



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 07:24 am BST

PDB ID : 9FQ7 / pdb_00009fq7
EMDB ID : EMD-50403
Title : Perkinsus marinus Respiratory supercomplex CII2CIII2CIV2 in c1 state
Authors : Wu, F.; Amunts, A.
Deposited on : 2024-06-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

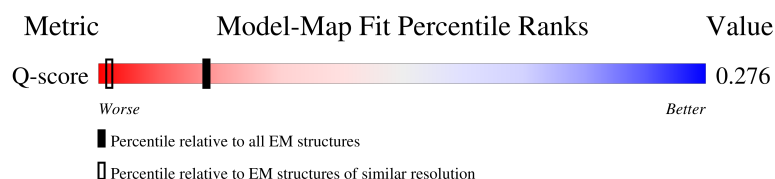
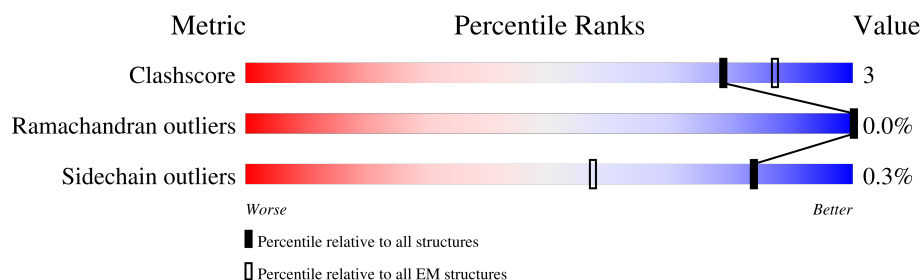
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	2M	604	94% 90% 9%
1	2m	604	93% 89% 10%
2	2N	259	62% 92% 8%
2	2n	259	61% 92% 8%

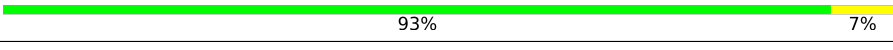
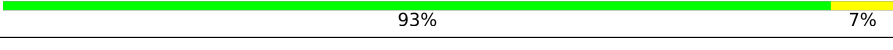
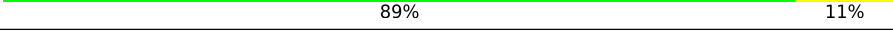
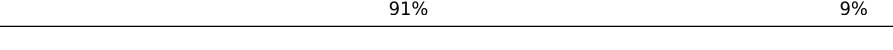
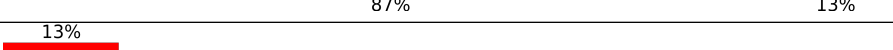
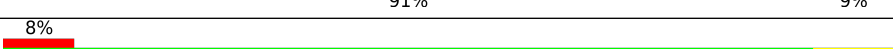
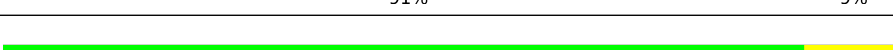
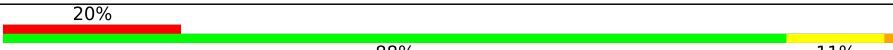
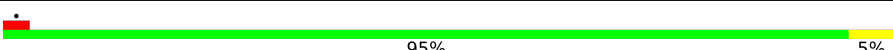
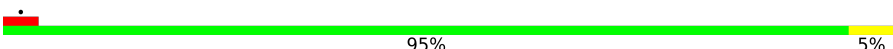
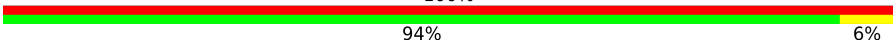
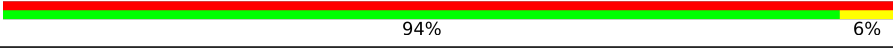
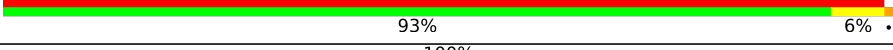
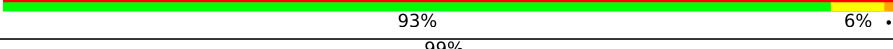
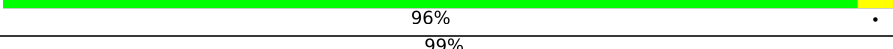
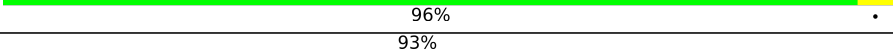
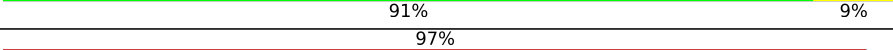
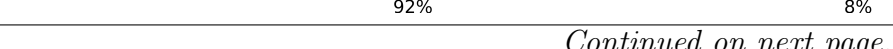
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Mol	Chain	Length	Quality of chain
3	2O	160	6% 96% .
3	2o	160	8% 95% 5% .
4	2P	158	11% 92% 7% .
4	2p	158	9% 91% 9% .
5	2Q	69	17% 96% .
5	2q	69	19% 94% 6% .
6	2R	117	13% 91% 9% .
6	2r	117	15% 91% 9% .
7	2S	164	23% 98% .
7	2s	164	21% 98% .
8	2T	82	10% 88% 9% .
8	2t	82	6% 89% 7% .
9	2U	48	46% 90% 10% .
9	2u	48	46% 88% 12% .
10	2V	86	58% 92% 8% .
10	2v	86	53% 93% 7% .
11	30	173	79% 91% 9% .
12	31	159	81% 82% 15% .
13	3A	454	. 96% .
13	3a	454	5% 97% .
14	3B	496	. 96% .
14	3b	496	. 96% .
15	3C	242	. 95% 5% .
15	3c	242	. 90% 9% .
16	3D	95	. 91% 9% .

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Mol	Chain	Length	Quality of chain
16	3d	95	
17	3E	92	
17	3e	92	
18	3F	84	
18	3f	84	
19	3G	354	
19	3g	354	
20	3H	326	
20	3h	326	
21	3I	176	
21	3i	176	
22	3J	92	
22	3j	92	
23	3K	79	
23	3k	79	
24	3L	68	
24	3l	68	
25	40	230	
25	41	230	
26	4A	100	
26	4a	100	
27	4B	93	
27	4b	93	
28	4C	75	
28	4c	75	

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Mol	Chain	Length	Quality of chain
29	4D	90	99% 86% 13%
29	4d	90	100% 86% 13%
30	4E	152	100% 95% 5%
30	4e	152	100% 94% 5%
31	4F	85	92% 88% 6% 6%
31	4f	85	98% 96%
32	4G	100	99% 95% 5%
32	4g	100	100% 95% 5%
33	4H	141	100% 96%
33	4h	141	100% 96%
34	4I	196	100% 93% 7%
34	4i	196	100% 93% 7%
35	4J	186	100% 90% 10%
35	4j	186	100% 92% 8%
36	4K	93	100% 90% 10%
36	4k	93	100% 88% 12%
37	4L	122	100% 93% 7%
37	4l	122	100% 91% 9%
38	4M	99	100% 91% 9%
38	4m	99	100% 90% 10%
39	4N	131	100% 96%
39	4n	131	100% 95% 5%
40	4O	47	100% 94% 6%
40	4o	47	100% 89% 11%
41	4P	180	100% 92% 8%

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Mol	Chain	Length	Quality of chain
41	4p	180	100% 92% 8%
42	4Q	459	100% 89% 11%
42	4q	459	100% 90% 10%
43	4R	103	100% 98% .
43	4r	103	100% 94% 6%
44	4S	65	100% 95% 5%
44	4s	65	100% 95% 5%
45	4T	121	100% 97% .
45	4t	121	100% 95% 5%
46	4U	91	100% 89% 11%
46	4u	91	100% 89% 11%
47	4V	185	100% 94% 6%
47	4v	185	100% 94% 6%
48	4W	141	100% 90% 10%
48	4w	141	100% 90% 10%
49	4X	226	100% 95% 5%
49	4x	226	100% 93% 7%
50	4Y	107	100% 95% 5%
50	4y	107	100% 94% 6%
51	4Z	186	99% 94% 6%
51	4z	186	99% 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	HEC	3C	302	X	-	-	-
61	HEC	3c	302	X	-	-	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 142971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2M	604	Total	C	N	O	S	0	0
			4602	2877	828	871	26		
1	2m	604	Total	C	N	O	S	0	0
			4602	2877	828	871	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2N	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		
2	2n	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		

- Molecule 3 is a protein called SDHG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2O	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		
3	2o	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2P	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		
4	2p	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		

- Molecule 5 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2Q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		
5	2q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		

- Molecule 6 is a protein called SDHH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2R	117	Total	C	N	O	S	0	0
			950	621	166	157	6		
6	2r	117	Total	C	N	O	S	0	0
			950	621	166	157	6		

- Molecule 7 is a protein called DUF6827 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2S	164	Total	C	N	O	S	0	0
			1323	832	223	257	11		
7	2s	164	Total	C	N	O	S	0	0
			1323	832	223	257	11		

- Molecule 8 is a protein called Rab-GAP TBC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2T	82	Total	C	N	O	S	0	0
			695	446	117	128	4		
8	2t	82	Total	C	N	O	S	0	0
			695	446	117	128	4		

- Molecule 9 is a protein called SDHC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2U	48	Total	C	N	O	S	0	0
			390	246	68	75	1		
9	2u	48	Total	C	N	O	S	0	0
			390	246	68	75	1		

- Molecule 10 is a protein called SDHI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2V	86	Total	C	N	O	S	0	0
			701	452	118	125	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2v	86	Total	C	N	O	S	0	0
			701	452	118	125	6		

- Molecule 11 is a protein called ISPR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	30	173	Total	C	N	O	S	0	0
			1181	723	209	242	7		

- Molecule 12 is a protein called ISPR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	31	159	Total	C	N	O	S	0	0
			1219	748	222	235	14		

- Molecule 13 is a protein called Mitochondrial processing peptidase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3A	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		
13	3a	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		

- Molecule 14 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3B	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		
14	3b	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		

- Molecule 15 is a protein called CytC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3C	241	Total	C	N	O	S	0	0
			1921	1225	334	349	13		
15	3c	242	Total	C	N	O	S	0	0
			1930	1230	335	352	13		

- Molecule 16 is a protein called QCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3D	95	Total	C	N	O	S	0	0
			836	551	146	135	4		
16	3d	95	Total	C	N	O	S	0	0
			836	551	146	135	4		

- Molecule 17 is a protein called QCR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3E	92	Total	C	N	O	S	0	0
			813	545	138	127	3		
17	3e	92	Total	C	N	O	S	0	0
			813	545	138	127	3		

- Molecule 18 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3F	84	Total	C	N	O	S	0	0
			734	493	123	114	4		
18	3f	84	Total	C	N	O	S	0	0
			734	493	123	114	4		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3G	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		
19	3g	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		

- Molecule 20 is a protein called Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3H	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		
20	3h	326	Total	C	N	O	S	0	0
			2621	1663	478	465	15		

- Molecule 21 is a protein called Ubiquinol-cytochrome C reductase complex 14kD subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3I	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		
21	3i	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		

- Molecule 22 is a protein called Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3J	92	Total	C	N	O	S	0	0
			755	471	134	139	11		
22	3j	92	Total	C	N	O	S	0	0
			755	471	134	139	11		

- Molecule 23 is a protein called QCR11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3K	79	Total	C	N	O	S	0	0
			608	391	110	103	4		
23	3k	79	Total	C	N	O	S	0	0
			608	391	110	103	4		

- Molecule 24 is a protein called Aurora kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3L	68	Total	C	N	O	S	0	0
			539	348	92	96	3		
24	3l	68	Total	C	N	O	S	0	0
			539	348	92	96	3		

- Molecule 25 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	40	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		
25	41	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4A	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	4a	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

- Molecule 27 is a protein called Peptidase M14 carboxypeptidase A domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4B	93	Total	C	N	O	S	0	0
			732	479	116	129	8		
27	4b	93	Total	C	N	O	S	0	0
			732	479	116	129	8		

- Molecule 28 is a protein called Cytochrome c oxidase subunit 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4C	75	Total	C	N	O	S	0	0
			626	414	95	113	4		
28	4c	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

- Molecule 29 is a protein called Cytochrome c oxidase subunit 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4D	90	Total	C	N	O	S	0	0
			787	525	128	131	3		
29	4d	90	Total	C	N	O	S	0	0
			787	525	128	131	3		

- Molecule 30 is a protein called Merozoite surface protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4E	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		
30	4e	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		

- Molecule 31 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4F	80	Total	C	N	O	S	0	0
			669	438	119	110	2		
31	4f	85	Total	C	N	O	S	0	0
			708	462	126	118	2		

- Molecule 32 is a protein called Cytochrome c oxidase subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4G	100	Total	C	N	O	S	0	0
			854	550	156	144	4		
32	4g	100	Total	C	N	O	S	0	0
			854	550	156	144	4		

- Molecule 33 is a protein called Cytochrome c oxidase subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4H	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		
33	4h	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		

- Molecule 34 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4I	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		
34	4i	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4J	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		
35	4j	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4K	93	Total	C	N	O	S	0	0
			722	473	129	118	2		
36	4k	93	Total	C	N	O	S	0	0
			722	473	129	118	2		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4L	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		
37	4l	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4M	99	Total	C	N	O	S	0	0
			778	501	148	128	1		
38	4m	99	Total	C	N	O	S	0	0
			778	501	148	128	1		

- Molecule 39 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4N	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		
39	4n	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		

- Molecule 40 is a protein called GINS subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4O	47	Total	C	N	O	S	0	0
			383	257	60	63	3		
40	4o	47	Total	C	N	O	S	0	0
			383	257	60	63	3		

- Molecule 41 is a protein called Cytochrome oxidase subunit II copper A binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	4P	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		
41	4p	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4Q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	4q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4R	103	Total	C	N	O	S	0	0
			916	609	156	145	6		
43	4r	103	Total	C	N	O	S	0	0
			916	609	156	145	6		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4S	65	Total	C	N	O	S	0	0
			541	350	85	100	6		
44	4s	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4T	121	Total	C	N	O	S	0	0
			983	634	170	167	12		
45	4t	121	Total	C	N	O	S	0	0
			983	634	170	167	12		

- Molecule 46 is a protein called Amino acid transporter transmembrane domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4U	91	Total	C	N	O	S	0	0
			758	503	125	127	3		
46	4u	91	Total	C	N	O	S	0	0
			758	503	125	127	3		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4V	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
47	4v	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4W	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		
48	4w	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		

- Molecule 49 is a protein called Cytochrome Coxidase subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	4X	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		
49	4x	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

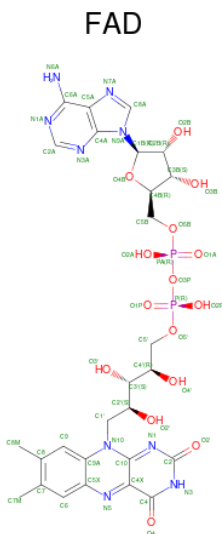
- Molecule 50 is a protein called Cytochrome c oxidase subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4Y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		
50	4y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 31.

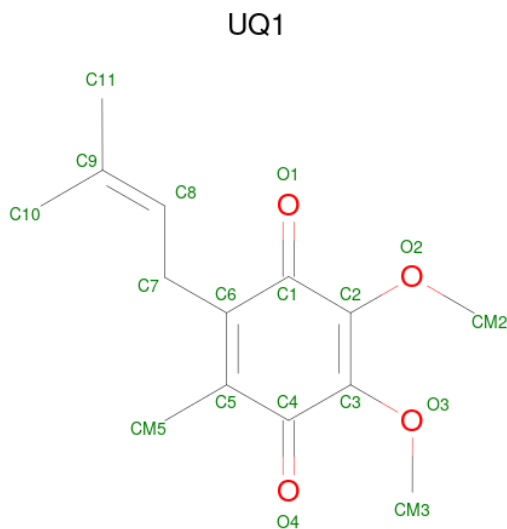
Mol	Chain	Residues	Atoms					AltConf	Trace
51	4Z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		
51	4z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		

- Molecule 52 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
52	2M	1	Total 53	C 27	N 9	O 15	P 2	0
52	2m	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 53 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



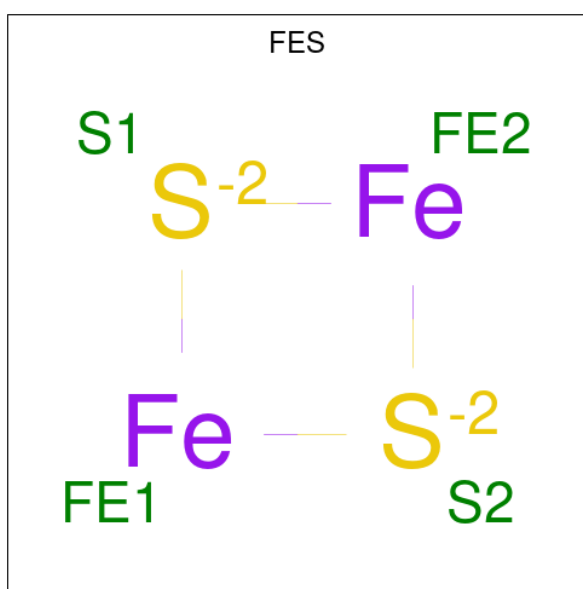
Mol	Chain	Residues	Atoms			AltConf
53	2N	1	Total 18	C 14	O 4	0
53	2p	1	Total 18	C 14	O 4	0

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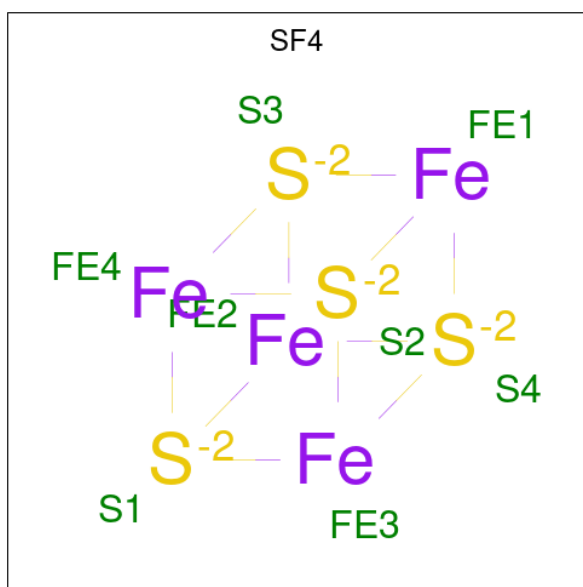
Mol	Chain	Residues	Atoms			AltConf
53	3G	1	Total	C	O	0
			18	14	4	
53	3G	1	Total	C	O	0
			18	14	4	
53	3g	1	Total	C	O	0
			18	14	4	
53	3g	1	Total	C	O	0
			18	14	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



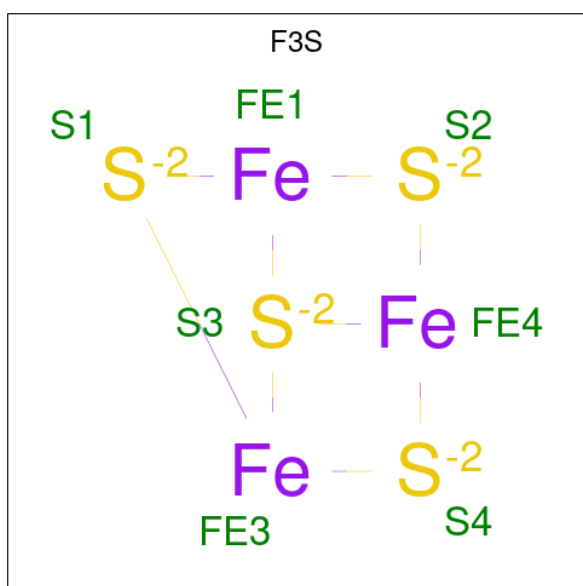
Mol	Chain	Residues	Atoms			AltConf
54	2N	1	Total	Fe	S	0
			4	2	2	
54	2n	1	Total	Fe	S	0
			4	2	2	
54	3H	1	Total	Fe	S	0
			4	2	2	
54	3h	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
55	2N	1	Total	Fe	S	0
			8	4	4	
55	2n	1	Total	Fe	S	0
			8	4	4	

- Molecule 56 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

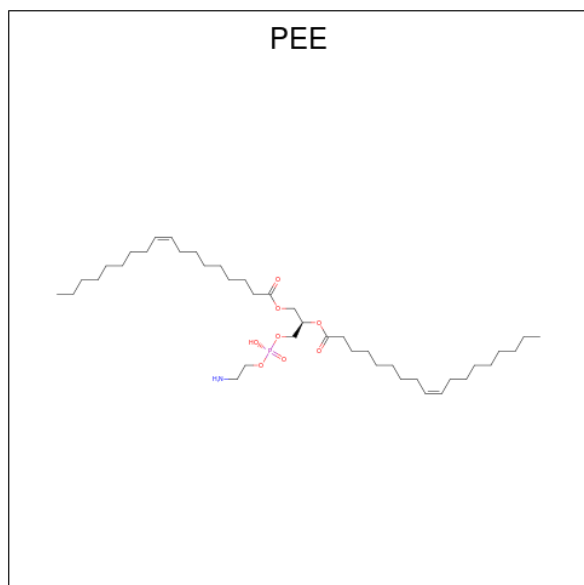


Mol	Chain	Residues	Atoms			AltConf
56	2N	1	Total	Fe	S	0
			7	3	4	
56	2n	1	Total	Fe	S	0
			7	3	4	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	2N	1	Total	K	0
			1	1	
57	2n	1	Total	K	0
			1	1	
57	4Q	1	Total	K	0
			1	1	
57	4q	1	Total	K	0
			1	1	

- Molecule 58 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
58	2O	1	Total	C	N	O	P	0
			39	29	1	8	1	
58	2O	1	Total	C	N	O	P	0
			41	31	1	8	1	
58	2P	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	2T	1	Total	C	N	O	P	0
			45	35	1	8	1	
58	2o	1	Total	C	N	O	P	0
			24	14	1	8	1	
58	2p	1	Total	C	N	O	P	0
			24	14	1	8	1	

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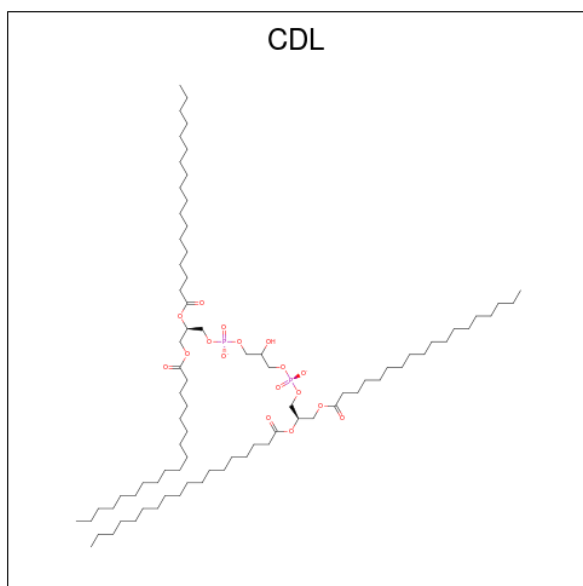
Mol	Chain	Residues	Atoms					AltConf
58	2r	1	Total	C	N	O	P	0
			39	29	1	8	1	
58	2t	1	Total	C	N	O	P	0
			42	32	1	8	1	
58	3C	1	Total	C	N	O	P	0
			30	20	1	8	1	
58	3H	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	3c	1	Total	C	N	O	P	0
			33	23	1	8	1	
58	3f	1	Total	C	N	O	P	0
			38	28	1	8	1	
58	40	1	Total	C	N	O	P	0
			45	35	1	8	1	
58	40	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	40	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	40	1	Total	C	N	O	P	0
			31	21	1	8	1	
58	41	1	Total	C	N	O	P	0
			45	35	1	8	1	
58	41	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	41	1	Total	C	N	O	P	0
			36	26	1	8	1	
58	4D	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	4Q	1	Total	C	N	O	P	0
			36	26	1	8	1	
58	4R	1	Total	C	N	O	P	0
			43	33	1	8	1	
58	4S	1	Total	C	N	O	P	0
			27	17	1	8	1	
58	4W	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4d	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4l	1	Total	C	N	O	P	0
			38	28	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
58	4q	1	Total	C	N	O	P	0
			37	27	1	8	1	
58	4q	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	4s	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	4w	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4z	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 59 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
59	2O	1	Total	C	O	P	0
			67	48	17	2	
59	2P	1	Total	C	O	P	0
			81	62	17	2	
59	2Q	1	Total	C	O	P	0
			100	81	17	2	
59	2T	1	Total	C	O	P	0
			71	52	17	2	
59	2o	1	Total	C	O	P	0
			86	67	17	2	
59	2p	1	Total	C	O	P	0
			74	55	17	2	

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Mol	Chain	Residues	Atoms				AltConf
59	2q	1	Total 100	C 81	O 17	P 2	0
59	2t	1	Total 66	C 47	O 17	P 2	0
59	3D	1	Total 84	C 65	O 17	P 2	0
59	3D	1	Total 100	C 81	O 17	P 2	0
59	3E	1	Total 93	C 74	O 17	P 2	0
59	3G	1	Total 100	C 81	O 17	P 2	0
59	3G	1	Total 75	C 56	O 17	P 2	0
59	3H	1	Total 89	C 70	O 17	P 2	0
59	3H	1	Total 84	C 65	O 17	P 2	0
59	3I	1	Total 68	C 49	O 17	P 2	0
59	3I	1	Total 81	C 62	O 17	P 2	0
59	3I	1	Total 63	C 44	O 17	P 2	0
59	3L	1	Total 85	C 66	O 17	P 2	0
59	3L	1	Total 81	C 62	O 17	P 2	0
59	3L	1	Total 93	C 74	O 17	P 2	0
59	3e	1	Total 71	C 52	O 17	P 2	0
59	3e	1	Total 77	C 58	O 17	P 2	0
59	3g	1	Total 70	C 51	O 17	P 2	0
59	3g	1	Total 89	C 70	O 17	P 2	0
59	3g	1	Total 90	C 71	O 17	P 2	0
59	3g	1	Total 58	C 39	O 17	P 2	0

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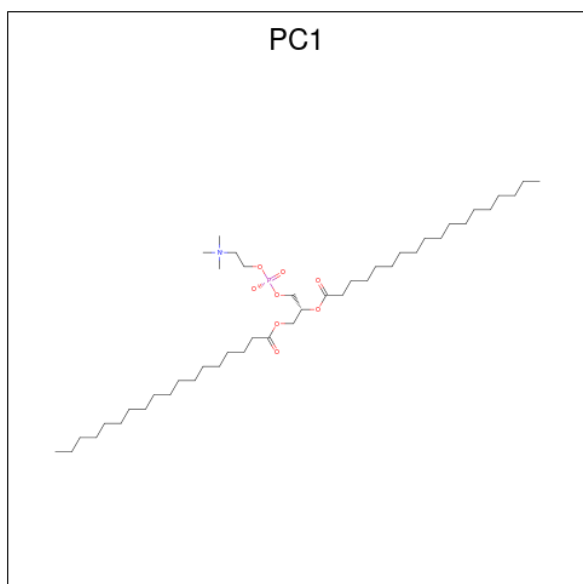
Mol	Chain	Residues	Atoms				AltConf
59	3h	1	Total	C	O	P	0
			85	66	17	2	
59	3i	1	Total	C	O	P	0
			51	32	17	2	
59	3i	1	Total	C	O	P	0
			76	57	17	2	
59	3l	1	Total	C	O	P	0
			100	81	17	2	
59	3l	1	Total	C	O	P	0
			81	62	17	2	
59	4l	1	Total	C	O	P	0
			92	73	17	2	
59	4E	1	Total	C	O	P	0
			89	70	17	2	
59	4E	1	Total	C	O	P	0
			46	27	17	2	
59	4F	1	Total	C	O	P	0
			100	81	17	2	
59	4J	1	Total	C	O	P	0
			59	40	17	2	
59	4K	1	Total	C	O	P	0
			90	71	17	2	
59	4L	1	Total	C	O	P	0
			94	75	17	2	
59	4M	1	Total	C	O	P	0
			75	56	17	2	
59	4O	1	Total	C	O	P	0
			97	78	17	2	
59	4Q	1	Total	C	O	P	0
			95	76	17	2	
59	4Q	1	Total	C	O	P	0
			75	56	17	2	
59	4S	1	Total	C	O	P	0
			100	81	17	2	
59	4U	1	Total	C	O	P	0
			72	53	17	2	
59	4W	1	Total	C	O	P	0
			73	54	17	2	
59	4Z	1	Total	C	O	P	0
			48	29	17	2	
59	4e	1	Total	C	O	P	0
			50	31	17	2	

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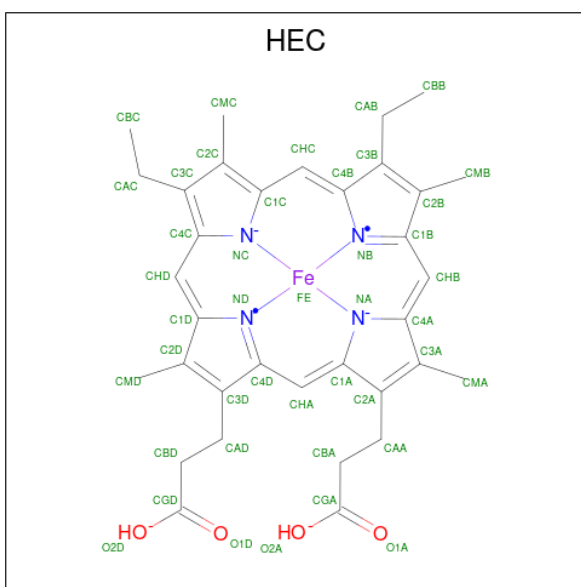
Mol	Chain	Residues	Atoms				AltConf
59	4e	1	Total	C	O	P	0
			96	77	17	2	
59	4f	1	Total	C	O	P	0
			92	73	17	2	
59	4g	1	Total	C	O	P	0
			66	47	17	2	
59	4j	1	Total	C	O	P	0
			51	32	17	2	
59	4j	1	Total	C	O	P	0
			88	69	17	2	
59	4m	1	Total	C	O	P	0
			100	81	17	2	
59	4o	1	Total	C	O	P	0
			93	74	17	2	
59	4q	1	Total	C	O	P	0
			93	74	17	2	
59	4s	1	Total	C	O	P	0
			100	81	17	2	
59	4t	1	Total	C	O	P	0
			61	42	17	2	
59	4z	1	Total	C	O	P	0
			93	74	17	2	
59	4z	1	Total	C	O	P	0
			86	67	17	2	

- Molecule 60 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



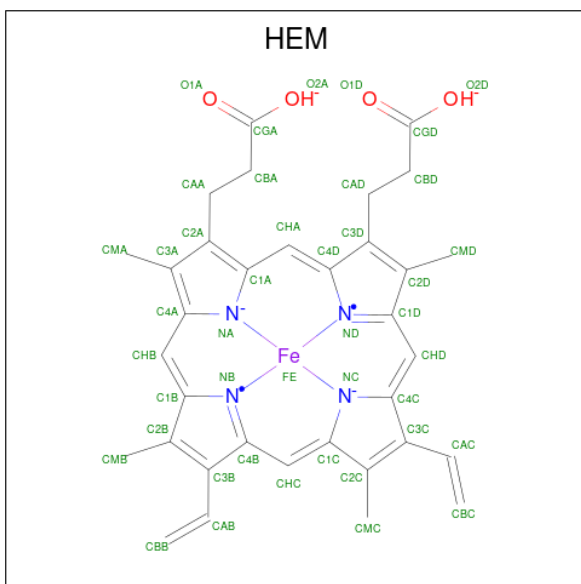
Mol	Chain	Residues	Atoms					AltConf
60	2P	1	Total	C	N	O	P	0
			35	25	1	8	1	
60	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2T	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2T	1	Total	C	N	O	P	0
			45	35	1	8	1	
60	2o	1	Total	C	N	O	P	0
			39	29	1	8	1	
60	2p	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	2r	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2r	1	Total	C	N	O	P	0
			52	42	1	8	1	
60	3A	1	Total	C	N	O	P	0
			38	28	1	8	1	
60	3H	1	Total	C	N	O	P	0
			34	24	1	8	1	
60	3H	1	Total	C	N	O	P	0
			33	23	1	8	1	
60	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	3f	1	Total	C	N	O	P	0
			46	36	1	8	1	
60	3h	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	3h	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	4F	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	4e	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 61 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
61	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
61	3c	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 62 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



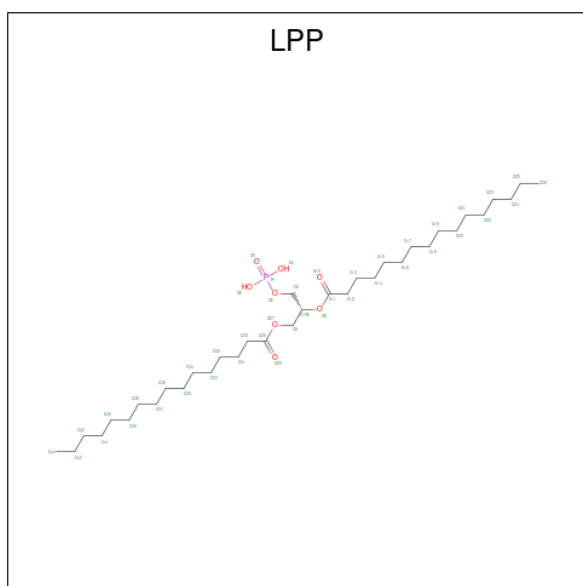
Mol	Chain	Residues	Atoms					AltConf
62	3G	1	Total 43	C 34	Fe 1	N 4	O 4	0

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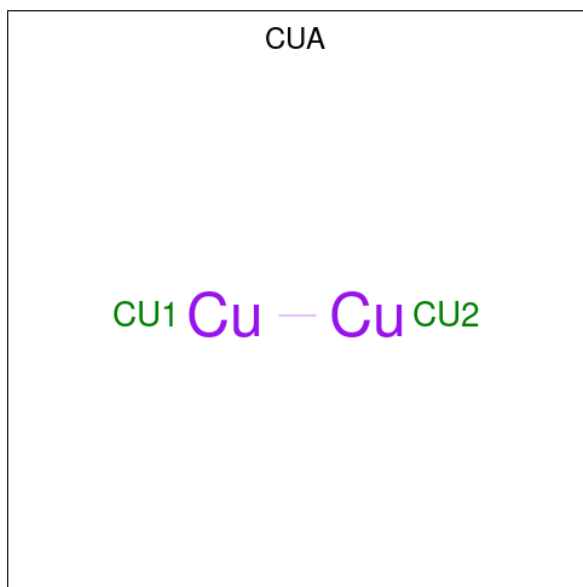
Mol	Chain	Residues	Atoms					AltConf
62	3G	1	Total 43	C 34	Fe 1	N 4	O 4	0
62	3g	1	Total 43	C 34	Fe 1	N 4	O 4	0
62	3g	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 63 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
63	4C	1	Total	C	O	P	0
			44	35	8	1	
63	4Z	1	Total	C	O	P	0
			44	35	8	1	
63	4g	1	Total	C	O	P	0
			39	30	8	1	
63	4z	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 64 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
64	4N	1	Total 2	Cu 2	0
64	4n	1	Total 2	Cu 2	0

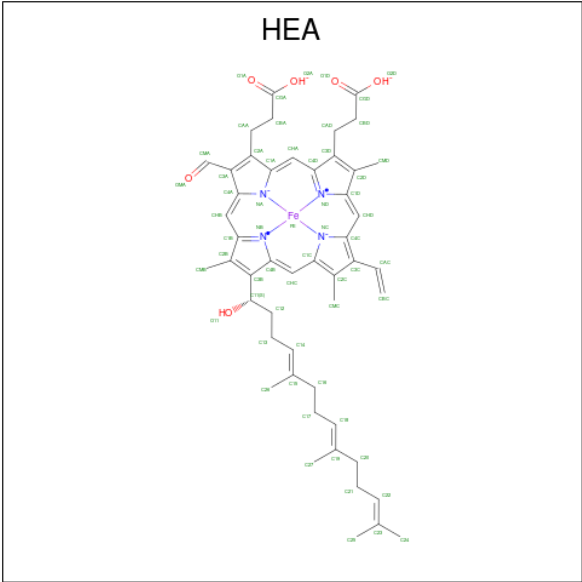
- Molecule 65 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
65	4Q	1	Total 1	Cu 1	0
65	4q	1	Total 1	Cu 1	0

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

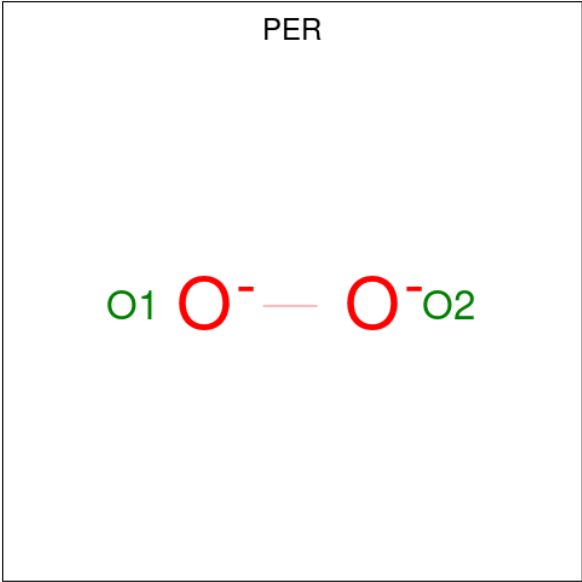
Mol	Chain	Residues	Atoms		AltConf
66	4Q	1	Total 1	Mg 1	0
66	4q	1	Total 1	Mg 1	0

- Molecule 67 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
67	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 68 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		AltConf
68	4Q	1	Total	O	0
			2	2	
68	4q	1	Total	O	0
			2	2	

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
69	4T	2	Total	Zn	0
			2	2	
69	4X	1	Total	Zn	0
			1	1	
69	4t	2	Total	Zn	0
			2	2	
69	4x	1	Total	Zn	0
			1	1	

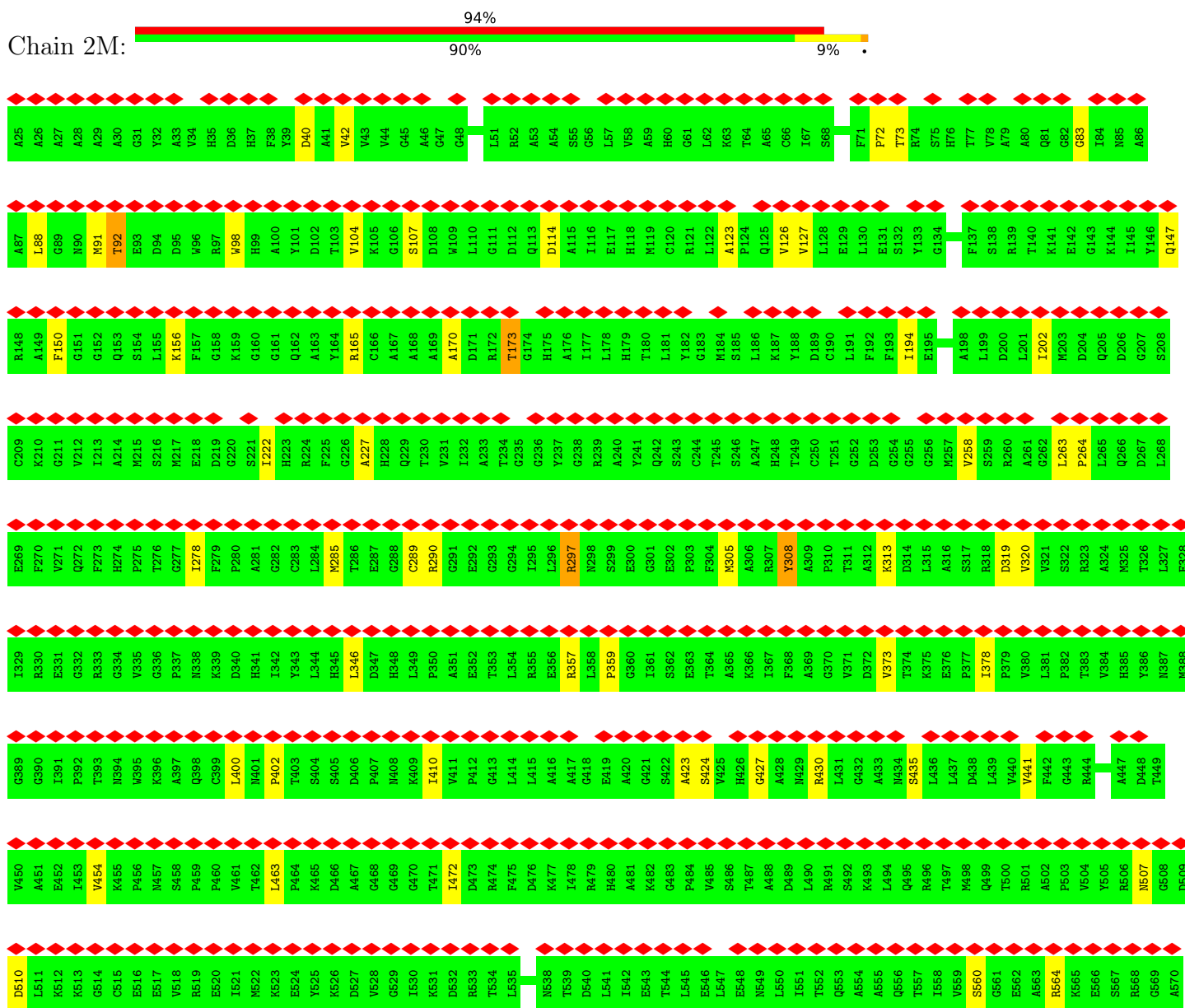
- Molecule 70 is water.

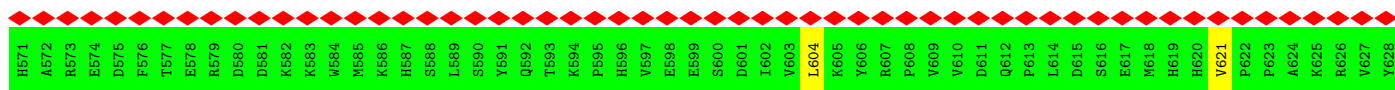
Mol	Chain	Residues	Atoms		AltConf
70	4Q	1	Total	O	0
			1	1	
70	4n	1	Total	O	0
			1	1	

3 Residue-property plots

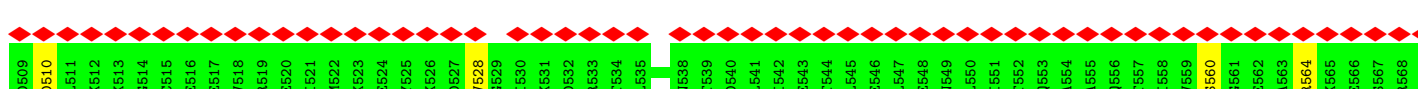
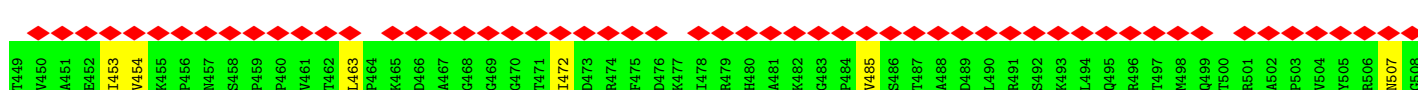
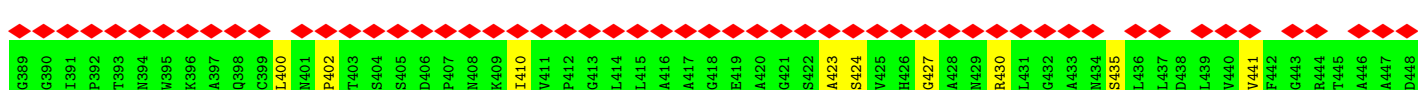
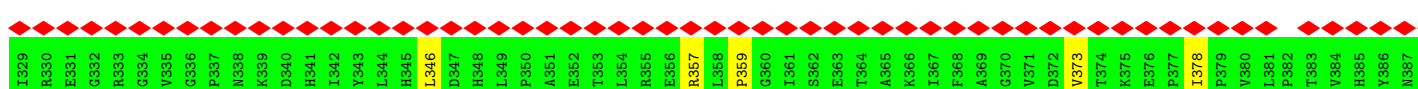
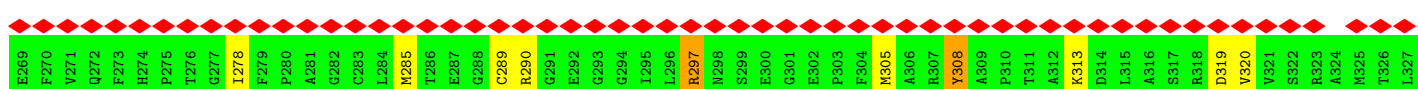
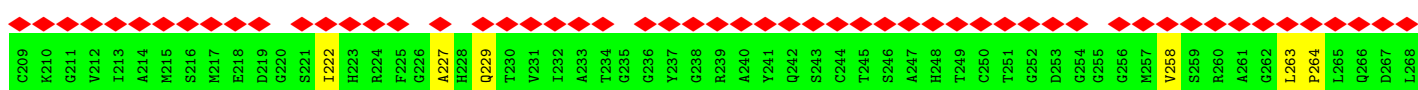
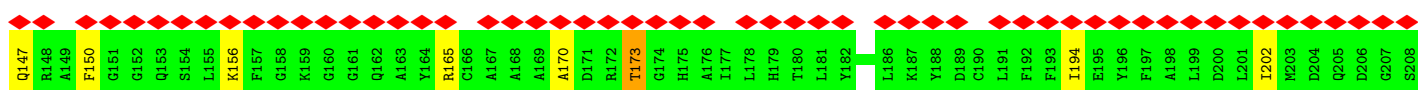
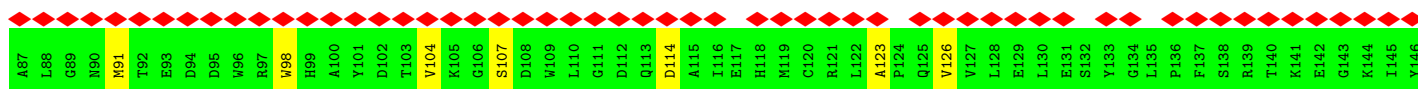
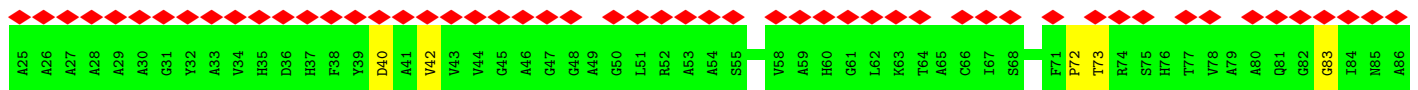
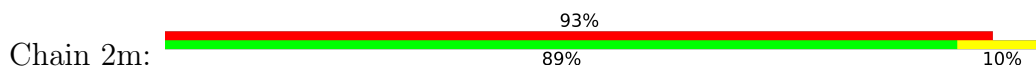
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



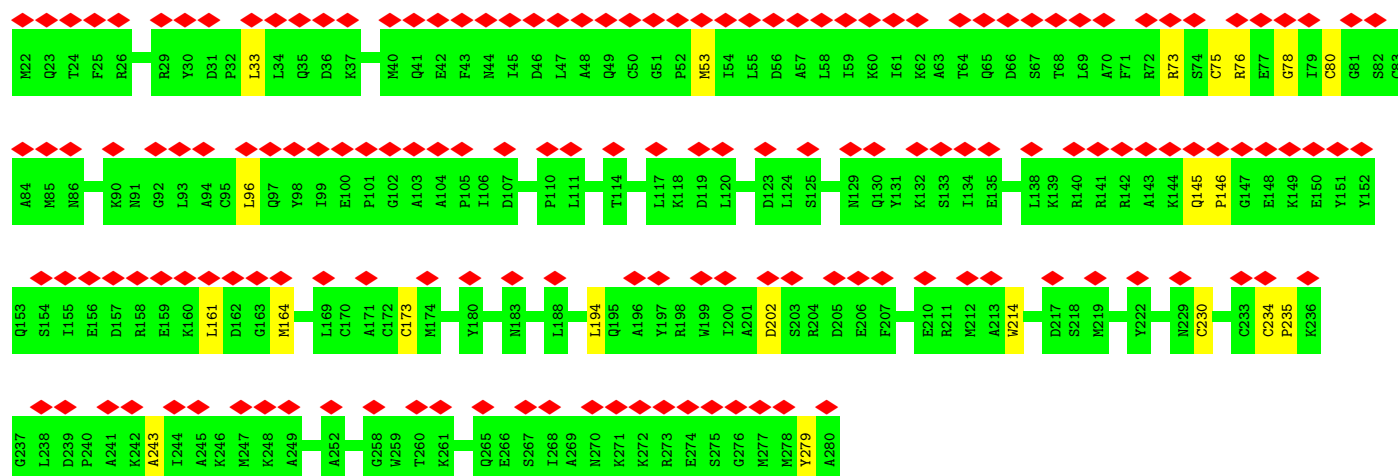


- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

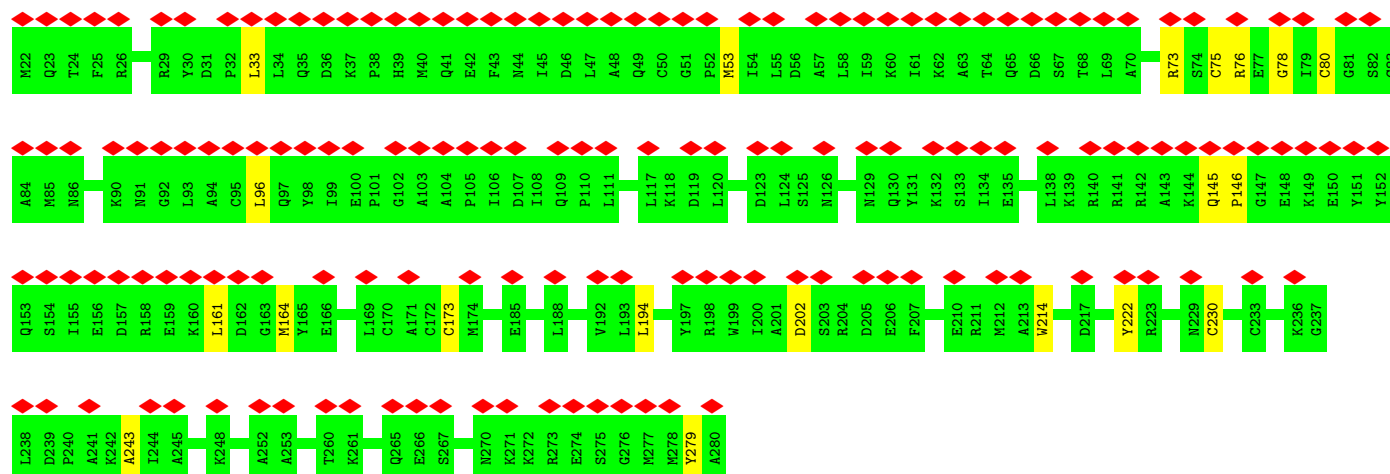


- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

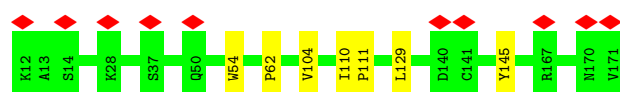




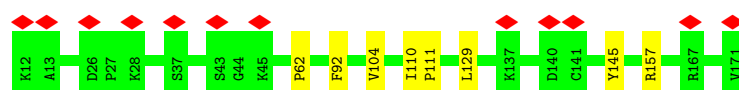
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



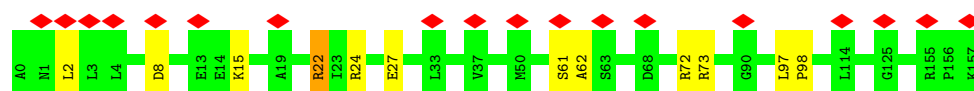
- Molecule 3: SDHG



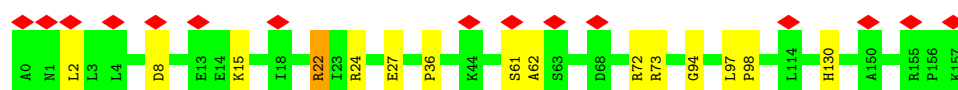
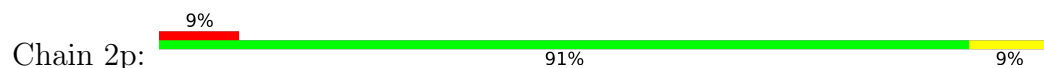
- Molecule 3: SDHG



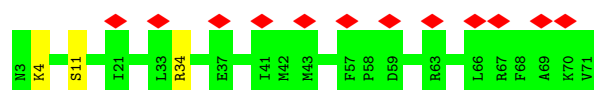
- Molecule 4: Transmembrane protein



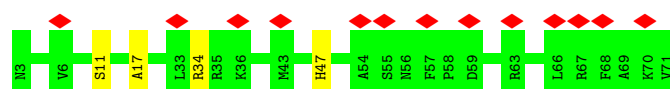
- Molecule 4: Transmembrane protein



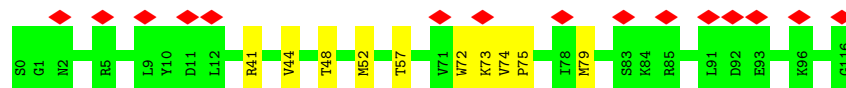
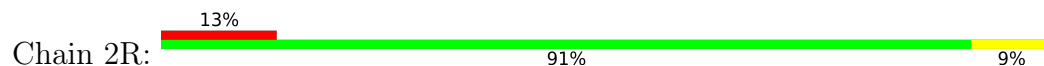
- Molecule 5: Kinesin-like protein



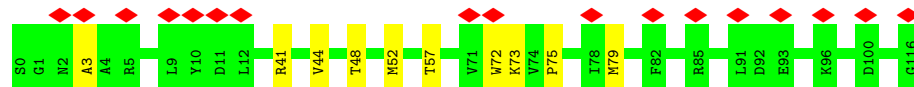
- Molecule 5: Kinesin-like protein



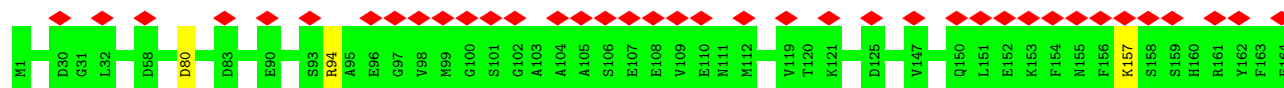
- Molecule 6: SDHH



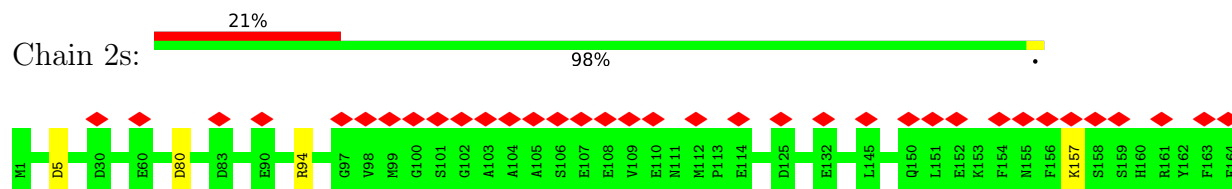
- Molecule 6: SDHH



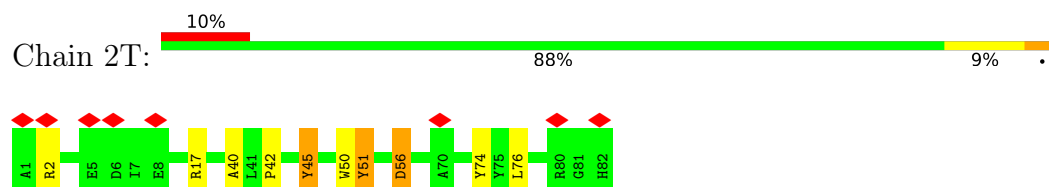
- Molecule 7: DUF6827 domain-containing protein



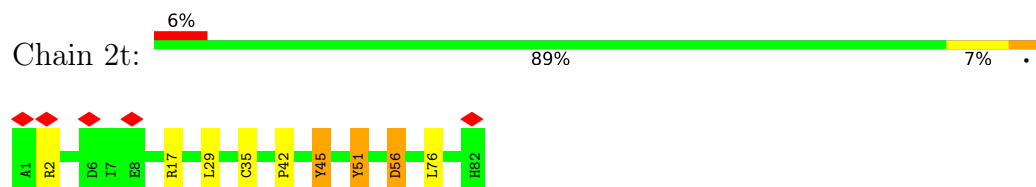
- Molecule 7: DUF6827 domain-containing protein



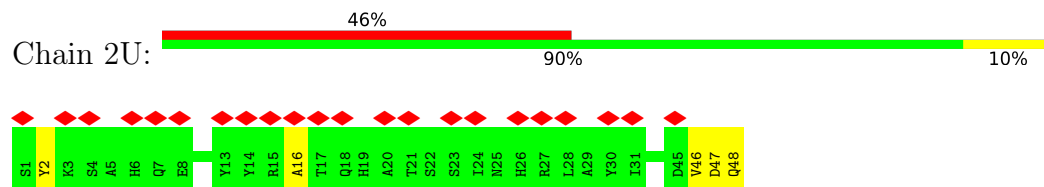
- Molecule 8: Rab-GAP TBC domain-containing protein



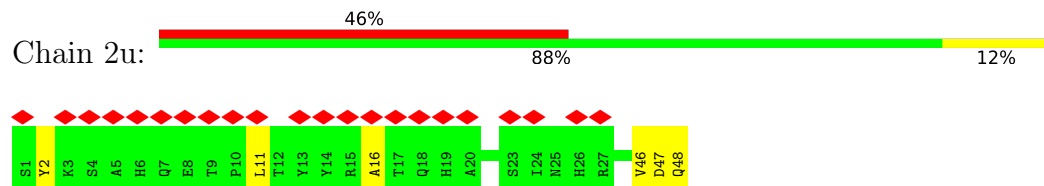
- Molecule 8: Rab-GAP TBC domain-containing protein



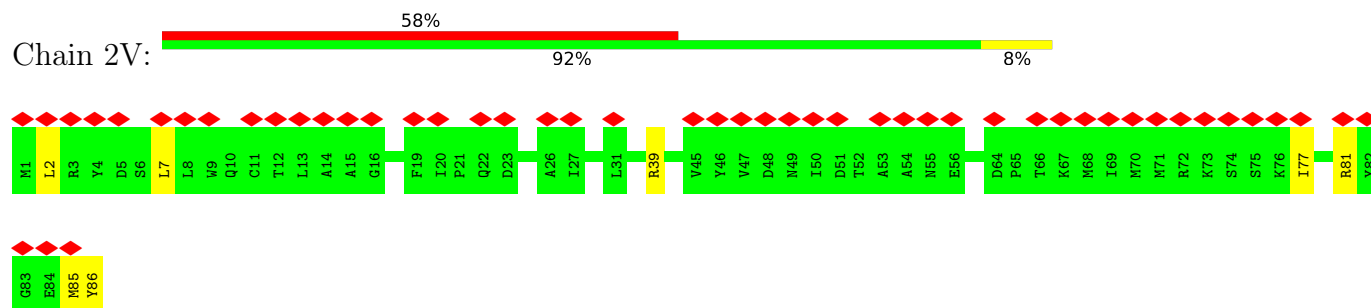
- Molecule 9: SDHC



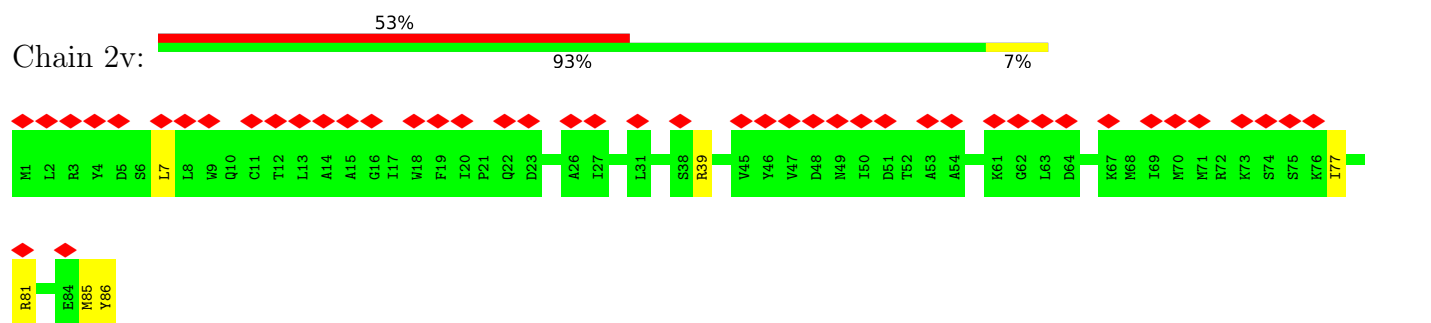
- Molecule 9: SDHC



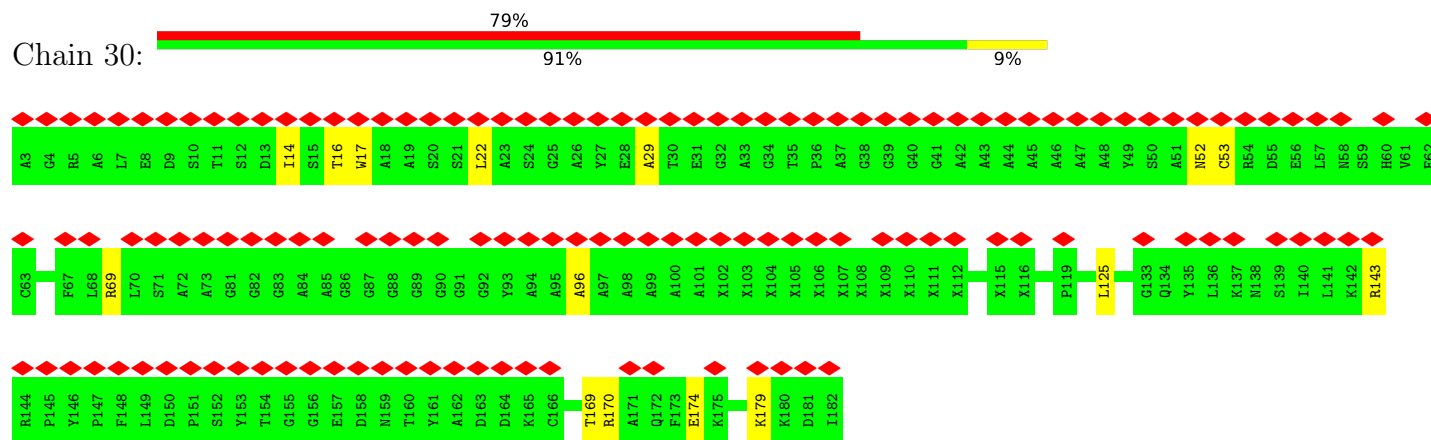
- Molecule 10: SDHI



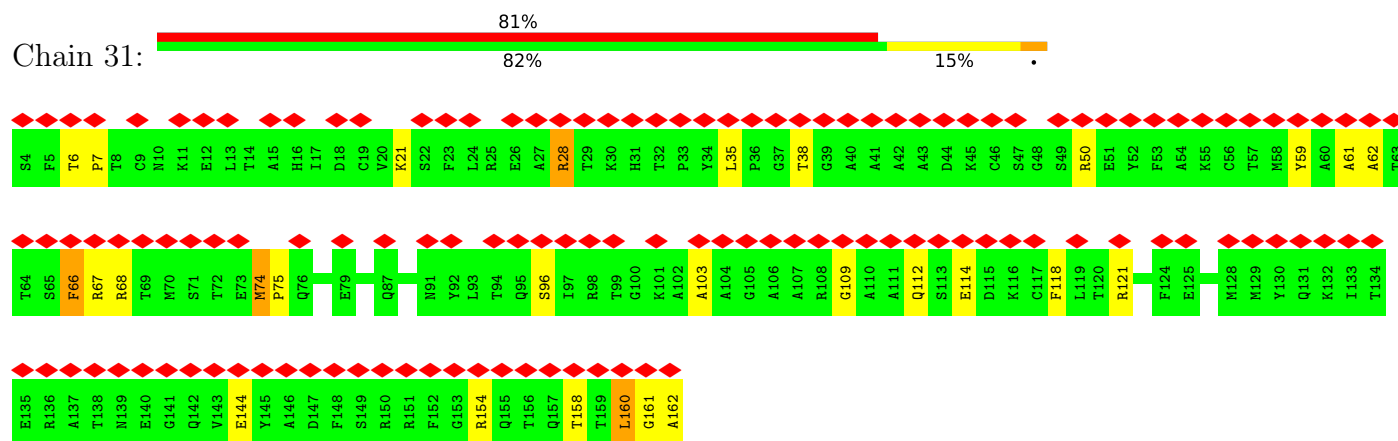
- Molecule 10: SDHI



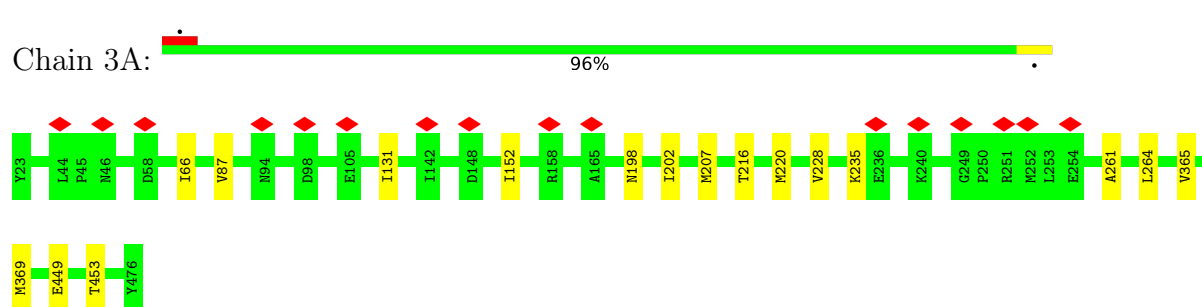
- Molecule 11: ISPR2



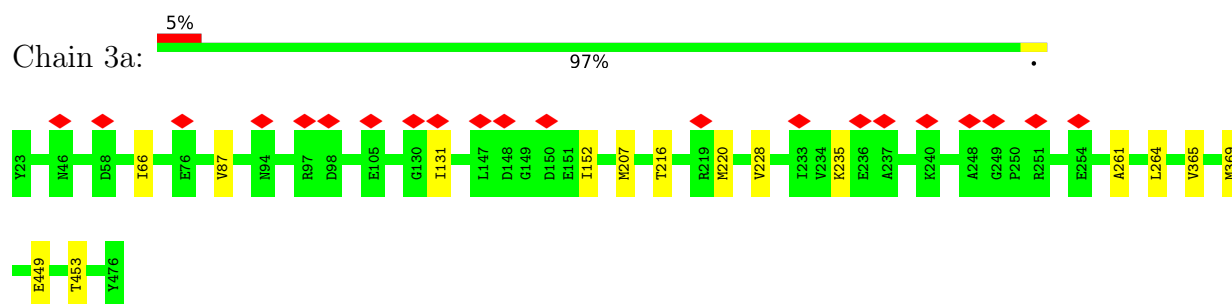
- Molecule 12: ISPR1



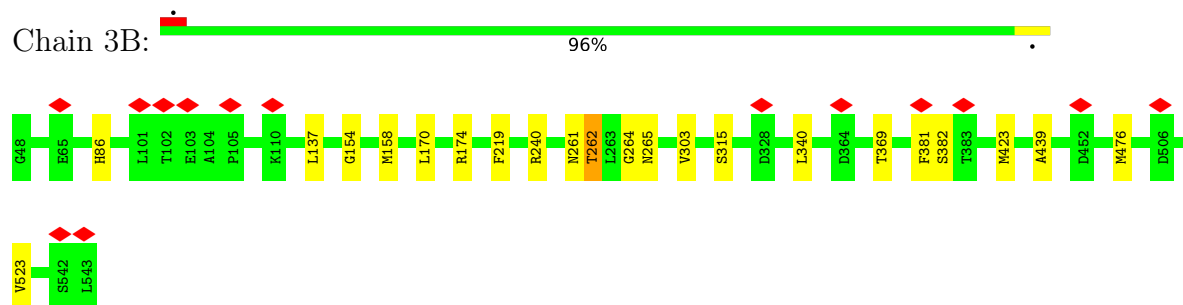
- Molecule 13: Mitochondrial processing peptidase beta subunit



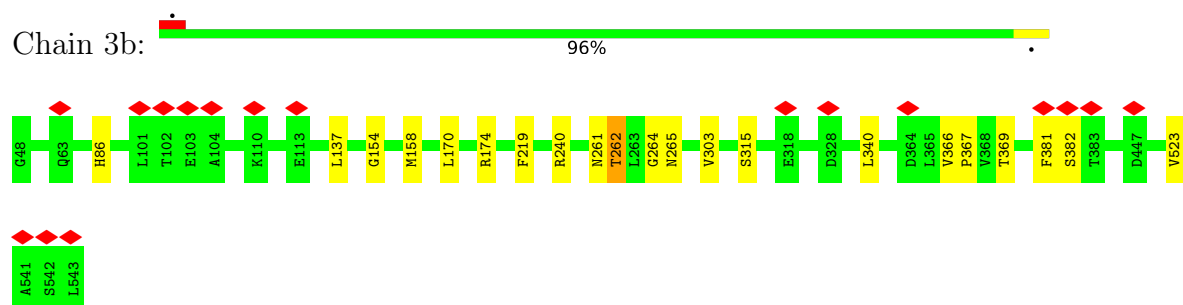
- Molecule 13: Mitochondrial processing peptidase beta subunit



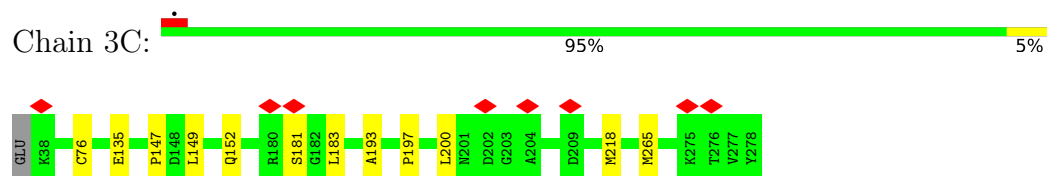
- Molecule 14: Alpha-MPP



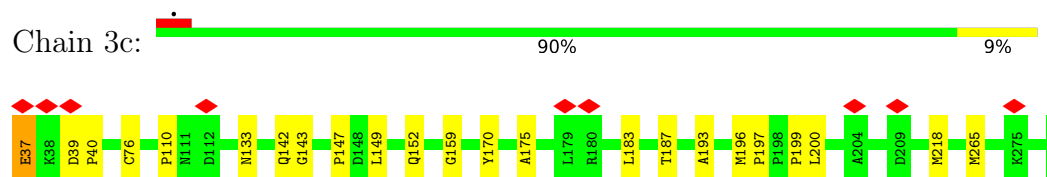
- Molecule 14: Alpha-MPP



- Molecule 15: CytC1

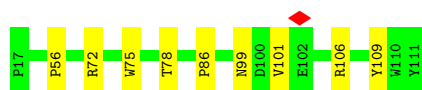


- Molecule 15: CytC1

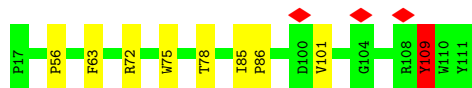
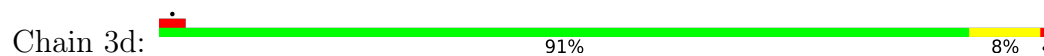


- Molecule 16: QCR8

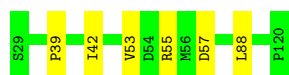




- Molecule 16: QCR8



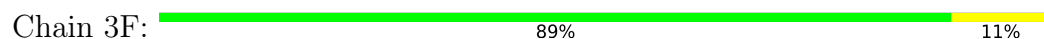
- Molecule 17: QCR9



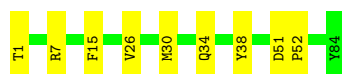
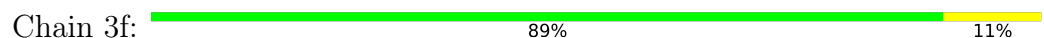
- Molecule 17: QCR9



- Molecule 18: QCR10



- Molecule 18: QCR10

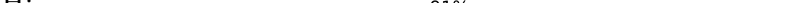


- Molecule 19: Cytochrome b

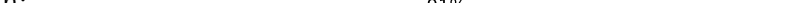


- Molecule 19: Cytochrome b

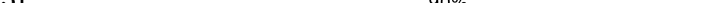
L288	G274	I277	V278	N280	I294	Y291	I296	M300	L305	M316	E327	L343	I344	M345	Y348	K352	K353												
F0 I1 L2	L20	I23	N42	M45	M46 I47	I57	Y79	V80	R88	N98	I101	G105	M108	L112	Y120 I121	S128	I136	T156	K161	Y164	F168	Y176	E195	N244	I245	L246	V247	P254	L259

- Chain 3H: 

Category	Item	Value	Color
Category 1	P273	100	Blue
	E274	100	Blue
	R275	100	Blue
	D276	100	Blue
	K277	100	Blue
	D278	100	Blue
	R279	100	Blue
	K282	100	Blue
	P283	100	Blue
	E284	100	Blue
Category 2	M288	100	Blue
	L295	100	Blue
	D302	100	Blue
	Q303	100	Blue
	G304	100	Blue
	L305	100	Blue
	Y306	100	Blue
	F310	100	Blue
	C311	100	Blue
	P312	100	Blue
Category 3	C313	100	Blue
	H314	100	Blue
	G315	100	Blue
	S316	100	Blue
	G327	100	Blue
	L335	100	Blue
	P336	100	Blue
	T337	100	Blue
	F340	100	Blue
	T341	100	Blue
Category 4	D342	100	Blue
	D343	100	Blue
	D344	100	Blue
	G349	100	Blue
	H24	100	Orange
	T27	100	Orange
	T37	100	Orange
	E38	100	Orange
	P62	100	Orange
	D72	100	Orange
Category 5	H100	100	Orange
	R108	100	Orange
	T126	100	Orange
	D127	100	Orange
	P145	100	Orange
	Y153	100	Orange
	I157	100	Orange
	P160	100	Orange
	H180	100	Orange
	W214	100	Orange
Category 6	P215	100	Orange
	D228	100	Orange
	L229	100	Orange
	R230	100	Orange
	G231	100	Orange
	I232	100	Orange
	Q233	100	Orange
	P234	100	Orange
	G235	100	Orange
	Q236	100	Orange
Category 7	R250	100	Orange
	R251	100	Orange
	M256	100	Orange
	T257	100	Orange
	D258	100	Orange
	A259	100	Orange
	A260	100	Orange
	T261	100	Orange
	A262	100	Orange
	D263	100	Orange
D264	100	Orange	
Category 8	A265	100	Orange
	T266	100	Orange
	N267	100	Orange
	D268	100	Orange
	S269	100	Orange
	P270	100	Orange

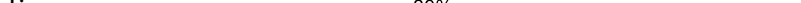
- Chain 3h: 

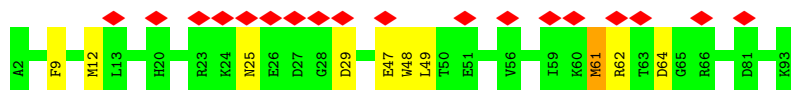
Bar chart showing the distribution of 2500 genes across 10 categories. The categories are: D278, R279, V280, K281, K282, P283, E284, M288, L295, D302, Q303, G304, L305, H314, G315, S316, G327, I335, D342, G349, H24, T27, I32, T37, E38, P62, P69, H100, R108, T126, D127, R131, P145, Y153, I157, P160, H180, W14, P215, G223, R230, G231, T232, D236, R251, T257, D258, A262, D263, D264, A265, T266, V267, H268, E274, R275, D276, and V277. The bars are color-coded: yellow for 'Other', green for 'Highly expressed', and red for 'Lowly expressed'. The height of each bar represents the number of genes in that category. The chart shows a high proportion of genes in the 'Highly expressed' category, particularly in the 'D278' and 'R279' categories.

