



Full wwPDB EM Validation Report ⓘ

Sep 24, 2024 – 02:09 am BST

PDB ID : 8PW5
EMDB ID : EMD-17989
Title : CS respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.60 Å(reported)
Based on initial models : 6g2j, 7o3c

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:

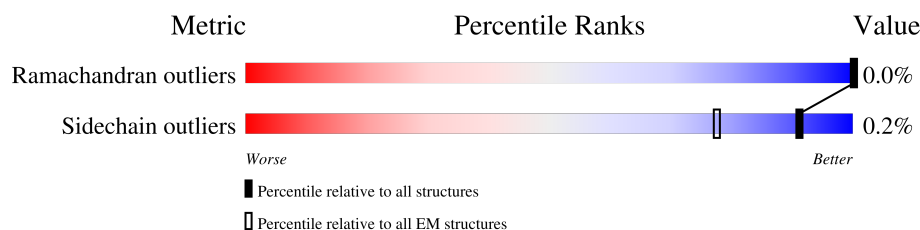
EMDB validation analysis : 0.0.1.dev112
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

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 3.60 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.



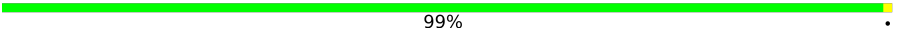















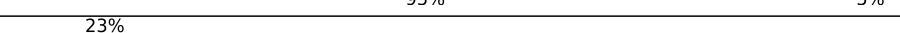
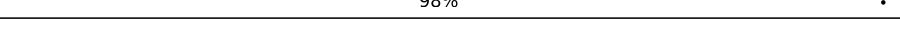
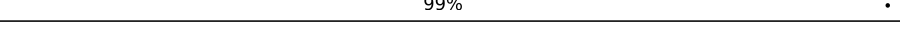
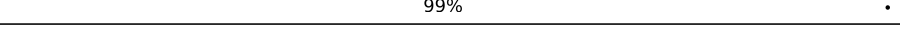
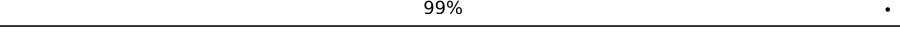
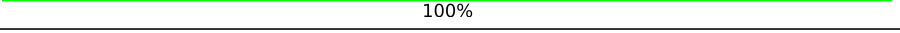
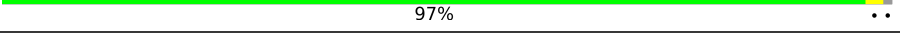
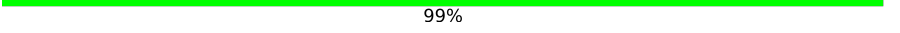

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	g	111	
1	t	111	
2	m	69	
2	z	69	
3	A	480	
3	L	480	
4	B	453	
4	M	453	
5	C	381	







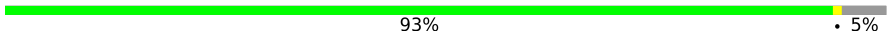










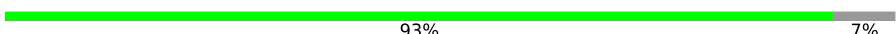
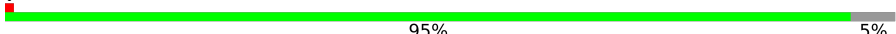






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Mol	Chain	Length	Quality of chain
5	N	381	 99%
6	D	325	 74% 26%
6	O	325	 74% 26%
7	E	274	 32% 72% 28%
7	P	274	 35% 71% 28%
7	T	274	 28% 72%
8	F	111	 87% 12%
8	Q	111	 91% 8%
9	G	82	 94% 6%
9	R	82	 94% 6%
10	H	89	 73% 26%
10	S	89	 76% 24%
11	J	64	 94% 6%
11	U	64	 5% 94% 6%
12	K	56	 18% 91% 7%
12	V	56	 11% 95% 5%
13	I	113	 23% 98%
14	a	514	 99%
14	n	514	 99%
15	b	227	 99%
15	o	227	 100%
16	c	261	 97%
16	p	261	 99%
17	d	169	 82% 18%
17	q	169	 82% 18%


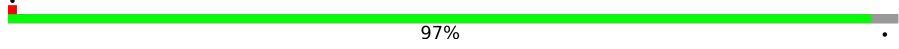

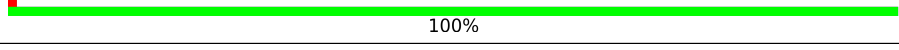

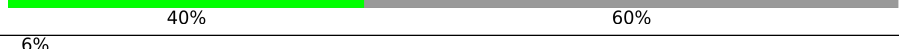
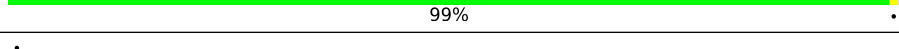
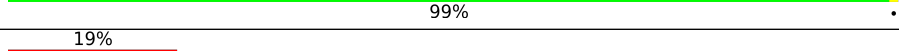
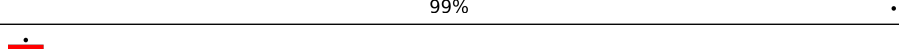
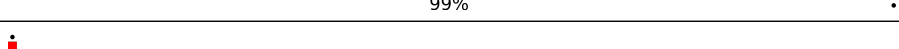
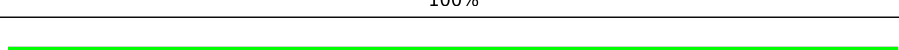
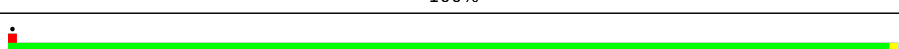
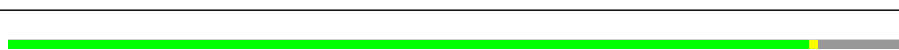
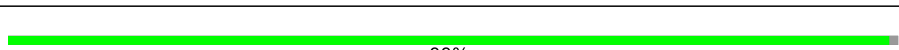
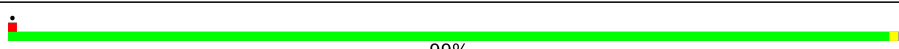

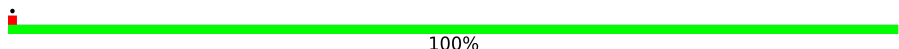
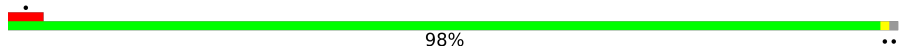

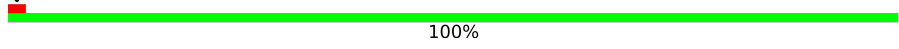
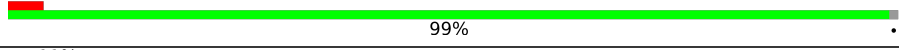
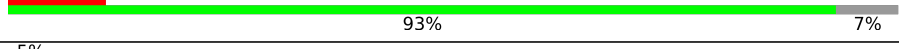



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Mol	Chain	Length	Quality of chain
18	e	146	
18	r	146	
19	f	128	
19	s	128	
20	h	86	
20	u	86	
21	i	76	
21	v	76	
22	k	80	
22	x	80	
23	l	63	
23	y	63	
24	w	83	
25	6	224	
26	C1	263	
27	D1	463	
28	2	248	
29	1	464	
30	3	727	
31	9	212	
32	P1	377	
33	Q1	175	
34	7	116	
35	S1	99	
36	T1	156	

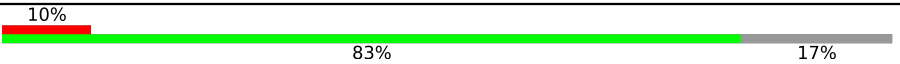

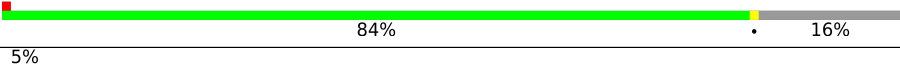
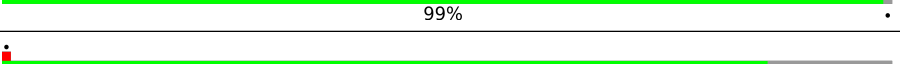
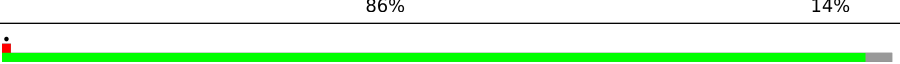
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Mol	Chain	Length	Quality of chain
36	U1	156	
37	V1	116	
38	W1	131	
39	q1	145	
40	r1	113	
41	s1	104	
42	A1	115	
43	H1	318	
44	J1	172	
45	K1	98	
46	L1	607	
47	M1	459	
48	N1	345	
49	O1	355	
50	X1	172	
51	Y1	141	
52	Z1	144	
53	a1	70	
54	b1	84	
55	c1	76	
56	d1	120	
57	e1	106	
58	f1	57	
59	g1	151	
60	h1	189	

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Mol	Chain	Length	Quality of chain
61	i1	128	
62	j1	105	
63	k1	104	
64	l1	186	
65	m1	129	
66	n1	179	
67	o1	137	
68	p1	176	

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 130610 atoms, of which 0 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 Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	76	Total	C	N	O	S	0	0
			620	404	112	102	2		
1	g	76	Total	C	N	O	S	0	0
			620	404	112	102	2		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	44	Total	C	N	O	S	0	0
			343	220	59	61	3		
2	z	44	Total	C	N	O	S	0	0
			343	220	59	61	3		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
3	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
4	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 5 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
5	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 6 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		
6	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	196	Total	C	N	O	S	0	0
			1167	705	219	237	6		
7	P	196	Total	C	N	O	S	0	0
			1164	702	219	237	6		
7	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	98	Total	C	N	O	S	0	0
			865	552	154	156	3		
8	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	77	Total	C	N	O	S	0	0
			654	424	120	109	1		
9	R	77	Total	C	N	O	S	0	0
			654	424	120	109	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
10	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	60	Total	C	N	O		0	0
			495	323	86	86			
11	U	60	Total	C	N	O		0	0
			495	323	86	86			

- Molecule 12 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	52	Total	C	N	O	S	0	0
			430	287	76	66	1		
12	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 13 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	111	Total	C	N	O	S	0	0
			807	520	138	144	5		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		
14	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		
15	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		
16	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		
17	d	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		
18	e	103	Total	C	N	O	S	0	0
			833	533	140	158	2		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	94	Total	C	N	O	S	0	0
			721	449	126	138	8		
19	f	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	79	Total	C	N	O	S	0	0
			654	416	116	117	5		
20	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		
21	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		
22	k	48	Total	C	N	O	S	0	0
			378	245	64	67	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		
23	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	57	Total	C	N	O	S	0	0
			435	283	71	78	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C1	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D1	430	Total	C	N	O	S	0	0
			3464	2215	595	630	24		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P1	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q1	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S1	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 36 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T1	79	Total	C	N	O	S	0	0
			637	410	95	127	5		
36	U1	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V1	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W1	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q1	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r1	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	s1	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A1	115	Total	C	N	O	S	0	0
			932	633	132	160	7		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	H1	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	J1	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	K1	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L1	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M1	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N1	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O1	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	X1	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Y1	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Z1	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a1	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	b1	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	c1	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	d1	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	e1	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	f1	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	g1	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	h1	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	i1	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	j1	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	k1	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	l1	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	m1	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	n1	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

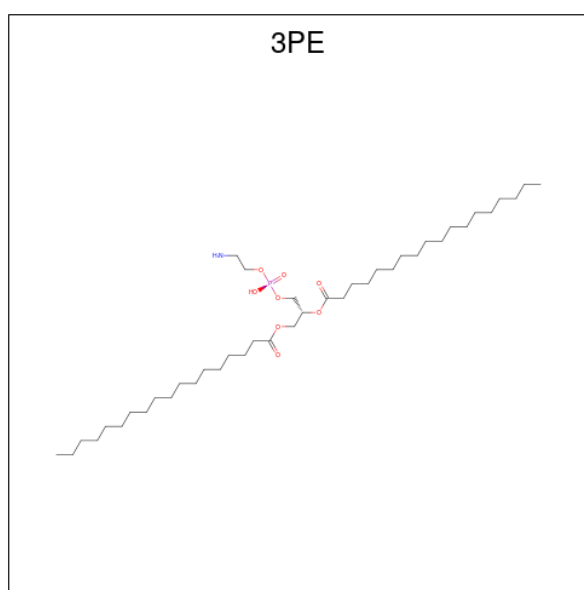
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	o1	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	p1	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



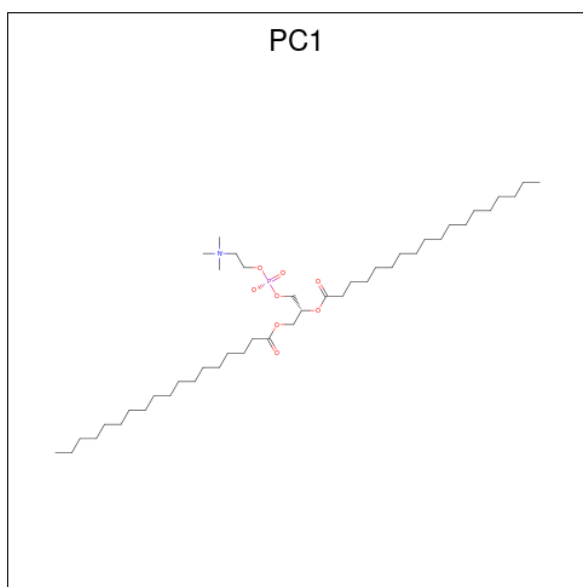
Mol	Chain	Residues	Atoms					AltConf
69	t	1	Total	C	N	O	P	0
			25	15	1	8	1	
69	z	1	Total	C	N	O	P	0
			26	16	1	8	1	
69	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
69	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
69	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
69	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	n	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	r1	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	H1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	

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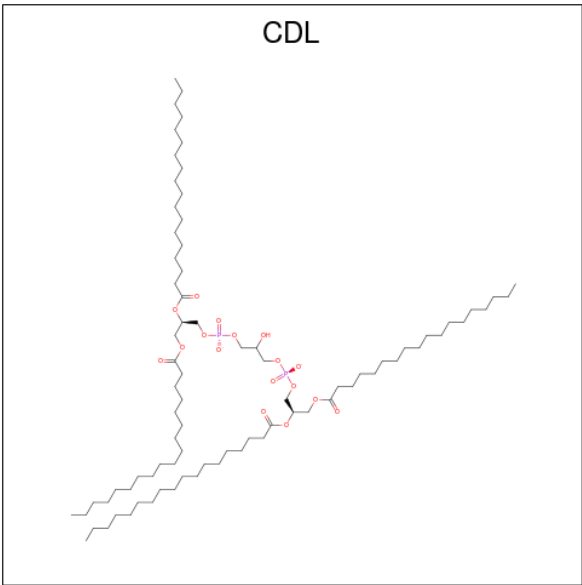
Mol	Chain	Residues	Atoms					AltConf
69	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	b1	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	m1	1	Total	C	N	O	P	0
			36	26	1	8	1	
69	a	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	a	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	c	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	d	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	g	1	Total	C	N	O	P	0
			25	15	1	8	1	
69	i	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
70	z	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	K	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
70	V	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	I	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	p	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
70	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	P1	1	Total	C	N	O	P	0
			31	21	1	8	1	
70	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	g	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 71 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



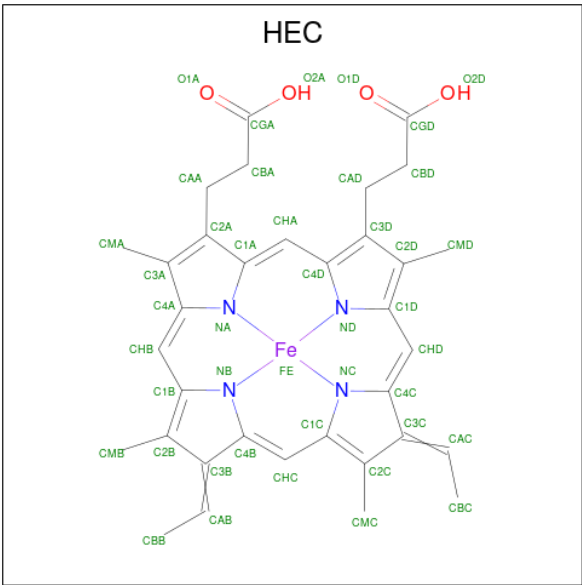
Mol	Chain	Residues	Atoms				AltConf
71	A	1	Total	C	O	P	0
			46	27	17	2	
71	D	1	Total	C	O	P	0
			56	37	17	2	
71	G	1	Total	C	O	P	0
			42	23	17	2	
71	L	1	Total	C	O	P	0
			46	27	17	2	
71	O	1	Total	C	O	P	0
			57	38	17	2	
71	R	1	Total	C	O	P	0
			41	22	17	2	
71	R	1	Total	C	O	P	0
			57	38	17	2	
71	R	1	Total	C	O	P	0
			72	53	17	2	
71	V	1	Total	C	O	P	0
			46	27	17	2	
71	r1	1	Total	C	O	P	0
			57	38	17	2	
71	H1	1	Total	C	O	P	0
			51	33	16	2	
71	L1	1	Total	C	O	P	0
			78	59	17	2	
71	L1	1	Total	C	O	P	0
			46	27	17	2	
71	N1	1	Total	C	O	P	0
			90	71	17	2	

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Mol	Chain	Residues	Atoms				AltConf
71	Y1	1	Total 94	C 75	O 17	P 2	0
71	d1	1	Total 67	C 48	O 17	P 2	0
71	h1	1	Total 70	C 51	O 17	P 2	0
71	g	1	Total 38	C 20	O 16	P 2	0

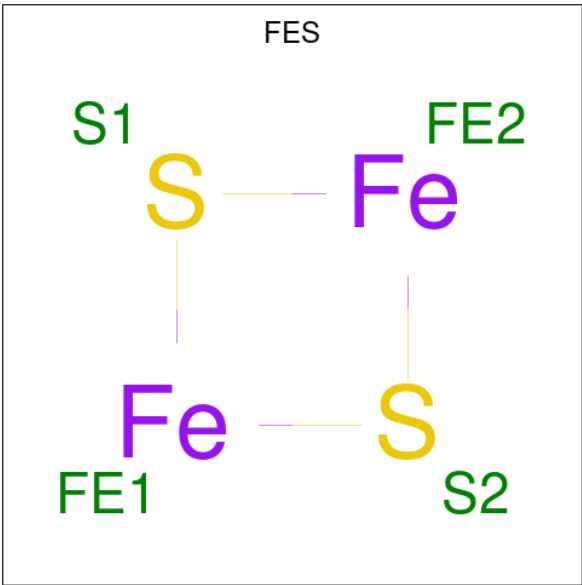
- # HEM

- Molecule 73 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
73	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
74	E	1	Total	Fe	S	0
			4	2	2	
74	P	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
74	2	1	Total	Fe	S	0
			4	2	2	
74	3	1	Total	Fe	S	0
			4	2	2	

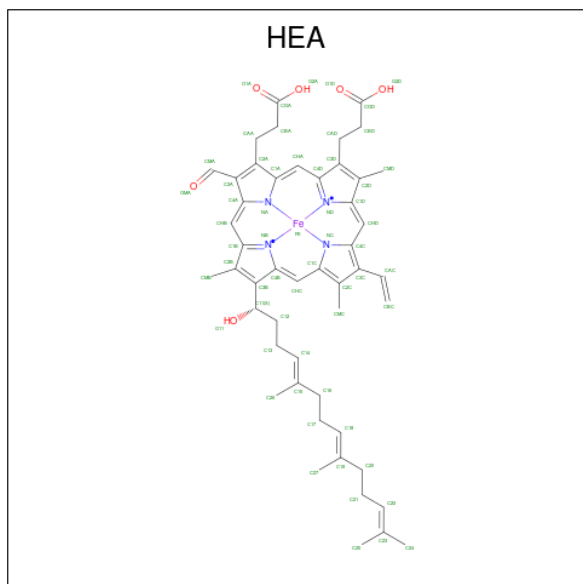
- Molecule 75 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total	Cu	0
			1	1	
75	a	1	Total	Cu	0
			1	1	

- Molecule 76 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
76	n	1	Total	Na	0
			1	1	
76	a	1	Total	Na	0
			1	1	

- Molecule 77 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
77	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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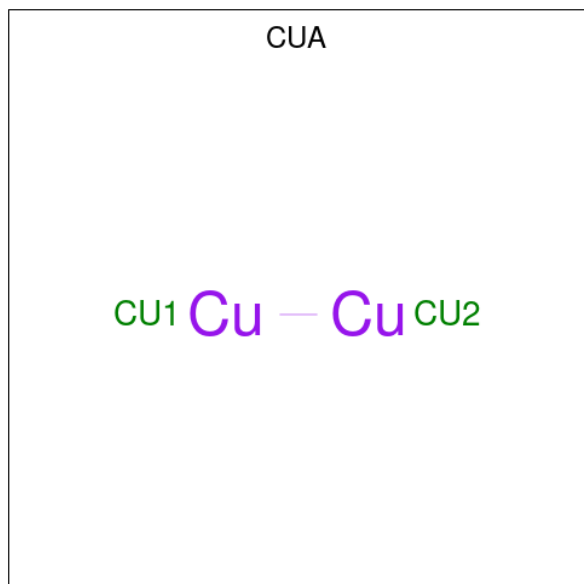
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Mol	Chain	Residues	Atoms					AltConf
77	n	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	o	1	Total	Mg	0
			1	1	
78	O1	1	Total	Mg	0
			1	1	
78	a	1	Total	Mg	0
			1	1	

- Molecule 79 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).

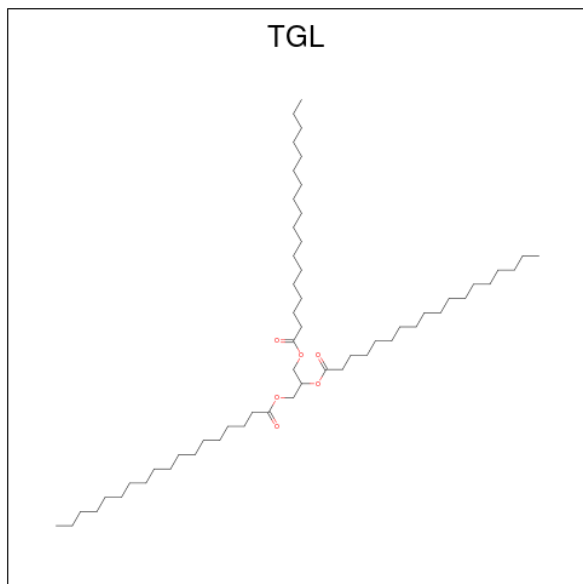


Mol	Chain	Residues	Atoms		AltConf
79	o	1	Total	Cu	0
			2	2	
79	b	1	Total	Cu	0
			2	2	

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

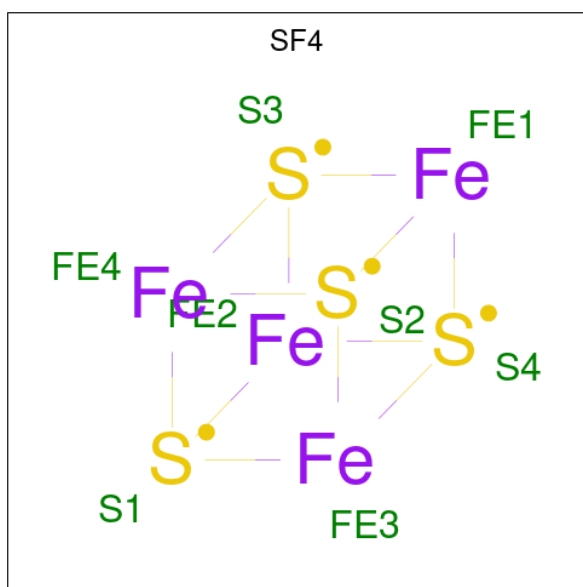
Mol	Chain	Residues	Atoms		AltConf
80	s	1	Total	Zn	0
			1	1	
80	7	1	Total	Zn	0
			1	1	
80	f	1	Total	Zn	0
			1	1	

- Molecule 81 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



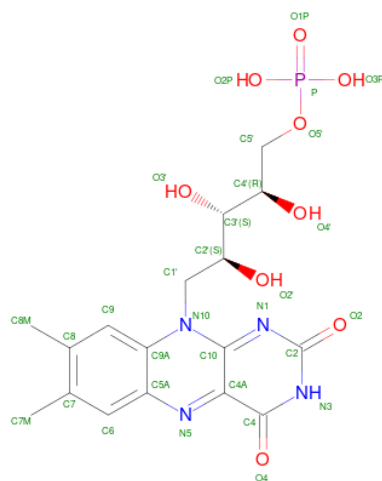
Mol	Chain	Residues	Atoms			AltConf
81	y	1	Total	C	O	0
			37	31	6	
81	l	1	Total	C	O	0
			37	31	6	

- Molecule 82 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
82	6	1	Total	Fe	S	0
			8	4	4	
82	1	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 83 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

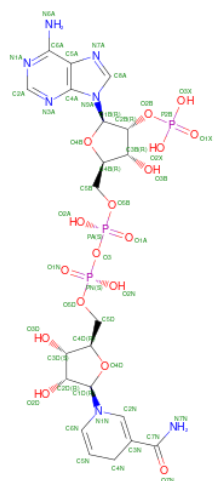


Mol	Chain	Residues	Atoms					AltConf
83	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

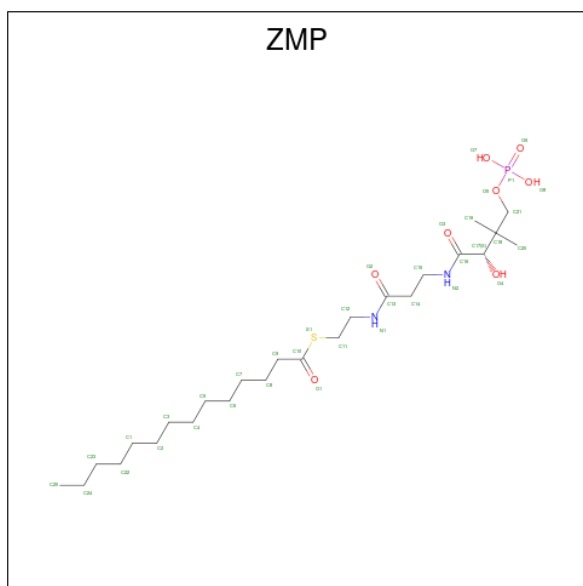
Mol	Chain	Residues	Atoms	AltConf
84	3	1	Total K 1 1	0

- Molecule 85 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
85	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 86 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
86	W1	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
86	n1	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

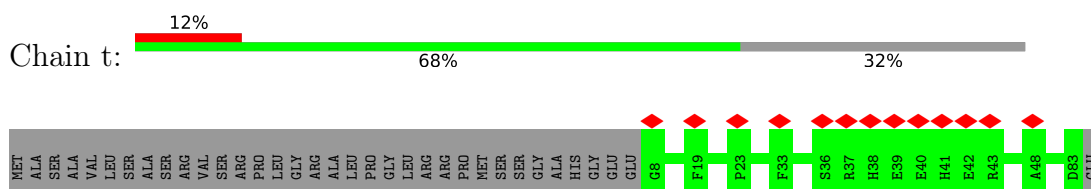
- Molecule 87 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



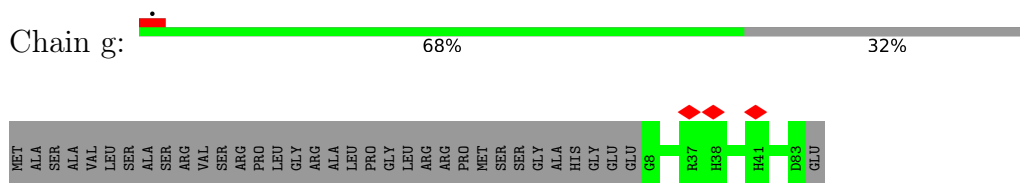
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

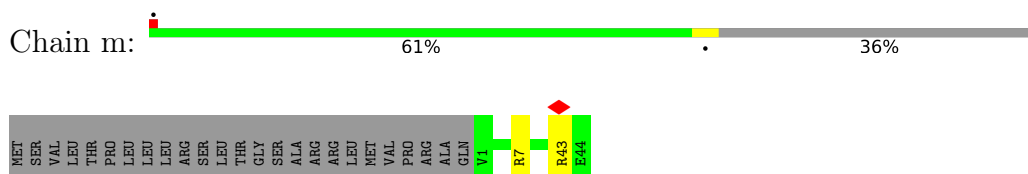
- Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial



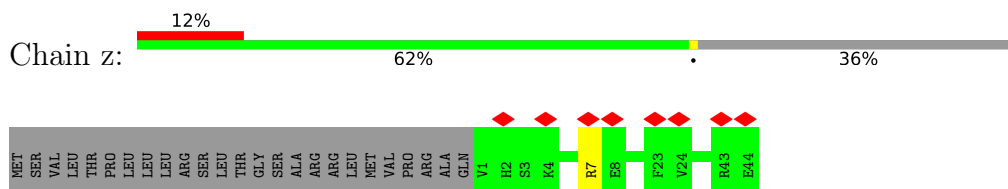
- Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial



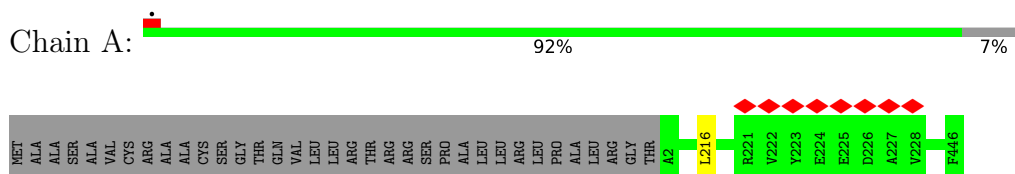
- Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial



- Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial

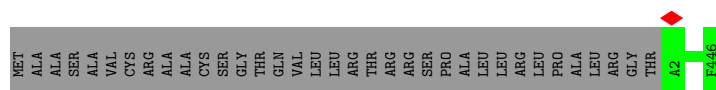


- Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial



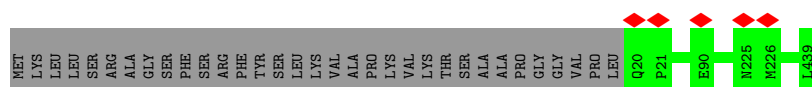
- Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:  93% 7%



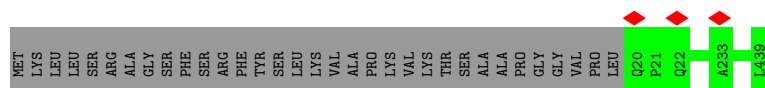
- Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  93% 7%



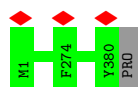
- Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  93% 7%



- Molecule 5: Cytochrome b

Chain C:  100%



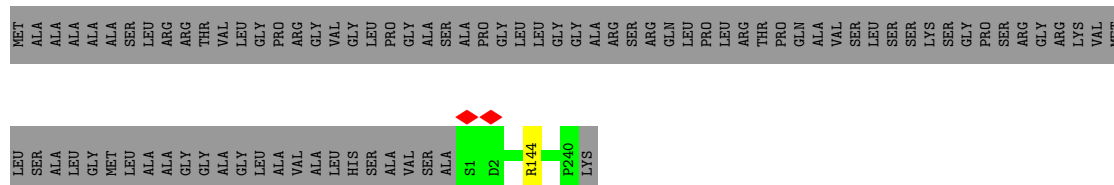
- Molecule 5: Cytochrome b

Chain N:  99%



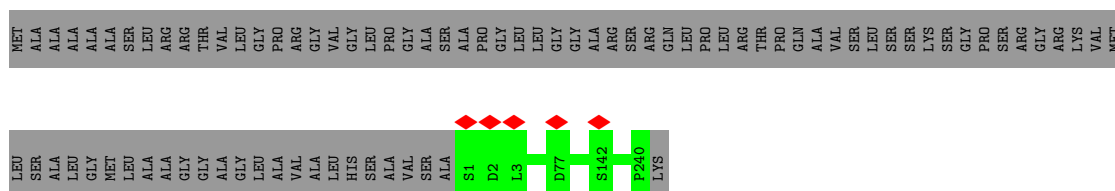
- Molecule 6: Cytochrome c1, heme protein, mitochondrial

Chain D:  74% 26%

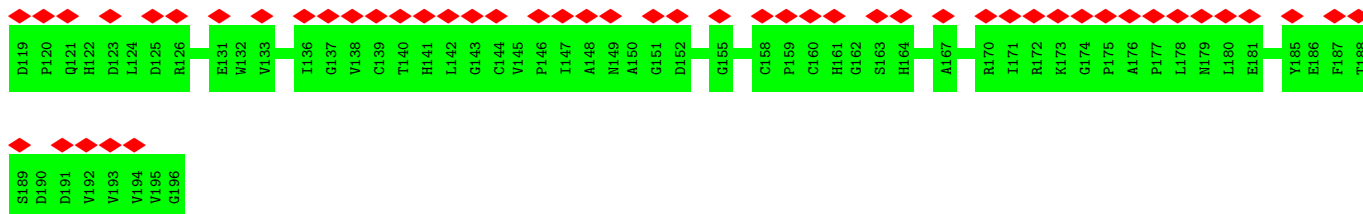
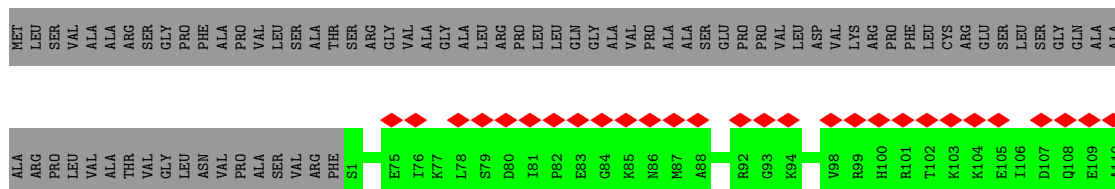
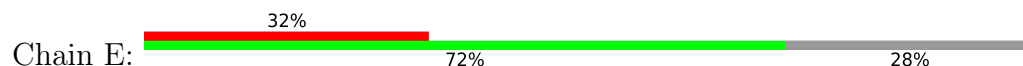


- Molecule 6: Cytochrome c1, heme protein, mitochondrial

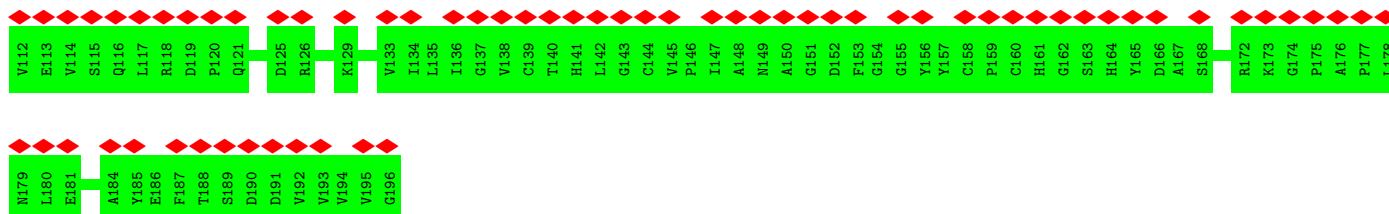
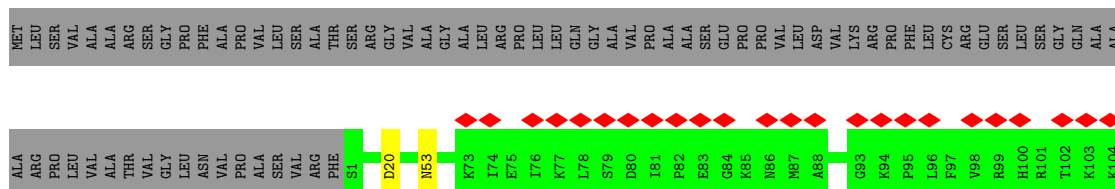
Chain O:  74% 26%



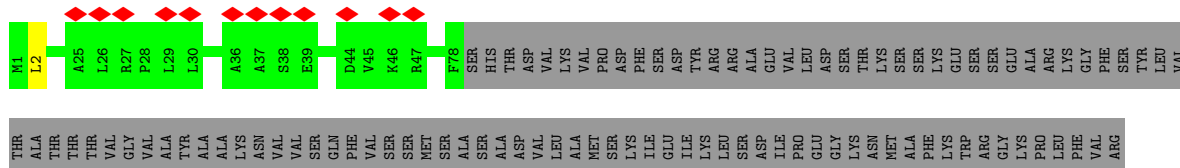
• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

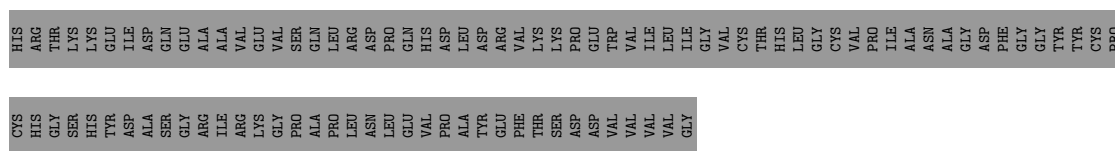


• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

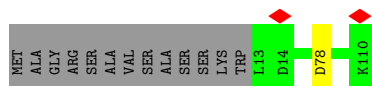
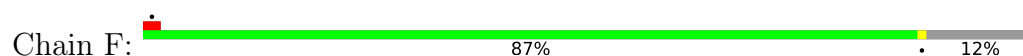


• Molecule 7: Cytochrome b-c1 complex subunit Rieske, mitochondrial

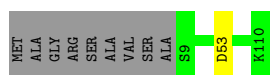




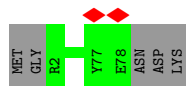
- Molecule 8: Cytochrome b-c1 complex subunit 7



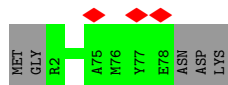
- Molecule 8: Cytochrome b-c1 complex subunit 7



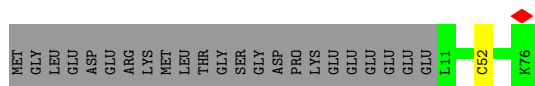
- Molecule 9: Cytochrome b-c1 complex subunit 8



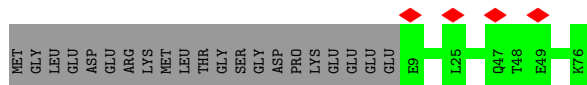
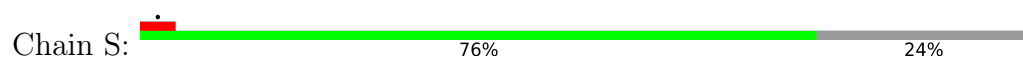
- Molecule 9: Cytochrome b-c1 complex subunit 8



- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial

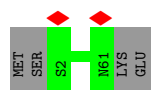


- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial



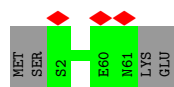
- Molecule 11: Cytochrome b-c1 complex subunit 9

Chain J:  94% 6%




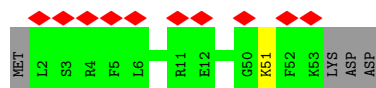
- Molecule 11: Cytochrome b-c1 complex subunit 9

Chain U:  94% 6%



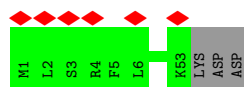
- Molecule 12: Cytochrome b-c1 complex subunit 10

Chain K:  91% 7%



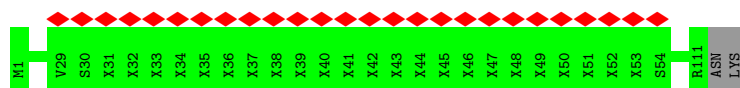
- Molecule 12: Cytochrome b-c1 complex subunit 10

Chain V:  95% 5%



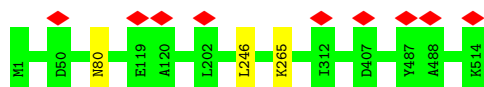
- Molecule 13: Cox7a2l protein

Chain I:  98%



- Molecule 14: Cytochrome c oxidase subunit 1

Chain n:  99%



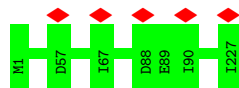
- Molecule 14: Cytochrome c oxidase subunit 1

Chain a:  99%



- Molecule 15: Cytochrome c oxidase subunit 2

Chain o: 100%



- Molecule 15: Cytochrome c oxidase subunit 2

Chain b: 99%



- Molecule 16: Cytochrome c oxidase subunit 3

Chain p: 99%



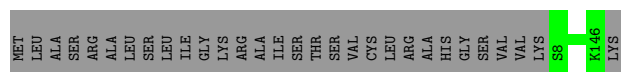
- Molecule 16: Cytochrome c oxidase subunit 3

Chain c: 97%



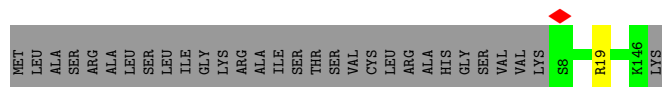
- Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q: 82% 18%



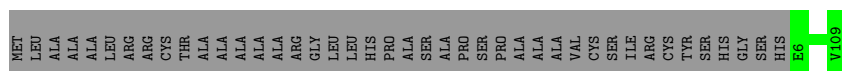
- Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d: 82% 18%



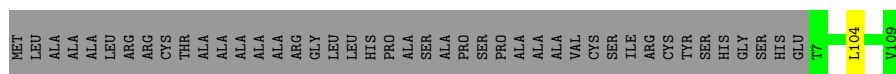
- Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:  71% 29%



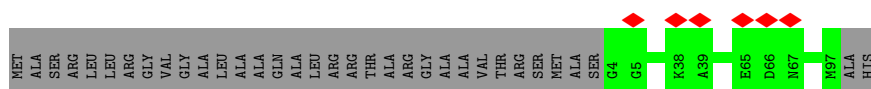
- Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:  70% 29%



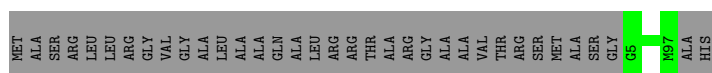
- Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain s:  5% 73% 27%



- Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:  73% 27%




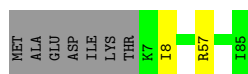
- Molecule 20: Cytochrome c oxidase subunit 6B1

Chain u:  91% 8%



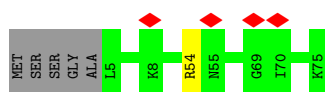
- Molecule 20: Cytochrome c oxidase subunit 6B1

Chain h:  90% 8%



- Molecule 21: Cytochrome c oxidase subunit 6C

Chain v:  5% 92% 7%



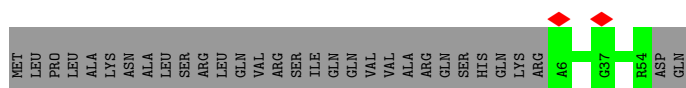
- Molecule 21: Cytochrome c oxidase subunit 6C

Chain i:  93% 5%



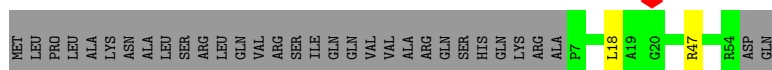
- Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain x:  61% 39%




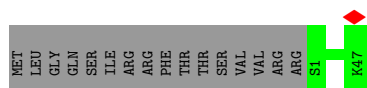
- Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:  58% 40%



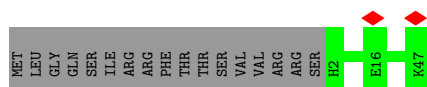
- Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

Chain y:  75% 25%



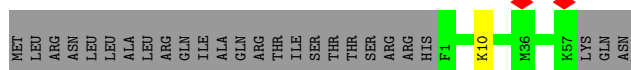
- Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

Chain l:  73% 27%



- Molecule 24: Cytochrome c oxidase subunit 7A2, mitochondrial

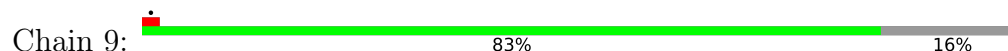
Chain w:  67% 31%

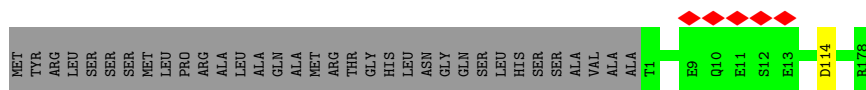


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

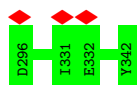
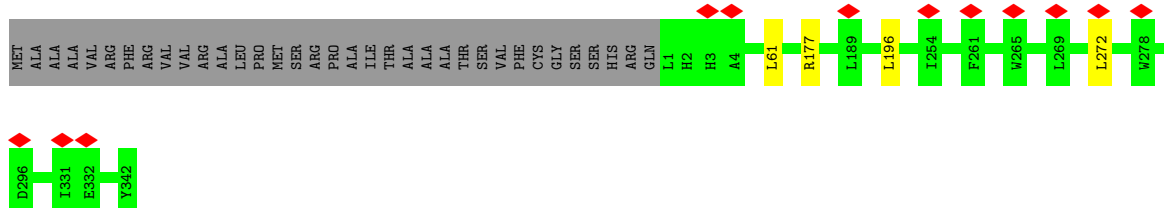
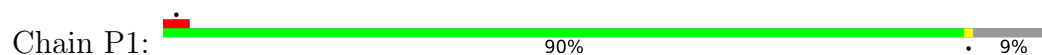
Chain 6:  69% 30%



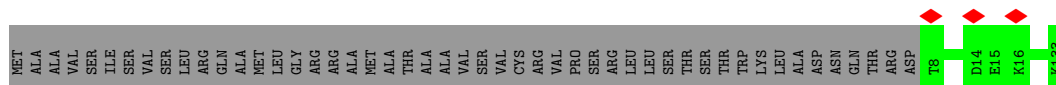
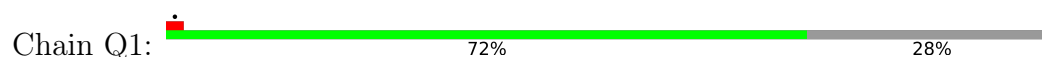




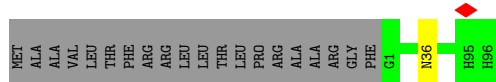
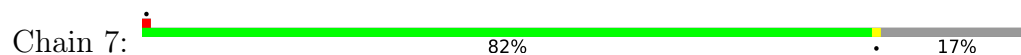
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



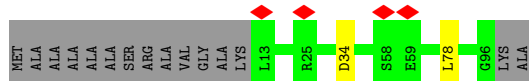
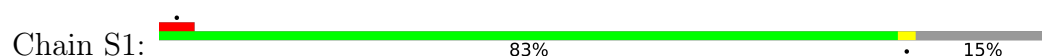
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



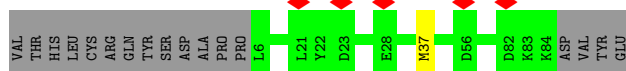
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 36: Acyl carrier protein, mitochondrial



- Molecule 36: Acyl carrier protein, mitochondrial

Chain U1:  56% 44%

MET ALA SER ARG VAL LEU CYS CYS VAL ARG ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO ARG LEU PRO THR LEU ALA ALA ARG PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU ALA ALA VAL PRO GLY THR


VAL THR HIS LEU CYS ARG GLN THR S1 D2 A3 E38

- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:  97% .

