



Full wwPDB EM Validation Report ⓘ

Apr 3, 2025 – 06:49 pm BST

PDB ID : 6YNZ / pdb_00006ynz
EMDB ID : EMD-10861
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- F1Fo composite tetramer model
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

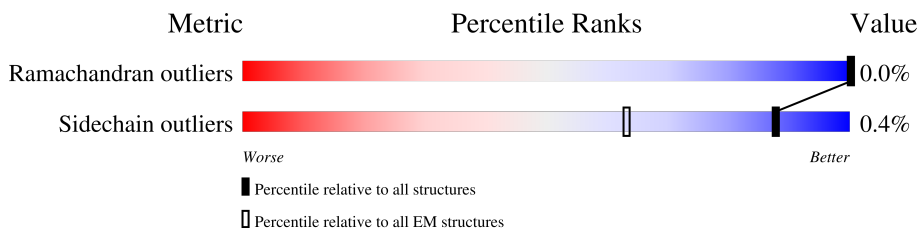
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

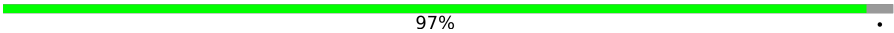
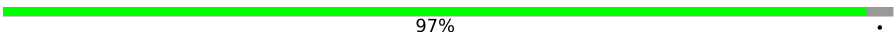
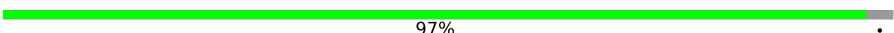
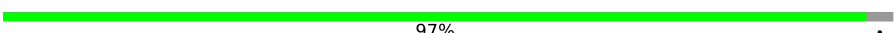





The reported resolution of this entry is 3.10 Å.

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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	
1	A3	446	
1	a	446	
1	a3	446	
2	B	381	
2	B3	381	
2	b	381	
2	b3	381	
3	D	234	

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Mol	Chain	Length	Quality of chain
3	D3	234	
3	d	234	
3	d3	234	
4	F	204	
4	F3	204	
4	f	204	
4	f3	204	
5	I	209	
5	I3	209	
5	i	209	
5	i3	209	
6	K	179	
6	K3	179	
6	k	179	
6	k3	179	
7	C	100	
7	C3	100	
7	c	100	
7	c3	100	
8	G	286	
8	G3	286	
8	g	286	
8	g3	286	
9	H	268	
9	H3	268	

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Mol	Chain	Length	Quality of chain
9	h	268	 13% 86% 14%
9	h3	268	 7% 86% 14%
10	J	273	 98%
10	J3	273	 98%
10	j	273	 99%
10	j3	273	 99%
11	L	247	 99%
11	L3	247	 99%
11	l	247	 99%
11	l3	247	 99%
12	M	221	 100%
12	M3	221	 100%
12	m	221	 100%
12	m3	221	 100%
13	N	179	 66% 34%
13	N3	179	 66% 34%
13	n	179	 66% 34%
13	n3	179	 66% 34%
14	O	154	 64% 36%
14	O3	154	 64% 36%
14	o	154	 64% 36%
14	o3	154	 64% 36%
15	P	152	 9% 99%
15	P3	152	 99%
15	p	152	 99%



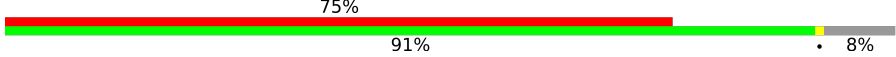
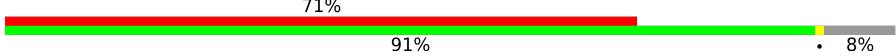
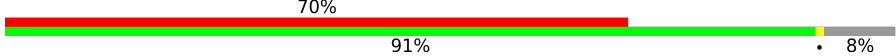
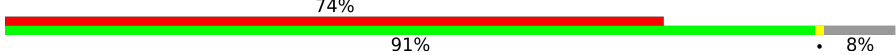
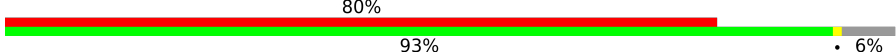
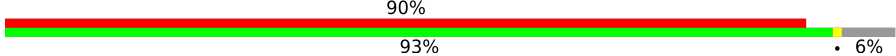
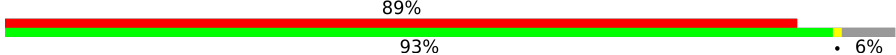
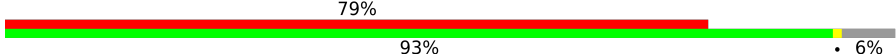
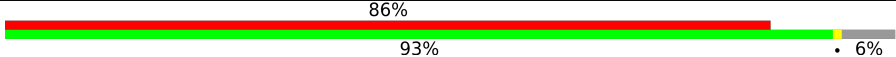

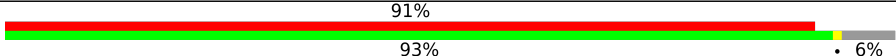
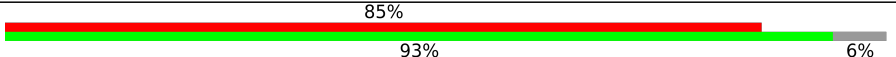
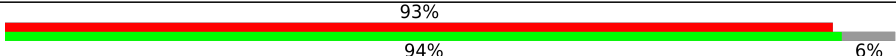
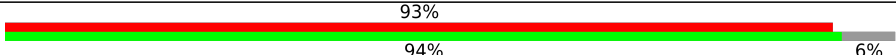
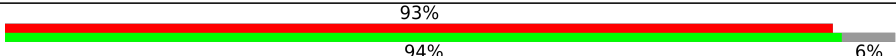
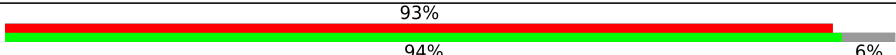
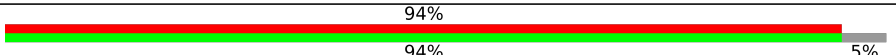
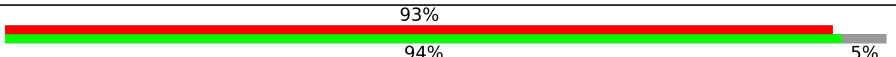
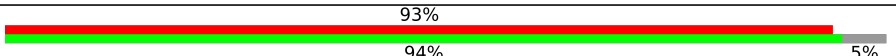
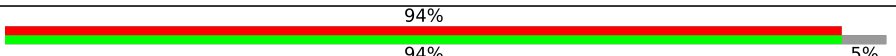
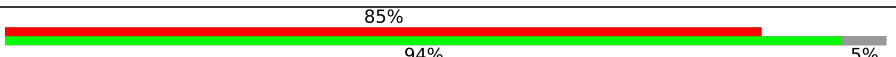
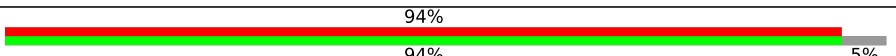
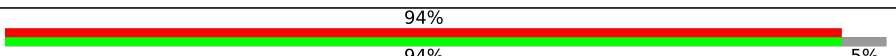
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Mol	Chain	Length	Quality of chain
15	p3	152	
16	Q	152	
16	Q3	152	
16	q	152	
16	q3	152	
17	R	149	
17	R3	149	
17	r	149	
17	r3	149	
18	S	145	
18	S3	145	
18	s	145	
18	s3	145	
19	E	480	
19	E3	480	
19	e	480	
19	e3	480	
20	i1	108	
20	i2	108	
20	i4	108	
20	i5	108	
21	t	460	
21	t3	460	
22	G1	219	
22	G2	219	

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Mol	Chain	Length	Quality of chain
22	G4	219	86% 
22	G5	219	86% 
23	g1	299	75% 
23	g2	299	71% 
23	g4	299	70% 
23	g5	299	74% 
24	A1	546	80% 
24	A2	546	90% 
24	A4	546	89% 
24	A5	546	79% 
24	B1	546	86% 
24	B2	546	91% 
24	B4	546	91% 
24	B5	546	85% 
24	C1	546	93% 
24	C2	546	93% 
24	C4	546	93% 
24	C5	546	93% 
25	D1	497	94% 
25	D2	497	93% 
25	D4	497	93% 
25	D5	497	94% 
25	E1	497	85% 
25	E2	497	94% 
25	E4	497	94% 

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Mol	Chain	Length	Quality of chain
25	E5	497	86% 94% 5%
25	F1	497	91% 94% 6%
25	F2	497	91% 94% 6%
25	F4	497	92% 94% 6%
25	F5	497	91% 94% 6%
26	H1	76	9% 99% .
26	H2	76	5% 99% .
26	H4	76	7% 99% .
26	H5	76	9% 99% .
26	I1	76	14% 96% ..
26	I2	76	. 99% .
26	I4	76	5% 96% ..
26	I5	76	14% 99% .
26	J1	76	24% 99% .
26	J2	76	8% 99% .
26	J4	76	8% 99% .
26	J5	76	26% 99% .
26	K1	76	32% 99% .
26	K2	76	13% 97% ..
26	K4	76	14% 99% .
26	K5	76	33% 97% ..
26	L1	76	30% 99% .
26	L2	76	12% 99% .
26	L4	76	12% 99% .
26	L5	76	30% 99% .

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Mol	Chain	Length	Quality of chain
26	M1	76	<div> <div>24%</div> <div>99%</div> </div>
26	M2	76	<div> <div>9%</div> <div>99%</div> </div>
26	M4	76	<div> <div>9%</div> <div>99%</div> </div>
26	M5	76	<div> <div>24%</div> <div>99%</div> </div>
26	N1	76	<div> <div>21%</div> <div>99%</div> </div>
26	N2	76	<div> <div>11%</div> <div>99%</div> </div>
26	N4	76	<div> <div>11%</div> <div>99%</div> </div>
26	N5	76	<div> <div>20%</div> <div>99%</div> </div>
26	O1	76	<div> <div>28%</div> <div>99%</div> </div>
26	O2	76	<div> <div>12%</div> <div>99%</div> </div>
26	O4	76	<div> <div>11%</div> <div>99%</div> </div>
26	O5	76	<div> <div>22%</div> <div>99%</div> </div>
26	P1	76	<div> <div>11%</div> <div>99%</div> </div>
26	P2	76	<div> <div>12%</div> <div>99%</div> </div>
26	P4	76	<div> <div>13%</div> <div>99%</div> </div>
26	P5	76	<div> <div>12%</div> <div>99%</div> </div>
26	Q1	76	<div> <div>9%</div> <div>99%</div> </div>
26	Q2	76	<div> <div>5%</div> <div>99%</div> </div>
26	Q4	76	<div> <div>7%</div> <div>99%</div> </div>
26	Q5	76	<div> <div>12%</div> <div>99%</div> </div>
27	d1	158	<div> <div>51%</div> <div>84%</div> <div>15%</div> </div>
27	d2	158	<div> <div>45%</div> <div>84%</div> <div>15%</div> </div>
27	d4	158	<div> <div>47%</div> <div>84%</div> <div>15%</div> </div>
27	d5	158	<div> <div>51%</div> <div>84%</div> <div>15%</div> </div>
28	e1	71	<div> <div>73%</div> <div>96%</div> </div>

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Mol	Chain	Length	Quality of chain
28	e2	71	<div><div></div><div>65%</div><div>94%</div><div>..</div></div>
28	e4	71	<div><div></div><div>65%</div><div>96%</div><div>.</div></div>
28	e5	71	<div><div></div><div>73%</div><div>94%</div><div>..</div></div>

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 571866 atoms, of which 287810 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Ymf66.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		
1	a3	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A3	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		
2	b3	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B3	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	d3	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D3	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		
4	f3	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F3	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		
5	i3	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I3	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		
6	k3	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K3	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called Ymf56.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	c3	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	C3	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	g3	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G3	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	h3	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H3	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	J	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	j3	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	J3	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	l	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	l3	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L3	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	m3	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M3	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	n3	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N3	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	o3	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
14	O3	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	p3	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P3	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	q3	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q3	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		
17	r3	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R3	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		
18	s3	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S3	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	e3	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E3	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	i2	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i1	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		
20	i5	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i4	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		
21	t3	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is a protein called Oligomycin sensitivity-conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	G1	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G2	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G4	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G5	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

- Molecule 23 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	g1	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g2	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g4	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g5	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		

- Molecule 24 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	C1	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B1	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A1	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C2	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B2	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A2	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C4	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B4	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A4	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C5	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		

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Mol	Chain	Residues	Atoms						AltConf	Trace
24	B5	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A5	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 25 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F1	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F2	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F4	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F5	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 26 is a protein called ATP synthase F0 subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	P1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	M1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	L4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

- Molecule 27 is a protein called subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d1	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d2	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d4	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

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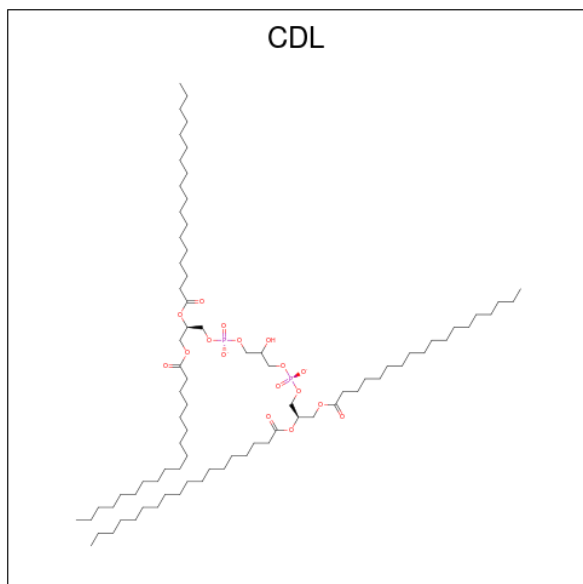
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Mol	Chain	Residues	Atoms						AltConf	Trace
27	d5	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- Molecule 28 is a protein called subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e1	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e2	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e4	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e5	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
29	f	1	Total 256	C 81	H 156	O 17	P 2	0
29	i	1	Total 256	C 81	H 156	O 17	P 2	0
29	k	1	Total 256	C 81	H 156	O 17	P 2	0
29	g	1	Total 256	C 81	H 156	O 17	P 2	0
29	j	1	Total 256	C 81	H 156	O 17	P 2	0
29	j	1	Total 256	C 81	H 156	O 17	P 2	0
29	l	1	Total 256	C 81	H 156	O 17	P 2	0
29	l	1	Total 256	C 81	H 156	O 17	P 2	0
29	p	1	Total 256	C 81	H 156	O 17	P 2	0
29	r	1	Total 256	C 81	H 156	O 17	P 2	0
29	A	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0

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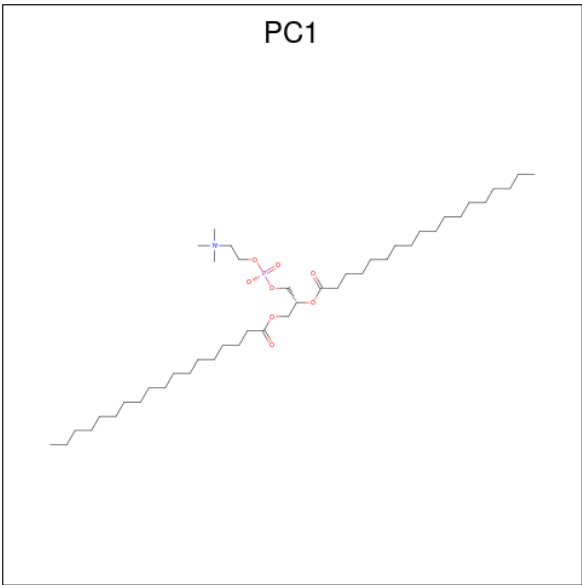
Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	P	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	b3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	k3	1	Total 256	C 81	H 156	O 17	P 2	0
29	g3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	p3	1	Total 256	C 81	H 156	O 17	P 2	0
29	A3	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	F3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	L3	1	Total 256	C 81	H 156	O 17	P 2	0
29	P3	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



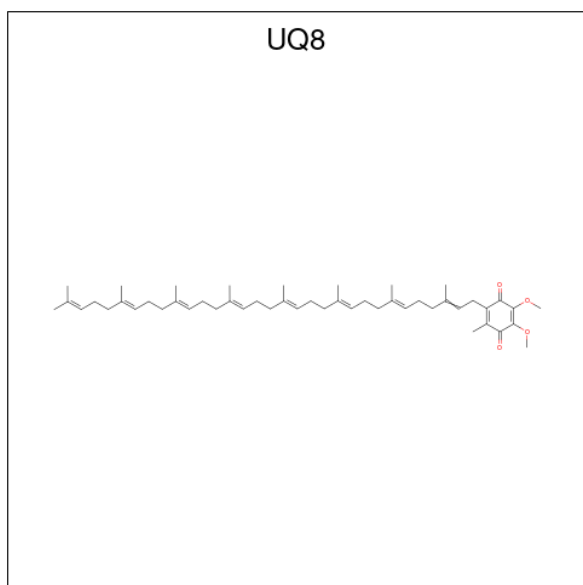
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	d3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



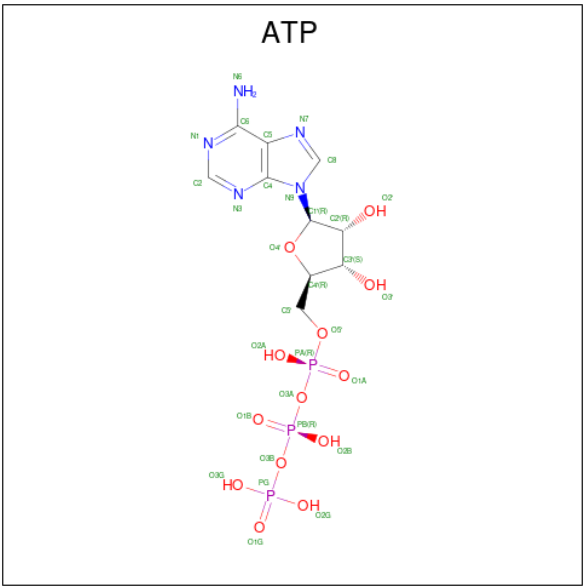
Mol	Chain	Residues	Atoms			AltConf
31	f	1	Total	O	P	0
			5	4	1	
31	F	1	Total	O	P	0
			5	4	1	
31	f3	1	Total	O	P	0
			5	4	1	
31	F3	1	Total	O	P	0
			5	4	1	

- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
32	i	1	Total	C	H	O	0
			127	49	74	4	
32	I	1	Total	C	H	O	0
			127	49	74	4	
32	i3	1	Total	C	H	O	0
			127	49	74	4	
32	I3	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
33	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

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Mol	Chain	Residues	Atoms						AltConf
33	g3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

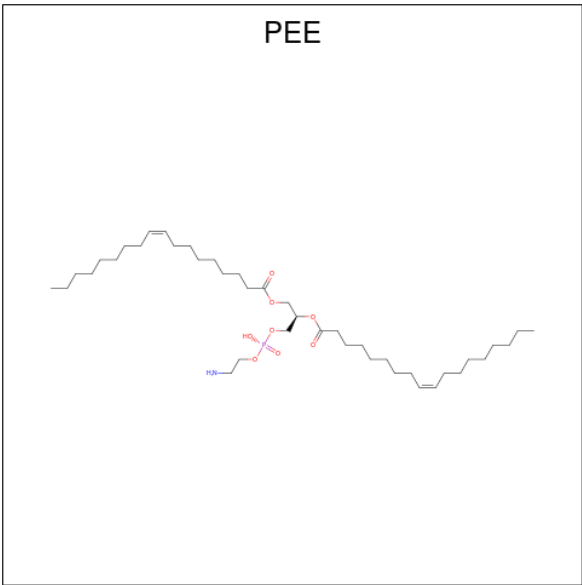
Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	C1	1	Total	Mg	0
			1	1	
34	D1	1	Total	Mg	0
			1	1	
34	B1	1	Total	Mg	0
			1	1	
34	A1	1	Total	Mg	0
			1	1	
34	E1	1	Total	Mg	0
			1	1	
34	C2	1	Total	Mg	0
			1	1	
34	D2	1	Total	Mg	0
			1	1	
34	B2	1	Total	Mg	0
			1	1	
34	A2	1	Total	Mg	0
			1	1	

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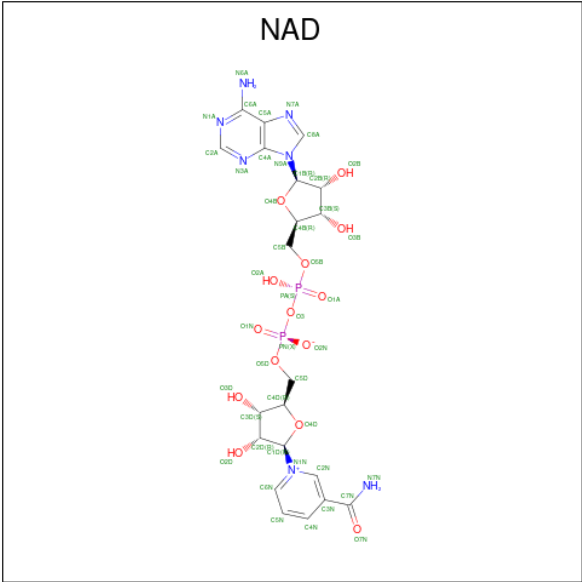
Mol	Chain	Residues	Atoms		AltConf
34	E2	1	Total 1	Mg 1	0
34	g3	1	Total 1	Mg 1	0
34	G3	1	Total 1	Mg 1	0
34	C4	1	Total 1	Mg 1	0
34	D4	1	Total 1	Mg 1	0
34	B4	1	Total 1	Mg 1	0
34	A4	1	Total 1	Mg 1	0
34	E4	1	Total 1	Mg 1	0
34	C5	1	Total 1	Mg 1	0
34	D5	1	Total 1	Mg 1	0
34	B5	1	Total 1	Mg 1	0
34	A5	1	Total 1	Mg 1	0
34	E5	1	Total 1	Mg 1	0

- Molecule 35 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



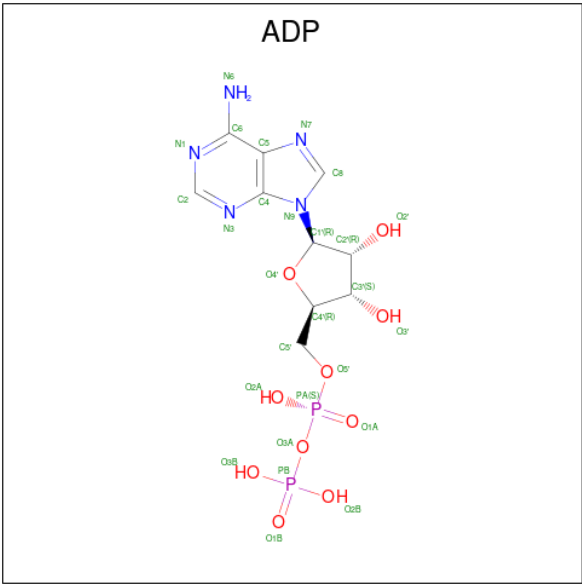
Mol	Chain	Residues	Atoms						AltConf
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	a3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	j3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	l3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	L3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						AltConf
36	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	e3	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E3	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

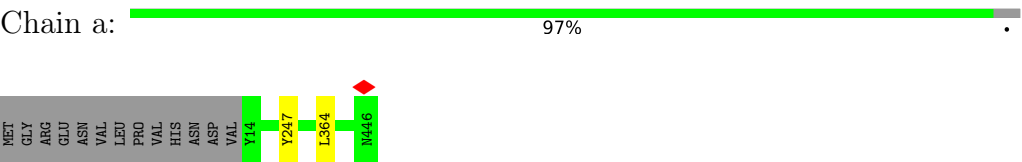


Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0

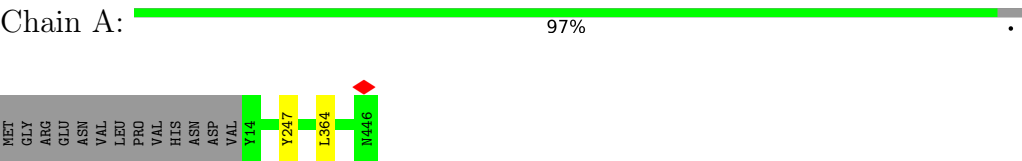
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

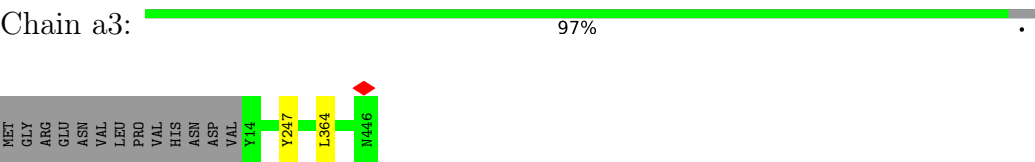
• Molecule 1: Ymf66



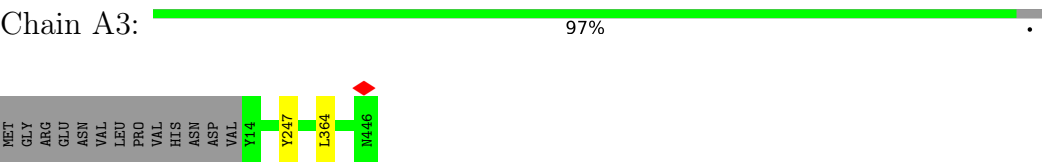
• Molecule 1: Ymf66



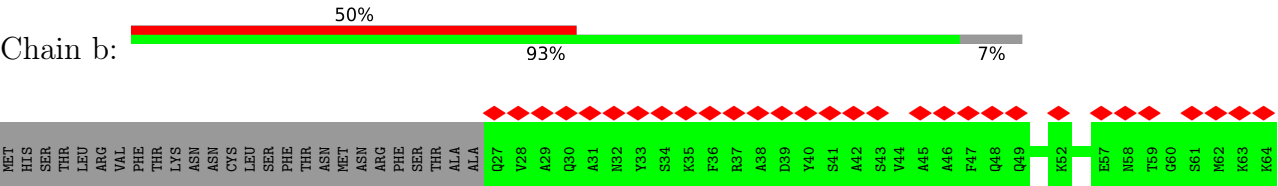
• Molecule 1: Ymf66

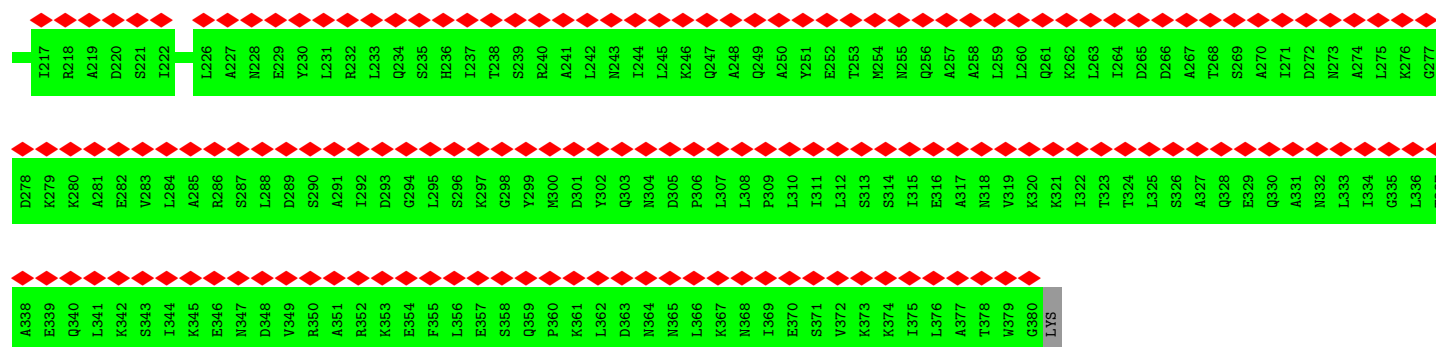


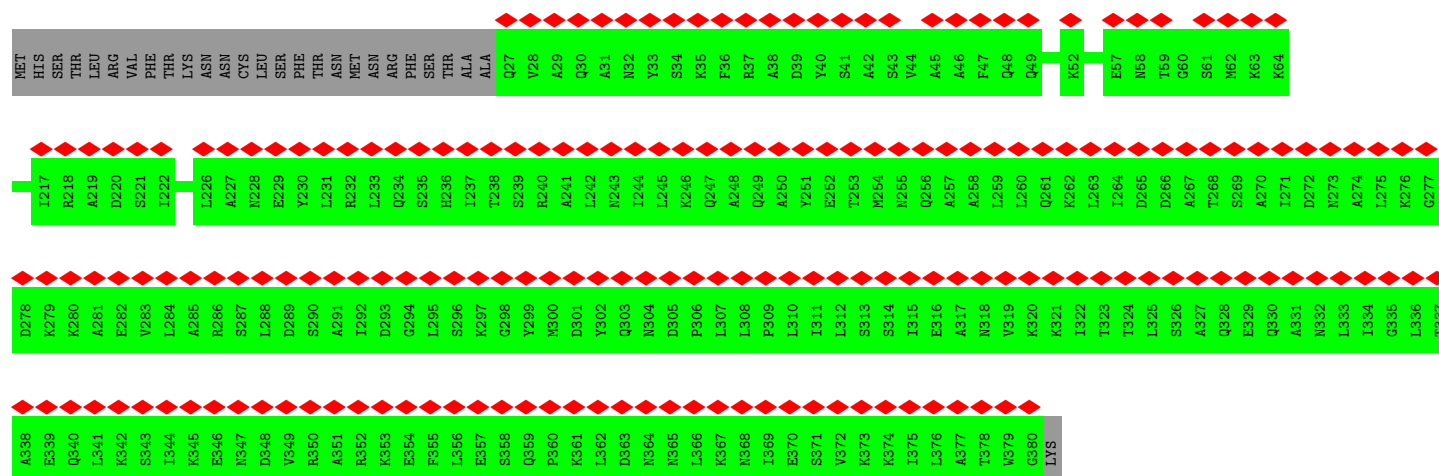
• Molecule 1: Ymf66



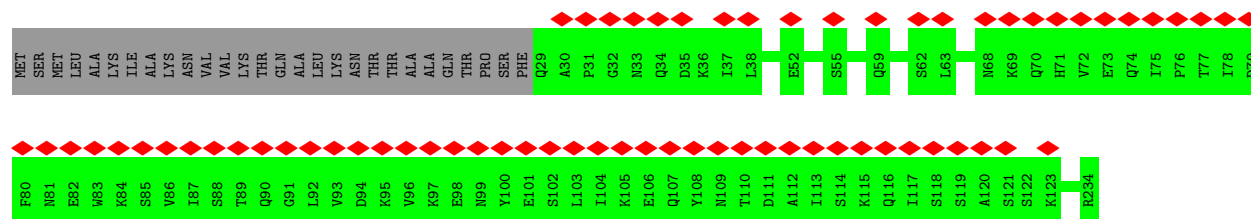
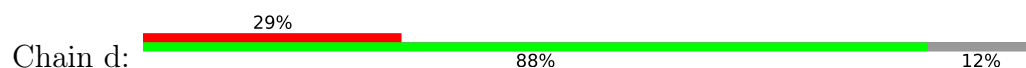
• Molecule 2: subunit b



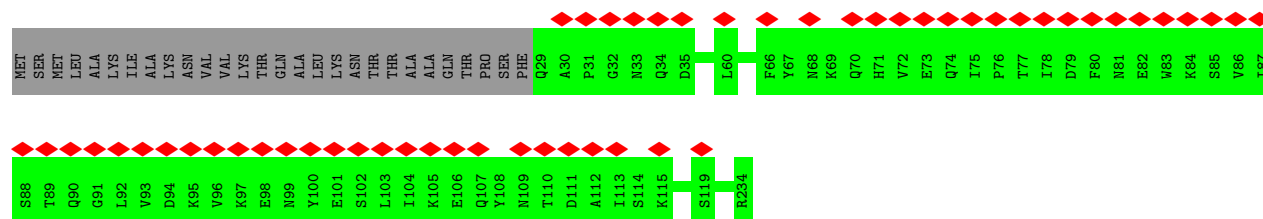
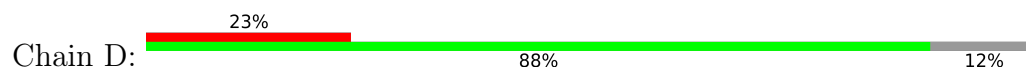




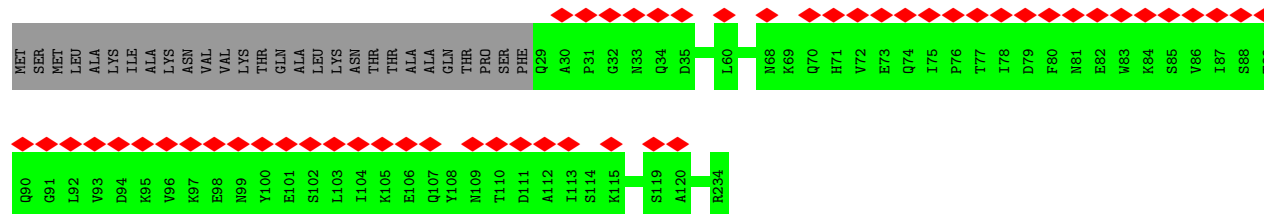
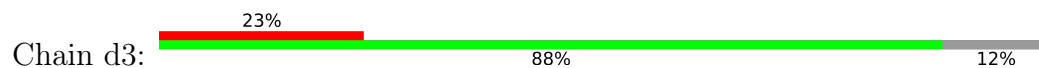
• Molecule 3: subunit d



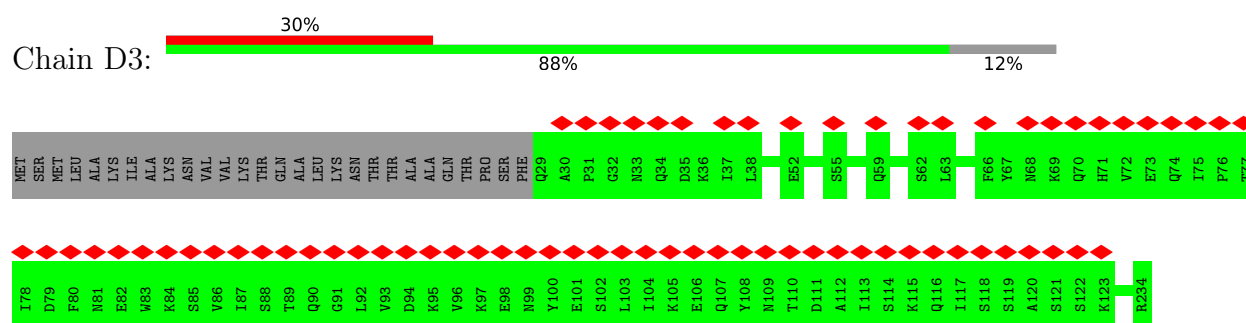
• Molecule 3: subunit d



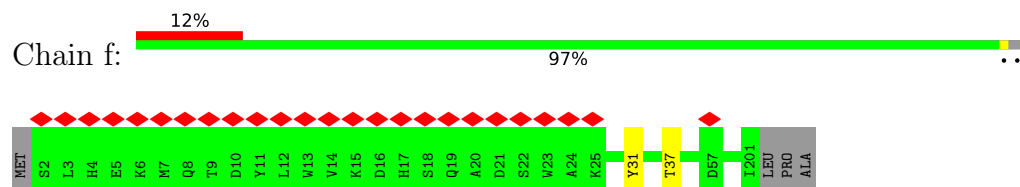
• Molecule 3: subunit d



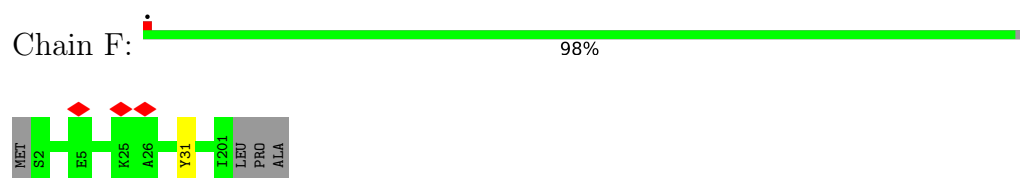
• Molecule 3: subunit d



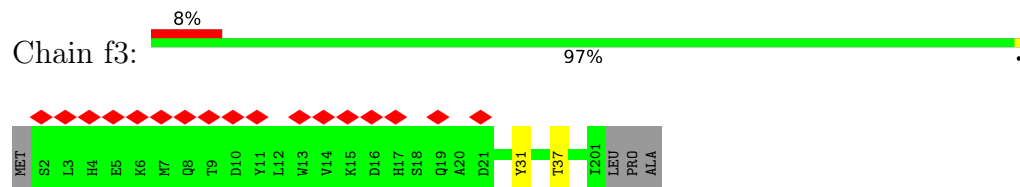
- Molecule 4: subunit f



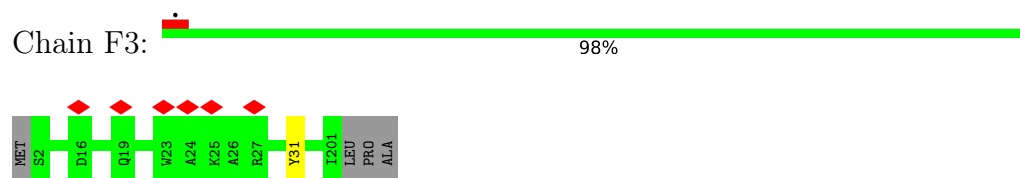
- Molecule 4: subunit f



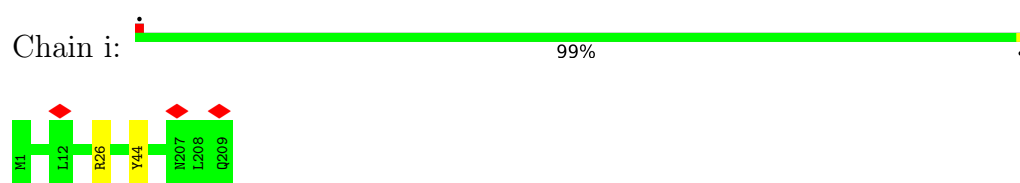
- Molecule 4: subunit f



- Molecule 4: subunit f

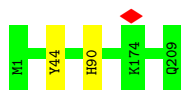


- Molecule 5: subunit i/j

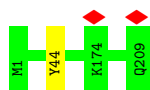


- Molecule 5: subunit i/j





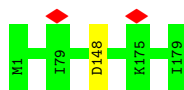
- Molecule 5: subunit i/j



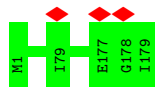
- Molecule 5: subunit i/j



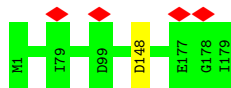
- Molecule 6: subunit k



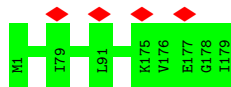
- Molecule 6: subunit k



- Molecule 6: subunit k



- Molecule 6: subunit k



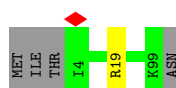
- Molecule 7: Ymf56

Chain c:  95%



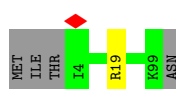
• Molecule 7: Ymf56

Chain C:  95%



• Molecule 7: Ymf56

Chain c3:  95%




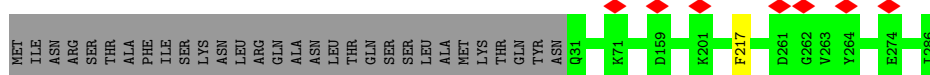
• Molecule 7: Ymf56

Chain C3:  95%




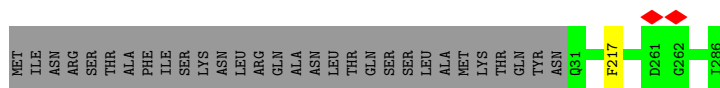
• Molecule 8: ATPTT3

Chain g:  89% 10%




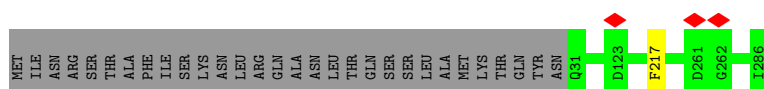
• Molecule 8: ATPTT3

Chain G:  89% 10%

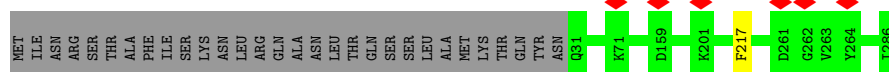


• Molecule 8: ATPTT3

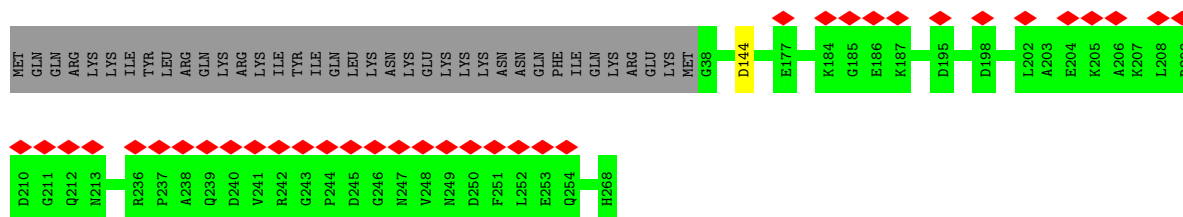
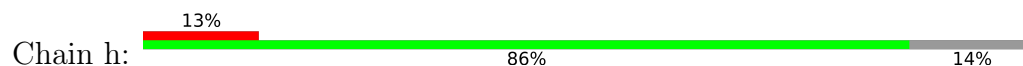
Chain g3:  89% 10%



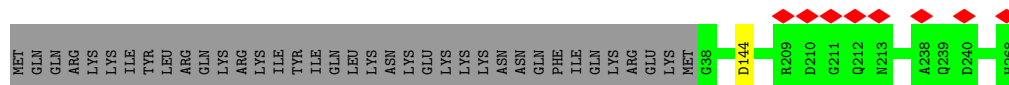
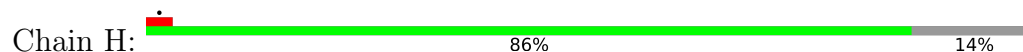
• Molecule 8: ATPTT3



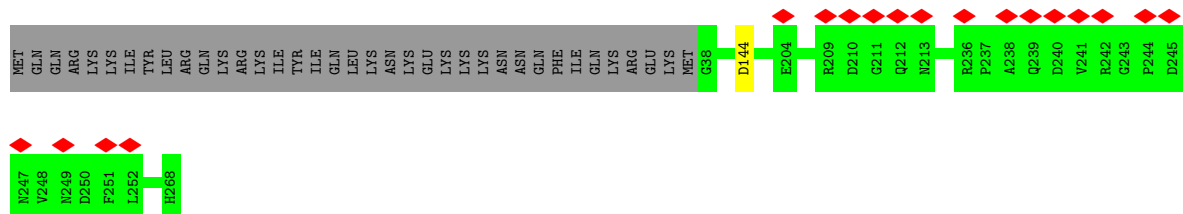
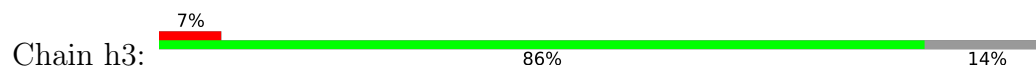
• Molecule 9: ATPTT4



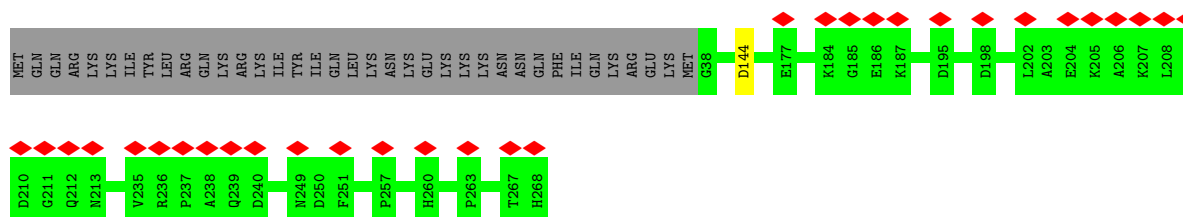
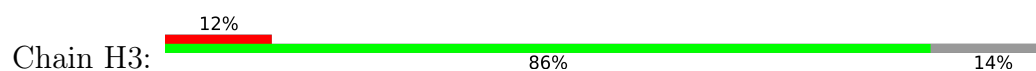
• Molecule 9: ATPTT4



• Molecule 9: ATPTT4

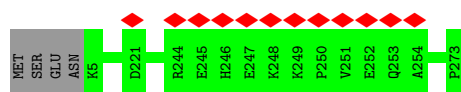


• Molecule 9: ATPTT4

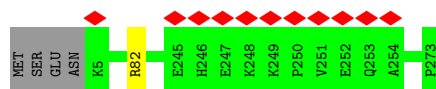


• Molecule 10: ATPTT5

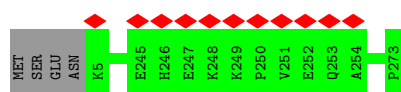




- Molecule 10: ATPTT5



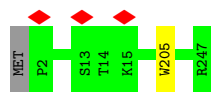
- Molecule 10: ATPTT5



- Molecule 10: ATPTT5



- Molecule 11: ATPTT6



- Molecule 11: ATPTT6

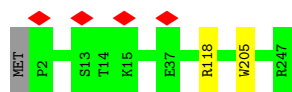


- Molecule 11: ATPTT6



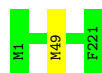
- Molecule 11: ATPTT6





- Molecule 12: ATPTT7

Chain m: 100%



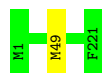
- Molecule 12: ATPPT7

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: ATPPT7

Chain m3: 



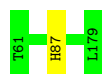
- Molecule 12: ATPPT7

Chain M3: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: ATPTT8

Chain n:  66% 34%



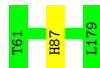
- Molecule 13: ATPTT8

Chain N:  66% 34%



- Molecule 13: ATPTT8

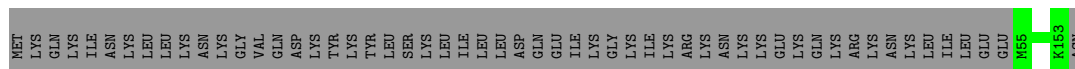
Chain n3:  66% 34%



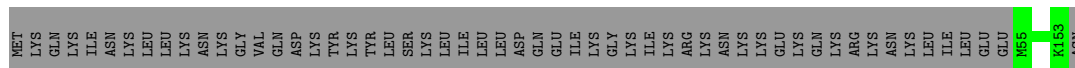
- Chain N3:  66% 34%



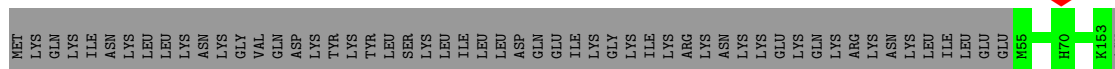
- Chain o:  64% 36%



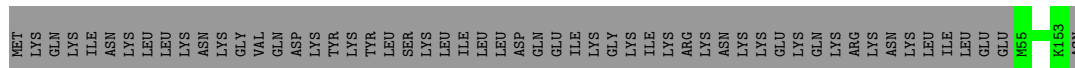
- Chain 0: 64% 36%



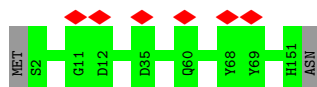
- Chain o3: 64% 36%



- Chain O3:  64% 36%

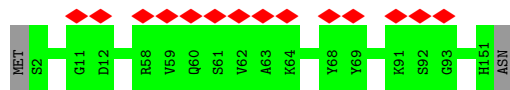


- Chain p:  99%



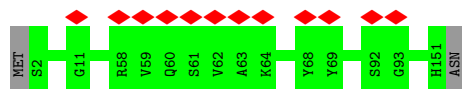
- Molecule 15: ATPTT10

Chain P:  9% 99%



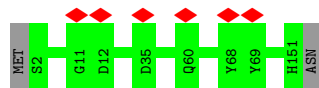
- Molecule 15: ATPTT10

Chain p3:  8% 99%



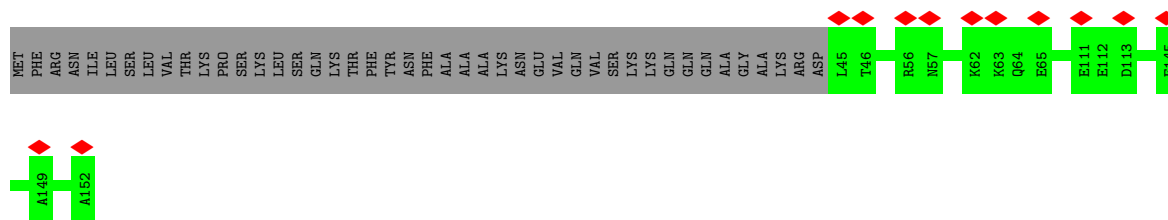
- Molecule 15: ATPTT10

Chain P3:  99%




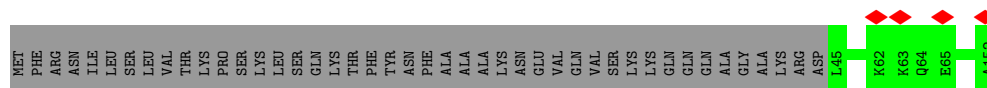
- Molecule 16: ATPTT11

Chain q:  8% 71% 29%




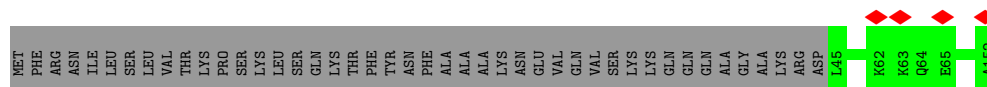
- Molecule 16: ATPTT11

Chain Q:  71% 29%

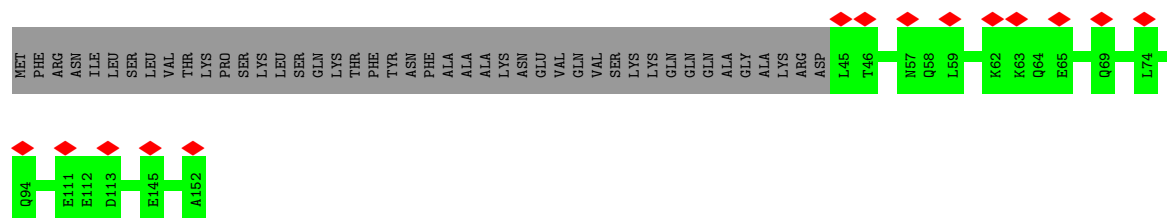
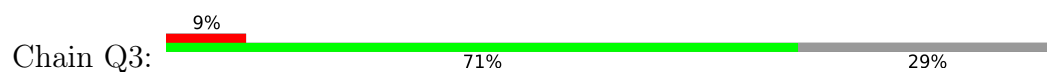


- Molecule 16: ATPTT11

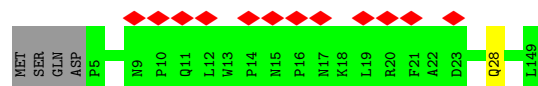
Chain q3:  71% 29%



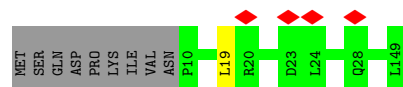
- Molecule 16: ATPTT11



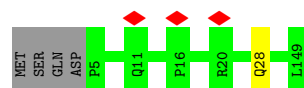
• Molecule 17: ATPTT12



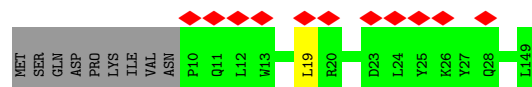
• Molecule 17: ATPTT12



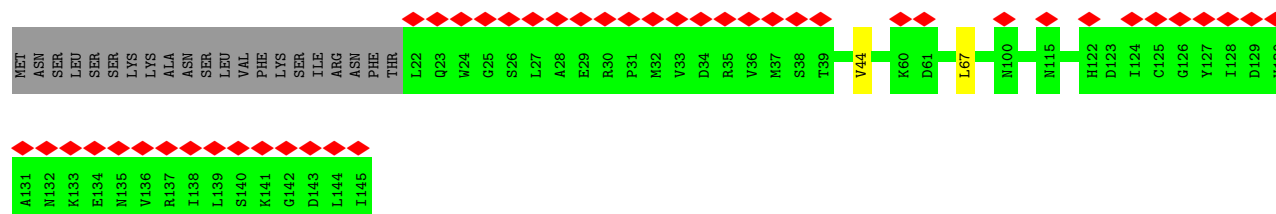
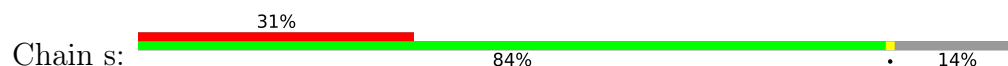
• Molecule 17: ATPTT12



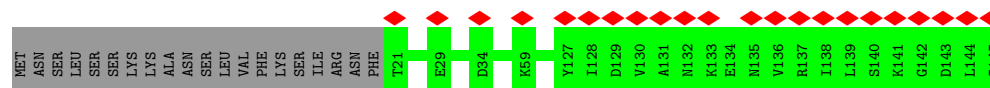
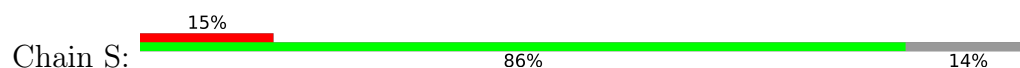
• Molecule 17: ATPTT12



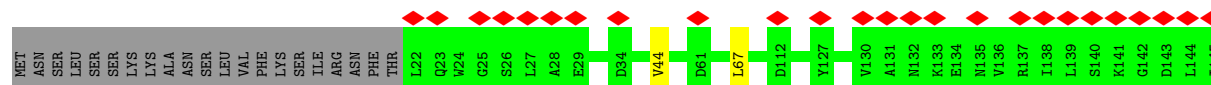
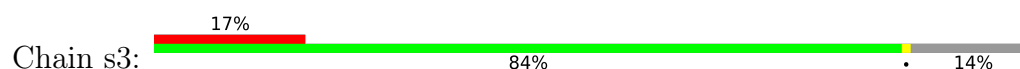
• Molecule 18: ATPTT13



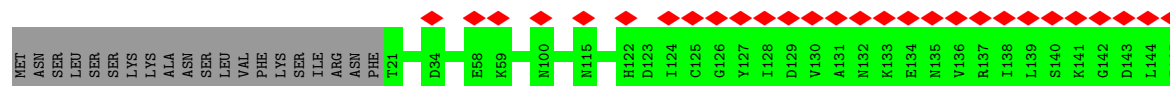
- Molecule 18: ATPTT13



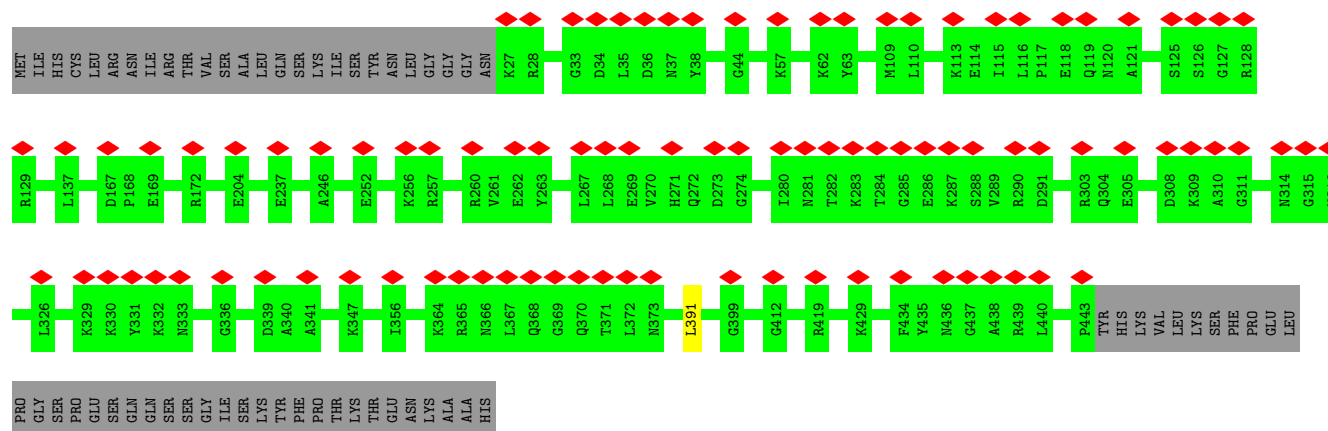
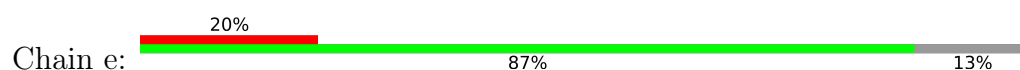
- Molecule 18: ATPTT13



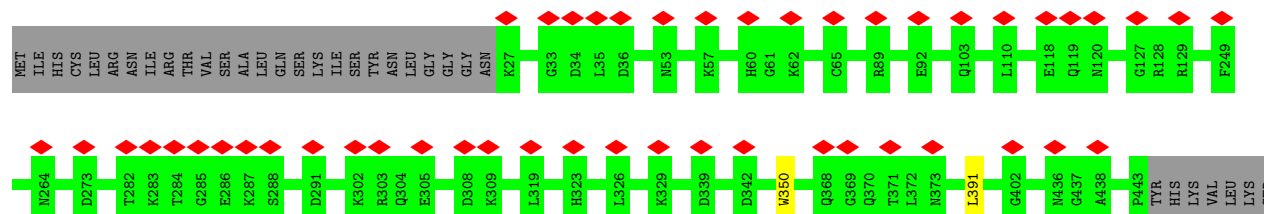
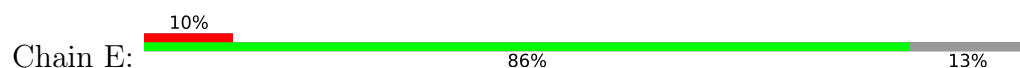
- Molecule 18: ATPTT13



- Molecule 19: ATPTT1



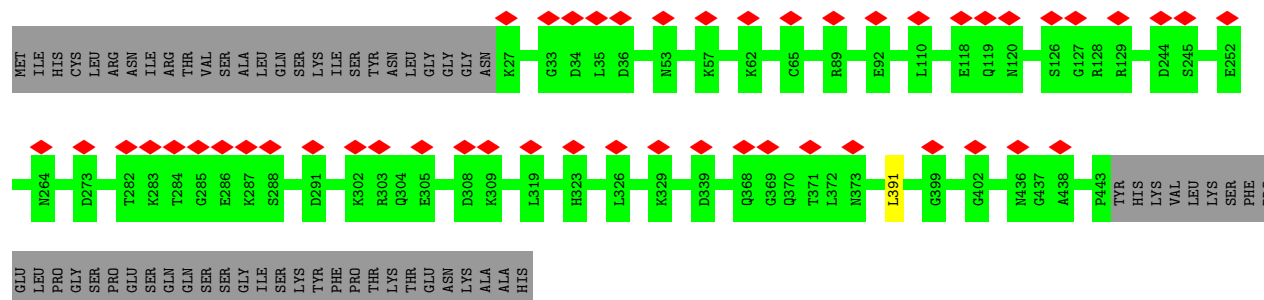
- Molecule 19: ATPTT1



PHE
PRO
GLU
LEU
PRO
PRO
GLY
SER
PRO
GLU
SER
GLN
GLN
SER
SER
GLY
SER
LYS
TYR
PHE
PRO
THR
LYS
GLY
THR
GLY
ASN
LYS
ALA
ALA
HIS

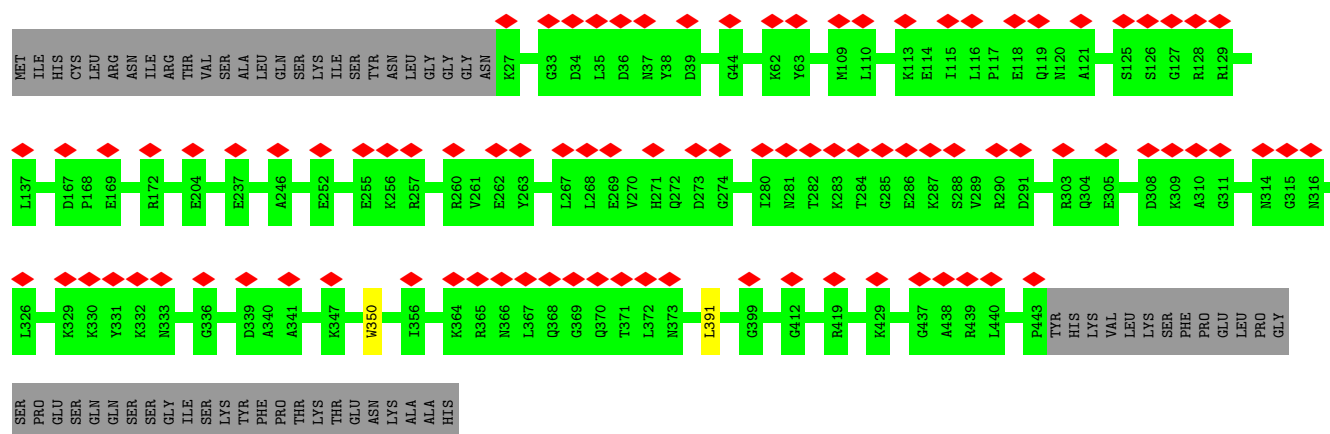
• Molecule 19: ATPTT1

Chain e3: 10% 87% 13%



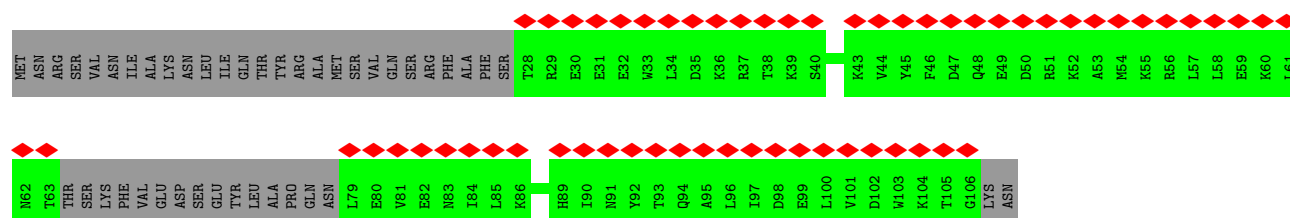
• Molecule 19: ATPTT1

Chain E3: 19% 86% 13%



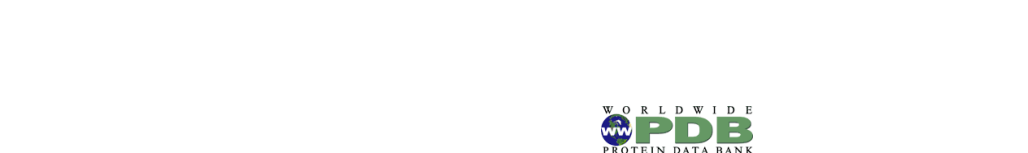
• Molecule 20: Inhibitor of F1 (IF1)

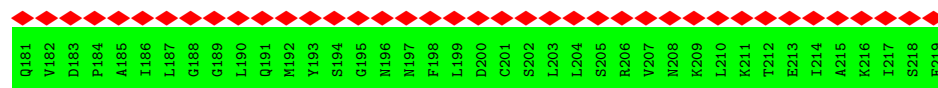
Chain i2: 56% 59% 41%



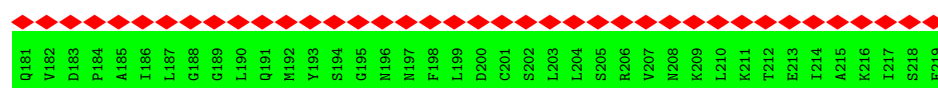
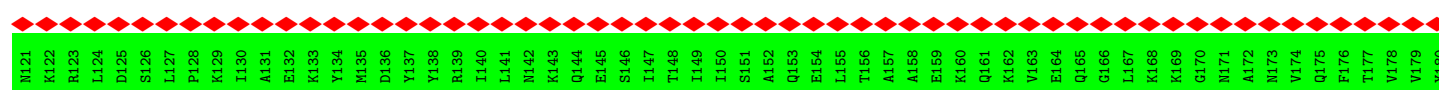
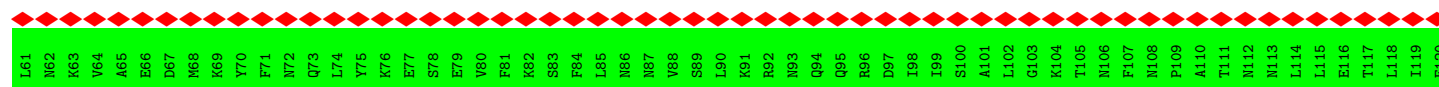
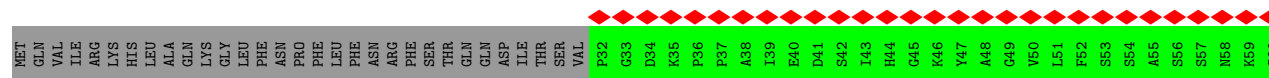
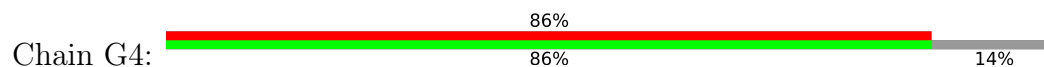
• Molecule 20: Inhibitor of F1 (IF1)

Chain i1: 60% 63% 37%

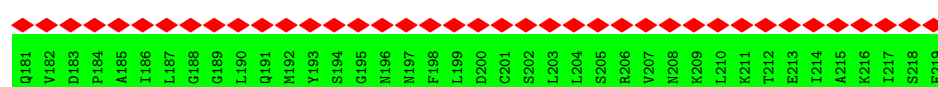
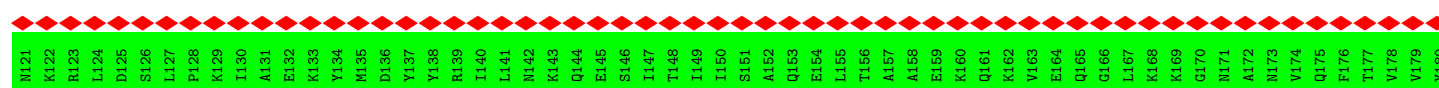
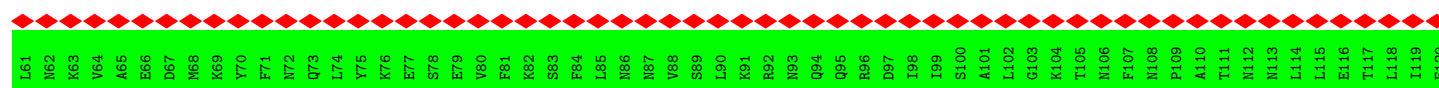
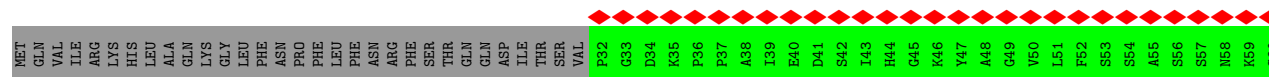
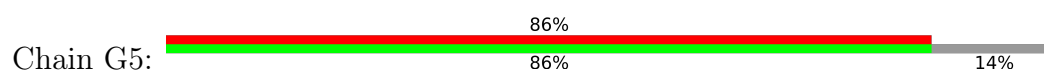




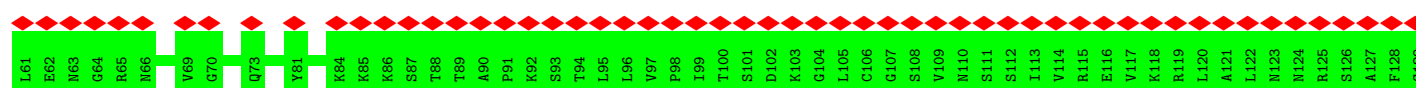
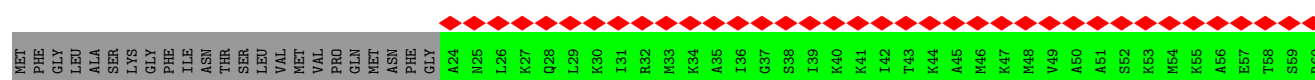
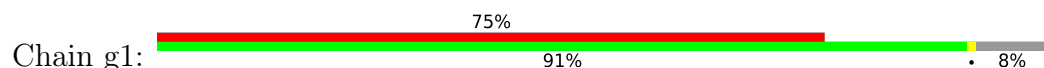
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

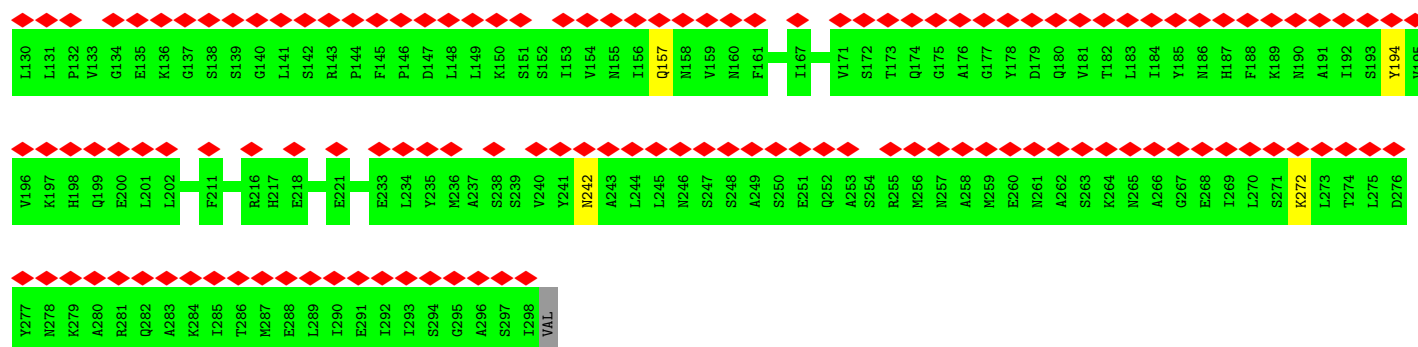


• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

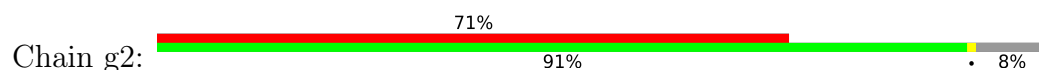


• Molecule 23: ATP synthase subunit gamma

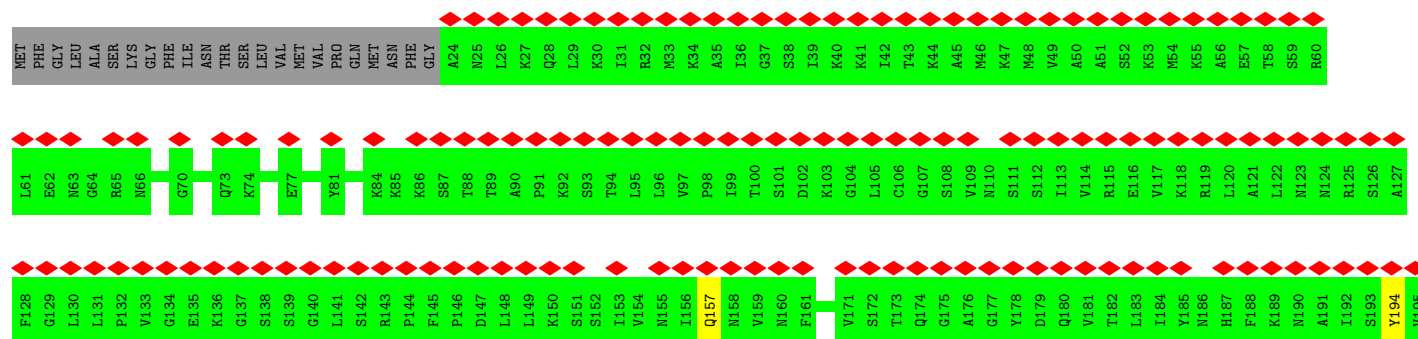
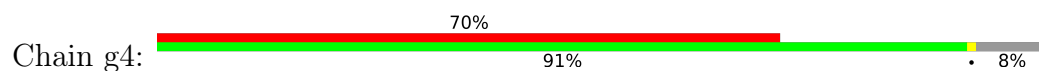




• Molecule 23: ATP synthase subunit gamma

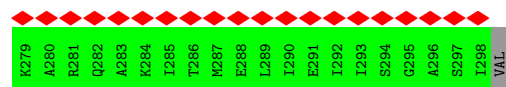
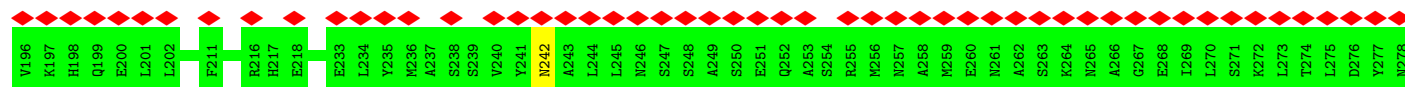
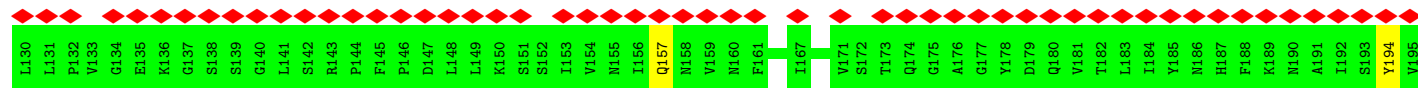
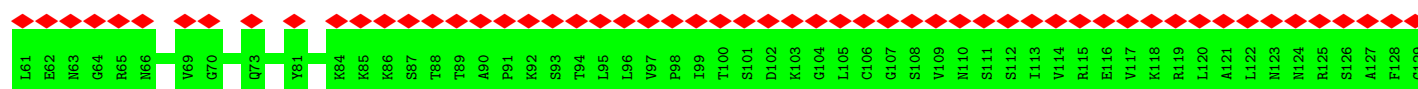
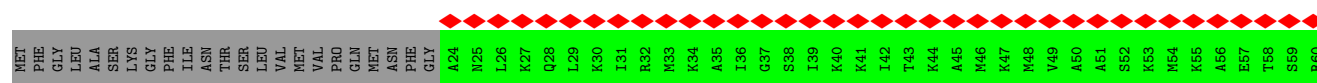
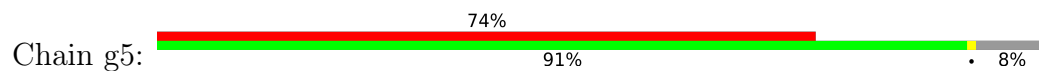


• Molecule 23: ATP synthase subunit gamma

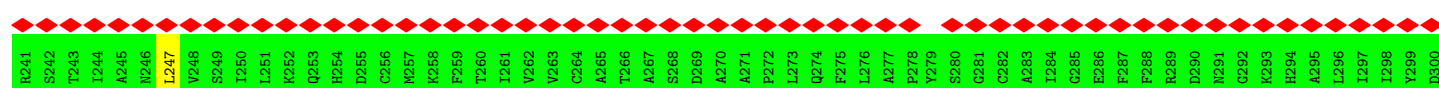
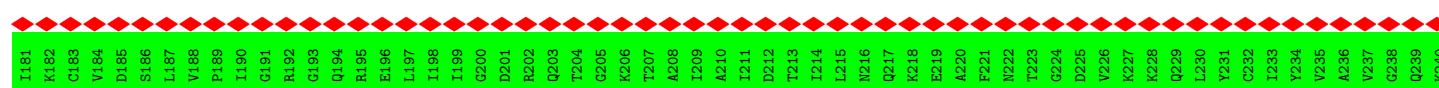
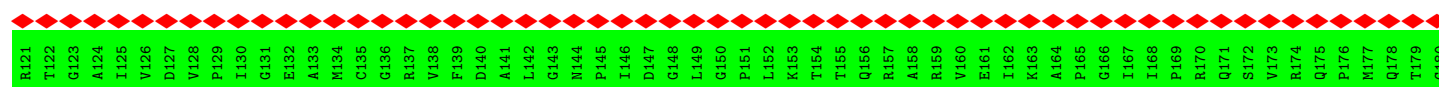
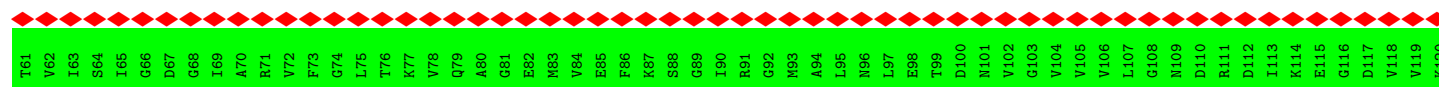
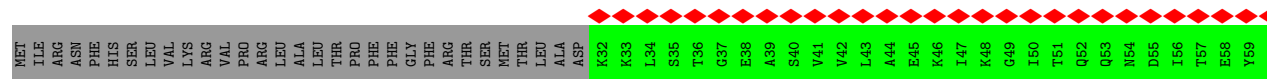




• Molecule 23: ATP synthase subunit gamma

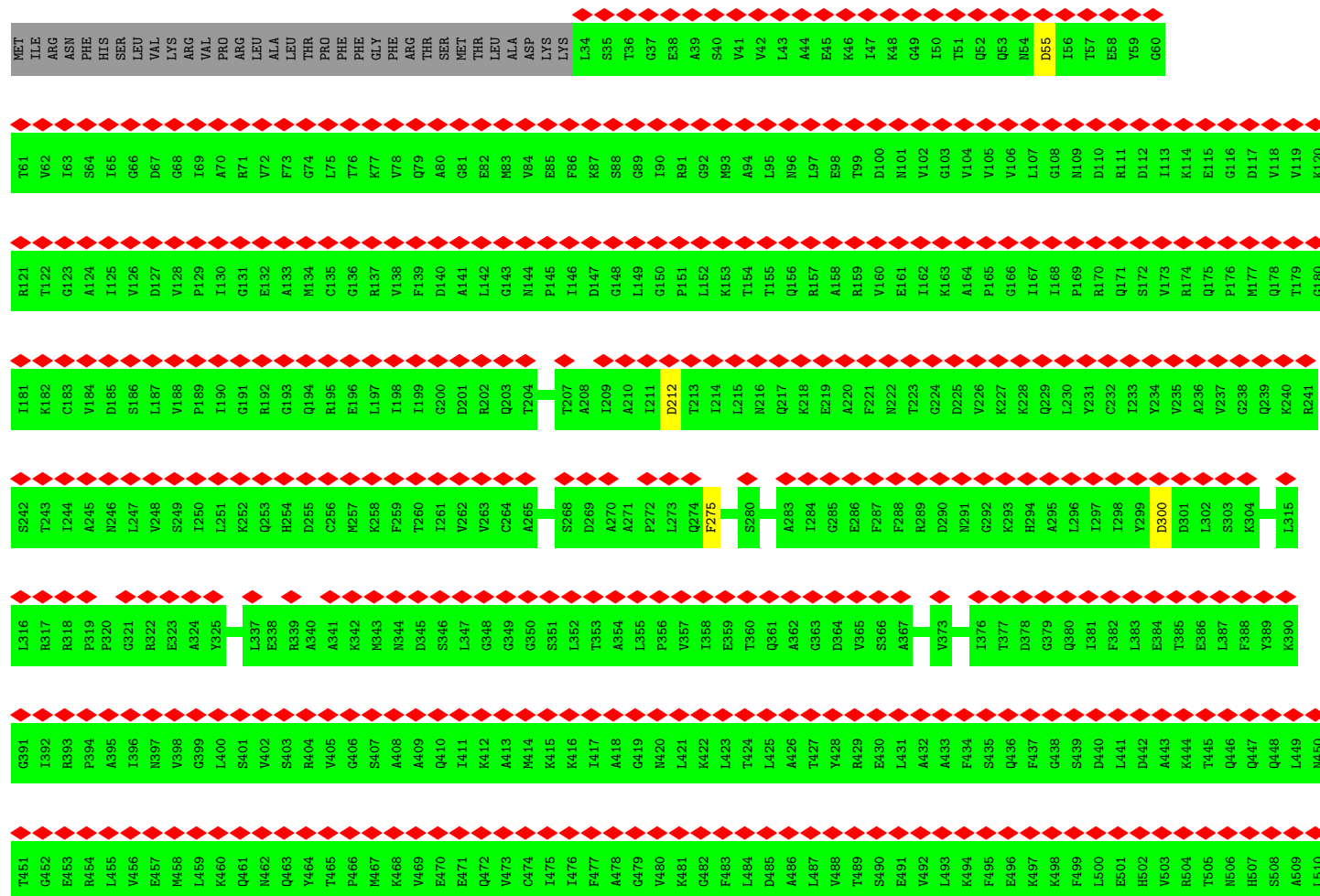
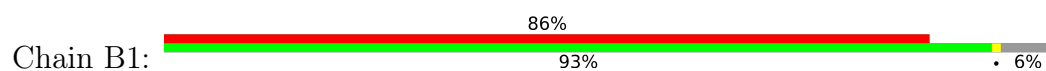


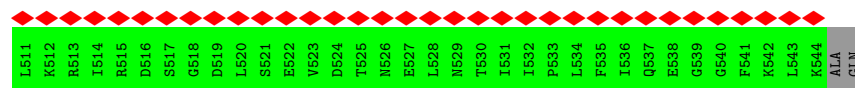
• Molecule 24: ATP synthase subunit alpha



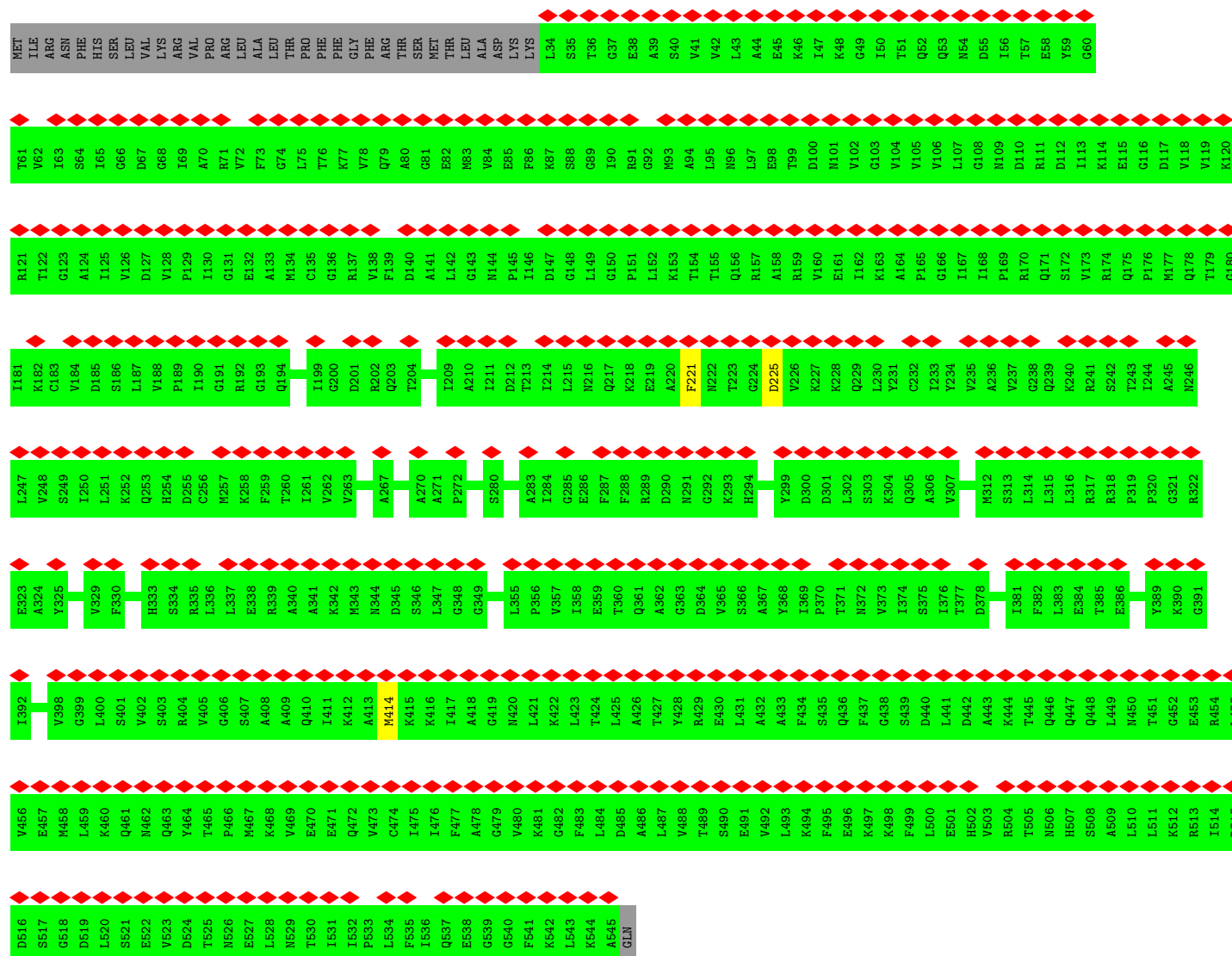
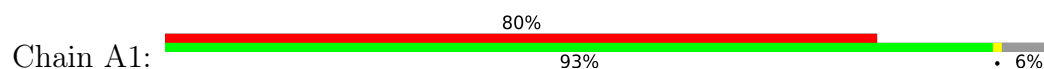


• Molecule 24: ATP synthase subunit alpha



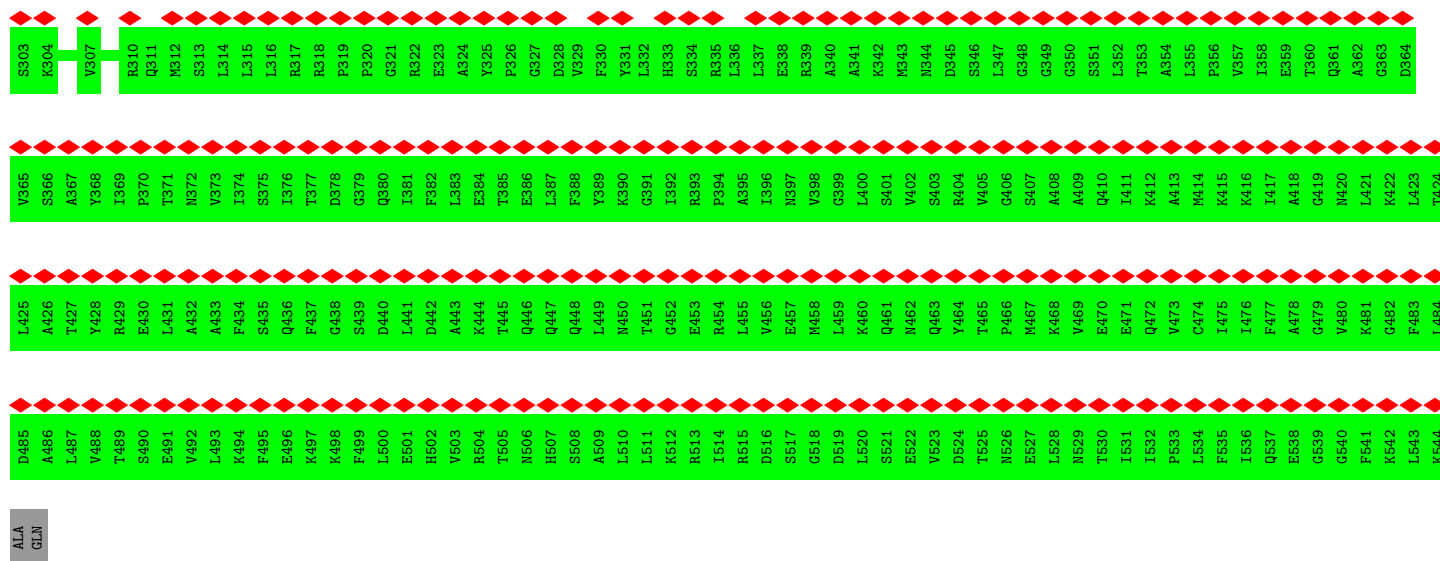


• Molecule 24: ATP synthase subunit alpha



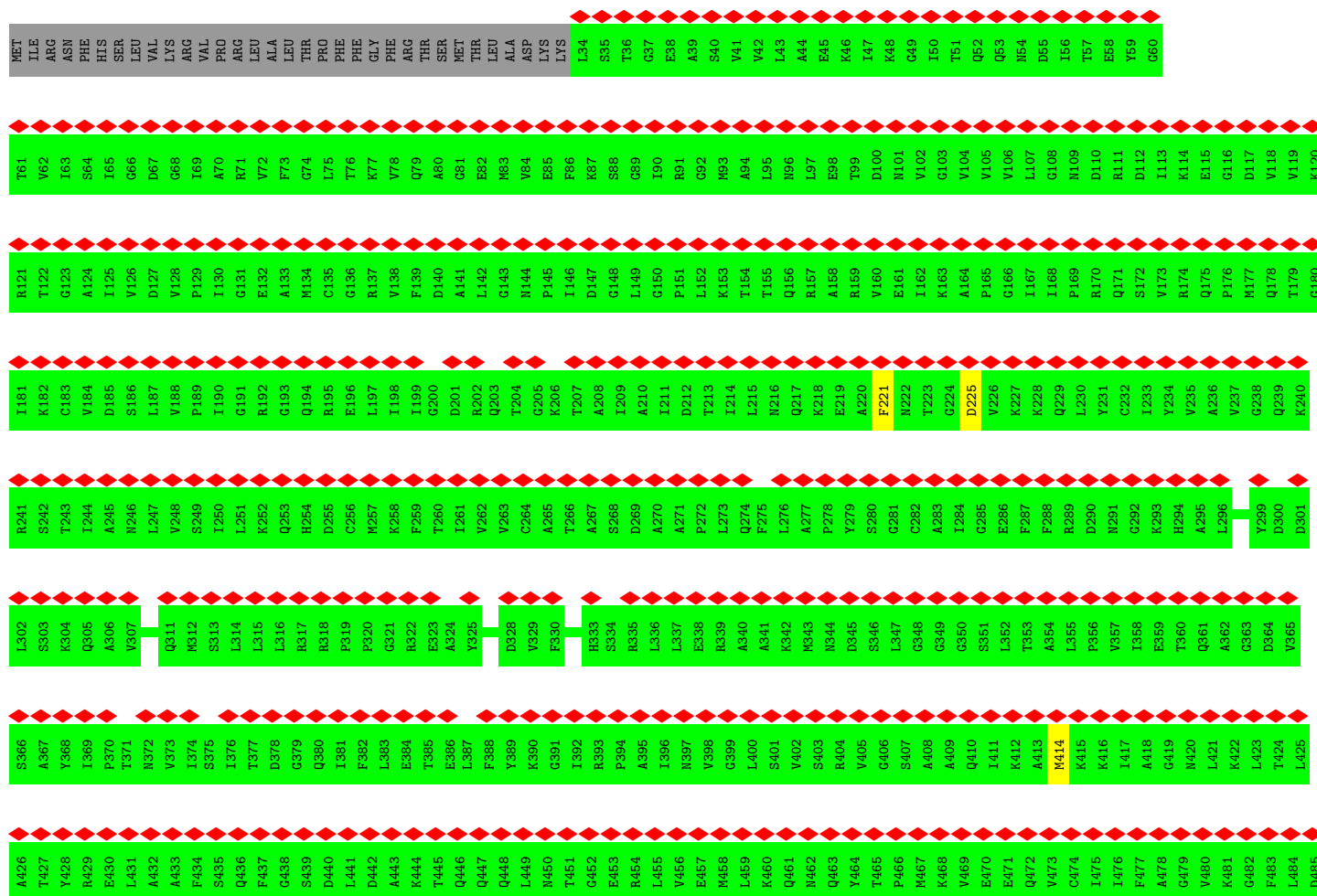
• Molecule 24: ATP synthase subunit alpha

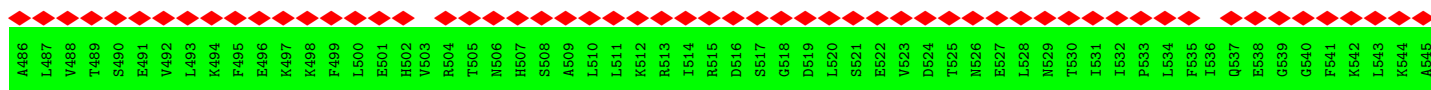




• Molecule 24: ATP synthase subunit alpha

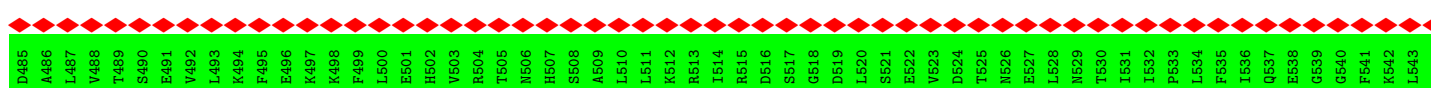
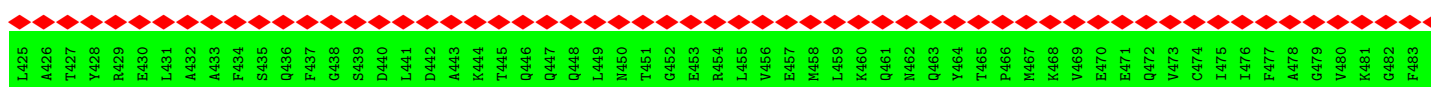
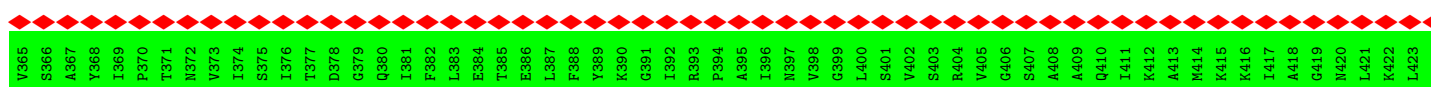
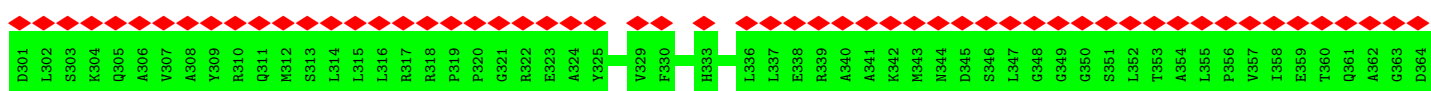
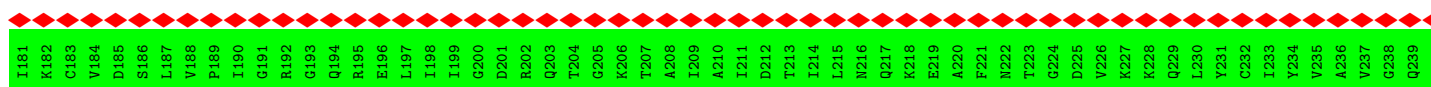
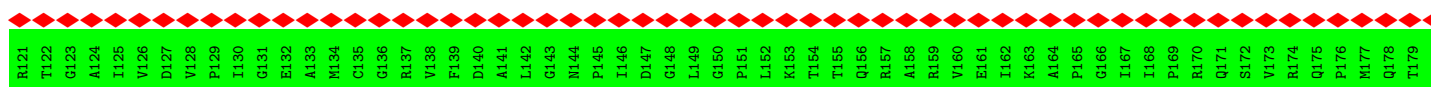
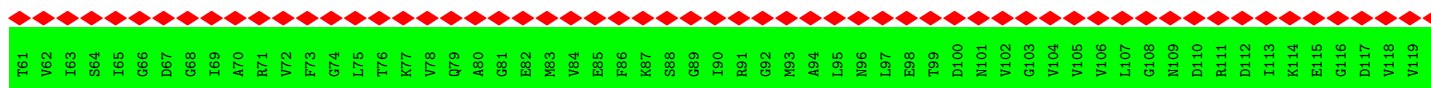
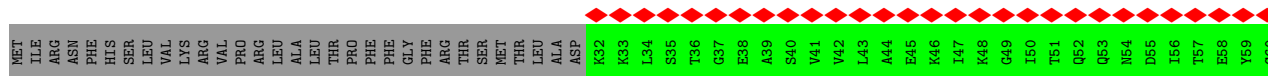
Chain A2: 90%
93% • 6%





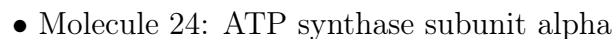
GLN

• Molecule 24: ATP synthase subunit alpha

ALA
GLN

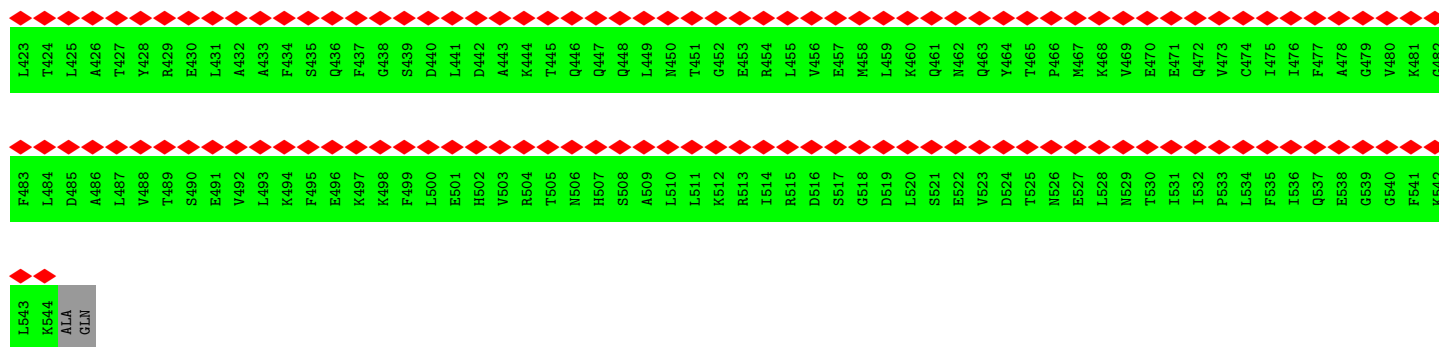
• Molecule 24: ATP synthase subunit alpha



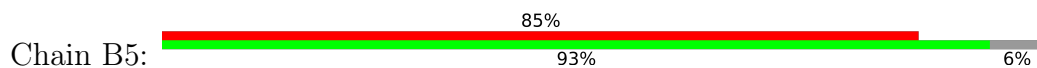


Group	Percentage
Group 1	89%
Group 2	93%
Group 3	6%

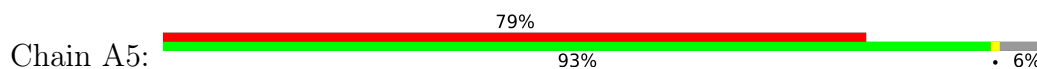


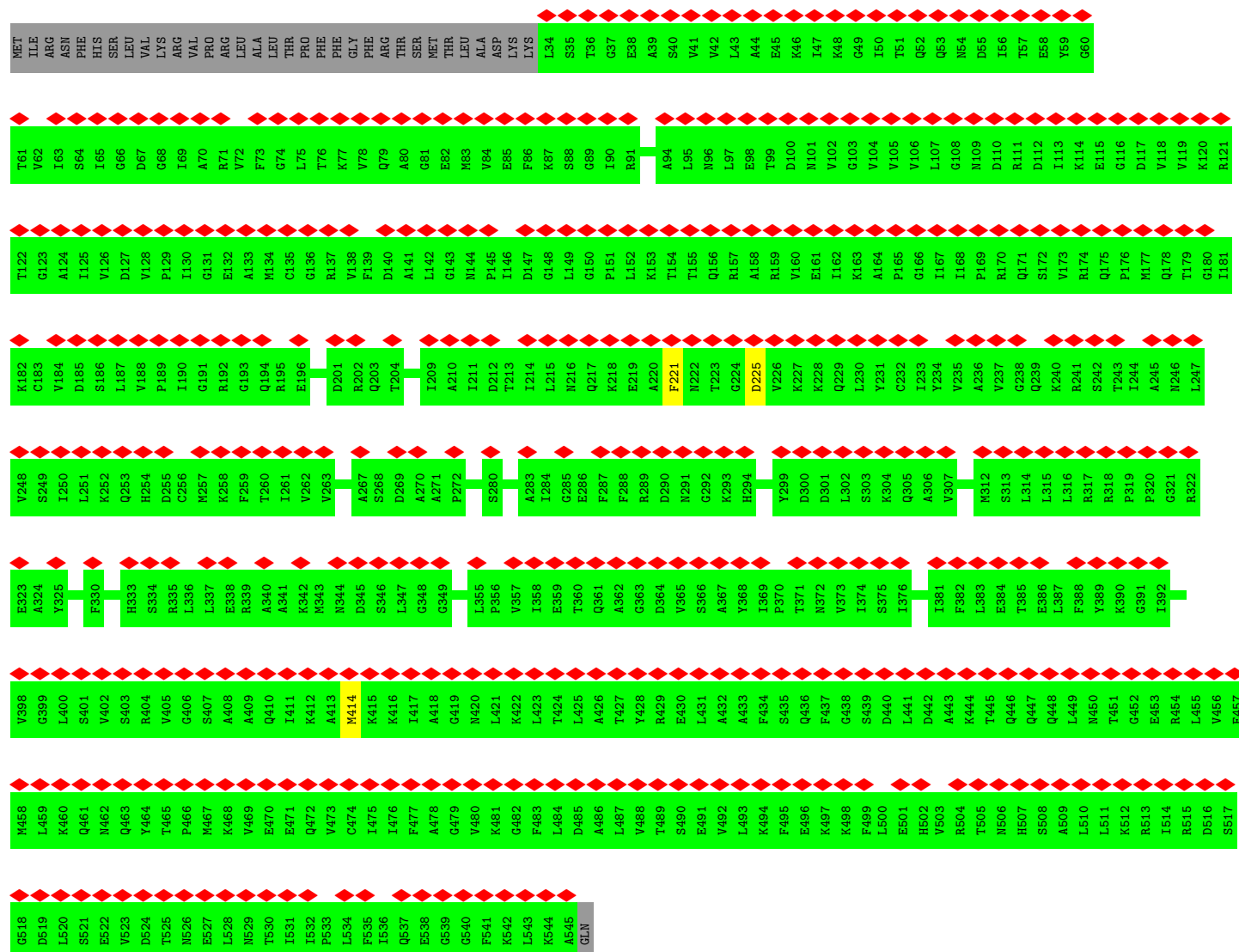


• Molecule 24: ATP synthase subunit alpha

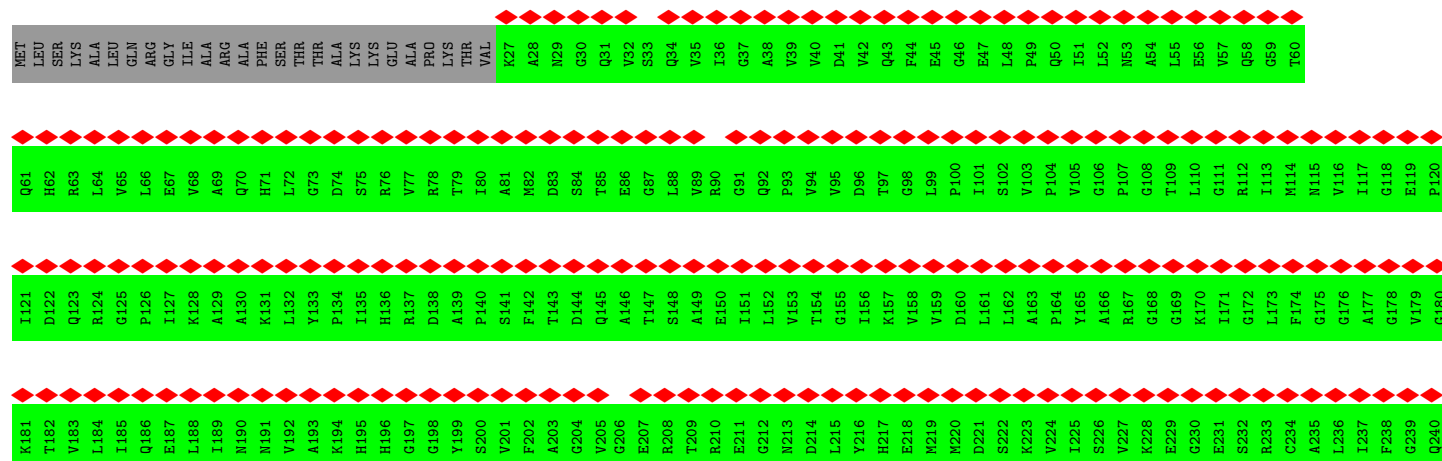


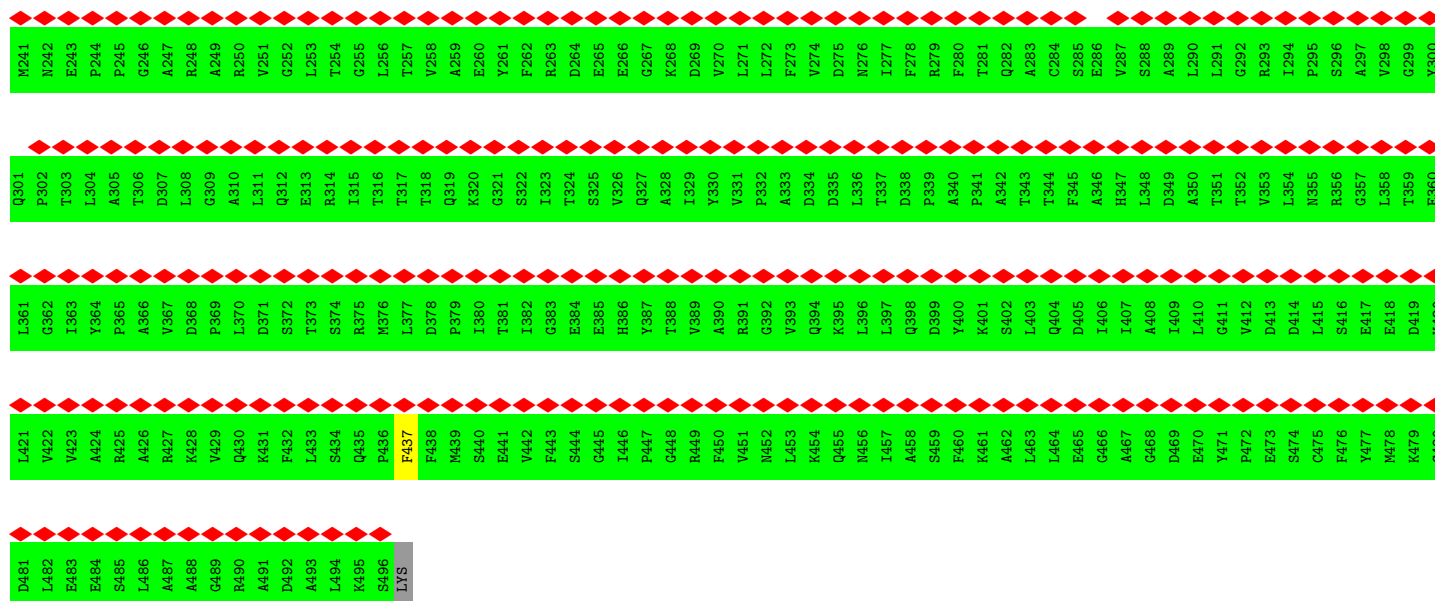
• Molecule 24: ATP synthase subunit alpha





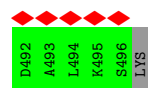
• Molecule 25: ATP synthase subunit beta



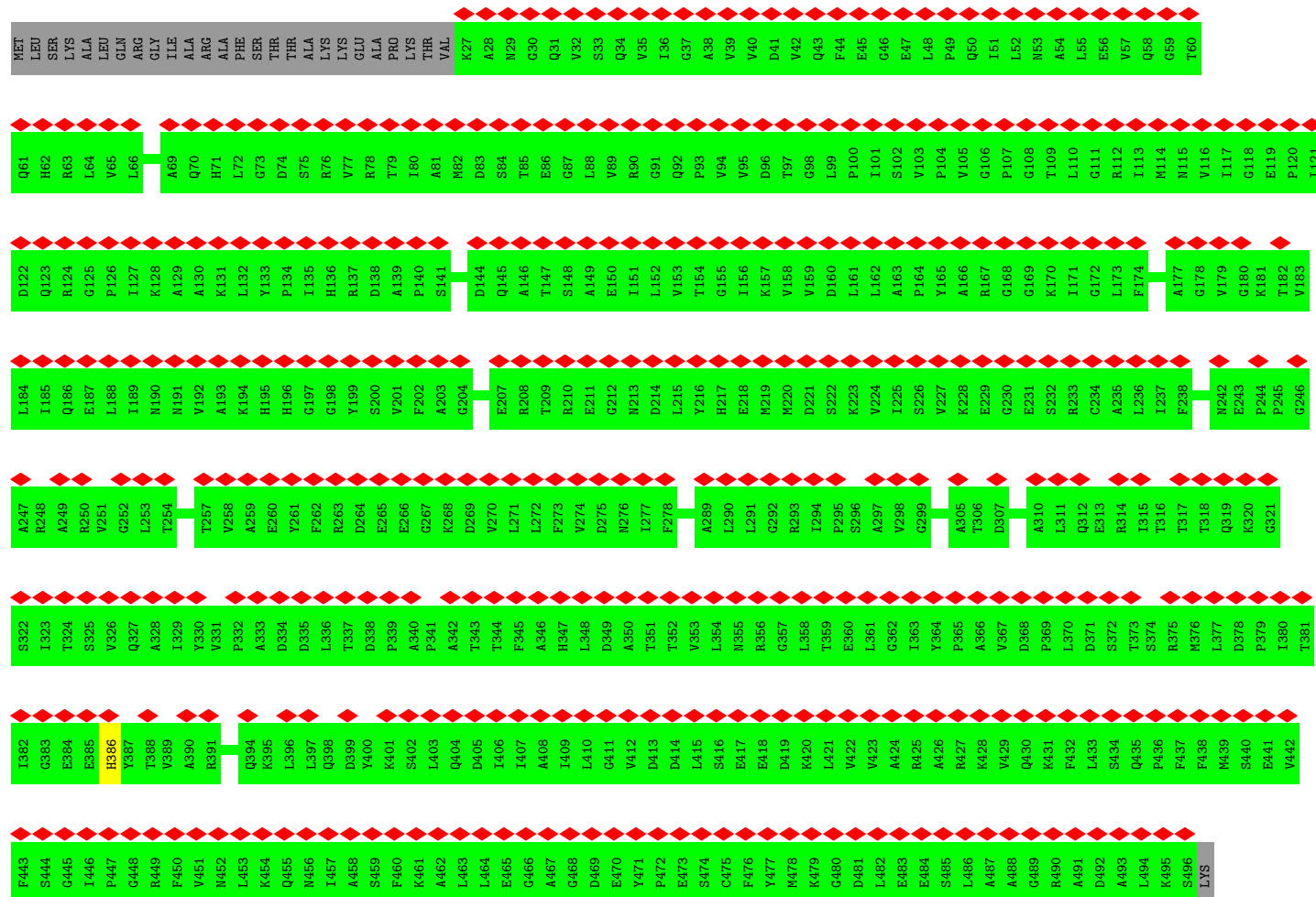
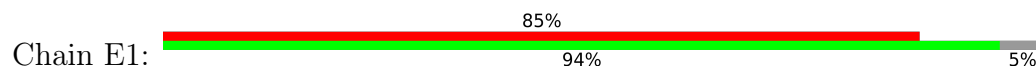


• Molecule 25: ATP synthase subunit beta

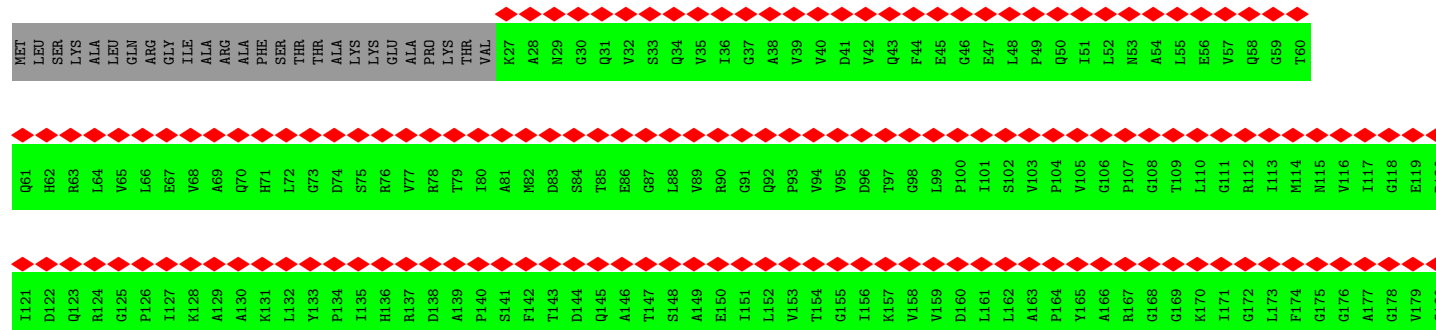




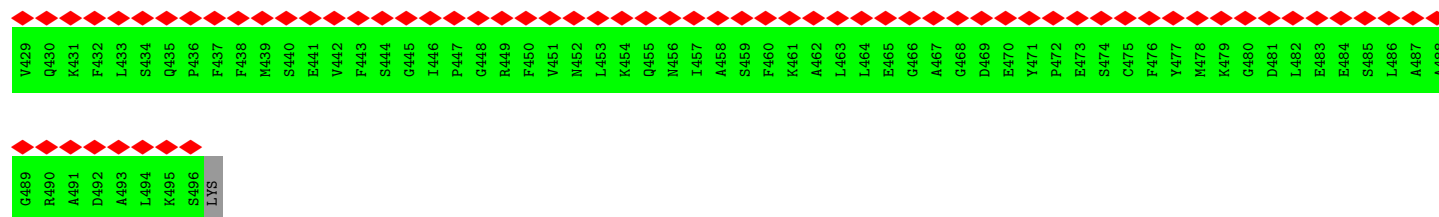
• Molecule 25: ATP synthase subunit beta



