



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 10:50 pm BST

PDB ID : 6T15 / pdb\_00006t15  
EMDB ID : EMD-10318  
Title : The III2-IV(5B)1 respiratory supercomplex from *S. cerevisiae*  
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.  
Deposited on : 2019-10-03  
Resolution : 3.29 Å (reported)  
Based on initial model : 6HU9

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.dev117  
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) : 2.42

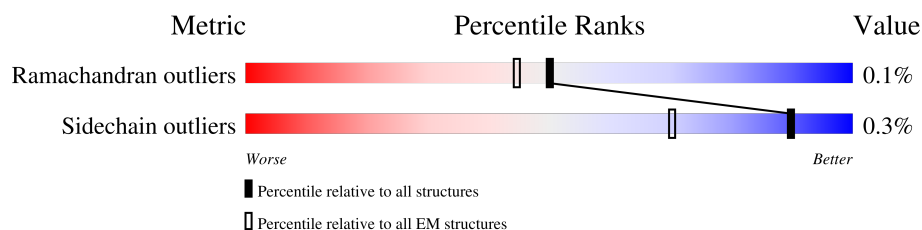
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.29 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.





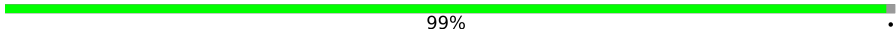
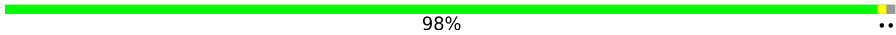
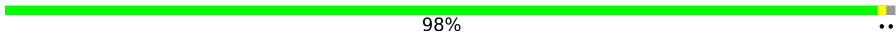
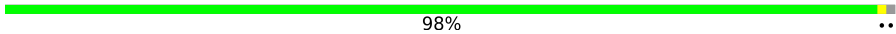


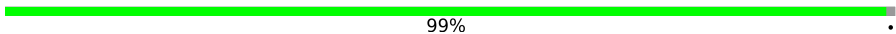
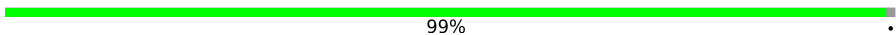
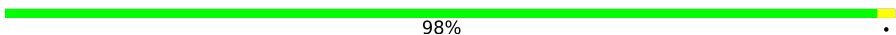




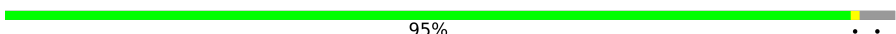
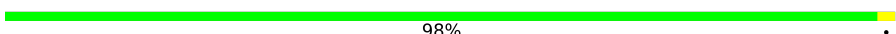
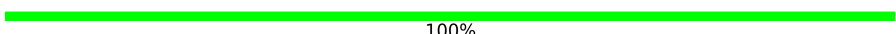
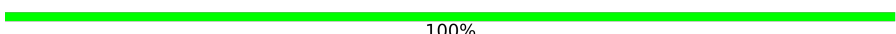




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	431	100%
1	L	431	100%
2	B	352	99% .
2	M	352	100%
3	C	385	100%
3	N	385	99% .
4	D	248	100%
4	O	248	100%
5	E	185	98% .
5	P	185	98% .

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Mol	Chain	Length	Quality of chain
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	94	
8	S	94	
9	I	66	
9	T	66	
10	J	77	
10	U	77	
11	a	534	
12	b	236	
13	c	269	
14	d	130	
15	e	134	
16	f	108	
17	g	59	
18	h	51	
19	i	55	
20	j	82	
21	k	131	
22	l	66	
23	m	224	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 48966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6, COMPLEX III SUBUNIT VI, CYTOCHROME C1 NON-HEME 17 KDA PROTEIN, MITOCHONDRIAL HINGE PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	57	Total	C	N	O		0	0
			465	310	77	78			
9	T	57	Total	C	N	O		0	0
			465	310	77	78			

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

- Molecule 11 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 12 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

- Molecule 13 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- Molecule 14 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 15 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	134	Total	C	N	O	S	0	0
			1083	694	188	199	2		

- Molecule 16 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	104	Total	C	N	O	S	0	0
			866	554	141	170	1		

- Molecule 17 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	59	Total	C	N	O	0	0
			484	328	83	73		

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	51	Total	C	N	O	S	0	0
			409	278	66	64	1		

- Molecule 19 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	77	Total	C	N	O	S	0	0
			642	410	109	118	5		

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	118	Total	C	N	O	S	0	0
			967	626	167	171	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799

- Molecule 22 is a protein called COX26; SYNONYM: Uncharacterized protein YDR119W-A.

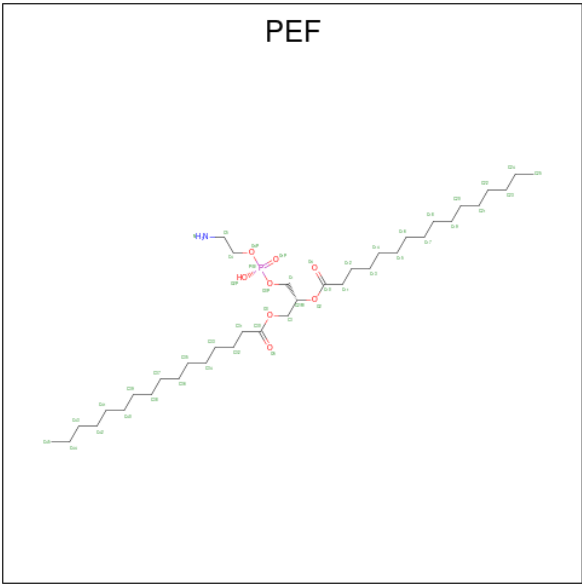
Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is a protein called RCF2; SYNONYM: Respiratory supercomplex factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	99	Total	C	N	O	S	0	0
			799	511	140	144	4		



- Molecule 24 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
24	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
24	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
24	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
24	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
24	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
24	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
24	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
24	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
24	P	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
24	U	1	Total	C	N	O	P	0
			47	37	1	8	1	

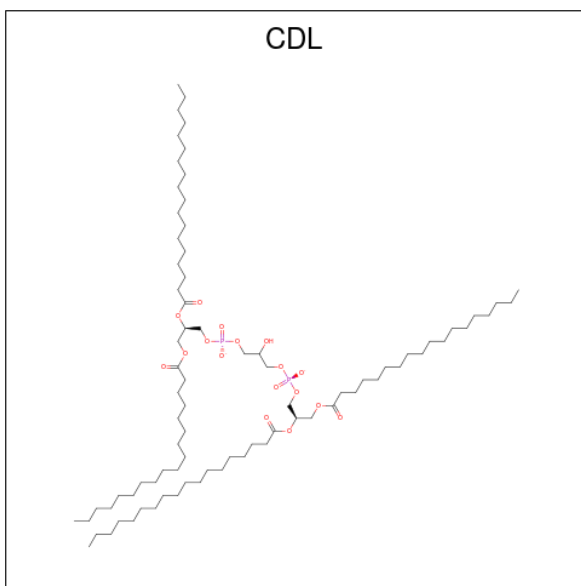
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Mol	Chain	Residues	Atoms					AltConf
24	a	1	Total 33	C 23	N 1	O 8	P 1	0
24	b	1	Total 40	C 30	N 1	O 8	P 1	0
24	b	1	Total 33	C 23	N 1	O 8	P 1	0
24	c	1	Total 36	C 26	N 1	O 8	P 1	0
24	c	1	Total 41	C 31	N 1	O 8	P 1	0
24	e	1	Total 42	C 32	N 1	O 8	P 1	0

- # HEM

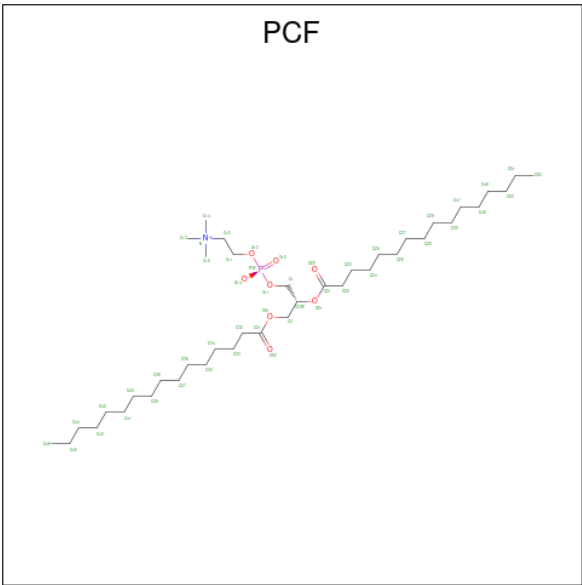
- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand

of Interest" by depositor).



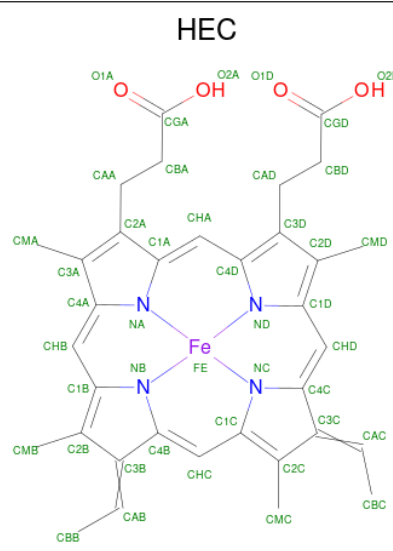
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			55	36	17	2	
26	D	1	Total	C	O	P	0
			67	48	17	2	
26	H	1	Total	C	O	P	0
			53	34	17	2	
26	L	1	Total	C	O	P	0
			58	39	17	2	
26	N	1	Total	C	O	P	0
			66	47	17	2	
26	O	1	Total	C	O	P	0
			71	52	17	2	
26	S	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula:  $C_{40}H_{80}NO_8P$ ).



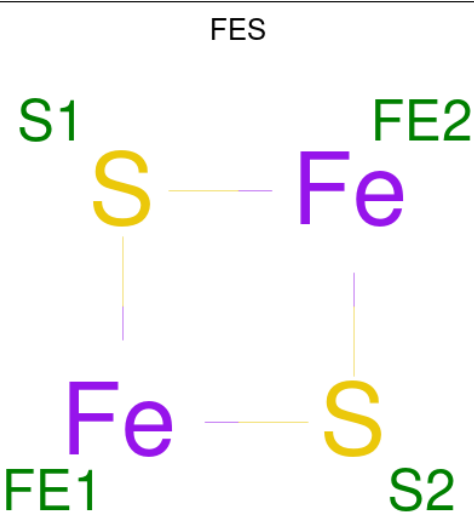
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	T	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

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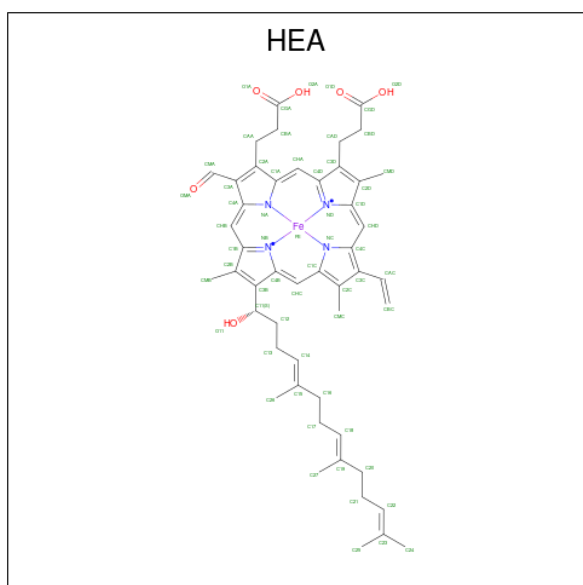
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Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

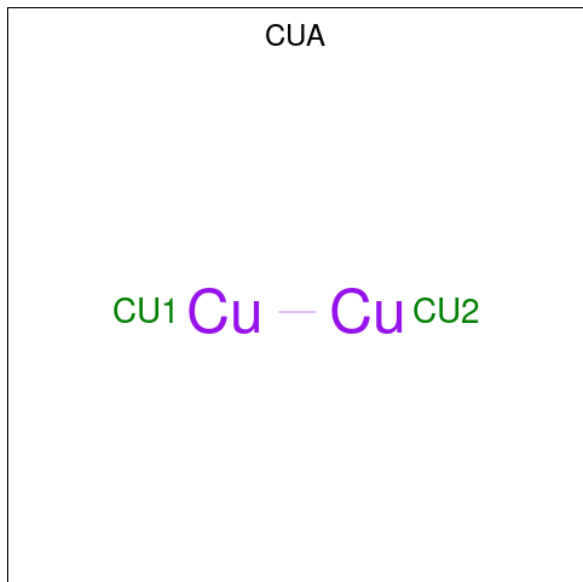


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Mg	0
			1	1	

- Molecule 33 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula:  $\text{Cu}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Cu	0
			2	2	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
34	d	1	Total	Zn	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. 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.

