0.29	96,96,96,96	0
84	MG	5	3591	1/1	0.64	0.54	61,61,61,61	0
84	MG	5	3937	1/1	0.65	0.35	60,60,60,60	0
84	MG	1	3590	1/1	0.65	0.39	58,58,58,58	0
84	MG	5	3896	1/1	0.65	0.83	71,71,71,71	0
84	MG	m8	203	1/1	0.65	0.39	69,69,69,69	0
84	MG	2	2007	1/1	0.65	0.24	88,88,88,88	0
84	MG	4	202	1/1	0.65	0.31	59,59,59,59	0
84	MG	2	1955	1/1	0.65	0.33	86,86,86,86	0
84	MG	6	2149	1/1	0.65	0.18	73,73,73,73	0
84	MG	1	3818	1/1	0.65	0.54	88,88,88,88	0
84	MG	1	3955	1/1	0.65	0.47	69,69,69,69	0
84	MG	2	2036	1/1	0.65	0.18	113,113,113,113	0
84	MG	l8	301	1/1	0.66	0.45	99,99,99,99	0
84	MG	m6	208	1/1	0.66	0.50	56,56,56,56	0
84	MG	5	3840	1/1	0.66	0.30	61,61,61,61	0
84	MG	6	2034	1/1	0.66	0.39	69,69,69,69	0
84	MG	5	3711	1/1	0.66	0.34	70,70,70,70	0
84	MG	6	1968	1/1	0.66	0.55	65,65,65,65	0
84	MG	5	3803	1/1	0.66	0.17	76,76,76,76	0
84	MG	2	2001	1/1	0.66	0.61	146,146,146,146	0
84	MG	O7	104	1/1	0.66	0.22	88,88,88,88	0
84	MG	1	3658	1/1	0.66	0.37	70,70,70,70	0
84	MG	5	3975	1/1	0.66	0.57	71,71,71,71	0
84	MG	5	3863	1/1	0.66	0.53	76,76,76,76	0
84	MG	d1	101	1/1	0.66	0.40	93,93,93,93	0
84	MG	S4	301	1/1	0.66	0.20	120,120,120,120	0
84	MG	n5	202	1/1	0.66	0.32	78,78,78,78	0
84	MG	1	3769	1/1	0.66	0.89	65,65,65,65	0
84	MG	4	211	1/1	0.67	0.27	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	4	208	1/1	0.67	0.40	60,60,60,60	0
84	MG	6	2134	1/1	0.67	0.14	99,99,99,99	0
84	MG	5	3794	1/1	0.67	0.23	61,61,61,61	0
84	MG	c1	201	1/1	0.67	0.40	78,78,78,78	0
84	MG	2	1906	1/1	0.67	0.40	86,86,86,86	0
84	MG	6	1993	1/1	0.67	0.72	71,71,71,71	0
84	MG	6	1989	1/1	0.67	0.44	67,67,67,67	0
84	MG	O4	503	1/1	0.67	0.13	127,127,127,127	0
84	MG	5	3825	1/1	0.67	0.35	58,58,58,58	0
84	MG	6	1903	1/1	0.68	0.77	67,67,67,67	0
84	MG	L2	303	1/1	0.68	0.27	88,88,88,88	0
84	MG	2	1905	1/1	0.68	0.09	127,127,127,127	0
84	MG	6	2148	1/1	0.68	0.26	78,78,78,78	0
84	MG	5	4135	1/1	0.68	0.32	77,77,77,77	0
84	MG	1	3447	1/1	0.68	0.45	58,58,58,58	0
84	MG	8	209	1/1	0.68	0.23	80,80,80,80	0
84	MG	5	4071	1/1	0.68	0.13	103,103,103,103	0
84	MG	5	3664	1/1	0.68	0.41	56,56,56,56	0
84	MG	5	4003	1/1	0.68	0.26	77,77,77,77	0
84	MG	1	3788	1/1	0.68	0.19	76,76,76,76	1
84	MG	5	4129	1/1	0.68	0.57	90,90,90,90	0
84	MG	5	3999	1/1	0.68	0.31	52,52,52,52	0
84	MG	6	1918	1/1	0.68	0.22	84,84,84,84	0
84	MG	6	2128	1/1	0.68	0.32	77,77,77,77	0
84	MG	5	3808	1/1	0.68	0.23	66,66,66,66	0
84	MG	5	3768	1/1	0.68	0.41	73,73,73,73	0
84	MG	6	1945	1/1	0.69	0.49	70,70,70,70	0
84	MG	1	3804	1/1	0.69	0.57	91,91,91,91	0
84	MG	6	2059	1/1	0.69	0.18	76,76,76,76	0
84	MG	N0	201	1/1	0.69	0.35	67,67,67,67	0
84	MG	6	1951	1/1	0.69	0.21	74,74,74,74	0
84	MG	1	3865	1/1	0.69	0.55	81,81,81,81	0
84	MG	1	3461	1/1	0.69	0.43	59,59,59,59	0
84	MG	m4	201	1/1	0.69	0.21	69,69,69,69	1
84	MG	5	3795	1/1	0.69	0.22	74,74,74,74	0
84	MG	1	3481	1/1	0.69	0.79	73,73,73,73	0
84	MG	1	3958	1/1	0.69	0.19	88,88,88,88	0
84	MG	n0	204	1/1	0.69	0.28	57,57,57,57	0
84	MG	1	3579	1/1	0.69	0.25	71,71,71,71	0
84	MG	5	4040	1/1	0.69	0.29	74,74,74,74	0
84	MG	5	3704	1/1	0.70	0.38	77,77,77,77	0
84	MG	5	3558	1/1	0.70	0.46	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	2	1979	1/1	0.70	0.84	68,68,68,68	0
84	MG	5	4007	1/1	0.70	0.46	63,63,63,63	0
84	MG	5	3868	1/1	0.70	0.74	57,57,57,57	0
84	MG	6	2114	1/1	0.70	0.23	96,96,96,96	0
84	MG	6	1943	1/1	0.70	0.35	65,65,65,65	0
84	MG	5	4134	1/1	0.70	0.30	73,73,73,73	0
84	MG	1	3545	1/1	0.70	0.55	62,62,62,62	0
84	MG	3	215	1/1	0.70	0.17	74,74,74,74	0
84	MG	1	3627	1/1	0.70	0.44	81,81,81,81	0
84	MG	1	3934	1/1	0.70	0.48	65,65,65,65	0
84	MG	6	2108	1/1	0.70	0.33	79,79,79,79	0
84	MG	5	4086	1/1	0.70	0.17	96,96,96,96	0
84	MG	6	1983	1/1	0.70	0.18	100,100,100,100	0
84	MG	2	1997	1/1	0.70	0.36	98,98,98,98	0
84	MG	6	1942	1/1	0.70	0.40	60,60,60,60	0
84	MG	2	1977	1/1	0.71	1.32	77,77,77,77	0
84	MG	5	3594	1/1	0.71	0.47	77,77,77,77	0
84	MG	N1	202	1/1	0.71	0.34	98,98,98,98	0
84	MG	2	1954	1/1	0.71	0.29	106,106,106,106	0
84	MG	5	3936	1/1	0.71	0.45	55,55,55,55	0
84	MG	5	3948	1/1	0.71	0.65	58,58,58,58	0
84	MG	2	2017	1/1	0.71	0.57	86,86,86,86	0
84	MG	6	2118	1/1	0.71	0.33	148,148,148,148	0
84	MG	1	3904	1/1	0.71	0.27	76,76,76,76	0
84	MG	2	1913	1/1	0.71	0.62	81,81,81,81	0
84	MG	1	3823	1/1	0.71	0.69	89,89,89,89	0
84	MG	C3	201	1/1	0.72	0.20	102,102,102,102	0
84	MG	1	3854	1/1	0.72	0.31	60,60,60,60	0
84	MG	5	3867	1/1	0.72	0.39	55,55,55,55	0
84	MG	7	219	1/1	0.72	0.17	62,62,62,62	0
84	MG	5	3601	1/1	0.72	0.46	89,89,89,89	0
84	MG	12	304	1/1	0.72	0.39	76,76,76,76	0
84	MG	1	3815	1/1	0.72	0.74	77,77,77,77	0
84	MG	5	4073	1/1	0.72	0.12	97,97,97,97	0
84	MG	6	2100	1/1	0.72	0.28	84,84,84,84	0
84	MG	6	2018	1/1	0.72	0.31	81,81,81,81	0
84	MG	1	3571	1/1	0.72	0.27	71,71,71,71	0
84	MG	M8	201	1/1	0.72	0.23	67,67,67,67	0
84	MG	1	3723	1/1	0.72	0.32	47,47,47,47	0
84	MG	1	3960	1/1	0.73	0.20	79,79,79,79	0
84	MG	5	3942	1/1	0.73	0.39	79,79,79,79	0
84	MG	5	3690	1/1	0.73	0.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3763	1/1	0.73	0.42	66,66,66,66	0
84	MG	6	2139	1/1	0.73	0.19	82,82,82,82	0
84	MG	3	208	1/1	0.73	0.46	64,64,64,64	0
84	MG	1	3900	1/1	0.73	0.11	85,85,85,85	0
84	MG	1	3495	1/1	0.73	0.62	75,75,75,75	0
84	MG	5	3764	1/1	0.73	0.32	78,78,78,78	0
84	MG	1	3782	1/1	0.73	0.74	69,69,69,69	0
84	MG	7	223	1/1	0.73	0.22	75,75,75,75	0
84	MG	6	2070	1/1	0.73	0.17	128,128,128,128	0
84	MG	1	3467	1/1	0.73	0.38	58,58,58,58	0
84	MG	1	3456	1/1	0.73	0.36	67,67,67,67	0
84	MG	6	2161	1/1	0.73	0.27	75,75,75,75	0
84	MG	D3	204	1/1	0.73	0.51	94,94,94,94	0
84	MG	5	3974	1/1	0.73	0.43	67,67,67,67	0
84	MG	2	1984	1/1	0.74	0.43	113,113,113,113	0
84	MG	l5	302	1/1	0.74	0.14	78,78,78,78	0
84	MG	8	202	1/1	0.74	0.19	90,90,90,90	0
84	MG	1	3694	1/1	0.74	0.38	62,62,62,62	0
84	MG	m7	207	1/1	0.74	0.53	66,66,66,66	0
84	MG	5	4130	1/1	0.74	0.21	81,81,81,81	0
84	MG	6	1960	1/1	0.74	0.41	62,62,62,62	0
84	MG	6	2142	1/1	0.74	0.24	89,89,89,89	0
84	MG	5	3934	1/1	0.74	0.46	48,48,48,48	1
84	MG	5	3856	1/1	0.74	0.34	61,61,61,61	0
84	MG	2	2037	1/1	0.74	0.35	99,99,99,99	0
84	MG	1	3565	1/1	0.74	0.20	71,71,71,71	0
84	MG	2	2000	1/1	0.74	0.36	164,164,164,164	0
84	MG	1	3580	1/1	0.74	0.24	75,75,75,75	0
84	MG	1	3738	1/1	0.74	0.73	75,75,75,75	0
84	MG	6	1977	1/1	0.74	0.26	103,103,103,103	0
84	MG	d9	102	1/1	0.74	0.22	94,94,94,94	0
84	MG	1	3681	1/1	0.75	0.36	62,62,62,62	0
84	MG	5	3780	1/1	0.75	0.30	64,64,64,64	0
84	MG	l3	410	1/1	0.75	0.17	73,73,73,73	0
84	MG	8	201	1/1	0.75	0.42	81,81,81,81	0
84	MG	1	3555	1/1	0.75	0.16	92,92,92,92	0
84	MG	5	3793	1/1	0.75	0.37	68,68,68,68	0
84	MG	C1	201	1/1	0.75	0.20	103,103,103,103	0
84	MG	5	4046	1/1	0.75	0.43	67,67,67,67	0
84	MG	2	1953	1/1	0.75	0.33	96,96,96,96	0
84	MG	6	1920	1/1	0.75	0.23	81,81,81,81	0
84	MG	1	3426	1/1	0.75	0.31	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3651	1/1	0.75	0.38	77,77,77,77	0
84	MG	Q2	504	1/1	0.75	0.37	59,59,59,59	0
84	MG	m4	206	1/1	0.75	0.35	58,58,58,58	0
84	MG	2	2004	1/1	0.75	0.72	81,81,81,81	0
84	MG	1	3454	1/1	0.75	0.37	61,61,61,61	0
84	MG	1	3893	1/1	0.75	0.30	57,57,57,57	0
84	MG	8	208	1/1	0.75	0.21	79,79,79,79	0
84	MG	4	210	1/1	0.75	0.14	90,90,90,90	0
84	MG	1	3948	1/1	0.75	0.51	82,82,82,82	0
84	MG	1	3584	1/1	0.75	0.36	76,76,76,76	0
84	MG	8	216	1/1	0.75	0.68	67,67,67,67	0
84	MG	1	3566	1/1	0.75	0.22	74,74,74,74	0
84	MG	5	3577	1/1	0.75	0.57	54,54,54,54	0
84	MG	sR	401	1/1	0.75	0.18	76,76,76,76	0
84	MG	1	3764	1/1	0.75	0.57	69,69,69,69	0
84	MG	6	1974	1/1	0.75	0.17	90,90,90,90	0
84	MG	1	3560	1/1	0.75	0.20	78,78,78,78	0
84	MG	m6	202	1/1	0.76	0.29	47,47,47,47	0
84	MG	6	1996	1/1	0.76	0.32	74,74,74,74	0
84	MG	1	3499	1/1	0.76	0.46	61,61,61,61	0
84	MG	5	3469	1/1	0.76	0.46	54,54,54,54	0
84	MG	5	3617	1/1	0.76	0.30	75,75,75,75	0
84	MG	1	3859	1/1	0.76	0.16	67,67,67,67	0
84	MG	1	3827	1/1	0.76	0.47	61,61,61,61	0
84	MG	5	3622	1/1	0.76	0.19	84,84,84,84	0
84	MG	1	3668	1/1	0.76	0.32	74,74,74,74	0
84	MG	5	3563	1/1	0.76	0.46	55,55,55,55	0
84	MG	5	4117	1/1	0.76	0.18	82,82,82,82	0
84	MG	5	3593	1/1	0.76	0.50	68,68,68,68	0
84	MG	q2	507	1/1	0.76	0.20	51,51,51,51	0
84	MG	1	3977	1/1	0.76	0.16	87,87,87,87	0
84	MG	5	4033	1/1	0.76	0.13	74,74,74,74	0
84	MG	l2	303	1/1	0.76	0.36	72,72,72,72	0
84	MG	5	3722	1/1	0.76	0.38	77,77,77,77	0
84	MG	5	3624	1/1	0.76	0.57	65,65,65,65	0
84	MG	1	3879	1/1	0.76	0.69	63,63,63,63	0
84	MG	5	3693	1/1	0.76	0.32	81,81,81,81	0
84	MG	d6	104	1/1	0.76	0.30	76,76,76,76	0
84	MG	O7	102	1/1	0.76	0.39	61,61,61,61	0
84	MG	5	3755	1/1	0.76	0.44	59,59,59,59	0
84	MG	1	3514	1/1	0.76	0.61	63,63,63,63	0
84	MG	q2	502	1/1	0.76	0.27	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	q3	503	1/1	0.76	0.26	79,79,79,79	0
84	MG	6	2064	1/1	0.76	0.15	126,126,126,126	0
84	MG	5	3675	1/1	0.76	0.25	67,67,67,67	0
84	MG	5	3775	1/1	0.76	0.45	120,120,120,120	0
84	MG	5	3954	1/1	0.76	0.62	58,58,58,58	0
84	MG	1	3578	1/1	0.76	0.21	78,78,78,78	0
84	MG	5	3526	1/1	0.76	0.62	61,61,61,61	0
84	MG	5	3855	1/1	0.76	0.57	69,69,69,69	0
84	MG	5	4120	1/1	0.76	0.10	90,90,90,90	0
84	MG	4	223	1/1	0.77	0.26	72,72,72,72	0
84	MG	6	1940	1/1	0.77	0.80	69,69,69,69	0
84	MG	5	3819	1/1	0.77	0.24	57,57,57,57	0
84	MG	5	3828	1/1	0.77	0.32	46,46,46,46	0
84	MG	2	1978	1/1	0.77	0.50	64,64,64,64	0
84	MG	1	3741	1/1	0.77	0.34	80,80,80,80	0
84	MG	8	214	1/1	0.77	0.39	54,54,54,54	0
84	MG	c3	201	1/1	0.77	0.61	89,89,89,89	0
84	MG	8	207	1/1	0.77	0.31	74,74,74,74	0
84	MG	5	4041	1/1	0.77	0.30	79,79,79,79	0
84	MG	5	3857	1/1	0.77	0.21	65,65,65,65	0
84	MG	1	3663	1/1	0.77	0.29	69,69,69,69	0
84	MG	5	3766	1/1	0.77	0.49	57,57,57,57	0
84	MG	5	3492	1/1	0.77	0.42	74,74,74,74	0
84	MG	l6	202	1/1	0.77	0.39	66,66,66,66	0
84	MG	L5	301	1/1	0.77	0.13	89,89,89,89	0
84	MG	5	4063	1/1	0.77	0.17	94,94,94,94	0
84	MG	l5	305	1/1	0.77	0.08	77,77,77,77	0
84	MG	1	3886	1/1	0.77	0.22	83,83,83,83	0
84	MG	1	3746	1/1	0.77	0.39	69,69,69,69	0
84	MG	1	3444	1/1	0.77	0.68	70,70,70,70	0
84	MG	l9	208	1/1	0.77	0.18	54,54,54,54	0
84	MG	5	3524	1/1	0.77	0.48	53,53,53,53	0
84	MG	m8	202	1/1	0.77	0.53	63,63,63,63	0
84	MG	1	3873	1/1	0.77	0.44	65,65,65,65	0
84	MG	8	205	1/1	0.77	0.17	111,111,111,111	0
84	MG	5	3802	1/1	0.77	0.15	75,75,75,75	0
84	MG	6	2085	1/1	0.77	0.15	88,88,88,88	0
84	MG	m6	203	1/1	0.78	0.34	55,55,55,55	0
84	MG	5	3706	1/1	0.78	0.62	71,71,71,71	0
84	MG	6	1992	1/1	0.78	0.47	78,78,78,78	0
84	MG	1	3711	1/1	0.78	0.19	84,84,84,84	0
84	MG	1	3577	1/1	0.78	0.23	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1988	1/1	0.78	0.39	66,66,66,66	0
84	MG	5	4149	1/1	0.78	0.32	74,74,74,74	0
84	MG	N4	201	1/1	0.78	0.39	70,70,70,70	0
84	MG	5	3915	1/1	0.78	0.49	78,78,78,78	0
84	MG	7	225	1/1	0.78	0.20	71,71,71,71	0
84	MG	5	3805	1/1	0.78	0.15	75,75,75,75	0
84	MG	5	3838	1/1	0.78	0.31	57,57,57,57	0
84	MG	5	3542	1/1	0.78	0.42	54,54,54,54	0
84	MG	5	3564	1/1	0.78	0.47	59,59,59,59	0
84	MG	1	3742	1/1	0.78	0.51	78,78,78,78	0
84	MG	6	1997	1/1	0.78	0.28	78,78,78,78	0
84	MG	1	3515	1/1	0.78	1.17	64,64,64,64	0
84	MG	1	3686	1/1	0.78	0.34	57,57,57,57	0
84	MG	5	4112	1/1	0.78	0.18	52,52,52,52	0
84	MG	d3	201	1/1	0.78	0.48	65,65,65,65	0
84	MG	1	3665	1/1	0.78	0.22	67,67,67,67	0
84	MG	3	211	1/1	0.78	0.24	71,71,71,71	0
84	MG	5	3574	1/1	0.78	0.61	58,58,58,58	0
84	MG	2	2013	1/1	0.78	0.12	120,120,120,120	0
84	MG	5	3960	1/1	0.78	0.18	74,74,74,74	0
84	MG	1	3805	1/1	0.78	0.32	74,74,74,74	0
84	MG	1	3932	1/1	0.79	0.69	71,71,71,71	0
84	MG	6	2026	1/1	0.79	0.28	78,78,78,78	0
84	MG	1	3829	1/1	0.79	0.53	71,71,71,71	0
84	MG	1	3847	1/1	0.79	0.51	53,53,53,53	0
84	MG	5	3878	1/1	0.79	0.47	79,79,79,79	0
84	MG	2	2026	1/1	0.79	0.22	126,126,126,126	0
84	MG	4	215	1/1	0.79	0.38	69,69,69,69	0
84	MG	5	3483	1/1	0.79	0.36	57,57,57,57	0
84	MG	5	3437	1/1	0.79	0.25	59,59,59,59	0
84	MG	m6	207	1/1	0.79	0.29	47,47,47,47	0
84	MG	5	3965	1/1	0.79	0.57	65,65,65,65	0
84	MG	1	3880	1/1	0.79	0.45	73,73,73,73	0
84	MG	1	3634	1/1	0.79	0.26	105,105,105,105	0
84	MG	l3	408	1/1	0.79	0.41	64,64,64,64	0
84	MG	1	3541	1/1	0.79	0.32	58,58,58,58	0
84	MG	5	4024	1/1	0.79	0.39	68,68,68,68	0
84	MG	1	3704	1/1	0.79	0.32	55,55,55,55	0
84	MG	2	2010	1/1	0.79	0.29	98,98,98,98	0
84	MG	2	1992	1/1	0.79	0.14	98,98,98,98	0
84	MG	1	3949	1/1	0.79	0.14	79,79,79,79	0
84	MG	5	3442	1/1	0.79	0.45	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	2058	1/1	0.79	0.30	81,81,81,81	0
85	LLL	5	4178	31/31	0.79	0.35	69,69,69,69	31
84	MG	5	3697	1/1	0.79	0.44	65,65,65,65	0
84	MG	1	3508	1/1	0.79	0.89	60,60,60,60	0
84	MG	m3	202	1/1	0.79	0.23	82,82,82,82	0
84	MG	1	3501	1/1	0.79	0.24	64,64,64,64	0
84	MG	2	2024	1/1	0.79	0.07	130,130,130,130	0
84	MG	6	2066	1/1	0.79	0.10	121,121,121,121	0
84	MG	5	3434	1/1	0.79	0.27	60,60,60,60	0
84	MG	1	3707	1/1	0.79	0.37	59,59,59,59	0
84	MG	8	219	1/1	0.79	0.38	90,90,90,90	0
84	MG	6	2035	1/1	0.79	0.21	82,82,82,82	0
84	MG	l3	406	1/1	0.79	0.44	63,63,63,63	0
84	MG	1	3792	1/1	0.79	0.23	94,94,94,94	0
84	MG	5	3588	1/1	0.79	0.94	62,62,62,62	0
84	MG	1	3820	1/1	0.79	0.45	76,76,76,76	0
84	MG	5	4098	1/1	0.79	0.36	81,81,81,81	0
84	MG	1	3465	1/1	0.79	0.37	56,56,56,56	0
84	MG	5	3833	1/1	0.79	0.36	53,53,53,53	0
84	MG	5	4012	1/1	0.79	0.31	61,61,61,61	0
84	MG	D3	201	1/1	0.79	0.32	72,72,72,72	0
84	MG	1	3953	1/1	0.79	0.30	72,72,72,72	0
84	MG	6	1913	1/1	0.79	0.15	107,107,107,107	0
84	MG	7	227	1/1	0.80	0.28	76,76,76,76	0
84	MG	5	3458	1/1	0.80	0.29	57,57,57,57	0
84	MG	7	203	1/1	0.80	0.36	52,52,52,52	0
84	MG	1	3928	1/1	0.80	0.23	64,64,64,64	0
84	MG	L4	405	1/1	0.80	0.43	63,63,63,63	0
84	MG	5	3859	1/1	0.80	0.56	71,71,71,71	0
84	MG	1	3457	1/1	0.80	0.25	63,63,63,63	0
84	MG	m3	201	1/1	0.80	0.28	88,88,88,88	0
84	MG	m5	303	1/1	0.80	0.17	79,79,79,79	0
84	MG	1	3469	1/1	0.80	0.21	59,59,59,59	1
84	MG	6	2062	1/1	0.80	0.11	111,111,111,111	0
84	MG	5	3899	1/1	0.80	0.81	59,59,59,59	0
84	MG	5	4052	1/1	0.80	0.43	77,77,77,77	0
84	MG	1	3696	1/1	0.80	0.50	55,55,55,55	0
84	MG	5	3958	1/1	0.80	0.62	66,66,66,66	0
84	MG	M0	303	1/1	0.80	0.33	66,66,66,66	0
84	MG	1	3669	1/1	0.80	0.30	78,78,78,78	0
84	MG	6	2111	1/1	0.80	0.19	113,113,113,113	0
84	MG	6	2063	1/1	0.80	0.13	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3881	1/1	0.80	0.18	78,78,78,78	0
84	MG	5	3583	1/1	0.80	0.59	59,59,59,59	0
84	MG	1	3670	1/1	0.80	0.31	76,76,76,76	0
84	MG	19	206	1/1	0.80	0.32	68,68,68,68	0
84	MG	5	4114	1/1	0.80	0.20	83,83,83,83	0
84	MG	5	3967	1/1	0.80	0.62	71,71,71,71	0
84	MG	2	2034	1/1	0.80	0.19	92,92,92,92	0
84	MG	1	3975	1/1	0.80	0.28	63,63,63,63	0
84	MG	5	4056	1/1	0.80	0.16	95,95,95,95	0
84	MG	1	3662	1/1	0.80	0.28	78,78,78,78	0
84	MG	1	3853	1/1	0.80	0.29	60,60,60,60	0
84	MG	O2	203	1/1	0.80	0.35	57,57,57,57	0
84	MG	6	1934	1/1	0.80	0.36	67,67,67,67	0
84	MG	1	3430	1/1	0.80	0.39	54,54,54,54	0
84	MG	1	3715	1/1	0.80	0.18	83,83,83,83	0
84	MG	6	2049	1/1	0.80	0.14	78,78,78,78	0
84	MG	1	3909	1/1	0.80	0.29	73,73,73,73	0
84	MG	5	3869	1/1	0.80	0.87	67,67,67,67	0
84	MG	6	2124	1/1	0.80	0.26	76,76,76,76	0
84	MG	6	2014	1/1	0.80	0.21	74,74,74,74	0
84	MG	1	3800	1/1	0.81	0.52	67,67,67,67	0
84	MG	5	3946	1/1	0.81	0.69	64,64,64,64	0
84	MG	6	1994	1/1	0.81	0.60	69,69,69,69	0
84	MG	5	3419	1/1	0.81	0.37	49,49,49,49	0
84	MG	5	3635	1/1	0.81	0.29	55,55,55,55	0
84	MG	6	1937	1/1	0.81	0.93	62,62,62,62	0
84	MG	1	3529	1/1	0.81	0.76	66,66,66,66	0
84	MG	O3	201	1/1	0.81	0.41	64,64,64,64	0
84	MG	1	3937	1/1	0.81	0.42	73,73,73,73	0
84	MG	5	3968	1/1	0.81	0.26	56,56,56,56	0
84	MG	5	4085	1/1	0.81	0.16	79,79,79,79	0
84	MG	5	3552	1/1	0.81	0.52	68,68,68,68	0
84	MG	2	2035	1/1	0.81	0.27	101,101,101,101	0
84	MG	2	1990	1/1	0.81	0.21	116,116,116,116	0
84	MG	1	3409	1/1	0.81	0.40	49,49,49,49	0
84	MG	N8	203	1/1	0.81	0.44	63,63,63,63	0
84	MG	5	3772	1/1	0.81	0.32	128,128,128,128	0
84	MG	n1	201	1/1	0.81	0.15	61,61,61,61	0
84	MG	5	4018	1/1	0.81	0.50	66,66,66,66	0
84	MG	5	4104	1/1	0.81	0.30	56,56,56,56	0
84	MG	5	4008	1/1	0.81	0.36	56,56,56,56	0
84	MG	2	2016	1/1	0.81	0.39	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	D3	202	1/1	0.81	0.51	67,67,67,67	0
84	MG	1	3739	1/1	0.81	0.42	72,72,72,72	0
84	MG	1	3556	1/1	0.81	0.35	73,73,73,73	0
84	MG	5	3792	1/1	0.81	0.26	63,63,63,63	1
84	MG	1	3506	1/1	0.81	0.35	57,57,57,57	0
84	MG	O2	204	1/1	0.81	0.32	58,58,58,58	0
84	MG	5	3992	1/1	0.81	0.42	49,49,49,49	0
84	MG	6	1987	1/1	0.81	0.31	79,79,79,79	0
84	MG	5	3520	1/1	0.81	0.36	54,54,54,54	0
84	MG	3	210	1/1	0.81	0.22	65,65,65,65	0
84	MG	5	4078	1/1	0.81	0.25	67,67,67,67	0
84	MG	1	3817	1/1	0.81	0.66	72,72,72,72	0
84	MG	6	2115	1/1	0.81	0.12	93,93,93,93	0
84	MG	1	3652	1/1	0.81	0.23	59,59,59,59	0
84	MG	5	3696	1/1	0.81	0.39	94,94,94,94	0
84	MG	6	2037	1/1	0.81	0.17	87,87,87,87	0
84	MG	1	3698	1/1	0.81	0.54	69,69,69,69	0
84	MG	1	3810	1/1	0.81	0.27	70,70,70,70	0
84	MG	5	3725	1/1	0.81	0.37	71,71,71,71	0
84	MG	8	206	1/1	0.81	0.25	81,81,81,81	0
84	MG	M0	302	1/1	0.81	0.83	64,64,64,64	0
84	MG	5	4019	1/1	0.81	0.63	66,66,66,66	0
84	MG	1	3840	1/1	0.81	0.67	67,67,67,67	0
84	MG	1	3766	1/1	0.82	0.27	58,58,58,58	0
84	MG	2	2027	1/1	0.82	0.55	95,95,95,95	0
84	MG	5	3752	1/1	0.82	0.36	59,59,59,59	0
84	MG	6	2021	1/1	0.82	0.09	86,86,86,86	0
84	MG	5	3546	1/1	0.82	0.37	63,63,63,63	0
84	MG	5	4083	1/1	0.82	0.15	88,88,88,88	0
84	MG	7	230	1/1	0.82	0.45	75,75,75,75	0
84	MG	5	3686	1/1	0.82	0.30	68,68,68,68	0
84	MG	5	4060	1/1	0.82	0.32	68,68,68,68	0
84	MG	6	1980	1/1	0.82	0.24	108,108,108,108	0
84	MG	1	3976	1/1	0.82	0.23	71,71,71,71	0
84	MG	1	3559	1/1	0.82	0.24	73,73,73,73	0
84	MG	L8	301	1/1	0.82	0.18	103,103,103,103	0
84	MG	5	3943	1/1	0.82	0.69	75,75,75,75	0
84	MG	5	3488	1/1	0.82	0.21	55,55,55,55	0
84	MG	5	3565	1/1	0.82	0.39	57,57,57,57	0
84	MG	1	3963	1/1	0.82	0.33	76,76,76,76	0
84	MG	5	3812	1/1	0.82	0.53	46,46,46,46	0
84	MG	5	3927	1/1	0.82	0.40	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1976	1/1	0.82	0.22	84,84,84,84	0
84	MG	1	3477	1/1	0.82	0.38	51,51,51,51	0
84	MG	2	1975	1/1	0.82	0.46	87,87,87,87	0
84	MG	2	1967	1/1	0.82	0.35	90,90,90,90	0
84	MG	s6	301	1/1	0.82	0.28	78,78,78,78	0
84	MG	1	3494	1/1	0.82	0.40	81,81,81,81	0
84	MG	1	3509	1/1	0.82	0.54	60,60,60,60	0
84	MG	2	2022	1/1	0.82	0.09	132,132,132,132	0
84	MG	N1	201	1/1	0.82	0.29	68,68,68,68	0
84	MG	1	3446	1/1	0.82	0.22	62,62,62,62	0
84	MG	5	3616	1/1	0.82	0.17	82,82,82,82	0
84	MG	5	3692	1/1	0.82	0.26	73,73,73,73	0
86	ZN	d7	101	1/1	0.82	0.15	272,272,272,272	0
84	MG	5	3694	1/1	0.82	0.22	84,84,84,84	0
84	MG	O4	504	1/1	0.82	0.48	76,76,76,76	0
84	MG	q2	503	1/1	0.82	0.35	52,52,52,52	0
84	MG	5	4015	1/1	0.82	0.41	59,59,59,59	0
84	MG	6	1950	1/1	0.82	0.28	72,72,72,72	0
84	MG	2	2033	1/1	0.82	0.23	108,108,108,108	0
84	MG	D3	205	1/1	0.82	0.23	86,86,86,86	0
84	MG	1	3936	1/1	0.82	0.37	67,67,67,67	0
84	MG	8	212	1/1	0.82	0.34	66,66,66,66	0
84	MG	1	3575	1/1	0.82	0.18	61,61,61,61	0
84	MG	5	3786	1/1	0.82	0.38	43,43,43,43	0
84	MG	1	3505	1/1	0.82	0.37	67,67,67,67	0
84	MG	5	3728	1/1	0.82	0.21	51,51,51,51	0
84	MG	M5	301	1/1	0.82	0.35	69,69,69,69	0
84	MG	5	3953	1/1	0.82	0.60	62,62,62,62	0
84	MG	1	3418	1/1	0.82	0.57	65,65,65,65	0
84	MG	1	3699	1/1	0.82	0.53	82,82,82,82	0
84	MG	5	3754	1/1	0.83	0.46	69,69,69,69	0
84	MG	5	3939	1/1	0.83	0.24	76,76,76,76	0
84	MG	M3	205	1/1	0.83	0.26	82,82,82,82	0
84	MG	1	3629	1/1	0.83	0.14	136,136,136,136	0
84	MG	6	2153	1/1	0.83	0.19	68,68,68,68	0
84	MG	5	4021	1/1	0.83	0.28	60,60,60,60	0
84	MG	1	3558	1/1	0.83	0.20	68,68,68,68	0
84	MG	6	2130	1/1	0.83	0.16	95,95,95,95	0
84	MG	m3	203	1/1	0.83	0.48	81,81,81,81	0
84	MG	N0	203	1/1	0.83	0.09	80,80,80,80	0
84	MG	1	3492	1/1	0.83	0.38	80,80,80,80	0
84	MG	D3	203	1/1	0.83	0.36	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	2	1919	1/1	0.83	0.28	84,84,84,84	0
84	MG	1	3922	1/1	0.83	0.25	61,61,61,61	0
84	MG	5	3897	1/1	0.83	0.42	76,76,76,76	0
84	MG	1	3807	1/1	0.83	0.46	77,77,77,77	0
84	MG	5	3839	1/1	0.83	0.25	68,68,68,68	0
84	MG	m9	201	1/1	0.83	0.24	74,74,74,74	0
84	MG	1	3941	1/1	0.83	0.17	66,66,66,66	0
84	MG	2	2018	1/1	0.83	0.10	135,135,135,135	0
84	MG	1	3837	1/1	0.83	0.48	58,58,58,58	0
85	LLL	5	4173	31/31	0.83	0.30	106,106,107,107	31
84	MG	M7	205	1/1	0.83	0.30	59,59,59,59	0
84	MG	5	3944	1/1	0.83	0.67	61,61,61,61	0
84	MG	1	3445	1/1	0.83	0.41	64,64,64,64	0
84	MG	5	4074	1/1	0.83	0.08	105,105,105,105	0
84	MG	5	3841	1/1	0.83	0.25	61,61,61,61	0
84	MG	1	3972	1/1	0.83	0.20	65,65,65,65	0
84	MG	5	4101	1/1	0.83	0.21	75,75,75,75	0
85	LLL	6	2174	31/31	0.83	0.29	81,81,81,81	31
84	MG	6	2065	1/1	0.83	0.20	104,104,104,104	0
84	MG	1	3824	1/1	0.83	0.37	62,62,62,62	0
84	MG	5	3980	1/1	0.83	0.39	52,52,52,52	0
84	MG	d3	202	1/1	0.83	0.35	69,69,69,69	0
84	MG	1	3502	1/1	0.83	0.37	64,64,64,64	0
84	MG	5	3566	1/1	0.83	0.27	60,60,60,60	0
84	MG	4	203	1/1	0.83	0.27	61,61,61,61	0
84	MG	5	3922	1/1	0.83	0.30	56,56,56,56	0
84	MG	2	1960	1/1	0.83	0.20	94,94,94,94	0
84	MG	s3	301	1/1	0.83	0.29	84,84,84,84	0
84	MG	5	3423	1/1	0.83	0.29	54,54,54,54	1
84	MG	s0	301	1/1	0.83	0.16	103,103,103,103	0
84	MG	6	1998	1/1	0.83	0.26	78,78,78,78	0
84	MG	5	3861	1/1	0.83	0.34	63,63,63,63	0
84	MG	2	1991	1/1	0.83	0.15	103,103,103,103	0
84	MG	8	220	1/1	0.83	0.35	94,94,94,94	0
84	MG	5	4072	1/1	0.83	0.09	109,109,109,109	0
84	MG	1	3695	1/1	0.83	0.64	67,67,67,67	0
84	MG	1	3935	1/1	0.83	0.26	68,68,68,68	0
84	MG	2	1901	1/1	0.83	0.21	92,92,92,92	0
84	MG	5	3708	1/1	0.83	0.30	75,75,75,75	0
84	MG	m6	205	1/1	0.83	0.27	51,51,51,51	1
84	MG	5	3691	1/1	0.83	0.43	74,74,74,74	0
84	MG	3	212	1/1	0.83	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3914	1/1	0.83	0.27	59,59,59,59	0
84	MG	6	2150	1/1	0.83	0.21	81,81,81,81	0
84	MG	5	3858	1/1	0.83	0.32	55,55,55,55	0
84	MG	13	411	1/1	0.83	0.16	53,53,53,53	0
84	MG	5	4027	1/1	0.83	0.54	50,50,50,50	0
84	MG	1	3957	1/1	0.83	0.21	71,71,71,71	0
84	MG	1	3929	1/1	0.83	0.54	63,63,63,63	0
84	MG	6	2061	1/1	0.84	0.20	80,80,80,80	0
84	MG	6	1912	1/1	0.84	0.13	95,95,95,95	0
84	MG	5	3512	1/1	0.84	0.36	56,56,56,56	0
84	MG	1	3984	1/1	0.84	0.32	65,65,65,65	0
84	MG	6	2125	1/1	0.84	0.22	71,71,71,71	0
84	MG	5	3571	1/1	0.84	0.18	77,77,77,77	0
84	MG	5	3609	1/1	0.84	0.20	87,87,87,87	0
84	MG	5	4125	1/1	0.84	0.44	55,55,55,55	0
84	MG	1	3799	1/1	0.84	0.14	93,93,93,93	0
84	MG	1	3412	1/1	0.84	0.30	51,51,51,51	0
84	MG	5	3414	1/1	0.84	0.51	54,54,54,54	0
84	MG	5	4023	1/1	0.84	0.17	58,58,58,58	1
84	MG	1	3554	1/1	0.84	0.21	67,67,67,67	0
84	MG	1	3543	1/1	0.84	0.64	51,51,51,51	0
84	MG	6	2094	1/1	0.84	0.30	69,69,69,69	0
84	MG	6	2123	1/1	0.84	0.59	142,142,142,142	0
84	MG	1	3884	1/1	0.84	0.22	80,80,80,80	0
84	MG	6	1917	1/1	0.84	0.28	89,89,89,89	0
84	MG	6	2144	1/1	0.84	0.15	76,76,76,76	0
84	MG	5	4132	1/1	0.84	0.34	94,94,94,94	0
84	MG	1	3821	1/1	0.84	0.75	68,68,68,68	0
84	MG	1	3576	1/1	0.84	0.26	72,72,72,72	0
84	MG	5	3509	1/1	0.84	0.48	65,65,65,65	0
84	MG	5	3604	1/1	0.84	0.23	78,78,78,78	0
84	MG	2	2042	1/1	0.84	0.17	101,101,101,101	0
84	MG	2	1947	1/1	0.84	0.48	92,92,92,92	0
84	MG	2	1914	1/1	0.84	0.50	83,83,83,83	0
84	MG	6	2079	1/1	0.84	0.38	63,63,63,63	0
84	MG	1	3790	1/1	0.84	0.33	78,78,78,78	0
84	MG	7	216	1/1	0.84	0.09	74,74,74,74	1
84	MG	1	3718	1/1	0.84	0.26	60,60,60,60	0
84	MG	7	222	1/1	0.84	0.13	66,66,66,66	0
84	MG	5	3598	1/1	0.84	0.55	84,84,84,84	0
84	MG	1	3908	1/1	0.84	0.36	60,60,60,60	0
84	MG	5	4128	1/1	0.84	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3624	1/1	0.84	0.23	74,74,74,74	0
84	MG	5	3688	1/1	0.84	0.39	73,73,73,73	0
84	MG	n9	101	1/1	0.84	0.44	49,49,49,49	0
84	MG	2	1908	1/1	0.84	0.37	104,104,104,104	0
84	MG	5	3940	1/1	0.84	0.36	71,71,71,71	0
84	MG	5	4118	1/1	0.84	0.17	87,87,87,87	0
84	MG	5	3709	1/1	0.84	0.17	75,75,75,75	0
84	MG	6	2089	1/1	0.84	0.25	71,71,71,71	0
84	MG	5	4141	1/1	0.84	0.29	62,62,62,62	0
84	MG	1	3925	1/1	0.84	0.30	83,83,83,83	0
84	MG	5	4004	1/1	0.84	0.32	80,80,80,80	0
85	LLL	5	4176	31/31	0.84	0.27	74,74,74,74	31
84	MG	1	3834	1/1	0.84	0.70	70,70,70,70	0
84	MG	6	2154	1/1	0.84	0.15	78,78,78,78	0
84	MG	M5	302	1/1	0.84	0.32	58,58,58,58	0
84	MG	1	3666	1/1	0.84	0.27	72,72,72,72	0
84	MG	5	3543	1/1	0.84	0.32	52,52,52,52	1
84	MG	1	3930	1/1	0.84	0.38	73,73,73,73	0
84	MG	2	1952	1/1	0.84	0.47	99,99,99,99	0
84	MG	2	2020	1/1	0.84	0.21	111,111,111,111	0
84	MG	6	2127	1/1	0.84	0.44	76,76,76,76	0
84	MG	1	3623	1/1	0.84	0.35	68,68,68,68	0
84	MG	1	3822	1/1	0.84	0.30	86,86,86,86	0
84	MG	1	3664	1/1	0.84	0.14	63,63,63,63	0
84	MG	5	3551	1/1	0.84	0.48	56,56,56,56	0
84	MG	M3	204	1/1	0.84	0.29	69,69,69,69	0
84	MG	2	1956	1/1	0.84	0.38	72,72,72,72	0
84	MG	5	3823	1/1	0.84	0.20	57,57,57,57	1
84	MG	5	3710	1/1	0.84	0.24	72,72,72,72	0
84	MG	L9	201	1/1	0.84	0.27	59,59,59,59	0
84	MG	2	1930	1/1	0.84	0.71	81,81,81,81	0
84	MG	2	2031	1/1	0.84	0.35	105,105,105,105	0
85	LLL	7	233	31/31	0.84	0.23	82,82,82,82	31
84	MG	5	3660	1/1	0.84	0.17	96,96,96,96	0
84	MG	5	3597	1/1	0.84	0.35	70,70,70,70	0
85	LLL	1	4000	31/31	0.84	0.29	84,85,85,85	31
84	MG	2	1923	1/1	0.84	0.41	87,87,87,87	0
84	MG	5	3891	1/1	0.84	0.70	75,75,75,75	0
84	MG	2	2003	1/1	0.84	0.28	118,118,118,118	0
84	MG	1	3896	1/1	0.84	0.19	73,73,73,73	0
84	MG	6	2027	1/1	0.84	0.19	61,61,61,61	0
84	MG	1	3730	1/1	0.84	0.38	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	2117	1/1	0.85	0.53	56,56,56,56	0
84	MG	3	219	1/1	0.85	0.31	79,79,79,79	0
84	MG	7	229	1/1	0.85	0.27	72,72,72,72	0
84	MG	1	3831	1/1	0.85	0.38	59,59,59,59	0
84	MG	5	3935	1/1	0.85	0.28	52,52,52,52	0
84	MG	6	1929	1/1	0.85	0.38	69,69,69,69	0
84	MG	1	3700	1/1	0.85	0.91	52,52,52,52	0
85	LLL	6	2175	31/31	0.85	0.30	66,66,66,66	31
84	MG	2	2009	1/1	0.85	0.19	117,117,117,117	0
84	MG	5	3822	1/1	0.85	0.16	60,60,60,60	0
84	MG	5	3610	1/1	0.85	0.24	110,110,110,110	0
84	MG	1	3468	1/1	0.85	0.45	61,61,61,61	0
84	MG	5	3924	1/1	0.85	0.30	56,56,56,56	0
84	MG	5	3732	1/1	0.85	0.32	70,70,70,70	0
84	MG	6	1906	1/1	0.85	0.29	76,76,76,76	0
84	MG	5	4077	1/1	0.85	0.26	70,70,70,70	0
84	MG	1	3413	1/1	0.85	0.21	55,55,55,55	1
85	LLL	1	4002	31/31	0.85	0.35	136,137,137,137	0
84	MG	5	4148	1/1	0.85	0.47	54,54,54,54	0
84	MG	1	3965	1/1	0.85	0.32	67,67,67,67	1
84	MG	1	3735	1/1	0.85	0.45	77,77,77,77	0
84	MG	5	3650	1/1	0.85	0.51	80,80,80,80	0
84	MG	1	3615	1/1	0.85	0.26	59,59,59,59	0
84	MG	6	2083	1/1	0.85	0.29	78,78,78,78	0
84	MG	l3	407	1/1	0.85	0.33	55,55,55,55	0
84	MG	6	1975	1/1	0.85	0.23	83,83,83,83	0
84	MG	1	3863	1/1	0.85	0.29	74,74,74,74	0
84	MG	1	3878	1/1	0.85	0.44	60,60,60,60	0
84	MG	L3	402	1/1	0.85	0.58	60,60,60,60	0
84	MG	1	3905	1/1	0.85	0.22	76,76,76,76	0
84	MG	5	4020	1/1	0.85	0.34	72,72,72,72	0
84	MG	5	4144	1/1	0.85	0.18	58,58,58,58	0
84	MG	5	3477	1/1	0.85	0.42	60,60,60,60	0
84	MG	1	3978	1/1	0.85	0.31	89,89,89,89	0
84	MG	5	4099	1/1	0.85	0.27	105,105,105,105	0
84	MG	n0	206	1/1	0.85	0.44	48,48,48,48	0
84	MG	6	2110	1/1	0.85	0.12	124,124,124,124	0
84	MG	q2	504	1/1	0.85	0.56	60,60,60,60	0
84	MG	5	3919	1/1	0.85	0.30	51,51,51,51	0
84	MG	5	4136	1/1	0.85	0.25	70,70,70,70	0
84	MG	1	3593	1/1	0.85	0.47	63,63,63,63	0
84	MG	5	3969	1/1	0.85	0.49	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3794	1/1	0.85	0.32	68,68,68,68	0
84	MG	5	3837	1/1	0.85	0.30	72,72,72,72	0
84	MG	1	3961	1/1	0.85	0.18	80,80,80,80	0
84	MG	5	3800	1/1	0.85	0.21	69,69,69,69	0
84	MG	5	4116	1/1	0.85	0.13	82,82,82,82	0
84	MG	5	3881	1/1	0.85	0.43	63,63,63,63	0
84	MG	6	1971	1/1	0.85	0.36	73,73,73,73	0
85	LLL	5	4175	31/31	0.85	0.29	60,60,60,60	31
85	LLL	4	224	31/31	0.85	0.36	99,99,99,99	0
84	MG	5	3653	1/1	0.85	0.26	76,76,76,76	0
84	MG	m8	201	1/1	0.85	0.28	55,55,55,55	0
84	MG	6	2145	1/1	0.85	0.20	77,77,77,77	0
84	MG	5	4140	1/1	0.85	0.33	57,57,57,57	0
84	MG	m4	203	1/1	0.85	0.21	59,59,59,59	0
84	MG	1	3785	1/1	0.85	0.26	73,73,73,73	0
84	MG	5	3923	1/1	0.85	0.90	67,67,67,67	0
84	MG	5	3441	1/1	0.85	0.25	72,72,72,72	0
84	MG	1	3903	1/1	0.86	0.23	80,80,80,80	0
84	MG	1	3547	1/1	0.86	0.30	65,65,65,65	0
84	MG	1	3609	1/1	0.86	0.36	52,52,52,52	0
84	MG	5	3880	1/1	0.86	0.22	73,73,73,73	0
84	MG	5	4059	1/1	0.86	0.37	66,66,66,66	0
84	MG	5	4069	1/1	0.86	0.12	110,110,110,110	0
84	MG	1	3747	1/1	0.86	0.23	71,71,71,71	0
84	MG	5	3649	1/1	0.86	0.14	63,63,63,63	1
85	LLL	7	232	31/31	0.86	0.34	81,81,81,81	31
84	MG	5	3806	1/1	0.86	0.39	73,73,73,73	0
84	MG	6	2023	1/1	0.86	0.19	79,79,79,79	0
84	MG	1	3841	1/1	0.86	0.45	92,92,92,92	0
84	MG	5	3494	1/1	0.86	0.23	59,59,59,59	0
84	MG	m7	203	1/1	0.86	0.38	63,63,63,63	0
84	MG	1	3875	1/1	0.86	0.37	64,64,64,64	0
84	MG	1	3969	1/1	0.86	0.34	72,72,72,72	0
84	MG	5	4146	1/1	0.86	0.22	63,63,63,63	0
84	MG	1	3828	1/1	0.86	0.58	67,67,67,67	0
84	MG	c3	202	1/1	0.86	0.29	87,87,87,87	0
84	MG	M7	201	1/1	0.86	0.29	59,59,59,59	0
84	MG	1	3813	1/1	0.86	0.29	80,80,80,80	0
84	MG	5	3962	1/1	0.86	0.53	95,95,95,95	0
84	MG	1	3569	1/1	0.86	0.16	75,75,75,75	0
84	MG	5	4084	1/1	0.86	0.19	96,96,96,96	0
84	MG	6	2133	1/1	0.86	0.20	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	l3	403	1/1	0.86	0.45	43,43,43,43	0
84	MG	6	1947	1/1	0.86	0.42	64,64,64,64	0
84	MG	6	2073	1/1	0.86	0.27	80,80,80,80	0
84	MG	1	3641	1/1	0.86	0.29	104,104,104,104	0
84	MG	5	3557	1/1	0.86	0.24	62,62,62,62	1
84	MG	1	3791	1/1	0.86	0.18	83,83,83,83	0
84	MG	5	3951	1/1	0.86	0.92	68,68,68,68	0
84	MG	6	1916	1/1	0.86	0.22	94,94,94,94	0
84	MG	1	3979	1/1	0.86	0.19	69,69,69,69	0
84	MG	5	3781	1/1	0.86	0.21	56,56,56,56	0
84	MG	1	3592	1/1	0.86	0.35	62,62,62,62	1
84	MG	5	3894	1/1	0.86	0.51	72,72,72,72	0
84	MG	3	209	1/1	0.86	0.18	70,70,70,70	0
84	MG	1	3466	1/1	0.86	0.45	54,54,54,54	0
84	MG	5	3981	1/1	0.86	0.31	46,46,46,46	0
84	MG	1	3431	1/1	0.86	0.35	56,56,56,56	0
85	LLL	5	4177	31/31	0.86	0.32	51,51,51,51	31
84	MG	1	3835	1/1	0.86	0.24	58,58,58,58	0
84	MG	1	3703	1/1	0.86	0.47	65,65,65,65	0
85	LLL	2	2044	31/31	0.86	0.28	116,116,116,116	0
84	MG	5	3528	1/1	0.86	0.89	56,56,56,56	0
84	MG	5	3627	1/1	0.86	0.32	53,53,53,53	1
84	MG	6	1938	1/1	0.86	0.36	59,59,59,59	0
84	MG	1	3622	1/1	0.86	0.38	87,87,87,87	0
85	LLL	2	2045	31/31	0.86	0.41	117,117,117,118	0
84	MG	5	4043	1/1	0.86	0.33	51,51,51,51	0
84	MG	2	2038	1/1	0.86	0.12	117,117,117,117	0
84	MG	3	205	1/1	0.86	0.21	61,61,61,61	1
84	MG	6	1990	1/1	0.86	0.26	73,73,73,73	0
84	MG	1	3774	1/1	0.86	0.30	61,61,61,61	0
84	MG	5	3674	1/1	0.86	0.45	65,65,65,65	0
84	MG	2	1942	1/1	0.86	0.45	84,84,84,84	0
85	LLL	5	4156	31/31	0.86	0.28	83,84,84,84	31
84	MG	5	3453	1/1	0.86	0.36	56,56,56,56	0
84	MG	7	214	1/1	0.86	0.33	80,80,80,80	0
84	MG	5	3972	1/1	0.86	0.45	60,60,60,60	0
84	MG	5	3576	1/1	0.86	0.33	52,52,52,52	0
84	MG	2	1989	1/1	0.86	0.10	114,114,114,114	0
85	LLL	6	2173	31/31	0.86	0.35	102,102,103,103	31
84	MG	5	4150	1/1	0.86	0.19	81,81,81,81	0
84	MG	5	3550	1/1	0.86	0.39	59,59,59,59	0
84	MG	5	3950	1/1	0.86	0.66	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	4067	1/1	0.86	0.24	76,76,76,76	0
84	MG	1	3476	1/1	0.86	0.49	54,54,54,54	0
84	MG	5	3403	1/1	0.86	0.37	54,54,54,54	0
84	MG	1	3626	1/1	0.86	0.26	63,63,63,63	0
84	MG	d3	204	1/1	0.86	0.27	66,66,66,66	0
84	MG	5	4035	1/1	0.86	0.27	76,76,76,76	0
84	MG	L4	401	1/1	0.86	0.32	69,69,69,69	0
84	MG	2	2019	1/1	0.86	0.09	127,127,127,127	0
84	MG	q1	102	1/1	0.86	0.34	64,64,64,64	0
84	MG	1	3573	1/1	0.86	0.13	65,65,65,65	0
84	MG	2	1968	1/1	0.87	0.29	95,95,95,95	0
84	MG	2	1941	1/1	0.87	0.36	60,60,60,60	0
84	MG	5	3809	1/1	0.87	0.20	60,60,60,60	0
84	MG	5	3947	1/1	0.87	0.48	57,57,57,57	0
84	MG	5	3907	1/1	0.87	0.33	41,41,41,41	0
84	MG	5	3743	1/1	0.87	0.44	61,61,61,61	0
84	MG	5	3608	1/1	0.87	0.13	95,95,95,95	0
84	MG	5	3523	1/1	0.87	0.33	55,55,55,55	0
84	MG	5	3454	1/1	0.87	0.42	46,46,46,46	0
84	MG	5	3618	1/1	0.87	0.43	83,83,83,83	0
85	LLL	5	4169	31/31	0.87	0.31	51,51,51,51	31
84	MG	5	3596	1/1	0.87	0.34	82,82,82,82	0
84	MG	1	3727	1/1	0.87	0.48	55,55,55,55	0
84	MG	5	3581	1/1	0.87	0.45	53,53,53,53	0
84	MG	2	2005	1/1	0.87	0.16	83,83,83,83	0
84	MG	3	213	1/1	0.87	0.14	90,90,90,90	0
84	MG	5	4115	1/1	0.87	0.44	59,59,59,59	0
84	MG	1	3819	1/1	0.87	0.30	80,80,80,80	0
84	MG	6	1914	1/1	0.87	0.08	114,114,114,114	0
84	MG	1	3620	1/1	0.87	0.66	65,65,65,65	0
84	MG	2	2029	1/1	0.87	0.18	110,110,110,110	0
84	MG	6	2091	1/1	0.87	0.49	68,68,68,68	0
84	MG	5	3491	1/1	0.87	0.14	62,62,62,62	0
84	MG	5	3605	1/1	0.87	0.12	76,76,76,76	0
84	MG	o3	201	1/1	0.87	0.23	56,56,56,56	0
84	MG	6	2160	1/1	0.87	0.29	88,88,88,88	0
84	MG	5	3466	1/1	0.87	0.34	50,50,50,50	0
84	MG	1	3869	1/1	0.87	0.39	62,62,62,62	0
84	MG	5	4034	1/1	0.87	0.24	68,68,68,68	0
84	MG	5	3698	1/1	0.87	0.32	81,81,81,81	0
84	MG	2	2028	1/1	0.87	0.21	117,117,117,117	0
84	MG	6	1961	1/1	0.87	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3874	1/1	0.87	0.27	70,70,70,70	0
84	MG	6	2101	1/1	0.87	0.34	82,82,82,82	0
84	MG	2	1951	1/1	0.87	0.70	95,95,95,95	0
84	MG	5	3925	1/1	0.87	0.31	53,53,53,53	0
84	MG	o2	203	1/1	0.87	0.27	51,51,51,51	0
84	MG	5	4051	1/1	0.87	0.31	77,77,77,77	0
84	MG	6	1984	1/1	0.87	0.18	89,89,89,89	0
84	MG	5	3938	1/1	0.87	0.16	66,66,66,66	0
84	MG	6	2163	1/1	0.87	0.43	66,66,66,66	1
84	MG	S1	301	1/1	0.87	0.27	94,94,94,94	0
84	MG	n0	201	1/1	0.87	0.15	68,68,68,68	0
84	MG	1	3625	1/1	0.87	0.17	71,71,71,71	0
84	MG	2	2025	1/1	0.87	0.20	123,123,123,123	0
84	MG	1	3488	1/1	0.87	0.26	73,73,73,73	0
84	MG	6	2010	1/1	0.87	0.33	68,68,68,68	0
84	MG	3	207	1/1	0.87	0.21	58,58,58,58	0
84	MG	1	3687	1/1	0.87	0.36	51,51,51,51	0
85	LLL	5	4171	31/31	0.87	0.24	107,107,107,107	0
84	MG	1	3775	1/1	0.87	0.36	62,62,62,62	0
84	MG	7	228	1/1	0.87	0.27	73,73,73,73	0
84	MG	l5	306	1/1	0.87	0.13	70,70,70,70	0
85	LLL	5	4174	31/31	0.87	0.33	47,47,47,47	31
84	MG	1	3582	1/1	0.87	0.28	65,65,65,65	0
85	LLL	5	4155	31/31	0.87	0.30	81,81,82,82	0
84	MG	6	1921	1/1	0.87	0.22	76,76,76,76	0
84	MG	1	3549	1/1	0.87	0.27	67,67,67,67	0
84	MG	5	3741	1/1	0.87	0.45	58,58,58,58	0
84	MG	5	3484	1/1	0.87	0.47	74,74,74,74	0
84	MG	4	204	1/1	0.87	0.30	69,69,69,69	0
84	MG	1	3913	1/1	0.87	0.29	59,59,59,59	0
84	MG	5	3744	1/1	0.87	0.40	65,65,65,65	0
84	MG	1	3713	1/1	0.87	0.12	81,81,81,81	0
84	MG	5	3887	1/1	0.87	0.12	84,84,84,84	0
84	MG	5	3749	1/1	0.87	0.39	77,77,77,77	0
84	MG	6	2131	1/1	0.87	0.16	89,89,89,89	0
84	MG	5	4006	1/1	0.87	0.44	64,64,64,64	0
84	MG	6	2152	1/1	0.87	0.19	68,68,68,68	0
84	MG	5	3446	1/1	0.87	0.33	53,53,53,53	0
84	MG	1	3691	1/1	0.87	0.26	59,59,59,59	0
84	MG	1	3784	1/1	0.87	0.51	72,72,72,72	0
84	MG	2	1917	1/1	0.87	0.22	88,88,88,88	0
84	MG	1	3459	1/1	0.87	0.47	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	m5	302	1/1	0.87	0.33	71,71,71,71	0
84	MG	5	4119	1/1	0.88	0.09	142,142,142,142	0
84	MG	5	3893	1/1	0.88	0.62	65,65,65,65	0
84	MG	4	218	1/1	0.88	0.23	60,60,60,60	0
84	MG	5	3909	1/1	0.88	0.27	48,48,48,48	1
84	MG	5	3629	1/1	0.88	0.33	60,60,60,60	0
84	MG	5	3510	1/1	0.88	0.27	62,62,62,62	0
84	MG	5	3718	1/1	0.88	0.34	68,68,68,68	0
84	MG	5	4133	1/1	0.88	0.28	114,114,114,114	0
84	MG	L3	401	1/1	0.88	0.17	76,76,76,76	0
84	MG	1	3455	1/1	0.88	0.42	70,70,70,70	0
84	MG	2	1912	1/1	0.88	0.55	86,86,86,86	0
84	MG	7	224	1/1	0.88	0.18	71,71,71,71	0
84	MG	5	3850	1/1	0.88	0.24	58,58,58,58	0
85	LLL	7	231	31/31	0.88	0.20	81,82,82,82	31
84	MG	1	3654	1/1	0.88	0.34	53,53,53,53	0
84	MG	1	3614	1/1	0.88	0.32	58,58,58,58	0
84	MG	1	3570	1/1	0.88	0.34	71,71,71,71	0
84	MG	1	3503	1/1	0.88	0.31	61,61,61,61	0
84	MG	5	3941	1/1	0.88	0.62	78,78,78,78	0
84	MG	1	3452	1/1	0.88	0.19	65,65,65,65	0
84	MG	5	3424	1/1	0.88	0.32	54,54,54,54	0
84	MG	5	3723	1/1	0.88	0.26	74,74,74,74	0
84	MG	1	3710	1/1	0.88	0.28	90,90,90,90	0
84	MG	m9	202	1/1	0.88	0.62	90,90,90,90	0
84	MG	2	1935	1/1	0.88	0.44	66,66,66,66	0
84	MG	1	3973	1/1	0.88	0.34	64,64,64,64	0
84	MG	4	222	1/1	0.88	0.20	79,79,79,79	0
84	MG	6	1941	1/1	0.88	0.45	66,66,66,66	1
84	MG	6	2093	1/1	0.88	0.25	75,75,75,75	0
84	MG	7	205	1/1	0.88	0.38	55,55,55,55	0
84	MG	6	1915	1/1	0.88	0.13	74,74,74,74	0
84	MG	1	3910	1/1	0.88	0.64	56,56,56,56	0
85	LLL	1	3995	31/31	0.88	0.24	124,125,125,125	0
84	MG	6	1919	1/1	0.88	0.11	80,80,80,80	0
84	MG	5	3455	1/1	0.88	0.34	55,55,55,55	0
84	MG	6	1954	1/1	0.88	0.27	80,80,80,80	0
84	MG	1	3660	1/1	0.88	0.15	72,72,72,72	0
84	MG	1	3970	1/1	0.88	0.42	50,50,50,50	0
84	MG	1	3611	1/1	0.88	0.40	47,47,47,47	0
84	MG	6	2067	1/1	0.88	0.24	92,92,92,92	0
84	MG	5	3873	1/1	0.88	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3487	1/1	0.88	0.27	79,79,79,79	0
84	MG	5	4002	1/1	0.88	0.22	64,64,64,64	0
84	MG	1	3683	1/1	0.88	0.29	64,64,64,64	0
84	MG	1	3586	1/1	0.88	0.28	58,58,58,58	0
84	MG	5	3763	1/1	0.88	0.35	78,78,78,78	0
84	MG	m4	205	1/1	0.88	0.15	58,58,58,58	0
84	MG	5	3632	1/1	0.88	0.38	49,49,49,49	0
84	MG	3	217	1/1	0.88	0.13	100,100,100,100	0
84	MG	5	3456	1/1	0.88	0.23	53,53,53,53	0
84	MG	O2	202	1/1	0.88	0.32	55,55,55,55	0
84	MG	6	2039	1/1	0.88	0.20	83,83,83,83	0
84	MG	N3	203	1/1	0.88	0.25	75,75,75,75	0
84	MG	1	3786	1/1	0.88	0.78	70,70,70,70	0
84	MG	6	2147	1/1	0.88	0.18	78,78,78,78	0
84	MG	5	4047	1/1	0.88	0.33	52,52,52,52	0
85	LLL	1	3996	31/31	0.88	0.28	107,107,108,108	31
84	MG	1	3546	1/1	0.88	0.27	63,63,63,63	0
84	MG	l9	202	1/1	0.88	0.35	58,58,58,58	0
84	MG	5	3932	1/1	0.88	0.25	52,52,52,52	0
84	MG	6	1966	1/1	0.88	0.18	73,73,73,73	0
84	MG	m5	301	1/1	0.88	0.29	62,62,62,62	0
85	LLL	1	3997	31/31	0.88	0.36	108,108,108,108	0
84	MG	1	3838	1/1	0.88	0.32	50,50,50,50	0
84	MG	6	2050	1/1	0.88	0.17	71,71,71,71	0
84	MG	1	3812	1/1	0.88	0.19	82,82,82,82	0
84	MG	1	3440	1/1	0.88	0.23	82,82,82,82	0
84	MG	5	4001	1/1	0.88	0.25	59,59,59,59	0
85	LLL	1	4001	31/31	0.88	0.22	121,121,121,121	0
84	MG	5	4014	1/1	0.88	0.32	62,62,62,62	0
84	MG	1	3692	1/1	0.88	0.39	64,64,64,64	0
84	MG	6	2068	1/1	0.88	0.14	83,83,83,83	0
84	MG	5	3910	1/1	0.88	0.27	52,52,52,52	0
84	MG	M3	202	1/1	0.88	0.20	80,80,80,80	0
84	MG	5	4065	1/1	0.88	0.36	58,58,58,58	0
84	MG	2	1946	1/1	0.88	0.55	80,80,80,80	0
84	MG	2	1949	1/1	0.89	0.32	102,102,102,102	0
84	MG	1	3402	1/1	0.89	0.24	60,60,60,60	0
84	MG	1	3512	1/1	0.89	0.50	66,66,66,66	0
84	MG	1	3753	1/1	0.89	0.46	64,64,64,64	0
84	MG	5	3448	1/1	0.89	0.35	49,49,49,49	0
84	MG	n8	202	1/1	0.89	0.20	73,73,73,73	0
84	MG	5	3769	1/1	0.89	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3489	1/1	0.89	0.24	79,79,79,79	0
84	MG	5	3736	1/1	0.89	0.43	59,59,59,59	0
84	MG	6	2053	1/1	0.89	0.16	74,74,74,74	0
84	MG	1	3524	1/1	0.89	0.40	71,71,71,71	0
84	MG	c8	202	1/1	0.89	0.19	75,75,75,75	0
84	MG	5	3846	1/1	0.89	0.21	55,55,55,55	0
84	MG	2	1939	1/1	0.89	0.26	80,80,80,80	0
84	MG	5	3435	1/1	0.89	0.20	50,50,50,50	0
84	MG	6	2102	1/1	0.89	0.29	80,80,80,80	0
84	MG	1	3887	1/1	0.89	0.35	55,55,55,55	0
84	MG	5	3748	1/1	0.89	0.33	46,46,46,46	0
84	MG	1	3806	1/1	0.89	0.24	65,65,65,65	0
84	MG	1	3931	1/1	0.89	0.25	79,79,79,79	0
85	LLL	1	3998	31/31	0.89	0.35	99,100,100,100	31
84	MG	m4	204	1/1	0.89	0.38	57,57,57,57	0
84	MG	5	3990	1/1	0.89	0.34	47,47,47,47	0
84	MG	6	1949	1/1	0.89	0.18	74,74,74,74	0
84	MG	5	3821	1/1	0.89	0.27	53,53,53,53	0
84	MG	1	3441	1/1	0.89	0.33	62,62,62,62	0
84	MG	5	3449	1/1	0.89	0.42	50,50,50,50	0
84	MG	l6	201	1/1	0.89	0.26	60,60,60,60	0
84	MG	5	3495	1/1	0.89	0.26	58,58,58,58	0
84	MG	5	3888	1/1	0.89	0.32	62,62,62,62	0
84	MG	5	3530	1/1	0.89	0.37	47,47,47,47	1
84	MG	5	3699	1/1	0.89	0.31	63,63,63,63	0
84	MG	5	3474	1/1	0.89	0.18	67,67,67,67	0
84	MG	5	3420	1/1	0.89	0.29	50,50,50,50	0
84	MG	5	3431	1/1	0.89	0.33	53,53,53,53	0
84	MG	c4	201	1/1	0.89	0.20	87,87,87,87	0
84	MG	1	3443	1/1	0.89	0.26	58,58,58,58	0
84	MG	7	212	1/1	0.89	0.25	65,65,65,65	0
84	MG	7	209	1/1	0.89	0.12	64,64,64,64	0
84	MG	5	3971	1/1	0.89	0.84	72,72,72,72	0
84	MG	s5	301	1/1	0.89	0.38	74,74,74,74	0
84	MG	M7	203	1/1	0.89	0.22	59,59,59,59	0
84	MG	1	3898	1/1	0.89	0.09	99,99,99,99	0
84	MG	1	3677	1/1	0.89	0.54	66,66,66,66	0
84	MG	s5	302	1/1	0.89	0.31	76,76,76,76	0
84	MG	5	3746	1/1	0.89	0.41	40,40,40,40	0
85	LLL	5	4166	31/31	0.89	0.26	77,78,78,78	31
84	MG	m3	204	1/1	0.89	0.35	59,59,59,59	0
84	MG	5	3620	1/1	0.89	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3899	1/1	0.89	0.11	82,82,82,82	0
84	MG	6	2038	1/1	0.89	0.30	85,85,85,85	0
84	MG	1	3462	1/1	0.89	0.21	54,54,54,54	1
84	MG	5	4143	1/1	0.89	0.17	72,72,72,72	0
84	MG	5	3762	1/1	0.89	0.38	65,65,65,65	0
84	MG	2	1958	1/1	0.89	0.15	108,108,108,108	0
84	MG	1	3808	1/1	0.89	0.24	71,71,71,71	0
84	MG	5	3496	1/1	0.89	0.24	56,56,56,56	0
84	MG	5	4058	1/1	0.89	0.13	95,95,95,95	0
84	MG	6	1936	1/1	0.89	0.79	65,65,65,65	0
84	MG	5	3621	1/1	0.89	0.15	77,77,77,77	0
85	LLL	5	4158	31/31	0.89	0.28	60,60,60,60	31
84	MG	5	3862	1/1	0.89	0.34	67,67,67,67	0
84	MG	1	3661	1/1	0.89	0.26	78,78,78,78	0
84	MG	1	3915	1/1	0.89	0.16	78,78,78,78	0
84	MG	5	3845	1/1	0.89	0.24	48,48,48,48	1
84	MG	2	1993	1/1	0.89	0.21	99,99,99,99	0
84	MG	5	3657	1/1	0.89	0.27	73,73,73,73	0
84	MG	5	3829	1/1	0.89	0.20	57,57,57,57	0
84	MG	5	3834	1/1	0.89	0.32	60,60,60,60	0
84	MG	5	4053	1/1	0.89	0.15	94,94,94,94	0
84	MG	5	3592	1/1	0.89	0.33	57,57,57,57	0
84	MG	5	4126	1/1	0.89	0.48	60,60,60,60	0
84	MG	5	3729	1/1	0.89	0.36	57,57,57,57	0
84	MG	1	3901	1/1	0.89	0.20	74,74,74,74	0
85	LLL	1	3999	31/31	0.89	0.29	85,86,86,86	31
84	MG	m6	201	1/1	0.89	0.25	52,52,52,52	0
84	MG	5	3964	1/1	0.89	0.59	82,82,82,82	0
84	MG	5	3730	1/1	0.89	0.30	74,74,74,74	0
84	MG	c3	205	1/1	0.89	0.28	84,84,84,84	0
84	MG	1	3988	1/1	0.89	0.23	53,53,53,53	0
84	MG	1	3451	1/1	0.89	0.11	69,69,69,69	0
84	MG	2	1911	1/1	0.89	0.16	91,91,91,91	0
84	MG	5	3765	1/1	0.89	0.24	64,64,64,64	0
84	MG	1	3864	1/1	0.89	0.21	61,61,61,61	0
84	MG	5	3977	1/1	0.89	0.27	67,67,67,67	0
84	MG	5	3628	1/1	0.89	0.40	60,60,60,60	0
84	MG	l9	204	1/1	0.89	0.21	57,57,57,57	0
84	MG	1	3632	1/1	0.89	0.10	72,72,72,72	0
84	MG	1	3877	1/1	0.89	0.31	68,68,68,68	0
84	MG	1	3653	1/1	0.89	0.26	59,59,59,59	0
84	MG	1	3867	1/1	0.89	0.33	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3486	1/1	0.89	0.31	52,52,52,52	0
84	MG	8	204	1/1	0.89	0.30	70,70,70,70	0
84	MG	5	3567	1/1	0.89	0.19	62,62,62,62	0
84	MG	2	1924	1/1	0.89	0.24	90,90,90,90	0
84	MG	n8	203	1/1	0.90	0.20	70,70,70,70	0
85	LLL	5	4162	31/31	0.90	0.16	117,118,118,118	0
84	MG	n1	202	1/1	0.90	0.26	61,61,61,61	0
84	MG	5	3619	1/1	0.90	0.18	86,86,86,86	0
85	LLL	8	221	31/31	0.90	0.22	100,100,100,100	31
84	MG	1	3768	1/1	0.90	0.44	67,67,67,67	0
84	MG	1	3552	1/1	0.90	0.14	84,84,84,84	0
84	MG	1	3709	1/1	0.90	0.27	60,60,60,60	0
84	MG	8	218	1/1	0.90	0.32	84,84,84,84	0
84	MG	1	3737	1/1	0.90	0.33	73,73,73,73	0
84	MG	5	3714	1/1	0.90	0.23	71,71,71,71	0
84	MG	14	1102	1/1	0.90	0.27	57,57,57,57	0
84	MG	1	3551	1/1	0.90	0.22	68,68,68,68	0
84	MG	6	1902	1/1	0.90	0.34	51,51,51,51	0
84	MG	5	3801	1/1	0.90	0.17	61,61,61,61	0
84	MG	1	3536	1/1	0.90	0.31	64,64,64,64	0
84	MG	1	3924	1/1	0.90	0.35	65,65,65,65	0
85	LLL	1	4004	31/31	0.90	0.23	100,101,101,101	31
84	MG	8	211	1/1	0.90	0.58	63,63,63,63	0
84	MG	5	3978	1/1	0.90	0.37	51,51,51,51	0
85	LLL	5	4167	31/31	0.90	0.17	125,126,126,126	0
84	MG	5	3647	1/1	0.90	0.36	58,58,58,58	0
84	MG	6	2008	1/1	0.90	0.25	67,67,67,67	0
84	MG	17	303	1/1	0.90	0.20	56,56,56,56	0
84	MG	13	409	1/1	0.90	0.22	70,70,70,70	0
84	MG	5	4138	1/1	0.90	0.24	48,48,48,48	0
84	MG	7	226	1/1	0.90	0.14	72,72,72,72	0
84	MG	1	3618	1/1	0.90	0.61	58,58,58,58	1
84	MG	5	3525	1/1	0.90	0.17	51,51,51,51	1
84	MG	1	3424	1/1	0.90	0.38	61,61,61,61	0
84	MG	5	3844	1/1	0.90	0.28	52,52,52,52	0
84	MG	1	3702	1/1	0.90	0.63	64,64,64,64	0
84	MG	5	3460	1/1	0.90	0.20	49,49,49,49	0
84	MG	1	3767	1/1	0.90	0.56	57,57,57,57	0
84	MG	m6	206	1/1	0.90	0.36	51,51,51,51	0
84	MG	2	2002	1/1	0.90	0.47	117,117,117,117	0
84	MG	5	3700	1/1	0.90	0.32	65,65,65,65	0
84	MG	L4	404	1/1	0.90	0.58	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	d6	103	1/1	0.90	0.24	77,77,77,77	0
84	MG	1	3825	1/1	0.90	0.74	77,77,77,77	0
84	MG	1	3572	1/1	0.90	0.17	70,70,70,70	0
84	MG	2	1907	1/1	0.90	0.17	95,95,95,95	0
84	MG	6	2136	1/1	0.90	0.16	85,85,85,85	0
84	MG	1	3645	1/1	0.90	0.55	55,55,55,55	0
84	MG	s4	301	1/1	0.90	0.23	103,103,103,103	0
84	MG	1	3714	1/1	0.90	0.16	90,90,90,90	0
85	LLL	8	222	31/31	0.90	0.36	102,102,102,102	31
84	MG	1	3939	1/1	0.90	0.30	61,61,61,61	0
84	MG	l9	203	1/1	0.90	0.24	49,49,49,49	0
84	MG	1	3724	1/1	0.90	0.15	63,63,63,63	0
84	MG	6	2012	1/1	0.90	0.21	61,61,61,61	0
84	MG	1	3916	1/1	0.90	0.15	70,70,70,70	0
84	MG	5	3631	1/1	0.90	0.21	55,55,55,55	0
84	MG	1	3680	1/1	0.90	0.35	59,59,59,59	0
84	MG	m7	205	1/1	0.90	0.21	53,53,53,53	0
84	MG	5	3590	1/1	0.90	0.35	59,59,59,59	0
84	MG	1	3798	1/1	0.90	0.36	60,60,60,60	0
84	MG	5	3554	1/1	0.90	0.22	60,60,60,60	0
85	LLL	6	2172	31/31	0.90	0.26	103,104,104,104	0
84	MG	5	3756	1/1	0.90	0.38	61,61,61,61	0
84	MG	1	3500	1/1	0.90	0.51	68,68,68,68	0
84	MG	5	3467	1/1	0.90	0.25	48,48,48,48	0
84	MG	1	3550	1/1	0.90	0.24	69,69,69,69	0