• Molecule 25: ATP synthase subunit beta



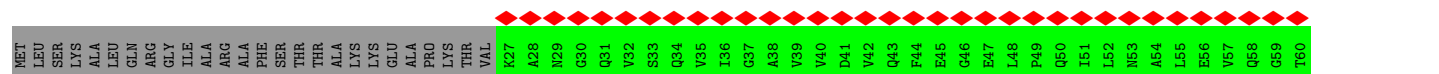


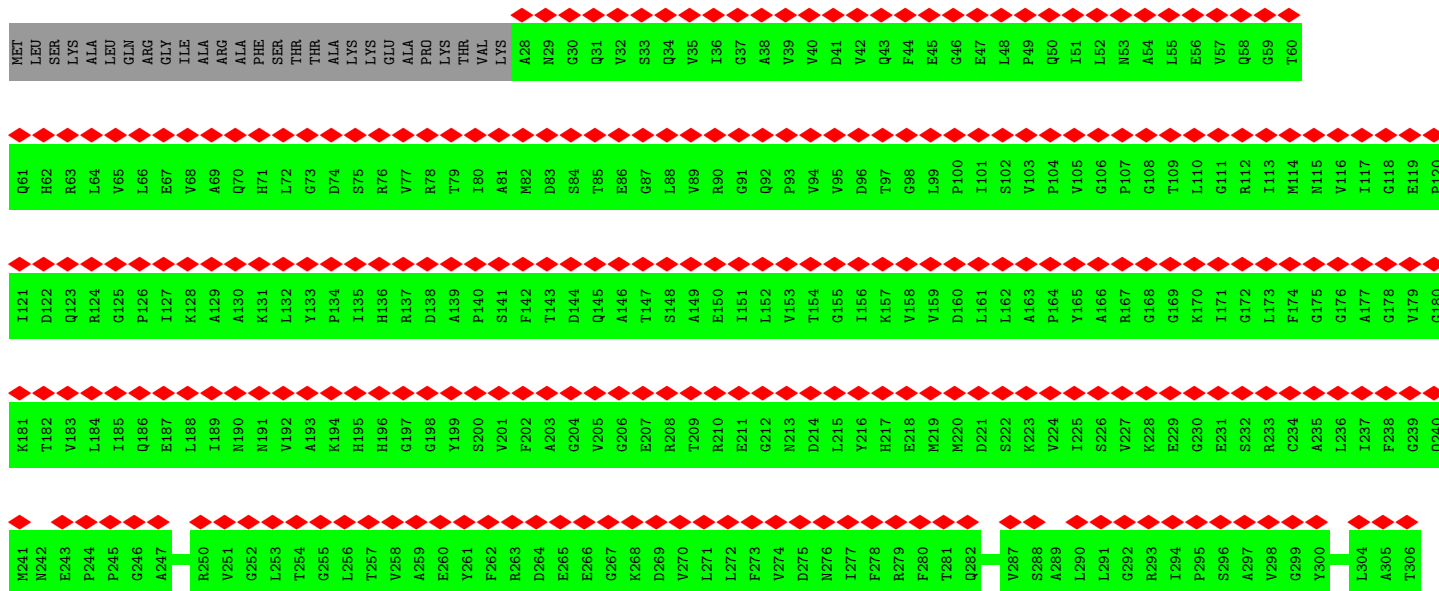


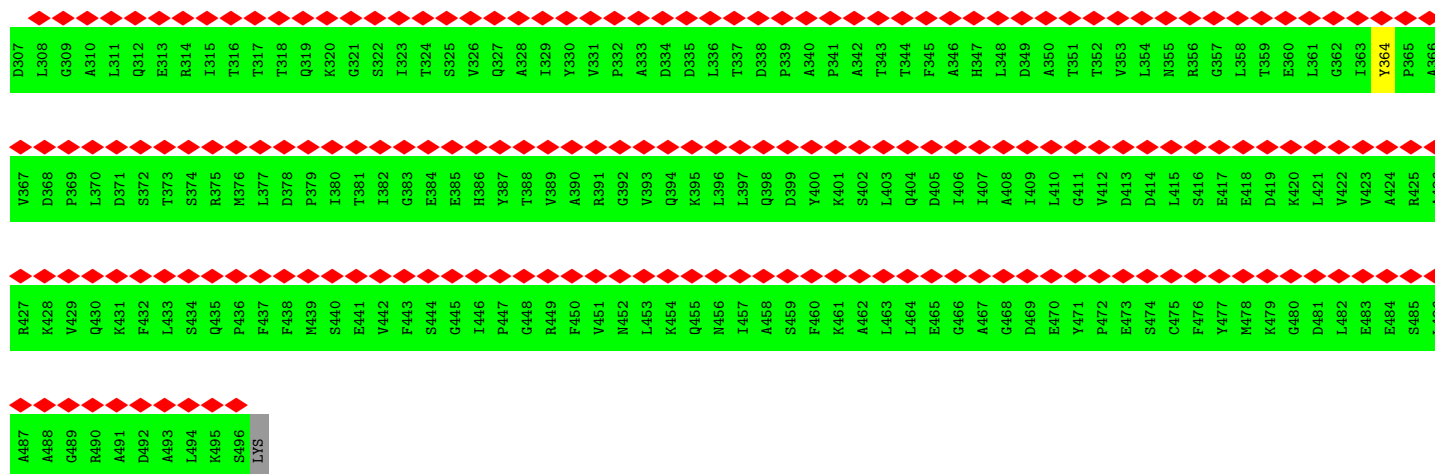
• Molecule 25: ATP synthase subunit beta



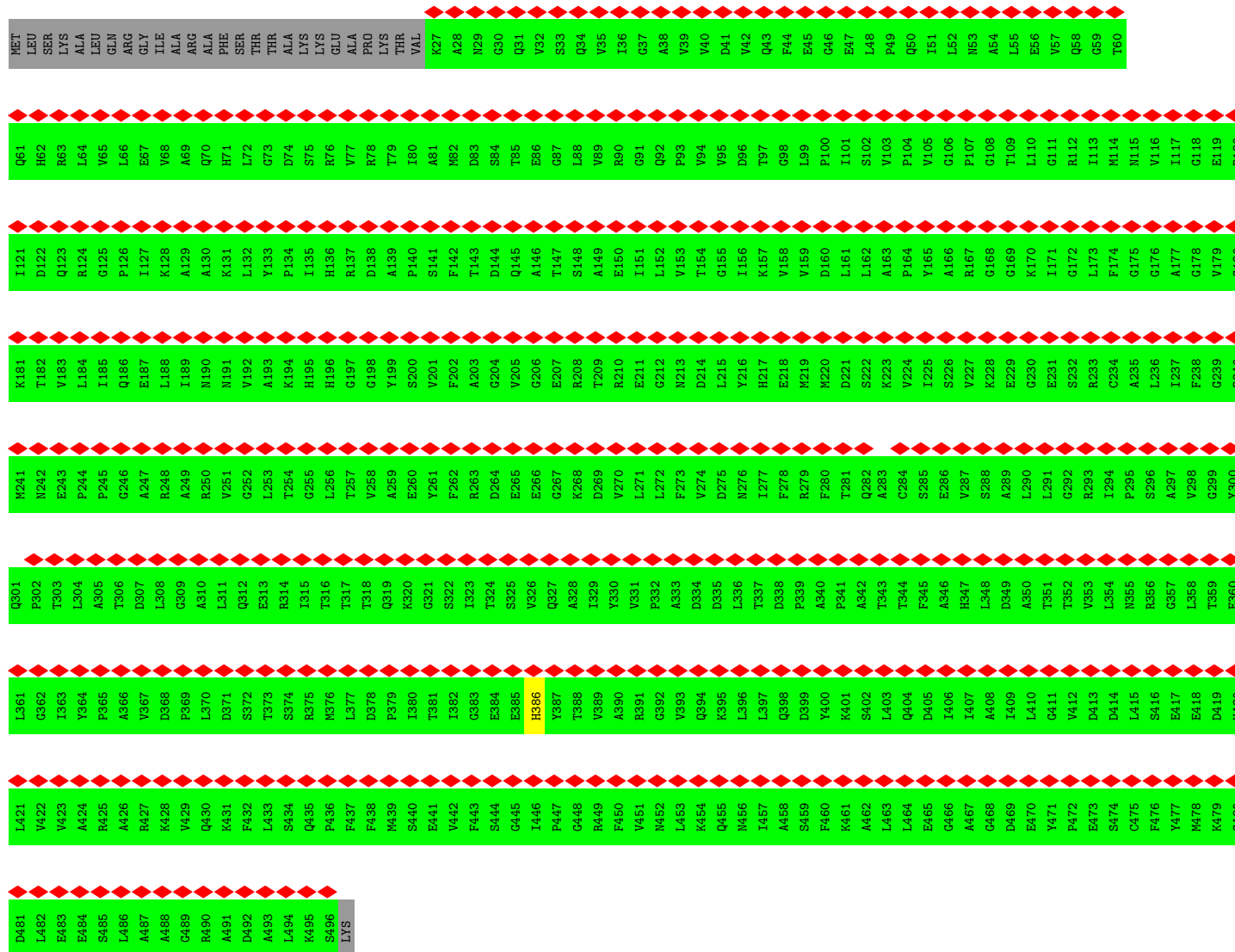
• Molecule 25: ATP synthase subunit beta





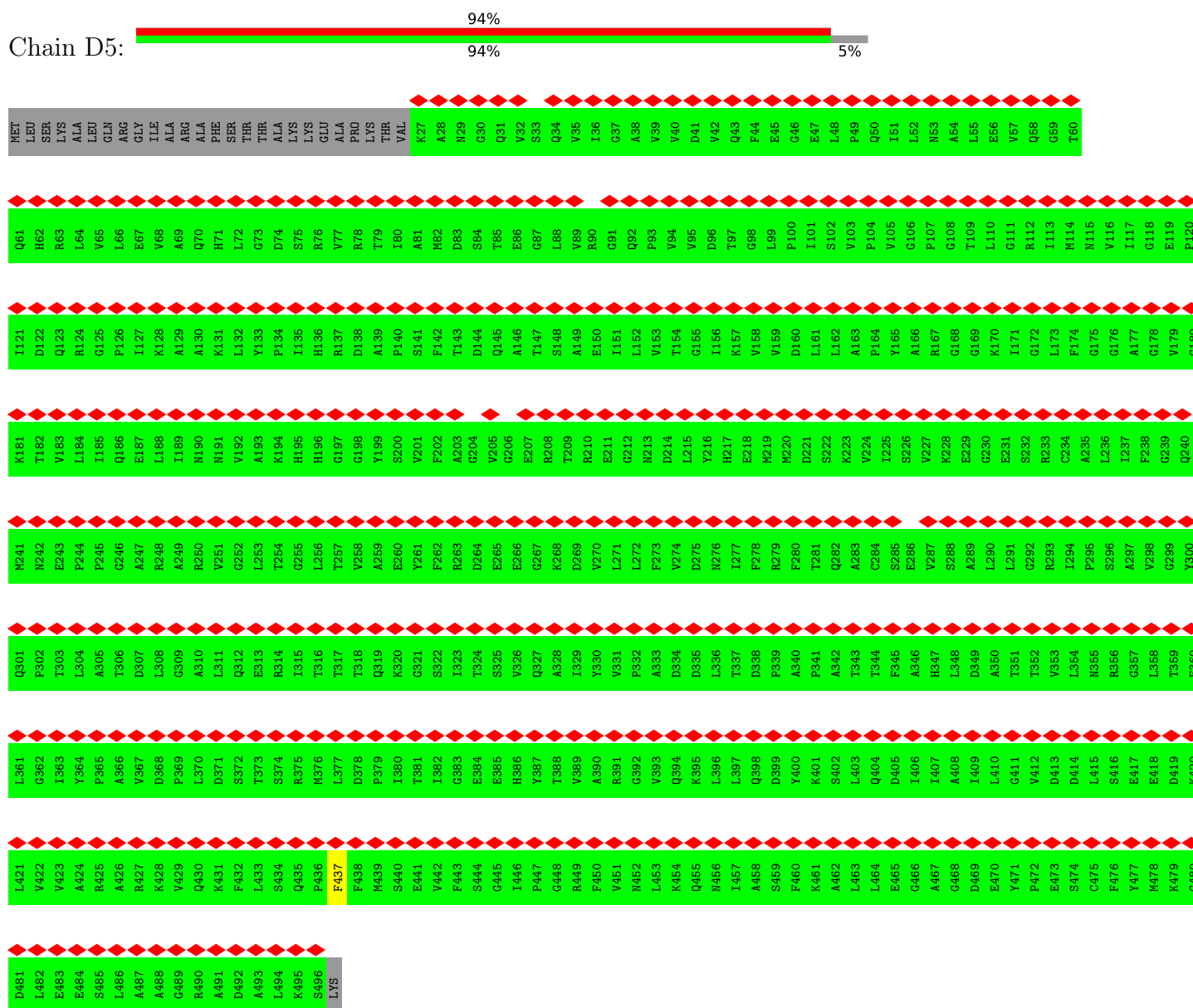


● Molecule 25: ATP synthase subunit beta



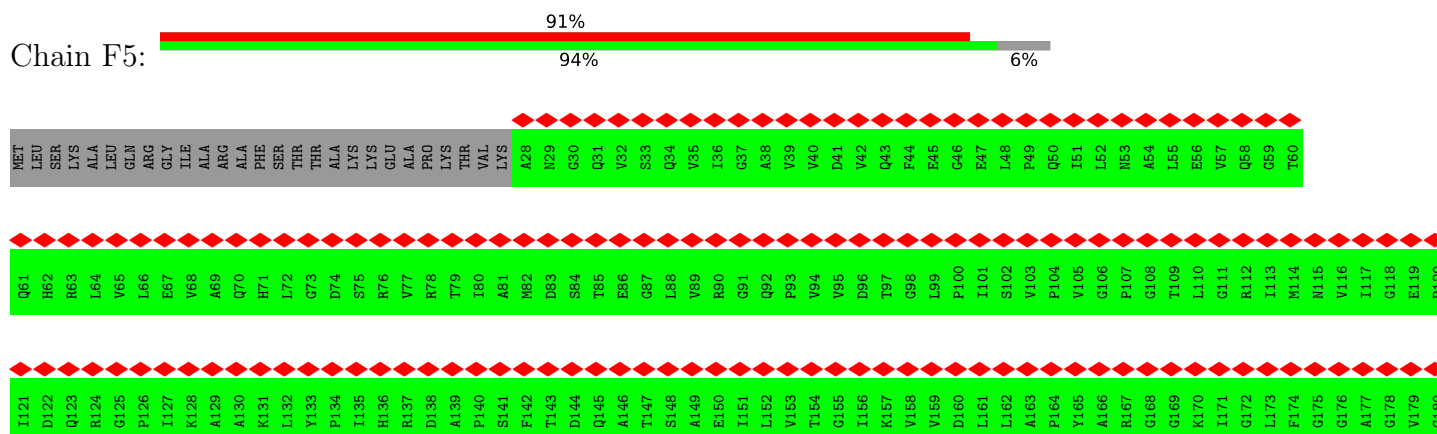
- Molecule 25: ATP synthase subunit beta

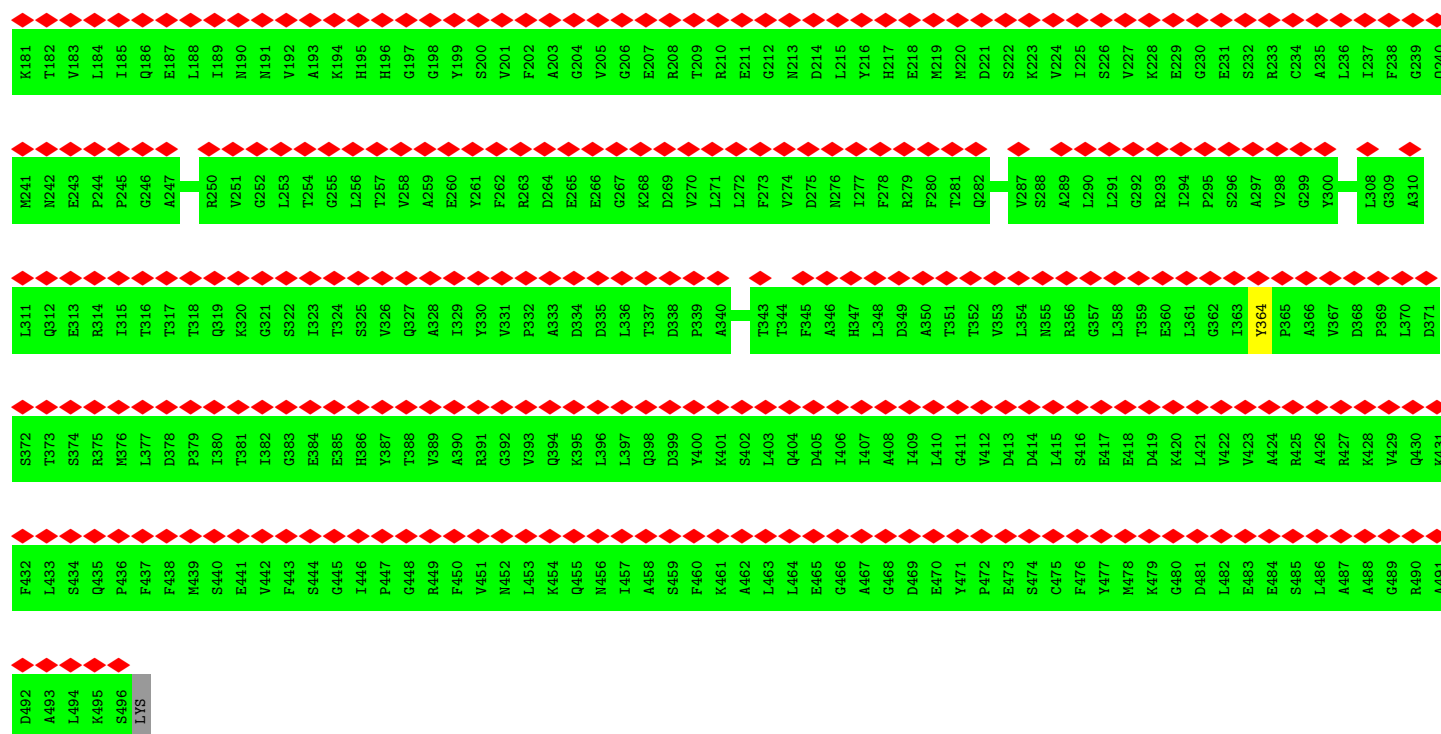
Chain D5:



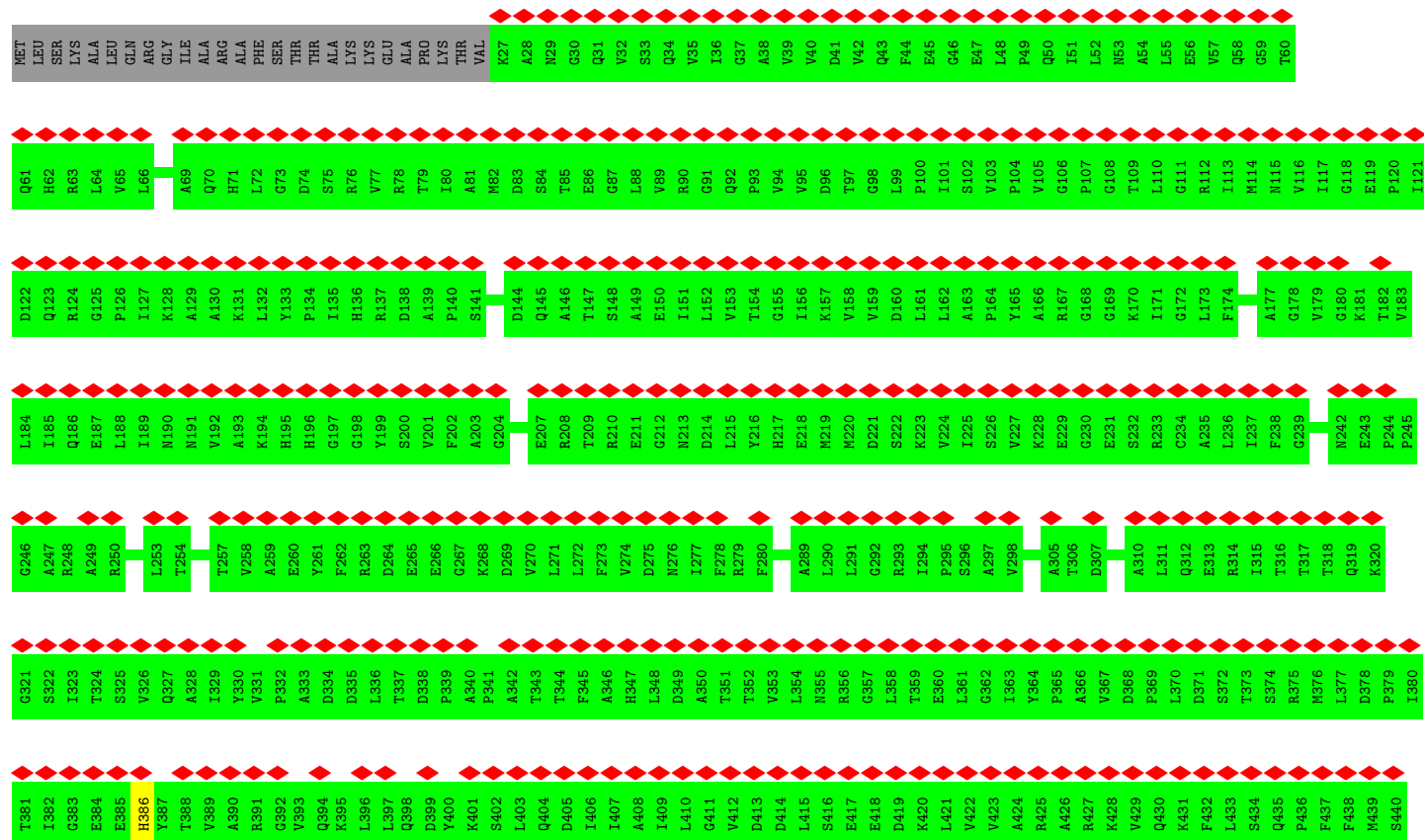
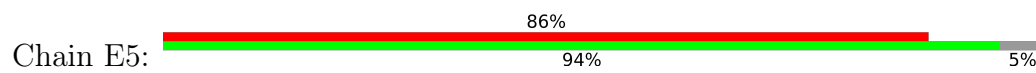
- Molecule 25: ATP synthase subunit beta

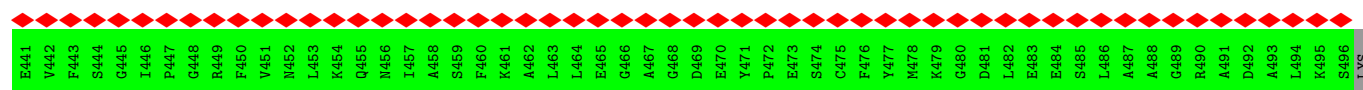
Chain F5:





● Molecule 25: ATP synthase subunit beta





- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



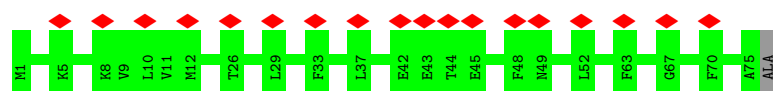
- Molecule 26: ATP synthase F0 subunit 9



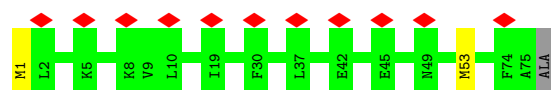
- Molecule 26: ATP synthase F0 subunit 9



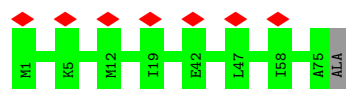
- Molecule 26: ATP synthase F0 subunit 9



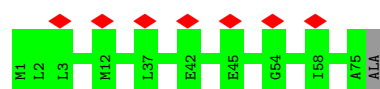
- Molecule 26: ATP synthase F0 subunit 9



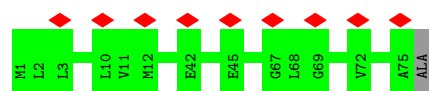
- Molecule 26: ATP synthase F0 subunit 9



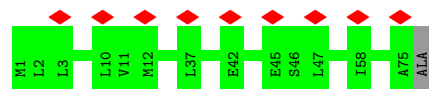
- Molecule 26: ATP synthase F0 subunit 9



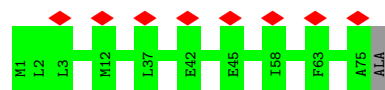
- Molecule 26: ATP synthase F0 subunit 9



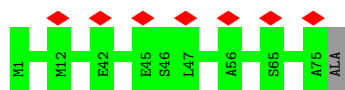
- Molecule 26: ATP synthase F0 subunit 9



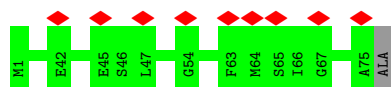
- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



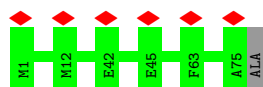
- Molecule 26: ATP synthase F0 subunit 9



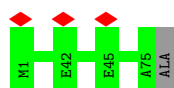
- Molecule 26: ATP synthase F0 subunit 9



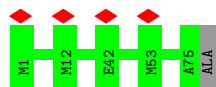
- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9

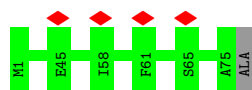


- Molecule 26: ATP synthase F0 subunit 9

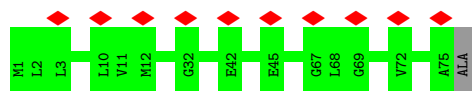


- Molecule 26: ATP synthase F0 subunit 9

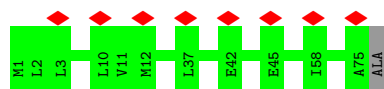




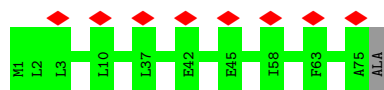
- Molecule 26: ATP synthase F0 subunit 9



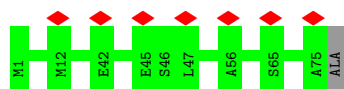
- Molecule 26: ATP synthase F0 subunit 9



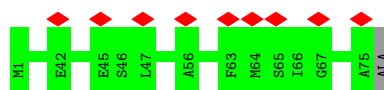
- Molecule 26: ATP synthase F0 subunit 9



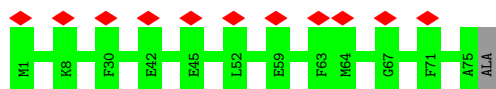
- Molecule 26: ATP synthase F0 subunit 9



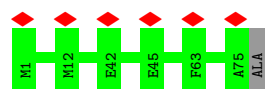
- Molecule 26: ATP synthase F0 subunit 9



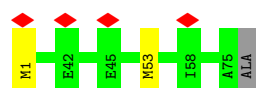
- Molecule 26: ATP synthase F0 subunit 9



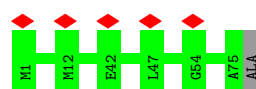
- Molecule 26: ATP synthase F0 subunit 9



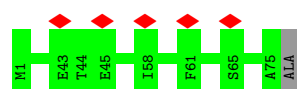
- Molecule 26: ATP synthase F0 subunit 9



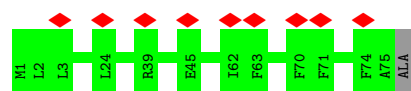
- Molecule 26: ATP synthase F0 subunit 9



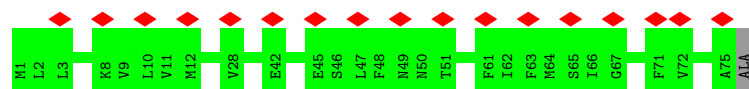
- Molecule 26: ATP synthase F0 subunit 9



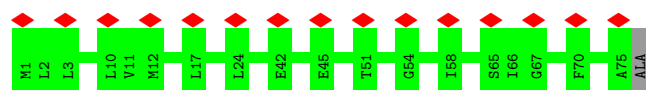
- Molecule 26: ATP synthase F0 subunit 9



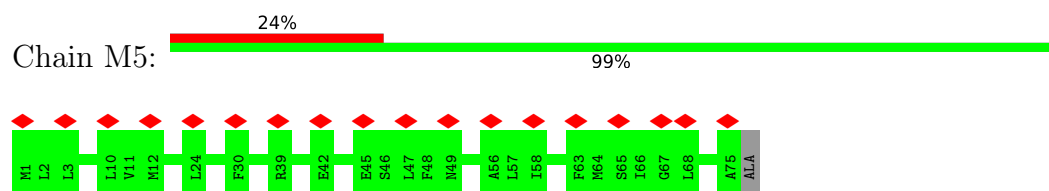
- Molecule 26: ATP synthase F0 subunit 9



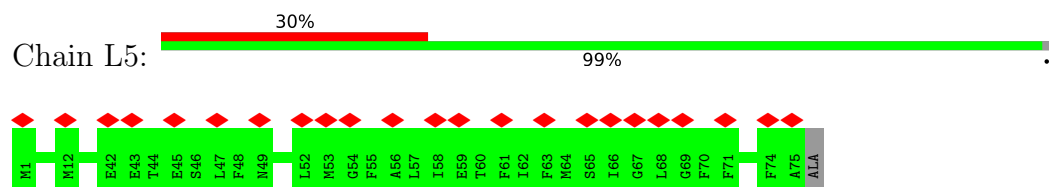
- Molecule 26: ATP synthase F0 subunit 9



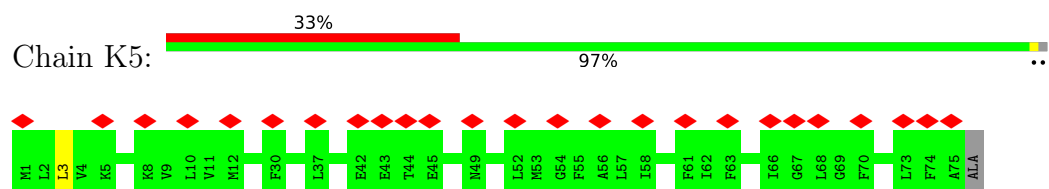
● Molecule 26: ATP synthase F0 subunit 9



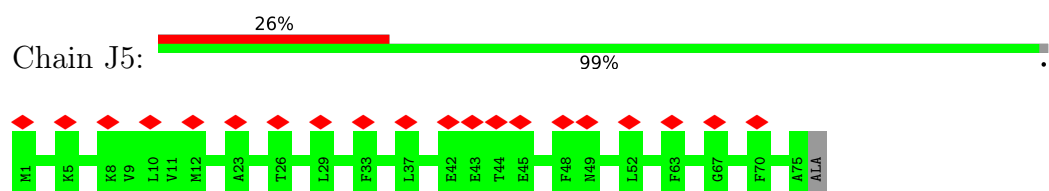
● Molecule 26: ATP synthase F0 subunit 9



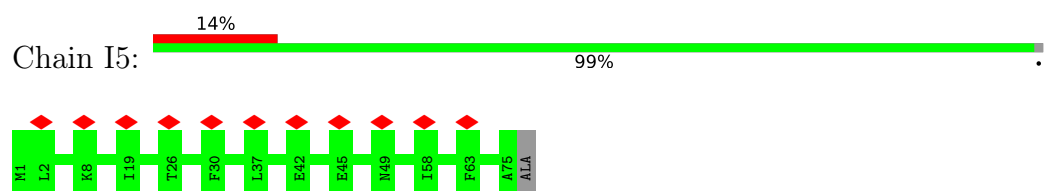
● Molecule 26: ATP synthase F0 subunit 9



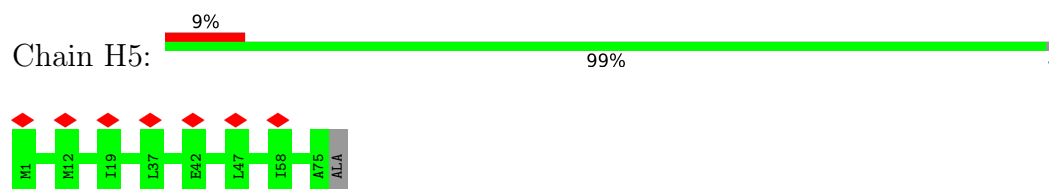
● Molecule 26: ATP synthase F0 subunit 9



● Molecule 26: ATP synthase F0 subunit 9



● Molecule 26: ATP synthase F0 subunit 9

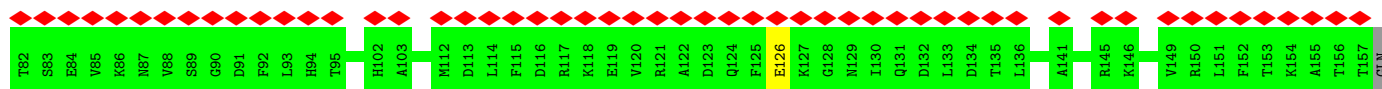
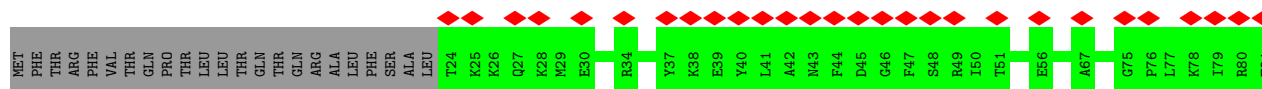
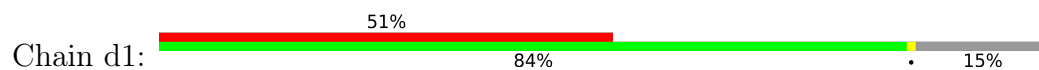


● Molecule 26: ATP synthase F0 subunit 9

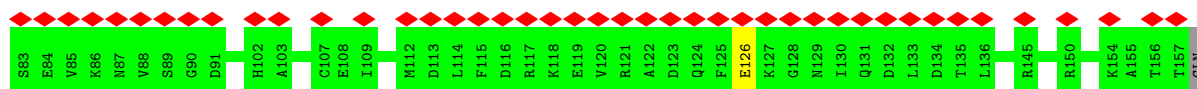
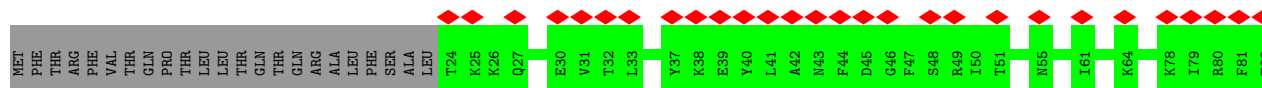
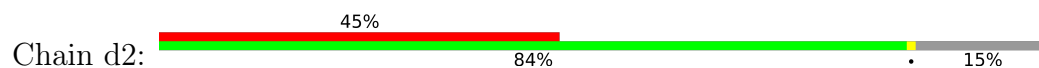




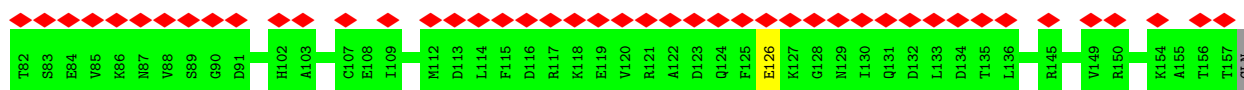
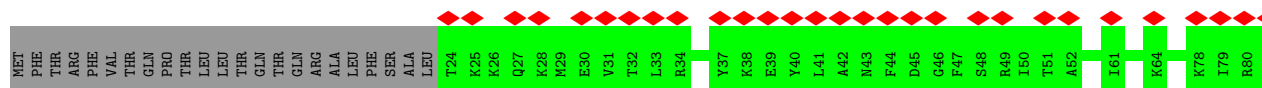
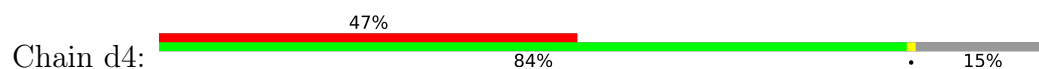
- Molecule 27: subunit delta



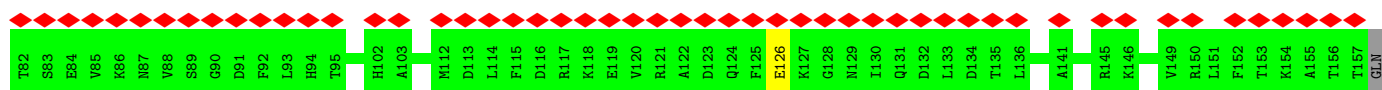
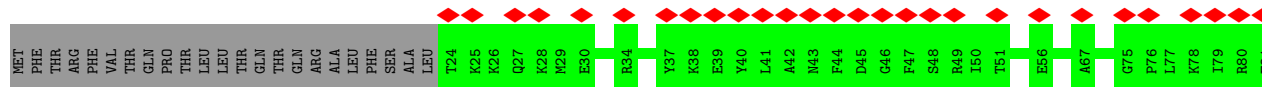
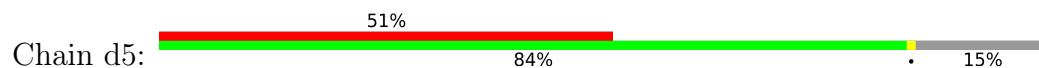
- Molecule 27: subunit delta



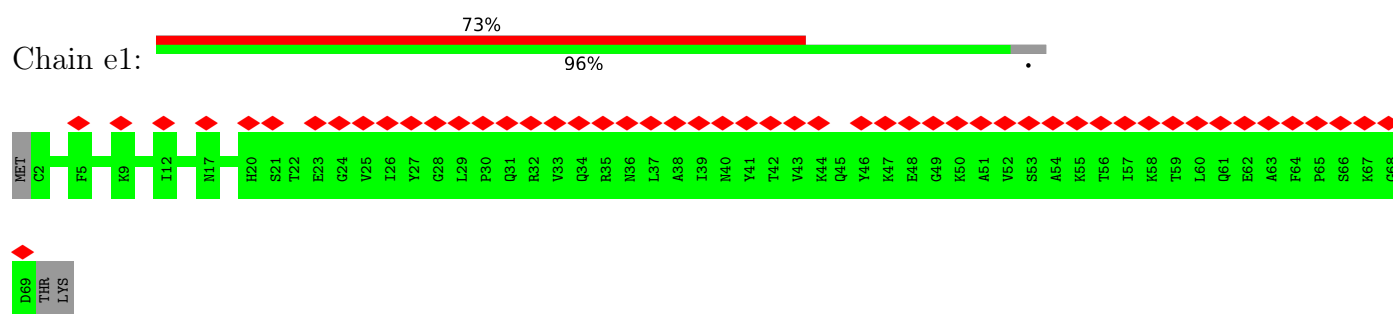
- Molecule 27: subunit delta



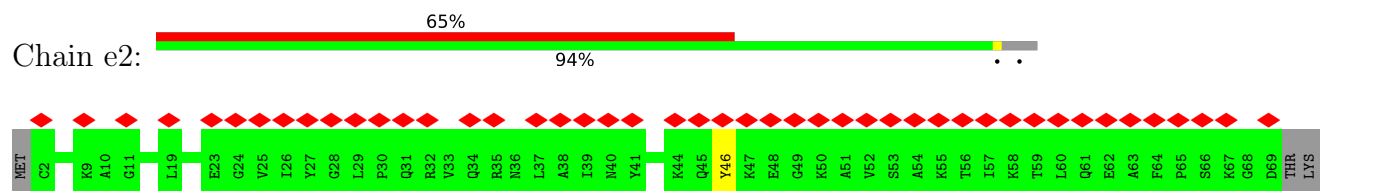
- Molecule 27: subunit delta



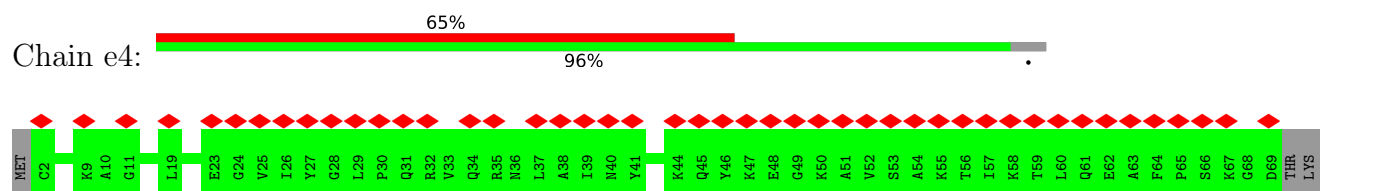
- Molecule 28: subunit epsilon



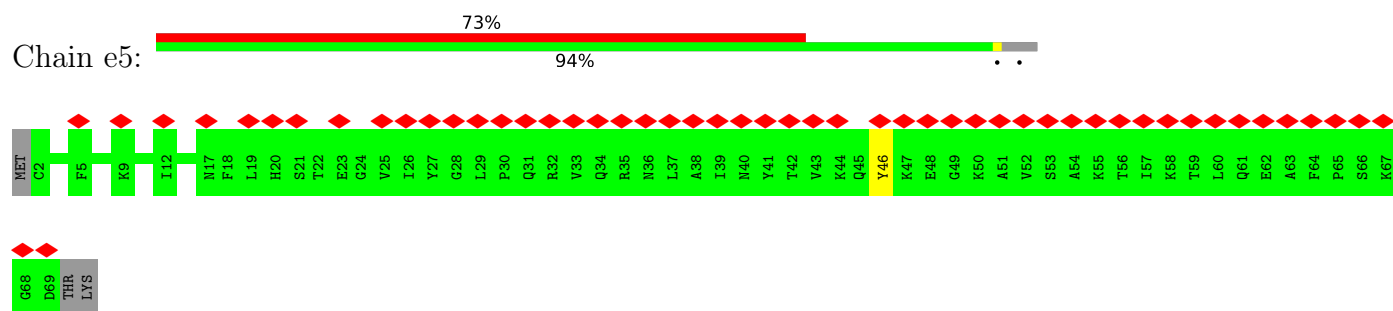
- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	40691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CDL, PO4, MG, PEE, PC1, UQ8, NAD, ATP

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	A	0.29	0/3752	0.38	0/5109
1	A3	0.29	0/3752	0.38	0/5109
1	a	0.29	0/3752	0.38	0/5109
1	a3	0.30	0/3752	0.38	0/5109
2	B	0.26	0/2940	0.36	0/3969
2	B3	0.26	0/2940	0.36	0/3969
2	b	0.26	0/2940	0.36	0/3969
2	b3	0.26	0/2940	0.36	0/3969
3	D	0.26	0/1715	0.37	0/2321
3	D3	0.26	0/1715	0.37	0/2321
3	d	0.26	0/1715	0.37	0/2321
3	d3	0.26	0/1715	0.37	0/2321
4	F	0.29	0/1733	0.40	0/2327
4	F3	0.29	0/1733	0.39	0/2327
4	f	0.29	0/1733	0.39	0/2327
4	f3	0.29	0/1733	0.39	0/2327
5	I	0.29	0/1771	0.38	0/2394
5	I3	0.28	0/1771	0.38	0/2394
5	i	0.28	0/1771	0.39	0/2394
5	i3	0.29	0/1771	0.38	0/2394
6	K	0.26	0/1508	0.37	0/2024
6	K3	0.26	0/1508	0.37	0/2024
6	k	0.26	0/1508	0.38	0/2024
6	k3	0.26	0/1508	0.38	0/2024
7	C	0.28	0/866	0.39	0/1176
7	C3	0.27	0/866	0.39	0/1176
7	c	0.27	0/866	0.39	0/1176
7	c3	0.28	0/866	0.38	0/1176
8	G	0.28	0/2302	0.40	0/3115
8	G3	0.27	0/2302	0.40	0/3115
8	g	0.27	0/2302	0.40	0/3115
8	g3	0.28	0/2302	0.40	0/3115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	H	0.26	0/2006	0.39	0/2704
9	H3	0.26	0/2006	0.39	0/2704
9	h	0.25	0/2006	0.39	0/2704
9	h3	0.26	0/2006	0.38	0/2704
10	J	0.28	0/2256	0.40	0/3069
10	J3	0.27	0/2256	0.40	0/3069
10	j	0.27	0/2256	0.40	0/3069
10	j3	0.28	0/2256	0.40	0/3069
11	L	0.29	0/2140	0.39	0/2903
11	L3	0.29	0/2140	0.39	0/2903
11	l	0.29	0/2140	0.39	0/2903
11	l3	0.29	0/2140	0.38	0/2903
12	M	0.28	0/1912	0.37	0/2598
12	M3	0.27	0/1912	0.37	0/2598
12	m	0.27	0/1912	0.37	0/2598
12	m3	0.28	0/1912	0.37	0/2598
13	N	0.30	0/1030	0.39	0/1393
13	N3	0.29	0/1030	0.39	0/1393
13	n	0.29	0/1030	0.40	0/1393
13	n3	0.30	0/1030	0.40	0/1393
14	O	0.26	0/821	0.39	0/1104
14	O3	0.26	0/821	0.40	0/1104
14	o	0.27	0/821	0.40	0/1104
14	o3	0.26	0/821	0.40	0/1104
15	P	0.25	0/1249	0.37	0/1695
15	P3	0.24	0/1249	0.37	0/1695
15	p	0.24	0/1249	0.38	0/1695
15	p3	0.25	0/1249	0.38	0/1695
16	Q	0.26	0/888	0.39	0/1200
16	Q3	0.25	0/888	0.39	0/1200
16	q	0.25	0/888	0.39	0/1200
16	q3	0.26	0/888	0.39	0/1200
17	R	0.28	0/1185	0.38	0/1594
17	R3	0.28	0/1185	0.38	0/1594
17	r	0.28	0/1225	0.38	0/1649
17	r3	0.29	0/1225	0.38	0/1649
18	S	0.26	0/1044	0.41	0/1414
18	S3	0.26	0/1044	0.41	0/1414
18	s	0.25	0/1037	0.41	0/1404
18	s3	0.26	0/1037	0.41	0/1404
19	E	0.25	0/3492	0.40	0/4720
19	E3	0.25	0/3492	0.40	0/4720
19	e	0.24	0/3492	0.40	0/4720

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	e3	0.25	0/3492	0.40	0/4720
20	i1	0.22	0/593	0.34	0/795
20	i2	0.22	0/563	0.34	0/753
20	i4	0.22	0/593	0.34	0/795
20	i5	0.22	0/563	0.34	0/753
21	t	0.25	0/3103	0.39	0/4200
21	t3	0.25	0/3103	0.39	0/4200
22	G1	0.24	0/1507	0.37	0/2027
22	G2	0.24	0/1507	0.37	0/2027
22	G4	0.24	0/1507	0.37	0/2027
22	G5	0.24	0/1507	0.37	0/2027
23	g1	0.24	0/2156	0.38	0/2900
23	g2	0.24	0/2156	0.38	0/2900
23	g4	0.24	0/2156	0.38	0/2900
23	g5	0.24	0/2156	0.38	0/2900
24	A1	0.24	0/3961	0.40	0/5346
24	A2	0.24	0/3961	0.40	0/5346
24	A4	0.24	0/3961	0.40	0/5346
24	A5	0.24	0/3961	0.40	0/5346
24	B1	0.24	0/3956	0.40	0/5339
24	B2	0.24	0/3956	0.40	0/5339
24	B4	0.23	0/3956	0.40	0/5339
24	B5	0.24	0/3956	0.40	0/5339
24	C1	0.24	0/3974	0.40	0/5361
24	C2	0.24	0/3974	0.40	0/5361
24	C4	0.24	0/3974	0.40	0/5361
24	C5	0.24	0/3974	0.40	0/5361
25	D1	0.24	0/3613	0.39	0/4900
25	D2	0.24	0/3613	0.40	0/4900
25	D4	0.24	0/3613	0.39	0/4900
25	D5	0.24	0/3613	0.39	0/4900
25	E1	0.24	0/3613	0.40	0/4900
25	E2	0.24	0/3613	0.40	0/4900
25	E4	0.24	0/3613	0.40	0/4900
25	E5	0.24	0/3613	0.40	0/4900
25	F1	0.24	0/3604	0.40	0/4889
25	F2	0.24	0/3604	0.40	0/4889
25	F4	0.24	0/3604	0.40	0/4889
25	F5	0.24	0/3604	0.40	0/4889
26	H1	0.27	0/572	0.35	0/771
26	H2	0.27	0/572	0.37	0/771
26	H4	0.27	0/572	0.35	0/771
26	H5	0.27	0/572	0.36	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	I1	0.27	0/572	0.36	0/771
26	I2	0.27	0/572	0.37	0/771
26	I4	0.27	0/572	0.36	0/771
26	I5	0.27	0/572	0.37	0/771
26	J1	0.27	0/572	0.35	0/771
26	J2	0.26	0/572	0.35	0/771
26	J4	0.27	0/572	0.35	0/771
26	J5	0.27	0/572	0.35	0/771
26	K1	0.27	0/572	0.35	0/771
26	K2	0.26	0/572	0.36	0/771
26	K4	0.26	0/572	0.35	0/771
26	K5	0.26	0/572	0.36	0/771
26	L1	0.26	0/572	0.35	0/771
26	L2	0.26	0/572	0.35	0/771
26	L4	0.26	0/572	0.35	0/771
26	L5	0.26	0/572	0.35	0/771
26	M1	0.26	0/572	0.35	0/771
26	M2	0.26	0/572	0.35	0/771
26	M4	0.26	0/572	0.35	0/771
26	M5	0.26	0/572	0.35	0/771
26	N1	0.26	0/572	0.35	0/771
26	N2	0.26	0/572	0.35	0/771
26	N4	0.26	0/572	0.35	0/771
26	N5	0.26	0/572	0.35	0/771
26	O1	0.26	0/572	0.35	0/771
26	O2	0.27	0/572	0.35	0/771
26	O4	0.26	0/572	0.35	0/771
26	O5	0.26	0/572	0.35	0/771
26	P1	0.26	0/572	0.36	0/771
26	P2	0.26	0/572	0.35	0/771
26	P4	0.26	0/572	0.36	0/771
26	P5	0.26	0/572	0.35	0/771
26	Q1	0.27	0/572	0.35	0/771
26	Q2	0.26	0/572	0.34	0/771
26	Q4	0.27	0/572	0.35	0/771
26	Q5	0.26	0/572	0.35	0/771
27	d1	0.25	0/1081	0.45	0/1459
27	d2	0.25	0/1081	0.45	0/1459
27	d4	0.25	0/1081	0.44	0/1459
27	d5	0.25	0/1081	0.45	0/1459
28	e1	0.24	0/547	0.41	0/735
28	e2	0.24	0/547	0.42	0/735
28	e4	0.24	0/547	0.41	0/735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	e5	0.24	0/547	0.41	0/735
All	All	0.26	0/281952	0.39	0/381166

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
25	F1	0	1
25	F2	0	1
25	F4	0	1
25	F5	0	1
28	e2	0	1
28	e5	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	F1	364	TYR	Peptide
25	F2	364	TYR	Peptide
25	F4	364	TYR	Peptide
25	F5	364	TYR	Peptide
28	e2	46	TYR	Peptide
28	e5	46	TYR	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	A3	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	a	431/446 (97%)	423 (98%)	8 (2%)	0	100	100
1	a3	431/446 (97%)	421 (98%)	10 (2%)	0	100	100
2	B	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	B3	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	b	352/381 (92%)	340 (97%)	12 (3%)	0	100	100
2	b3	352/381 (92%)	339 (96%)	13 (4%)	0	100	100
3	D	204/234 (87%)	199 (98%)	5 (2%)	0	100	100
3	D3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	F3	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f3	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	I3	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	i	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	i3	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
6	K	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	K3	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	k	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k3	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
8	G	254/286 (89%)	245 (96%)	9 (4%)	0	100	100
8	G3	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
8	g3	254/286 (89%)	244 (96%)	10 (4%)	0	100	100
9	H	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
9	H3	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h3	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
10	J	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	J3	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	j	267/273 (98%)	263 (98%)	4 (2%)	0	100	100
10	j3	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	L3	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
11	l3	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
12	M	219/221 (99%)	219 (100%)	0	0	100	100
12	M3	219/221 (99%)	219 (100%)	0	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
12	m3	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
13	N	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	N3	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	n	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
13	n3	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	O3	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
14	o3	97/154 (63%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	P3	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	p	148/152 (97%)	139 (94%)	9 (6%)	0	100	100
15	p3	148/152 (97%)	138 (93%)	10 (7%)	0	100	100
16	Q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	Q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
17	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	R3	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	r	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
17	r3	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
18	S	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
18	S3	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
18	s	122/145 (84%)	122 (100%)	0	0	100	100
18	s3	122/145 (84%)	122 (100%)	0	0	100	100
19	E	415/480 (86%)	407 (98%)	8 (2%)	0	100	100
19	E3	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
19	e	415/480 (86%)	405 (98%)	10 (2%)	0	100	100
19	e3	415/480 (86%)	403 (97%)	12 (3%)	0	100	100
20	i1	64/108 (59%)	64 (100%)	0	0	100	100
20	i2	60/108 (56%)	60 (100%)	0	0	100	100
20	i4	64/108 (59%)	64 (100%)	0	0	100	100
20	i5	60/108 (56%)	60 (100%)	0	0	100	100
21	t	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
21	t3	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
22	G1	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G2	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G4	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G5	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
23	g1	273/299 (91%)	265 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	g2	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g4	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g5	273/299 (91%)	264 (97%)	9 (3%)	0	100	100
24	A1	510/546 (93%)	504 (99%)	6 (1%)	0	100	100
24	A2	510/546 (93%)	502 (98%)	8 (2%)	0	100	100
24	A4	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	A5	510/546 (93%)	502 (98%)	8 (2%)	0	100	100
24	B1	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	44	74
24	B2	509/546 (93%)	500 (98%)	9 (2%)	0	100	100
24	B4	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	44	74
24	B5	509/546 (93%)	499 (98%)	10 (2%)	0	100	100
24	C1	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C2	511/546 (94%)	508 (99%)	3 (1%)	0	100	100
24	C4	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C5	511/546 (94%)	507 (99%)	4 (1%)	0	100	100
25	D1	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D2	468/497 (94%)	463 (99%)	5 (1%)	0	100	100
25	D4	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D5	468/497 (94%)	462 (99%)	6 (1%)	0	100	100
25	E1	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E2	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	E4	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E5	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	F1	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F2	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
25	F4	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F5	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
26	H1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	I1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	I4	73/76 (96%)	73 (100%)	0	0	100	100
26	I5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	J1	73/76 (96%)	73 (100%)	0	0	100	100
26	J2	73/76 (96%)	73 (100%)	0	0	100	100
26	J4	73/76 (96%)	73 (100%)	0	0	100	100
26	J5	73/76 (96%)	73 (100%)	0	0	100	100
26	K1	73/76 (96%)	73 (100%)	0	0	100	100
26	K2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	K4	73/76 (96%)	73 (100%)	0	0	100	100
26	K5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	L4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	M1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N5	73/76 (96%)	73 (100%)	0	0	100	100
26	O1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	O2	73/76 (96%)	73 (100%)	0	0	100	100
26	O4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	O5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	P1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	P4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	P5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q2	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
26	Q4	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q5	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
27	d1	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d2	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d4	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d5	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
28	e1	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e2	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e4	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e5	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
All	All	34342/37732 (91%)	33598 (98%)	742 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	B1	55	ASP
24	B4	55	ASP

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	397/409 (97%)	395 (100%)	2 (0%)	86	92
1	A3	397/409 (97%)	395 (100%)	2 (0%)	86	92
1	a	397/409 (97%)	395 (100%)	2 (0%)	86	92
1	a3	397/409 (97%)	395 (100%)	2 (0%)	86	92
2	B	306/331 (92%)	306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B3	306/331 (92%)	306 (100%)	0	100	100
2	b	306/331 (92%)	306 (100%)	0	100	100
2	b3	306/331 (92%)	306 (100%)	0	100	100
3	D	183/206 (89%)	183 (100%)	0	100	100
3	D3	183/206 (89%)	183 (100%)	0	100	100
3	d	183/206 (89%)	183 (100%)	0	100	100
3	d3	183/206 (89%)	183 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	84	91
4	F3	175/178 (98%)	174 (99%)	1 (1%)	84	91
4	f	175/178 (98%)	173 (99%)	2 (1%)	70	84
4	f3	175/178 (98%)	173 (99%)	2 (1%)	70	84
5	I	182/182 (100%)	180 (99%)	2 (1%)	70	84
5	I3	182/182 (100%)	180 (99%)	2 (1%)	70	84
5	i	182/182 (100%)	180 (99%)	2 (1%)	70	84
5	i3	182/182 (100%)	181 (100%)	1 (0%)	86	92
6	K	152/152 (100%)	152 (100%)	0	100	100
6	K3	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	151 (99%)	1 (1%)	81	90
6	k3	152/152 (100%)	151 (99%)	1 (1%)	81	90
7	C	93/97 (96%)	92 (99%)	1 (1%)	70	84
7	C3	93/97 (96%)	92 (99%)	1 (1%)	70	84
7	c	93/97 (96%)	92 (99%)	1 (1%)	70	84
7	c3	93/97 (96%)	92 (99%)	1 (1%)	70	84
8	G	235/262 (90%)	234 (100%)	1 (0%)	89	94
8	G3	235/262 (90%)	234 (100%)	1 (0%)	89	94
8	g	235/262 (90%)	234 (100%)	1 (0%)	89	94
8	g3	235/262 (90%)	234 (100%)	1 (0%)	89	94
9	H	208/245 (85%)	207 (100%)	1 (0%)	86	92
9	H3	208/245 (85%)	207 (100%)	1 (0%)	86	92
9	h	208/245 (85%)	207 (100%)	1 (0%)	86	92
9	h3	208/245 (85%)	207 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	235/239 (98%)	234 (100%)	1 (0%)	89	94
10	J3	235/239 (98%)	234 (100%)	1 (0%)	89	94
10	j	235/239 (98%)	235 (100%)	0	100	100
10	j3	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	217 (99%)	2 (1%)	75	88
11	L3	219/220 (100%)	217 (99%)	2 (1%)	75	88
11	l	219/220 (100%)	218 (100%)	1 (0%)	86	92
11	l3	219/220 (100%)	218 (100%)	1 (0%)	86	92
12	M	202/202 (100%)	202 (100%)	0	100	100
12	M3	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	201 (100%)	1 (0%)	86	92
12	m3	202/202 (100%)	201 (100%)	1 (0%)	86	92
13	N	104/162 (64%)	104 (100%)	0	100	100
13	N3	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	103 (99%)	1 (1%)	73	86
13	n3	104/162 (64%)	103 (99%)	1 (1%)	73	86
14	O	89/142 (63%)	89 (100%)	0	100	100
14	O3	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
14	o3	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	131 (100%)	0	100	100
15	P3	131/133 (98%)	131 (100%)	0	100	100
15	p	131/133 (98%)	131 (100%)	0	100	100
15	p3	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100
16	Q3	97/135 (72%)	97 (100%)	0	100	100
16	q	97/135 (72%)	97 (100%)	0	100	100
16	q3	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	119 (99%)	1 (1%)	79	89
17	R3	120/129 (93%)	119 (99%)	1 (1%)	79	89
17	r	125/129 (97%)	124 (99%)	1 (1%)	79	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	r3	125/129 (97%)	124 (99%)	1 (1%)	79	89
18	S	112/131 (86%)	112 (100%)	0	100	100
18	S3	112/131 (86%)	112 (100%)	0	100	100
18	s	111/131 (85%)	109 (98%)	2 (2%)	54	76
18	s3	111/131 (85%)	109 (98%)	2 (2%)	54	76
19	E	359/414 (87%)	357 (99%)	2 (1%)	84	91
19	E3	359/414 (87%)	357 (99%)	2 (1%)	84	91
19	e	359/414 (87%)	358 (100%)	1 (0%)	91	95
19	e3	359/414 (87%)	358 (100%)	1 (0%)	91	95
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	61 (100%)	0	100	100
20	i4	64/101 (63%)	64 (100%)	0	100	100
20	i5	61/101 (60%)	61 (100%)	0	100	100
21	t	325/414 (78%)	322 (99%)	3 (1%)	75	88
21	t3	325/414 (78%)	322 (99%)	3 (1%)	75	88
22	G1	166/195 (85%)	166 (100%)	0	100	100
22	G2	166/195 (85%)	166 (100%)	0	100	100
22	G4	166/195 (85%)	166 (100%)	0	100	100
22	G5	166/195 (85%)	166 (100%)	0	100	100
23	g1	234/254 (92%)	230 (98%)	4 (2%)	56	78
23	g2	234/254 (92%)	231 (99%)	3 (1%)	65	82
23	g4	234/254 (92%)	230 (98%)	4 (2%)	56	78
23	g5	234/254 (92%)	231 (99%)	3 (1%)	65	82
24	A1	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	A2	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	A4	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	A5	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	B1	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	B2	422/453 (93%)	421 (100%)	1 (0%)	92	96
24	B4	422/453 (93%)	419 (99%)	3 (1%)	81	90
24	B5	422/453 (93%)	421 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	C1	424/453 (94%)	423 (100%)	1 (0%)	92	96
24	C2	424/453 (94%)	423 (100%)	1 (0%)	92	96
24	C4	424/453 (94%)	423 (100%)	1 (0%)	92	96
24	C5	424/453 (94%)	423 (100%)	1 (0%)	92	96
25	D1	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	D2	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	D4	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	D5	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	E1	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	E2	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	E4	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	E5	381/402 (95%)	380 (100%)	1 (0%)	91	95
25	F1	380/402 (94%)	380 (100%)	0	100	100
25	F2	380/402 (94%)	380 (100%)	0	100	100
25	F4	380/402 (94%)	380 (100%)	0	100	100
25	F5	380/402 (94%)	380 (100%)	0	100	100
26	H1	59/59 (100%)	59 (100%)	0	100	100
26	H2	59/59 (100%)	59 (100%)	0	100	100
26	H4	59/59 (100%)	59 (100%)	0	100	100
26	H5	59/59 (100%)	59 (100%)	0	100	100
26	I1	59/59 (100%)	57 (97%)	2 (3%)	32	62
26	I2	59/59 (100%)	59 (100%)	0	100	100
26	I4	59/59 (100%)	57 (97%)	2 (3%)	32	62
26	I5	59/59 (100%)	59 (100%)	0	100	100
26	J1	59/59 (100%)	59 (100%)	0	100	100
26	J2	59/59 (100%)	59 (100%)	0	100	100
26	J4	59/59 (100%)	59 (100%)	0	100	100
26	J5	59/59 (100%)	59 (100%)	0	100	100
26	K1	59/59 (100%)	59 (100%)	0	100	100
26	K2	59/59 (100%)	58 (98%)	1 (2%)	56	78
26	K4	59/59 (100%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	K5	59/59 (100%)	58 (98%)	1 (2%)	56	78
26	L1	59/59 (100%)	59 (100%)	0	100	100
26	L2	59/59 (100%)	59 (100%)	0	100	100
26	L4	59/59 (100%)	59 (100%)	0	100	100
26	L5	59/59 (100%)	59 (100%)	0	100	100
26	M1	59/59 (100%)	59 (100%)	0	100	100
26	M2	59/59 (100%)	59 (100%)	0	100	100
26	M4	59/59 (100%)	59 (100%)	0	100	100
26	M5	59/59 (100%)	59 (100%)	0	100	100
26	N1	59/59 (100%)	59 (100%)	0	100	100
26	N2	59/59 (100%)	59 (100%)	0	100	100
26	N4	59/59 (100%)	59 (100%)	0	100	100
26	N5	59/59 (100%)	59 (100%)	0	100	100
26	O1	59/59 (100%)	59 (100%)	0	100	100
26	O2	59/59 (100%)	59 (100%)	0	100	100
26	O4	59/59 (100%)	59 (100%)	0	100	100
26	O5	59/59 (100%)	59 (100%)	0	100	100
26	P1	59/59 (100%)	59 (100%)	0	100	100
26	P2	59/59 (100%)	59 (100%)	0	100	100
26	P4	59/59 (100%)	59 (100%)	0	100	100
26	P5	59/59 (100%)	59 (100%)	0	100	100
26	Q1	59/59 (100%)	59 (100%)	0	100	100
26	Q2	59/59 (100%)	59 (100%)	0	100	100
26	Q4	59/59 (100%)	59 (100%)	0	100	100
26	Q5	59/59 (100%)	59 (100%)	0	100	100
27	d1	117/139 (84%)	116 (99%)	1 (1%)	75	88
27	d2	117/139 (84%)	116 (99%)	1 (1%)	75	88
27	d4	117/139 (84%)	116 (99%)	1 (1%)	75	88
27	d5	117/139 (84%)	116 (99%)	1 (1%)	75	88
28	e1	57/60 (95%)	57 (100%)	0	100	100
28	e2	57/60 (95%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	e4	57/60 (95%)	57 (100%)	0	100	100
28	e5	57/60 (95%)	57 (100%)	0	100	100
All	All	29600/32320 (92%)	29477 (100%)	123 (0%)	88	94

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	247	TYR
1	a	364	LEU
4	f	31	TYR
4	f	37	THR
5	i	26	ARG
5	i	44	TYR
6	k	148	ASP
7	c	19	ARG
8	g	217	PHE
9	h	144	ASP
11	l	205	TRP
12	m	49	MET
13	n	87	HIS
17	r	28	GLN
18	s	44	VAL
18	s	67	LEU
19	e	391	LEU
1	A	247	TYR
1	A	364	LEU
4	F	31	TYR
5	I	44	TYR
5	I	90	HIS
7	C	19	ARG
8	G	217	PHE
9	H	144	ASP
10	J	82	ARG
11	L	118	ARG
11	L	205	TRP
17	R	19	LEU
19	E	350	TRP
19	E	391	LEU
21	t	135	GLU
21	t	140	THR
21	t	158	ARG

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Mol	Chain	Res	Type
23	g1	157	GLN
23	g1	194	TYR
23	g1	242	ASN
23	g1	272	LYS
24	C1	247	LEU
25	D1	437	PHE
24	B1	212	ASP
24	B1	275	PHE
24	B1	300	ASP
24	A1	221	PHE
24	A1	225	ASP
24	A1	414	MET
25	E1	386	HIS
26	I1	1	MET
26	I1	53	MET
27	d1	126	GLU
23	g2	157	GLN
23	g2	194	TYR
23	g2	242	ASN
24	C2	247	LEU
25	D2	437	PHE
24	B2	300	ASP
24	A2	221	PHE
24	A2	225	ASP
24	A2	414	MET
25	E2	386	HIS
26	K2	3	LEU
27	d2	126	GLU
1	a3	247	TYR
1	a3	364	LEU
4	f3	31	TYR
4	f3	37	THR
5	i3	44	TYR
6	k3	148	ASP
7	c3	19	ARG
8	g3	217	PHE
9	h3	144	ASP
11	l3	205	TRP
12	m3	49	MET
13	n3	87	HIS
17	r3	28	GLN
18	s3	44	VAL

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Mol	Chain	Res	Type
18	s3	67	LEU
19	e3	391	LEU
1	A3	247	TYR
1	A3	364	LEU
4	F3	31	TYR
5	I3	44	TYR
5	I3	90	HIS
7	C3	19	ARG
8	G3	217	PHE
9	H3	144	ASP
10	J3	82	ARG
11	L3	118	ARG
11	L3	205	TRP
17	R3	19	LEU
19	E3	350	TRP
19	E3	391	LEU
21	t3	135	GLU
21	t3	140	THR
21	t3	158	ARG
23	g4	157	GLN
23	g4	194	TYR
23	g4	242	ASN
23	g4	272	LYS
24	C4	247	LEU
25	D4	437	PHE
24	B4	212	ASP
24	B4	275	PHE
24	B4	300	ASP
24	A4	221	PHE
24	A4	225	ASP
24	A4	414	MET
25	E4	386	HIS
26	I4	1	MET
26	I4	53	MET
27	d4	126	GLU
23	g5	157	GLN
23	g5	194	TYR
23	g5	242	ASN
24	C5	247	LEU
25	D5	437	PHE
24	B5	300	ASP
24	A5	221	PHE

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Mol	Chain	Res	Type
24	A5	225	ASP
24	A5	414	MET
25	E5	386	HIS
26	K5	3	LEU
27	d5	126	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	124	HIS
1	a	399	GLN
4	f	4	HIS
9	h	171	HIS
9	h	260	HIS
11	l	50	GLN
11	l	95	ASN
11	l	194	GLN
11	l	217	HIS
12	m	215	HIS
19	e	165	ASN
19	e	361	ASN
1	A	391	HIS
2	B	255	ASN
3	D	29	GLN
4	F	81	ASN
5	I	20	ASN
5	I	201	ASN
5	I	209	GLN
9	H	101	GLN
9	H	171	HIS
10	J	130	GLN
12	M	3	ASN
15	P	150	GLN
16	Q	69	GLN
19	E	361	ASN
22	G1	161	GLN
22	G1	165	GLN
25	D1	145	GLN
24	A1	171	GLN
24	A1	436	GLN
25	E1	92	GLN
26	M1	40	ASN

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Mol	Chain	Res	Type
26	K1	50	ASN
27	d1	63	ASN
22	G2	161	GLN
22	G2	165	GLN
23	g2	242	ASN
24	A2	171	GLN
25	E2	92	GLN
26	M2	40	ASN
1	a3	124	HIS
1	a3	399	GLN
2	b3	255	ASN
9	h3	171	HIS
11	l3	50	GLN
12	m3	215	HIS
19	e3	361	ASN
2	B3	255	ASN
3	D3	29	GLN
5	I3	20	ASN
5	I3	201	ASN
5	I3	209	GLN
9	H3	101	GLN
9	H3	171	HIS
12	M3	3	ASN
15	P3	150	GLN
16	Q3	69	GLN
19	E3	165	ASN
19	E3	361	ASN
21	t3	349	HIS
22	G4	161	GLN
22	G4	165	GLN
23	g4	242	ASN
25	D4	145	GLN
24	A4	171	GLN
25	E4	92	GLN
26	K4	50	ASN
27	d4	62	GLN
27	d4	63	ASN
22	G5	161	GLN
22	G5	165	GLN
23	g5	242	ASN
24	A5	171	GLN
25	E5	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 140 ligands modelled in this entry, 24 are monoatomic - leaving 116 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$
35	PEE	l3	302	-	47,47,50	1.17	6 (12%)	50,52,55	1.21	2 (4%)
33	ATP	g	301	34	26,33,33	4.79	8 (30%)	31,52,52	2.45	7 (22%)
35	PEE	a3	503	-	47,47,50	1.17	6 (12%)	50,52,55	1.17	4 (8%)
30	PC1	G3	304	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
37	ADP	B2	1002	34	24,29,29	3.71	9 (37%)	29,45,45	3.57	6 (20%)
29	CDL	g3	305	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
29	CDL	F	303	-	99,99,99	0.87	6 (6%)	105,111,111	1.08	4 (3%)
29	CDL	a3	501	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	5 (4%)
29	CDL	A3	501	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
31	PO4	F	301	-	4,4,4	0.99	0	6,6,6	0.45	0
35	PEE	m	301	-	50,50,50	1.14	6 (12%)	53,55,55	1.10	4 (7%)
29	CDL	B3	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
35	PEE	A	501	-	47,47,50	1.18	6 (12%)	50,52,55	1.21	2 (4%)
29	CDL	B	403	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	l3	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
33	ATP	G3	301	34	26,33,33	4.77	8 (30%)	31,52,52	2.47	7 (22%)
33	ATP	B4	1003	34	26,33,33	4.79	8 (30%)	31,52,52	2.44	8 (25%)
35	PEE	j3	303	-	50,50,50	1.14	6 (12%)	53,55,55	1.10	5 (9%)
29	CDL	K	202	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
30	PC1	d	301	-	53,53,53	0.94	4 (7%)	59,61,61	1.07	2 (3%)
30	PC1	G	304	-	53,53,53	0.95	4 (7%)	59,61,61	0.98	2 (3%)
33	ATP	C2	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.42	7 (22%)
29	CDL	K3	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	k	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
37	ADP	D2	501	34	24,29,29	3.69	9 (37%)	29,45,45	3.54	7 (24%)
29	CDL	b	401	-	99,99,99	0.87	7 (7%)	105,111,111	1.10	4 (3%)
32	UQ8	i3	303	-	53,53,53	1.79	7 (13%)	64,67,67	1.61	16 (25%)
37	ADP	D5	501	34	24,29,29	3.69	9 (37%)	29,45,45	3.55	7 (24%)
33	ATP	B1	1003	34	26,33,33	4.80	8 (30%)	31,52,52	2.45	8 (25%)
29	CDL	P	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.02	5 (4%)
29	CDL	J	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	i3	301	-	99,99,99	0.87	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	a	501	-	99,99,99	0.88	8 (8%)	105,111,111	1.06	5 (4%)
29	CDL	l3	303	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	k3	201	-	99,99,99	0.89	6 (6%)	105,111,111	1.02	4 (3%)
37	ADP	B1	1002	34	24,29,29	3.71	9 (37%)	29,45,45	3.58	7 (24%)
32	UQ8	i	302	-	53,53,53	1.81	7 (13%)	64,67,67	1.60	16 (25%)
29	CDL	B	402	-	99,99,99	0.87	8 (8%)	105,111,111	1.12	5 (4%)
29	CDL	A	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
33	ATP	C1	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.40	7 (22%)
29	CDL	B3	403	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
35	PEE	L3	302	-	50,50,50	1.15	6 (12%)	53,55,55	1.15	4 (7%)
30	PC1	g3	304	-	53,53,53	0.95	4 (7%)	59,61,61	0.93	2 (3%)
31	PO4	f	301	-	4,4,4	0.96	0	6,6,6	0.41	0
29	CDL	l3	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
30	PC1	g	303	-	53,53,53	0.95	4 (7%)	59,61,61	0.98	2 (3%)
30	PC1	g	304	-	53,53,53	0.95	4 (7%)	59,61,61	0.96	2 (3%)
31	PO4	f3	301	-	4,4,4	0.98	0	6,6,6	0.45	0
33	ATP	g3	301	34	26,33,33	4.78	7 (26%)	31,52,52	2.46	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	B	404	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	5 (4%)
29	CDL	f	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
29	CDL	J3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	a3	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	5 (4%)
29	CDL	B3	402	-	99,99,99	0.87	7 (7%)	105,111,111	1.12	5 (4%)
33	ATP	A1	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.41	7 (22%)
33	ATP	A4	601	34	26,33,33	4.80	8 (30%)	31,52,52	2.42	7 (22%)
33	ATP	A5	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.40	7 (22%)
30	PC1	g3	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
30	PC1	d3	301	-	53,53,53	0.94	4 (7%)	59,61,61	1.07	2 (3%)
37	ADP	B4	1002	34	24,29,29	3.71	9 (37%)	29,45,45	3.57	7 (24%)
36	NAD	e	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.16	7 (14%)
36	NAD	E	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.14	7 (14%)
29	CDL	f	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	5 (4%)
29	CDL	I3	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	J3	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.03	4 (3%)
29	CDL	P3	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)
29	CDL	L	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
33	ATP	B2	1003	34	26,33,33	4.81	8 (30%)	31,52,52	2.44	8 (25%)
32	UQ8	I3	304	-	53,53,53	1.81	7 (13%)	64,67,67	1.65	15 (23%)
36	NAD	E3	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.15	7 (14%)
29	CDL	f3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
33	ATP	A2	601	34	26,33,33	4.81	8 (30%)	31,52,52	2.42	7 (22%)
35	PEE	L	303	-	47,47,50	1.17	6 (12%)	50,52,55	1.17	3 (6%)
31	PO4	F3	301	-	4,4,4	0.96	0	6,6,6	0.42	0
29	CDL	L3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	l	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	3 (2%)
30	PC1	G3	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	B	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.97	4 (3%)
29	CDL	F3	302	-	99,99,99	0.88	6 (6%)	105,111,111	1.08	4 (3%)
32	UQ8	I	303	-	53,53,53	1.80	7 (13%)	64,67,67	1.67	15 (23%)
29	CDL	j	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.04	4 (3%)
29	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	f	304	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	l	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.04	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	L	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.04	4 (3%)
33	ATP	G	301	34	26,33,33	4.77	7 (26%)	31,52,52	2.48	7 (22%)
29	CDL	j3	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	g	305	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	j	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	p3	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	r	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
37	ADP	D4	501	34	24,29,29	3.66	9 (37%)	29,45,45	3.79	7 (24%)
29	CDL	I	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
30	PC1	D3	301	-	53,53,53	0.93	4 (7%)	59,61,61	1.09	2 (3%)
29	CDL	F	302	-	99,99,99	0.87	8 (8%)	105,111,111	1.02	5 (4%)
36	NAD	e3	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.16	7 (14%)
37	ADP	D1	501	34	24,29,29	3.66	9 (37%)	29,45,45	3.80	7 (24%)
33	ATP	B5	1003	34	26,33,33	4.80	9 (34%)	31,52,52	2.45	8 (25%)
33	ATP	C4	601	34	26,33,33	4.78	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	f3	304	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
30	PC1	G	303	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	j3	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
33	ATP	C5	601	34	26,33,33	4.81	8 (30%)	31,52,52	2.42	7 (22%)
29	CDL	i	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	4 (3%)
35	PEE	J	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.15	4 (7%)
29	CDL	b3	401	-	99,99,99	0.88	7 (7%)	105,111,111	1.12	4 (3%)
29	CDL	K3	202	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
30	PC1	D	301	-	53,53,53	0.94	4 (7%)	59,61,61	1.08	2 (3%)
29	CDL	B3	404	-	99,99,99	0.89	8 (8%)	105,111,111	1.11	5 (4%)
29	CDL	I3	302	-	99,99,99	0.88	6 (6%)	105,111,111	1.02	4 (3%)
29	CDL	f3	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
29	CDL	J	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	i3	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	I	301	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
29	CDL	K	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
37	ADP	B5	1002	34	24,29,29	3.71	9 (37%)	29,45,45	3.58	6 (20%)

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
35	PEE	l3	302	-	-	21/51/51/54	-
33	ATP	g	301	34	-	0/18/38/38	0/3/3/3
35	PEE	a3	503	-	-	22/51/51/54	-
30	PC1	G3	304	-	-	19/57/57/57	-
37	ADP	B2	1002	34	-	2/12/32/32	0/3/3/3
29	CDL	g3	305	-	-	36/110/110/110	-
29	CDL	F	303	-	-	46/110/110/110	-
29	CDL	a3	501	-	-	34/110/110/110	-
29	CDL	A3	501	-	-	46/110/110/110	-
35	PEE	m	301	-	-	24/54/54/54	-
29	CDL	B3	401	-	-	44/110/110/110	-
35	PEE	A	501	-	-	21/51/51/54	-
29	CDL	B	403	-	-	33/110/110/110	-
29	CDL	l3	301	-	-	39/110/110/110	-
33	ATP	G3	301	34	-	0/18/38/38	0/3/3/3
33	ATP	B4	1003	34	-	2/18/38/38	0/3/3/3
35	PEE	j3	303	-	-	23/54/54/54	-
29	CDL	K	202	-	-	35/110/110/110	-
30	PC1	d	301	-	-	23/57/57/57	-
30	PC1	G	304	-	-	19/57/57/57	-
33	ATP	C2	601	34	-	4/18/38/38	0/3/3/3
29	CDL	K3	201	-	-	28/110/110/110	-
29	CDL	k	201	-	-	37/110/110/110	-
37	ADP	D2	501	34	-	2/12/32/32	0/3/3/3
29	CDL	b	401	-	-	44/110/110/110	-
32	UQ8	i3	303	-	-	8/51/75/75	0/1/1/1
37	ADP	D5	501	34	-	2/12/32/32	0/3/3/3
33	ATP	B1	1003	34	-	2/18/38/38	0/3/3/3
29	CDL	P	201	-	-	35/110/110/110	-
29	CDL	J	302	-	-	38/110/110/110	-
29	CDL	i3	301	-	-	36/110/110/110	-
29	CDL	a	501	-	-	34/110/110/110	-
29	CDL	I3	303	-	-	38/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	k3	201	-	-	38/110/110/110	-
37	ADP	B1	1002	34	-	1/12/32/32	0/3/3/3
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
29	CDL	B	402	-	-	39/110/110/110	-
29	CDL	A	502	-	-	46/110/110/110	-
33	ATP	C1	601	34	-	5/18/38/38	0/3/3/3
29	CDL	B3	403	-	-	33/110/110/110	-
35	PEE	L3	302	-	-	29/54/54/54	-
30	PC1	g3	304	-	-	18/57/57/57	-
29	CDL	l3	303	-	-	41/110/110/110	-
30	PC1	g	303	-	-	21/57/57/57	-
30	PC1	g	304	-	-	20/57/57/57	-
33	ATP	g3	301	34	-	0/18/38/38	0/3/3/3
29	CDL	B	404	-	-	46/110/110/110	-
29	CDL	f	302	-	-	54/110/110/110	-
29	CDL	J3	302	-	-	40/110/110/110	-
29	CDL	a3	502	-	-	39/110/110/110	-
29	CDL	B3	402	-	-	40/110/110/110	-
33	ATP	A1	601	34	-	5/18/38/38	0/3/3/3
33	ATP	A4	601	34	-	5/18/38/38	0/3/3/3
33	ATP	A5	601	34	-	5/18/38/38	0/3/3/3
30	PC1	g3	303	-	-	21/57/57/57	-
30	PC1	d3	301	-	-	23/57/57/57	-
37	ADP	B4	1002	34	-	1/12/32/32	0/3/3/3
36	NAD	e	900	-	-	6/26/62/62	0/5/5/5
36	NAD	E	900	-	-	8/26/62/62	0/5/5/5
29	CDL	f	303	-	-	41/110/110/110	-
29	CDL	I3	301	-	-	42/110/110/110	-
29	CDL	J3	301	-	-	42/110/110/110	-
29	CDL	P3	201	-	-	37/110/110/110	-
29	CDL	L	301	-	-	37/110/110/110	-
33	ATP	B2	1003	34	-	2/18/38/38	0/3/3/3
32	UQ8	I3	304	-	-	9/51/75/75	0/1/1/1
36	NAD	E3	900	-	-	7/26/62/62	0/5/5/5
29	CDL	f3	302	-	-	54/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ATP	A2	601	34	-	5/18/38/38	0/3/3/3
35	PEE	L	303	-	-	22/51/51/54	-
29	CDL	L3	301	-	-	38/110/110/110	-
29	CDL	l	302	-	-	41/110/110/110	-
30	PC1	G3	303	-	-	28/57/57/57	-
29	CDL	B	401	-	-	44/110/110/110	-
29	CDL	F3	302	-	-	45/110/110/110	-
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
29	CDL	j	301	-	-	40/110/110/110	-
29	CDL	p	201	-	-	45/110/110/110	-
29	CDL	f	304	-	-	49/110/110/110	-
29	CDL	l	301	-	-	38/110/110/110	-
29	CDL	L	302	-	-	45/110/110/110	-
33	ATP	G	301	34	-	0/18/38/38	0/3/3/3
29	CDL	j3	302	-	-	40/110/110/110	-
29	CDL	g	305	-	-	36/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
29	CDL	p3	201	-	-	44/110/110/110	-
29	CDL	r	201	-	-	36/110/110/110	-
37	ADP	D4	501	34	-	2/12/32/32	0/3/3/3
29	CDL	I	302	-	-	38/110/110/110	-
30	PC1	D3	301	-	-	22/57/57/57	-
29	CDL	F	302	-	-	39/110/110/110	-
36	NAD	e3	900	-	-	7/26/62/62	0/5/5/5
37	ADP	D1	501	34	-	2/12/32/32	0/3/3/3
33	ATP	B5	1003	34	-	2/18/38/38	0/3/3/3
33	ATP	C4	601	34	-	5/18/38/38	0/3/3/3
29	CDL	f3	304	-	-	48/110/110/110	-
30	PC1	G	303	-	-	29/57/57/57	-
29	CDL	j3	301	-	-	40/110/110/110	-
33	ATP	C5	601	34	-	4/18/38/38	0/3/3/3
29	CDL	i	301	-	-	39/110/110/110	-
35	PEE	J	303	-	-	29/54/54/54	-
29	CDL	b3	401	-	-	44/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	K3	202	-	-	35/110/110/110	-
30	PC1	D	301	-	-	22/57/57/57	-
29	CDL	B3	404	-	-	46/110/110/110	-
29	CDL	I3	302	-	-	45/110/110/110	-
29	CDL	f3	303	-	-	41/110/110/110	-
29	CDL	J	301	-	-	42/110/110/110	-
29	CDL	i3	302	-	-	38/110/110/110	-
29	CDL	I	301	-	-	43/110/110/110	-
29	CDL	K	201	-	-	28/110/110/110	-
37	ADP	B5	1002	34	-	2/12/32/32	0/3/3/3