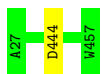
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

Chain A:  100%

There are no outlier residues recorded for this chain.

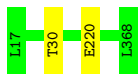
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

Chain L:  100%



- Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:  99%



- Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2

Chain C:  100%





- Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2

Chain N: 99%



- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1

Chain D: 100%



- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1

Chain O: 100%



- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E: 98%



- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain P: 98%







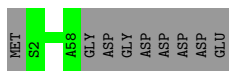
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S: 98% ..



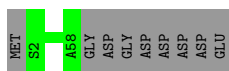
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

Chain I: 86% 14%



- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

Chain T: 86% 14%



- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN

Chain J: 99% .



- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN

Chain U: 99% .



- Molecule 11: CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1

Chain a:  98%



- Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2

Chain b:  99%



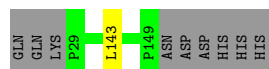
- Molecule 13: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

Chain c:  99%



- Molecule 14: CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4

Chain d:  92% 7%



- Molecule 15: CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B

Chain e:  99%



- Molecule 16: CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6

Chain f:  95%



- Molecule 17: CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7

Chain g:  98%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:  100%


There are no outlier residues recorded for this chain.

- Molecule 19: CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9

Chain i:  100%

There are no outlier residues recorded for this chain.

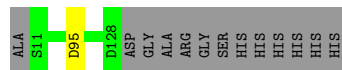
- Molecule 20: Cytochrome c oxidase subunit 6B

Chain j:  91% 6%



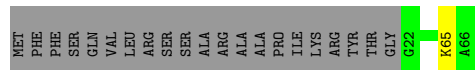
- Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13

Chain k:  89% 10%



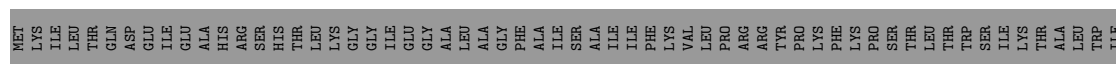
- Molecule 22: COX26; SYNONYM: Uncharacterized protein YDR119W-A

Chain l:  67% 32%



- Molecule 23: RCF2; SYNONYM: Respiratory supercomplex factor 2

Chain m:  44% 56%



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73042	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 ( $e^-/\text{\AA}^2$ )	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCF, MG, HEM, FES, HEC, CU, ZN, CDL, CUA, HEA, PEF

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	0.29	0/3406	0.52	0/4615
1	L	0.30	0/3406	0.55	0/4615
2	B	0.31	0/2781	0.54	0/3764
2	M	0.31	0/2781	0.54	0/3764
3	C	0.34	0/3192	0.56	1/4354 (0.0%)
3	N	0.34	0/3192	0.56	1/4354 (0.0%)
4	D	0.30	0/2012	0.46	0/2740
4	O	0.31	0/2012	0.46	0/2740
5	E	0.31	0/1444	0.60	1/1957 (0.1%)
5	P	0.33	0/1444	0.66	2/1957 (0.1%)
6	F	0.36	0/647	0.66	1/870 (0.1%)
6	Q	0.38	1/647 (0.2%)	0.57	0/870
7	G	0.31	0/1040	0.54	0/1408
7	R	0.28	0/1040	0.52	1/1408 (0.1%)
8	H	0.29	0/804	0.46	0/1088
8	S	0.30	0/804	0.49	0/1088
9	I	0.29	0/479	0.45	0/646
9	T	0.29	0/479	0.45	0/646
10	J	0.30	0/619	0.58	0/841
10	U	0.31	0/619	0.57	0/841
11	a	0.35	0/4290	0.64	6/5857 (0.1%)
12	b	0.34	0/1941	0.64	2/2653 (0.1%)
13	c	0.34	0/2218	0.59	1/3036 (0.0%)
14	d	0.31	0/932	0.58	0/1269
15	e	0.31	0/1111	0.57	0/1503
16	f	0.36	0/884	0.54	0/1196
17	g	0.35	0/500	0.67	1/681 (0.1%)
18	h	0.34	0/424	0.60	0/569
19	i	0.33	0/468	0.49	0/626
20	j	0.37	0/664	0.58	0/899
21	k	0.29	0/1002	0.54	0/1364
22	l	0.30	0/372	0.59	0/502



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
23	m	0.34	0/813	0.58	0/1093
All	All	0.32	1/48467 (0.0%)	0.56	17/65814 (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	L	0	1
2	B	0	1
3	N	0	1
5	E	0	1
5	P	0	1
11	a	0	4
13	c	0	1
14	d	0	1
21	k	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	101	CYS	CB-SG	-5.00	1.73	1.81

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	156	LEU	CA-CB-CG	7.14	131.73	115.30
12	b	172	ASP	CB-CG-OD2	7.14	124.72	118.30
5	E	156	LEU	CA-CB-CG	6.23	129.62	115.30
11	a	200	LEU	CA-CB-CG	6.18	129.52	115.30
3	C	300	LEU	CA-CB-CG	6.17	129.48	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	GLU	Peptide
5	E	167	ILE	Peptide
1	L	444	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	N	345	GLU	Peptide
5	P	125	GLU	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	429/431 (100%)	397 (92%)	32 (8%)	0	100	100
1	L	429/431 (100%)	394 (92%)	35 (8%)	0	100	100
2	B	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
2	M	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
3	C	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
3	N	383/385 (100%)	357 (93%)	26 (7%)	0	100	100
4	D	245/248 (99%)	239 (98%)	6 (2%)	0	100	100
4	O	245/248 (99%)	241 (98%)	4 (2%)	0	100	100
5	E	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
5	P	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
6	F	73/147 (50%)	68 (93%)	5 (7%)	0	100	100
6	Q	73/147 (50%)	70 (96%)	3 (4%)	0	100	100
7	G	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
8	S	91/94 (97%)	85 (93%)	6 (7%)	0	100	100
9	I	55/66 (83%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	55/66 (83%)	55 (100%)	0	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	490 (92%)	40 (8%)	2 (0%)	30	61
12	b	234/236 (99%)	214 (92%)	20 (8%)	0	100	100
13	c	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	30	61
14	d	119/130 (92%)	101 (85%)	18 (15%)	0	100	100
15	e	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
16	f	102/108 (94%)	96 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
18	h	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
20	j	75/82 (92%)	67 (89%)	8 (11%)	0	100	100
21	k	116/131 (88%)	103 (89%)	13 (11%)	0	100	100
22	l	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
23	m	97/224 (43%)	91 (94%)	6 (6%)	0	100	100
All	All	5890/6303 (93%)	5521 (94%)	366 (6%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	a	121	SER
11	a	521	PRO
13	c	23	PRO

### 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	370/370 (100%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	300 (100%)	1 (0%)	91	94
2	M	301/301 (100%)	301 (100%)	0	100	100
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	336 (99%)	2 (1%)	84	90
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	150 (99%)	1 (1%)	81	88
5	P	151/151 (100%)	151 (100%)	0	100	100
6	F	68/131 (52%)	67 (98%)	1 (2%)	60	77
6	Q	68/131 (52%)	67 (98%)	1 (2%)	60	77
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	76 (99%)	1 (1%)	65	79
8	S	77/78 (99%)	76 (99%)	1 (1%)	65	79
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	65 (100%)	0	100	100
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	446 (100%)	1 (0%)	92	95
12	b	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	227 (100%)	1 (0%)	89	93
14	d	102/111 (92%)	102 (100%)	0	100	100
15	e	115/115 (100%)	114 (99%)	1 (1%)	75	85
16	f	92/96 (96%)	91 (99%)	1 (1%)	70	82
17	g	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
20	j	69/73 (94%)	67 (97%)	2 (3%)	37	63
21	k	104/113 (92%)	104 (100%)	0	100	100
22	l	36/53 (68%)	35 (97%)	1 (3%)	38	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	m	84/191 (44%)	84 (100%)	0	100	100
All	All	5087/5385 (94%)	5072 (100%)	15 (0%)	90	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	7	LYS
20	j	41	LYS
11	a	244	VAL
22	l	65	LYS
16	f	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
10	U	29	ASN
13	c	47	ASN
11	a	99	ASN
11	a	482	ASN
23	m	149	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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	$\# Z  > 2$
26	CDL	D	402	-	66,66,99	1.12	4 (6%)	72,78,111	1.19	6 (8%)
24	PEF	E	302	-	42,42,46	1.01	2 (4%)	45,47,51	1.10	3 (6%)
24	PEF	e	201	-	41,41,46	1.03	2 (4%)	44,46,51	0.97	2 (4%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
24	PEF	C	605	-	42,42,46	1.01	2 (4%)	45,47,51	1.15	3 (6%)
24	PEF	N	605	-	38,38,46	1.08	2 (5%)	41,43,51	0.99	2 (4%)
26	CDL	H	601	-	52,52,99	1.26	4 (7%)	58,64,111	1.26	5 (8%)
26	CDL	L	501	-	57,57,99	1.21	4 (7%)	63,69,111	1.20	4 (6%)
24	PEF	U	101	-	46,46,46	0.96	2 (4%)	49,51,51	1.03	2 (4%)
27	PCF	e	202	15	35,35,49	1.13	2 (5%)	41,43,57	1.06	3 (7%)
24	PEF	a	605	11	32,32,46	1.16	2 (6%)	35,37,51	1.19	3 (8%)
24	PEF	b	302	-	39,39,46	1.04	2 (5%)	42,44,51	1.05	2 (4%)
24	PEF	N	604	-	43,43,46	0.97	2 (4%)	46,48,51	1.05	3 (6%)
24	PEF	J	101	-	28,28,46	1.22	2 (7%)	31,33,51	1.18	2 (6%)
24	PEF	c	302	-	40,40,46	1.02	2 (5%)	43,45,51	1.04	1 (2%)
27	PCF	C	606	-	49,49,49	0.96	2 (4%)	55,57,57	1.00	4 (7%)
27	PCF	T	101	-	49,49,49	0.97	2 (4%)	55,57,57	1.02	3 (5%)
27	PCF	S	103	8	31,31,49	1.19	2 (6%)	37,39,57	1.09	4 (10%)
24	PEF	L	502	1	35,35,46	1.08	2 (5%)	38,40,51	1.14	4 (10%)
27	PCF	I	101	24	38,38,49	1.07	2 (5%)	44,46,57	1.08	4 (9%)
24	PEF	c	301	-	35,35,46	1.08	2 (5%)	38,40,51	1.14	3 (7%)
26	CDL	N	603	26	65,65,99	1.12	4 (6%)	71,77,111	1.16	6 (8%)
24	PEF	A	501	1	30,30,46	1.17	2 (6%)	33,35,51	1.12	3 (9%)
25	HEM	C	602	3	41,50,50	1.37	4 (9%)	45,82,82	1.83	11 (24%)
31	HEA	a	602	11	57,67,67	2.04	16 (28%)	61,103,103	2.63	27 (44%)
33	CUA	b	301	12	0,1,1	-	-	-	-	-
25	HEM	C	601	3	41,50,50	1.34	5 (12%)	45,82,82	1.93	12 (26%)
25	HEM	N	601	3	41,50,50	1.34	4 (9%)	45,82,82	1.88	11 (24%)
26	CDL	C	603	1,3	54,54,99	1.16	4 (7%)	60,66,111	1.24	5 (8%)
26	CDL	S	101	-	52,52,99	1.26	4 (7%)	58,64,111	1.25	7 (12%)
24	PEF	C	604	27	39,39,46	1.04	2 (5%)	42,44,51	1.10	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PEF	b	303	-	32,32,46	1.12	2 (6%)	35,37,51	1.23	4 (11%)
25	HEM	N	602	3	41,50,50	1.35	4 (9%)	45,82,82	1.85	11 (24%)
24	PEF	H	602	-	31,31,46	1.16	2 (6%)	34,36,51	1.24	4 (11%)
26	CDL	O	402	26	70,70,99	1.09	4 (5%)	76,82,111	1.22	6 (7%)
28	HEC	D	401	4	32,50,50	2.54	12 (37%)	24,82,82	2.79	9 (37%)
27	PCF	N	606	-	38,38,49	1.10	2 (5%)	44,46,57	1.05	3 (6%)
29	FES	P	301	5	0,4,4	-	-	-	-	-
24	PEF	S	102	-	35,35,46	1.08	2 (5%)	38,40,51	1.11	3 (7%)
31	HEA	a	603	11	57,67,67	2.03	16 (28%)	61,103,103	2.66	27 (44%)
24	PEF	P	302	-	41,41,46	1.00	2 (4%)	44,46,51	1.04	3 (6%)
28	HEC	O	401	4	32,50,50	2.52	12 (37%)	24,82,82	2.85	9 (37%)

