



## wwPDB EM Validation Summary Report ⓘ

Sep 24, 2024 – 01:58 am BST

PDB ID : 8PW7  
EMDB ID : EMD-17991  
Title : A respirasome from murine liver  
Authors : Vercellino, I.; Sazanov, L.A.  
Deposited on : 2023-07-19  
Resolution : 3.50 Å(reported)  
Based on initial models : 7o3c, 6g2j

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

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

A user guide is available at

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

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

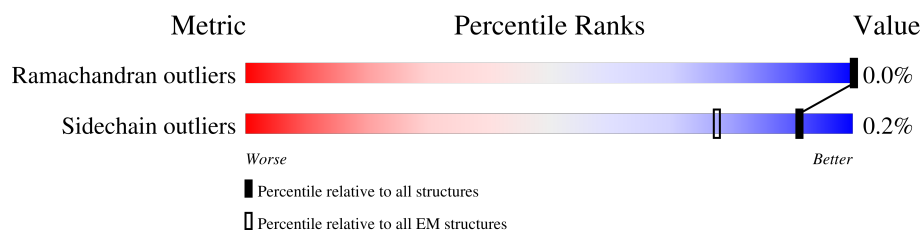
EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 3.50 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	n	514	99%
2	o	227	99%
3	p	261	99%
4	q	169	81% 18%
5	r	146	71% 29%
6	s	128	7% 73% 27%
7	t	111	5% 68% 32%
8	u	86	90% 8%
9	v	76	93% 7%





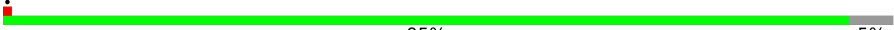








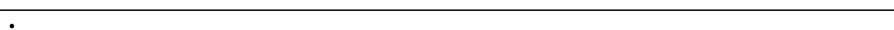

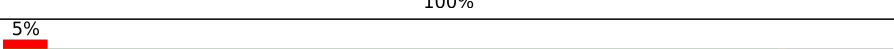

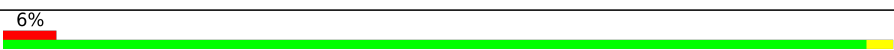




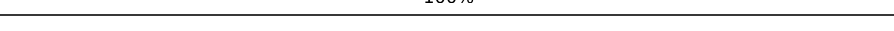
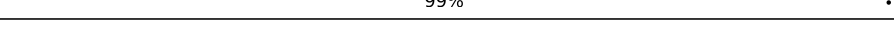
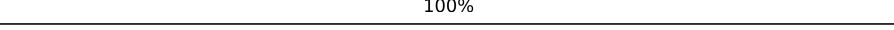
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Mol	Chain	Length	Quality of chain
10	x	80	
11	y	63	
12	w	83	
13	A	480	
13	L	480	
14	B	453	
14	M	453	
15	C	381	
15	N	381	
16	D	325	
16	O	325	
17	E	274	
17	P	274	
17	T	274	
18	F	111	
18	Q	111	
19	G	82	
19	R	82	
20	H	89	
20	S	89	
21	J	64	
21	U	64	
22	K	56	
22	V	56	
23	6	224	

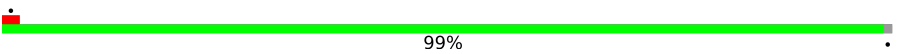
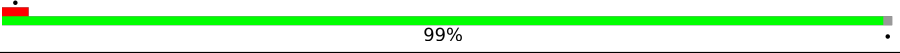
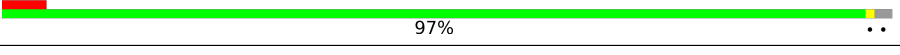
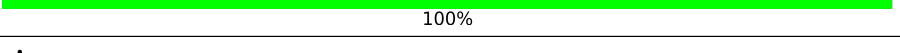
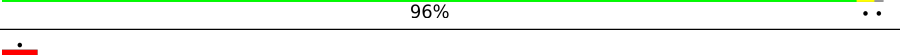
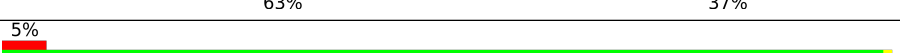
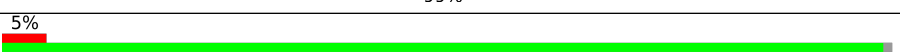
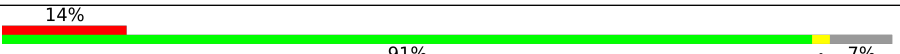


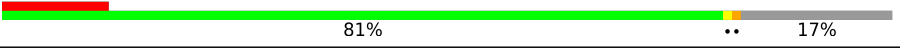



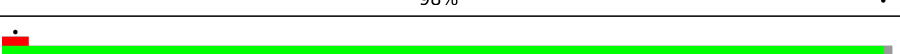
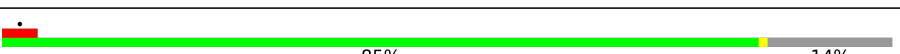
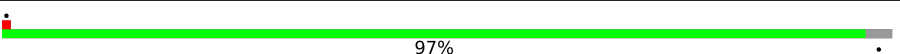



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Mol	Chain	Length	Quality of chain
24	C1	263	
25	D1	463	
26	2	248	
27	1	464	
28	3	727	
29	9	212	
30	P1	377	
31	Q1	175	
32	7	116	
33	S1	99	
34	T1	156	
34	U1	156	
35	V1	116	
36	W1	131	
37	q1	145	
38	r1	113	
39	s1	104	
40	A1	115	
41	H1	318	
42	J1	172	
43	K1	98	
44	L1	607	
45	M1	459	
46	N1	345	
47	O1	355	

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Mol	Chain	Length	Quality of chain
48	X1	172	 99%
49	Y1	141	 99%
50	Z1	144	 97%
51	a1	70	 100%
52	b1	84	 96%
53	c1	76	 63% 37%
54	d1	120	 99%
55	e1	106	 99%
56	f1	57	 91% 7%
57	g1	151	 67% 33%
58	h1	189	 74% 26%
59	i1	128	 81% 17%
60	j1	105	 62% 38%
61	k1	104	 73% 26%
62	l1	186	 84% 16%
63	m1	129	 98%
64	n1	179	 99%
65	o1	137	 85% 14%
66	p1	176	 97%
67	z	69	 59% 36%

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 115575 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 1.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	s	94	Total	C	N	O	S	0	0
			721	449	126	138	8		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

- Molecule 15 is a protein called Cytochrome b.

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

- Molecule 16 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 17 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
18	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

- Molecule 19 is a protein called Cytochrome b-c1 complex subunit 8.



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

- Molecule 20 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

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

- Molecule 21 is a protein called Cytochrome b-c1 complex subunit 9.

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

- Molecule 22 is a protein called Cytochrome b-c1 complex subunit 10.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 34 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

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

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

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 67 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

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

- Molecule 68 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

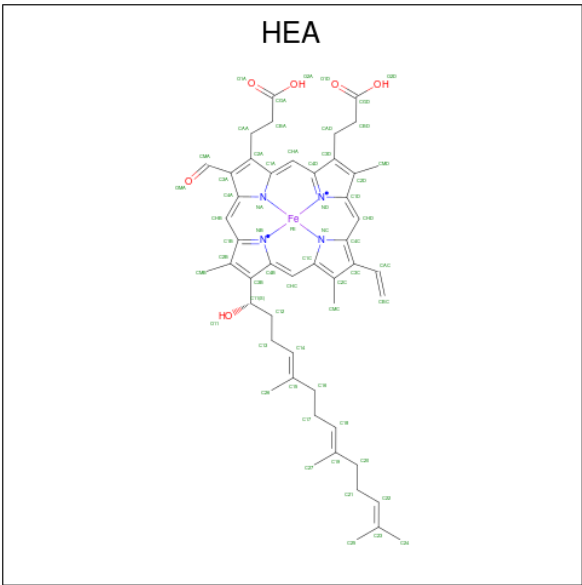
Mol	Chain	Residues	Atoms		AltConf
68	n	1	Total	Cu	0
			1	1	

- Molecule 69 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
69	n	1	Total	Na	0
			1	1	

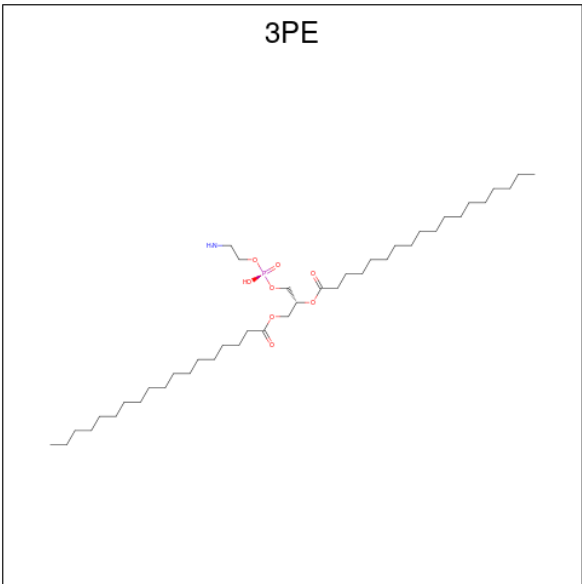
- Molecule 70 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).





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

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
71	n	1	Total	C	N	O	P	0
			34	24	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	n	1	Total 28	C 18	N 1	O 8	P 1	0
71	n	1	Total 27	C 17	N 1	O 8	P 1	0
71	o	1	Total 29	C 19	N 1	O 8	P 1	0
71	p	1	Total 45	C 35	N 1	O 8	P 1	0
71	t	1	Total 25	C 15	N 1	O 8	P 1	0
71	v	1	Total 28	C 18	N 1	O 8	P 1	0
71	A	1	Total 23	C 13	N 1	O 8	P 1	0
71	C	1	Total 35	C 25	N 1	O 8	P 1	0
71	C	1	Total 31	C 21	N 1	O 8	P 1	0
71	E	1	Total 32	C 22	N 1	O 8	P 1	0
71	G	1	Total 51	C 41	N 1	O 8	P 1	0
71	L	1	Total 23	C 13	N 1	O 8	P 1	0
71	N	1	Total 34	C 24	N 1	O 8	P 1	0
71	N	1	Total 37	C 27	N 1	O 8	P 1	0
71	O	1	Total 33	C 23	N 1	O 8	P 1	0
71	R	1	Total 30	C 20	N 1	O 8	P 1	0
71	6	1	Total 32	C 22	N 1	O 8	P 1	0
71	D1	1	Total 51	C 41	N 1	O 8	P 1	0
71	r1	1	Total 46	C 36	N 1	O 8	P 1	0
71	A1	1	Total 43	C 33	N 1	O 8	P 1	0
71	H1	1	Total 51	C 41	N 1	O 8	P 1	0

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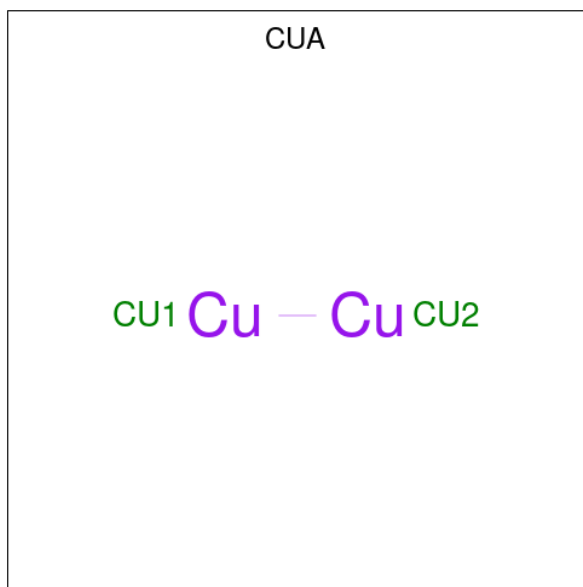
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Mol	Chain	Residues	Atoms					AltConf
71	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
71	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
72	o	1	Total	Mg	0
			1	1	
72	O1	1	Total	Mg	0
			1	1	

- Molecule 73 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).

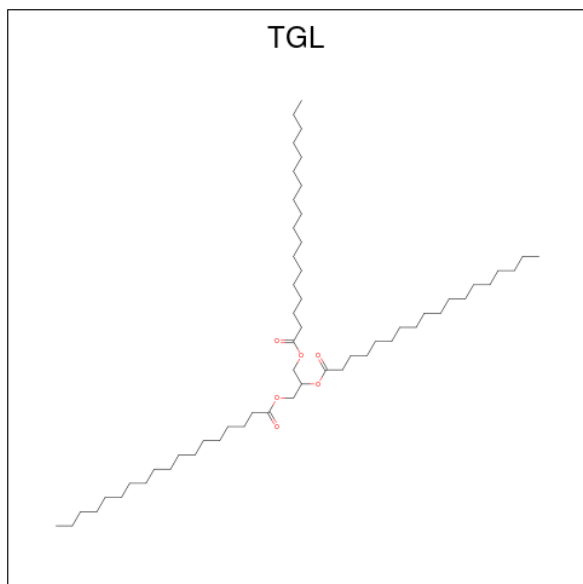


Mol	Chain	Residues	Atoms		AltConf
73	o	1	Total	Cu	0
			2	2	

- Molecule 74 is ZINC ION (three-letter code: ZN) (formula: Zn).

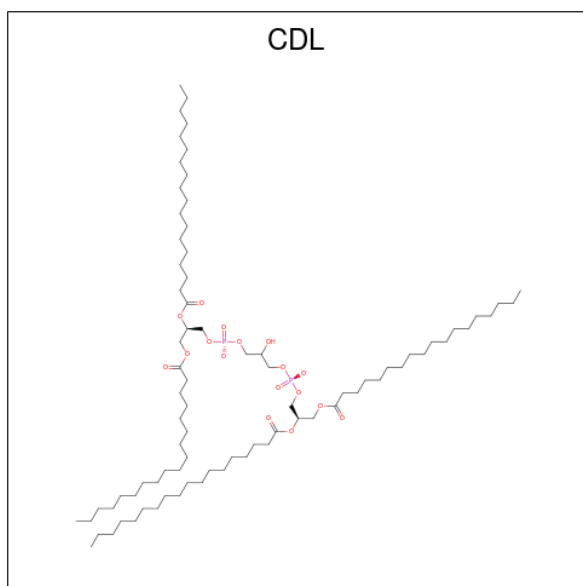
Mol	Chain	Residues	Atoms		AltConf
74	s	1	Total	Zn	0
			1	1	
74	7	1	Total	Zn	0
			1	1	

- Molecule 75 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



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

- Molecule 76 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



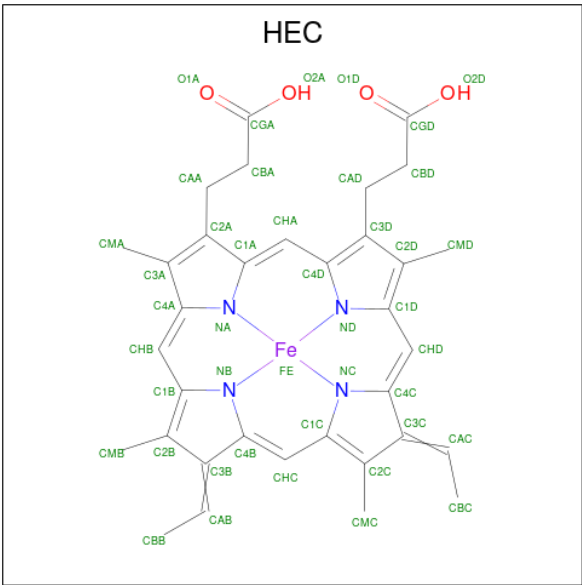
Mol	Chain	Residues	Atoms				AltConf
76	A	1	Total	C	O	P	0
			46	27	17	2	
76	C	1	Total	C	O	P	0
			42	23	17	2	
76	G	1	Total	C	O	P	0
			56	37	17	2	
76	N	1	Total	C	O	P	0
			46	27	17	2	
76	O	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			41	22	17	2	
76	R	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			72	53	17	2	
76	H1	1	Total	C	O	P	0
			51	33	16	2	
76	L1	1	Total	C	O	P	0
			78	59	17	2	
76	L1	1	Total	C	O	P	0
			46	27	17	2	

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Mol	Chain	Residues	Atoms				AltConf
76	N1	1	Total 90	C 71	O 17	P 2	0
76	Y1	1	Total 94	C 75	O 17	P 2	0
76	a1	1	Total 57	C 38	O 17	P 2	0
76	d1	1	Total 67	C 48	O 17	P 2	0
76	h1	1	Total 70	C 51	O 17	P 2	0

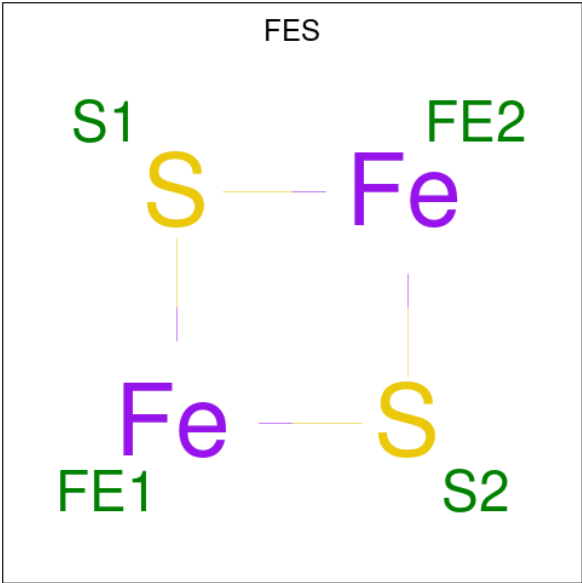
- # HEM

- Molecule 78 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
78	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
78	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 79 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



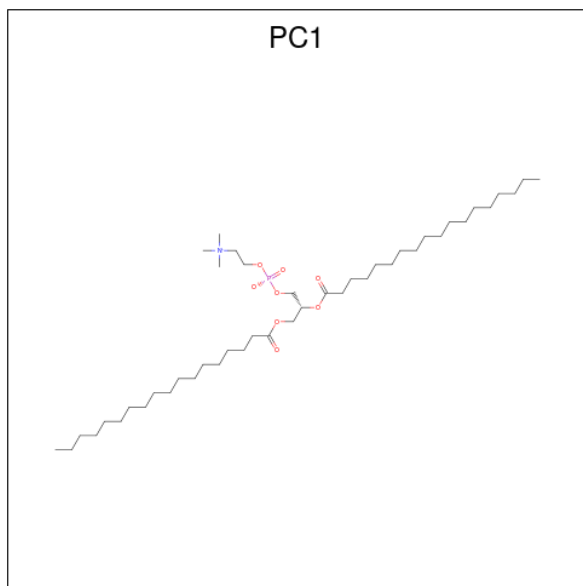
Mol	Chain	Residues	Atoms			AltConf
79	E	1	Total	Fe	S	0
			4	2	2	
79	P	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
79	2	1	Total	Fe	S	0
			4	2	2	
79	3	1	Total	Fe	S	0
			4	2	2	

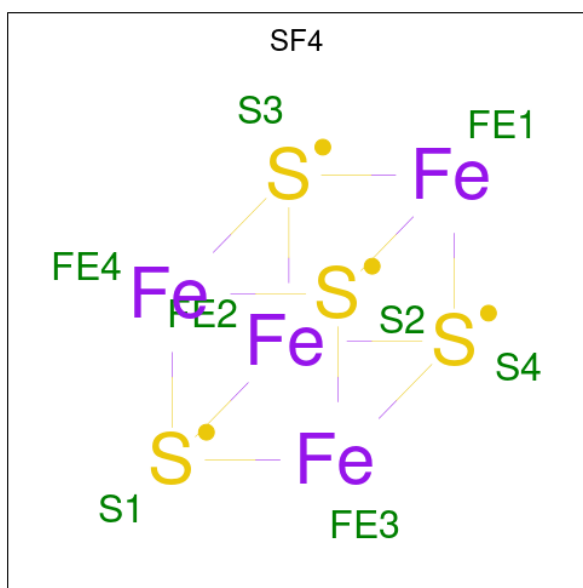
- Molecule 80 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
80	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
80	K	1	Total	C	N	O	P	0
			28	18	1	8	1	
80	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
80	V	1	Total	C	N	O	P	0
			28	18	1	8	1	
80	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
80	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
80	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
80	P1	1	Total	C	N	O	P	0
			31	21	1	8	1	
80	Y1	1	Total	C	N	O	P	0
			54	44	1	8	1	

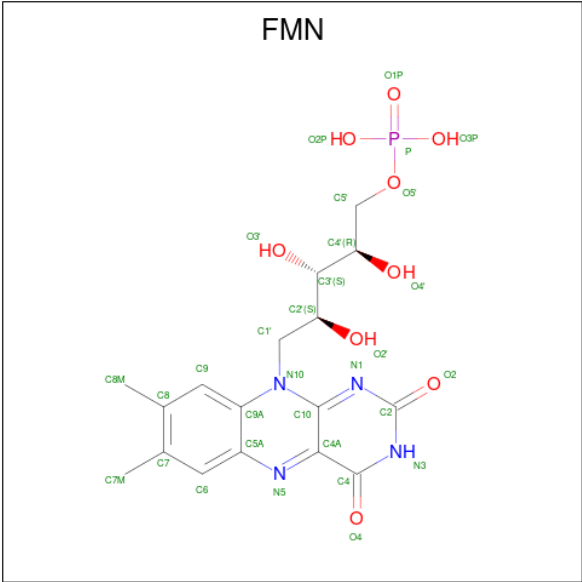


- Molecule 81 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



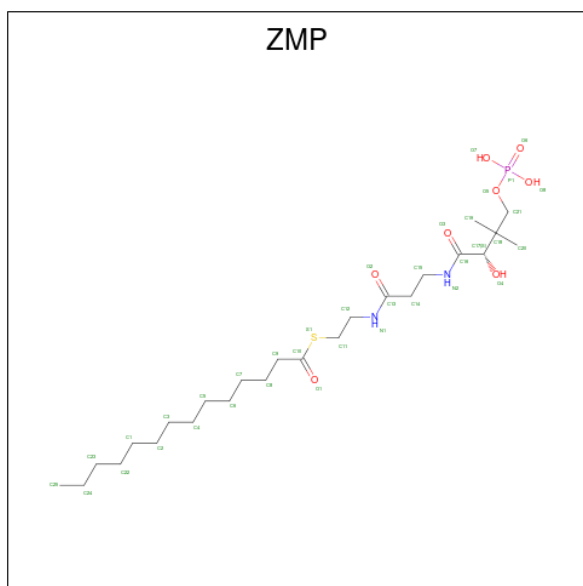
Mol	Chain	Residues	Atoms			AltConf
81	6	1	Total	Fe	S	0
			8	4	4	
81	1	1	Total	Fe	S	0
			8	4	4	
81	3	1	Total	Fe	S	0
			8	4	4	
81	3	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 82 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



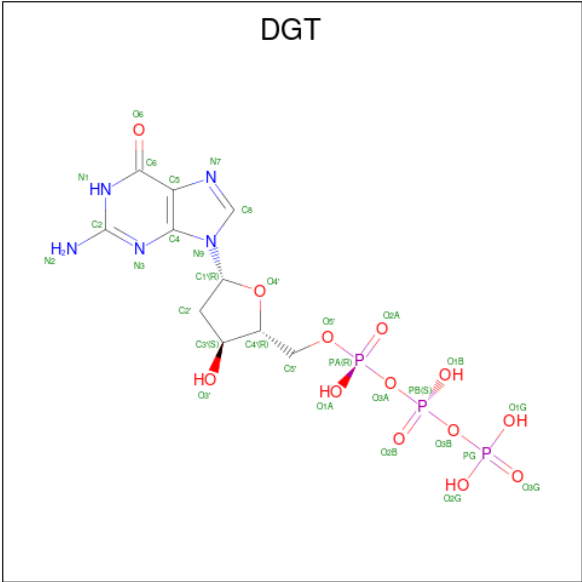
Mol	Chain	Residues	Atoms					AltConf
84	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 85 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



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

- Molecule 86 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

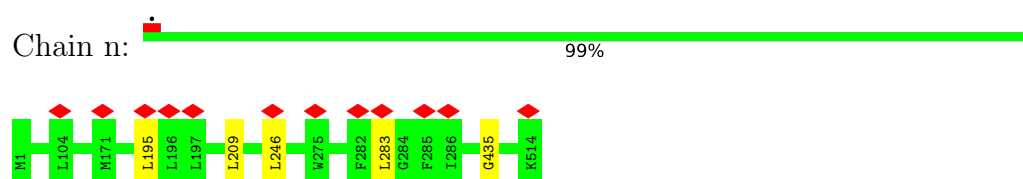


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	O1	1	31	10	5	13	3	0

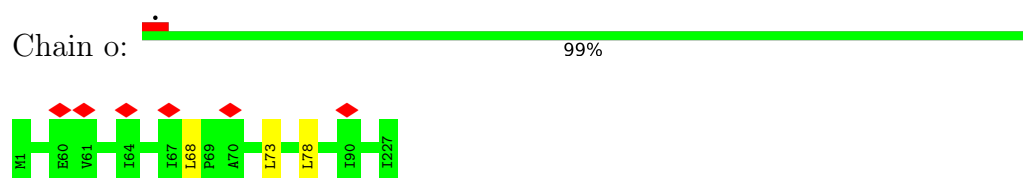
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

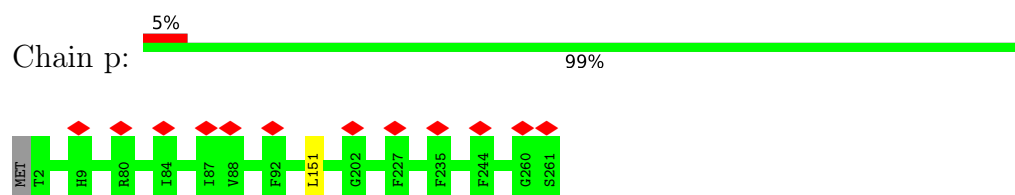
- Molecule 1: Cytochrome c oxidase subunit 1



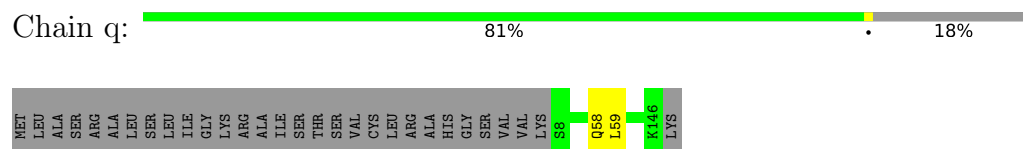
- Molecule 2: Cytochrome c oxidase subunit 2



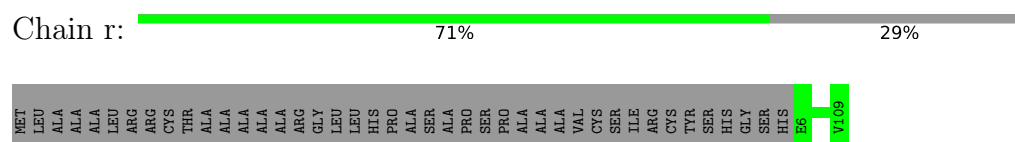
- Molecule 3: Cytochrome c oxidase subunit 3



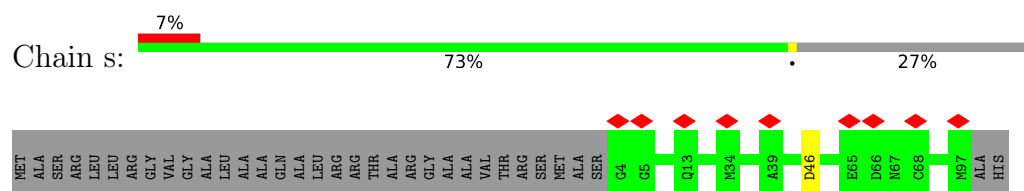
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



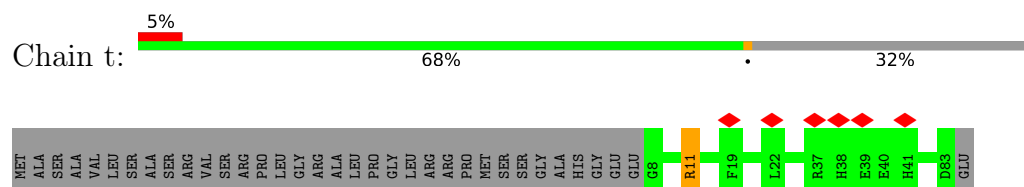
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



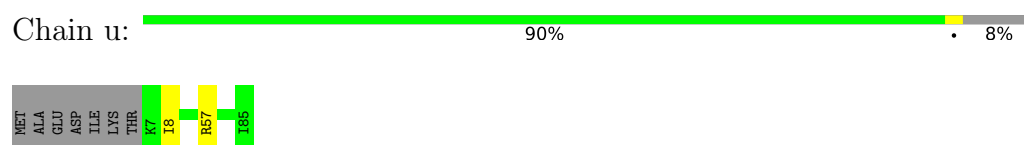
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



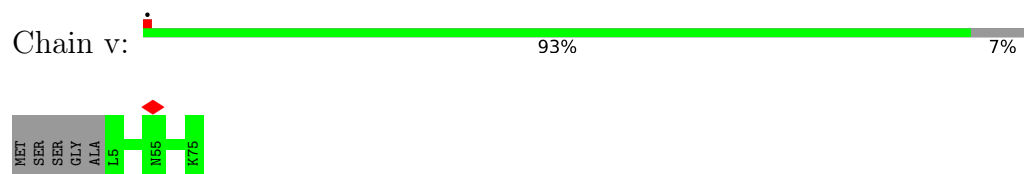
- Molecule 7: Cytochrome c oxidase subunit 6A1, mitochondrial



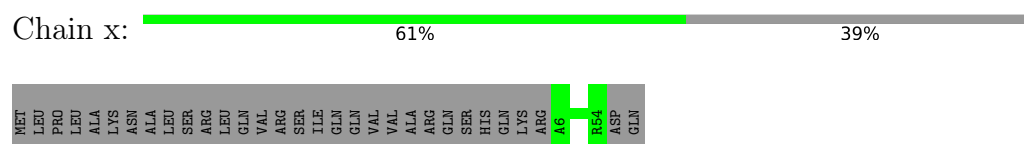
- Molecule 8: Cytochrome c oxidase subunit 6B1



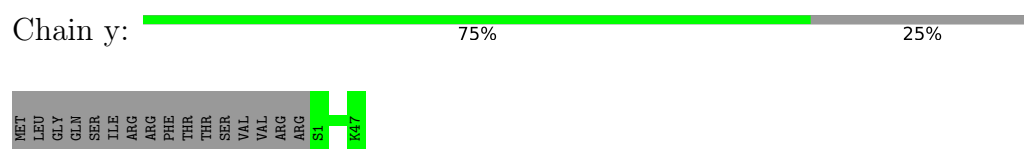
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase subunit 7B, mitochondrial

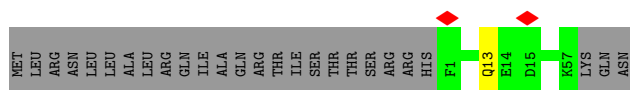


- Molecule 11: Cytochrome c oxidase subunit 7C, mitochondrial



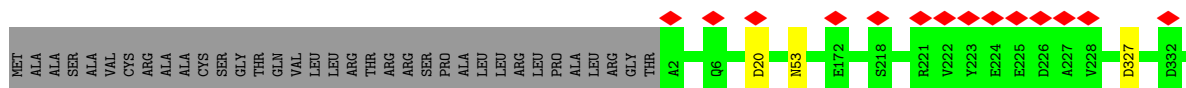
- Molecule 12: Cytochrome c oxidase subunit 7A2, mitochondrial





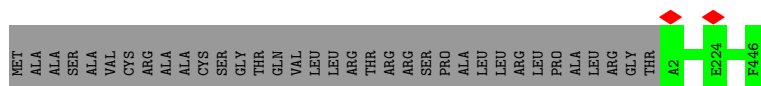
- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A: 92% 7%



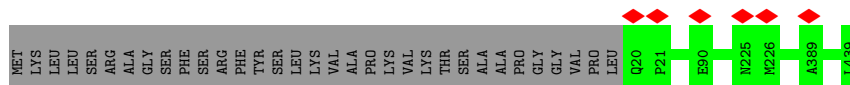
- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L: 93% 7%



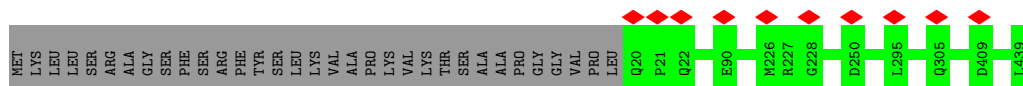
- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 93% 7%



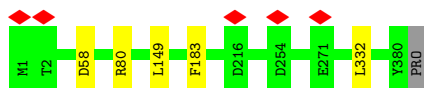
- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 93% 7%



- Molecule 15: Cytochrome b

Chain C: 98% 0%

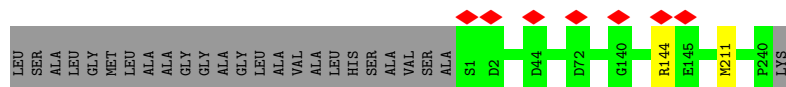
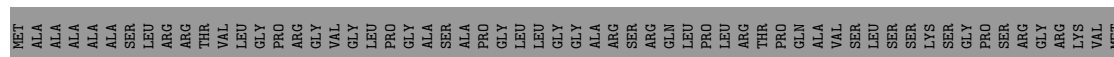


- Molecule 15: Cytochrome b

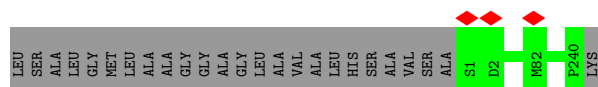
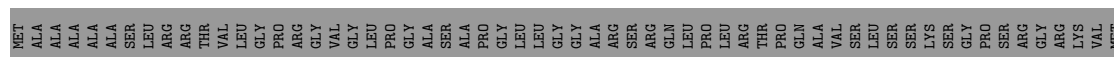
Chain N: 98% 0%



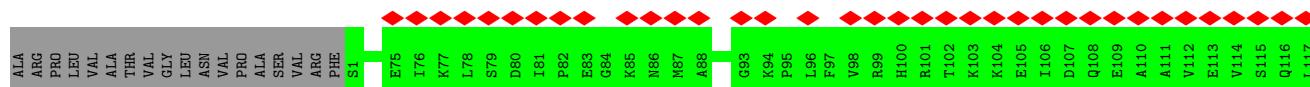
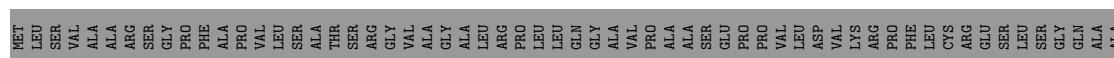
- Molecule 16: Cytochrome c1, heme protein, mitochondrial



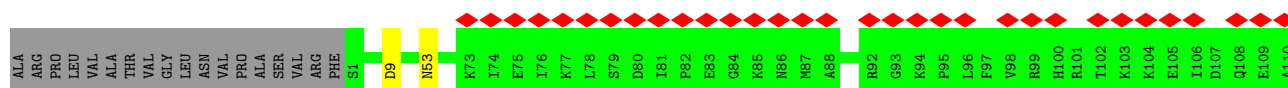
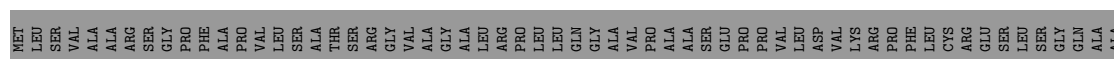
- Molecule 16: Cytochrome c1, heme protein, mitochondrial



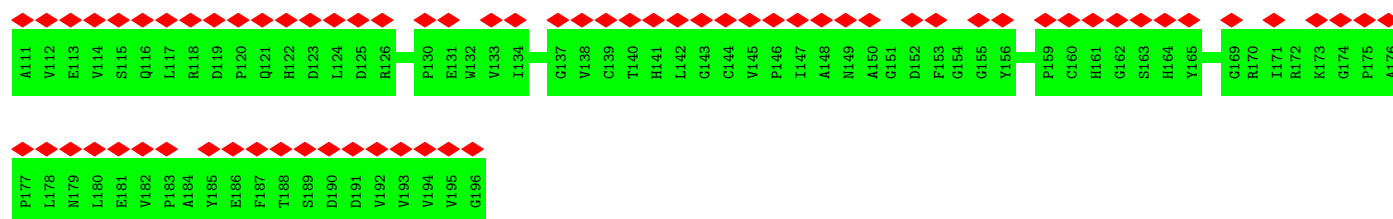
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial



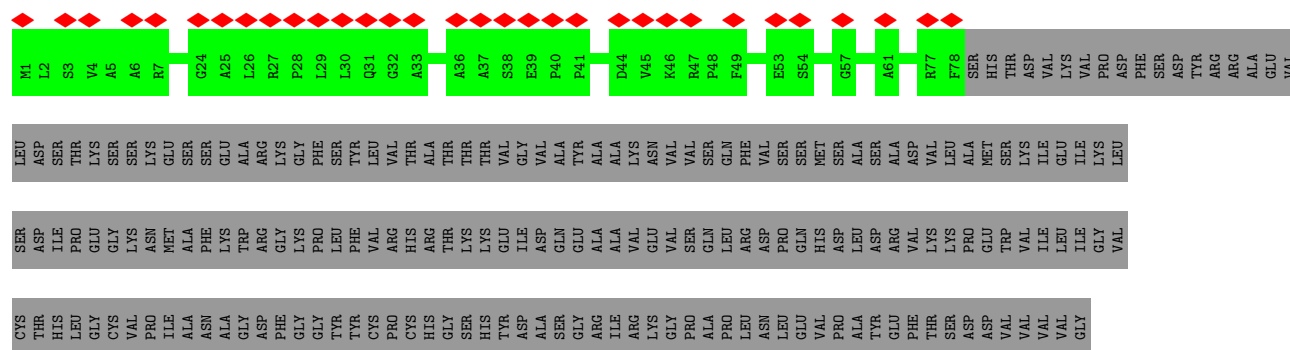
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial



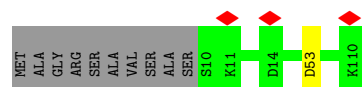




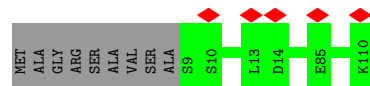
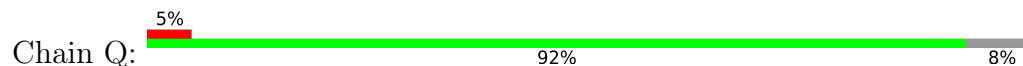
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 18: Cytochrome b-c1 complex subunit 7



- Molecule 18: Cytochrome b-c1 complex subunit 7

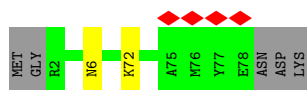


- Molecule 19: Cytochrome b-c1 complex subunit 8

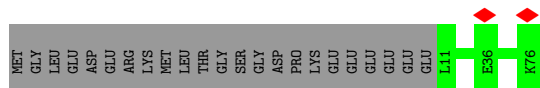
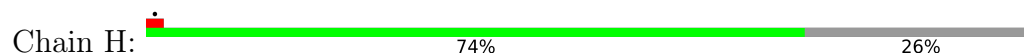


- Molecule 19: Cytochrome b-c1 complex subunit 8

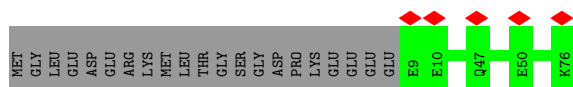
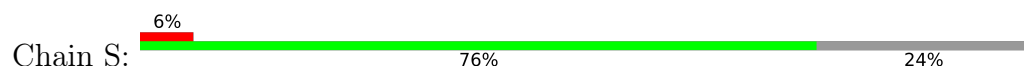




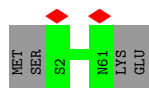
- Molecule 20: Cytochrome b-c1 complex subunit 6, mitochondrial



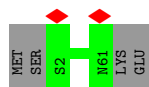
- Molecule 20: Cytochrome b-c1 complex subunit 6, mitochondrial



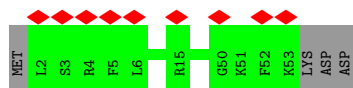
- Molecule 21: Cytochrome b-c1 complex subunit 9



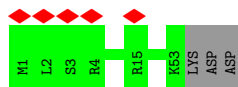
- Molecule 21: Cytochrome b-c1 complex subunit 9



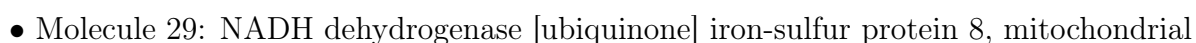
- Molecule 22: Cytochrome b-c1 complex subunit 10

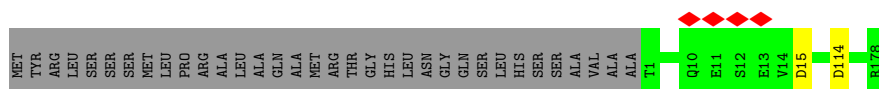
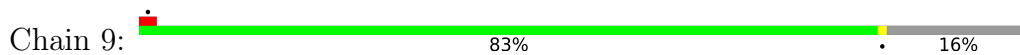