All (855) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C5	601	ATP	C2'-C1'	-17.26	1.27	1.53
33	B2	1003	ATP	C2'-C1'	-17.25	1.27	1.53
33	A1	601	ATP	C2'-C1'	-17.22	1.27	1.53
33	A5	601	ATP	C2'-C1'	-17.19	1.27	1.53
33	B5	1003	ATP	C2'-C1'	-17.15	1.27	1.53
33	B1	1003	ATP	C2'-C1'	-17.15	1.27	1.53
33	C2	601	ATP	C2'-C1'	-17.14	1.27	1.53
33	A4	601	ATP	C2'-C1'	-17.10	1.27	1.53
33	g	301	ATP	C2'-C1'	-17.10	1.27	1.53
33	C1	601	ATP	C2'-C1'	-17.09	1.27	1.53
33	A2	601	ATP	C2'-C1'	-17.09	1.27	1.53
33	B4	1003	ATP	C2'-C1'	-17.08	1.27	1.53
33	g3	301	ATP	C2'-C1'	-17.01	1.28	1.53
33	G3	301	ATP	C2'-C1'	-17.00	1.28	1.53
33	G	301	ATP	C2'-C1'	-16.99	1.28	1.53
33	C4	601	ATP	C2'-C1'	-16.98	1.28	1.53
33	A2	601	ATP	O4'-C1'	11.52	1.57	1.41
33	A1	601	ATP	O4'-C1'	11.50	1.57	1.41
33	A5	601	ATP	O4'-C1'	11.49	1.57	1.41
33	C1	601	ATP	O4'-C1'	11.45	1.57	1.41
33	C4	601	ATP	O4'-C1'	11.43	1.57	1.41
33	g3	301	ATP	O4'-C1'	11.42	1.57	1.41
33	A4	601	ATP	O4'-C1'	11.39	1.57	1.41
33	B1	1003	ATP	O4'-C1'	11.36	1.56	1.41
33	C2	601	ATP	O4'-C1'	11.36	1.56	1.41
33	B5	1003	ATP	O4'-C1'	11.36	1.56	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	G	301	ATP	O4'-C1'	11.35	1.56	1.41
33	B4	1003	ATP	O4'-C1'	11.35	1.56	1.41
33	g	301	ATP	O4'-C1'	11.33	1.56	1.41
33	B2	1003	ATP	O4'-C1'	11.32	1.56	1.41
33	C5	601	ATP	O4'-C1'	11.31	1.56	1.41
33	G3	301	ATP	O4'-C1'	11.27	1.56	1.41
37	D2	501	ADP	C2'-C3'	-10.53	1.24	1.53
37	D5	501	ADP	C2'-C3'	-10.48	1.24	1.53
37	B2	1002	ADP	C2'-C3'	-10.46	1.24	1.53
37	D1	501	ADP	C2'-C3'	-10.46	1.24	1.53
37	B4	1002	ADP	C2'-C3'	-10.45	1.24	1.53
37	D4	501	ADP	C2'-C3'	-10.43	1.24	1.53
37	B1	1002	ADP	C2'-C3'	-10.42	1.24	1.53
37	B5	1002	ADP	C2'-C3'	-10.40	1.24	1.53
36	e	900	NAD	O4D-C1D	-9.86	1.27	1.41
32	I3	304	UQ8	C6-C1	9.83	1.53	1.35
36	E3	900	NAD	O4D-C1D	-9.82	1.27	1.41
32	i	302	UQ8	C6-C1	9.82	1.53	1.35
36	e3	900	NAD	O4D-C1D	-9.75	1.27	1.41
36	E	900	NAD	O4D-C1D	-9.75	1.27	1.41
32	i3	303	UQ8	C6-C1	9.69	1.52	1.35
32	I	303	UQ8	C6-C1	9.65	1.52	1.35
33	g3	301	ATP	C3'-C4'	-9.60	1.28	1.53
33	G	301	ATP	C3'-C4'	-9.55	1.28	1.53
33	g	301	ATP	C3'-C4'	-9.55	1.28	1.53
33	G3	301	ATP	C3'-C4'	-9.53	1.28	1.53
33	A4	601	ATP	C3'-C4'	-9.51	1.28	1.53
33	A2	601	ATP	C3'-C4'	-9.49	1.28	1.53
33	A1	601	ATP	C3'-C4'	-9.48	1.28	1.53
33	A5	601	ATP	C3'-C4'	-9.47	1.28	1.53
33	C4	601	ATP	C3'-C4'	-9.46	1.28	1.53
33	C1	601	ATP	C3'-C4'	-9.42	1.28	1.53
33	C2	601	ATP	C3'-C4'	-9.41	1.29	1.53
33	B1	1003	ATP	C3'-C4'	-9.40	1.29	1.53
33	B4	1003	ATP	C3'-C4'	-9.38	1.29	1.53
33	C5	601	ATP	C3'-C4'	-9.38	1.29	1.53
33	B5	1003	ATP	C3'-C4'	-9.38	1.29	1.53
33	B2	1003	ATP	C3'-C4'	-9.35	1.29	1.53
36	E3	900	NAD	C3B-C4B	-9.15	1.29	1.53
36	e	900	NAD	C3B-C4B	-9.10	1.29	1.53
36	E	900	NAD	C3B-C4B	-9.10	1.29	1.53
36	e3	900	NAD	C3B-C4B	-9.10	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	900	NAD	C7N-N7N	8.49	1.49	1.33
36	e3	900	NAD	C7N-N7N	8.46	1.49	1.33
36	E3	900	NAD	C7N-N7N	8.45	1.49	1.33
36	E	900	NAD	C7N-N7N	8.42	1.49	1.33
36	e3	900	NAD	C3D-C4D	-8.41	1.31	1.53
36	E	900	NAD	C3D-C4D	-8.39	1.31	1.53
36	E3	900	NAD	C3D-C4D	-8.35	1.31	1.53
36	e	900	NAD	C3D-C4D	-8.33	1.31	1.53
37	B2	1002	ADP	O4'-C1'	7.97	1.52	1.41
37	B5	1002	ADP	O4'-C1'	7.95	1.52	1.41
37	B4	1002	ADP	O4'-C1'	7.93	1.52	1.41
37	B1	1002	ADP	O4'-C1'	7.91	1.52	1.41
37	D5	501	ADP	O4'-C1'	7.90	1.52	1.41
37	D2	501	ADP	O4'-C1'	7.88	1.52	1.41
37	D1	501	ADP	O4'-C1'	7.70	1.51	1.41
37	D4	501	ADP	O4'-C1'	7.69	1.51	1.41
36	e3	900	NAD	O4B-C4B	7.68	1.62	1.45
36	E	900	NAD	O4B-C4B	7.63	1.62	1.45
36	e	900	NAD	O4B-C4B	7.63	1.62	1.45
36	E3	900	NAD	O4B-C4B	7.59	1.62	1.45
36	E	900	NAD	O4D-C4D	7.44	1.61	1.45
36	e3	900	NAD	O4D-C4D	7.42	1.61	1.45
36	e	900	NAD	O4D-C4D	7.39	1.61	1.45
36	E3	900	NAD	O4D-C4D	7.37	1.61	1.45
37	B5	1002	ADP	O4'-C4'	-6.46	1.30	1.45
37	B4	1002	ADP	O4'-C4'	-6.46	1.30	1.45
37	B2	1002	ADP	O4'-C4'	-6.45	1.30	1.45
37	B1	1002	ADP	O4'-C4'	-6.43	1.30	1.45
37	D1	501	ADP	O4'-C4'	-6.40	1.30	1.45
37	D4	501	ADP	O4'-C4'	-6.39	1.30	1.45
36	E3	900	NAD	O4B-C1B	-6.30	1.32	1.41
37	D5	501	ADP	O4'-C4'	-6.30	1.30	1.45
36	e	900	NAD	O4B-C1B	-6.27	1.32	1.41
36	E	900	NAD	O4B-C1B	-6.24	1.32	1.41
37	D2	501	ADP	O4'-C4'	-6.24	1.31	1.45
36	e3	900	NAD	O4B-C1B	-6.22	1.32	1.41
37	D5	501	ADP	C3'-C4'	5.95	1.68	1.53
37	D2	501	ADP	C3'-C4'	5.94	1.68	1.53
37	D4	501	ADP	C3'-C4'	5.86	1.68	1.53
37	D1	501	ADP	C3'-C4'	5.81	1.67	1.53
37	B5	1002	ADP	C3'-C4'	5.80	1.67	1.53
37	B4	1002	ADP	C3'-C4'	5.78	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B1	1002	ADP	C3'-C4'	5.77	1.67	1.53
37	B2	1002	ADP	C3'-C4'	5.76	1.67	1.53
37	B1	1002	ADP	C2'-C1'	5.40	1.62	1.53
37	B5	1002	ADP	C2'-C1'	5.38	1.61	1.53
37	B4	1002	ADP	C2'-C1'	5.29	1.61	1.53
37	B2	1002	ADP	C2'-C1'	5.28	1.61	1.53
37	D5	501	ADP	C2'-C1'	5.01	1.61	1.53
37	D2	501	ADP	C2'-C1'	4.97	1.61	1.53
37	D1	501	ADP	C2'-C1'	4.89	1.61	1.53
36	E3	900	NAD	C3N-C7N	4.86	1.57	1.50
37	D4	501	ADP	C2'-C1'	4.84	1.61	1.53
33	B5	1003	ATP	C2'-C3'	4.82	1.66	1.53
33	B1	1003	ATP	C2'-C3'	4.80	1.66	1.53
36	e	900	NAD	C3N-C7N	4.79	1.57	1.50
36	e3	900	NAD	C3N-C7N	4.79	1.57	1.50
36	E	900	NAD	C3N-C7N	4.78	1.57	1.50
33	B2	1003	ATP	C2'-C3'	4.78	1.66	1.53
33	B4	1003	ATP	C2'-C3'	4.78	1.66	1.53
33	A2	601	ATP	C2'-C3'	4.77	1.66	1.53
33	C2	601	ATP	C2'-C3'	4.77	1.66	1.53
33	C5	601	ATP	C2'-C3'	4.76	1.66	1.53
33	C1	601	ATP	C2'-C3'	4.75	1.66	1.53
33	A4	601	ATP	C2'-C3'	4.74	1.66	1.53
33	C5	601	ATP	O4'-C4'	4.74	1.55	1.45
33	B2	1003	ATP	O4'-C4'	4.74	1.55	1.45
33	C4	601	ATP	C2'-C3'	4.74	1.66	1.53
33	A5	601	ATP	C2'-C3'	4.73	1.66	1.53
33	A4	601	ATP	O4'-C4'	4.72	1.55	1.45
33	A1	601	ATP	O4'-C4'	4.72	1.55	1.45
33	B1	1003	ATP	O4'-C4'	4.71	1.55	1.45
33	A1	601	ATP	C2'-C3'	4.70	1.66	1.53
33	C2	601	ATP	O4'-C4'	4.70	1.55	1.45
33	B4	1003	ATP	O4'-C4'	4.70	1.55	1.45
33	G	301	ATP	C2'-C3'	4.69	1.66	1.53
33	A5	601	ATP	O4'-C4'	4.69	1.55	1.45
33	G3	301	ATP	C2'-C3'	4.69	1.66	1.53
33	B5	1003	ATP	O4'-C4'	4.68	1.55	1.45
33	g	301	ATP	C2'-C3'	4.67	1.66	1.53
33	C1	601	ATP	O4'-C4'	4.66	1.55	1.45
33	C4	601	ATP	O4'-C4'	4.66	1.55	1.45
33	A2	601	ATP	O4'-C4'	4.65	1.55	1.45
33	g3	301	ATP	C2'-C3'	4.63	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e3	900	NAD	O3D-C3D	4.55	1.53	1.43
36	E3	900	NAD	O3D-C3D	4.55	1.53	1.43
36	E	900	NAD	O3D-C3D	4.53	1.53	1.43
36	e	900	NAD	O3D-C3D	4.51	1.53	1.43
33	g	301	ATP	O4'-C4'	4.50	1.55	1.45
33	G3	301	ATP	O4'-C4'	4.47	1.55	1.45
33	g3	301	ATP	O4'-C4'	4.44	1.54	1.45
33	G	301	ATP	O4'-C4'	4.43	1.54	1.45
36	E	900	NAD	C6A-N6A	4.23	1.49	1.34
36	e3	900	NAD	C6A-N6A	4.23	1.49	1.34
36	e	900	NAD	C6A-N6A	4.20	1.49	1.34
36	E3	900	NAD	C6A-N6A	4.19	1.49	1.34
32	I	303	UQ8	C4-C3	4.13	1.53	1.36
32	i3	303	UQ8	C4-C3	4.11	1.53	1.36
32	I3	304	UQ8	C4-C3	4.07	1.52	1.36
32	i	302	UQ8	C4-C3	4.04	1.52	1.36
37	B2	1002	ADP	O2'-C2'	3.87	1.52	1.43
37	D4	501	ADP	O2'-C2'	3.86	1.52	1.43
37	B4	1002	ADP	O2'-C2'	3.85	1.52	1.43
37	B1	1002	ADP	O2'-C2'	3.84	1.52	1.43
37	D5	501	ADP	O2'-C2'	3.84	1.52	1.43
37	D1	501	ADP	O2'-C2'	3.84	1.52	1.43
37	D2	501	ADP	O2'-C2'	3.83	1.52	1.43
37	B5	1002	ADP	O2'-C2'	3.82	1.52	1.43
35	J	303	PEE	C18-C19	3.72	1.53	1.31
35	m	301	PEE	C18-C19	3.70	1.53	1.31
35	j3	303	PEE	C18-C19	3.70	1.53	1.31
35	j3	303	PEE	C39-C38	3.70	1.53	1.31
35	A	501	PEE	C39-C38	3.70	1.53	1.31
35	m	301	PEE	C39-C38	3.70	1.53	1.31
35	a3	503	PEE	C39-C38	3.69	1.53	1.31
35	L3	302	PEE	C18-C19	3.69	1.53	1.31
35	L3	302	PEE	C39-C38	3.68	1.53	1.31
35	A	501	PEE	C18-C19	3.68	1.53	1.31
35	l3	302	PEE	C18-C19	3.67	1.53	1.31
35	J	303	PEE	C39-C38	3.67	1.53	1.31
35	l3	302	PEE	C39-C38	3.67	1.53	1.31
35	L	303	PEE	C39-C38	3.65	1.52	1.31
35	a3	503	PEE	C18-C19	3.65	1.52	1.31
35	L	303	PEE	C18-C19	3.65	1.52	1.31
33	A4	601	ATP	C6-N6	3.31	1.46	1.34
33	C1	601	ATP	C6-N6	3.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A1	601	ATP	C6-N6	3.30	1.46	1.34
33	A2	601	ATP	C6-N6	3.29	1.46	1.34
33	B2	1003	ATP	C6-N6	3.29	1.46	1.34
33	A5	601	ATP	C6-N6	3.29	1.46	1.34
33	B5	1003	ATP	C6-N6	3.29	1.46	1.34
33	C5	601	ATP	C6-N6	3.29	1.46	1.34
33	B1	1003	ATP	C6-N6	3.28	1.46	1.34
33	B4	1003	ATP	C6-N6	3.28	1.46	1.34
33	C4	601	ATP	C6-N6	3.28	1.46	1.34
37	D2	501	ADP	C5-C4	-3.27	1.32	1.40
37	B1	1002	ADP	C5-C4	-3.27	1.32	1.40
37	B5	1002	ADP	C5-C4	-3.26	1.32	1.40
33	C2	601	ATP	C6-N6	3.26	1.45	1.34
37	D5	501	ADP	C5-C4	-3.25	1.32	1.40
33	g3	301	ATP	C6-N6	3.25	1.45	1.34
33	G	301	ATP	C6-N6	3.25	1.45	1.34
37	B2	1002	ADP	C5-C4	-3.24	1.32	1.40
37	B4	1002	ADP	C5-C4	-3.24	1.32	1.40
37	D4	501	ADP	C5-C4	-3.24	1.32	1.40
33	G3	301	ATP	C6-N6	3.23	1.45	1.34
33	g	301	ATP	C6-N6	3.23	1.45	1.34
36	E	900	NAD	O3B-C3B	3.21	1.50	1.43
36	e3	900	NAD	O3B-C3B	3.21	1.50	1.43
37	D1	501	ADP	C5-C4	-3.20	1.32	1.40
36	e	900	NAD	O3B-C3B	3.19	1.50	1.43
37	B5	1002	ADP	C6-N6	3.19	1.45	1.34
37	B1	1002	ADP	C6-N6	3.19	1.45	1.34
37	D2	501	ADP	C6-N6	3.18	1.45	1.34
37	B2	1002	ADP	C6-N6	3.18	1.45	1.34
37	B4	1002	ADP	C6-N6	3.18	1.45	1.34
36	E3	900	NAD	O3B-C3B	3.18	1.50	1.43
37	D5	501	ADP	C6-N6	3.17	1.45	1.34
37	D4	501	ADP	C6-N6	3.15	1.45	1.34
37	D1	501	ADP	C6-N6	3.14	1.45	1.34
29	I3	302	CDL	OA6-CA4	-2.83	1.39	1.46
29	L	302	CDL	OA6-CA4	-2.78	1.39	1.46
36	e3	900	NAD	O2B-C2B	-2.77	1.36	1.43
29	I3	301	CDL	OA6-CA4	-2.75	1.39	1.46
29	A3	501	CDL	OA6-CA4	-2.75	1.39	1.46
29	f3	304	CDL	OB6-CB4	-2.74	1.39	1.46
36	E	900	NAD	O2B-C2B	-2.74	1.36	1.43
29	l	301	CDL	OA6-CA4	-2.73	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E3	900	NAD	O2B-C2B	-2.71	1.36	1.43
29	A	502	CDL	OA6-CA4	-2.71	1.39	1.46
36	E	900	NAD	C2N-N1N	2.71	1.38	1.35
29	f	304	CDL	OB6-CB4	-2.71	1.39	1.46
29	a3	501	CDL	OA6-CA4	-2.71	1.39	1.46
29	a	501	CDL	OB6-CB4	-2.70	1.39	1.46
29	a	501	CDL	OA6-CA4	-2.70	1.39	1.46
33	g	301	ATP	C5-C4	-2.70	1.33	1.40
29	b	401	CDL	OA6-CA4	-2.70	1.39	1.46
33	G	301	ATP	C5-C4	-2.69	1.33	1.40
33	g3	301	ATP	C5-C4	-2.69	1.33	1.40
29	b3	401	CDL	OA6-CA4	-2.68	1.39	1.46
29	J	301	CDL	OA6-CA4	-2.68	1.39	1.46
36	e	900	NAD	O2B-C2B	-2.68	1.36	1.43
29	g	305	CDL	OA6-CA4	-2.68	1.39	1.46
29	J3	301	CDL	OA6-CA4	-2.68	1.39	1.46
36	e	900	NAD	C2N-N1N	2.67	1.38	1.35
29	i3	302	CDL	OA6-CA4	-2.67	1.39	1.46
36	e3	900	NAD	C2N-N1N	2.66	1.38	1.35
33	G3	301	ATP	C5-C4	-2.66	1.33	1.40
29	f3	302	CDL	OB6-CB4	-2.66	1.39	1.46
29	j	301	CDL	OA6-CA4	-2.66	1.39	1.46
36	E3	900	NAD	C2N-N1N	2.65	1.38	1.35
29	j3	301	CDL	OA6-CA4	-2.64	1.40	1.46
29	a3	501	CDL	OB6-CB4	-2.64	1.40	1.46
29	K	202	CDL	OA6-CA4	-2.63	1.40	1.46
29	l3	301	CDL	OB6-CB4	-2.63	1.40	1.46
29	I	302	CDL	OA6-CA4	-2.63	1.40	1.46
33	A2	601	ATP	C5-C4	-2.62	1.34	1.40
29	K3	202	CDL	OA6-CA4	-2.62	1.40	1.46
33	A1	601	ATP	C5-C4	-2.61	1.34	1.40
29	f	302	CDL	OB6-CB4	-2.61	1.40	1.46
29	F	302	CDL	OB6-CB4	-2.61	1.40	1.46
29	I3	302	CDL	OB6-CB4	-2.61	1.40	1.46
29	I	301	CDL	OB6-CB4	-2.61	1.40	1.46
36	e	900	NAD	C2A-N1A	2.61	1.38	1.33
29	b3	401	CDL	OB6-CB4	-2.61	1.40	1.46
29	b	401	CDL	OB6-CB4	-2.61	1.40	1.46
33	C5	601	ATP	C5-C4	-2.61	1.34	1.40
29	i3	301	CDL	OB6-CB4	-2.61	1.40	1.46
29	B	402	CDL	OB6-CB4	-2.60	1.40	1.46
33	A4	601	ATP	C5-C4	-2.60	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	403	CDL	OB6-CB4	-2.60	1.40	1.46
29	A3	501	CDL	OB6-CB4	-2.60	1.40	1.46
29	l	301	CDL	OB6-CB4	-2.60	1.40	1.46
35	j3	303	PEE	O2-C2	-2.60	1.40	1.46
33	C2	601	ATP	C5-C4	-2.60	1.34	1.40
29	r	201	CDL	OB6-CB4	-2.60	1.40	1.46
29	B3	402	CDL	OA6-CA4	-2.59	1.40	1.46
30	g	304	PC1	O21-C2	-2.59	1.40	1.46
33	B1	1003	ATP	C5-C4	-2.59	1.34	1.40
29	g3	305	CDL	OA6-CA4	-2.59	1.40	1.46
33	C1	601	ATP	C5-C4	-2.59	1.34	1.40
29	K	202	CDL	OB6-CB4	-2.59	1.40	1.46
29	P	201	CDL	OB8-CB7	2.59	1.40	1.33
29	J	302	CDL	OB6-CB4	-2.59	1.40	1.46
33	C4	601	ATP	C5-C4	-2.59	1.34	1.40
33	B4	1003	ATP	C5-C4	-2.58	1.34	1.40
29	B	402	CDL	OA6-CA4	-2.58	1.40	1.46
29	A	502	CDL	OB6-CB4	-2.58	1.40	1.46
29	P3	201	CDL	OB8-CB7	2.58	1.40	1.33
29	f	303	CDL	OB6-CB4	-2.58	1.40	1.46
36	E	900	NAD	C2A-N1A	2.58	1.38	1.33
33	B5	1003	ATP	C5-C4	-2.58	1.34	1.40
33	B2	1003	ATP	C5-C4	-2.58	1.34	1.40
29	a3	502	CDL	OB6-CB4	-2.57	1.40	1.46
29	L	302	CDL	OB6-CB4	-2.57	1.40	1.46
29	L	301	CDL	OB8-CB7	2.57	1.40	1.33
29	I	301	CDL	OA8-CA7	2.57	1.40	1.33
29	K3	202	CDL	OB6-CB4	-2.57	1.40	1.46
29	J3	301	CDL	OA8-CA7	2.57	1.40	1.33
35	J	303	PEE	O2-C2	-2.57	1.40	1.46
29	B3	403	CDL	OB6-CB4	-2.56	1.40	1.46
30	g3	304	PC1	O21-C2	-2.56	1.40	1.46
29	f	304	CDL	OA6-CA4	-2.56	1.40	1.46
29	J	301	CDL	OB6-CB4	-2.56	1.40	1.46
29	P3	201	CDL	OA6-CA4	-2.56	1.40	1.46
29	B	401	CDL	OB6-CB4	-2.56	1.40	1.46
29	L3	301	CDL	OB8-CB7	2.56	1.40	1.33
29	f3	303	CDL	OB6-CB4	-2.56	1.40	1.46
29	I3	303	CDL	OA6-CA4	-2.56	1.40	1.46
29	b3	401	CDL	OA8-CA7	2.55	1.40	1.33
29	j3	301	CDL	OB6-CB4	-2.55	1.40	1.46
29	g	305	CDL	OB6-CB4	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K3	202	CDL	OA8-CA7	2.55	1.40	1.33
36	e3	900	NAD	C2A-N1A	2.55	1.38	1.33
29	j	301	CDL	OA8-CA7	2.55	1.40	1.33
33	A5	601	ATP	C5-C4	-2.55	1.34	1.40
29	J3	301	CDL	OB6-CB4	-2.55	1.40	1.46
29	A	502	CDL	OA8-CA7	2.55	1.40	1.33
29	J	301	CDL	OB8-CB7	2.54	1.40	1.33
29	a3	501	CDL	OA8-CA7	2.54	1.40	1.33
29	f	302	CDL	OA8-CA7	2.54	1.40	1.33
29	i	301	CDL	OA8-CA7	2.54	1.40	1.33
29	I3	301	CDL	OA8-CA7	2.54	1.40	1.33
29	l3	303	CDL	OA8-CA7	2.54	1.40	1.33
29	L	302	CDL	OA8-CA7	2.54	1.40	1.33
29	j	301	CDL	OB8-CB7	2.54	1.40	1.33
29	j3	301	CDL	OB8-CB7	2.54	1.40	1.33
29	A3	501	CDL	OA8-CA7	2.54	1.40	1.33
29	k	201	CDL	OB8-CB7	2.53	1.40	1.33
29	k3	201	CDL	OB8-CB7	2.53	1.40	1.33
29	J3	302	CDL	OB6-CB4	-2.53	1.40	1.46
29	B3	402	CDL	OB6-CB4	-2.53	1.40	1.46
29	i	301	CDL	OB6-CB4	-2.53	1.40	1.46
29	I3	301	CDL	OB6-CB4	-2.53	1.40	1.46
29	f3	304	CDL	OA6-CA4	-2.53	1.40	1.46
29	k	201	CDL	OA8-CA7	2.53	1.40	1.33
29	F3	302	CDL	OA8-CA7	2.53	1.40	1.33
29	i	301	CDL	OA6-CA4	-2.53	1.40	1.46
29	g3	305	CDL	OB6-CB4	-2.53	1.40	1.46
29	b	401	CDL	OA8-CA7	2.52	1.40	1.33
29	K	201	CDL	OB8-CB7	2.52	1.40	1.33
29	l	302	CDL	OA8-CA7	2.52	1.40	1.33
29	J3	301	CDL	OB8-CB7	2.52	1.40	1.33
29	I	302	CDL	OA8-CA7	2.52	1.40	1.33
29	P	201	CDL	OA6-CA4	-2.52	1.40	1.46
29	f3	302	CDL	OA8-CA7	2.52	1.40	1.33
29	g3	305	CDL	OA8-CA7	2.52	1.40	1.33
29	B	404	CDL	OB8-CB7	2.52	1.40	1.33
29	k3	201	CDL	OA8-CA7	2.52	1.40	1.33
36	E3	900	NAD	C2D-C1D	2.52	1.57	1.53
30	D	301	PC1	O21-C2	-2.52	1.40	1.46
29	B	402	CDL	OA8-CA7	2.52	1.40	1.33
29	I3	303	CDL	OA8-CA7	2.52	1.40	1.33
36	E3	900	NAD	C2A-N1A	2.51	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j3	302	CDL	OB6-CB4	-2.51	1.40	1.46
29	j	302	CDL	OA8-CA7	2.51	1.40	1.33
29	I3	302	CDL	OA8-CA7	2.51	1.40	1.33
30	g3	303	PC1	O21-C2	-2.51	1.40	1.46
35	m	301	PEE	O2-C2	-2.51	1.40	1.46
29	L3	301	CDL	OA8-CA7	2.51	1.40	1.33
30	G3	303	PC1	O21-C2	-2.51	1.40	1.46
36	e	900	NAD	C2D-C1D	2.51	1.57	1.53
29	i3	301	CDL	OA6-CA4	-2.51	1.40	1.46
29	i3	302	CDL	OA8-CA7	2.51	1.40	1.33
29	F3	302	CDL	OA6-CA4	-2.51	1.40	1.46
29	g	305	CDL	OA8-CA7	2.50	1.40	1.33
29	B3	401	CDL	OB6-CB4	-2.50	1.40	1.46
29	F	303	CDL	OA8-CA7	2.50	1.40	1.33
30	G	304	PC1	O21-C2	-2.50	1.40	1.46
29	B3	402	CDL	OA8-CA7	2.50	1.40	1.33
29	j	301	CDL	OB6-CB4	-2.50	1.40	1.46
29	f3	303	CDL	OB8-CB7	2.50	1.40	1.33
30	G	303	PC1	O21-C2	-2.50	1.40	1.46
29	k	201	CDL	OA6-CA4	-2.50	1.40	1.46
29	g	305	CDL	OB8-CB7	2.50	1.40	1.33
29	p	201	CDL	OA6-CA4	-2.49	1.40	1.46
29	k3	201	CDL	OA6-CA4	-2.49	1.40	1.46
29	p	201	CDL	OA8-CA7	2.49	1.40	1.33
29	a	501	CDL	OA8-CA7	2.49	1.40	1.33
29	B3	404	CDL	OB8-CB7	2.49	1.40	1.33
29	J3	302	CDL	OB8-CB7	2.49	1.40	1.33
36	E	900	NAD	C2D-C1D	2.49	1.57	1.53
29	B	404	CDL	OB6-CB4	-2.49	1.40	1.46
29	g3	305	CDL	OB8-CB7	2.49	1.40	1.33
36	e3	900	NAD	C2D-C1D	2.49	1.57	1.53
29	K3	201	CDL	OB8-CB7	2.48	1.40	1.33
35	L3	302	PEE	O2-C2	-2.48	1.40	1.46
29	k	201	CDL	OB6-CB4	-2.48	1.40	1.46
29	f3	303	CDL	OA6-CA4	-2.48	1.40	1.46
29	f	304	CDL	OB8-CB7	2.48	1.40	1.33
29	B	401	CDL	OA8-CA7	2.48	1.40	1.33
29	j	302	CDL	OB6-CB4	-2.48	1.40	1.46
29	i3	302	CDL	OB6-CB4	-2.48	1.40	1.46
29	B3	401	CDL	OA8-CA7	2.48	1.40	1.33
29	p	201	CDL	OB6-CB4	-2.48	1.40	1.46
36	e3	900	NAD	C5A-C4A	-2.48	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	201	CDL	OA8-CA7	2.48	1.40	1.33
29	K	202	CDL	OA8-CA7	2.48	1.40	1.33
29	L	301	CDL	OA8-CA7	2.48	1.40	1.33
29	p3	201	CDL	OA8-CA7	2.48	1.40	1.33
36	e	900	NAD	C5A-C4A	-2.48	1.34	1.40
29	K3	201	CDL	OA6-CA4	-2.48	1.40	1.46
29	j	302	CDL	OB8-CB7	2.47	1.40	1.33
35	a3	503	PEE	O2-C2	-2.47	1.40	1.46
29	F	303	CDL	OB8-CB7	2.47	1.40	1.33
29	K	201	CDL	OA6-CA4	-2.47	1.40	1.46
29	J3	302	CDL	OA8-CA7	2.47	1.40	1.33
30	G3	304	PC1	O21-C2	-2.47	1.40	1.46
29	F3	302	CDL	OB8-CB7	2.47	1.40	1.33
29	f	303	CDL	OB8-CB7	2.47	1.40	1.33
30	g3	304	PC1	O31-C31	2.47	1.40	1.33
29	F	303	CDL	OA6-CA4	-2.47	1.40	1.46
29	i	301	CDL	OB8-CB7	2.47	1.40	1.33
29	I3	301	CDL	OB8-CB7	2.47	1.40	1.33
29	L3	301	CDL	OB6-CB4	-2.47	1.40	1.46
30	D3	301	PC1	O21-C2	-2.47	1.40	1.46
36	E3	900	NAD	C5A-C4A	-2.47	1.34	1.40
29	p3	201	CDL	OB6-CB4	-2.47	1.40	1.46
29	f3	304	CDL	OB8-CB7	2.47	1.40	1.33
29	B	404	CDL	OA6-CA4	-2.47	1.40	1.46
35	A	501	PEE	O2-C2	-2.46	1.40	1.46
29	k3	201	CDL	OB6-CB4	-2.46	1.40	1.46
29	B	403	CDL	OB8-CB7	2.46	1.40	1.33
29	I	301	CDL	OA6-CA4	-2.46	1.40	1.46
35	l3	302	PEE	O2-C2	-2.46	1.40	1.46
29	j3	302	CDL	OA8-CA7	2.46	1.40	1.33
29	K3	202	CDL	OB8-CB7	2.46	1.40	1.33
29	p	201	CDL	OB8-CB7	2.45	1.40	1.33
29	I3	302	CDL	OB8-CB7	2.45	1.40	1.33
29	J	302	CDL	OB8-CB7	2.45	1.40	1.33
29	J	302	CDL	OA8-CA7	2.45	1.40	1.33
29	J	301	CDL	OA8-CA7	2.45	1.40	1.33
29	P	201	CDL	OB6-CB4	-2.45	1.40	1.46
30	g	303	PC1	O21-C2	-2.45	1.40	1.46
29	r	201	CDL	OB8-CB7	2.45	1.40	1.33
29	K	202	CDL	OB8-CB7	2.45	1.40	1.33
29	i3	301	CDL	OA8-CA7	2.45	1.40	1.33
29	B3	404	CDL	OA8-CA7	2.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	p3	201	CDL	OB8-CB7	2.45	1.40	1.33
29	I3	303	CDL	OB6-CB4	-2.45	1.40	1.46
29	i3	302	CDL	OB8-CB7	2.44	1.40	1.33
30	G	304	PC1	O31-C31	2.44	1.40	1.33
29	P3	201	CDL	OA8-CA7	2.44	1.40	1.33
29	p3	201	CDL	OA6-CA4	-2.44	1.40	1.46
29	l	302	CDL	OB8-CB7	2.44	1.40	1.33
35	L3	302	PEE	O3-C30	2.44	1.40	1.33
29	P	201	CDL	OA8-CA7	2.44	1.40	1.33
29	f	303	CDL	OA6-CA4	-2.44	1.40	1.46
29	I3	303	CDL	OB8-CB7	2.44	1.40	1.33
29	r	201	CDL	OA8-CA7	2.44	1.40	1.33
29	r	201	CDL	OA6-CA4	-2.44	1.40	1.46
29	I	302	CDL	OB6-CB4	-2.44	1.40	1.46
29	l	301	CDL	OA8-CA7	2.44	1.40	1.33
29	a3	502	CDL	OB8-CB7	2.44	1.40	1.33
36	E	900	NAD	C5A-C4A	-2.43	1.34	1.40
29	f3	302	CDL	OA6-CA4	-2.43	1.40	1.46
29	b	401	CDL	OB8-CB7	2.43	1.40	1.33
30	d3	301	PC1	O21-C2	-2.43	1.40	1.46
29	L	301	CDL	OB6-CB4	-2.43	1.40	1.46
30	g	304	PC1	O31-C31	2.43	1.40	1.33
29	l	302	CDL	OB6-CB4	-2.43	1.40	1.46
29	B3	404	CDL	OB6-CB4	-2.42	1.40	1.46
29	P3	201	CDL	OB6-CB4	-2.42	1.40	1.46
29	L3	301	CDL	OA6-CA4	-2.42	1.40	1.46
29	L	302	CDL	OB8-CB7	2.42	1.40	1.33
29	l3	301	CDL	OA8-CA7	2.42	1.40	1.33
29	l3	303	CDL	OB8-CB7	2.42	1.40	1.33
29	I	302	CDL	OB8-CB7	2.42	1.40	1.33
29	K3	201	CDL	OA8-CA7	2.42	1.40	1.33
29	K3	201	CDL	OB6-CB4	-2.42	1.40	1.46
29	B3	403	CDL	OB8-CB7	2.42	1.40	1.33
30	G3	303	PC1	O31-C31	2.42	1.40	1.33
29	I	301	CDL	OB8-CB7	2.41	1.40	1.33
29	K	201	CDL	OB6-CB4	-2.41	1.40	1.46
29	b3	401	CDL	OB8-CB7	2.41	1.40	1.33
29	j3	301	CDL	OA8-CA7	2.41	1.40	1.33
29	f	302	CDL	OA6-CA4	-2.41	1.40	1.46
29	B	403	CDL	OA6-CA4	-2.41	1.40	1.46
30	G3	304	PC1	O31-C31	2.41	1.40	1.33
29	B3	404	CDL	OA6-CA4	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	J	303	PEE	O3-C30	2.41	1.40	1.33
30	g	303	PC1	O31-C31	2.41	1.40	1.33
29	f3	302	CDL	OB8-CB7	2.40	1.40	1.33
29	l3	303	CDL	OB6-CB4	-2.40	1.40	1.46
29	B3	403	CDL	OA8-CA7	2.40	1.40	1.33
29	f	302	CDL	OB8-CB7	2.40	1.40	1.33
29	j3	302	CDL	OB8-CB7	2.40	1.40	1.33
35	L	303	PEE	O2-C2	-2.40	1.40	1.46
29	B	403	CDL	OA8-CA7	2.40	1.40	1.33
29	i3	301	CDL	OB8-CB7	2.40	1.40	1.33
29	f3	303	CDL	OA8-CA7	2.39	1.40	1.33
30	d	301	PC1	O21-C2	-2.39	1.40	1.46
29	a3	501	CDL	OB8-CB7	2.39	1.40	1.33
29	f	303	CDL	OA8-CA7	2.39	1.40	1.33
29	F3	302	CDL	OB6-CB4	-2.38	1.40	1.46
29	l3	301	CDL	OB8-CB7	2.38	1.40	1.33
29	B3	403	CDL	OA6-CA4	-2.38	1.40	1.46
29	L	301	CDL	OA6-CA4	-2.38	1.40	1.46
29	f3	304	CDL	OA8-CA7	2.38	1.40	1.33
29	B	404	CDL	OA8-CA7	2.37	1.40	1.33
29	A	502	CDL	OB8-CB7	2.37	1.40	1.33
29	I3	301	CDL	OA6-CA4	-2.37	1.40	1.46
29	B3	402	CDL	OB8-CB7	2.37	1.40	1.33
29	a	501	CDL	OB8-CB7	2.37	1.40	1.33
29	F	302	CDL	OB8-CB7	2.36	1.40	1.33
35	L	303	PEE	O3-C30	2.36	1.40	1.33
29	l	302	CDL	OA6-CA4	-2.36	1.40	1.46
30	g3	303	PC1	O31-C31	2.36	1.40	1.33
29	l3	303	CDL	OA6-CA4	-2.36	1.40	1.46
29	l	301	CDL	OB8-CB7	2.35	1.40	1.33
29	A3	501	CDL	OB8-CB7	2.35	1.40	1.33
35	m	301	PEE	O3-C30	2.35	1.40	1.33
29	B	401	CDL	OA6-CA4	-2.35	1.40	1.46
29	a3	502	CDL	OA8-CA7	2.35	1.40	1.33
30	d	301	PC1	O31-C31	2.35	1.40	1.33
29	B3	401	CDL	OB8-CB7	2.35	1.40	1.33
29	B	401	CDL	OB8-CB7	2.34	1.40	1.33
30	G	303	PC1	O31-C31	2.34	1.40	1.33
30	D3	301	PC1	O31-C31	2.34	1.40	1.33
35	A	501	PEE	O3-C30	2.34	1.40	1.33
29	F	303	CDL	OB6-CB4	-2.34	1.40	1.46
29	B3	404	CDL	OA6-CA5	2.34	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	301	PC1	O31-C31	2.33	1.40	1.33
35	a3	503	PEE	O3-C30	2.33	1.40	1.33
36	E	900	NAD	O7N-C7N	-2.33	1.19	1.24
35	j3	303	PEE	O3-C30	2.33	1.40	1.33
29	B	402	CDL	OB8-CB7	2.33	1.40	1.33
29	A3	501	CDL	OB8-CB6	-2.33	1.39	1.45
35	l3	302	PEE	O3-C30	2.33	1.40	1.33
32	i3	303	UQ8	C6-C5	2.33	1.53	1.46
36	e	900	NAD	O7N-C7N	-2.32	1.19	1.24
29	f	304	CDL	OA8-CA7	2.32	1.40	1.33
30	d3	301	PC1	O31-C31	2.32	1.40	1.33
29	B3	401	CDL	OA6-CA4	-2.32	1.40	1.46
29	F	302	CDL	OA8-CA7	2.31	1.40	1.33
29	B3	404	CDL	OB6-CB5	2.31	1.40	1.34
32	I3	304	UQ8	C6-C5	2.31	1.53	1.46
32	I	303	UQ8	C6-C5	2.31	1.53	1.46
29	a3	502	CDL	OA6-CA4	-2.31	1.40	1.46
36	E3	900	NAD	O7N-C7N	-2.31	1.19	1.24
36	e3	900	NAD	O7N-C7N	-2.30	1.19	1.24
29	J	302	CDL	OA6-CA4	-2.30	1.40	1.46
29	B	402	CDL	OB8-CB6	-2.30	1.39	1.45
32	i	302	UQ8	C6-C5	2.29	1.53	1.46
29	l3	303	CDL	OA6-CA5	2.28	1.40	1.34
29	B	404	CDL	OA6-CA5	2.28	1.40	1.34
29	F	302	CDL	OA8-CA6	-2.28	1.40	1.45
29	B	404	CDL	OB6-CB5	2.27	1.40	1.34
29	F	302	CDL	OA6-CA5	2.27	1.40	1.34
29	L3	301	CDL	OB6-CB5	2.27	1.40	1.34
29	I3	303	CDL	OB6-CB5	2.27	1.40	1.34
29	l	302	CDL	OA6-CA5	2.27	1.40	1.34
29	A	502	CDL	OB8-CB6	-2.27	1.40	1.45
29	F	302	CDL	OA6-CA4	-2.26	1.40	1.46
32	I	303	UQ8	O3-C3M	-2.26	1.40	1.45
29	I	302	CDL	OB6-CB5	2.26	1.40	1.34
30	d3	301	PC1	O21-C21	2.26	1.40	1.34
29	j3	302	CDL	OA6-CA4	-2.26	1.40	1.46
29	a3	502	CDL	OA6-CA5	2.26	1.40	1.34
29	J3	302	CDL	OA6-CA4	-2.26	1.41	1.46
29	j	302	CDL	OB6-CB5	2.25	1.40	1.34
29	K	201	CDL	OB6-CB5	2.25	1.40	1.34
29	L	301	CDL	OB6-CB5	2.25	1.40	1.34
29	l3	301	CDL	OA8-CA6	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	301	PC1	O21-C21	2.25	1.40	1.34
29	f	303	CDL	OA6-CA5	2.25	1.40	1.34
32	i3	303	UQ8	O3-C3M	-2.25	1.40	1.45
29	F3	302	CDL	OB6-CB5	2.25	1.40	1.34
29	f	304	CDL	OA8-CA6	-2.25	1.40	1.45
29	a3	502	CDL	OA8-CA6	-2.25	1.40	1.45
29	K3	201	CDL	OB6-CB5	2.25	1.40	1.34
29	B	403	CDL	OA6-CA5	2.24	1.40	1.34
29	B3	401	CDL	OA6-CA5	2.24	1.40	1.34
35	L	303	PEE	O2-C10	2.24	1.40	1.34
29	k3	201	CDL	OA6-CA5	2.24	1.40	1.34
29	K	201	CDL	OA6-CA5	2.23	1.40	1.34
29	l	302	CDL	OB6-CB5	2.23	1.40	1.34
29	F3	302	CDL	OA6-CA5	2.23	1.40	1.34
29	k	201	CDL	OB6-CB5	2.23	1.40	1.34
29	f3	302	CDL	OB8-CB6	-2.23	1.40	1.45
29	B3	403	CDL	OA6-CA5	2.23	1.40	1.34
29	F	302	CDL	OB8-CB6	-2.23	1.40	1.45
29	f3	303	CDL	OA6-CA5	2.23	1.40	1.34
35	a3	503	PEE	O3-C3	-2.23	1.40	1.45
30	G3	303	PC1	O31-C3	-2.22	1.40	1.45
29	f3	304	CDL	OA6-CA5	2.22	1.40	1.34
29	F	303	CDL	OA6-CA5	2.22	1.40	1.34
35	a3	503	PEE	O2-C10	2.22	1.40	1.34
29	L	301	CDL	OA6-CA5	2.22	1.40	1.34
29	F	303	CDL	OB6-CB5	2.22	1.40	1.34
29	j	302	CDL	OA6-CA4	-2.22	1.41	1.46
30	G	303	PC1	O31-C3	-2.22	1.40	1.45
32	I	303	UQ8	O4-C4M	-2.22	1.40	1.45
29	i3	302	CDL	OB6-CB5	2.22	1.40	1.34
32	I3	304	UQ8	O4-C4M	-2.21	1.40	1.45
35	A	501	PEE	O3-C3	-2.21	1.40	1.45
30	G	304	PC1	O21-C21	2.21	1.40	1.34
29	B	403	CDL	OA8-CA6	-2.21	1.40	1.45
29	p3	201	CDL	OB6-CB5	2.21	1.40	1.34
29	k	201	CDL	OA6-CA5	2.21	1.40	1.34
30	G3	304	PC1	O21-C21	2.21	1.40	1.34
35	l3	302	PEE	O2-C10	2.21	1.40	1.34
29	j3	302	CDL	OB6-CB5	2.21	1.40	1.34
29	g	305	CDL	OB6-CB5	2.21	1.40	1.34
32	I3	304	UQ8	O3-C3M	-2.21	1.40	1.45
29	p	201	CDL	OA6-CA5	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	PEE	O2-C10	2.21	1.40	1.34
30	d3	301	PC1	O31-C3	-2.20	1.40	1.45
29	B	401	CDL	OB6-CB5	2.20	1.40	1.34
29	P3	201	CDL	OB6-CB5	2.20	1.40	1.34
29	f	302	CDL	OA6-CA5	2.20	1.40	1.34
32	i	302	UQ8	O4-C4M	-2.20	1.40	1.45
29	l3	303	CDL	OB6-CB5	2.20	1.40	1.34
29	J3	302	CDL	OA6-CA5	2.20	1.40	1.34
29	l	301	CDL	OB8-CB6	-2.20	1.40	1.45
29	B	401	CDL	OB8-CB6	-2.20	1.40	1.45
29	I3	301	CDL	OB6-CB5	2.20	1.40	1.34
30	g3	303	PC1	O31-C3	-2.20	1.40	1.45
29	K3	201	CDL	OA6-CA5	2.20	1.40	1.34
32	i	302	UQ8	O3-C3M	-2.19	1.40	1.45
30	D3	301	PC1	O31-C3	-2.19	1.40	1.45
29	f	304	CDL	OA6-CA5	2.19	1.40	1.34
29	k3	201	CDL	OB6-CB5	2.19	1.40	1.34
29	p	201	CDL	OB6-CB5	2.19	1.40	1.34
30	D	301	PC1	O31-C3	-2.19	1.40	1.45
29	f	303	CDL	OB6-CB5	2.19	1.40	1.34
29	J	302	CDL	OA6-CA5	2.19	1.40	1.34
32	i3	303	UQ8	O4-C4M	-2.19	1.40	1.45
29	j	302	CDL	OA6-CA5	2.19	1.40	1.34
29	B	401	CDL	OA6-CA5	2.18	1.40	1.34
29	f3	302	CDL	OA6-CA5	2.18	1.40	1.34
29	A3	501	CDL	OB6-CB5	2.18	1.40	1.34
29	j3	301	CDL	OB6-CB5	2.18	1.40	1.34
29	B3	403	CDL	OB8-CB6	-2.18	1.40	1.45
29	B3	401	CDL	OB6-CB5	2.18	1.40	1.34
29	B3	401	CDL	OB8-CB6	-2.18	1.40	1.45
29	j3	302	CDL	OA6-CA5	2.18	1.40	1.34
29	I	301	CDL	OB6-CB5	2.18	1.40	1.34
29	P	201	CDL	OB6-CB5	2.18	1.40	1.34
29	p3	201	CDL	OA6-CA5	2.17	1.40	1.34
29	f	302	CDL	OB8-CB6	-2.17	1.40	1.45
29	J	301	CDL	OB6-CB5	2.17	1.40	1.34
29	F	302	CDL	OB6-CB5	2.17	1.40	1.34
29	B	404	CDL	OA8-CA6	-2.17	1.40	1.45
29	i	301	CDL	OB6-CB5	2.17	1.40	1.34
29	a3	502	CDL	OB8-CB6	-2.17	1.40	1.45
30	g	303	PC1	O31-C3	-2.17	1.40	1.45
30	D	301	PC1	O21-C21	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	403	CDL	OB8-CB6	-2.17	1.40	1.45
29	B3	402	CDL	OB6-CB5	2.17	1.40	1.34
35	j3	303	PEE	O3-C3	-2.17	1.40	1.45
29	L3	301	CDL	OA6-CA5	2.17	1.40	1.34
35	L	303	PEE	O3-C3	-2.17	1.40	1.45
29	J3	302	CDL	OB6-CB5	2.16	1.40	1.34
29	g3	305	CDL	OB6-CB5	2.16	1.40	1.34
29	A	502	CDL	OB6-CB5	2.16	1.40	1.34
29	I3	303	CDL	OA6-CA5	2.16	1.40	1.34
29	B3	402	CDL	OB8-CB6	-2.16	1.40	1.45
29	b3	401	CDL	OB8-CB6	-2.16	1.40	1.45
29	K3	202	CDL	OB6-CB5	2.16	1.40	1.34
29	a	501	CDL	OB8-CB6	-2.16	1.40	1.45
29	A3	501	CDL	OA8-CA6	-2.16	1.40	1.45
29	J3	301	CDL	OB6-CB5	2.16	1.40	1.34
35	l3	302	PEE	O3-C3	-2.16	1.40	1.45
29	a3	502	CDL	OB6-CB5	2.15	1.40	1.34
29	f3	304	CDL	OA8-CA6	-2.15	1.40	1.45
29	I	302	CDL	OA6-CA5	2.15	1.40	1.34
30	g3	303	PC1	O21-C21	2.15	1.40	1.34
29	j	301	CDL	OB6-CB5	2.15	1.40	1.34
36	e3	900	NAD	C2A-N3A	2.15	1.35	1.32
36	E3	900	NAD	C2A-N3A	2.15	1.35	1.32
29	B3	402	CDL	OA6-CA5	2.15	1.40	1.34
30	g	303	PC1	O21-C21	2.15	1.40	1.34
30	D3	301	PC1	O21-C21	2.14	1.40	1.34
35	m	301	PEE	O2-C10	2.14	1.40	1.34
35	L3	302	PEE	O2-C10	2.14	1.40	1.34
29	l	302	CDL	OB8-CB6	-2.14	1.40	1.45
29	j	301	CDL	OA6-CA5	2.14	1.40	1.34
29	l3	303	CDL	OB8-CB6	-2.14	1.40	1.45
29	B3	403	CDL	OA8-CA6	-2.14	1.40	1.45
29	B	402	CDL	OA6-CA5	2.14	1.40	1.34
29	j3	302	CDL	OB8-CB6	-2.13	1.40	1.45
36	E	900	NAD	C2A-N3A	2.13	1.35	1.32
29	a3	501	CDL	OB8-CB6	-2.13	1.40	1.45
29	I	302	CDL	OB8-CB6	-2.13	1.40	1.45
29	r	201	CDL	OB6-CB5	2.13	1.40	1.34
30	G	303	PC1	O21-C21	2.13	1.40	1.34
29	B3	404	CDL	OA8-CA6	-2.13	1.40	1.45
29	B	403	CDL	OB6-CB5	2.13	1.40	1.34
36	E3	900	NAD	PA-O5B	2.13	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I3	301	CDL	OB8-CB6	-2.13	1.40	1.45
29	K	202	CDL	OB6-CB5	2.13	1.40	1.34
29	B3	404	CDL	OB8-CB6	-2.13	1.40	1.45
29	A3	501	CDL	OA6-CA5	2.13	1.40	1.34
29	I3	303	CDL	OB8-CB6	-2.12	1.40	1.45
29	P3	201	CDL	OA6-CA5	2.12	1.40	1.34
29	l	302	CDL	OA8-CA6	-2.12	1.40	1.45
35	J	303	PEE	O3-C3	-2.12	1.40	1.45
29	f	303	CDL	OA8-CA6	-2.12	1.40	1.45
37	B1	1002	ADP	C2-N3	2.12	1.35	1.32
32	i	302	UQ8	O5-C5	-2.12	1.18	1.23
29	I3	302	CDL	OB6-CB5	2.12	1.40	1.34
29	J	302	CDL	OB6-CB5	2.12	1.40	1.34
29	f3	303	CDL	OB6-CB5	2.12	1.40	1.34
29	J	302	CDL	OA8-CA6	-2.12	1.40	1.45
30	d	301	PC1	O31-C3	-2.12	1.40	1.45
32	I3	304	UQ8	O5-C5	-2.12	1.18	1.23
29	f3	303	CDL	OA8-CA6	-2.12	1.40	1.45
29	j	302	CDL	OB8-CB6	-2.12	1.40	1.45
29	I3	302	CDL	OB8-CB6	-2.12	1.40	1.45
35	J	303	PEE	O2-C10	2.12	1.40	1.34
29	i	301	CDL	OA6-CA5	2.12	1.40	1.34
29	a3	501	CDL	OA6-CA5	2.11	1.40	1.34
33	C1	601	ATP	C5'-C4'	2.11	1.58	1.51
37	B4	1002	ADP	C2-N3	2.11	1.35	1.32
29	i3	301	CDL	OB6-CB5	2.11	1.40	1.34
36	e	900	NAD	PA-O5B	2.11	1.67	1.59
29	b	401	CDL	OB6-CB5	2.11	1.40	1.34
29	B	402	CDL	OB6-CB5	2.11	1.40	1.34
29	j3	301	CDL	OA6-CA5	2.11	1.40	1.34
32	I3	304	UQ8	O2-C2	-2.11	1.18	1.23
29	r	201	CDL	OA6-CA5	2.11	1.40	1.34
29	A	502	CDL	OA6-CA5	2.11	1.40	1.34
32	i	302	UQ8	O2-C2	-2.11	1.18	1.23
29	l	301	CDL	OB6-CB5	2.10	1.40	1.34
29	B3	403	CDL	OB6-CB5	2.10	1.40	1.34
29	i3	301	CDL	OB8-CB6	-2.10	1.40	1.45
29	f3	304	CDL	OB6-CB5	2.10	1.40	1.34
29	f	304	CDL	OB6-CB5	2.10	1.40	1.34
29	i3	302	CDL	OA6-CA5	2.10	1.40	1.34
30	G3	303	PC1	O21-C21	2.10	1.40	1.34
32	i3	303	UQ8	O2-C2	-2.10	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	303	UQ8	O2-C2	-2.10	1.18	1.23
29	K3	201	CDL	OA8-CA6	-2.10	1.40	1.45
32	i3	303	UQ8	O5-C5	-2.10	1.18	1.23
37	B2	1002	ADP	C2-N3	2.10	1.35	1.32
29	L	302	CDL	OB6-CB5	2.10	1.40	1.34
36	e	900	NAD	C2A-N3A	2.10	1.35	1.32
29	a	501	CDL	OB6-CB5	2.10	1.40	1.34
29	a	501	CDL	OA6-CA5	2.10	1.40	1.34
29	P	201	CDL	OA6-CA5	2.10	1.40	1.34
32	I	303	UQ8	O5-C5	-2.10	1.18	1.23
29	b3	401	CDL	OB6-CB5	2.09	1.40	1.34
29	f	303	CDL	OB8-CB6	-2.09	1.40	1.45
30	G3	304	PC1	O31-C3	-2.09	1.40	1.45
29	a3	501	CDL	OB6-CB5	2.09	1.40	1.34
33	C4	601	ATP	C5'-C4'	2.09	1.58	1.51
29	B	401	CDL	OA8-CA6	-2.09	1.40	1.45
29	K3	202	CDL	OA8-CA6	-2.09	1.40	1.45
35	m	301	PEE	O3-C3	-2.09	1.40	1.45
29	I3	301	CDL	OA6-CA5	2.09	1.40	1.34
29	i3	301	CDL	OA8-CA6	-2.09	1.40	1.45
29	r	201	CDL	OA8-CA6	-2.09	1.40	1.45
29	l	301	CDL	OA8-CA6	-2.09	1.40	1.45
29	a3	501	CDL	OA8-CA6	-2.09	1.40	1.45
29	K	202	CDL	OA6-CA5	2.09	1.40	1.34
33	B2	1003	ATP	C5'-C4'	2.08	1.58	1.51
29	g	305	CDL	OA6-CA5	2.08	1.40	1.34
29	f	304	CDL	OB8-CB6	-2.08	1.40	1.45
30	g	304	PC1	O21-C21	2.08	1.40	1.34
29	I	301	CDL	OA6-CA5	2.08	1.40	1.34
29	g	305	CDL	OA8-CA6	-2.08	1.40	1.45
29	B3	401	CDL	OA8-CA6	-2.08	1.40	1.45
29	K	202	CDL	OA8-CA6	-2.08	1.40	1.45
29	g3	305	CDL	OA6-CA5	2.08	1.40	1.34
29	J3	302	CDL	OA8-CA6	-2.08	1.40	1.45
36	e3	900	NAD	PA-O5B	2.08	1.67	1.59
35	L3	302	PEE	O3-C3	-2.08	1.40	1.45
29	K3	202	CDL	OB8-CB6	-2.08	1.40	1.45
29	L	302	CDL	OA8-CA6	-2.08	1.40	1.45
29	f3	304	CDL	OB8-CB6	-2.08	1.40	1.45
29	b	401	CDL	OA6-CA5	2.08	1.40	1.34
29	b3	401	CDL	OA6-CA5	2.08	1.40	1.34
30	g3	304	PC1	O21-C21	2.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K3	202	CDL	OA6-CA5	2.07	1.40	1.34
29	L	302	CDL	OB8-CB6	-2.07	1.40	1.45
29	L3	301	CDL	OB8-CB6	-2.07	1.40	1.45
33	G3	301	ATP	C5'-C4'	2.07	1.58	1.51
33	B4	1003	ATP	C5'-C4'	2.07	1.58	1.51
35	j3	303	PEE	O2-C10	2.07	1.40	1.34
29	P	201	CDL	OA8-CA6	-2.07	1.40	1.45
29	K3	201	CDL	OB8-CB6	-2.07	1.40	1.45
37	D5	501	ADP	C2-N3	2.07	1.35	1.32
29	f3	302	CDL	OB6-CB5	2.07	1.40	1.34
29	J3	301	CDL	OA6-CA5	2.06	1.40	1.34
37	D1	501	ADP	C2-N3	2.06	1.35	1.32
36	E	900	NAD	PA-O5B	2.06	1.67	1.59
29	j3	301	CDL	OA8-CA6	-2.06	1.40	1.45
33	A2	601	ATP	C5'-C4'	2.06	1.58	1.51
29	j3	302	CDL	OA8-CA6	-2.06	1.40	1.45
33	A4	601	ATP	C5'-C4'	2.06	1.58	1.51
29	l3	303	CDL	OA8-CA6	-2.06	1.40	1.45
29	J	301	CDL	OA6-CA5	2.06	1.40	1.34
29	J3	302	CDL	OB8-CB6	-2.06	1.40	1.45
29	g	305	CDL	OB8-CB6	-2.06	1.40	1.45
37	B5	1002	ADP	C2-N3	2.06	1.35	1.32
29	g3	305	CDL	OA8-CA6	-2.05	1.40	1.45
29	K	201	CDL	OB8-CB6	-2.05	1.40	1.45
33	B1	1003	ATP	C5'-C4'	2.05	1.58	1.51
33	B5	1003	ATP	C5'-C4'	2.05	1.58	1.51
33	A5	601	ATP	C5'-C4'	2.05	1.58	1.51
29	g3	305	CDL	OB8-CB6	-2.04	1.40	1.45
29	p3	201	CDL	OB8-CB6	-2.04	1.40	1.45
29	A	502	CDL	OA8-CA6	-2.04	1.40	1.45
29	i	301	CDL	OB8-CB6	-2.04	1.40	1.45
30	g3	304	PC1	O31-C3	-2.04	1.40	1.45
29	r	201	CDL	OB8-CB6	-2.04	1.40	1.45
30	g	304	PC1	O31-C3	-2.04	1.40	1.45
29	f	302	CDL	OB6-CB5	2.04	1.40	1.34
29	f	302	CDL	OA8-CA6	-2.04	1.40	1.45
29	k	201	CDL	OA8-CA6	-2.04	1.40	1.45
29	b	401	CDL	OB8-CB6	-2.04	1.40	1.45
29	p3	201	CDL	OA8-CA6	-2.04	1.40	1.45
29	B	404	CDL	OB8-CB6	-2.04	1.40	1.45
29	i3	302	CDL	OB8-CB6	-2.04	1.40	1.45
29	l3	301	CDL	OA6-CA5	2.04	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P3	201	CDL	OA8-CA6	-2.04	1.40	1.45
37	D2	501	ADP	C2-N3	2.04	1.35	1.32
29	i3	301	CDL	OA6-CA5	2.04	1.40	1.34
37	D4	501	ADP	C2-N3	2.04	1.35	1.32
29	a	501	CDL	OA8-CA6	-2.03	1.40	1.45
29	f3	303	CDL	OB8-CB6	-2.03	1.40	1.45
33	C2	601	ATP	C5'-C4'	2.03	1.57	1.51
29	j	302	CDL	OA8-CA6	-2.03	1.40	1.45
29	K	201	CDL	OA8-CA6	-2.03	1.40	1.45
29	p	201	CDL	OA8-CA6	-2.03	1.40	1.45
30	G	304	PC1	O31-C3	-2.03	1.40	1.45
29	J3	301	CDL	OB8-CB6	-2.03	1.40	1.45
29	J	301	CDL	OA8-CA6	-2.03	1.40	1.45
29	L3	301	CDL	OA8-CA6	-2.03	1.40	1.45
33	C5	601	ATP	C5'-C4'	2.03	1.57	1.51
29	K	202	CDL	OB8-CB6	-2.02	1.40	1.45
29	L	301	CDL	OA8-CA6	-2.02	1.40	1.45
33	A1	601	ATP	C5'-C4'	2.02	1.57	1.51
29	I	301	CDL	OB8-CB6	-2.02	1.40	1.45
29	I3	301	CDL	OB8-CB6	-2.02	1.40	1.45
29	I3	301	CDL	OB6-CB5	2.02	1.40	1.34
29	L	301	CDL	OB8-CB6	-2.02	1.40	1.45
29	B	402	CDL	OA8-CA6	-2.02	1.40	1.45
29	J	302	CDL	OB8-CB6	-2.02	1.40	1.45
29	f3	302	CDL	OA8-CA6	-2.01	1.40	1.45
29	p	201	CDL	OB8-CB6	-2.01	1.40	1.45
33	B5	1003	ATP	C2-N3	2.01	1.35	1.32
29	I3	301	CDL	OA8-CA6	-2.01	1.40	1.45
29	I	301	CDL	OA8-CA6	-2.01	1.40	1.45
33	g	301	ATP	C5'-C4'	2.01	1.57	1.51
29	k	201	CDL	OB8-CB6	-2.00	1.40	1.45

All (562) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D4	501	ADP	C1'-N9-C4	15.99	154.74	126.64
37	D1	501	ADP	C1'-N9-C4	15.96	154.69	126.64
37	B5	1002	ADP	C1'-N9-C4	14.92	152.85	126.64
37	B1	1002	ADP	C1'-N9-C4	14.91	152.84	126.64
37	B2	1002	ADP	C1'-N9-C4	14.87	152.77	126.64
37	B4	1002	ADP	C1'-N9-C4	14.86	152.75	126.64
37	D5	501	ADP	C1'-N9-C4	14.68	152.43	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D2	501	ADP	C1'-N9-C4	14.63	152.35	126.64
36	e	900	NAD	C1B-N9A-C4A	-8.75	111.28	126.64
36	e3	900	NAD	C1B-N9A-C4A	-8.67	111.41	126.64
36	E3	900	NAD	C1B-N9A-C4A	-8.51	111.70	126.64
36	E	900	NAD	C1B-N9A-C4A	-8.43	111.83	126.64
36	e3	900	NAD	C5A-C6A-N6A	8.02	132.54	120.35
36	E	900	NAD	C5A-C6A-N6A	8.00	132.50	120.35
36	E3	900	NAD	C5A-C6A-N6A	7.94	132.42	120.35
36	e	900	NAD	C5A-C6A-N6A	7.85	132.28	120.35
33	A1	601	ATP	C5-C6-N6	7.64	131.96	120.35
33	G	301	ATP	C5-C6-N6	7.63	131.94	120.35
37	D1	501	ADP	C5-C6-N6	7.61	131.92	120.35
33	B1	1003	ATP	C5-C6-N6	7.61	131.92	120.35
33	g3	301	ATP	C5-C6-N6	7.60	131.90	120.35
33	B2	1003	ATP	C5-C6-N6	7.57	131.86	120.35
33	B4	1003	ATP	C5-C6-N6	7.57	131.86	120.35
33	A5	601	ATP	C5-C6-N6	7.57	131.86	120.35
33	C5	601	ATP	C5-C6-N6	7.56	131.84	120.35
33	A4	601	ATP	C5-C6-N6	7.55	131.82	120.35
33	A2	601	ATP	C5-C6-N6	7.54	131.81	120.35
33	G3	301	ATP	C5-C6-N6	7.53	131.80	120.35
37	B5	1002	ADP	C5-C6-N6	7.53	131.80	120.35
33	B5	1003	ATP	C5-C6-N6	7.53	131.80	120.35
37	B1	1002	ADP	C5-C6-N6	7.53	131.80	120.35
33	C4	601	ATP	C5-C6-N6	7.53	131.79	120.35
37	B4	1002	ADP	C5-C6-N6	7.52	131.78	120.35
33	C2	601	ATP	C5-C6-N6	7.51	131.77	120.35
37	B2	1002	ADP	C5-C6-N6	7.51	131.76	120.35
37	D4	501	ADP	C5-C6-N6	7.51	131.76	120.35
33	g	301	ATP	C5-C6-N6	7.50	131.75	120.35
33	C1	601	ATP	C5-C6-N6	7.49	131.74	120.35
37	D2	501	ADP	C5-C6-N6	7.47	131.70	120.35
37	D5	501	ADP	C5-C6-N6	7.46	131.69	120.35
33	g	301	ATP	C1'-N9-C4	5.71	136.67	126.64
33	G3	301	ATP	C1'-N9-C4	5.69	136.64	126.64
33	A2	601	ATP	C1'-N9-C4	5.68	136.62	126.64
33	g3	301	ATP	C1'-N9-C4	5.67	136.59	126.64
33	A4	601	ATP	C1'-N9-C4	5.66	136.59	126.64
33	A5	601	ATP	C1'-N9-C4	5.64	136.56	126.64
33	C2	601	ATP	C1'-N9-C4	5.64	136.55	126.64
33	A1	601	ATP	C1'-N9-C4	5.62	136.51	126.64
33	C4	601	ATP	C1'-N9-C4	5.61	136.49	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	G	301	ATP	C1'-N9-C4	5.59	136.47	126.64
33	C5	601	ATP	C1'-N9-C4	5.59	136.47	126.64
33	B2	1003	ATP	C1'-N9-C4	5.59	136.46	126.64
33	C1	601	ATP	C1'-N9-C4	5.59	136.46	126.64
33	B5	1003	ATP	C1'-N9-C4	5.58	136.44	126.64
33	B4	1003	ATP	C1'-N9-C4	5.57	136.43	126.64
37	B5	1002	ADP	N3-C2-N1	-5.55	120.00	128.68
37	B2	1002	ADP	N3-C2-N1	-5.55	120.01	128.68
37	D1	501	ADP	N3-C2-N1	-5.54	120.01	128.68
37	B4	1002	ADP	N3-C2-N1	-5.54	120.02	128.68
33	B1	1003	ATP	C1'-N9-C4	5.53	136.36	126.64
37	D5	501	ADP	N3-C2-N1	-5.53	120.04	128.68
37	D2	501	ADP	N3-C2-N1	-5.51	120.06	128.68
33	B5	1003	ATP	N3-C2-N1	-5.51	120.07	128.68
37	B1	1002	ADP	N3-C2-N1	-5.51	120.07	128.68
37	D4	501	ADP	N3-C2-N1	-5.51	120.07	128.68
33	C4	601	ATP	N3-C2-N1	-5.51	120.07	128.68
33	G	301	ATP	N3-C2-N1	-5.50	120.08	128.68
33	g	301	ATP	N3-C2-N1	-5.50	120.08	128.68
33	B1	1003	ATP	N3-C2-N1	-5.50	120.09	128.68
33	A5	601	ATP	N3-C2-N1	-5.49	120.09	128.68
33	C2	601	ATP	N3-C2-N1	-5.49	120.09	128.68
33	C5	601	ATP	N3-C2-N1	-5.49	120.11	128.68
33	g3	301	ATP	N3-C2-N1	-5.48	120.11	128.68
33	A4	601	ATP	N3-C2-N1	-5.48	120.11	128.68
33	B4	1003	ATP	N3-C2-N1	-5.48	120.11	128.68
33	G3	301	ATP	N3-C2-N1	-5.48	120.11	128.68
33	A1	601	ATP	N3-C2-N1	-5.48	120.11	128.68
33	B2	1003	ATP	N3-C2-N1	-5.47	120.13	128.68
33	C1	601	ATP	N3-C2-N1	-5.47	120.13	128.68
33	A2	601	ATP	N3-C2-N1	-5.46	120.14	128.68
36	e	900	NAD	N3A-C2A-N1A	-5.41	120.22	128.68
36	e3	900	NAD	N3A-C2A-N1A	-5.40	120.24	128.68
36	E3	900	NAD	N3A-C2A-N1A	-5.40	120.24	128.68
36	E	900	NAD	N3A-C2A-N1A	-5.39	120.26	128.68
36	E	900	NAD	N6A-C6A-N1A	-5.38	107.41	118.57
36	E3	900	NAD	N6A-C6A-N1A	-5.36	107.44	118.57
36	e3	900	NAD	N6A-C6A-N1A	-5.34	107.50	118.57
36	e	900	NAD	N6A-C6A-N1A	-5.31	107.56	118.57
33	G	301	ATP	N6-C6-N1	-5.08	108.02	118.57
33	A1	601	ATP	N6-C6-N1	-5.05	108.10	118.57
37	D1	501	ADP	N6-C6-N1	-5.04	108.11	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	g3	301	ATP	N6-C6-N1	-5.04	108.12	118.57
33	B1	1003	ATP	N6-C6-N1	-5.03	108.13	118.57
33	B4	1003	ATP	N6-C6-N1	-5.02	108.15	118.57
37	D4	501	ADP	N6-C6-N1	-5.02	108.16	118.57
37	B2	1002	ADP	N6-C6-N1	-5.01	108.18	118.57
33	B2	1003	ATP	N6-C6-N1	-5.00	108.19	118.57
33	A4	601	ATP	N6-C6-N1	-5.00	108.20	118.57
33	A5	601	ATP	N6-C6-N1	-5.00	108.20	118.57
33	C5	601	ATP	N6-C6-N1	-5.00	108.20	118.57
33	A2	601	ATP	N6-C6-N1	-5.00	108.20	118.57
33	G3	301	ATP	N6-C6-N1	-5.00	108.20	118.57
37	B5	1002	ADP	N6-C6-N1	-5.00	108.20	118.57
37	B4	1002	ADP	N6-C6-N1	-4.99	108.21	118.57
37	B1	1002	ADP	N6-C6-N1	-4.99	108.21	118.57
33	g	301	ATP	N6-C6-N1	-4.99	108.22	118.57
33	B5	1003	ATP	N6-C6-N1	-4.98	108.23	118.57
37	D2	501	ADP	N6-C6-N1	-4.98	108.23	118.57
29	l	302	CDL	OB6-CB5-C51	4.97	122.21	111.50
33	C4	601	ATP	N6-C6-N1	-4.97	108.26	118.57
33	C2	601	ATP	N6-C6-N1	-4.97	108.26	118.57
37	D5	501	ADP	N6-C6-N1	-4.96	108.27	118.57
33	C1	601	ATP	N6-C6-N1	-4.95	108.30	118.57
29	l3	303	CDL	OB6-CB5-C51	4.94	122.16	111.50
29	B3	402	CDL	OB6-CB5-C51	4.92	122.10	111.50
29	B	402	CDL	OB6-CB5-C51	4.87	122.00	111.50
29	F3	302	CDL	OB6-CB5-C51	4.56	121.32	111.50
30	d3	301	PC1	O21-C21-C22	4.55	121.32	111.50
32	I3	304	UQ8	C25-C24-C26	4.55	122.92	115.27
30	d	301	PC1	O21-C21-C22	4.52	121.24	111.50
29	f3	304	CDL	OA6-CA5-C11	4.51	121.21	111.50
32	I	303	UQ8	C25-C24-C26	4.45	122.75	115.27
29	B3	401	CDL	OA6-CA5-C11	4.42	121.02	111.50
29	B	401	CDL	OA6-CA5-C11	4.39	120.97	111.50
29	F	303	CDL	OB6-CB5-C51	4.37	120.93	111.50
29	f	304	CDL	OA6-CA5-C11	4.34	120.86	111.50
29	K3	201	CDL	OA6-CA5-C11	4.31	120.80	111.50
29	A	502	CDL	OB6-CB5-C51	4.31	120.78	111.50
29	k	201	CDL	OA6-CA5-C11	4.30	120.77	111.50
35	A	501	PEE	O2-C10-C11	4.27	120.70	111.50
29	a	501	CDL	OB6-CB5-C51	4.23	120.62	111.50
30	G3	304	PC1	O21-C21-C22	4.21	120.57	111.50
29	K3	202	CDL	OA6-CA5-C11	4.19	120.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	G	301	ATP	C3'-C2'-C1'	4.19	107.29	100.98
29	k3	201	CDL	OA6-CA5-C11	4.18	120.52	111.50
35	a3	503	PEE	O2-C10-C11	4.18	120.51	111.50
35	l3	302	PEE	O2-C10-C11	4.18	120.50	111.50
29	f	303	CDL	OA6-CA5-C11	4.15	120.44	111.50
33	G3	301	ATP	C3'-C2'-C1'	4.15	107.22	100.98
29	K	201	CDL	OA6-CA5-C11	4.14	120.42	111.50
29	a3	501	CDL	OB6-CB5-C51	4.12	120.37	111.50
29	F	303	CDL	OA6-CA5-C11	4.11	120.36	111.50
30	D3	301	PC1	O21-C21-C22	4.11	120.36	111.50
29	p3	201	CDL	OB6-CB5-C51	4.11	120.35	111.50
29	I	302	CDL	OA6-CA5-C11	4.10	120.34	111.50
29	P	201	CDL	OA6-CA5-C11	4.09	120.32	111.50
29	B3	404	CDL	OB6-CB5-C51	4.08	120.29	111.50
29	A3	501	CDL	OB6-CB5-C51	4.08	120.29	111.50
29	J	301	CDL	OB6-CB5-C51	4.08	120.29	111.50
29	P3	201	CDL	OA6-CA5-C11	4.08	120.29	111.50
29	j	301	CDL	OB6-CB5-C51	4.07	120.27	111.50
30	G	304	PC1	O21-C21-C22	4.07	120.27	111.50
29	f3	303	CDL	OA6-CA5-C11	4.06	120.26	111.50
29	i	301	CDL	OA6-CA5-C11	4.06	120.25	111.50
35	L	303	PEE	O2-C10-C11	4.06	120.24	111.50
29	I3	303	CDL	OA6-CA5-C11	4.03	120.20	111.50
30	D	301	PC1	O21-C21-C22	4.02	120.17	111.50
29	p	201	CDL	OB6-CB5-C51	4.02	120.16	111.50
29	F3	302	CDL	OA6-CA5-C11	4.02	120.16	111.50
29	f	302	CDL	OA6-CA5-C11	4.01	120.14	111.50
29	L	302	CDL	OB6-CB5-C51	4.01	120.13	111.50
29	B	404	CDL	OA6-CA5-C11	4.00	120.13	111.50
29	b	401	CDL	OB6-CB5-C51	3.99	120.09	111.50
29	b3	401	CDL	OA6-CA5-C11	3.98	120.09	111.50
29	f	304	CDL	OB6-CB5-C51	3.98	120.08	111.50
29	j3	301	CDL	OA6-CA5-C11	3.98	120.07	111.50
30	G	303	PC1	O21-C21-C22	3.98	120.07	111.50
29	K	202	CDL	OA6-CA5-C11	3.98	120.07	111.50
29	f3	302	CDL	OB6-CB5-C51	3.97	120.06	111.50
29	b3	401	CDL	OB6-CB5-C51	3.97	120.06	111.50
29	j3	301	CDL	OB6-CB5-C51	3.97	120.05	111.50
29	J3	301	CDL	OA6-CA5-C11	3.96	120.04	111.50
32	I3	304	UQ8	C40-C39-C41	3.96	121.94	115.27
29	f3	304	CDL	OB6-CB5-C51	3.96	120.04	111.50
29	g3	305	CDL	OB6-CB5-C51	3.96	120.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	g3	303	PC1	O21-C21-C22	3.96	120.04	111.50
29	P3	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
37	D4	501	ADP	C3'-C2'-C1'	3.94	106.92	100.98
33	g3	301	ATP	C3'-C2'-C1'	3.94	106.91	100.98
29	g3	305	CDL	OA6-CA5-C11	3.94	119.98	111.50
29	b	401	CDL	OA6-CA5-C11	3.93	119.97	111.50
29	f	302	CDL	OB6-CB5-C51	3.93	119.97	111.50
30	g	303	PC1	O21-C21-C22	3.93	119.97	111.50
29	j	301	CDL	OA6-CA5-C11	3.93	119.97	111.50
29	I3	303	CDL	OB6-CB5-C51	3.92	119.95	111.50
29	B	404	CDL	OB6-CB5-C51	3.91	119.93	111.50
30	G3	303	PC1	O21-C21-C22	3.91	119.93	111.50
29	f3	302	CDL	OA6-CA5-C11	3.91	119.93	111.50
29	I	302	CDL	OB6-CB5-C51	3.91	119.93	111.50
29	f3	303	CDL	OB6-CB5-C51	3.91	119.93	111.50
29	F	302	CDL	OA6-CA5-C11	3.90	119.90	111.50
33	g	301	ATP	C3'-C2'-C1'	3.90	106.85	100.98
37	D1	501	ADP	C3'-C2'-C1'	3.90	106.84	100.98
29	J	301	CDL	OA6-CA5-C11	3.87	119.85	111.50
29	i3	302	CDL	OB6-CB5-C51	3.86	119.83	111.50
29	I3	302	CDL	OB6-CB5-C51	3.85	119.81	111.50
29	a	501	CDL	OA6-CA5-C11	3.85	119.80	111.50
29	a3	502	CDL	OA6-CA5-C11	3.85	119.79	111.50
35	L3	302	PEE	O2-C10-C11	3.85	119.79	111.50
32	I	303	UQ8	C40-C39-C41	3.84	121.74	115.27
29	B	403	CDL	OB6-CB5-C51	3.84	119.79	111.50
29	g	305	CDL	OA6-CA5-C11	3.84	119.78	111.50
29	I3	301	CDL	OB6-CB5-C51	3.84	119.78	111.50
29	B3	402	CDL	OA6-CA5-C11	3.82	119.73	111.50
29	a3	501	CDL	OA6-CA5-C11	3.82	119.73	111.50
29	l	301	CDL	OB6-CB5-C51	3.81	119.72	111.50
29	i	301	CDL	OB6-CB5-C51	3.81	119.71	111.50
29	i3	302	CDL	OA6-CA5-C11	3.80	119.69	111.50
29	L	301	CDL	OB6-CB5-C51	3.80	119.69	111.50
29	L	302	CDL	OA6-CA5-C11	3.79	119.68	111.50
29	p3	201	CDL	OA6-CA5-C11	3.79	119.68	111.50
29	f	303	CDL	OB6-CB5-C51	3.79	119.67	111.50
29	P	201	CDL	OB6-CB5-C51	3.79	119.67	111.50
29	g	305	CDL	OB6-CB5-C51	3.79	119.67	111.50
29	J3	302	CDL	OA6-CA5-C11	3.79	119.66	111.50
29	B3	404	CDL	OA6-CA5-C11	3.78	119.64	111.50
29	L	301	CDL	OA6-CA5-C11	3.78	119.64	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J3	301	CDL	OB6-CB5-C51	3.77	119.62	111.50
29	p	201	CDL	OA6-CA5-C11	3.76	119.61	111.50
29	K3	201	CDL	OB6-CB5-C51	3.75	119.59	111.50
29	l	301	CDL	OA6-CA5-C11	3.73	119.55	111.50
29	K	201	CDL	OB6-CB5-C51	3.73	119.53	111.50
29	k3	201	CDL	OB6-CB5-C51	3.73	119.53	111.50
29	B3	403	CDL	OA6-CA5-C11	3.73	119.53	111.50
29	l3	301	CDL	OA6-CA5-C11	3.72	119.52	111.50
29	B3	403	CDL	OB6-CB5-C51	3.72	119.51	111.50
29	I	301	CDL	OA6-CA5-C11	3.71	119.50	111.50
29	B	402	CDL	OA6-CA5-C11	3.71	119.49	111.50
29	J3	302	CDL	OB6-CB5-C51	3.70	119.48	111.50
29	I3	301	CDL	OA6-CA5-C11	3.67	119.42	111.50
29	J	302	CDL	OA6-CA5-C11	3.67	119.40	111.50
29	j	302	CDL	OA6-CA5-C11	3.66	119.39	111.50
29	j	302	CDL	OB6-CB5-C51	3.66	119.39	111.50
29	B	403	CDL	OA6-CA5-C11	3.66	119.38	111.50
35	J	303	PEE	O2-C10-C11	3.65	119.37	111.50
29	A	502	CDL	OA6-CA5-C11	3.64	119.34	111.50
29	J	302	CDL	OB6-CB5-C51	3.62	119.31	111.50
29	i3	301	CDL	OA6-CA5-C11	3.61	119.29	111.50
37	B4	1002	ADP	C3'-C2'-C1'	3.60	106.39	100.98
29	a3	502	CDL	OB6-CB5-C51	3.60	119.25	111.50
29	L3	301	CDL	OA6-CA5-C11	3.58	119.22	111.50
29	K	202	CDL	OB6-CB5-C51	3.58	119.22	111.50
29	I3	302	CDL	OA6-CA5-C11	3.57	119.20	111.50
37	B1	1002	ADP	C3'-C2'-C1'	3.57	106.36	100.98
29	L3	301	CDL	OB6-CB5-C51	3.56	119.18	111.50
29	j3	302	CDL	OB6-CB5-C51	3.56	119.17	111.50
29	l3	301	CDL	OB6-CB5-C51	3.56	119.17	111.50
29	k	201	CDL	OB6-CB5-C51	3.55	119.14	111.50
29	I	301	CDL	OB6-CB5-C51	3.55	119.14	111.50
37	B2	1002	ADP	C3'-C2'-C1'	3.54	106.31	100.98
29	A3	501	CDL	OA6-CA5-C11	3.54	119.13	111.50
37	B5	1002	ADP	C3'-C2'-C1'	3.54	106.30	100.98
29	r	201	CDL	OA6-CA5-C11	3.52	119.08	111.50
29	B3	401	CDL	OB6-CB5-C51	3.50	119.05	111.50
29	r	201	CDL	OB6-CB5-C51	3.50	119.04	111.50
32	i	302	UQ8	C30-C29-C31	3.49	121.15	115.27
32	i3	303	UQ8	C25-C24-C26	3.49	121.15	115.27
33	B5	1003	ATP	C3'-C2'-C1'	3.49	106.23	100.98
30	g	304	PC1	O21-C21-C22	3.49	119.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j3	302	CDL	OA6-CA5-C11	3.49	119.01	111.50
29	K3	202	CDL	OB6-CB5-C51	3.44	118.91	111.50
35	m	301	PEE	O2-C10-C11	3.41	118.84	111.50
30	g3	304	PC1	O21-C21-C22	3.37	118.76	111.50
32	i3	303	UQ8	C30-C29-C31	3.36	120.92	115.27
32	i	302	UQ8	C25-C24-C26	3.36	120.92	115.27
29	B	401	CDL	OB6-CB5-C51	3.34	118.69	111.50
35	j3	303	PEE	O2-C10-C11	3.33	118.69	111.50
29	F	302	CDL	OB6-CB5-C51	3.32	118.65	111.50
29	i3	301	CDL	OB6-CB5-C51	3.31	118.63	111.50
33	B1	1003	ATP	C3'-C2'-C1'	3.30	105.95	100.98
29	l3	303	CDL	OA6-CA5-C11	3.28	118.57	111.50
32	i3	303	UQ8	C17-C18-C19	-3.28	119.77	127.66
32	I	303	UQ8	C20-C19-C21	3.27	120.78	115.27
33	B4	1003	ATP	C3'-C2'-C1'	3.27	105.90	100.98
29	l	302	CDL	OA6-CA5-C11	3.27	118.54	111.50
32	I	303	UQ8	C17-C18-C19	-3.25	119.83	127.66
32	I3	304	UQ8	C17-C18-C19	-3.21	119.94	127.66
33	B2	1003	ATP	C3'-C2'-C1'	3.20	105.79	100.98
32	i	302	UQ8	C17-C18-C19	-3.20	119.97	127.66
32	i3	303	UQ8	C20-C19-C21	3.19	120.64	115.27
33	A2	601	ATP	C3'-C2'-C1'	3.17	105.75	100.98
32	I3	304	UQ8	C7-C8-C9	-3.16	121.53	126.79
29	i3	302	CDL	OB8-CB7-C71	3.08	121.57	111.91
32	i3	303	UQ8	C22-C23-C24	-3.03	120.36	127.66
32	I	303	UQ8	C12-C13-C14	-3.03	120.36	127.66
32	i	302	UQ8	C20-C19-C21	3.03	120.37	115.27
29	b3	401	CDL	OA8-CA7-C31	3.03	121.41	111.91
29	i	301	CDL	OB8-CB7-C71	3.02	121.38	111.91
33	A4	601	ATP	C3'-C2'-C1'	3.02	105.52	100.98
32	I	303	UQ8	C7-C8-C9	-3.01	121.77	126.79
33	C4	601	ATP	C3'-C2'-C1'	3.01	105.52	100.98
37	D4	501	ADP	C2'-C3'-C4'	3.01	108.50	102.64
32	I3	304	UQ8	C20-C19-C21	2.99	120.30	115.27
33	C2	601	ATP	C3'-C2'-C1'	2.98	105.47	100.98
33	G3	301	ATP	PB-O3B-PG	-2.98	122.59	132.83
29	b	401	CDL	OA8-CA7-C31	2.97	121.23	111.91
33	g	301	ATP	PB-O3B-PG	-2.96	122.67	132.83
35	L3	302	PEE	O3-C30-C31	2.95	121.15	111.91
37	D1	501	ADP	PA-O3A-PB	-2.94	122.73	132.83
32	i	302	UQ8	C22-C23-C24	-2.93	120.60	127.66
33	G	301	ATP	PB-O3B-PG	-2.93	122.78	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	302	UQ8	C7-C8-C9	-2.92	121.94	126.79
35	J	303	PEE	O3-C30-C31	2.89	120.99	111.91
32	i	302	UQ8	C40-C39-C41	2.89	120.13	115.27
33	g3	301	ATP	PB-O3B-PG	-2.88	122.95	132.83
37	D4	501	ADP	PA-O3A-PB	-2.88	122.95	132.83
29	i3	301	CDL	OA8-CA7-C31	2.87	120.91	111.91
29	B3	402	CDL	OA8-CA7-C31	2.86	120.90	111.91
32	I	303	UQ8	C22-C23-C24	-2.85	120.79	127.66
32	i3	303	UQ8	C40-C39-C38	-2.85	116.37	123.68
29	r	201	CDL	OB8-CB7-C71	2.85	120.85	111.91
29	K3	201	CDL	OB8-CB7-C71	2.84	120.83	111.91
32	i3	303	UQ8	C40-C39-C41	2.84	120.04	115.27
33	C1	601	ATP	C3'-C2'-C1'	2.83	105.25	100.98
37	D1	501	ADP	C2'-C3'-C4'	2.83	108.15	102.64
29	l3	301	CDL	OB8-CB7-C71	2.83	120.79	111.91
32	I3	304	UQ8	C12-C13-C14	-2.83	120.86	127.66
32	I	303	UQ8	C1M-C1-C6	-2.82	119.79	124.40
29	B3	404	CDL	OB8-CB7-C71	2.82	120.75	111.91
33	B1	1003	ATP	PB-O3B-PG	-2.81	123.17	132.83
36	E	900	NAD	PN-O3-PA	-2.81	123.17	132.83
29	I	302	CDL	OA8-CA7-C31	2.80	120.71	111.91
29	l	301	CDL	OA8-CA7-C31	2.79	120.65	111.91
29	F	303	CDL	OB8-CB7-C71	2.79	120.65	111.91
35	m	301	PEE	O3-C30-C31	2.78	120.65	111.91
32	i	302	UQ8	C32-C33-C34	-2.78	120.96	127.66
29	K	202	CDL	OA8-CA7-C31	2.78	120.64	111.91
36	e	900	NAD	C3D-C2D-C1D	2.78	105.16	100.98
32	i	302	UQ8	C40-C39-C38	-2.78	116.56	123.68
33	B4	1003	ATP	PB-O3B-PG	-2.77	123.32	132.83
37	D5	501	ADP	PA-O3A-PB	-2.77	123.33	132.83
29	f	303	CDL	OB8-CB7-C71	2.77	120.59	111.91
29	B	402	CDL	OA8-CA7-C31	2.77	120.59	111.91
30	D	301	PC1	O31-C31-C32	2.76	120.58	111.91
33	B5	1003	ATP	PB-O3B-PG	-2.76	123.36	132.83
32	i3	303	UQ8	C32-C33-C34	-2.76	121.02	127.66
29	K	201	CDL	OB8-CB7-C71	2.75	120.55	111.91
33	A1	601	ATP	PA-O3A-PB	-2.74	123.41	132.83
36	E3	900	NAD	C3D-C2D-C1D	2.74	105.11	100.98
36	E3	900	NAD	PN-O3-PA	-2.74	123.43	132.83
29	A	502	CDL	OA8-CA7-C31	2.74	120.50	111.91
37	B4	1002	ADP	PA-O3A-PB	-2.74	123.44	132.83
33	C1	601	ATP	PB-O3B-PG	-2.73	123.44	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D3	301	PC1	O31-C31-C32	2.73	120.49	111.91
29	i3	301	CDL	OB8-CB7-C71	2.73	120.48	111.91
33	A2	601	ATP	PB-O3B-PG	-2.73	123.46	132.83
33	C4	601	ATP	PB-O3B-PG	-2.73	123.46	132.83
29	B3	404	CDL	OA8-CA7-C31	2.73	120.47	111.91
37	B2	1002	ADP	PA-O3A-PB	-2.73	123.47	132.83
29	p3	201	CDL	OB8-CB7-C71	2.72	120.46	111.91
29	B3	403	CDL	OB8-CB7-C71	2.72	120.45	111.91
29	p	201	CDL	OB8-CB7-C71	2.72	120.44	111.91
37	D2	501	ADP	PA-O3A-PB	-2.72	123.50	132.83
33	C5	601	ATP	PB-O3B-PG	-2.72	123.50	132.83
29	l3	301	CDL	OA8-CA7-C31	2.71	120.43	111.91
29	F3	302	CDL	OA8-CA7-C31	2.71	120.41	111.91
33	A5	601	ATP	PA-O3A-PB	-2.71	123.53	132.83
30	g3	304	PC1	O31-C31-C32	2.71	120.40	111.91
37	B5	1002	ADP	PA-O3A-PB	-2.71	123.54	132.83
33	B2	1003	ATP	PB-O3B-PG	-2.70	123.55	132.83
29	k	201	CDL	OB8-CB7-C71	2.70	120.39	111.91
33	A4	601	ATP	PB-O3B-PG	-2.70	123.55	132.83
29	r	201	CDL	OA8-CA7-C31	2.70	120.39	111.91
32	I3	304	UQ8	C22-C23-C24	-2.70	121.17	127.66
33	C2	601	ATP	PB-O3B-PG	-2.69	123.59	132.83
29	f3	303	CDL	OB8-CB7-C71	2.69	120.35	111.91
29	B	404	CDL	OA8-CA7-C31	2.69	120.35	111.91
29	J	301	CDL	OB8-CB7-C71	2.69	120.34	111.91
29	B	404	CDL	OB8-CB7-C71	2.68	120.33	111.91
33	A1	601	ATP	PB-O3B-PG	-2.68	123.62	132.83
37	B1	1002	ADP	PA-O3A-PB	-2.68	123.63	132.83
29	J	301	CDL	OA8-CA7-C31	2.68	120.32	111.91
33	A5	601	ATP	PB-O3B-PG	-2.68	123.63	132.83
33	A4	601	ATP	PA-O3A-PB	-2.68	123.64	132.83
29	b3	401	CDL	OB8-CB7-C71	2.67	120.30	111.91
29	k3	201	CDL	OA8-CA7-C31	2.67	120.30	111.91
29	j3	302	CDL	OB8-CB7-C71	2.67	120.29	111.91
29	A3	501	CDL	OA8-CA7-C31	2.67	120.28	111.91
29	i3	302	CDL	OA8-CA7-C31	2.67	120.28	111.91
33	C5	601	ATP	C3'-C2'-C1'	2.67	104.99	100.98
37	D5	501	ADP	C2'-C3'-C4'	2.66	107.82	102.64
30	G	303	PC1	O31-C31-C32	2.66	120.26	111.91
29	g3	305	CDL	OA8-CA7-C31	2.66	120.24	111.91
29	b	401	CDL	OB8-CB7-C71	2.65	120.23	111.91
35	j3	303	PEE	O3-C30-C31	2.65	120.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l3	302	PEE	O3-C30-C31	2.65	120.22	111.91
29	J3	301	CDL	OA8-CA7-C31	2.65	120.22	111.91
37	D2	501	ADP	C2'-C3'-C4'	2.65	107.78	102.64
29	g	305	CDL	OA8-CA7-C31	2.65	120.21	111.91
37	D5	501	ADP	C3'-C2'-C1'	2.65	104.96	100.98
33	C2	601	ATP	PA-O3A-PB	-2.64	123.75	132.83
32	i3	303	UQ8	C7-C8-C9	-2.64	122.39	126.79
29	K	201	CDL	OA8-CA7-C31	2.64	120.19	111.91
29	l	301	CDL	OB8-CB7-C71	2.64	120.18	111.91
29	L	301	CDL	OB8-CB7-C71	2.64	120.18	111.91
29	B	403	CDL	OB8-CB7-C71	2.63	120.18	111.91
29	F	303	CDL	OA8-CA7-C31	2.63	120.17	111.91
29	J	302	CDL	OB8-CB7-C71	2.63	120.17	111.91
29	j	302	CDL	OB8-CB7-C71	2.63	120.16	111.91
29	I3	303	CDL	OA8-CA7-C31	2.63	120.15	111.91
33	C5	601	ATP	PA-O3A-PB	-2.62	123.83	132.83
29	I3	301	CDL	OA8-CA7-C31	2.62	120.14	111.91
30	d	301	PC1	O31-C31-C32	2.62	120.13	111.91
29	a3	501	CDL	OB8-CB7-C71	2.62	120.12	111.91
30	g	304	PC1	O31-C31-C32	2.62	120.12	111.91
36	e3	900	NAD	PN-O3-PA	-2.62	123.85	132.83
32	I3	304	UQ8	C1M-C1-C6	-2.61	120.14	124.40
29	F3	302	CDL	OB8-CB7-C71	2.61	120.11	111.91
29	g	305	CDL	OB8-CB7-C71	2.61	120.10	111.91
32	i	302	UQ8	C35-C34-C36	2.61	119.66	115.27
33	A2	601	ATP	PA-O3A-PB	-2.61	123.88	132.83
29	j	301	CDL	OA8-CA7-C31	2.61	120.08	111.91
29	B3	402	CDL	OB8-CB7-C71	2.60	120.08	111.91
29	j3	302	CDL	OA8-CA7-C31	2.59	120.05	111.91
29	j3	301	CDL	OA8-CA7-C31	2.59	120.03	111.91
30	d3	301	PC1	O31-C31-C32	2.58	120.01	111.91
29	L3	301	CDL	OB8-CB7-C71	2.58	120.00	111.91
33	A5	601	ATP	C3'-C2'-C1'	2.57	104.85	100.98
29	L3	301	CDL	OA8-CA7-C31	2.57	119.98	111.91
33	C1	601	ATP	PA-O3A-PB	-2.57	124.02	132.83
29	f3	303	CDL	OA8-CA7-C31	2.57	119.96	111.91
29	I3	301	CDL	OB8-CB7-C71	2.56	119.95	111.91
29	J	302	CDL	OA8-CA7-C31	2.56	119.94	111.91
29	J3	302	CDL	OB8-CB7-C71	2.56	119.93	111.91
30	G	304	PC1	O31-C31-C32	2.56	119.93	111.91
29	a	501	CDL	OB8-CB7-C71	2.55	119.92	111.91
29	f3	302	CDL	OA8-CA7-C31	2.55	119.92	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I3	303	CDL	OB8-CB7-C71	2.55	119.91	111.91
30	g3	303	PC1	O31-C31-C32	2.55	119.91	111.91
36	e	900	NAD	PN-O3-PA	-2.55	124.09	132.83
29	L	301	CDL	OA8-CA7-C31	2.54	119.88	111.91
29	K3	202	CDL	OA8-CA7-C31	2.53	119.86	111.91
29	K	202	CDL	OB8-CB7-C71	2.53	119.86	111.91
29	I3	302	CDL	OA8-CA7-C31	2.53	119.85	111.91
33	C4	601	ATP	PA-O3A-PB	-2.53	124.15	132.83
29	g3	305	CDL	OB8-CB7-C71	2.53	119.84	111.91
29	A	502	CDL	OB8-CB7-C71	2.52	119.83	111.91
32	i3	303	UQ8	C1M-C1-C6	-2.52	120.29	124.40
32	i3	303	UQ8	C27-C28-C29	-2.52	121.59	127.66
29	f	302	CDL	OA8-CA7-C31	2.52	119.81	111.91
29	J3	301	CDL	OB8-CB7-C71	2.52	119.80	111.91
32	I	303	UQ8	C37-C38-C39	-2.51	121.61	127.66
36	e3	900	NAD	C3D-C2D-C1D	2.51	104.76	100.98
33	G3	301	ATP	PA-O3A-PB	-2.50	124.26	132.83
30	G3	304	PC1	O31-C31-C32	2.50	119.74	111.91
33	G	301	ATP	PA-O3A-PB	-2.50	124.26	132.83
29	k3	201	CDL	OB8-CB7-C71	2.50	119.74	111.91
35	A	501	PEE	O3-C30-C31	2.49	119.74	111.91
32	i	302	UQ8	C1M-C1-C6	-2.49	120.33	124.40
29	i	301	CDL	OA8-CA7-C31	2.49	119.73	111.91
29	f	303	CDL	OA8-CA7-C31	2.49	119.72	111.91
32	I	303	UQ8	C27-C28-C29	-2.49	121.67	127.66
29	K3	202	CDL	OB8-CB7-C71	2.48	119.70	111.91
33	B1	1003	ATP	PA-O3A-PB	-2.48	124.32	132.83
29	l3	303	CDL	OA8-CA7-C31	2.48	119.69	111.91
33	A1	601	ATP	C3'-C2'-C1'	2.47	104.70	100.98
33	g3	301	ATP	PA-O3A-PB	-2.47	124.36	132.83
32	I	303	UQ8	C15-C14-C16	2.47	119.42	115.27
29	a	501	CDL	OA8-CA7-C31	2.46	119.64	111.91
32	i3	303	UQ8	C35-C34-C36	2.46	119.41	115.27
29	I	302	CDL	OB8-CB7-C71	2.46	119.63	111.91
29	l	302	CDL	OA8-CA7-C31	2.45	119.60	111.91
37	D2	501	ADP	C3'-C2'-C1'	2.45	104.67	100.98
29	P3	201	CDL	OB8-CB7-C71	2.45	119.59	111.91
32	I3	304	UQ8	C27-C28-C29	-2.45	121.77	127.66
29	P3	201	CDL	OA8-CA7-C31	2.44	119.57	111.91
33	B5	1003	ATP	PA-O3A-PB	-2.44	124.45	132.83
33	g	301	ATP	PA-O3A-PB	-2.44	124.45	132.83
33	B4	1003	ATP	PA-O3A-PB	-2.44	124.45	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	g	303	PC1	O31-C31-C32	2.44	119.56	111.91
29	B	402	CDL	OB8-CB7-C71	2.43	119.55	111.91
29	f3	304	CDL	OB8-CB7-C71	2.43	119.52	111.91
36	E	900	NAD	C3D-C2D-C1D	2.43	104.63	100.98
32	i	302	UQ8	C27-C28-C29	-2.42	121.83	127.66
29	K3	201	CDL	OA8-CA7-C31	2.41	119.48	111.91
29	j	301	CDL	OB8-CB7-C71	2.41	119.47	111.91
29	B3	403	CDL	OA8-CA7-C31	2.41	119.47	111.91
29	a3	502	CDL	OB8-CB7-C71	2.41	119.47	111.91
29	p	201	CDL	OA8-CA7-C31	2.41	119.46	111.91
29	P	201	CDL	OB8-CB7-C71	2.41	119.46	111.91
29	j3	301	CDL	OB8-CB7-C71	2.40	119.45	111.91
33	B2	1003	ATP	PA-O3A-PB	-2.40	124.58	132.83
29	k	201	CDL	OA8-CA7-C31	2.40	119.44	111.91
29	P	201	CDL	OA8-CA7-C31	2.40	119.43	111.91
29	p3	201	CDL	OA8-CA7-C31	2.39	119.42	111.91
29	F	302	CDL	OB8-CB7-C71	2.39	119.41	111.91
29	I	301	CDL	OB8-CB7-C71	2.39	119.41	111.91
29	L	302	CDL	OB8-CB7-C71	2.39	119.41	111.91
29	I	301	CDL	OA8-CA7-C31	2.39	119.40	111.91
29	B3	401	CDL	OA8-CA7-C31	2.38	119.39	111.91
30	G3	303	PC1	O31-C31-C32	2.38	119.38	111.91
29	f	302	CDL	OB8-CB7-C71	2.38	119.37	111.91
35	L	303	PEE	O3-C30-C31	2.38	119.36	111.91
29	f3	304	CDL	OA8-CA7-C31	2.37	119.36	111.91
29	A3	501	CDL	OB8-CB7-C71	2.37	119.34	111.91
32	i3	303	UQ8	C12-C13-C14	-2.37	121.97	127.66
29	B	401	CDL	OA8-CA7-C31	2.36	119.32	111.91
32	i3	303	UQ8	C46-C44-C45	2.36	119.81	114.60
29	f	304	CDL	OB8-CB7-C71	2.34	119.25	111.91
29	a3	501	CDL	OA8-CA7-C31	2.32	119.19	111.91
29	B	403	CDL	OA8-CA7-C31	2.32	119.18	111.91
32	i	302	UQ8	C46-C44-C45	2.31	119.71	114.60
29	I3	302	CDL	OB8-CB7-C71	2.31	119.16	111.91
33	B5	1003	ATP	C2'-C3'-C4'	2.31	107.12	102.64
29	L	302	CDL	OA8-CA7-C31	2.30	119.13	111.91
29	J3	302	CDL	OA8-CA7-C31	2.30	119.11	111.91
29	j	302	CDL	OA8-CA7-C31	2.30	119.11	111.91
29	f	304	CDL	OA8-CA7-C31	2.29	119.11	111.91
32	I3	304	UQ8	C37-C38-C39	-2.26	122.22	127.66
32	I	303	UQ8	C46-C44-C45	2.26	119.60	114.60
29	P	201	CDL	CA4-OA6-CA5	-2.25	112.26	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B2	1003	ATP	C2'-C3'-C4'	2.25	107.01	102.64
29	f3	302	CDL	OB8-CB7-C71	2.24	118.92	111.91
33	B1	1003	ATP	C2'-C3'-C4'	2.23	106.97	102.64
29	a3	502	CDL	OA8-CA7-C31	2.22	118.89	111.91
29	K3	202	CDL	CA4-OA6-CA5	-2.21	112.36	117.79
29	B	402	CDL	CB6-CB4-CB3	-2.20	106.58	111.79
32	I3	304	UQ8	C15-C14-C16	2.20	118.98	115.27
35	J	303	PEE	C40-C39-C38	-2.20	107.86	124.73
32	I	303	UQ8	C10-C9-C11	2.19	118.96	115.27
33	B4	1003	ATP	C2'-C3'-C4'	2.19	106.90	102.64
32	i3	303	UQ8	C42-C43-C44	-2.18	120.28	127.75
32	I3	304	UQ8	C46-C44-C45	2.18	119.42	114.60
32	i	302	UQ8	C42-C43-C44	-2.17	120.33	127.75
32	I	303	UQ8	C42-C43-C44	-2.17	120.33	127.75
35	a3	503	PEE	O3-C30-C31	2.17	118.70	111.91
29	a	501	CDL	OB6-CB5-OB7	-2.15	118.50	123.70
32	I3	304	UQ8	C35-C34-C33	-2.14	118.18	123.68
35	m	301	PEE	C17-C18-C19	-2.13	108.40	124.73
32	I3	304	UQ8	C42-C43-C44	-2.13	120.48	127.75
35	m	301	PEE	C40-C39-C38	-2.12	108.43	124.73
29	B	401	CDL	OB8-CB7-C71	2.12	118.57	111.91
29	F	302	CDL	OA8-CA7-C31	2.12	118.56	111.91
35	j3	303	PEE	C17-C18-C19	-2.12	108.47	124.73
29	B3	401	CDL	OB8-CB7-C71	2.11	118.52	111.91
32	i	302	UQ8	C12-C13-C14	-2.09	122.62	127.66
36	E	900	NAD	C6N-N1N-C2N	-2.09	120.07	121.97
29	a3	502	CDL	C41-C40-C39	-2.09	103.82	114.42
35	L3	302	PEE	C17-C18-C19	-2.09	108.72	124.73
36	e3	900	NAD	C6N-N1N-C2N	-2.08	120.08	121.97
32	i	302	UQ8	C15-C14-C16	2.08	118.77	115.27
32	I3	304	UQ8	C30-C29-C31	2.08	118.77	115.27
35	j3	303	PEE	C40-C39-C38	-2.08	108.78	124.73
29	a3	501	CDL	OB6-CB5-OB7	-2.07	118.70	123.70
29	F	302	CDL	C41-C40-C39	-2.07	103.94	114.42
29	B3	404	CDL	CB6-CB4-CB3	-2.07	106.90	111.79
36	E3	900	NAD	C6N-N1N-C2N	-2.06	120.09	121.97
37	B4	1002	ADP	C2'-C3'-C4'	2.06	106.64	102.64
29	B3	402	CDL	OB6-CB5-OB7	-2.05	118.75	123.70
36	e	900	NAD	C6N-N1N-C2N	-2.05	120.11	121.97
35	L3	302	PEE	C40-C39-C38	-2.04	109.04	124.73
35	j3	303	PEE	C37-C38-C39	-2.04	109.08	124.73
37	B1	1002	ADP	C2'-C3'-C4'	2.04	106.60	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a3	503	PEE	C17-C18-C19	-2.04	109.11	124.73
35	L	303	PEE	C40-C39-C38	-2.03	109.14	124.73
29	f	303	CDL	CA6-CA4-CA3	-2.03	106.99	111.79
32	I	303	UQ8	C35-C34-C33	-2.03	118.47	123.68
32	i3	303	UQ8	C15-C14-C16	2.02	118.67	115.27
29	l3	303	CDL	CB4-OB6-CB5	-2.02	112.82	117.79
35	J	303	PEE	C17-C18-C19	-2.01	109.30	124.73
35	a3	503	PEE	C37-C38-C39	-2.01	109.33	124.73
29	B	404	CDL	CA6-CA4-CA3	-2.00	107.05	111.79

There are no chirality outliers.

