



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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **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

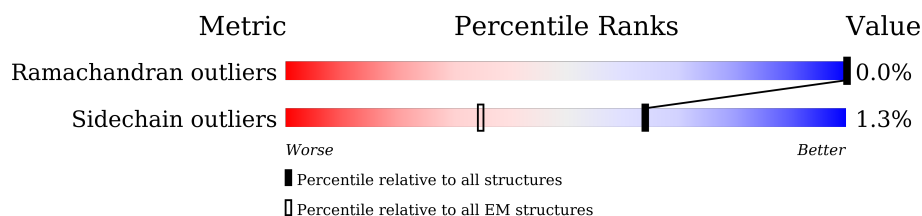
1 Overall quality at a glance

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.







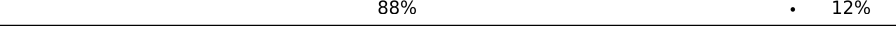
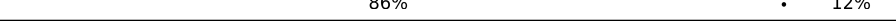
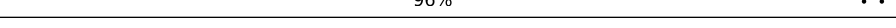
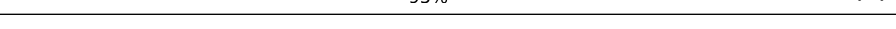
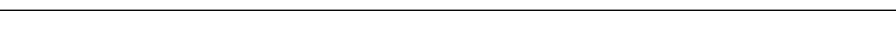
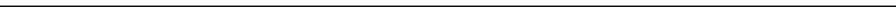





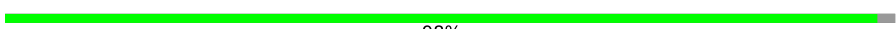
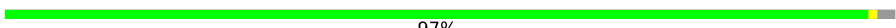


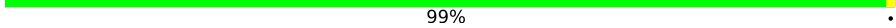
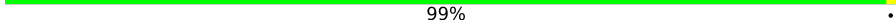
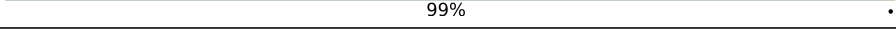
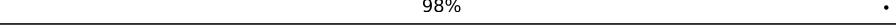
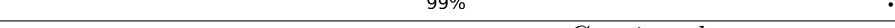

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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% ..

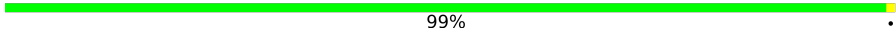
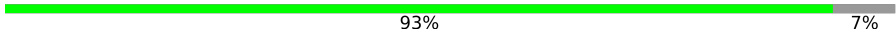





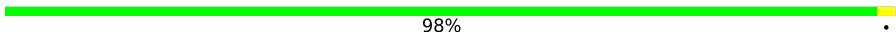
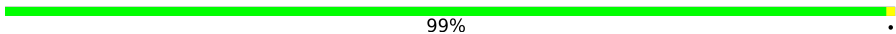
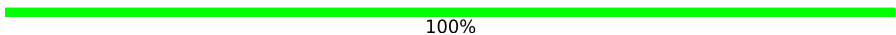
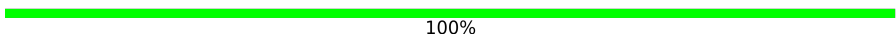
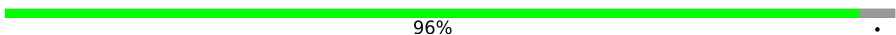



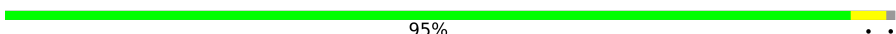
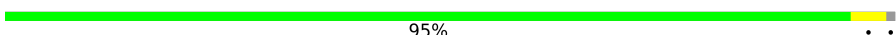
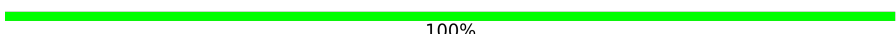
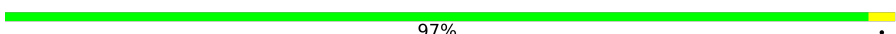
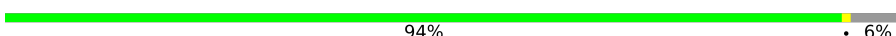
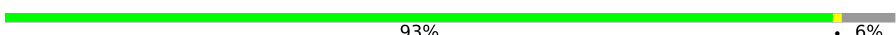
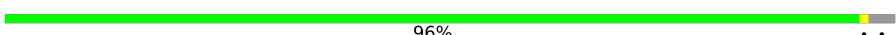
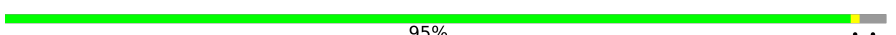


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Mol	Chain	Length	Quality of chain
6	QK	100	
6	Qk	100	
7	4A	246	
7	4a	246	
8	4C	139	
8	4c	139	
9	4E	165	
9	4e	165	
10	4H	221	
10	4h	221	
11	4J	88	
11	4j	88	
12	5C	208	
12	5c	208	
13	6A	112	
13	6a	112	
14	6B	287	
14	6b	287	
15	7C	171	
15	7c	171	
16	C1	495	
16	c1	495	
17	C2	196	
17	c2	196	
18	C3	161	

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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 [i](#)

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		

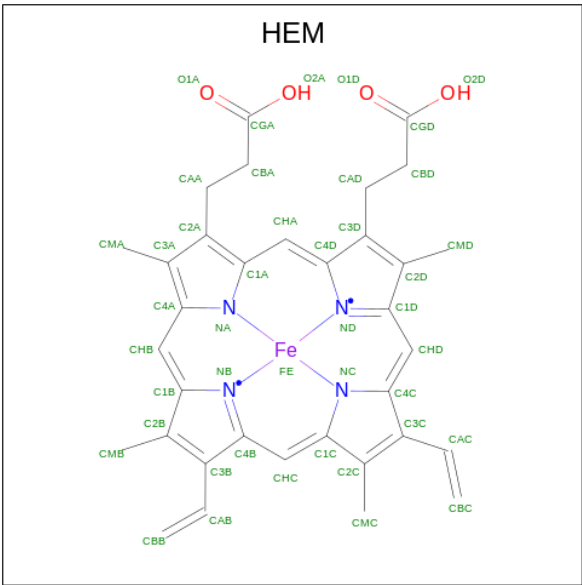
- Molecule 29 is a protein called COXEG9.

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.

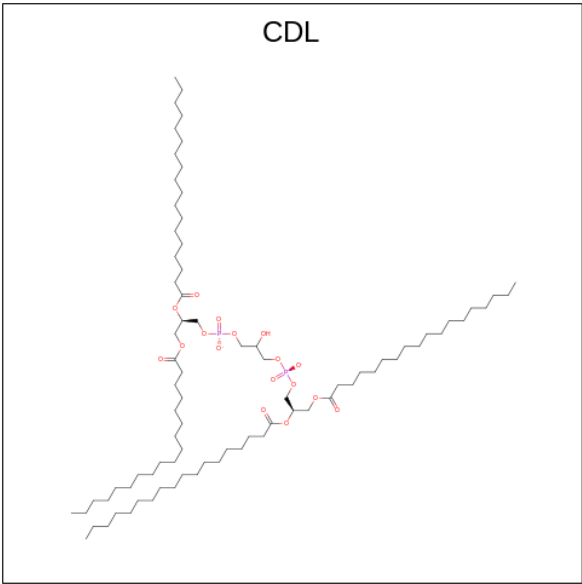
Mol	Chain	Residues	Atoms						AltConf	Trace
30	7a	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		
30	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- 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).



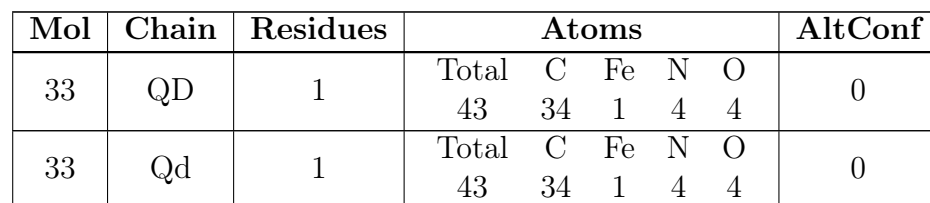
Mol	Chain	Residues	Atoms					AltConf
31	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

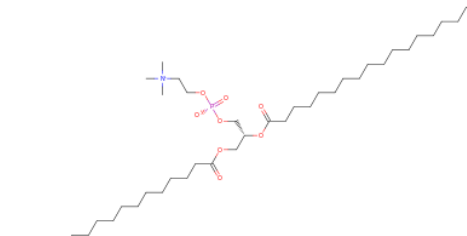
- Molecule 32 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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).



- PC1
- 
- The chemical structure of PC1 is a phosphazene-based polymer. It consists of a central phosphorus atom (P) bonded to two nitrogen atoms (N). Each nitrogen atom is part of a repeating unit that includes a long, zigzag alkyl chain and a phosphate group. The phosphate groups are linked together, forming a continuous backbone structure.

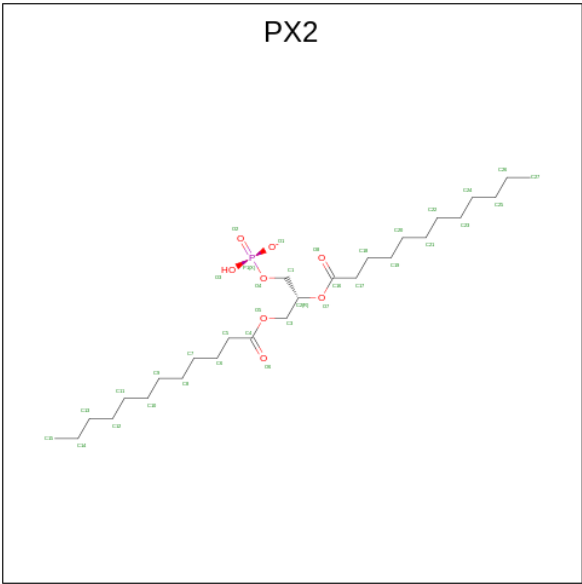
Mol	Chain	Residues	Atoms					AltConf	
34	QD	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	



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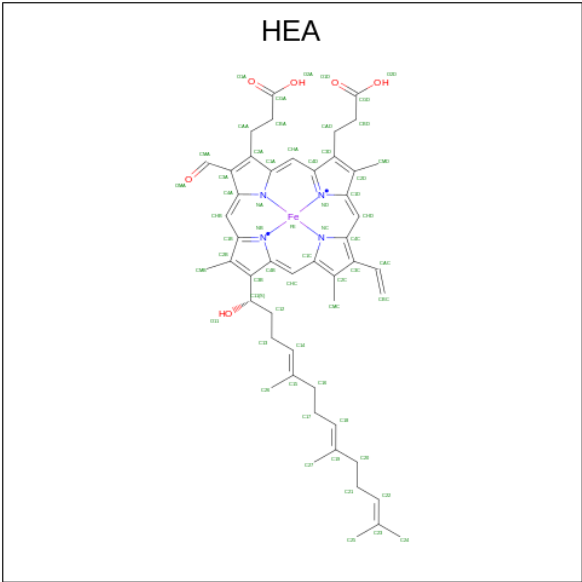
Mol	Chain	Residues	Atoms						AltConf
34	Qc	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
34	Qd	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
34	Qj	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
34	4a	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
34	4e	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
34	7c	1	Total	C	H	N	O	P	0
			142	44	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: C₂₇H₅₂O₈P).



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 60	C 49	Fe 1	N 4	O 6	0
37	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
37	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

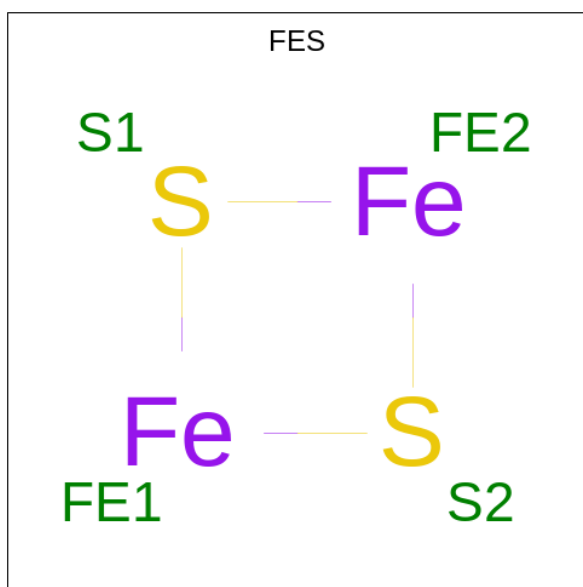
- Molecule 38 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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).

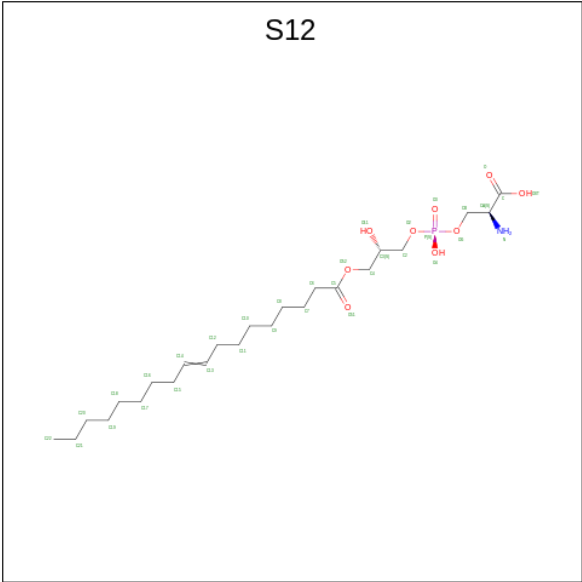


Mol	Chain	Residues	Atoms			AltConf
40	QE	1	Total	Fe	S	0
			4	2	2	
40	Qe	1	Total	Fe	S	0
			4	2	2	

- 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% ..



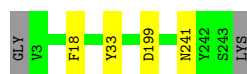
- Molecule 2: Cytochrome b

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%



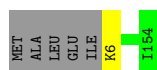
- Molecule 4: UQCRQ

Chain Qh: 99%



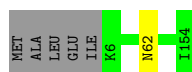
- Molecule 5: UQCR10

Chain QJ: 96%



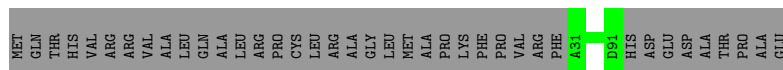
- Molecule 5: UQCR10

Chain Qj: 96%



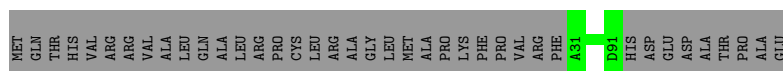
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK: 61%



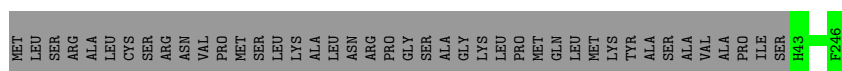
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain Qk: 61%



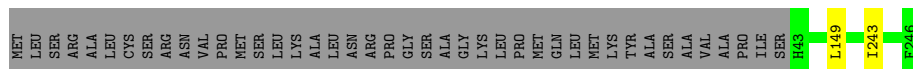
- Molecule 7: COXEG1

Chain 4a: 83%



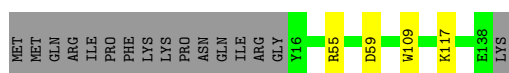
- Molecule 7: COXEG1

Chain 4A: 82% 17%



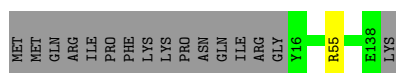
- Molecule 8: COXEG3

Chain 4c: 86% 12%



- Molecule 8: COXEG3

Chain 4C: 88% 12%



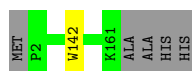
- Molecule 9: COXEG5

Chain 4e: 95% ..



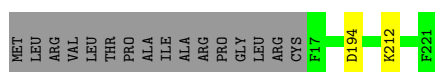
- Molecule 9: COXEG5

Chain 4E: 96% ..



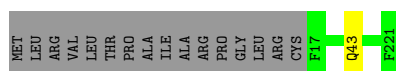
- Molecule 10: COXEG8

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.

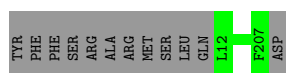
- Molecule 11: COXEG10

Chain 4J: 99%



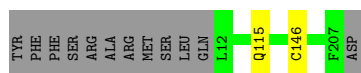
- Molecule 12: COX5c

Chain 5c: 94%



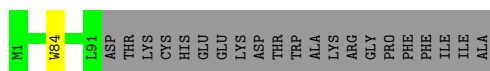
- Molecule 12: COX5c

Chain 5C: 93%



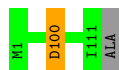
- Molecule 13: COX6a

Chain 6a: 80%



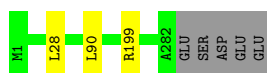
- Molecule 13: COX6a

Chain 6A: 98%

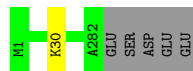


- Molecule 14: COX6b-1


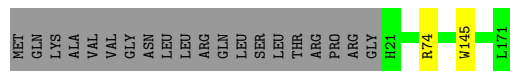
Chain 6b: 97%




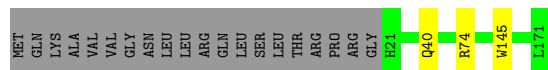
• Molecule 14: COX6b-1

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%

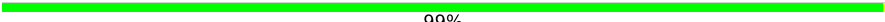
• Molecule 17: Cytochrome c oxidase subunit 2

Chain c2:  98%

• Molecule 17: Cytochrome c oxidase subunit 2

Chain C2:  99%

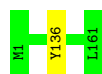
• Molecule 18: Putative NADH dehydrogenase subunit 6

Chain c3:  99%



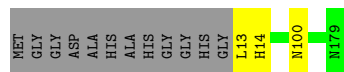
- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain C3:  99%



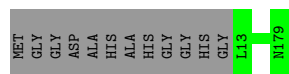
- Molecule 19: COX4

Chain dc:  92%



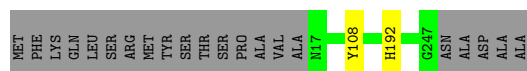
- Molecule 19: COX4

Chain DC:  93%



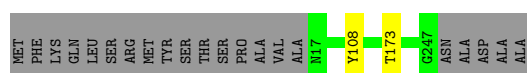
- Molecule 20: UQCRFS1

Chain QE:  91%




- Molecule 20: UQCRFS1

Chain Qe:  91%




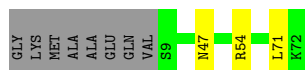
- Molecule 21: UQCRH

Chain QF:  85%



- 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.

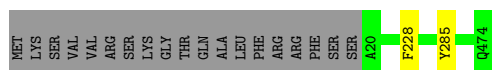
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain Qb:  93%




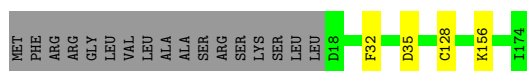
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain QB:  96%

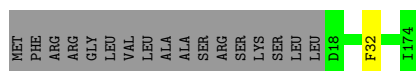
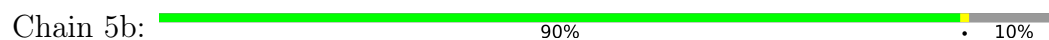


- Molecule 25: COX5b-2

Chain 5B:  88% 10%



- Molecule 25: COX5b-2



- Molecule 26: COXEG4



- Molecule 26: COXEG4

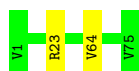


- Molecule 27: COXEG6

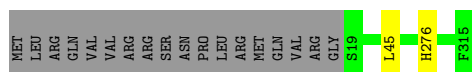


There are no outlier residues recorded for this chain.

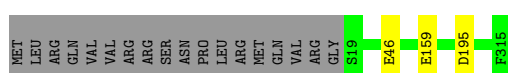
- Molecule 27: COXEG6



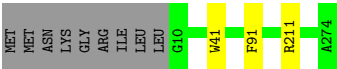
- Molecule 28: COXEG7



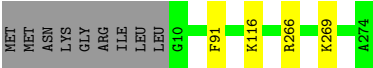
- Molecule 28: COXEG7



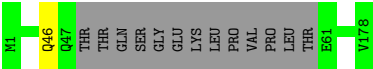
● Molecule 29: COXEG9



● Molecule 29: COXEG9



● Molecule 30: COX7a



● Molecule 30: COX7a



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

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	QA	71	PHE
1	QA	348	TYR
1	QA	474	VAL
2	QC	173	TYR
2	QC	316	LEU

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Mol	Chain	Res	Type
3	QD	18	PHE
3	QD	33	TYR
3	QD	199	ASP
3	QD	241	ASN
5	QJ	6	LYS
1	Qa	71	PHE
1	Qa	293	ASP
1	Qa	348	TYR
1	Qa	443	GLU
2	Qc	191	HIS
2	Qc	329	CYS
3	Qd	33	TYR
3	Qd	97	GLU
5	Qj	62	ASN
8	4c	55	ARG
8	4c	59	ASP
8	4c	109	TRP
8	4c	117	LYS
9	4e	39	GLU
9	4e	81	LYS
9	4e	100	GLU
9	4e	142	TRP
10	4h	194	ASP
10	4h	212	LYS
13	6a	84	TRP
14	6b	28	LEU
14	6b	90	LEU
14	6b	199	ARG
15	7c	74	ARG
15	7c	145	TRP
16	c1	154	ASN
16	c1	156	ASP
16	c1	416	PHE
16	c1	419	PHE
16	c1	465	PHE
17	c2	60	TRP
17	c2	133	HIS
17	c2	140	ASP
18	c3	93	PHE
18	c3	156	HIS
19	dc	13	LEU
19	dc	14	HIS

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Mol	Chain	Res	Type
19	dc	100	ASN
7	4A	149	LEU
7	4A	243	ILE
8	4C	55	ARG
9	4E	142	TRP
10	4H	43	GLN
11	4J	29	THR
12	5C	115	GLN
12	5C	146	CYS
14	6B	30	LYS
15	7C	40	GLN
15	7C	74	ARG
15	7C	145	TRP
16	C1	1	MET
16	C1	154	ASN
16	C1	416	PHE
16	C1	465	PHE
17	C2	60	TRP
17	C2	133	HIS
18	C3	136	TYR
13	6A	100	ASP
20	QE	108	TYR
20	QE	192	HIS
20	Qe	108	TYR
20	Qe	173	THR
21	QF	36	CYS
21	QF	47	ASN
21	QF	55	LEU
22	QG	29	LEU
22	QG	62	GLU
22	QG	126	CYS
22	QG	228	ARG
24	Qb	106	ASP
24	Qb	141	VAL
24	Qb	173	GLU
24	Qb	201	THR
24	Qb	279	TYR
24	Qb	285	TYR
24	Qb	286	ASP
24	Qb	303	SER
24	Qb	413	GLN
24	Qb	459	VAL

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Mol	Chain	Res	Type
21	Qf	47	ASN
21	Qf	54	ARG
21	Qf	71	LEU
22	Qg	126	CYS
22	Qg	149	LYS
22	Qg	226	TYR
24	QB	228	PHE
24	QB	285	TYR
25	5B	32	PHE
25	5B	35	ASP
25	5B	128	CYS
25	5B	156	LYS
26	4D	81	ILE
26	4D	125	HIS
26	4D	126	VAL
26	4D	168	ASP
26	4D	169	ASP
26	4D	171	GLN
26	4D	173	ARG
28	4G	45	LEU
28	4G	276	HIS
29	4I	41	TRP
29	4I	91	PHE
29	4I	211	ARG
30	7a	46	GLN
26	4d	81	ILE
26	4d	126	VAL
26	4d	160	ASP
26	4d	166	ILE
26	4d	167	LEU
26	4d	171	GLN
26	4d	172	LYS
27	4f	23	ARG
27	4f	64	VAL
28	4g	46	GLU
28	4g	159	GLU
28	4g	195	ASP
29	4i	91	PHE
29	4i	116	LYS
29	4i	266	ARG
29	4i	269	LYS
25	5b	32	PHE

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Mol	Chain	Res	Type
30	7A	1	MET
30	7A	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	QA	29	GLN
1	QA	65	ASN
1	QA	167	HIS
1	QA	333	ASN
1	QA	398	GLN
2	QC	56	HIS
2	QC	204	ASN
3	QD	16	GLN
3	QD	19	GLN
3	QD	147	GLN
3	QD	241	ASN
4	QH	40	GLN
6	QK	89	HIS
1	Qa	70	HIS
1	Qa	167	HIS
1	Qa	268	GLN
2	Qc	56	HIS
2	Qc	73	HIS
2	Qc	204	ASN
3	Qd	147	GLN
5	Qj	62	ASN
5	Qj	116	HIS
7	4a	186	HIS
11	4j	23	GLN
11	4j	34	ASN
12	5c	22	GLN
12	5c	24	ASN
12	5c	63	ASN
14	6b	105	GLN
14	6b	111	ASN
14	6b	252	HIS
15	7c	32	ASN
15	7c	134	GLN
16	c1	154	ASN
16	c1	194	ASN
16	c1	299	HIS

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Mol	Chain	Res	Type
16	c1	346	ASN
16	c1	423	HIS
16	c1	439	HIS
16	c1	466	HIS
16	c1	488	HIS
16	c1	490	ASN
17	c2	17	GLN
17	c2	133	HIS
18	c3	8	ASN
18	c3	128	ASN
19	dc	29	GLN
19	dc	54	HIS
19	dc	76	ASN
7	4A	130	ASN
7	4A	161	HIS
7	4A	186	HIS
10	4H	92	HIS
11	4J	3	HIS
12	5C	22	GLN
12	5C	24	ASN
12	5C	48	HIS
12	5C	63	ASN
12	5C	79	GLN
12	5C	115	GLN
14	6B	252	HIS
15	7C	32	ASN
15	7C	112	HIS
15	7C	134	GLN
16	C1	154	ASN
16	C1	194	ASN
16	C1	242	GLN
16	C1	346	ASN
16	C1	423	HIS
16	C1	439	HIS
16	C1	484	GLN
17	C2	90	ASN
17	C2	98	ASN
18	C3	8	ASN
18	C3	124	HIS
19	DC	29	GLN
13	6A	68	ASN
13	6A	72	ASN

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Mol	Chain	Res	Type
20	Qe	112	GLN
22	QG	2	ASN
22	QG	25	HIS
22	QG	96	HIS
22	QG	105	GLN
22	QG	196	HIS
23	QI	15	GLN
24	Qb	40	ASN
24	Qb	76	GLN
24	Qb	133	ASN
24	Qb	199	HIS
24	Qb	289	HIS
24	Qb	413	GLN
24	Qb	474	GLN
22	Qg	2	ASN
22	Qg	21	GLN
22	Qg	25	HIS
22	Qg	96	HIS
22	Qg	105	GLN
22	Qg	125	HIS
22	Qg	196	HIS
24	QB	50	GLN
24	QB	133	ASN
24	QB	199	HIS
24	QB	289	HIS
24	QB	413	GLN
24	QB	461	HIS
25	5B	47	GLN
25	5B	131	HIS
26	4D	37	GLN
26	4D	64	HIS
26	4D	94	GLN
26	4D	118	HIS
26	4D	120	ASN
26	4D	125	HIS
28	4G	22	ASN
28	4G	24	GLN
28	4G	141	ASN
28	4G	197	GLN
28	4G	266	ASN
29	4I	62	HIS
29	4I	153	ASN