- Molecule 22: Cytochrome b-c1 complex subunit 10

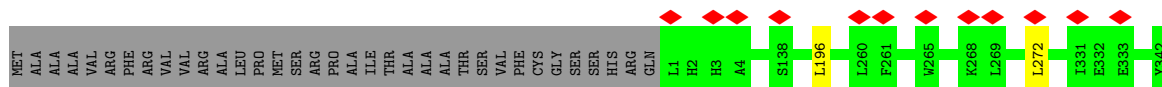
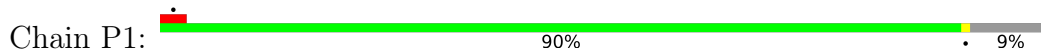


- Molecule 23: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

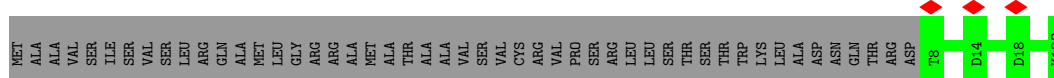
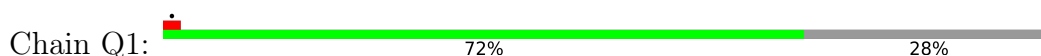




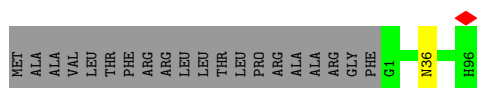
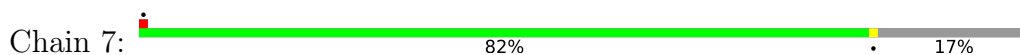
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



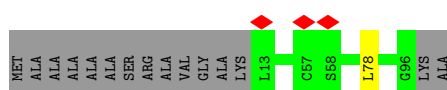
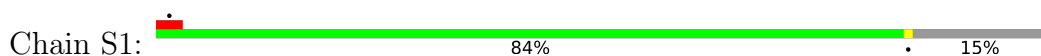
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



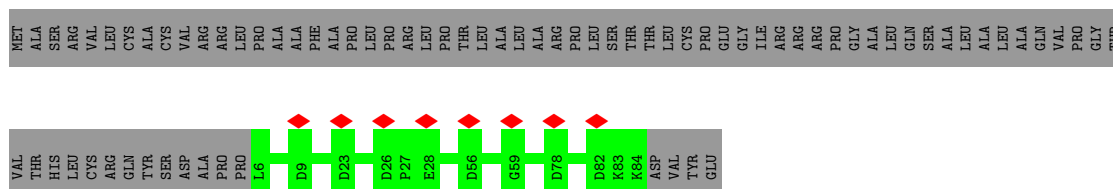
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 34: Acyl carrier protein, mitochondrial



- Molecule 34: Acyl carrier protein, mitochondrial



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

VAL THR HIS LEU CYS ARG GLN TYR S1 D2 A3 E55 E88

- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:  97%

MET ALA GLY L3 T115

- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:  87% 13%


MET ALA ALA ALA ALA THR GLY LEU ARG GLN ALA ALA ALA ALA ALA SER T17 D55 R115 P130

- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1:  100%

R1 K145

- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1:  5% 87% 12%

MET A1 Q72 K73 A74 L75 V76 SER GLY LYS ALA ALA GLU SER SER ALA MET ALA ALA THR E90 L112

- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s1:  39% 60%

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

PRO T27 D28 N49 E65 H68 HIS

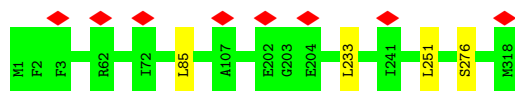
- Molecule 40: NADH-ubiquinone oxidoreductase chain 3

Chain A1:  6% 97%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain H1: 99%



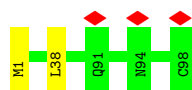
- Molecule 42: NADH-ubiquinone oxidoreductase chain 6

Chain J1: 18% 100%



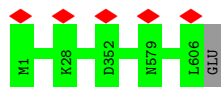
- Molecule 43: NADH-ubiquinone oxidoreductase chain 4L

Chain K1: 98%



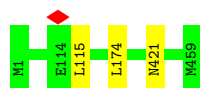
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain L1: 100%



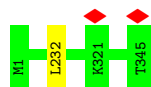
- Molecule 45: NADH-ubiquinone oxidoreductase chain 4

Chain M1: 99%




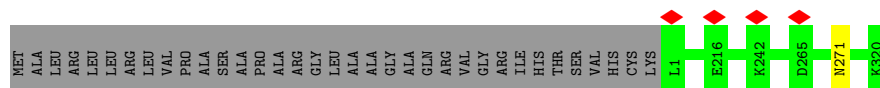
- Molecule 46: NADH-ubiquinone oxidoreductase chain 2

Chain N1: 100%



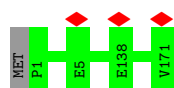
- Molecule 47: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:  90% 10%



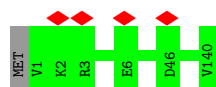
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:  99%



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1:  99%



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1:  5% 97%



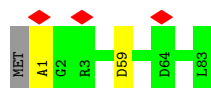
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1:  100%



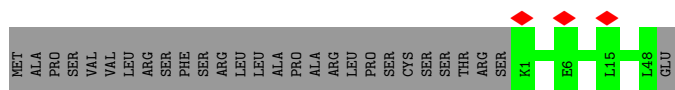
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b1:  96%

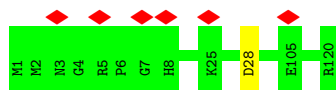


- Molecule 53: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

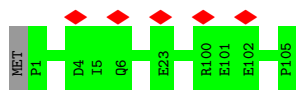
Chain c1:  63% 37%



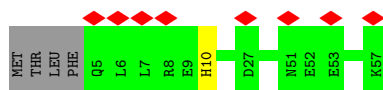
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C2



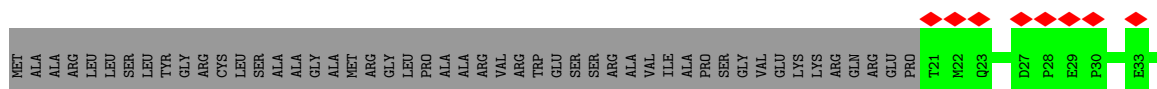
- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



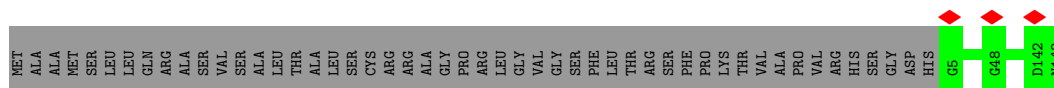
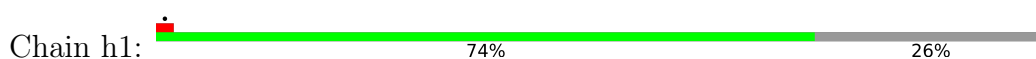
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



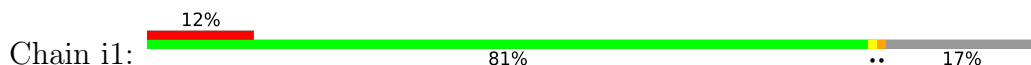
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



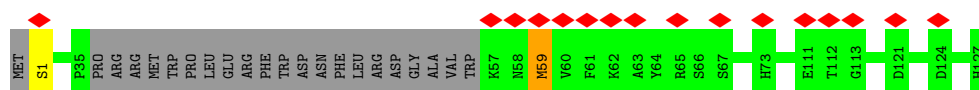
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



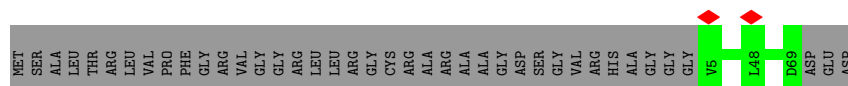
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



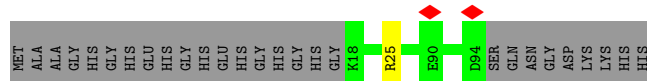
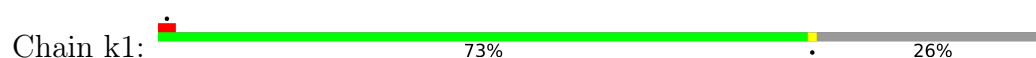




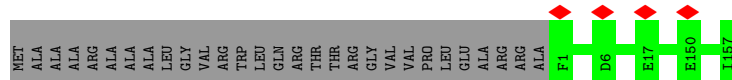
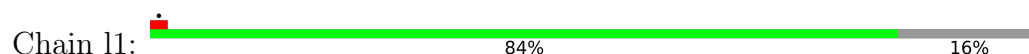
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



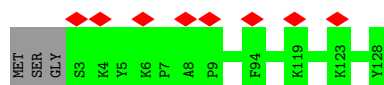
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



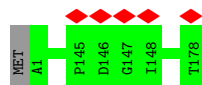
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



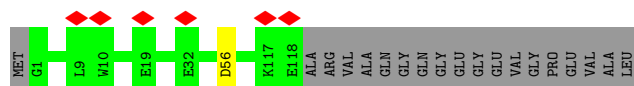
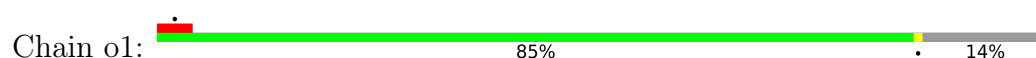
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



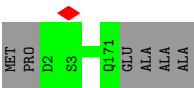
- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



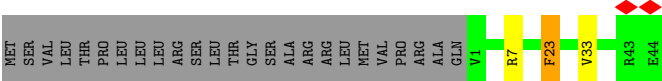
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 67: Cytochrome c oxidase subunit 8A, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57506	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	0.139	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	227.9, 263.93997, 262.87997	wwPDB
Map dimensions	215, 249, 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: HEA, CU, SF4, HEC, K, ZMP, CDL, 3PE, FMN, HEM, CUA, PC1, NDP, SAC, NA, 2MR, AYA, ZN, MG, DGT, FME, TGL, FES

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	n	0.32	0/4162	0.65	6/5686 (0.1%)
2	o	0.31	0/1863	0.75	3/2542 (0.1%)
3	p	0.31	0/2202	0.68	1/3010 (0.0%)
4	q	0.31	0/1190	0.67	2/1609 (0.1%)
5	r	0.30	0/860	0.67	0/1167
6	s	0.29	0/738	0.67	1/1001 (0.1%)
7	t	0.70	0/646	0.86	0/882
8	u	0.33	0/674	0.67	1/910 (0.1%)
9	v	0.33	0/579	0.76	0/771
10	x	0.29	0/396	0.60	0/541
11	y	0.30	0/399	0.62	0/535
12	w	0.27	0/444	0.62	0/598
13	A	0.27	0/3529	0.56	2/4793 (0.0%)
13	L	0.28	0/3530	0.56	0/4793
14	B	0.27	0/3205	0.53	0/4332
14	M	0.27	0/3205	0.51	0/4332
15	C	0.29	0/3147	0.57	3/4297 (0.1%)
15	N	0.29	0/3147	0.56	4/4297 (0.1%)
16	D	0.28	0/1968	0.55	1/2674 (0.0%)
16	O	0.28	0/1968	0.55	0/2674
17	E	0.28	0/1173	0.52	0/1605
17	P	0.28	0/1173	0.51	1/1605 (0.1%)
17	T	0.29	0/565	0.64	0/772
18	F	0.26	0/916	0.61	1/1226 (0.1%)
18	Q	0.27	0/922	0.54	0/1234
19	G	0.34	0/673	0.67	0/909
19	R	0.33	0/673	0.60	0/909
20	H	0.32	0/552	0.69	0/739
20	S	0.30	0/570	0.67	0/763
21	J	0.28	0/509	0.56	0/687
21	U	0.27	0/509	0.50	0/687

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
22	K	0.27	0/446	0.63	0/609
22	V	0.25	0/454	0.59	0/619
23	6	0.35	0/1289	0.67	0/1744
24	C1	0.29	0/1780	0.56	1/2424 (0.0%)
25	D1	0.29	0/3540	0.54	1/4795 (0.0%)
26	2	0.29	0/1700	0.54	0/2316
27	1	0.29	0/3396	0.57	0/4586
28	3	0.28	0/5392	0.54	0/7305
29	9	0.30	0/1461	0.59	2/1974 (0.1%)
30	P1	0.28	0/2823	0.59	2/3828 (0.1%)
31	Q1	0.27	0/1045	0.55	0/1411
32	7	0.28	0/773	0.51	0/1041
33	S1	0.28	0/682	0.64	1/920 (0.1%)
34	T1	0.30	0/646	0.62	0/869
34	U1	0.30	0/718	0.53	0/970
35	V1	0.26	0/945	0.44	0/1281
36	W1	0.29	0/993	0.60	0/1335
37	q1	0.29	0/1251	0.58	0/1702
38	r1	0.28	0/806	0.57	0/1090
39	s1	0.26	0/360	0.54	0/489
40	A1	0.31	0/948	0.66	2/1295 (0.2%)
41	H1	0.34	0/2607	0.70	4/3564 (0.1%)
42	J1	0.33	0/1330	0.60	0/1810
43	K1	0.31	0/738	0.66	2/1002 (0.2%)
44	L1	0.31	0/4913	0.57	0/6686
45	M1	0.30	0/3709	0.62	2/5052 (0.0%)
46	N1	0.30	0/2755	0.60	1/3751 (0.0%)
47	O1	0.28	0/2674	0.51	0/3626
48	X1	0.29	0/1434	0.55	0/1937
49	Y1	0.30	0/1061	0.58	0/1439
50	Z1	0.28	0/1198	0.61	0/1616
51	a1	0.29	0/585	0.63	0/788
52	b1	0.29	0/666	0.58	1/914 (0.1%)
53	c1	0.31	0/409	0.55	0/555
54	d1	0.29	0/1028	0.61	1/1387 (0.1%)
55	e1	0.27	0/900	0.53	0/1199
56	f1	0.29	0/468	0.60	0/630
57	g1	0.28	0/878	0.52	0/1196
58	h1	0.30	0/1201	0.55	0/1626
59	i1	0.28	0/917	0.54	1/1243 (0.1%)
60	j1	0.27	0/587	0.51	0/804
61	k1	0.27	0/646	0.52	0/873
62	l1	0.28	0/1379	0.54	0/1882

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
63	m1	0.30	0/1079	0.59	0/1463
64	n1	0.28	0/1596	0.55	0/2162
65	o1	0.33	0/1039	0.65	1/1394 (0.1%)
66	p1	0.28	0/1471	0.53	0/1988
67	z	0.66	0/350	0.71	0/472
All	All	0.30	0/115153	0.59	48/156242 (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
7	t	0	1
67	z	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	195	LEU	CA-CB-CG	11.02	140.66	115.30
40	A1	98	LEU	CA-CB-CG	8.11	133.96	115.30
15	C	332	LEU	CA-CB-CG	8.05	133.81	115.30
6	s	46	ASP	CB-CG-OD1	7.98	125.48	118.30
43	K1	38	LEU	CA-CB-CG	7.77	133.18	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	t	11	ARG	Sidechain
67	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	n	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	o	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
3	p	258/261 (99%)	248 (96%)	10 (4%)	0	100	100
4	q	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
5	r	102/146 (70%)	98 (96%)	4 (4%)	0	100	100
6	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
7	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
8	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
9	v	69/76 (91%)	65 (94%)	4 (6%)	0	100	100
10	x	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
11	y	45/63 (71%)	43 (96%)	2 (4%)	0	100	100
12	w	55/83 (66%)	54 (98%)	1 (2%)	0	100	100
13	A	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
13	L	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
14	B	418/453 (92%)	408 (98%)	10 (2%)	0	100	100
14	M	418/453 (92%)	399 (96%)	19 (4%)	0	100	100
15	C	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
15	N	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
16	D	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
16	O	238/325 (73%)	226 (95%)	12 (5%)	0	100	100
17	E	194/274 (71%)	184 (95%)	10 (5%)	0	100	100
17	P	194/274 (71%)	185 (95%)	9 (5%)	0	100	100
17	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
18	F	99/111 (89%)	97 (98%)	2 (2%)	0	100	100
18	Q	100/111 (90%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
19	R	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
20	H	64/89 (72%)	64 (100%)	0	0	100	100
20	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
21	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
21	U	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
22	K	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
22	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
23	6	155/224 (69%)	149 (96%)	6 (4%)	0	100	100
24	C1	206/263 (78%)	197 (96%)	9 (4%)	0	100	100
25	D1	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
26	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	25	59
27	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
28	3	688/727 (95%)	659 (96%)	29 (4%)	0	100	100
29	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
30	P1	340/377 (90%)	327 (96%)	13 (4%)	0	100	100
31	Q1	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
32	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
33	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
34	T1	77/156 (49%)	77 (100%)	0	0	100	100
34	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
35	V1	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
36	W1	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
37	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
38	r1	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
39	s1	40/104 (38%)	40 (100%)	0	0	100	100
40	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
41	H1	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
42	J1	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
43	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
44	L1	604/607 (100%)	566 (94%)	38 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	M1	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
46	N1	343/345 (99%)	330 (96%)	13 (4%)	0	100	100
47	O1	318/355 (90%)	298 (94%)	20 (6%)	0	100	100
48	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
49	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
50	Z1	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
51	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
52	b1	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
53	c1	46/76 (60%)	46 (100%)	0	0	100	100
54	d1	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
55	e1	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
56	f1	51/57 (90%)	51 (100%)	0	0	100	100
57	g1	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
58	h1	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
59	i1	102/128 (80%)	98 (96%)	3 (3%)	1 (1%)	13	46
60	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
61	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
62	l1	155/186 (83%)	153 (99%)	2 (1%)	0	100	100
63	m1	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
64	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
65	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
66	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
67	z	42/69 (61%)	36 (86%)	4 (10%)	2 (5%)	2	17
All	All	13990/16129 (87%)	13464 (96%)	522 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	2	183	LYS
67	z	23	PHE
59	i1	59	MET
67	z	33	VAL

### 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	n	425/425 (100%)	425 (100%)	0	100	100
2	o	210/210 (100%)	210 (100%)	0	100	100
3	p	226/227 (100%)	226 (100%)	0	100	100
4	q	122/146 (84%)	122 (100%)	0	100	100
5	r	91/118 (77%)	91 (100%)	0	100	100
6	s	80/101 (79%)	80 (100%)	0	100	100
7	t	66/92 (72%)	65 (98%)	1 (2%)	60	77
8	u	70/76 (92%)	69 (99%)	1 (1%)	62	79
9	v	54/57 (95%)	54 (100%)	0	100	100
10	x	39/67 (58%)	39 (100%)	0	100	100
11	y	40/55 (73%)	40 (100%)	0	100	100
12	w	43/67 (64%)	42 (98%)	1 (2%)	45	69
13	A	372/398 (94%)	371 (100%)	1 (0%)	91	96
13	L	372/398 (94%)	372 (100%)	0	100	100
14	B	330/356 (93%)	330 (100%)	0	100	100
14	M	330/356 (93%)	330 (100%)	0	100	100
15	C	332/333 (100%)	330 (99%)	2 (1%)	84	91
15	N	332/333 (100%)	331 (100%)	1 (0%)	91	96
16	D	205/260 (79%)	204 (100%)	1 (0%)	86	93
16	O	205/260 (79%)	205 (100%)	0	100	100
17	E	68/224 (30%)	68 (100%)	0	100	100
17	P	68/224 (30%)	67 (98%)	1 (2%)	60	77
17	T	58/224 (26%)	58 (100%)	0	100	100
18	F	93/99 (94%)	93 (100%)	0	100	100
18	Q	94/99 (95%)	94 (100%)	0	100	100
19	G	70/74 (95%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	70/74 (95%)	68 (97%)	2 (3%)	37	64
20	H	63/83 (76%)	63 (100%)	0	100	100
20	S	65/83 (78%)	65 (100%)	0	100	100
21	J	51/55 (93%)	51 (100%)	0	100	100
21	U	51/55 (93%)	51 (100%)	0	100	100
22	K	42/46 (91%)	42 (100%)	0	100	100
22	V	43/46 (94%)	43 (100%)	0	100	100
23	6	133/185 (72%)	132 (99%)	1 (1%)	79	88
24	C1	190/227 (84%)	190 (100%)	0	100	100
25	D1	370/394 (94%)	370 (100%)	0	100	100
26	2	184/206 (89%)	183 (100%)	1 (0%)	86	93
27	1	345/370 (93%)	345 (100%)	0	100	100
28	3	580/610 (95%)	579 (100%)	1 (0%)	92	97
29	9	152/178 (85%)	152 (100%)	0	100	100
30	P1	299/325 (92%)	299 (100%)	0	100	100
31	Q1	113/153 (74%)	113 (100%)	0	100	100
32	7	81/96 (84%)	80 (99%)	1 (1%)	67	82
33	S1	74/80 (92%)	74 (100%)	0	100	100
34	T1	73/135 (54%)	73 (100%)	0	100	100
34	U1	81/135 (60%)	81 (100%)	0	100	100
35	V1	101/102 (99%)	101 (100%)	0	100	100
36	W1	108/114 (95%)	108 (100%)	0	100	100
37	q1	131/131 (100%)	131 (100%)	0	100	100
38	r1	88/96 (92%)	88 (100%)	0	100	100
39	s1	41/95 (43%)	40 (98%)	1 (2%)	44	68
40	A1	103/103 (100%)	102 (99%)	1 (1%)	73	84
41	H1	279/279 (100%)	279 (100%)	0	100	100
42	J1	137/137 (100%)	137 (100%)	0	100	100
43	K1	87/87 (100%)	87 (100%)	0	100	100
44	L1	548/549 (100%)	548 (100%)	0	100	100
45	M1	414/414 (100%)	413 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	N1	307/307 (100%)	307 (100%)	0	100	100
47	O1	284/309 (92%)	283 (100%)	1 (0%)	89	95
48	X1	153/154 (99%)	153 (100%)	0	100	100
49	Y1	105/106 (99%)	105 (100%)	0	100	100
50	Z1	122/123 (99%)	121 (99%)	1 (1%)	79	88
51	a1	60/60 (100%)	60 (100%)	0	100	100
52	b1	72/73 (99%)	72 (100%)	0	100	100
53	c1	42/67 (63%)	42 (100%)	0	100	100
54	d1	107/107 (100%)	107 (100%)	0	100	100
55	e1	93/94 (99%)	93 (100%)	0	100	100
56	f1	49/53 (92%)	48 (98%)	1 (2%)	50	72
57	g1	92/129 (71%)	92 (100%)	0	100	100
58	h1	123/162 (76%)	123 (100%)	0	100	100
59	i1	99/119 (83%)	99 (100%)	0	100	100
60	j1	61/87 (70%)	61 (100%)	0	100	100
61	k1	60/78 (77%)	59 (98%)	1 (2%)	56	75
62	l1	142/161 (88%)	142 (100%)	0	100	100
63	m1	112/114 (98%)	112 (100%)	0	100	100
64	n1	163/164 (99%)	163 (100%)	0	100	100
65	o1	109/121 (90%)	109 (100%)	0	100	100
66	p1	155/158 (98%)	155 (100%)	0	100	100
67	z	39/61 (64%)	38 (97%)	1 (3%)	41	66
All	All	12041/13729 (88%)	12018 (100%)	23 (0%)	91	97

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	7	36	ASN
45	M1	421	ASN
40	A1	108	GLN
47	O1	271	ASN
16	D	144	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
66	p1	106	GLN
62	l1	131	GLN
30	P1	136	ASN
58	h1	108	GLN
17	E	161	HIS

### 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	$\# Z  > 2$
41	FME	H1	1	41	8,9,10	0.95	0	7,9,11	0.89	0
40	FME	A1	1	40	8,9,10	0.94	0	7,9,11	0.82	0
44	FME	L1	1	44	8,9,10	0.92	0	7,9,11	0.96	0
25	2MR	D1	85	25	10,12,13	2.60	2 (20%)	5,13,15	2.77	2 (40%)
59	SAC	i1	1	59	7,8,9	1.02	0	8,9,11	0.85	1 (12%)
42	FME	J1	1	42	8,9,10	0.91	0	7,9,11	0.88	0
46	FME	N1	1	46	8,9,10	0.93	0	7,9,11	0.90	0
52	AYA	b1	1	52	6,7,8	1.22	1 (16%)	5,8,10	1.30	1 (20%)
38	AYA	r1	1	38	6,7,8	1.27	1 (16%)	5,8,10	1.40	1 (20%)
43	FME	K1	1	43	8,9,10	0.88	0	7,9,11	2.22	2 (28%)
45	FME	M1	1	45	8,9,10	0.95	0	7,9,11	0.77	0

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
41	FME	H1	1	41	-	2/7/9/11	-
40	FME	A1	1	40	-	1/7/9/11	-
44	FME	L1	1	44	-	4/7/9/11	-
25	2MR	D1	85	25	-	2/10/13/15	-
59	SAC	i1	1	59	-	2/7/8/10	-
42	FME	J1	1	42	-	4/7/9/11	-
46	FME	N1	1	46	-	4/7/9/11	-
52	AYA	b1	1	52	-	0/4/6/8	-
38	AYA	r1	1	38	-	0/4/6/8	-
43	FME	K1	1	43	-	4/7/9/11	-
45	FME	M1	1	45	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D1	85	2MR	CZ-NE	5.93	1.47	1.34
25	D1	85	2MR	CZ-NH2	5.15	1.44	1.33
38	r1	1	AYA	CA-N	-2.43	1.44	1.46
52	b1	1	AYA	CA-N	-2.23	1.44	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	K1	1	FME	C-CA-N	4.96	118.69	109.73
25	D1	85	2MR	CD-NE-CZ	4.81	132.41	123.41
25	D1	85	2MR	NE-CZ-NH2	-3.53	116.24	119.48
38	r1	1	AYA	CB-CA-N	2.96	112.90	109.61
52	b1	1	AYA	CB-CA-N	2.70	112.61	109.61

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	H1	1	FME	N-CA-CB-CG
42	J1	1	FME	C-CA-CB-CG
42	J1	1	FME	O-C-CA-CB
43	K1	1	FME	O1-CN-N-CA
43	K1	1	FME	N-CA-CB-CG

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 90 ligands modelled in this entry, 7 are monoatomic - leaving 83 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
80	PC1	K	101	-	27,27,53	0.40	0	33,35,61	0.37	0
71	3PE	C	405	-	30,30,50	0.38	0	33,35,55	0.35	0
71	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
80	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.49	0
79	FES	2	301	26	0,4,4	-	-	-		
71	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.34	0
71	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0
80	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.56	0
76	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
76	CDL	Y1	202	-	93,93,99	0.31	0	99,105,111	0.27	0
76	CDL	G	101	-	55,55,99	0.39	0	61,67,111	0.32	0
84	NDP	P1	501	-	45,52,52	0.52	0	53,80,80	0.59	1 (1%)
71	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.65	0
79	FES	P	201	17	0,4,4	-	-	-		
76	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
76	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.42	1 (1%)
80	PC1	L	502	-	23,23,53	0.44	0	29,31,61	0.61	0
78	HEC	D	301	16	32,50,50	2.19	4 (12%)	24,82,82	1.57	3 (12%)
79	FES	3	803	28	0,4,4	-	-	-		
71	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.63	0
71	3PE	p	301	-	44,44,50	0.33	0	47,49,55	0.30	0
80	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.33	0
71	3PE	L	501	-	22,22,50	0.44	0	25,27,55	0.36	0
79	FES	E	201	17	0,4,4	-	-	-		
71	3PE	A1	201	-	42,42,50	0.32	0	45,47,55	0.33	0
71	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.28	0
76	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
76	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
81	SF4	9	202	29	0,12,12	-	-	-		
71	3PE	M1	501	-	50,50,50	0.30	0	53,55,55	0.30	0
81	SF4	3	801	28	0,12,12	-	-	-		
71	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.35	0
76	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.36	0
71	3PE	v	101	-	27,27,50	0.39	0	30,32,55	0.34	0
76	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.40	1 (1%)
76	CDL	L1	703	-	45,45,99	0.42	0	51,57,111	0.35	0
80	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.28	0
76	CDL	L1	702	-	77,77,99	0.34	0	83,89,111	0.29	0
71	3PE	D1	501	-	50,50,50	0.31	0	53,55,55	0.29	0
85	ZMP	W1	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.03	2 (6%)
71	3PE	Y1	204	-	41,41,50	0.33	0	44,46,55	0.32	0
70	HEA	n	604	1	57,67,67	1.48	8 (14%)	61,103,103	2.52	22 (36%)
73	CUA	o	303	2	0,1,1	-	-	-		
71	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.31	0
71	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
77	HEM	C	402	15	41,50,50	1.47	4 (9%)	45,82,82	1.60	9 (20%)
71	3PE	M1	503	-	35,35,50	0.36	0	38,40,55	0.30	0
80	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.44	0
71	3PE	K1	201	-	40,40,50	0.34	0	43,45,55	0.29	0
80	PC1	Y1	201	-	53,53,53	0.30	0	59,61,61	0.32	0
71	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.38	0
82	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.46	1 (2%)
71	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.44	0
75	TGL	y	601	-	36,36,62	0.23	0	39,39,65	0.18	0
71	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.35	0
81	SF4	9	201	29	0,12,12	-	-	-		
77	HEM	N	402	15	41,50,50	1.43	3 (7%)	45,82,82	1.59	10 (22%)
77	HEM	N	403	15	41,50,50	1.45	4 (9%)	45,82,82	1.56	8 (17%)
71	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.35	0
77	HEM	C	401	15	41,50,50	1.42	3 (7%)	45,82,82	1.52	9 (20%)
85	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.96	1 (3%)
71	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.34	0
70	HEA	n	603	1	57,67,67	1.45	8 (14%)	61,103,103	2.36	22 (36%)
71	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
71	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.33	0
71	3PE	Y1	203	-	27,27,50	0.40	0	30,32,55	0.34	0
80	PC1	V	101	-	27,27,53	0.40	0	33,35,61	0.34	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
76	CDL	R	101	-	40,40,99	0.46	0	46,52,111	0.54	0
81	SF4	3	802	28	0,12,12	-	-	-		
76	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.43	0
76	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
71	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.34	0
86	DGT	O1	401	72	26,33,33	0.79	1 (3%)	32,52,52	0.47	0
71	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
81	SF4	6	201	23	0,12,12	-	-	-		
71	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.31	0
78	HEC	O	303	16	32,50,50	2.19	3 (9%)	24,82,82	1.60	4 (16%)
76	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.46	0
76	CDL	N	405	-	45,45,99	0.44	0	51,57,111	0.51	0
81	SF4	1	502	27	0,12,12	-	-	-		
71	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.32	0
71	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	0
71	3PE	G	102	-	50,50,50	0.30	0	53,55,55	0.28	0

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
80	PC1	K	101	-	-	9/31/31/57	-
71	3PE	C	405	-	-	6/34/34/54	-
71	3PE	6	202	-	-	6/35/35/54	-
80	PC1	6	203	-	-	11/46/46/57	-
79	FES	2	301	26	-	-	0/1/1/1
71	3PE	N1	402	-	-	7/41/41/54	-
71	3PE	M1	502	-	-	12/54/54/54	-
80	PC1	P1	502	-	-	16/34/34/57	-
76	CDL	A	502	-	-	21/56/56/110	-
76	CDL	Y1	202	-	-	16/104/104/110	-
76	CDL	G	101	-	-	14/66/66/110	-
84	NDP	P1	501	-	-	8/30/77/77	0/5/5/5
71	3PE	A	501	-	-	9/26/26/54	-
79	FES	P	201	17	-	-	0/1/1/1
76	CDL	H1	402	-	-	12/59/59/110	-
76	CDL	R	103	-	-	17/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PC1	L	502	-	-	7/27/27/57	-
78	HEC	D	301	16	-	2/10/54/54	-
79	FES	3	803	28	-	-	0/1/1/1
71	3PE	t	101	-	-	6/28/28/54	-
71	3PE	p	301	-	-	8/48/48/54	-
80	PC1	J	101	-	-	7/38/38/57	-
71	3PE	L	501	-	-	7/26/26/54	-
79	FES	E	201	17	-	-	0/1/1/1
71	3PE	A1	201	-	-	9/46/46/54	-
71	3PE	r1	201	-	-	6/49/49/54	-
76	CDL	O	301	-	-	14/67/67/110	-
76	CDL	d1	201	-	-	14/77/77/110	-
81	SF4	9	202	29	-	-	0/6/5/5
71	3PE	M1	501	-	-	12/54/54/54	-
81	SF4	3	801	28	-	-	0/6/5/5
71	3PE	O	302	-	-	6/36/36/54	-
76	CDL	C	404	-	-	13/52/52/110	-
71	3PE	v	101	-	-	10/31/31/54	-
76	CDL	N1	401	-	-	18/100/100/110	-
76	CDL	L1	703	-	-	8/56/56/110	-
80	PC1	9	204	-	-	11/50/50/57	-
76	CDL	L1	702	-	-	20/88/88/110	-
71	3PE	D1	501	-	-	9/54/54/54	-
85	ZMP	W1	201	-	-	6/38/40/43	-
71	3PE	Y1	204	-	-	8/45/45/54	-
70	HEA	n	604	1	-	7/32/76/76	-
71	3PE	i1	201	-	-	6/45/45/54	-
71	3PE	n	605	-	-	9/37/37/54	-
77	HEM	C	402	15	-	2/12/54/54	-
71	3PE	M1	503	-	-	9/39/39/54	-
80	PC1	9	203	-	-	10/57/57/57	-
71	3PE	K1	201	-	-	10/44/44/54	-
80	PC1	Y1	201	-	-	14/57/57/57	-
71	3PE	o	302	-	-	9/32/32/54	-
82	FMN	1	501	-	-	5/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	3PE	n	606	-	-	13/31/31/54	-
75	TGL	y	601	-	-	2/39/39/65	-
71	3PE	E	202	-	-	6/35/35/54	-
81	SF4	9	201	29	-	-	0/6/5/5
77	HEM	N	402	15	-	1/12/54/54	-
77	HEM	N	403	15	-	4/12/54/54	-
71	3PE	d1	203	-	-	6/35/35/54	-
77	HEM	C	401	15	-	3/12/54/54	-
85	ZMP	n1	201	-	-	17/36/38/43	-
71	3PE	N	401	-	-	5/37/37/54	-
70	HEA	n	603	1	-	10/32/76/76	-
71	3PE	C	403	-	-	11/38/38/54	-
71	3PE	d1	202	-	-	8/34/34/54	-
71	3PE	Y1	203	-	-	7/31/31/54	-
80	PC1	V	101	-	-	4/31/31/57	-
76	CDL	R	101	-	-	11/51/51/110	-
81	SF4	3	802	28	-	-	0/6/5/5
76	CDL	h1	201	-	-	21/80/80/110	-
76	CDL	R	102	-	-	20/67/67/110	-
71	3PE	n	607	-	-	5/30/30/54	-
86	DGT	O1	401	72	-	7/18/34/34	0/3/3/3
71	3PE	L1	701	-	-	7/54/54/54	-
81	SF4	6	201	23	-	-	0/6/5/5
71	3PE	N	404	-	-	5/40/40/54	-
78	HEC	O	303	16	-	0/10/54/54	-
76	CDL	a1	101	-	-	13/67/67/110	-
76	CDL	N	405	-	-	10/56/56/110	-
81	SF4	1	502	27	-	-	0/6/5/5
71	3PE	R	104	-	-	9/33/33/54	-
71	3PE	H1	401	-	-	10/54/54/54	-
71	3PE	G	102	-	-	10/54/54/54	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	O	303	HEC	C2B-C3B	-6.40	1.34	1.40
78	O	303	HEC	C3C-C2C	-6.30	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	D	301	HEC	C3C-C2C	-6.27	1.34	1.40
78	D	301	HEC	C2B-C3B	-6.14	1.34	1.40
78	D	301	HEC	C3D-C2D	5.44	1.53	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	n	604	HEA	CMC-C2C-C3C	7.86	139.38	124.68
70	n	603	HEA	CMC-C2C-C3C	7.15	138.06	124.68
70	n	604	HEA	CMC-C2C-C1C	-7.13	117.50	128.46
70	n	603	HEA	CMC-C2C-C1C	-6.56	118.39	128.46
70	n	604	HEA	C3D-C4D-ND	5.38	115.57	110.36

There are no chirality outliers.