All (2998) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4
29	b	401	CDL	CB3-OB5-PB2-OB4
29	b	401	CDL	OB7-CB5-OB6-CB4
29	b	401	CDL	C51-CB5-OB6-CB4
29	f	302	CDL	C1-CA2-OA2-PA1
29	f	302	CDL	CA4-CA3-OA5-PA1
29	f	302	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	CB2-OB2-PB2-OB3
29	f	302	CDL	CB2-OB2-PB2-OB4
29	f	302	CDL	CB2-OB2-PB2-OB5
29	f	302	CDL	CB3-OB5-PB2-OB2
29	f	302	CDL	CB3-OB5-PB2-OB3
29	f	302	CDL	CB3-OB5-PB2-OB4
29	f	303	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	CB3-OB5-PB2-OB2
29	f	303	CDL	CB3-OB5-PB2-OB3
29	f	303	CDL	CB3-OB5-PB2-OB4
29	f	303	CDL	OB6-CB4-CB6-OB8
29	f	303	CDL	C51-CB5-OB6-CB4
29	f	304	CDL	C1-CA2-OA2-PA1
29	f	304	CDL	CA3-OA5-PA1-OA3
29	f	304	CDL	OA5-CA3-CA4-OA6
29	f	304	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	CB3-OB5-PB2-OB2
29	i	301	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	i	301	CDL	OB7-CB5-OB6-CB4
29	k	201	CDL	CA3-OA5-PA1-OA3
29	k	201	CDL	OA7-CA5-OA6-CA4
29	k	201	CDL	C11-CA5-OA6-CA4
29	k	201	CDL	CB2-OB2-PB2-OB4
29	k	201	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB3-OB5-PB2-OB4
29	g	305	CDL	OA5-CA3-CA4-OA6
29	g	305	CDL	CB3-OB5-PB2-OB2
29	g	305	CDL	CB3-OB5-PB2-OB3
29	g	305	CDL	CB3-OB5-PB2-OB4
29	j	301	CDL	CB3-OB5-PB2-OB3
29	j	302	CDL	CA3-OA5-PA1-OA4
29	j	302	CDL	CB3-OB5-PB2-OB2
29	j	302	CDL	CB3-OB5-PB2-OB3
29	j	302	CDL	CB3-OB5-PB2-OB4
29	l	302	CDL	CB3-OB5-PB2-OB3
29	p	201	CDL	CA2-OA2-PA1-OA3
29	p	201	CDL	CA3-OA5-PA1-OA3
29	p	201	CDL	C11-CA5-OA6-CA4
29	p	201	CDL	CB2-OB2-PB2-OB3
29	p	201	CDL	CB3-OB5-PB2-OB2
29	p	201	CDL	CB3-OB5-PB2-OB3
29	p	201	CDL	CB3-OB5-PB2-OB4
29	r	201	CDL	CA3-OA5-PA1-OA2
29	r	201	CDL	CB2-OB2-PB2-OB3
29	A	502	CDL	C1-CA2-OA2-PA1
29	A	502	CDL	C11-CA5-OA6-CA4
29	A	502	CDL	CB3-OB5-PB2-OB2
29	A	502	CDL	CB3-OB5-PB2-OB3
29	A	502	CDL	CB3-OB5-PB2-OB4
29	A	502	CDL	C51-CB5-OB6-CB4
29	B	401	CDL	CA4-CA3-OA5-PA1
29	B	401	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	OA7-CA5-OA6-CA4
29	B	402	CDL	CB3-OB5-PB2-OB2
29	B	402	CDL	CB3-OB5-PB2-OB3
29	B	402	CDL	CB3-OB5-PB2-OB4
29	B	402	CDL	OB7-CB5-OB6-CB4
29	B	402	CDL	C51-CB5-OB6-CB4
29	B	404	CDL	O1-C1-CB2-OB2
29	B	404	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
29	B	404	CDL	C11-CA5-OA6-CA4
29	B	404	CDL	OA9-CA7-OA8-CA6
29	B	404	CDL	CB3-OB5-PB2-OB2
29	B	404	CDL	CB3-OB5-PB2-OB3
29	B	404	CDL	CB3-OB5-PB2-OB4
29	B	404	CDL	OB6-CB4-CB6-OB8
29	F	302	CDL	CA3-OA5-PA1-OA3
29	F	303	CDL	CB2-OB2-PB2-OB3
29	F	303	CDL	CB2-OB2-PB2-OB5
29	F	303	CDL	CB3-OB5-PB2-OB3
29	F	303	CDL	CB3-OB5-PB2-OB4
29	F	303	CDL	OB7-CB5-OB6-CB4
29	I	301	CDL	CB2-C1-CA2-OA2
29	I	301	CDL	CA3-OA5-PA1-OA3
29	I	301	CDL	CA3-OA5-PA1-OA4
29	I	301	CDL	CB3-OB5-PB2-OB3
29	I	301	CDL	CB3-OB5-PB2-OB4
29	I	302	CDL	CA3-OA5-PA1-OA2
29	I	302	CDL	CB3-OB5-PB2-OB2
29	I	302	CDL	CB3-OB5-PB2-OB3
29	I	302	CDL	CB3-OB5-PB2-OB4
29	I	302	CDL	OB7-CB5-OB6-CB4
29	I	302	CDL	C51-CB5-OB6-CB4
29	K	201	CDL	CA3-OA5-PA1-OA3
29	K	201	CDL	OA7-CA5-OA6-CA4
29	K	201	CDL	C11-CA5-OA6-CA4
29	K	202	CDL	OA5-CA3-CA4-OA6
29	K	202	CDL	CB3-OB5-PB2-OB3
29	K	202	CDL	CB3-OB5-PB2-OB4
29	J	301	CDL	CA2-OA2-PA1-OA3
29	J	301	CDL	OB7-CB5-OB6-CB4
29	J	301	CDL	C51-CB5-OB6-CB4
29	J	302	CDL	CB3-OB5-PB2-OB3
29	J	302	CDL	CB3-OB5-PB2-OB4
29	L	301	CDL	CA3-OA5-PA1-OA3
29	L	301	CDL	C11-CA5-OA6-CA4
29	L	301	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CA3-OA5-PA1-OA3
29	L	302	CDL	CA3-OA5-PA1-OA4
29	P	201	CDL	C11-CA5-OA6-CA4
29	P	201	CDL	CB2-OB2-PB2-OB3
29	P	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
29	P	201	CDL	CB3-OB5-PB2-OB2
29	P	201	CDL	CB3-OB5-PB2-OB3
29	P	201	CDL	CB3-OB5-PB2-OB4
29	a3	501	CDL	OA5-CA3-CA4-OA6
29	a3	501	CDL	CB3-OB5-PB2-OB4
29	a3	501	CDL	OB7-CB5-OB6-CB4
29	a3	501	CDL	C51-CB5-OB6-CB4
29	a3	502	CDL	CA3-OA5-PA1-OA3
29	b3	401	CDL	CB3-OB5-PB2-OB4
29	b3	401	CDL	OB7-CB5-OB6-CB4
29	b3	401	CDL	C51-CB5-OB6-CB4
29	f3	302	CDL	C1-CA2-OA2-PA1
29	f3	302	CDL	CA4-CA3-OA5-PA1
29	f3	302	CDL	C11-CA5-OA6-CA4
29	f3	302	CDL	CB2-OB2-PB2-OB3
29	f3	302	CDL	CB2-OB2-PB2-OB4
29	f3	302	CDL	CB2-OB2-PB2-OB5
29	f3	302	CDL	CB3-OB5-PB2-OB2
29	f3	302	CDL	CB3-OB5-PB2-OB3
29	f3	302	CDL	CB3-OB5-PB2-OB4
29	f3	303	CDL	OA7-CA5-OA6-CA4
29	f3	303	CDL	CB3-OB5-PB2-OB2
29	f3	303	CDL	CB3-OB5-PB2-OB3
29	f3	303	CDL	CB3-OB5-PB2-OB4
29	f3	303	CDL	OB6-CB4-CB6-OB8
29	f3	303	CDL	C51-CB5-OB6-CB4
29	f3	304	CDL	C1-CA2-OA2-PA1
29	f3	304	CDL	CA3-OA5-PA1-OA3
29	f3	304	CDL	OA5-CA3-CA4-OA6
29	f3	304	CDL	C51-CB5-OB6-CB4
29	i3	301	CDL	CA3-OA5-PA1-OA2
29	i3	301	CDL	CB2-OB2-PB2-OB3
29	i3	302	CDL	CB3-OB5-PB2-OB2
29	i3	302	CDL	CB3-OB5-PB2-OB4
29	i3	302	CDL	OB7-CB5-OB6-CB4
29	k3	201	CDL	CA3-OA5-PA1-OA3
29	k3	201	CDL	OA7-CA5-OA6-CA4
29	k3	201	CDL	C11-CA5-OA6-CA4
29	k3	201	CDL	CB2-OB2-PB2-OB4
29	k3	201	CDL	CB3-OB5-PB2-OB3
29	k3	201	CDL	CB3-OB5-PB2-OB4
29	g3	305	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
29	g3	305	CDL	CB3-OB5-PB2-OB2
29	g3	305	CDL	CB3-OB5-PB2-OB3
29	g3	305	CDL	CB3-OB5-PB2-OB4
29	j3	301	CDL	CB3-OB5-PB2-OB3
29	j3	302	CDL	CA3-OA5-PA1-OA4
29	j3	302	CDL	CB3-OB5-PB2-OB2
29	j3	302	CDL	CB3-OB5-PB2-OB3
29	j3	302	CDL	CB3-OB5-PB2-OB4
29	l3	303	CDL	CB3-OB5-PB2-OB3
29	p3	201	CDL	CA2-OA2-PA1-OA3
29	p3	201	CDL	CA3-OA5-PA1-OA3
29	p3	201	CDL	C11-CA5-OA6-CA4
29	p3	201	CDL	CB2-OB2-PB2-OB3
29	p3	201	CDL	CB3-OB5-PB2-OB2
29	p3	201	CDL	CB3-OB5-PB2-OB3
29	p3	201	CDL	CB3-OB5-PB2-OB4
29	A3	501	CDL	C1-CA2-OA2-PA1
29	A3	501	CDL	C11-CA5-OA6-CA4
29	A3	501	CDL	CB3-OB5-PB2-OB2
29	A3	501	CDL	CB3-OB5-PB2-OB3
29	A3	501	CDL	CB3-OB5-PB2-OB4
29	A3	501	CDL	C51-CB5-OB6-CB4
29	B3	401	CDL	CA4-CA3-OA5-PA1
29	B3	401	CDL	C11-CA5-OA6-CA4
29	B3	402	CDL	OA7-CA5-OA6-CA4
29	B3	402	CDL	CB3-OB5-PB2-OB2
29	B3	402	CDL	CB3-OB5-PB2-OB3
29	B3	402	CDL	CB3-OB5-PB2-OB4
29	B3	402	CDL	OB7-CB5-OB6-CB4
29	B3	402	CDL	C51-CB5-OB6-CB4
29	B3	404	CDL	O1-C1-CB2-OB2
29	B3	404	CDL	CA2-C1-CB2-OB2
29	B3	404	CDL	C11-CA5-OA6-CA4
29	B3	404	CDL	OA9-CA7-OA8-CA6
29	B3	404	CDL	CB3-OB5-PB2-OB2
29	B3	404	CDL	CB3-OB5-PB2-OB3
29	B3	404	CDL	CB3-OB5-PB2-OB4
29	B3	404	CDL	OB6-CB4-CB6-OB8
29	F3	302	CDL	CB2-OB2-PB2-OB3
29	F3	302	CDL	CB2-OB2-PB2-OB5
29	F3	302	CDL	CB3-OB5-PB2-OB3
29	F3	302	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	F3	302	CDL	OB7-CB5-OB6-CB4
29	I3	301	CDL	CB2-C1-CA2-OA2
29	I3	301	CDL	CA3-OA5-PA1-OA3
29	I3	301	CDL	CA3-OA5-PA1-OA4
29	I3	301	CDL	CB3-OB5-PB2-OB3
29	I3	301	CDL	CB3-OB5-PB2-OB4
29	I3	302	CDL	CA3-OA5-PA1-OA3
29	I3	302	CDL	CA3-OA5-PA1-OA4
29	I3	303	CDL	CA3-OA5-PA1-OA2
29	I3	303	CDL	CB3-OB5-PB2-OB2
29	I3	303	CDL	CB3-OB5-PB2-OB3
29	I3	303	CDL	CB3-OB5-PB2-OB4
29	I3	303	CDL	OB7-CB5-OB6-CB4
29	K3	201	CDL	CA3-OA5-PA1-OA3
29	K3	201	CDL	OA7-CA5-OA6-CA4
29	K3	201	CDL	C11-CA5-OA6-CA4
29	K3	202	CDL	OA5-CA3-CA4-OA6
29	K3	202	CDL	CB3-OB5-PB2-OB3
29	K3	202	CDL	CB3-OB5-PB2-OB4
29	J3	301	CDL	CA2-OA2-PA1-OA3
29	J3	301	CDL	OB7-CB5-OB6-CB4
29	J3	301	CDL	C51-CB5-OB6-CB4
29	J3	302	CDL	CB3-OB5-PB2-OB3
29	J3	302	CDL	CB3-OB5-PB2-OB4
29	L3	301	CDL	CA3-OA5-PA1-OA3
29	L3	301	CDL	C11-CA5-OA6-CA4
29	L3	301	CDL	CB3-OB5-PB2-OB3
29	P3	201	CDL	C11-CA5-OA6-CA4
29	P3	201	CDL	CB2-OB2-PB2-OB3
29	P3	201	CDL	CB2-OB2-PB2-OB5
29	P3	201	CDL	CB3-OB5-PB2-OB2
29	P3	201	CDL	CB3-OB5-PB2-OB3
29	P3	201	CDL	CB3-OB5-PB2-OB4
30	d	301	PC1	C1-O11-P-O14
30	d	301	PC1	O13-C11-C12-N
30	d	301	PC1	O22-C21-O21-C2
30	g	303	PC1	O13-C11-C12-N
30	g	303	PC1	C2-C1-O11-P
30	g	304	PC1	O22-C21-O21-C2
30	g	304	PC1	C22-C21-O21-C2
30	D	301	PC1	C1-O11-P-O14
30	D	301	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
30	D	301	PC1	O22-C21-O21-C2
30	D	301	PC1	C22-C21-O21-C2
30	G	303	PC1	C1-O11-P-O12
30	G	304	PC1	O22-C21-O21-C2
30	d3	301	PC1	C1-O11-P-O14
30	d3	301	PC1	O13-C11-C12-N
30	d3	301	PC1	O22-C21-O21-C2
30	g3	303	PC1	O13-C11-C12-N
30	g3	303	PC1	C2-C1-O11-P
30	g3	304	PC1	O22-C21-O21-C2
30	g3	304	PC1	C22-C21-O21-C2
30	D3	301	PC1	C1-O11-P-O14
30	D3	301	PC1	O13-C11-C12-N
30	D3	301	PC1	O22-C21-O21-C2
30	D3	301	PC1	C22-C21-O21-C2
30	G3	303	PC1	C1-O11-P-O12
30	G3	304	PC1	O22-C21-O21-C2
32	i	302	UQ8	C34-C36-C37-C38
32	I	303	UQ8	C29-C31-C32-C33
32	i3	303	UQ8	C34-C36-C37-C38
32	I3	304	UQ8	C29-C31-C32-C33
33	B1	1003	ATP	C5'-O5'-PA-O1A
33	A1	601	ATP	C5'-O5'-PA-O3A
33	A1	601	ATP	C3'-C4'-C5'-O5'
33	C2	601	ATP	C5'-O5'-PA-O3A
33	B2	1003	ATP	C5'-O5'-PA-O1A
33	A2	601	ATP	C5'-O5'-PA-O3A
33	A2	601	ATP	C3'-C4'-C5'-O5'
33	B4	1003	ATP	C5'-O5'-PA-O1A
33	A4	601	ATP	C5'-O5'-PA-O3A
33	A4	601	ATP	C3'-C4'-C5'-O5'
33	C5	601	ATP	C5'-O5'-PA-O3A
33	B5	1003	ATP	C5'-O5'-PA-O1A
33	A5	601	ATP	C5'-O5'-PA-O3A
33	A5	601	ATP	C3'-C4'-C5'-O5'
35	m	301	PEE	C1-O3P-P-O2P
35	m	301	PEE	C4-O4P-P-O2P
35	m	301	PEE	C4-O4P-P-O1P
35	A	501	PEE	C1-O3P-P-O2P
35	A	501	PEE	C1-O3P-P-O1P
35	A	501	PEE	C4-O4P-P-O1P
35	J	303	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
35	J	303	PEE	C1-O3P-P-O2P
35	J	303	PEE	C4-O4P-P-O2P
35	J	303	PEE	C4-O4P-P-O1P
35	L	303	PEE	C1-O3P-P-O2P
35	L	303	PEE	C1-O3P-P-O1P
35	L	303	PEE	C4-O4P-P-O1P
35	a3	503	PEE	C1-O3P-P-O2P
35	a3	503	PEE	C1-O3P-P-O1P
35	a3	503	PEE	C4-O4P-P-O1P
35	j3	303	PEE	C1-O3P-P-O2P
35	j3	303	PEE	C4-O4P-P-O2P
35	j3	303	PEE	C4-O4P-P-O1P
35	l3	302	PEE	C1-O3P-P-O2P
35	l3	302	PEE	C1-O3P-P-O1P
35	l3	302	PEE	C4-O4P-P-O1P
35	L3	302	PEE	O2-C2-C3-O3
35	L3	302	PEE	C1-O3P-P-O2P
35	L3	302	PEE	C4-O4P-P-O2P
35	L3	302	PEE	C4-O4P-P-O1P
36	e	900	NAD	O4B-C4B-C5B-O5B
36	E	900	NAD	C5B-O5B-PA-O1A
36	E	900	NAD	O4D-C4D-C5D-O5D
36	E	900	NAD	O4D-C1D-N1N-C2N
36	e3	900	NAD	O4B-C4B-C5B-O5B
36	e3	900	NAD	O4D-C1D-N1N-C2N
36	E3	900	NAD	C5B-O5B-PA-O1A
37	D1	501	ADP	C5'-O5'-PA-O1A
37	D2	501	ADP	C5'-O5'-PA-O1A
37	B2	1002	ADP	PA-O3A-PB-O2B
37	D4	501	ADP	C5'-O5'-PA-O1A
37	D5	501	ADP	C5'-O5'-PA-O1A
37	B5	1002	ADP	PA-O3A-PB-O2B
37	B5	1002	ADP	PA-O3A-PB-O3B
29	B	403	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OB9-CB7-OB8-CB6
29	B3	403	CDL	OB9-CB7-OB8-CB6
29	I3	301	CDL	OB9-CB7-OB8-CB6
29	B	403	CDL	C71-CB7-OB8-CB6
29	B3	403	CDL	C71-CB7-OB8-CB6
35	m	301	PEE	C31-C30-O3-C3
35	j3	303	PEE	C31-C30-O3-C3
29	f	303	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	f	303	CDL	OB9-CB7-OB8-CB6
29	j	302	CDL	OA9-CA7-OA8-CA6
29	l	302	CDL	OB9-CB7-OB8-CB6
29	r	201	CDL	OA9-CA7-OA8-CA6
29	B	404	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OA9-CA7-OA8-CA6
29	J	302	CDL	OA9-CA7-OA8-CA6
29	f3	303	CDL	OA9-CA7-OA8-CA6
29	f3	303	CDL	OB9-CB7-OB8-CB6
29	i3	301	CDL	OA9-CA7-OA8-CA6
29	j3	302	CDL	OA9-CA7-OA8-CA6
29	l3	303	CDL	OB9-CB7-OB8-CB6
29	B3	404	CDL	OB9-CB7-OB8-CB6
29	I3	301	CDL	OA9-CA7-OA8-CA6
29	J3	302	CDL	OA9-CA7-OA8-CA6
35	m	301	PEE	O5-C30-O3-C3
35	A	501	PEE	O5-C30-O3-C3
35	L	303	PEE	O5-C30-O3-C3
35	a3	503	PEE	O5-C30-O3-C3
35	j3	303	PEE	O5-C30-O3-C3
35	l3	302	PEE	O5-C30-O3-C3
29	f	302	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	OB7-CB5-OB6-CB4
29	g	305	CDL	OA7-CA5-OA6-CA4
29	p	201	CDL	OA7-CA5-OA6-CA4
29	A	502	CDL	OA7-CA5-OA6-CA4
29	A	502	CDL	OB7-CB5-OB6-CB4
29	B	401	CDL	OA7-CA5-OA6-CA4
29	B	404	CDL	OA7-CA5-OA6-CA4
29	L	301	CDL	OA7-CA5-OA6-CA4
29	f3	302	CDL	OA7-CA5-OA6-CA4
29	f3	303	CDL	OB7-CB5-OB6-CB4
29	p3	201	CDL	OA7-CA5-OA6-CA4
29	A3	501	CDL	OA7-CA5-OA6-CA4
29	A3	501	CDL	OB7-CB5-OB6-CB4
29	B3	401	CDL	OA7-CA5-OA6-CA4
29	B3	404	CDL	OA7-CA5-OA6-CA4
29	L3	301	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	C31-CA7-OA8-CA6
29	f	303	CDL	C71-CB7-OB8-CB6
29	l	302	CDL	C71-CB7-OB8-CB6
29	r	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	B	404	CDL	C31-CA7-OA8-CA6
29	B	404	CDL	C71-CB7-OB8-CB6
29	I	301	CDL	C71-CB7-OB8-CB6
29	f3	303	CDL	C31-CA7-OA8-CA6
29	f3	303	CDL	C71-CB7-OB8-CB6
29	i3	301	CDL	C31-CA7-OA8-CA6
29	l3	303	CDL	C71-CB7-OB8-CB6
29	B3	404	CDL	C31-CA7-OA8-CA6
29	B3	404	CDL	C71-CB7-OB8-CB6
29	I3	301	CDL	C71-CB7-OB8-CB6
30	d	301	PC1	C32-C31-O31-C3
30	d3	301	PC1	C32-C31-O31-C3
29	f	303	CDL	C11-CA5-OA6-CA4
29	i	301	CDL	C51-CB5-OB6-CB4
29	g	305	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	C11-CA5-OA6-CA4
29	F	303	CDL	C51-CB5-OB6-CB4
29	f3	303	CDL	C11-CA5-OA6-CA4
29	i3	302	CDL	C51-CB5-OB6-CB4
29	g3	305	CDL	C11-CA5-OA6-CA4
29	B3	402	CDL	C11-CA5-OA6-CA4
29	F3	302	CDL	C51-CB5-OB6-CB4
29	I3	303	CDL	C51-CB5-OB6-CB4
30	d	301	PC1	C22-C21-O21-C2
30	G	304	PC1	C22-C21-O21-C2
30	d3	301	PC1	C22-C21-O21-C2
30	G3	304	PC1	C22-C21-O21-C2
29	r	201	CDL	OB9-CB7-OB8-CB6
29	i3	301	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	C31-CA7-OA8-CA6
29	f	304	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C31-CA7-OA8-CA6
29	I	301	CDL	C31-CA7-OA8-CA6
29	K	201	CDL	C71-CB7-OB8-CB6
29	K	202	CDL	C31-CA7-OA8-CA6
29	J	302	CDL	C31-CA7-OA8-CA6
29	f3	304	CDL	C31-CA7-OA8-CA6
29	f3	304	CDL	C71-CB7-OB8-CB6
29	j3	302	CDL	C31-CA7-OA8-CA6
29	I3	301	CDL	C31-CA7-OA8-CA6
29	K3	201	CDL	C71-CB7-OB8-CB6
29	K3	202	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	J3	302	CDL	C31-CA7-OA8-CA6
29	L3	301	CDL	C71-CB7-OB8-CB6
35	A	501	PEE	C31-C30-O3-C3
35	L	303	PEE	C31-C30-O3-C3
35	a3	503	PEE	C31-C30-O3-C3
35	l3	302	PEE	C31-C30-O3-C3
29	f	304	CDL	OB7-CB5-OB6-CB4
29	P	201	CDL	OA7-CA5-OA6-CA4
29	f3	304	CDL	OB7-CB5-OB6-CB4
29	g3	305	CDL	OA7-CA5-OA6-CA4
29	P3	201	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	OA9-CA7-OA8-CA6
29	F	302	CDL	OB9-CB7-OB8-CB6
29	K	201	CDL	OB9-CB7-OB8-CB6
29	K	202	CDL	OA9-CA7-OA8-CA6
29	a3	502	CDL	OB9-CB7-OB8-CB6
29	f3	304	CDL	OA9-CA7-OA8-CA6
29	K3	201	CDL	OB9-CB7-OB8-CB6
29	K3	202	CDL	OA9-CA7-OA8-CA6
29	B	402	CDL	O1-C1-CA2-OA2
29	B3	402	CDL	O1-C1-CA2-OA2
29	k	201	CDL	C71-CB7-OB8-CB6
29	g	305	CDL	C31-CA7-OA8-CA6
29	r	201	CDL	C71-CB7-OB8-CB6
29	L	301	CDL	C71-CB7-OB8-CB6
29	i3	301	CDL	C71-CB7-OB8-CB6
29	k3	201	CDL	C71-CB7-OB8-CB6
29	g3	305	CDL	C31-CA7-OA8-CA6
29	k	201	CDL	OB9-CB7-OB8-CB6
29	k3	201	CDL	OB9-CB7-OB8-CB6
30	d	301	PC1	O32-C31-O31-C3
30	d3	301	PC1	O32-C31-O31-C3
29	i	301	CDL	C11-CA5-OA6-CA4
29	r	201	CDL	C11-CA5-OA6-CA4
29	K	202	CDL	C11-CA5-OA6-CA4
29	i3	301	CDL	C11-CA5-OA6-CA4
29	i3	302	CDL	C11-CA5-OA6-CA4
29	K3	202	CDL	C11-CA5-OA6-CA4
29	K	201	CDL	C62-C63-C64-C65
29	f	304	CDL	OB9-CB7-OB8-CB6
29	f3	304	CDL	OB9-CB7-OB8-CB6
29	g3	305	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	I	302	CDL	C76-C77-C78-C79
29	I3	303	CDL	C76-C77-C78-C79
29	K3	201	CDL	C62-C63-C64-C65
33	A1	601	ATP	O4'-C4'-C5'-O5'
33	A2	601	ATP	O4'-C4'-C5'-O5'
33	A4	601	ATP	O4'-C4'-C5'-O5'
33	A5	601	ATP	O4'-C4'-C5'-O5'
36	e	900	NAD	O4D-C4D-C5D-O5D
36	e	900	NAD	C3D-C4D-C5D-O5D
36	E	900	NAD	O4B-C4B-C5B-O5B
36	e3	900	NAD	O4D-C4D-C5D-O5D
36	e3	900	NAD	C3D-C4D-C5D-O5D
36	E3	900	NAD	O4B-C4B-C5B-O5B
36	E3	900	NAD	O4D-C4D-C5D-O5D
29	F	302	CDL	C71-CB7-OB8-CB6
29	a3	502	CDL	C71-CB7-OB8-CB6
29	g	305	CDL	OA9-CA7-OA8-CA6
29	L3	301	CDL	OB9-CB7-OB8-CB6
29	L	301	CDL	OB9-CB7-OB8-CB6
32	I	303	UQ8	C34-C36-C37-C38
32	I3	304	UQ8	C34-C36-C37-C38
29	l	301	CDL	C31-CA7-OA8-CA6
29	l	301	CDL	C71-CB7-OB8-CB6
29	l3	301	CDL	C31-CA7-OA8-CA6
29	l3	301	CDL	C71-CB7-OB8-CB6
29	I	302	CDL	C22-C23-C24-C25
29	I3	303	CDL	C22-C23-C24-C25
29	f	304	CDL	C22-C23-C24-C25
29	B	403	CDL	CB2-C1-CA2-OA2
29	F	302	CDL	CB2-C1-CA2-OA2
29	a3	502	CDL	CB2-C1-CA2-OA2
29	B3	403	CDL	CB2-C1-CA2-OA2
29	K	202	CDL	OA7-CA5-OA6-CA4
29	K3	202	CDL	OA7-CA5-OA6-CA4
29	f3	304	CDL	C22-C23-C24-C25
29	B	401	CDL	C71-CB7-OB8-CB6
29	B3	401	CDL	C71-CB7-OB8-CB6
30	D	301	PC1	C32-C31-O31-C3
30	D3	301	PC1	C32-C31-O31-C3
29	b	401	CDL	C16-C17-C18-C19
29	b3	401	CDL	C16-C17-C18-C19
29	f	303	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
29	F	302	CDL	O1-C1-CA2-OA2
29	a3	502	CDL	O1-C1-CA2-OA2
29	f3	303	CDL	O1-C1-CB2-OB2
29	B	404	CDL	CB7-C71-C72-C73
29	B3	404	CDL	CB7-C71-C72-C73
30	D	301	PC1	O32-C31-O31-C3
30	D3	301	PC1	O32-C31-O31-C3
29	r	201	CDL	OA7-CA5-OA6-CA4
29	i3	301	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	C11-CA5-OA6-CA4
29	f3	304	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	CA5-C11-C12-C13
29	B3	402	CDL	CA5-C11-C12-C13
29	i	301	CDL	C31-CA7-OA8-CA6
29	I	302	CDL	C31-CA7-OA8-CA6
29	i3	302	CDL	C31-CA7-OA8-CA6
29	I3	303	CDL	C31-CA7-OA8-CA6
29	i	301	CDL	CB5-C51-C52-C53
29	B	404	CDL	CA5-C11-C12-C13
29	i3	302	CDL	CB5-C51-C52-C53
29	B3	404	CDL	CA5-C11-C12-C13
29	B	401	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	CA7-C31-C32-C33
29	f	303	CDL	CB7-C71-C72-C73
29	k	201	CDL	CA7-C31-C32-C33
29	l	302	CDL	CA5-C11-C12-C13
29	B	401	CDL	CA5-C11-C12-C13
29	P	201	CDL	CA5-C11-C12-C13
29	f3	302	CDL	CA7-C31-C32-C33
29	f3	303	CDL	CB7-C71-C72-C73
29	k3	201	CDL	CA7-C31-C32-C33
29	l3	303	CDL	CA5-C11-C12-C13
29	B3	401	CDL	CA5-C11-C12-C13
29	P3	201	CDL	CA5-C11-C12-C13
29	l	301	CDL	C54-C55-C56-C57
35	m	301	PEE	C43-C44-C45-C46
35	j3	303	PEE	C43-C44-C45-C46
36	e	900	NAD	C3B-C4B-C5B-O5B
36	E	900	NAD	C3B-C4B-C5B-O5B
36	E	900	NAD	C3D-C4D-C5D-O5D
36	e3	900	NAD	C3B-C4B-C5B-O5B
36	E3	900	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
36	E3	900	NAD	C3D-C4D-C5D-O5D
29	l3	301	CDL	C54-C55-C56-C57
29	i	301	CDL	OA7-CA5-OA6-CA4
29	i3	302	CDL	OA7-CA5-OA6-CA4
30	g	304	PC1	C21-C22-C23-C24
30	g3	304	PC1	C21-C22-C23-C24
29	B3	401	CDL	OB9-CB7-OB8-CB6
32	i	302	UQ8	C29-C31-C32-C33
32	i3	303	UQ8	C29-C31-C32-C33
29	B	403	CDL	O1-C1-CA2-OA2
29	B3	403	CDL	O1-C1-CA2-OA2
29	l	301	CDL	OA9-CA7-OA8-CA6
29	l	301	CDL	OB9-CB7-OB8-CB6
29	l3	301	CDL	OA9-CA7-OA8-CA6
29	l3	301	CDL	OB9-CB7-OB8-CB6
29	B	401	CDL	CB5-C51-C52-C53
29	B3	401	CDL	CB5-C51-C52-C53
29	i	301	CDL	OA9-CA7-OA8-CA6
29	I	302	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	OA9-CA7-OA8-CA6
29	J	301	CDL	C11-CA5-OA6-CA4
29	J3	301	CDL	C11-CA5-OA6-CA4
29	l	302	CDL	C20-C21-C22-C23
29	L	301	CDL	C81-C82-C83-C84
29	L	302	CDL	C40-C41-C42-C43
29	l3	303	CDL	C20-C21-C22-C23
29	I3	302	CDL	C40-C41-C42-C43
29	L3	301	CDL	C81-C82-C83-C84
29	a	501	CDL	CB3-OB5-PB2-OB2
29	f	302	CDL	CA2-OA2-PA1-OA5
29	f	303	CDL	CB2-OB2-PB2-OB5
29	i	301	CDL	CA3-OA5-PA1-OA2
29	k	201	CDL	CB2-OB2-PB2-OB5
29	k	201	CDL	CB3-OB5-PB2-OB2
29	g	305	CDL	CB2-OB2-PB2-OB5
29	j	302	CDL	CA3-OA5-PA1-OA2
29	l	301	CDL	CA3-OA5-PA1-OA2
29	l	301	CDL	CB3-OB5-PB2-OB2
29	r	201	CDL	CB2-OB2-PB2-OB5
29	B	401	CDL	CB3-OB5-PB2-OB2
29	B	404	CDL	CB2-OB2-PB2-OB5
29	F	303	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
29	I	301	CDL	CA3-OA5-PA1-OA2
29	I	301	CDL	CB2-OB2-PB2-OB5
29	K	201	CDL	CB2-OB2-PB2-OB5
29	K	202	CDL	CB3-OB5-PB2-OB2
29	J	301	CDL	CB3-OB5-PB2-OB2
29	J	302	CDL	CA3-OA5-PA1-OA2
29	J	302	CDL	CB3-OB5-PB2-OB2
29	L	301	CDL	CA3-OA5-PA1-OA2
29	L	301	CDL	CB3-OB5-PB2-OB2
29	L	302	CDL	CA3-OA5-PA1-OA2
29	L	302	CDL	CB3-OB5-PB2-OB2
29	a3	501	CDL	CB3-OB5-PB2-OB2
29	f3	302	CDL	CA2-OA2-PA1-OA5
29	f3	303	CDL	CB2-OB2-PB2-OB5
29	i3	301	CDL	CB2-OB2-PB2-OB5
29	i3	302	CDL	CA3-OA5-PA1-OA2
29	k3	201	CDL	CB2-OB2-PB2-OB5
29	k3	201	CDL	CB3-OB5-PB2-OB2
29	g3	305	CDL	CB2-OB2-PB2-OB5
29	j3	302	CDL	CA3-OA5-PA1-OA2
29	l3	301	CDL	CA3-OA5-PA1-OA2
29	l3	301	CDL	CB3-OB5-PB2-OB2
29	B3	401	CDL	CB3-OB5-PB2-OB2
29	B3	404	CDL	CB2-OB2-PB2-OB5
29	F3	302	CDL	CB3-OB5-PB2-OB2
29	I3	301	CDL	CA3-OA5-PA1-OA2
29	I3	301	CDL	CB2-OB2-PB2-OB5
29	I3	302	CDL	CA3-OA5-PA1-OA2
29	I3	302	CDL	CB3-OB5-PB2-OB2
29	K3	201	CDL	CB2-OB2-PB2-OB5
29	K3	202	CDL	CB3-OB5-PB2-OB2
29	J3	301	CDL	CB3-OB5-PB2-OB2
29	J3	302	CDL	CA3-OA5-PA1-OA2
29	J3	302	CDL	CB3-OB5-PB2-OB2
29	L3	301	CDL	CA3-OA5-PA1-OA2
29	L3	301	CDL	CB3-OB5-PB2-OB2
30	g	303	PC1	C1-O11-P-O13
30	g3	303	PC1	C1-O11-P-O13
35	m	301	PEE	C1-O3P-P-O4P
35	m	301	PEE	C4-O4P-P-O3P
35	A	501	PEE	C1-O3P-P-O4P
35	J	303	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
35	L	303	PEE	C1-O3P-P-O4P
35	a3	503	PEE	C1-O3P-P-O4P
35	j3	303	PEE	C1-O3P-P-O4P
35	j3	303	PEE	C4-O4P-P-O3P
35	l3	302	PEE	C1-O3P-P-O4P
35	L3	302	PEE	C1-O3P-P-O4P
35	L3	302	PEE	C4-O4P-P-O3P
29	F	302	CDL	CA5-C11-C12-C13
29	a3	502	CDL	CA5-C11-C12-C13
30	G	304	PC1	C32-C31-O31-C3
30	G3	304	PC1	C32-C31-O31-C3
29	I3	303	CDL	OA9-CA7-OA8-CA6
29	a	501	CDL	CA7-C31-C32-C33
29	a3	501	CDL	CA7-C31-C32-C33
30	g	303	PC1	C31-C32-C33-C34
30	g3	303	PC1	C31-C32-C33-C34
29	f	304	CDL	OA7-CA5-OA6-CA4
29	J	301	CDL	OA7-CA5-OA6-CA4
29	f3	304	CDL	OA7-CA5-OA6-CA4
29	J3	301	CDL	OA7-CA5-OA6-CA4
29	g	305	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C71-CB7-OB8-CB6
29	K	202	CDL	C71-CB7-OB8-CB6
29	g3	305	CDL	C71-CB7-OB8-CB6
29	j3	302	CDL	C71-CB7-OB8-CB6
29	K3	202	CDL	C71-CB7-OB8-CB6
35	A	501	PEE	C10-C11-C12-C13
35	L	303	PEE	C10-C11-C12-C13
35	a3	503	PEE	C10-C11-C12-C13
35	l3	302	PEE	C10-C11-C12-C13
29	j	302	CDL	C36-C37-C38-C39
29	j	302	CDL	C41-C42-C43-C44
29	B	402	CDL	C54-C55-C56-C57
29	j3	302	CDL	C41-C42-C43-C44
29	B3	402	CDL	C54-C55-C56-C57
29	K3	202	CDL	C74-C75-C76-C77
29	a	501	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	C51-CB5-OB6-CB4
29	j	302	CDL	C11-CA5-OA6-CA4
29	F	302	CDL	C11-CA5-OA6-CA4
29	I	301	CDL	C11-CA5-OA6-CA4
29	I	302	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
29	a3	501	CDL	C11-CA5-OA6-CA4
29	a3	502	CDL	C11-CA5-OA6-CA4
29	f3	302	CDL	C51-CB5-OB6-CB4
29	j3	302	CDL	C11-CA5-OA6-CA4
29	I3	301	CDL	C11-CA5-OA6-CA4
29	I3	303	CDL	C11-CA5-OA6-CA4
35	J	303	PEE	C11-C10-O2-C2
35	L3	302	PEE	C11-C10-O2-C2
29	f	302	CDL	C62-C63-C64-C65
29	l	302	CDL	C22-C23-C24-C25
29	A	502	CDL	C56-C57-C58-C59
29	B	403	CDL	C18-C19-C20-C21
29	F	303	CDL	C35-C36-C37-C38
29	K	202	CDL	C58-C59-C60-C61
29	K	202	CDL	C74-C75-C76-C77
29	K	202	CDL	C83-C84-C85-C86
29	P	201	CDL	C54-C55-C56-C57
29	f3	302	CDL	C62-C63-C64-C65
29	j3	302	CDL	C36-C37-C38-C39
29	B3	403	CDL	C18-C19-C20-C21
29	F3	302	CDL	C35-C36-C37-C38
29	I3	303	CDL	C13-C14-C15-C16
29	K3	202	CDL	C83-C84-C85-C86
29	J3	301	CDL	C35-C36-C37-C38
29	P3	201	CDL	C54-C55-C56-C57
35	J	303	PEE	C41-C42-C43-C44
35	L	303	PEE	C34-C35-C36-C37
35	a3	503	PEE	C34-C35-C36-C37
35	L3	302	PEE	C41-C42-C43-C44
29	b	401	CDL	C81-C82-C83-C84
29	g	305	CDL	C74-C75-C76-C77
29	l	302	CDL	C74-C75-C76-C77
29	B	403	CDL	C76-C77-C78-C79
29	I	302	CDL	C13-C14-C15-C16
29	J	301	CDL	C35-C36-C37-C38
29	J	301	CDL	C72-C73-C74-C75
29	P	201	CDL	C74-C75-C76-C77
29	b3	401	CDL	C81-C82-C83-C84
29	f3	302	CDL	C35-C36-C37-C38
29	l3	303	CDL	C22-C23-C24-C25
29	l3	303	CDL	C74-C75-C76-C77
29	A3	501	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
29	B3	403	CDL	C76-C77-C78-C79
29	K3	202	CDL	C58-C59-C60-C61
29	J3	301	CDL	C72-C73-C74-C75
29	P3	201	CDL	C74-C75-C76-C77
30	g	303	PC1	C2D-C2E-C2F-C2G
30	g3	303	PC1	C2D-C2E-C2F-C2G
29	a	501	CDL	OA7-CA5-OA6-CA4
29	j	302	CDL	OA7-CA5-OA6-CA4
29	F	302	CDL	OA7-CA5-OA6-CA4
29	I	301	CDL	OA7-CA5-OA6-CA4
29	I	302	CDL	OA7-CA5-OA6-CA4
29	a3	501	CDL	OA7-CA5-OA6-CA4
29	a3	502	CDL	OA7-CA5-OA6-CA4
29	j3	302	CDL	OA7-CA5-OA6-CA4
29	I3	301	CDL	OA7-CA5-OA6-CA4
29	I3	303	CDL	OA7-CA5-OA6-CA4
35	J	303	PEE	O4-C10-O2-C2
35	L3	302	PEE	O4-C10-O2-C2
29	j	302	CDL	CA7-C31-C32-C33
29	A3	501	CDL	CB5-C51-C52-C53
29	f	302	CDL	C35-C36-C37-C38
29	j	301	CDL	C72-C73-C74-C75
29	j	302	CDL	C54-C55-C56-C57
29	B	402	CDL	C83-C84-C85-C86
29	g3	305	CDL	C74-C75-C76-C77
29	j3	301	CDL	C72-C73-C74-C75
29	j3	302	CDL	C54-C55-C56-C57
29	I3	302	CDL	C21-C22-C23-C24
29	J3	302	CDL	C77-C78-C79-C80
29	a	501	CDL	C60-C61-C62-C63
29	K	201	CDL	C74-C75-C76-C77
29	J	302	CDL	C77-C78-C79-C80
29	L	301	CDL	C83-C84-C85-C86
29	L	302	CDL	C21-C22-C23-C24
29	a3	501	CDL	C60-C61-C62-C63
29	b3	401	CDL	C11-C12-C13-C14
29	B3	402	CDL	C83-C84-C85-C86
29	K3	201	CDL	C74-C75-C76-C77
29	L3	301	CDL	C83-C84-C85-C86
30	D	301	PC1	C27-C28-C29-C2A
30	D3	301	PC1	C27-C28-C29-C2A
29	b	401	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
29	I	301	CDL	O1-C1-CA2-OA2
29	I	302	CDL	O1-C1-CA2-OA2
29	b3	401	CDL	O1-C1-CA2-OA2
29	I3	301	CDL	O1-C1-CA2-OA2
29	I3	303	CDL	O1-C1-CA2-OA2
29	b	401	CDL	C11-C12-C13-C14
29	f	303	CDL	C51-C52-C53-C54
29	g	305	CDL	C19-C20-C21-C22
29	l	301	CDL	C21-C22-C23-C24
29	I	302	CDL	C82-C83-C84-C85
29	a3	501	CDL	C58-C59-C60-C61
29	f3	303	CDL	C51-C52-C53-C54
29	g3	305	CDL	C19-C20-C21-C22
29	j3	301	CDL	C22-C23-C24-C25
29	I3	303	CDL	C82-C83-C84-C85
29	L3	301	CDL	C74-C75-C76-C77
29	B	403	CDL	CA5-C11-C12-C13
29	j3	302	CDL	CA7-C31-C32-C33
29	B3	403	CDL	CA5-C11-C12-C13
29	j	301	CDL	C11-C12-C13-C14
29	j	301	CDL	C22-C23-C24-C25
29	j	301	CDL	C31-C32-C33-C34
29	A	502	CDL	C14-C15-C16-C17
29	B	401	CDL	C41-C42-C43-C44
29	F	303	CDL	C52-C53-C54-C55
29	L	301	CDL	C71-C72-C73-C74
29	a3	501	CDL	C53-C54-C55-C56
29	j3	301	CDL	C31-C32-C33-C34
29	l3	301	CDL	C21-C22-C23-C24
29	l3	301	CDL	C34-C35-C36-C37
29	A3	501	CDL	C14-C15-C16-C17
29	B3	401	CDL	C41-C42-C43-C44
29	F3	302	CDL	C52-C53-C54-C55
29	L3	301	CDL	C71-C72-C73-C74
29	a	501	CDL	C53-C54-C55-C56
29	a	501	CDL	C58-C59-C60-C61
29	f	304	CDL	C11-C12-C13-C14
29	l	301	CDL	C34-C35-C36-C37
29	B	401	CDL	C81-C82-C83-C84
29	K	202	CDL	C43-C44-C45-C46
29	L	301	CDL	C74-C75-C76-C77
29	j3	301	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	B3	401	CDL	C81-C82-C83-C84
29	i	301	CDL	CB7-C71-C72-C73
29	A	502	CDL	CB5-C51-C52-C53
29	i3	302	CDL	CB7-C71-C72-C73
29	f	303	CDL	C76-C77-C78-C79
29	f	304	CDL	C75-C76-C77-C78
29	i	301	CDL	C19-C20-C21-C22
29	k	201	CDL	C76-C77-C78-C79
29	l	302	CDL	C15-C16-C17-C18
29	B	401	CDL	C38-C39-C40-C41
29	J	302	CDL	C38-C39-C40-C41
29	f3	303	CDL	C76-C77-C78-C79
29	f3	304	CDL	C11-C12-C13-C14
29	f3	304	CDL	C75-C76-C77-C78
29	i3	302	CDL	C19-C20-C21-C22
29	k3	201	CDL	C76-C77-C78-C79
29	j3	301	CDL	C16-C17-C18-C19
29	A3	501	CDL	C80-C81-C82-C83
29	B3	401	CDL	C38-C39-C40-C41
29	K3	202	CDL	C43-C44-C45-C46
29	J3	302	CDL	C38-C39-C40-C41
30	d	301	PC1	C28-C29-C2A-C2B
30	d3	301	PC1	C28-C29-C2A-C2B
35	A	501	PEE	C42-C43-C44-C45
35	l3	302	PEE	C42-C43-C44-C45
29	i	301	CDL	C74-C75-C76-C77
29	j	301	CDL	C16-C17-C18-C19
29	A	502	CDL	C80-C81-C82-C83
29	B	402	CDL	C22-C23-C24-C25
29	I	302	CDL	C72-C73-C74-C75
29	i3	302	CDL	C74-C75-C76-C77
29	l3	303	CDL	C15-C16-C17-C18
29	l3	303	CDL	C83-C84-C85-C86
29	B3	402	CDL	C22-C23-C24-C25
29	I3	303	CDL	C72-C73-C74-C75
29	f	302	CDL	OB7-CB5-OB6-CB4
29	j	301	CDL	OA7-CA5-OA6-CA4
29	f3	302	CDL	OB7-CB5-OB6-CB4
29	j3	301	CDL	OA7-CA5-OA6-CA4
29	j	301	CDL	C11-CA5-OA6-CA4
29	j3	301	CDL	C11-CA5-OA6-CA4
29	b	401	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
29	f	302	CDL	C19-C20-C21-C22
29	i	301	CDL	C81-C82-C83-C84
29	k	201	CDL	C36-C37-C38-C39
29	l	302	CDL	C83-C84-C85-C86
29	B	401	CDL	C22-C23-C24-C25
29	B	404	CDL	C12-C13-C14-C15
29	f3	302	CDL	C19-C20-C21-C22
29	k3	201	CDL	C36-C37-C38-C39
29	B3	401	CDL	C22-C23-C24-C25
29	B3	404	CDL	C12-C13-C14-C15
29	F3	302	CDL	C38-C39-C40-C41
29	F3	302	CDL	C78-C79-C80-C81
30	d	301	PC1	C35-C36-C37-C38
30	d3	301	PC1	C35-C36-C37-C38
29	r	201	CDL	CA7-C31-C32-C33
29	r	201	CDL	CB7-C71-C72-C73
29	F	303	CDL	CB5-C51-C52-C53
29	i3	301	CDL	CA7-C31-C32-C33
29	F3	302	CDL	CB5-C51-C52-C53
29	a	501	CDL	C51-C52-C53-C54
29	f	302	CDL	C17-C18-C19-C20
29	k	201	CDL	C37-C38-C39-C40
29	j	301	CDL	C20-C21-C22-C23
29	p	201	CDL	C22-C23-C24-C25
29	p	201	CDL	C73-C74-C75-C76
29	B	402	CDL	C75-C76-C77-C78
29	B	403	CDL	C81-C82-C83-C84
29	B	404	CDL	C35-C36-C37-C38
29	F	302	CDL	C37-C38-C39-C40
29	F	303	CDL	C38-C39-C40-C41
29	I	301	CDL	C74-C75-C76-C77
29	I	302	CDL	C74-C75-C76-C77
29	J	301	CDL	C63-C64-C65-C66
29	L	301	CDL	C37-C38-C39-C40
29	P	201	CDL	C23-C24-C25-C26
29	a3	501	CDL	C51-C52-C53-C54
29	a3	502	CDL	C37-C38-C39-C40
29	b3	401	CDL	C56-C57-C58-C59
29	f3	302	CDL	C17-C18-C19-C20
29	i3	302	CDL	C81-C82-C83-C84
29	j3	301	CDL	C20-C21-C22-C23
29	l3	303	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
29	p3	201	CDL	C22-C23-C24-C25
29	p3	201	CDL	C73-C74-C75-C76
29	B3	402	CDL	C75-C76-C77-C78
29	B3	403	CDL	C81-C82-C83-C84
29	I3	301	CDL	C74-C75-C76-C77
29	I3	303	CDL	C74-C75-C76-C77
29	J3	301	CDL	C63-C64-C65-C66
29	L3	301	CDL	C37-C38-C39-C40
29	P3	201	CDL	C23-C24-C25-C26
30	g	303	PC1	C2C-C2D-C2E-C2F
30	G	304	PC1	C2C-C2D-C2E-C2F
30	g3	303	PC1	C2C-C2D-C2E-C2F
30	G3	304	PC1	C2C-C2D-C2E-C2F
29	l	302	CDL	C55-C56-C57-C58
29	A	502	CDL	C72-C73-C74-C75
29	B	401	CDL	C63-C64-C65-C66
29	F	303	CDL	C78-C79-C80-C81
29	J	302	CDL	C16-C17-C18-C19
29	f3	302	CDL	C78-C79-C80-C81
29	k3	201	CDL	C37-C38-C39-C40
29	j3	301	CDL	C37-C38-C39-C40
29	A3	501	CDL	C72-C73-C74-C75
29	B3	401	CDL	C63-C64-C65-C66
29	B3	404	CDL	C35-C36-C37-C38
29	K3	201	CDL	C54-C55-C56-C57
30	g3	304	PC1	C24-C25-C26-C27
29	f	302	CDL	C56-C57-C58-C59
29	f	302	CDL	C78-C79-C80-C81
29	f	303	CDL	C80-C81-C82-C83
29	j	301	CDL	C37-C38-C39-C40
29	K	201	CDL	C54-C55-C56-C57
29	L	302	CDL	C83-C84-C85-C86
29	f3	302	CDL	C56-C57-C58-C59
29	f3	303	CDL	C80-C81-C82-C83
29	J3	302	CDL	C16-C17-C18-C19
29	L3	301	CDL	C31-C32-C33-C34
30	g	304	PC1	C24-C25-C26-C27
30	G3	304	PC1	C34-C35-C36-C37
35	m	301	PEE	C14-C15-C16-C17
35	j3	303	PEE	C14-C15-C16-C17
29	K	202	CDL	CA5-C11-C12-C13
29	i3	301	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
29	K3	202	CDL	CA5-C11-C12-C13
29	g	305	CDL	OB9-CB7-OB8-CB6
29	j	302	CDL	OB9-CB7-OB8-CB6
29	g3	305	CDL	OB9-CB7-OB8-CB6
29	j3	302	CDL	OB9-CB7-OB8-CB6
29	j	301	CDL	C33-C34-C35-C36
29	B	404	CDL	C57-C58-C59-C60
29	F	303	CDL	C20-C21-C22-C23
29	J	302	CDL	C74-C75-C76-C77
29	L	301	CDL	C31-C32-C33-C34
29	j3	301	CDL	C33-C34-C35-C36
29	B3	404	CDL	C57-C58-C59-C60
29	F3	302	CDL	C20-C21-C22-C23
29	I3	302	CDL	C83-C84-C85-C86
29	J3	302	CDL	C74-C75-C76-C77
30	G	304	PC1	C29-C2A-C2B-C2C
30	G	304	PC1	C34-C35-C36-C37
30	G3	304	PC1	C29-C2A-C2B-C2C
35	J	303	PEE	C23-C24-C25-C26
35	L3	302	PEE	C23-C24-C25-C26
30	g	304	PC1	C32-C31-O31-C3
30	g3	304	PC1	C32-C31-O31-C3
29	a	501	CDL	C38-C39-C40-C41
29	A	502	CDL	C21-C22-C23-C24
29	I	301	CDL	C60-C61-C62-C63
29	a3	501	CDL	C38-C39-C40-C41
29	b3	401	CDL	C40-C41-C42-C43
29	A3	501	CDL	C21-C22-C23-C24
29	I3	301	CDL	C60-C61-C62-C63
29	b	401	CDL	C40-C41-C42-C43
29	l	302	CDL	C36-C37-C38-C39
29	p	201	CDL	C54-C55-C56-C57
29	A	502	CDL	C74-C75-C76-C77
29	L	301	CDL	C54-C55-C56-C57
29	a3	501	CDL	C43-C44-C45-C46
29	l3	303	CDL	C36-C37-C38-C39
29	p3	201	CDL	C54-C55-C56-C57
29	A3	501	CDL	C74-C75-C76-C77
29	L3	301	CDL	C54-C55-C56-C57
30	d	301	PC1	C37-C38-C39-C3A
30	d3	301	PC1	C37-C38-C39-C3A
35	A	501	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	l3	302	PEE	C32-C33-C34-C35
29	f	304	CDL	CA7-C31-C32-C33
30	G	304	PC1	O32-C31-O31-C3
30	G3	304	PC1	O32-C31-O31-C3
29	a	501	CDL	C43-C44-C45-C46
29	j	302	CDL	C74-C75-C76-C77
29	A	502	CDL	C16-C17-C18-C19
29	J	301	CDL	C33-C34-C35-C36
29	J	302	CDL	C13-C14-C15-C16
29	j3	302	CDL	C74-C75-C76-C77
29	A3	501	CDL	C16-C17-C18-C19
29	J3	302	CDL	C13-C14-C15-C16
29	J3	302	CDL	CA3-CA4-CA6-OA8
35	J	303	PEE	C17-C18-C19-C20
35	L3	302	PEE	C17-C18-C19-C20
29	f	303	CDL	C35-C36-C37-C38
29	f	304	CDL	C18-C19-C20-C21
29	l	301	CDL	C37-C38-C39-C40
29	J	302	CDL	C31-C32-C33-C34
29	f3	303	CDL	C35-C36-C37-C38
29	f3	304	CDL	C18-C19-C20-C21
29	l3	301	CDL	C37-C38-C39-C40
29	J3	301	CDL	C33-C34-C35-C36
29	J3	302	CDL	C31-C32-C33-C34
29	f	304	CDL	CB5-C51-C52-C53
29	f3	304	CDL	CA7-C31-C32-C33
29	a3	501	CDL	C56-C57-C58-C59
29	b	401	CDL	C71-CB7-OB8-CB6
29	b3	401	CDL	C71-CB7-OB8-CB6
29	j	301	CDL	C51-CB5-OB6-CB4
29	j3	301	CDL	C51-CB5-OB6-CB4
29	r	201	CDL	CB4-CB6-OB8-CB7
29	i3	301	CDL	CB4-CB6-OB8-CB7
29	a	501	CDL	C56-C57-C58-C59
29	j	301	CDL	C82-C83-C84-C85
29	F	302	CDL	C57-C58-C59-C60
29	a3	502	CDL	C57-C58-C59-C60
29	j3	301	CDL	C82-C83-C84-C85
29	f	302	CDL	C80-C81-C82-C83
29	k	201	CDL	C18-C19-C20-C21
29	j	302	CDL	C13-C14-C15-C16
29	j	302	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
29	A	502	CDL	C83-C84-C85-C86
29	K	201	CDL	C56-C57-C58-C59
29	f3	302	CDL	C80-C81-C82-C83
29	k3	201	CDL	C18-C19-C20-C21
29	j3	302	CDL	C13-C14-C15-C16
29	j3	302	CDL	C52-C53-C54-C55
29	A3	501	CDL	C83-C84-C85-C86
29	K3	201	CDL	C56-C57-C58-C59
35	m	301	PEE	C19-C20-C21-C22
35	j3	303	PEE	C19-C20-C21-C22
29	K3	202	CDL	OB9-CB7-OB8-CB6
29	K	202	CDL	CB5-C51-C52-C53
29	f3	302	CDL	CA5-C11-C12-C13
29	f3	304	CDL	CB5-C51-C52-C53
29	K3	202	CDL	CB5-C51-C52-C53
29	B	404	CDL	C43-C44-C45-C46
29	L	301	CDL	C38-C39-C40-C41
29	L	301	CDL	C78-C79-C80-C81
29	L3	301	CDL	C38-C39-C40-C41
29	B	404	CDL	O1-C1-CA2-OA2
29	B3	404	CDL	O1-C1-CA2-OA2
29	F	302	CDL	C22-C23-C24-C25
29	a3	502	CDL	C22-C23-C24-C25
29	B3	404	CDL	C43-C44-C45-C46
29	L3	301	CDL	C78-C79-C80-C81
29	b	401	CDL	C53-C54-C55-C56
29	I	302	CDL	C79-C80-C81-C82
29	L	302	CDL	C72-C73-C74-C75
29	b3	401	CDL	C53-C54-C55-C56
29	I3	302	CDL	C72-C73-C74-C75
29	I3	303	CDL	C79-C80-C81-C82
29	K	202	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	CA5-C11-C12-C13
29	f	304	CDL	CA5-C11-C12-C13
29	F	303	CDL	CB7-C71-C72-C73
29	f3	304	CDL	CA5-C11-C12-C13
29	a	501	CDL	C74-C75-C76-C77
29	f	302	CDL	C23-C24-C25-C26
29	f	303	CDL	C77-C78-C79-C80
29	l	302	CDL	C17-C18-C19-C20
29	a3	501	CDL	C74-C75-C76-C77
29	f3	302	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	f3	303	CDL	C77-C78-C79-C80
29	l3	303	CDL	C17-C18-C19-C20
29	I3	303	CDL	C60-C61-C62-C63
29	f	302	CDL	C42-C43-C44-C45
29	I	302	CDL	C60-C61-C62-C63
29	J	301	CDL	C21-C22-C23-C24
29	L	302	CDL	C76-C77-C78-C79
29	I3	302	CDL	C74-C75-C76-C77
29	I3	302	CDL	C76-C77-C78-C79
29	J3	301	CDL	C21-C22-C23-C24
29	a	501	CDL	C1-CB2-OB2-PB2
29	a3	501	CDL	C1-CB2-OB2-PB2
30	g	304	PC1	O32-C31-O31-C3
30	g3	304	PC1	O32-C31-O31-C3
29	r	201	CDL	C82-C83-C84-C85
29	F	303	CDL	C39-C40-C41-C42
29	J	302	CDL	C52-C53-C54-C55
29	L	302	CDL	C74-C75-C76-C77
29	f3	302	CDL	C42-C43-C44-C45
29	p3	201	CDL	C52-C53-C54-C55
29	p3	201	CDL	C58-C59-C60-C61
29	F3	302	CDL	C39-C40-C41-C42
29	J3	302	CDL	C52-C53-C54-C55
30	d	301	PC1	C2B-C2C-C2D-C2E
30	d3	301	PC1	C2B-C2C-C2D-C2E
29	F3	302	CDL	CB7-C71-C72-C73
29	p	201	CDL	C52-C53-C54-C55
29	p	201	CDL	C58-C59-C60-C61
29	i3	301	CDL	C82-C83-C84-C85
29	l3	301	CDL	C11-CA5-OA6-CA4
29	a	501	CDL	C21-C22-C23-C24
29	l	301	CDL	C60-C61-C62-C63
29	l	302	CDL	C62-C63-C64-C65
29	F	302	CDL	C51-C52-C53-C54
29	a3	501	CDL	C21-C22-C23-C24
29	a3	502	CDL	C51-C52-C53-C54
29	l3	301	CDL	C60-C61-C62-C63
29	l3	303	CDL	C62-C63-C64-C65
29	B3	402	CDL	C71-C72-C73-C74
29	l	302	CDL	C71-C72-C73-C74
29	B	402	CDL	C71-C72-C73-C74
29	K	201	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
29	l3	303	CDL	C71-C72-C73-C74
29	K3	201	CDL	C40-C41-C42-C43
29	K	201	CDL	C71-C72-C73-C74
29	i3	302	CDL	C76-C77-C78-C79
29	K3	201	CDL	C71-C72-C73-C74
30	g	303	PC1	C3D-C3E-C3F-C3G
30	g3	303	PC1	C3D-C3E-C3F-C3G
29	b	401	CDL	OB9-CB7-OB8-CB6
29	b3	401	CDL	OB9-CB7-OB8-CB6
29	i	301	CDL	C76-C77-C78-C79
30	g	303	PC1	C37-C38-C39-C3A
30	d3	301	PC1	C24-C25-C26-C27
35	m	301	PEE	C35-C36-C37-C38
35	J	303	PEE	C19-C20-C21-C22
35	j3	303	PEE	C35-C36-C37-C38
35	L3	302	PEE	C19-C20-C21-C22
29	j	301	CDL	OB7-CB5-OB6-CB4
29	j	302	CDL	OB7-CB5-OB6-CB4
29	B	403	CDL	OA7-CA5-OA6-CA4
29	j3	301	CDL	OB7-CB5-OB6-CB4
29	j3	302	CDL	OB7-CB5-OB6-CB4
29	B3	403	CDL	OA7-CA5-OA6-CA4
35	m	301	PEE	O4-C10-O2-C2
35	j3	303	PEE	O4-C10-O2-C2
29	f	303	CDL	CA5-C11-C12-C13
29	g	305	CDL	CA5-C11-C12-C13
29	f3	303	CDL	CA5-C11-C12-C13
29	g3	305	CDL	CA5-C11-C12-C13
29	j	301	CDL	C31-CA7-OA8-CA6
29	I	302	CDL	C71-CB7-OB8-CB6
29	P	201	CDL	C31-CA7-OA8-CA6
29	j3	301	CDL	C31-CA7-OA8-CA6
29	I3	303	CDL	C71-CB7-OB8-CB6
29	P3	201	CDL	C31-CA7-OA8-CA6
29	B	404	CDL	C13-C14-C15-C16
29	F	302	CDL	C76-C77-C78-C79
29	J	301	CDL	C52-C53-C54-C55
29	B3	402	CDL	C60-C61-C62-C63
29	B3	404	CDL	C13-C14-C15-C16
30	d	301	PC1	C24-C25-C26-C27
30	g3	303	PC1	C37-C38-C39-C3A
35	A	501	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
29	A	502	CDL	C35-C36-C37-C38
29	B	401	CDL	C36-C37-C38-C39
29	B	402	CDL	C60-C61-C62-C63
29	a3	502	CDL	C76-C77-C78-C79
29	f3	302	CDL	C38-C39-C40-C41
29	i3	302	CDL	C61-C62-C63-C64
29	A3	501	CDL	C35-C36-C37-C38
29	B3	401	CDL	C36-C37-C38-C39
29	J3	301	CDL	C52-C53-C54-C55
35	a3	503	PEE	C32-C33-C34-C35
35	l3	302	PEE	C41-C42-C43-C44
29	f	302	CDL	C38-C39-C40-C41
29	i	301	CDL	C61-C62-C63-C64
29	i3	302	CDL	C36-C37-C38-C39
29	L3	301	CDL	C52-C53-C54-C55
35	L	303	PEE	C32-C33-C34-C35
29	L3	301	CDL	CA5-C11-C12-C13
29	a	501	CDL	C83-C84-C85-C86
29	i	301	CDL	C36-C37-C38-C39
29	I	301	CDL	C78-C79-C80-C81
29	I	302	CDL	C56-C57-C58-C59
29	L	301	CDL	C15-C16-C17-C18
29	L	301	CDL	C52-C53-C54-C55
29	L	302	CDL	C42-C43-C44-C45
29	a3	501	CDL	C83-C84-C85-C86
29	I3	301	CDL	C71-C72-C73-C74
29	I3	301	CDL	C78-C79-C80-C81
29	I3	302	CDL	C42-C43-C44-C45
29	I3	303	CDL	C56-C57-C58-C59
29	L3	301	CDL	C15-C16-C17-C18
29	j	302	CDL	C72-C73-C74-C75
29	I	301	CDL	C71-C72-C73-C74
29	j3	302	CDL	C72-C73-C74-C75
29	f	302	CDL	C81-C82-C83-C84
29	F	302	CDL	C43-C44-C45-C46
29	I	301	CDL	C19-C20-C21-C22
29	L	302	CDL	C19-C20-C21-C22
29	a3	502	CDL	C43-C44-C45-C46
29	f3	302	CDL	C81-C82-C83-C84
29	I3	301	CDL	C19-C20-C21-C22
29	I3	302	CDL	C19-C20-C21-C22
30	g	303	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	D	301	PC1	C28-C29-C2A-C2B
30	g3	303	PC1	C24-C25-C26-C27
30	D3	301	PC1	C28-C29-C2A-C2B
29	L	301	CDL	CA5-C11-C12-C13
29	L	302	CDL	CA5-C11-C12-C13
29	I3	302	CDL	CA5-C11-C12-C13
29	j	302	CDL	C51-CB5-OB6-CB4
29	l	301	CDL	C11-CA5-OA6-CA4
29	B	403	CDL	C11-CA5-OA6-CA4
29	J	302	CDL	C51-CB5-OB6-CB4
29	j3	302	CDL	C51-CB5-OB6-CB4
29	B3	403	CDL	C11-CA5-OA6-CA4
29	J3	302	CDL	C51-CB5-OB6-CB4
35	m	301	PEE	C11-C10-O2-C2
35	j3	303	PEE	C11-C10-O2-C2
29	i3	302	CDL	OB5-CB3-CB4-OB6
29	g	305	CDL	C40-C41-C42-C43
29	f3	303	CDL	C13-C14-C15-C16
29	b	401	CDL	C42-C43-C44-C45
29	f	303	CDL	C13-C14-C15-C16
29	k	201	CDL	C40-C41-C42-C43
29	b3	401	CDL	C42-C43-C44-C45
29	k3	201	CDL	C40-C41-C42-C43
29	g3	305	CDL	C40-C41-C42-C43
29	F3	302	CDL	C11-C12-C13-C14
29	F	303	CDL	C11-C12-C13-C14
29	K	202	CDL	C77-C78-C79-C80
29	f	302	CDL	C77-C78-C79-C80
29	f3	302	CDL	C77-C78-C79-C80
29	K3	202	CDL	C77-C78-C79-C80
29	F	303	CDL	C82-C83-C84-C85
32	I	303	UQ8	C40-C39-C41-C42
32	I3	304	UQ8	C40-C39-C41-C42
29	f	302	CDL	C51-C52-C53-C54
29	f3	302	CDL	C51-C52-C53-C54
29	F3	302	CDL	C82-C83-C84-C85
29	a	501	CDL	C31-C32-C33-C34
29	j	302	CDL	C22-C23-C24-C25
29	r	201	CDL	C58-C59-C60-C61
29	B	401	CDL	C59-C60-C61-C62
29	J	301	CDL	C31-C32-C33-C34
29	a3	501	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	i3	301	CDL	C58-C59-C60-C61
29	j3	302	CDL	C22-C23-C24-C25
29	B3	401	CDL	C59-C60-C61-C62
29	B	403	CDL	C52-C53-C54-C55
29	J	301	CDL	C22-C23-C24-C25
29	B3	403	CDL	C52-C53-C54-C55
29	J3	301	CDL	C22-C23-C24-C25
29	J3	301	CDL	C31-C32-C33-C34
30	D	301	PC1	C39-C3A-C3B-C3C
30	D3	301	PC1	C39-C3A-C3B-C3C
29	l	301	CDL	OA7-CA5-OA6-CA4
29	J	302	CDL	OB7-CB5-OB6-CB4
29	l3	301	CDL	OA7-CA5-OA6-CA4
29	J3	302	CDL	OB7-CB5-OB6-CB4
29	j	302	CDL	C20-C21-C22-C23
29	B	402	CDL	C74-C75-C76-C77
29	b3	401	CDL	C38-C39-C40-C41
29	B3	402	CDL	C74-C75-C76-C77
30	D	301	PC1	C25-C26-C27-C28
30	G3	304	PC1	C27-C28-C29-C2A
29	b	401	CDL	CB3-OB5-PB2-OB2
29	j	301	CDL	CB3-OB5-PB2-OB2
29	p	201	CDL	CA3-OA5-PA1-OA2
29	p	201	CDL	CB2-OB2-PB2-OB5
29	B	401	CDL	CA2-OA2-PA1-OA5
29	B	403	CDL	CB2-OB2-PB2-OB5
29	F	302	CDL	CA3-OA5-PA1-OA2
29	I	301	CDL	CB3-OB5-PB2-OB2
29	a3	502	CDL	CA3-OA5-PA1-OA2
29	b3	401	CDL	CB3-OB5-PB2-OB2
29	j3	301	CDL	CB3-OB5-PB2-OB2
29	p3	201	CDL	CA3-OA5-PA1-OA2
29	p3	201	CDL	CB2-OB2-PB2-OB5
29	B3	401	CDL	CA2-OA2-PA1-OA5
29	B3	403	CDL	CB2-OB2-PB2-OB5
29	I3	301	CDL	CB3-OB5-PB2-OB2
30	d	301	PC1	C1-O11-P-O13
30	D	301	PC1	C1-O11-P-O13
30	G	303	PC1	C11-O13-P-O11
30	d3	301	PC1	C1-O11-P-O13
30	D3	301	PC1	C1-O11-P-O13
30	G3	303	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
30	G3	303	PC1	C1-O11-P-O13
35	A	501	PEE	C4-O4P-P-O3P
35	J	303	PEE	C1-O3P-P-O4P
35	L	303	PEE	C4-O4P-P-O3P
35	a3	503	PEE	C4-O4P-P-O3P
35	l3	302	PEE	C4-O4P-P-O3P
29	b	401	CDL	C38-C39-C40-C41
29	j3	302	CDL	C20-C21-C22-C23
30	D3	301	PC1	C25-C26-C27-C28
35	a3	503	PEE	C43-C44-C45-C46
29	B	401	CDL	C1-CA2-OA2-PA1
29	B3	401	CDL	C1-CA2-OA2-PA1
30	G	304	PC1	C27-C28-C29-C2A
35	L	303	PEE	C43-C44-C45-C46
29	a	501	CDL	OA5-CA3-CA4-CA6
29	b	401	CDL	OA5-CA3-CA4-CA6
29	f	304	CDL	OA5-CA3-CA4-CA6
29	F	303	CDL	OB5-CB3-CB4-CB6
29	K	202	CDL	OA5-CA3-CA4-CA6
29	a3	501	CDL	OA5-CA3-CA4-CA6
29	b3	401	CDL	OA5-CA3-CA4-CA6
29	f3	304	CDL	OA5-CA3-CA4-CA6
29	i3	301	CDL	OA5-CA3-CA4-CA6
29	j3	301	CDL	OA5-CA3-CA4-CA6
29	F3	302	CDL	OB5-CB3-CB4-CB6
29	K3	202	CDL	OA5-CA3-CA4-CA6
29	P3	201	CDL	OB5-CB3-CB4-CB6
35	L3	302	PEE	O3P-C1-C2-C3
29	B3	404	CDL	C79-C80-C81-C82
29	B	404	CDL	C79-C80-C81-C82
35	J	303	PEE	C31-C32-C33-C34
35	L3	302	PEE	C31-C32-C33-C34
29	f	302	CDL	C74-C75-C76-C77
29	f3	302	CDL	C74-C75-C76-C77
29	f	302	CDL	C33-C34-C35-C36
29	F3	302	CDL	C41-C42-C43-C44
30	d3	301	PC1	C2A-C2B-C2C-C2D
29	f	303	CDL	C38-C39-C40-C41
29	B	401	CDL	C39-C40-C41-C42
29	F	303	CDL	C41-C42-C43-C44
29	f3	302	CDL	C33-C34-C35-C36
30	d	301	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
30	g	304	PC1	C33-C34-C35-C36
30	g3	304	PC1	C33-C34-C35-C36
29	j	302	CDL	C16-C17-C18-C19
29	f3	303	CDL	C38-C39-C40-C41
29	j3	302	CDL	C16-C17-C18-C19
29	l3	301	CDL	C32-C33-C34-C35
35	l3	302	PEE	C33-C34-C35-C36
29	g	305	CDL	C31-C32-C33-C34
29	l	301	CDL	C32-C33-C34-C35
29	a3	501	CDL	C72-C73-C74-C75
29	b3	401	CDL	C71-C72-C73-C74
29	B3	401	CDL	C39-C40-C41-C42
35	A	501	PEE	C33-C34-C35-C36
29	j3	301	CDL	OA9-CA7-OA8-CA6
29	I3	303	CDL	OB9-CB7-OB8-CB6
29	P3	201	CDL	OA9-CA7-OA8-CA6
29	a	501	CDL	C72-C73-C74-C75
29	b	401	CDL	C71-C72-C73-C74
29	p	201	CDL	C63-C64-C65-C66
29	g3	305	CDL	C31-C32-C33-C34
29	p3	201	CDL	C63-C64-C65-C66
29	b	401	CDL	CB3-CB4-CB6-OB8
29	f	303	CDL	CB3-CB4-CB6-OB8
29	p	201	CDL	C64-C65-C66-C67
29	r	201	CDL	CB3-CB4-CB6-OB8
29	B	404	CDL	CB3-CB4-CB6-OB8
29	F	303	CDL	CA3-CA4-CA6-OA8
29	I	302	CDL	CB3-CB4-CB6-OB8
29	b3	401	CDL	CB3-CB4-CB6-OB8
29	f3	303	CDL	CB3-CB4-CB6-OB8
29	i3	301	CDL	CB3-CB4-CB6-OB8
29	j3	302	CDL	CA3-CA4-CA6-OA8
29	p3	201	CDL	C64-C65-C66-C67
29	B3	404	CDL	CB3-CB4-CB6-OB8
29	F3	302	CDL	CA3-CA4-CA6-OA8
29	I3	303	CDL	C36-C37-C38-C39
29	K3	202	CDL	CB3-CB4-CB6-OB8
29	P3	201	CDL	CA3-CA4-CA6-OA8
30	d	301	PC1	C1-C2-C3-O31
30	D	301	PC1	C1-C2-C3-O31
30	D3	301	PC1	C1-C2-C3-O31
29	I	302	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
29	f3	302	CDL	C58-C59-C60-C61
30	D	301	PC1	C29-C2A-C2B-C2C
29	P	201	CDL	OA9-CA7-OA8-CA6
29	f	302	CDL	C58-C59-C60-C61
29	p	201	CDL	C41-C42-C43-C44
29	F	303	CDL	C51-C52-C53-C54
30	G	303	PC1	C3F-C3G-C3H-C3I
30	D3	301	PC1	C29-C2A-C2B-C2C
30	G3	303	PC1	C3F-C3G-C3H-C3I
29	a	501	CDL	C11-C12-C13-C14
29	F	302	CDL	C80-C81-C82-C83
29	I	301	CDL	C17-C18-C19-C20
29	a3	501	CDL	C11-C12-C13-C14
29	p3	201	CDL	C41-C42-C43-C44
30	G	303	PC1	C22-C23-C24-C25
29	B	401	CDL	C32-C31-CA7-OA8
29	B3	401	CDL	C32-C31-CA7-OA8
29	j	301	CDL	OA9-CA7-OA8-CA6
29	I	302	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	C44-C45-C46-C47
29	F	302	CDL	C24-C25-C26-C27
29	F	303	CDL	C74-C75-C76-C77
29	F	303	CDL	C83-C84-C85-C86
29	a3	502	CDL	C80-C81-C82-C83
29	f3	302	CDL	C44-C45-C46-C47
29	F3	302	CDL	C51-C52-C53-C54
29	F3	302	CDL	C74-C75-C76-C77
29	I3	301	CDL	C17-C18-C19-C20
30	g	303	PC1	C3F-C3G-C3H-C3I
29	r	201	CDL	C74-C75-C76-C77
29	I	301	CDL	C53-C54-C55-C56
29	J	302	CDL	C18-C19-C20-C21
29	F3	302	CDL	C83-C84-C85-C86
29	I3	301	CDL	C53-C54-C55-C56
29	J3	302	CDL	C18-C19-C20-C21
29	J3	302	CDL	C59-C60-C61-C62
30	G3	303	PC1	C22-C23-C24-C25
29	F	303	CDL	CB4-CB6-OB8-CB7
29	F3	302	CDL	CB4-CB6-OB8-CB7
29	J	302	CDL	C59-C60-C61-C62
29	a3	502	CDL	C24-C25-C26-C27
29	i3	301	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
29	g3	305	CDL	C79-C80-C81-C82
30	g3	303	PC1	C3F-C3G-C3H-C3I
29	L	302	CDL	CA7-C31-C32-C33
29	I3	302	CDL	CA7-C31-C32-C33
29	g	305	CDL	C79-C80-C81-C82
29	p	201	CDL	C72-C73-C74-C75
30	g	304	PC1	C27-C28-C29-C2A
30	g3	304	PC1	C27-C28-C29-C2A
37	B2	1002	ADP	PA-O3A-PB-O1B
37	B4	1002	ADP	PA-O3A-PB-O1B
29	p	201	CDL	CA7-C31-C32-C33
29	p3	201	CDL	CA7-C31-C32-C33
30	G	303	PC1	C31-C32-C33-C34
30	G3	303	PC1	C31-C32-C33-C34
29	p3	201	CDL	C72-C73-C74-C75
29	A3	501	CDL	C38-C39-C40-C41
29	A	502	CDL	C38-C39-C40-C41
29	K	201	CDL	C78-C79-C80-C81
29	A	502	CDL	C60-C61-C62-C63
29	K3	201	CDL	C78-C79-C80-C81
29	f	302	CDL	C84-C85-C86-C87
29	f3	302	CDL	C84-C85-C86-C87
29	f	304	CDL	OB5-CB3-CB4-OB6
29	i	301	CDL	OB5-CB3-CB4-OB6
29	A	502	CDL	OB5-CB3-CB4-OB6
29	L	302	CDL	OA5-CA3-CA4-OA6
29	A3	501	CDL	C60-C61-C62-C63
29	j	302	CDL	C24-C25-C26-C27
29	j3	302	CDL	C24-C25-C26-C27
29	I3	302	CDL	C59-C60-C61-C62
29	K	202	CDL	C51-C52-C53-C54
29	L	302	CDL	C59-C60-C61-C62
29	j3	301	CDL	C12-C13-C14-C15
29	a	501	CDL	C16-C17-C18-C19
29	j	301	CDL	C12-C13-C14-C15
29	I	302	CDL	C81-C82-C83-C84
29	a3	502	CDL	C58-C59-C60-C61
29	I	301	CDL	CB4-CB6-OB8-CB7
29	f	303	CDL	C58-C59-C60-C61
29	J	301	CDL	C12-C13-C14-C15
29	a3	501	CDL	C16-C17-C18-C19
29	f3	304	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	K3	202	CDL	C51-C52-C53-C54
29	J3	301	CDL	C12-C13-C14-C15
29	f	304	CDL	C35-C36-C37-C38
29	l	302	CDL	C76-C77-C78-C79
29	F	302	CDL	C41-C42-C43-C44
29	F	302	CDL	C58-C59-C60-C61
29	L	301	CDL	C44-C45-C46-C47
29	a3	502	CDL	C41-C42-C43-C44
29	f3	303	CDL	C58-C59-C60-C61
29	l3	303	CDL	C76-C77-C78-C79
29	I3	303	CDL	C81-C82-C83-C84
29	L3	301	CDL	C16-C17-C18-C19
29	L3	301	CDL	C44-C45-C46-C47
30	g	304	PC1	C23-C24-C25-C26
30	g3	304	PC1	C23-C24-C25-C26
32	I	303	UQ8	C30-C29-C31-C32
32	I3	304	UQ8	C30-C29-C31-C32
29	J	301	CDL	C78-C79-C80-C81
29	L	301	CDL	C16-C17-C18-C19
29	k3	201	CDL	C38-C39-C40-C41
29	J3	301	CDL	C78-C79-C80-C81
29	k	201	CDL	C38-C39-C40-C41
29	L	301	CDL	C33-C34-C35-C36
29	I3	301	CDL	CB4-CB6-OB8-CB7
29	L3	301	CDL	C33-C34-C35-C36
29	L	302	CDL	C31-CA7-OA8-CA6
29	I3	302	CDL	C31-CA7-OA8-CA6
29	B	401	CDL	C84-C85-C86-C87
29	f3	303	CDL	C73-C74-C75-C76
29	B3	401	CDL	C84-C85-C86-C87
29	f	302	CDL	C36-C37-C38-C39
29	f3	302	CDL	C36-C37-C38-C39
30	D	301	PC1	C3F-C3G-C3H-C3I
30	D3	301	PC1	C3F-C3G-C3H-C3I
29	A	502	CDL	CB2-C1-CA2-OA2
29	B	402	CDL	CB2-C1-CA2-OA2
29	I	302	CDL	CB2-C1-CA2-OA2
29	A3	501	CDL	CB2-C1-CA2-OA2
29	B3	402	CDL	CB2-C1-CA2-OA2
29	I3	303	CDL	CB2-C1-CA2-OA2
29	b	401	CDL	C11-CA5-OA6-CA4
29	L	302	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	b3	401	CDL	C11-CA5-OA6-CA4
29	I3	302	CDL	C51-CB5-OB6-CB4
29	f	303	CDL	C73-C74-C75-C76
29	I	302	CDL	C58-C59-C60-C61
29	L	302	CDL	C11-C12-C13-C14
29	B3	404	CDL	C77-C78-C79-C80
29	I3	302	CDL	C11-C12-C13-C14
29	I3	303	CDL	C58-C59-C60-C61
29	p	201	CDL	C31-CA7-OA8-CA6
29	J	302	CDL	C71-CB7-OB8-CB6
29	p3	201	CDL	C31-CA7-OA8-CA6
29	J3	302	CDL	C71-CB7-OB8-CB6
29	B	404	CDL	C77-C78-C79-C80
29	j3	302	CDL	CB5-C51-C52-C53
29	i	301	CDL	C22-C23-C24-C25
29	i3	302	CDL	C22-C23-C24-C25
29	r	201	CDL	C52-C53-C54-C55
33	C4	601	ATP	O4'-C4'-C5'-O5'
29	f	302	CDL	OA5-CA3-CA4-CA6
29	i	301	CDL	OB5-CB3-CB4-CB6
29	r	201	CDL	OA5-CA3-CA4-CA6
29	A	502	CDL	OB5-CB3-CB4-CB6
29	B	401	CDL	OB5-CB3-CB4-CB6
29	B	404	CDL	OA5-CA3-CA4-CA6
29	I	301	CDL	OA5-CA3-CA4-CA6
29	J	301	CDL	OA5-CA3-CA4-CA6
29	L	302	CDL	OA5-CA3-CA4-CA6
29	P	201	CDL	OB5-CB3-CB4-CB6
29	f3	302	CDL	OA5-CA3-CA4-CA6
29	i3	302	CDL	OB5-CB3-CB4-CB6
29	B3	404	CDL	OA5-CA3-CA4-CA6
29	I3	302	CDL	OA5-CA3-CA4-CA6
29	J3	301	CDL	OA5-CA3-CA4-CA6
30	G	303	PC1	O11-C1-C2-C3
30	G3	304	PC1	O11-C1-C2-C3
35	m	301	PEE	O3P-C1-C2-C3
35	J	303	PEE	O3P-C1-C2-C3
29	k	201	CDL	C16-C17-C18-C19
29	j	302	CDL	CB5-C51-C52-C53
29	A	502	CDL	CA7-C31-C32-C33
29	j	301	CDL	C74-C75-C76-C77
29	i3	301	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
29	k3	201	CDL	C16-C17-C18-C19
29	j3	301	CDL	C74-C75-C76-C77
30	G	304	PC1	C3D-C3E-C3F-C3G
30	G3	304	PC1	C3D-C3E-C3F-C3G
29	l	302	CDL	C31-CA7-OA8-CA6
29	B	402	CDL	C71-CB7-OB8-CB6
29	l3	303	CDL	C31-CA7-OA8-CA6
29	B3	402	CDL	C71-CB7-OB8-CB6
29	J3	301	CDL	C74-C75-C76-C77
32	i	302	UQ8	C40-C39-C41-C42
32	i3	303	UQ8	C40-C39-C41-C42
29	A3	501	CDL	CA7-C31-C32-C33
29	J	301	CDL	C74-C75-C76-C77
29	l	302	CDL	C58-C59-C60-C61
29	l3	303	CDL	C58-C59-C60-C61
35	L	303	PEE	C14-C15-C16-C17
35	a3	503	PEE	C14-C15-C16-C17
29	B3	401	CDL	C31-CA7-OA8-CA6
29	B	403	CDL	C1-CB2-OB2-PB2
29	B3	403	CDL	C1-CB2-OB2-PB2
29	f	304	CDL	C40-C41-C42-C43
29	a	501	CDL	C13-C14-C15-C16
29	f	304	CDL	C63-C64-C65-C66
29	i	301	CDL	C51-C52-C53-C54
29	p	201	CDL	C59-C60-C61-C62
29	K	201	CDL	C52-C53-C54-C55
29	a3	501	CDL	C13-C14-C15-C16
29	f3	304	CDL	C40-C41-C42-C43
29	f3	304	CDL	C63-C64-C65-C66
29	l3	303	CDL	C64-C65-C66-C67
29	K3	201	CDL	C52-C53-C54-C55
30	G	304	PC1	C2F-C2G-C2H-C2I
30	G3	304	PC1	C2F-C2G-C2H-C2I
29	l	302	CDL	C64-C65-C66-C67
29	p	201	CDL	C61-C62-C63-C64
29	i3	302	CDL	C51-C52-C53-C54
29	p3	201	CDL	C59-C60-C61-C62
29	B	401	CDL	C31-CA7-OA8-CA6
29	F	302	CDL	C52-C53-C54-C55
29	B3	404	CDL	C32-C33-C34-C35
29	j	301	CDL	CB3-CB4-CB6-OB8
29	j	302	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	CA3-CA4-CA6-OA8
29	F	303	CDL	CB3-CB4-CB6-OB8
29	I	301	CDL	CB3-CB4-CB6-OB8
29	K	202	CDL	CB3-CB4-CB6-OB8
29	J	302	CDL	CA3-CA4-CA6-OA8
29	a3	501	CDL	CB3-CB4-CB6-OB8
29	I3	301	CDL	CB3-CB4-CB6-OB8
29	I3	303	CDL	CB3-CB4-CB6-OB8
30	g	303	PC1	C1-C2-C3-O31
30	G	303	PC1	C1-C2-C3-O31
30	d3	301	PC1	C1-C2-C3-O31
30	g3	303	PC1	C1-C2-C3-O31
30	G3	303	PC1	C1-C2-C3-O31
35	J	303	PEE	C1-C2-C3-O3
35	L3	302	PEE	C1-C2-C3-O3
29	l	302	CDL	C77-C78-C79-C80
29	a3	502	CDL	C52-C53-C54-C55
29	i3	301	CDL	C35-C36-C37-C38
29	l3	303	CDL	C77-C78-C79-C80
29	r	201	CDL	C35-C36-C37-C38
29	B	404	CDL	C32-C33-C34-C35
29	L3	301	CDL	C61-C62-C63-C64
35	A	501	PEE	C14-C15-C16-C17
35	l3	302	PEE	C14-C15-C16-C17
29	f	303	CDL	C79-C80-C81-C82
29	l	301	CDL	C11-C12-C13-C14
29	B	402	CDL	C40-C41-C42-C43
29	j3	301	CDL	C61-C62-C63-C64
29	l3	301	CDL	C11-C12-C13-C14
29	p3	201	CDL	C61-C62-C63-C64
29	a3	502	CDL	CA7-C31-C32-C33
29	j	301	CDL	C61-C62-C63-C64
29	B	404	CDL	C74-C75-C76-C77
29	f3	303	CDL	C79-C80-C81-C82
29	B3	404	CDL	C74-C75-C76-C77
35	J	303	PEE	C34-C35-C36-C37
32	I	303	UQ8	C38-C39-C41-C42
32	I	303	UQ8	C28-C29-C31-C32
29	k	201	CDL	C54-C55-C56-C57
29	B	403	CDL	C57-C58-C59-C60
29	B3	403	CDL	C57-C58-C59-C60
35	L3	302	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	k3	201	CDL	CB4-CB6-OB8-CB7
29	f	303	CDL	C16-C17-C18-C19
29	I	301	CDL	C21-C22-C23-C24
29	I	301	CDL	C76-C77-C78-C79
29	K	202	CDL	C64-C65-C66-C67
29	L	301	CDL	C61-C62-C63-C64
29	P	201	CDL	C58-C59-C60-C61
29	k3	201	CDL	C54-C55-C56-C57
29	K3	202	CDL	C64-C65-C66-C67
29	P3	201	CDL	C58-C59-C60-C61
29	A	502	CDL	CA3-OA5-PA1-OA2
29	F	302	CDL	CB2-OB2-PB2-OB5
29	J	301	CDL	CA2-OA2-PA1-OA5
29	J	302	CDL	CA2-OA2-PA1-OA5
29	a3	502	CDL	CB2-OB2-PB2-OB5
29	A3	501	CDL	CA3-OA5-PA1-OA2
29	J3	301	CDL	CA2-OA2-PA1-OA5
29	J3	302	CDL	CA2-OA2-PA1-OA5
30	g	303	PC1	C11-O13-P-O11
30	G	303	PC1	C1-O11-P-O13
29	F	302	CDL	CA7-C31-C32-C33
29	f3	303	CDL	C16-C17-C18-C19
29	I3	301	CDL	C21-C22-C23-C24
29	I3	301	CDL	C76-C77-C78-C79
29	b	401	CDL	OA5-CA3-CA4-OA6
29	f	302	CDL	OA5-CA3-CA4-OA6
29	j	302	CDL	OB5-CB3-CB4-OB6
29	B	403	CDL	OA5-CA3-CA4-OA6
29	B	403	CDL	OB5-CB3-CB4-OB6
29	F	302	CDL	OA5-CA3-CA4-OA6
29	F	302	CDL	OB5-CB3-CB4-OB6
29	F	303	CDL	OB5-CB3-CB4-OB6
29	a3	502	CDL	OA5-CA3-CA4-OA6
29	a3	502	CDL	OB5-CB3-CB4-OB6
29	b3	401	CDL	OA5-CA3-CA4-OA6
29	f3	302	CDL	OA5-CA3-CA4-OA6
29	A3	501	CDL	OB5-CB3-CB4-OB6
29	B3	403	CDL	OA5-CA3-CA4-OA6
29	I3	302	CDL	OA5-CA3-CA4-OA6
35	L3	302	PEE	O3P-C1-C2-O2
29	j3	301	CDL	C80-C81-C82-C83
29	B3	402	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
29	j	301	CDL	C80-C81-C82-C83
29	f	302	CDL	C72-C71-CB7-OB8
29	f3	302	CDL	C72-C71-CB7-OB8
33	C4	601	ATP	C3'-C4'-C5'-O5'
29	L	302	CDL	OA9-CA7-OA8-CA6
29	I3	302	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	C84-C85-C86-C87
29	l3	301	CDL	C44-C45-C46-C47
29	i	301	CDL	C84-C85-C86-C87
29	l	301	CDL	C44-C45-C46-C47
29	p	201	CDL	C23-C24-C25-C26
29	p3	201	CDL	C23-C24-C25-C26
29	a	501	CDL	OB6-CB4-CB6-OB8
29	r	201	CDL	OB6-CB4-CB6-OB8
29	F	303	CDL	OA6-CA4-CA6-OA8
29	I	301	CDL	OB6-CB4-CB6-OB8
29	I	302	CDL	OB6-CB4-CB6-OB8
29	K	201	CDL	OA6-CA4-CA6-OA8
29	a3	501	CDL	OB6-CB4-CB6-OB8
29	i3	301	CDL	OB6-CB4-CB6-OB8
29	F3	302	CDL	OA6-CA4-CA6-OA8
29	I3	301	CDL	OB6-CB4-CB6-OB8
29	I3	303	CDL	OB6-CB4-CB6-OB8
30	d	301	PC1	O21-C2-C3-O31
30	d3	301	PC1	O21-C2-C3-O31
29	r	201	CDL	C16-C17-C18-C19
29	i3	301	CDL	C16-C17-C18-C19
29	l3	301	CDL	C62-C63-C64-C65
35	L	303	PEE	C44-C45-C46-C47
35	a3	503	PEE	C44-C45-C46-C47
29	B3	401	CDL	C12-C13-C14-C15
29	k	201	CDL	C75-C76-C77-C78
29	l	301	CDL	C62-C63-C64-C65
29	B	401	CDL	C12-C13-C14-C15
29	b3	401	CDL	OA7-CA5-OA6-CA4
32	I3	304	UQ8	C38-C39-C41-C42
32	I3	304	UQ8	C28-C29-C31-C32
29	j	301	CDL	C52-C53-C54-C55
29	k3	201	CDL	C24-C25-C26-C27
29	k3	201	CDL	C75-C76-C77-C78
29	j3	301	CDL	C52-C53-C54-C55
29	k	201	CDL	CB4-CB6-OB8-CB7

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Mol	Chain	Res	Type	Atoms
29	i	301	CDL	C41-C42-C43-C44
29	l	301	CDL	C24-C25-C26-C27
29	a3	501	CDL	C33-C34-C35-C36
29	F3	302	CDL	C40-C41-C42-C43
29	a	501	CDL	C33-C34-C35-C36
29	b	401	CDL	C23-C24-C25-C26
29	k	201	CDL	C24-C25-C26-C27
29	F	303	CDL	C40-C41-C42-C43
29	l3	301	CDL	C24-C25-C26-C27
29	f	304	CDL	CA4-CA3-OA5-PA1
29	F	302	CDL	C1-CB2-OB2-PB2
29	F	302	CDL	CB4-CB3-OB5-PB2
29	L	302	CDL	CA4-CA3-OA5-PA1
29	a3	502	CDL	C1-CB2-OB2-PB2
29	a3	502	CDL	CB4-CB3-OB5-PB2
29	f3	304	CDL	CA4-CA3-OA5-PA1
29	I3	302	CDL	CA4-CA3-OA5-PA1
30	G	303	PC1	C2-C1-O11-P
30	G3	303	PC1	C2-C1-O11-P
35	l3	302	PEE	C35-C36-C37-C38
29	b3	401	CDL	C23-C24-C25-C26
29	i3	302	CDL	C41-C42-C43-C44
30	D	301	PC1	C32-C33-C34-C35
30	D3	301	PC1	C32-C33-C34-C35
29	f	303	CDL	C11-C12-C13-C14
29	J	302	CDL	C72-C73-C74-C75
29	l	302	CDL	C32-C31-CA7-OA8
29	B	402	CDL	C32-C31-CA7-OA8
29	l3	303	CDL	C32-C31-CA7-OA8
29	k	201	CDL	C22-C23-C24-C25
29	k3	201	CDL	C22-C23-C24-C25
29	f	303	CDL	C12-C13-C14-C15
29	r	201	CDL	C64-C65-C66-C67
29	B	402	CDL	C63-C64-C65-C66
29	i3	301	CDL	C64-C65-C66-C67
29	B3	402	CDL	C63-C64-C65-C66
29	b	401	CDL	OA7-CA5-OA6-CA4
29	L	302	CDL	OB7-CB5-OB6-CB4
29	I3	302	CDL	OB7-CB5-OB6-CB4
29	p	201	CDL	C51-CB5-OB6-CB4
29	F	303	CDL	C11-CA5-OA6-CA4
29	p3	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	F3	302	CDL	C11-CA5-OA6-CA4
29	l	301	CDL	C40-C41-C42-C43
29	l3	301	CDL	C40-C41-C42-C43
29	l3	301	CDL	C75-C76-C77-C78
29	j	302	CDL	CA5-C11-C12-C13
29	J	301	CDL	CA5-C11-C12-C13
29	j3	302	CDL	CA5-C11-C12-C13
29	J3	301	CDL	CA5-C11-C12-C13
29	f3	303	CDL	C11-C12-C13-C14
29	J3	302	CDL	C41-C42-C43-C44
30	d3	301	PC1	C33-C34-C35-C36
36	e	900	NAD	PA-O3-PN-O5D
36	E	900	NAD	PA-O3-PN-O5D
36	e3	900	NAD	PA-O3-PN-O5D
36	E3	900	NAD	PA-O3-PN-O5D
29	l	301	CDL	C75-C76-C77-C78
29	F	303	CDL	C57-C58-C59-C60
29	f3	303	CDL	C12-C13-C14-C15
29	F3	302	CDL	C57-C58-C59-C60
30	d	301	PC1	C33-C34-C35-C36
29	p	201	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	C31-C32-C33-C34
29	J3	302	CDL	C72-C73-C74-C75
29	f	302	CDL	OB5-CB3-CB4-CB6
29	f	304	CDL	OB5-CB3-CB4-CB6
29	g	305	CDL	OA5-CA3-CA4-CA6
29	j	301	CDL	OA5-CA3-CA4-CA6
29	B	403	CDL	OB5-CB3-CB4-CB6
29	f3	302	CDL	OB5-CB3-CB4-CB6
29	g3	305	CDL	OA5-CA3-CA4-CA6
29	A3	501	CDL	OB5-CB3-CB4-CB6
29	B3	403	CDL	OA5-CA3-CA4-CA6
29	I3	301	CDL	OA5-CA3-CA4-CA6
30	g	304	PC1	O11-C1-C2-C3
30	G	304	PC1	O11-C1-C2-C3
29	B3	402	CDL	C32-C31-CA7-OA8
29	i	301	CDL	C31-C32-C33-C34
29	J	302	CDL	C41-C42-C43-C44
30	G	304	PC1	C37-C38-C39-C3A
30	G3	304	PC1	C37-C38-C39-C3A
29	b	401	CDL	C75-C76-C77-C78
29	b3	401	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
29	j3	302	CDL	C34-C35-C36-C37
29	f	304	CDL	C78-C79-C80-C81
29	l	301	CDL	C61-C62-C63-C64
29	f3	304	CDL	C78-C79-C80-C81
29	l3	301	CDL	C61-C62-C63-C64
29	p3	201	CDL	OA9-CA7-OA8-CA6
29	j	302	CDL	C34-C35-C36-C37
29	J3	301	CDL	C82-C83-C84-C85
35	m	301	PEE	C40-C41-C42-C43
29	J	301	CDL	C82-C83-C84-C85
29	B	403	CDL	CB5-C51-C52-C53
29	B3	403	CDL	CB5-C51-C52-C53
29	I	301	CDL	C22-C23-C24-C25
35	j3	303	PEE	C40-C41-C42-C43
29	p	201	CDL	C71-CB7-OB8-CB6
29	L	302	CDL	C71-CB7-OB8-CB6
29	p3	201	CDL	C71-CB7-OB8-CB6
29	I3	302	CDL	C71-CB7-OB8-CB6
29	L	302	CDL	C72-C71-CB7-OB8
29	I3	302	CDL	C72-C71-CB7-OB8
29	I3	301	CDL	C22-C23-C24-C25
29	A	502	CDL	C34-C35-C36-C37
29	i3	301	CDL	C20-C21-C22-C23
29	B3	403	CDL	C72-C73-C74-C75
29	j	301	CDL	C63-C64-C65-C66
29	j3	301	CDL	C63-C64-C65-C66
29	j	302	CDL	CA6-CA4-OA6-CA5
29	B	401	CDL	CA3-CA4-OA6-CA5
29	B	403	CDL	CA6-CA4-OA6-CA5
29	F	302	CDL	CA6-CA4-OA6-CA5
29	I	301	CDL	CA6-CA4-OA6-CA5
29	J	302	CDL	CA6-CA4-OA6-CA5
29	i3	301	CDL	CA6-CA4-OA6-CA5
29	j3	302	CDL	CA6-CA4-OA6-CA5
29	B3	401	CDL	CA3-CA4-OA6-CA5
29	B3	403	CDL	CA6-CA4-OA6-CA5
29	I3	301	CDL	CA6-CA4-OA6-CA5
29	J3	302	CDL	CA6-CA4-OA6-CA5
29	F	303	CDL	OA7-CA5-OA6-CA4
29	F3	302	CDL	OA7-CA5-OA6-CA4
29	A	502	CDL	C84-C85-C86-C87
29	A3	501	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	B3	402	CDL	C33-C34-C35-C36
29	K3	202	CDL	C81-C82-C83-C84
30	G	303	PC1	C3E-C3F-C3G-C3H
30	G3	303	PC1	C3E-C3F-C3G-C3H
29	j	301	CDL	CB5-C51-C52-C53
29	j3	301	CDL	CB5-C51-C52-C53
29	i	301	CDL	C72-C71-CB7-OB8
29	l	301	CDL	C80-C81-C82-C83
29	B	403	CDL	C72-C73-C74-C75
29	K	202	CDL	C81-C82-C83-C84
29	A3	501	CDL	C84-C85-C86-C87
32	I	303	UQ8	C15-C14-C16-C17
32	I3	304	UQ8	C15-C14-C16-C17
29	B	401	CDL	C56-C57-C58-C59
32	i	302	UQ8	C13-C14-C16-C17
32	I	303	UQ8	C13-C14-C16-C17
32	i3	303	UQ8	C13-C14-C16-C17
32	I3	304	UQ8	C13-C14-C16-C17
35	A	501	PEE	C35-C36-C37-C38
29	r	201	CDL	C20-C21-C22-C23
29	k	201	CDL	CB3-CB4-CB6-OB8
29	g	305	CDL	CB3-CB4-CB6-OB8
29	B	402	CDL	C1-CA2-OA2-PA1
29	P	201	CDL	CA3-CA4-CA6-OA8
29	f3	304	CDL	CA3-CA4-CA6-OA8
29	k3	201	CDL	CB3-CB4-CB6-OB8
29	g3	305	CDL	CB3-CB4-CB6-OB8
29	j3	301	CDL	CB3-CB4-CB6-OB8
29	B3	402	CDL	C1-CA2-OA2-PA1
29	F3	302	CDL	CB3-CB4-CB6-OB8
29	l	302	CDL	OA9-CA7-OA8-CA6
29	J	302	CDL	OB9-CB7-OB8-CB6
29	l3	303	CDL	OA9-CA7-OA8-CA6
29	J3	302	CDL	OB9-CB7-OB8-CB6
29	B	402	CDL	C33-C34-C35-C36
29	f3	304	CDL	C39-C40-C41-C42
29	f	302	CDL	OB5-CB3-CB4-OB6
29	r	201	CDL	OA5-CA3-CA4-OA6
29	B	401	CDL	OB5-CB3-CB4-OB6
29	B	404	CDL	OA5-CA3-CA4-OA6
29	I	302	CDL	OB5-CB3-CB4-OB6
29	J	301	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
29	f3	304	CDL	OB5-CB3-CB4-OB6
29	i3	301	CDL	OA5-CA3-CA4-OA6
29	j3	301	CDL	OA5-CA3-CA4-OA6
29	j3	301	CDL	OB5-CB3-CB4-OB6
29	B3	403	CDL	OB5-CB3-CB4-OB6
29	B3	404	CDL	OA5-CA3-CA4-OA6
29	F3	302	CDL	OB5-CB3-CB4-OB6
29	I3	301	CDL	OA5-CA3-CA4-OA6
29	I3	303	CDL	OB5-CB3-CB4-OB6
29	J3	301	CDL	OA5-CA3-CA4-OA6
29	P3	201	CDL	OB5-CB3-CB4-OB6
30	G	303	PC1	O11-C1-C2-O21
35	J	303	PEE	O3P-C1-C2-O2
29	J	301	CDL	C72-C71-CB7-OB8
29	i3	302	CDL	C72-C71-CB7-OB8
29	J3	301	CDL	C72-C71-CB7-OB8
29	f	304	CDL	C54-C55-C56-C57
29	g	305	CDL	C83-C84-C85-C86
29	L	301	CDL	C77-C78-C79-C80
29	f3	304	CDL	C13-C14-C15-C16
29	g3	305	CDL	C83-C84-C85-C86
29	l3	301	CDL	C80-C81-C82-C83
29	L3	301	CDL	C77-C78-C79-C80
30	G	304	PC1	C3B-C3C-C3D-C3E
29	f	304	CDL	C13-C14-C15-C16
29	P	201	CDL	C11-C12-C13-C14
29	b	401	CDL	O1-C1-CB2-OB2
29	f	304	CDL	O1-C1-CA2-OA2
29	i	301	CDL	O1-C1-CA2-OA2
29	b3	401	CDL	O1-C1-CB2-OB2
29	f3	304	CDL	O1-C1-CA2-OA2
29	i3	302	CDL	O1-C1-CA2-OA2
29	f	304	CDL	C39-C40-C41-C42
29	f3	304	CDL	C54-C55-C56-C57
29	B	402	CDL	OB9-CB7-OB8-CB6
29	B3	402	CDL	OB9-CB7-OB8-CB6
29	B3	401	CDL	C56-C57-C58-C59
29	F3	302	CDL	C72-C73-C74-C75
29	P3	201	CDL	C11-C12-C13-C14
30	G3	304	PC1	C3B-C3C-C3D-C3E
29	F	303	CDL	C72-C73-C74-C75
29	k	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	j	301	CDL	OB6-CB4-CB6-OB8
29	A	502	CDL	OB6-CB4-CB6-OB8
29	k3	201	CDL	OB6-CB4-CB6-OB8
29	j3	302	CDL	OA6-CA4-CA6-OA8
29	K3	202	CDL	OB6-CB4-CB6-OB8
29	J3	302	CDL	OA6-CA4-CA6-OA8
29	J3	302	CDL	OB6-CB4-CB6-OB8
29	P3	201	CDL	OA6-CA4-CA6-OA8
30	g	303	PC1	O21-C2-C3-O31
30	G	303	PC1	O21-C2-C3-O31
30	g3	303	PC1	O21-C2-C3-O31
30	G3	303	PC1	O21-C2-C3-O31
30	G	303	PC1	C35-C36-C37-C38
35	A	501	PEE	C43-C44-C45-C46
29	B	401	CDL	OA9-CA7-OA8-CA6
30	G3	303	PC1	C35-C36-C37-C38
35	l3	302	PEE	C43-C44-C45-C46
33	C1	601	ATP	C5'-O5'-PA-O3A
33	B1	1003	ATP	C5'-O5'-PA-O3A
33	B2	1003	ATP	C5'-O5'-PA-O3A
33	C4	601	ATP	C5'-O5'-PA-O3A
33	B4	1003	ATP	C5'-O5'-PA-O3A
33	B5	1003	ATP	C5'-O5'-PA-O3A
36	E	900	NAD	C5B-O5B-PA-O3
36	E3	900	NAD	C5B-O5B-PA-O3
29	L	302	CDL	C78-C79-C80-C81
35	L	303	PEE	C35-C36-C37-C38
35	a3	503	PEE	C35-C36-C37-C38
32	i	302	UQ8	C15-C14-C16-C17
32	i3	303	UQ8	C15-C14-C16-C17
29	I3	302	CDL	C78-C79-C80-C81
29	B3	401	CDL	OA9-CA7-OA8-CA6
30	D	301	PC1	C2A-C2B-C2C-C2D
30	D3	301	PC1	C2A-C2B-C2C-C2D
29	p	201	CDL	OB7-CB5-OB6-CB4
29	p3	201	CDL	OB7-CB5-OB6-CB4
29	L	302	CDL	OB9-CB7-OB8-CB6
29	I	302	CDL	C20-C21-C22-C23
29	f3	304	CDL	C51-C52-C53-C54
29	i3	301	CDL	C33-C34-C35-C36
29	I3	303	CDL	C20-C21-C22-C23
29	f	304	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
29	I3	302	CDL	OB9-CB7-OB8-CB6
29	b3	401	CDL	CA7-C31-C32-C33
29	r	201	CDL	C33-C34-C35-C36
29	f	304	CDL	C42-C43-C44-C45
29	a3	502	CDL	C75-C76-C77-C78
30	G	303	PC1	C2F-C2G-C2H-C2I
29	f3	304	CDL	C42-C43-C44-C45
30	G3	303	PC1	C2F-C2G-C2H-C2I
29	l3	303	CDL	OA7-CA5-OA6-CA4
29	f	302	CDL	C31-C32-C33-C34
29	F	302	CDL	C75-C76-C77-C78
29	f3	302	CDL	C31-C32-C33-C34
29	I3	301	CDL	C39-C40-C41-C42
29	l	302	CDL	CB3-OB5-PB2-OB2
29	B	402	CDL	CA3-OA5-PA1-OA2
29	K	202	CDL	CA3-OA5-PA1-OA2
29	l3	303	CDL	CB3-OB5-PB2-OB2
29	B3	402	CDL	CA3-OA5-PA1-OA2
29	K3	202	CDL	CA3-OA5-PA1-OA2
29	i	301	CDL	C57-C58-C59-C60
29	I	301	CDL	C39-C40-C41-C42
29	A	502	CDL	O1-C1-CA2-OA2
29	A3	501	CDL	O1-C1-CA2-OA2
29	b	401	CDL	CA7-C31-C32-C33
29	I3	303	CDL	C38-C39-C40-C41
29	j	301	CDL	C1-CB2-OB2-PB2
29	l	302	CDL	C1-CA2-OA2-PA1
29	J	301	CDL	C1-CB2-OB2-PB2
29	j3	301	CDL	C1-CB2-OB2-PB2
29	l3	303	CDL	C1-CA2-OA2-PA1
29	J3	301	CDL	C1-CB2-OB2-PB2
32	i	302	UQ8	C38-C39-C41-C42
29	B	404	CDL	C22-C23-C24-C25
29	I	302	CDL	C38-C39-C40-C41
29	i3	302	CDL	C57-C58-C59-C60
29	B3	401	CDL	C72-C73-C74-C75
29	B3	404	CDL	C22-C23-C24-C25
29	b	401	CDL	CA3-OA5-PA1-OA3
29	b	401	CDL	CB3-OB5-PB2-OB3
29	f	302	CDL	CA2-OA2-PA1-OA4
29	f	303	CDL	CB2-OB2-PB2-OB3
29	f	303	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	i	301	CDL	CA3-OA5-PA1-OA4
29	i	301	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB2-OB2-PB2-OB3
29	g	305	CDL	CB2-OB2-PB2-OB4
29	l	301	CDL	CA3-OA5-PA1-OA4
29	l	301	CDL	CB3-OB5-PB2-OB3
29	l	301	CDL	CB3-OB5-PB2-OB4
29	l	302	CDL	CA3-OA5-PA1-OA4
29	l	302	CDL	CB3-OB5-PB2-OB4
29	p	201	CDL	CA3-OA5-PA1-OA4
29	r	201	CDL	CB3-OB5-PB2-OB3
29	B	401	CDL	CA2-OA2-PA1-OA4
29	B	401	CDL	CB3-OB5-PB2-OB3
29	B	401	CDL	CB3-OB5-PB2-OB4
29	B	404	CDL	CB2-OB2-PB2-OB3
29	B	404	CDL	CB2-OB2-PB2-OB4
29	F	302	CDL	CA3-OA5-PA1-OA4
29	F	303	CDL	CA2-OA2-PA1-OA4
29	F	303	CDL	CB2-OB2-PB2-OB4
29	I	301	CDL	CB2-OB2-PB2-OB3
29	I	301	CDL	CB2-OB2-PB2-OB4
29	K	201	CDL	CB2-OB2-PB2-OB3
29	K	201	CDL	CB3-OB5-PB2-OB4
29	J	301	CDL	CB3-OB5-PB2-OB3
29	J	301	CDL	CB3-OB5-PB2-OB4
29	J	302	CDL	CA3-OA5-PA1-OA4
29	L	301	CDL	CA3-OA5-PA1-OA4
29	L	301	CDL	CB3-OB5-PB2-OB4
29	L	302	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CB3-OB5-PB2-OB4
29	P	201	CDL	CA3-OA5-PA1-OA4
29	a3	502	CDL	CA3-OA5-PA1-OA4
29	b3	401	CDL	CA3-OA5-PA1-OA3
29	b3	401	CDL	CB3-OB5-PB2-OB3
29	f3	302	CDL	CA2-OA2-PA1-OA4
29	f3	303	CDL	CB2-OB2-PB2-OB3
29	f3	303	CDL	CB2-OB2-PB2-OB4
29	i3	301	CDL	CB3-OB5-PB2-OB3
29	i3	302	CDL	CA3-OA5-PA1-OA4
29	i3	302	CDL	CB3-OB5-PB2-OB3
29	k3	201	CDL	CB2-OB2-PB2-OB3
29	g3	305	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	l3	301	CDL	CA3-OA5-PA1-OA4
29	l3	301	CDL	CB3-OB5-PB2-OB3
29	l3	301	CDL	CB3-OB5-PB2-OB4
29	l3	303	CDL	CA3-OA5-PA1-OA4
29	l3	303	CDL	CB3-OB5-PB2-OB4
29	p3	201	CDL	CA3-OA5-PA1-OA4
29	B3	401	CDL	CA2-OA2-PA1-OA4
29	B3	401	CDL	CB3-OB5-PB2-OB3
29	B3	401	CDL	CB3-OB5-PB2-OB4
29	B3	404	CDL	CB2-OB2-PB2-OB3
29	B3	404	CDL	CB2-OB2-PB2-OB4
29	F3	302	CDL	CA2-OA2-PA1-OA4
29	F3	302	CDL	CB2-OB2-PB2-OB4
29	I3	301	CDL	CB2-OB2-PB2-OB3
29	I3	301	CDL	CB2-OB2-PB2-OB4
29	I3	302	CDL	CB3-OB5-PB2-OB3
29	I3	302	CDL	CB3-OB5-PB2-OB4
29	K3	201	CDL	CB2-OB2-PB2-OB3
29	K3	201	CDL	CB3-OB5-PB2-OB4
29	J3	301	CDL	CB3-OB5-PB2-OB3
29	J3	301	CDL	CB3-OB5-PB2-OB4
29	J3	302	CDL	CA3-OA5-PA1-OA4
29	L3	301	CDL	CA3-OA5-PA1-OA4
29	L3	301	CDL	CB3-OB5-PB2-OB4
29	P3	201	CDL	CA3-OA5-PA1-OA4
30	g	303	PC1	C1-O11-P-O14
30	G	303	PC1	C11-O13-P-O14
30	G	303	PC1	C1-O11-P-O14
30	g3	303	PC1	C1-O11-P-O14
30	G3	303	PC1	C11-O13-P-O12
30	G3	303	PC1	C11-O13-P-O14
30	G3	303	PC1	C1-O11-P-O14
33	A1	601	ATP	C5'-O5'-PA-O2A
33	C2	601	ATP	C5'-O5'-PA-O2A
33	A2	601	ATP	C5'-O5'-PA-O2A
33	A4	601	ATP	C5'-O5'-PA-O2A
33	C5	601	ATP	C5'-O5'-PA-O2A
33	A5	601	ATP	C5'-O5'-PA-O2A
35	m	301	PEE	C1-O3P-P-O1P
35	A	501	PEE	C4-O4P-P-O2P
35	J	303	PEE	C1-O3P-P-O1P
35	L	303	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
35	a3	503	PEE	C4-O4P-P-O2P
35	j3	303	PEE	C1-O3P-P-O1P
35	l3	302	PEE	C4-O4P-P-O2P
35	L3	302	PEE	C1-O3P-P-O1P
29	B	401	CDL	C72-C73-C74-C75
29	B	403	CDL	OA5-CA3-CA4-CA6
29	F	302	CDL	OA5-CA3-CA4-CA6
29	F	302	CDL	OB5-CB3-CB4-CB6
29	I	302	CDL	OB5-CB3-CB4-CB6
29	a3	502	CDL	OB5-CB3-CB4-CB6
29	f3	304	CDL	OB5-CB3-CB4-CB6
29	B3	401	CDL	OB5-CB3-CB4-CB6
29	B3	403	CDL	OB5-CB3-CB4-CB6
29	I3	303	CDL	OB5-CB3-CB4-CB6
29	p3	201	CDL	C39-C40-C41-C42
29	L3	301	CDL	C76-C77-C78-C79
35	m	301	PEE	O4P-C4-C5-N
35	J	303	PEE	O4P-C4-C5-N
35	j3	303	PEE	O4P-C4-C5-N
35	L3	302	PEE	O4P-C4-C5-N
29	p	201	CDL	C39-C40-C41-C42
29	L	301	CDL	C76-C77-C78-C79
29	l	302	CDL	OA7-CA5-OA6-CA4
29	g	305	CDL	C15-C16-C17-C18
35	L	303	PEE	C12-C13-C14-C15
29	k	201	CDL	C57-C58-C59-C60
29	g3	305	CDL	C15-C16-C17-C18
35	a3	503	PEE	C12-C13-C14-C15
29	k3	201	CDL	C57-C58-C59-C60
29	B	401	CDL	C72-C71-CB7-OB8
29	B3	401	CDL	C72-C71-CB7-OB8
29	j	301	CDL	C18-C19-C20-C21
29	j3	301	CDL	C18-C19-C20-C21
29	J3	302	CDL	C20-C21-C22-C23
29	p	201	CDL	OB9-CB7-OB8-CB6
29	K	202	CDL	C61-C62-C63-C64
29	J	302	CDL	C20-C21-C22-C23
29	K3	202	CDL	C61-C62-C63-C64
30	d3	301	PC1	C3C-C3D-C3E-C3F
29	B	404	CDL	C72-C73-C74-C75
29	A	502	CDL	C71-CB7-OB8-CB6
29	A3	501	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	f	303	CDL	CA2-C1-CB2-OB2
29	f3	303	CDL	CA2-C1-CB2-OB2
29	B	403	CDL	C19-C20-C21-C22
29	F	303	CDL	C43-C44-C45-C46
29	B3	404	CDL	C72-C73-C74-C75
29	K3	202	CDL	C31-C32-C33-C34
29	b	401	CDL	CB7-C71-C72-C73
29	j	301	CDL	OA5-CA3-CA4-OA6
29	P	201	CDL	OB5-CB3-CB4-OB6
29	f3	302	CDL	OB5-CB3-CB4-OB6
29	B3	401	CDL	OB5-CB3-CB4-OB6
30	G	304	PC1	O11-C1-C2-O21
35	m	301	PEE	O3P-C1-C2-O2
29	B3	403	CDL	C19-C20-C21-C22
29	F3	302	CDL	C43-C44-C45-C46
29	L3	301	CDL	C11-C12-C13-C14
30	d	301	PC1	C3C-C3D-C3E-C3F
29	p3	201	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	C64-C65-C66-C67
29	r	201	CDL	C84-C85-C86-C87
29	K	202	CDL	C31-C32-C33-C34
29	L	301	CDL	C11-C12-C13-C14
29	l	301	CDL	C72-C71-CB7-OB8
29	I	302	CDL	C72-C71-CB7-OB8
29	l3	301	CDL	C72-C71-CB7-OB8
29	I3	303	CDL	C72-C71-CB7-OB8
29	i3	301	CDL	C84-C85-C86-C87
29	b3	401	CDL	CB7-C71-C72-C73
29	f3	302	CDL	C64-C65-C66-C67
29	K3	202	CDL	C17-C18-C19-C20
29	j	301	CDL	C34-C35-C36-C37
29	K	202	CDL	C17-C18-C19-C20
29	J	302	CDL	C61-C62-C63-C64
29	j3	301	CDL	C34-C35-C36-C37
29	b3	401	CDL	C32-C31-CA7-OA8
29	f	304	CDL	CA3-CA4-CA6-OA8
29	A	502	CDL	C13-C14-C15-C16
29	K	201	CDL	CA3-CA4-CA6-OA8
29	J3	302	CDL	C61-C62-C63-C64
30	g	304	PC1	O13-C11-C12-N
30	G	303	PC1	C25-C26-C27-C28
30	G	304	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
30	g3	304	PC1	O13-C11-C12-N
30	G3	304	PC1	O13-C11-C12-N
29	b	401	CDL	OB6-CB4-CB6-OB8
29	f	304	CDL	OA6-CA4-CA6-OA8
29	J	301	CDL	OB6-CB4-CB6-OB8
29	J	302	CDL	OA6-CA4-CA6-OA8
29	b3	401	CDL	OB6-CB4-CB6-OB8
29	f3	304	CDL	OA6-CA4-CA6-OA8
29	A3	501	CDL	OB6-CB4-CB6-OB8
29	K3	201	CDL	OA6-CA4-CA6-OA8
29	J3	301	CDL	OB6-CB4-CB6-OB8
30	D	301	PC1	O21-C2-C3-O31
30	D3	301	PC1	O21-C2-C3-O31
29	A3	501	CDL	C40-C41-C42-C43
30	G3	303	PC1	C25-C26-C27-C28
35	J	303	PEE	C33-C34-C35-C36
35	L3	302	PEE	C33-C34-C35-C36
29	j	302	CDL	C31-C32-C33-C34
29	A	502	CDL	C40-C41-C42-C43
29	j3	302	CDL	C31-C32-C33-C34
29	p3	201	CDL	C36-C37-C38-C39
29	A3	501	CDL	C13-C14-C15-C16
30	d	301	PC1	C38-C39-C3A-C3B
29	P	201	CDL	C37-C38-C39-C40
29	g3	305	CDL	C13-C14-C15-C16
29	b	401	CDL	C32-C31-CA7-OA8
29	p	201	CDL	C36-C37-C38-C39
29	L	302	CDL	C36-C37-C38-C39
29	j3	301	CDL	C13-C14-C15-C16
30	d3	301	PC1	C38-C39-C3A-C3B
29	f	303	CDL	CA4-CA3-OA5-PA1
29	I	302	CDL	CB4-CB3-OB5-PB2
29	L	302	CDL	C1-CA2-OA2-PA1
29	f3	303	CDL	CA4-CA3-OA5-PA1
29	I3	302	CDL	C1-CA2-OA2-PA1
29	I3	303	CDL	CB4-CB3-OB5-PB2
29	j	301	CDL	C13-C14-C15-C16
29	g	305	CDL	C13-C14-C15-C16
29	A3	501	CDL	C61-C62-C63-C64
29	B3	404	CDL	C17-C18-C19-C20
29	I3	302	CDL	C36-C37-C38-C39
29	K3	201	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	P3	201	CDL	C37-C38-C39-C40
32	i3	303	UQ8	C38-C39-C41-C42
29	l3	303	CDL	C11-CA5-OA6-CA4
29	K	201	CDL	C33-C34-C35-C36
29	J	301	CDL	C17-C18-C19-C20
29	K	202	CDL	C55-C56-C57-C58
29	P	201	CDL	C34-C35-C36-C37
29	J3	301	CDL	C17-C18-C19-C20
29	P3	201	CDL	C34-C35-C36-C37
29	a	501	CDL	C75-C76-C77-C78
29	B	404	CDL	C17-C18-C19-C20
29	a3	501	CDL	C75-C76-C77-C78
29	A	502	CDL	C61-C62-C63-C64
29	I3	301	CDL	C15-C16-C17-C18
35	J	303	PEE	C14-C15-C16-C17
29	B	403	CDL	C22-C23-C24-C25
29	I	301	CDL	C15-C16-C17-C18
29	K3	202	CDL	C55-C56-C57-C58
29	B3	403	CDL	C22-C23-C24-C25
35	L3	302	PEE	C14-C15-C16-C17
29	i	301	CDL	C71-CB7-OB8-CB6
29	B3	402	CDL	C16-C17-C18-C19
29	f	303	CDL	O1-C1-CA2-OA2
29	I	301	CDL	C44-C45-C46-C47
29	L	302	CDL	C24-C25-C26-C27
33	C1	601	ATP	C3'-C4'-C5'-O5'
29	k	201	CDL	C20-C21-C22-C23
29	I3	301	CDL	C44-C45-C46-C47
29	I3	302	CDL	C24-C25-C26-C27
35	l3	302	PEE	C12-C13-C14-C15
29	j	301	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C32-C31-CA7-OA8
29	j3	301	CDL	C72-C71-CB7-OB8
29	A3	501	CDL	C32-C31-CA7-OA8
29	B	402	CDL	C16-C17-C18-C19
29	K	201	CDL	C75-C76-C77-C78
35	A	501	PEE	C12-C13-C14-C15
29	k3	201	CDL	C20-C21-C22-C23
29	a	501	CDL	C34-C35-C36-C37
29	j	301	CDL	C55-C56-C57-C58
29	L	302	CDL	C34-C35-C36-C37
29	a3	501	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	f3	303	CDL	C72-C73-C74-C75
29	j3	301	CDL	C55-C56-C57-C58
29	p3	201	CDL	C11-C12-C13-C14
29	p	201	CDL	C11-C12-C13-C14
29	L	302	CDL	C33-C34-C35-C36
29	l	302	CDL	CA6-CA4-OA6-CA5
29	p	201	CDL	CA6-CA4-OA6-CA5
29	r	201	CDL	CA6-CA4-OA6-CA5
29	B	402	CDL	CB3-CB4-OB6-CB5
29	F	303	CDL	CB3-CB4-OB6-CB5
29	a3	502	CDL	CA6-CA4-OA6-CA5
29	l3	303	CDL	CA6-CA4-OA6-CA5
29	p3	201	CDL	CA6-CA4-OA6-CA5
30	d	301	PC1	C1-C2-O21-C21
30	d3	301	PC1	C1-C2-O21-C21
29	f	302	CDL	CB2-C1-CA2-OA2
29	f3	302	CDL	CB2-C1-CA2-OA2
29	f	303	CDL	C72-C73-C74-C75
29	I3	302	CDL	C33-C34-C35-C36
29	K3	201	CDL	C75-C76-C77-C78
29	i3	302	CDL	C71-CB7-OB8-CB6
35	L3	302	PEE	C12-C13-C14-C15
29	A3	501	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	C22-C23-C24-C25
29	I3	302	CDL	C34-C35-C36-C37
29	g3	305	CDL	C80-C81-C82-C83
35	J	303	PEE	C12-C13-C14-C15
29	j	302	CDL	CB4-CB3-OB5-PB2
29	l	302	CDL	CB4-CB3-OB5-PB2
29	l3	303	CDL	CB4-CB3-OB5-PB2
29	f3	302	CDL	C22-C23-C24-C25
29	A	502	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OA5-CA3-CA4-OA6
29	j3	302	CDL	OB5-CB3-CB4-OB6
29	l3	303	CDL	OB5-CB3-CB4-OB6
30	G3	304	PC1	O11-C1-C2-O21
29	b	401	CDL	C61-C62-C63-C64
29	g	305	CDL	C80-C81-C82-C83
29	a	501	CDL	C15-C16-C17-C18
29	a3	501	CDL	C15-C16-C17-C18
29	b3	401	CDL	C61-C62-C63-C64
29	P	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
29	L	301	CDL	C31-CA7-OA8-CA6
29	L3	301	CDL	C31-CA7-OA8-CA6
29	I	301	CDL	C43-C44-C45-C46
29	I3	301	CDL	C33-C34-C35-C36
29	I3	301	CDL	C43-C44-C45-C46
29	l	302	CDL	C11-CA5-OA6-CA4
29	l	301	CDL	C33-C34-C35-C36
29	L	301	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	OB9-CB7-OB8-CB6
29	L3	301	CDL	OA9-CA7-OA8-CA6
29	p	201	CDL	OA6-CA4-CA6-OA8
29	B	402	CDL	OB6-CB4-CB6-OB8
29	K	202	CDL	OB6-CB4-CB6-OB8
29	j3	301	CDL	OB6-CB4-CB6-OB8
29	F	303	CDL	C14-C15-C16-C17
29	j3	302	CDL	C58-C59-C60-C61
29	A3	501	CDL	C33-C34-C35-C36
29	F3	302	CDL	C14-C15-C16-C17
29	b	401	CDL	CA3-OA5-PA1-OA2
29	f	304	CDL	CA2-OA2-PA1-OA5
29	i	301	CDL	CB2-OB2-PB2-OB5
29	g	305	CDL	CA3-OA5-PA1-OA2
29	l	302	CDL	CA3-OA5-PA1-OA2
29	l	302	CDL	CB2-OB2-PB2-OB5
29	L	301	CDL	CB2-OB2-PB2-OB5
29	P	201	CDL	CA3-OA5-PA1-OA2
29	b3	401	CDL	CA3-OA5-PA1-OA2
29	f3	304	CDL	CA2-OA2-PA1-OA5
29	i3	302	CDL	CB2-OB2-PB2-OB5
29	g3	305	CDL	CA3-OA5-PA1-OA2
29	l3	303	CDL	CA3-OA5-PA1-OA2
29	l3	303	CDL	CB2-OB2-PB2-OB5
29	L3	301	CDL	CB2-OB2-PB2-OB5
29	P3	201	CDL	CA3-OA5-PA1-OA2
30	g3	303	PC1	C11-O13-P-O11
29	P3	201	CDL	CB7-C71-C72-C73
29	j	302	CDL	C58-C59-C60-C61
29	A	502	CDL	C33-C34-C35-C36
33	C1	601	ATP	O4'-C4'-C5'-O5'
29	l	301	CDL	CA7-C31-C32-C33
29	B3	404	CDL	C14-C15-C16-C17
29	a	501	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	J3	301	CDL	CB3-CB4-CB6-OB8
30	g	304	PC1	C1-C2-C3-O31
30	g	304	PC1	C32-C33-C34-C35
29	l3	301	CDL	CA7-C31-C32-C33
29	k	201	CDL	C14-C15-C16-C17
30	g3	304	PC1	C32-C33-C34-C35
30	g3	304	PC1	C3C-C3D-C3E-C3F
29	I	301	CDL	CA5-C11-C12-C13
29	I3	301	CDL	CA5-C11-C12-C13
29	f	304	CDL	C53-C54-C55-C56
29	r	201	CDL	C78-C79-C80-C81
29	f3	304	CDL	C53-C54-C55-C56
29	f3	304	CDL	C72-C73-C74-C75
29	i3	301	CDL	C78-C79-C80-C81
29	k3	201	CDL	C14-C15-C16-C17
33	C2	601	ATP	PB-O3A-PA-O2A
33	C5	601	ATP	PB-O3A-PA-O2A
29	I	301	CDL	C14-C15-C16-C17
29	f3	304	CDL	C36-C37-C38-C39
30	g	304	PC1	C3C-C3D-C3E-C3F
29	f	304	CDL	C72-C73-C74-C75
29	L	302	CDL	C44-C45-C46-C47
30	G	303	PC1	C3D-C3E-C3F-C3G
29	l3	303	CDL	C16-C17-C18-C19
29	I3	303	CDL	C31-C32-C33-C34
29	i	301	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	C36-C37-C38-C39
29	I	302	CDL	C31-C32-C33-C34
29	I3	302	CDL	C44-C45-C46-C47
30	G3	303	PC1	C3D-C3E-C3F-C3G
29	l	301	CDL	CA4-CA3-OA5-PA1
29	L	301	CDL	C1-CA2-OA2-PA1
29	L	302	CDL	CB4-CB3-OB5-PB2
29	j3	302	CDL	CB4-CB3-OB5-PB2
29	l3	301	CDL	CA4-CA3-OA5-PA1
29	I3	302	CDL	CB4-CB3-OB5-PB2
29	L3	301	CDL	C1-CA2-OA2-PA1
29	J3	302	CDL	C22-C23-C24-C25
30	d3	301	PC1	C3B-C3C-C3D-C3E
29	l	302	CDL	C16-C17-C18-C19
29	J	302	CDL	C22-C23-C24-C25
30	D3	301	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	k	201	CDL	C12-C13-C14-C15
29	B	404	CDL	C14-C15-C16-C17
30	D	301	PC1	C34-C35-C36-C37
29	I3	301	CDL	C14-C15-C16-C17
29	k	201	CDL	C31-CA7-OA8-CA6
29	k3	201	CDL	C31-CA7-OA8-CA6
29	k3	201	CDL	C12-C13-C14-C15
29	l3	301	CDL	C17-C18-C19-C20
29	l	301	CDL	C17-C18-C19-C20
30	d	301	PC1	C3B-C3C-C3D-C3E
29	b	401	CDL	C60-C61-C62-C63
29	B	401	CDL	C24-C25-C26-C27
29	b3	401	CDL	C60-C61-C62-C63
30	G3	303	PC1	C33-C34-C35-C36
29	i3	301	CDL	C22-C23-C24-C25
29	B3	401	CDL	C24-C25-C26-C27
29	I3	303	CDL	C34-C35-C36-C37
35	J	303	PEE	C18-C19-C20-C21
35	L3	302	PEE	C18-C19-C20-C21
29	r	201	CDL	C22-C23-C24-C25
29	B3	403	CDL	C56-C57-C58-C59
29	I	302	CDL	C34-C35-C36-C37
29	f3	303	CDL	C23-C24-C25-C26
29	a3	502	CDL	OA5-CA3-CA4-CA6
30	g3	304	PC1	O11-C1-C2-C3
30	G3	303	PC1	O11-C1-C2-C3
29	k3	201	CDL	OA9-CA7-OA8-CA6
30	G	303	PC1	C33-C34-C35-C36
29	f	303	CDL	C23-C24-C25-C26
29	L	302	CDL	C31-C32-C33-C34
29	I3	302	CDL	C31-C32-C33-C34
29	j	301	CDL	OB5-CB3-CB4-OB6
29	l	302	CDL	OB5-CB3-CB4-OB6
29	A	502	CDL	OA5-CA3-CA4-OA6
29	k	201	CDL	C59-C60-C61-C62
29	B	404	CDL	C20-C21-C22-C23
29	k3	201	CDL	C59-C60-C61-C62
29	B3	404	CDL	C20-C21-C22-C23
29	B	403	CDL	C56-C57-C58-C59
29	k	201	CDL	OA9-CA7-OA8-CA6
30	G3	303	PC1	C23-C24-C25-C26
29	f3	303	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
29	B	404	CDL	C78-C79-C80-C81
29	i3	301	CDL	C11-C12-C13-C14
30	G	303	PC1	C23-C24-C25-C26
29	P	201	CDL	C72-C71-CB7-OB8
29	P3	201	CDL	C72-C71-CB7-OB8
30	G	304	PC1	O31-C31-C32-C33
30	G3	304	PC1	O31-C31-C32-C33
29	B3	404	CDL	C78-C79-C80-C81
29	g	305	CDL	C52-C53-C54-C55
29	J	302	CDL	OB6-CB4-CB6-OB8
29	J3	301	CDL	OA6-CA4-CA6-OA8
29	r	201	CDL	C11-C12-C13-C14
29	B3	403	CDL	CB4-CB3-OB5-PB2
29	B	401	CDL	C32-C31-CA7-OA9
29	B3	401	CDL	C32-C31-CA7-OA9
29	g3	305	CDL	C52-C53-C54-C55
29	g	305	CDL	C58-C59-C60-C61
29	B	402	CDL	C72-C71-CB7-OB8
29	J	302	CDL	C72-C71-CB7-OB8
29	J3	302	CDL	C72-C71-CB7-OB8
29	B	403	CDL	C36-C37-C38-C39
29	l3	303	CDL	C19-C20-C21-C22
29	l	302	CDL	C19-C20-C21-C22
29	j3	302	CDL	C18-C19-C20-C21
29	l3	303	CDL	C14-C15-C16-C17
29	B3	403	CDL	C36-C37-C38-C39
29	j	302	CDL	C18-C19-C20-C21
29	g3	305	CDL	C58-C59-C60-C61
29	B3	401	CDL	C11-C12-C13-C14
29	J3	301	CDL	C39-C40-C41-C42
29	B3	402	CDL	C72-C71-CB7-OB8
29	B	401	CDL	C11-C12-C13-C14
29	J	301	CDL	C39-C40-C41-C42
29	l	302	CDL	C14-C15-C16-C17
29	B	401	CDL	C20-C21-C22-C23
29	B3	401	CDL	C20-C21-C22-C23
30	g3	303	PC1	C3E-C3F-C3G-C3H
29	A	502	CDL	CA3-CA4-CA6-OA8
29	A	502	CDL	CB3-CB4-CB6-OB8
29	B	402	CDL	CB3-CB4-CB6-OB8
29	p3	201	CDL	CA3-CA4-CA6-OA8
29	K3	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
29	J3	302	CDL	CB3-CB4-CB6-OB8
29	P3	201	CDL	C76-C77-C78-C79
30	g	303	PC1	C3E-C3F-C3G-C3H
29	B3	401	CDL	C35-C36-C37-C38
29	B	401	CDL	C35-C36-C37-C38
29	p3	201	CDL	C37-C38-C39-C40
29	g	305	CDL	C56-C57-C58-C59
29	P	201	CDL	C76-C77-C78-C79
29	B3	401	CDL	C71-C72-C73-C74
29	B	401	CDL	C71-C72-C73-C74
29	g3	305	CDL	C56-C57-C58-C59
35	j3	303	PEE	C15-C16-C17-C18
29	L3	301	CDL	C17-C18-C19-C20
29	f	302	CDL	CA6-CA4-OA6-CA5
29	B	404	CDL	CA3-CA4-OA6-CA5
29	L	301	CDL	CA6-CA4-OA6-CA5
29	f3	302	CDL	CA6-CA4-OA6-CA5
29	B3	402	CDL	CB3-CB4-OB6-CB5
29	B3	404	CDL	CA3-CA4-OA6-CA5
29	F3	302	CDL	CB3-CB4-OB6-CB5
29	L3	301	CDL	CA6-CA4-OA6-CA5
30	d	301	PC1	C3-C2-O21-C21
30	D	301	PC1	C1-C2-O21-C21
30	D	301	PC1	C3-C2-O21-C21
30	d3	301	PC1	C3-C2-O21-C21
30	D3	301	PC1	C3-C2-O21-C21
29	p	201	CDL	C37-C38-C39-C40
29	B	403	CDL	C11-C12-C13-C14
29	L	301	CDL	C17-C18-C19-C20
29	b	401	CDL	C21-C22-C23-C24
29	p	201	CDL	C78-C79-C80-C81
29	P	201	CDL	C40-C41-C42-C43
29	a3	502	CDL	C71-C72-C73-C74
29	p3	201	CDL	C78-C79-C80-C81
29	j	302	CDL	C72-C71-CB7-OB8
29	j3	302	CDL	C72-C71-CB7-OB8
29	B3	403	CDL	C11-C12-C13-C14
29	b3	401	CDL	C21-C22-C23-C24
29	B	403	CDL	CB4-CB3-OB5-PB2
29	B	404	CDL	C58-C59-C60-C61
29	J	301	CDL	C41-C42-C43-C44
29	B3	404	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
29	J3	301	CDL	C41-C42-C43-C44
29	J3	302	CDL	C24-C25-C26-C27
29	P3	201	CDL	C40-C41-C42-C43
29	b3	401	CDL	OB5-CB3-CB4-OB6
29	A3	501	CDL	OA5-CA3-CA4-OA6
29	J3	302	CDL	OB5-CB3-CB4-OB6
30	g	304	PC1	O11-C1-C2-O21
29	J	302	CDL	C24-C25-C26-C27
35	m	301	PEE	C15-C16-C17-C18
35	L	303	PEE	C19-C20-C21-C22
35	a3	503	PEE	C19-C20-C21-C22
35	j3	303	PEE	O3P-C1-C2-C3
35	m	301	PEE	C36-C37-C38-C39
35	j3	303	PEE	C36-C37-C38-C39
29	F	302	CDL	C71-C72-C73-C74
29	A3	501	CDL	C20-C21-C22-C23
29	k3	201	CDL	C72-C73-C74-C75
29	k	201	CDL	C72-C73-C74-C75
29	A	502	CDL	C20-C21-C22-C23
29	A	502	CDL	C53-C54-C55-C56
29	K	201	CDL	C60-C61-C62-C63
29	A3	501	CDL	C53-C54-C55-C56
29	K3	201	CDL	C60-C61-C62-C63
30	G	304	PC1	C3A-C3B-C3C-C3D
29	L	302	CDL	CB5-C51-C52-C53
29	K	201	CDL	C37-C38-C39-C40
29	K3	201	CDL	C37-C38-C39-C40
30	g	304	PC1	C2F-C2G-C2H-C2I
30	g3	304	PC1	C2F-C2G-C2H-C2I
35	L	303	PEE	C20-C21-C22-C23
35	a3	503	PEE	C20-C21-C22-C23
29	a	501	CDL	OA6-CA4-CA6-OA8
29	g	305	CDL	OB6-CB4-CB6-OB8
29	f3	302	CDL	OA6-CA4-CA6-OA8
29	g3	305	CDL	OB6-CB4-CB6-OB8
30	G3	304	PC1	C3A-C3B-C3C-C3D
29	I3	302	CDL	CB5-C51-C52-C53
30	g	304	PC1	O31-C31-C32-C33
30	g3	304	PC1	O31-C31-C32-C33
29	i	301	CDL	C24-C25-C26-C27
29	J	302	CDL	C11-C12-C13-C14
29	J3	302	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	f	303	CDL	C20-C21-C22-C23
29	B	402	CDL	C41-C42-C43-C44
29	f3	303	CDL	C20-C21-C22-C23
29	i3	302	CDL	C24-C25-C26-C27
29	P3	201	CDL	C59-C60-C61-C62
29	f	304	CDL	CB2-C1-CA2-OA2
29	i	301	CDL	CB2-C1-CA2-OA2
29	K	201	CDL	CB2-C1-CA2-OA2
29	f3	304	CDL	CB2-C1-CA2-OA2
29	i3	302	CDL	CB2-C1-CA2-OA2
29	K3	201	CDL	CB2-C1-CA2-OA2
29	B3	402	CDL	C41-C42-C43-C44
30	d	301	PC1	C3F-C3G-C3H-C3I
29	P	201	CDL	C59-C60-C61-C62
30	d3	301	PC1	C3F-C3G-C3H-C3I
29	j3	302	CDL	C32-C33-C34-C35
29	B3	403	CDL	C53-C54-C55-C56
29	B	403	CDL	C53-C54-C55-C56
29	a3	502	CDL	C11-C12-C13-C14
29	f3	304	CDL	C83-C84-C85-C86
29	j	302	CDL	C32-C33-C34-C35
33	A2	601	ATP	PB-O3A-PA-O1A
33	A5	601	ATP	PB-O3A-PA-O1A
29	B3	403	CDL	OB7-CB5-OB6-CB4
29	f	304	CDL	C83-C84-C85-C86
29	r	201	CDL	C81-C82-C83-C84
29	K	201	CDL	C72-C73-C74-C75
29	J3	302	CDL	C15-C16-C17-C18
29	F	302	CDL	C11-C12-C13-C14
29	A3	501	CDL	CA3-CA4-CA6-OA8
29	K3	201	CDL	C72-C73-C74-C75
29	f	303	CDL	C14-C15-C16-C17
29	A	502	CDL	C52-C53-C54-C55
30	g3	304	PC1	C39-C3A-C3B-C3C
35	A	501	PEE	C34-C35-C36-C37
35	l3	302	PEE	C34-C35-C36-C37
29	l	301	CDL	C13-C14-C15-C16
29	K	201	CDL	C16-C17-C18-C19
29	J	302	CDL	C15-C16-C17-C18
29	f3	303	CDL	C14-C15-C16-C17
29	i3	301	CDL	C81-C82-C83-C84
29	l3	301	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	K3	201	CDL	C16-C17-C18-C19
29	A3	501	CDL	C52-C53-C54-C55
29	p	201	CDL	C82-C83-C84-C85
29	J	302	CDL	C34-C35-C36-C37
29	K3	202	CDL	C73-C74-C75-C76
30	g3	303	PC1	C23-C24-C25-C26
29	K	202	CDL	C73-C74-C75-C76
29	J3	302	CDL	C34-C35-C36-C37
30	g	303	PC1	C23-C24-C25-C26
30	g	304	PC1	C39-C3A-C3B-C3C
35	J	303	PEE	C38-C39-C40-C41
35	L3	302	PEE	C38-C39-C40-C41
29	b	401	CDL	OB5-CB3-CB4-OB6
29	F3	302	CDL	C63-C64-C65-C66
29	f	302	CDL	C24-C25-C26-C27
29	p3	201	CDL	C82-C83-C84-C85
29	J3	301	CDL	C59-C60-C61-C62
30	d3	301	PC1	C22-C23-C24-C25
29	B	401	CDL	C12-C11-CA5-OA6
29	B3	401	CDL	C12-C11-CA5-OA6
29	f3	302	CDL	C24-C25-C26-C27
29	f3	302	CDL	C72-C73-C74-C75
29	f	302	CDL	C72-C73-C74-C75
30	d	301	PC1	C22-C23-C24-C25
30	G3	303	PC1	C2C-C2D-C2E-C2F
29	F	303	CDL	C63-C64-C65-C66
29	k3	201	CDL	C56-C57-C58-C59
30	G	303	PC1	C2C-C2D-C2E-C2F
29	l3	303	CDL	OB5-CB3-CB4-CB6
29	k	201	CDL	C56-C57-C58-C59
29	P	201	CDL	C61-C62-C63-C64
29	P	201	CDL	C80-C81-C82-C83
29	b	401	CDL	CA5-C11-C12-C13
29	J	301	CDL	C59-C60-C61-C62
29	f3	304	CDL	C12-C11-CA5-OA6
30	G	303	PC1	O21-C21-C22-C23
30	G3	303	PC1	O21-C21-C22-C23
29	j3	302	CDL	C1-CB2-OB2-PB2
29	b	401	CDL	CB2-C1-CA2-OA2
29	j	302	CDL	OA6-CA4-CA6-OA8
29	J	301	CDL	OA6-CA4-CA6-OA8
29	L	302	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
29	B3	402	CDL	OB6-CB4-CB6-OB8
29	I3	302	CDL	OA6-CA4-CA6-OA8
29	g	305	CDL	C53-C54-C55-C56
29	a3	502	CDL	C55-C56-C57-C58
29	J3	302	CDL	C82-C83-C84-C85
29	F	302	CDL	C55-C56-C57-C58
29	A3	501	CDL	C36-C37-C38-C39
29	J3	301	CDL	C34-C35-C36-C37
29	f	304	CDL	C12-C11-CA5-OA6
30	g3	303	PC1	O31-C31-C32-C33
29	J	301	CDL	C34-C35-C36-C37
29	J	302	CDL	C82-C83-C84-C85
29	g3	305	CDL	C53-C54-C55-C56
29	P3	201	CDL	C61-C62-C63-C64
29	P3	201	CDL	C80-C81-C82-C83
29	b	401	CDL	C44-C45-C46-C47
29	b3	401	CDL	C44-C45-C46-C47
29	b3	401	CDL	CA5-C11-C12-C13
29	b	401	CDL	C52-C51-CB5-OB6
29	g	305	CDL	C12-C11-CA5-OA6
29	L	302	CDL	C32-C31-CA7-OA8
29	b3	401	CDL	C52-C51-CB5-OB6
29	i	301	CDL	C58-C59-C60-C61
29	B	401	CDL	C33-C34-C35-C36
29	i3	302	CDL	C58-C59-C60-C61
29	B	403	CDL	OB7-CB5-OB6-CB4
29	B	404	CDL	C54-C55-C56-C57
29	B3	404	CDL	C54-C55-C56-C57
29	J3	301	CDL	C80-C81-C82-C83
29	g3	305	CDL	C12-C11-CA5-OA6
30	g	303	PC1	O31-C31-C32-C33
29	B3	401	CDL	C33-C34-C35-C36
29	f3	302	CDL	CA4-CA6-OA8-CA7
29	A	502	CDL	C36-C37-C38-C39
29	B	401	CDL	C54-C55-C56-C57
29	B3	401	CDL	C54-C55-C56-C57
35	J	303	PEE	C13-C14-C15-C16
35	L3	302	PEE	C13-C14-C15-C16
29	l	301	CDL	C58-C59-C60-C61
29	l3	301	CDL	C58-C59-C60-C61
29	J	301	CDL	C80-C81-C82-C83
29	p	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
29	B	402	CDL	C52-C51-CB5-OB6
29	B3	402	CDL	C52-C51-CB5-OB6
29	I3	302	CDL	C32-C31-CA7-OA8
35	L3	302	PEE	C36-C37-C38-C39
29	F	303	CDL	C36-C37-C38-C39
29	B3	402	CDL	CB6-CB4-OB6-CB5
30	D3	301	PC1	C1-C2-O21-C21
29	A	502	CDL	C44-C45-C46-C47
29	f	303	CDL	C72-C71-CB7-OB8
29	F	303	CDL	C72-C71-CB7-OB8
29	P	201	CDL	C12-C11-CA5-OA6
29	f3	303	CDL	C72-C71-CB7-OB8
29	f3	304	CDL	C72-C71-CB7-OB8
29	p3	201	CDL	C72-C71-CB7-OB8
29	A3	501	CDL	C52-C51-CB5-OB6
29	A3	501	CDL	C44-C45-C46-C47
29	f	302	CDL	CA4-CA6-OA8-CA7
29	B	402	CDL	C84-C85-C86-C87
29	B3	402	CDL	C84-C85-C86-C87
29	B3	403	CDL	C63-C64-C65-C66
29	B	403	CDL	C63-C64-C65-C66
29	P3	201	CDL	C41-C42-C43-C44
29	f	304	CDL	C72-C71-CB7-OB8
29	g	305	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C52-C51-CB5-OB6
29	g3	305	CDL	C72-C71-CB7-OB8
29	F3	302	CDL	C72-C71-CB7-OB8
29	b	401	CDL	C73-C74-C75-C76
29	F	303	CDL	C13-C14-C15-C16
29	F	303	CDL	C22-C23-C24-C25
29	F3	302	CDL	C22-C23-C24-C25
35	J	303	PEE	C36-C37-C38-C39
35	L	303	PEE	C36-C37-C38-C39
35	a3	503	PEE	C36-C37-C38-C39
29	l	302	CDL	C12-C13-C14-C15
29	B3	404	CDL	C16-C17-C18-C19
29	F3	302	CDL	C13-C14-C15-C16
29	i	301	CDL	CB3-CB4-CB6-OB8
29	j	302	CDL	C1-CB2-OB2-PB2
29	K	201	CDL	CB3-CB4-CB6-OB8
29	J	301	CDL	CA3-CA4-CA6-OA8
29	J	301	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	B3	402	CDL	CB3-CB4-CB6-OB8
29	J3	301	CDL	CA3-CA4-CA6-OA8
29	f	304	CDL	C16-C17-C18-C19
29	F3	302	CDL	C36-C37-C38-C39
29	l3	303	CDL	C12-C13-C14-C15
29	F3	302	CDL	C60-C61-C62-C63
29	B	404	CDL	C16-C17-C18-C19
29	P	201	CDL	C41-C42-C43-C44
29	b3	401	CDL	C73-C74-C75-C76
29	P3	201	CDL	C12-C11-CA5-OA6
35	a3	503	PEE	C38-C39-C40-C41
30	G	304	PC1	C22-C23-C24-C25
29	i	301	CDL	C60-C61-C62-C63
29	k3	201	CDL	C42-C43-C44-C45
37	B1	1002	ADP	PA-O3A-PB-O3B
29	k	201	CDL	C42-C43-C44-C45
29	F	303	CDL	C60-C61-C62-C63
29	f3	304	CDL	C16-C17-C18-C19
29	j	302	CDL	OB5-CB3-CB4-CB6
29	l	302	CDL	OB5-CB3-CB4-CB6
29	j3	301	CDL	OB5-CB3-CB4-CB6
29	l	301	CDL	C12-C13-C14-C15
29	I3	303	CDL	C41-C42-C43-C44
29	b	401	CDL	C72-C71-CB7-OB8
29	r	201	CDL	C72-C71-CB7-OB8
29	B	404	CDL	C72-C71-CB7-OB8
29	K	202	CDL	C72-C71-CB7-OB8
29	i3	301	CDL	C72-C71-CB7-OB8
29	F	302	CDL	C53-C54-C55-C56
29	I	302	CDL	C41-C42-C43-C44
29	l3	301	CDL	C12-C13-C14-C15
29	f	302	CDL	OA6-CA4-CA6-OA8
29	l	302	CDL	OA6-CA4-CA6-OA8
29	B	401	CDL	OB6-CB4-CB6-OB8
29	K	201	CDL	OB6-CB4-CB6-OB8
29	a3	501	CDL	OA6-CA4-CA6-OA8
29	l3	303	CDL	OA6-CA4-CA6-OA8
29	B3	401	CDL	OB6-CB4-CB6-OB8
29	K3	201	CDL	OB6-CB4-CB6-OB8
29	l	302	CDL	C24-C25-C26-C27
29	i3	302	CDL	C60-C61-C62-C63
29	l3	303	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	D3	301	PC1	C24-C25-C26-C27
30	G3	304	PC1	C22-C23-C24-C25
35	L	303	PEE	C38-C39-C40-C41
30	D	301	PC1	C24-C25-C26-C27
29	a	501	CDL	C32-C31-CA7-OA8
29	a3	501	CDL	C32-C31-CA7-OA8
29	b3	401	CDL	C72-C71-CB7-OB8
29	B3	404	CDL	C72-C71-CB7-OB8
29	K3	202	CDL	C72-C71-CB7-OB8
37	D1	501	ADP	C5'-O5'-PA-O3A
37	D2	501	ADP	C5'-O5'-PA-O3A
37	D4	501	ADP	C5'-O5'-PA-O3A
37	D5	501	ADP	C5'-O5'-PA-O3A
29	B	402	CDL	C52-C53-C54-C55
29	B3	402	CDL	C52-C53-C54-C55
29	f	302	CDL	C72-C71-CB7-OB9
29	f3	302	CDL	C72-C71-CB7-OB9
29	B3	403	CDL	C51-CB5-OB6-CB4
29	p	201	CDL	C34-C35-C36-C37
29	f	304	CDL	CB4-CB3-OB5-PB2
29	J	302	CDL	CA4-CA3-OA5-PA1
29	J3	302	CDL	CA4-CA3-OA5-PA1
29	J	301	CDL	C71-C72-C73-C74
30	g	303	PC1	C2A-C2B-C2C-C2D
30	g3	303	PC1	C2A-C2B-C2C-C2D
35	A	501	PEE	C36-C37-C38-C39
35	l3	302	PEE	C36-C37-C38-C39
35	L	303	PEE	O2-C10-C11-C12
35	a3	503	PEE	O2-C10-C11-C12
29	p3	201	CDL	C34-C35-C36-C37
29	I	301	CDL	C20-C21-C22-C23
29	a3	502	CDL	C53-C54-C55-C56
29	p3	201	CDL	C79-C80-C81-C82
29	K	202	CDL	C12-C11-CA5-OA6
33	C1	601	ATP	PB-O3A-PA-O2A
33	A1	601	ATP	PB-O3A-PA-O1A
33	C2	601	ATP	PB-O3A-PA-O1A
33	C4	601	ATP	PB-O3A-PA-O2A
33	A4	601	ATP	PB-O3A-PA-O1A
33	C5	601	ATP	PB-O3A-PA-O1A
29	B	403	CDL	C51-C52-C53-C54
29	I3	301	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
30	G	303	PC1	C3B-C3C-C3D-C3E
29	B	403	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	CA5-C11-C12-C13
32	i	302	UQ8	C21-C22-C23-C24
32	I	303	UQ8	C16-C17-C18-C19
32	i3	303	UQ8	C21-C22-C23-C24
32	I3	304	UQ8	C16-C17-C18-C19
29	A3	501	CDL	C52-C51-CB5-OB7
29	B3	403	CDL	C51-C52-C53-C54
29	J3	301	CDL	C71-C72-C73-C74
29	f	302	CDL	C52-C51-CB5-OB6
29	K3	202	CDL	C12-C11-CA5-OA6
30	G	303	PC1	O31-C31-C32-C33
30	G3	303	PC1	O31-C31-C32-C33
29	I	302	CDL	C64-C65-C66-C67
29	P	201	CDL	C31-C32-C33-C34
29	P3	201	CDL	C52-C53-C54-C55
29	A	502	CDL	C52-C51-CB5-OB7
29	a3	502	CDL	C64-C65-C66-C67
29	I3	303	CDL	C64-C65-C66-C67
29	F	302	CDL	C64-C65-C66-C67
29	f3	302	CDL	C52-C51-CB5-OB6
35	m	301	PEE	O2-C10-C11-C12
35	A	501	PEE	O2-C10-C11-C12
35	j3	303	PEE	O2-C10-C11-C12
35	l3	302	PEE	O2-C10-C11-C12
29	p	201	CDL	C79-C80-C81-C82
29	P	201	CDL	C52-C53-C54-C55
29	P3	201	CDL	C31-C32-C33-C34
30	G3	303	PC1	C3B-C3C-C3D-C3E
29	i3	302	CDL	CA5-C11-C12-C13
29	I3	302	CDL	C32-C31-CA7-OA9
29	l	301	CDL	C16-C17-C18-C19
29	b3	401	CDL	C20-C21-C22-C23
29	f3	302	CDL	C59-C60-C61-C62
29	K3	201	CDL	C44-C45-C46-C47
29	K	201	CDL	C44-C45-C46-C47
29	b	401	CDL	C52-C51-CB5-OB7
29	g	305	CDL	C12-C11-CA5-OA7
29	L	302	CDL	C32-C31-CA7-OA9
29	b3	401	CDL	C52-C51-CB5-OB7
29	b	401	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	B	401	CDL	C16-C17-C18-C19
29	l3	301	CDL	C16-C17-C18-C19
29	B3	401	CDL	C31-C32-C33-C34
32	i	302	UQ8	C16-C17-C18-C19
32	i3	303	UQ8	C16-C17-C18-C19
29	f	302	CDL	C59-C60-C61-C62
29	B3	404	CDL	C38-C39-C40-C41
29	F	303	CDL	C72-C71-CB7-OB9
29	f3	304	CDL	C72-C71-CB7-OB9
29	F3	302	CDL	C72-C71-CB7-OB9
30	G	303	PC1	O22-C21-C22-C23
30	G3	303	PC1	O22-C21-C22-C23
29	K3	201	CDL	CB3-CB4-CB6-OB8
29	I3	301	CDL	C72-C71-CB7-OB8
29	B3	401	CDL	C16-C17-C18-C19
29	K3	202	CDL	C56-C57-C58-C59
29	k3	201	CDL	CA3-OA5-PA1-OA2
29	B	401	CDL	C31-C32-C33-C34
29	B	404	CDL	C38-C39-C40-C41
29	B	402	CDL	CB5-C51-C52-C53
29	f	304	CDL	C72-C71-CB7-OB9
29	g3	305	CDL	C12-C11-CA5-OA7
30	g	303	PC1	O32-C31-C32-C33
30	g3	303	PC1	O32-C31-C32-C33
29	I3	302	CDL	C13-C14-C15-C16
30	g	303	PC1	C32-C33-C34-C35
29	I	301	CDL	C72-C71-CB7-OB8
29	f3	304	CDL	CB4-CB3-OB5-PB2
35	J	303	PEE	C2-C1-O3P-P
35	L3	302	PEE	C2-C1-O3P-P
29	K	202	CDL	C56-C57-C58-C59
29	B3	402	CDL	CB5-C51-C52-C53
29	g3	305	CDL	C72-C71-CB7-OB9
29	K3	202	CDL	C72-C71-CB7-OB9
30	G	303	PC1	O32-C31-C32-C33
30	G3	303	PC1	O32-C31-C32-C33
35	J	303	PEE	C16-C17-C18-C19
35	L3	302	PEE	C16-C17-C18-C19
29	L	301	CDL	C59-C60-C61-C62
29	f3	304	CDL	C34-C35-C36-C37
29	L3	301	CDL	C18-C19-C20-C21
29	f	302	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
29	f	304	CDL	CA2-OA2-PA1-OA3
29	g	305	CDL	CA2-OA2-PA1-OA3
29	g	305	CDL	CB2-OB2-PB2-OB3
29	j	301	CDL	CA2-OA2-PA1-OA3
29	j	301	CDL	CB2-OB2-PB2-OB3
29	K	202	CDL	CA2-OA2-PA1-OA3
29	L	302	CDL	CB2-OB2-PB2-OB3
29	P	201	CDL	CA2-OA2-PA1-OA3
29	f3	302	CDL	CA2-OA2-PA1-OA3
29	f3	304	CDL	CA2-OA2-PA1-OA3
29	g3	305	CDL	CA2-OA2-PA1-OA3
29	g3	305	CDL	CB2-OB2-PB2-OB3
29	j3	301	CDL	CA2-OA2-PA1-OA3
29	j3	301	CDL	CB2-OB2-PB2-OB3
29	l3	302	CDL	CB2-OB2-PB2-OB3
29	K3	202	CDL	CA2-OA2-PA1-OA3
29	P3	201	CDL	CA2-OA2-PA1-OA3
30	g	304	PC1	C1-O11-P-O14
30	G	303	PC1	C11-O13-P-O12
30	G	304	PC1	C1-O11-P-O14
30	g3	304	PC1	C1-O11-P-O14
30	G3	304	PC1	C1-O11-P-O14
33	C1	601	ATP	C5'-O5'-PA-O2A
33	C4	601	ATP	C5'-O5'-PA-O2A
36	e	900	NAD	C5B-O5B-PA-O1A
36	e3	900	NAD	C5B-O5B-PA-O1A
29	F	303	CDL	OB6-CB4-CB6-OB8
29	f	304	CDL	C34-C35-C36-C37
29	L	302	CDL	C13-C14-C15-C16
29	p3	201	CDL	C75-C76-C77-C78
29	L3	301	CDL	C59-C60-C61-C62
30	g3	303	PC1	C32-C33-C34-C35
29	g	305	CDL	C72-C71-CB7-OB9
29	l	302	CDL	C32-C31-CA7-OA9
29	B	402	CDL	C52-C51-CB5-OB7
29	K	202	CDL	C72-C71-CB7-OB9
29	P	201	CDL	C12-C11-CA5-OA7
29	l3	303	CDL	C32-C31-CA7-OA9
29	B3	402	CDL	C52-C51-CB5-OB7
29	j	301	CDL	OB5-CB3-CB4-CB6
29	p	201	CDL	C75-C76-C77-C78
29	f3	304	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
29	f	303	CDL	C72-C71-CB7-OB9
29	K	202	CDL	C12-C11-CA5-OA7
29	i3	301	CDL	C72-C71-CB7-OB9
29	K3	202	CDL	C12-C11-CA5-OA7
29	P3	201	CDL	C12-C11-CA5-OA7
29	L	301	CDL	C18-C19-C20-C21
30	g3	303	PC1	O21-C21-C22-C23
29	f	304	CDL	C57-C58-C59-C60
29	B	402	CDL	C32-C31-CA7-OA9
29	f3	303	CDL	C72-C71-CB7-OB9
29	B3	402	CDL	C32-C31-CA7-OA9
29	p3	201	CDL	C43-C44-C45-C46
35	m	301	PEE	C32-C33-C34-C35
30	g	303	PC1	O21-C21-C22-C23
29	B	404	CDL	C72-C71-CB7-OB9
29	L	302	CDL	C72-C71-CB7-OB9
29	I3	302	CDL	C72-C71-CB7-OB9
29	B	402	CDL	C11-C12-C13-C14
29	I3	302	CDL	C58-C59-C60-C61
30	G3	303	PC1	C2B-C2C-C2D-C2E
29	B	402	CDL	CB6-CB4-OB6-CB5
29	B	404	CDL	CA6-CA4-OA6-CA5
29	B3	404	CDL	CA6-CA4-OA6-CA5
30	g	304	PC1	C12-C11-O13-P
30	g3	304	PC1	C12-C11-O13-P
29	B3	404	CDL	C72-C71-CB7-OB9
29	p	201	CDL	C43-C44-C45-C46
29	J	301	CDL	C18-C19-C20-C21
29	B3	402	CDL	C11-C12-C13-C14
30	D3	301	PC1	C22-C23-C24-C25
35	j3	303	PEE	C32-C33-C34-C35
29	J	301	CDL	C32-C31-CA7-OA8
29	J3	301	CDL	C18-C19-C20-C21
30	G	303	PC1	C2B-C2C-C2D-C2E
29	r	201	CDL	C72-C71-CB7-OB9
29	a3	501	CDL	C32-C31-CA7-OA9
29	l	302	CDL	C53-C54-C55-C56
29	L	302	CDL	C58-C59-C60-C61
29	i3	301	CDL	C12-C13-C14-C15
29	l	301	CDL	C32-C31-CA7-OA8
29	l3	301	CDL	C32-C31-CA7-OA8
29	F	302	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	a3	502	CDL	C54-C55-C56-C57
30	D	301	PC1	C22-C23-C24-C25
29	B	403	CDL	C20-C21-C22-C23
30	G	303	PC1	C29-C2A-C2B-C2C
29	B3	403	CDL	C20-C21-C22-C23
29	r	201	CDL	C12-C13-C14-C15
29	a3	502	CDL	C12-C13-C14-C15
29	J3	301	CDL	C32-C33-C34-C35
29	B	404	CDL	C32-C31-CA7-OA8
29	j3	301	CDL	C32-C31-CA7-OA8
29	b3	401	CDL	CB2-C1-CA2-OA2
29	F	302	CDL	C54-C55-C56-C57
29	l3	303	CDL	C53-C54-C55-C56
29	p3	201	CDL	C31-C32-C33-C34
29	J3	302	CDL	C83-C84-C85-C86
29	I	301	CDL	C72-C71-CB7-OB9
35	j3	303	PEE	O4-C10-C11-C12
29	J	301	CDL	C51-C52-C53-C54
29	J	302	CDL	C83-C84-C85-C86
29	j	302	CDL	CA4-CA3-OA5-PA1
29	I	301	CDL	C1-CA2-OA2-PA1
29	j3	302	CDL	CA4-CA3-OA5-PA1
35	m	301	PEE	C2-C1-O3P-P
35	j3	303	PEE	C2-C1-O3P-P
29	a	501	CDL	C32-C31-CA7-OA9
29	I3	301	CDL	C72-C71-CB7-OB9
29	f	302	CDL	C12-C11-CA5-OA6
29	j	301	CDL	C32-C31-CA7-OA8
29	f3	302	CDL	C12-C11-CA5-OA6
29	B3	404	CDL	C32-C31-CA7-OA8
29	J3	301	CDL	C32-C31-CA7-OA8
29	p	201	CDL	C31-C32-C33-C34
29	r	201	CDL	C17-C18-C19-C20
29	J	301	CDL	C32-C33-C34-C35
29	J3	301	CDL	C51-C52-C53-C54
35	a3	503	PEE	O4-C10-C11-C12
35	l3	302	PEE	O4-C10-C11-C12
29	k	201	CDL	C32-C31-CA7-OA8
29	F3	302	CDL	C52-C51-CB5-OB6
29	B3	402	CDL	C19-C20-C21-C22
30	G3	303	PC1	C29-C2A-C2B-C2C
29	a3	502	CDL	C42-C43-C44-C45