84	MG	1	3564	1/1	0.90	0.14	71,71,71,71	0
84	MG	6	1927	1/1	0.90	0.28	78,78,78,78	0
84	MG	4	213	1/1	0.90	0.42	80,80,80,80	0
84	MG	6	2028	1/1	0.90	0.12	99,99,99,99	0
84	MG	5	3606	1/1	0.90	0.10	84,84,84,84	0
84	MG	2	1972	1/1	0.90	0.22	88,88,88,88	0
84	MG	5	3804	1/1	0.90	0.06	73,73,73,73	1
84	MG	1	3911	1/1	0.90	0.40	56,56,56,56	0
84	MG	1	3672	1/1	0.90	0.31	52,52,52,52	0
84	MG	1	3874	1/1	0.90	0.21	66,66,66,66	0
84	MG	N8	202	1/1	0.90	0.72	73,73,73,73	0
84	MG	5	3602	1/1	0.90	0.26	81,81,81,81	0
84	MG	5	3642	1/1	0.90	0.47	52,52,52,52	0
84	MG	L2	305	1/1	0.90	0.31	60,60,60,60	0
84	MG	5	4013	1/1	0.90	0.31	58,58,58,58	0
84	MG	5	3433	1/1	0.90	0.38	48,48,48,48	0
84	MG	5	4082	1/1	0.90	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3642	1/1	0.90	0.25	71,71,71,71	0
84	MG	4	205	1/1	0.90	0.20	87,87,87,87	0
84	MG	5	3854	1/1	0.90	0.23	60,60,60,60	0
84	MG	5	3875	1/1	0.90	0.39	80,80,80,80	0
84	MG	1	3757	1/1	0.90	0.56	62,62,62,62	0
84	MG	14	1101	1/1	0.90	0.29	65,65,65,65	0
85	LLL	6	2168	31/31	0.90	0.24	86,86,86,87	0
84	MG	1	3538	1/1	0.90	0.35	64,64,64,64	0
84	MG	5	3921	1/1	0.90	0.19	52,52,52,52	0
84	MG	2	1962	1/1	0.90	0.19	100,100,100,100	0
84	MG	5	3933	1/1	0.90	0.34	55,55,55,55	0
84	MG	5	3747	1/1	0.90	0.24	46,46,46,46	0
84	MG	5	3779	1/1	0.90	0.38	67,67,67,67	0
84	MG	1	3708	1/1	0.90	0.38	66,66,66,66	0
84	MG	6	2158	1/1	0.91	0.22	77,77,77,77	0
84	MG	5	4062	1/1	0.91	0.16	86,86,86,86	0
84	MG	6	2080	1/1	0.91	0.31	62,62,62,62	0
84	MG	5	4089	1/1	0.91	0.70	62,62,62,62	0
84	MG	5	4107	1/1	0.91	0.27	59,59,59,59	0
84	MG	5	3892	1/1	0.91	0.80	68,68,68,68	0
84	MG	5	3928	1/1	0.91	0.22	46,46,46,46	0
84	MG	1	3633	1/1	0.91	0.29	79,79,79,79	0
84	MG	1	3923	1/1	0.91	0.47	72,72,72,72	0
84	MG	5	3871	1/1	0.91	0.24	71,71,71,71	0
84	MG	1	3733	1/1	0.91	0.61	80,80,80,80	0
84	MG	5	3787	1/1	0.91	0.24	48,48,48,48	1
84	MG	2	2012	1/1	0.91	0.11	127,127,127,127	0
84	MG	6	2017	1/1	0.91	0.12	81,81,81,81	0
84	MG	Q2	505	1/1	0.91	0.35	59,59,59,59	0
84	MG	5	3430	1/1	0.91	0.33	49,49,49,49	0
84	MG	6	1946	1/1	0.91	0.14	70,70,70,70	0
84	MG	1	3956	1/1	0.91	0.25	71,71,71,71	0
84	MG	5	3753	1/1	0.91	0.47	85,85,85,85	0
84	MG	6	1978	1/1	0.91	0.13	93,93,93,93	0
84	MG	1	3531	1/1	0.91	0.30	68,68,68,68	0
84	MG	1	3987	1/1	0.91	0.20	60,60,60,60	0
84	MG	6	2112	1/1	0.91	0.27	81,81,81,81	0
84	MG	5	3917	1/1	0.91	0.31	62,62,62,62	0
84	MG	5	3895	1/1	0.91	0.32	57,57,57,57	0
84	MG	4	219	1/1	0.91	0.26	68,68,68,68	0
84	MG	1	3933	1/1	0.91	0.71	84,84,84,84	0
84	MG	1	3643	1/1	0.91	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3991	1/1	0.91	0.59	57,57,57,57	0
84	MG	5	4137	1/1	0.91	0.31	58,58,58,58	0
85	LLL	5	4164	31/31	0.91	0.23	62,62,62,62	31
84	MG	6	1909	1/1	0.91	0.28	67,67,67,67	0
84	MG	6	2016	1/1	0.91	0.17	79,79,79,79	0
84	MG	1	3906	1/1	0.91	0.19	67,67,67,67	0
84	MG	6	2042	1/1	0.91	0.15	77,77,77,77	0
85	LLL	3	220	31/31	0.91	0.24	98,98,99,99	0
85	LLL	6	2164	31/31	0.91	0.27	73,74,74,74	0
84	MG	5	3961	1/1	0.91	0.33	53,53,53,53	0
84	MG	6	2075	1/1	0.91	0.28	61,61,61,61	0
84	MG	6	2032	1/1	0.91	0.06	77,77,77,77	0
84	MG	6	2096	1/1	0.91	0.40	65,65,65,65	0
84	MG	1	3773	1/1	0.91	0.33	62,62,62,62	0
84	MG	1	3449	1/1	0.91	0.26	56,56,56,56	0
84	MG	2	1915	1/1	0.91	0.25	95,95,95,95	0
84	MG	5	3485	1/1	0.91	0.29	57,57,57,57	0
84	MG	5	3889	1/1	0.91	0.21	55,55,55,55	0
84	MG	l5	303	1/1	0.91	0.19	74,74,74,74	0
84	MG	5	3703	1/1	0.91	0.20	70,70,70,70	0
84	MG	5	3505	1/1	0.91	0.19	50,50,50,50	0
84	MG	1	3862	1/1	0.91	0.20	63,63,63,63	0
84	MG	5	3773	1/1	0.91	0.10	139,139,139,139	0
84	MG	2	1944	1/1	0.91	0.72	87,87,87,87	0
84	MG	4	220	1/1	0.91	0.25	71,71,71,71	0
84	MG	5	3527	1/1	0.91	0.59	53,53,53,53	0
85	LLL	5	4172	31/31	0.91	0.18	77,77,77,77	31
84	MG	5	4111	1/1	0.91	0.43	46,46,46,46	0
84	MG	1	3872	1/1	0.91	0.31	73,73,73,73	0
84	MG	5	3603	1/1	0.91	0.15	80,80,80,80	0
84	MG	1	3751	1/1	0.91	0.80	72,72,72,72	0
84	MG	1	3781	1/1	0.91	0.33	69,69,69,69	1
84	MG	c3	206	1/1	0.91	0.24	80,80,80,80	0
84	MG	6	1953	1/1	0.91	0.18	83,83,83,83	0
84	MG	5	3529	1/1	0.91	0.35	47,47,47,47	0
84	MG	q2	508	1/1	0.91	0.17	62,62,62,62	0
84	MG	5	3614	1/1	0.91	0.21	81,81,81,81	0
84	MG	6	2140	1/1	0.91	0.33	65,65,65,65	0
84	MG	1	3755	1/1	0.91	0.72	60,60,60,60	0
84	MG	c3	203	1/1	0.91	0.10	108,108,108,108	0
84	MG	1	3926	1/1	0.91	0.33	54,54,54,54	0
84	MG	6	2132	1/1	0.91	0.13	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	4010	1/1	0.91	0.33	53,53,53,53	0
84	MG	6	2048	1/1	0.91	0.40	68,68,68,68	0
84	MG	1	3849	1/1	0.91	0.22	58,58,58,58	0
84	MG	6	2041	1/1	0.91	0.16	73,73,73,73	0
84	MG	6	2092	1/1	0.91	0.21	66,66,66,66	0
85	LLL	6	2167	31/31	0.91	0.35	97,98,98,98	0
84	MG	6	2011	1/1	0.91	0.29	68,68,68,68	0
84	MG	5	3876	1/1	0.91	0.14	66,66,66,66	0
85	LLL	5	4153	31/31	0.91	0.28	64,64,65,65	0
84	MG	5	3476	1/1	0.91	0.19	53,53,53,53	0
84	MG	2	1904	1/1	0.91	0.27	91,91,91,91	0
84	MG	5	3945	1/1	0.91	0.45	59,59,59,59	0
84	MG	m7	204	1/1	0.91	0.30	62,62,62,62	0
84	MG	6	2126	1/1	0.91	0.33	92,92,92,92	0
84	MG	6	2103	1/1	0.91	0.13	94,94,94,94	0
84	MG	5	4102	1/1	0.91	0.33	47,47,47,47	0
85	LLL	6	2176	31/31	0.91	0.24	80,80,80,80	31
84	MG	5	3503	1/1	0.91	0.31	42,42,42,42	0
84	MG	5	4079	1/1	0.91	0.14	70,70,70,70	0
84	MG	1	3563	1/1	0.91	0.13	76,76,76,76	0
84	MG	1	3649	1/1	0.91	0.19	61,61,61,61	0
84	MG	1	3912	1/1	0.91	0.17	58,58,58,58	0
84	MG	5	3553	1/1	0.91	0.39	59,59,59,59	0
84	MG	6	1973	1/1	0.91	0.38	65,65,65,65	0
84	MG	5	3785	1/1	0.91	0.38	51,51,51,51	0
84	MG	5	4068	1/1	0.91	0.12	112,112,112,112	0
84	MG	2	1910	1/1	0.91	0.79	80,80,80,80	0
84	MG	6	2046	1/1	0.91	0.11	72,72,72,72	0
84	MG	1	3749	1/1	0.91	0.37	60,60,60,60	0
84	MG	1	3594	1/1	0.91	0.18	53,53,53,53	0
84	MG	6	2025	1/1	0.91	0.18	81,81,81,81	1
84	MG	2	1938	1/1	0.91	0.51	76,76,76,76	0
84	MG	o1	201	1/1	0.92	0.18	79,79,79,79	0
84	MG	n0	205	1/1	0.92	0.16	47,47,47,47	0
84	MG	2	1950	1/1	0.92	0.34	94,94,94,94	0
84	MG	5	3929	1/1	0.92	0.27	43,43,43,43	0
84	MG	1	3811	1/1	0.92	0.20	80,80,80,80	0
84	MG	1	3968	1/1	0.92	0.11	74,74,74,74	0
84	MG	5	3409	1/1	0.92	0.18	45,45,45,45	0
84	MG	5	3734	1/1	0.92	0.17	67,67,67,67	0
84	MG	5	3827	1/1	0.92	0.16	51,51,51,51	1
84	MG	5	3815	1/1	0.92	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	s2	301	1/1	0.92	0.34	69,69,69,69	0
84	MG	5	3760	1/1	0.92	0.29	59,59,59,59	0
84	MG	5	4092	1/1	0.92	0.43	71,71,71,71	0
84	MG	L4	406	1/1	0.92	0.29	48,48,48,48	0
84	MG	5	3644	1/1	0.92	0.25	64,64,64,64	0
84	MG	6	2020	1/1	0.92	0.13	85,85,85,85	0
84	MG	6	2157	1/1	0.92	0.24	63,63,63,63	0
85	LLL	5	4163	31/31	0.92	0.17	112,112,112,112	0
84	MG	2	1964	1/1	0.92	0.20	90,90,90,90	0
84	MG	2	1948	1/1	0.92	0.47	82,82,82,82	0
85	LLL	L3	404	31/31	0.92	0.22	82,82,82,82	0
84	MG	1	3722	1/1	0.92	0.10	68,68,68,68	0
84	MG	q2	505	1/1	0.92	0.26	63,63,63,63	0
84	MG	q3	502	1/1	0.92	0.38	68,68,68,68	0
84	MG	6	1995	1/1	0.92	0.11	117,117,117,117	0
84	MG	1	3983	1/1	0.92	0.20	61,61,61,61	0
84	MG	1	3845	1/1	0.92	0.17	53,53,53,53	0
84	MG	5	3778	1/1	0.92	0.24	92,92,92,92	0
84	MG	5	3470	1/1	0.92	0.35	54,54,54,54	0
84	MG	5	4087	1/1	0.92	0.28	52,52,52,52	0
84	MG	1	3890	1/1	0.92	0.39	50,50,50,50	0
84	MG	5	3882	1/1	0.92	0.28	67,67,67,67	0
84	MG	2	1981	1/1	0.92	0.61	58,58,58,58	0
84	MG	5	3987	1/1	0.92	0.35	48,48,48,48	0
84	MG	2	1996	1/1	0.92	0.15	111,111,111,111	0
84	MG	2	1999	1/1	0.92	0.63	73,73,73,73	0
84	MG	6	1910	1/1	0.92	0.29	60,60,60,60	0
84	MG	5	4147	1/1	0.92	0.17	61,61,61,61	0
84	MG	1	3801	1/1	0.92	0.19	69,69,69,69	0
84	MG	1	3605	1/1	0.92	0.72	46,46,46,46	0
84	MG	5	3918	1/1	0.92	0.31	58,58,58,58	0
84	MG	1	3685	1/1	0.92	0.40	56,56,56,56	0
84	MG	8	203	1/1	0.92	0.18	83,83,83,83	1
84	MG	5	4076	1/1	0.92	0.29	77,77,77,77	0
84	MG	5	3586	1/1	0.92	0.42	55,55,55,55	0
84	MG	d3	205	1/1	0.92	0.29	98,98,98,98	0
84	MG	5	3866	1/1	0.92	0.27	51,51,51,51	1
84	MG	2	1920	1/1	0.92	0.28	88,88,88,88	0
84	MG	5	3549	1/1	0.92	0.40	63,63,63,63	0
84	MG	5	4016	1/1	0.92	0.25	62,62,62,62	0
84	MG	5	3796	1/1	0.92	0.10	67,67,67,67	0
86	ZN	e1	501	1/1	0.92	0.10	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1986	1/1	0.92	0.28	82,82,82,82	0
84	MG	5	3860	1/1	0.92	0.18	56,56,56,56	0
84	MG	6	1939	1/1	0.92	0.40	58,58,58,58	0
84	MG	5	4039	1/1	0.92	0.22	77,77,77,77	0
84	MG	1	3437	1/1	0.92	0.19	51,51,51,51	0
84	MG	5	3777	1/1	0.92	0.35	70,70,70,70	0
84	MG	2	1986	1/1	0.92	0.13	117,117,117,117	0
84	MG	1	3585	1/1	0.92	0.29	52,52,52,52	0
84	MG	5	4113	1/1	0.92	0.18	72,72,72,72	0
84	MG	5	4054	1/1	0.92	0.12	97,97,97,97	0
84	MG	5	3955	1/1	0.92	0.32	52,52,52,52	0
84	MG	1	3945	1/1	0.92	0.28	54,54,54,54	0
84	MG	2	1994	1/1	0.92	0.14	109,109,109,109	0
84	MG	5	3998	1/1	0.92	0.23	54,54,54,54	0
84	MG	5	3976	1/1	0.92	0.20	68,68,68,68	0
84	MG	1	3651	1/1	0.92	0.26	59,59,59,59	0
84	MG	6	2074	1/1	0.92	0.15	64,64,64,64	0
84	MG	o2	202	1/1	0.92	0.43	55,55,55,55	0
84	MG	1	3712	1/1	0.92	0.17	82,82,82,82	0
84	MG	6	2146	1/1	0.92	0.12	87,87,87,87	0
84	MG	1	3535	1/1	0.92	0.48	62,62,62,62	0
84	MG	6	2006	1/1	0.92	0.39	63,63,63,63	0
84	MG	L4	403	1/1	0.92	0.22	55,55,55,55	0
84	MG	6	2069	1/1	0.92	0.12	86,86,86,86	0
84	MG	l2	305	1/1	0.92	0.27	50,50,50,50	0
84	MG	l2	301	1/1	0.92	0.30	59,59,59,59	0
84	MG	6	2001	1/1	0.92	0.36	79,79,79,79	0
84	MG	L3	403	1/1	0.92	0.27	62,62,62,62	0
85	LLL	5	4152	31/31	0.92	0.27	79,79,79,79	31
84	MG	1	3527	1/1	0.92	0.45	70,70,70,70	0
84	MG	5	3429	1/1	0.92	0.36	48,48,48,48	0
84	MG	1	3754	1/1	0.92	0.68	68,68,68,68	0
84	MG	6	2113	1/1	0.92	0.17	67,67,67,67	0
84	MG	1	3464	1/1	0.92	0.32	51,51,51,51	0
84	MG	o3	202	1/1	0.92	0.22	70,70,70,70	0
84	MG	5	3879	1/1	0.92	0.31	64,64,64,64	0
84	MG	5	4121	1/1	0.92	0.14	84,84,84,84	0
84	MG	5	3912	1/1	0.92	0.28	45,45,45,45	0
84	MG	1	3648	1/1	0.92	0.29	57,57,57,57	0
84	MG	2	2008	1/1	0.92	0.16	117,117,117,117	0
84	MG	5	3870	1/1	0.92	0.37	54,54,54,54	0
85	LLL	6	2170	31/31	0.92	0.19	82,82,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3568	1/1	0.92	0.14	83,83,83,83	0
84	MG	6	2109	1/1	0.92	0.11	91,91,91,91	0
84	MG	5	3468	1/1	0.92	0.14	55,55,55,55	0
84	MG	5	3996	1/1	0.92	0.26	44,44,44,44	0
85	LLL	6	2165	31/31	0.92	0.22	76,77,77,77	31
84	MG	1	3920	1/1	0.92	0.29	53,53,53,53	0
84	MG	O7	103	1/1	0.92	0.18	59,59,59,59	0
84	MG	5	3504	1/1	0.92	0.18	54,54,54,54	0
84	MG	m6	204	1/1	0.92	0.35	48,48,48,48	0
84	MG	2	1963	1/1	0.92	0.14	117,117,117,117	0
84	MG	6	1982	1/1	0.92	0.21	104,104,104,104	0
84	MG	6	2022	1/1	0.92	0.26	88,88,88,88	0
84	MG	1	3921	1/1	0.92	0.18	72,72,72,72	0
84	MG	1	3962	1/1	0.92	0.28	78,78,78,78	0
84	MG	5	3712	1/1	0.92	0.13	75,75,75,75	0
84	MG	5	3767	1/1	0.92	0.34	60,60,60,60	0
84	MG	1	3705	1/1	0.92	0.25	59,59,59,59	0
84	MG	6	2156	1/1	0.92	0.42	77,77,77,77	0
84	MG	5	3817	1/1	0.92	0.25	41,41,41,41	0
84	MG	5	3534	1/1	0.92	0.39	50,50,50,50	0
84	MG	5	4037	1/1	0.92	0.17	77,77,77,77	0
84	MG	5	3443	1/1	0.92	0.33	49,49,49,49	0
84	MG	5	3613	1/1	0.92	0.31	79,79,79,79	0
84	MG	d2	201	1/1	0.92	0.22	80,80,80,80	0
84	MG	5	3595	1/1	0.93	0.17	74,74,74,74	0
84	MG	5	4032	1/1	0.93	0.06	69,69,69,69	1
84	MG	5	3438	1/1	0.93	0.16	64,64,64,64	1
85	LLL	5	4159	31/31	0.93	0.23	59,59,60,60	0
84	MG	5	3865	1/1	0.93	0.37	56,56,56,56	0
84	MG	1	3613	1/1	0.93	0.43	48,48,48,48	0
84	MG	5	3883	1/1	0.93	0.23	67,67,67,67	0
84	MG	6	1904	1/1	0.93	0.29	65,65,65,65	0
84	MG	l5	304	1/1	0.93	0.07	80,80,80,80	0
84	MG	4	214	1/1	0.93	0.36	63,63,63,63	0
84	MG	5	3532	1/1	0.93	0.18	43,43,43,43	0
84	MG	5	3983	1/1	0.93	0.21	50,50,50,50	0
84	MG	5	3421	1/1	0.93	0.20	51,51,51,51	0
84	MG	5	4081	1/1	0.93	0.08	79,79,79,79	0
84	MG	5	3731	1/1	0.93	0.11	69,69,69,69	0
84	MG	5	3911	1/1	0.93	0.32	43,43,43,43	0
84	MG	m7	202	1/1	0.93	0.38	49,49,49,49	0
84	MG	1	3532	1/1	0.93	0.66	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	4	217	1/1	0.93	0.25	79,79,79,79	0
85	LLL	6	2171	31/31	0.93	0.21	87,88,88,88	0
84	MG	1	3617	1/1	0.93	0.60	70,70,70,70	0
84	MG	6	2095	1/1	0.93	0.33	65,65,65,65	0
84	MG	1	3830	1/1	0.93	0.51	72,72,72,72	0
84	MG	5	3701	1/1	0.93	0.18	66,66,66,66	0
84	MG	5	3519	1/1	0.93	0.33	42,42,42,42	0
84	MG	5	3638	1/1	0.93	0.23	51,51,51,51	0
84	MG	5	3791	1/1	0.93	0.33	54,54,54,54	0
84	MG	6	2155	1/1	0.93	0.11	84,84,84,84	0
84	MG	5	3913	1/1	0.93	0.31	57,57,57,57	0
84	MG	5	3797	1/1	0.93	0.24	57,57,57,57	0
84	MG	5	4103	1/1	0.93	0.20	50,50,50,50	0
85	LLL	5	4165	31/31	0.93	0.21	84,84,84,84	0
85	LLL	5	4170	31/31	0.93	0.21	61,61,61,61	31
84	MG	5	3810	1/1	0.93	0.33	59,59,59,59	0
84	MG	6	2015	1/1	0.93	0.37	68,68,68,68	0
84	MG	5	3685	1/1	0.93	0.31	66,66,66,66	0
84	MG	19	205	1/1	0.93	0.13	72,72,72,72	0
84	MG	7	221	1/1	0.93	0.09	75,75,75,75	0
84	MG	1	3971	1/1	0.93	0.40	56,56,56,56	0
84	MG	5	3672	1/1	0.93	0.46	67,67,67,67	0
84	MG	5	3648	1/1	0.93	0.17	65,65,65,65	0
84	MG	1	3621	1/1	0.93	0.48	68,68,68,68	0
84	MG	6	2007	1/1	0.93	0.35	61,61,61,61	0
84	MG	5	3465	1/1	0.93	0.29	41,41,41,41	0
84	MG	6	1981	1/1	0.93	0.13	97,97,97,97	0
84	MG	N8	201	1/1	0.93	0.24	75,75,75,75	0
84	MG	6	1923	1/1	0.93	0.17	71,71,71,71	0
84	MG	5	3687	1/1	0.93	0.40	69,69,69,69	0
84	MG	7	210	1/1	0.93	0.14	67,67,67,67	0
84	MG	19	201	1/1	0.93	0.18	53,53,53,53	0
84	MG	6	1922	1/1	0.93	0.17	74,74,74,74	0
84	MG	1	3777	1/1	0.93	0.61	62,62,62,62	0
84	MG	5	3615	1/1	0.93	0.21	89,89,89,89	0
84	MG	5	3600	1/1	0.93	0.21	92,92,92,92	0
84	MG	5	4070	1/1	0.93	0.11	99,99,99,99	0
84	MG	1	3964	1/1	0.93	0.60	87,87,87,87	0
84	MG	5	3852	1/1	0.93	0.31	57,57,57,57	0
84	MG	5	4064	1/1	0.93	0.36	44,44,44,44	0
84	MG	5	3799	1/1	0.93	0.25	64,64,64,64	0
84	MG	5	3482	1/1	0.93	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	2	1987	1/1	0.93	0.17	110,110,110,110	0
84	MG	1	3486	1/1	0.93	0.33	62,62,62,62	0
84	MG	5	3506	1/1	0.93	0.32	49,49,49,49	0
84	MG	5	3451	1/1	0.93	0.44	45,45,45,45	0
84	MG	1	3676	1/1	0.93	0.52	53,53,53,53	0
85	LLL	1	3992	31/31	0.93	0.32	78,79,79,79	31
84	MG	6	1911	1/1	0.93	0.21	71,71,71,71	0
84	MG	5	4048	1/1	0.93	0.56	64,64,64,64	0
84	MG	1	3760	1/1	0.93	0.34	69,69,69,69	0
84	MG	1	3752	1/1	0.93	0.28	62,62,62,62	0
84	MG	1	3855	1/1	0.93	0.28	55,55,55,55	1
85	LLL	6	2169	31/31	0.93	0.20	89,89,90,90	0
85	LLL	1	4003	31/31	0.93	0.23	79,80,80,80	31
84	MG	1	3779	1/1	0.93	0.35	58,58,58,58	0
84	MG	6	1970	1/1	0.93	0.35	63,63,63,63	0
84	MG	1	3814	1/1	0.93	0.16	103,103,103,103	0
84	MG	5	3959	1/1	0.93	0.36	51,51,51,51	0
84	MG	6	2077	1/1	0.93	0.32	65,65,65,65	0
84	MG	5	3914	1/1	0.93	0.24	56,56,56,56	0
84	MG	5	3661	1/1	0.93	0.34	61,61,61,61	0
84	MG	1	3448	1/1	0.93	0.52	68,68,68,68	0
84	MG	1	3748	1/1	0.93	0.37	61,61,61,61	0
84	MG	6	1952	1/1	0.93	0.14	68,68,68,68	0
84	MG	5	3832	1/1	0.93	0.24	50,50,50,50	0
84	MG	6	2071	1/1	0.93	0.14	76,76,76,76	1
84	MG	5	3849	1/1	0.93	0.27	50,50,50,50	0
84	MG	L7	301	1/1	0.93	0.34	58,58,58,58	0
84	MG	7	220	1/1	0.93	0.21	66,66,66,66	0
84	MG	2	1969	1/1	0.93	0.22	100,100,100,100	0
84	MG	2	2030	1/1	0.93	0.08	122,122,122,122	0
84	MG	5	3427	1/1	0.93	0.30	45,45,45,45	0
84	MG	5	3541	1/1	0.93	0.31	52,52,52,52	0
84	MG	6	1985	1/1	0.93	0.14	92,92,92,92	0
84	MG	5	4025	1/1	0.93	0.18	55,55,55,55	0
84	MG	1	3548	1/1	0.93	0.33	70,70,70,70	0
84	MG	1	3967	1/1	0.93	0.20	72,72,72,72	0
84	MG	c8	203	1/1	0.93	0.11	74,74,74,74	0
85	LLL	1	3994	31/31	0.93	0.23	68,69,69,69	0
84	MG	L2	302	1/1	0.93	0.46	43,43,43,43	0
84	MG	5	3705	1/1	0.93	0.32	81,81,81,81	0
84	MG	1	3458	1/1	0.93	0.39	64,64,64,64	0
84	MG	5	4139	1/1	0.93	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3920	1/1	0.93	0.35	55,55,55,55	0
84	MG	2	1921	1/1	0.93	0.20	91,91,91,91	0
84	MG	5	3993	1/1	0.93	0.44	56,56,56,56	0
84	MG	1	3659	1/1	0.93	0.15	69,69,69,69	0
84	MG	1	3706	1/1	0.93	0.26	51,51,51,51	0
84	MG	6	2036	1/1	0.93	0.09	83,83,83,83	0
84	MG	6	2060	1/1	0.93	0.13	86,86,86,86	0
84	MG	5	3570	1/1	0.93	0.24	67,67,67,67	0
84	MG	1	3657	1/1	0.93	0.26	50,50,50,50	0
84	MG	5	4096	1/1	0.93	0.34	54,54,54,54	0
84	MG	5	4026	1/1	0.93	0.26	66,66,66,66	0
84	MG	1	3616	1/1	0.93	0.21	54,54,54,54	0
84	MG	1	3860	1/1	0.93	0.19	65,65,65,65	0
84	MG	7	217	1/1	0.93	0.13	63,63,63,63	0
84	MG	1	3463	1/1	0.93	0.28	52,52,52,52	0
84	MG	1	3504	1/1	0.93	0.28	66,66,66,66	0
84	MG	l3	401	1/1	0.93	0.28	57,57,57,57	0
84	MG	1	3889	1/1	0.93	0.31	54,54,54,54	0
84	MG	5	3735	1/1	0.93	0.13	64,64,64,64	0
84	MG	6	2088	1/1	0.93	0.38	83,83,83,83	0
84	MG	o4	503	1/1	0.93	0.11	94,94,94,94	0
84	MG	1	3894	1/1	0.93	0.35	60,60,60,60	0
84	MG	2	1974	1/1	0.93	0.27	96,96,96,96	0
84	MG	2	1976	1/1	0.93	0.35	92,92,92,92	0
84	MG	5	3501	1/1	0.93	0.19	54,54,54,54	0
85	LLL	5	4168	31/31	0.93	0.27	76,76,76,76	0
84	MG	1	3583	1/1	0.93	0.19	63,63,63,63	0
84	MG	1	3607	1/1	0.93	0.59	58,58,58,58	0
84	MG	5	3535	1/1	0.93	0.44	57,57,57,57	0
84	MG	1	3871	1/1	0.94	0.14	73,73,73,73	0
84	MG	5	3636	1/1	0.94	0.41	53,53,53,53	0
84	MG	5	3807	1/1	0.94	0.27	71,71,71,71	0
84	MG	6	2098	1/1	0.94	0.32	63,63,63,63	0
84	MG	1	3743	1/1	0.94	0.63	72,72,72,72	0
84	MG	1	3982	1/1	0.94	0.12	90,90,90,90	0
84	MG	5	3680	1/1	0.94	0.15	73,73,73,73	0
84	MG	1	3496	1/1	0.94	0.58	73,73,73,73	0
84	MG	6	2005	1/1	0.94	0.19	83,83,83,83	0
84	MG	5	3410	1/1	0.94	0.52	46,46,46,46	0
84	MG	5	4066	1/1	0.94	0.12	84,84,84,84	0
84	MG	2	1985	1/1	0.94	0.28	122,122,122,122	0
84	MG	1	3836	1/1	0.94	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1907	1/1	0.94	0.21	69,69,69,69	0
84	MG	6	2029	1/1	0.94	0.27	75,75,75,75	0
84	MG	2	2011	1/1	0.94	0.19	102,102,102,102	0
84	MG	1	3861	1/1	0.94	0.30	58,58,58,58	0
84	MG	5	3842	1/1	0.94	0.24	46,46,46,46	0
84	MG	2	1937	1/1	0.94	0.23	80,80,80,80	0
84	MG	1	3497	1/1	0.94	0.22	73,73,73,73	0
84	MG	5	3612	1/1	0.94	0.20	80,80,80,80	0
84	MG	5	3926	1/1	0.94	0.21	55,55,55,55	1
84	MG	5	3742	1/1	0.94	0.27	67,67,67,67	0
84	MG	5	3462	1/1	0.94	0.21	53,53,53,53	0
84	MG	1	3470	1/1	0.94	0.38	56,56,56,56	0
84	MG	l3	402	1/1	0.94	0.35	51,51,51,51	0
84	MG	3	214	1/1	0.94	0.07	86,86,86,86	0
84	MG	5	3463	1/1	0.94	0.28	49,49,49,49	0
84	MG	5	3562	1/1	0.94	0.41	57,57,57,57	0
84	MG	2	1998	1/1	0.94	0.10	154,154,154,154	0
84	MG	1	3601	1/1	0.94	0.35	53,53,53,53	0
84	MG	N5	201	1/1	0.94	0.15	95,95,95,95	0
84	MG	5	3415	1/1	0.94	0.24	48,48,48,48	1
84	MG	5	3973	1/1	0.94	0.33	69,69,69,69	0
84	MG	1	3693	1/1	0.94	0.26	64,64,64,64	0
84	MG	2	1934	1/1	0.94	0.29	87,87,87,87	0
84	MG	6	2105	1/1	0.94	0.25	67,67,67,67	0
84	MG	1	3883	1/1	0.94	0.11	75,75,75,75	0
84	MG	m7	206	1/1	0.94	0.36	55,55,55,55	0
84	MG	1	3809	1/1	0.94	0.14	59,59,59,59	0
84	MG	M0	301	1/1	0.94	0.23	51,51,51,51	0
84	MG	2	1933	1/1	0.94	0.16	88,88,88,88	0
84	MG	5	3498	1/1	0.94	0.15	52,52,52,52	0
84	MG	5	3985	1/1	0.94	0.25	56,56,56,56	0
84	MG	5	3665	1/1	0.94	0.54	56,56,56,56	0
84	MG	6	1959	1/1	0.94	0.22	68,68,68,68	0
84	MG	1	3761	1/1	0.94	0.17	73,73,73,73	1
84	MG	Q2	502	1/1	0.94	0.14	65,65,65,65	0
84	MG	1	3966	1/1	0.94	0.17	68,68,68,68	0
84	MG	1	3581	1/1	0.94	0.15	64,64,64,64	0
84	MG	1	3597	1/1	0.94	0.37	46,46,46,46	0
84	MG	C8	201	1/1	0.94	0.05	138,138,138,138	0
84	MG	5	3905	1/1	0.94	0.45	44,44,44,44	0
84	MG	5	4123	1/1	0.94	0.28	53,53,53,53	0
84	MG	6	2056	1/1	0.94	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3604	1/1	0.94	0.26	52,52,52,52	0
84	MG	5	4110	1/1	0.94	0.17	47,47,47,47	0
84	MG	6	1972	1/1	0.94	0.42	70,70,70,70	0
84	MG	6	1962	1/1	0.94	0.20	69,69,69,69	0
84	MG	2	2040	1/1	0.94	0.34	95,95,95,95	0
84	MG	6	2116	1/1	0.94	0.24	71,71,71,71	0
84	MG	1	3750	1/1	0.94	0.57	70,70,70,70	0
84	MG	1	3959	1/1	0.94	0.34	61,61,61,61	0
84	MG	6	2143	1/1	0.94	0.26	104,104,104,104	0
84	MG	1	3602	1/1	0.94	0.43	49,49,49,49	0
84	MG	5	3478	1/1	0.94	0.42	50,50,50,50	0
84	MG	5	3931	1/1	0.94	0.51	44,44,44,44	0
84	MG	5	4094	1/1	0.94	0.14	63,63,63,63	0
85	LLL	6	2166	31/31	0.94	0.26	77,77,77,77	31
84	MG	5	4108	1/1	0.94	0.19	59,59,59,59	0
84	MG	3	204	1/1	0.94	0.15	85,85,85,85	0
84	MG	5	4100	1/1	0.94	0.45	90,90,90,90	0
85	LLL	2	2043	31/31	0.94	0.31	101,101,101,101	0
84	MG	5	4022	1/1	0.94	0.28	50,50,50,50	0
84	MG	M5	303	1/1	0.94	0.19	65,65,65,65	0
84	MG	1	3780	1/1	0.94	0.34	64,64,64,64	0
84	MG	5	3607	1/1	0.94	0.21	83,83,83,83	0
84	MG	L2	304	1/1	0.94	0.32	73,73,73,73	0
84	MG	4	209	1/1	0.94	0.50	59,59,59,59	0
84	MG	7	213	1/1	0.94	0.17	71,71,71,71	0
85	LLL	5	4154	31/31	0.94	0.25	67,67,67,67	0
84	MG	2	1936	1/1	0.94	0.35	86,86,86,86	0
84	MG	1	3526	1/1	0.94	0.57	65,65,65,65	0
84	MG	6	1958	1/1	0.94	0.26	66,66,66,66	0
84	MG	1	3540	1/1	0.94	0.27	54,54,54,54	0
85	LLL	l3	412	31/31	0.94	0.20	69,69,70,70	0
84	MG	2	1918	1/1	0.94	0.22	91,91,91,91	0
84	MG	3	218	1/1	0.94	0.13	97,97,97,97	0
84	MG	5	3684	1/1	0.94	0.12	79,79,79,79	0
84	MG	2	1925	1/1	0.94	0.28	90,90,90,90	0
84	MG	7	215	1/1	0.94	0.28	63,63,63,63	0
84	MG	5	3826	1/1	0.94	0.21	56,56,56,56	0
84	MG	2	1943	1/1	0.94	0.27	95,95,95,95	0
84	MG	5	4028	1/1	0.94	0.10	59,59,59,59	0
84	MG	6	2137	1/1	0.94	0.29	76,76,76,76	0
84	MG	5	3646	1/1	0.94	0.17	65,65,65,65	0
84	MG	5	3659	1/1	0.94	0.13	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	8	210	1/1	0.94	0.18	96,96,96,96	0
84	MG	7	218	1/1	0.94	0.09	68,68,68,68	0
84	MG	d5	201	1/1	0.94	0.17	90,90,90,90	0
84	MG	2	2032	1/1	0.94	0.10	111,111,111,111	0
84	MG	6	1969	1/1	0.94	0.15	69,69,69,69	1
84	MG	5	3916	1/1	0.94	0.19	51,51,51,51	0
84	MG	6	2051	1/1	0.94	0.16	69,69,69,69	0
84	MG	5	3517	1/1	0.94	0.60	49,49,49,49	0
84	MG	1	3776	1/1	0.94	0.27	68,68,68,68	1
84	MG	1	3410	1/1	0.94	0.55	56,56,56,56	0
85	LLL	1	3990	31/31	0.94	0.20	75,75,75,75	0
84	MG	1	3635	1/1	0.94	0.09	117,117,117,117	0
84	MG	5	3502	1/1	0.94	0.18	50,50,50,50	0
84	MG	1	3852	1/1	0.94	0.51	65,65,65,65	0
84	MG	N3	201	1/1	0.94	0.30	67,67,67,67	0
84	MG	5	3599	1/1	0.94	0.24	92,92,92,92	0
84	MG	6	2000	1/1	0.94	0.17	84,84,84,84	0
84	MG	1	3656	1/1	0.94	0.24	52,52,52,52	0
84	MG	2	2014	1/1	0.94	0.24	88,88,88,88	0
84	MG	5	3539	1/1	0.94	0.49	54,54,54,54	0
84	MG	5	4145	1/1	0.94	0.13	54,54,54,54	0
84	MG	c8	201	1/1	0.94	0.18	75,75,75,75	0
84	MG	5	3540	1/1	0.94	0.32	49,49,49,49	0
84	MG	5	3759	1/1	0.94	0.32	67,67,67,67	0
84	MG	5	3436	1/1	0.94	0.22	66,66,66,66	0
84	MG	6	2135	1/1	0.94	0.25	77,77,77,77	0
84	MG	5	3531	1/1	0.94	0.35	43,43,43,43	0
84	MG	1	3640	1/1	0.94	0.19	100,100,100,100	0
84	MG	5	3872	1/1	0.94	0.14	76,76,76,76	0
84	MG	5	3726	1/1	0.94	0.45	52,52,52,52	0
84	MG	5	3721	1/1	0.94	0.21	65,65,65,65	0
84	MG	q1	101	1/1	0.94	0.39	67,67,67,67	0
84	MG	5	3835	1/1	0.94	0.30	62,62,62,62	0
84	MG	5	3439	1/1	0.95	0.25	54,54,54,54	0
84	MG	5	3843	1/1	0.95	0.11	50,50,50,50	0
84	MG	1	3833	1/1	0.95	0.27	64,64,64,64	0
84	MG	5	3739	1/1	0.95	0.33	52,52,52,52	0
84	MG	M5	304	1/1	0.95	0.26	67,67,67,67	0
84	MG	1	3574	1/1	0.95	0.12	67,67,67,67	0
84	MG	q0	202	1/1	0.95	0.18	51,51,51,51	0
84	MG	1	3608	1/1	0.95	0.19	57,57,57,57	0
84	MG	1	3793	1/1	0.95	0.16	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3658	1/1	0.95	0.17	71,71,71,71	0
84	MG	5	3584	1/1	0.95	0.48	51,51,51,51	0
84	MG	1	3519	1/1	0.95	0.35	70,70,70,70	0
84	MG	2	1957	1/1	0.95	0.13	95,95,95,95	0
84	MG	6	2082	1/1	0.95	0.26	67,67,67,67	0
84	MG	5	4090	1/1	0.95	0.39	60,60,60,60	0
85	LLL	5	4161	31/31	0.95	0.22	69,70,70,70	0
84	MG	1	3986	1/1	0.95	0.41	68,68,68,68	0
84	MG	5	3432	1/1	0.95	0.19	54,54,54,54	0
84	MG	6	2087	1/1	0.95	0.22	82,82,82,82	0
84	MG	1	3427	1/1	0.95	0.27	51,51,51,51	0
84	MG	n0	207	1/1	0.95	0.23	56,56,56,56	0
84	MG	8	217	1/1	0.95	0.22	64,64,64,64	0
84	MG	5	3569	1/1	0.95	0.43	64,64,64,64	0
84	MG	Q2	503	1/1	0.95	0.27	67,67,67,67	0
84	MG	5	3516	1/1	0.95	0.18	49,49,49,49	0
84	MG	l7	302	1/1	0.95	0.30	55,55,55,55	0
84	MG	5	3667	1/1	0.95	0.56	49,49,49,49	0
84	MG	1	3518	1/1	0.95	0.28	64,64,64,64	0
84	MG	5	4000	1/1	0.95	0.27	45,45,45,45	0
84	MG	5	3425	1/1	0.95	0.17	46,46,46,46	0
84	MG	M6	201	1/1	0.95	0.43	60,60,60,60	0
84	MG	5	4042	1/1	0.95	0.27	46,46,46,46	0
84	MG	5	3784	1/1	0.95	0.37	44,44,44,44	0
84	MG	5	4131	1/1	0.95	0.30	70,70,70,70	0
84	MG	1	3907	1/1	0.95	0.31	62,62,62,62	0
84	MG	1	3561	1/1	0.95	0.15	79,79,79,79	0
84	MG	5	3416	1/1	0.95	0.31	45,45,45,45	0
84	MG	5	4122	1/1	0.95	0.18	89,89,89,89	0
84	MG	1	3728	1/1	0.95	0.13	83,83,83,83	0
84	MG	2	1909	1/1	0.95	0.45	94,94,94,94	0
84	MG	5	3707	1/1	0.95	0.18	73,73,73,73	0
84	MG	1	3603	1/1	0.95	0.35	45,45,45,45	0
85	LLL	1	3989	31/31	0.95	0.21	69,69,69,69	0
84	MG	6	2052	1/1	0.95	0.11	73,73,73,73	0
84	MG	6	2151	1/1	0.95	0.20	67,67,67,67	0
84	MG	5	3547	1/1	0.95	0.49	54,54,54,54	0
84	MG	1	3414	1/1	0.95	0.21	56,56,56,56	0
84	MG	5	3652	1/1	0.95	0.19	76,76,76,76	0
85	LLL	5	4160	31/31	0.95	0.28	49,50,50,50	31
84	MG	1	3892	1/1	0.95	0.23	64,64,64,64	0
84	MG	1	3720	1/1	0.95	0.47	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3598	1/1	0.95	0.42	52,52,52,52	0
84	MG	5	4045	1/1	0.95	0.21	71,71,71,71	0
84	MG	5	3757	1/1	0.95	0.09	64,64,64,64	0
84	MG	5	3740	1/1	0.95	0.28	56,56,56,56	0
84	MG	6	1957	1/1	0.95	0.17	66,66,66,66	0
84	MG	5	3668	1/1	0.95	0.44	49,49,49,49	0
84	MG	2	2041	1/1	0.95	0.08	94,94,94,94	0
84	MG	5	4142	1/1	0.95	0.33	69,69,69,69	0
84	MG	5	3798	1/1	0.95	0.39	58,58,58,58	0
84	MG	6	1925	1/1	0.95	0.28	68,68,68,68	0
84	MG	1	3719	1/1	0.95	0.25	55,55,55,55	0
84	MG	1	3944	1/1	0.95	0.20	67,67,67,67	0
84	MG	1	3530	1/1	0.95	0.28	67,67,67,67	0
84	MG	6	1935	1/1	0.95	0.24	73,73,73,73	0
84	MG	5	3514	1/1	0.95	0.26	65,65,65,65	0
84	MG	2	2006	1/1	0.95	0.28	106,106,106,106	0
84	MG	M3	201	1/1	0.95	0.16	65,65,65,65	0
84	MG	5	3556	1/1	0.95	0.49	57,57,57,57	0
84	MG	5	3982	1/1	0.95	0.15	50,50,50,50	0
84	MG	1	3919	1/1	0.95	0.25	69,69,69,69	0
84	MG	1	3479	1/1	0.95	0.41	59,59,59,59	0
84	MG	5	3440	1/1	0.95	0.16	56,56,56,56	0
84	MG	7	208	1/1	0.95	0.11	65,65,65,65	0
84	MG	5	3637	1/1	0.95	0.30	48,48,48,48	0
84	MG	2	1995	1/1	0.95	0.40	100,100,100,100	0
84	MG	2	1973	1/1	0.95	0.20	96,96,96,96	0
84	MG	2	1902	1/1	0.95	0.09	95,95,95,95	0
84	MG	6	2003	1/1	0.95	0.16	64,64,64,64	0
84	MG	1	3797	1/1	0.95	0.54	56,56,56,56	0
84	MG	5	3555	1/1	0.95	0.21	62,62,62,62	1
84	MG	1	3421	1/1	0.95	0.25	50,50,50,50	0
84	MG	1	3843	1/1	0.95	0.28	58,58,58,58	0
84	MG	M7	204	1/1	0.95	0.25	60,60,60,60	0
84	MG	3	203	1/1	0.95	0.12	103,103,103,103	0
84	MG	5	3487	1/1	0.95	0.16	61,61,61,61	0
84	MG	5	3641	1/1	0.95	0.24	51,51,51,51	0
84	MG	5	3490	1/1	0.95	0.24	58,58,58,58	0
84	MG	3	216	1/1	0.95	0.08	74,74,74,74	0
84	MG	5	3401	1/1	0.95	0.36	49,49,49,49	0
84	MG	1	3484	1/1	0.95	0.31	60,60,60,60	0
84	MG	1	3533	1/1	0.95	0.56	75,75,75,75	0
84	MG	1	3954	1/1	0.95	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3517	1/1	0.95	0.43	54,54,54,54	0
84	MG	6	1926	1/1	0.95	0.24	75,75,75,75	0
84	MG	5	3538	1/1	0.95	0.28	52,52,52,52	0
84	MG	2	1922	1/1	0.95	0.28	84,84,84,84	0
84	MG	5	3518	1/1	0.95	0.44	53,53,53,53	0
84	MG	1	3482	1/1	0.95	0.25	72,72,72,72	0
84	MG	1	3885	1/1	0.95	0.19	80,80,80,80	0
84	MG	5	3745	1/1	0.95	0.34	52,52,52,52	0
84	MG	6	2047	1/1	0.95	0.12	79,79,79,79	0
84	MG	1	3423	1/1	0.95	0.30	51,51,51,51	0
84	MG	1	3882	1/1	0.95	0.24	71,71,71,71	0
84	MG	5	3497	1/1	0.95	0.17	49,49,49,49	0
84	MG	5	3404	1/1	0.95	0.22	55,55,55,55	0
84	MG	5	3814	1/1	0.95	0.13	48,48,48,48	0
84	MG	5	3716	1/1	0.95	0.57	62,62,62,62	0
84	MG	5	3853	1/1	0.95	0.15	58,58,58,58	0
84	MG	n3	202	1/1	0.95	0.51	62,62,62,62	1
84	MG	5	3818	1/1	0.95	0.18	54,54,54,54	0
84	MG	d1	102	1/1	0.95	0.10	106,106,106,106	0
84	MG	L2	301	1/1	0.95	0.20	55,55,55,55	0
84	MG	1	3844	1/1	0.95	0.22	56,56,56,56	0
84	MG	1	3868	1/1	0.95	0.21	61,61,61,61	0
84	MG	5	4075	1/1	0.95	0.12	97,97,97,97	0
84	MG	5	4088	1/1	0.95	0.22	69,69,69,69	0
84	MG	5	3445	1/1	0.95	0.21	50,50,50,50	0
84	MG	1	3802	1/1	0.95	0.20	98,98,98,98	0
84	MG	l3	405	1/1	0.95	0.30	43,43,43,43	0
84	MG	5	3671	1/1	0.95	0.37	63,63,63,63	0
84	MG	5	3790	1/1	0.95	0.32	47,47,47,47	0
84	MG	1	3951	1/1	0.95	0.06	82,82,82,82	0
84	MG	5	3884	1/1	0.95	0.09	69,69,69,69	0
84	MG	1	3596	1/1	0.96	0.36	55,55,55,55	0
84	MG	1	3787	1/1	0.96	0.85	67,67,67,67	0
84	MG	5	3475	1/1	0.96	0.17	64,64,64,64	0
84	MG	5	3507	1/1	0.96	0.20	55,55,55,55	0
84	MG	5	3997	1/1	0.96	0.16	50,50,50,50	0
84	MG	5	3774	1/1	0.96	0.29	116,116,116,116	0
84	MG	6	1956	1/1	0.96	0.33	69,69,69,69	0
84	MG	1	3425	1/1	0.96	0.26	57,57,57,57	0
84	MG	5	3587	1/1	0.96	0.35	55,55,55,55	0
84	MG	n8	201	1/1	0.96	0.30	54,54,54,54	0
84	MG	2	1983	1/1	0.96	0.22	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3557	1/1	0.96	0.18	71,71,71,71	0
84	MG	5	3493	1/1	0.96	0.18	57,57,57,57	0
84	MG	5	3783	1/1	0.96	0.31	41,41,41,41	0
84	MG	1	3408	1/1	0.96	0.27	51,51,51,51	0
86	ZN	E1	501	1/1	0.96	0.09	182,182,182,182	0
84	MG	1	3732	1/1	0.96	0.35	75,75,75,75	0
84	MG	1	3778	1/1	0.96	0.39	61,61,61,61	0
84	MG	1	3736	1/1	0.96	0.15	82,82,82,82	0
84	MG	1	3419	1/1	0.96	0.22	55,55,55,55	0
84	MG	1	3553	1/1	0.96	0.20	71,71,71,71	0
84	MG	6	2031	1/1	0.96	0.18	73,73,73,73	0
84	MG	1	3528	1/1	0.96	0.41	63,63,63,63	0
84	MG	1	3770	1/1	0.96	0.36	55,55,55,55	0
84	MG	5	4009	1/1	0.96	0.38	53,53,53,53	0
84	MG	5	3580	1/1	0.96	0.43	48,48,48,48	0
84	MG	1	3438	1/1	0.96	0.30	51,51,51,51	0
84	MG	1	3417	1/1	0.96	0.28	52,52,52,52	0
84	MG	5	3457	1/1	0.96	0.14	51,51,51,51	0
84	MG	5	3776	1/1	0.96	0.12	65,65,65,65	0
84	MG	1	3405	1/1	0.96	0.35	53,53,53,53	0
84	MG	5	3963	1/1	0.96	0.12	102,102,102,102	0
84	MG	5	3789	1/1	0.96	0.35	48,48,48,48	0
84	MG	5	4036	1/1	0.96	0.30	56,56,56,56	0
84	MG	5	3473	1/1	0.96	0.22	63,63,63,63	0
84	MG	n0	203	1/1	0.96	0.19	49,49,49,49	0
84	MG	1	3600	1/1	0.96	0.34	54,54,54,54	0
84	MG	1	3450	1/1	0.96	0.35	62,62,62,62	0
84	MG	1	3721	1/1	0.96	0.26	59,59,59,59	0
84	MG	1	3765	1/1	0.96	0.29	61,61,61,61	0
84	MG	2	2021	1/1	0.96	0.40	90,90,90,90	0
84	MG	1	3981	1/1	0.96	0.39	63,63,63,63	0
85	LLL	5	4157	31/31	0.96	0.25	49,49,49,49	0
84	MG	1	3432	1/1	0.96	0.43	46,46,46,46	0
84	MG	5	3782	1/1	0.96	0.16	67,67,67,67	0
84	MG	1	3612	1/1	0.96	0.37	55,55,55,55	0
84	MG	7	211	1/1	0.96	0.14	67,67,67,67	0
84	MG	5	3515	1/1	0.96	0.21	43,43,43,43	0
84	MG	1	3918	1/1	0.96	0.16	59,59,59,59	0
84	MG	5	3561	1/1	0.96	0.29	57,57,57,57	0
84	MG	5	3461	1/1	0.96	0.24	50,50,50,50	0
84	MG	5	4061	1/1	0.96	0.37	68,68,68,68	0
84	MG	1	3655	1/1	0.96	0.31	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3453	1/1	0.96	0.09	70,70,70,70	0
84	MG	1	3631	1/1	0.96	0.12	76,76,76,76	0
84	MG	6	2104	1/1	0.96	0.11	89,89,89,89	0
84	MG	6	1979	1/1	0.96	0.09	100,100,100,100	0
84	MG	1	3974	1/1	0.96	0.19	79,79,79,79	0
84	MG	1	3689	1/1	0.96	0.26	58,58,58,58	0
84	MG	m8	204	1/1	0.96	0.50	63,63,63,63	0
84	MG	1	3439	1/1	0.96	0.27	49,49,49,49	0
84	MG	1	3772	1/1	0.96	0.23	59,59,59,59	1
84	MG	5	4017	1/1	0.96	0.19	63,63,63,63	0
84	MG	6	2138	1/1	0.96	0.13	84,84,84,84	0
84	MG	1	3942	1/1	0.96	0.27	49,49,49,49	0
84	MG	1	3789	1/1	0.96	0.27	80,80,80,80	0
84	MG	1	3701	1/1	0.96	0.29	59,59,59,59	0
84	MG	4	207	1/1	0.96	0.24	59,59,59,59	0
84	MG	n3	201	1/1	0.96	0.25	43,43,43,43	0
84	MG	5	4011	1/1	0.96	0.16	45,45,45,45	0
84	MG	5	3903	1/1	0.96	1.06	61,61,61,61	0
84	MG	6	2054	1/1	0.96	0.14	76,76,76,76	0
84	MG	1	3610	1/1	0.96	0.29	52,52,52,52	0
84	MG	5	3719	1/1	0.96	0.24	66,66,66,66	0
84	MG	5	4091	1/1	0.96	0.41	68,68,68,68	0
84	MG	1	3589	1/1	0.96	0.09	55,55,55,55	0
84	MG	1	3858	1/1	0.96	0.37	46,46,46,46	0
84	MG	6	2019	1/1	0.96	0.18	81,81,81,81	0
84	MG	6	2045	1/1	0.96	0.12	68,68,68,68	0
84	MG	5	3450	1/1	0.96	0.34	42,42,42,42	0
85	LLL	5	4151	31/31	0.96	0.22	48,48,49,49	0
84	MG	5	3682	1/1	0.96	0.17	73,73,73,73	0
84	MG	1	3674	1/1	0.96	0.25	63,63,63,63	0
84	MG	6	2097	1/1	0.96	0.35	63,63,63,63	0
84	MG	6	2078	1/1	0.96	0.28	65,65,65,65	0
84	MG	8	215	1/1	0.96	0.44	58,58,58,58	0
85	LLL	1	3993	31/31	0.96	0.22	61,61,61,61	0
84	MG	5	3750	1/1	0.96	0.26	52,52,52,52	0
84	MG	5	3663	1/1	0.96	0.31	46,46,46,46	0
84	MG	1	3940	1/1	0.96	0.13	64,64,64,64	0
84	MG	5	4127	1/1	0.96	0.22	62,62,62,62	0
84	MG	5	3770	1/1	0.96	0.12	79,79,79,79	0
84	MG	5	3689	1/1	0.96	0.14	78,78,78,78	0
84	MG	7	207	1/1	0.96	0.16	62,62,62,62	0
85	LLL	1	3991	31/31	0.96	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3771	1/1	0.96	0.14	77,77,77,77	0
84	MG	5	3957	1/1	0.96	0.31	57,57,57,57	0
84	MG	1	3851	1/1	0.96	0.20	57,57,57,57	0
84	MG	5	3713	1/1	0.96	0.21	78,78,78,78	0
84	MG	5	3623	1/1	0.96	0.30	62,62,62,62	0
84	MG	6	2043	1/1	0.96	0.21	96,96,96,96	0
84	MG	5	3480	1/1	0.96	0.25	49,49,49,49	0
84	MG	6	2084	1/1	0.96	0.27	67,67,67,67	0
84	MG	1	3891	1/1	0.96	0.21	60,60,60,60	0
84	MG	5	3986	1/1	0.96	0.34	45,45,45,45	1
84	MG	1	3675	1/1	0.96	0.11	62,62,62,62	0
84	MG	6	2033	1/1	0.97	0.18	74,74,74,74	0
84	MG	6	2055	1/1	0.97	0.17	77,77,77,77	0
84	MG	5	4029	1/1	0.97	0.27	52,52,52,52	0
84	MG	1	3404	1/1	0.97	0.34	53,53,53,53	0
84	MG	5	3890	1/1	0.97	0.19	62,62,62,62	0
84	MG	m7	201	1/1	0.97	0.25	57,57,57,57	0
84	MG	1	3403	1/1	0.97	0.35	58,58,58,58	0
84	MG	1	3474	1/1	0.97	0.29	59,59,59,59	0
84	MG	5	3417	1/1	0.97	0.38	43,43,43,43	0
84	MG	6	2009	1/1	0.97	0.12	73,73,73,73	0
84	MG	1	3534	1/1	0.97	0.46	63,63,63,63	0
84	MG	5	3464	1/1	0.97	0.29	52,52,52,52	0
84	MG	5	3717	1/1	0.97	0.31	52,52,52,52	0
84	MG	2	1926	1/1	0.97	0.52	89,89,89,89	0
84	MG	6	2081	1/1	0.97	0.20	69,69,69,69	0
84	MG	7	206	1/1	0.97	0.12	62,62,62,62	0
84	MG	5	4038	1/1	0.97	0.10	79,79,79,79	0
84	MG	5	3625	1/1	0.97	0.27	54,54,54,54	0
86	ZN	Q3	501	1/1	0.97	0.12	108,108,108,108	0
84	MG	6	2044	1/1	0.97	0.15	71,71,71,71	0
84	MG	6	1932	1/1	0.97	0.34	62,62,62,62	0
84	MG	1	3619	1/1	0.97	0.32	59,59,59,59	0
84	MG	1	3420	1/1	0.97	0.18	53,53,53,53	0
84	MG	1	3856	1/1	0.97	0.26	55,55,55,55	0
84	MG	1	3544	1/1	0.97	0.38	54,54,54,54	0
84	MG	19	207	1/1	0.97	0.11	52,52,52,52	0
84	MG	6	1908	1/1	0.97	0.18	70,70,70,70	0
84	MG	5	3626	1/1	0.97	0.28	52,52,52,52	0
84	MG	5	3428	1/1	0.97	0.14	47,47,47,47	0
84	MG	6	2099	1/1	0.97	0.31	57,57,57,57	0
84	MG	7	202	1/1	0.97	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3537	1/1	0.97	0.30	60,60,60,60	0
84	MG	1	3857	1/1	0.97	0.44	47,47,47,47	0
84	MG	5	3724	1/1	0.97	0.17	60,60,60,60	1
84	MG	1	3429	1/1	0.97	0.34	50,50,50,50	0
84	MG	5	3585	1/1	0.97	0.38	48,48,48,48	0
84	MG	5	3640	1/1	0.97	0.42	41,41,41,41	0
84	MG	6	2002	1/1	0.97	0.12	68,68,68,68	0
84	MG	1	3771	1/1	0.97	0.23	59,59,59,59	0
84	MG	5	3848	1/1	0.97	0.26	44,44,44,44	0
84	MG	2	1932	1/1	0.97	0.25	91,91,91,91	0
84	MG	O4	502	1/1	0.97	0.10	106,106,106,106	0
84	MG	2	1971	1/1	0.97	0.27	102,102,102,102	0
84	MG	N3	202	1/1	0.97	0.32	55,55,55,55	0
84	MG	5	3988	1/1	0.97	0.36	45,45,45,45	0
84	MG	5	3459	1/1	0.97	0.14	52,52,52,52	1
84	MG	1	3690	1/1	0.97	0.40	58,58,58,58	0
84	MG	1	3846	1/1	0.97	0.26	53,53,53,53	0
84	MG	5	3411	1/1	0.97	0.38	46,46,46,46	0
84	MG	5	3639	1/1	0.97	0.30	42,42,42,42	0
84	MG	5	3733	1/1	0.97	0.14	65,65,65,65	0
84	MG	5	3930	1/1	0.97	0.20	45,45,45,45	0
84	MG	1	3516	1/1	0.97	0.34	54,54,54,54	0
84	MG	1	3606	1/1	0.97	0.29	52,52,52,52	0
84	MG	5	4005	1/1	0.97	0.21	58,58,58,58	0
84	MG	1	3731	1/1	0.97	0.15	80,80,80,80	0
84	MG	n5	203	1/1	0.97	0.06	89,89,89,89	0
84	MG	5	3575	1/1	0.97	0.21	51,51,51,51	0
84	MG	5	3820	1/1	0.97	0.13	52,52,52,52	0
84	MG	2	1928	1/1	0.97	0.47	67,67,67,67	0
84	MG	M7	202	1/1	0.97	0.36	48,48,48,48	0
84	MG	6	2076	1/1	0.97	0.21	64,64,64,64	0
84	MG	5	3679	1/1	0.97	0.23	66,66,66,66	0
84	MG	1	3895	1/1	0.97	0.18	66,66,66,66	0
84	MG	5	4105	1/1	0.97	0.32	56,56,56,56	0
84	MG	5	3864	1/1	0.97	0.34	68,68,68,68	0
84	MG	5	3847	1/1	0.97	0.31	45,45,45,45	0
84	MG	o4	502	1/1	0.97	0.42	87,87,87,87	0
84	MG	5	3877	1/1	0.97	0.17	89,89,89,89	0
84	MG	1	3740	1/1	0.97	0.17	74,74,74,74	0
84	MG	6	2086	1/1	0.97	0.09	83,83,83,83	0
84	MG	o2	201	1/1	0.97	0.30	55,55,55,55	0
84	MG	2	1945	1/1	0.97	0.31	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3729	1/1	0.97	0.21	72,72,72,72	0
84	MG	6	1948	1/1	0.97	0.27	66,66,66,66	0
84	MG	6	2013	1/1	0.97	0.26	76,76,76,76	0
84	MG	S3	301	1/1	0.97	0.14	100,100,100,100	0
84	MG	5	3952	1/1	0.97	0.19	58,58,58,58	0
84	MG	5	3633	1/1	0.97	0.30	45,45,45,45	0
86	ZN	O4	501	1/1	0.97	0.08	141,141,141,141	0
84	MG	n0	202	1/1	0.97	0.26	52,52,52,52	0
84	MG	1	3415	1/1	0.97	0.39	55,55,55,55	0
84	MG	5	3568	1/1	0.97	0.20	67,67,67,67	0
84	MG	7	204	1/1	0.97	0.28	54,54,54,54	0
84	MG	5	3508	1/1	0.97	0.10	53,53,53,53	0
84	MG	1	3644	1/1	0.97	0.32	49,49,49,49	0
84	MG	5	3579	1/1	0.97	0.45	45,45,45,45	0
84	MG	6	2159	1/1	0.97	0.15	81,81,81,81	0
84	MG	1	3478	1/1	0.97	0.31	58,58,58,58	0
84	MG	1	3826	1/1	0.97	0.41	65,65,65,65	0
84	MG	5	3678	1/1	0.97	0.25	68,68,68,68	0
84	MG	6	1999	1/1	0.97	0.24	87,87,87,87	0
84	MG	5	3824	1/1	0.97	0.15	58,58,58,58	0
84	MG	5	3681	1/1	0.97	0.29	66,66,66,66	0
84	MG	1	3638	1/1	0.97	0.17	90,90,90,90	0
84	MG	5	3582	1/1	0.97	0.30	54,54,54,54	0
84	MG	2	1903	1/1	0.97	0.33	90,90,90,90	0
84	MG	1	3587	1/1	0.97	0.32	58,58,58,58	0
84	MG	5	3831	1/1	0.97	0.26	44,44,44,44	0
84	MG	5	3989	1/1	0.97	0.28	47,47,47,47	0
84	MG	1	3795	1/1	0.97	0.41	56,56,56,56	0
84	MG	5	3589	1/1	0.97	0.35	58,58,58,58	0
84	MG	M0	304	1/1	0.97	0.13	62,62,62,62	0
84	MG	1	3734	1/1	0.97	0.17	77,77,77,77	0
84	MG	5	3979	1/1	0.97	0.37	46,46,46,46	0
84	MG	1	3796	1/1	0.97	0.18	60,60,60,60	0
84	MG	Q1	101	1/1	0.97	0.25	83,83,83,83	0
84	MG	1	3678	1/1	0.97	0.28	69,69,69,69	0
84	MG	2	2039	1/1	0.97	0.20	95,95,95,95	0
84	MG	1	3938	1/1	0.97	0.30	62,62,62,62	0
84	MG	2	1959	1/1	0.97	0.15	110,110,110,110	0
84	MG	5	4093	1/1	0.97	0.15	73,73,73,73	0
84	MG	1	3897	1/1	0.97	0.14	104,104,104,104	0
84	MG	1	3866	1/1	0.97	0.28	55,55,55,55	0
84	MG	6	1965	1/1	0.97	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	6	1955	1/1	0.97	0.16	77,77,77,77	0
84	MG	5	3666	1/1	0.97	0.14	55,55,55,55	0
84	MG	1	3407	1/1	0.97	0.28	59,59,59,59	0
84	MG	1	3697	1/1	0.97	0.19	56,56,56,56	0
84	MG	5	3471	1/1	0.97	0.40	56,56,56,56	0
84	MG	5	3413	1/1	0.97	0.30	46,46,46,46	0
84	MG	1	3745	1/1	0.97	0.11	73,73,73,73	0
84	MG	5	3830	1/1	0.97	0.07	49,49,49,49	1
84	MG	5	4055	1/1	0.97	0.24	103,103,103,103	0
84	MG	s5	303	1/1	0.97	0.33	77,77,77,77	0
84	MG	5	3720	1/1	0.97	0.08	71,71,71,71	0
84	MG	5	3560	1/1	0.97	0.24	51,51,51,51	0
84	MG	l5	301	1/1	0.97	0.15	56,56,56,56	0
84	MG	N0	204	1/1	0.97	0.13	68,68,68,68	0
84	MG	1	3647	1/1	0.97	0.13	55,55,55,55	0
84	MG	5	3630	1/1	0.97	0.20	50,50,50,50	0
84	MG	5	3702	1/1	0.97	0.11	85,85,85,85	0
84	MG	1	3480	1/1	0.97	0.31	62,62,62,62	0
84	MG	1	3848	1/1	0.97	0.15	57,57,57,57	0
84	MG	5	3901	1/1	0.97	0.74	55,55,55,55	0
84	MG	5	3737	1/1	0.97	0.27	49,49,49,49	0
84	MG	5	3949	1/1	0.97	0.36	56,56,56,56	0
84	MG	1	3475	1/1	0.98	0.29	60,60,60,60	0
84	MG	5	3479	1/1	0.98	0.32	48,48,48,48	0
84	MG	1	3471	1/1	0.98	0.20	63,63,63,63	0
84	MG	5	3908	1/1	0.98	0.33	48,48,48,48	0
84	MG	1	3539	1/1	0.98	0.24	52,52,52,52	0
84	MG	1	3472	1/1	0.98	0.32	57,57,57,57	0
84	MG	5	3481	1/1	0.98	0.31	49,49,49,49	0
84	MG	5	3572	1/1	0.98	0.23	67,67,67,67	0
84	MG	5	3545	1/1	0.98	0.23	49,49,49,49	0
84	MG	5	4044	1/1	0.98	0.40	72,72,72,72	0
84	MG	5	3536	1/1	0.98	0.43	56,56,56,56	0
84	MG	5	3956	1/1	0.98	0.29	55,55,55,55	0
84	MG	d3	203	1/1	0.98	0.11	68,68,68,68	0
84	MG	4	201	1/1	0.98	0.34	55,55,55,55	0
84	MG	5	3677	1/1	0.98	0.22	59,59,59,59	0
84	MG	5	3418	1/1	0.98	0.29	44,44,44,44	0
84	MG	1	3433	1/1	0.98	0.30	49,49,49,49	0
84	MG	6	2057	1/1	0.98	0.24	81,81,81,81	0
84	MG	5	3522	1/1	0.98	0.22	42,42,42,42	0
84	MG	1	3832	1/1	0.98	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3513	1/1	0.98	0.34	55,55,55,55	0
84	MG	6	1930	1/1	0.98	0.22	70,70,70,70	0
84	MG	2	1927	1/1	0.98	0.26	95,95,95,95	0
84	MG	5	3676	1/1	0.98	0.10	65,65,65,65	0
84	MG	5	3422	1/1	0.98	0.27	49,49,49,49	0
84	MG	1	3498	1/1	0.98	0.19	62,62,62,62	0
84	MG	5	3408	1/1	0.98	0.26	45,45,45,45	0
84	MG	5	3405	1/1	0.98	0.42	47,47,47,47	0
84	MG	5	3407	1/1	0.98	0.37	43,43,43,43	0
84	MG	5	3683	1/1	0.98	0.23	73,73,73,73	0
84	MG	1	3591	1/1	0.98	0.41	46,46,46,46	0
84	MG	5	3412	1/1	0.98	0.27	47,47,47,47	0
84	MG	6	1905	1/1	0.98	0.26	64,64,64,64	0
84	MG	5	3758	1/1	0.98	0.25	65,65,65,65	0
84	MG	5	3851	1/1	0.98	0.20	54,54,54,54	0
84	MG	1	3688	1/1	0.98	0.26	61,61,61,61	0
84	MG	5	3544	1/1	0.98	0.30	61,61,61,61	0
84	MG	5	3489	1/1	0.98	0.16	55,55,55,55	0
84	MG	6	2040	1/1	0.98	0.16	78,78,78,78	0
84	MG	5	3643	1/1	0.98	0.26	55,55,55,55	0
84	MG	1	3762	1/1	0.98	0.26	70,70,70,70	0
84	MG	5	3472	1/1	0.98	0.17	57,57,57,57	0
84	MG	1	3850	1/1	0.98	0.29	57,57,57,57	0
84	MG	1	3595	1/1	0.98	0.27	54,54,54,54	0
84	MG	5	3811	1/1	0.98	0.30	44,44,44,44	0
84	MG	m0	302	1/1	0.98	0.21	53,53,53,53	0
84	MG	5	3670	1/1	0.98	0.30	63,63,63,63	0
84	MG	1	3673	1/1	0.98	0.12	66,66,66,66	0
84	MG	5	3513	1/1	0.98	0.22	48,48,48,48	0
84	MG	l7	301	1/1	0.98	0.24	45,45,45,45	0
84	MG	1	3401	1/1	0.98	0.31	56,56,56,56	0
84	MG	6	1964	1/1	0.98	0.40	73,73,73,73	0
84	MG	1	3542	1/1	0.98	0.26	52,52,52,52	0
84	MG	1	3416	1/1	0.98	0.17	56,56,56,56	0
84	MG	5	3669	1/1	0.98	0.23	63,63,63,63	0
86	ZN	o4	501	1/1	0.98	0.17	127,127,127,127	0
84	MG	1	3839	1/1	0.98	0.34	57,57,57,57	0
84	MG	N0	202	1/1	0.98	0.12	49,49,49,49	0
84	MG	1	3507	1/1	0.98	0.35	60,60,60,60	0
84	MG	q3	504	1/1	0.98	0.23	74,74,74,74	0
84	MG	5	4095	1/1	0.98	0.12	68,68,68,68	0
84	MG	5	3537	1/1	0.98	0.49	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3788	1/1	0.98	0.22	50,50,50,50	0
84	MG	5	3548	1/1	0.98	0.33	60,60,60,60	0
84	MG	1	3485	1/1	0.98	0.21	70,70,70,70	0
84	MG	6	1931	1/1	0.98	0.31	67,67,67,67	0
84	MG	1	3525	1/1	0.98	0.23	69,69,69,69	0
84	MG	5	3662	1/1	0.98	0.22	50,50,50,50	0
84	MG	2	1988	1/1	0.98	0.14	112,112,112,112	0
84	MG	5	3578	1/1	0.98	0.17	48,48,48,48	1
84	MG	2	1916	1/1	0.98	0.16	90,90,90,90	0
86	ZN	D9	101	1/1	0.98	0.11	121,121,121,121	0
84	MG	1	3947	1/1	0.98	0.48	79,79,79,79	0
84	MG	4	216	1/1	0.98	0.12	69,69,69,69	0
84	MG	m4	202	1/1	0.98	0.19	52,52,52,52	0
84	MG	1	3567	1/1	0.98	0.16	66,66,66,66	0
84	MG	1	3491	1/1	0.98	0.34	79,79,79,79	0
84	MG	5	3656	1/1	0.98	0.19	78,78,78,78	0
84	MG	6	2122	1/1	0.98	0.30	96,96,96,96	0
84	MG	1	3679	1/1	0.98	0.18	68,68,68,68	0
84	MG	L4	402	1/1	0.98	0.08	65,65,65,65	0
84	MG	5	3906	1/1	0.98	0.22	50,50,50,50	0
84	MG	1	3422	1/1	0.98	0.25	50,50,50,50	0
84	MG	5	3533	1/1	0.98	0.27	45,45,45,45	0
84	MG	5	3511	1/1	0.98	0.18	47,47,47,47	0
84	MG	7	201	1/1	0.98	0.27	45,45,45,45	0
84	MG	1	3434	1/1	0.98	0.24	53,53,53,53	0
84	MG	1	3511	1/1	0.98	0.39	59,59,59,59	0
84	MG	3	201	1/1	0.98	0.13	81,81,81,81	0
84	MG	5	3655	1/1	0.98	0.17	78,78,78,78	0
84	MG	5	3885	1/1	0.98	0.20	65,65,65,65	0
84	MG	5	3573	1/1	0.98	0.31	61,61,61,61	0
84	MG	1	3411	1/1	0.98	0.39	53,53,53,53	0
84	MG	2	1970	1/1	0.98	0.18	105,105,105,105	0
84	MG	5	3761	1/1	0.98	0.34	69,69,69,69	0
84	MG	1	3870	1/1	0.98	0.21	58,58,58,58	0
84	MG	1	3523	1/1	0.98	0.18	70,70,70,70	0
84	MG	1	3943	1/1	0.98	0.30	60,60,60,60	0
84	MG	1	3725	1/1	0.98	0.26	62,62,62,62	0
84	MG	5	3898	1/1	0.98	0.20	56,56,56,56	0
86	ZN	Q2	501	1/1	0.98	0.08	102,102,102,102	0
84	MG	1	3522	1/1	0.99	0.34	63,63,63,63	0
84	MG	1	3435	1/1	0.99	0.23	53,53,53,53	0
84	MG	1	3716	1/1	0.99	0.32	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	5	3521	1/1	0.99	0.19	50,50,50,50	0
84	MG	1	3756	1/1	0.99	0.24	62,62,62,62	0
84	MG	5	3902	1/1	0.99	0.42	55,55,55,55	0
84	MG	2	1982	1/1	0.99	0.13	97,97,97,97	0
84	MG	1	3436	1/1	0.99	0.28	49,49,49,49	0
86	ZN	d6	101	1/1	0.99	0.16	82,82,82,82	0
84	MG	1	3588	1/1	0.99	0.26	58,58,58,58	0
84	MG	1	3473	1/1	0.99	0.37	59,59,59,59	0
84	MG	5	3426	1/1	0.99	0.21	48,48,48,48	0
84	MG	5	4109	1/1	0.99	0.22	42,42,42,42	0
84	MG	O2	201	1/1	0.99	0.11	60,60,60,60	0
84	MG	5	3715	1/1	0.99	0.15	54,54,54,54	0
84	MG	5	3500	1/1	0.99	0.19	51,51,51,51	0
84	MG	5	3816	1/1	0.99	0.17	43,43,43,43	0
84	MG	1	3717	1/1	0.99	0.64	56,56,56,56	0
84	MG	5	3995	1/1	0.99	0.22	47,47,47,47	0
84	MG	1	3646	1/1	0.99	0.22	52,52,52,52	0
84	MG	1	3684	1/1	0.99	0.25	58,58,58,58	0
84	MG	5	3406	1/1	0.99	0.27	44,44,44,44	0
84	MG	1	3428	1/1	0.99	0.22	54,54,54,54	0
86	ZN	Q0	500	1/1	0.99	0.17	72,72,72,72	0
84	MG	m0	301	1/1	0.99	0.26	49,49,49,49	1
84	MG	1	3946	1/1	0.99	0.27	54,54,54,54	0
84	MG	5	3499	1/1	0.99	0.15	53,53,53,53	0
84	MG	1	3671	1/1	0.99	0.35	55,55,55,55	0
86	ZN	D6	500	1/1	0.99	0.13	101,101,101,101	0
84	MG	1	3460	1/1	0.99	0.27	58,58,58,58	0
84	MG	1	3599	1/1	0.99	0.28	52,52,52,52	0
84	MG	5	4050	1/1	0.99	0.10	80,80,80,80	0
84	MG	1	3562	1/1	0.99	0.10	80,80,80,80	0
84	MG	5	3900	1/1	0.99	0.41	51,51,51,51	0
86	ZN	d9	101	1/1	0.99	0.12	89,89,89,89	0
84	MG	1	3783	1/1	0.99	0.21	61,61,61,61	0
84	MG	6	1928	1/1	0.99	0.31	68,68,68,68	0
84	MG	l2	302	1/1	0.99	0.29	53,53,53,53	0
84	MG	5	4124	1/1	0.99	0.22	50,50,50,50	0
84	MG	5	3994	1/1	0.99	0.21	48,48,48,48	0
84	MG	5	3402	1/1	0.99	0.22	47,47,47,47	0
86	ZN	q3	501	1/1	0.99	0.14	102,102,102,102	0
86	ZN	o7	501	1/1	0.99	0.19	80,80,80,80	0
84	MG	1	3406	1/1	0.99	0.11	58,58,58,58	0
84	MG	5	3559	1/1	0.99	0.11	56,56,56,56	1