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Mol	Chain	Res	Type
29	4I	167	HIS
29	4I	223	HIS
30	7a	15	HIS
30	7a	19	HIS
30	7a	30	GLN
30	7a	84	GLN
30	7a	101	ASN
26	4d	22	ASN
26	4d	37	GLN
26	4d	94	GLN
26	4d	107	GLN
26	4d	118	HIS
26	4d	120	ASN
26	4d	133	ASN
28	4g	22	ASN
28	4g	24	GLN
28	4g	141	ASN
28	4g	243	ASN
28	4g	266	ASN
29	4i	62	HIS
29	4i	153	ASN
29	4i	167	HIS
29	4i	223	HIS
25	5b	47	GLN
25	5b	131	HIS
30	7A	15	HIS
30	7A	30	GLN
30	7A	84	GLN
30	7A	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
37	C1	502	HEA	C3B-C2B	5.27	1.46	1.34
37	C1	501	HEA	C3B-C2B	5.12	1.46	1.34
37	c1	501	HEA	C3B-C2B	5.06	1.46	1.34
37	c1	502	HEA	C3A-C2A	4.73	1.46	1.40
37	C1	502	HEA	C4B-NB	-4.64	1.32	1.40
37	c1	501	HEA	C4B-NB	-4.58	1.32	1.40
37	C1	502	HEA	C3A-C2A	4.57	1.46	1.40
37	c1	502	HEA	C4B-NB	-4.46	1.32	1.40
37	C1	502	HEA	CHC-C4B	4.45	1.46	1.35
37	c1	502	HEA	CHC-C4B	4.39	1.46	1.35
37	C1	501	HEA	CHC-C4B	4.39	1.46	1.35
37	c1	501	HEA	CHD-C1D	4.27	1.45	1.35
37	c1	502	HEA	C1D-ND	-4.24	1.33	1.40
37	c1	501	HEA	CHC-C4B	4.13	1.45	1.35
37	C1	501	HEA	C1D-ND	-4.09	1.33	1.40
37	C1	501	HEA	C4B-NB	-4.09	1.33	1.40
37	C1	501	HEA	CHD-C1D	4.00	1.45	1.35
37	C1	501	HEA	C3C-C2C	4.00	1.45	1.40
31	QC	401	HEM	C4D-ND	-3.95	1.33	1.40
37	c1	501	HEA	C1D-ND	-3.95	1.33	1.40
37	C1	501	HEA	C3D-C2D	3.93	1.45	1.36
37	c1	501	HEA	C3A-C2A	3.92	1.45	1.40
37	C1	502	HEA	C3C-C2C	3.86	1.45	1.40
37	C1	502	HEA	C3D-C2D	3.86	1.44	1.36
37	C1	502	HEA	CHD-C1D	3.85	1.44	1.35
37	c1	502	HEA	CHD-C1D	3.83	1.44	1.35
31	Qc	402	HEM	C4D-ND	-3.83	1.33	1.40
37	c1	502	HEA	C3C-C2C	3.83	1.45	1.40
31	QC	402	HEM	C4D-ND	-3.82	1.33	1.40
37	c1	501	HEA	C3D-C2D	3.82	1.44	1.36
37	c1	502	HEA	C3D-C2D	3.76	1.44	1.36
37	C1	501	HEA	C3A-C2A	3.73	1.45	1.40
31	Qc	401	HEM	C4D-ND	-3.70	1.33	1.40
37	c1	501	HEA	C3C-C2C	3.57	1.45	1.40
37	C1	502	HEA	C1D-ND	-3.53	1.34	1.40
33	QD	301	HEC	CBC-CAC	-3.44	1.36	1.49
31	Qc	401	HEM	C1B-NB	-3.42	1.34	1.40
33	Qd	301	HEC	CBC-CAC	-3.42	1.36	1.49
37	c1	501	HEA	C1B-NB	-3.26	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	502	HEA	C1B-NB	-3.23	1.32	1.38
31	QC	401	HEM	C1B-NB	-3.21	1.34	1.40
31	Qc	402	HEM	C1B-NB	-3.20	1.34	1.40
31	QC	402	HEM	C1B-NB	-3.16	1.34	1.40
37	c1	501	HEA	CAA-C2A	-3.11	1.46	1.52
37	C1	501	HEA	CAA-C2A	-3.11	1.46	1.52
37	c1	502	HEA	C1B-NB	-2.78	1.33	1.38
37	C1	502	HEA	CAA-C2A	-2.76	1.47	1.52
35	QD	304	PX2	O7-C2	-2.76	1.39	1.46
37	c1	502	HEA	CAA-C2A	-2.74	1.47	1.52
37	C1	501	HEA	FE-ND	2.74	2.10	1.96
31	QC	401	HEM	C1D-ND	-2.72	1.33	1.38
37	C1	502	HEA	FE-NB	2.71	2.10	1.96
35	4C	201	PX2	O7-C2	-2.70	1.39	1.46
37	C1	501	HEA	C1B-NB	-2.69	1.33	1.38
31	Qc	402	HEM	C1D-ND	-2.68	1.33	1.38
31	QC	402	HEM	C1D-ND	-2.66	1.33	1.38
37	c1	502	HEA	C4D-ND	-2.65	1.33	1.38
35	QJ	201	PX2	O7-C2	-2.63	1.40	1.46
37	c1	501	HEA	FE-ND	2.59	2.09	1.96
37	c1	502	HEA	FE-ND	2.56	2.09	1.96
37	c1	502	HEA	O2D-CGD	-2.49	1.22	1.30
37	c1	501	HEA	C4D-ND	-2.48	1.33	1.38
31	Qc	401	HEM	C1D-ND	-2.48	1.33	1.38
37	C1	501	HEA	O2D-CGD	-2.47	1.22	1.30
37	C1	502	HEA	O2D-CGD	-2.47	1.22	1.30
33	QD	301	HEC	CBB-CAB	-2.45	1.40	1.49
37	c1	501	HEA	O2D-CGD	-2.44	1.22	1.30
37	C1	501	HEA	FE-NB	2.44	2.08	1.96
37	C1	501	HEA	O2A-CGA	-2.44	1.22	1.30
37	C1	501	HEA	C4D-ND	-2.42	1.33	1.38
37	c1	502	HEA	O2A-CGA	-2.41	1.22	1.30
33	Qd	301	HEC	CBB-CAB	-2.40	1.40	1.49
35	QD	304	PX2	O5-C3	-2.39	1.39	1.45
37	C1	502	HEA	O2A-CGA	-2.38	1.22	1.30
37	c1	501	HEA	O2A-CGA	-2.37	1.22	1.30
37	C1	502	HEA	C4D-ND	-2.36	1.33	1.38
37	C1	502	HEA	FE-ND	2.34	2.08	1.96
37	c1	502	HEA	FE-NB	2.33	2.08	1.96
35	4C	201	PX2	O5-C4	2.27	1.40	1.33
35	QJ	201	PX2	O5-C4	2.26	1.39	1.33
37	c1	501	HEA	FE-NB	2.26	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4C	201	PX2	O5-C3	-2.21	1.40	1.45
35	QJ	201	PX2	O5-C3	-2.17	1.40	1.45
37	C1	501	HEA	C4B-C3B	2.14	1.48	1.44
31	Qc	401	HEM	C4B-NB	-2.13	1.34	1.38
31	QC	401	HEM	C4B-NB	-2.10	1.34	1.38
35	QD	304	PX2	O5-C4	2.10	1.39	1.33
31	QC	401	HEM	CHB-C1B	2.08	1.40	1.35
31	Qc	401	HEM	C3C-C2C	-2.03	1.37	1.40
31	Qc	402	HEM	C4B-NB	-2.02	1.34	1.38
35	QD	304	PX2	O7-C16	2.02	1.40	1.34
35	4C	201	PX2	O7-C16	2.00	1.40	1.34

All (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
37	C1	501	HEA	CAA-CBA-CGA	-5.79	97.52	113.76
37	c1	501	HEA	C13-C12-C11	-5.64	105.88	114.35
37	C1	501	HEA	C3D-C4D-ND	5.60	115.78	110.36
37	c1	501	HEA	CAA-CBA-CGA	-5.53	98.27	113.76
31	QC	401	HEM	CHC-C4B-NB	5.35	130.24	124.43
37	C1	502	HEA	C3D-C4D-ND	5.32	115.51	110.36
37	c1	502	HEA	CAA-CBA-CGA	-5.31	98.88	113.76
37	C1	502	HEA	C13-C12-C11	-5.25	106.46	114.35
37	c1	502	HEA	C13-C12-C11	-5.16	106.59	114.35
37	c1	501	HEA	CHB-C1B-C2B	-5.05	117.09	124.98
37	C1	501	HEA	C13-C12-C11	-5.03	106.80	114.35
37	c1	502	HEA	C3D-C4D-ND	5.02	115.22	110.36
37	C1	502	HEA	C2D-C1D-ND	5.01	115.78	109.84
37	C1	501	HEA	C2B-C1B-NB	4.99	115.86	109.88
31	Qc	402	HEM	CHC-C4B-NB	4.95	129.81	124.43
37	C1	502	HEA	C1D-C2D-C3D	-4.94	101.76	106.96
37	C1	501	HEA	C2D-C1D-ND	4.94	115.69	109.84
31	Qc	401	HEM	CHC-C4B-NB	4.88	129.74	124.43
37	C1	502	HEA	C2B-C1B-NB	4.87	115.71	109.88
37	C1	501	HEA	CHB-C1B-C2B	-4.84	117.42	124.98
42	4F	102	S12	OG-CB-CA	4.81	112.25	108.06
37	C1	502	HEA	CAA-CBA-CGA	-4.77	100.40	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c1	501	HEA	C2B-C1B-NB	4.75	115.57	109.88
37	c1	502	HEA	C2B-C1B-NB	4.67	115.48	109.88
37	C1	501	HEA	C1D-C2D-C3D	-4.60	102.12	106.96
31	QC	402	HEM	CHC-C4B-NB	4.57	129.39	124.43
37	c1	502	HEA	C1D-C2D-C3D	-4.55	102.18	106.96
37	c1	501	HEA	C3B-C4B-NB	4.53	115.21	109.84
37	c1	502	HEA	C3B-C4B-NB	4.50	115.17	109.84
37	c1	502	HEA	C2D-C1D-ND	4.49	115.16	109.84
37	C1	502	HEA	CHB-C1B-C2B	-4.45	118.03	124.98
35	QJ	201	PX2	O7-C16-C17	4.42	121.03	111.50
37	c1	501	HEA	C2D-C1D-ND	4.29	114.93	109.84
37	c1	502	HEA	CHB-C1B-C2B	-4.24	118.35	124.98
37	c1	501	HEA	C1D-C2D-C3D	-4.22	102.52	106.96
37	C1	502	HEA	C3B-C4B-NB	4.21	114.83	109.84
37	C1	501	HEA	C3B-C4B-NB	4.19	114.80	109.84
37	C1	501	HEA	C3C-C4C-NC	4.17	114.60	109.21
37	c1	502	HEA	C3C-C4C-NC	4.16	114.59	109.21
35	4C	201	PX2	O7-C16-C17	4.13	120.40	111.50
31	QC	402	HEM	CHB-C1B-NB	4.05	129.38	124.38
37	c1	502	HEA	CMC-C2C-C3C	4.04	132.24	124.68
42	4d	203	S12	OG-CB-CA	4.01	111.55	108.06
37	C1	502	HEA	C3C-C4C-NC	3.96	114.32	109.21
31	Qc	402	HEM	CHB-C1B-NB	3.93	129.24	124.38
37	c1	501	HEA	C3C-C4C-NC	3.91	114.27	109.21
33	QD	301	HEC	CMD-C2D-C1D	-3.90	122.47	128.46
31	Qc	401	HEM	C4D-ND-C1D	3.89	109.09	105.07
37	c1	501	HEA	C4B-C3B-C2B	-3.87	100.80	107.41
31	Qc	401	HEM	CHB-C1B-NB	3.84	129.12	124.38
35	QD	304	PX2	O7-C16-C17	3.80	119.68	111.50
37	c1	501	HEA	CHA-C4D-C3D	-3.69	119.42	124.84
37	C1	502	HEA	CMC-C2C-C3C	3.65	131.50	124.68
37	C1	502	HEA	C4B-C3B-C2B	-3.65	101.18	107.41
37	c1	502	HEA	C4B-C3B-C2B	-3.65	101.18	107.41
33	Qd	301	HEC	CMD-C2D-C1D	-3.60	122.93	128.46
37	C1	501	HEA	C4B-C3B-C2B	-3.59	101.27	107.41
31	QC	401	HEM	CHB-C1B-NB	3.59	128.81	124.38
37	C1	501	HEA	CMC-C2C-C3C	3.52	131.26	124.68
31	QC	402	HEM	C4D-ND-C1D	3.50	108.69	105.07
33	QD	301	HEC	CMB-C2B-C1B	-3.47	123.14	128.46
37	C1	501	HEA	CHA-C4D-C3D	-3.46	119.75	124.84
37	c1	502	HEA	CHA-C4D-C3D	-3.42	119.81	124.84
37	c1	501	HEA	CMC-C2C-C3C	3.40	131.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Qc	401	HEM	CHA-C4D-ND	3.40	128.58	124.38
31	Qc	402	HEM	C4D-ND-C1D	3.38	108.56	105.07
31	QC	401	HEM	C1B-NB-C4B	3.33	108.51	105.07
33	QD	301	HEC	CMB-C2B-C3B	3.32	129.72	125.82
31	QC	401	HEM	C4D-ND-C1D	3.29	108.47	105.07
31	Qc	402	HEM	CHA-C4D-ND	3.21	128.34	124.38
33	Qd	301	HEC	CMB-C2B-C1B	-3.20	123.55	128.46
31	Qc	402	HEM	C1B-NB-C4B	3.19	108.37	105.07
31	QC	401	HEM	CHA-C4D-ND	3.17	128.30	124.38
31	Qc	401	HEM	C1B-NB-C4B	3.12	108.29	105.07
33	QD	301	HEC	CMC-C2C-C3C	3.10	129.47	125.82
37	C1	502	HEA	CHA-C4D-C3D	-3.10	120.28	124.84
37	c1	501	HEA	C13-C14-C15	-3.09	120.21	127.66
33	Qd	301	HEC	CMC-C2C-C3C	3.02	129.37	125.82
33	Qd	301	HEC	C4C-C3C-C2C	2.96	109.55	106.35
31	QC	402	HEM	C1B-NB-C4B	2.96	108.13	105.07
31	QC	402	HEM	CHA-C4D-ND	2.94	128.01	124.38
33	QD	301	HEC	C4C-C3C-C2C	2.87	109.45	106.35
33	QD	301	HEC	O1D-CGD-CBD	-2.86	113.88	123.08
37	c1	501	HEA	C27-C19-C20	2.86	120.08	115.27
33	Qd	301	HEC	CMB-C2B-C3B	2.84	129.16	125.82
37	C1	501	HEA	CMB-C2B-C1B	-2.83	120.72	125.04
31	Qc	402	HEM	CHD-C1D-ND	2.82	127.50	124.43
37	c1	502	HEA	CMB-C2B-C1B	-2.82	120.75	125.04
33	Qd	301	HEC	O1D-CGD-CBD	-2.80	114.07	123.08
35	QD	304	PX2	O5-C4-C5	2.80	120.69	111.91
31	QC	401	HEM	CHD-C1D-ND	2.79	127.46	124.43
37	C1	501	HEA	C13-C14-C15	-2.79	120.94	127.66
37	C1	502	HEA	CMB-C2B-C1B	-2.74	120.86	125.04
37	C1	501	HEA	C27-C19-C20	2.72	119.85	115.27
37	C1	501	HEA	C17-C18-C19	-2.71	121.13	127.66
37	C1	501	HEA	CHC-C4B-NB	-2.70	121.04	124.38
37	c1	501	HEA	C17-C18-C19	-2.69	121.17	127.66
37	c1	501	HEA	CHB-C1B-NB	2.68	127.34	124.43
37	C1	502	HEA	CMB-C2B-C3B	2.67	135.43	130.34
37	C1	501	HEA	OMA-CMA-C3A	-2.67	119.10	124.91
31	Qc	402	HEM	CAD-CBD-CGD	-2.66	107.88	113.60
31	QC	402	HEM	CBA-CAA-C2A	-2.66	108.08	112.62
37	c1	502	HEA	CMB-C2B-C3B	2.65	135.40	130.34
33	QD	301	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
31	QC	402	HEM	CAD-CBD-CGD	-2.63	107.94	113.60
31	QC	402	HEM	CHD-C1D-ND	2.63	127.28	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c1	501	HEA	CMB-C2B-C1B	-2.62	121.05	125.04
37	C1	502	HEA	C1B-C2B-C3B	-2.59	103.70	106.80
37	C1	501	HEA	O1A-CGA-CBA	-2.59	114.77	123.08
37	c1	501	HEA	O1A-CGA-CBA	-2.58	114.78	123.08
37	c1	501	HEA	C4D-C3D-C2D	-2.58	103.14	106.90
31	Qc	401	HEM	CHD-C1D-ND	2.57	127.22	124.43
42	4d	203	S12	O4-P-O3	2.57	124.93	112.24
37	C1	501	HEA	CMB-C2B-C3B	2.56	135.22	130.34
33	Qd	301	HEC	CMC-C2C-C1C	-2.55	124.55	128.46
37	c1	501	HEA	C26-C15-C16	2.55	119.56	115.27
35	4C	201	PX2	O5-C4-C5	2.53	119.84	111.91
35	QJ	201	PX2	O5-C4-C5	2.53	119.84	111.91
42	4F	102	S12	O4-P-O3	2.50	124.62	112.24
31	QC	402	HEM	CHB-C1B-C2B	-2.50	119.82	126.72
37	c1	502	HEA	CAA-C2A-C3A	2.49	133.00	126.86
37	C1	502	HEA	C27-C19-C18	-2.48	117.31	123.68
37	c1	502	HEA	C1B-C2B-C3B	-2.47	103.85	106.80
37	C1	501	HEA	C27-C19-C18	-2.47	117.34	123.68
37	C1	501	HEA	C4D-C3D-C2D	-2.46	103.32	106.90
37	C1	502	HEA	O1A-CGA-CBA	-2.45	115.20	123.08
37	c1	501	HEA	C27-C19-C18	-2.45	117.39	123.68
37	c1	502	HEA	O1A-CGA-CBA	-2.45	115.22	123.08
33	QD	301	HEC	CMD-C2D-C3D	2.42	129.50	124.94
33	Qd	301	HEC	O1A-CGA-CBA	-2.41	115.33	123.08
33	QD	301	HEC	O1A-CGA-CBA	-2.38	115.42	123.08
37	C1	502	HEA	C13-C14-C15	-2.37	121.95	127.66
37	c1	502	HEA	C27-C19-C18	-2.37	117.60	123.68
33	Qd	301	HEC	O2A-CGA-O1A	2.36	129.18	123.30
37	c1	501	HEA	CMB-C2B-C3B	2.32	134.76	130.34
31	QC	401	HEM	CAD-CBD-CGD	-2.32	108.61	113.60
37	c1	502	HEA	C17-C18-C19	-2.31	122.10	127.66
37	C1	501	HEA	C1B-C2B-C3B	-2.30	104.05	106.80
37	c1	502	HEA	C13-C14-C15	-2.28	122.17	127.66
31	Qc	402	HEM	CHB-C1B-C2B	-2.27	120.43	126.72
33	QD	301	HEC	O2A-CGA-O1A	2.27	128.96	123.30
31	Qc	401	HEM	CAA-CBA-CGA	-2.25	107.46	113.76
37	c1	501	HEA	CAD-C3D-C2D	2.23	132.03	127.88
33	Qd	301	HEC	CMA-C3A-C2A	2.23	129.14	124.94
37	c1	501	HEA	O1D-CGD-CBD	-2.23	115.93	123.08
37	c1	502	HEA	OMA-CMA-C3A	-2.22	120.08	124.91
42	4d	203	S12	O52-C5-O51	-2.22	117.99	123.59
37	C1	501	HEA	O1D-CGD-CBD	-2.21	115.98	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c1	502	HEA	C4D-C3D-C2D	-2.21	103.68	106.90
37	C1	502	HEA	C17-C18-C19	-2.19	122.38	127.66
33	QD	301	HEC	CMA-C3A-C2A	2.19	129.07	124.94
31	Qc	401	HEM	CHB-C1B-C2B	-2.19	120.66	126.72
37	c1	501	HEA	C1B-C2B-C3B	-2.19	104.19	106.80
37	C1	502	HEA	C25-C23-C22	-2.14	116.46	122.65
37	C1	502	HEA	O1D-CGD-CBD	-2.12	116.27	123.08
37	C1	502	HEA	C27-C19-C20	2.12	118.83	115.27
37	C1	502	HEA	C1D-ND-C4D	-2.10	102.91	105.07
37	C1	501	HEA	CHB-C1B-NB	2.10	126.71	124.43
37	c1	502	HEA	C26-C15-C14	-2.09	118.30	123.68
37	C1	501	HEA	CHD-C1D-C2D	-2.09	120.94	126.72
37	C1	502	HEA	CHD-C1D-C2D	-2.08	120.96	126.72
37	c1	501	HEA	CMD-C2D-C1D	2.08	128.21	125.04
34	DC	201	PC1	O21-C2-C1	2.08	115.92	108.40
33	QD	301	HEC	C2B-C3B-C4B	2.07	108.59	106.35
33	Qd	301	HEC	C2B-C3B-C4B	2.07	108.59	106.35
37	c1	502	HEA	O1D-CGD-CBD	-2.07	116.45	123.08
33	Qd	301	HEC	CMD-C2D-C3D	2.05	128.81	124.94
37	c1	501	HEA	C4D-CHA-C1A	2.04	125.25	122.56
31	Qc	402	HEM	CBA-CAA-C2A	-2.04	109.14	112.62
31	QC	401	HEM	CHB-C1B-C2B	-2.04	121.09	126.72
37	c1	501	HEA	OMA-CMA-C3A	-2.03	120.48	124.91
31	Qc	401	HEM	O2A-CGA-CBA	2.02	120.51	114.03
37	C1	502	HEA	CHC-C4B-NB	-2.00	121.91	124.38

There are no chirality outliers.

All (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
32	QH	101	CDL	CA2-OA2-PA1-OA4
32	QH	101	CDL	CA2-OA2-PA1-OA5
32	QJ	202	CDL	CB2-OB2-PB2-OB4
32	QJ	202	CDL	CB2-OB2-PB2-OB5
32	Qc	404	CDL	CA3-OA5-PA1-OA4
32	Qd	302	CDL	CA2-OA2-PA1-OA3
32	Qd	302	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
32	Qd	302	CDL	CA3-OA5-PA1-OA3
32	Qd	302	CDL	CA3-OA5-PA1-OA4
32	Qd	302	CDL	CB2-OB2-PB2-OB3
32	Qh	102	CDL	CA2-OA2-PA1-OA4
32	Qh	102	CDL	CB2-OB2-PB2-OB3
32	Qj	202	CDL	CA2-OA2-PA1-OA4
32	Qj	202	CDL	CB2-OB2-PB2-OB3
32	Qj	202	CDL	CB3-OB5-PB2-OB4
32	4c	201	CDL	CA2-OA2-PA1-OA3
32	4c	201	CDL	CA2-OA2-PA1-OA4
32	4c	201	CDL	CA3-OA5-PA1-OA4
32	4c	201	CDL	CA4-CA3-OA5-PA1
32	4c	201	CDL	CB2-OB2-PB2-OB3
32	4c	201	CDL	CB2-OB2-PB2-OB4
32	4c	201	CDL	CB2-OB2-PB2-OB5
32	4c	201	CDL	OB5-CB3-CB4-OB6
32	4e	202	CDL	CA2-OA2-PA1-OA4
32	4e	202	CDL	CB3-OB5-PB2-OB4
32	7c	201	CDL	CA2-OA2-PA1-OA3
32	7c	201	CDL	CA2-OA2-PA1-OA4
32	7c	201	CDL	CA2-OA2-PA1-OA5
32	7c	201	CDL	CB3-OB5-PB2-OB4
32	4E	202	CDL	CA2-OA2-PA1-OA3
32	4E	202	CDL	CA2-OA2-PA1-OA4
32	4E	202	CDL	CB3-OB5-PB2-OB3
32	QE	302	CDL	CA2-OA2-PA1-OA3
32	QE	302	CDL	CA2-OA2-PA1-OA4
32	QE	302	CDL	CA2-OA2-PA1-OA5
32	QE	302	CDL	CB2-OB2-PB2-OB3
32	QE	302	CDL	CB2-OB2-PB2-OB5
32	QE	302	CDL	CB3-OB5-PB2-OB3
34	QD	303	PC1	C1-O11-P-O14
34	QD	303	PC1	C1-O11-P-O13
34	Qc	403	PC1	C11-O13-P-O12
34	Qc	403	PC1	C11-O13-P-O14
34	Qc	403	PC1	C11-O13-P-O11
34	Qd	303	PC1	C1-O11-P-O12
34	Qd	303	PC1	C1-O11-P-O14
34	Qj	201	PC1	C1-O11-P-O12
34	Qj	201	PC1	C1-O11-P-O14
34	Qj	201	PC1	C1-O11-P-O13
34	4a	301	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
34	4a	301	PC1	C1-O11-P-O14
34	7c	202	PC1	C11-O13-P-O12
34	7c	202	PC1	C11-O13-P-O14
34	7c	202	PC1	C1-O11-P-O13
34	c1	505	PC1	C11-O13-P-O12
34	c1	505	PC1	C11-O13-P-O14
34	c1	505	PC1	C1-O11-P-O14
34	c1	505	PC1	O21-C2-C3-O31
34	c1	508	PC1	C11-O13-P-O12
34	c3	201	PC1	C11-O13-P-O14
34	c3	201	PC1	C1-O11-P-O13
34	4A	301	PC1	C11-O13-P-O12
34	4A	301	PC1	C1-O11-P-O14
34	4A	302	PC1	O21-C2-C3-O31
34	C1	505	PC1	C1-O11-P-O12
34	C1	509	PC1	C11-O13-P-O12
34	C3	201	PC1	C11-O13-P-O14
34	DC	201	PC1	C11-O13-P-O14
34	DC	201	PC1	C1-O11-P-O12
34	DC	201	PC1	O13-C11-C12-N
34	QE	303	PC1	C11-O13-P-O14
34	QE	303	PC1	C1-O11-P-O12
34	Qe	301	PC1	C11-O13-P-O11
34	Qe	302	PC1	C11-O13-P-O12
34	Qg	301	PC1	C1-O11-P-O12
34	Qg	301	PC1	C1-O11-P-O14
35	QD	304	PX2	C1-O4-P1-O1
35	QD	304	PX2	C1-O4-P1-O2
35	QD	304	PX2	C1-O4-P1-O3
35	QJ	201	PX2	C1-O4-P1-O1
35	QJ	201	PX2	C1-O4-P1-O2
35	QJ	201	PX2	C1-O4-P1-O3
35	4C	201	PX2	C1-O4-P1-O1
35	4C	201	PX2	C1-O4-P1-O2
36	4a	302	3PE	C1-O11-P-O12
36	4a	302	3PE	C1-O11-P-O14
36	4a	302	3PE	C11-O13-P-O12
36	4a	302	3PE	O13-C11-C12-N
36	c1	506	3PE	O13-C11-C12-N
36	c1	507	3PE	C1-O11-P-O13
36	c1	507	3PE	C11-O13-P-O12
36	c1	507	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
36	C1	507	3PE	C1-O11-P-O13
36	C1	507	3PE	C2-C1-O11-P
36	C1	507	3PE	C12-C11-O13-P
36	C1	507	3PE	O13-C11-C12-N
36	C1	508	3PE	C1-O11-P-O14
36	C1	508	3PE	C11-O13-P-O14
36	4D	201	3PE	C11-O13-P-O14
36	4F	101	3PE	O13-C11-C12-N
36	4d	201	3PE	C11-O13-P-O14
36	4d	202	3PE	O13-C11-C12-N
36	7A	201	3PE	C1-O11-P-O12
36	7A	201	3PE	C11-O13-P-O12
36	7A	201	3PE	O13-C11-C12-N
37	c1	501	HEA	C1A-C2A-CAA-CBA
37	c1	501	HEA	C3A-C2A-CAA-CBA
37	c1	501	HEA	C17-C18-C19-C27
37	c1	501	HEA	C19-C20-C21-C22
37	c1	502	HEA	C1A-C2A-CAA-CBA
37	c1	502	HEA	C3A-C2A-CAA-CBA
37	c1	502	HEA	C3B-C11-C12-C13
37	c1	502	HEA	O11-C11-C12-C13
37	c1	502	HEA	C13-C14-C15-C16
37	c1	502	HEA	C13-C14-C15-C26
37	c1	502	HEA	C17-C18-C19-C27
37	c1	502	HEA	C27-C19-C20-C21
37	C1	501	HEA	C1A-C2A-CAA-CBA
37	C1	501	HEA	C3A-C2A-CAA-CBA
37	C1	501	HEA	C17-C18-C19-C27
37	C1	502	HEA	C3A-C2A-CAA-CBA
37	C1	502	HEA	C3B-C11-C12-C13
37	C1	502	HEA	O11-C11-C12-C13
37	C1	502	HEA	C13-C14-C15-C16
37	C1	502	HEA	C13-C14-C15-C26
37	C1	502	HEA	C15-C16-C17-C18
37	C1	502	HEA	C17-C18-C19-C20
37	C1	502	HEA	C19-C20-C21-C22
42	4F	102	S12	O-C-CA-CB
42	4F	102	S12	OXT-C-CA-CB
42	4F	102	S12	O11-C3-C4-O52
42	4d	203	S12	C2-O2-P-OG
42	4d	203	S12	C2-O2-P-O3
42	4d	203	S12	C2-O2-P-O4