- Chain 3I:  90% 10%

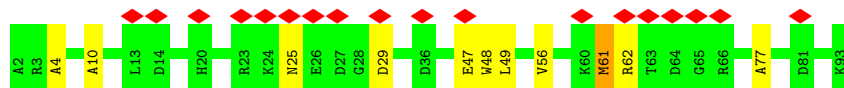
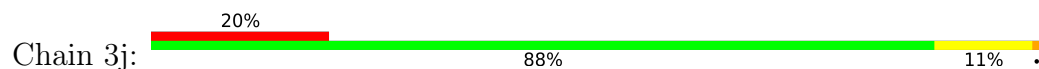
S2	R5	R9	F34	Q35	Q36	E40	R65	M82	I83	R101	N122	A131	P132	E135	E136	A137	K138	Q145	G161	T176	M177
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- Chain 3i: 91% 9%

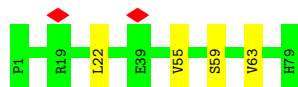
- Chain 3J: 



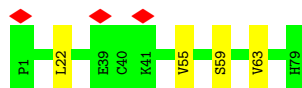
- Molecule 22: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative



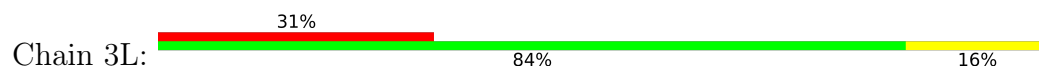
- Molecule 23: QCR11



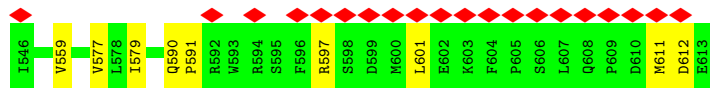
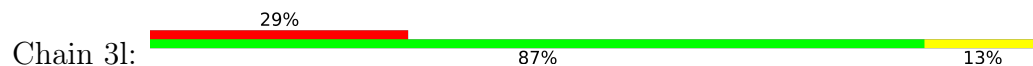
- Molecule 23: QCR11



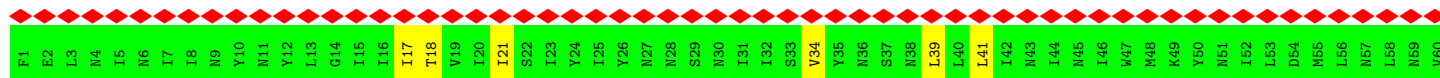
- Molecule 24: Aurora kinase



- Molecule 24: Aurora kinase

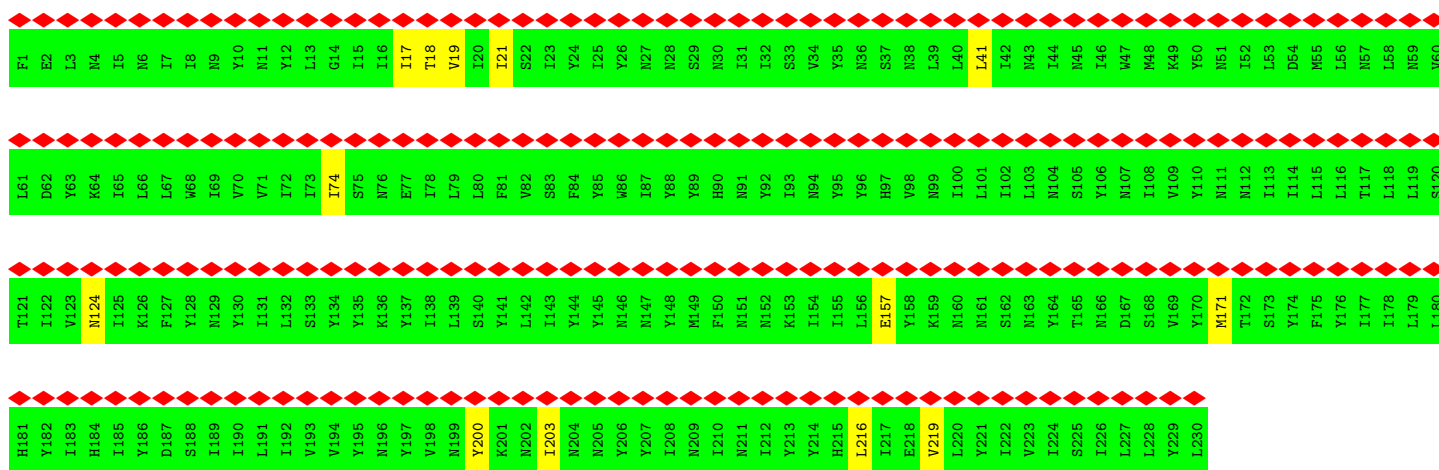


- Molecule 25: Cytochrome c oxidase subunit 3





• Molecule 25: Cytochrome c oxidase subunit 3



• Molecule 26: Cytochrome c oxidase subunit 6B

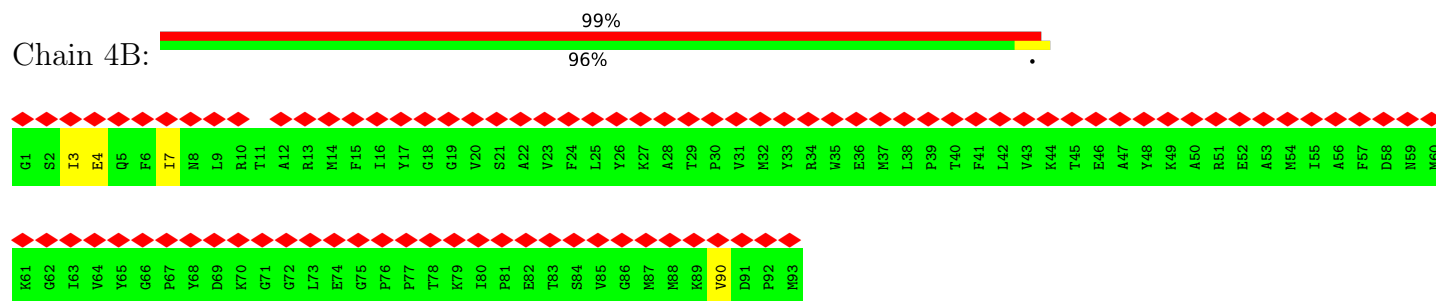


• Molecule 26: Cytochrome c oxidase subunit 6B



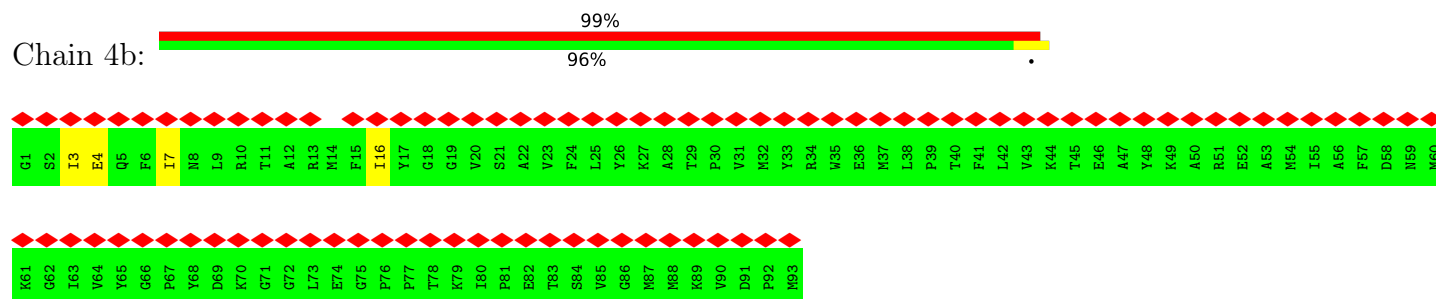
● Molecule 27: Peptidase M14 carboxypeptidase A domain-containing protein

Chain 4B:



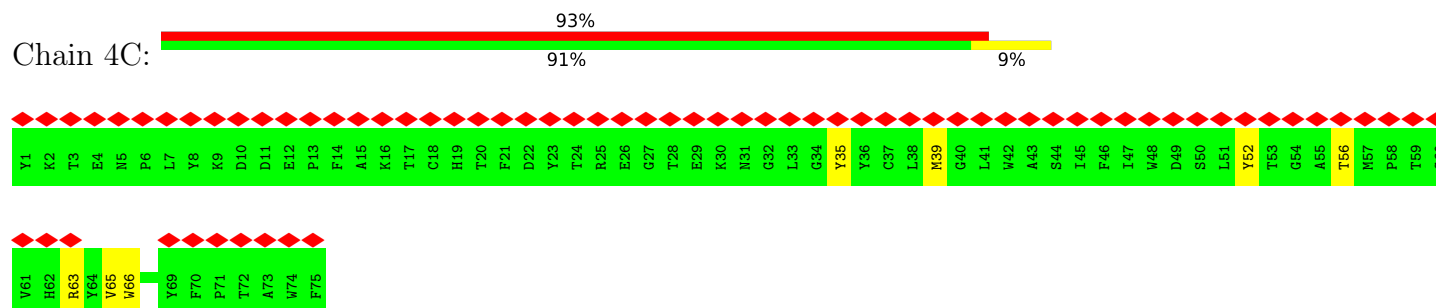
● Molecule 27: Peptidase M14 carboxypeptidase A domain-containing protein

Chain 4b:



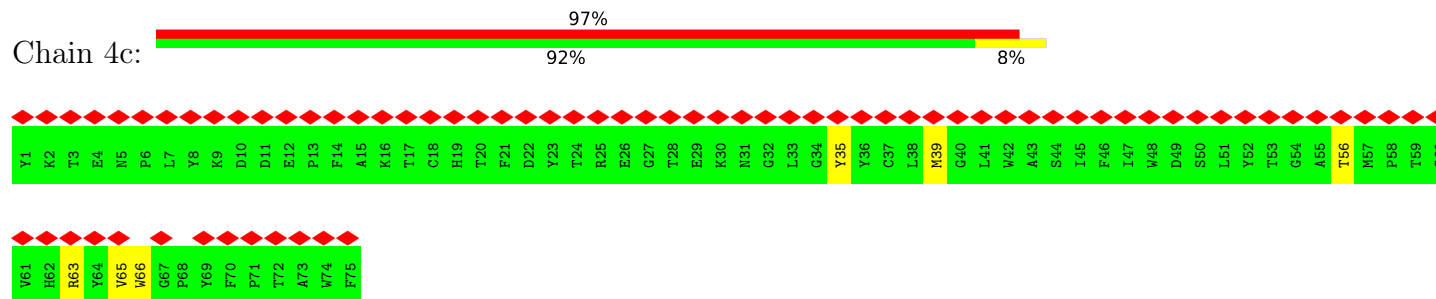
● Molecule 28: Cytochrome c oxidase subunit 40

Chain 4C:



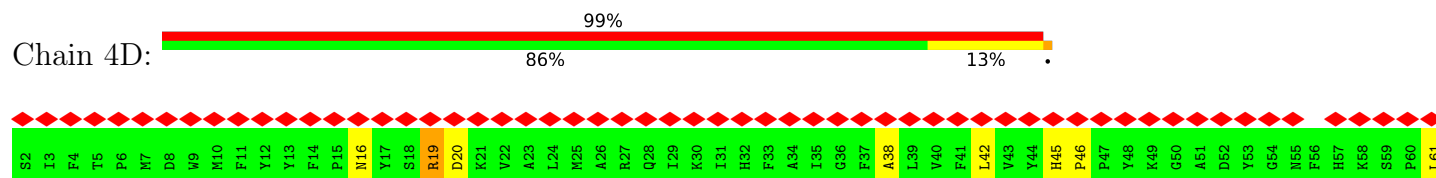
● Molecule 28: Cytochrome c oxidase subunit 40

Chain 4c:



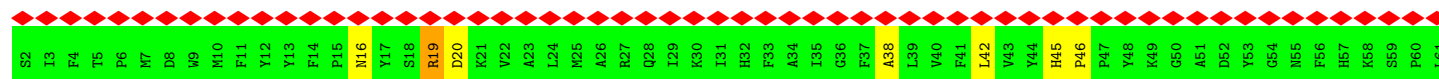
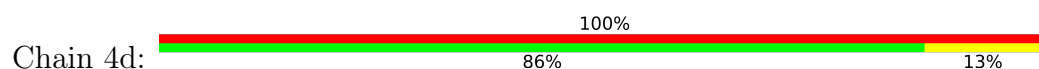
● Molecule 29: Cytochrome c oxidase subunit 34

Chain 4D:

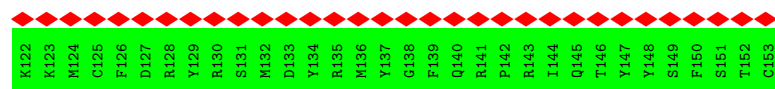
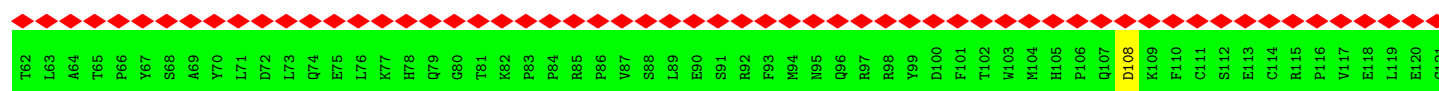




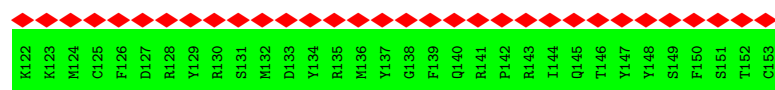
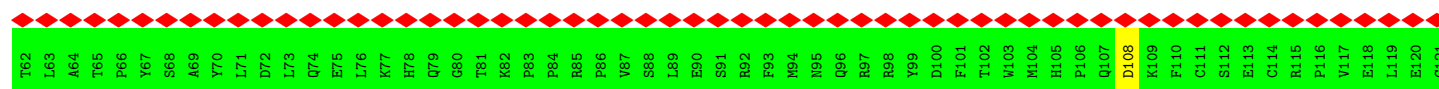
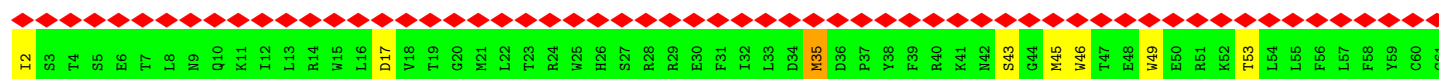
• Molecule 29: Cytochrome c oxidase subunit 34



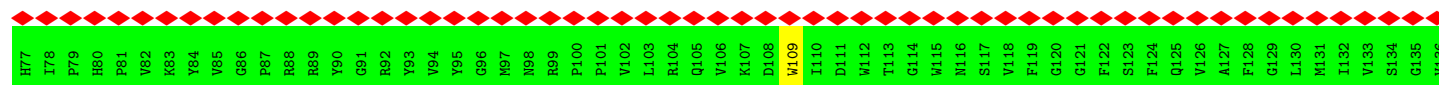
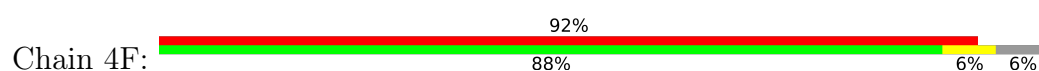
• Molecule 30: Merozoite surface protein, putative

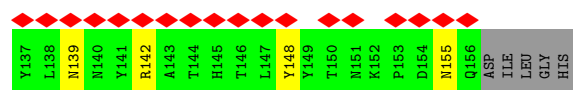


• Molecule 30: Merozoite surface protein, putative

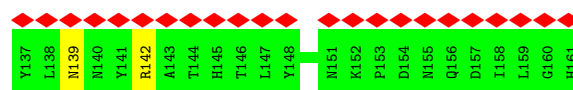
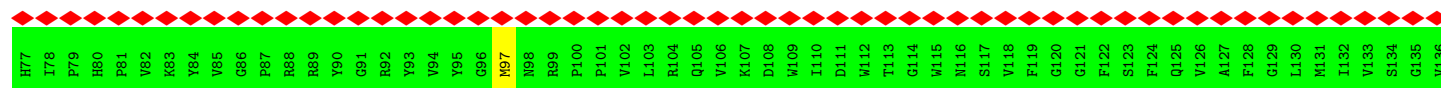


• Molecule 31: Ubiquitin, putative

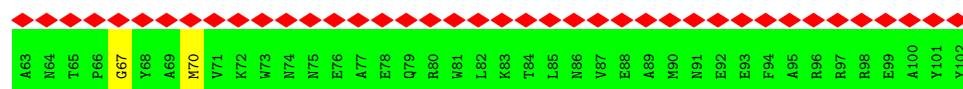




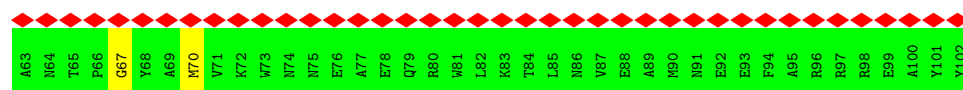
- Molecule 31: Ubiquitin, putative



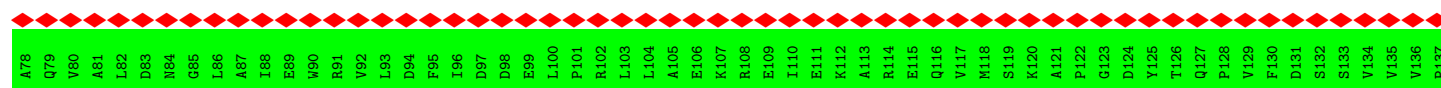
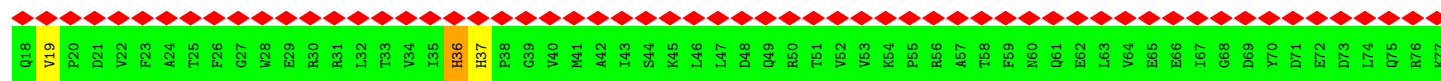
- Molecule 32: Cytochrome c oxidase subunit 33

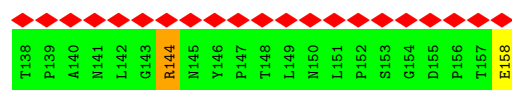


- Molecule 32: Cytochrome c oxidase subunit 33

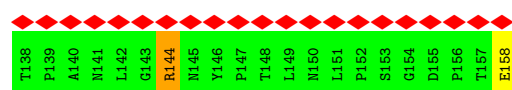
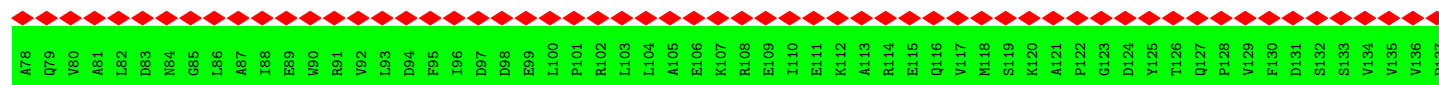
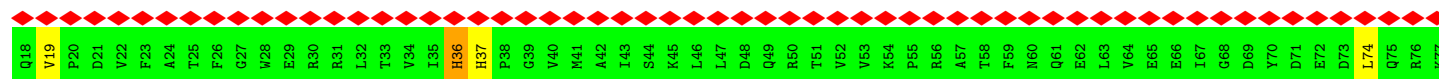


- Molecule 33: Cytochrome c oxidase subunit 30

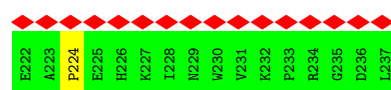
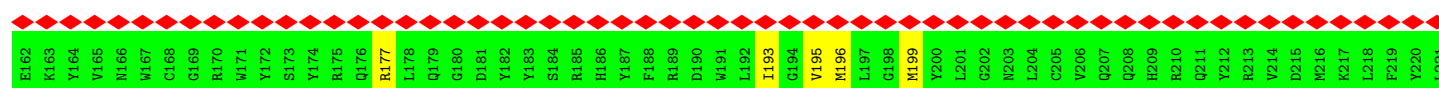
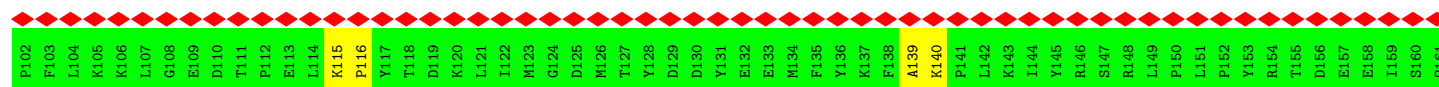
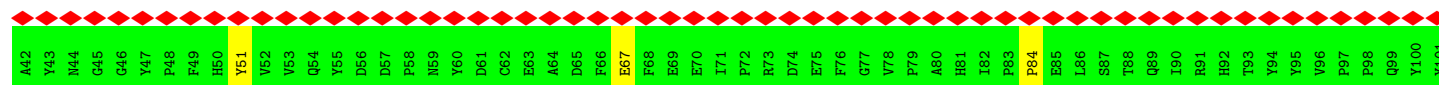
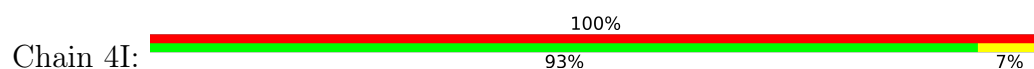




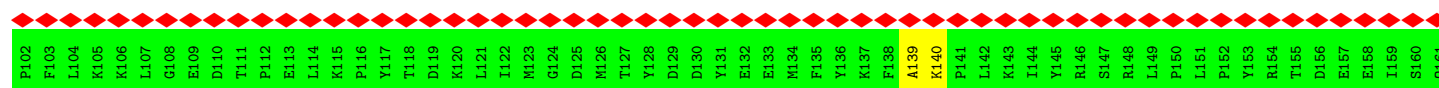
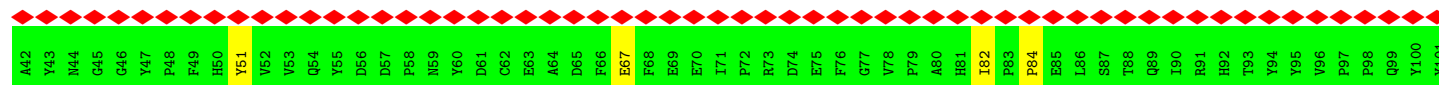
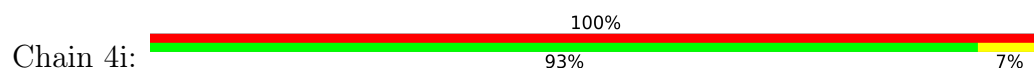
• Molecule 33: Cytochrome c oxidase subunit 30

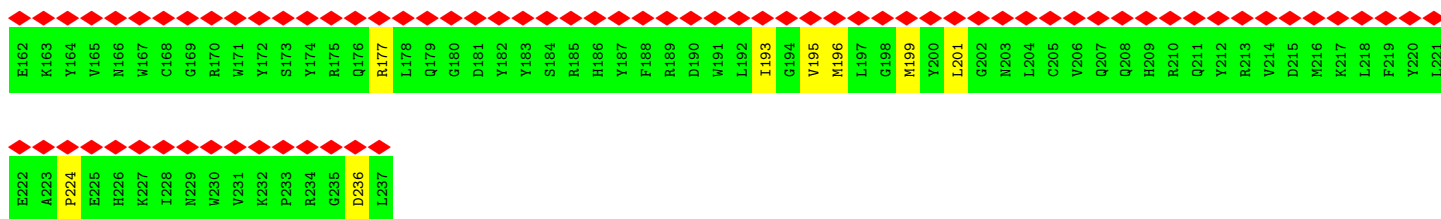


• Molecule 34: Cytochrome c oxidase subunit 6C

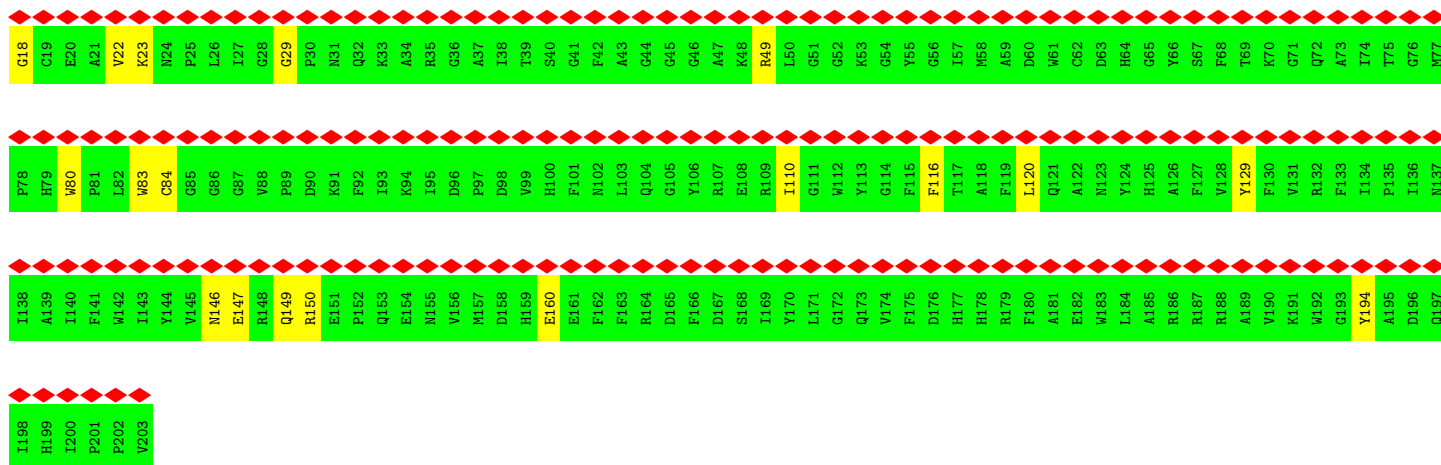
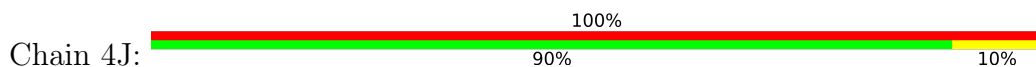


• Molecule 34: Cytochrome c oxidase subunit 6C

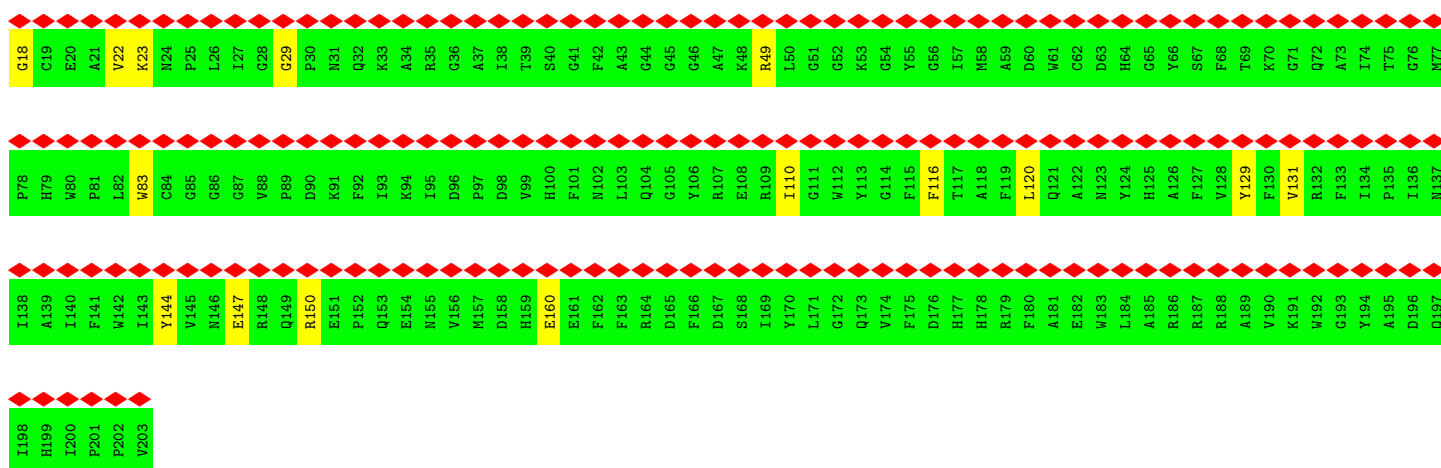
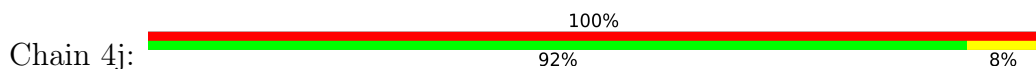




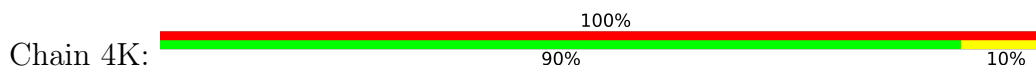
• Molecule 35: Cytochrome c oxidase subunit 24

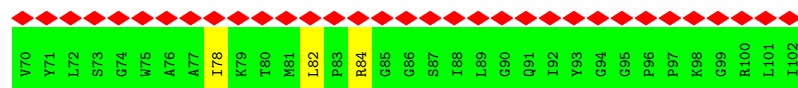


• Molecule 35: Cytochrome c oxidase subunit 24

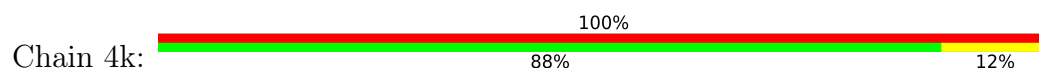


• Molecule 36: Cytochrome c oxidase subunit 37

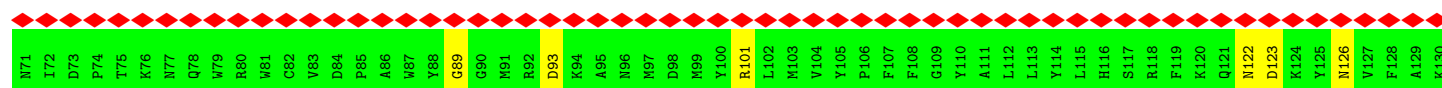
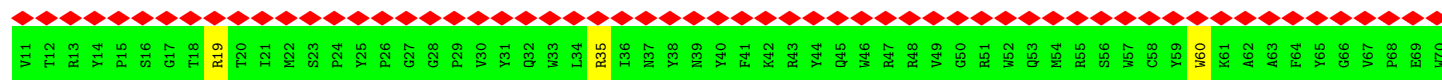




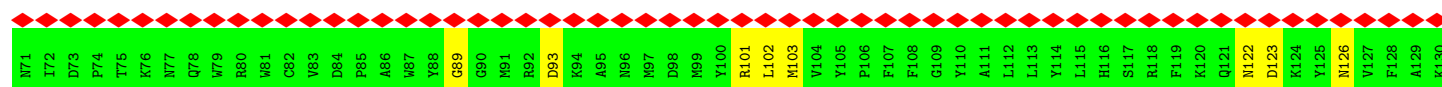
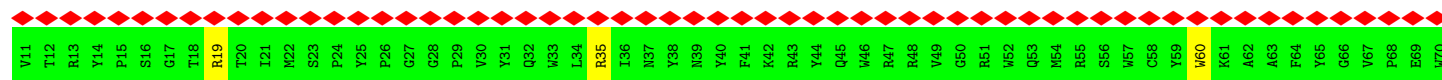
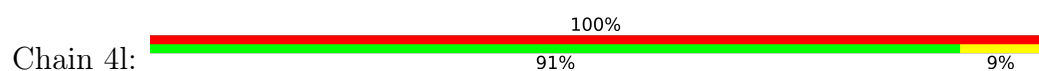
• Molecule 36: Cytochrome c oxidase subunit 37



• Molecule 37: Cytochrome c oxidase subunit 7A

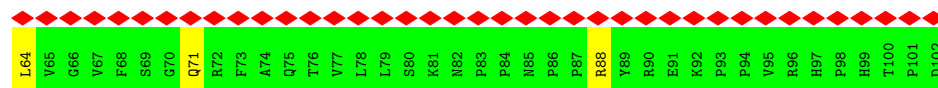


• Molecule 37: Cytochrome c oxidase subunit 7A

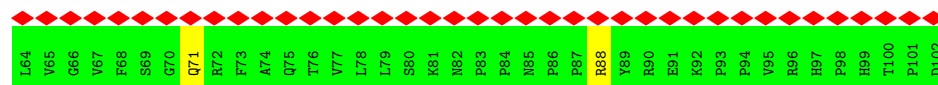
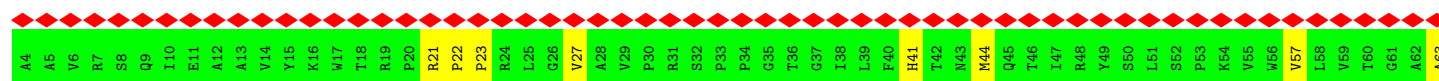
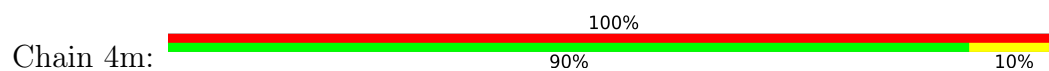


• Molecule 38: Cytochrome c oxidase subunit 35

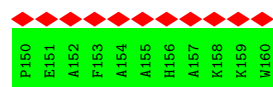
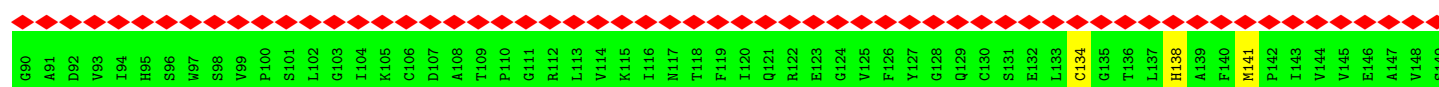
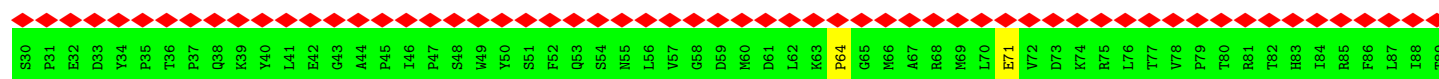




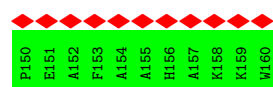
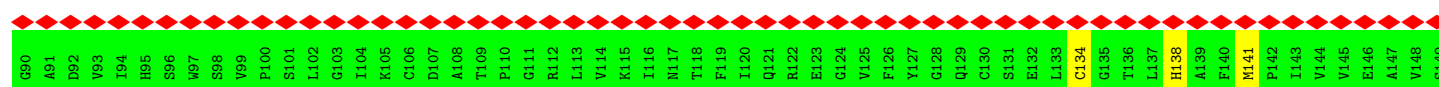
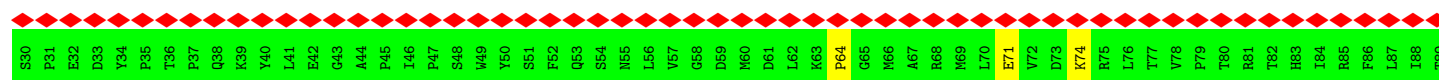
• Molecule 38: Cytochrome c oxidase subunit 35



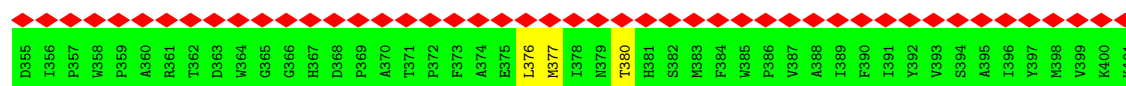
• Molecule 39: Cytochrome c oxidase polypeptide II



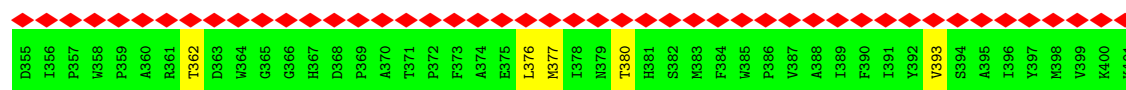
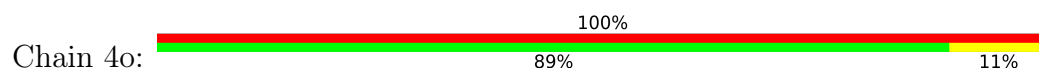
• Molecule 39: Cytochrome c oxidase polypeptide II



• Molecule 40: GINS subunit domain-containing protein



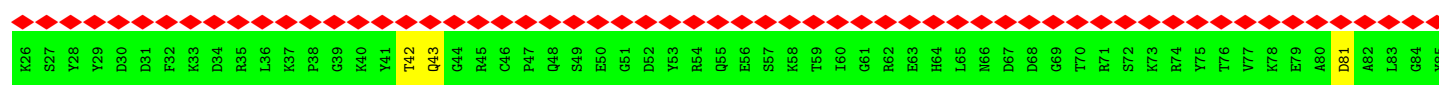
- Molecule 40: GINS subunit domain-containing protein



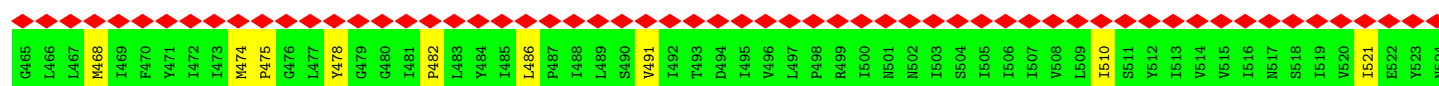
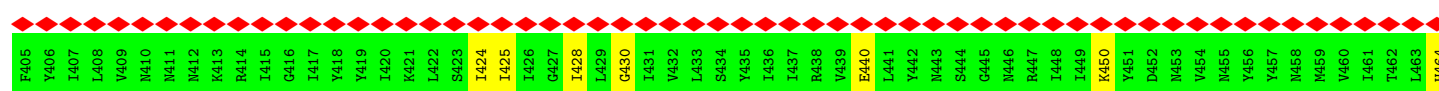
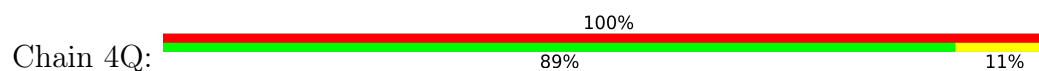
- Molecule 41: Cytochrome oxidase subunit II copper A binding domain-containing protein

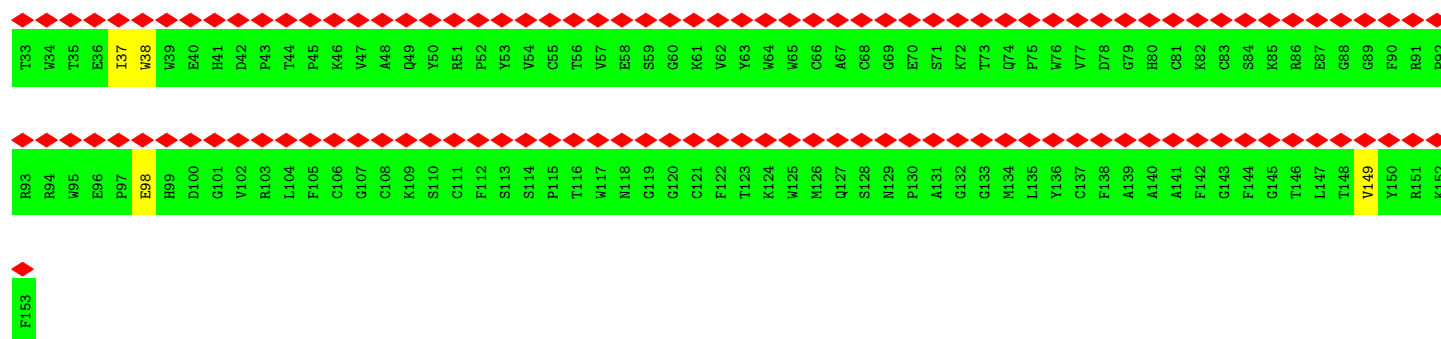


- Molecule 41: Cytochrome oxidase subunit II copper A binding domain-containing protein

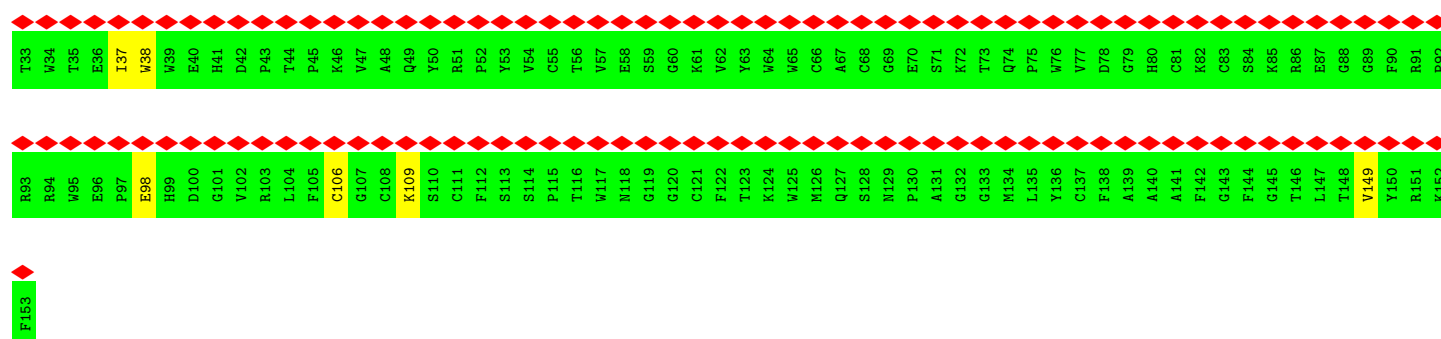


- Molecule 42: Cytochrome c oxidase subunit 1

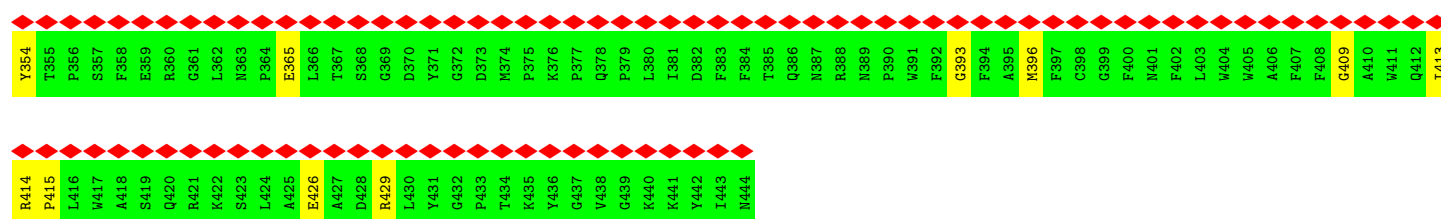
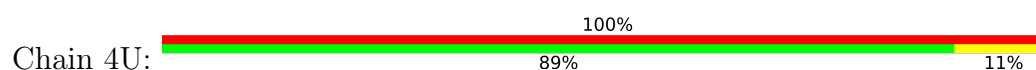




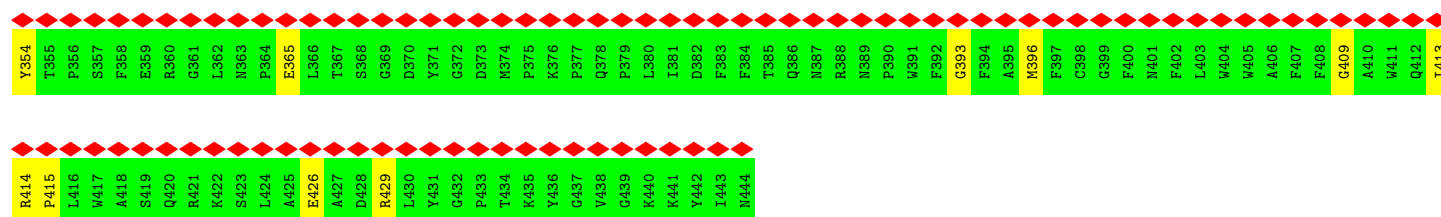
• Molecule 45: Cytochrome c oxidase subunit 13



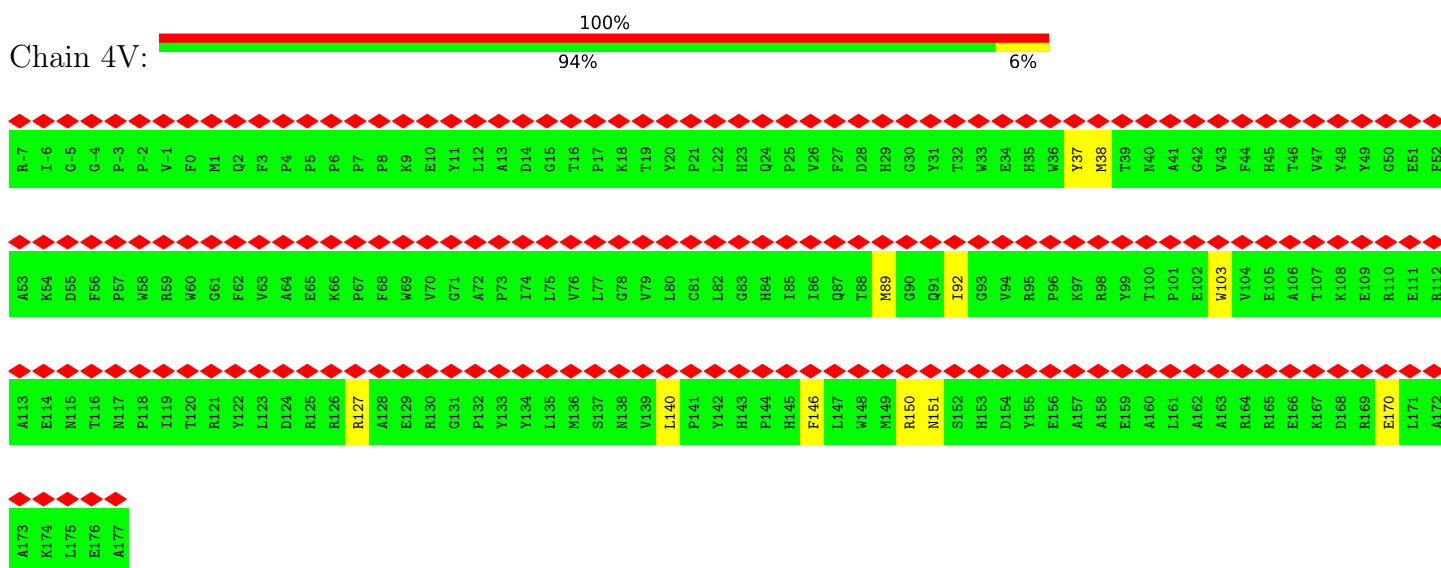
• Molecule 46: Amino acid transporter transmembrane domain-containing protein



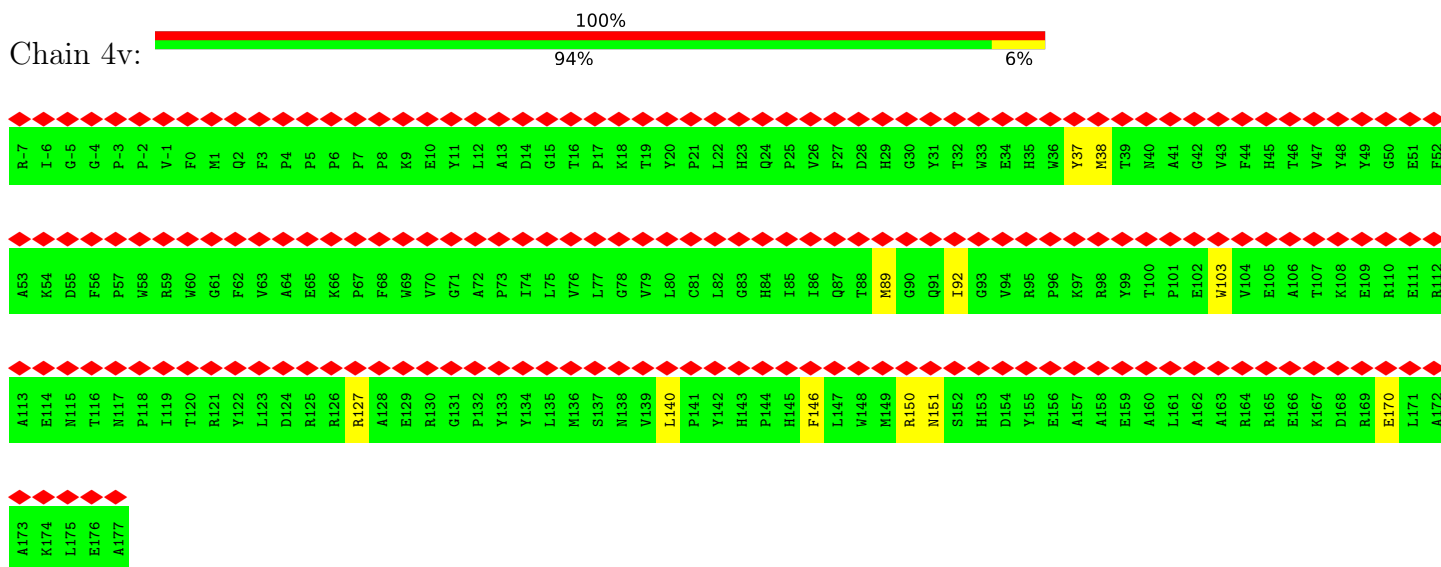
• Molecule 46: Amino acid transporter transmembrane domain-containing protein



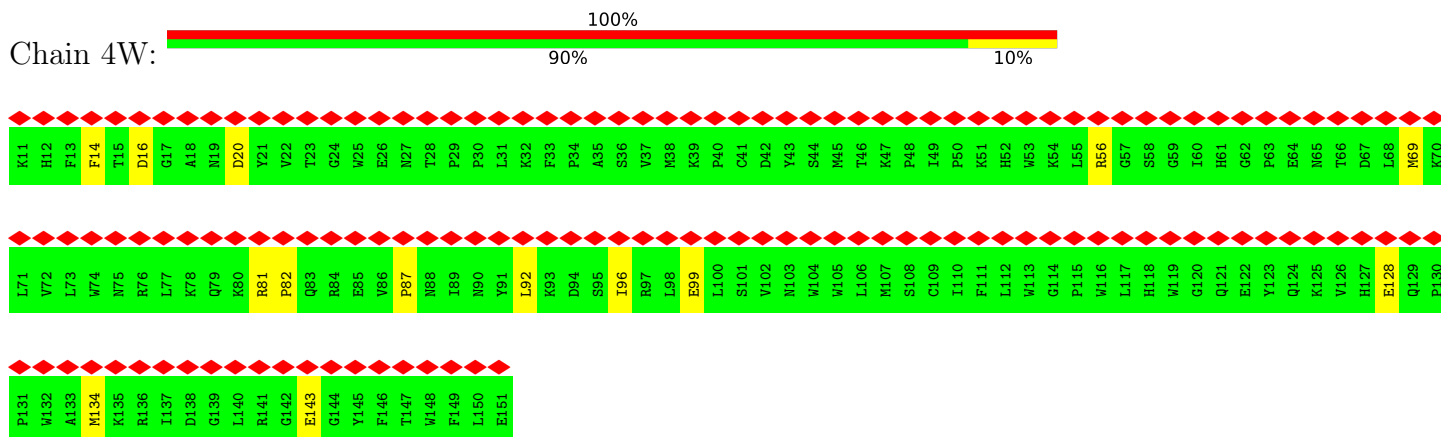
• Molecule 47: Cytochrome c oxidase subunit 4



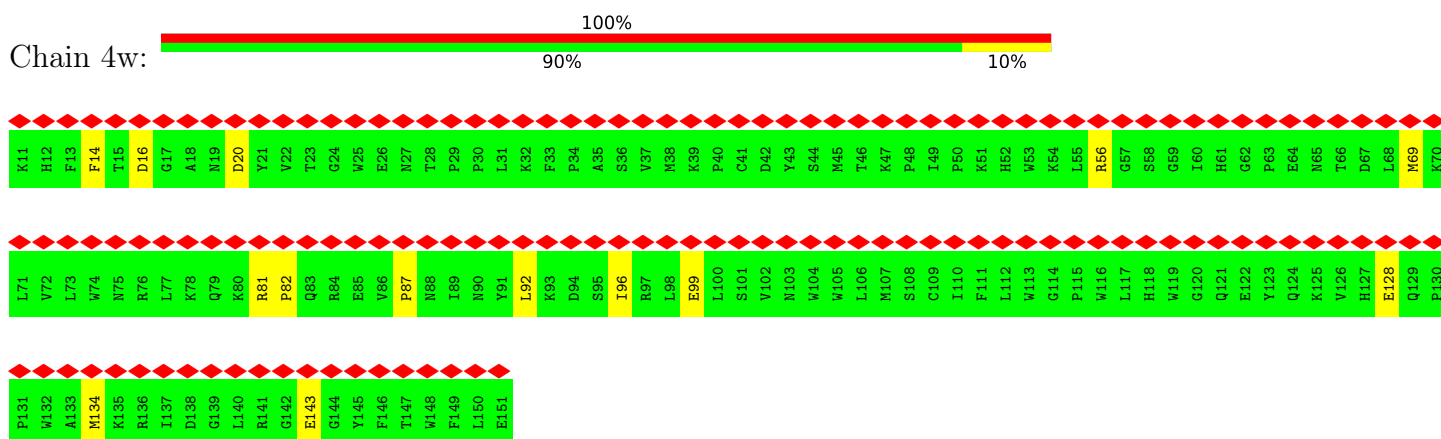
- Molecule 47: Cytochrome c oxidase subunit 4



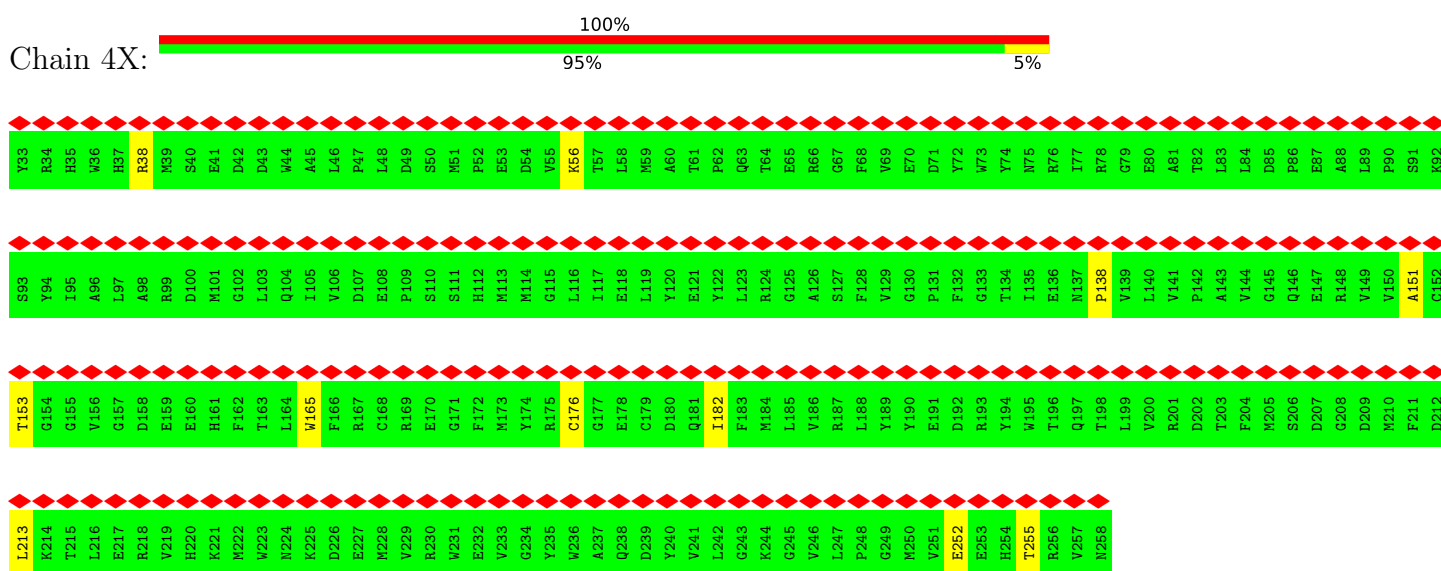
- Molecule 48: Cytochrome c oxidase subunit 19



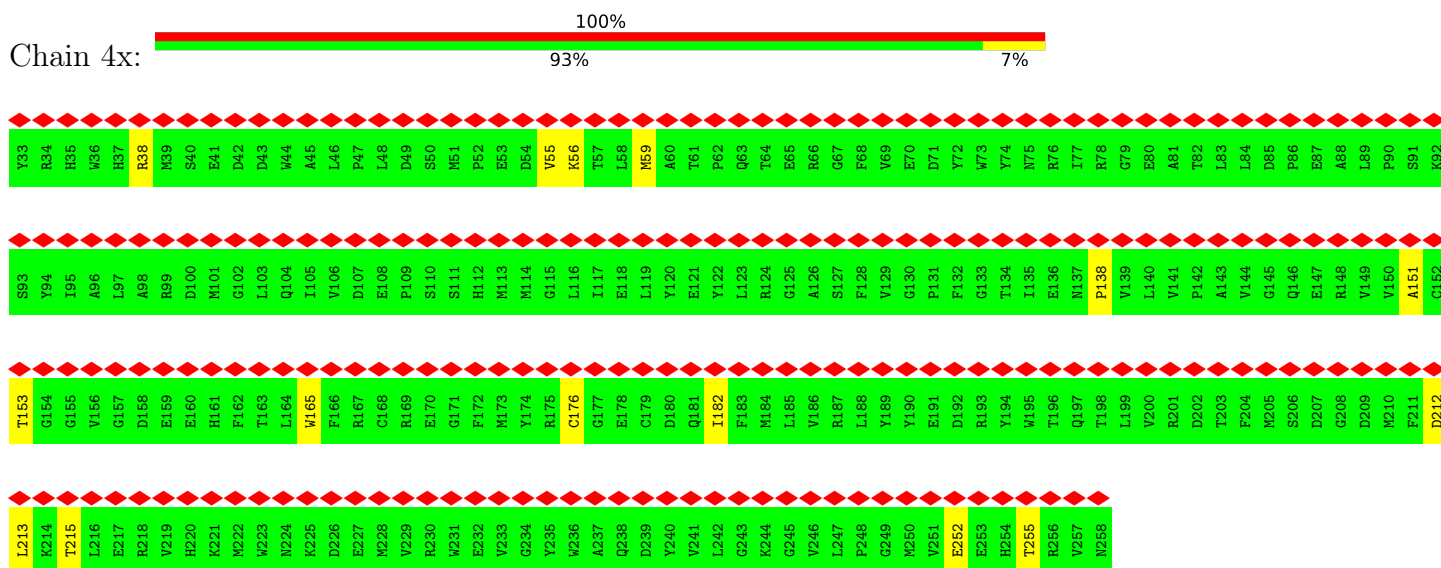
- Molecule 48: Cytochrome c oxidase subunit 19



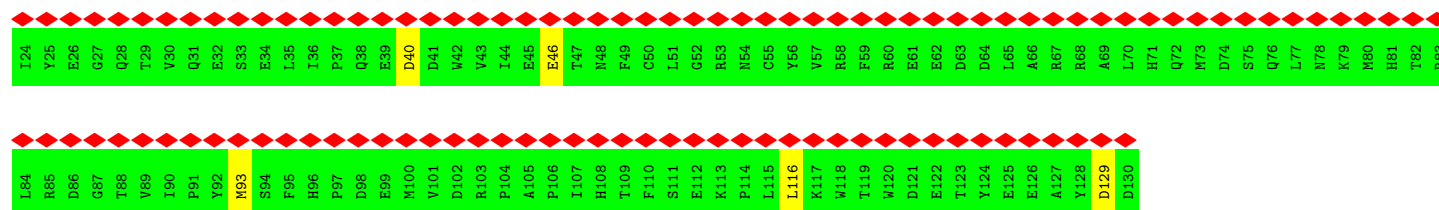
- Molecule 49: Cytochrome Coxidase subunit, putative



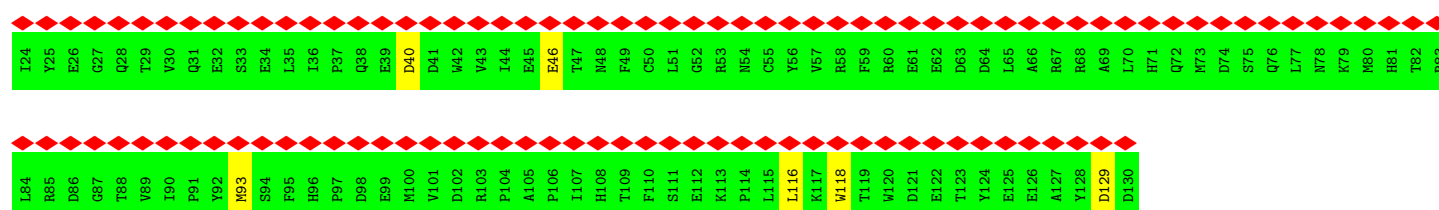
- Molecule 49: Cytochrome Coxidase subunit, putative



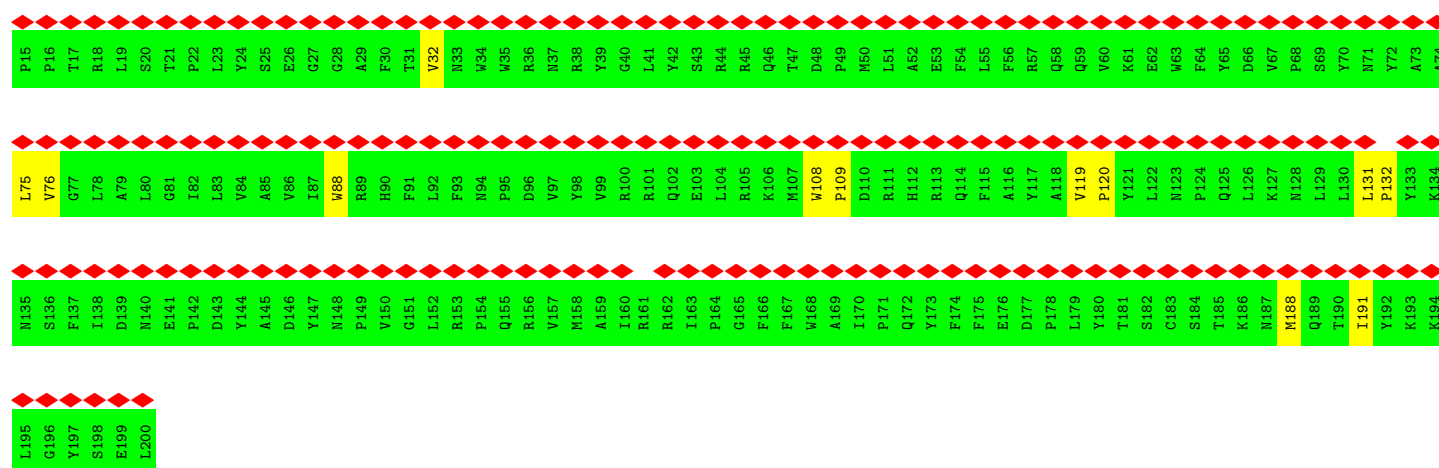
- Molecule 50: Cytochrome c oxidase subunit 18



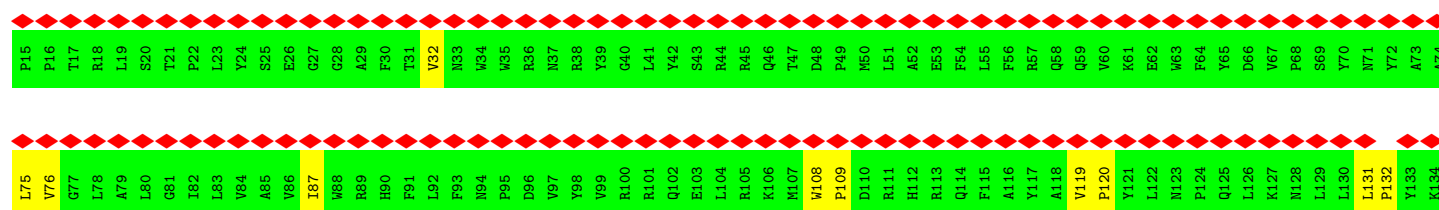
• Molecule 50: Cytochrome c oxidase subunit 18



• Molecule 51: Cytochrome c oxidase subunit 31



• Molecule 51: Cytochrome c oxidase subunit 31



L195	L196	Y197	S198	E199	L200	N135	S136	F137	I138	D139	N140	E141	P142	D143	Y144	A145	D146	Y147	N148	P149	V150	G151	L152	R153	P154	Q155	R156	V157	M158	A159	I160	R161	R162	I163	P164	G165	F166	F167	V168	A169	I170	P171	Q172	Y173	F174	F175	E176	D177	P178	L179	Y180	T181	S182	C183	S184	T185	K186	N187	M188	Q189	T190	I191	Y192	K193	K194
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111717	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	423.2, 423.2, 423.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HEM, PEE, AME, FES, PC1, SF4, F3S, MG, CDL, FAD, K, PER, UQ1, HEA, CUA, LPP, CU, HEC

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	2M	0.44	6/4701 (0.1%)	0.54	5/6363 (0.1%)
1	2m	0.44	5/4701 (0.1%)	0.53	4/6363 (0.1%)
2	2N	0.23	0/2118	0.38	0/2863
2	2n	0.23	0/2118	0.38	0/2863
3	2O	0.24	0/1292	0.38	0/1759
3	2o	0.24	0/1292	0.38	0/1759
4	2P	0.17	0/1342	0.32	0/1812
4	2p	0.17	0/1342	0.32	0/1812
5	2Q	0.17	0/580	0.36	0/788
5	2q	0.17	0/580	0.36	0/788
6	2R	0.23	0/985	0.31	0/1336
6	2r	0.23	0/985	0.31	0/1336
7	2S	0.19	0/1341	0.31	0/1816
7	2s	0.18	0/1341	0.32	0/1816
8	2T	1.31	10/714 (1.4%)	1.29	11/971 (1.1%)
8	2t	1.31	10/714 (1.4%)	1.29	11/971 (1.1%)
9	2U	0.18	0/400	0.33	0/547
9	2u	0.18	0/400	0.33	0/547
10	2V	0.21	0/716	0.40	0/965
10	2v	0.21	0/716	0.39	0/965
11	30	0.35	0/1124	0.56	0/1518
12	31	0.30	0/1240	0.57	0/1667
13	3A	0.19	0/3701	0.28	0/5025
13	3a	0.19	0/3701	0.28	0/5025
14	3B	0.21	0/3967	0.31	0/5371
14	3b	0.21	0/3967	0.31	0/5371
15	3C	0.22	0/1988	0.34	0/2712
15	3c	0.21	0/1997	0.35	0/2724
16	3D	0.32	0/872	0.44	1/1182 (0.1%)
16	3d	0.88	5/872 (0.6%)	0.66	3/1182 (0.3%)
17	3E	0.24	0/848	0.33	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	3e	0.25	0/848	0.33	0/1148
18	3F	0.21	0/767	0.33	0/1042
18	3f	0.21	0/767	0.33	0/1042
19	3G	0.20	0/3098	0.35	0/4231
19	3g	0.21	0/3098	0.40	0/4231
20	3H	0.18	0/2713	0.36	0/3693
20	3h	0.18	0/2705	0.36	0/3682
21	3I	0.20	0/1514	0.34	0/2045
21	3i	0.20	0/1514	0.34	0/2045
22	3J	0.29	0/776	0.42	1/1045 (0.1%)
22	3j	0.29	0/776	0.42	1/1045 (0.1%)
23	3K	0.15	0/627	0.32	0/847
23	3k	0.15	0/627	0.32	0/847
24	3L	0.19	0/554	0.40	0/755
24	3l	0.19	0/554	0.41	0/755
25	40	0.20	0/2060	0.36	0/2822
25	41	0.20	0/2060	0.36	0/2822
26	4A	0.16	0/863	0.32	0/1166
26	4a	0.16	0/863	0.32	0/1166
27	4B	0.17	0/751	0.30	0/1013
27	4b	0.17	0/751	0.30	0/1013
28	4C	0.16	0/653	0.30	0/891
28	4c	0.16	0/653	0.30	0/891
29	4D	0.16	0/819	0.31	0/1110
29	4d	0.16	0/819	0.31	0/1110
30	4E	0.17	0/1353	0.34	0/1824
30	4e	0.17	0/1353	0.34	0/1824
31	4F	0.22	0/695	0.34	0/948
31	4f	0.22	0/735	0.35	0/1001
32	4G	0.16	0/883	0.26	0/1199
32	4g	0.16	0/883	0.26	0/1199
33	4H	0.14	0/1149	0.26	0/1565
33	4h	0.14	0/1149	0.26	0/1565
34	4I	0.22	0/1757	0.28	0/2386
34	4i	0.22	0/1757	0.29	0/2386
35	4J	0.22	0/1573	0.33	0/2131
35	4j	0.22	0/1573	0.33	0/2131
36	4K	0.21	0/745	0.34	0/1017
36	4k	0.21	0/745	0.34	0/1017
37	4L	0.17	0/1131	0.27	0/1537
37	4l	0.17	0/1131	0.27	0/1537
38	4M	0.17	0/805	0.30	0/1104
38	4m	0.16	0/805	0.30	0/1104

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	4N	0.18	0/1055	0.32	0/1436
39	4n	0.18	0/1055	0.32	0/1436
40	4O	0.29	0/400	0.36	0/549
40	4o	0.29	0/400	0.36	0/549
41	4P	0.17	0/1551	0.30	0/2106
41	4p	0.16	0/1551	0.30	0/2106
42	4Q	0.24	0/3774	0.36	0/5155
42	4q	0.24	0/3774	0.37	0/5155
43	4R	0.14	0/958	0.25	0/1301
43	4r	0.14	0/958	0.25	0/1301
44	4S	0.15	0/560	0.24	0/760
44	4s	0.15	0/560	0.24	0/760
45	4T	0.18	0/1024	0.27	0/1391
45	4t	0.18	0/1024	0.27	0/1391
46	4U	0.14	0/790	0.35	0/1073
46	4u	0.14	0/790	0.35	0/1073
47	4V	0.23	0/1600	0.32	0/2183
47	4v	0.23	0/1600	0.32	0/2183
48	4W	0.17	0/1240	0.32	0/1686
48	4w	0.17	0/1240	0.33	0/1686
49	4X	0.18	0/1912	0.32	0/2592
49	4x	0.18	0/1912	0.32	0/2592
50	4Y	0.17	0/929	0.27	0/1261
50	4y	0.16	0/929	0.27	0/1261
51	4Z	0.18	0/1639	0.32	0/2233
51	4z	0.18	0/1639	0.32	0/2233
All	All	0.27	36/138971 (0.0%)	0.38	37/188749 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2M	0	3
1	2m	0	3
4	2P	0	3
4	2p	0	3
5	2Q	0	1
5	2q	0	1
7	2S	0	1
7	2s	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	2T	0	3
8	2t	0	3
10	2V	0	2
10	2v	0	2
11	3O	0	3
12	3I	0	6
16	3D	0	1
16	3d	0	2
18	3F	0	1
18	3f	0	1
20	3H	0	1
20	3h	0	1
21	3I	0	2
21	3i	0	2
26	4A	0	1
26	4a	0	1
28	4C	0	1
28	4c	0	1
29	4D	0	1
29	4d	0	1
31	4F	0	1
31	4f	0	1
33	4H	0	1
33	4h	0	1
35	4J	0	1
35	4j	0	1
36	4K	0	2
36	4k	0	2
47	4V	0	1
47	4v	0	1
49	4X	0	1
49	4x	0	1
All	All	0	66

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3d	109	TYR	CG-CD2	-16.85	1.03	1.39
8	2t	45	TYR	CG-CD2	-13.32	1.11	1.39
8	2T	45	TYR	CG-CD2	-13.25	1.11	1.39
8	2t	45	TYR	CG-CD1	-12.97	1.12	1.39
8	2T	45	TYR	CG-CD1	-12.96	1.12	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2T	76	LEU	CD1-CG-CD2	-20.95	64.71	110.80
8	2t	76	LEU	CD1-CG-CD2	-20.94	64.74	110.80
8	2T	51	TYR	CE1-CZ-CE2	-14.89	90.51	120.30
8	2t	51	TYR	CE1-CZ-CE2	-14.85	90.59	120.30
8	2t	45	TYR	CE1-CZ-CE2	-13.43	93.43	120.30

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2M	165	ARG	Sidechain
1	2M	290	ARG	Sidechain
1	2M	564	ARG	Sidechain
4	2P	22	ARG	Sidechain
4	2P	72	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2M	4602	0	4530	32	0
1	2m	4602	0	4530	35	0
2	2N	2068	0	2025	14	0
2	2n	2068	0	2025	14	0
3	2O	1254	0	1263	6	0
3	2o	1254	0	1263	7	0
4	2P	1309	0	1367	7	0
4	2p	1309	0	1367	10	0
5	2Q	564	0	567	2	0
5	2q	564	0	567	3	0
6	2R	950	0	935	7	0
6	2r	950	0	935	7	0
7	2S	1323	0	1261	2	0
7	2s	1323	0	1261	3	0
8	2T	695	0	672	6	0
8	2t	695	0	672	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2U	390	0	369	4	0
9	2u	390	0	369	6	0
10	2V	701	0	714	4	0
10	2v	701	0	714	3	0
11	30	1181	0	1061	10	0
12	31	1219	0	1185	14	0
13	3A	3622	0	3508	11	0
13	3a	3622	0	3508	10	0
14	3B	3884	0	3842	13	0
14	3b	3884	0	3842	12	0
15	3C	1921	0	1816	10	0
15	3c	1930	0	1822	22	0
16	3D	836	0	798	7	0
16	3d	836	0	798	6	0
17	3E	813	0	776	5	0
17	3e	813	0	776	6	0
18	3F	734	0	704	5	0
18	3f	734	0	704	5	0
19	3G	3016	0	3162	30	0
19	3g	3016	0	3162	42	0
20	3H	2628	0	2541	23	0
20	3h	2621	0	2534	24	0
21	3I	1472	0	1436	14	0
21	3i	1472	0	1436	12	0
22	3J	755	0	693	7	0
22	3j	755	0	693	10	0
23	3K	608	0	617	3	0
23	3k	608	0	617	3	0
24	3L	539	0	536	8	0
24	3l	539	0	536	7	0
25	40	2004	0	2032	11	0
25	41	2004	0	2032	13	0
26	4A	841	0	766	7	0
26	4a	841	0	766	7	0
27	4B	732	0	746	3	0
27	4b	732	0	746	4	0
28	4C	626	0	575	4	0
28	4c	626	0	575	3	0
29	4D	787	0	745	8	0
29	4d	787	0	745	8	0
30	4E	1313	0	1269	8	0
30	4e	1313	0	1269	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4F	669	0	642	5	0
31	4f	708	0	678	2	0
32	4G	854	0	811	3	0
32	4g	854	0	811	3	0
33	4H	1125	0	1112	4	0
33	4h	1125	0	1112	5	0
34	4I	1695	0	1593	11	0
34	4i	1695	0	1593	13	0
35	4J	1517	0	1435	11	0
35	4j	1517	0	1435	10	0
36	4K	722	0	760	4	0
36	4k	722	0	760	5	0
37	4L	1083	0	1027	9	0
37	4l	1083	0	1027	12	0
38	4M	778	0	802	8	0
38	4m	778	0	802	11	0
39	4N	1025	0	1018	6	0
39	4n	1025	0	1018	6	0
40	4O	383	0	368	3	0
40	4o	383	0	368	5	0
41	4P	1504	0	1461	12	0
41	4p	1504	0	1461	13	0
42	4Q	3687	0	3956	45	0
42	4q	3687	0	3956	45	0
43	4R	916	0	854	1	0
43	4r	916	0	854	3	0
44	4S	541	0	489	2	0
44	4s	541	0	489	2	0
45	4T	983	0	902	3	0
45	4t	983	0	902	4	0
46	4U	758	0	713	8	0
46	4u	758	0	713	8	0
47	4V	1539	0	1482	10	0
47	4v	1539	0	1482	10	0
48	4W	1193	0	1164	10	0
48	4w	1193	0	1164	11	0
49	4X	1860	0	1764	7	0
49	4x	1860	0	1764	9	0
50	4Y	905	0	835	5	0
50	4y	905	0	835	6	0
51	4Z	1582	0	1548	8	0
51	4z	1582	0	1548	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	2M	53	0	30	0	0
52	2m	53	0	29	0	0
53	2N	18	0	18	0	0
53	2p	18	0	18	1	0
53	3G	36	0	36	5	0
53	3g	36	0	36	4	0
54	2N	4	0	0	0	0
54	2n	4	0	0	0	0
54	3H	4	0	0	1	0
54	3h	4	0	0	1	0
55	2N	8	0	0	0	0
55	2n	8	0	0	0	0
56	2N	7	0	0	0	0
56	2n	7	0	0	0	0
57	2N	1	0	0	0	0
57	2n	1	0	0	0	0
57	4Q	1	0	0	0	0
57	4q	1	0	0	0	0
58	2O	80	0	114	1	0
58	2P	46	0	69	0	0
58	2T	45	0	67	1	0
58	2o	24	0	24	0	0
58	2p	24	0	22	0	0
58	2r	39	0	55	0	0
58	2t	42	0	61	0	0
58	3C	30	0	34	0	0
58	3H	46	0	69	0	0
58	3c	33	0	40	1	0
58	3f	38	0	50	0	0
58	40	158	0	218	1	0
58	41	125	0	175	2	0
58	4D	40	0	57	0	0
58	4Q	36	0	46	0	0
58	4R	43	0	63	0	0
58	4S	27	0	28	0	0
58	4W	51	0	82	0	0
58	4Z	51	0	82	2	0
58	4d	51	0	82	0	0
58	4l	38	0	50	2	0
58	4q	77	0	102	0	0
58	4s	47	0	71	0	0
58	4w	51	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	4z	44	0	62	1	0
59	2O	67	0	78	2	0
59	2P	81	0	112	0	0
59	2Q	100	0	156	0	0
59	2T	71	0	89	0	0
59	2o	86	0	122	0	0
59	2p	74	0	95	1	0
59	2q	100	0	156	7	0
59	2t	66	0	76	2	0
59	3D	184	0	274	0	0
59	3E	93	0	136	0	0
59	3G	175	0	253	0	0
59	3H	173	0	246	2	0
59	3I	212	0	261	1	0
59	3L	259	0	371	5	0
59	3e	148	0	193	5	0
59	3g	307	0	405	3	0
59	3h	85	0	120	2	0
59	3i	127	0	148	3	0
59	3l	181	0	265	7	0
59	4I	92	0	137	0	0
59	4E	135	0	167	2	0
59	4F	100	0	156	0	0
59	4J	59	0	64	0	0
59	4K	90	0	133	1	0
59	4L	94	0	141	1	0
59	4M	75	0	100	1	0
59	4O	97	0	147	0	0
59	4Q	170	0	243	2	0
59	4S	100	0	156	0	0
59	4U	72	0	88	0	0
59	4W	73	0	93	0	0
59	4Z	48	0	40	1	0
59	4e	146	0	189	5	0
59	4f	92	0	137	4	0
59	4g	66	0	78	1	0
59	4j	139	0	179	2	0
59	4m	100	0	156	3	0
59	4o	93	0	139	4	0
59	4q	93	0	139	3	0
59	4s	100	0	156	0	0
59	4t	61	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	4z	179	0	264	1	0
60	2P	35	0	44	0	0
60	2R	108	0	176	1	0
60	2T	99	0	155	3	0
60	2o	39	0	52	0	0
60	2p	41	0	56	0	0
60	2r	106	0	169	2	0
60	3A	38	0	53	0	0
60	3H	67	0	82	0	0
60	3a	54	0	88	0	0
60	3f	46	0	69	1	0
60	3h	81	0	116	1	0
60	4F	54	0	88	2	0
60	4e	54	0	88	0	0
61	3C	43	0	31	4	0
61	3c	43	0	31	6	0
62	3G	86	0	60	4	0
62	3g	86	0	60	7	0
63	4C	44	0	67	1	0
63	4Z	44	0	67	0	0
63	4g	39	0	54	0	0
63	4z	38	0	49	0	0
64	4N	2	0	0	0	0
64	4n	2	0	0	0	0
65	4Q	1	0	0	0	0
65	4q	1	0	0	0	0
66	4Q	1	0	0	0	0
66	4q	1	0	0	0	0
67	4Q	120	0	108	9	0
67	4q	120	0	108	11	0
68	4Q	2	0	0	0	0
68	4q	2	0	0	0	0
69	4T	2	0	0	0	0
69	4X	1	0	0	0	0
69	4t	2	0	0	0	0
69	4x	1	0	0	0	0
70	4Q	1	0	0	0	0
70	4n	1	0	0	0	0
All	All	142971	0	142850	813	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 813 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:4q:632:HIS:NE2	42:4q:636:TYR:HE2	1.60	0.98
42:4Q:632:HIS:NE2	42:4Q:636:TYR:HE2	1.60	0.97
15:3c:76:CYS:SG	61:3c:302:HEC:CAC	2.69	0.80
19:3G:268:LEU:HD21	19:3G:277:ILE:HG13	1.63	0.80
19:3g:268:LEU:HD21	19:3g:277:ILE:HG13	1.64	0.79

There are no symmetry-related clashes.

