



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 10:23 am BST

PDB ID : 6RFR  
EMDB ID : EMD-4873  
Title : Cryo-EM structure of respiratory complex I from *Yarrowia lipolytica* at 3.2 Å resolution  
Authors : Parey, K.; Vonck, J.  
Deposited on : 2019-04-16  
Resolution : 3.20 Å (reported)  
Based on initial model : 6GCS

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

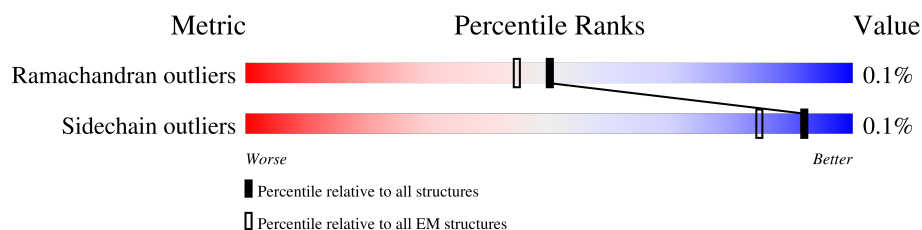
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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




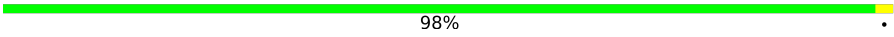


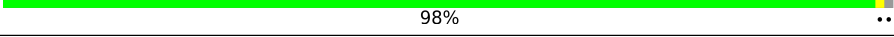

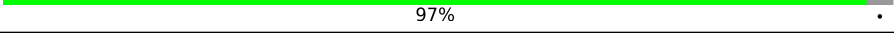

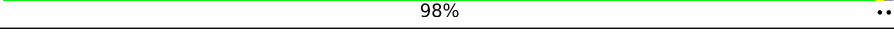
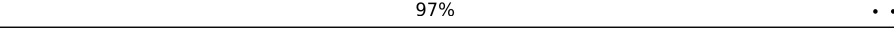
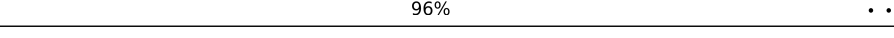
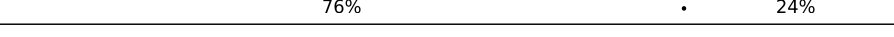
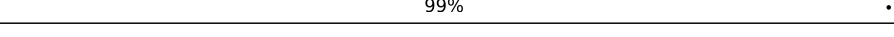
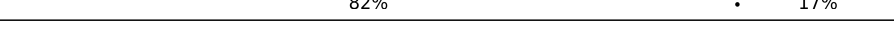


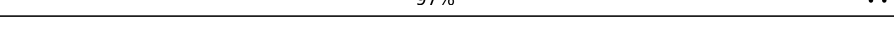

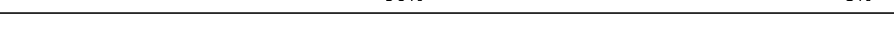






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	728	94% • 5%
2	B	488	93% • 7%
3	C	466	93% • 6%
4	D	87	98% ..
5	E	375	93% • 7%
6	F	144	83% • 16%
7	G	281	83% • 15%
8	H	243	87% • 11%
9	I	229	82% • 17%
10	J	198	89% • 10%

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Mol	Chain	Length	Quality of chain
11	K	210	
12	L	89	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	249	
19	U	172	
20	W	123	
21	X	169	
22	Y	161	
23	Z	182	
24	a	149	
25	b	74	
26	c	60	
27	d	92	
28	e	67	
29	f	87	
30	g	78	
31	h	138	
32	i	90	
33	j	93	
34	n	120	
35	1	341	

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Mol	Chain	Length	Quality of chain
36	2	469	97% .
37	3	128	98% ..
38	4	486	97% .
39	5	655	98% .
40	6	185	97% ..
41	8	99	81% . 17%
42	9	89	97% .

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 65934 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 Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	692	Total	C	N	O	S	0	0
			5258	3263	926	1040	29		

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	0	0
			3528	2229	621	654	24		

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	438	Total	C	N	O	S	0	0
			3472	2205	596	649	22		

- Molecule 4 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	349	Total	C	N	O	S	0	0
			2798	1778	489	521	10		

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 10 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	179	Total	C	N	O	S	0	0
			1329	844	241	239	5		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	177	Total	C	N	O	S	0	0
			1395	885	246	249	15		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	89	Total	C	N	O	S	0	0
			691	464	109	115	3		

- Molecule 13 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	77	Total	C	N	O	S	0	0
			591	373	93	125			

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 18 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 19 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 21 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1296	839	221	232	4		

- Molecule 22 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

- Molecule 23 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	181	Total	C	N	O	S	0	0
			1389	893	240	255	1		

- Molecule 24 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 25 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	64	Total	C	N	O	S	0	0
			490	326	83	81			

- Molecule 26 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	44	Total	C	N	O	S	0	0
			353	229	67	57			

- Molecule 27 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	90	Total	C	N	O	S	0	0
			760	472	137	148	3		

- Molecule 28 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 29 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 30 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 31 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 32 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 33 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	90	Total	C	N	O	0	0
			724	465	132	127		

- Molecule 34 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	114	Total	C	N	O	S	0	0
			914	588	156	169	1		

- Molecule 35 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	340	Total	C	N	O	S	0	0
			2714	1849	393	465	7		

- Molecule 36 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 37 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	127	Total	C	N	O	S	0	0
			1017	694	150	170	3		

- Molecule 38 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	486	Total	C	N	O	S	0	0
			3855	2600	586	654	15		

- Molecule 39 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 40 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	183	Total	C	N	O	S	0	0
			1443	979	207	249	8		

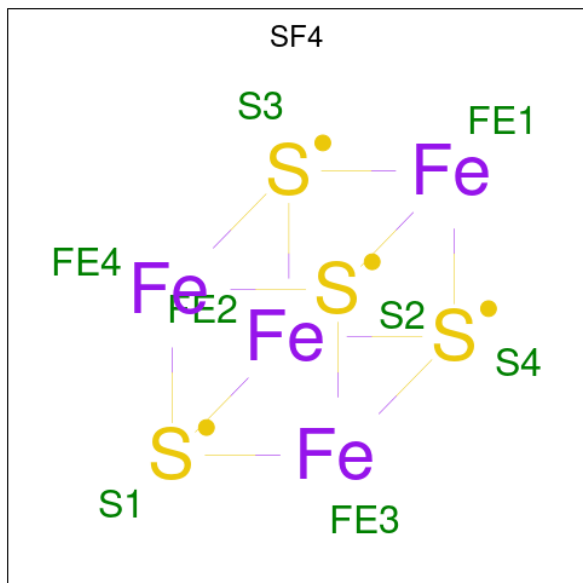
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

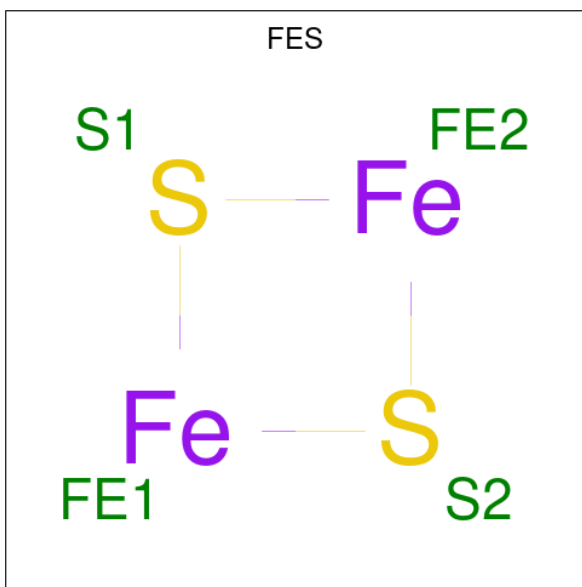
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



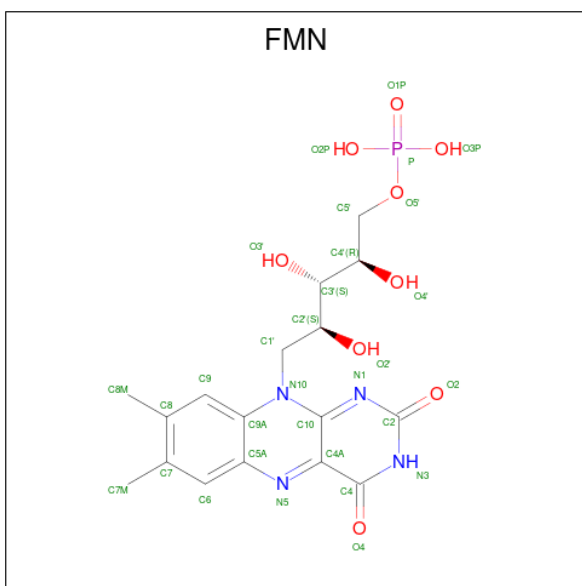
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total 4	Fe 2	S 2	0
44	H	1	Total 4	Fe 2	S 2	0

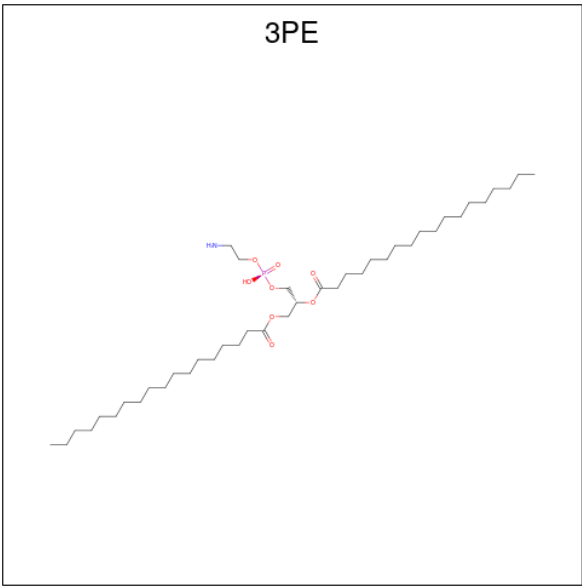
- Molecule 45 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE)

(formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



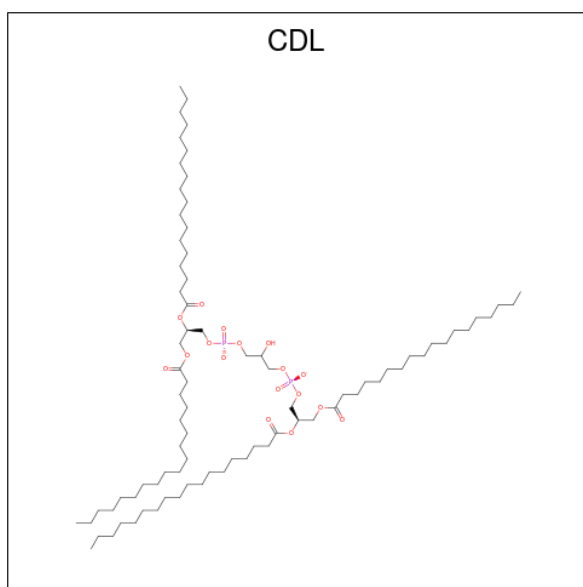
Mol	Chain	Residues	Atoms					AltConf
46	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	E	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	b	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	5	1	Total 42	C 32	N 1	O 8	P 1	0
46	5	1	Total 51	C 41	N 1	O 8	P 1	0

- # NDP

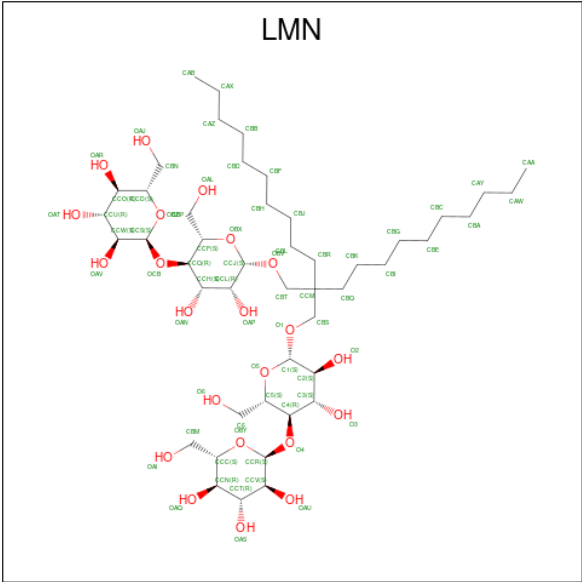
- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ).



Mol	Chain	Residues	Atoms				AltConf
48	E	1	Total	C	O	P	0
			72	53	17	2	
48	X	1	Total	C	O	P	0
			86	67	17	2	
48	Z	1	Total	C	O	P	0
			76	57	17	2	
48	g	1	Total	C	O	P	0
			83	64	17	2	
48	j	1	Total	C	O	P	0
			78	59	17	2	
48	4	1	Total	C	O	P	0
			92	73	17	2	

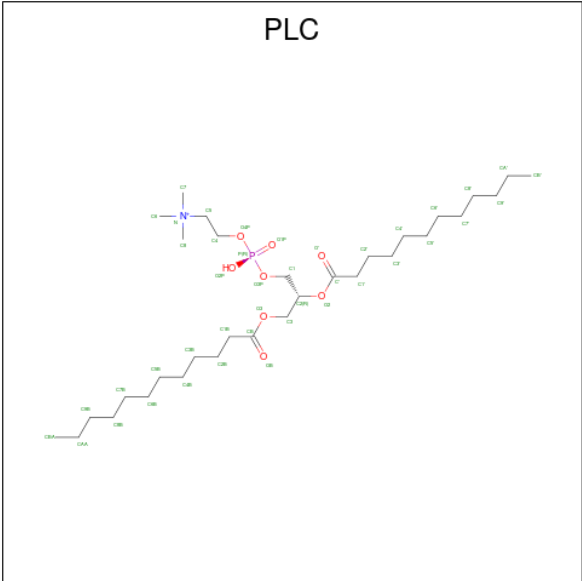
- Molecule 49 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C<sub>47</sub>H<sub>88</sub>O<sub>22</sub>).





Mol	Chain	Residues	Atoms			AltConf
49	J	1	Total	C	O	0
			69	47	22	
49	j	1	Total	C	O	0
			65	43	22	

- Molecule 50 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
50	K	1	Total	C	N	O	P	0
			39	29	1	8	1	

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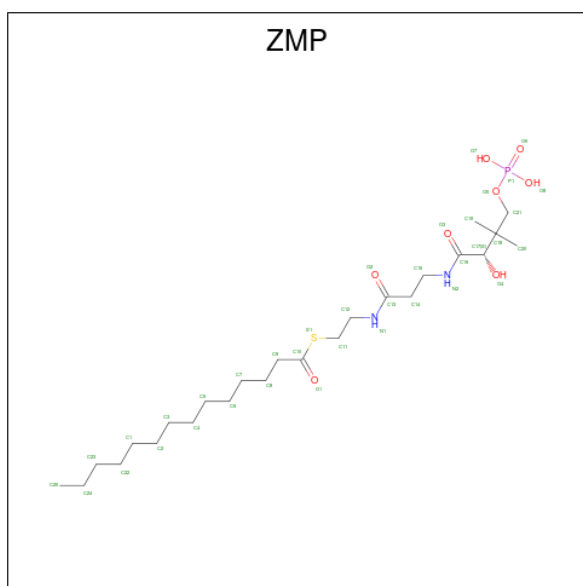
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Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	n	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

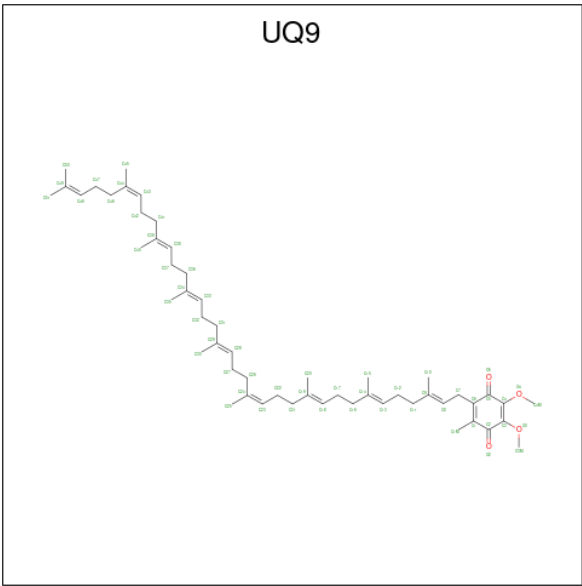
Mol	Chain	Residues	Atoms		AltConf
51	M	1	Total	Zn	0
			1	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



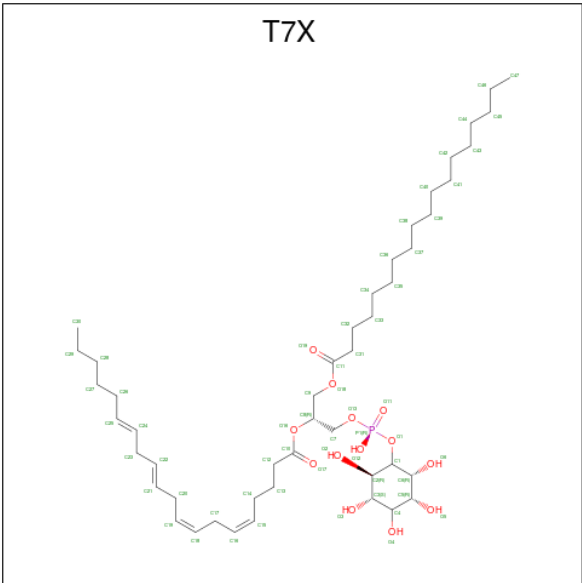
Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 53 is Ubiquinone-9 (three-letter code: UQ9) (formula: C<sub>54</sub>H<sub>82</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
53	1	1	Total	C	O	0
			35	31	4	

- Molecule 54 is Phosphatidylinositol (three-letter code: T7X) (formula: C<sub>47</sub>H<sub>83</sub>O<sub>13</sub>P).



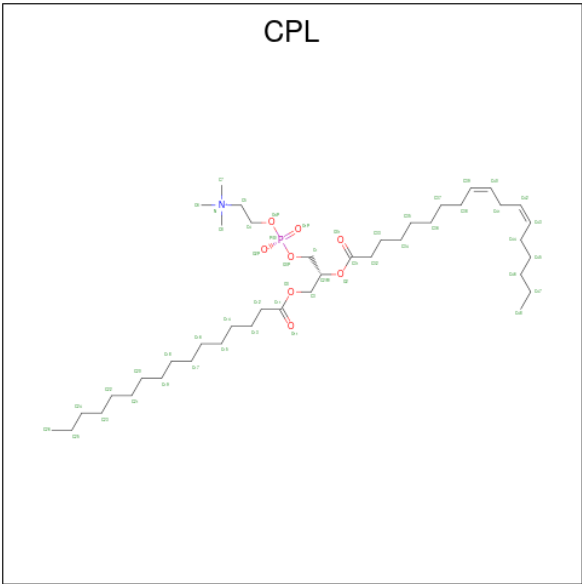
Mol	Chain	Residues	Atoms				AltConf
54	2	1	Total	C	O	P	0
			48	34	13	1	
54	2	1	Total	C	O	P	0
			52	38	13	1	

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Mol	Chain	Residues	Atoms				AltConf
54	3	1	Total	C	O	P	0
			49	35	13	1	
54	5	1	Total	C	O	P	0
			43	29	13	1	

- Molecule 55 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C<sub>42</sub>H<sub>80</sub>NO<sub>8</sub>P).



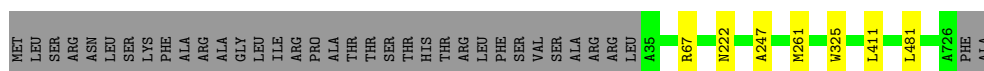
Mol	Chain	Residues	Atoms					AltConf
55	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

### 3 Residue-property plots [i](#)

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

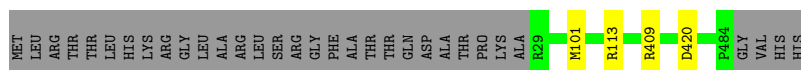
- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain A:  94% 5%



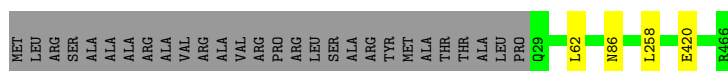
- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain B:  93% 7%



- Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain C:  93% 6%



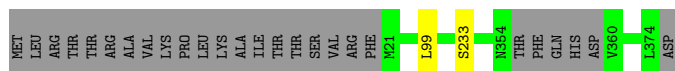
- Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain D:  98% ..




- Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

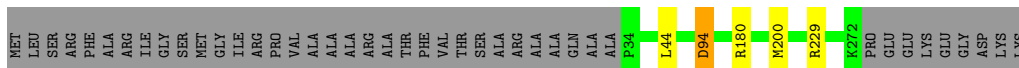
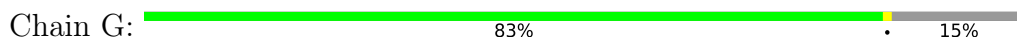
Chain E:  93% 7%



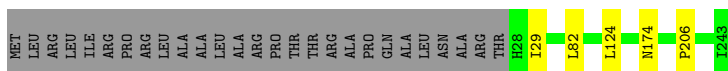
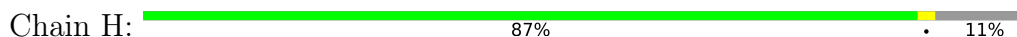
- Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain F:  83% 16%

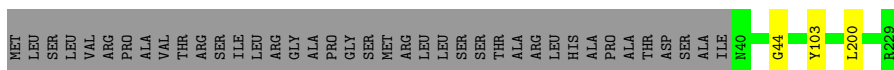
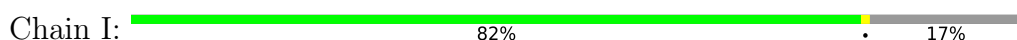
- Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)



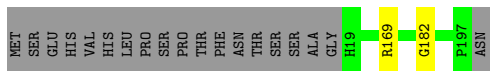
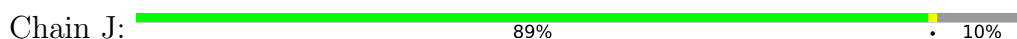
- Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



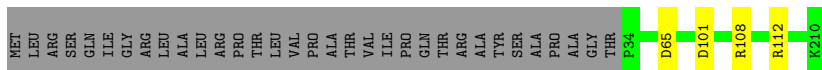
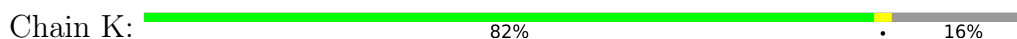
- Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)



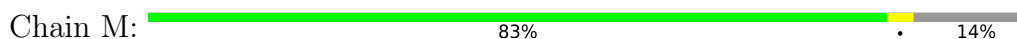
- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

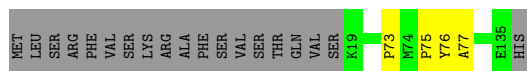


- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)

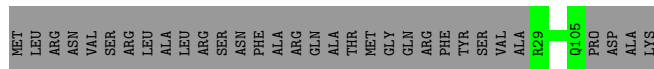


- Molecule 13: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

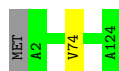




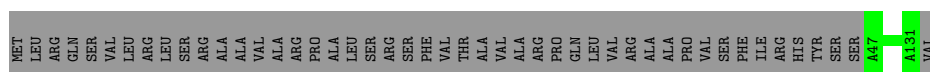
- Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



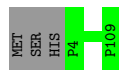
- Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



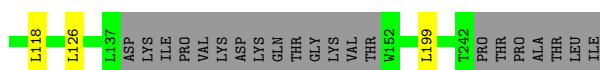
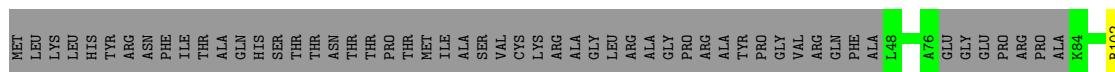
- Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



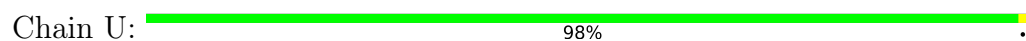
- Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

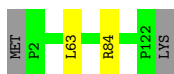


- Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain W:  97% ..



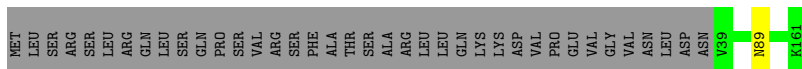
- Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain X:  96% ..



- Molecule 22: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Y:  76% . 24%




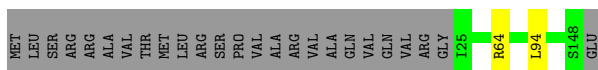
- Molecule 23: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Z:  99% ..




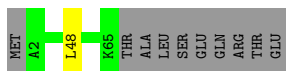
- Molecule 24: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain a:  82% . 17%



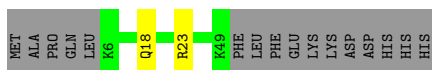
- Molecule 25: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:  85% . 14%



- Molecule 26: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

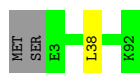
Chain c:  70% . 27%




- Molecule 27: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



Chain d:  97% ..




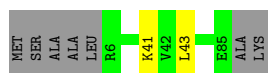
- Molecule 28: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:  78% 22%



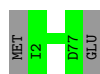
- Molecule 29: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:  90% • 8%



- Molecule 30: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain g:  97% •




- Molecule 31: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain h:  96% ..



- Molecule 32: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain i:  90% • 8%

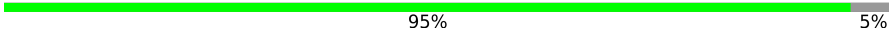


- Molecule 33: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain j:  96% ..



- Molecule 34: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n:  95% 5%



- Molecule 35: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 1:  96% .



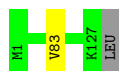
- Molecule 36: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 2:  97% .



- Molecule 37: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 3:  98% ..



- Molecule 38: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 4:  97% .



- Molecule 39: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 5:  98% .

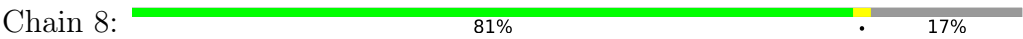


- Molecule 40: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)

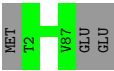
Chain 6:  97% ..



- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



● Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	297066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	46425	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T7X, 3PE, UQ9, ZN, CPL, CDL, FES, FMN, LMN, ZMP, PLC, NDP, SF4

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	A	0.53	1/5351 (0.0%)	0.69	3/7262 (0.0%)
2	B	0.49	1/3605 (0.0%)	0.68	4/4865 (0.1%)
3	C	0.63	0/3554	0.77	3/4817 (0.1%)
4	D	0.52	0/697	0.77	2/940 (0.2%)
5	E	0.48	0/2858	0.72	2/3870 (0.1%)
6	F	0.50	0/1011	0.73	1/1371 (0.1%)
7	G	0.62	1/2040 (0.0%)	0.79	7/2781 (0.3%)
8	H	0.45	0/1725	0.70	2/2343 (0.1%)
9	I	0.66	0/1557	0.76	3/2110 (0.1%)
10	J	0.44	1/1362 (0.1%)	0.69	1/1855 (0.1%)
11	K	0.63	0/1434	0.74	3/1950 (0.2%)
12	L	0.54	0/700	0.79	2/947 (0.2%)
13	M	0.51	0/935	0.68	2/1268 (0.2%)
14	O	0.34	0/598	0.57	0/813
15	P	0.54	1/1061 (0.1%)	0.69	0/1427
16	Q	0.36	0/654	0.63	0/890
17	R	0.41	0/909	0.65	0/1229
18	S	0.41	0/1454	0.72	3/1960 (0.2%)
19	U	0.45	0/1374	0.73	2/1856 (0.1%)
20	W	0.47	0/998	0.67	3/1346 (0.2%)
21	X	0.52	1/1335 (0.1%)	0.69	4/1811 (0.2%)
22	Y	0.48	0/1051	0.60	0/1420
23	Z	0.46	0/1430	0.66	1/1955 (0.1%)
24	a	0.40	0/1064	0.70	1/1439 (0.1%)
25	b	0.41	0/503	0.72	1/679 (0.1%)
26	c	0.43	0/364	0.56	0/491
27	d	0.54	0/776	0.67	1/1043 (0.1%)
28	e	0.38	0/456	0.62	0/619
29	f	0.44	0/639	0.70	1/856 (0.1%)
30	g	0.42	0/643	0.58	0/880
31	h	0.57	0/1168	0.78	2/1589 (0.1%)
32	i	0.44	0/666	0.57	1/907 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	j	0.45	0/745	0.60	0/1006
34	n	0.44	0/943	0.68	0/1279
35	1	0.61	0/2789	0.91	11/3808 (0.3%)
36	2	0.62	1/3854 (0.0%)	0.83	9/5252 (0.2%)
37	3	0.49	0/1041	0.80	1/1419 (0.1%)
38	4	0.56	0/3949	0.84	17/5392 (0.3%)
39	5	0.52	0/5327	0.76	12/7273 (0.2%)
40	6	0.49	0/1468	0.83	4/2003 (0.2%)
41	8	0.38	0/686	0.65	1/918 (0.1%)
42	9	0.45	0/684	0.64	0/918
All	All	0.52	7/65458 (0.0%)	0.74	110/88857 (0.1%)

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	A	0	3
3	C	0	1
8	H	0	2
10	J	0	1
11	K	0	1
18	S	0	1
26	c	0	2
31	h	0	1
32	i	0	1
33	j	0	1
35	1	0	1
36	2	0	1
38	4	0	1
39	5	0	3
41	8	0	1
All	All	0	21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	MET	CA-CB	-5.65	1.41	1.53
7	G	180	ARG	CB-CG	-5.58	1.37	1.52
10	J	169	ARG	C-N	-5.28	1.22	1.34
1	A	325	TRP	CB-CG	-5.26	1.40	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	74	VAL	CB-CG1	-5.24	1.41	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	258	LEU	CB-CG-CD2	-12.30	90.09	111.00
35	1	255	TYR	CB-CG-CD1	9.98	126.99	121.00
38	4	36	LEU	CB-CG-CD1	-9.88	94.21	111.00
36	2	277	LEU	CA-CB-CG	9.59	137.36	115.30
6	F	126	LEU	CA-CB-CG	9.10	136.22	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ASN	Peptide
1	A	247	ALA	Peptide
1	A	67	ARG	Sidechain
3	C	86	ASN	Peptide
8	H	29	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	690/728 (95%)	638 (92%)	52 (8%)	0	100	100
2	B	454/488 (93%)	425 (94%)	29 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	436/466 (94%)	402 (92%)	34 (8%)	0	100	100
4	D	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
5	E	345/375 (92%)	323 (94%)	22 (6%)	0	100	100
6	F	119/144 (83%)	111 (93%)	8 (7%)	0	100	100
7	G	237/281 (84%)	222 (94%)	14 (6%)	1 (0%)	30	64
8	H	214/243 (88%)	191 (89%)	22 (10%)	1 (0%)	25	60
9	I	188/229 (82%)	178 (95%)	10 (5%)	0	100	100
10	J	177/198 (89%)	171 (97%)	6 (3%)	0	100	100
11	K	175/210 (83%)	161 (92%)	14 (8%)	0	100	100
12	L	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
13	M	115/136 (85%)	106 (92%)	7 (6%)	2 (2%)	7	36
14	O	75/109 (69%)	71 (95%)	4 (5%)	0	100	100
15	P	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
16	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
17	R	104/109 (95%)	98 (94%)	6 (6%)	0	100	100
18	S	168/249 (68%)	164 (98%)	4 (2%)	0	100	100
19	U	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
20	W	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
21	X	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
22	Y	121/161 (75%)	113 (93%)	7 (6%)	1 (1%)	16	51
23	Z	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
24	a	122/149 (82%)	111 (91%)	11 (9%)	0	100	100
25	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100
26	c	42/60 (70%)	37 (88%)	5 (12%)	0	100	100
27	d	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
28	e	50/67 (75%)	48 (96%)	2 (4%)	0	100	100
29	f	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
30	g	74/78 (95%)	66 (89%)	8 (11%)	0	100	100
31	h	134/138 (97%)	127 (95%)	6 (4%)	1 (1%)	19	54
32	i	81/90 (90%)	76 (94%)	5 (6%)	0	100	100
33	j	88/93 (95%)	83 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	n	112/120 (93%)	103 (92%)	9 (8%)	0	100	100
35	1	338/341 (99%)	318 (94%)	20 (6%)	0	100	100
36	2	467/469 (100%)	435 (93%)	30 (6%)	2 (0%)	30	64
37	3	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
38	4	484/486 (100%)	466 (96%)	18 (4%)	0	100	100
39	5	652/655 (100%)	617 (95%)	34 (5%)	1 (0%)	44	75
40	6	181/185 (98%)	170 (94%)	11 (6%)	0	100	100
41	8	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
42	9	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
All	All	7967/8704 (92%)	7480 (94%)	478 (6%)	9 (0%)	50	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	5	555	VAL
13	M	77	ALA
31	h	108	PRO
22	Y	89	ASN
36	2	188	ASP

### 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	A	565/595 (95%)	565 (100%)	0	100	100
2	B	364/389 (94%)	364 (100%)	0	100	100
3	C	374/394 (95%)	374 (100%)	0	100	100
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	305/329 (93%)	305 (100%)	0	100	100
6	F	109/129 (84%)	109 (100%)	0	100	100
7	G	216/245 (88%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	191/212 (90%)	191 (100%)	0	100	100
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	154/180 (86%)	154 (100%)	0	100	100
12	L	77/77 (100%)	77 (100%)	0	100	100
13	M	97/115 (84%)	97 (100%)	0	100	100
14	O	65/91 (71%)	65 (100%)	0	100	100
15	P	109/110 (99%)	109 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	97/100 (97%)	97 (100%)	0	100	100
18	S	149/211 (71%)	149 (100%)	0	100	100
19	U	147/148 (99%)	147 (100%)	0	100	100
20	W	100/102 (98%)	100 (100%)	0	100	100
21	X	131/133 (98%)	131 (100%)	0	100	100
22	Y	105/140 (75%)	105 (100%)	0	100	100
23	Z	147/148 (99%)	147 (100%)	0	100	100
24	a	108/129 (84%)	107 (99%)	1 (1%)	75	89
25	b	50/59 (85%)	50 (100%)	0	100	100
26	c	30/45 (67%)	30 (100%)	0	100	100
27	d	83/85 (98%)	83 (100%)	0	100	100
28	e	44/55 (80%)	44 (100%)	0	100	100
29	f	69/73 (94%)	68 (99%)	1 (1%)	62	82
30	g	62/64 (97%)	62 (100%)	0	100	100
31	h	121/123 (98%)	120 (99%)	1 (1%)	79	90
32	i	64/68 (94%)	64 (100%)	0	100	100
33	j	71/73 (97%)	71 (100%)	0	100	100
34	n	98/102 (96%)	98 (100%)	0	100	100
35	1	301/302 (100%)	301 (100%)	0	100	100
36	2	433/433 (100%)	433 (100%)	0	100	100
37	3	113/114 (99%)	113 (100%)	0	100	100
38	4	434/434 (100%)	433 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	5	579/580 (100%)	579 (100%)	0	100	100
40	6	165/167 (99%)	165 (100%)	0	100	100
41	8	69/76 (91%)	69 (100%)	0	100	100
42	9	73/76 (96%)	73 (100%)	0	100	100
All	All	6895/7420 (93%)	6891 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	a	64	ARG
29	f	41	LYS
31	h	75	PRO
38	4	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
21	X	142	ASN
28	e	53	HIS
39	5	331	HIS
21	X	161	HIS
22	Y	135	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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$
46	3PE	4	502	-	42,42,50	0.93	4 (9%)	45,47,55	1.14	2 (4%)
50	PLC	K	302	-	38,38,41	1.35	5 (13%)	44,46,49	1.05	2 (4%)
50	PLC	5	803	-	30,30,41	1.47	4 (13%)	36,38,49	1.12	2 (5%)
43	SF4	A	802	1	0,12,12	-	-	-		
50	PLC	1	502	-	34,34,41	1.46	6 (17%)	40,42,49	1.22	2 (5%)
43	SF4	K	301	11	0,12,12	-	-	-		
43	SF4	A	801	1	0,12,12	-	-	-		
46	3PE	4	501	-	41,41,50	0.93	4 (9%)	44,46,55	1.11	2 (4%)
48	CDL	E	403	-	71,71,99	1.04	6 (8%)	77,83,111	1.17	4 (5%)
54	T7X	2	501	-	48,48,61	0.93	2 (4%)	57,60,73	1.41	8 (14%)
46	3PE	4	505	-	50,50,50	0.85	3 (6%)	53,55,55	1.22	2 (3%)
54	T7X	3	201	-	49,49,61	0.93	4 (8%)	59,61,73	1.33	7 (11%)
49	LMN	J	202	-	72,72,72	1.52	9 (12%)	96,98,98	1.72	19 (19%)
48	CDL	4	503	-	91,91,99	0.92	7 (7%)	97,103,111	1.22	6 (6%)
45	FMN	B	502	-	33,33,33	2.81	11 (33%)	48,50,50	1.62	11 (22%)
43	SF4	I	301	9	0,12,12	-	-	-		
50	PLC	W	402	-	41,41,41	1.30	5 (12%)	47,49,49	1.22	3 (6%)
44	FES	H	301	8	0,4,4	-	-	-		
48	CDL	X	201	-	85,85,99	0.92	8 (9%)	91,97,111	1.24	5 (5%)
50	PLC	n	1101	-	41,41,41	1.30	5 (12%)	47,49,49	1.09	2 (4%)
50	PLC	W	401	-	40,40,41	1.31	4 (10%)	46,48,49	1.14	3 (6%)
48	CDL	Z	201	-	75,75,99	0.99	7 (9%)	81,87,111	1.10	4 (4%)
52	ZMP	O	201	14	26,32,36	1.86	6 (23%)	31,39,45	1.93	7 (22%)
53	UQ9	1	501	-	35,35,58	2.48	15 (42%)	42,45,73	1.53	11 (26%)
46	3PE	b	201	-	41,41,50	0.93	4 (9%)	44,46,55	1.20	2 (4%)
46	3PE	g	202	-	42,42,50	0.94	4 (9%)	45,47,55	1.23	2 (4%)
48	CDL	g	201	-	82,82,99	0.95	6 (7%)	88,94,111	1.24	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	3PE	W	404	-	33,33,50	1.03	4 (12%)	36,38,55	1.12	2 (5%)
49	LMN	j	101	-	68,68,72	1.58	13 (19%)	92,94,98	1.63	15 (16%)
44	FES	A	803	1	0,4,4	-	-	-	-	-
48	CDL	j	102	-	77,77,99	0.99	7 (9%)	83,89,111	1.14	5 (6%)
46	3PE	J	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.22	3 (6%)
46	3PE	5	804	-	50,50,50	0.89	3 (6%)	53,55,55	1.04	2 (3%)
43	SF4	B	501	2	0,12,12	-	-	-	-	-
47	NDP	E	401	-	45,52,52	3.95	18 (40%)	53,80,80	2.31	6 (11%)
52	ZMP	Q	201	16	26,32,36	1.86	6 (23%)	31,39,45	1.84	4 (12%)
54	T7X	5	801	-	43,43,61	1.06	4 (9%)	53,55,73	1.65	10 (18%)
46	3PE	1	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.20	2 (5%)
55	CPL	2	502	-	51,51,51	0.98	4 (7%)	57,59,59	0.93	3 (5%)
54	T7X	2	503	-	52,52,61	0.90	4 (7%)	62,64,73	1.29	5 (8%)
43	SF4	I	302	9	0,12,12	-	-	-	-	-
46	3PE	4	504	-	41,41,50	0.93	4 (9%)	44,46,55	1.08	2 (4%)
46	3PE	C	501	-	50,50,50	0.89	4 (8%)	53,55,55	1.26	3 (5%)
46	3PE	E	402	-	35,35,50	1.03	4 (11%)	38,40,55	1.18	2 (5%)
50	PLC	W	403	-	41,41,41	1.30	4 (9%)	47,49,49	1.07	3 (6%)
46	3PE	5	802	-	41,41,50	0.98	4 (9%)	44,46,55	1.31	3 (6%)
46	3PE	1	504	-	35,35,50	1.01	4 (11%)	38,40,55	1.14	2 (5%)
46	3PE	J	203	-	43,43,50	0.93	4 (9%)	46,48,55	1.17	2 (4%)