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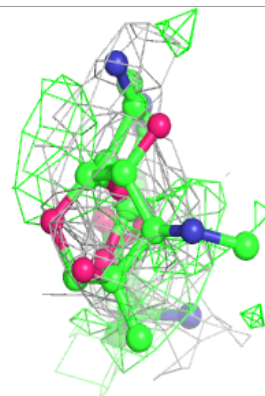
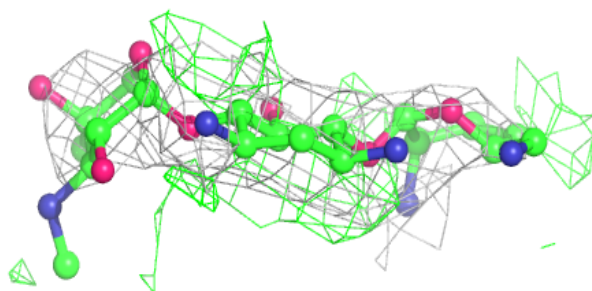
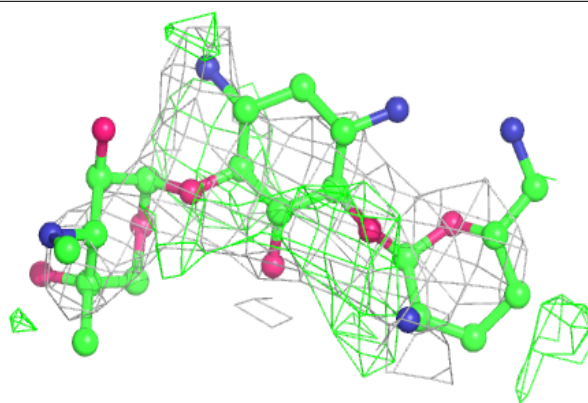
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3520	1/1	0.99	0.22	69,69,69,69	0
84	MG	5	3738	1/1	0.99	0.30	50,50,50,50	0
84	MG	l3	404	1/1	0.99	0.27	42,42,42,42	0
84	MG	5	3727	1/1	0.99	0.25	46,46,46,46	0
84	MG	5	3444	1/1	0.99	0.24	45,45,45,45	0
86	ZN	q2	501	1/1	0.99	0.10	94,94,94,94	0
84	MG	1	3682	1/1	0.99	0.09	65,65,65,65	0
84	MG	5	3673	1/1	0.99	0.33	55,55,55,55	0
84	MG	5	3447	1/1	0.99	0.34	49,49,49,49	0
84	MG	5	3452	1/1	0.99	0.16	48,48,48,48	0
84	MG	6	1963	1/1	0.99	0.32	68,68,68,68	0
84	MG	6	2004	1/1	0.99	0.22	67,67,67,67	0
86	ZN	q0	201	1/1	1.00	0.15	52,52,52,52	0
86	ZN	O7	101	1/1	1.00	0.14	77,77,77,77	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.