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Mol	Chain	Res	Type	Atoms
42	4d	203	S12	CA-CB-OG-P
42	4d	203	S12	O11-C3-C4-O52
42	4d	203	S12	N-CA-CB-OG
37	c1	502	HEA	C21-C22-C23-C24
37	C1	502	HEA	C17-C18-C19-C27
42	4F	102	S12	OXT-C-CA-N
42	4d	203	S12	OXT-C-CA-N
37	c1	501	HEA	C17-C18-C19-C20
37	C1	501	HEA	C17-C18-C19-C20
32	7c	201	CDL	O1-C1-CA2-OA2
35	QD	304	PX2	C16-C17-C18-C19
37	c1	502	HEA	C21-C22-C23-C25
36	4a	302	3PE	C37-C38-C39-C3A
36	4F	101	3PE	C39-C3A-C3B-C3C
32	QE	302	CDL	C1-CB2-OB2-PB2
37	c1	502	HEA	C15-C16-C17-C18
37	c1	502	HEA	C19-C20-C21-C22
36	4F	101	3PE	C28-C29-C2A-C2B
32	C1	506	CDL	C13-C14-C15-C16
34	7c	202	PC1	C33-C34-C35-C36
32	QD	302	CDL	OA6-CA4-CA6-OA8
34	7c	202	PC1	C39-C3A-C3B-C3C
35	QJ	201	PX2	C5-C4-O5-C3
31	QC	401	HEM	C2A-CAA-CBA-CGA
31	Qc	401	HEM	C2A-CAA-CBA-CGA
34	c3	201	PC1	C31-C32-C33-C34
42	4F	102	S12	C5-C6-C7-C8
32	QC	403	CDL	CA5-C11-C12-C13
35	QJ	201	PX2	C4-C5-C6-C7
34	DC	201	PC1	C32-C33-C34-C35
34	4a	301	PC1	C11-C12-N-C13
34	4A	302	PC1	C11-C12-N-C14
32	7c	201	CDL	CB5-C51-C52-C53
34	c1	505	PC1	C24-C25-C26-C27
37	C1	501	HEA	C19-C20-C21-C22
32	QD	302	CDL	CA2-OA2-PA1-OA5
32	QD	302	CDL	CA3-OA5-PA1-OA2
32	QD	302	CDL	CB3-OB5-PB2-OB2
32	Qd	302	CDL	CA2-OA2-PA1-OA5
32	Qd	302	CDL	CB2-OB2-PB2-OB5
32	Qh	101	CDL	CA3-OA5-PA1-OA2
32	Qh	101	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
32	Qh	102	CDL	CA2-OA2-PA1-OA5
32	Qj	202	CDL	CB3-OB5-PB2-OB2
32	4c	201	CDL	CA2-OA2-PA1-OA5
32	4c	201	CDL	CA3-OA5-PA1-OA2
32	4e	202	CDL	CA2-OA2-PA1-OA5
32	4e	202	CDL	CB3-OB5-PB2-OB2
32	7c	201	CDL	CB3-OB5-PB2-OB2
32	4E	202	CDL	CA2-OA2-PA1-OA5
32	4E	202	CDL	CB2-OB2-PB2-OB5
32	4E	202	CDL	CB3-OB5-PB2-OB2
32	QE	302	CDL	CB3-OB5-PB2-OB2
34	QD	303	PC1	C11-O13-P-O11
34	Qc	403	PC1	C1-O11-P-O13
34	Qd	303	PC1	C1-O11-P-O13
34	4a	301	PC1	C11-O13-P-O11
34	4a	301	PC1	C1-O11-P-O13
34	4e	201	PC1	C1-O11-P-O13
34	7c	202	PC1	C11-O13-P-O11
34	c1	505	PC1	C11-O13-P-O11
34	c1	508	PC1	C11-O13-P-O11
34	C1	505	PC1	C11-O13-P-O11
34	C1	505	PC1	C1-O11-P-O13
34	C1	509	PC1	C11-O13-P-O11
34	C3	201	PC1	C11-O13-P-O11
34	DC	201	PC1	C1-O11-P-O13
34	Qe	301	PC1	C1-O11-P-O13
34	Qe	302	PC1	C11-O13-P-O11
34	Qe	304	PC1	C1-O11-P-O13
34	Qg	301	PC1	C1-O11-P-O13
36	4a	302	3PE	C1-O11-P-O13
36	4a	302	3PE	C11-O13-P-O11
36	c1	506	3PE	C11-O13-P-O11
36	c1	507	3PE	C11-O13-P-O11
36	C1	507	3PE	C11-O13-P-O11
36	4D	201	3PE	C11-O13-P-O11
36	7a	201	3PE	C11-O13-P-O11
36	4d	202	3PE	C11-O13-P-O11
36	7A	201	3PE	C11-O13-P-O11
42	4F	102	S12	C2-O2-P-OG
32	C1	506	CDL	CA7-C31-C32-C33
34	Qc	403	PC1	C11-C12-N-C14
34	Qc	403	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
34	DC	201	PC1	C11-C12-N-C13
34	DC	201	PC1	C11-C12-N-C15
34	Qe	301	PC1	C11-C12-N-C13
34	Qe	301	PC1	C11-C12-N-C14
34	Qe	301	PC1	C11-C12-N-C15
34	DC	201	PC1	C35-C36-C37-C38
34	DC	201	PC1	C2D-C2E-C2F-C2G
35	QD	304	PX2	C18-C19-C20-C21
35	QJ	201	PX2	C6-C7-C8-C9
36	4F	101	3PE	C2E-C2F-C2G-C2H
36	4d	202	3PE	C32-C33-C34-C35
36	4d	202	3PE	C28-C29-C2A-C2B
42	4d	203	S12	C11-C10-C9-C8
42	4d	203	S12	C15-C16-C17-C18
32	Qd	302	CDL	C22-C23-C24-C25
35	QJ	201	PX2	C17-C18-C19-C20
36	4a	302	3PE	C33-C34-C35-C36
36	4a	302	3PE	C34-C35-C36-C37
36	4a	302	3PE	C39-C3A-C3B-C3C
36	4d	202	3PE	C27-C28-C29-C2A
35	QD	304	PX2	C11-C12-C13-C14
34	Qc	403	PC1	C2-C1-O11-P
35	QJ	201	PX2	O6-C4-O5-C3
34	C3	201	PC1	C33-C34-C35-C36
42	4F	102	S12	C15-C16-C17-C18
32	QH	101	CDL	O1-C1-CB2-OB2
35	4C	201	PX2	C22-C23-C24-C25
32	QE	302	CDL	C51-C52-C53-C54
34	7c	202	PC1	C34-C35-C36-C37
36	4a	302	3PE	C28-C29-C2A-C2B
37	c1	501	HEA	C27-C19-C20-C21
32	Qd	302	CDL	C17-C18-C19-C20
32	4e	202	CDL	C56-C57-C58-C59
34	7c	202	PC1	C35-C36-C37-C38
35	4C	201	PX2	C16-C17-C18-C19
32	4E	202	CDL	C56-C57-C58-C59
34	DC	201	PC1	C3B-C3C-C3D-C3E
32	Qd	302	CDL	C76-C77-C78-C79
36	c1	506	3PE	C33-C34-C35-C36
32	Qd	302	CDL	C21-C22-C23-C24
34	C1	505	PC1	C22-C23-C24-C25
34	DC	201	PC1	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
35	QJ	201	PX2	C9-C10-C11-C12
42	4F	102	S12	C10-C11-C12-C13
34	4E	201	PC1	C31-C32-C33-C34
34	C1	505	PC1	C21-C22-C23-C24
34	Qe	302	PC1	C2A-C2B-C2C-C2D
35	4C	201	PX2	C10-C11-C12-C13
34	Qc	403	PC1	C11-C12-N-C13
34	4a	301	PC1	C11-C12-N-C15
34	4A	302	PC1	C11-C12-N-C15
34	DC	201	PC1	C11-C12-N-C14
37	c1	501	HEA	C15-C16-C17-C18
34	4a	301	PC1	C28-C29-C2A-C2B
36	4a	302	3PE	C27-C28-C29-C2A
32	Qd	302	CDL	C58-C59-C60-C61
36	4F	101	3PE	C21-C22-C23-C24
36	4d	202	3PE	C31-C32-C33-C34
34	C1	505	PC1	C37-C38-C39-C3A
36	4F	101	3PE	C2B-C2C-C2D-C2E
36	4F	101	3PE	C2C-C2D-C2E-C2F
32	4E	202	CDL	C31-C32-C33-C34
35	QJ	201	PX2	C18-C19-C20-C21
35	4C	201	PX2	C19-C20-C21-C22
36	C1	507	3PE	C33-C34-C35-C36
32	Qh	101	CDL	C52-C53-C54-C55
32	4e	202	CDL	C31-C32-C33-C34
32	7c	201	CDL	C43-C44-C45-C46
34	c1	508	PC1	C23-C24-C25-C26
34	Qj	201	PC1	C1-C2-C3-O31
35	QD	304	PX2	C9-C10-C11-C12
36	4d	202	3PE	C24-C25-C26-C27
34	c1	505	PC1	C26-C27-C28-C29
34	DC	201	PC1	C23-C24-C25-C26
32	7c	201	CDL	C12-C13-C14-C15
32	C1	506	CDL	O1-C1-CB2-OB2
32	7c	201	CDL	CB2-C1-CA2-OA2
36	4d	202	3PE	C33-C34-C35-C36
32	4c	201	CDL	C36-C37-C38-C39
34	C1	505	PC1	C3B-C3C-C3D-C3E
34	Qe	301	PC1	C3D-C3E-C3F-C3G
34	7c	202	PC1	C11-C12-N-C13
34	4A	302	PC1	C11-C12-N-C13
34	Qe	302	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
34	Qe	304	PC1	C11-C12-N-C15
32	QH	101	CDL	CB7-C71-C72-C73
32	C1	506	CDL	C34-C35-C36-C37
34	7c	202	PC1	C3D-C3E-C3F-C3G
32	7c	201	CDL	C39-C40-C41-C42
42	4d	203	S12	C6-C5-O52-C4
36	c1	506	3PE	C35-C36-C37-C38
34	4A	301	PC1	C27-C28-C29-C2A
34	DC	201	PC1	C26-C27-C28-C29
34	c1	505	PC1	C3C-C3D-C3E-C3F
34	DC	201	PC1	C27-C28-C29-C2A
36	4F	101	3PE	C33-C34-C35-C36
36	4d	202	3PE	C39-C3A-C3B-C3C
42	4d	203	S12	C-CA-CB-OG
34	Qe	301	PC1	C33-C34-C35-C36
32	QH	101	CDL	CA5-C11-C12-C13
32	Qc	404	CDL	C53-C54-C55-C56
42	4F	102	S12	C7-C8-C9-C10
36	4F	101	3PE	O21-C2-C3-O31
36	c1	506	3PE	C25-C26-C27-C28
36	4d	202	3PE	C2D-C2E-C2F-C2G
42	4d	203	S12	C7-C8-C9-C10
34	4a	301	PC1	C11-C12-N-C14
32	Qc	404	CDL	C11-C12-C13-C14
34	4a	301	PC1	C25-C26-C27-C28
34	C3	201	PC1	C3D-C3E-C3F-C3G
35	QD	304	PX2	C7-C8-C9-C10
36	4F	101	3PE	C24-C25-C26-C27
32	QC	403	CDL	CA2-OA2-PA1-OA5
32	QJ	202	CDL	CA2-OA2-PA1-OA5
32	4e	202	CDL	CB2-OB2-PB2-OB5
34	c1	505	PC1	C1-O11-P-O13
34	c3	201	PC1	C11-O13-P-O11
36	C1	508	3PE	C1-O11-P-O13
36	4d	201	3PE	C11-O13-P-O11
36	4a	302	3PE	C23-C24-C25-C26
36	7a	201	3PE	C3A-C3B-C3C-C3D
32	QH	101	CDL	OB5-CB3-CB4-CB6
32	4c	201	CDL	OA5-CA3-CA4-CA6
32	4c	201	CDL	OB5-CB3-CB4-CB6
35	4C	201	PX2	C11-C12-C13-C14
42	4F	102	S12	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
36	4a	302	3PE	C25-C26-C27-C28
42	4F	102	S12	C9-C10-C11-C12
34	QE	303	PC1	C32-C33-C34-C35
42	4d	203	S12	O51-C5-O52-C4
32	Qh	101	CDL	CA3-CA4-CA6-OA8
34	c1	505	PC1	C1-C2-C3-O31
34	Qe	301	PC1	C1-C2-C3-O31
36	4a	302	3PE	C1-C2-C3-O31
34	4E	201	PC1	C24-C25-C26-C27
35	QJ	201	PX2	C24-C25-C26-C27
34	C3	201	PC1	C22-C23-C24-C25
36	c1	506	3PE	O31-C31-C32-C33
36	c1	507	3PE	C31-C32-C33-C34
35	4C	201	PX2	C17-C18-C19-C20
34	DC	201	PC1	C1-C2-O21-C21
34	C1	505	PC1	O11-C1-C2-O21
34	C1	509	PC1	O11-C1-C2-O21
36	c1	506	3PE	O11-C1-C2-O21
36	4F	101	3PE	O11-C1-C2-O21
34	C1	505	PC1	C28-C29-C2A-C2B
42	4d	203	S12	C18-C19-C20-C21
42	4F	102	S12	C19-C20-C21-C22
36	C1	507	3PE	C3A-C3B-C3C-C3D
32	4c	201	CDL	C72-C71-CB7-OB8
34	c3	201	PC1	C26-C27-C28-C29
37	C1	501	HEA	C27-C19-C20-C21
42	4d	203	S12	C16-C17-C18-C19
37	c1	501	HEA	C18-C19-C20-C21
34	C3	201	PC1	C3A-C3B-C3C-C3D
36	4d	202	3PE	C2C-C2D-C2E-C2F
35	4C	201	PX2	C5-C4-O5-C3
34	7c	202	PC1	C23-C24-C25-C26
42	4d	203	S12	O2-C2-C3-C4
32	4E	202	CDL	C62-C63-C64-C65
36	C1	507	3PE	C26-C27-C28-C29
36	C1	507	3PE	C32-C33-C34-C35
34	7c	202	PC1	C11-C12-N-C15
34	Qe	302	PC1	C11-C12-N-C15
34	Qe	304	PC1	C11-C12-N-C13
32	QH	101	CDL	OA5-CA3-CA4-CA6
32	Qh	102	CDL	OB5-CB3-CB4-CB6
36	4F	101	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
37	C1	501	HEA	C15-C16-C17-C18
34	7c	202	PC1	C3A-C3B-C3C-C3D
34	DC	201	PC1	C2F-C2G-C2H-C2I
36	C1	507	3PE	C31-C32-C33-C34
42	4F	102	S12	C16-C17-C18-C19
32	QJ	202	CDL	CA4-CA3-OA5-PA1
32	C1	506	CDL	CA4-CA3-OA5-PA1
42	4d	203	S12	C11-C12-C13-C14
36	4a	302	3PE	C24-C25-C26-C27
34	c3	201	PC1	C27-C28-C29-C2A
34	DC	201	PC1	C39-C3A-C3B-C3C
32	QD	302	CDL	CA3-CA4-CA6-OA8
32	Qh	101	CDL	CB3-CB4-CB6-OB8
32	Qh	102	CDL	CB3-CB4-CB6-OB8
32	4e	202	CDL	CB3-CB4-CB6-OB8
32	4E	202	CDL	CB3-CB4-CB6-OB8
32	QE	302	CDL	CA3-CA4-CA6-OA8
36	c1	506	3PE	C1-C2-C3-O31
32	C1	506	CDL	C39-C40-C41-C42
34	c3	201	PC1	C24-C25-C26-C27
36	4F	101	3PE	C3A-C3B-C3C-C3D
42	4d	203	S12	C2-C3-C4-O52
36	7a	201	3PE	C31-C32-C33-C34
32	C1	506	CDL	C11-C12-C13-C14
34	4A	302	PC1	C27-C28-C29-C2A
36	7a	201	3PE	C33-C34-C35-C36
34	7c	202	PC1	C2F-C2G-C2H-C2I
32	Qc	404	CDL	CA3-OA5-PA1-OA2
32	Qh	102	CDL	CA3-OA5-PA1-OA2
32	QE	302	CDL	CA3-OA5-PA1-OA2
34	Qj	201	PC1	C11-O13-P-O11
34	4A	301	PC1	C1-O11-P-O13
36	C1	508	3PE	C11-O13-P-O11
37	C1	502	HEA	C21-C22-C23-C24
32	QH	101	CDL	OB5-CB3-CB4-OB6
32	4c	201	CDL	OA5-CA3-CA4-OA6
36	C1	507	3PE	O11-C1-C2-O21
35	4C	201	PX2	O6-C4-O5-C3
36	c1	506	3PE	C3A-C3B-C3C-C3D
32	Qh	101	CDL	OA6-CA4-CA6-OA8
32	4e	202	CDL	OA6-CA4-CA6-OA8
32	4E	202	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
32	QE	302	CDL	OB6-CB4-CB6-OB8
36	4a	302	3PE	O21-C2-C3-O31
32	QE	302	CDL	CA2-C1-CB2-OB2
42	4F	102	S12	O-C-CA-N
42	4d	203	S12	O-C-CA-N
32	Qc	404	CDL	CA4-CA3-OA5-PA1
34	QD	303	PC1	C2-C1-O11-P
36	7a	201	3PE	C2-C1-O11-P
36	4d	202	3PE	C2B-C2C-C2D-C2E
36	c1	507	3PE	C2B-C2C-C2D-C2E
32	4E	202	CDL	C33-C34-C35-C36
35	QJ	201	PX2	O4-C1-C2-C3
36	c1	507	3PE	O11-C1-C2-C3
36	C1	507	3PE	O11-C1-C2-C3
32	QJ	202	CDL	C32-C33-C34-C35
32	4e	202	CDL	C64-C65-C66-C67
36	4d	202	3PE	C3D-C3E-C3F-C3G
36	4F	101	3PE	C3D-C3E-C3F-C3G
34	DC	201	PC1	C37-C38-C39-C3A
36	4F	101	3PE	C35-C36-C37-C38
34	7c	202	PC1	C27-C28-C29-C2A
36	c1	506	3PE	C3-C2-O21-C21
32	4e	202	CDL	C33-C34-C35-C36
32	4e	202	CDL	C62-C63-C64-C65
32	Qh	102	CDL	C1-CB2-OB2-PB2
32	QE	302	CDL	CB3-CB4-CB6-OB8
34	4A	302	PC1	C1-C2-C3-O31
34	Qe	301	PC1	C2-C1-O11-P
36	c1	506	3PE	C2-C1-O11-P
35	4C	201	PX2	C18-C19-C20-C21
32	QC	403	CDL	OB5-CB3-CB4-OB6
32	QD	302	CDL	OB5-CB3-CB4-OB6
32	Qh	102	CDL	OB5-CB3-CB4-OB6
35	QJ	201	PX2	O4-C1-C2-O7
36	4d	202	3PE	C3E-C3F-C3G-C3H
32	Qc	404	CDL	OA6-CA4-CA6-OA8
32	Qh	101	CDL	OB6-CB4-CB6-OB8
32	Qh	102	CDL	OB6-CB4-CB6-OB8
32	4e	202	CDL	OB6-CB4-CB6-OB8
32	QE	302	CDL	OA6-CA4-CA6-OA8
34	Qe	301	PC1	O21-C2-C3-O31
36	4D	201	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
36	4F	101	3PE	C2D-C2E-C2F-C2G
34	7c	202	PC1	C2C-C2D-C2E-C2F
32	4e	202	CDL	C51-C52-C53-C54
32	4E	202	CDL	C64-C65-C66-C67
32	QJ	202	CDL	CA3-OA5-PA1-OA2
32	Qd	302	CDL	CB3-OB5-PB2-OB2
32	Qj	202	CDL	CB2-OB2-PB2-OB5
34	C3	201	PC1	C1-O11-P-O13
34	QE	303	PC1	C1-O11-P-O13
36	4F	101	3PE	C1-O11-P-O13
34	7c	202	PC1	C38-C39-C3A-C3B
34	DC	201	PC1	C24-C25-C26-C27
32	Qh	102	CDL	C1-CA2-OA2-PA1
32	4c	201	CDL	C1-CB2-OB2-PB2
32	4e	202	CDL	CA4-CA3-OA5-PA1
32	4E	202	CDL	C1-CB2-OB2-PB2
34	c1	505	PC1	C2-C1-O11-P
32	4E	202	CDL	C71-C72-C73-C74
32	QC	403	CDL	CA2-OA2-PA1-OA4
32	QD	302	CDL	CA2-OA2-PA1-OA3
32	QD	302	CDL	CA2-OA2-PA1-OA4
32	QD	302	CDL	CA3-OA5-PA1-OA3
32	QJ	202	CDL	CB2-OB2-PB2-OB3
32	Qc	404	CDL	CA3-OA5-PA1-OA3
32	Qd	302	CDL	CA2-OA2-PA1-OA4
32	Qd	302	CDL	CB2-OB2-PB2-OB4
32	Qh	101	CDL	CA3-OA5-PA1-OA3
32	Qh	101	CDL	CB3-OB5-PB2-OB3
32	Qj	202	CDL	CA2-OA2-PA1-OA3
32	Qj	202	CDL	CB2-OB2-PB2-OB4
32	4e	202	CDL	CA2-OA2-PA1-OA3
32	4e	202	CDL	CB2-OB2-PB2-OB3
32	4e	202	CDL	CB2-OB2-PB2-OB4
32	4E	202	CDL	CB2-OB2-PB2-OB3
32	4E	202	CDL	CB2-OB2-PB2-OB4
32	4E	202	CDL	CB3-OB5-PB2-OB4
34	QD	303	PC1	C11-O13-P-O12
34	QD	303	PC1	C11-O13-P-O14
34	Qc	403	PC1	C1-O11-P-O14
34	4e	201	PC1	C1-O11-P-O14
34	7c	202	PC1	C1-O11-P-O12
34	c1	505	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
34	c3	201	PC1	C11-O13-P-O12
34	c3	201	PC1	C1-O11-P-O12
34	C1	505	PC1	C11-O13-P-O12
34	C1	505	PC1	C11-O13-P-O14
34	C3	201	PC1	C11-O13-P-O12
34	QE	303	PC1	C1-O11-P-O14
34	Qe	301	PC1	C11-O13-P-O12
34	Qe	301	PC1	C1-O11-P-O14
34	Qe	304	PC1	C1-O11-P-O12
34	Qe	304	PC1	C11-C12-N-C14
36	c1	506	3PE	C11-O13-P-O14
36	c1	507	3PE	C1-O11-P-O12
36	C1	507	3PE	C1-O11-P-O12
36	C1	507	3PE	C11-O13-P-O14
36	C1	508	3PE	C1-O11-P-O12
36	4D	201	3PE	C11-O13-P-O12
36	7a	201	3PE	C11-O13-P-O12
36	7a	201	3PE	C11-O13-P-O14
36	4d	201	3PE	C11-O13-P-O12
36	4d	202	3PE	C11-O13-P-O14
36	7A	201	3PE	C11-O13-P-O14
42	4F	102	S12	C2-O2-P-O3
34	c3	201	PC1	C36-C37-C38-C39
32	QD	302	CDL	OB5-CB3-CB4-CB6
34	C1	505	PC1	O11-C1-C2-C3
36	4F	101	3PE	C25-C26-C27-C28
42	4F	102	S12	C2-C3-C4-O52
34	7c	202	PC1	C12-C11-O13-P
34	c1	508	PC1	C12-C11-O13-P
36	c1	506	3PE	C12-C11-O13-P
36	c1	507	3PE	C12-C11-O13-P
36	7a	201	3PE	C12-C11-O13-P
36	4d	201	3PE	C23-C24-C25-C26
34	7c	202	PC1	C2B-C2C-C2D-C2E
32	QH	101	CDL	OA5-CA3-CA4-OA6
32	QJ	202	CDL	OA5-CA3-CA4-OA6
32	QJ	202	CDL	OB5-CB3-CB4-OB6
34	QD	303	PC1	O11-C1-C2-O21
34	Qg	301	PC1	O11-C1-C2-O21
36	c1	507	3PE	O11-C1-C2-O21
34	QD	303	PC1	C22-C23-C24-C25
34	Qj	201	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
34	Qe	301	PC1	C31-C32-C33-C34
32	Qh	101	CDL	O1-C1-CA2-OA2
32	QD	302	CDL	C52-C53-C54-C55
36	4a	302	3PE	C38-C39-C3A-C3B
34	7c	202	PC1	C11-C12-N-C14
34	C3	201	PC1	C11-C12-N-C15
34	QE	303	PC1	C31-C32-C33-C34
32	Qc	404	CDL	CA3-CA4-CA6-OA8
34	QD	303	PC1	O13-C11-C12-N
34	4a	301	PC1	O13-C11-C12-N
34	7c	202	PC1	O13-C11-C12-N
34	c1	508	PC1	O13-C11-C12-N
34	4A	301	PC1	O13-C11-C12-N
34	4A	302	PC1	O13-C11-C12-N
34	C1	509	PC1	O13-C11-C12-N
34	Qe	301	PC1	O13-C11-C12-N
34	Qe	302	PC1	O13-C11-C12-N
36	4F	101	3PE	C1-C2-C3-O31
37	C1	502	HEA	C1A-C2A-CAA-CBA
34	Qj	201	PC1	O21-C2-C3-O31
36	c1	506	3PE	O21-C2-C3-O31
36	7A	201	3PE	C3C-C3D-C3E-C3F
34	c1	505	PC1	C25-C26-C27-C28
36	C1	507	3PE	C35-C36-C37-C38
32	QC	403	CDL	CB4-CB3-OB5-PB2
34	4a	301	PC1	C26-C27-C28-C29
37	C1	501	HEA	C18-C19-C20-C21
36	4a	302	3PE	C2E-C2F-C2G-C2H
34	c3	201	PC1	C3E-C3F-C3G-C3H
34	Qe	302	PC1	C11-C12-N-C13
34	DC	201	PC1	C25-C26-C27-C28
32	QD	302	CDL	CB6-CB4-OB6-CB5
32	4c	201	CDL	CB6-CB4-OB6-CB5
34	c3	201	PC1	C1-C2-O21-C21
34	C3	201	PC1	C3-C2-O21-C21
32	QJ	202	CDL	OA5-CA3-CA4-CA6
32	QJ	202	CDL	OB5-CB3-CB4-CB6
37	C1	501	HEA	C11-C12-C13-C14
32	4e	202	CDL	C71-C72-C73-C74
32	Qd	302	CDL	C40-C41-C42-C43
34	Qe	304	PC1	C21-C22-C23-C24
32	Qj	202	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
35	QD	304	PX2	C21-C22-C23-C24
36	4F	101	3PE	C37-C38-C39-C3A
31	Qc	401	HEM	C3D-CAD-CBD-CGD
35	QJ	201	PX2	C23-C24-C25-C26
32	4E	202	CDL	OA6-CA4-CA6-OA8
34	7c	202	PC1	O21-C2-C3-O31
32	QC	403	CDL	CB3-OB5-PB2-OB2
32	Qh	102	CDL	CB2-OB2-PB2-OB5
32	Qj	202	CDL	CA2-OA2-PA1-OA5
32	Qj	202	CDL	CA3-OA5-PA1-OA2
34	4A	302	PC1	C11-O13-P-O11
34	DC	201	PC1	C11-O13-P-O11
36	c1	506	3PE	C1-O11-P-O13
32	C1	506	CDL	C12-C13-C14-C15
35	QJ	201	PX2	C10-C11-C12-C13
34	4E	201	PC1	C1-C2-C3-O31
34	Qe	304	PC1	C31-C32-C33-C34
34	QD	303	PC1	C32-C33-C34-C35
32	Qd	302	CDL	C13-C14-C15-C16
32	QH	101	CDL	CA4-CA3-OA5-PA1
32	Qd	302	CDL	CA4-CA3-OA5-PA1
32	Qh	101	CDL	CA4-CA3-OA5-PA1
32	QE	302	CDL	C1-CA2-OA2-PA1
32	Qd	302	CDL	C42-C43-C44-C45
33	Qd	301	HEC	CAD-CBD-CGD-O1D
32	QD	302	CDL	CB4-CB6-OB8-CB7
32	QC	403	CDL	OB5-CB3-CB4-CB6
34	QD	303	PC1	C33-C34-C35-C36
34	DC	201	PC1	C22-C23-C24-C25
42	4F	102	S12	C14-C15-C16-C17
36	7A	201	3PE	C3A-C3B-C3C-C3D
36	c1	507	3PE	C32-C33-C34-C35
34	4E	201	PC1	O21-C2-C3-O31
36	4d	201	3PE	O21-C2-C3-O31
34	DC	201	PC1	C3F-C3G-C3H-C3I
36	4D	201	3PE	C23-C24-C25-C26
32	4e	202	CDL	C1-CB2-OB2-PB2
34	7c	202	PC1	C2-C1-O11-P
34	4A	301	PC1	C28-C29-C2A-C2B
34	Qe	302	PC1	C29-C2A-C2B-C2C
31	QC	401	HEM	CAD-CBD-CGD-O1D
32	7c	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
34	Qj	201	PC1	C2-C3-O31-C31
42	4F	102	S12	C6-C5-O52-C4
42	4d	203	S12	O-C-CA-CB
42	4d	203	S12	OXT-C-CA-CB
34	4A	301	PC1	C21-C22-C23-C24
36	4a	302	3PE	C32-C31-O31-C3
34	4A	302	PC1	C39-C3A-C3B-C3C
35	4C	201	PX2	C9-C10-C11-C12
32	Qh	101	CDL	CB2-C1-CA2-OA2
34	QE	303	PC1	C1-C2-C3-O31
35	QD	304	PX2	C1-C2-C3-O5
36	c1	506	3PE	O32-C31-C32-C33
31	Qc	401	HEM	CAD-CBD-CGD-O2D
34	DC	201	PC1	C29-C2A-C2B-C2C
32	7c	201	CDL	C53-C54-C55-C56
31	Qc	402	HEM	CAD-CBD-CGD-O1D
32	QC	403	CDL	CB6-CB4-OB6-CB5
32	QH	101	CDL	CB3-CB4-OB6-CB5
32	QJ	202	CDL	CB6-CB4-OB6-CB5
32	Qh	101	CDL	CB3-CB4-OB6-CB5
32	4c	201	CDL	CA3-CA4-OA6-CA5
32	7c	201	CDL	CA6-CA4-OA6-CA5
32	C1	506	CDL	CA6-CA4-OA6-CA5
32	C1	506	CDL	CB3-CB4-OB6-CB5
32	C1	506	CDL	CB6-CB4-OB6-CB5
34	QD	303	PC1	C1-C2-O21-C21
34	Qc	403	PC1	C3-C2-O21-C21
34	Qd	303	PC1	C1-C2-O21-C21
34	Qe	302	PC1	C1-C2-O21-C21
34	Qe	302	PC1	C3-C2-O21-C21
36	C1	507	3PE	C3-C2-O21-C21
34	C3	201	PC1	C11-C12-N-C13
31	Qc	401	HEM	CAD-CBD-CGD-O1D
31	QC	402	HEM	CAD-CBD-CGD-O1D
31	QC	402	HEM	CAD-CBD-CGD-O2D
31	Qc	402	HEM	CAD-CBD-CGD-O2D
37	C1	501	HEA	CAD-CBD-CGD-O1D
34	Qe	302	PC1	C33-C34-C35-C36
34	C1	509	PC1	O11-C1-C2-C3
36	c1	506	3PE	O11-C1-C2-C3
36	4a	302	3PE	C2D-C2E-C2F-C2G
37	c1	501	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	QD	302	CDL	C33-C34-C35-C36
34	QE	303	PC1	C21-C22-C23-C24
42	4d	203	S12	O2-C2-C3-O11
34	4A	302	PC1	C25-C26-C27-C28
32	4c	201	CDL	C18-C19-C20-C21
42	4F	102	S12	O51-C5-O52-C4
34	C3	201	PC1	C11-C12-N-C14
33	Qd	301	HEC	CAD-CBD-CGD-O2D
34	C3	201	PC1	O21-C2-C3-O31
35	QD	304	PX2	O7-C2-C3-O5
32	4e	202	CDL	CA5-C11-C12-C13
32	7c	201	CDL	C32-C31-CA7-OA8
36	C1	507	3PE	O31-C31-C32-C33
32	QD	302	CDL	C36-C37-C38-C39
34	Qe	302	PC1	C3B-C3C-C3D-C3E
32	7c	201	CDL	C1-CA2-OA2-PA1
32	4E	202	CDL	CA4-CA3-OA5-PA1
34	C1	505	PC1	C33-C34-C35-C36
32	4c	201	CDL	C72-C71-CB7-OB9
34	c1	505	PC1	O21-C21-C22-C23
36	4d	202	3PE	C25-C26-C27-C28
32	QJ	202	CDL	C32-C31-CA7-OA8
31	QC	401	HEM	CAD-CBD-CGD-O2D
37	c1	501	HEA	CAD-CBD-CGD-O2D
32	Qd	302	CDL	C62-C63-C64-C65
34	QD	303	PC1	O11-C1-C2-C3
36	4d	202	3PE	C2A-C2B-C2C-C2D
34	C3	201	PC1	O31-C31-C32-C33
32	QH	101	CDL	OA6-CA4-CA6-OA8
32	C1	506	CDL	OA6-CA4-CA6-OA8
34	QD	303	PC1	O21-C2-C3-O31
34	4a	301	PC1	O21-C21-C22-C23
32	C1	506	CDL	C60-C61-C62-C63
33	QD	301	HEC	CAD-CBD-CGD-O1D
35	4C	201	PX2	C1-O4-P1-O3
32	Qc	404	CDL	C72-C71-CB7-OB8
31	QC	402	HEM	CAA-CBA-CGA-O2A
34	Qe	302	PC1	C38-C39-C3A-C3B
32	4e	202	CDL	C72-C73-C74-C75
36	4a	302	3PE	C2A-C2B-C2C-C2D
32	Qh	102	CDL	C12-C11-CA5-OA6
32	Qh	102	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
34	C1	509	PC1	O21-C21-C22-C23
36	C1	508	3PE	O21-C21-C22-C23
32	QC	403	CDL	CB3-CB4-OB6-CB5
32	7c	201	CDL	CA3-CA4-OA6-CA5
34	Qc	403	PC1	C1-C2-O21-C21
34	Qe	301	PC1	C1-C2-O21-C21
34	C1	509	PC1	C31-C32-C33-C34
37	C1	501	HEA	CAA-CBA-CGA-O2A
32	QD	302	CDL	C52-C51-CB5-OB6
32	QE	302	CDL	C32-C31-CA7-OA8
36	c1	507	3PE	O21-C21-C22-C23
34	Qe	301	PC1	C38-C39-C3A-C3B
31	Qc	402	HEM	CAA-CBA-CGA-O2A
34	Qc	403	PC1	C24-C25-C26-C27
32	Qd	302	CDL	OA5-CA3-CA4-OA6
35	QD	304	PX2	O4-C1-C2-O7
35	4C	201	PX2	O4-C1-C2-O7
34	Qd	303	PC1	O31-C31-C32-C33
34	c3	201	PC1	C32-C33-C34-C35
31	Qc	402	HEM	CAA-CBA-CGA-O1A
34	c3	201	PC1	C37-C38-C39-C3A
32	4E	202	CDL	C72-C73-C74-C75
32	C1	506	CDL	C12-C11-CA5-OA6
31	QC	402	HEM	CAA-CBA-CGA-O1A
37	C1	501	HEA	CAD-CBD-CGD-O2D
32	Qd	302	CDL	C52-C51-CB5-OB6
32	Qd	302	CDL	C77-C78-C79-C80
35	4C	201	PX2	O4-C1-C2-C3
35	QJ	201	PX2	C22-C23-C24-C25
32	4c	201	CDL	C52-C51-CB5-OB6
34	4A	302	PC1	O21-C21-C22-C23
32	QC	403	CDL	OB6-CB4-CB6-OB8
32	QD	302	CDL	OB6-CB4-CB6-OB8
32	7c	201	CDL	OA6-CA4-CA6-OA8
34	QE	303	PC1	O21-C2-C3-O31
34	DC	201	PC1	C28-C29-C2A-C2B
32	Qc	404	CDL	C32-C31-CA7-OA8
32	Qd	302	CDL	C72-C71-CB7-OB8
32	QE	302	CDL	C12-C11-CA5-OA6
34	Qe	302	PC1	O31-C31-C32-C33
32	4e	202	CDL	C60-C61-C62-C63
36	4F	101	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
34	4A	302	PC1	C23-C24-C25-C26
34	c1	505	PC1	C33-C34-C35-C36
32	QH	101	CDL	C12-C11-CA5-OA6
34	DC	201	PC1	O31-C31-C32-C33
42	4d	203	S12	C19-C20-C21-C22
34	4A	301	PC1	C36-C37-C38-C39
34	4A	301	PC1	O21-C21-C22-C23
33	QD	301	HEC	CAD-CBD-CGD-O2D
34	4a	301	PC1	O22-C21-C22-C23
36	4D	201	3PE	C24-C25-C26-C27
32	Qh	101	CDL	C32-C31-CA7-OA8
35	QJ	201	PX2	O5-C4-C5-C6
37	c1	502	HEA	C12-C13-C14-C15
34	4A	301	PC1	C2A-C2B-C2C-C2D
32	Qh	102	CDL	C12-C11-CA5-OA7
32	Qc	404	CDL	C32-C31-CA7-OA9
32	Qc	404	CDL	C72-C71-CB7-OB9
32	QE	302	CDL	C32-C31-CA7-OA9
32	QH	101	CDL	CA2-C1-CB2-OB2
34	7c	202	PC1	C3E-C3F-C3G-C3H
36	c1	506	3PE	C37-C38-C39-C3A
37	c1	501	HEA	CAA-CBA-CGA-O2A
32	4E	202	CDL	C61-C62-C63-C64
36	4d	202	3PE	C3F-C3G-C3H-C3I
32	Qd	302	CDL	C52-C51-CB5-OB7
34	QD	303	PC1	C1-C2-C3-O31
34	4e	201	PC1	C1-C2-C3-O31
34	QE	303	PC1	C11-O13-P-O11
34	Qd	303	PC1	O32-C31-C32-C33
36	c1	507	3PE	O22-C21-C22-C23
32	4c	201	CDL	C12-C13-C14-C15
32	QD	302	CDL	C12-C11-CA5-OA6
34	c3	201	PC1	O31-C31-C32-C33
32	C1	506	CDL	C38-C39-C40-C41
34	C3	201	PC1	O32-C31-C32-C33
32	QJ	202	CDL	CA2-OA2-PA1-OA3
32	Qh	101	CDL	CA2-OA2-PA1-OA3
32	Qj	202	CDL	CA3-OA5-PA1-OA3
32	C1	506	CDL	CB2-OB2-PB2-OB3
32	QE	302	CDL	CB3-OB5-PB2-OB4
34	4A	301	PC1	C11-O13-P-O14
34	4A	302	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
34	C1	509	PC1	C1-O11-P-O14
34	Qe	304	PC1	C11-O13-P-O14
34	Qg	301	PC1	C11-O13-P-O14
36	c1	506	3PE	C1-O11-P-O14
36	7A	201	3PE	C1-O11-P-O14
35	QJ	201	PX2	O6-C4-C5-C6
32	C1	506	CDL	CA5-C11-C12-C13
32	C1	506	CDL	C12-C11-CA5-OA7
34	Qe	302	PC1	O32-C31-C32-C33
32	QJ	202	CDL	C72-C71-CB7-OB8
36	c1	507	3PE	C29-C2A-C2B-C2C
35	QD	304	PX2	O7-C16-C17-C18
32	QD	302	CDL	C52-C51-CB5-OB7
32	QH	101	CDL	C12-C11-CA5-OA7
32	4E	202	CDL	C51-C52-C53-C54
32	QH	101	CDL	CB6-CB4-OB6-CB5
32	QJ	202	CDL	CB3-CB4-OB6-CB5
32	Qh	101	CDL	CB6-CB4-OB6-CB5
32	4c	201	CDL	CA6-CA4-OA6-CA5
32	C1	506	CDL	CA3-CA4-OA6-CA5
34	4a	301	PC1	C12-C11-O13-P
34	4A	302	PC1	C12-C11-O13-P
34	C3	201	PC1	C1-C2-O21-C21
34	DC	201	PC1	C12-C11-O13-P
34	Qe	301	PC1	C3-C2-O21-C21
37	C1	501	HEA	C3B-C11-C12-C13
36	4a	302	3PE	O32-C31-O31-C3
32	Qd	302	CDL	C72-C71-CB7-OB9
32	Qh	102	CDL	C32-C31-CA7-OA9
42	4d	203	S12	C17-C18-C19-C20
34	c1	508	PC1	O21-C21-C22-C23
32	Qd	302	CDL	C63-C64-C65-C66
35	QD	304	PX2	C12-C13-C14-C15
34	4A	301	PC1	O22-C21-C22-C23
36	4d	202	3PE	O31-C31-C32-C33
34	QD	303	PC1	C21-C22-C23-C24
42	4F	102	S12	C17-C18-C19-C20
36	7a	201	3PE	C39-C3A-C3B-C3C
32	QE	302	CDL	C52-C51-CB5-OB6
34	QD	303	PC1	O21-C21-C22-C23
32	QC	403	CDL	OA5-CA3-CA4-OA6
32	4E	202	CDL	OB5-CB3-CB4-OB6

