



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 10:51 AM JST

PDB ID : 8IUJ
EMDB ID : EMD-35723
Title : Cryo-EM structure of Euglena gracilis super-complex III2+IV2, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), 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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

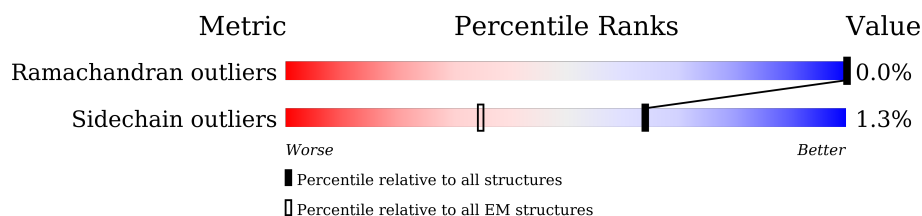
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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







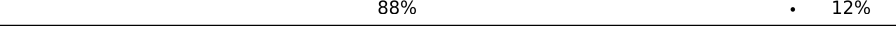
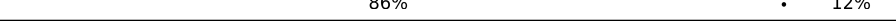
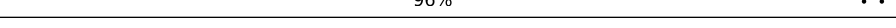
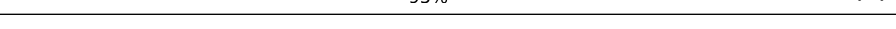
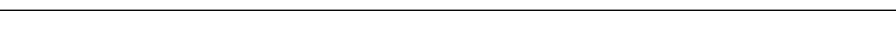
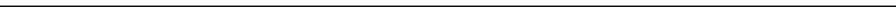





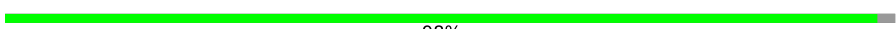
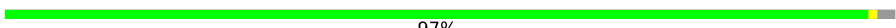


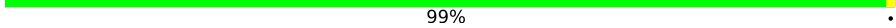
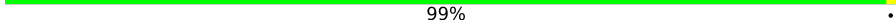
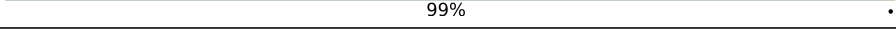
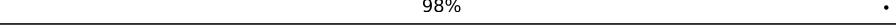
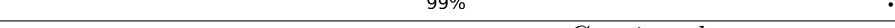

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	QA	479	99% ..
1	Qa	479	99% ..
2	QC	368	98% ..
2	Qc	368	98% ..
3	QD	243	98% ..
3	Qd	243	98% ..
4	QH	86	99% .
4	Qh	86	99% .
5	QJ	154	96% ..
5	Qj	154	96% ..

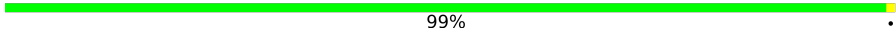
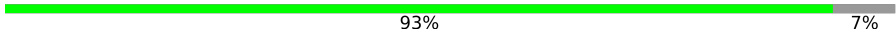





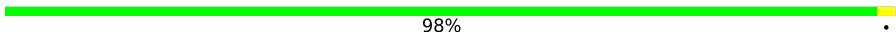
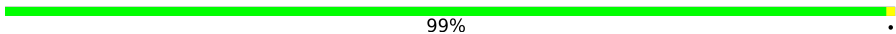
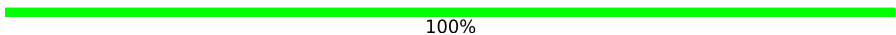
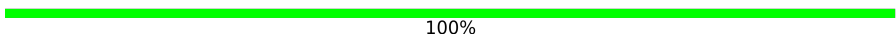
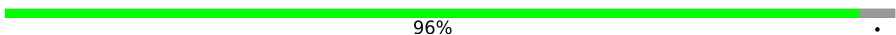



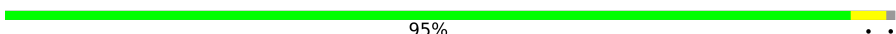
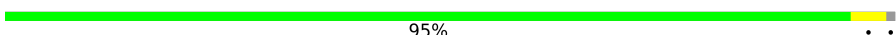
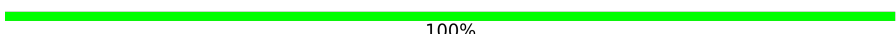
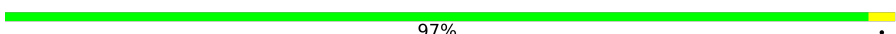
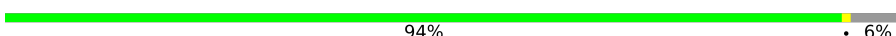
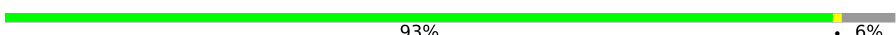
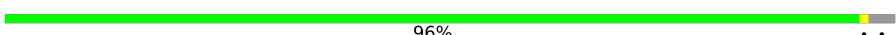
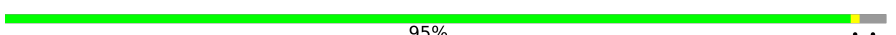


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Mol	Chain	Length	Quality of chain
6	QK	100	 61% 39%
6	Qk	100	 61% 39%
7	4A	246	 82% 17%
7	4a	246	 83% 17%
8	4C	139	 88% 12%
8	4c	139	 86% 12%
9	4E	165	 96% ..
9	4e	165	 95% ..
10	4H	221	 92% 7%
10	4h	221	 92% 7%
11	4J	88	 99% .
11	4j	88	 100%
12	5C	208	 93% 6%
12	5c	208	 94% 6%
13	6A	112	 98% ..
13	6a	112	 80% 19%
14	6B	287	 98% .
14	6b	287	 97% ..
15	7C	171	 87% 12%
15	7c	171	 87% 12%
16	C1	495	 99% .
16	c1	495	 99% .
17	C2	196	 99% .
17	c2	196	 98% .
18	C3	161	 99% .

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Mol	Chain	Length	Quality of chain
18	c3	161	 99% .
19	DC	179	 93% 7%
19	dc	179	 92% . 7%
20	QE	252	 91% . 8%
20	Qe	252	 91% . 8%
21	QF	72	 85% . 11%
21	Qf	72	 85% . 11%
22	QG	228	 98% .
22	Qg	228	 99% .
23	QI	70	 100%
23	Qi	70	 100%
24	QB	474	 96% .
24	Qb	474	 93% . .
25	5B	174	 88% . 10%
25	5b	174	 90% . 10%
26	4D	174	 95% . .
26	4d	174	 95% . .
27	4F	75	 100%
27	4f	75	 97% .
28	4G	315	 94% . 6%
28	4g	315	 93% . 6%
29	4I	274	 96% . .
29	4i	274	 95% . .
30	7A	178	 92% . 7%
30	7a	178	 92% . 7%

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 200404 atoms, of which 99661 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 MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
1	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
2	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

- Molecule 3 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
3	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 4 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
4	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 5 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
5	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 6 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		
6	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 7 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4a	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		
7	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 8 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4c	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		
8	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 9 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4e	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		
9	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4h	205	Total	C	H	N	O		0	0
			3250	1040	1644	260	306			

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	4H	205	Total	C	H	N	O	0	0
			3250	1040	1644	260	306		

- Molecule 11 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4j	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		
11	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 12 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	5c	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		
12	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 13 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	6a	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		
13	6A	111	Total	C	H	N	O	S	0	0
			1829	608	909	157	150	5		

- Molecule 14 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	6b	282	Total	C	H	N	O	S	0	0
			4512	1455	2227	396	427	7		
14	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 15 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	7c	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		
15	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	c1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		
16	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	c2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		
17	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 18 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		
18	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 19 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	dc	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		
19	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 20 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
20	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 21 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	QF	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		
21	Qf	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		

- Molecule 22 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
22	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 23 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	QI	70	Total	C	H	N	O	S	0	0
			741	290	292	77	81	1		
23	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 24 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Qb	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
24	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		

- Molecule 25 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		
25	5b	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 26 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	4d	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 27 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		
27	4f	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 28 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	4G	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		
28	4g	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		

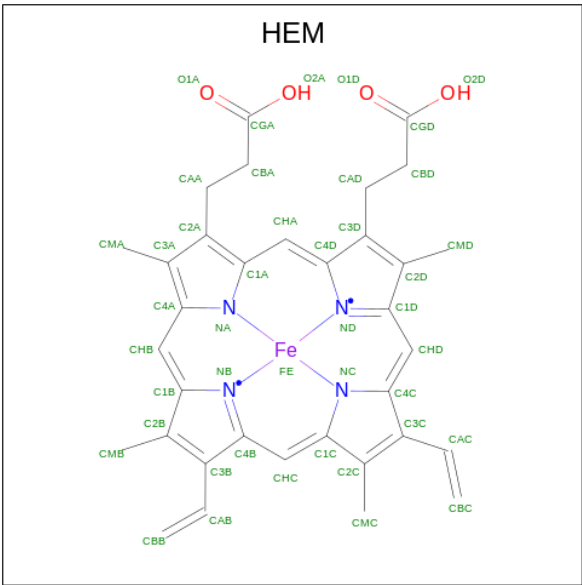
- Molecule 29 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		
29	4i	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 30 is a protein called COX7a.

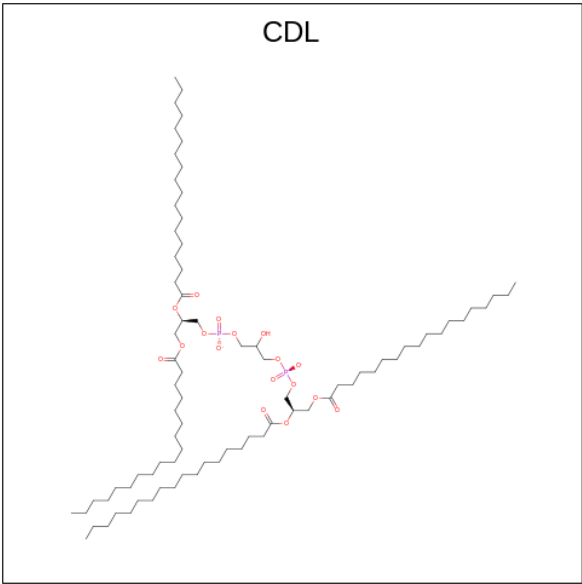
Mol	Chain	Residues	Atoms						AltConf	Trace
30	7a	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		
30	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



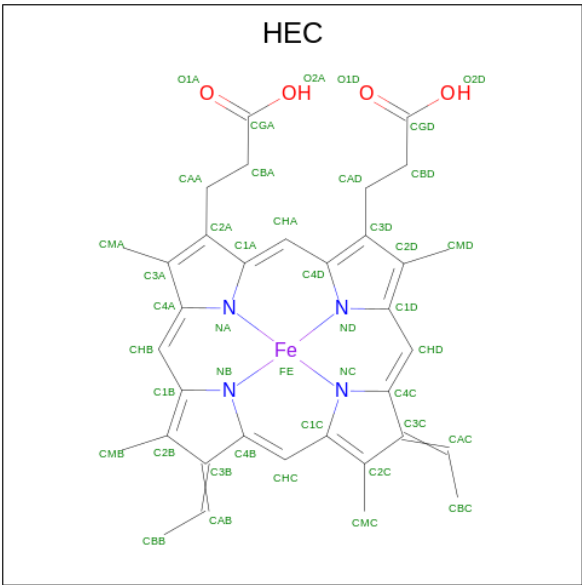
Mol	Chain	Residues	Atoms					AltConf
31	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



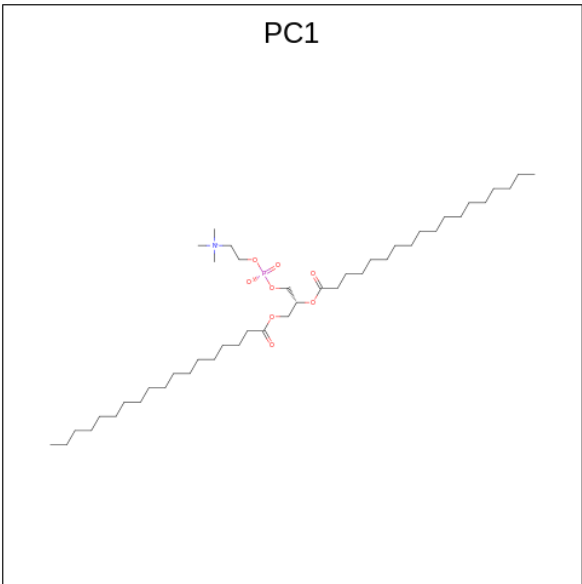
Mol	Chain	Residues	Atoms					AltConf
32	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
32	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
32	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
32	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
32	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
32	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
32	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
32	Qh	1	Total	C	H	O	P	0
			124	41	64	17	2	
32	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	
32	4c	1	Total	C	H	O	P	0
			157	51	87	17	2	
32	4e	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	7c	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	C1	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	QE	1	Total	C	H	O	P	0
			124	41	64	17	2	

- Molecule 33 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

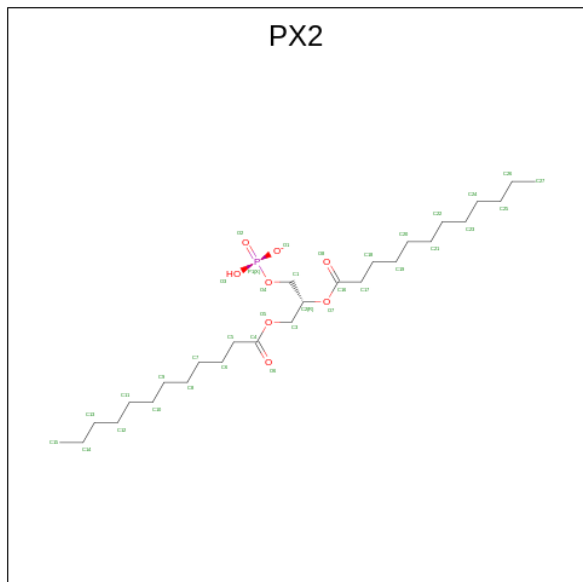
- Molecule 34 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



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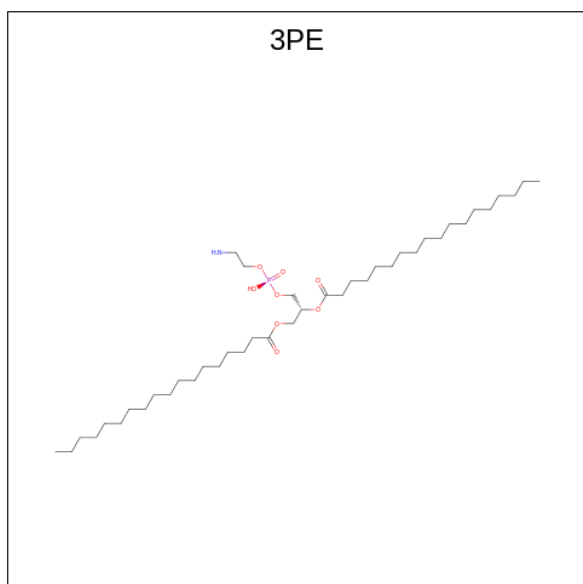
Mol	Chain	Residues	Atoms						AltConf
34	Qc	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qd	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
34	Qj	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	4a	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
34	4e	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
34	7c	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	c1	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
34	c1	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	c3	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	
34	4A	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
34	4A	1	Total	C	H	N	O	P	0
			112	36	66	1	8	1	
34	4E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
34	C1	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
34	C1	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	C3	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	
34	DC	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	QE	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	Qe	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qg	1	Total	C	H	N	O	P	0
			58	18	30	1	8	1	

- Molecule 35 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$).



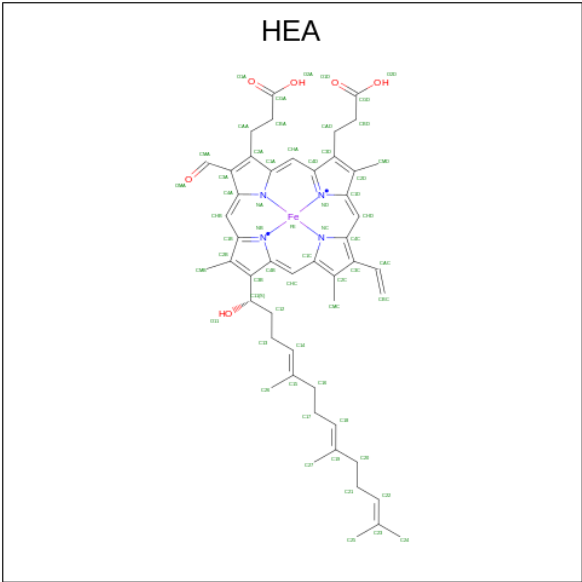
Mol	Chain	Residues	Atoms				AltConf
35	QD	1	Total	C	O	P	0
			36	27	8	1	
35	QJ	1	Total	C	O	P	0
			36	27	8	1	
35	4C	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 36 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
36	4a	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	4D	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4F	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7a	1	Total 100	C 31	H 59	N 1	O 8	P 1	0
36	4d	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4d	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7A	1	Total 100	C 31	H 59	N 1	O 8	P 1	0

- Molecule 37 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
37	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
37	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

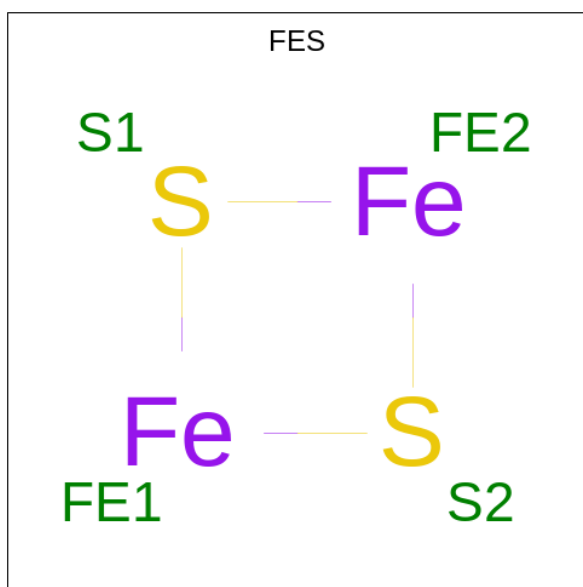
- Molecule 38 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	c1	1	Total	Cu	0
			1	1	
38	c2	2	Total	Cu	0
			2	2	
38	C1	1	Total	Cu	0
			1	1	
38	C2	2	Total	Cu	0
			2	2	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
39	c1	1	Total	Mg	0
			1	1	
39	C1	1	Total	Mg	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	QE	1	Total	Fe	S	0
			4	2	2	
40	Qe	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	5B	1	Total	Zn	0
			1	1	
41	5b	1	Total	Zn	0
			1	1	

- Molecule 42 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (three-letter code: S12) (formula: C₂₄H₄₆NO₉P).



Mol	Chain	Residues	Atoms						AltConf
42	4F	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	
42	4d	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

3 Residue-property plots [i](#)

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

Chain QA:  99% ..



- Molecule 1: MPP-beta

Chain Qa:  99% ..



- Molecule 2: Cytochrome b

Chain QC:  98% ..



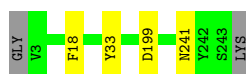
- Molecule 2: Cytochrome b

Chain Qc:  98% ..



- Molecule 3: Cytochrome c1, heme protein

Chain QD:  98% ..



- Molecule 3: Cytochrome c1, heme protein

Chain Qd:  98% ..



- Molecule 4: UQCRQ

Chain QH: 99%



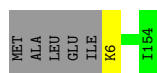
- Molecule 4: UQCRQ

Chain Qh: 99%



- Molecule 5: UQCR10

Chain QJ: 96%



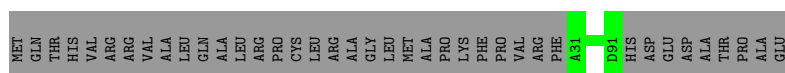
- Molecule 5: UQCR10

Chain Qj: 96%



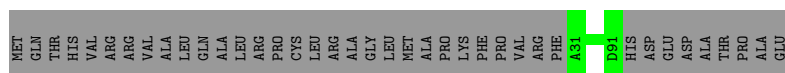
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK: 61% 39%



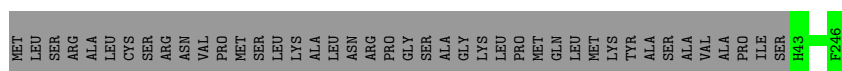
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain Qk: 61% 39%



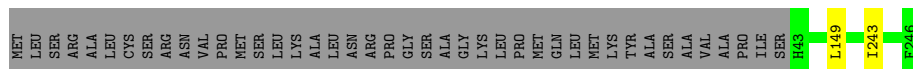
- Molecule 7: COXEG1

Chain 4a: 83% 17%



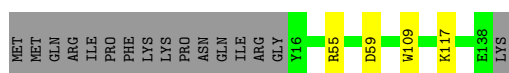
- Molecule 7: COXEG1

Chain 4A: 82% 17%



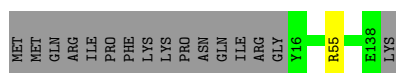
- Molecule 8: COXEG3

Chain 4c: 86% 12%



- Molecule 8: COXEG3

Chain 4C: 88% 12%



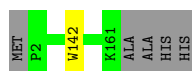
- Molecule 9: COXEG5

Chain 4e: 95% ..



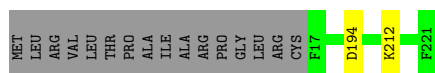
- Molecule 9: COXEG5

Chain 4E: 96% ..



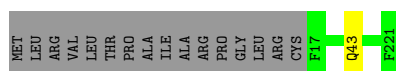
- Molecule 10: COXEG8

Chain 4h: 92% 7%



- Molecule 10: COXEG8

Chain 4H: 92% 7%



- Molecule 11: COXEG10

Chain 4j: 100%

There are no outlier residues recorded for this chain.

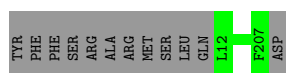
- Molecule 11: COXEG10

Chain 4J: 99%



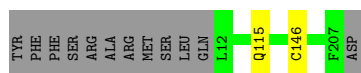
- Molecule 12: COX5c

Chain 5c: 94%



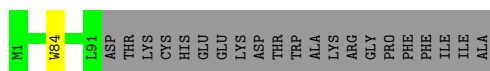
- Molecule 12: COX5c

Chain 5C: 93%



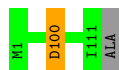
- Molecule 13: COX6a

Chain 6a: 80%



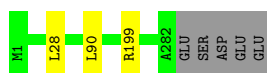
- Molecule 13: COX6a

Chain 6A: 98%

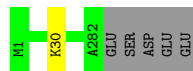


- Molecule 14: COX6b-1


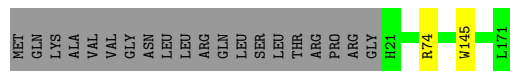
Chain 6b: 97%




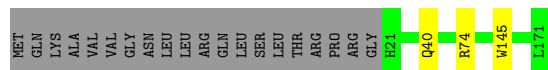
• Molecule 14: COX6b-1

Chain 6B:  98%

• Molecule 15: COX7c

Chain 7c:  87% 12%

• Molecule 15: COX7c

Chain 7C:  87% 12%

• Molecule 16: Cytochrome c oxidase subunit 1

Chain c1:  99%

• Molecule 16: Cytochrome c oxidase subunit 1

Chain C1:  99%

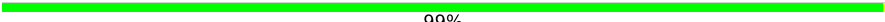
• Molecule 17: Cytochrome c oxidase subunit 2

Chain c2:  98%

• Molecule 17: Cytochrome c oxidase subunit 2

Chain C2:  99%

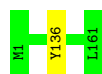
• Molecule 18: Putative NADH dehydrogenase subunit 6

Chain c3:  99%



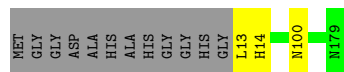
- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain C3:  99%



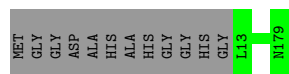
- Molecule 19: COX4

Chain dc:  92% 7%



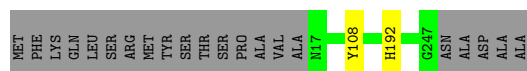
- Molecule 19: COX4

Chain DC:  93% 7%



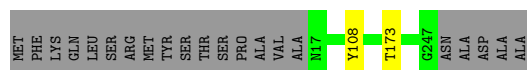
- Molecule 20: UQCRFS1

Chain QE:  91% 8%




- Molecule 20: UQCRFS1

Chain Qe:  91% 8%




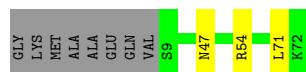
- Molecule 21: UQCRH

Chain QF:  85% 11%



- Molecule 21: UQCRH

Chain Qf:  85% 11%



- Molecule 22: UQCRB

Chain QG:  98%



- Molecule 22: UQCRB

Chain Qg:  99%



- Molecule 23: UQCR9

Chain QI:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: UQCR9

Chain Qi:  100%

There are no outlier residues recorded for this chain.