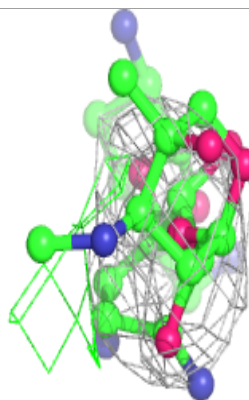
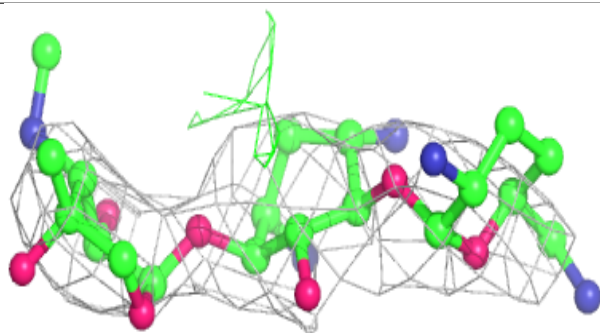
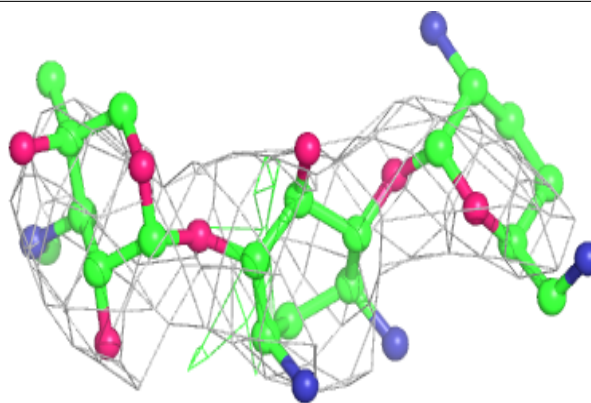
**Electron density around LLL 5 4178:**