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	2M	602/604 (100%)	579 (96%)	23 (4%)	0	100	100
1	2m	602/604 (100%)	579 (96%)	23 (4%)	0	100	100
2	2N	257/259 (99%)	244 (95%)	13 (5%)	0	100	100
2	2n	257/259 (99%)	244 (95%)	13 (5%)	0	100	100
3	2O	158/160 (99%)	158 (100%)	0	0	100	100
3	2o	158/160 (99%)	158 (100%)	0	0	100	100
4	2P	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	2p	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
5	2Q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
5	2q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
6	2R	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
6	2r	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
7	2S	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
7	2s	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	2T	80/82 (98%)	80 (100%)	0	0	100	100
8	2t	80/82 (98%)	80 (100%)	0	0	100	100
9	2U	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
9	2u	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
10	2V	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
10	2v	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
11	30	154/173 (89%)	149 (97%)	5 (3%)	0	100	100
12	31	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
13	3A	452/454 (100%)	445 (98%)	7 (2%)	0	100	100
13	3a	452/454 (100%)	445 (98%)	7 (2%)	0	100	100
14	3B	494/496 (100%)	489 (99%)	4 (1%)	1 (0%)	43	63
14	3b	494/496 (100%)	489 (99%)	4 (1%)	1 (0%)	43	63
15	3C	239/242 (99%)	232 (97%)	7 (3%)	0	100	100
15	3c	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
16	3D	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
16	3d	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
17	3E	90/92 (98%)	90 (100%)	0	0	100	100
17	3e	90/92 (98%)	90 (100%)	0	0	100	100
18	3F	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
18	3f	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
19	3G	352/354 (99%)	342 (97%)	10 (3%)	0	100	100
19	3g	352/354 (99%)	336 (96%)	16 (4%)	0	100	100
20	3H	324/326 (99%)	313 (97%)	11 (3%)	0	100	100
20	3h	324/326 (99%)	313 (97%)	11 (3%)	0	100	100
21	3I	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
21	3i	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
22	3J	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
22	3j	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
23	3K	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
23	3k	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
24	3L	66/68 (97%)	58 (88%)	8 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	3l	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
25	40	228/230 (99%)	225 (99%)	3 (1%)	0	100	100
25	41	228/230 (99%)	225 (99%)	3 (1%)	0	100	100
26	4A	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
26	4a	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
27	4B	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
27	4b	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
28	4C	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
28	4c	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
29	4D	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
29	4d	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
30	4E	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
30	4e	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
31	4F	78/85 (92%)	74 (95%)	4 (5%)	0	100	100
31	4f	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
32	4G	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
32	4g	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
33	4H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
33	4h	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
34	4I	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
34	4i	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
35	4J	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
35	4j	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
36	4K	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
36	4k	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
37	4L	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
37	4l	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
38	4M	97/99 (98%)	97 (100%)	0	0	100	100
38	4m	97/99 (98%)	97 (100%)	0	0	100	100
39	4N	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
39	4n	129/131 (98%)	126 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	4O	45/47 (96%)	45 (100%)	0	0	100	100
40	4o	45/47 (96%)	45 (100%)	0	0	100	100
41	4P	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
41	4p	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
42	4Q	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
42	4q	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
43	4R	101/103 (98%)	101 (100%)	0	0	100	100
43	4r	101/103 (98%)	101 (100%)	0	0	100	100
44	4S	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	4s	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
45	4T	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
45	4t	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
46	4U	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
46	4u	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
47	4V	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
47	4v	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
48	4W	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
48	4w	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
49	4X	224/226 (99%)	220 (98%)	4 (2%)	0	100	100
49	4x	224/226 (99%)	220 (98%)	4 (2%)	0	100	100
50	4Y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
50	4y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
51	4Z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
51	4z	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
All	All	16327/16550 (99%)	15930 (98%)	395 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	3B	262	THR
14	3b	262	THR

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	2M	478/478 (100%)	473 (99%)	5 (1%)	68	86
1	2m	478/478 (100%)	474 (99%)	4 (1%)	73	88
2	2N	221/221 (100%)	221 (100%)	0	100	100
2	2n	221/221 (100%)	221 (100%)	0	100	100
3	2O	130/130 (100%)	130 (100%)	0	100	100
3	2o	130/130 (100%)	130 (100%)	0	100	100
4	2P	139/139 (100%)	139 (100%)	0	100	100
4	2p	139/139 (100%)	139 (100%)	0	100	100
5	2Q	60/60 (100%)	60 (100%)	0	100	100
5	2q	60/60 (100%)	60 (100%)	0	100	100
6	2R	100/100 (100%)	100 (100%)	0	100	100
6	2r	100/100 (100%)	100 (100%)	0	100	100
7	2S	143/143 (100%)	143 (100%)	0	100	100
7	2s	143/143 (100%)	143 (100%)	0	100	100
8	2T	73/73 (100%)	72 (99%)	1 (1%)	59	81
8	2t	73/73 (100%)	72 (99%)	1 (1%)	59	81
9	2U	43/43 (100%)	43 (100%)	0	100	100
9	2u	43/43 (100%)	43 (100%)	0	100	100
10	2V	75/75 (100%)	75 (100%)	0	100	100
10	2v	75/75 (100%)	75 (100%)	0	100	100
11	30	102/102 (100%)	101 (99%)	1 (1%)	68	86
12	31	126/126 (100%)	121 (96%)	5 (4%)	28	54
13	3A	386/386 (100%)	386 (100%)	0	100	100
13	3a	386/386 (100%)	386 (100%)	0	100	100
14	3B	423/423 (100%)	422 (100%)	1 (0%)	87	95
14	3b	423/423 (100%)	422 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	3C	204/205 (100%)	204 (100%)	0	100	100
15	3c	205/205 (100%)	203 (99%)	2 (1%)	68	86
16	3D	88/88 (100%)	88 (100%)	0	100	100
16	3d	88/88 (100%)	88 (100%)	0	100	100
17	3E	81/81 (100%)	81 (100%)	0	100	100
17	3e	81/81 (100%)	81 (100%)	0	100	100
18	3F	72/72 (100%)	72 (100%)	0	100	100
18	3f	72/72 (100%)	72 (100%)	0	100	100
19	3G	336/336 (100%)	335 (100%)	1 (0%)	86	94
19	3g	336/336 (100%)	334 (99%)	2 (1%)	78	91
20	3H	280/280 (100%)	279 (100%)	1 (0%)	84	93
20	3h	279/280 (100%)	278 (100%)	1 (0%)	84	93
21	3I	154/154 (100%)	154 (100%)	0	100	100
21	3i	154/154 (100%)	154 (100%)	0	100	100
22	3J	79/79 (100%)	79 (100%)	0	100	100
22	3j	79/79 (100%)	79 (100%)	0	100	100
23	3K	67/67 (100%)	66 (98%)	1 (2%)	57	80
23	3k	67/67 (100%)	66 (98%)	1 (2%)	57	80
24	3L	59/59 (100%)	59 (100%)	0	100	100
24	3l	59/59 (100%)	59 (100%)	0	100	100
25	40	229/229 (100%)	229 (100%)	0	100	100
25	41	229/229 (100%)	229 (100%)	0	100	100
26	4A	91/91 (100%)	91 (100%)	0	100	100
26	4a	91/91 (100%)	91 (100%)	0	100	100
27	4B	77/77 (100%)	77 (100%)	0	100	100
27	4b	77/77 (100%)	77 (100%)	0	100	100
28	4C	64/64 (100%)	64 (100%)	0	100	100
28	4c	64/64 (100%)	64 (100%)	0	100	100
29	4D	81/81 (100%)	81 (100%)	0	100	100
29	4d	81/81 (100%)	81 (100%)	0	100	100
30	4E	146/146 (100%)	145 (99%)	1 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	4e	146/146 (100%)	145 (99%)	1 (1%)	76	89
31	4F	70/74 (95%)	70 (100%)	0	100	100
31	4f	74/74 (100%)	74 (100%)	0	100	100
32	4G	83/83 (100%)	82 (99%)	1 (1%)	63	83
32	4g	83/83 (100%)	82 (99%)	1 (1%)	63	83
33	4H	124/124 (100%)	123 (99%)	1 (1%)	73	88
33	4h	124/124 (100%)	123 (99%)	1 (1%)	73	88
34	4I	180/180 (100%)	179 (99%)	1 (1%)	78	91
34	4i	180/180 (100%)	179 (99%)	1 (1%)	78	91
35	4J	148/148 (100%)	148 (100%)	0	100	100
35	4j	148/148 (100%)	148 (100%)	0	100	100
36	4K	77/77 (100%)	77 (100%)	0	100	100
36	4k	77/77 (100%)	77 (100%)	0	100	100
37	4L	108/108 (100%)	108 (100%)	0	100	100
37	4l	108/108 (100%)	108 (100%)	0	100	100
38	4M	85/85 (100%)	85 (100%)	0	100	100
38	4m	85/85 (100%)	85 (100%)	0	100	100
39	4N	112/112 (100%)	112 (100%)	0	100	100
39	4n	112/112 (100%)	112 (100%)	0	100	100
40	4O	40/40 (100%)	40 (100%)	0	100	100
40	4o	40/40 (100%)	40 (100%)	0	100	100
41	4P	163/163 (100%)	162 (99%)	1 (1%)	78	91
41	4p	163/163 (100%)	162 (99%)	1 (1%)	78	91
42	4Q	419/419 (100%)	419 (100%)	0	100	100
42	4q	419/419 (100%)	419 (100%)	0	100	100
43	4R	92/92 (100%)	92 (100%)	0	100	100
43	4r	92/92 (100%)	92 (100%)	0	100	100
44	4S	59/59 (100%)	59 (100%)	0	100	100
44	4s	59/59 (100%)	59 (100%)	0	100	100
45	4T	102/102 (100%)	102 (100%)	0	100	100
45	4t	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	4U	76/76 (100%)	76 (100%)	0	100	100
46	4u	76/76 (100%)	76 (100%)	0	100	100
47	4V	156/156 (100%)	156 (100%)	0	100	100
47	4v	156/156 (100%)	156 (100%)	0	100	100
48	4W	128/128 (100%)	128 (100%)	0	100	100
48	4w	128/128 (100%)	128 (100%)	0	100	100
49	4X	198/198 (100%)	198 (100%)	0	100	100
49	4x	198/198 (100%)	198 (100%)	0	100	100
50	4Y	100/100 (100%)	100 (100%)	0	100	100
50	4y	100/100 (100%)	100 (100%)	0	100	100
51	4Z	167/167 (100%)	167 (100%)	0	100	100
51	4z	167/167 (100%)	167 (100%)	0	100	100
All	All	14364/14370 (100%)	14326 (100%)	38 (0%)	84	94

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	4E	35	MET
33	4h	36	HIS
32	4G	24	TRP
41	4P	186	MET
41	4p	186	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
49	4X	104	GLN
48	4w	61	HIS
29	4d	74	GLN
35	4j	123	ASN
24	3L	590	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	AME	2S	1	7	9,10,11	0.27	0	9,11,13	0.48	0
7	AME	2s	1	7	9,10,11	0.30	0	9,11,13	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AME	2S	1	7	-	2/9/10/12	-
7	AME	2s	1	7	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2S	1	AME	O-C-CA-CB
7	2S	1	AME	C-CA-N-CT1
7	2s	1	AME	O-C-CA-CB
7	2s	1	AME	C-CA-N-CT1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 158 ligands modelled in this entry, 14 are monoatomic - leaving 144 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$
59	CDL	3l	702	-	80,80,99	0.33	0	86,92,111	0.48	0
67	HEA	4q	907	42	66,67,67	1.35	7 (10%)	78,103,103	2.42	28 (35%)
55	SF4	2n	302	2	0,12,12	-	-	-	-	-
59	CDL	4f	201	-	91,91,99	0.32	0	97,103,111	0.45	0
59	CDL	3l	201	-	66,66,99	0.35	0	71,77,111	0.43	0
56	F3S	2N	304	2	0,9,9	-	-	-	-	-
68	PER	4Q	909	67,65	1,1,1	0.26	0	-	-	-
54	FES	3h	404	20	0,4,4	-	-	-	-	-
59	CDL	4M	201	-	74,74,99	0.32	0	80,86,111	0.43	0
59	CDL	4L	201	-	93,93,99	0.29	0	99,105,111	0.35	0
53	UQ1	2p	201	-	18,18,18	1.13	2 (11%)	22,25,25	0.63	0
58	PEE	4z	302	-	43,43,50	0.81	2 (4%)	46,48,55	0.56	0
60	PC1	3a	501	-	53,53,53	0.28	0	59,61,61	0.37	0
59	CDL	4m	201	-	99,99,99	0.28	0	105,111,111	0.50	0
60	PC1	4F	201	-	53,53,53	0.29	0	59,61,61	0.41	0
58	PEE	2P	202	-	45,45,50	0.77	2 (4%)	48,50,55	0.59	0
59	CDL	3i	202	-	75,75,99	0.33	0	81,87,111	0.49	0
68	PER	4q	909	67,65	1,1,1	0.25	0	-	-	-
58	PEE	4Z	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.55	0
59	CDL	3D	201	-	83,83,99	0.31	0	89,95,111	0.41	0
60	PC1	2R	201	-	53,53,53	0.29	0	59,61,61	0.48	1 (1%)
59	CDL	3D	202	-	99,99,99	0.29	0	105,111,111	0.39	0
61	HEC	3C	302	15	50,50,50	1.48	9 (18%)	68,82,82	1.99	12 (17%)
64	CUA	4n	201	39	0,1,1	-	-	-	-	-
59	CDL	2q	101	-	99,99,99	0.30	0	105,111,111	0.47	0
59	CDL	4Q	902	-	94,94,99	0.30	0	100,106,111	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	LPP	4z	301	-	37,37,43	0.24	0	41,42,48	0.47	0
58	PEE	4S	101	-	26,26,50	0.37	0	29,31,55	0.34	0
58	PEE	40	304	-	30,30,50	0.32	0	33,35,55	0.52	0
62	HEM	3g	407	19	50,50,50	1.43	7 (14%)	66,82,82	1.42	11 (16%)
59	CDL	3H	405	-	83,83,99	0.32	0	89,95,111	0.39	0
53	UQ1	2N	301	-	18,18,18	1.07	2 (11%)	22,25,25	0.75	0
58	PEE	2r	203	-	38,38,50	0.61	1 (2%)	41,43,55	0.46	0
59	CDL	4t	201	-	60,60,99	0.37	0	66,72,111	0.45	0
59	CDL	4U	501	-	71,71,99	0.34	0	77,83,111	0.44	0
60	PC1	3H	401	-	33,33,53	0.35	0	39,41,61	0.77	1 (2%)
59	CDL	3I	202	-	80,80,99	0.32	0	86,92,111	0.44	0
54	FES	2n	301	2	0,4,4	-	-	-	-	-
58	PEE	40	301	-	44,44,50	0.78	2 (4%)	46,49,55	0.55	0
60	PC1	2o	202	-	38,38,53	0.33	0	44,46,61	0.48	0
59	CDL	3e	202	-	76,76,99	0.33	0	82,88,111	0.43	0
60	PC1	3h	402	-	40,40,53	0.34	0	46,48,61	0.44	0
63	LPP	4Z	301	-	43,43,43	0.23	0	47,48,48	0.44	0
58	PEE	4q	902	-	39,39,50	0.85	2 (5%)	41,44,55	0.64	0
63	LPP	4C	101	-	43,43,43	0.24	0	47,48,48	0.38	0
60	PC1	2r	201	-	53,53,53	0.30	0	59,61,61	0.57	1 (1%)
59	CDL	3g	406	-	57,57,99	0.38	0	63,69,111	0.55	0
60	PC1	2r	202	-	51,51,53	0.29	0	57,59,61	0.40	0
58	PEE	4q	901	-	36,36,50	0.89	2 (5%)	38,41,55	0.64	0
60	PC1	3h	401	-	39,39,53	0.33	0	45,47,61	0.46	0
58	PEE	4D	101	-	39,39,50	0.66	1 (2%)	42,44,55	0.45	0
52	FAD	2M	701	1	56,58,58	0.73	2 (3%)	81,89,89	1.01	4 (4%)
59	CDL	4J	301	-	58,58,99	0.36	0	62,69,111	0.49	0
59	CDL	2p	204	-	73,73,99	0.33	0	79,85,111	0.50	0
67	HEA	4q	908	42,68	66,67,67	1.38	7 (10%)	78,103,103	2.38	29 (37%)
59	CDL	4z	303	-	92,92,99	0.30	0	98,104,111	0.51	1 (1%)
59	CDL	4E	201	-	88,88,99	0.30	0	94,100,111	0.37	0
58	PEE	4s	101	-	46,46,50	0.80	2 (4%)	49,51,55	0.52	0
58	PEE	3H	403	-	45,45,50	0.79	2 (4%)	48,50,55	0.75	1 (2%)
59	CDL	4Z	303	-	47,47,99	0.40	0	53,59,111	0.49	0
59	CDL	4O	501	-	96,96,99	0.30	0	102,108,111	0.41	0
62	HEM	3G	406	19	50,50,50	1.51	8 (16%)	66,82,82	1.54	9 (13%)
54	FES	3H	406	20	0,4,4	-	-	-	-	-
60	PC1	4e	201	-	53,53,53	0.28	0	59,61,61	0.35	0
59	CDL	4I	304	-	91,91,99	0.29	0	97,103,111	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PEE	3c	301	-	32,32,50	0.70	1 (3%)	34,37,55	0.43	0
59	CDL	3E	201	-	92,92,99	0.30	0	98,104,111	0.37	0
58	PEE	4l	301	-	44,44,50	0.80	2 (4%)	46,49,55	0.43	0
59	CDL	2T	104	-	70,70,99	0.34	0	76,82,111	0.56	1 (1%)
58	PEE	3f	102	-	37,37,50	0.66	1 (2%)	40,42,55	0.51	0
58	PEE	4w	201	-	50,50,50	0.75	2 (4%)	53,55,55	0.52	0
53	UQ1	3g	402	-	18,18,18	1.07	2 (11%)	22,25,25	0.64	0
59	CDL	2O	203	-	66,66,99	0.35	0	72,78,111	0.56	0
60	PC1	2T	102	-	44,44,53	0.31	0	50,52,61	0.37	0
58	PEE	4l	303	-	35,35,50	0.67	1 (2%)	38,40,55	0.56	0
58	PEE	2t	101	-	41,41,50	0.62	1 (2%)	44,46,55	0.46	0
53	UQ1	3G	402	-	18,18,18	1.06	2 (11%)	22,25,25	0.65	0
59	CDL	4q	903	-	92,92,99	0.29	0	98,104,111	0.51	0
60	PC1	2p	202	-	40,40,53	0.31	0	46,48,61	0.35	0
58	PEE	2O	202	-	40,40,50	0.64	1 (2%)	43,45,55	0.52	0
53	UQ1	3g	401	-	18,18,18	1.02	1 (5%)	22,25,25	1.04	2 (9%)
59	CDL	2o	201	-	85,85,99	0.31	0	91,97,111	0.42	0
59	CDL	3L	701	-	84,84,99	0.31	0	90,96,111	0.44	0
53	UQ1	3G	401	-	18,18,18	0.95	2 (11%)	22,25,25	1.33	4 (18%)
59	CDL	4g	202	-	65,65,99	0.35	0	69,76,111	0.47	0
61	HEC	3c	302	15	50,50,50	1.45	10 (20%)	68,82,82	1.48	10 (14%)
59	CDL	3h	403	-	84,84,99	0.32	0	90,96,111	0.48	1 (1%)
60	PC1	3A	501	-	37,37,53	0.32	0	43,45,61	0.36	0
56	F3S	2n	303	2	0,9,9	-	-	-	-	-
52	FAD	2m	701	1	56,58,58	0.72	3 (5%)	81,89,89	0.98	4 (4%)
59	CDL	3g	404	-	88,88,99	0.30	0	94,100,111	0.42	0
58	PEE	4W	201	-	50,50,50	0.74	2 (4%)	53,55,55	0.56	0
59	CDL	2t	102	-	65,65,99	0.36	0	71,77,111	0.48	0
59	CDL	3g	403	-	69,69,99	0.35	0	75,81,111	0.53	0
59	CDL	4e	203	-	95,95,99	0.31	0	101,107,111	0.47	0
59	CDL	3G	403	-	99,99,99	0.29	0	105,111,111	0.46	0
59	CDL	4S	102	-	99,99,99	0.29	0	105,111,111	0.44	1 (0%)
59	CDL	4e	202	-	49,49,99	0.41	0	55,61,111	0.62	1 (1%)
59	CDL	4j	301	-	50,50,99	0.41	0	52,60,111	0.58	0
58	PEE	40	302	-	46,46,50	0.81	2 (4%)	49,51,55	0.61	0
59	CDL	4j	302	-	87,87,99	0.30	0	93,99,111	0.33	0
59	CDL	4E	202	-	45,45,99	0.40	0	51,57,111	0.52	0
59	CDL	3g	405	-	89,89,99	0.31	0	95,101,111	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	CDL	4Q	903	-	74,74,99	0.32	0	80,86,111	0.42	0
59	CDL	4z	304	-	85,85,99	0.30	0	91,97,111	0.53	1 (1%)
59	CDL	3L	702	-	80,80,99	0.32	0	86,92,111	0.41	0
58	PEE	4l	201	-	37,37,50	0.82	2 (5%)	39,42,55	0.69	1 (2%)
59	CDL	3L	703	-	92,92,99	0.30	0	98,104,111	0.42	0
59	CDL	3i	201	-	50,50,99	0.40	0	56,62,111	0.48	0
64	CUA	4N	201	39	0,1,1	-	-	-	-	-
59	CDL	4K	201	-	89,89,99	0.30	0	95,101,111	0.38	0
58	PEE	4l	302	-	43,43,50	0.78	2 (4%)	46,48,55	0.54	0
59	CDL	2P	203	-	80,80,99	0.31	0	86,92,111	0.34	0
60	PC1	3f	101	-	45,45,53	0.31	0	51,53,61	0.36	0
58	PEE	2O	201	-	38,38,50	0.63	1 (2%)	41,43,55	0.45	0
55	SF4	2N	303	2	0,12,12	-	-	-	-	-
58	PEE	4o	303	-	34,34,50	0.66	1 (2%)	36,39,55	0.45	0
60	PC1	2R	202	-	53,53,53	0.28	0	59,61,61	0.50	1 (1%)
59	CDL	3l	701	-	99,99,99	0.29	0	105,111,111	0.47	0
59	CDL	2Q	101	-	99,99,99	0.28	0	105,111,111	0.37	0
58	PEE	2T	103	-	44,44,50	0.79	2 (4%)	46,49,55	0.53	0
59	CDL	4F	202	-	99,99,99	0.30	0	105,111,111	0.42	0
58	PEE	2o	203	-	23,23,50	0.36	0	24,27,55	0.35	0
59	CDL	3I	203	-	62,62,99	0.36	0	68,74,111	0.43	0
67	HEA	4Q	907	42	66,67,67	1.36	7 (10%)	78,103,103	2.43	28 (35%)
54	FES	2N	302	2	0,4,4	-	-	-	-	-
58	PEE	4d	101	-	50,50,50	0.75	2 (4%)	53,55,55	0.46	0
59	CDL	4s	102	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
63	LPP	4g	201	-	38,38,43	0.25	0	42,43,48	0.44	0
60	PC1	3H	402	-	32,32,53	0.37	0	38,40,61	0.58	0
58	PEE	2p	203	-	23,23,50	0.38	0	26,28,55	0.41	0
59	CDL	3G	404	-	74,74,99	0.33	0	80,86,111	0.45	0
60	PC1	2P	201	-	34,34,53	0.34	0	40,42,61	0.41	0
60	PC1	2T	101	-	53,53,53	0.28	0	59,61,61	0.30	0
59	CDL	4o	501	-	92,92,99	0.30	0	98,104,111	0.41	0
59	CDL	3H	404	-	88,88,99	0.31	0	94,100,111	0.39	0
59	CDL	3e	201	-	70,70,99	0.34	0	76,82,111	0.48	0
62	HEM	3g	408	19	50,50,50	1.46	8 (16%)	66,82,82	1.52	11 (16%)
59	CDL	4W	202	-	72,72,99	0.34	0	78,84,111	0.40	0
67	HEA	4Q	908	42,68	66,67,67	1.38	6 (9%)	78,103,103	2.37	29 (37%)
58	PEE	4Q	901	-	35,35,50	0.84	2 (5%)	38,40,55	0.71	1 (2%)
58	PEE	3C	301	-	29,29,50	0.74	1 (3%)	32,34,55	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	HEM	3G	405	19	50,50,50	1.43	7 (14%)	66,82,82	1.37	9 (13%)
58	PEE	4R	201	-	42,42,50	0.83	2 (4%)	45,47,55	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CDL	3l	702	-	-	14/91/91/110	-
67	HEA	4q	907	42	-	6/36/76/76	-
55	SF4	2n	302	2	-	-	0/6/5/5
59	CDL	4f	201	-	-	26/102/102/110	-
59	CDL	3l	201	-	-	14/75/75/110	-
56	F3S	2N	304	2	-	-	0/3/3/3
54	FES	3h	404	20	-	-	0/1/1/1
59	CDL	4M	201	-	-	22/85/85/110	-
59	CDL	4L	201	-	-	21/104/104/110	-
53	UQ1	2p	201	-	-	1/9/33/33	0/1/1/1
58	PEE	4z	302	-	-	22/47/47/54	-
60	PC1	3a	501	-	-	15/57/57/57	-
59	CDL	4m	201	-	-	23/110/110/110	-
60	PC1	4F	201	-	-	15/57/57/57	-
58	PEE	2P	202	-	-	15/49/49/54	-
59	CDL	3i	202	-	-	24/86/86/110	-
58	PEE	4Z	302	-	-	20/54/54/54	-
59	CDL	3D	201	-	-	26/94/94/110	-
60	PC1	2R	201	-	-	16/57/57/57	-
59	CDL	3D	202	-	-	10/110/110/110	-
59	CDL	2q	101	-	-	32/110/110/110	-
59	CDL	4Q	902	-	-	32/105/105/110	-
63	LPP	4z	301	-	-	10/39/39/45	-
58	PEE	4S	101	-	-	3/30/30/54	-
58	PEE	40	304	-	-	7/34/34/54	-
62	HEM	3g	407	19	-	7/14/54/54	-
59	CDL	3H	405	-	-	23/94/94/110	-
53	UQ1	2N	301	-	-	1/9/33/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PEE	2r	203	-	-	8/42/42/54	-
59	CDL	4t	201	-	-	22/71/71/110	-
59	CDL	4U	501	-	-	21/82/82/110	-
60	PC1	3H	401	-	-	10/37/37/57	-
59	CDL	3I	202	-	-	24/91/91/110	-
58	PEE	40	301	-	-	19/48/48/54	-
54	FES	2n	301	2	-	-	0/1/1/1
60	PC1	2o	202	-	-	12/42/42/57	-
59	CDL	3e	202	-	-	27/87/87/110	-
60	PC1	3h	402	-	-	10/44/44/57	-
63	LPP	4Z	301	-	-	5/45/45/45	-
58	PEE	4q	902	-	-	14/43/43/54	-
63	LPP	4C	101	-	-	8/45/45/45	-
60	PC1	2r	201	-	-	7/57/57/57	-
59	CDL	3g	406	-	-	24/68/68/110	-
60	PC1	2r	202	-	-	12/55/55/57	-
58	PEE	4q	901	-	-	13/40/40/54	-
60	PC1	3h	401	-	-	13/43/43/57	-
58	PEE	4D	101	-	-	5/43/43/54	-
52	FAD	2M	701	1	-	8/34/50/50	0/6/6/6
59	CDL	4J	301	-	-	22/68/68/110	-
59	CDL	2p	204	-	-	14/84/84/110	-
67	HEA	4q	908	42,68	-	8/36/76/76	-
59	CDL	4z	303	-	-	16/103/103/110	-
59	CDL	4E	201	-	-	11/99/99/110	-
58	PEE	4s	101	-	-	9/50/50/54	-
58	PEE	3H	403	-	-	11/49/49/54	-
59	CDL	4Z	303	-	-	20/58/58/110	-
59	CDL	4O	501	-	-	24/107/107/110	-
62	HEM	3G	406	19	-	6/14/54/54	-
54	FES	3H	406	20	-	-	0/1/1/1
60	PC1	4e	201	-	-	10/57/57/57	-
59	CDL	4I	304	-	-	21/102/102/110	-
58	PEE	3c	301	-	-	13/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CDL	3E	201	-	-	37/103/103/110	-
58	PEE	41	301	-	-	9/48/48/54	-
59	CDL	2T	104	-	-	18/81/81/110	-
58	PEE	3f	102	-	-	13/41/41/54	-
58	PEE	4w	201	-	-	12/54/54/54	-
53	UQ1	3g	402	-	-	1/9/33/33	0/1/1/1
59	CDL	2O	203	-	-	24/77/77/110	-
60	PC1	2T	102	-	-	8/48/48/57	-
58	PEE	41	303	-	-	12/39/39/54	-
58	PEE	2t	101	-	-	10/45/45/54	-
53	UQ1	3G	402	-	-	1/9/33/33	0/1/1/1
59	CDL	4q	903	-	-	28/103/103/110	-
60	PC1	2p	202	-	-	2/44/44/57	-
58	PEE	2O	202	-	-	16/44/44/54	-
53	UQ1	3g	401	-	-	4/9/33/33	0/1/1/1
59	CDL	2o	201	-	-	18/96/96/110	-
59	CDL	3L	701	-	-	25/95/95/110	-
61	HEC	3c	302	15	1/1/3/7	5/14/54/54	-
53	UQ1	3G	401	-	-	4/9/33/33	0/1/1/1
59	CDL	4g	202	-	-	18/75/75/110	-
59	CDL	3h	403	-	-	24/95/95/110	-
60	PC1	3A	501	-	-	7/40/40/57	-
58	PEE	3C	301	-	-	3/33/33/54	-
56	F3S	2n	303	2	-	-	0/3/3/3
52	FAD	2m	701	1	-	8/34/50/50	0/6/6/6
59	CDL	3g	404	-	-	10/99/99/110	-
58	PEE	4W	201	-	-	9/54/54/54	-
59	CDL	2t	102	-	-	9/76/76/110	-
59	CDL	3g	403	-	-	25/80/80/110	-
59	CDL	4e	203	-	-	8/106/106/110	-
59	CDL	3G	403	-	-	19/110/110/110	-
59	CDL	4S	102	-	-	17/110/110/110	-
59	CDL	4e	202	-	-	15/60/60/110	-
59	CDL	4j	301	-	-	16/59/59/110	-
58	PEE	40	302	-	-	15/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CDL	4j	302	-	-	22/98/98/110	-
59	CDL	4E	202	-	-	12/55/55/110	-
59	CDL	3g	405	-	-	18/100/100/110	-
59	CDL	4Q	903	-	-	15/84/84/110	-
59	CDL	4z	304	-	-	23/96/96/110	-
59	CDL	3L	702	-	-	17/91/91/110	-
58	PEE	4l	201	-	-	16/41/41/54	-
59	CDL	3L	703	-	-	32/103/103/110	-
59	CDL	3i	201	-	-	19/61/61/110	-
59	CDL	4K	201	-	-	26/100/100/110	-
58	PEE	4l	302	-	-	13/47/47/54	-
59	CDL	2P	203	-	-	17/91/91/110	-
60	PC1	3f	101	-	-	8/49/49/57	-
58	PEE	2O	201	-	-	15/42/42/54	-
58	PEE	40	303	-	-	12/38/38/54	-
55	SF4	2N	303	2	-	-	0/6/5/5
60	PC1	2R	202	-	-	14/57/57/57	-
59	CDL	3l	701	-	-	24/110/110/110	-
59	CDL	2Q	101	-	-	29/110/110/110	-
58	PEE	2T	103	-	-	12/48/48/54	-
59	CDL	4F	202	-	-	31/110/110/110	-
58	PEE	2o	203	-	-	8/26/26/54	-
59	CDL	3I	203	-	-	22/73/73/110	-
67	HEA	4Q	907	42	-	6/36/76/76	-
58	PEE	4d	101	-	-	6/54/54/54	-
59	CDL	4s	102	-	-	14/110/110/110	-
54	FES	2N	302	2	-	-	0/1/1/1
63	LPP	4g	201	-	-	8/40/40/45	-
60	PC1	3H	402	-	-	16/36/36/57	-
58	PEE	2p	203	-	-	8/27/27/54	-
59	CDL	3G	404	-	-	12/85/85/110	-
60	PC1	2P	201	-	-	0/38/38/57	-
60	PC1	2T	101	-	-	8/57/57/57	-
59	CDL	4o	501	-	-	19/103/103/110	-
59	CDL	3H	404	-	-	23/99/99/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CDL	3e	201	-	-	14/81/81/110	-
62	HEM	3g	408	19	-	6/14/54/54	-
59	CDL	4W	202	-	-	22/83/83/110	-
67	HEA	4Q	908	42,68	-	8/36/76/76	-
58	PEE	4Q	901	-	-	13/39/39/54	-
61	HEC	3C	302	15	1/1/3/7	5/14/54/54	-
62	HEM	3G	405	19	-	7/14/54/54	-
58	PEE	4R	201	-	-	12/46/46/54	-

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	4q	908	HEA	C3B-C2B	4.59	1.45	1.34
67	4Q	908	HEA	C3B-C2B	4.58	1.45	1.34
67	4Q	907	HEA	C3B-C2B	4.49	1.44	1.34
67	4q	907	HEA	C3B-C2B	4.47	1.44	1.34
67	4Q	908	HEA	C3A-C2A	4.01	1.45	1.36

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	3C	302	HEC	CAB-C3B-C4B	10.29	138.17	124.81
61	3C	302	HEC	CAB-C3B-C2B	-7.23	115.17	127.53
67	4Q	907	HEA	C3A-C2A-C1A	-6.80	100.59	107.08
67	4q	908	HEA	C3A-C2A-C1A	-6.79	100.60	107.08
67	4q	907	HEA	C3A-C2A-C1A	-6.75	100.63	107.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
61	3C	302	HEC	NA
61	3c	302	HEC	NA

5 of 1914 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	2M	701	FAD	N10-C1'-C2'-O2'
52	2M	701	FAD	N10-C1'-C2'-C3'
52	2m	701	FAD	N10-C1'-C2'-O2'
52	2m	701	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
58	2O	201	PEE	C1-O3P-P-O2P

There are no ring outliers.

63 monomers are involved in 145 short contacts:

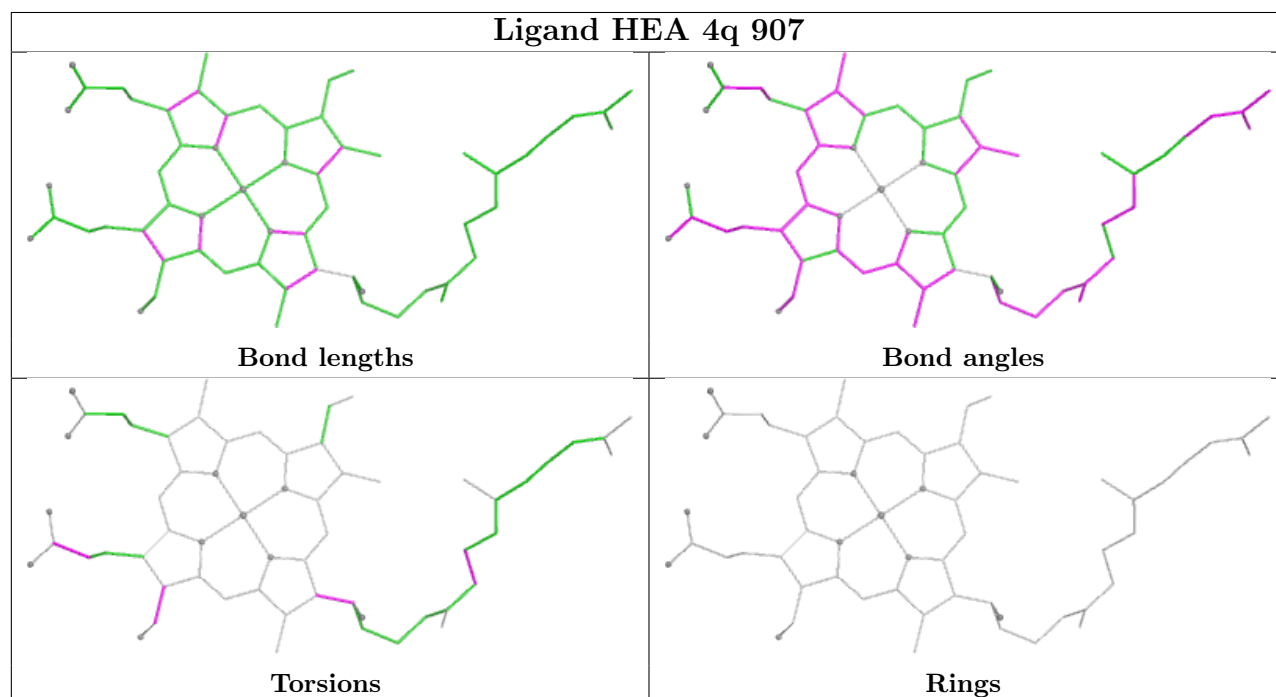
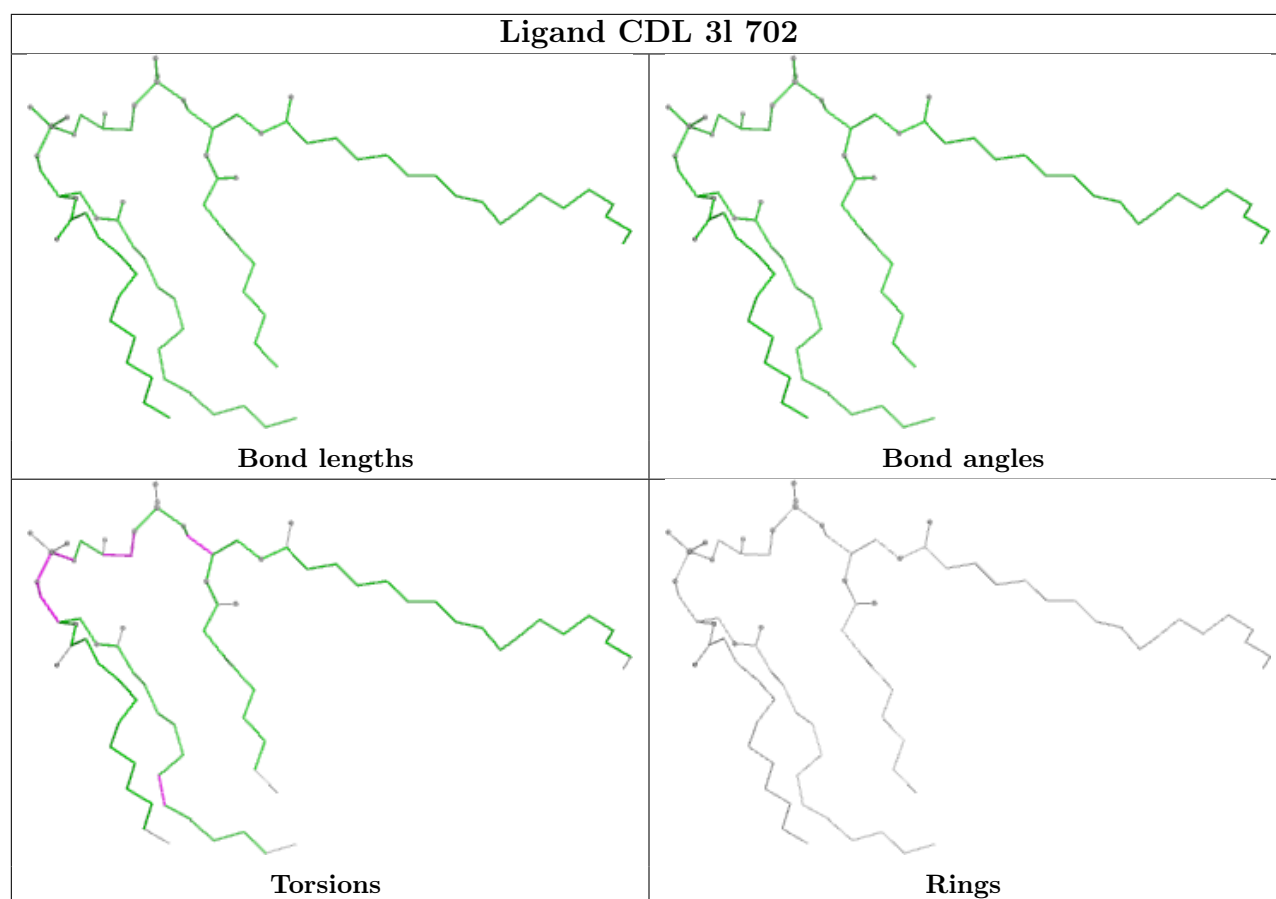
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	4q	907	HEA	5	0
59	4f	201	CDL	4	0
54	3h	404	FES	1	0
59	4M	201	CDL	1	0
59	4L	201	CDL	1	0
53	2p	201	UQ1	1	0
58	4z	302	PEE	1	0
59	4m	201	CDL	3	0
60	4F	201	PC1	2	0
59	3i	202	CDL	2	0
58	4Z	302	PEE	2	0
60	2R	201	PC1	1	0
61	3C	302	HEC	4	0
59	2q	101	CDL	7	0
59	4Q	902	CDL	2	0
58	40	304	PEE	1	0
62	3g	407	HEM	7	0
59	3H	405	CDL	1	0
59	4t	201	CDL	1	0
59	3I	202	CDL	1	0
59	3e	202	CDL	2	0
60	3h	402	PC1	1	0
63	4C	101	LPP	1	0
60	2r	201	PC1	2	0
59	2p	204	CDL	1	0
67	4q	908	HEA	6	0
59	4z	303	CDL	1	0
59	4Z	303	CDL	1	0
54	3H	406	FES	1	0
58	3c	301	PEE	1	0
58	41	301	PEE	1	0
59	2O	203	CDL	2	0
60	2T	102	PC1	3	0
58	41	303	PEE	1	0
59	4q	903	CDL	3	0
58	2O	202	PEE	1	0

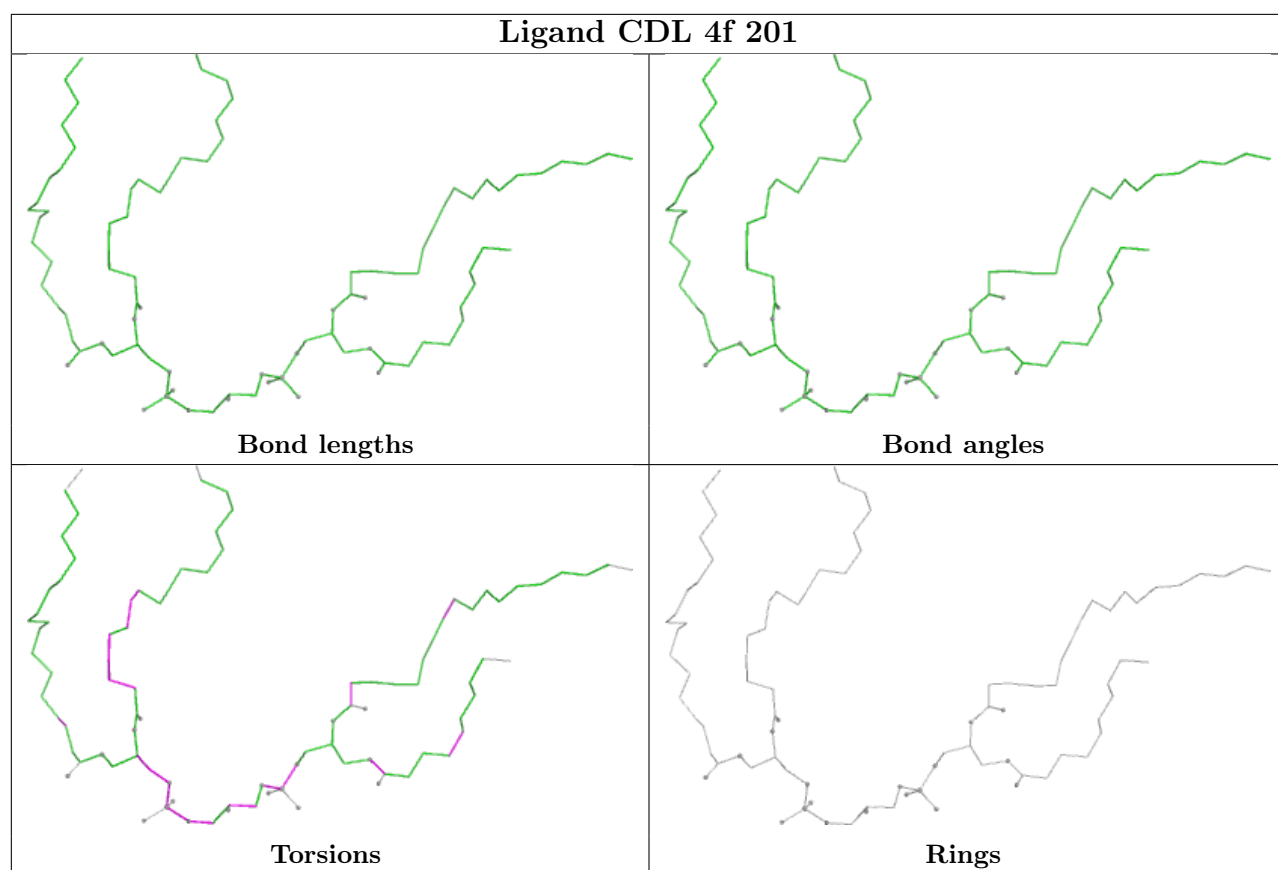
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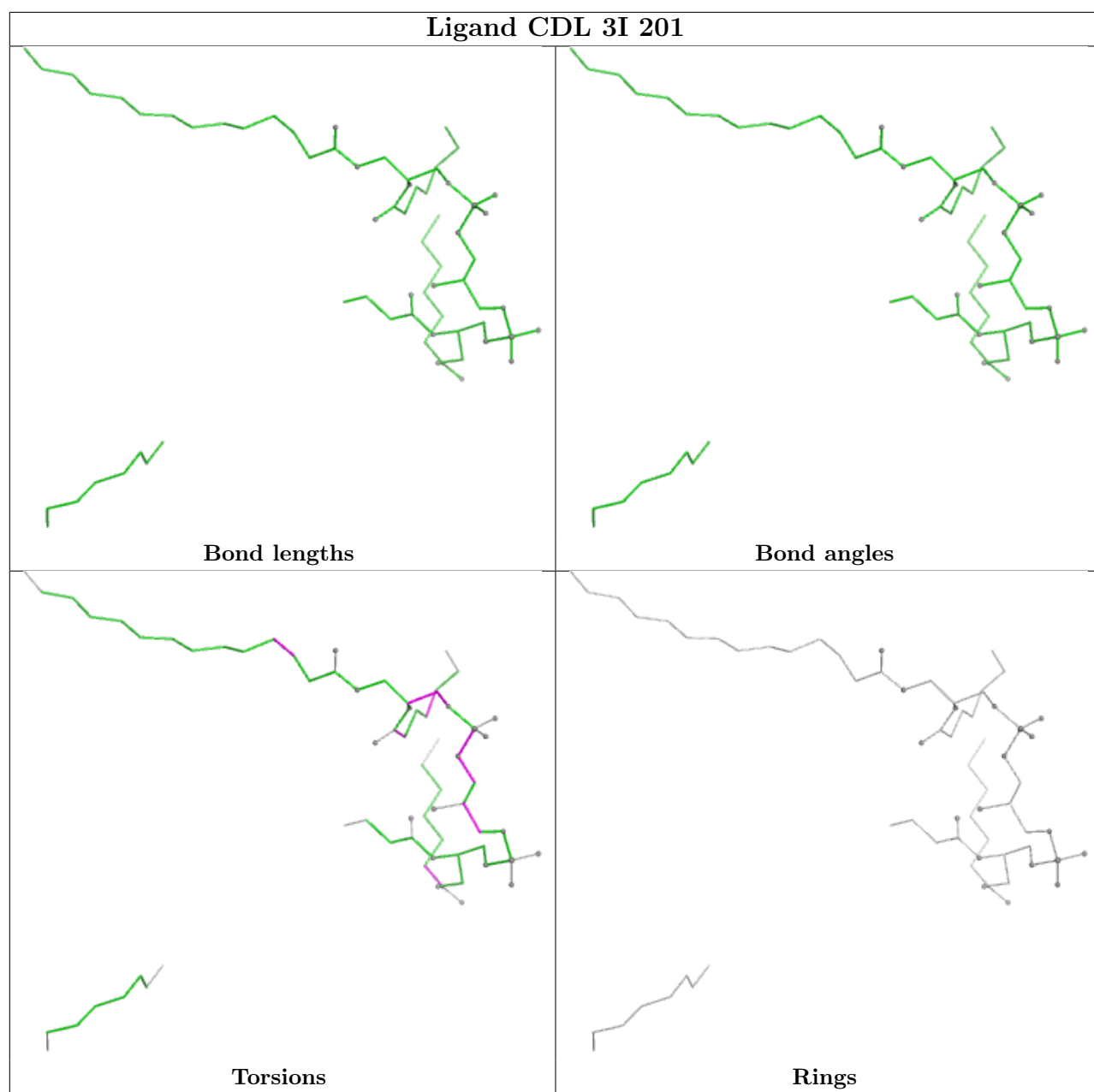
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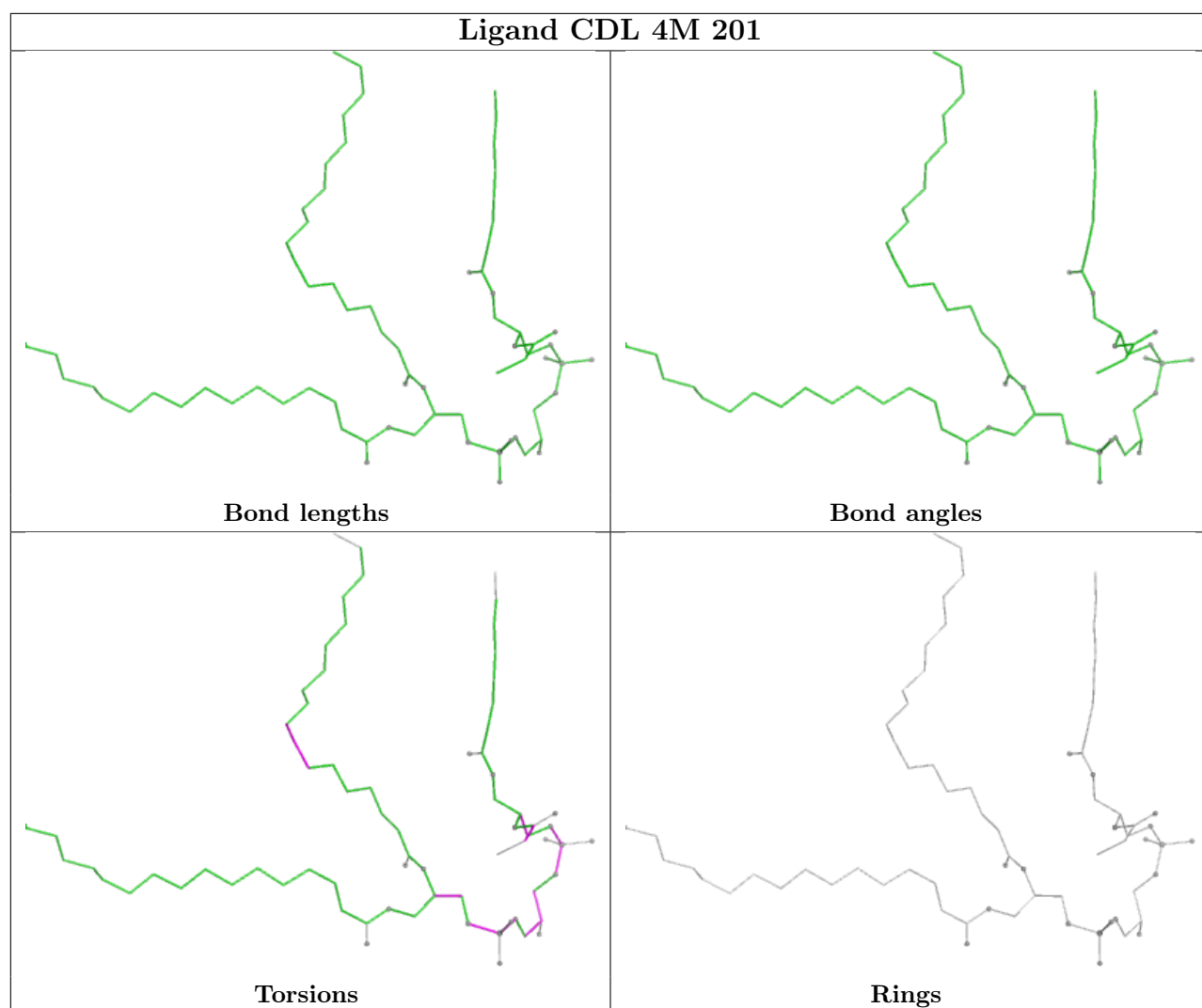
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	3g	401	UQ1	4	0
53	3G	401	UQ1	5	0
59	4g	202	CDL	1	0
61	3c	302	HEC	6	0
59	3h	403	CDL	2	0
59	3g	404	CDL	1	0
59	2t	102	CDL	2	0
59	3g	403	CDL	2	0
59	4e	203	CDL	3	0
59	4e	202	CDL	2	0
59	4j	301	CDL	1	0
59	4j	302	CDL	1	0
59	4E	202	CDL	2	0
58	4l	201	PEE	2	0
59	3L	703	CDL	5	0
59	3i	201	CDL	1	0
59	4K	201	CDL	1	0
60	3f	101	PC1	1	0
58	2O	201	PEE	1	0
59	3l	701	CDL	7	0
58	2T	103	PEE	1	0
67	4Q	907	HEA	4	0
59	4o	501	CDL	4	0
59	3H	404	CDL	1	0
59	3e	201	CDL	3	0
67	4Q	908	HEA	5	0
62	3G	405	HEM	4	0

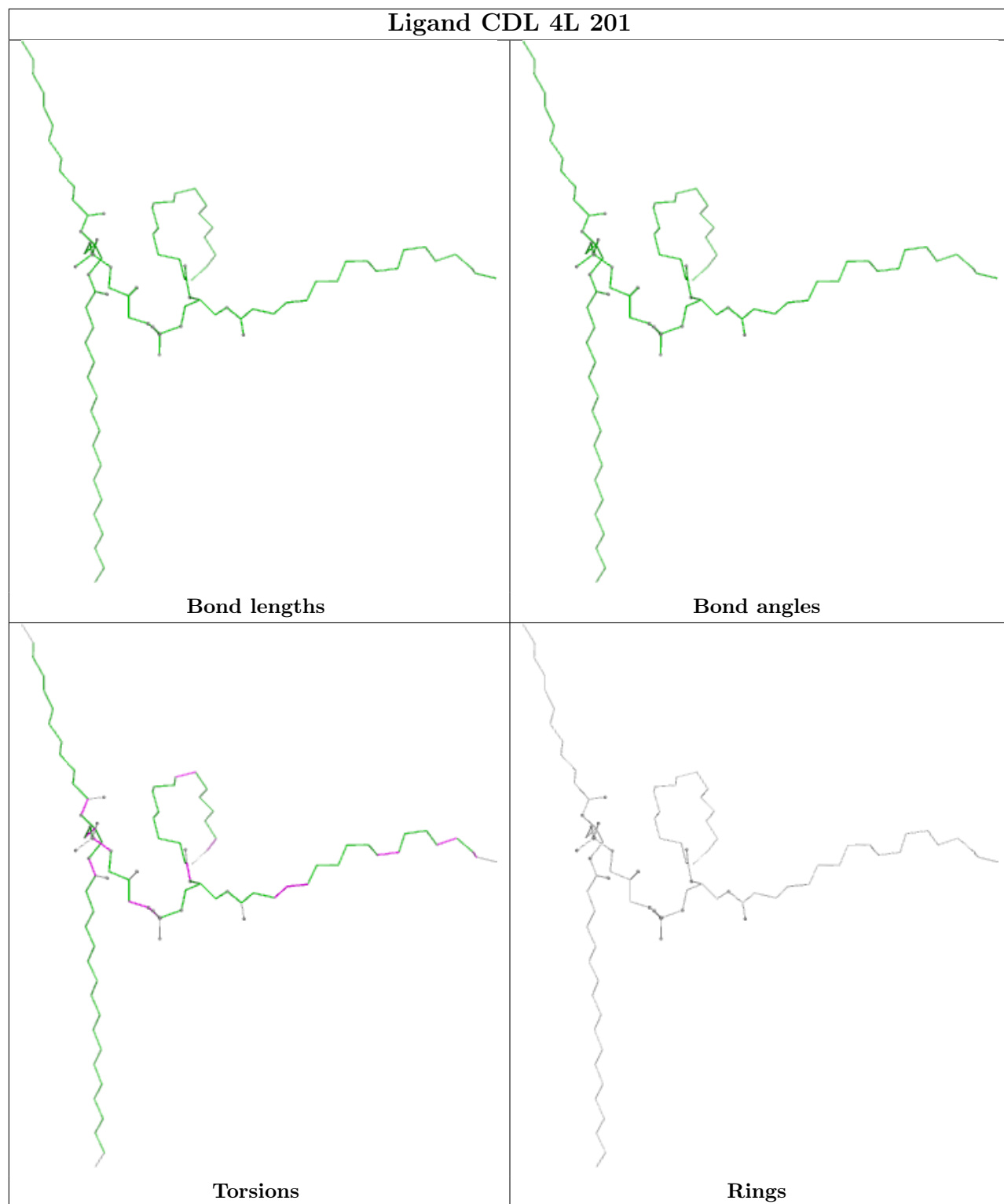
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

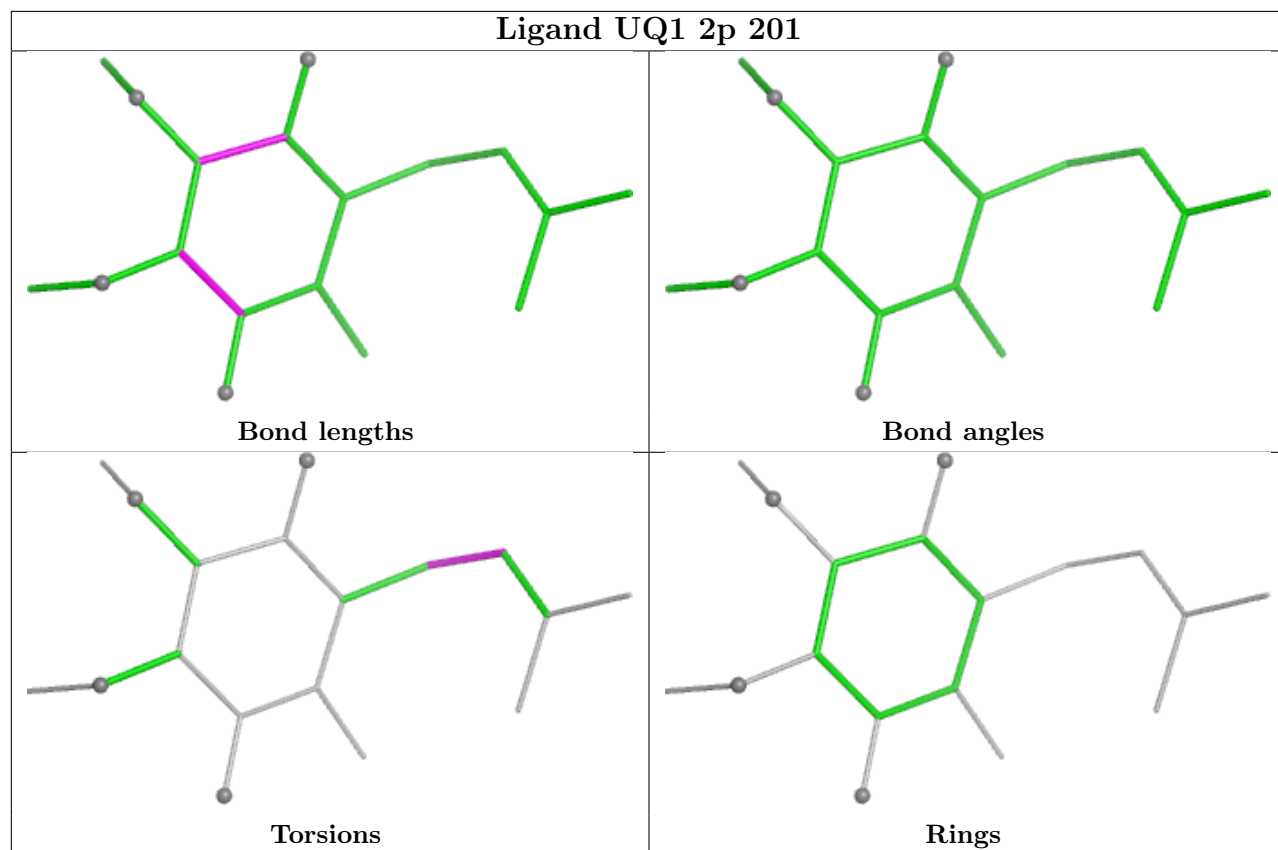


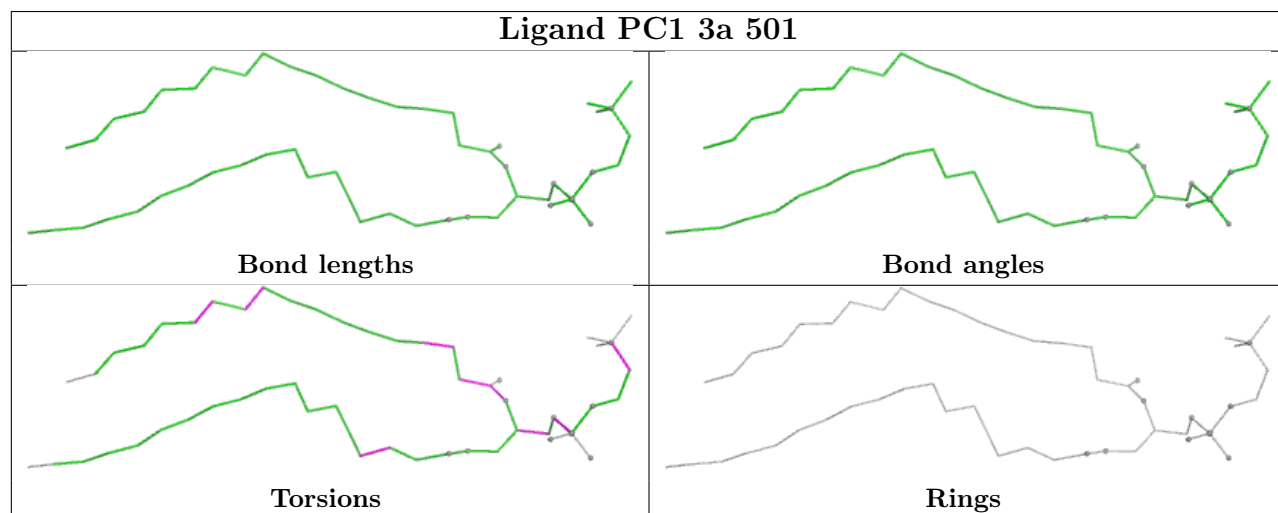
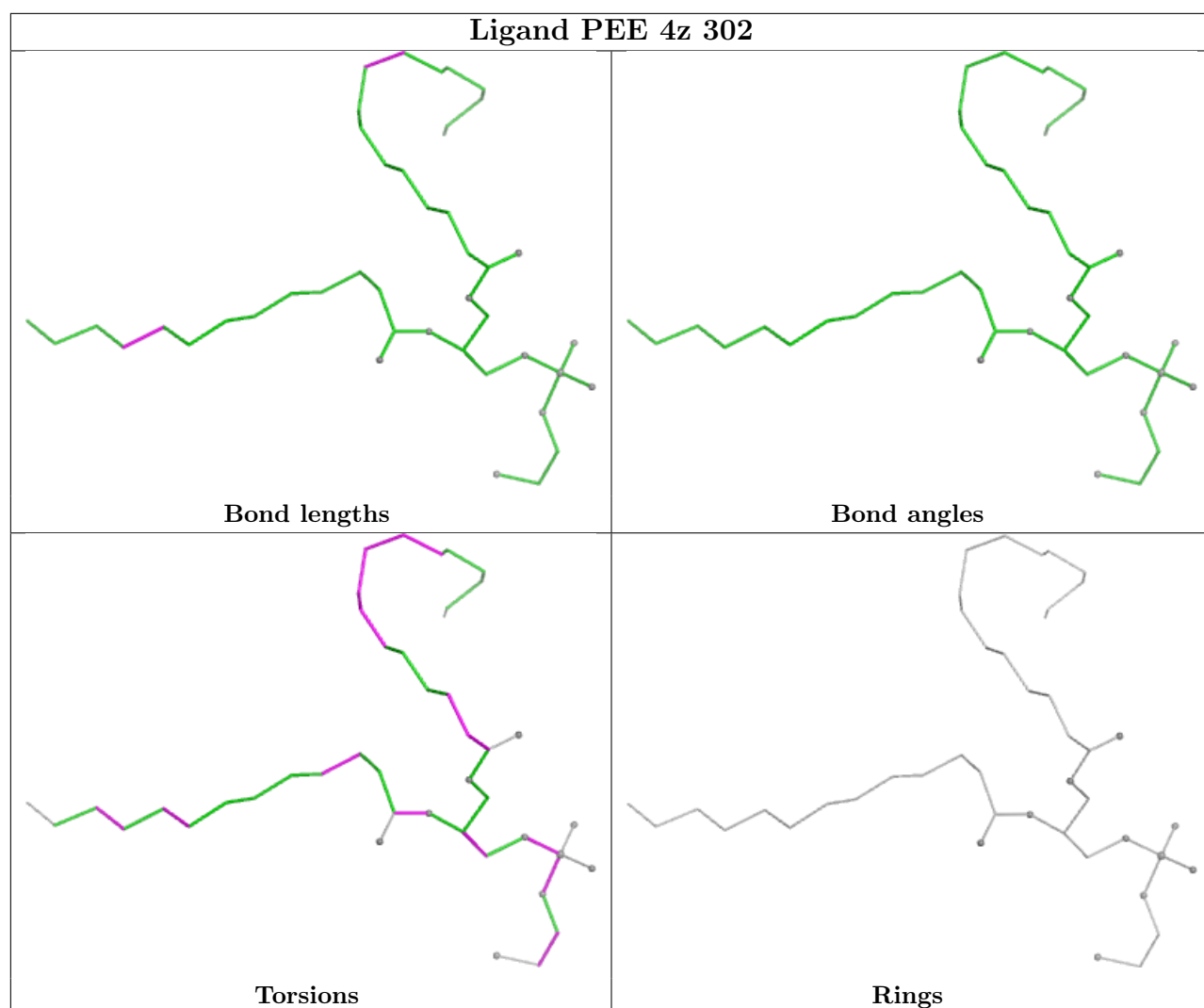


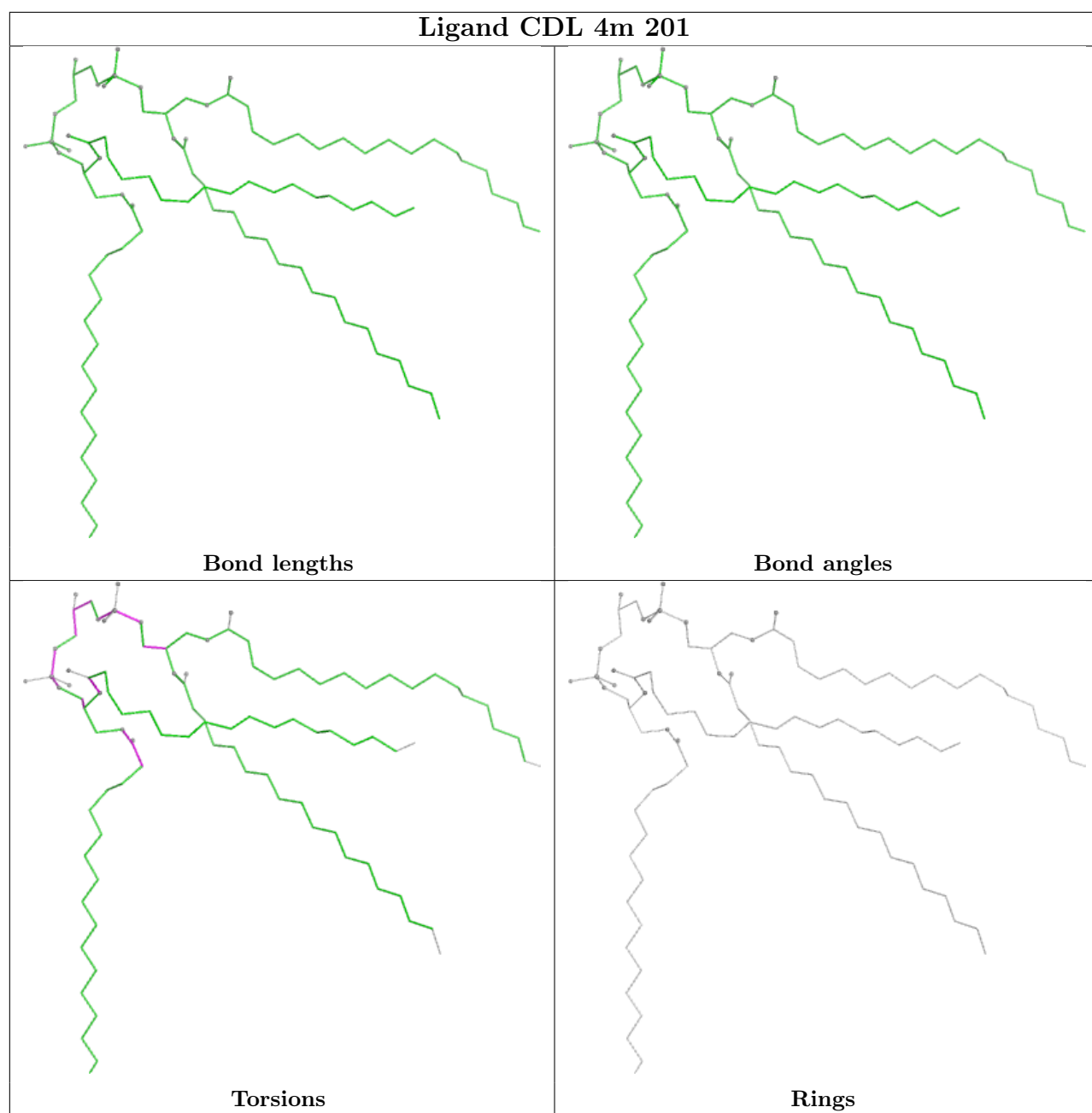


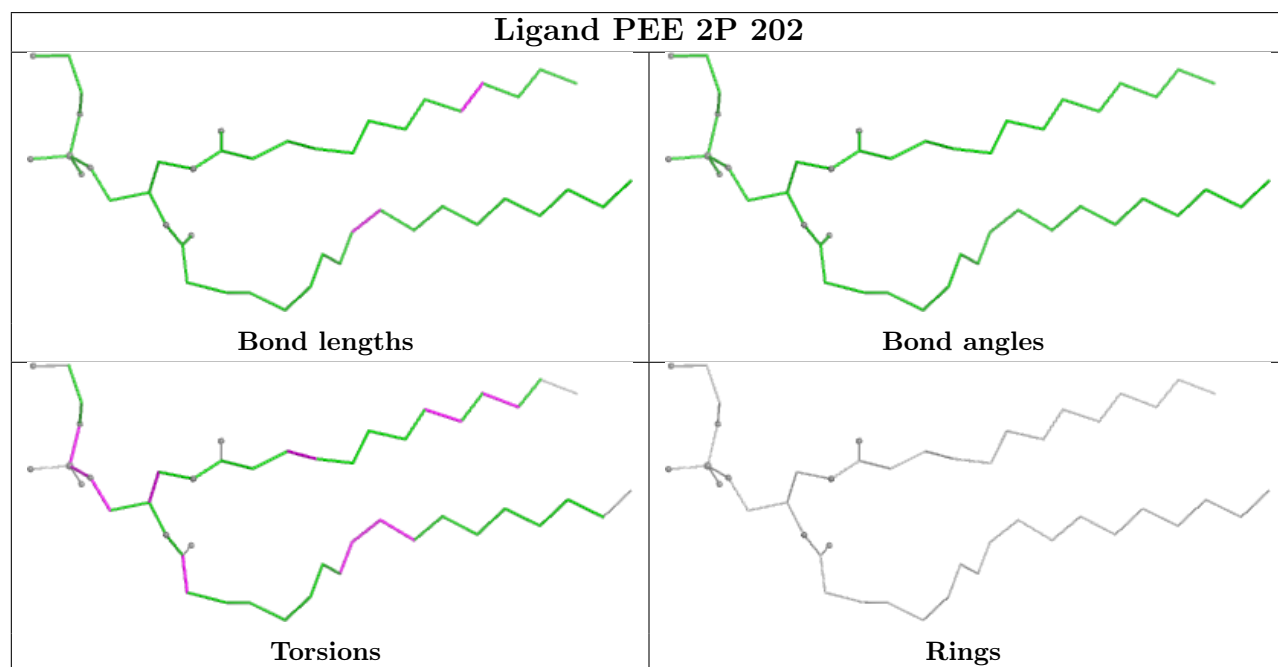
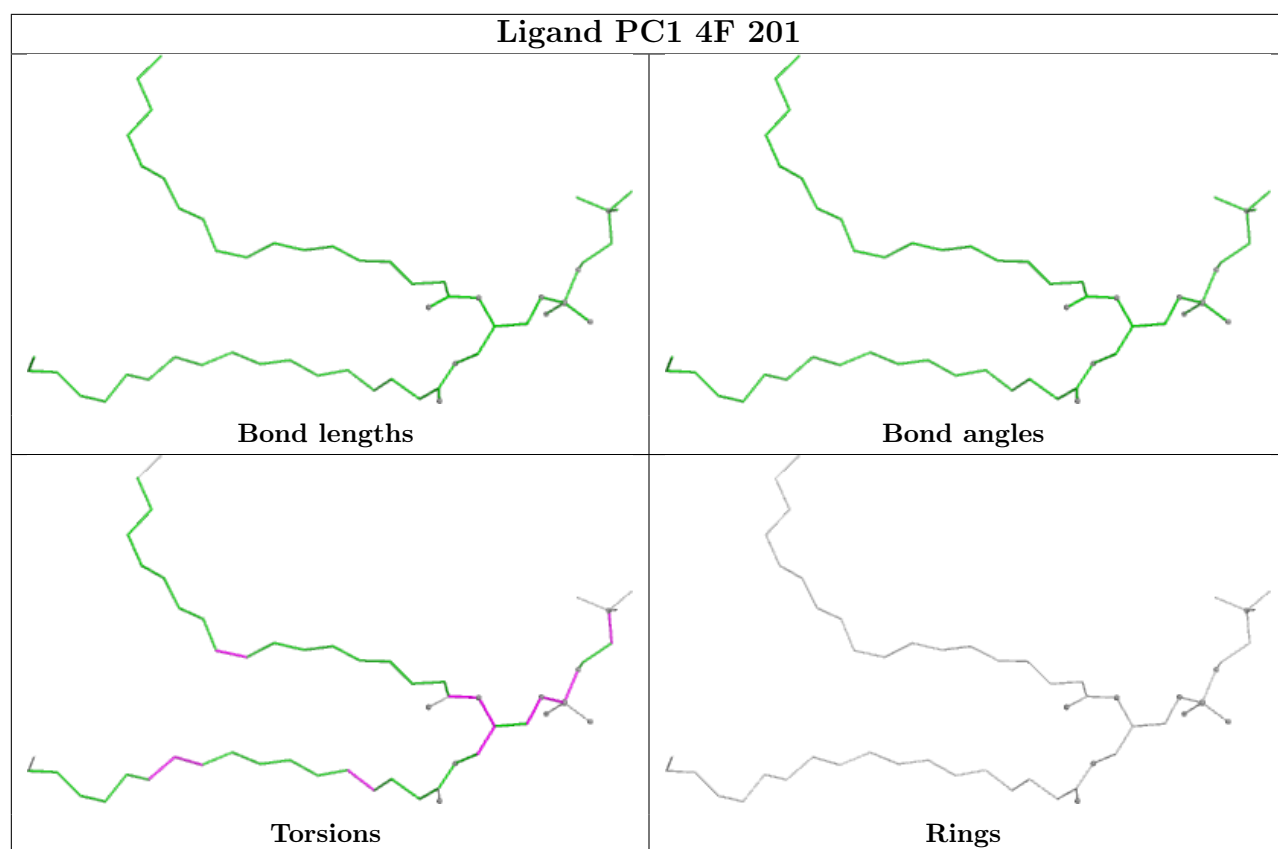