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
26	CDL	D	402	-	-	29/77/77/110	-
24	PEF	E	302	-	-	14/46/46/50	-
24	PEF	e	201	-	-	13/45/45/50	-
29	FES	E	301	5	-	-	0/1/1/1
24	PEF	C	605	-	-	13/46/46/50	-
24	PEF	N	605	-	-	10/42/42/50	-
26	CDL	H	601	-	-	19/63/63/110	-
26	CDL	L	501	-	-	19/68/68/110	-
24	PEF	U	101	-	-	14/50/50/50	-
27	PCF	e	202	15	-	7/39/39/53	-
24	PEF	a	605	11	-	6/36/36/50	-
24	PEF	b	302	-	-	19/43/43/50	-
24	PEF	N	604	-	-	9/47/47/50	-
24	PEF	J	101	-	-	15/32/32/50	-
24	PEF	c	302	-	-	11/44/44/50	-
27	PCF	C	606	-	-	15/53/53/53	-
27	PCF	T	101	-	-	9/53/53/53	-
27	PCF	S	103	8	-	8/35/35/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEF	L	502	1	-	15/39/39/50	-
27	PCF	I	101	24	-	6/42/42/53	-
24	PEF	c	301	-	-	10/39/39/50	-
26	CDL	N	603	26	-	11/76/76/110	-
24	PEF	A	501	1	-	7/34/34/50	-
25	HEM	C	602	3	-	4/12/54/54	-
31	HEA	a	602	11	-	10/32/76/76	-
25	HEM	C	601	3	-	8/12/54/54	-
25	HEM	N	601	3	-	8/12/54/54	-
26	CDL	C	603	1,3	-	21/64/64/110	-
26	CDL	S	101	-	-	23/63/63/110	-
24	PEF	C	604	27	-	9/43/43/50	-
24	PEF	b	303	-	-	14/36/36/50	-
25	HEM	N	602	3	-	4/12/54/54	-
24	PEF	H	602	-	-	6/35/35/50	-
26	CDL	O	402	26	-	19/81/81/110	-
28	HEC	D	401	4	-	0/10/54/54	-
27	PCF	N	606	-	-	11/42/42/53	-
29	FES	P	301	5	-	-	0/1/1/1
24	PEF	S	102	-	-	10/39/39/50	-
31	HEA	a	603	11	-	4/32/76/76	-
24	PEF	P	302	-	-	13/45/45/50	-
28	HEC	O	401	4	-	3/10/54/54	-

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C2B-C3B	7.64	1.48	1.40
28	D	401	HEC	C2B-C3B	7.62	1.48	1.40
28	D	401	HEC	C3C-C2C	7.50	1.48	1.40
28	O	401	HEC	C3C-C2C	7.36	1.48	1.40
31	a	602	HEA	C3B-C2B	5.41	1.46	1.34

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	HEC	CMB-C2B-C3B	7.99	135.22	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	401	HEC	CMB-C2B-C3B	7.61	134.76	125.82
31	a	603	HEA	C3D-C4D-ND	6.65	116.80	110.36
28	D	401	HEC	CMC-C2C-C3C	6.56	133.53	125.82
31	a	603	HEA	C2D-C1D-ND	6.36	117.38	109.84

There are no chirality outliers.

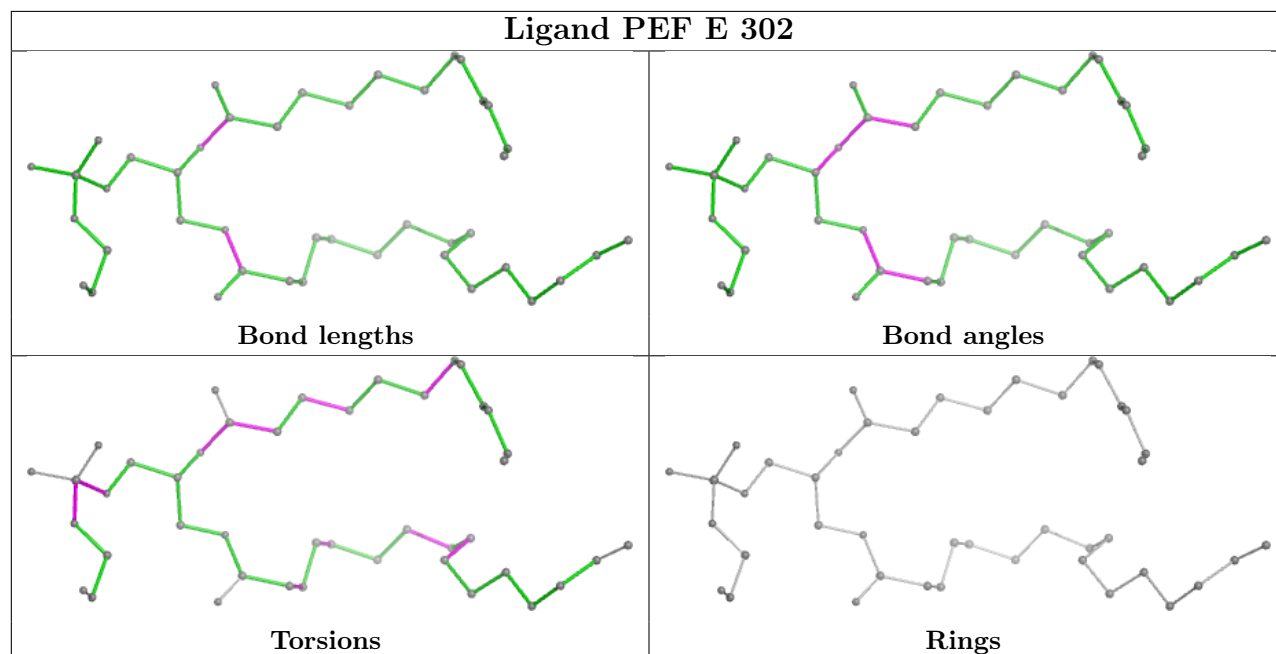
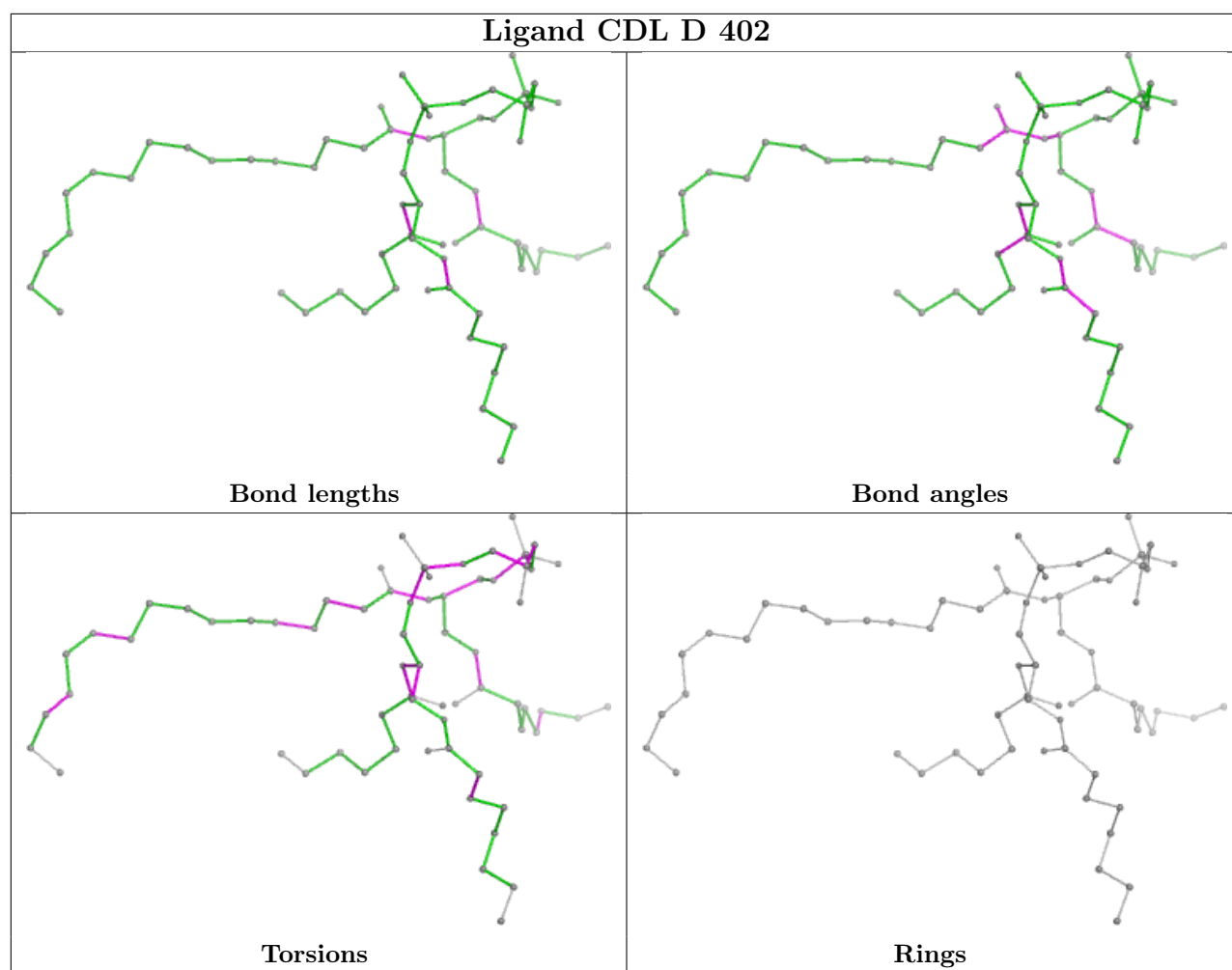
5 of 446 torsion outliers are listed below:

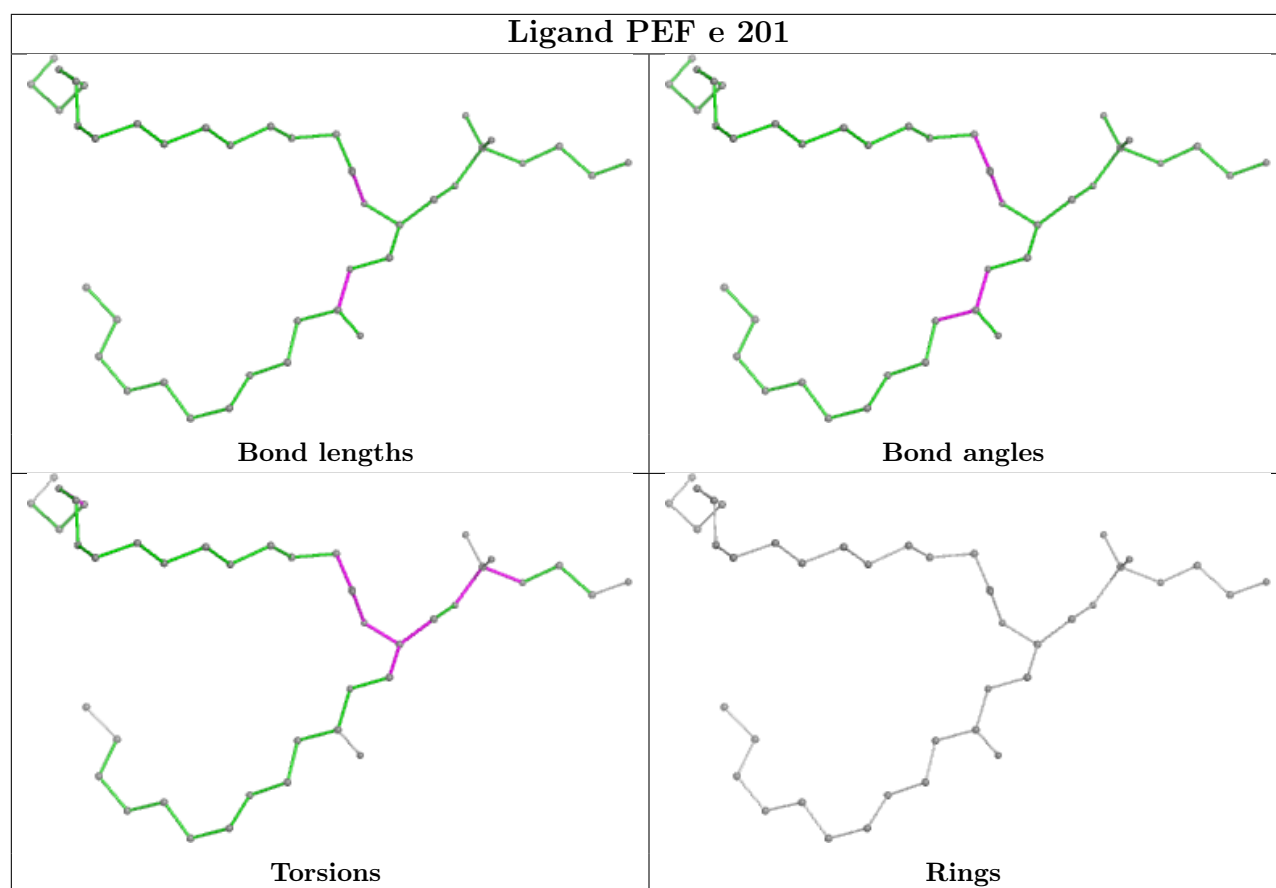
Mol	Chain	Res	Type	Atoms
24	A	501	PEF	C1-O3P-P-O1P
24	A	501	PEF	C1-O3P-P-O2P
24	A	501	PEF	C1-O3P-P-O4P
24	C	605	PEF	C11-C10-O2-C2
24	C	605	PEF	O4-C10-O2-C2

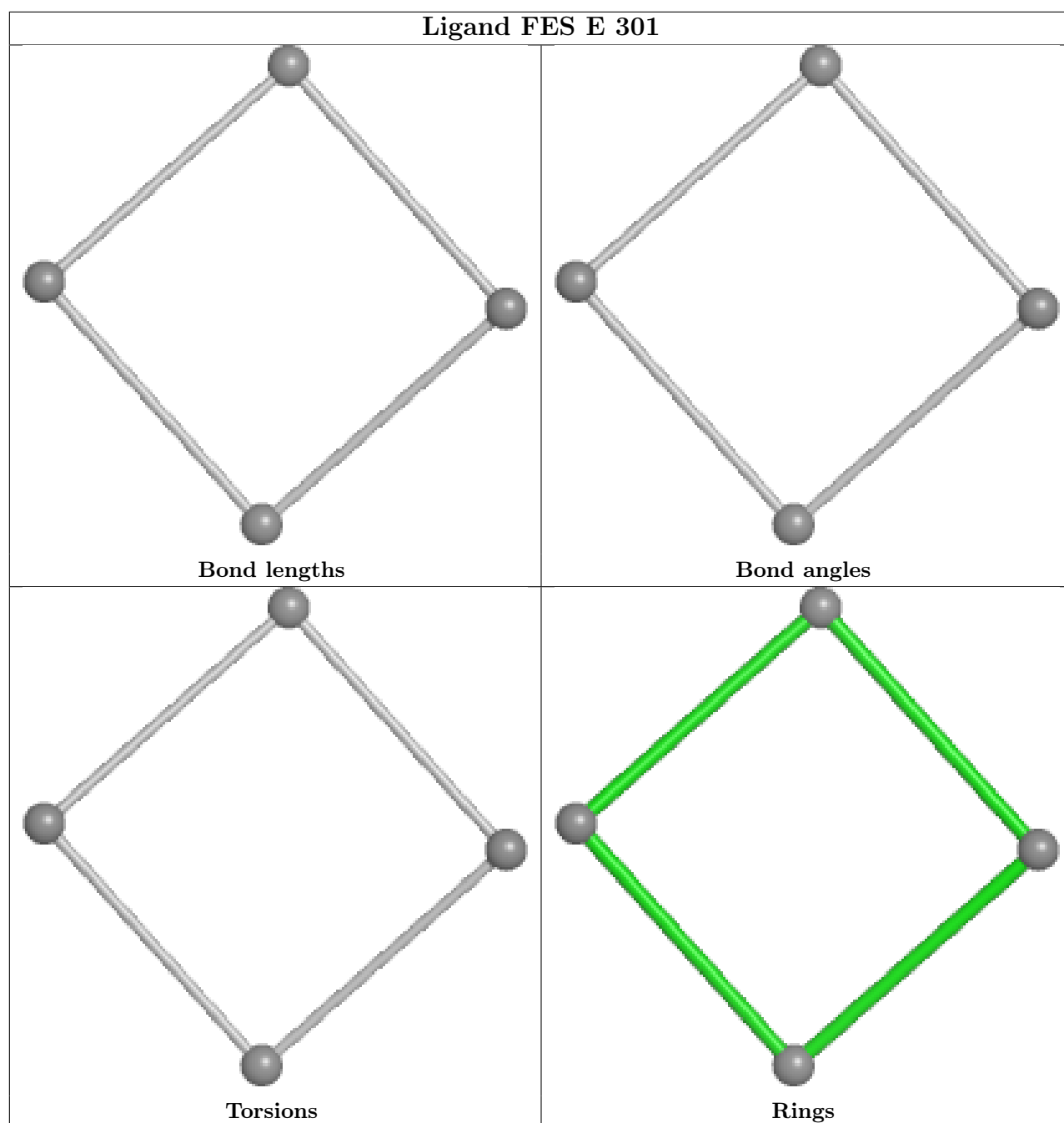
There are no ring outliers.

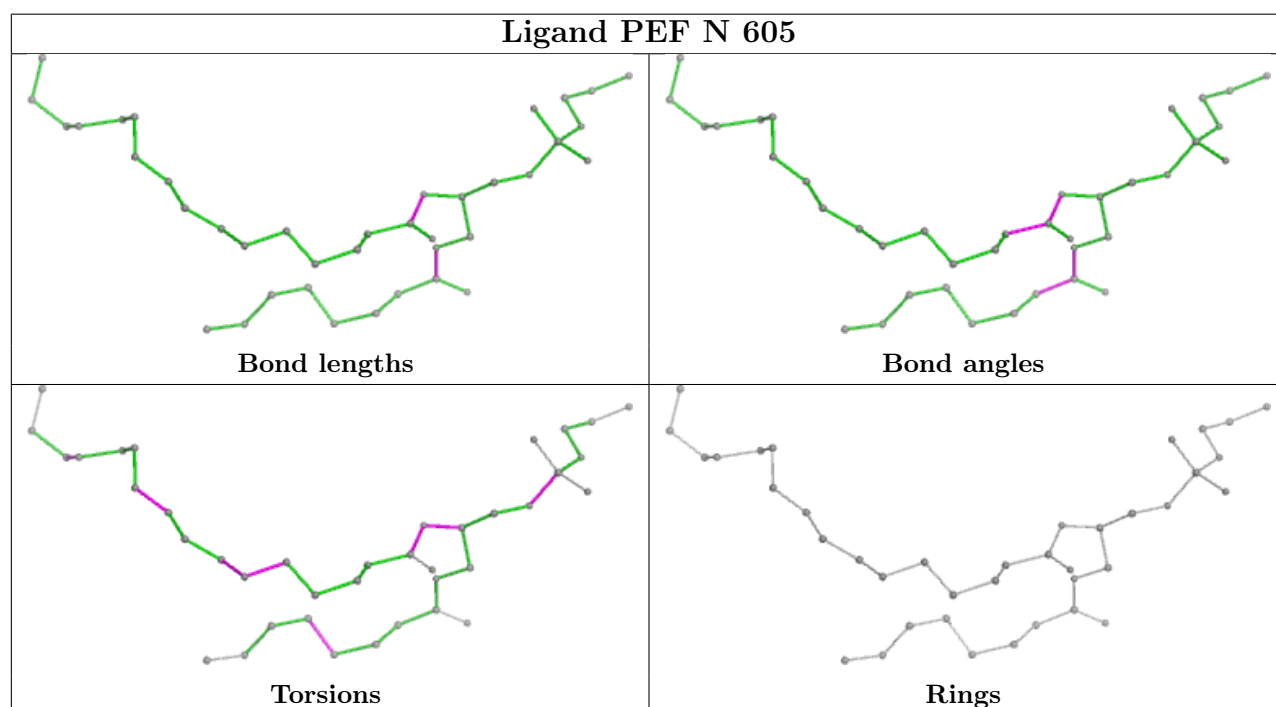
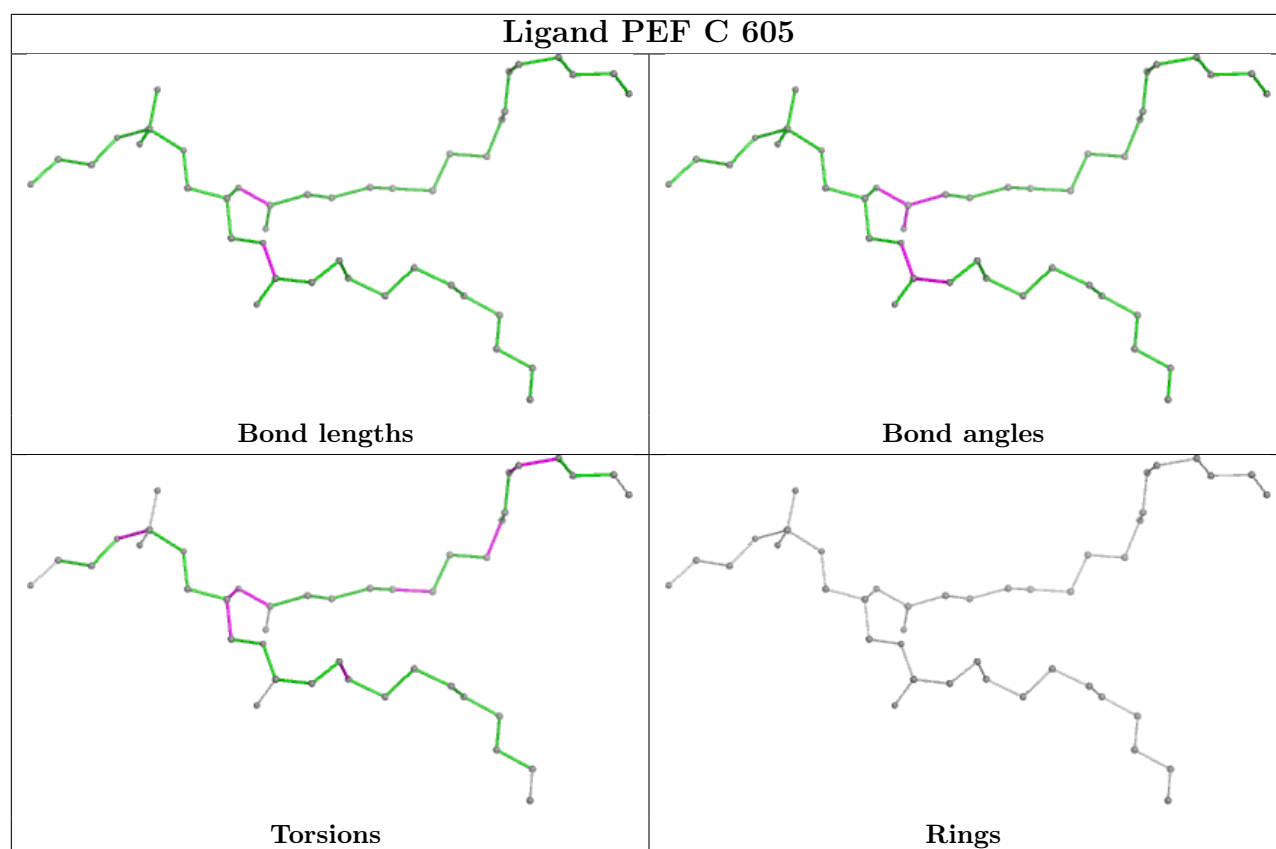
No monomer is involved in short contacts.