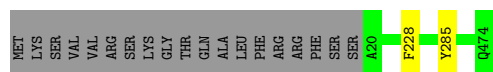
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain Qb:  93%




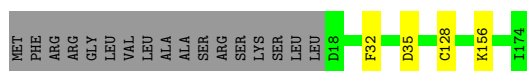
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain QB:  96%



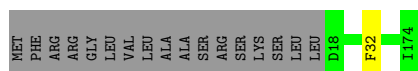
- Molecule 25: COX5b-2

Chain 5B:  88% 10%



- Molecule 25: COX5b-2

Chain 5b: 90% • 10%



- Molecule 26: COXEG4

Chain 4D: 95% • •



- Molecule 26: COXEG4

Chain 4d: 95% • •



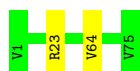
- Molecule 27: COXEG6

Chain 4F: 100%

There are no outlier residues recorded for this chain.

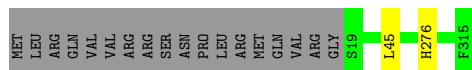
- Molecule 27: COXEG6

Chain 4f: 97% •



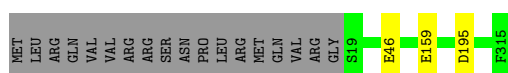
- Molecule 28: COXEG7

Chain 4G: 94% • 6%

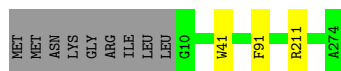


- Molecule 28: COXEG7

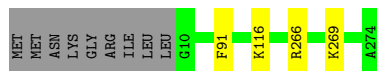
Chain 4g: 93% • 6%



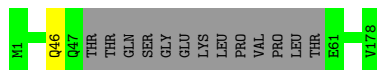
● Molecule 29: COXEG9

Chain 4I:  96% 

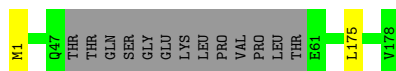
● Molecule 29: COXEG9

Chain 4i:  95% 

● Molecule 30: COX7a

Chain 7a:  92%  7%

● Molecule 30: COX7a

Chain 7A:  92%  7%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135598	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 ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, HEC, ZN, CU, FES, CDL, 3PE, MG, PX2, HEA, HEM, S12

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	QA	0.31	0/3838	0.50	0/5193
1	Qa	0.32	0/3838	0.50	0/5193
2	QC	0.35	0/3058	0.47	0/4178
2	Qc	0.35	0/3058	0.47	0/4178
3	QD	0.35	0/2027	0.49	0/2760
3	Qd	0.35	0/2027	0.50	0/2760
4	QH	0.33	0/717	0.54	0/966
4	Qh	0.32	0/717	0.54	0/966
5	QJ	0.29	0/1243	0.51	0/1693
5	Qj	0.30	0/1243	0.51	0/1693
6	QK	0.32	0/498	0.48	0/677
6	Qk	0.32	0/498	0.47	0/677
7	4A	0.29	0/1650	0.44	0/2235
7	4a	0.29	0/1650	0.45	0/2235
8	4C	0.32	0/1051	0.46	0/1432
8	4c	0.31	0/1051	0.46	0/1432
9	4E	0.29	0/1376	0.44	0/1864
9	4e	0.29	0/1376	0.45	0/1864
10	4H	0.31	0/1640	0.44	0/2224
10	4h	0.30	0/1640	0.43	0/2224
11	4J	0.30	0/736	0.48	0/1008
11	4j	0.31	0/736	0.48	0/1008
12	5C	0.36	0/1616	0.46	0/2192
12	5c	0.36	0/1616	0.46	0/2192
13	6A	0.30	0/953	0.45	0/1292
13	6a	0.30	0/777	0.44	0/1055
14	6B	0.32	0/2343	0.45	0/3174
14	6b	0.31	0/2343	0.45	0/3174
15	7C	0.35	0/1299	0.45	0/1777
15	7c	0.36	0/1299	0.45	0/1777
16	C1	0.36	0/4054	0.48	0/5516
16	c1	0.39	0/4054	0.48	0/5516

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C2	0.34	0/1620	0.50	0/2207
17	c2	0.36	0/1620	0.50	0/2207
18	C3	0.35	0/1416	0.44	0/1945
18	c3	0.34	0/1416	0.45	0/1945
19	DC	0.35	0/1410	0.50	0/1914
19	dc	0.34	0/1410	0.51	0/1914
20	QE	0.29	0/1842	0.50	0/2502
20	Qe	0.29	0/1842	0.50	0/2502
21	QF	0.27	0/526	0.40	0/702
21	Qf	0.27	0/526	0.40	0/702
22	QG	0.35	0/1987	0.53	0/2696
22	Qg	0.35	0/1987	0.53	0/2696
23	QI	0.35	0/251	0.42	0/340
23	Qi	0.35	0/251	0.43	0/340
24	QB	0.32	0/3532	0.48	0/4805
24	Qb	0.33	0/3532	0.50	0/4805
25	5B	0.36	0/1294	0.49	0/1759
25	5b	0.38	0/1294	0.49	0/1759
26	4D	0.31	0/1379	0.50	0/1867
26	4d	0.31	0/1379	0.50	0/1867
27	4F	0.34	0/641	0.45	0/867
27	4f	0.35	0/641	0.45	0/867
28	4G	0.30	0/2391	0.49	0/3240
28	4g	0.30	0/2391	0.48	0/3240
29	4I	0.34	0/2255	0.48	0/3059
29	4i	0.35	0/2255	0.48	0/3059
30	7A	0.31	0/1359	0.50	0/1835
30	7a	0.30	0/1359	0.49	0/1835
All	All	0.33	0/99828	0.48	0/135601

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
24	Qb	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	Qb	283	GLU	Peptide
24	Qb	284	GLY	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	QA	476/479 (99%)	460 (97%)	16 (3%)	0	100	100
1	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
2	QC	362/368 (98%)	354 (98%)	7 (2%)	1 (0%)	37	64
2	Qc	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
3	QD	239/243 (98%)	225 (94%)	14 (6%)	0	100	100
3	Qd	239/243 (98%)	218 (91%)	21 (9%)	0	100	100
4	QH	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
4	Qh	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
5	QJ	147/154 (96%)	141 (96%)	6 (4%)	0	100	100
5	Qj	147/154 (96%)	139 (95%)	8 (5%)	0	100	100
6	QK	59/100 (59%)	59 (100%)	0	0	100	100
6	Qk	59/100 (59%)	59 (100%)	0	0	100	100
7	4A	202/246 (82%)	195 (96%)	7 (4%)	0	100	100
7	4a	202/246 (82%)	191 (95%)	11 (5%)	0	100	100
8	4C	121/139 (87%)	115 (95%)	6 (5%)	0	100	100
8	4c	121/139 (87%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	4E	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
9	4e	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
10	4H	203/221 (92%)	200 (98%)	3 (2%)	0	100	100
10	4h	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
11	4J	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
11	4j	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
12	5C	194/208 (93%)	189 (97%)	5 (3%)	0	100	100
12	5c	194/208 (93%)	185 (95%)	9 (5%)	0	100	100
13	6A	109/112 (97%)	101 (93%)	7 (6%)	1 (1%)	14	40
13	6a	89/112 (80%)	86 (97%)	3 (3%)	0	100	100
14	6B	280/287 (98%)	274 (98%)	6 (2%)	0	100	100
14	6b	280/287 (98%)	271 (97%)	9 (3%)	0	100	100
15	7C	149/171 (87%)	143 (96%)	6 (4%)	0	100	100
15	7c	149/171 (87%)	142 (95%)	7 (5%)	0	100	100
16	C1	493/495 (100%)	479 (97%)	14 (3%)	0	100	100
16	c1	493/495 (100%)	473 (96%)	20 (4%)	0	100	100
17	C2	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
17	c2	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
18	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
18	c3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
19	DC	165/179 (92%)	159 (96%)	6 (4%)	0	100	100
19	dc	165/179 (92%)	157 (95%)	8 (5%)	0	100	100
20	QE	229/252 (91%)	219 (96%)	10 (4%)	0	100	100
20	Qe	229/252 (91%)	216 (94%)	13 (6%)	0	100	100
21	QF	62/72 (86%)	62 (100%)	0	0	100	100
21	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
22	QG	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
22	Qg	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
23	QI	28/70 (40%)	28 (100%)	0	0	100	100
23	Qi	28/70 (40%)	27 (96%)	1 (4%)	0	100	100
24	QB	453/474 (96%)	438 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Qb	453/474 (96%)	429 (95%)	24 (5%)	0	100	100
25	5B	155/174 (89%)	149 (96%)	6 (4%)	0	100	100
25	5b	155/174 (89%)	148 (96%)	7 (4%)	0	100	100
26	4D	171/174 (98%)	157 (92%)	14 (8%)	0	100	100
26	4d	171/174 (98%)	161 (94%)	10 (6%)	0	100	100
27	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
27	4f	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
28	4G	295/315 (94%)	286 (97%)	9 (3%)	0	100	100
28	4g	295/315 (94%)	283 (96%)	12 (4%)	0	100	100
29	4I	263/274 (96%)	255 (97%)	8 (3%)	0	100	100
29	4i	263/274 (96%)	252 (96%)	11 (4%)	0	100	100
30	7A	161/178 (90%)	155 (96%)	6 (4%)	0	100	100
30	7a	161/178 (90%)	156 (97%)	5 (3%)	0	100	100
All	All	11970/12768 (94%)	11501 (96%)	467 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	6A	100	ASP
2	QC	145	PHE

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	QA	400/401 (100%)	397 (99%)	3 (1%)	79	88
1	Qa	400/401 (100%)	396 (99%)	4 (1%)	73	85
2	QC	337/341 (99%)	335 (99%)	2 (1%)	84	90
2	Qc	337/341 (99%)	335 (99%)	2 (1%)	84	90
3	QD	206/207 (100%)	202 (98%)	4 (2%)	52	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Qd	206/207 (100%)	204 (99%)	2 (1%)	73	85
4	QH	71/72 (99%)	71 (100%)	0	100	100
4	Qh	71/72 (99%)	71 (100%)	0	100	100
5	QJ	124/128 (97%)	123 (99%)	1 (1%)	79	88
5	Qj	124/128 (97%)	123 (99%)	1 (1%)	79	88
6	QK	50/82 (61%)	50 (100%)	0	100	100
6	Qk	50/82 (61%)	50 (100%)	0	100	100
7	4A	173/207 (84%)	171 (99%)	2 (1%)	67	82
7	4a	173/207 (84%)	173 (100%)	0	100	100
8	4C	112/127 (88%)	111 (99%)	1 (1%)	75	86
8	4c	112/127 (88%)	108 (96%)	4 (4%)	30	57
9	4E	142/145 (98%)	141 (99%)	1 (1%)	81	89
9	4e	142/145 (98%)	138 (97%)	4 (3%)	38	63
10	4H	176/189 (93%)	175 (99%)	1 (1%)	84	90
10	4h	176/189 (93%)	174 (99%)	2 (1%)	70	83
11	4J	75/75 (100%)	74 (99%)	1 (1%)	65	80
11	4j	75/75 (100%)	75 (100%)	0	100	100
12	5C	167/178 (94%)	165 (99%)	2 (1%)	67	82
12	5c	167/178 (94%)	167 (100%)	0	100	100
13	6A	97/97 (100%)	96 (99%)	1 (1%)	73	85
13	6a	79/97 (81%)	78 (99%)	1 (1%)	65	80
14	6B	238/243 (98%)	237 (100%)	1 (0%)	89	93
14	6b	238/243 (98%)	235 (99%)	3 (1%)	65	80
15	7C	135/152 (89%)	132 (98%)	3 (2%)	47	68
15	7c	135/152 (89%)	133 (98%)	2 (2%)	60	77
16	C1	438/438 (100%)	434 (99%)	4 (1%)	75	86
16	c1	438/438 (100%)	433 (99%)	5 (1%)	70	83
17	C2	178/178 (100%)	176 (99%)	2 (1%)	70	83
17	c2	178/178 (100%)	175 (98%)	3 (2%)	56	75
18	C3	155/155 (100%)	154 (99%)	1 (1%)	84	90
18	c3	155/155 (100%)	153 (99%)	2 (1%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	DC	148/153 (97%)	148 (100%)	0	100	100
19	dc	148/153 (97%)	145 (98%)	3 (2%)	50	71
20	QE	193/209 (92%)	191 (99%)	2 (1%)	73	85
20	Qe	193/209 (92%)	191 (99%)	2 (1%)	73	85
21	QF	58/63 (92%)	55 (95%)	3 (5%)	19	45
21	Qf	58/63 (92%)	55 (95%)	3 (5%)	19	45
22	QG	207/207 (100%)	203 (98%)	4 (2%)	52	72
22	Qg	207/207 (100%)	204 (99%)	3 (1%)	62	79
23	QI	27/27 (100%)	27 (100%)	0	100	100
23	Qi	27/27 (100%)	27 (100%)	0	100	100
24	QB	369/386 (96%)	367 (100%)	2 (0%)	86	91
24	Qb	369/386 (96%)	359 (97%)	10 (3%)	40	64
25	5B	134/148 (90%)	130 (97%)	4 (3%)	36	61
25	5b	134/148 (90%)	133 (99%)	1 (1%)	81	89
26	4D	146/147 (99%)	139 (95%)	7 (5%)	21	48
26	4d	146/147 (99%)	139 (95%)	7 (5%)	21	48
27	4F	62/62 (100%)	62 (100%)	0	100	100
27	4f	62/62 (100%)	60 (97%)	2 (3%)	34	60
28	4G	247/264 (94%)	245 (99%)	2 (1%)	79	88
28	4g	247/264 (94%)	244 (99%)	3 (1%)	67	82
29	4I	230/238 (97%)	227 (99%)	3 (1%)	65	80
29	4i	230/238 (97%)	226 (98%)	4 (2%)	56	75
30	7A	138/150 (92%)	136 (99%)	2 (1%)	62	79
30	7a	138/150 (92%)	137 (99%)	1 (1%)	81	89
All	All	10448/10938 (96%)	10315 (99%)	133 (1%)	64	80

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	4d	126	VAL
26	4d	171	GLN
25	5b	32	PHE
7	4A	149	LEU
19	dc	100	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
28	4G	141	ASN
25	5b	47	GLN
29	4I	153	ASN
26	4d	107	GLN
19	dc	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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	$\# Z > 2$
36	3PE	4F	101	-	50,50,50	0.31	0	53,55,55	0.32	0
33	HEC	Qd	301	3	32,50,50	2.05	4 (12%)	24,82,82	2.16	12 (50%)
31	HEM	Qc	402	2	41,50,50	1.26	4 (9%)	45,82,82	1.75	9 (20%)
34	PC1	c1	508	-	35,35,53	0.36	0	41,43,61	0.31	0
32	CDL	7c	201	-	89,89,99	0.32	0	95,101,111	0.35	0
34	PC1	Qe	302	-	53,53,53	0.30	0	59,61,61	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	S12	4F	102	-	33,34,34	0.79	0	36,40,40	1.18	2 (5%)
31	HEM	QC	401	2	41,50,50	1.26	5 (12%)	45,82,82	1.75	8 (17%)
34	PC1	4A	301	-	46,46,53	0.32	0	52,54,61	0.33	0
32	CDL	QJ	202	-	57,57,99	0.39	0	63,69,111	0.33	0
34	PC1	DC	201	-	53,53,53	0.32	0	59,61,61	0.51	1 (1%)
34	PC1	QD	303	-	30,30,53	0.38	0	36,38,61	0.37	0
37	HEA	c1	502	16	57,67,67	2.04	15 (26%)	61,103,103	2.59	25 (40%)
34	PC1	c3	201	-	50,50,53	0.31	0	56,58,61	0.29	0
34	PC1	Qe	304	-	35,35,53	0.35	0	41,43,61	0.36	0
36	3PE	4a	302	-	50,50,50	0.31	0	53,55,55	0.42	0
34	PC1	Qe	301	-	53,53,53	0.30	0	59,61,61	0.35	0
36	3PE	c1	507	-	39,39,50	0.34	0	42,44,55	0.33	0
36	3PE	4d	202	-	50,50,50	0.31	0	53,55,55	0.27	0
37	HEA	C1	501	16	57,67,67	2.00	16 (28%)	61,103,103	2.73	27 (44%)
31	HEM	QC	402	2	41,50,50	1.27	3 (7%)	45,82,82	1.71	9 (20%)
34	PC1	4a	301	-	46,46,53	0.32	0	52,54,61	0.31	0
34	PC1	C3	201	-	50,50,53	0.32	0	56,58,61	0.30	0
34	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.32	0
32	CDL	QC	403	-	55,55,99	0.40	0	61,67,111	0.33	0
35	PX2	QJ	201	-	35,35,35	0.98	3 (8%)	39,40,40	1.11	2 (5%)
34	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.33	0
36	3PE	7a	201	-	40,40,50	0.34	0	43,45,55	0.29	0
37	HEA	C1	502	16	57,67,67	2.03	15 (26%)	61,103,103	2.60	26 (42%)
34	PC1	Qd	303	-	30,30,53	0.38	0	36,38,61	0.34	0
32	CDL	Qh	101	-	64,64,99	0.37	0	70,76,111	0.32	0
32	CDL	QH	101	-	75,75,99	0.34	0	81,87,111	0.32	0
32	CDL	4e	202	-	71,71,99	0.36	0	77,83,111	0.33	0
36	3PE	4d	201	-	34,34,50	0.37	0	37,39,55	0.34	0
34	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.35	0
34	PC1	4e	201	-	34,34,53	0.36	0	40,42,61	0.32	0
32	CDL	QD	302	-	68,68,99	0.38	0	74,80,111	0.37	0
33	HEC	QD	301	3	32,50,50	2.05	4 (12%)	24,82,82	2.20	12 (50%)
34	PC1	4E	201	-	34,34,53	0.36	0	40,42,61	0.33	0
32	CDL	Qc	404	-	53,53,99	0.40	0	59,65,111	0.34	0
34	PC1	Qj	201	-	53,53,53	0.30	0	59,61,61	0.28	0
34	PC1	C1	509	-	35,35,53	0.37	0	41,43,61	0.32	0
32	CDL	Qh	102	-	59,59,99	0.38	0	65,71,111	0.37	0
32	CDL	4c	201	-	69,69,99	0.35	0	75,81,111	0.32	0
40	FES	Qe	303	20	0,4,4	-	-	-	-	-
32	CDL	C1	506	-	89,89,99	0.32	0	95,101,111	0.28	0
34	PC1	Qc	403	-	35,35,53	0.36	0	41,43,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PE	c1	506	-	39,39,50	0.35	0	42,44,55	0.39	0
36	3PE	C1	508	-	39,39,50	0.35	0	42,44,55	0.34	0
36	3PE	7A	201	-	40,40,50	0.34	0	43,45,55	0.30	0
32	CDL	QE	302	-	59,59,99	0.38	0	65,71,111	0.33	0
36	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.34	0
34	PC1	c1	505	-	49,49,53	0.31	0	55,57,61	0.31	0
34	PC1	7c	202	-	53,53,53	0.30	0	59,61,61	0.30	0
36	3PE	C1	507	-	39,39,50	0.36	0	42,44,55	0.35	0
32	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
31	HEM	Qc	401	2	41,50,50	1.27	5 (12%)	45,82,82	1.78	9 (20%)
32	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.37	0
40	FES	QE	301	20	0,4,4	-	-	-	-	-
35	PX2	4C	201	-	35,35,35	0.99	4 (11%)	39,40,40	1.06	2 (5%)
34	PC1	QE	303	-	35,35,53	0.35	0	41,43,61	0.37	0
42	S12	4d	203	-	33,34,34	0.77	0	36,40,40	1.10	3 (8%)
35	PX2	QD	304	-	35,35,35	0.99	4 (11%)	39,40,40	1.02	2 (5%)
32	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.29	0
37	HEA	c1	501	16	57,67,67	2.00	15 (26%)	61,103,103	2.74	29 (47%)

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
36	3PE	4F	101	-	-	21/54/54/54	-
33	HEC	Qd	301	3	-	3/10/54/54	-
31	HEM	Qc	402	2	-	4/12/54/54	-
34	PC1	c1	508	-	-	6/39/39/57	-
32	CDL	7c	201	-	-	18/100/100/110	-
34	PC1	Qe	302	-	-	15/57/57/57	-
42	S12	4F	102	-	-	20/38/38/38	-
31	HEM	QC	401	2	-	3/12/54/54	-
34	PC1	4A	301	-	-	12/50/50/57	-
32	CDL	QJ	202	-	-	17/68/68/110	-
34	PC1	DC	201	-	-	29/57/57/57	-
34	PC1	QD	303	-	-	17/34/34/57	-
37	HEA	c1	502	16	-	13/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PC1	c3	201	-	-	16/54/54/57	-
34	PC1	Qe	304	-	-	8/39/39/57	-
36	3PE	4a	302	-	-	23/54/54/54	-
34	PC1	Qe	301	-	-	17/57/57/57	-
36	3PE	c1	507	-	-	14/43/43/54	-
36	3PE	4d	202	-	-	19/54/54/54	-
37	HEA	C1	501	16	-	13/32/76/76	-
31	HEM	QC	402	2	-	4/12/54/54	-
34	PC1	4a	301	-	-	14/50/50/57	-
34	PC1	C3	201	-	-	16/54/54/57	-
34	PC1	C1	505	-	-	13/53/53/57	-
32	CDL	QC	403	-	-	13/66/66/110	-
35	PX2	QJ	201	-	-	18/37/37/37	-
34	PC1	4A	302	-	-	15/49/49/57	-
36	3PE	7a	201	-	-	9/44/44/54	-
37	HEA	C1	502	16	-	11/32/76/76	-
34	PC1	Qd	303	-	-	6/34/34/57	-
32	CDL	Qh	101	-	-	18/75/75/110	-
32	CDL	QH	101	-	-	17/86/86/110	-
32	CDL	4e	202	-	-	23/82/82/110	-
36	3PE	4d	201	-	-	5/38/38/54	-
34	PC1	Qg	301	-	-	5/31/31/57	-
34	PC1	4e	201	-	-	3/38/38/57	-
32	CDL	QD	302	-	-	22/79/79/110	-
33	HEC	QD	301	3	-	2/10/54/54	-
34	PC1	4E	201	-	-	5/38/38/57	-
32	CDL	Qc	404	-	-	12/64/64/110	-
34	PC1	Qj	201	-	-	8/57/57/57	-
34	PC1	C1	509	-	-	8/39/39/57	-
32	CDL	Qh	102	-	-	15/70/70/110	-
32	CDL	4c	201	-	-	25/80/80/110	-
40	FES	Qe	303	20	-	-	0/1/1/1
32	CDL	C1	506	-	-	19/100/100/110	-
34	PC1	Qc	403	-	-	12/39/39/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	3PE	c1	506	-	-	19/43/43/54	-
36	3PE	C1	508	-	-	6/43/43/54	-
36	3PE	7A	201	-	-	8/44/44/54	-
32	CDL	QE	302	-	-	24/70/70/110	-
36	3PE	4D	201	-	-	6/38/38/54	-
34	PC1	c1	505	-	-	16/53/53/57	-
34	PC1	7c	202	-	-	26/57/57/57	-
36	3PE	C1	507	-	-	17/43/43/54	-
32	CDL	4E	202	-	-	24/82/82/110	-
31	HEM	Qc	401	2	-	4/12/54/54	-
32	CDL	Qj	202	-	-	11/58/58/110	-
40	FES	QE	301	20	-	-	0/1/1/1
35	PX2	4C	201	-	-	16/37/37/37	-
34	PC1	QE	303	-	-	10/39/39/57	-
42	S12	4d	203	-	-	24/38/38/38	-
35	PX2	QD	304	-	-	15/37/37/37	-
32	CDL	Qd	302	-	-	28/110/110/110	-
37	HEA	c1	501	16	-	11/32/76/76	-

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	QD	301	HEC	C3C-C2C	-6.84	1.33	1.40
33	Qd	301	HEC	C3C-C2C	-6.59	1.33	1.40
33	Qd	301	HEC	C2B-C3B	-6.44	1.34	1.40
33	QD	301	HEC	C2B-C3B	-6.27	1.34	1.40
37	c1	502	HEA	C3B-C2B	5.42	1.46	1.34

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	501	HEA	CAD-CBD-CGD	-8.18	96.01	113.60
37	c1	501	HEA	CAD-CBD-CGD	-7.67	97.11	113.60
37	C1	502	HEA	CAD-CBD-CGD	-7.16	98.20	113.60
37	c1	502	HEA	CAD-CBD-CGD	-6.93	98.70	113.60
37	c1	501	HEA	C3D-C4D-ND	6.03	116.20	110.36

There are no chirality outliers.