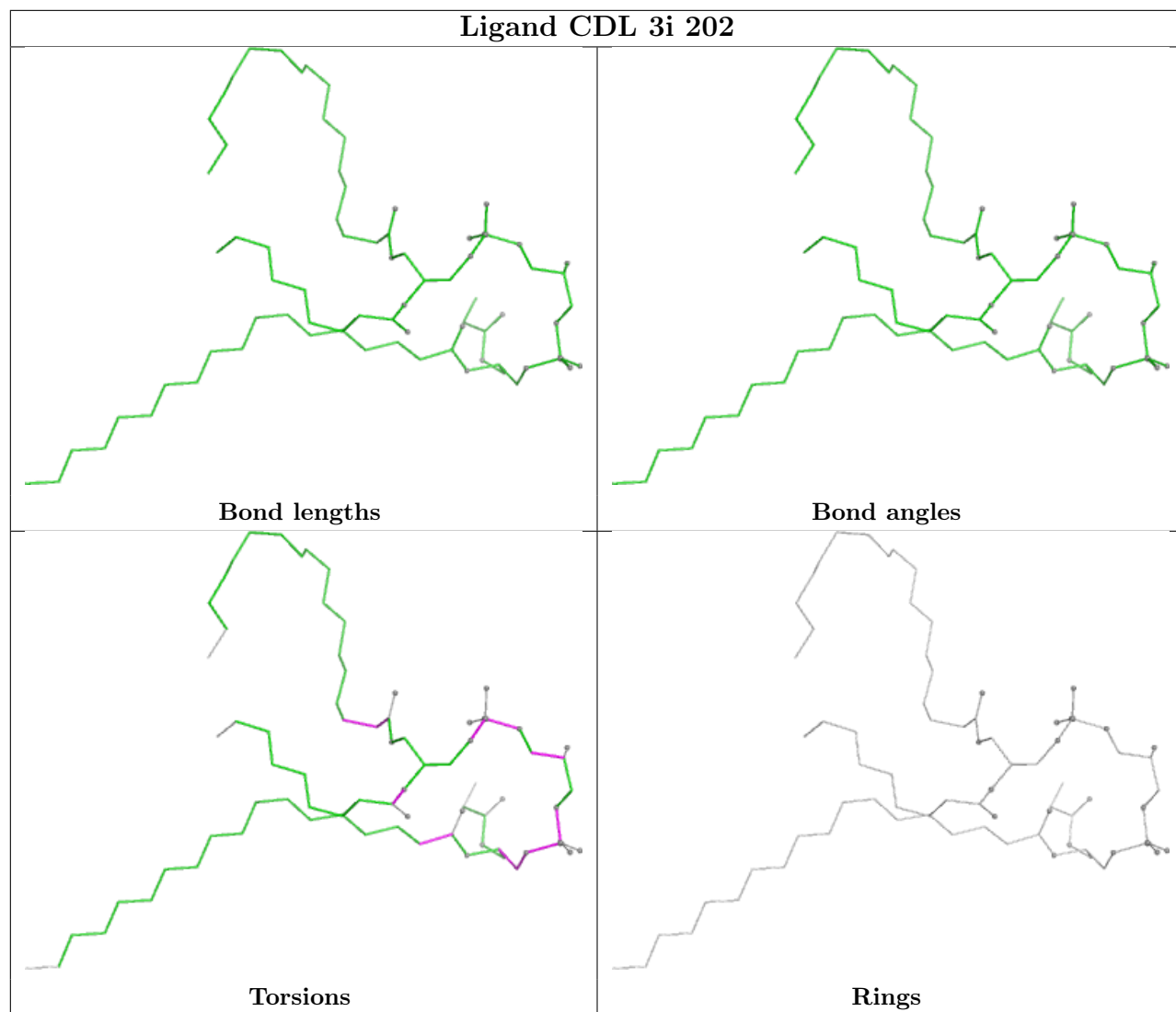


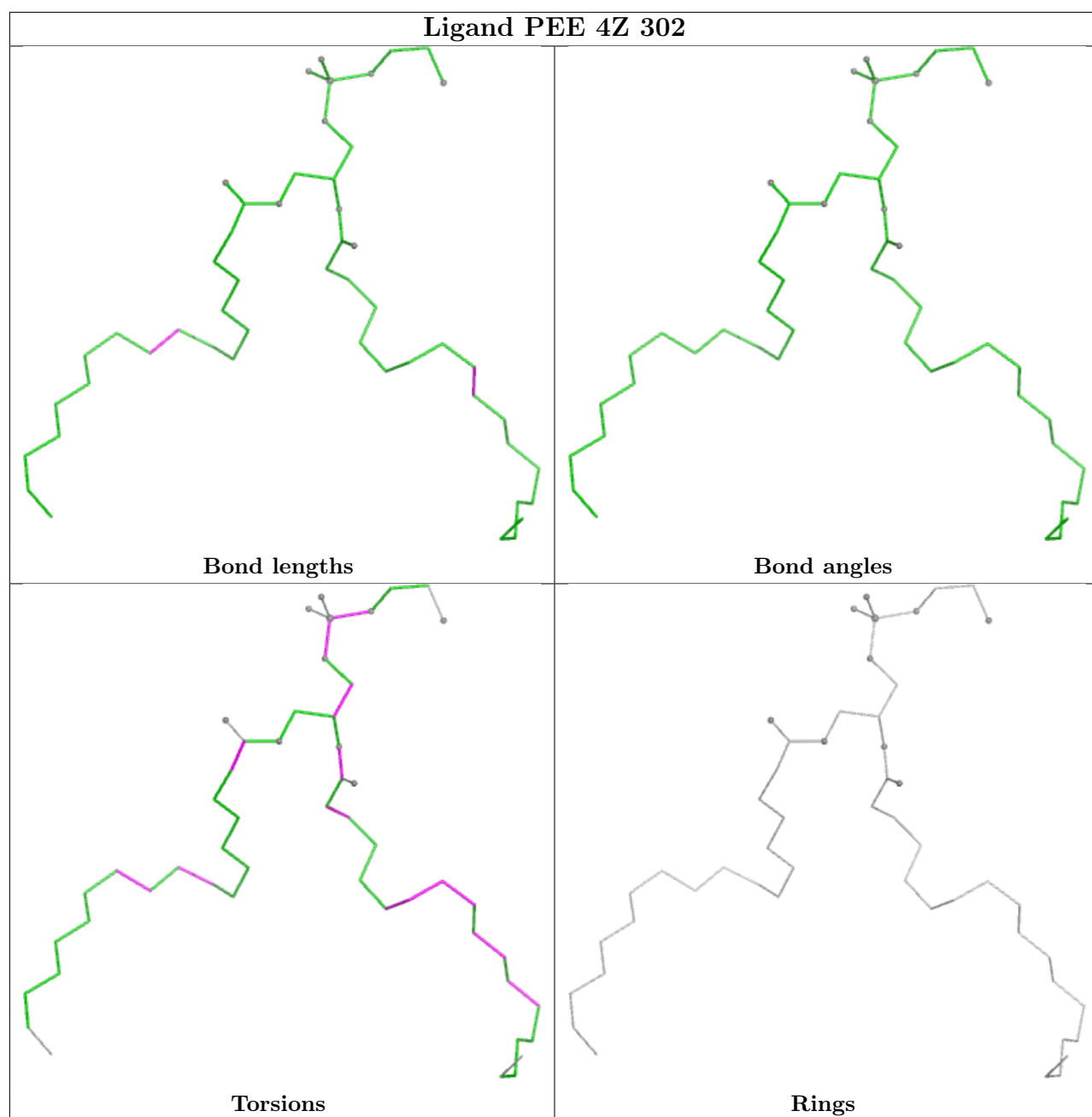


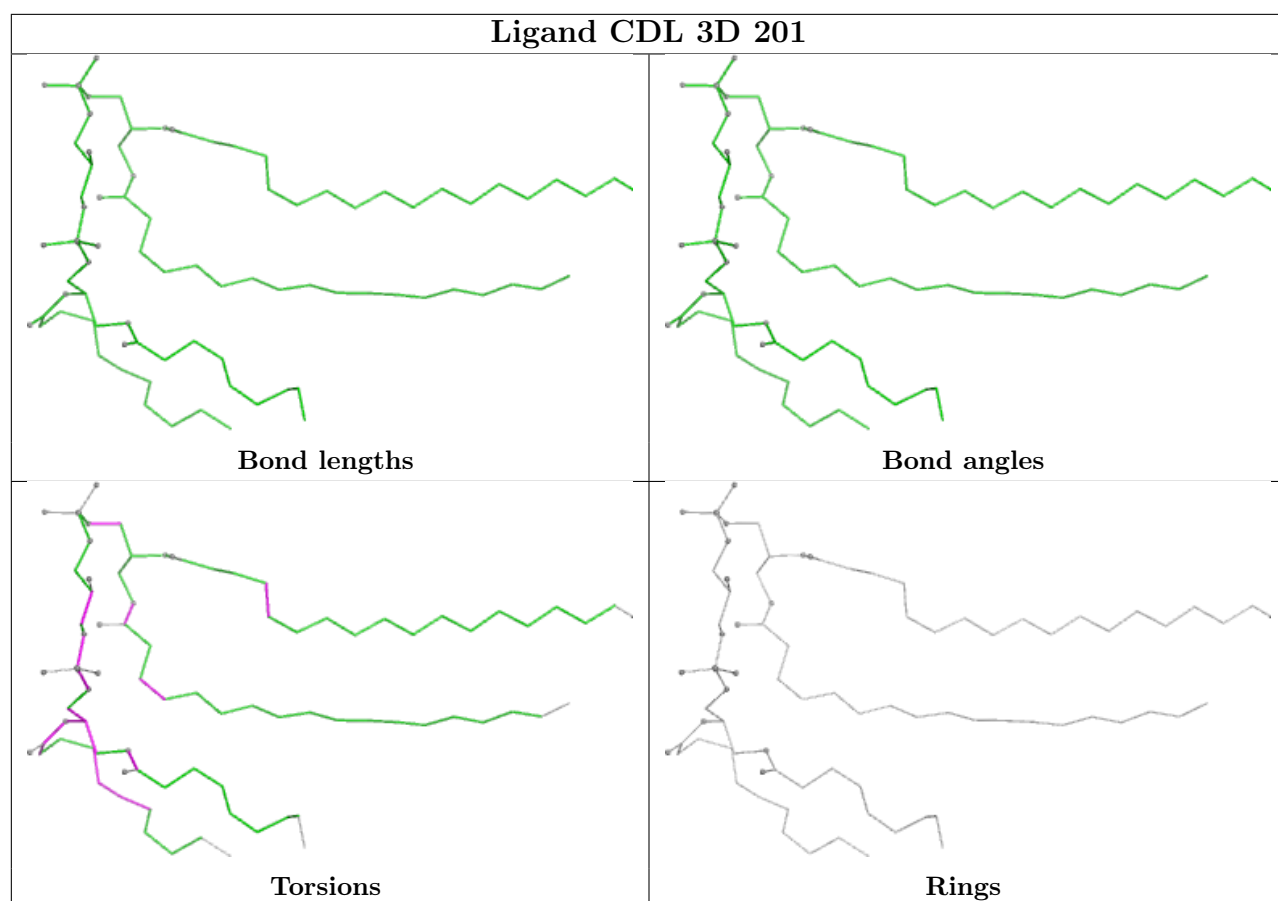


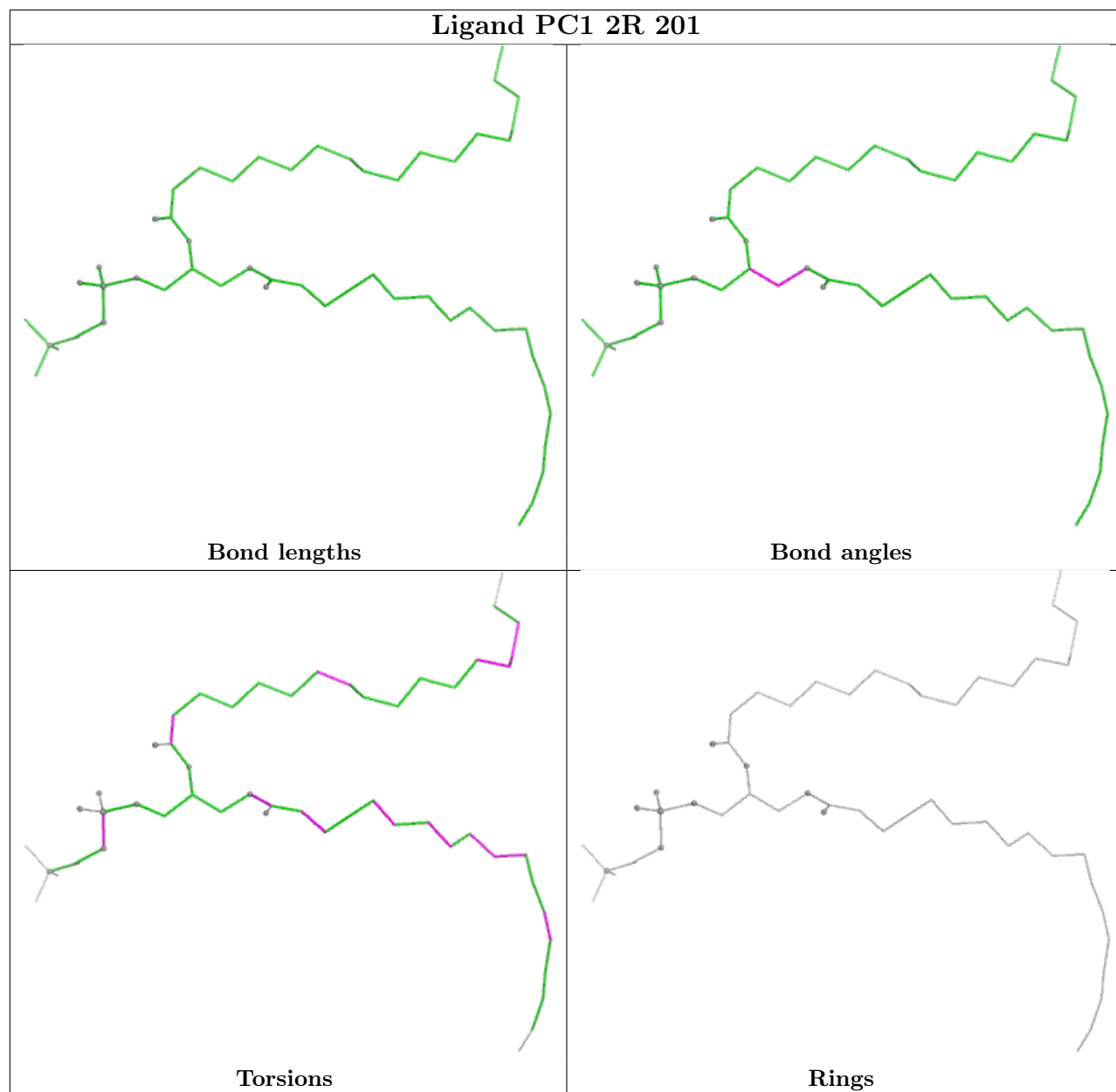


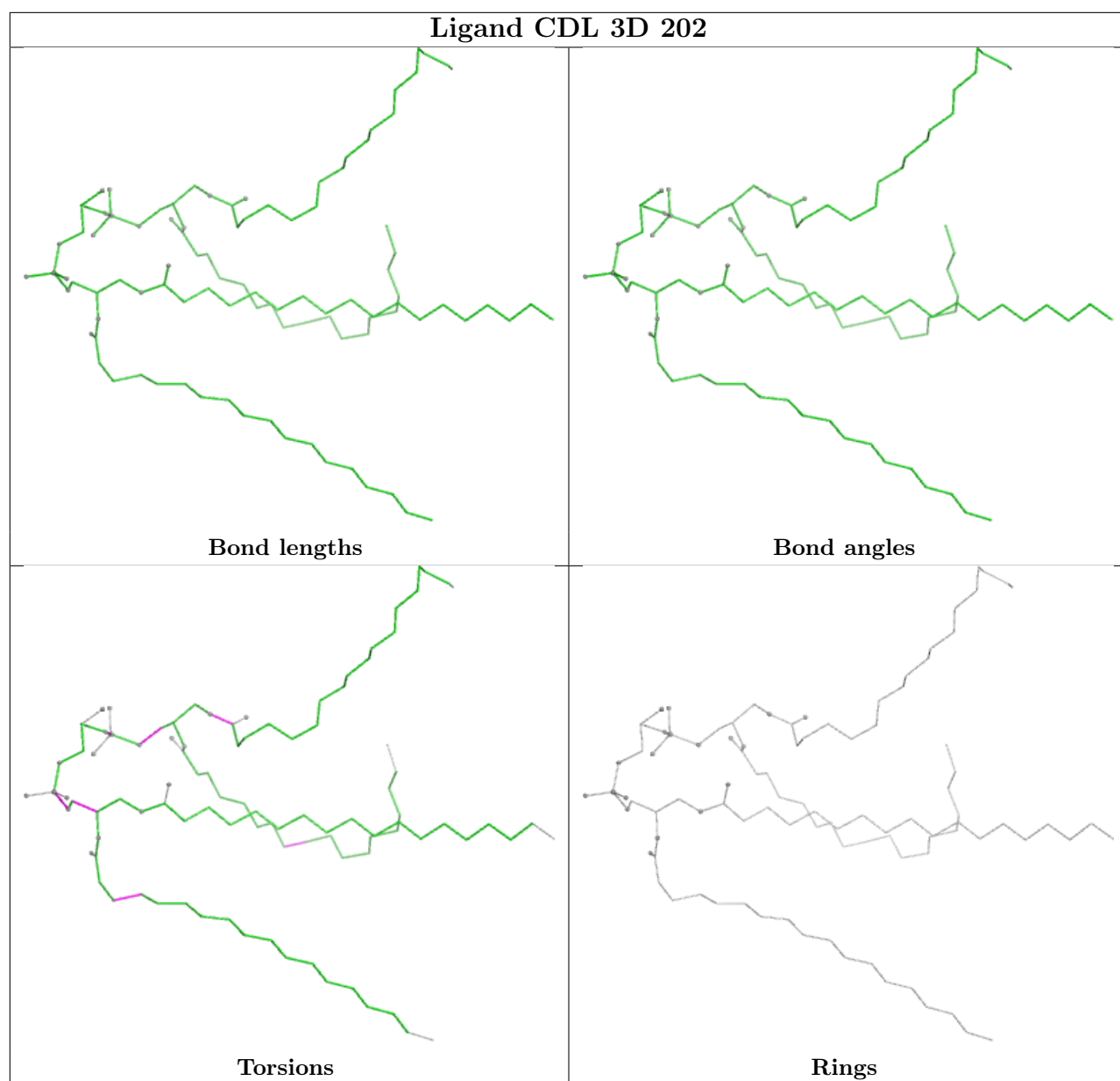




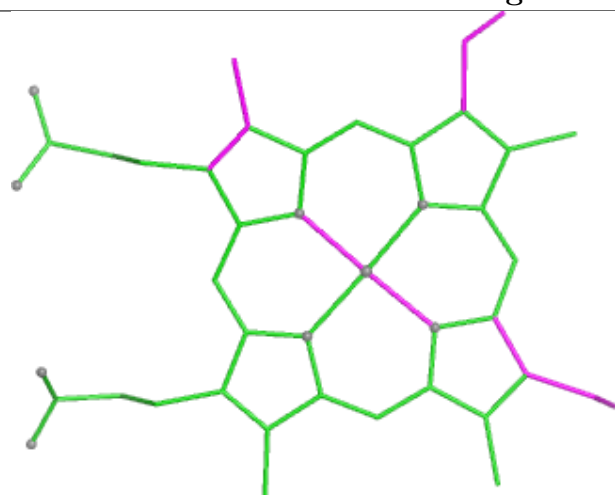




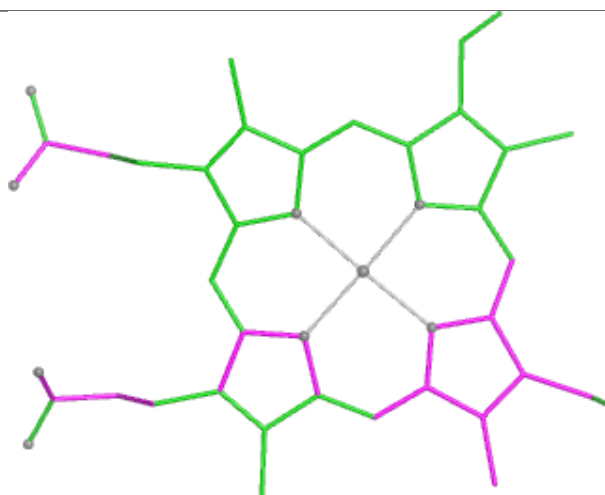




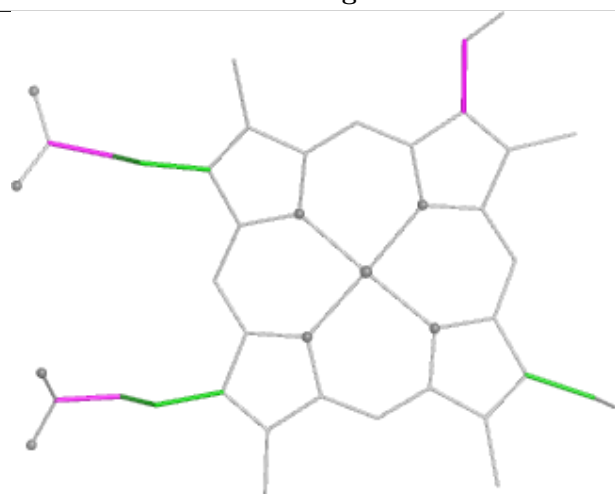
Ligand HEC 3C 302



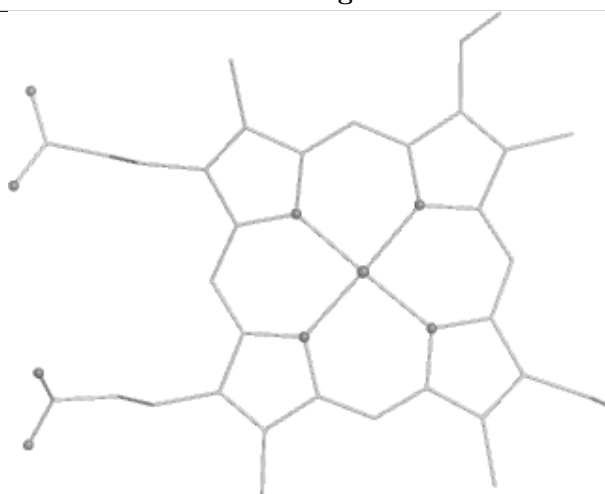
Bond lengths



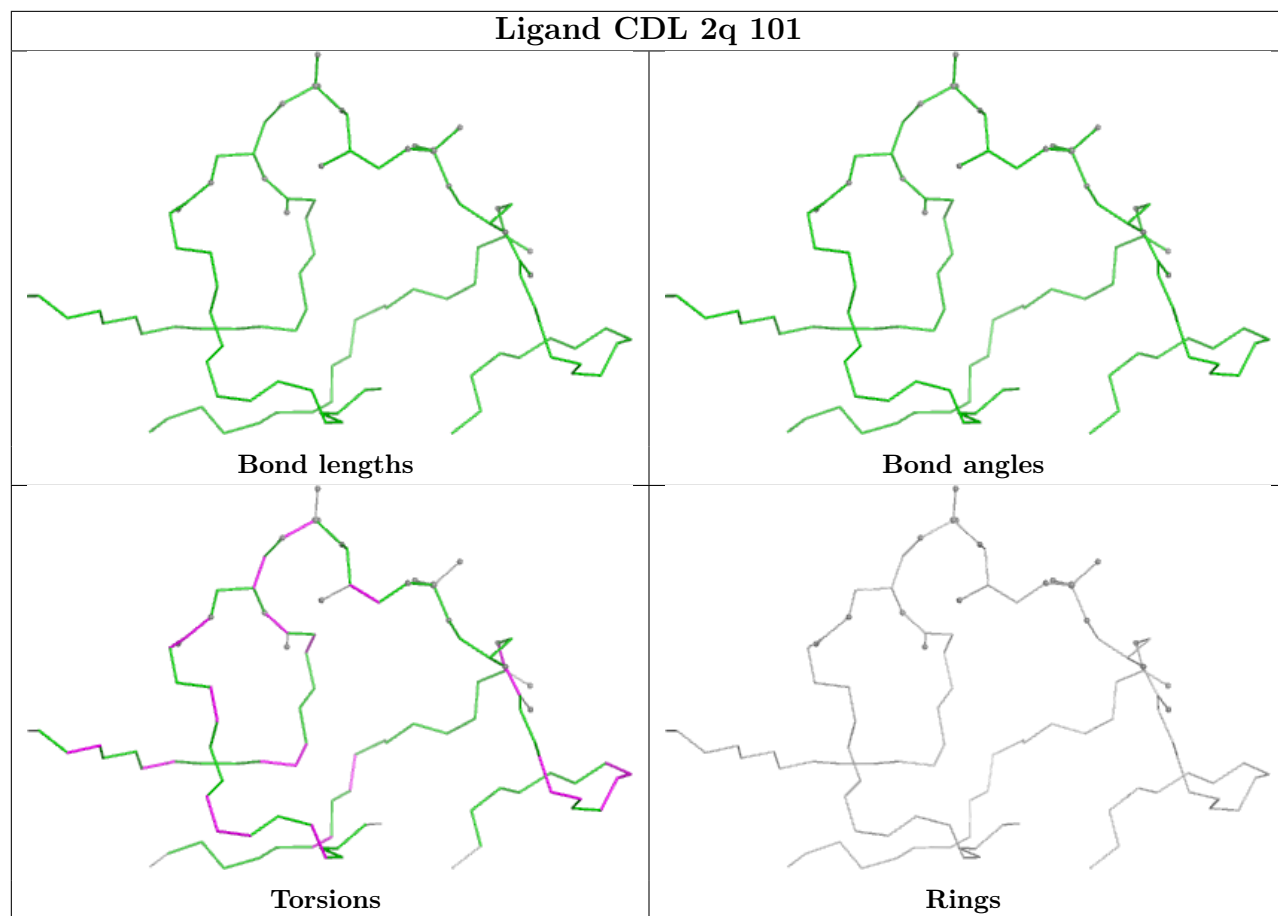
Bond angles

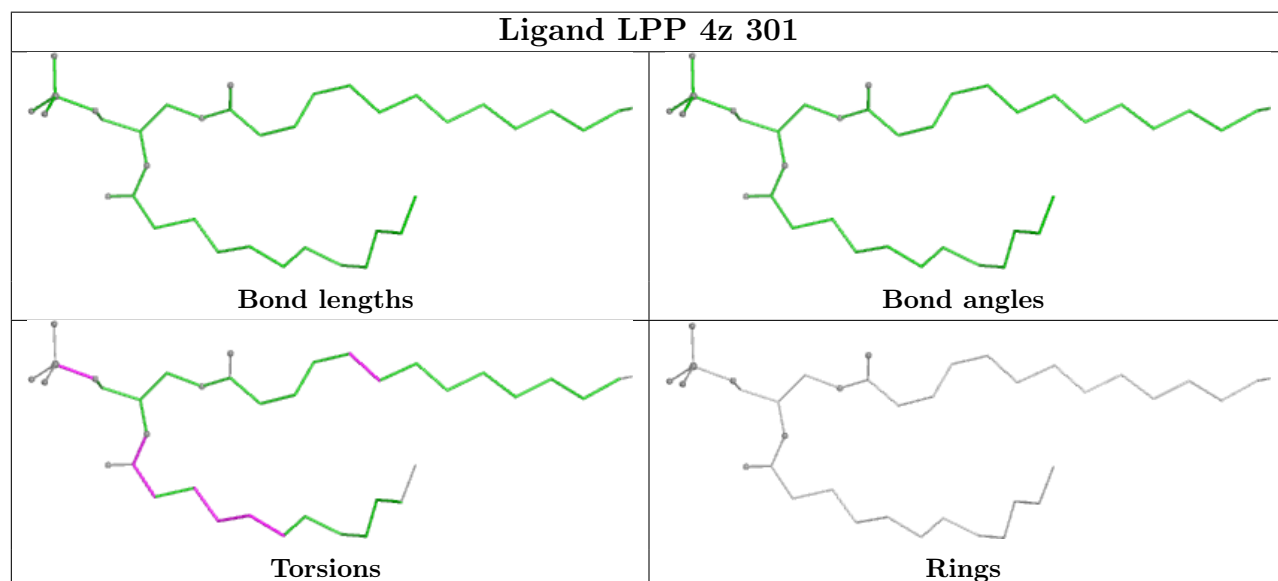
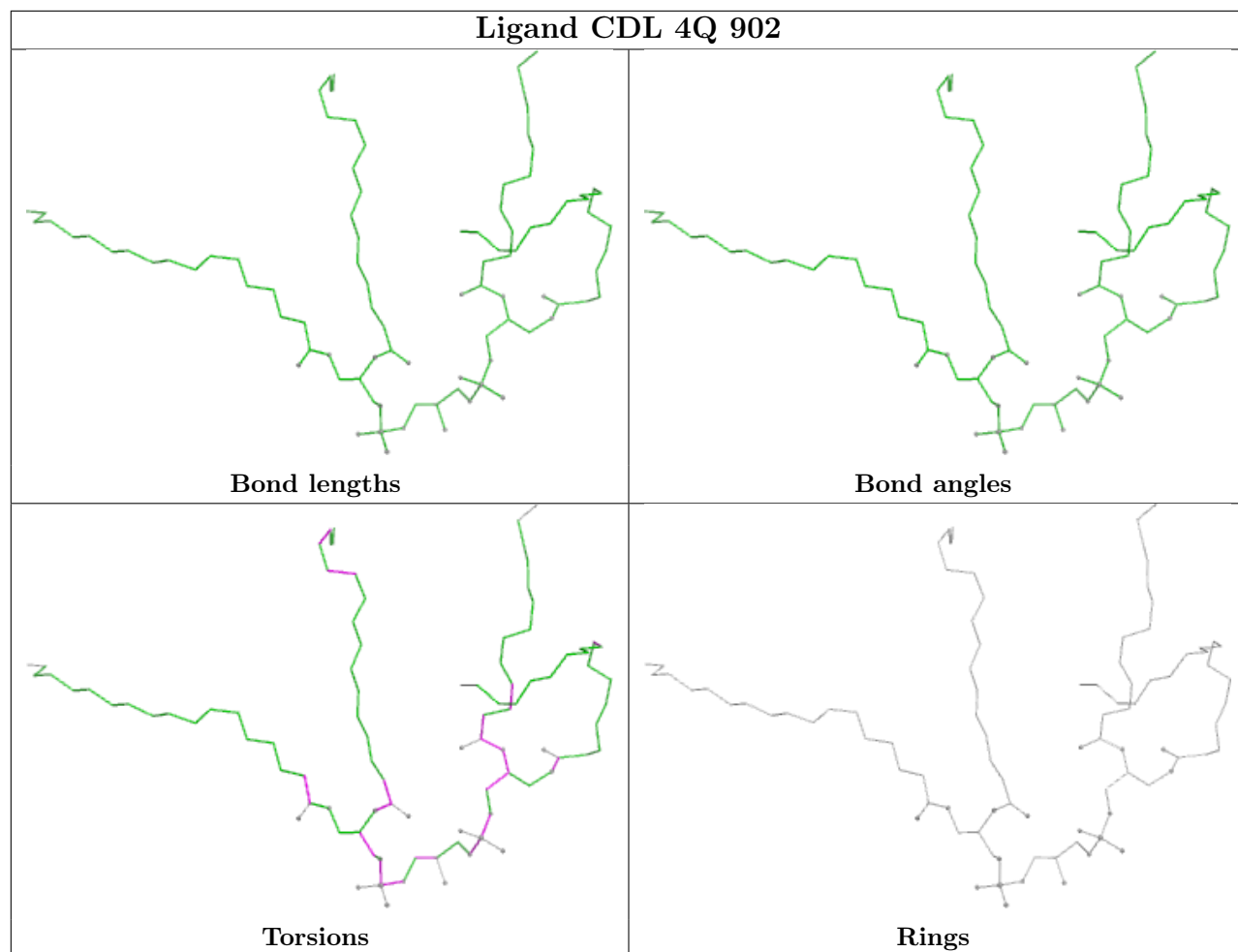


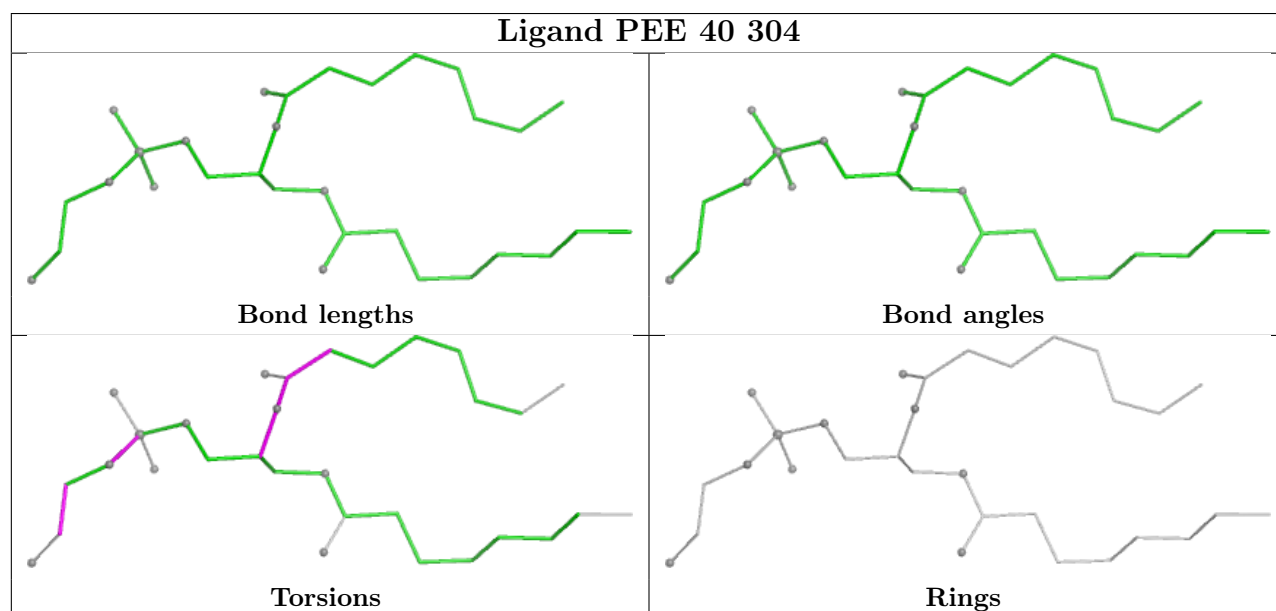
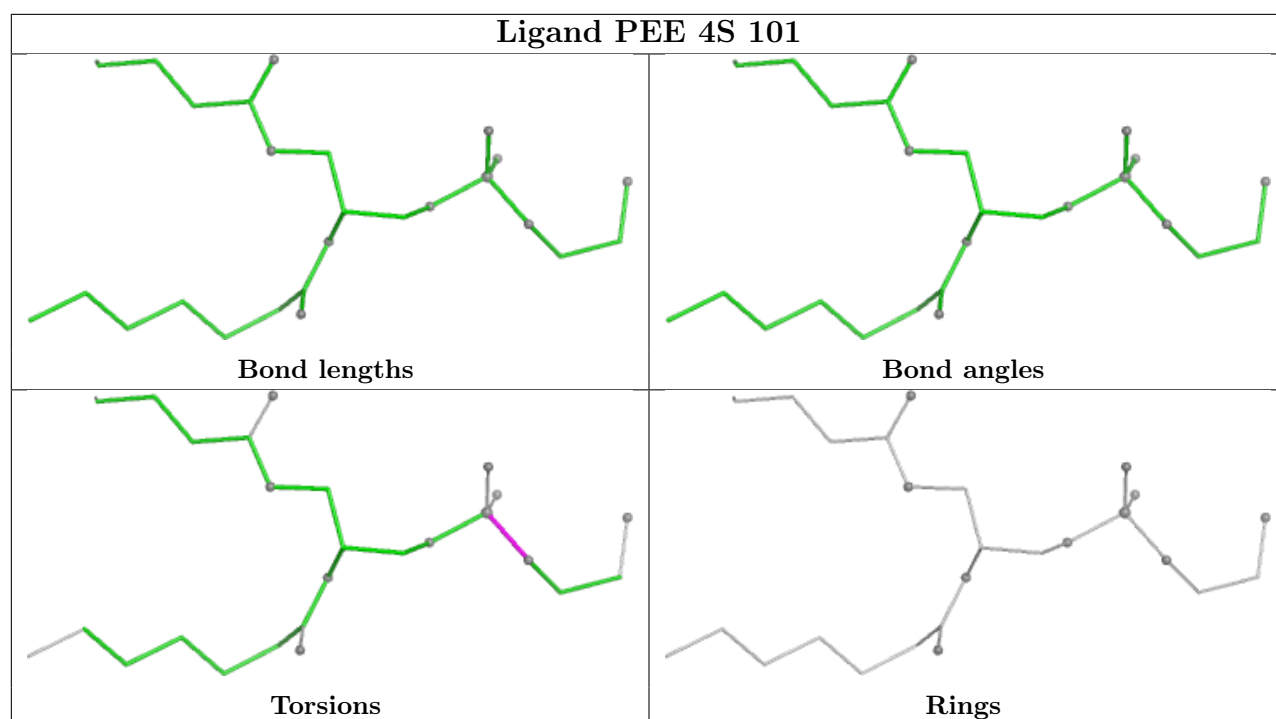
Torsions

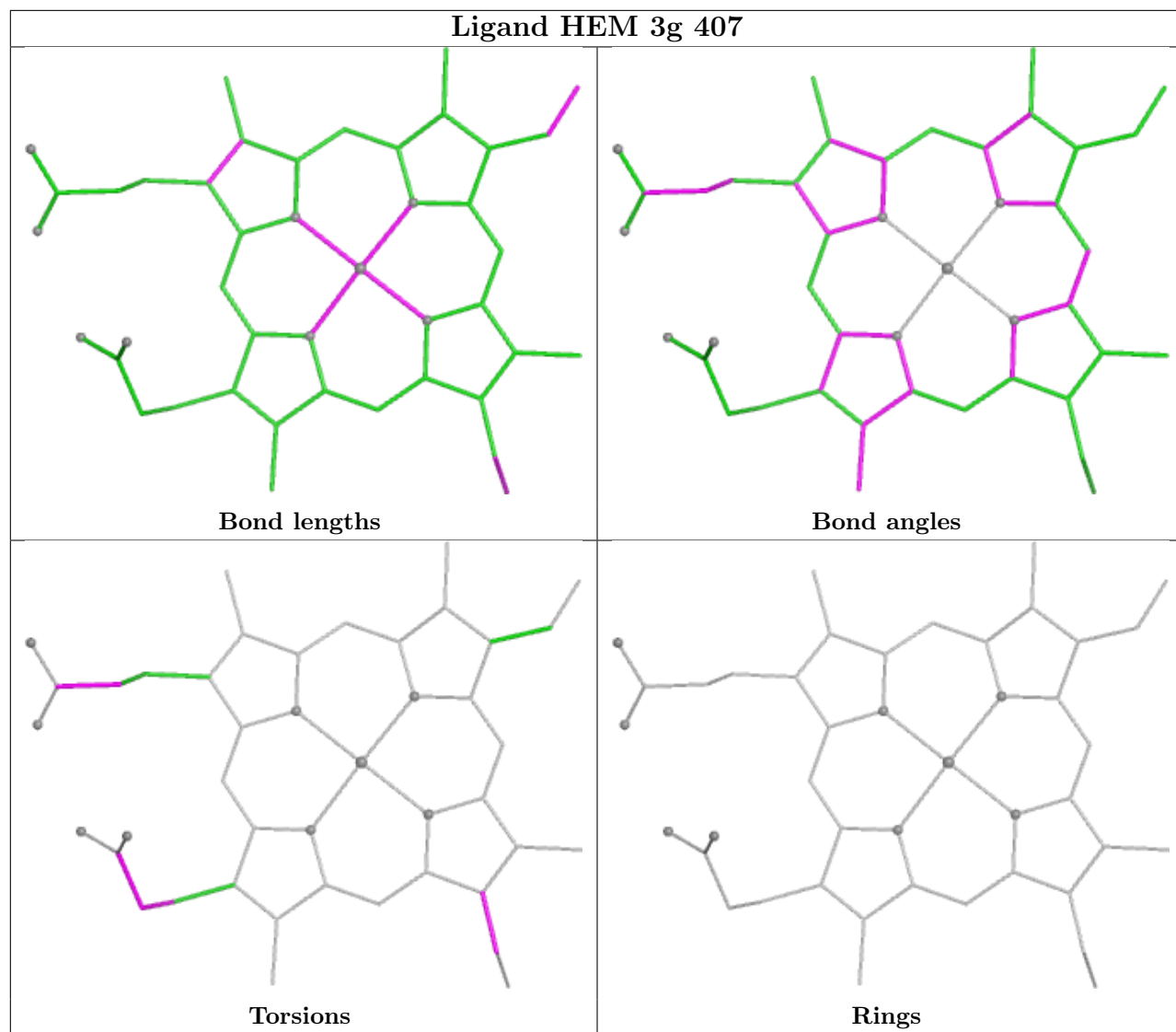


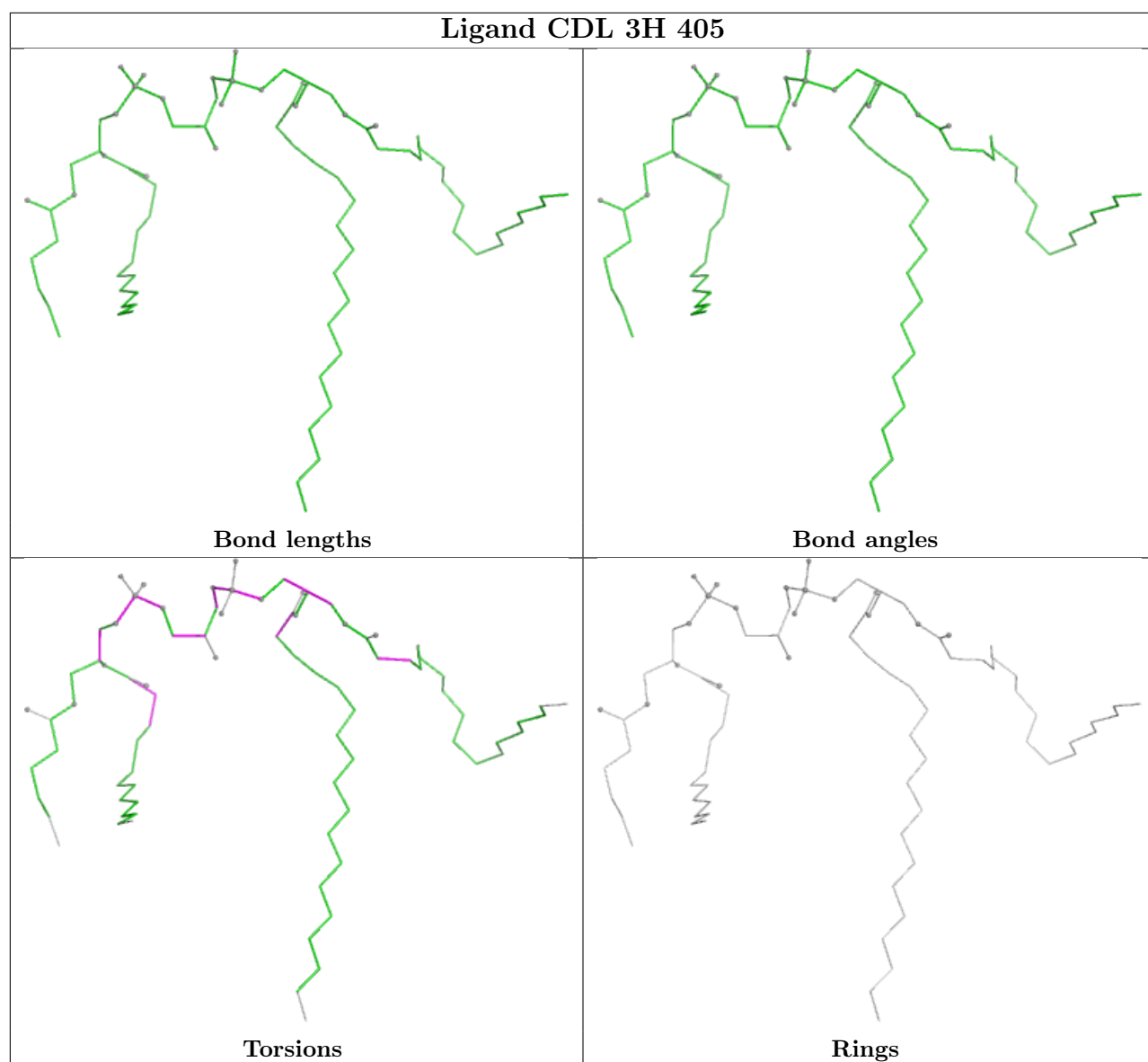
Rings

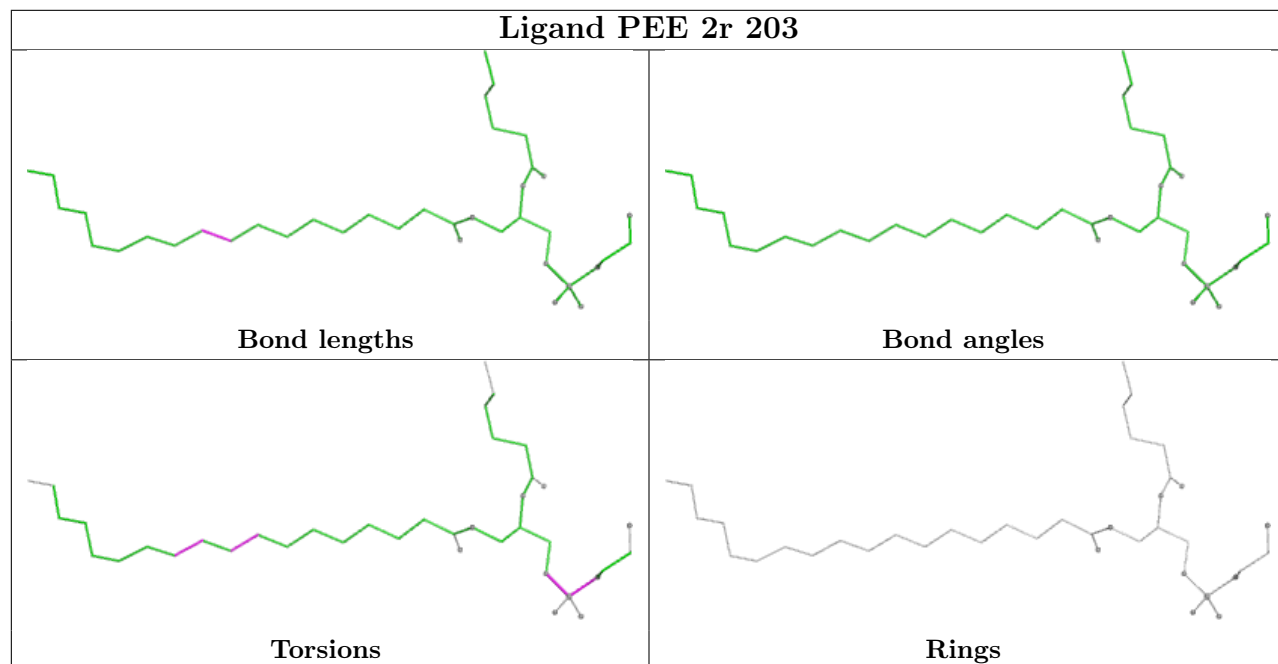
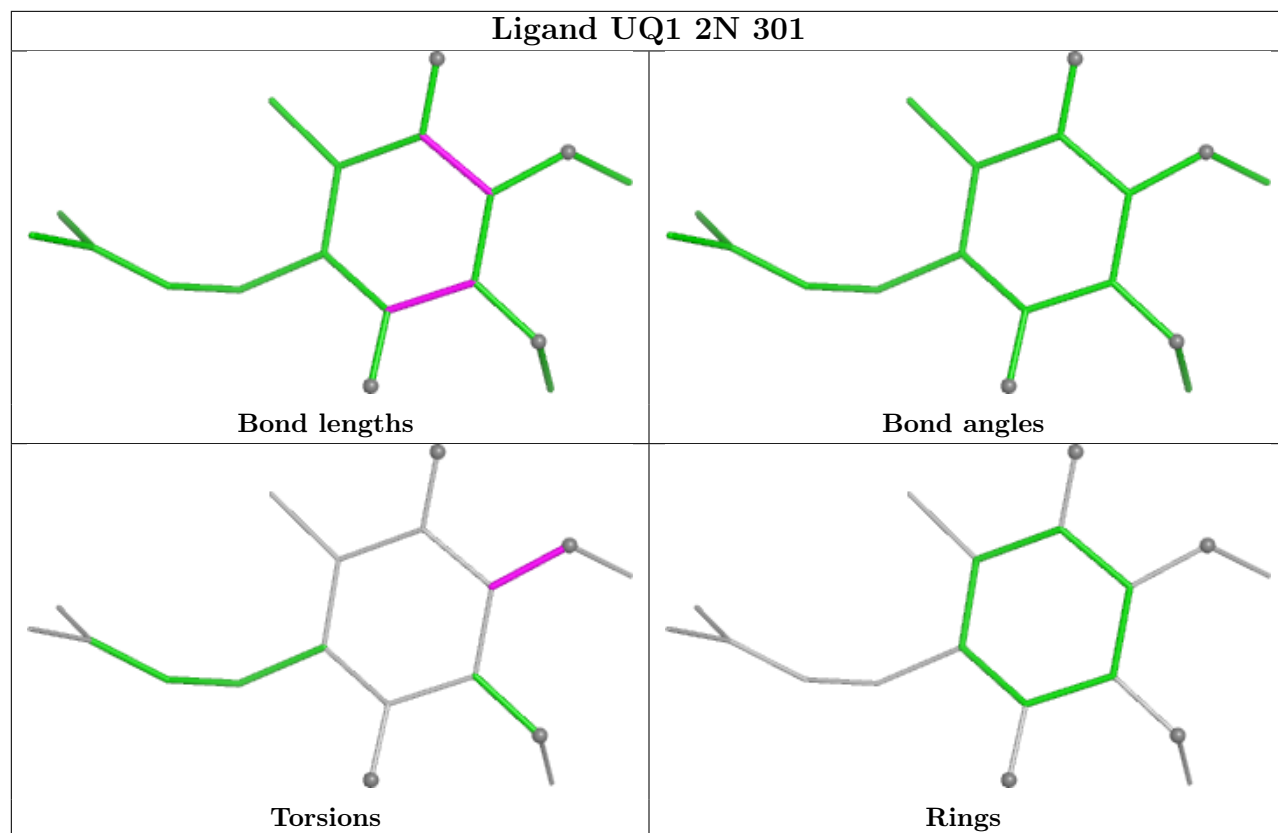


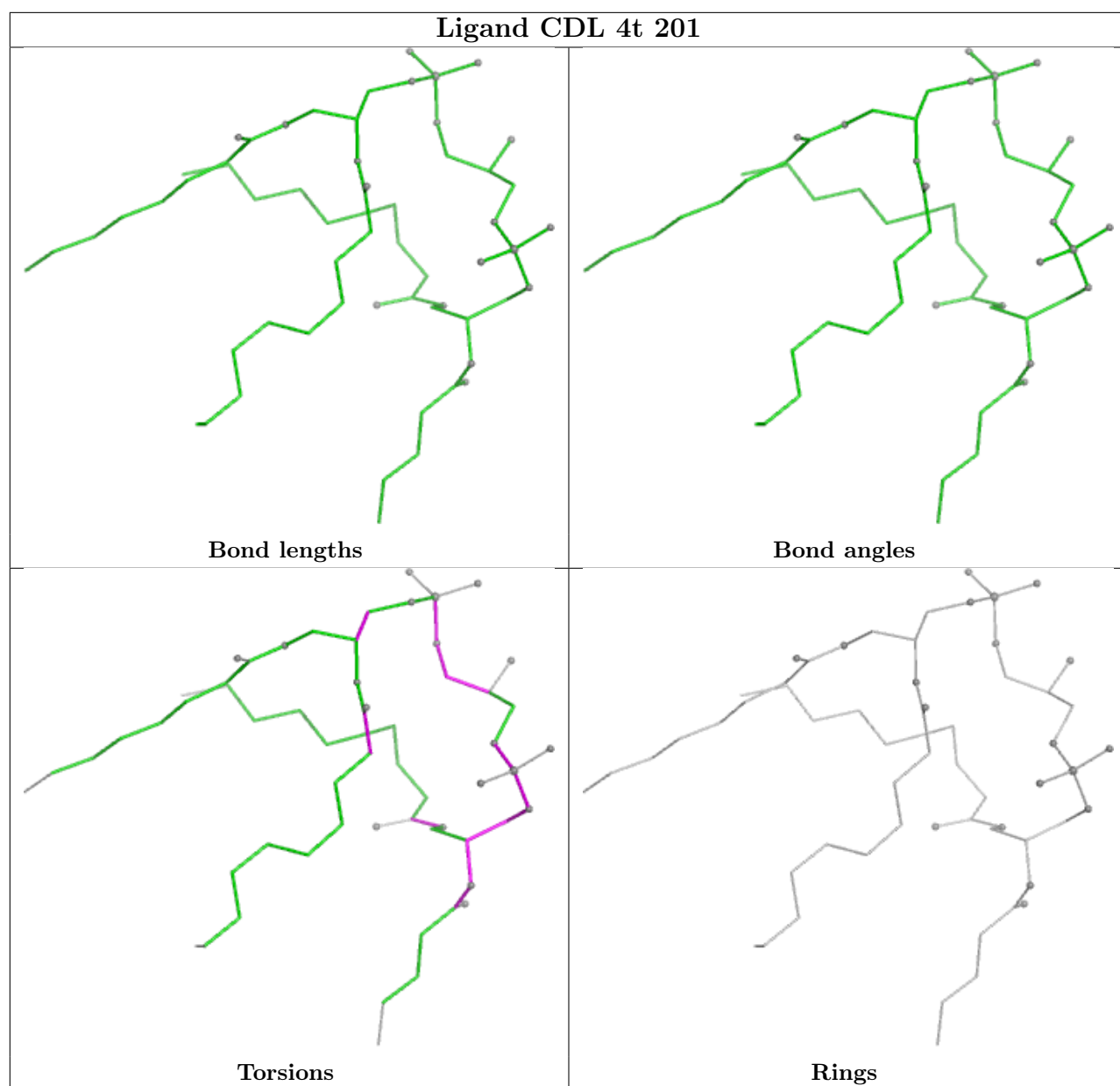


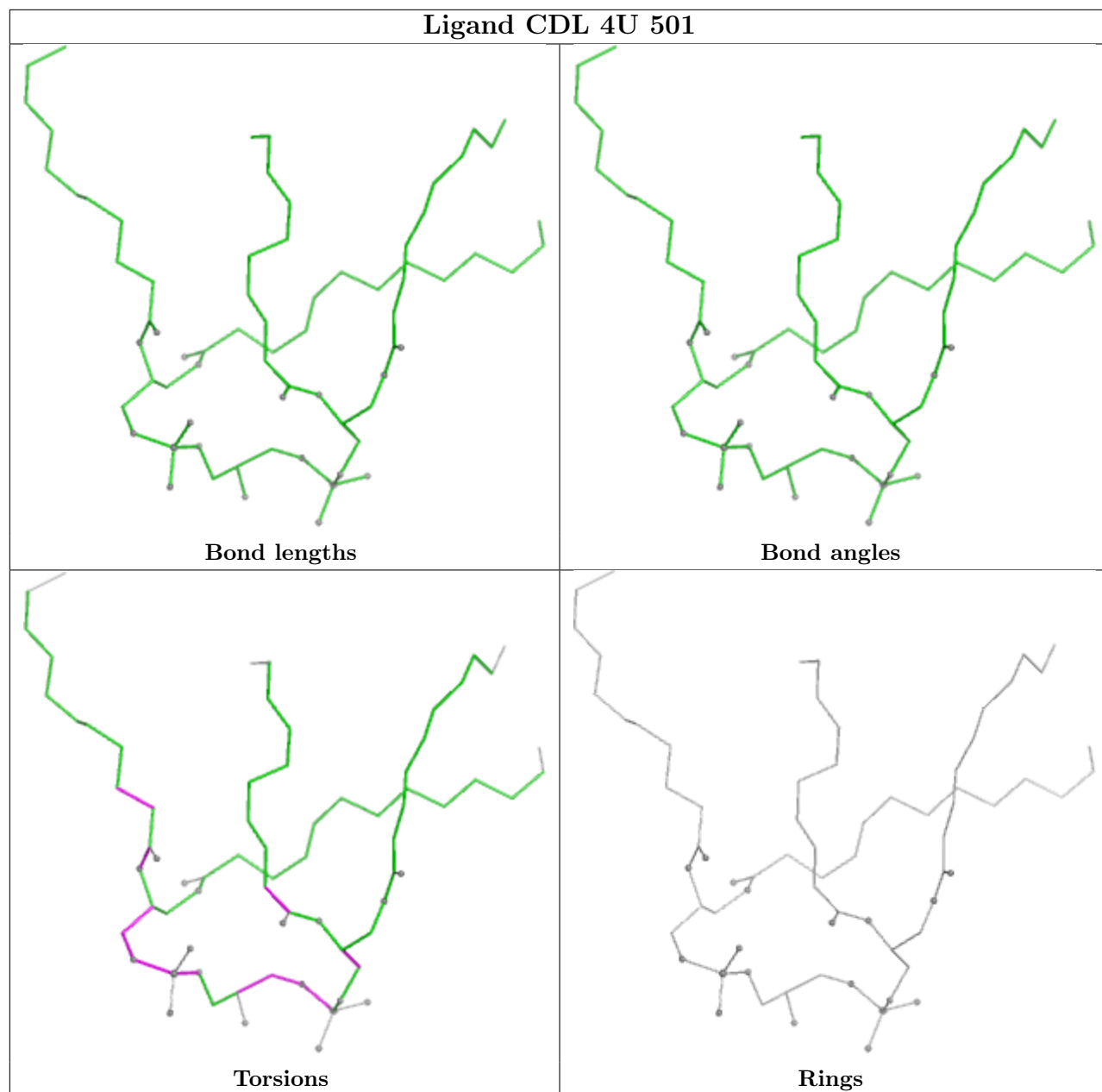


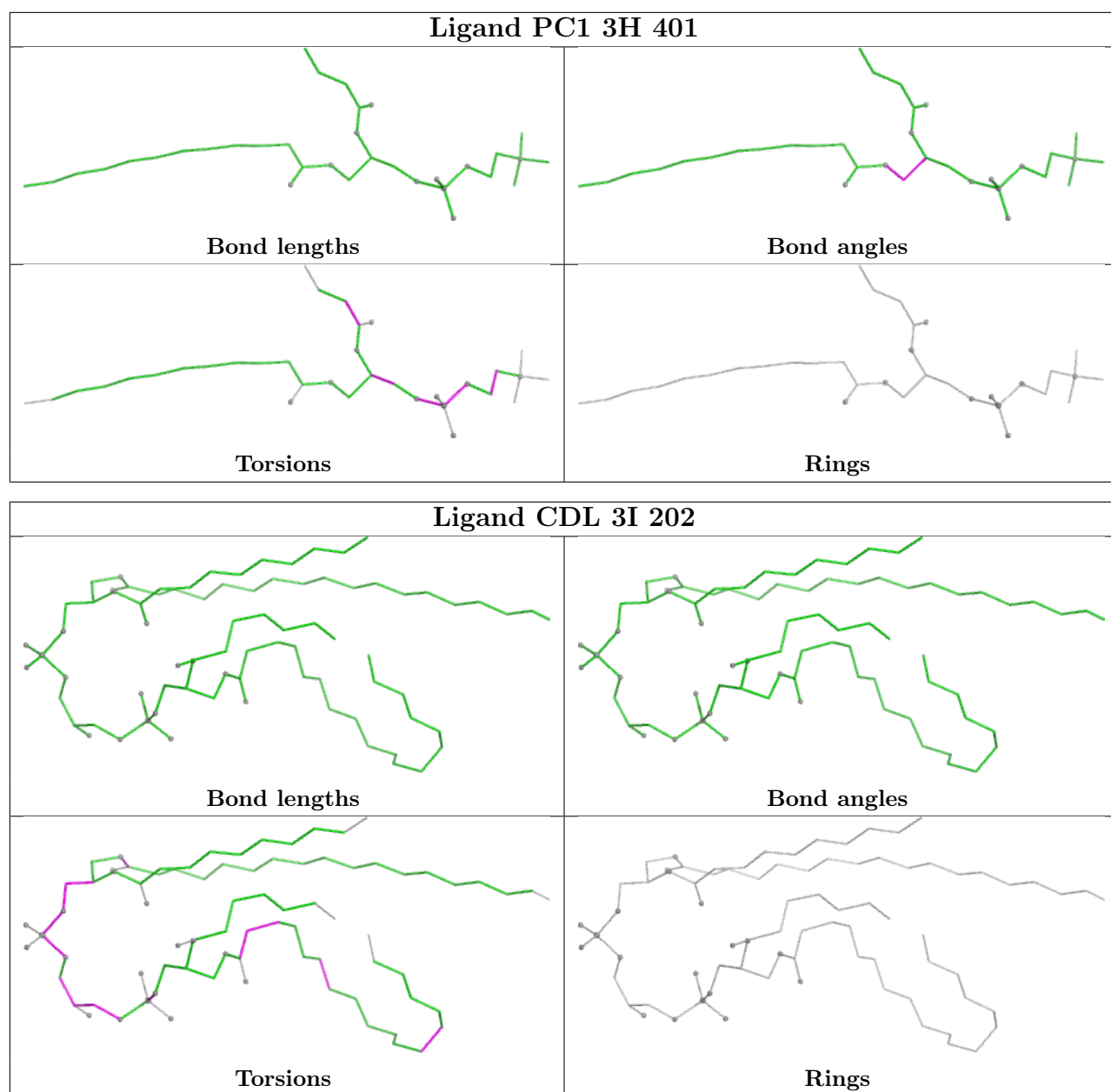


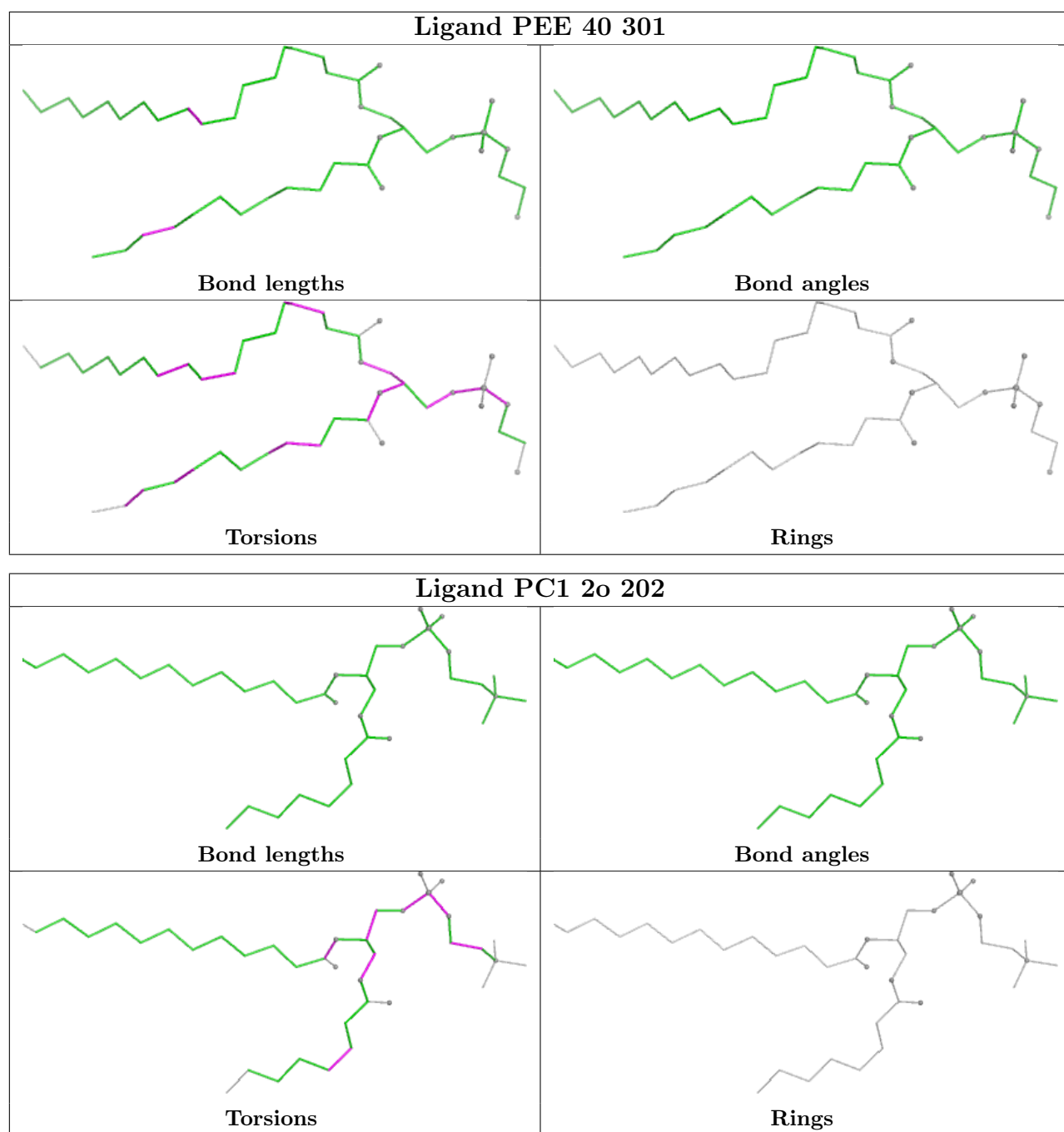


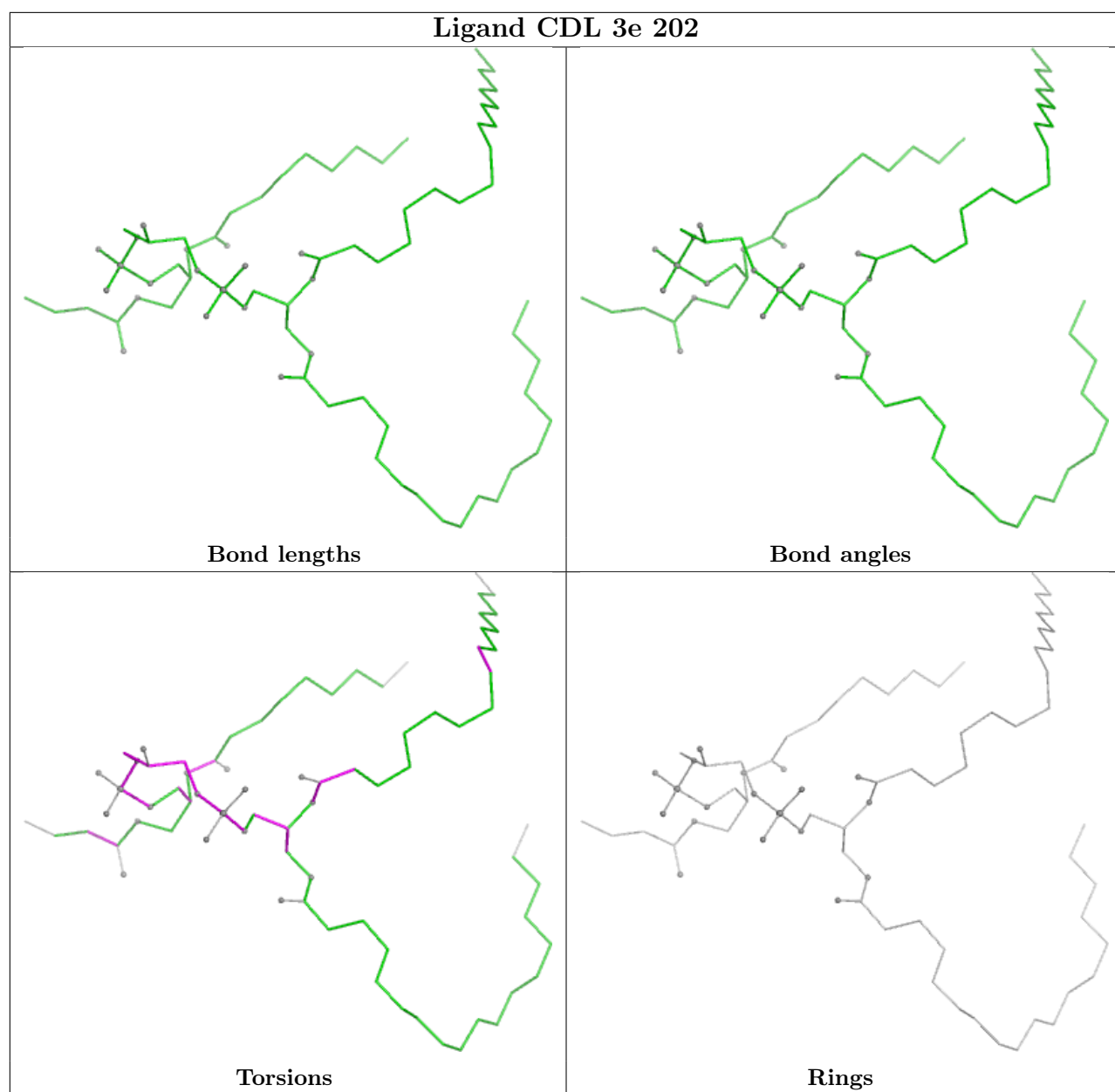


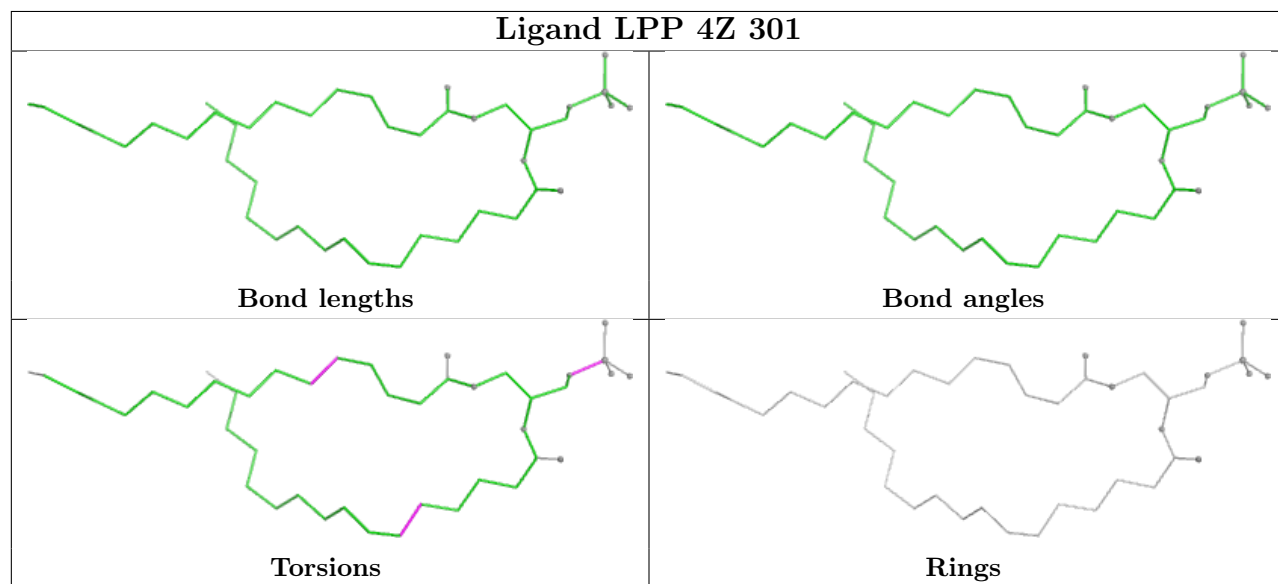
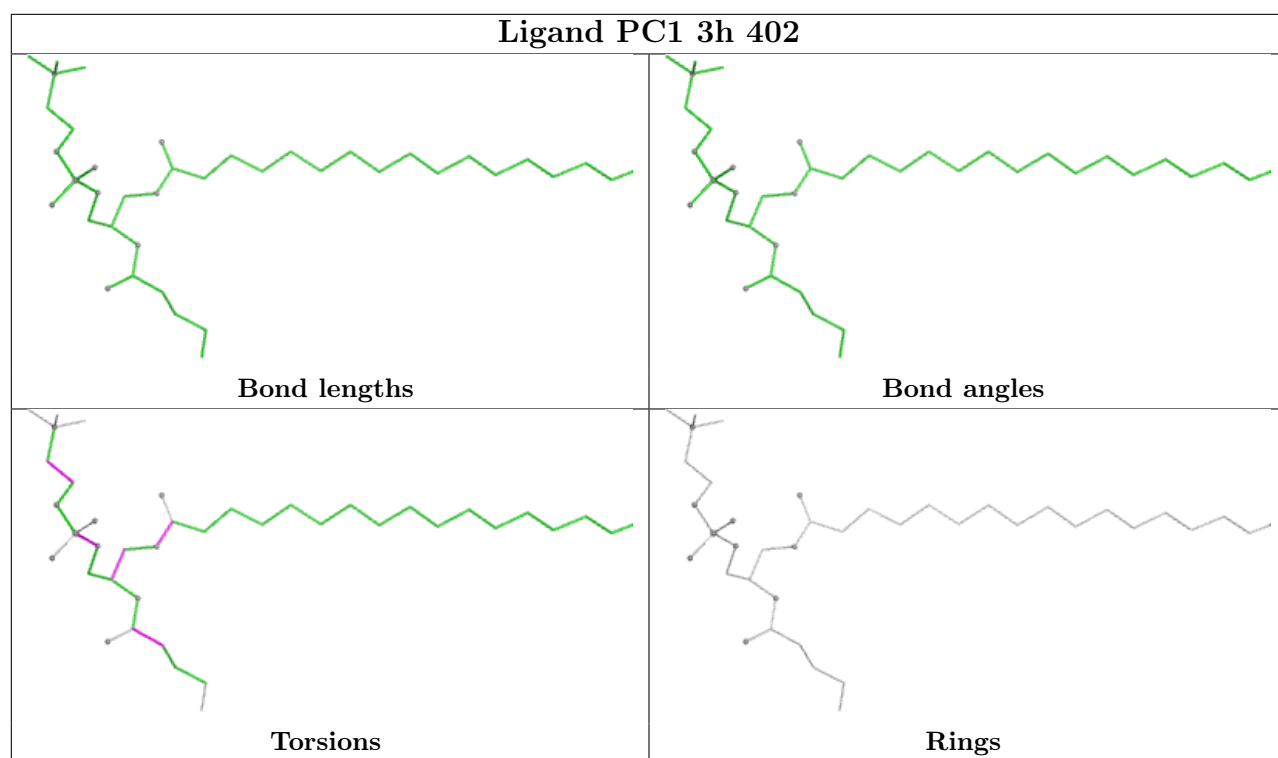


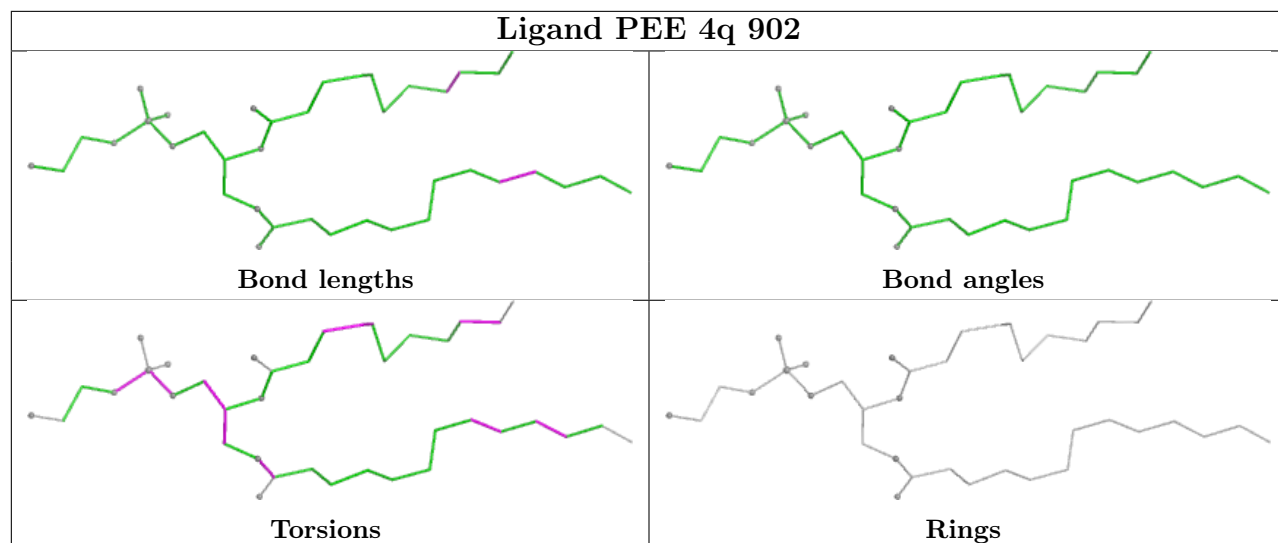


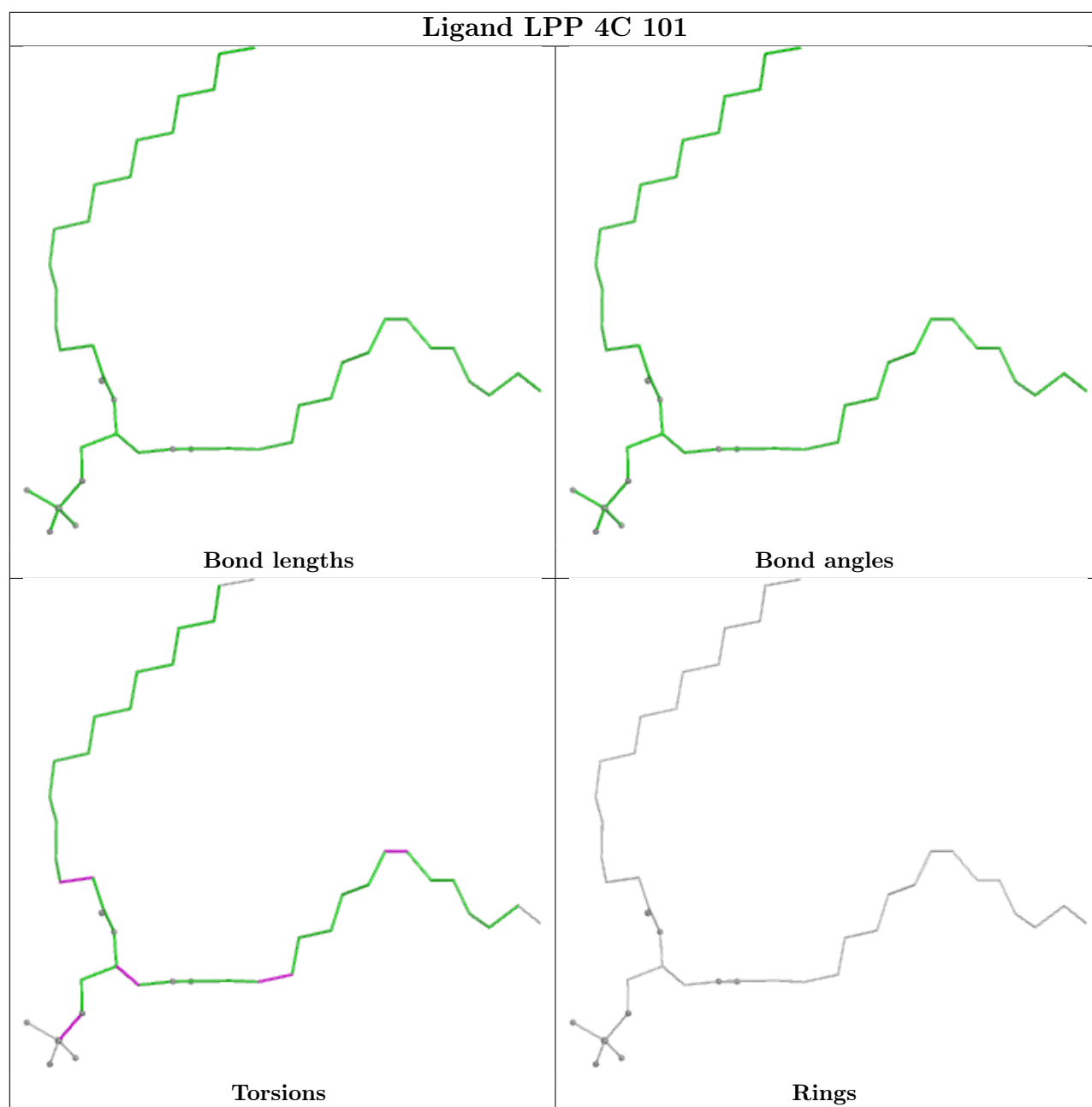


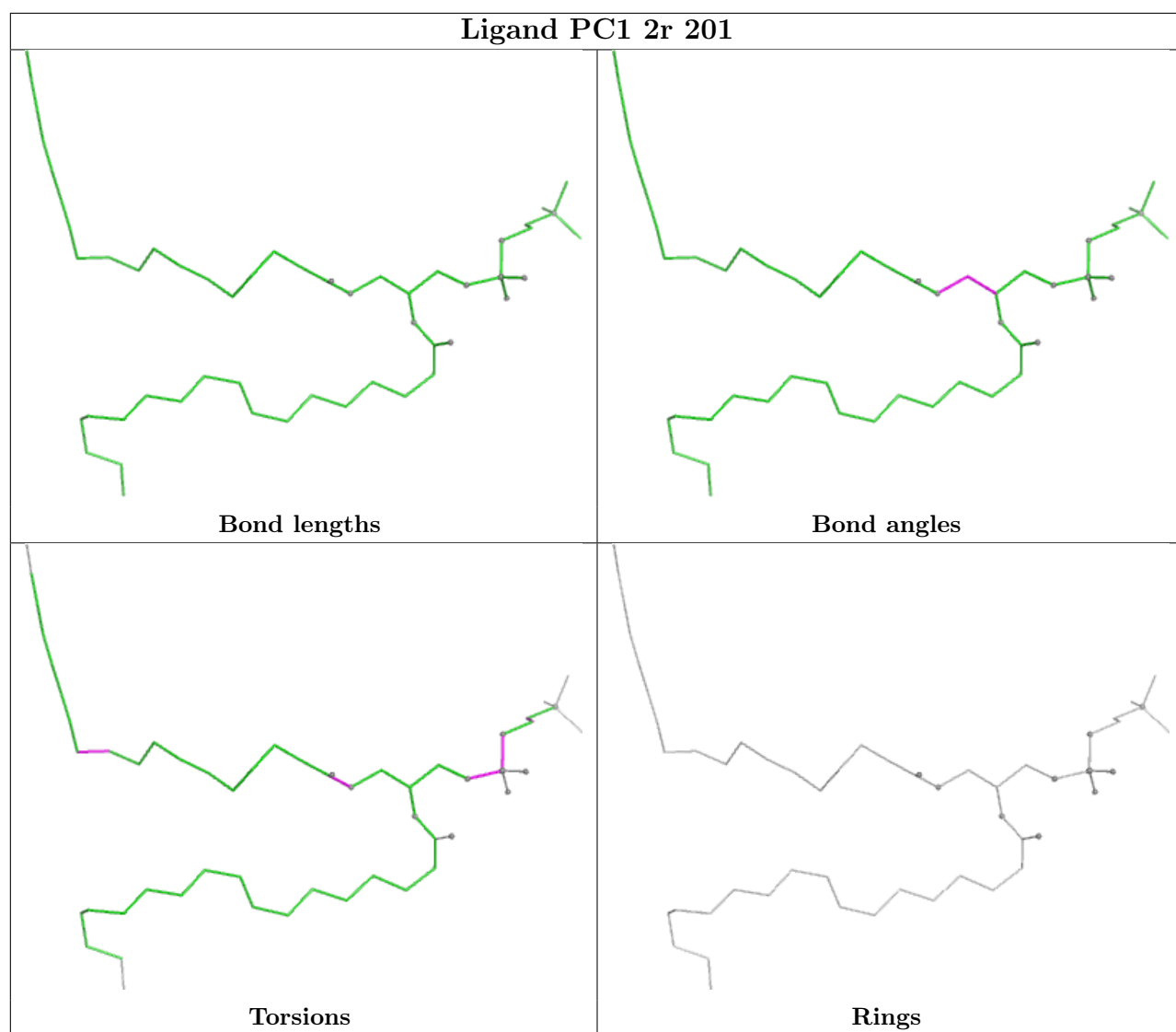


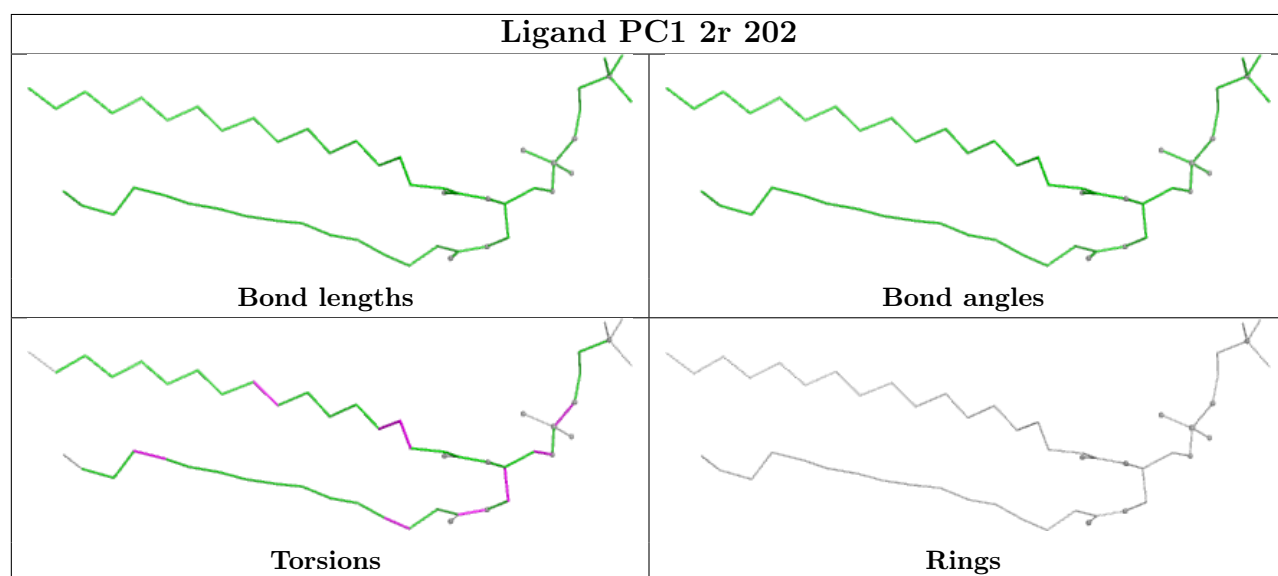
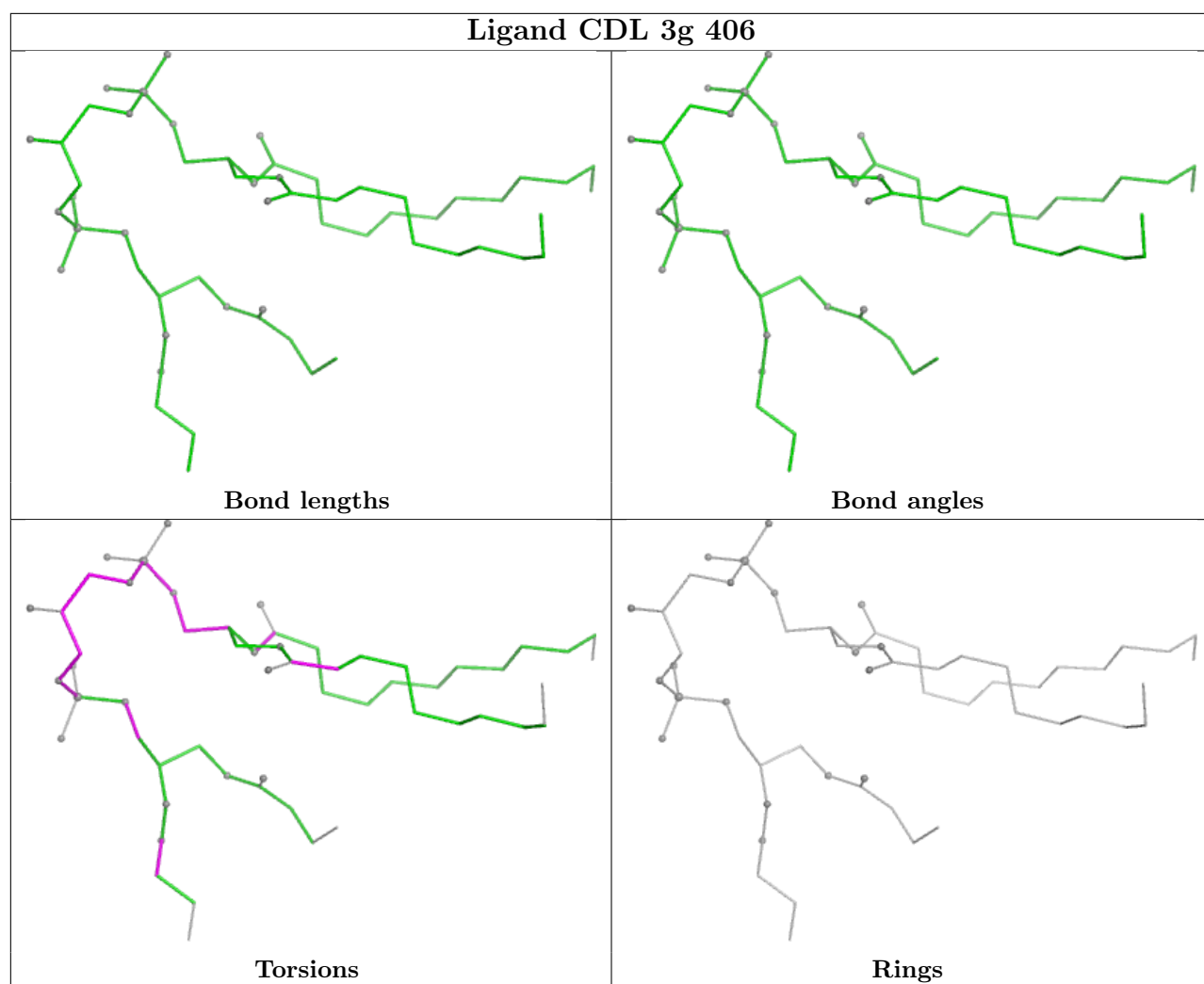


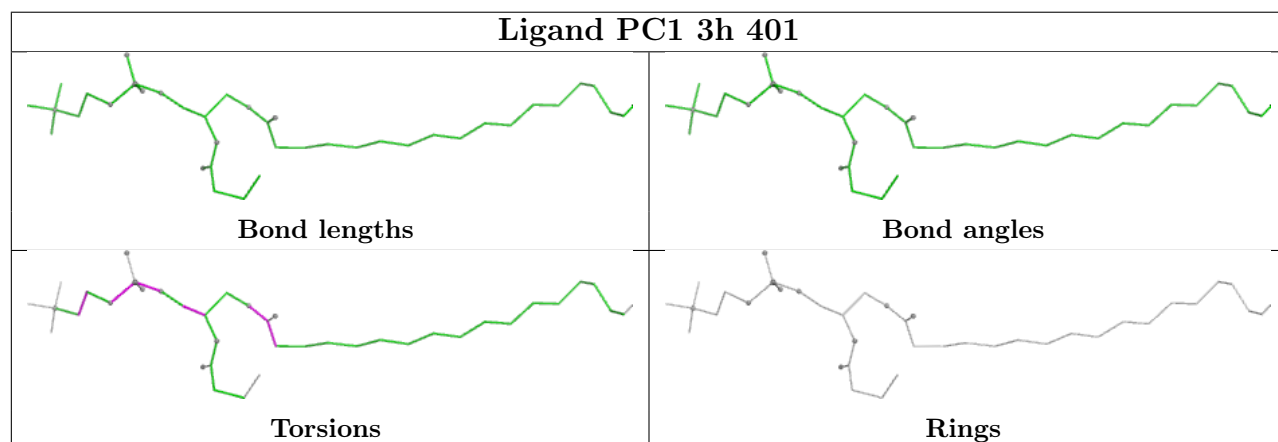
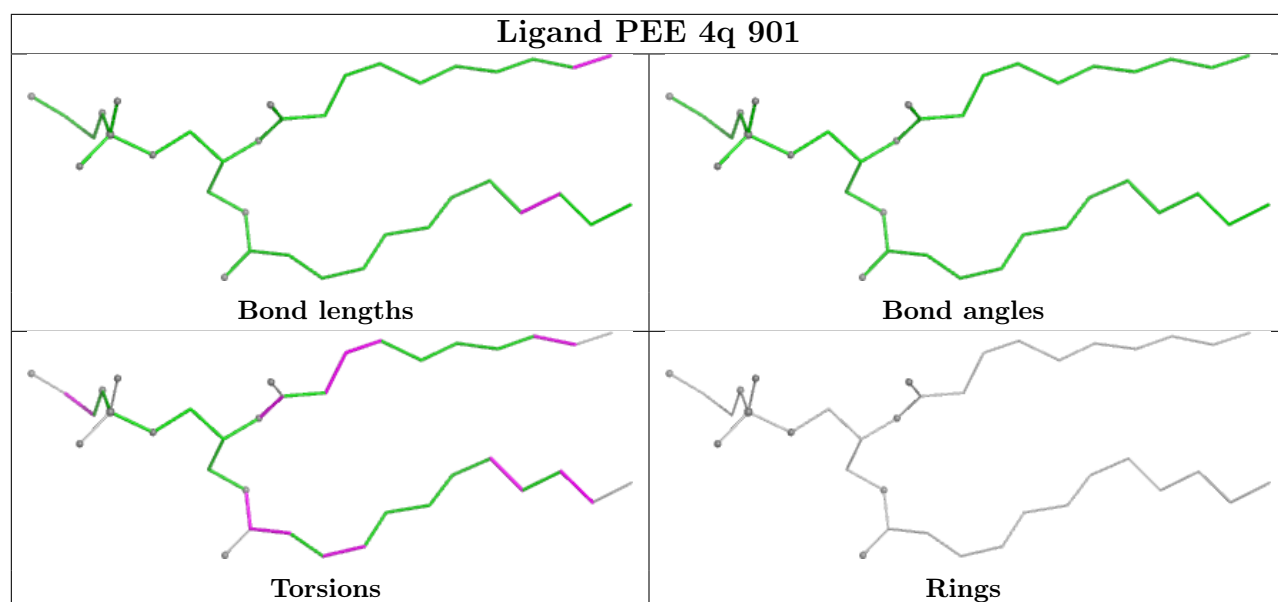