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
46	3PE	4	502	-	-	21/46/46/54	-
50	PLC	K	302	-	-	15/42/42/45	-
50	PLC	5	803	-	-	15/34/34/45	-
43	SF4	A	802	1	-	-	0/6/5/5
50	PLC	1	502	-	-	12/38/38/45	-
46	3PE	4	501	-	-	18/45/45/54	-
43	SF4	A	801	1	-	-	0/6/5/5
48	CDL	E	403	-	-	35/82/82/110	-
43	SF4	K	301	11	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	T7X	2	501	-	-	16/43/67/80	0/1/1/1
46	3PE	4	505	-	-	22/54/54/54	-
54	T7X	3	201	-	-	21/44/68/80	0/1/1/1
49	LMN	J	202	-	-	22/50/130/130	0/4/4/4
48	CDL	4	503	-	-	48/102/102/110	-
45	FMN	B	502	-	-	10/18/18/18	0/3/3/3
50	PLC	W	402	-	-	24/45/45/45	-
43	SF4	I	301	9	-	-	0/6/5/5
44	FES	H	301	8	-	-	0/1/1/1
48	CDL	X	201	-	-	34/96/96/110	-
50	PLC	n	1101	-	-	11/45/45/45	-
50	PLC	W	401	-	-	19/44/44/45	-
48	CDL	Z	201	-	-	43/86/86/110	-
52	ZMP	O	201	14	-	5/37/39/43	-
53	UQ9	1	501	-	-	7/30/54/81	0/1/1/1
46	3PE	b	201	-	-	21/45/45/54	-
46	3PE	g	202	-	-	18/46/46/54	-
48	CDL	g	201	-	-	39/93/93/110	-
46	3PE	W	404	-	-	15/37/37/54	-
49	LMN	j	101	-	-	21/46/126/130	0/4/4/4
44	FES	A	803	1	-	-	0/1/1/1
48	CDL	j	102	-	-	32/88/88/110	-
46	3PE	J	201	-	-	13/44/44/54	-
46	3PE	5	804	-	-	12/54/54/54	-
52	ZMP	Q	201	16	-	10/37/39/43	-
47	NDP	E	401	-	-	13/30/77/77	0/5/5/5
43	SF4	B	501	2	-	-	0/6/5/5
54	T7X	5	801	-	-	15/38/62/80	0/1/1/1
46	3PE	1	503	-	-	21/39/39/54	-
55	CPL	2	502	-	-	31/55/55/55	-
54	T7X	2	503	-	-	12/47/71/80	0/1/1/1
43	SF4	I	302	9	-	-	0/6/5/5
46	3PE	4	504	-	-	23/45/45/54	-
46	3PE	C	501	-	-	28/54/54/54	-
46	3PE	E	402	-	-	14/39/39/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PLC	W	403	-	-	18/45/45/45	-
46	3PE	5	802	-	-	19/45/45/54	-
46	3PE	1	504	-	-	21/39/39/54	-
46	3PE	J	203	-	-	21/47/47/54	-

The worst 5 of 228 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	E	401	NDP	O4B-C1B	13.51	1.59	1.41
47	E	401	NDP	C6N-C5N	12.21	1.55	1.33
53	1	501	UQ9	C6-C1	9.39	1.52	1.35
45	B	502	FMN	C4A-N5	7.65	1.45	1.30
47	E	401	NDP	O4D-C1D	7.48	1.59	1.42

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	E	401	NDP	C5A-C6A-N6A	9.69	135.07	120.35
47	E	401	NDP	C1B-N9A-C4A	-8.46	111.77	126.64
52	Q	201	ZMP	C9-C10-S1	6.79	121.36	113.46
47	E	401	NDP	N6A-C6A-N1A	-6.64	104.79	118.57
52	O	201	ZMP	C9-C10-S1	6.29	120.78	113.46

There are no chirality outliers.

5 of 815 torsion outliers are listed below:

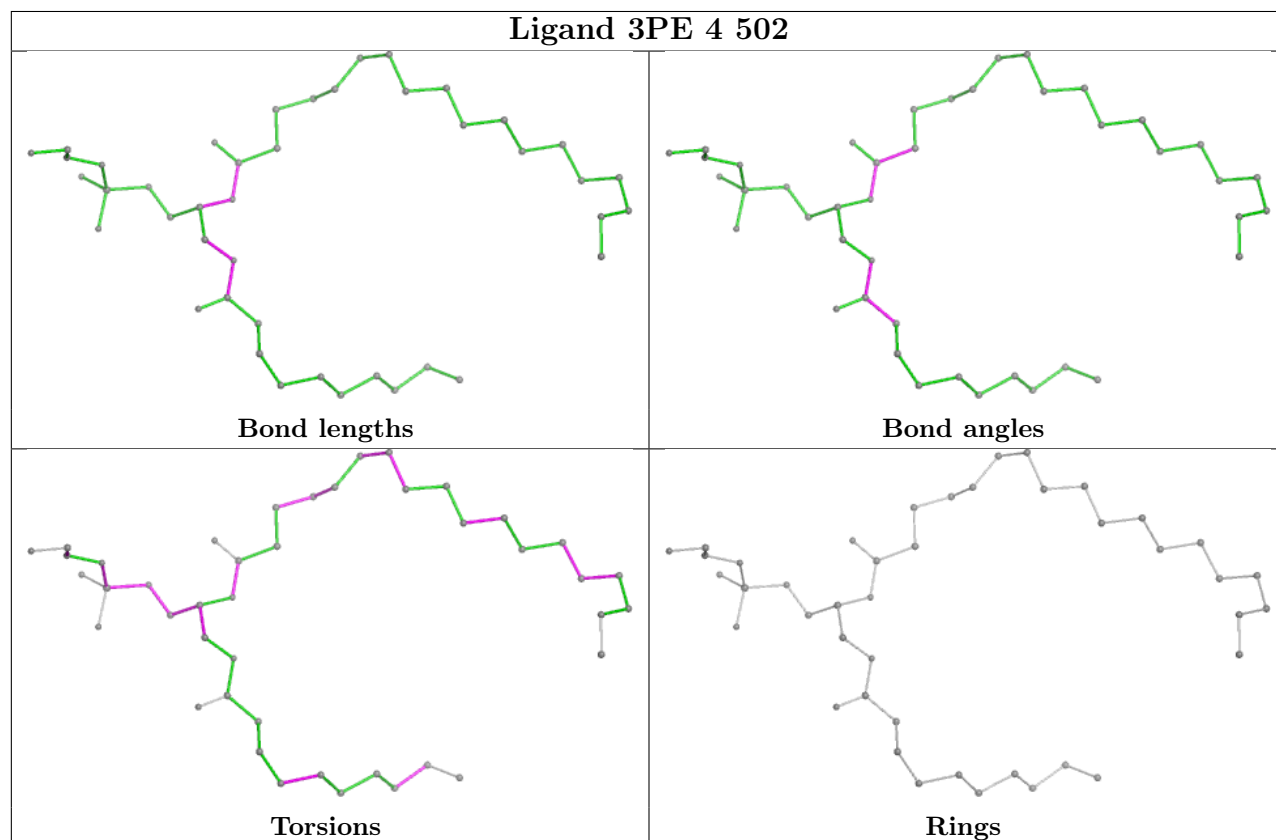
Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O2'-C2'-C3'-O3'

There are no ring outliers.

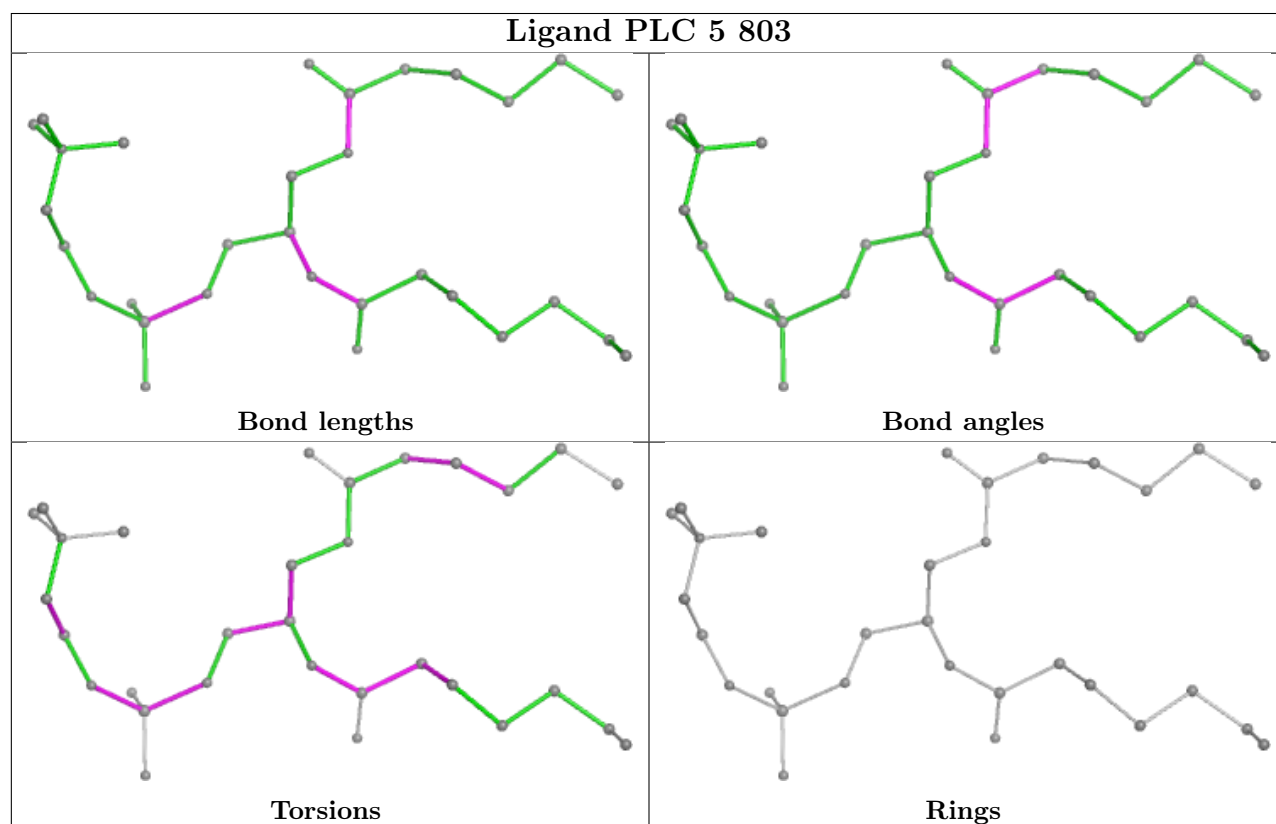
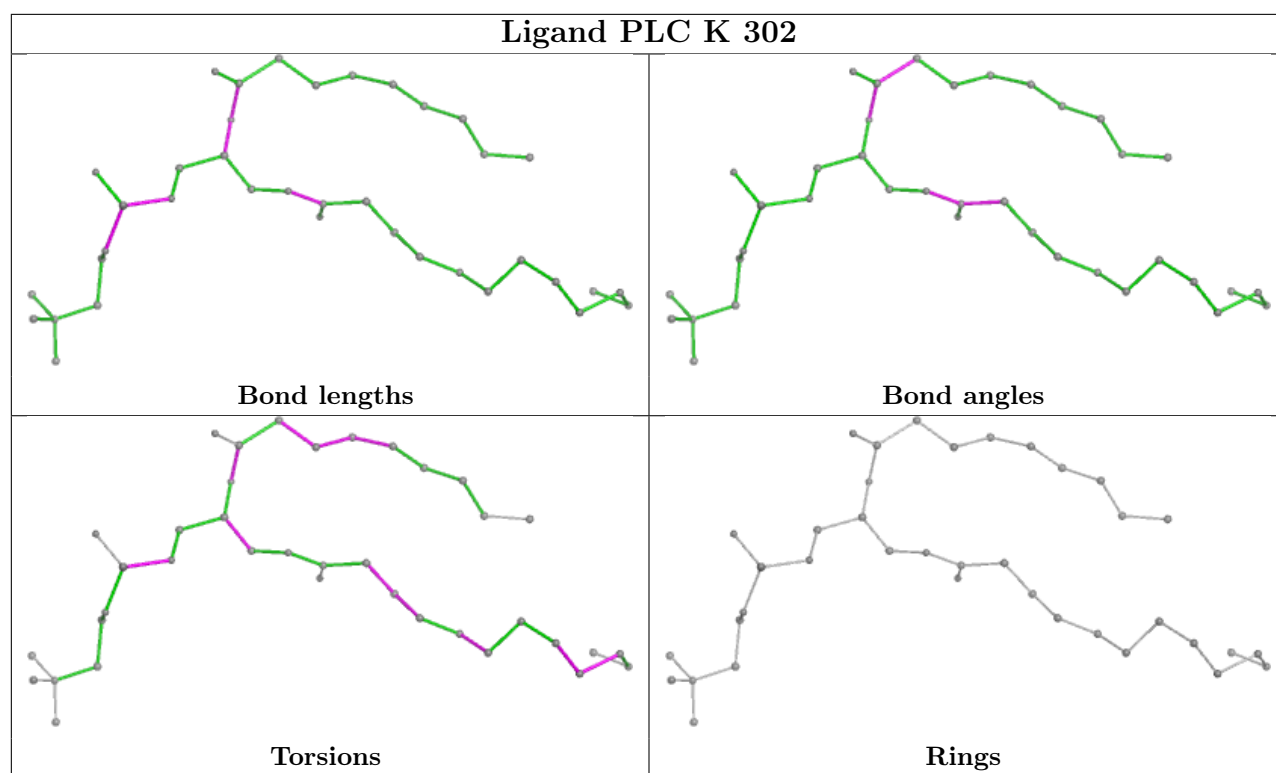
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

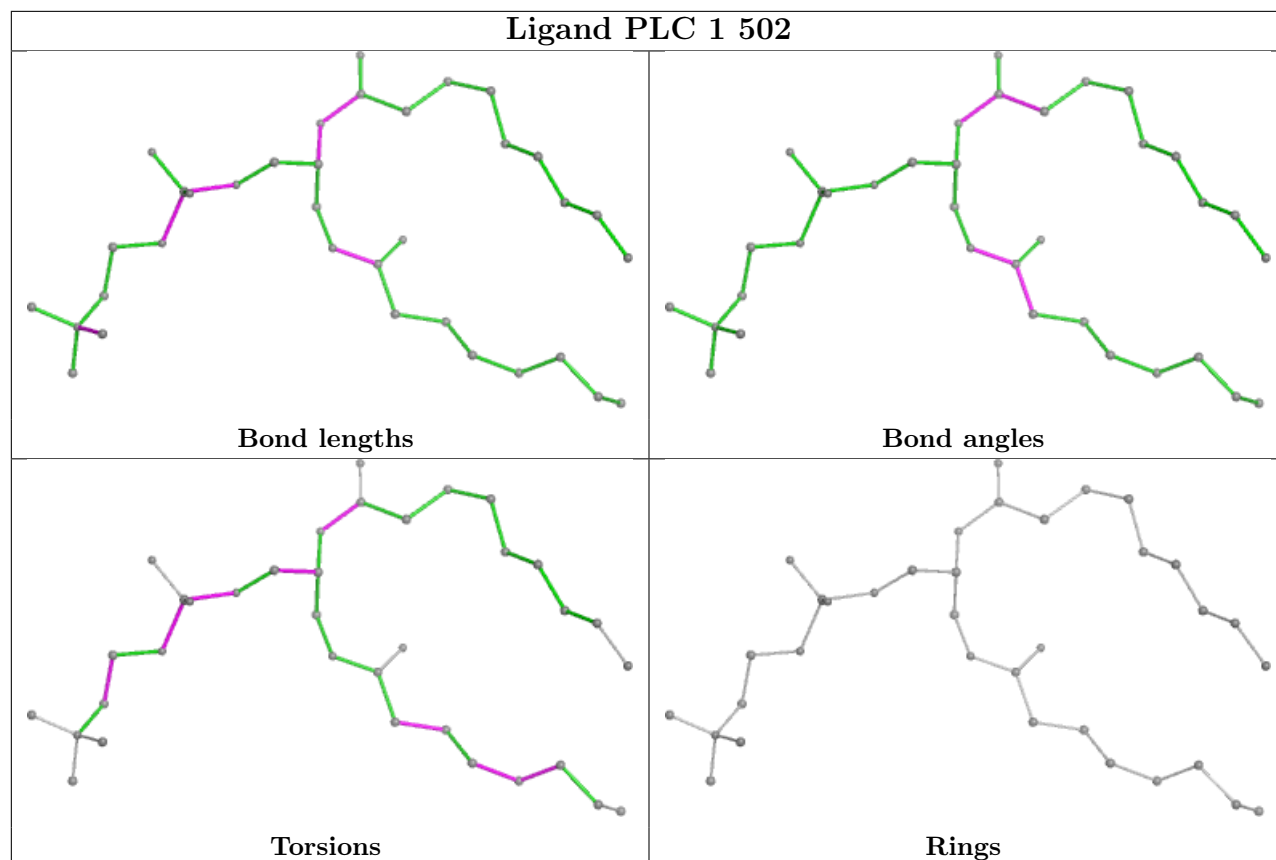
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