MET ALA GLY L3 I15

- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:  87% 13%


MET ALA ALA ALA THR GLY LEU ARG GLN ALA ALA ALA ALA ALA SER T17 D55 R116 P130

- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1:  100%

W1 K145

- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1:  87% 12%

MET A1 A74 L75 V76 SER GLY LYS ALA ALA GLU ALA SER SER ALA MET ALA ALA THR E90 L112

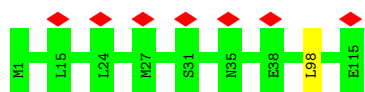
- Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s1:  40% 60%

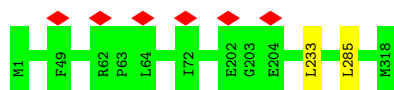
MET ALA VAL SER LEU LEU ARG GLY GLY ARG ARG ILE ARG ALA LEU LYS ALA VAL LEU LEU LEU GLU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL VAL ARG LEU SER THR THR GLU SER GLU LYS SER ALA LYS GLU LYS GLU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO GLU

PRO T27 D28 T29 R68 HIS

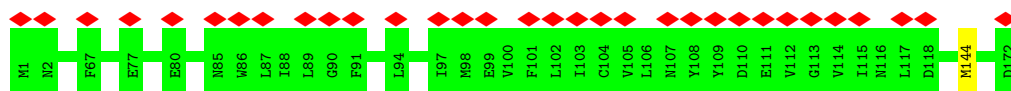
- Molecule 42: NADH-ubiquinone oxidoreductase chain 3



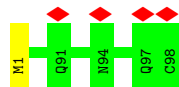
- Molecule 43: NADH-ubiquinone oxidoreductase chain 1



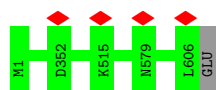
- Molecule 44: NADH-ubiquinone oxidoreductase chain 6



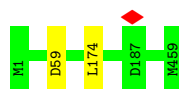
- Molecule 45: NADH-ubiquinone oxidoreductase chain 4L



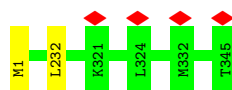
- Molecule 46: NADH-ubiquinone oxidoreductase chain 5



- Molecule 47: NADH-ubiquinone oxidoreductase chain 4

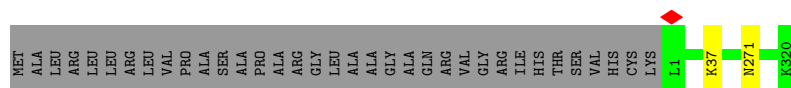


- Molecule 48: NADH-ubiquinone oxidoreductase chain 2



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:  90% 10%



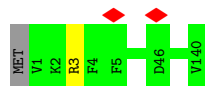
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:  99%



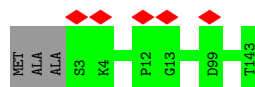
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1:  99%



- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1:  98%



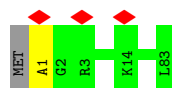
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1:  100%



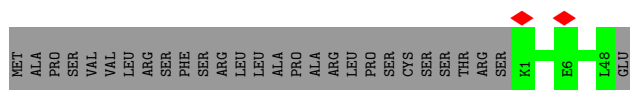
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b1:  98%

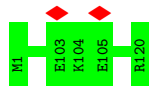


- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

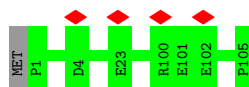
Chain c1:  63% 37%



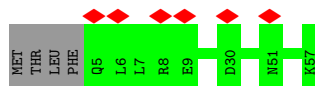
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 subunit C2



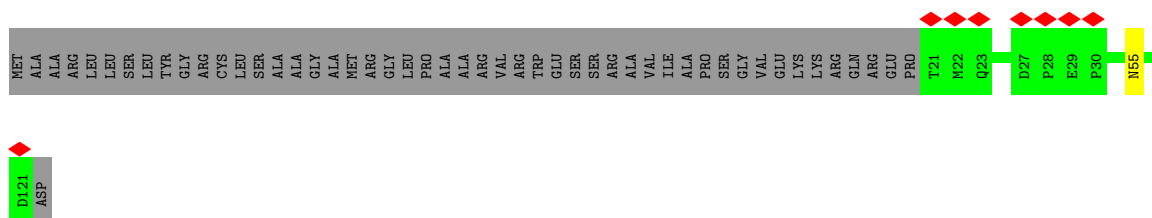
- Molecule 57: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



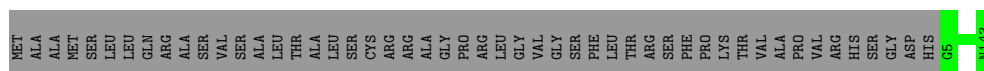
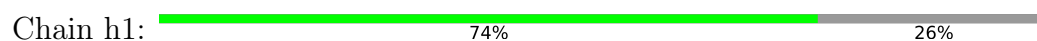
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



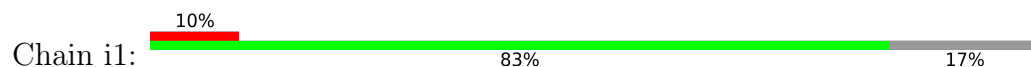
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

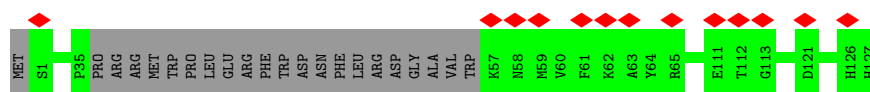


- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

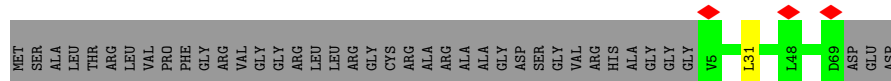


- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

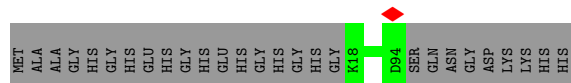
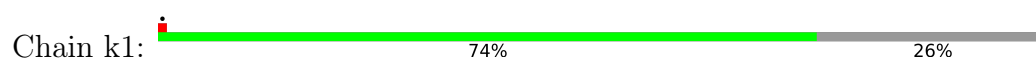




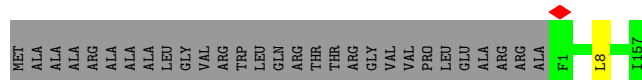
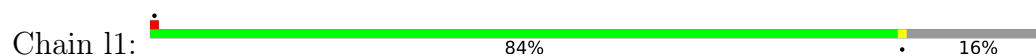
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



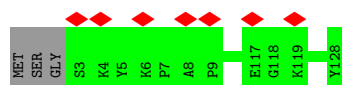
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



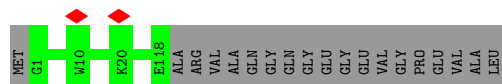
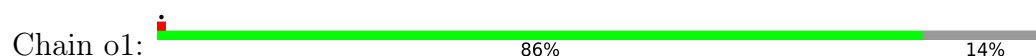
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

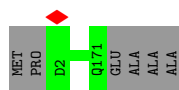


- Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 68: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p1:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51488	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	299.97998, 218.35999, 262.87997	wwPDB
Map dimensions	283, 206, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, HEM, HEC, FMN, DGT, SF4, FME, K, FES, NA, SAC, AYA, 3PE, CU, CDL, TGL, HEA, NDP, PC1, ZMP, MG, ZN, CUA

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	g	0.70	0/646	0.87	0/882
1	t	0.70	0/646	0.87	0/882
2	m	0.69	0/350	0.61	0/472
2	z	0.69	0/350	0.58	0/472
3	A	0.27	0/3529	0.56	1/4793 (0.0%)
3	L	0.28	0/3530	0.53	0/4793
4	B	0.27	0/3205	0.50	0/4332
4	M	0.27	0/3205	0.50	0/4332
5	C	0.29	0/3147	0.52	0/4297
5	N	0.30	0/3147	0.55	3/4297 (0.1%)
6	D	0.27	0/1968	0.53	0/2674
6	O	0.28	0/1968	0.53	0/2674
7	E	0.27	0/1176	0.49	0/1609
7	P	0.27	0/1173	0.52	1/1605 (0.1%)
7	T	0.28	0/565	0.66	1/772 (0.1%)
8	F	0.28	0/885	0.65	1/1184 (0.1%)
8	Q	0.29	0/922	0.60	1/1234 (0.1%)
9	G	0.31	0/673	0.63	0/909
9	R	0.32	0/673	0.63	0/909
10	H	0.35	0/552	0.76	1/739 (0.1%)
10	S	0.34	0/570	0.70	0/763
11	J	0.28	0/509	0.54	0/687
11	U	0.31	0/509	0.58	0/687
12	K	0.29	0/446	0.62	0/609
12	V	0.27	0/454	0.64	0/619
13	I	0.29	0/709	0.66	0/955
14	a	0.33	0/4162	0.68	5/5686 (0.1%)
14	n	0.33	0/4162	0.59	1/5686 (0.0%)
15	b	0.31	0/1863	0.73	2/2542 (0.1%)
15	o	0.30	0/1863	0.64	0/2542
16	c	0.29	0/2195	0.59	2/3000 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	p	0.30	0/2202	0.58	1/3010 (0.0%)
17	d	0.29	0/1190	0.68	0/1609
17	q	0.31	0/1190	0.64	0/1609
18	e	0.30	0/851	0.70	1/1155 (0.1%)
18	r	0.28	0/860	0.65	0/1167
19	f	0.30	0/734	0.64	0/996
19	s	0.30	0/738	0.60	0/1001
20	h	0.32	0/674	0.74	0/910
20	u	0.34	0/674	0.69	1/910 (0.1%)
21	i	0.38	0/584	0.85	1/778 (0.1%)
21	v	0.34	0/579	0.71	0/771
22	k	0.26	0/391	0.54	1/533 (0.2%)
22	x	0.32	0/396	0.61	0/541
23	l	0.30	0/393	0.62	0/527
23	y	0.35	0/399	0.61	0/535
24	w	0.28	0/444	0.55	0/598
25	6	0.34	0/1289	0.69	2/1744 (0.1%)
26	C1	0.28	0/1780	0.56	0/2424
27	D1	0.31	0/3540	0.56	0/4795
28	2	0.29	0/1700	0.51	0/2316
29	1	0.29	0/3396	0.55	0/4586
30	3	0.28	0/5392	0.54	0/7305
31	9	0.35	0/1461	0.58	1/1974 (0.1%)
32	P1	0.28	0/2823	0.60	3/3828 (0.1%)
33	Q1	0.27	0/1045	0.52	0/1411
34	7	0.28	0/773	0.52	0/1041
35	S1	0.30	0/682	0.68	2/920 (0.2%)
36	T1	0.27	0/646	0.59	0/869
36	U1	0.32	0/718	0.56	0/970
37	V1	0.25	0/945	0.41	0/1281
38	W1	0.28	0/993	0.57	0/1335
39	q1	0.28	0/1251	0.53	0/1702
40	r1	0.27	0/806	0.55	0/1090
41	s1	0.27	0/360	0.67	0/489
42	A1	0.30	0/948	0.60	1/1295 (0.1%)
43	H1	0.35	0/2607	0.63	2/3564 (0.1%)
44	J1	0.32	0/1330	0.59	1/1810 (0.1%)
45	K1	0.31	0/738	0.57	0/1002
46	L1	0.31	0/4913	0.56	0/6686
47	M1	0.30	0/3709	0.60	2/5052 (0.0%)
48	N1	0.29	0/2755	0.57	1/3751 (0.0%)
49	O1	0.28	0/2674	0.51	0/3626
50	X1	0.27	0/1434	0.55	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
51	Y1	0.28	0/1061	0.56	0/1439
52	Z1	0.27	0/1198	0.56	0/1616
53	a1	0.32	0/585	0.61	0/788
54	b1	0.28	0/666	0.55	0/914
55	c1	0.27	0/409	0.53	0/555
56	d1	0.29	0/1028	0.55	0/1387
57	e1	0.29	0/900	0.54	0/1199
58	f1	0.28	0/468	0.65	0/630
59	g1	0.28	0/878	0.51	0/1196
60	h1	0.29	0/1201	0.55	0/1626
61	i1	0.27	0/917	0.54	0/1243
62	j1	0.30	0/587	0.64	1/804 (0.1%)
63	k1	0.30	0/646	0.60	0/873
64	l1	0.29	0/1379	0.55	1/1882 (0.1%)
65	m1	0.33	0/1079	0.64	0/1463
66	n1	0.28	0/1596	0.53	0/2162
67	o1	0.29	0/1039	0.59	0/1394
68	p1	0.28	0/1471	0.52	0/1988
All	All	0.31	0/129867	0.58	41/176249 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	m	0	2
2	z	0	1
All	All	0	3

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	468	MET	CG-SD-CE	9.76	115.81	100.20
32	P1	196	LEU	CA-CB-CG	7.44	132.41	115.30
25	6	80	ASP	CB-CG-OD1	6.95	124.55	118.30
8	Q	53	ASP	CB-CG-OD1	6.53	124.18	118.30
32	P1	272	LEU	CA-CB-CG	6.49	130.22	115.30
35	S1	34	ASP	CB-CG-OD1	6.48	124.13	118.30
8	F	78	ASP	CB-CG-OD1	6.41	124.07	118.30
47	M1	59	ASP	CB-CG-OD1	6.40	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	20	ASP	CB-CG-OD1	6.39	124.05	118.30
14	a	208	MET	CA-CB-CG	6.38	124.14	113.30
44	J1	144	MET	CA-CB-CG	6.25	123.93	113.30
14	a	417	MET	CB-CG-SD	-6.12	94.05	112.40
5	N	149	LEU	CB-CG-CD2	-5.88	101.01	111.00
47	M1	174	LEU	CA-CB-CG	5.81	128.66	115.30
43	H1	233	LEU	CB-CG-CD1	-5.79	101.16	111.00
31	9	114	ASP	CB-CG-OD1	5.77	123.49	118.30
14	a	417	MET	CA-CB-CG	5.72	123.03	113.30
32	P1	61	LEU	CA-CB-CG	5.70	128.40	115.30
3	A	216	LEU	CA-CB-CG	5.68	128.37	115.30
16	c	164	LEU	CA-CB-CG	5.62	128.23	115.30
18	e	104	LEU	CA-CB-CG	5.62	128.23	115.30
42	A1	98	LEU	CA-CB-CG	5.53	128.02	115.30
64	l1	8	LEU	CA-CB-CG	5.53	128.02	115.30
14	a	215	LEU	CA-CB-CG	5.50	127.94	115.30
7	T	2	LEU	CA-CB-CG	5.48	127.91	115.30
5	N	58	ASP	CB-CG-OD1	5.43	123.18	118.30
16	p	111	ASP	CB-CG-OD1	5.40	123.16	118.30
5	N	149	LEU	CB-CG-CD1	5.38	120.15	111.00
10	H	52	CYS	CA-CB-SG	5.38	123.68	114.00
48	N1	232	LEU	CA-CB-CG	5.30	127.49	115.30
14	n	246	LEU	CB-CG-CD1	5.26	119.94	111.00
15	b	207	MET	CA-CB-CG	5.18	122.11	113.30
21	i	65	MET	CA-CB-CG	5.18	122.11	113.30
15	b	33	LEU	CA-CB-CG	5.14	127.12	115.30
16	c	48	LEU	CA-CB-CG	5.09	127.00	115.30
25	6	62	LEU	CA-CB-CG	5.07	126.96	115.30
20	u	63	LEU	C-N-CA	-5.07	109.04	121.70
62	j1	31	LEU	CA-CB-CG	5.06	126.95	115.30
43	H1	285	LEU	CA-CB-CG	5.05	126.92	115.30
35	S1	78	LEU	CA-CB-CG	5.01	126.82	115.30
22	k	18	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	m	43	ARG	Sidechain
2	m	7	ARG	Sidechain
2	z	7	ARG	Sidechain

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	g	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
1	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
2	m	42/69 (61%)	41 (98%)	1 (2%)	0	100	100
2	z	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
3	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
3	L	443/480 (92%)	429 (97%)	14 (3%)	0	100	100
4	B	418/453 (92%)	409 (98%)	9 (2%)	0	100	100
4	M	418/453 (92%)	403 (96%)	15 (4%)	0	100	100
5	C	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
5	N	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
6	D	238/325 (73%)	233 (98%)	5 (2%)	0	100	100
6	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
7	E	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	P	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
8	F	96/111 (86%)	96 (100%)	0	0	100	100
8	Q	100/111 (90%)	100 (100%)	0	0	100	100
9	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
9	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
10	H	64/89 (72%)	64 (100%)	0	0	100	100
10	S	66/89 (74%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
11	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
12	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
12	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
13	I	86/113 (76%)	82 (95%)	4 (5%)	0	100	100
14	a	512/514 (100%)	491 (96%)	20 (4%)	1 (0%)	44	73
14	n	512/514 (100%)	489 (96%)	23 (4%)	0	100	100
15	b	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
15	o	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
16	c	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
16	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
17	d	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
17	q	137/169 (81%)	127 (93%)	10 (7%)	0	100	100
18	e	101/146 (69%)	100 (99%)	1 (1%)	0	100	100
18	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
19	f	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
19	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
20	h	77/86 (90%)	73 (95%)	3 (4%)	1 (1%)	10	41
20	u	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
21	i	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
21	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
22	k	46/80 (58%)	44 (96%)	2 (4%)	0	100	100
22	x	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
23	l	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
23	y	45/63 (71%)	45 (100%)	0	0	100	100
24	w	55/83 (66%)	55 (100%)	0	0	100	100
25	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
26	C1	206/263 (78%)	200 (97%)	6 (3%)	0	100	100
27	D1	427/463 (92%)	412 (96%)	15 (4%)	0	100	100
28	2	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
29	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	3	688/727 (95%)	666 (97%)	22 (3%)	0	100	100
31	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
32	P1	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
33	Q1	124/175 (71%)	120 (97%)	4 (3%)	0	100	100
34	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
35	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
36	T1	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
36	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
37	V1	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
38	W1	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
39	q1	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
40	r1	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
41	s1	40/104 (38%)	38 (95%)	2 (5%)	0	100	100
42	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
43	H1	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
44	J1	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
45	K1	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
46	L1	604/607 (100%)	567 (94%)	37 (6%)	0	100	100
47	M1	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
48	N1	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
49	O1	318/355 (90%)	300 (94%)	18 (6%)	0	100	100
50	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
51	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
52	Z1	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
53	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
54	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
55	c1	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
56	d1	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
57	e1	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
58	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
59	g1	99/151 (66%)	95 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	h1	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
61	i1	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
62	j1	63/105 (60%)	61 (97%)	2 (3%)	0	100	100
63	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
64	l1	155/186 (83%)	152 (98%)	3 (2%)	0	100	100
65	m1	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
66	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
67	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
68	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	15749/18172 (87%)	15149 (96%)	598 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	h	8	ILE
14	a	376	HIS

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	g	66/92 (72%)	66 (100%)	0	100	100
1	t	66/92 (72%)	66 (100%)	0	100	100
2	m	39/61 (64%)	39 (100%)	0	100	100
2	z	39/61 (64%)	39 (100%)	0	100	100
3	A	372/398 (94%)	372 (100%)	0	100	100
3	L	372/398 (94%)	372 (100%)	0	100	100
4	B	330/356 (93%)	330 (100%)	0	100	100
4	M	330/356 (93%)	330 (100%)	0	100	100
5	C	332/333 (100%)	332 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	N	332/333 (100%)	332 (100%)	0	100	100
6	D	205/260 (79%)	204 (100%)	1 (0%)	86	93
6	O	205/260 (79%)	205 (100%)	0	100	100
7	E	69/224 (31%)	69 (100%)	0	100	100
7	P	68/224 (30%)	67 (98%)	1 (2%)	60	78
7	T	58/224 (26%)	58 (100%)	0	100	100
8	F	90/99 (91%)	90 (100%)	0	100	100
8	Q	94/99 (95%)	94 (100%)	0	100	100
9	G	70/74 (95%)	70 (100%)	0	100	100
9	R	70/74 (95%)	70 (100%)	0	100	100
10	H	63/83 (76%)	63 (100%)	0	100	100
10	S	65/83 (78%)	65 (100%)	0	100	100
11	J	51/55 (93%)	51 (100%)	0	100	100
11	U	51/55 (93%)	51 (100%)	0	100	100
12	K	42/46 (91%)	41 (98%)	1 (2%)	44	67
12	V	43/46 (94%)	43 (100%)	0	100	100
13	I	73/75 (97%)	73 (100%)	0	100	100
14	a	425/425 (100%)	424 (100%)	1 (0%)	92	96
14	n	425/425 (100%)	423 (100%)	2 (0%)	86	93
15	b	210/210 (100%)	210 (100%)	0	100	100
15	o	210/210 (100%)	210 (100%)	0	100	100
16	c	225/227 (99%)	222 (99%)	3 (1%)	65	81
16	p	226/227 (100%)	226 (100%)	0	100	100
17	d	122/146 (84%)	121 (99%)	1 (1%)	79	88
17	q	122/146 (84%)	122 (100%)	0	100	100
18	e	90/118 (76%)	90 (100%)	0	100	100
18	r	91/118 (77%)	91 (100%)	0	100	100
19	f	80/101 (79%)	80 (100%)	0	100	100
19	s	80/101 (79%)	80 (100%)	0	100	100
20	h	70/76 (92%)	69 (99%)	1 (1%)	62	79
20	u	70/76 (92%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	i	54/57 (95%)	54 (100%)	0	100	100
21	v	54/57 (95%)	53 (98%)	1 (2%)	52	73
22	k	39/67 (58%)	38 (97%)	1 (3%)	41	65
22	x	39/67 (58%)	39 (100%)	0	100	100
23	l	39/55 (71%)	39 (100%)	0	100	100
23	y	40/55 (73%)	40 (100%)	0	100	100
24	w	43/67 (64%)	42 (98%)	1 (2%)	45	68
25	6	133/185 (72%)	132 (99%)	1 (1%)	79	88
26	C1	190/227 (84%)	190 (100%)	0	100	100
27	D1	370/394 (94%)	368 (100%)	2 (0%)	86	93
28	2	184/206 (89%)	184 (100%)	0	100	100
29	1	345/370 (93%)	345 (100%)	0	100	100
30	3	580/610 (95%)	579 (100%)	1 (0%)	92	96
31	9	152/178 (85%)	152 (100%)	0	100	100
32	P1	299/325 (92%)	298 (100%)	1 (0%)	91	96
33	Q1	113/153 (74%)	113 (100%)	0	100	100
34	7	81/96 (84%)	80 (99%)	1 (1%)	67	82
35	S1	74/80 (92%)	74 (100%)	0	100	100
36	T1	73/135 (54%)	72 (99%)	1 (1%)	62	79
36	U1	81/135 (60%)	81 (100%)	0	100	100
37	V1	101/102 (99%)	101 (100%)	0	100	100
38	W1	108/114 (95%)	108 (100%)	0	100	100
39	q1	131/131 (100%)	131 (100%)	0	100	100
40	r1	88/96 (92%)	88 (100%)	0	100	100
41	s1	41/95 (43%)	41 (100%)	0	100	100
42	A1	103/103 (100%)	103 (100%)	0	100	100
43	H1	279/279 (100%)	279 (100%)	0	100	100
44	J1	137/137 (100%)	137 (100%)	0	100	100
45	K1	87/87 (100%)	87 (100%)	0	100	100
46	L1	548/549 (100%)	548 (100%)	0	100	100
47	M1	414/414 (100%)	414 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	N1	307/307 (100%)	307 (100%)	0	100	100
49	O1	284/309 (92%)	282 (99%)	2 (1%)	81	90
50	X1	153/154 (99%)	153 (100%)	0	100	100
51	Y1	105/106 (99%)	104 (99%)	1 (1%)	73	85
52	Z1	122/123 (99%)	122 (100%)	0	100	100
53	a1	60/60 (100%)	60 (100%)	0	100	100
54	b1	72/73 (99%)	72 (100%)	0	100	100
55	c1	42/67 (63%)	42 (100%)	0	100	100
56	d1	107/107 (100%)	107 (100%)	0	100	100
57	e1	93/94 (99%)	93 (100%)	0	100	100
58	f1	49/53 (92%)	49 (100%)	0	100	100
59	g1	92/129 (71%)	91 (99%)	1 (1%)	70	83
60	h1	123/162 (76%)	123 (100%)	0	100	100
61	i1	99/119 (83%)	99 (100%)	0	100	100
62	j1	61/87 (70%)	61 (100%)	0	100	100
63	k1	60/78 (77%)	60 (100%)	0	100	100
64	l1	142/161 (88%)	142 (100%)	0	100	100
65	m1	112/114 (98%)	112 (100%)	0	100	100
66	n1	163/164 (99%)	163 (100%)	0	100	100
67	o1	109/121 (90%)	109 (100%)	0	100	100
68	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	13571/15439 (88%)	13546 (100%)	25 (0%)	91	96

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	144	ARG
12	K	51	LYS
7	P	53	ASN
14	n	80	ASN
14	n	265	LYS
21	v	54	ARG
24	w	10	LYS
25	6	33	ARG
27	D1	164	MET

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Mol	Chain	Res	Type
27	D1	385	ARG
30	3	444	LYS
32	P1	177	ARG
34	7	36	ASN
36	T1	37	MET
49	O1	37	LYS
49	O1	271	ASN
51	Y1	3	ARG
59	g1	55	ASN
14	a	480	ARG
16	c	12	ASN
16	c	77	LYS
16	c	222	GLN
17	d	19	ARG
20	h	57	ARG
22	k	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	t	75	ASN
2	m	2	HIS
3	A	53	ASN
3	A	339	GLN
5	C	16	HIS
7	E	161	HIS
3	L	53	ASN
3	L	323	HIS
3	L	363	ASN
13	I	24	GLN
13	I	63	GLN
14	n	151	HIS
16	p	161	GLN
22	x	41	ASN
43	H1	138	GLN
46	L1	170	GLN
50	X1	98	HIS
66	n1	12	GLN
14	a	98	ASN
14	a	135	ASN
14	a	216	ASN
14	a	429	HIS

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Mol	Chain	Res	Type
16	c	157	ASN
16	c	160	ASN
16	c	161	GLN
16	c	222	GLN
16	c	231	HIS
1	g	75	ASN
23	l	10	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
48	FME	N1	1	48	8,9,10	0.96	0	7,9,11	1.04	1 (14%)
45	FME	K1	1	45	8,9,10	0.94	0	7,9,11	1.66	2 (28%)
46	FME	L1	1	46	8,9,10	0.92	0	7,9,11	0.91	0
40	AYA	r1	1	40	6,7,8	1.28	1 (16%)	5,8,10	1.28	1 (20%)
42	FME	A1	1	42	8,9,10	0.94	0	7,9,11	0.79	0
47	FME	M1	1	47	8,9,10	0.96	0	7,9,11	0.76	0
54	AYA	b1	1	54	6,7,8	1.25	1 (16%)	5,8,10	1.28	1 (20%)
61	SAC	i1	1	61	7,8,9	1.02	0	8,9,11	0.81	0
44	FME	J1	1	44	8,9,10	0.95	0	7,9,11	0.85	0
43	FME	H1	1	43	8,9,10	0.96	0	7,9,11	0.89	0
27	2MR	D1	85	27	10,12,13	2.58	2 (20%)	5,13,15	2.84	2 (40%)

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
48	FME	N1	1	48	-	2/7/9/11	-
45	FME	K1	1	45	-	3/7/9/11	-
46	FME	L1	1	46	-	4/7/9/11	-
40	AYA	r1	1	40	-	0/4/6/8	-
42	FME	A1	1	42	-	1/7/9/11	-
47	FME	M1	1	47	-	2/7/9/11	-
54	AYA	b1	1	54	-	0/4/6/8	-
61	SAC	i1	1	61	-	2/7/8/10	-
44	FME	J1	1	44	-	4/7/9/11	-
43	FME	H1	1	43	-	3/7/9/11	-
27	2MR	D1	85	27	-	4/10/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D1	85	2MR	CZ-NE	5.89	1.46	1.34
27	D1	85	2MR	CZ-NH2	5.11	1.44	1.33
40	r1	1	AYA	CA-N	-2.49	1.43	1.46
54	b1	1	AYA	CA-N	-2.30	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D1	85	2MR	CD-NE-CZ	4.86	132.50	123.41
27	D1	85	2MR	NE-CZ-NH2	-3.72	116.07	119.48
45	K1	1	FME	C-CA-N	3.51	116.06	109.73
40	r1	1	AYA	CB-CA-N	2.70	112.61	109.61
54	b1	1	AYA	CB-CA-N	2.57	112.47	109.61
45	K1	1	FME	O-C-CA	-2.14	119.18	124.78
48	N1	1	FME	C-CA-N	2.12	113.56	109.73

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D1	85	2MR	O-C-CA-CB
43	H1	1	FME	N-CA-CB-CG
44	J1	1	FME	C-CA-CB-CG
44	J1	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
45	K1	1	FME	O1-CN-N-CA
46	L1	1	FME	CB-CA-N-CN
46	L1	1	FME	N-CA-CB-CG
47	M1	1	FME	N-CA-CB-CG
48	N1	1	FME	C-CA-CB-CG
27	D1	85	2MR	NE-CD-CG-CB
44	J1	1	FME	CB-CG-SD-CE
45	K1	1	FME	CA-CB-CG-SD
27	D1	85	2MR	CA-CB-CG-CD
48	N1	1	FME	CA-CB-CG-SD
42	A1	1	FME	N-CA-CB-CG
44	J1	1	FME	N-CA-CB-CG
45	K1	1	FME	N-CA-CB-CG
46	L1	1	FME	CB-CG-SD-CE
43	H1	1	FME	CB-CA-N-CN
47	M1	1	FME	CB-CA-N-CN
43	H1	1	FME	C-CA-CB-CG
46	L1	1	FME	C-CA-CB-CG
27	D1	85	2MR	CG-CD-NE-CZ
61	i1	1	SAC	C-CA-CB-OG
61	i1	1	SAC	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 11 are monoatomic - leaving 101 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
69	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.32	0
82	SF4	1	502	29	0,12,12	-	-	-		
69	3PE	L1	704	-	50,50,50	0.31	0	53,55,55	0.28	0
73	HEC	D	301	6	32,50,50	2.23	3 (9%)	24,82,82	1.63	5 (20%)
69	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.39	0
69	3PE	C	404	-	30,30,50	0.38	0	33,35,55	0.34	0
70	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.28	0
77	HEA	a	604	14	57,67,67	1.41	8 (14%)	61,103,103	2.39	23 (37%)
81	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.17	0
69	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.30	0
74	FES	3	803	30	0,4,4	-	-	-		
69	3PE	b1	101	-	42,42,50	0.33	0	45,47,55	0.35	0
69	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
69	3PE	M1	503	-	50,50,50	0.30	0	53,55,55	0.27	0
69	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.41	0
69	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
69	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.31	0
69	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
69	3PE	i	101	-	27,27,50	0.39	0	30,32,55	0.33	0
70	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.47	0
71	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
71	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.38	0
82	SF4	9	201	31	0,12,12	-	-	-		
70	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
77	HEA	n	604	14	57,67,67	1.44	8 (14%)	61,103,103	2.48	23 (37%)
72	HEM	C	402	5	41,50,50	1.43	5 (12%)	45,82,82	1.41	6 (13%)
74	FES	E	201	7	0,4,4	-	-	-		
70	PC1	z	101	-	27,27,53	0.40	0	33,35,61	0.35	0
69	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.37	0
74	FES	2	301	28	0,4,4	-	-	-		
69	3PE	a	606	-	26,26,50	0.40	0	29,31,55	0.36	0
70	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.36	0
82	SF4	9	202	31	0,12,12	-	-	-		
69	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.30	0
71	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
70	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.61	0
69	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.32	0
86	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.93	1 (3%)
71	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
69	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.33	0
71	CDL	r1	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
82	SF4	3	802	30	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	CDL	R	101	-	40,40,99	0.45	0	46,52,111	0.53	0
72	HEM	N	402	5	41,50,50	1.45	4 (9%)	45,82,82	1.58	10 (22%)
69	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
82	SF4	6	201	25	0,12,12	-	-	-	-	-
69	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.30	0
77	HEA	n	603	14	57,67,67	1.40	7 (12%)	61,103,103	2.47	22 (36%)
71	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.51	0
69	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
69	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.32	0
69	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
69	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.36	0
69	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
69	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.34	0
81	TGL	y	601	-	36,36,62	0.24	0	39,39,65	0.18	0
79	CUA	b	302	15	0,1,1	-	-	-	-	-
71	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
86	ZMP	W1	201	-	27,33,36	0.68	1 (3%)	32,40,45	0.93	1 (3%)
71	CDL	V	101	-	45,45,99	0.34	0	51,57,111	0.45	0
69	3PE	Y1	402	-	27,27,50	0.39	0	30,32,55	0.37	0
71	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.34	0
85	NDP	P1	501	-	45,52,52	0.52	0	53,80,80	0.60	1 (1%)
83	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.47	1 (2%)
72	HEM	N	401	5	41,50,50	1.46	3 (7%)	45,82,82	1.74	9 (20%)
69	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.30	0
74	FES	P	201	7	0,4,4	-	-	-	-	-
70	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.47	0
70	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
69	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.34	0
69	3PE	b	301	-	28,28,50	0.40	0	31,33,55	0.37	0
73	HEC	O	303	6	32,50,50	2.17	4 (12%)	24,82,82	1.60	3 (12%)
77	HEA	a	603	14	57,67,67	1.49	7 (12%)	61,103,103	2.43	23 (37%)
71	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.28	0
69	3PE	d	201	-	33,33,50	0.37	0	36,38,55	0.53	0
69	3PE	m1	601	-	35,35,50	0.36	0	38,40,55	0.30	0
71	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
70	PC1	I	201	-	49,49,53	0.32	0	55,57,61	0.52	1 (1%)
71	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.42	0
69	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.33	0
70	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
70	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	CDL	G	101	-	41,41,99	0.44	0	47,53,111	0.36	0
69	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.66	0
69	3PE	a	605	-	27,27,50	0.40	0	30,32,55	0.46	0
71	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.28	0
82	SF4	3	801	30	0,12,12	-	-	-		
79	CUA	o	303	15	0,1,1	-	-	-		
87	DGT	O1	401	78	26,33,33	0.79	1 (3%)	32,52,52	0.46	0
69	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
69	3PE	E	203	-	33,33,50	0.36	0	36,38,55	0.33	0
69	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.29	0
71	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)
70	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.58	0
71	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.33	0
70	PC1	V	102	-	27,27,53	0.40	0	33,35,61	0.35	0
69	3PE	g	303	-	24,24,50	0.43	0	27,29,55	0.63	0
71	CDL	g	301	-	34,37,99	0.37	0	37,47,111	0.53	0
69	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
69	3PE	G	102	-	50,50,50	0.31	0	53,55,55	0.28	0
72	HEM	C	401	5	41,50,50	1.44	3 (7%)	45,82,82	1.59	7 (15%)

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
69	3PE	c	301	-	-	10/48/48/54	-
82	SF4	1	502	29	-	-	0/6/5/5
69	3PE	L1	704	-	-	7/54/54/54	-
73	HEC	D	301	6	-	2/10/54/54	-
69	3PE	z	102	-	-	1/29/29/54	-
69	3PE	C	404	-	-	4/34/34/54	-
70	PC1	g	302	-	-	8/53/53/57	-
77	HEA	a	604	14	-	11/32/76/76	-
81	TGL	l	601	-	-	0/39/39/65	-
69	3PE	p	301	-	-	12/48/48/54	-
74	FES	3	803	30	-	-	0/1/1/1
69	3PE	b1	101	-	-	10/46/46/54	-
69	3PE	L	501	-	-	6/26/26/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	M1	503	-	-	14/54/54/54	-
69	3PE	n	606	-	-	9/31/31/54	-
69	3PE	C	403	-	-	9/38/38/54	-
69	3PE	N	403	-	-	7/40/40/54	-
69	3PE	L1	701	-	-	9/54/54/54	-
69	3PE	i	101	-	-	8/31/31/54	-
70	PC1	6	203	-	-	12/46/46/57	-
71	CDL	A	502	-	-	13/56/56/110	-
71	CDL	N1	401	-	-	21/100/100/110	-
82	SF4	9	201	31	-	-	0/6/5/5
70	PC1	p	302	-	-	10/38/38/57	-
77	HEA	n	604	14	-	7/32/76/76	-
72	HEM	C	402	5	-	1/12/54/54	-
74	FES	E	201	7	-	-	0/1/1/1
70	PC1	z	101	-	-	6/31/31/57	-
69	3PE	d1	203	-	-	7/35/35/54	-
74	FES	2	301	28	-	-	0/1/1/1
69	3PE	a	606	-	-	9/30/30/54	-
70	PC1	M1	501	-	-	9/57/57/57	-
82	SF4	9	202	31	-	-	0/6/5/5
69	3PE	M1	502	-	-	17/54/54/54	-
71	CDL	H1	402	-	-	12/59/59/110	-
70	PC1	L	503	-	-	9/27/27/57	-
69	3PE	E	202	-	-	9/35/35/54	-
86	ZMP	n1	201	-	-	20/36/38/43	-
71	CDL	d1	201	-	-	16/77/77/110	-
69	3PE	v	101	-	-	7/31/31/54	-
71	CDL	r1	202	-	-	13/67/67/110	-
82	SF4	3	802	30	-	-	0/6/5/5
71	CDL	R	101	-	-	15/51/51/110	-
72	HEM	N	402	5	-	4/12/54/54	-
69	3PE	d1	202	-	-	7/34/34/54	-
82	SF4	6	201	25	-	-	0/6/5/5
69	3PE	i1	201	-	-	6/45/45/54	-
77	HEA	n	603	14	-	9/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	CDL	L	502	-	-	9/56/56/110	-
69	3PE	n	605	-	-	10/37/37/54	-
69	3PE	Y1	403	-	-	7/45/45/54	-
69	3PE	N1	402	-	-	6/41/41/54	-
69	3PE	n	607	-	-	8/30/30/54	-
69	3PE	H1	401	-	-	9/54/54/54	-
69	3PE	O	302	-	-	9/36/36/54	-
81	TGL	y	601	-	-	3/39/39/65	-
86	ZMP	W1	201	-	-	5/38/40/43	-
71	CDL	R	102	-	-	17/67/67/110	-
71	CDL	V	101	-	-	18/55/55/110	-
69	3PE	Y1	402	-	-	4/31/31/54	-
71	CDL	L1	703	-	-	15/56/56/110	-
85	NDP	P1	501	-	-	5/30/77/77	0/5/5/5
83	FMN	1	501	-	-	5/18/18/18	0/3/3/3
72	HEM	N	401	5	-	3/12/54/54	-
69	3PE	K1	201	-	-	12/44/44/54	-
74	FES	P	201	7	-	-	0/1/1/1
70	PC1	K	101	-	-	4/31/31/57	-
70	PC1	9	204	-	-	10/50/50/57	-
69	3PE	R	104	-	-	5/33/33/54	-
69	3PE	b	301	-	-	9/32/32/54	-
73	HEC	O	303	6	-	4/10/54/54	-
77	HEA	a	603	14	-	13/32/76/76	-
71	CDL	Y1	401	-	-	11/104/104/110	-
69	3PE	d	201	-	-	6/37/37/54	-
69	3PE	m1	601	-	-	13/39/39/54	-
71	CDL	O	301	-	-	15/67/67/110	-
70	PC1	I	201	-	-	9/53/53/57	-
71	CDL	h1	201	-	-	20/80/80/110	-
69	3PE	6	202	-	-	4/35/35/54	-
70	PC1	9	203	-	-	12/57/57/57	-
70	PC1	J	101	-	-	7/38/38/57	-
71	CDL	G	101	-	-	13/52/52/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	A	501	-	-	9/26/26/54	-
69	3PE	a	605	-	-	6/31/31/54	-
71	CDL	L1	702	-	-	15/88/88/110	-
82	SF4	3	801	30	-	-	0/6/5/5
87	DGT	O1	401	78	-	1/18/34/34	0/3/3/3
69	3PE	o	302	-	-	10/32/32/54	-
69	3PE	E	203	-	-	9/37/37/54	-
69	3PE	r1	201	-	-	8/49/49/54	-
71	CDL	R	103	-	-	19/82/82/110	-
70	PC1	P1	502	-	-	15/34/34/57	-
71	CDL	D	302	-	-	19/66/66/110	-
70	PC1	V	102	-	-	4/31/31/57	-
69	3PE	g	303	-	-	9/28/28/54	-
71	CDL	g	301	-	-	9/41/45/110	-
69	3PE	t	101	-	-	7/28/28/54	-
69	3PE	G	102	-	-	11/54/54/54	-
72	HEM	C	401	5	-	1/12/54/54	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	D	301	HEC	C2B-C3B	-6.73	1.33	1.40
73	D	301	HEC	C3C-C2C	-6.41	1.34	1.40
73	O	303	HEC	C2B-C3B	-6.33	1.34	1.40
73	O	303	HEC	C3C-C2C	-6.09	1.34	1.40
73	D	301	HEC	C3D-C2D	5.45	1.53	1.37
73	O	303	HEC	C3D-C2D	5.35	1.53	1.37
77	a	603	HEA	C3B-C2B	4.57	1.45	1.34
77	n	604	HEA	C3D-C2D	4.46	1.46	1.36
77	n	604	HEA	C3B-C2B	4.32	1.44	1.34
77	n	603	HEA	C3B-C2B	4.17	1.44	1.34
77	a	604	HEA	C3B-C2B	4.14	1.44	1.34
77	a	603	HEA	C3D-C2D	4.10	1.45	1.36
77	a	603	HEA	C3A-C2A	4.06	1.46	1.40
72	C	402	HEM	C3C-CAC	3.94	1.55	1.47
72	N	401	HEM	C3C-CAC	3.93	1.55	1.47
72	C	401	HEM	C3C-C2C	-3.91	1.34	1.40
72	N	401	HEM	C3C-C2C	-3.90	1.35	1.40
72	N	402	HEM	C3C-CAC	3.87	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	C	401	HEM	C3C-CAC	3.86	1.55	1.47
77	n	603	HEA	C3D-C2D	3.84	1.44	1.36
77	a	604	HEA	C3D-C2D	3.69	1.44	1.36
77	a	604	HEA	C3A-C2A	3.69	1.45	1.40
72	N	402	HEM	C3C-C2C	-3.64	1.35	1.40
72	C	402	HEM	C3C-C2C	-3.49	1.35	1.40
77	a	604	HEA	C3C-C2C	3.45	1.45	1.40
77	a	603	HEA	C3C-C2C	3.43	1.45	1.40
77	n	603	HEA	C3C-C2C	3.38	1.45	1.40
77	n	604	HEA	C3C-C2C	3.34	1.45	1.40
77	n	603	HEA	C3A-C2A	3.33	1.45	1.40
77	n	604	HEA	C3A-C2A	3.19	1.44	1.40
72	C	401	HEM	CAB-C3B	3.15	1.56	1.47
72	C	402	HEM	CAB-C3B	3.11	1.55	1.47
77	a	603	HEA	C4B-C3B	3.06	1.49	1.44
72	N	401	HEM	CAB-C3B	3.04	1.55	1.47
77	n	604	HEA	C4B-C3B	3.01	1.49	1.44
77	n	603	HEA	C4B-C3B	2.97	1.49	1.44
72	N	402	HEM	CAB-C3B	2.95	1.55	1.47
77	a	604	HEA	C4B-C3B	2.84	1.49	1.44
77	a	603	HEA	C2A-C1A	2.65	1.48	1.42
77	n	604	HEA	C1D-ND	-2.46	1.36	1.40
86	n1	201	ZMP	C9-C10	2.44	1.53	1.50
77	n	604	HEA	C2A-C1A	2.43	1.48	1.42
77	n	603	HEA	C1D-ND	-2.41	1.36	1.40
86	W1	201	ZMP	C9-C10	2.40	1.53	1.50
77	a	603	HEA	C1D-ND	-2.40	1.36	1.40
77	a	604	HEA	C2A-C1A	2.32	1.47	1.42
77	a	604	HEA	C1D-C2D	2.32	1.49	1.44
72	N	402	HEM	FE-NB	2.27	2.08	1.96
87	O1	401	DGT	C5-C6	-2.20	1.42	1.47
77	n	603	HEA	C2A-C1A	2.16	1.47	1.42
77	a	604	HEA	C1D-ND	-2.15	1.36	1.40
72	C	402	HEM	FE-NB	2.08	2.07	1.96
72	C	402	HEM	CMB-C2B	2.07	1.55	1.50
77	n	604	HEA	C4D-C3D	2.03	1.48	1.45
73	O	303	HEC	CAD-C3D	2.03	1.55	1.52

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	604	HEA	CMC-C2C-C3C	7.88	139.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	603	HEA	CMC-C2C-C3C	7.77	139.22	124.68
77	n	604	HEA	CMC-C2C-C3C	7.59	138.87	124.68
77	n	603	HEA	CMC-C2C-C3C	7.42	138.56	124.68
77	a	604	HEA	CMC-C2C-C1C	-6.87	117.91	128.46
77	n	604	HEA	CMC-C2C-C1C	-6.75	118.09	128.46
77	n	603	HEA	CMC-C2C-C1C	-6.73	118.11	128.46
77	a	603	HEA	CMC-C2C-C1C	-6.68	118.20	128.46
77	n	603	HEA	C13-C12-C11	-5.79	105.64	114.35
77	n	604	HEA	CMD-C2D-C1D	-5.25	117.05	125.04
77	n	604	HEA	C3D-C4D-ND	5.14	115.33	110.36
77	n	603	HEA	C3D-C4D-ND	4.97	115.17	110.36
77	a	604	HEA	C3D-C4D-ND	4.96	115.16	110.36
72	N	401	HEM	C3B-C2B-C1B	4.88	110.11	106.49
77	a	603	HEA	CMD-C2D-C1D	-4.59	118.05	125.04
77	a	603	HEA	C3D-C4D-ND	4.59	114.80	110.36
72	C	401	HEM	C3B-C2B-C1B	4.56	109.87	106.49
77	a	603	HEA	CMB-C2B-C1B	-4.35	118.41	125.04
77	n	604	HEA	C13-C12-C11	-4.29	107.91	114.35
77	n	603	HEA	CHA-C4D-C3D	-4.24	118.60	124.84
77	a	603	HEA	C13-C12-C11	-4.05	108.27	114.35
77	n	604	HEA	CMD-C2D-C3D	4.04	137.08	126.12
77	n	603	HEA	C4D-C3D-C2D	-4.00	101.07	106.90
77	a	604	HEA	CHA-C4D-C3D	-3.98	118.99	124.84
77	n	604	HEA	CHA-C4D-C3D	-3.95	119.03	124.84
73	O	303	HEC	CMC-C2C-C1C	-3.91	122.46	128.46
77	n	604	HEA	CMB-C2B-C1B	-3.86	119.16	125.04
77	n	603	HEA	CMB-C2B-C1B	-3.85	119.17	125.04
77	a	603	HEA	C4D-C3D-C2D	-3.84	101.31	106.90
77	n	604	HEA	C4D-C3D-C2D	-3.80	101.36	106.90
77	a	604	HEA	CAD-CBD-CGD	-3.73	105.57	113.60
72	N	401	HEM	CHB-C1B-NB	3.72	128.98	124.38
77	n	603	HEA	CMD-C2D-C1D	-3.71	119.39	125.04
73	D	301	HEC	CMC-C2C-C1C	-3.66	122.83	128.46
72	C	401	HEM	CMC-C2C-C3C	3.66	131.52	124.68
77	a	604	HEA	C4D-C3D-C2D	-3.64	101.59	106.90
77	n	603	HEA	CAA-CBA-CGA	-3.59	103.70	113.76
77	a	603	HEA	CHA-C4D-C3D	-3.58	119.58	124.84
77	n	603	HEA	C13-C14-C15	-3.57	119.07	127.66
77	a	604	HEA	C13-C12-C11	-3.49	109.11	114.35
72	N	401	HEM	CMC-C2C-C3C	3.40	131.05	124.68
72	N	401	HEM	C4C-CHD-C1D	3.35	126.98	122.56
77	a	603	HEA	CMD-C2D-C3D	3.33	135.15	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	C	402	HEM	C4D-ND-C1D	3.31	108.50	105.07
77	a	604	HEA	CMB-C2B-C1B	-3.25	120.09	125.04
77	a	604	HEA	C26-C15-C16	3.23	120.70	115.27
77	a	604	HEA	CAD-C3D-C4D	3.17	130.20	124.66
72	N	401	HEM	CMB-C2B-C1B	-3.16	120.23	125.04
77	a	603	HEA	CMB-C2B-C3B	3.15	136.34	130.34
77	a	604	HEA	CAA-CBA-CGA	-3.12	105.02	113.76
77	n	604	HEA	C26-C15-C16	3.11	120.50	115.27
77	n	603	HEA	CHB-C1B-C2B	-3.07	120.18	124.98
72	N	402	HEM	C4D-ND-C1D	3.07	108.24	105.07
72	N	402	HEM	C3B-C2B-C1B	3.06	108.76	106.49
77	a	603	HEA	C26-C15-C16	3.04	120.38	115.27
77	n	604	HEA	OMA-CMA-C3A	-2.89	118.60	124.91
72	N	402	HEM	CBA-CAA-C2A	-2.89	107.69	112.62
77	n	603	HEA	CMB-C2B-C3B	2.86	135.80	130.34
77	a	604	HEA	C13-C14-C15	-2.86	120.77	127.66
73	O	303	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
72	N	402	HEM	C1B-NB-C4B	2.79	107.96	105.07
77	n	604	HEA	CAA-CBA-CGA	-2.79	105.94	113.76
72	C	401	HEM	C4D-ND-C1D	2.78	107.95	105.07
72	N	402	HEM	CMC-C2C-C3C	2.78	129.88	124.68
77	a	604	HEA	C27-C19-C20	2.77	119.93	115.27
72	C	402	HEM	CMC-C2C-C3C	2.77	129.85	124.68
73	D	301	HEC	CBD-CAD-C3D	-2.72	107.98	112.62
72	C	402	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
77	n	604	HEA	C25-C23-C24	2.70	120.58	114.60
77	n	603	HEA	CMD-C2D-C3D	2.68	133.40	126.12
77	a	603	HEA	CAA-C2A-C3A	2.68	133.46	126.86
77	n	604	HEA	C17-C18-C19	-2.67	121.24	127.66
77	a	603	HEA	CHB-C1B-C2B	-2.66	120.82	124.98
73	O	303	HEC	CAA-CBA-CGA	-2.66	106.31	113.76
72	N	402	HEM	C4B-CHC-C1C	2.66	126.06	122.56
72	C	401	HEM	C4C-CHD-C1D	2.64	126.05	122.56
77	a	603	HEA	C13-C14-C15	-2.64	121.30	127.66
72	N	402	HEM	CHC-C4B-C3B	2.64	128.61	124.57
72	N	401	HEM	C4D-ND-C1D	2.64	107.80	105.07
77	n	604	HEA	C13-C14-C15	-2.61	121.38	127.66
77	n	604	HEA	CAD-C3D-C2D	2.61	132.73	127.88
86	W1	201	ZMP	O1-C10-C9	-2.60	120.91	123.99
77	n	603	HEA	C26-C15-C16	2.60	119.65	115.27
86	n1	201	ZMP	O1-C10-C9	-2.57	120.95	123.99
77	a	604	HEA	C17-C18-C19	-2.57	121.47	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	n	603	HEA	CHB-C1B-NB	2.56	127.22	124.43
77	a	604	HEA	C25-C23-C24	2.56	120.27	114.60
77	a	603	HEA	C17-C18-C19	-2.56	121.50	127.66
77	n	603	HEA	CAD-C3D-C4D	2.54	129.10	124.66
77	a	603	HEA	CAA-CBA-CGA	-2.54	106.64	113.76
72	C	402	HEM	C3D-C4D-ND	-2.53	107.35	110.17
77	n	604	HEA	C4B-C3B-C2B	-2.52	103.10	107.41
77	a	604	HEA	CAA-C2A-C3A	2.52	133.07	126.86
77	a	603	HEA	C3B-C4B-NB	2.44	112.73	109.84
77	a	603	HEA	C27-C19-C20	2.43	119.35	115.27
77	n	603	HEA	C27-C19-C20	2.43	119.35	115.27
77	n	603	HEA	C17-C18-C19	-2.42	121.83	127.66
77	a	603	HEA	CAD-C3D-C4D	2.40	128.85	124.66
77	a	604	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
72	C	401	HEM	CAD-CBD-CGD	-2.39	108.46	113.60
77	n	604	HEA	CMB-C2B-C3B	2.38	134.89	130.34
77	n	604	HEA	C3B-C4B-NB	2.38	112.66	109.84
72	N	401	HEM	CAD-CBD-CGD	-2.38	108.48	113.60
77	a	604	HEA	C3B-C4B-NB	2.37	112.65	109.84
77	n	603	HEA	C25-C23-C24	2.36	119.81	114.60
77	a	603	HEA	C4B-C3B-C2B	-2.35	103.39	107.41
77	a	603	HEA	C2B-C1B-NB	2.34	112.69	109.88
72	N	402	HEM	C3D-C4D-ND	-2.31	107.59	110.17
77	a	604	HEA	CMD-C2D-C1D	-2.31	121.52	125.04
77	n	604	HEA	CHB-C1B-C2B	-2.31	121.37	124.98
77	n	604	HEA	CAD-CBD-CGD	-2.31	108.64	113.60
77	a	603	HEA	C25-C23-C24	2.29	119.66	114.60
77	n	604	HEA	C27-C19-C20	2.28	119.11	115.27
85	P1	501	NDP	C5A-C6A-N6A	2.28	123.82	120.35
77	n	603	HEA	C2B-C1B-NB	2.27	112.60	109.88
72	N	401	HEM	CMA-C3A-C4A	-2.26	124.98	128.46
77	n	604	HEA	C2D-C1D-ND	2.25	112.50	109.84
72	C	402	HEM	C1B-NB-C4B	2.19	107.34	105.07
83	1	501	FMN	P-O5'-C5'	2.18	124.31	118.30
72	C	402	HEM	C4B-CHC-C1C	2.17	125.42	122.56
77	n	603	HEA	CAD-CBD-CGD	-2.17	108.94	113.60
72	C	401	HEM	C2B-C1B-NB	-2.16	107.27	109.84
70	I	201	PC1	C2-O21-C21	2.16	123.11	117.79
73	D	301	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
77	a	604	HEA	CBA-CAA-C2A	2.14	116.21	112.60
73	D	301	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
77	a	603	HEA	CAD-CBD-CGD	-2.13	109.03	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	604	HEA	CHB-C1B-C2B	-2.12	121.67	124.98
77	n	603	HEA	CAA-C2A-C3A	2.11	132.07	126.86
72	C	401	HEM	C3D-C4D-ND	-2.11	107.82	110.17
77	a	604	HEA	CMD-C2D-C3D	2.10	131.82	126.12
72	N	402	HEM	CAD-CBD-CGD	-2.09	109.10	113.60
71	R	103	CDL	CA4-OA6-CA5	2.05	122.83	117.79
72	N	401	HEM	CHD-C1D-ND	2.04	126.64	124.43
71	r1	202	CDL	CA4-OA6-CA5	2.03	122.79	117.79
69	H1	401	3PE	C2-O21-C21	2.02	122.78	117.79
71	R	102	CDL	CA4-OA6-CA5	2.02	122.76	117.79
73	D	301	HEC	C2B-C3B-C4B	2.02	108.53	106.35
77	a	604	HEA	CHB-C1B-NB	2.02	126.62	124.43
72	N	402	HEM	CAB-C3B-C2B	-2.01	121.97	128.60
69	n	605	3PE	C2-O21-C21	2.01	122.75	117.79
69	t	101	3PE	C2-O21-C21	2.01	122.73	117.79

There are no chirality outliers.