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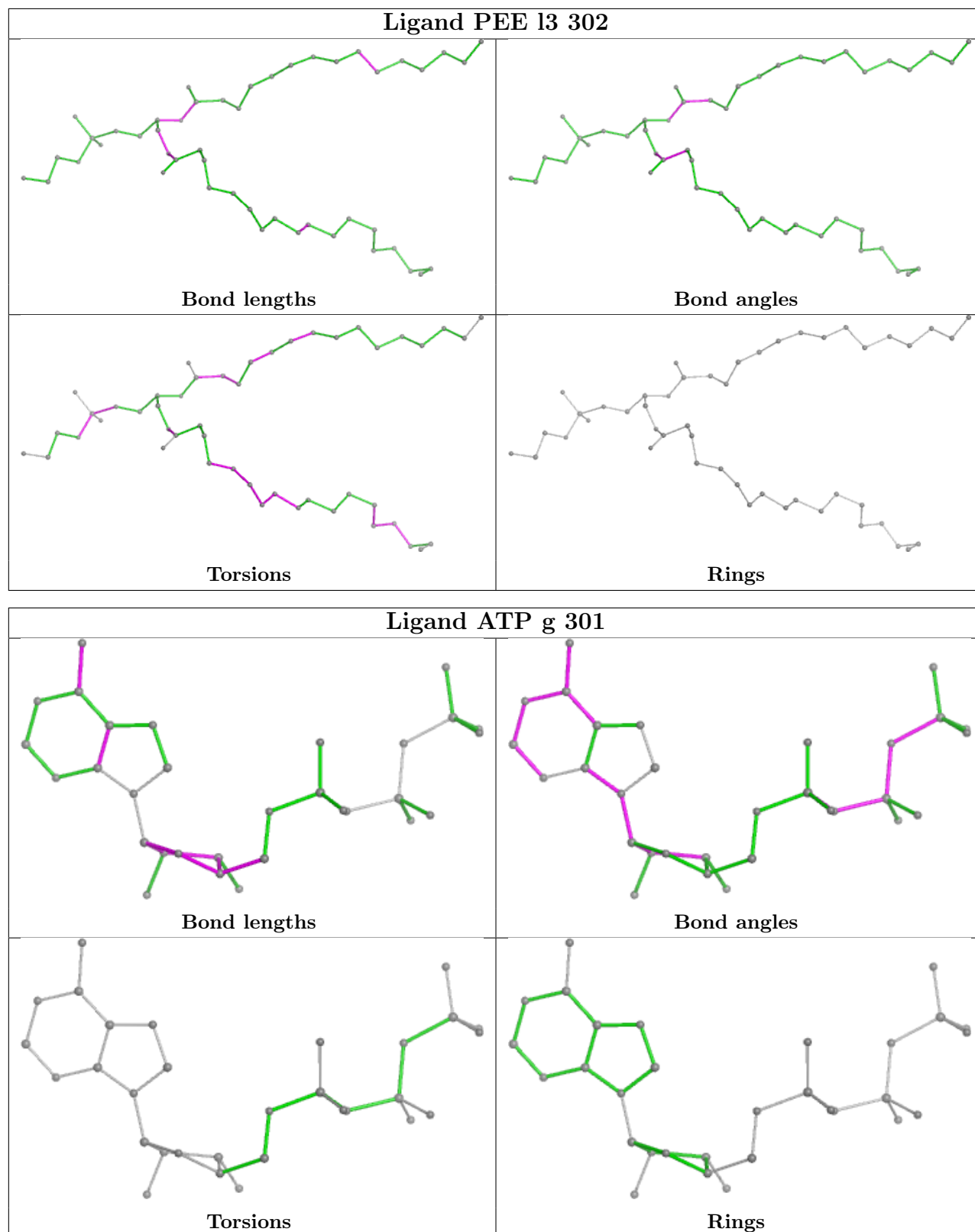
Mol	Chain	Res	Type	Atoms
29	B	404	CDL	C32-C31-CA7-OA9
29	J	301	CDL	C32-C31-CA7-OA9
29	B3	404	CDL	C32-C31-CA7-OA9
29	J3	301	CDL	C32-C31-CA7-OA9
35	m	301	PEE	O4-C10-C11-C12
35	A	501	PEE	O4-C10-C11-C12
35	L	303	PEE	O4-C10-C11-C12
29	l	301	CDL	C52-C53-C54-C55
29	F	302	CDL	C42-C43-C44-C45
29	l	301	CDL	C52-C51-CB5-OB6
29	F	303	CDL	C52-C51-CB5-OB6
29	l3	301	CDL	C52-C51-CB5-OB6
35	J	303	PEE	O2-C10-C11-C12
29	l	301	CDL	C32-C31-CA7-OA9
29	l3	301	CDL	C32-C31-CA7-OA9
29	i3	302	CDL	C56-C57-C58-C59
29	l3	301	CDL	C52-C53-C54-C55
29	L3	301	CDL	C14-C15-C16-C17
29	b3	401	CDL	C72-C73-C74-C75
29	b	401	CDL	C72-C73-C74-C75
29	f	304	CDL	C64-C65-C66-C67
29	i	301	CDL	C56-C57-C58-C59
29	i3	301	CDL	C17-C18-C19-C20
29	l3	301	CDL	C42-C43-C44-C45
29	A3	501	CDL	C71-C72-C73-C74
29	j	301	CDL	C12-C11-CA5-OA6
29	k3	201	CDL	C32-C31-CA7-OA8
29	j3	301	CDL	C12-C11-CA5-OA6
29	P3	201	CDL	C32-C31-CA7-OA8
35	L3	302	PEE	O2-C10-C11-C12

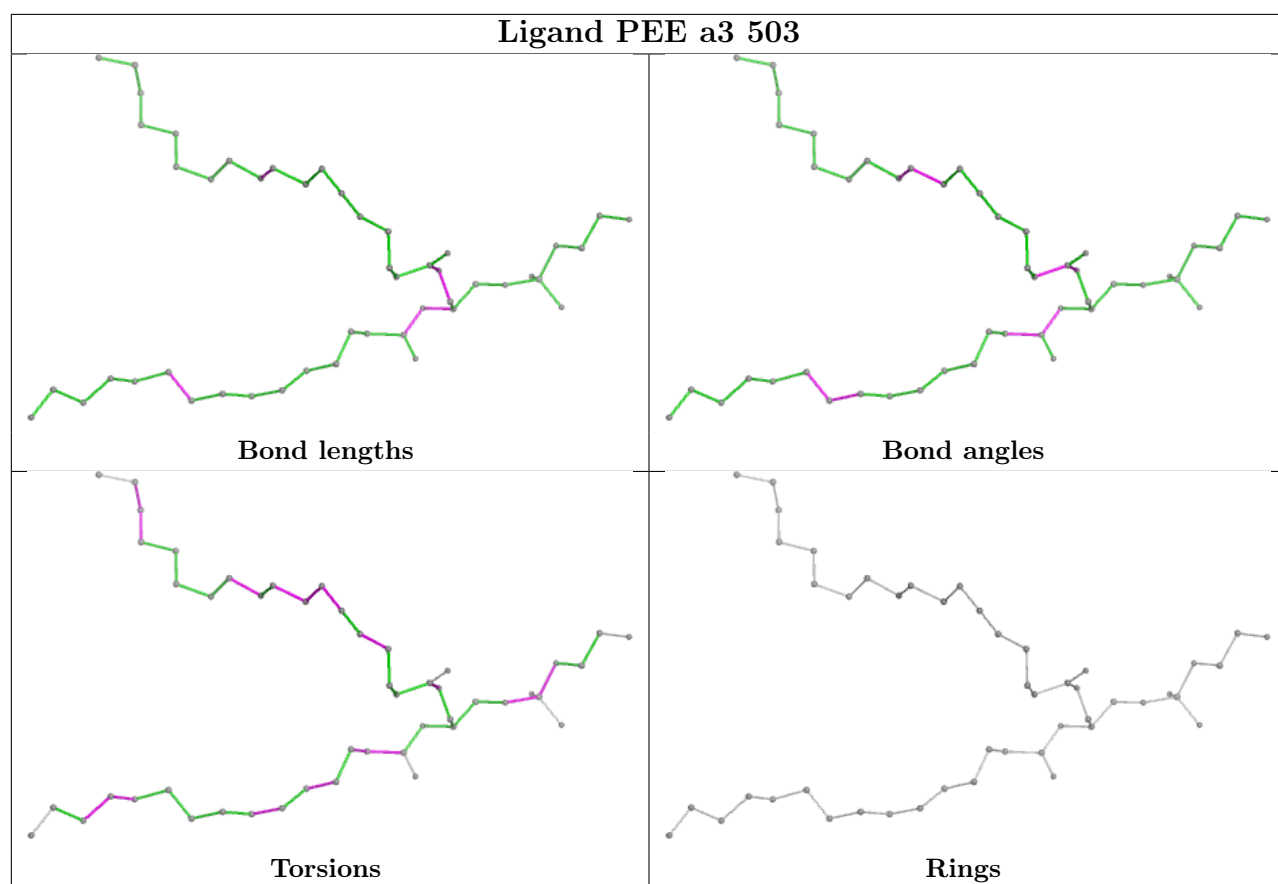
There are no ring outliers.

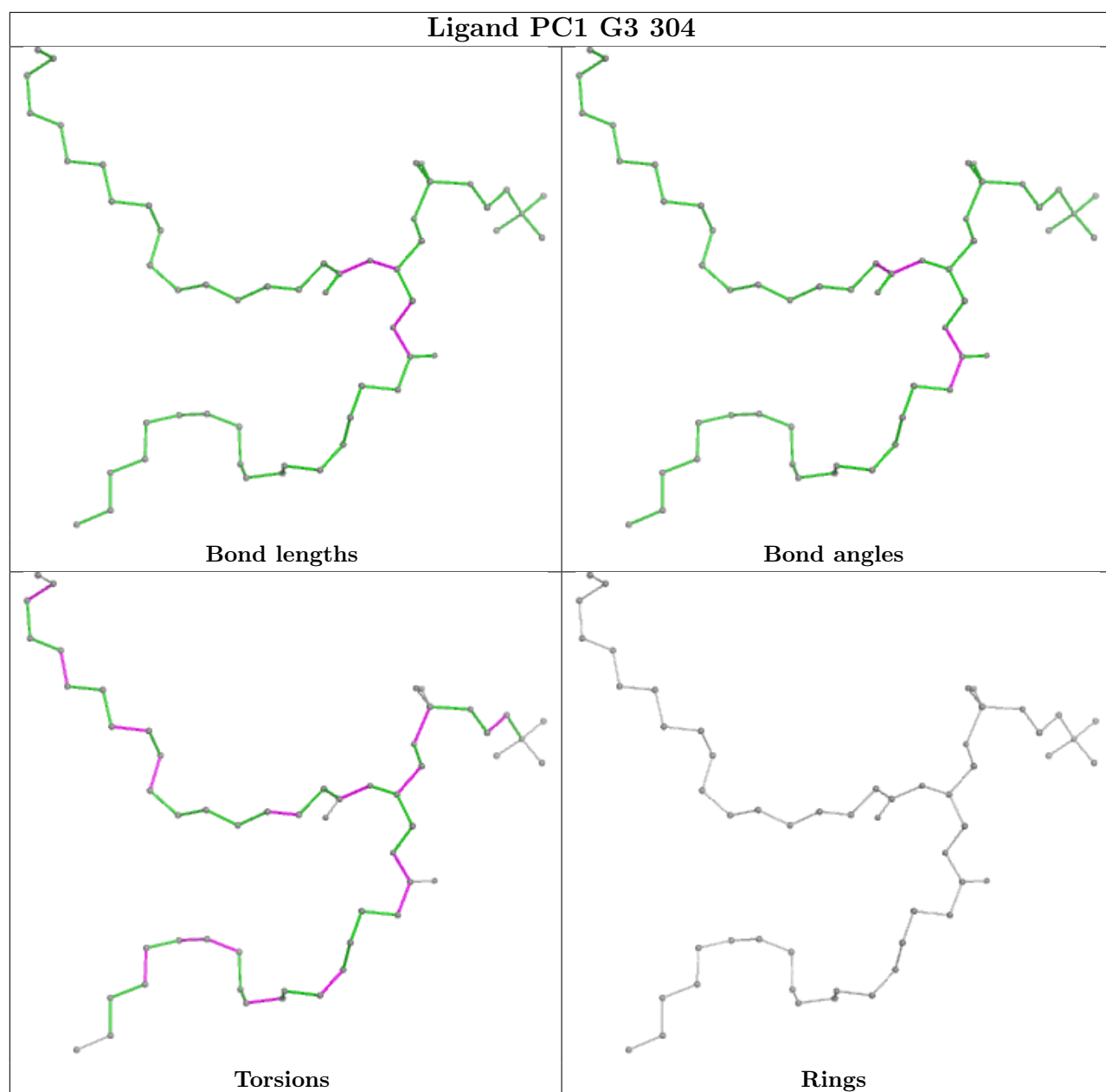
No monomer is involved in short contacts.

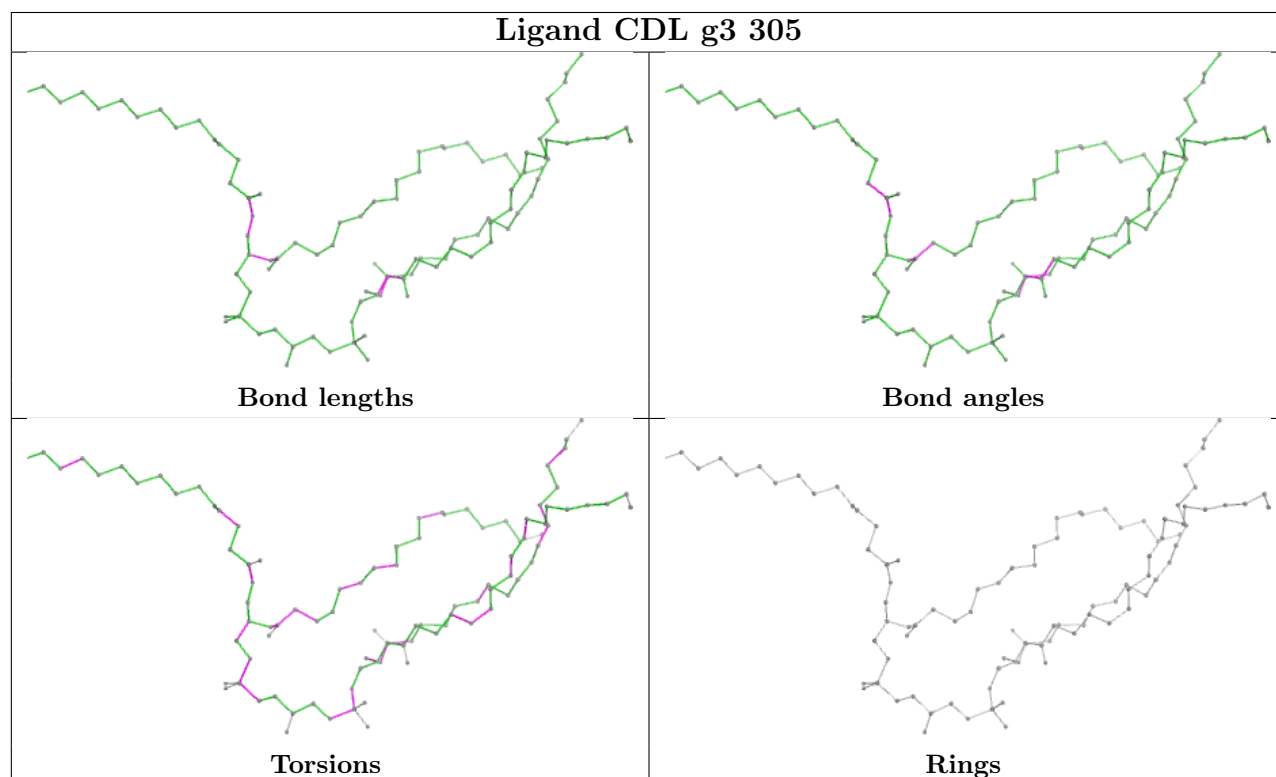
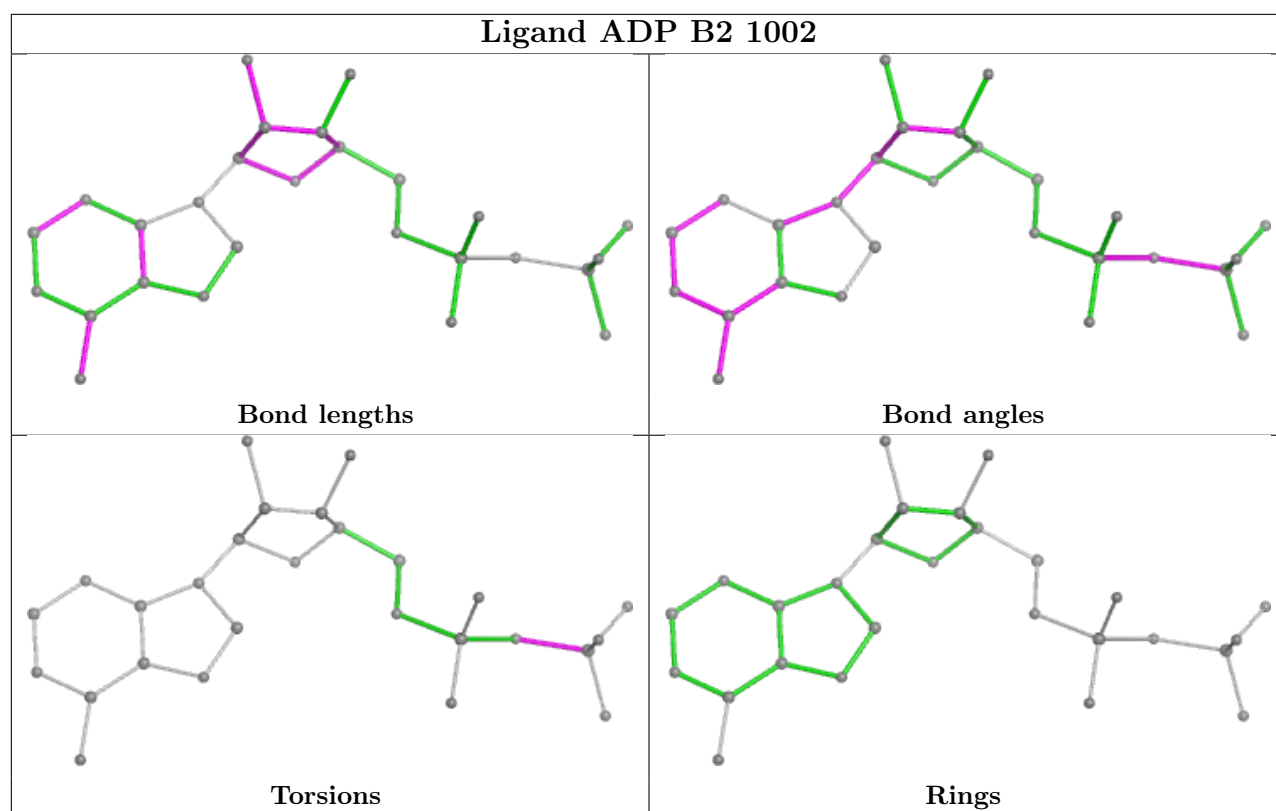
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

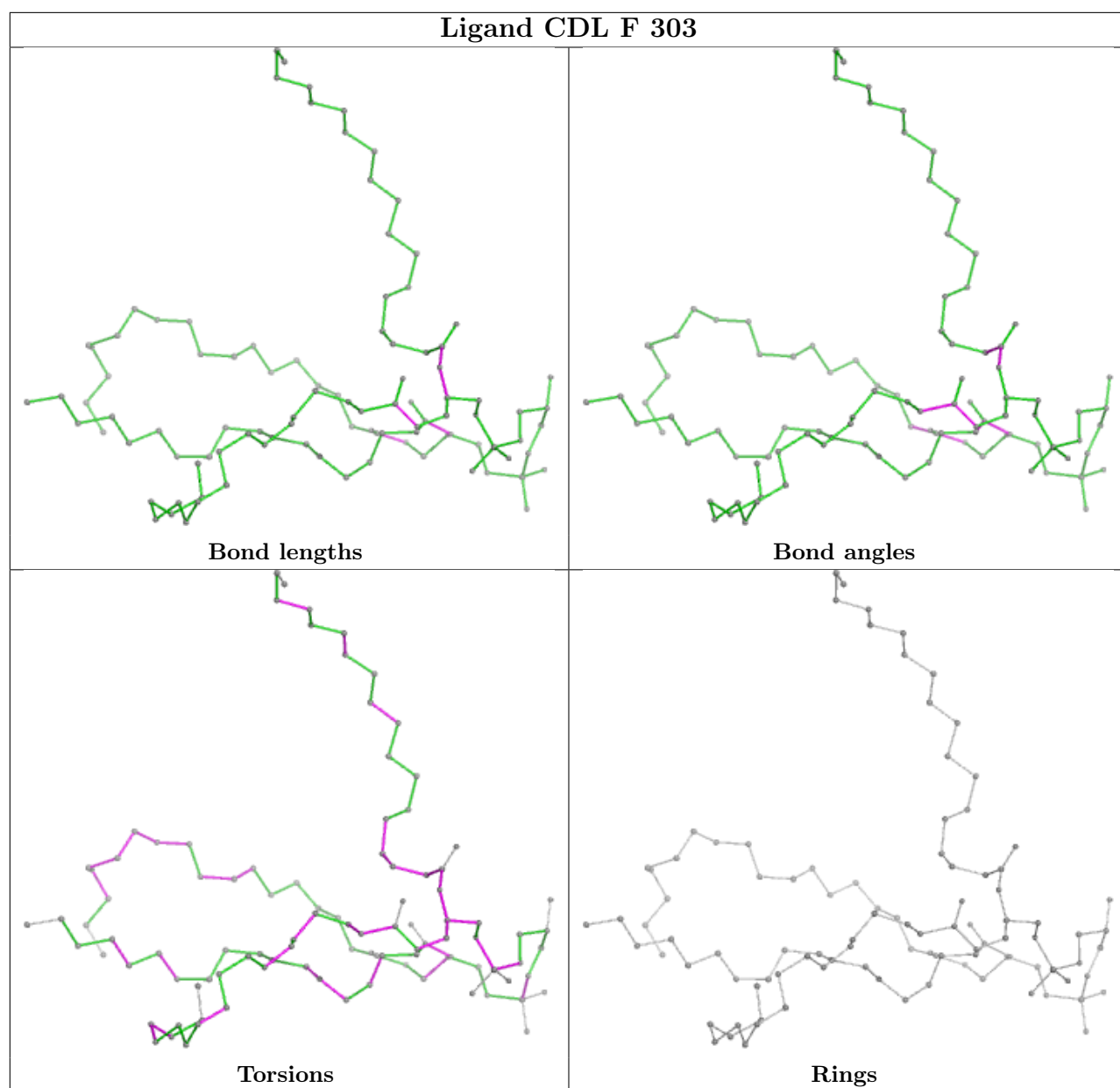
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

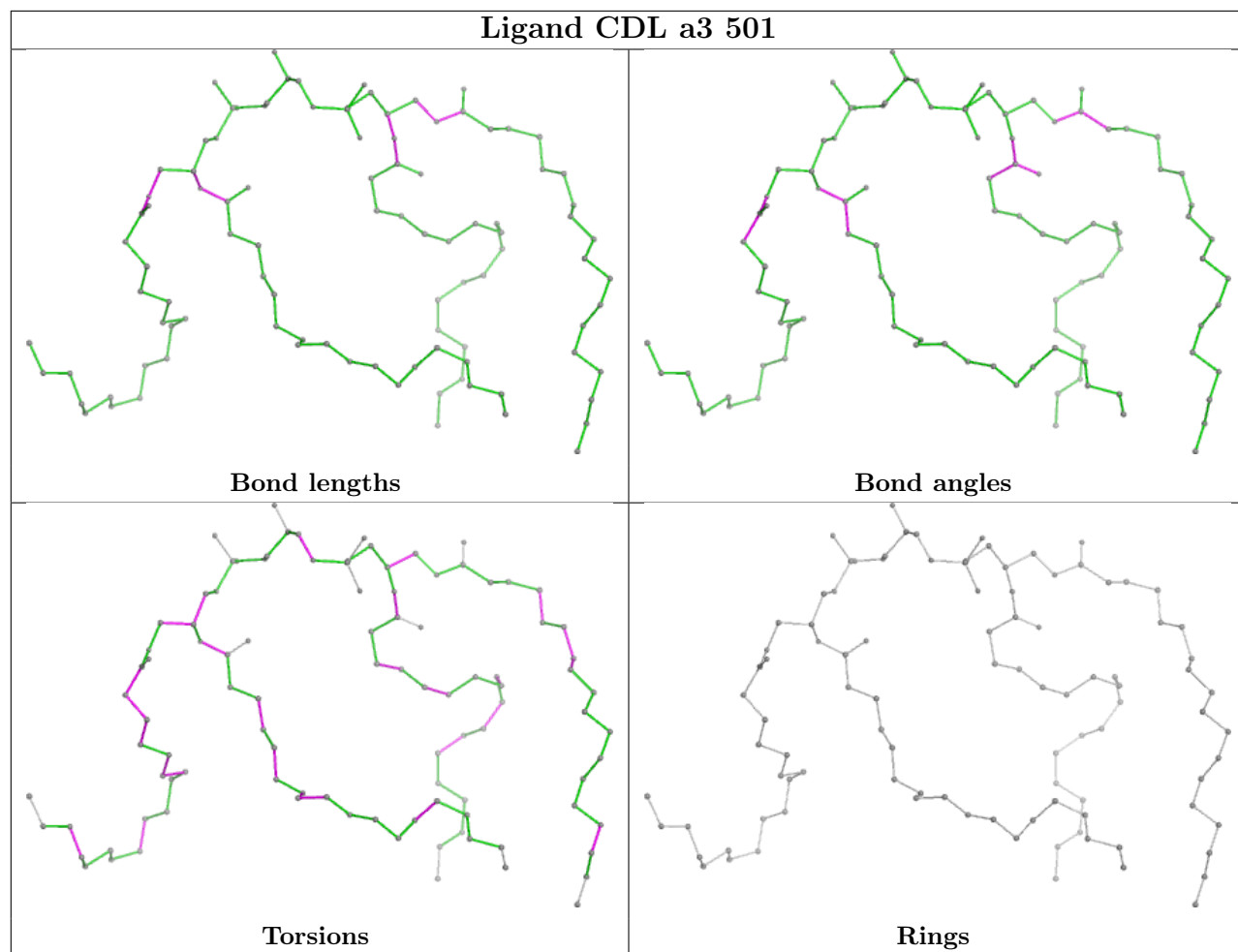


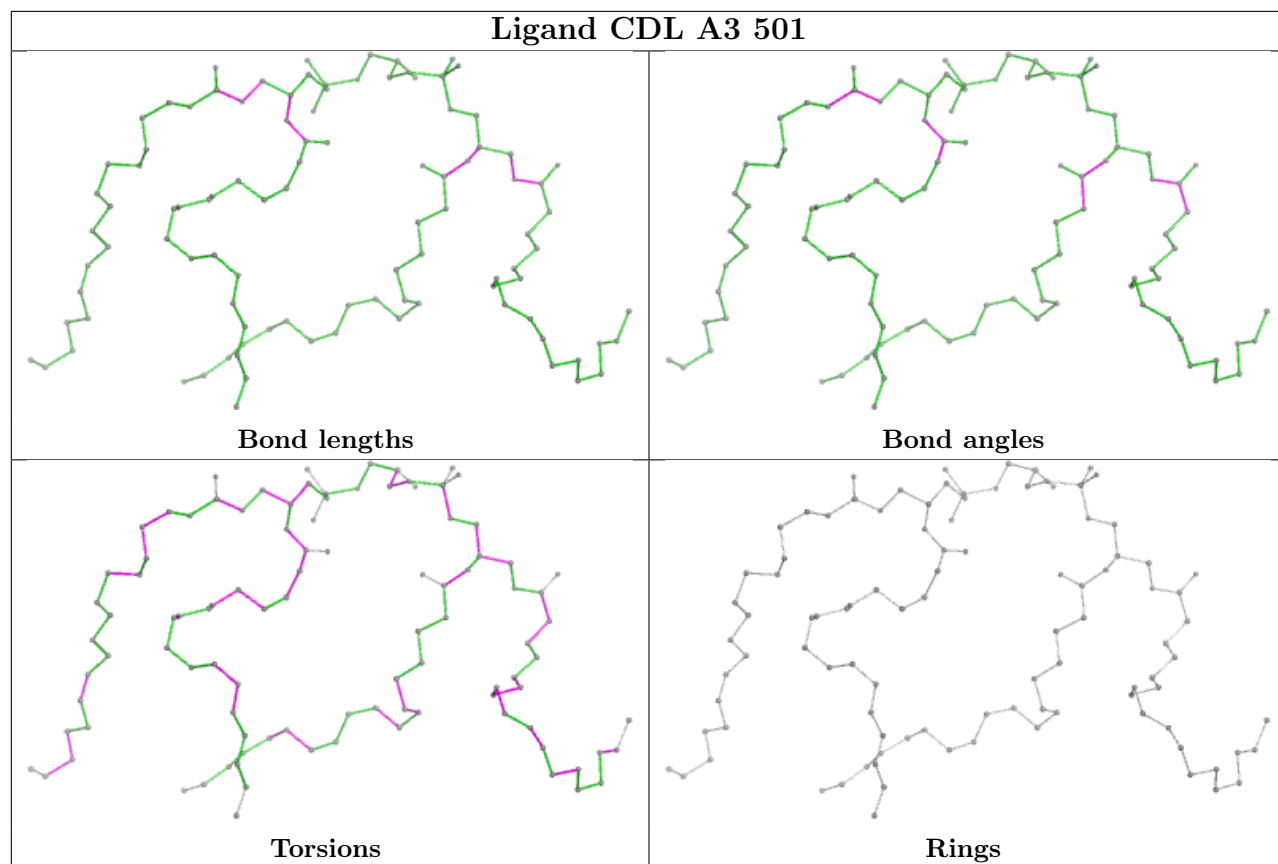


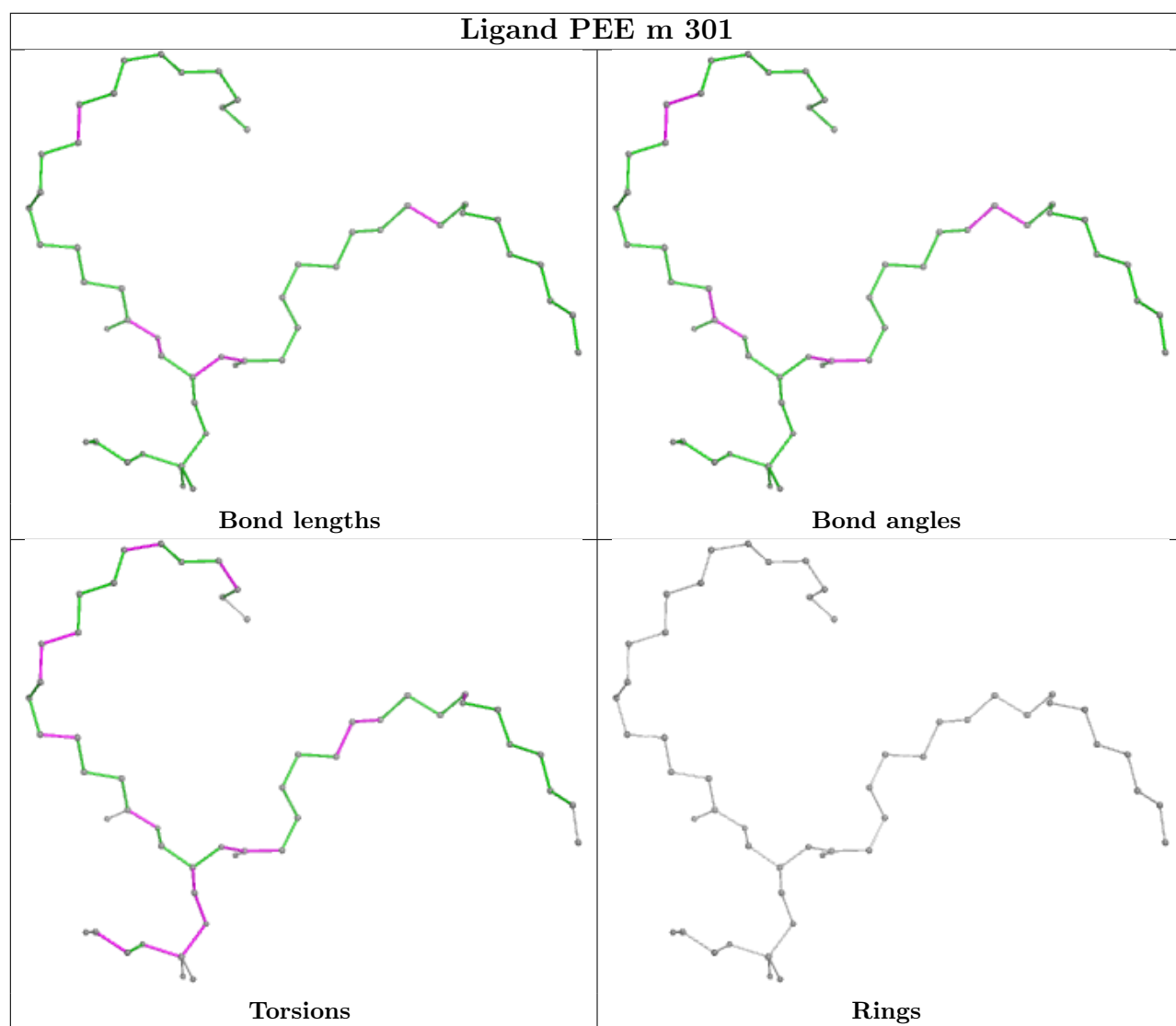


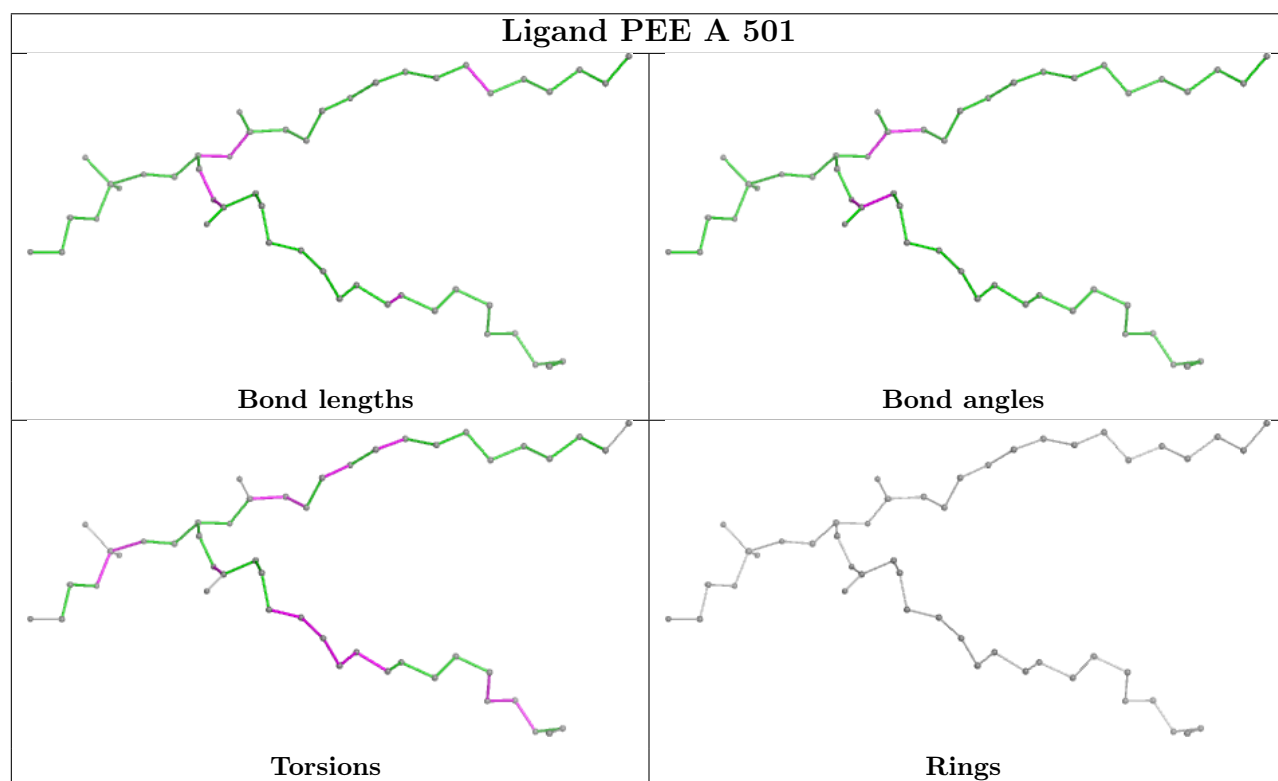
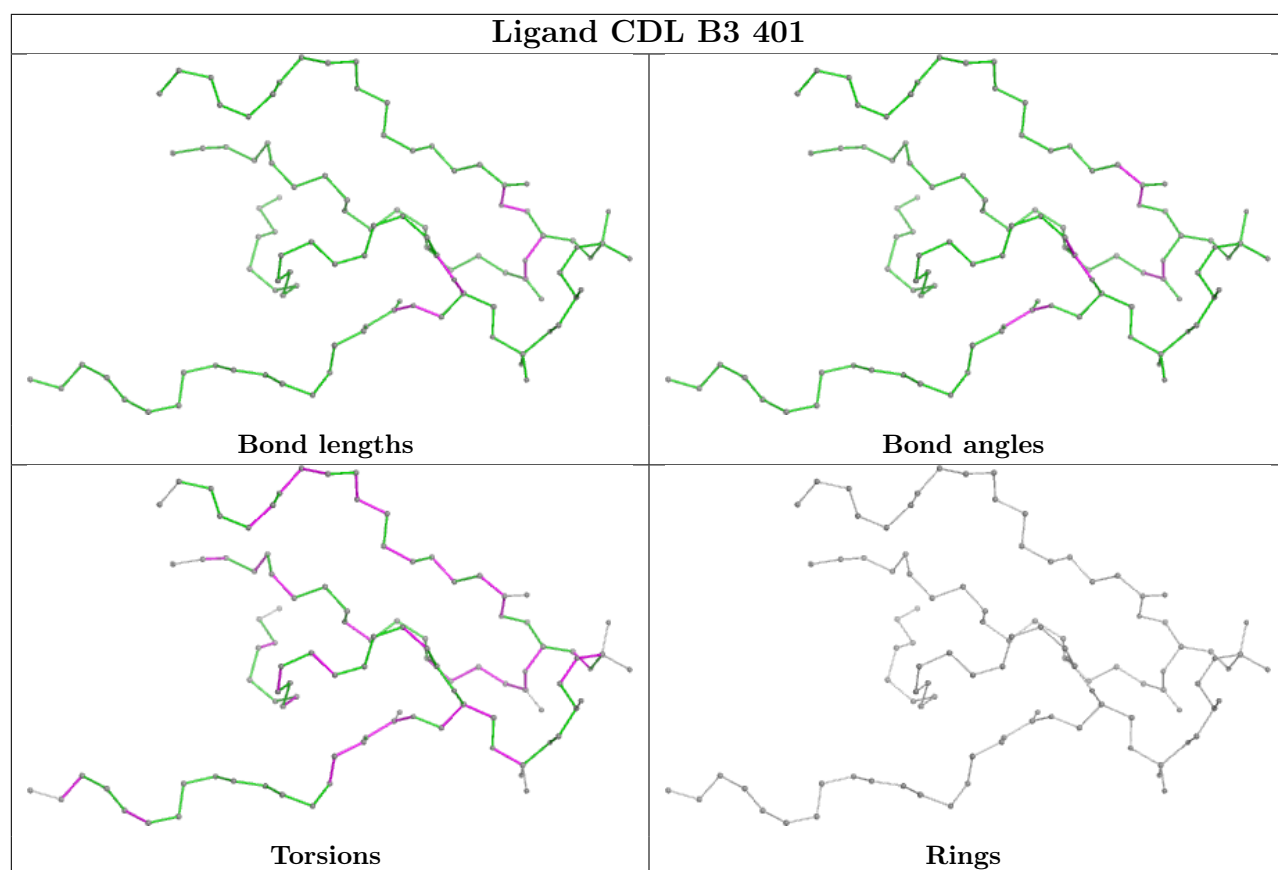


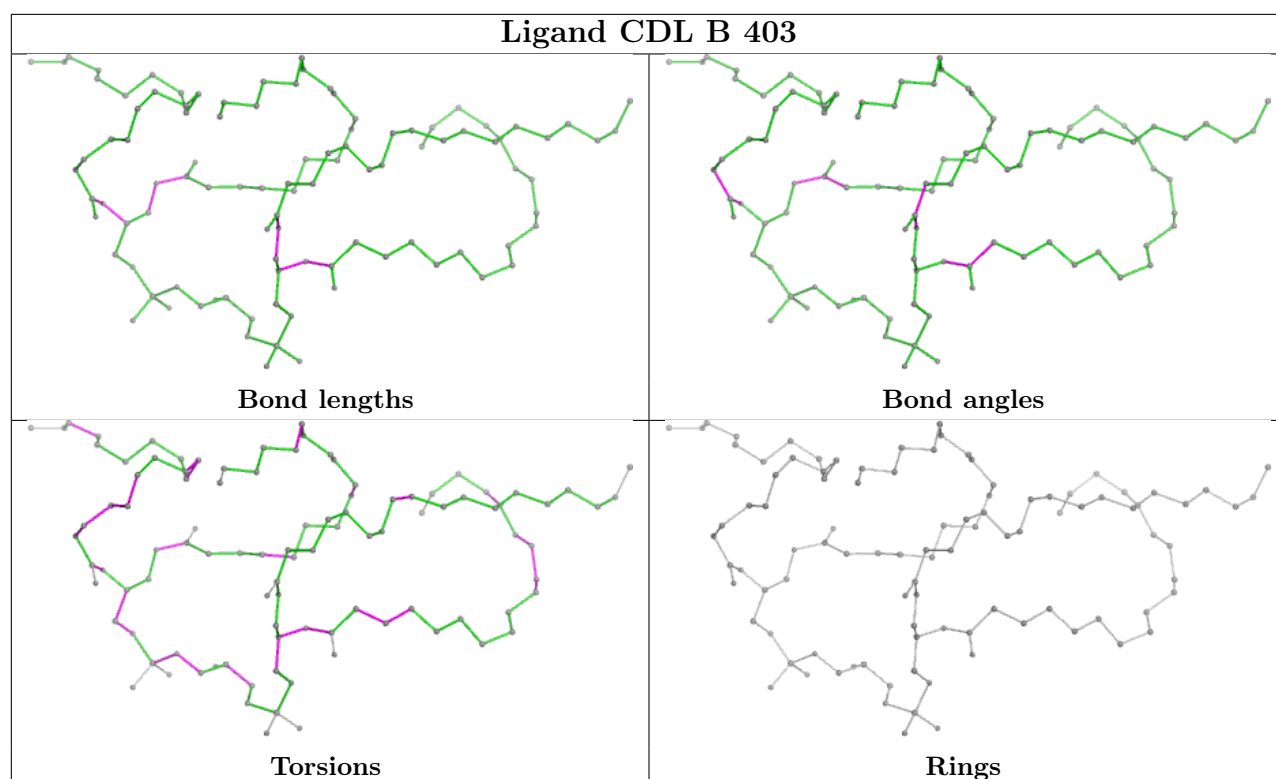


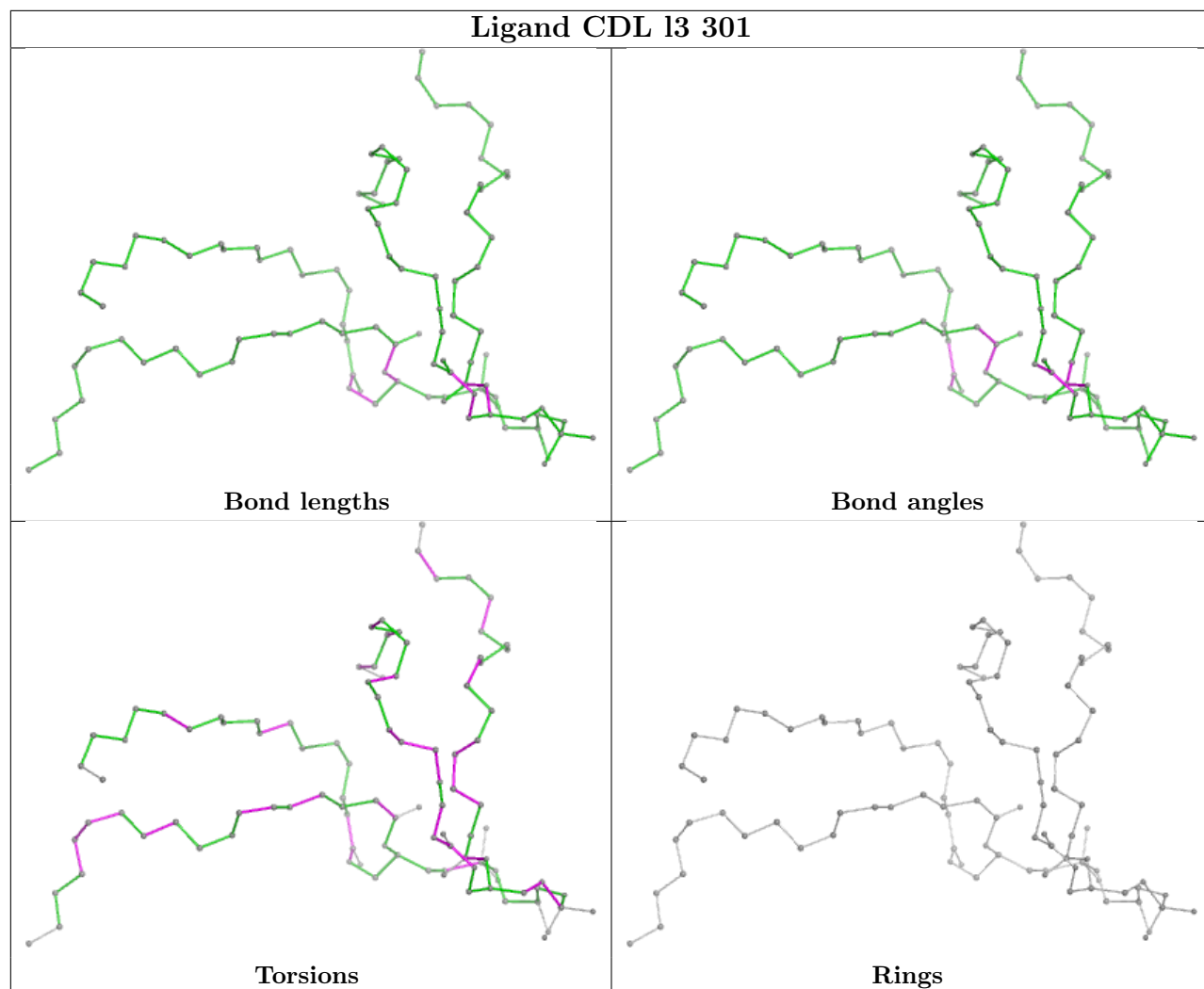


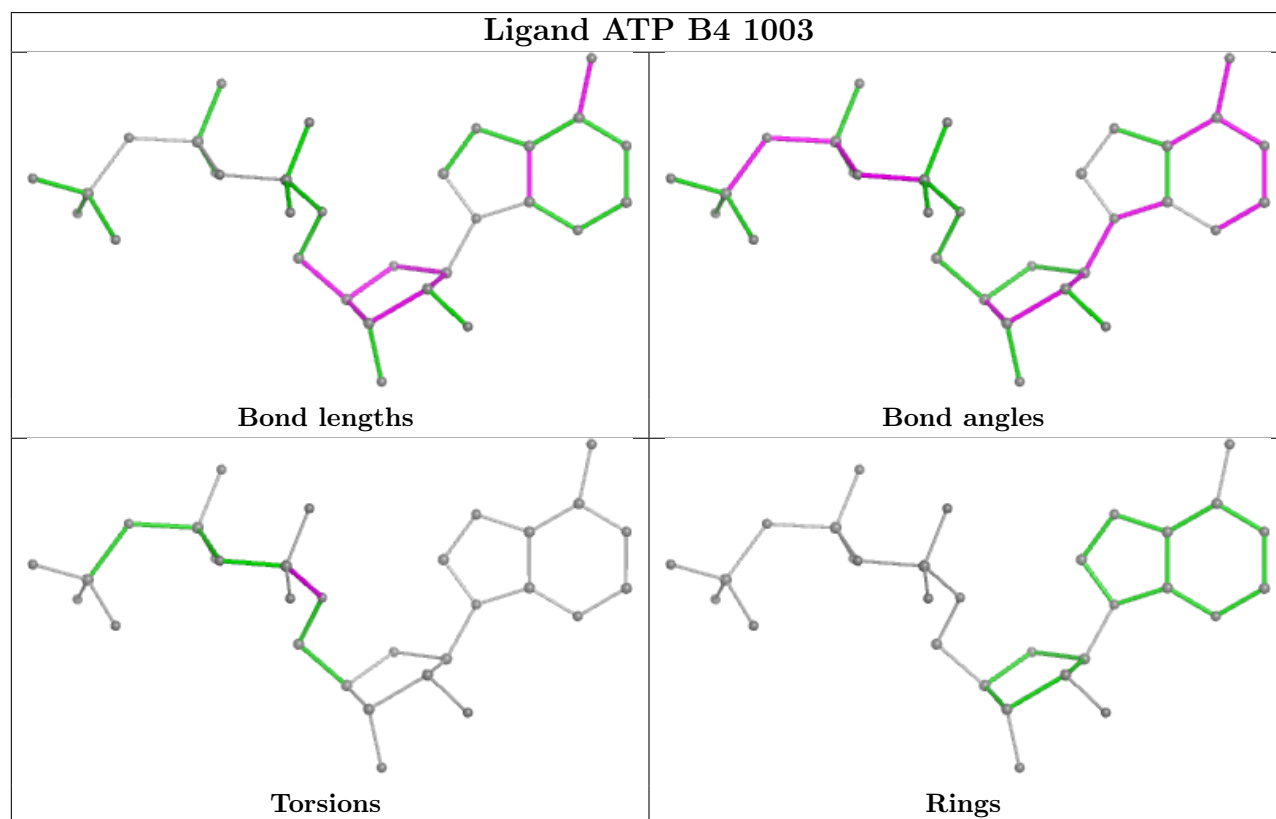
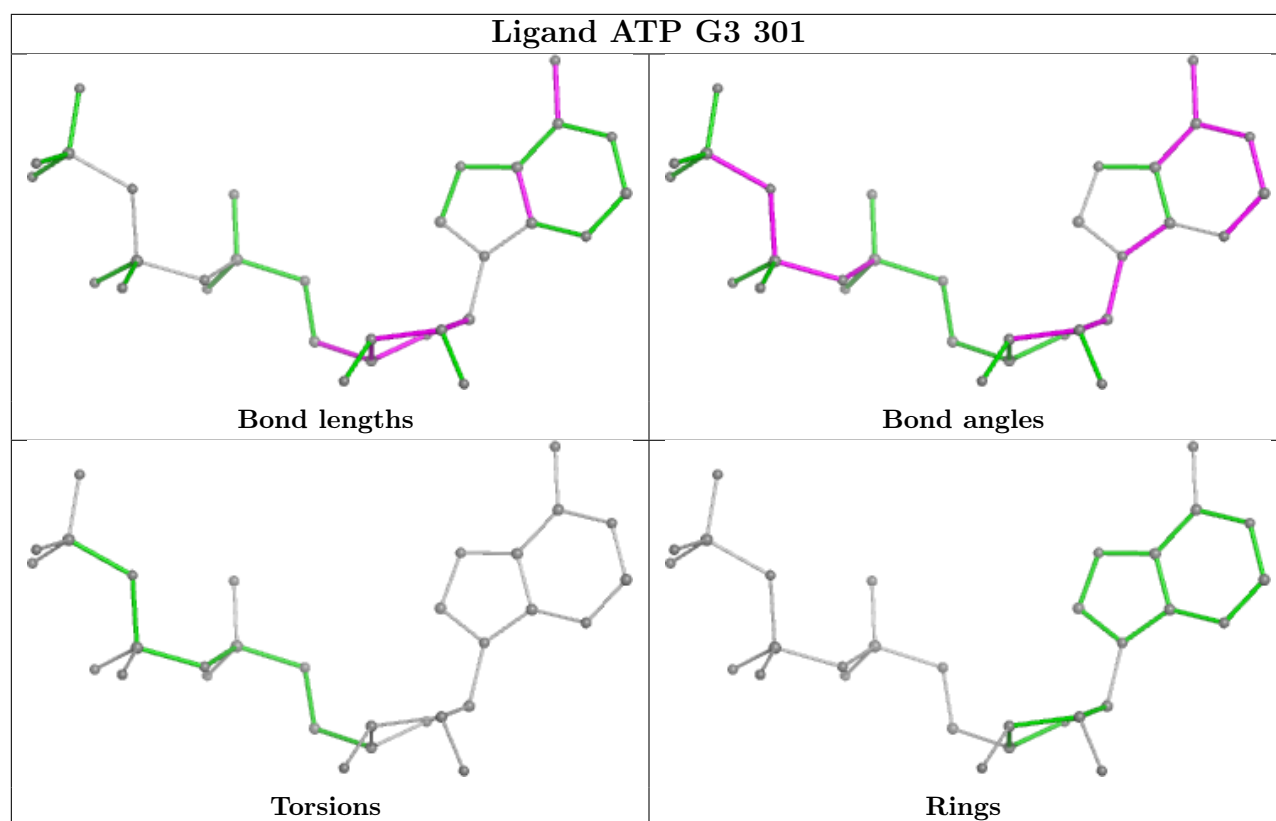


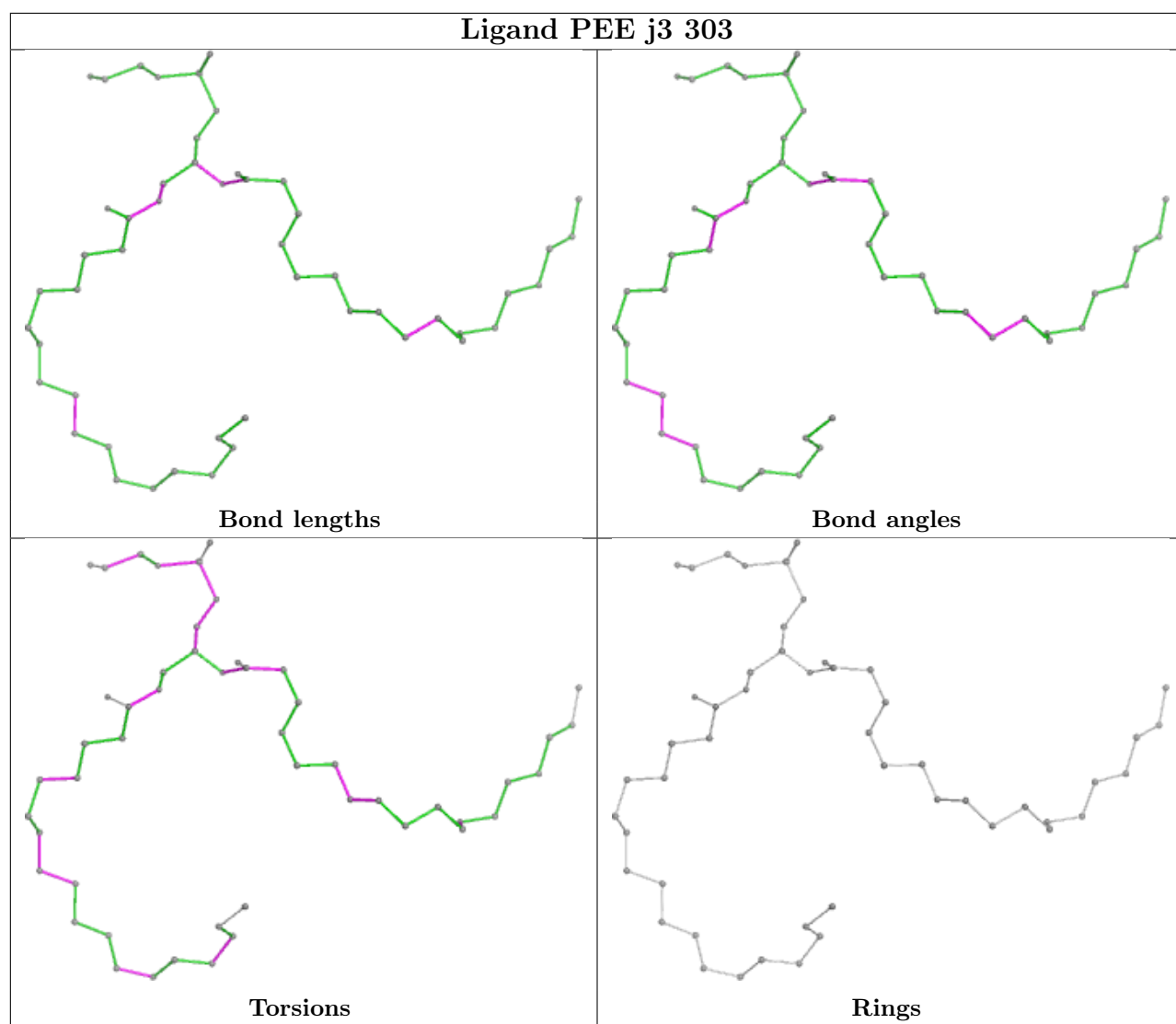


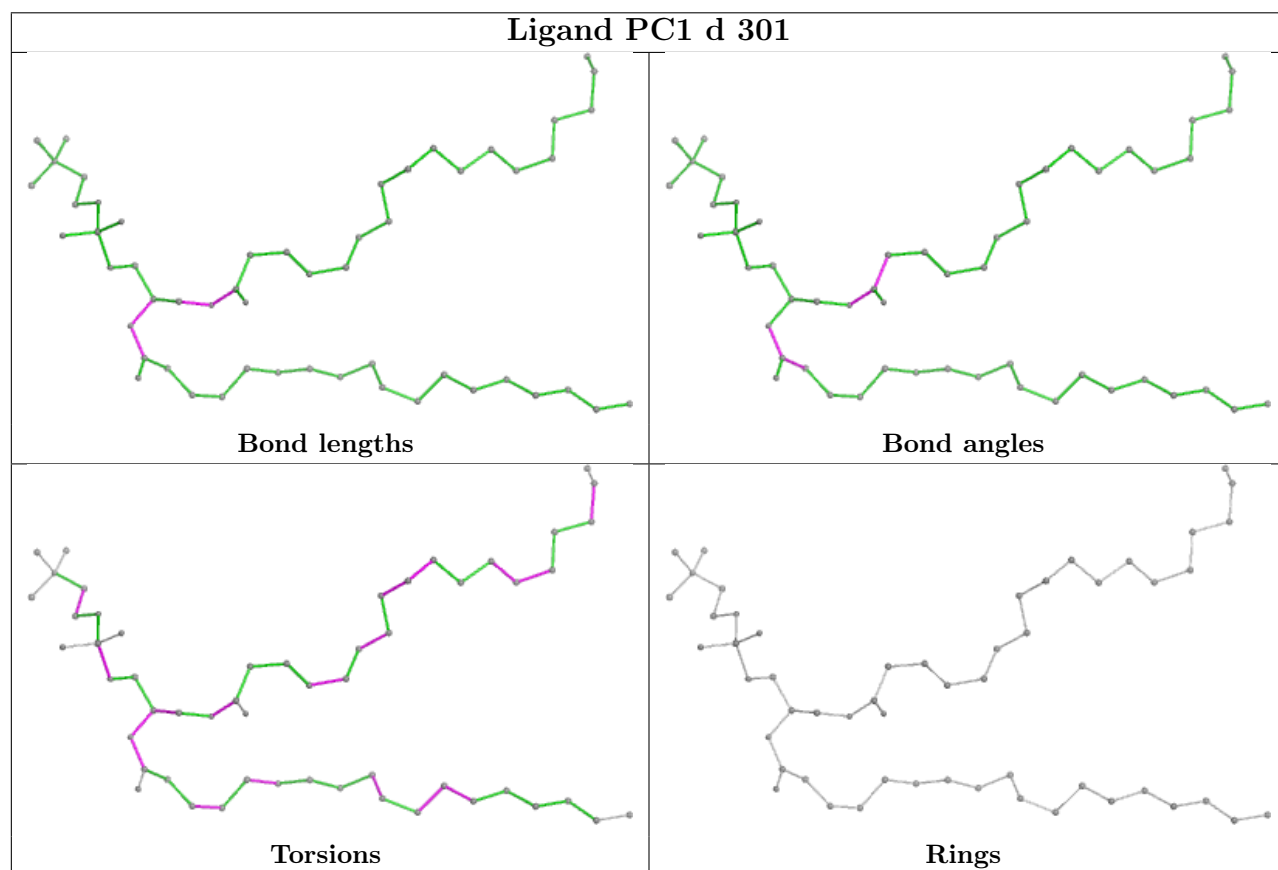
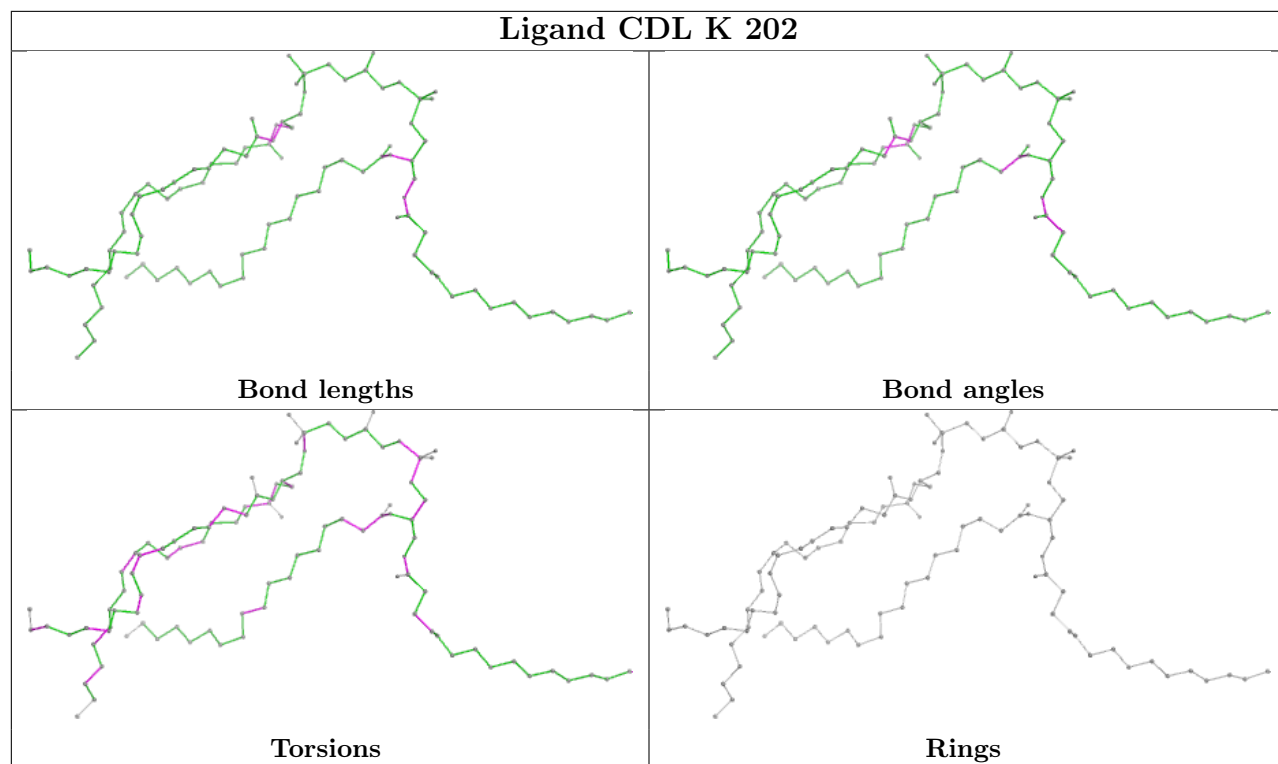


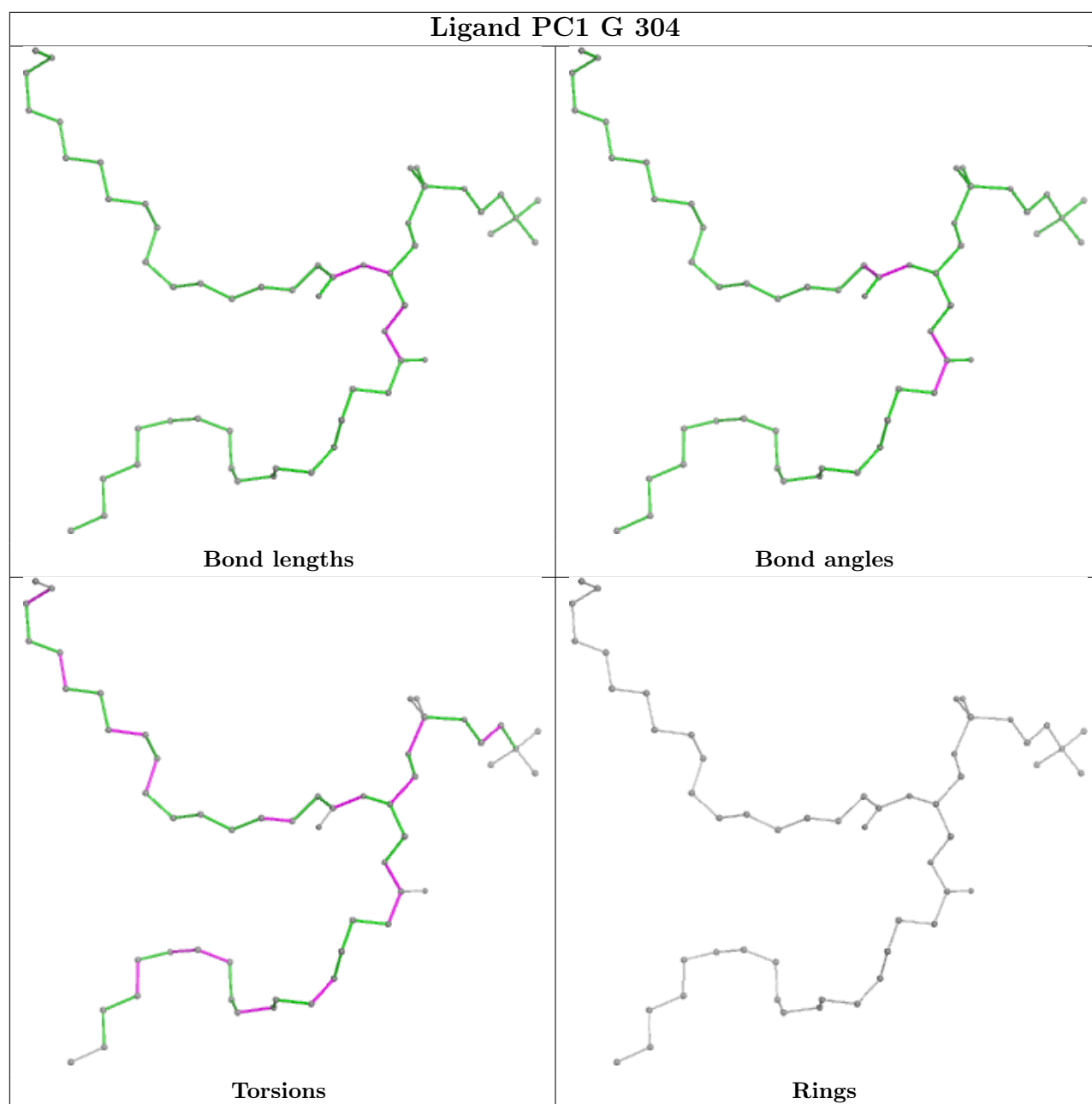


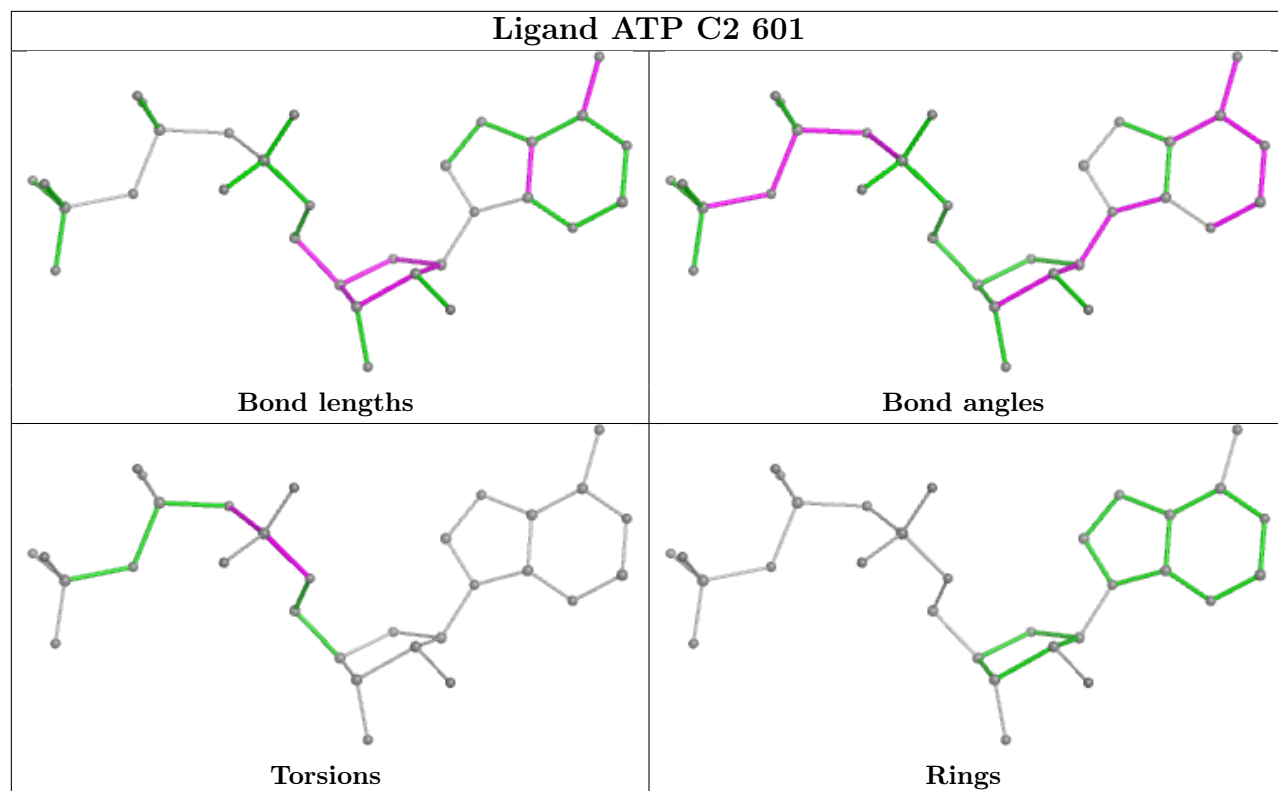


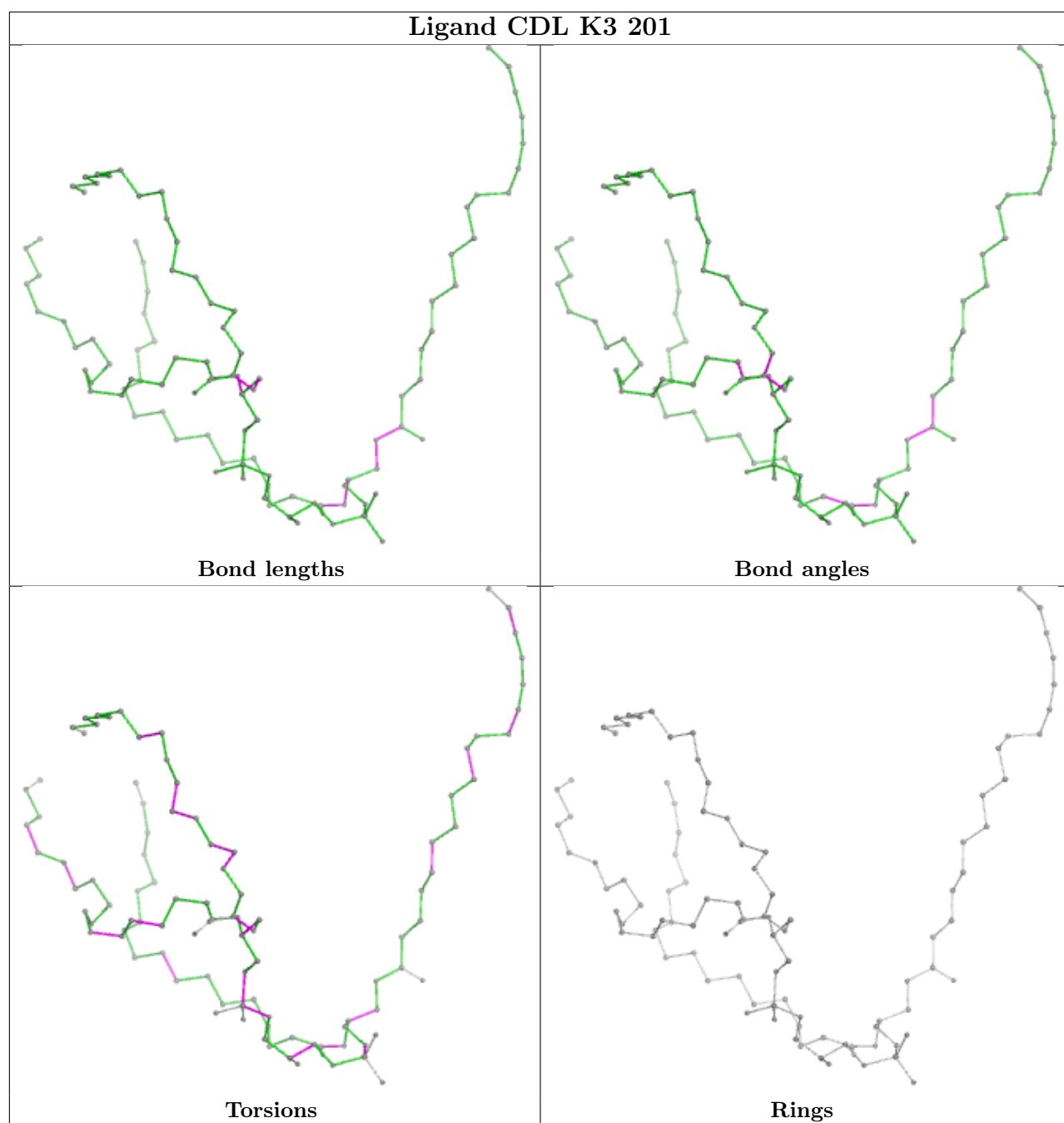


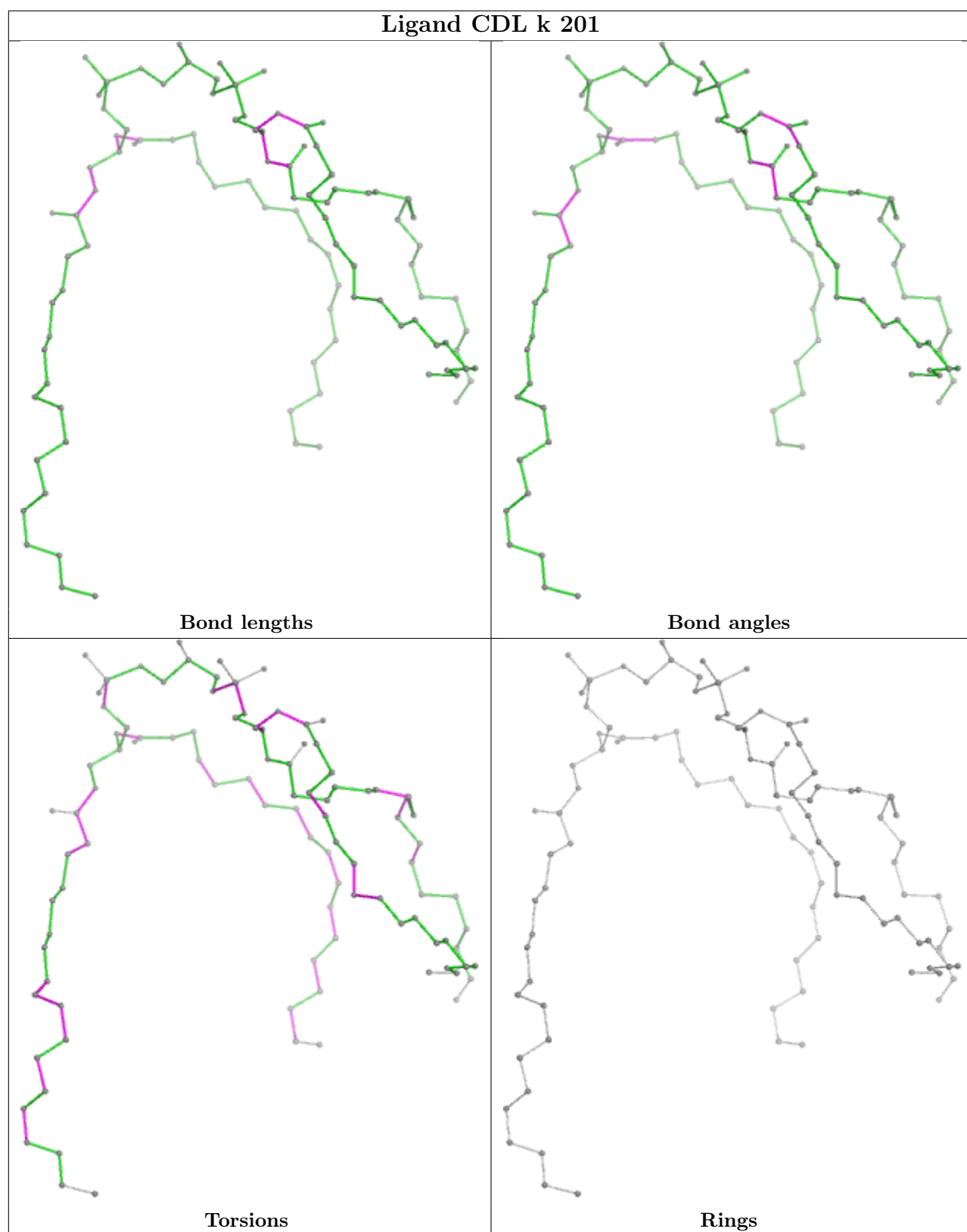


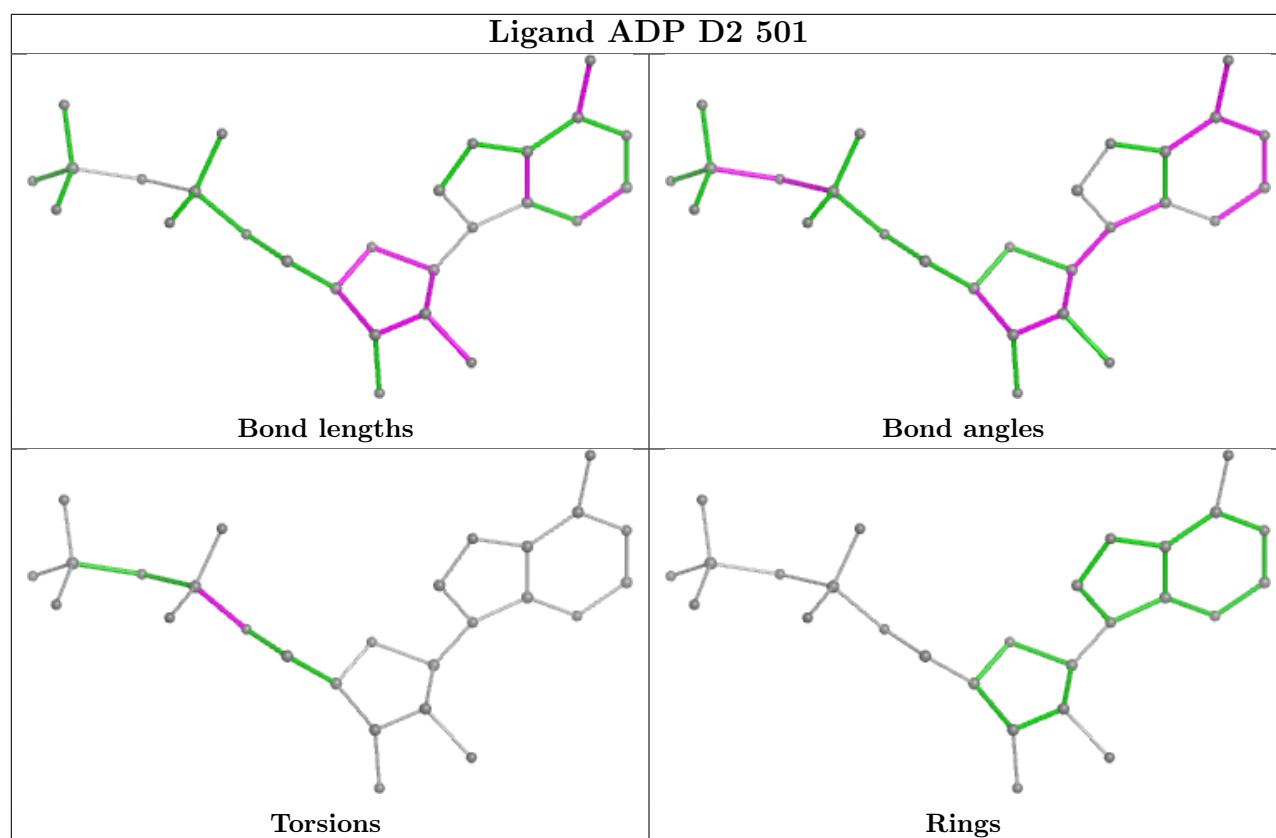


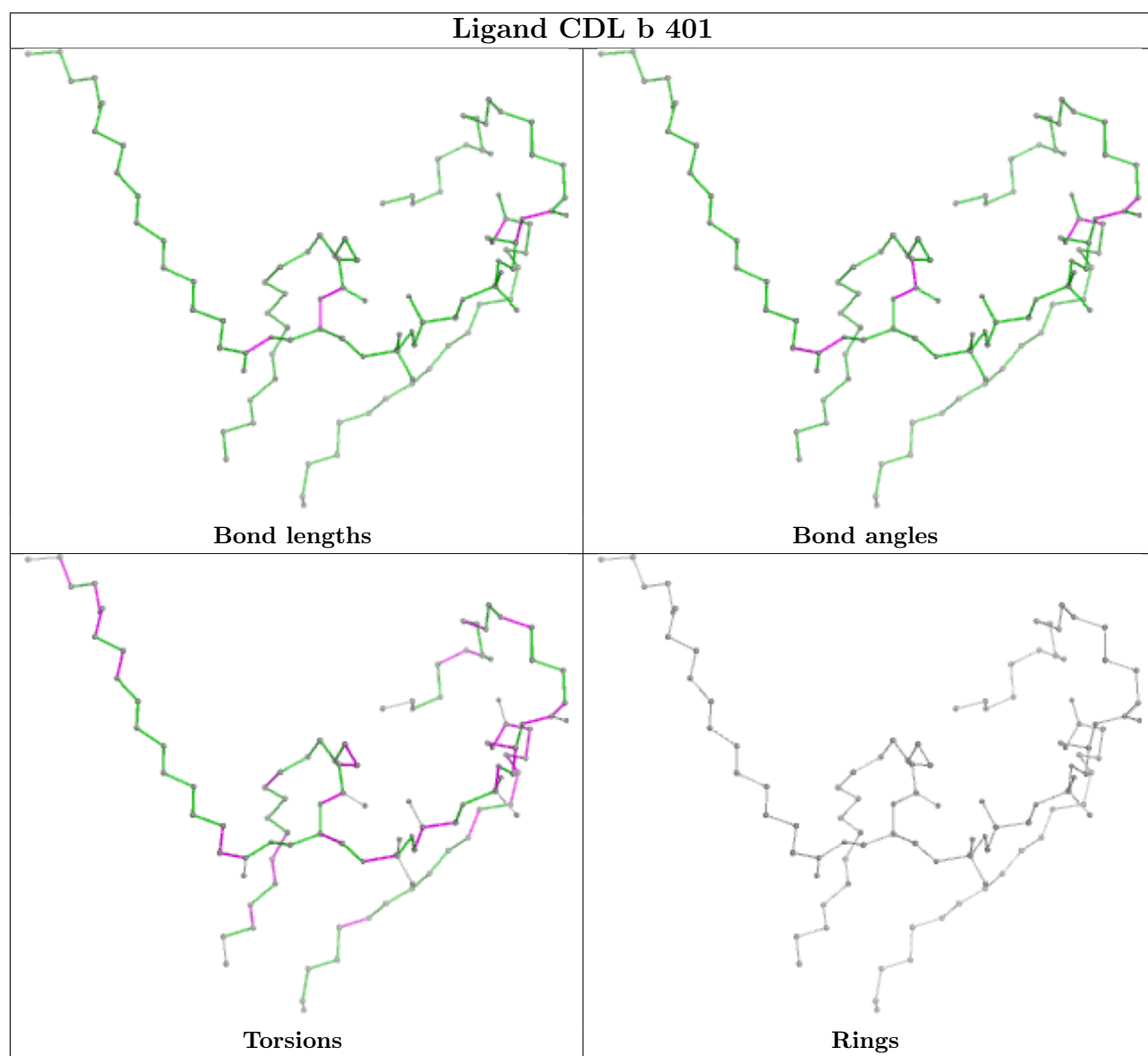


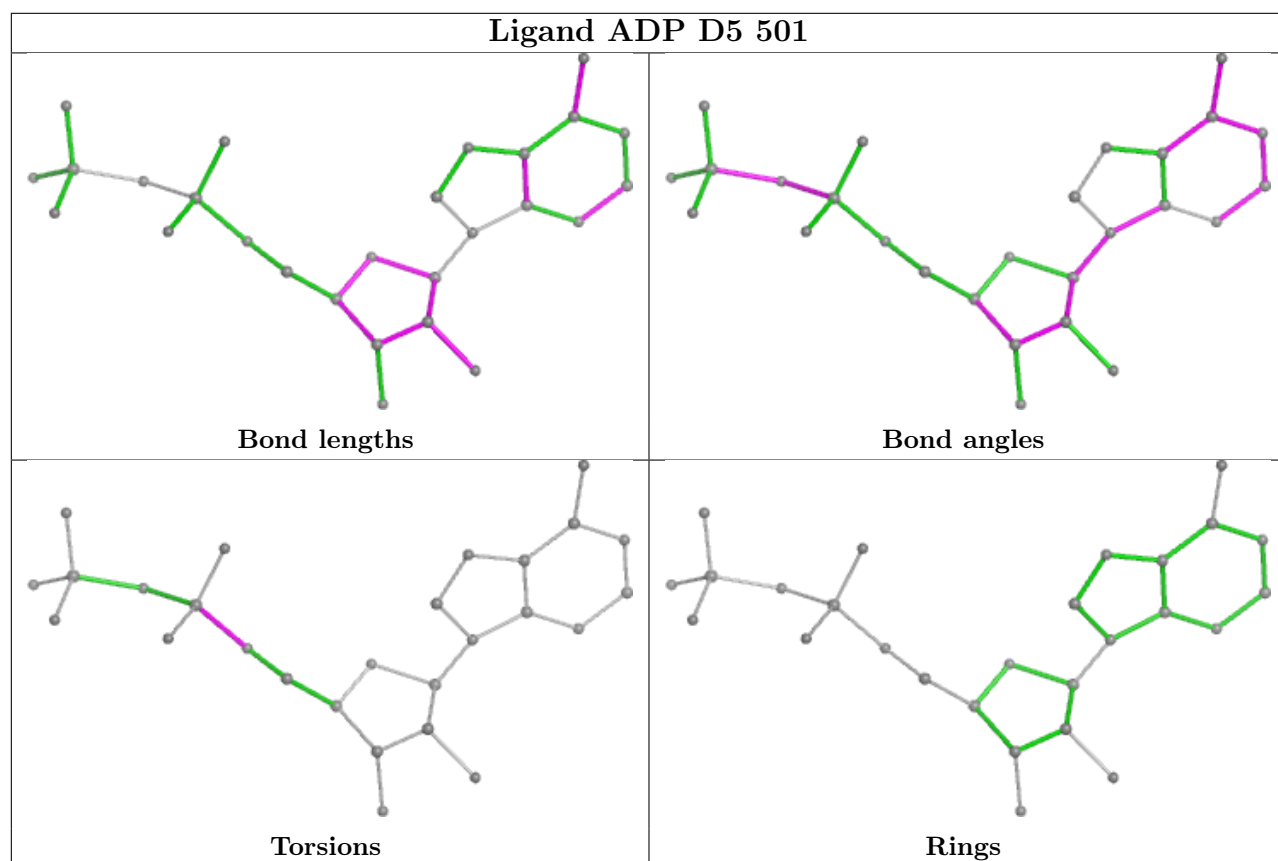
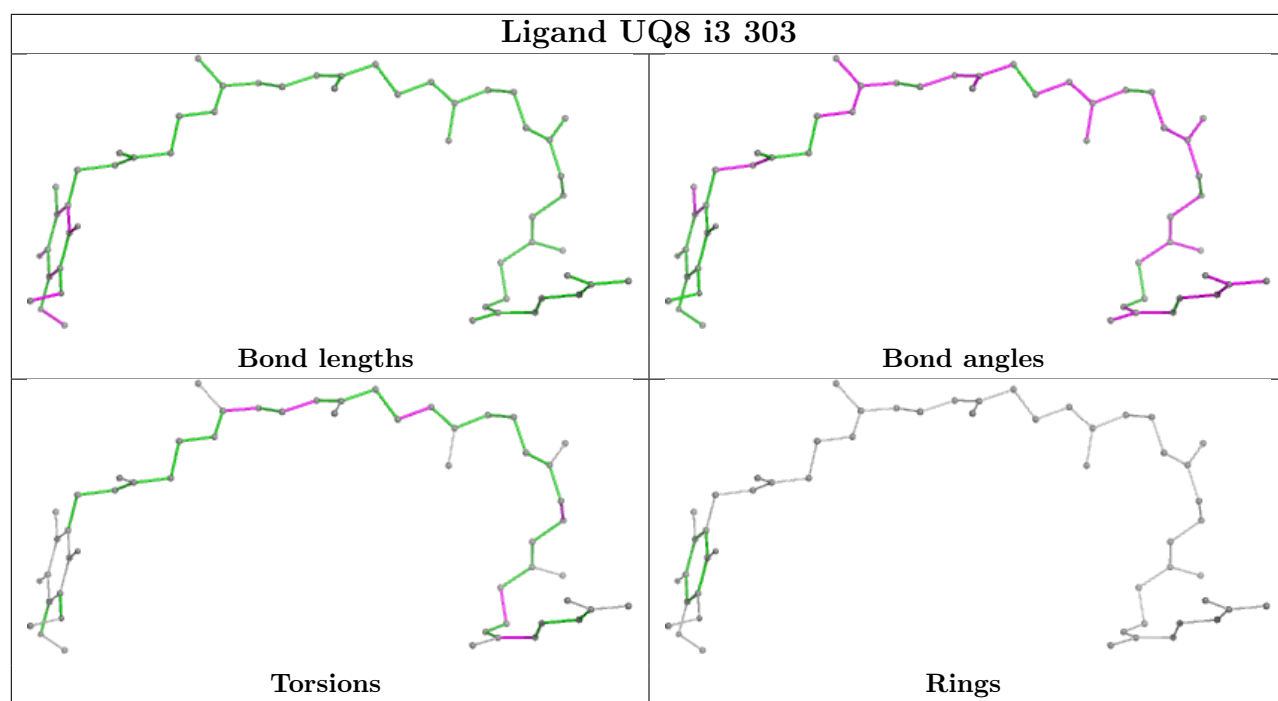