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

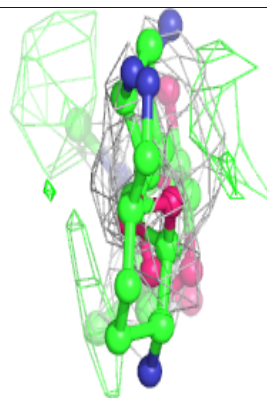
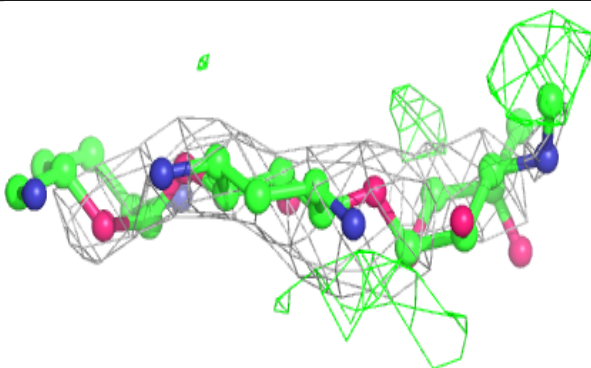
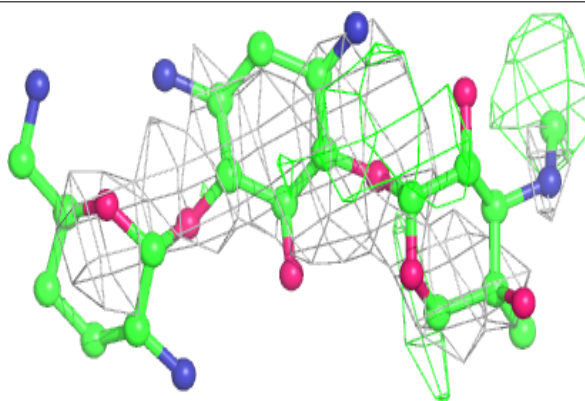


**Electron density around LLL 5 4173:**

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

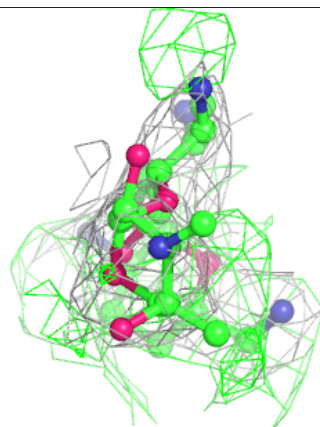
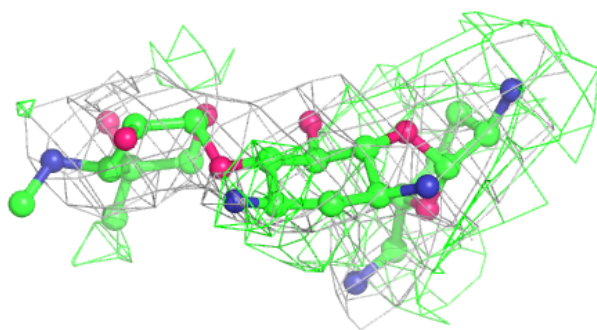
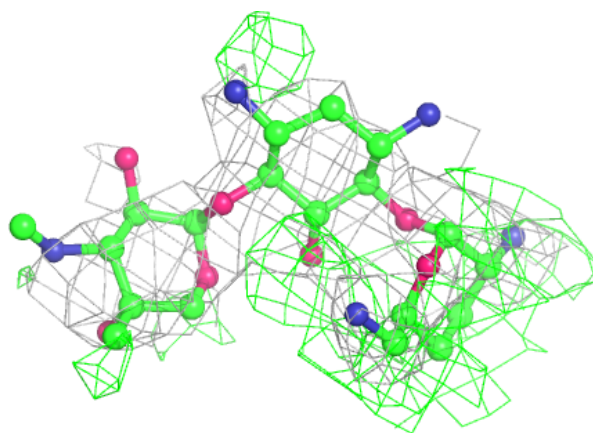
**Electron density around LLL 6 2174:**

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



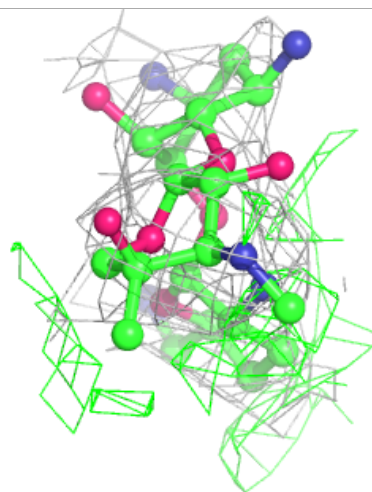
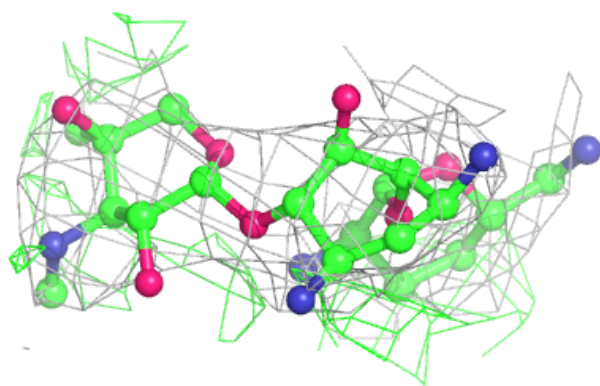
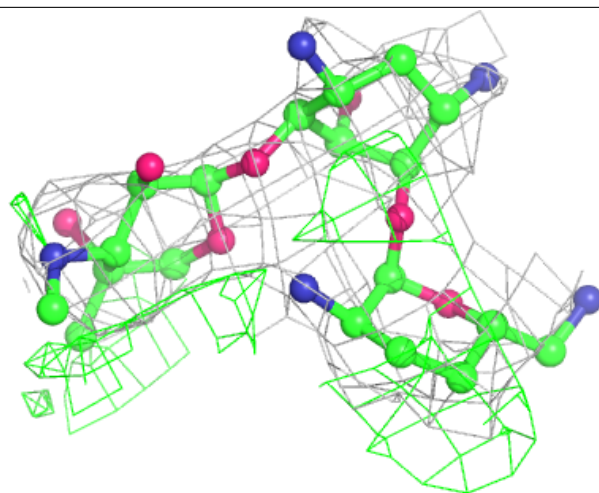
**Electron density around LLL 5 4176:**

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



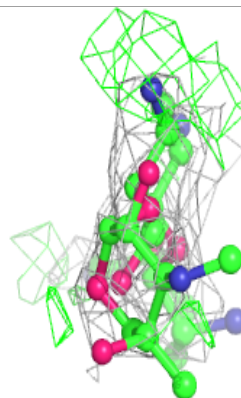
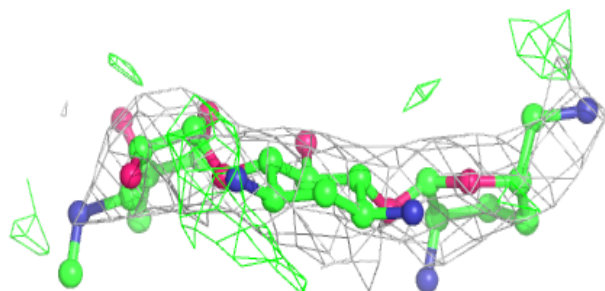
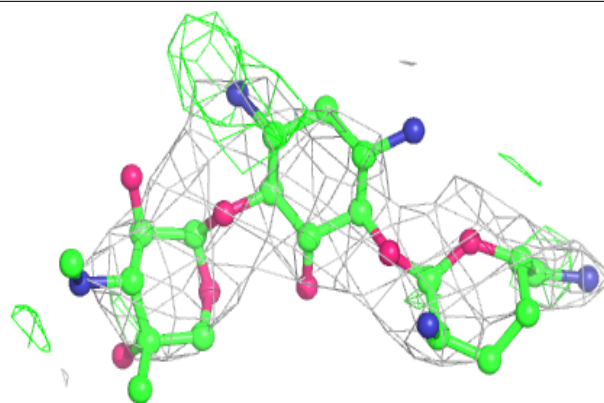
**Electron density around LLL 7 233:**

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

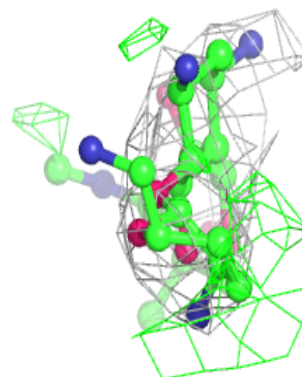
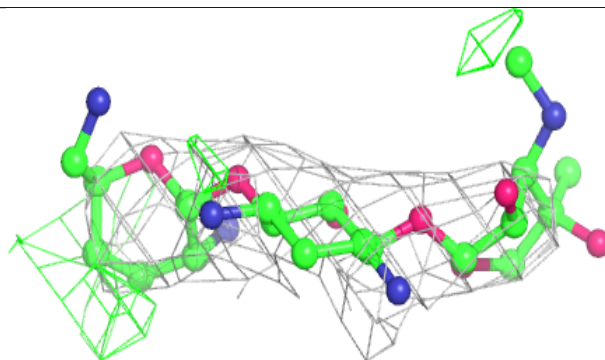
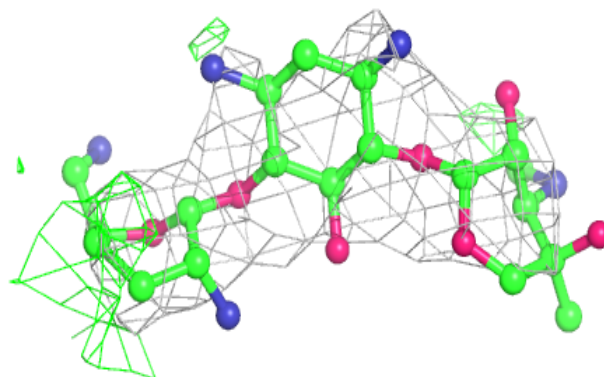


**Electron density around LLL 1 4000:**

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

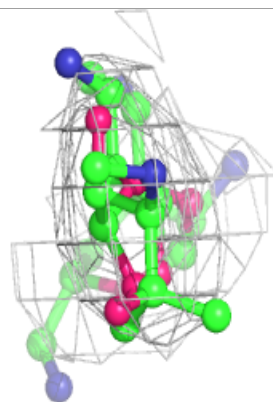
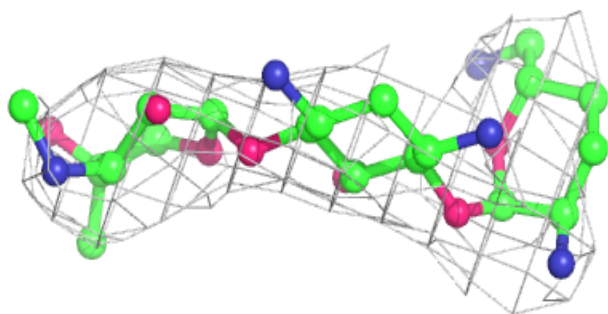
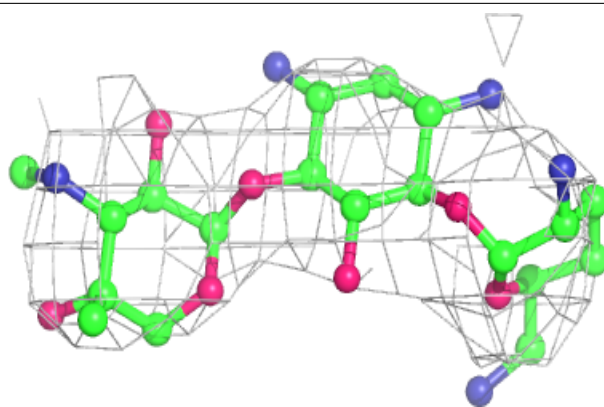
**Electron density around LLL 6 2175:**

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

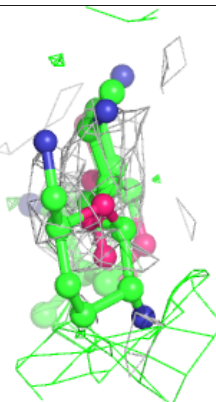
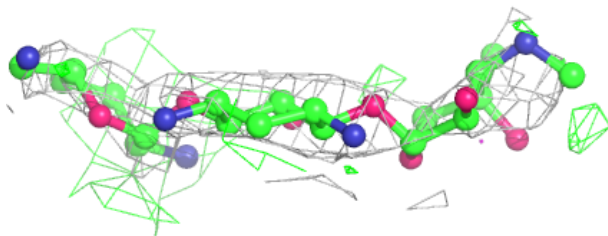
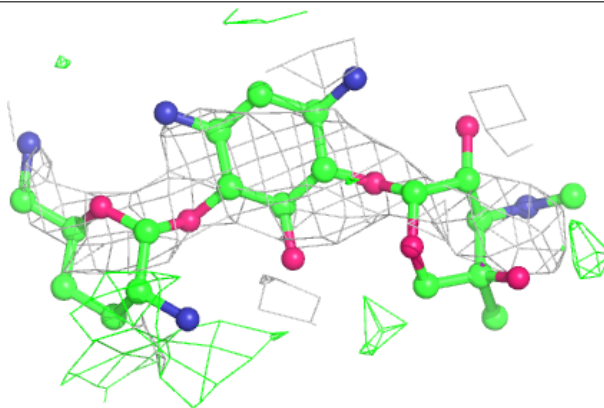