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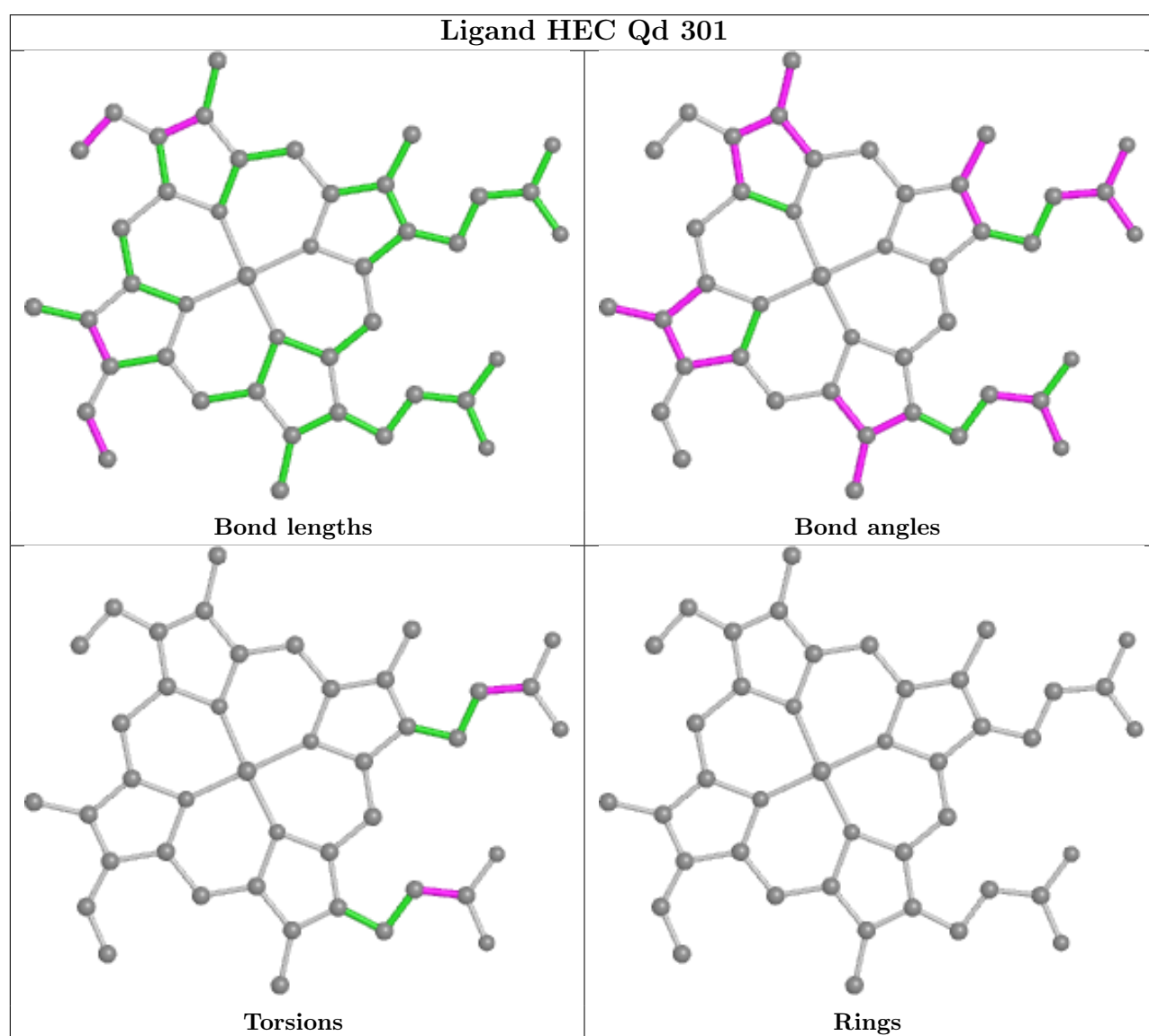
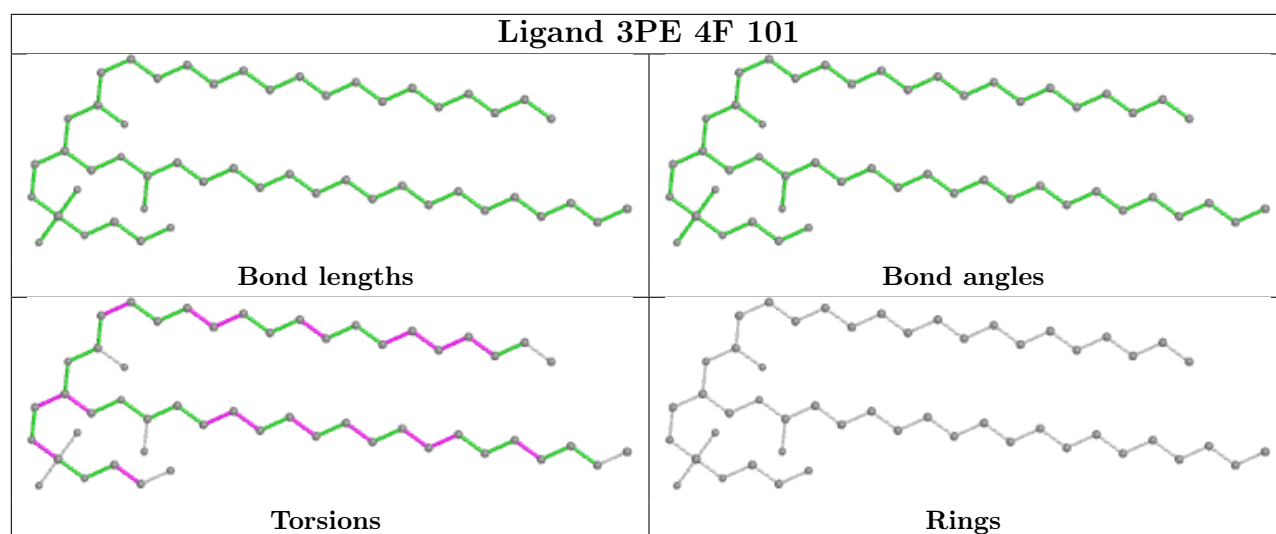
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Mol	Chain	Res	Type	Atoms
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32	Qh	101	CDL	C52-C51-CB5-OB6
32	4c	201	CDL	C12-C11-CA5-OA6
32	QD	302	CDL	C12-C11-CA5-OA7
32	Qh	101	CDL	C32-C31-CA7-OA9
34	7c	202	PC1	O21-C21-C22-C23
35	QD	304	PX2	C6-C7-C8-C9
34	c1	505	PC1	C21-C22-C23-C24
32	4c	201	CDL	C52-C51-CB5-OB7
32	QE	302	CDL	C12-C11-CA5-OA7
34	DC	201	PC1	O32-C31-C32-C33
32	QE	302	CDL	O1-C1-CB2-OB2
34	4E	201	PC1	O21-C21-C22-C23
32	QE	302	CDL	C52-C51-CB5-OB7
34	4A	302	PC1	O22-C21-C22-C23
33	Qd	301	HEC	CAA-CBA-CGA-O2A
32	Qd	302	CDL	C83-C84-C85-C86
32	QJ	202	CDL	C72-C71-CB7-OB9
35	4C	201	PX2	O7-C16-C17-C18

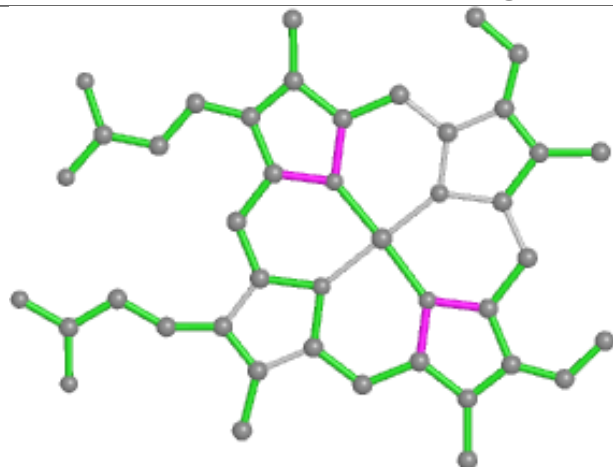
There are no ring outliers.

No monomer is involved in short contacts.

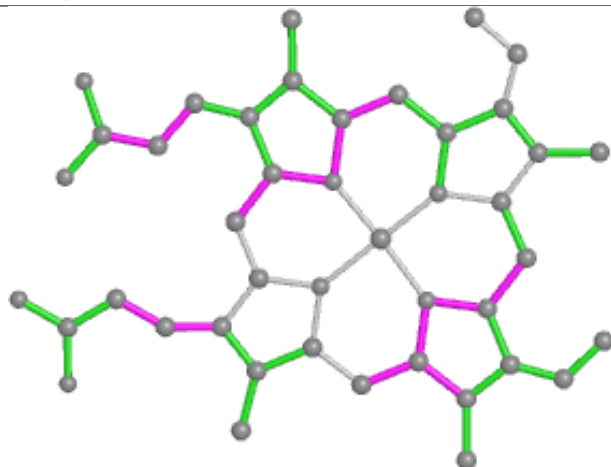
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



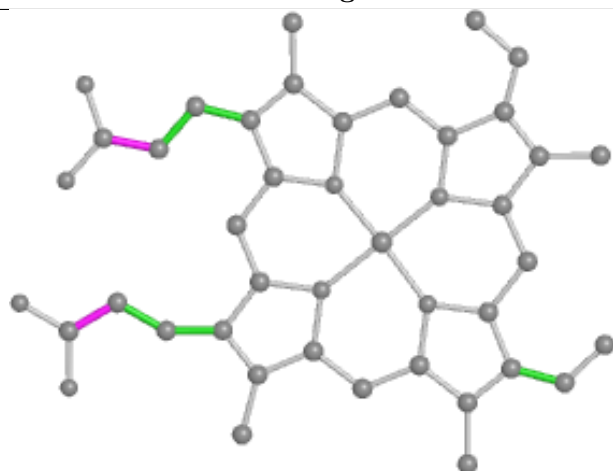
Ligand HEM Qc 402



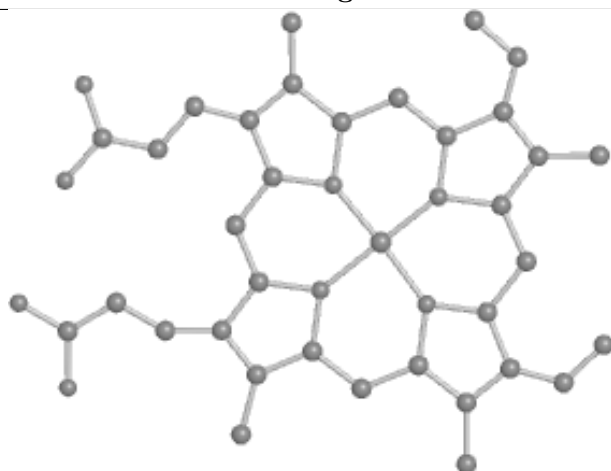
Bond lengths



Bond angles

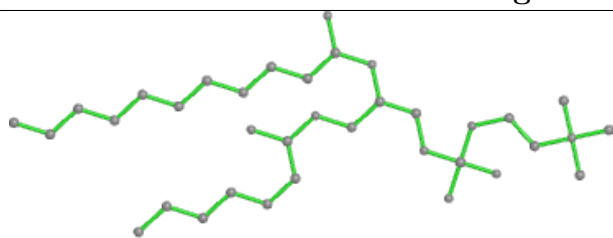


Torsions

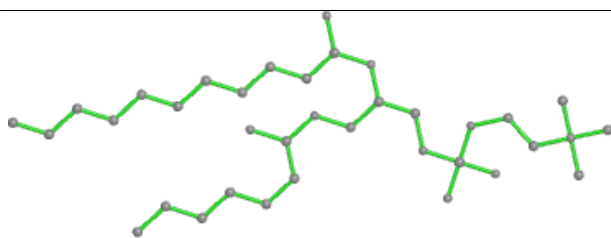


Rings

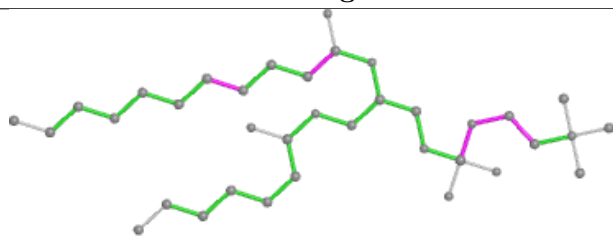
Ligand PC1 c1 508



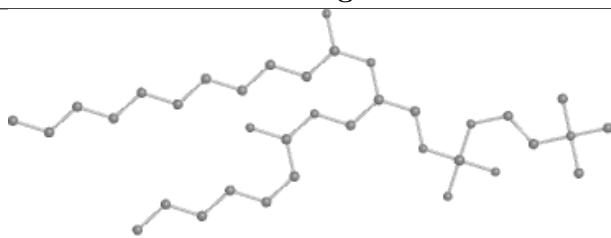
Bond lengths



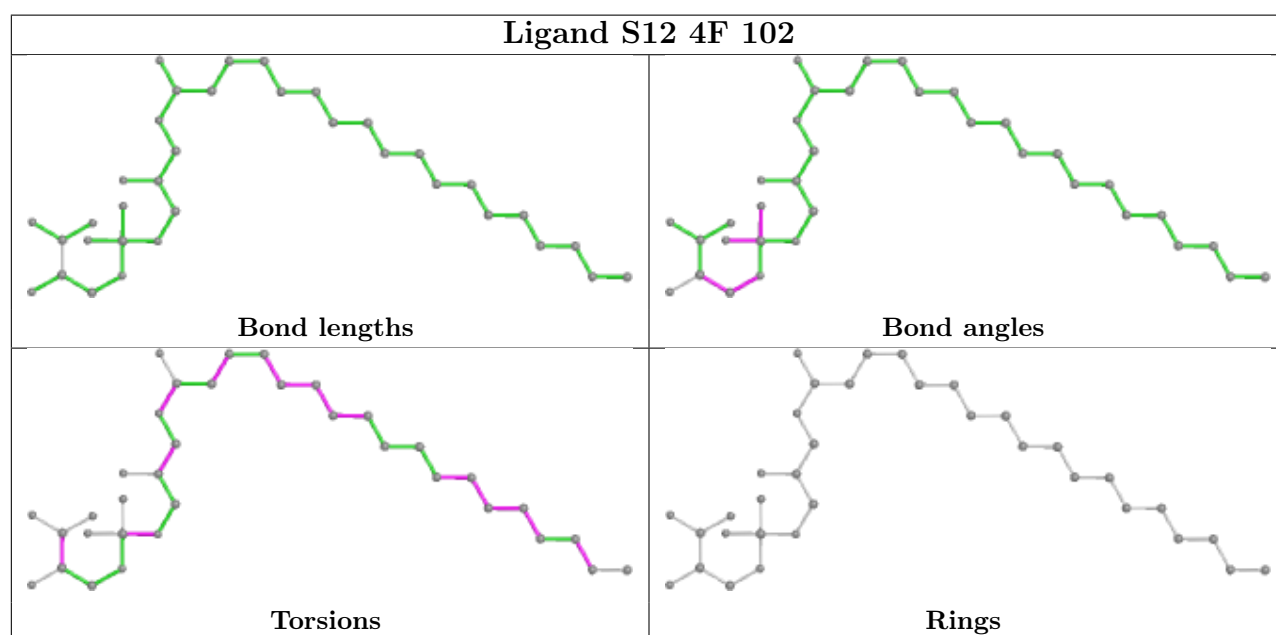
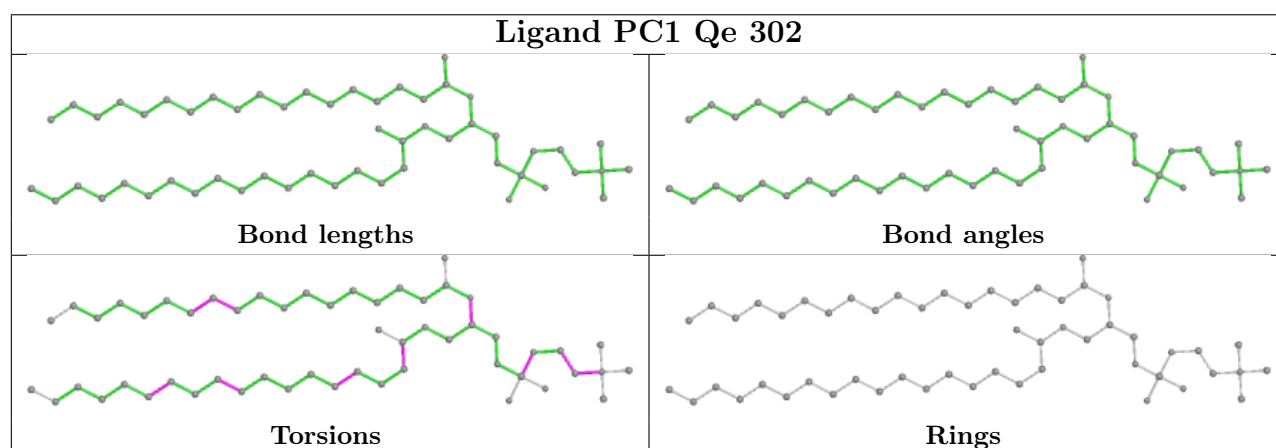
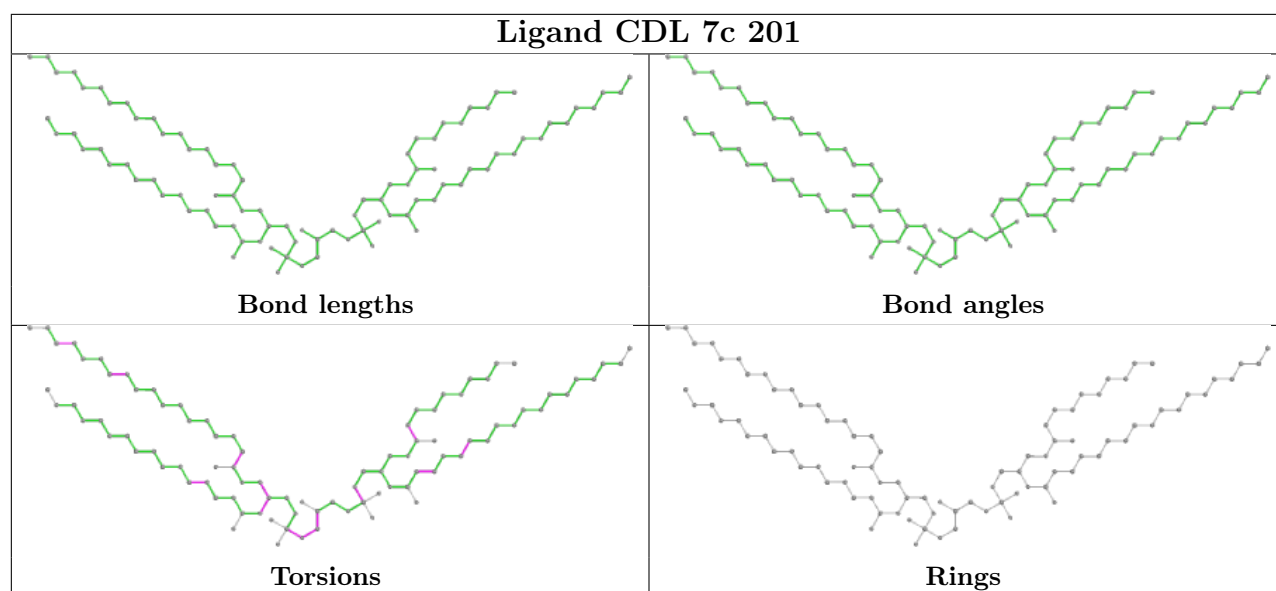
Bond angles