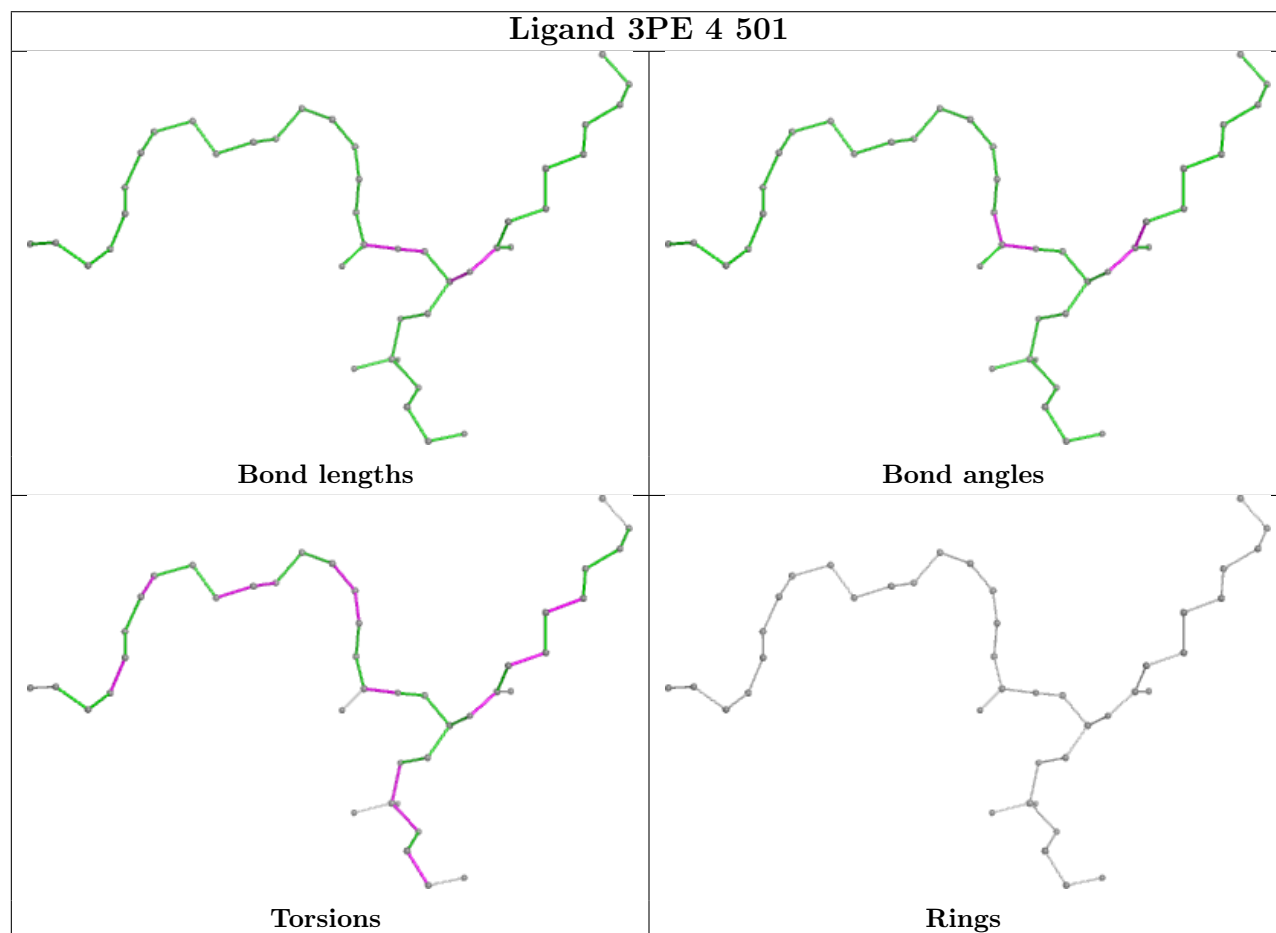




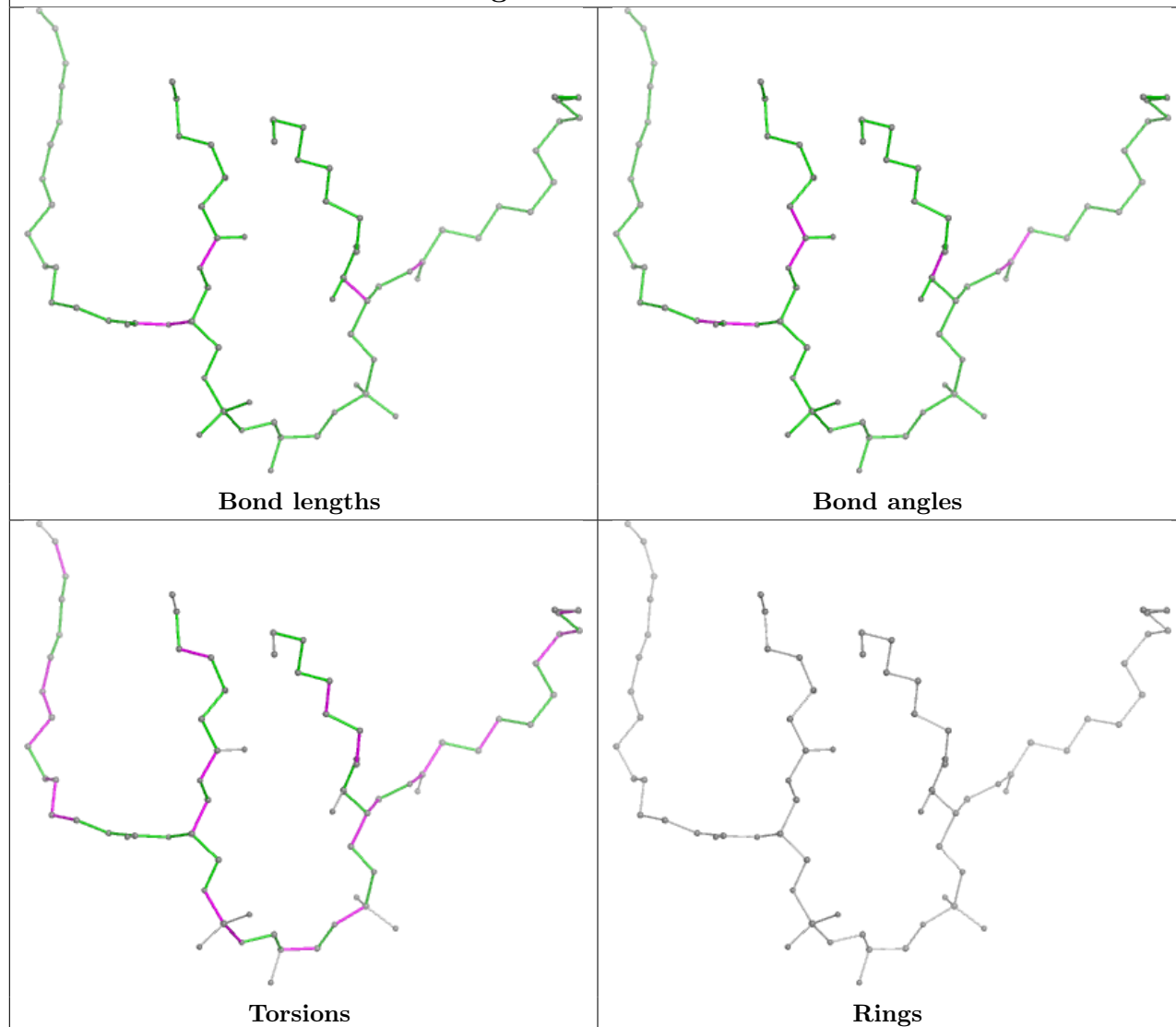
## Ligand PLC 1 502



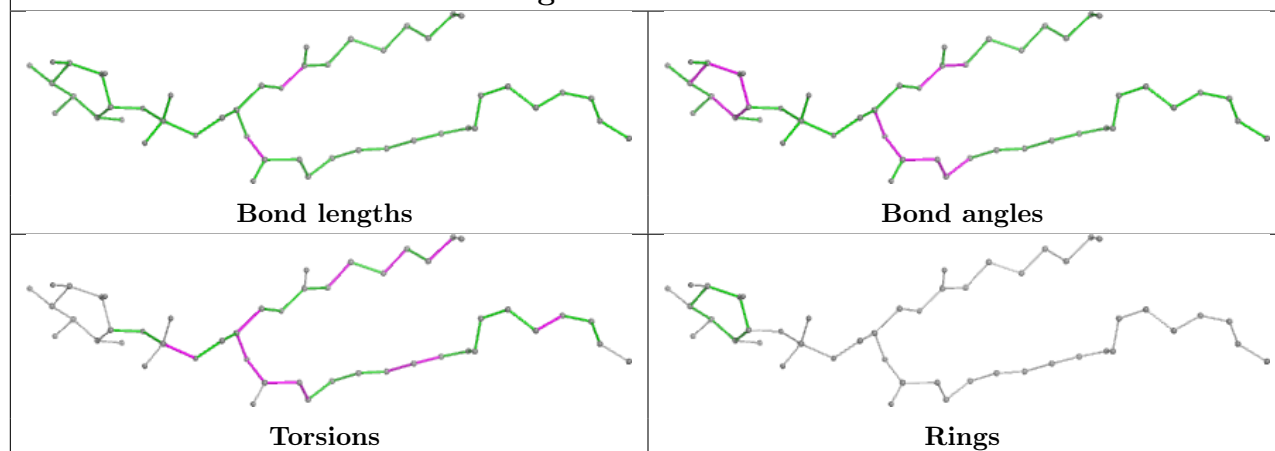
## Ligand 3PE 4 501

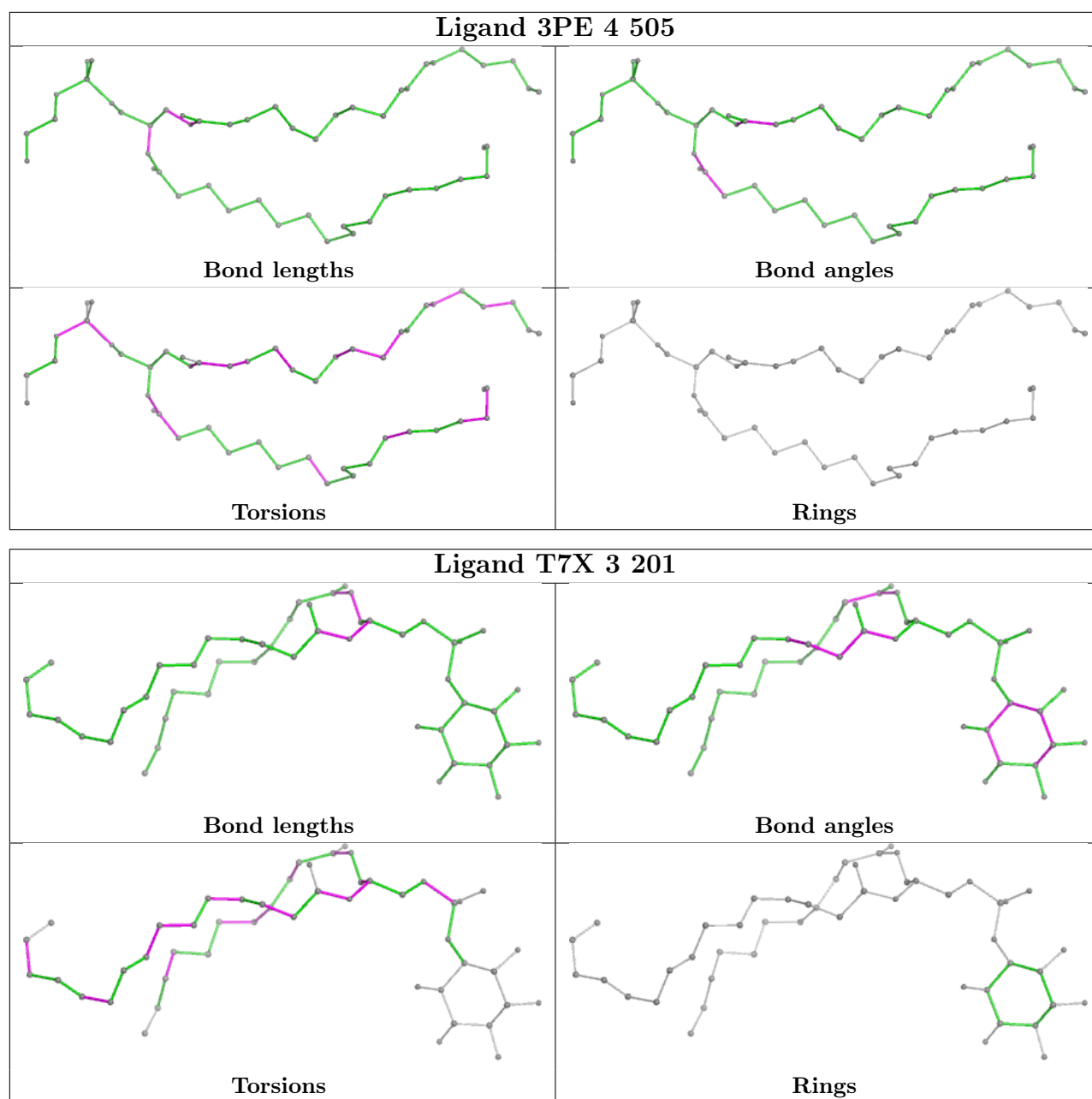


## Ligand CDL E 403

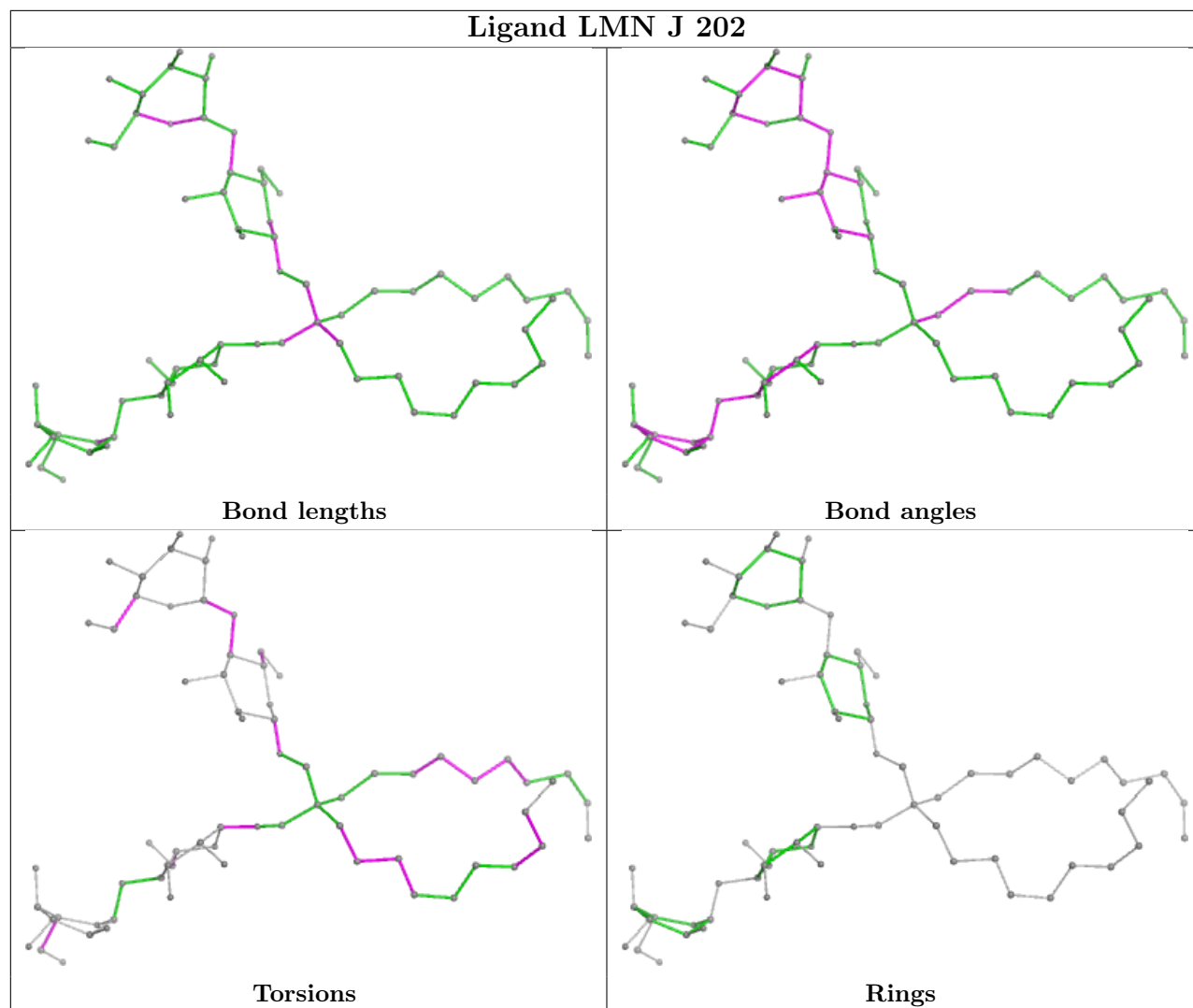