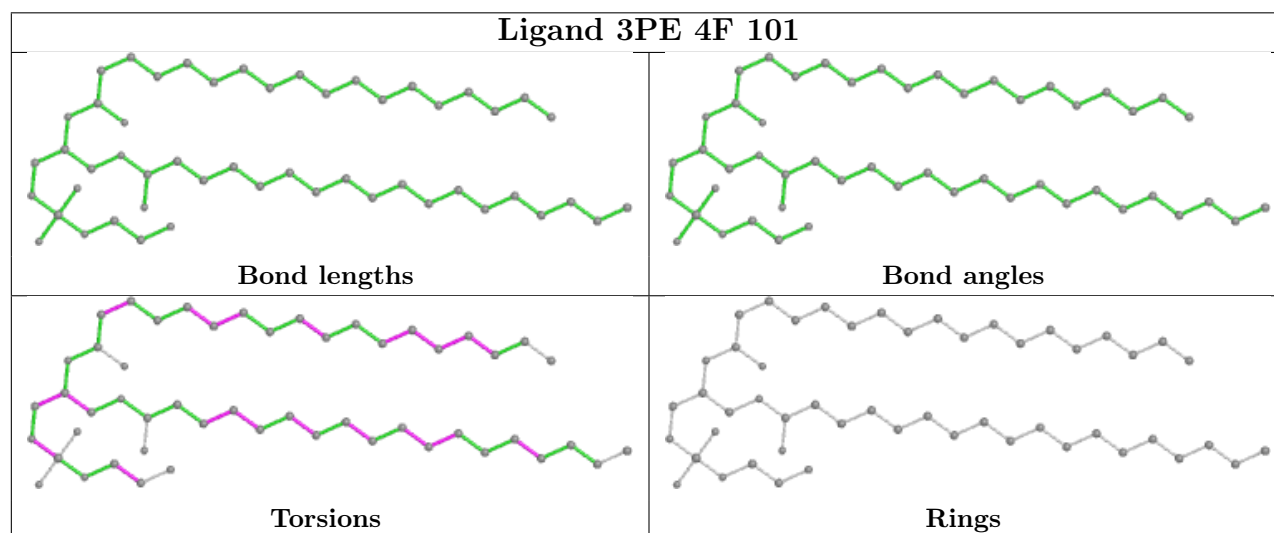
5 of 871 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	QC	403	CDL	CA2-OA2-PA1-OA3
32	QC	403	CDL	CB3-OB5-PB2-OB3
32	QD	302	CDL	CB3-OB5-PB2-OB3
32	QD	302	CDL	CB3-OB5-PB2-OB4
32	QH	101	CDL	CA2-OA2-PA1-OA3

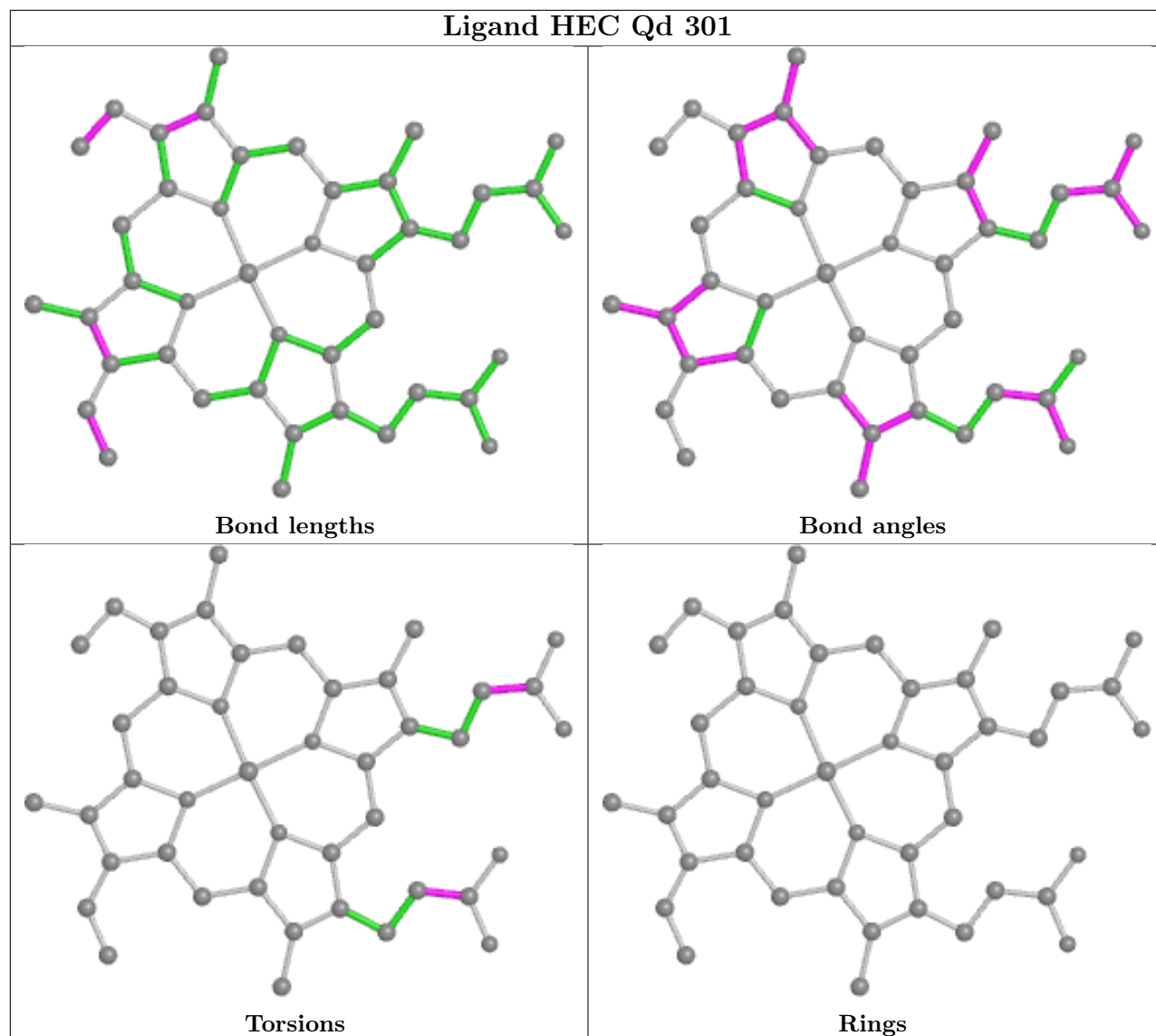
There are no ring outliers.

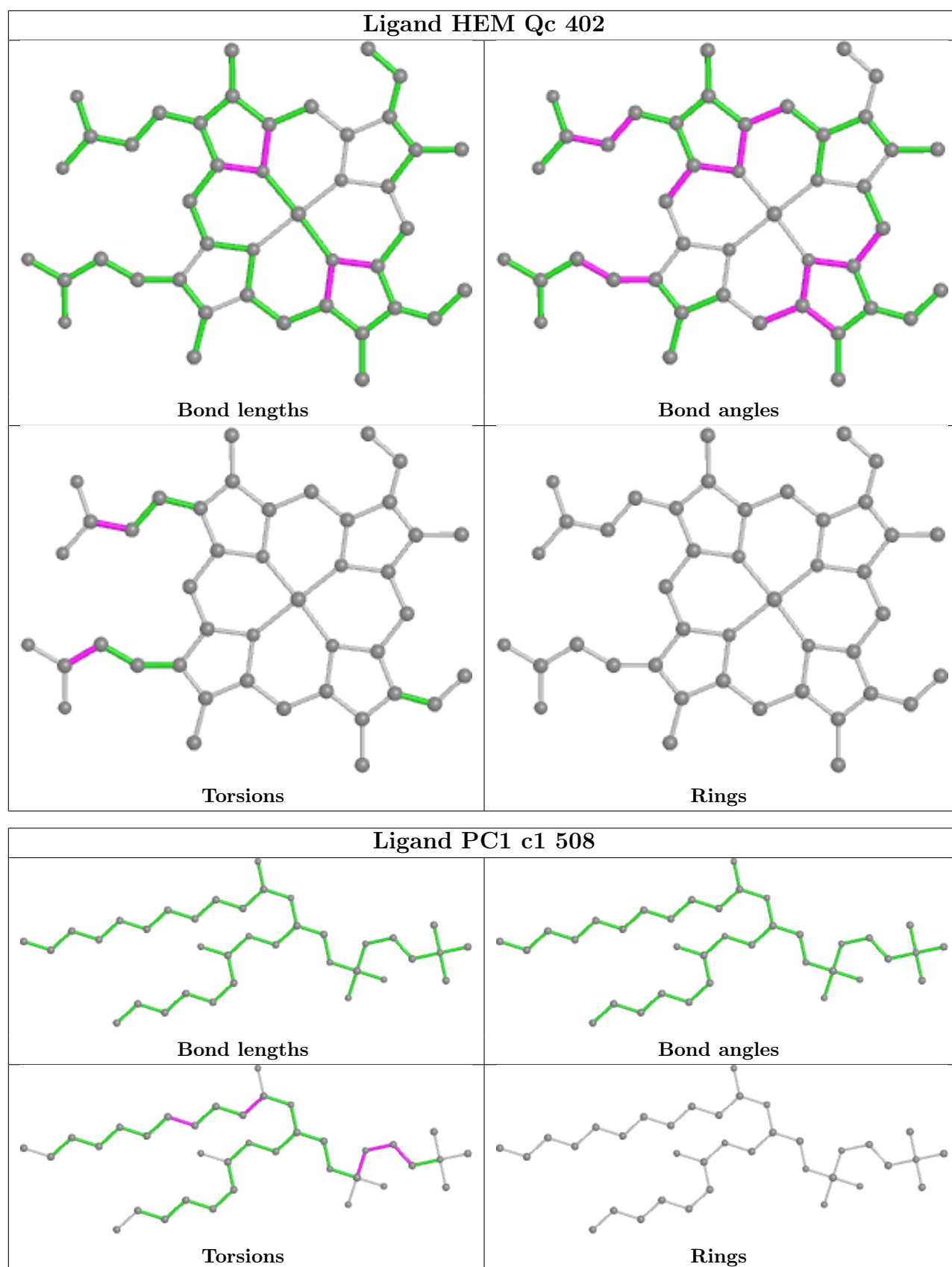
No monomer is involved in short contacts.

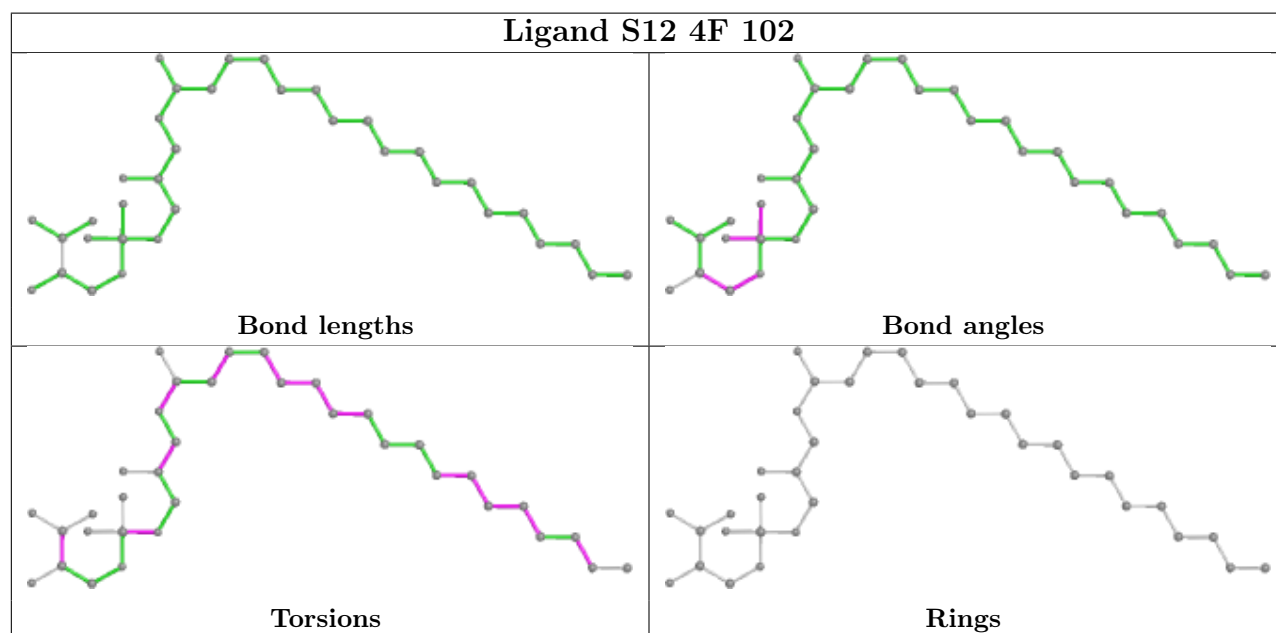
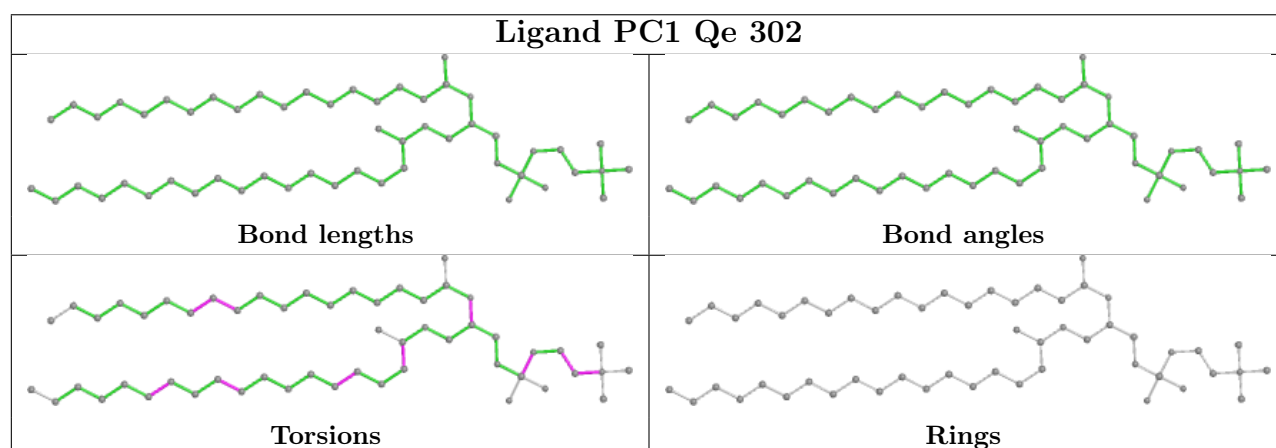
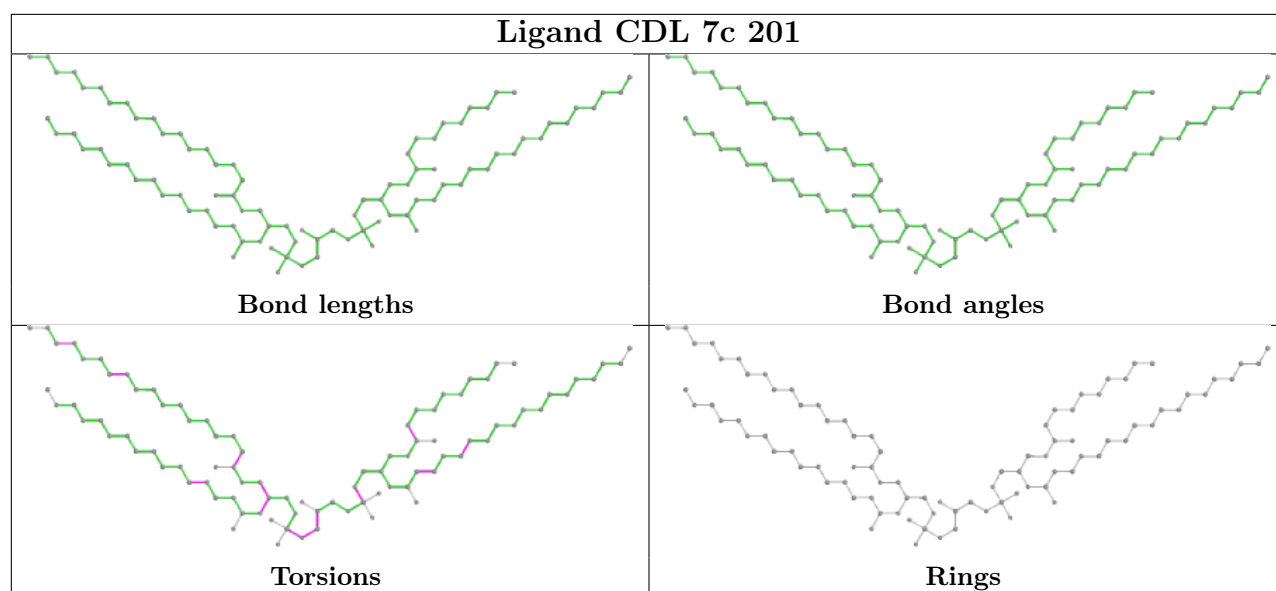
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