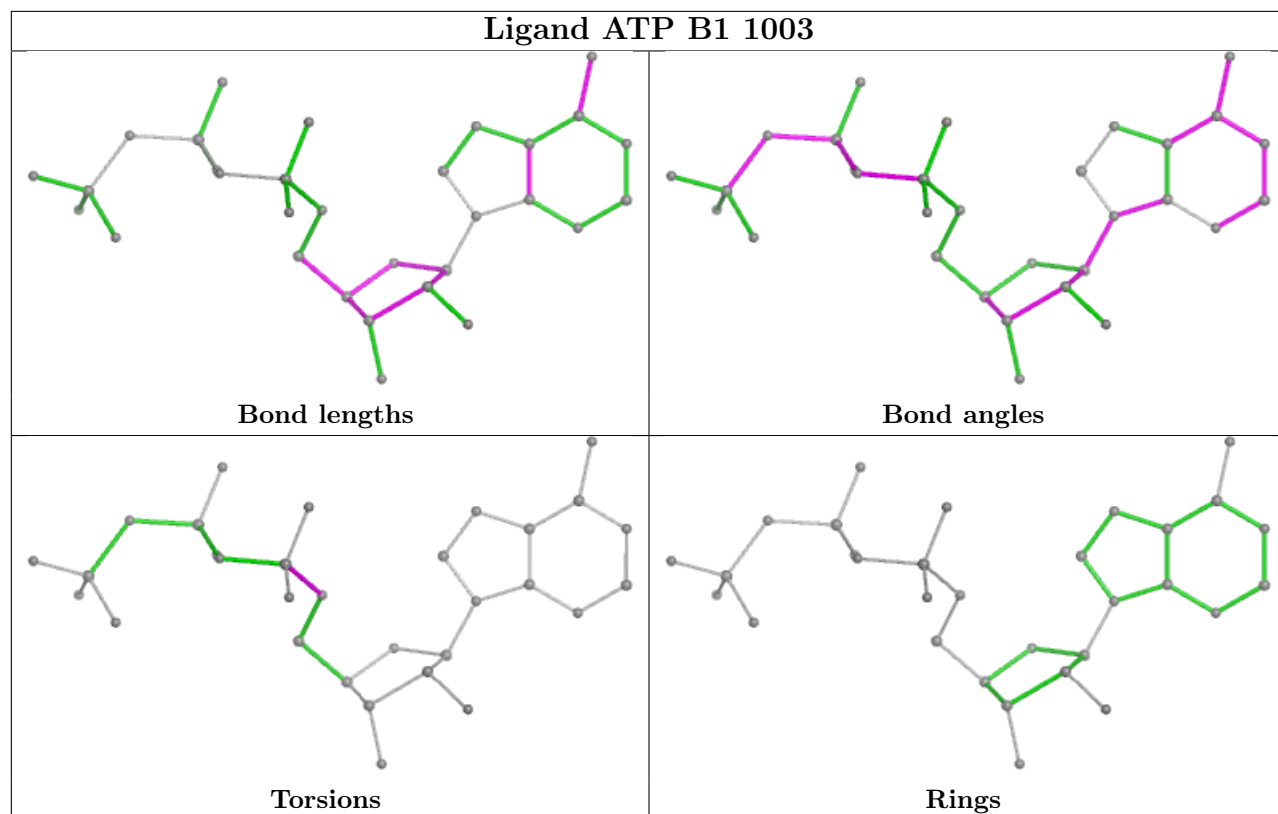




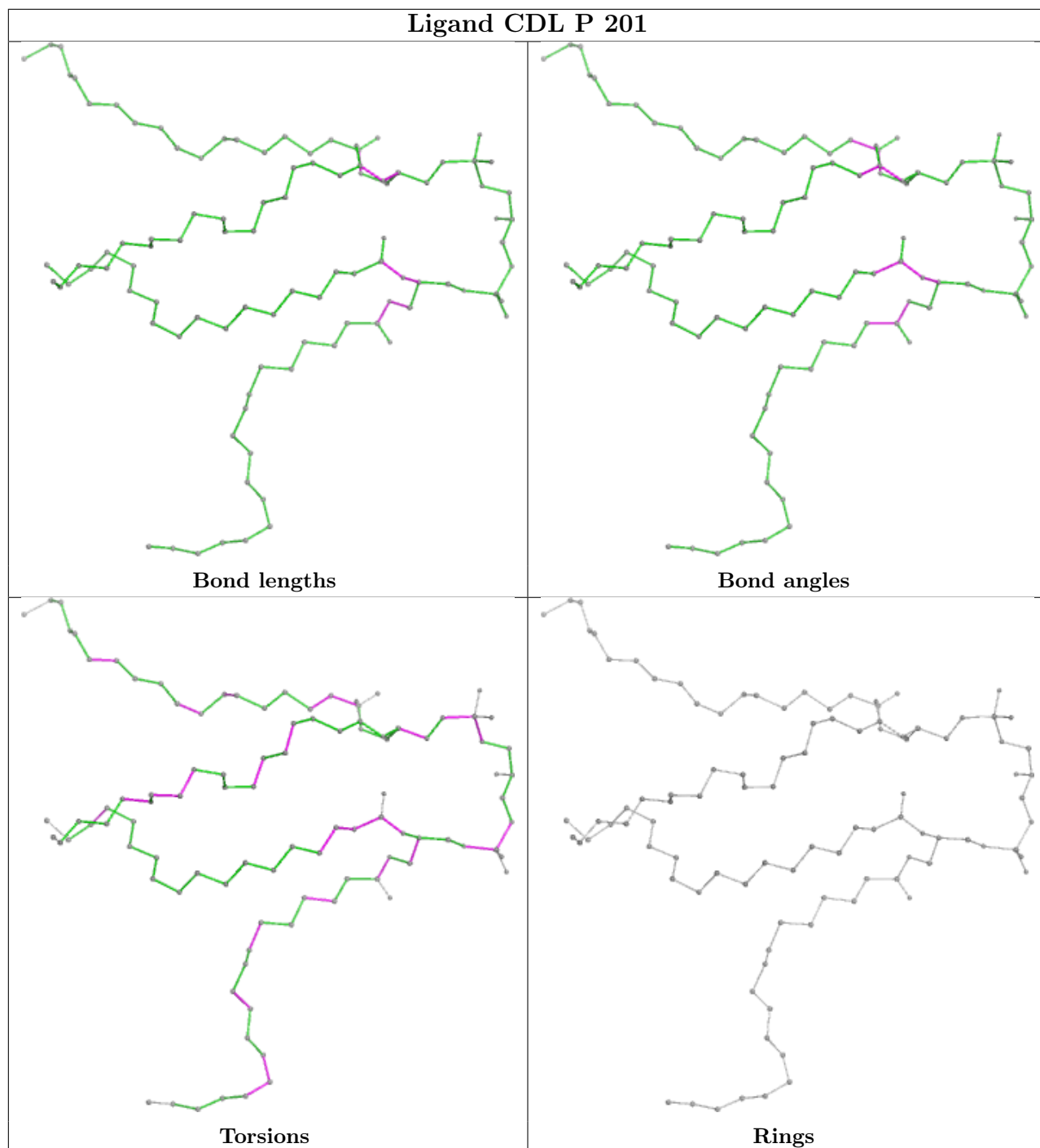


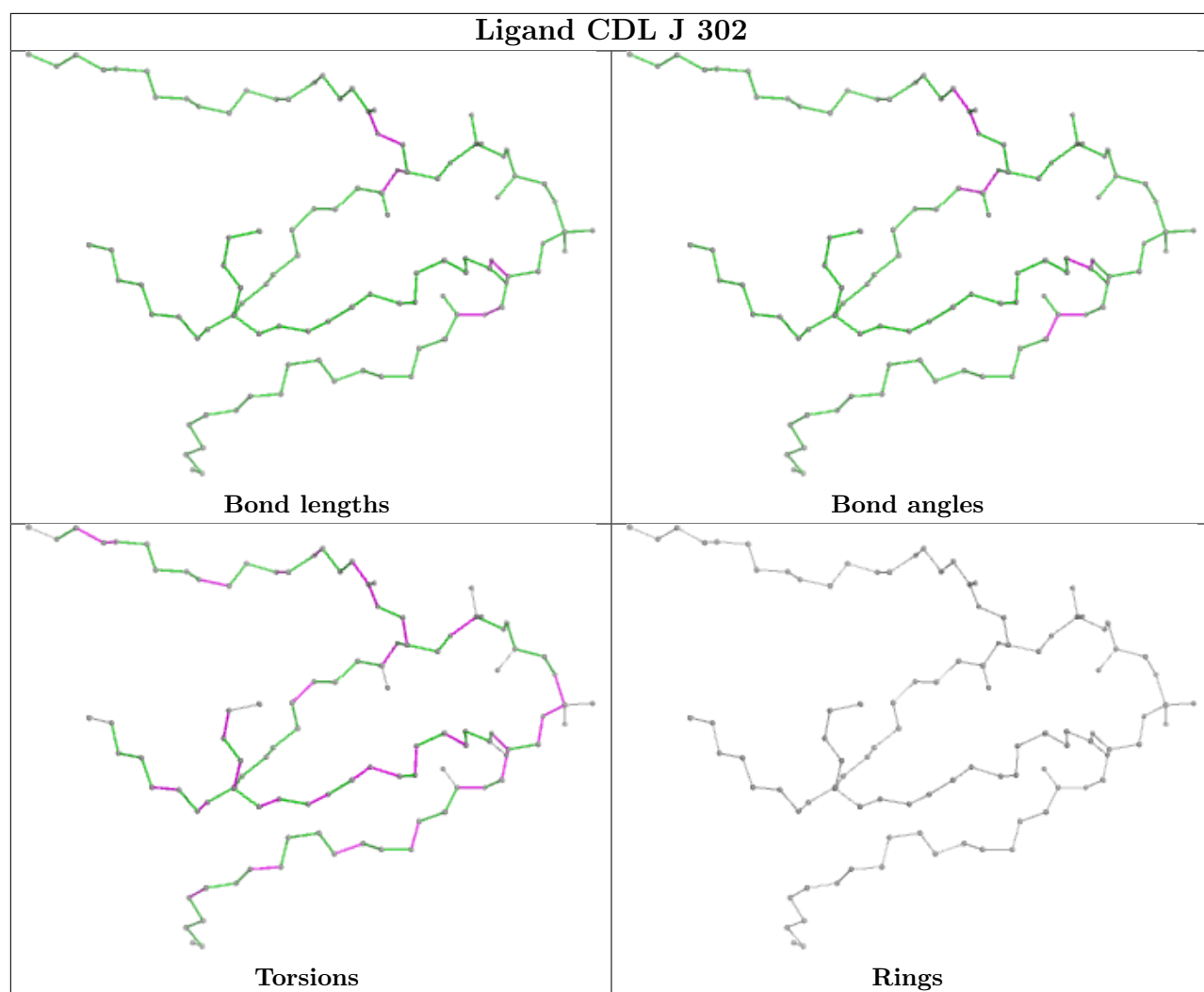


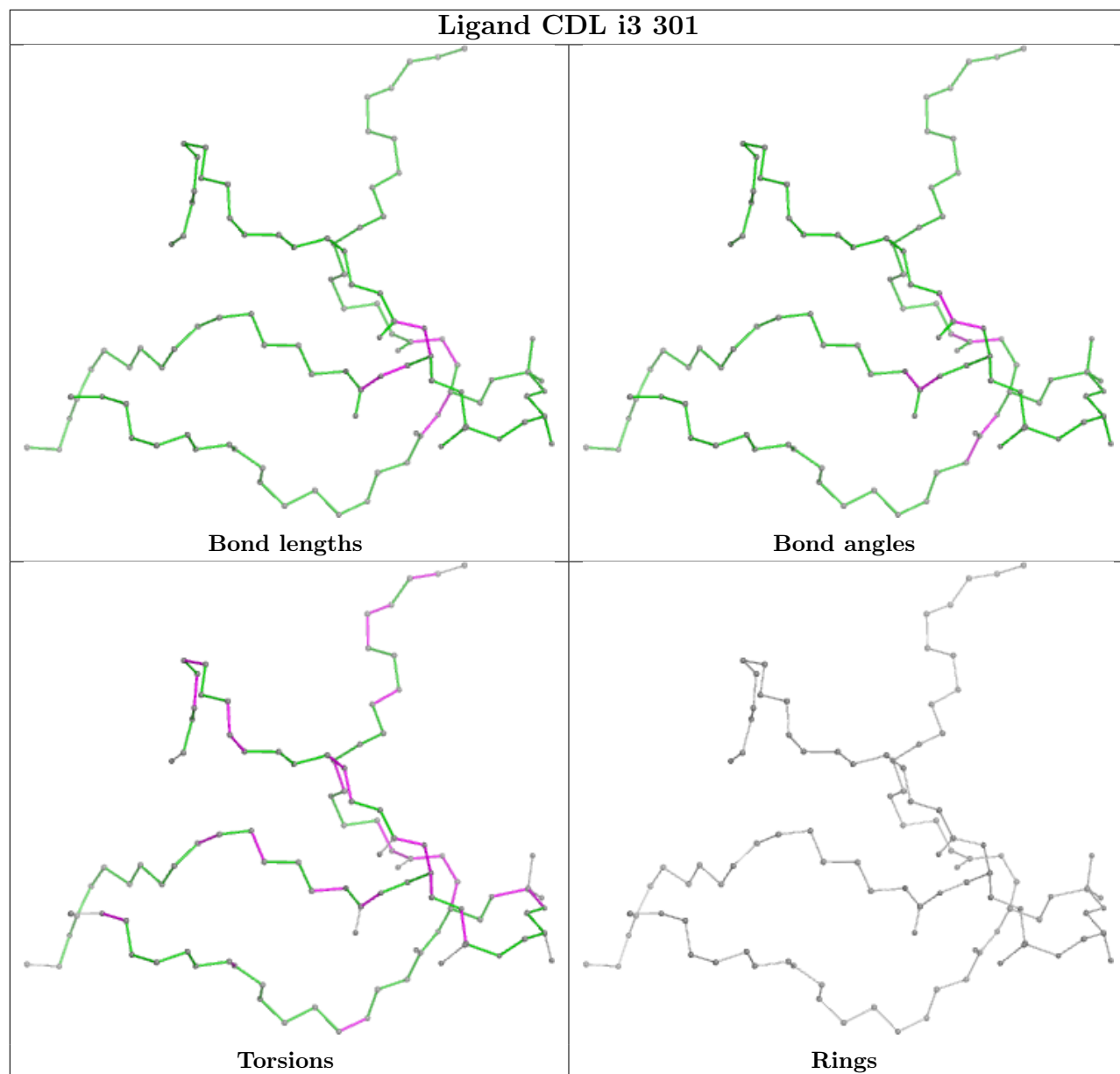


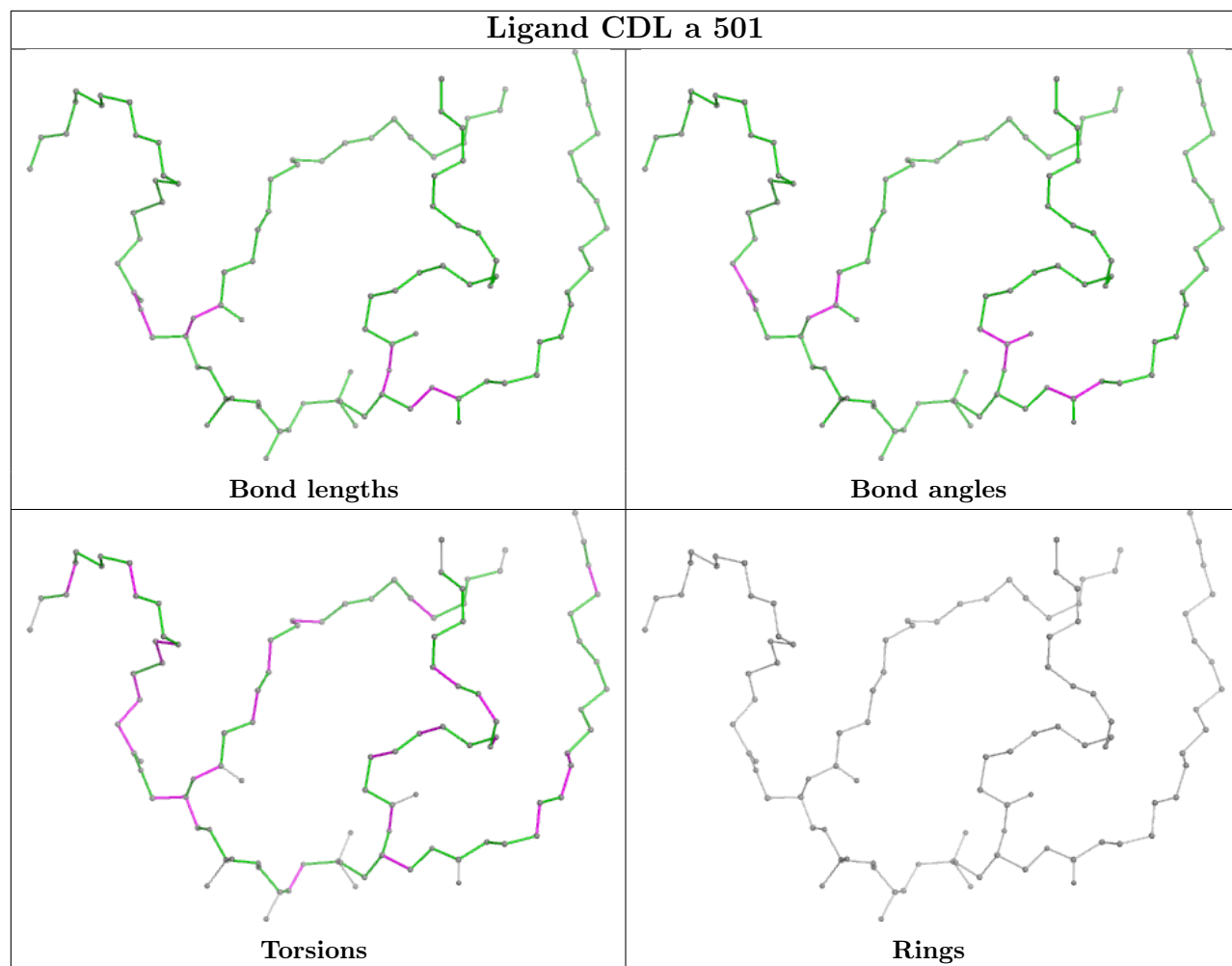


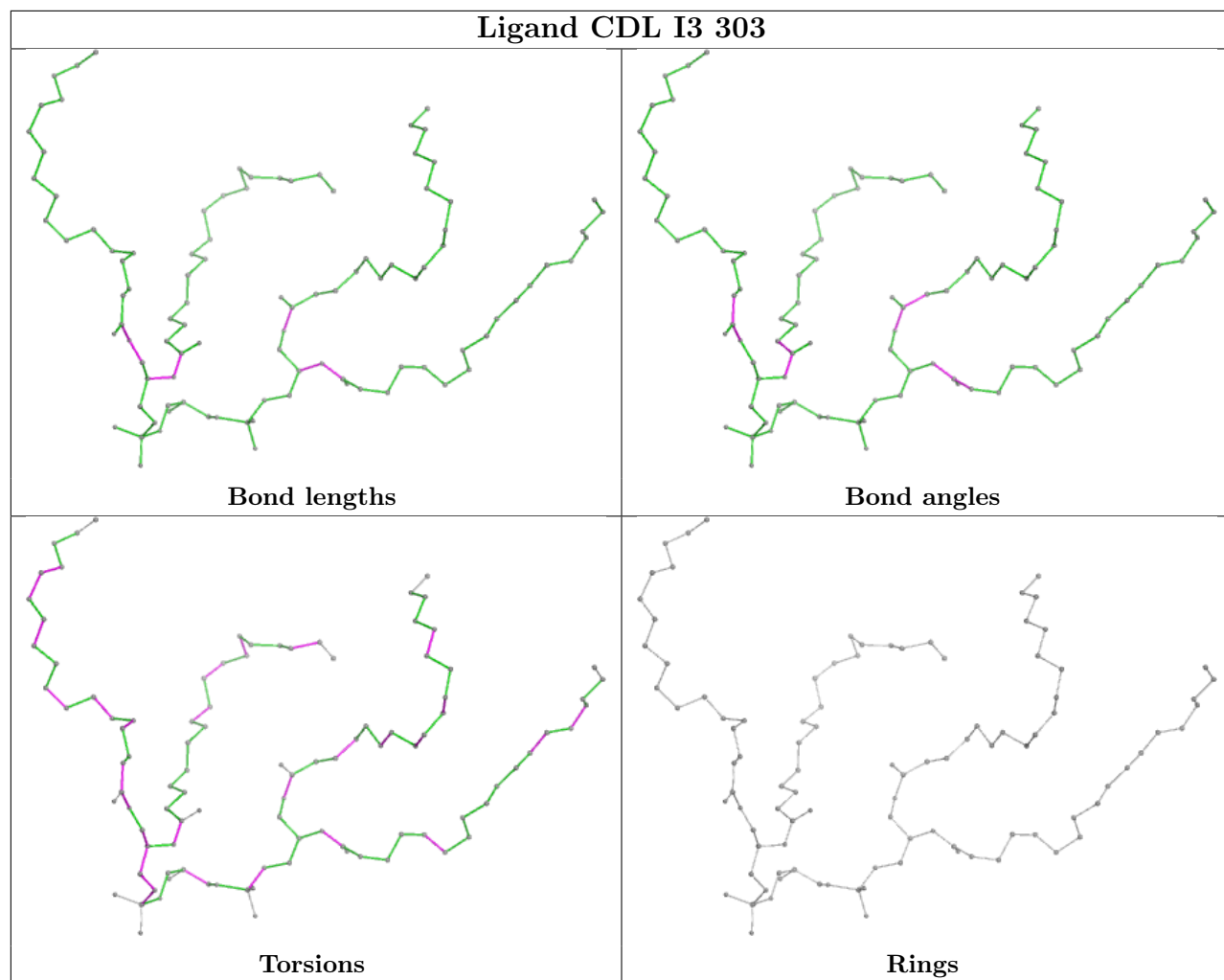
Ligand CDL P 201

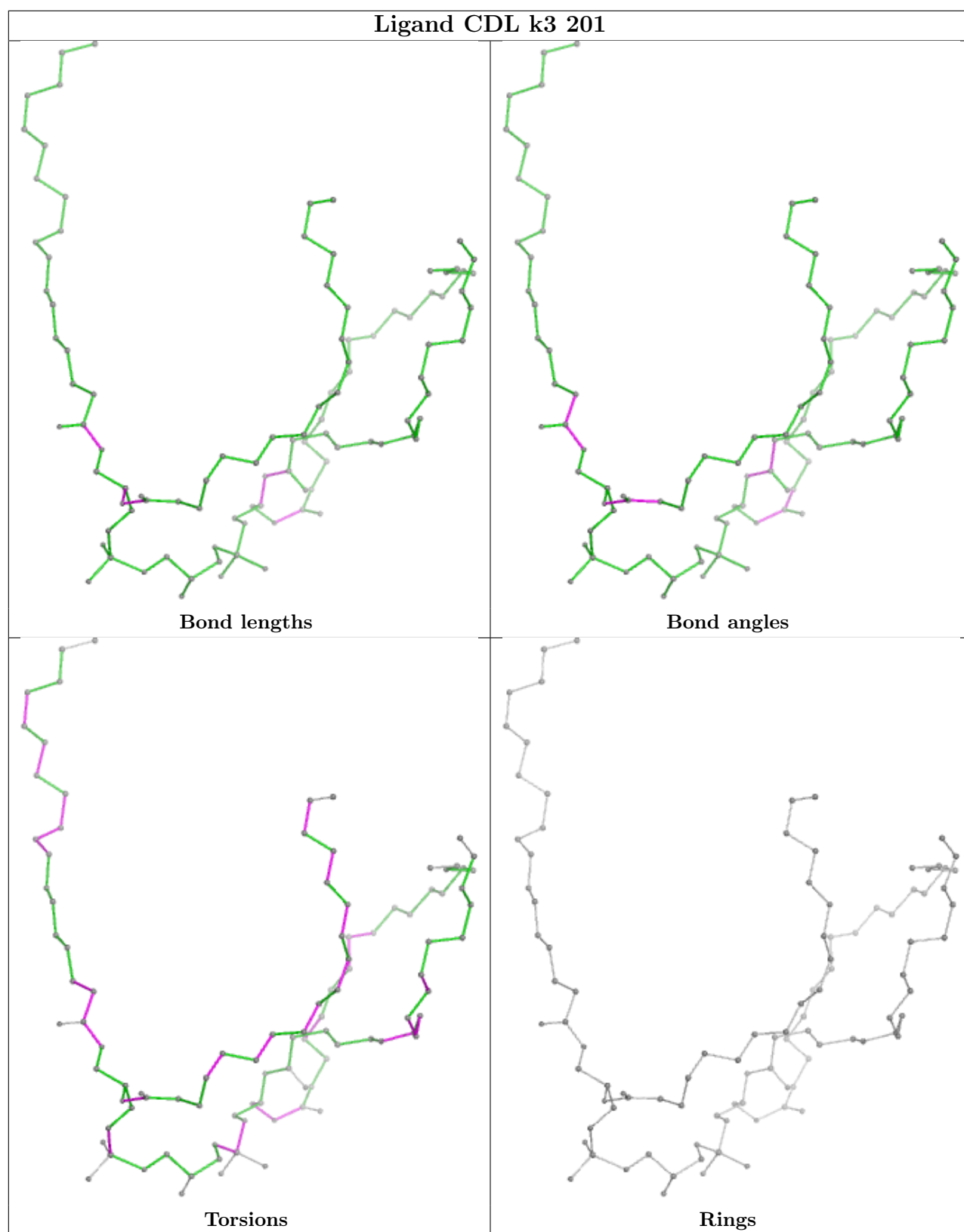




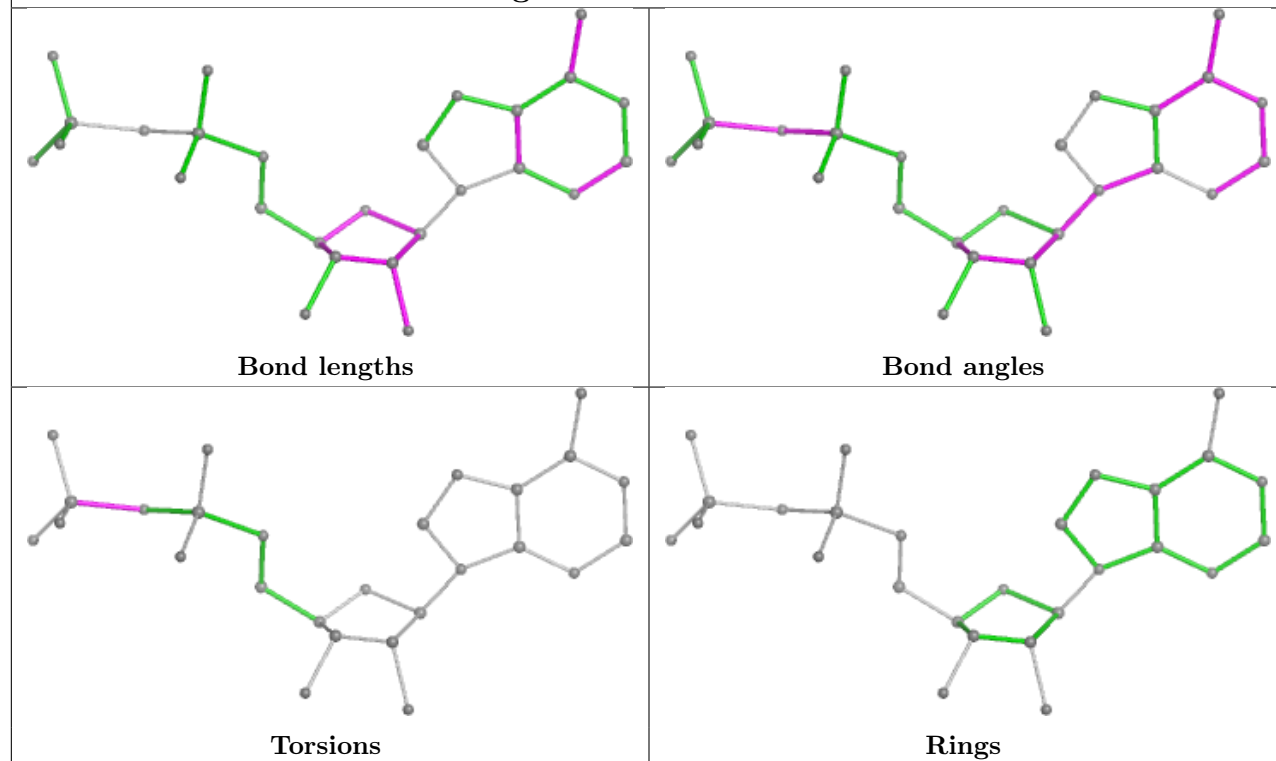




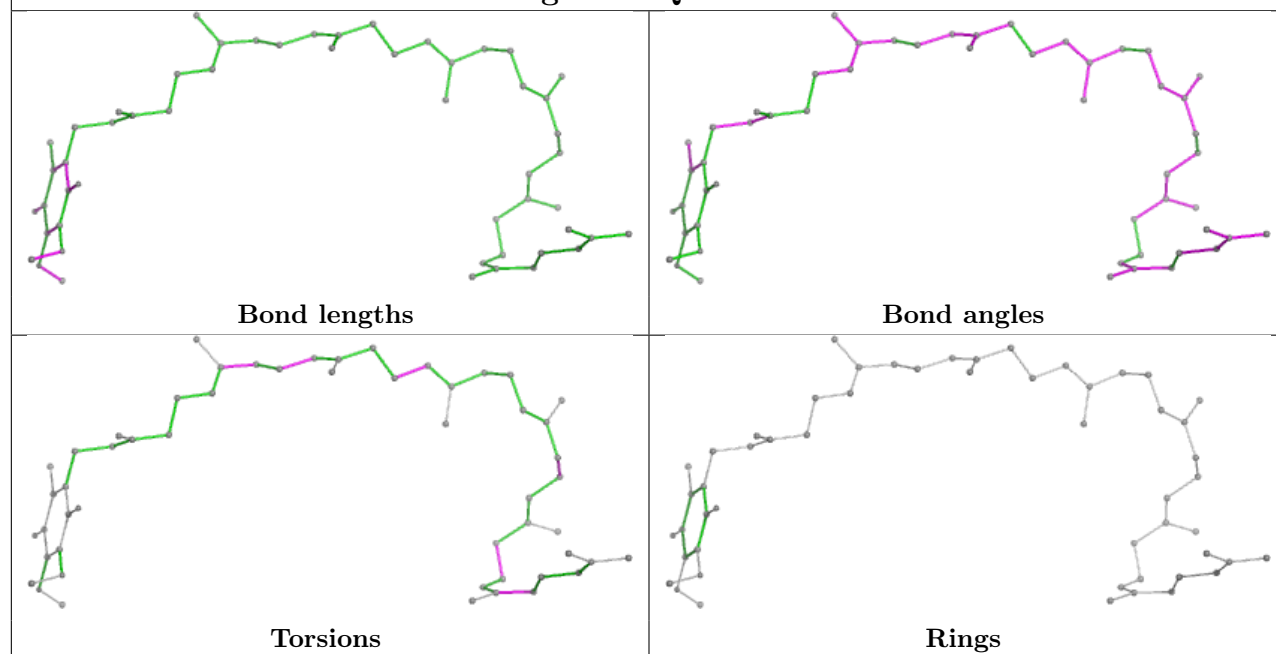


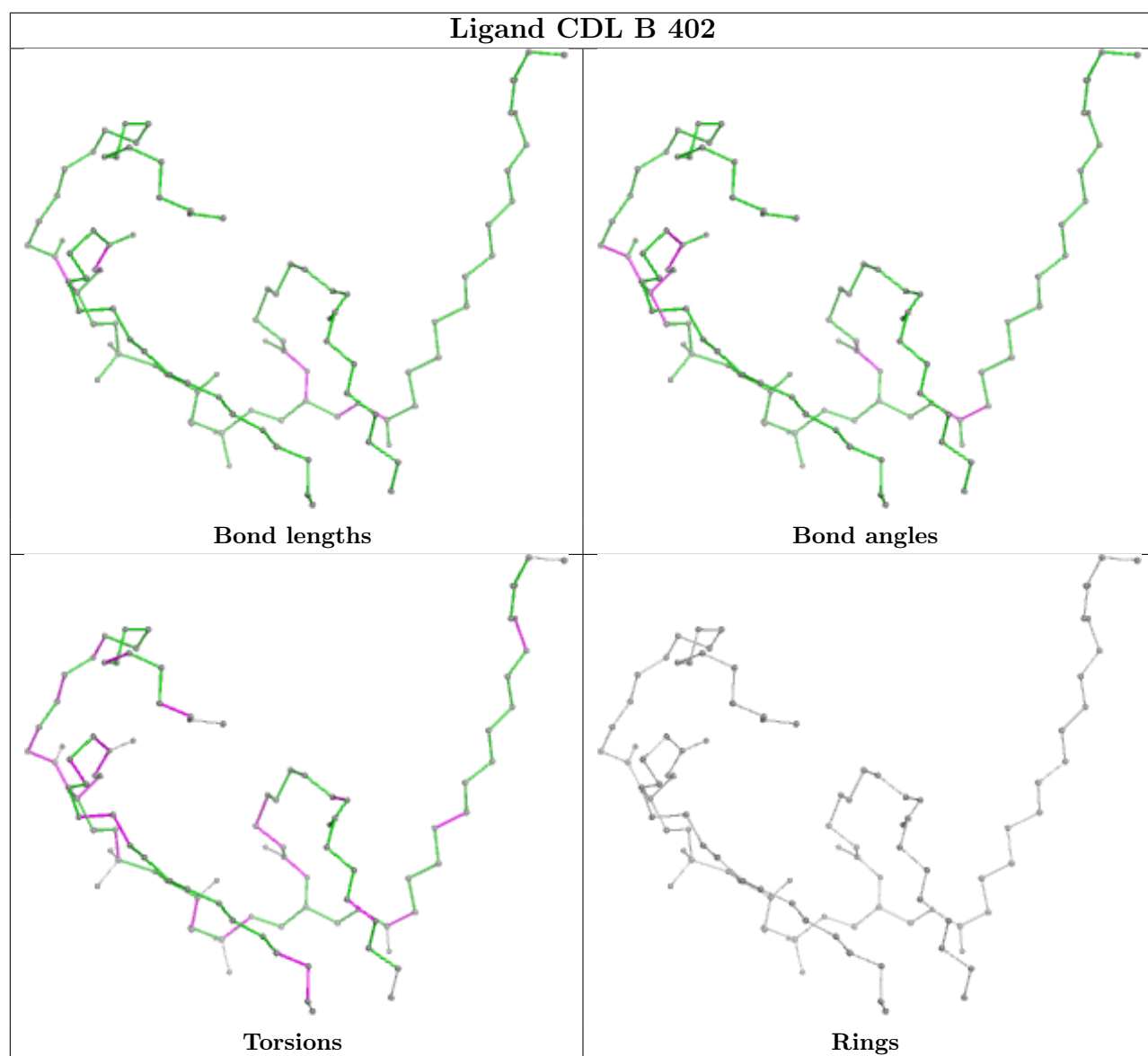


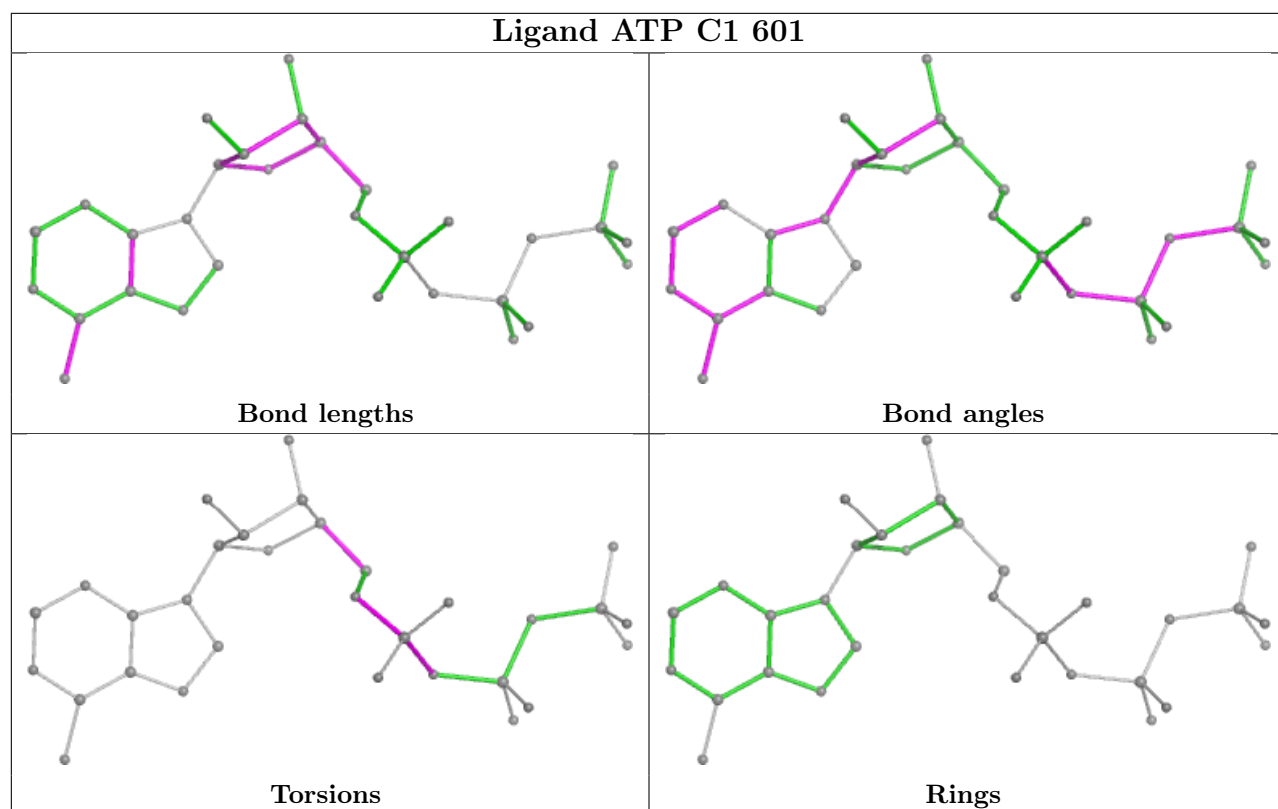
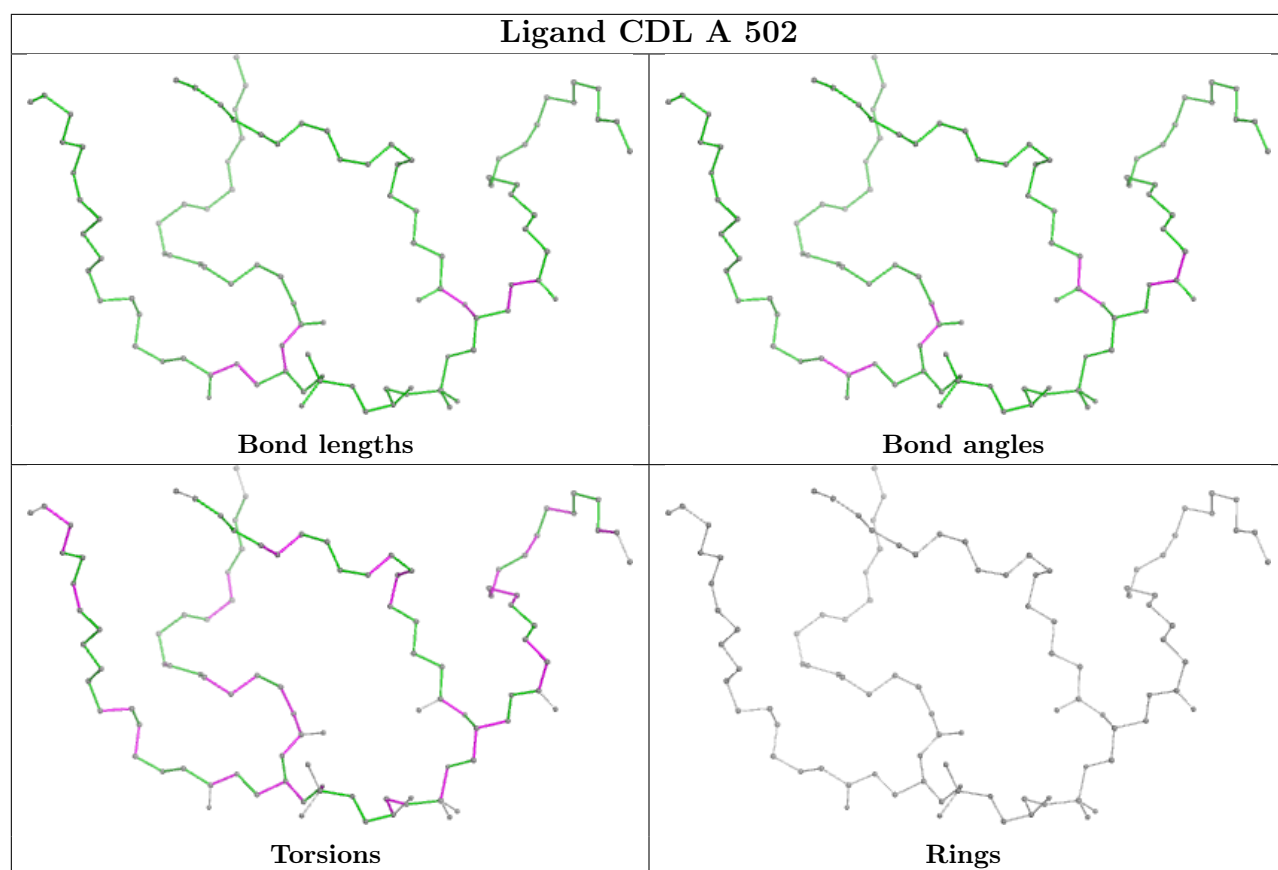
Ligand ADP B1 1002

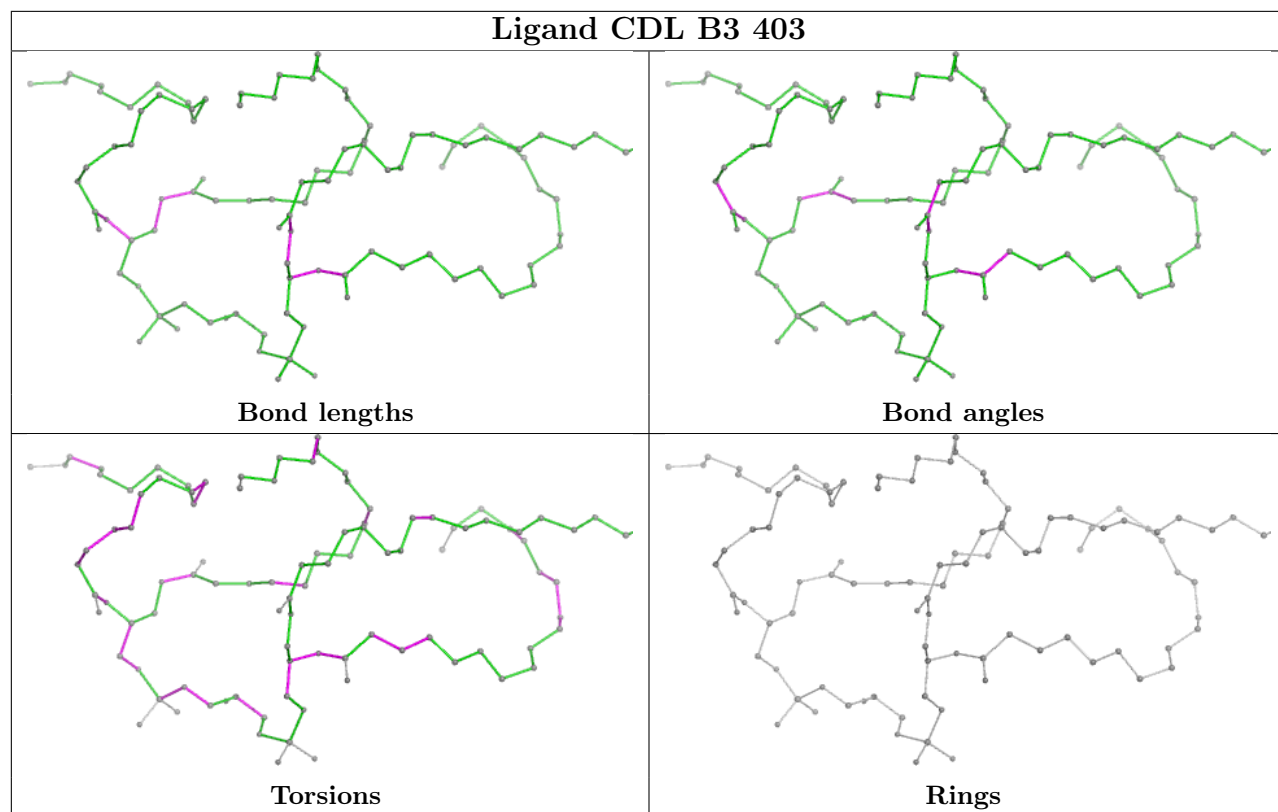


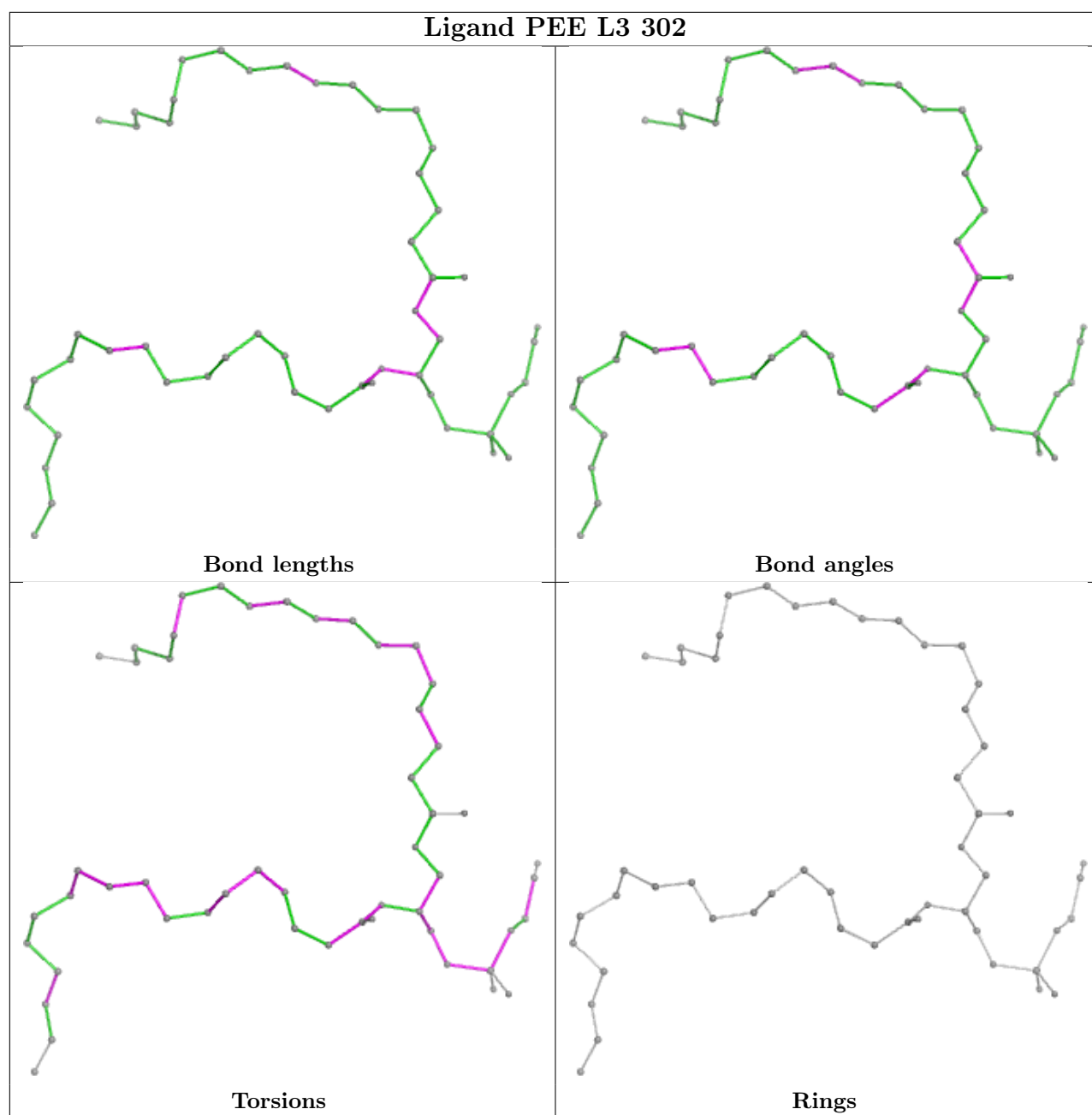
Ligand UQ8 i 302

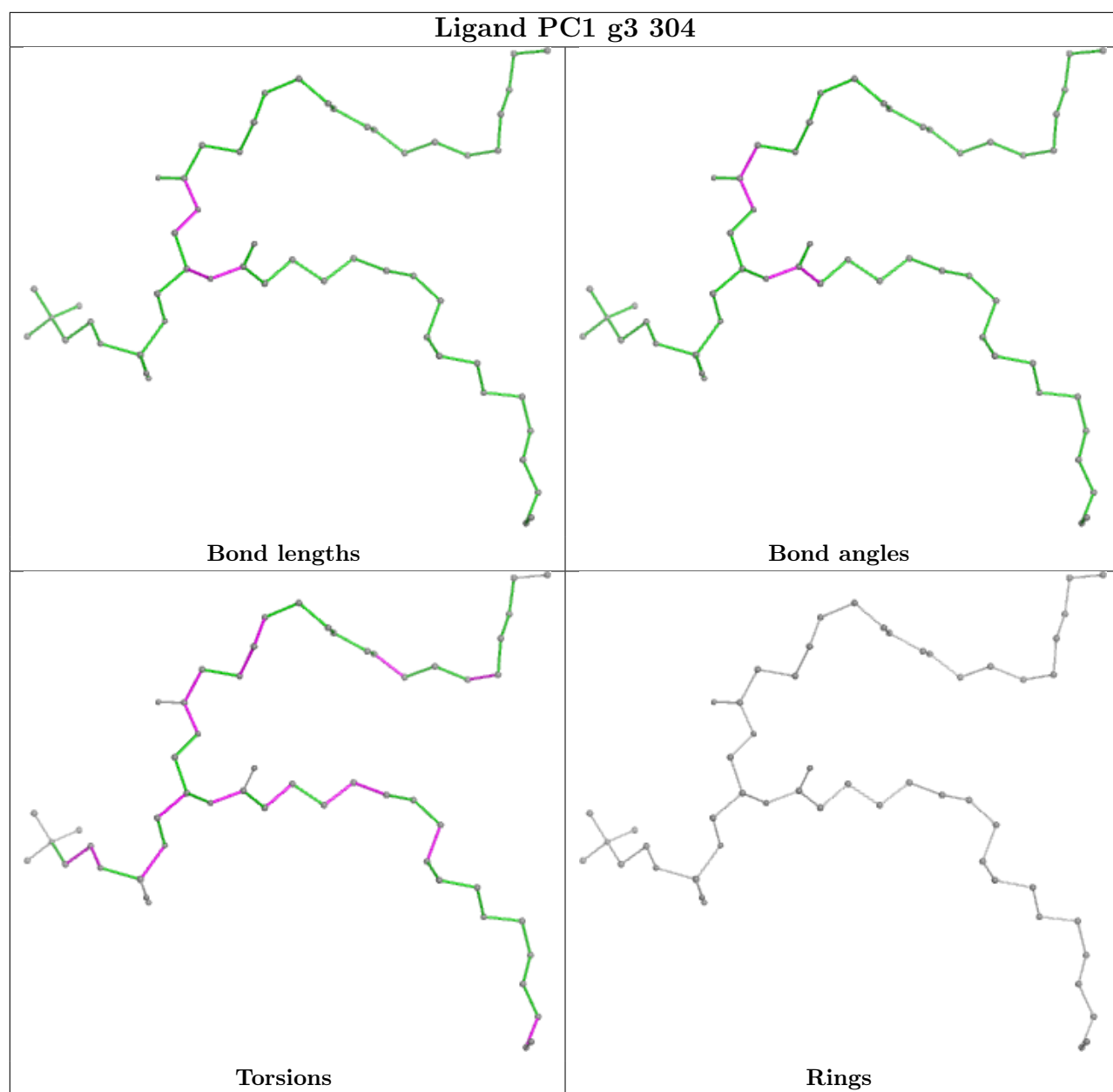


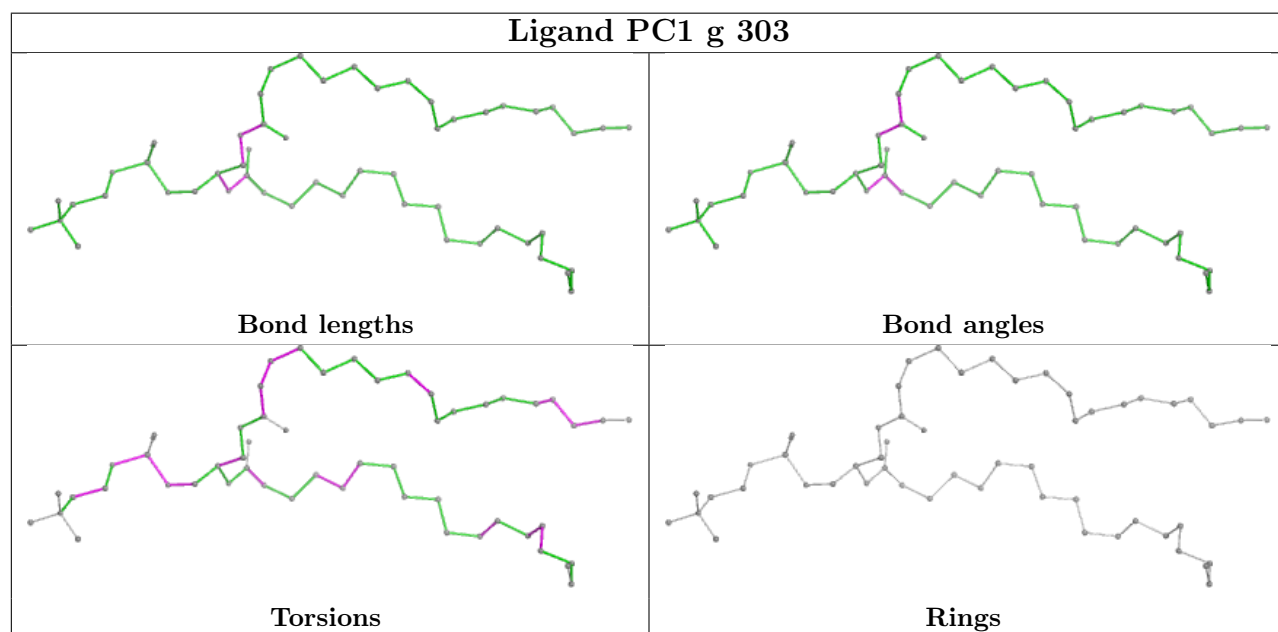
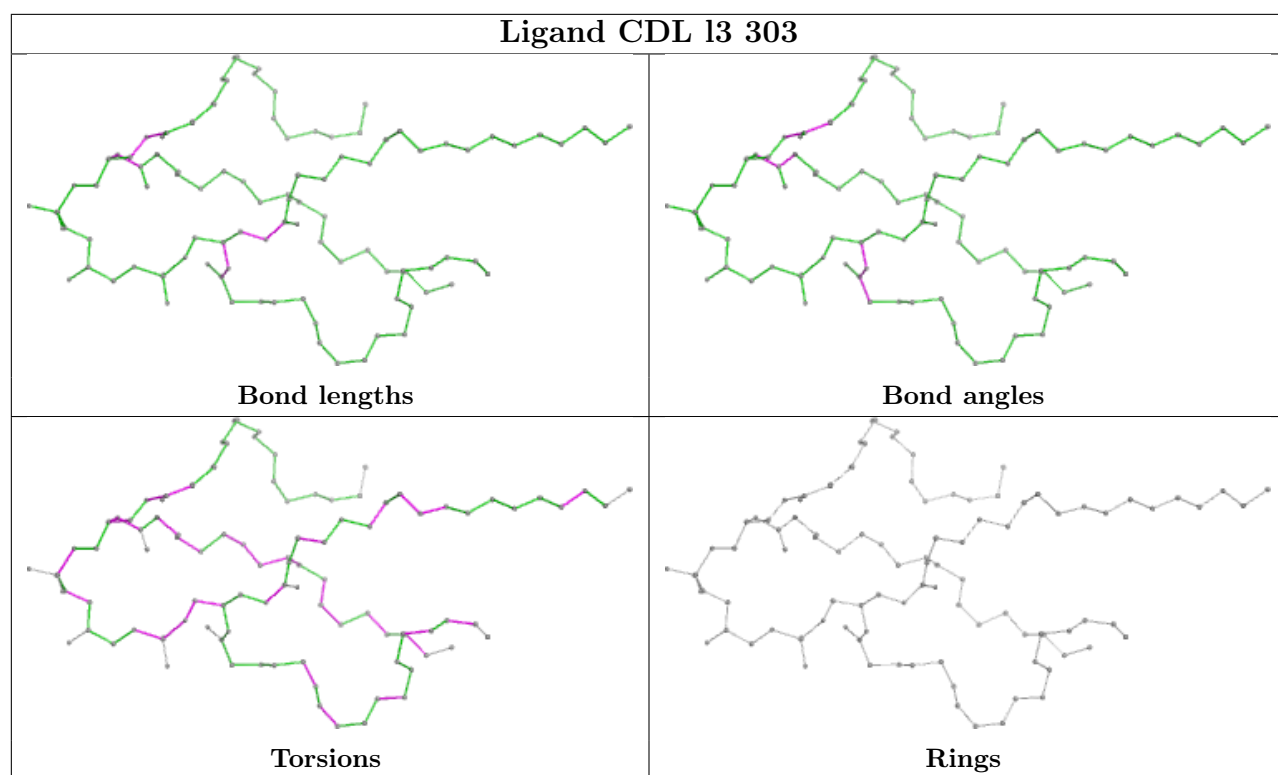


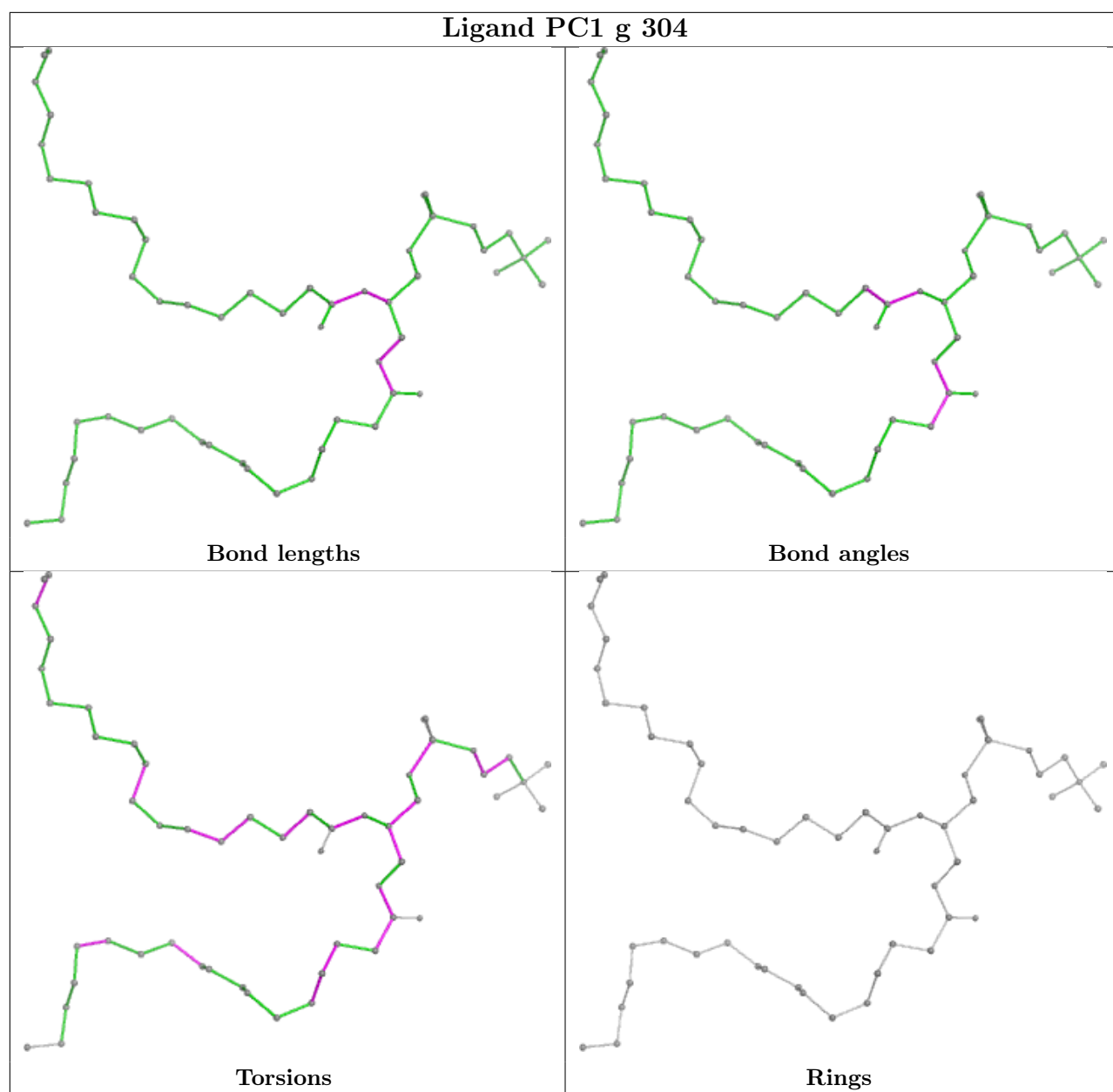


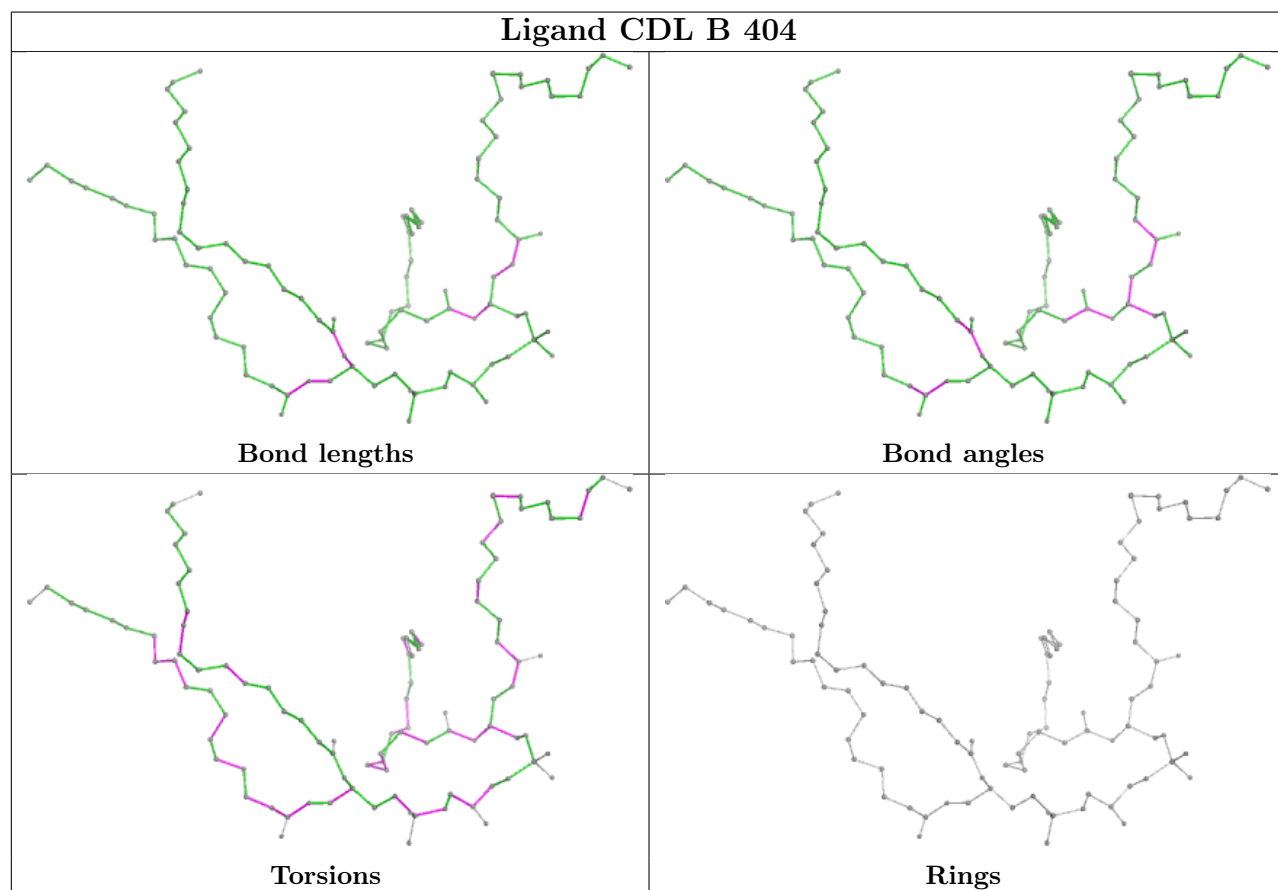
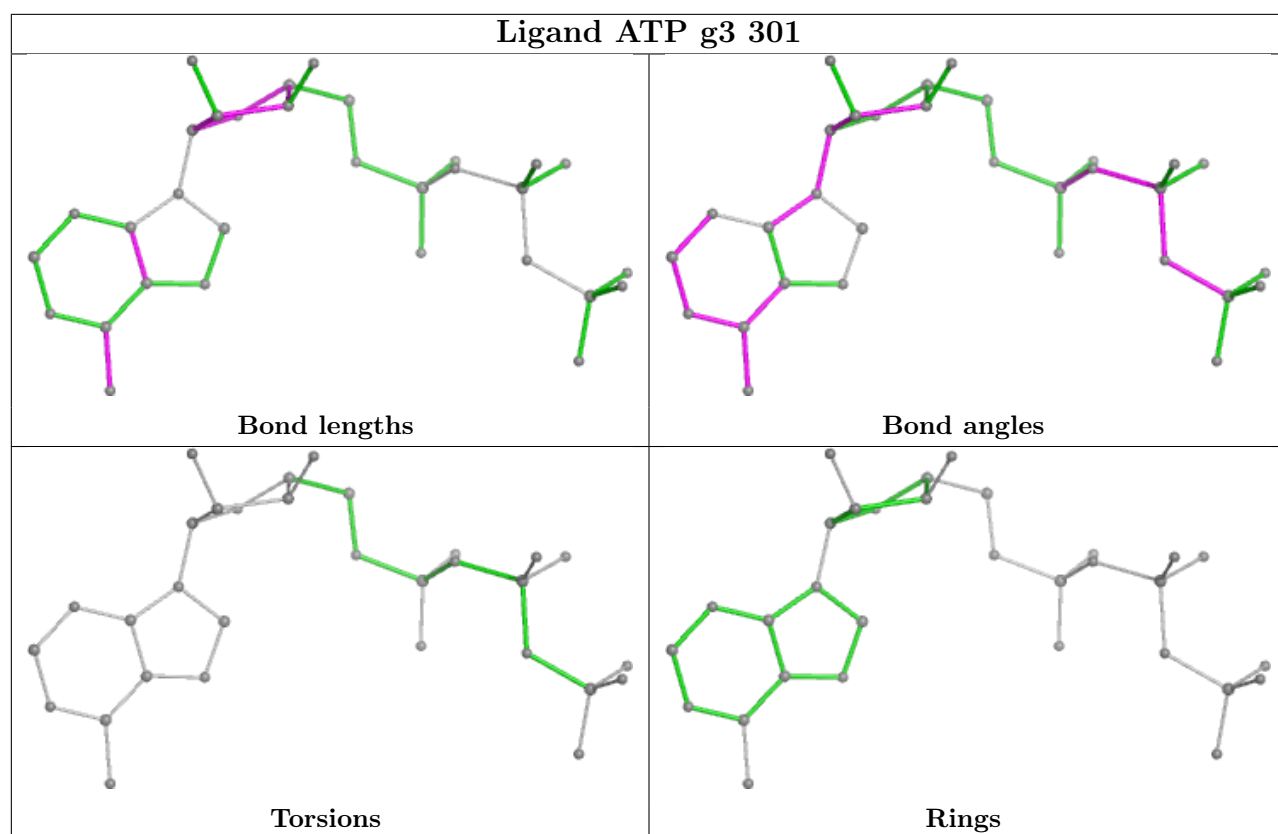


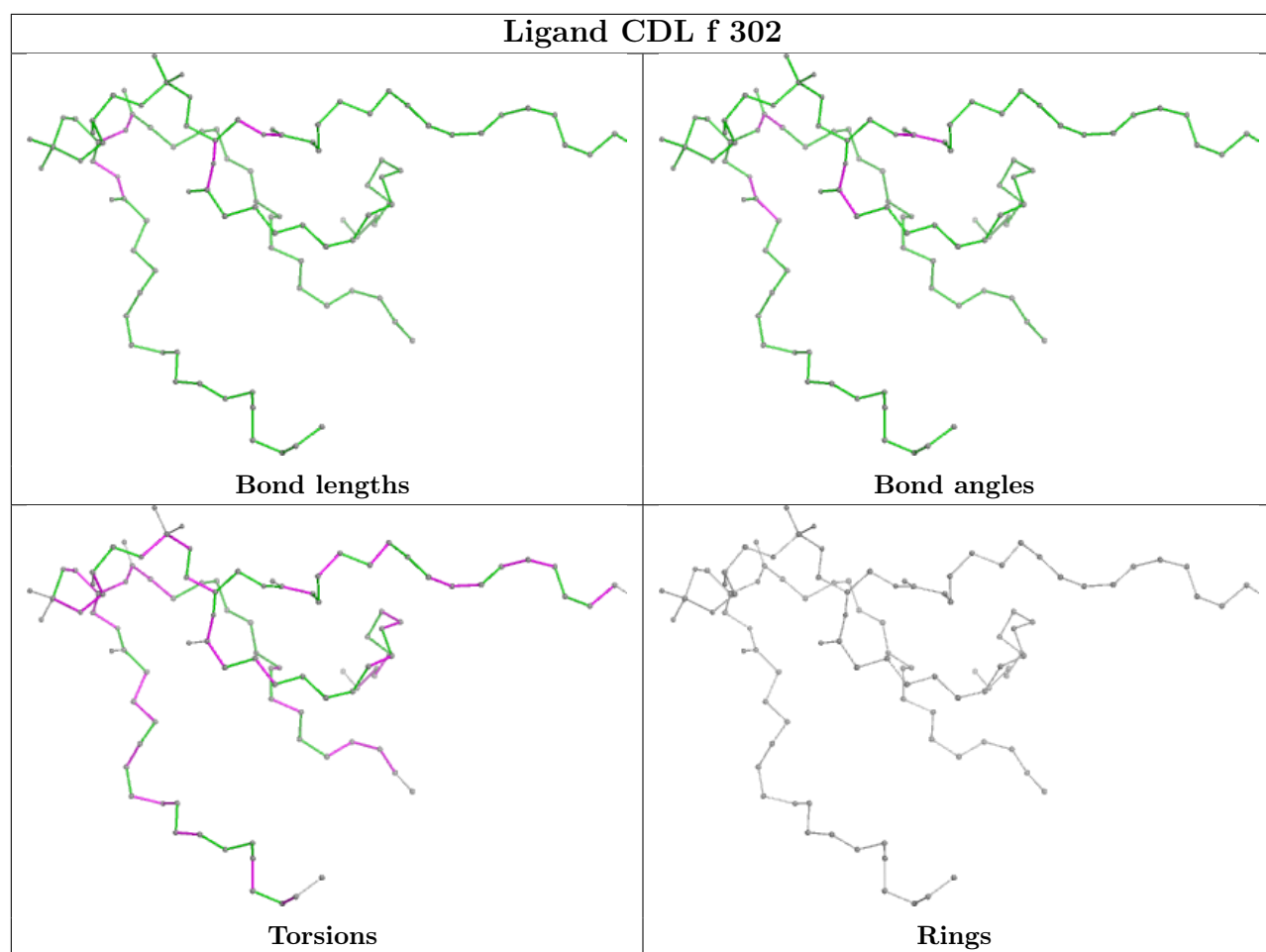


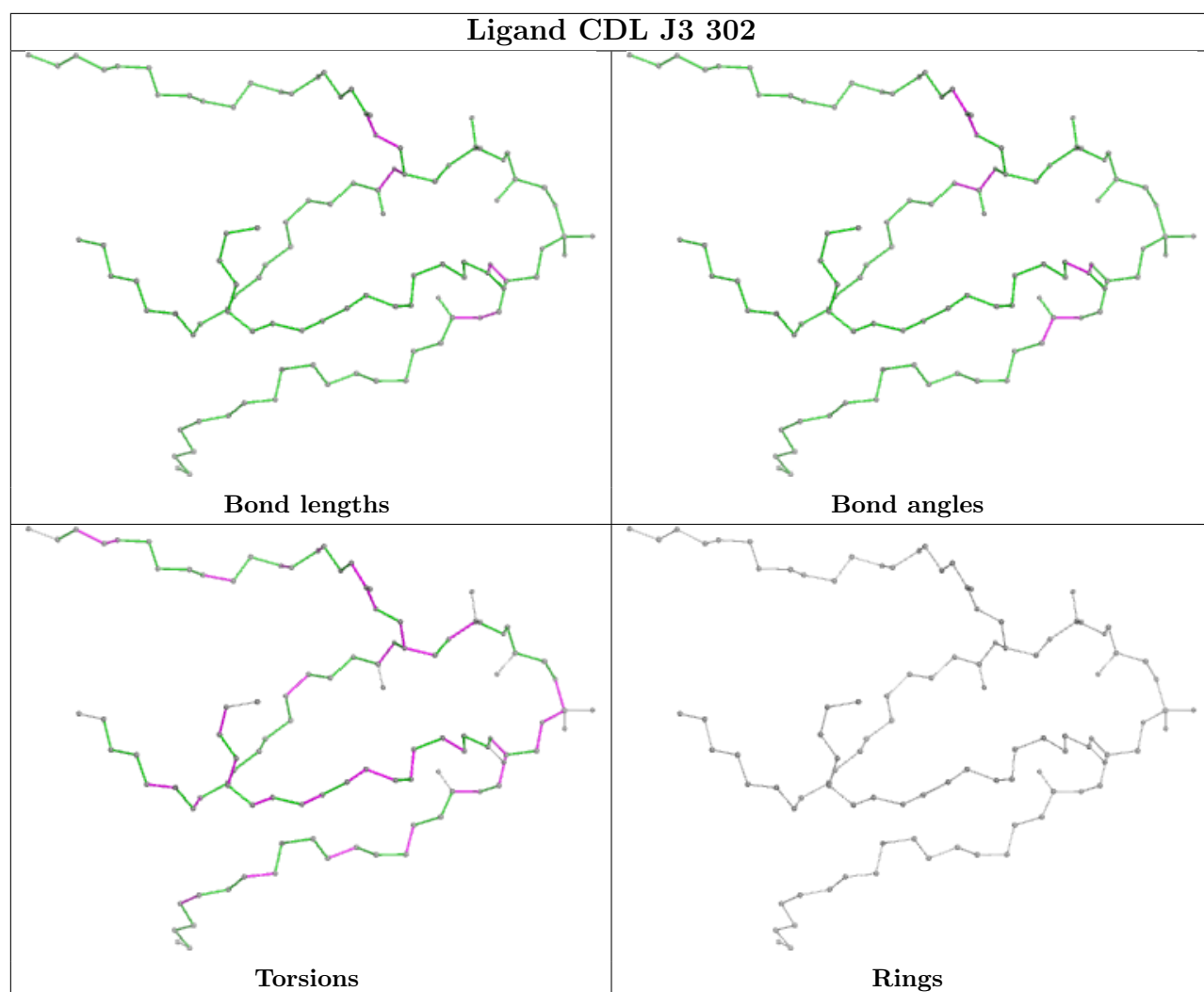


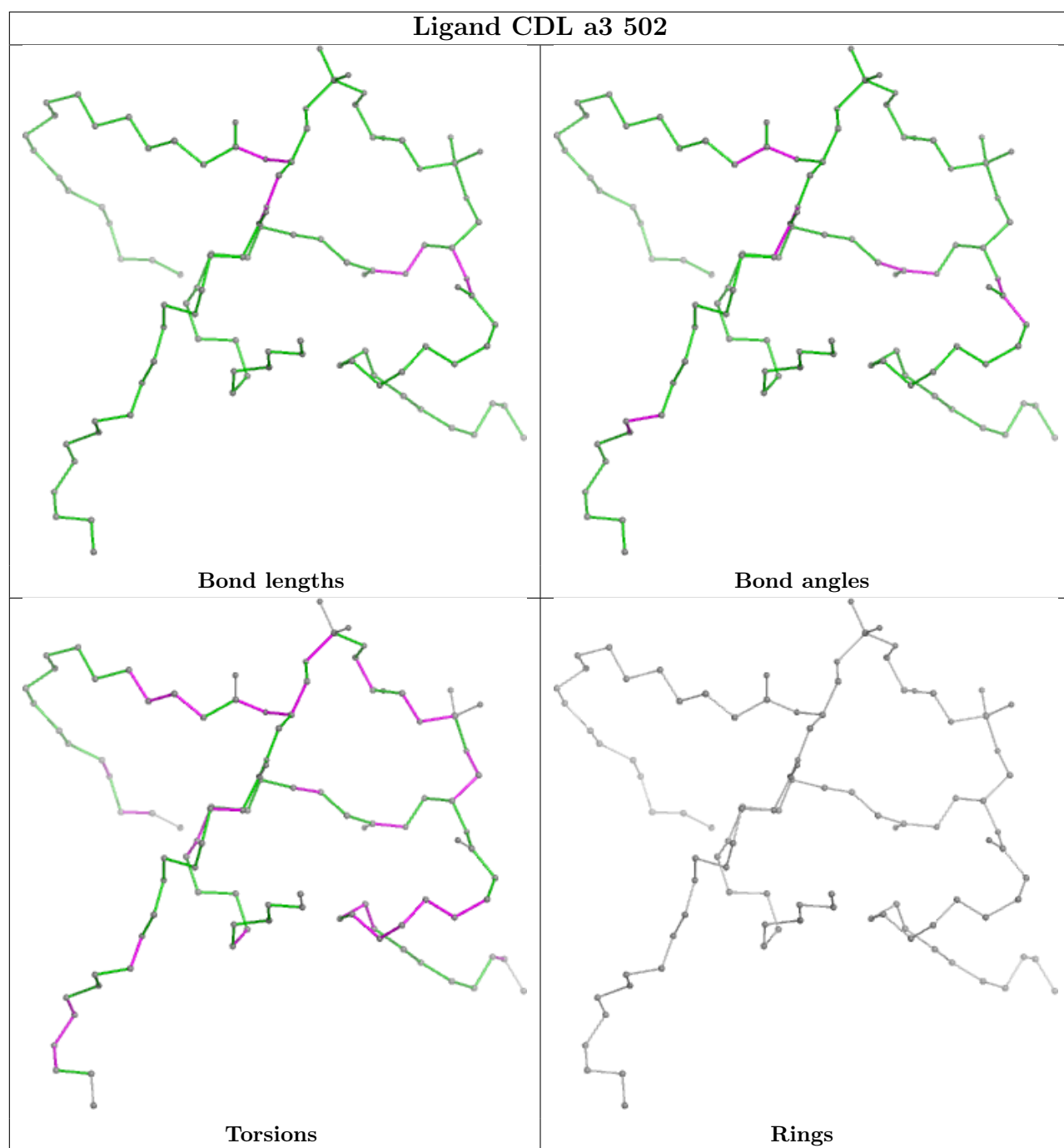


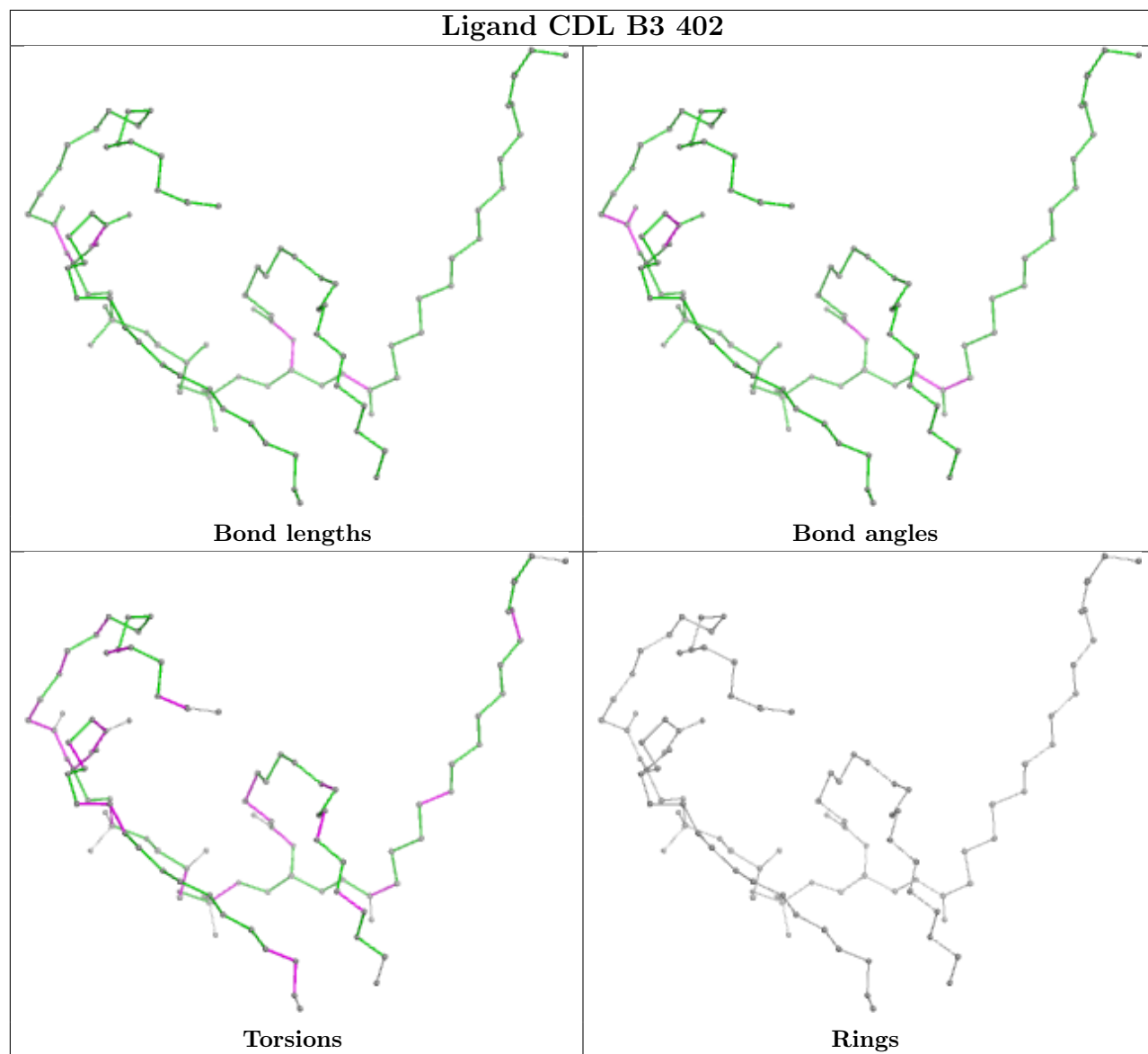




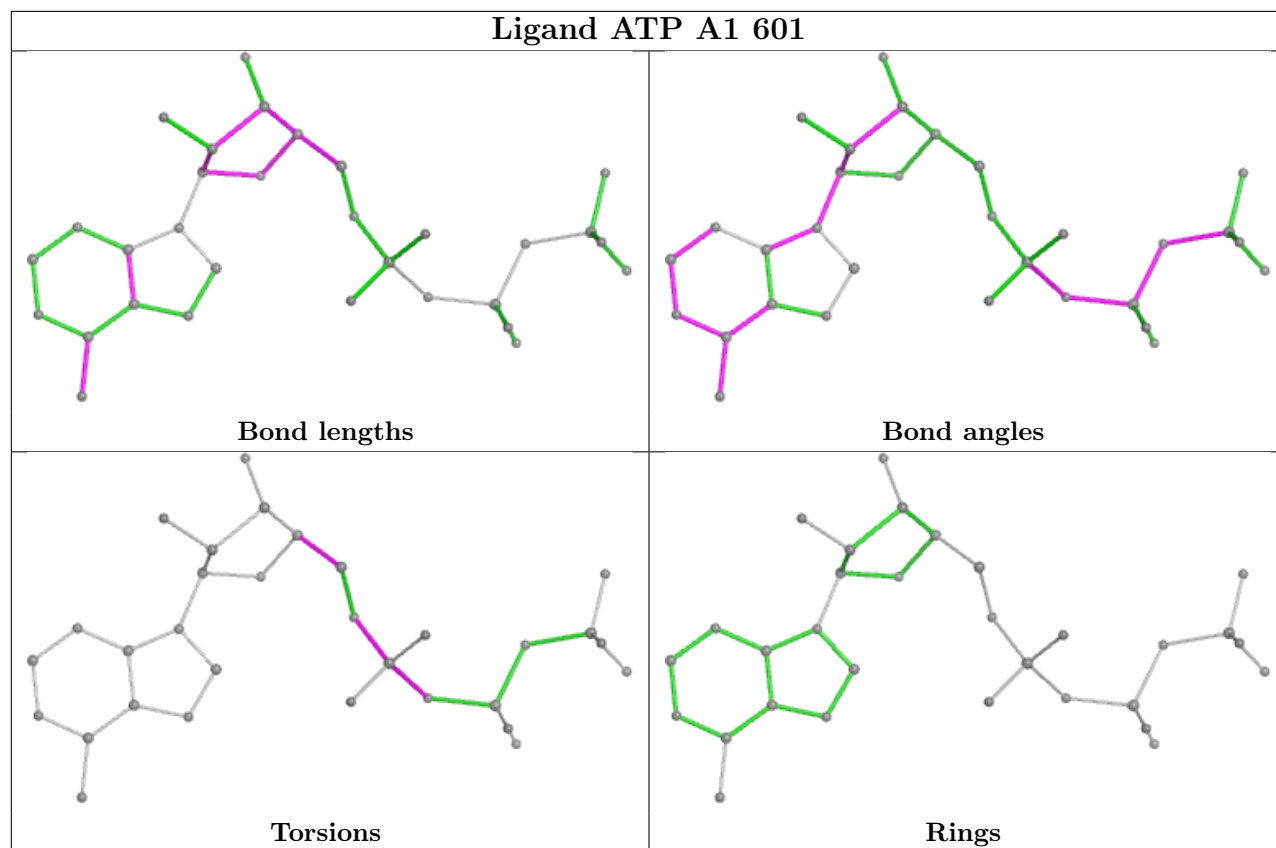




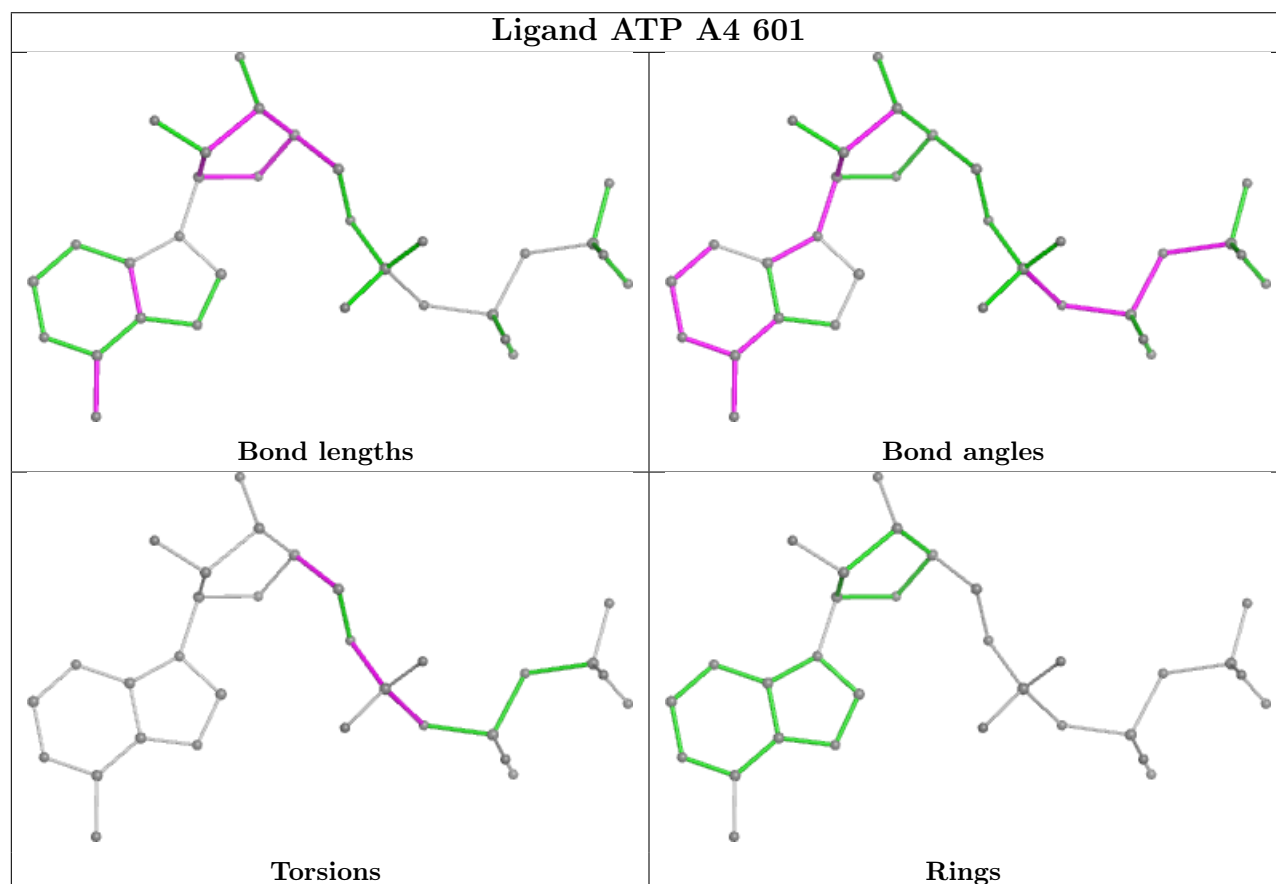


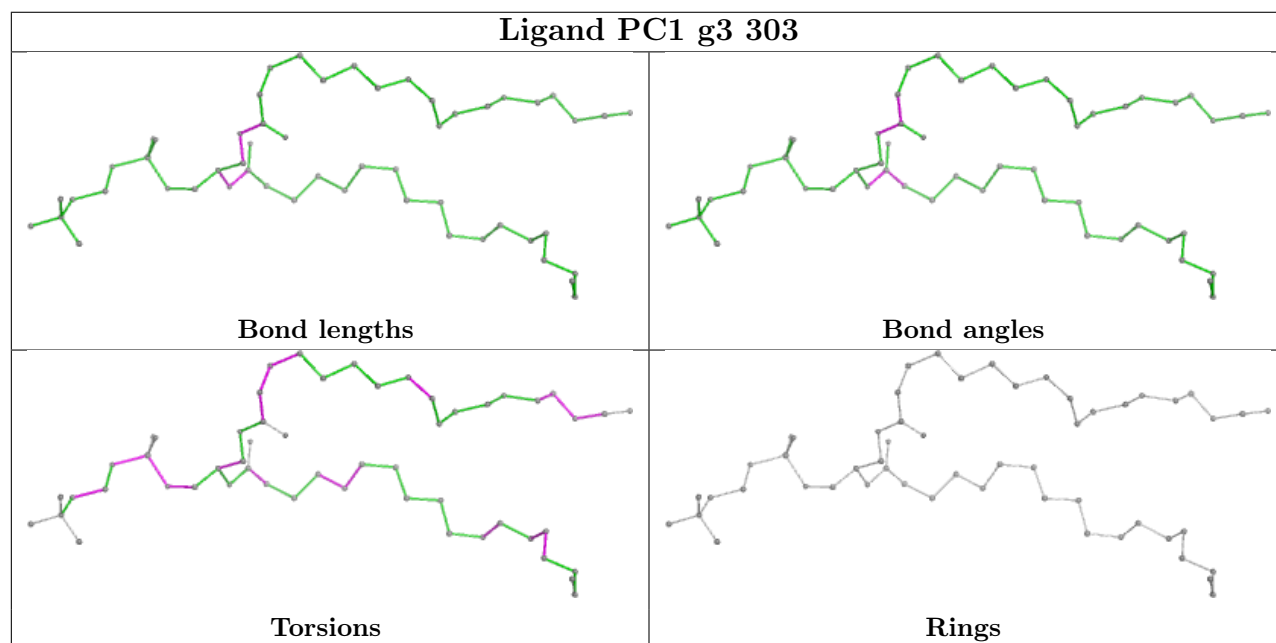
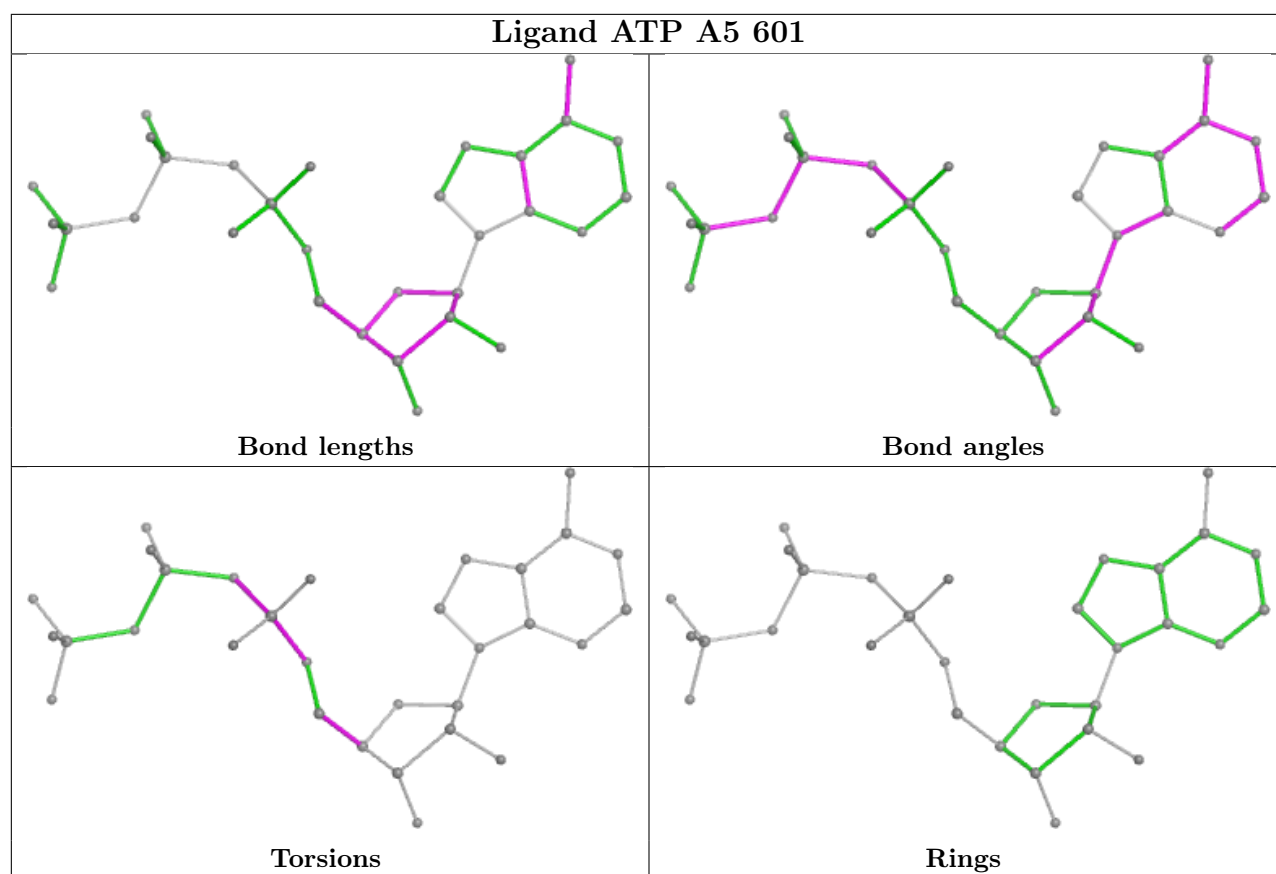


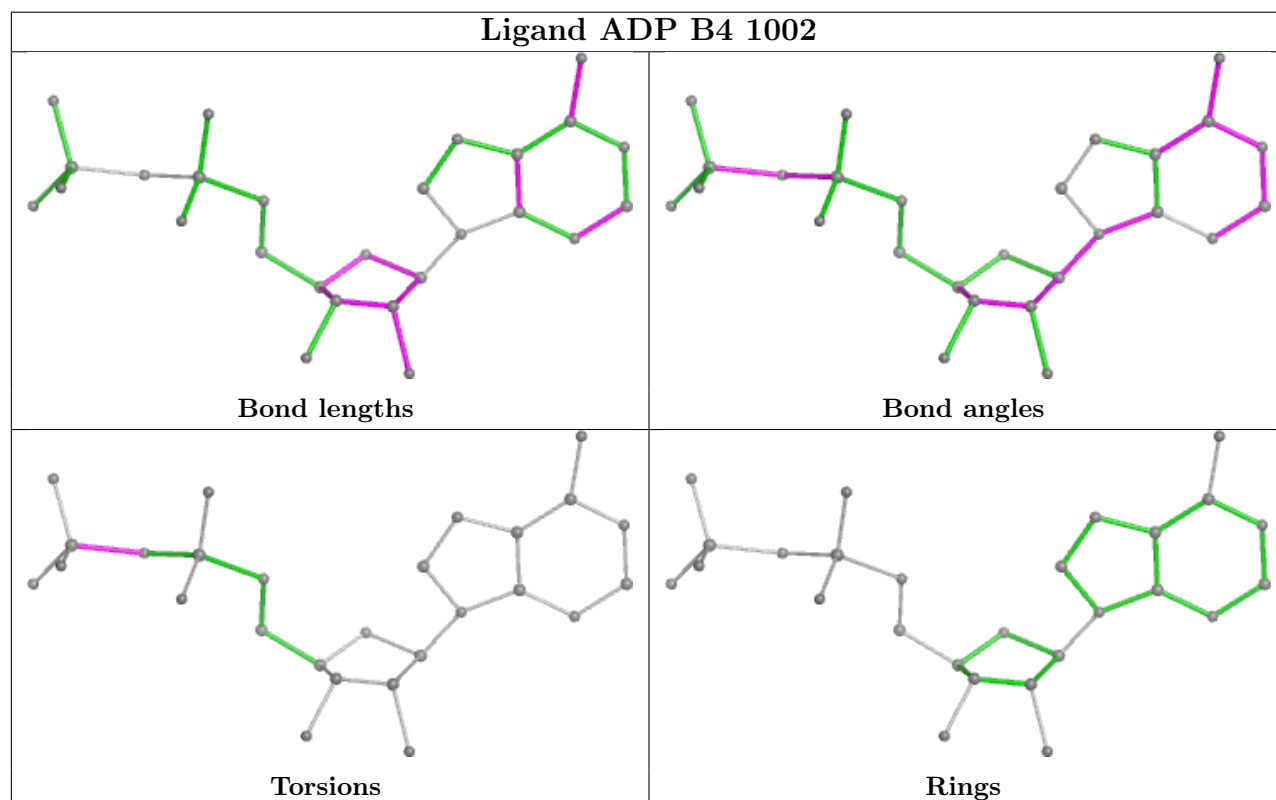
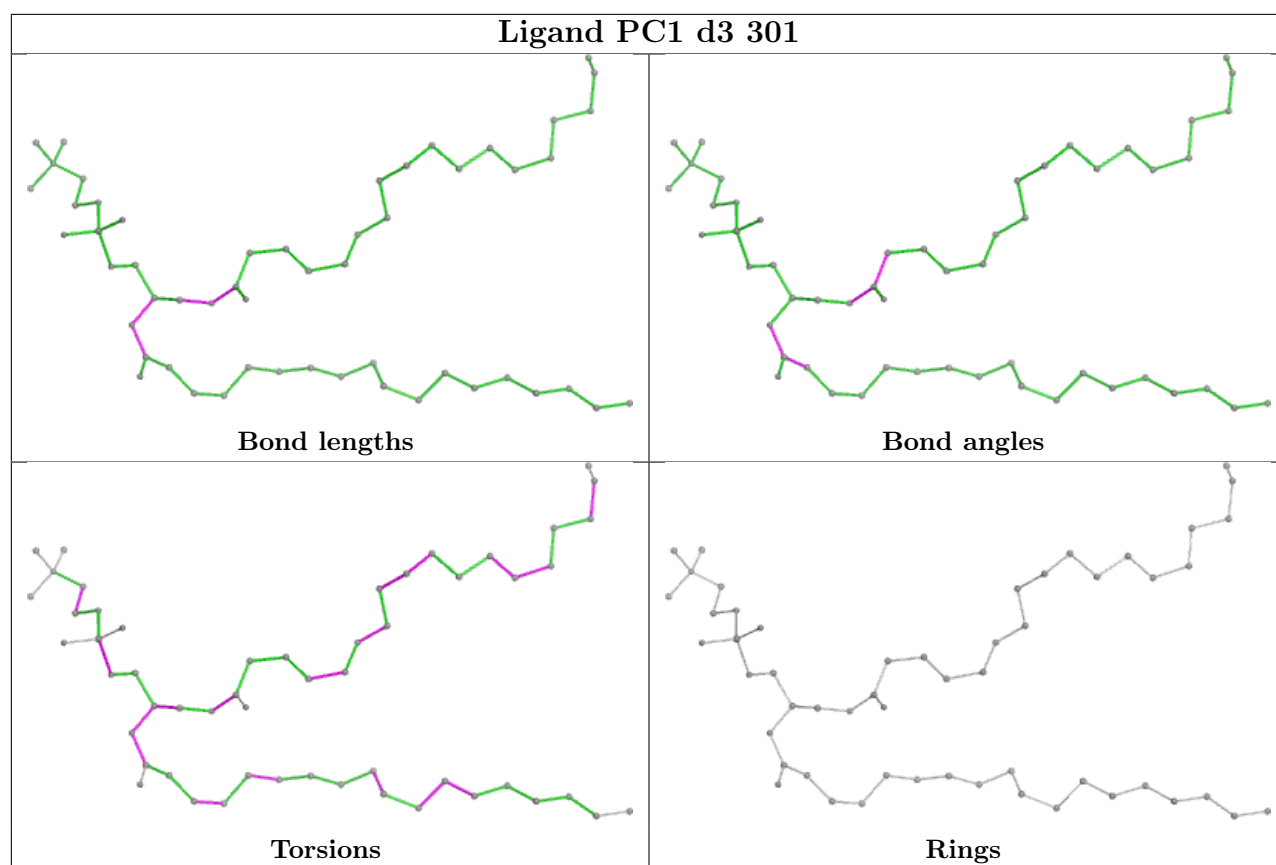
Ligand ATP A1 601

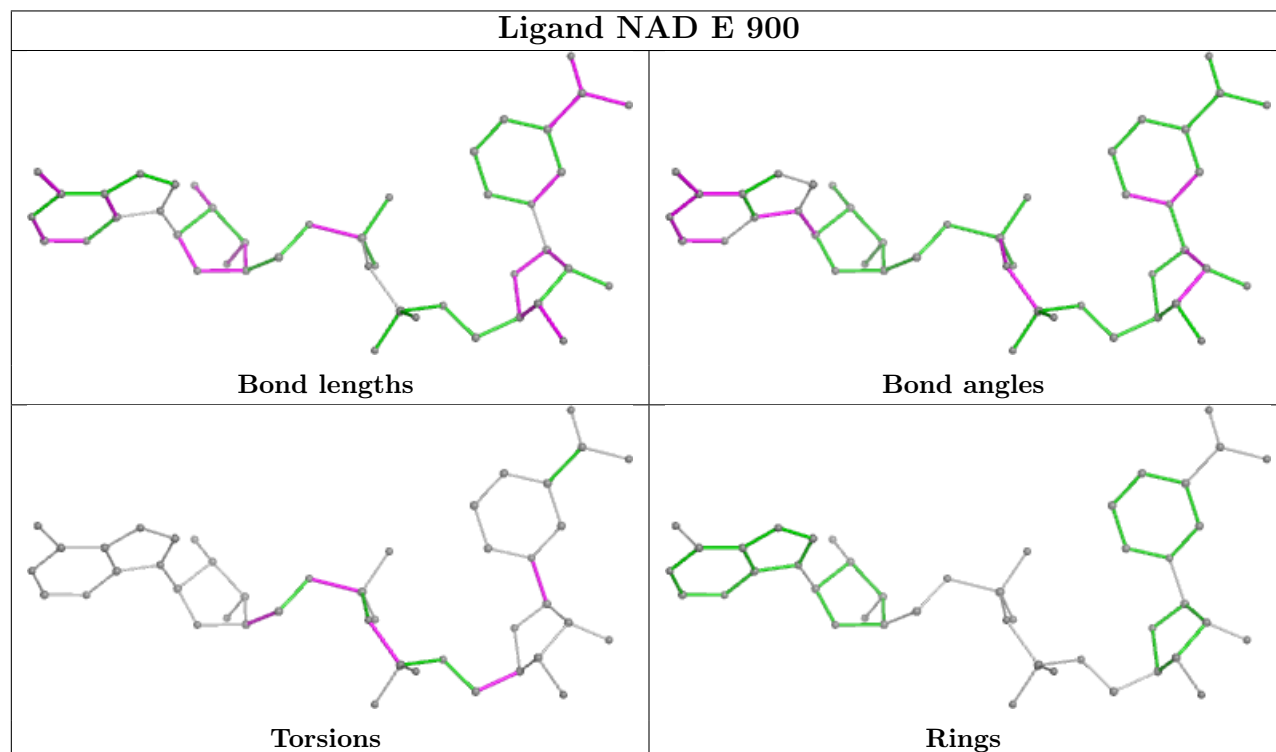
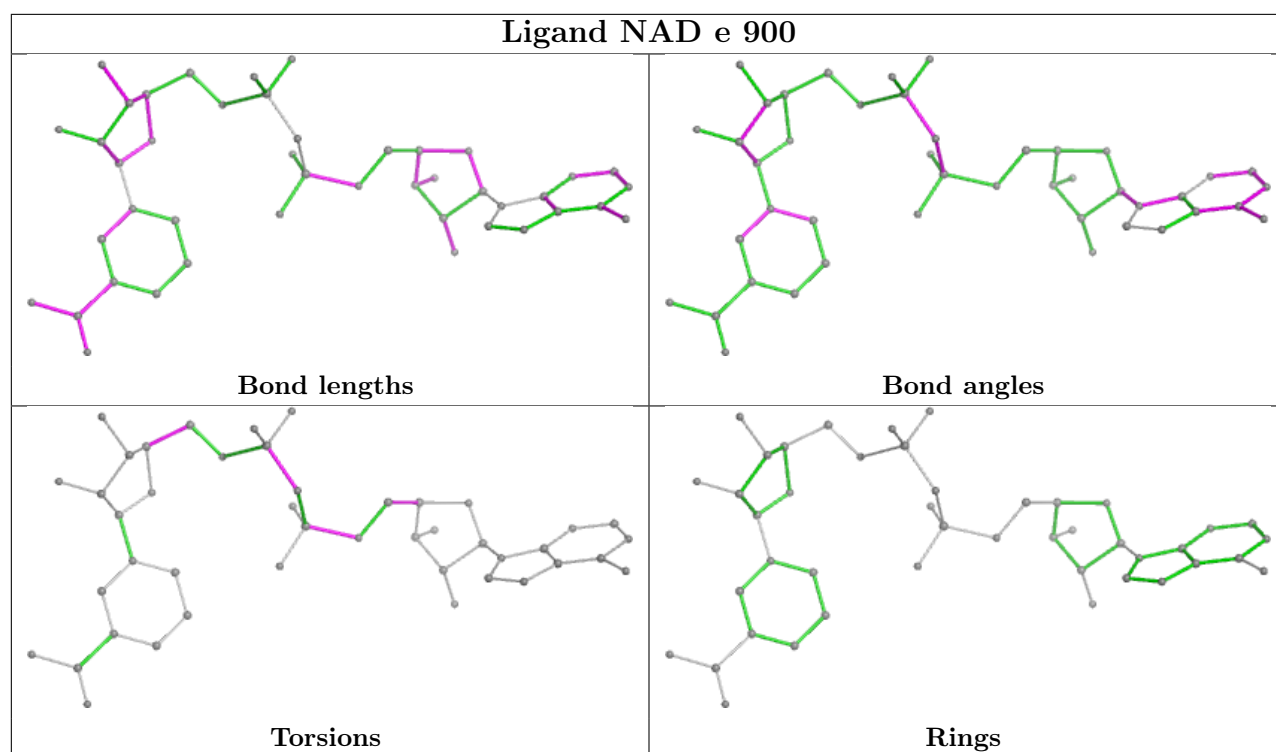