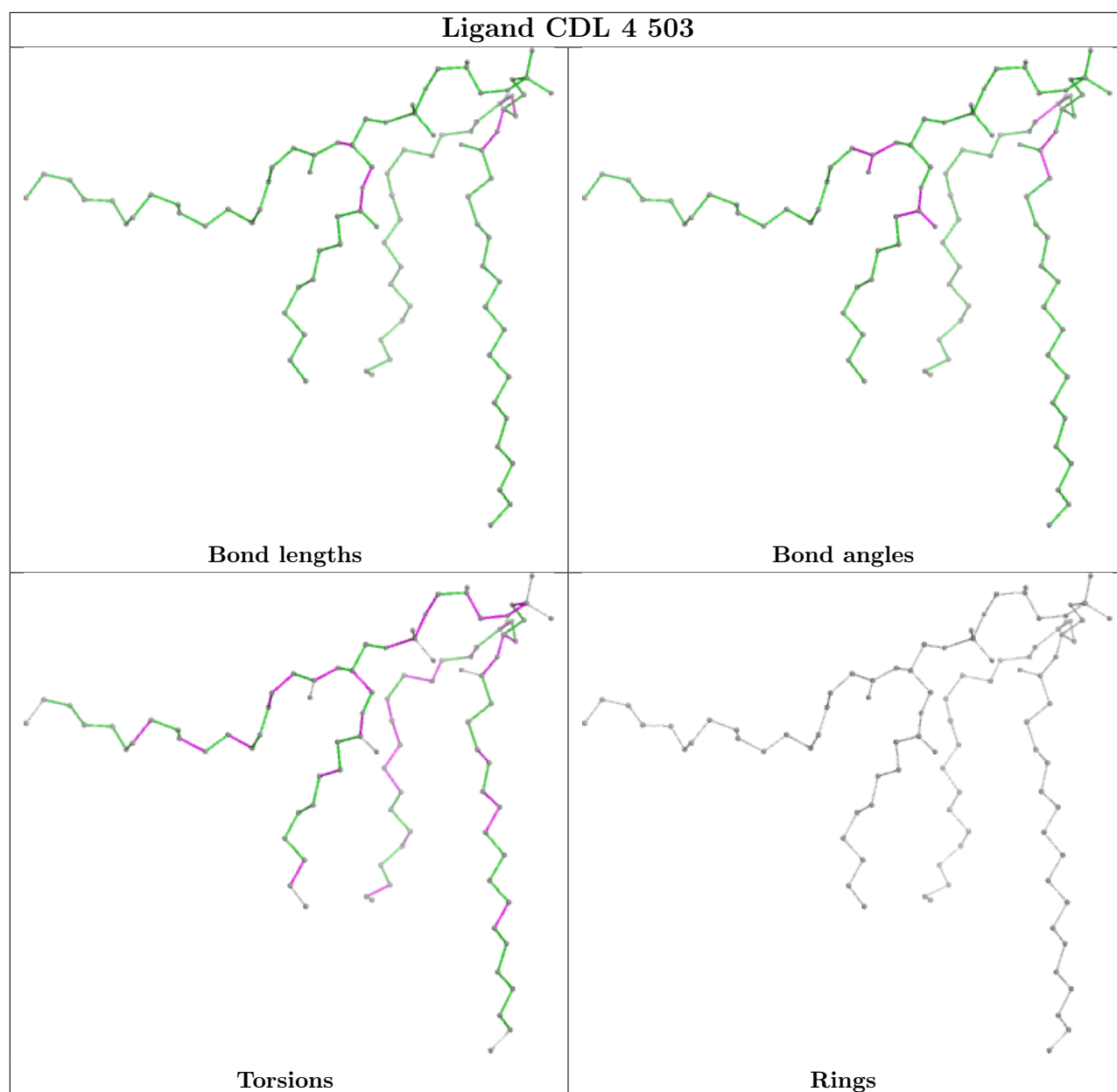
## Ligand T7X 2 501

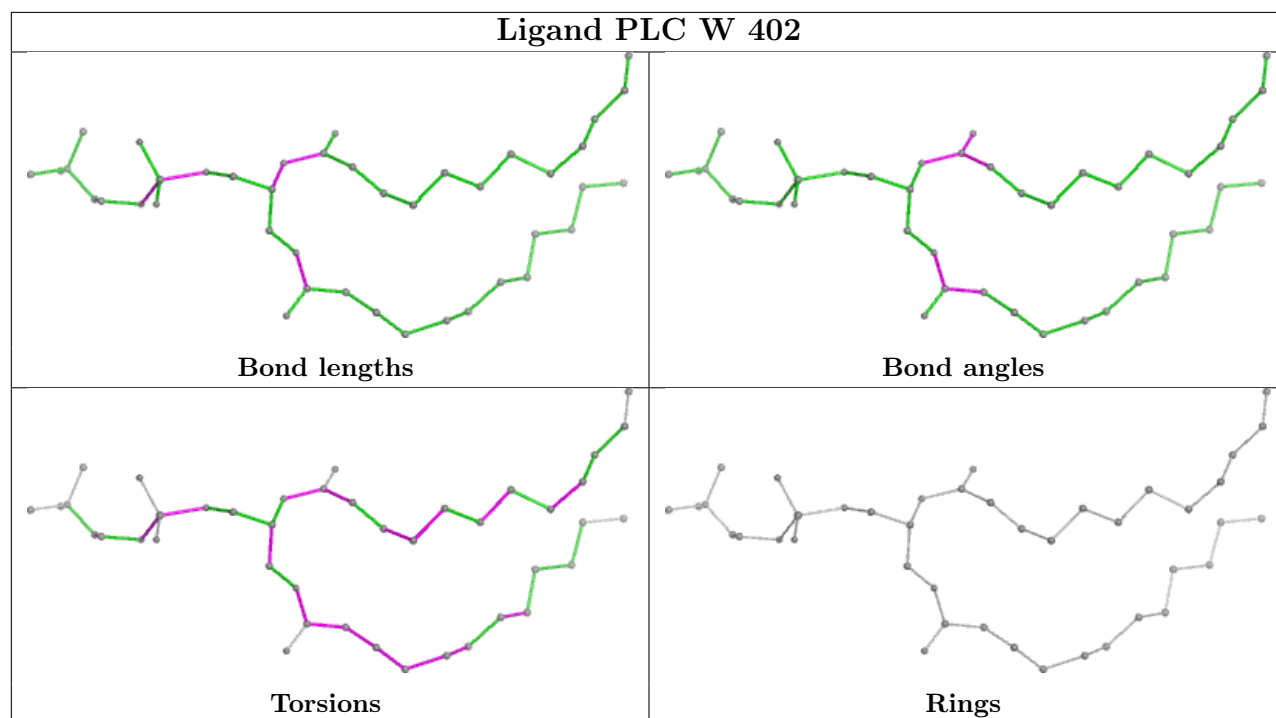
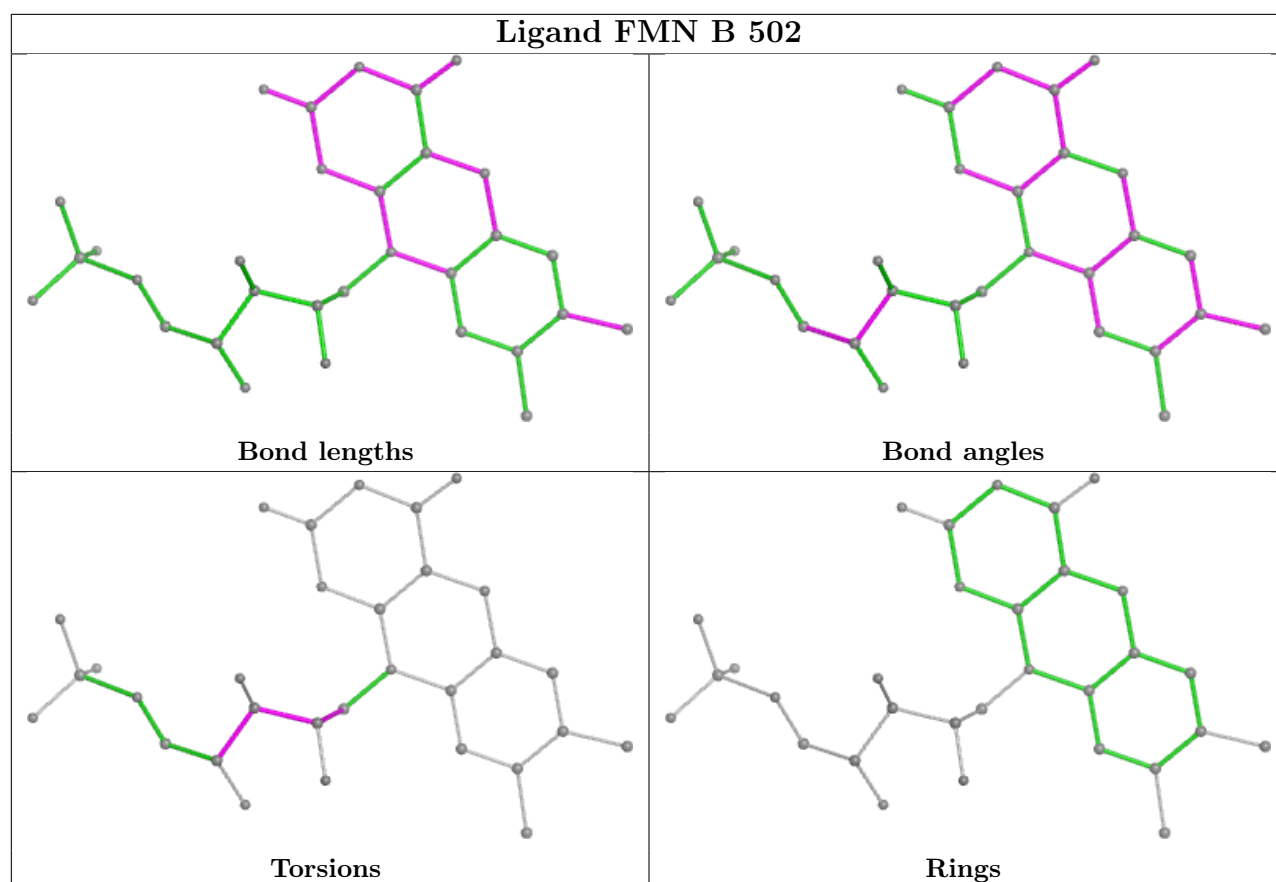


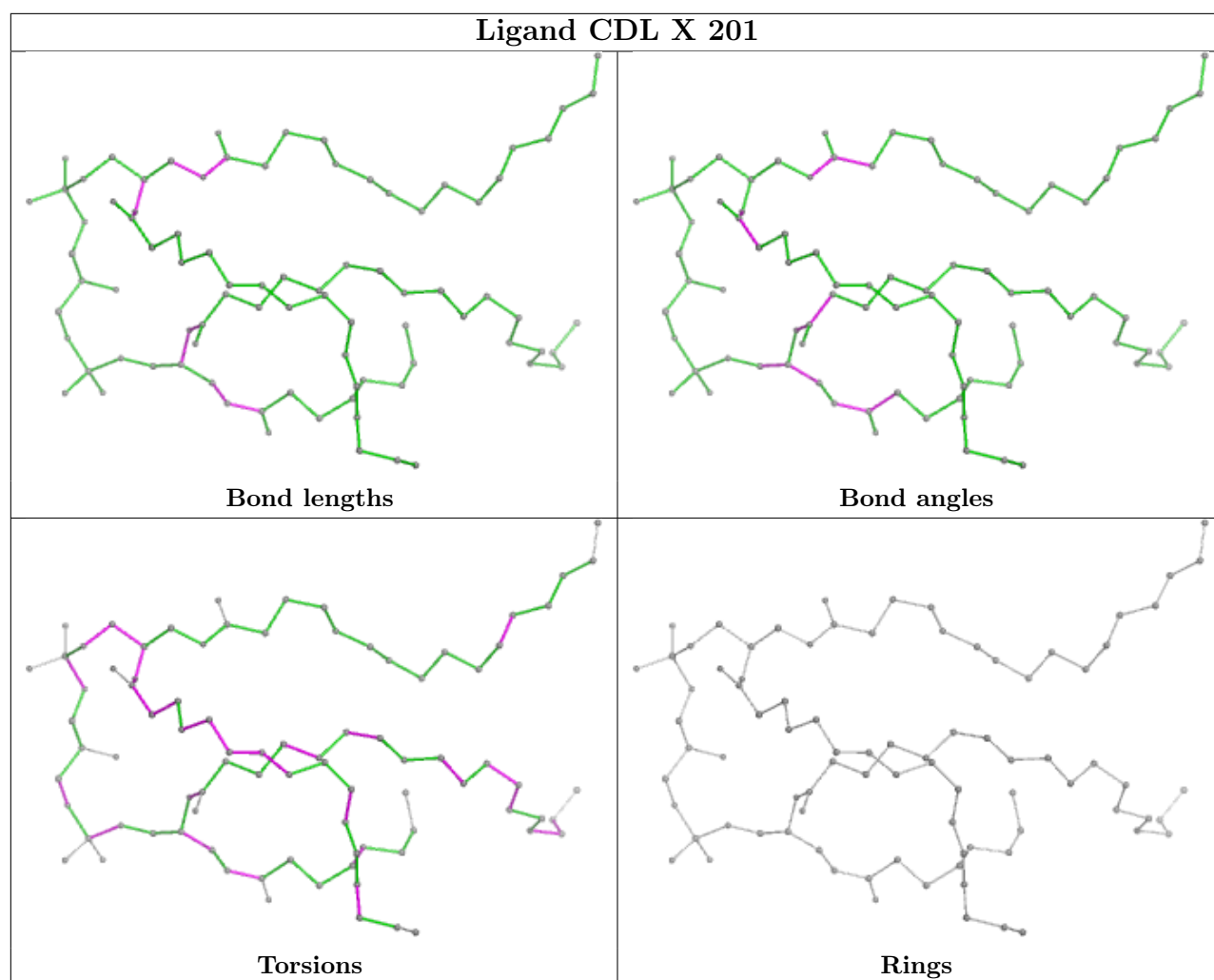


## Ligand LMN J 202

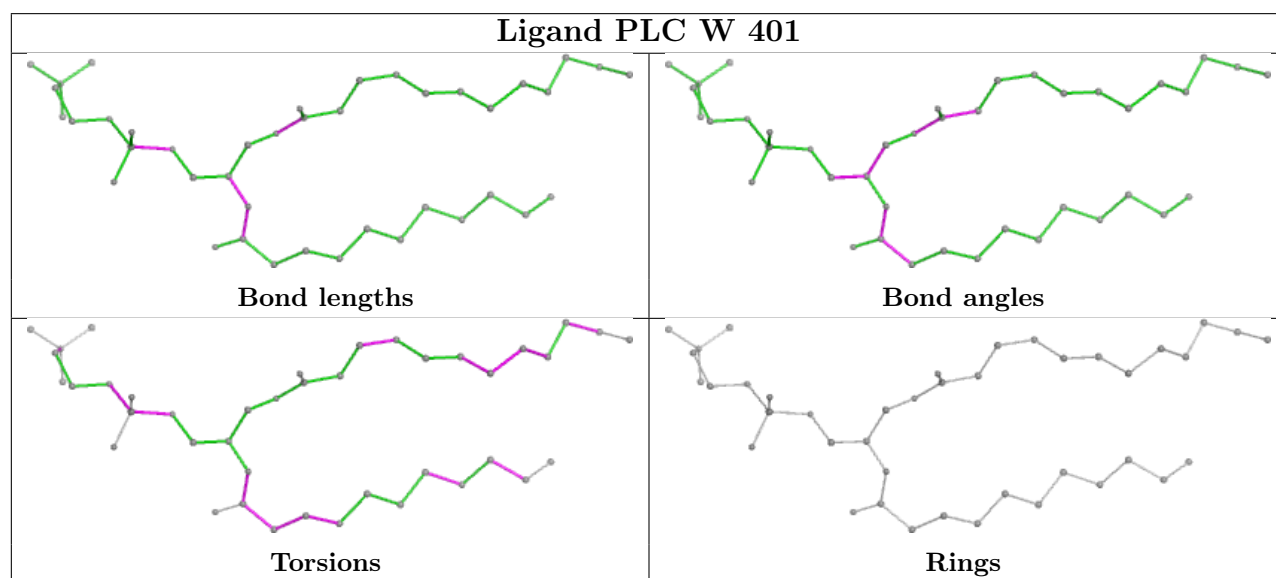
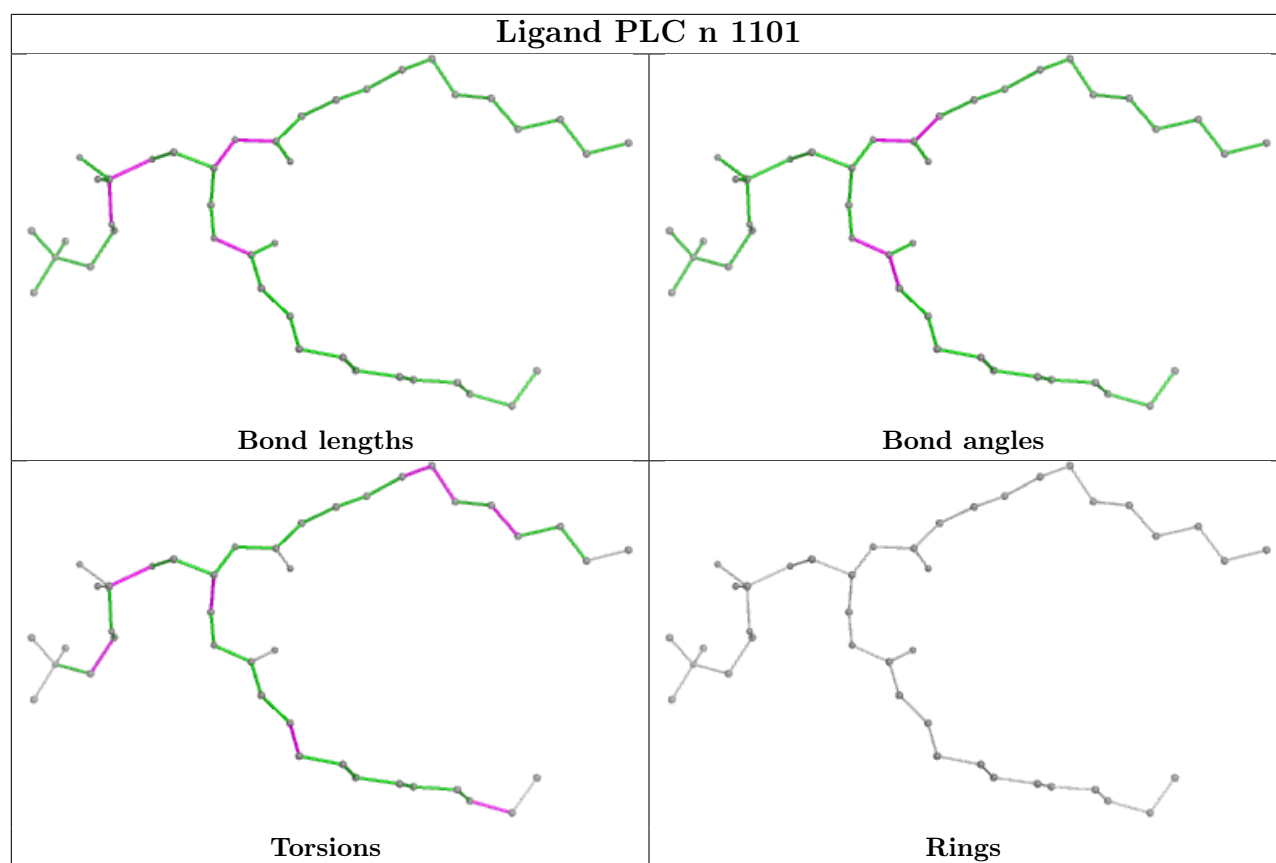