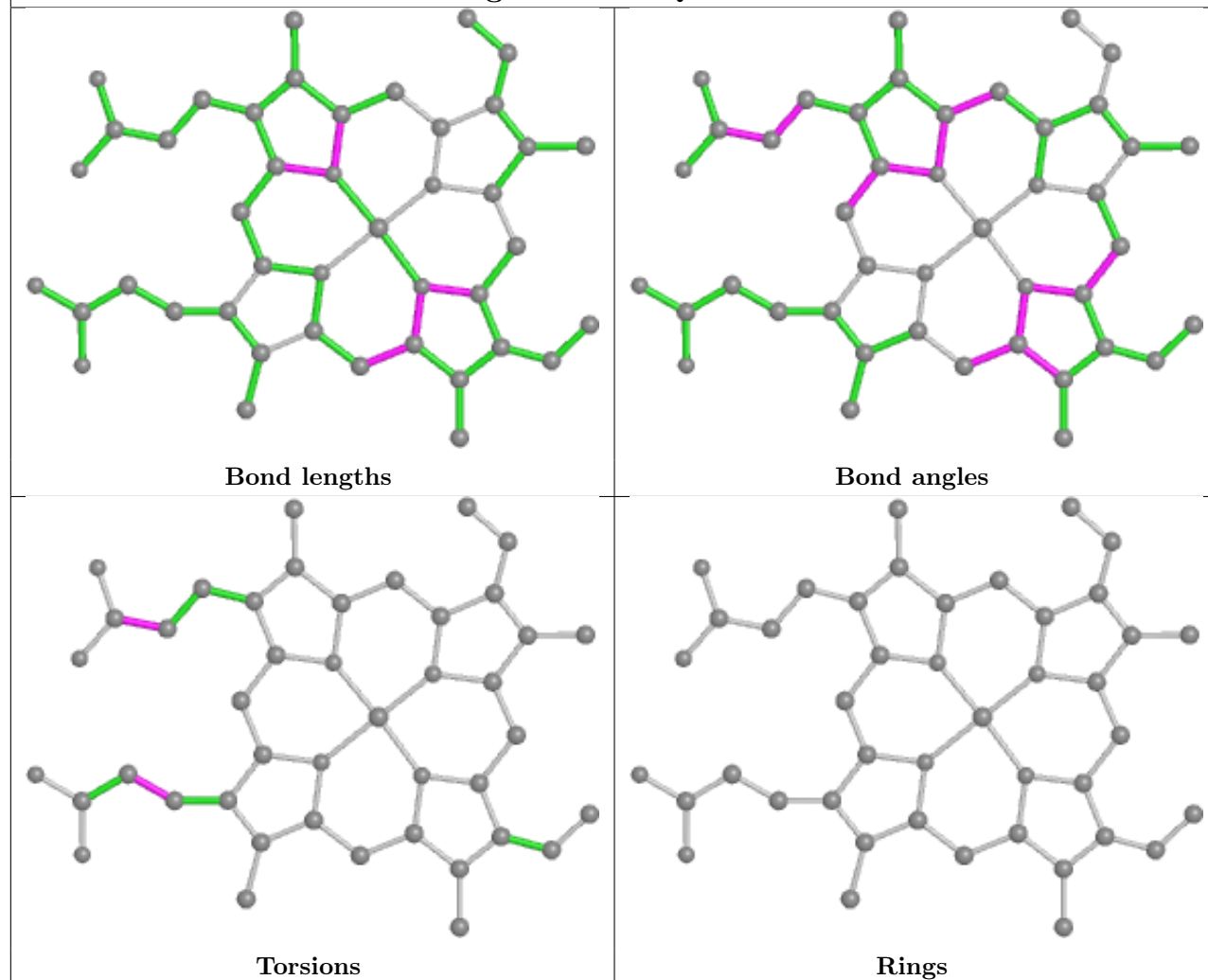
Ligand HEC Qd 301



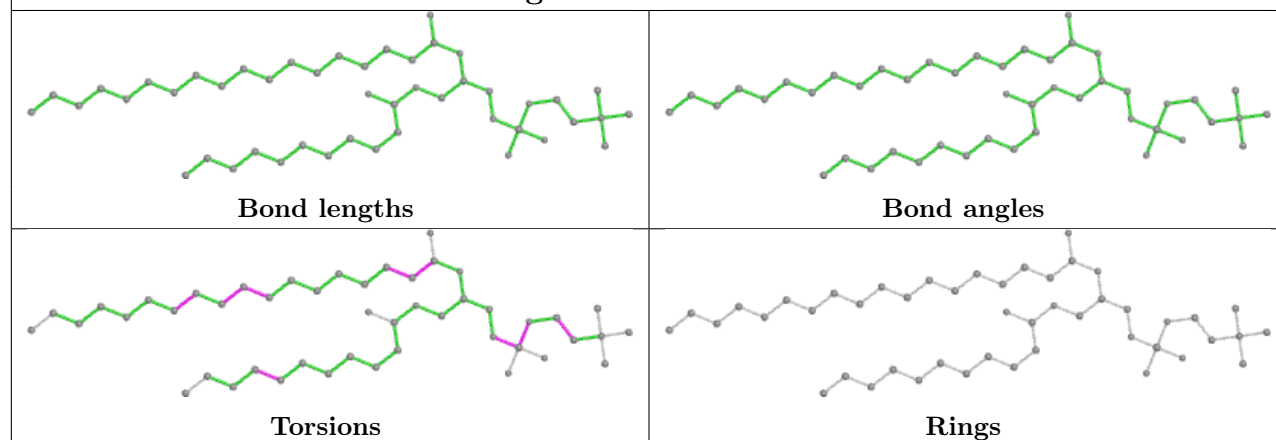


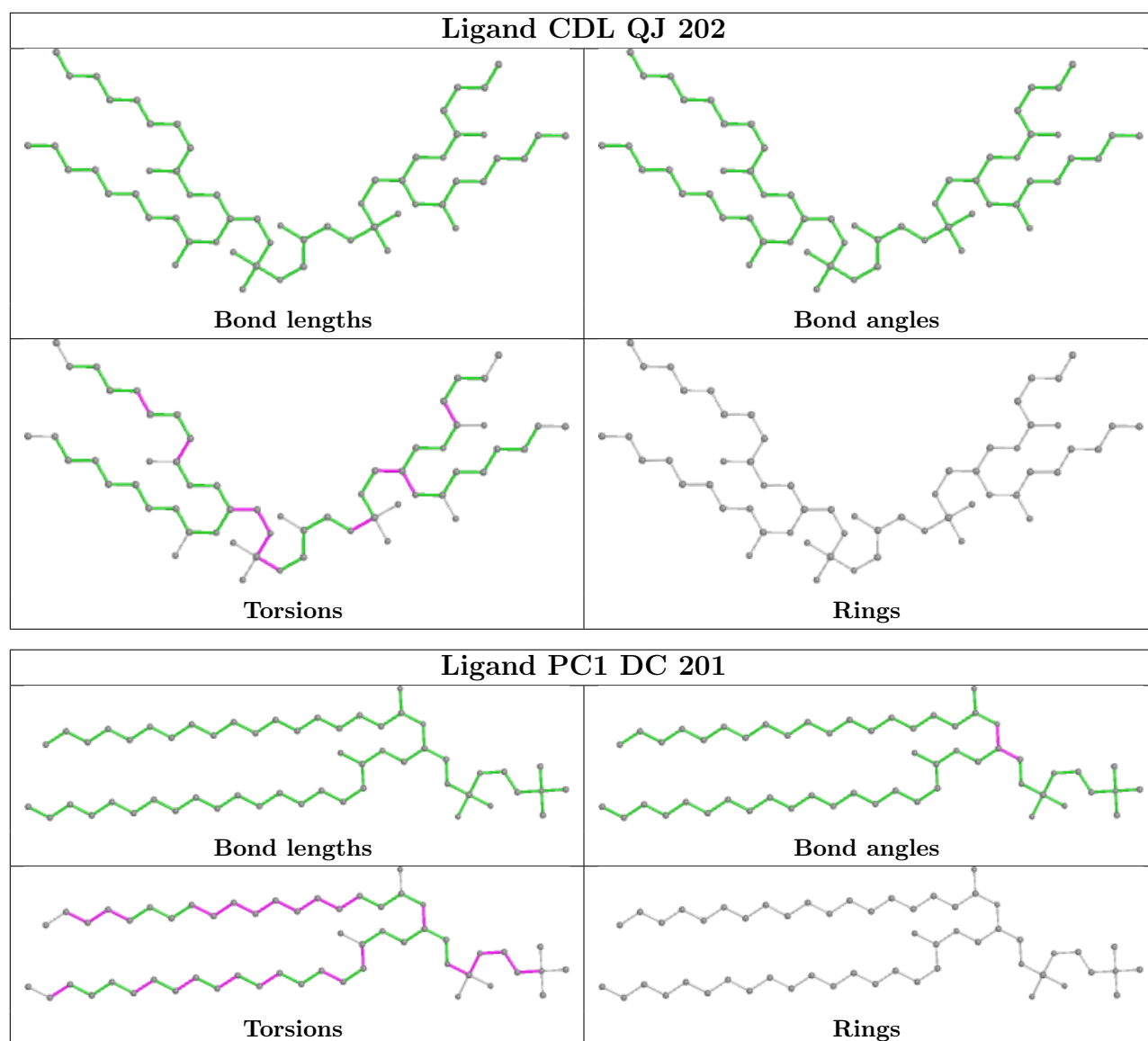


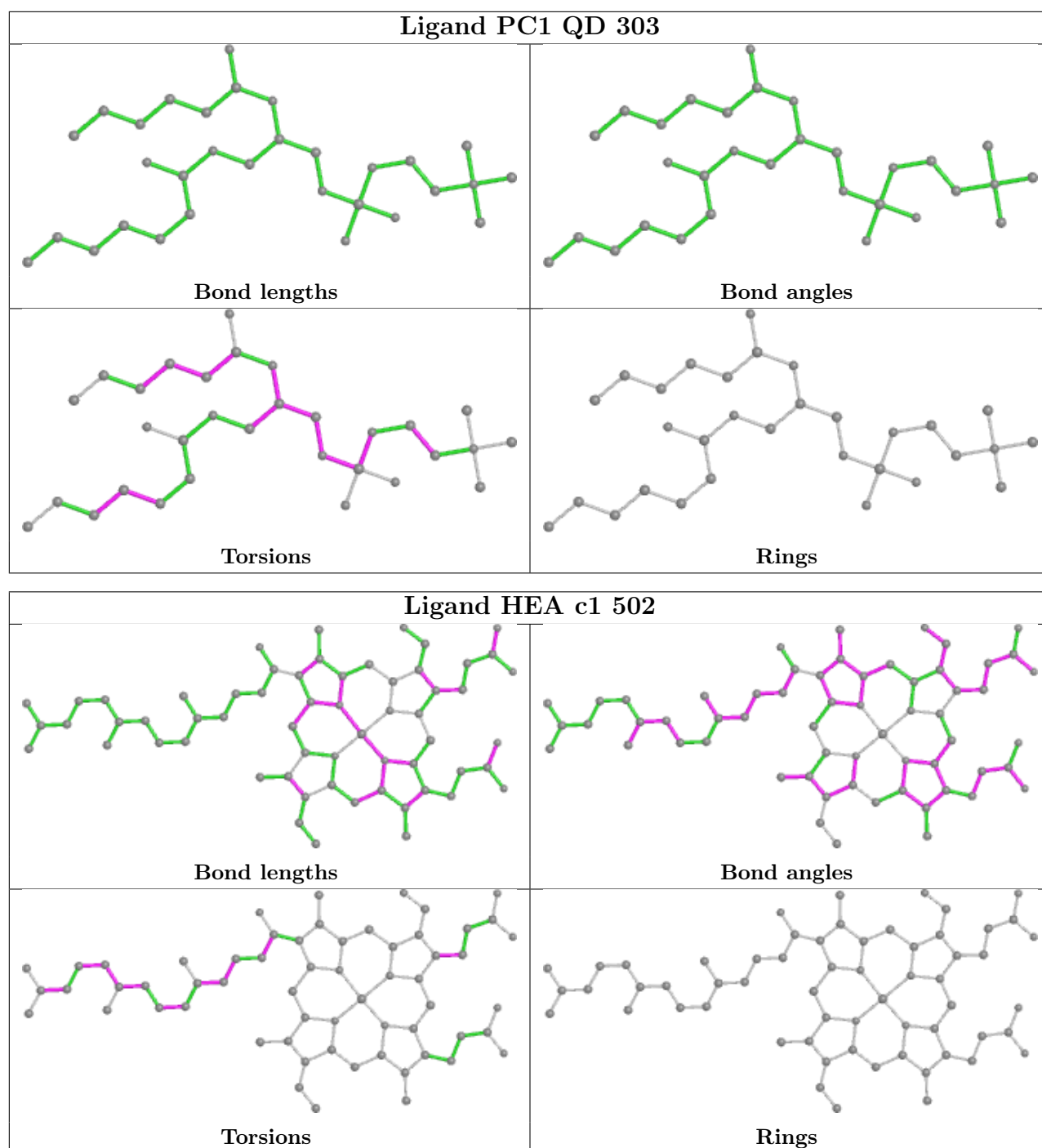
Ligand HEM QC 401

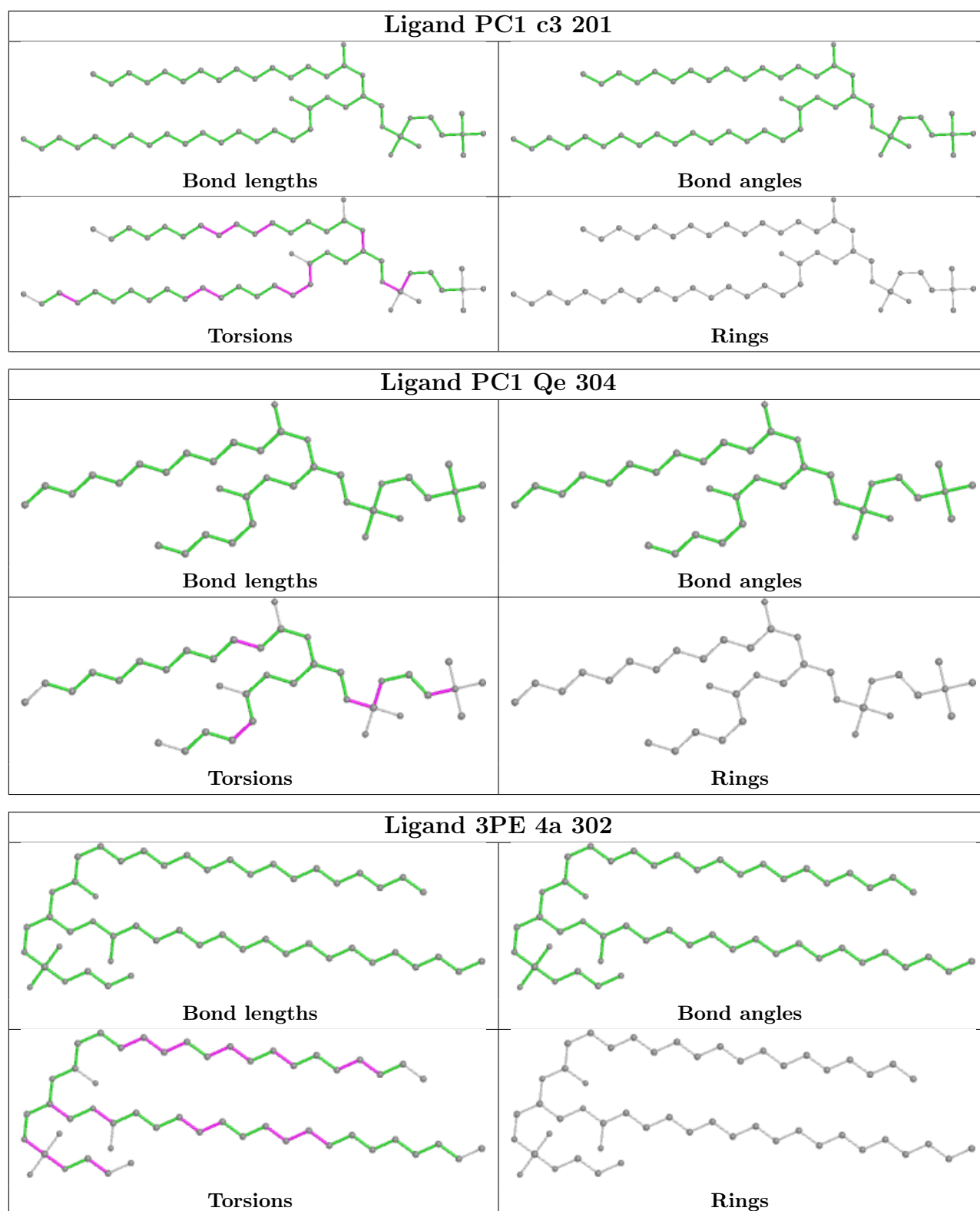


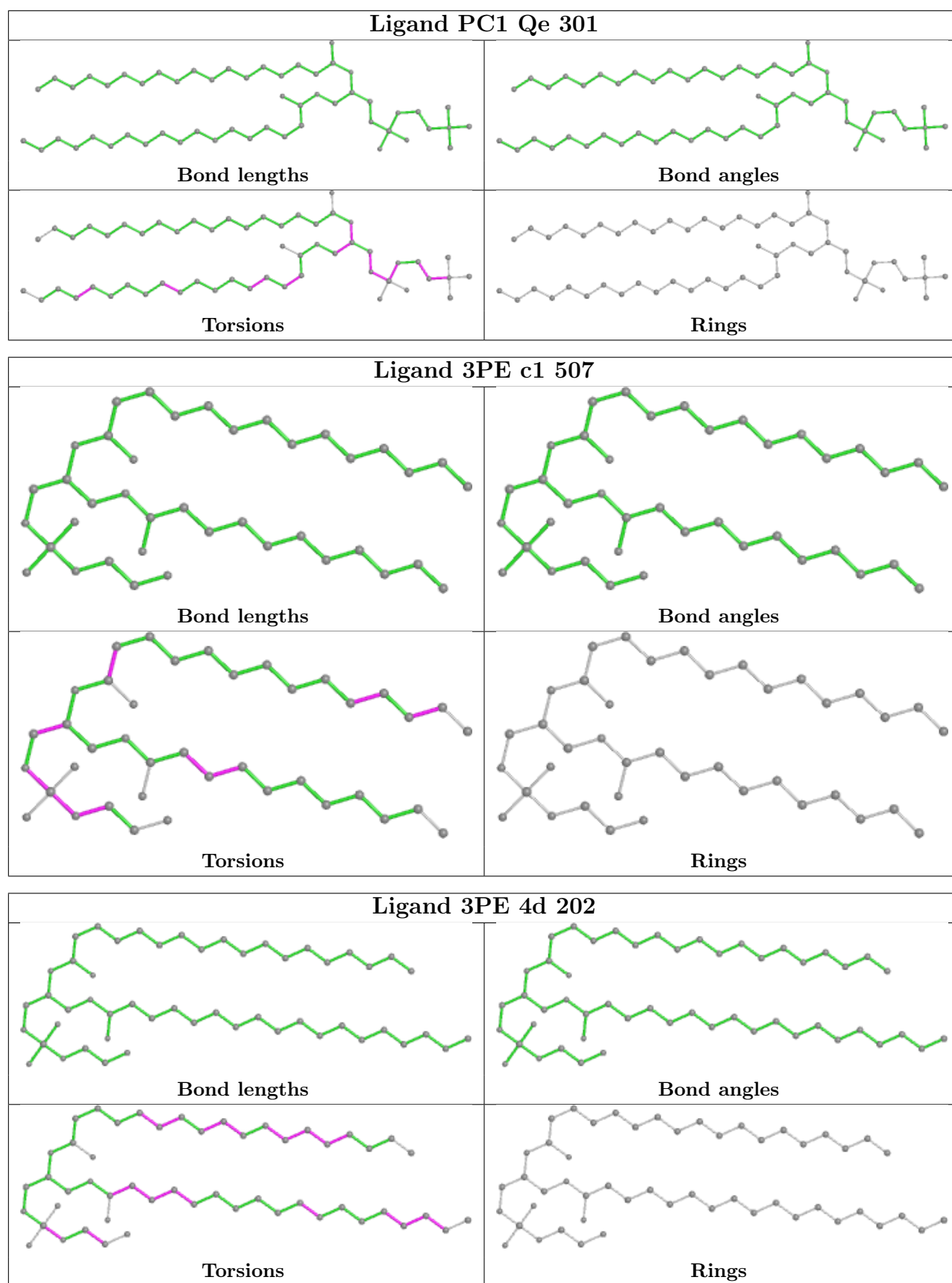
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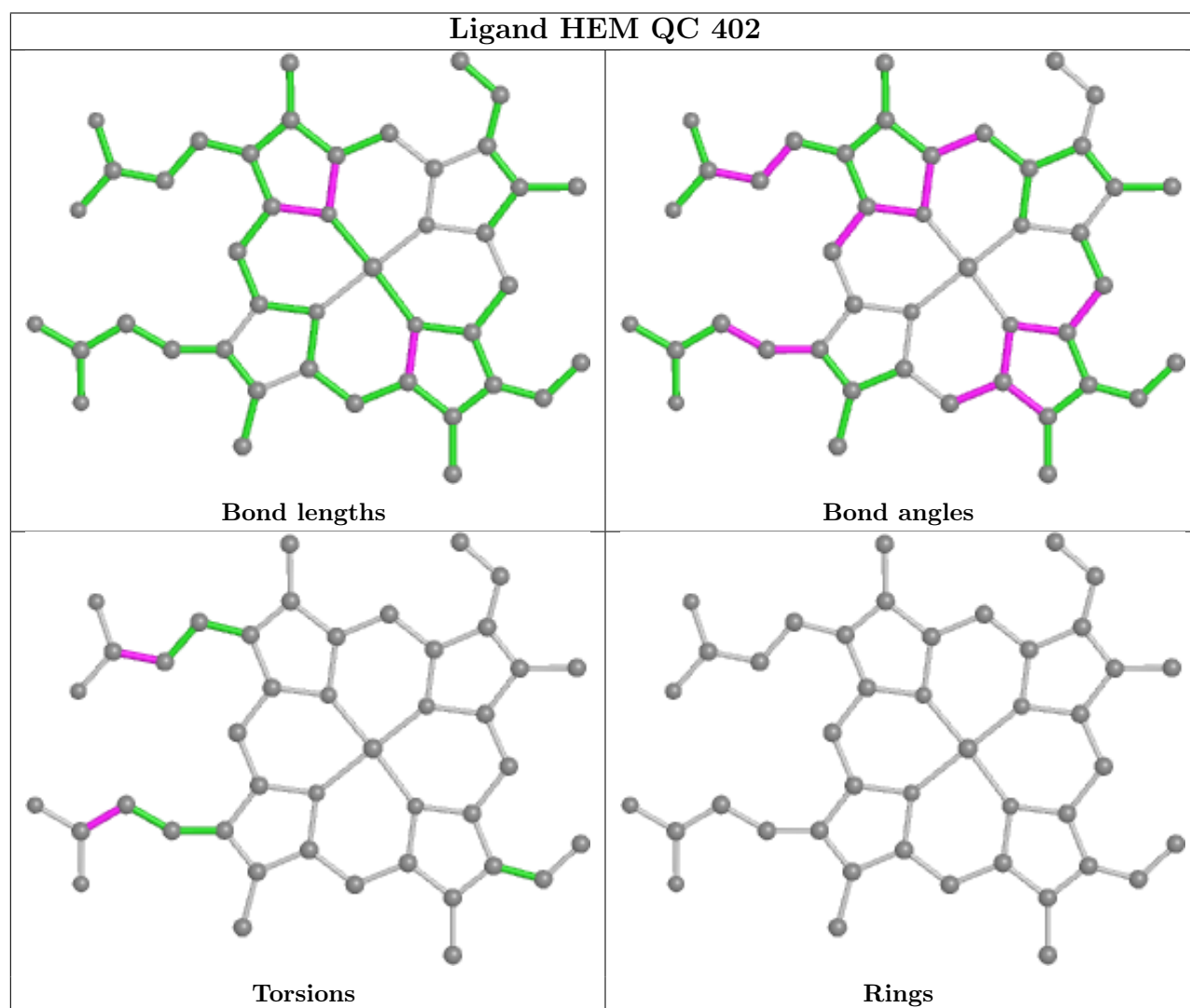
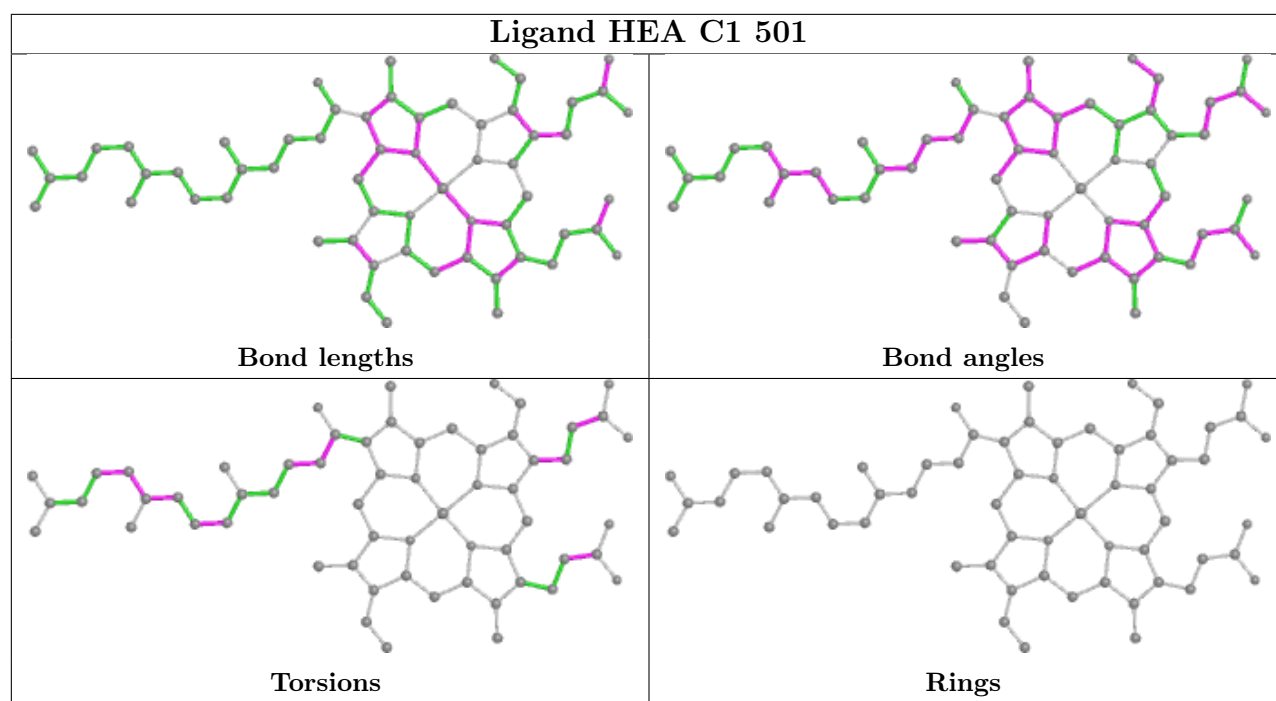