All (818) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	t	101	3PE	C11-O13-P-O12
69	t	101	3PE	C11-O13-P-O14
69	t	101	3PE	O13-C11-C12-N
69	z	102	3PE	O13-C11-C12-N
69	A	501	3PE	C1-O11-P-O12
69	A	501	3PE	C1-O11-P-O13
69	A	501	3PE	C1-O11-P-O14
69	A	501	3PE	C11-O13-P-O11
69	A	501	3PE	C11-O13-P-O12
69	A	501	3PE	C11-O13-P-O14
69	A	501	3PE	O13-C11-C12-N
69	C	403	3PE	C1-O11-P-O12
69	C	403	3PE	C1-O11-P-O14
69	C	403	3PE	C11-O13-P-O12
69	C	403	3PE	C11-O13-P-O14
69	E	202	3PE	C11-O13-P-O14
69	E	202	3PE	O13-C11-C12-N
69	E	203	3PE	C1-O11-P-O12
69	E	203	3PE	O13-C11-C12-N
69	G	102	3PE	C1-O11-P-O14
69	G	102	3PE	C11-O13-P-O14
69	L	501	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	L	501	3PE	O13-C11-C12-N
69	N	403	3PE	C11-O13-P-O11
69	N	403	3PE	C11-O13-P-O12
69	N	403	3PE	C11-O13-P-O14
69	N	403	3PE	O13-C11-C12-N
69	O	302	3PE	C1-O11-P-O14
69	O	302	3PE	C11-O13-P-O11
69	O	302	3PE	C11-O13-P-O14
69	O	302	3PE	O13-C11-C12-N
69	R	104	3PE	O13-C11-C12-N
69	n	605	3PE	C1-O11-P-O12
69	n	605	3PE	C1-O11-P-O14
69	n	605	3PE	C11-O13-P-O11
69	n	605	3PE	C11-O13-P-O12
69	n	605	3PE	C11-O13-P-O14
69	n	605	3PE	O13-C11-C12-N
69	n	606	3PE	C1-O11-P-O12
69	n	606	3PE	C1-O11-P-O14
69	n	606	3PE	O11-C1-C2-O21
69	n	607	3PE	C11-O13-P-O14
69	n	607	3PE	C2-C1-O11-P
69	n	607	3PE	O13-C11-C12-N
69	o	302	3PE	C12-C11-O13-P
69	p	301	3PE	C1-O11-P-O12
69	p	301	3PE	C1-O11-P-O13
69	p	301	3PE	C1-O11-P-O14
69	p	301	3PE	C11-O13-P-O14
69	p	301	3PE	O13-C11-C12-N
69	v	101	3PE	C1-O11-P-O12
69	v	101	3PE	O13-C11-C12-N
69	6	202	3PE	C11-O13-P-O11
69	6	202	3PE	C11-O13-P-O14
69	6	202	3PE	O13-C11-C12-N
69	r1	201	3PE	C1-O11-P-O14
69	r1	201	3PE	C11-O13-P-O11
69	r1	201	3PE	C11-O13-P-O12
69	r1	201	3PE	C11-O13-P-O14
69	r1	201	3PE	O13-C11-C12-N
69	K1	201	3PE	C1-O11-P-O12
69	K1	201	3PE	C1-O11-P-O13
69	K1	201	3PE	C1-O11-P-O14
69	L1	701	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	L1	701	3PE	C11-O13-P-O14
69	L1	704	3PE	C1-O11-P-O12
69	L1	704	3PE	O13-C11-C12-N
69	M1	502	3PE	C1-O11-P-O12
69	M1	502	3PE	C11-O13-P-O11
69	M1	502	3PE	C11-O13-P-O12
69	M1	502	3PE	C11-O13-P-O14
69	M1	502	3PE	O13-C11-C12-N
69	M1	503	3PE	C11-O13-P-O11
69	M1	503	3PE	C11-O13-P-O12
69	M1	503	3PE	C11-O13-P-O14
69	M1	503	3PE	O13-C11-C12-N
69	N1	402	3PE	O13-C11-C12-N
69	Y1	402	3PE	C1-O11-P-O12
69	Y1	402	3PE	C1-O11-P-O13
69	Y1	402	3PE	C1-O11-P-O14
69	Y1	402	3PE	O13-C11-C12-N
69	Y1	403	3PE	C11-O13-P-O11
69	Y1	403	3PE	C11-O13-P-O14
69	d1	202	3PE	C11-O13-P-O12
69	d1	202	3PE	C11-O13-P-O14
69	d1	202	3PE	O13-C11-C12-N
69	d1	203	3PE	C1-O11-P-O12
69	d1	203	3PE	C1-O11-P-O14
69	m1	601	3PE	C1-O11-P-O14
69	m1	601	3PE	C11-O13-P-O12
69	m1	601	3PE	C11-O13-P-O14
69	a	605	3PE	C1-O11-P-O12
69	a	606	3PE	C11-O13-P-O14
69	a	606	3PE	O13-C11-C12-N
69	c	301	3PE	O13-C11-C12-N
69	d	201	3PE	C11-O13-P-O14
69	d	201	3PE	O13-C11-C12-N
69	g	303	3PE	C11-O13-P-O12
69	g	303	3PE	C11-O13-P-O14
69	g	303	3PE	O13-C11-C12-N
69	i	101	3PE	C11-O13-P-O12
69	i	101	3PE	O13-C11-C12-N
70	J	101	PC1	C1-O11-P-O12
70	J	101	PC1	C1-O11-P-O14
70	J	101	PC1	C1-O11-P-O13
70	K	101	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
70	L	503	PC1	C11-O13-P-O12
70	L	503	PC1	C11-O13-P-O14
70	L	503	PC1	C11-O13-P-O11
70	L	503	PC1	C1-O11-P-O12
70	L	503	PC1	C1-O11-P-O13
70	I	201	PC1	C11-O13-P-O12
70	I	201	PC1	C1-O11-P-O13
70	p	302	PC1	C11-O13-P-O12
70	p	302	PC1	C11-O13-P-O14
70	p	302	PC1	C1-O11-P-O14
70	6	203	PC1	C1-O11-P-O12
70	6	203	PC1	C1-O11-P-O14
70	9	203	PC1	C11-O13-P-O11
70	9	203	PC1	C1-O11-P-O12
70	9	203	PC1	C1-O11-P-O14
70	9	204	PC1	C1-O11-P-O14
70	P1	502	PC1	C11-O13-P-O12
70	P1	502	PC1	C11-O13-P-O14
70	P1	502	PC1	C1-O11-P-O12
70	P1	502	PC1	C1-O11-P-O14
70	M1	501	PC1	C11-O13-P-O12
70	g	302	PC1	C1-O11-P-O14
71	A	502	CDL	CB2-OB2-PB2-OB3
71	A	502	CDL	CB2-OB2-PB2-OB4
71	A	502	CDL	CB2-OB2-PB2-OB5
71	D	302	CDL	CA3-OA5-PA1-OA3
71	D	302	CDL	CB2-OB2-PB2-OB5
71	D	302	CDL	CB3-OB5-PB2-OB4
71	G	101	CDL	CA2-OA2-PA1-OA4
71	G	101	CDL	CB2-OB2-PB2-OB3
71	G	101	CDL	CB2-OB2-PB2-OB4
71	G	101	CDL	CB3-OB5-PB2-OB3
71	L	502	CDL	CA3-OA5-PA1-OA3
71	O	301	CDL	CB2-OB2-PB2-OB3
71	O	301	CDL	CB3-OB5-PB2-OB4
71	R	101	CDL	CA2-OA2-PA1-OA3
71	R	101	CDL	CA2-OA2-PA1-OA4
71	R	101	CDL	CB2-OB2-PB2-OB3
71	R	102	CDL	CA3-OA5-PA1-OA2
71	R	102	CDL	CA3-OA5-PA1-OA3
71	R	102	CDL	CA3-OA5-PA1-OA4
71	R	102	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
71	R	103	CDL	CA3-OA5-PA1-OA2
71	R	103	CDL	CA3-OA5-PA1-OA3
71	R	103	CDL	CA3-OA5-PA1-OA4
71	R	103	CDL	CB2-OB2-PB2-OB3
71	R	103	CDL	CB2-OB2-PB2-OB4
71	R	103	CDL	CB3-OB5-PB2-OB2
71	R	103	CDL	CB3-OB5-PB2-OB3
71	R	103	CDL	CB3-OB5-PB2-OB4
71	V	101	CDL	CA3-OA5-PA1-OA2
71	V	101	CDL	CA3-OA5-PA1-OA3
71	V	101	CDL	CA3-OA5-PA1-OA4
71	V	101	CDL	CB2-OB2-PB2-OB3
71	r1	202	CDL	CA2-OA2-PA1-OA3
71	r1	202	CDL	CA2-OA2-PA1-OA4
71	r1	202	CDL	CA2-OA2-PA1-OA5
71	H1	402	CDL	CA2-OA2-PA1-OA3
71	H1	402	CDL	CA2-OA2-PA1-OA4
71	H1	402	CDL	CA2-OA2-PA1-OA5
71	H1	402	CDL	CB2-OB2-PB2-OB3
71	H1	402	CDL	CB2-OB2-PB2-OB4
71	L1	702	CDL	CB2-OB2-PB2-OB3
71	L1	702	CDL	CB2-OB2-PB2-OB4
71	L1	702	CDL	CB3-OB5-PB2-OB2
71	L1	702	CDL	CB3-OB5-PB2-OB4
71	L1	703	CDL	CA2-OA2-PA1-OA3
71	L1	703	CDL	CA2-OA2-PA1-OA4
71	L1	703	CDL	CA3-OA5-PA1-OA3
71	N1	401	CDL	CA2-OA2-PA1-OA4
71	N1	401	CDL	OA6-CA4-CA6-OA8
71	N1	401	CDL	CB2-OB2-PB2-OB3
71	N1	401	CDL	CB2-OB2-PB2-OB4
71	Y1	401	CDL	CA2-OA2-PA1-OA3
71	Y1	401	CDL	CA2-OA2-PA1-OA4
71	d1	201	CDL	CA2-OA2-PA1-OA3
71	d1	201	CDL	CA2-OA2-PA1-OA4
71	d1	201	CDL	OB5-CB3-CB4-OB6
71	h1	201	CDL	CA2-OA2-PA1-OA3
71	h1	201	CDL	CB2-OB2-PB2-OB4
71	h1	201	CDL	CB3-OB5-PB2-OB3
71	g	301	CDL	CA2-OA2-PA1-OA3
71	g	301	CDL	CA2-OA2-PA1-OA4
71	g	301	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
72	N	402	HEM	C2A-CAA-CBA-CGA
77	n	603	HEA	C11-C12-C13-C14
77	n	603	HEA	C15-C16-C17-C18
77	n	603	HEA	C19-C20-C21-C22
77	n	604	HEA	C2D-C3D-CAD-CBD
77	n	604	HEA	C4D-C3D-CAD-CBD
77	n	604	HEA	C15-C16-C17-C18
77	a	603	HEA	C1A-C2A-CAA-CBA
77	a	603	HEA	C3A-C2A-CAA-CBA
77	a	603	HEA	C11-C12-C13-C14
77	a	603	HEA	C14-C15-C16-C17
77	a	603	HEA	C26-C15-C16-C17
77	a	604	HEA	C1A-C2A-CAA-CBA
77	a	604	HEA	C3A-C2A-CAA-CBA
77	a	604	HEA	C14-C15-C16-C17
77	a	604	HEA	C26-C15-C16-C17
83	1	501	FMN	N10-C1'-C2'-O2'
83	1	501	FMN	N10-C1'-C2'-C3'
83	1	501	FMN	C5'-O5'-P-O1P
83	1	501	FMN	C5'-O5'-P-O2P
86	W1	201	ZMP	S1-C11-C12-N1
86	n1	201	ZMP	C17-C18-C21-O5
86	n1	201	ZMP	O4-C17-C18-C21
86	n1	201	ZMP	C16-C17-C18-C21
86	n1	201	ZMP	O4-C17-C18-C19
86	n1	201	ZMP	C16-C17-C18-C20
86	n1	201	ZMP	O3-C16-C17-O4
86	n1	201	ZMP	C17-C16-N2-C15
86	n1	201	ZMP	C13-C14-C15-N2
86	n1	201	ZMP	O1-C10-S1-C11
86	n1	201	ZMP	C9-C10-S1-C11
86	n1	201	ZMP	C7-C8-C9-C10
71	V	101	CDL	OA9-CA7-OA8-CA6
71	V	101	CDL	C31-CA7-OA8-CA6
86	n1	201	ZMP	O3-C16-N2-C15
77	a	604	HEA	C15-C16-C17-C18
71	O	301	CDL	OB5-CB3-CB4-OB6
71	R	103	CDL	OB5-CB3-CB4-OB6
69	M1	502	3PE	C31-C32-C33-C34
72	C	401	HEM	C2A-CAA-CBA-CGA
72	C	402	HEM	C2A-CAA-CBA-CGA
72	N	401	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
70	M1	501	PC1	C21-C22-C23-C24
70	V	102	PC1	C11-C12-N-C13
70	p	302	PC1	C11-C12-N-C13
70	6	203	PC1	C11-C12-N-C14
70	9	204	PC1	C11-C12-N-C15
70	P1	502	PC1	C11-C12-N-C15
77	a	603	HEA	C15-C16-C17-C18
69	t	101	3PE	C11-O13-P-O11
69	C	403	3PE	C1-O11-P-O13
69	C	403	3PE	C11-O13-P-O11
69	E	203	3PE	C1-O11-P-O13
69	E	203	3PE	C11-O13-P-O11
69	G	102	3PE	C1-O11-P-O13
69	R	104	3PE	C11-O13-P-O11
69	n	605	3PE	C1-O11-P-O13
69	n	606	3PE	C1-O11-P-O13
69	n	607	3PE	C1-O11-P-O13
69	o	302	3PE	C1-O11-P-O13
69	o	302	3PE	C11-O13-P-O11
69	p	301	3PE	C11-O13-P-O11
69	v	101	3PE	C1-O11-P-O13
69	v	101	3PE	C11-O13-P-O11
69	r1	201	3PE	C1-O11-P-O13
69	K1	201	3PE	C11-O13-P-O11
69	L1	701	3PE	C1-O11-P-O13
69	L1	704	3PE	C1-O11-P-O13
69	M1	502	3PE	C1-O11-P-O13
69	b1	101	3PE	C11-O13-P-O11
69	d1	202	3PE	C1-O11-P-O13
69	d1	202	3PE	C11-O13-P-O11
69	d1	203	3PE	C1-O11-P-O13
69	i1	201	3PE	C11-O13-P-O11
69	m1	601	3PE	C1-O11-P-O13
69	m1	601	3PE	C11-O13-P-O11
69	a	606	3PE	C11-O13-P-O11
69	b	301	3PE	C11-O13-P-O11
69	c	301	3PE	C11-O13-P-O11
69	g	303	3PE	C11-O13-P-O11
69	i	101	3PE	C1-O11-P-O13
69	i	101	3PE	C11-O13-P-O11
70	J	101	PC1	C11-O13-P-O11
70	I	201	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
70	p	302	PC1	C11-O13-P-O11
70	p	302	PC1	C1-O11-P-O13
70	6	203	PC1	C11-O13-P-O11
70	6	203	PC1	C1-O11-P-O13
70	9	203	PC1	C1-O11-P-O13
70	P1	502	PC1	C11-O13-P-O11
70	P1	502	PC1	C1-O11-P-O13
70	M1	501	PC1	C11-O13-P-O11
71	A	502	CDL	CB3-OB5-PB2-OB2
71	D	302	CDL	CA2-OA2-PA1-OA5
71	D	302	CDL	CA3-OA5-PA1-OA2
71	D	302	CDL	CB3-OB5-PB2-OB2
71	G	101	CDL	CB2-OB2-PB2-OB5
71	O	301	CDL	CB3-OB5-PB2-OB2
71	R	101	CDL	CA2-OA2-PA1-OA5
71	R	102	CDL	CB2-OB2-PB2-OB5
71	R	102	CDL	CB3-OB5-PB2-OB2
71	R	103	CDL	CB2-OB2-PB2-OB5
71	r1	202	CDL	CB2-OB2-PB2-OB5
71	H1	402	CDL	CB2-OB2-PB2-OB5
71	L1	702	CDL	CA2-OA2-PA1-OA5
71	L1	702	CDL	CB2-OB2-PB2-OB5
71	L1	703	CDL	CA2-OA2-PA1-OA5
71	L1	703	CDL	CA3-OA5-PA1-OA2
71	L1	703	CDL	CB2-OB2-PB2-OB5
71	N1	401	CDL	CA2-OA2-PA1-OA5
71	N1	401	CDL	CB2-OB2-PB2-OB5
71	N1	401	CDL	CB3-OB5-PB2-OB2
71	Y1	401	CDL	CA2-OA2-PA1-OA5
71	Y1	401	CDL	CB3-OB5-PB2-OB2
71	d1	201	CDL	CA2-OA2-PA1-OA5
71	d1	201	CDL	CA3-OA5-PA1-OA2
71	h1	201	CDL	CA2-OA2-PA1-OA5
71	h1	201	CDL	CB2-OB2-PB2-OB5
71	h1	201	CDL	CB3-OB5-PB2-OB2
71	V	101	CDL	C11-CA5-OA6-CA4
71	N1	401	CDL	C81-C82-C83-C84
69	L1	704	3PE	C38-C39-C3A-C3B
71	H1	402	CDL	C13-C14-C15-C16
71	V	101	CDL	OA7-CA5-OA6-CA4
69	M1	503	3PE	C28-C29-C2A-C2B
69	G	102	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
69	b1	101	3PE	C3A-C3B-C3C-C3D
69	M1	502	3PE	C36-C37-C38-C39
69	H1	401	3PE	C31-C32-C33-C34
71	Y1	401	CDL	C82-C83-C84-C85
70	z	101	PC1	C11-C12-N-C13
69	L1	701	3PE	O13-C11-C12-N
69	b1	101	3PE	O13-C11-C12-N
69	b	301	3PE	O13-C11-C12-N
69	L1	701	3PE	C21-C22-C23-C24
70	9	204	PC1	C2A-C2B-C2C-C2D
70	M1	501	PC1	C37-C38-C39-C3A
69	M1	502	3PE	C23-C24-C25-C26
69	N1	402	3PE	C36-C37-C38-C39
71	d1	201	CDL	C55-C56-C57-C58
86	n1	201	ZMP	C6-C7-C8-C9
69	N1	402	3PE	C1-C2-C3-O31
71	Y1	401	CDL	C73-C74-C75-C76
71	R	103	CDL	CA5-C11-C12-C13
69	c	301	3PE	C23-C24-C25-C26
70	V	102	PC1	C11-C12-N-C14
70	p	302	PC1	C11-C12-N-C14
70	p	302	PC1	C11-C12-N-C15
70	6	203	PC1	C11-C12-N-C15
70	9	204	PC1	C11-C12-N-C14
69	p	301	3PE	C23-C24-C25-C26
70	I	201	PC1	C25-C26-C27-C28
71	V	101	CDL	C12-C11-CA5-OA6
70	9	204	PC1	C34-C35-C36-C37
71	D	302	CDL	C74-C75-C76-C77
69	L1	704	3PE	C32-C33-C34-C35
69	n	607	3PE	O21-C2-C3-O31
70	z	101	PC1	C11-C12-N-C15
70	V	102	PC1	C11-C12-N-C15
70	6	203	PC1	C11-C12-N-C13
70	9	204	PC1	C11-C12-N-C13
70	P1	502	PC1	C11-C12-N-C13
70	P1	502	PC1	C11-C12-N-C14
77	n	604	HEA	C26-C15-C16-C17
69	L	501	3PE	C11-O13-P-O11
69	O	302	3PE	C1-O11-P-O13
71	G	101	CDL	CB3-OB5-PB2-OB2
71	O	301	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
71	r1	202	CDL	CA3-OA5-PA1-OA2
77	a	603	HEA	O11-C11-C12-C13
69	G	102	3PE	C32-C33-C34-C35
71	d1	201	CDL	C63-C64-C65-C66
69	C	404	3PE	C1-C2-C3-O31
86	W1	201	ZMP	C19-C18-C21-O5
86	W1	201	ZMP	C20-C18-C21-O5
86	n1	201	ZMP	C5-C6-C7-C8
71	D	302	CDL	C1-CB2-OB2-PB2
70	z	101	PC1	C11-C12-N-C14
69	o	302	3PE	O21-C2-C3-O31
69	N1	402	3PE	O21-C2-C3-O31
86	n1	201	ZMP	O4-C17-C18-C20
69	n	606	3PE	O11-C1-C2-C3
71	O	301	CDL	OB5-CB3-CB4-CB6
71	R	103	CDL	OB5-CB3-CB4-CB6
71	L1	703	CDL	OB5-CB3-CB4-CB6
71	d1	201	CDL	OB5-CB3-CB4-CB6
69	L	501	3PE	C31-C32-C33-C34
69	G	102	3PE	O13-C11-C12-N
69	K1	201	3PE	O13-C11-C12-N
69	i1	201	3PE	O13-C11-C12-N
69	g	303	3PE	O31-C31-C32-C33
69	p	301	3PE	C2-C1-O11-P
69	a	606	3PE	C2-C1-O11-P
69	g	303	3PE	C2-C1-O11-P
70	J	101	PC1	C2-C1-O11-P
71	R	103	CDL	CB3-CB4-CB6-OB8
71	Y1	401	CDL	CB3-CB4-CB6-OB8
69	d1	203	3PE	C21-C22-C23-C24
70	P1	502	PC1	O11-C1-C2-O21
71	L1	702	CDL	OB5-CB3-CB4-OB6
69	C	404	3PE	O21-C2-C3-O31
69	n	606	3PE	O21-C2-C3-O31
71	R	103	CDL	OB6-CB4-CB6-OB8
71	Y1	401	CDL	OB6-CB4-CB6-OB8
69	m1	601	3PE	C2-C1-O11-P
69	c	301	3PE	C2-C1-O11-P
71	D	302	CDL	C1-CA2-OA2-PA1
71	G	101	CDL	C1-CA2-OA2-PA1
71	O	301	CDL	CB4-CB3-OB5-PB2
71	R	101	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
71	R	103	CDL	C1-CB2-OB2-PB2
71	H1	402	CDL	C1-CB2-OB2-PB2
71	h1	201	CDL	C1-CA2-OA2-PA1
70	P1	502	PC1	O21-C21-C22-C23
86	W1	201	ZMP	O1-C10-S1-C11
71	R	101	CDL	OB5-CB3-CB4-CB6
71	D	302	CDL	C52-C51-CB5-OB6
71	L1	702	CDL	CA5-C11-C12-C13
69	b1	101	3PE	C21-C22-C23-C24
86	W1	201	ZMP	C9-C10-S1-C11
69	E	202	3PE	C1-C2-C3-O31
69	n	607	3PE	C1-C2-C3-O31
69	K1	201	3PE	C2-C1-O11-P
71	H1	402	CDL	C1-CA2-OA2-PA1
71	N1	401	CDL	CA3-CA4-CA6-OA8
71	d1	201	CDL	C1-CB2-OB2-PB2
71	h1	201	CDL	CA4-CA3-OA5-PA1
69	b	301	3PE	O11-C1-C2-O21
71	R	101	CDL	OB5-CB3-CB4-OB6
69	N	403	3PE	C25-C26-C27-C28
72	N	402	HEM	C4B-C3B-CAB-CBB
86	n1	201	ZMP	C16-C17-C18-C19
69	b1	101	3PE	C23-C24-C25-C26
69	c	301	3PE	C32-C33-C34-C35
77	n	604	HEA	C14-C15-C16-C17
71	L	502	CDL	C31-C32-C33-C34
69	G	102	3PE	C11-O13-P-O11
69	n	607	3PE	C11-O13-P-O11
69	d	201	3PE	C11-O13-P-O11
70	g	302	PC1	C1-O11-P-O13
71	G	101	CDL	CA2-OA2-PA1-OA5
71	L	502	CDL	CA3-OA5-PA1-OA2
71	R	101	CDL	CB2-OB2-PB2-OB5
71	g	301	CDL	CA3-OA5-PA1-OA2
71	N1	401	CDL	C78-C79-C80-C81
69	t	101	3PE	C2-C1-O11-P
69	a	605	3PE	C2-C1-O11-P
71	D	302	CDL	CB4-CB3-OB5-PB2
71	L	502	CDL	CB4-CB3-OB5-PB2
71	O	301	CDL	C1-CA2-OA2-PA1
71	g	301	CDL	CA4-CA3-OA5-PA1
69	E	203	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	E	203	3PE	C11-O13-P-O14
69	G	102	3PE	C1-O11-P-O12
69	L	501	3PE	C11-O13-P-O14
69	O	302	3PE	C1-O11-P-O12
69	R	104	3PE	C11-O13-P-O14
69	n	607	3PE	C1-O11-P-O14
69	o	302	3PE	C1-O11-P-O14
69	o	302	3PE	C11-O13-P-O14
69	p	301	3PE	C11-O13-P-O12
69	v	101	3PE	C1-O11-P-O14
69	v	101	3PE	C11-O13-P-O12
69	v	101	3PE	C11-O13-P-O14
69	r1	201	3PE	C1-O11-P-O12
69	K1	201	3PE	C11-O13-P-O14
69	L1	701	3PE	C1-O11-P-O12
69	M1	502	3PE	C1-O11-P-O14
69	b1	101	3PE	C11-O13-P-O14
69	d1	202	3PE	C1-O11-P-O12
69	d1	202	3PE	C1-O11-P-O14
69	i1	201	3PE	C11-O13-P-O12
69	m1	601	3PE	C1-O11-P-O12
69	a	606	3PE	C11-O13-P-O12
69	b	301	3PE	C11-O13-P-O14
69	c	301	3PE	C11-O13-P-O12
69	i	101	3PE	C1-O11-P-O14
69	i	101	3PE	C11-O13-P-O14
70	J	101	PC1	C11-O13-P-O14
70	L	503	PC1	C1-O11-P-O14
70	I	201	PC1	C1-O11-P-O12
70	p	302	PC1	C1-O11-P-O12
70	6	203	PC1	C11-O13-P-O12
70	6	203	PC1	C11-O13-P-O14
70	9	203	PC1	C11-O13-P-O12
70	g	302	PC1	C1-O11-P-O12
71	A	502	CDL	CB3-OB5-PB2-OB3
71	A	502	CDL	CB3-OB5-PB2-OB4
71	D	302	CDL	CA2-OA2-PA1-OA3
71	D	302	CDL	CA3-OA5-PA1-OA4
71	D	302	CDL	CB2-OB2-PB2-OB4
71	G	101	CDL	CA2-OA2-PA1-OA3
71	G	101	CDL	CB3-OB5-PB2-OB4
71	O	301	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
71	O	301	CDL	CA2-OA2-PA1-OA4
71	O	301	CDL	CB2-OB2-PB2-OB4
71	R	102	CDL	CB2-OB2-PB2-OB3
71	r1	202	CDL	CA3-OA5-PA1-OA3
71	r1	202	CDL	CA3-OA5-PA1-OA4
71	r1	202	CDL	CB2-OB2-PB2-OB3
71	L1	702	CDL	CA2-OA2-PA1-OA3
71	L1	702	CDL	CB3-OB5-PB2-OB3
71	L1	703	CDL	CA3-OA5-PA1-OA4
71	L1	703	CDL	CB2-OB2-PB2-OB3
71	N1	401	CDL	CA2-OA2-PA1-OA3
71	N1	401	CDL	CB3-OB5-PB2-OB3
71	N1	401	CDL	CB3-OB5-PB2-OB4
71	Y1	401	CDL	CB3-OB5-PB2-OB3
71	d1	201	CDL	CA3-OA5-PA1-OA3
71	h1	201	CDL	CA2-OA2-PA1-OA4
71	h1	201	CDL	CB3-OB5-PB2-OB4
71	L1	702	CDL	OB5-CB3-CB4-CB6
71	h1	201	CDL	OB5-CB3-CB4-CB6
77	a	604	HEA	O11-C11-C12-C13
69	M1	502	3PE	C12-C11-O13-P
69	b	301	3PE	C12-C11-O13-P
69	c	301	3PE	C12-C11-O13-P
69	g	303	3PE	C12-C11-O13-P
69	i	101	3PE	C12-C11-O13-P
71	g	301	CDL	CB4-CB3-OB5-PB2
70	K	101	PC1	O11-C1-C2-O21
71	L1	703	CDL	OB5-CB3-CB4-OB6
71	N1	401	CDL	OB5-CB3-CB4-OB6
71	h1	201	CDL	OB5-CB3-CB4-OB6
77	a	603	HEA	C2A-CAA-CBA-CGA
71	G	101	CDL	C72-C71-CB7-OB8
71	L	502	CDL	C52-C51-CB5-OB6
70	p	302	PC1	C21-C22-C23-C24
69	n	606	3PE	C1-C2-C3-O31
69	o	302	3PE	C1-C2-C3-O31
69	c	301	3PE	C25-C26-C27-C28
70	J	101	PC1	O13-C11-C12-N
70	L	503	PC1	O13-C11-C12-N
70	I	201	PC1	O13-C11-C12-N
70	9	203	PC1	O13-C11-C12-N
70	M1	501	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
70	g	302	PC1	O13-C11-C12-N
77	n	603	HEA	C1A-C2A-CAA-CBA
71	N1	401	CDL	C80-C81-C82-C83
69	H1	401	3PE	C2-C1-O11-P
69	i1	201	3PE	C2-C1-O11-P
69	b1	101	3PE	C38-C39-C3A-C3B
71	D	302	CDL	C72-C73-C74-C75
69	H1	401	3PE	O31-C31-C32-C33
69	M1	502	3PE	C3D-C3E-C3F-C3G
71	R	102	CDL	C31-C32-C33-C34
69	6	202	3PE	C32-C33-C34-C35
86	n1	201	ZMP	C19-C18-C21-O5
86	n1	201	ZMP	C20-C18-C21-O5
69	t	101	3PE	C3-C2-O21-C21
70	9	203	PC1	C3-C2-O21-C21
71	V	101	CDL	CA3-CA4-OA6-CA5
69	r1	201	3PE	O31-C31-C32-C33
71	L1	702	CDL	C12-C11-CA5-OA6
69	E	202	3PE	O21-C2-C3-O31
69	E	202	3PE	C11-O13-P-O11
69	n	606	3PE	C11-O13-P-O11
69	L1	701	3PE	C11-O13-P-O11
69	M1	503	3PE	C1-O11-P-O13
69	N1	402	3PE	C11-O13-P-O11
69	a	605	3PE	C11-O13-P-O11
69	a	606	3PE	C1-O11-P-O13
69	b	301	3PE	C1-O11-P-O13
70	z	101	PC1	C11-O13-P-O11
70	g	302	PC1	C11-O13-P-O11
71	A	502	CDL	CA2-OA2-PA1-OA5
71	L	502	CDL	CA2-OA2-PA1-OA5
71	O	301	CDL	CA3-OA5-PA1-OA2
71	O	301	CDL	CB2-OB2-PB2-OB5
71	R	103	CDL	CA2-OA2-PA1-OA5
71	V	101	CDL	CA2-OA2-PA1-OA5
71	V	101	CDL	CB2-OB2-PB2-OB5
71	V	101	CDL	CB3-OB5-PB2-OB2
71	r1	202	CDL	CB3-OB5-PB2-OB2
71	H1	402	CDL	CA3-OA5-PA1-OA2
71	H1	402	CDL	CB3-OB5-PB2-OB2
71	N1	401	CDL	CA3-OA5-PA1-OA2
71	d1	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
85	P1	501	NDP	O4D-C1D-N1N-C6N
71	G	101	CDL	C72-C71-CB7-OB9
69	H1	401	3PE	C21-C22-C23-C24
85	P1	501	NDP	PN-O3-PA-O2A
69	M1	502	3PE	C37-C38-C39-C3A
69	n	606	3PE	C2-C1-O11-P
71	N1	401	CDL	C1-CA2-OA2-PA1
69	O	302	3PE	C34-C35-C36-C37
69	H1	401	3PE	C2A-C2B-C2C-C2D
69	L1	704	3PE	O21-C21-C22-C23
70	I	201	PC1	C36-C37-C38-C39
70	6	203	PC1	O11-C1-C2-C3
71	D	302	CDL	OB5-CB3-CB4-CB6
69	m1	601	3PE	O13-C11-C12-N
77	n	604	HEA	CAA-CBA-CGA-O2A
77	a	604	HEA	CAA-CBA-CGA-O2A
69	M1	503	3PE	O11-C1-C2-O21
71	D	302	CDL	OB5-CB3-CB4-OB6
69	N1	402	3PE	C2-C1-O11-P
70	V	102	PC1	C2-C1-O11-P
85	P1	501	NDP	C2D-C1D-N1N-C6N
69	d1	203	3PE	O21-C21-C22-C23
77	a	603	HEA	CAD-CBD-CGD-O1D
77	a	604	HEA	CAA-CBA-CGA-O1A
69	p	301	3PE	C22-C23-C24-C25
71	g	301	CDL	CA3-CA4-CA6-OA8
69	c	301	3PE	C28-C29-C2A-C2B
77	a	604	HEA	C19-C20-C21-C22
77	a	604	HEA	CAD-CBD-CGD-O1D
69	H1	401	3PE	C3-C2-O21-C21
69	d	201	3PE	C3-C2-O21-C21
69	g	303	3PE	C3-C2-O21-C21
71	h1	201	CDL	CB6-CB4-OB6-CB5
77	a	603	HEA	CAD-CBD-CGD-O2D
71	R	101	CDL	C72-C71-CB7-OB8
71	O	301	CDL	C1-CB2-OB2-PB2
71	r1	202	CDL	C52-C51-CB5-OB6
71	V	101	CDL	C12-C11-CA5-OA7
70	9	204	PC1	C35-C36-C37-C38
69	H1	401	3PE	O11-C1-C2-C3
71	V	101	CDL	OB5-CB3-CB4-CB6
71	r1	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
77	n	603	HEA	O11-C11-C12-C13
86	n1	201	ZMP	C12-C11-S1-C10
70	M1	501	PC1	O21-C2-C3-O31
73	O	303	HEC	CAD-CBD-CGD-O2D
71	N1	401	CDL	C79-C80-C81-C82
69	M1	503	3PE	C27-C28-C29-C2A
72	N	402	HEM	CAD-CBD-CGD-O2D
77	n	604	HEA	CAA-CBA-CGA-O1A
70	I	201	PC1	O21-C21-C22-C23
77	a	604	HEA	CAD-CBD-CGD-O2D
71	D	302	CDL	CA4-CA3-OA5-PA1
69	M1	502	3PE	C33-C34-C35-C36
77	n	603	HEA	CAD-CBD-CGD-O1D
71	R	103	CDL	C75-C76-C77-C78
71	d1	201	CDL	CA3-CA4-CA6-OA8
71	r1	202	CDL	OB5-CB3-CB4-OB6
70	9	203	PC1	C37-C38-C39-C3A
73	O	303	HEC	CAD-CBD-CGD-O1D
69	M1	503	3PE	O11-C1-C2-C3
69	c	301	3PE	O11-C1-C2-C3
71	h1	201	CDL	C12-C11-CA5-OA6
69	b1	101	3PE	C34-C35-C36-C37
69	g	303	3PE	O32-C31-C32-C33
72	N	402	HEM	CAD-CBD-CGD-O1D
71	G	101	CDL	C32-C31-CA7-OA8
69	G	102	3PE	C35-C36-C37-C38
83	1	501	FMN	C5'-O5'-P-O3P
86	n1	201	ZMP	N2-C16-C17-O4
69	K1	201	3PE	O21-C21-C22-C23
69	d	201	3PE	O21-C21-C22-C23
77	n	603	HEA	C27-C19-C20-C21
69	E	202	3PE	O31-C31-C32-C33
69	C	403	3PE	O31-C31-C32-C33
69	N	403	3PE	O31-C31-C32-C33
70	K	101	PC1	O21-C21-C22-C23
71	A	502	CDL	C12-C11-CA5-OA6
71	N1	401	CDL	C51-C52-C53-C54
69	L1	701	3PE	C3-C2-O21-C21
70	I	201	PC1	C1-C2-O21-C21
70	6	203	PC1	C3-C2-O21-C21
70	9	204	PC1	O31-C31-C32-C33
70	P1	502	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
71	A	502	CDL	C32-C31-CA7-OA8
69	C	404	3PE	O21-C21-C22-C23
69	i1	201	3PE	O31-C31-C32-C33
71	R	102	CDL	C32-C31-CA7-OA8
71	g	301	CDL	C12-C11-CA5-OA6
70	9	204	PC1	C21-C22-C23-C24
69	Y1	403	3PE	C1-C2-C3-O31
69	b	301	3PE	C1-C2-C3-O31
71	R	102	CDL	OA5-CA3-CA4-OA6
71	d1	201	CDL	C72-C71-CB7-OB8
71	h1	201	CDL	C52-C51-CB5-OB6
71	V	101	CDL	C75-C76-C77-C78
69	E	203	3PE	O31-C31-C32-C33
69	o	302	3PE	O21-C21-C22-C23
69	K1	201	3PE	O31-C31-C32-C33
71	R	102	CDL	C52-C51-CB5-OB6
70	9	203	PC1	C29-C2A-C2B-C2C
71	O	301	CDL	O1-C1-CA2-OA2
71	R	101	CDL	C32-C31-CA7-OA8
69	L	501	3PE	O11-C1-C2-C3
71	A	502	CDL	OB5-CB3-CB4-CB6
69	O	302	3PE	O21-C21-C22-C23
69	M1	502	3PE	O21-C21-C22-C23
69	a	606	3PE	O31-C31-C32-C33
71	L1	702	CDL	C72-C71-CB7-OB8
69	E	203	3PE	O21-C2-C3-O31
69	M1	503	3PE	O21-C2-C3-O31
69	m1	601	3PE	O21-C2-C3-O31
71	R	101	CDL	C12-C11-CA5-OA7
81	y	601	TGL	CC1-CC2-CC3-CC4
77	a	603	HEA	CAA-CBA-CGA-O1A
69	o	302	3PE	C22-C23-C24-C25
69	b1	101	3PE	O31-C31-C32-C33
71	L1	703	CDL	C32-C31-CA7-OA8
71	h1	201	CDL	C32-C31-CA7-OA8
77	n	603	HEA	CAD-CBD-CGD-O2D
85	P1	501	NDP	C5B-O5B-PA-O3
71	R	102	CDL	C72-C71-CB7-OB8
69	C	403	3PE	C2A-C2B-C2C-C2D
69	M1	503	3PE	C2-C1-O11-P
69	R	104	3PE	O31-C31-C32-C33
71	h1	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
81	y	601	TGL	OG1-CA1-CA2-CA3
69	K1	201	3PE	C25-C26-C27-C28
69	i	101	3PE	O31-C31-C32-C33
71	R	101	CDL	C52-C51-CB5-OB6
69	K1	201	3PE	O22-C21-C22-C23
69	Y1	403	3PE	C23-C24-C25-C26
69	E	202	3PE	O21-C21-C22-C23
69	M1	503	3PE	O31-C31-C32-C33
85	P1	501	NDP	PN-O3-PA-O1A
87	O1	401	DGT	PB-O3A-PA-O1A
71	R	102	CDL	C32-C31-CA7-OA9
71	g	301	CDL	C12-C11-CA5-OA7
73	O	303	HEC	CAA-CBA-CGA-O2A
69	C	403	3PE	O32-C31-C32-C33
70	K	101	PC1	O22-C21-C22-C23
69	G	102	3PE	O21-C21-C22-C23
69	m1	601	3PE	O21-C21-C22-C23
69	C	404	3PE	O22-C21-C22-C23
69	N	403	3PE	O32-C31-C32-C33
69	i1	201	3PE	O32-C31-C32-C33
70	P1	502	PC1	O22-C21-C22-C23
71	r1	202	CDL	C17-C18-C19-C20
71	L1	702	CDL	C12-C13-C14-C15
69	d	201	3PE	O22-C21-C22-C23
73	D	301	HEC	CAD-CBD-CGD-O2D
69	p	301	3PE	C25-C26-C27-C28
69	K1	201	3PE	O32-C31-C32-C33
71	h1	201	CDL	C52-C51-CB5-OB7
69	O	302	3PE	O22-C21-C22-C23
69	a	606	3PE	O32-C31-C32-C33
71	A	502	CDL	C12-C11-CA5-OA7
71	R	101	CDL	C32-C31-CA7-OA9
69	Y1	403	3PE	O31-C31-C32-C33
69	E	202	3PE	O32-C31-C32-C33
70	9	204	PC1	O32-C31-C32-C33
70	P1	502	PC1	O32-C31-C32-C33
81	y	601	TGL	OA1-CA1-CA2-CA3
77	n	603	HEA	CAA-CBA-CGA-O2A
69	m1	601	3PE	C32-C33-C34-C35
69	H1	401	3PE	C1-O11-P-O14
69	L1	701	3PE	C11-O13-P-O12
69	a	605	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	a	605	3PE	C11-O13-P-O14
69	a	606	3PE	C1-O11-P-O14
69	b	301	3PE	C1-O11-P-O14
70	z	101	PC1	C1-O11-P-O14
70	g	302	PC1	C11-O13-P-O14
71	L	502	CDL	CA3-OA5-PA1-OA4
71	V	101	CDL	CB3-OB5-PB2-OB3
71	L1	703	CDL	CB3-OB5-PB2-OB3
71	N1	401	CDL	CA3-OA5-PA1-OA3
71	d1	201	CDL	CB2-OB2-PB2-OB3
69	o	302	3PE	O22-C21-C22-C23
71	D	302	CDL	C52-C51-CB5-OB7
69	b	301	3PE	O11-C1-C2-C3
70	M1	501	PC1	O11-C1-C2-C3
71	R	102	CDL	C52-C51-CB5-OB7
71	h1	201	CDL	C72-C71-CB7-OB9
69	M1	502	3PE	O31-C31-C32-C33
71	Y1	401	CDL	C32-C31-CA7-OA8
69	E	203	3PE	O32-C31-C32-C33
69	M1	502	3PE	O22-C21-C22-C23
71	h1	201	CDL	C32-C31-CA7-OA9
71	d1	201	CDL	C62-C63-C64-C65
71	A	502	CDL	C32-C31-CA7-OA9
77	a	603	HEA	CAA-CBA-CGA-O2A
69	t	101	3PE	C12-C11-O13-P
69	A	501	3PE	C1-C2-O21-C21
69	n	605	3PE	C1-C2-O21-C21
69	Y1	403	3PE	C12-C11-O13-P
69	d1	203	3PE	C12-C11-O13-P
69	m1	601	3PE	C12-C11-O13-P
69	a	605	3PE	C12-C11-O13-P
70	L	503	PC1	C1-C2-O21-C21
70	9	203	PC1	C12-C11-O13-P
70	P1	502	PC1	C3-C2-O21-C21
70	M1	501	PC1	C12-C11-O13-P
71	R	101	CDL	CA6-CA4-OA6-CA5
71	R	102	CDL	CA3-CA4-OA6-CA5
71	R	103	CDL	CA6-CA4-OA6-CA5
71	N1	401	CDL	CB6-CB4-OB6-CB5
77	a	603	HEA	C3B-C11-C12-C13
69	M1	503	3PE	O32-C31-C32-C33
71	L1	703	CDL	C32-C31-CA7-OA9

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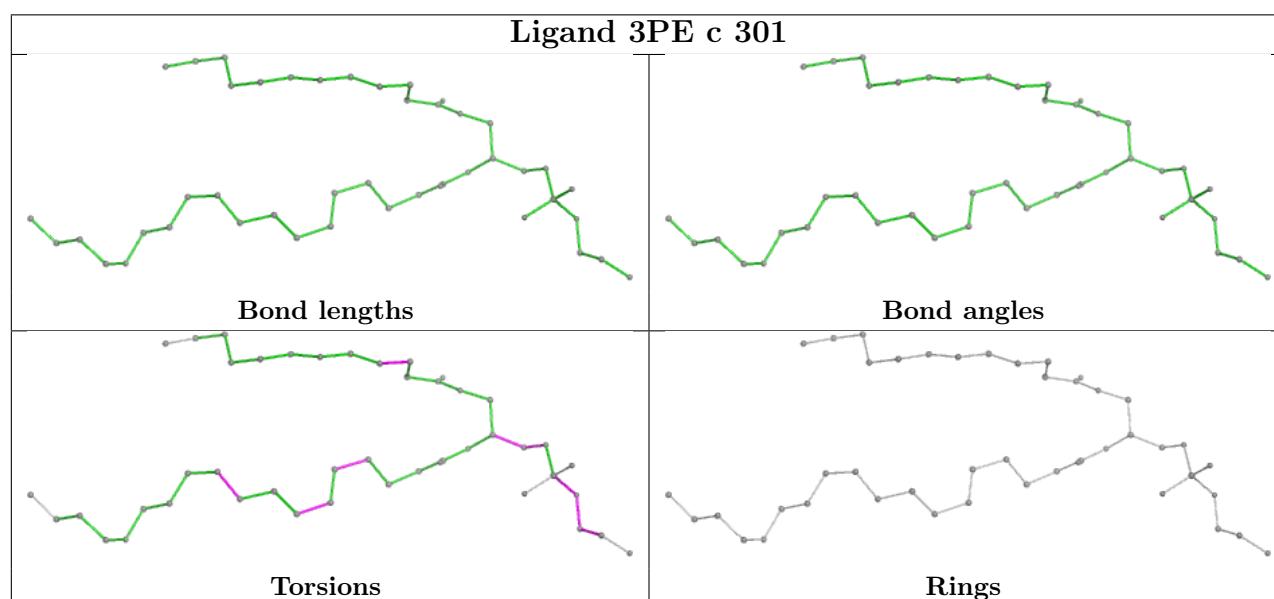
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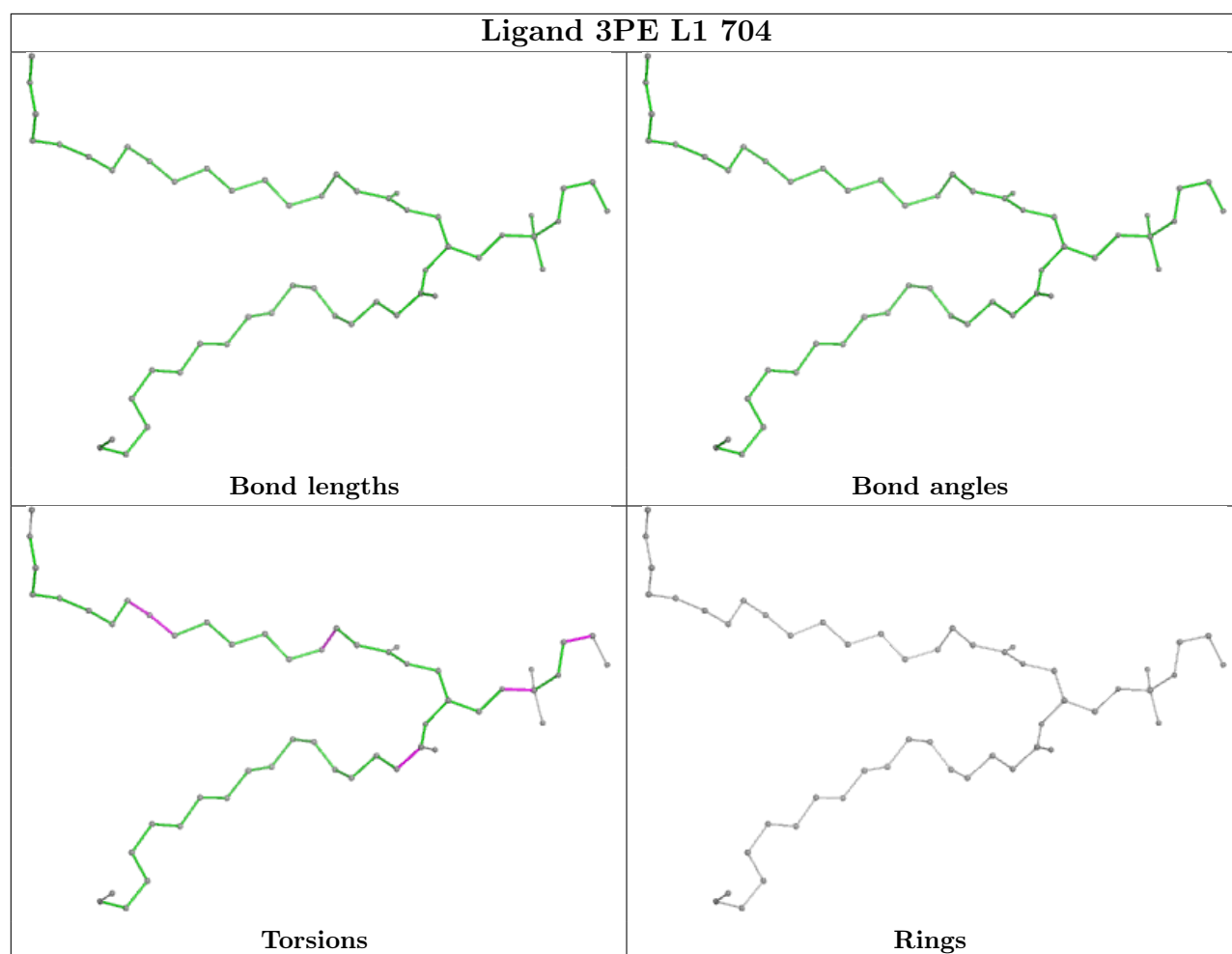
Mol	Chain	Res	Type	Atoms
71	d1	201	CDL	C72-C71-CB7-OB9
71	R	103	CDL	C81-C82-C83-C84
70	M1	501	PC1	C3B-C3C-C3D-C3E
69	d1	203	3PE	C31-C32-C33-C34
69	n	605	3PE	O21-C21-C22-C23
70	g	302	PC1	O31-C31-C32-C33
71	L	502	CDL	C12-C11-CA5-OA6
72	N	401	HEM	CAA-CBA-CGA-O1A
73	O	303	HEC	CAA-CBA-CGA-O1A
71	V	101	CDL	C72-C73-C74-C75
69	b1	101	3PE	O32-C31-C32-C33
69	H1	401	3PE	C23-C24-C25-C26
69	A	501	3PE	O31-C31-C32-C33
69	p	301	3PE	O31-C31-C32-C33
70	9	203	PC1	O21-C21-C22-C23
71	L1	703	CDL	C52-C51-CB5-OB6
69	L1	704	3PE	C39-C3A-C3B-C3C
69	M1	503	3PE	C29-C2A-C2B-C2C
71	L1	702	CDL	C72-C71-CB7-OB9
70	6	203	PC1	C3A-C3B-C3C-C3D
69	R	104	3PE	O32-C31-C32-C33
69	m1	601	3PE	O22-C21-C22-C23
73	D	301	HEC	CAD-CBD-CGD-O1D
70	L	503	PC1	O21-C21-C22-C23
71	A	502	CDL	C52-C51-CB5-OB6
71	R	101	CDL	C12-C11-CA5-OA6
69	E	202	3PE	O22-C21-C22-C23
69	G	102	3PE	O22-C21-C22-C23
71	H1	402	CDL	C17-C18-C19-C20
69	n	605	3PE	O22-C21-C22-C23
70	9	203	PC1	O22-C21-C22-C23
71	L	502	CDL	C12-C11-CA5-OA7
71	R	102	CDL	C72-C71-CB7-OB9
71	L1	703	CDL	C52-C51-CB5-OB7
70	g	302	PC1	O32-C31-C32-C33
71	Y1	401	CDL	C32-C31-CA7-OA9
72	N	401	HEM	CAA-CBA-CGA-O2A
69	Y1	403	3PE	O32-C31-C32-C33
70	z	101	PC1	O21-C21-C22-C23
71	R	102	CDL	C12-C11-CA5-OA6

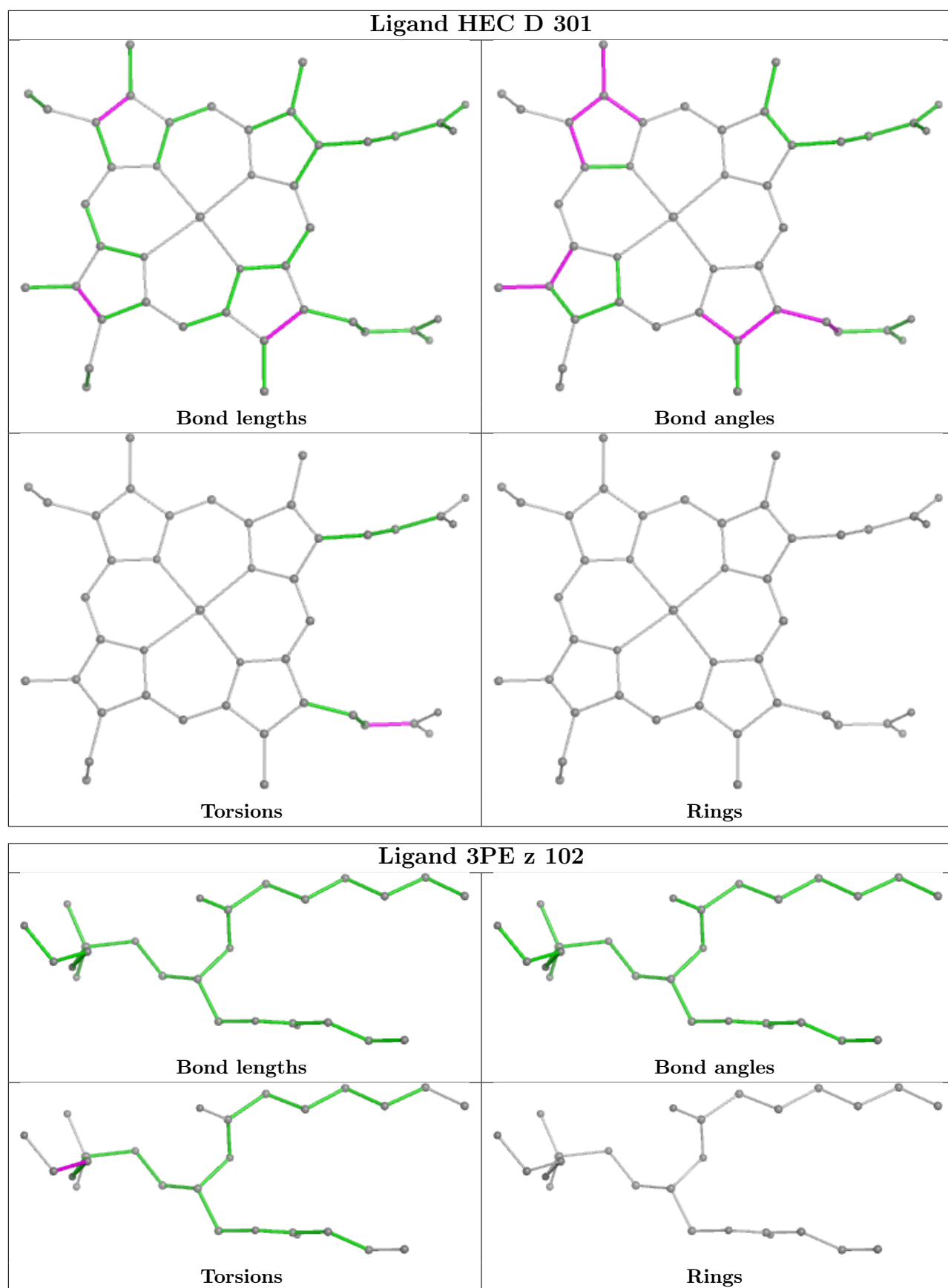
There are no ring outliers.

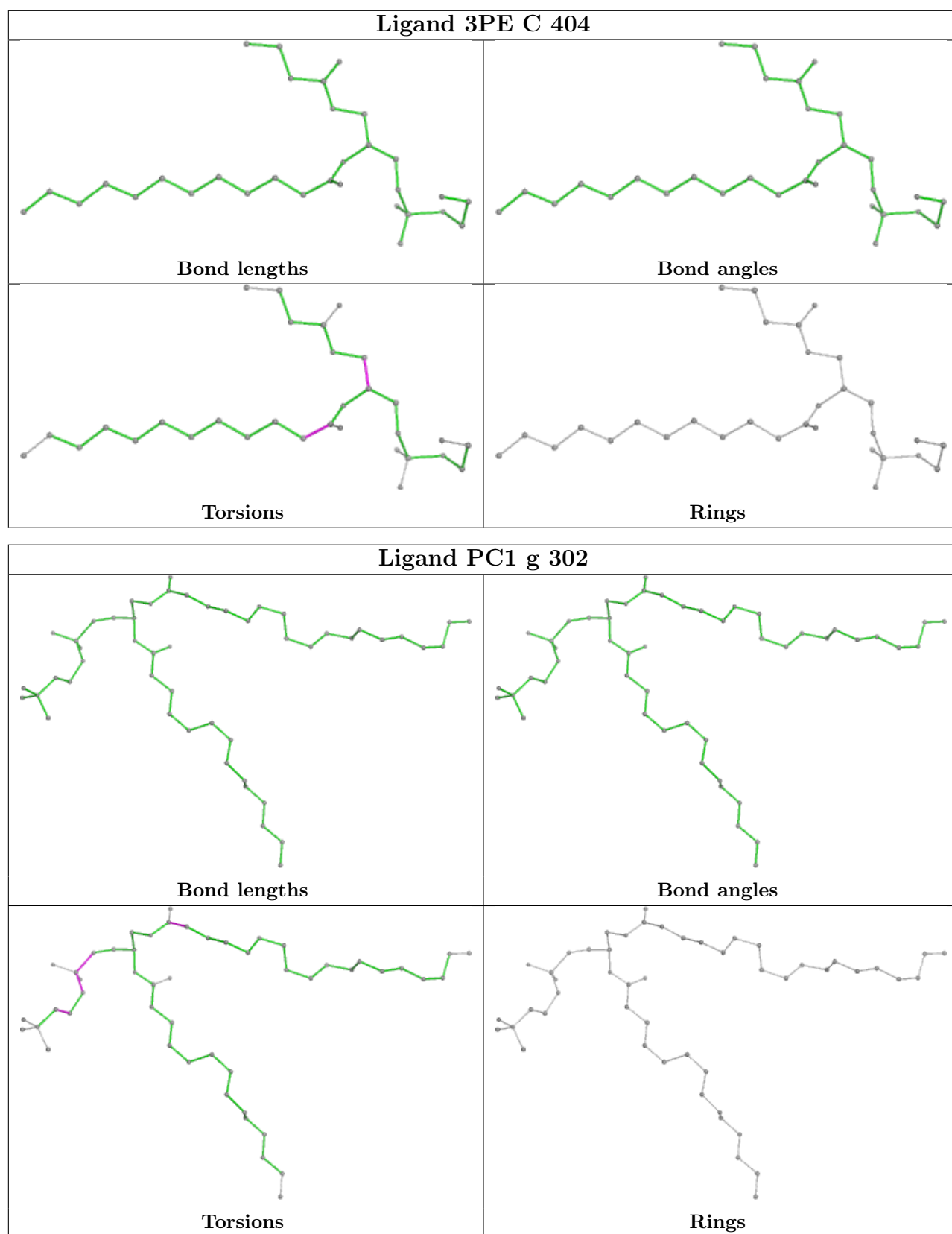
No monomer is involved in short contacts.