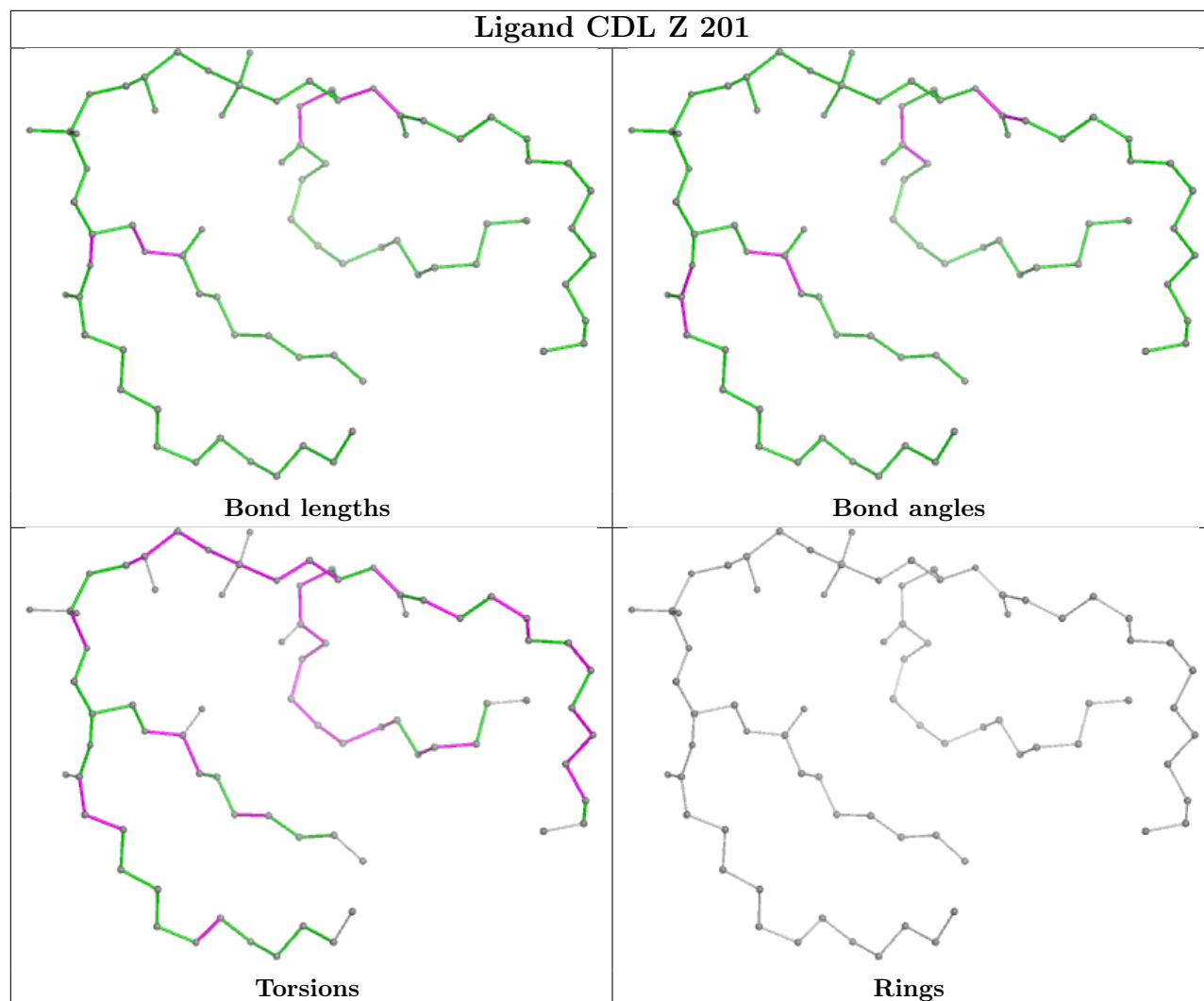




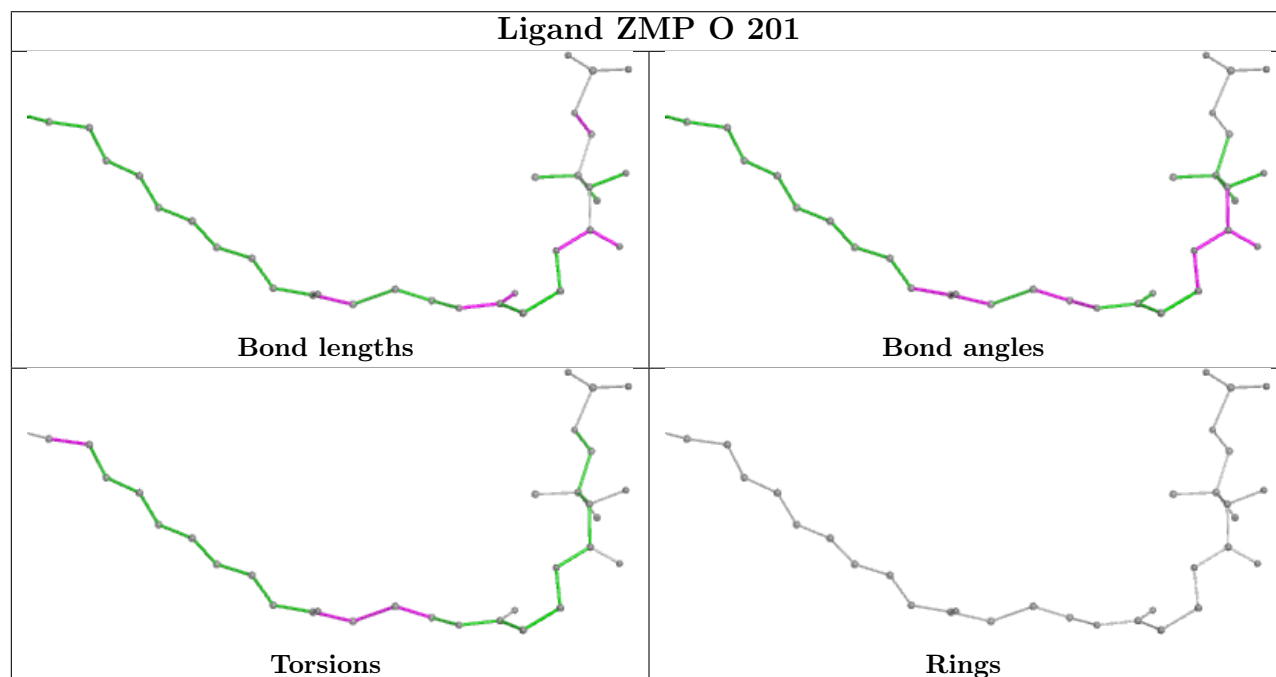


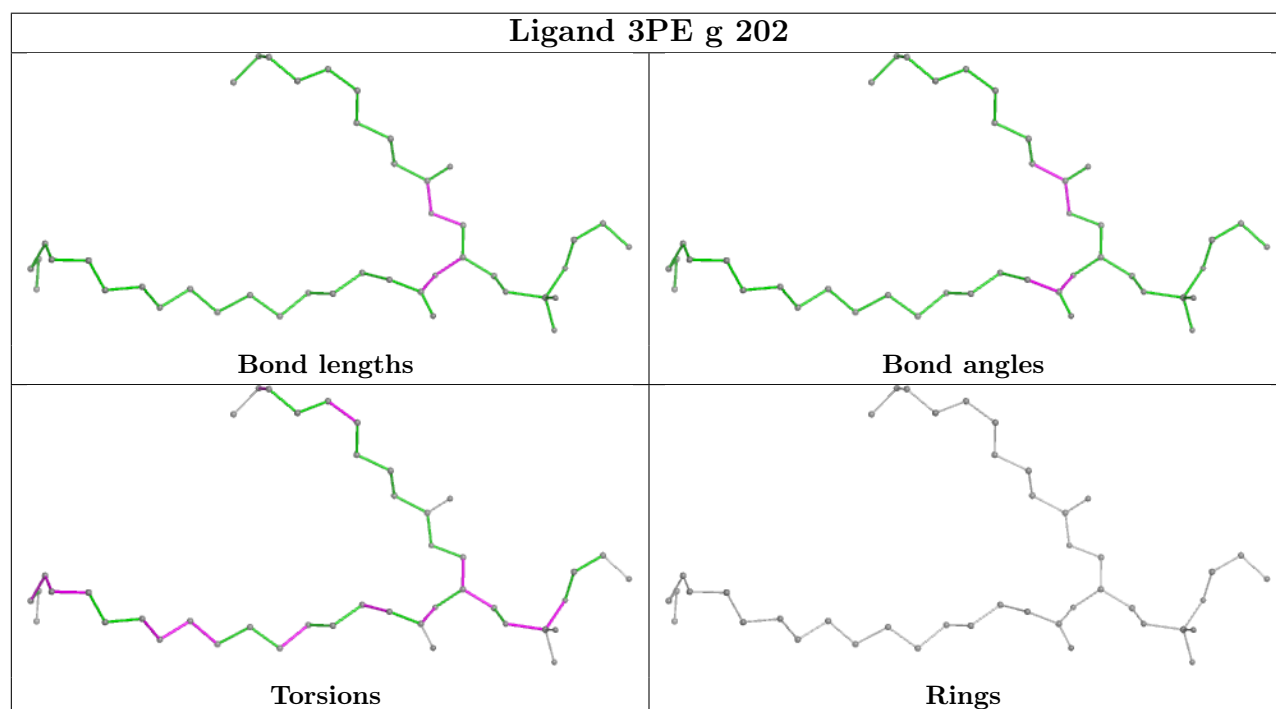
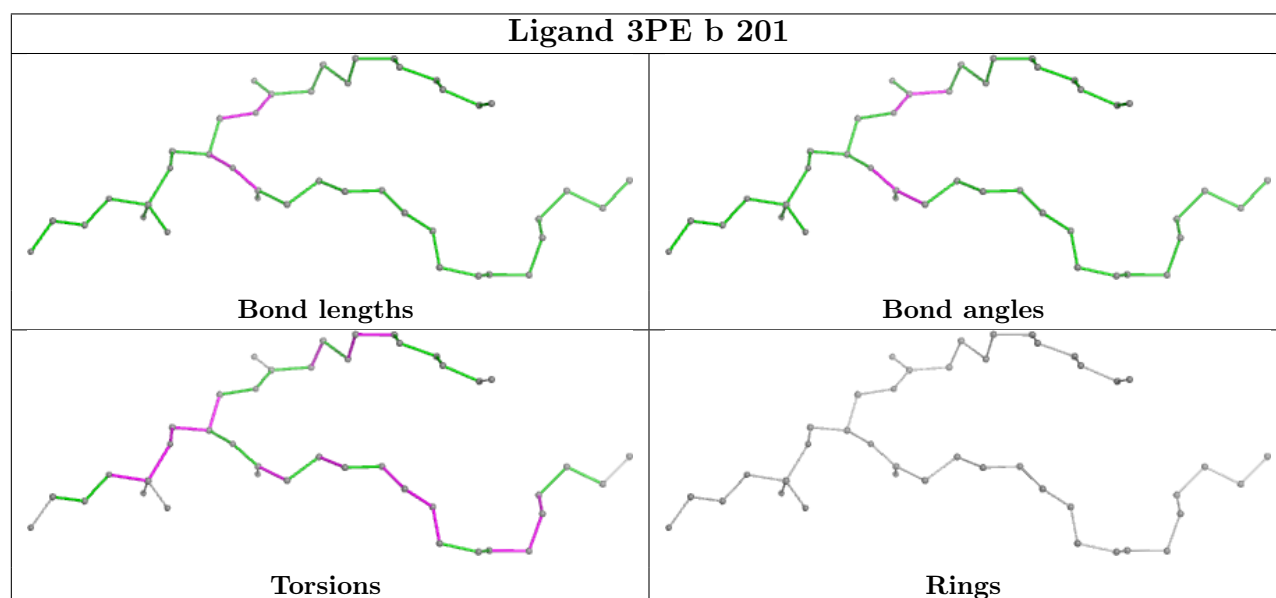
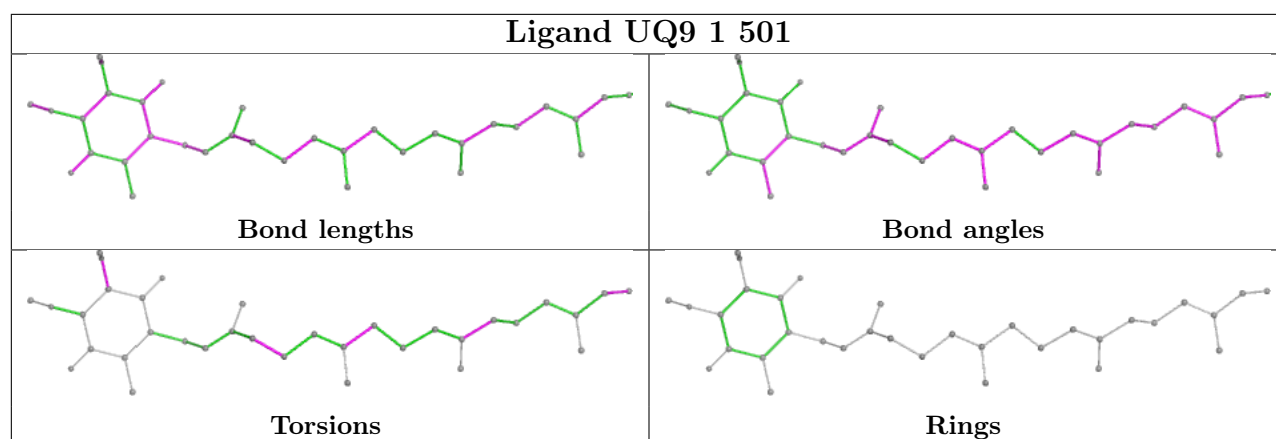