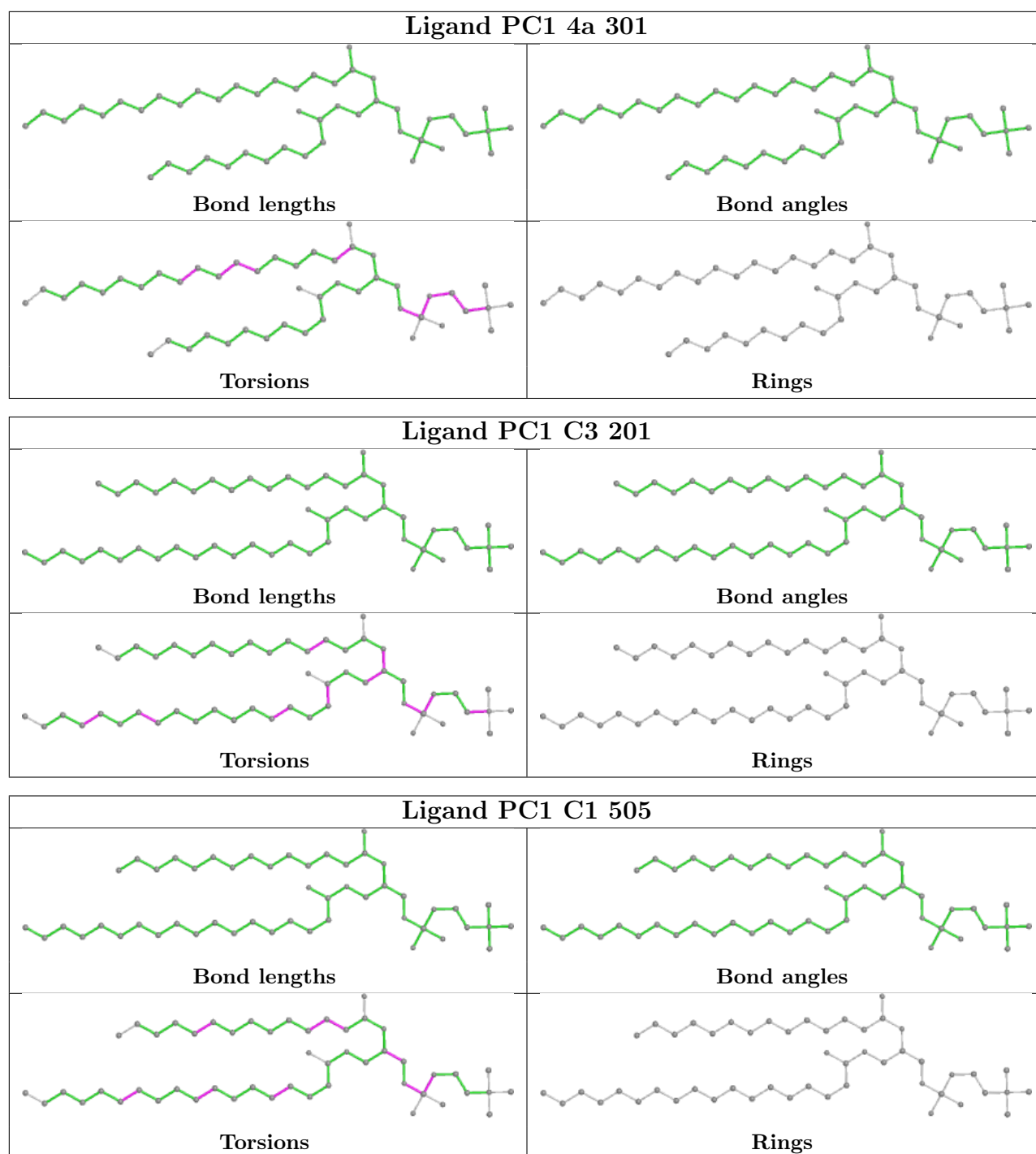


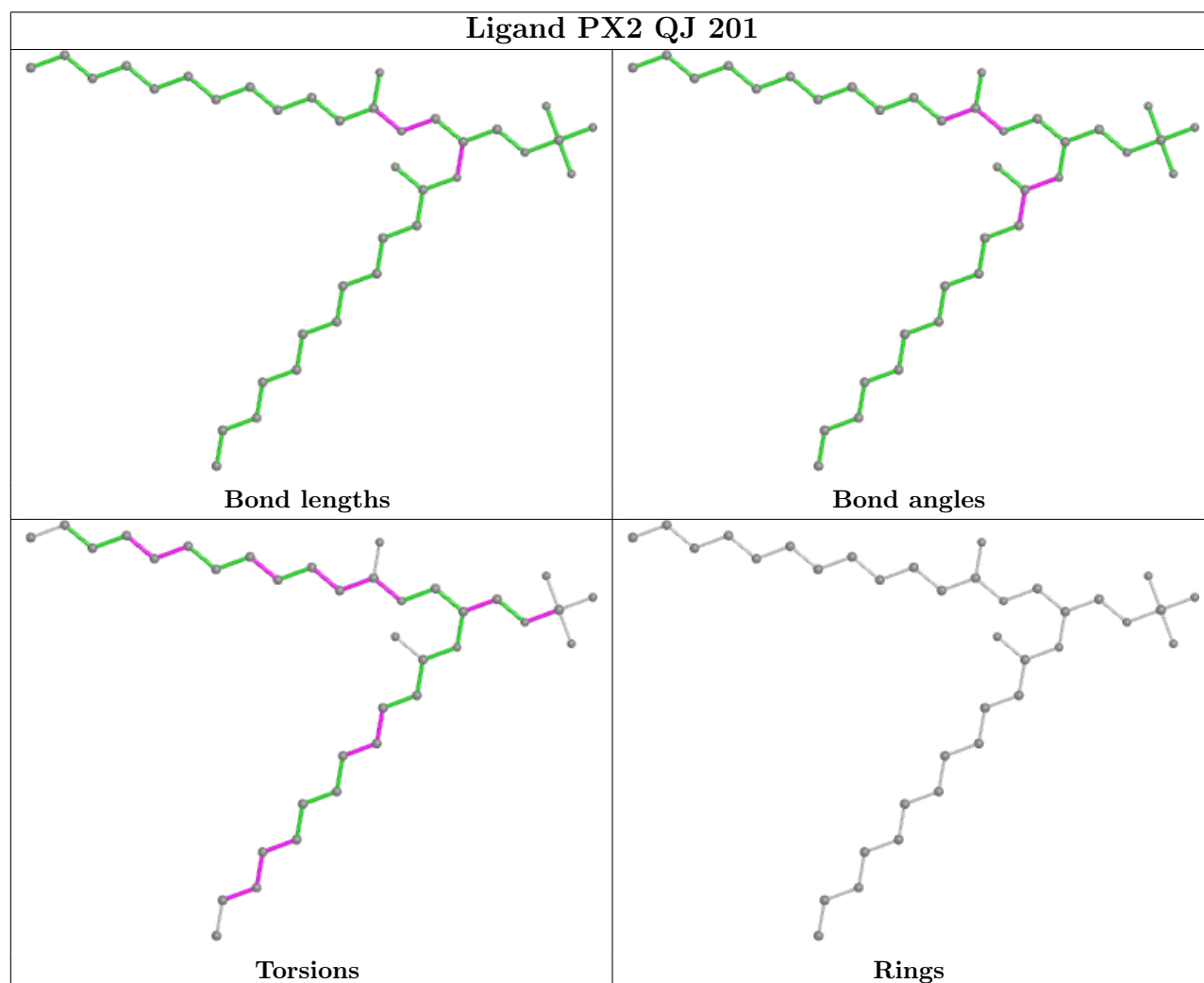
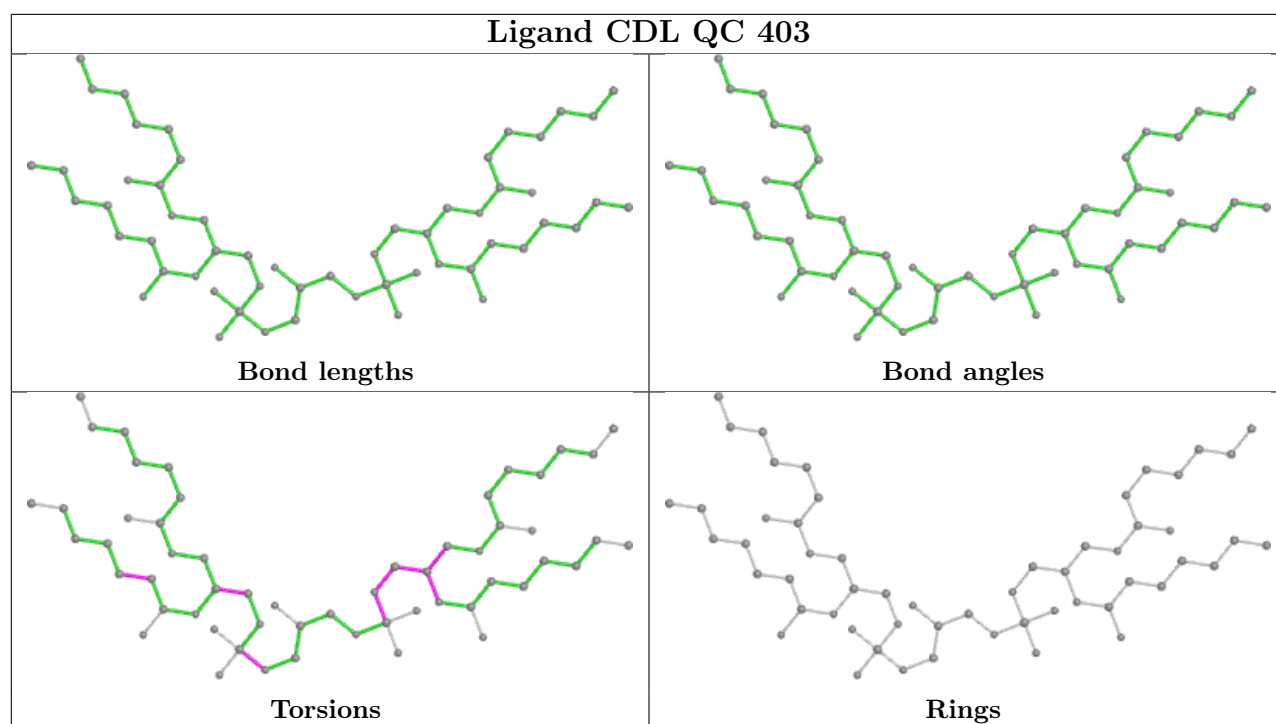


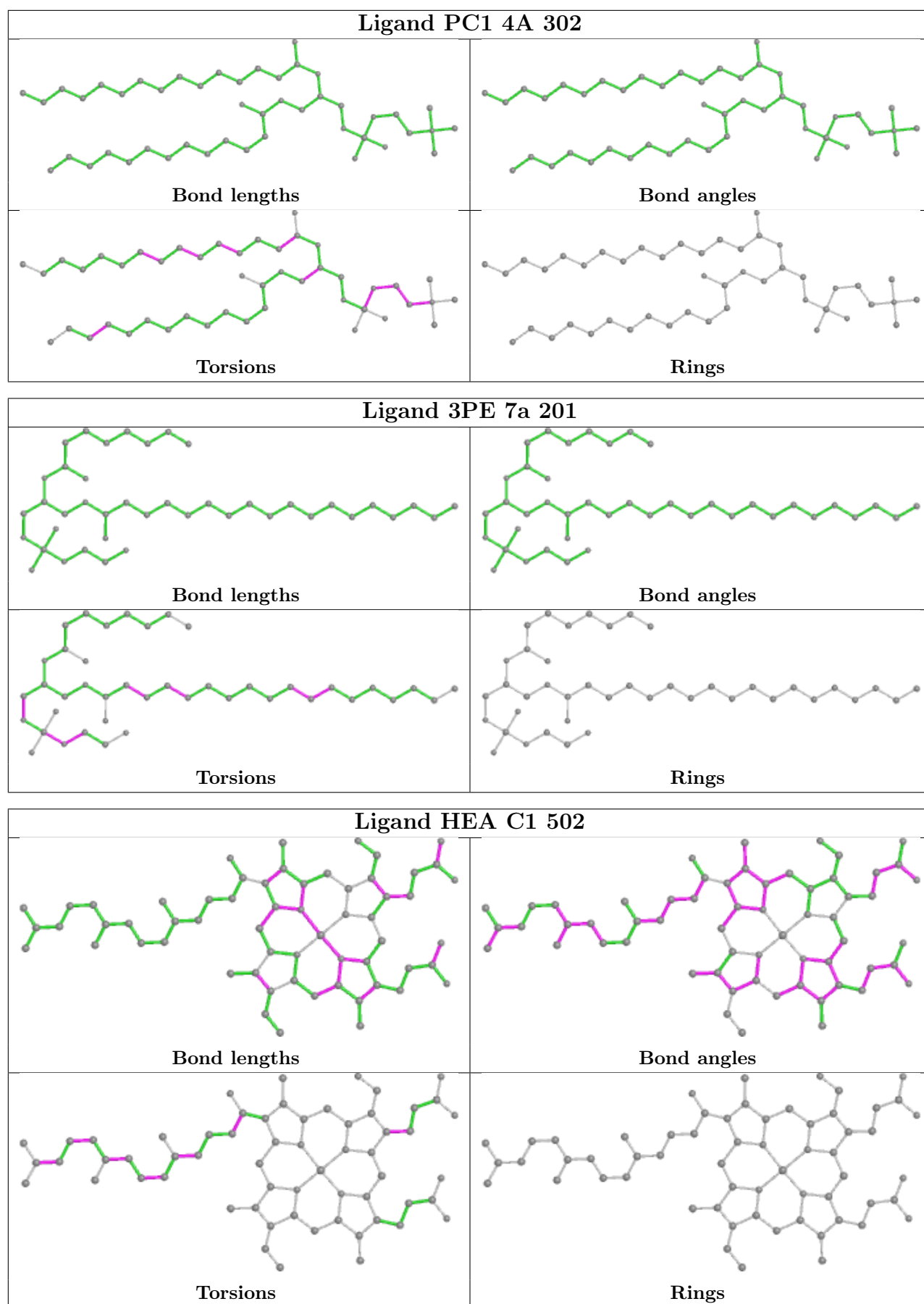


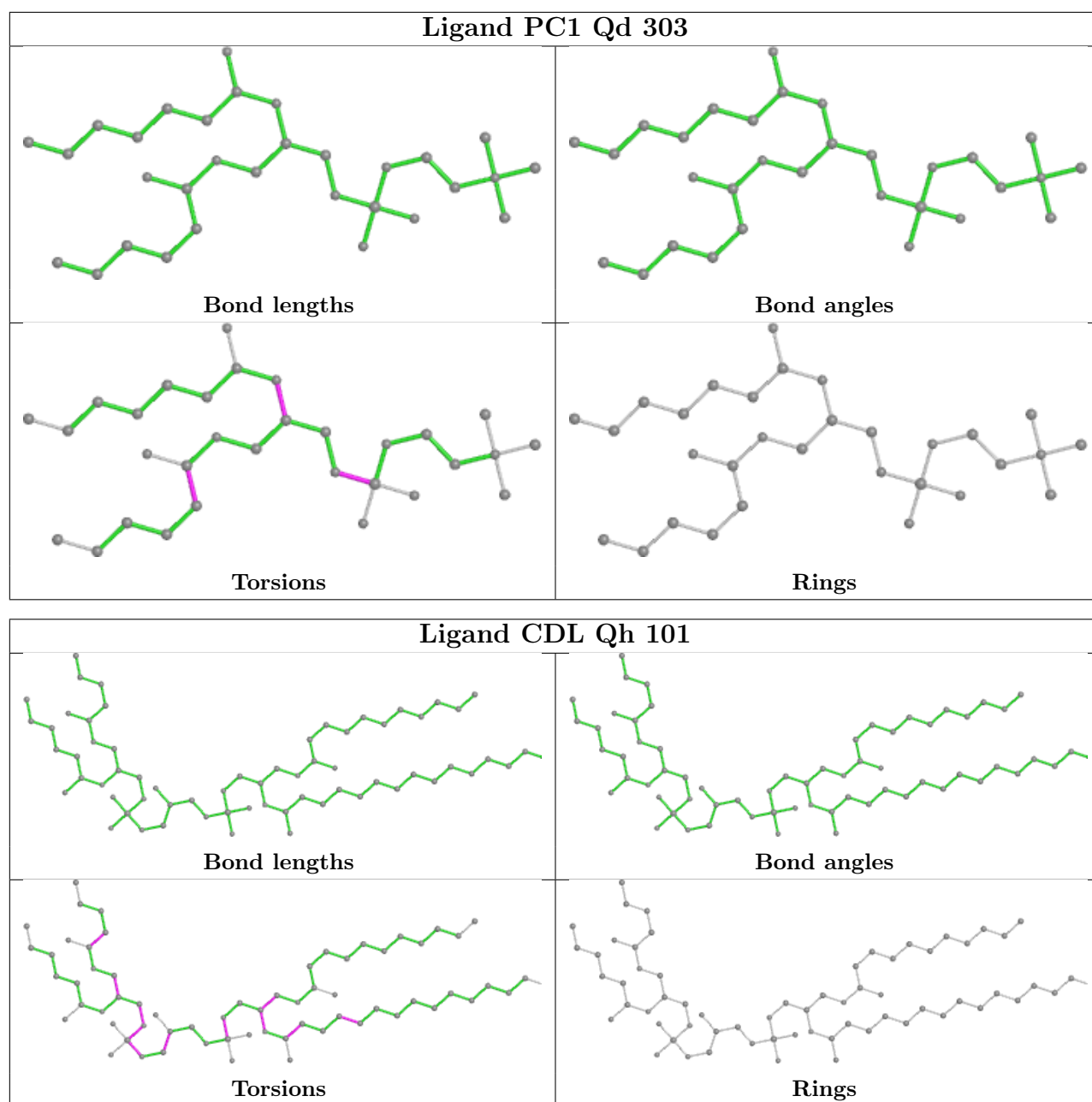


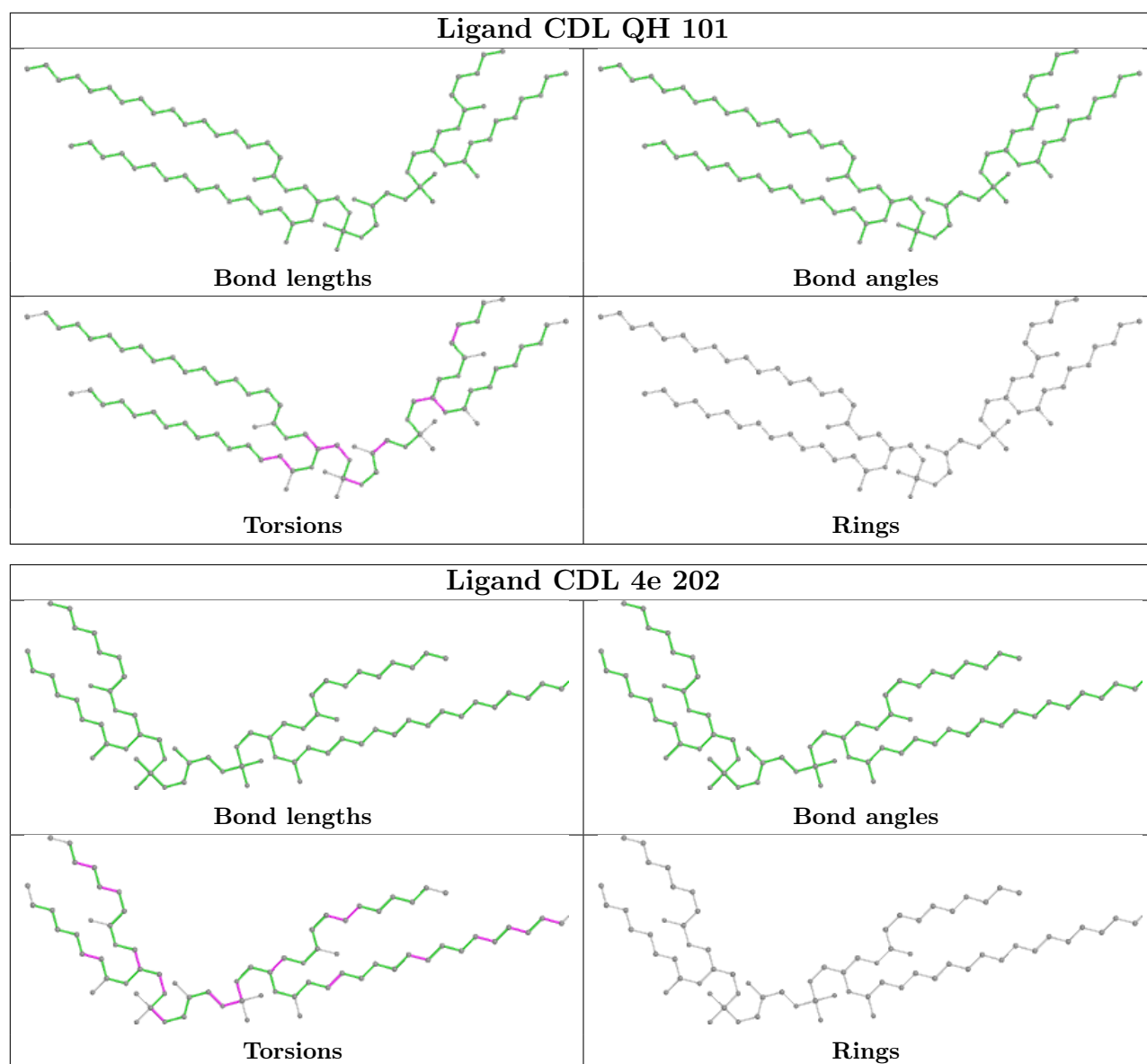


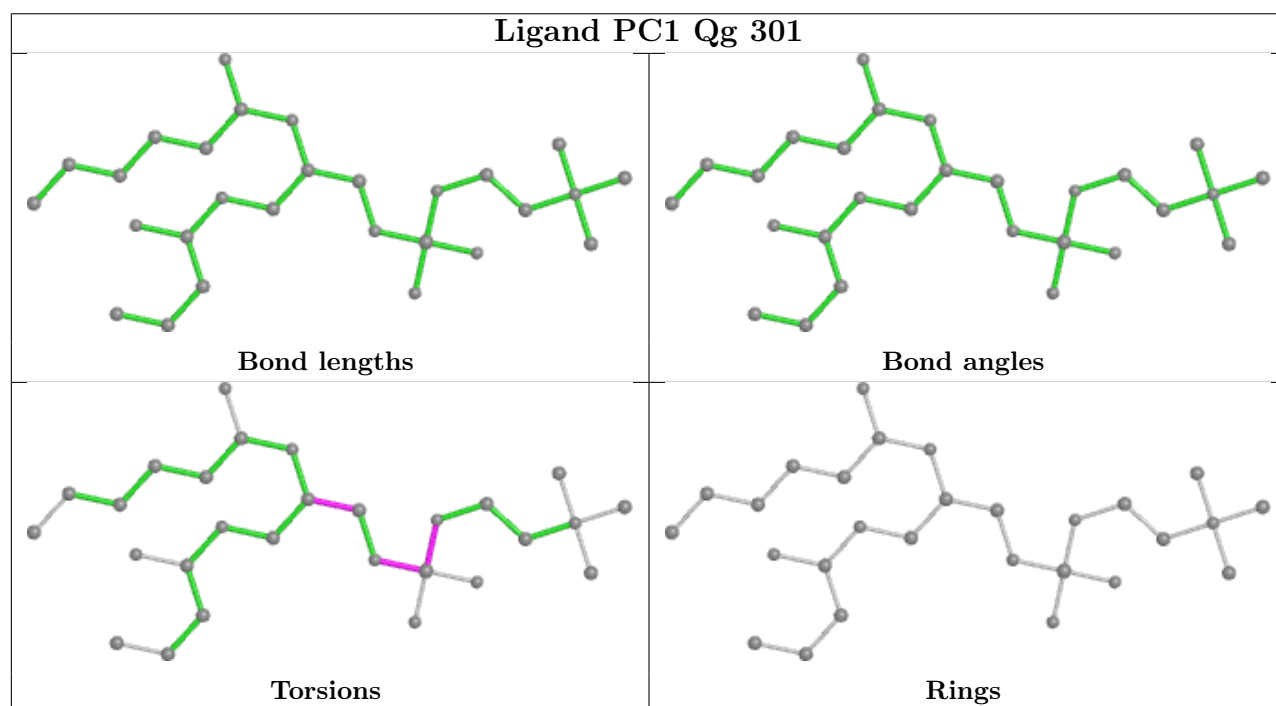
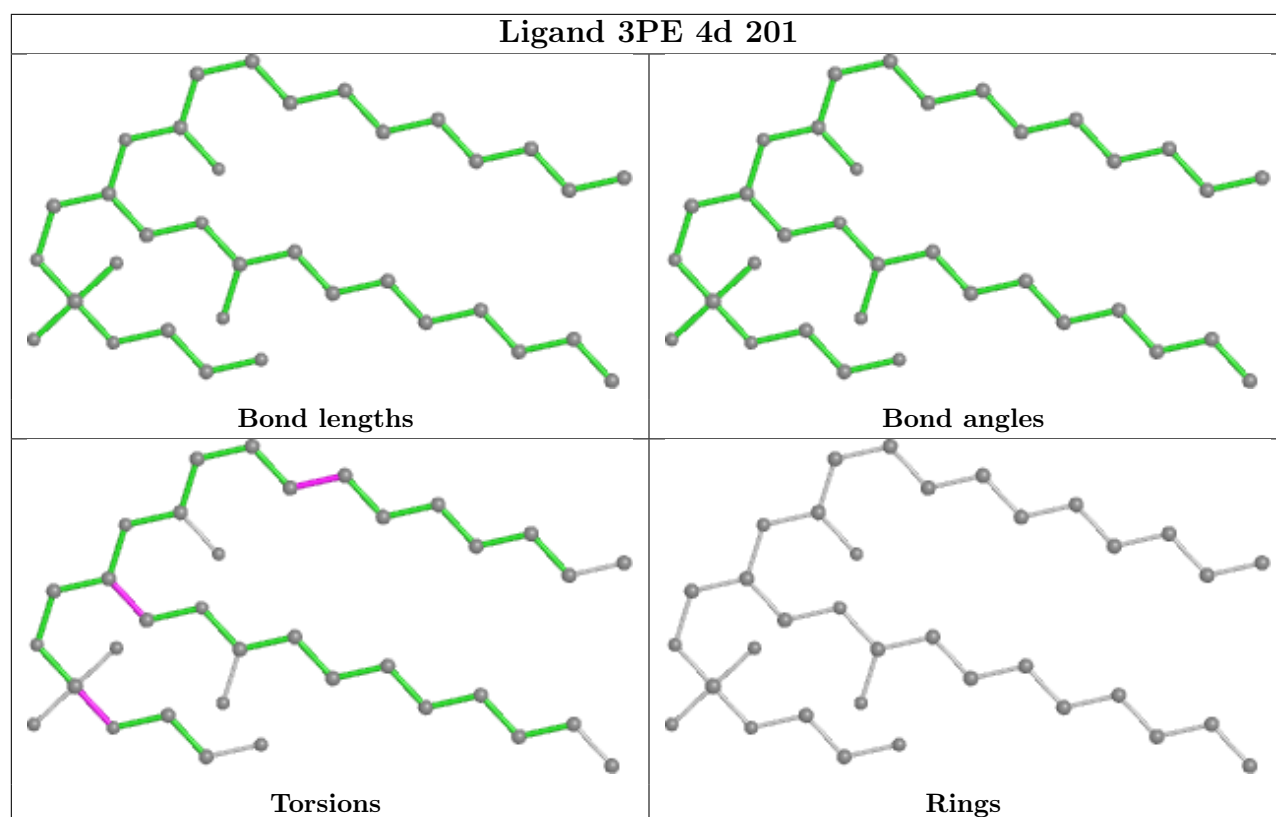