**Electron density around LLL 1 4002:**

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

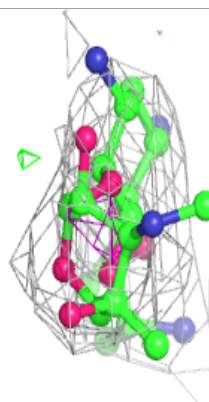
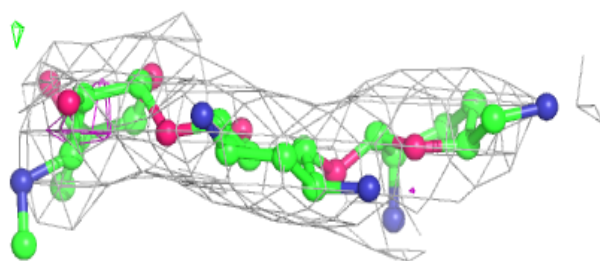
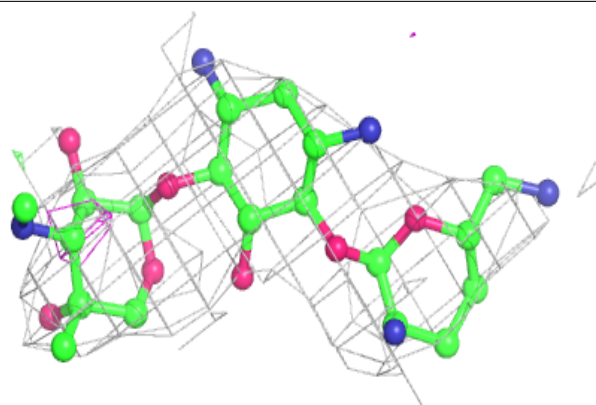
**Electron density around LLL 5 4175:**

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

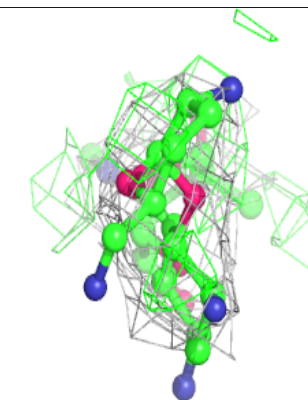
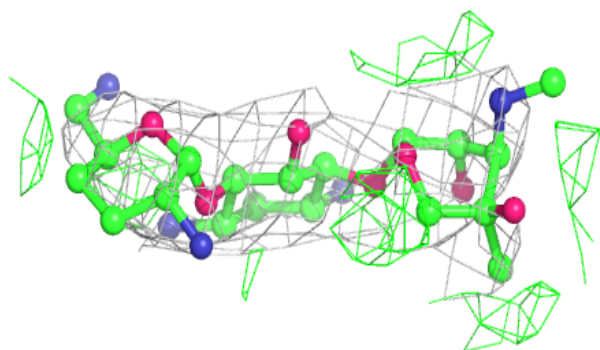
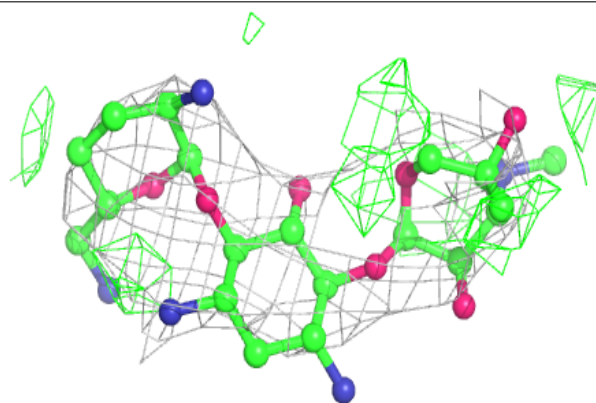


**Electron density around LLL 4 224:**

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

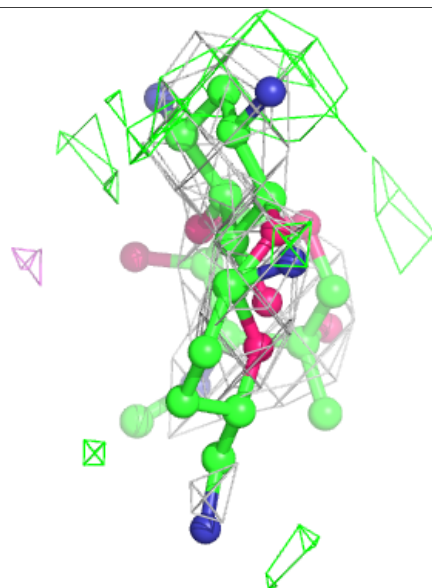
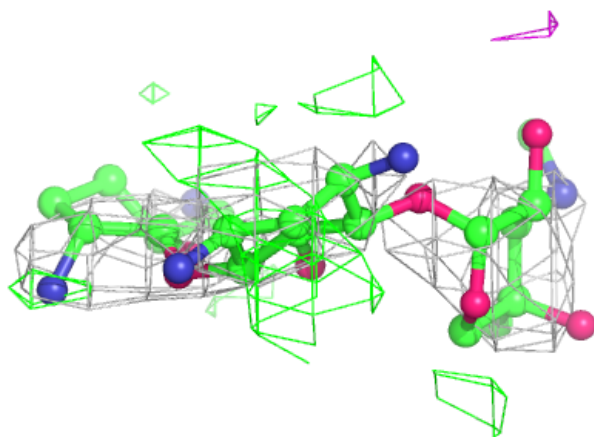
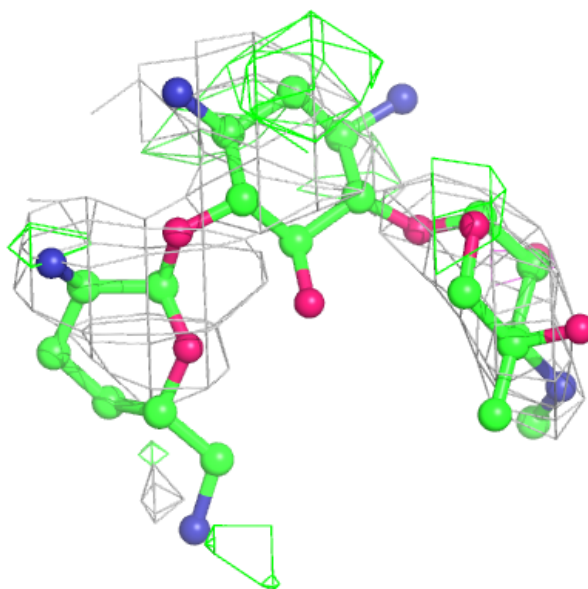
**Electron density around LLL 7 232:**

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



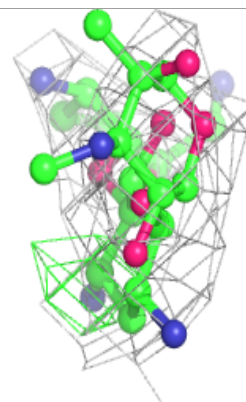
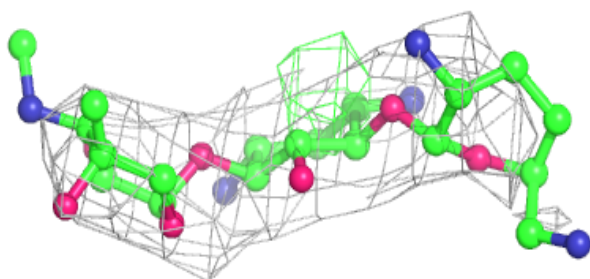
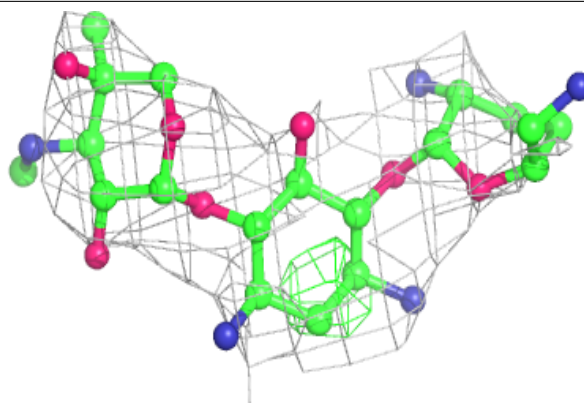
**Electron density around LLL 5 4177:**

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

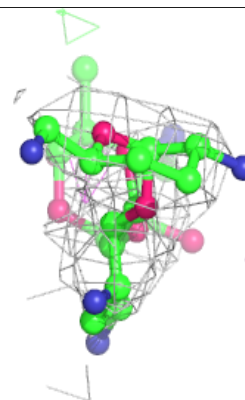
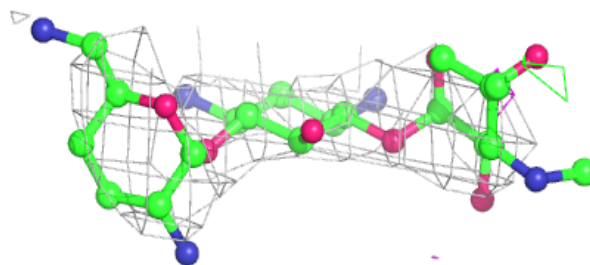
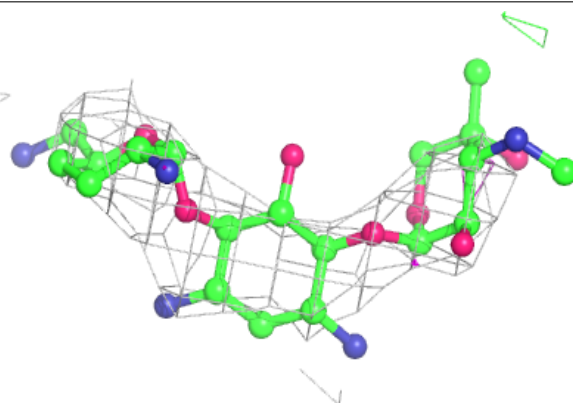


**Electron density around LLL 2 2044:**

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

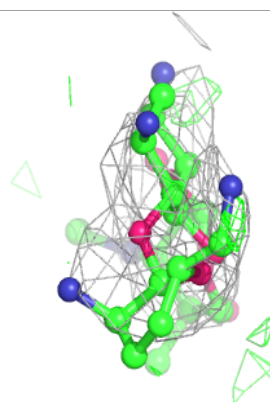
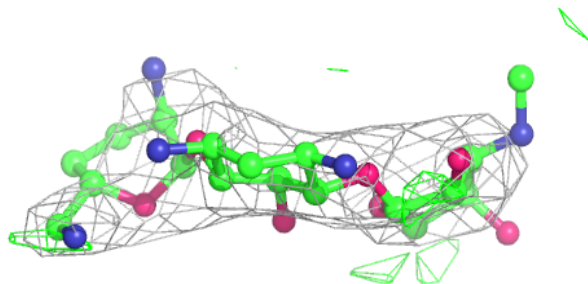
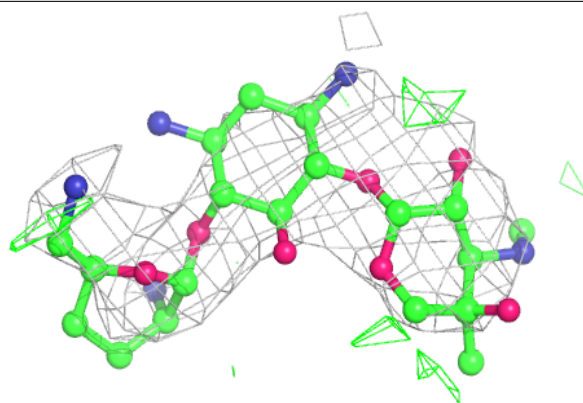
**Electron density around LLL 2 2045:**

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

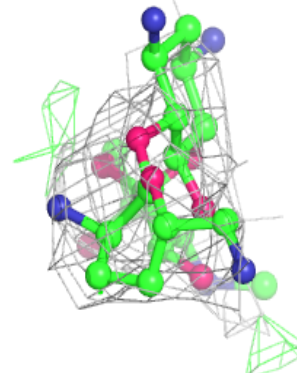
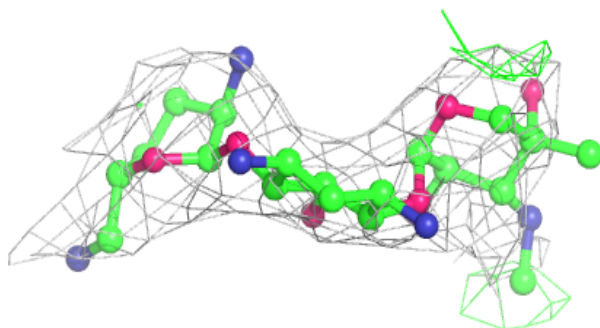
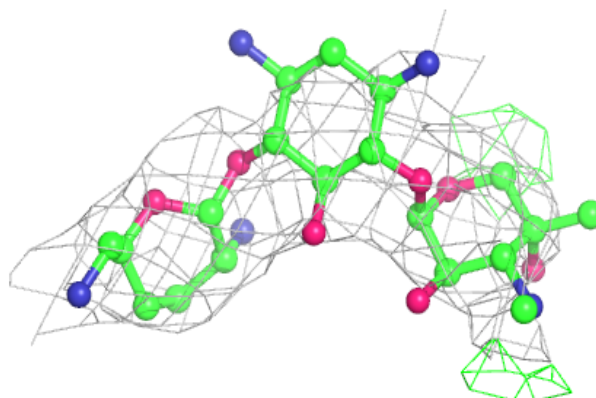


**Electron density around LLL 5 4156:**

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

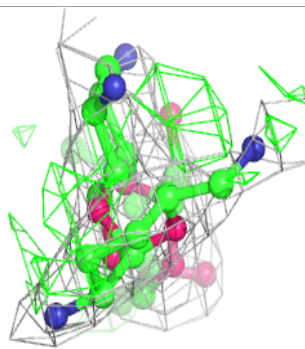
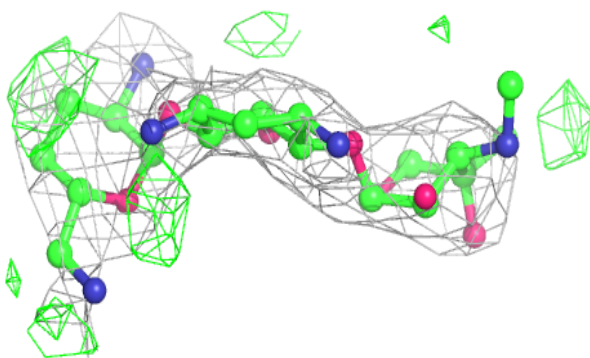
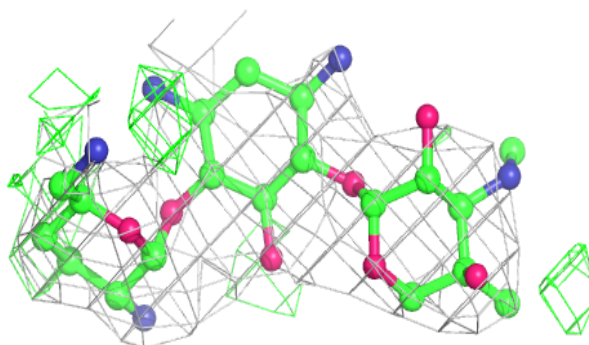
**Electron density around LLL 6 2173:**

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

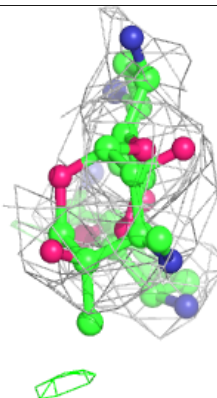
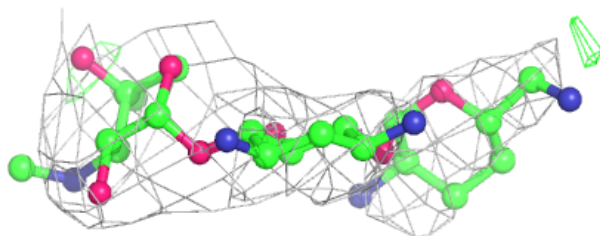
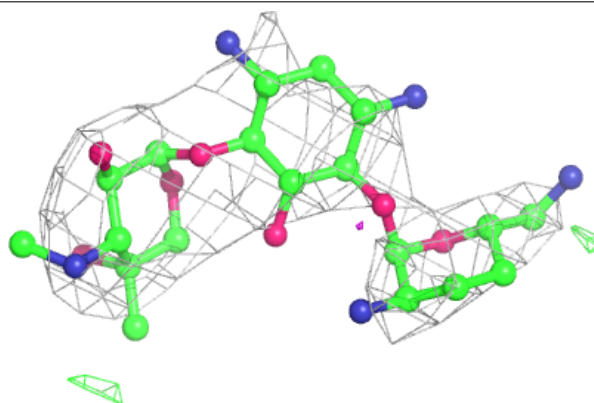


**Electron density around LLL 5 4169:**

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

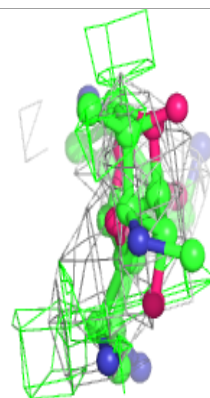
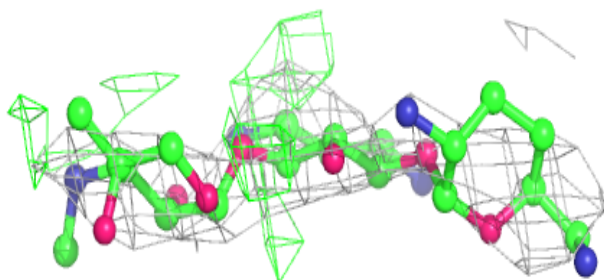
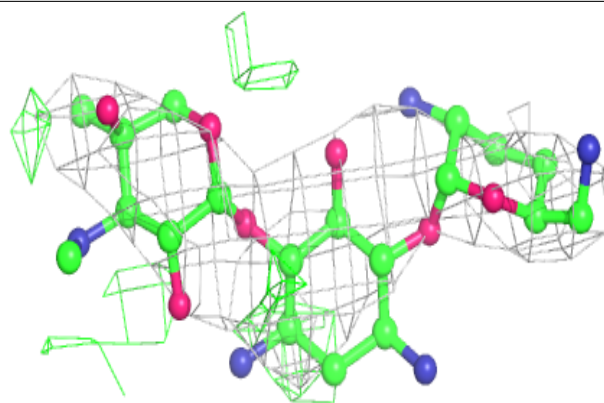
**Electron density around LLL 5 4171:**

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

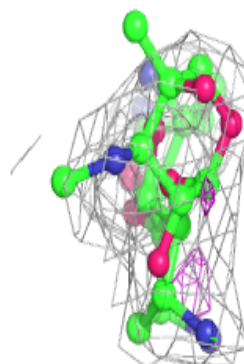
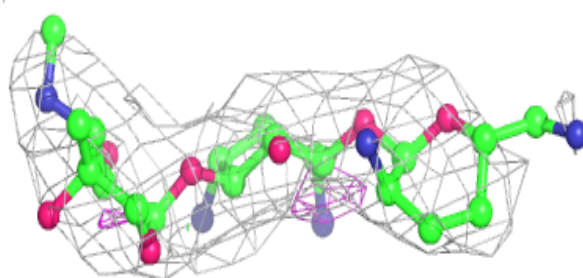
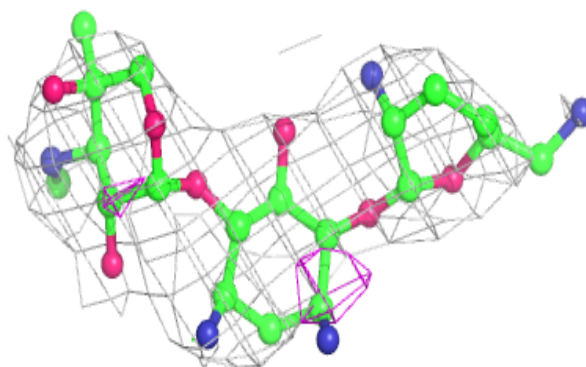


**Electron density around LLL 5 4174:**

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

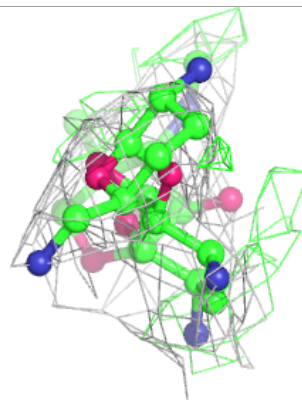
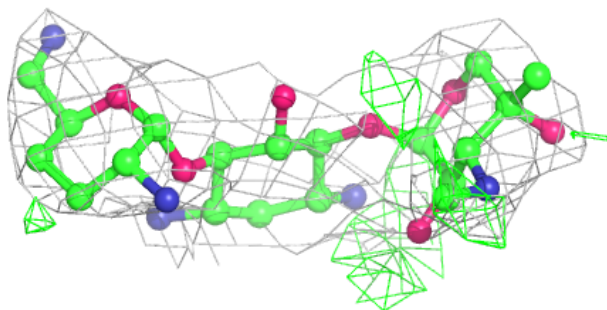
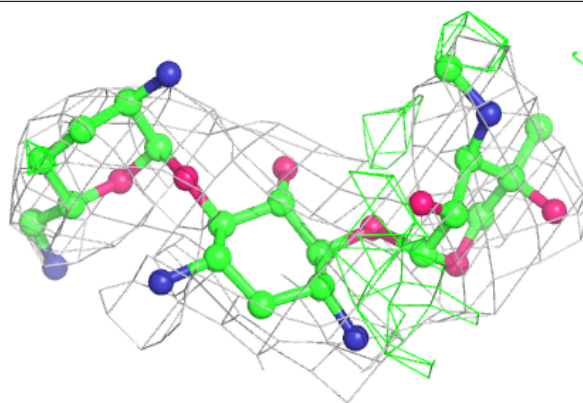
**Electron density around LLL 5 4155:**

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

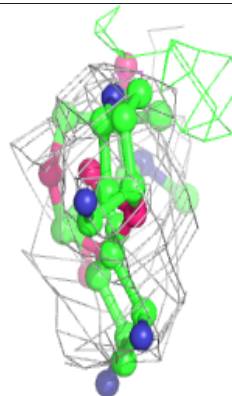
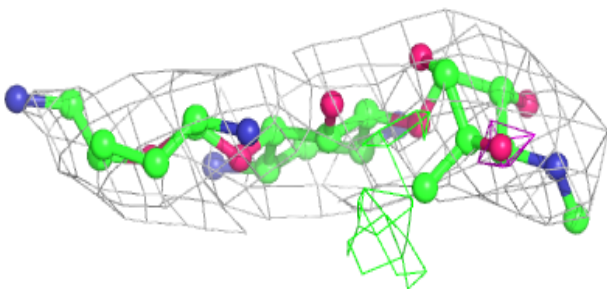
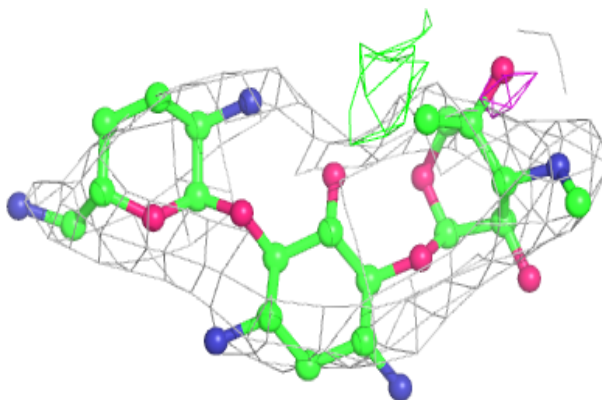


**Electron density around LLL 7 231:**

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

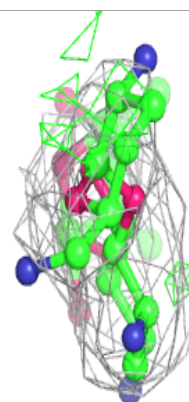
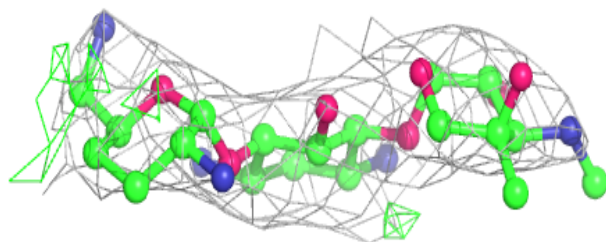
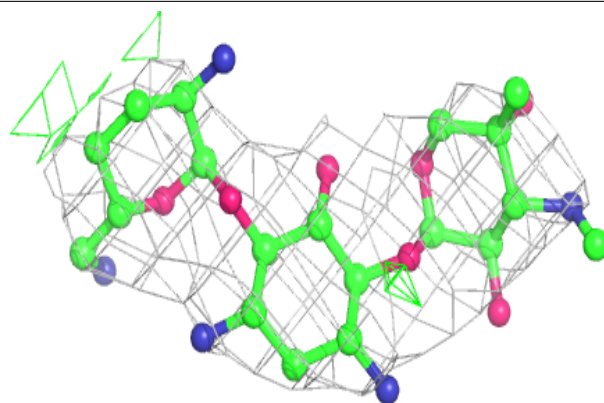
**Electron density around LLL 1 3995:**

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

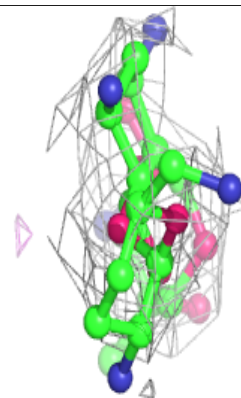
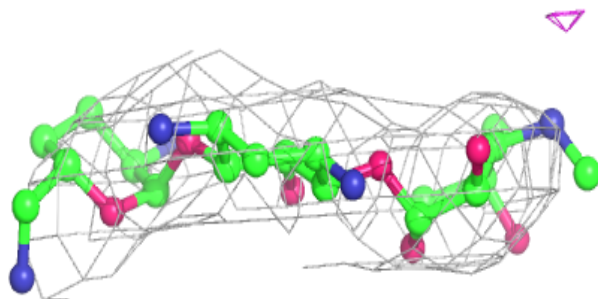
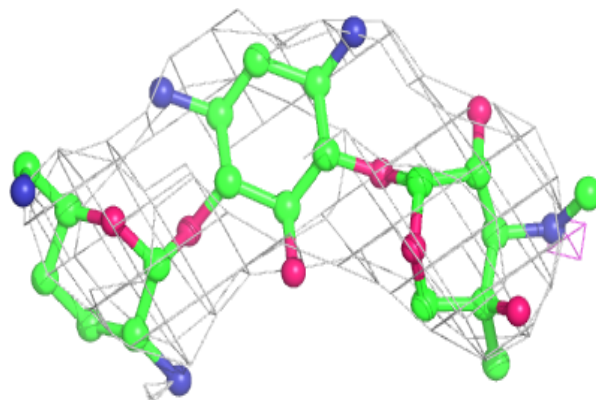


**Electron density around LLL 1 3996:**

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

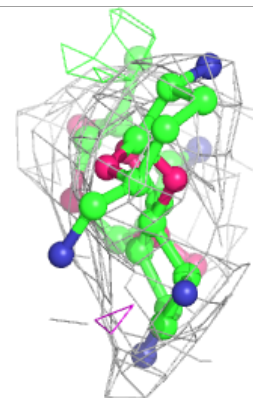
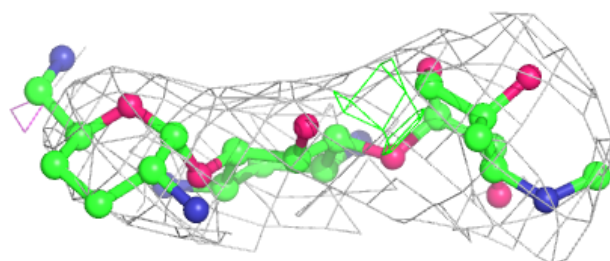
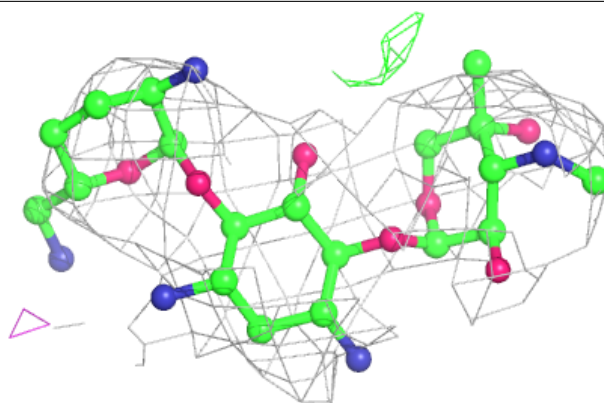
**Electron density around LLL 1 3997:**

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

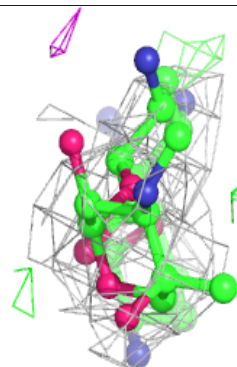
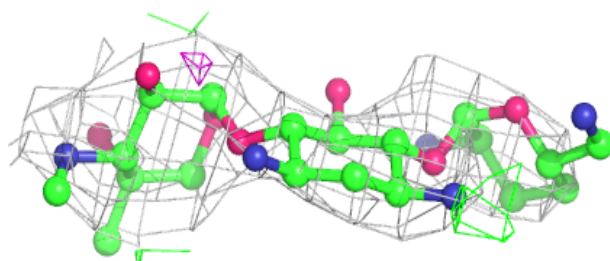
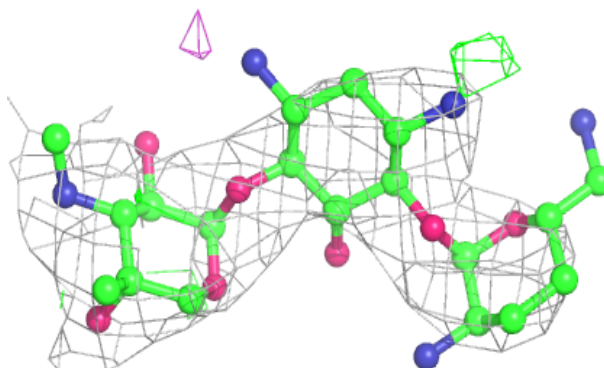


**Electron density around LLL 1 4001:**

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

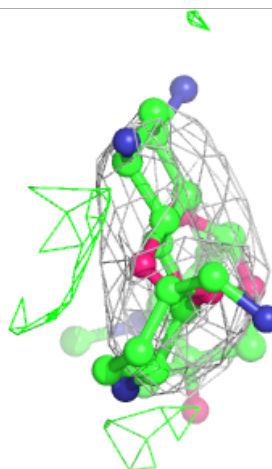
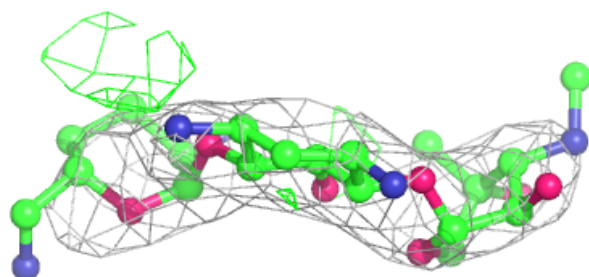
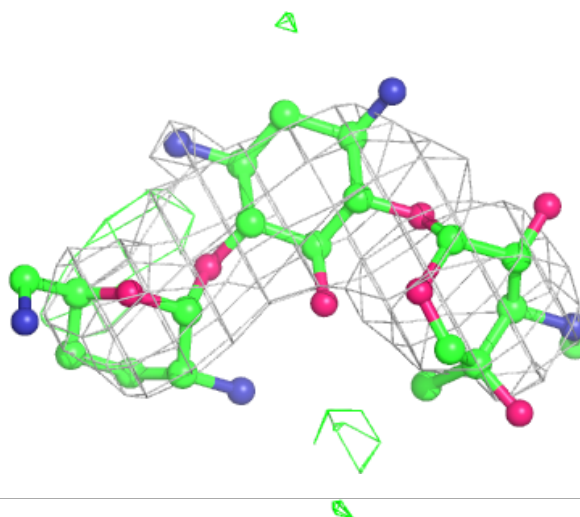
**Electron density around LLL 1 3998:**

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



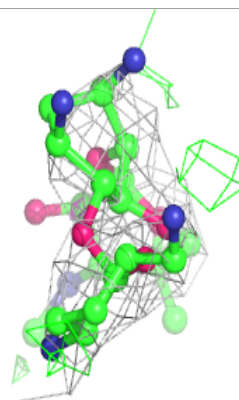
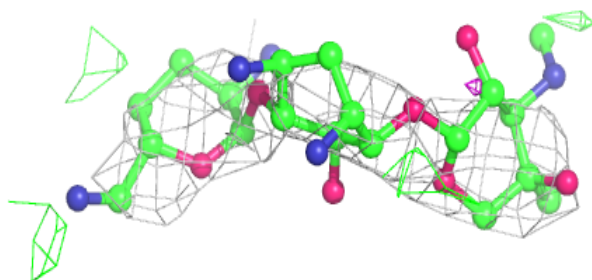
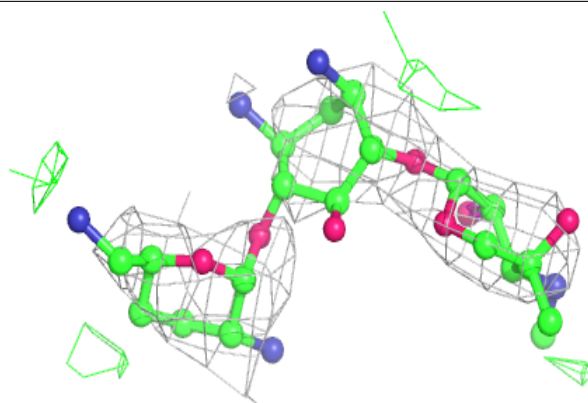
**Electron density around LLL 5 4166:**

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

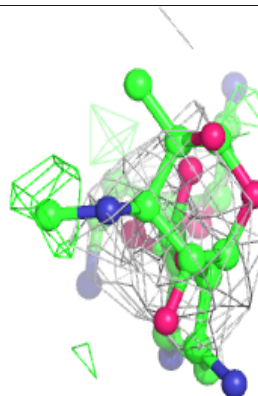
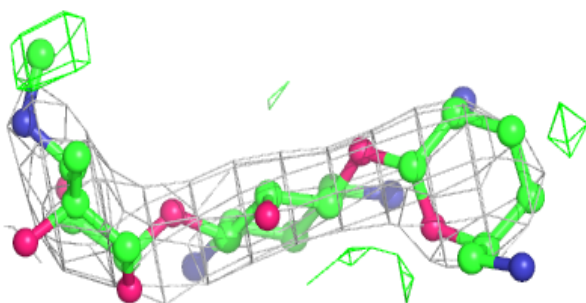
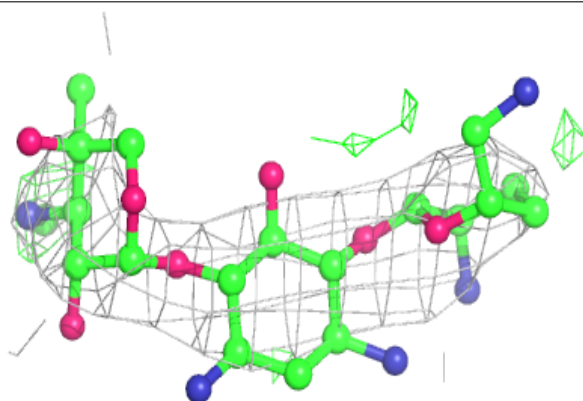