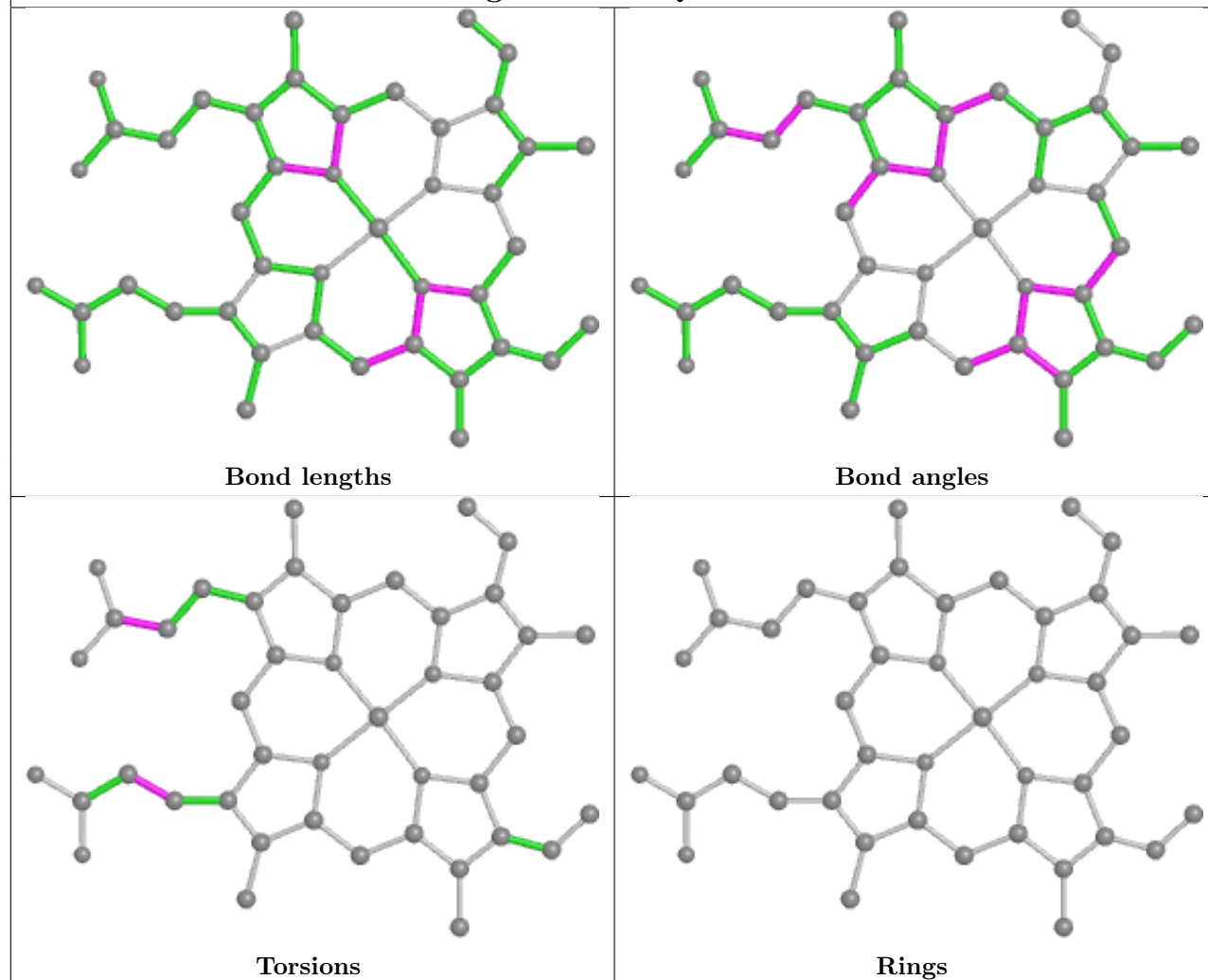
Torsions



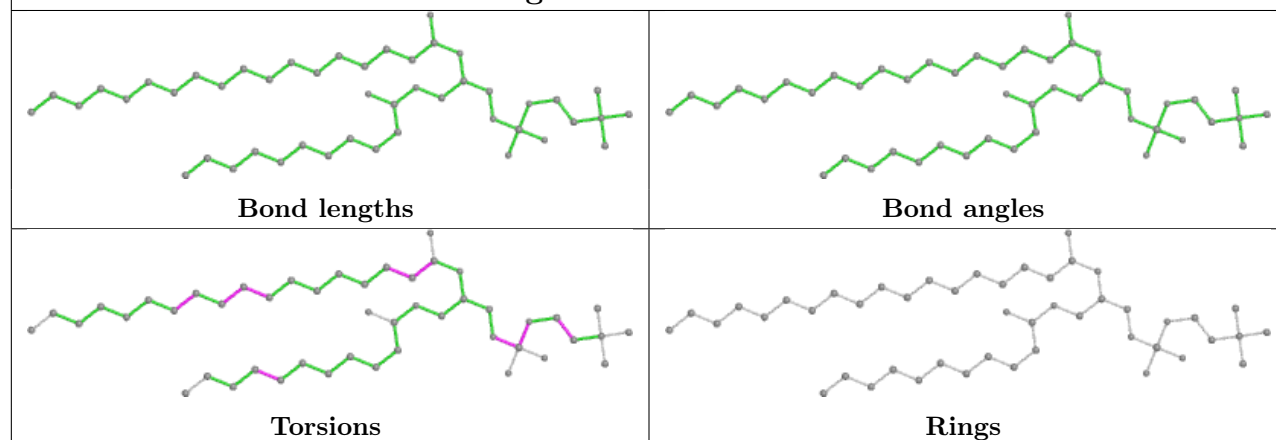
Rings

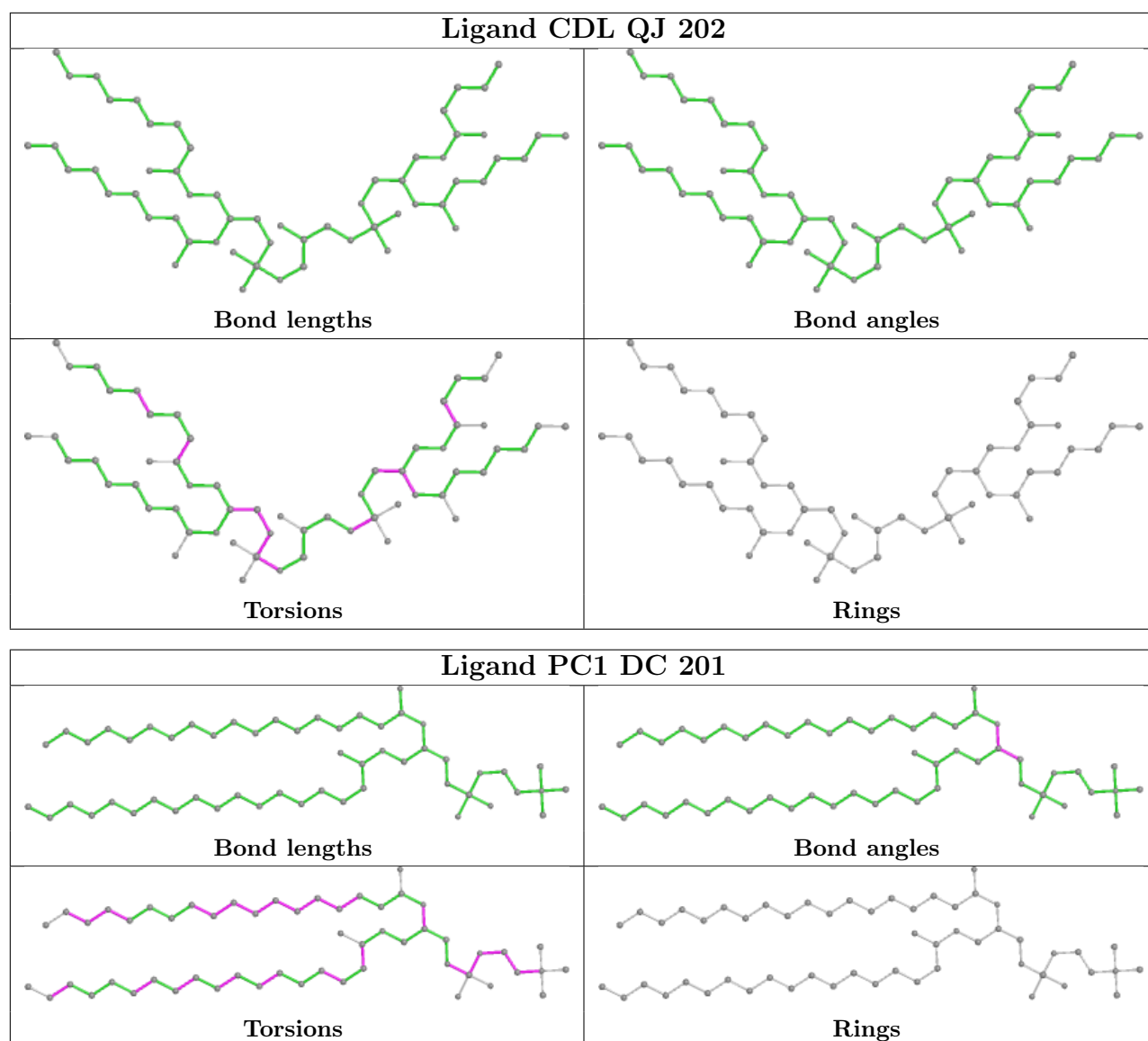


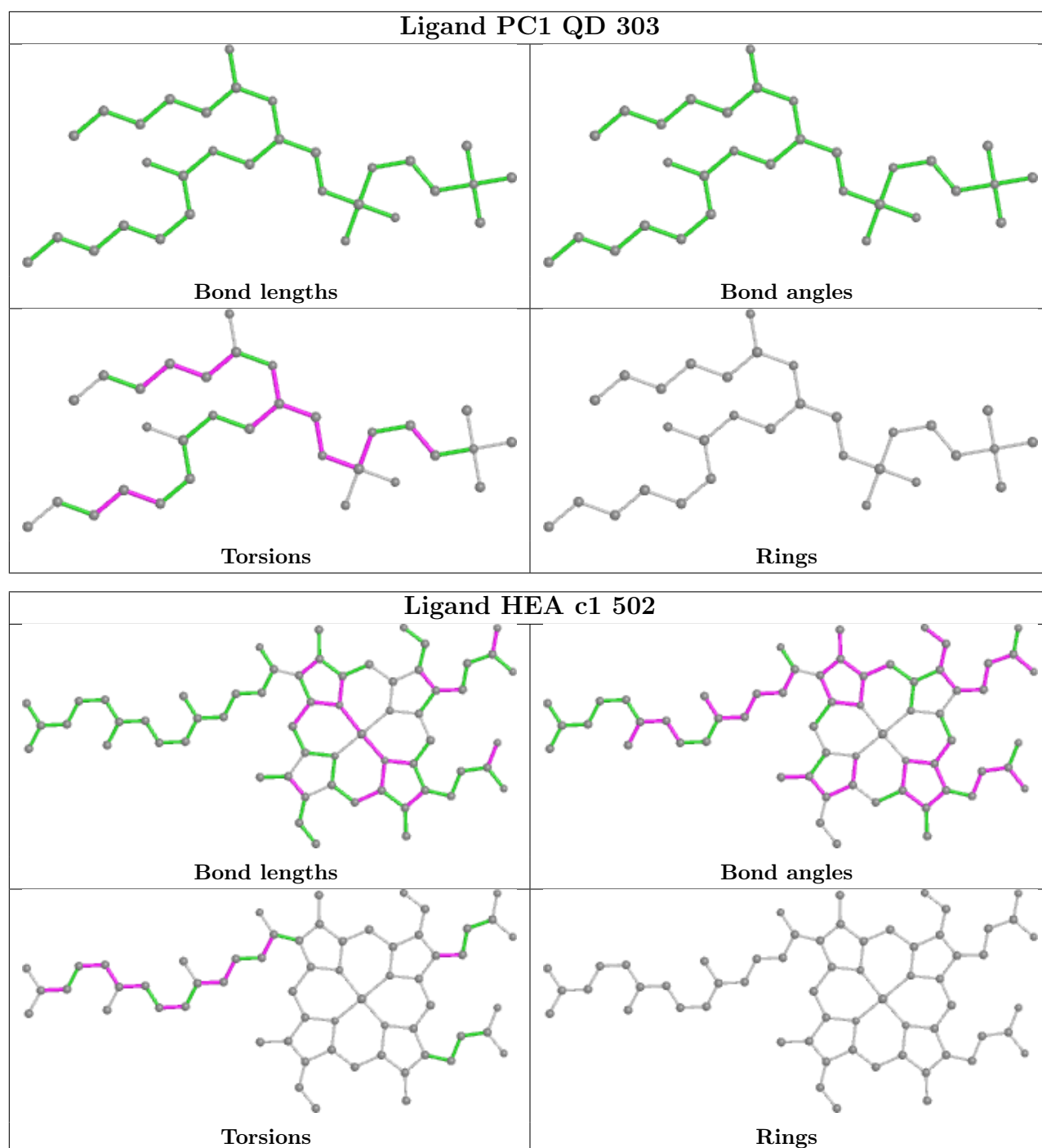
Ligand HEM QC 401

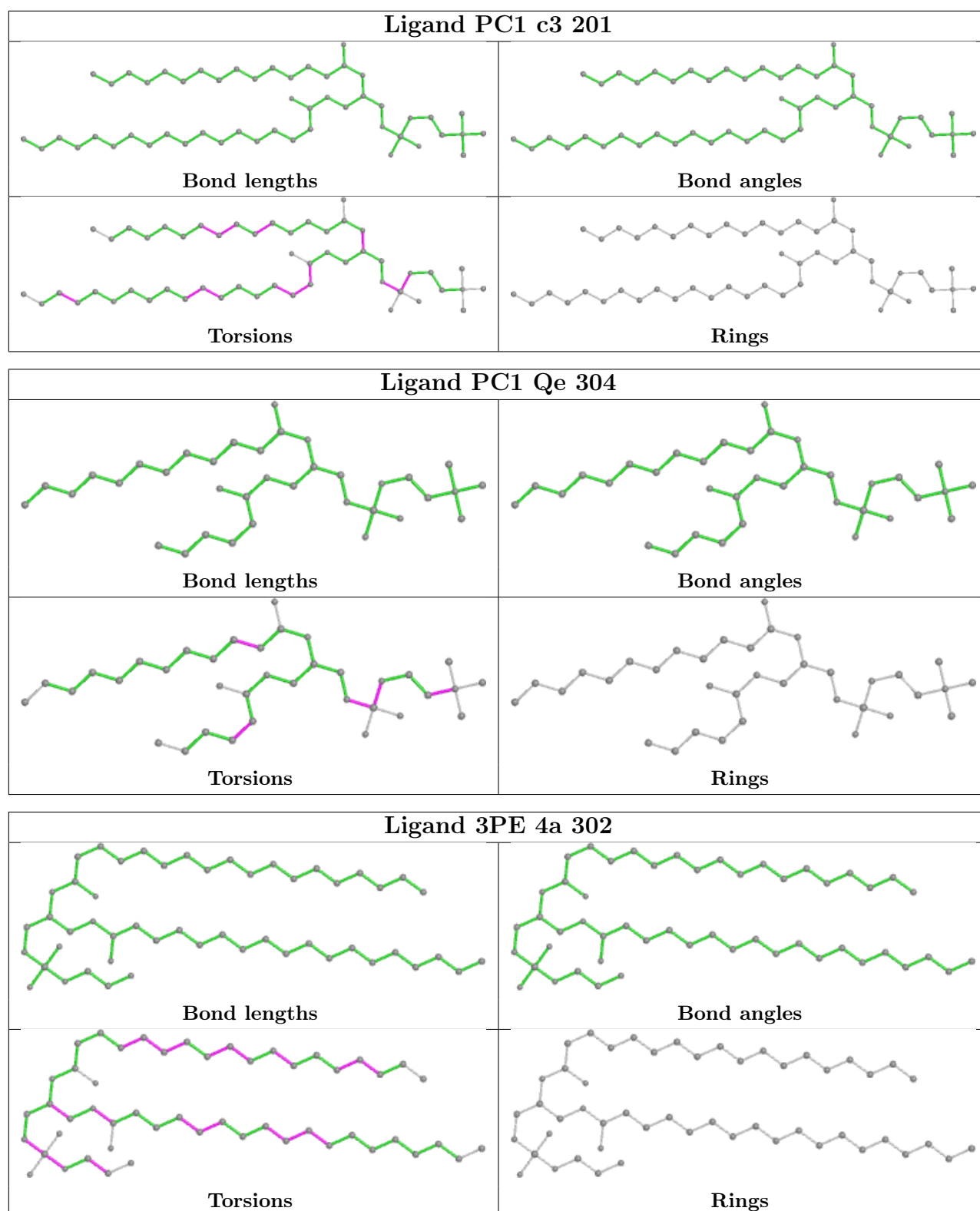


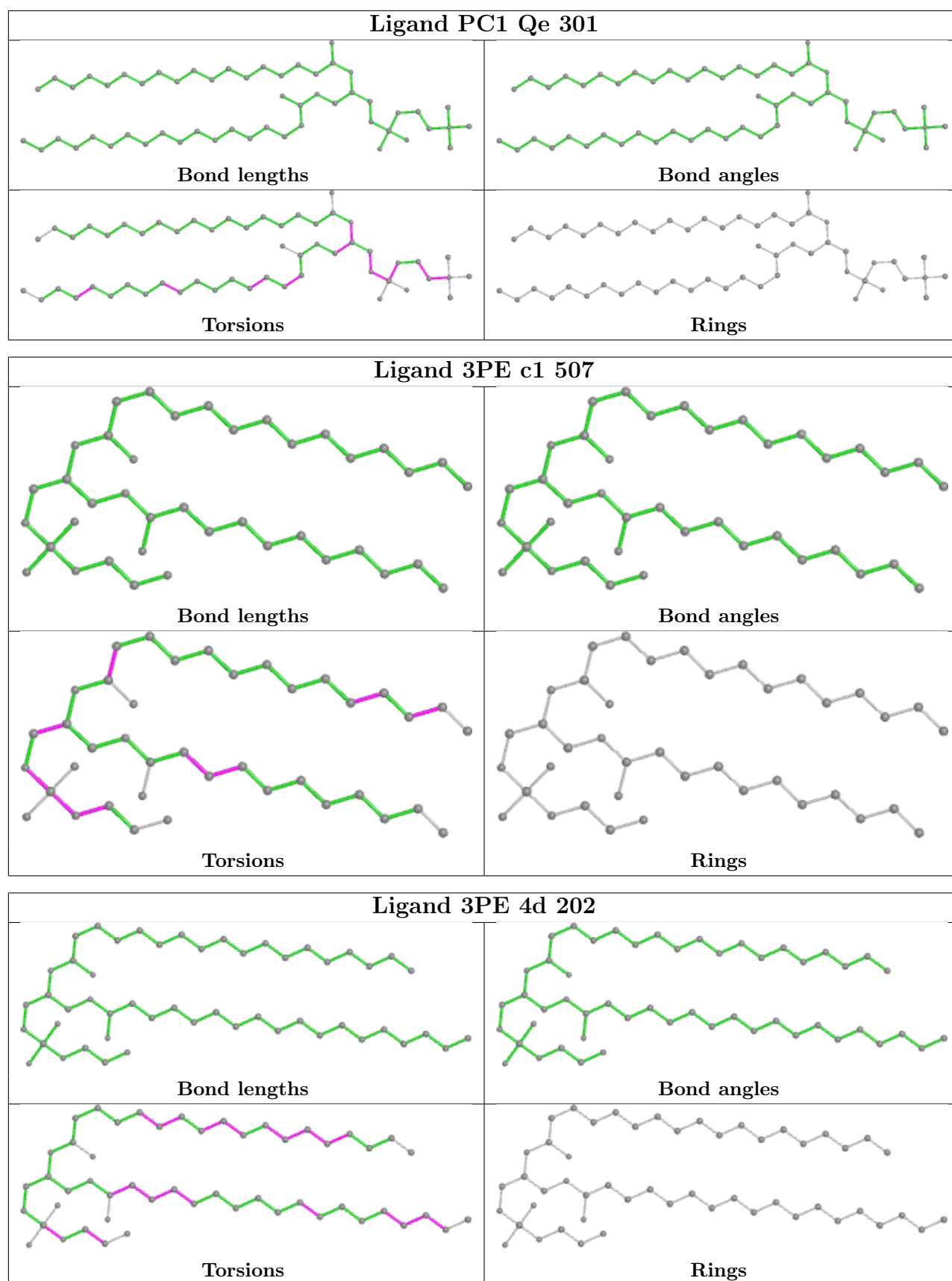
Ligand PC1 4A 301



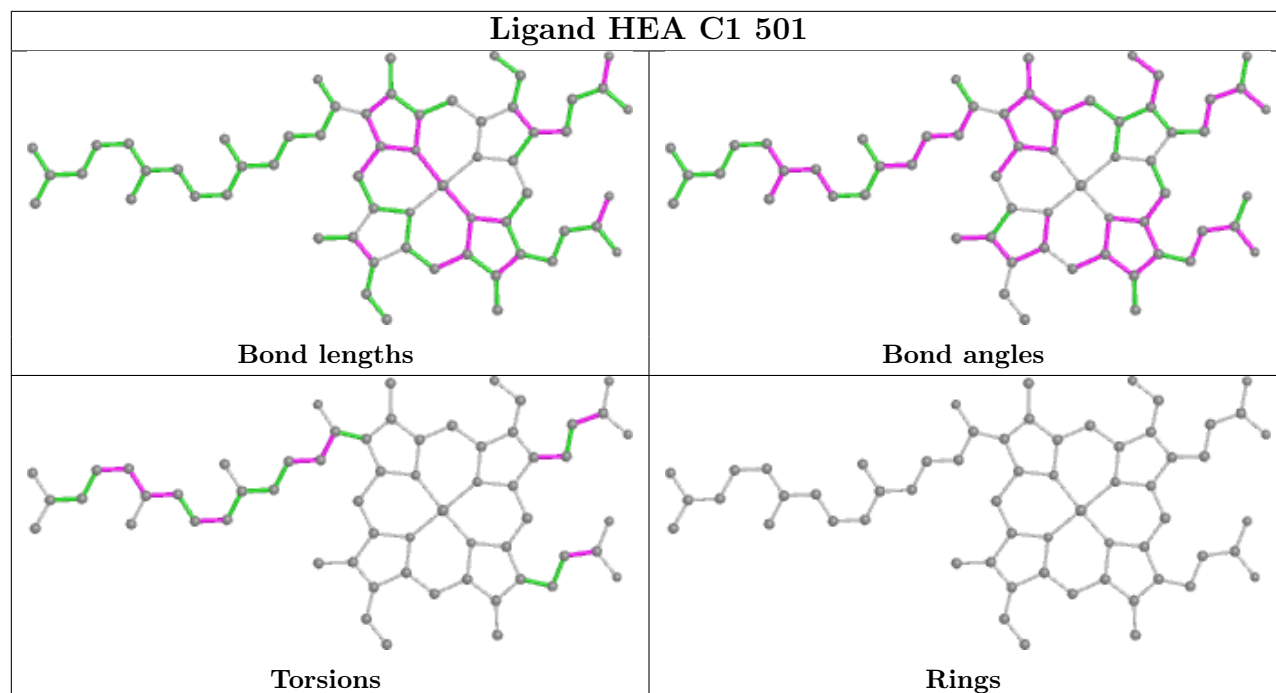




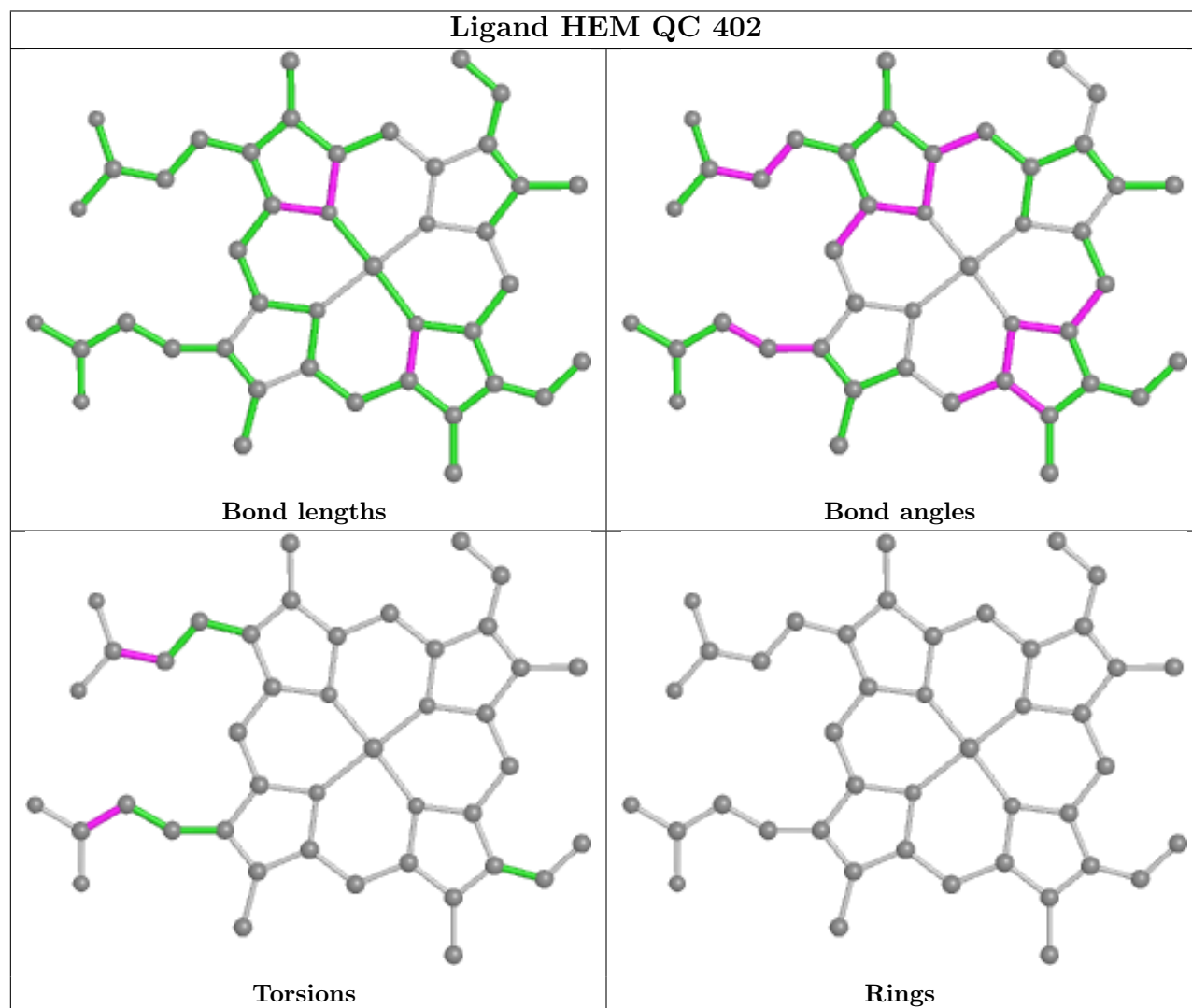


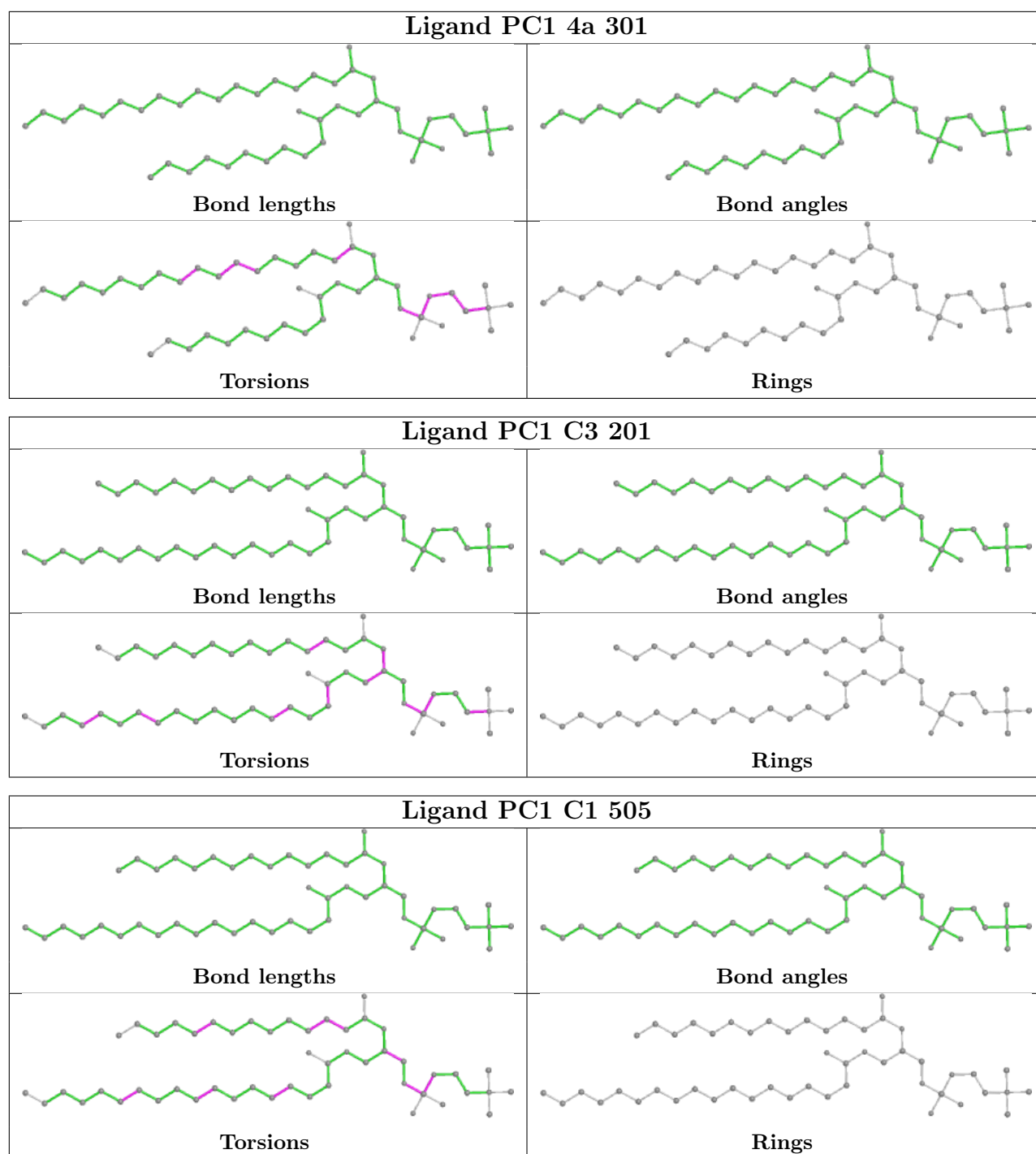


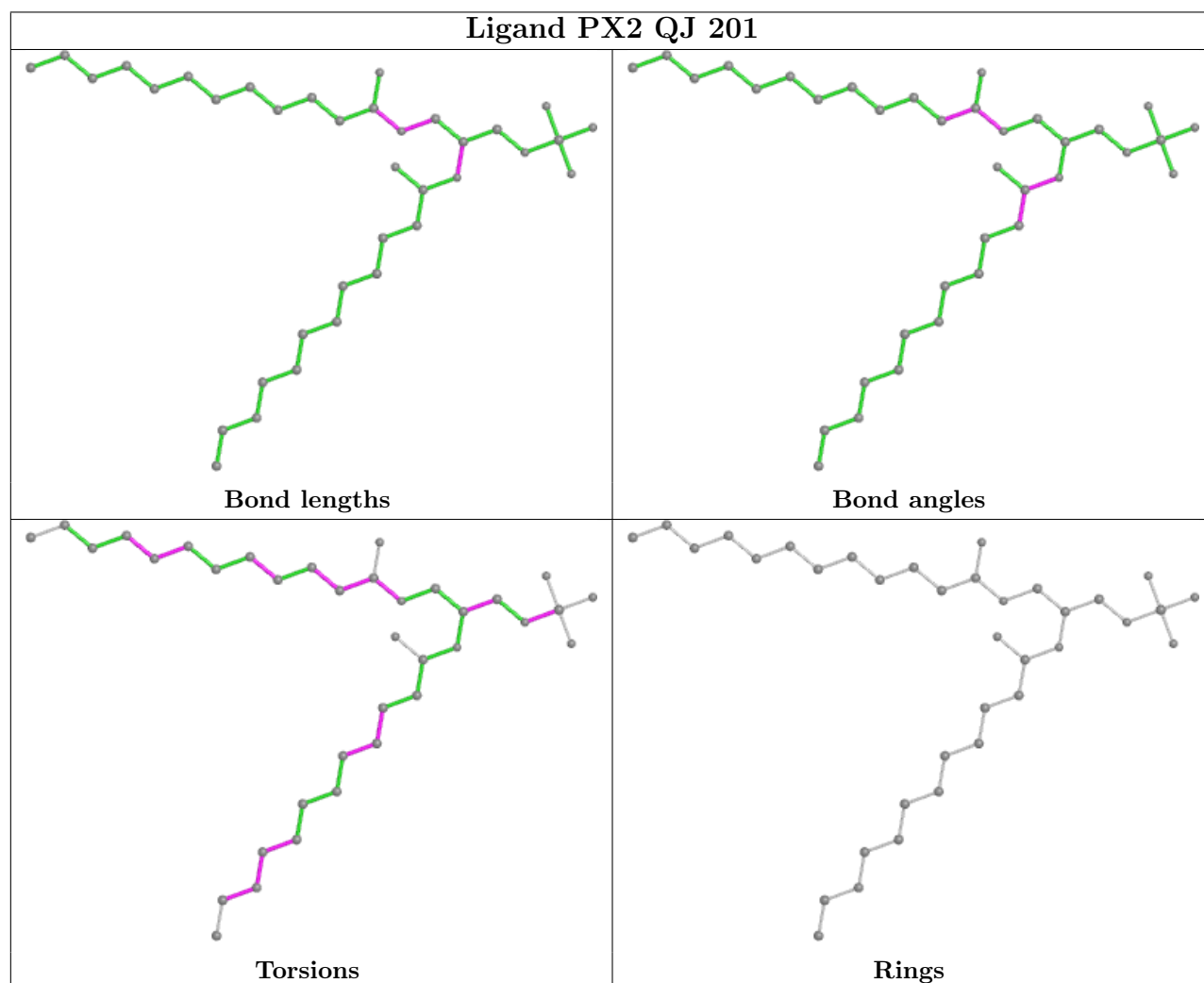
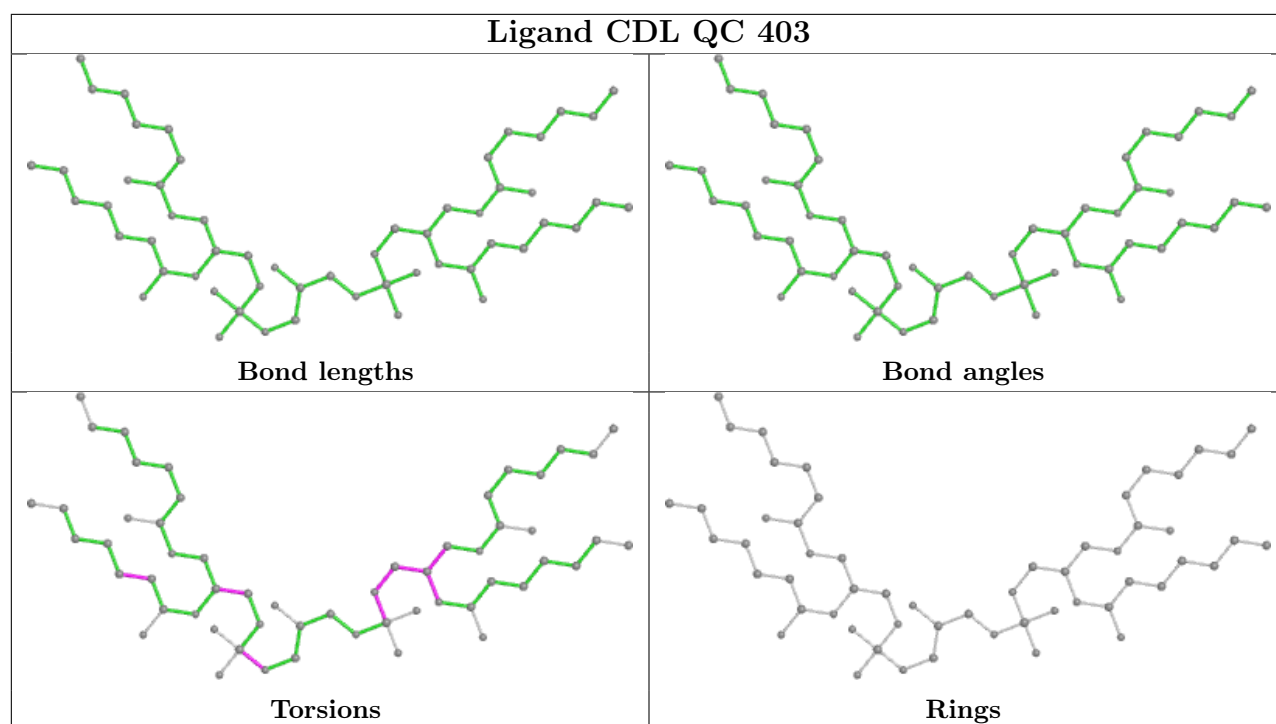
Ligand HEA C1 501