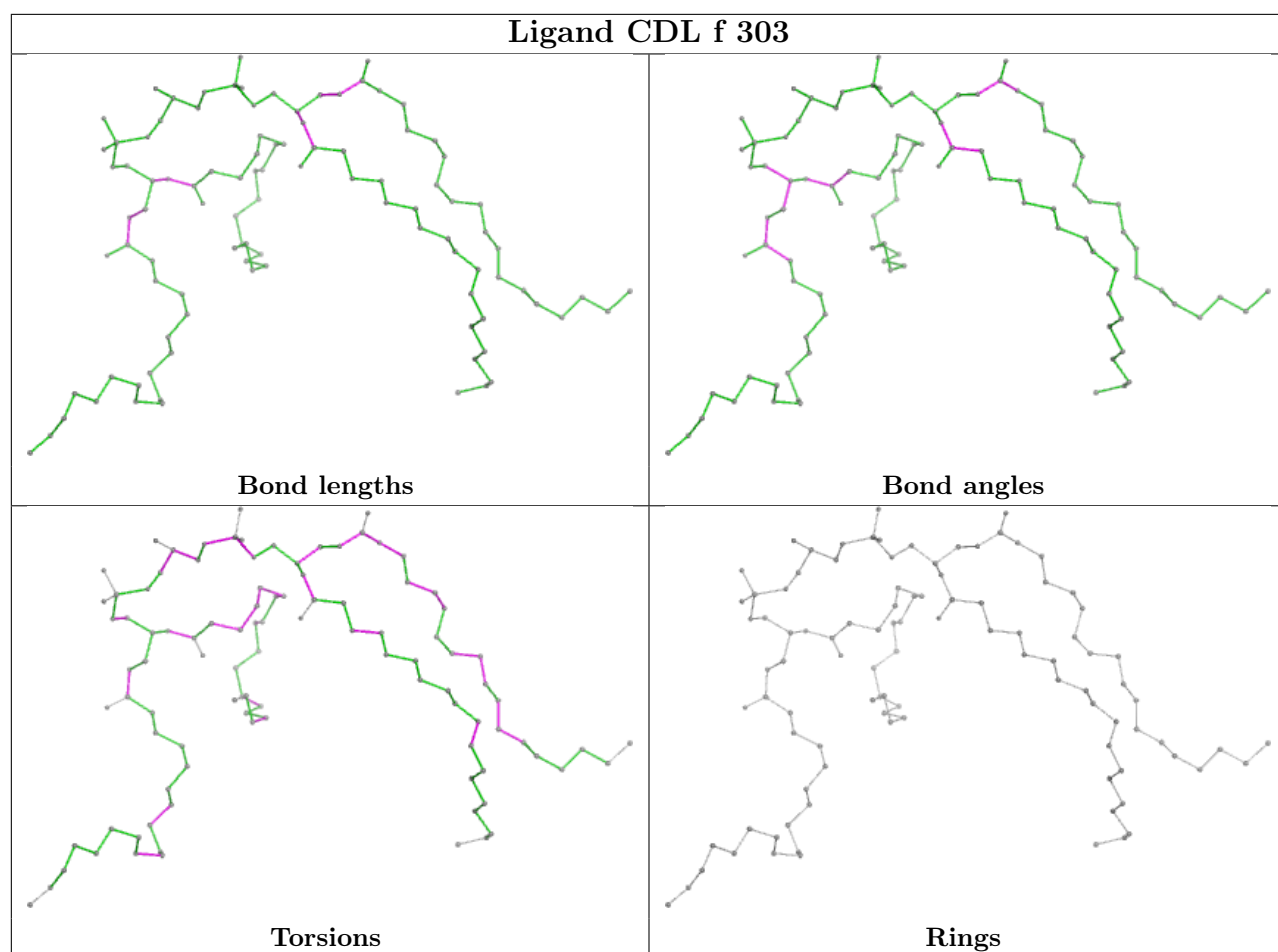
Ligand ATP A4 601

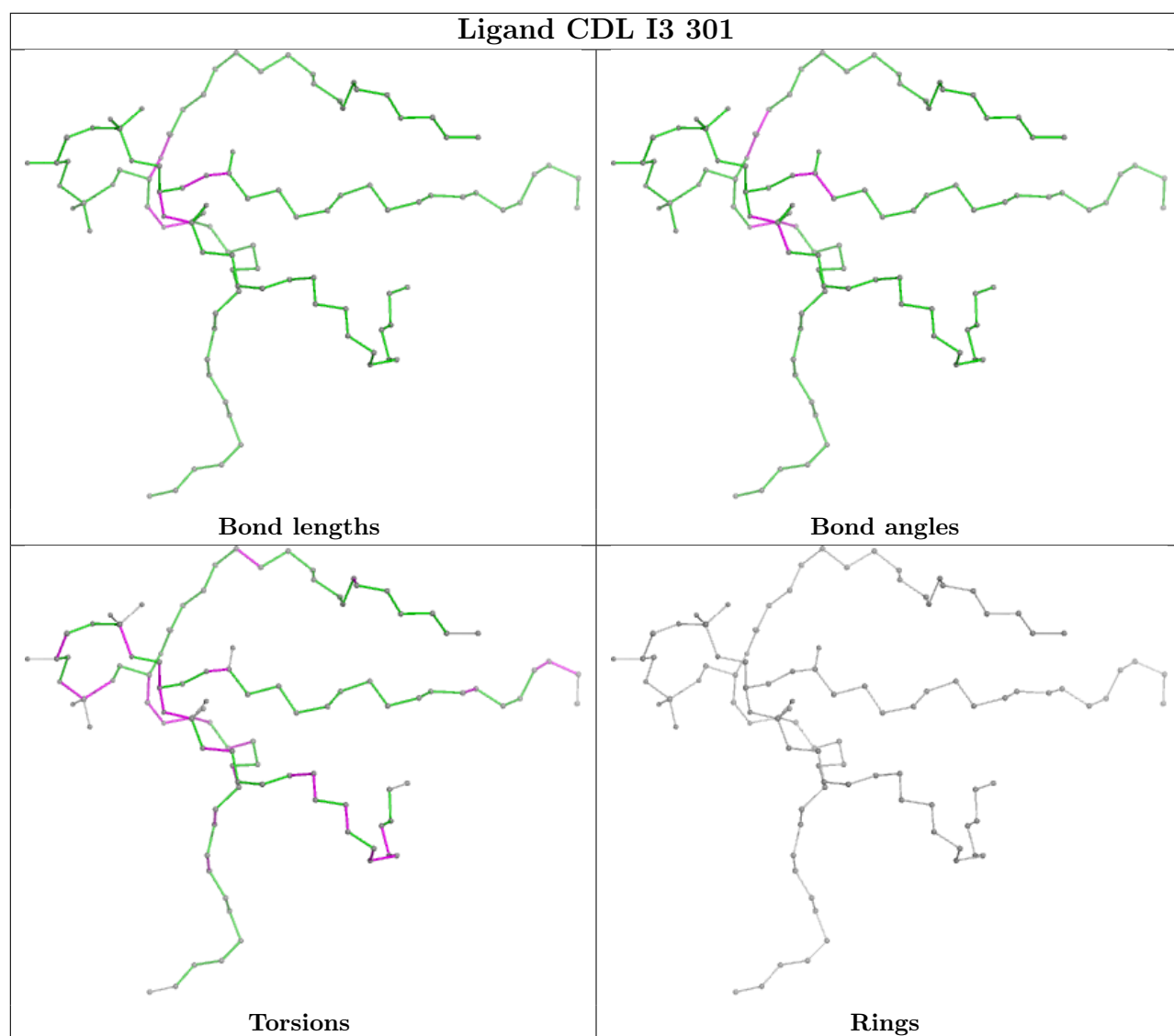


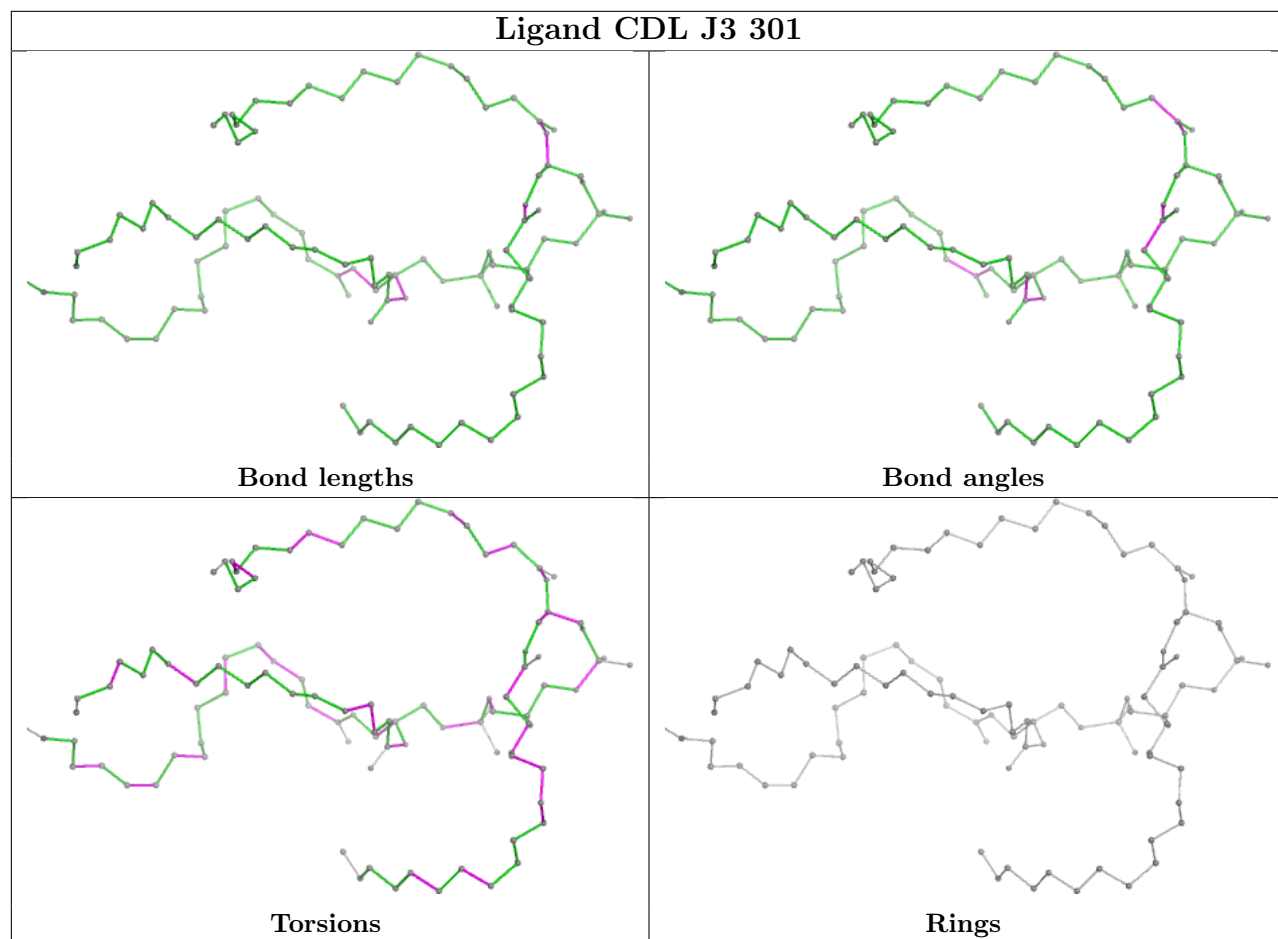


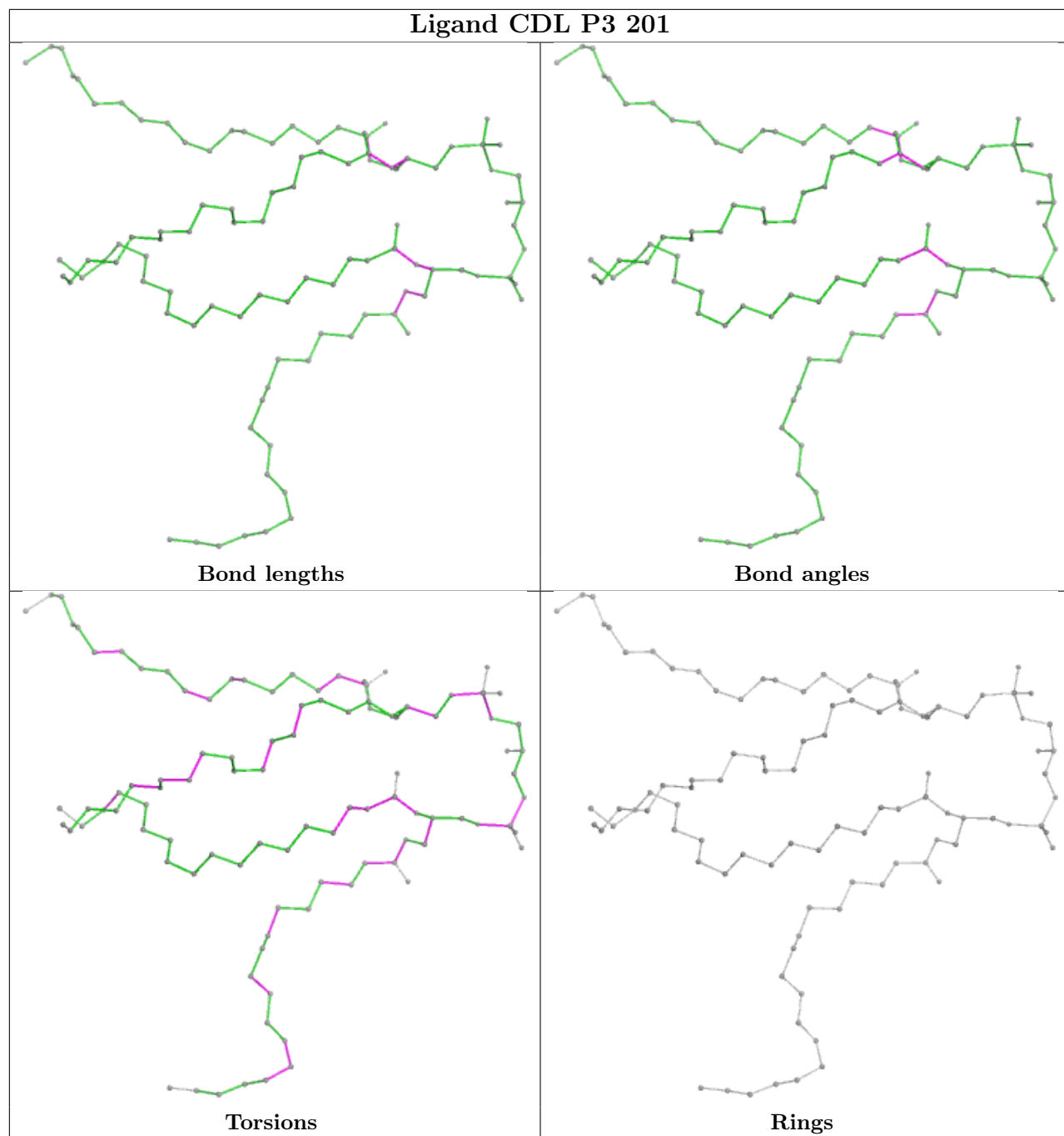




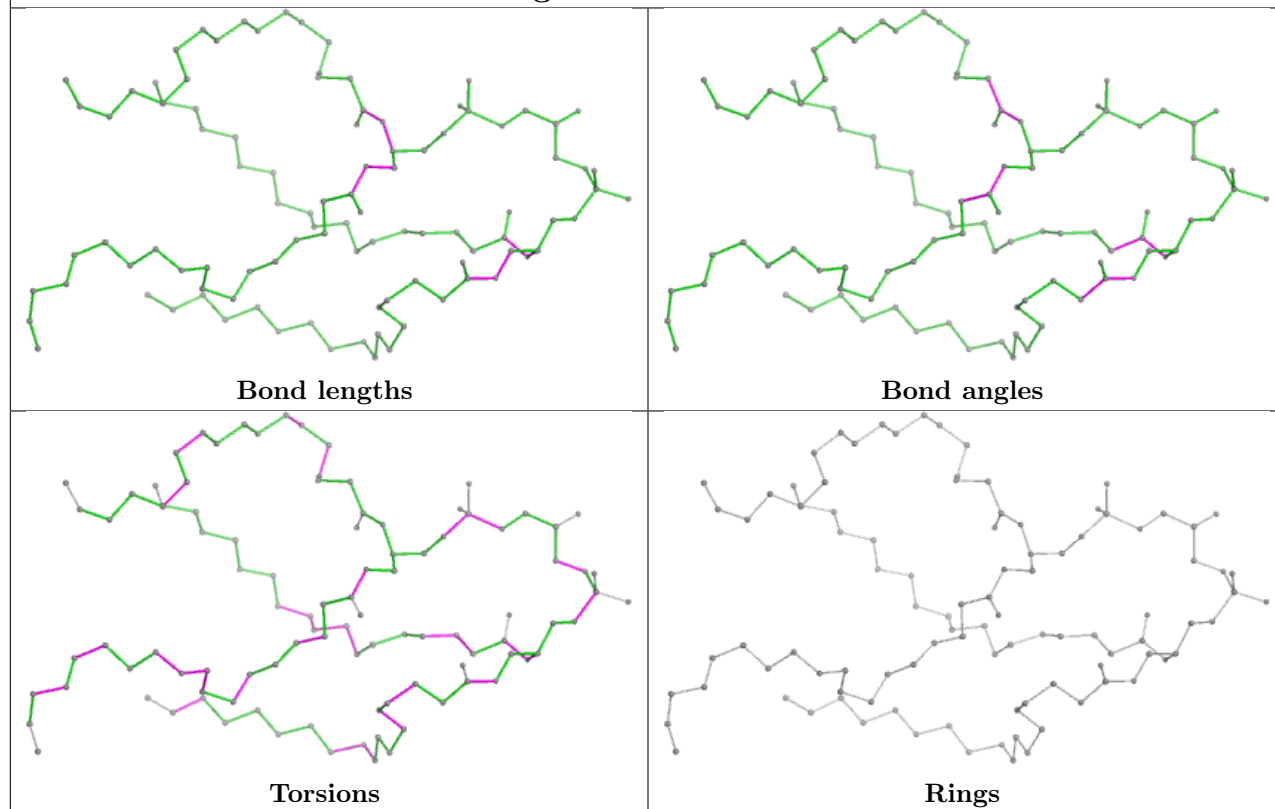




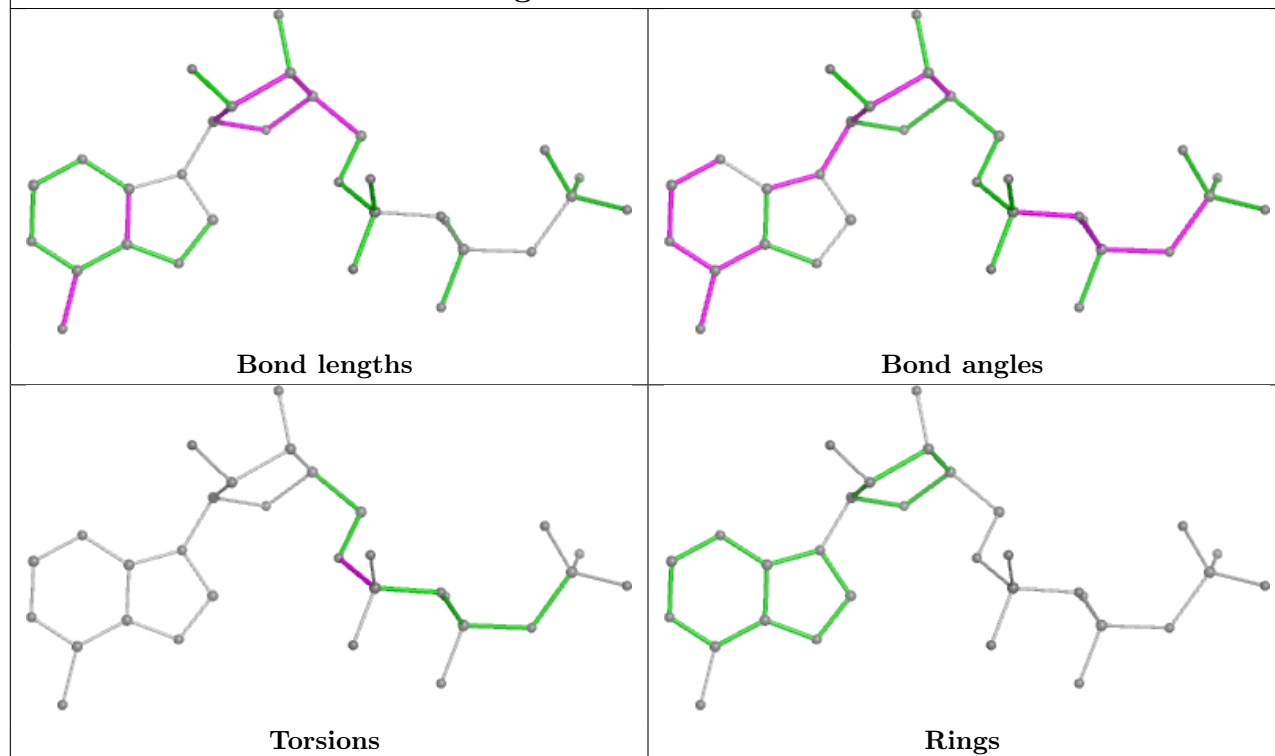


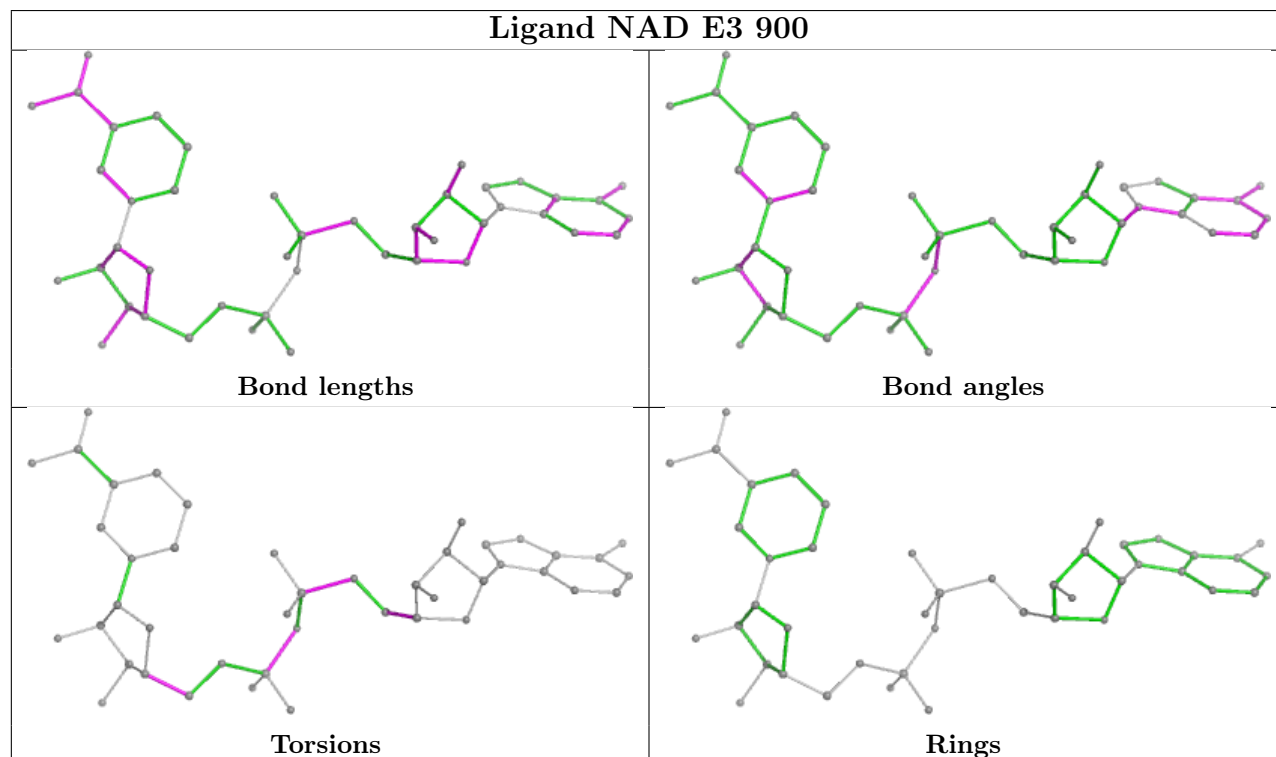
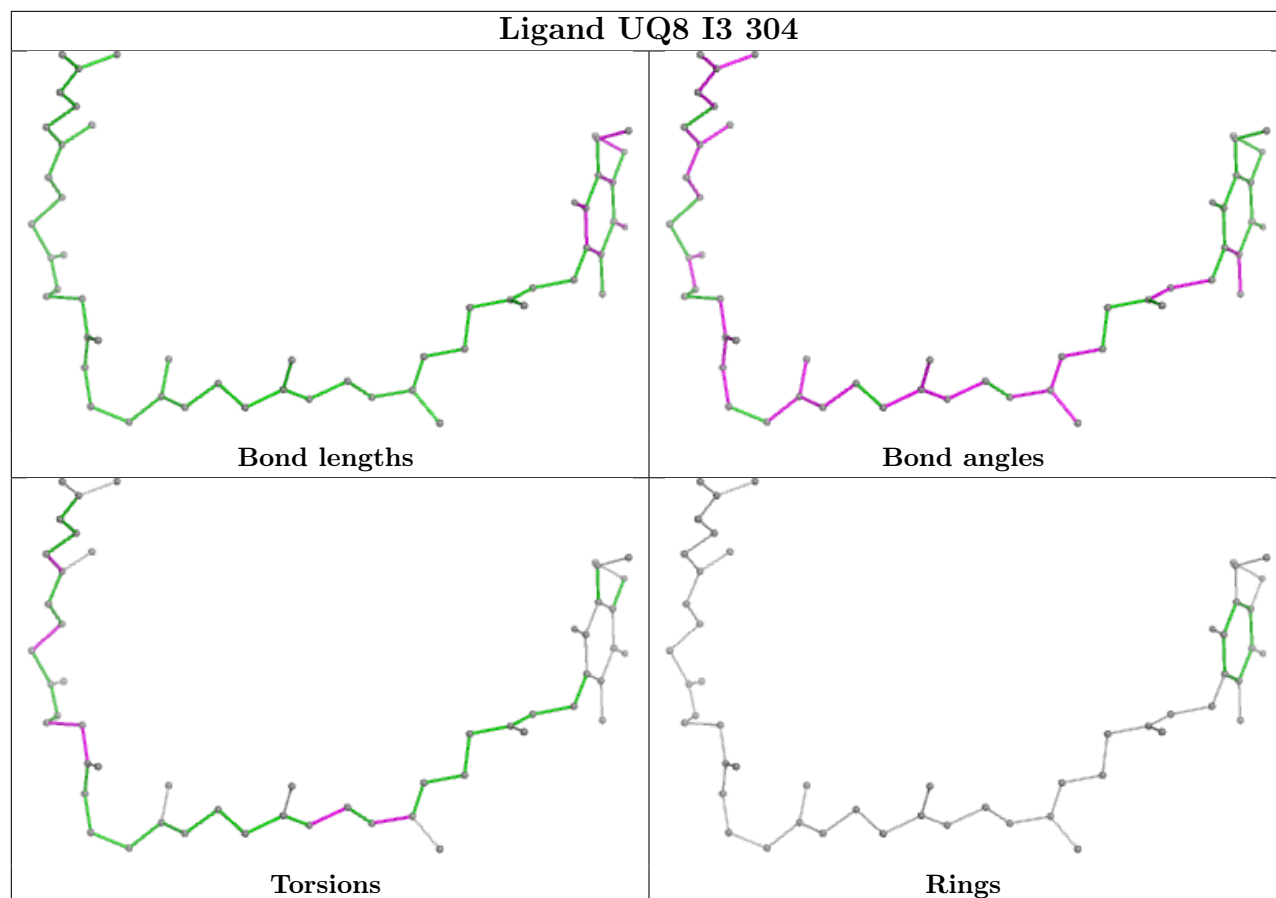


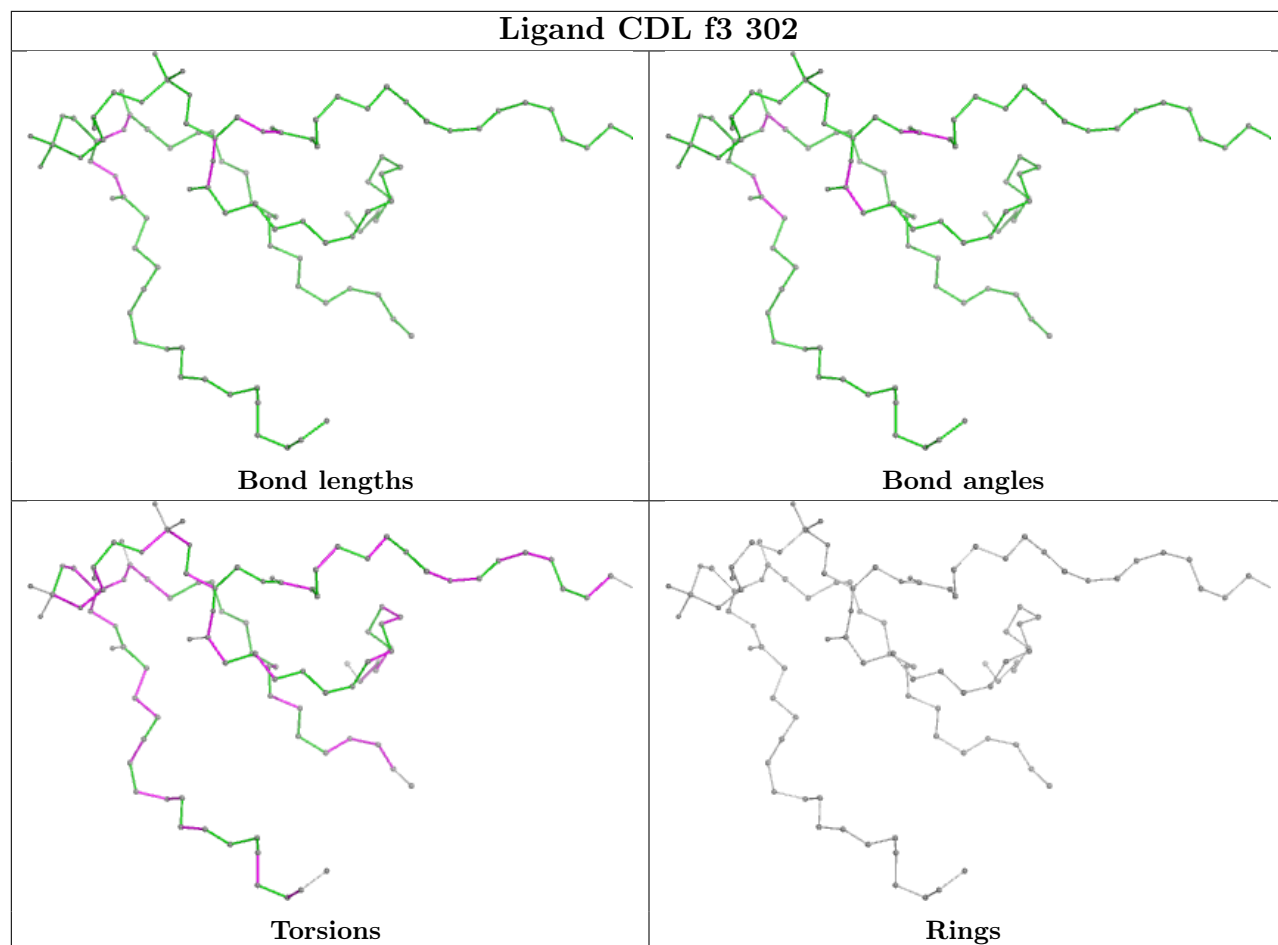
Ligand CDL L 301

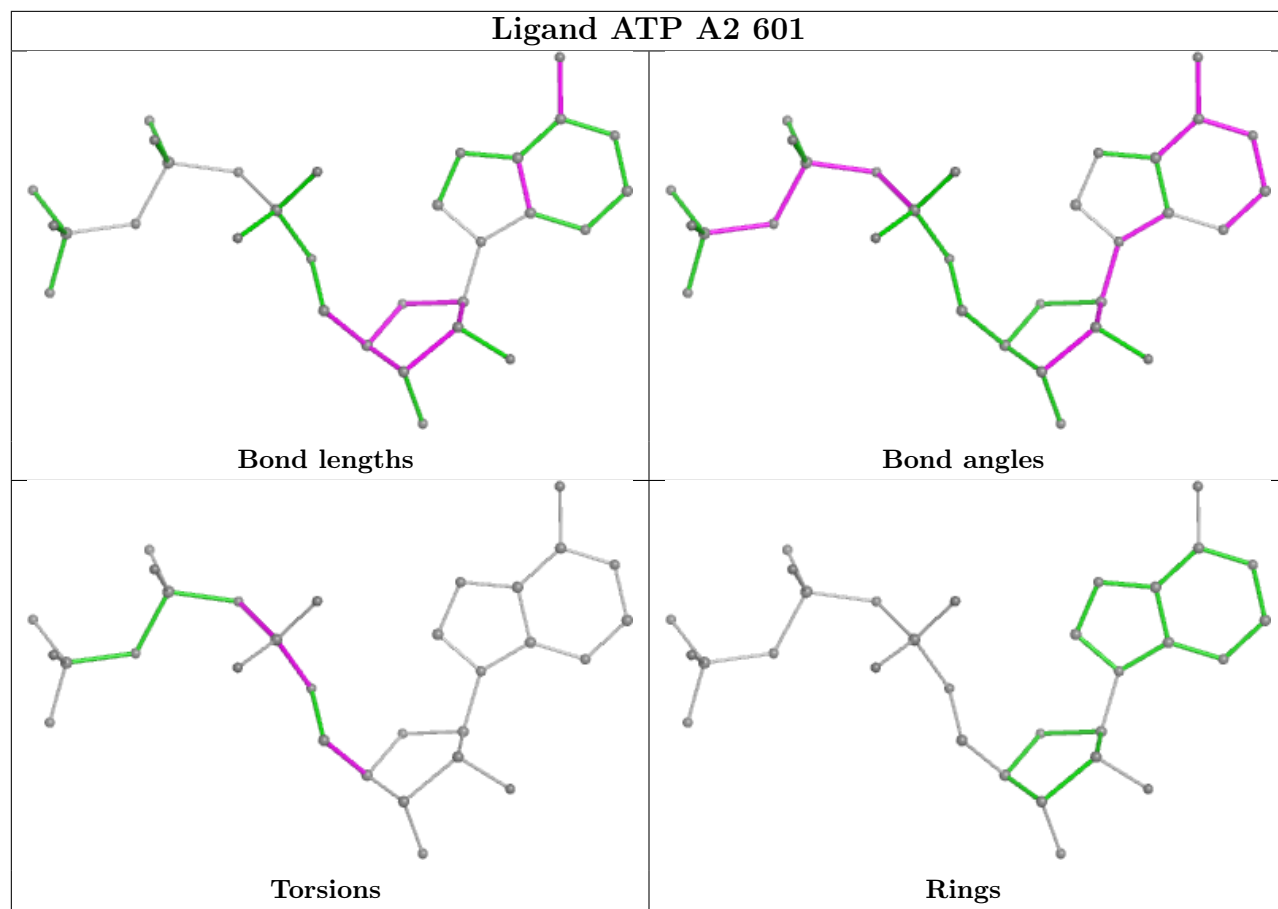


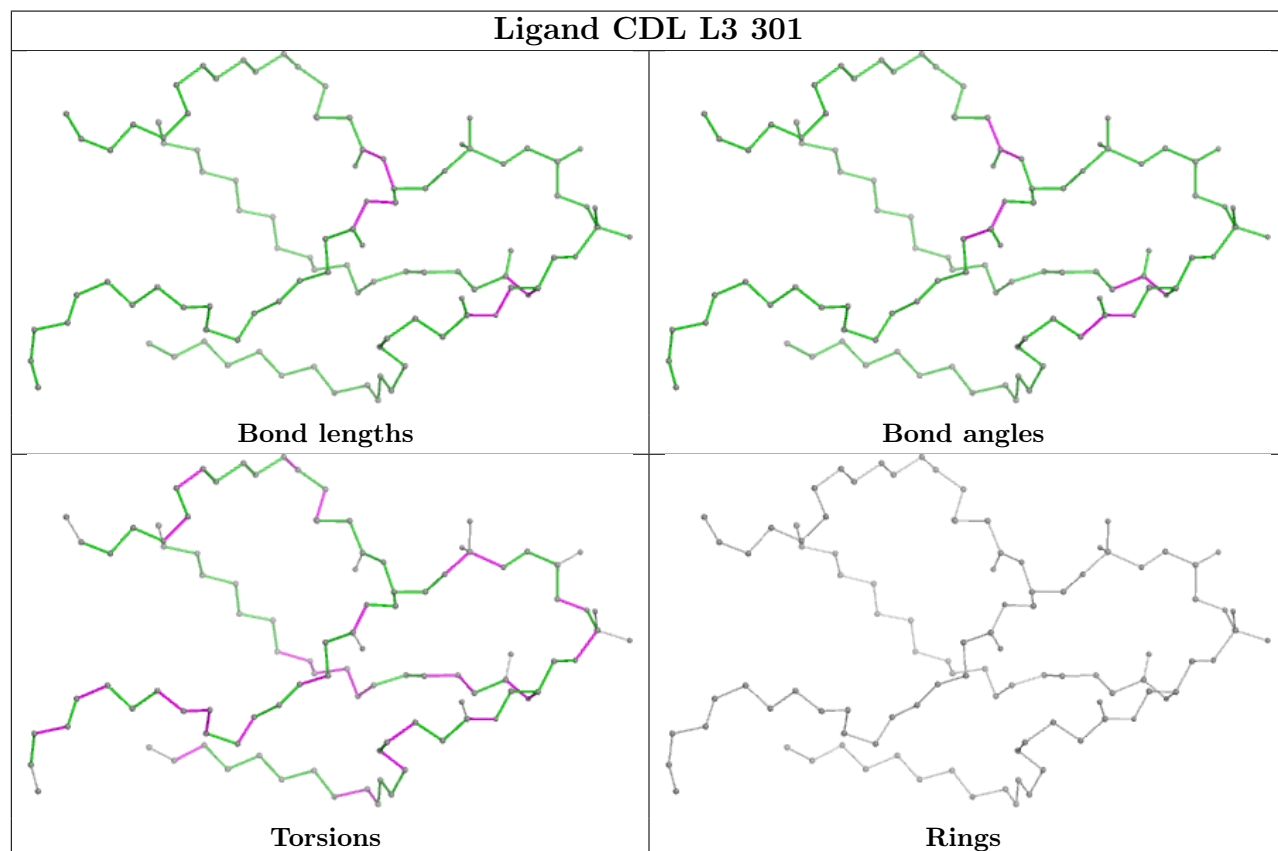
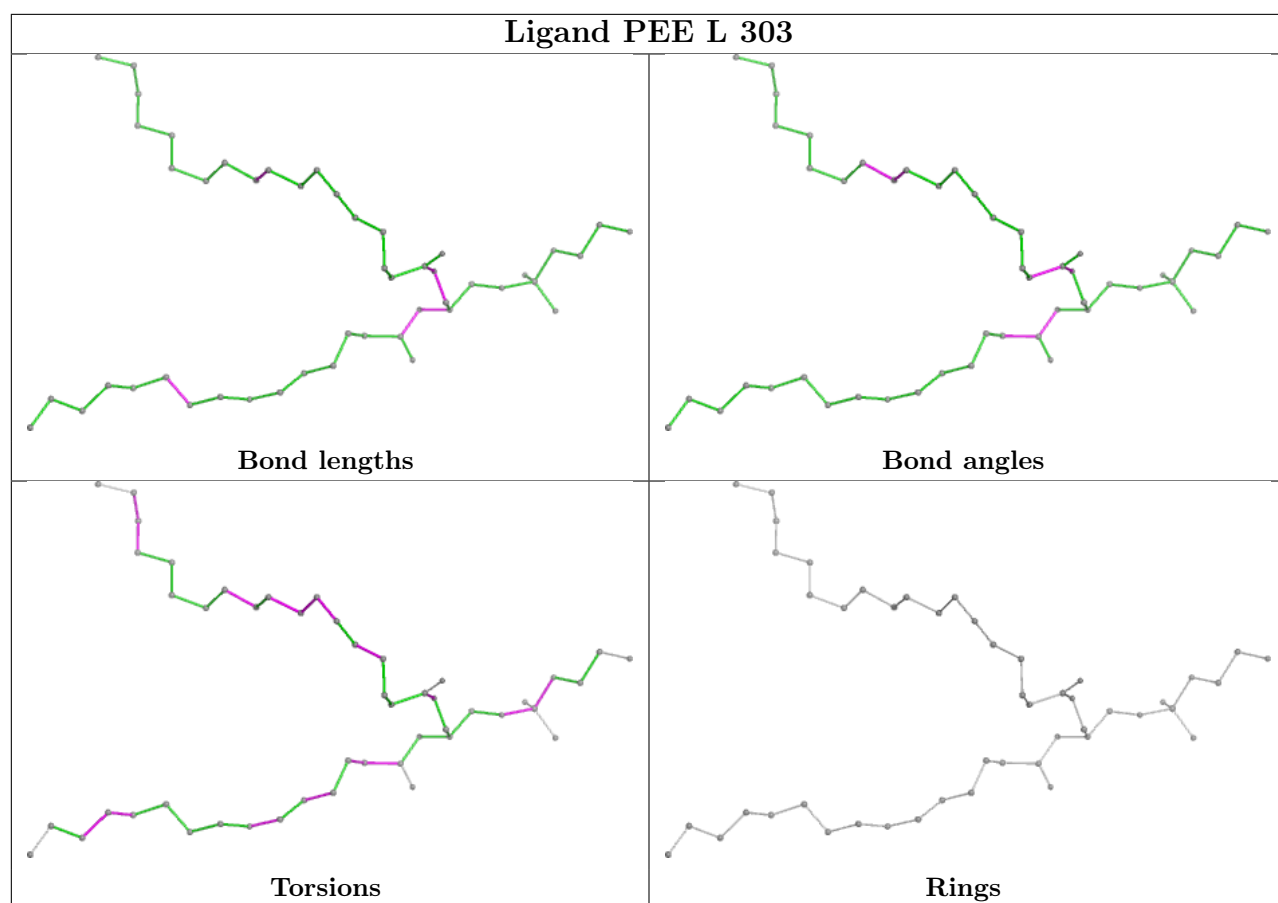
Ligand ATP B2 1003

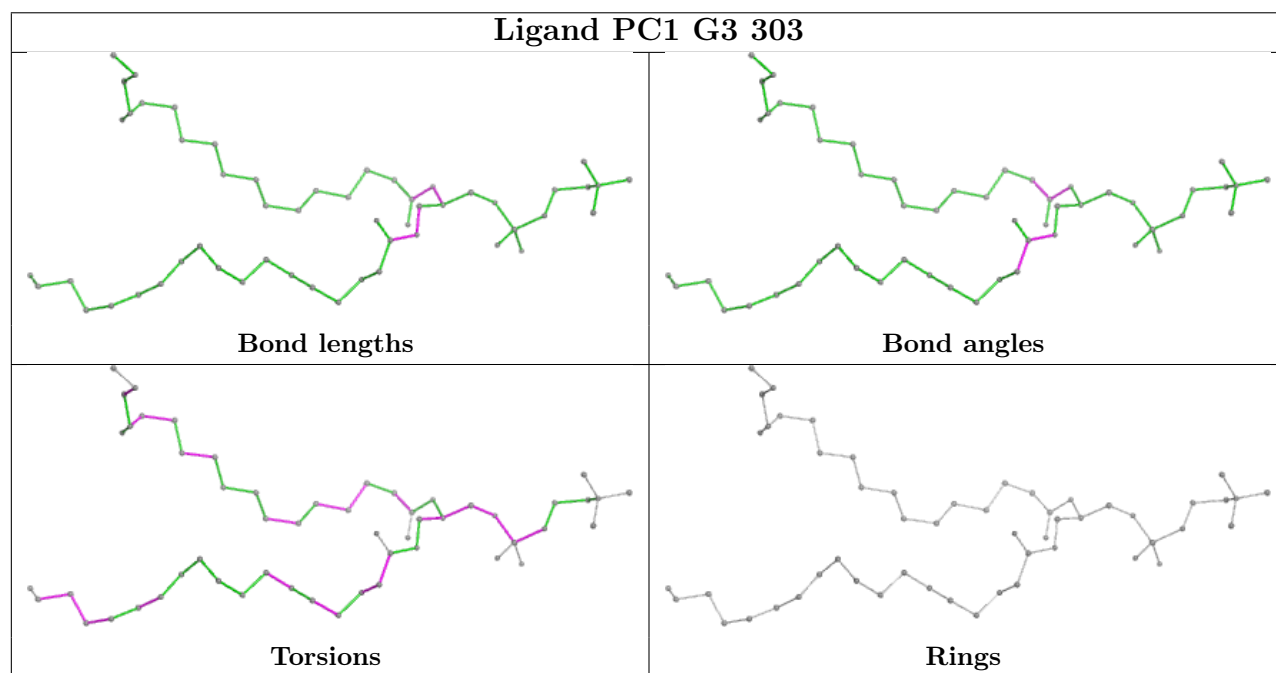
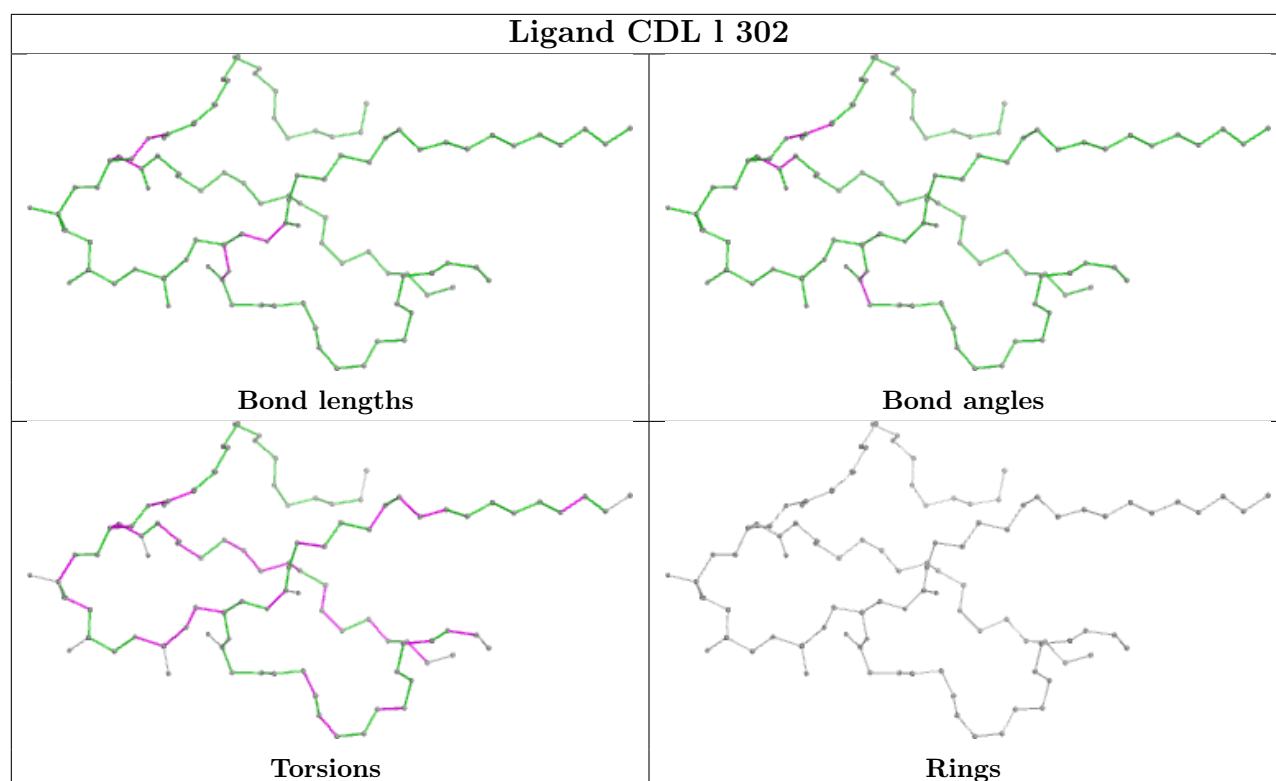


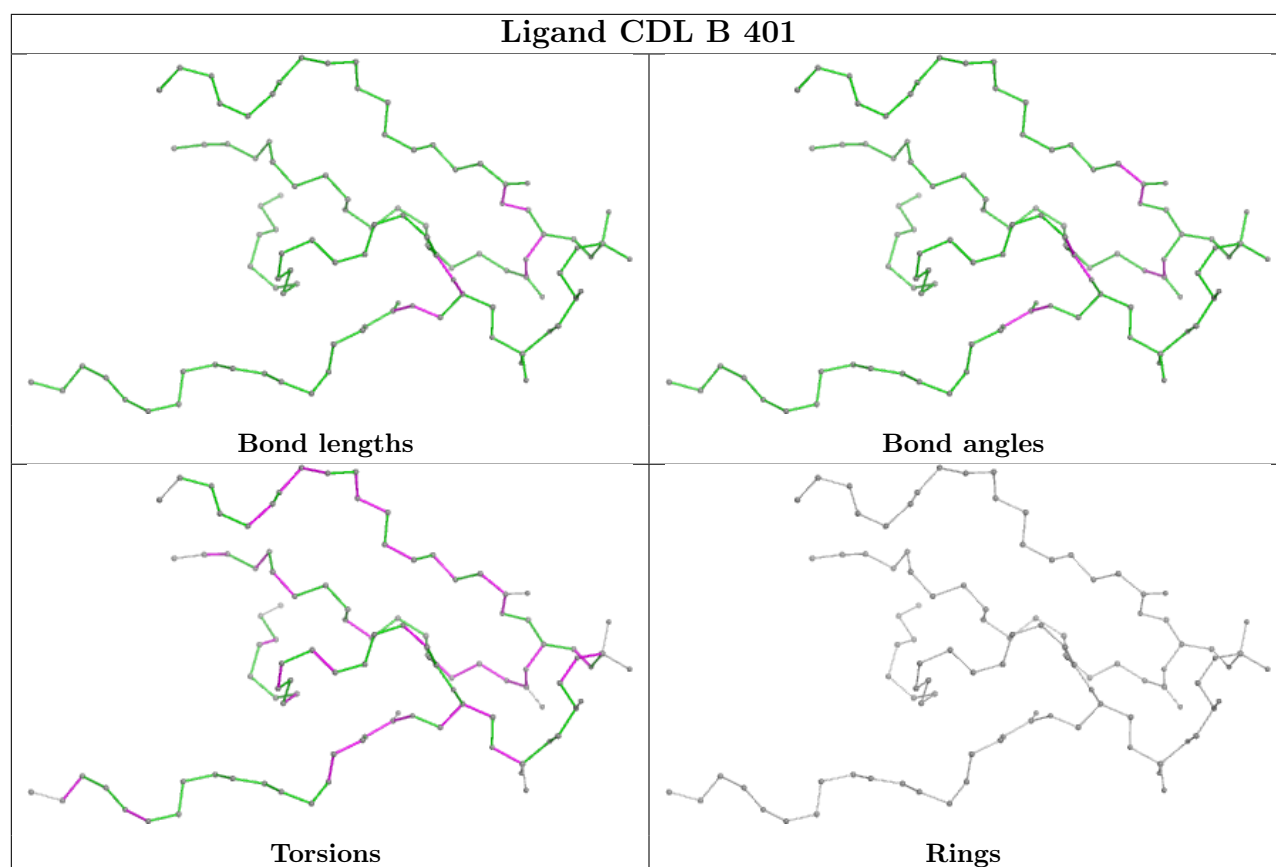


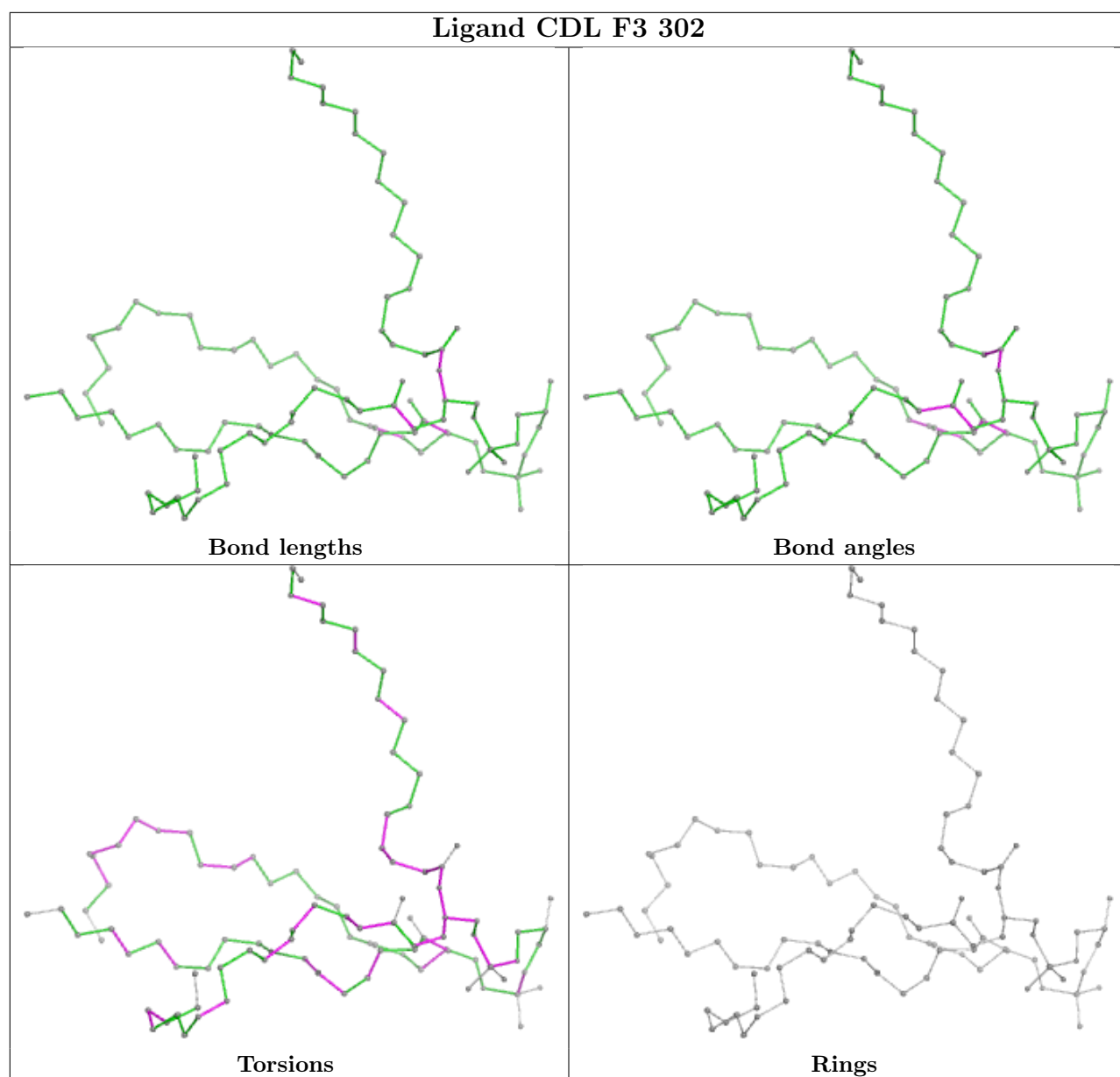


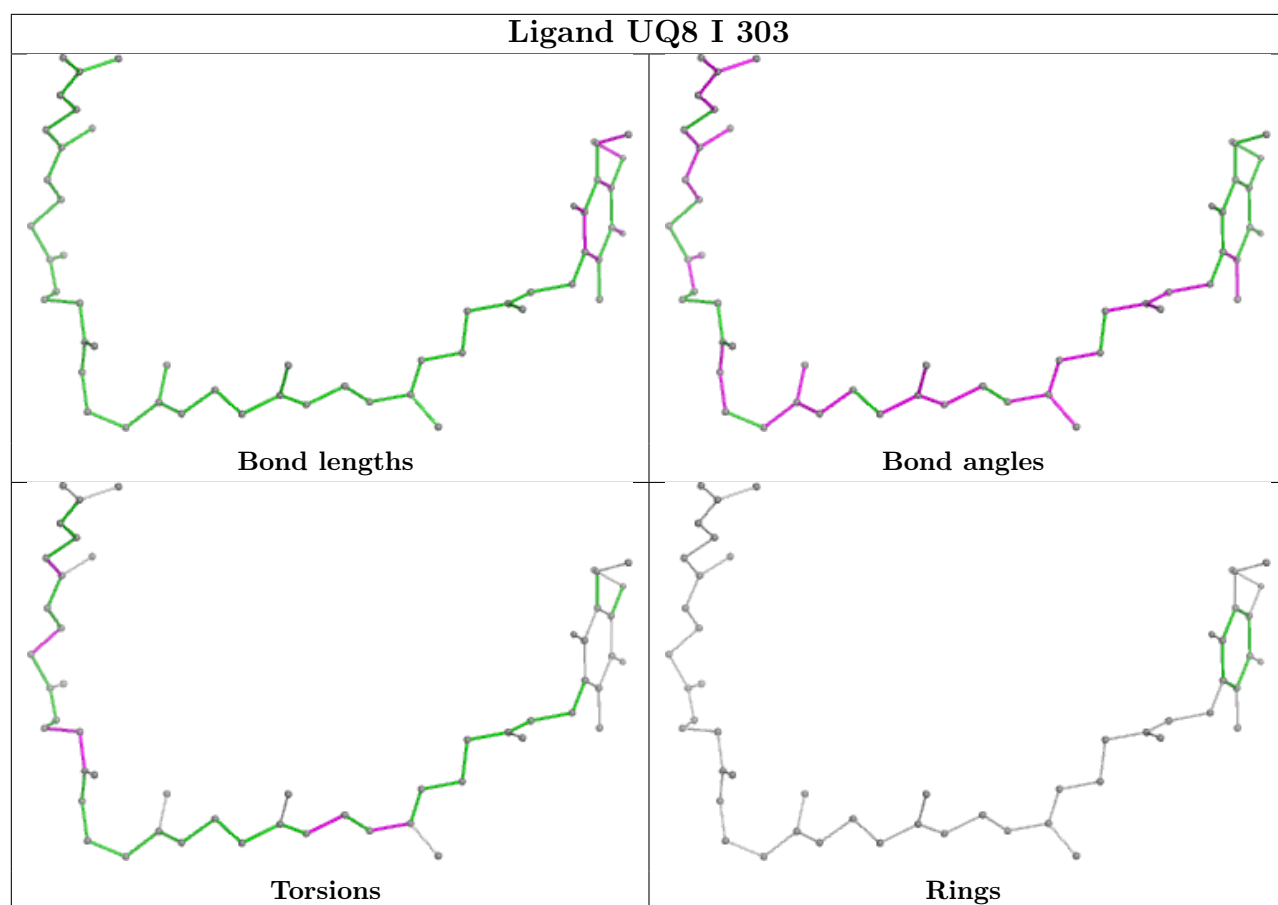


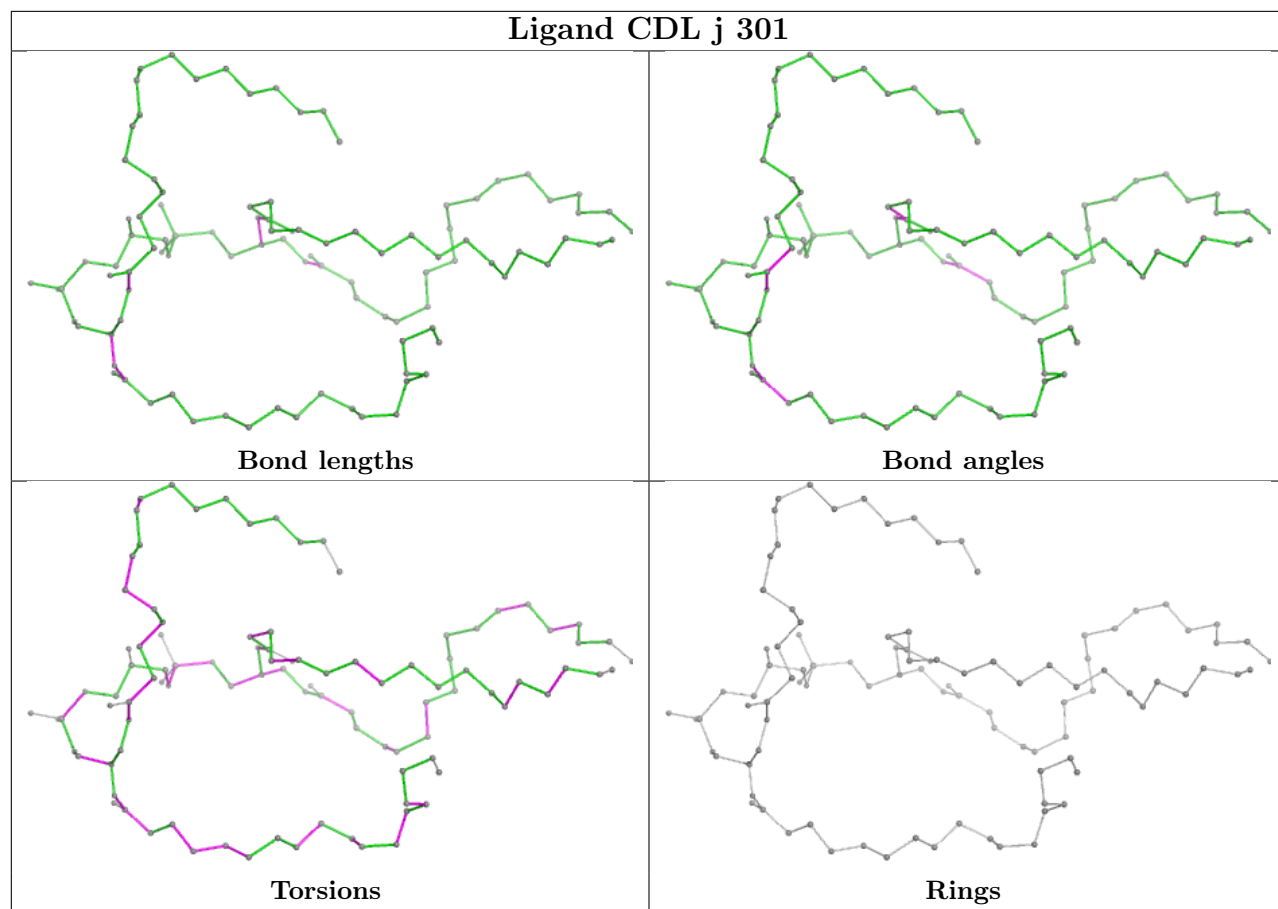


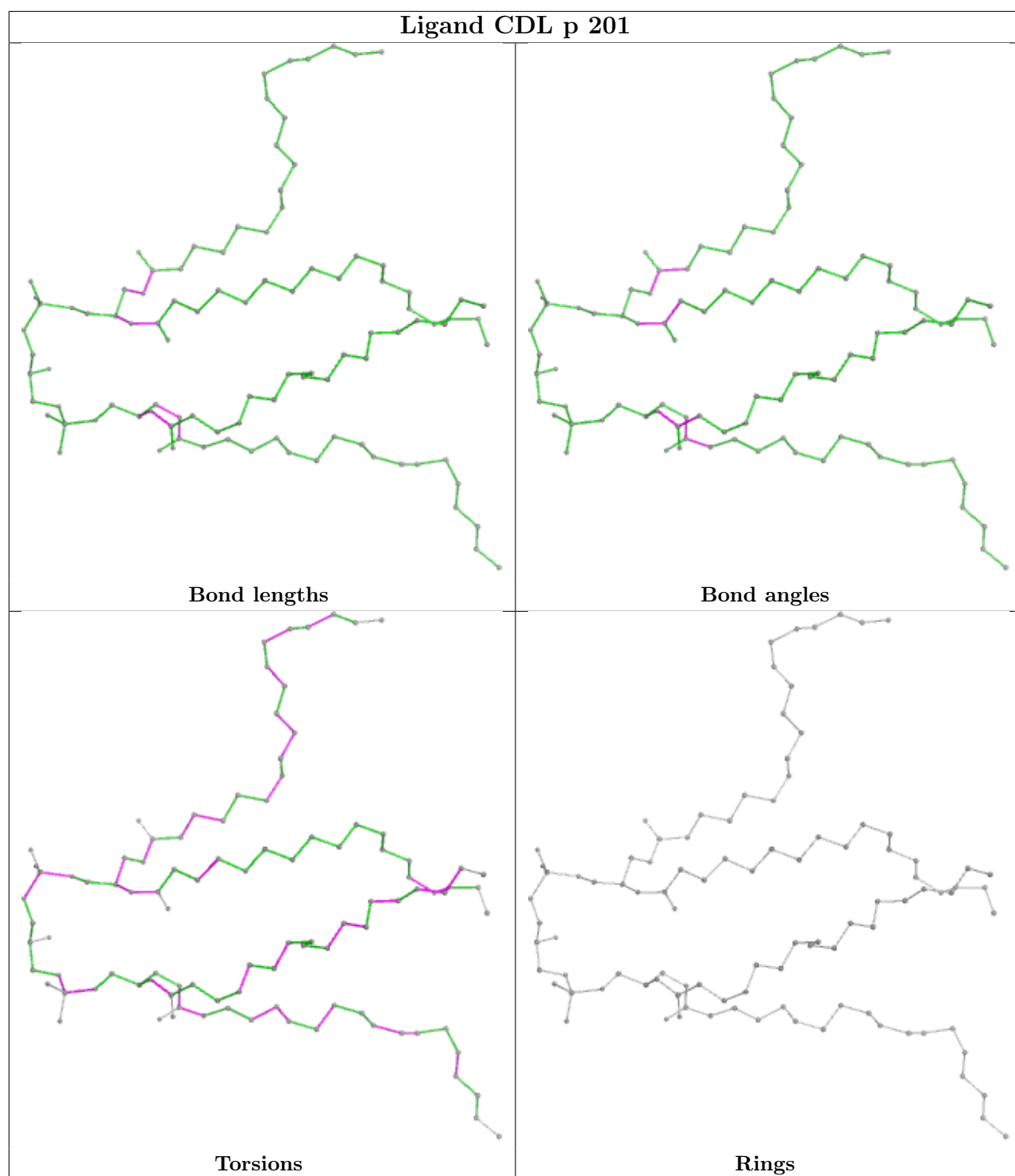


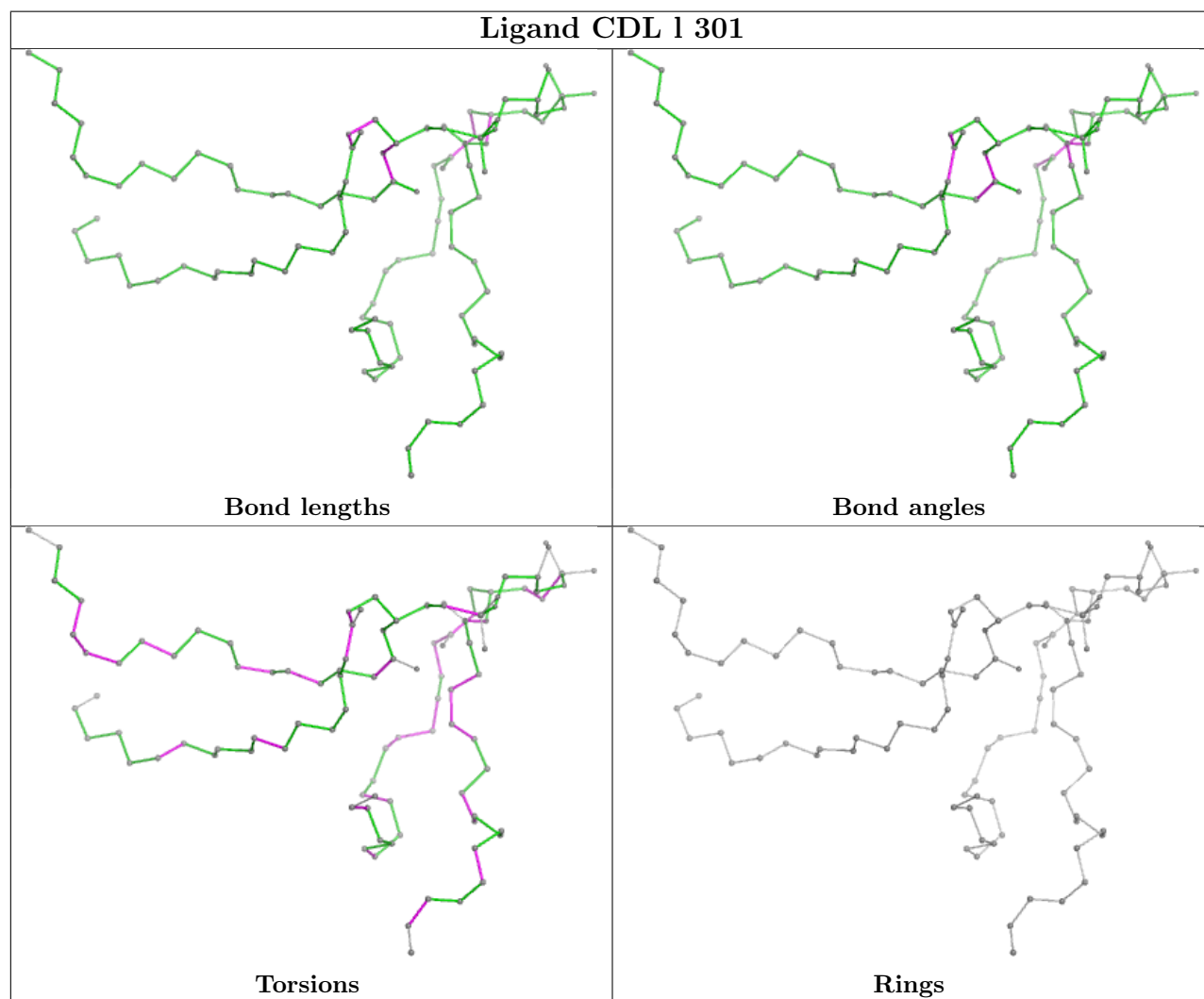
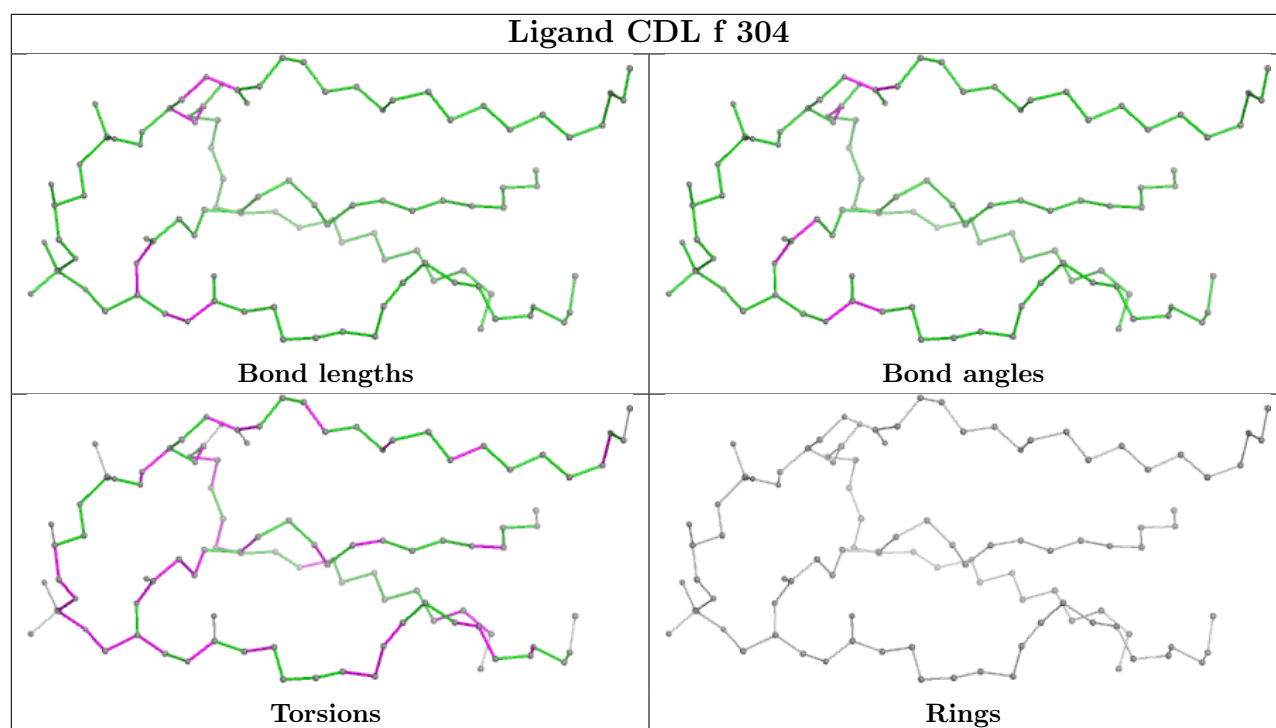


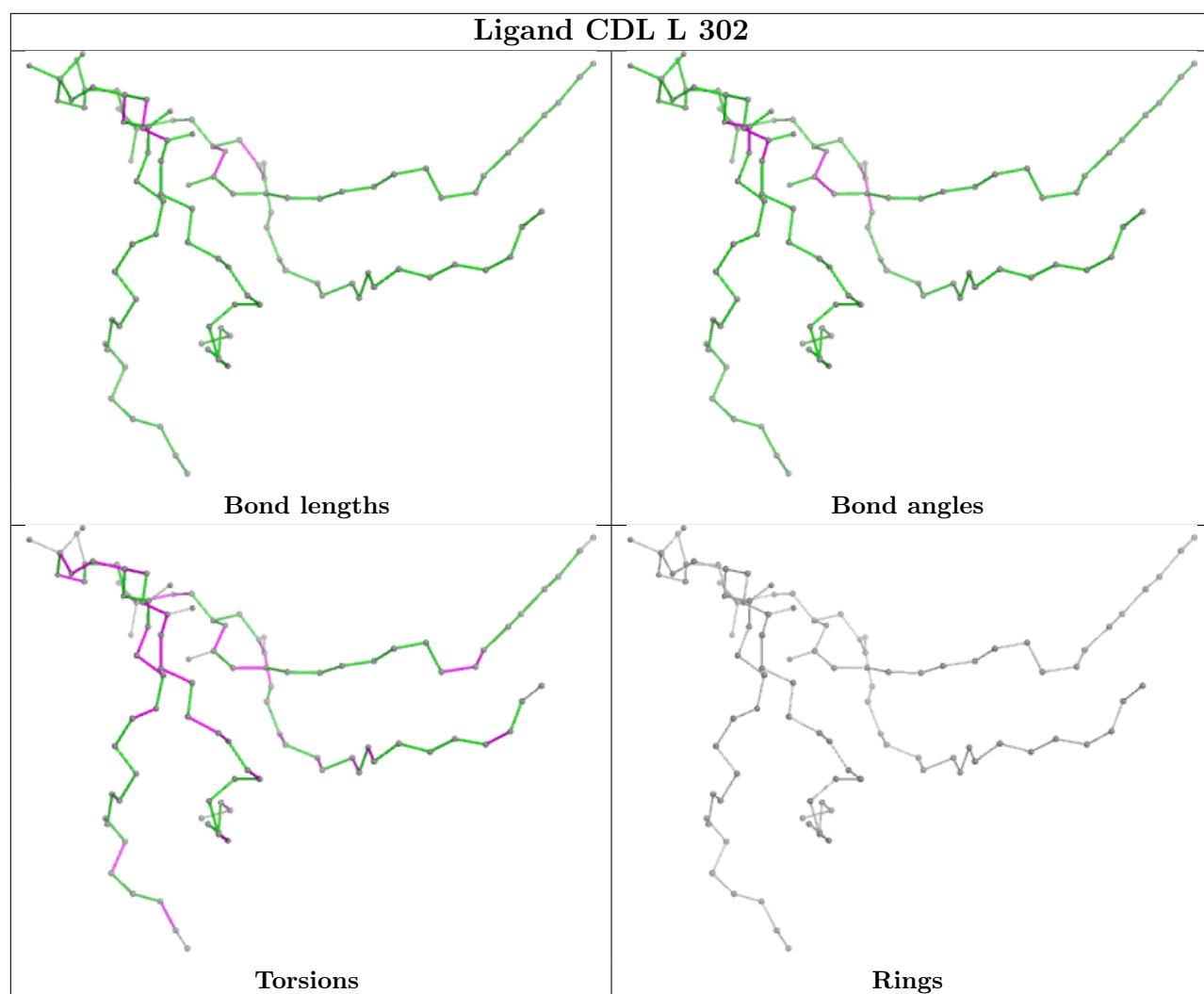


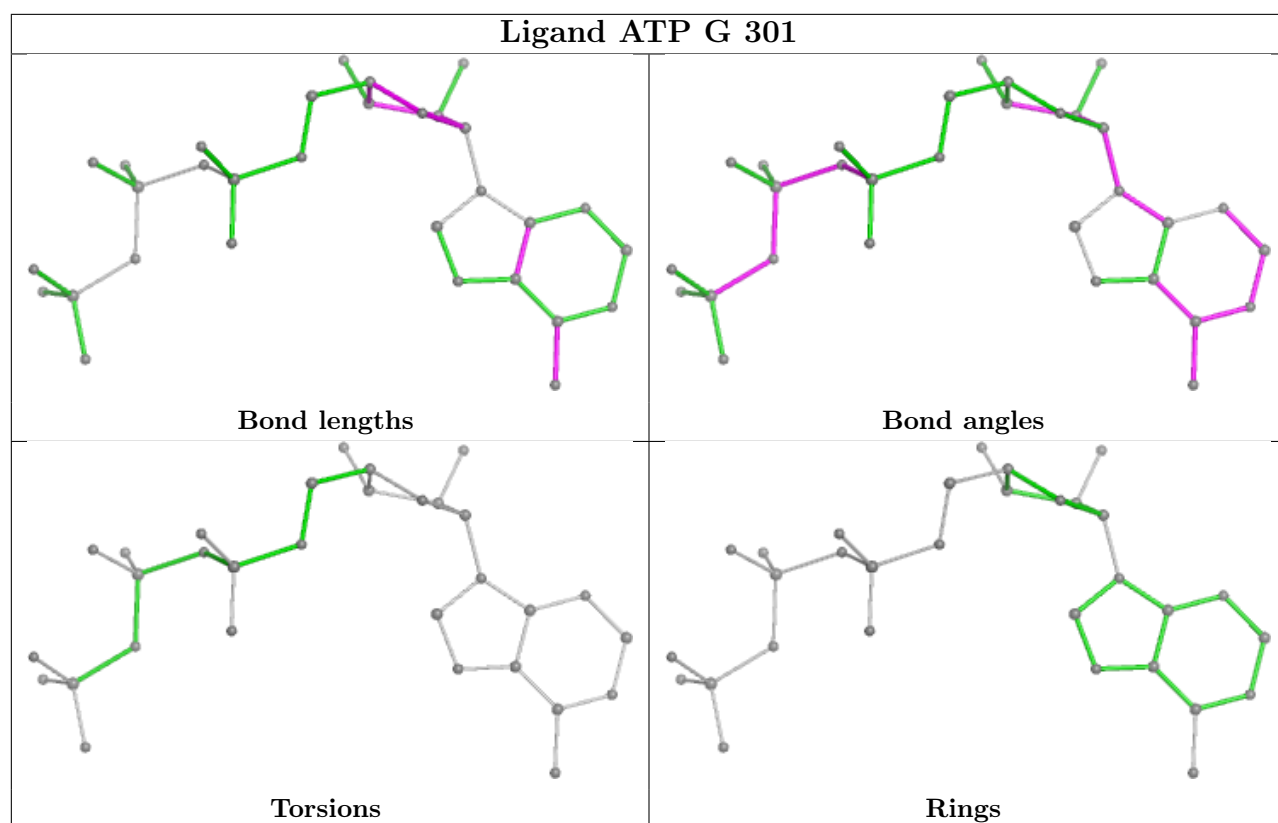


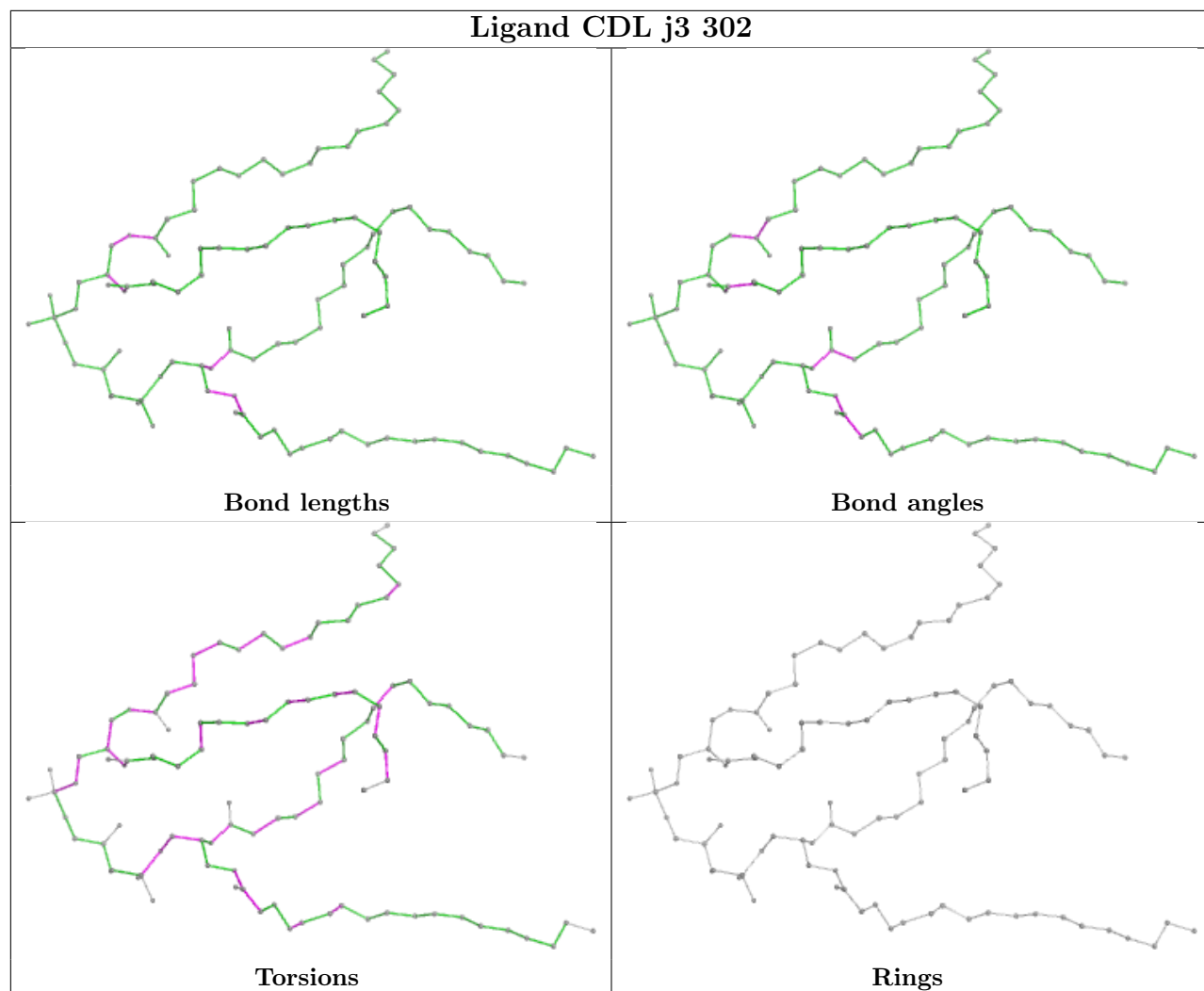


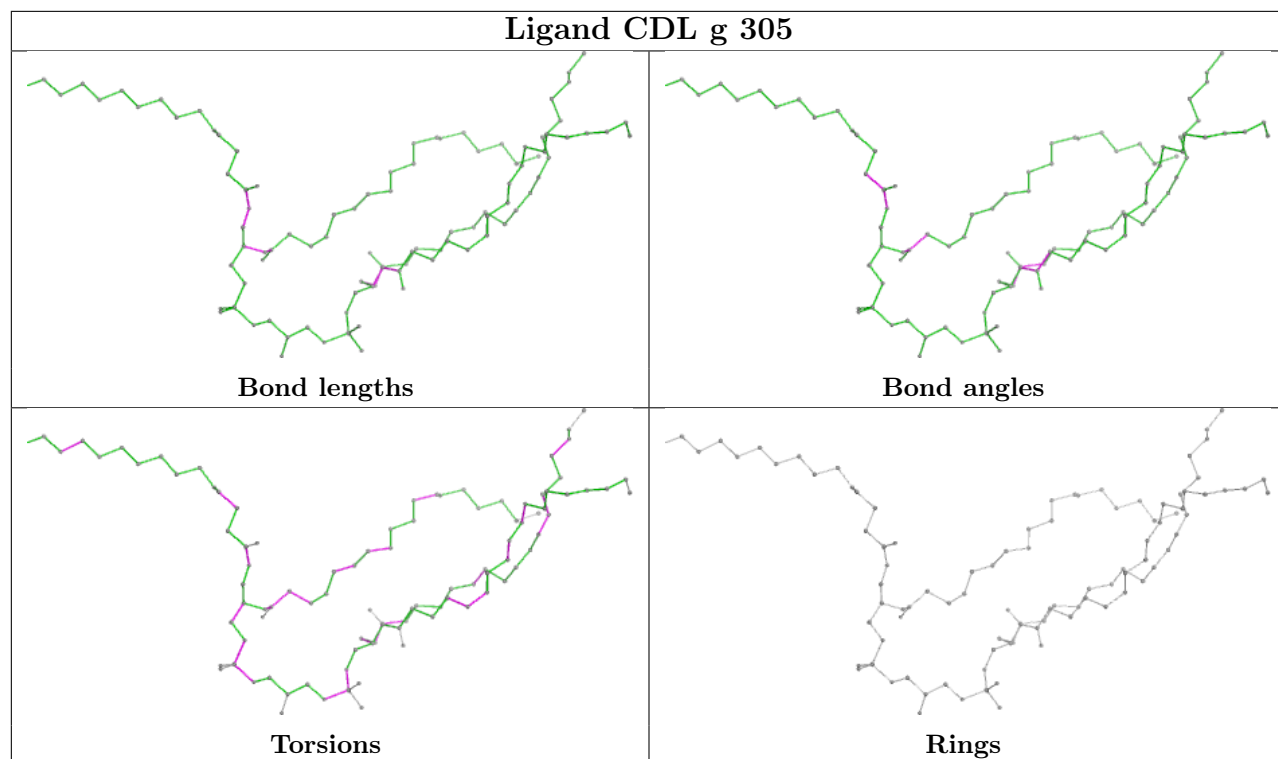




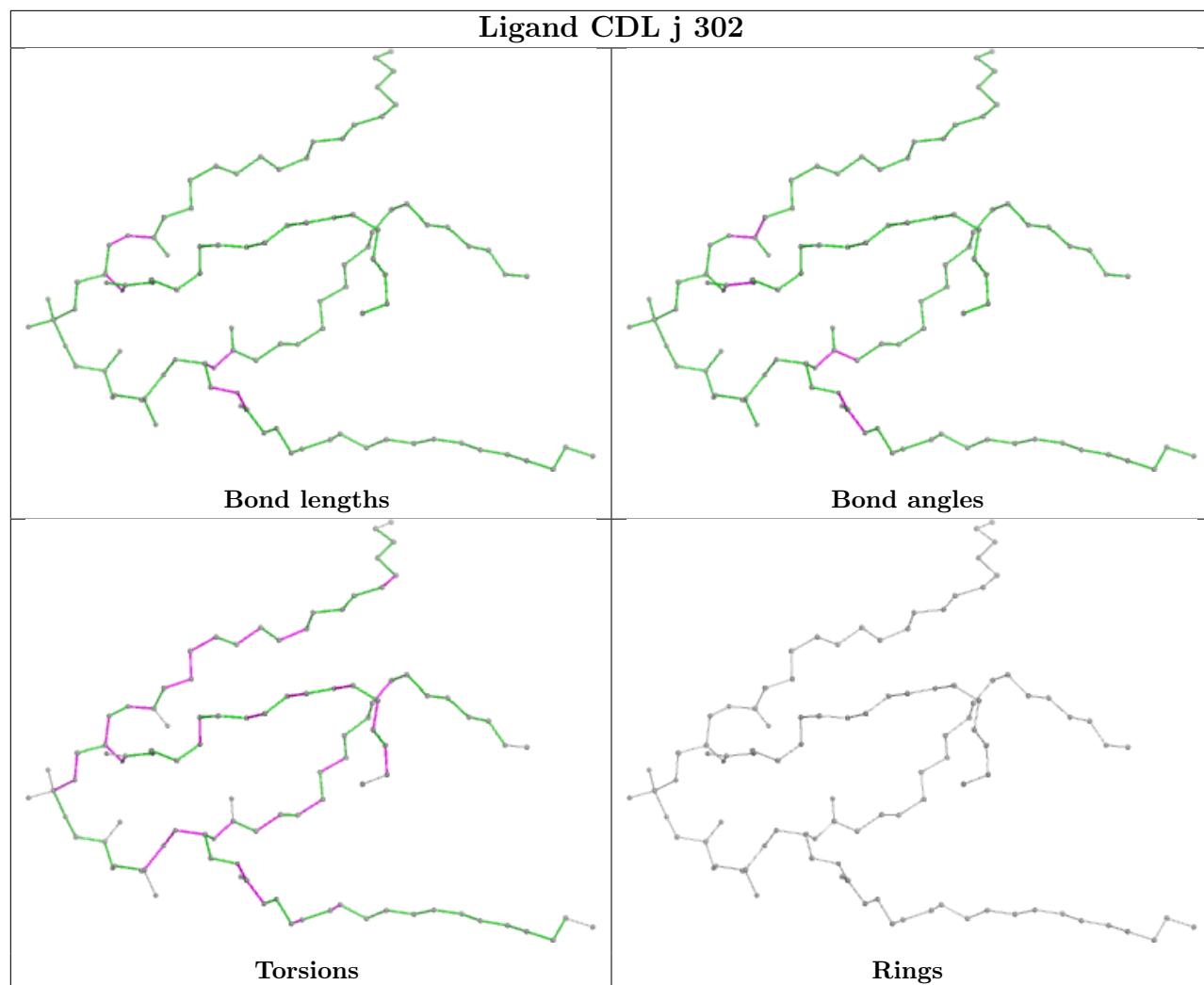


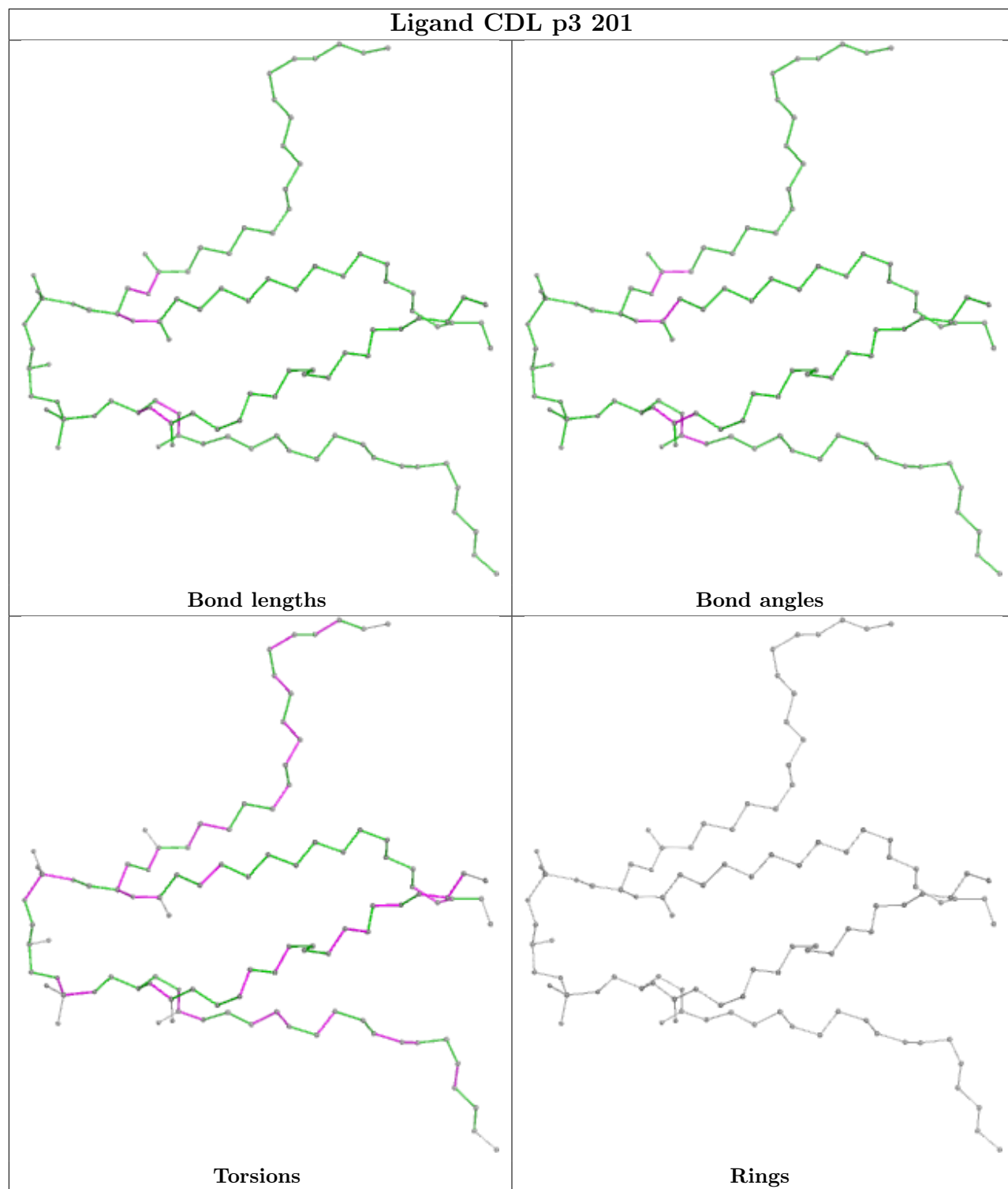


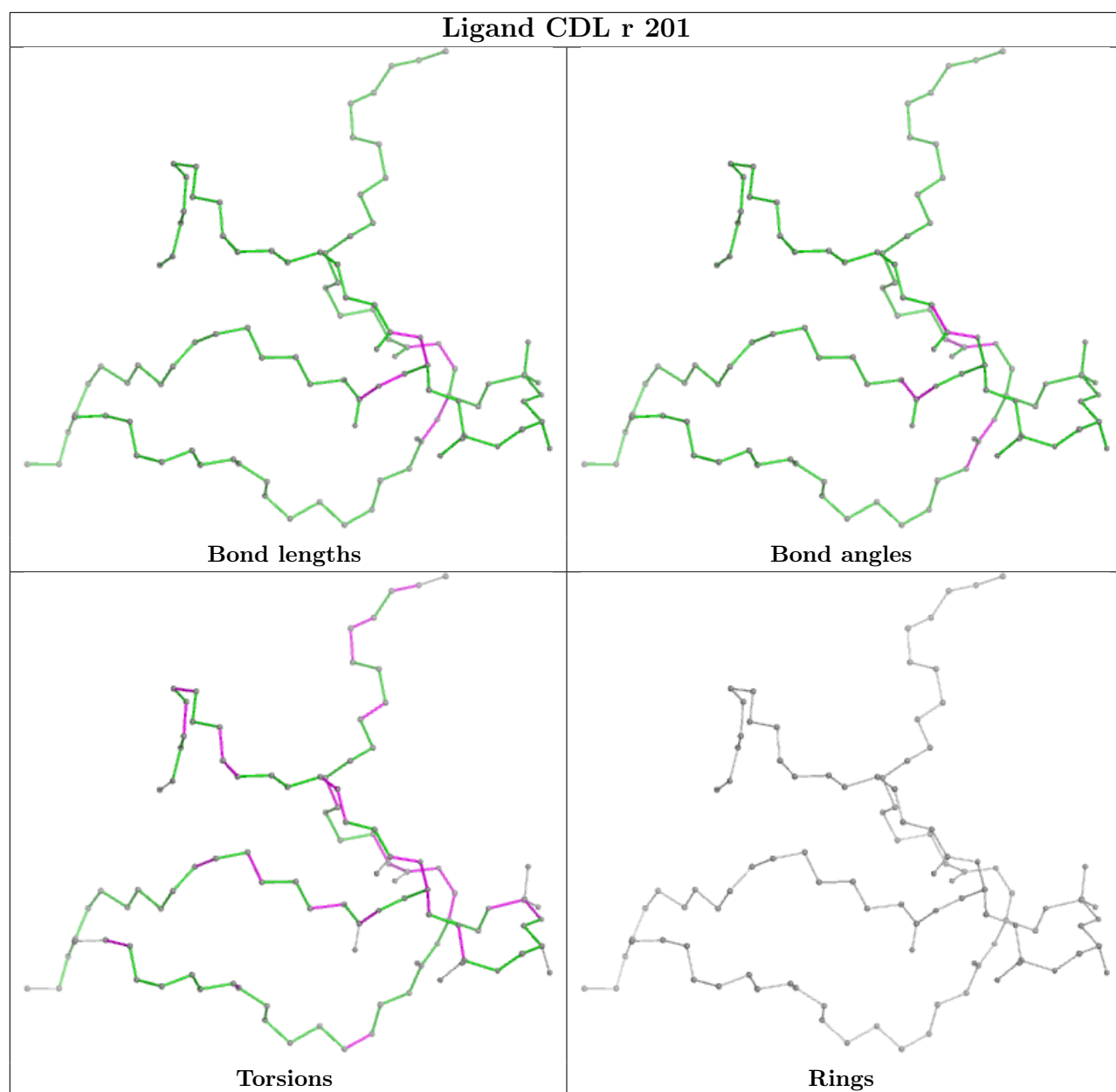


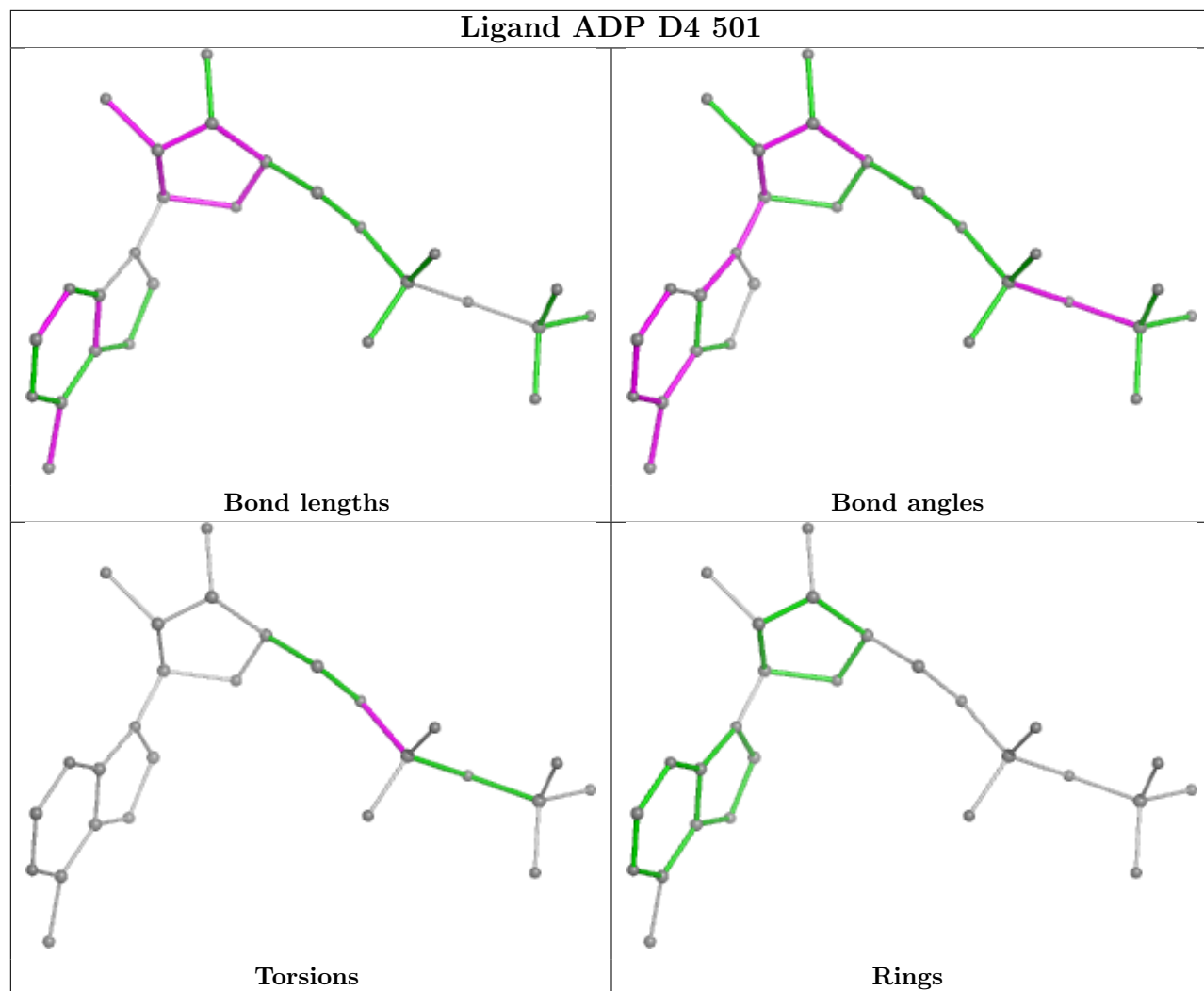


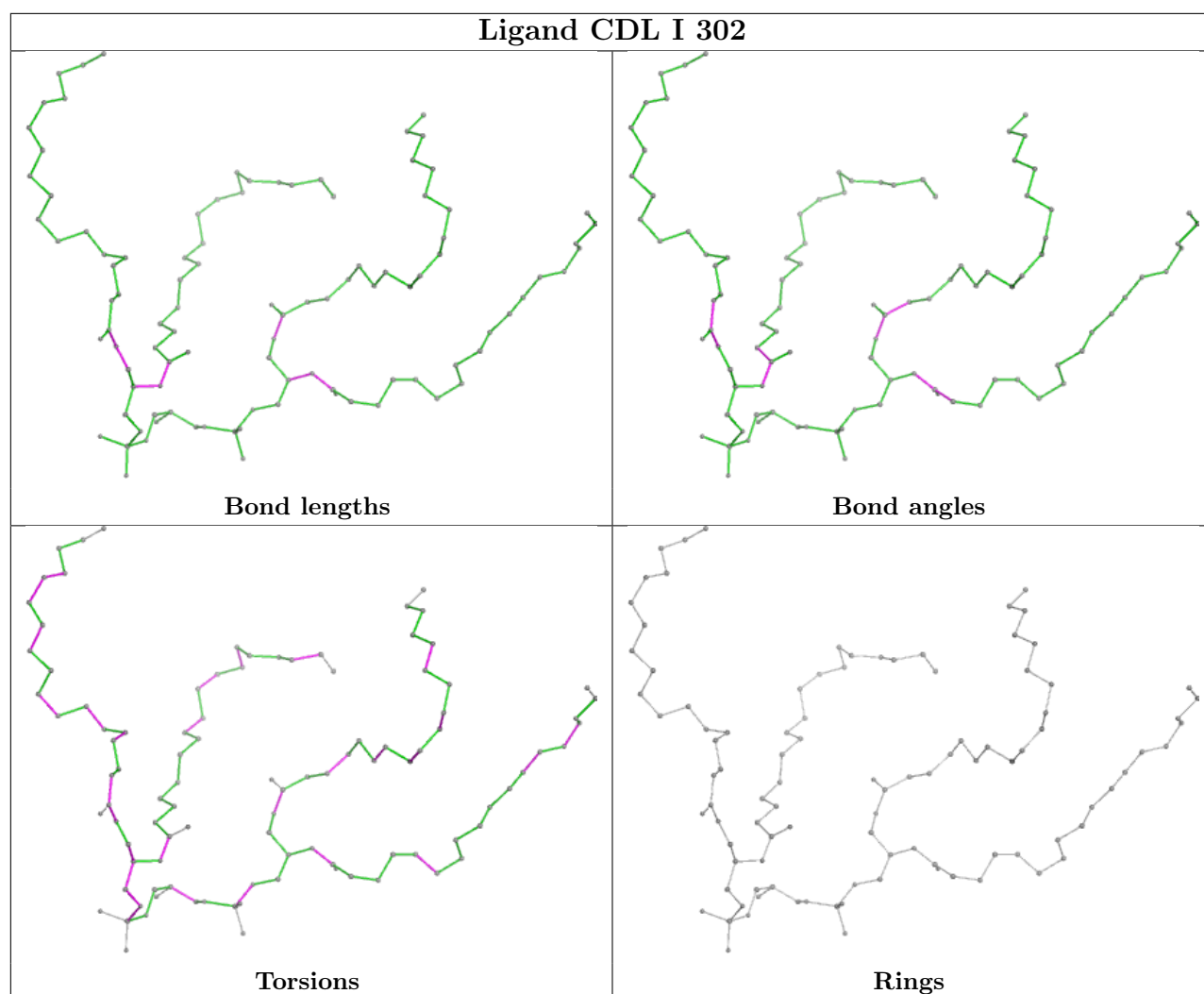
Ligand CDL j 302

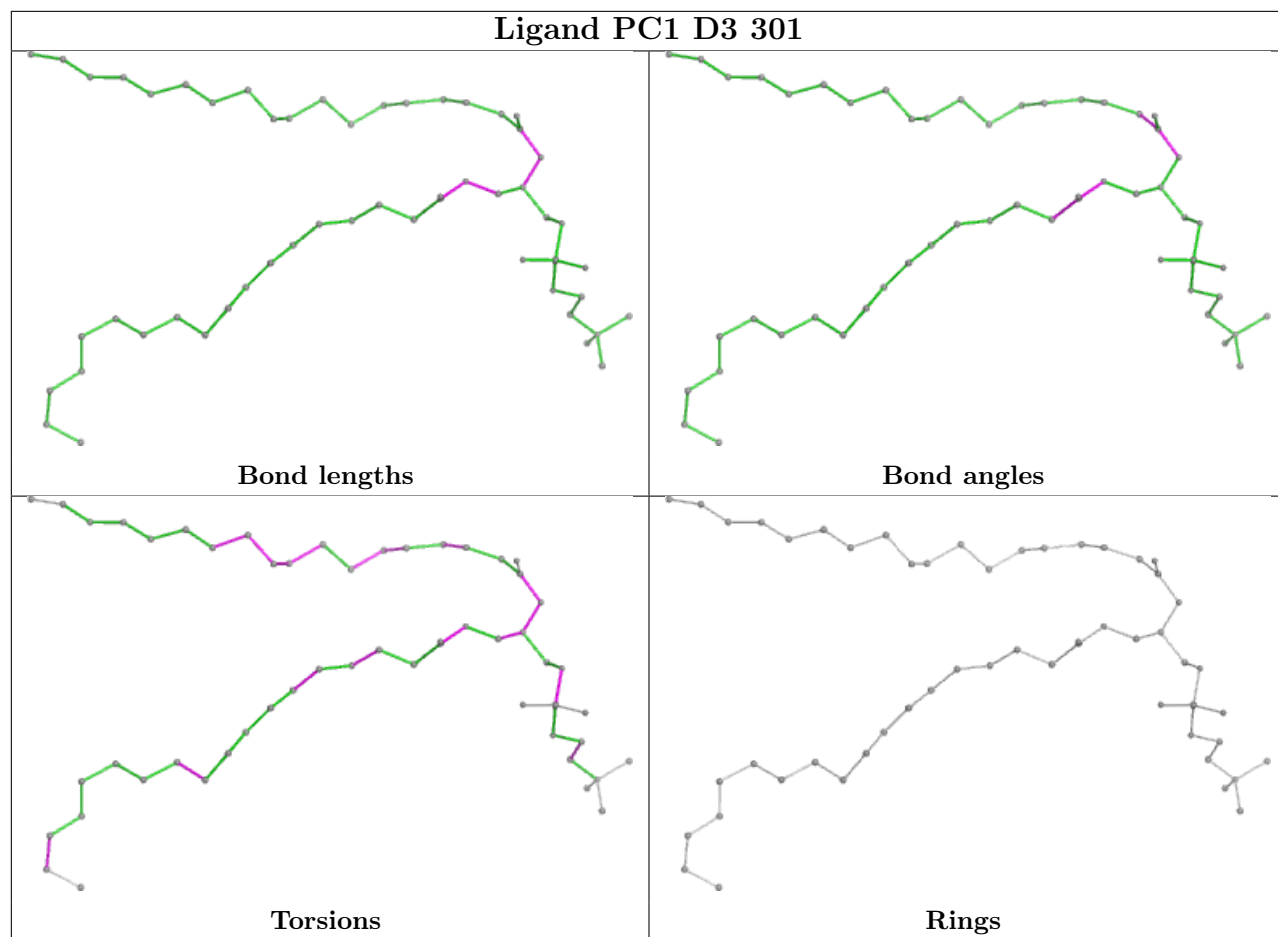


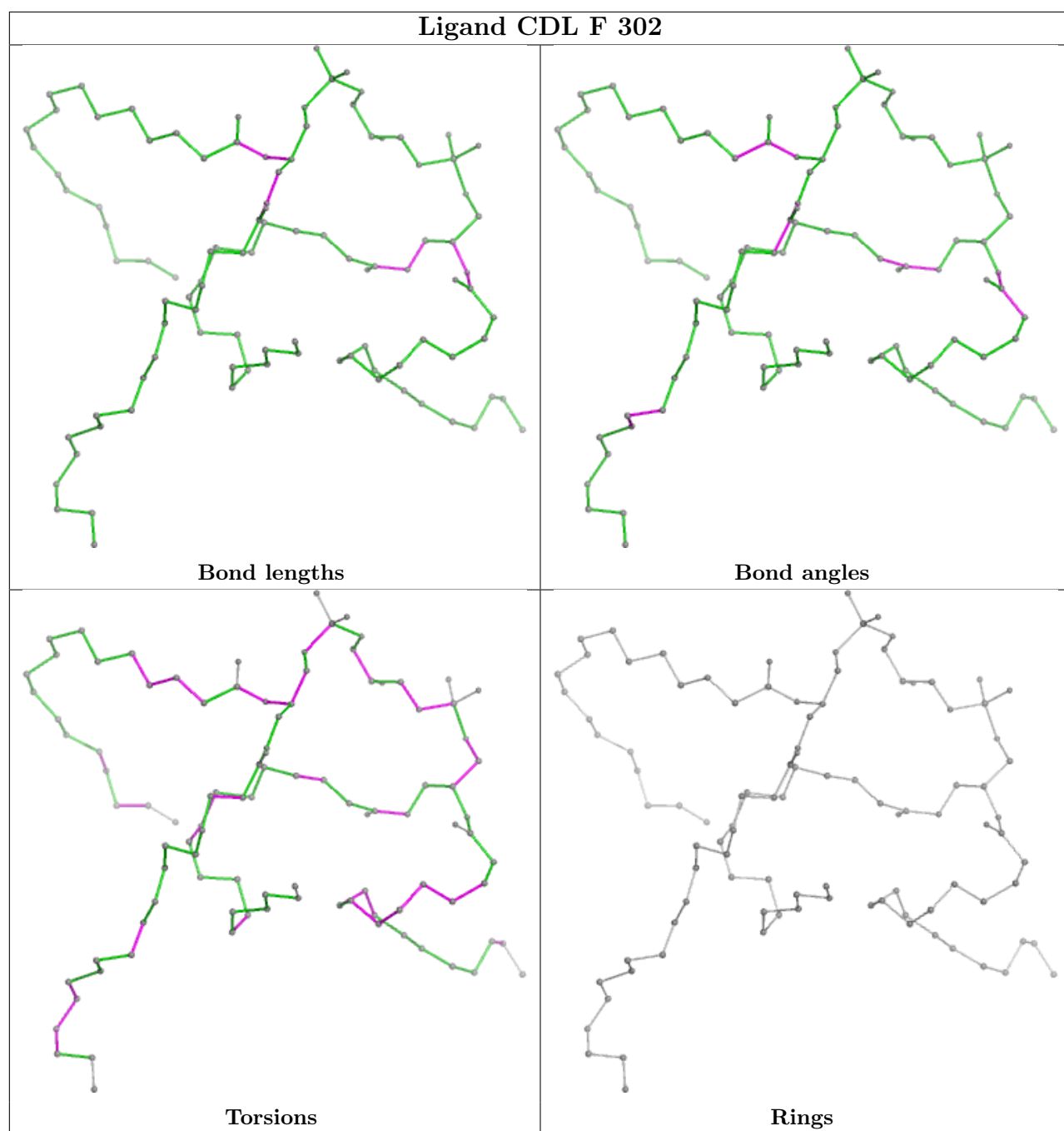


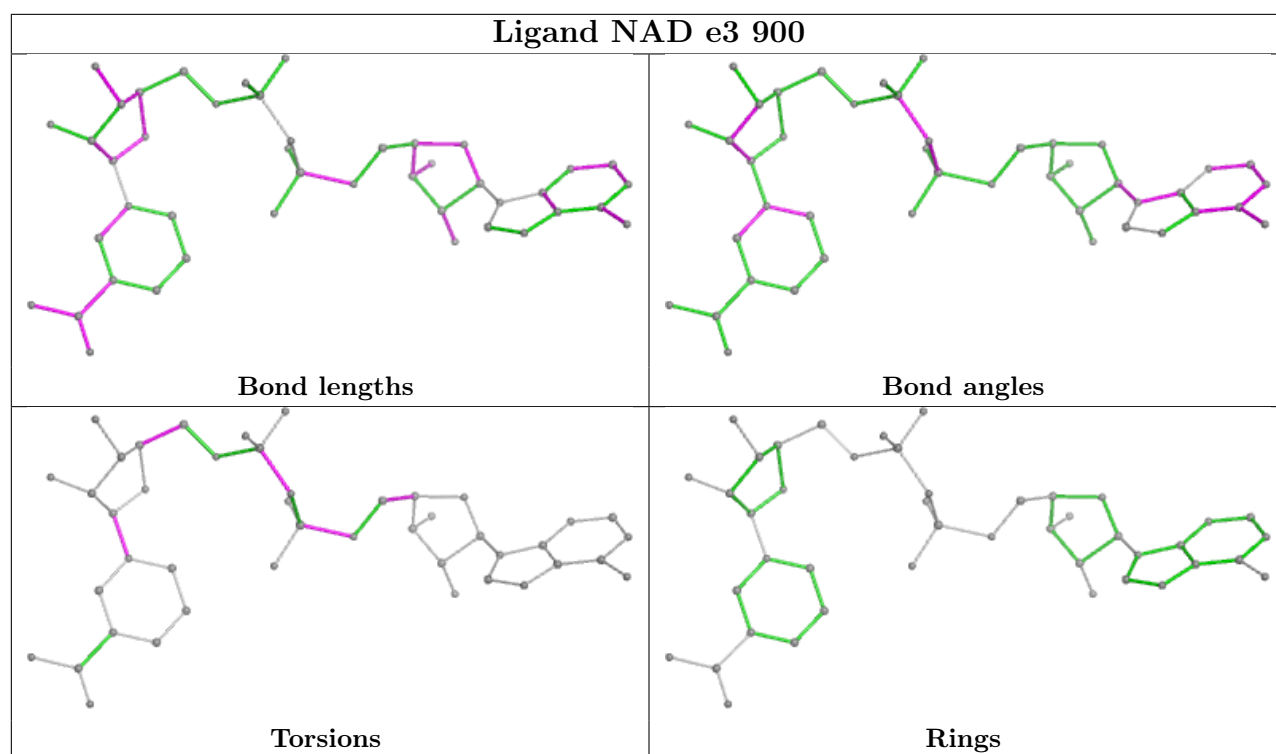


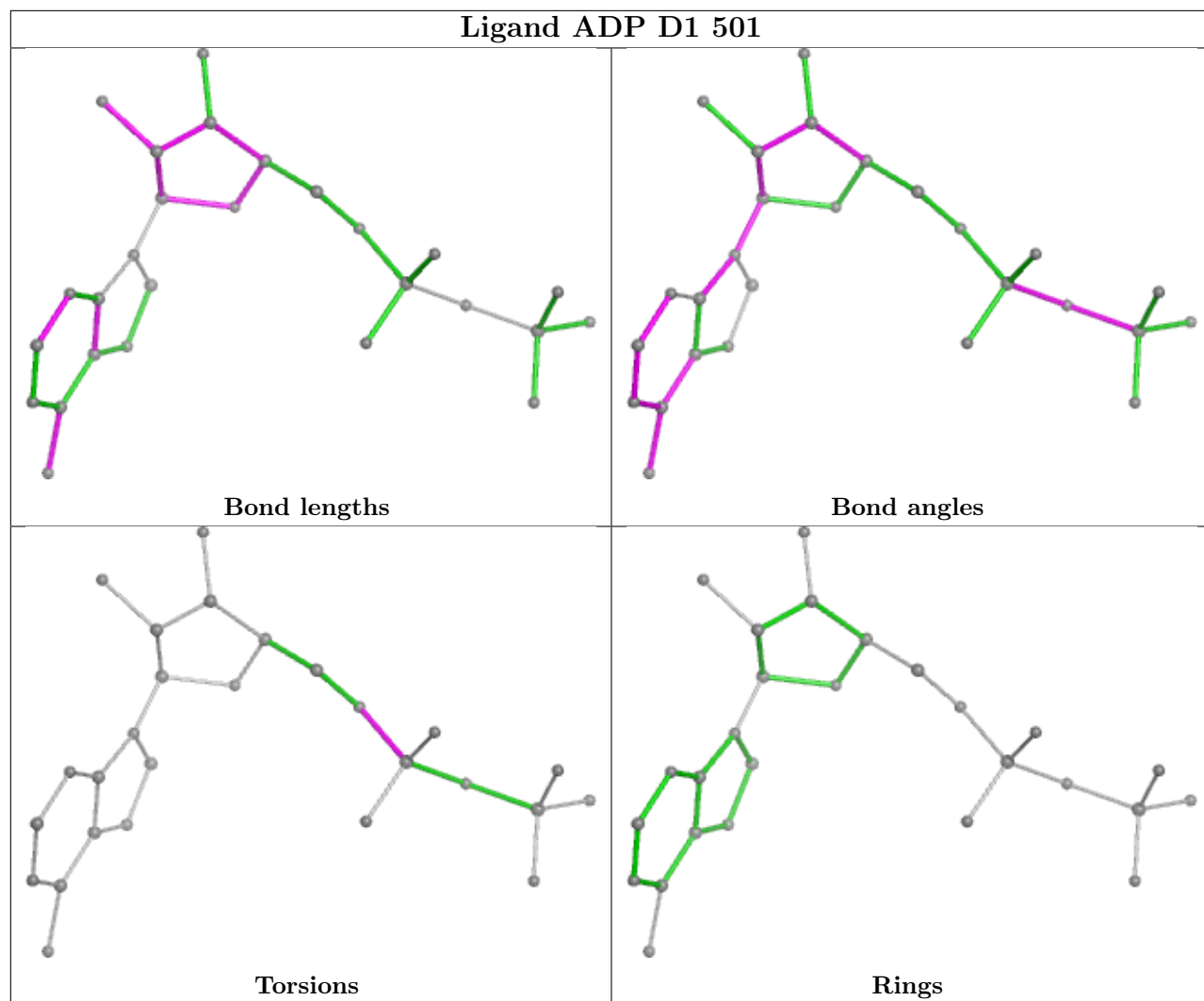




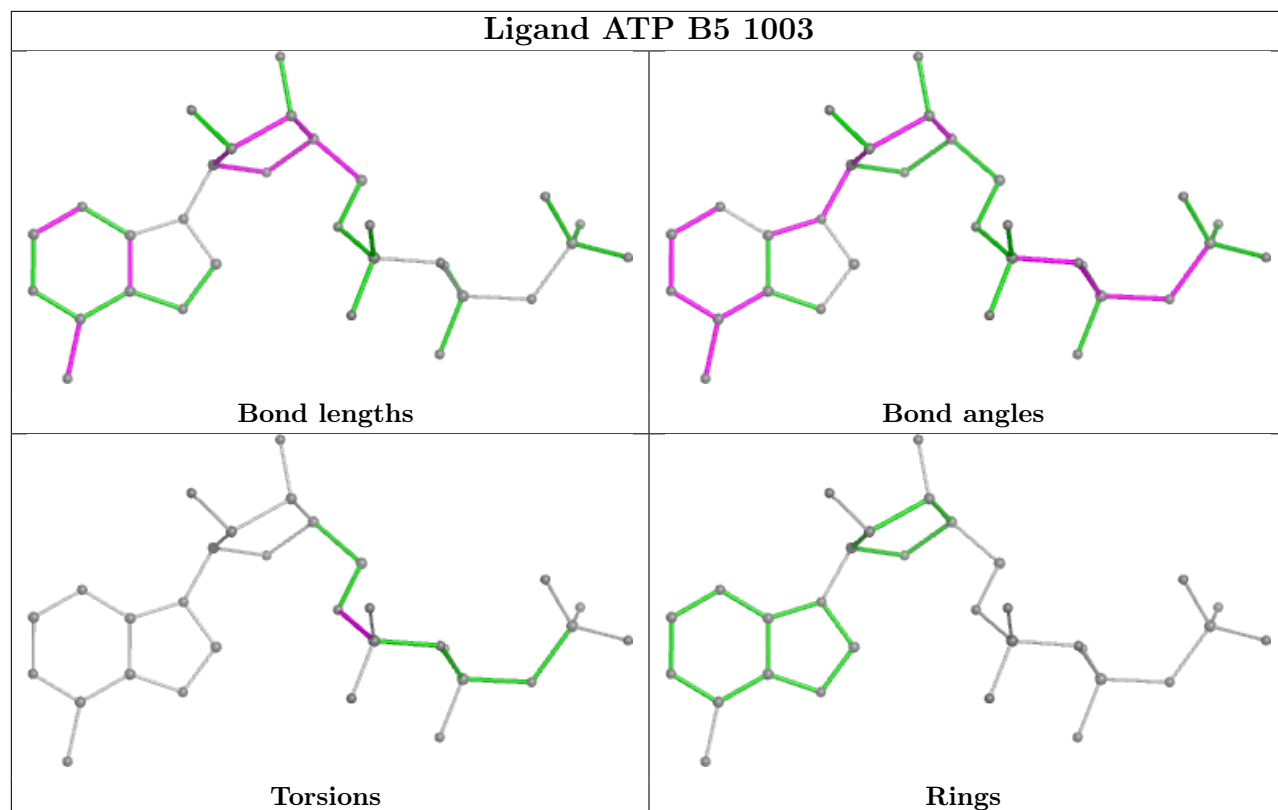




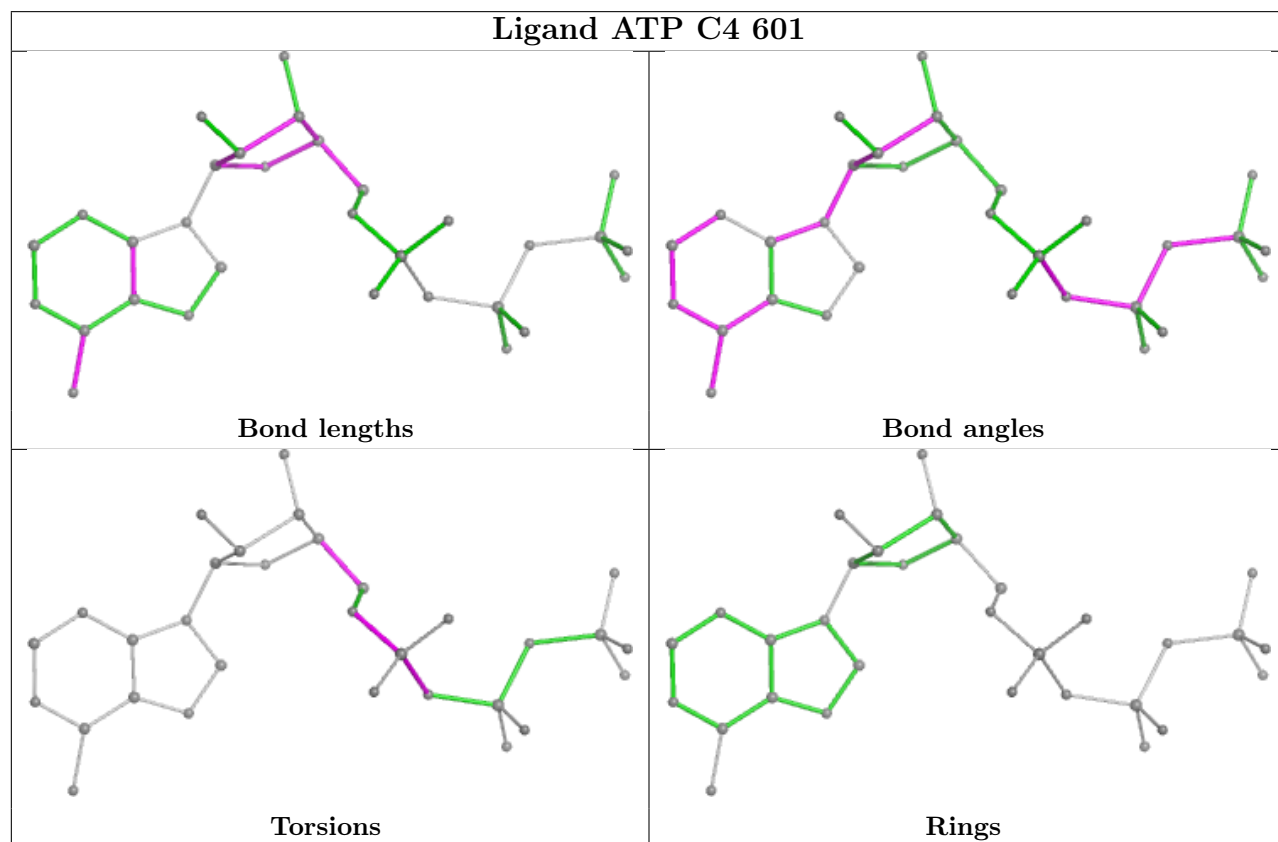


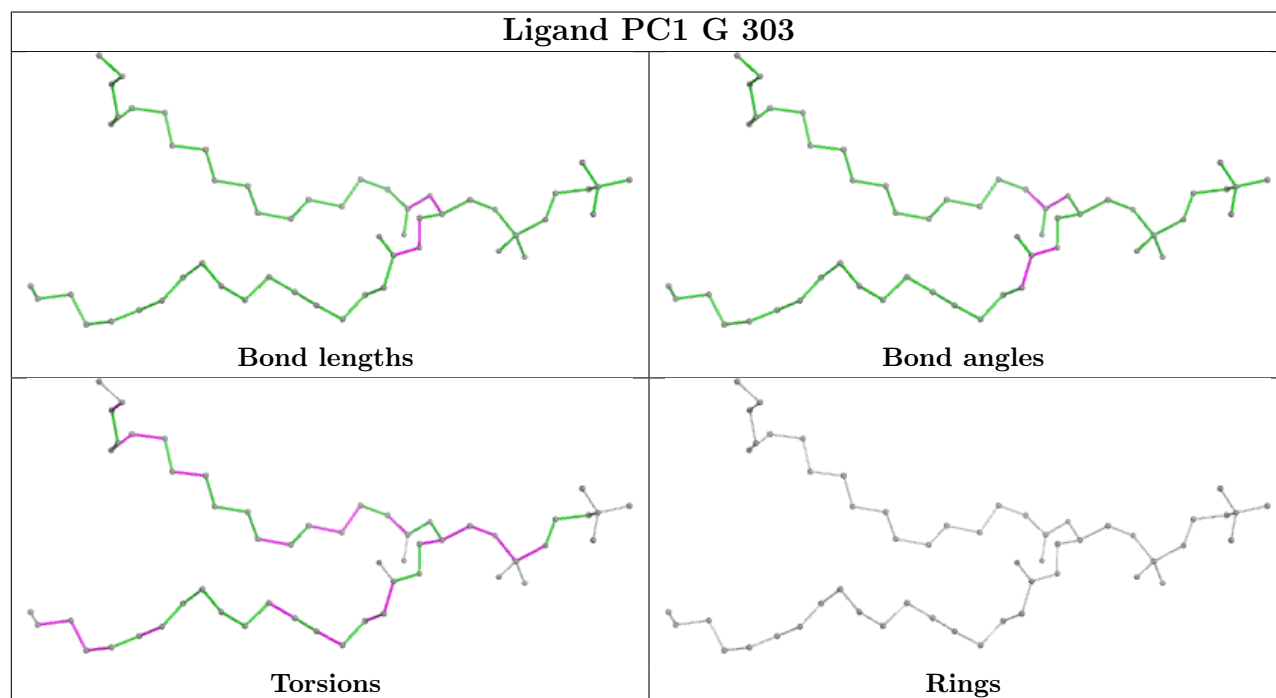
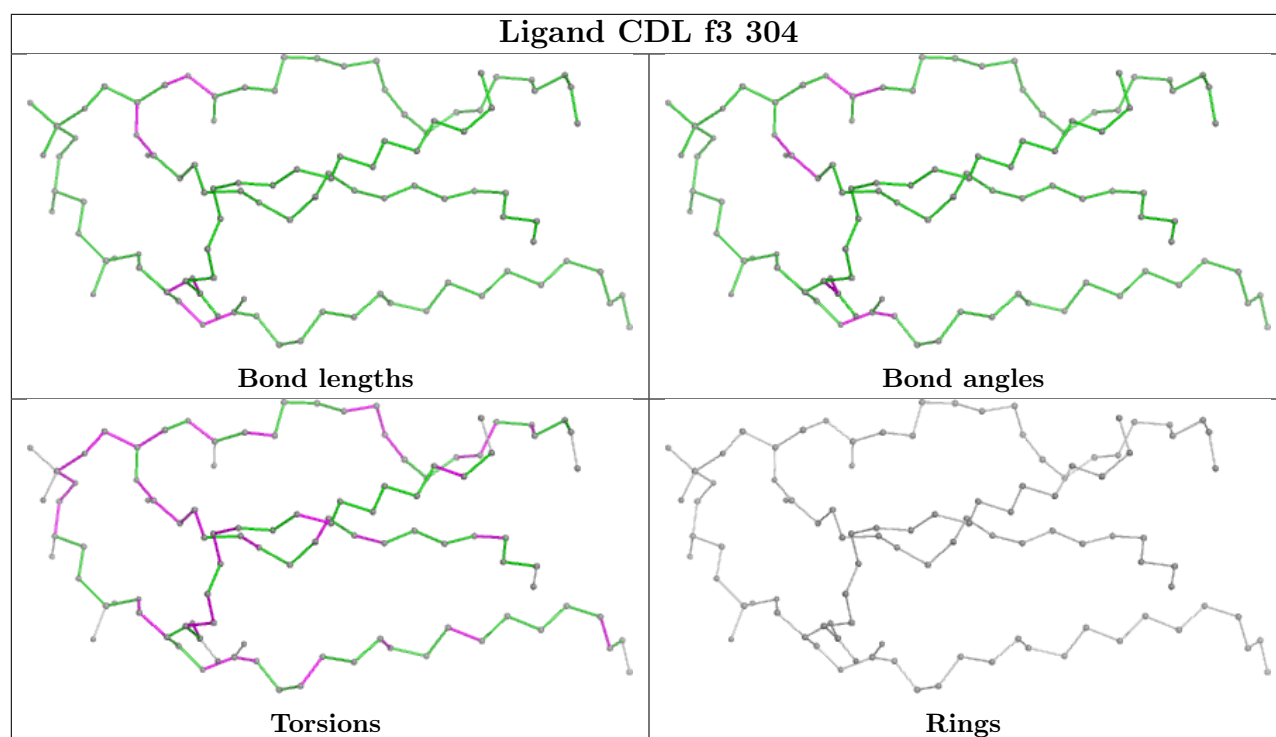