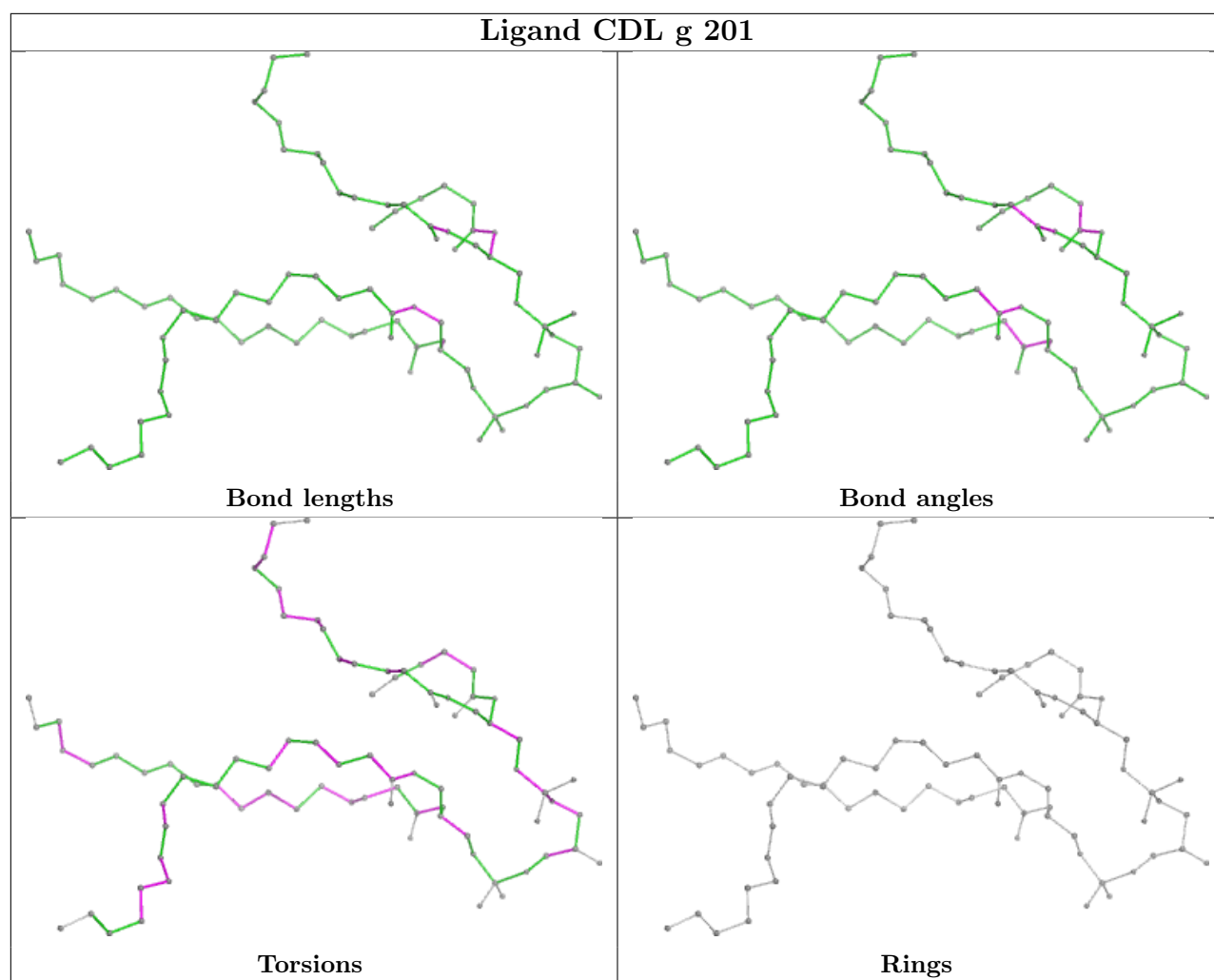
## Ligand CDL Z 201

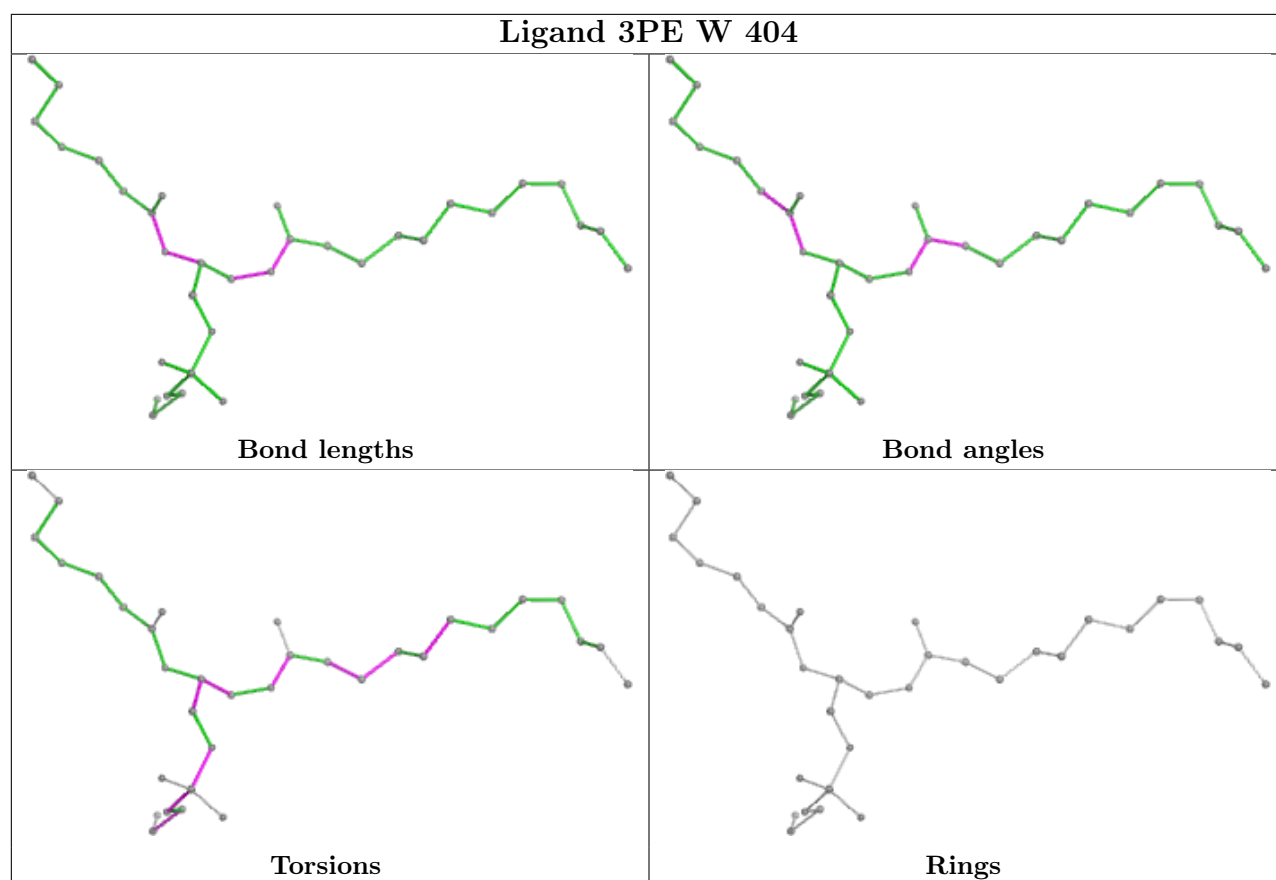


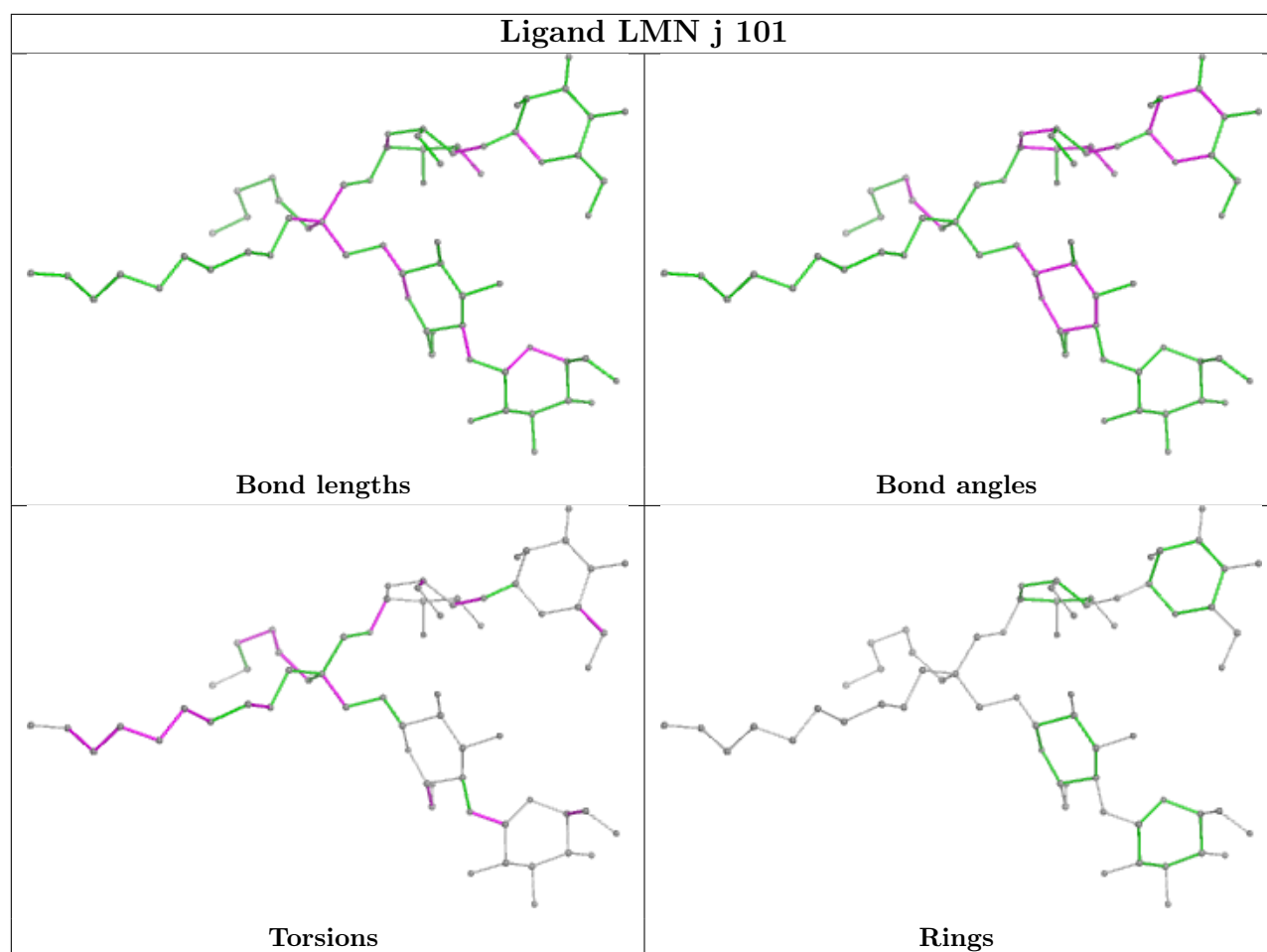
## Ligand ZMP O 201

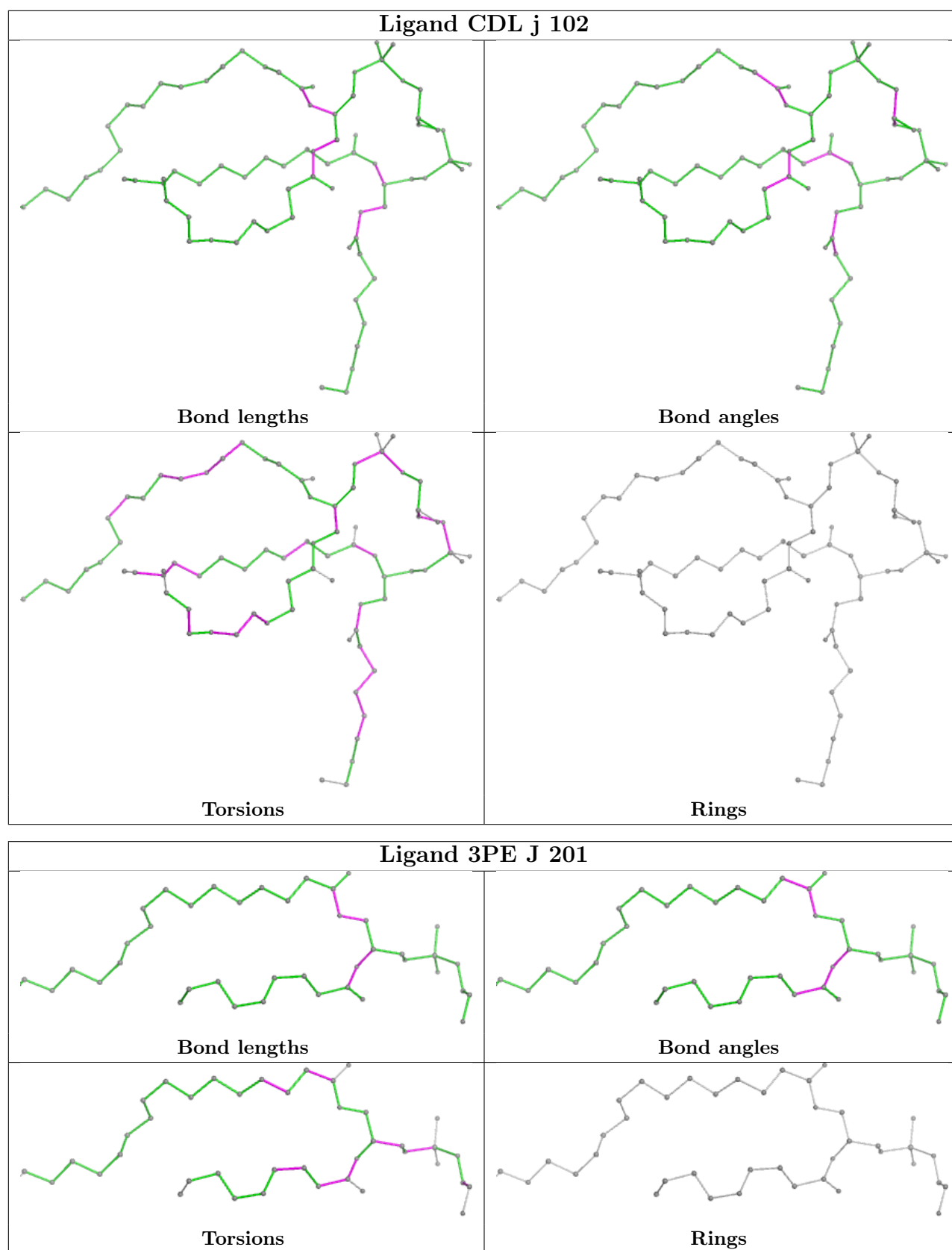


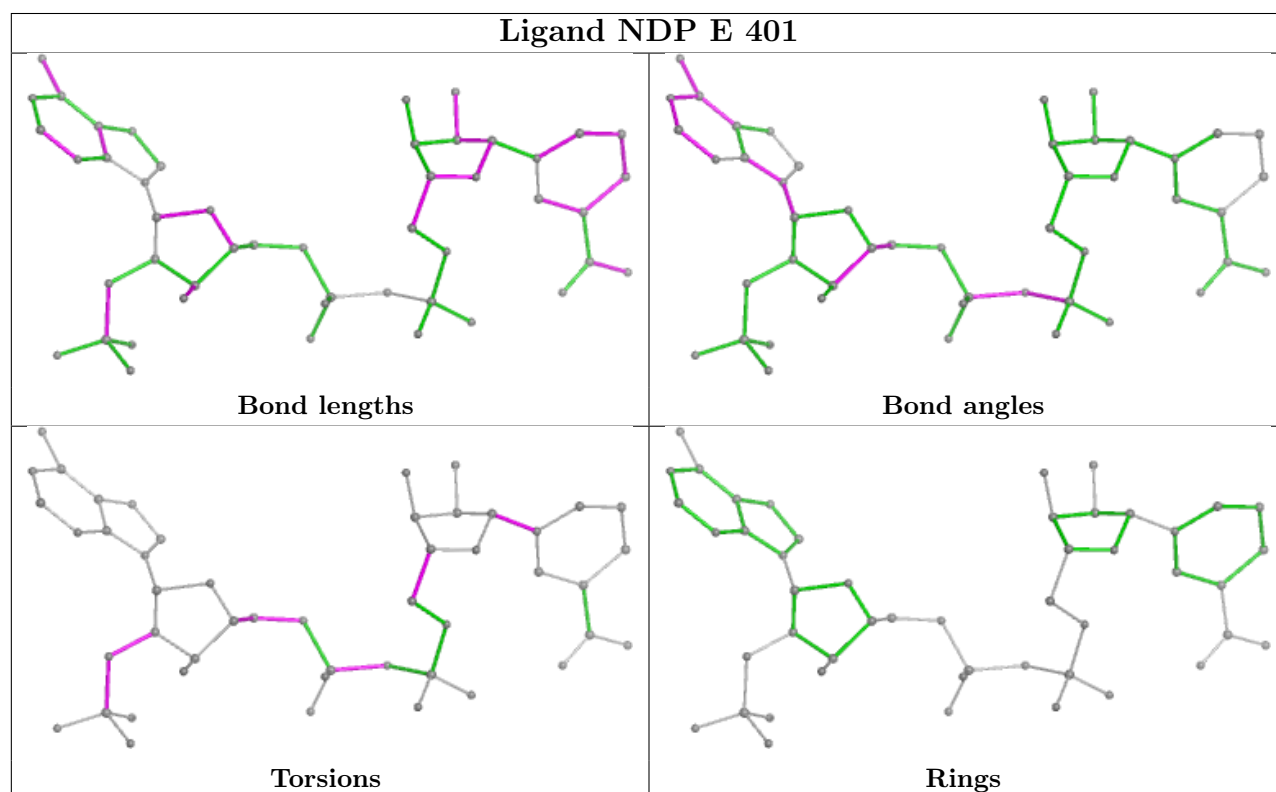
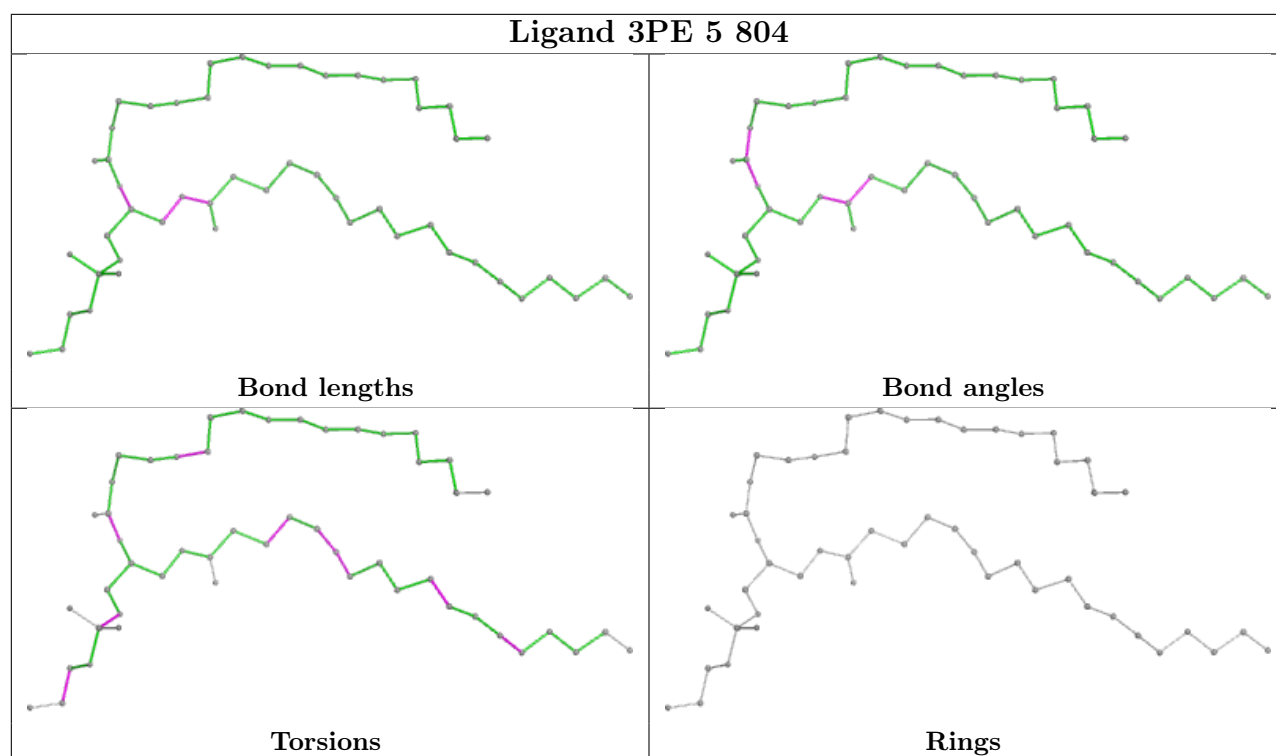




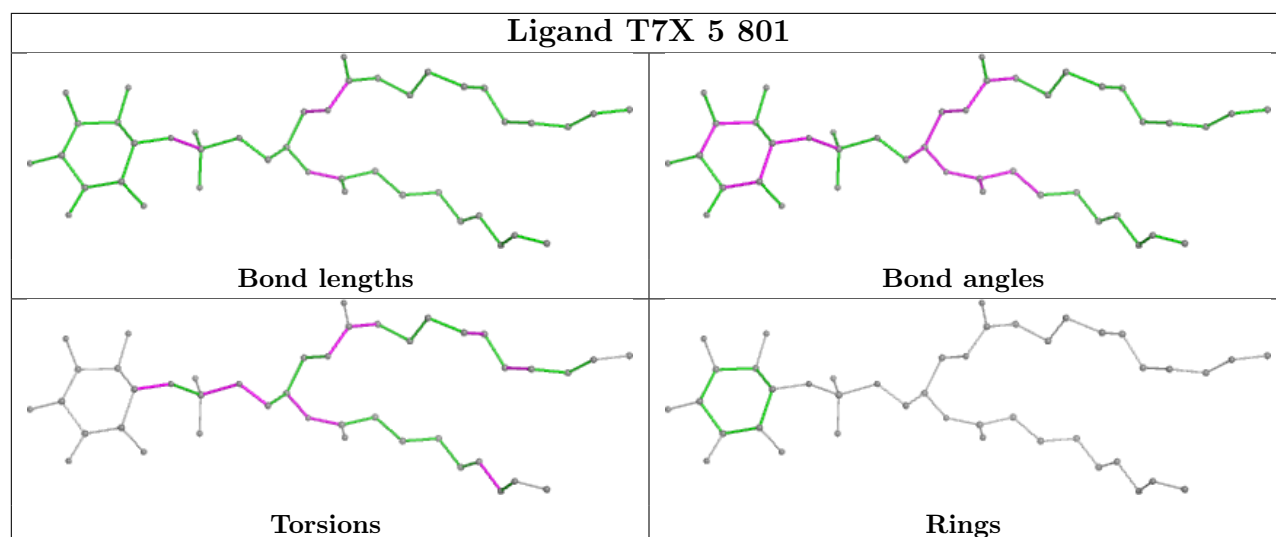
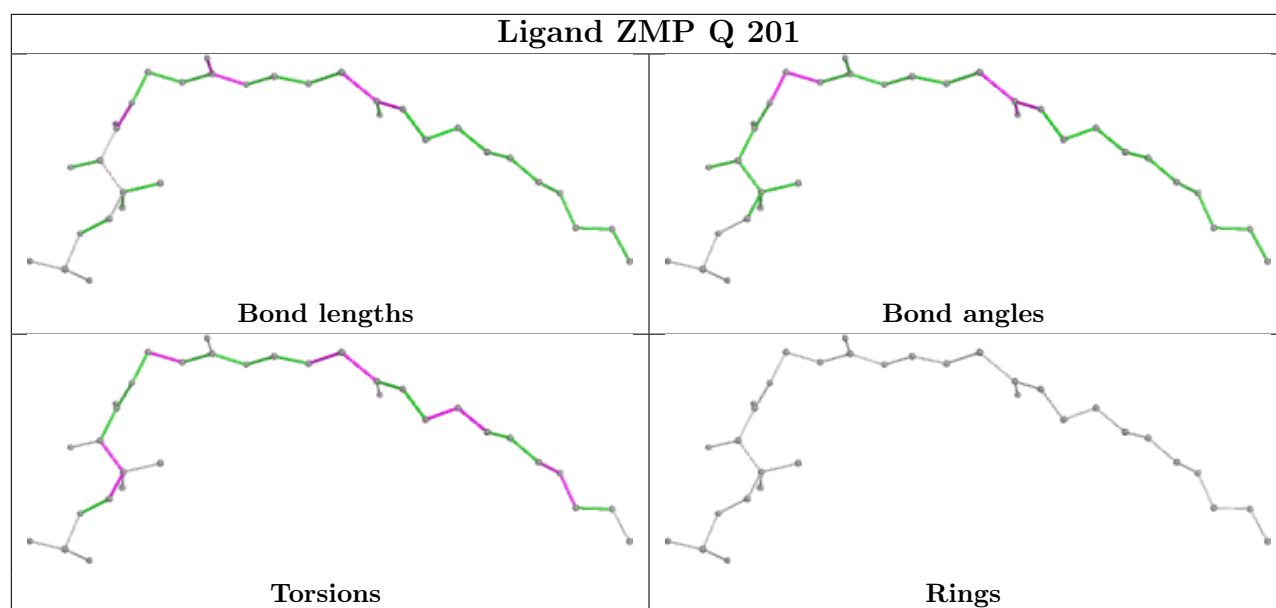