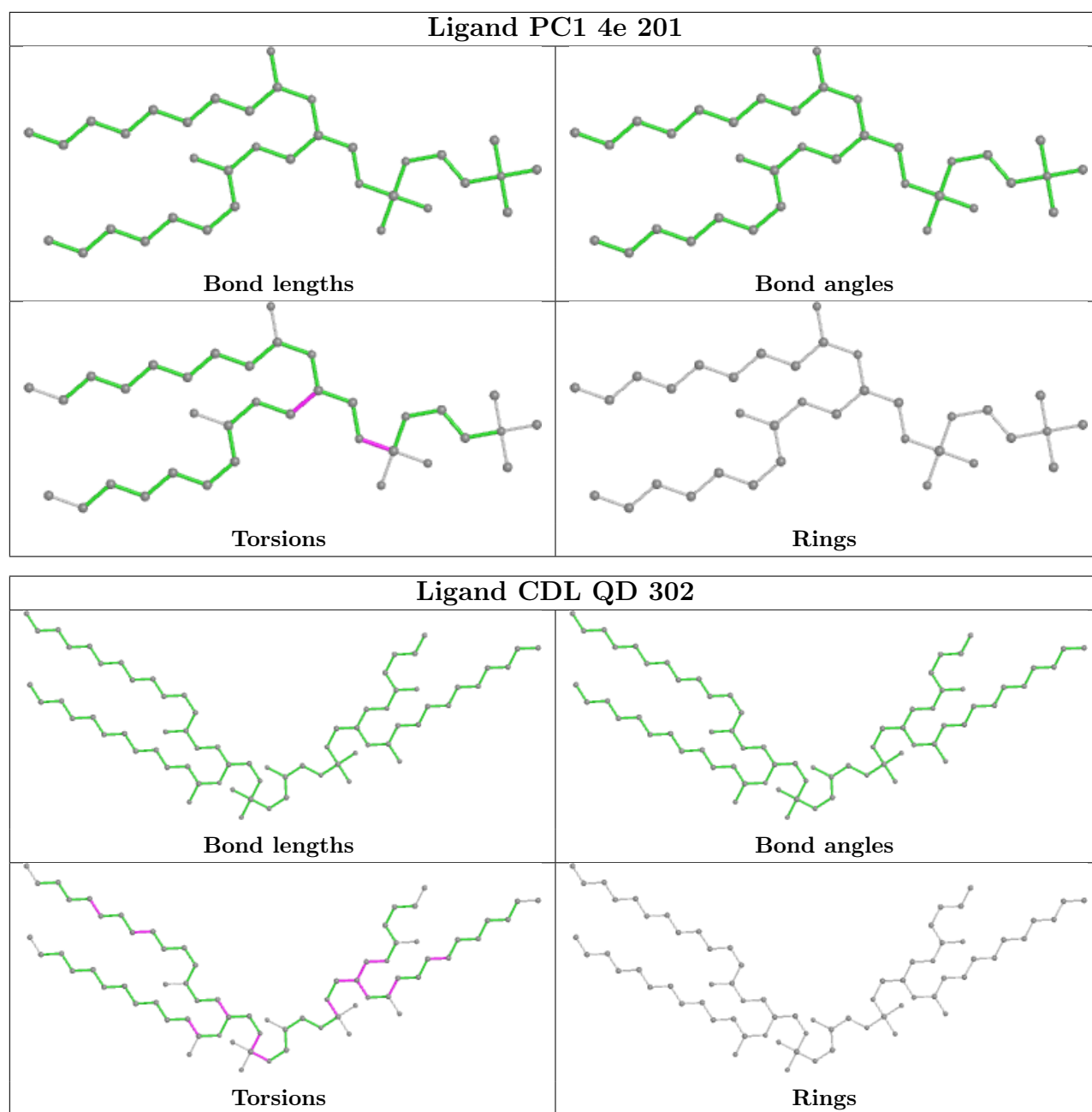




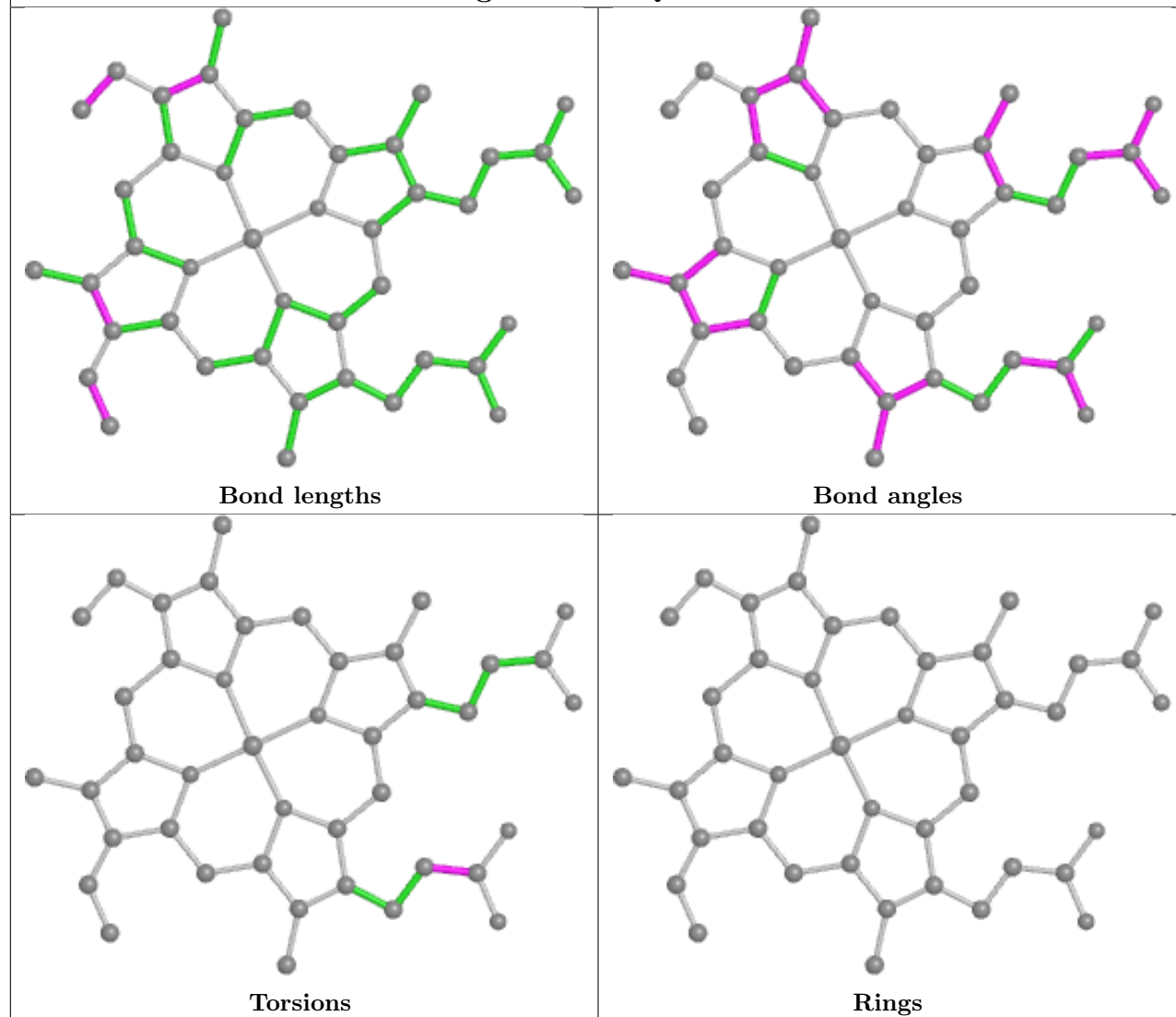




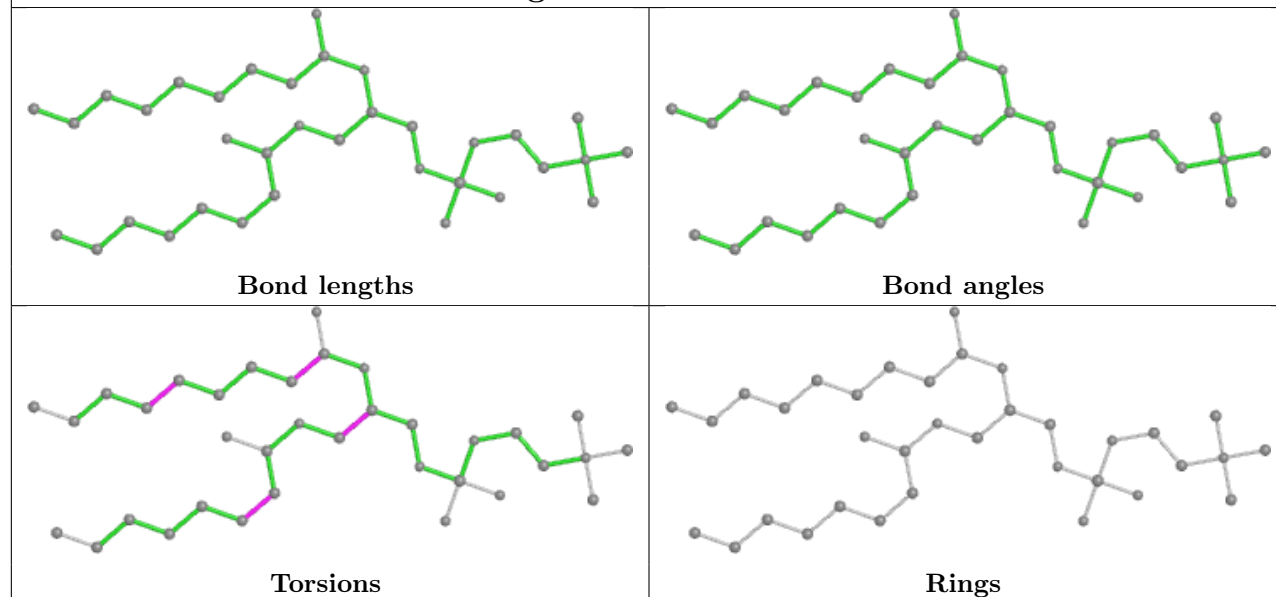


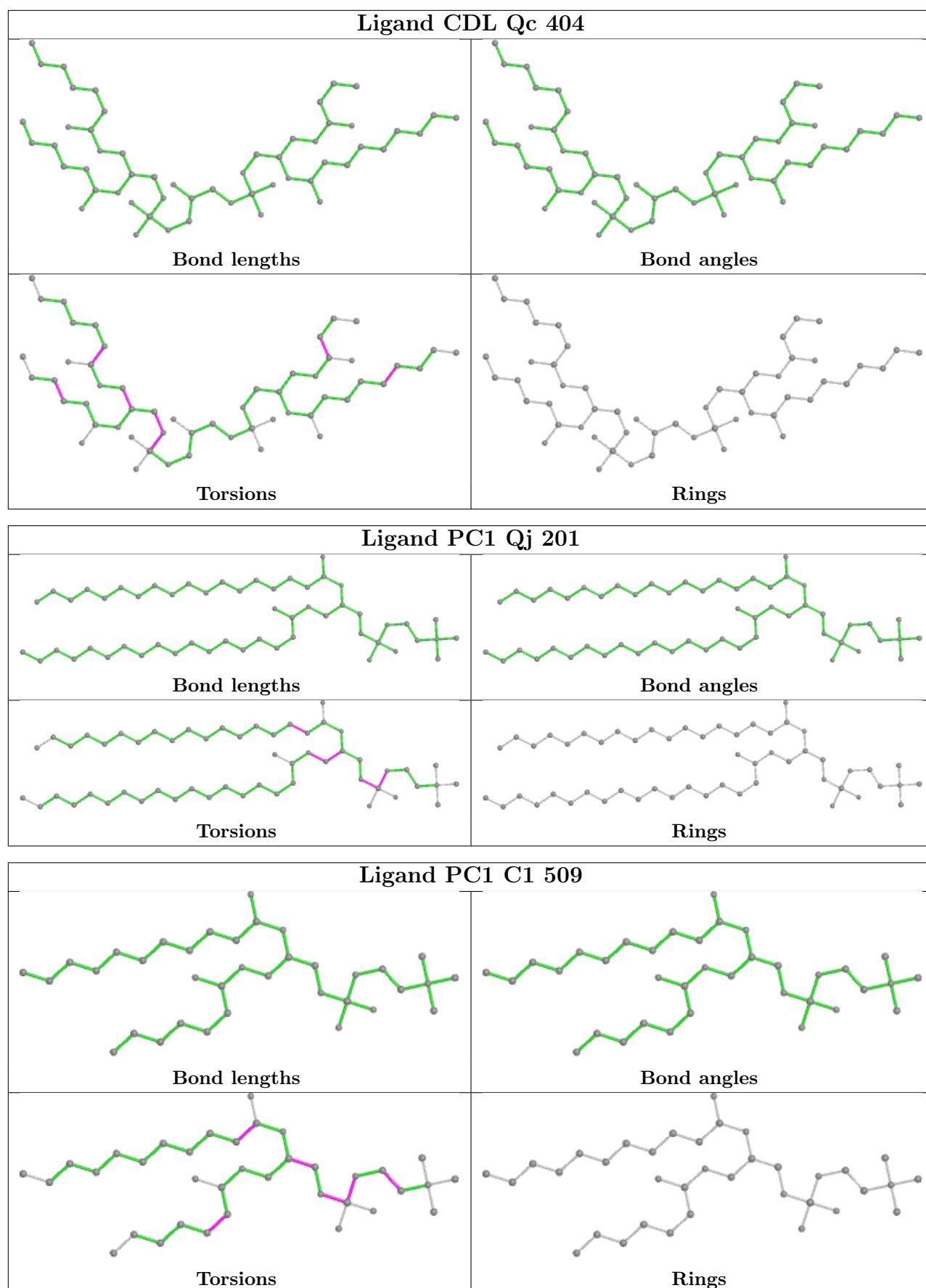


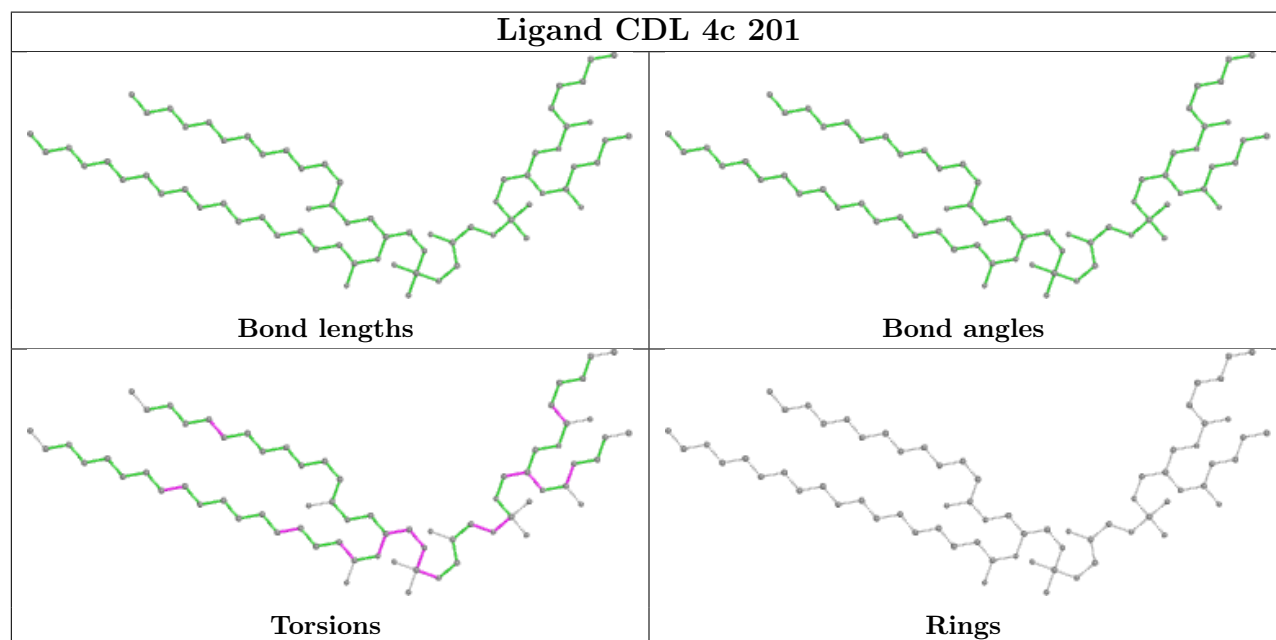
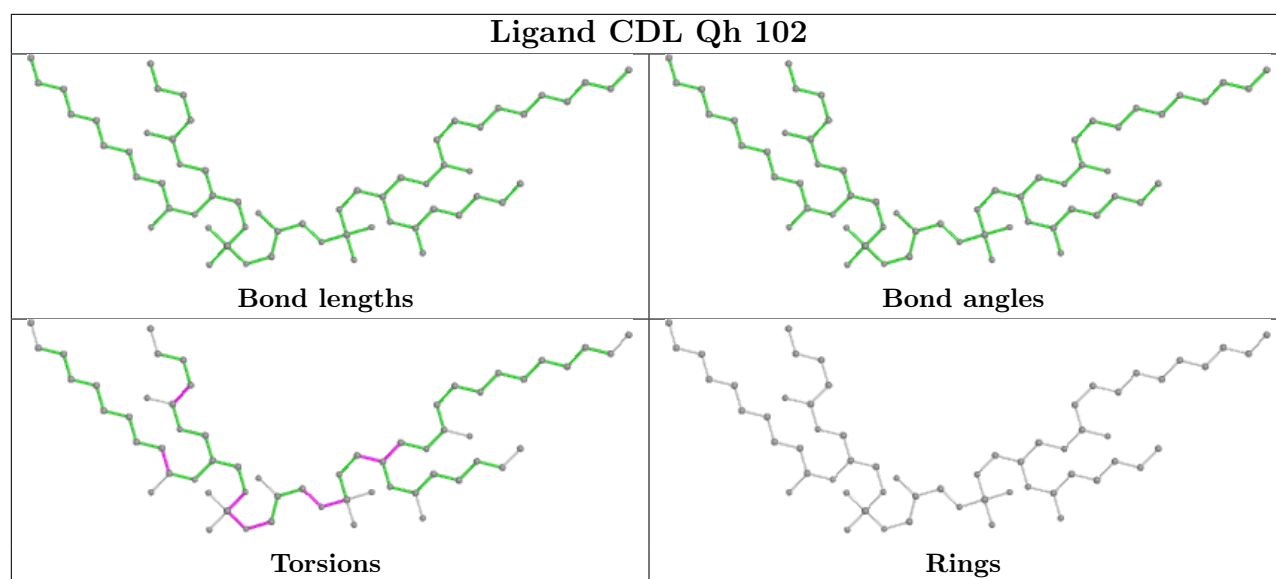
Ligand HEC QD 301

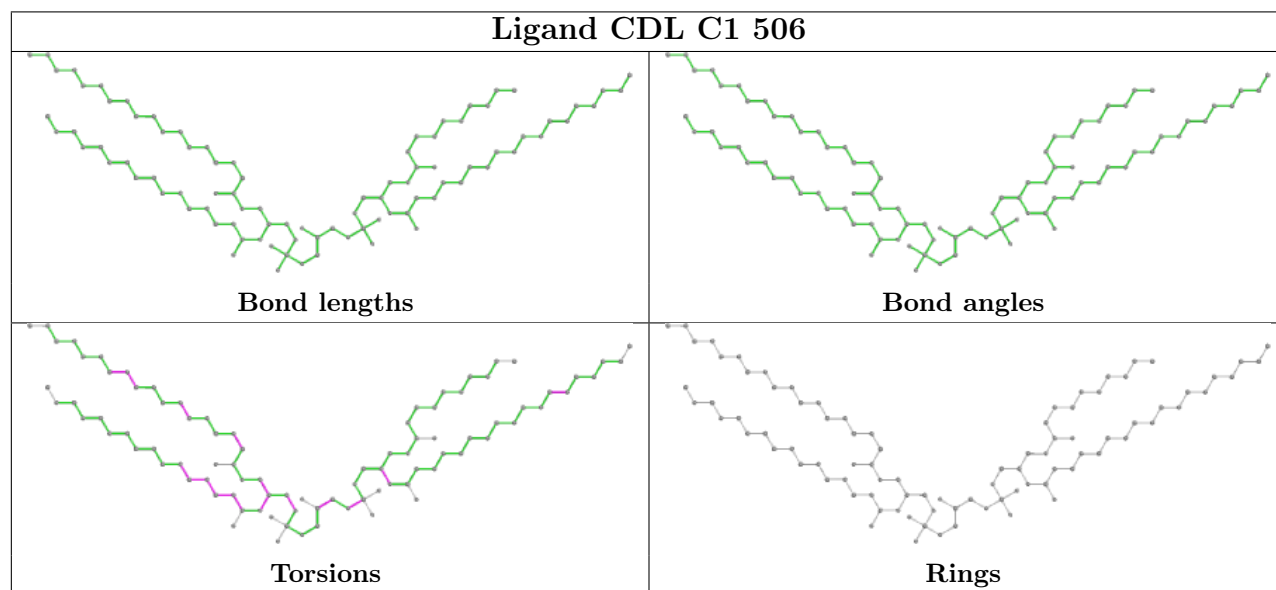
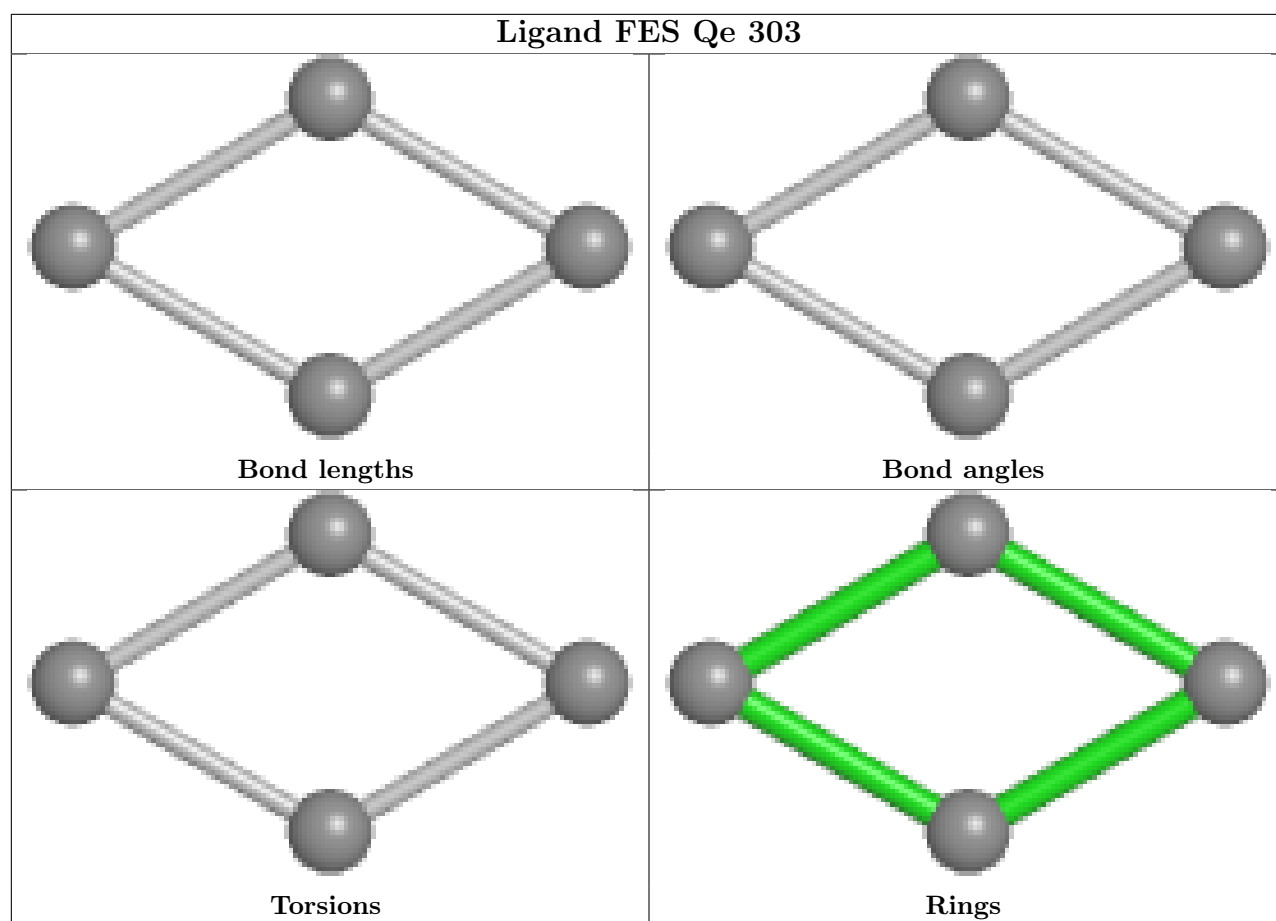