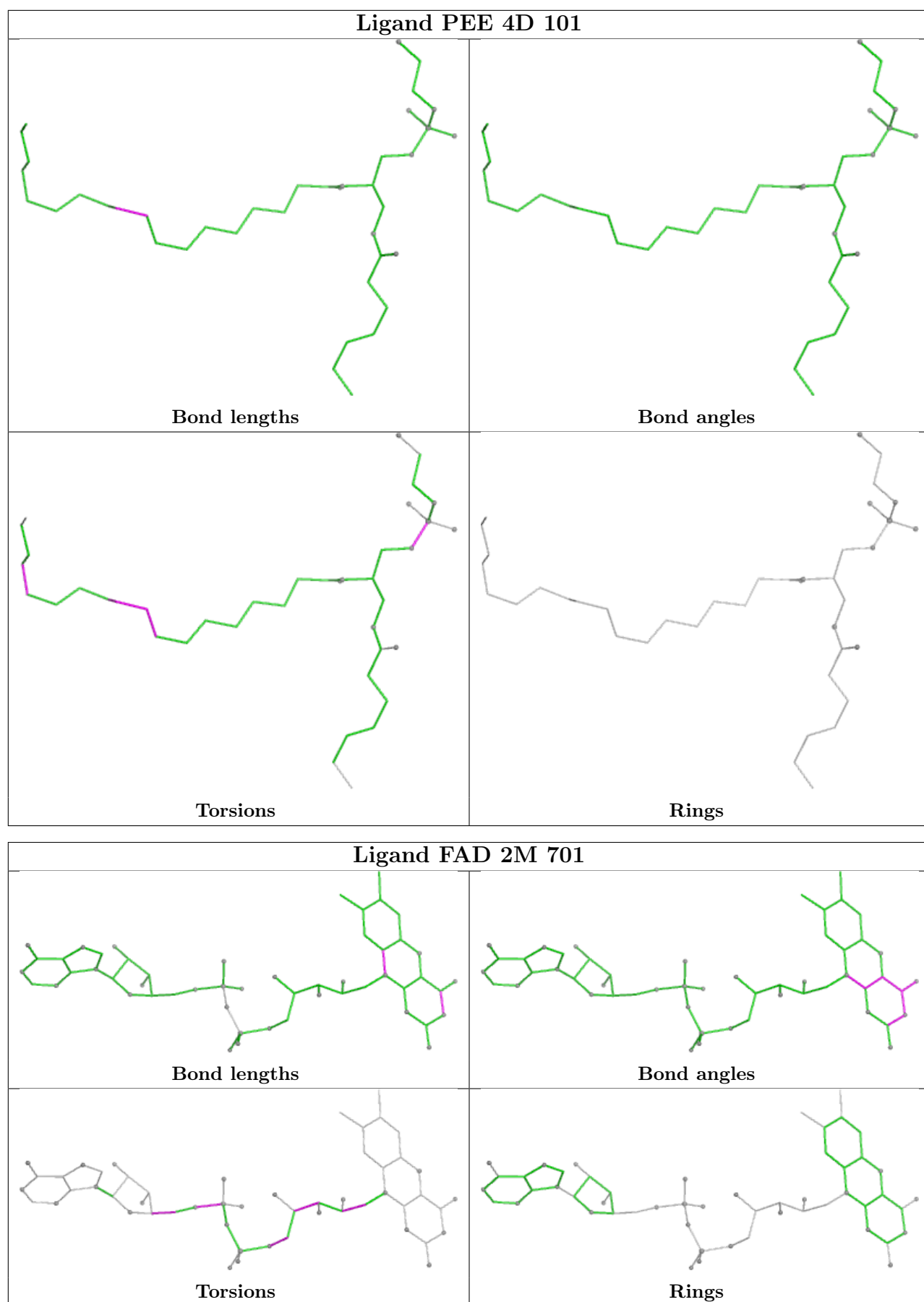


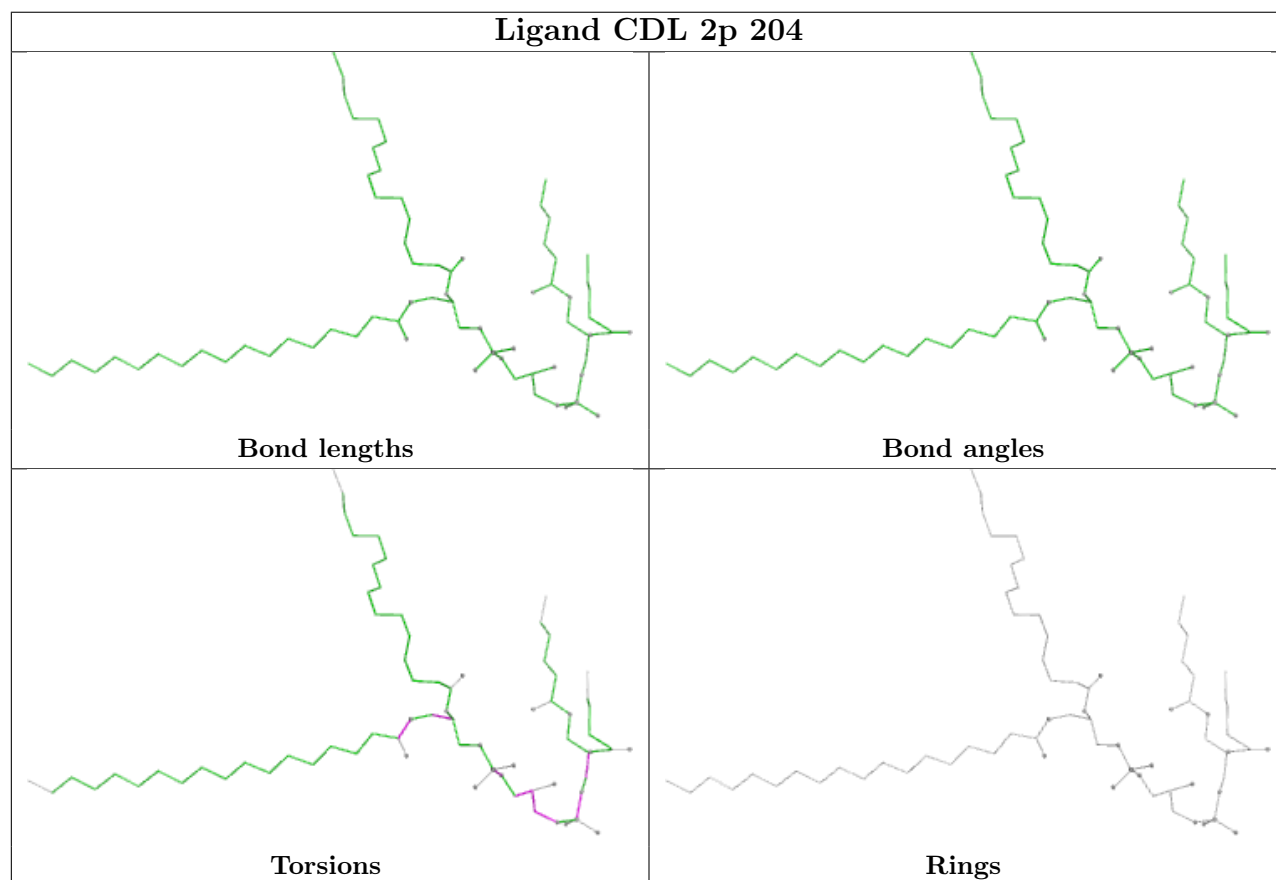
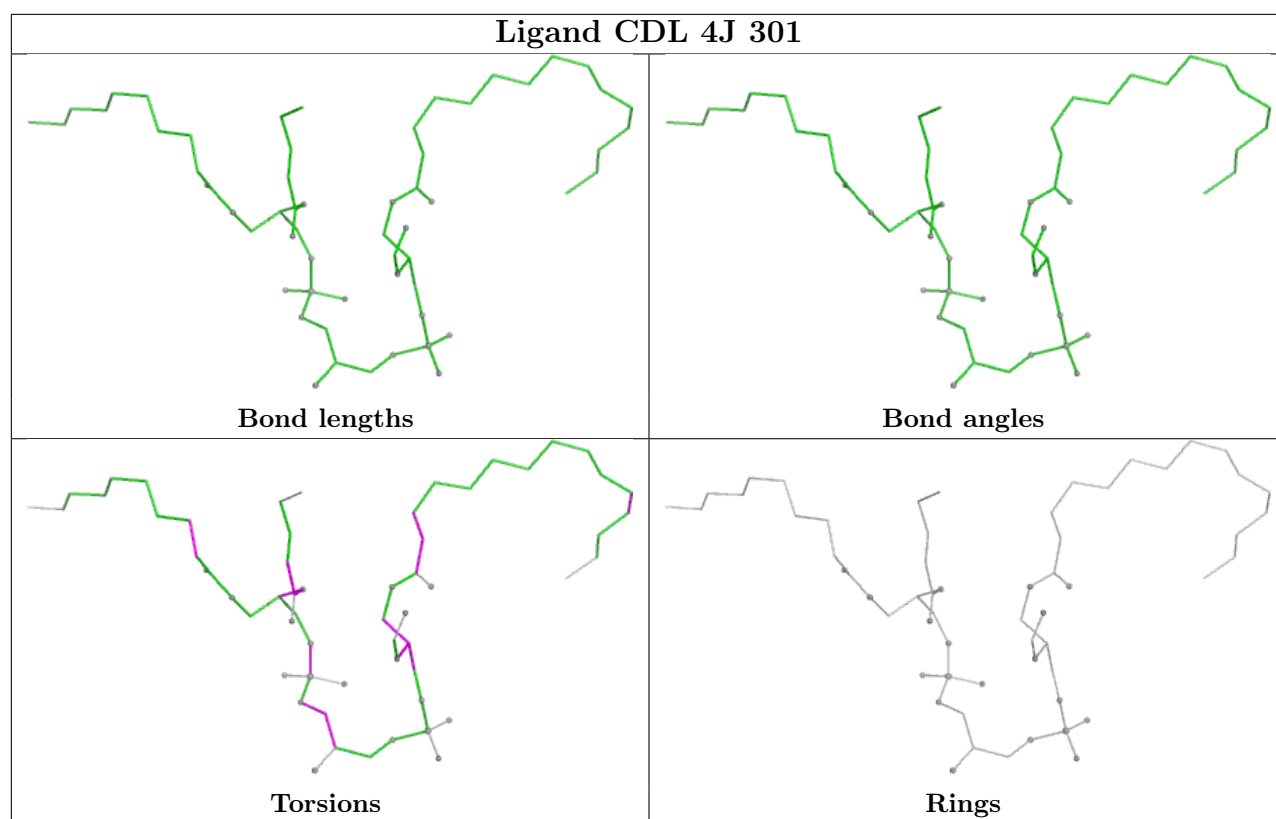


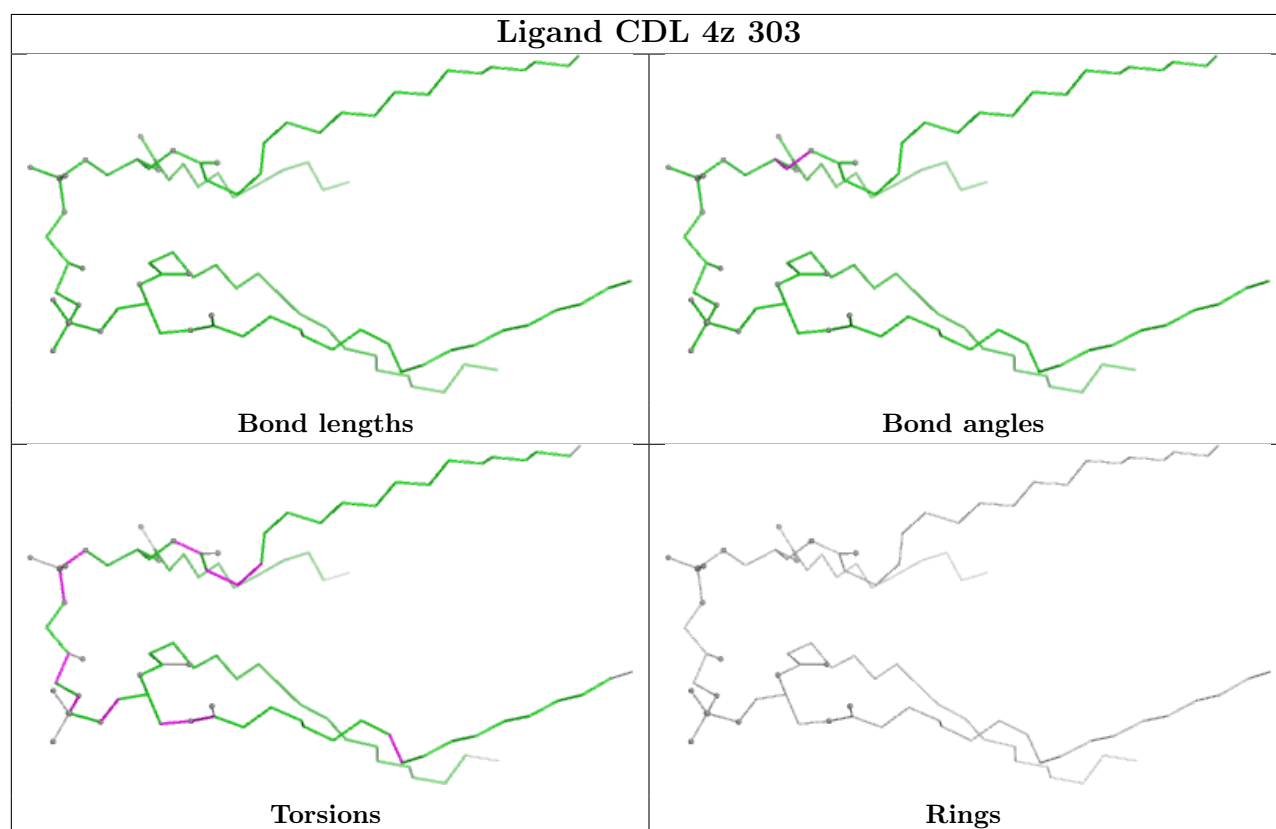
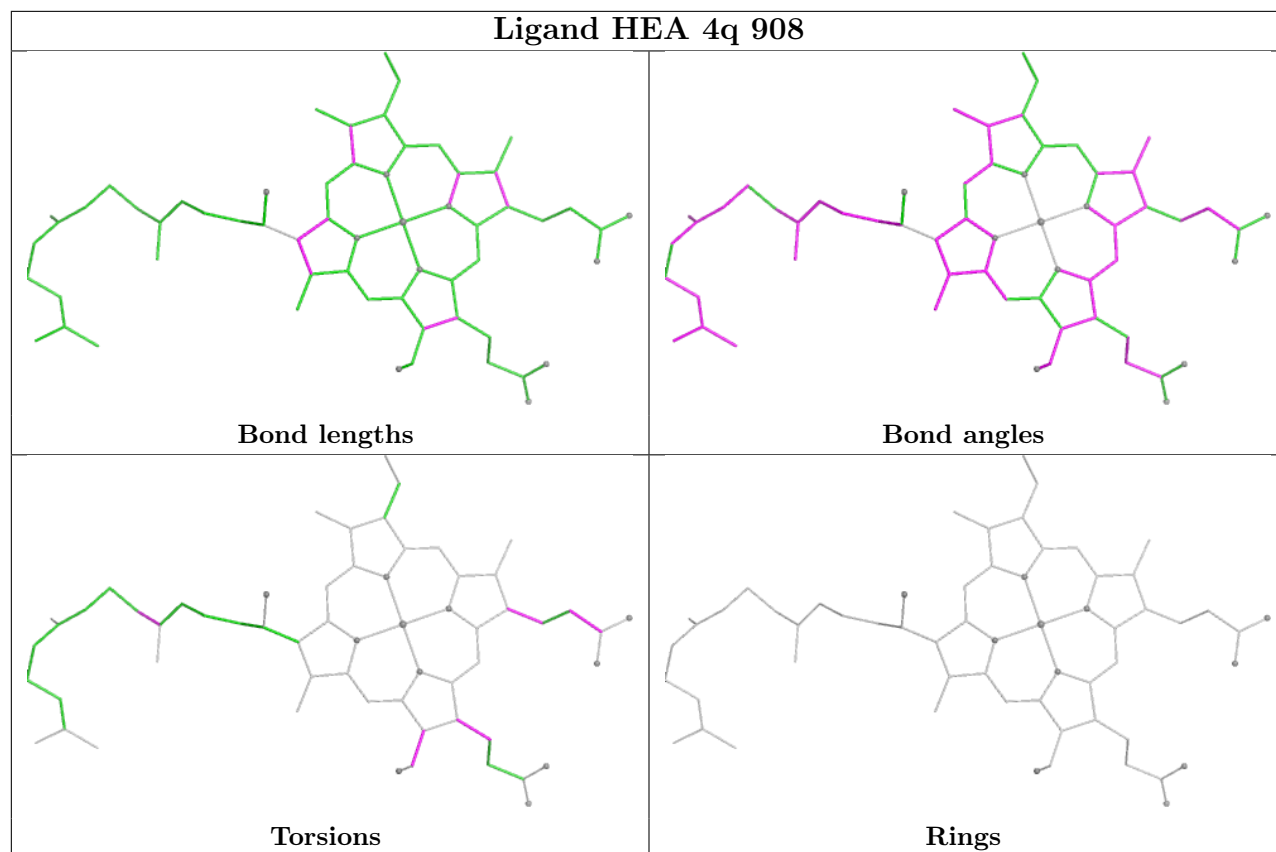


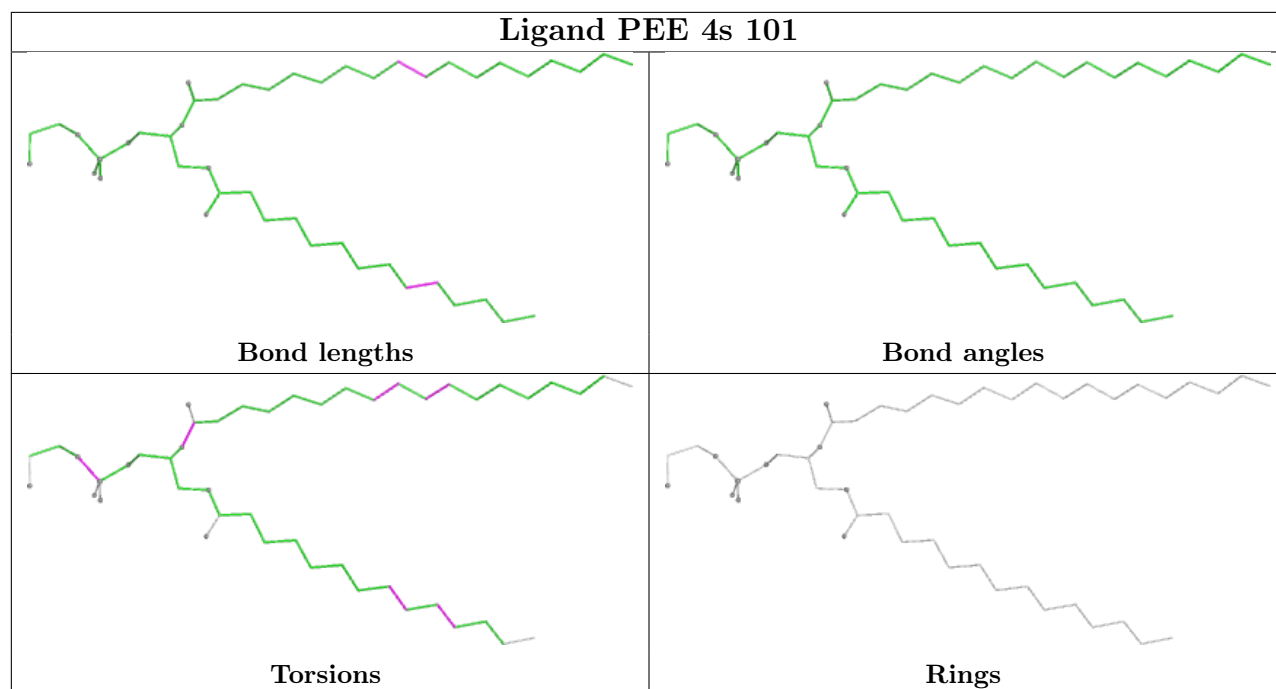
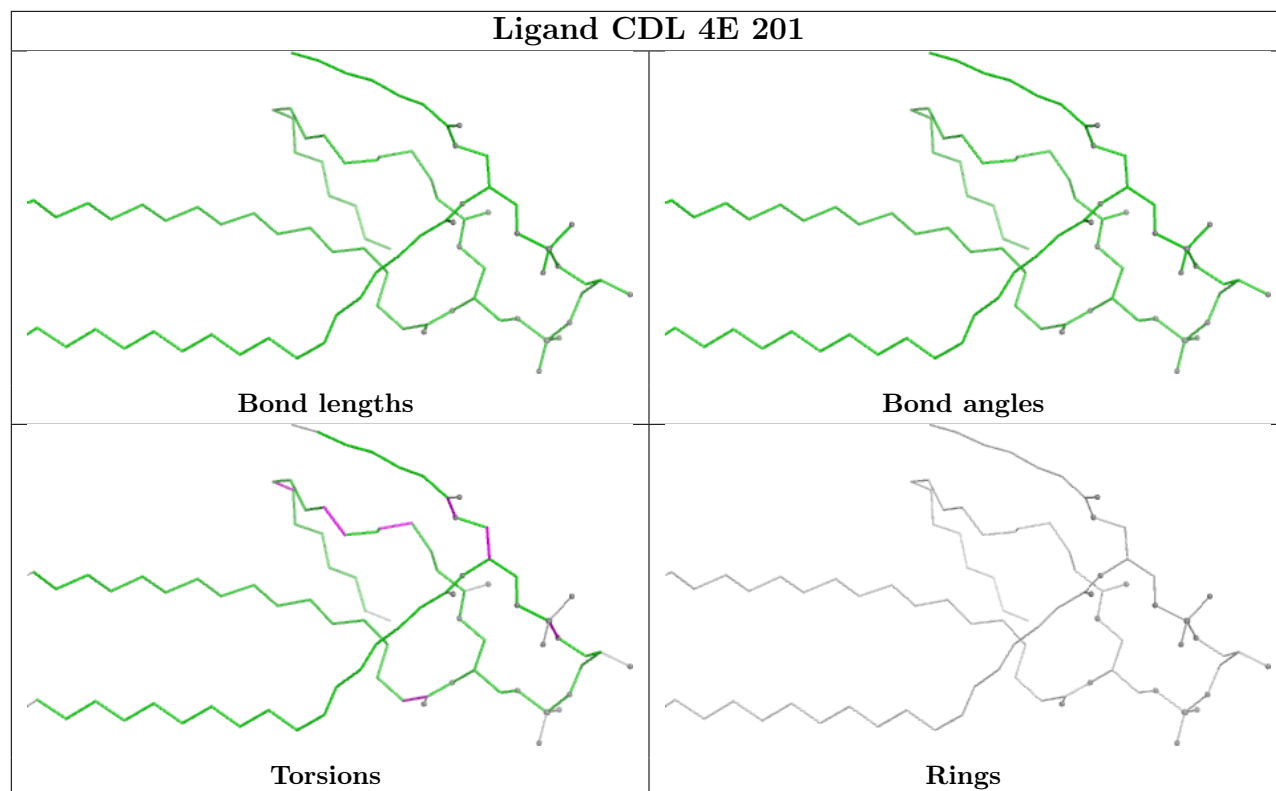


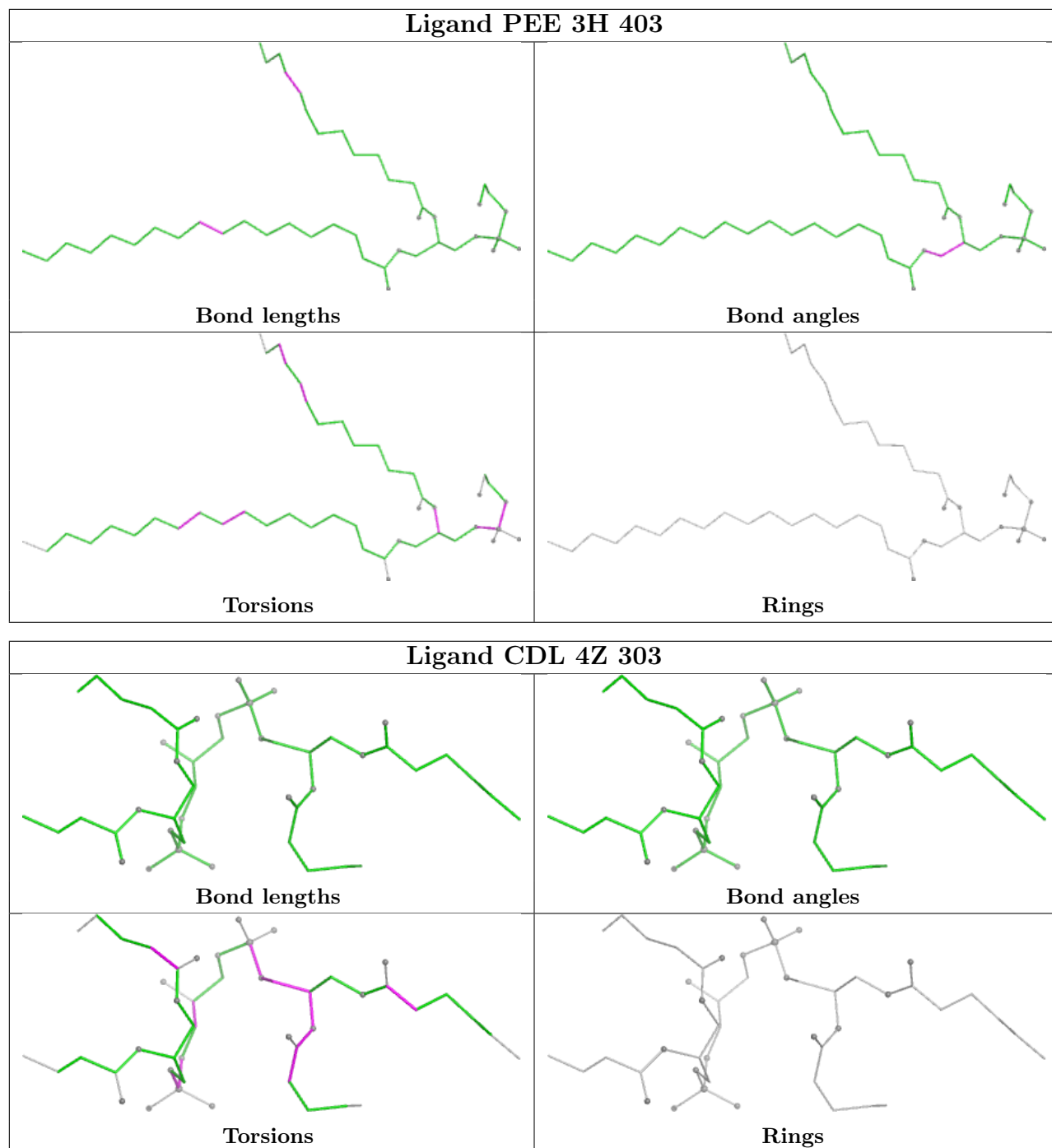


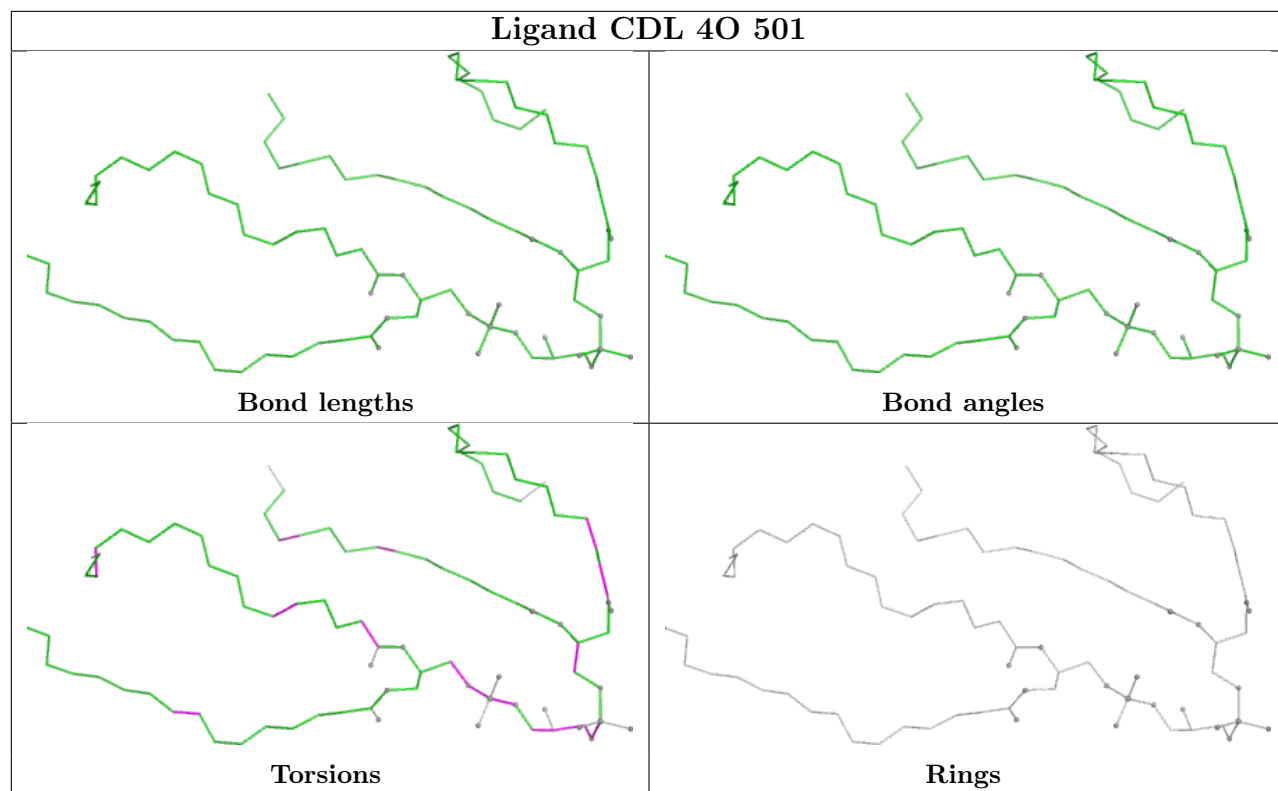




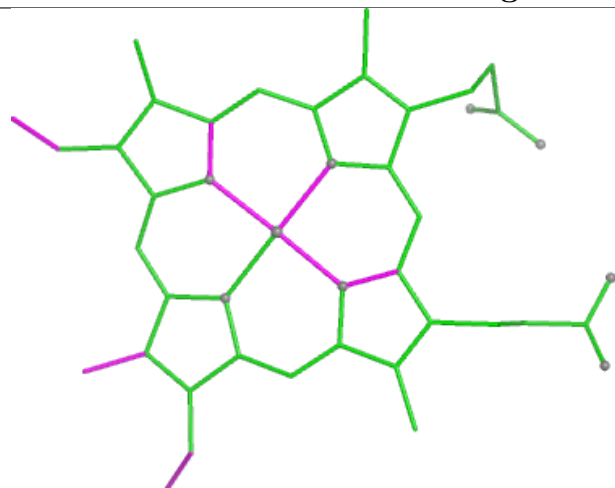




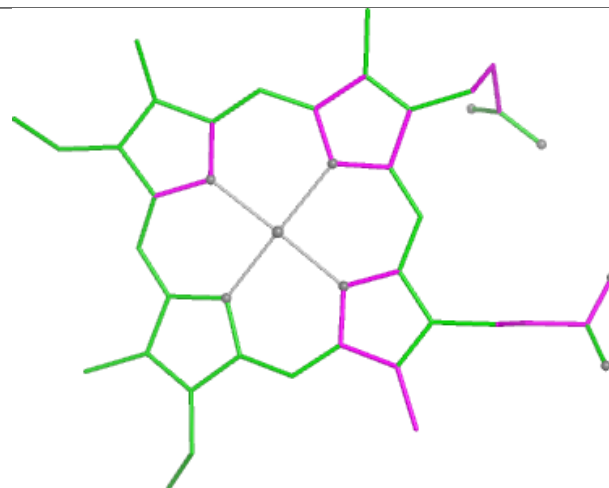




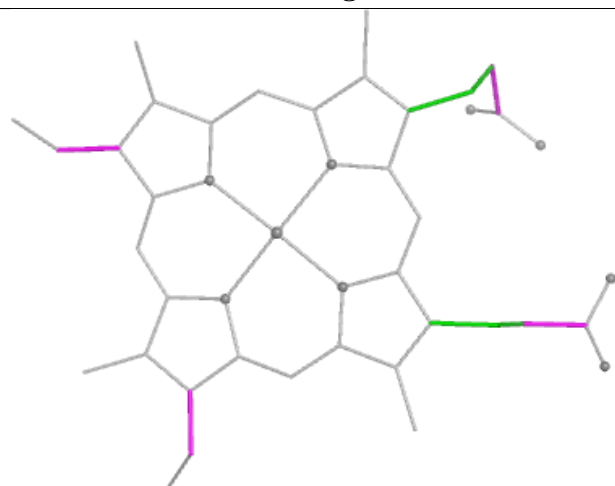
Ligand HEM 3G 406



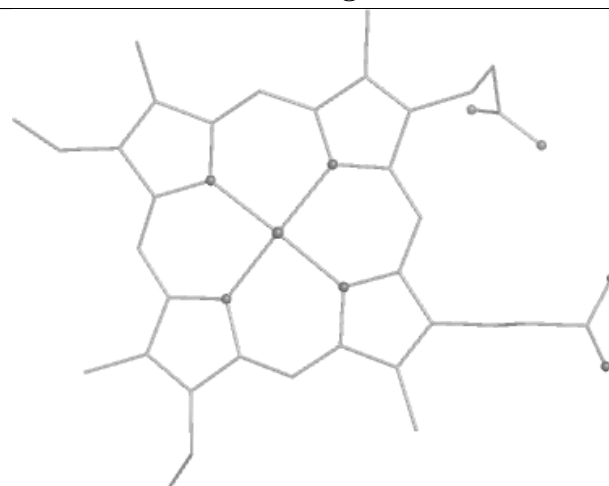
Bond lengths



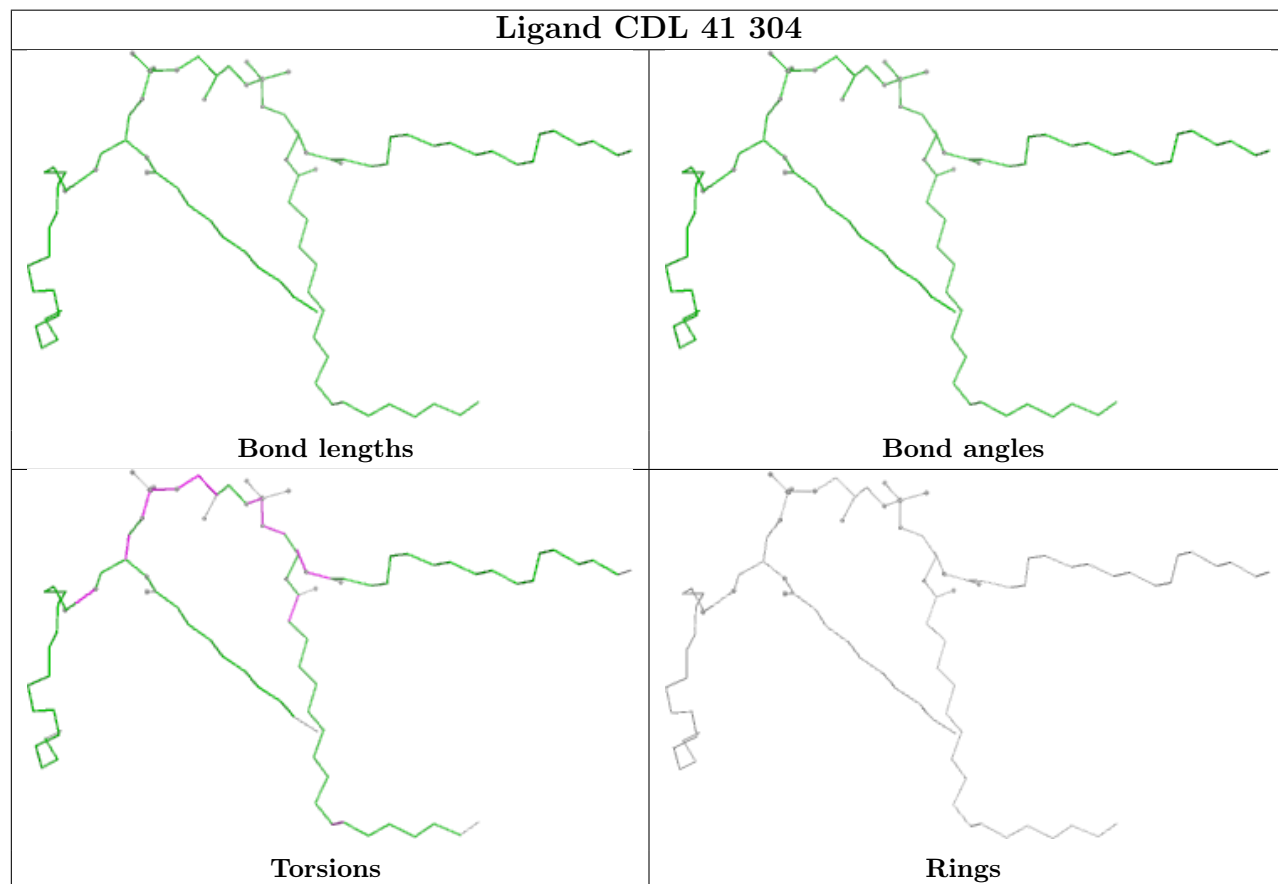
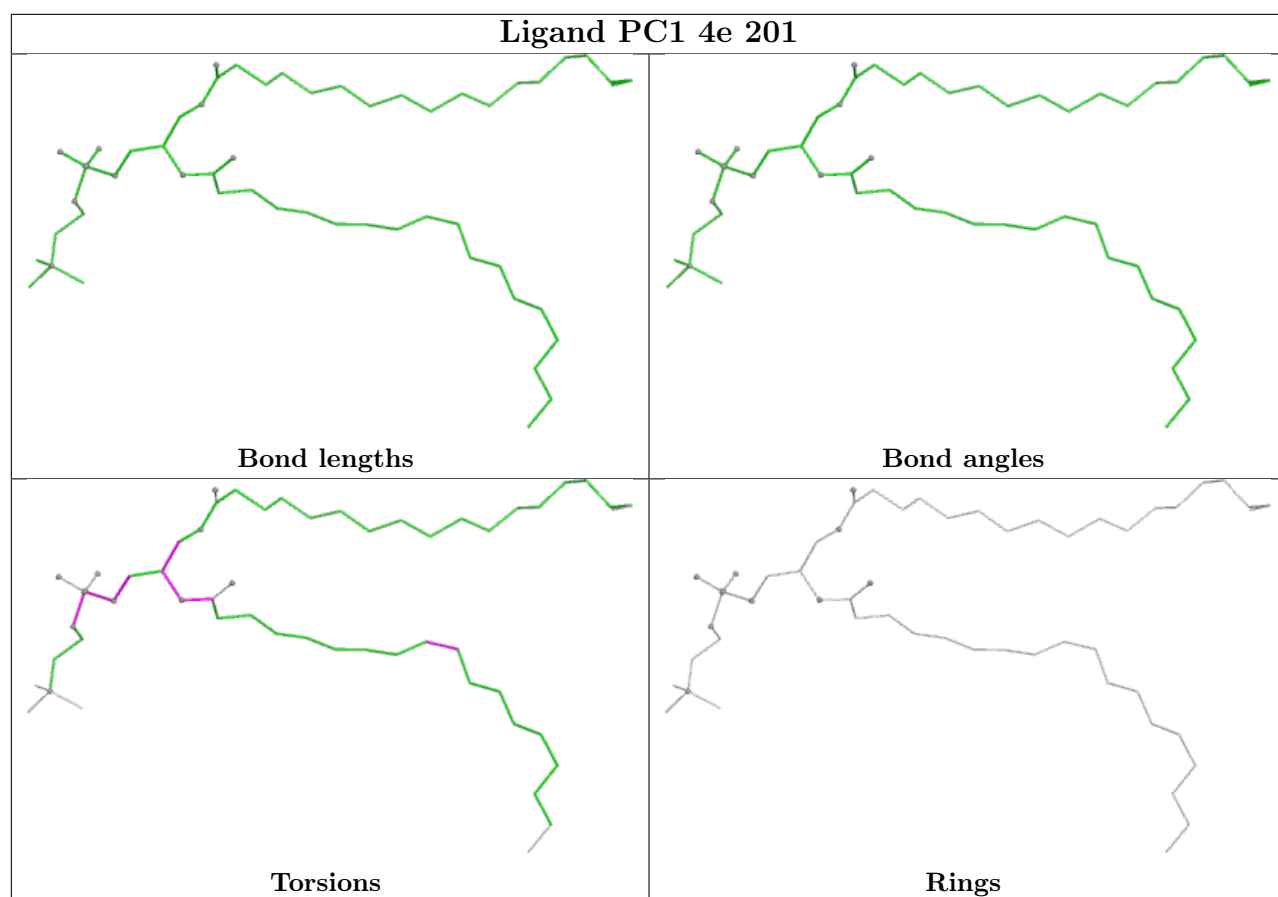
Bond angles

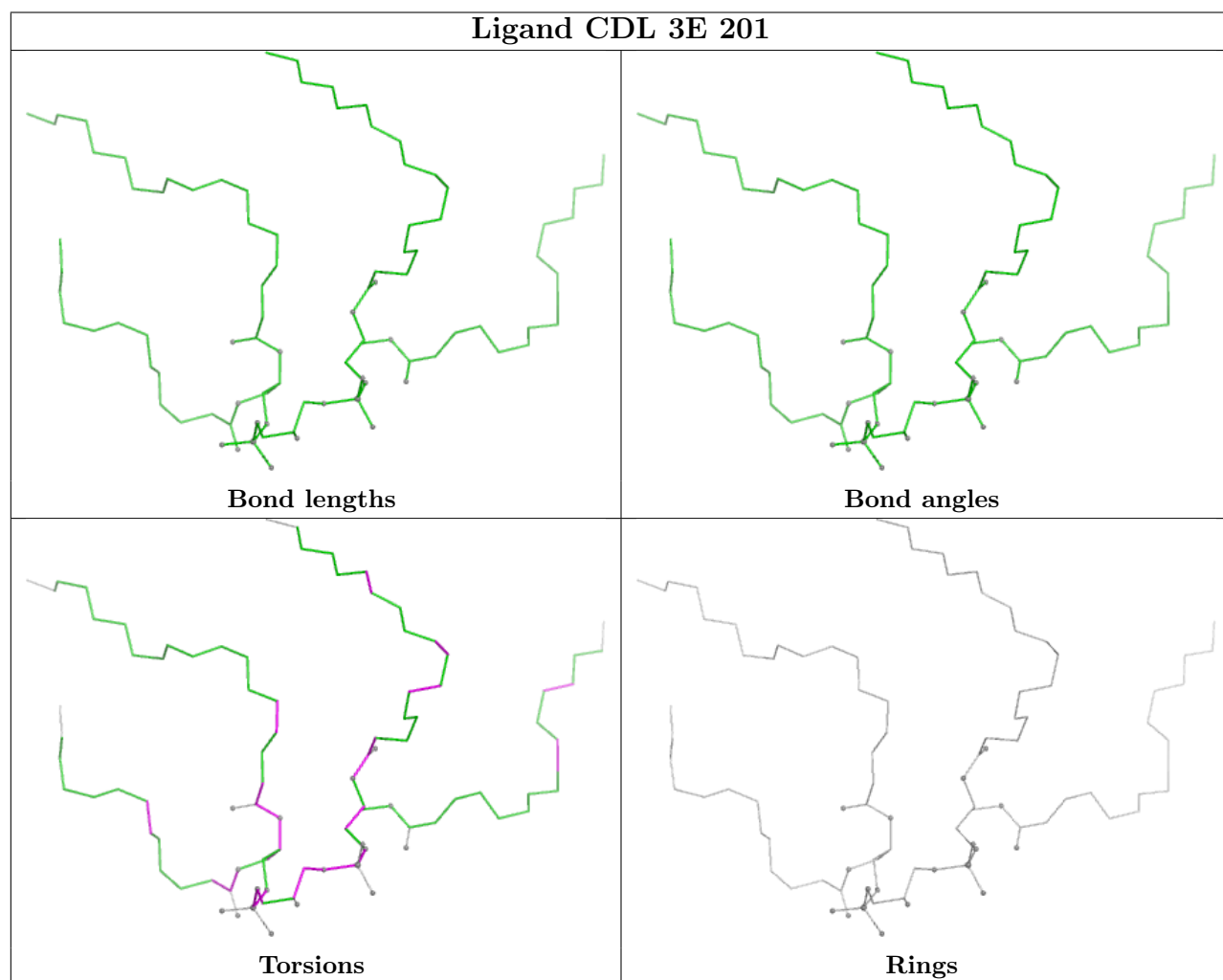
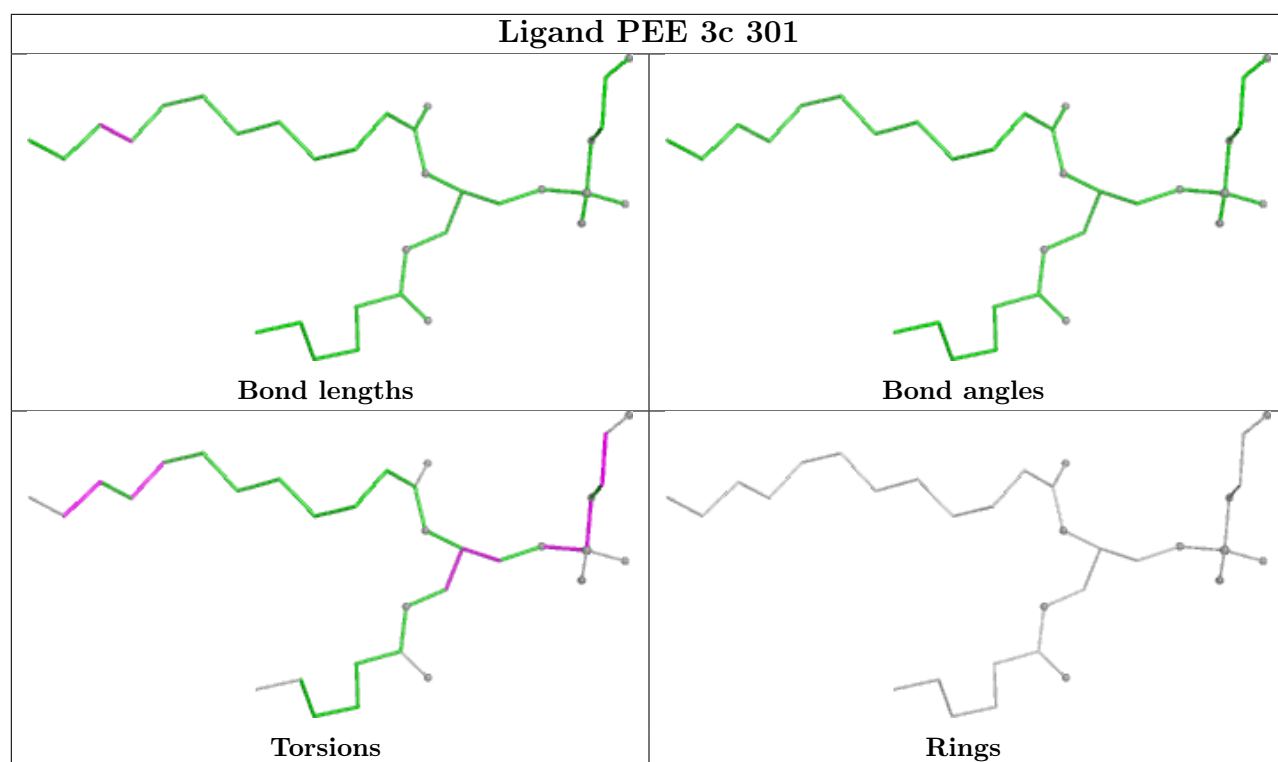


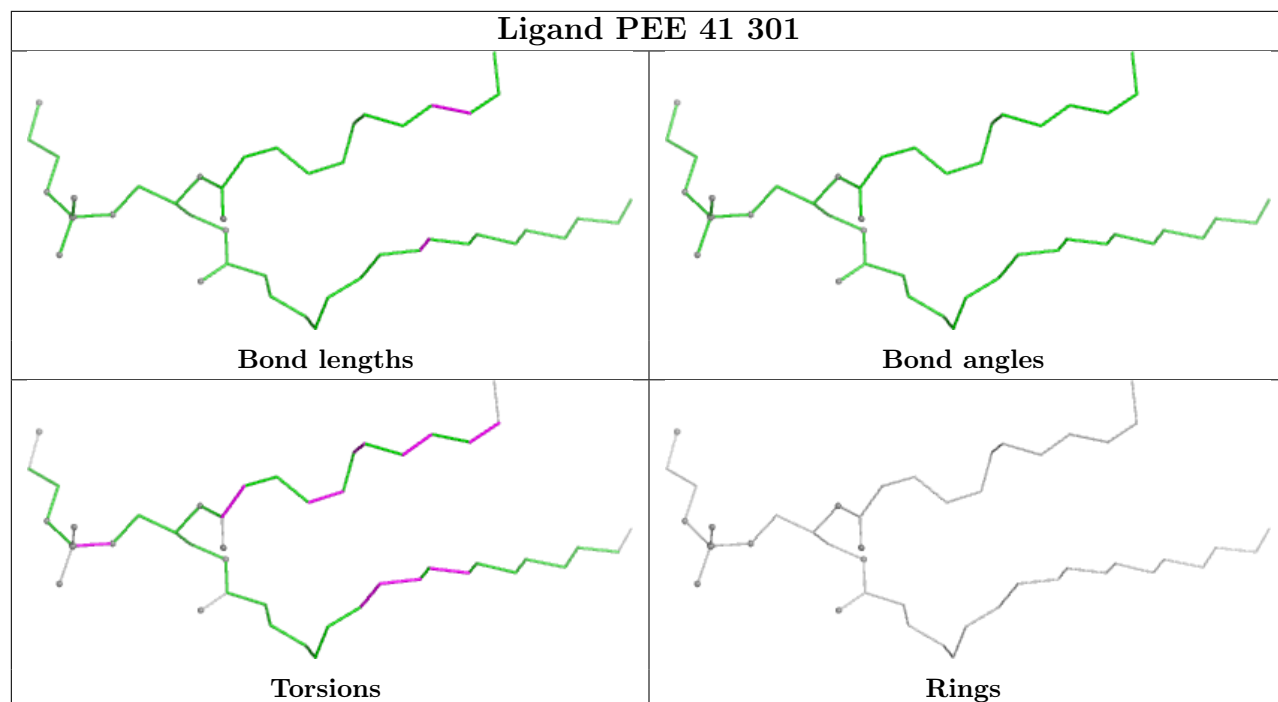
Torsions

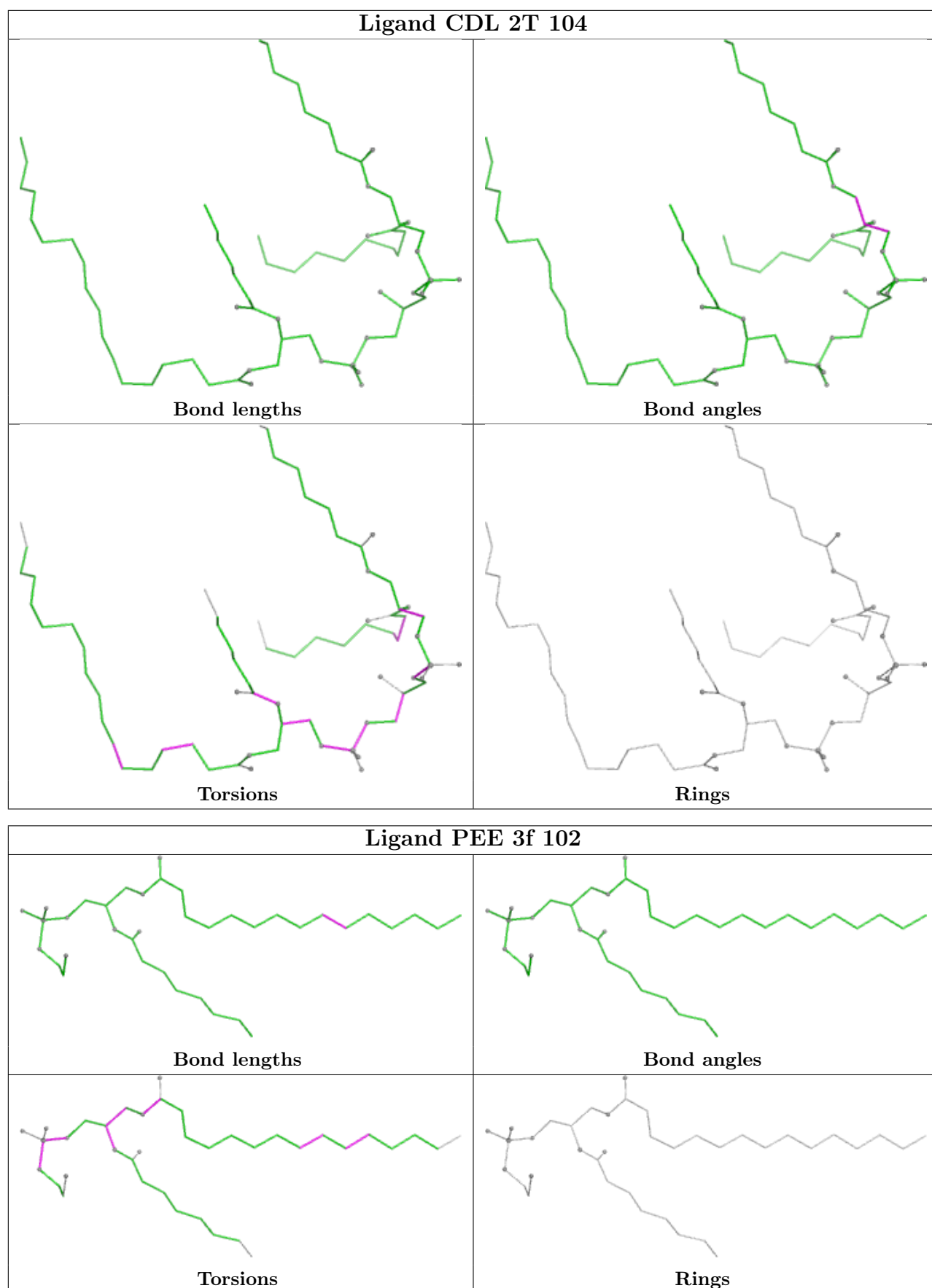


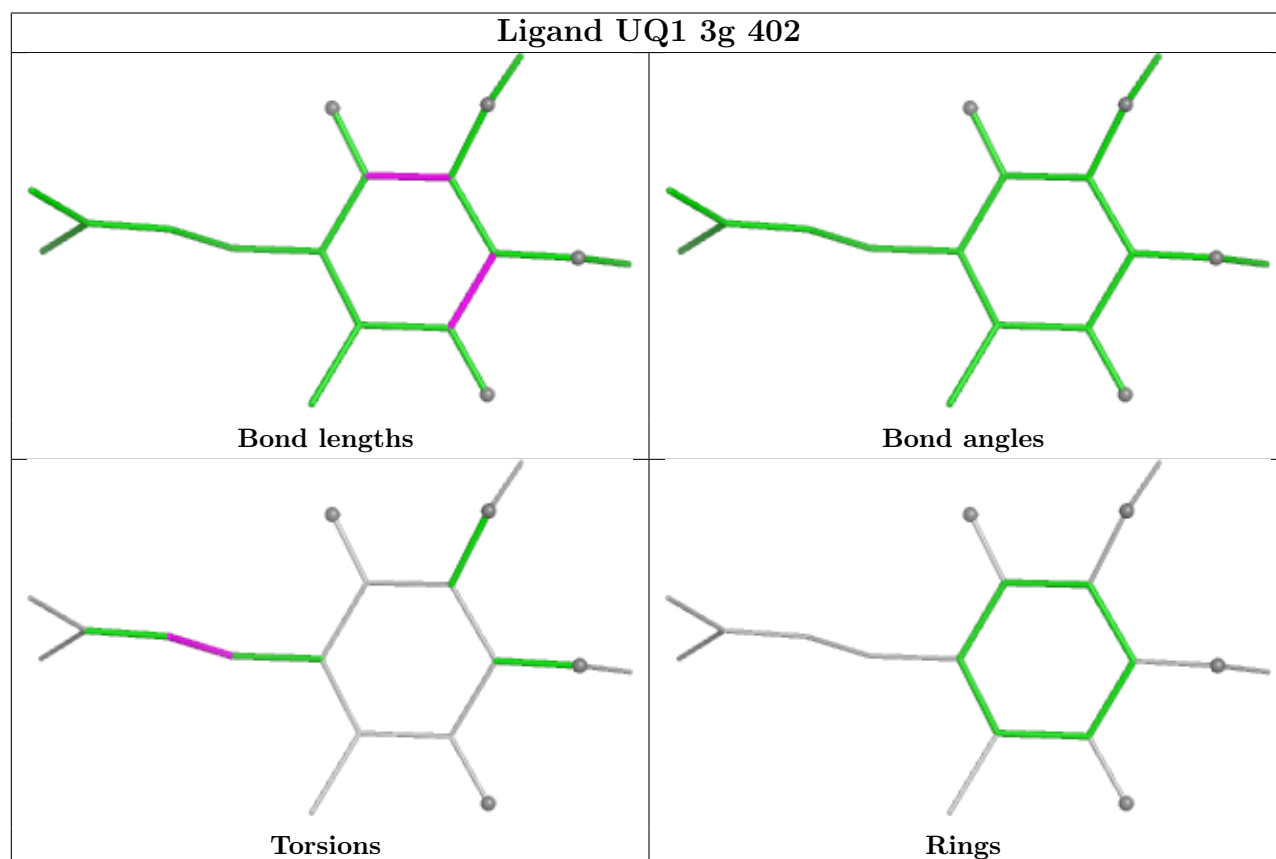
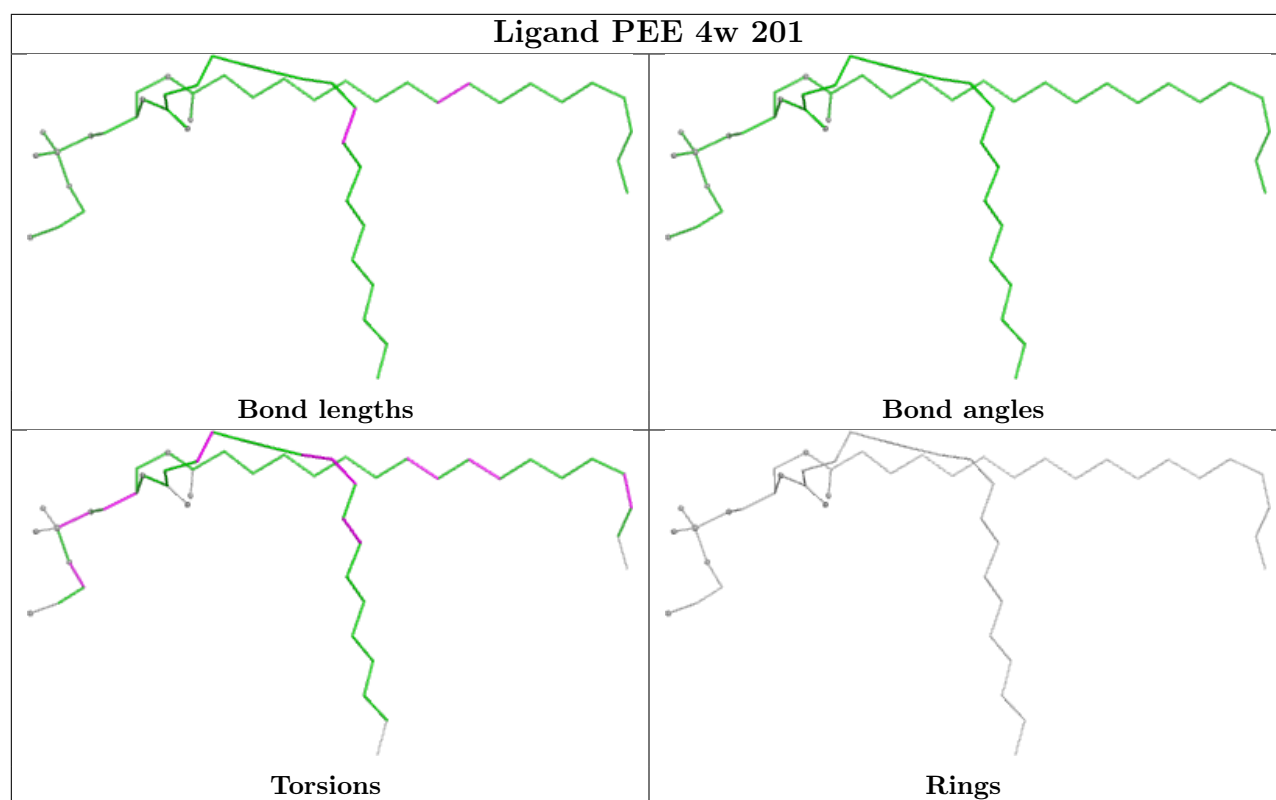
Rings

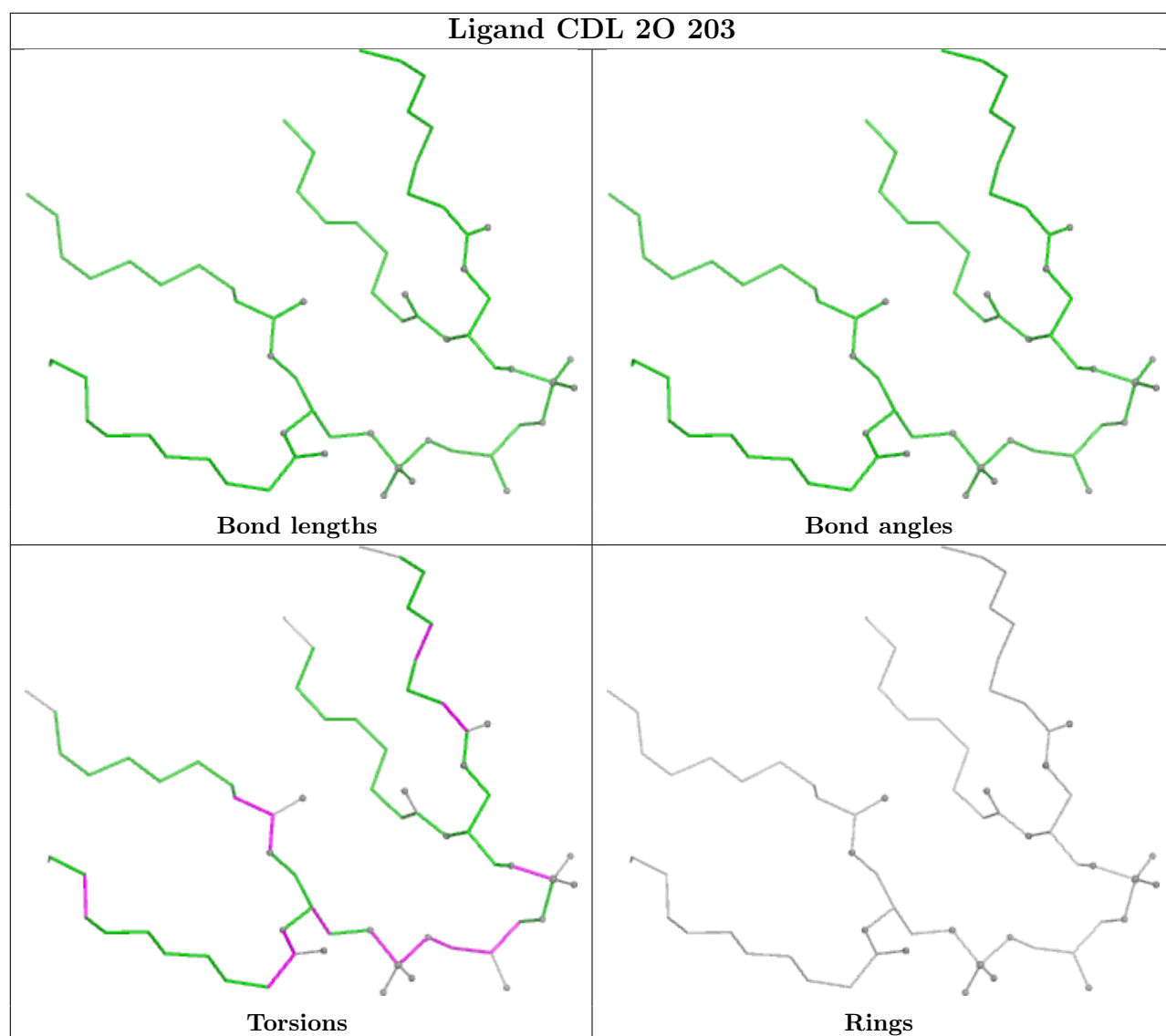


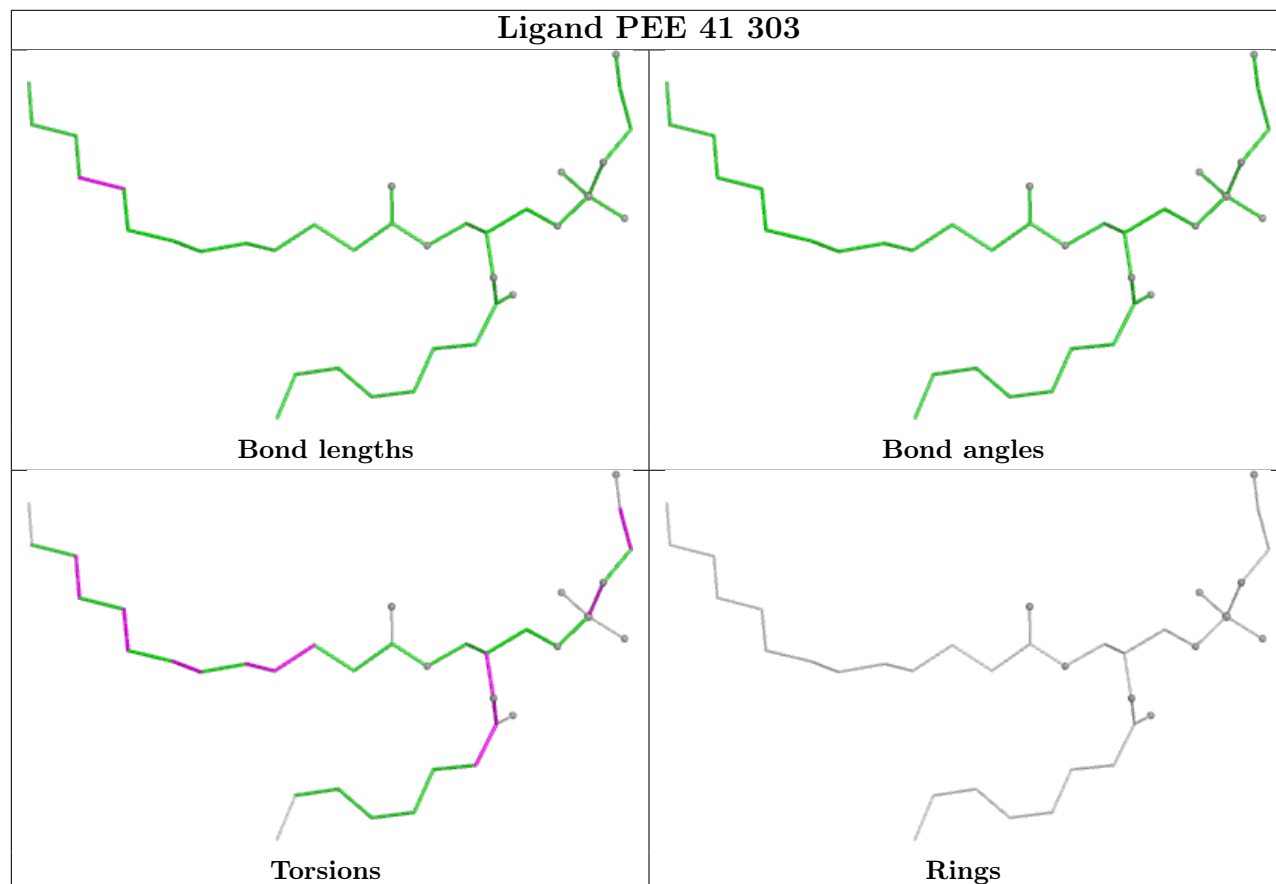
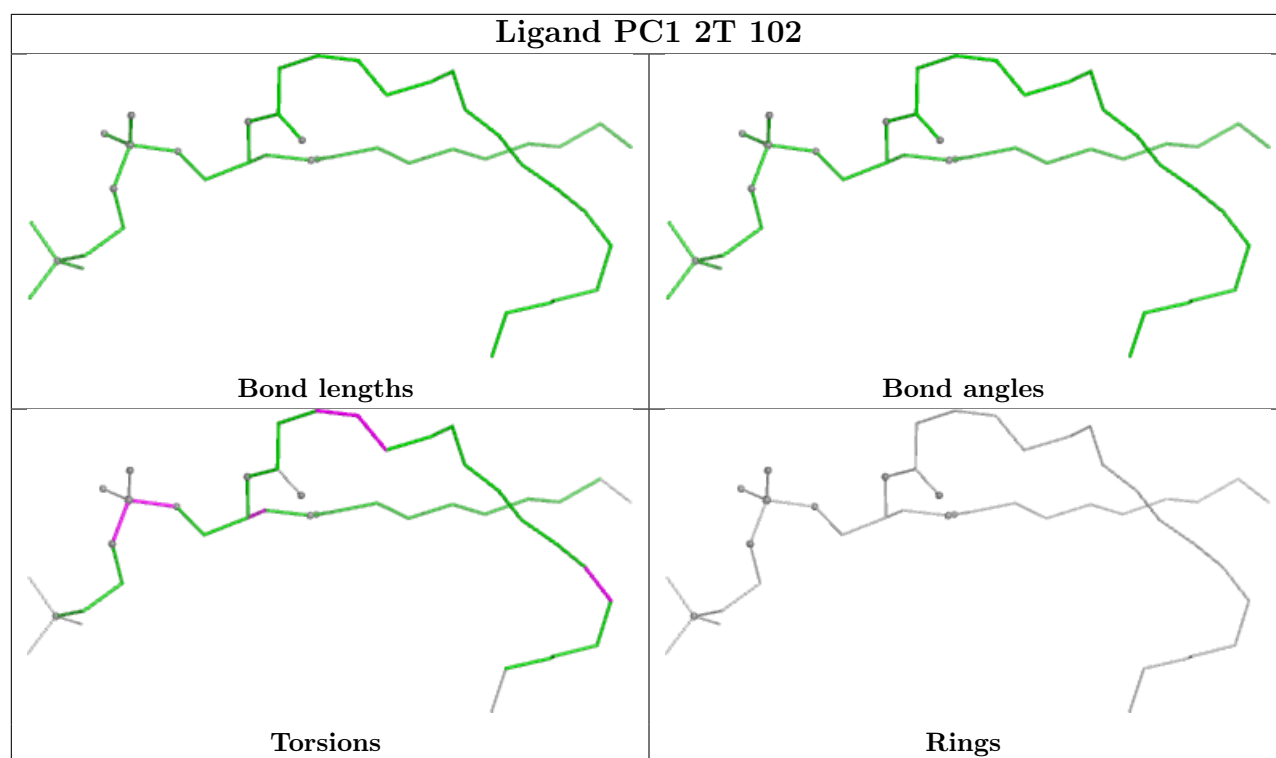


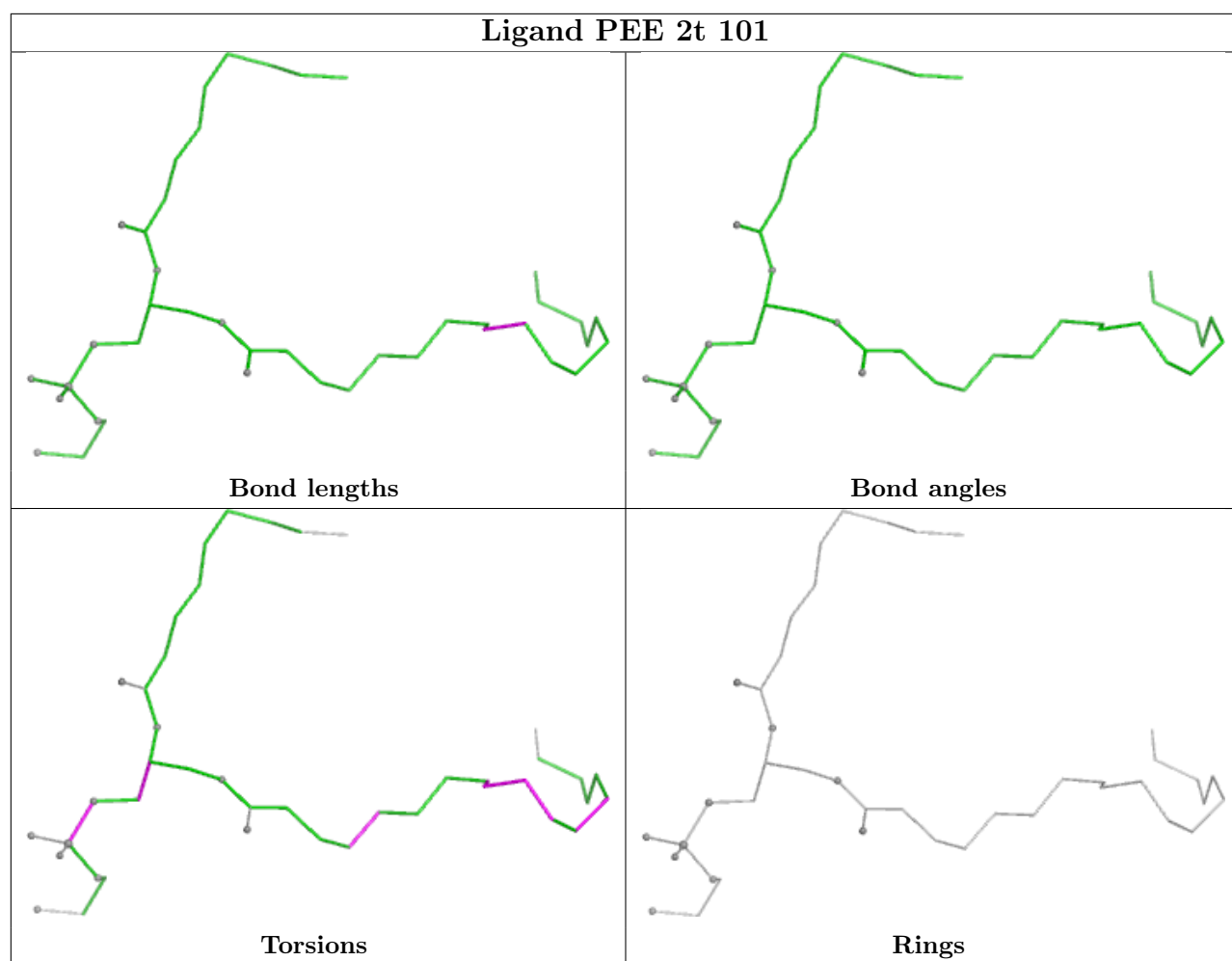


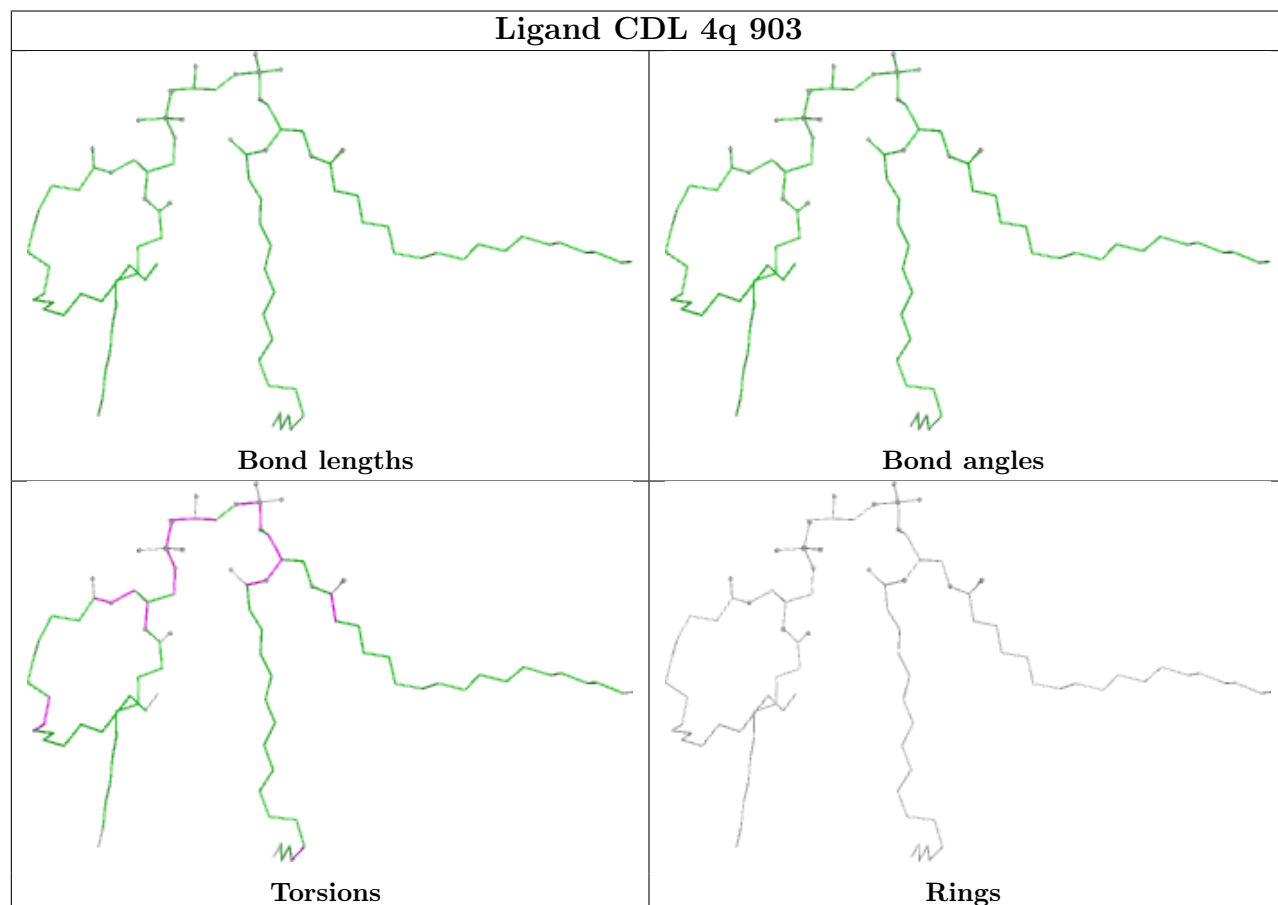
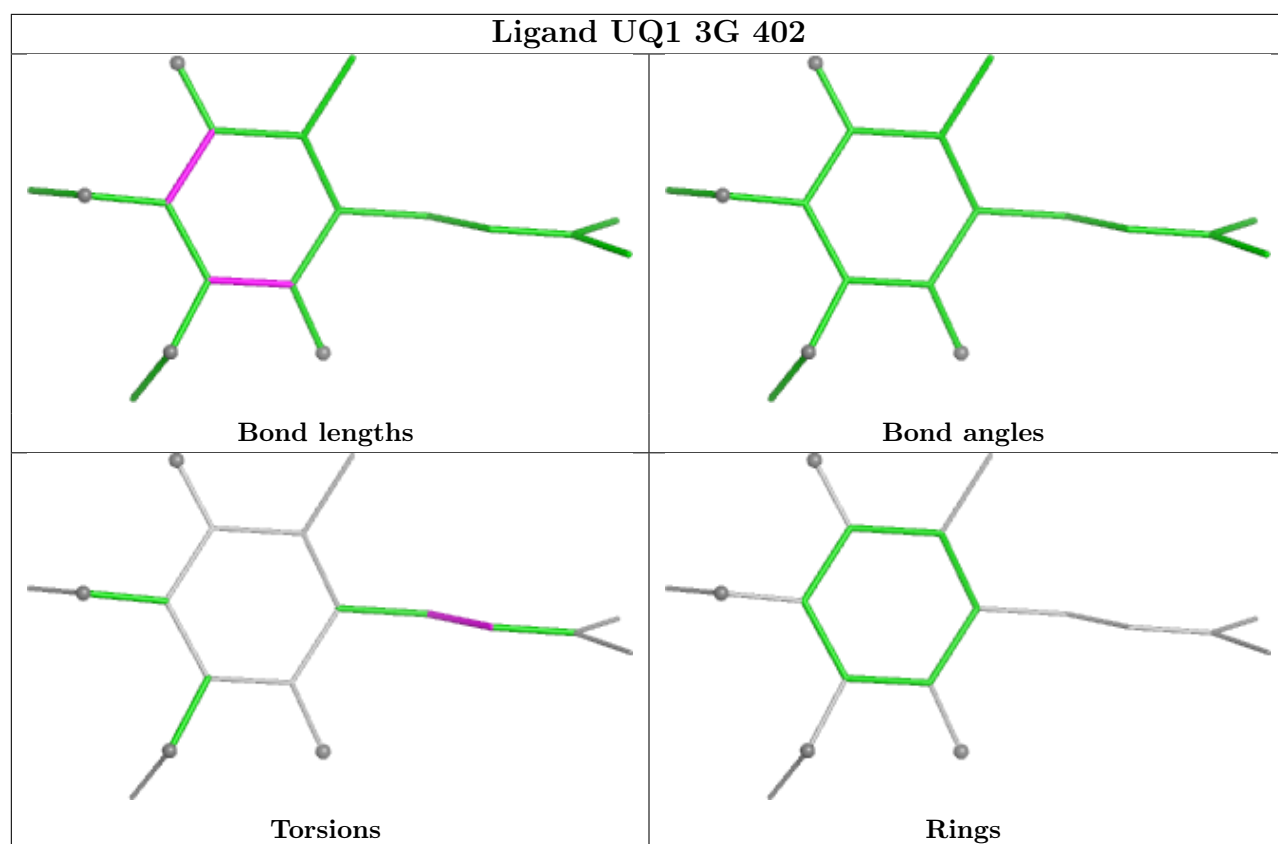