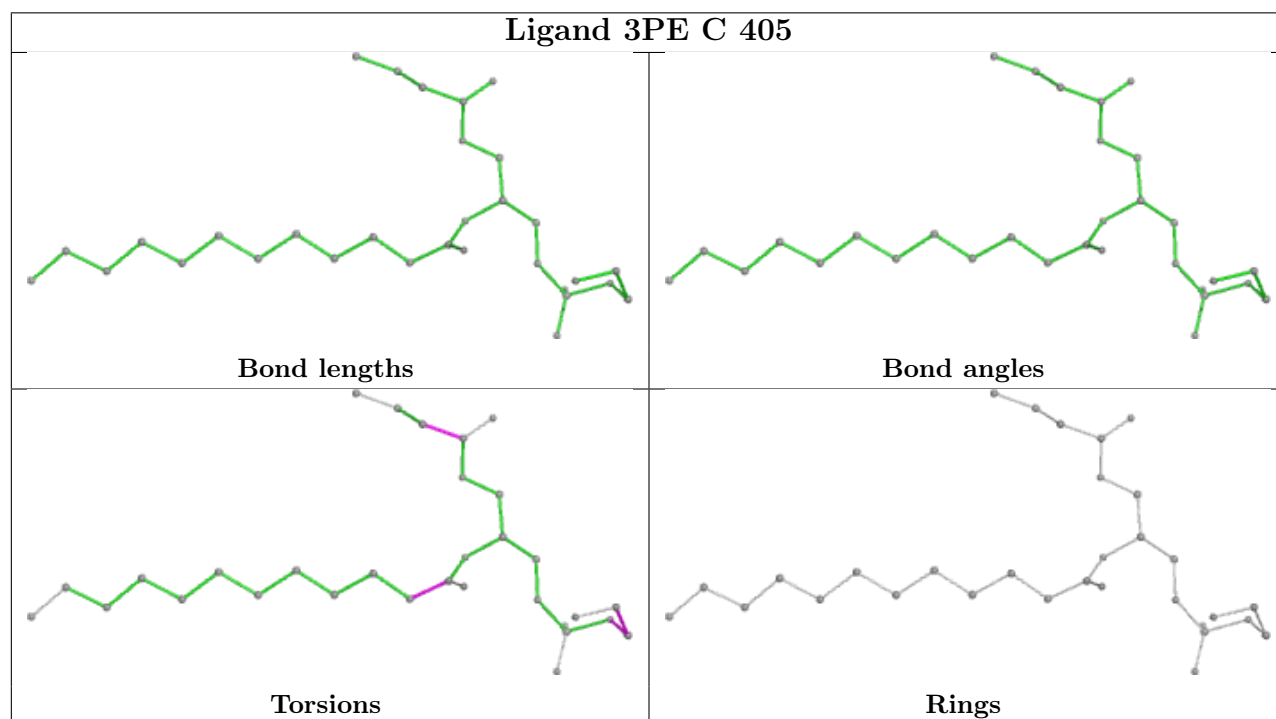
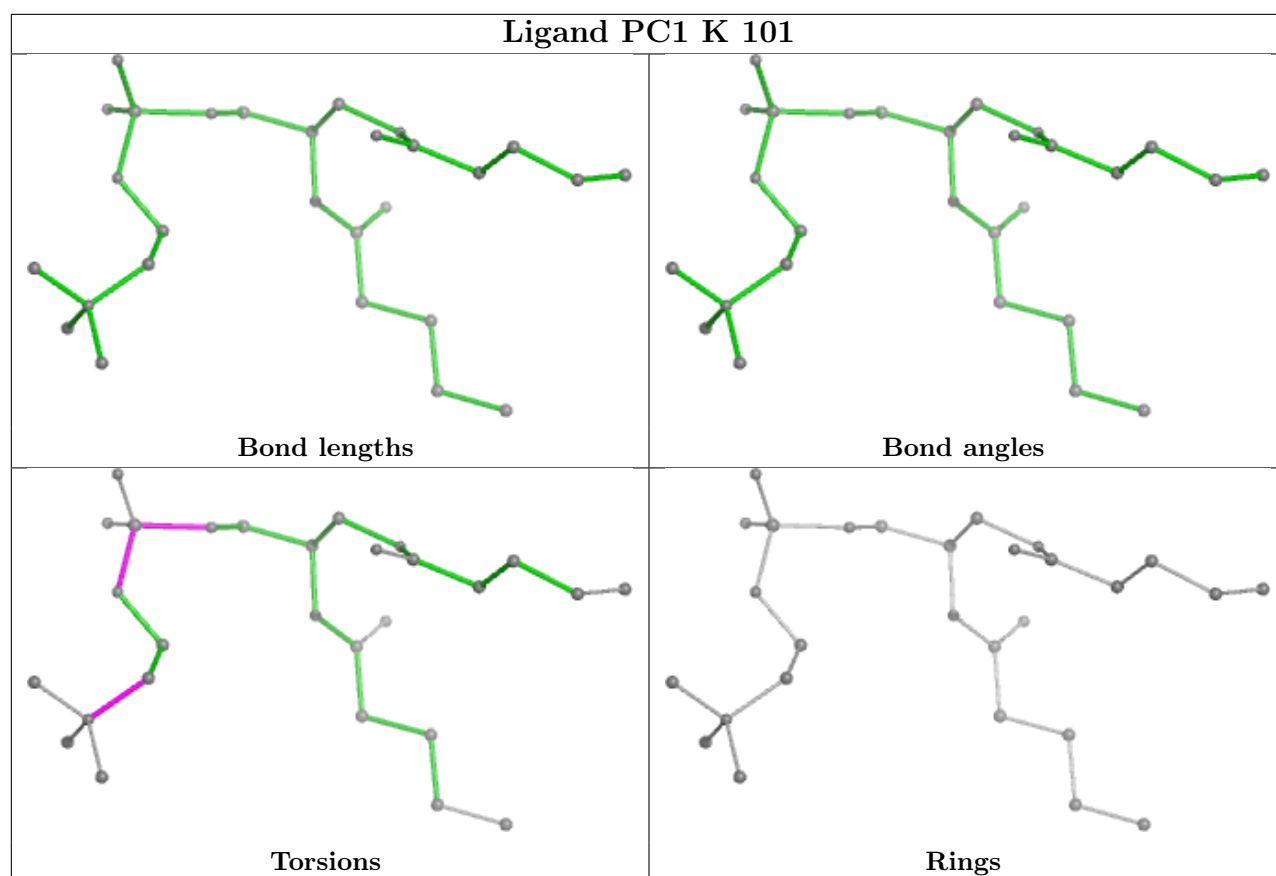
5 of 671 torsion outliers are listed below:

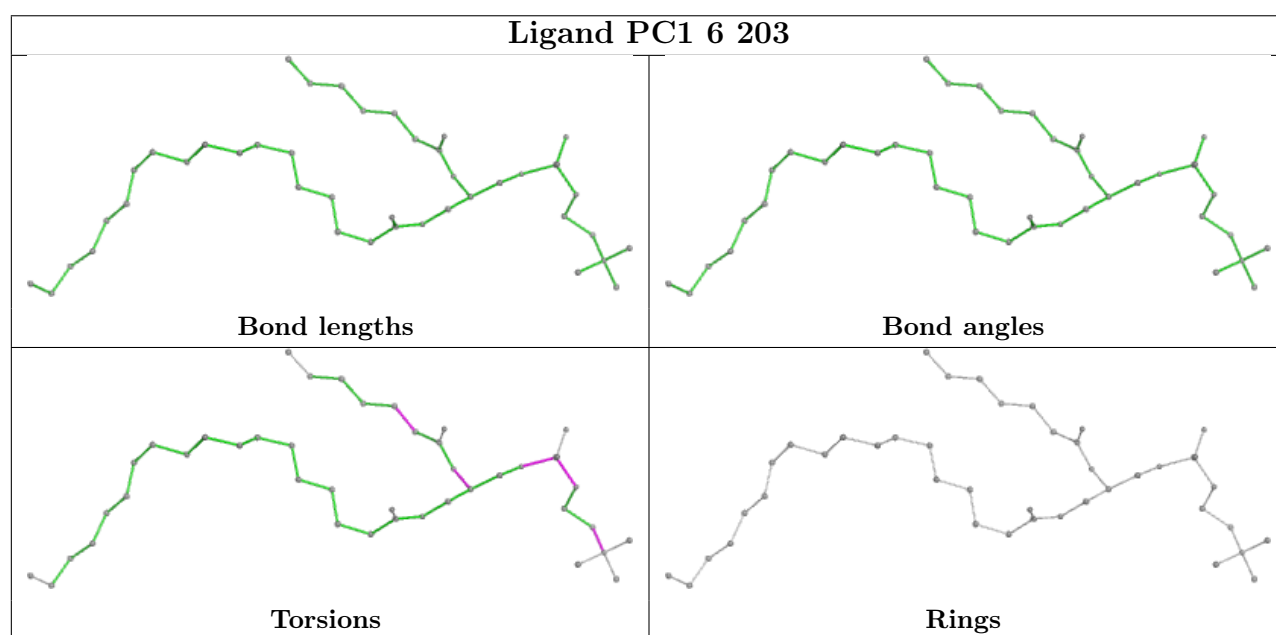
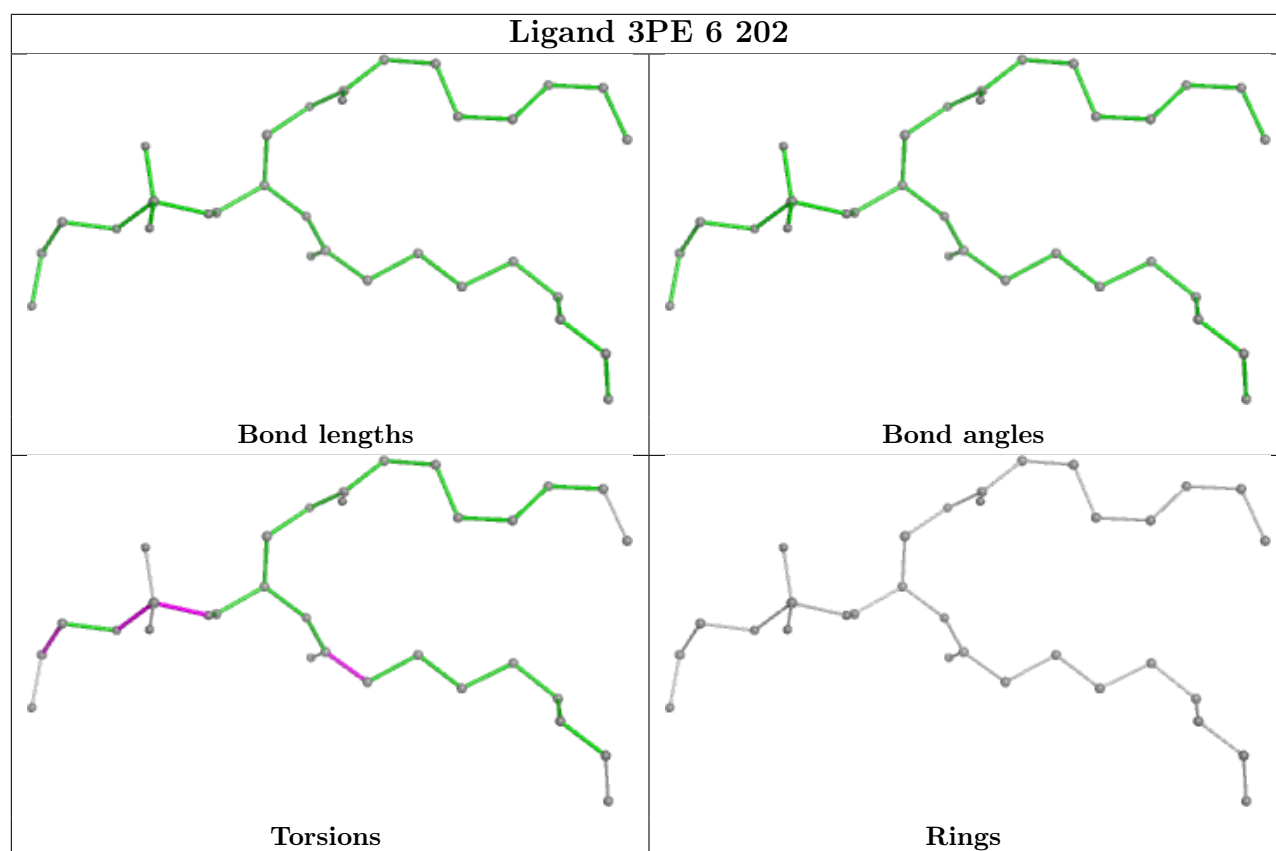
Mol	Chain	Res	Type	Atoms
70	n	603	HEA	C15-C16-C17-C18
70	n	604	HEA	C2D-C3D-CAD-CBD
70	n	604	HEA	C15-C16-C17-C18
71	n	605	3PE	C11-O13-P-O12
71	n	605	3PE	C11-O13-P-O14

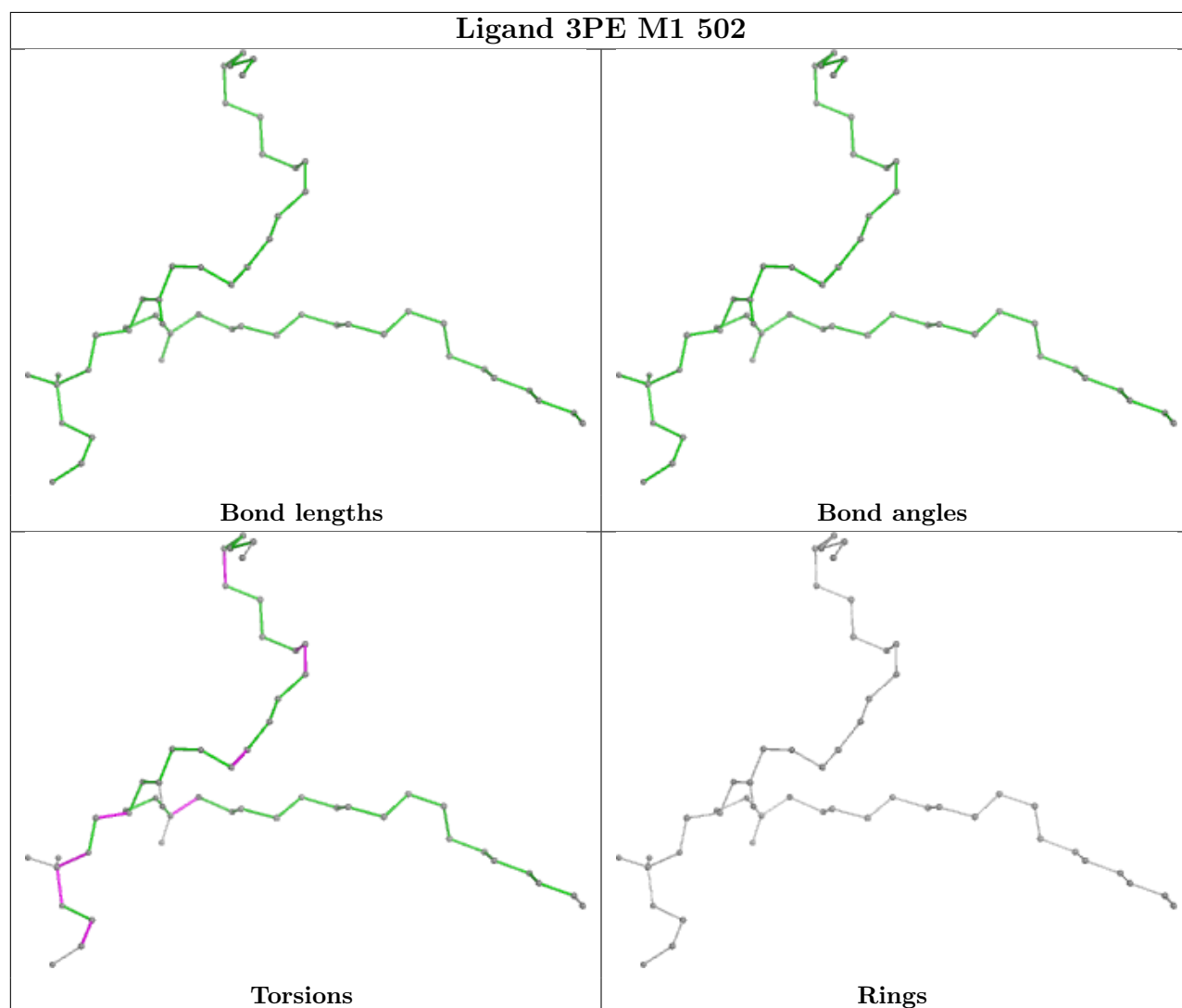
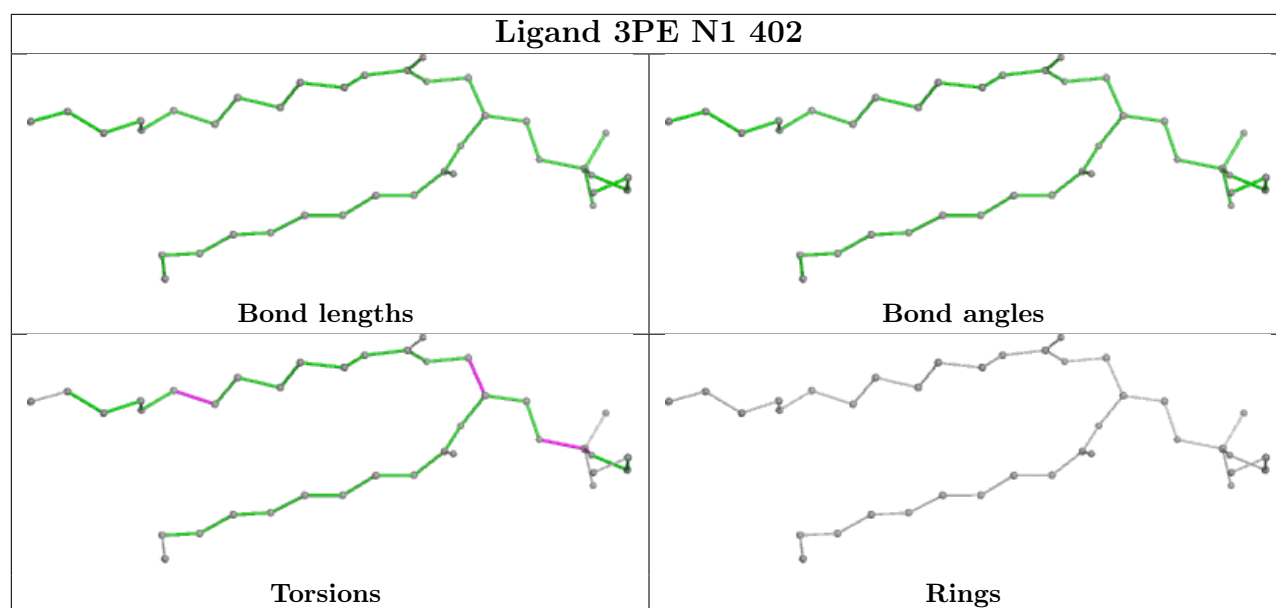
There are no ring outliers.

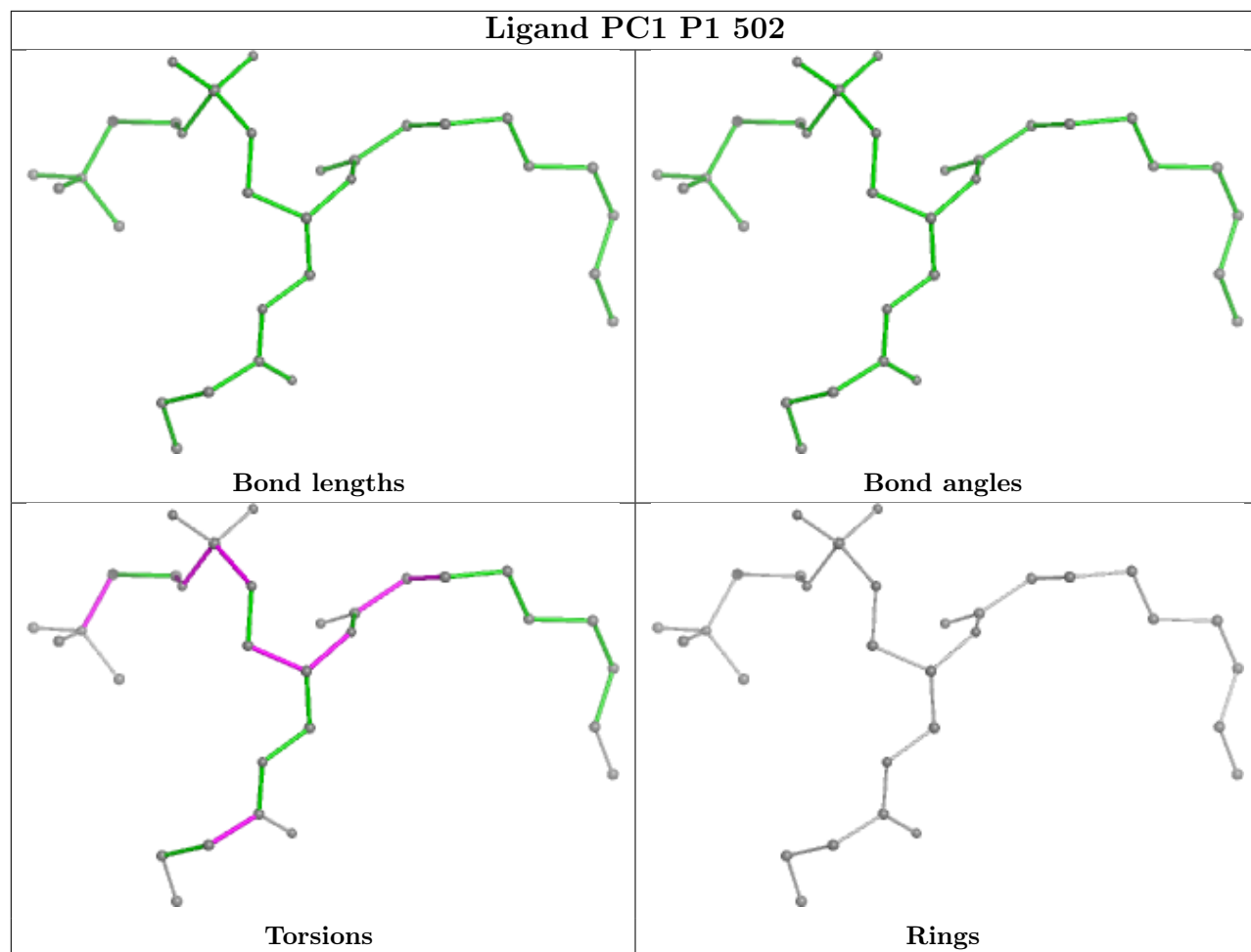
No monomer is involved in short contacts.

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.

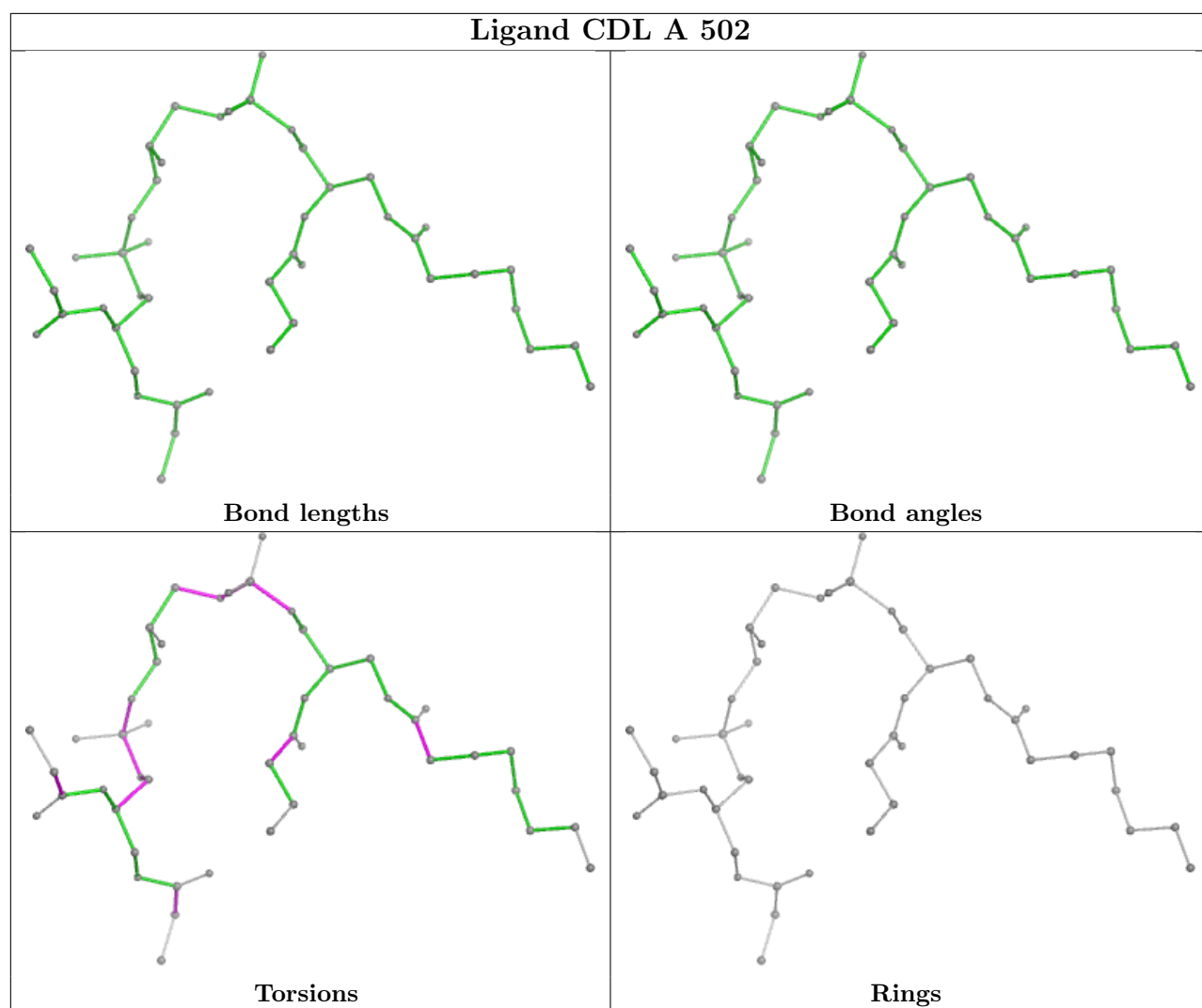


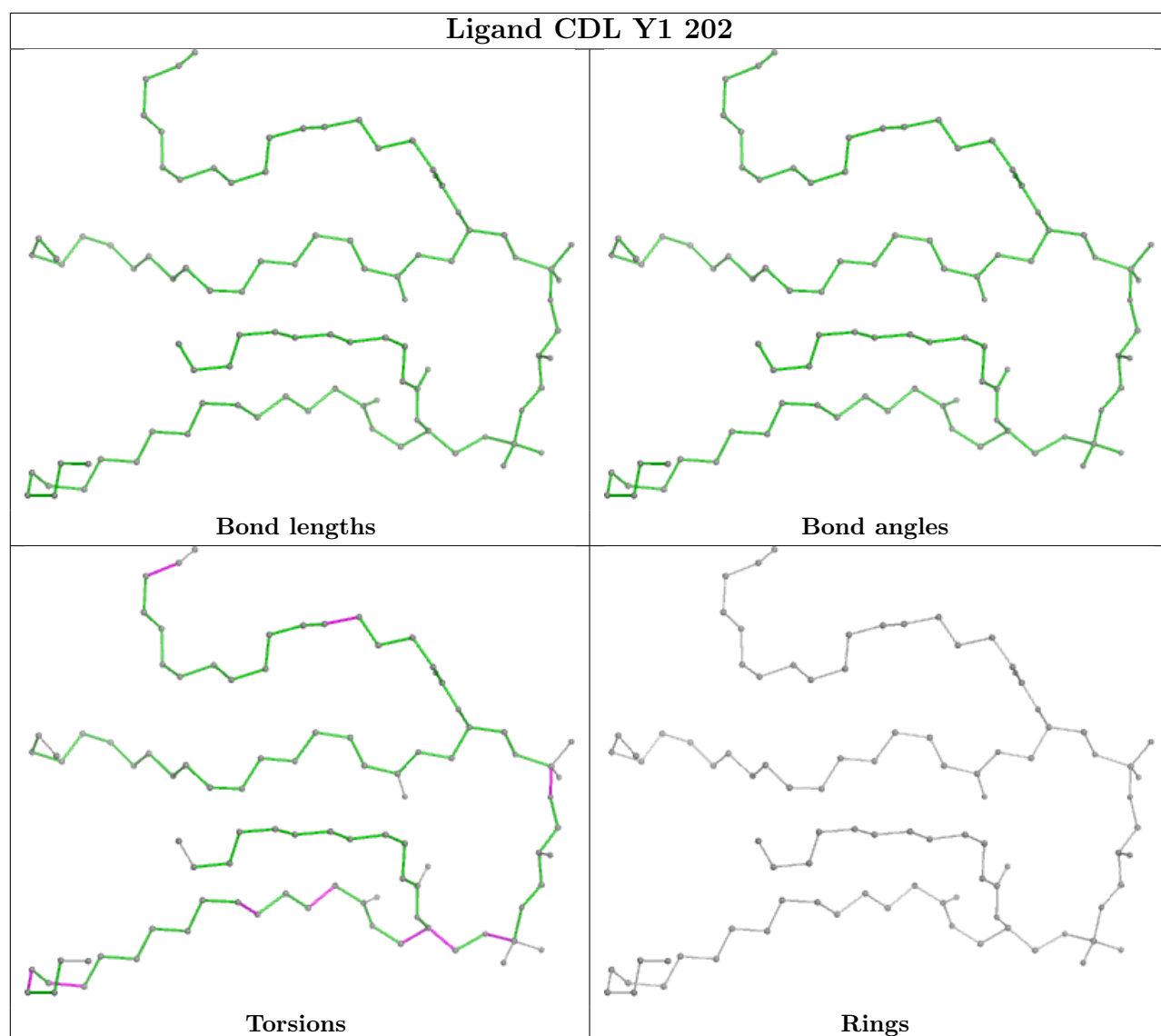


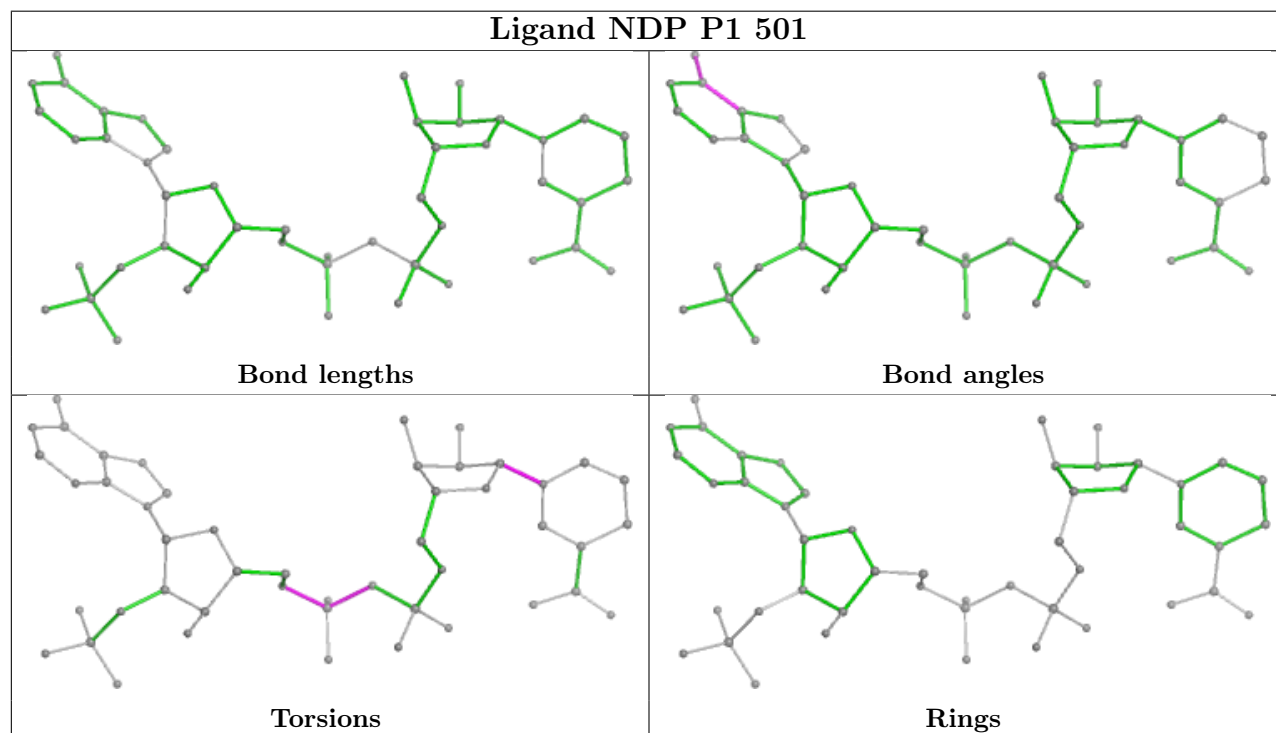
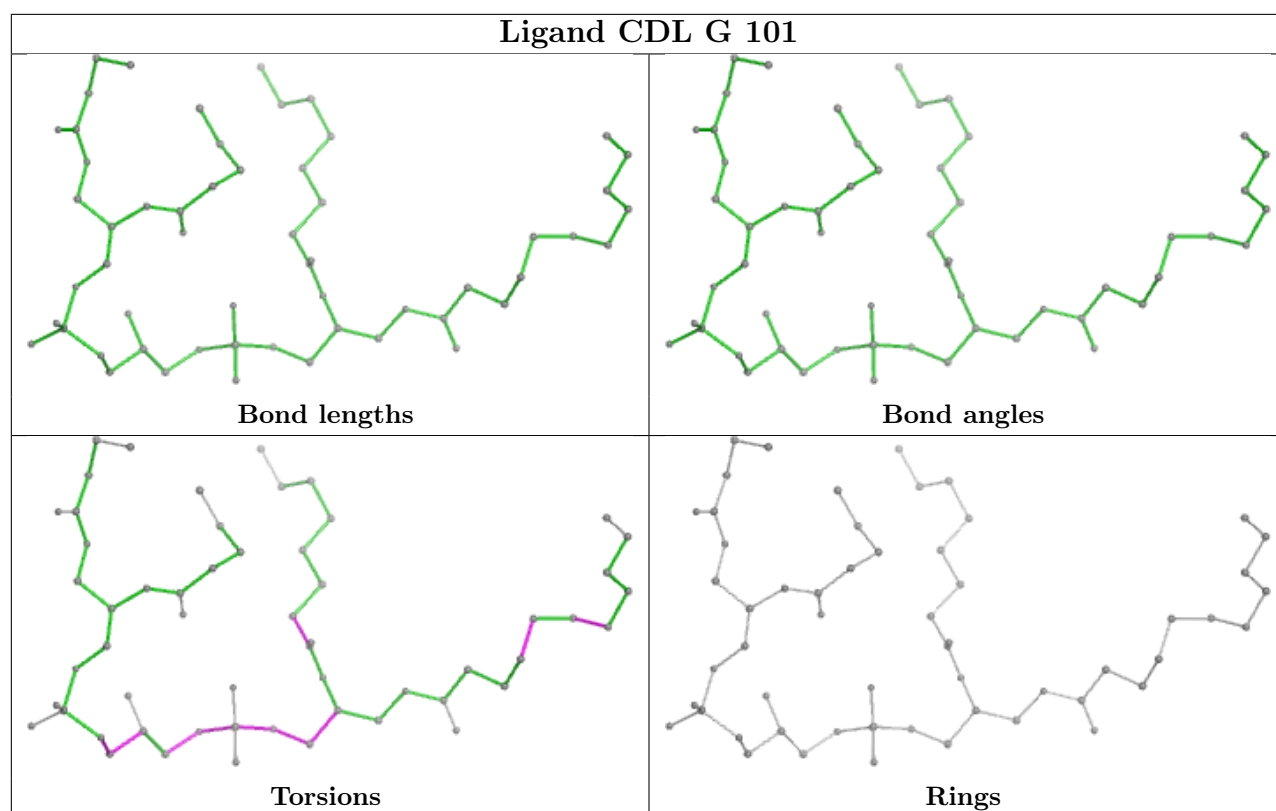


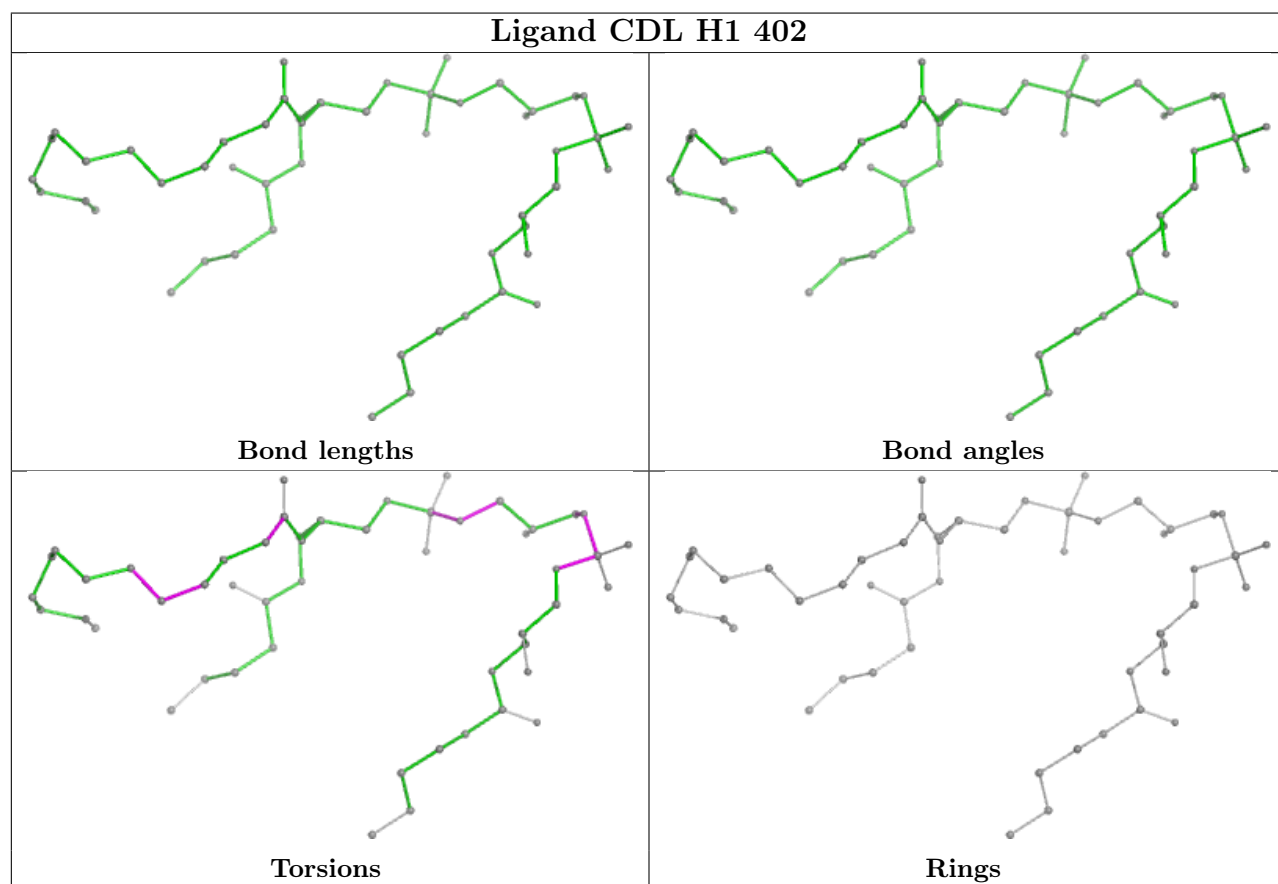
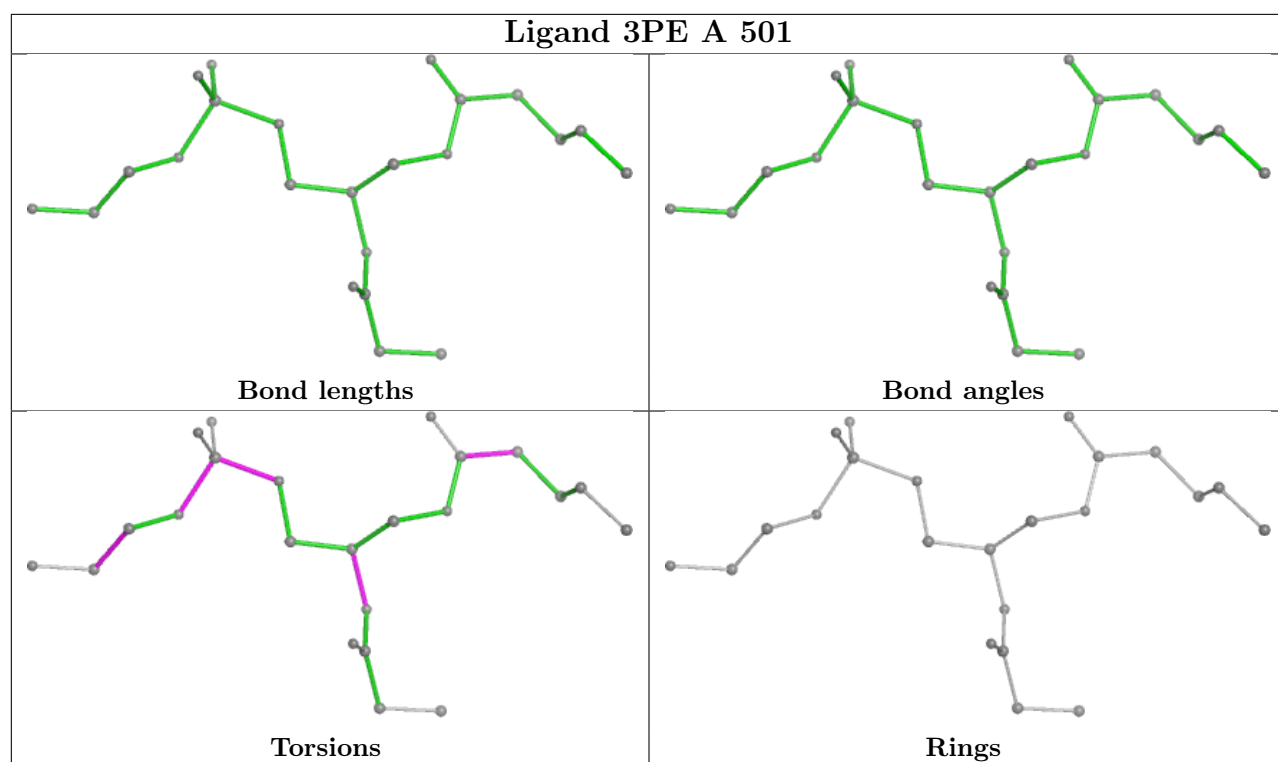