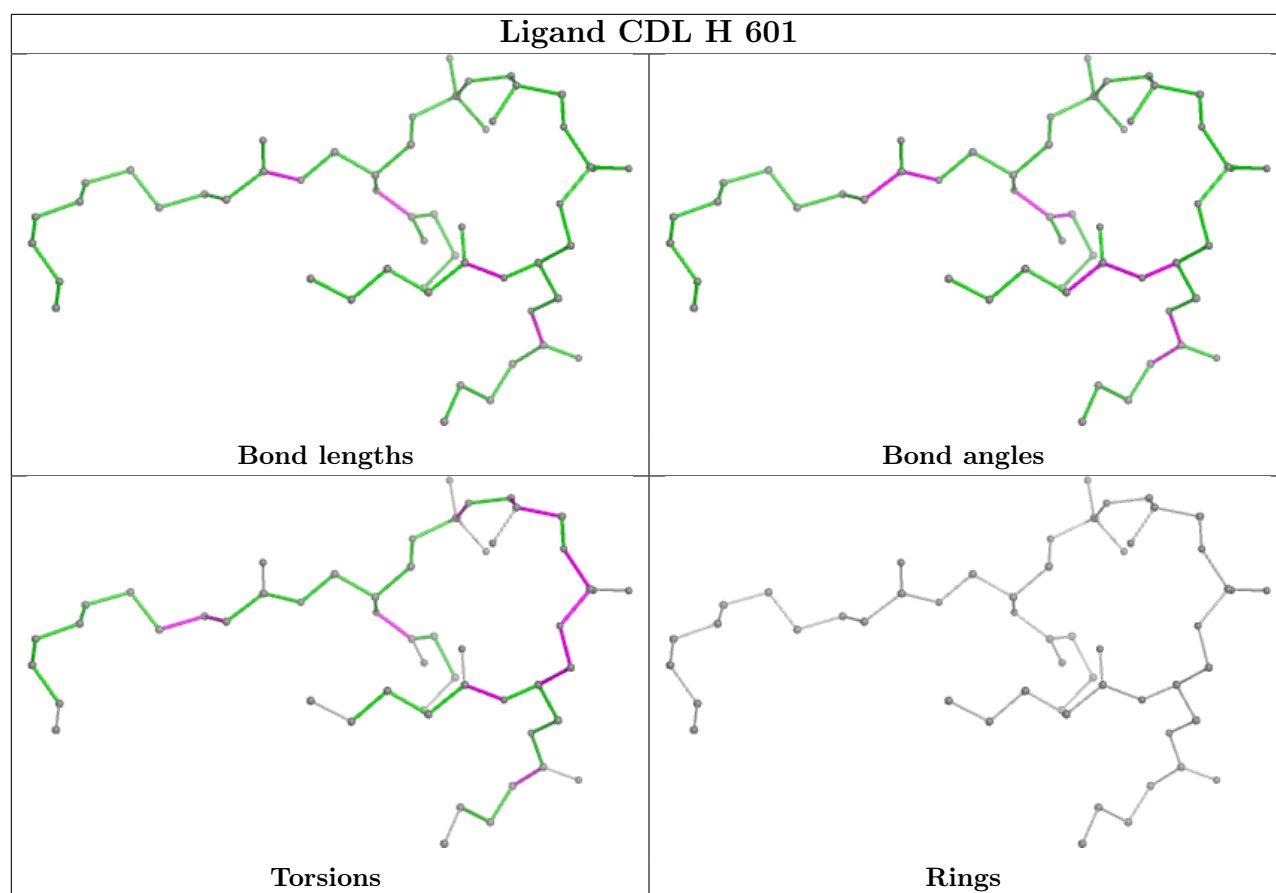
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