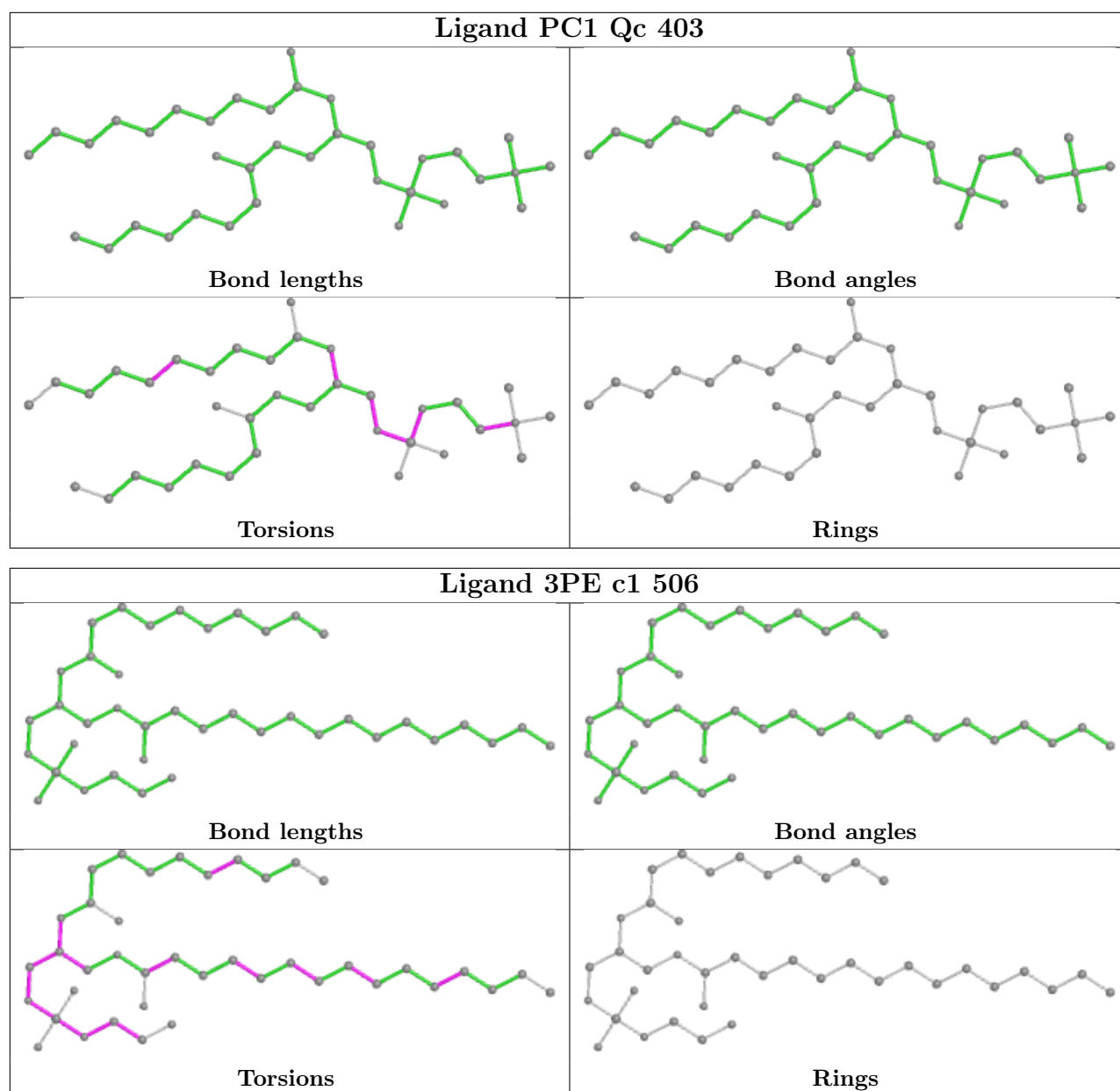
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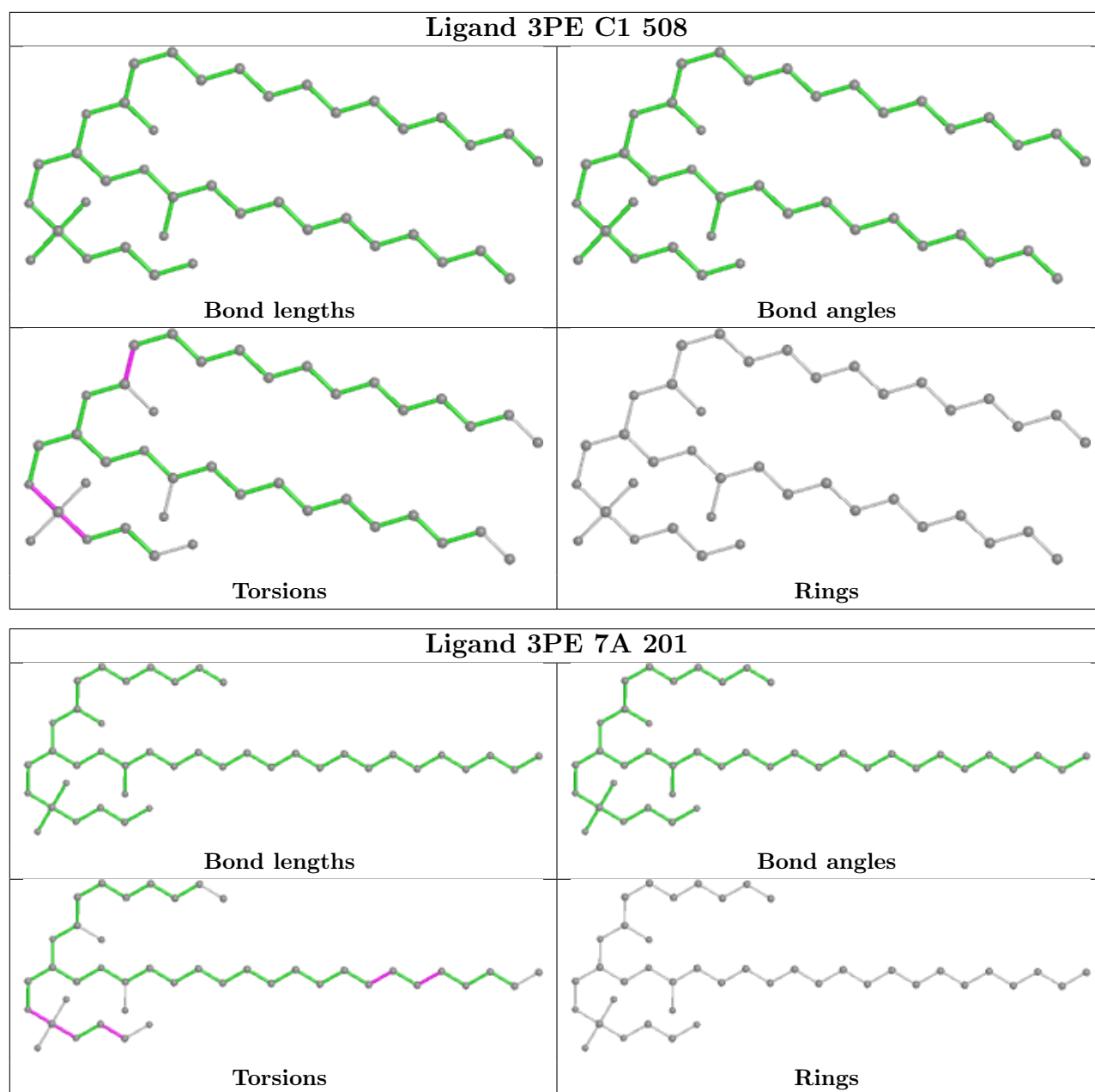


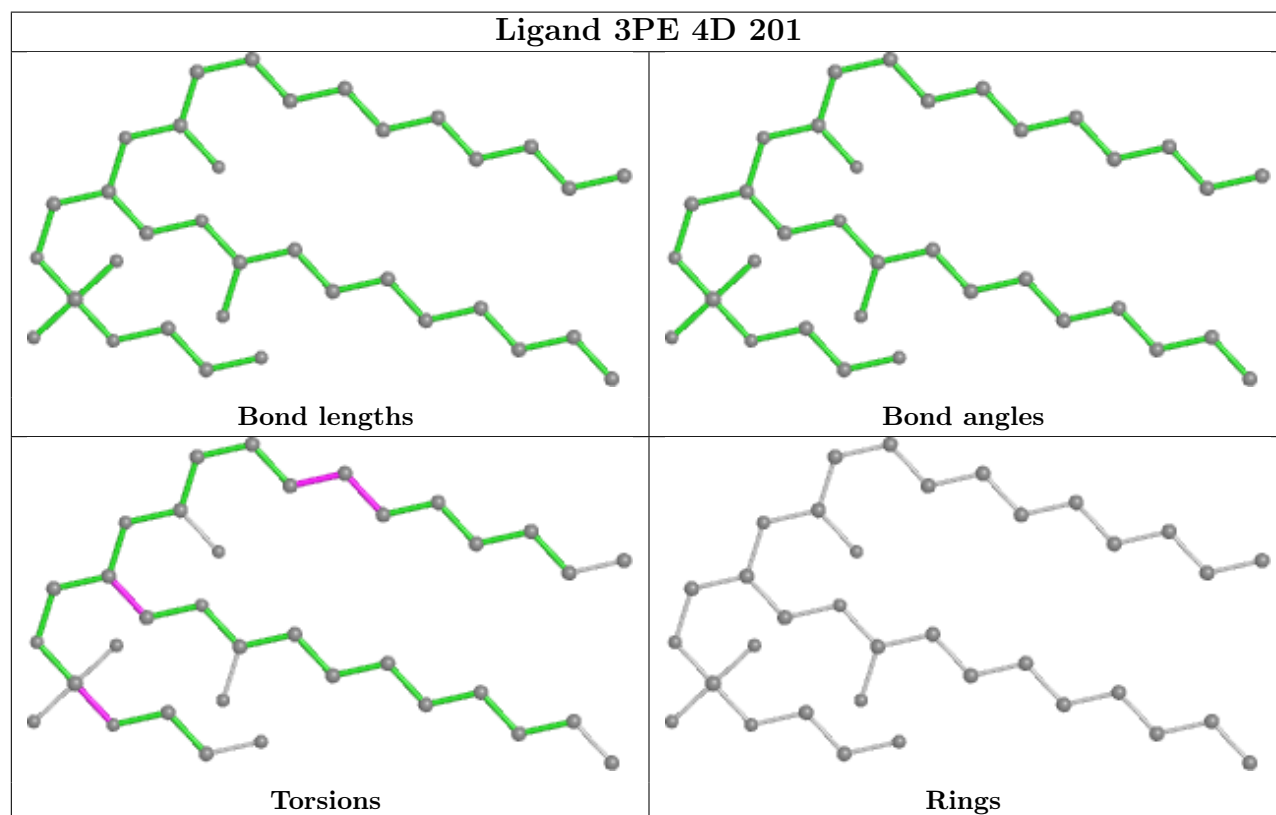
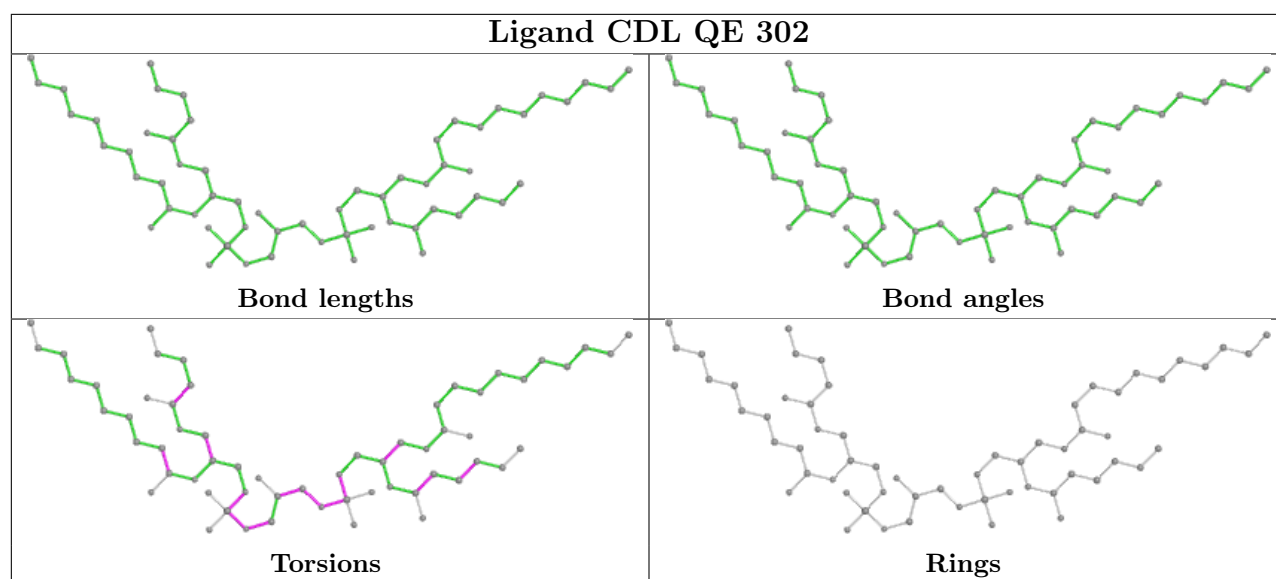


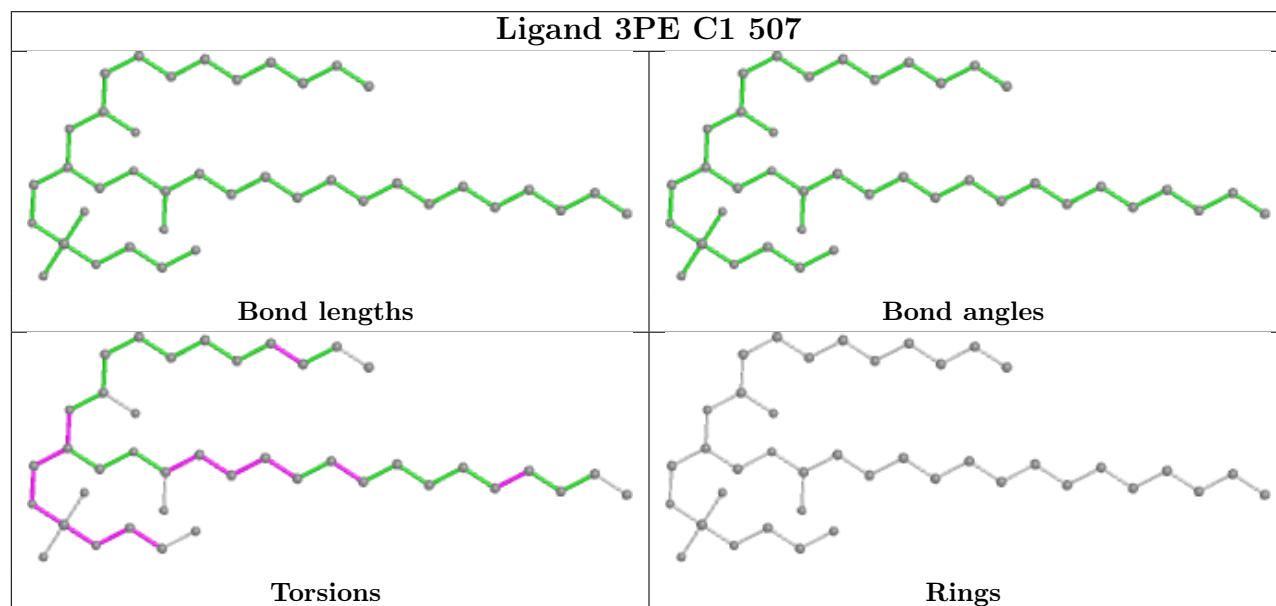
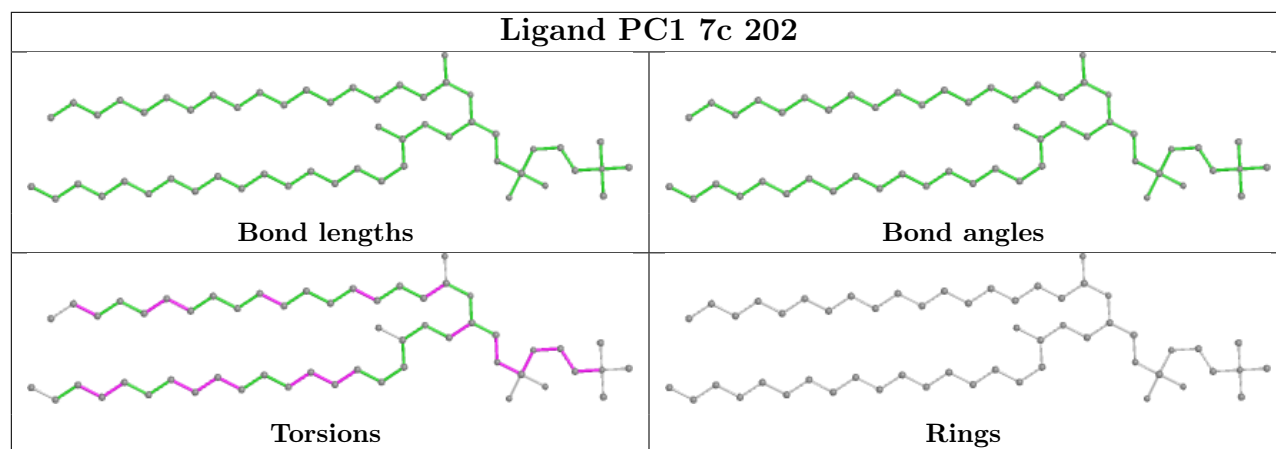
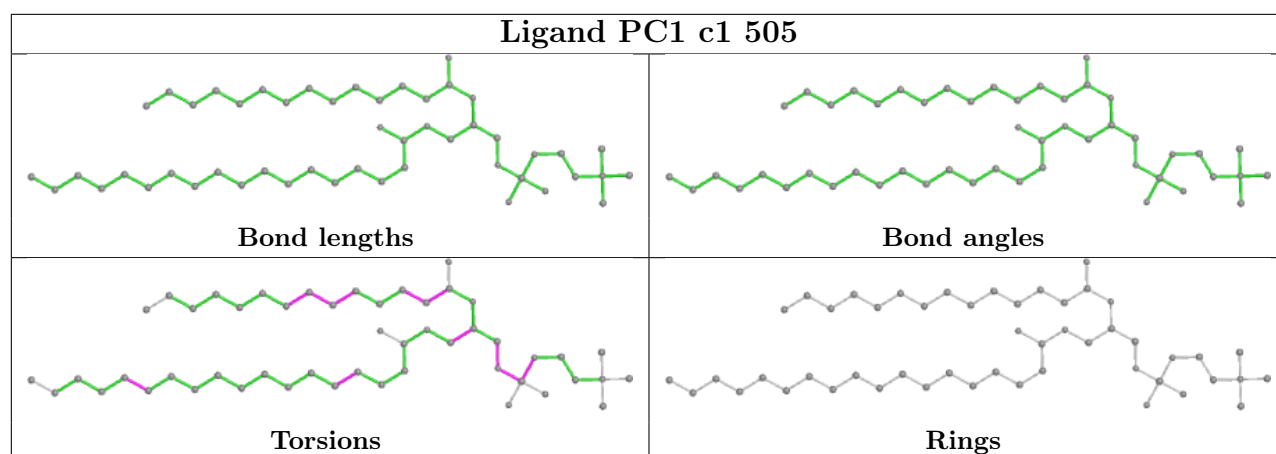


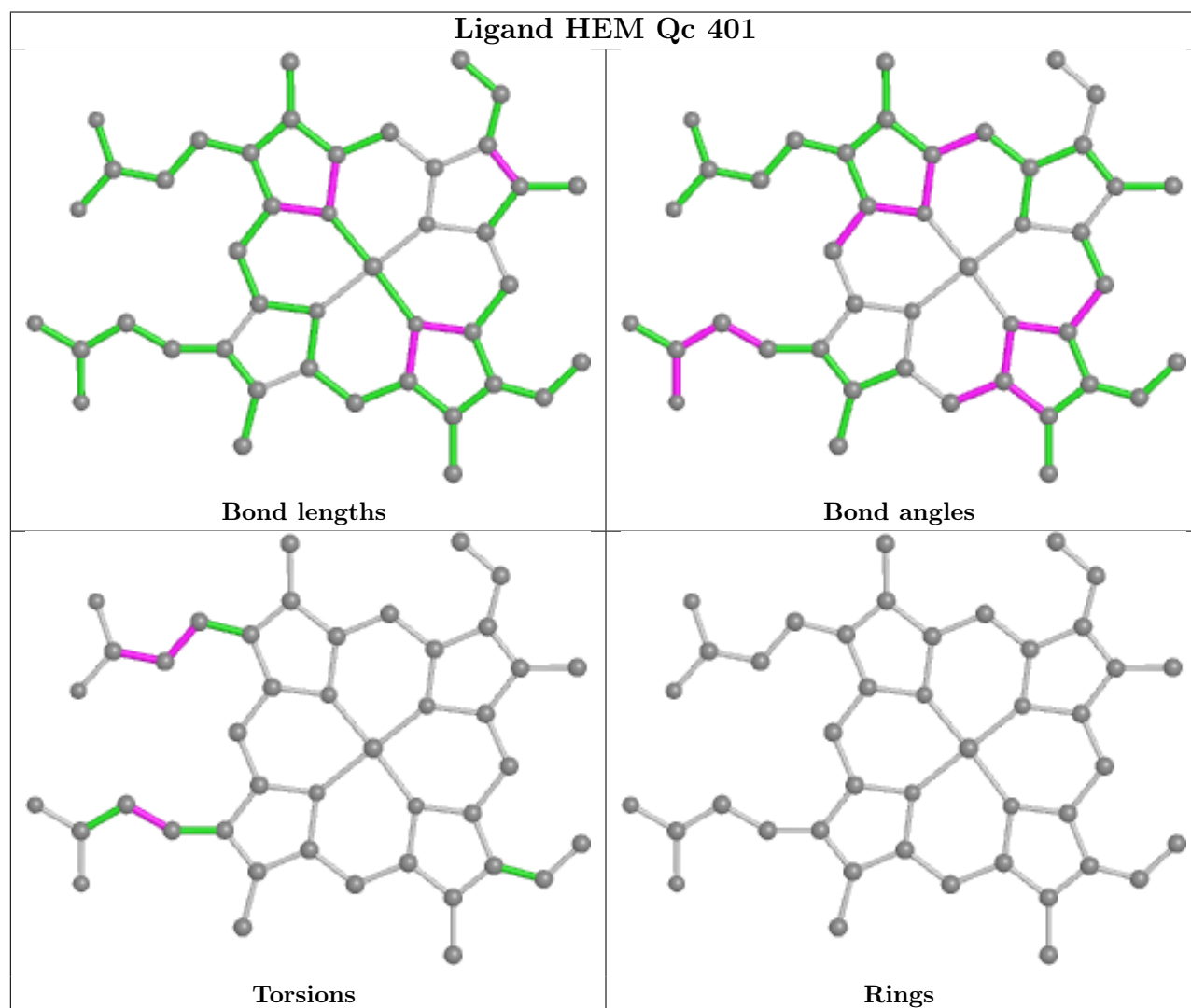
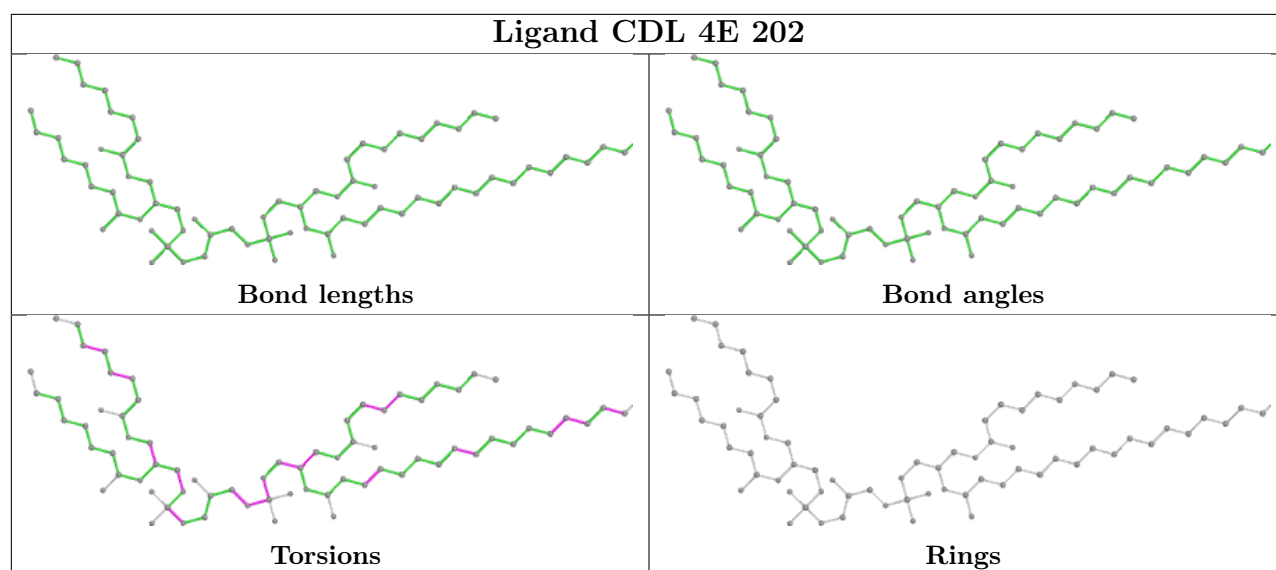