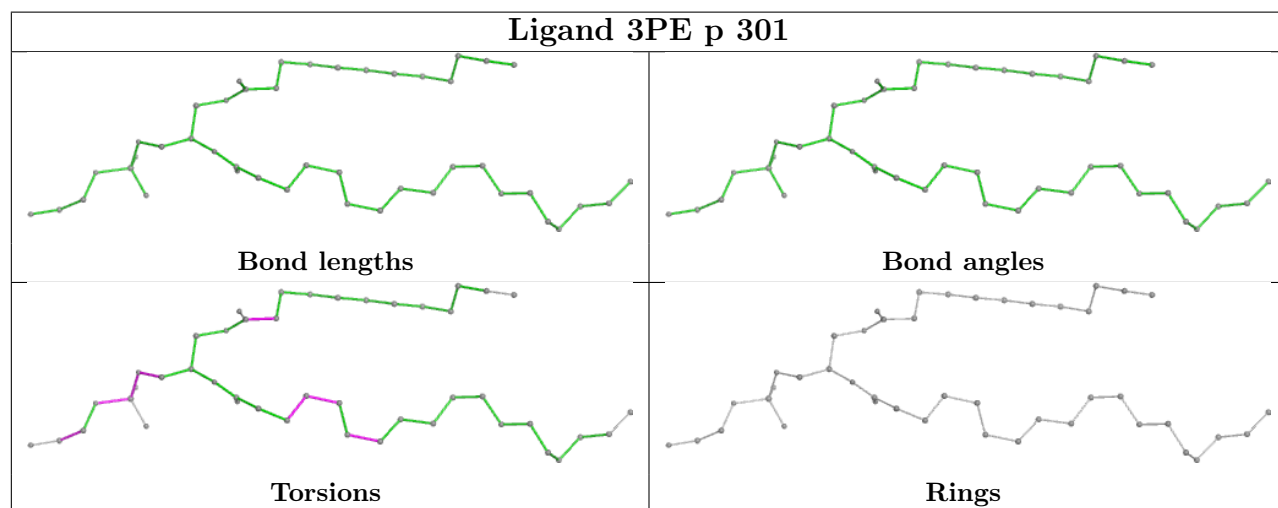
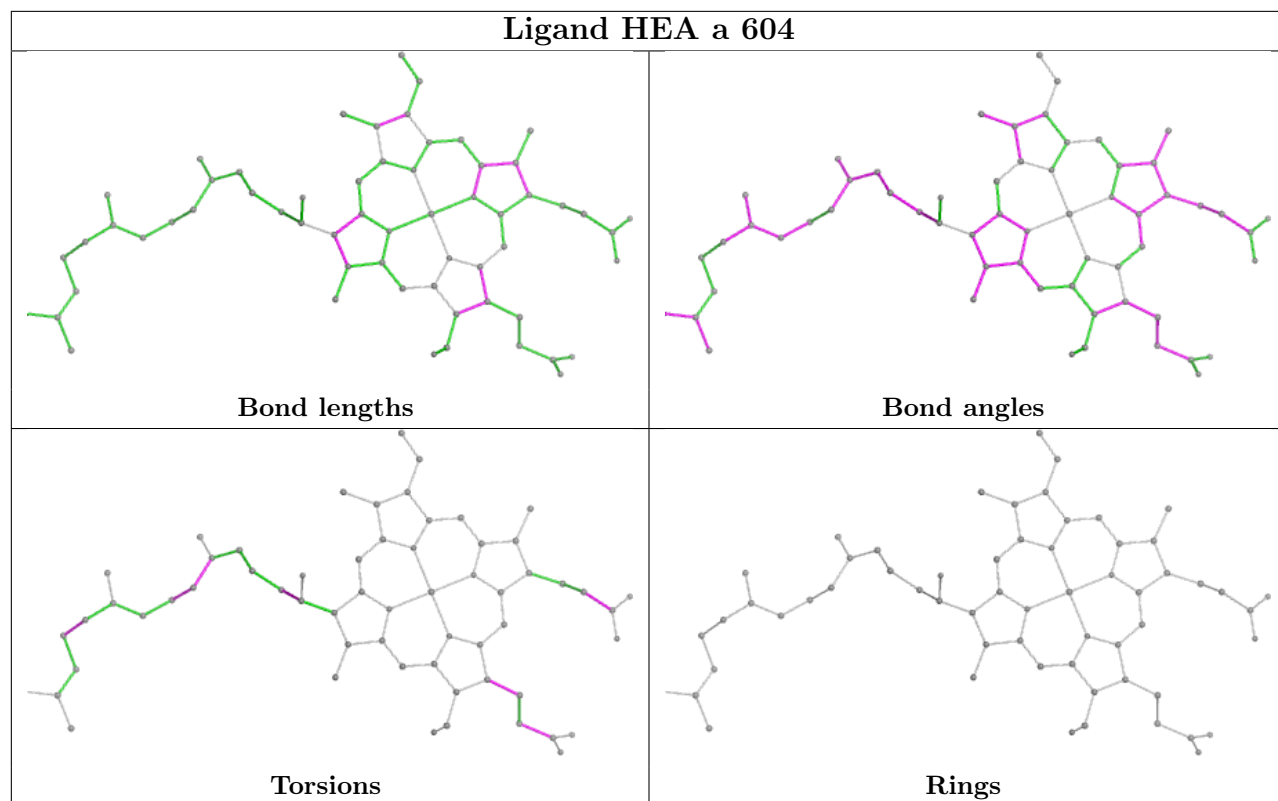
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

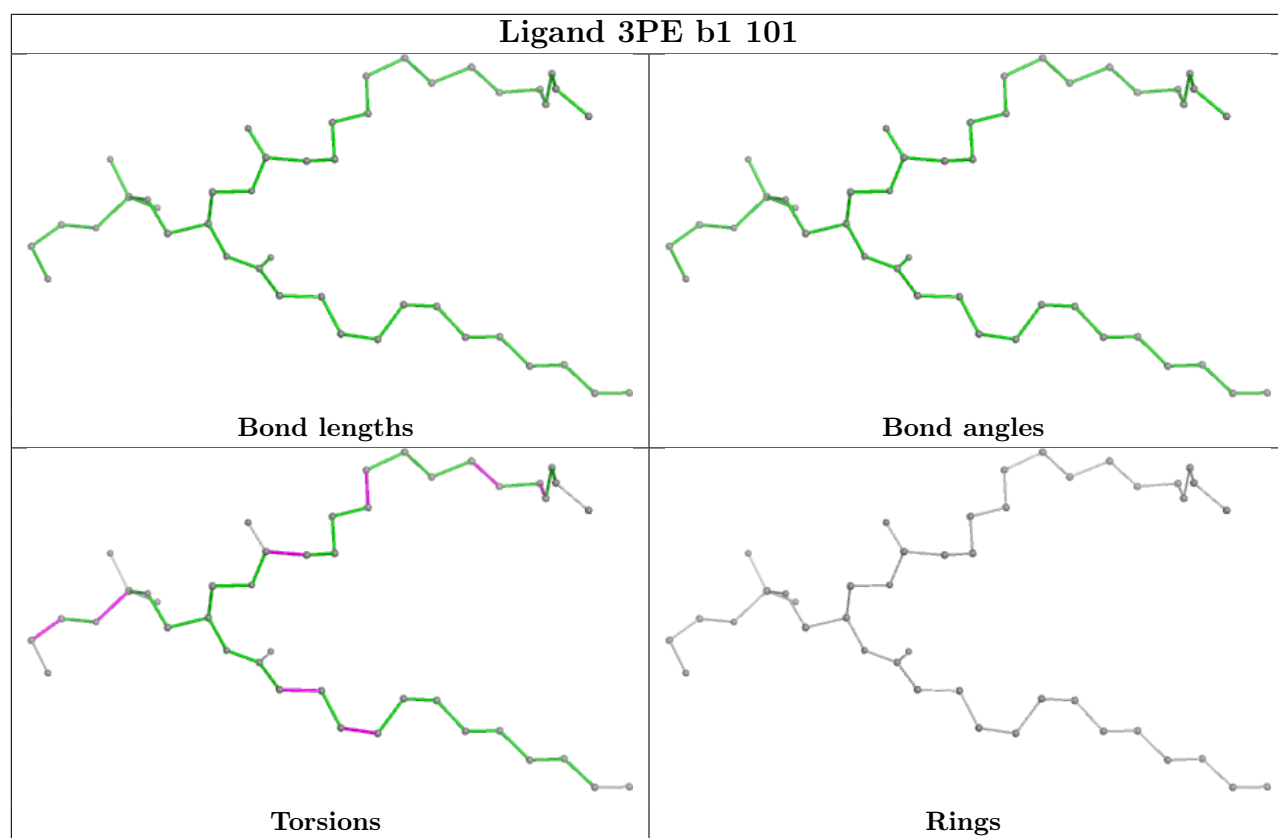


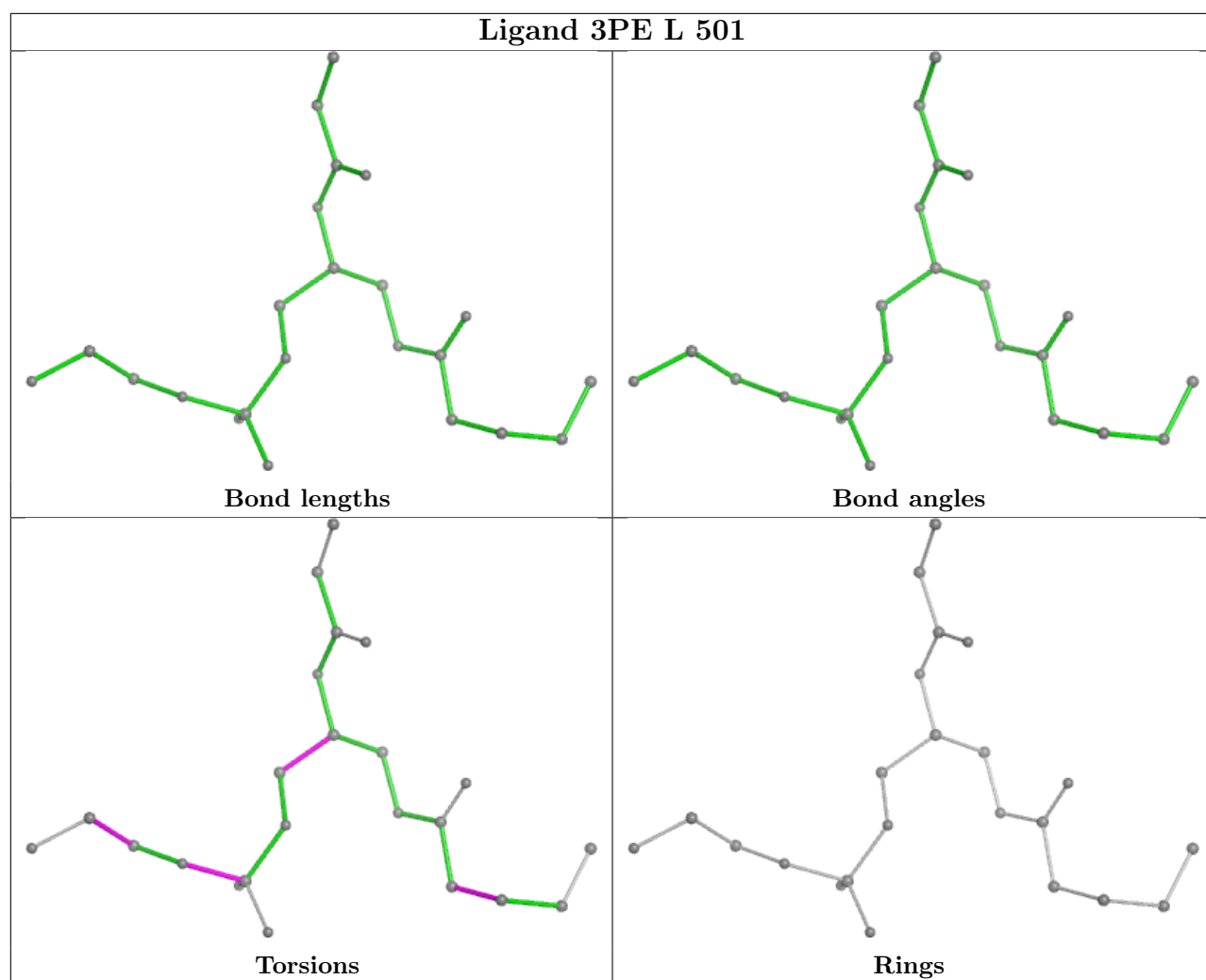


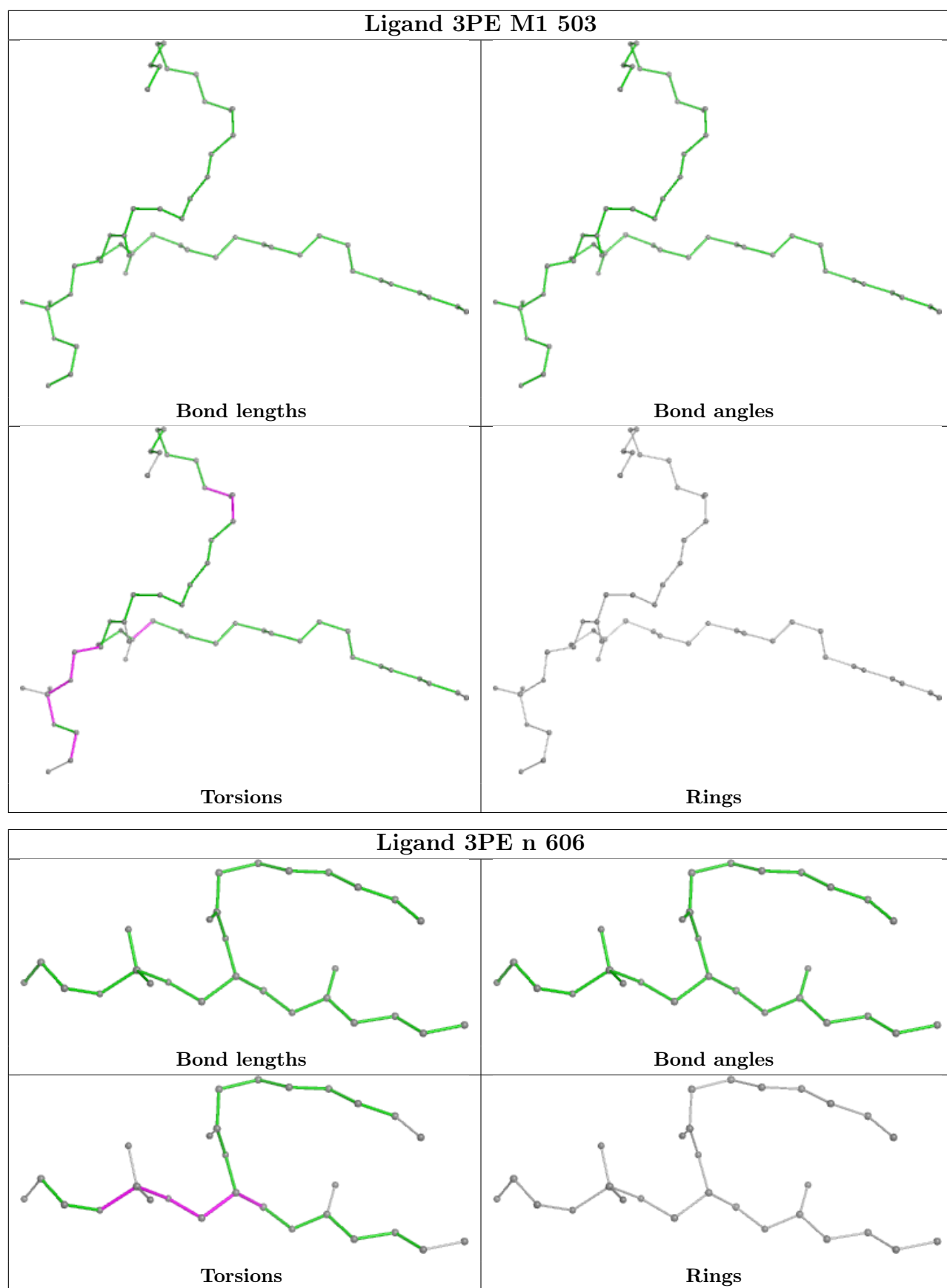


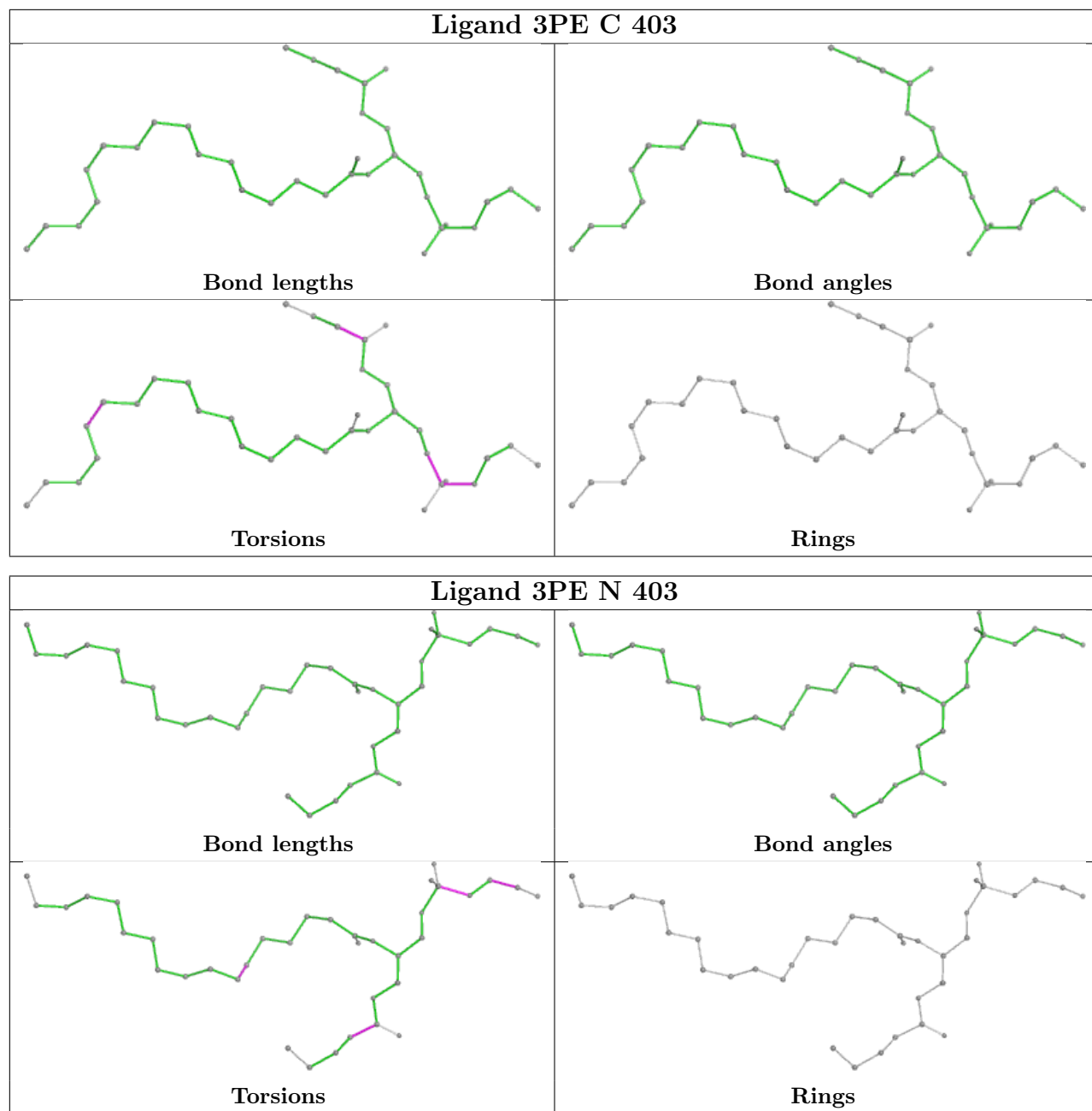


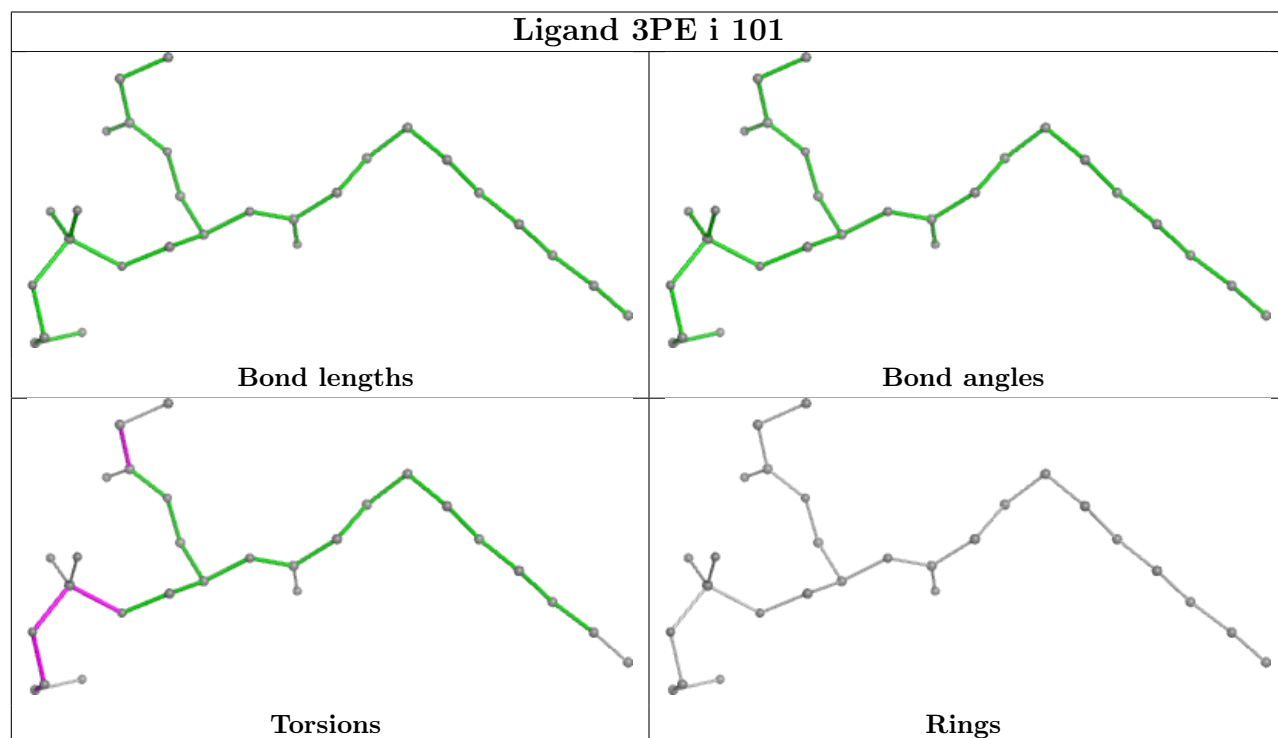
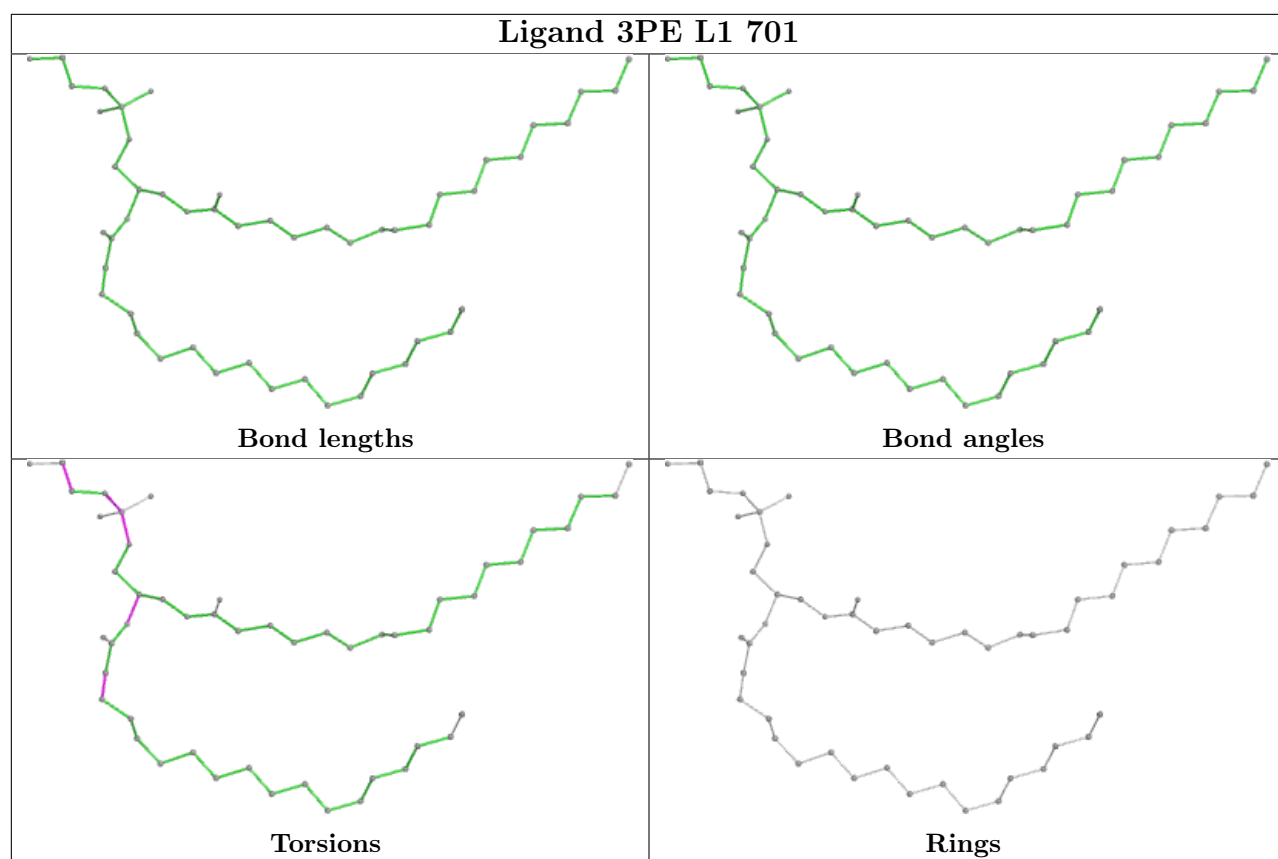


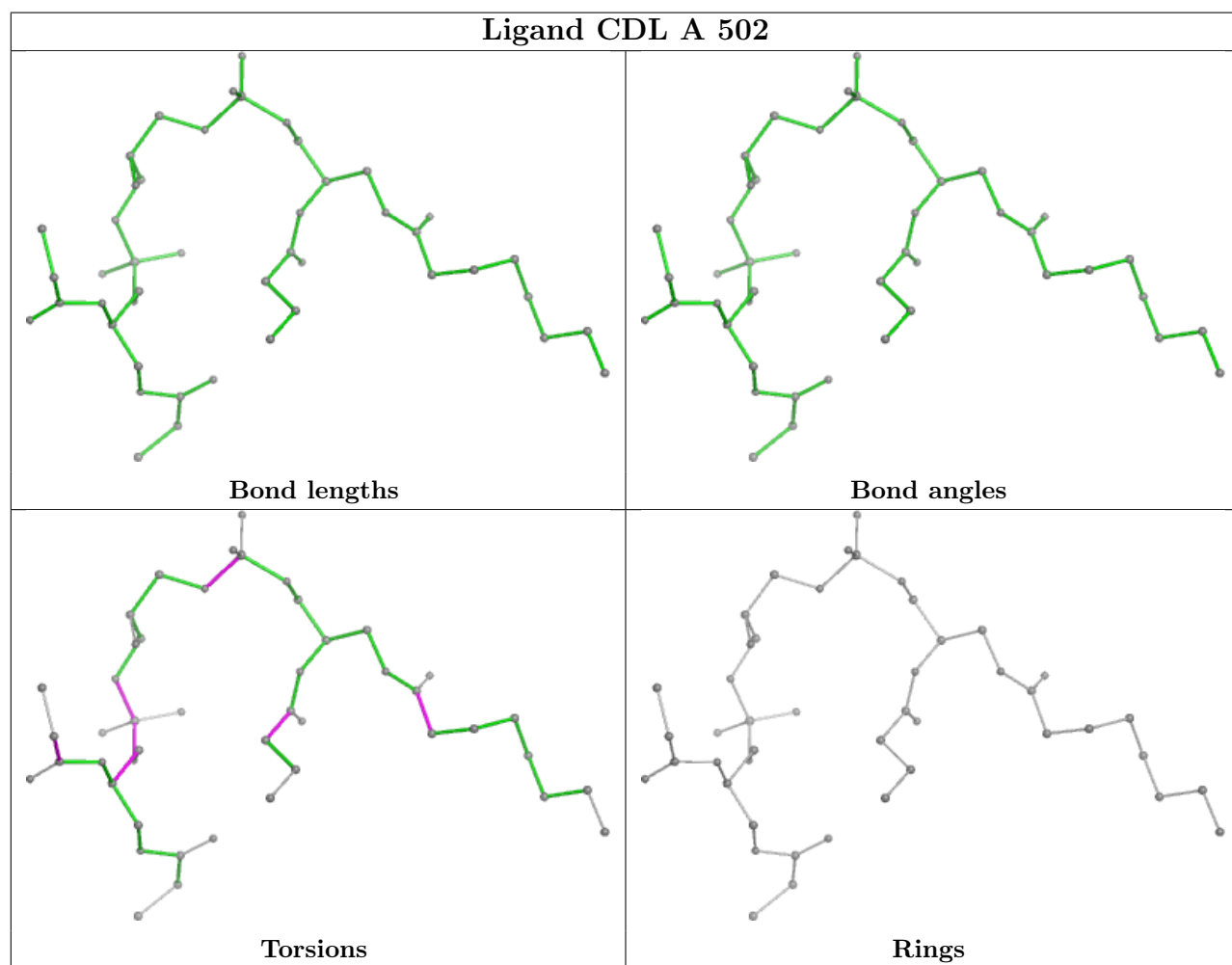
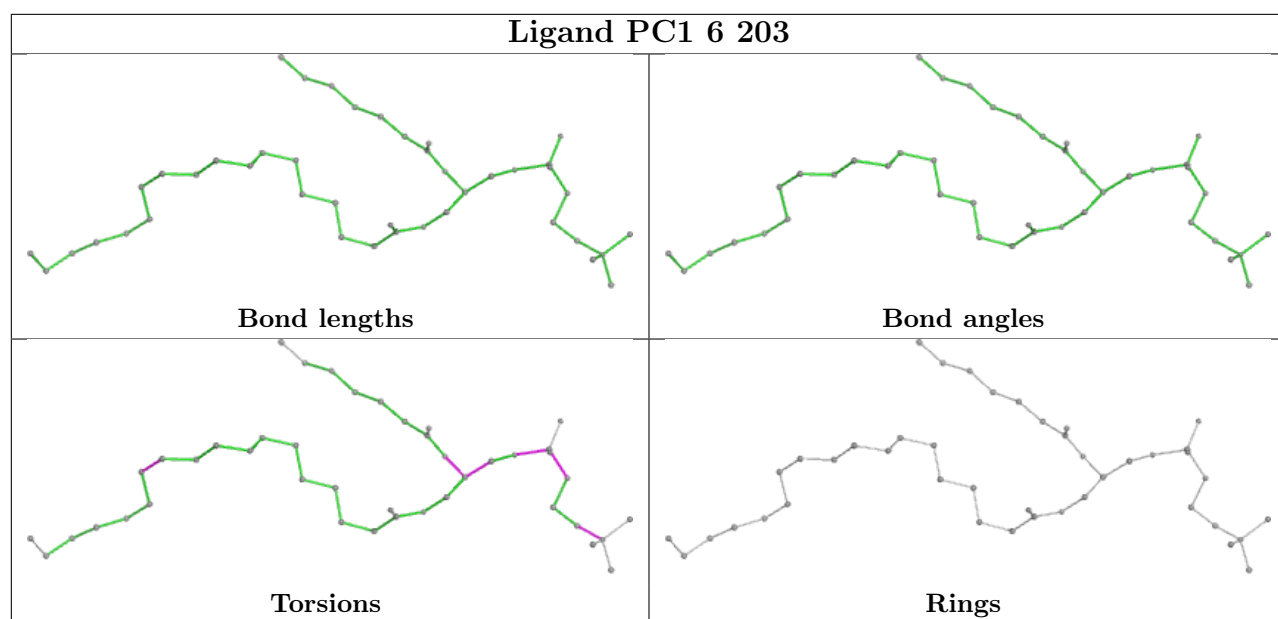


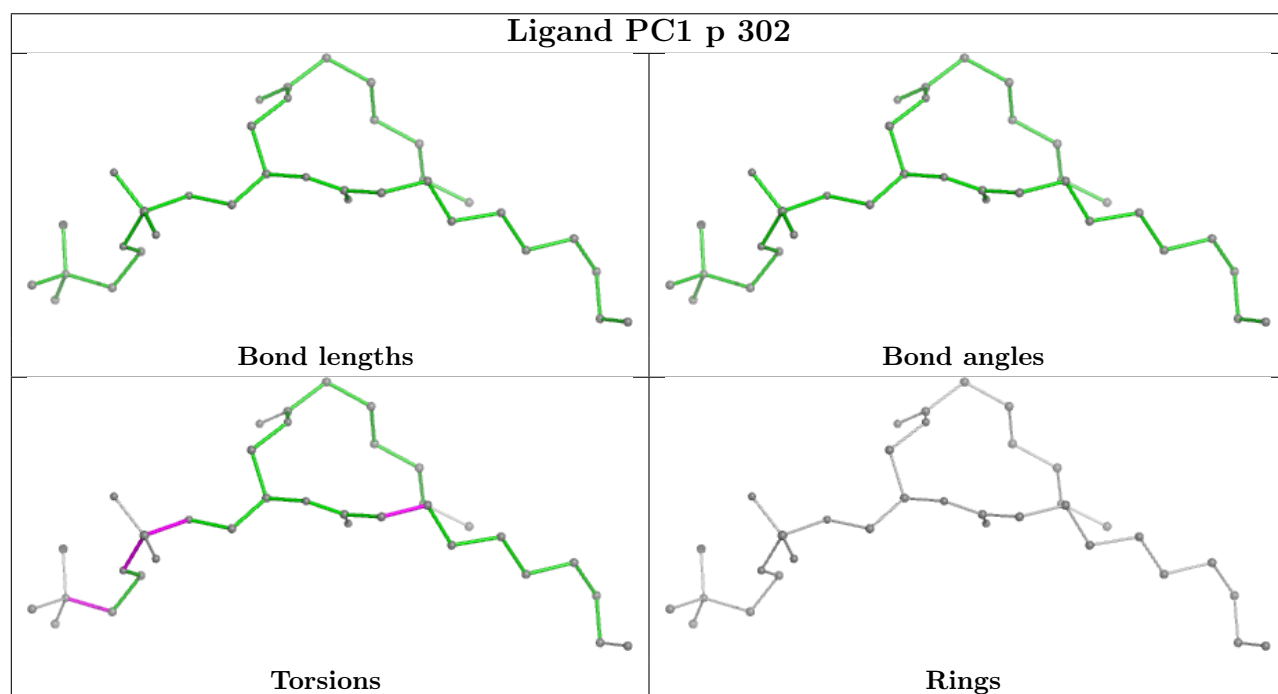
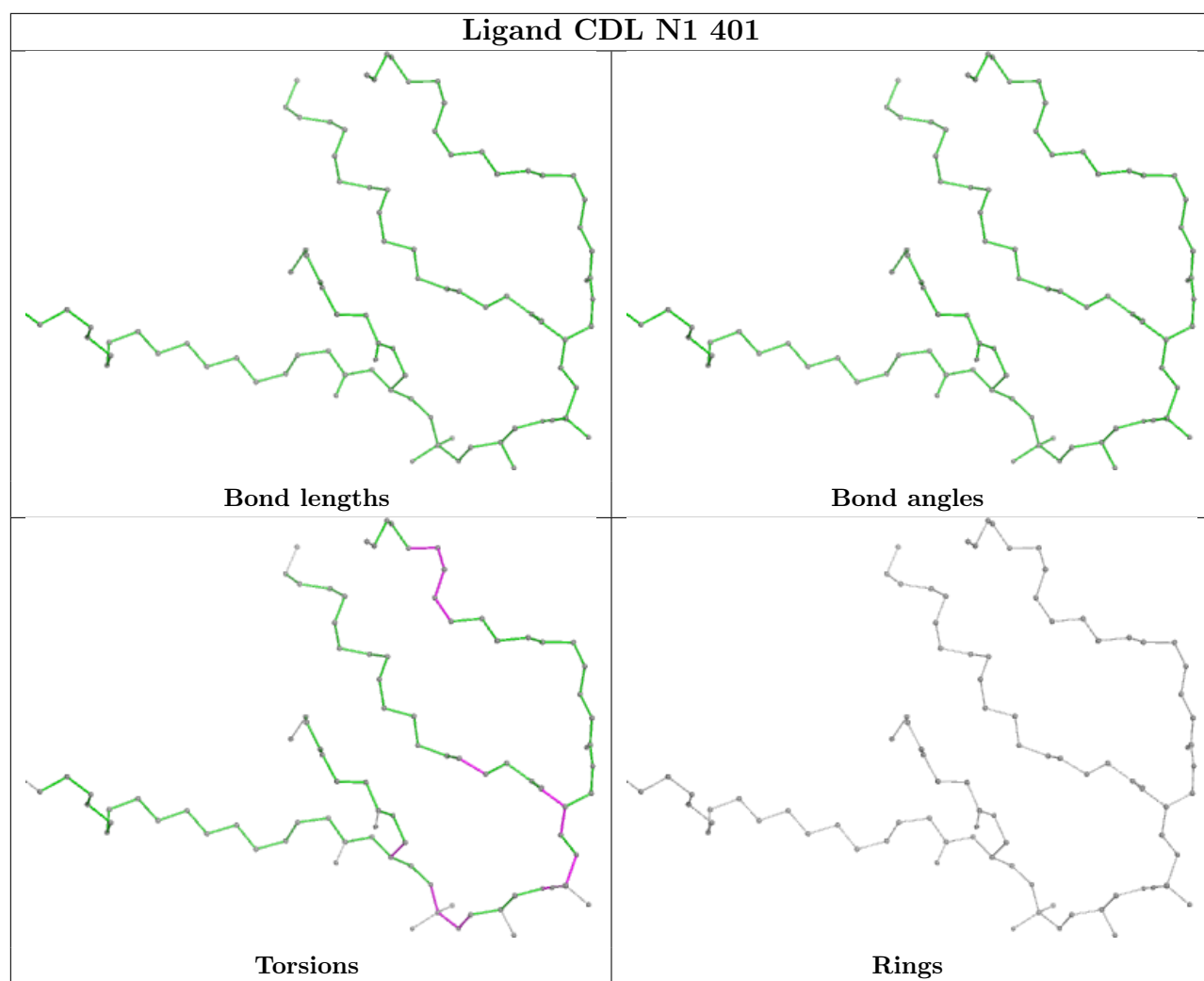


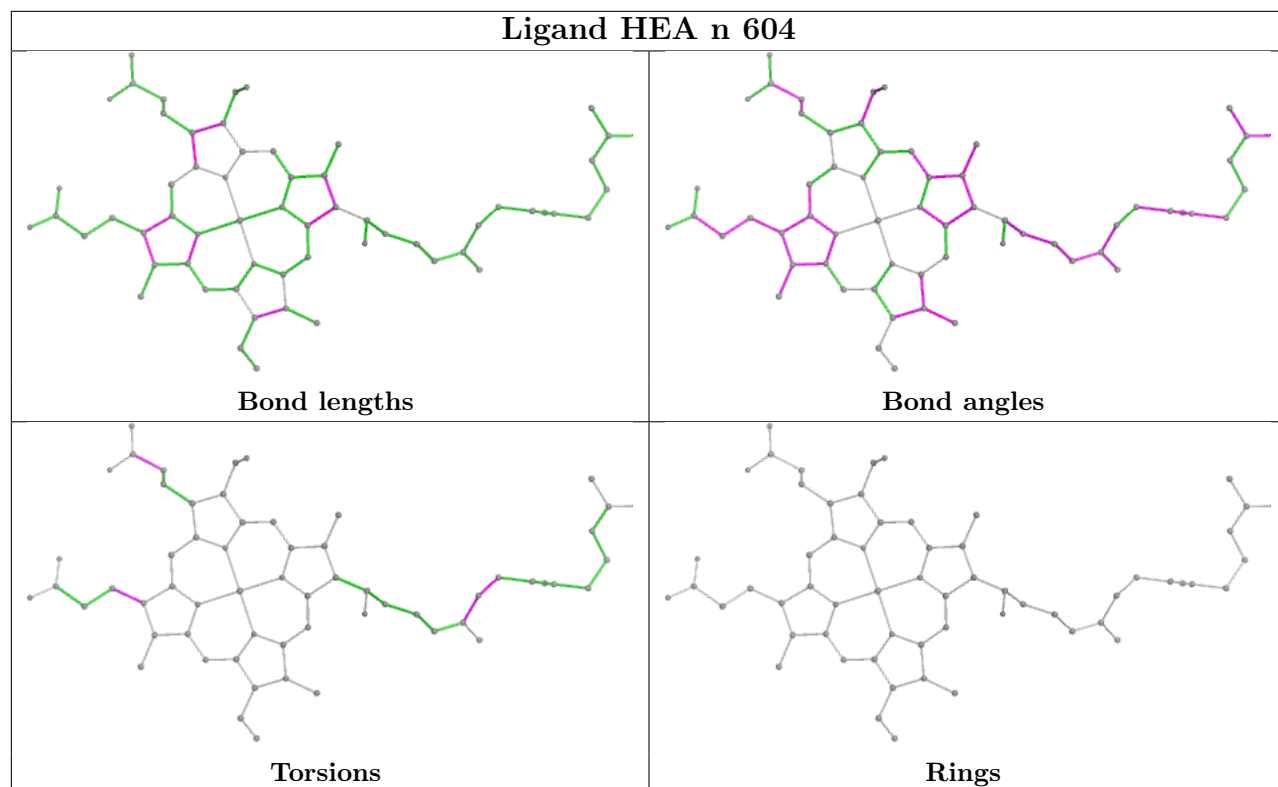


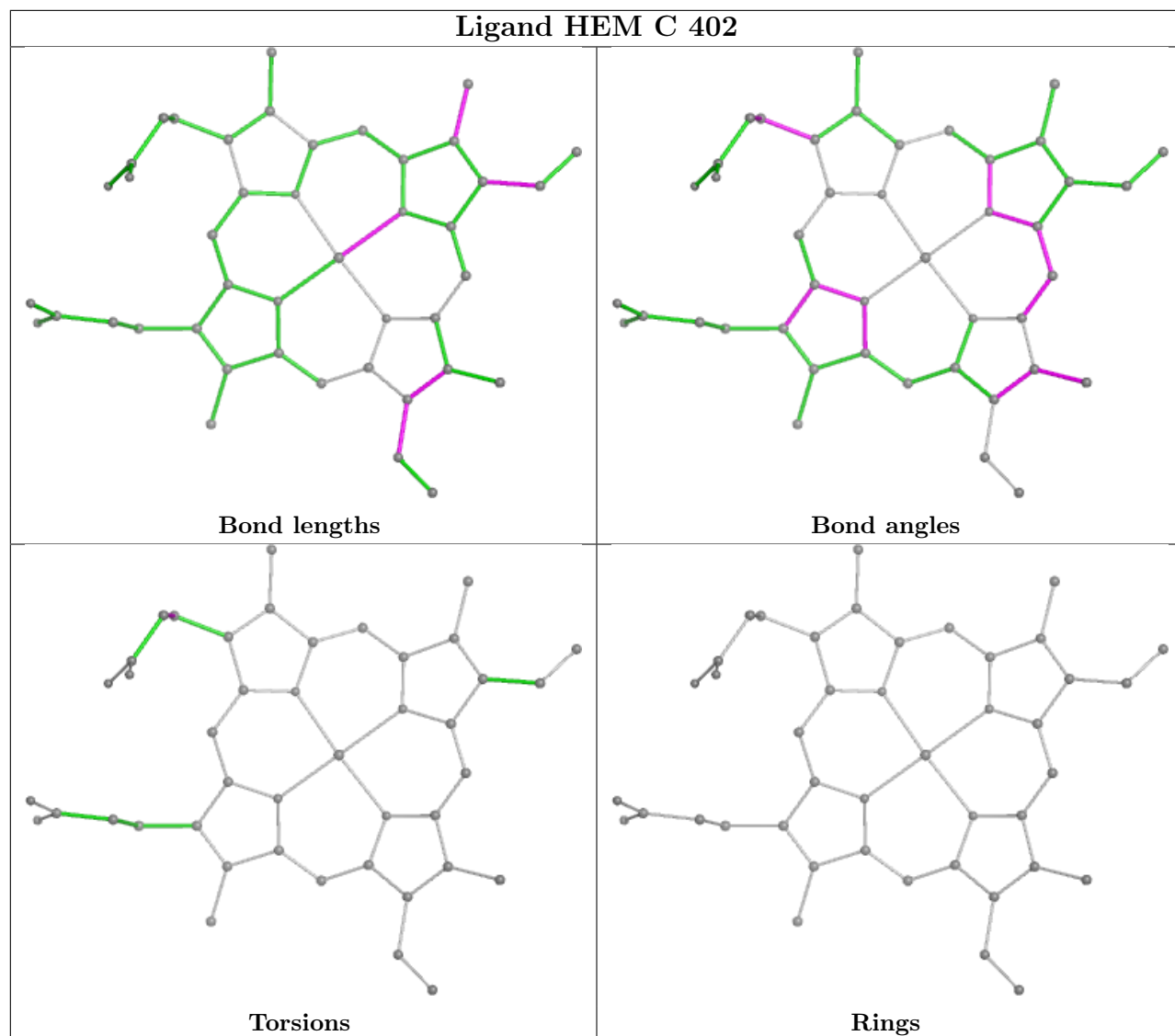


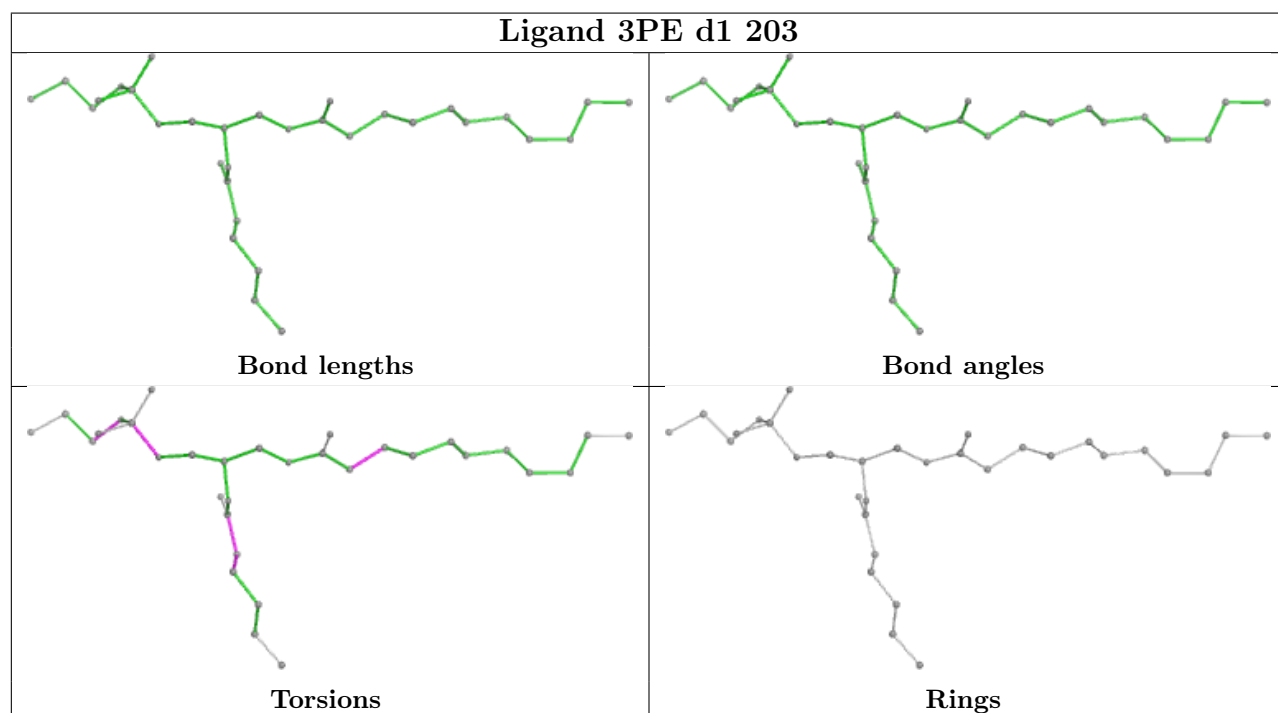
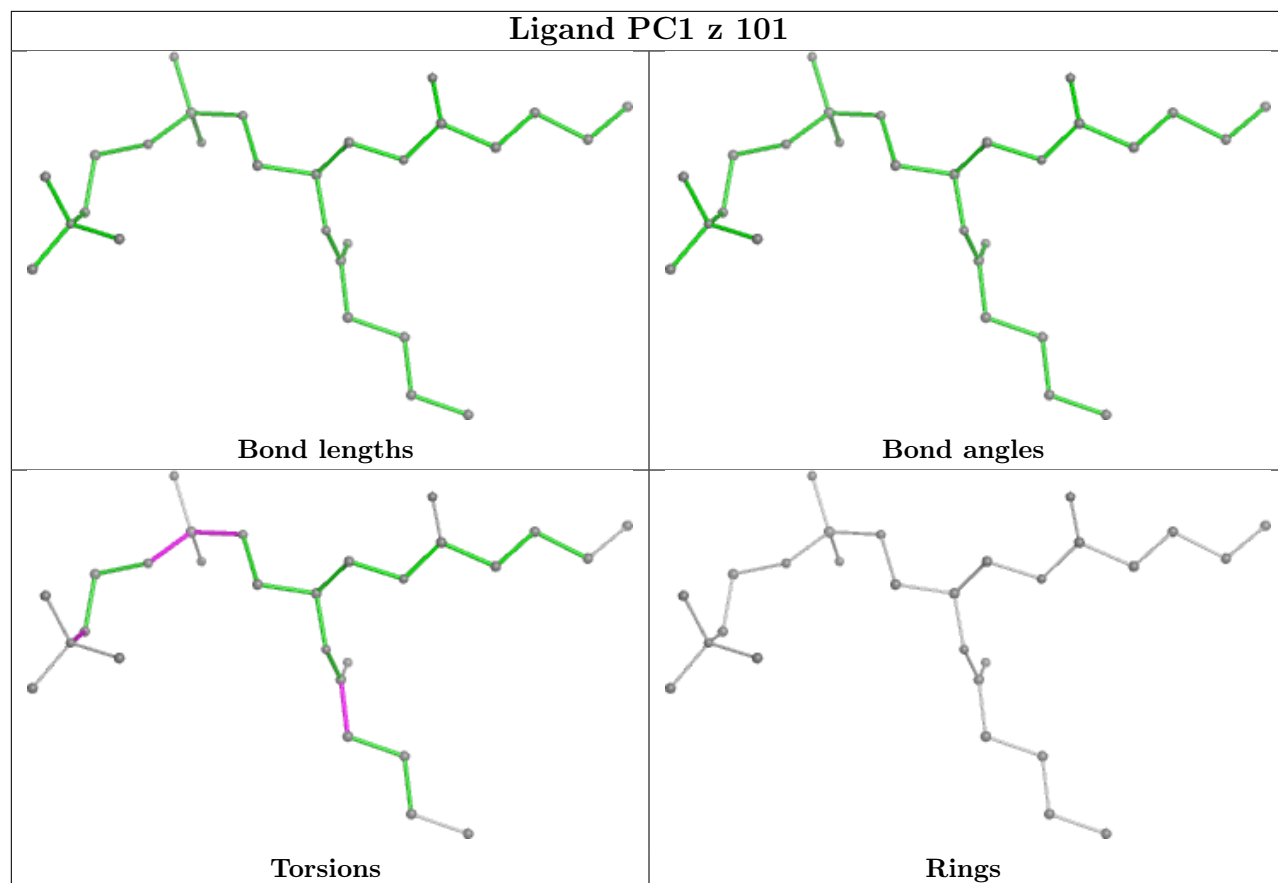