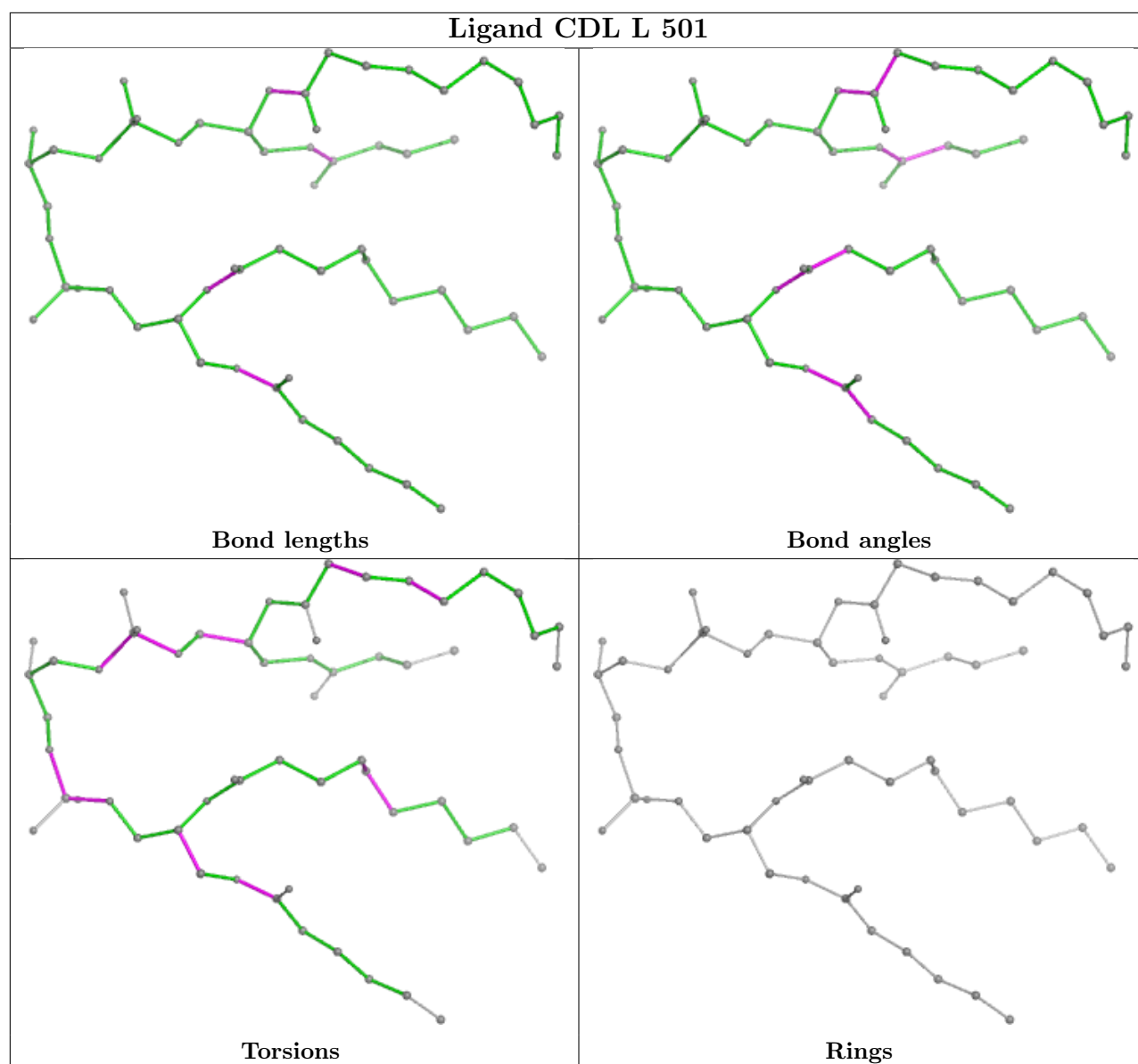


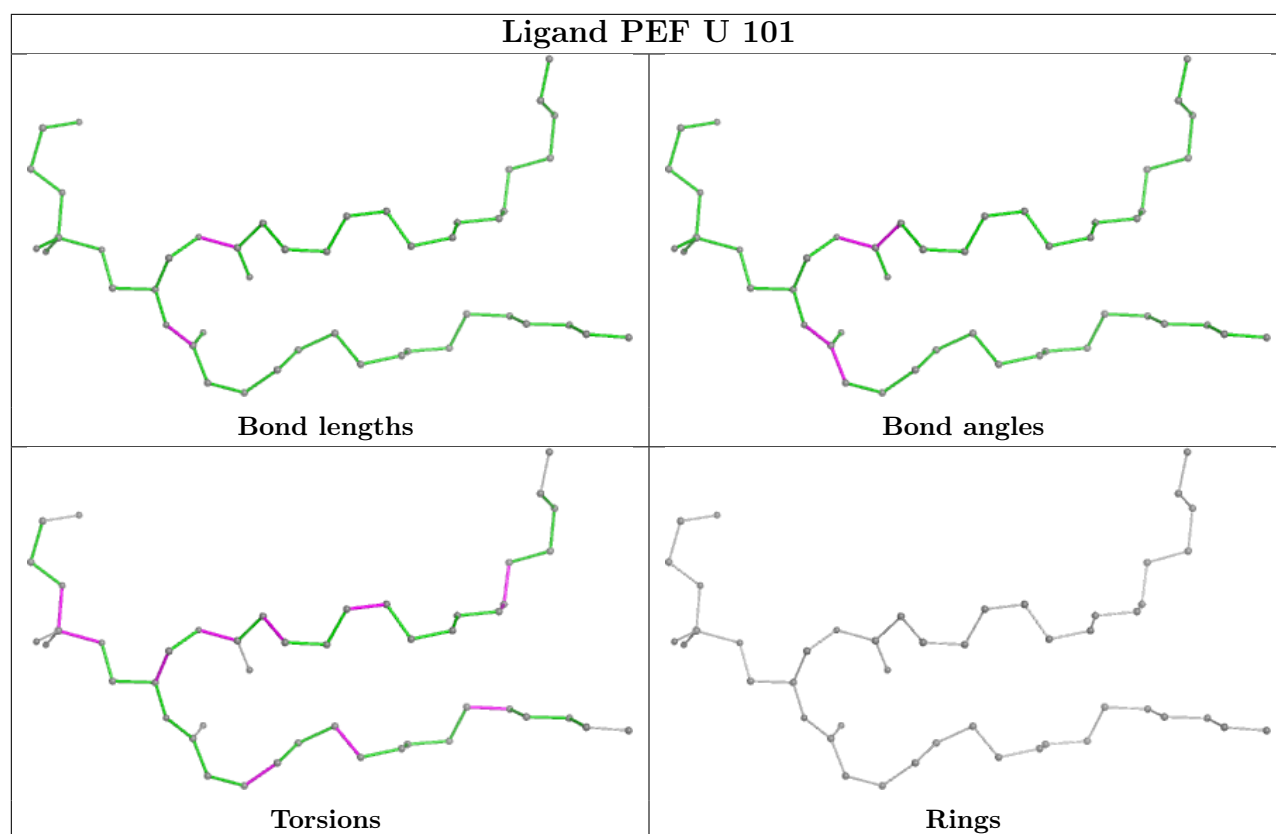




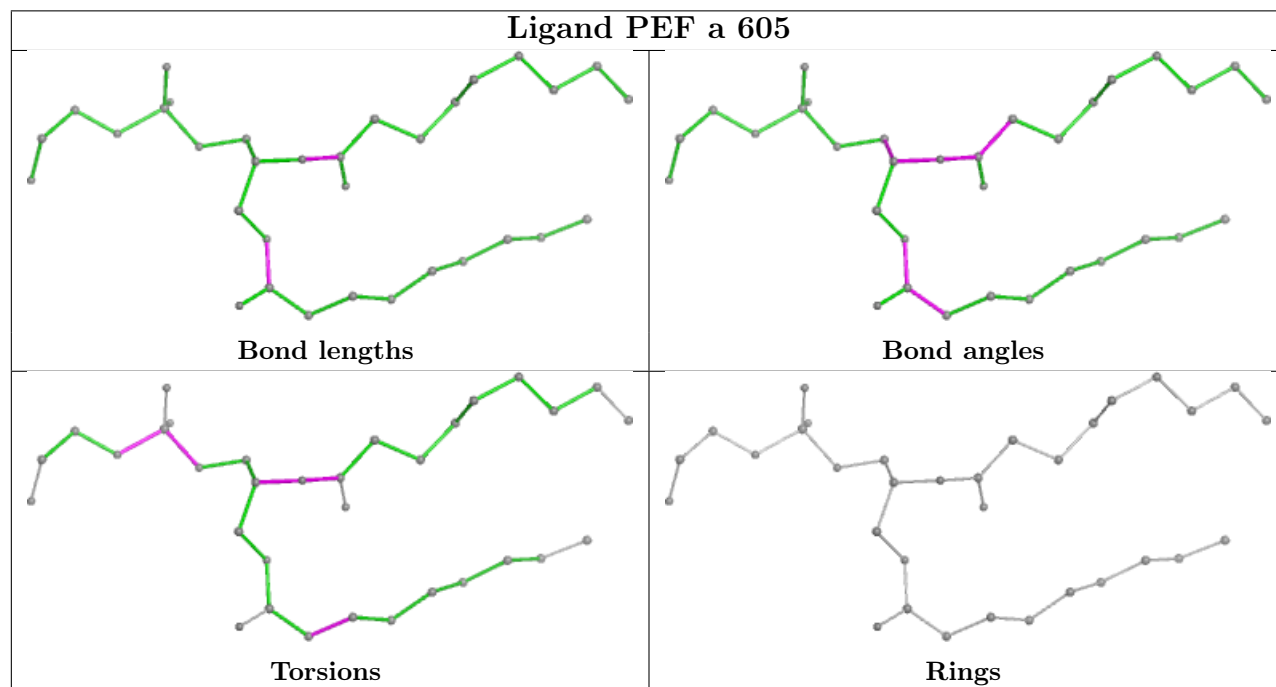
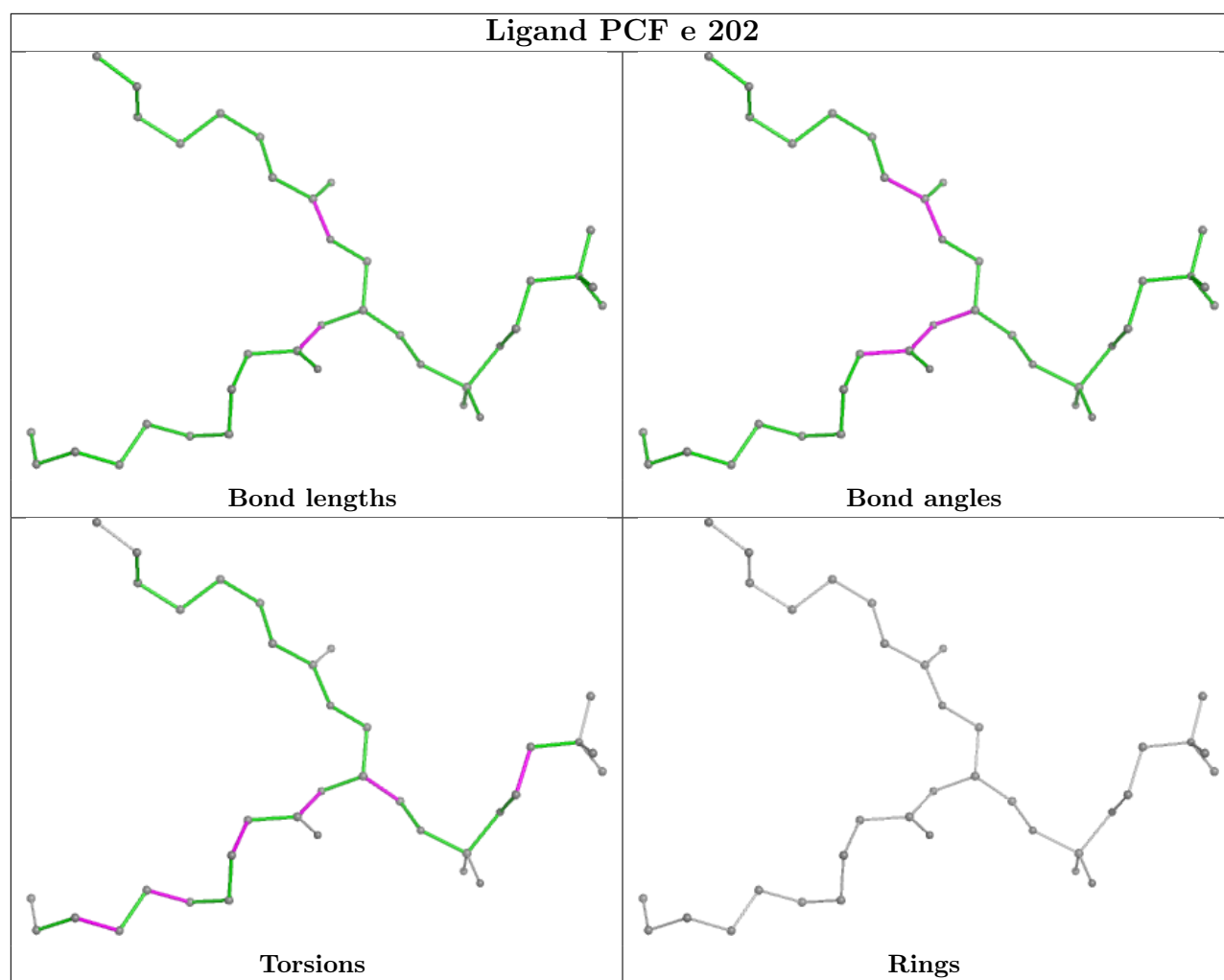


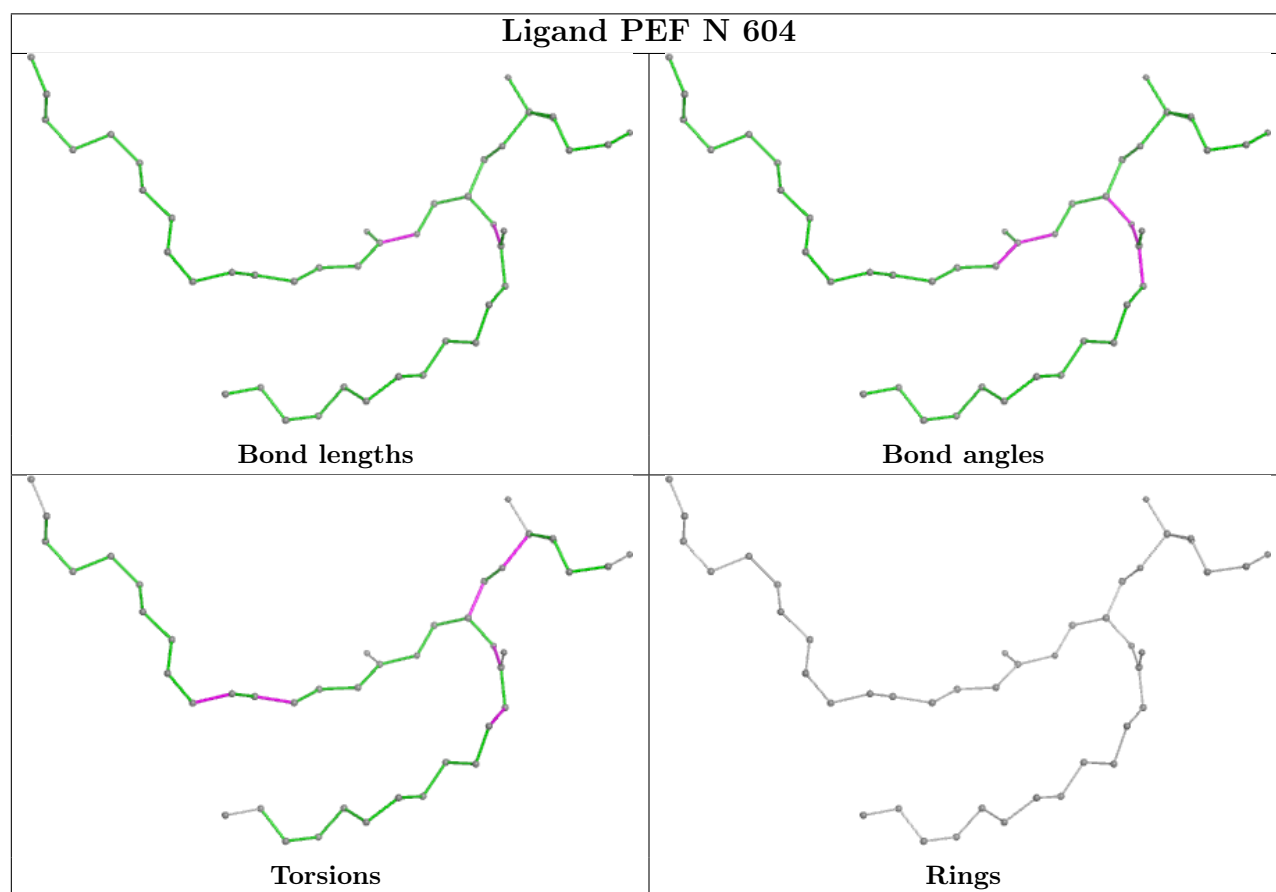
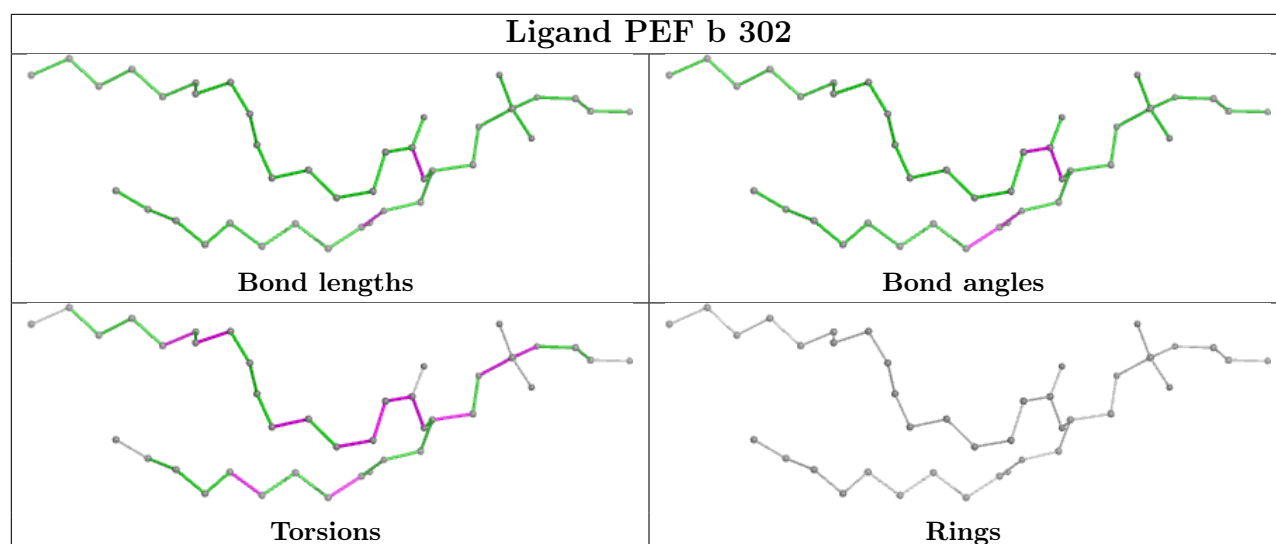