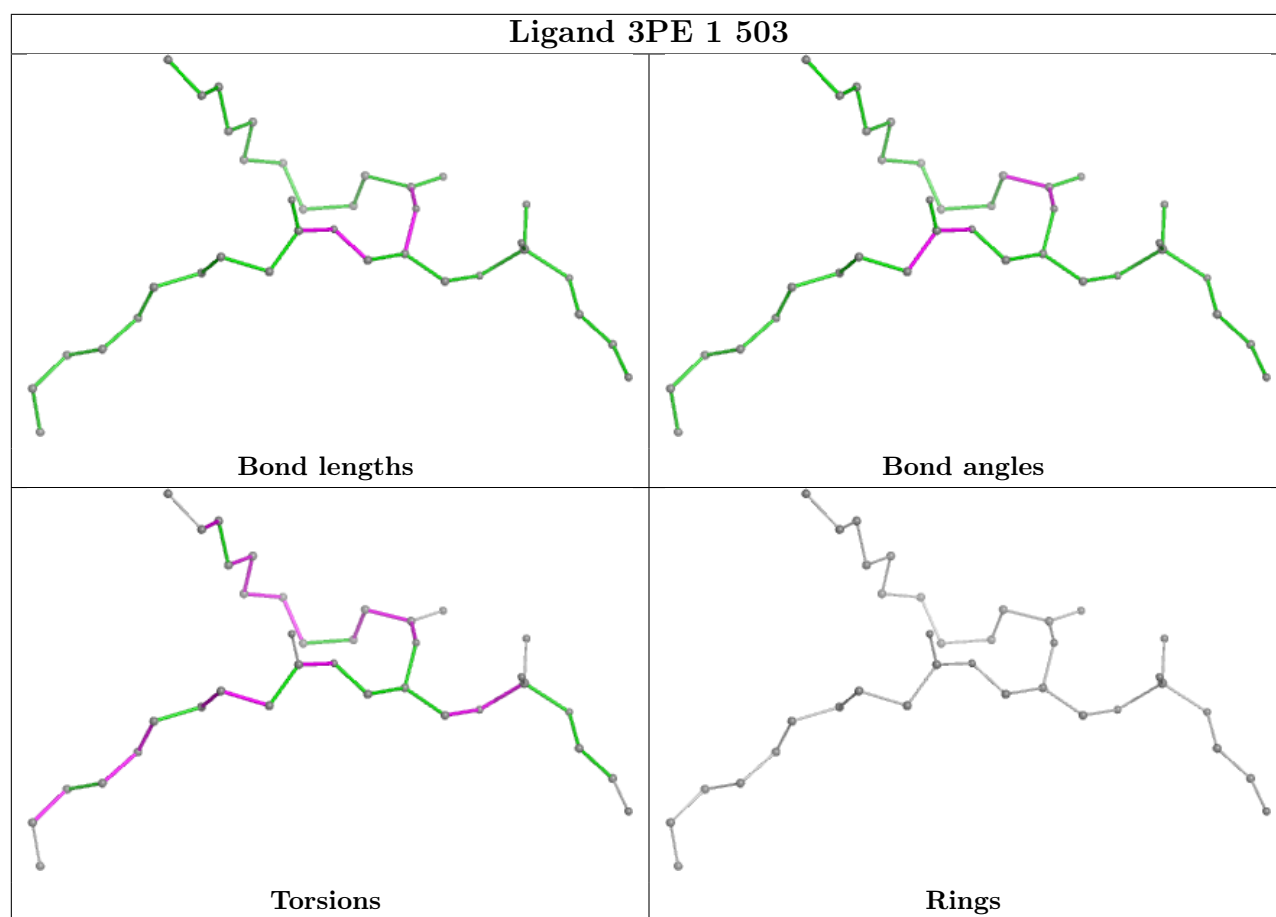


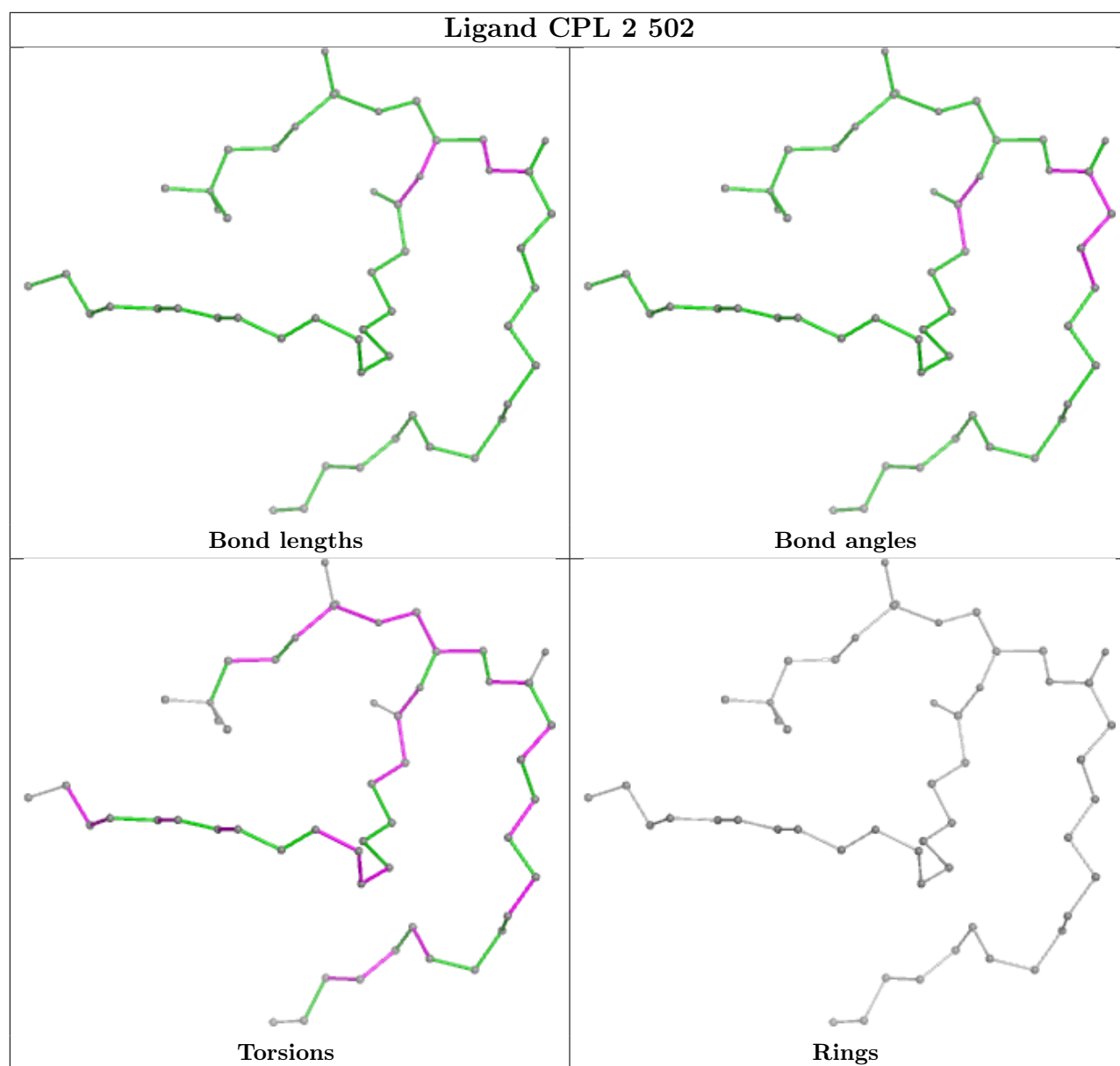


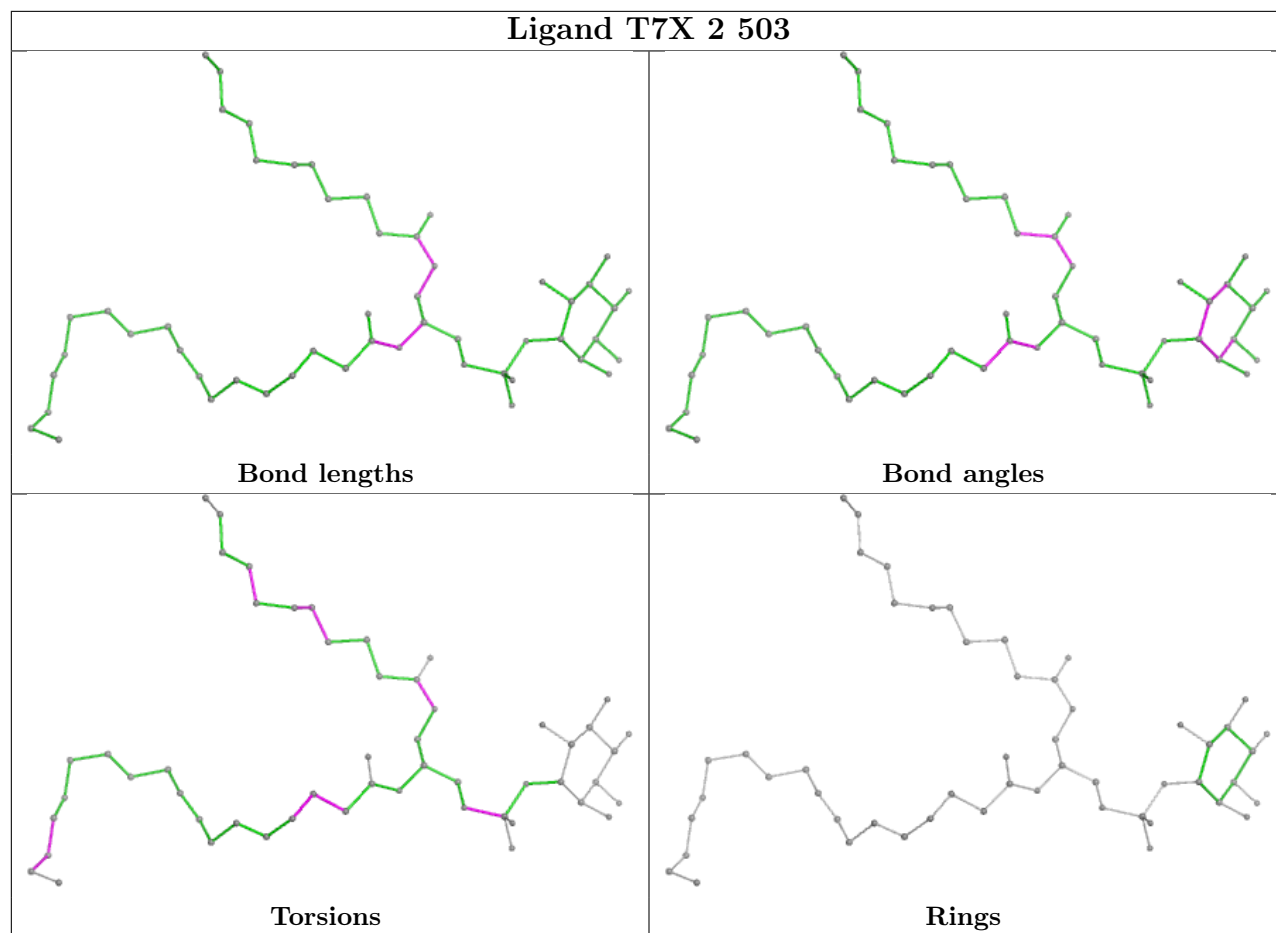
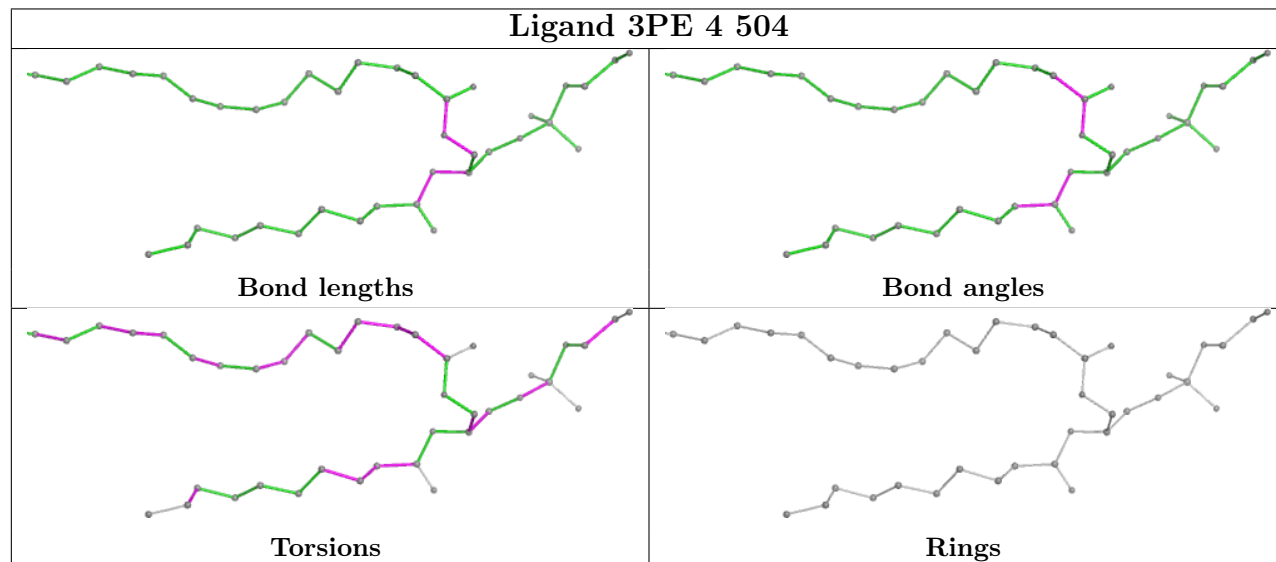


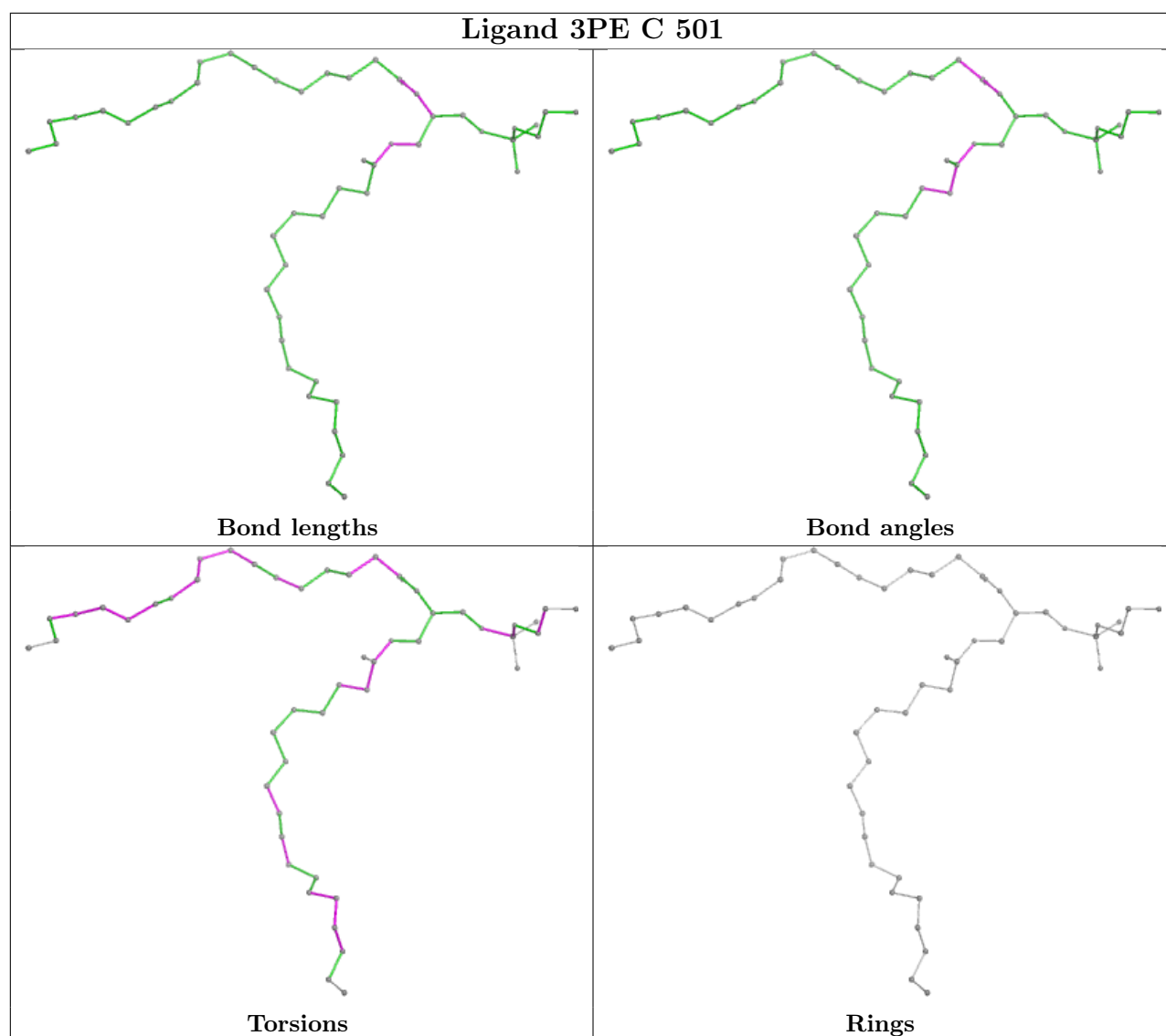


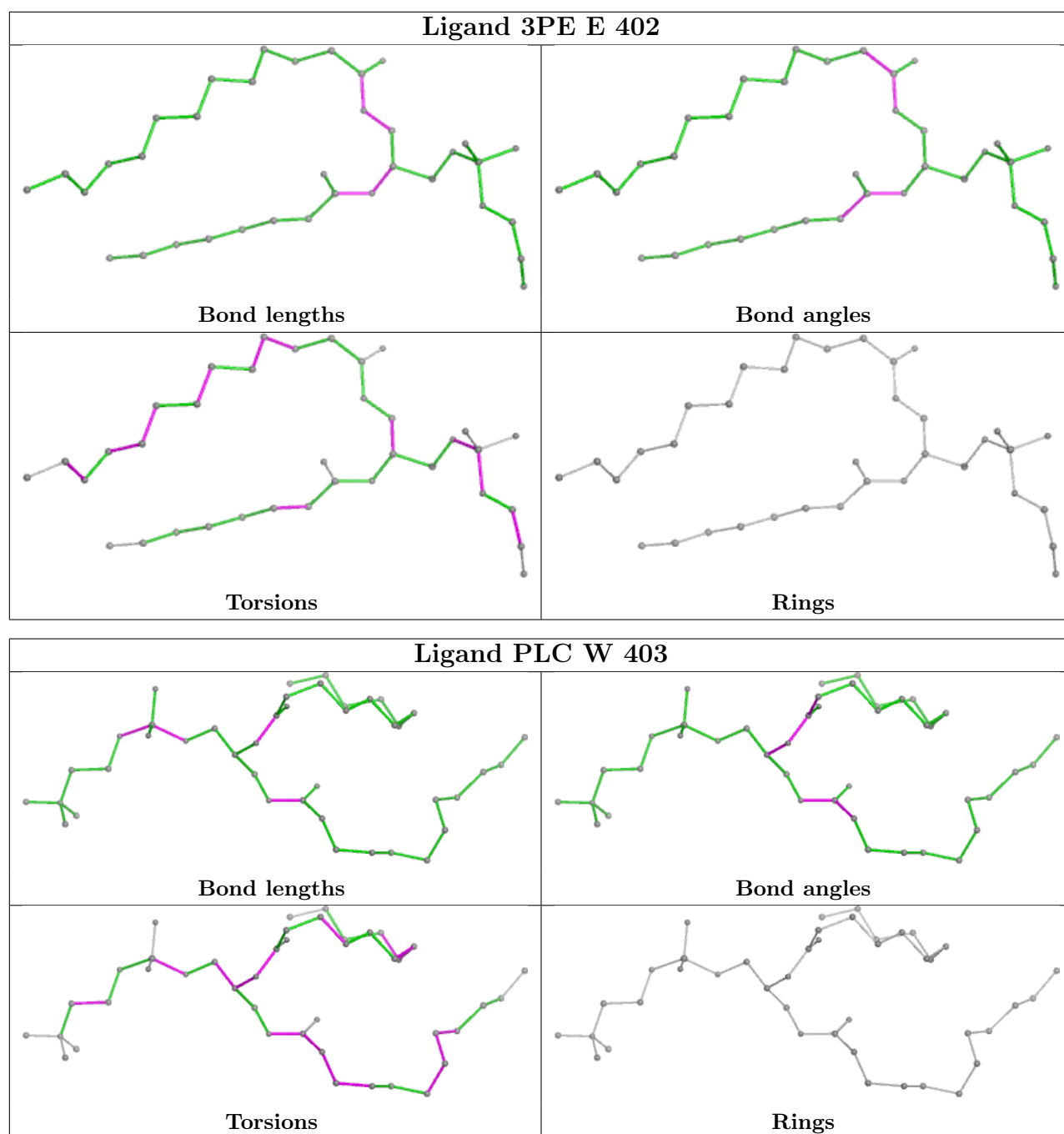


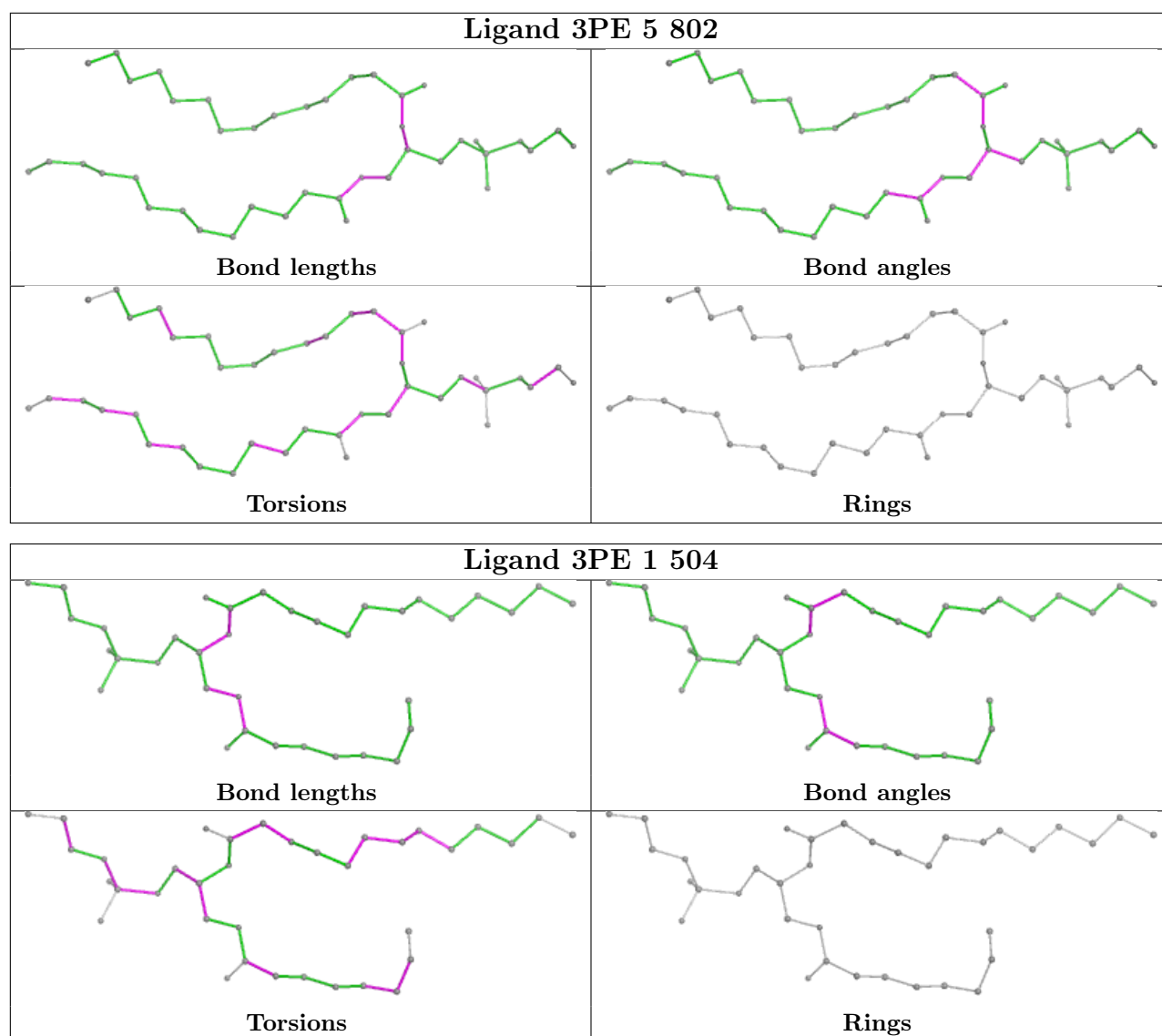


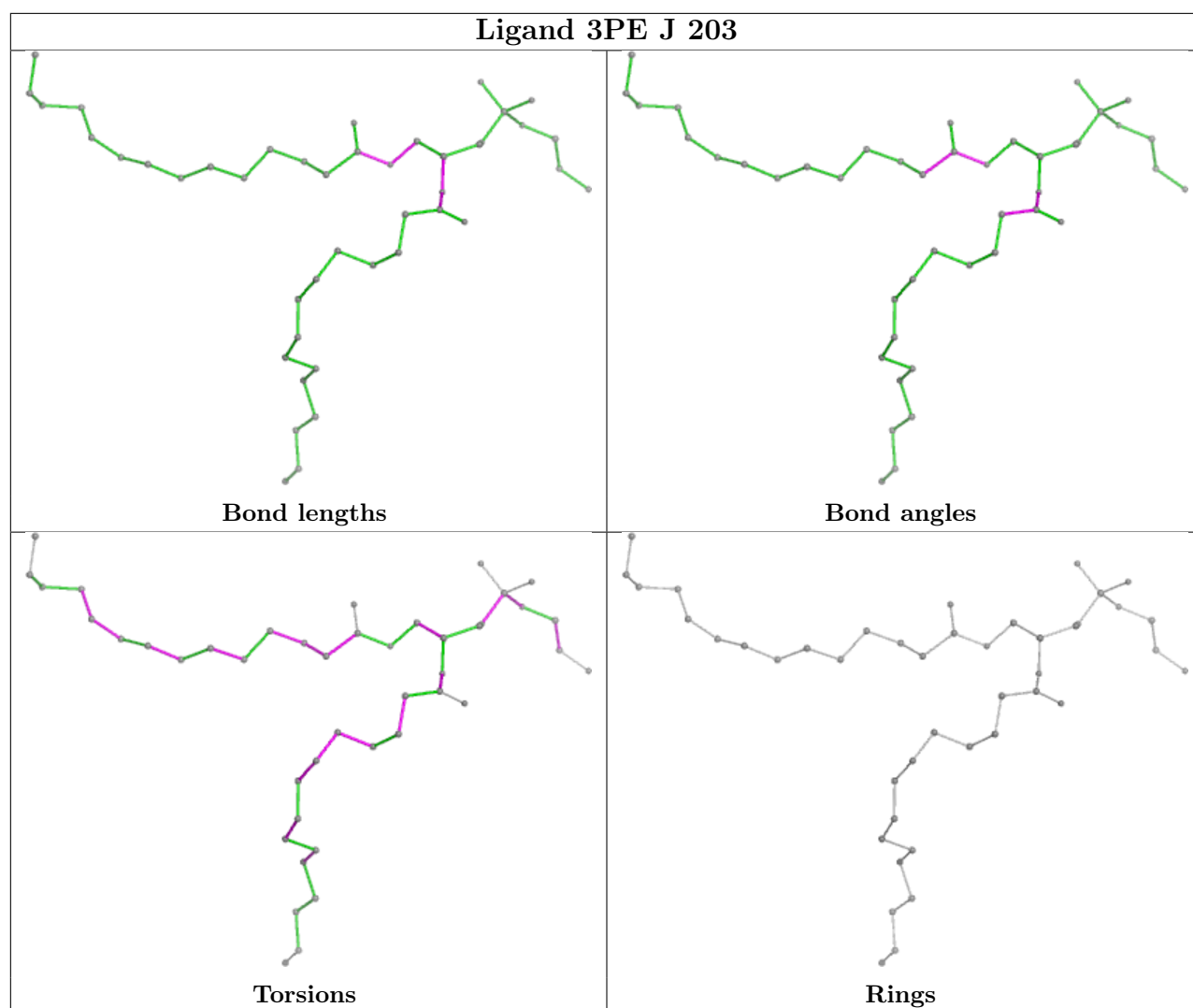


**Ligand T7X 2 503****Ligand 3PE 4 504**









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4873. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.