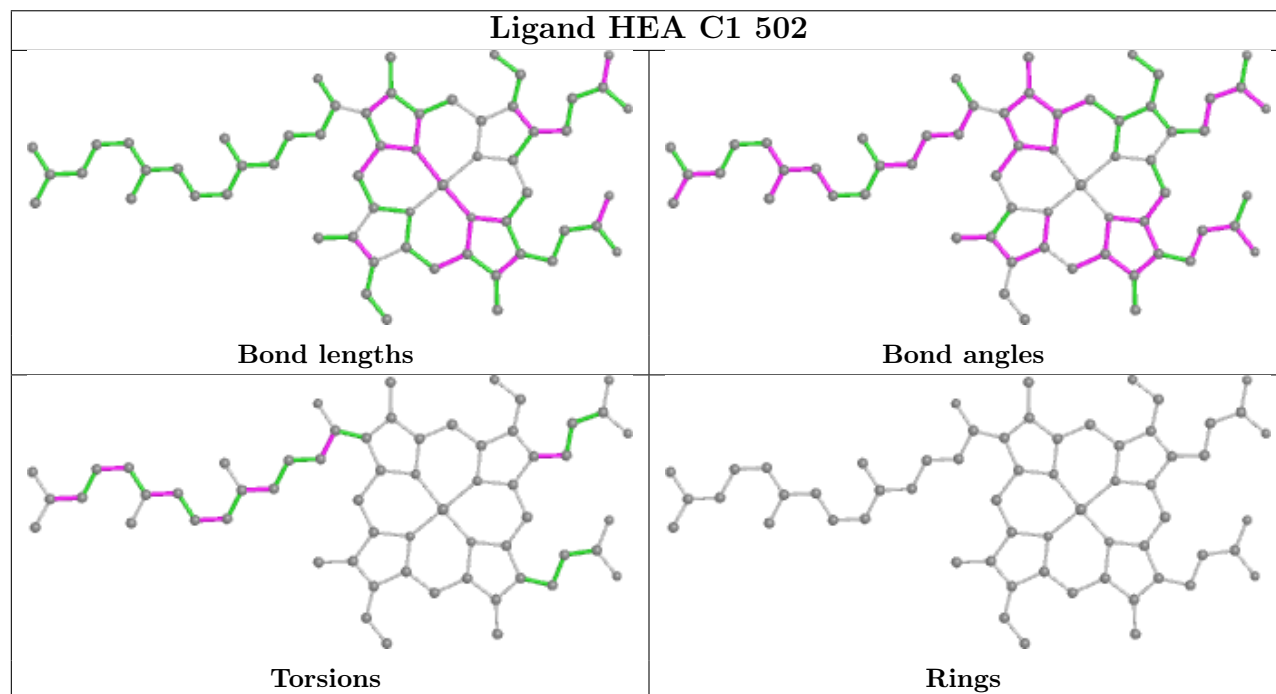
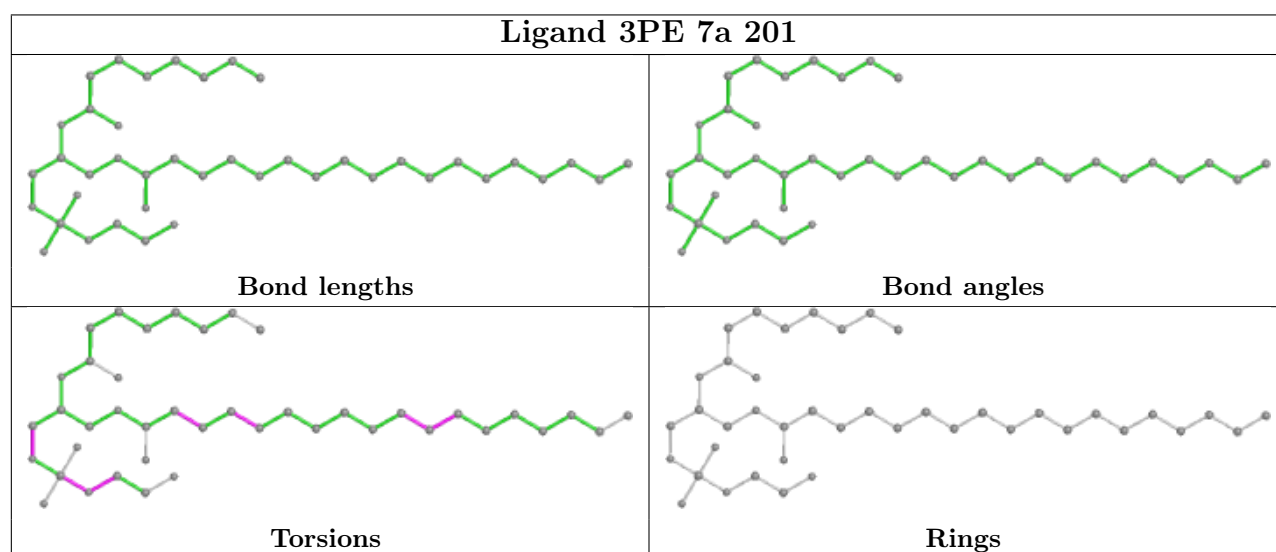
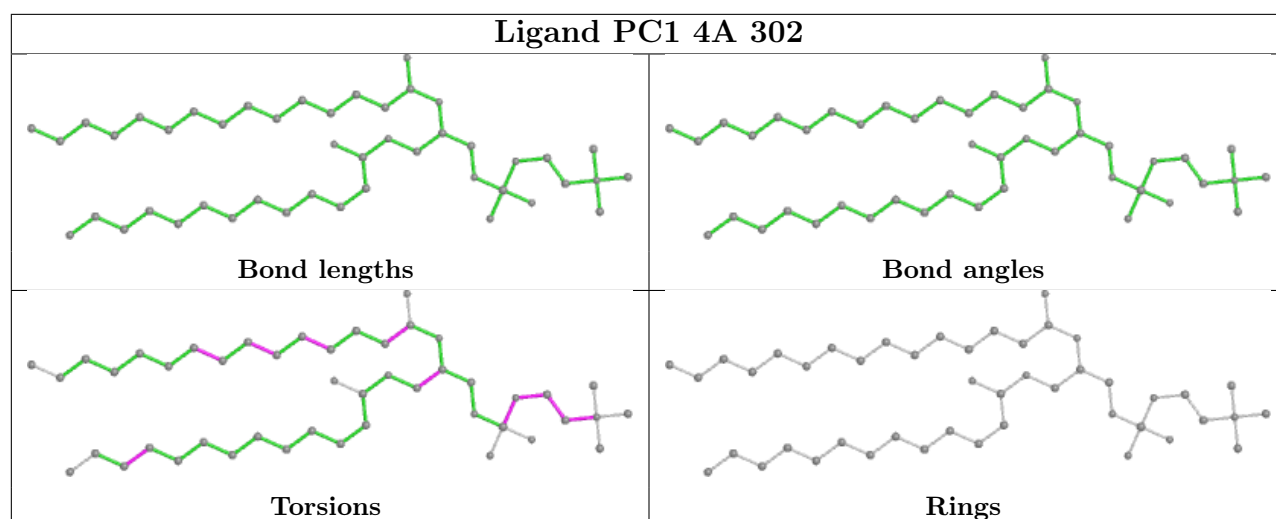


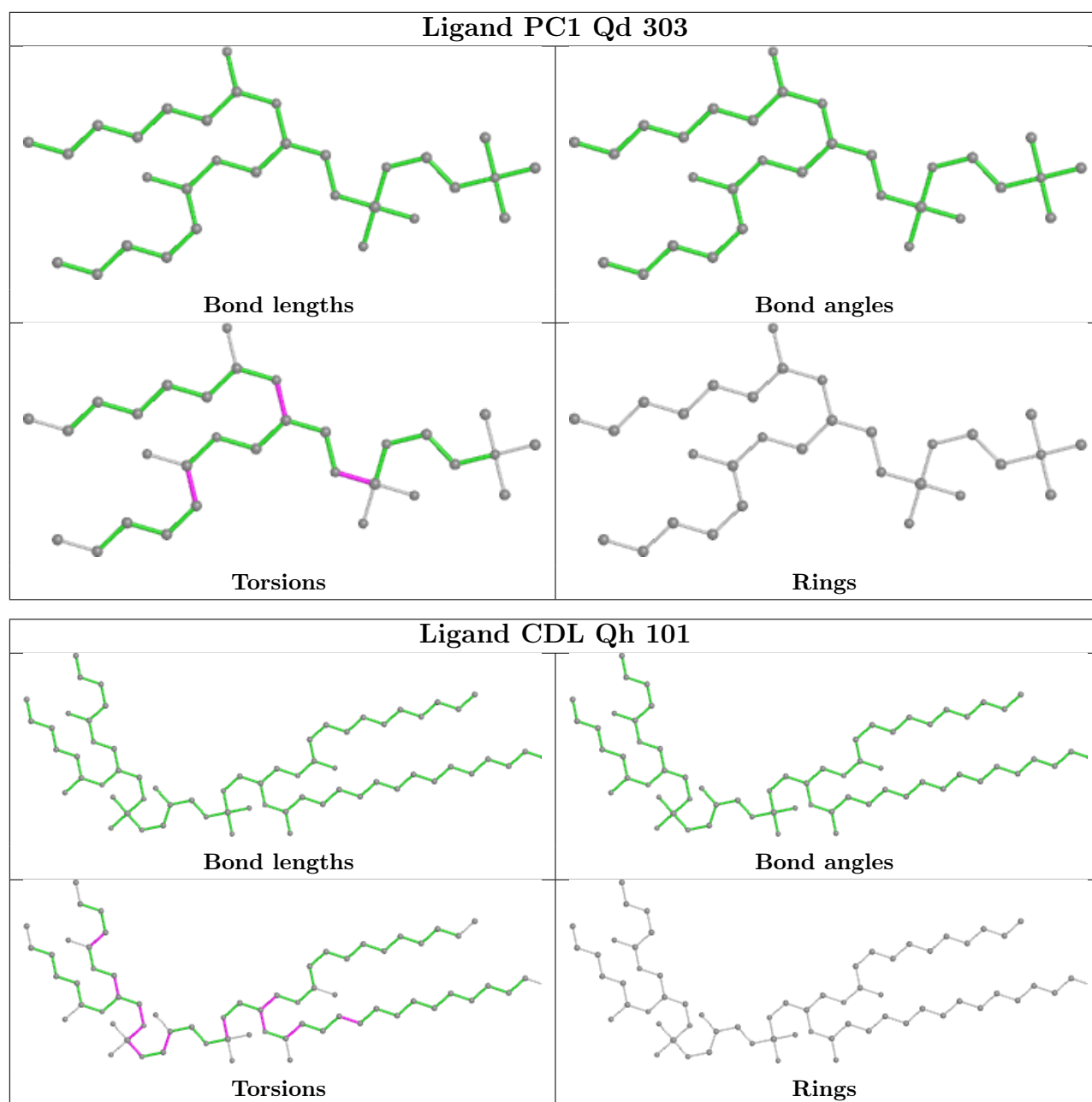
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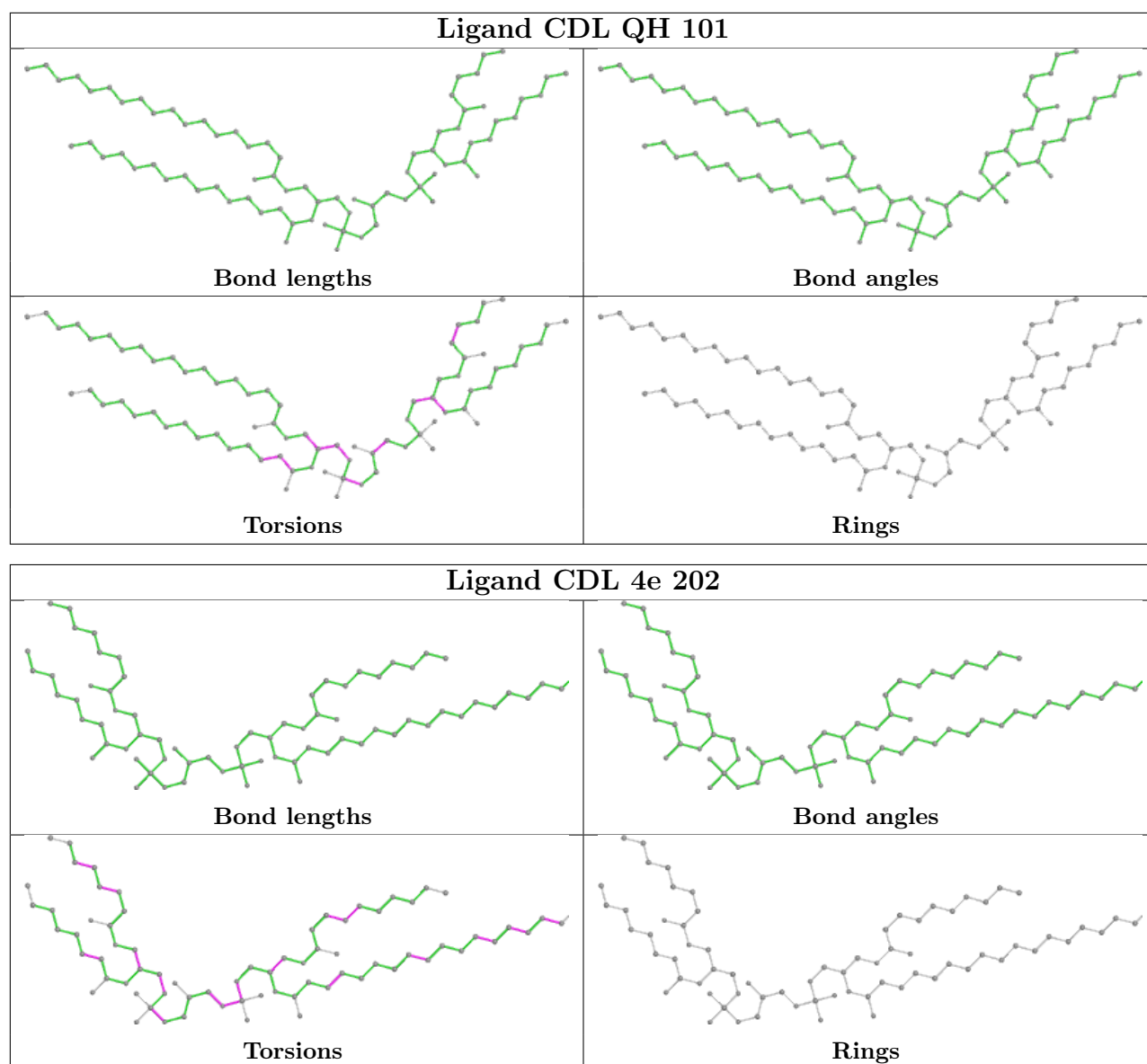


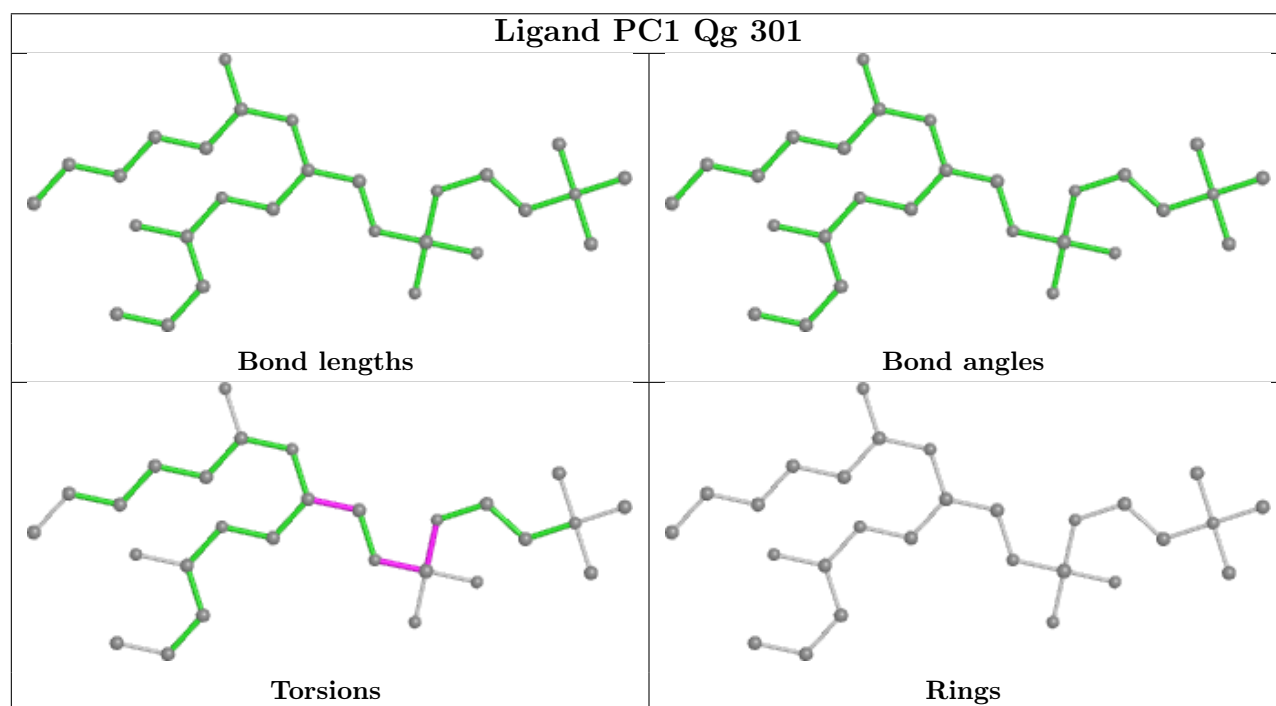
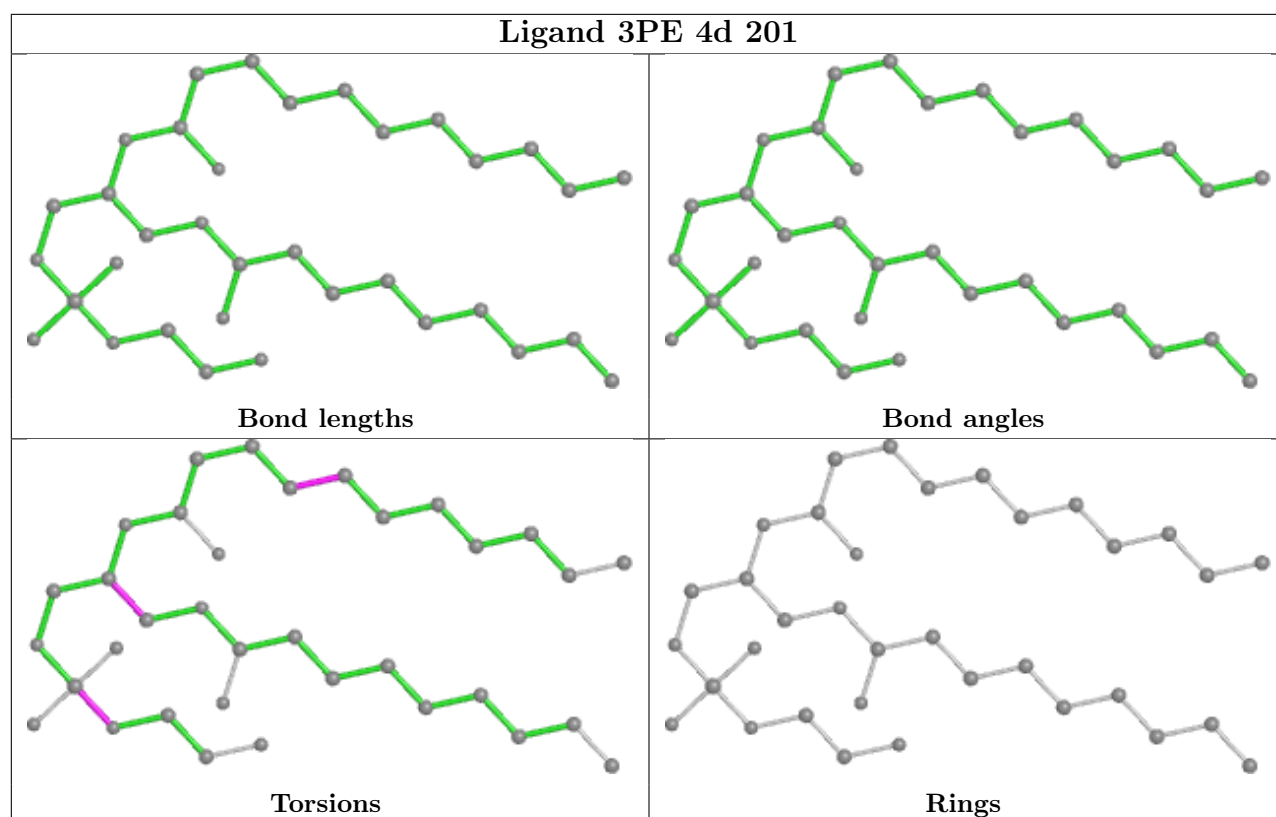