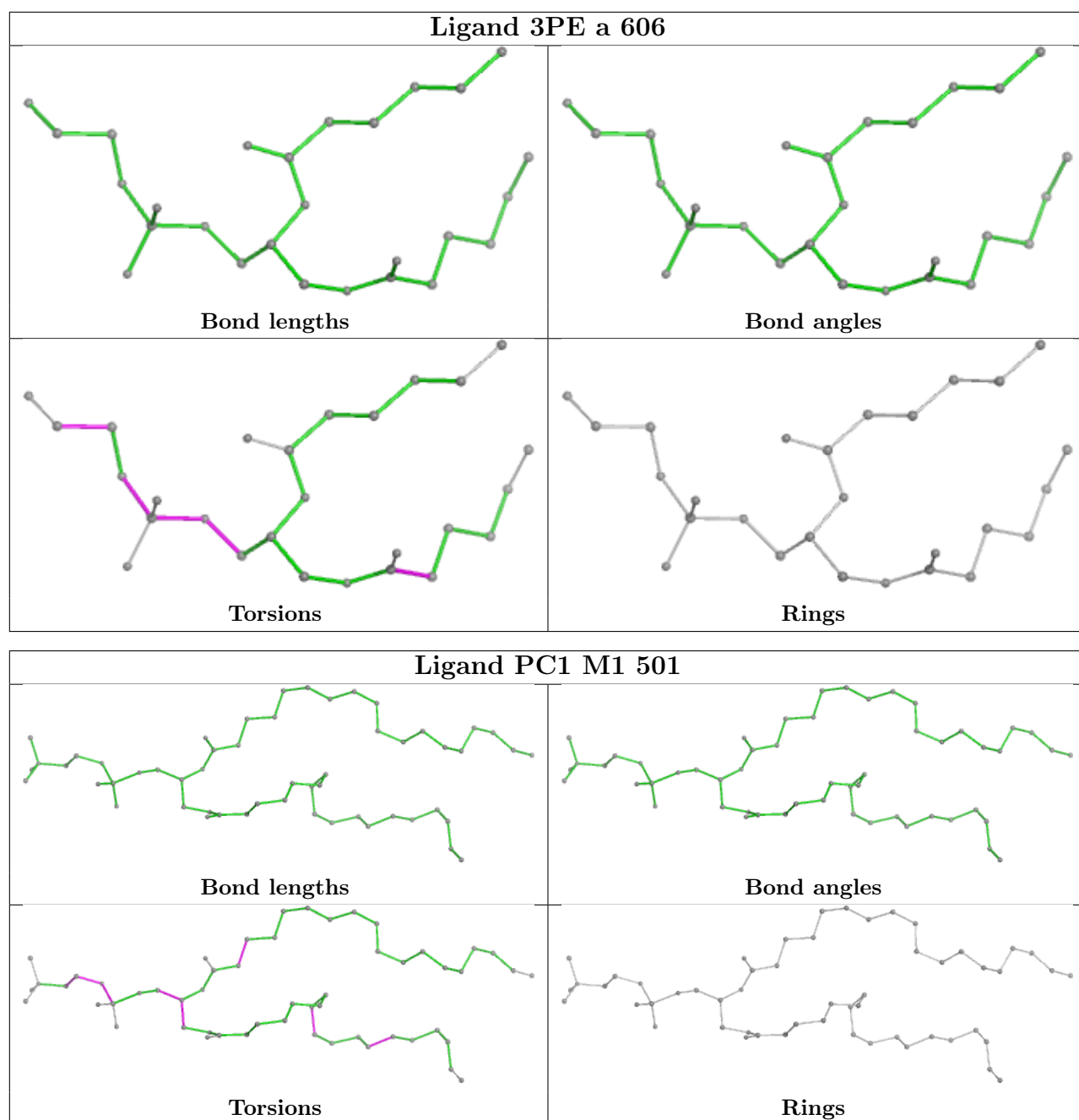


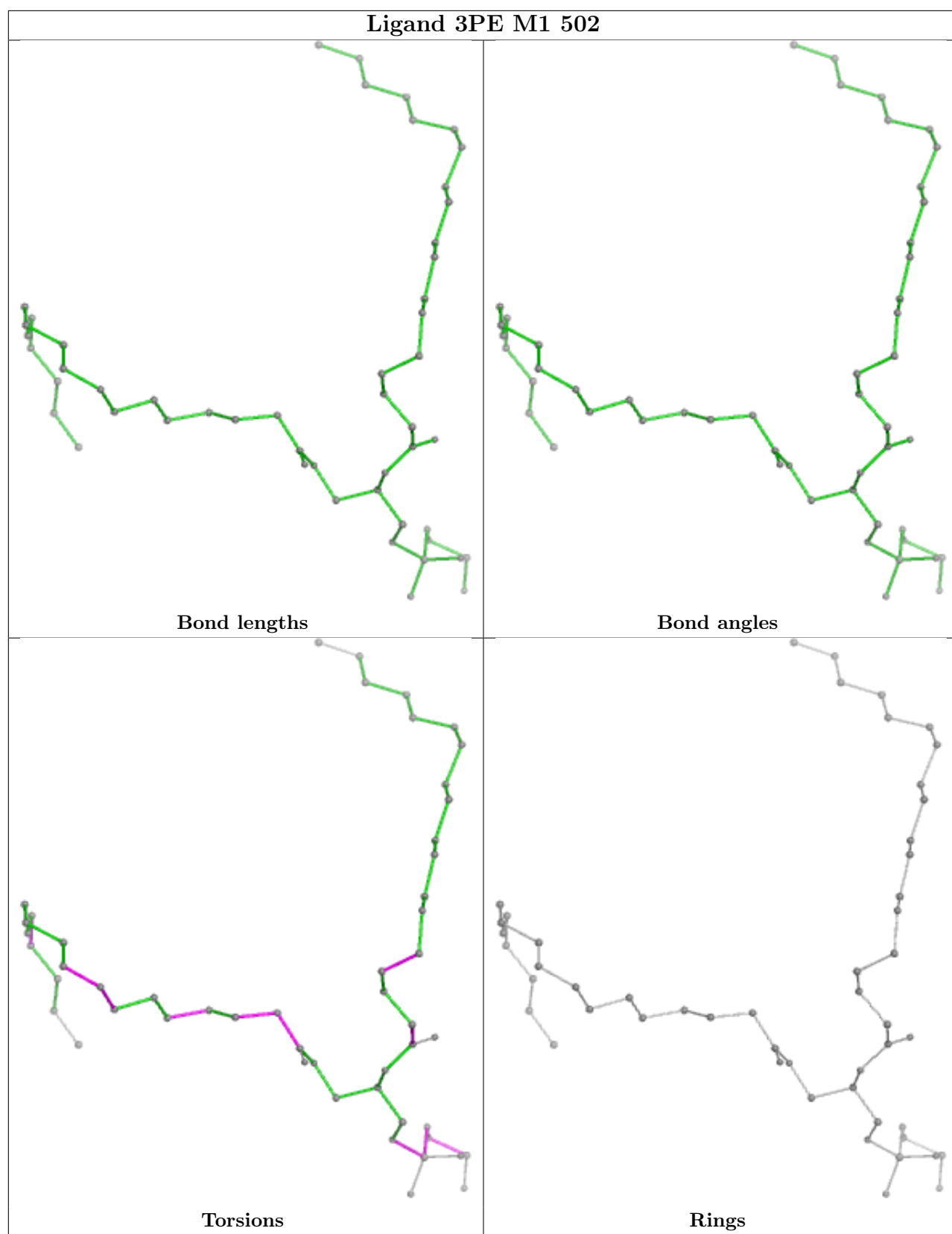


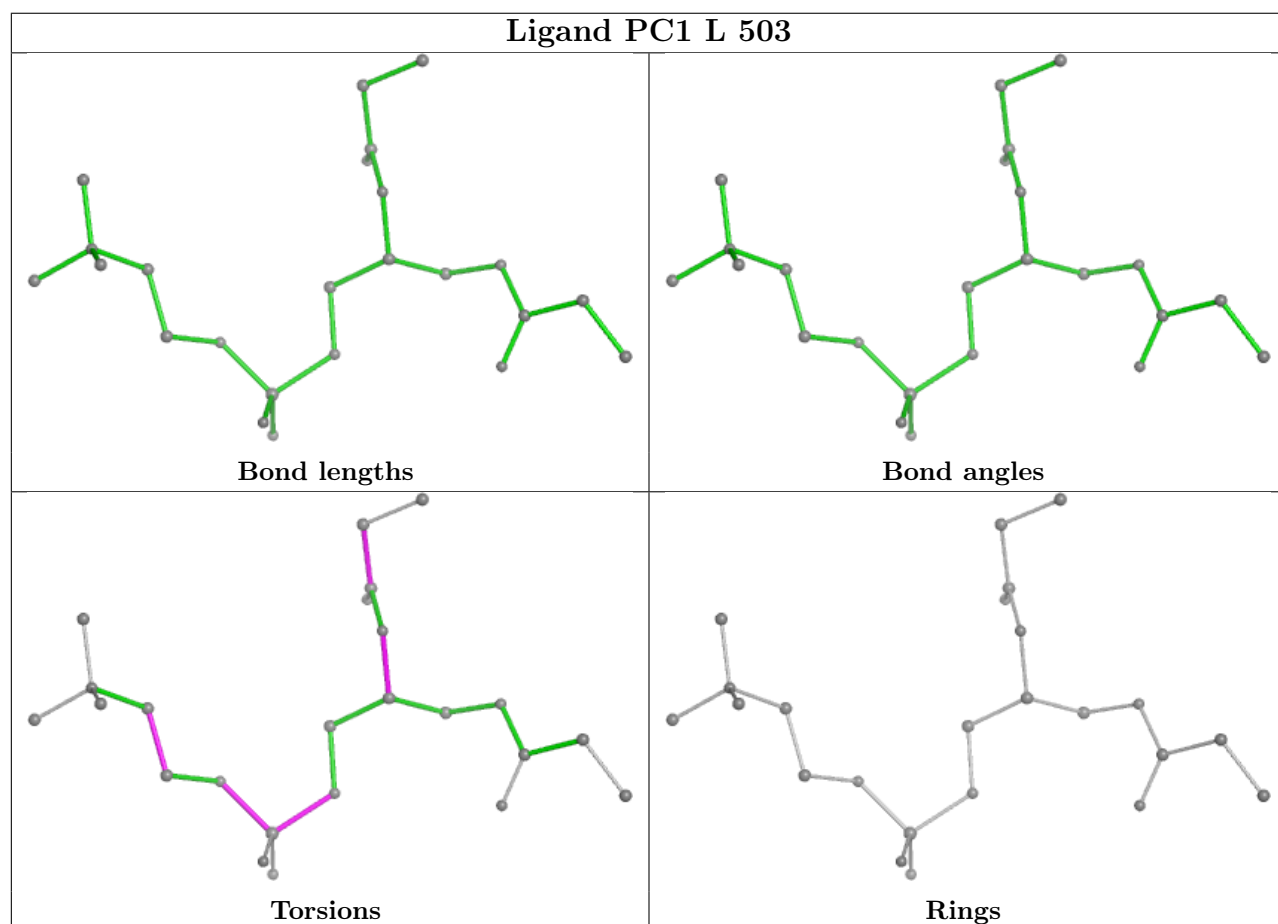
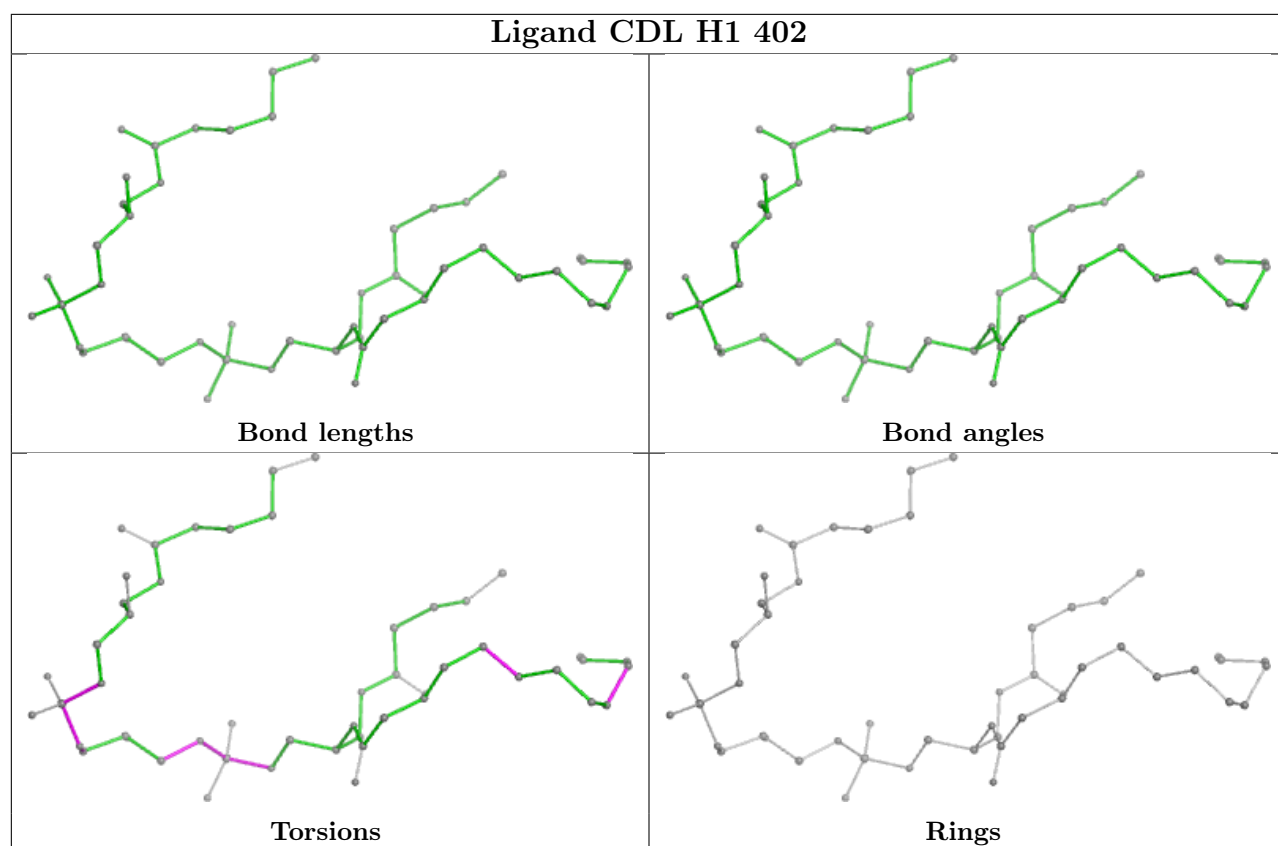


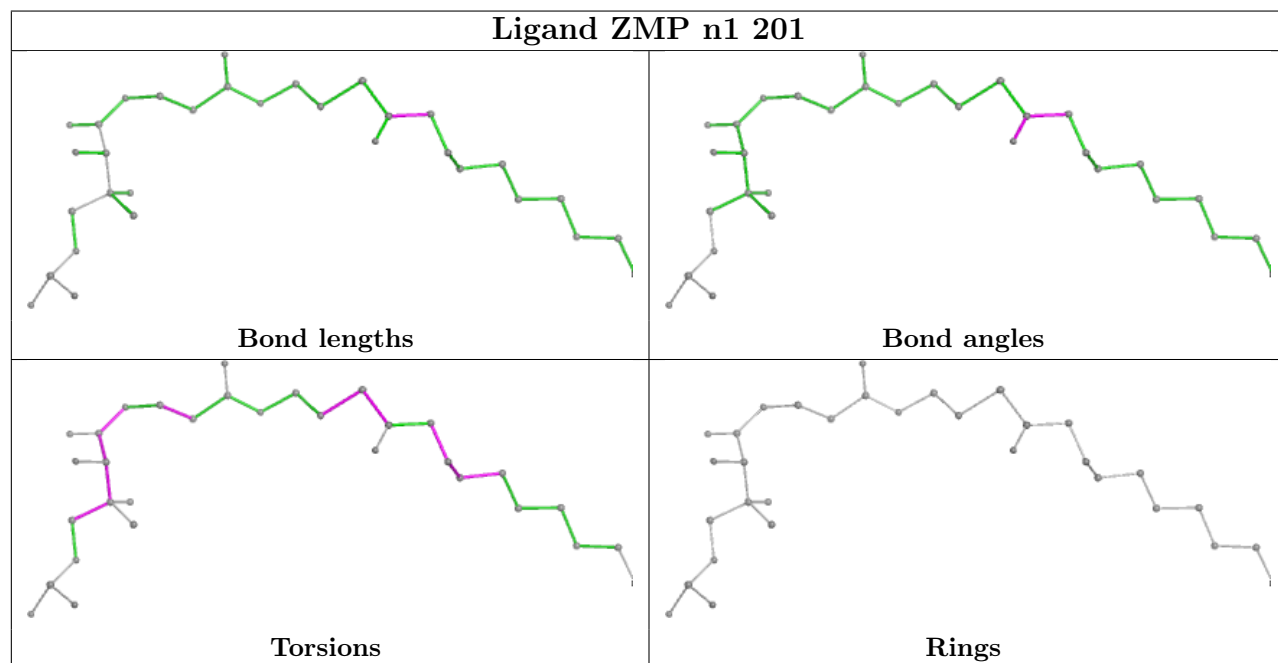
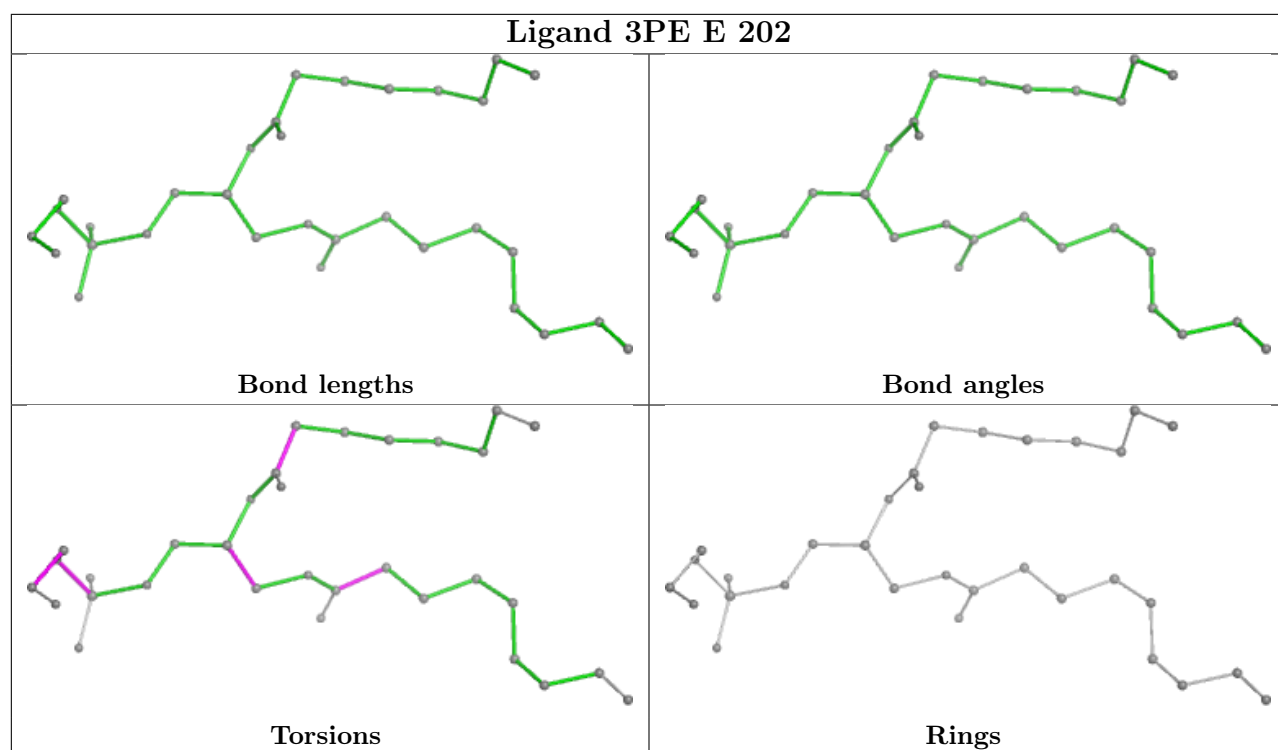


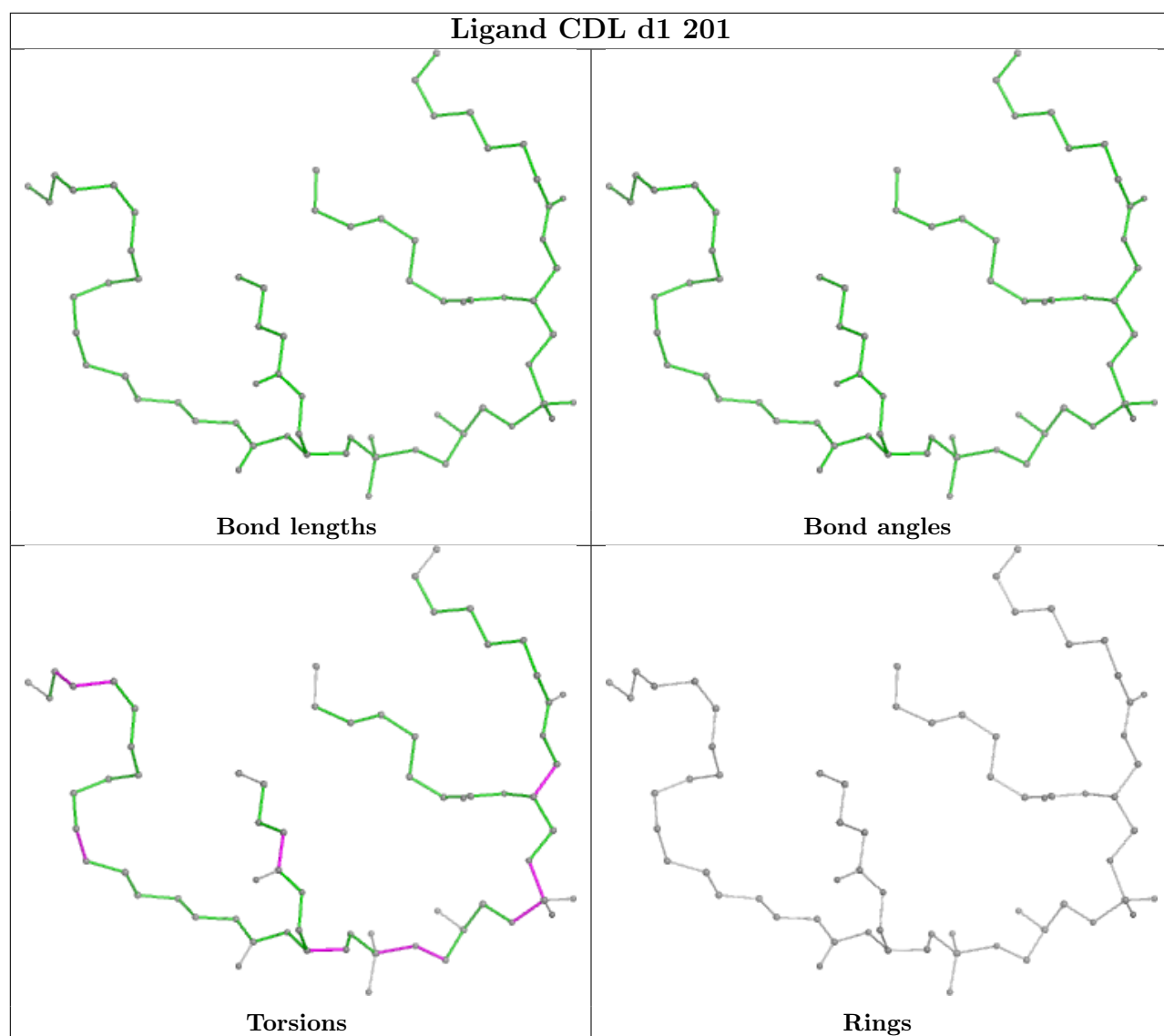


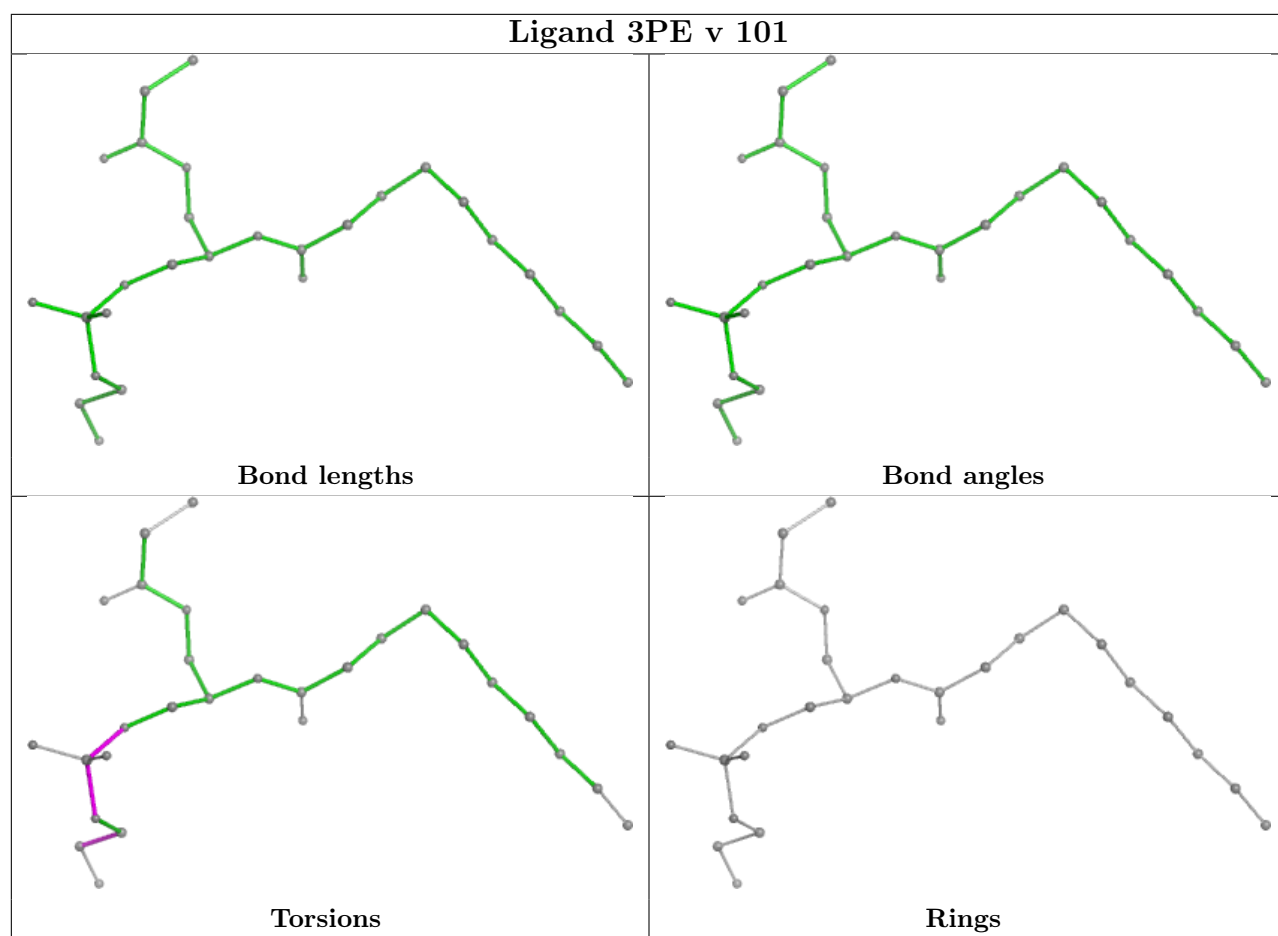


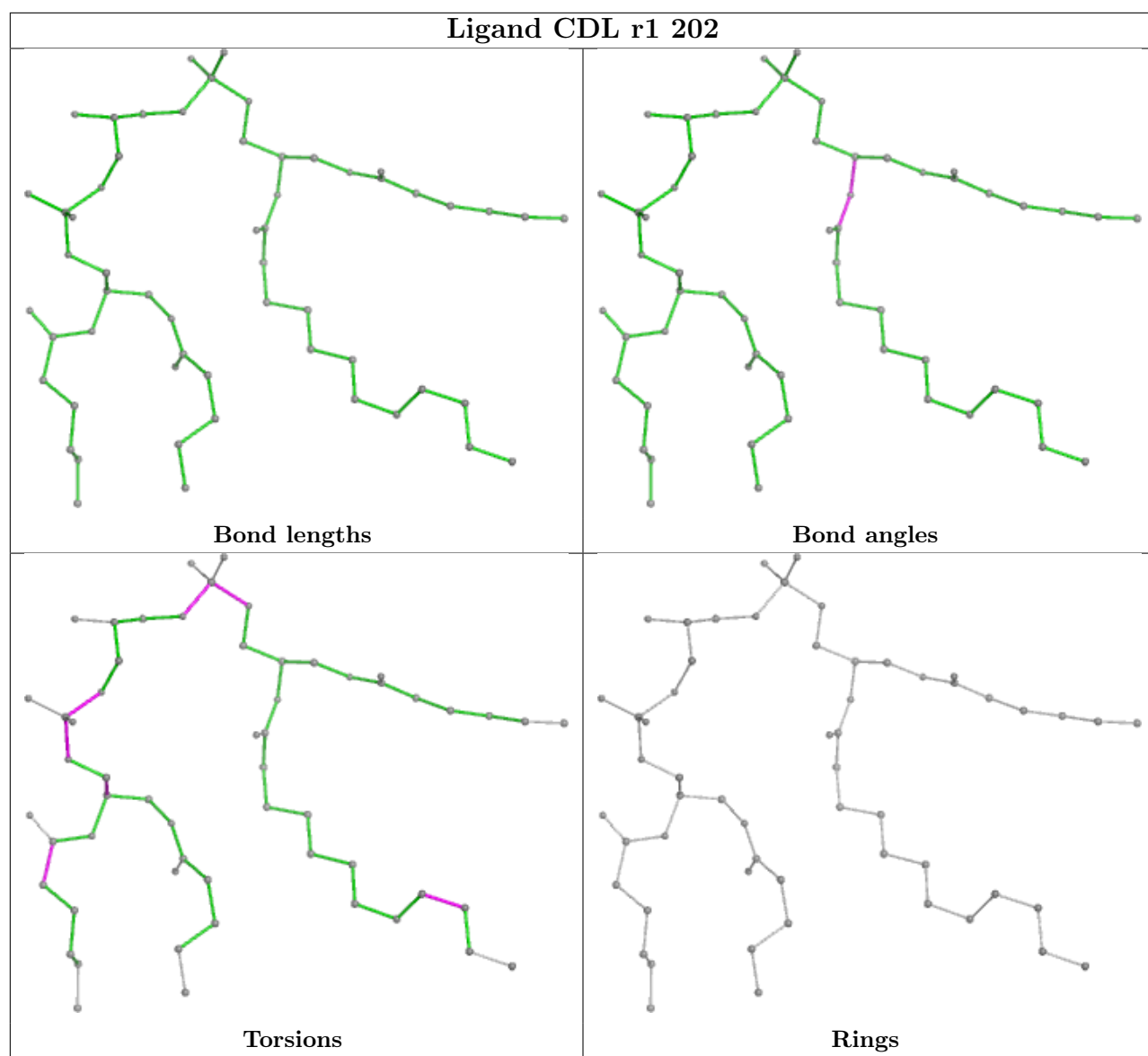


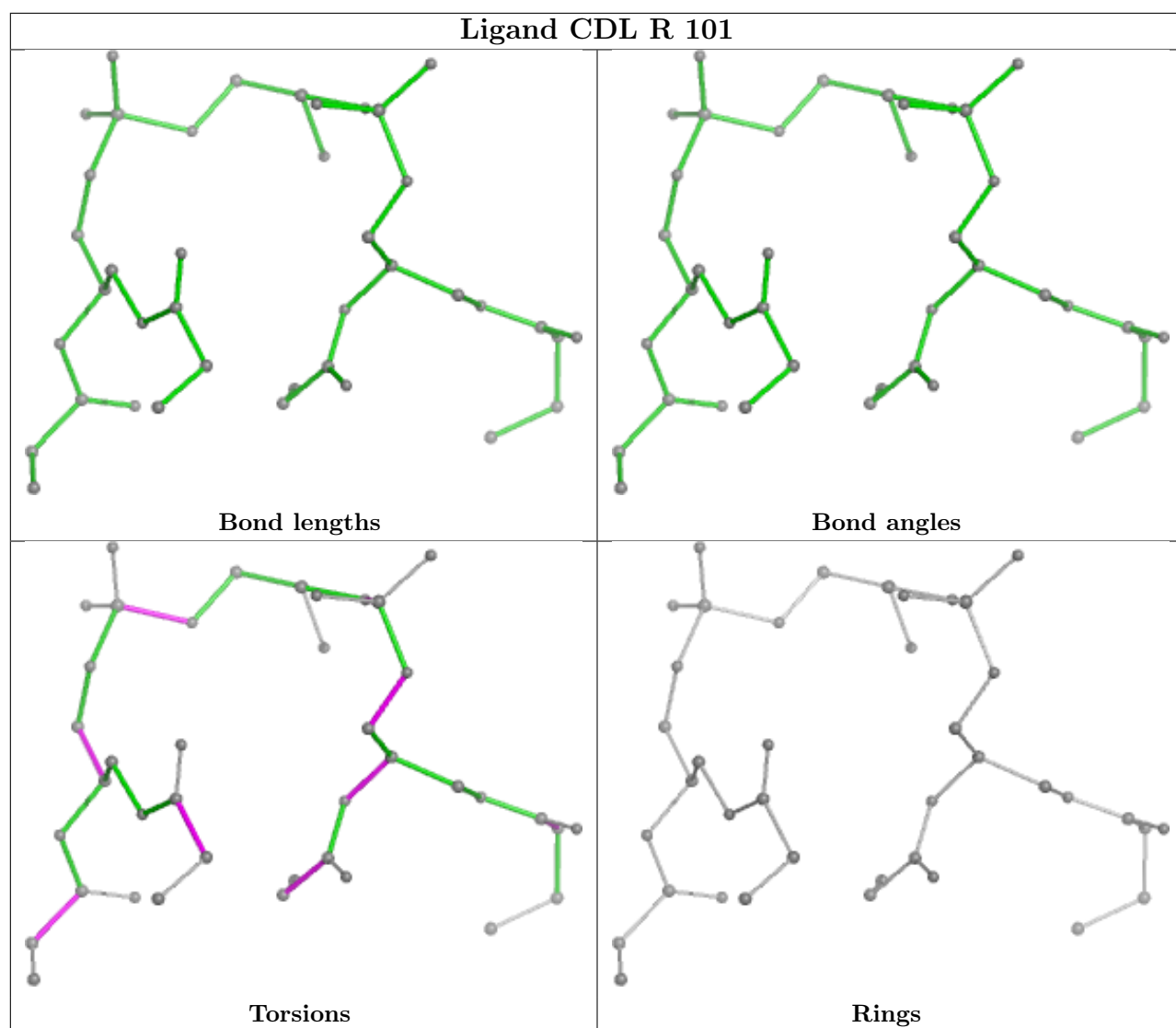




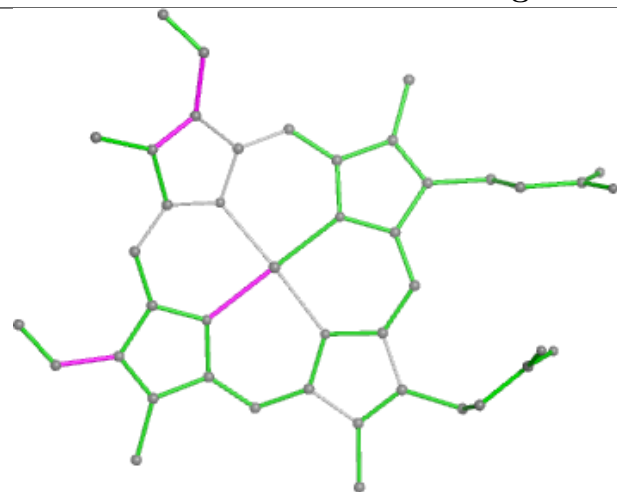




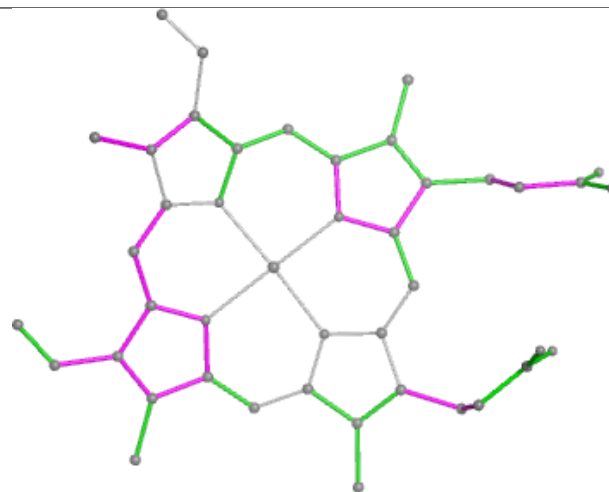




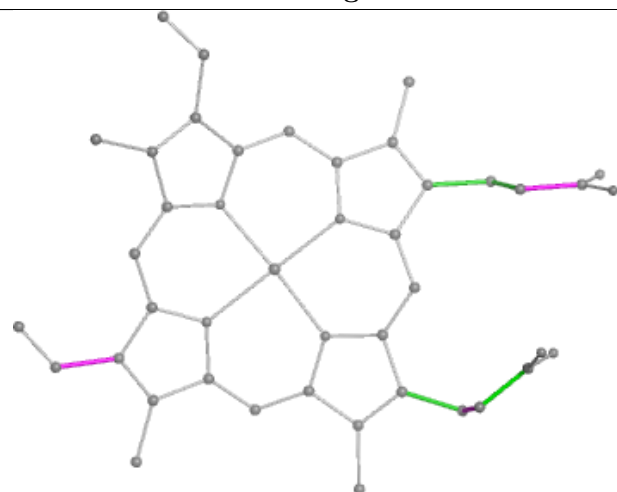
Ligand HEM N 402



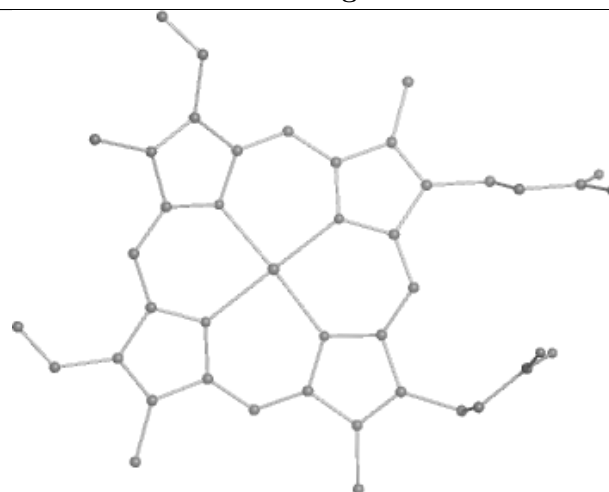
Bond lengths



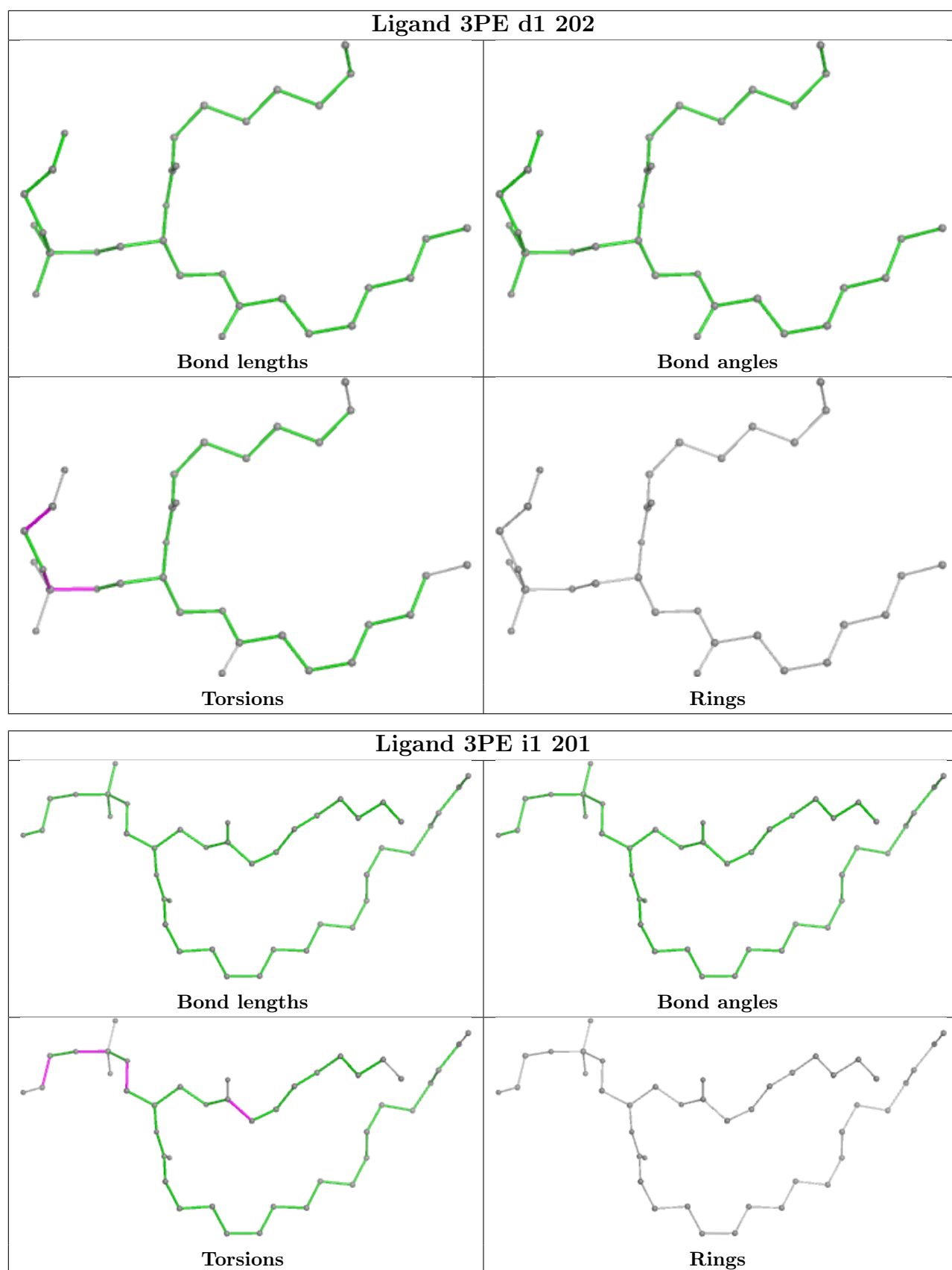
Bond angles

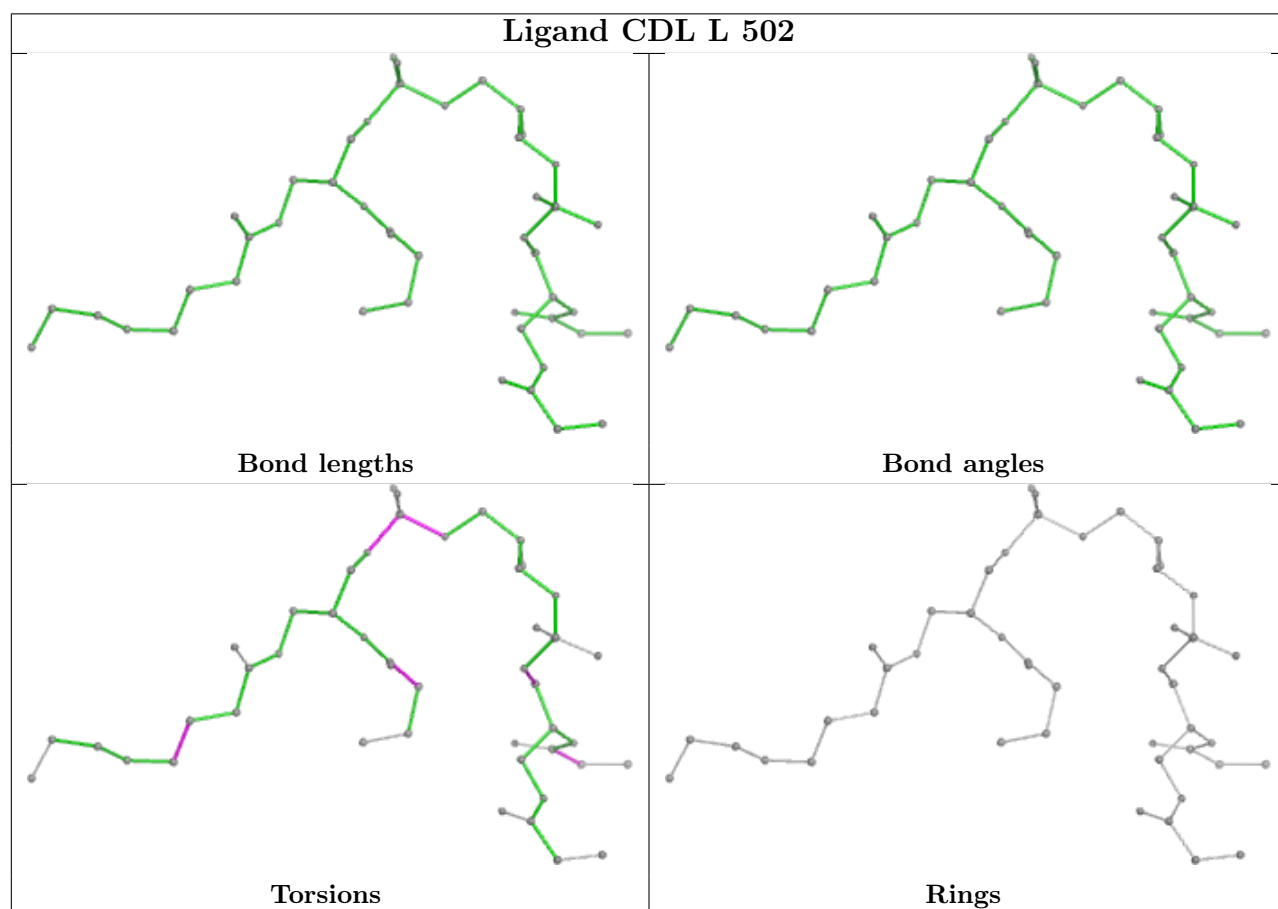
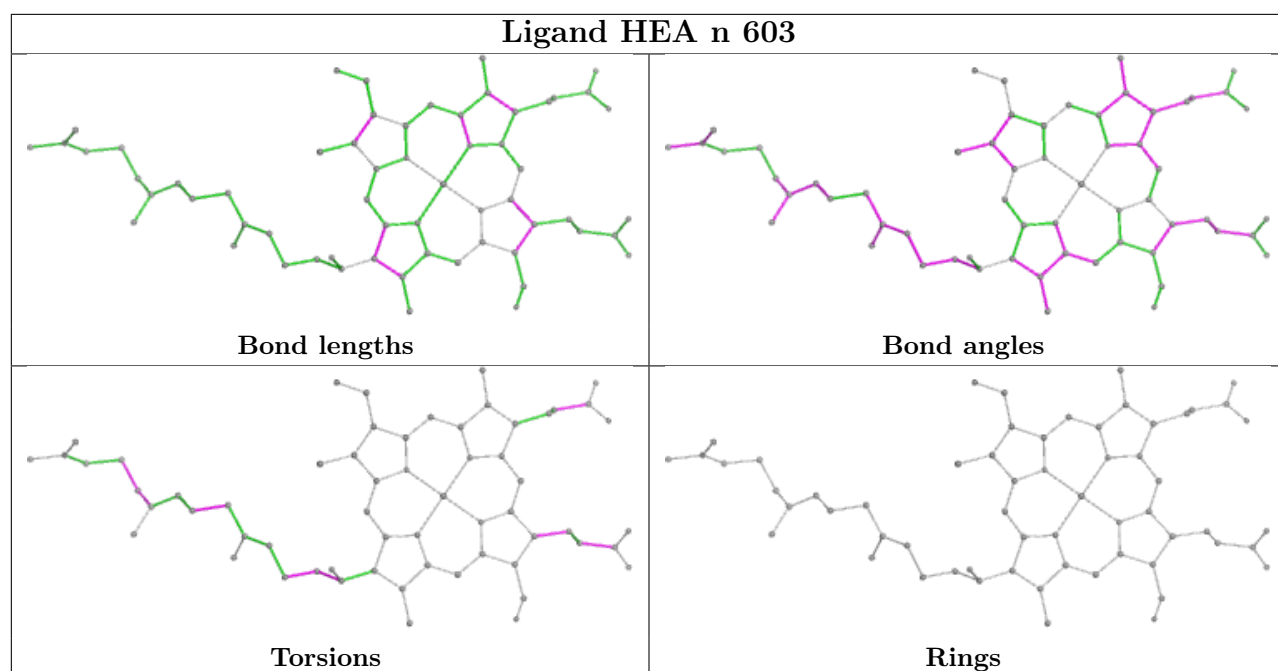


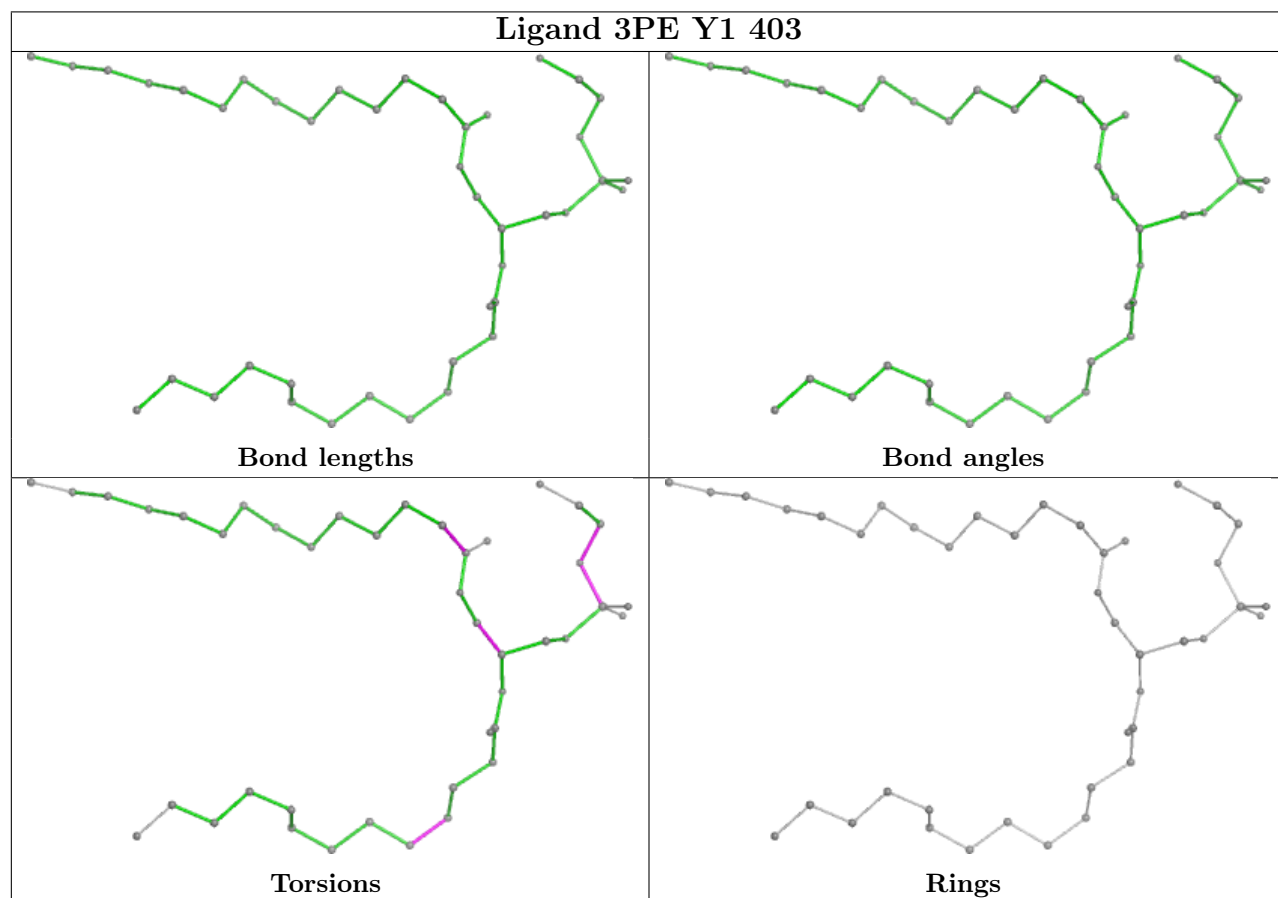
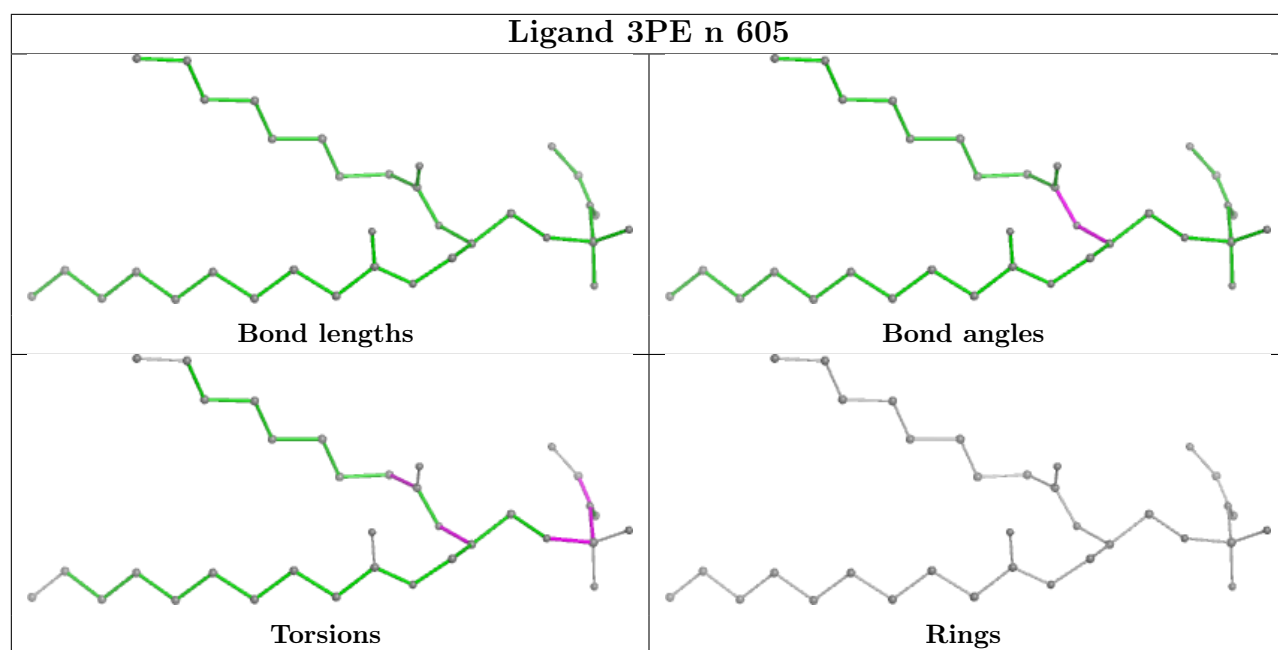
Torsions

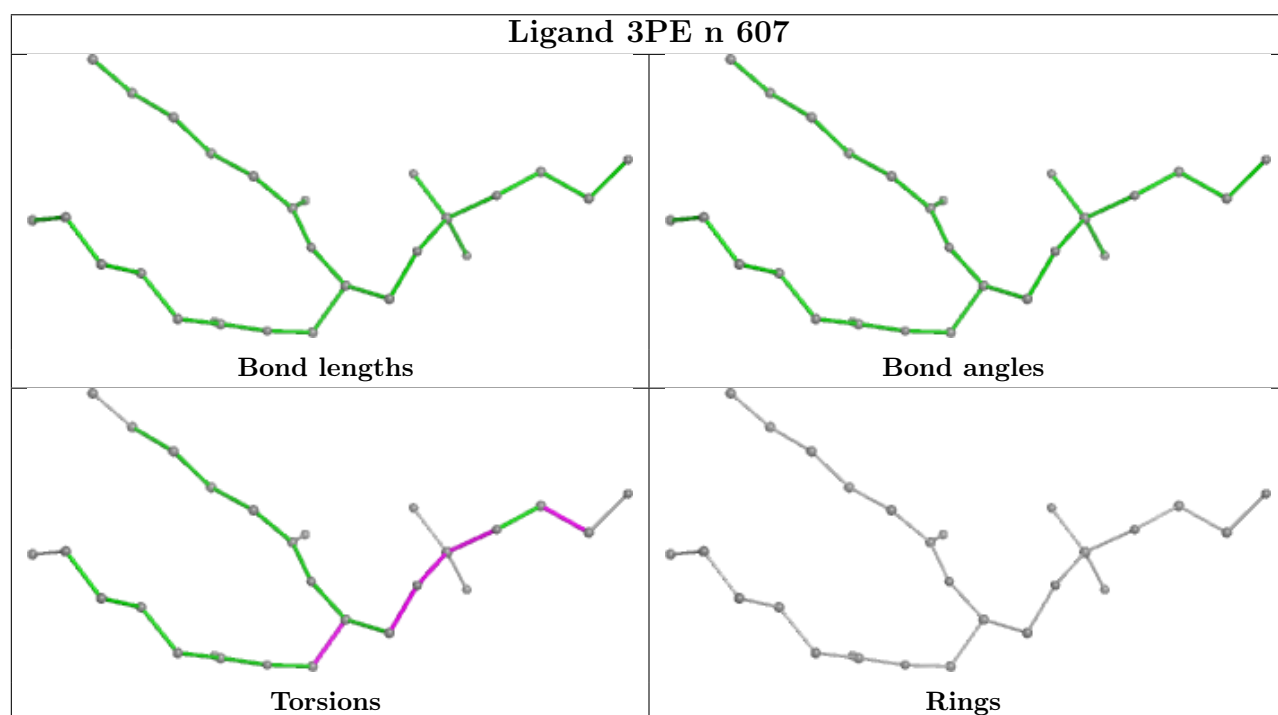
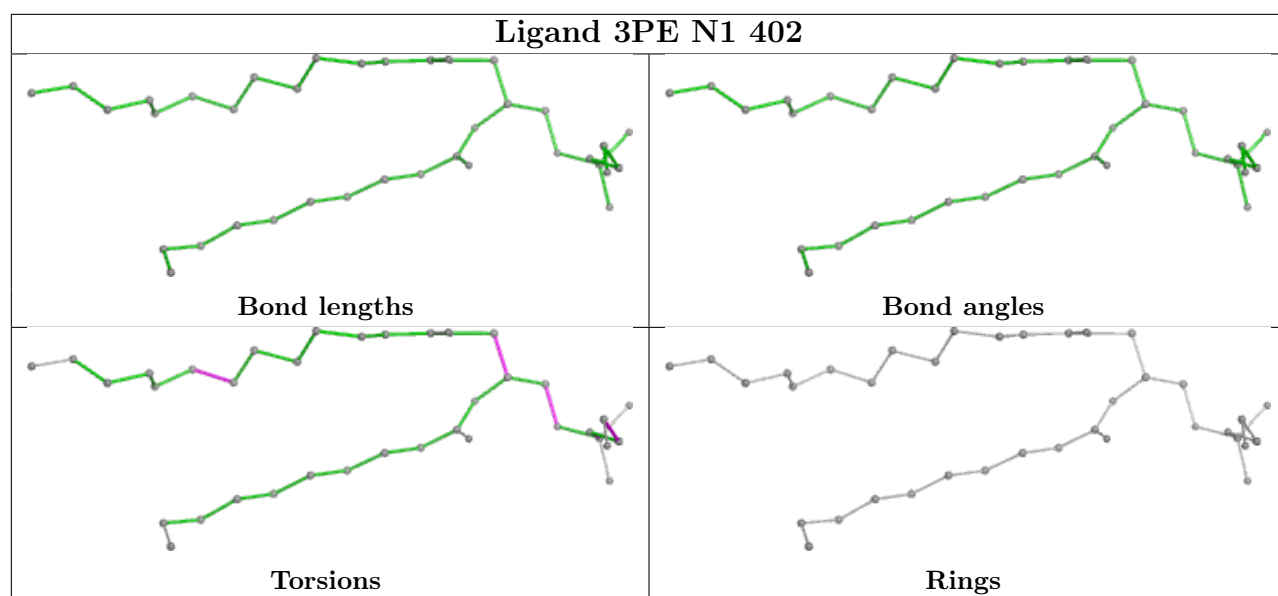