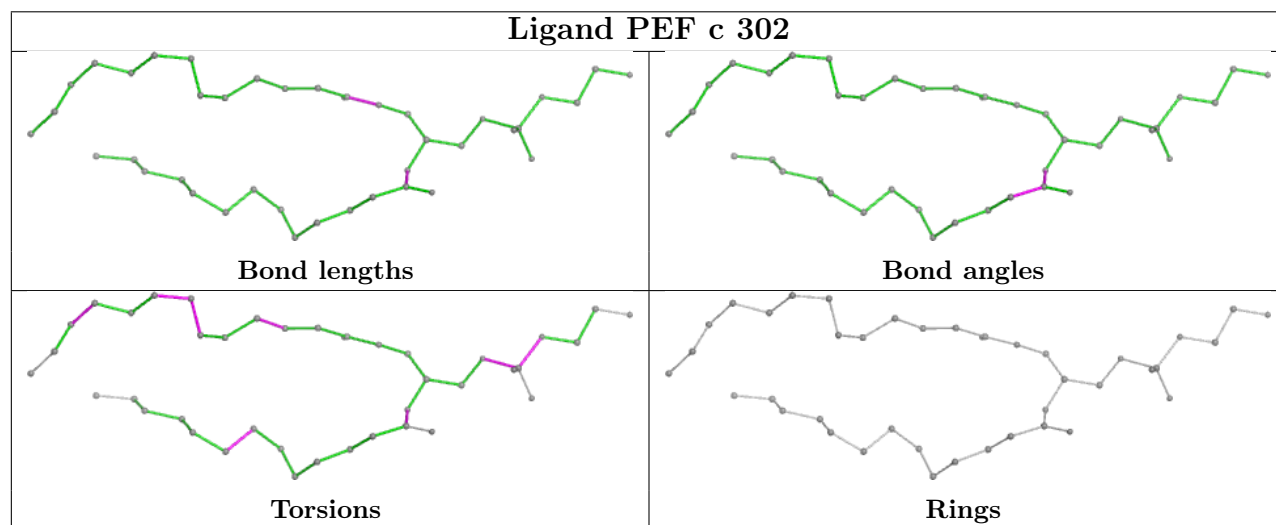
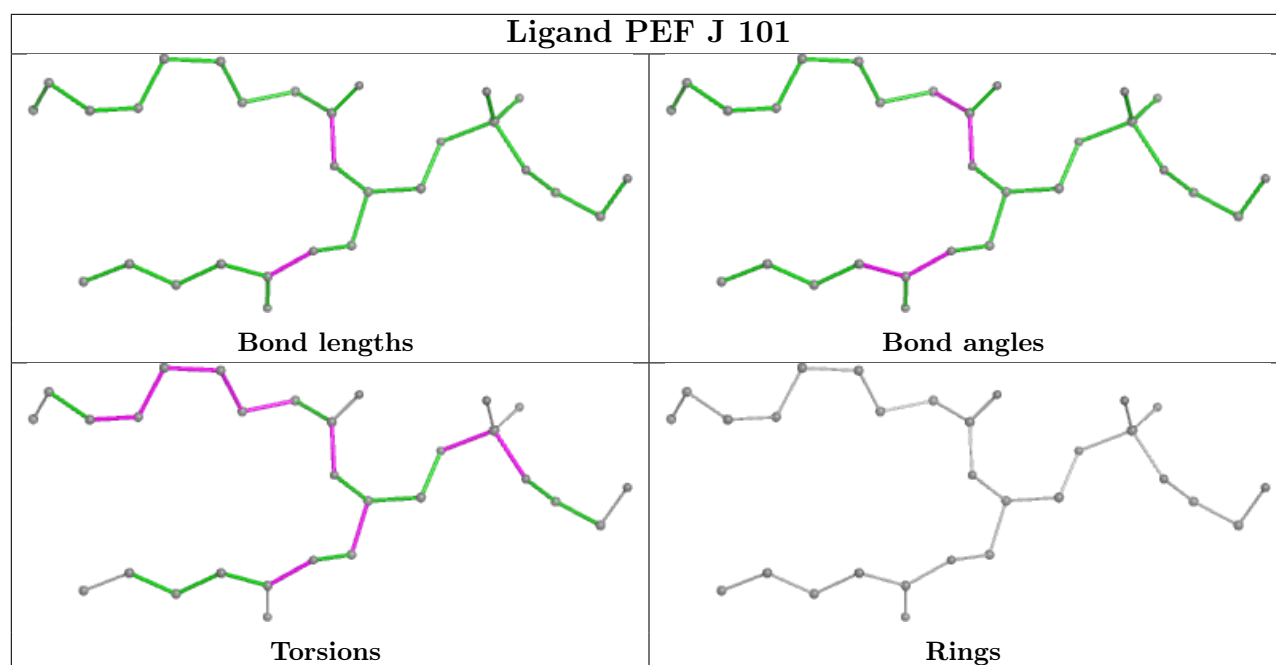


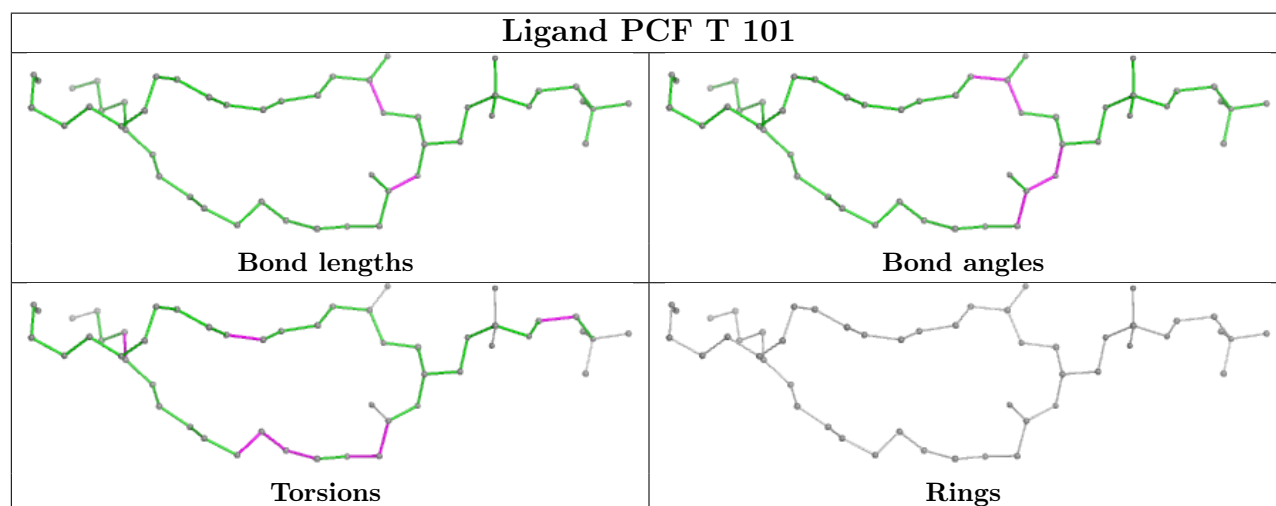
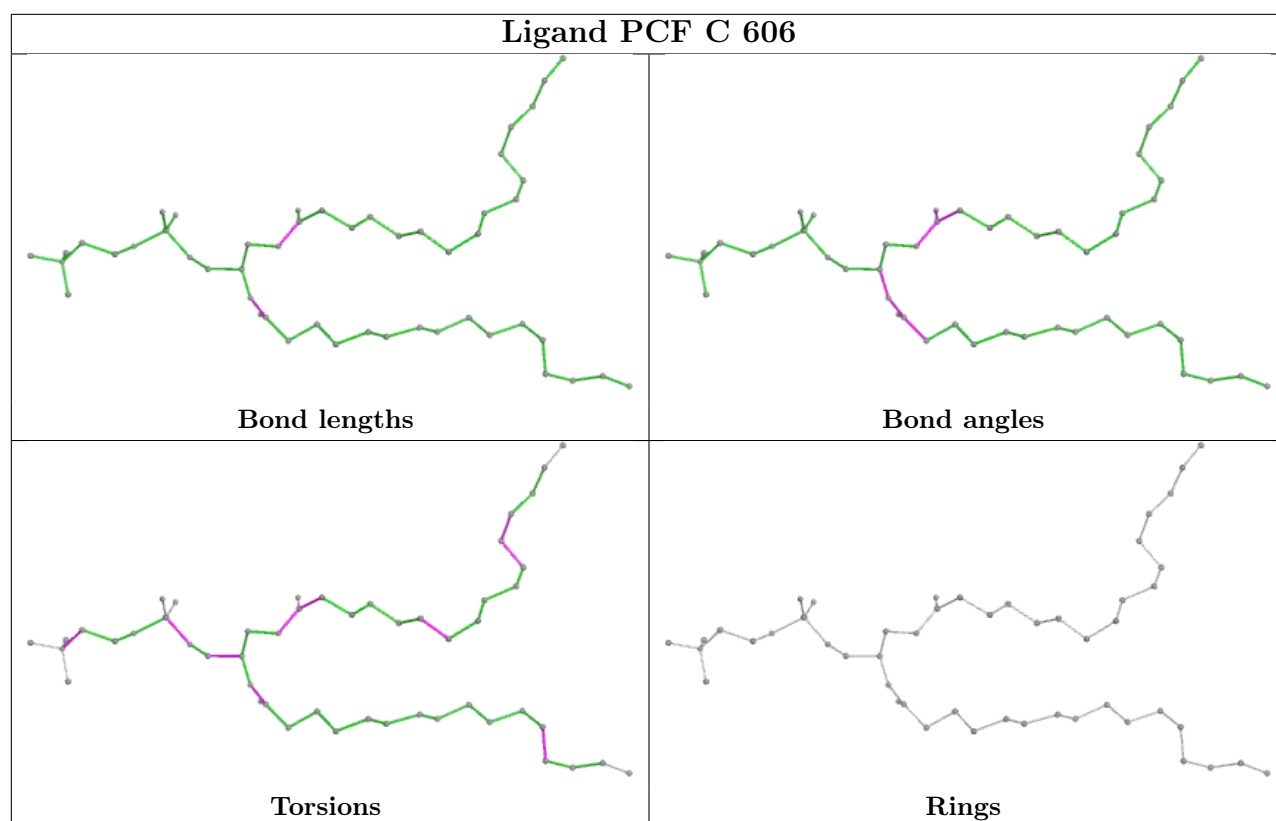