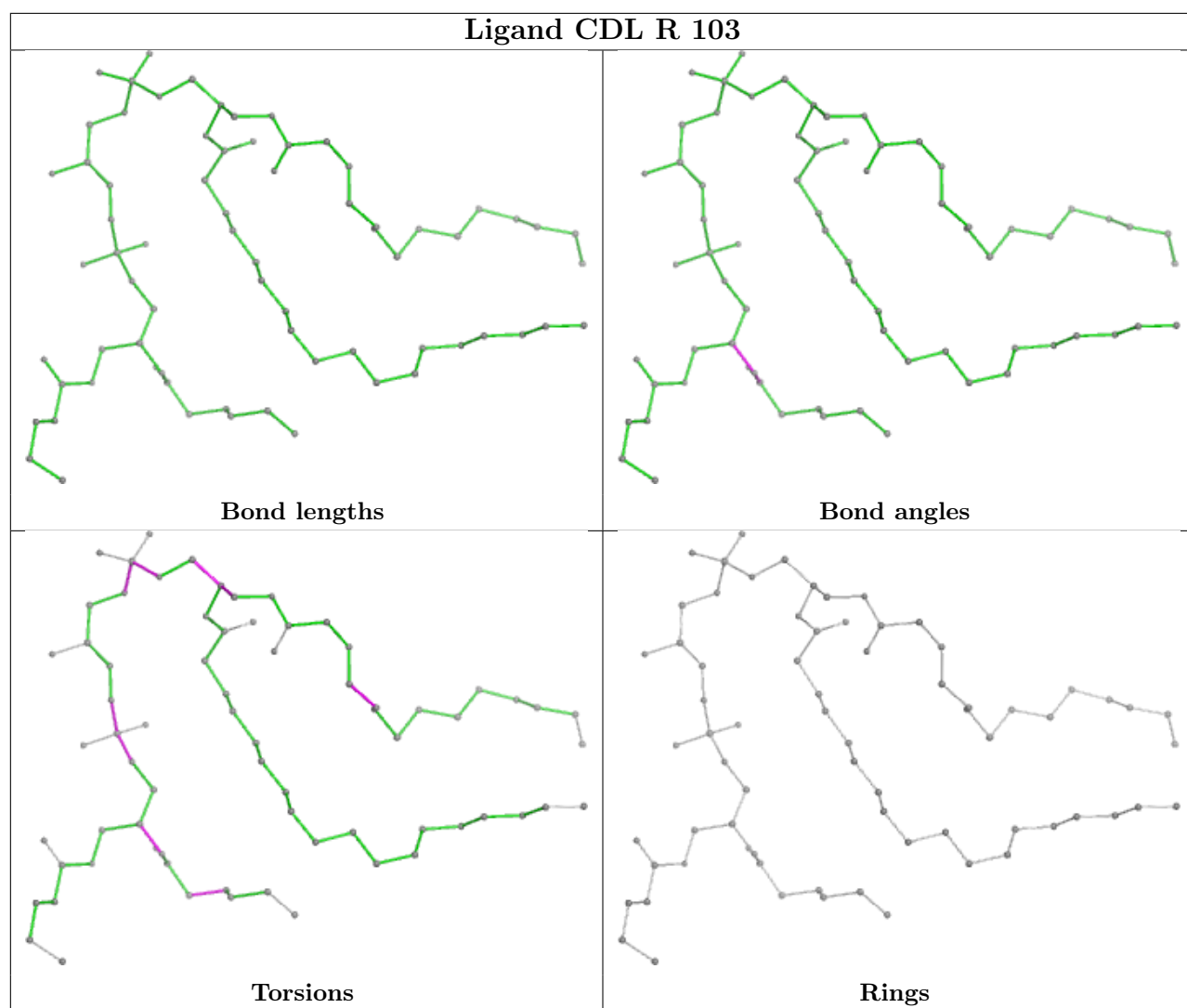


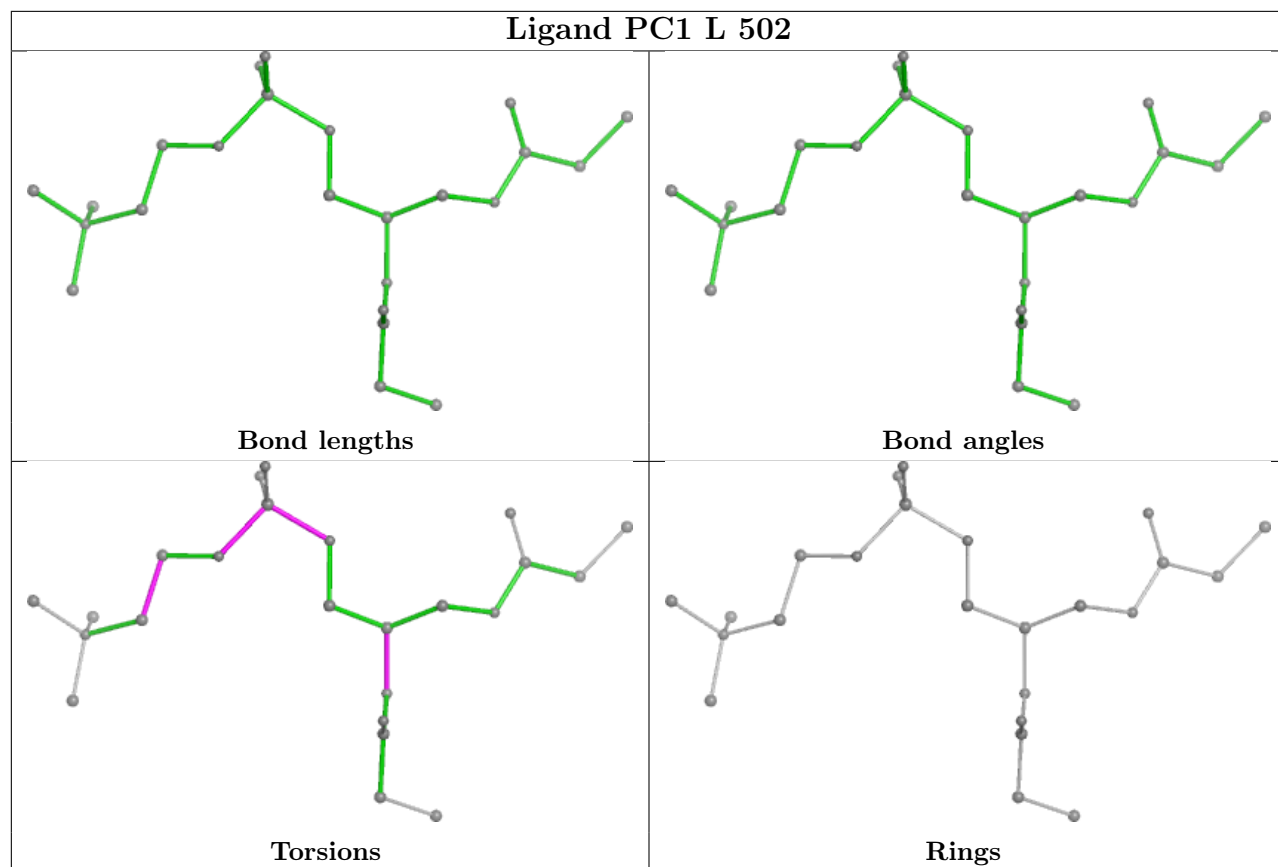


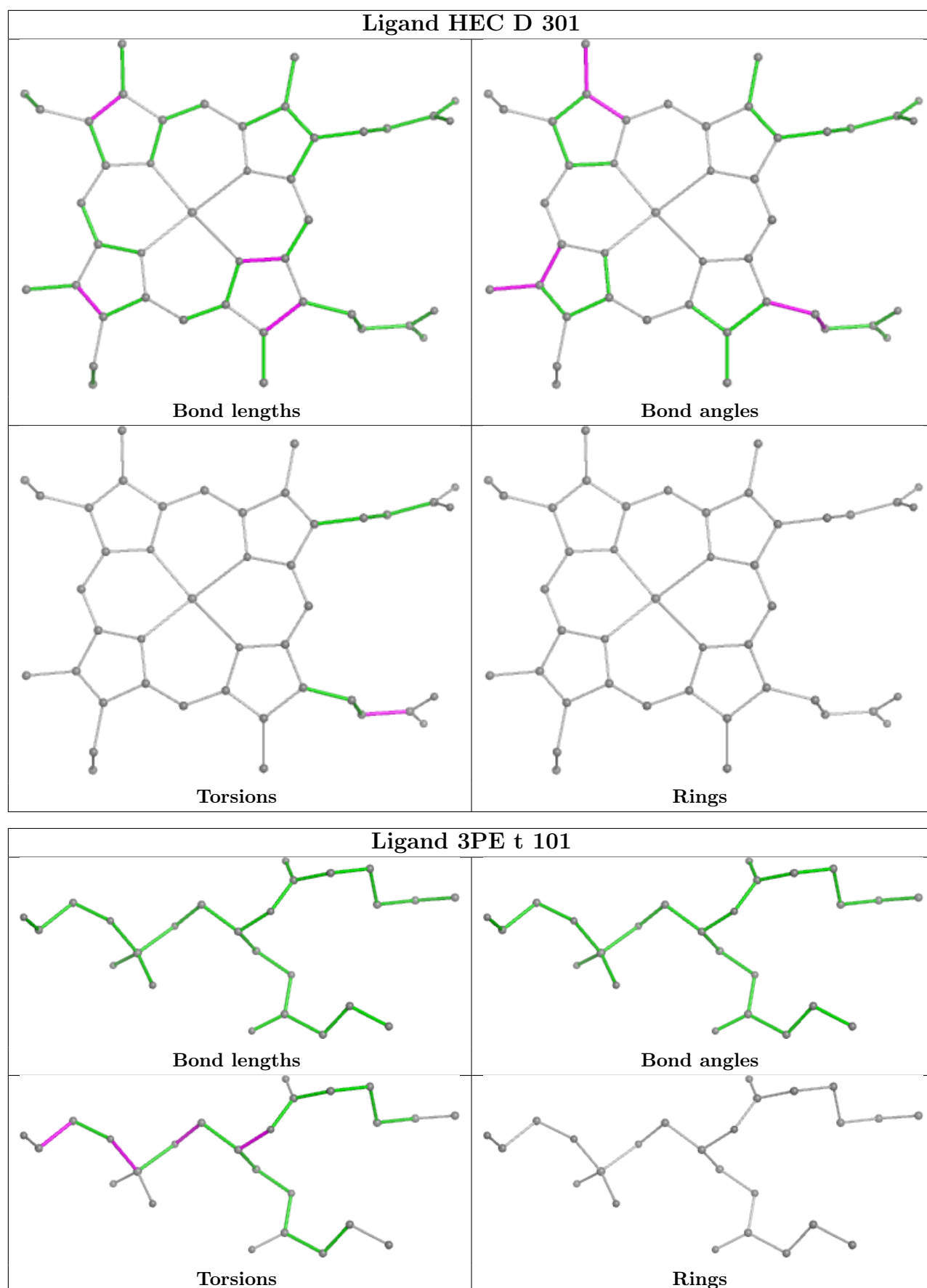


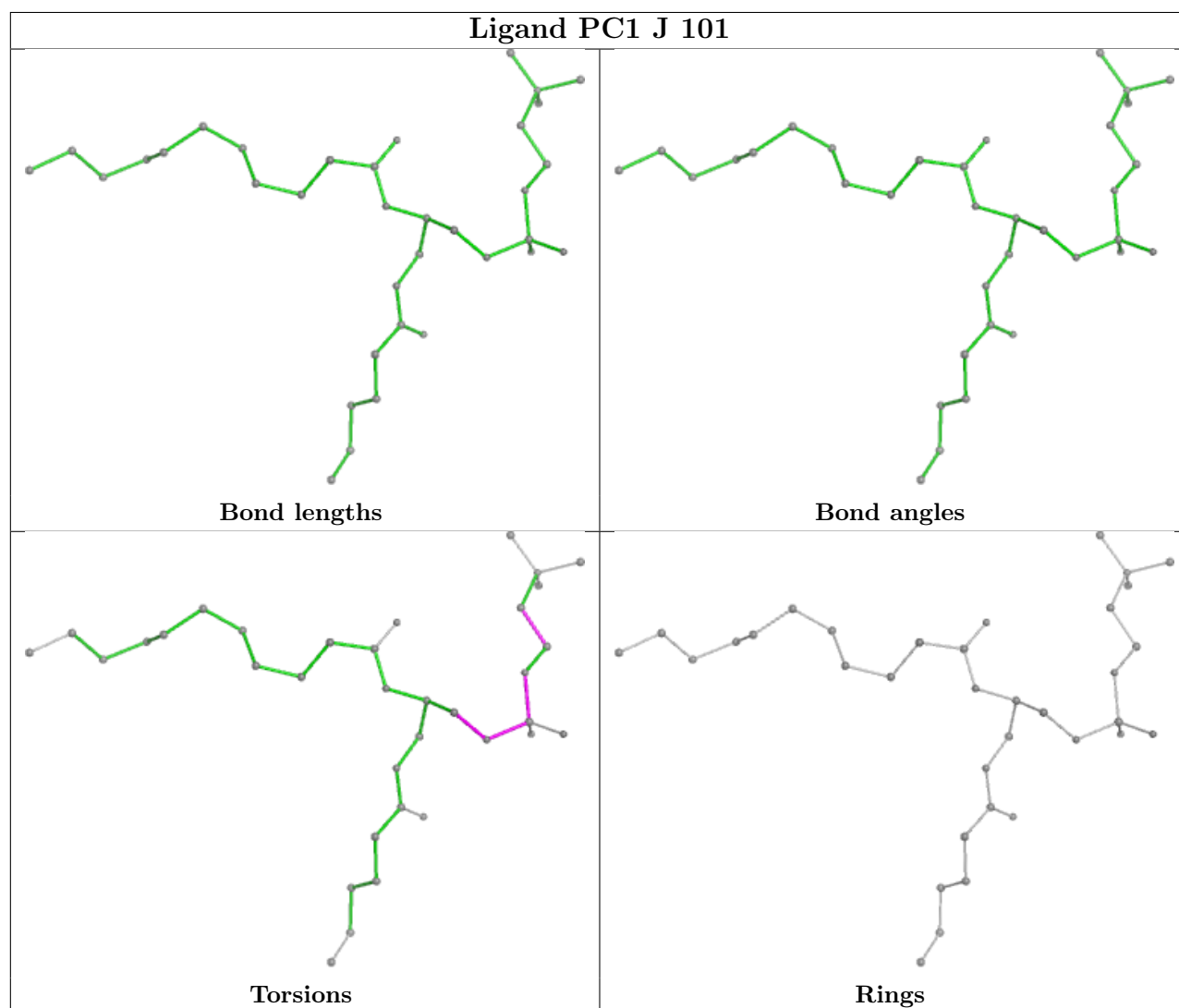
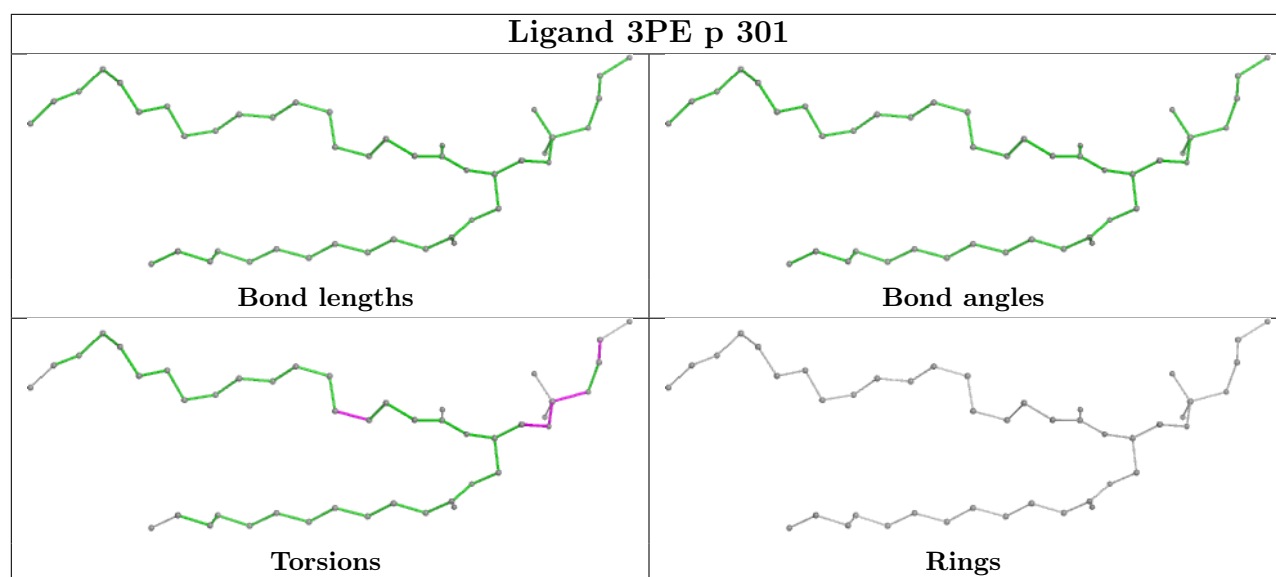






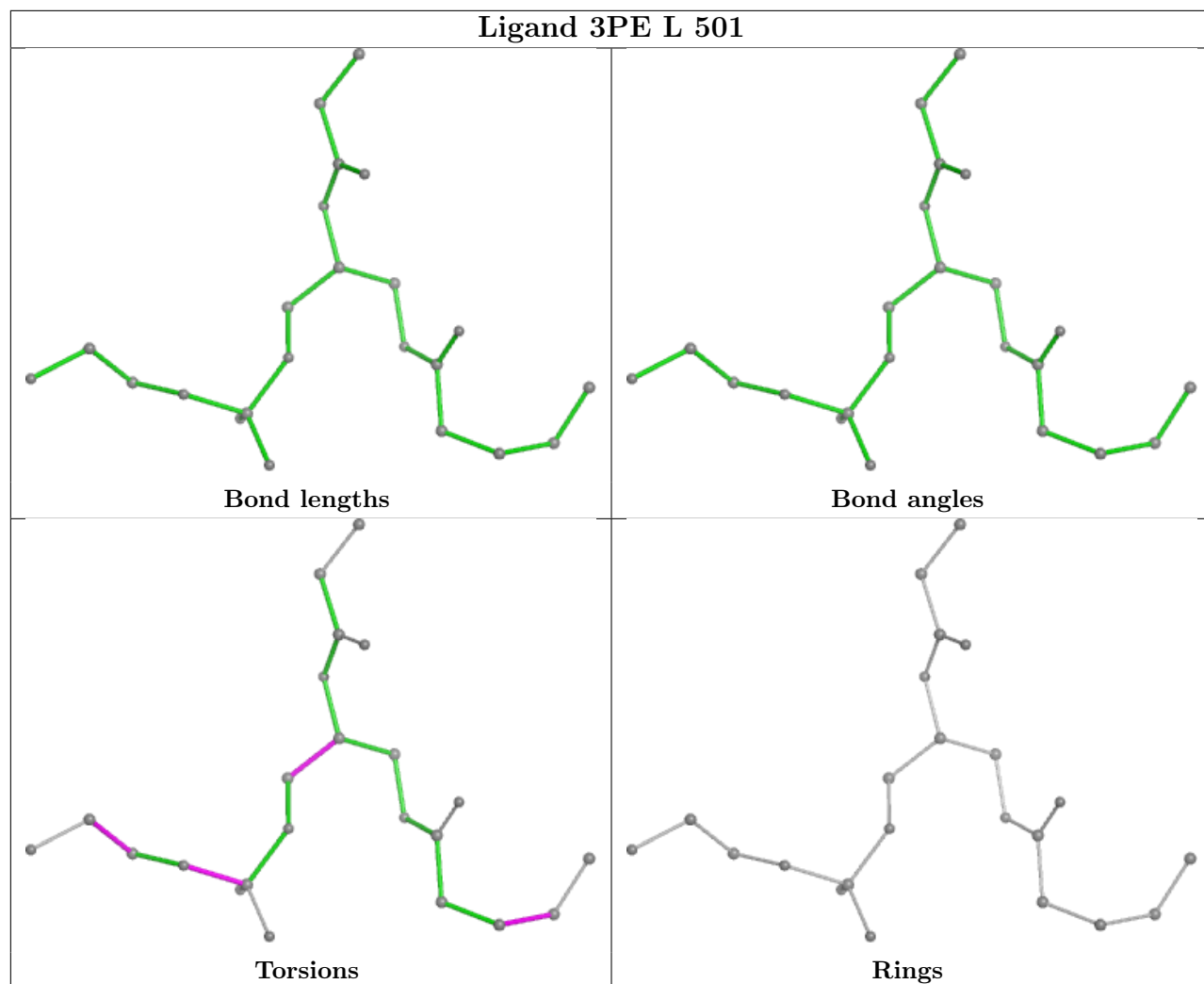


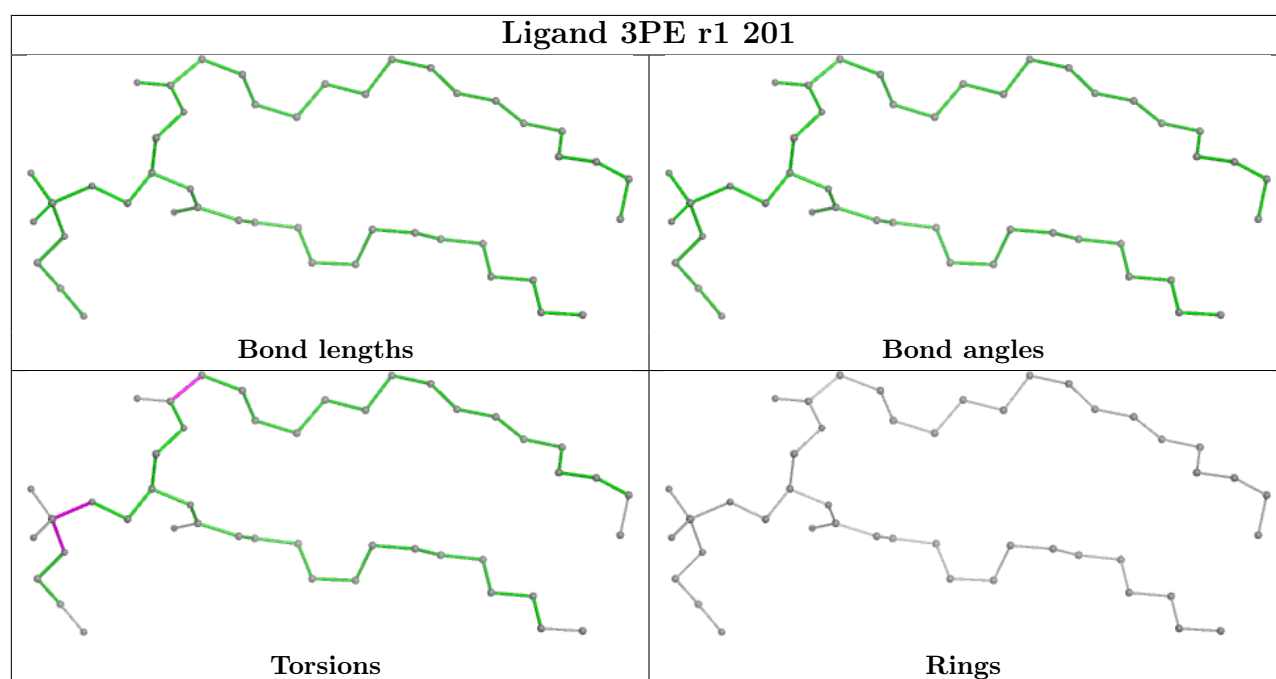
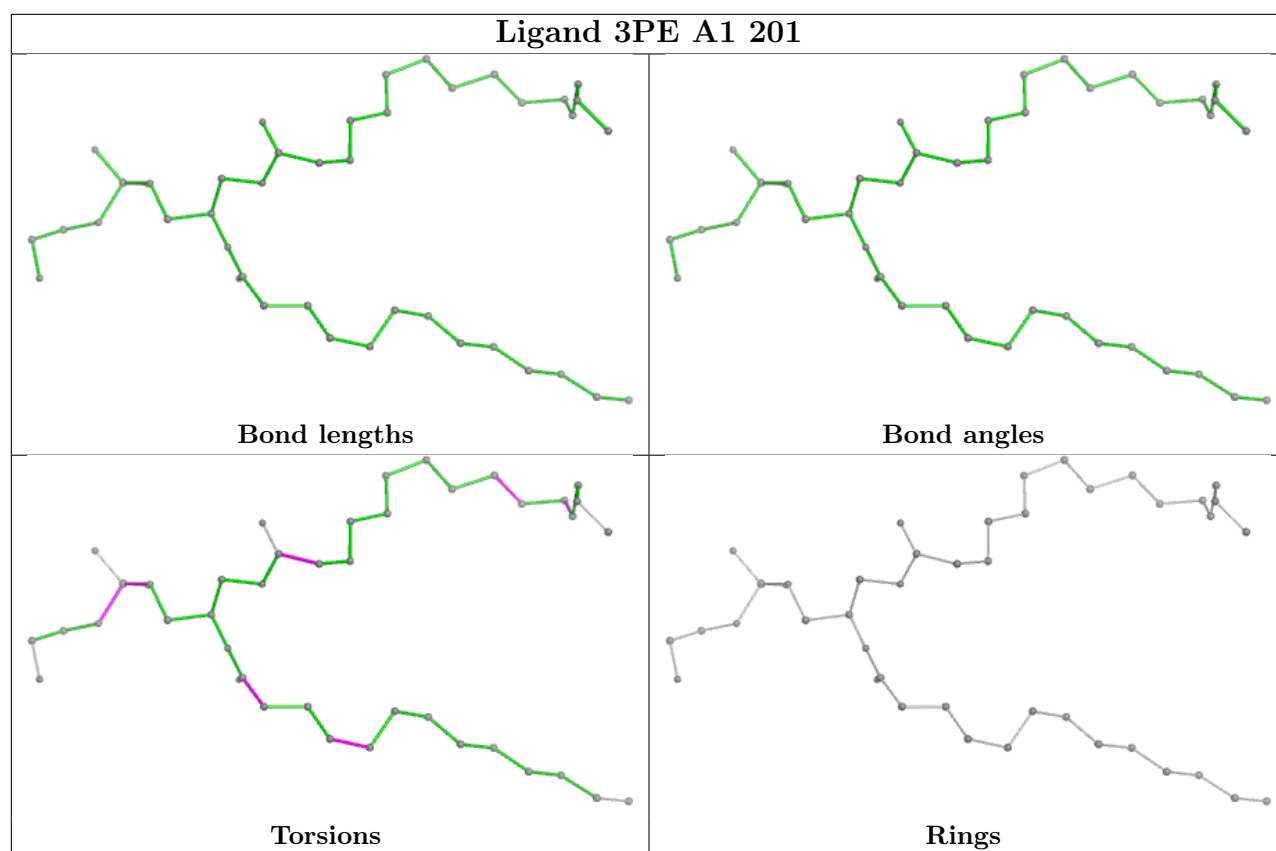