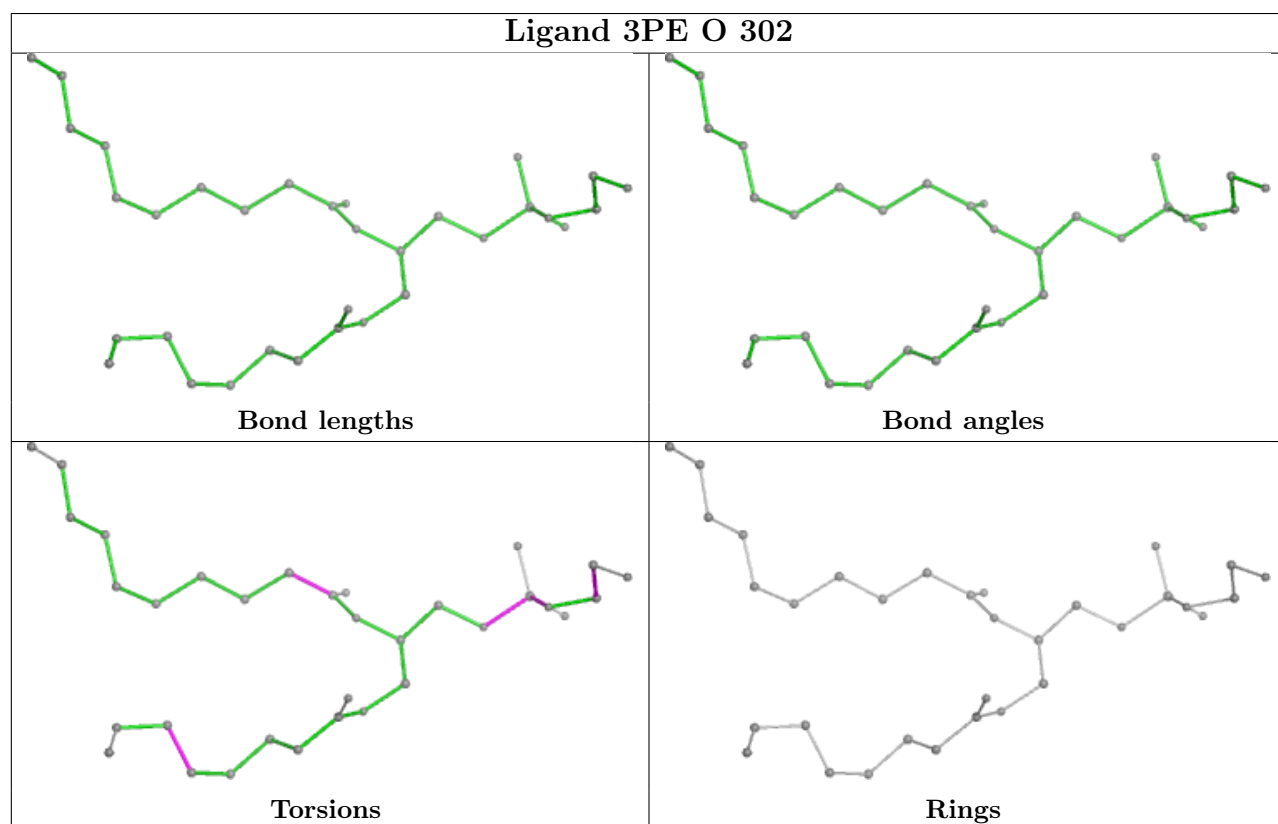
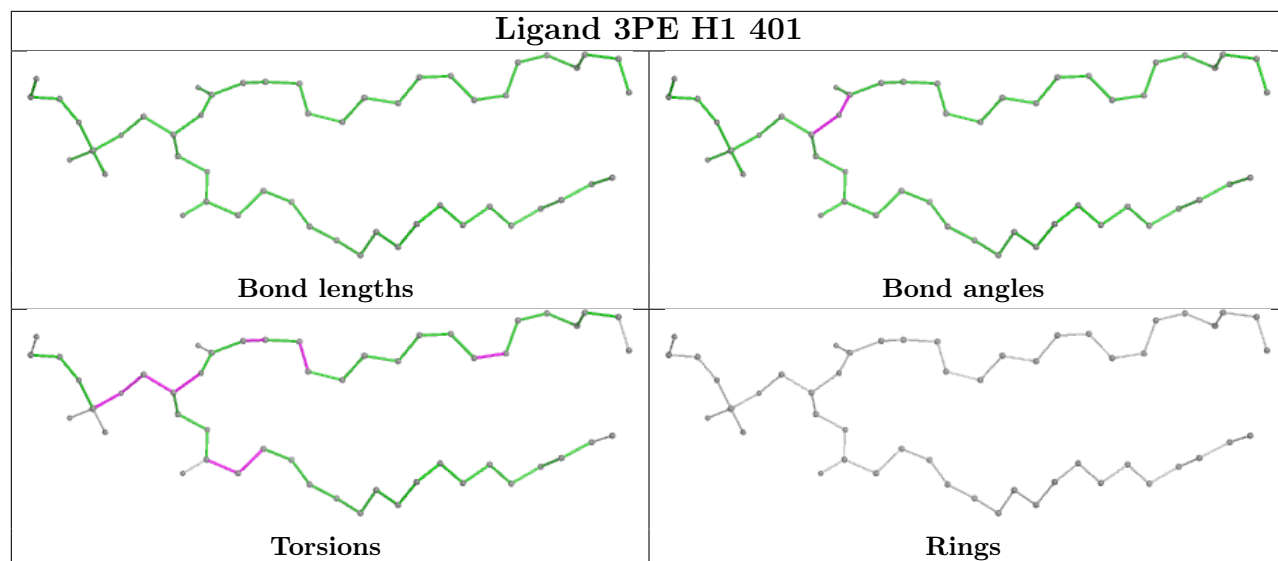
Rings

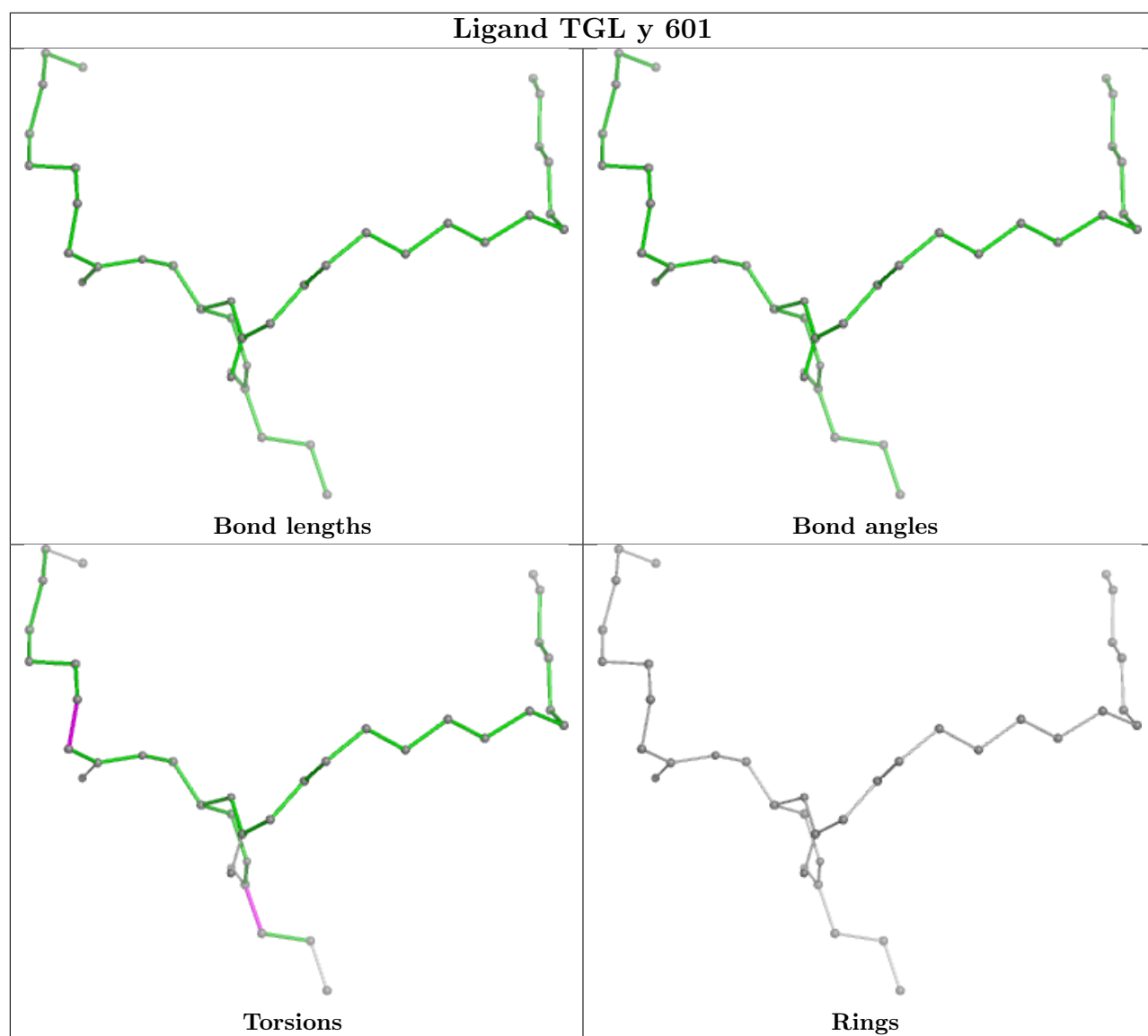


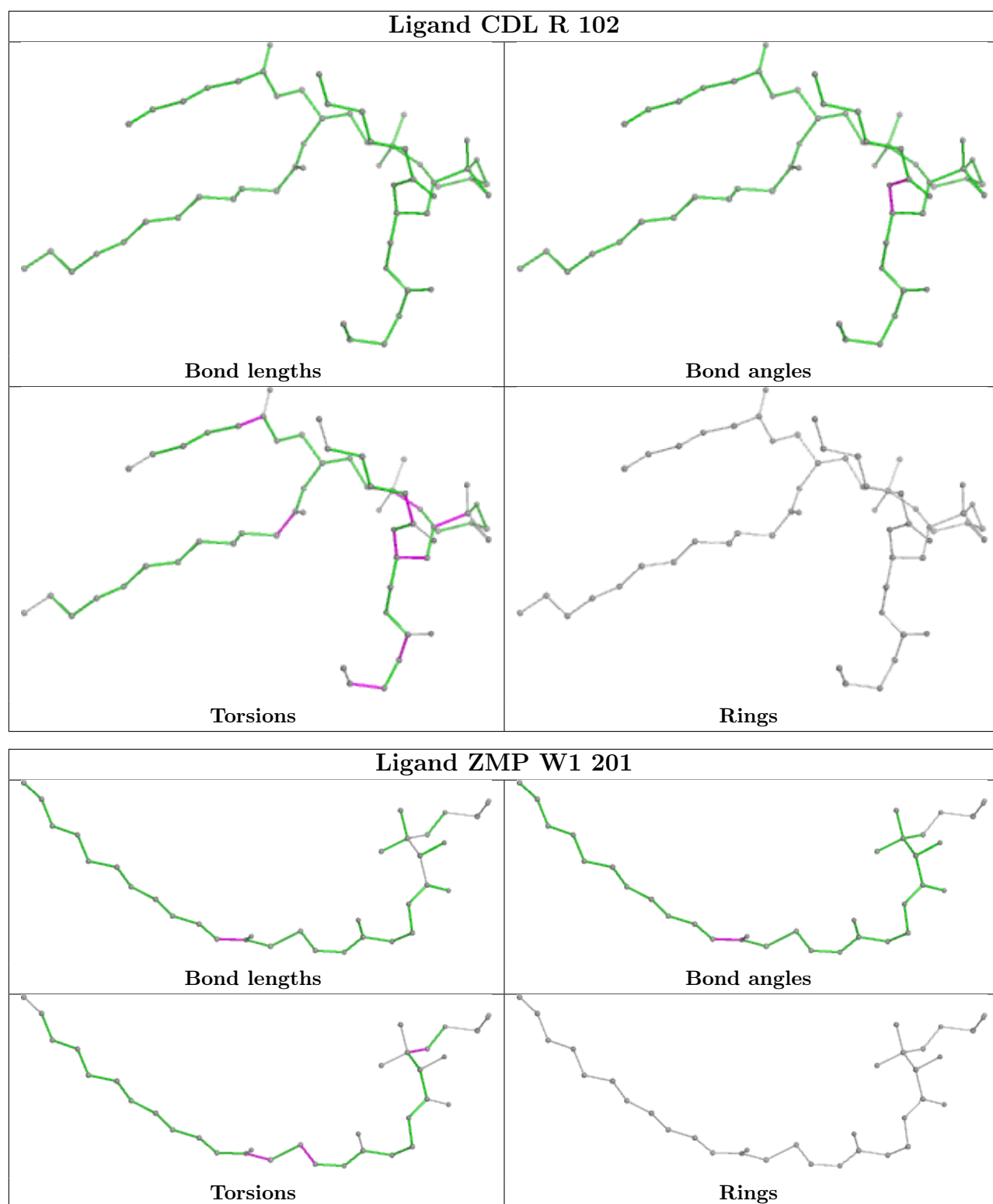


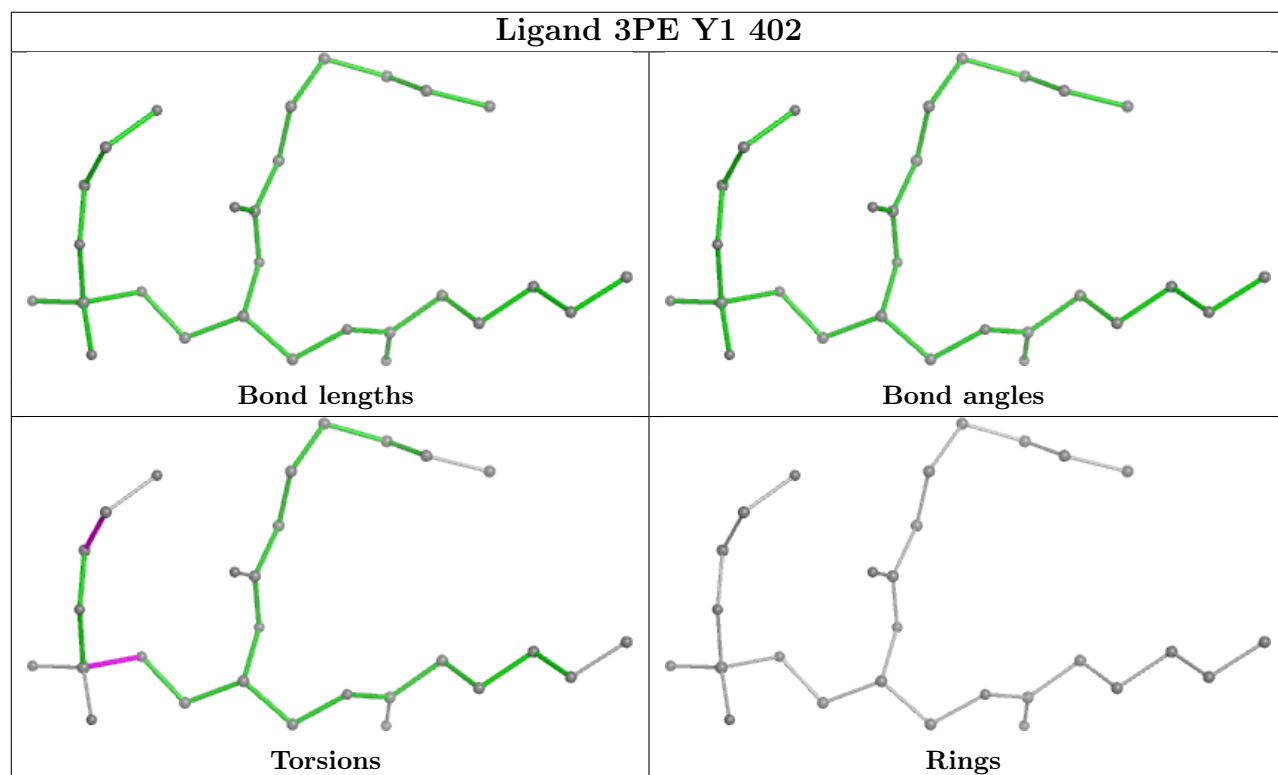
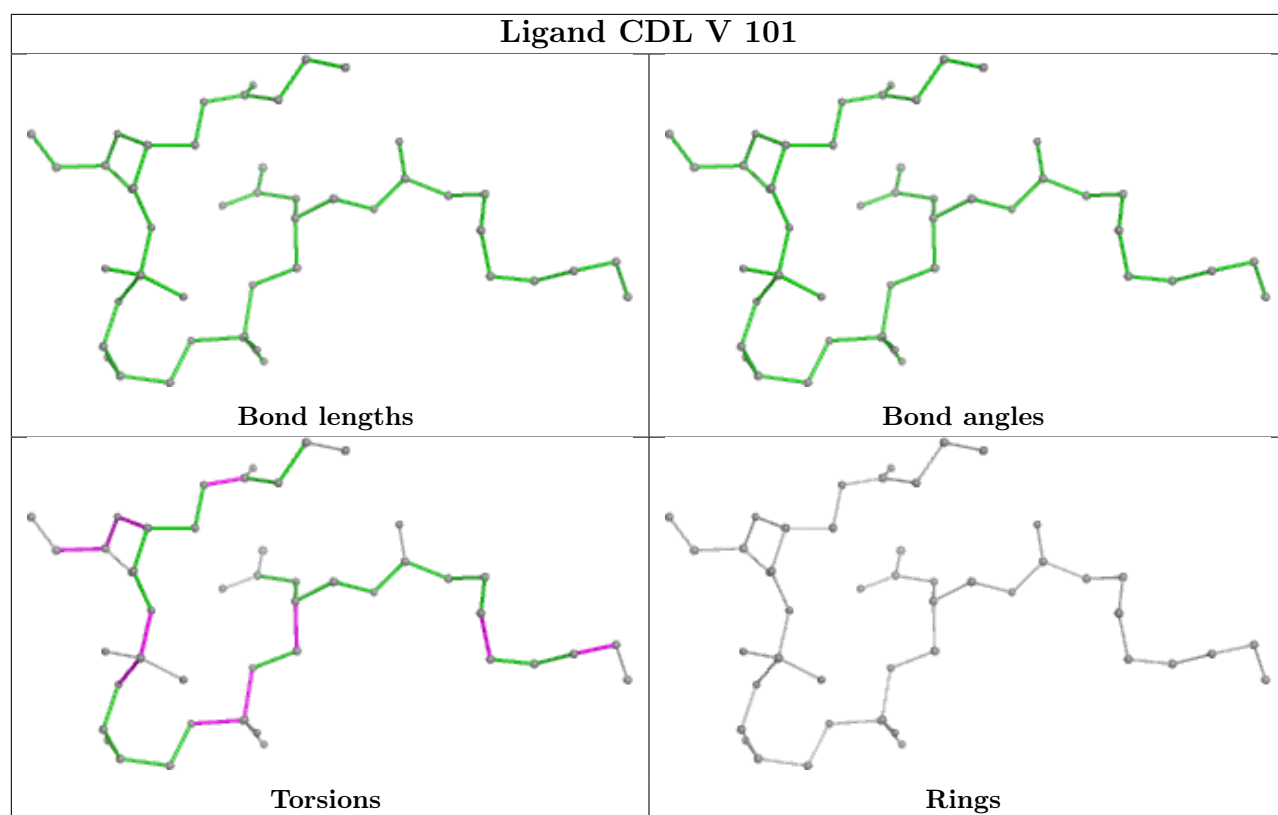


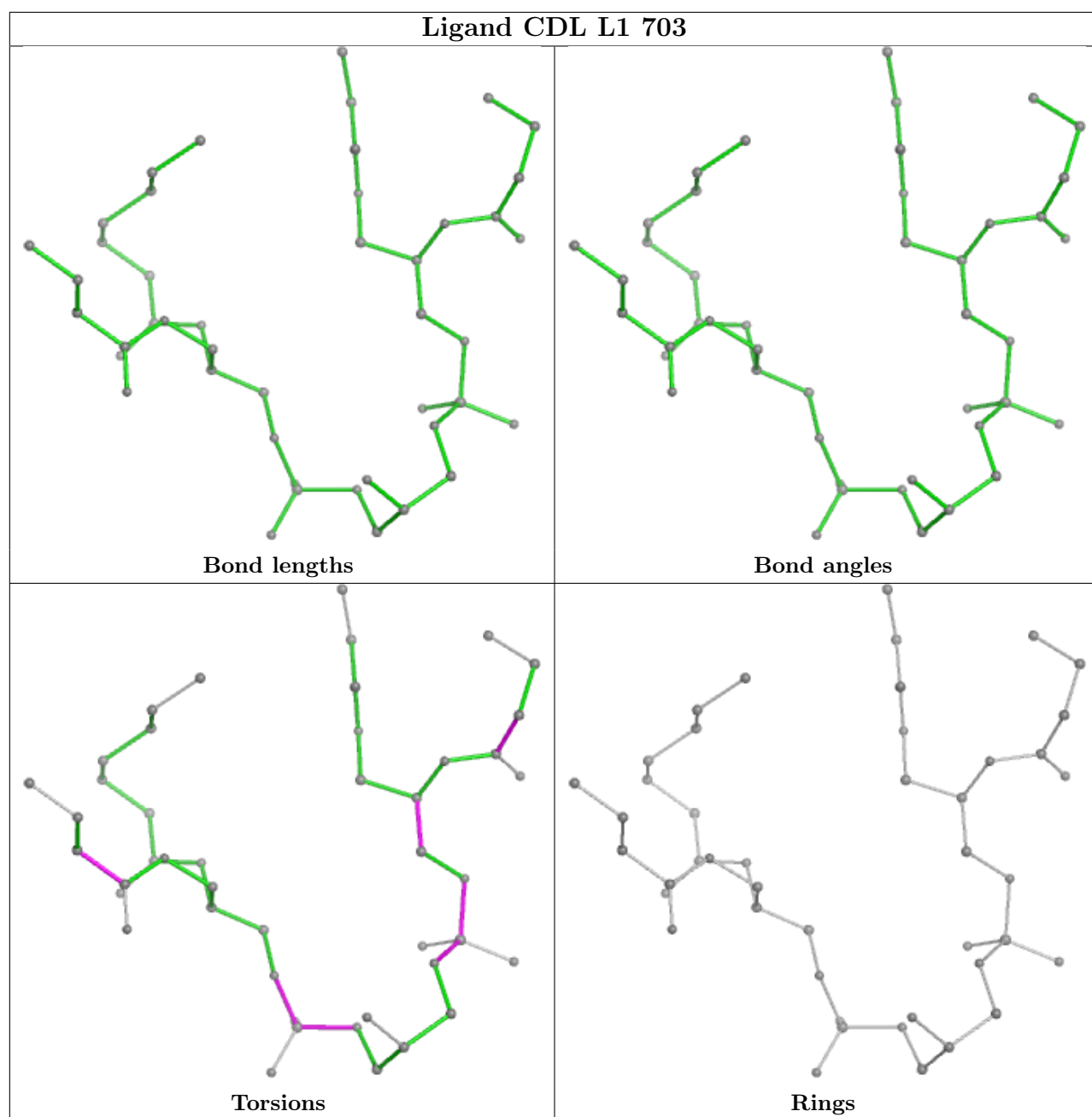




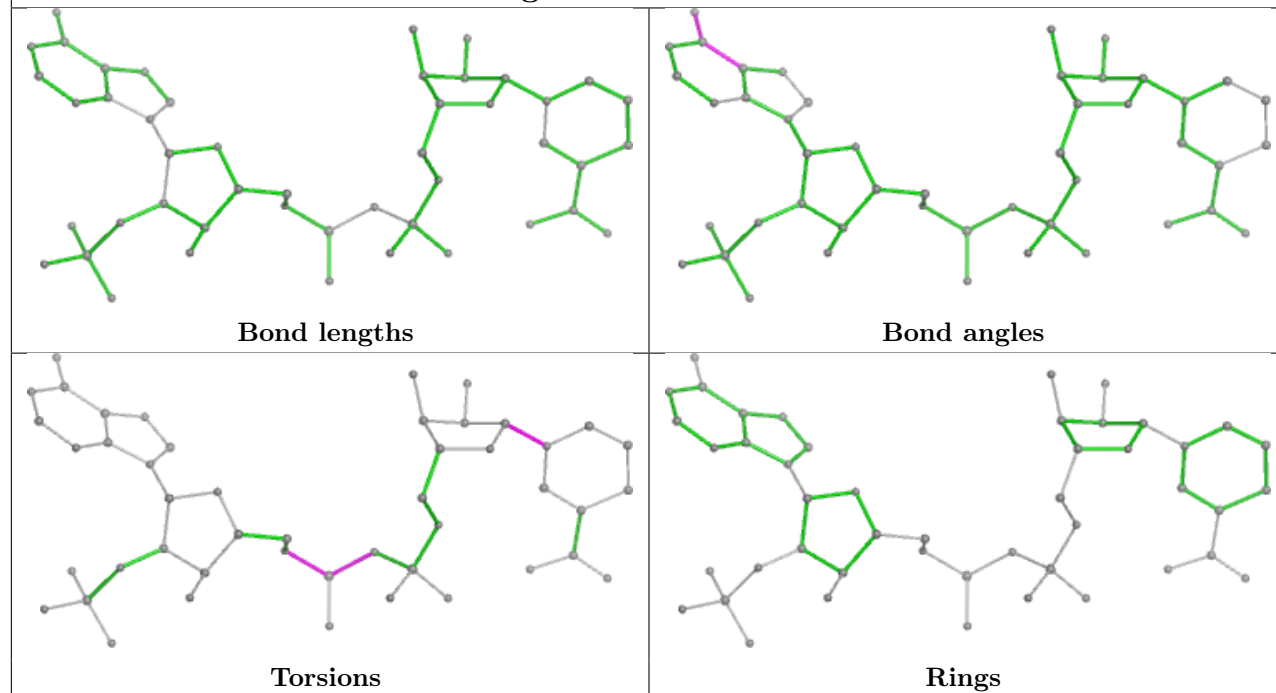




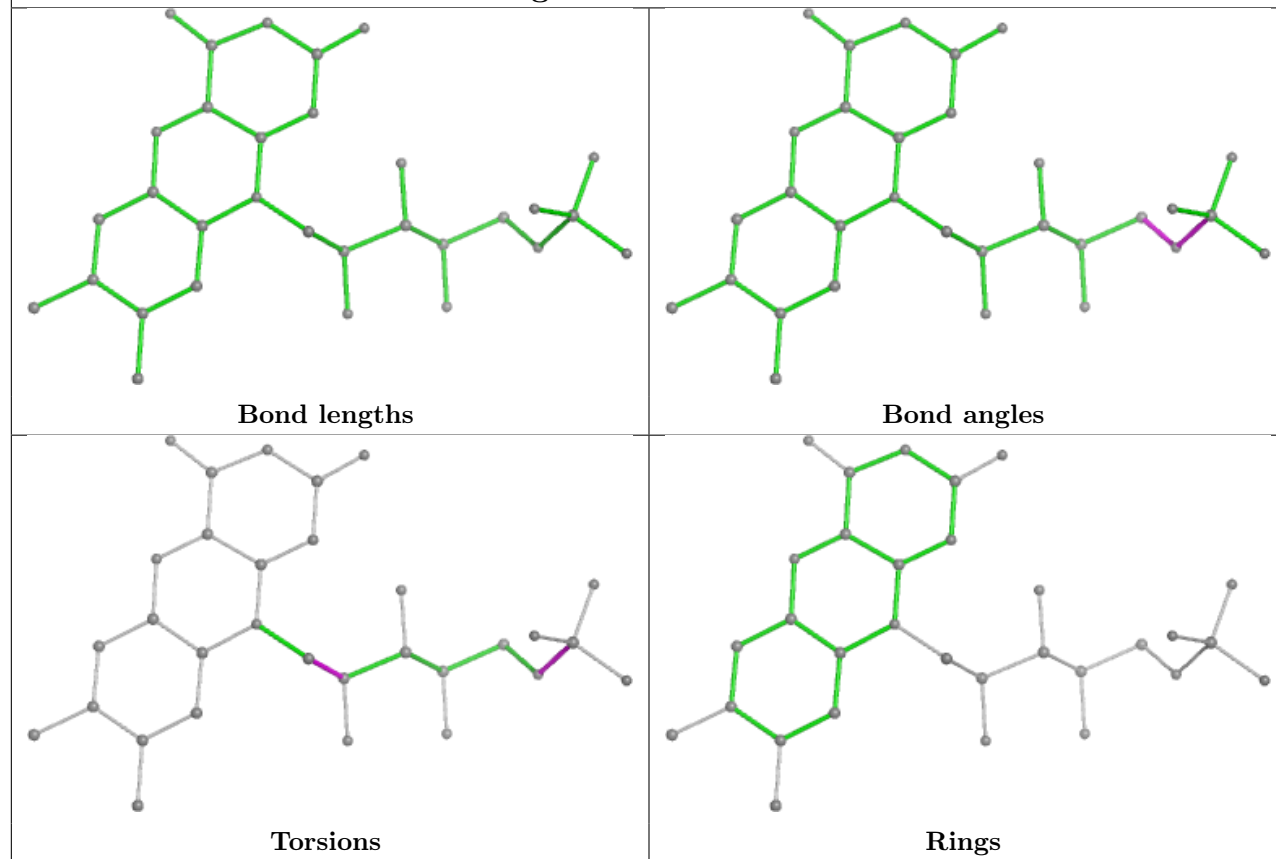


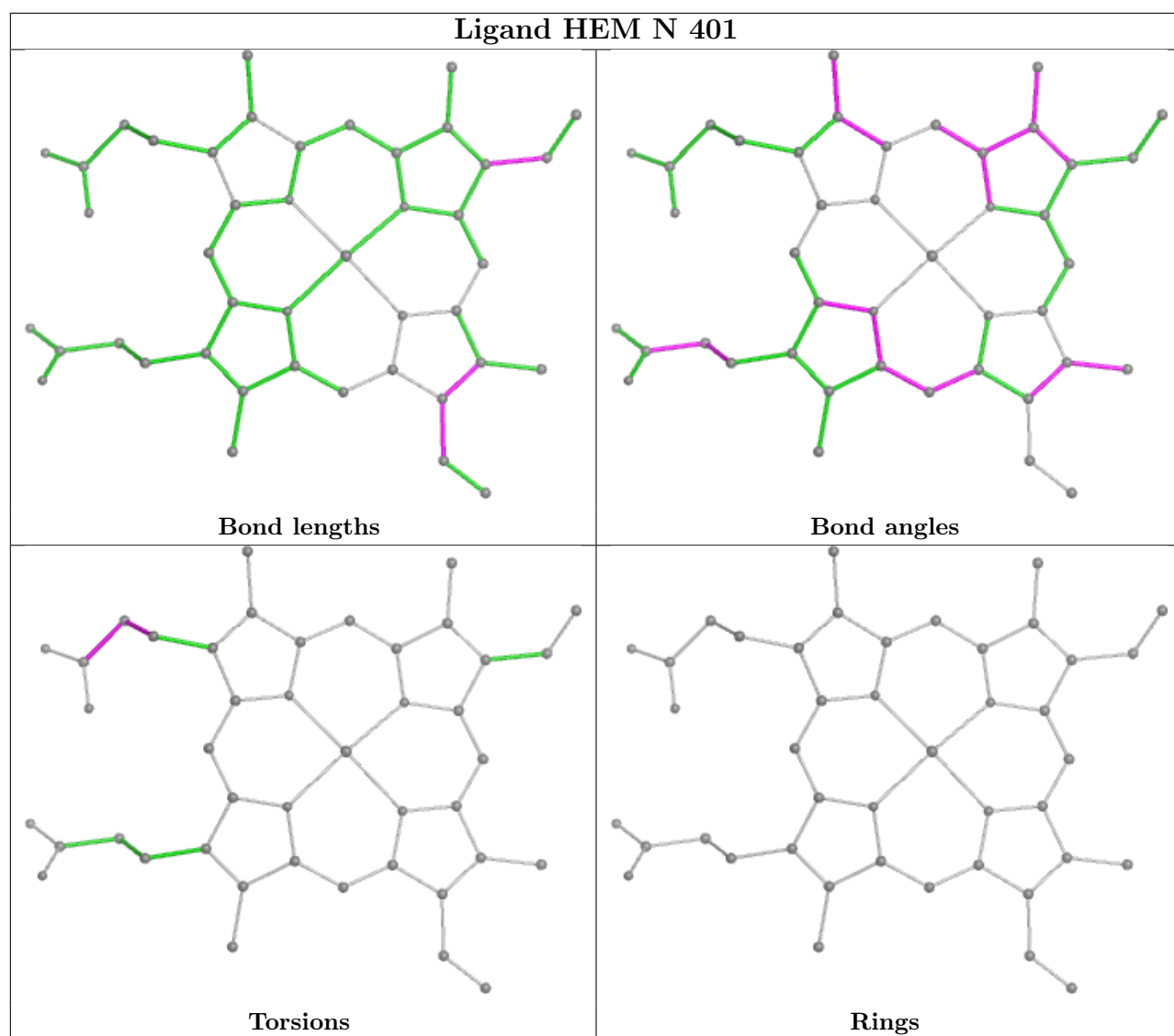


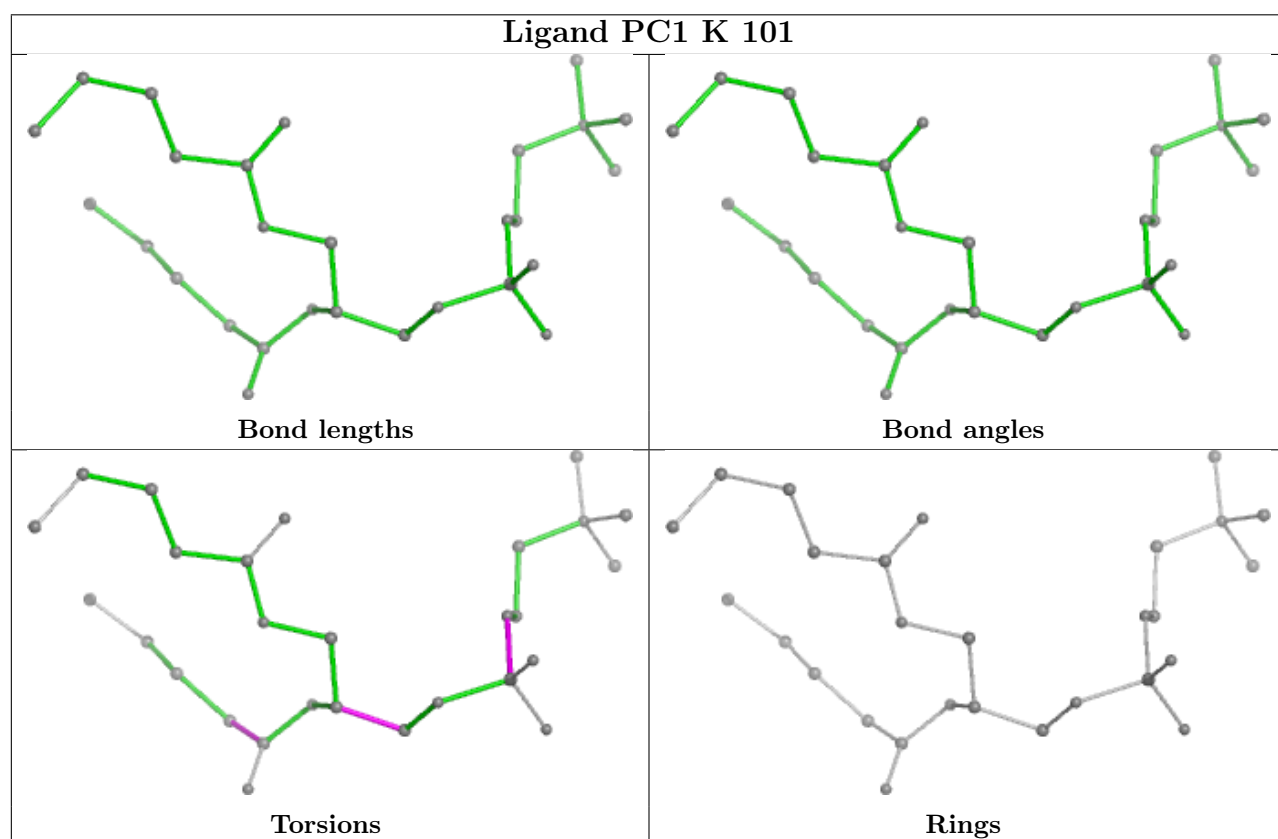
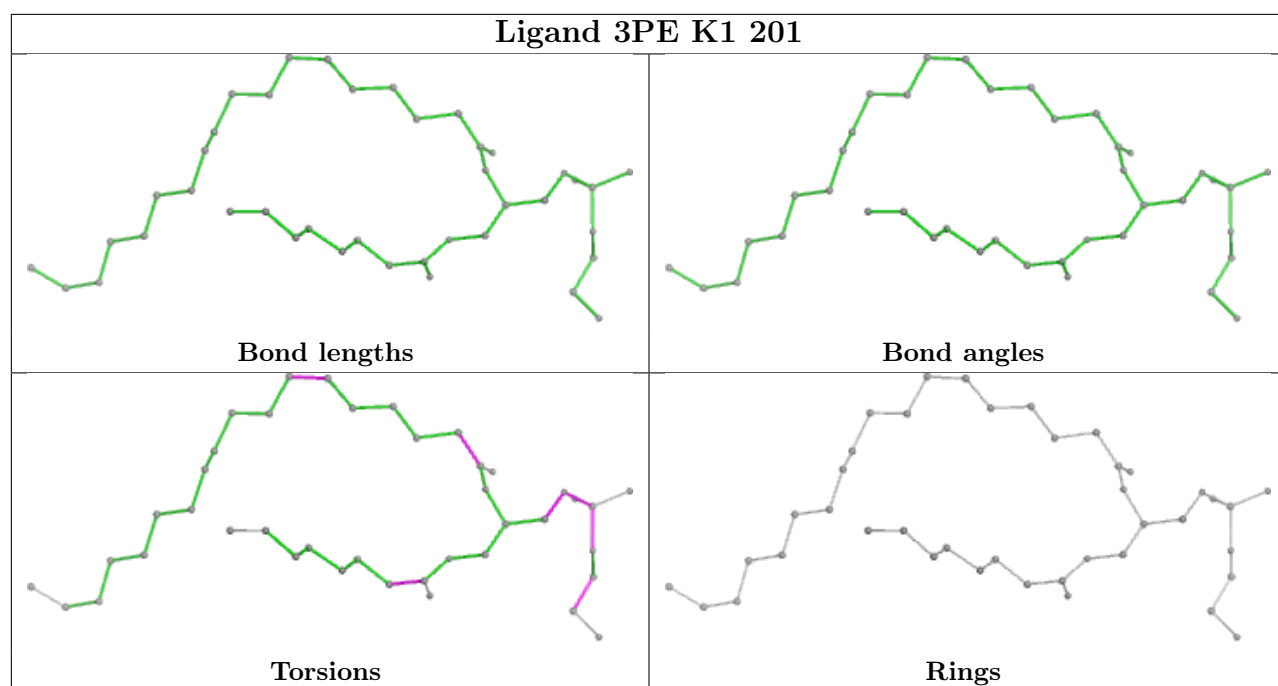
Ligand NDP P1 501

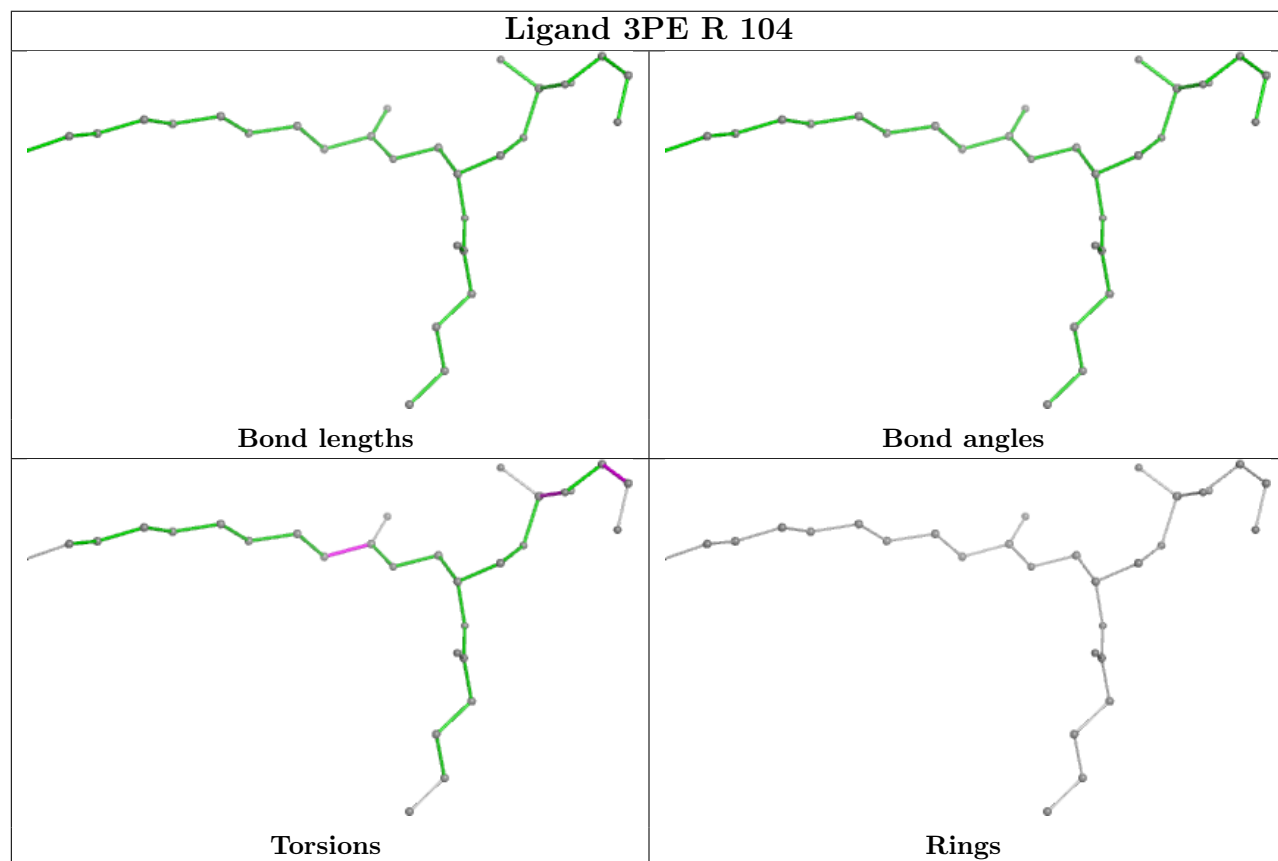
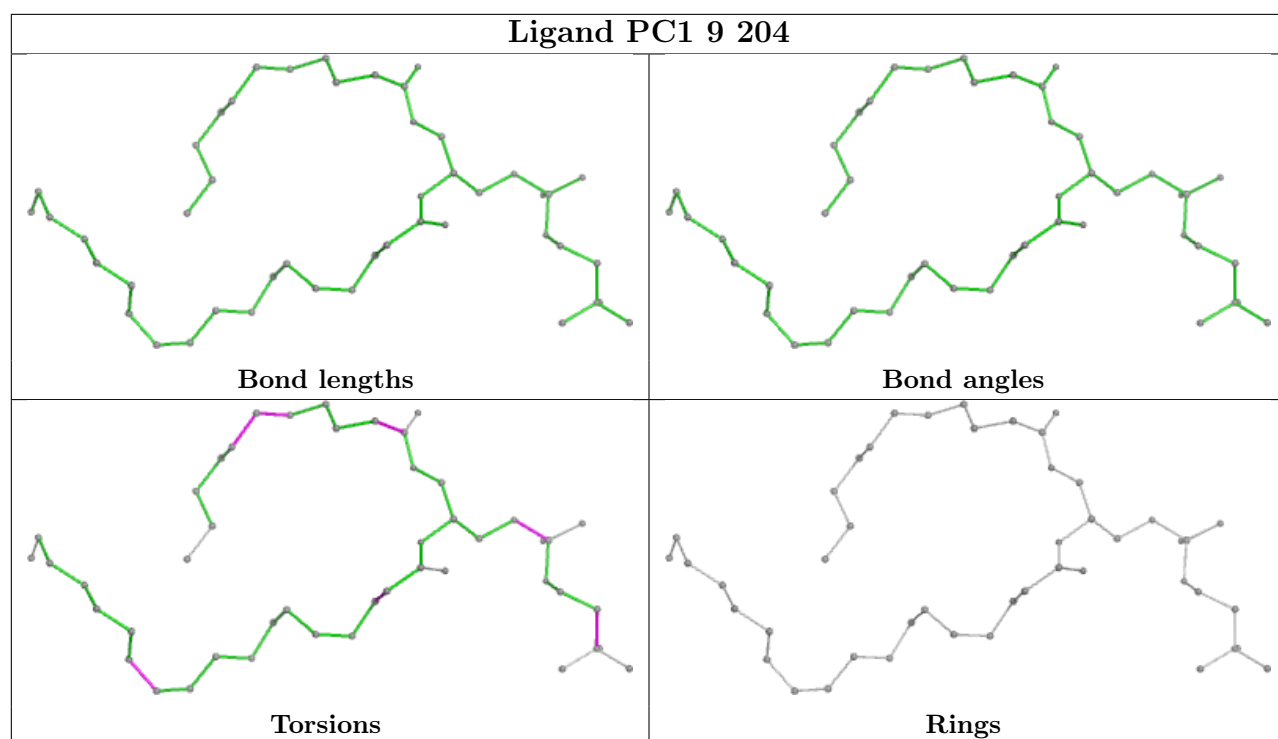


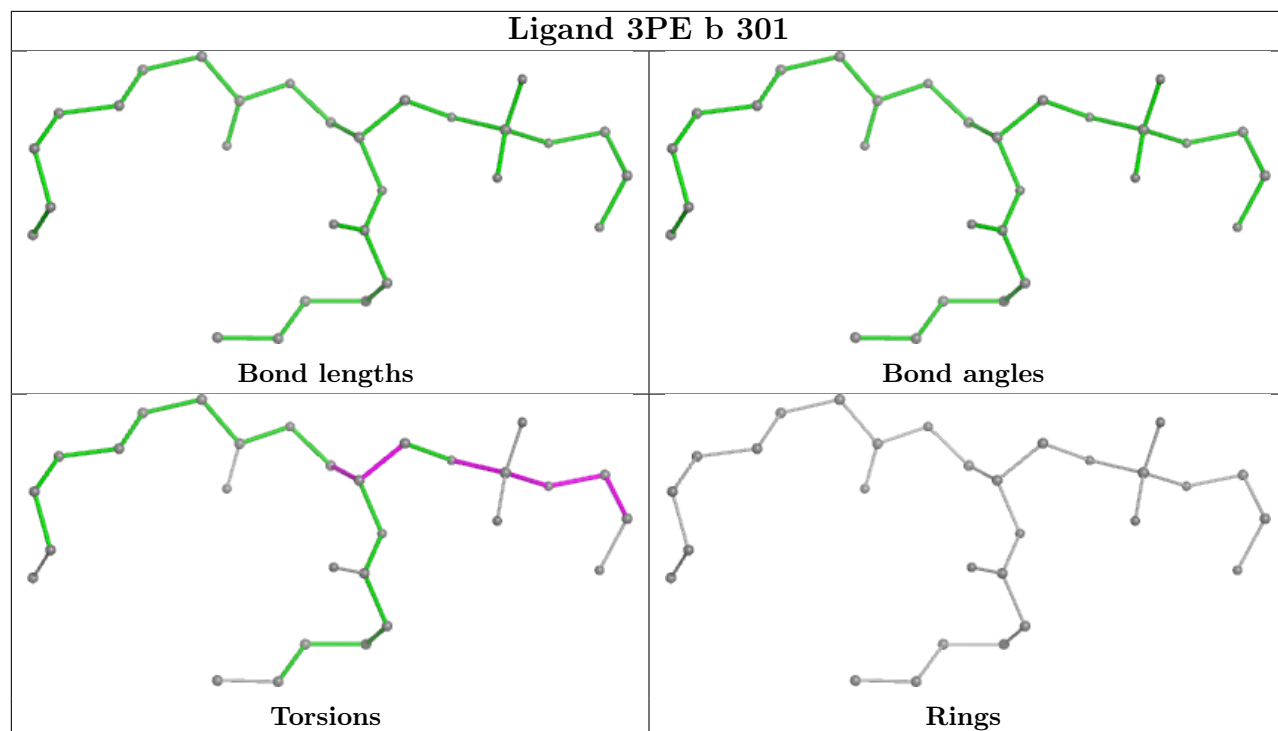
Ligand FMN 1 501

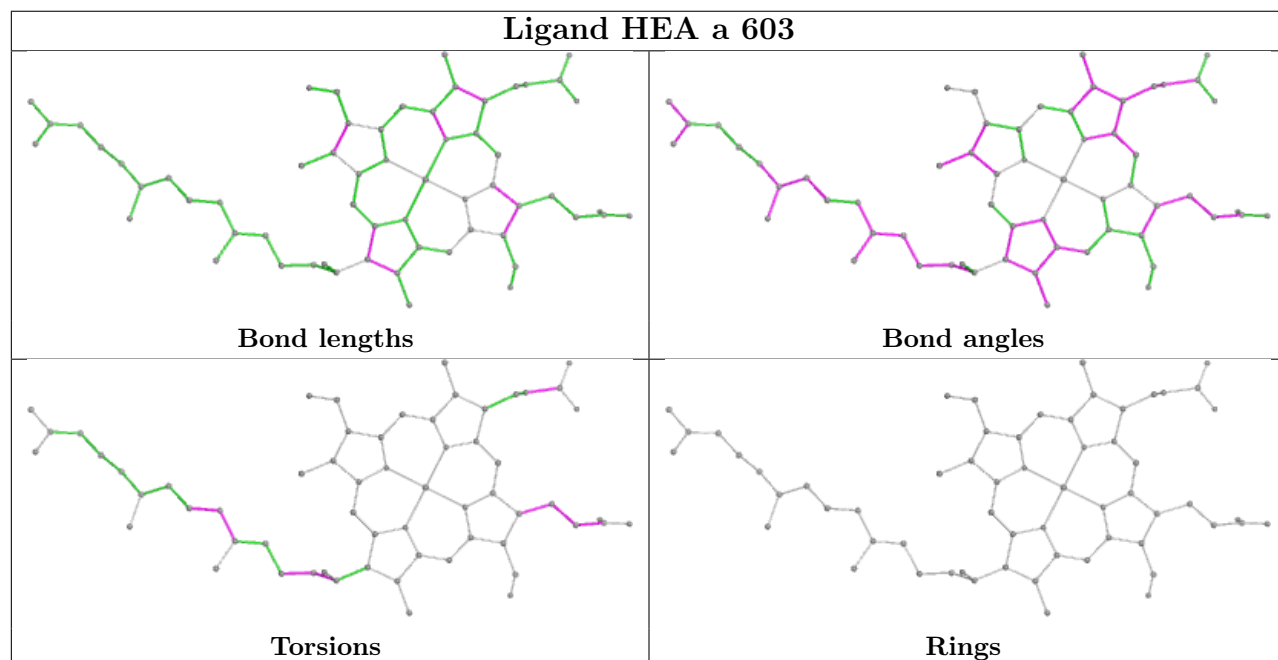
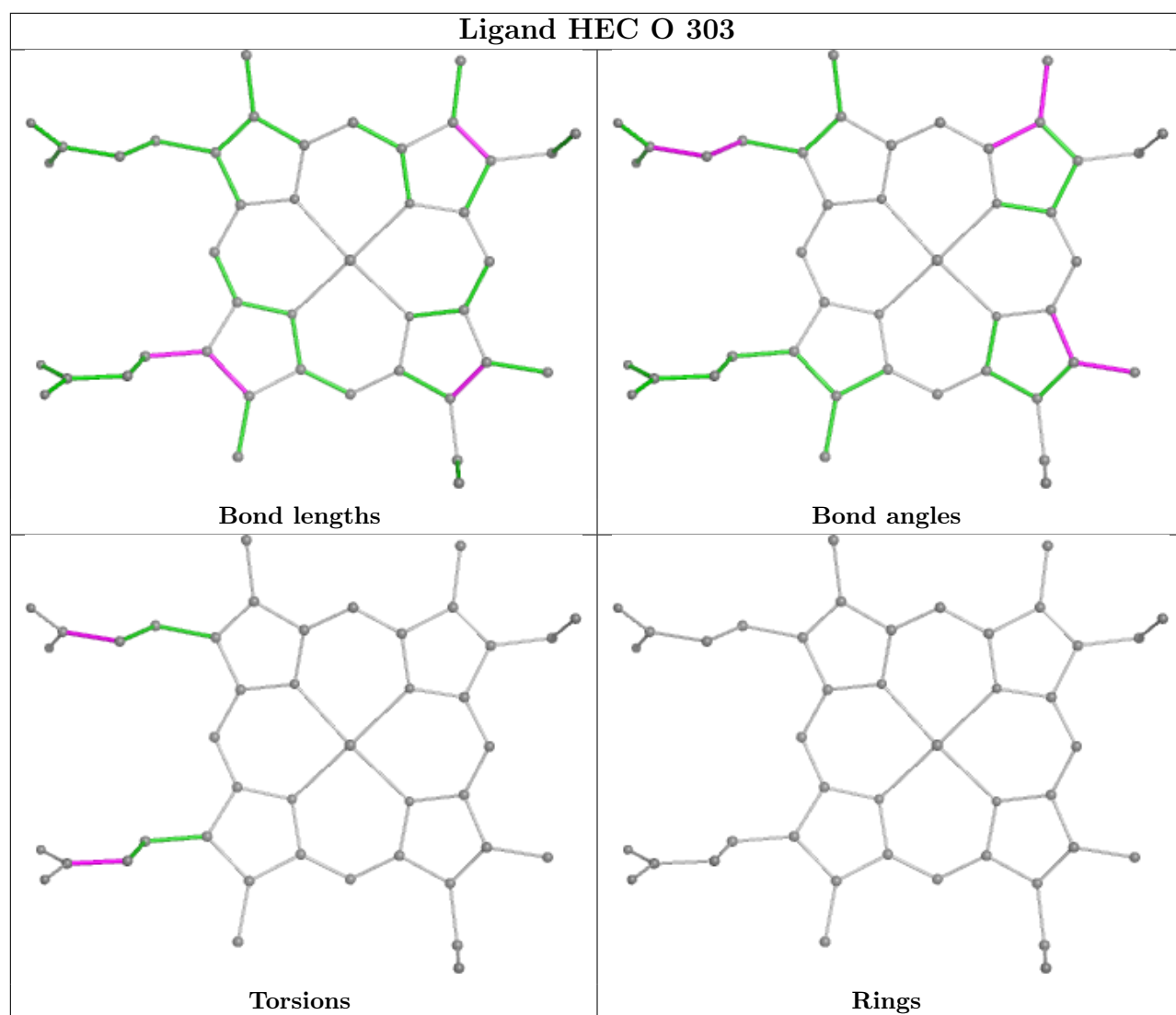