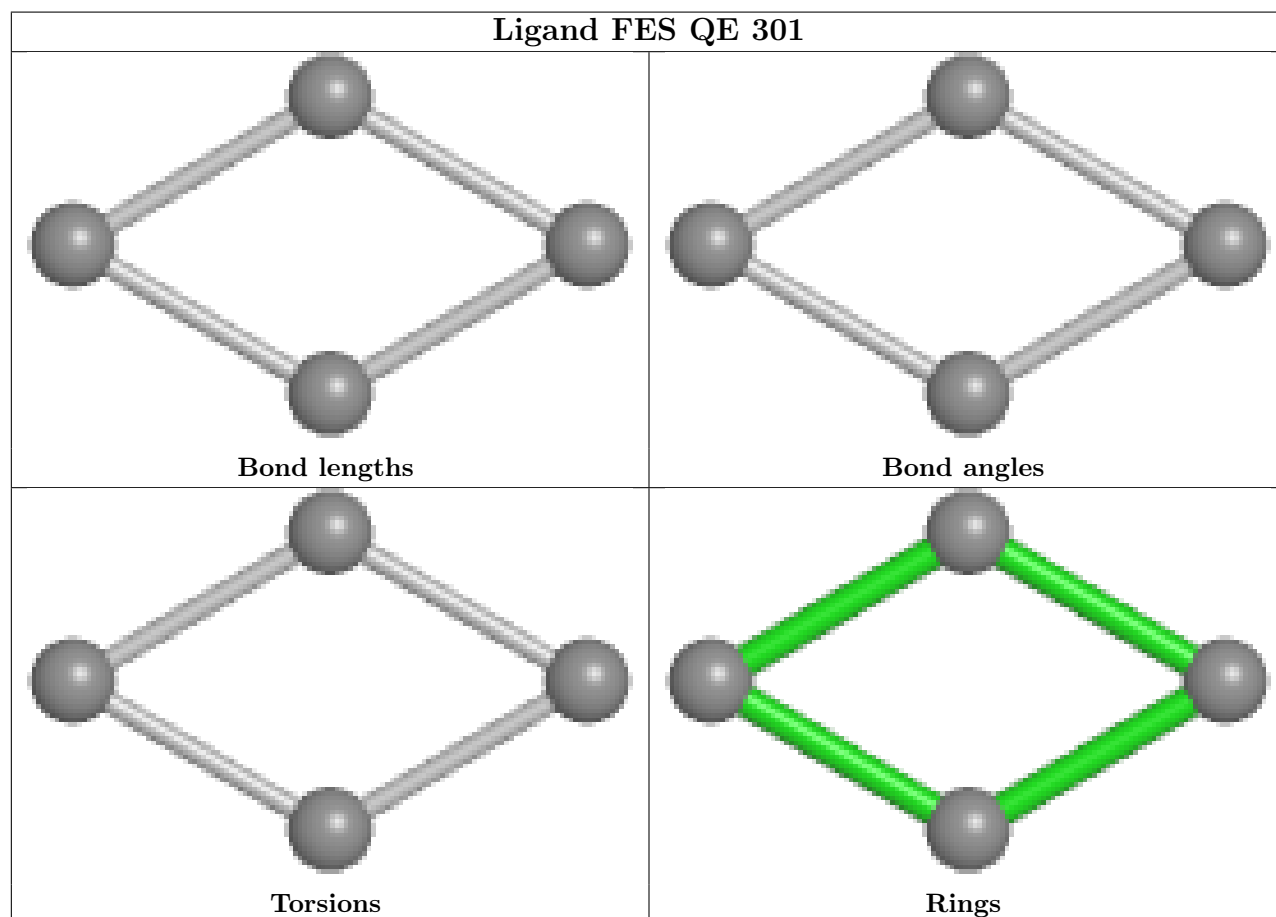
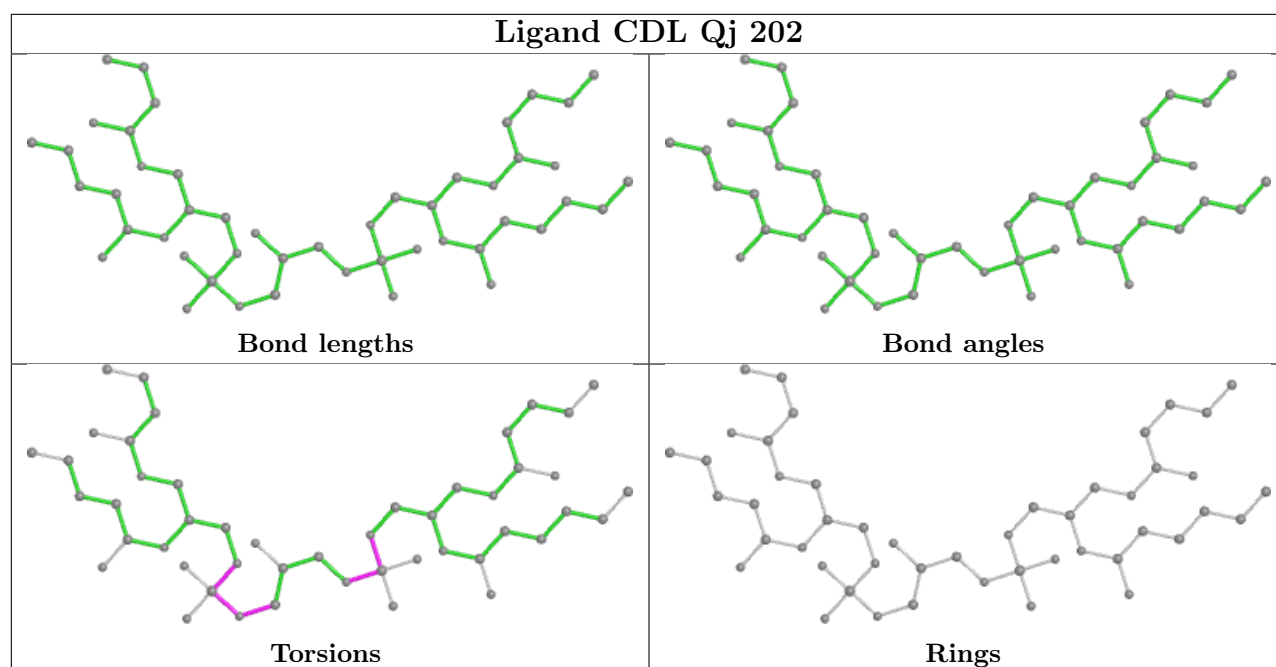


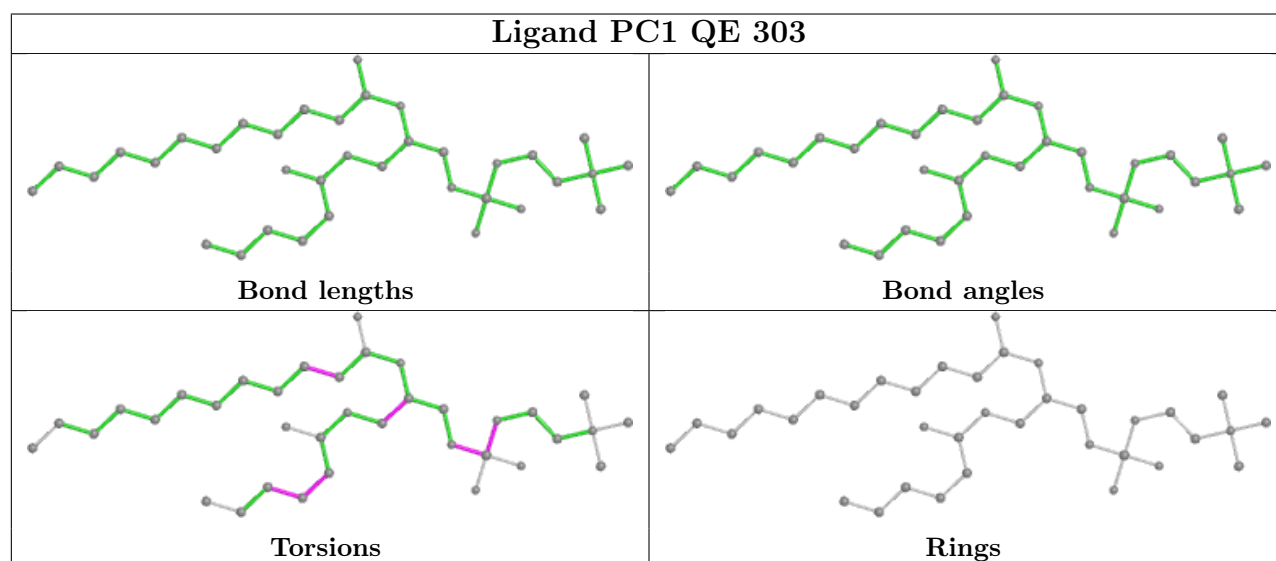
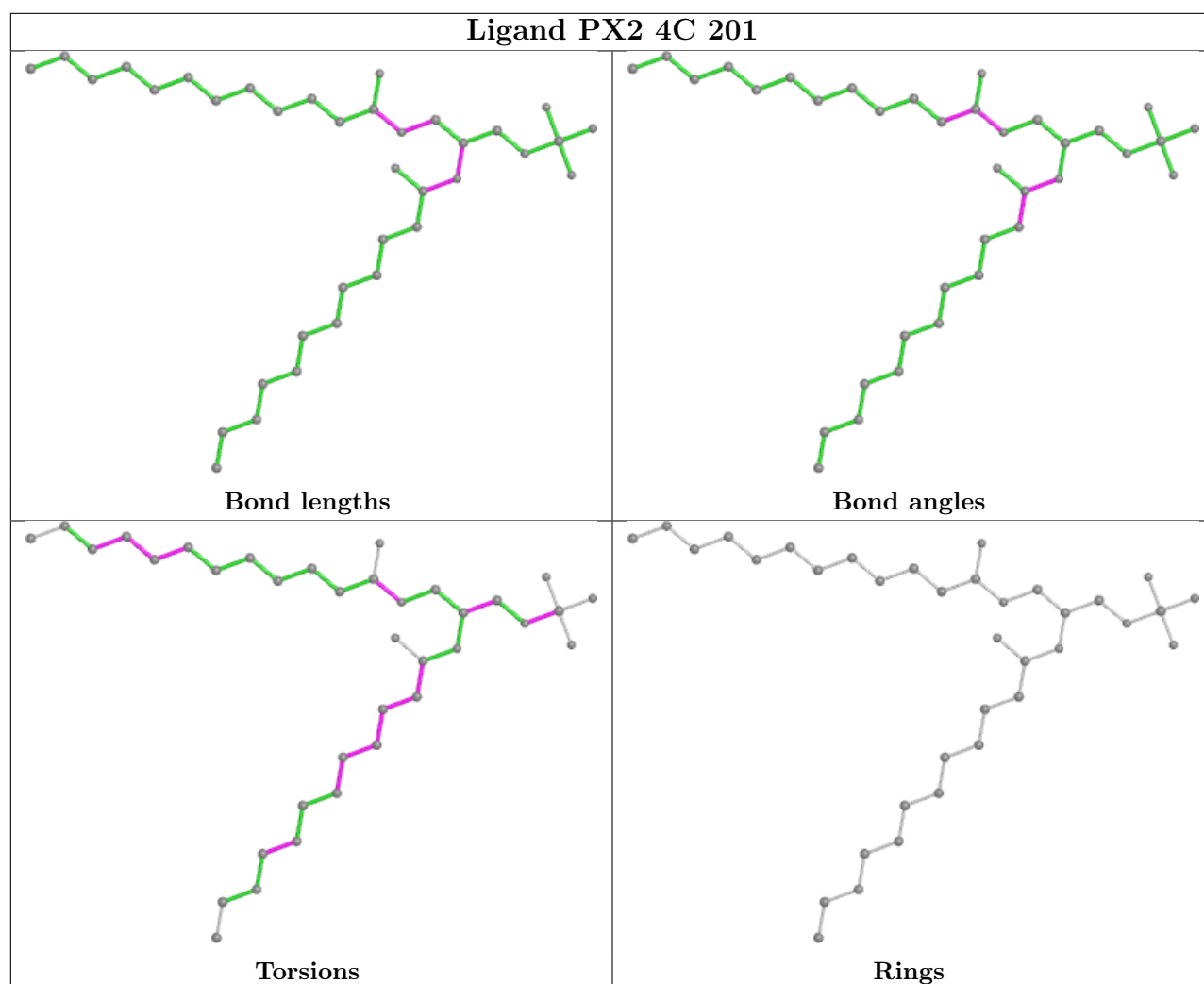


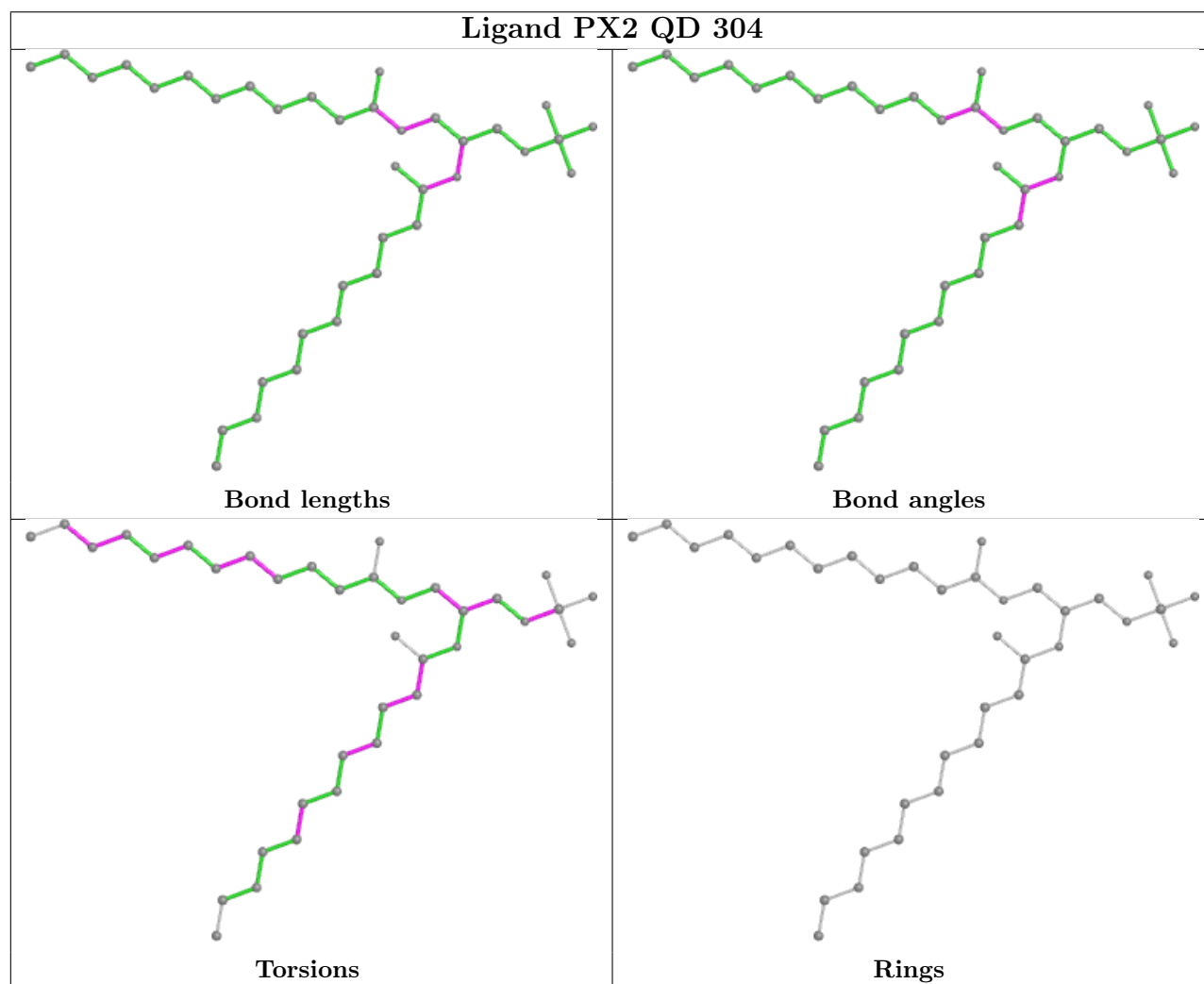
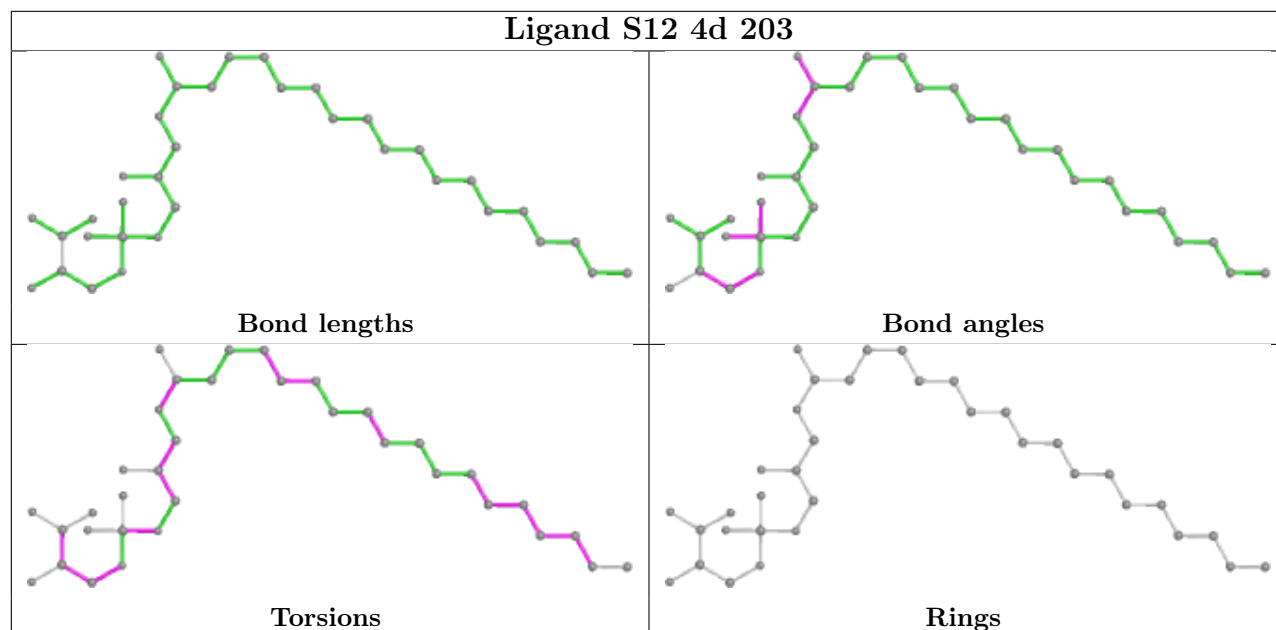


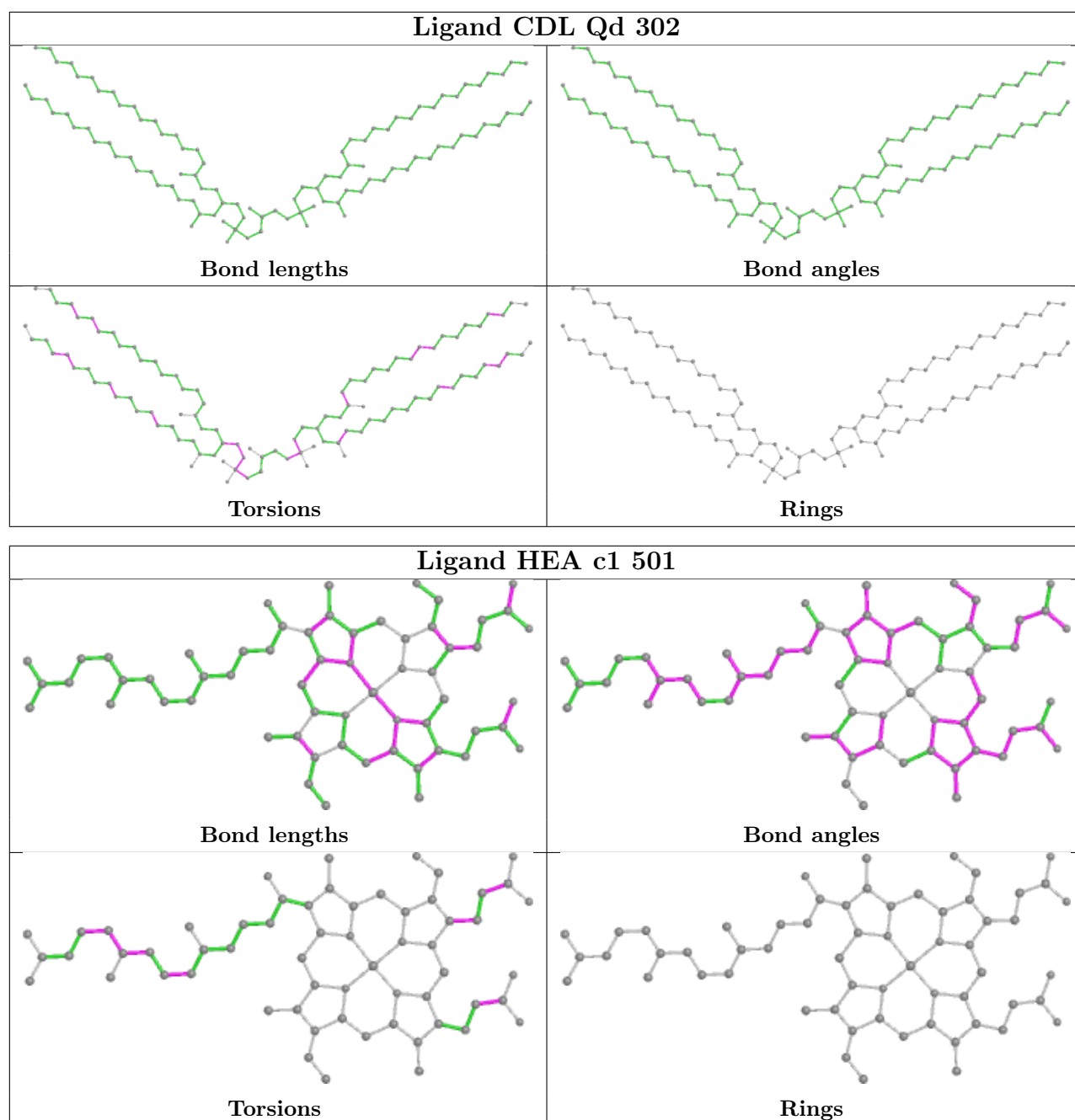












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.