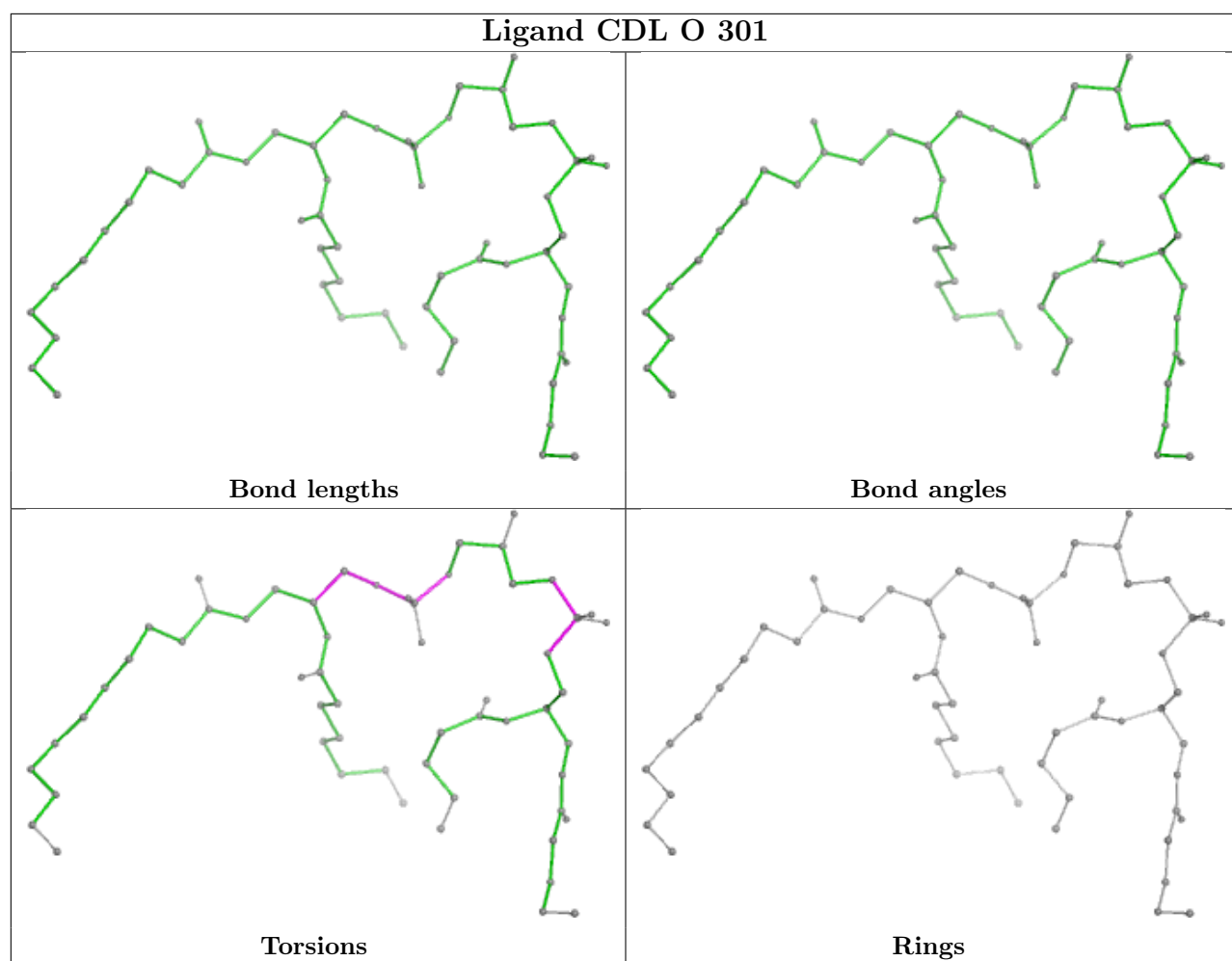


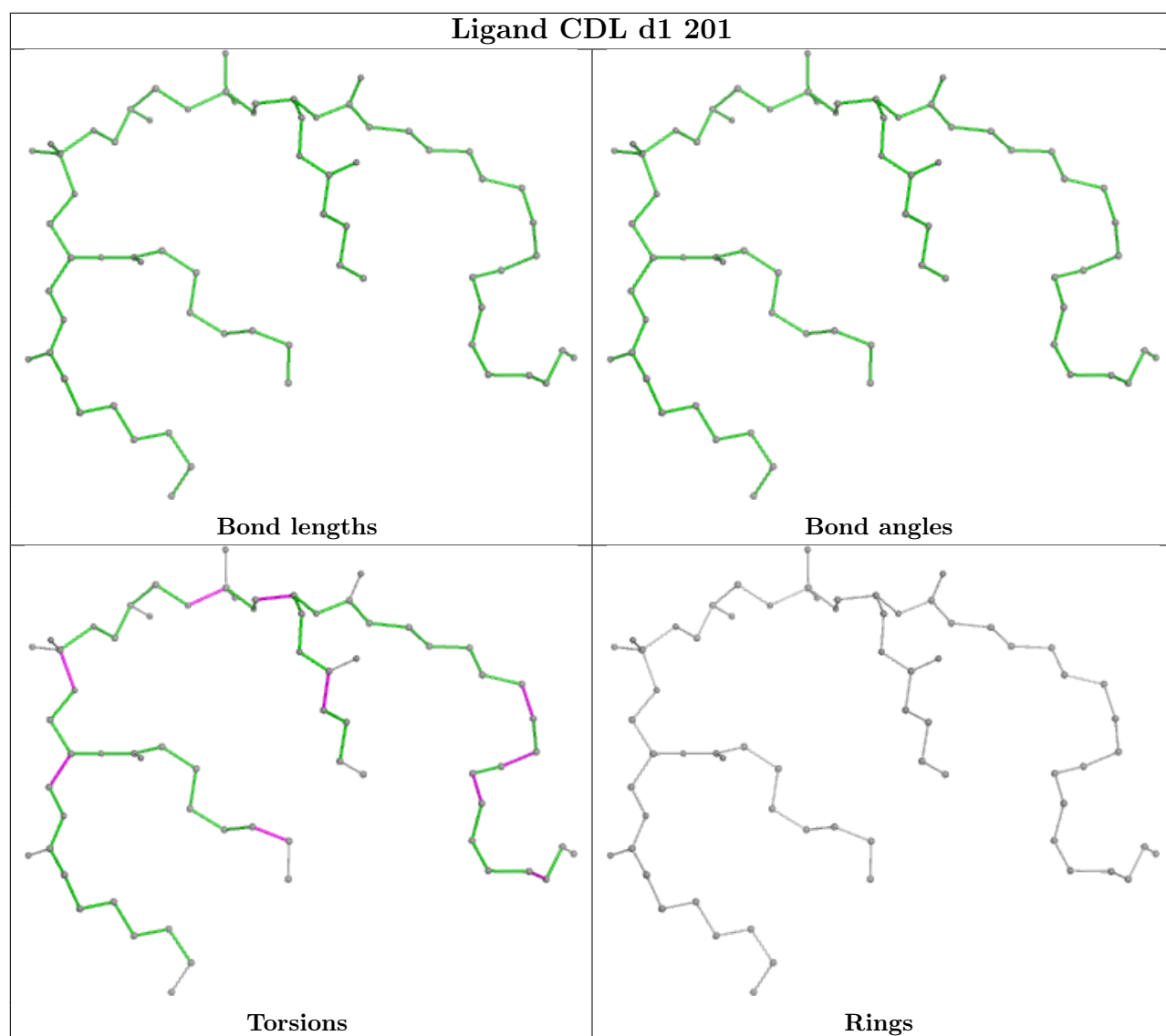


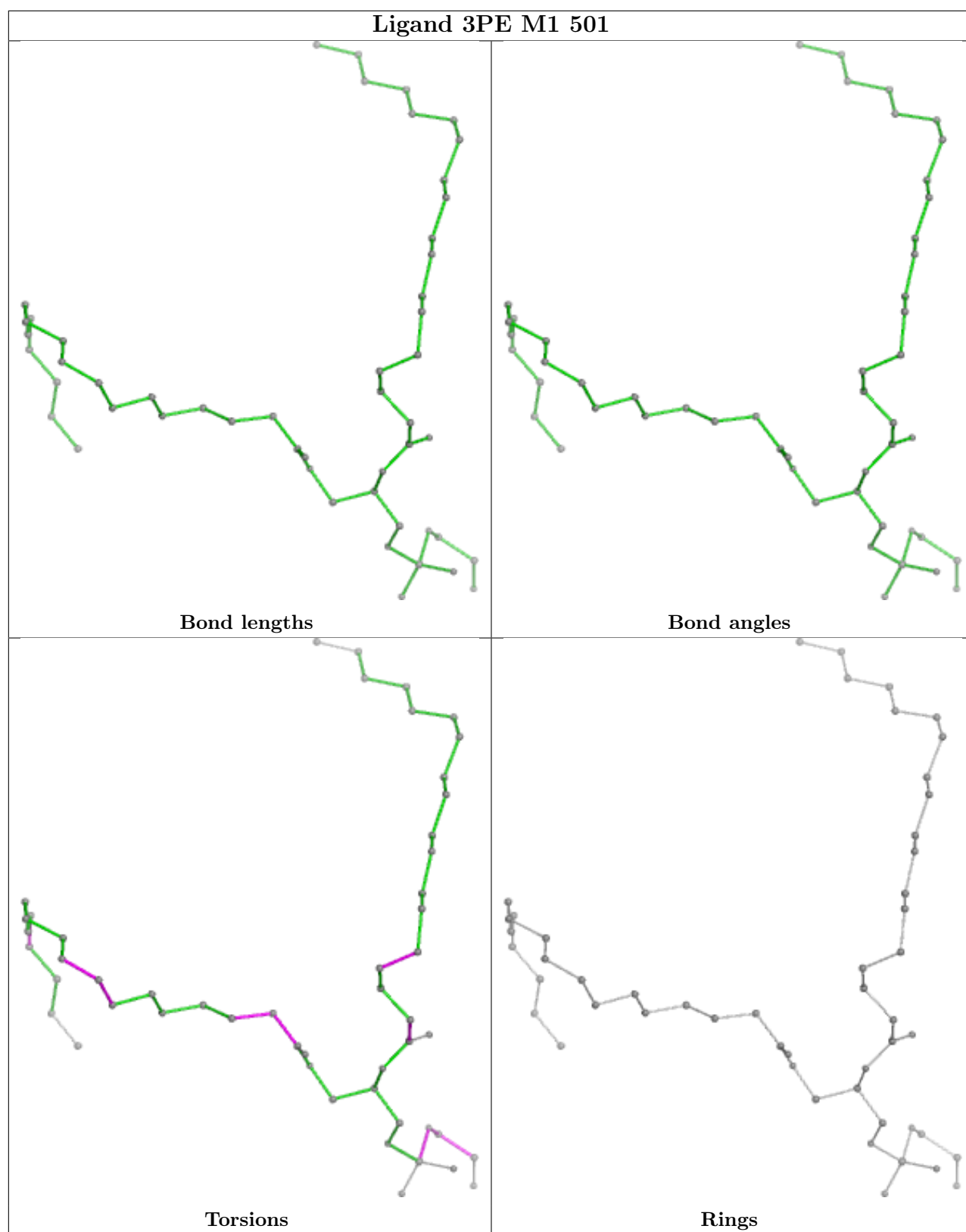
## Ligand 3PE L 501

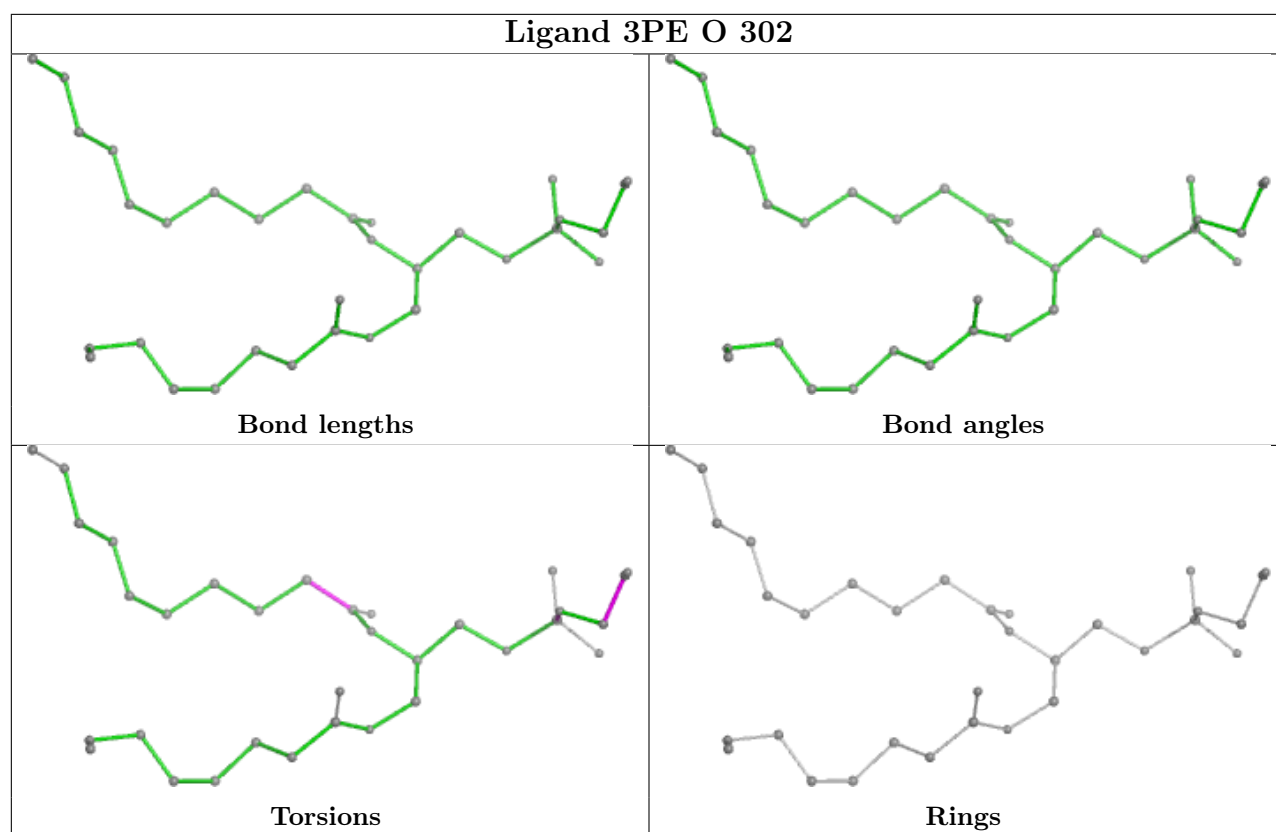


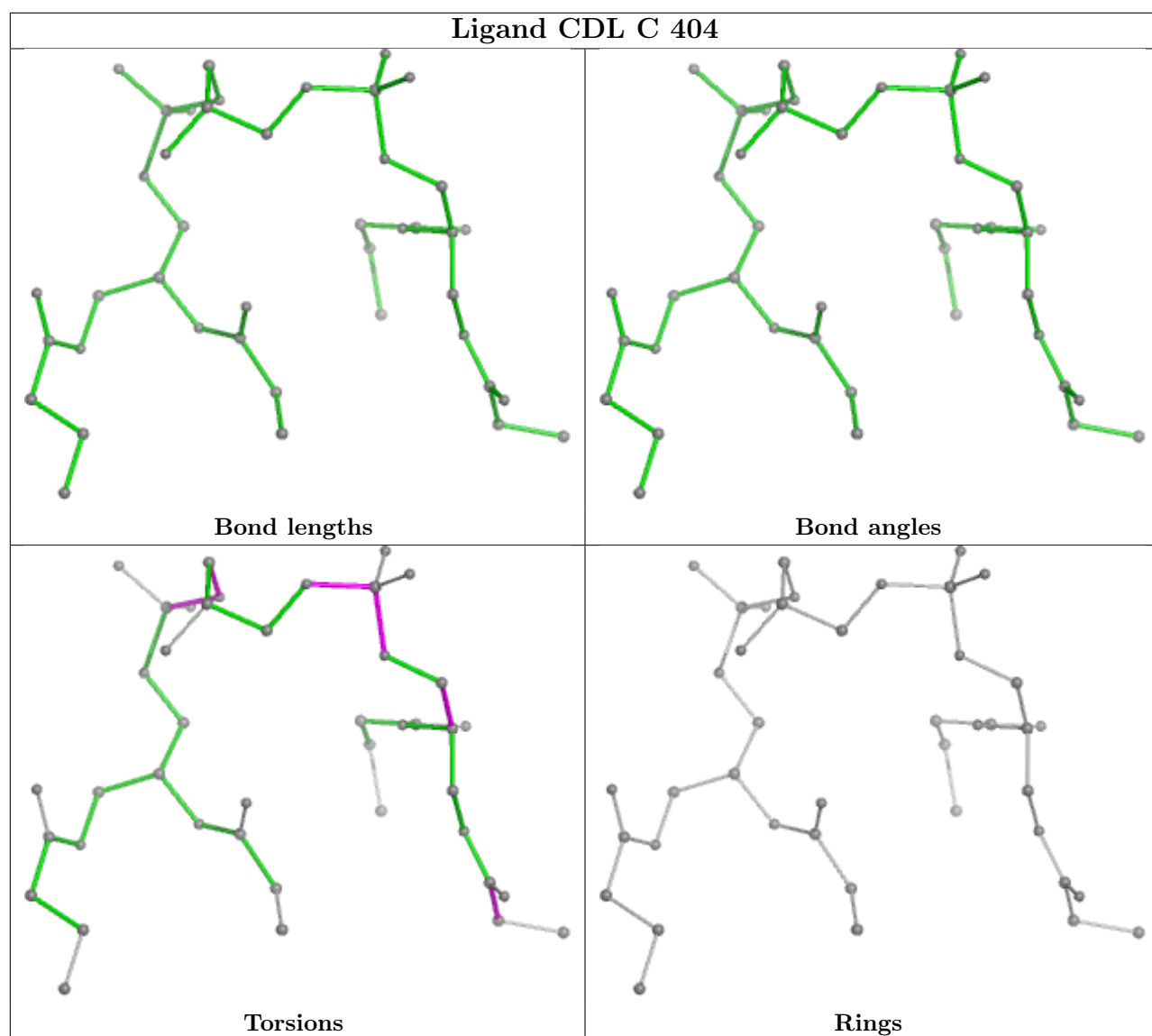


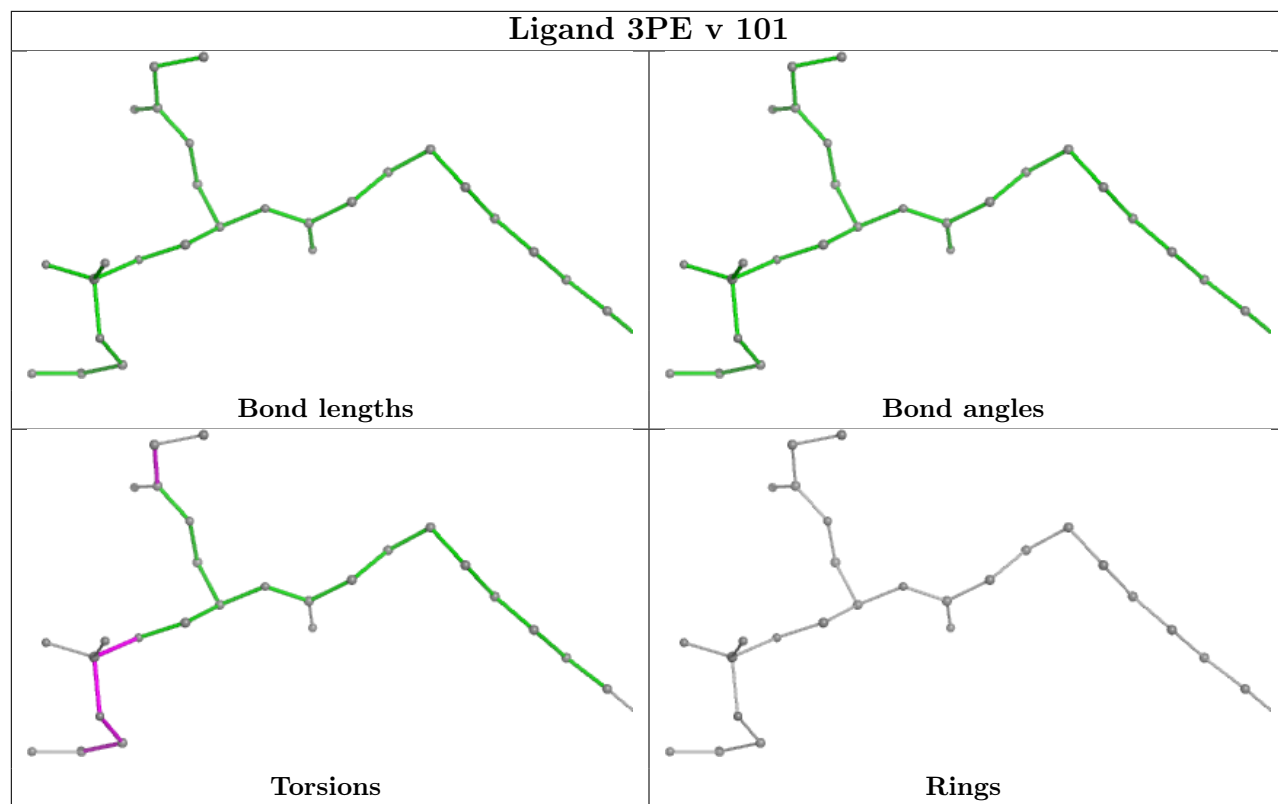




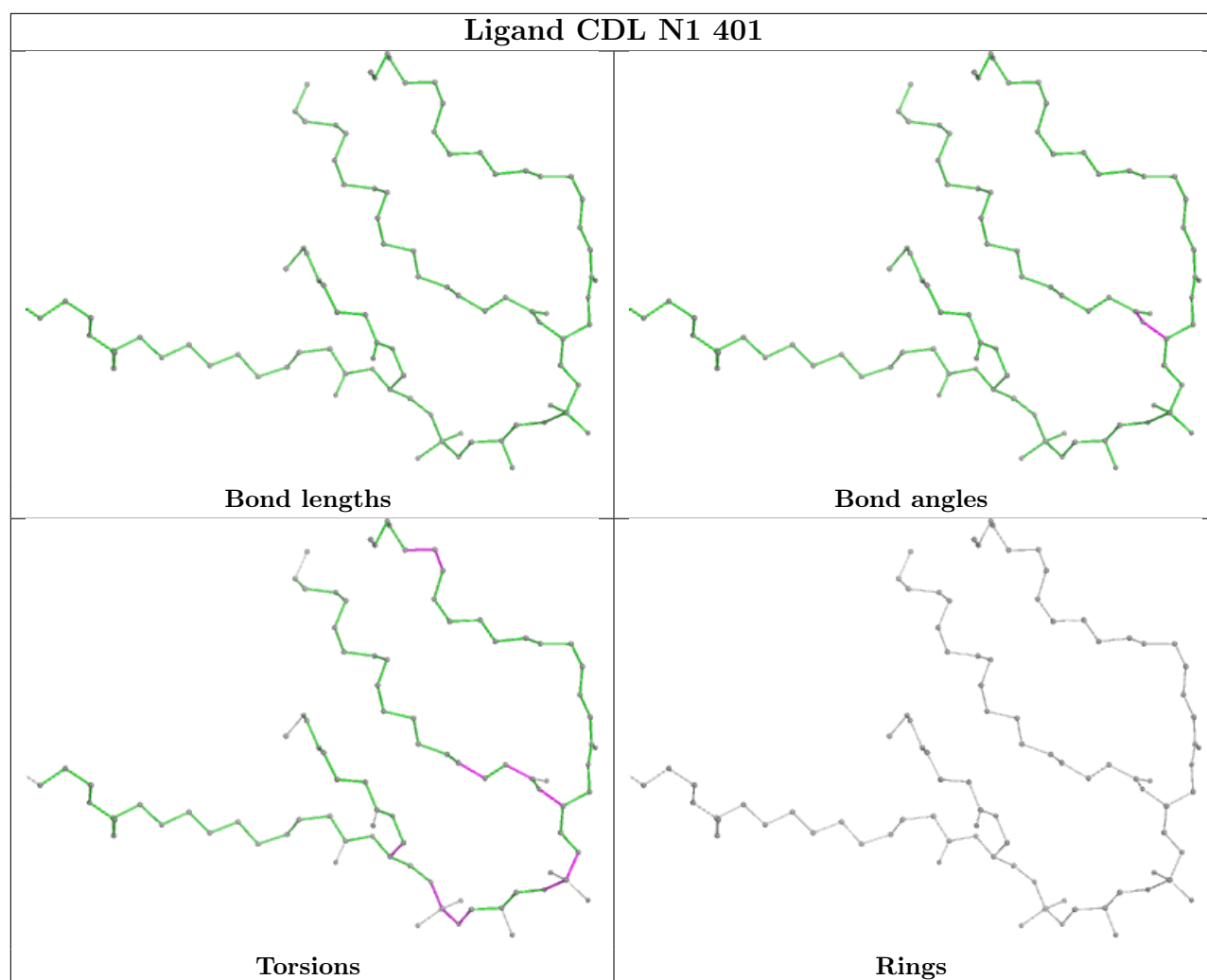


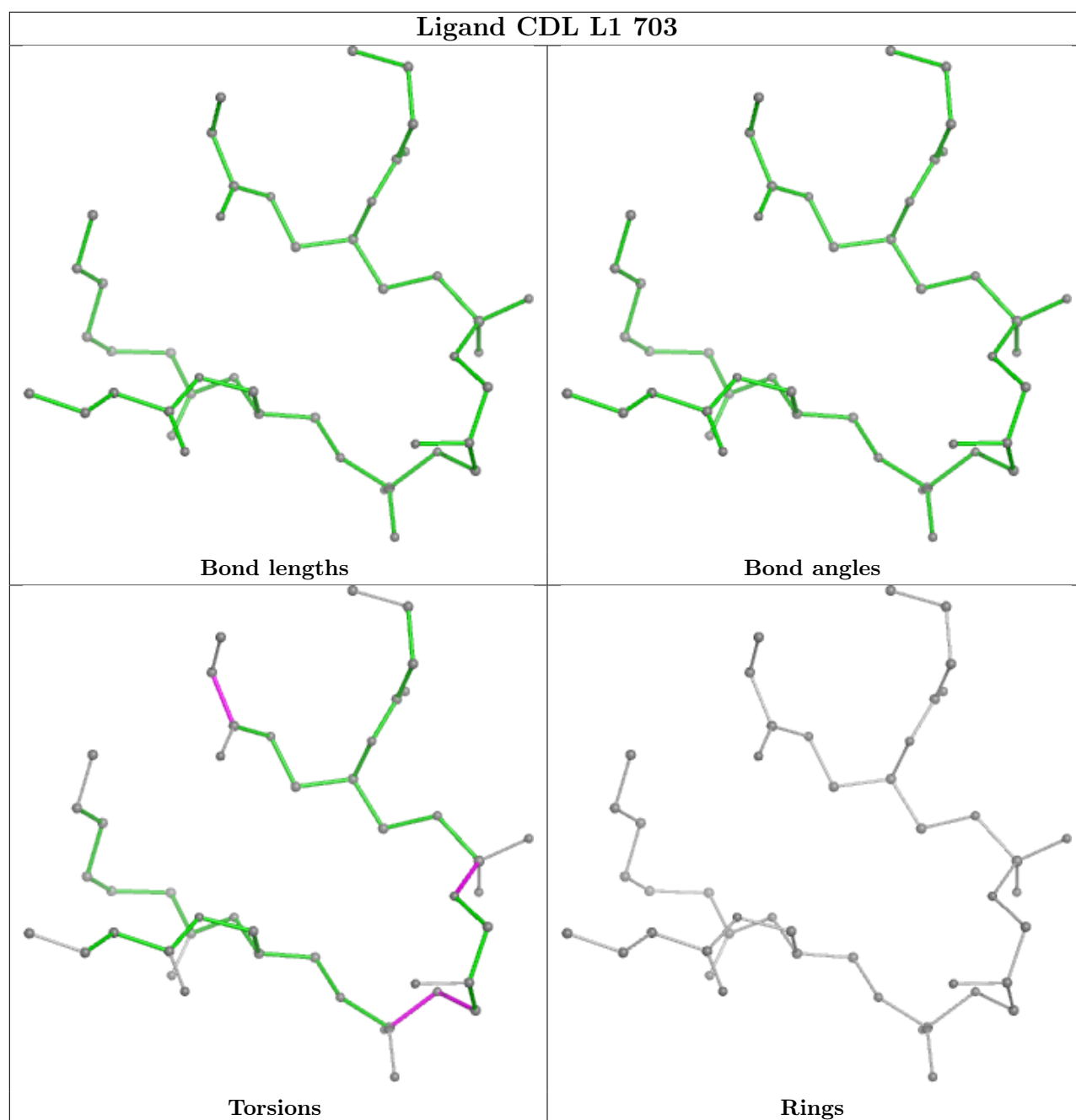


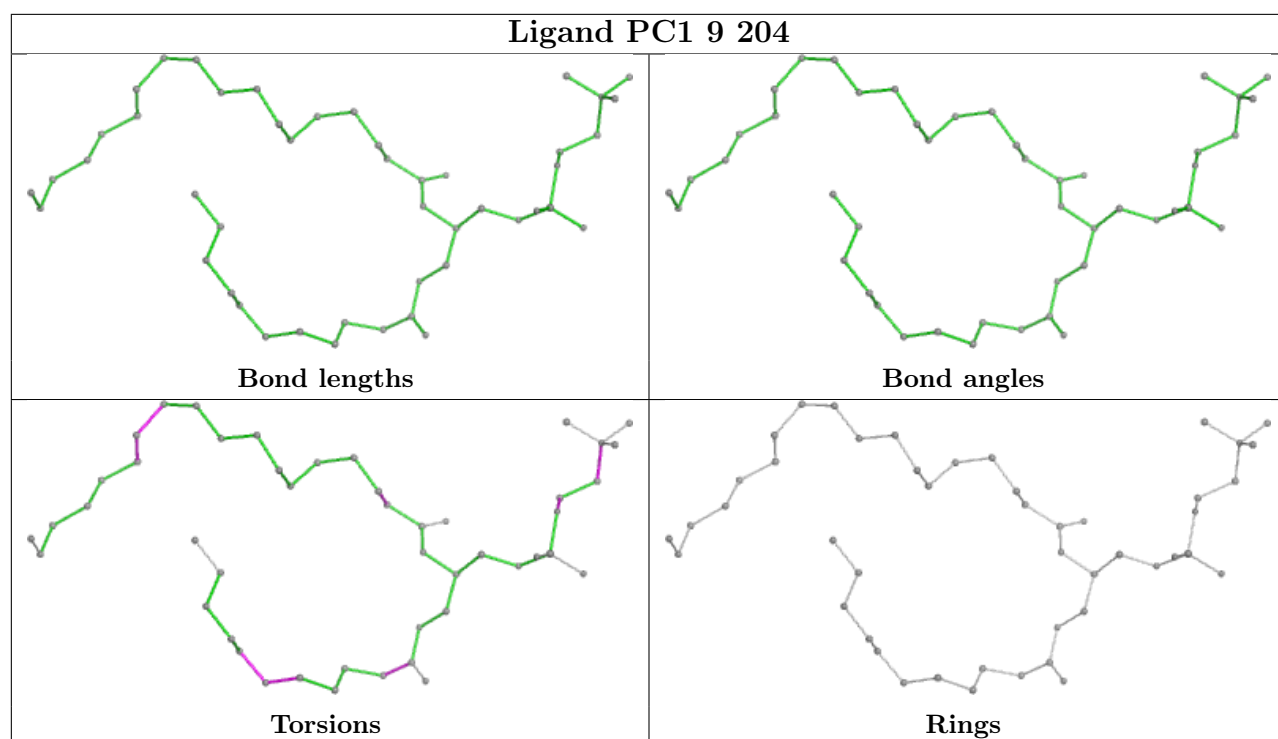


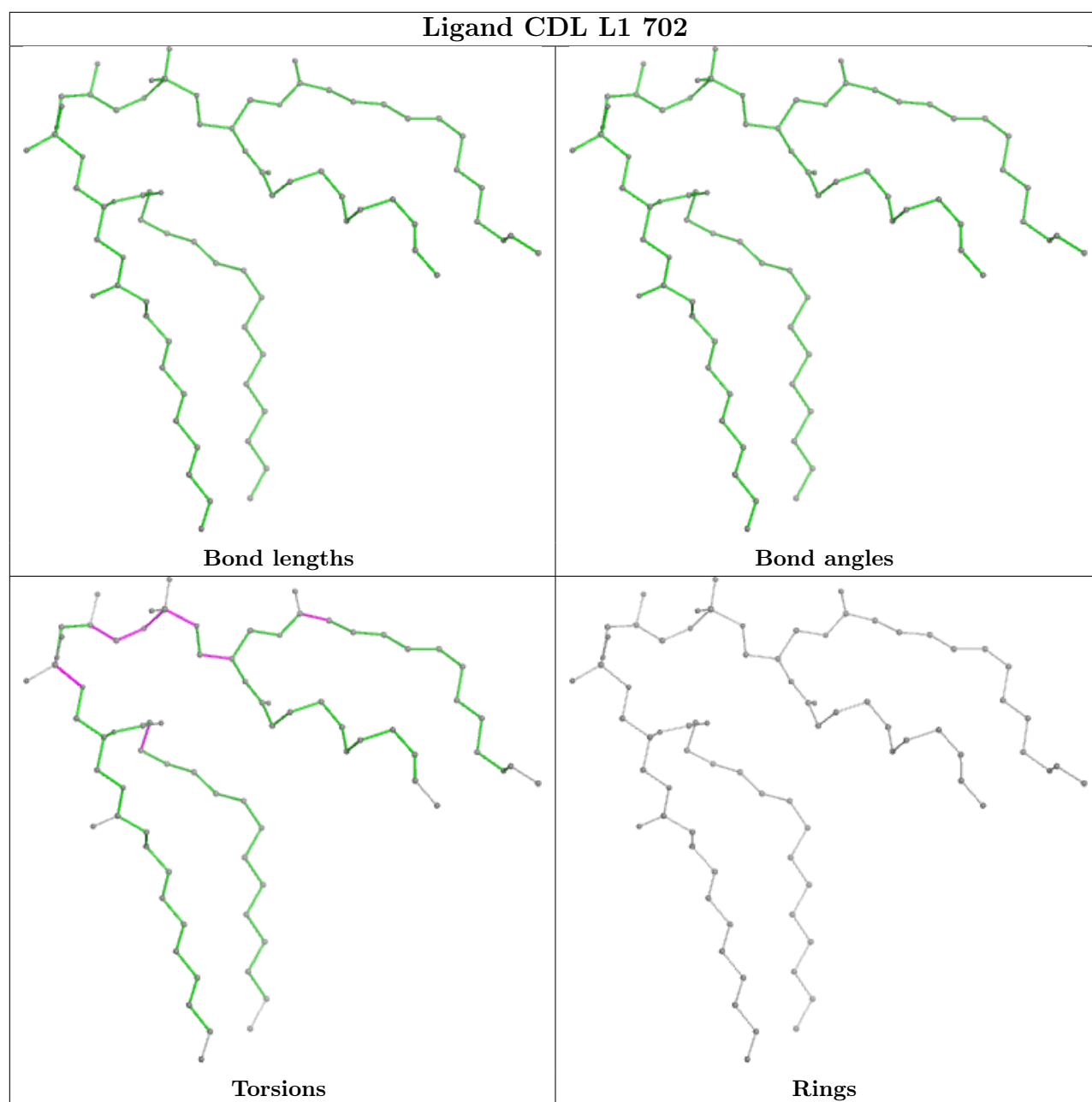


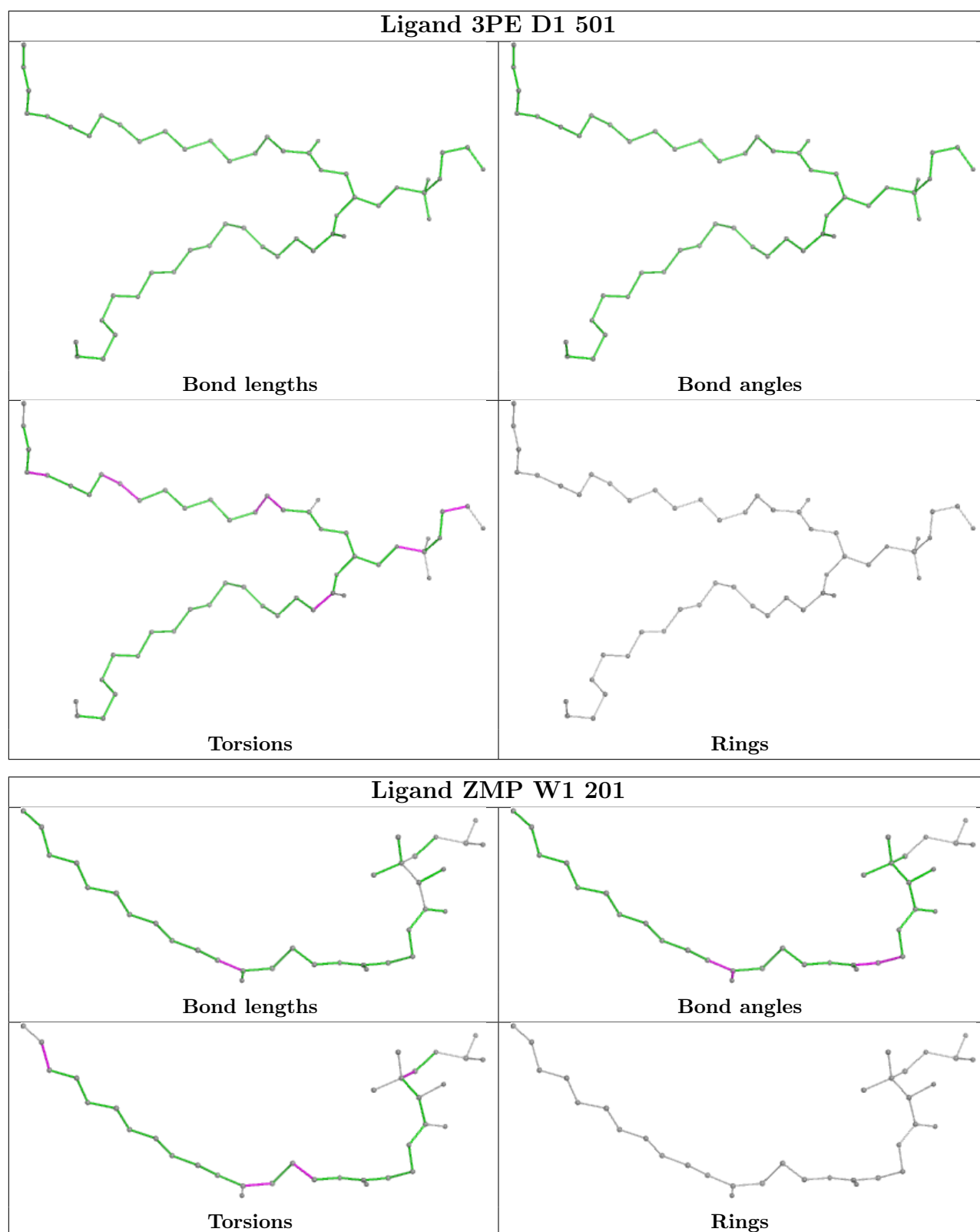


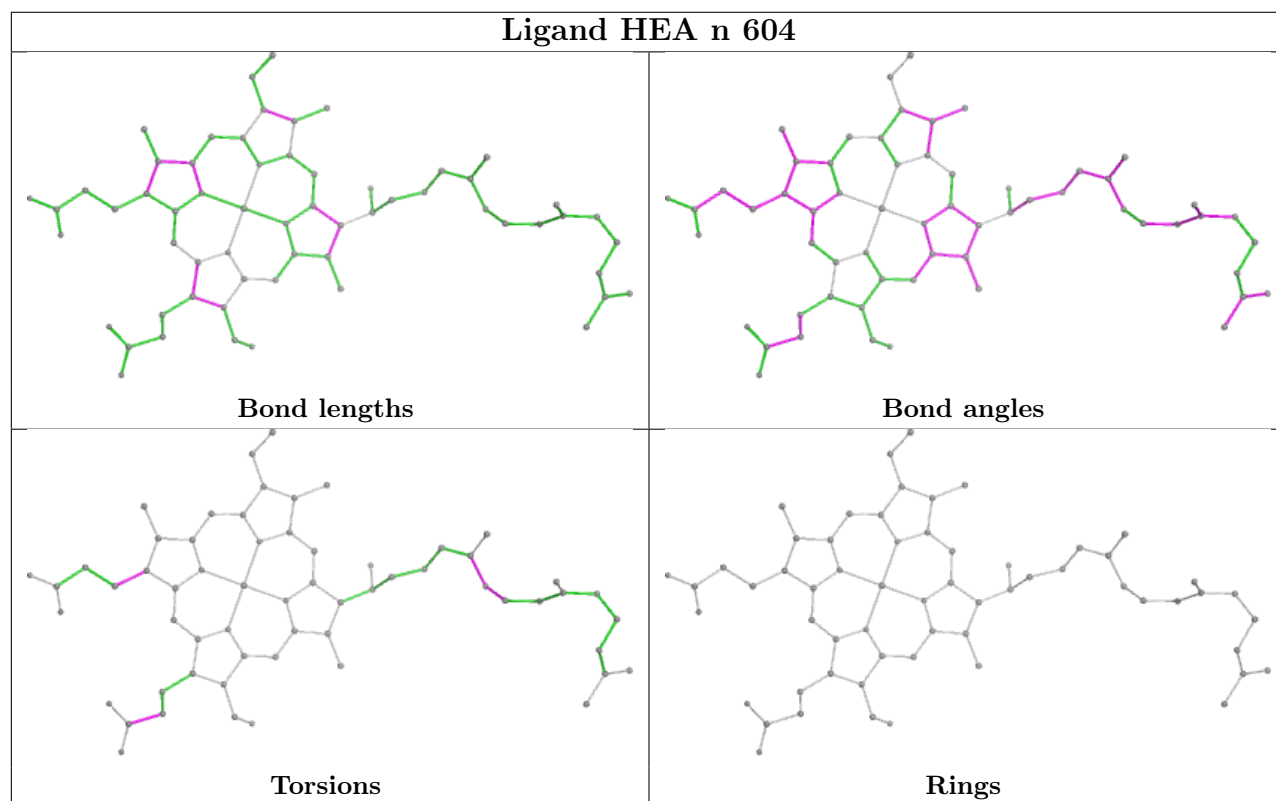
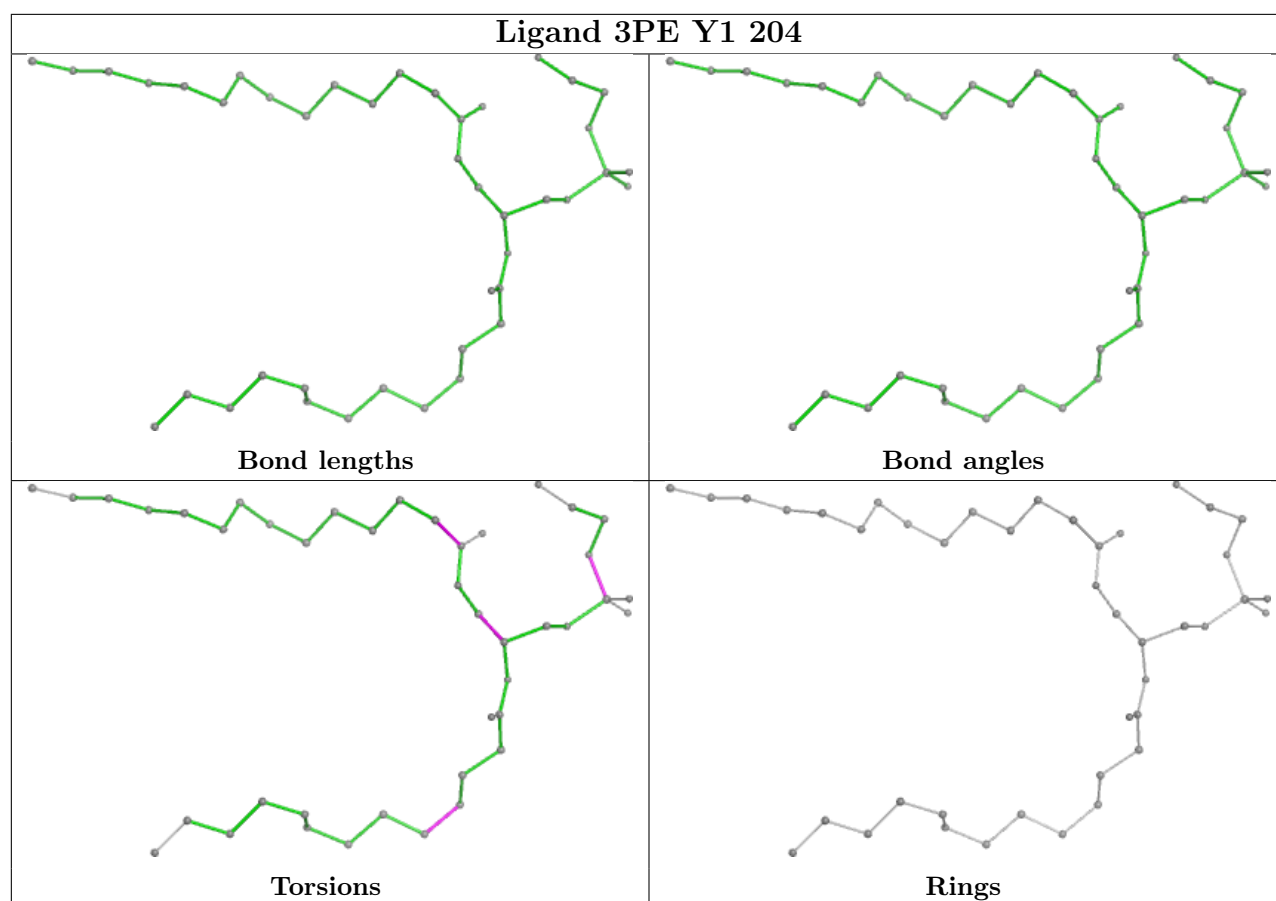