**Electron density around LLL 5 4158:**

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

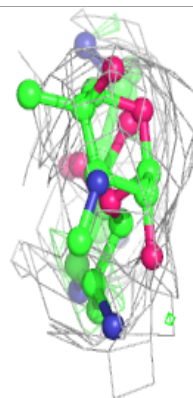
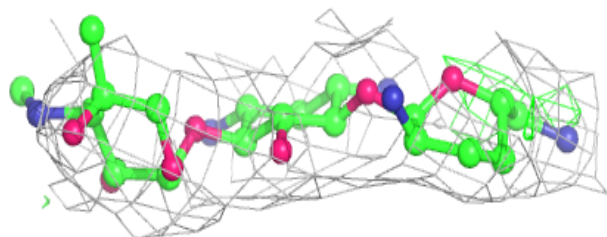
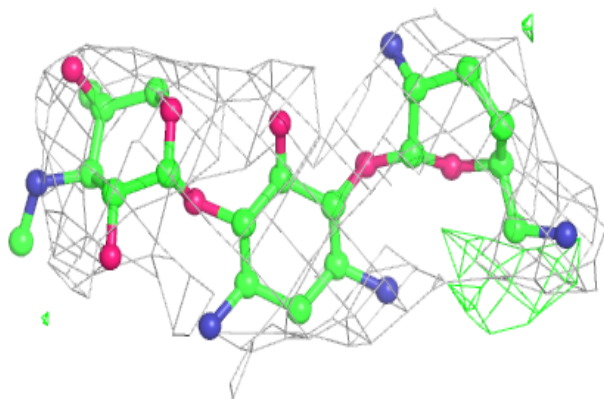
**Electron density around LLL 1 3999:**

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

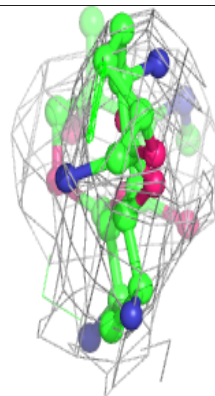
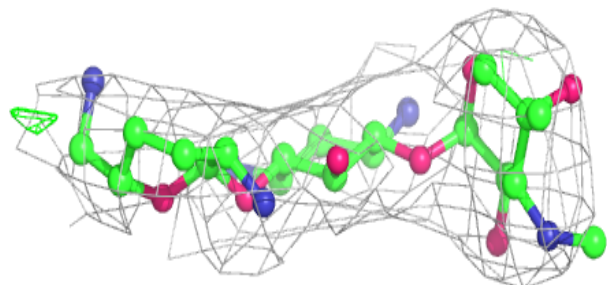
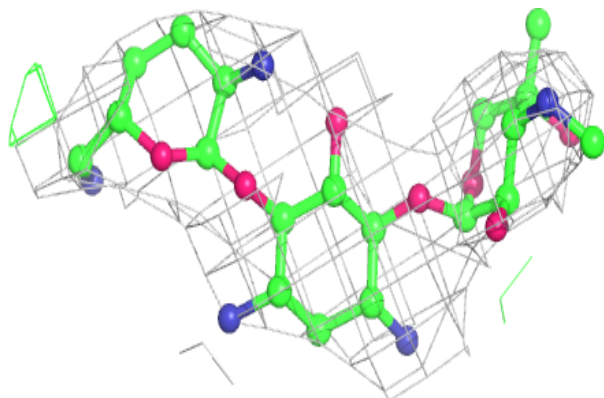


**Electron density around LLL 5 4162:**

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

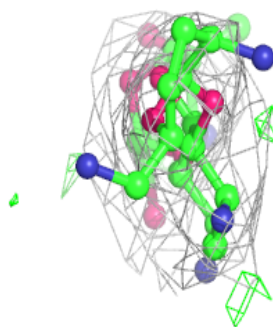
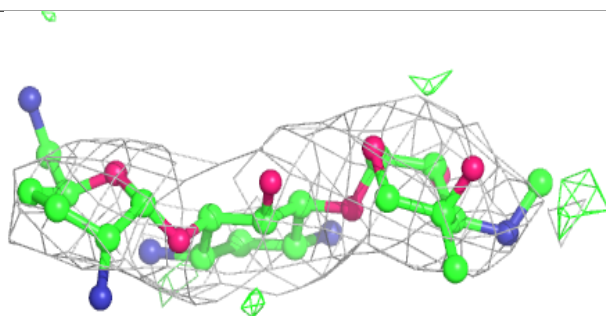
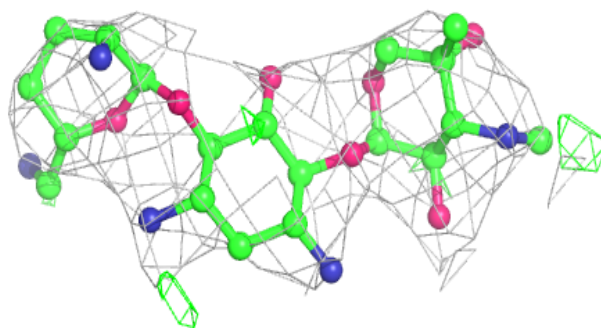
**Electron density around LLL 8 221:**

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

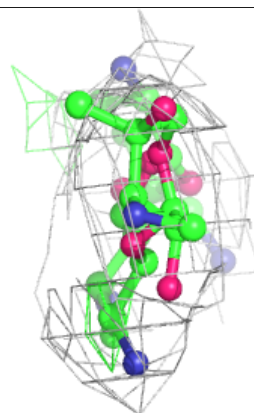
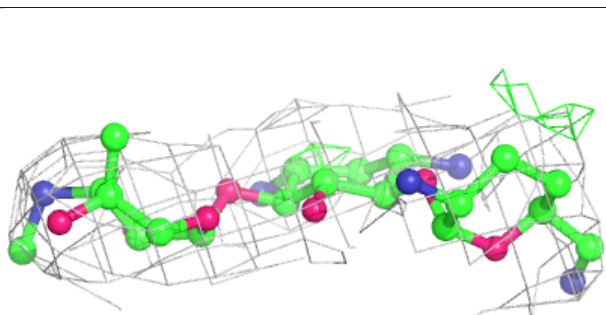
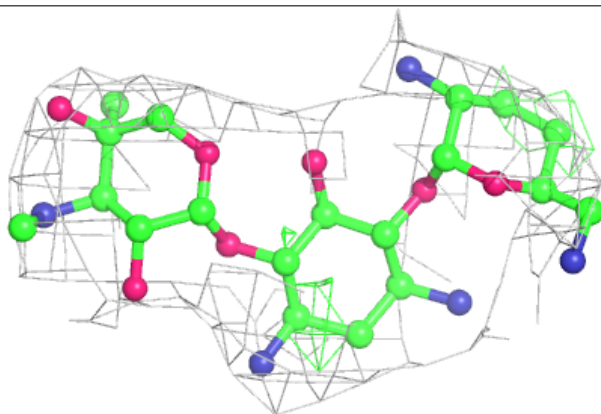


**Electron density around LLL 1 4004:**

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

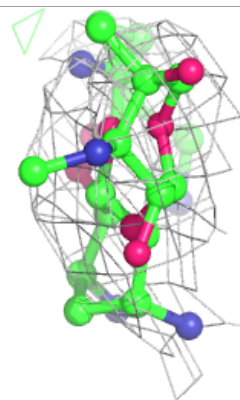
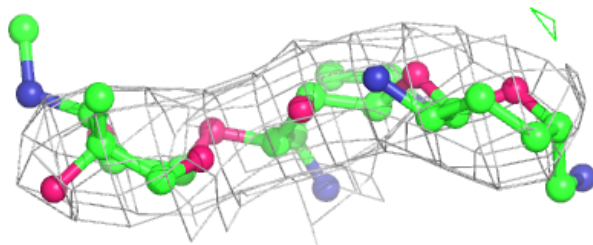
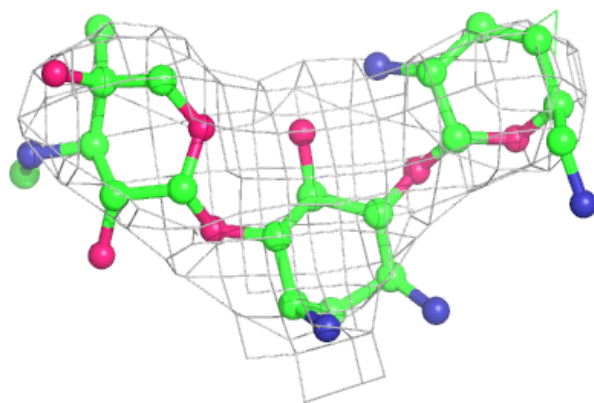
**Electron density around LLL 5 4167:**

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

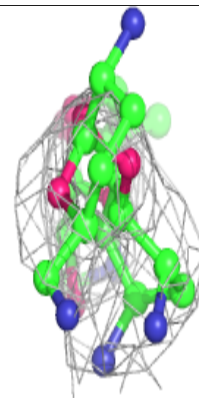
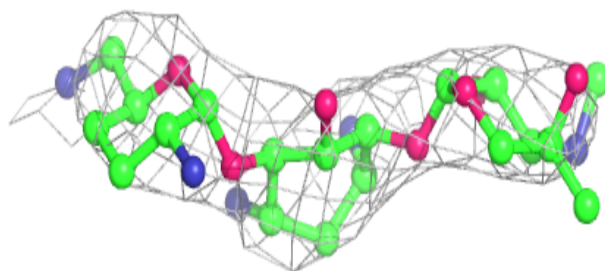
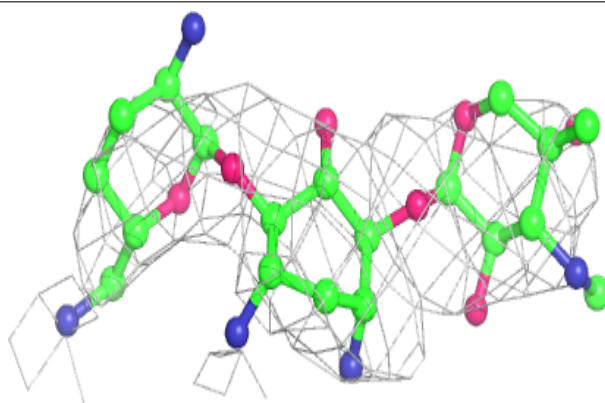


**Electron density around LLL 8 222:**

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

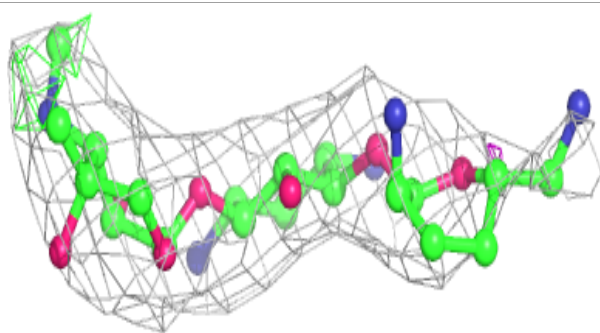
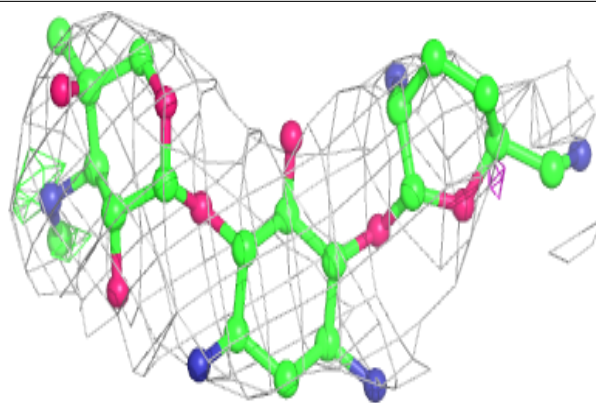
**Electron density around LLL 6 2172:**

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

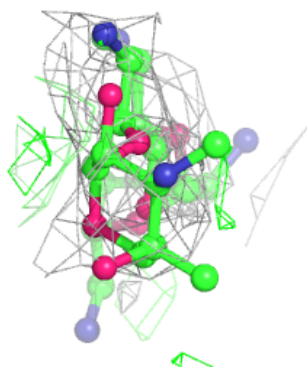
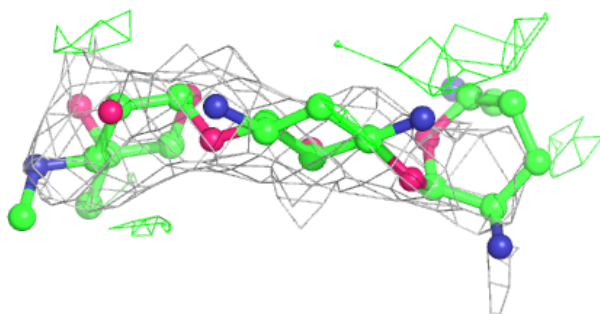
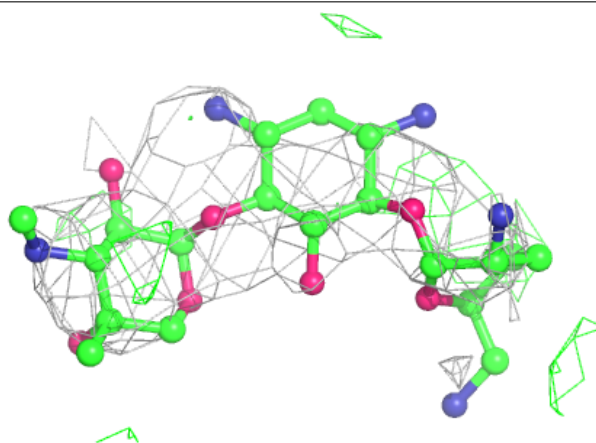


**Electron density around LLL 6 2168:**

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

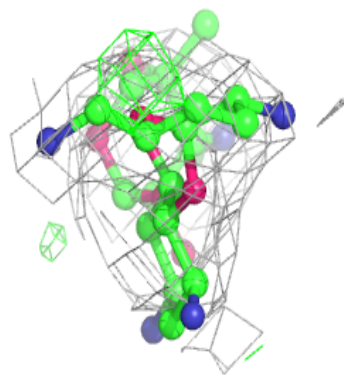
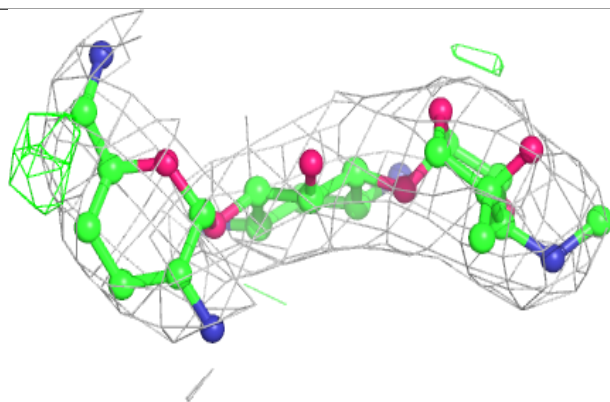
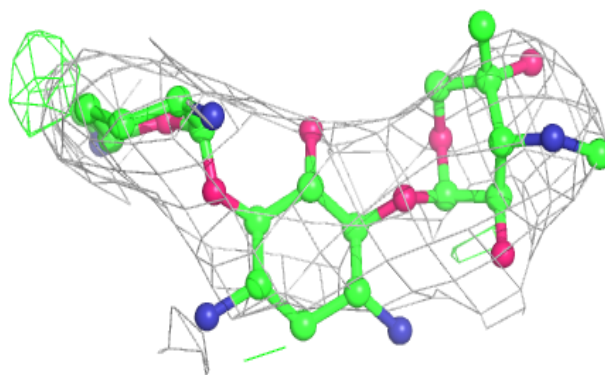
**Electron density around LLL 5 4164:**

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

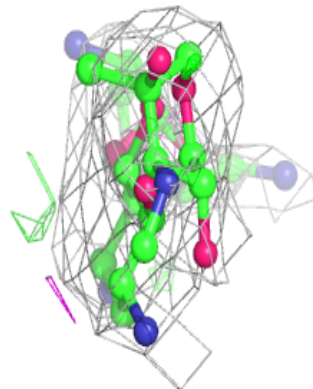
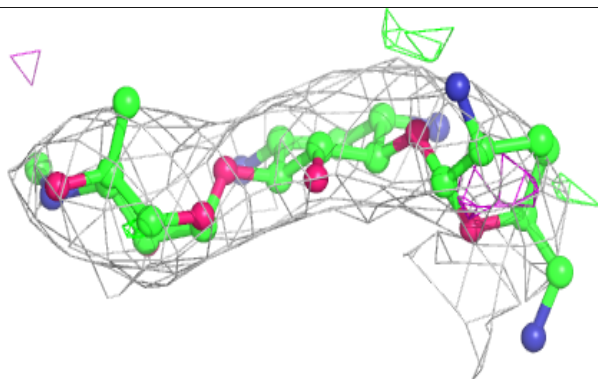
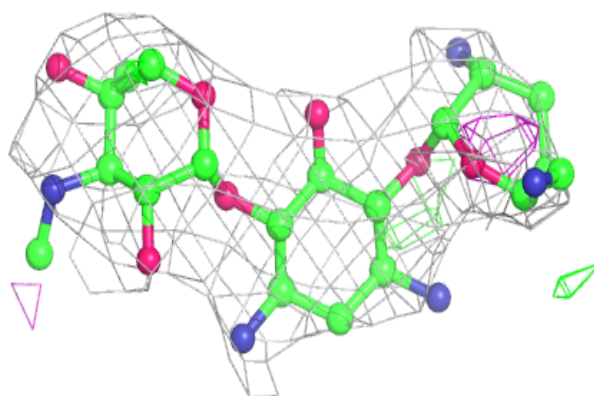


**Electron density around LLL 3 220:**

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

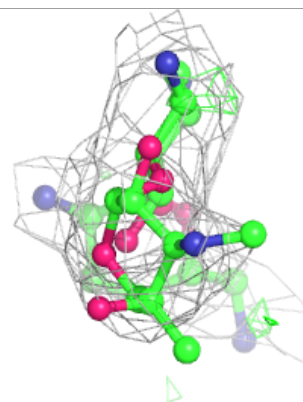
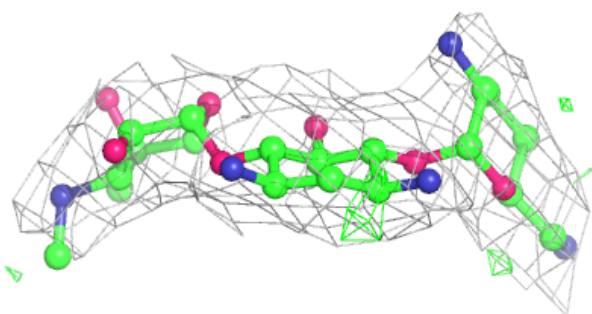
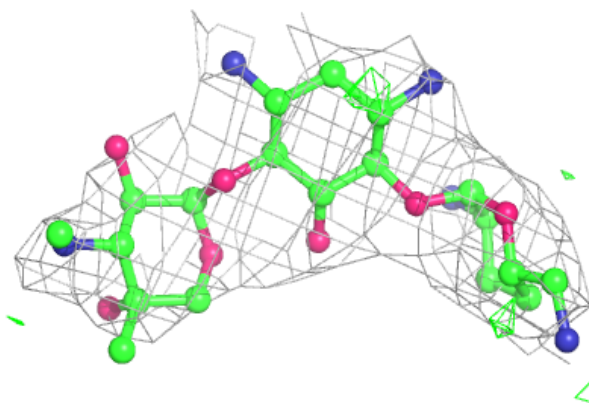
**Electron density around LLL 6 2164:**

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

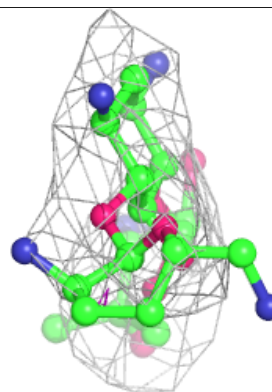
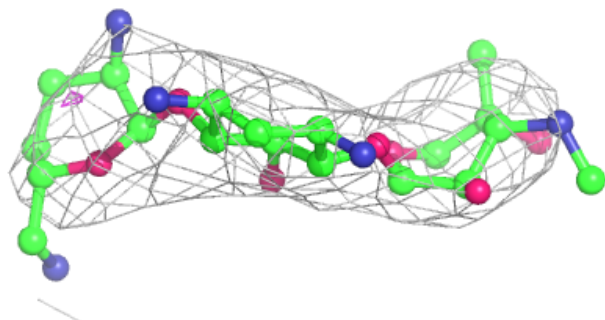
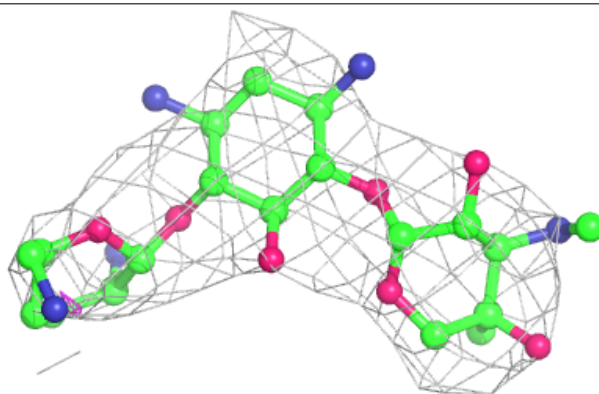


**Electron density around LLL 5 4172:**

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

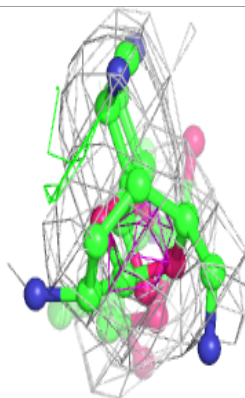
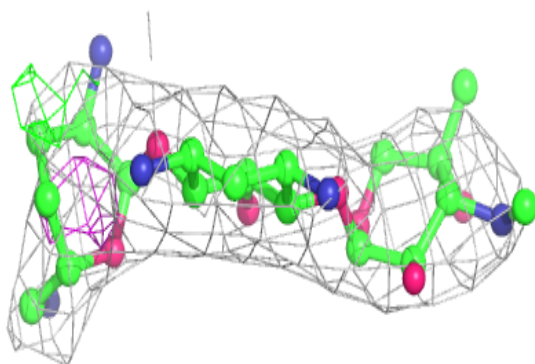
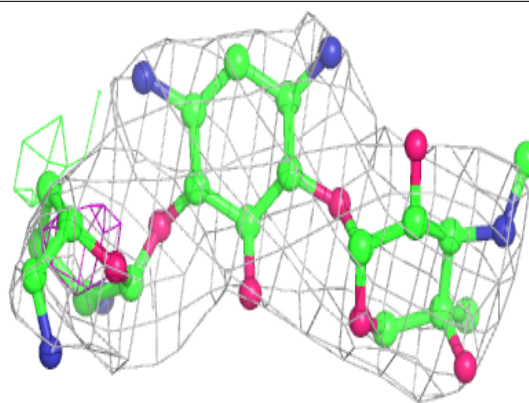
**Electron density around LLL 6 2167:**

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

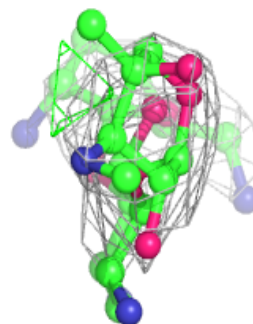
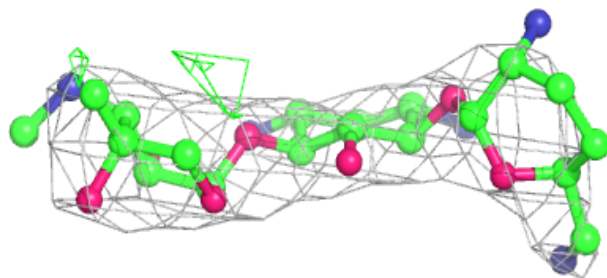
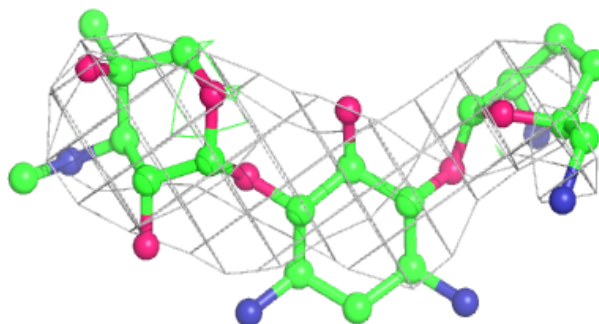


**Electron density around LLL 5 4153:**

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

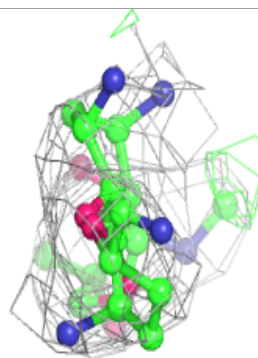
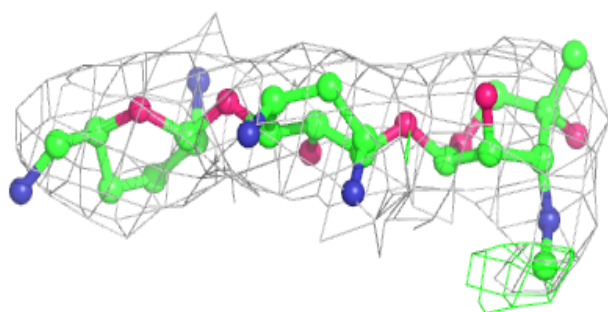
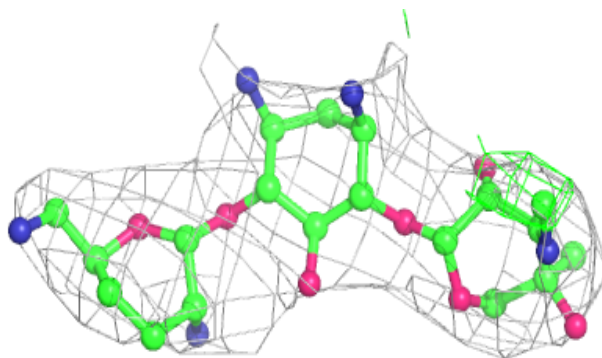
**Electron density around LLL 6 2176:**

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

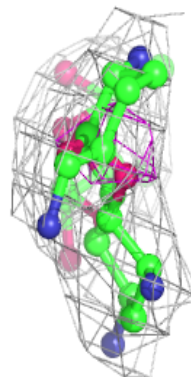
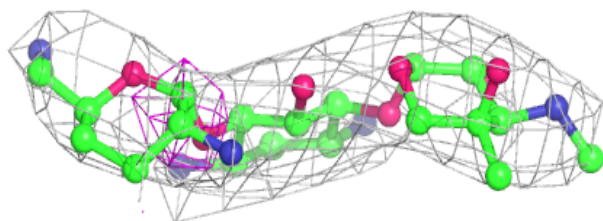
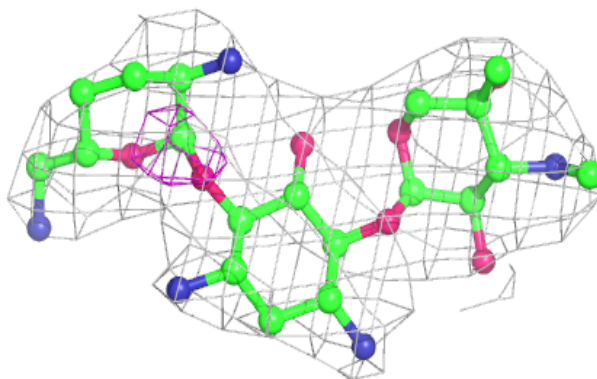


**Electron density around LLL 5 4163:**

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

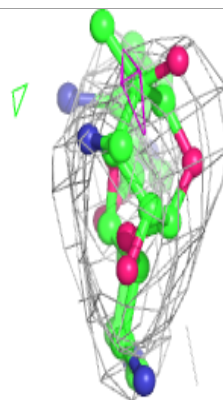
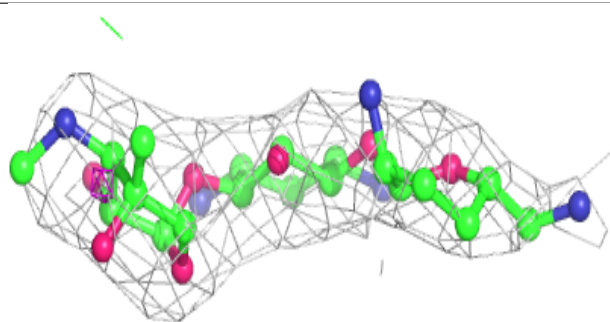
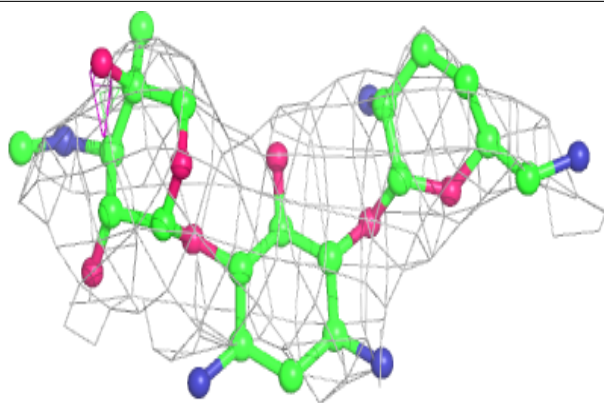
**Electron density around LLL L3 404:**

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

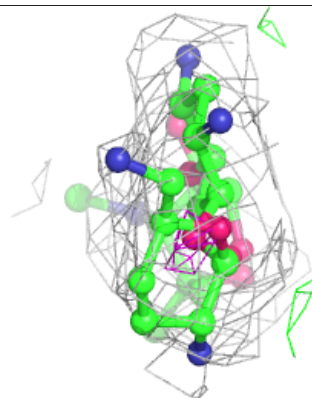
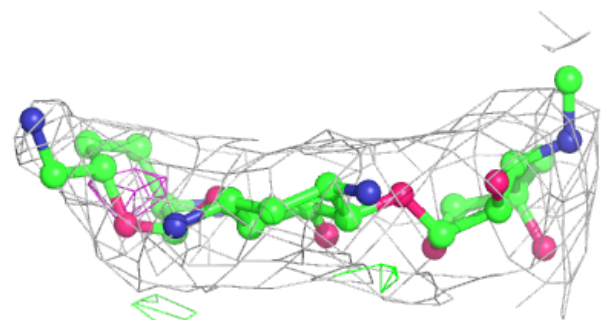
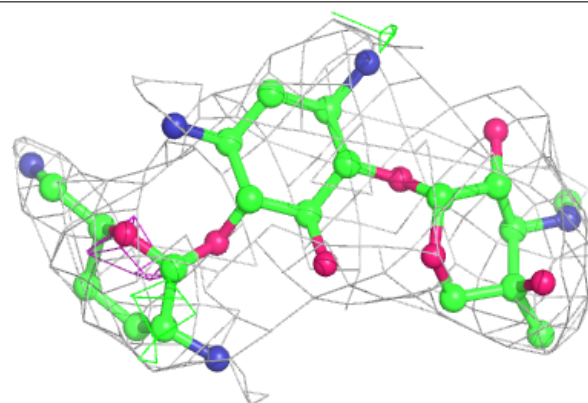


**Electron density around LLL 5 4152:**

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

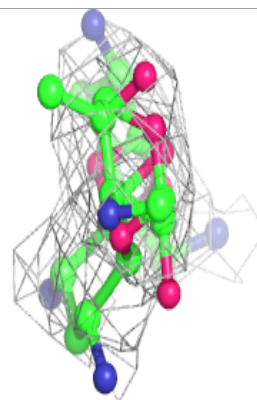
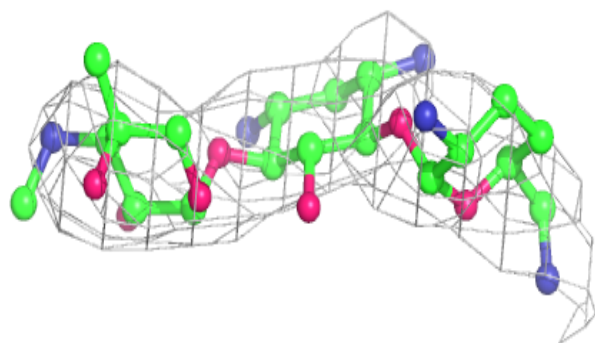
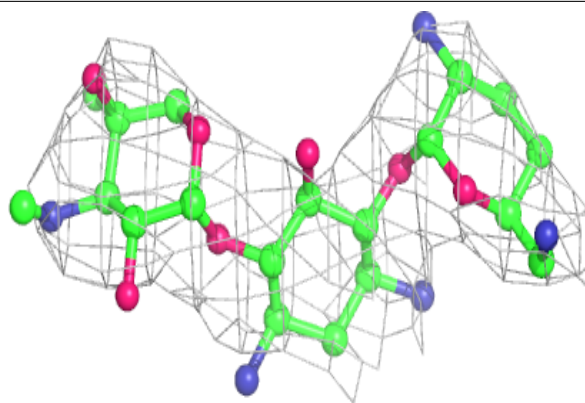
**Electron density around LLL 6 2170:**

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

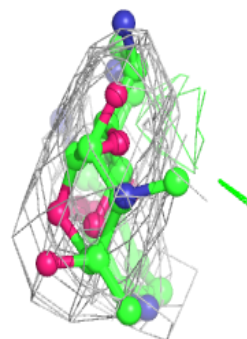
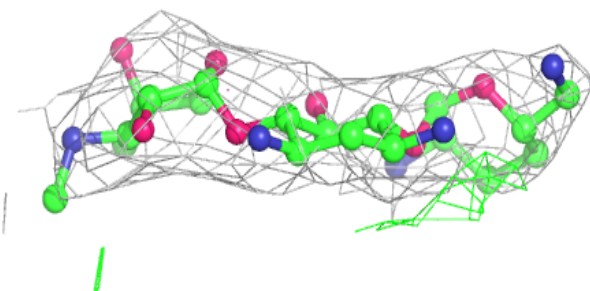
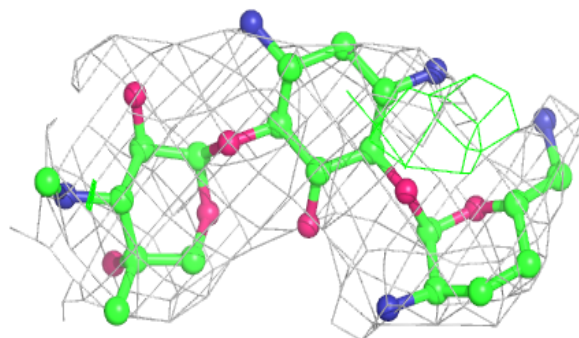