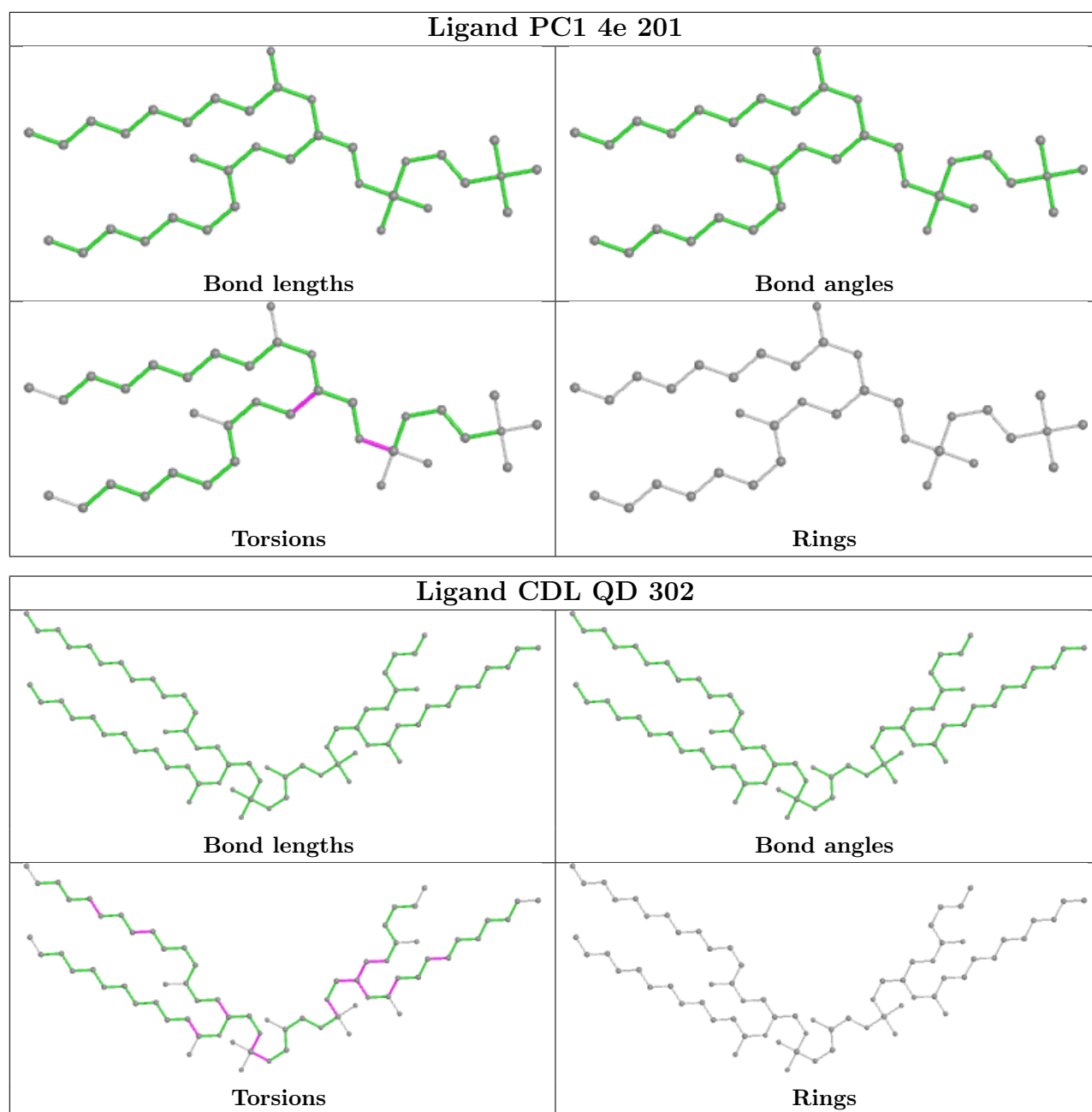




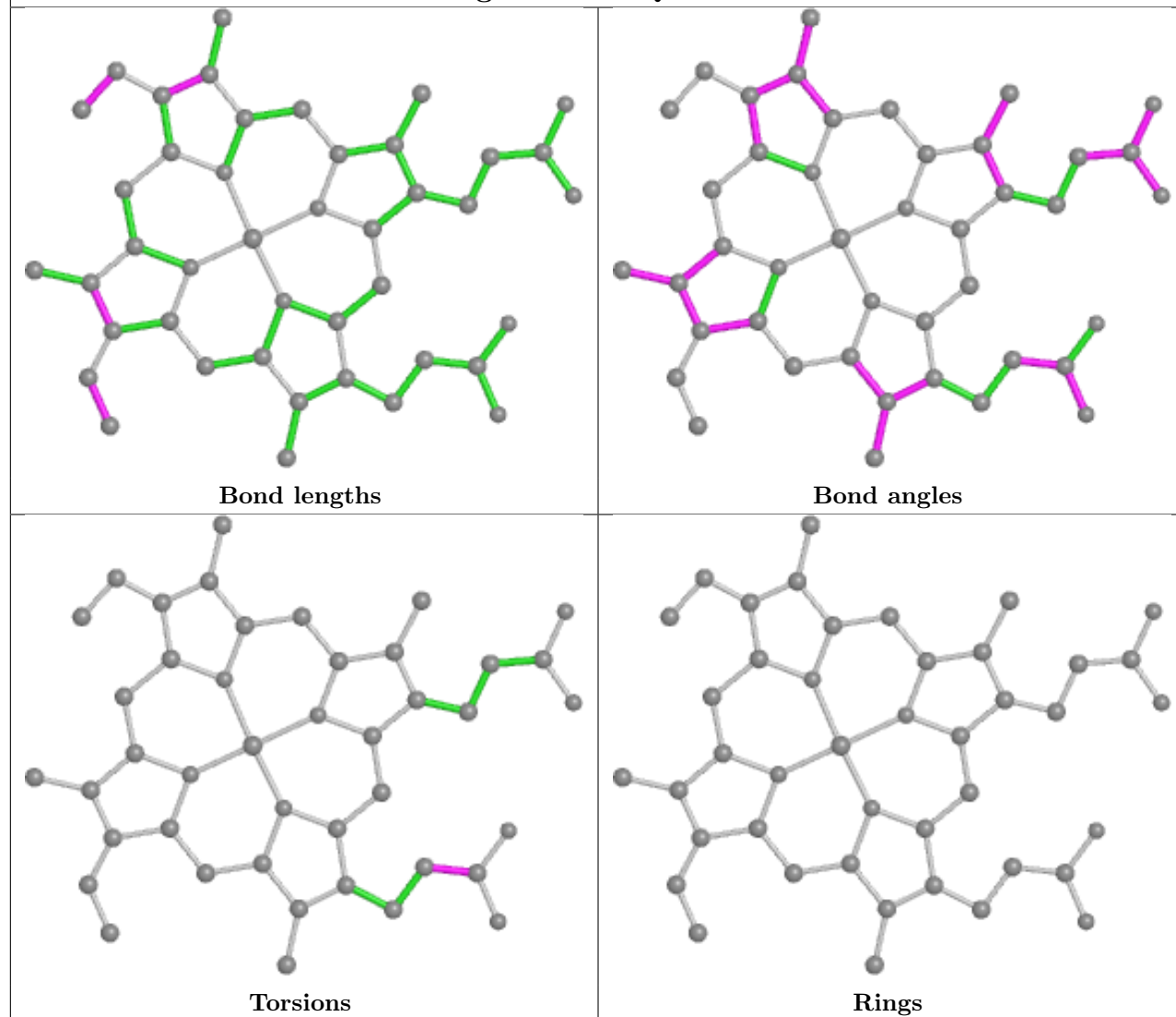




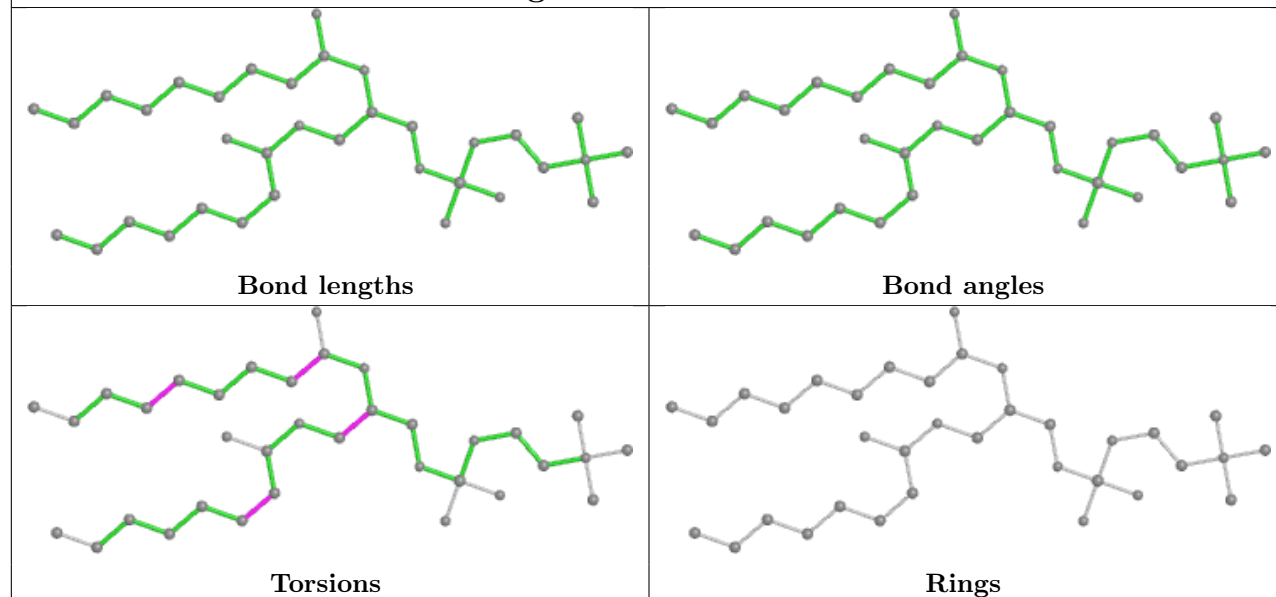


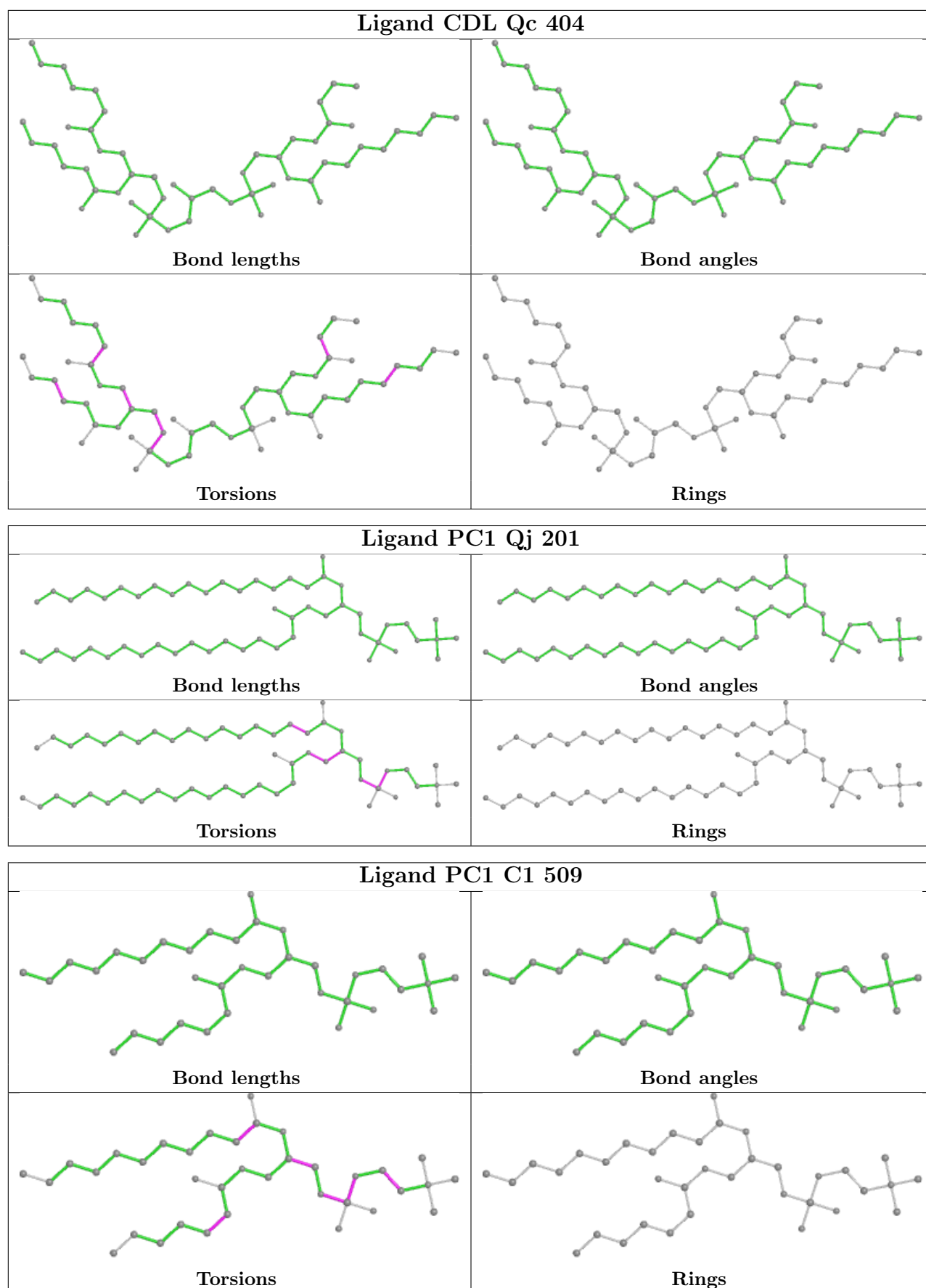


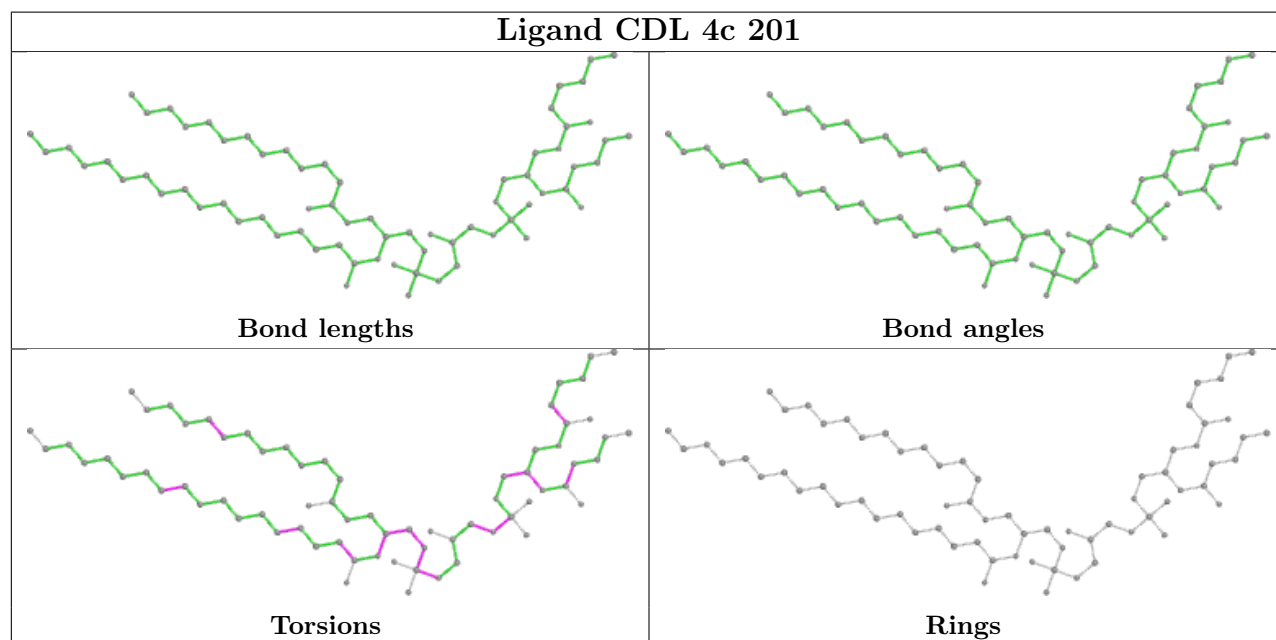
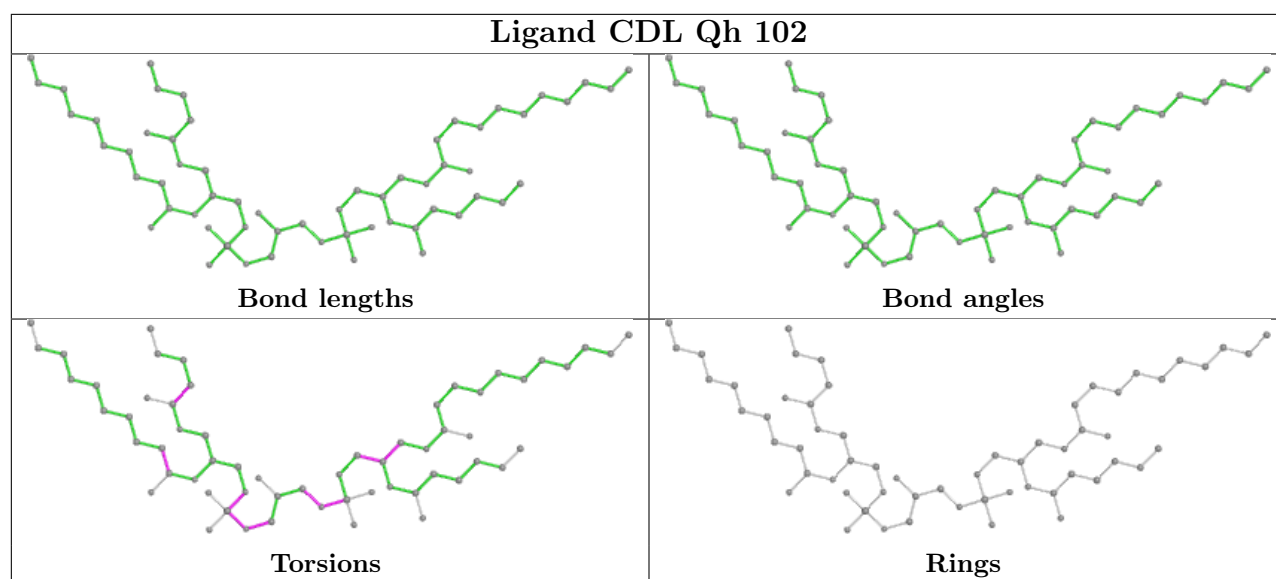
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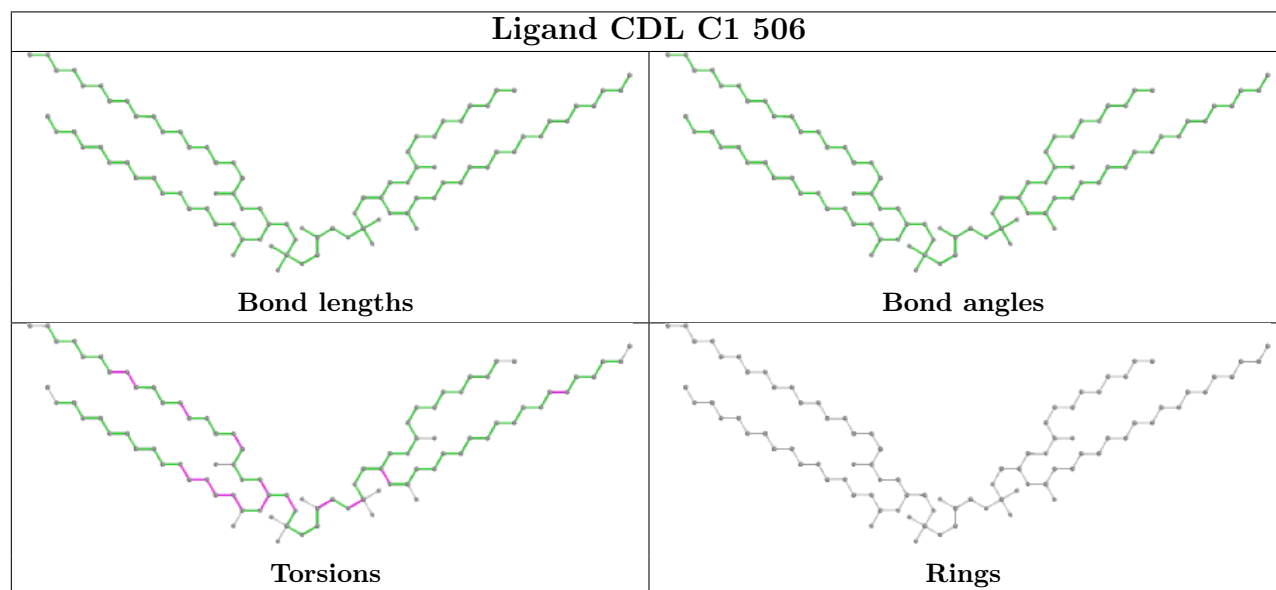
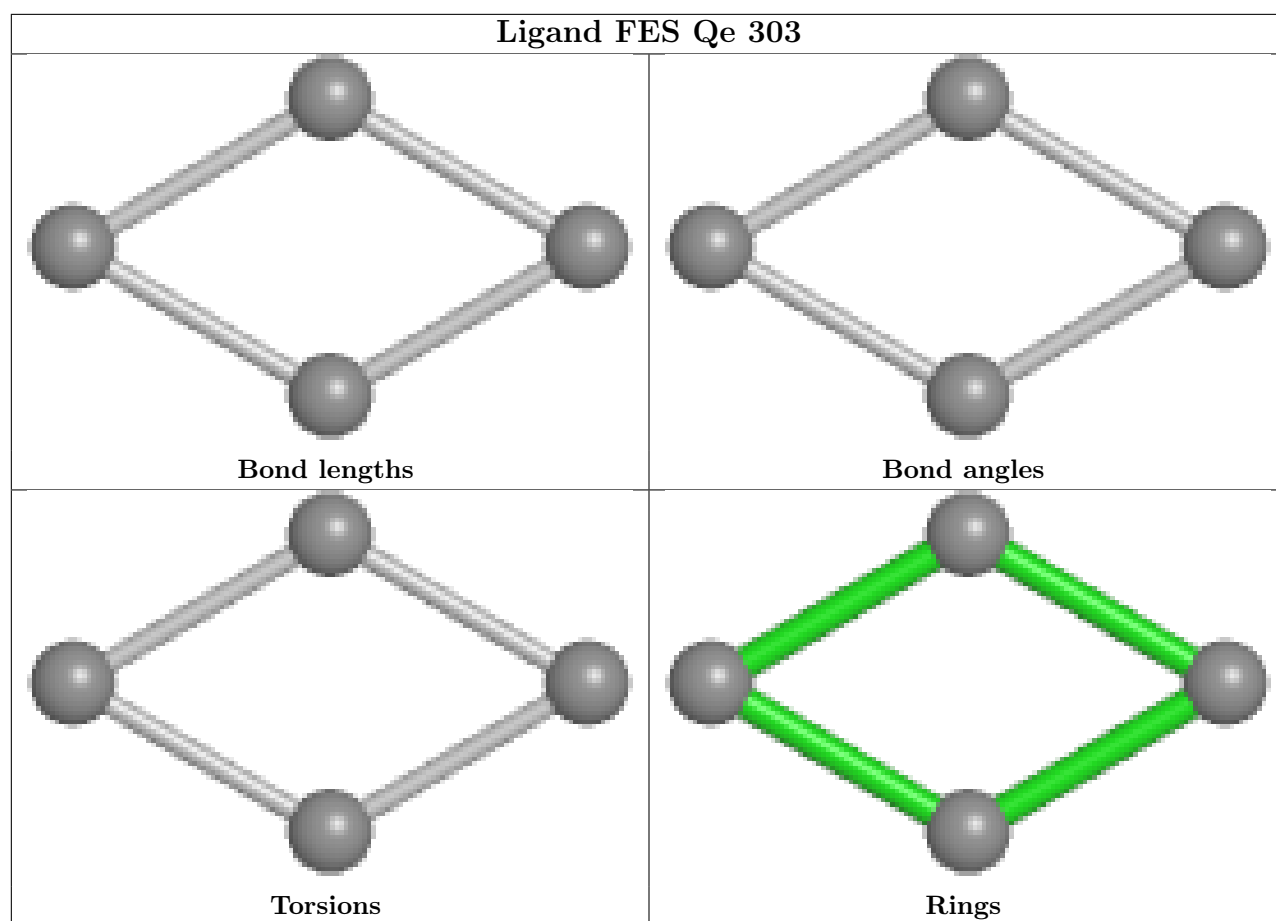


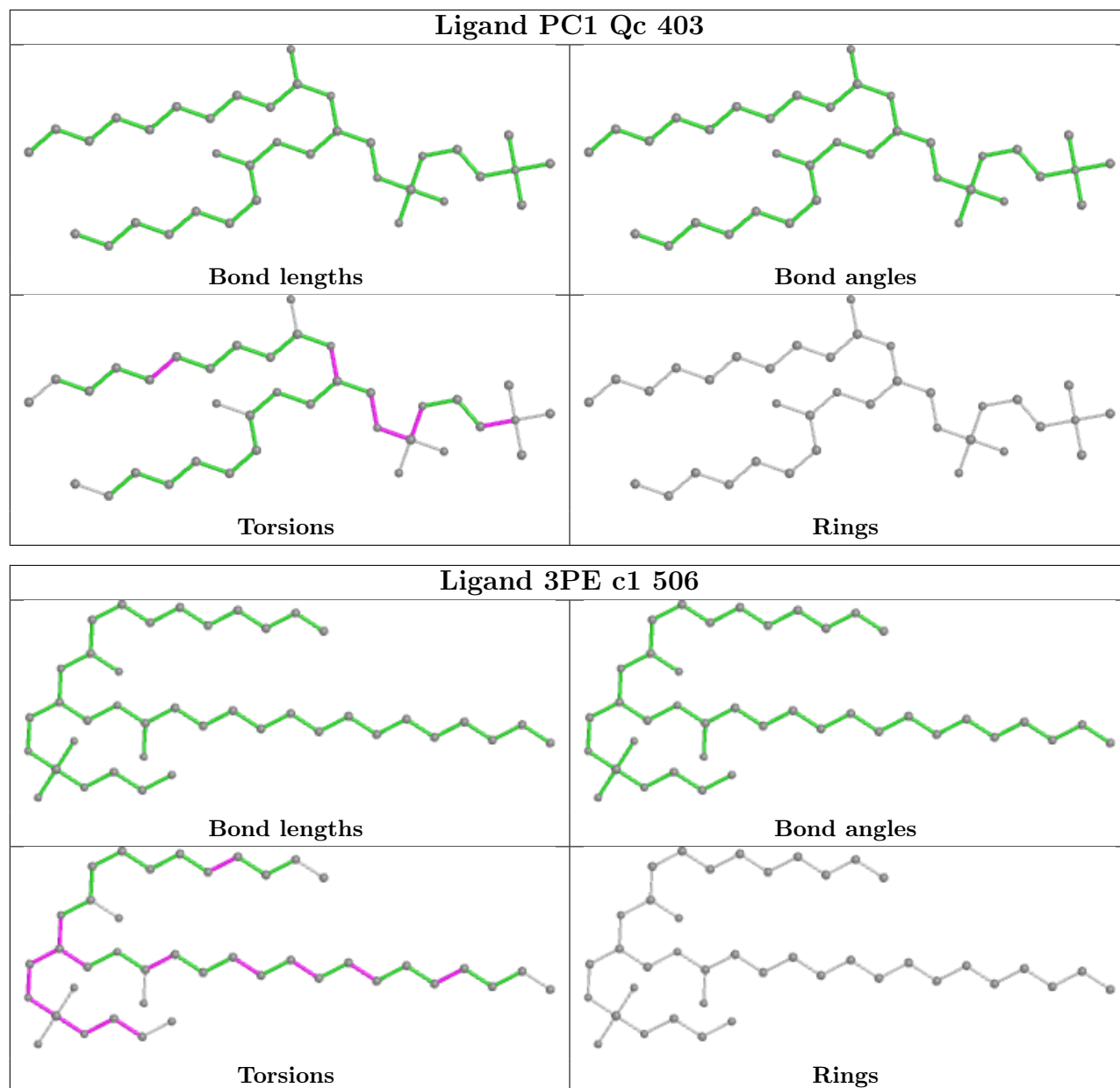
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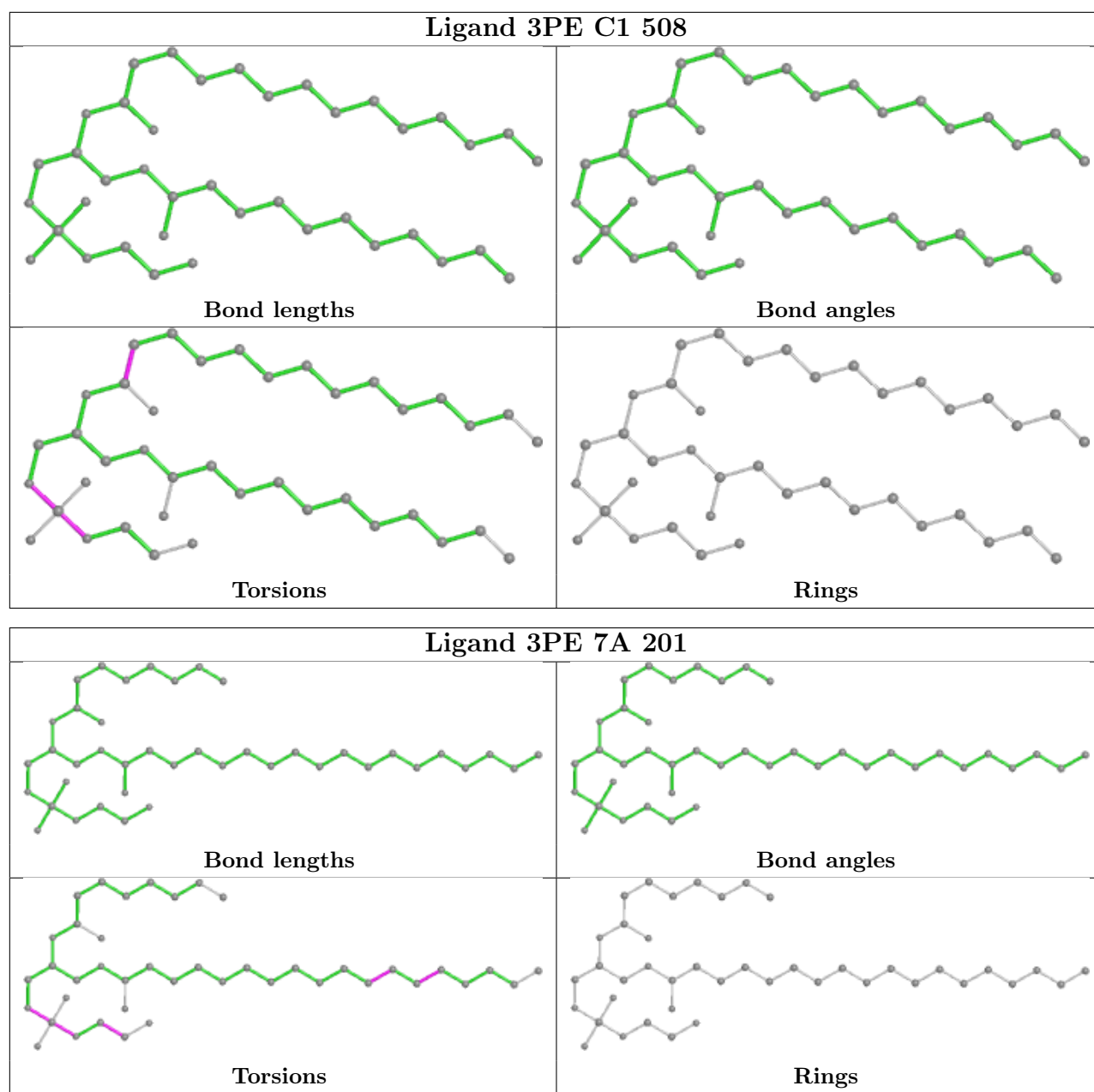


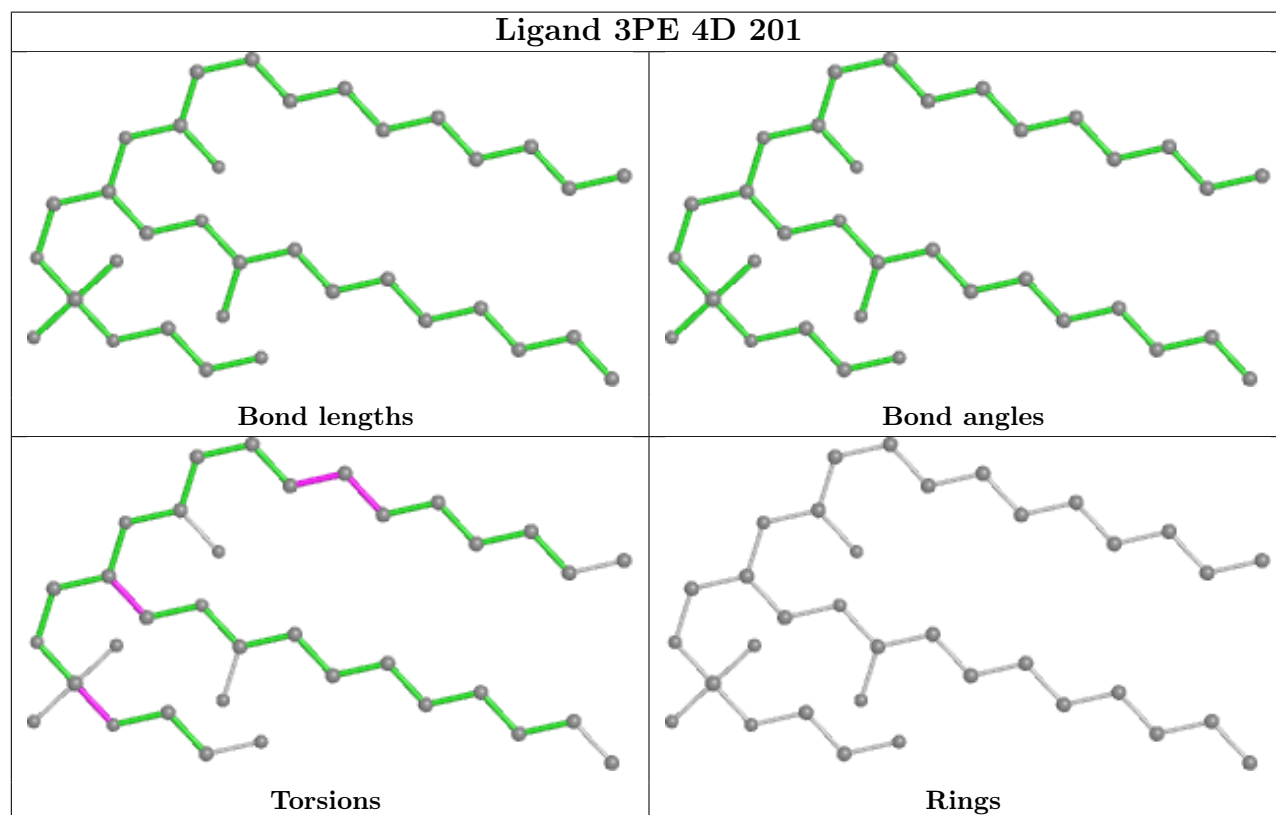
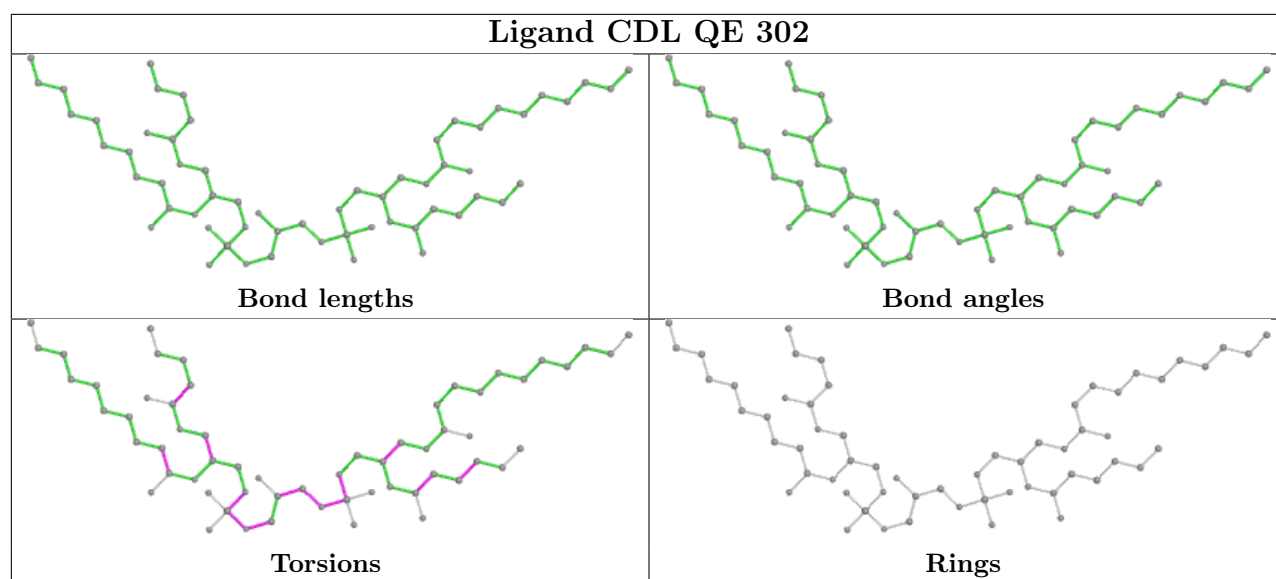


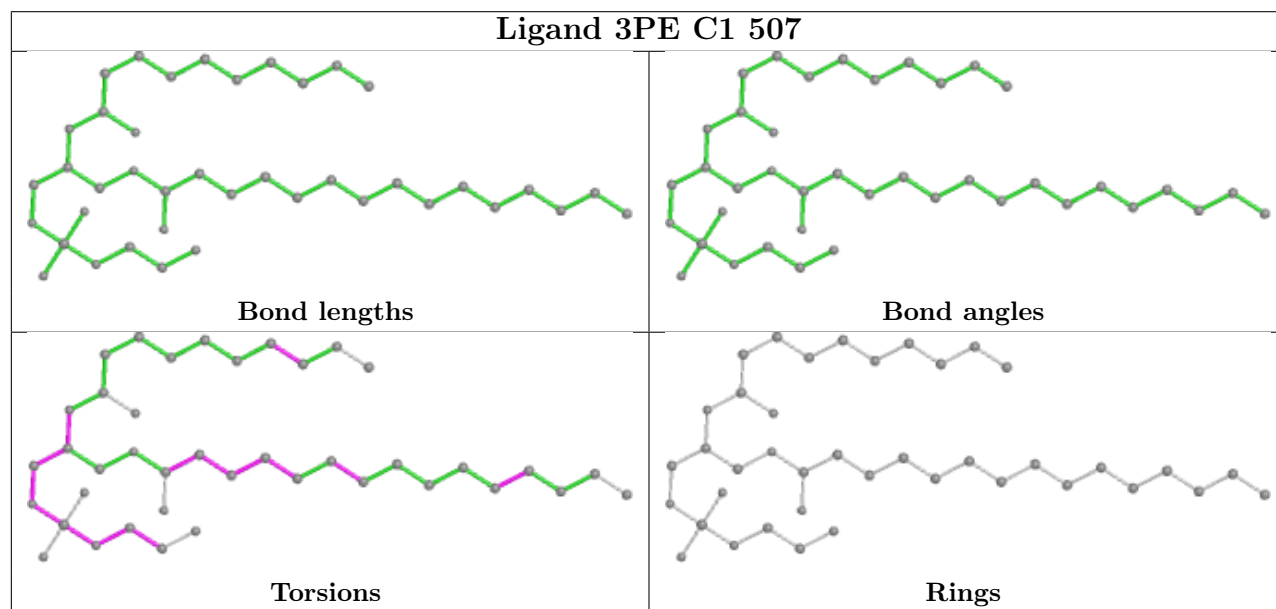
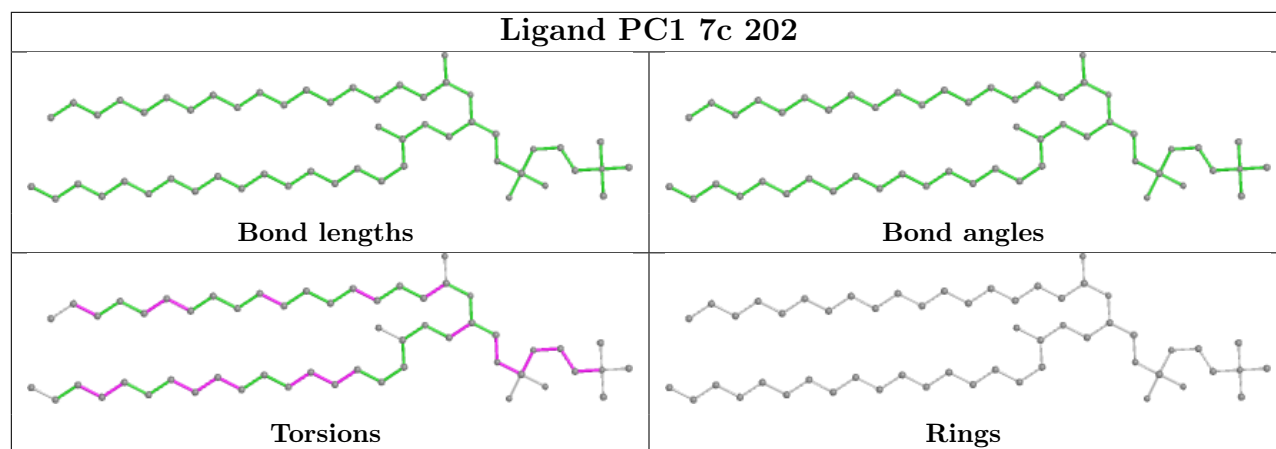
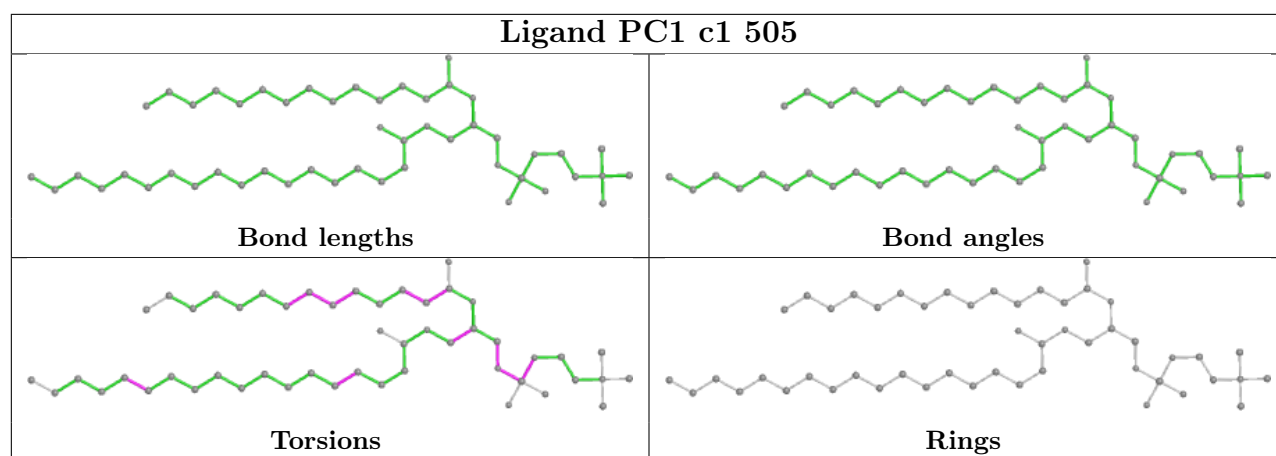