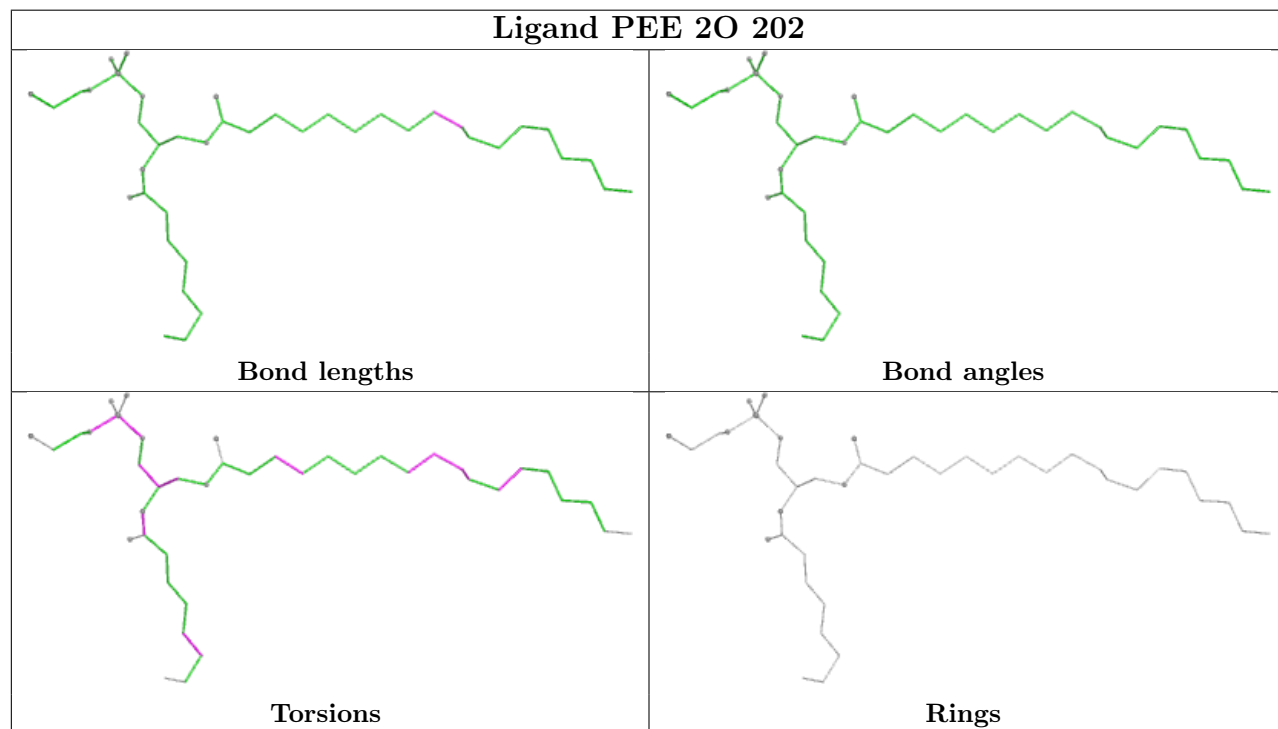
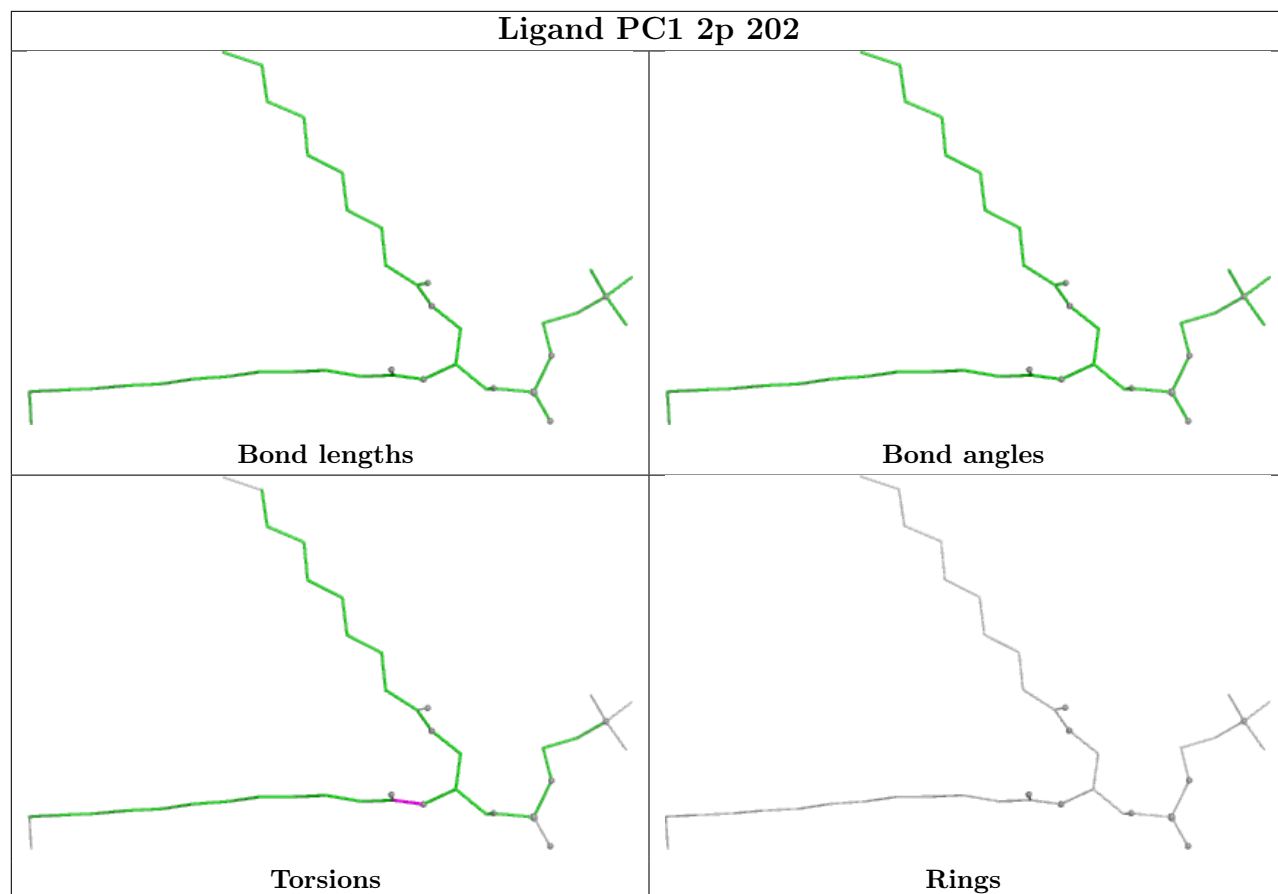


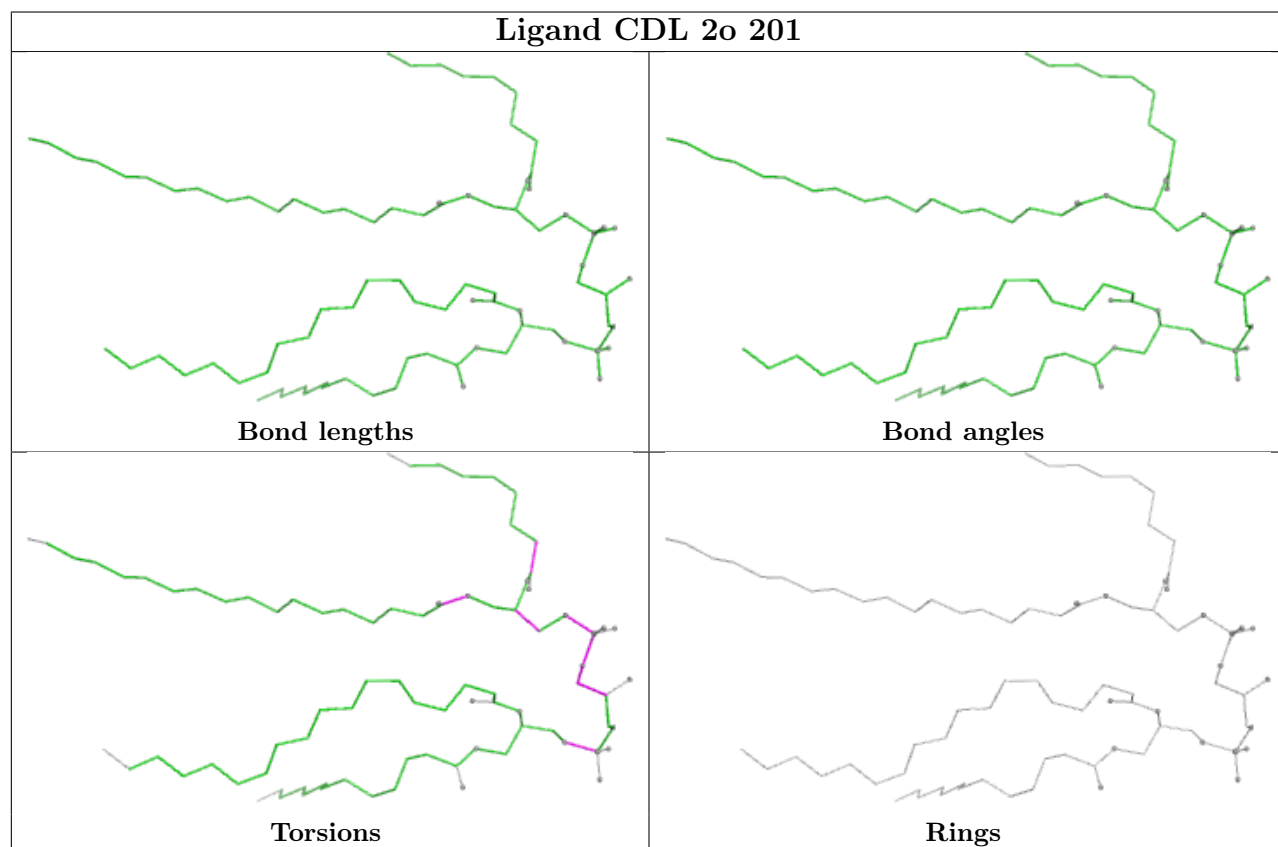
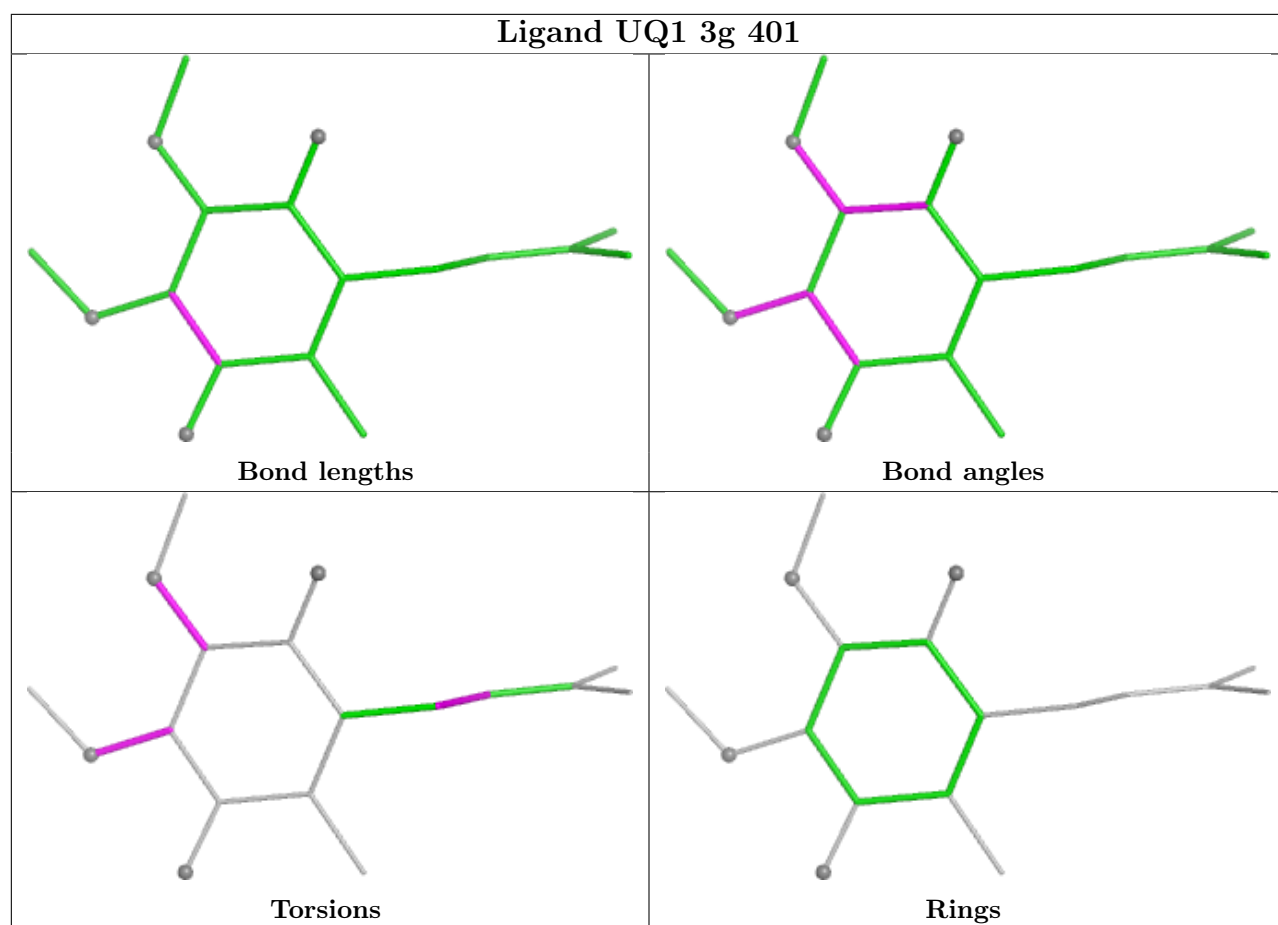


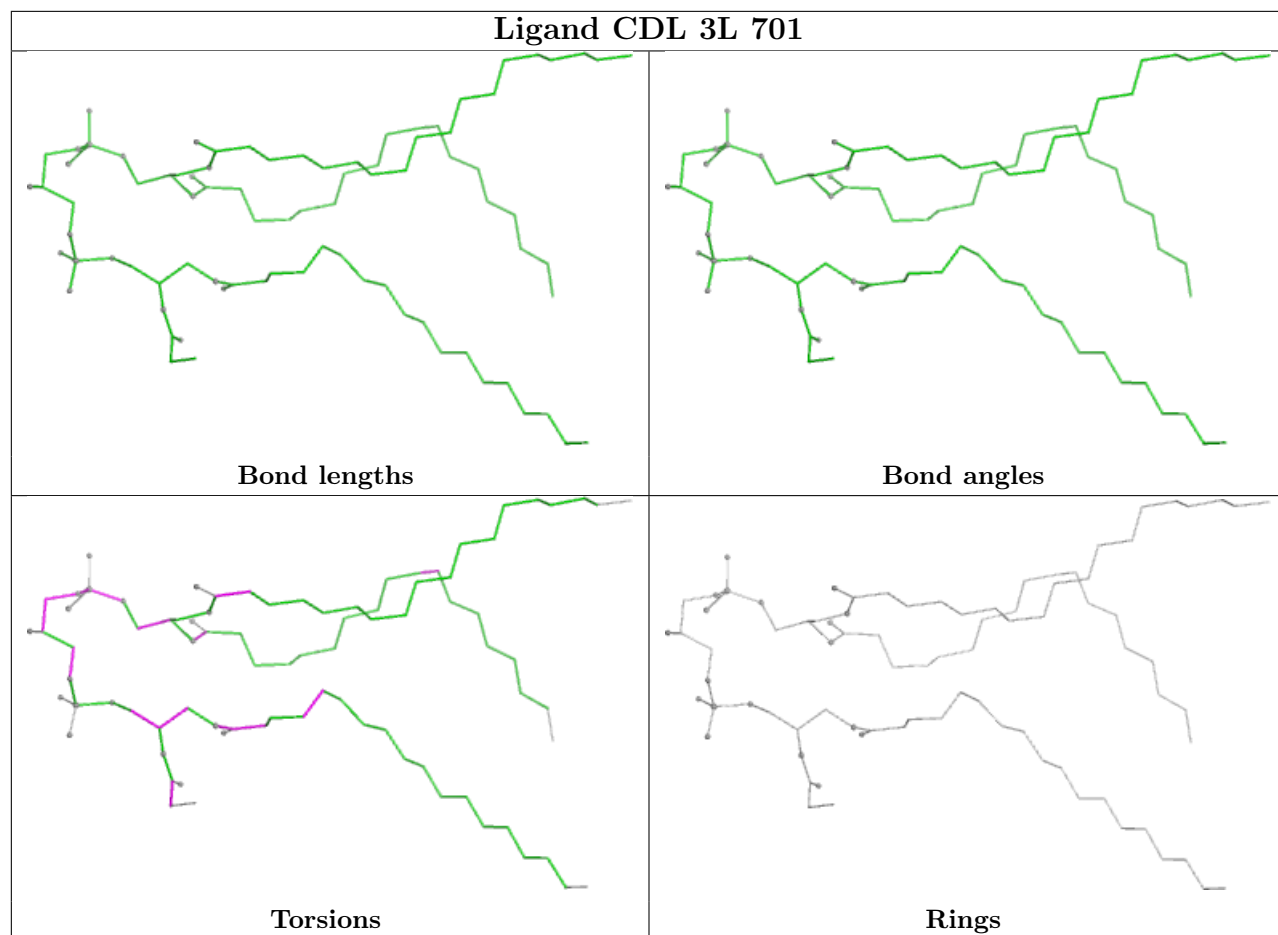


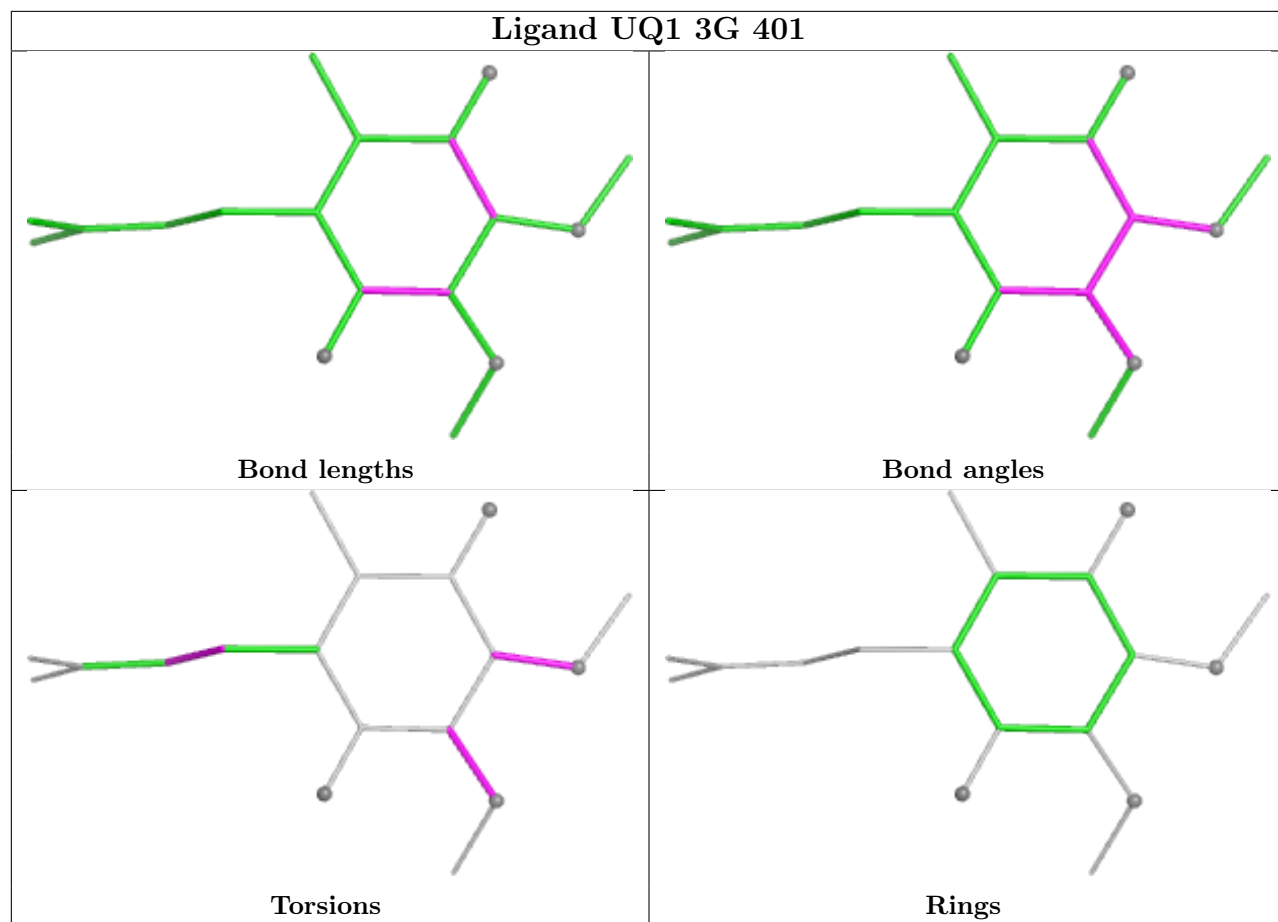


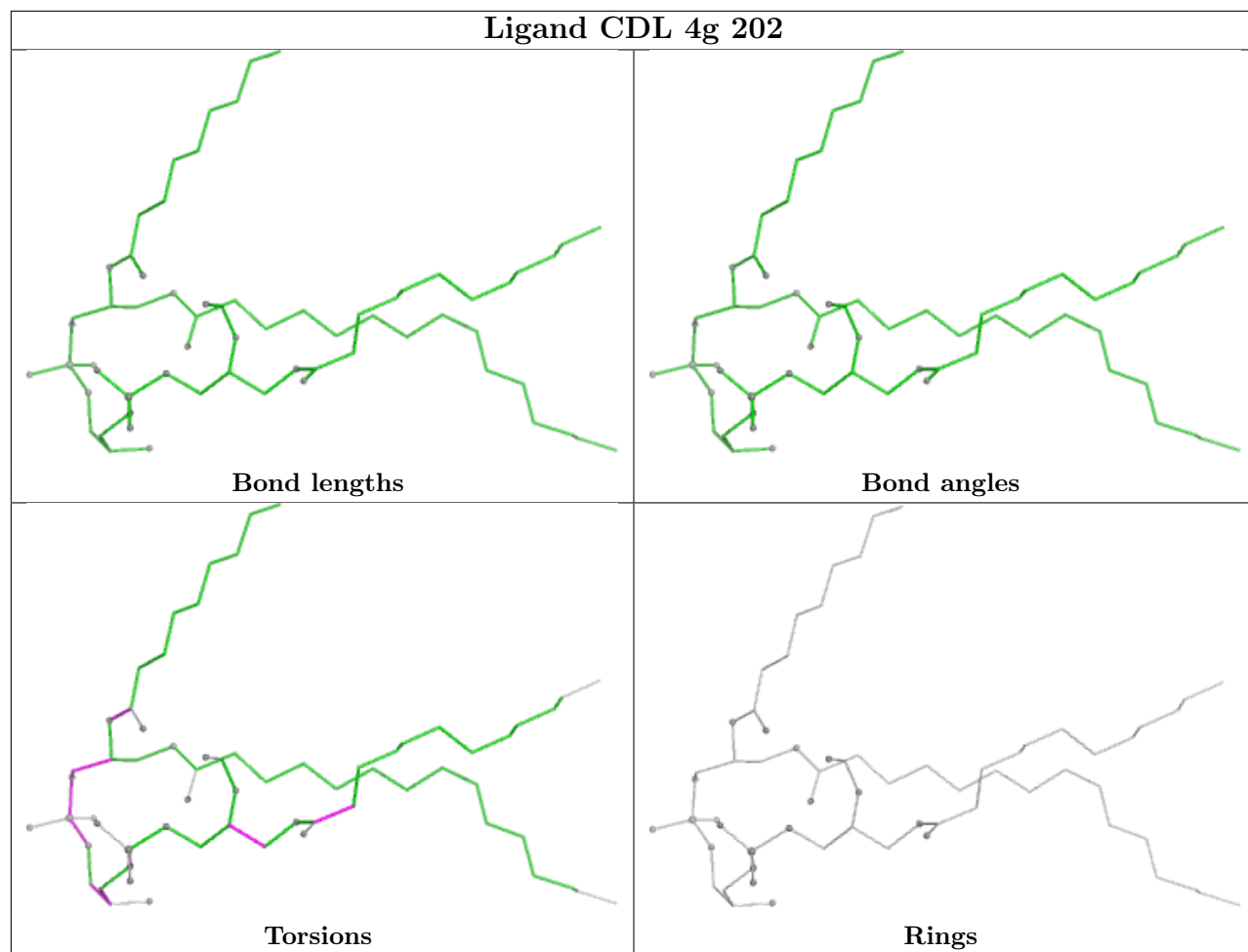


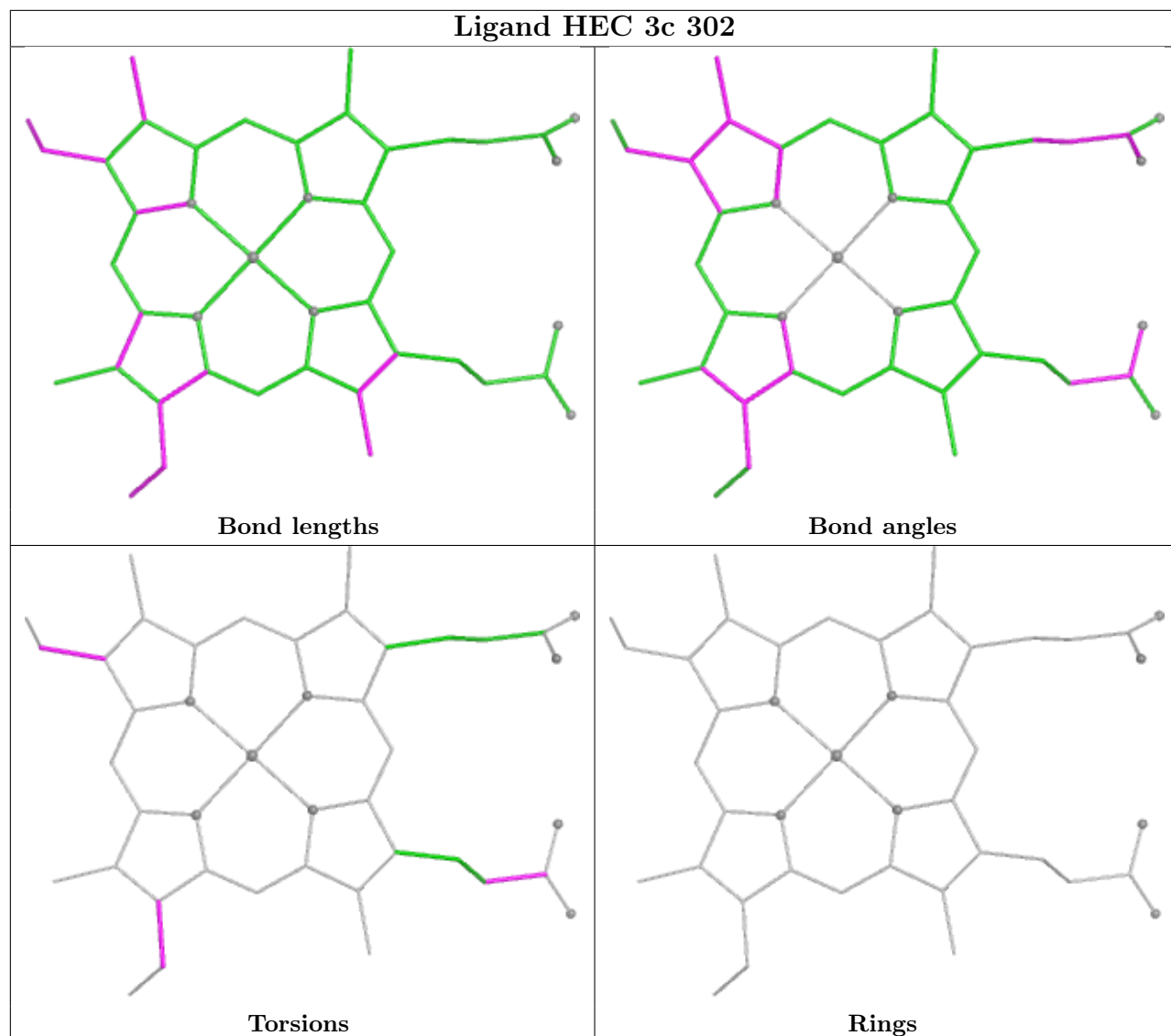


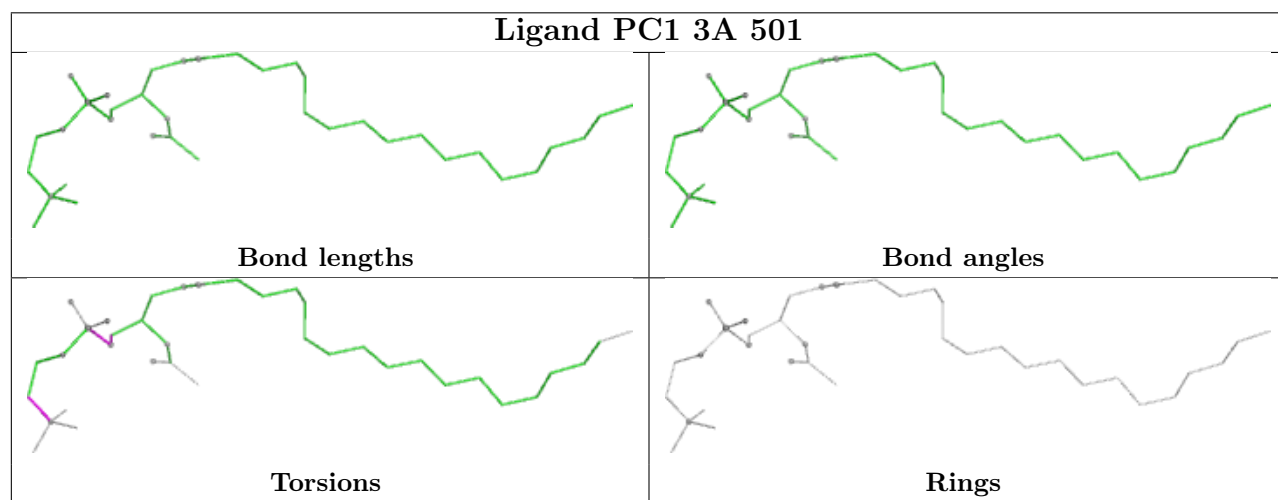
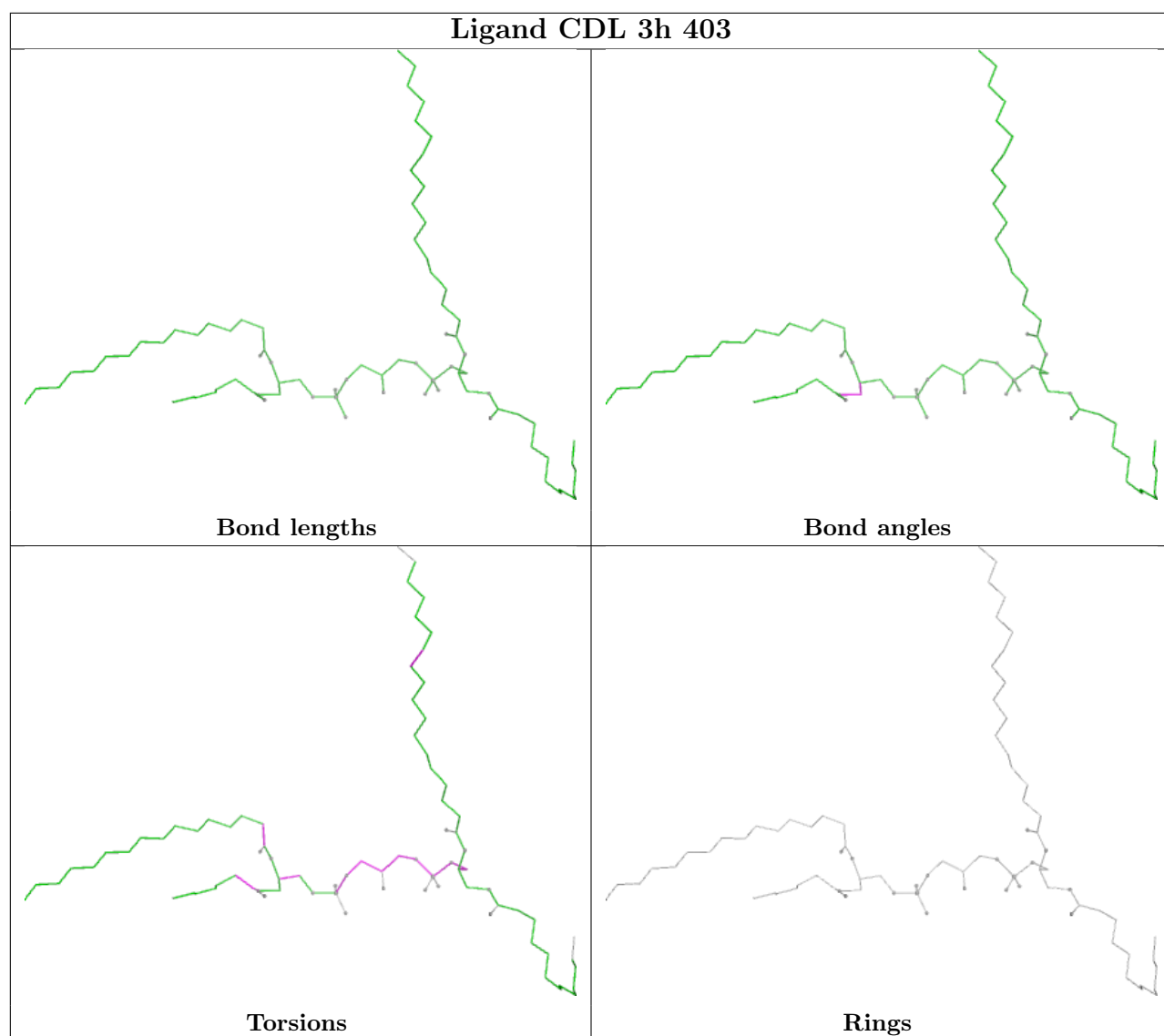


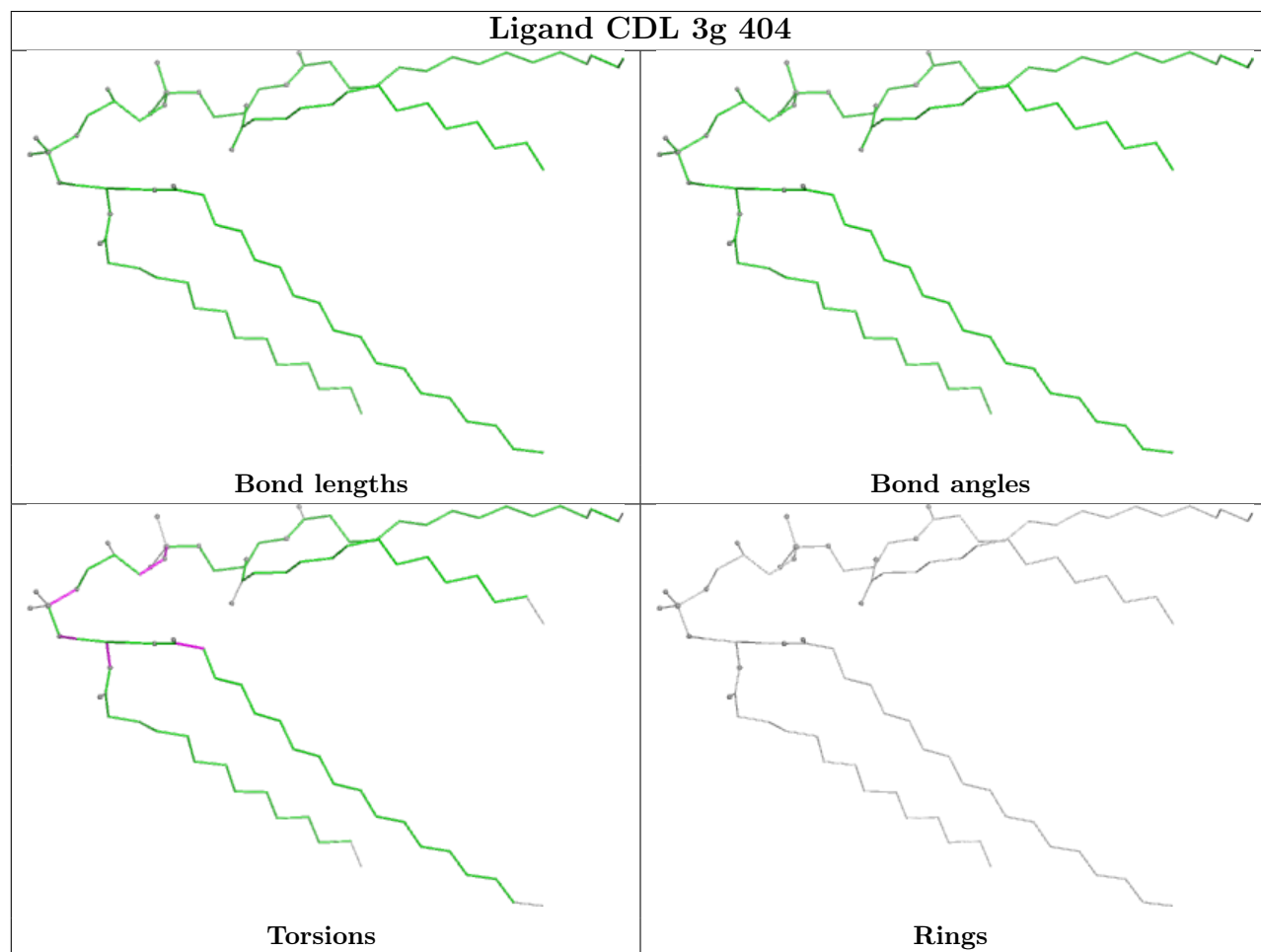
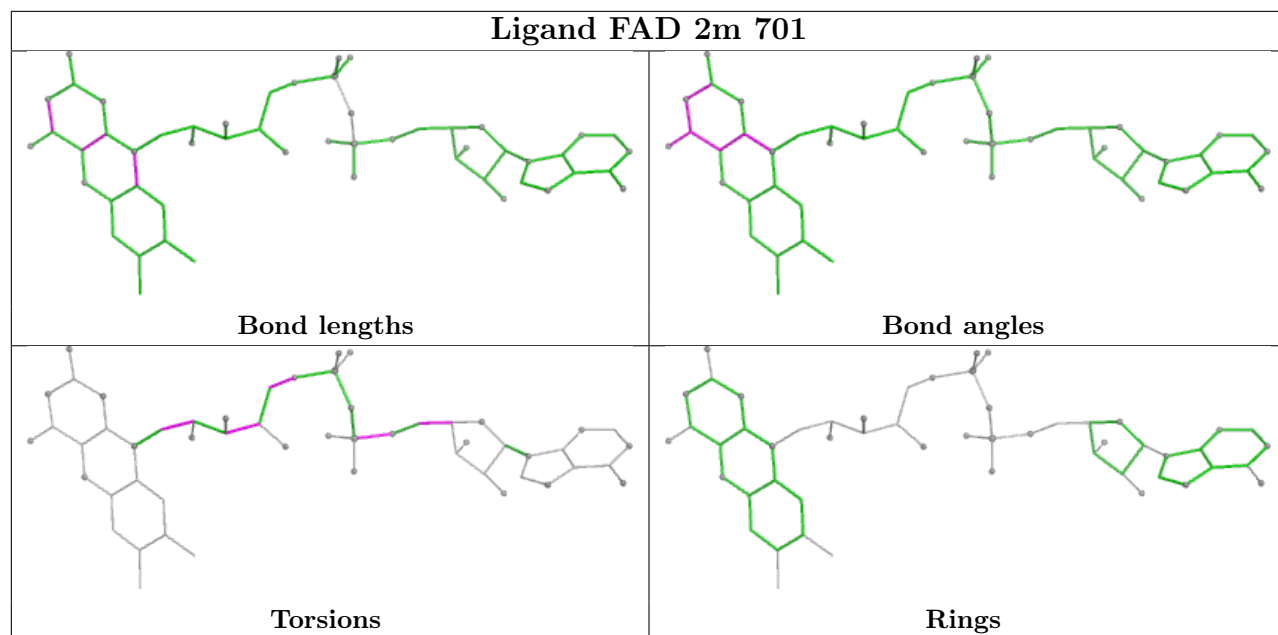


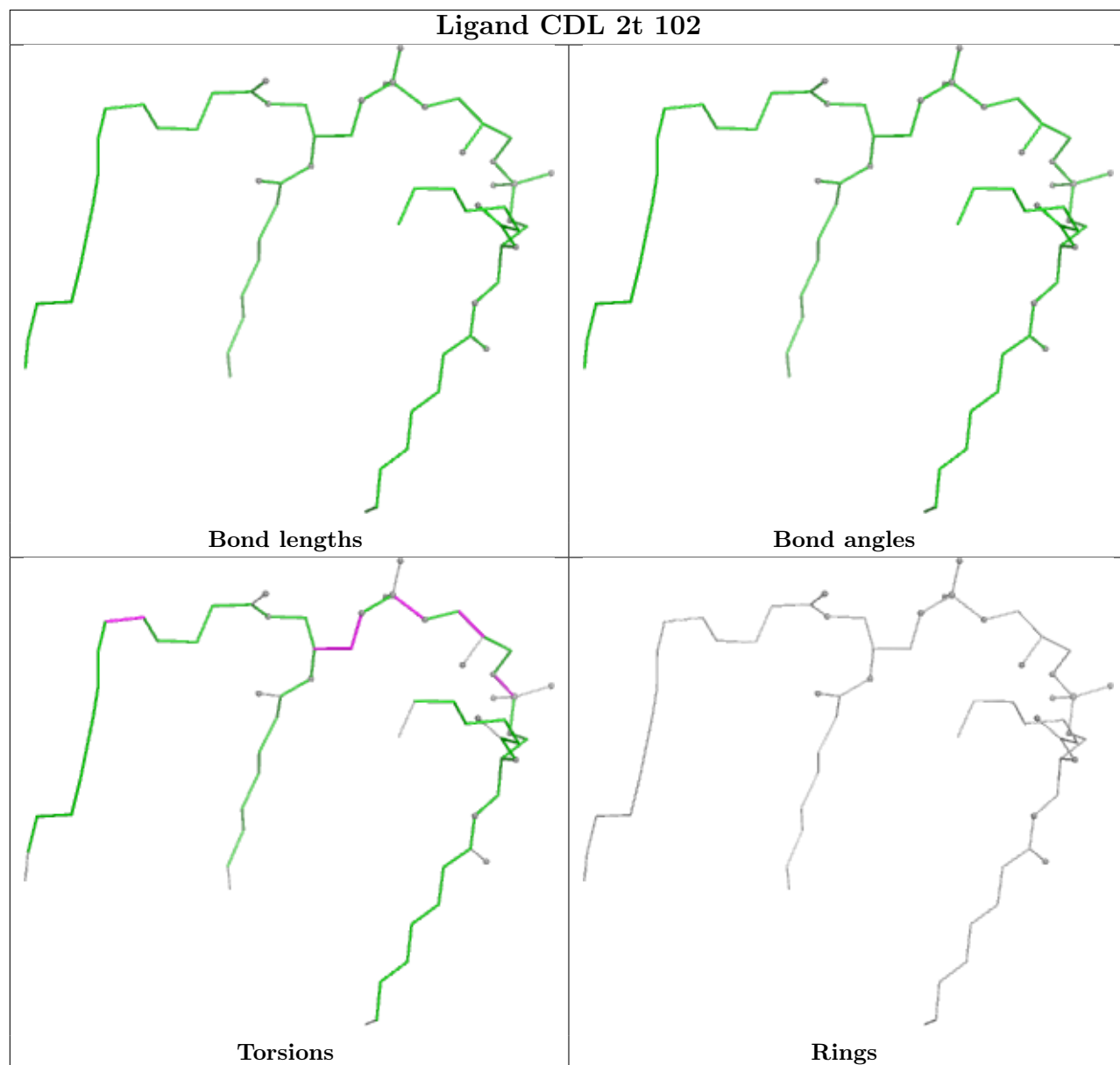
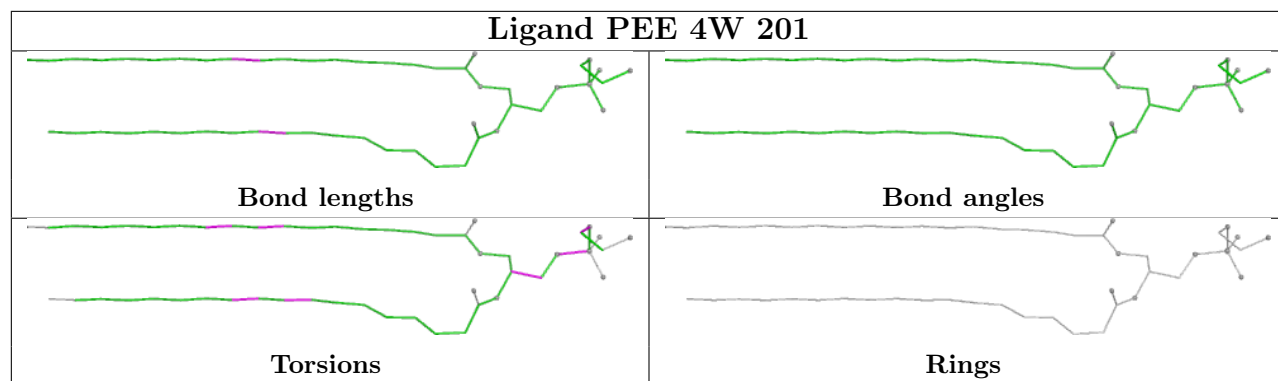


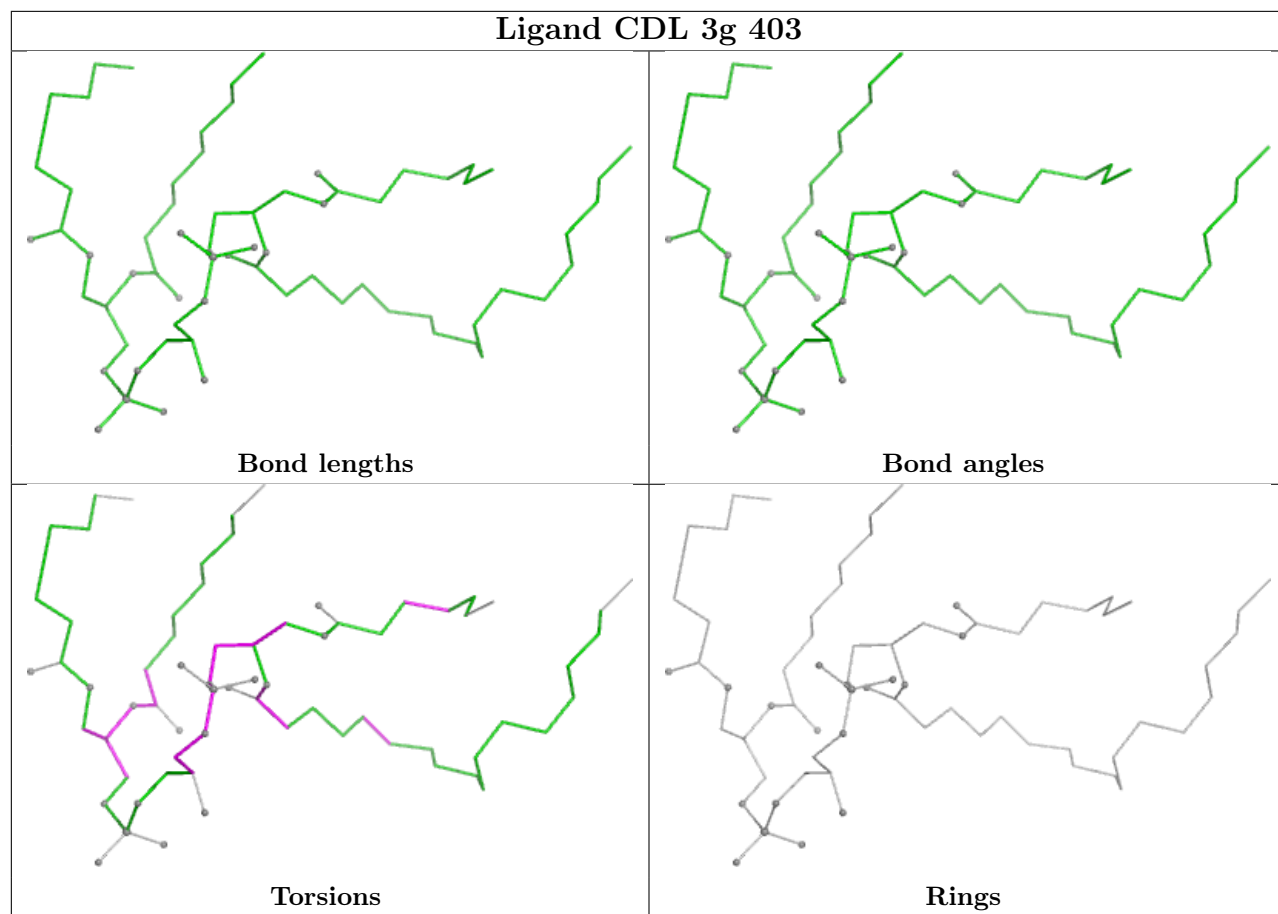


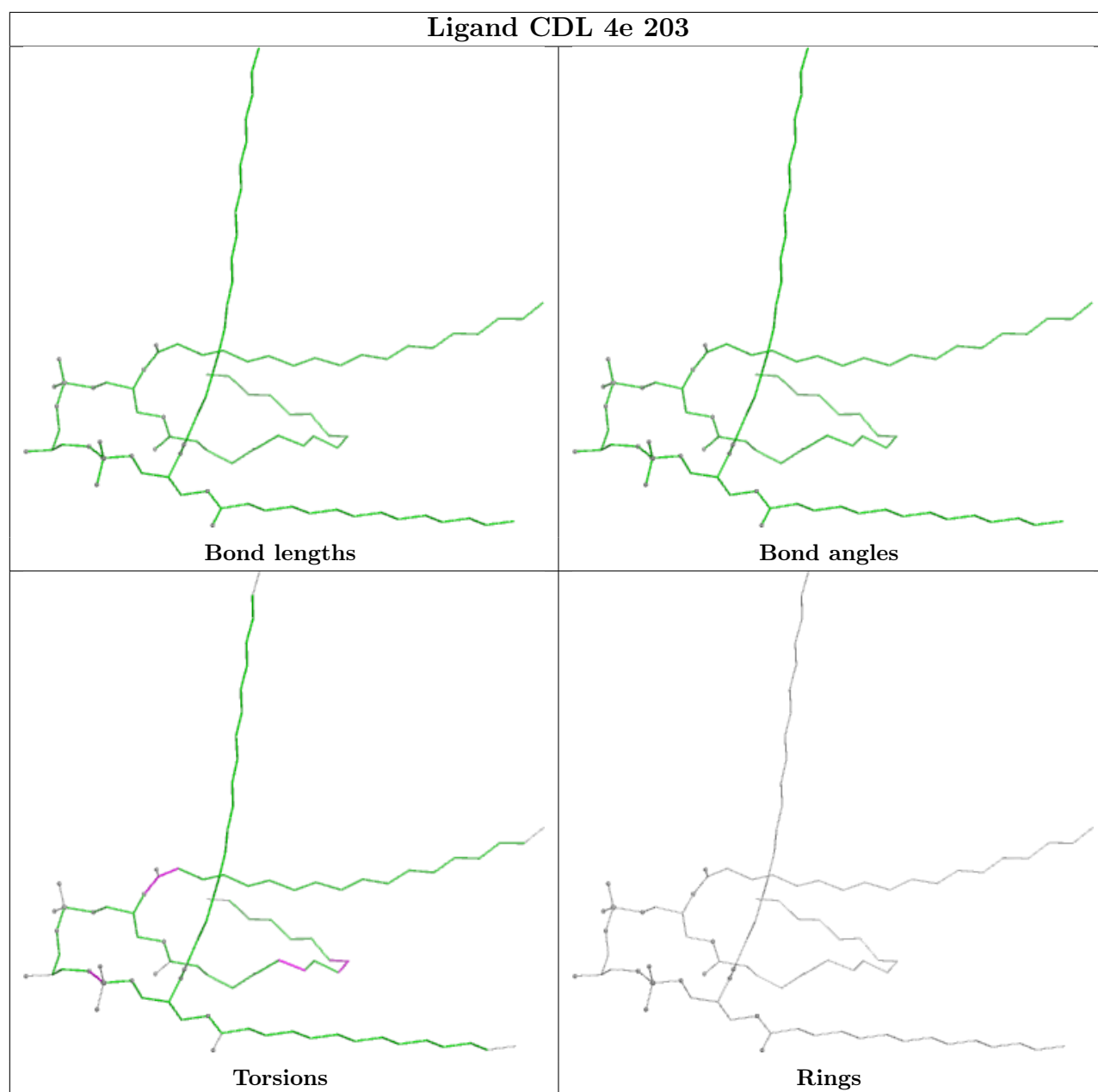


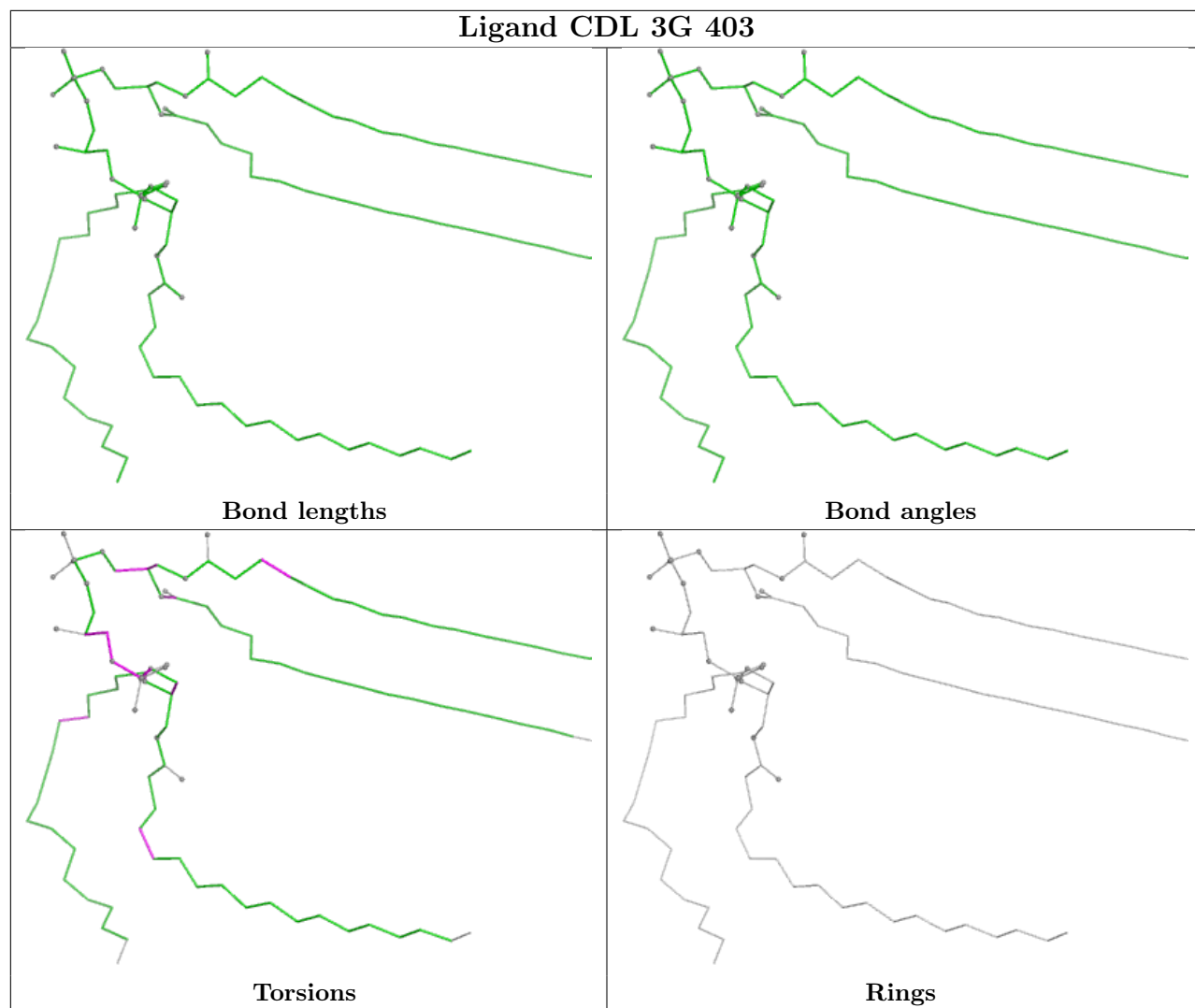


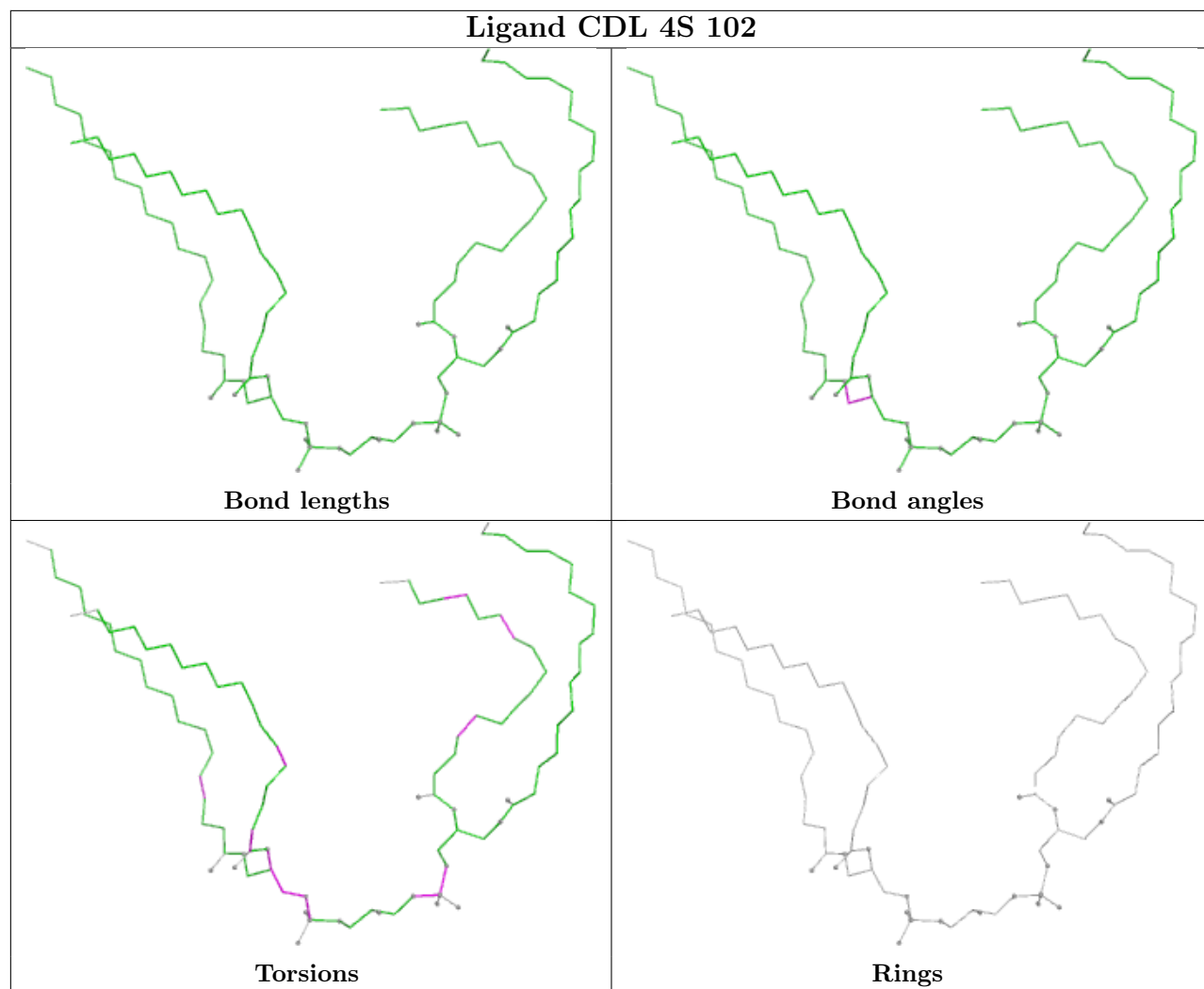


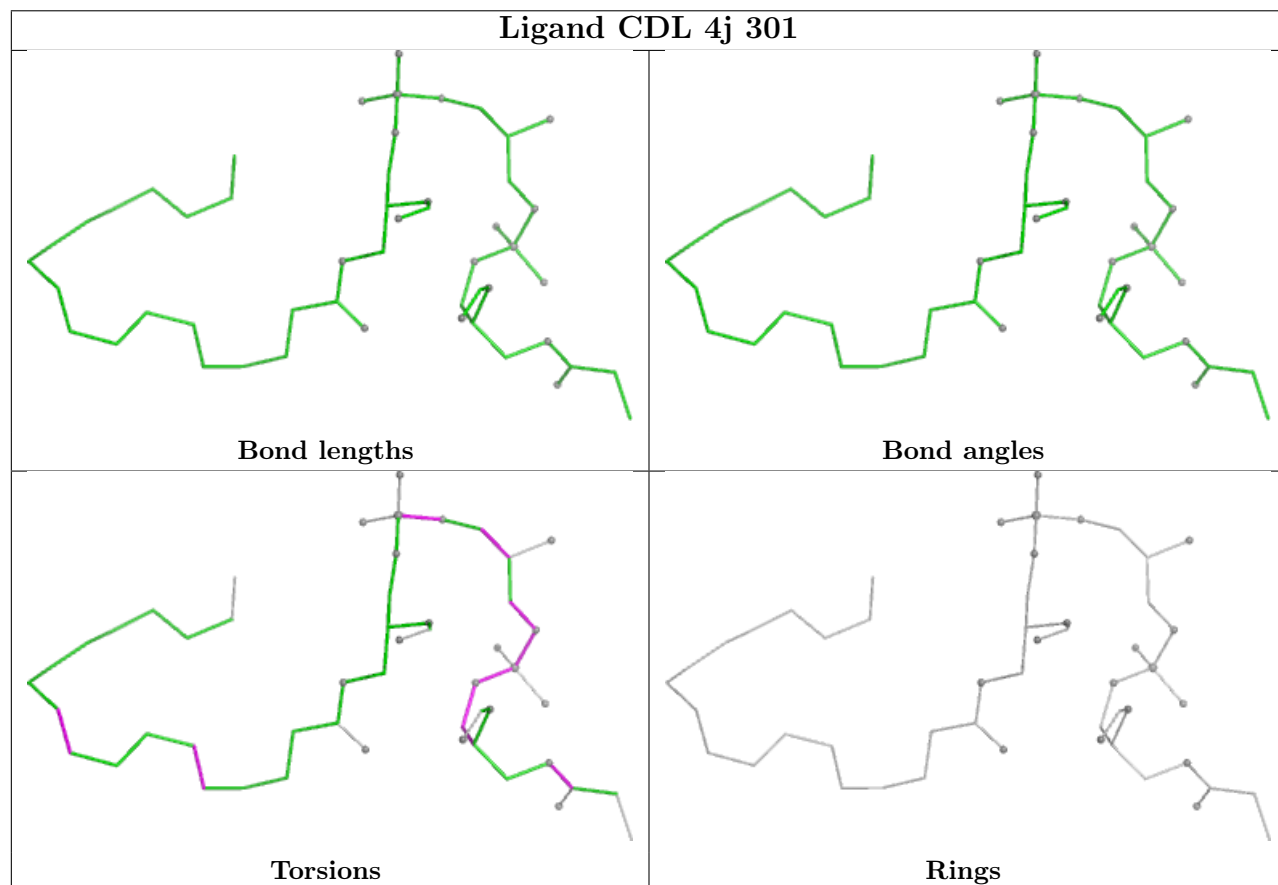
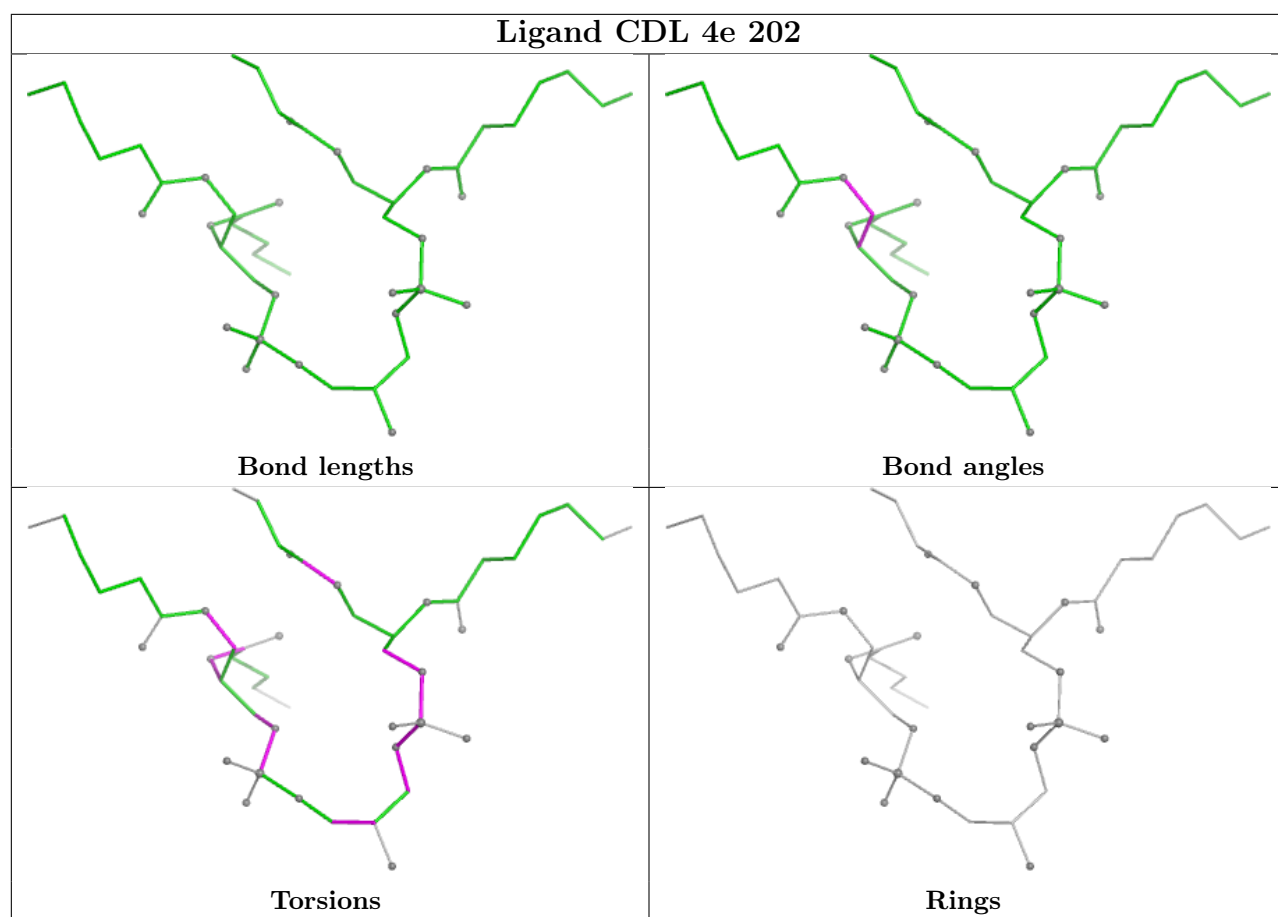