**Electron density around LLL 6 2165:**

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

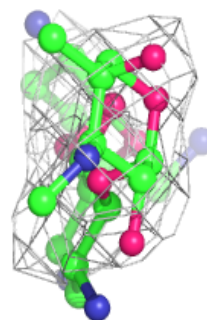
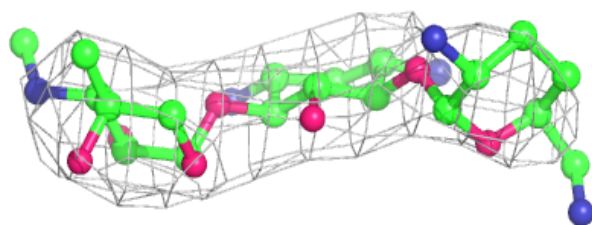
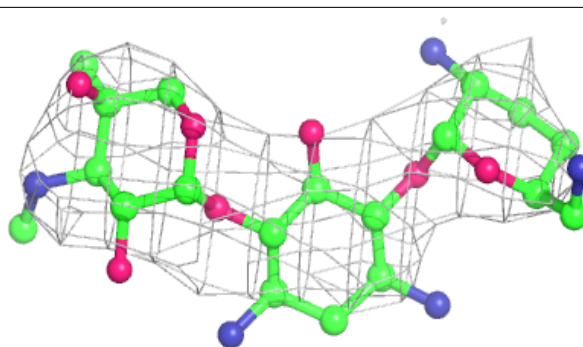
**Electron density around LLL 5 4159:**

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

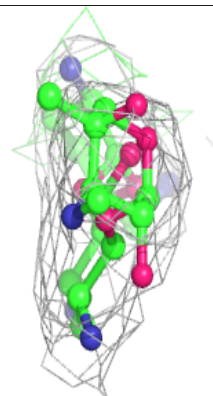
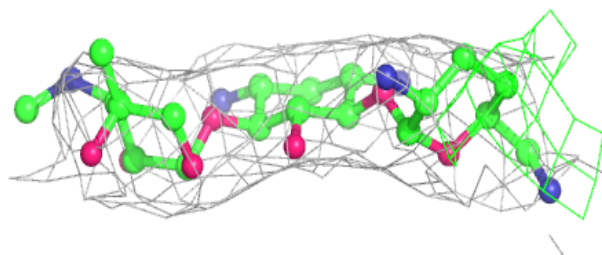
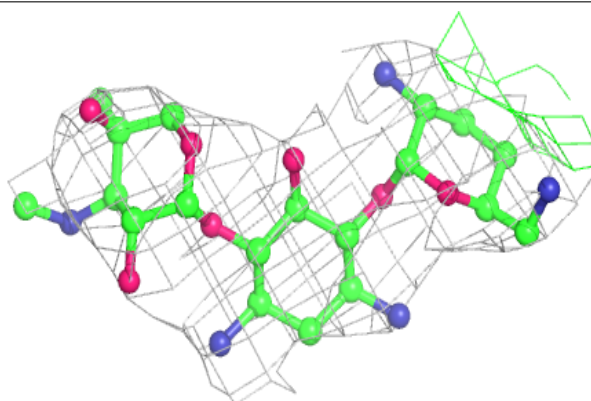


**Electron density around LLL 6 2171:**

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

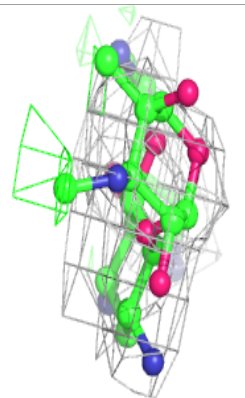
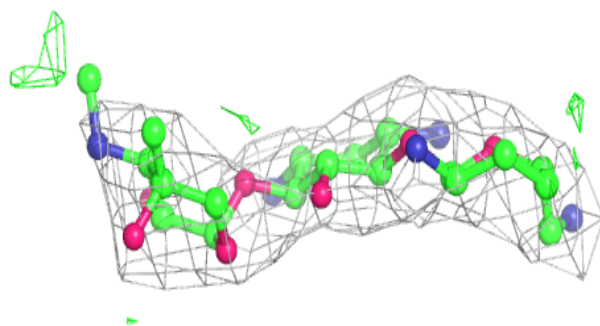
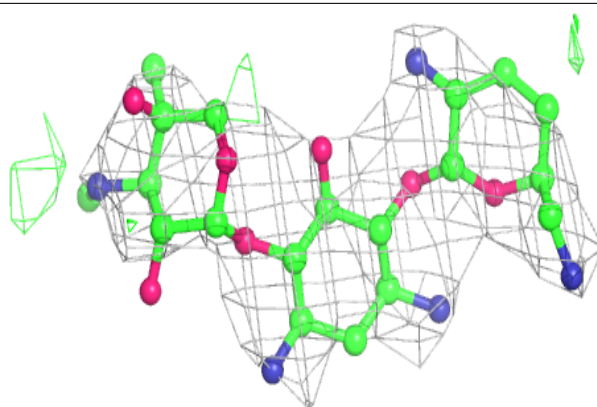
**Electron density around LLL 5 4165:**

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

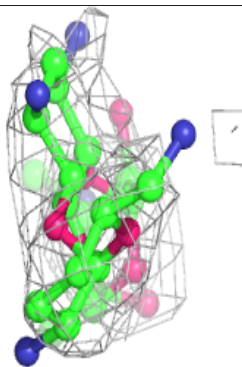
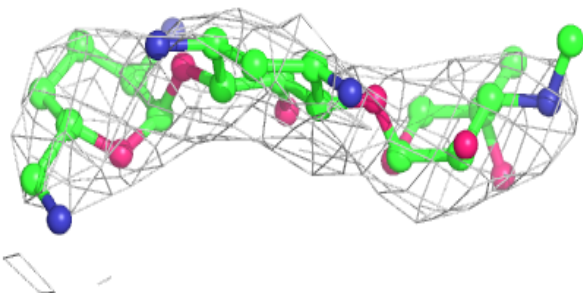
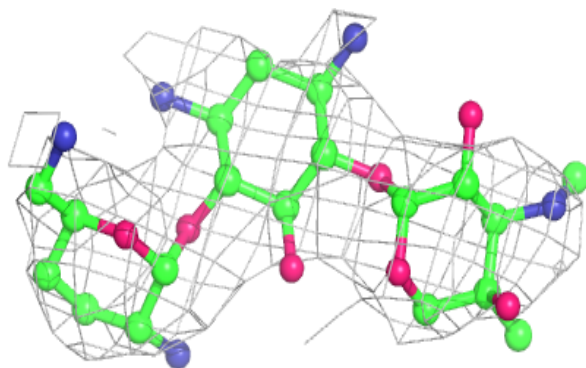


**Electron density around LLL 5 4170:**

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

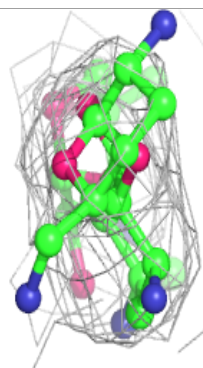
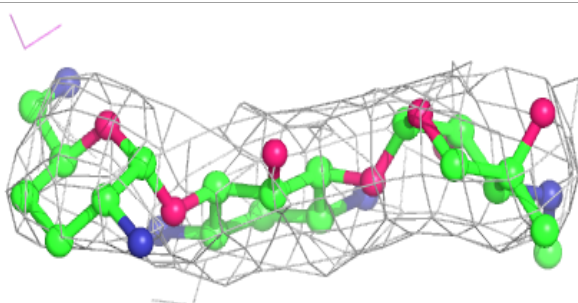
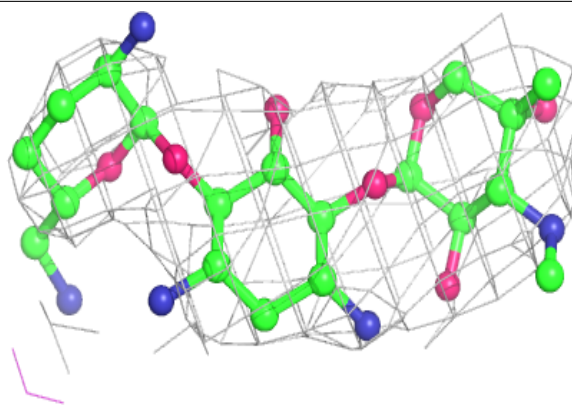
**Electron density around LLL 1 3992:**

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

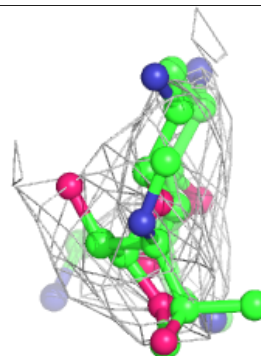
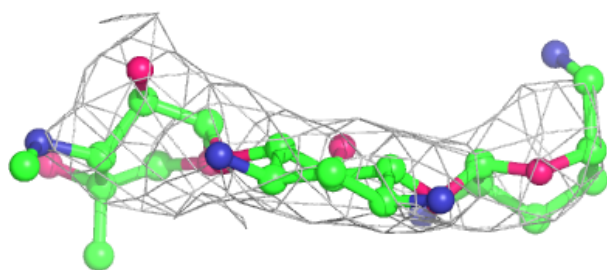
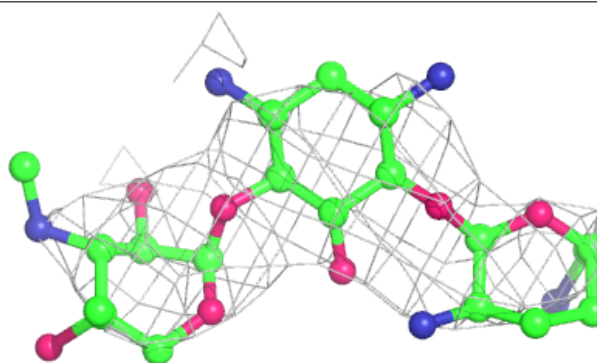


**Electron density around LLL 6 2169:**

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

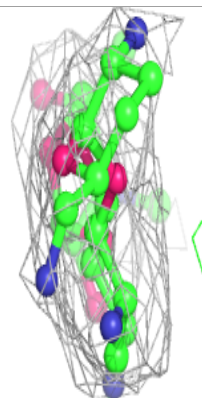
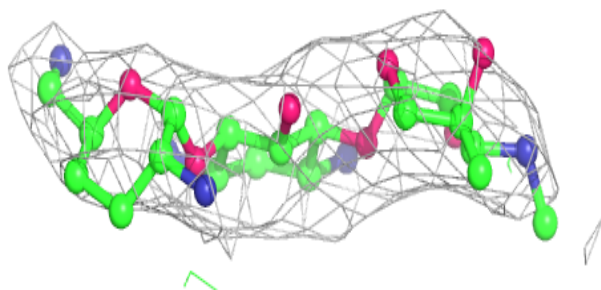
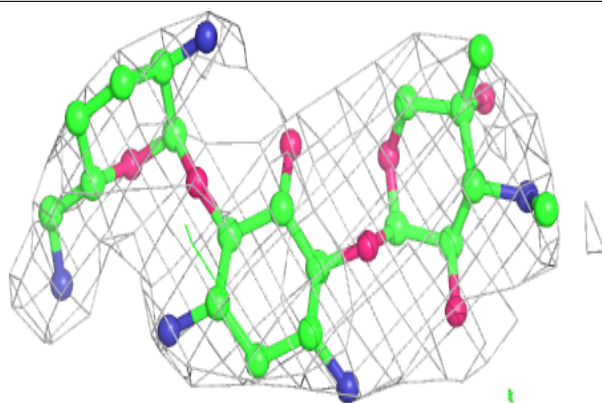
**Electron density around LLL 1 4003:**

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

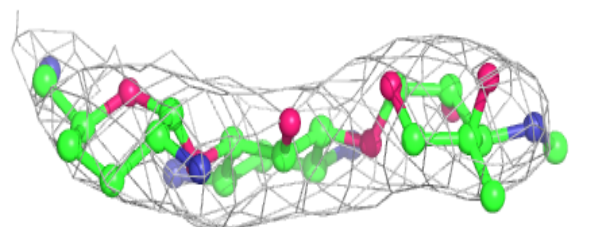
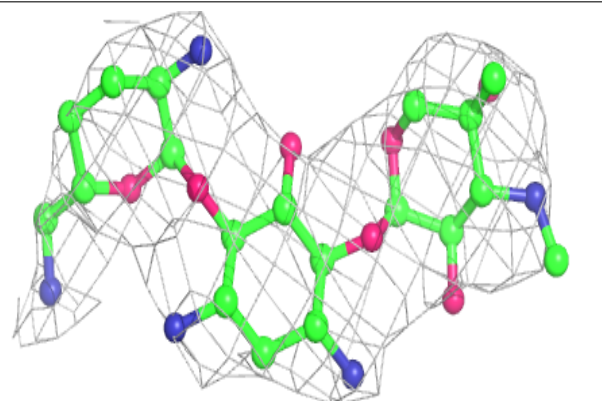


**Electron density around LLL 1 3994:**

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

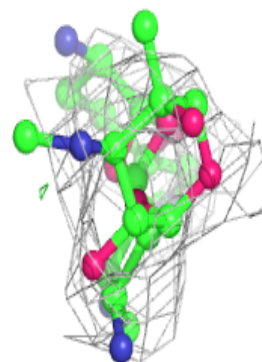
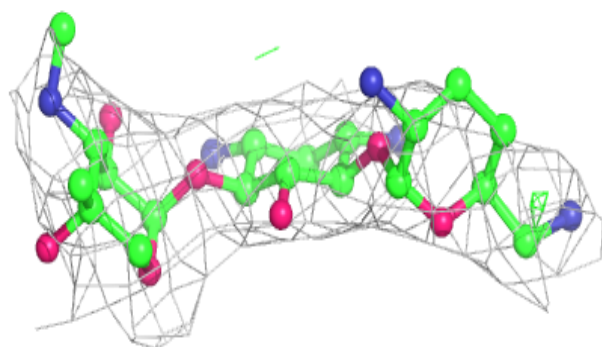
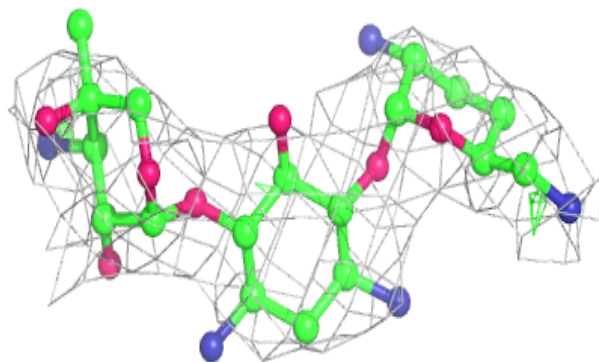
**Electron density around LLL 5 4168:**

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

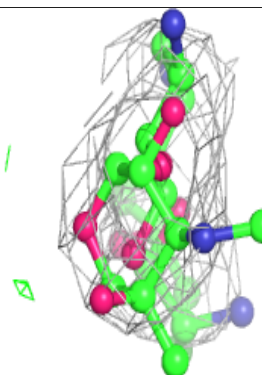
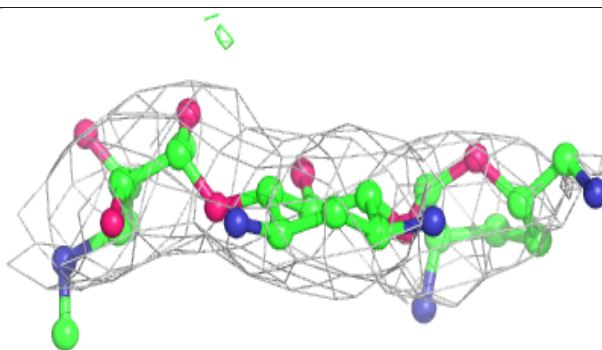
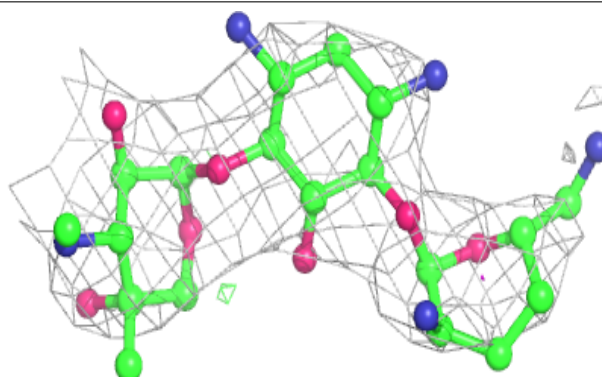


**Electron density around LLL 6 2166:**

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

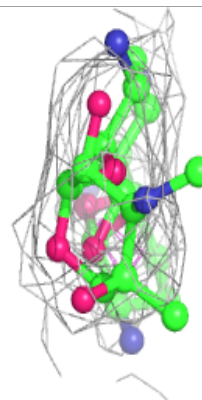
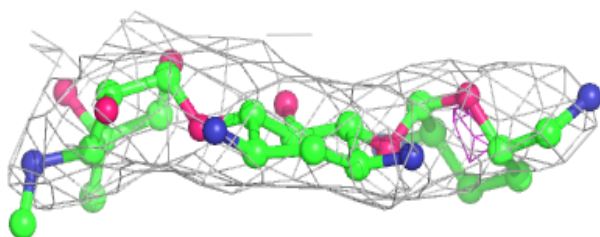
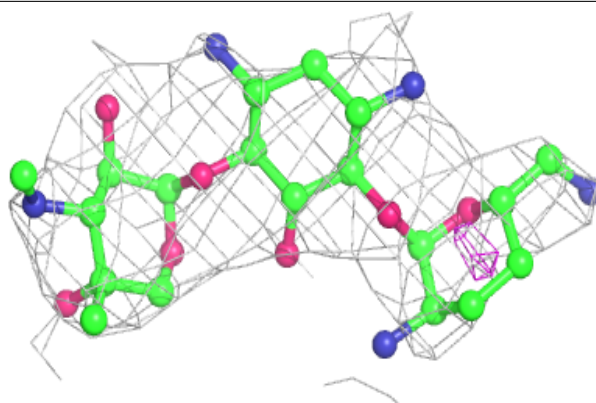
**Electron density around LLL 2 2043:**

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

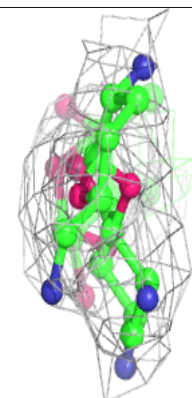
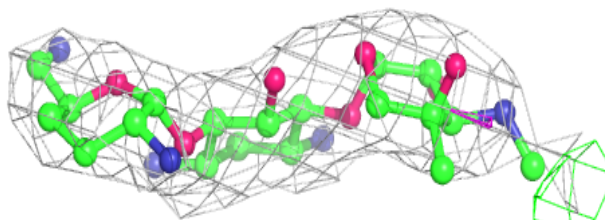
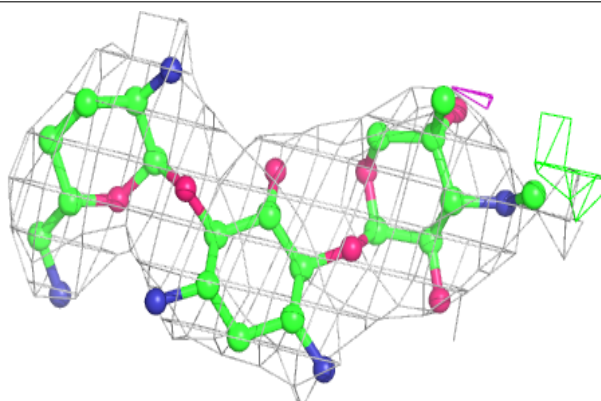


**Electron density around LLL 5 4154:**

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

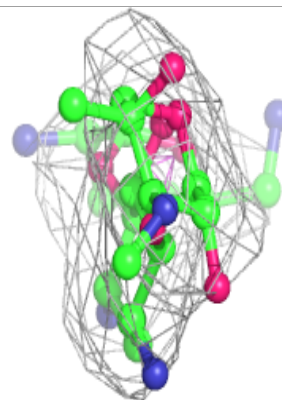
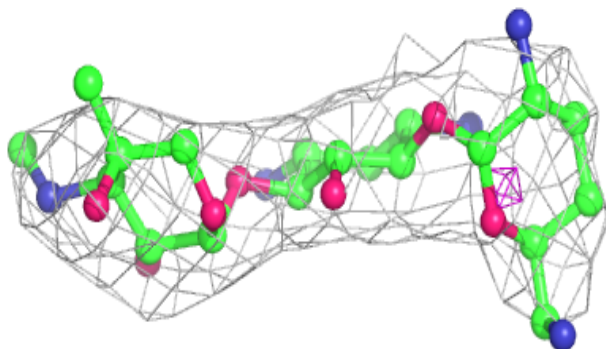
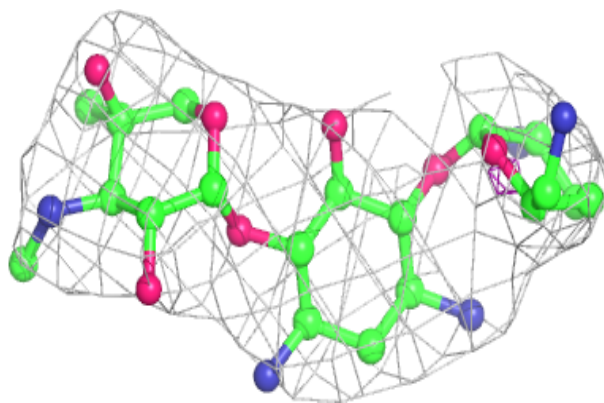
**Electron density around LLL 13 412:**

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

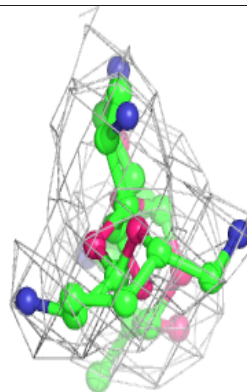
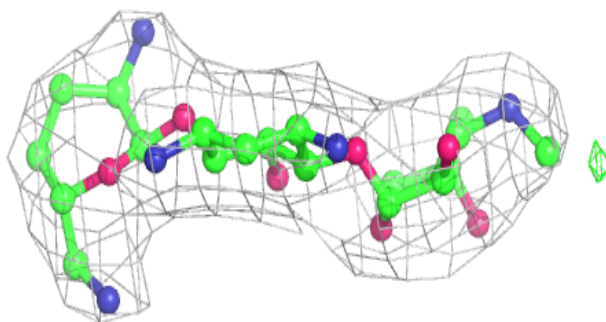
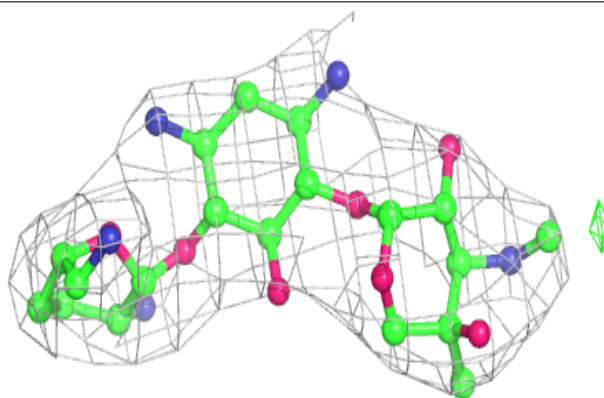


**Electron density around LLL 1 3990:**

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

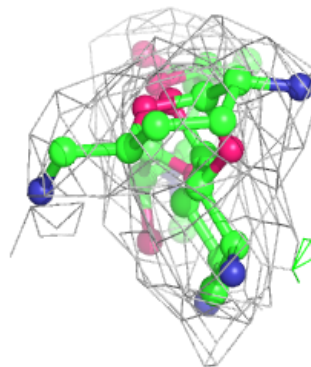
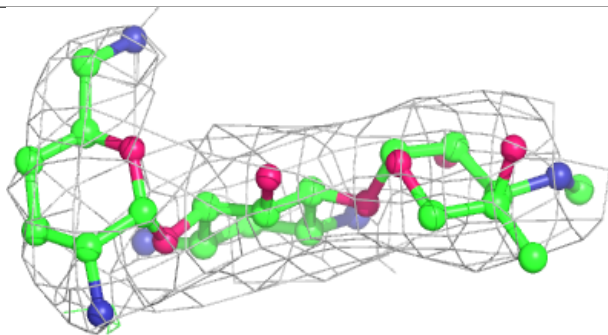
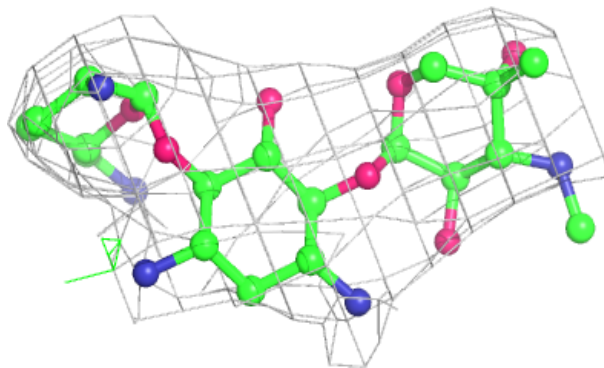
**Electron density around LLL 5 4161:**

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

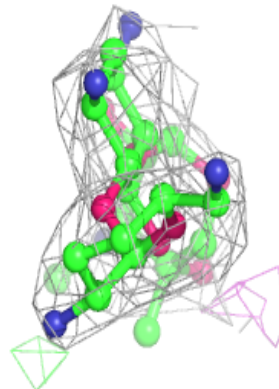
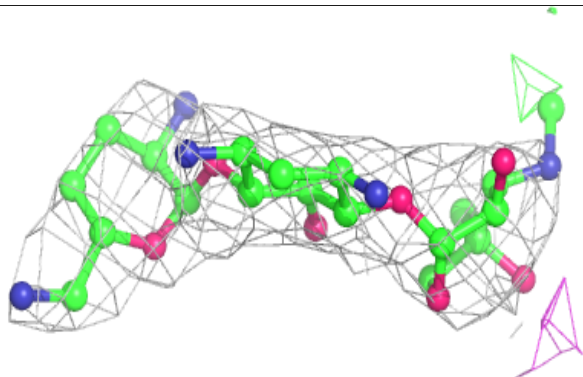
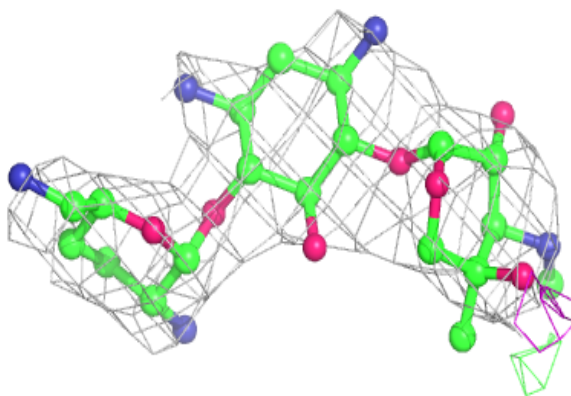


**Electron density around LLL 1 3989:**

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

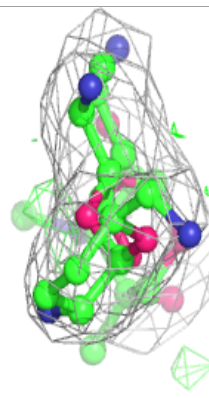
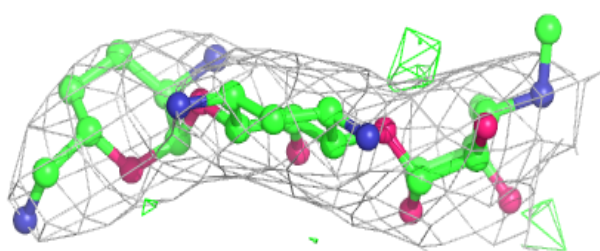
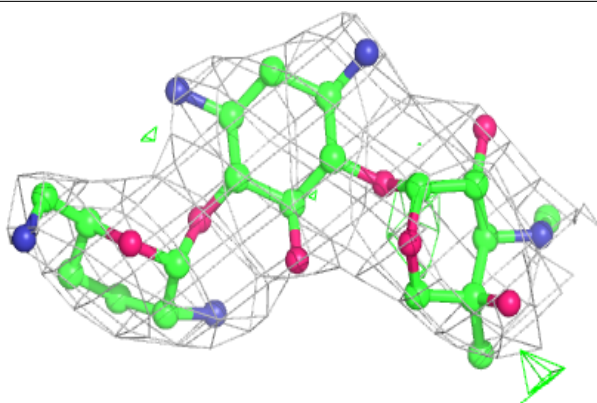
**Electron density around LLL 5 4160:**

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

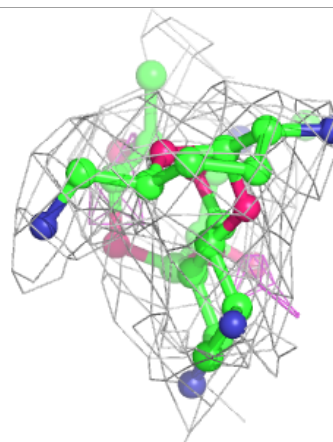
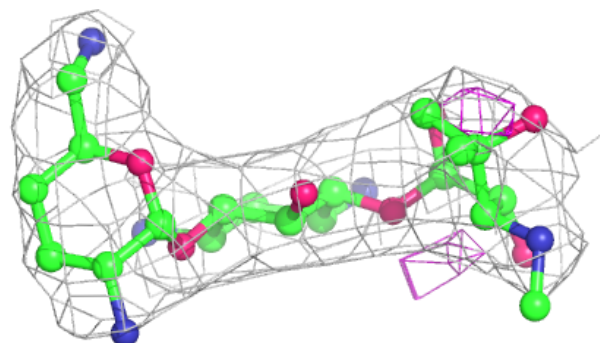
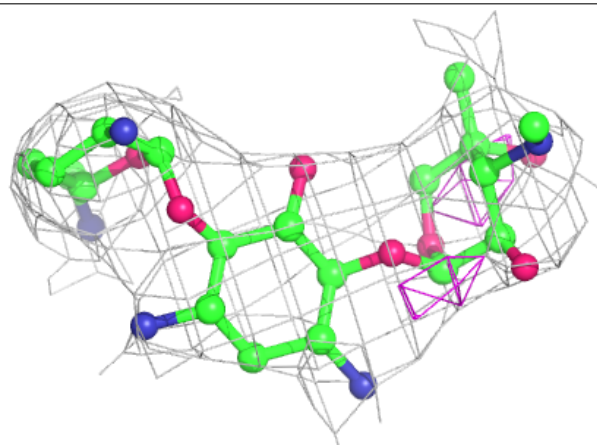


**Electron density around LLL 5 4157:**

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

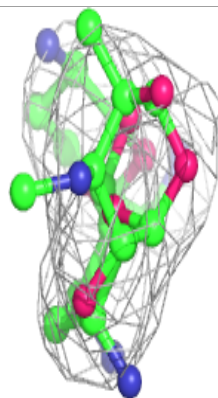
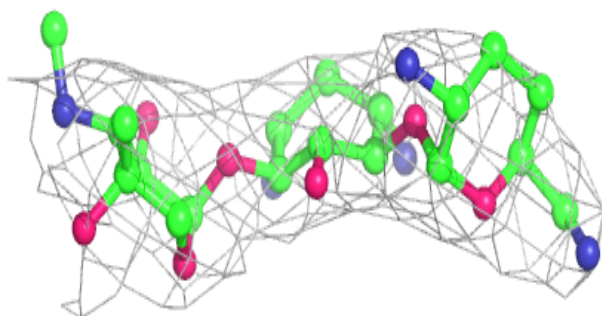
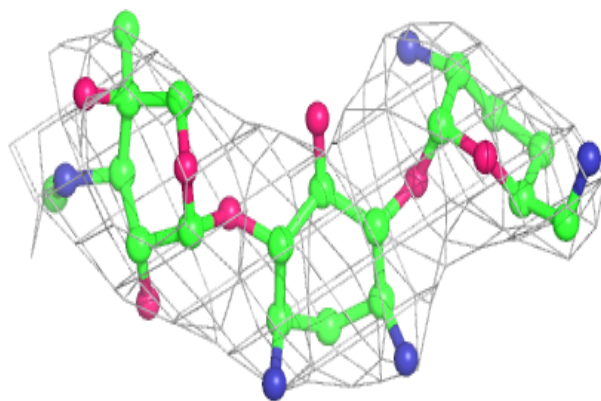
**Electron density around LLL 5 4151:**

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

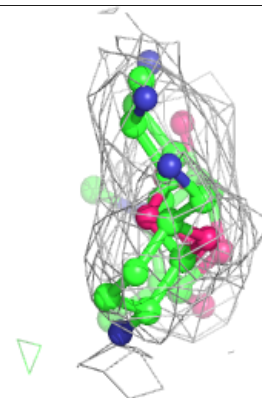
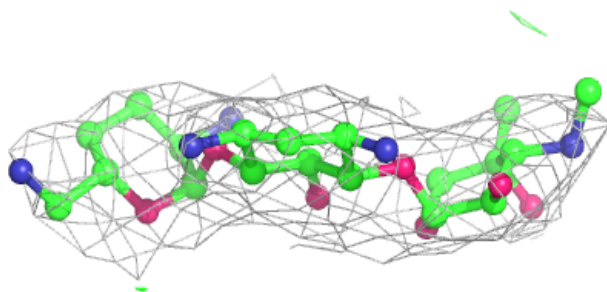
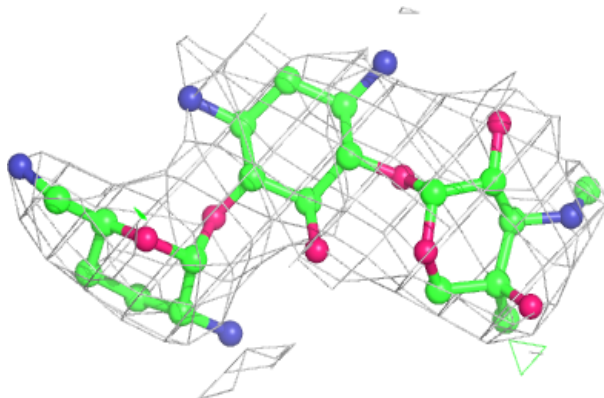


**Electron density around LLL 1 3993:**

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

**Electron density around LLL 1 3991:**

$2mF_o-DF_c$  (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.