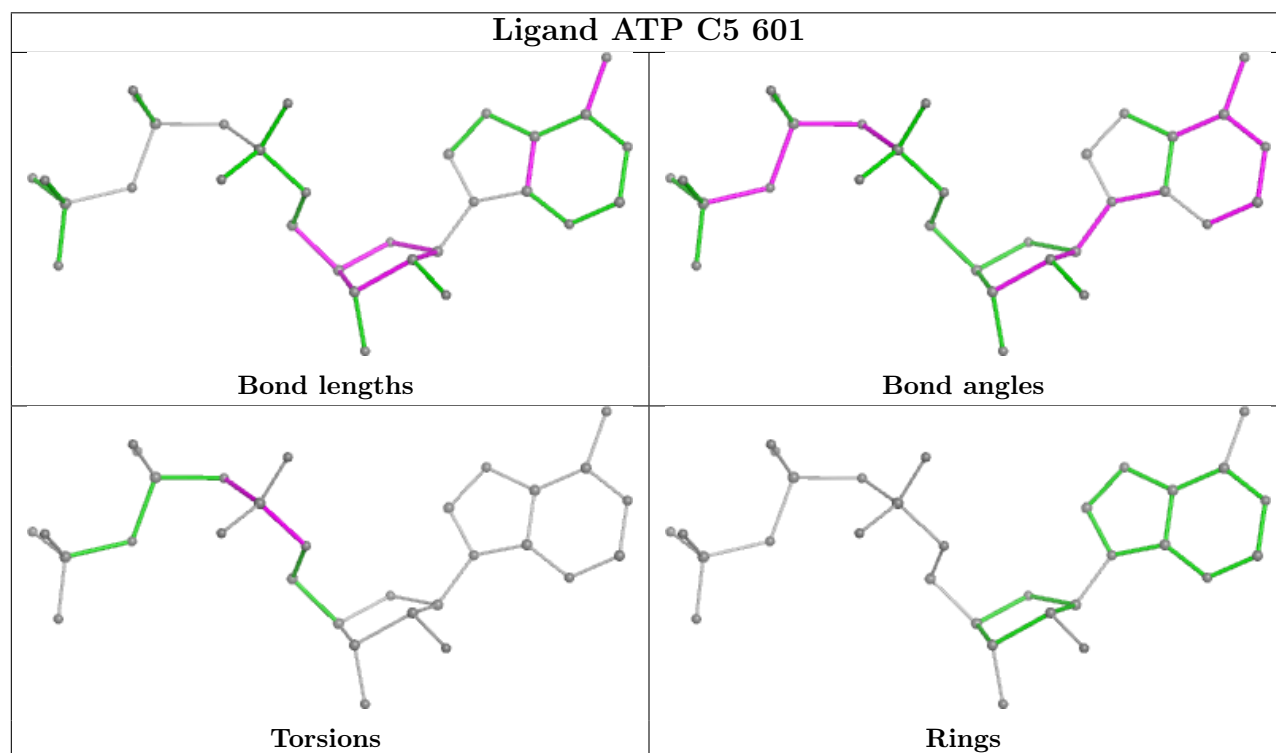
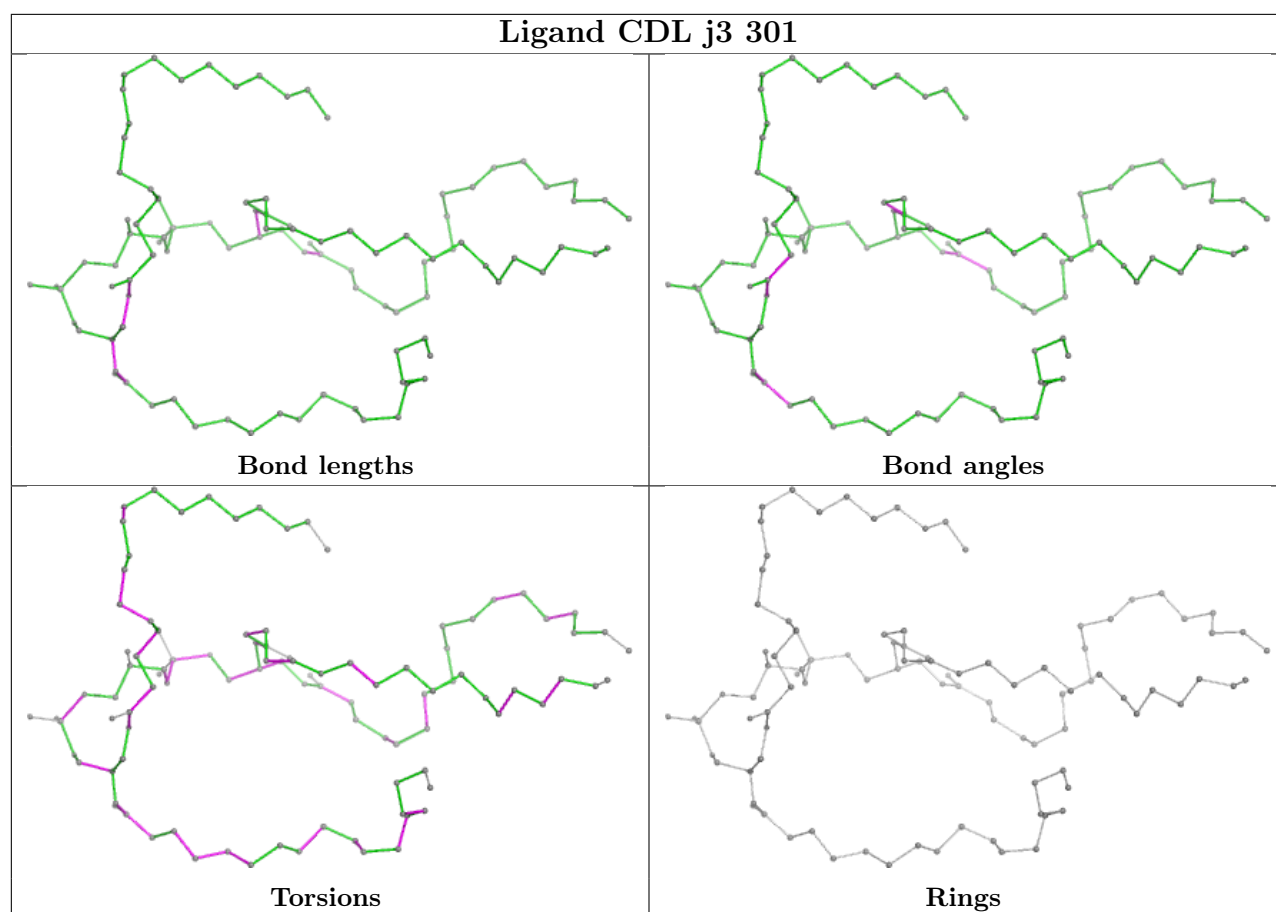
Ligand ATP B5 1003

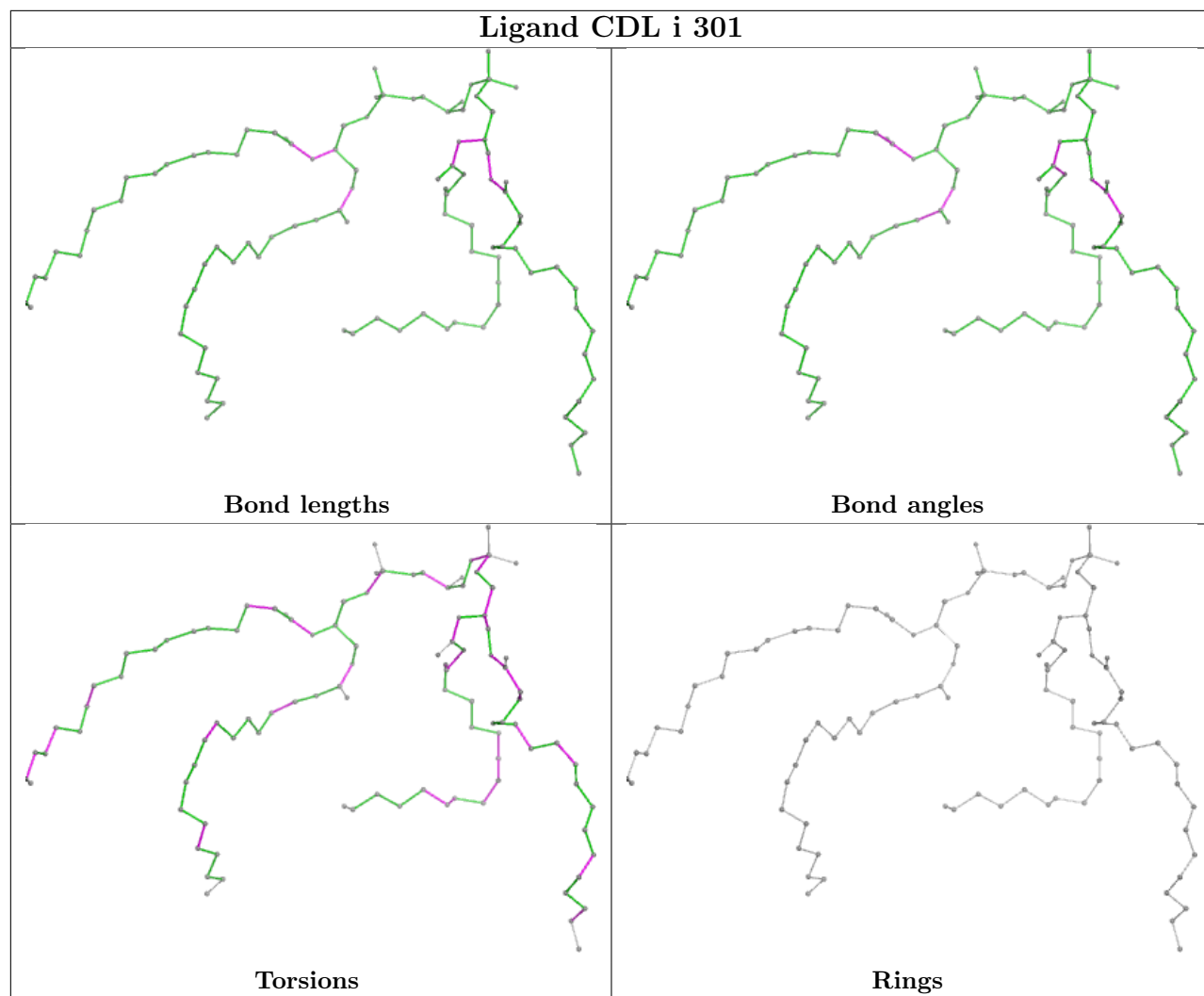


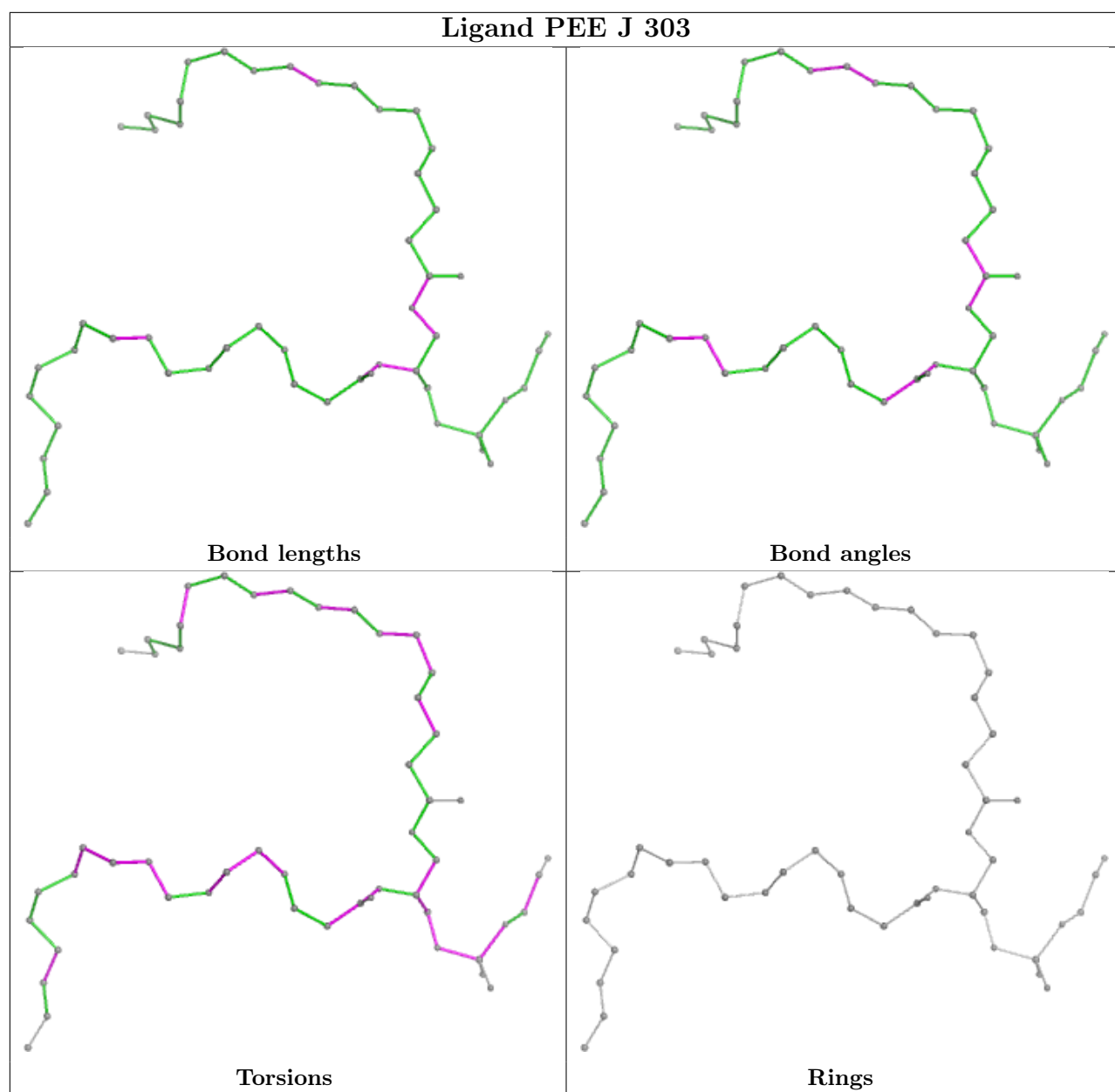
Ligand ATP C4 601

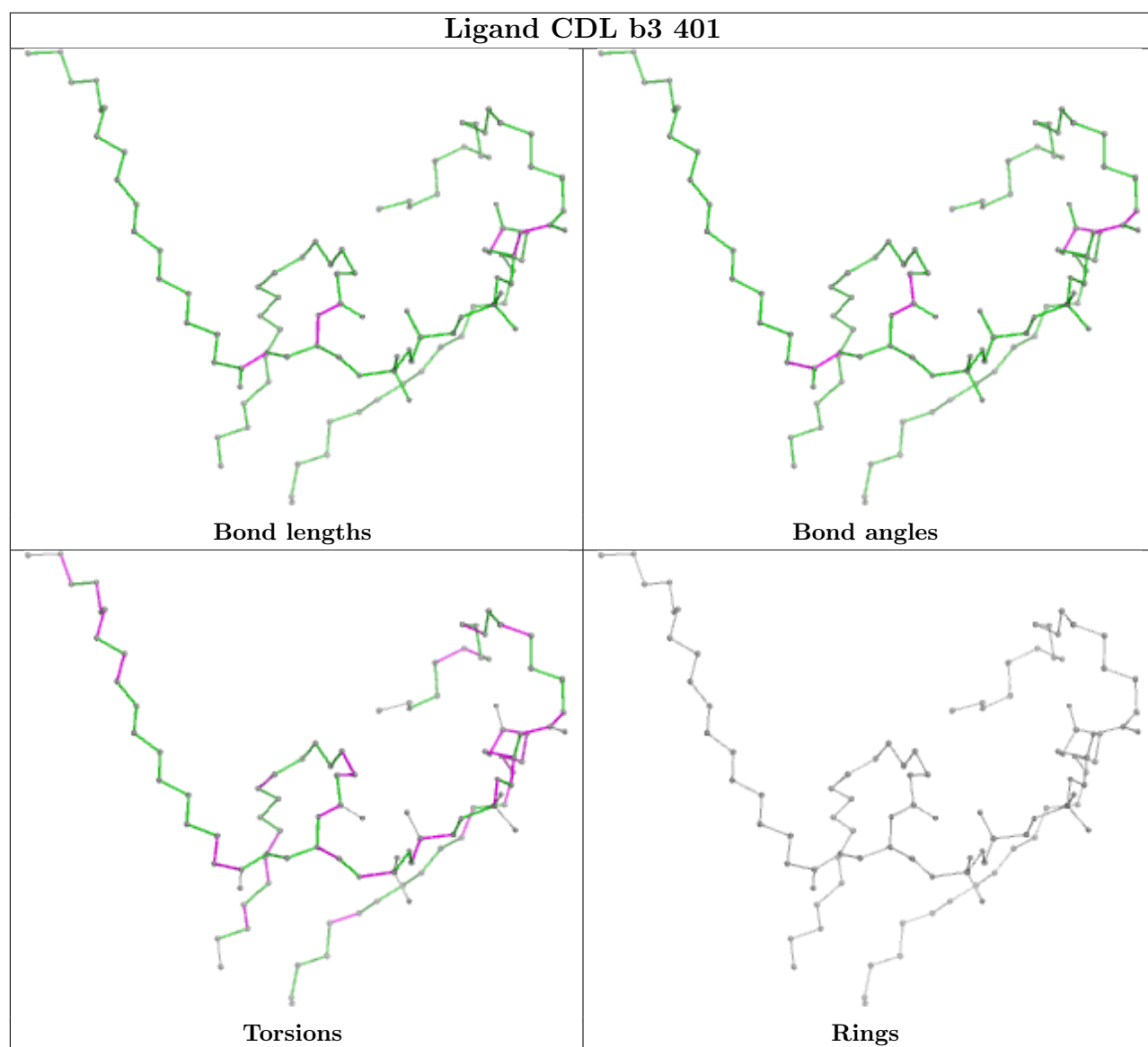


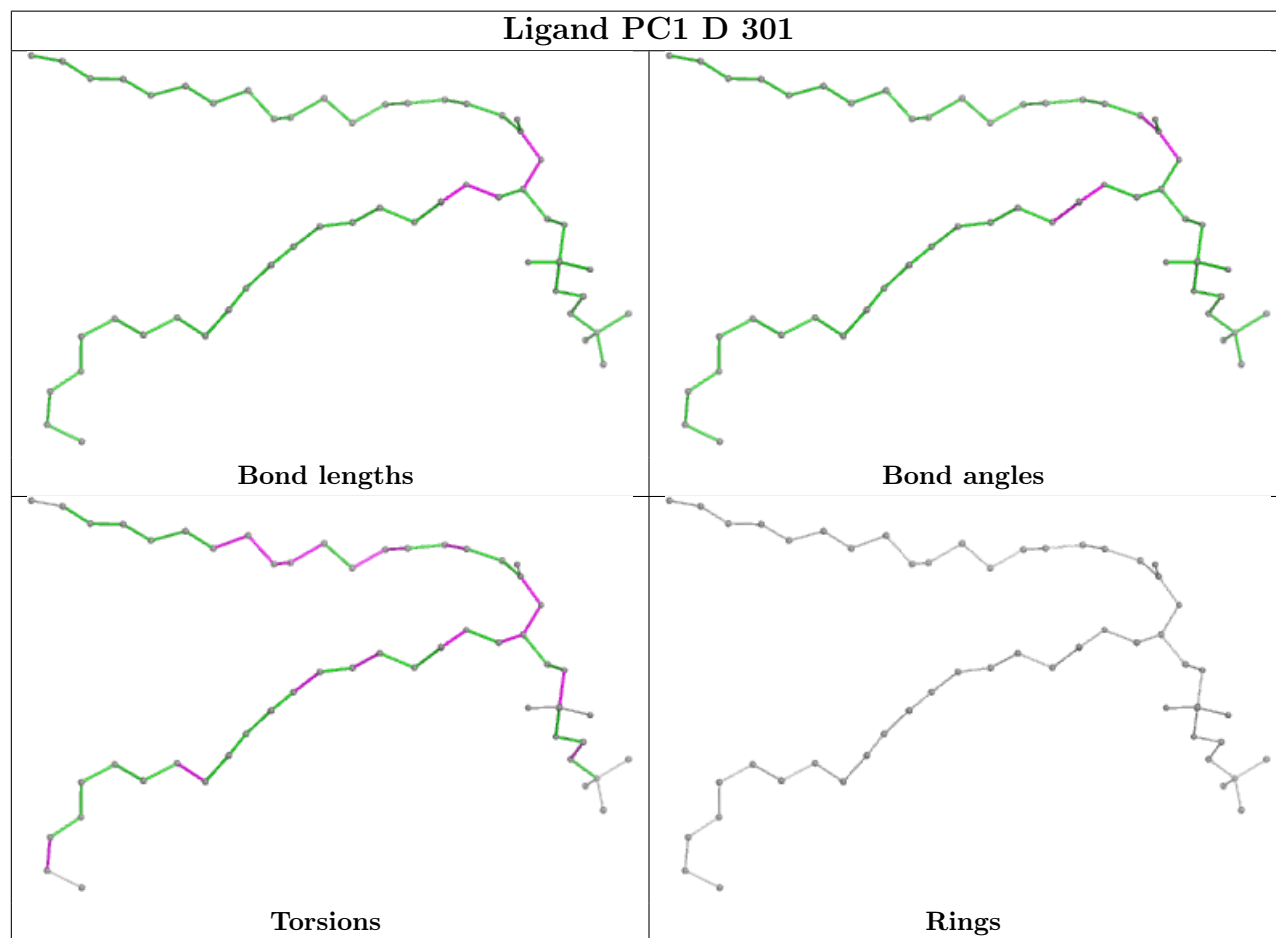
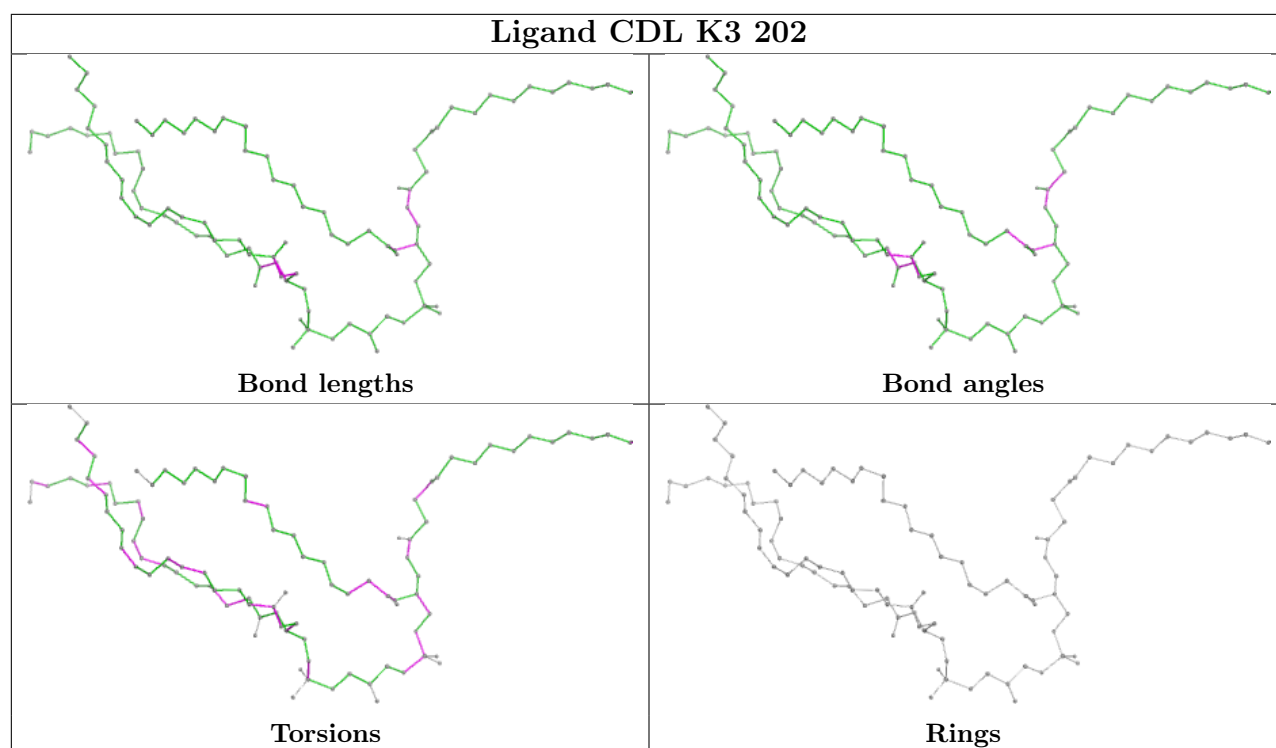


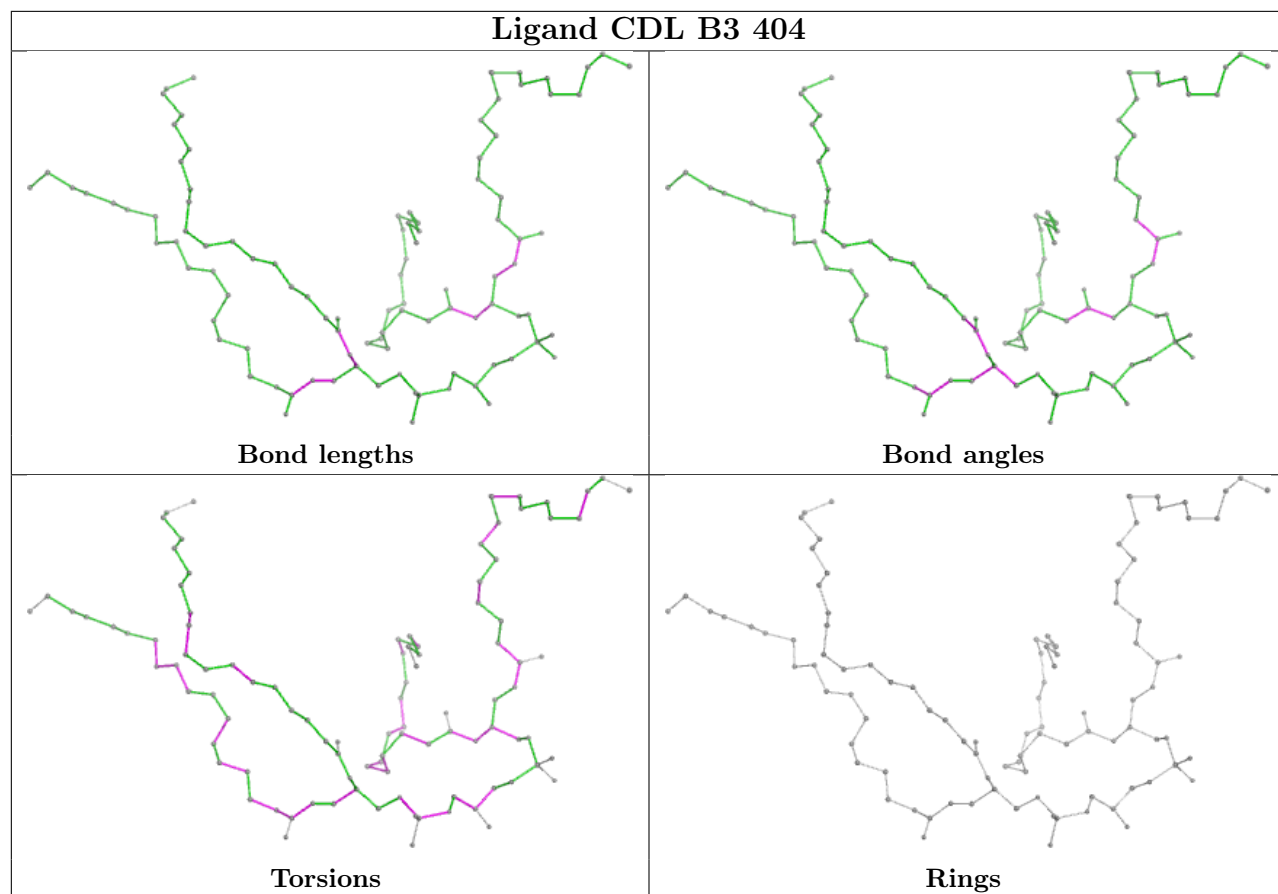


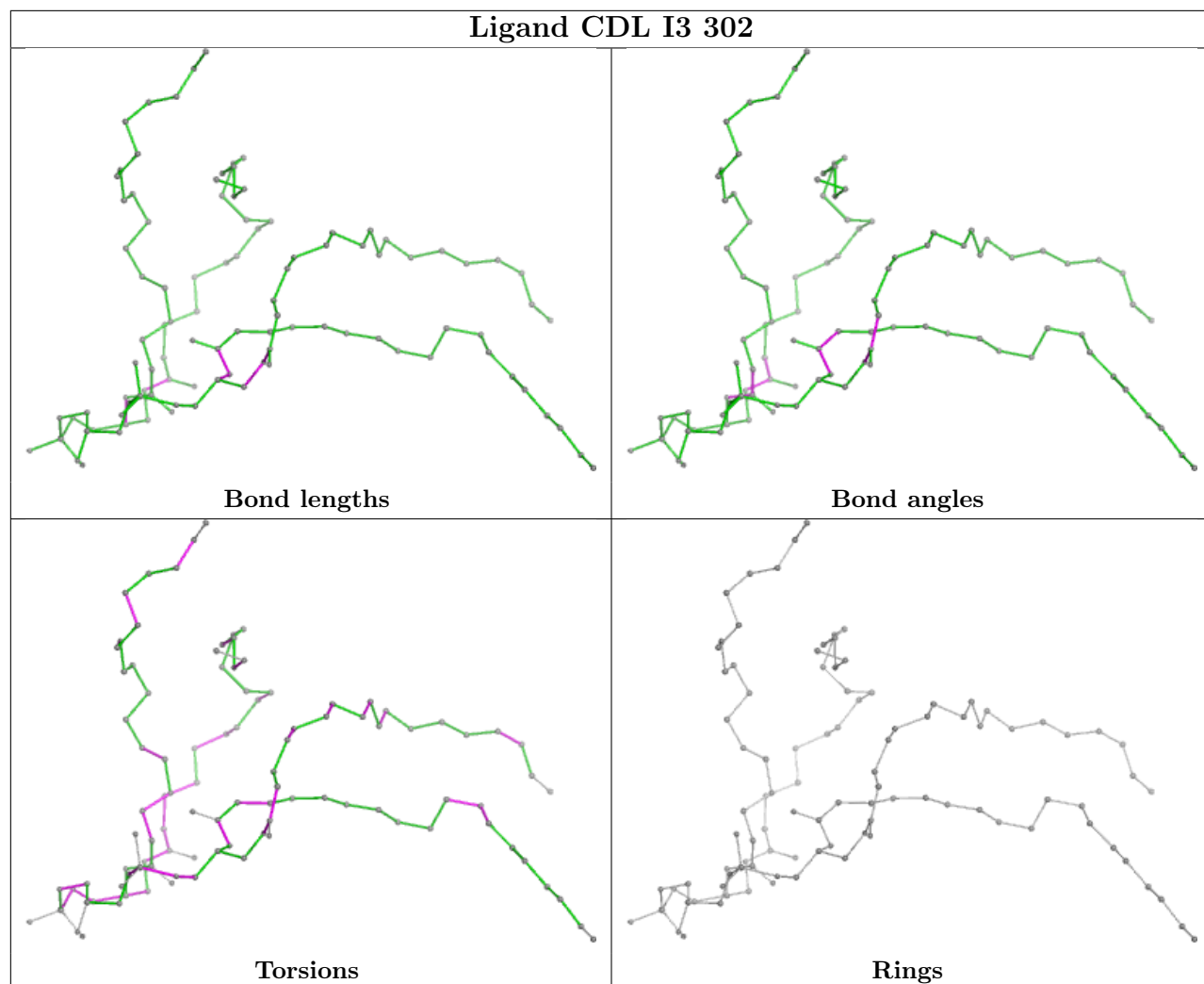


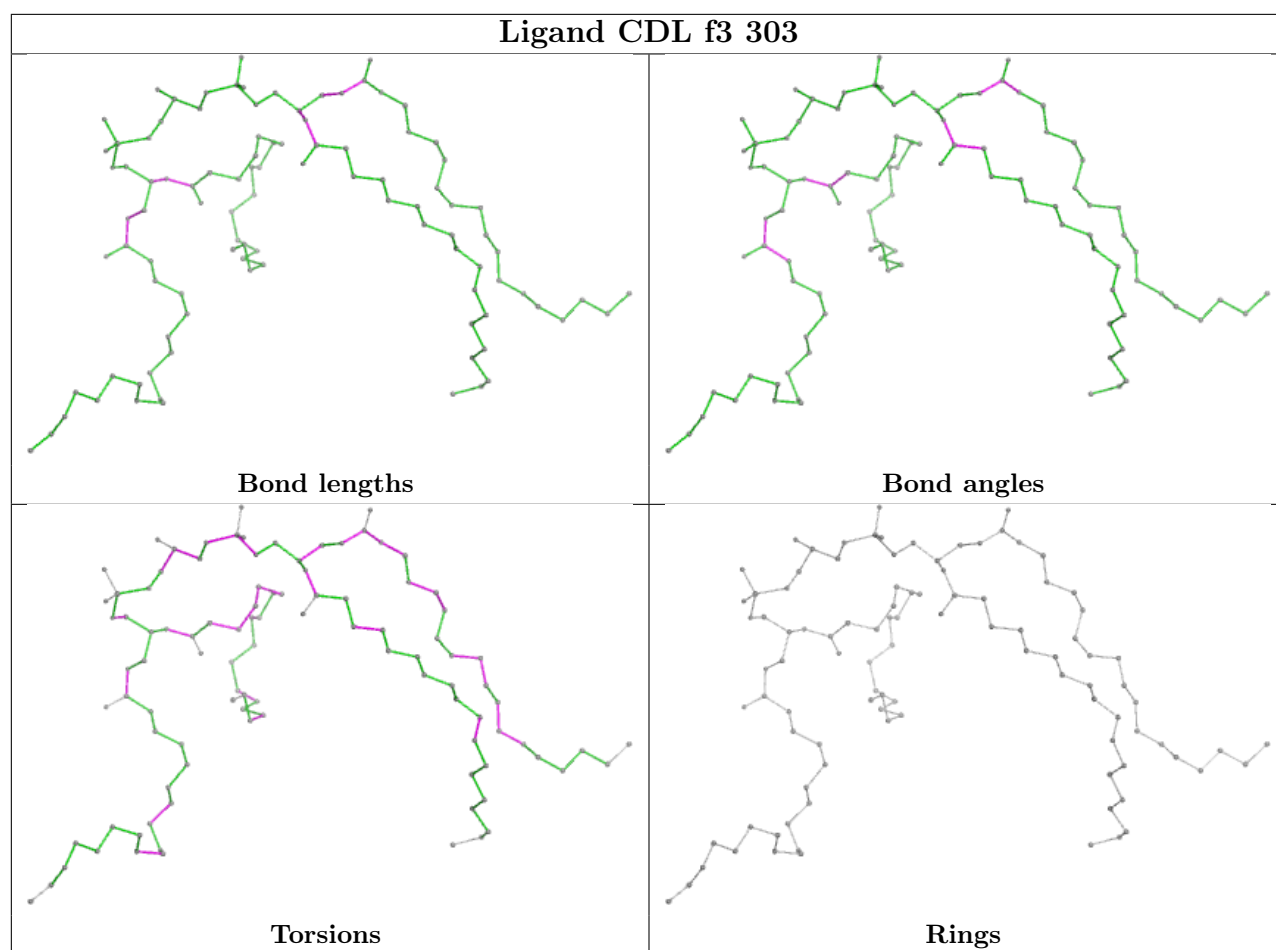


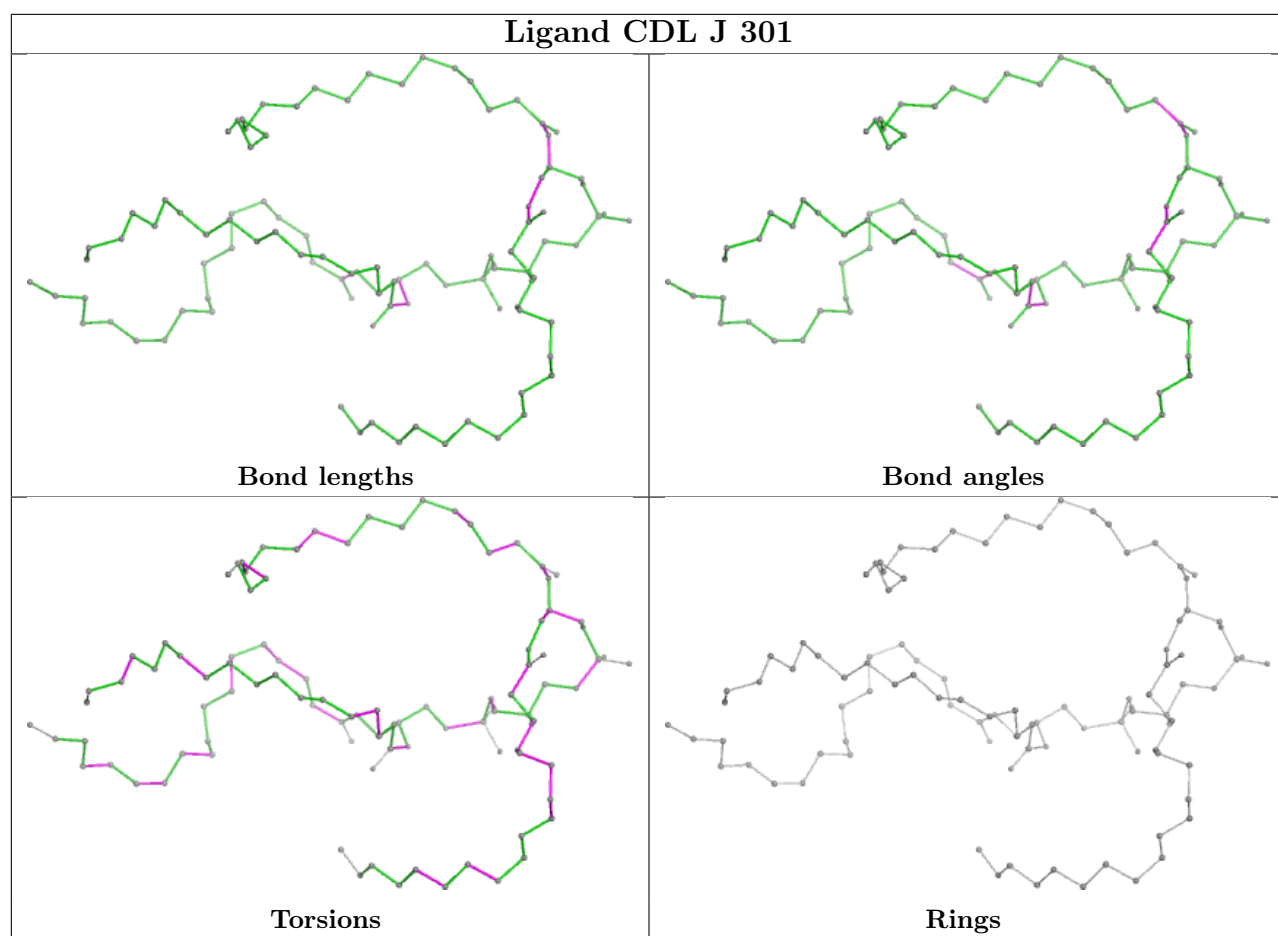


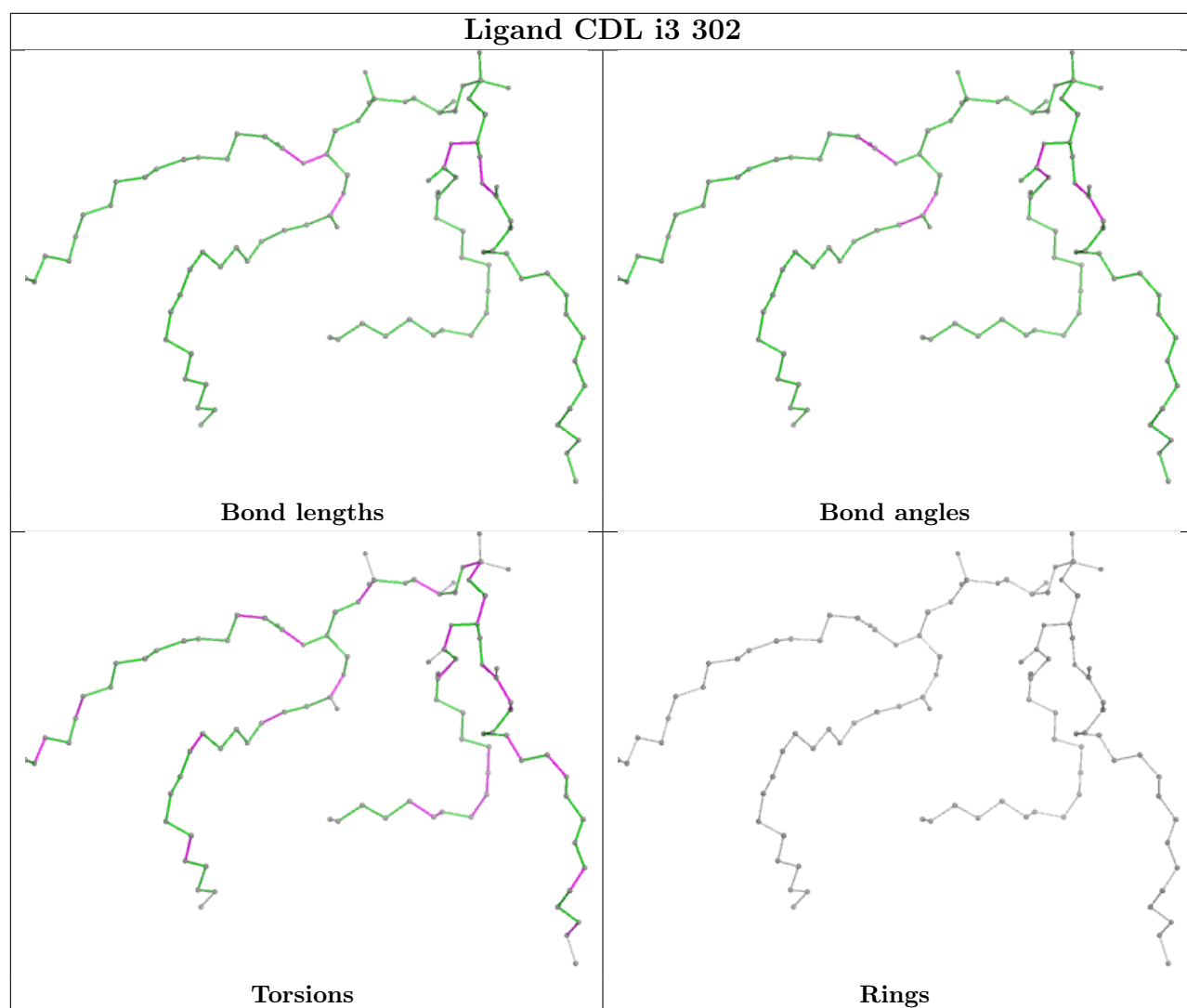


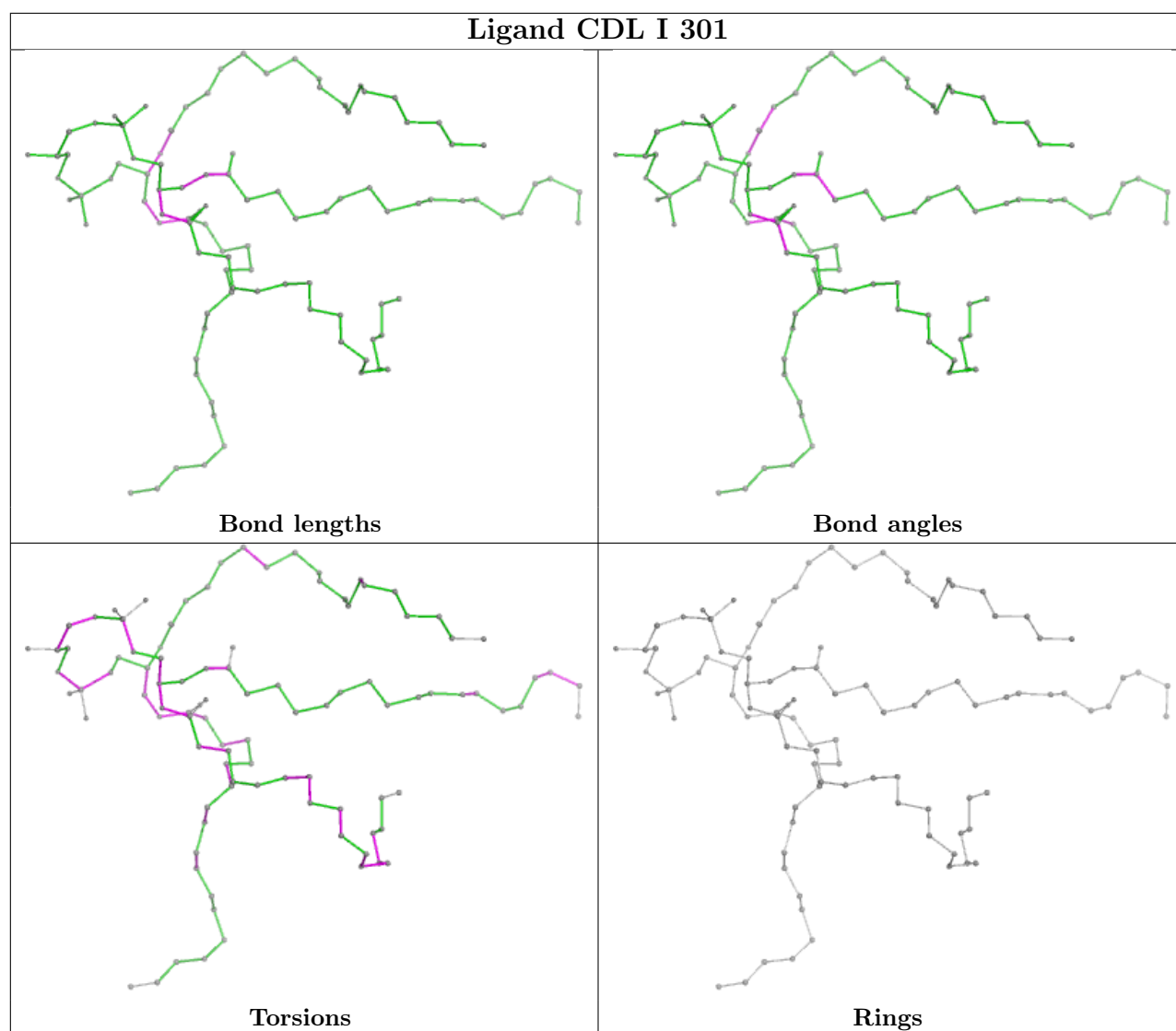


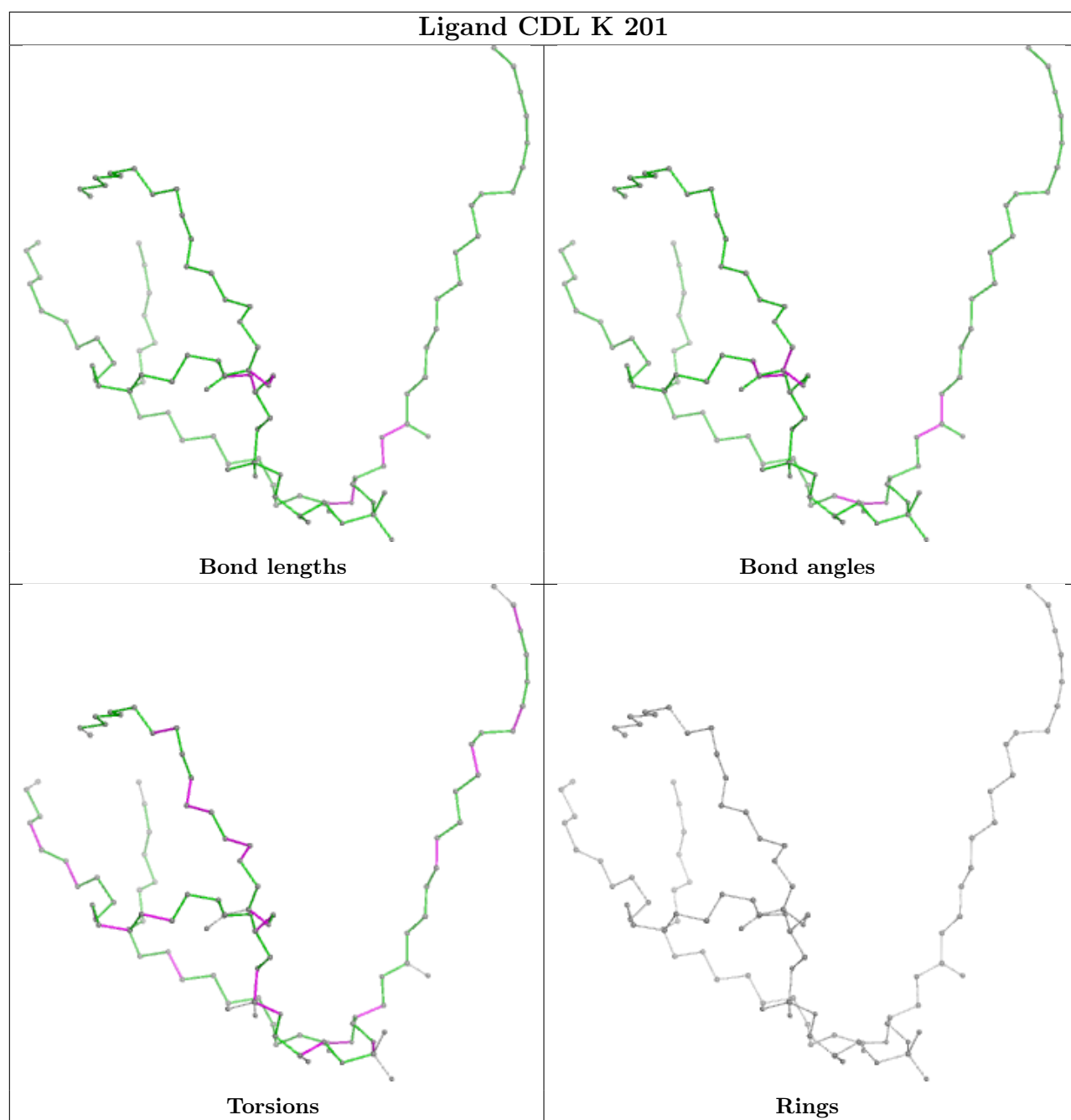


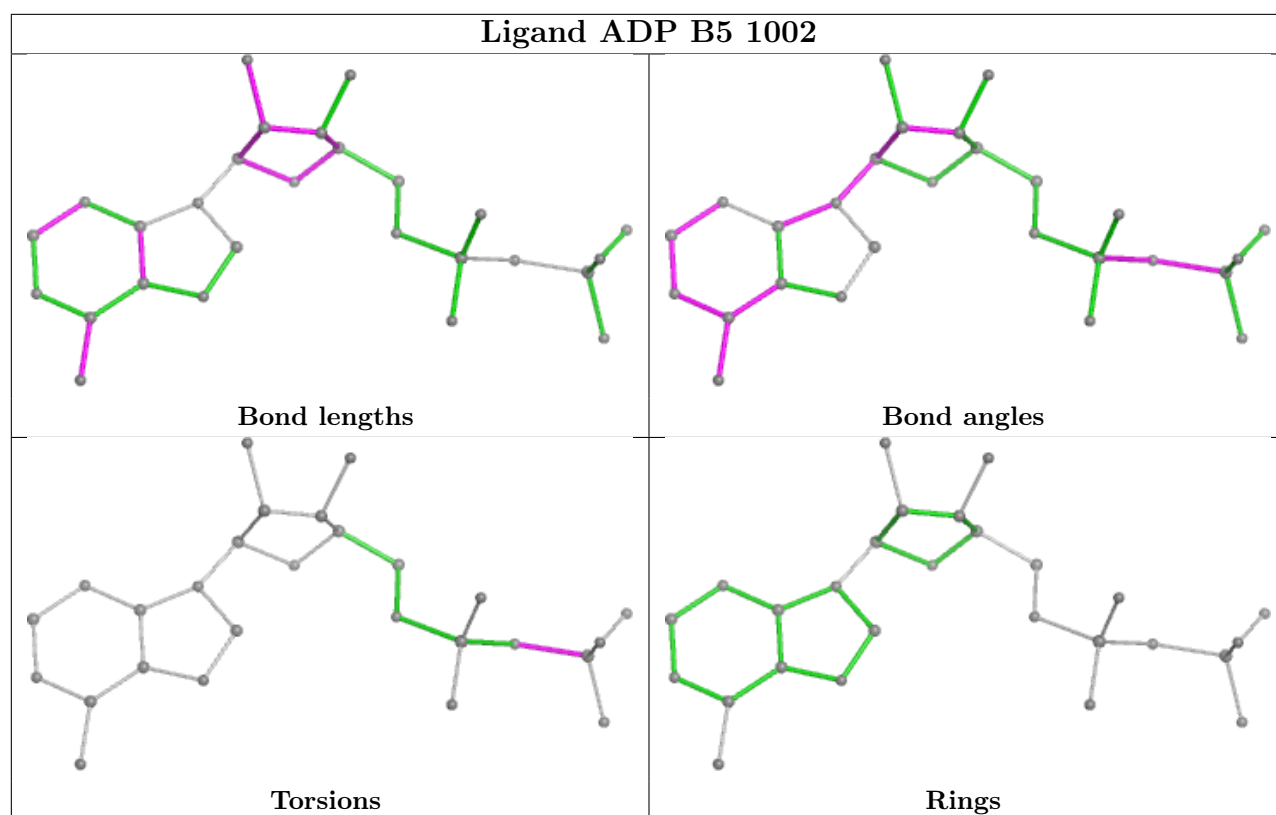












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

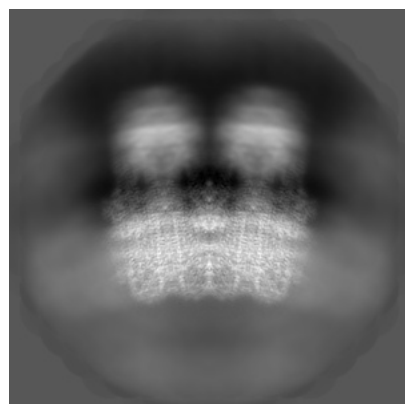
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10861. These allow visual inspection of the internal detail of the map and identification of artifacts.

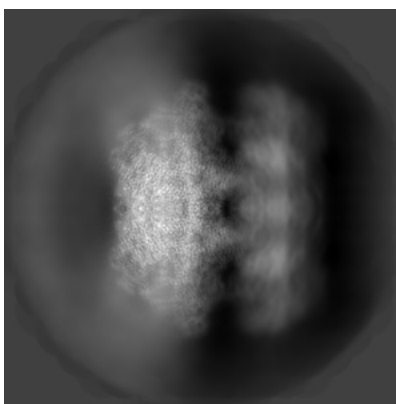
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

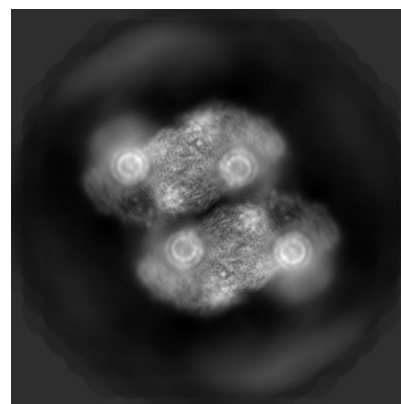
6.1.1 Primary map



X

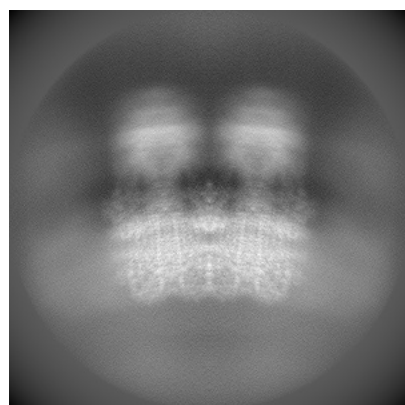


Y

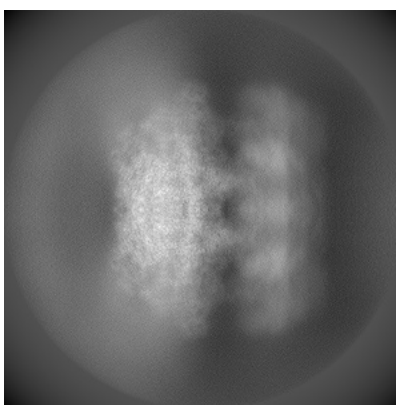


Z

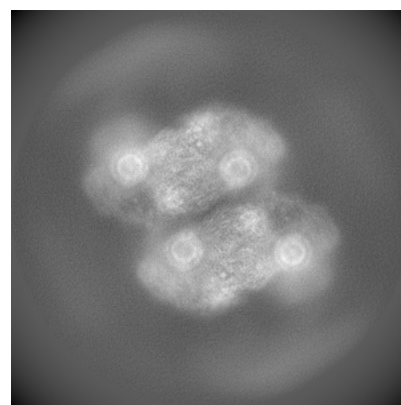
6.1.2 Raw map



X



Y

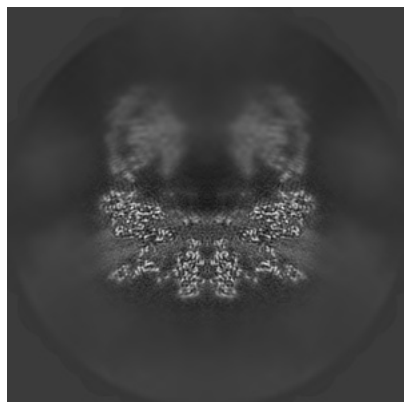


Z

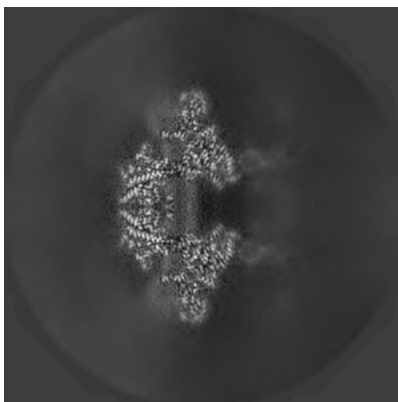
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

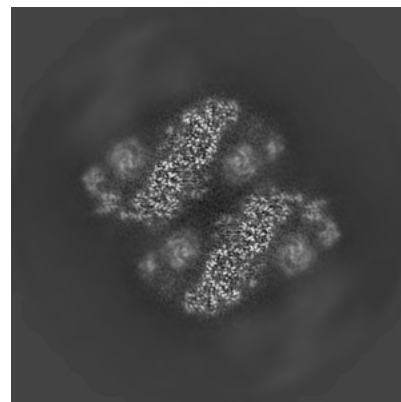
6.2.1 Primary map



X Index: 300

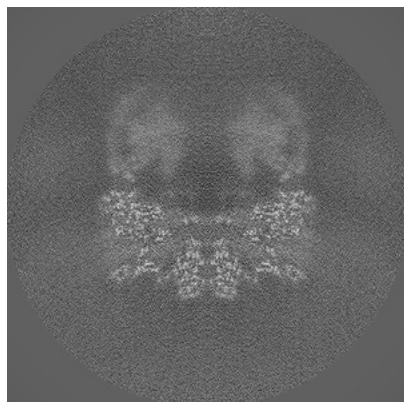


Y Index: 300

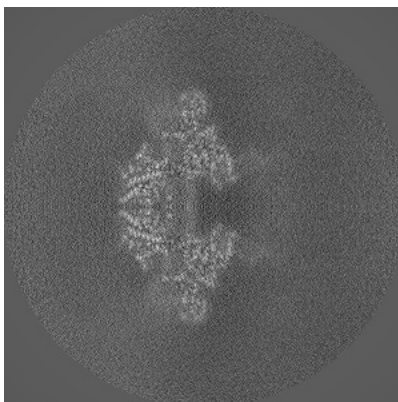


Z Index: 300

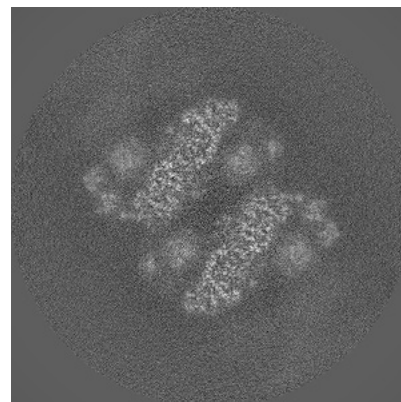
6.2.2 Raw map



X Index: 300



Y Index: 300

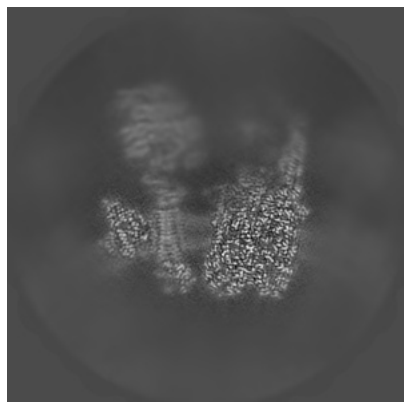


Z Index: 300

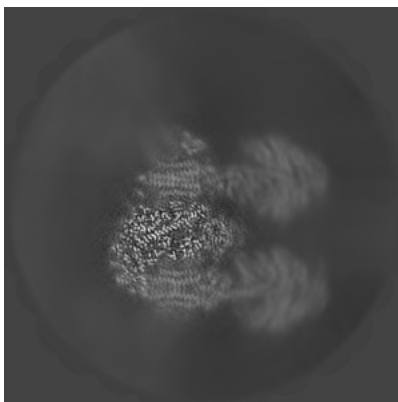
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

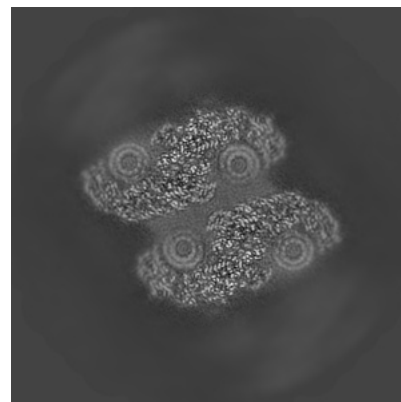
6.3.1 Primary map



X Index: 275

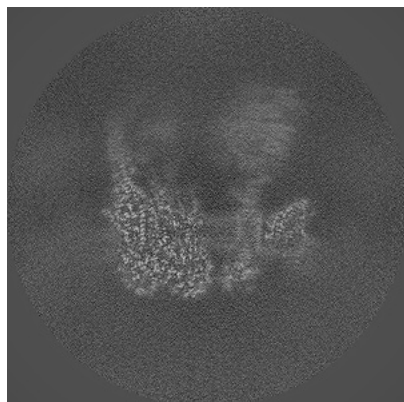


Y Index: 376

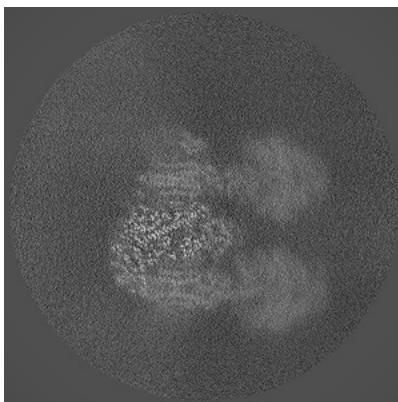


Z Index: 278

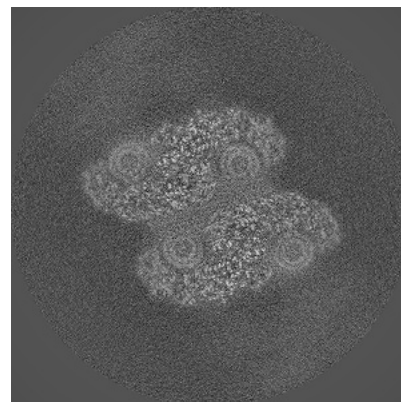
6.3.2 Raw map



X Index: 320



Y Index: 376

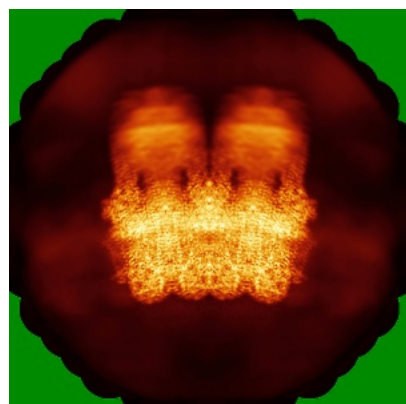


Z Index: 278

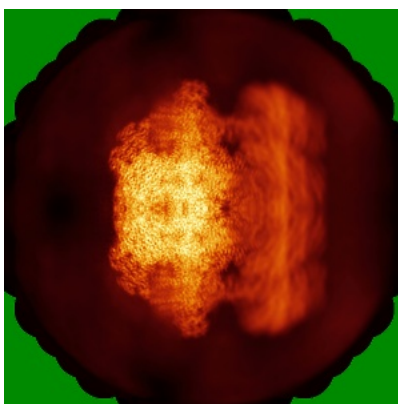
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

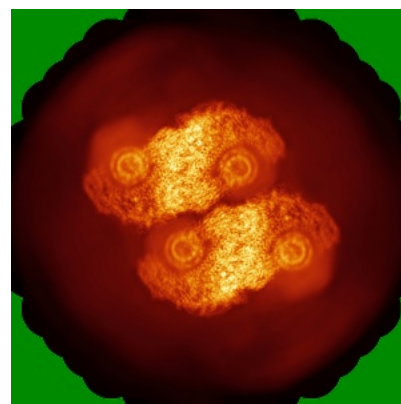
6.4.1 Primary map



X

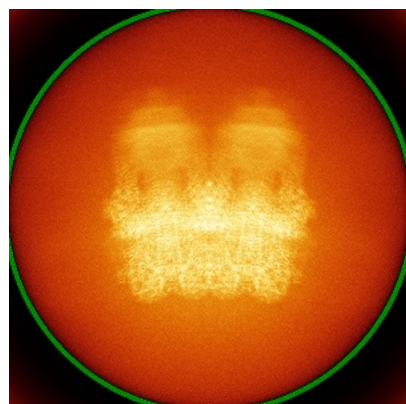


Y

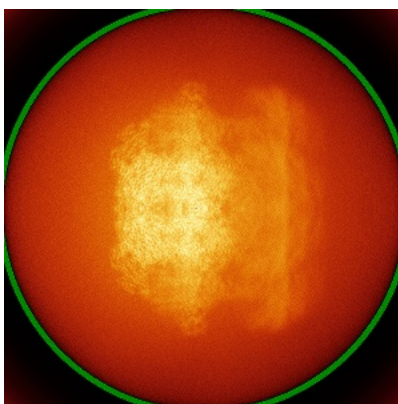


Z

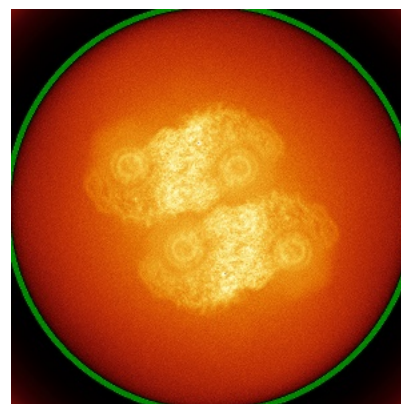
6.4.2 Raw map



X



Y



Z

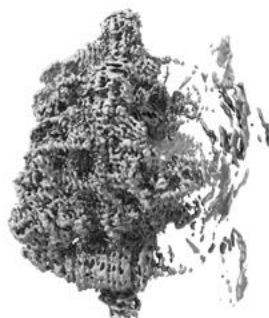
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

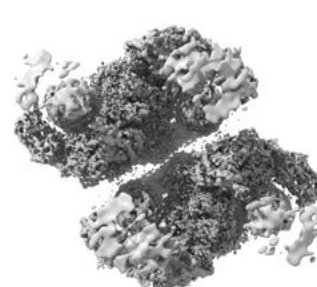
6.5.1 Primary map



X



Y



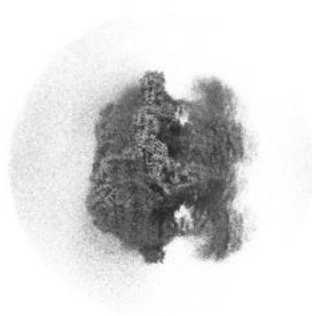
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

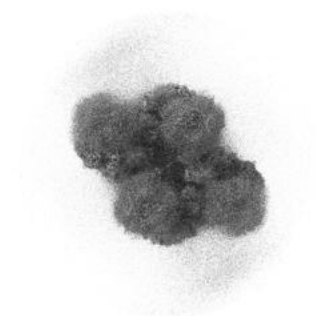
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

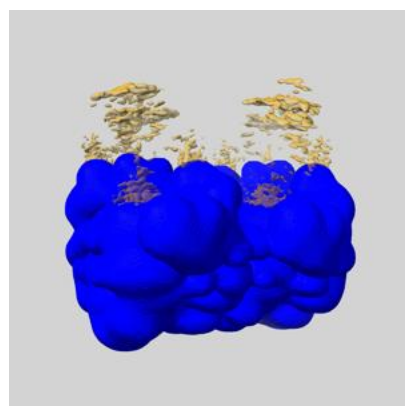
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

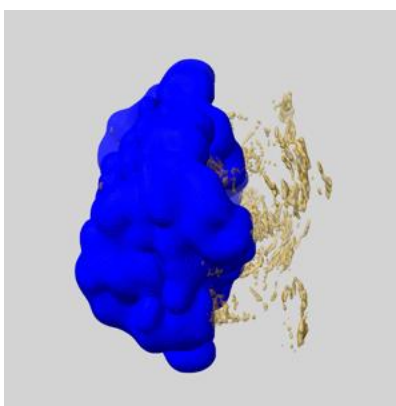
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

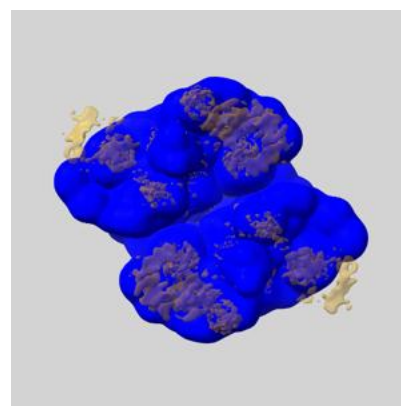
6.6.1 emd_10861_msk_1.map [i](#)



X



Y

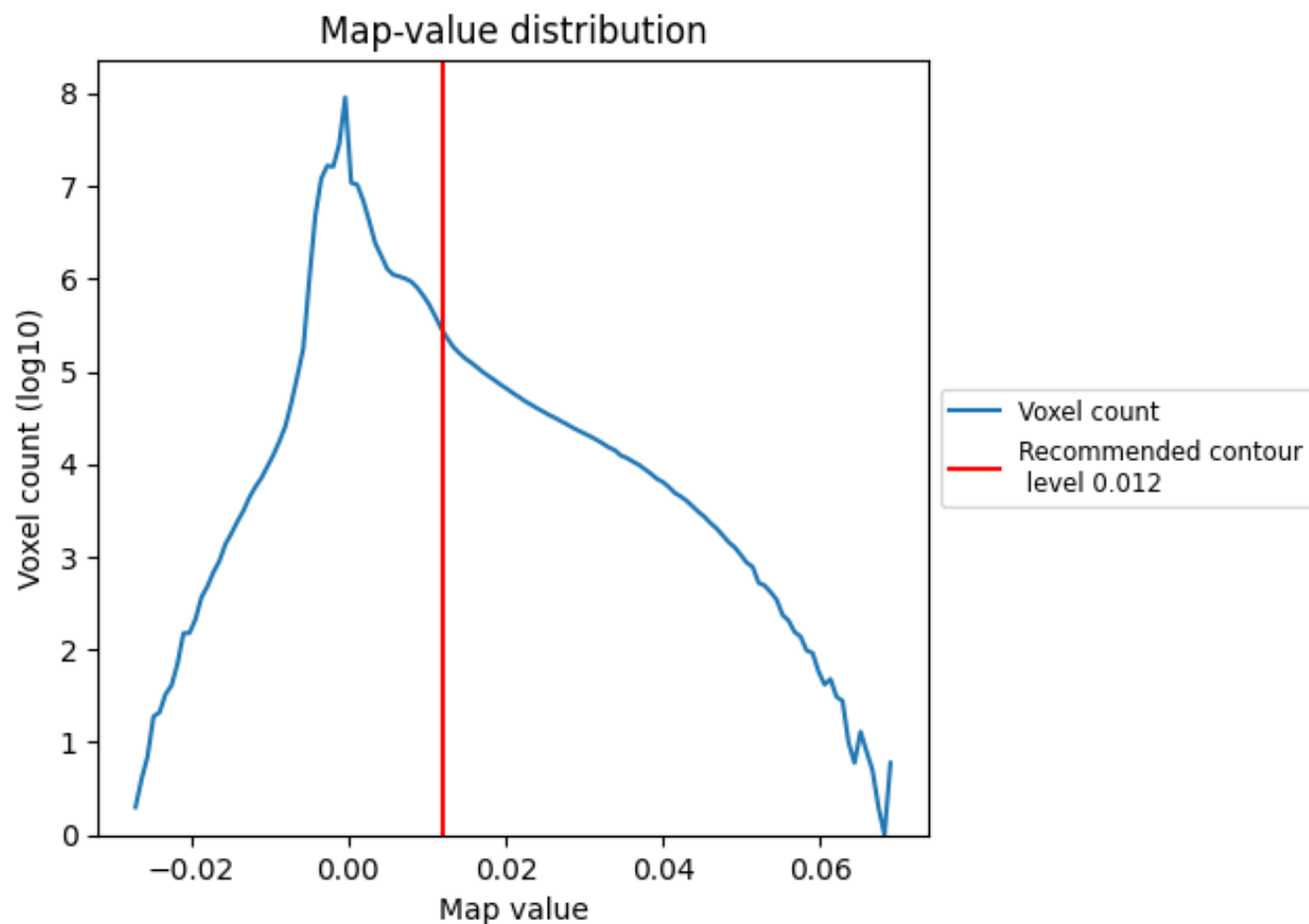


Z

7 Map analysis [i](#)

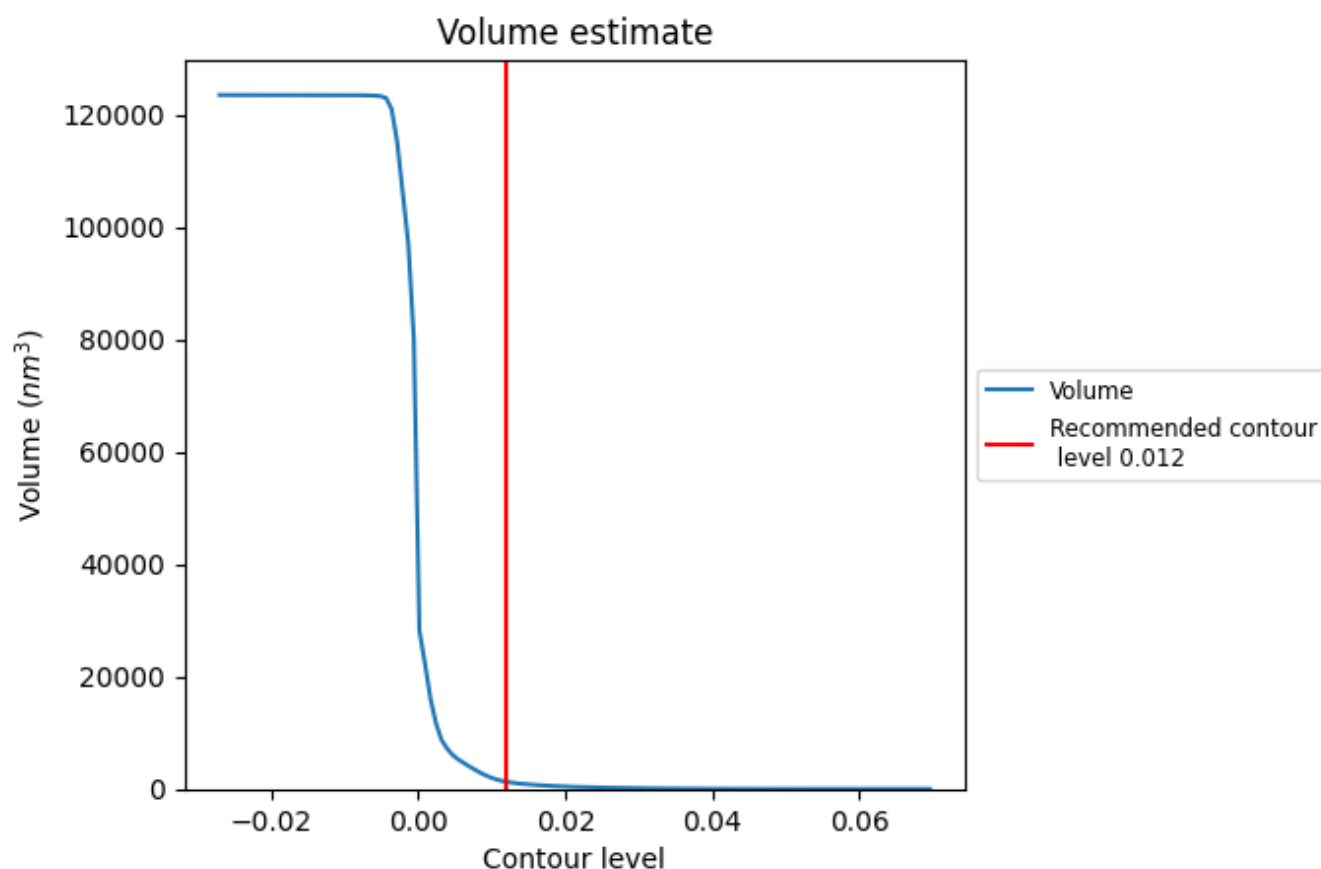
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

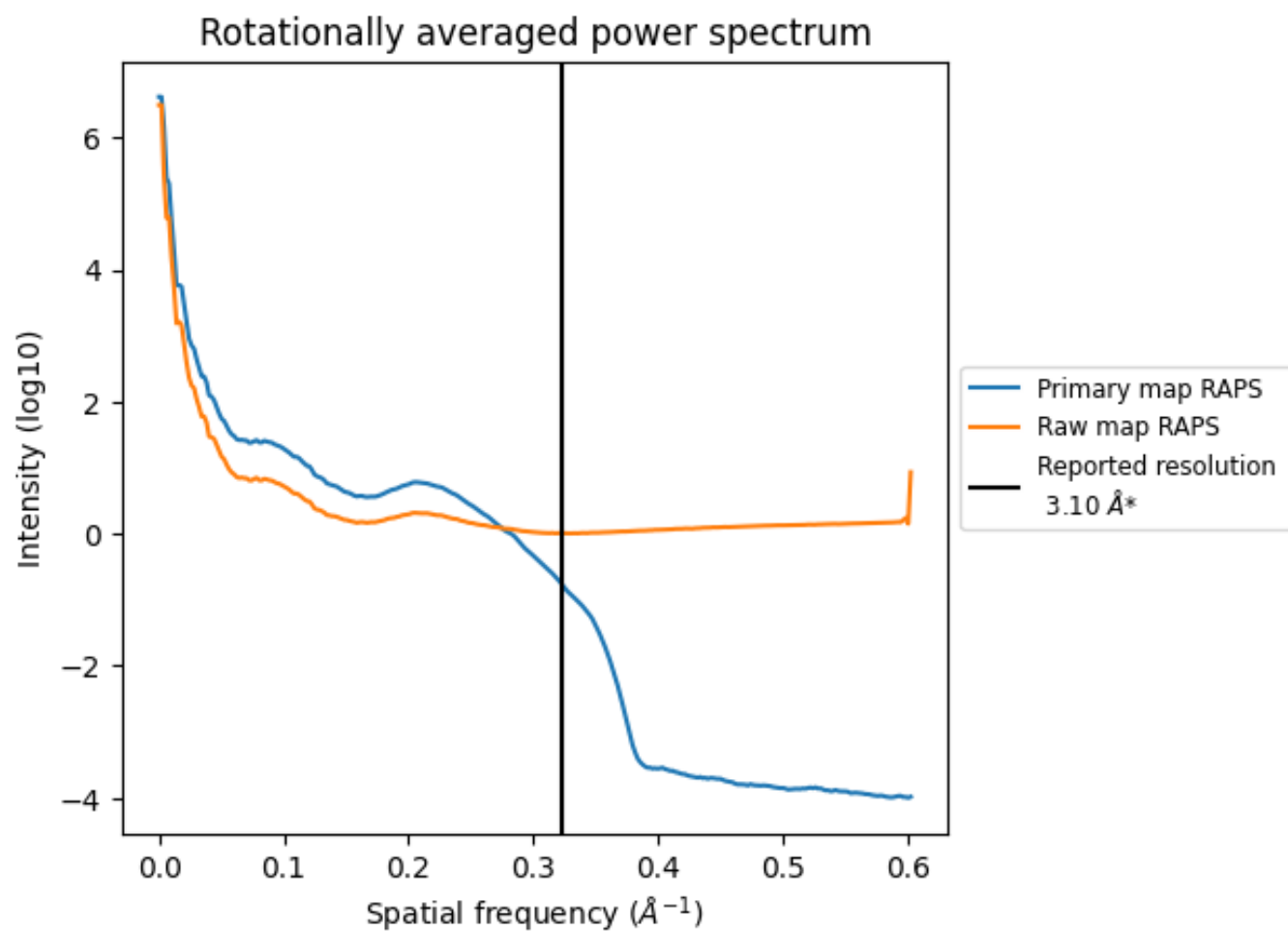
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280 nm^3 ; this corresponds to an approximate mass of 1157 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

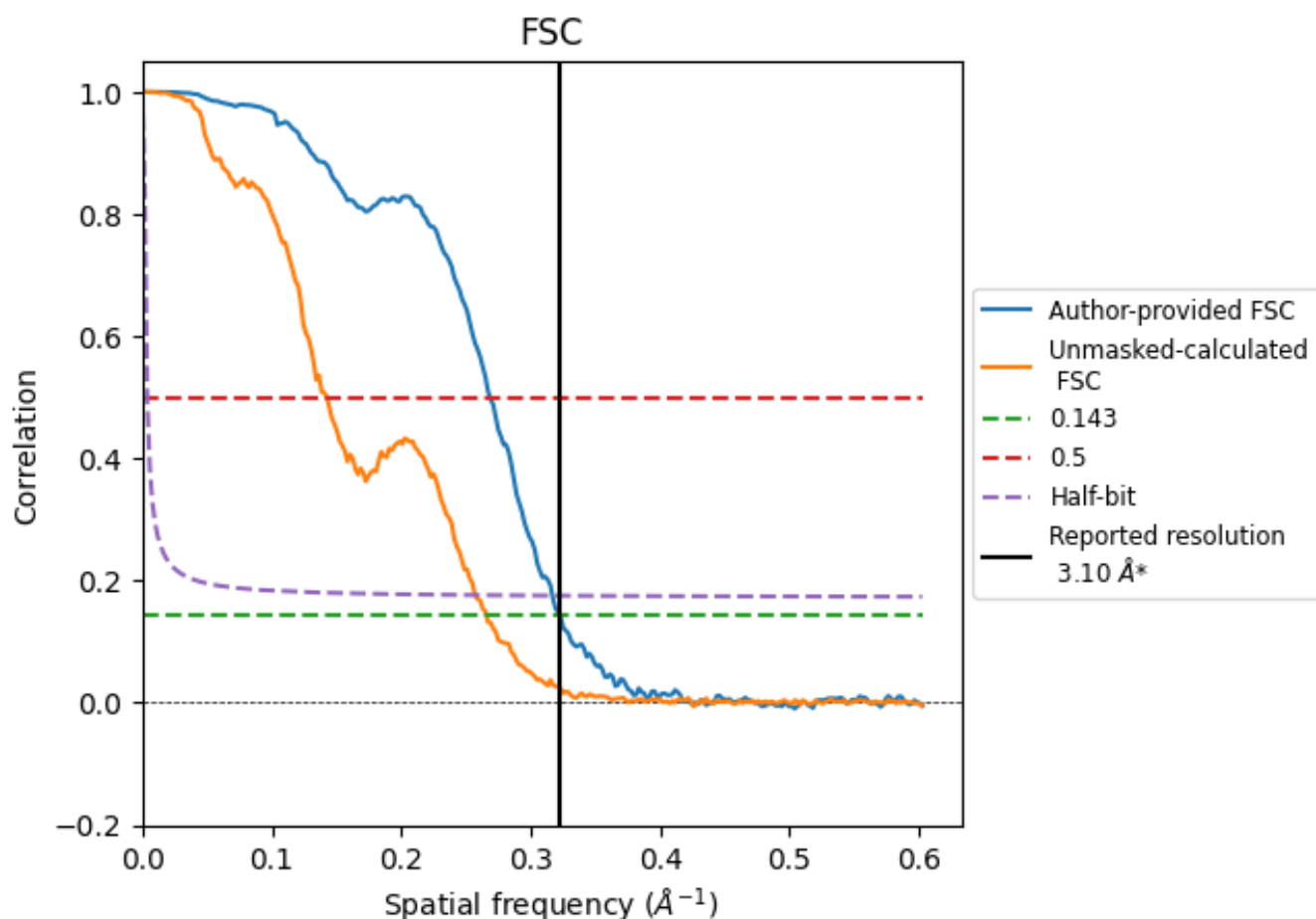


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

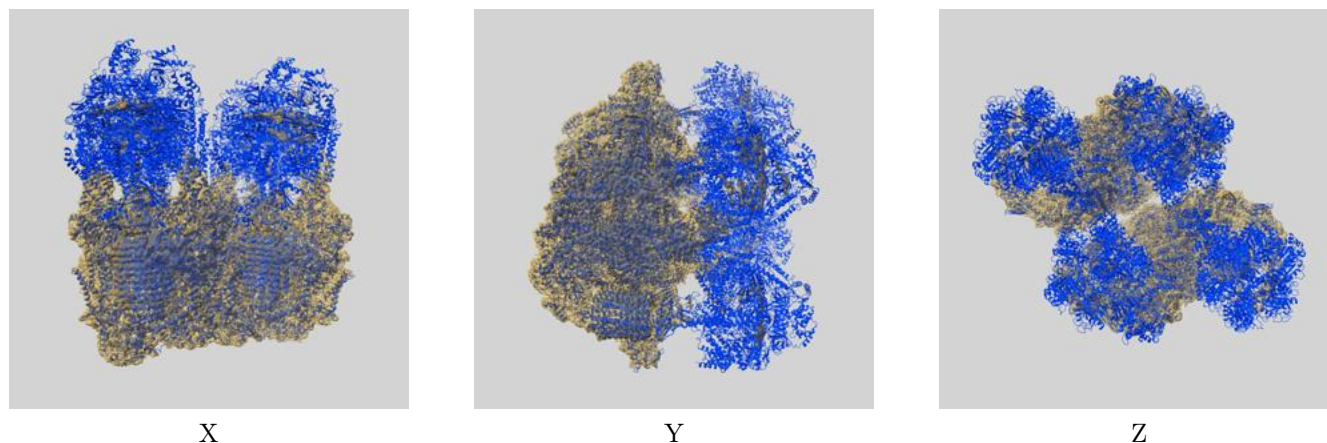
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.72	3.16
Unmasked-calculated*	3.76	7.01	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

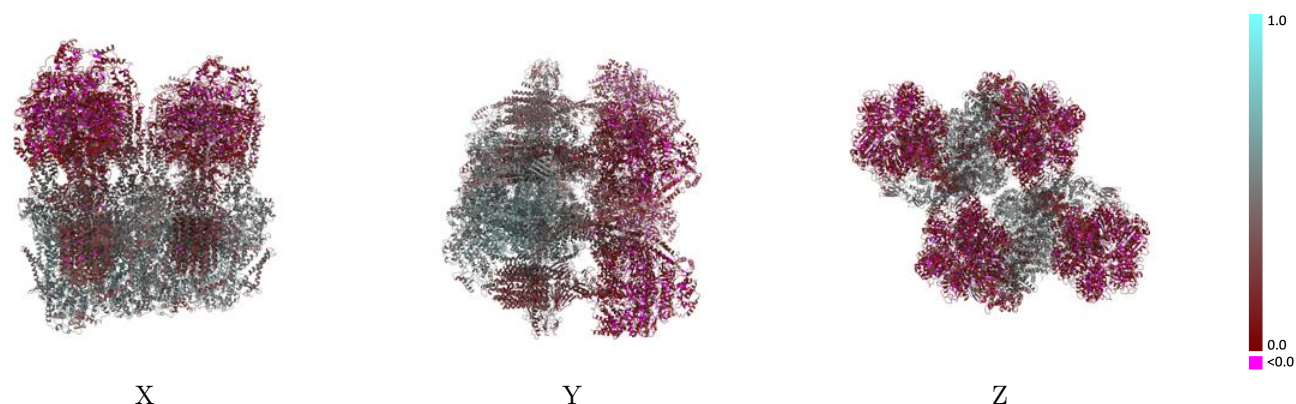
This section contains information regarding the fit between EMDB map EMD-10861 and PDB model 6YNZ. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



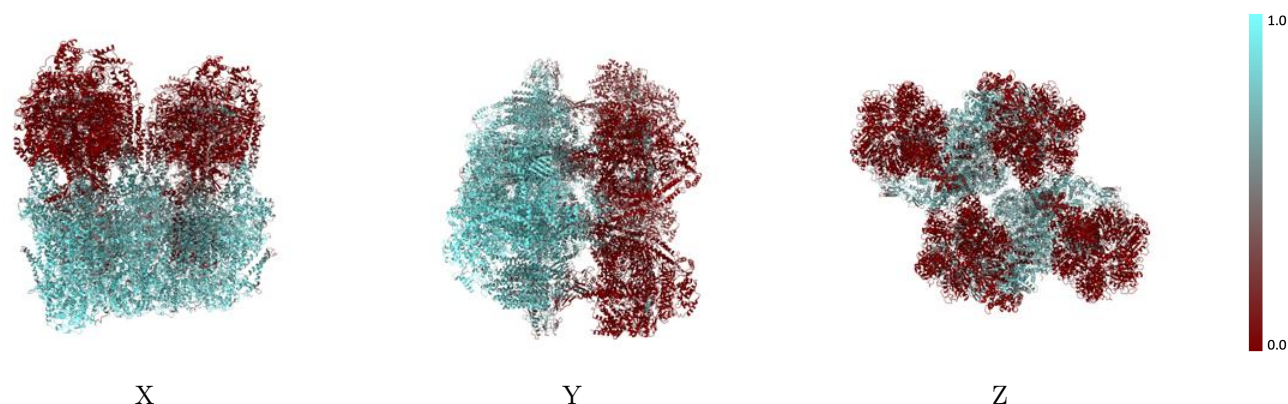
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



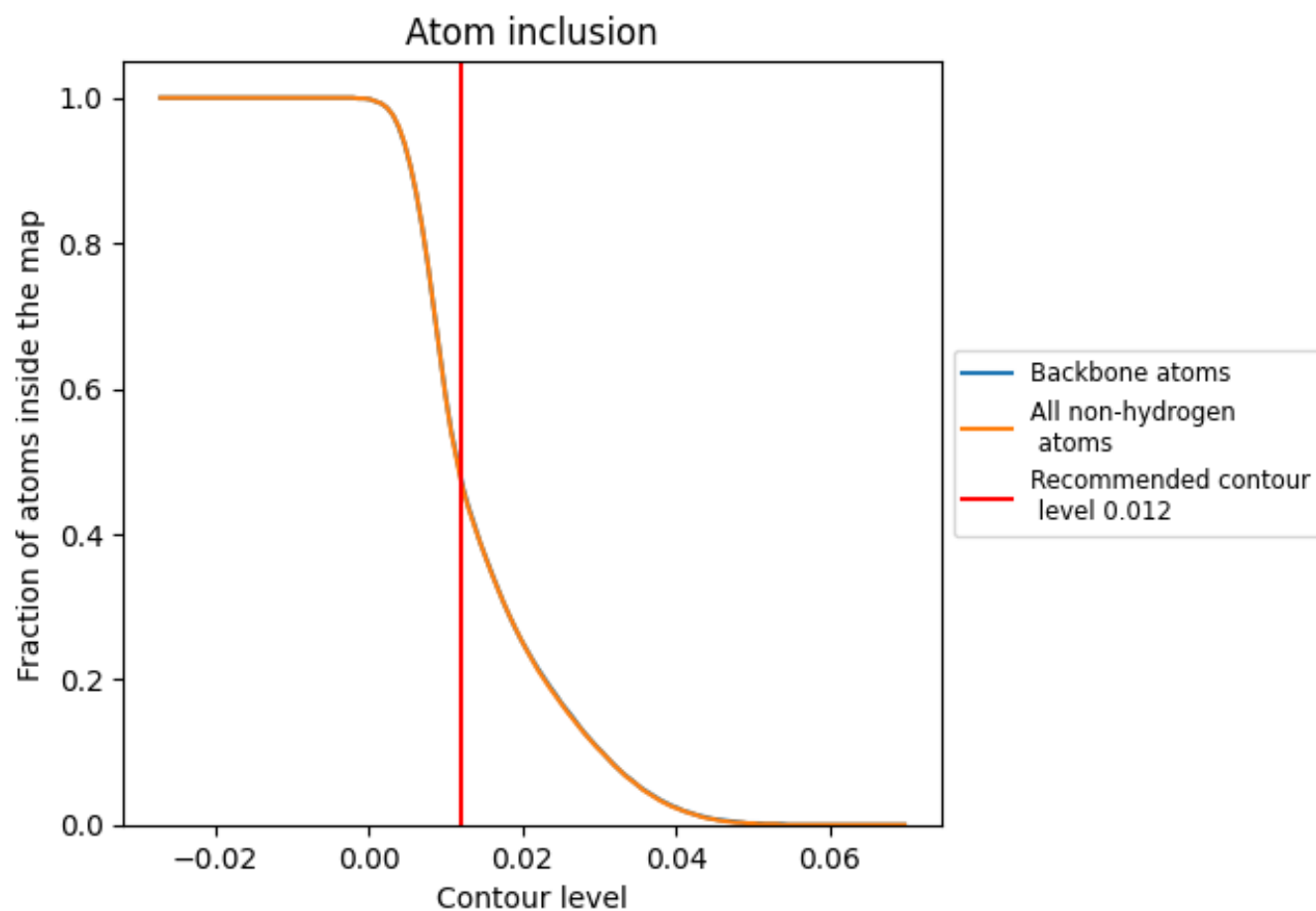
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4740	 0.3170
A	 0.8900	 0.5390
A1	 0.1400	 0.1480
A2	 0.0490	 0.1350
A3	 0.8860	 0.5350
A4	 0.0500	 0.1360
A5	 0.1440	 0.1460
B	 0.4990	 0.3720
B1	 0.0720	 0.1030
B2	 0.0260	 0.0960
B3	 0.4380	 0.3590
B4	 0.0260	 0.0910
B5	 0.0750	 0.1090
C	 0.9210	 0.5390
C1	 0.0110	 0.1020
C2	 0.0100	 0.0850
C3	 0.9010	 0.5170
C4	 0.0100	 0.0910
C5	 0.0110	 0.0980
D	 0.6370	 0.4190
D1	 0.0110	 0.1130
D2	 0.0140	 0.1060
D3	 0.5740	 0.4000
D4	 0.0150	 0.1120
D5	 0.0110	 0.1070
E	 0.6940	 0.3810
E1	 0.0850	 0.1090
E2	 0.0070	 0.0990
E3	 0.5910	 0.3760
E4	 0.0060	 0.0930
E5	 0.0840	 0.1120
F	 0.8620	 0.5330
F1	 0.0330	 0.1050
F2	 0.0300	 0.0930
F3	 0.8620	 0.5410























































































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Chain	Atom inclusion	Q-score
F4	 0.0270	 0.0900
F5	 0.0340	 0.1070
G	 0.8260	 0.4910
G1	 0.0000	 0.1100
G2	 0.0000	 0.1040
G3	 0.7570	 0.4600
G4	 0.0000	 0.1020
G5	 0.0000	 0.1110
H	 0.8440	 0.4920
H1	 0.7070	 0.3200
H2	 0.7480	 0.3540
H3	 0.7470	 0.4600
H4	 0.7370	 0.3510
H5	 0.7070	 0.3140
I	 0.8520	 0.5090
I1	 0.6670	 0.3080
I2	 0.7480	 0.3210
I3	 0.7920	 0.4940
I4	 0.7480	 0.3170
I5	 0.6640	 0.3040
J	 0.8320	 0.4970
J1	 0.5780	 0.3010
J2	 0.7500	 0.3050
J3	 0.8030	 0.4820
J4	 0.7420	 0.3020
J5	 0.5730	 0.3020
K	 0.7860	 0.4370
K1	 0.5560	 0.2960
K2	 0.6910	 0.2760
K3	 0.7690	 0.4430
K4	 0.6960	 0.2740
K5	 0.5510	 0.2980
L	 0.8910	 0.5260
L1	 0.5580	 0.3000
L2	 0.7080	 0.2540
L3	 0.8580	 0.5160
L4	 0.7000	 0.2520
L5	 0.5730	 0.3000
M	 0.9330	 0.5270
M1	 0.6370	 0.2900
M2	 0.7510	 0.2800
M3	 0.9140	 0.5170





















































































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Chain	Atom inclusion	Q-score
M4	 0.7580	 0.2820
M5	 0.6350	 0.2930
N	 0.9300	 0.5530
N1	 0.6210	 0.2830
N2	 0.7460	 0.2890
N3	 0.9090	 0.5410
N4	 0.7530	 0.2920
N5	 0.6230	 0.2860
O	 0.8700	 0.4970
O1	 0.6400	 0.2950
O2	 0.6960	 0.2760
O3	 0.8960	 0.4930
O4	 0.6920	 0.2730
O5	 0.6420	 0.2900
P	 0.7080	 0.4440
P1	 0.6820	 0.3080
P2	 0.6800	 0.3040
P3	 0.7280	 0.4340
P4	 0.6780	 0.3030
P5	 0.6890	 0.3090
Q	 0.7870	 0.4740
Q1	 0.6800	 0.3010
Q2	 0.7120	 0.3370
Q3	 0.6750	 0.4400
Q4	 0.7190	 0.3330
Q5	 0.6670	 0.3010
R	 0.8680	 0.5130
R3	 0.8260	 0.5040
S	 0.7340	 0.4300
S3	 0.6440	 0.4040
a	 0.8850	 0.5360
a3	 0.8680	 0.5290
b	 0.4400	 0.3580
b3	 0.5050	 0.3720
c	 0.8960	 0.5180
c3	 0.9180	 0.5400
d	 0.5720	 0.3980
d1	 0.2940	 0.2560
d2	 0.3590	 0.2310
d3	 0.6370	 0.4210
d4	 0.3510	 0.2340
d5	 0.2900	 0.2610




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Chain	Atom inclusion	Q-score
e	 0.5840	 0.3730
e1	 0.2350	 0.2080
e2	 0.2600	 0.2250
e3	 0.6960	 0.3810
e4	 0.2630	 0.2310
e5	 0.2270	 0.2020
f	 0.7670	 0.5250
f3	 0.8120	 0.5360
g	 0.7460	 0.4620
g1	 0.1590	 0.2070
g2	 0.1950	 0.2080
g3	 0.8180	 0.4890
g4	 0.1970	 0.2050
g5	 0.1610	 0.2050
h	 0.7220	 0.4690
h3	 0.8190	 0.5010
i	 0.8250	 0.4940
i1	 0.0400	 0.1780
i2	 0.0700	 0.1820
i3	 0.8470	 0.5160
i4	 0.0910	 0.2000
i5	 0.0300	 0.1910
j	 0.8010	 0.4810
j3	 0.8380	 0.4910
k	 0.7840	 0.4400
k3	 0.7920	 0.4370
l	 0.8520	 0.5170
l3	 0.8930	 0.5230
m	 0.9040	 0.5140
m3	 0.9320	 0.5230
n	 0.9070	 0.5410
n3	 0.9280	 0.5530
o	 0.8960	 0.4970
o3	 0.8580	 0.4950
p	 0.7170	 0.4310
p3	 0.7090	 0.4430
q	 0.6780	 0.4440
q3	 0.7860	 0.4720
r	 0.7860	 0.4940
r3	 0.8700	 0.5200
s	 0.5440	 0.3940
s3	 0.7000	 0.4300

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Chain	Atom inclusion	Q-score
t	 0.5330	 0.3790
t3	 0.6050	 0.4000