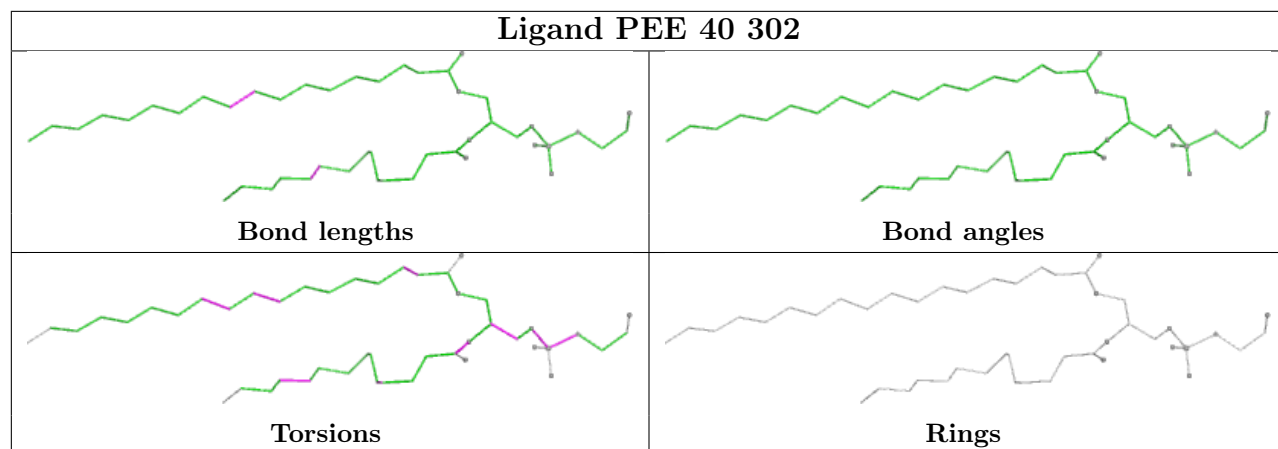


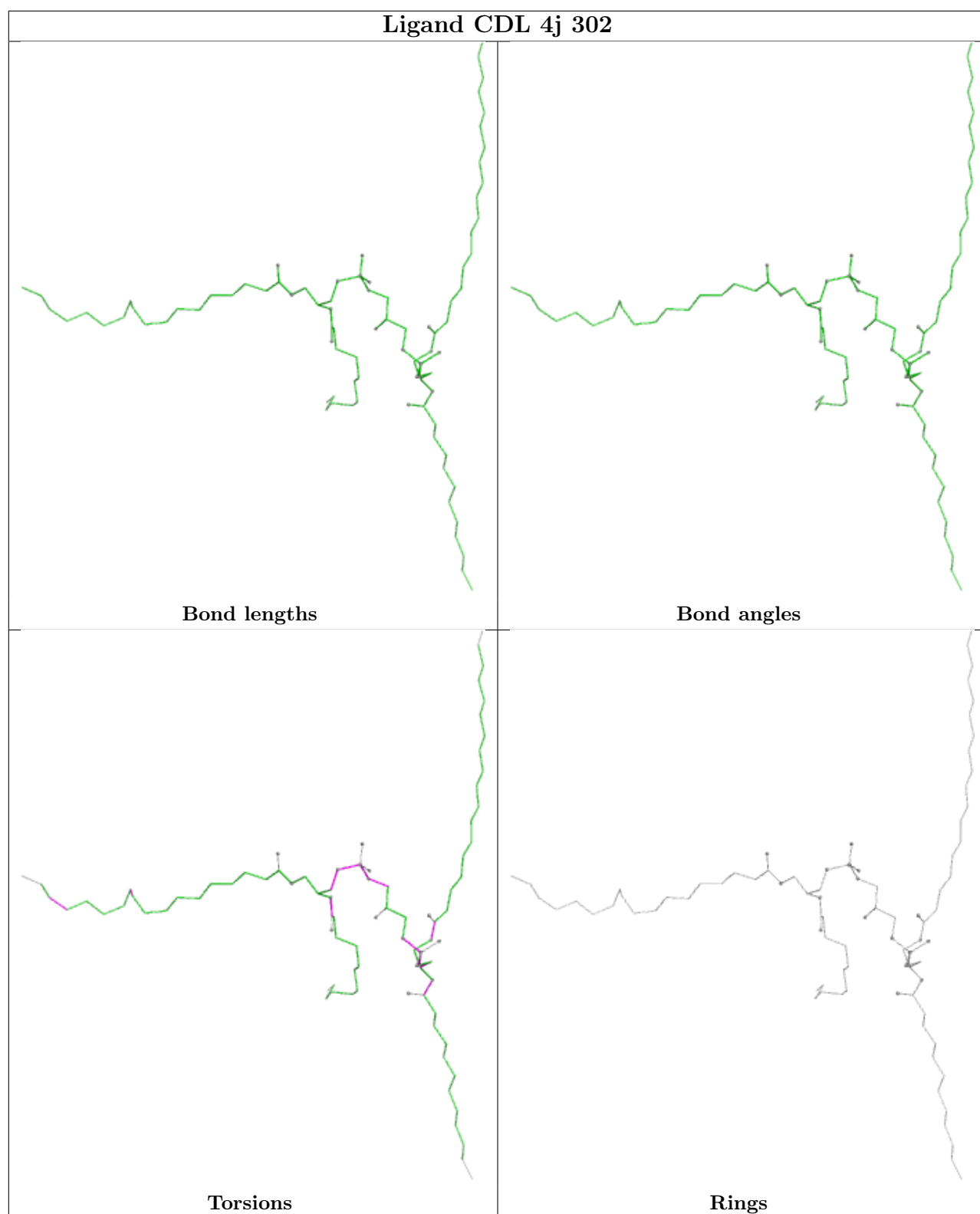


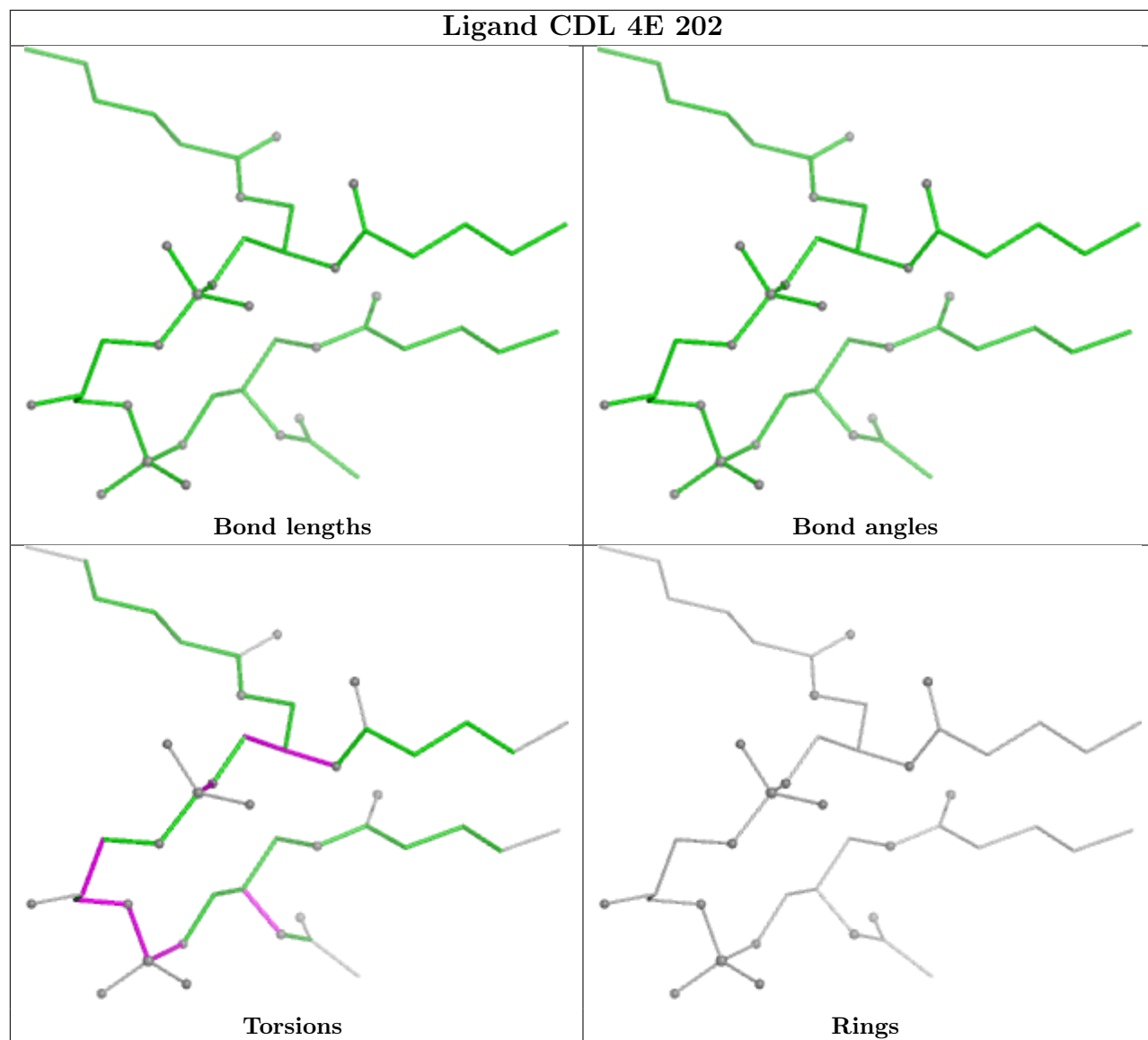


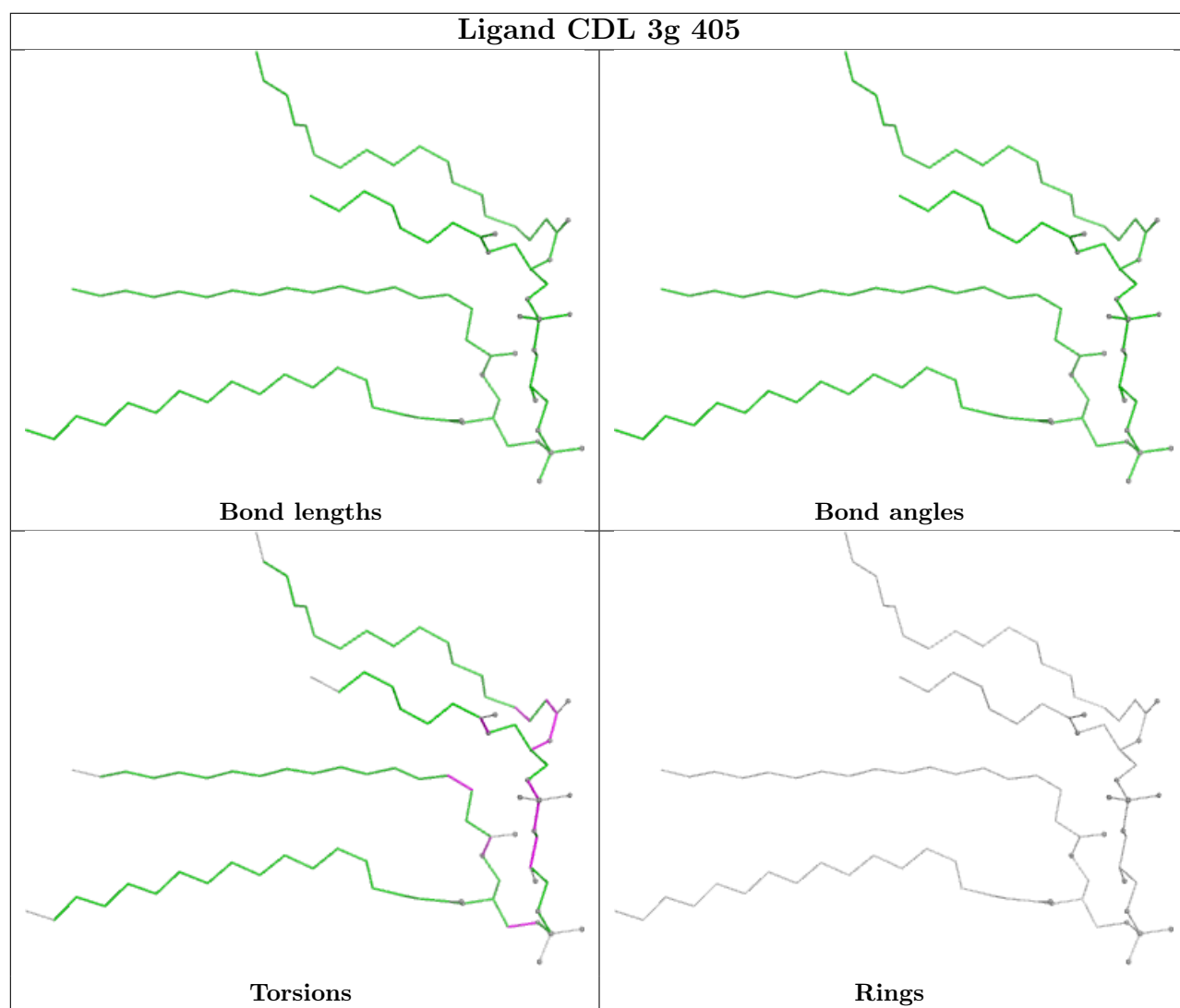


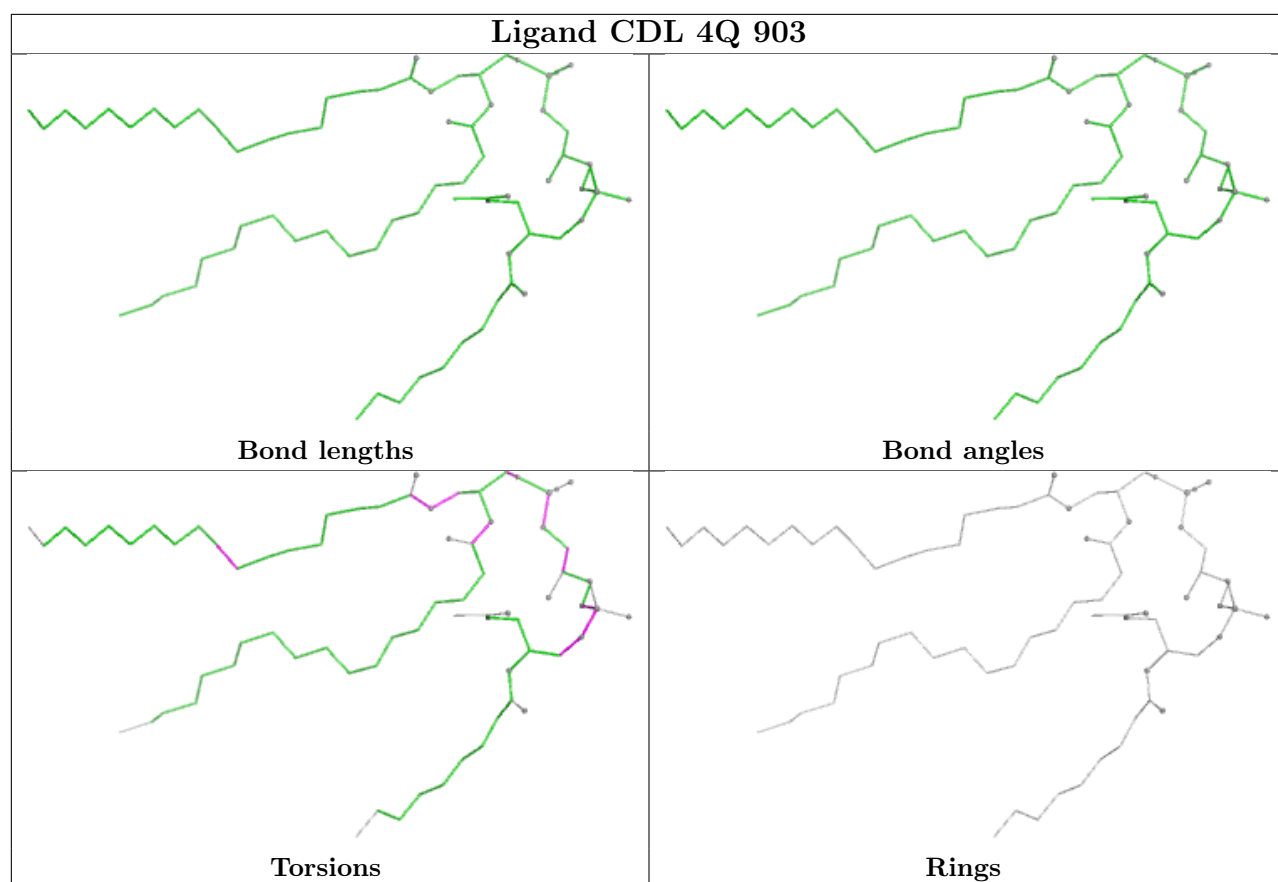


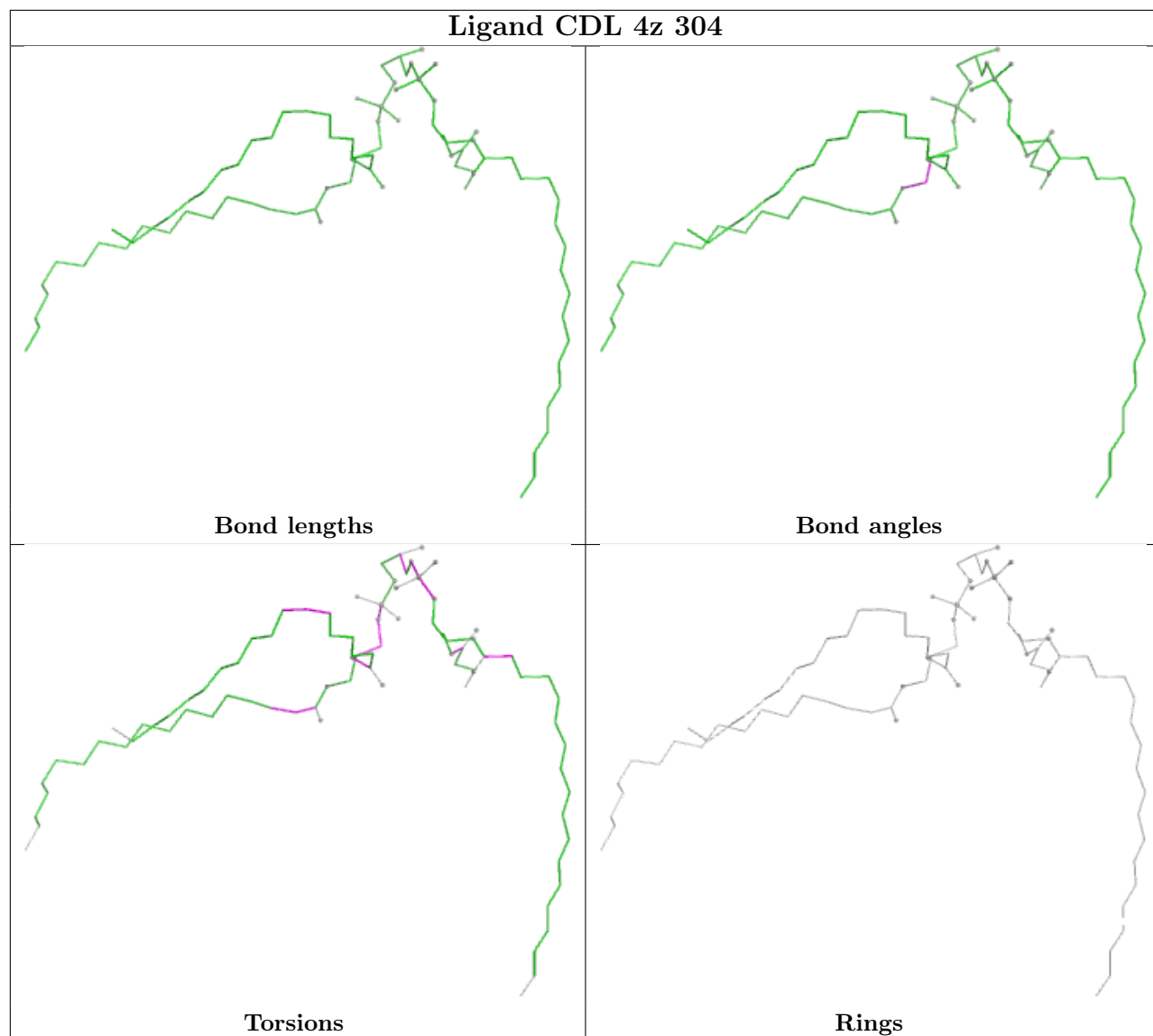


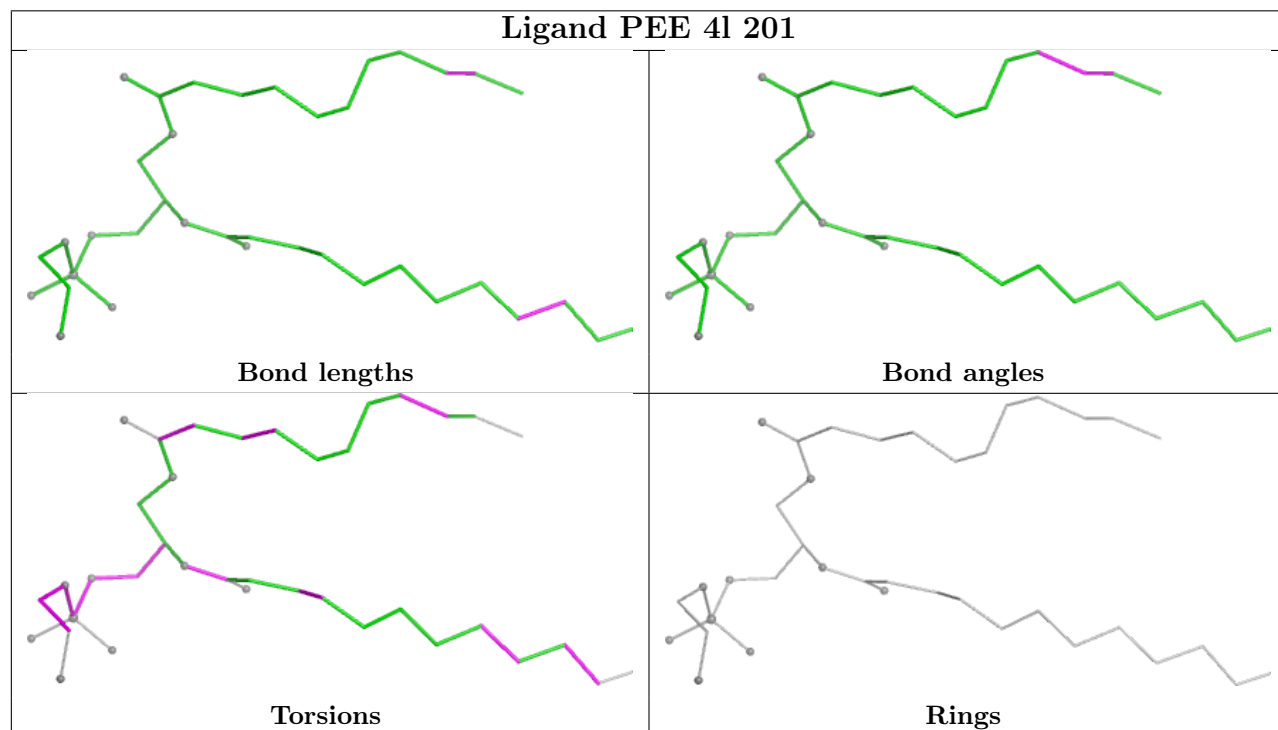
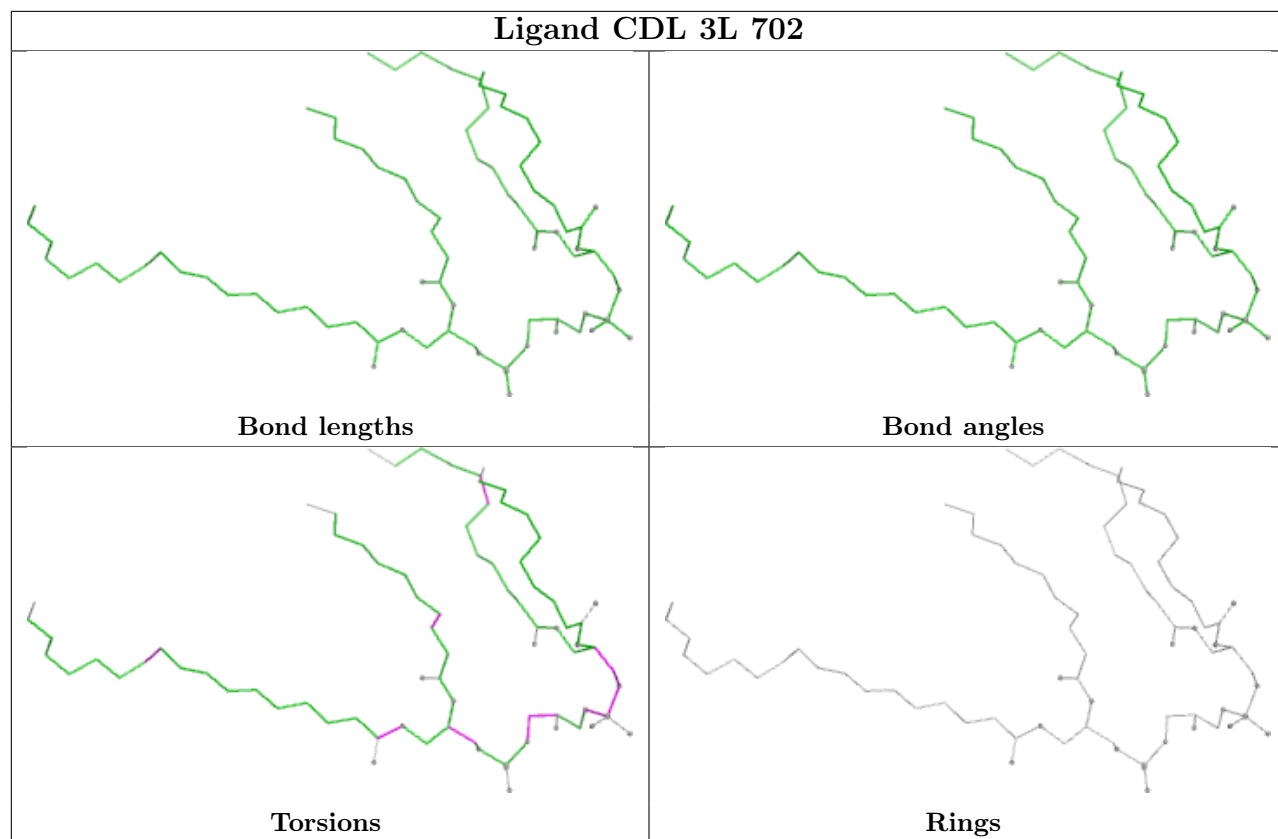


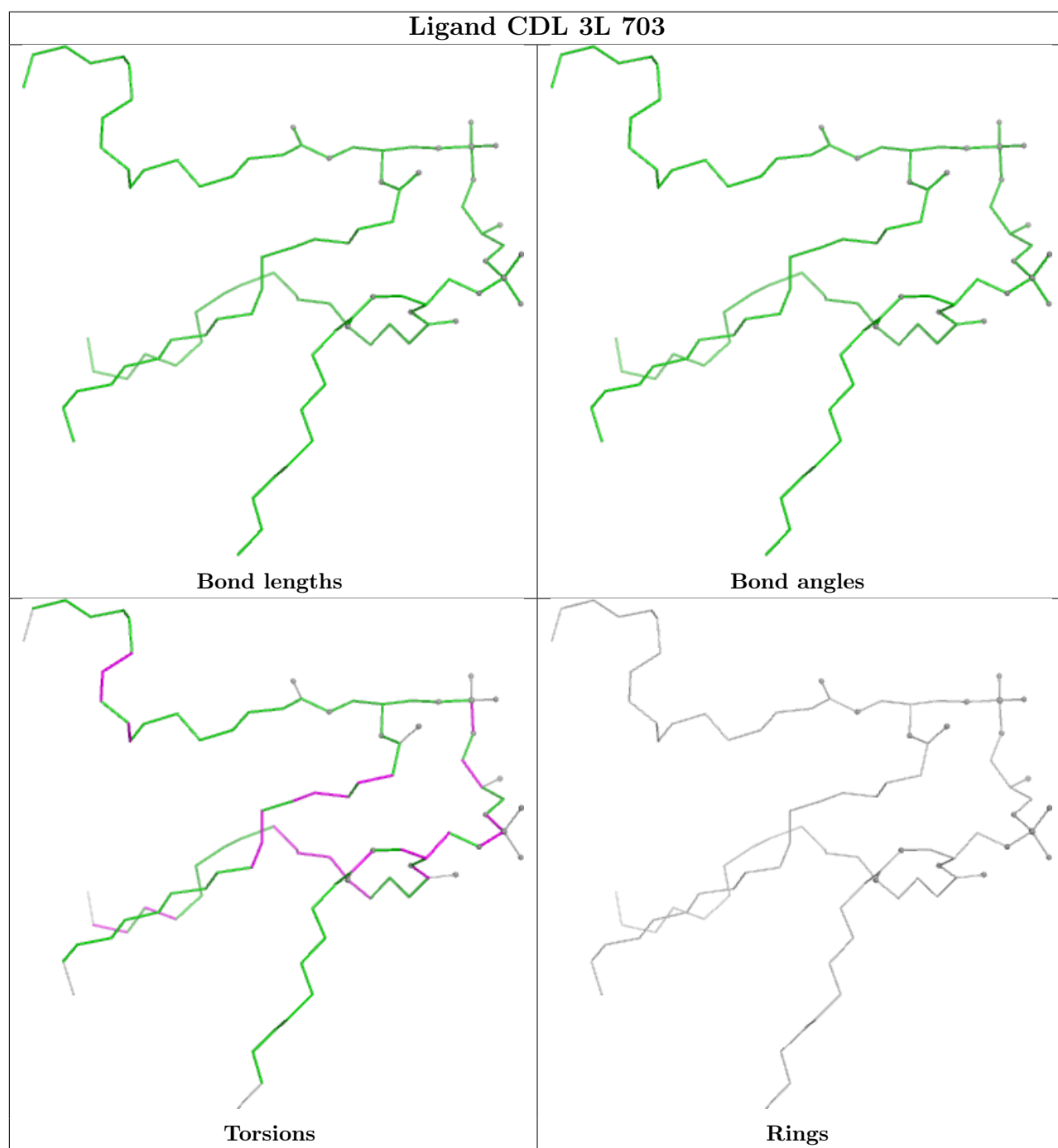


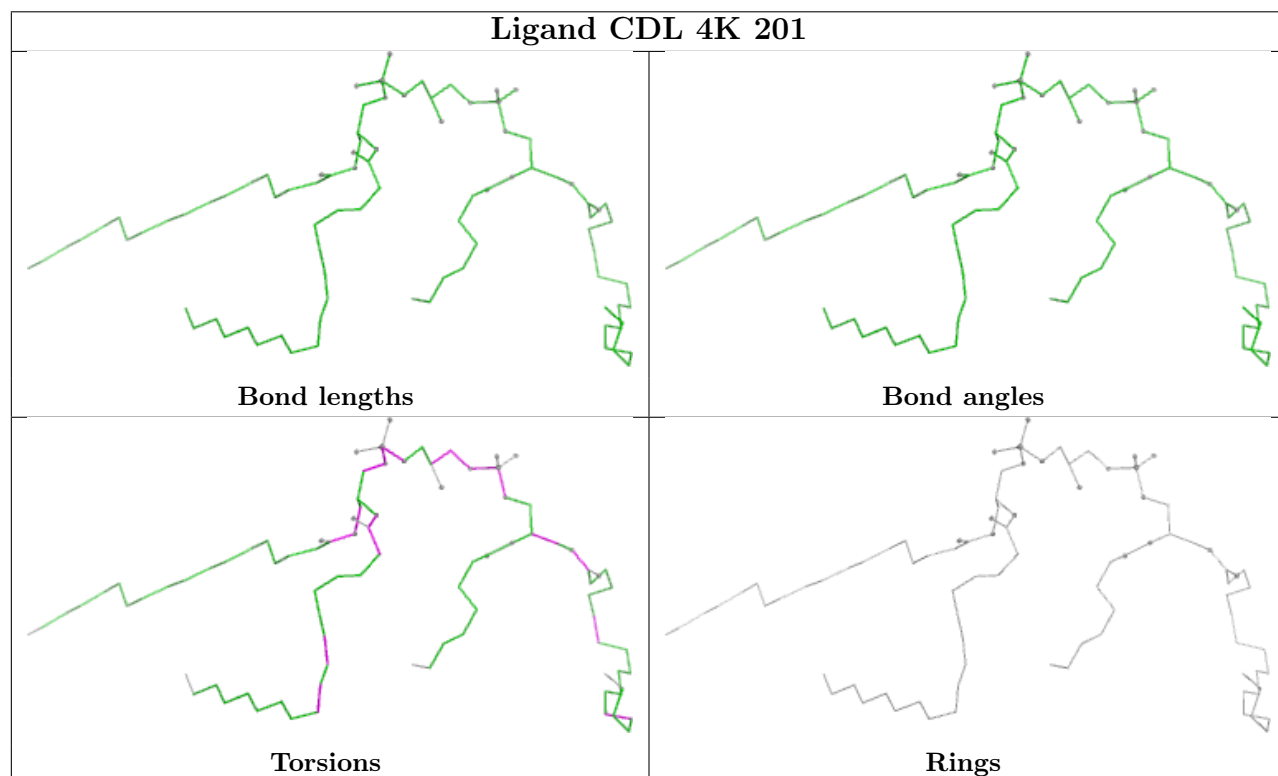
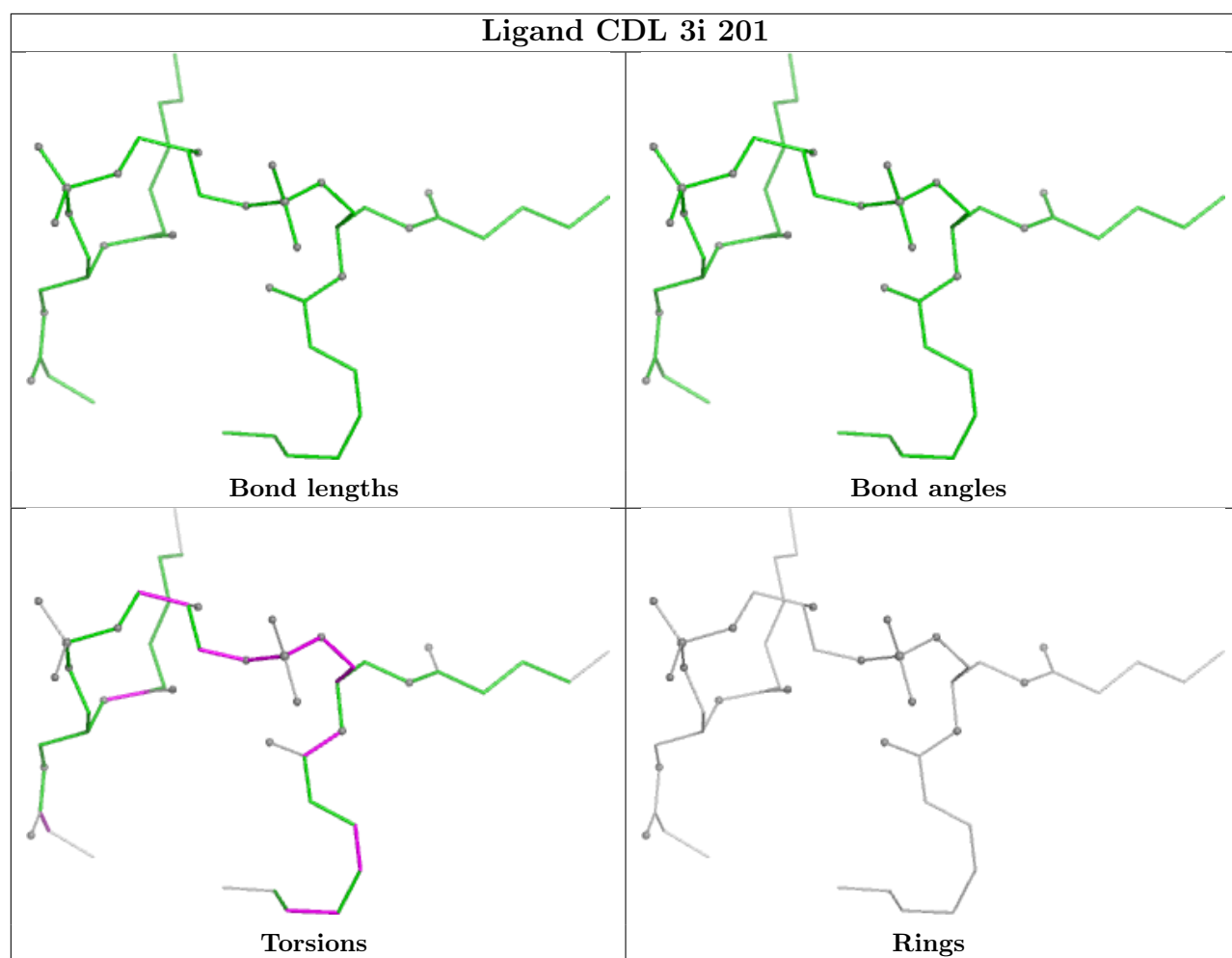


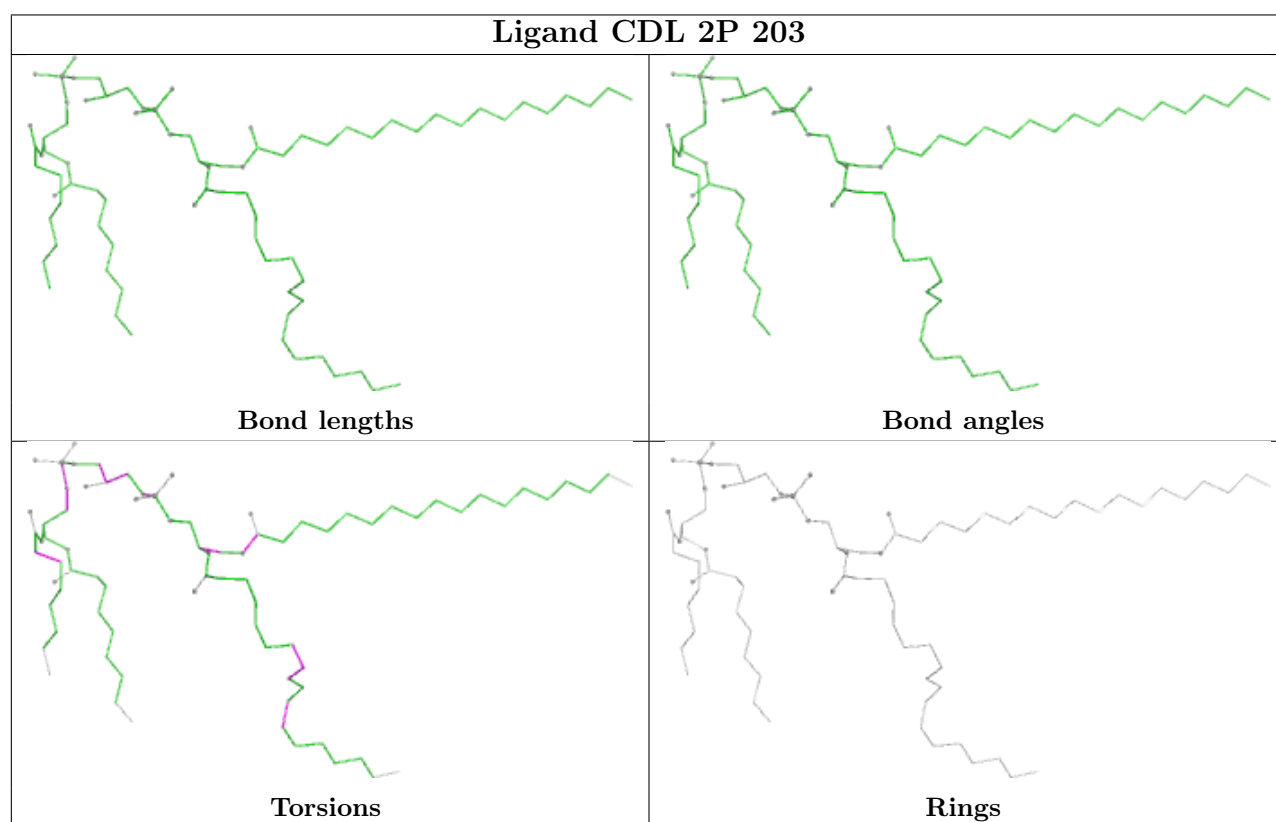
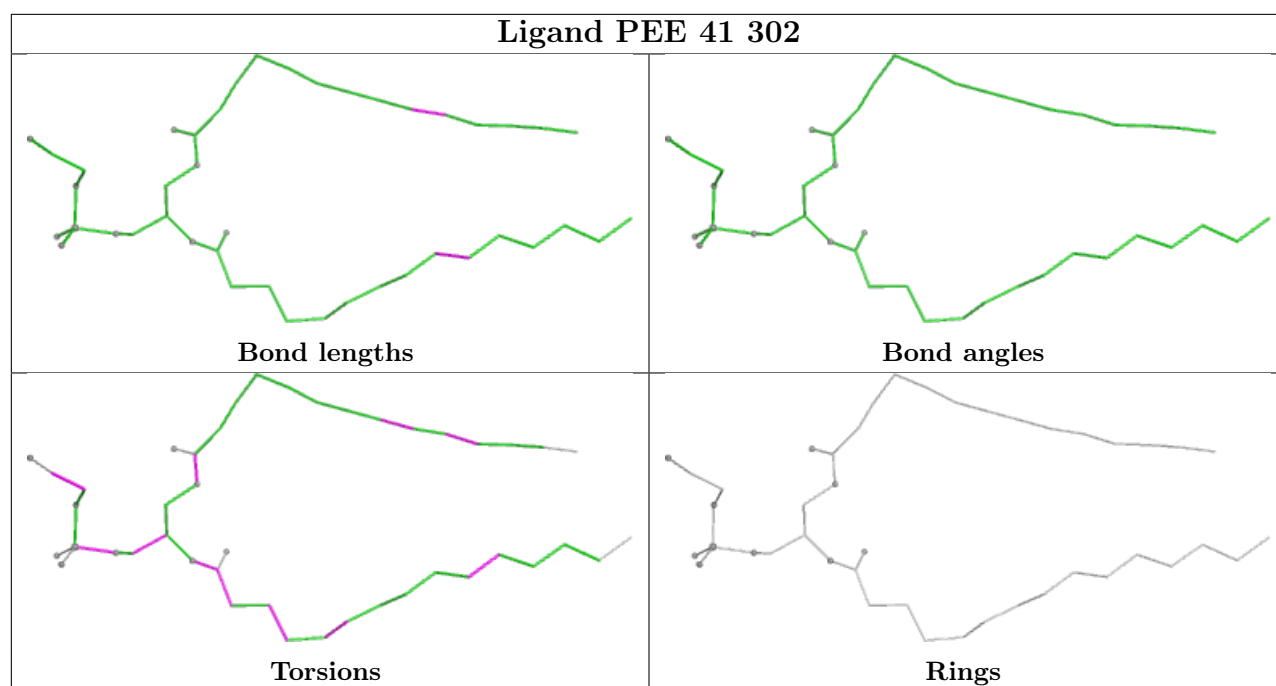


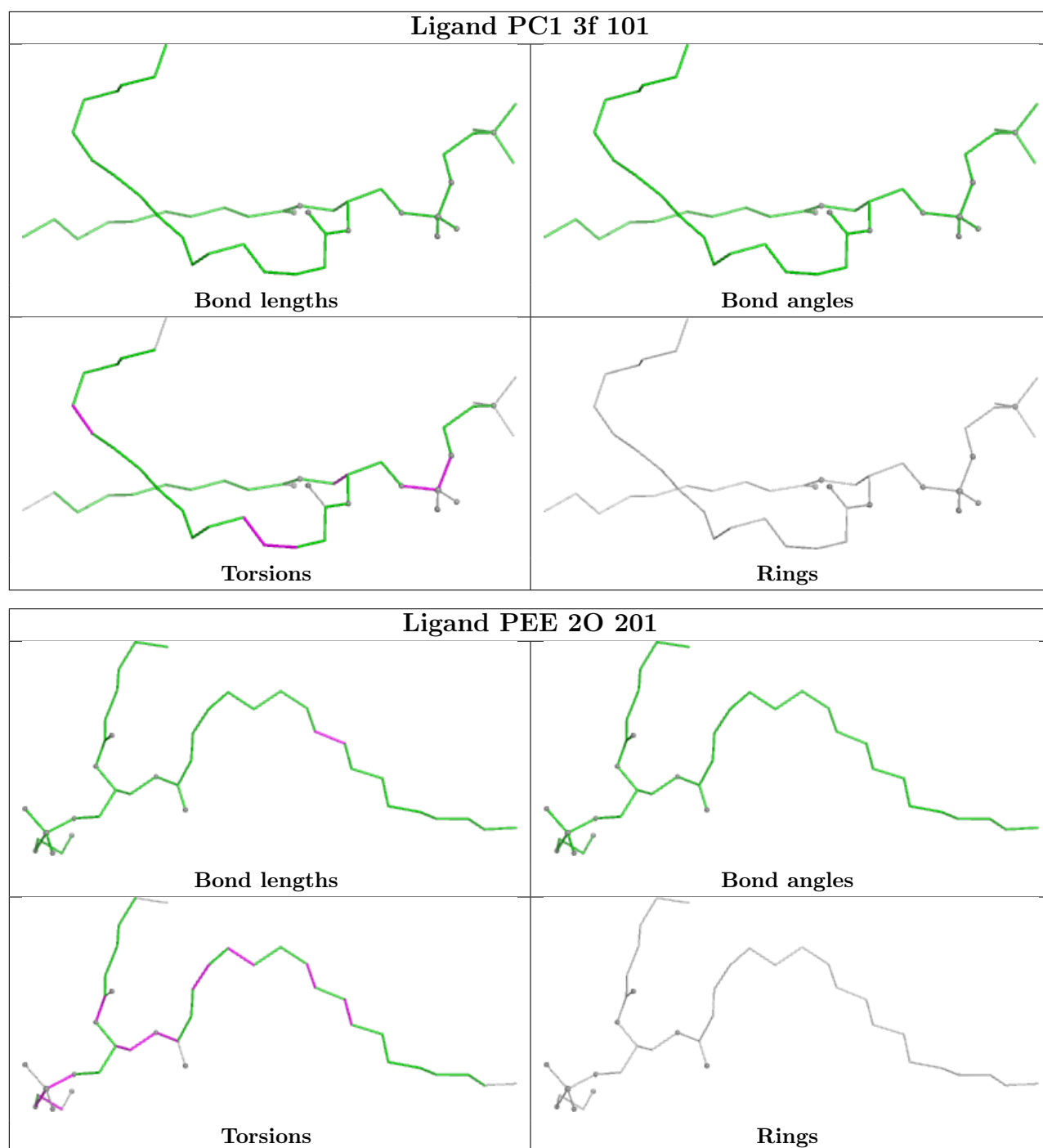


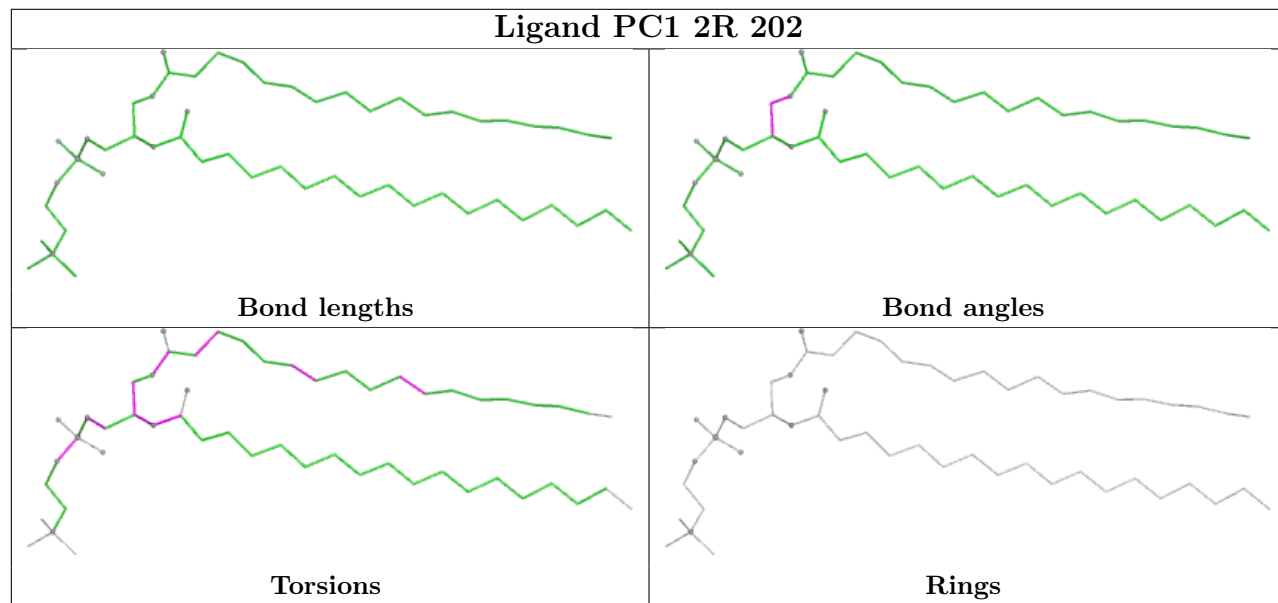
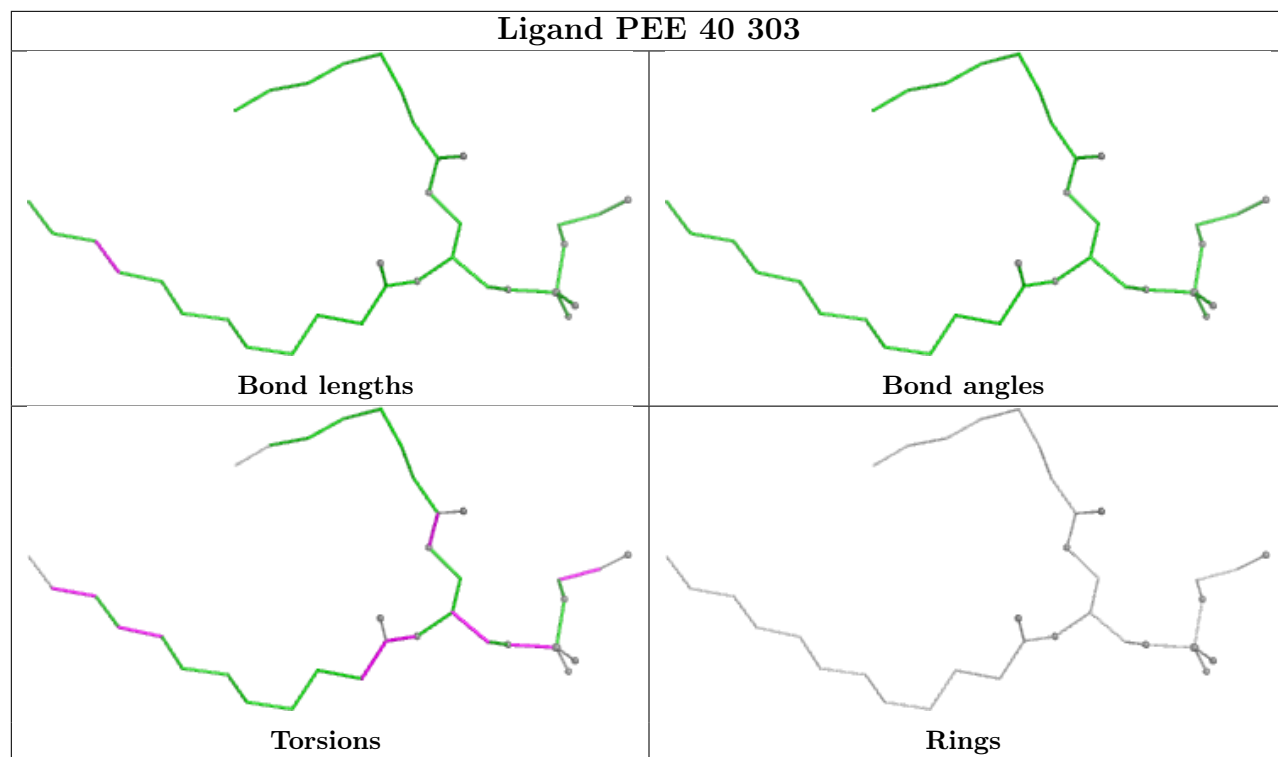


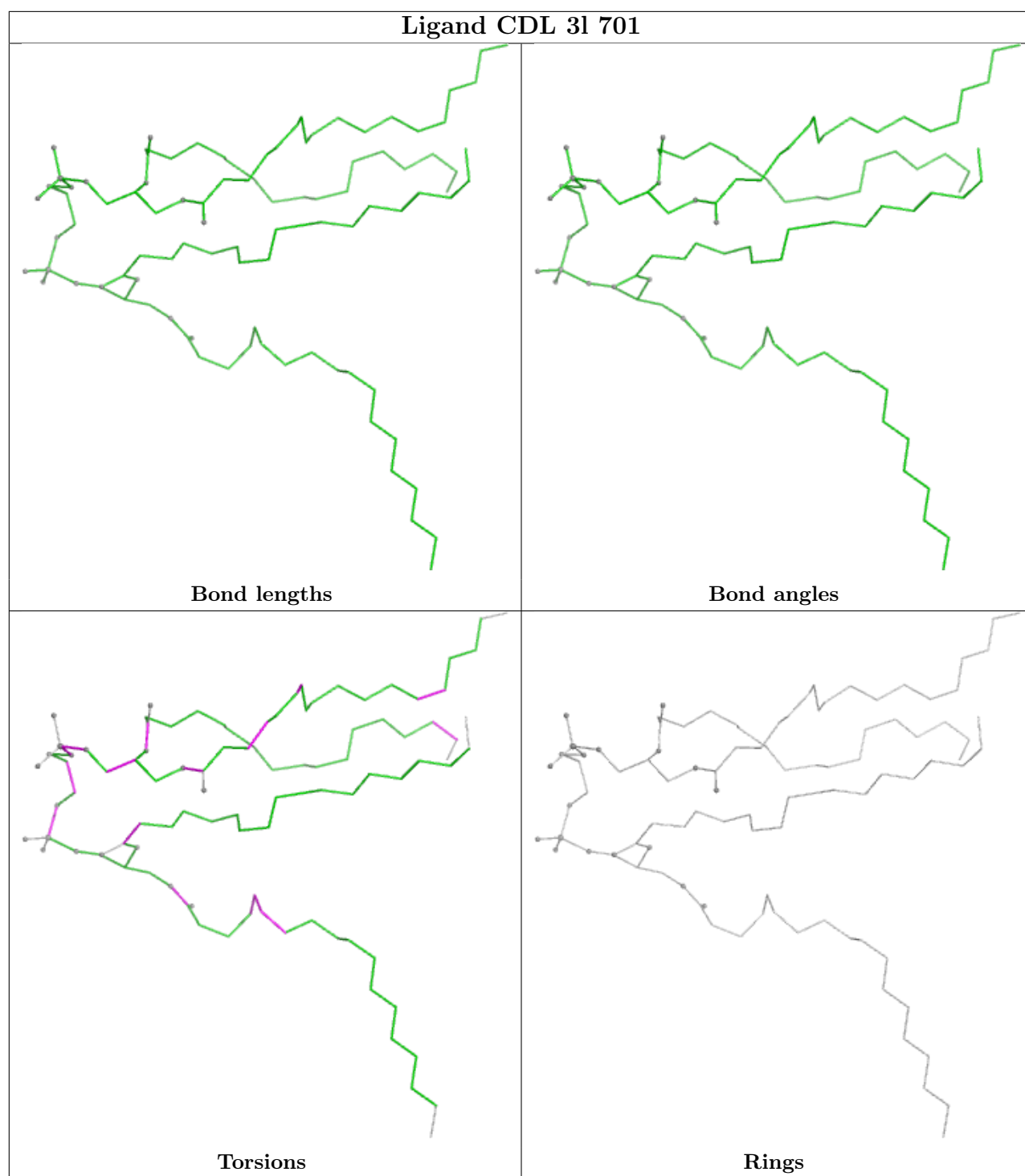


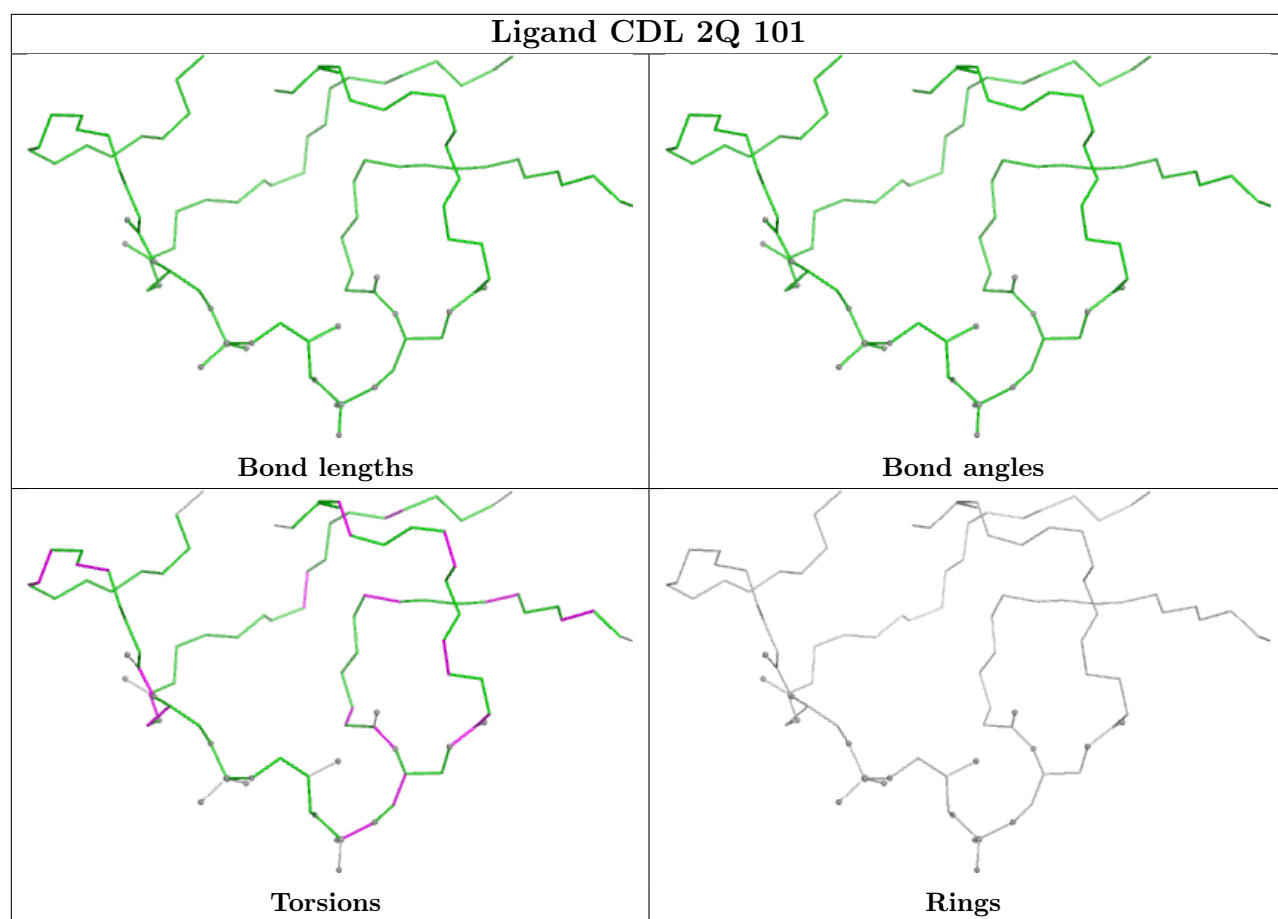


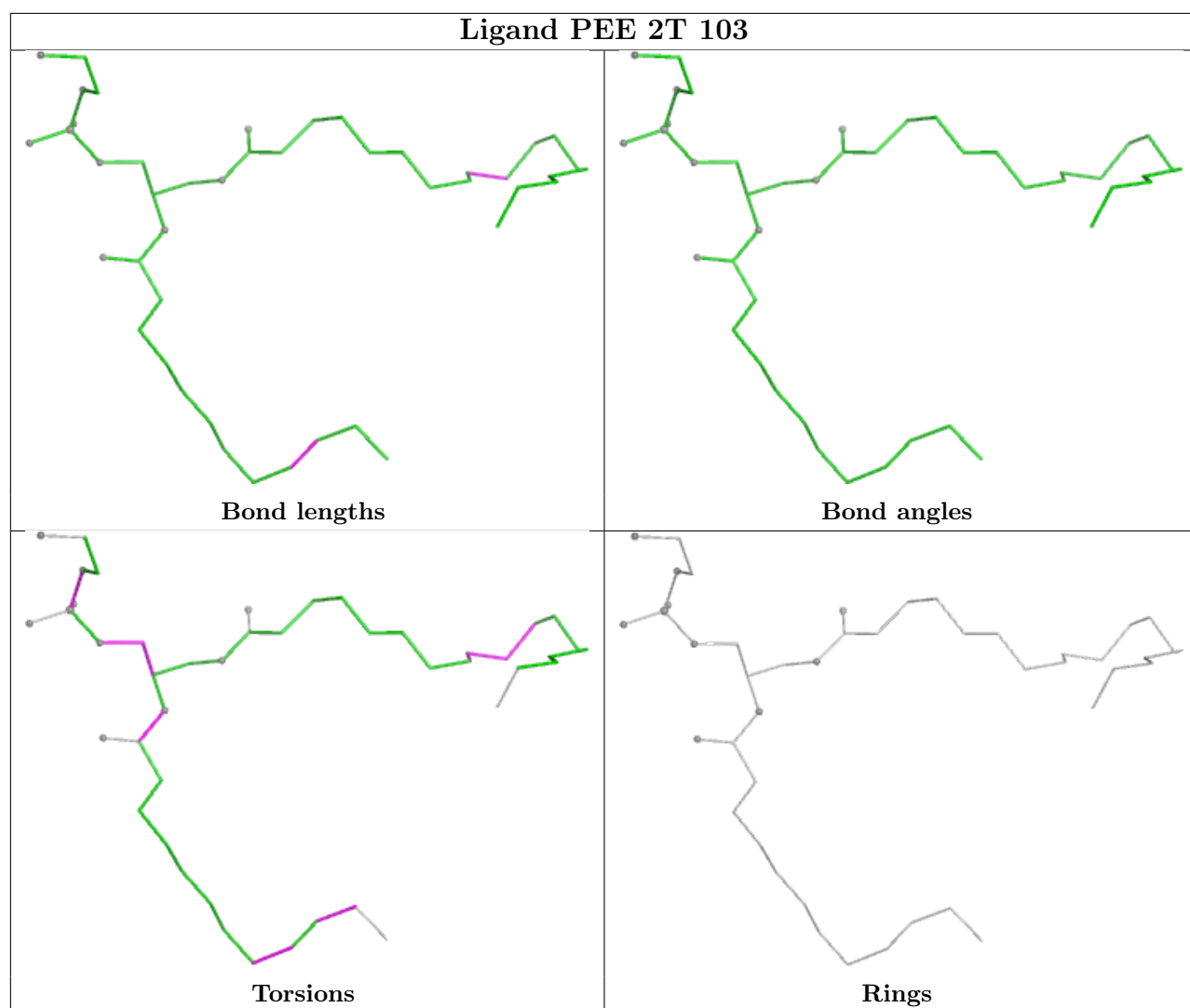


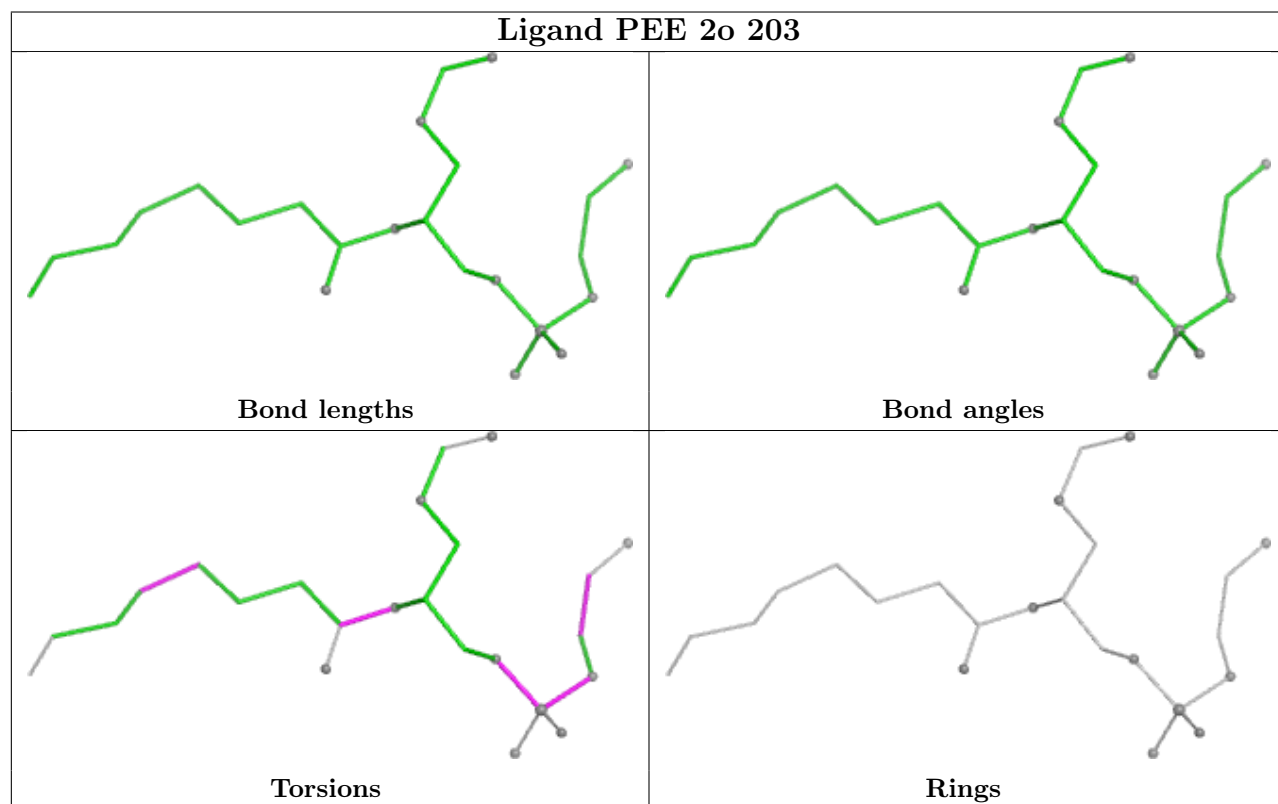
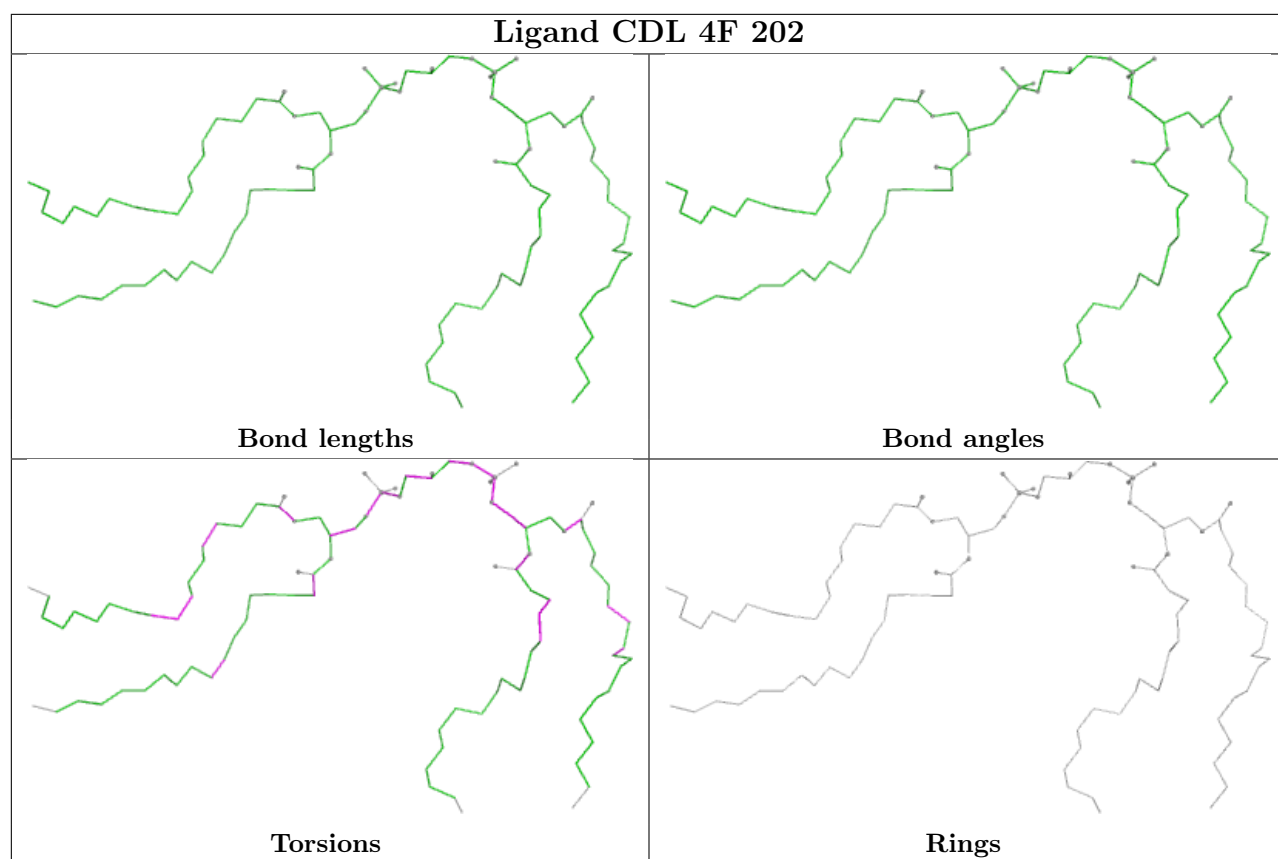


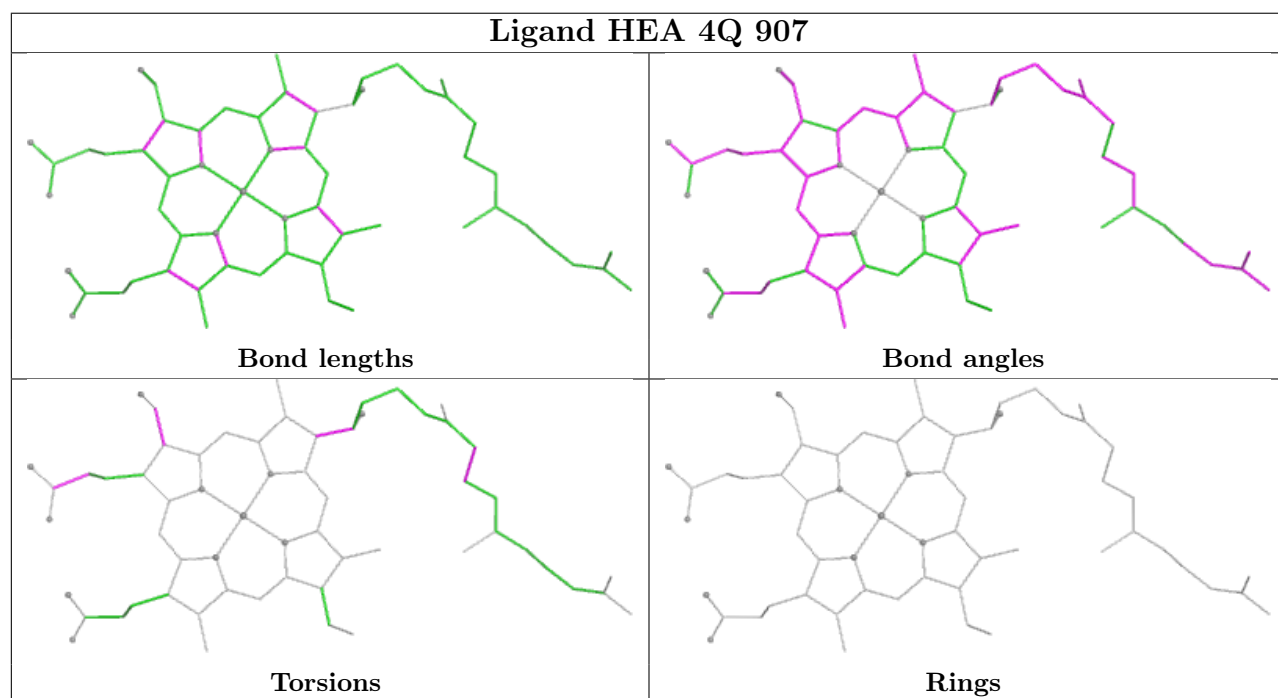
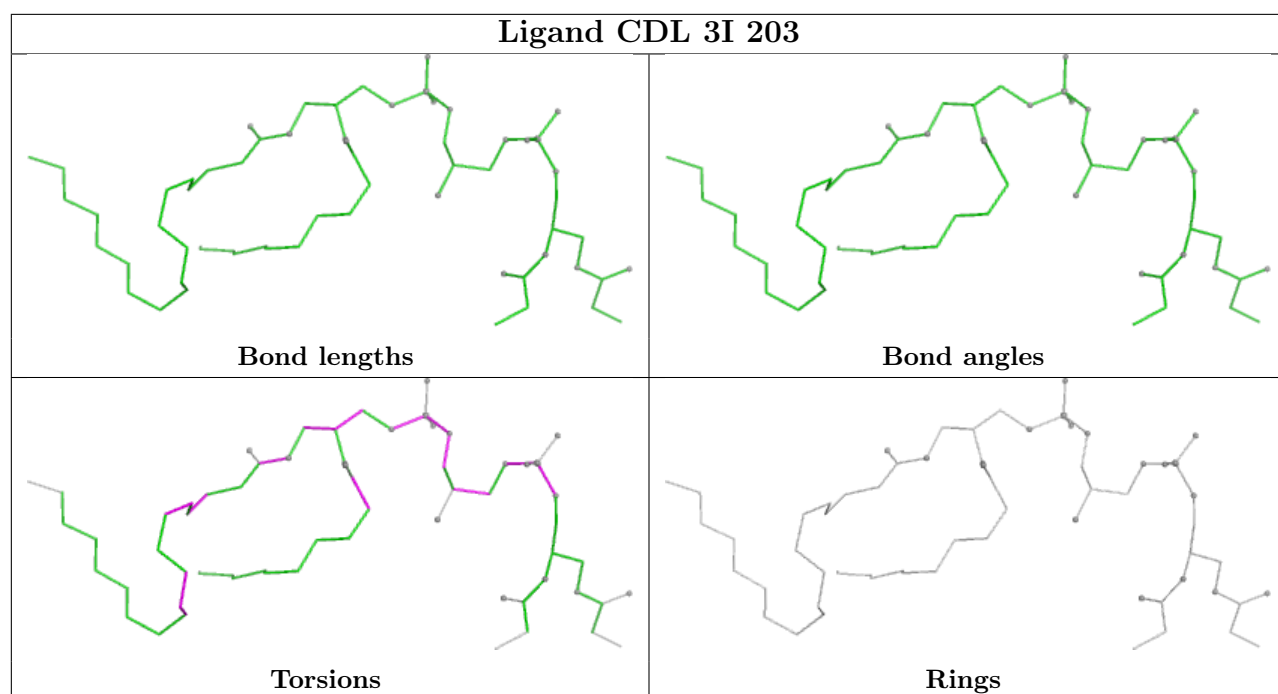


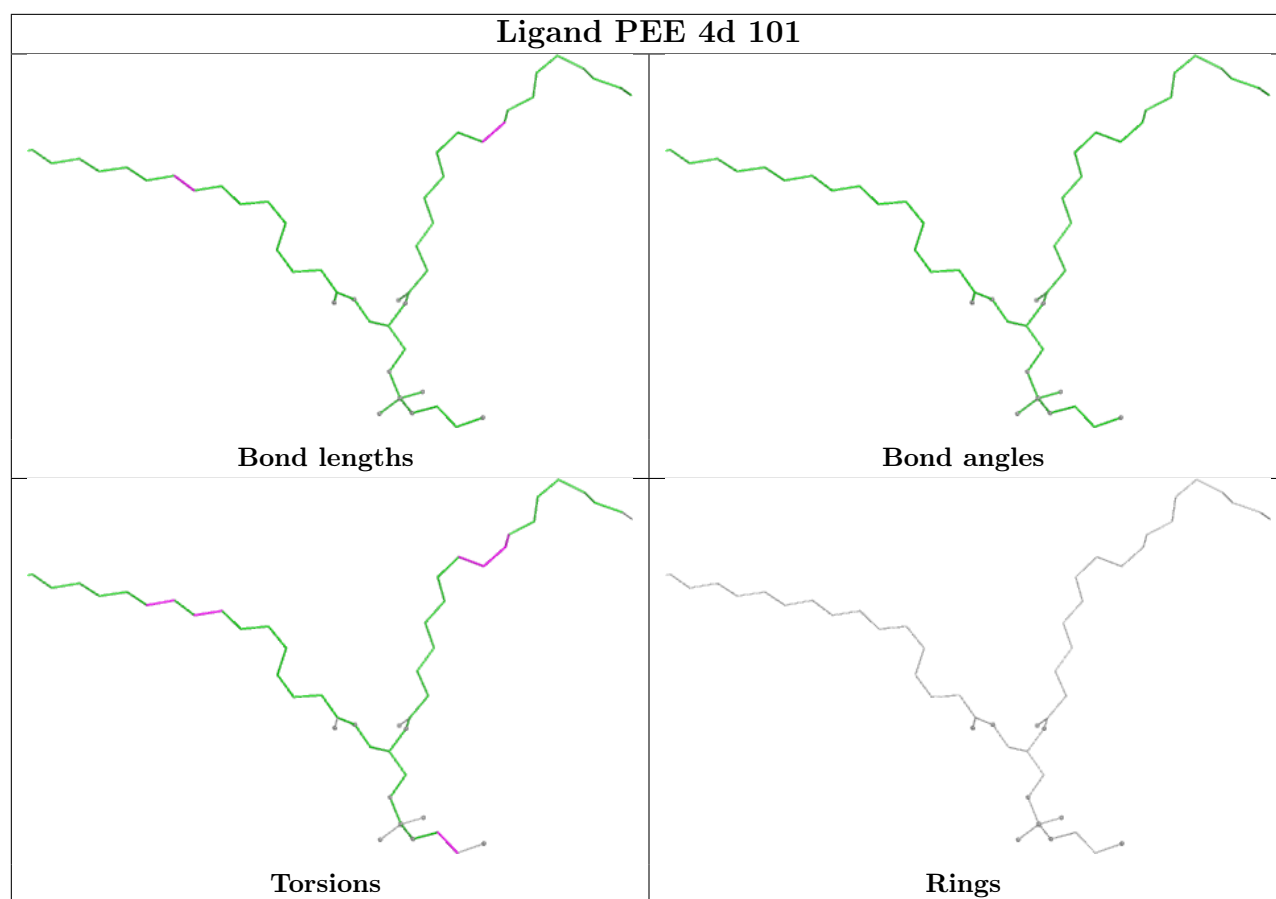


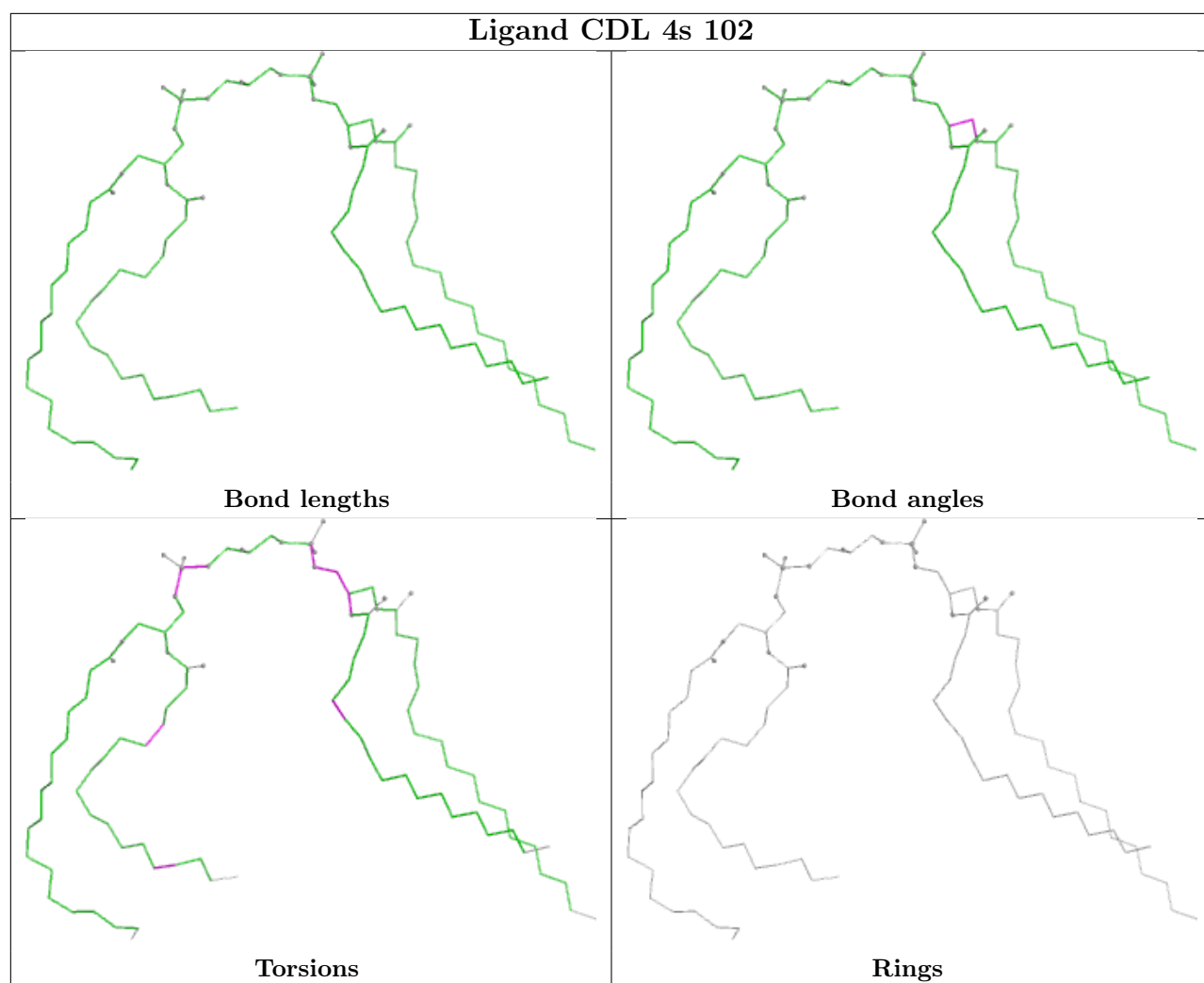


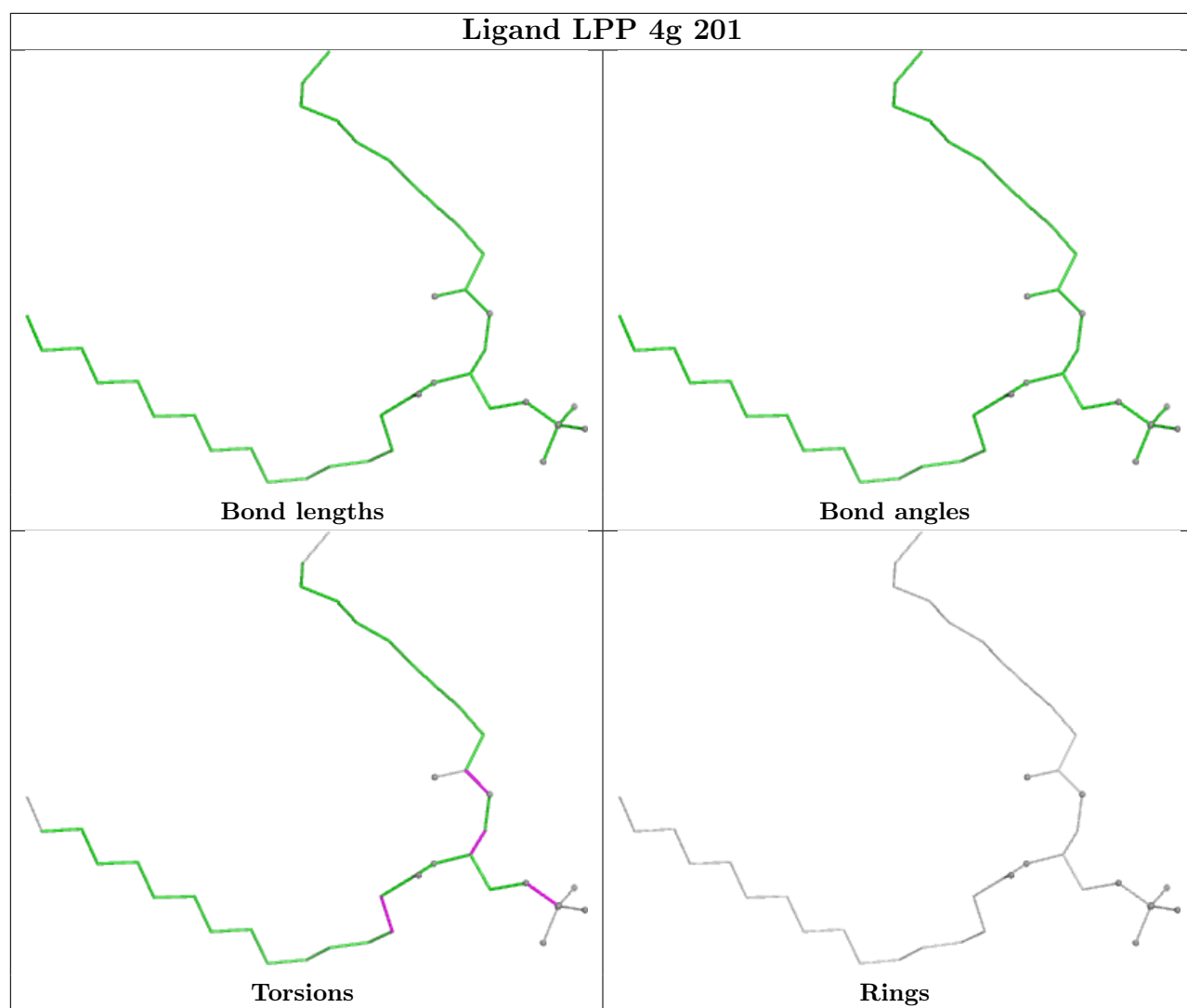


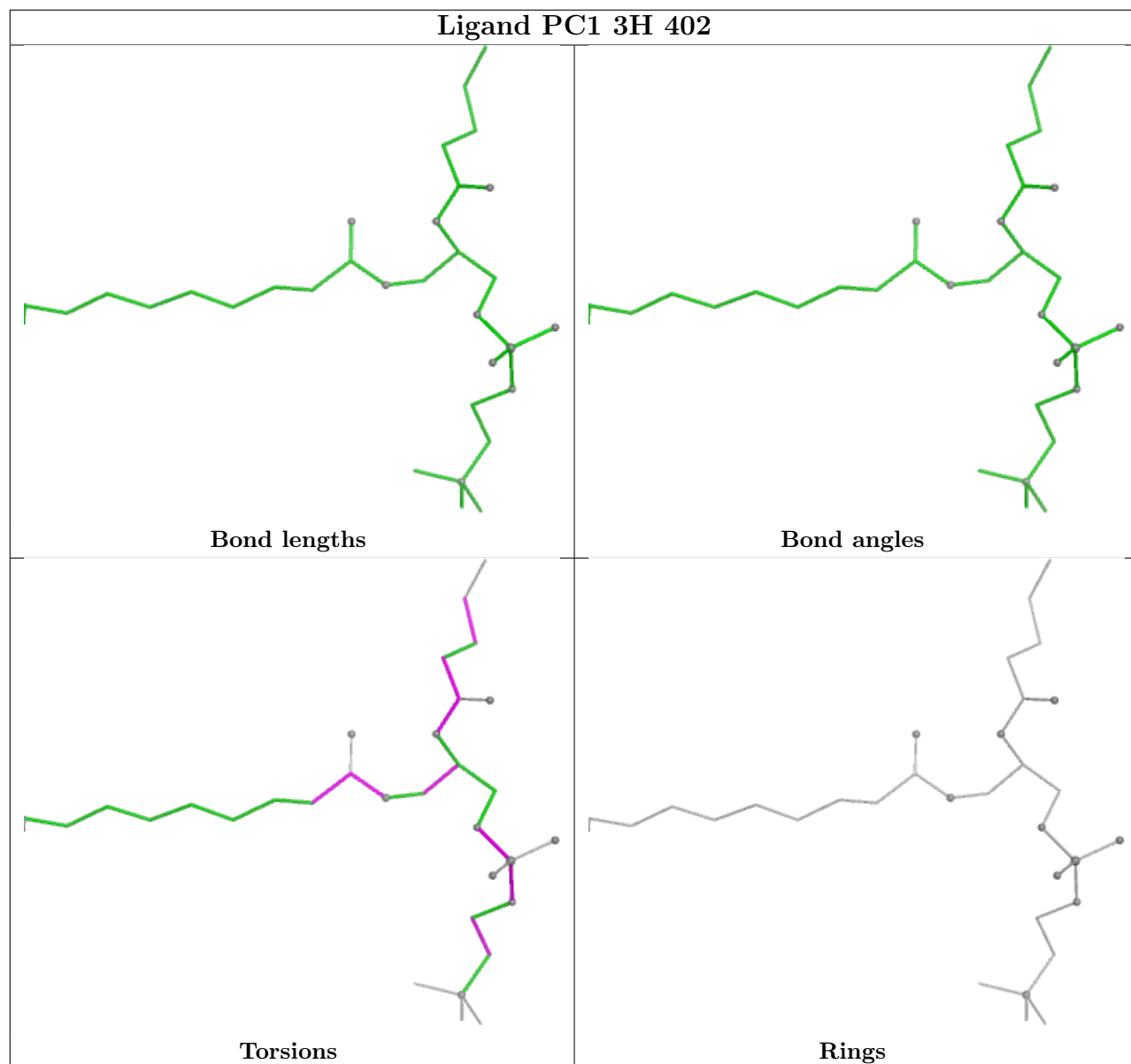


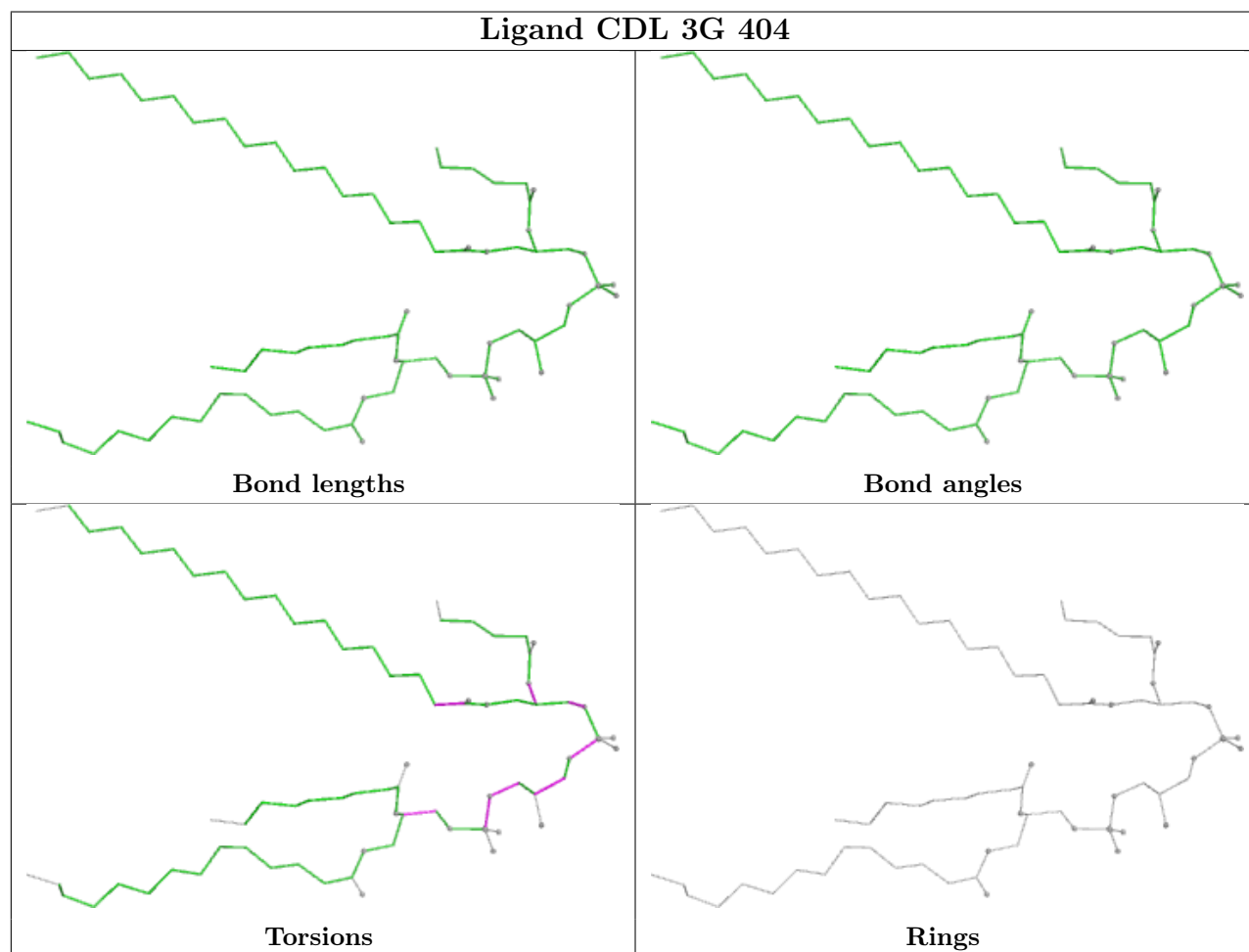
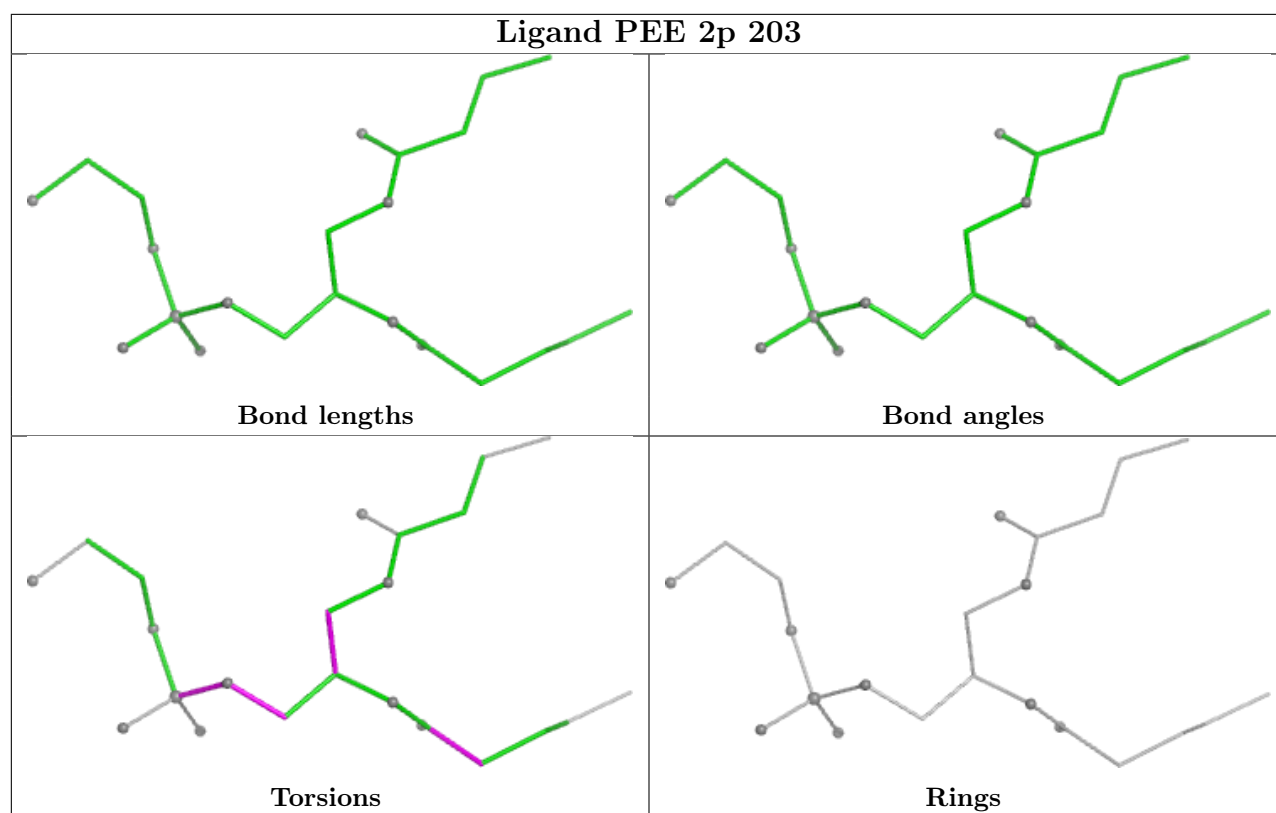