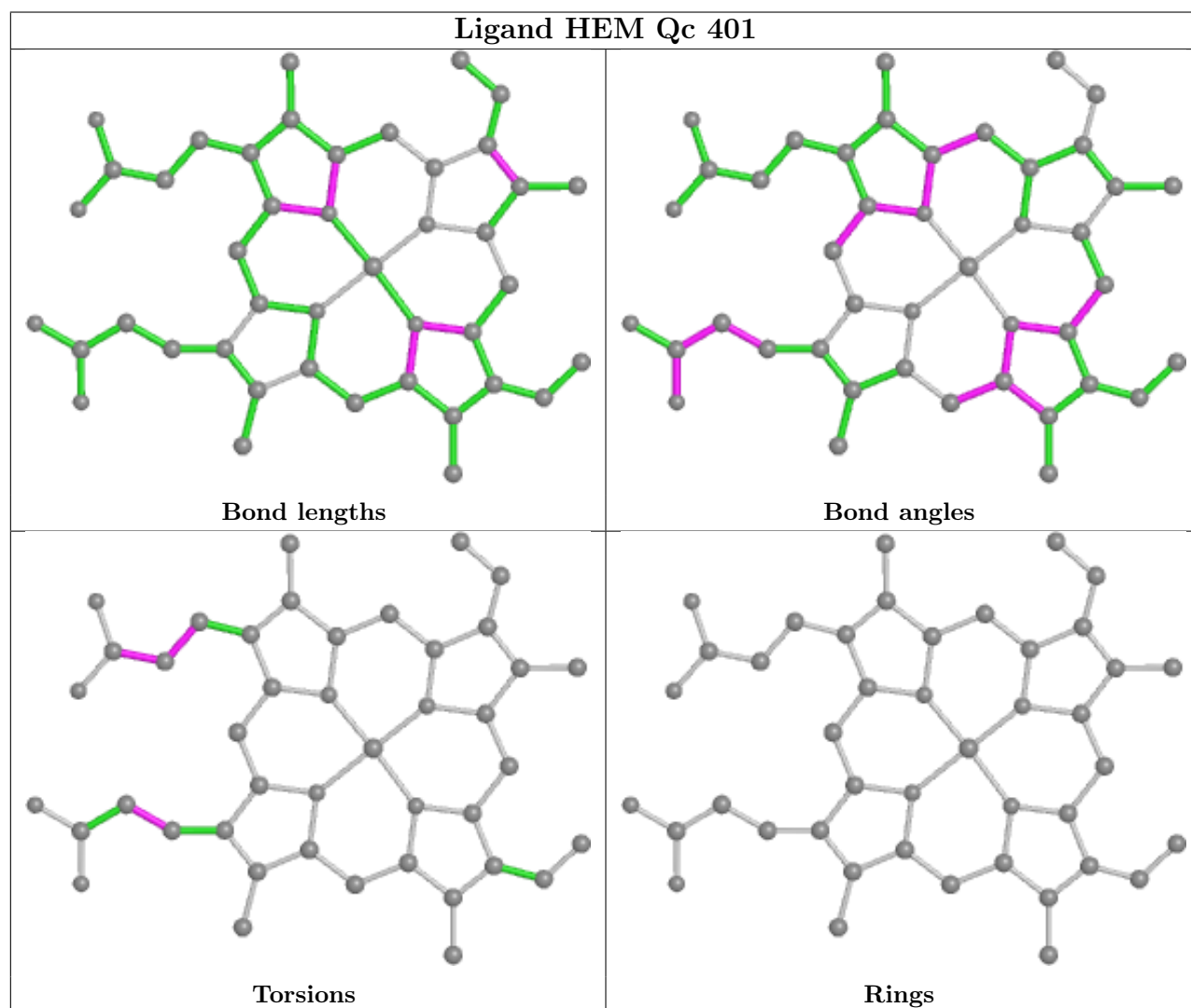
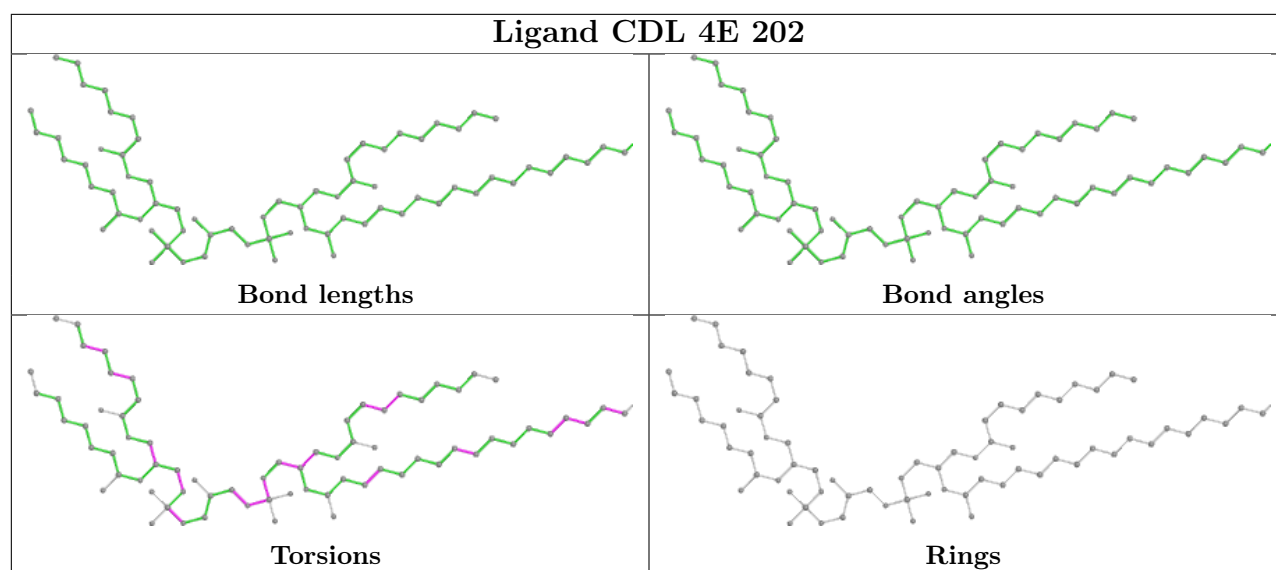


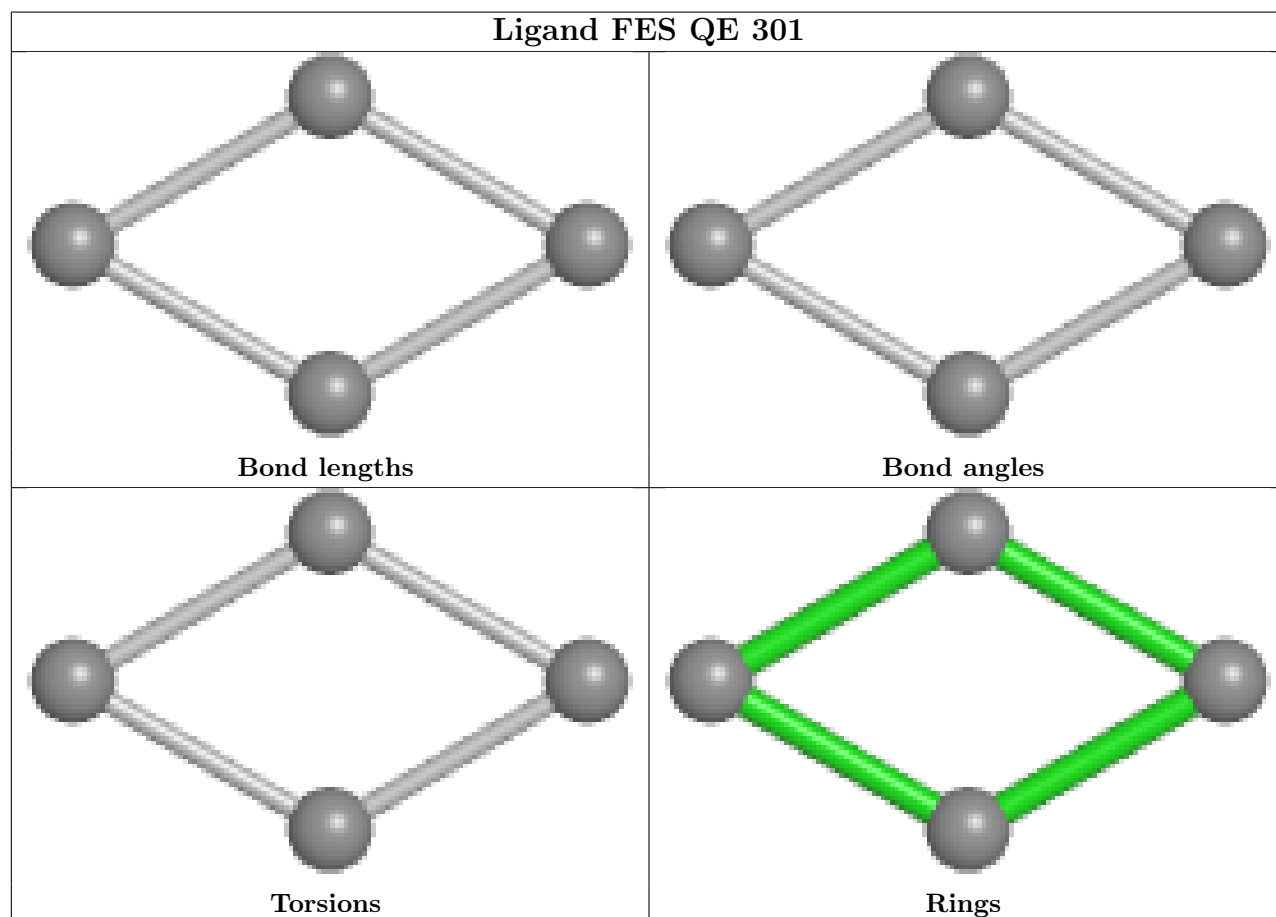
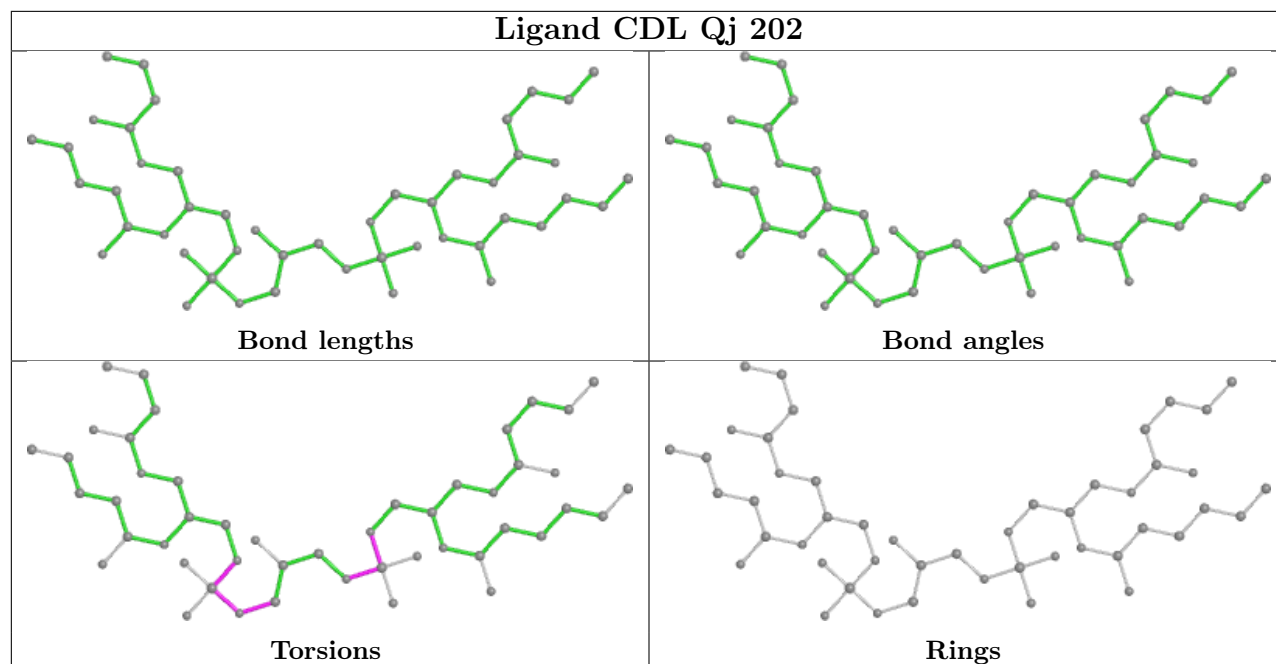


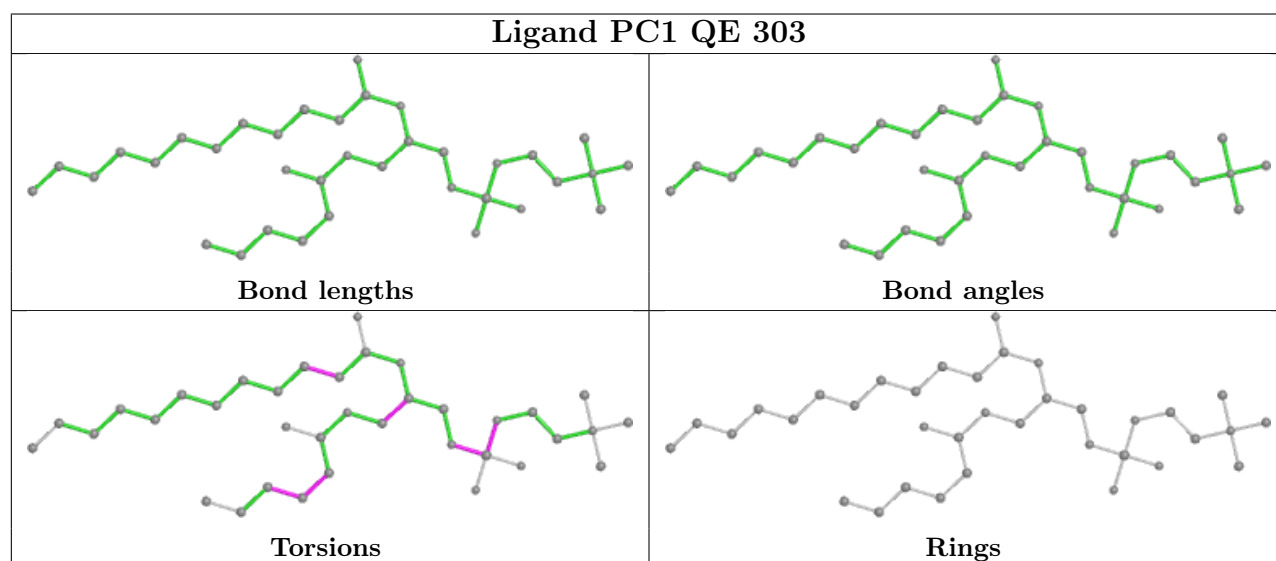
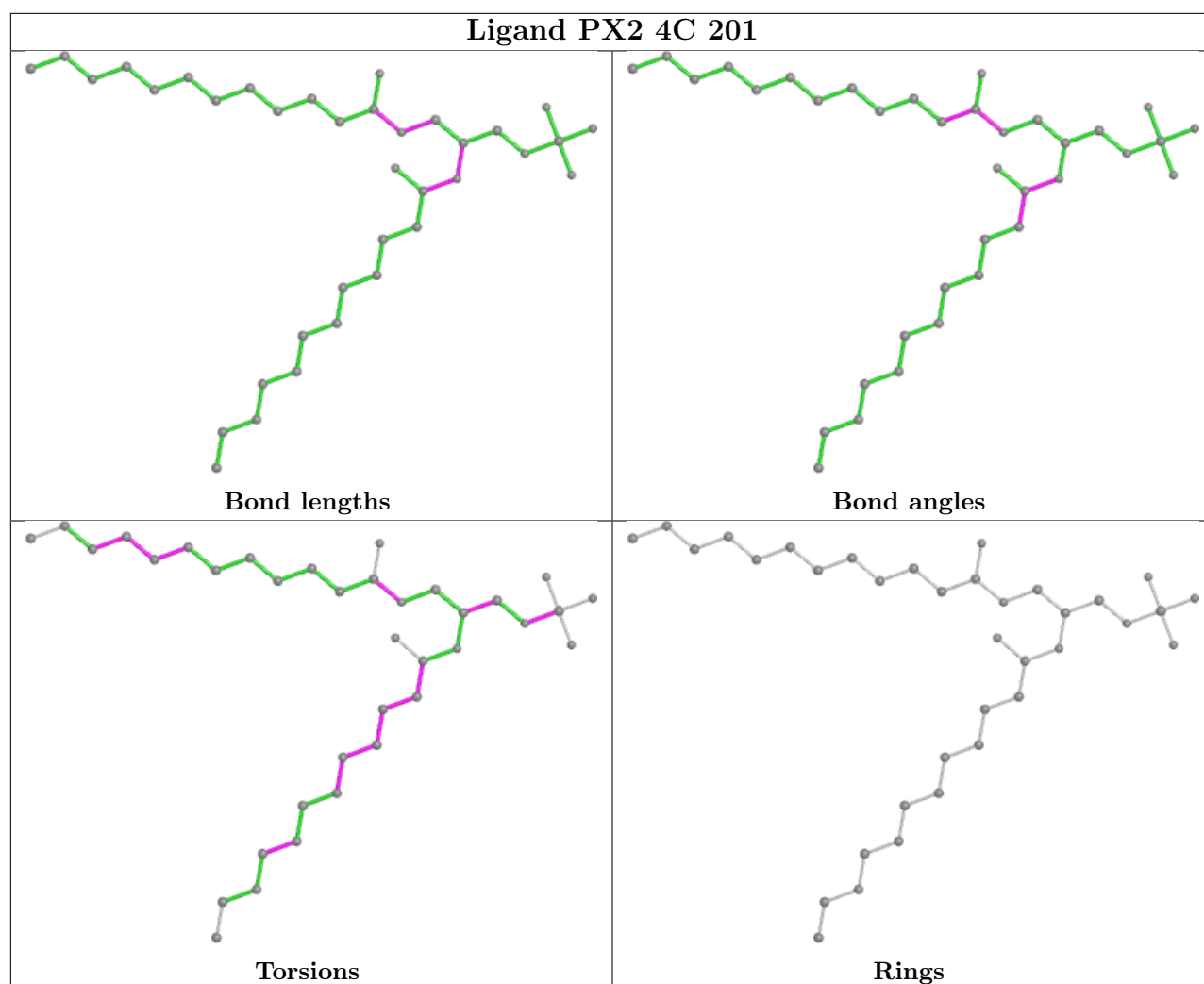


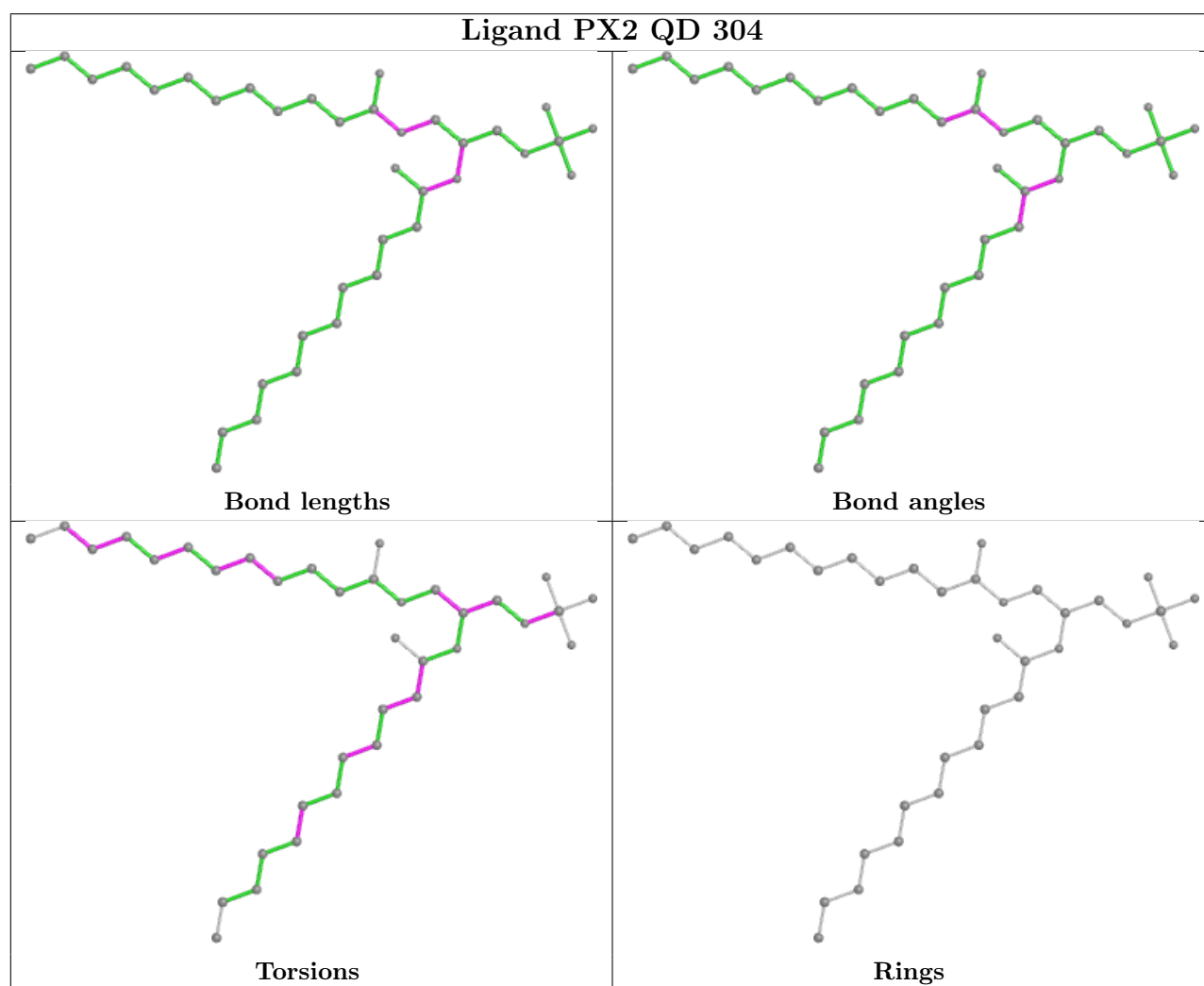
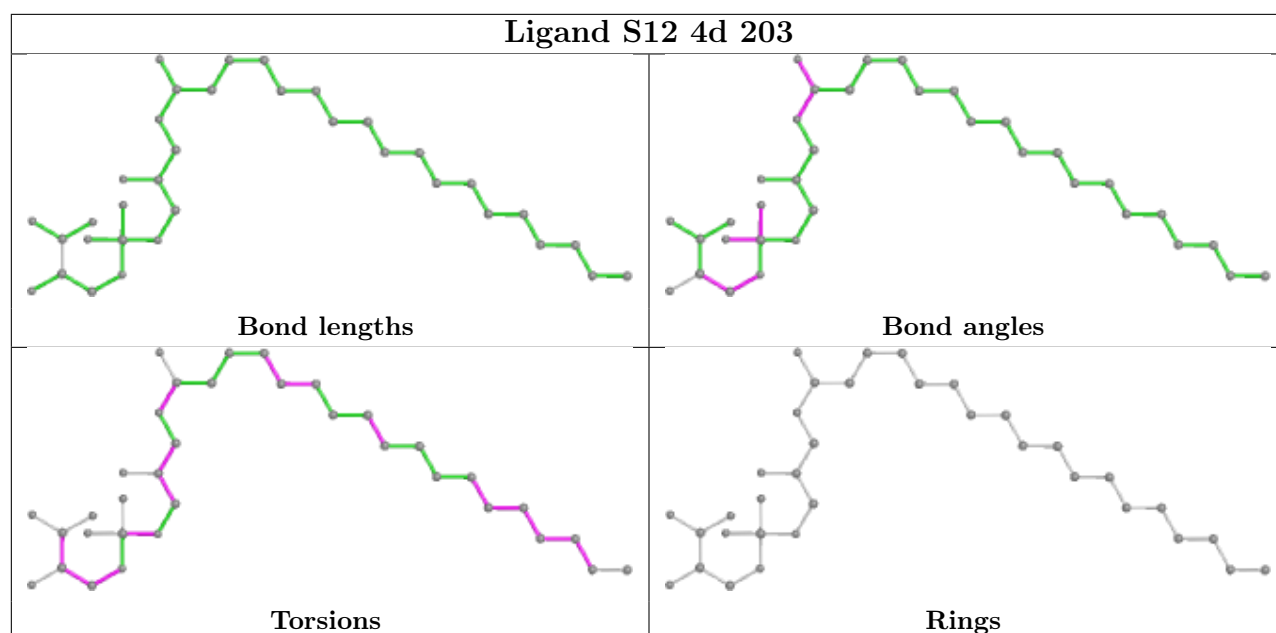


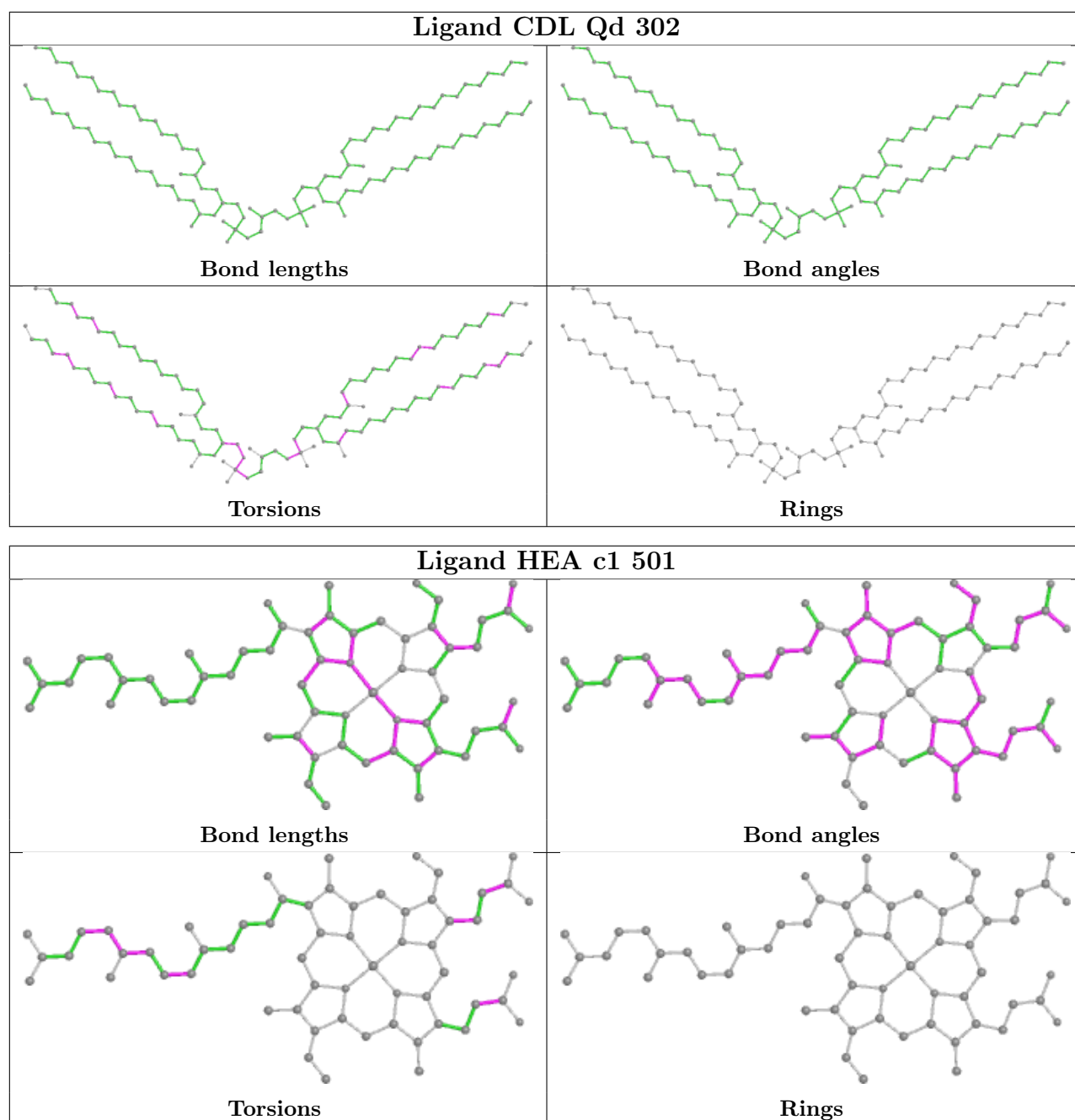












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.