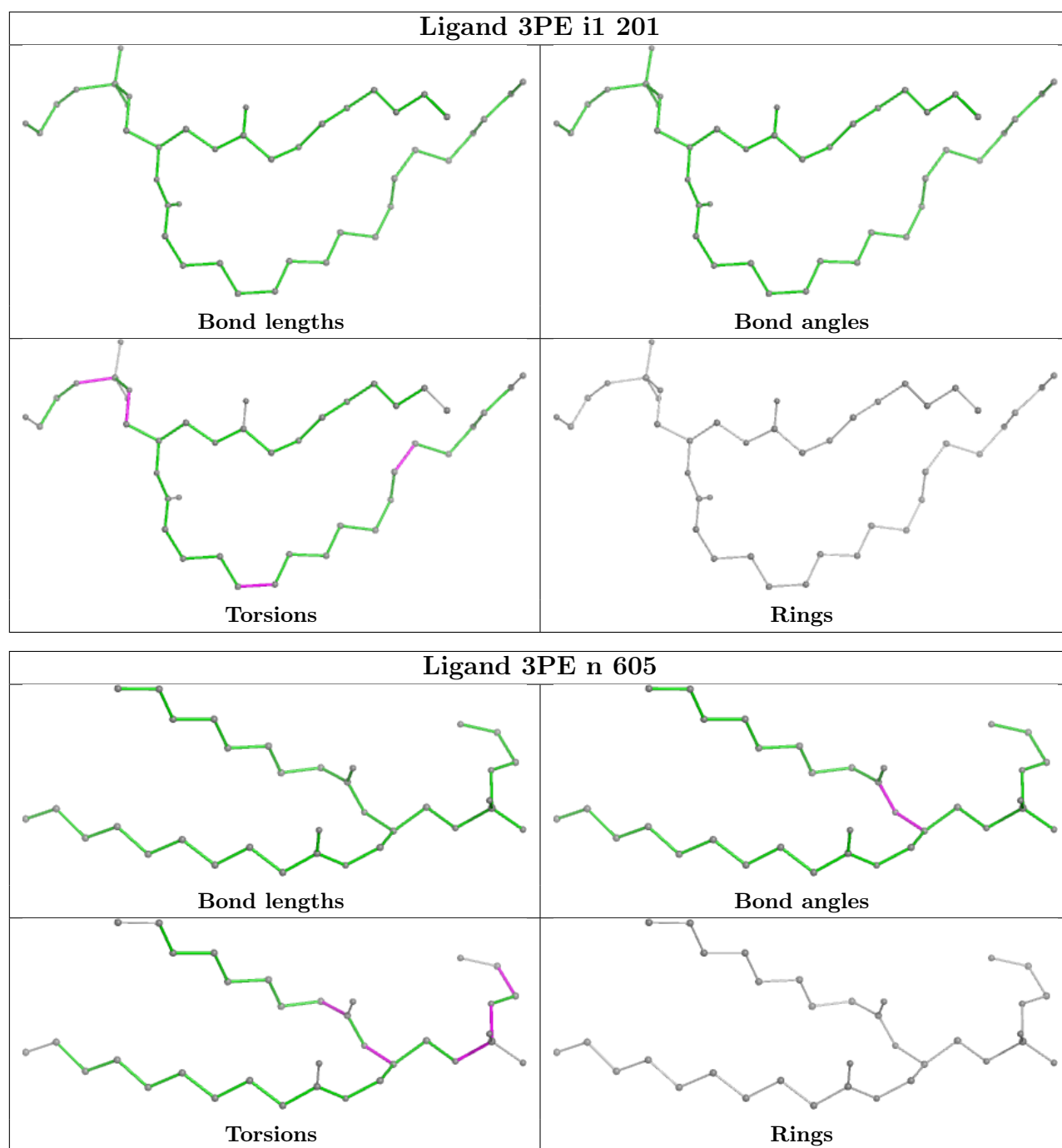


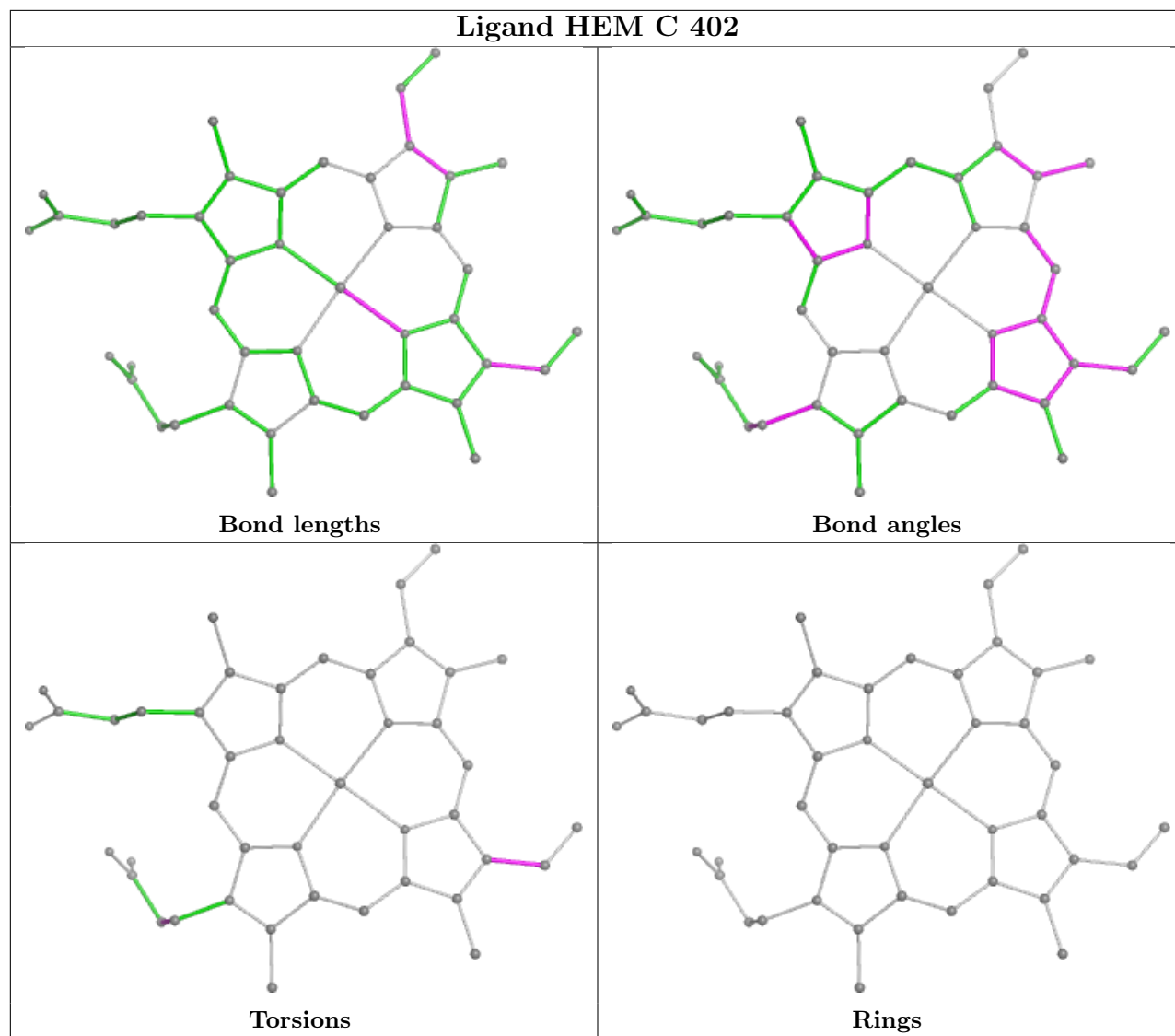




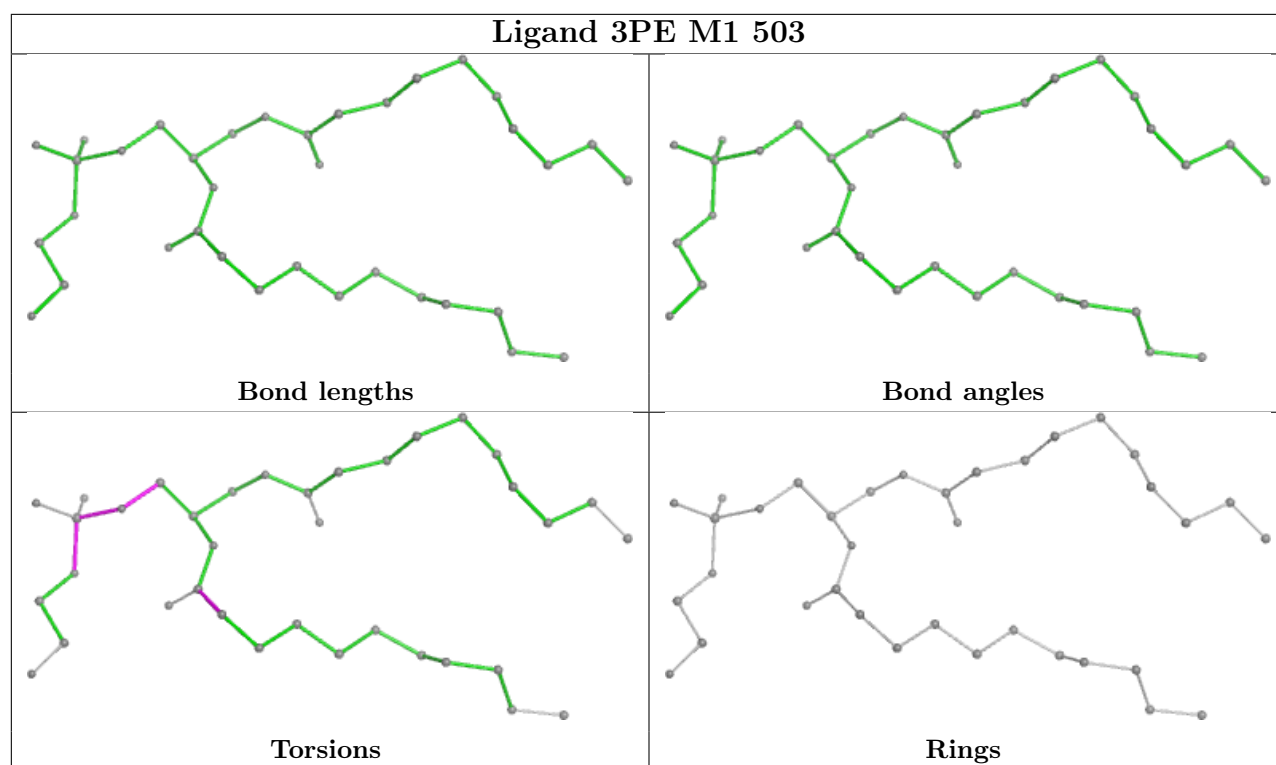


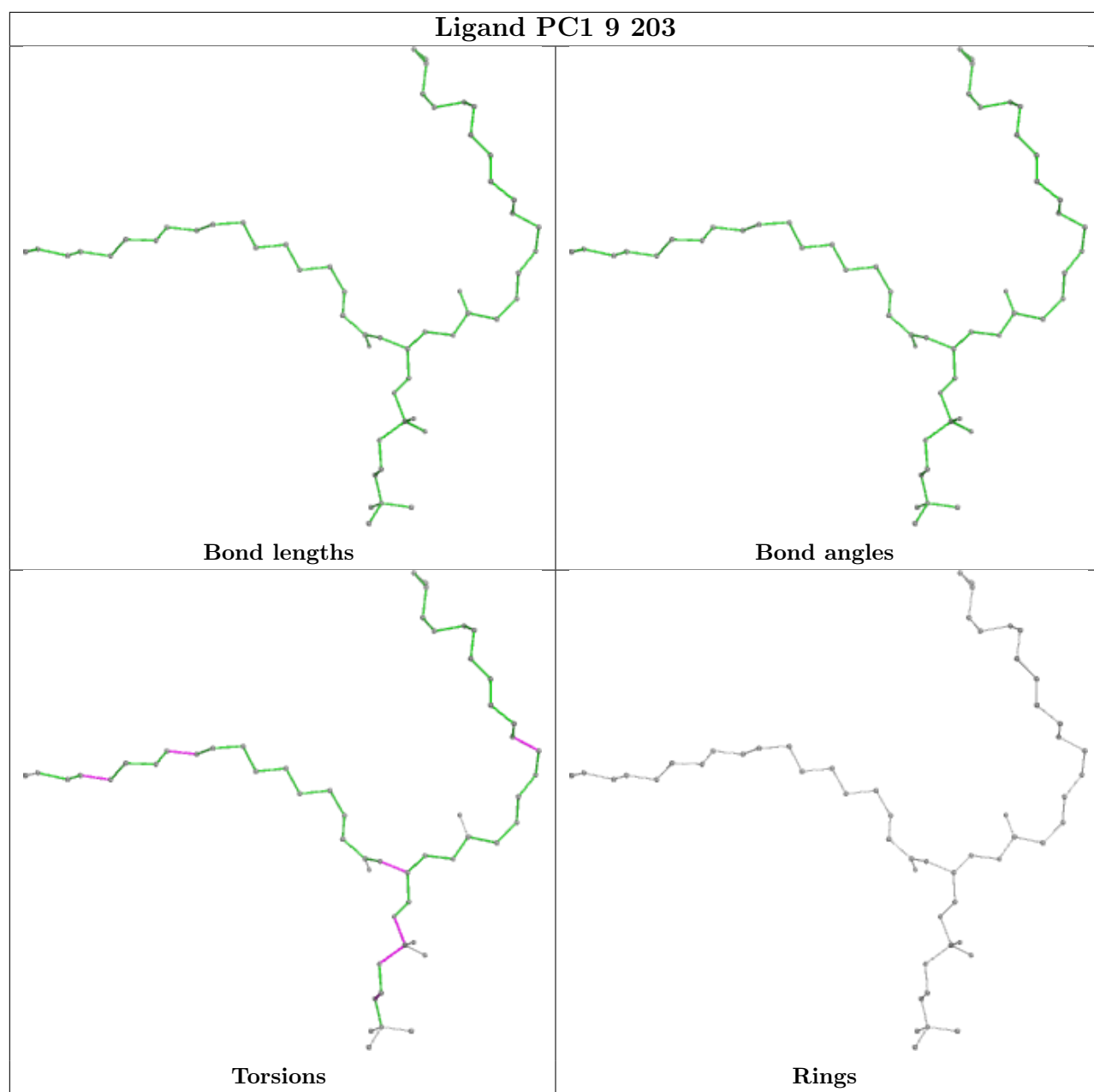


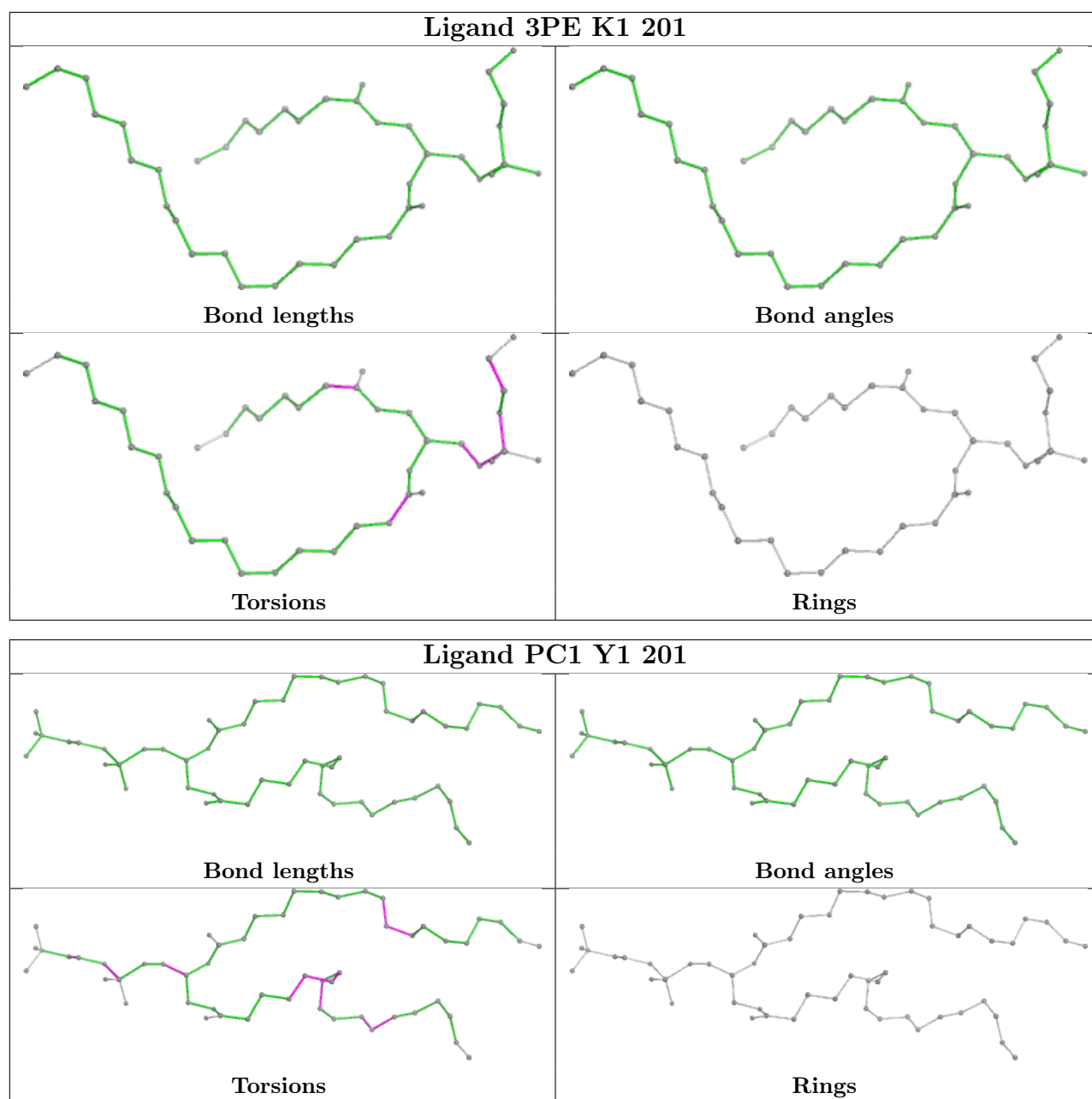


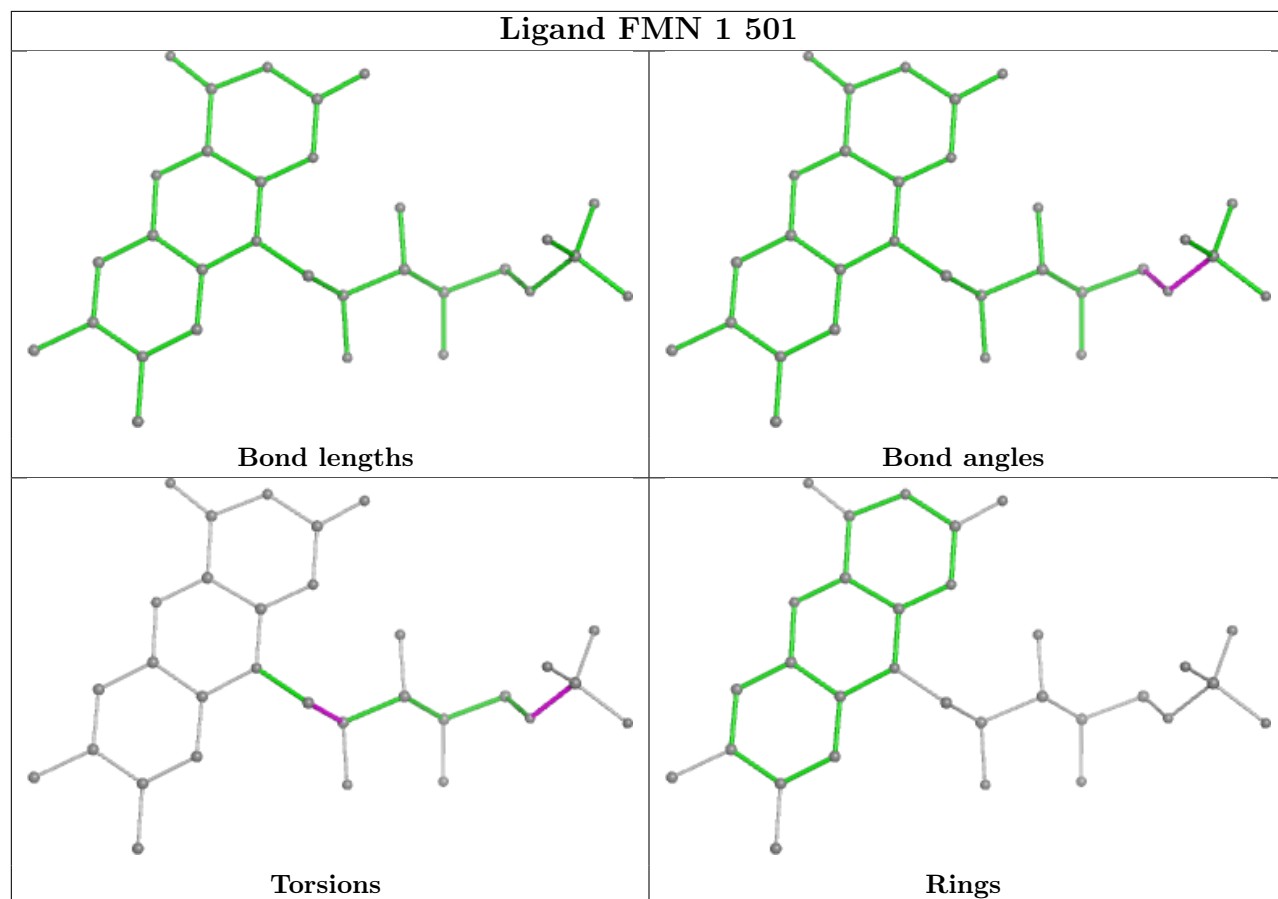
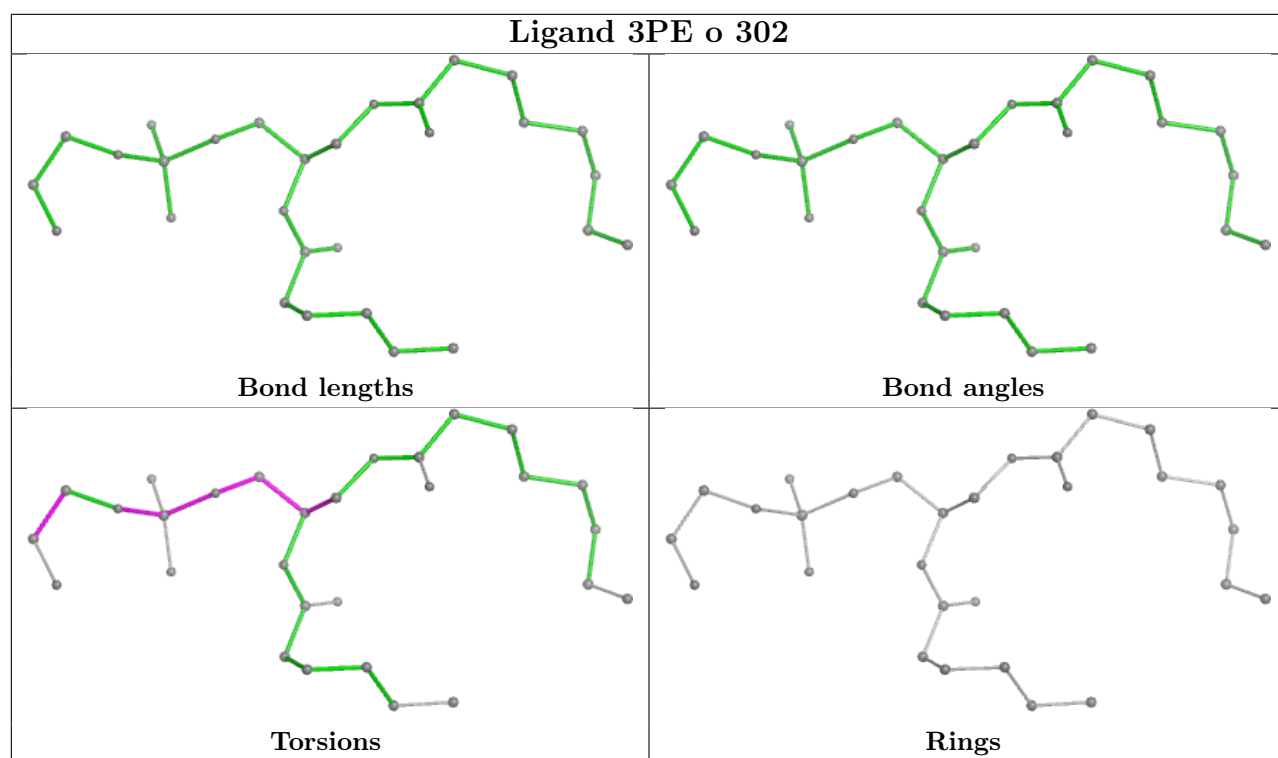


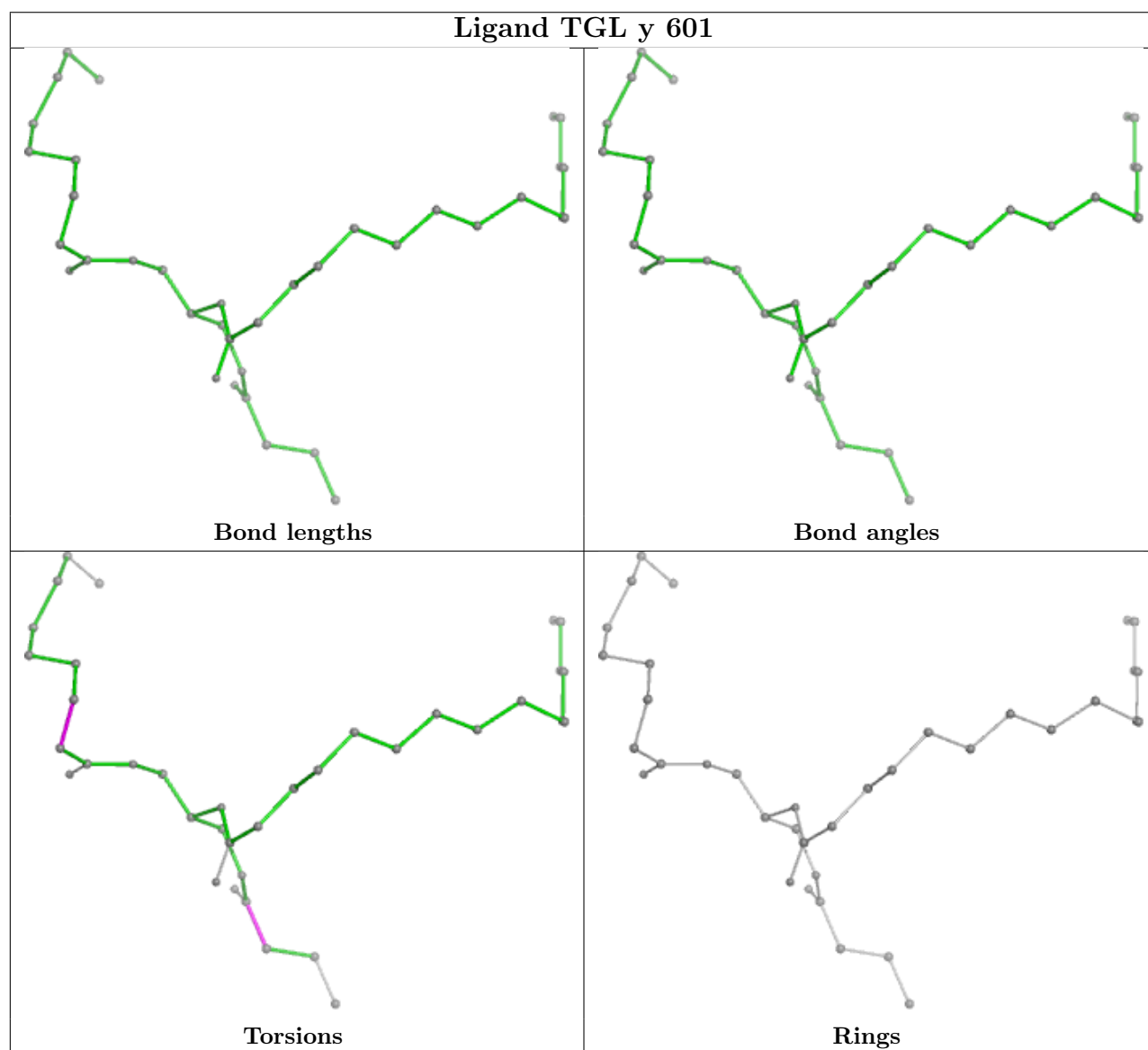
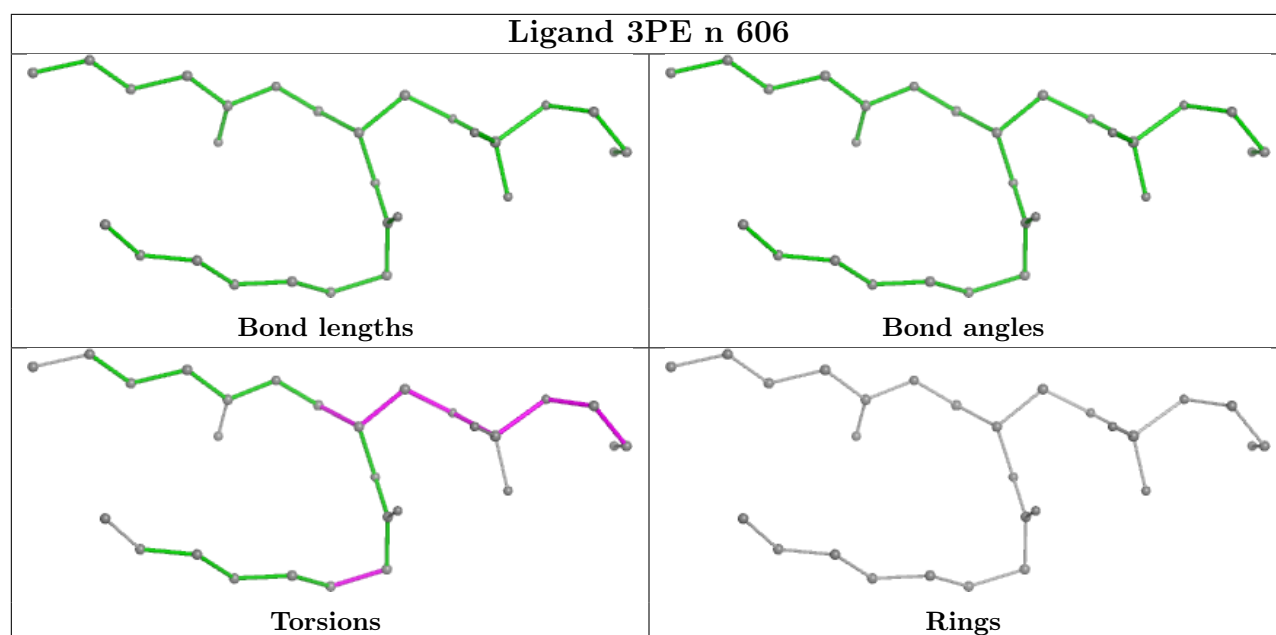


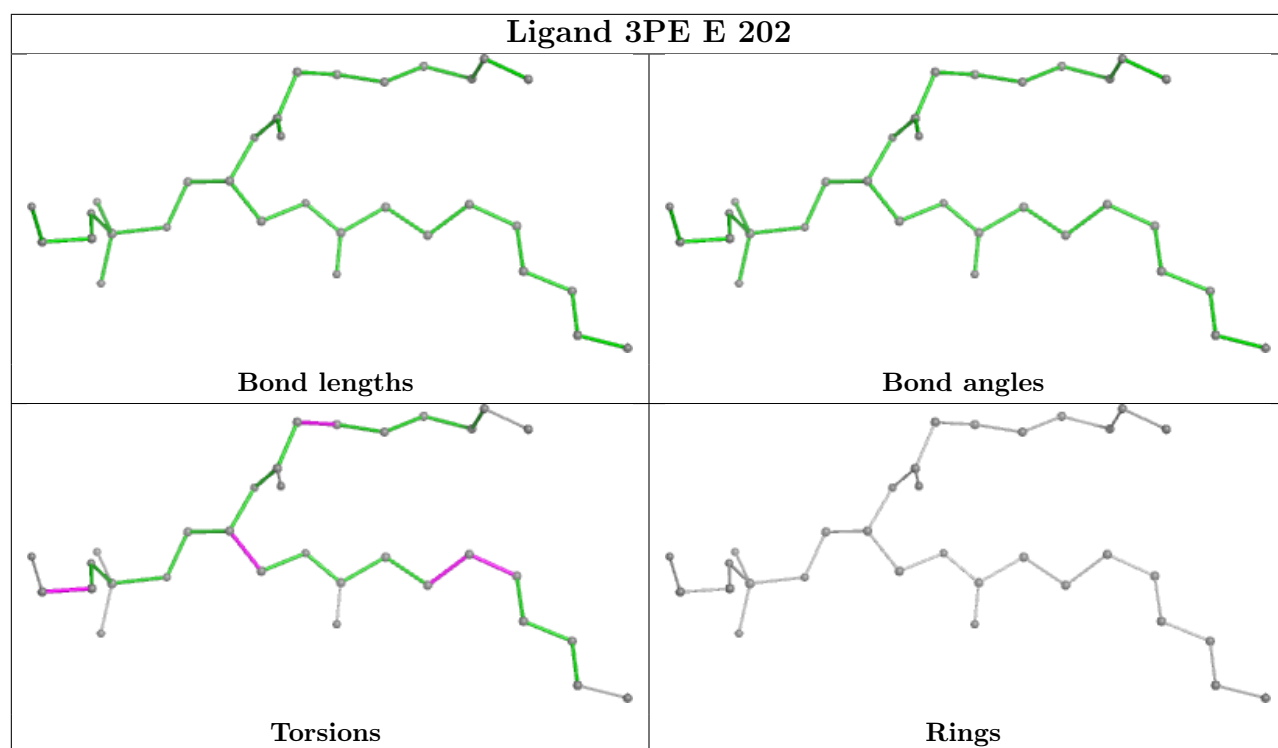


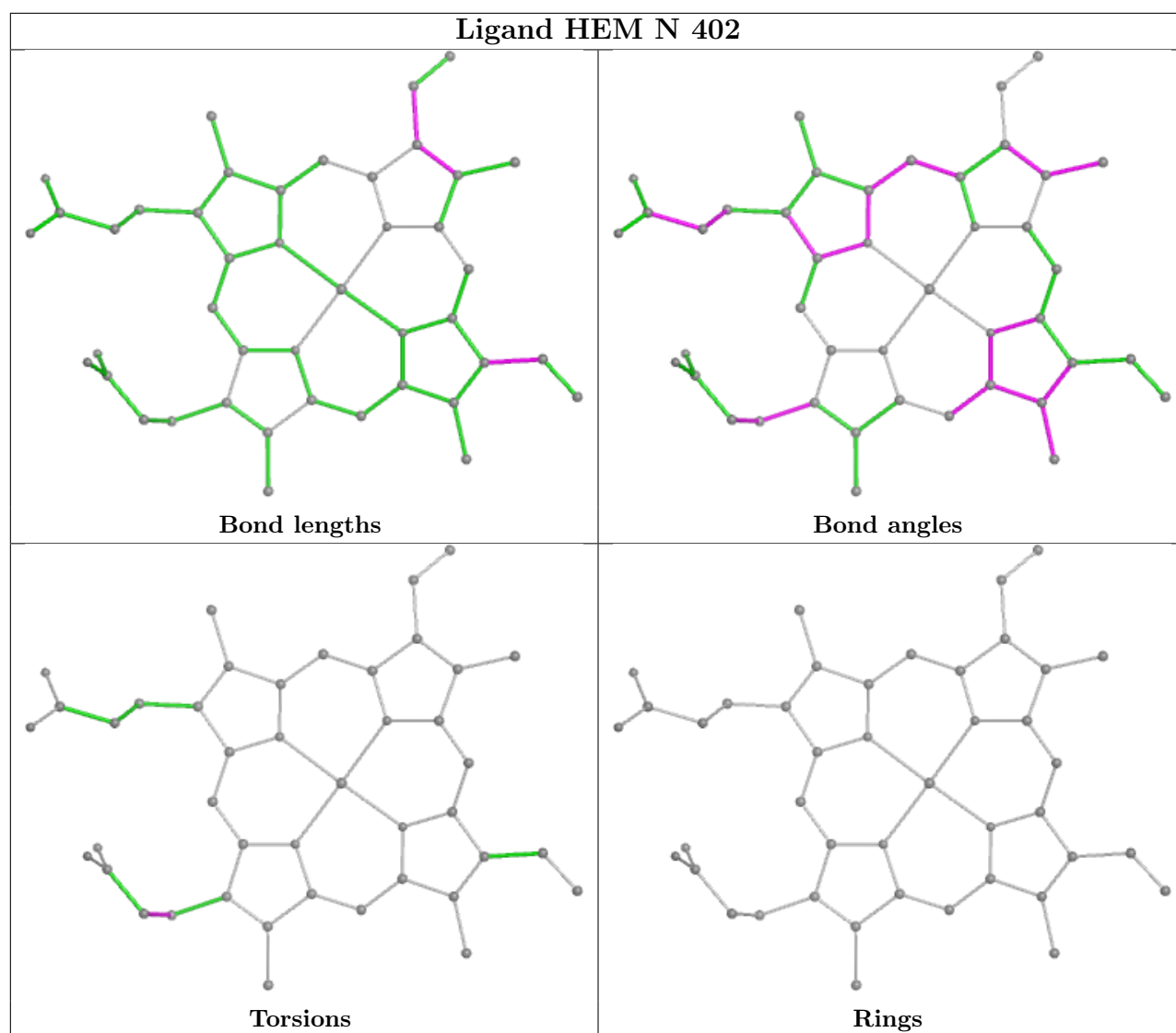


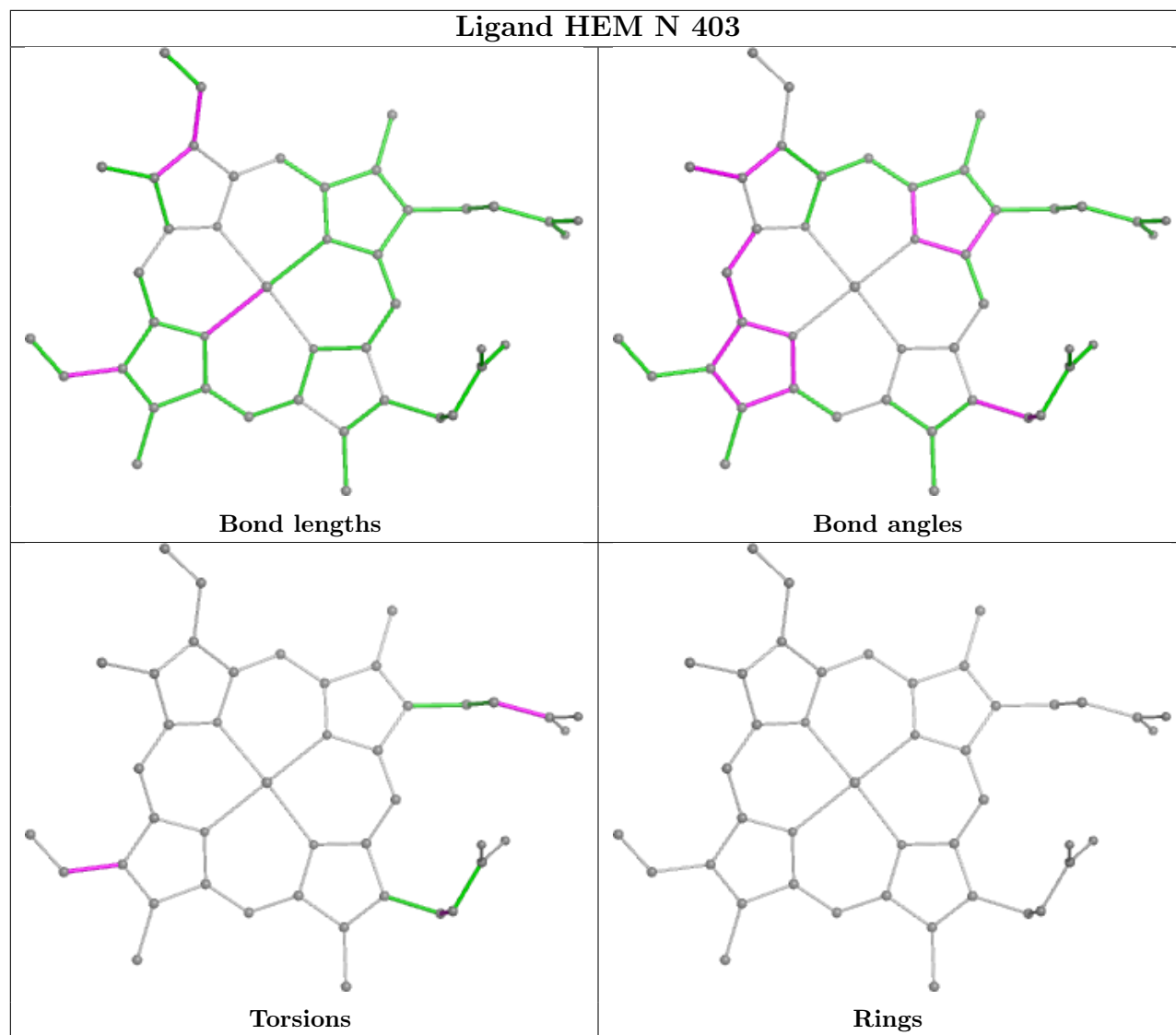




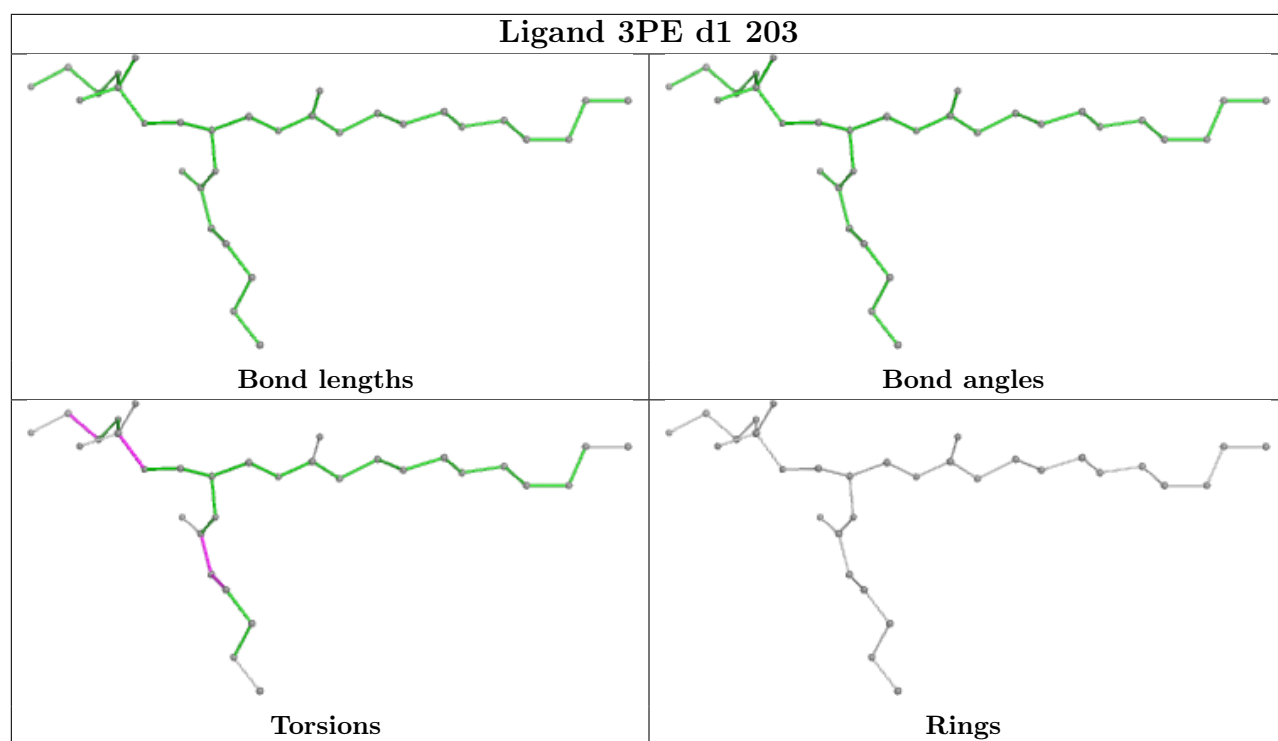


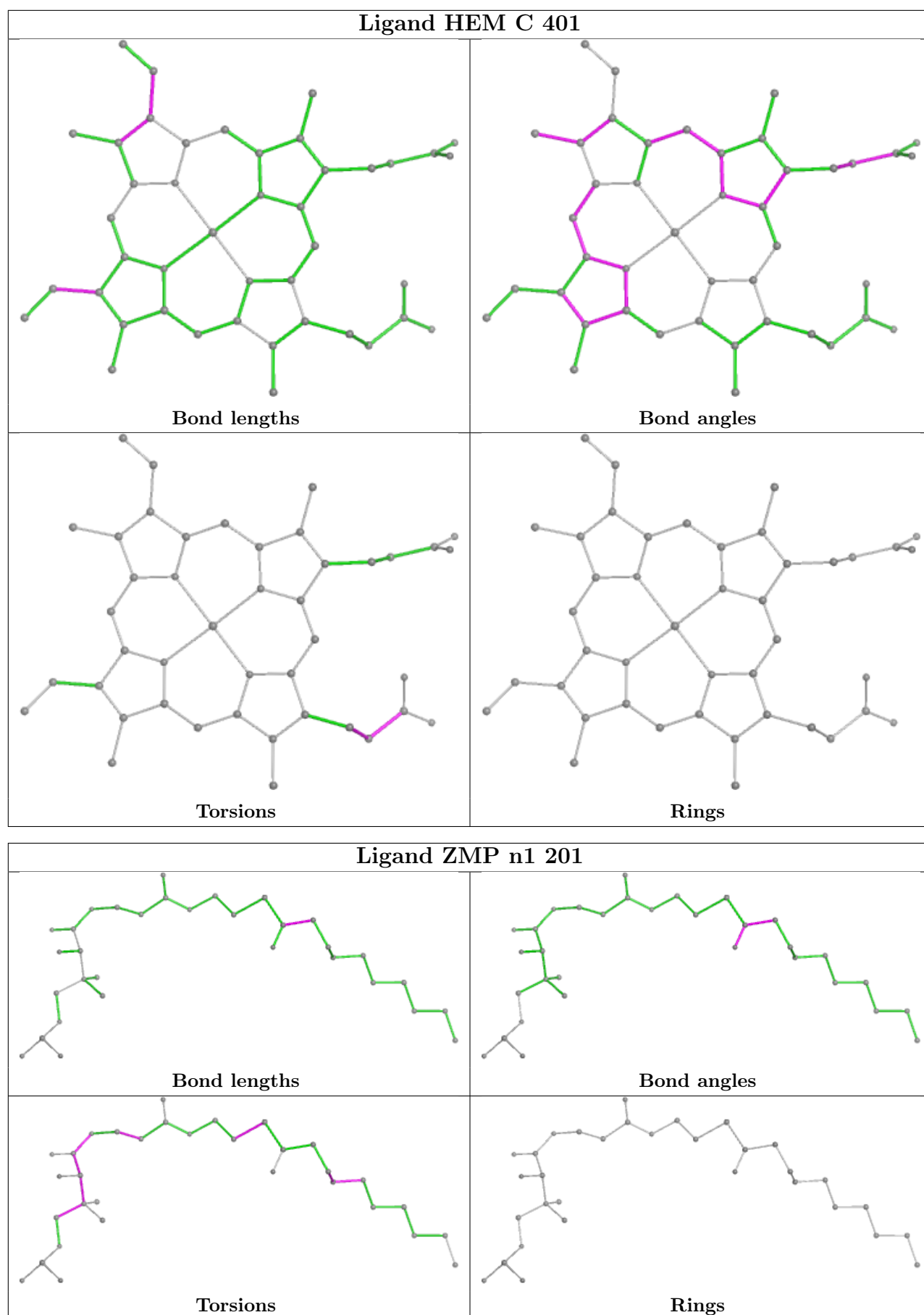


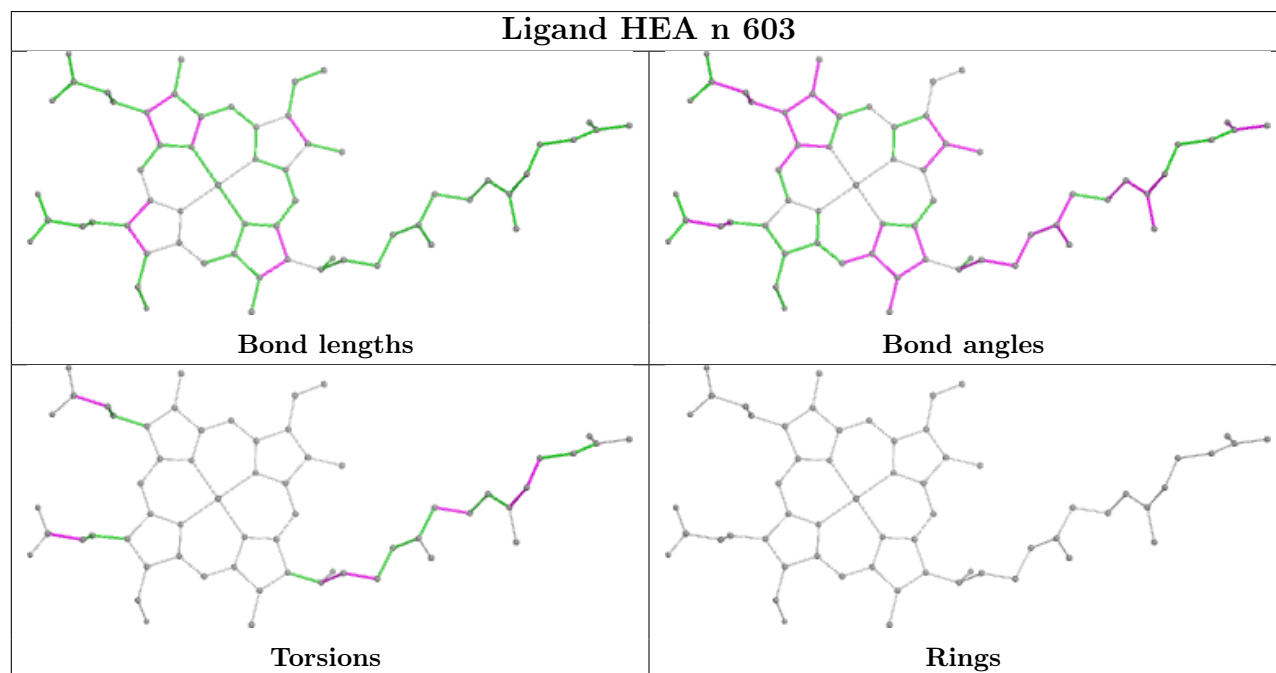
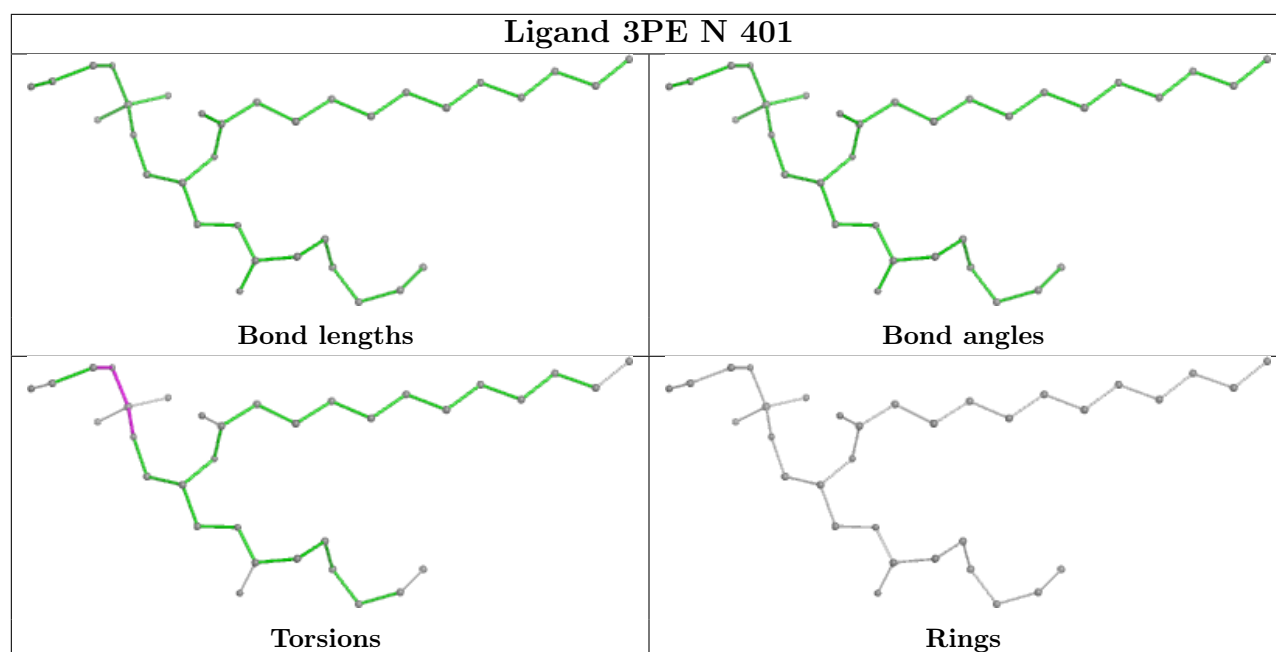