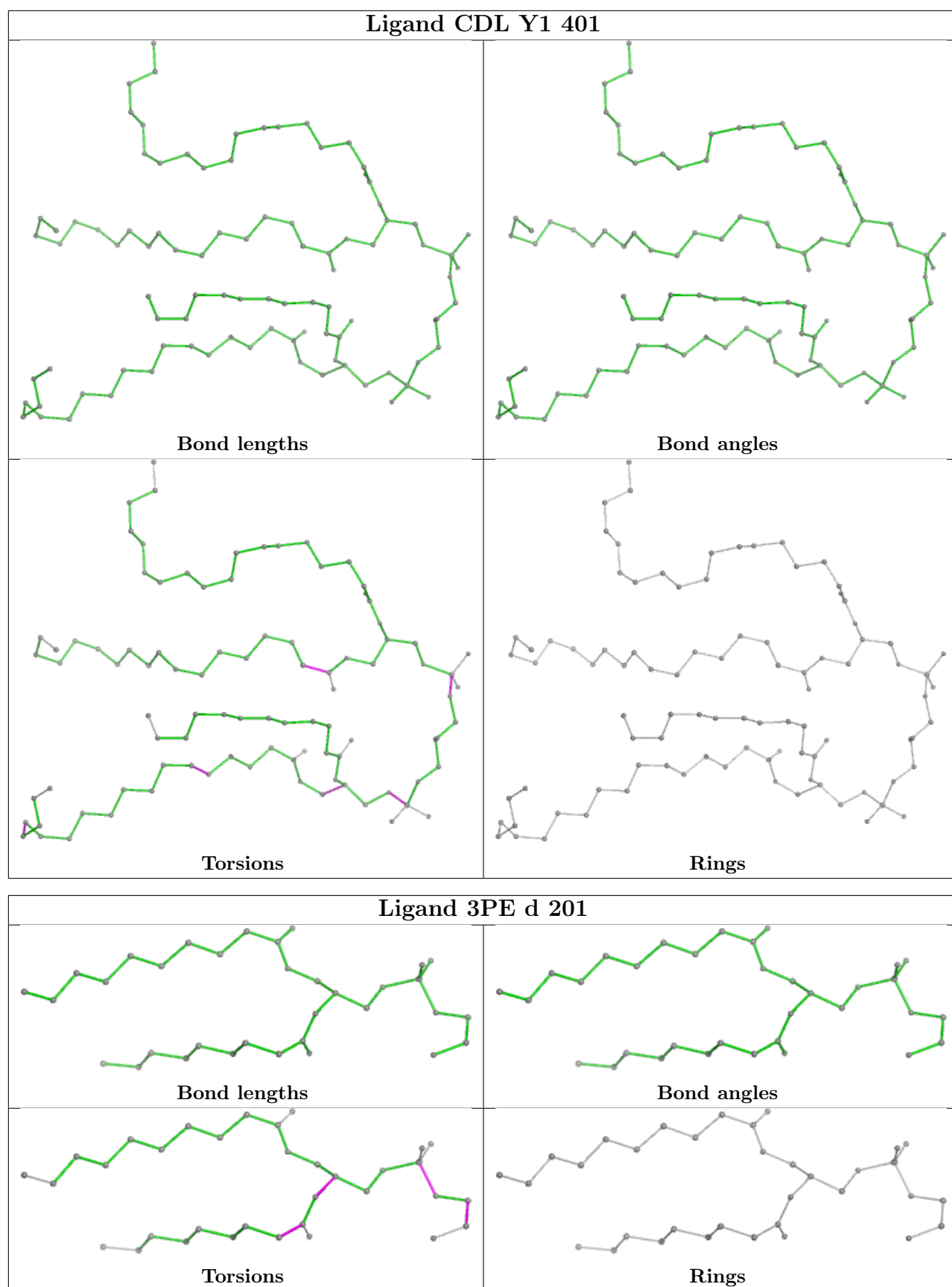


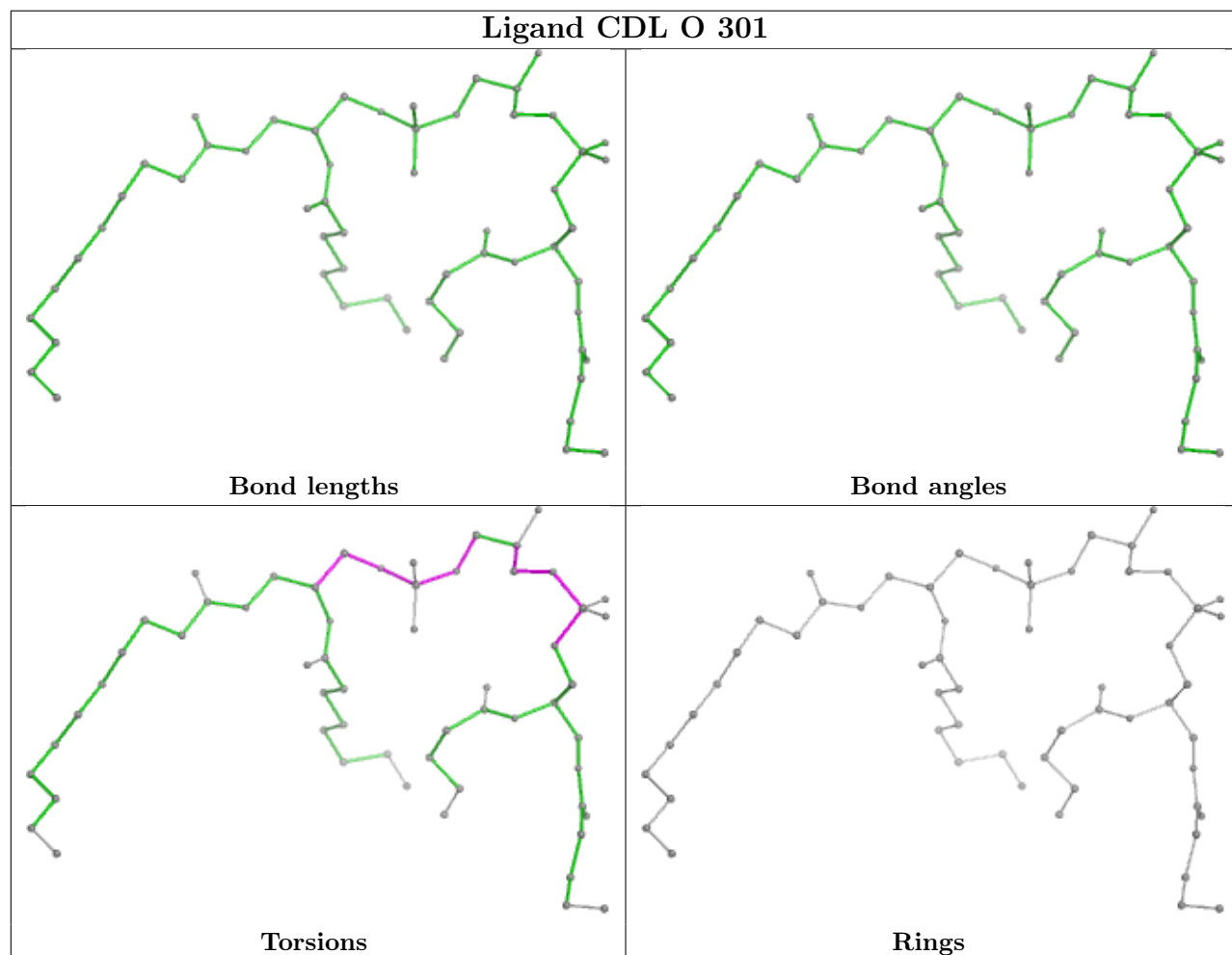
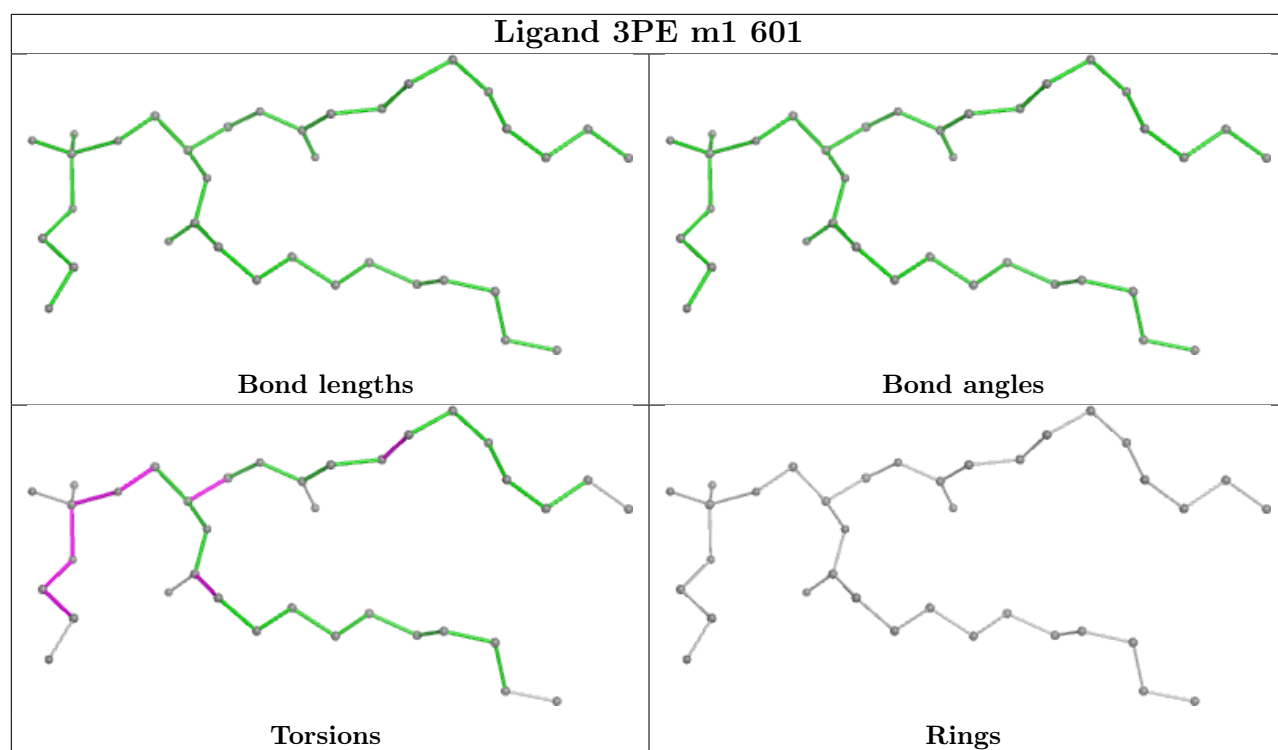


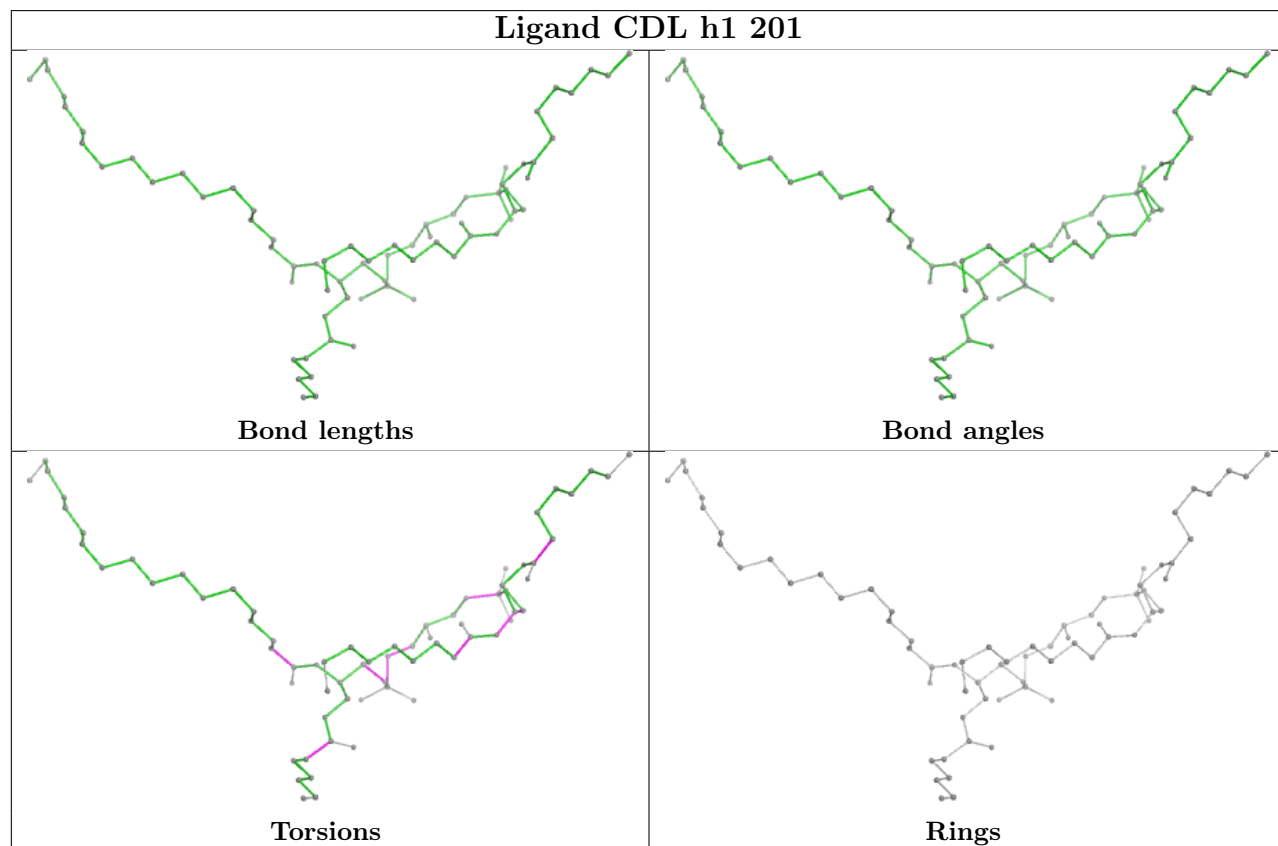
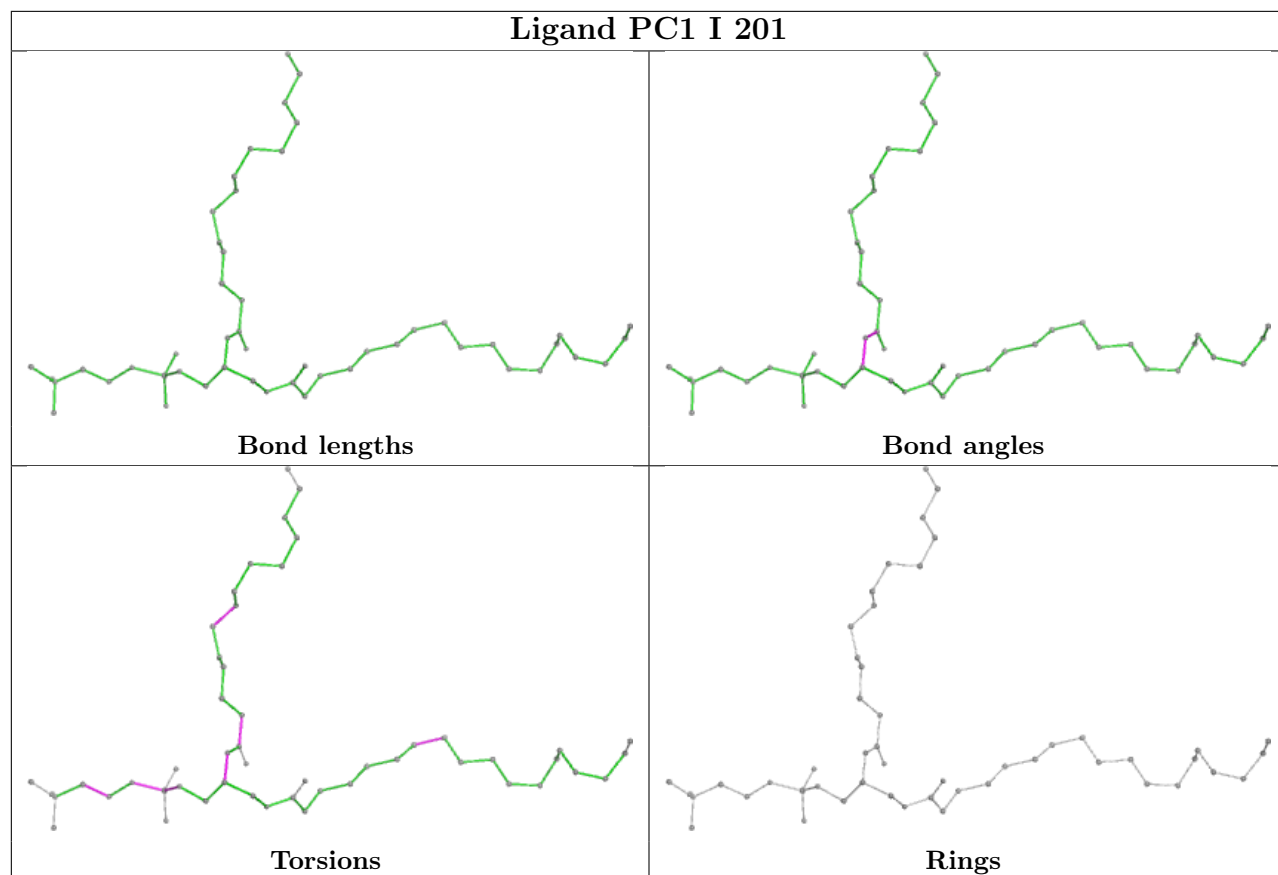


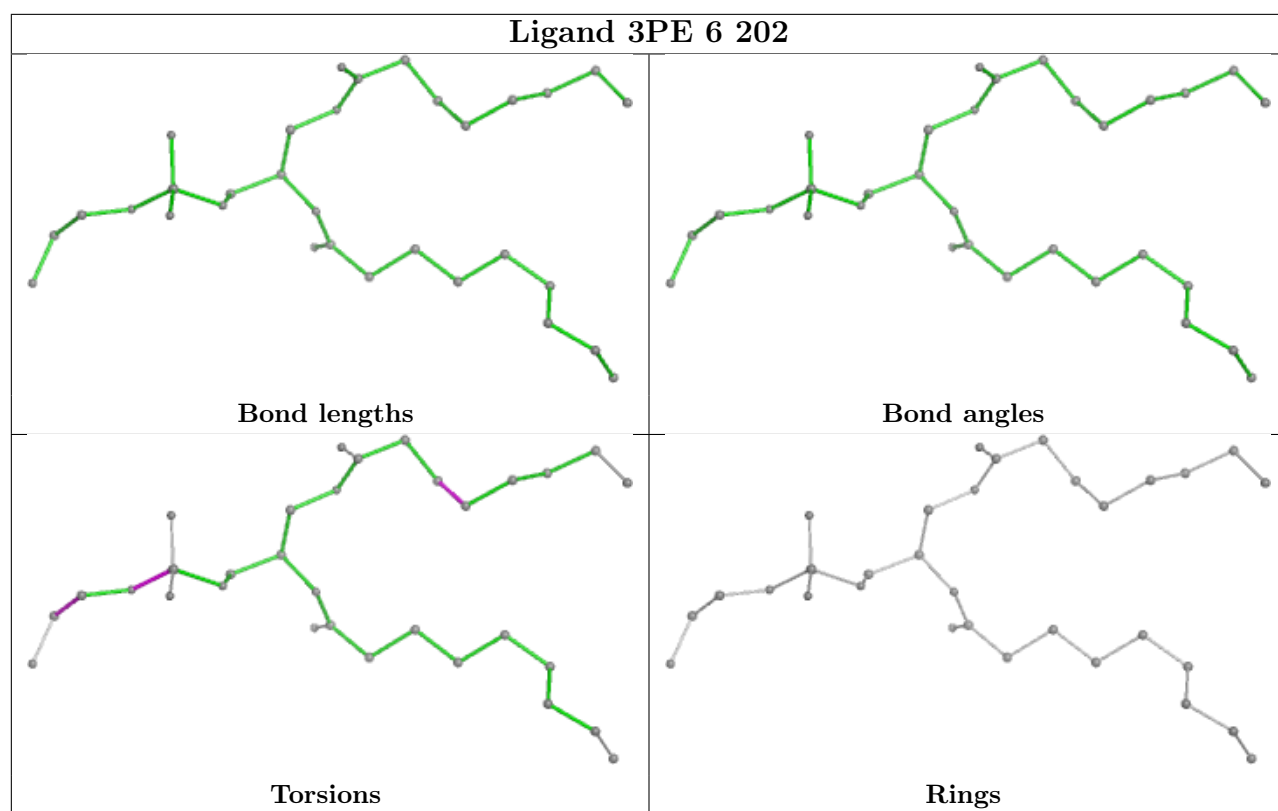


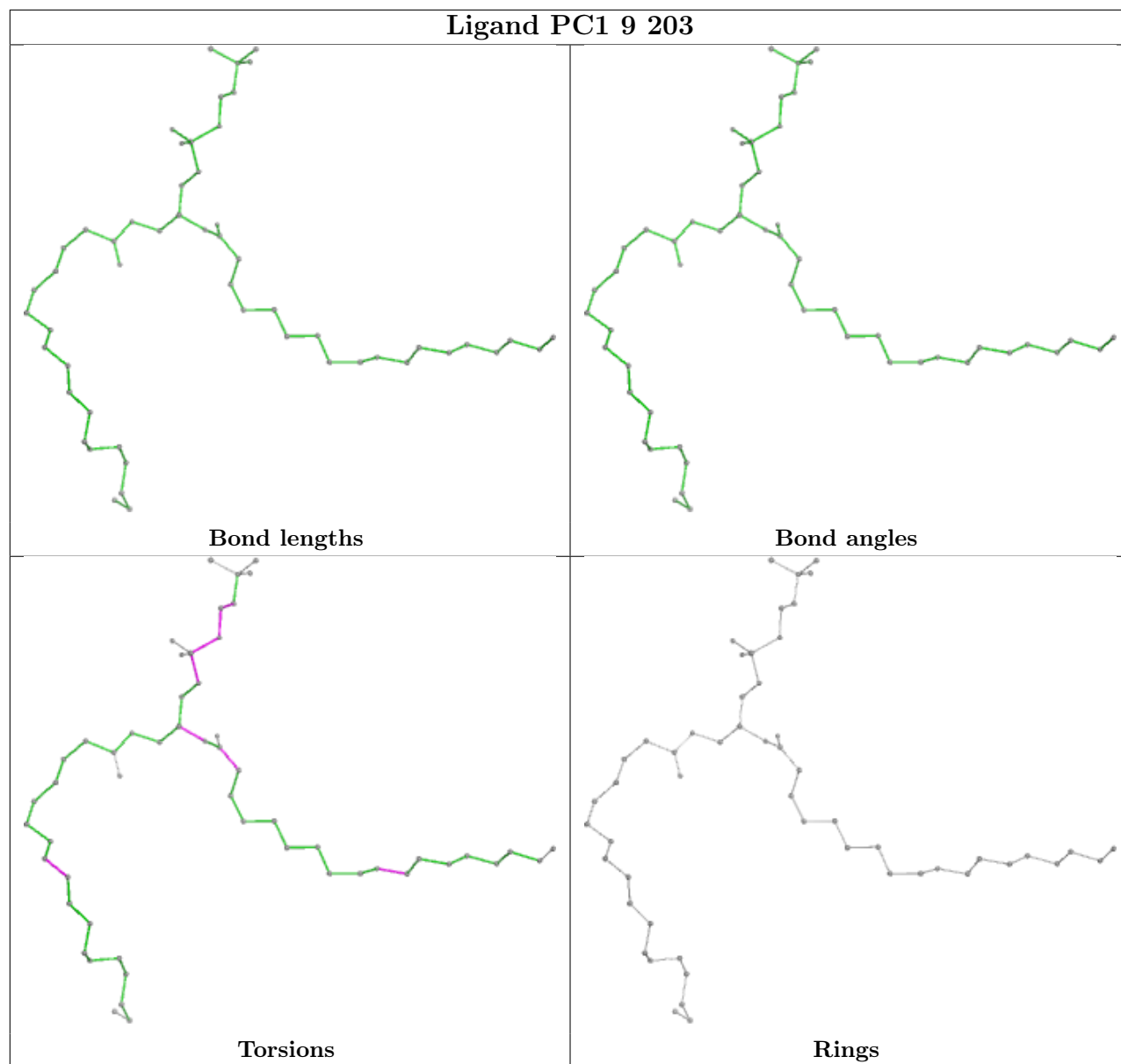


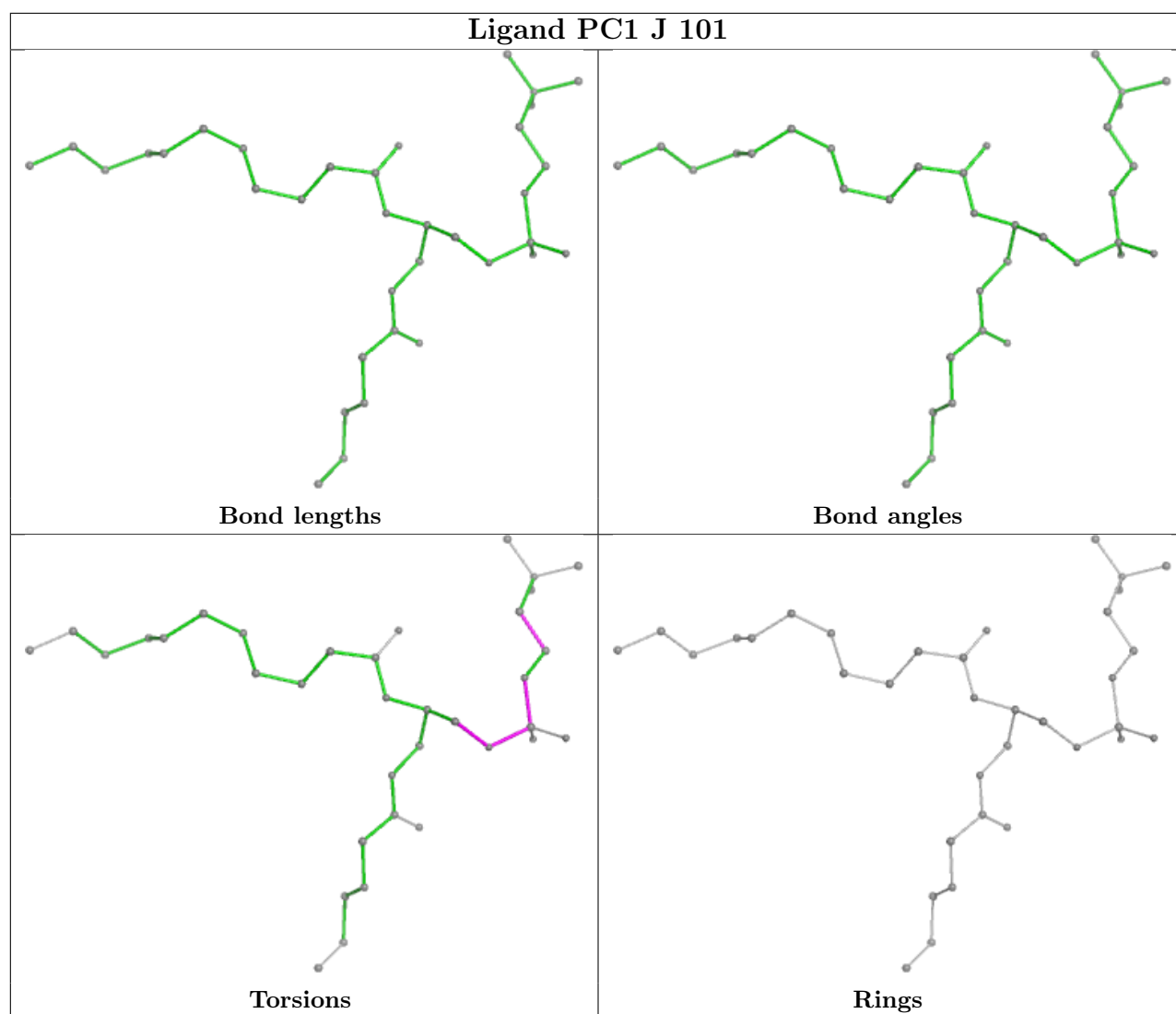


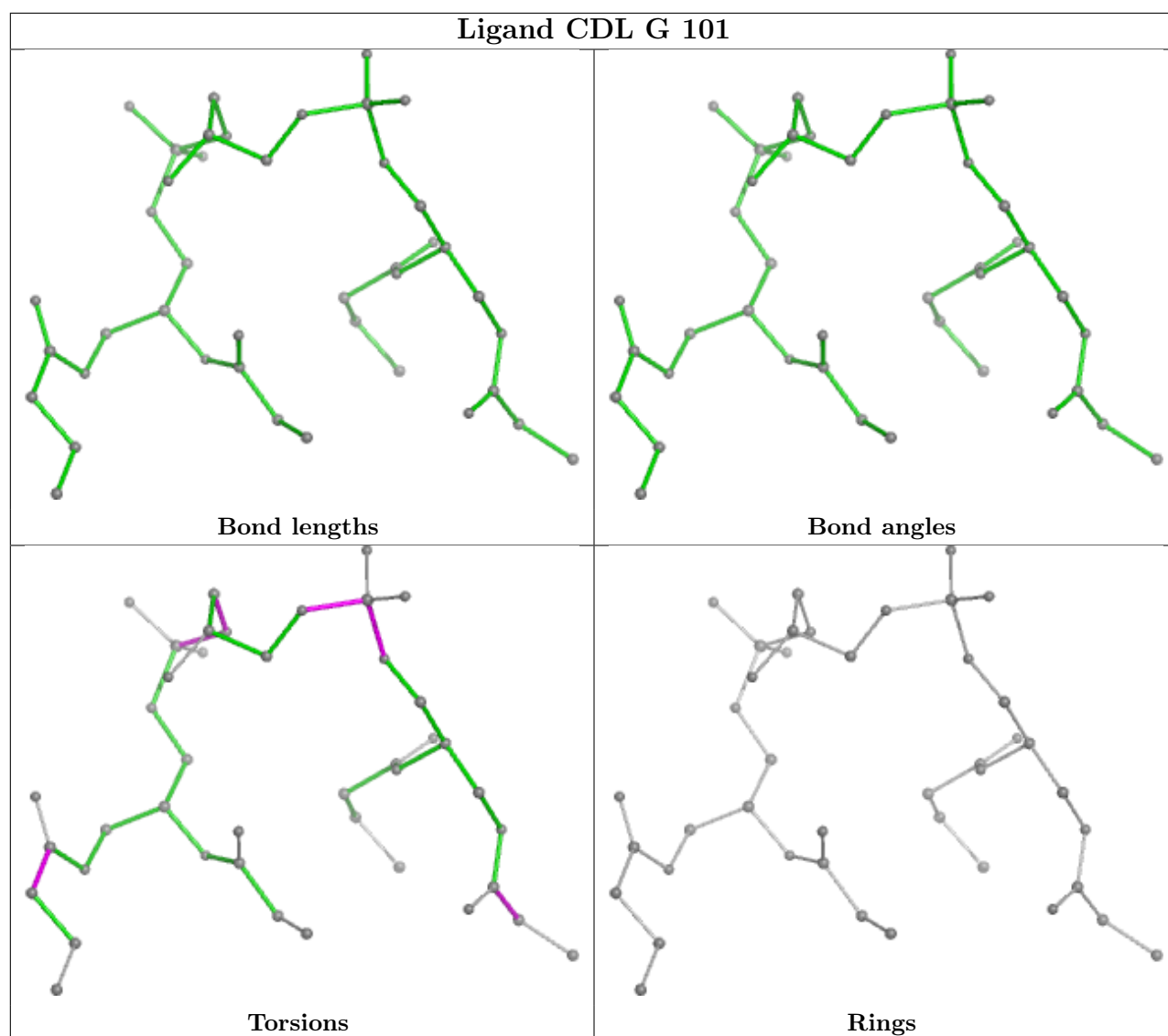


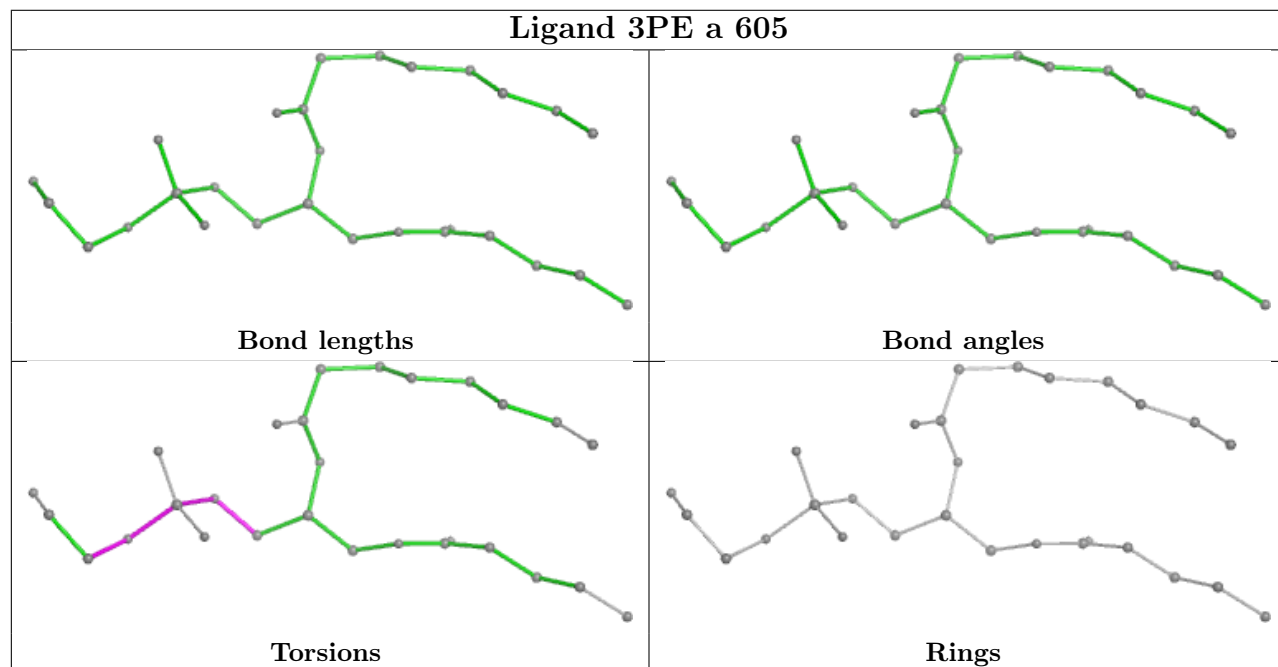
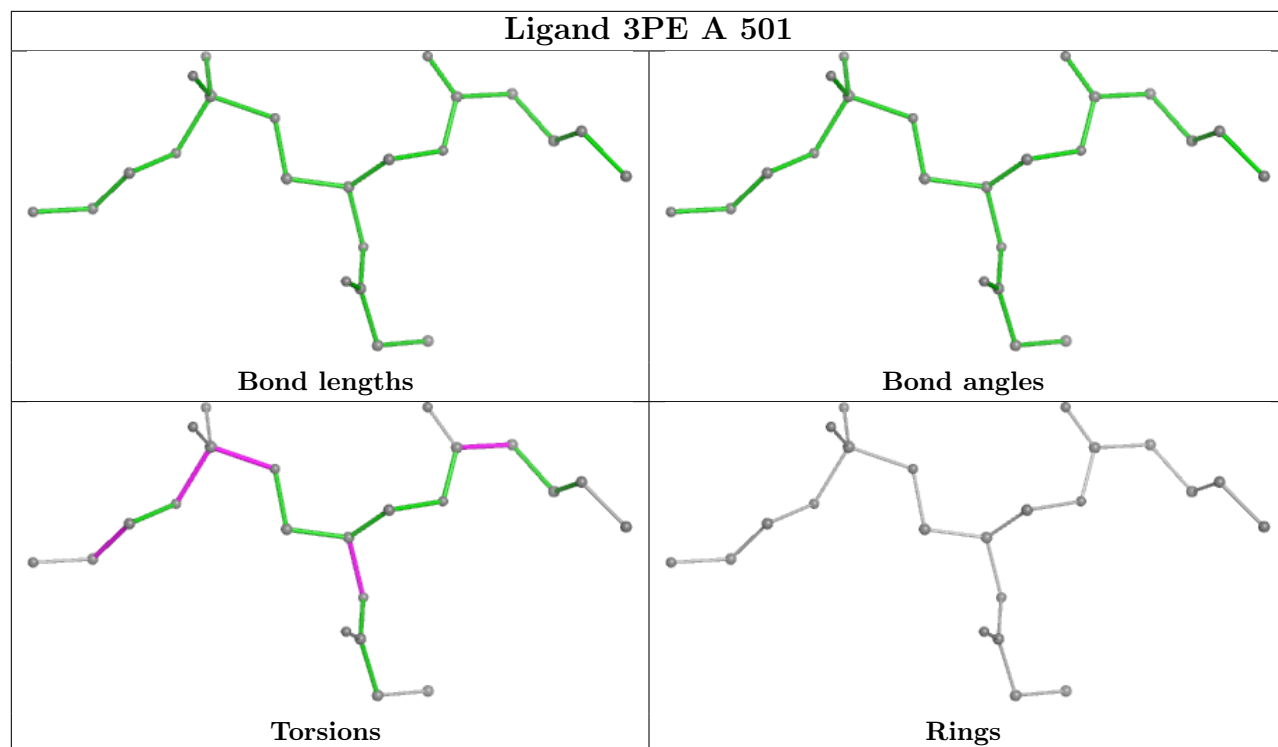


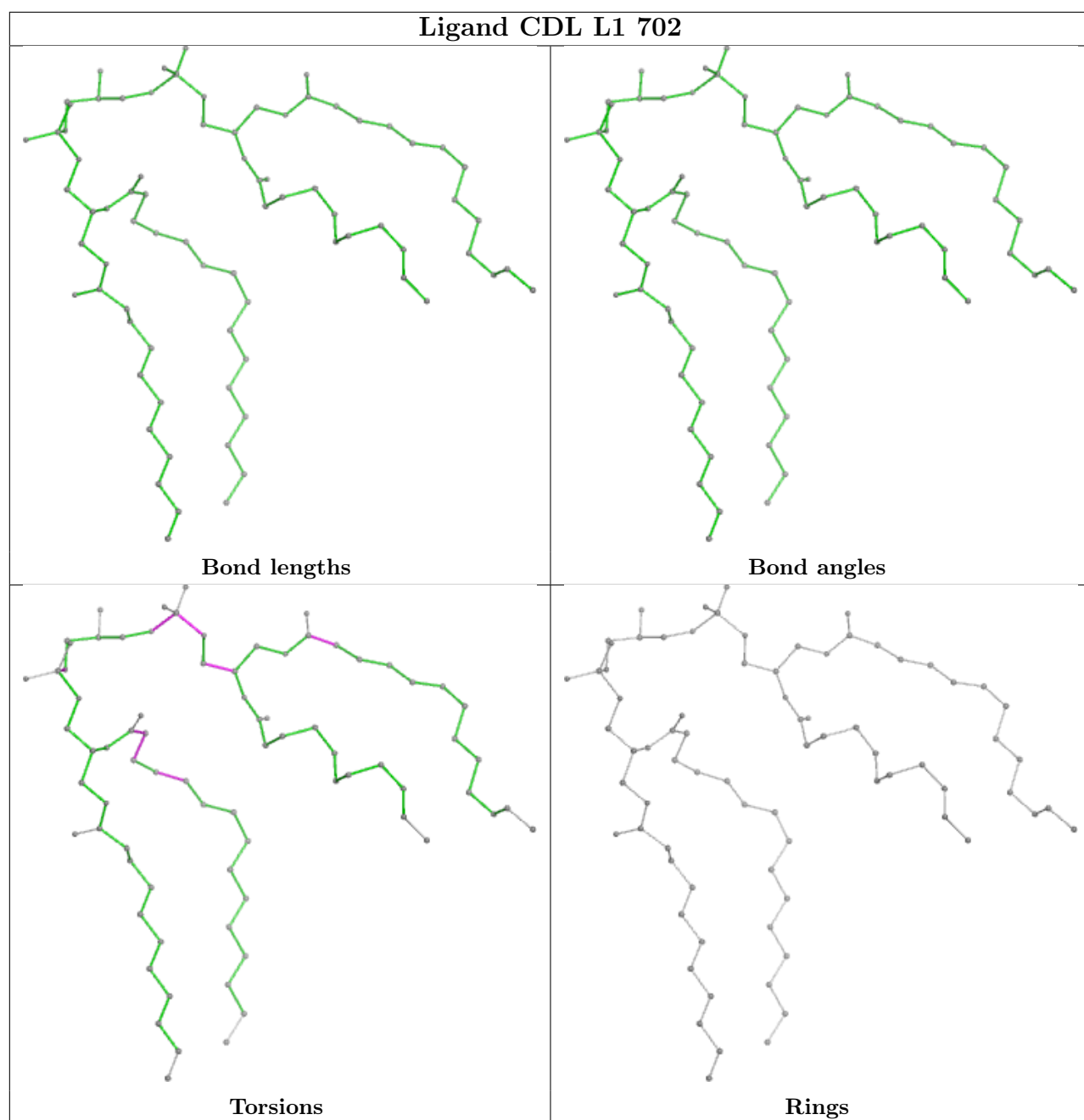




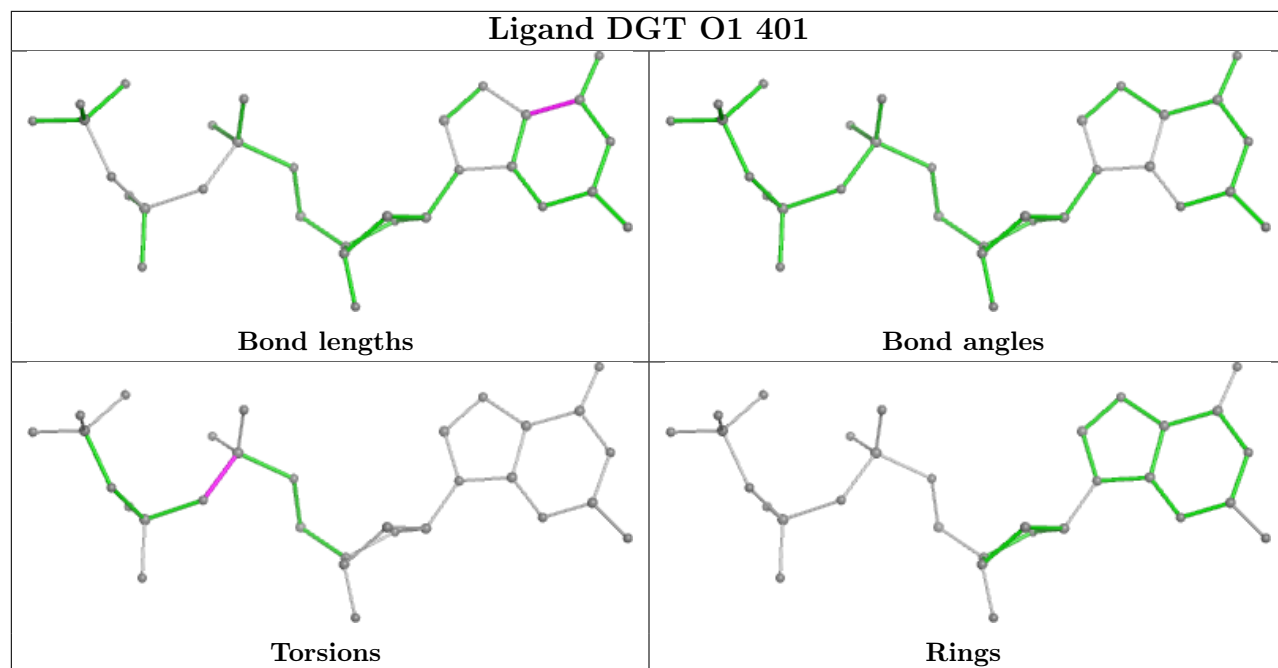




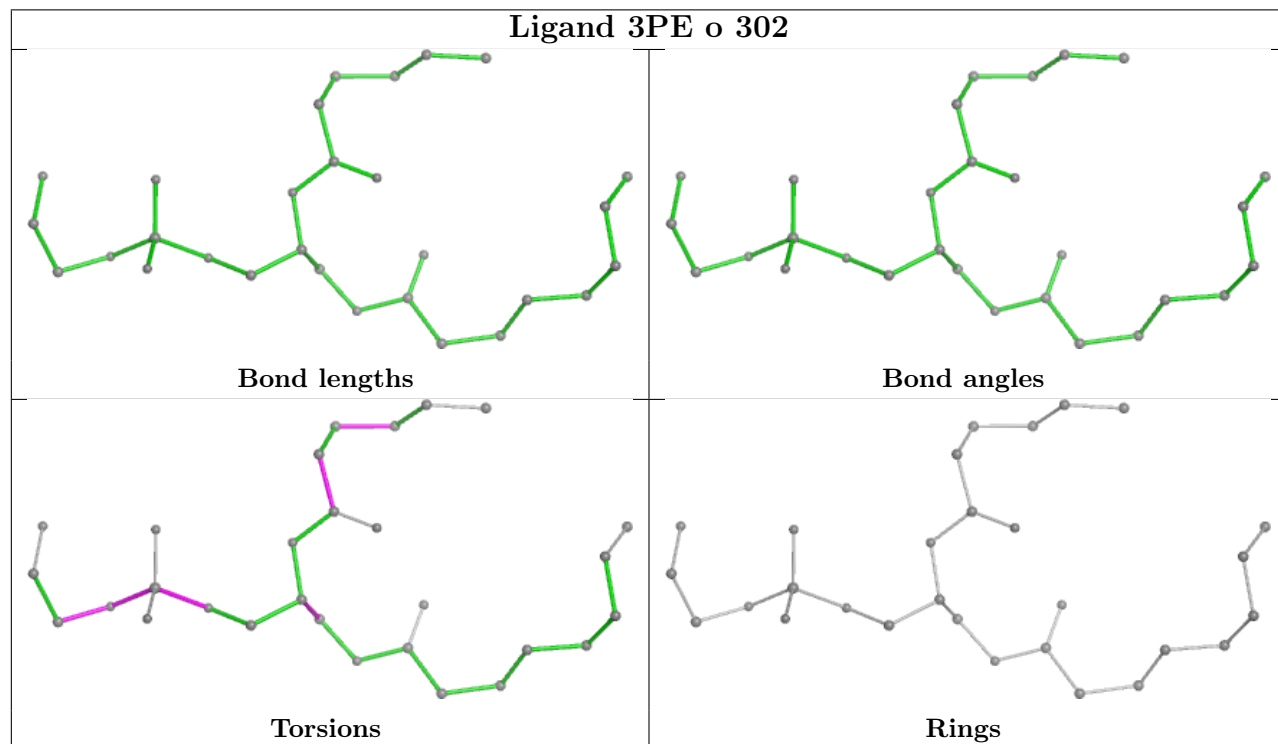


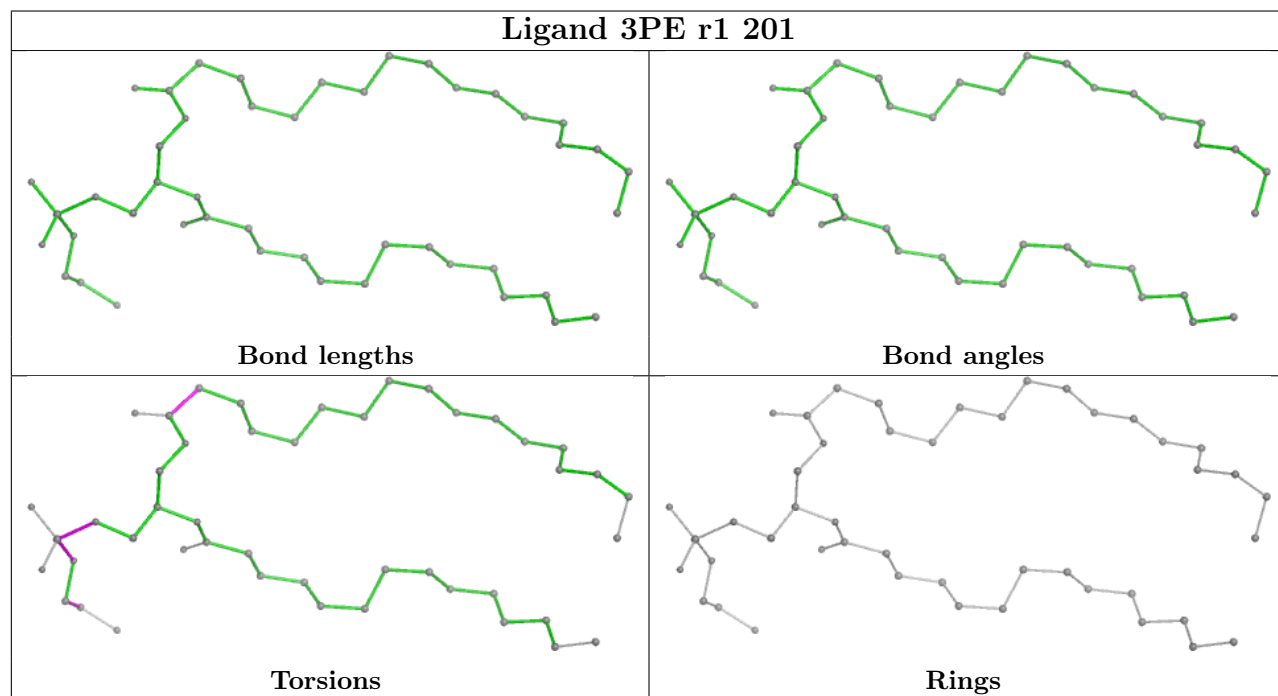
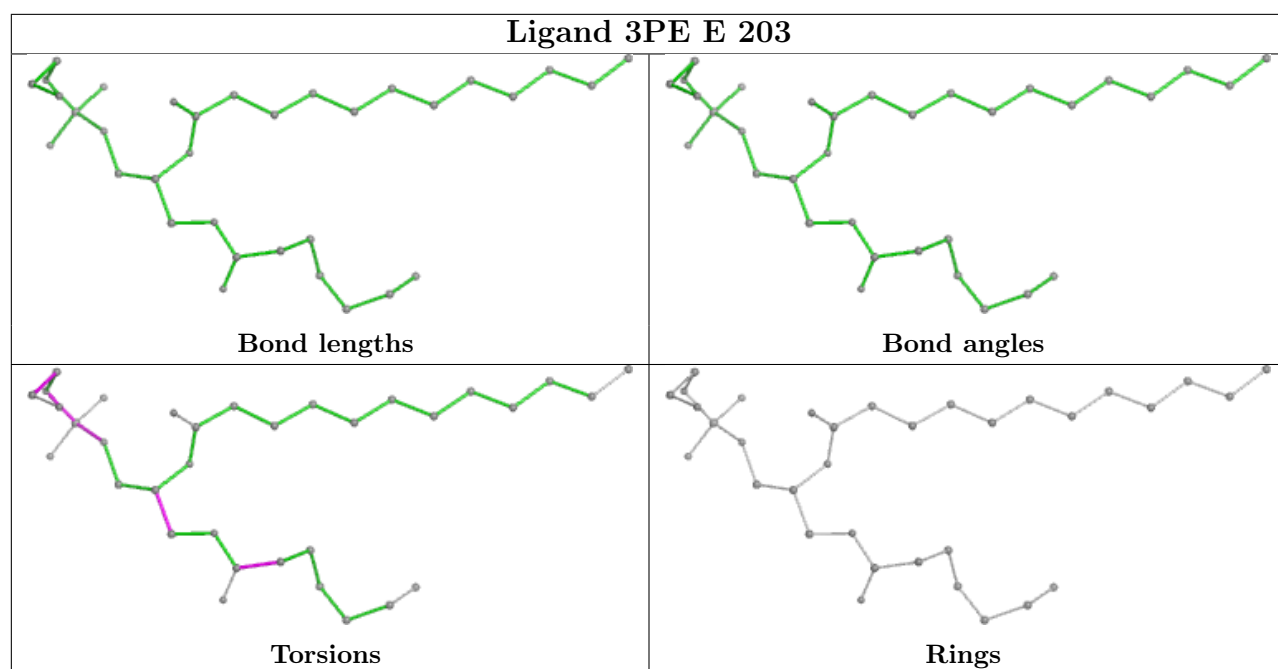