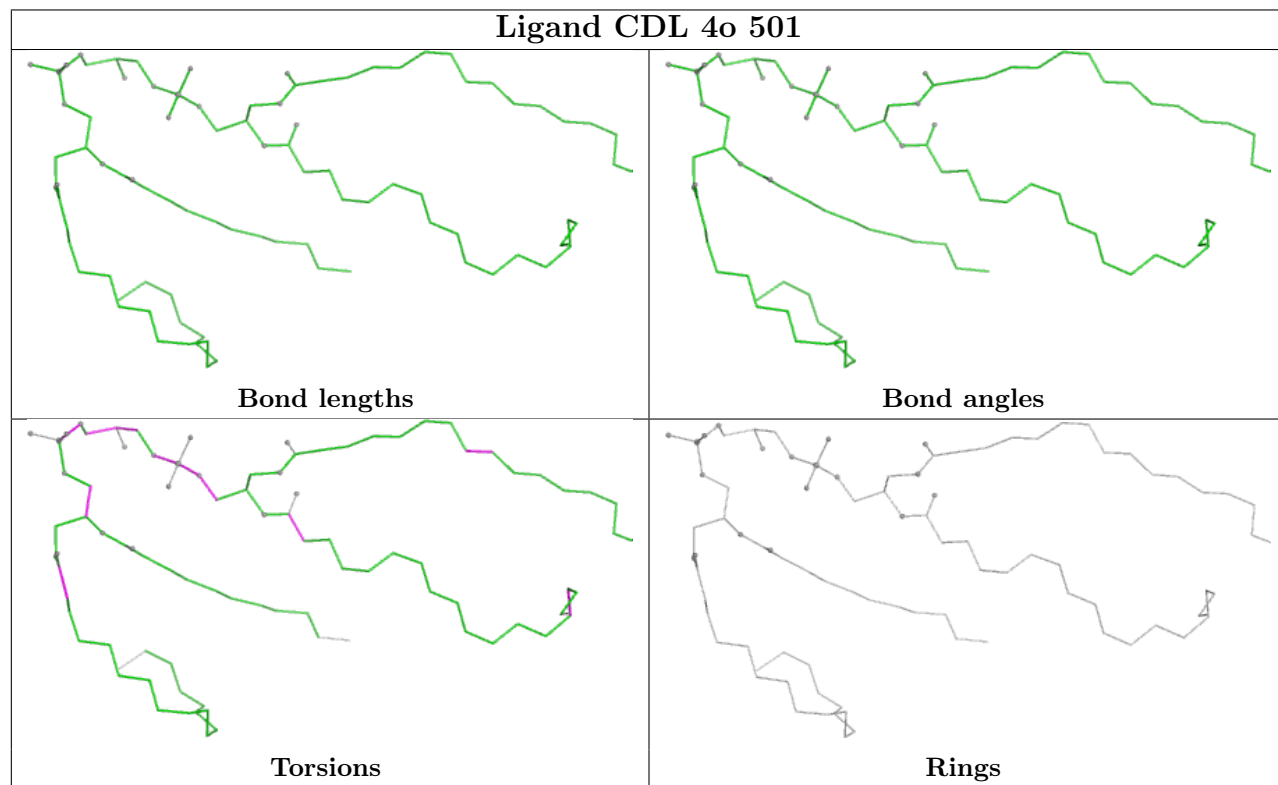
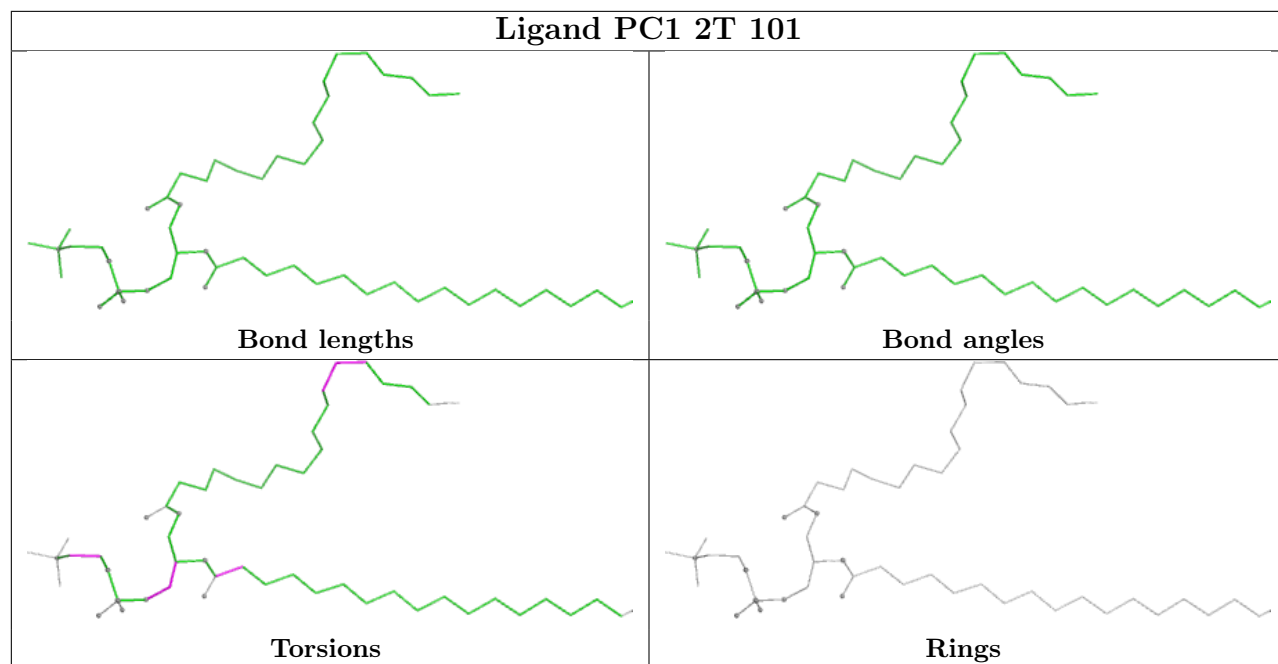


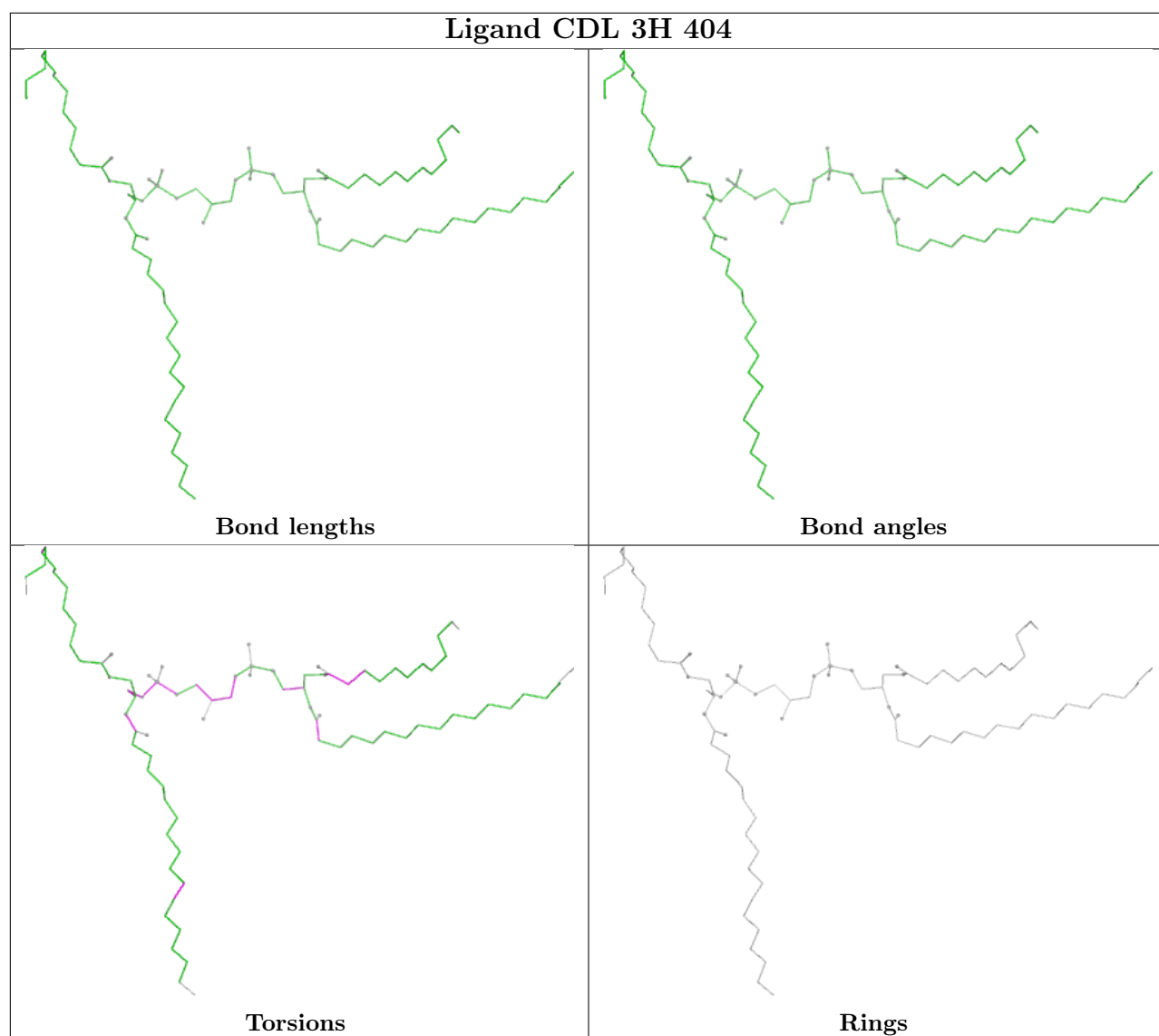


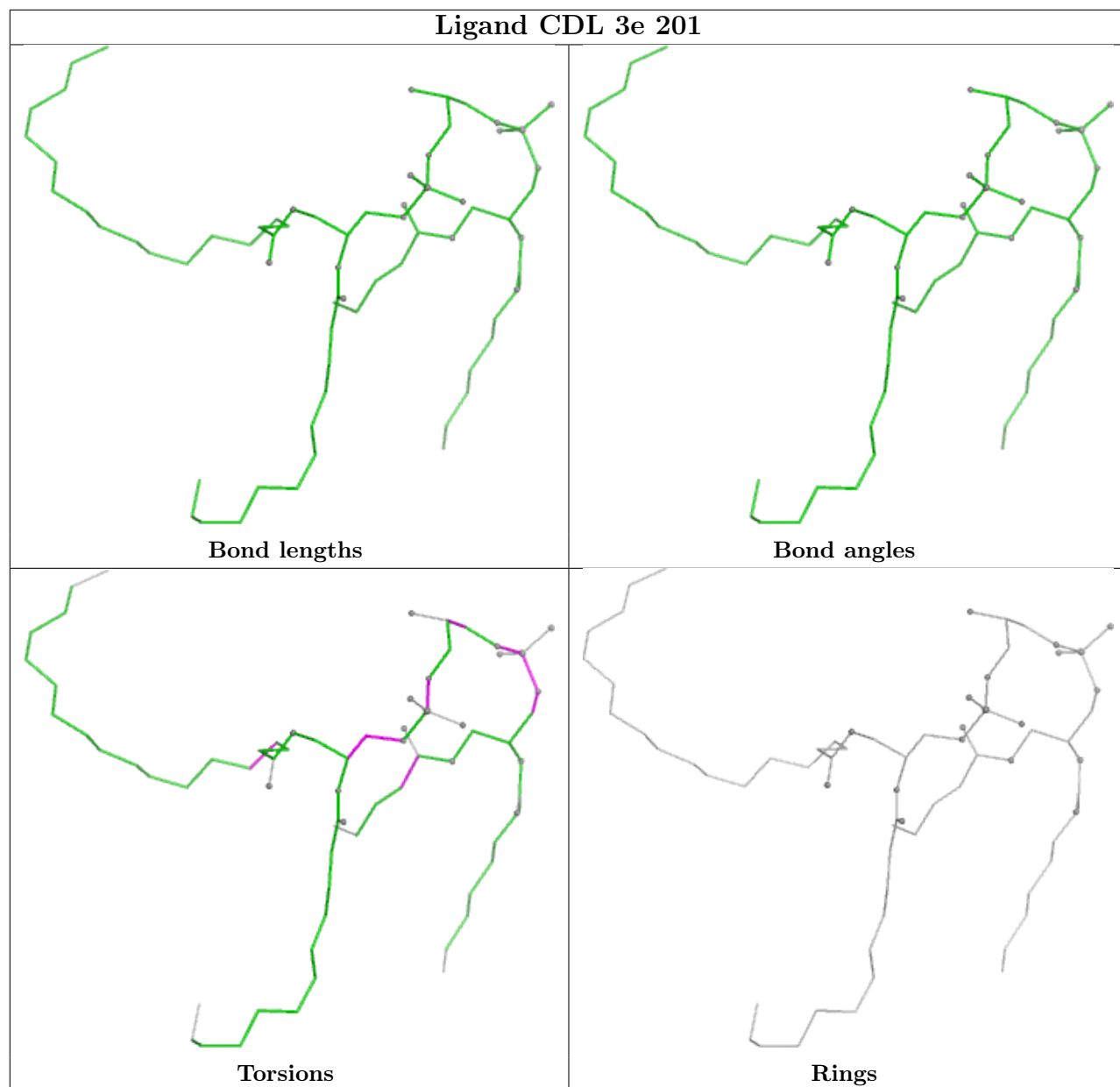




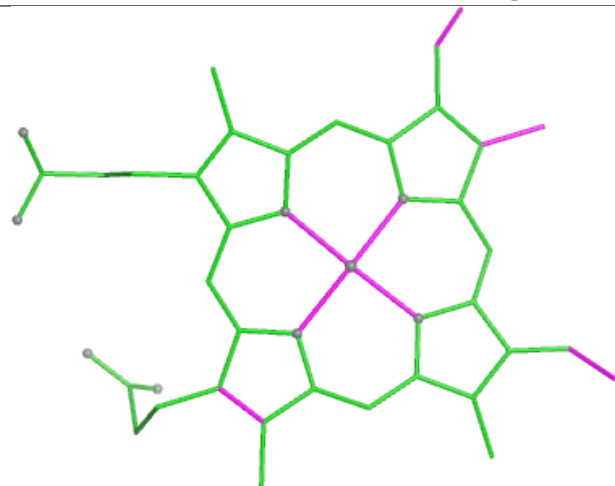




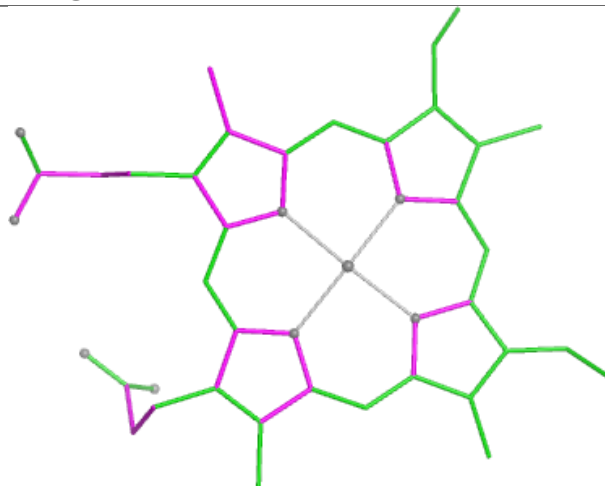




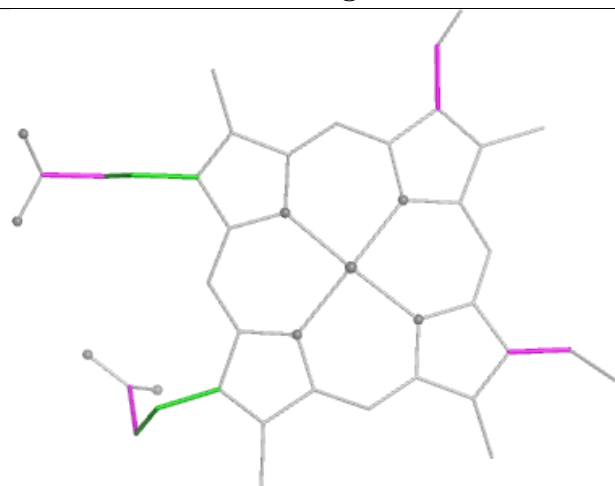
Ligand HEM 3g 408



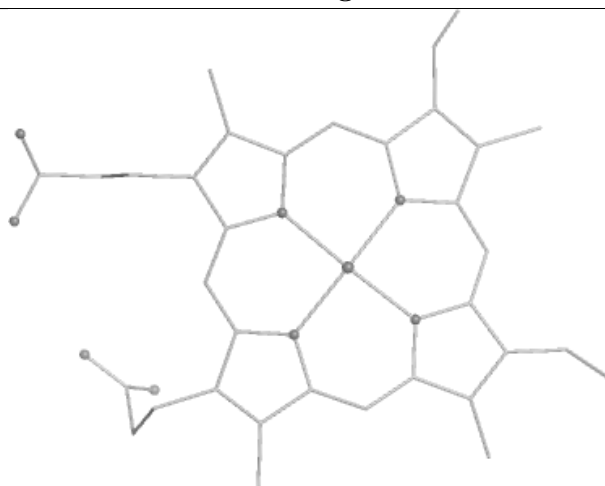
Bond lengths



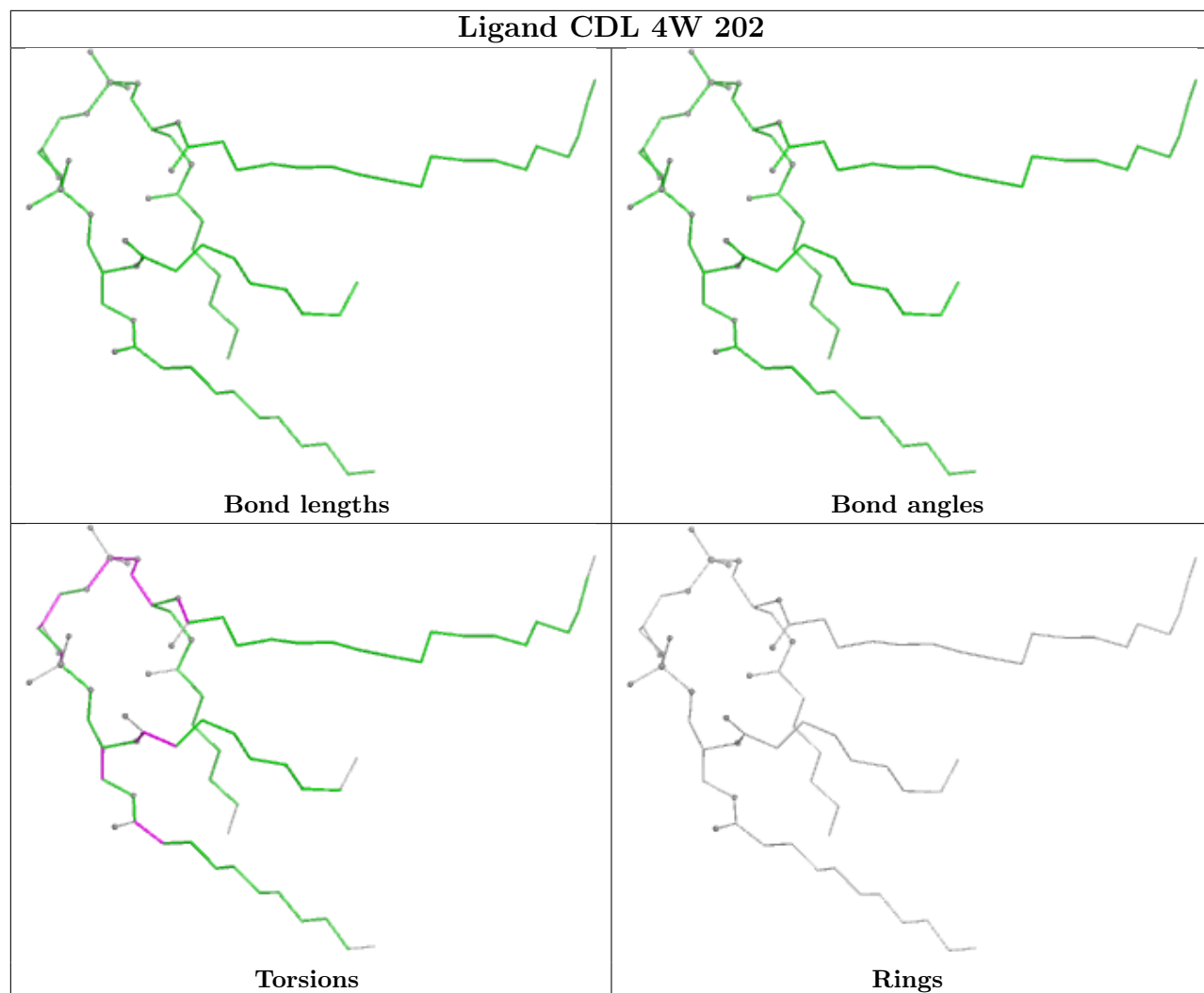
Bond angles

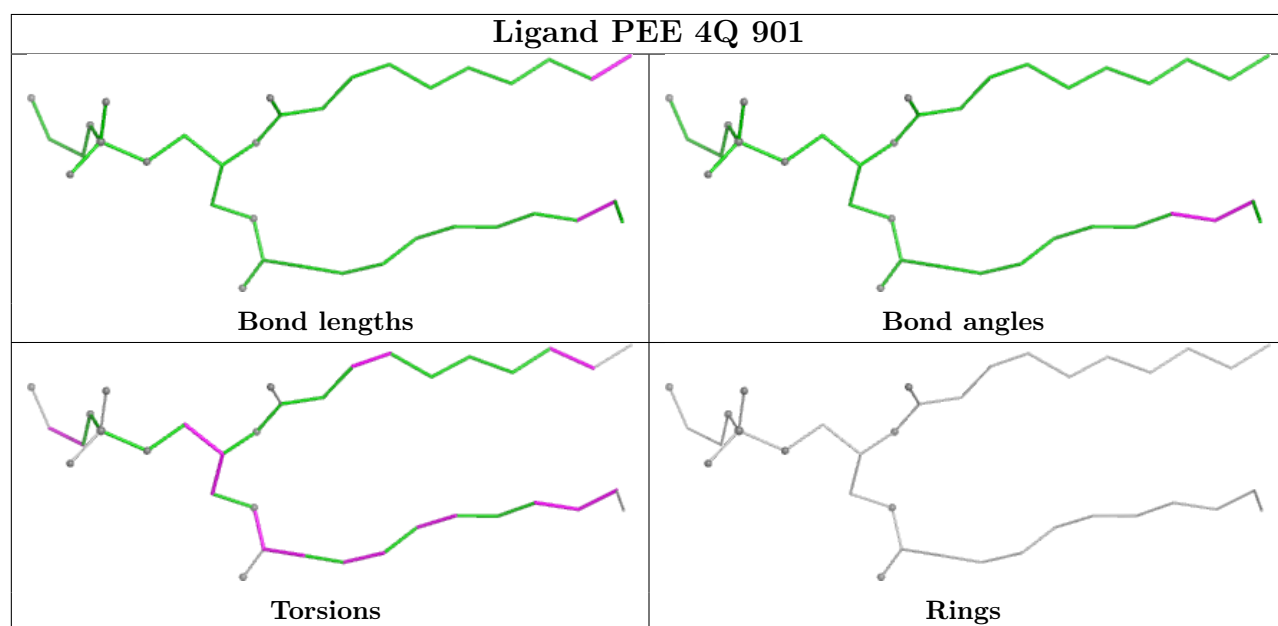
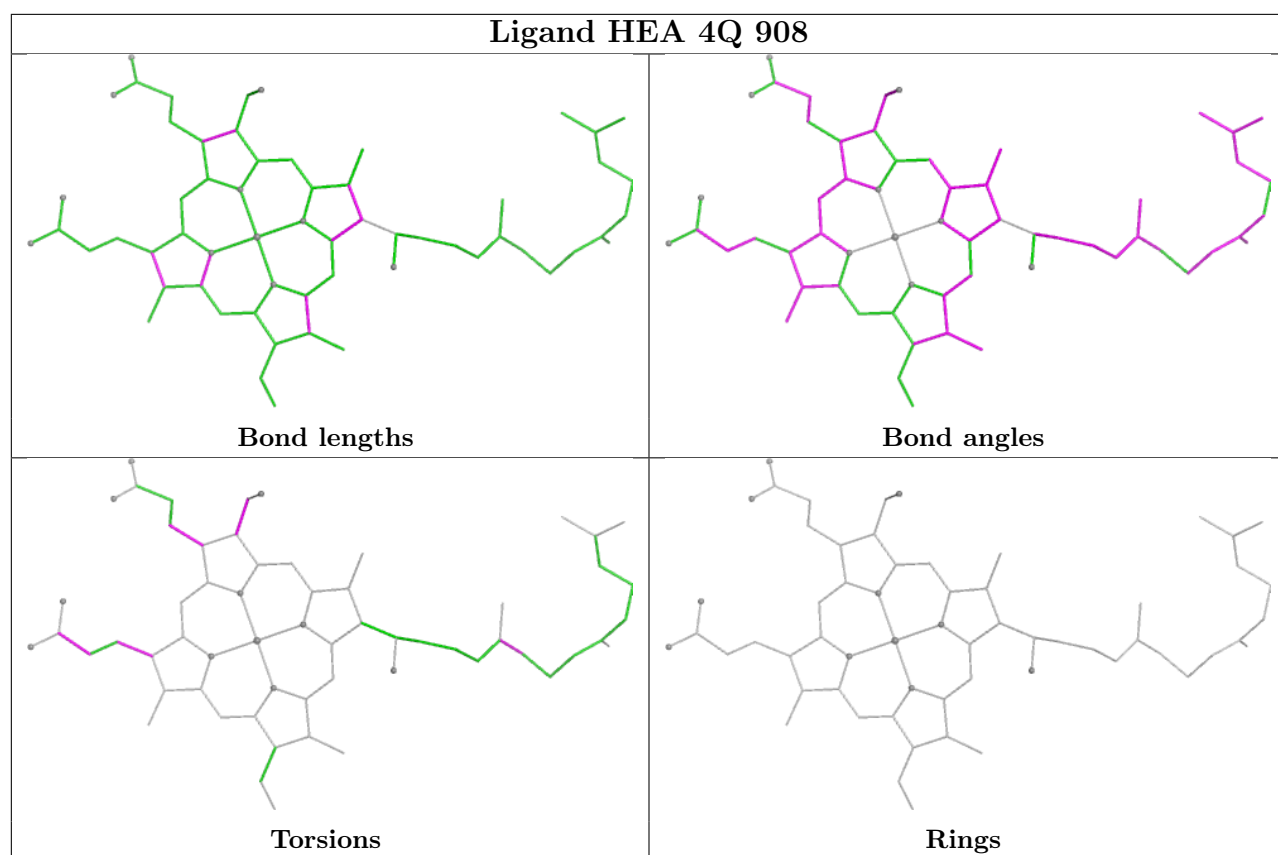


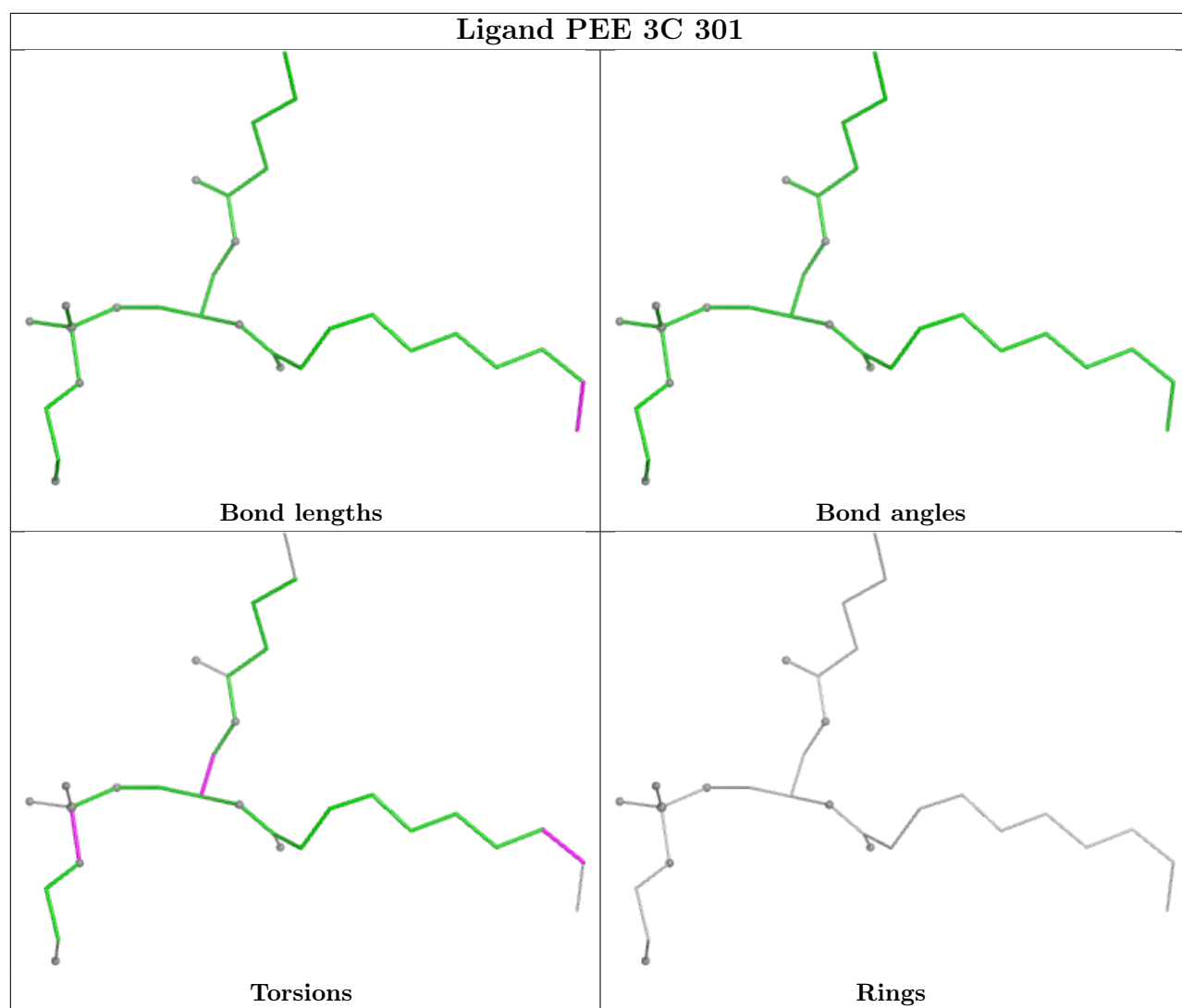
Torsions



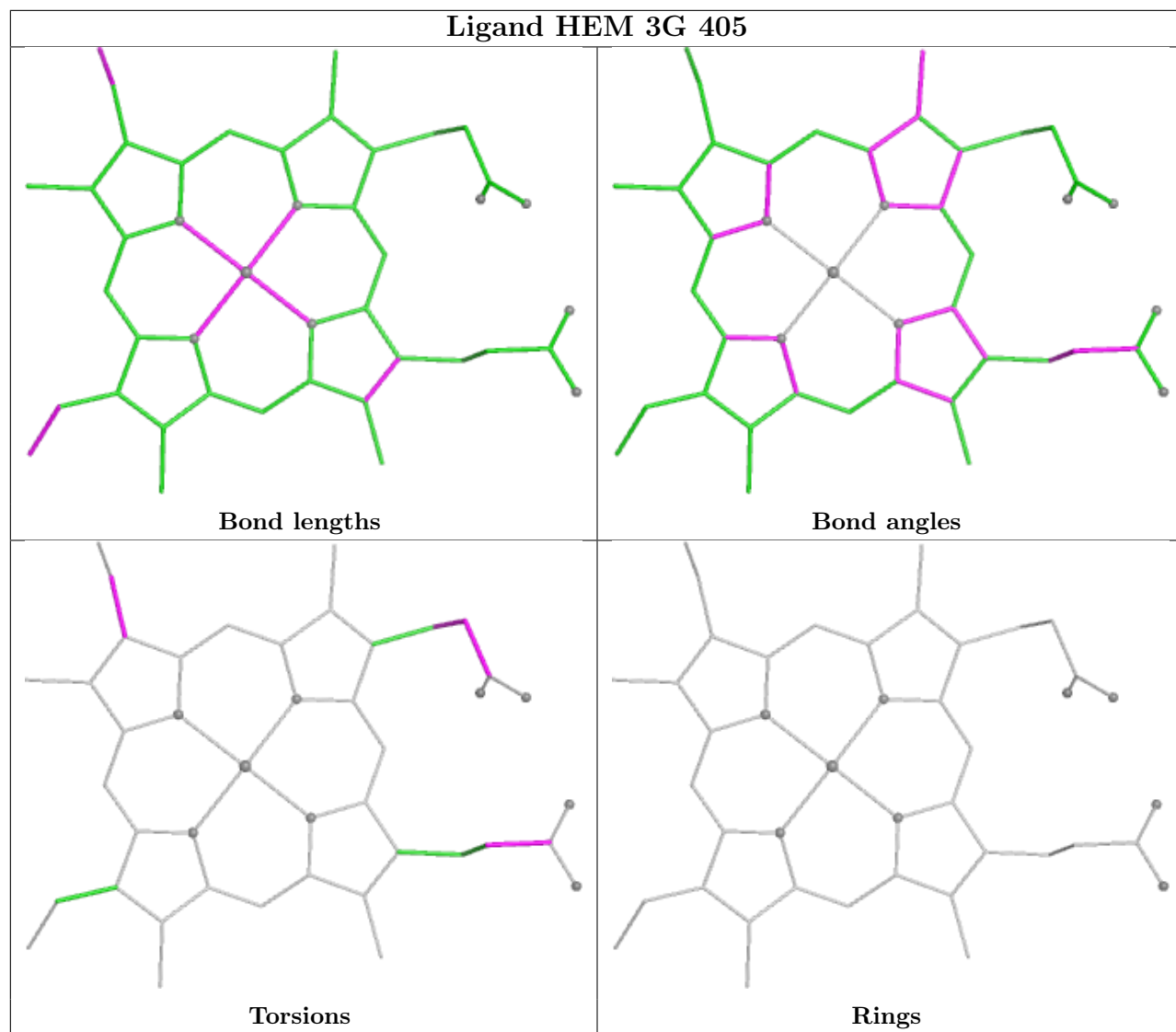
Rings



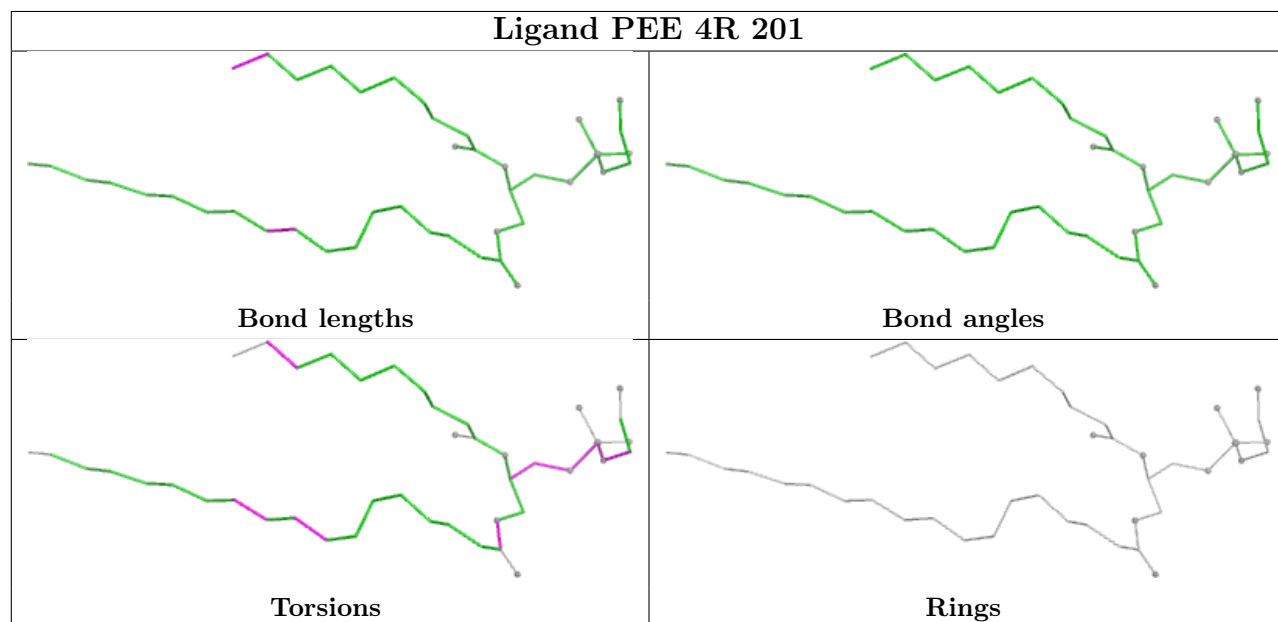




Ligand HEM 3G 405



Ligand PEE 4R 201



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	30	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	30	73:ALA	C	81:GLY	N	8.69

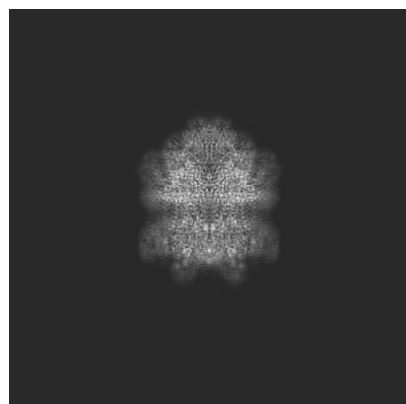
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50403. These allow visual inspection of the internal detail of the map and identification of artifacts.

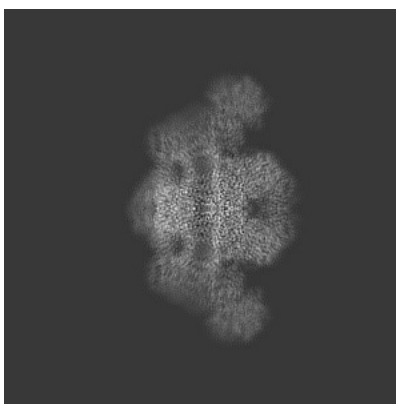
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

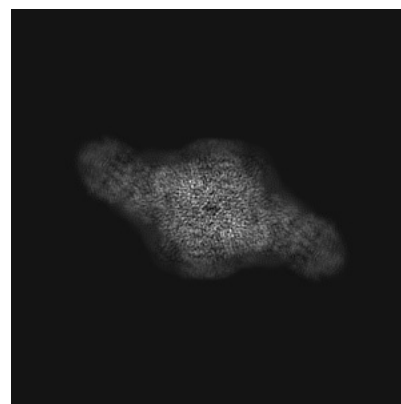
6.1.1 Primary map



X

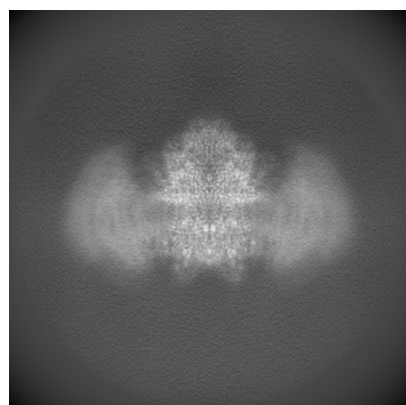


Y

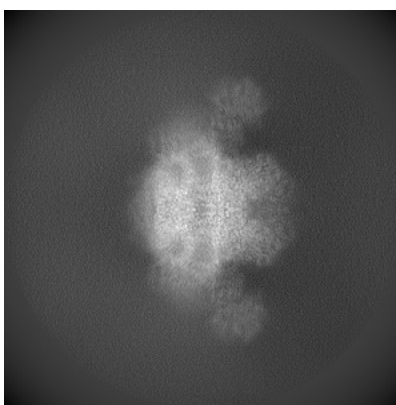


Z

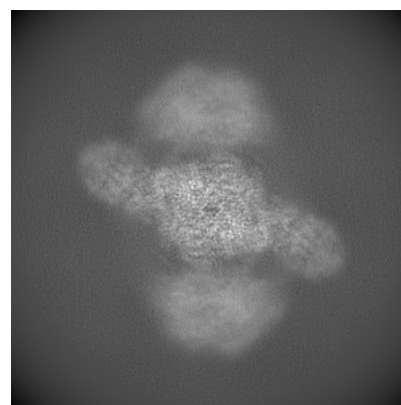
6.1.2 Raw map



X



Y



Z

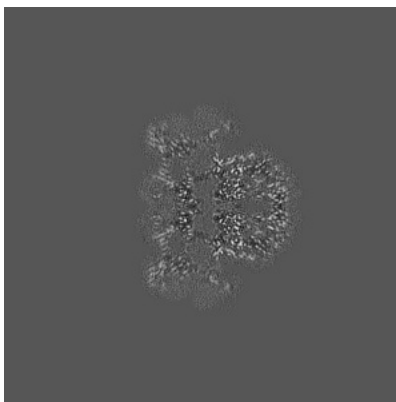
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

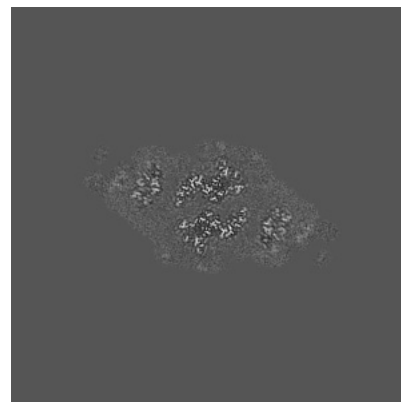
6.2.1 Primary map



X Index: 250

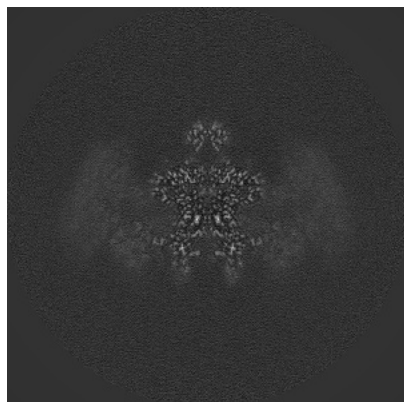


Y Index: 250

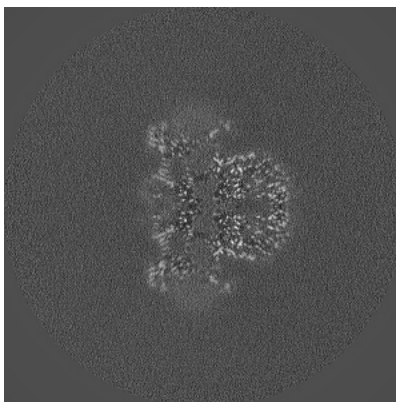


Z Index: 250

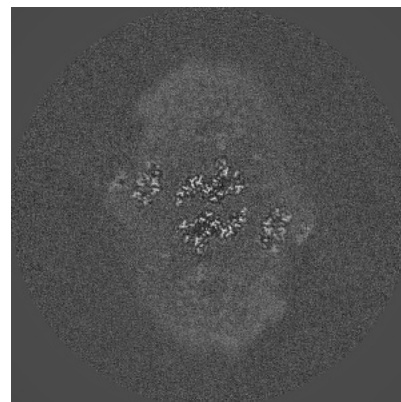
6.2.2 Raw map



X Index: 250



Y Index: 250

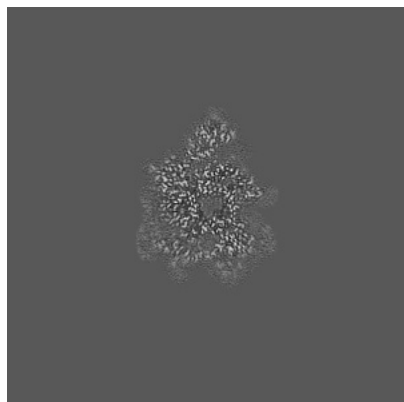


Z Index: 250

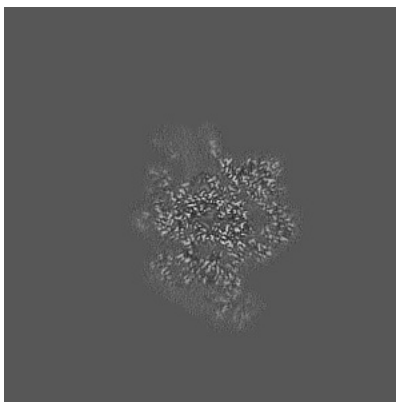
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

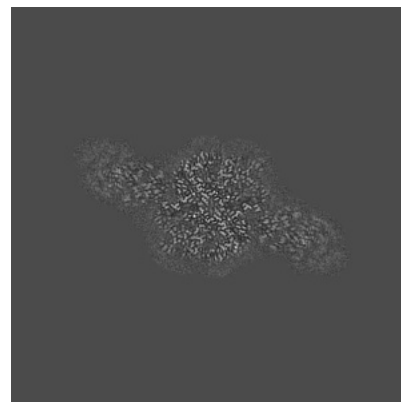
6.3.1 Primary map



X Index: 237

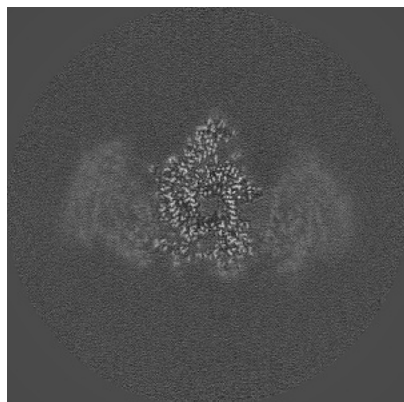


Y Index: 267

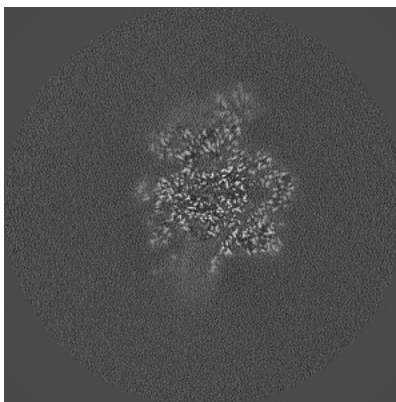


Z Index: 268

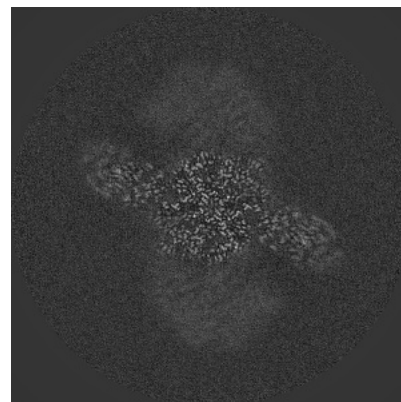
6.3.2 Raw map



X Index: 235



Y Index: 233

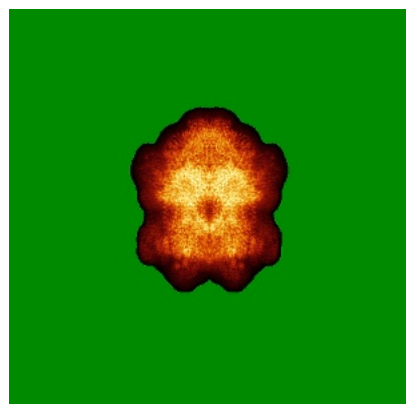


Z Index: 268

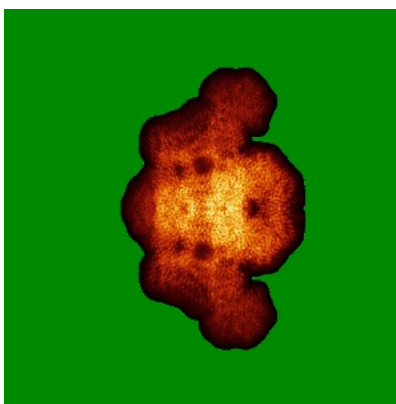
The images above show the largest variance slices of the map in three orthogonal directions.

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

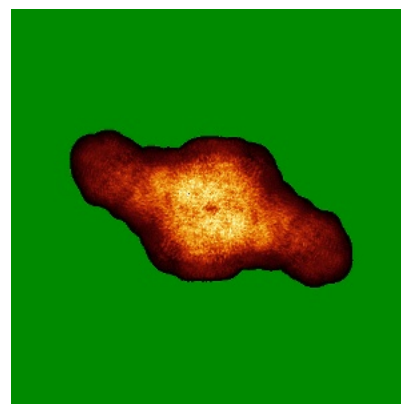
6.4.1 Primary map



X

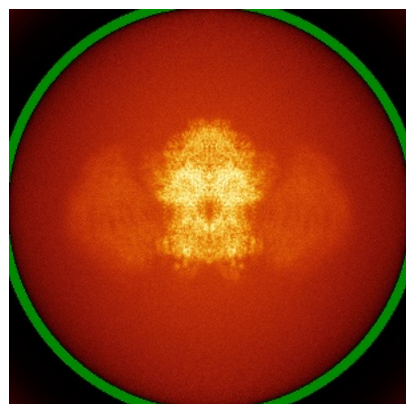


Y

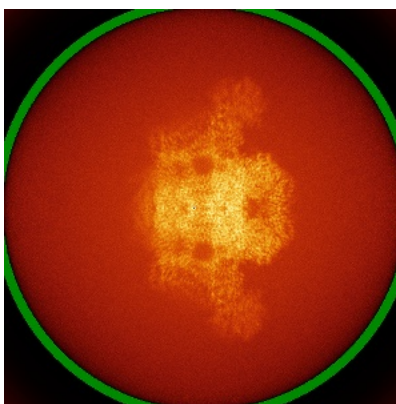


Z

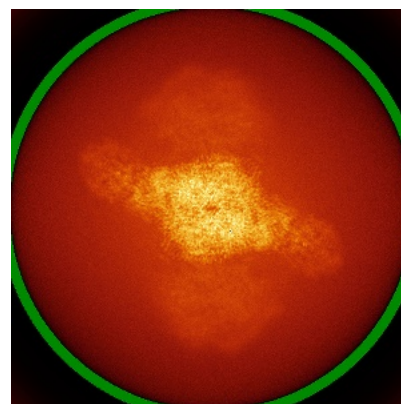
6.4.2 Raw map



X



Y

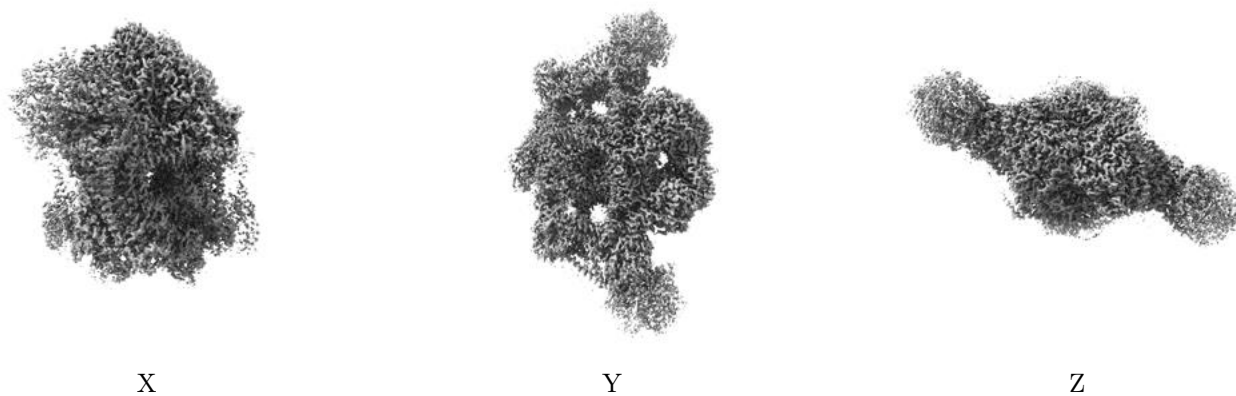


Z

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

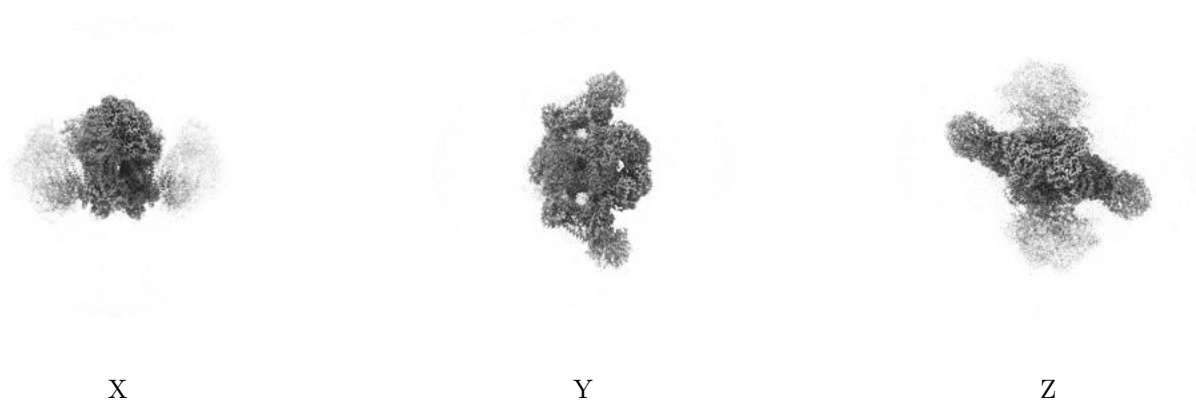
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

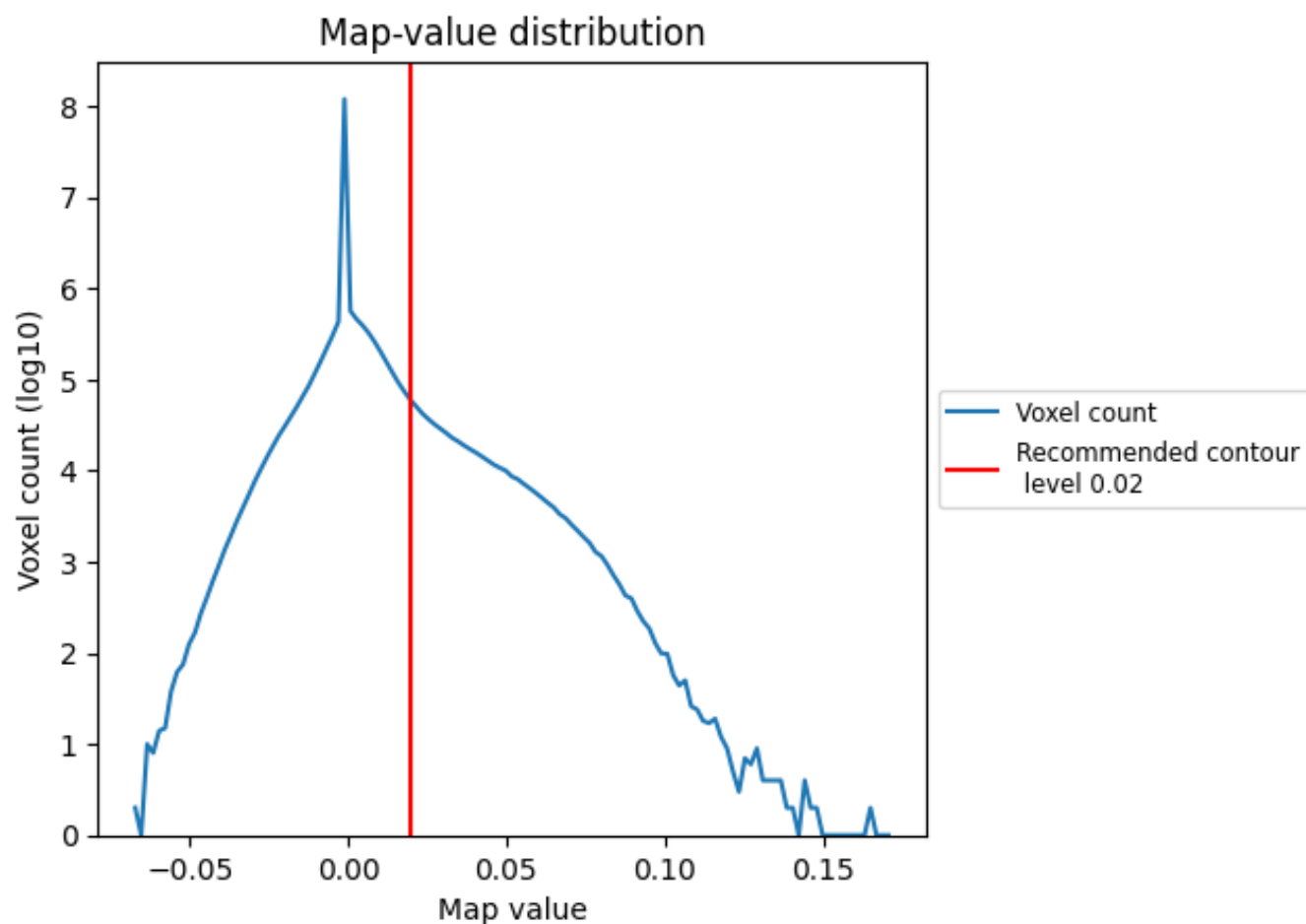
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

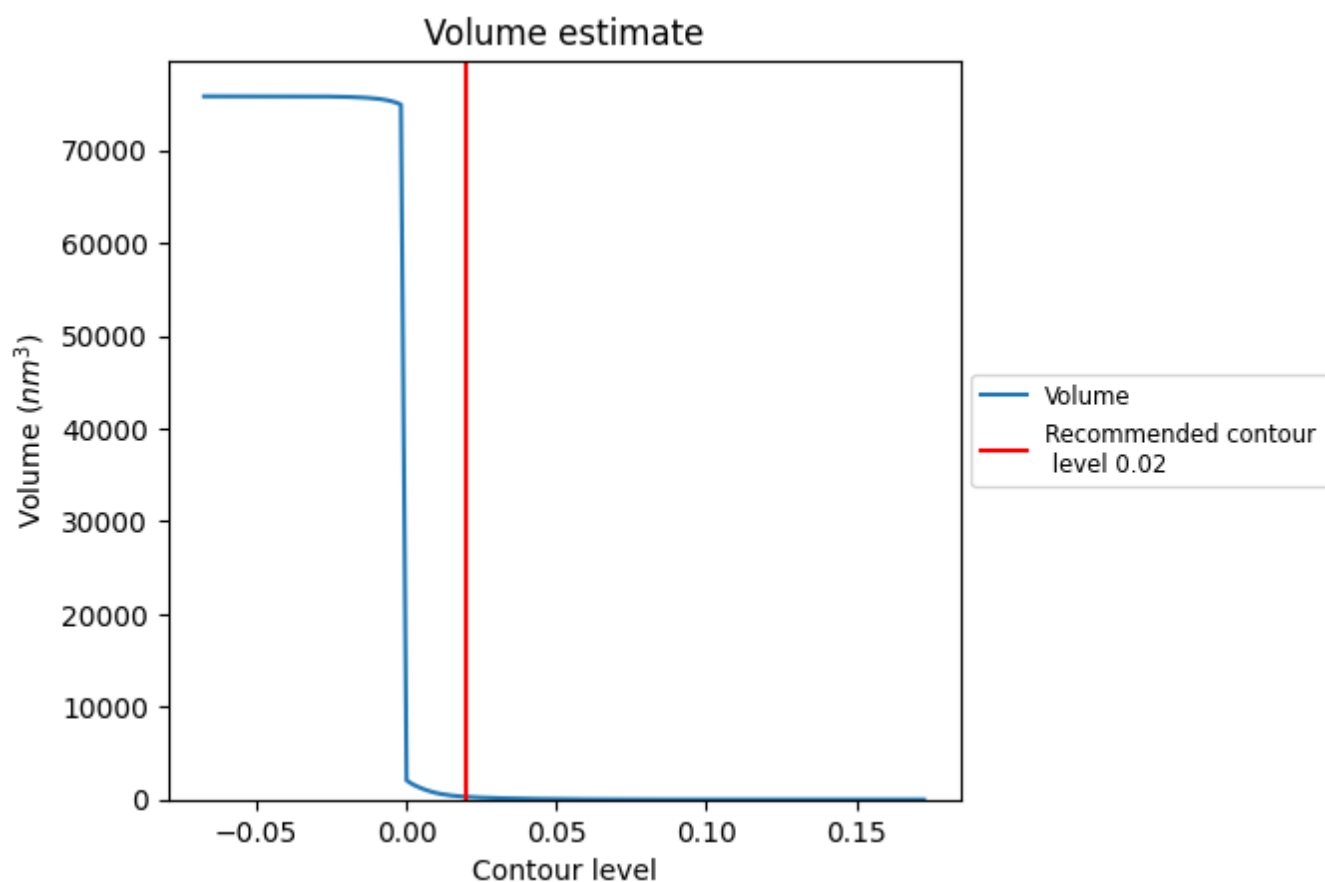
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

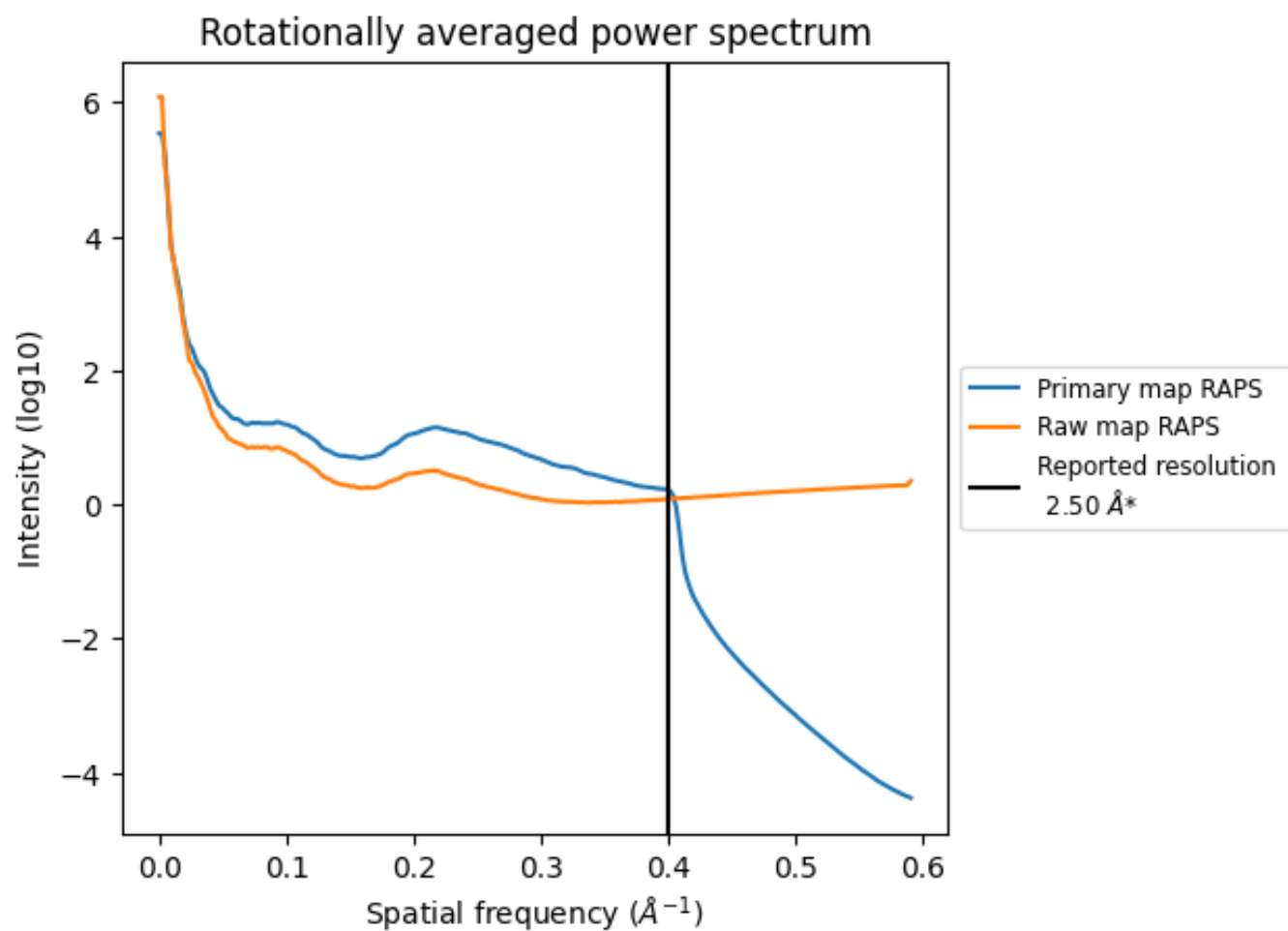
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm^3 ; this corresponds to an approximate mass of 271 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

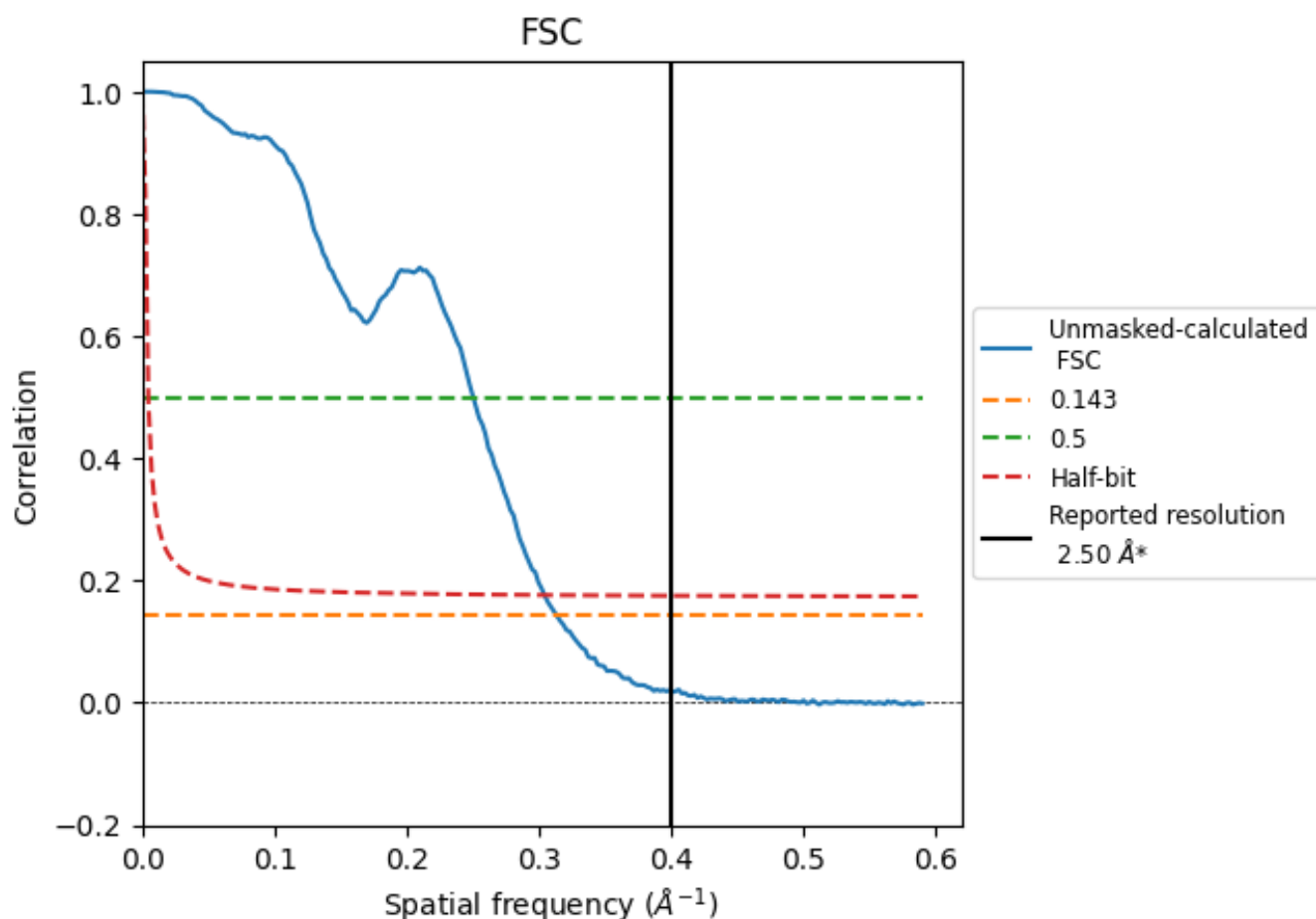


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

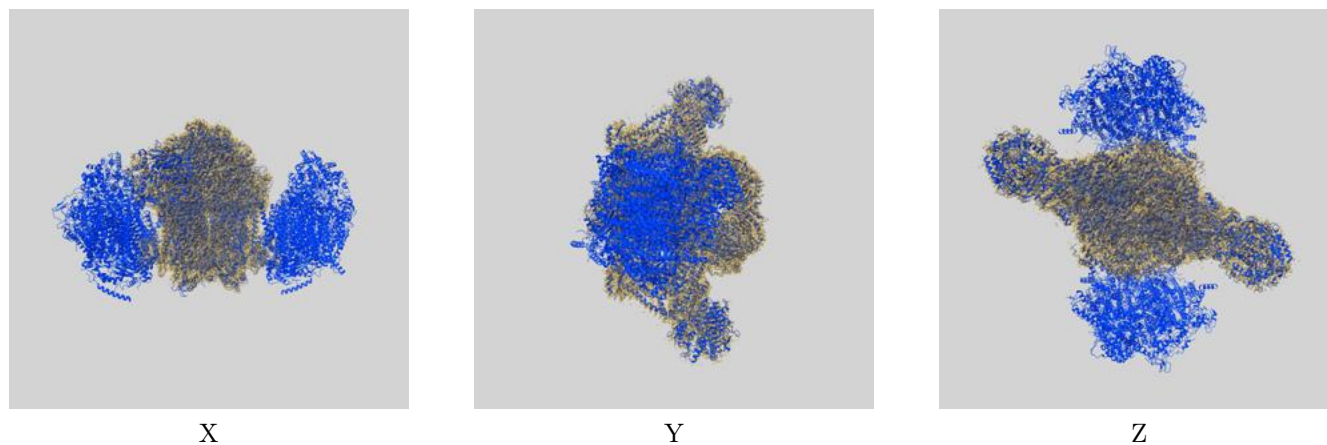
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.99	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

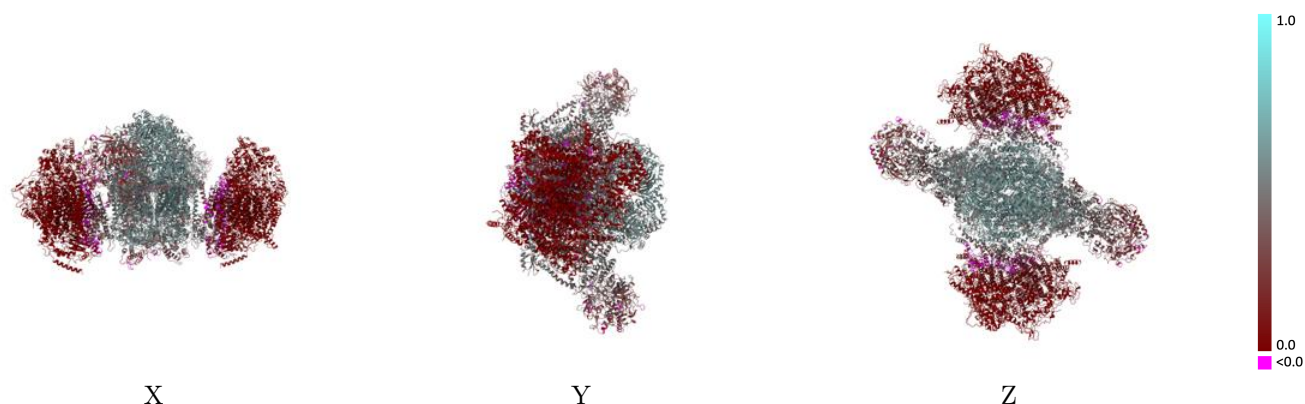
This section contains information regarding the fit between EMDB map EMD-50403 and PDB model 9FQ7. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



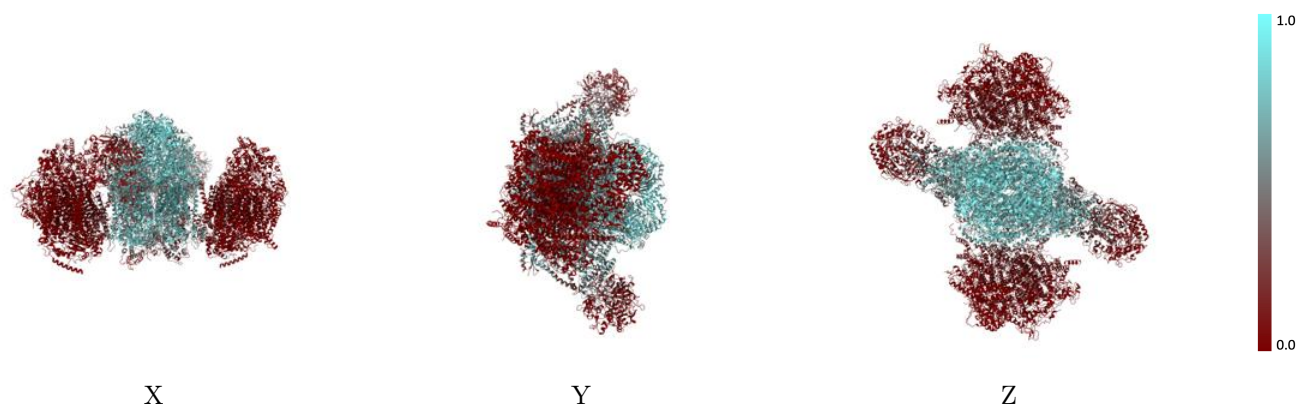
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



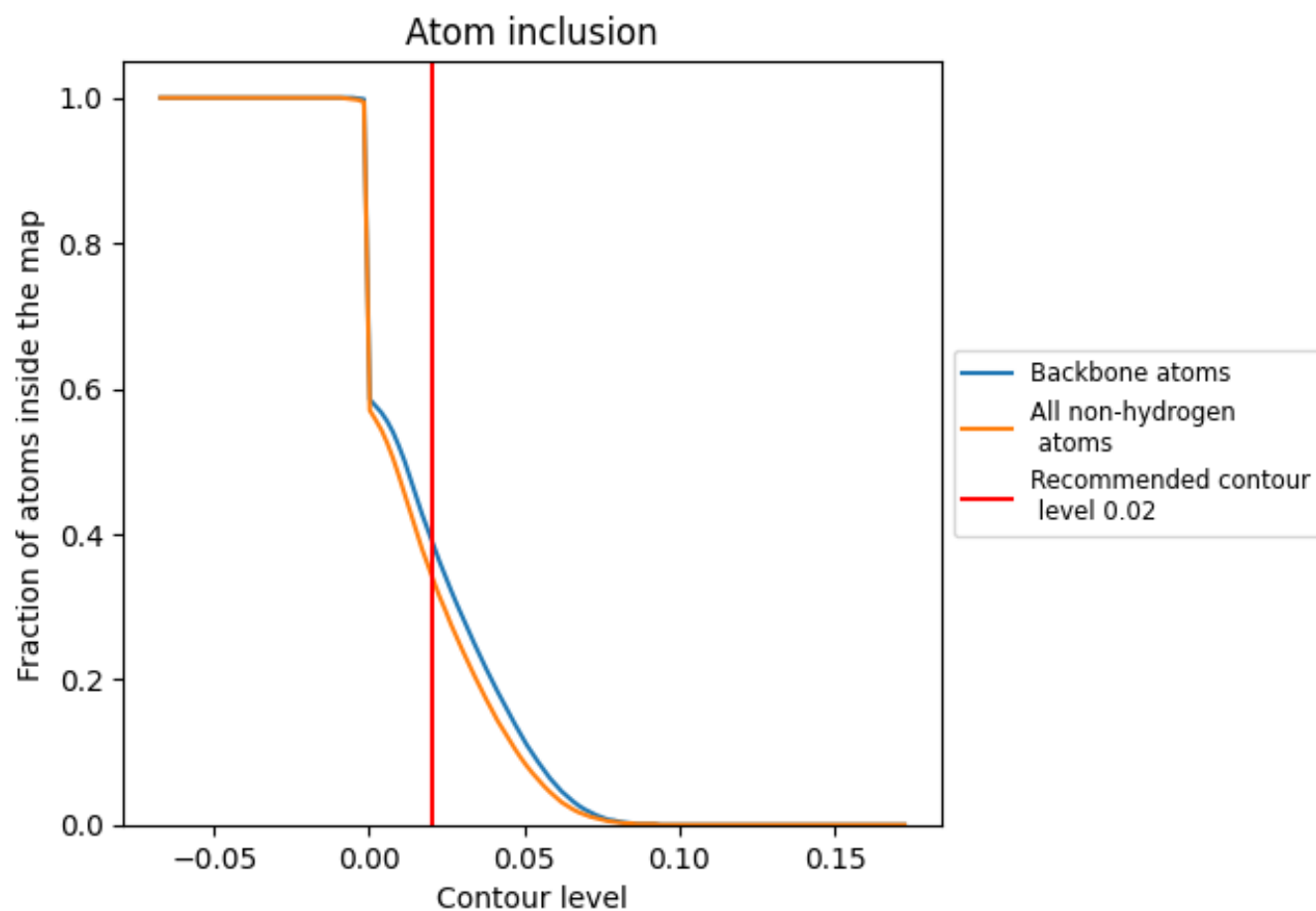
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3440	 0.2760
2M	 0.1330	 0.2740
2N	 0.3560	 0.3680
2O	 0.6730	 0.4980
2P	 0.6050	 0.4880
2Q	 0.5500	 0.4370
2R	 0.6300	 0.4740
2S	 0.6240	 0.4770
2T	 0.6430	 0.4960
2U	 0.4150	 0.3900
2V	 0.3670	 0.3800
2m	 0.1310	 0.2860
2n	 0.3680	 0.3720
2o	 0.6880	 0.5050
2p	 0.6390	 0.5030
2q	 0.5560	 0.4470
2r	 0.5950	 0.4780
2s	 0.6460	 0.4760
2t	 0.6790	 0.5040
2u	 0.4200	 0.4020
2v	 0.4200	 0.4110
30	 0.2220	 0.2470
31	 0.1960	 0.2440
3A	 0.8110	 0.5670
3B	 0.8090	 0.5660
3C	 0.8610	 0.5990
3D	 0.8220	 0.5810
3E	 0.8140	 0.5750
3F	 0.8970	 0.6110
3G	 0.8870	 0.6240
3H	 0.7290	 0.5430
3I	 0.8170	 0.5850
3J	 0.6480	 0.5000
3K	 0.8240	 0.6060
3L	 0.5730	 0.4820



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Chain	Atom inclusion	Q-score
3a	 0.8070	 0.5650
3b	 0.8050	 0.5610
3c	 0.8540	 0.5970
3d	 0.8750	 0.6130
3e	 0.8250	 0.5680
3f	 0.8820	 0.5990
3g	 0.8600	 0.6140
3h	 0.7870	 0.5650
3i	 0.8450	 0.5950
3j	 0.6290	 0.4780
3k	 0.8130	 0.6010
3l	 0.5860	 0.4810
40	 0.0000	 -0.0020
41	 0.0000	 -0.0010
4A	 0.0130	 0.0850
4B	 0.0380	 0.0870
4C	 0.0960	 0.2500
4D	 0.0750	 0.2040
4E	 0.0000	 0.0000
4F	 0.0510	 0.0910
4G	 0.0340	 0.1010
4H	 0.0000	 0.0000
4I	 0.0000	 0.0000
4J	 0.0000	 0.0000
4K	 0.0000	 0.0000
4L	 0.0000	 0.0000
4M	 0.0000	 0.0000
4N	 0.0000	 0.0100
4O	 0.0000	 -0.0010
4P	 0.0010	 0.0130
4Q	 0.0000	 -0.0000
4R	 0.0000	 0.0000
4S	 0.0000	 0.0000
4T	 0.0000	 0.0000
4U	 0.0000	 0.0000
4V	 0.0000	 0.0000
4W	 0.0010	 0.0090
4X	 0.0000	 0.0000
4Y	 0.0000	 0.0000
4Z	 0.0460	 0.1300
4a	 0.0220	 0.0930
4b	 0.0310	 0.0670

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Chain	Atom inclusion	Q-score
4c	 0.0670	 0.2310
4d	 0.0340	 0.1560
4e	 0.0000	 -0.0000
4f	 0.0210	 0.0700
4g	 0.0250	 0.0950
4h	 0.0000	 0.0000
4i	 0.0000	 0.0000
4j	 0.0000	 0.0000
4k	 0.0000	 0.0000
4l	 0.0000	 0.0000
4m	 0.0000	 0.0000
4n	 0.0000	 0.0100
4o	 0.0000	 -0.0030
4p	 0.0010	 0.0090
4q	 0.0000	 -0.0000
4r	 0.0000	 0.0000
4s	 0.0000	 0.0000
4t	 0.0000	 0.0000
4u	 0.0000	 0.0000
4v	 0.0000	 0.0000
4w	 0.0010	 0.0140
4x	 0.0000	 0.0000
4y	 0.0000	 0.0000
4z	 0.0280	 0.1170