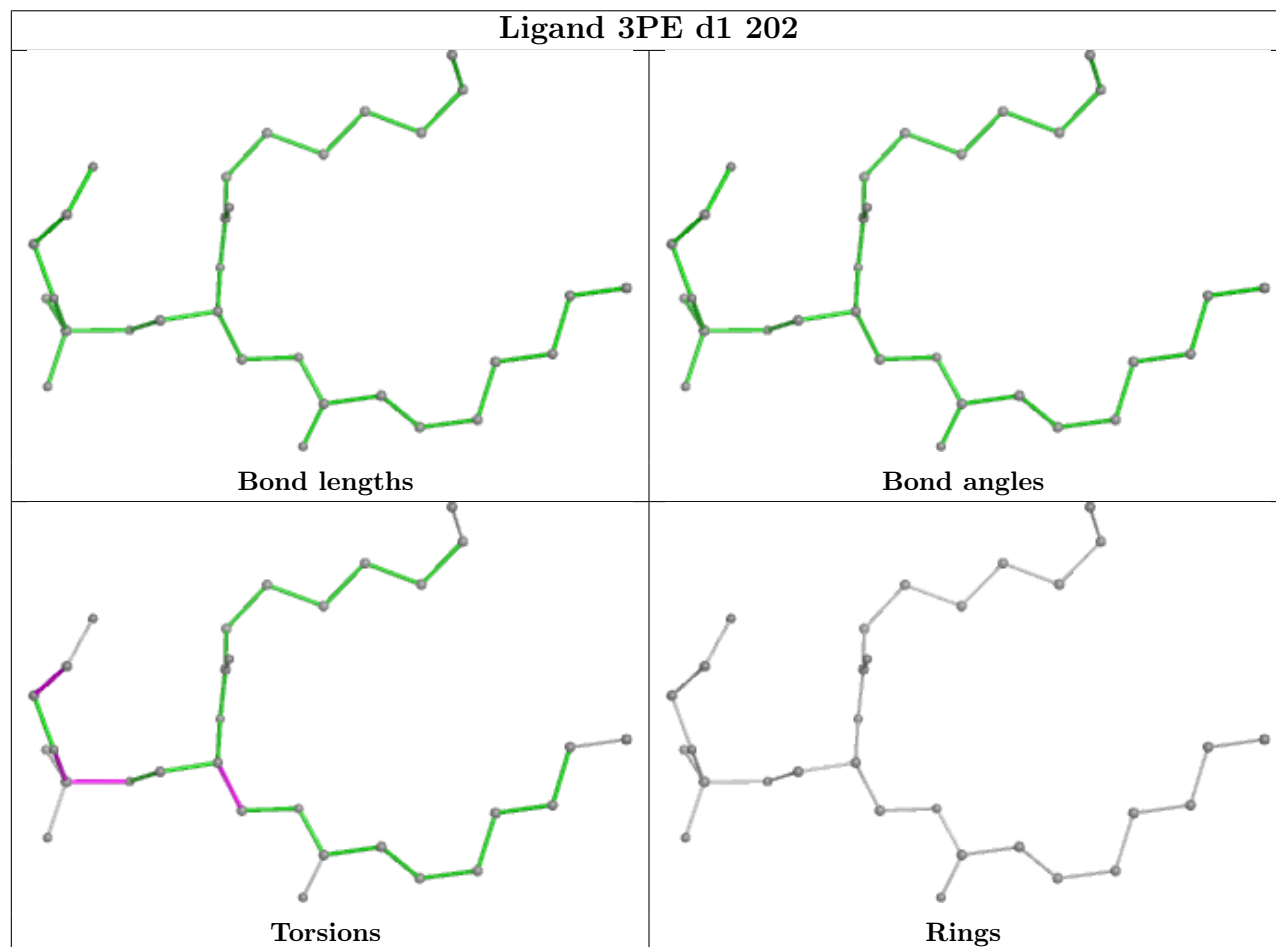
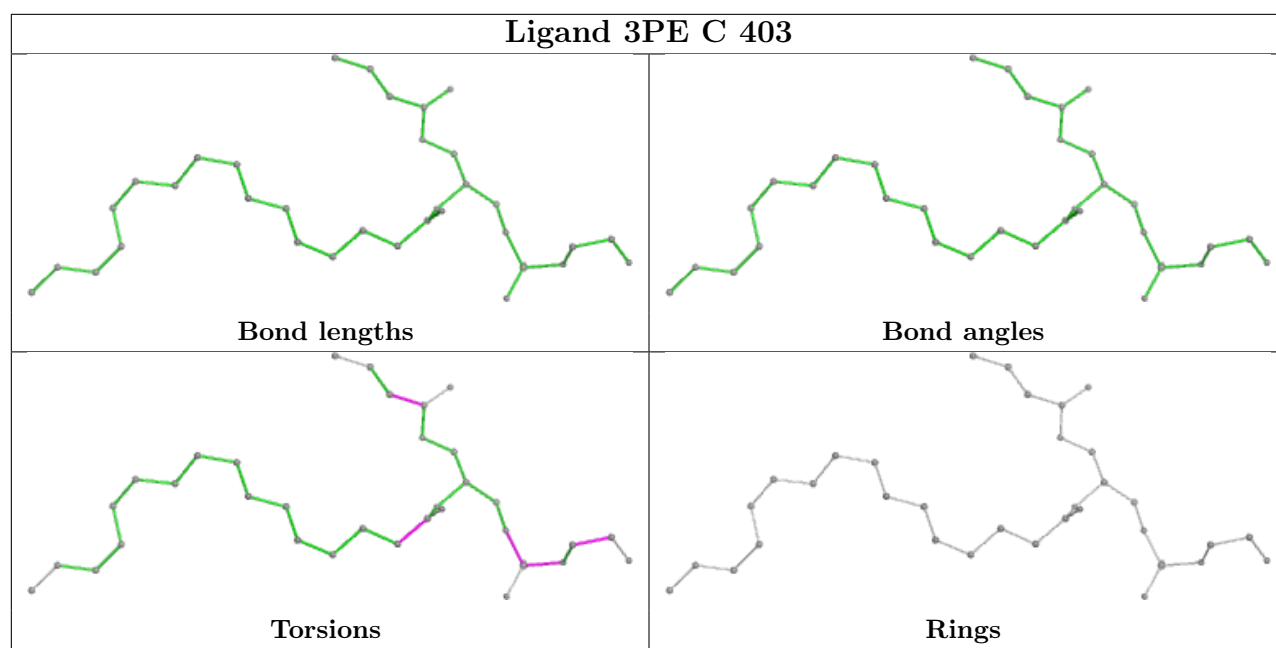


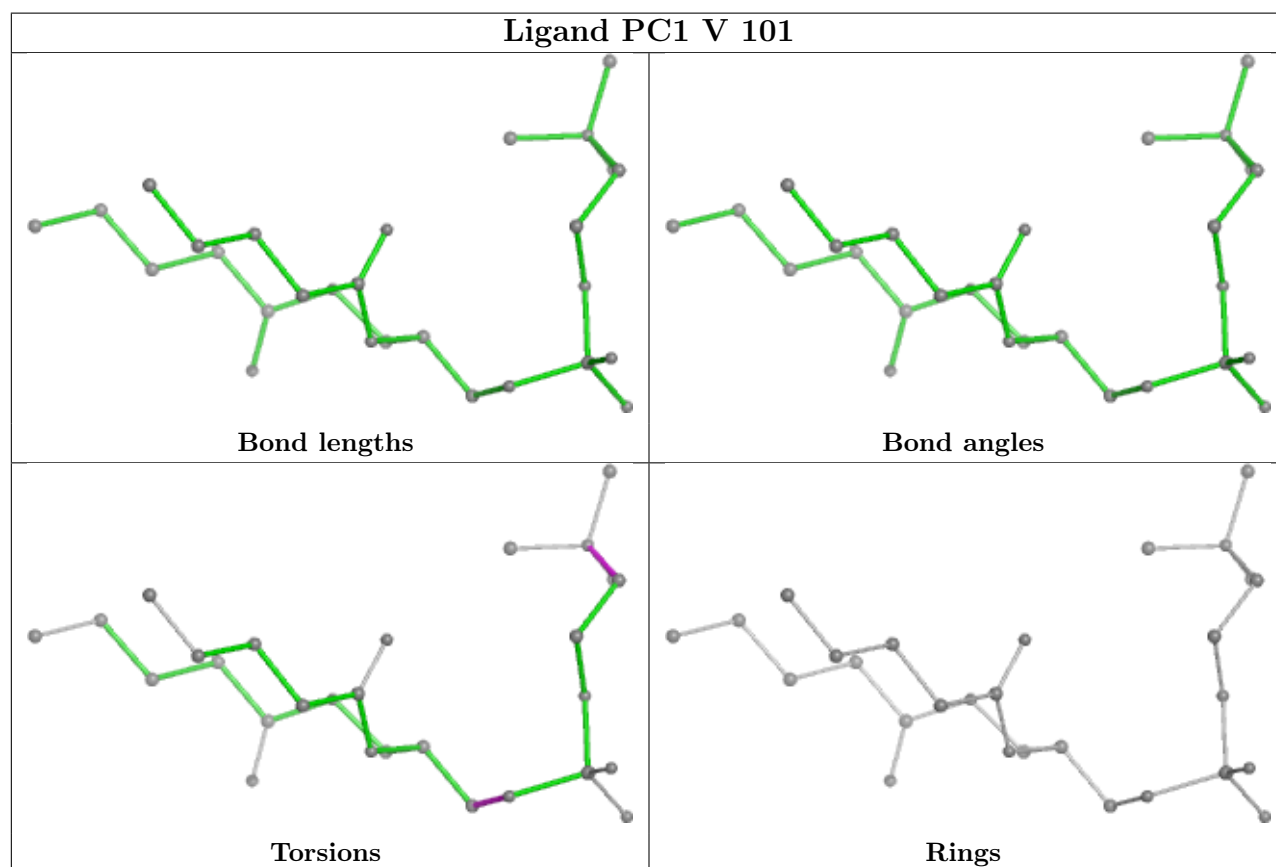
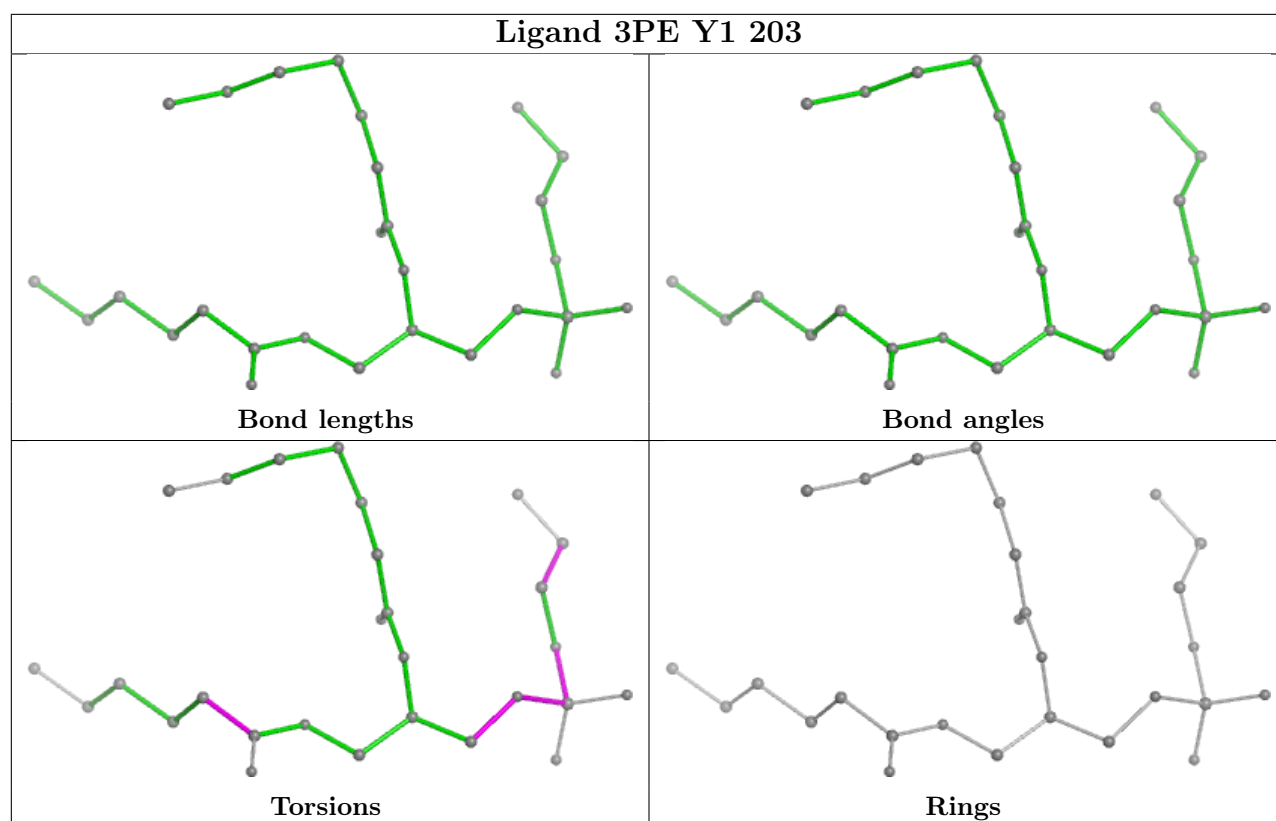


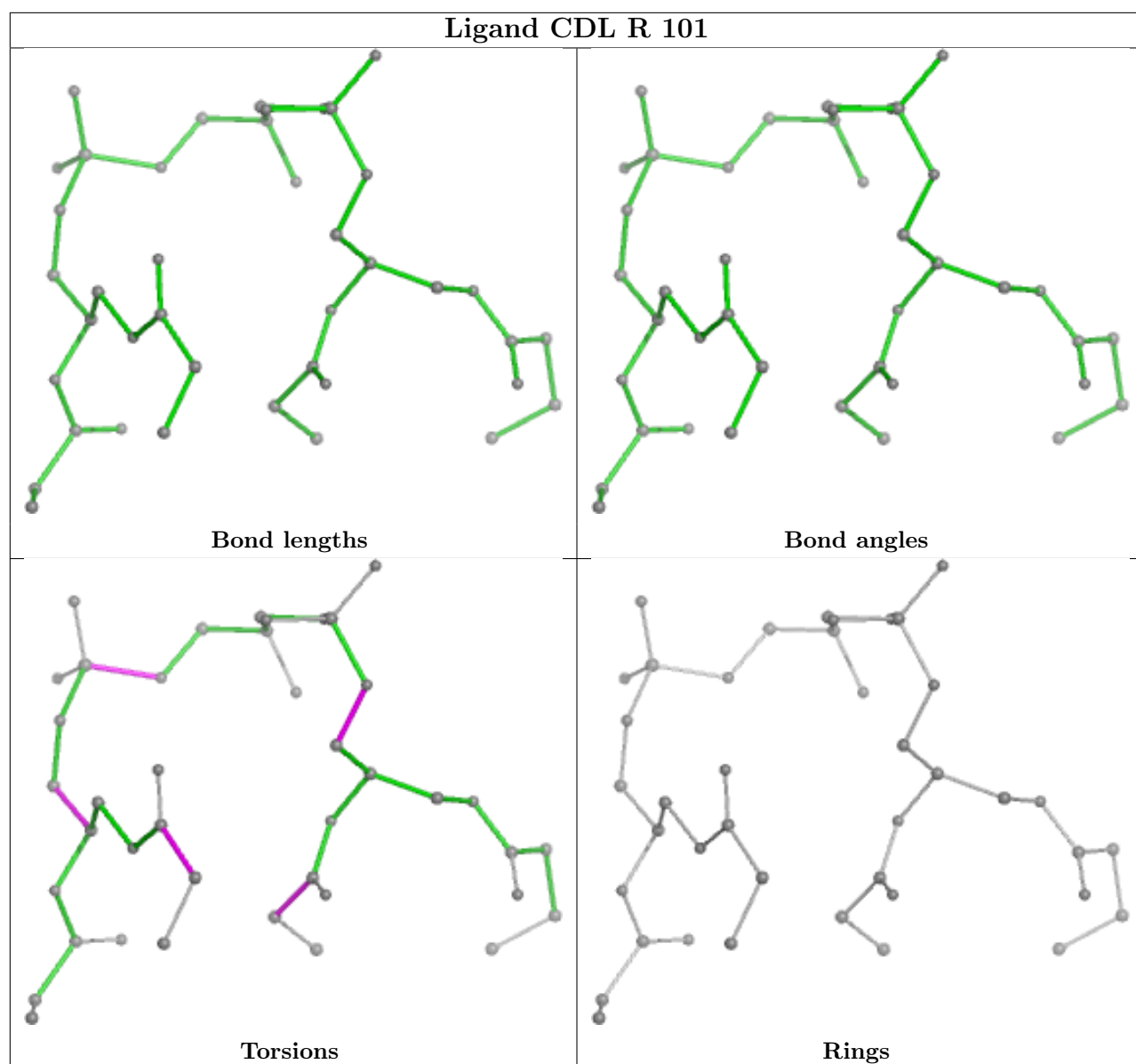


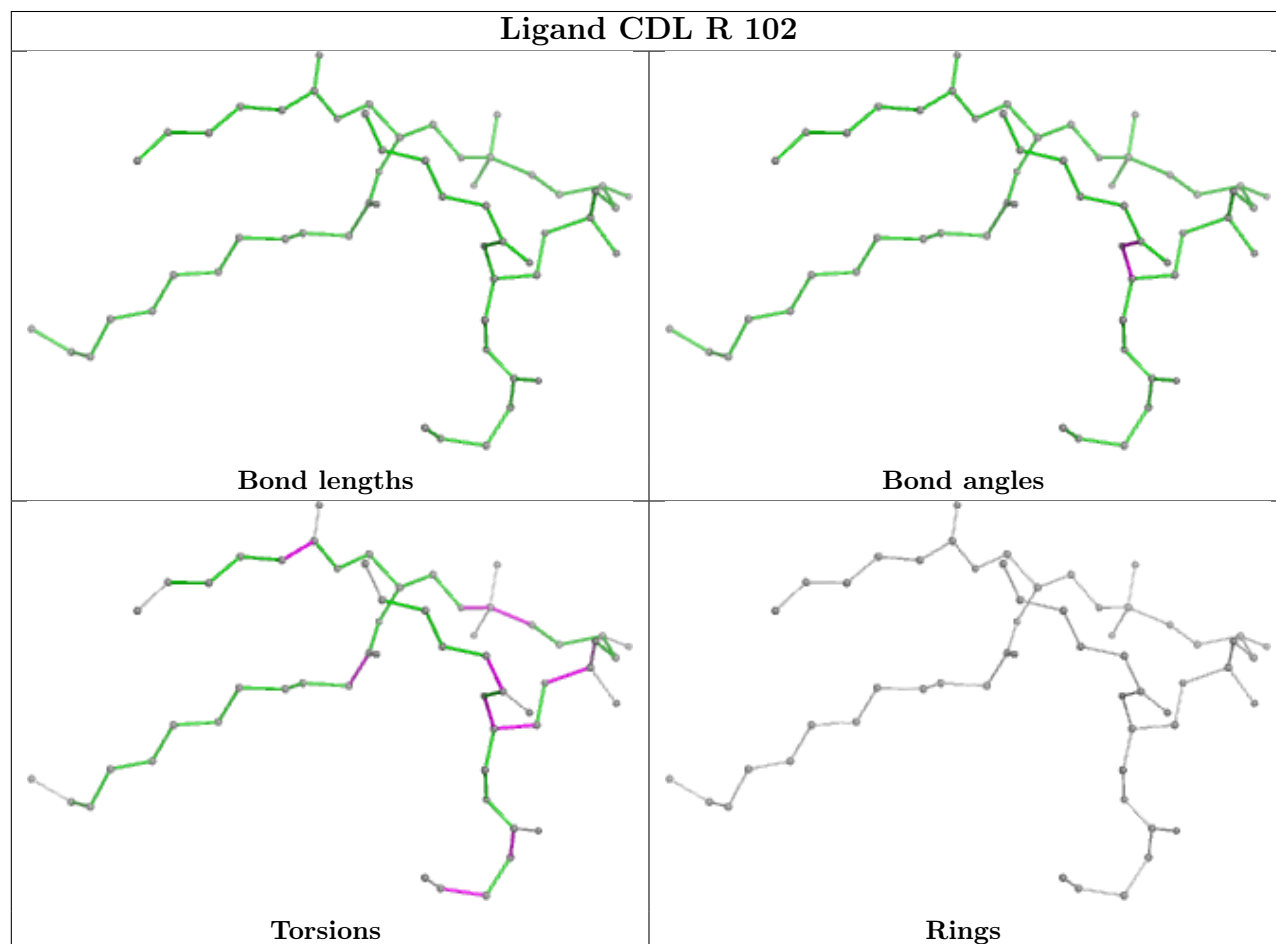
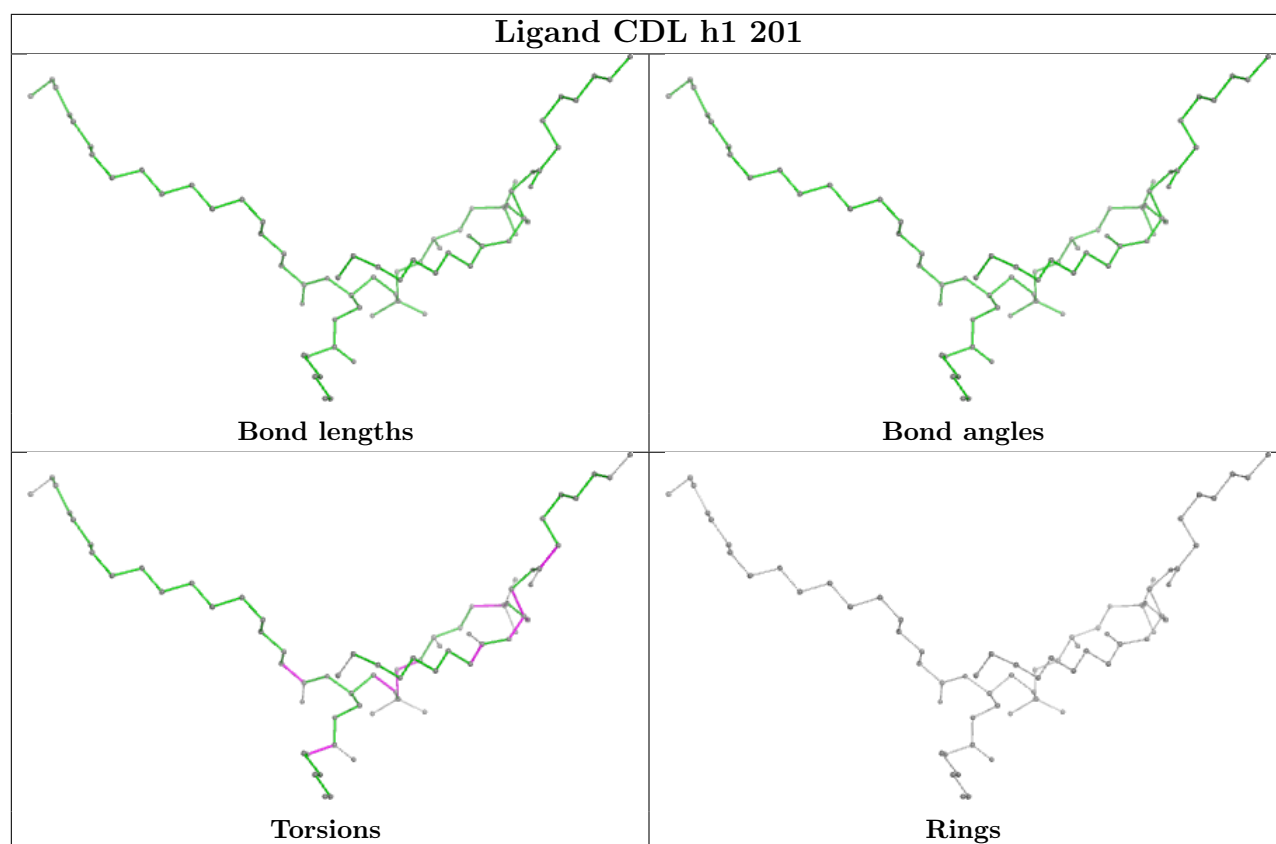


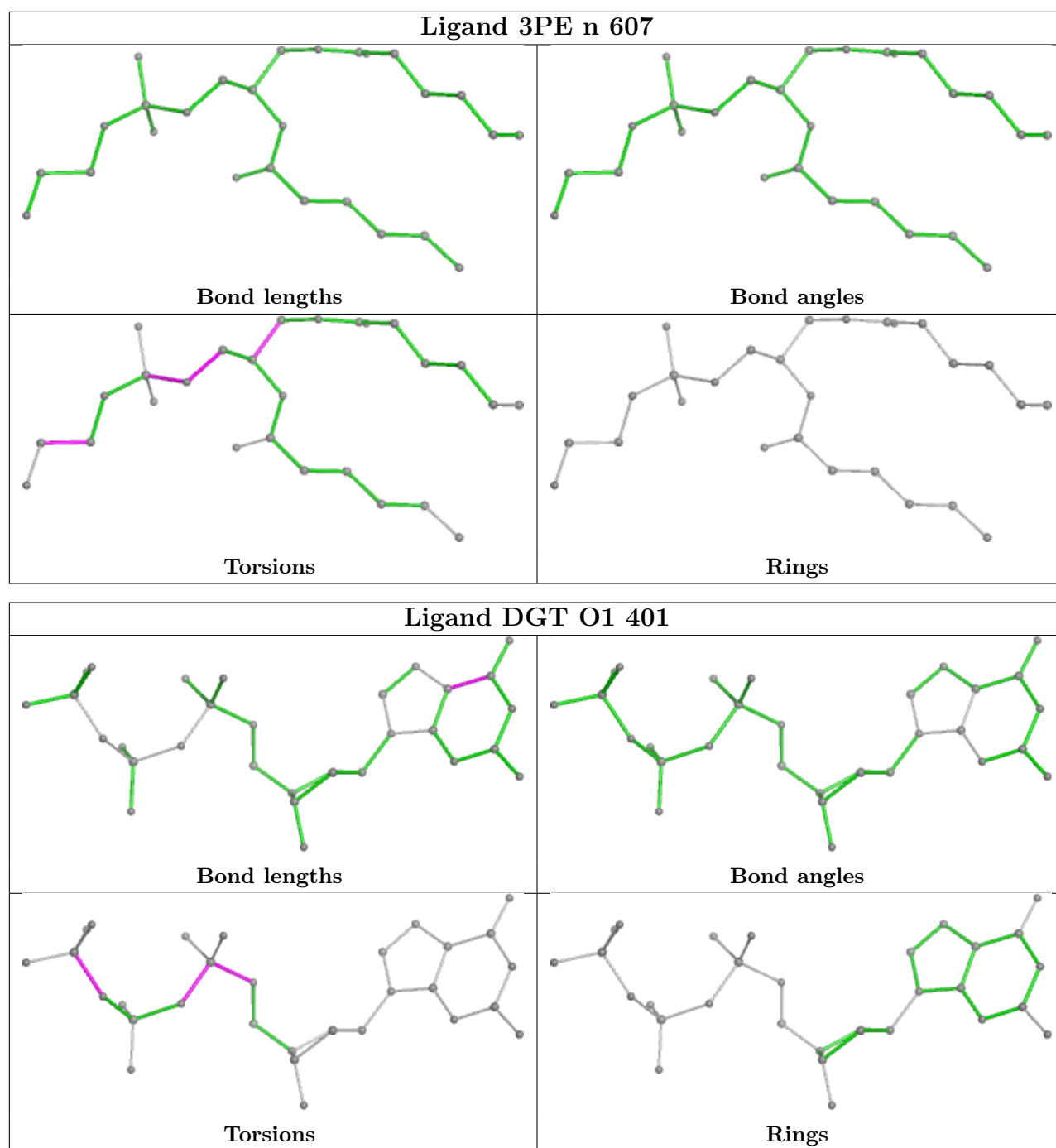




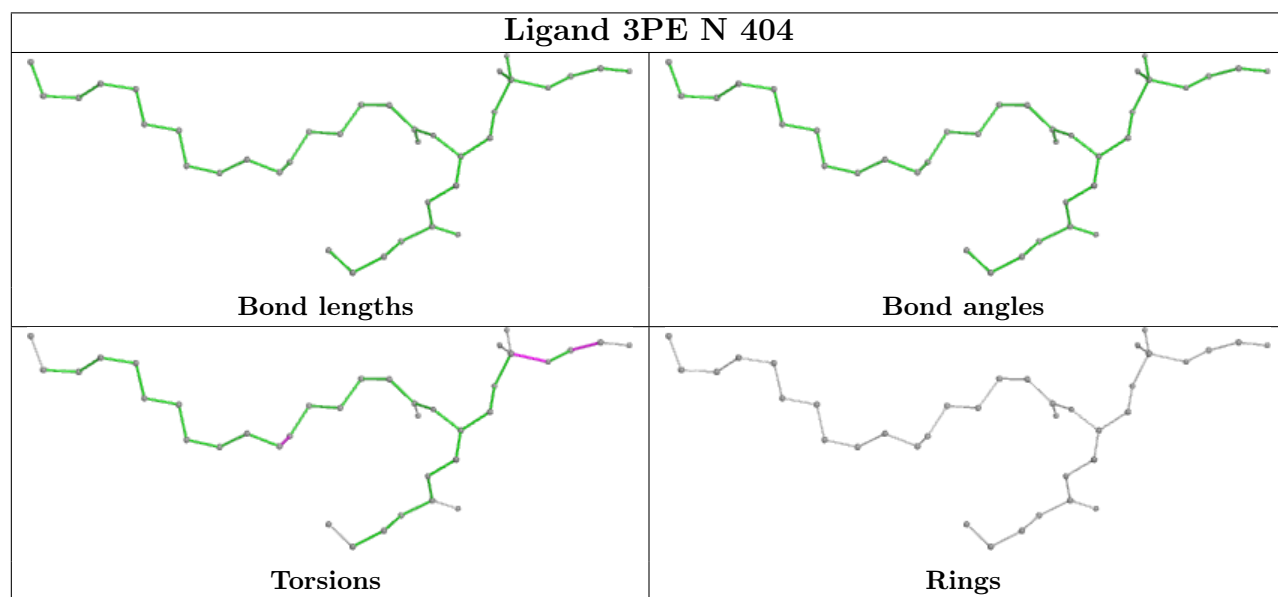
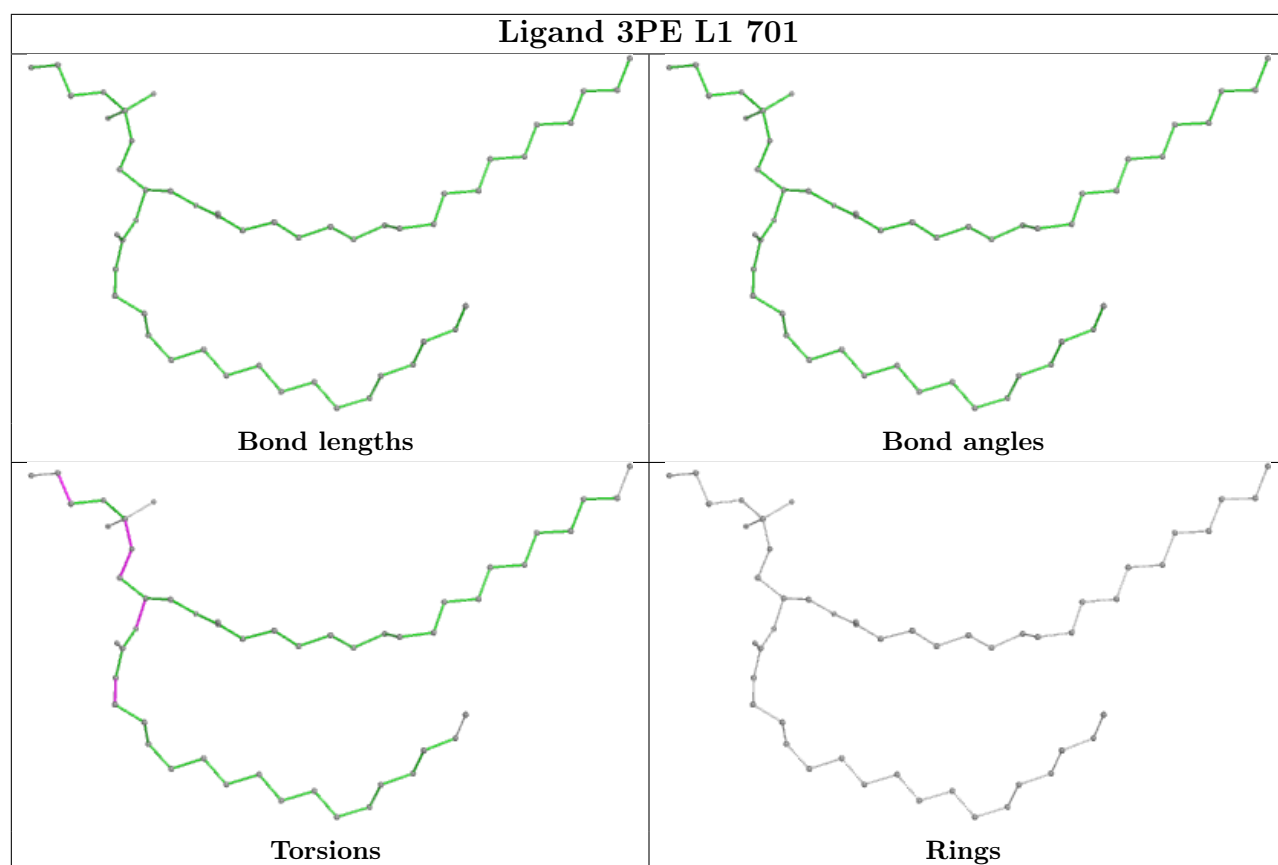