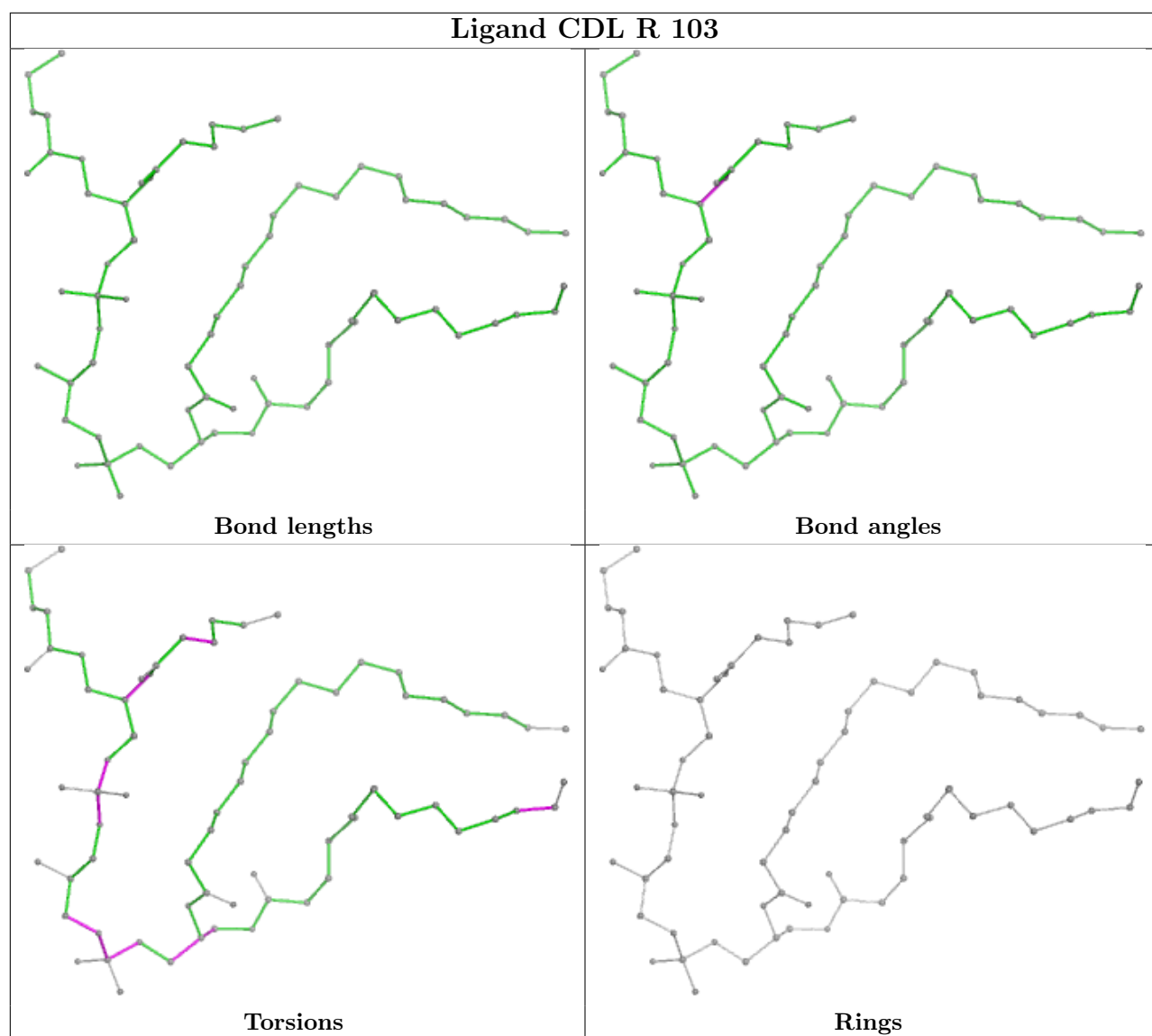
Ligand DGT O1 401

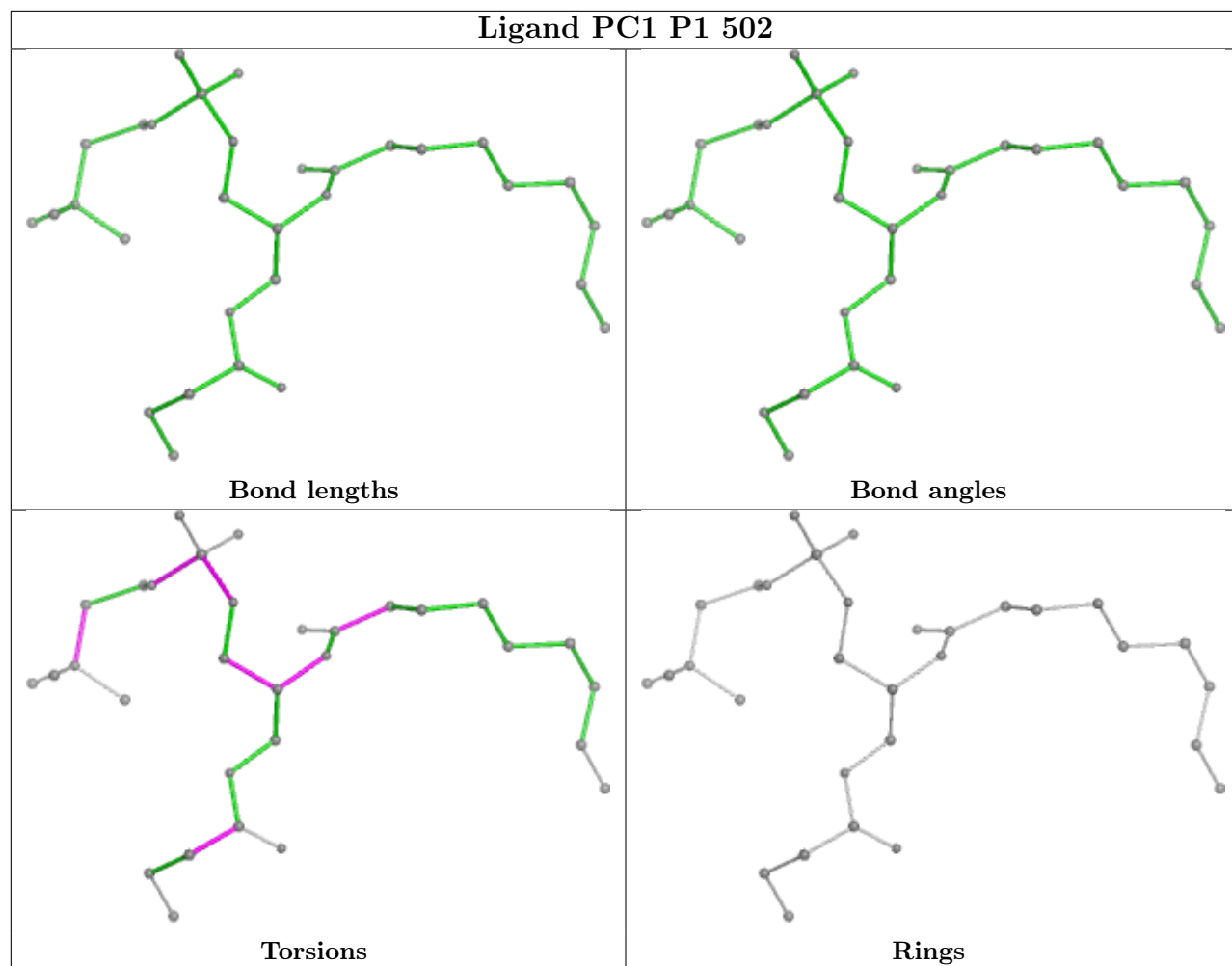


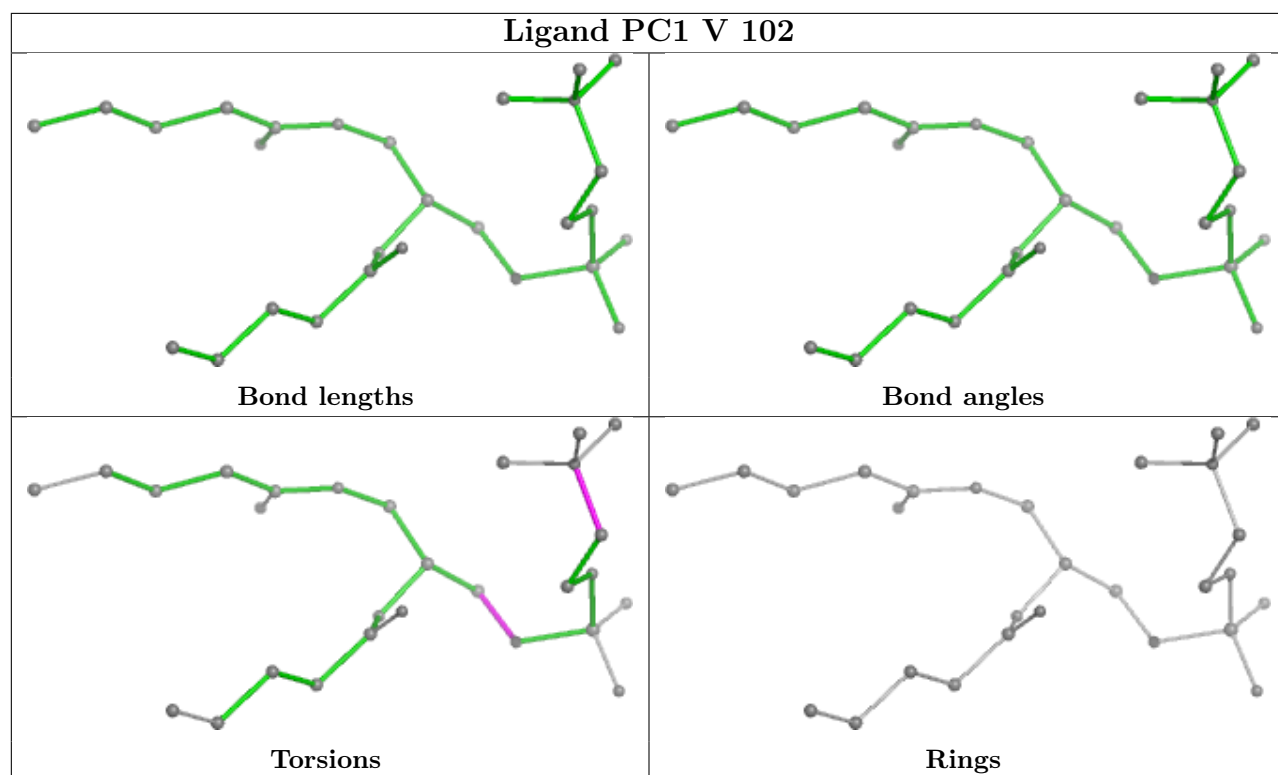
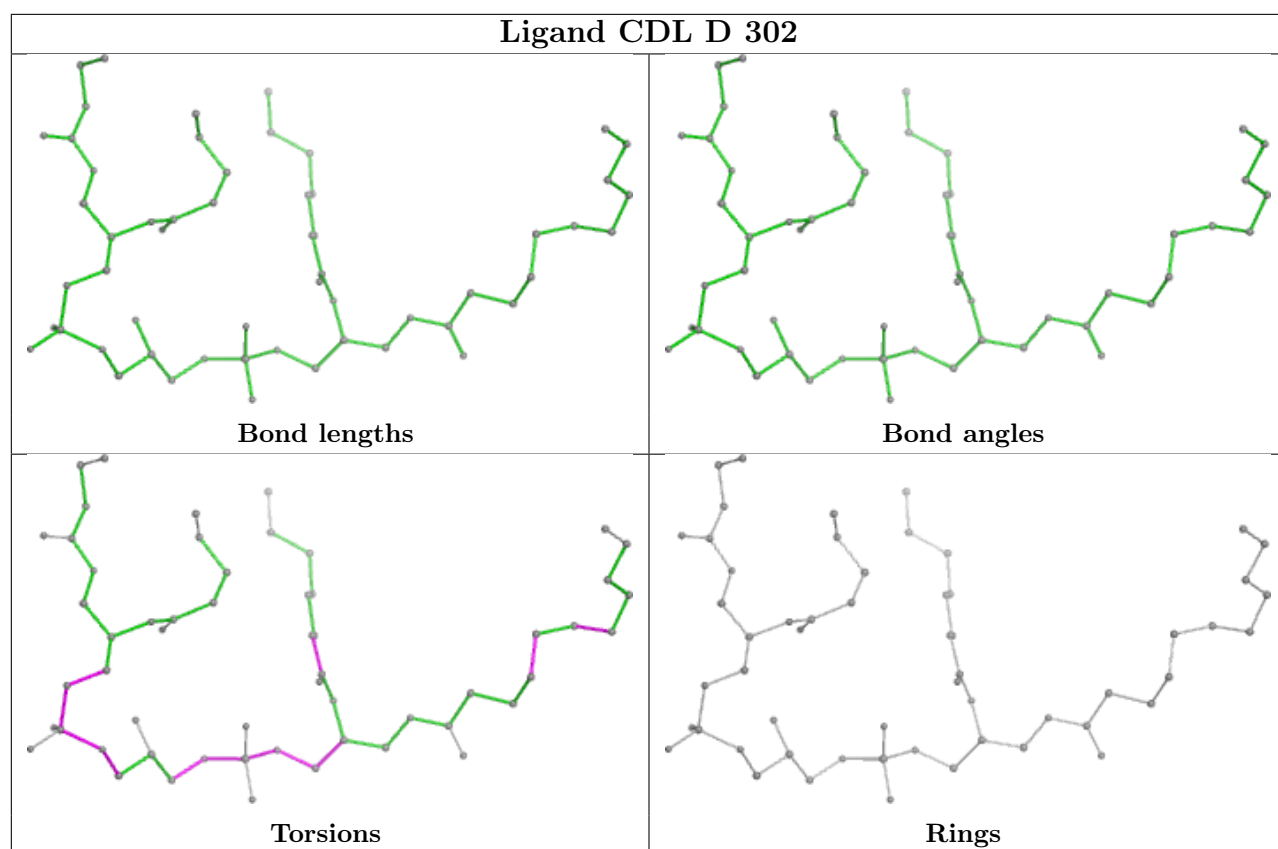
Ligand 3PE o 302

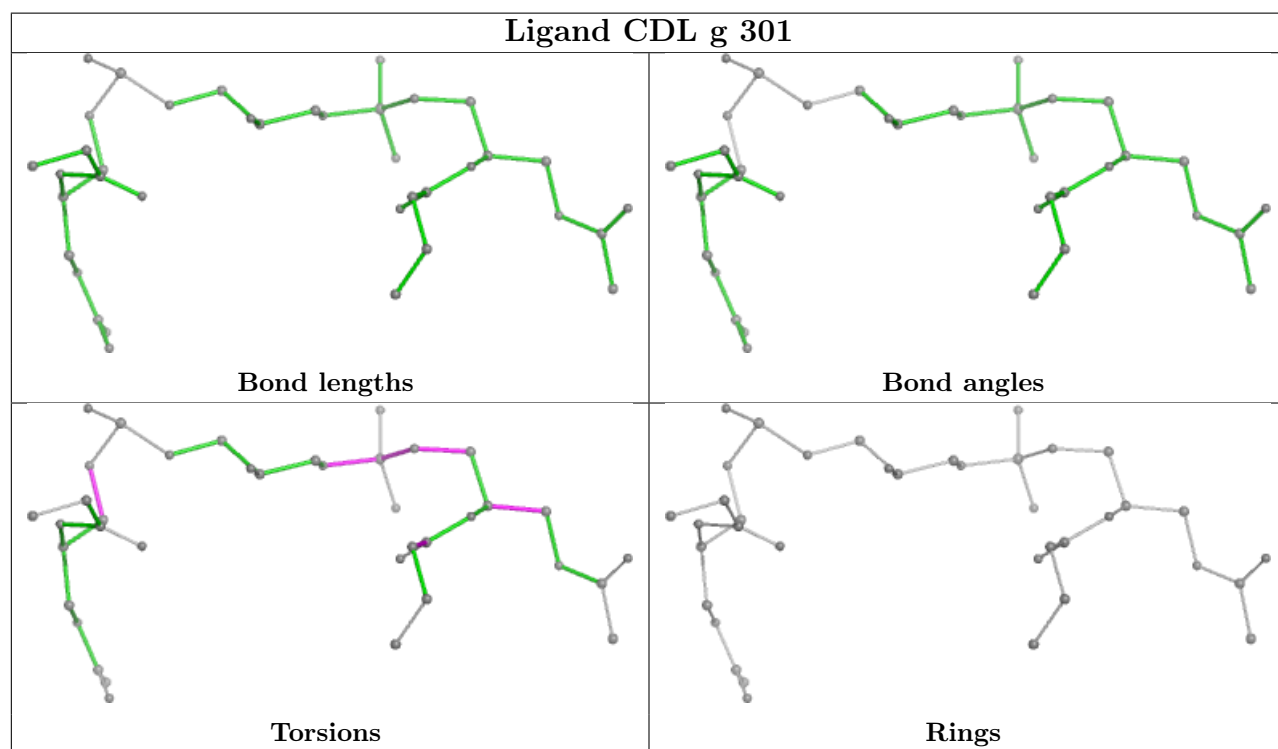
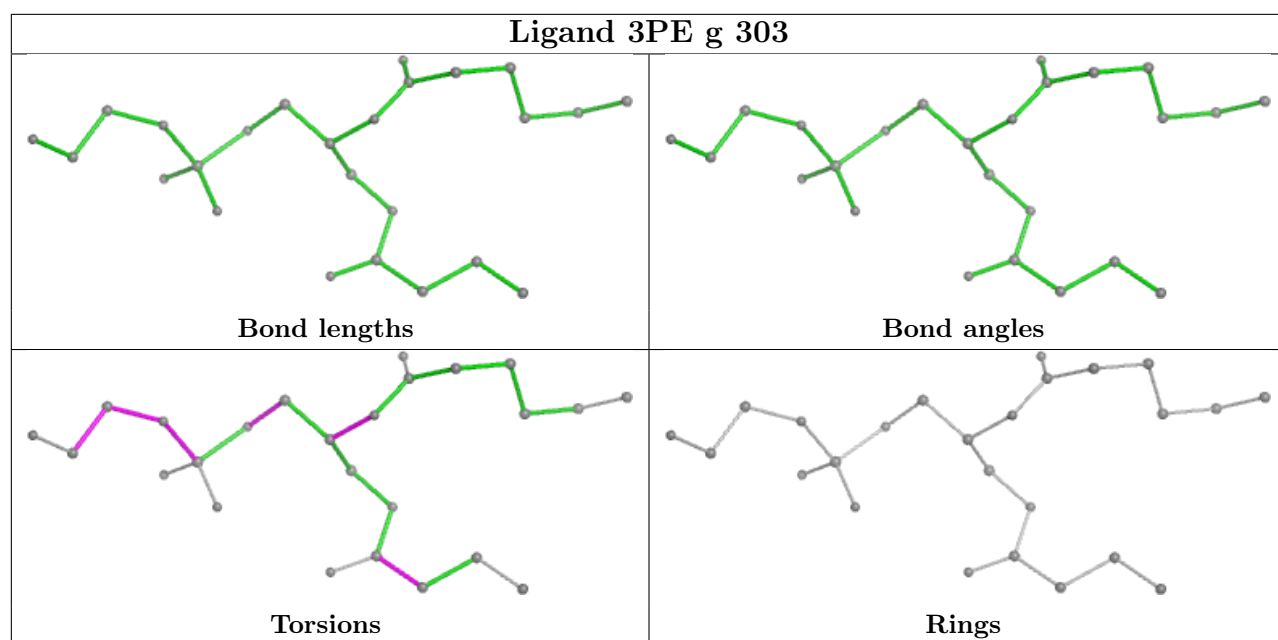


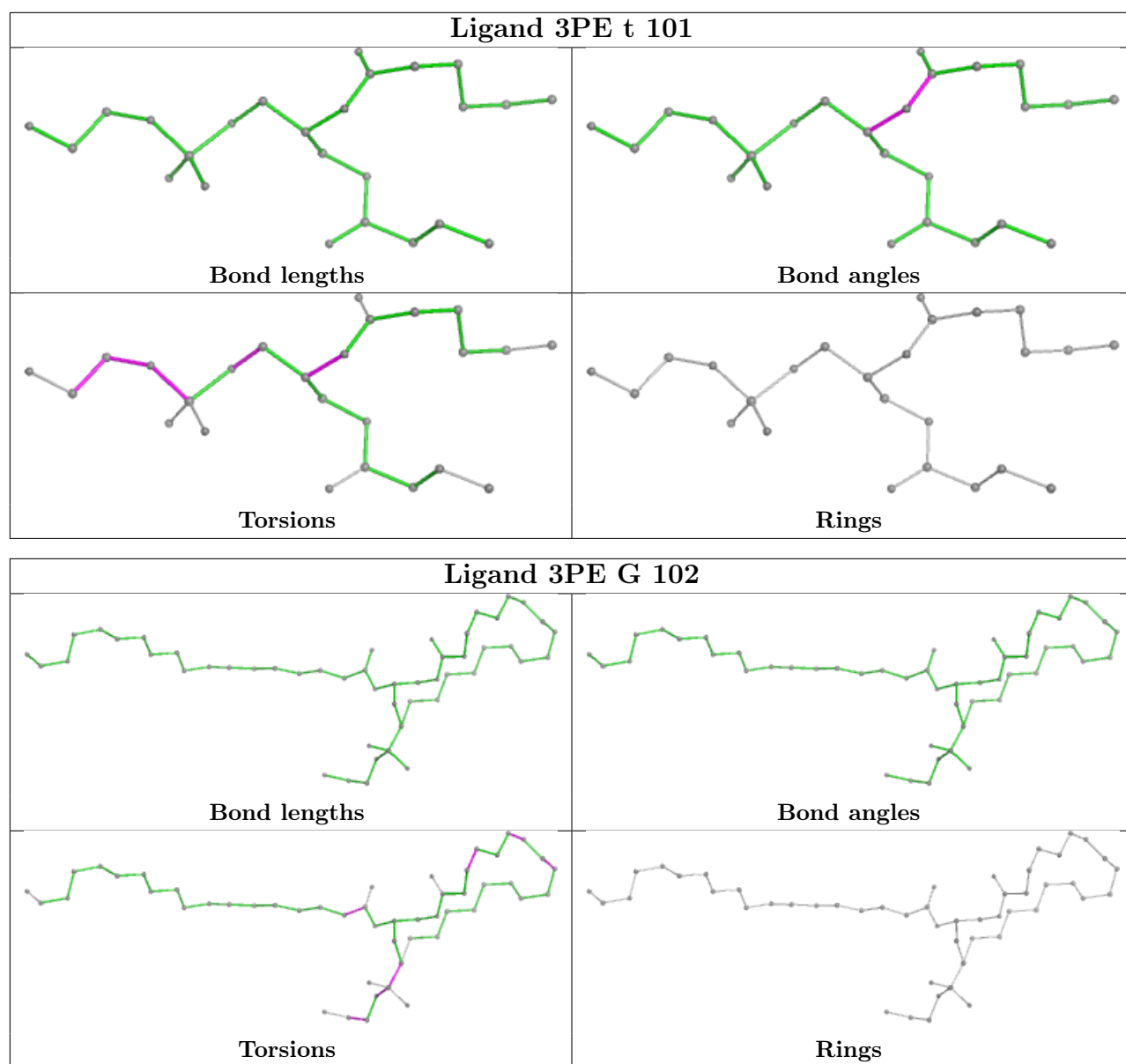


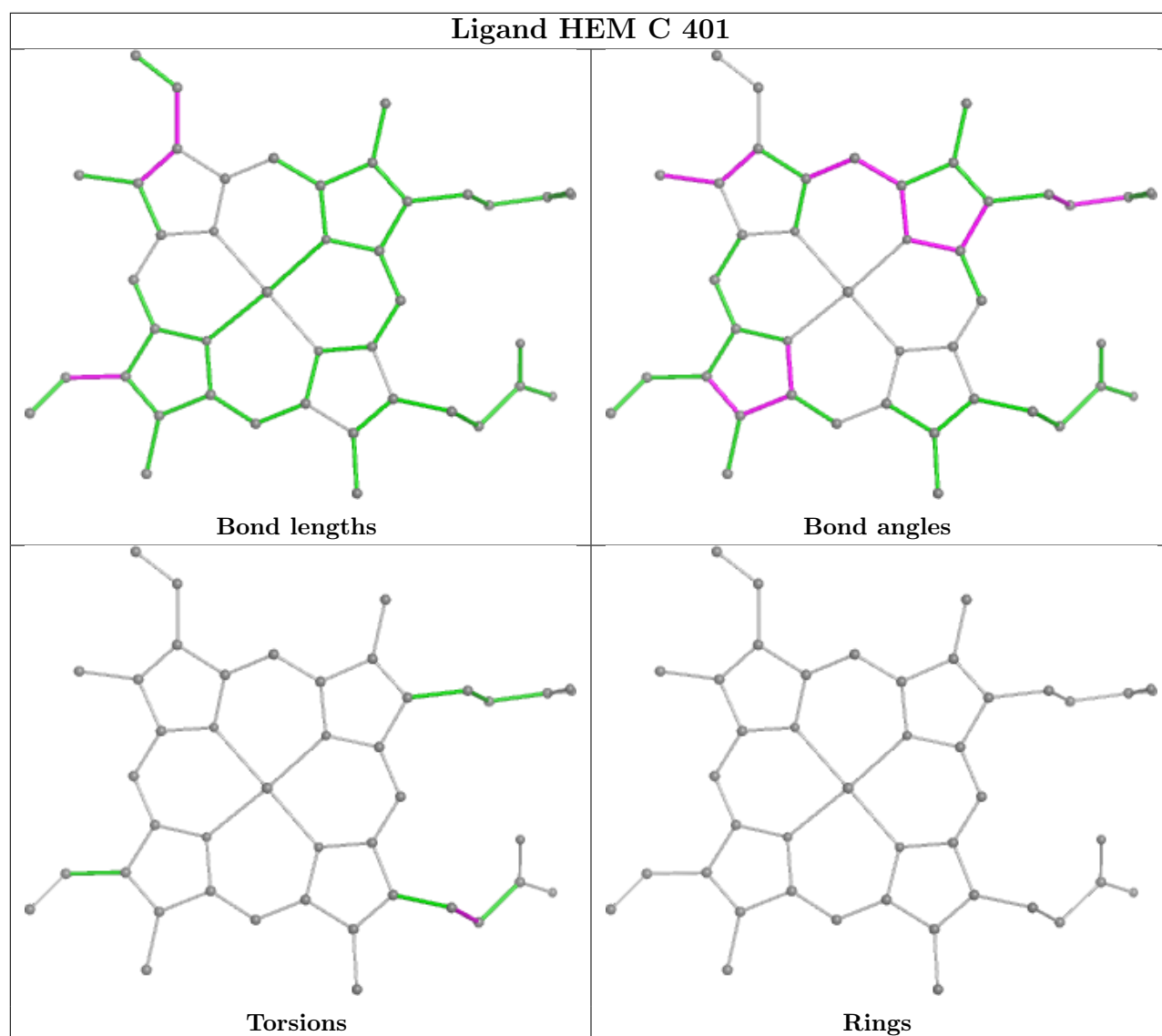












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

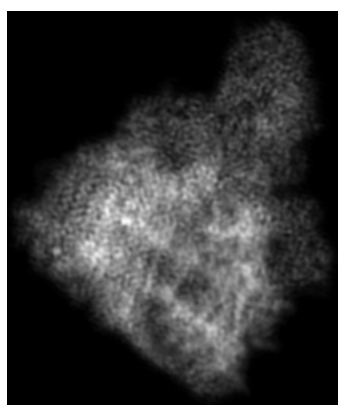
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17989. These allow visual inspection of the internal detail of the map and identification of artifacts.

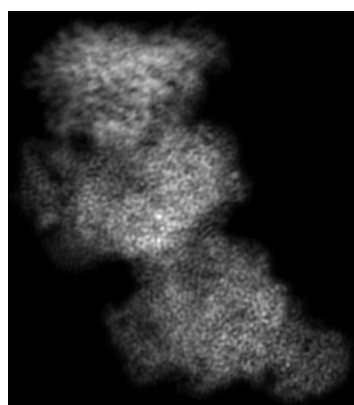
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

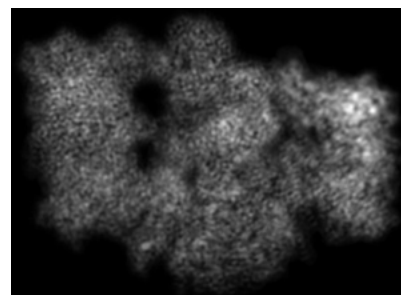
6.1.1 Primary map



X



Y



Z

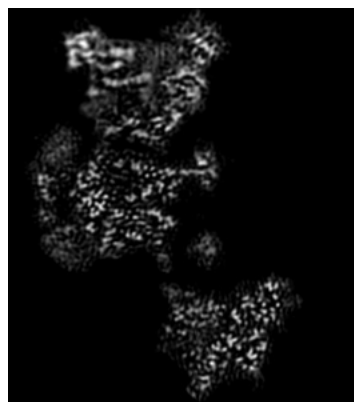
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

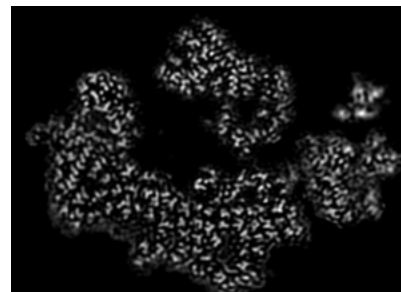
6.2.1 Primary map



X Index: 141



Y Index: 103

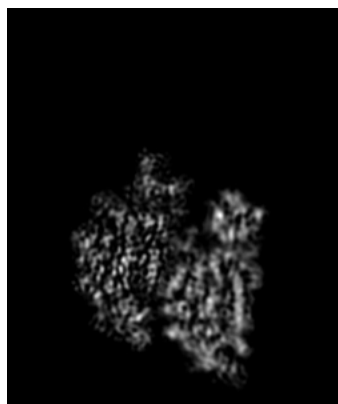


Z Index: 124

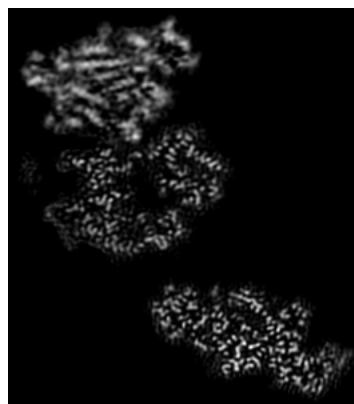
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

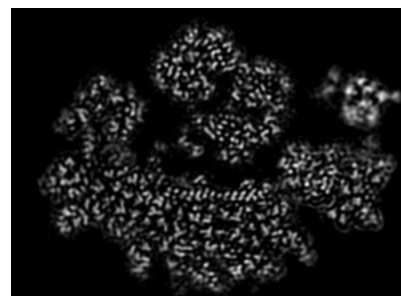
6.3.1 Primary map



X Index: 243



Y Index: 143

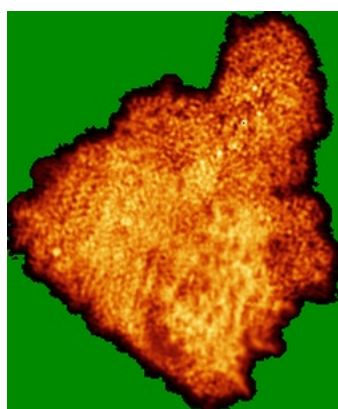


Z Index: 115

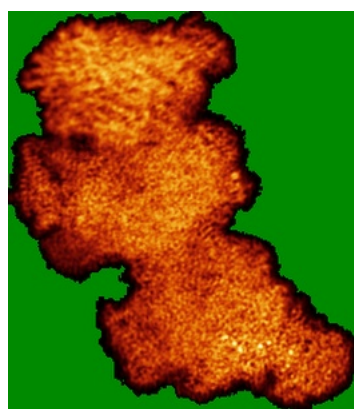
The images above show the largest variance slices of the map in three orthogonal directions.

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

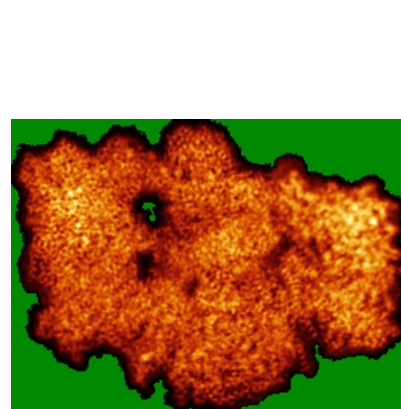
6.4.1 Primary map



X



Y

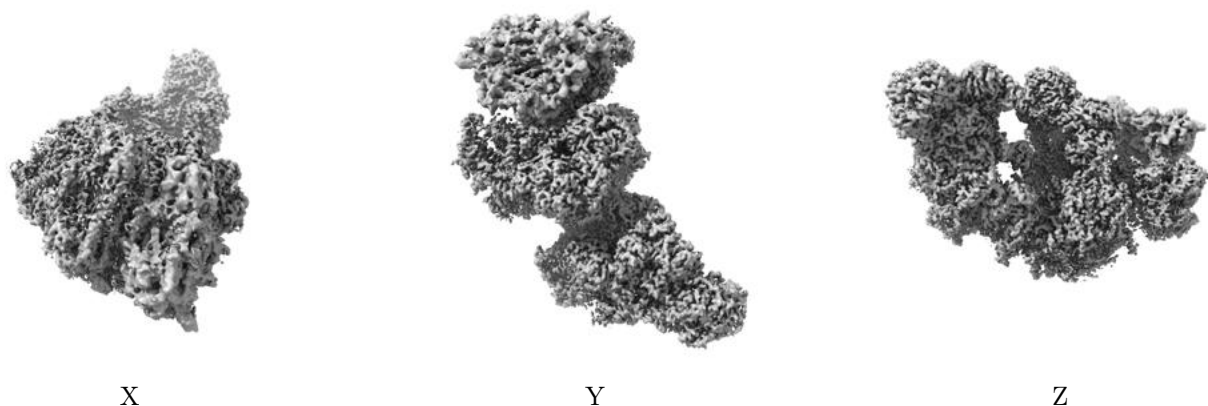


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

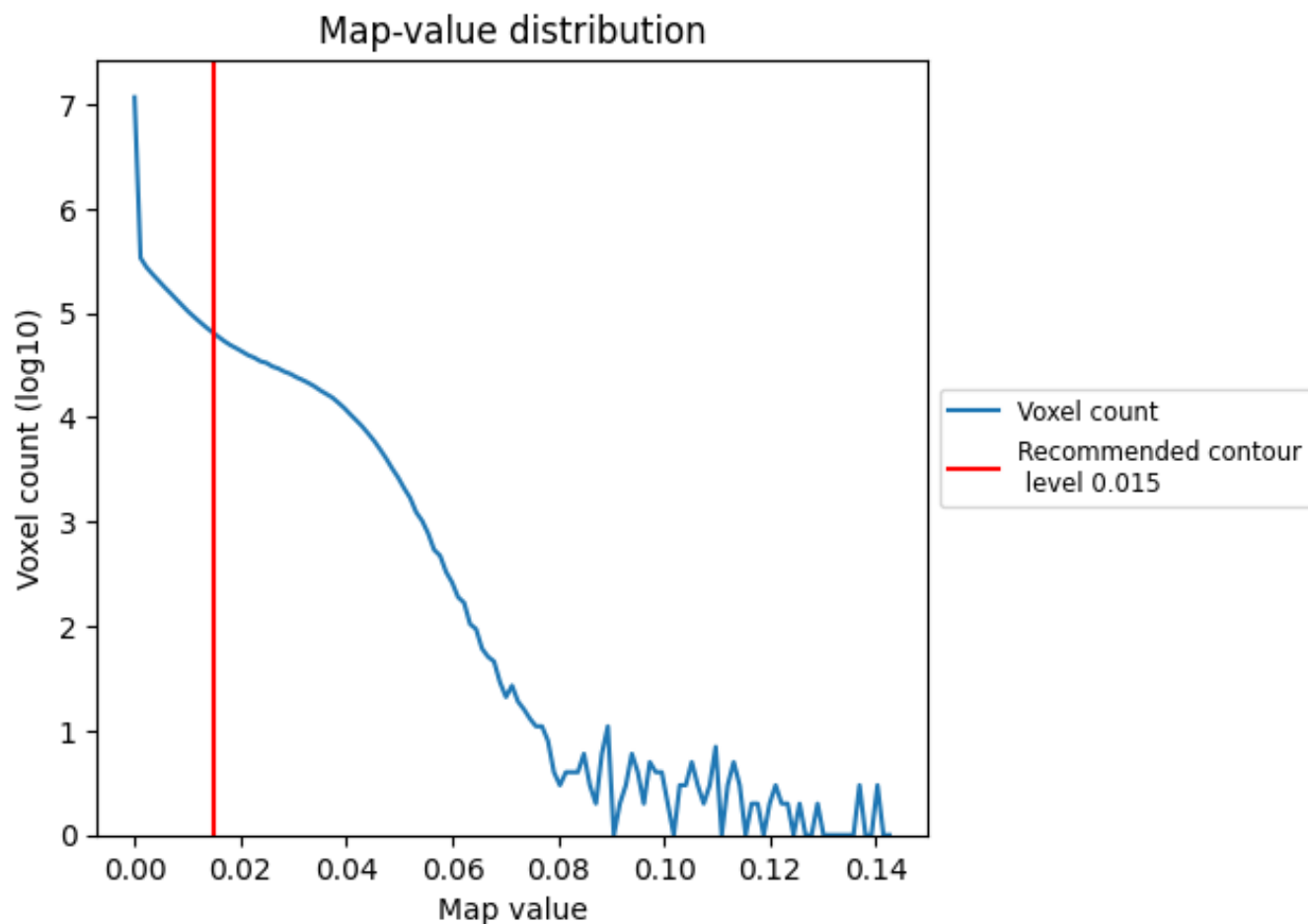
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

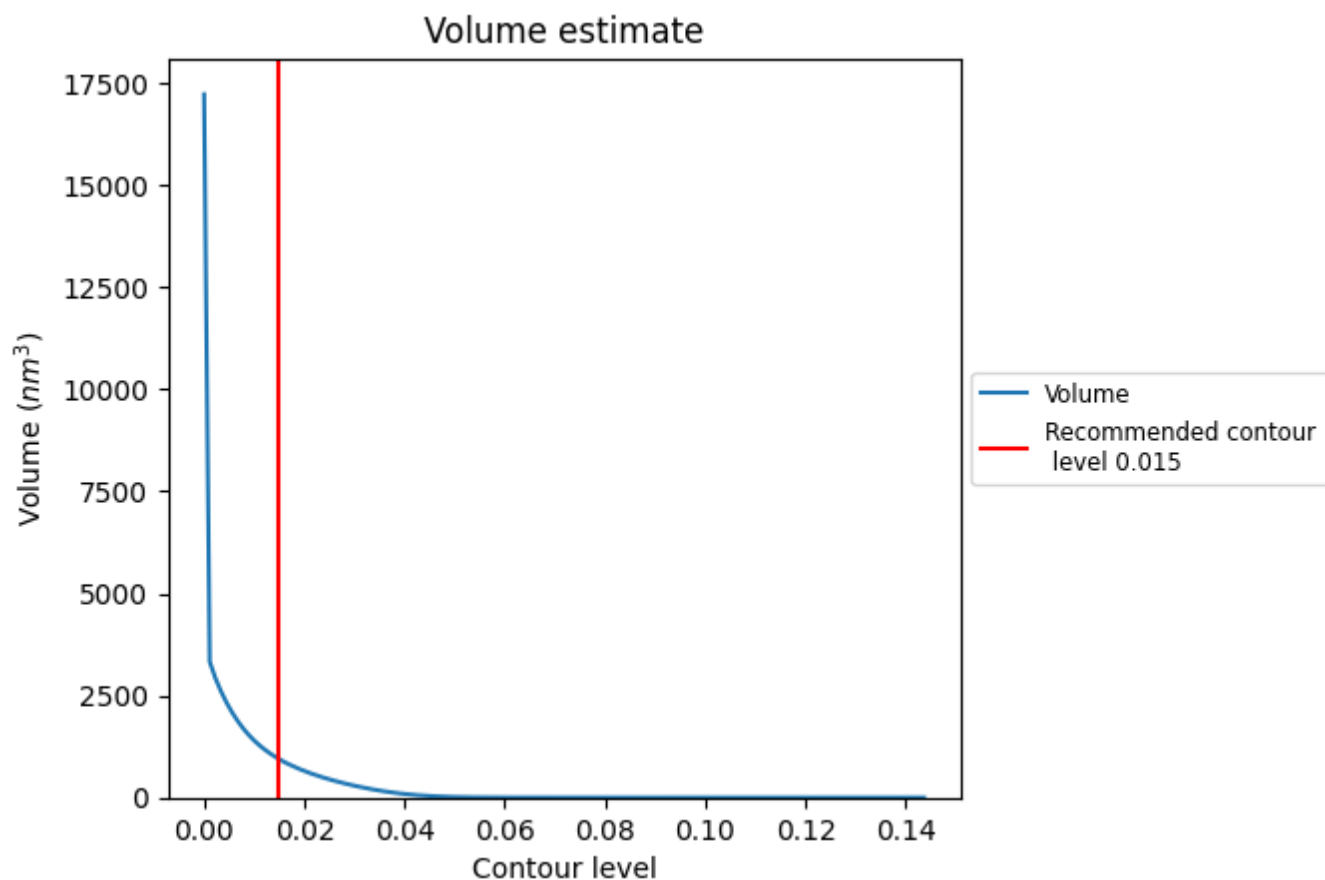
This section contains the results of statistical analysis of the map.

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 940 nm³; this corresponds to an approximate mass of 849 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.

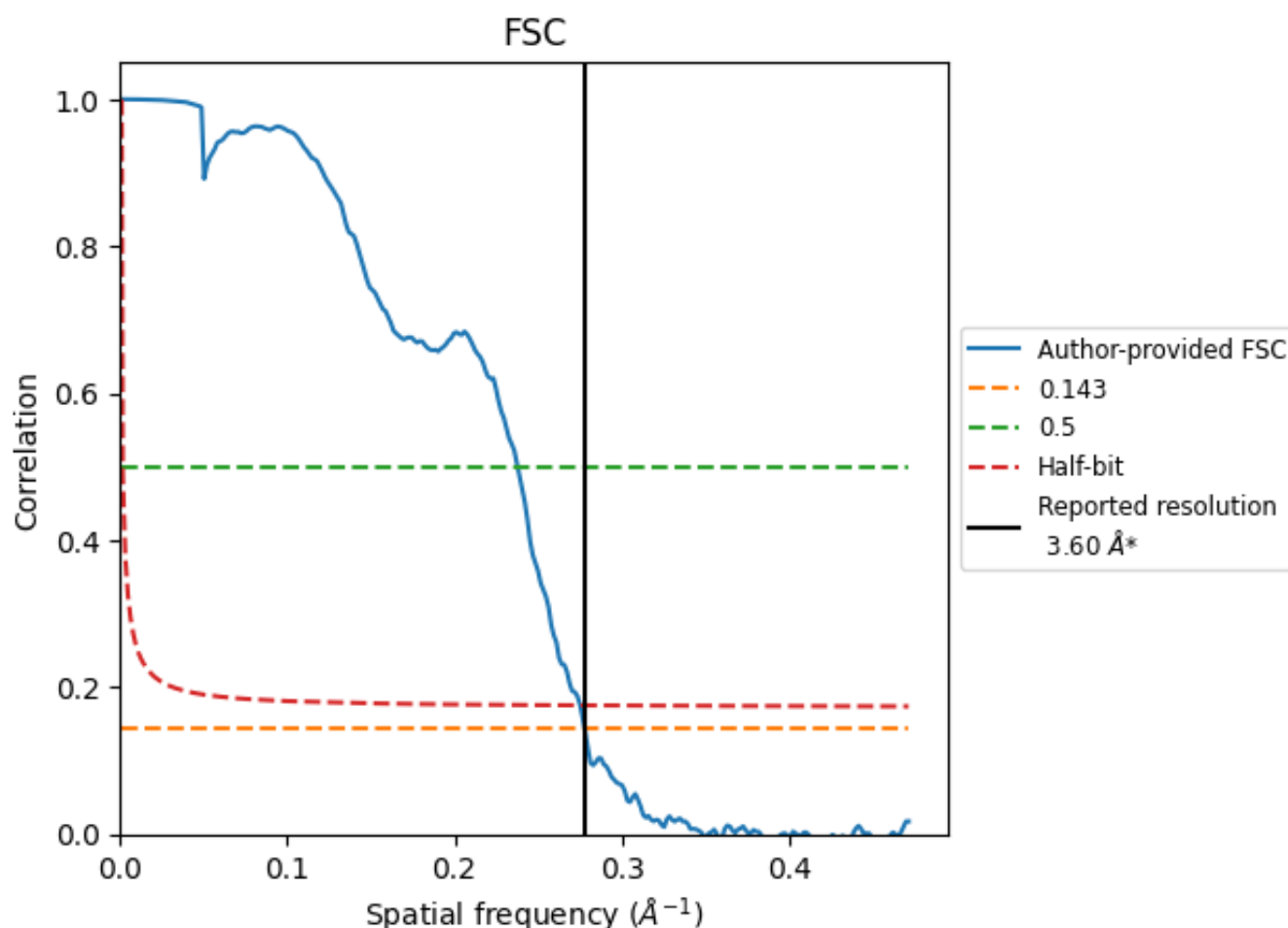
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

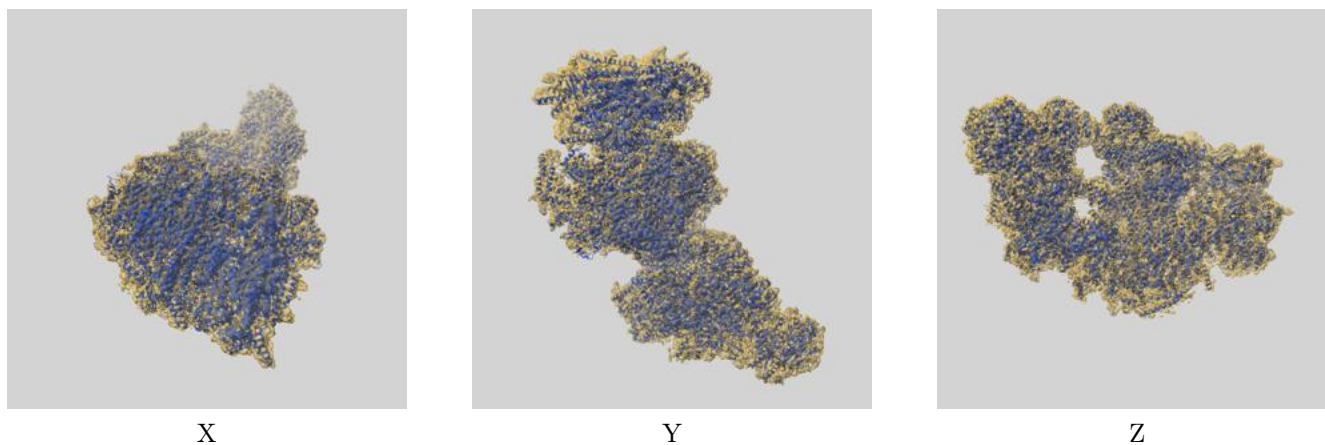
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.21	3.63
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

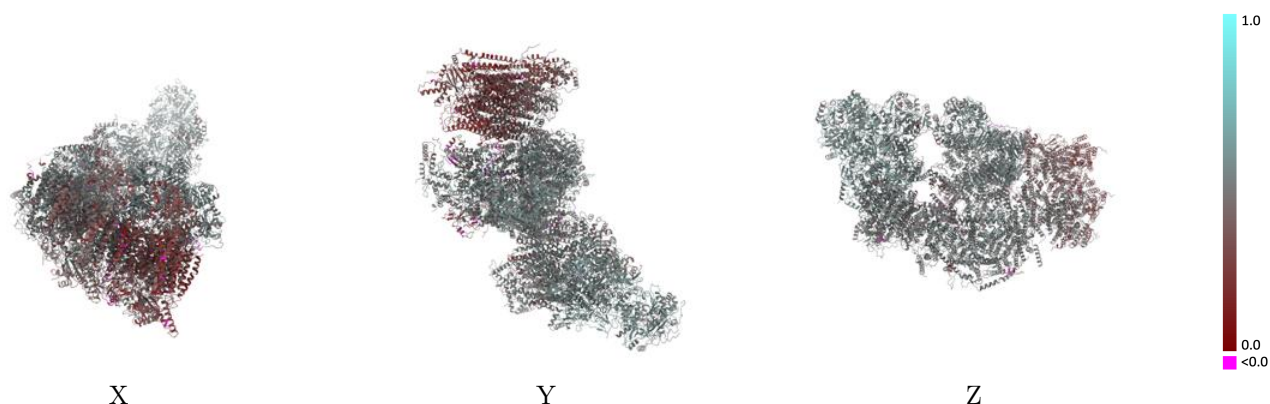
This section contains information regarding the fit between EMDB map EMD-17989 and PDB model 8PW5. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



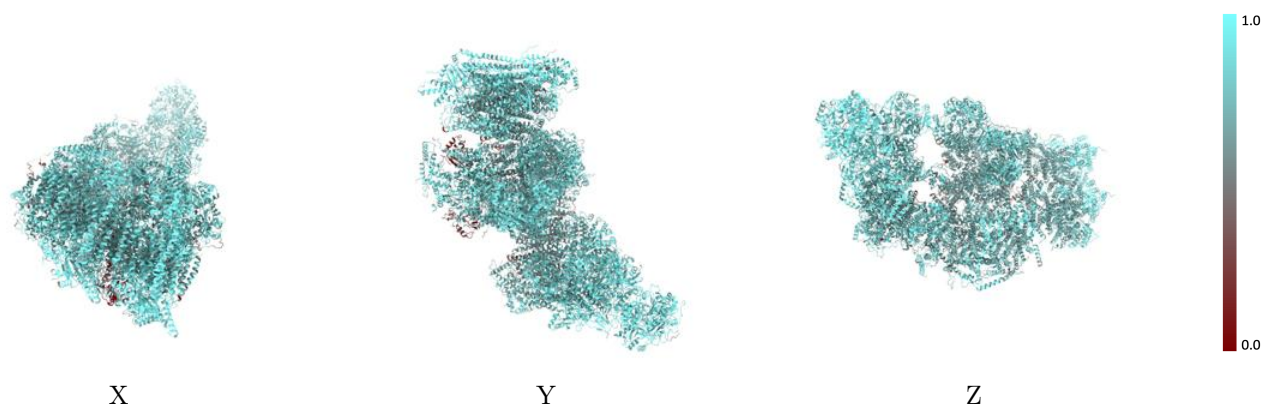
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



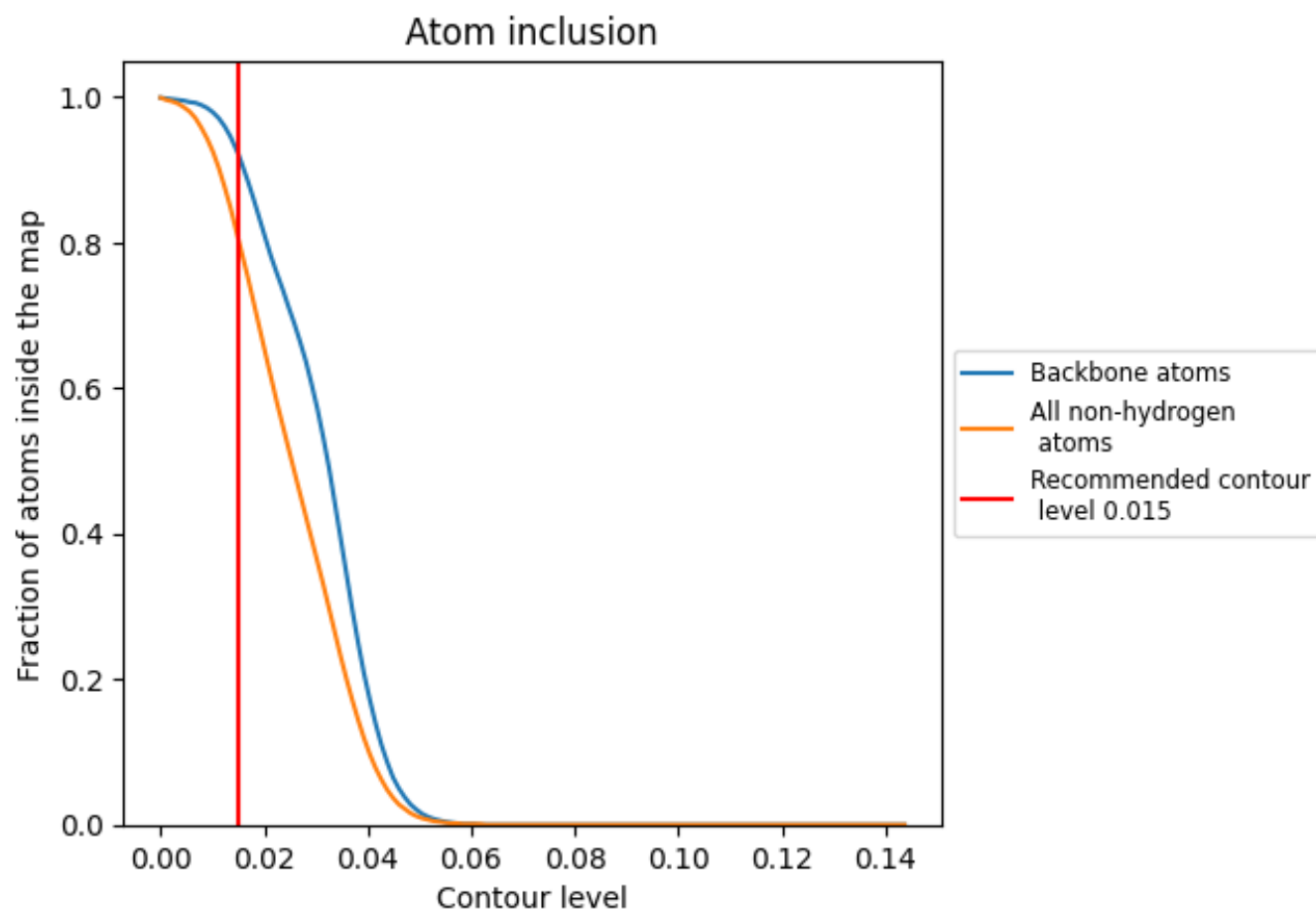
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.4640
1	 0.8980	 0.5360
2	 0.8890	 0.5310
3	 0.8580	 0.5280
6	 0.8540	 0.5200
7	 0.8730	 0.5440
9	 0.8630	 0.5330
A	 0.8270	 0.5110
A1	 0.7140	 0.4720
B	 0.8420	 0.5200
C	 0.7850	 0.4980
C1	 0.8800	 0.5470
D	 0.8520	 0.5090
D1	 0.8130	 0.5020
E	 0.5370	 0.3560
F	 0.8000	 0.5020
G	 0.7650	 0.4990
H	 0.7730	 0.4440
H1	 0.7390	 0.4660
I	 0.6610	 0.3060
J	 0.7720	 0.5000
J1	 0.6380	 0.4250
K	 0.6100	 0.4630
K1	 0.7170	 0.4750
L	 0.8180	 0.5060
L1	 0.7810	 0.4900
M	 0.8460	 0.5150
M1	 0.7950	 0.5010
N	 0.8000	 0.5010
N1	 0.7660	 0.4930
O	 0.8200	 0.5070
O1	 0.8260	 0.4900
P	 0.4970	 0.3440
P1	 0.7980	 0.5010
Q	 0.7900	 0.5140



































Continued on next page...

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Chain	Atom inclusion	Q-score
Q1	 0.8470	 0.5420
R	 0.6750	 0.4690
S	 0.7460	 0.4470
S1	 0.8470	 0.4820
T	 0.7060	 0.4930
T1	 0.7500	 0.4280
U	 0.7500	 0.5020
U1	 0.8090	 0.4890
V	 0.6460	 0.4590
V1	 0.8620	 0.5210
W1	 0.8470	 0.5290
X1	 0.8360	 0.4840
Y1	 0.6780	 0.4530
Z1	 0.8260	 0.4950
a	 0.8350	 0.3120
a1	 0.8170	 0.4920
b	 0.9150	 0.3000
b1	 0.7670	 0.4650
c	 0.8060	 0.2880
c1	 0.7670	 0.4680
d	 0.9240	 0.3070
d1	 0.7590	 0.4940
e	 0.9290	 0.3000
e1	 0.7840	 0.4850
f	 0.8860	 0.3030
f1	 0.7310	 0.4540
g	 0.7920	 0.2650
g1	 0.7600	 0.4690
h	 0.9070	 0.2810
h1	 0.8220	 0.4900
i	 0.8940	 0.2620
i1	 0.7470	 0.4570
j1	 0.7900	 0.4620
k	 0.9290	 0.2960
k1	 0.7960	 0.4800
l	 0.7370	 0.2750
l1	 0.8240	 0.5090
m	 0.7180	 0.2200
m1	 0.7540	 0.4750
n	 0.8060	 0.4290
n1	 0.8350	 0.5020
o	 0.8340	 0.4160

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Chain	Atom inclusion	Q-score
o1	 0.7940	 0.4630
p	 0.7830	 0.4190
p1	 0.8270	 0.4910
q	 0.8680	 0.4120
q1	 0.8950	 0.5450
r	 0.8580	 0.3740
r1	 0.8280	 0.5340
s	 0.8090	 0.4010
s1	 0.8040	 0.4860
t	 0.6790	 0.3260
u	 0.8840	 0.3990
v	 0.7940	 0.3500
w	 0.7670	 0.4310
x	 0.8420	 0.3890
y	 0.8030	 0.4430
z	 0.6440	 0.2910