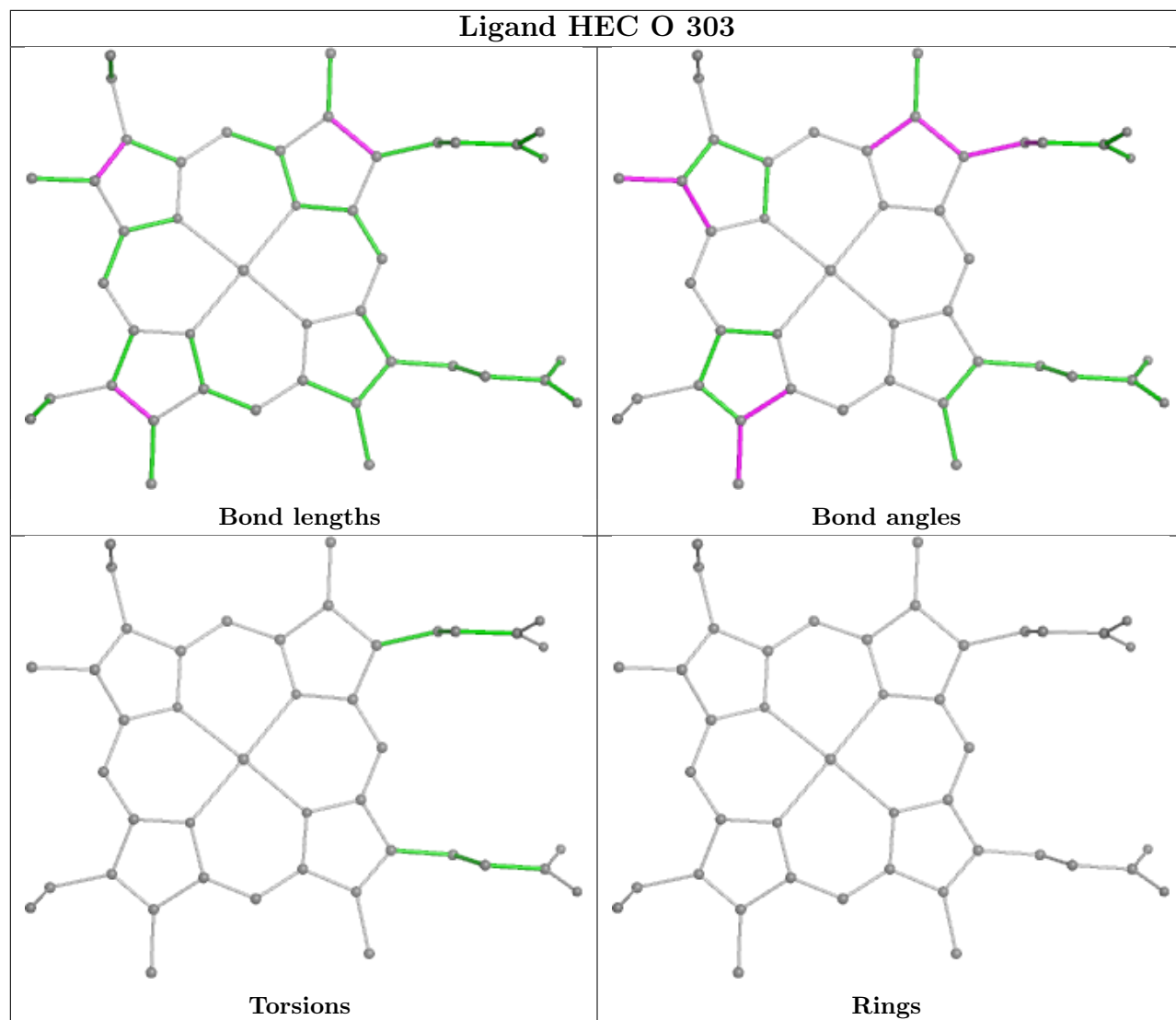


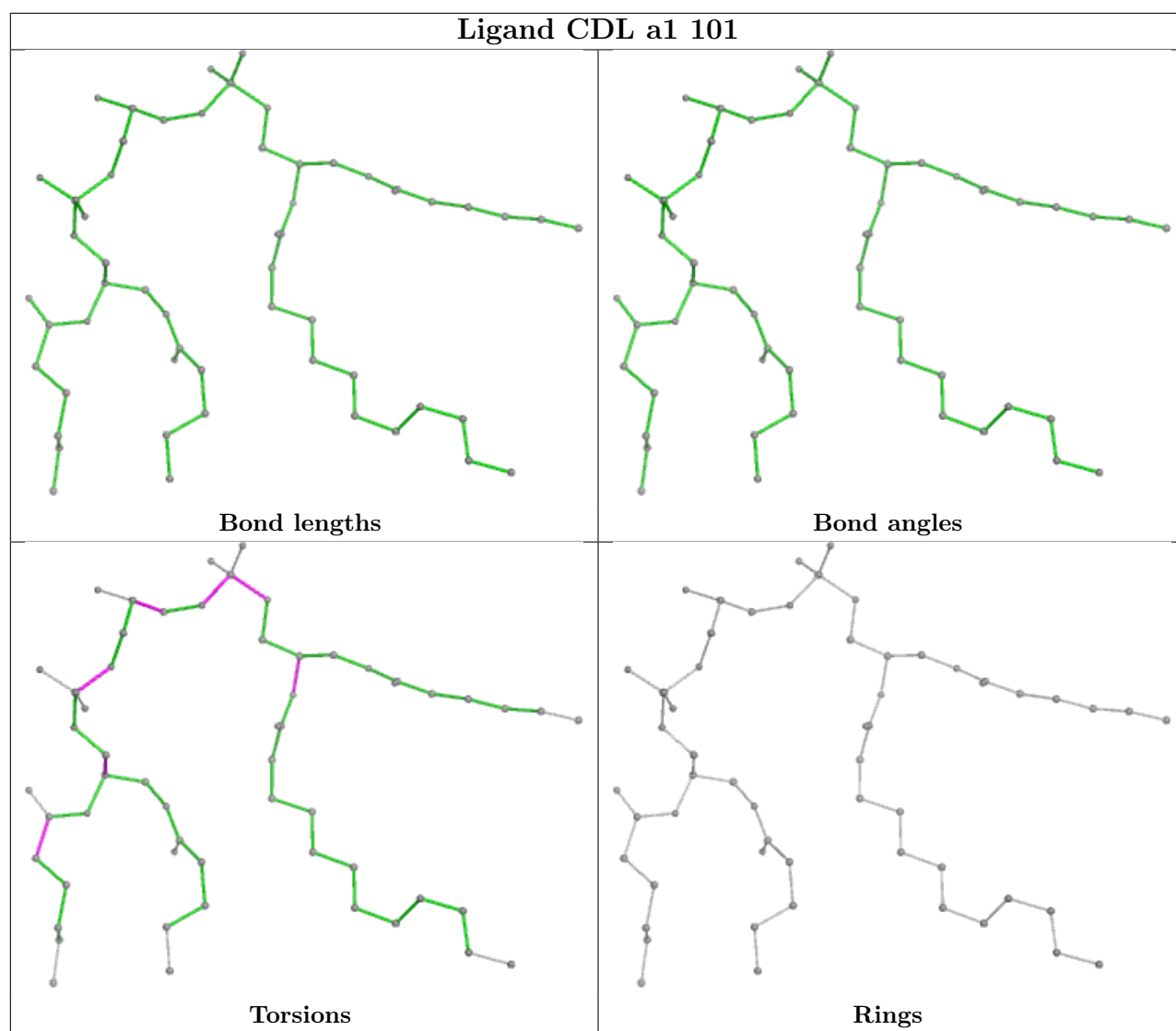


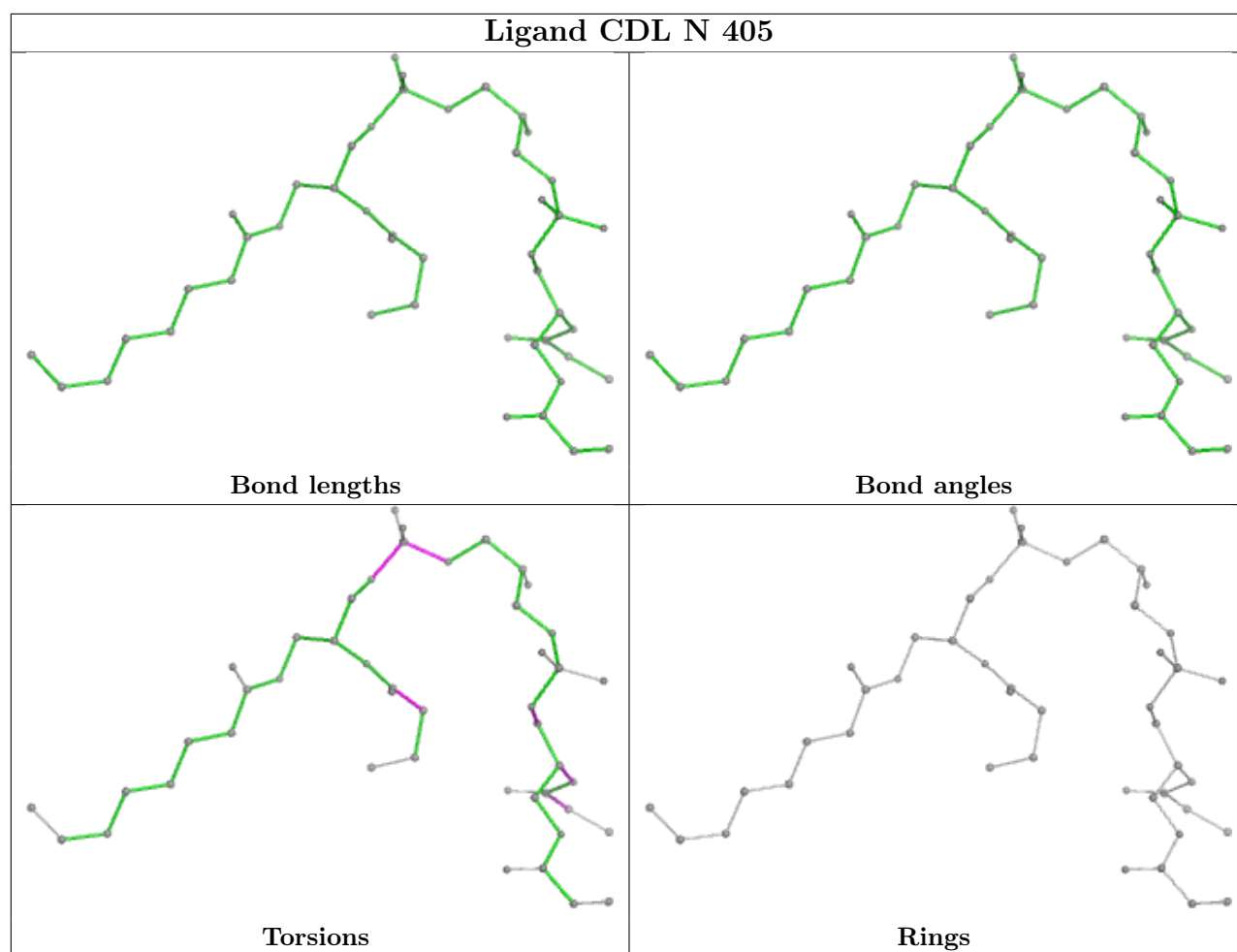


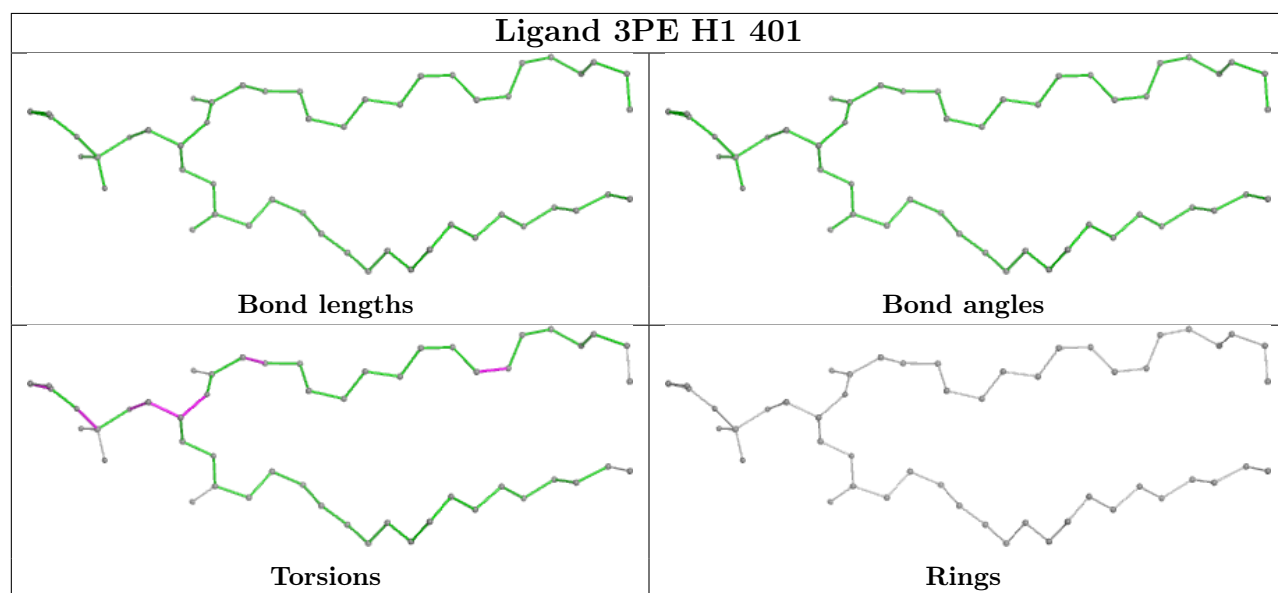
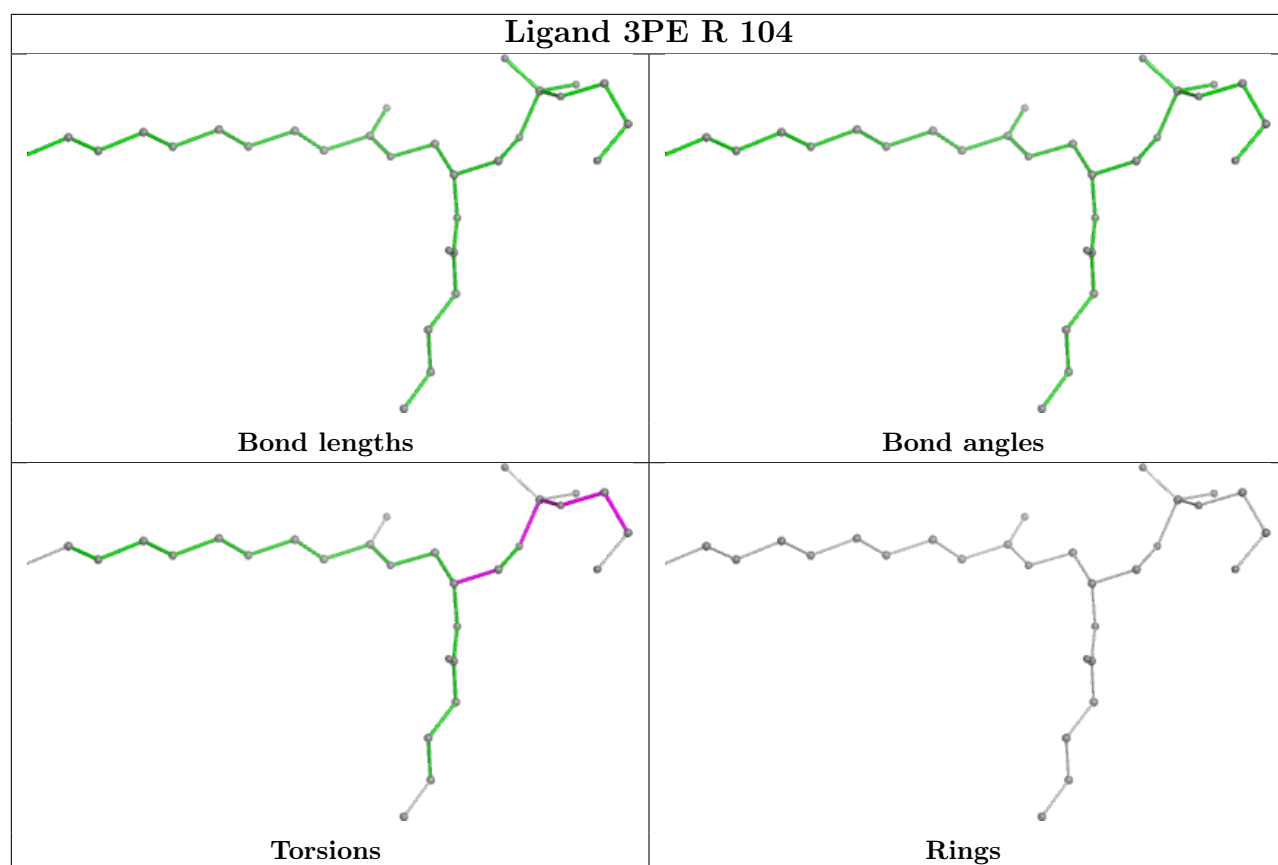


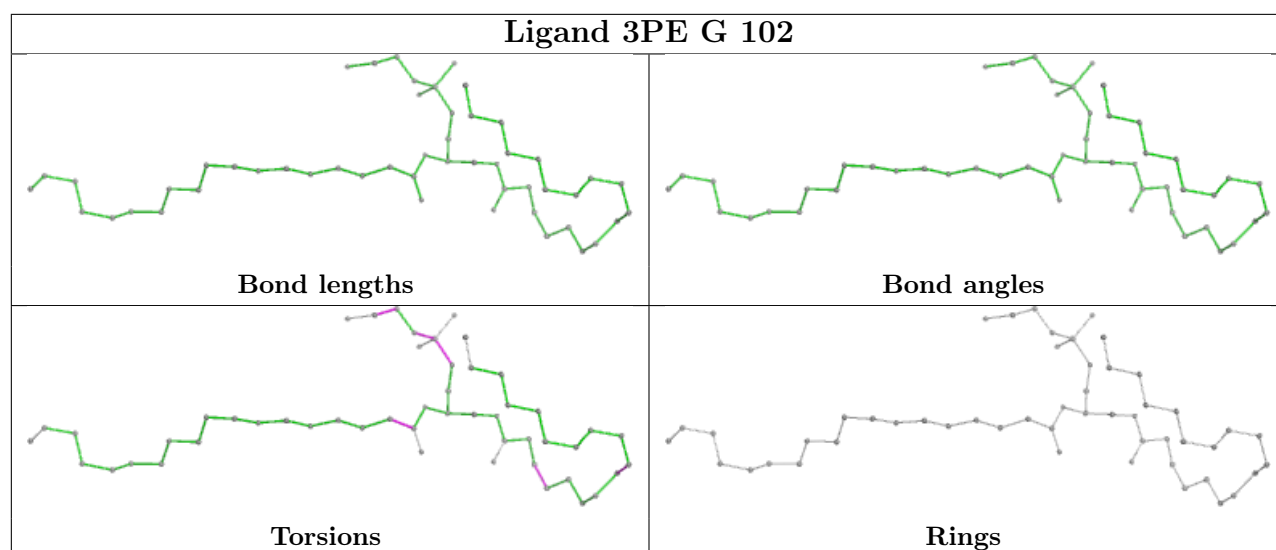












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

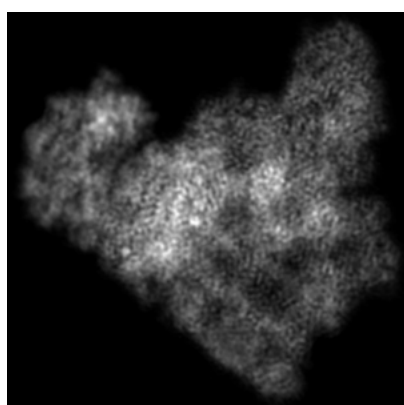
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17991. These allow visual inspection of the internal detail of the map and identification of artifacts.

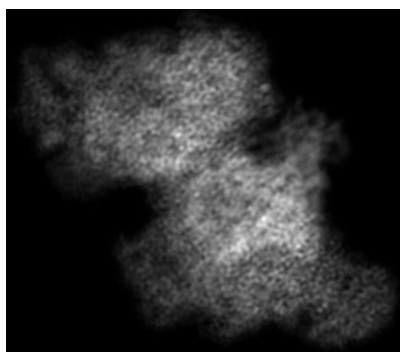
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

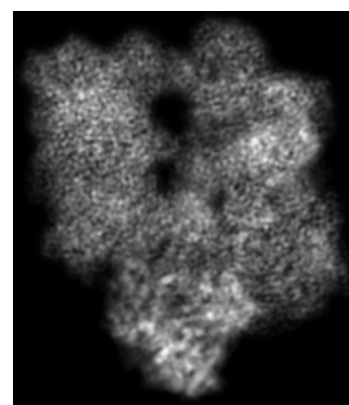
#### 6.1.1 Primary map



X



Y

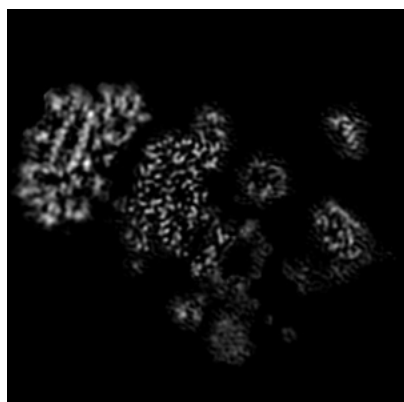


Z

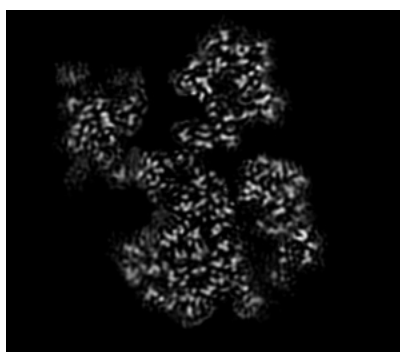
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

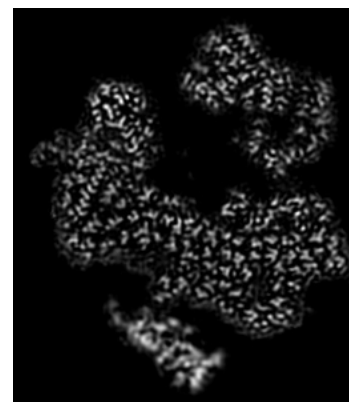
#### 6.2.1 Primary map



X Index: 107



Y Index: 124



Z Index: 124

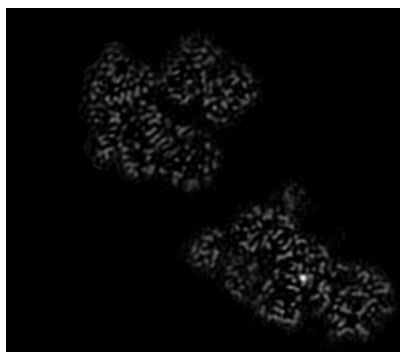
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

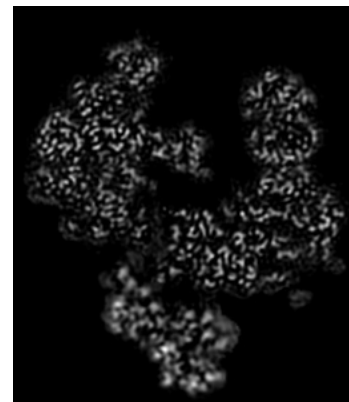
### 6.3.1 Primary map



X Index: 141



Y Index: 198

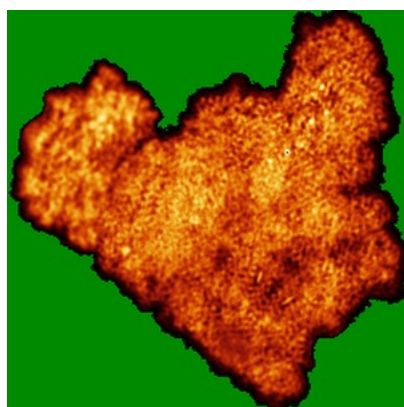


Z Index: 142

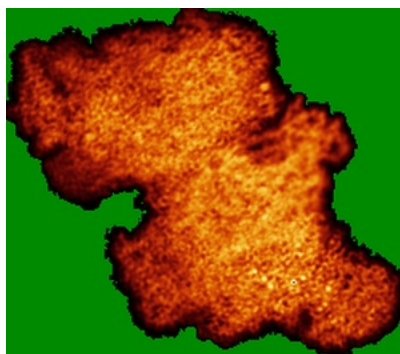
The images above show the largest variance slices of the map in three orthogonal directions.

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

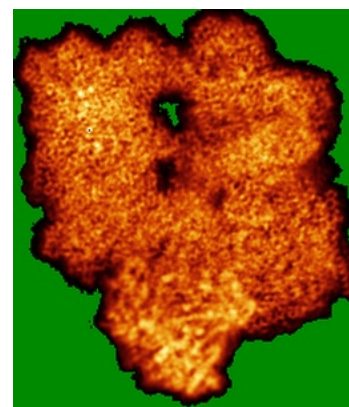
### 6.4.1 Primary map



X



Y



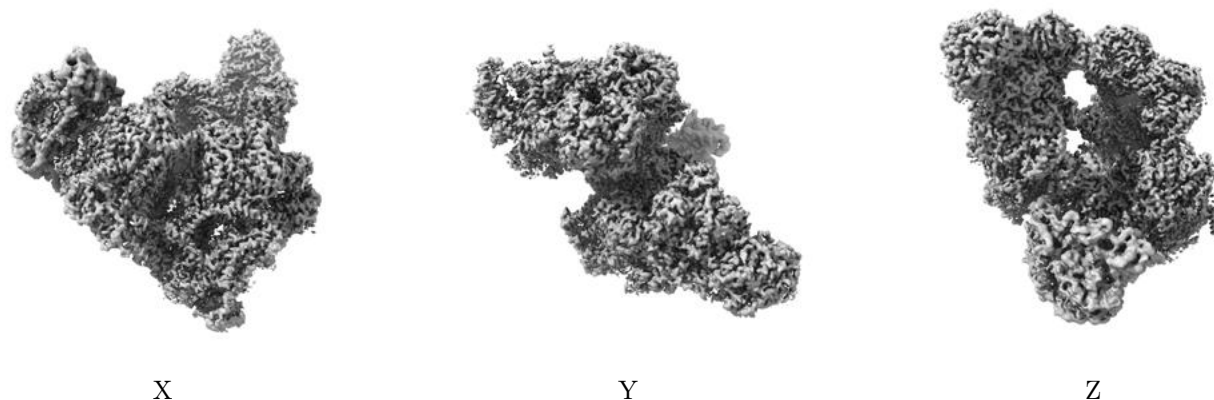
Z

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.

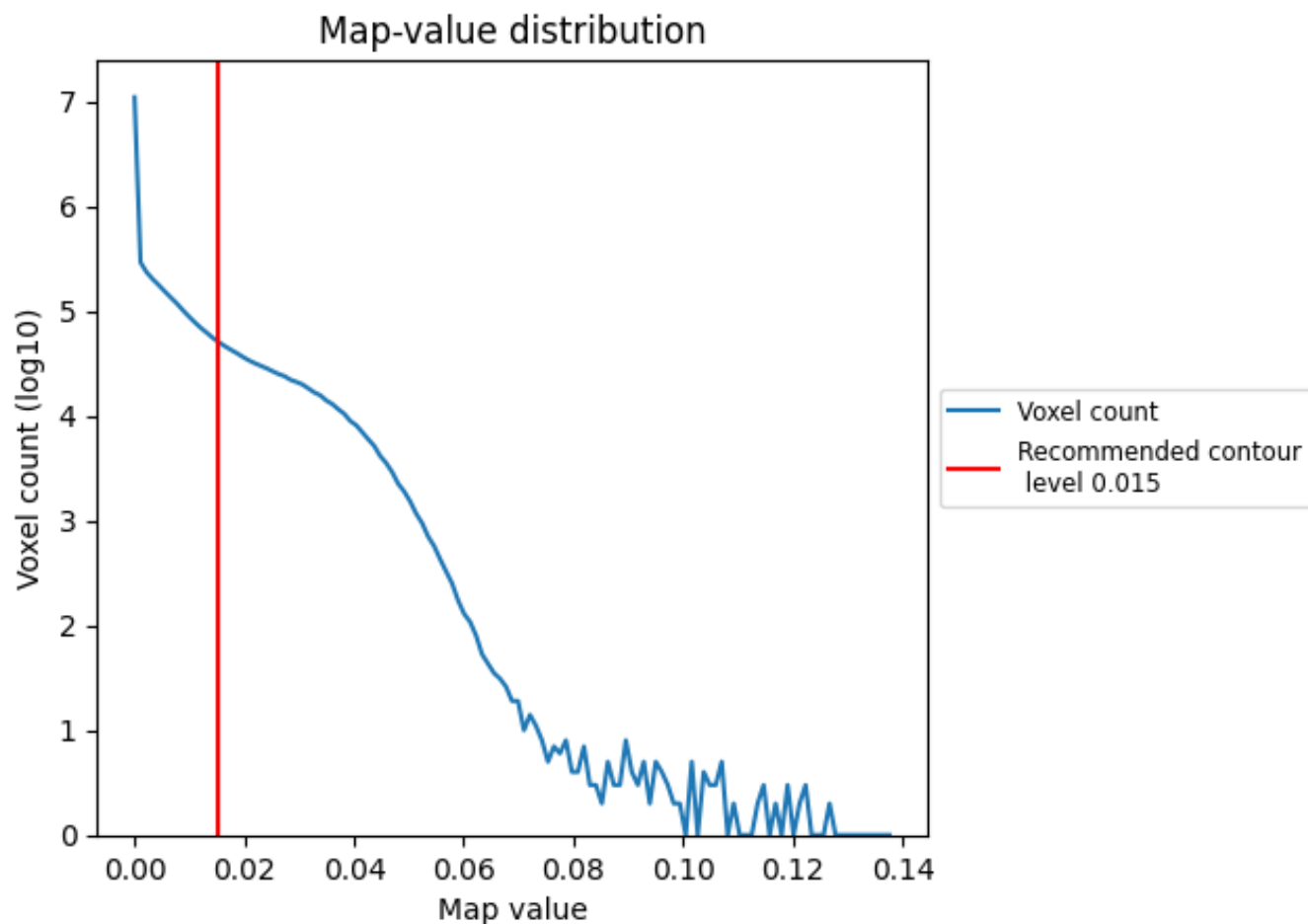
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

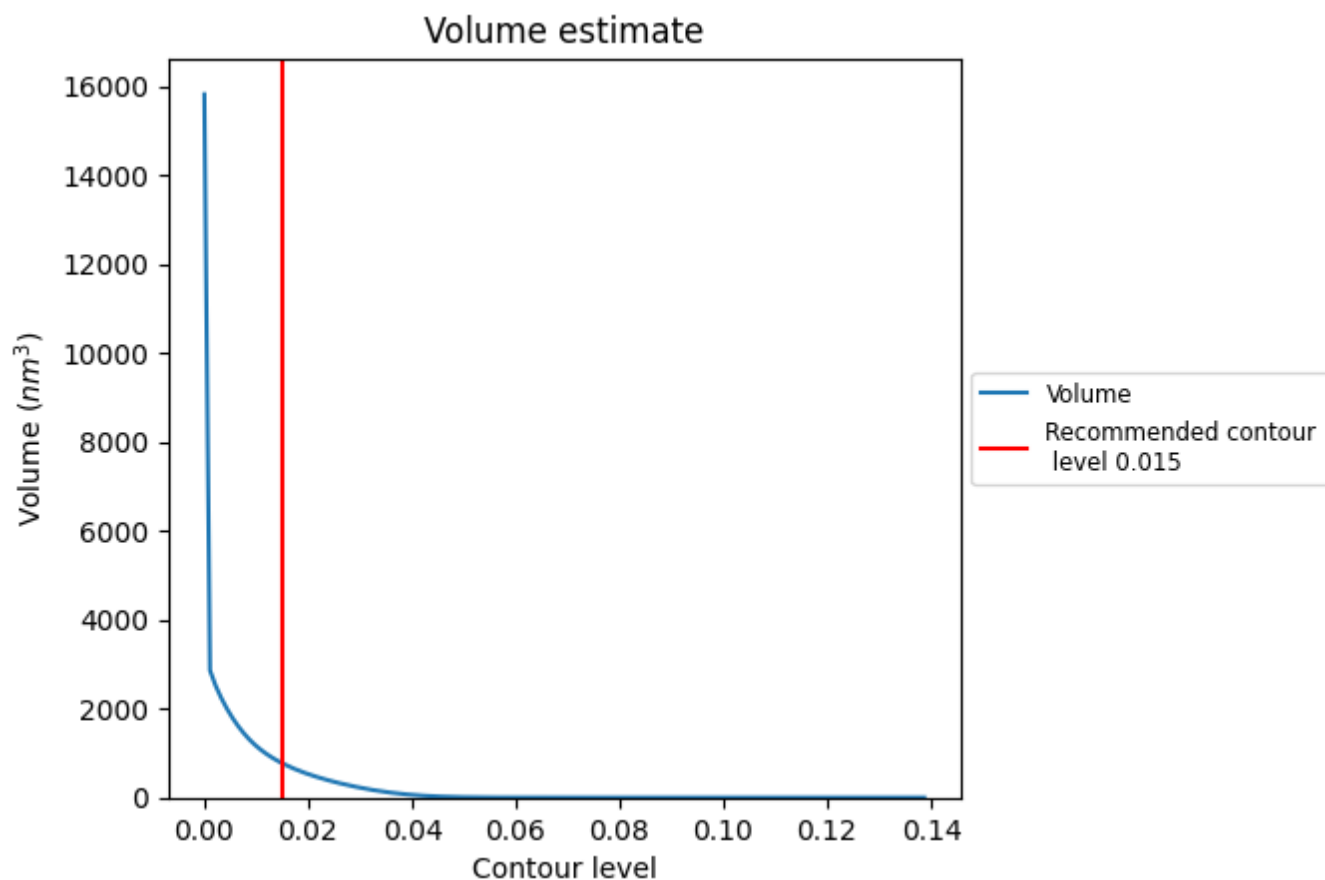
This section contains the results of statistical analysis of the map.

### 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 772 nm<sup>3</sup>; this corresponds to an approximate mass of 698 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.

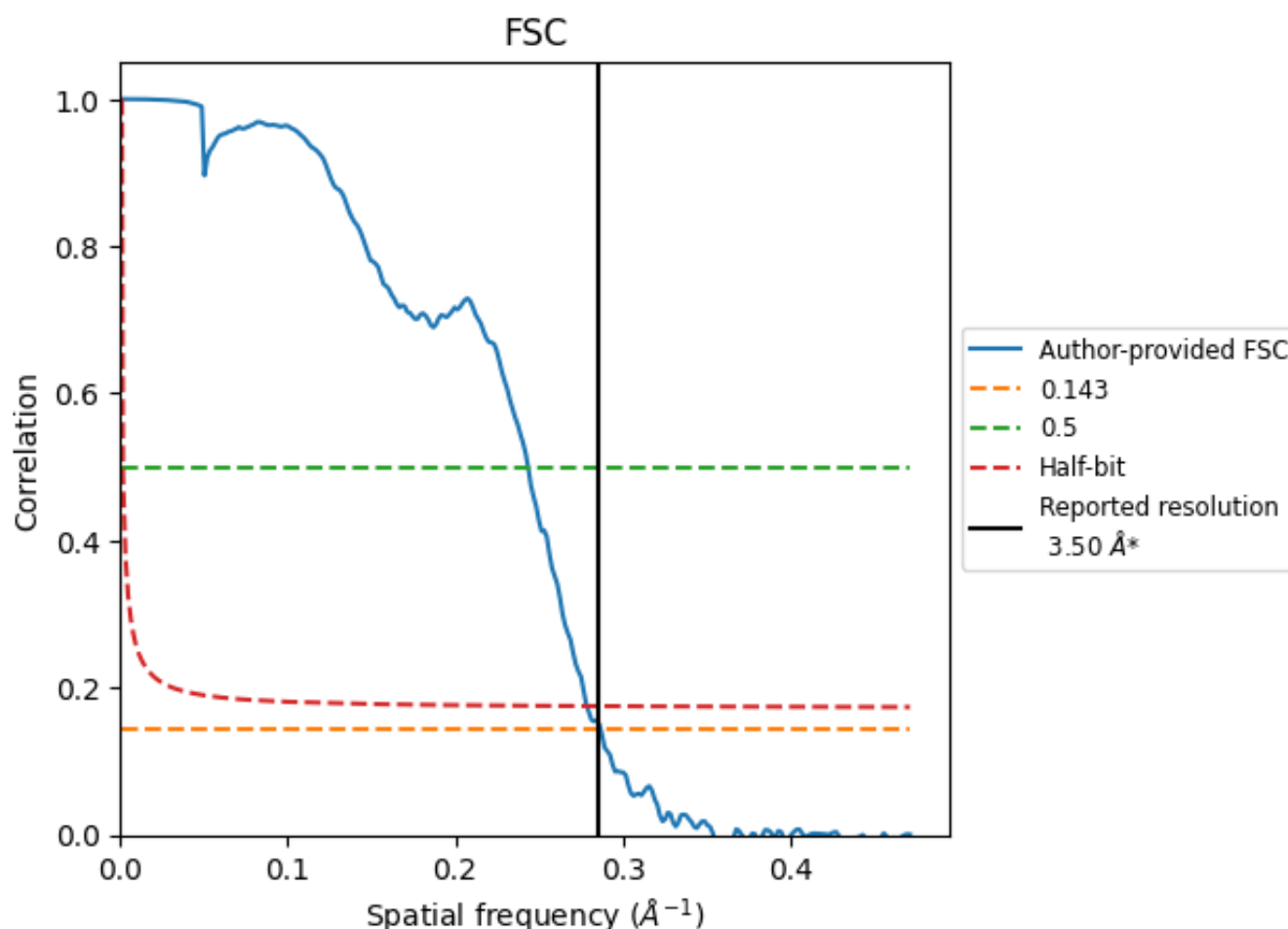
## 7.3 Rotationally averaged power spectrum [i](#)

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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

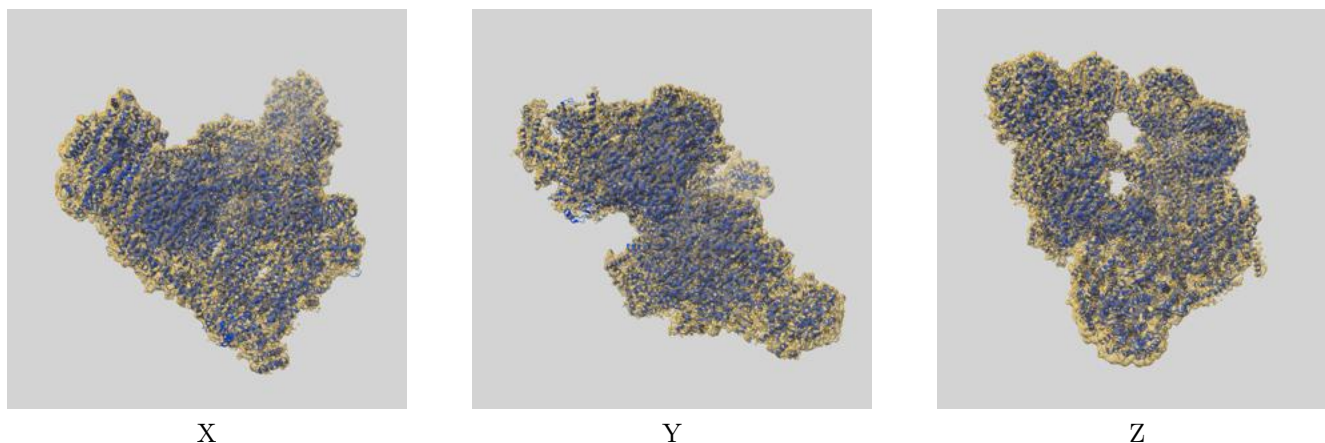
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.11	3.59
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

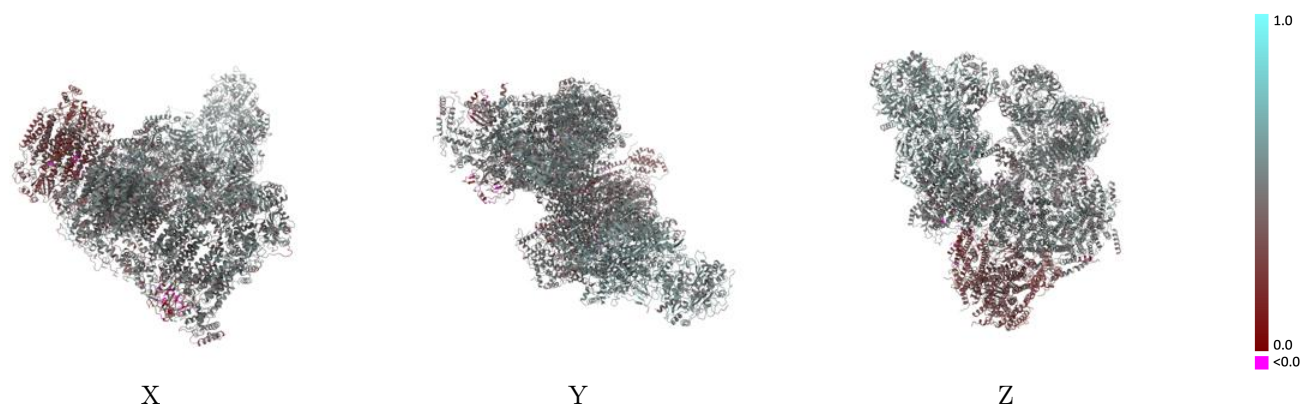
This section contains information regarding the fit between EMDB map EMD-17991 and PDB model 8PW7. Per-residue inclusion information can be found in section [3](#) on page [29](#).

### 9.1 Map-model overlay [i](#)



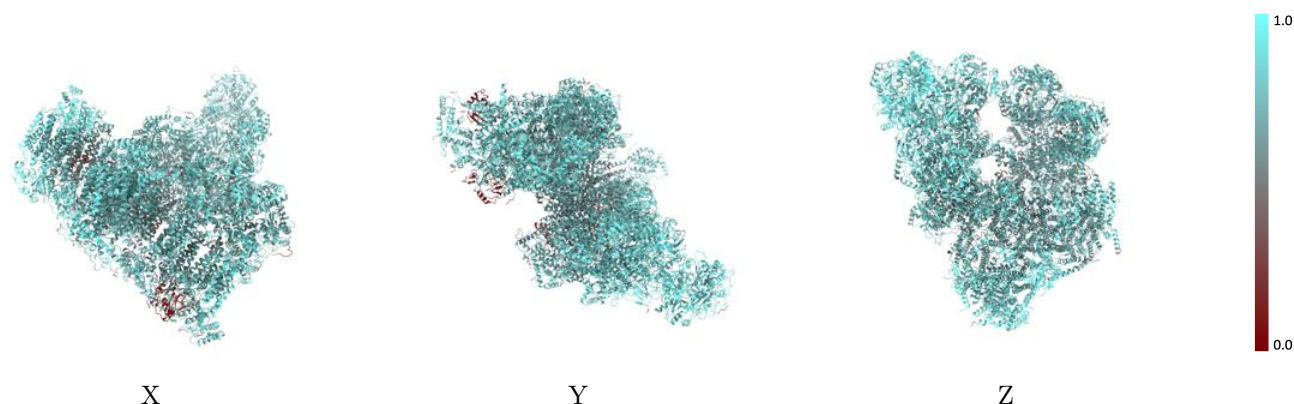
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



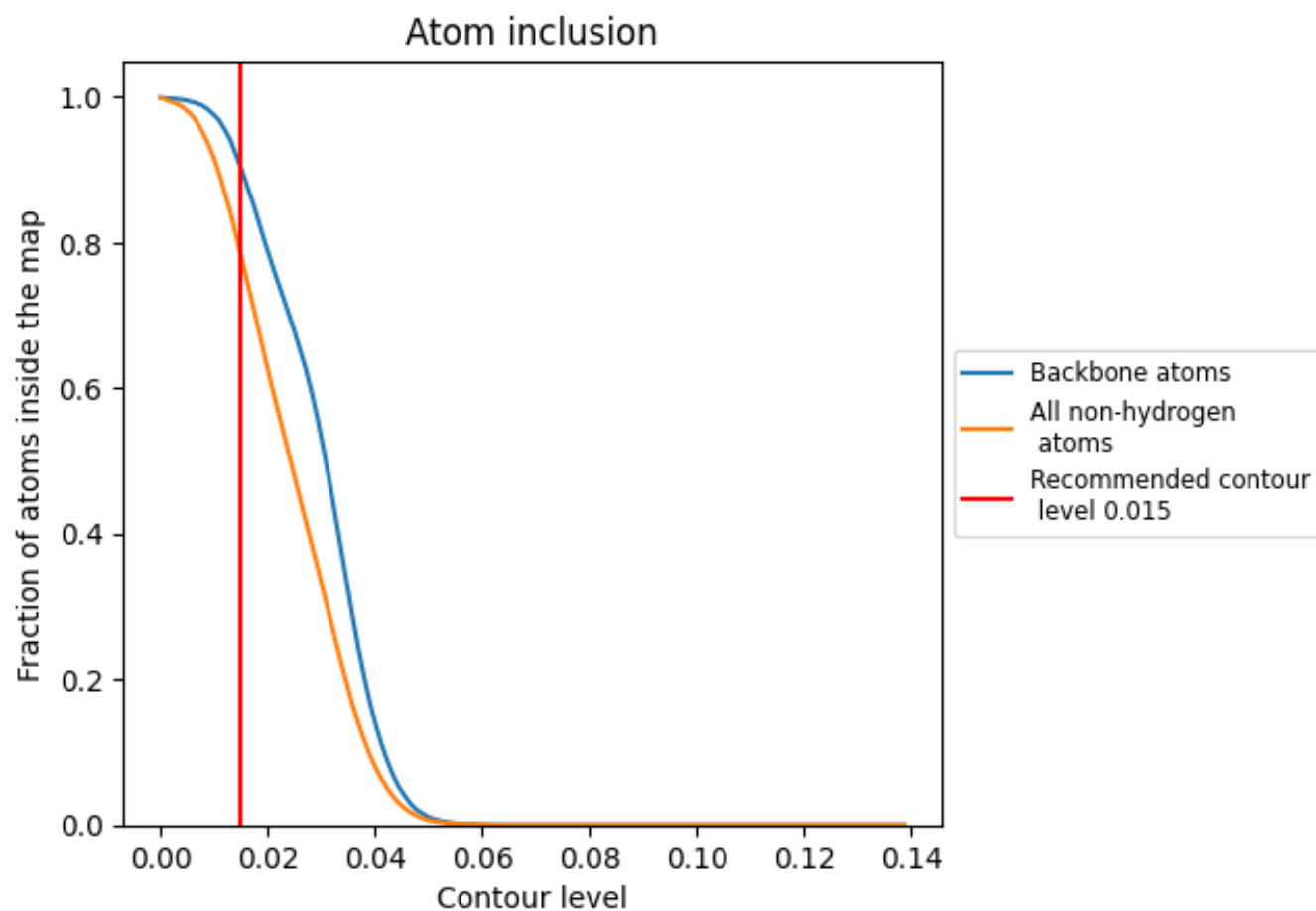
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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









































































At the recommended contour level, 90% of all backbone atoms, 78% 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	 0.7830	 0.4710
1	 0.8740	 0.5240
2	 0.8610	 0.5270
3	 0.8540	 0.5320
6	 0.8450	 0.5240
7	 0.8580	 0.5350
9	 0.8540	 0.5370
A	 0.7730	 0.4960
A1	 0.7010	 0.4750
B	 0.7960	 0.5030
C	 0.7900	 0.5000
C1	 0.8710	 0.5530
D	 0.8200	 0.4890
D1	 0.8040	 0.5120
E	 0.4810	 0.3500
F	 0.8050	 0.4930
G	 0.7560	 0.4890
H	 0.7620	 0.4360
H1	 0.7470	 0.4730
J	 0.7620	 0.4930
J1	 0.6160	 0.4290
K	 0.6280	 0.4510
K1	 0.7050	 0.4750
L	 0.7970	 0.4980
L1	 0.7750	 0.4950
M	 0.7860	 0.4950
M1	 0.7770	 0.5060
N	 0.7770	 0.4960
N1	 0.7370	 0.4940
O	 0.8040	 0.4940
O1	 0.8120	 0.4950
P	 0.4740	 0.3380
P1	 0.7910	 0.5100
Q	 0.7570	 0.5060
Q1	 0.8250	 0.5480









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Chain	Atom inclusion	Q-score
R	 0.6420	 0.4600
S	 0.7110	 0.4250
S1	 0.8250	 0.4910
T	 0.4570	 0.4300
T1	 0.7090	 0.4280
U	 0.7930	 0.5030
U1	 0.7660	 0.4830
V	 0.6770	 0.4710
V1	 0.8330	 0.5180
W1	 0.8280	 0.5200
X1	 0.7920	 0.4770
Y1	 0.6420	 0.4410
Z1	 0.8010	 0.4820
a1	 0.7820	 0.4810
b1	 0.7800	 0.4740
c1	 0.7260	 0.4580
d1	 0.7070	 0.4870
e1	 0.7230	 0.4870
f1	 0.6770	 0.4560
g1	 0.7600	 0.4840
h1	 0.7990	 0.4980
i1	 0.7030	 0.4470
j1	 0.7900	 0.4530
k1	 0.7850	 0.4850
l1	 0.8010	 0.5060
m1	 0.7560	 0.4760
n	 0.7730	 0.3330
n1	 0.8200	 0.4970
o	 0.8290	 0.3160
o1	 0.7730	 0.4550
p	 0.7160	 0.2880
p1	 0.8230	 0.4980
q	 0.9180	 0.3150
q1	 0.8730	 0.5400
r	 0.8890	 0.2870
r1	 0.7980	 0.5290
s	 0.7890	 0.3170
s1	 0.7860	 0.4960
t	 0.7970	 0.2640
u	 0.9120	 0.2960
v	 0.8570	 0.2900
w	 0.8260	 0.3100

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Chain	Atom inclusion	Q-score
x	 0.9440	 0.3210
y	 0.8150	 0.3300
z	 0.7890	 0.2780