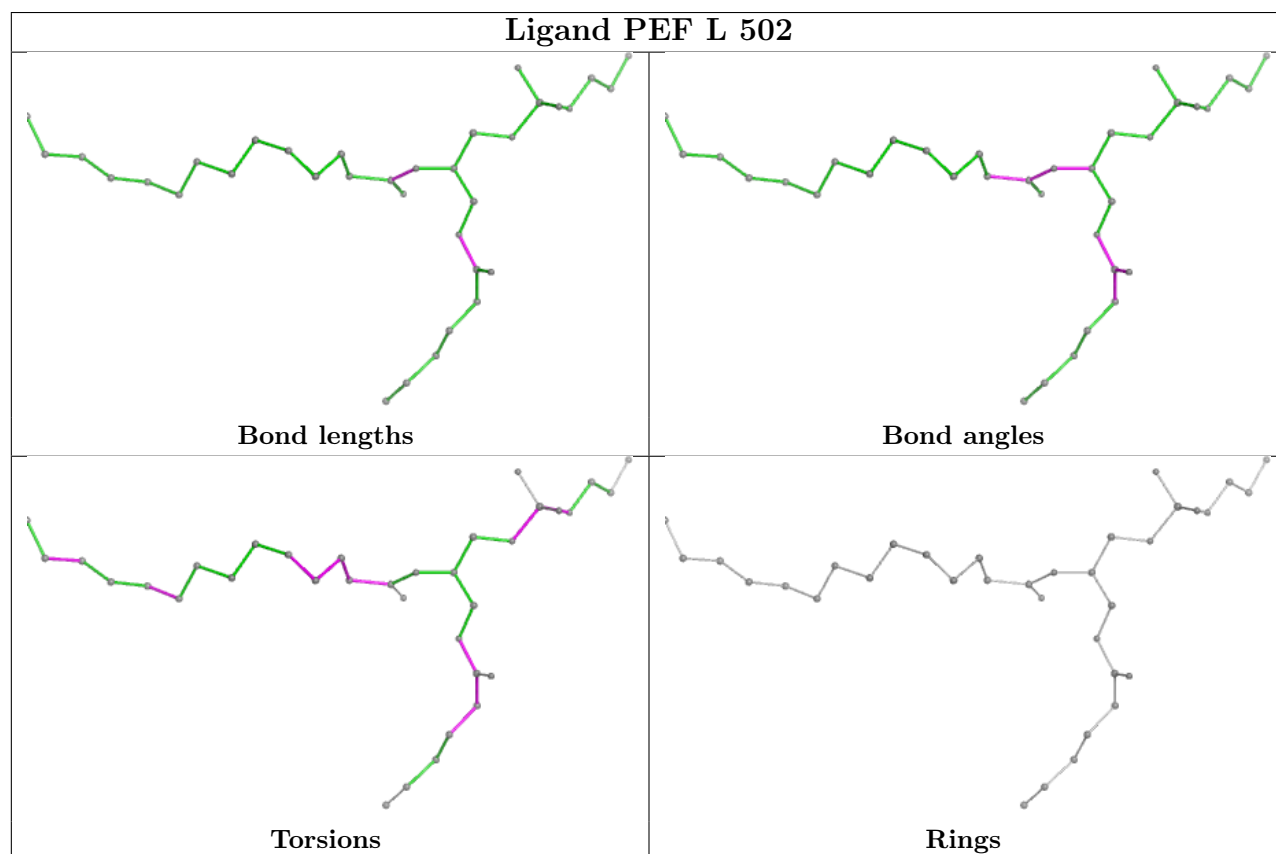
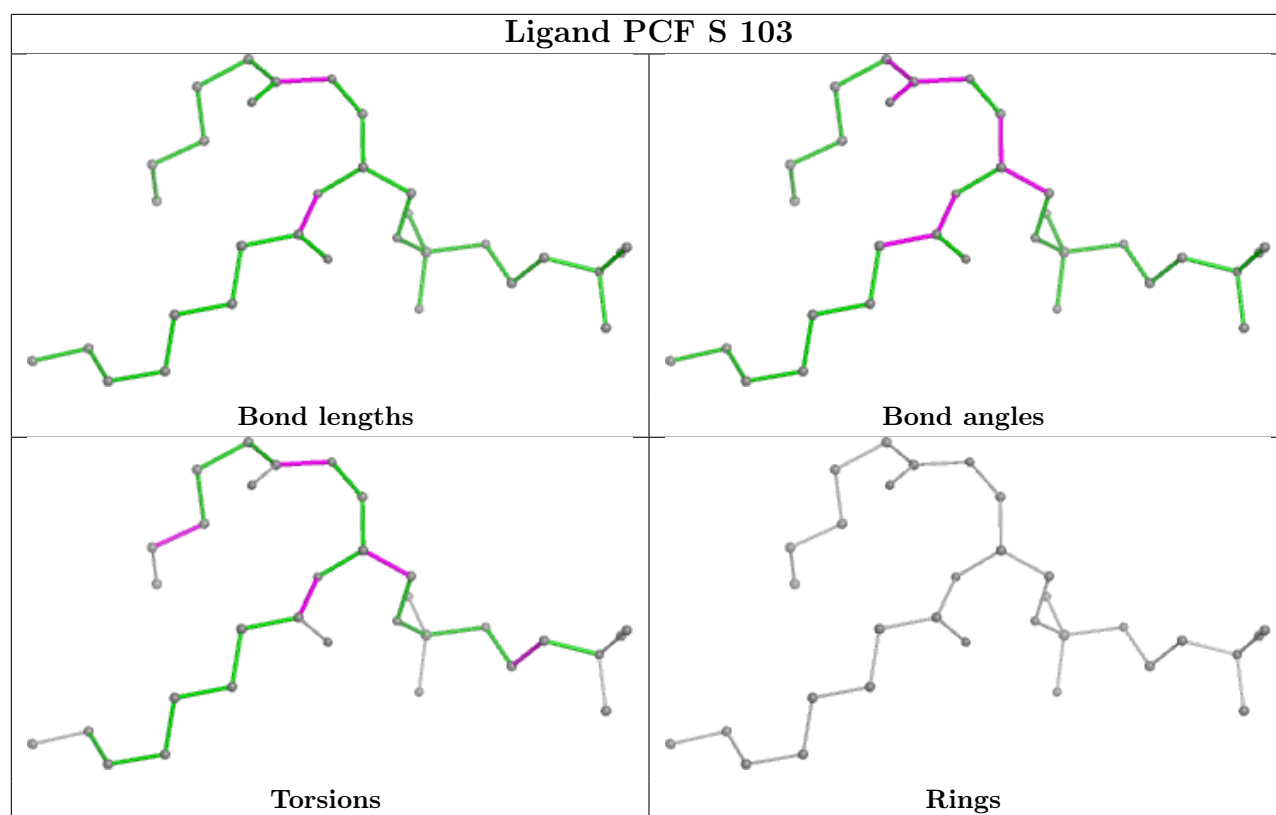


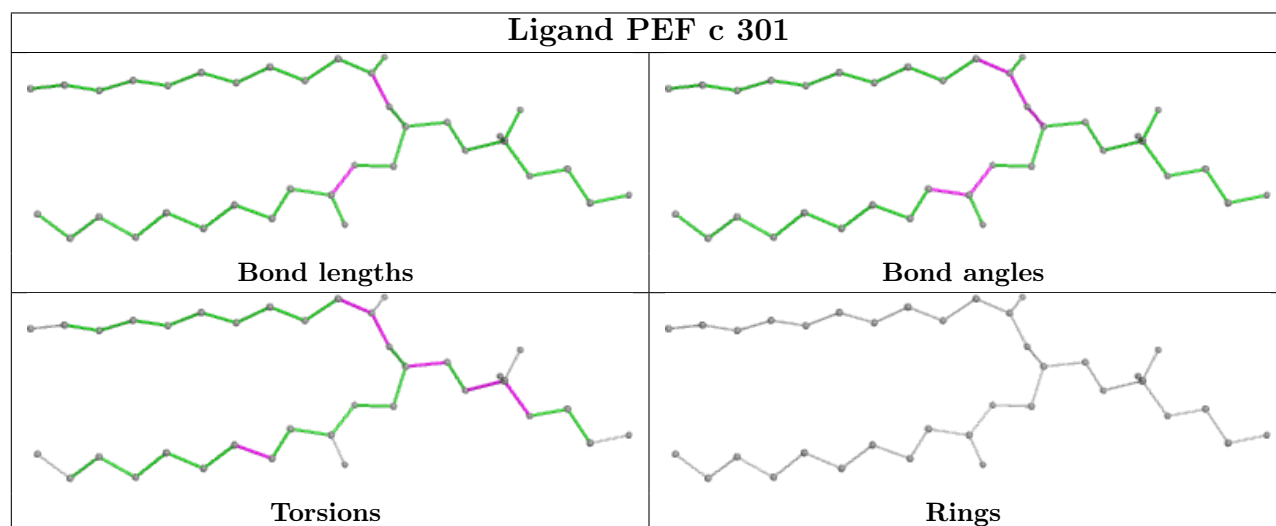
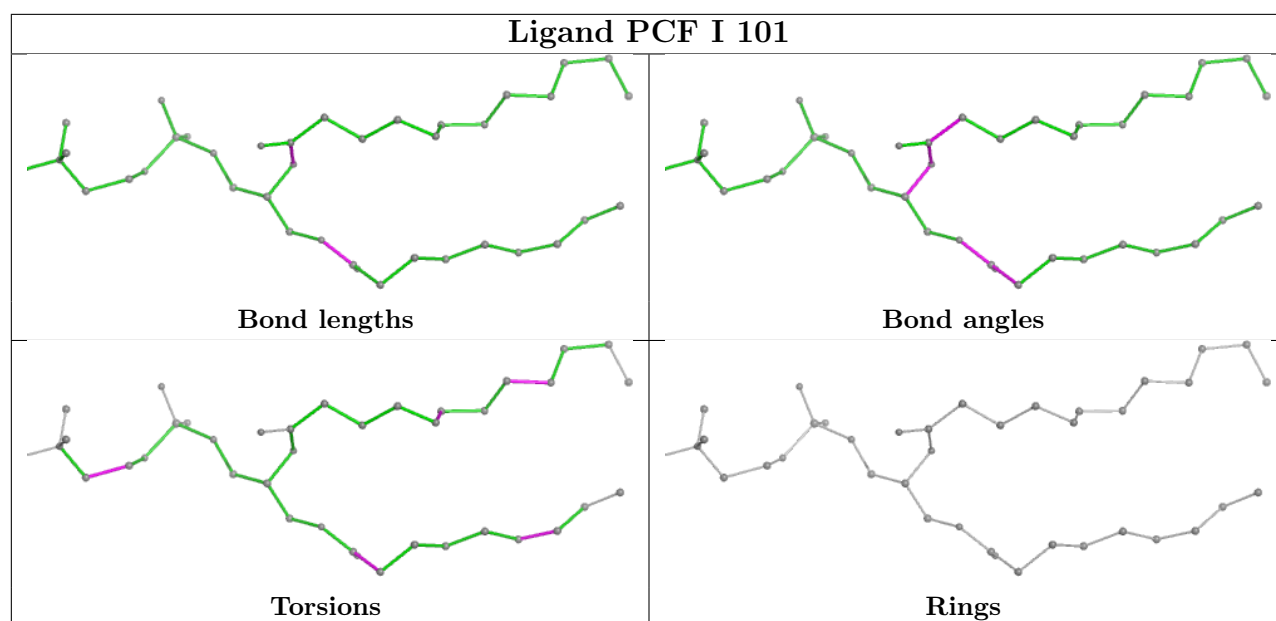


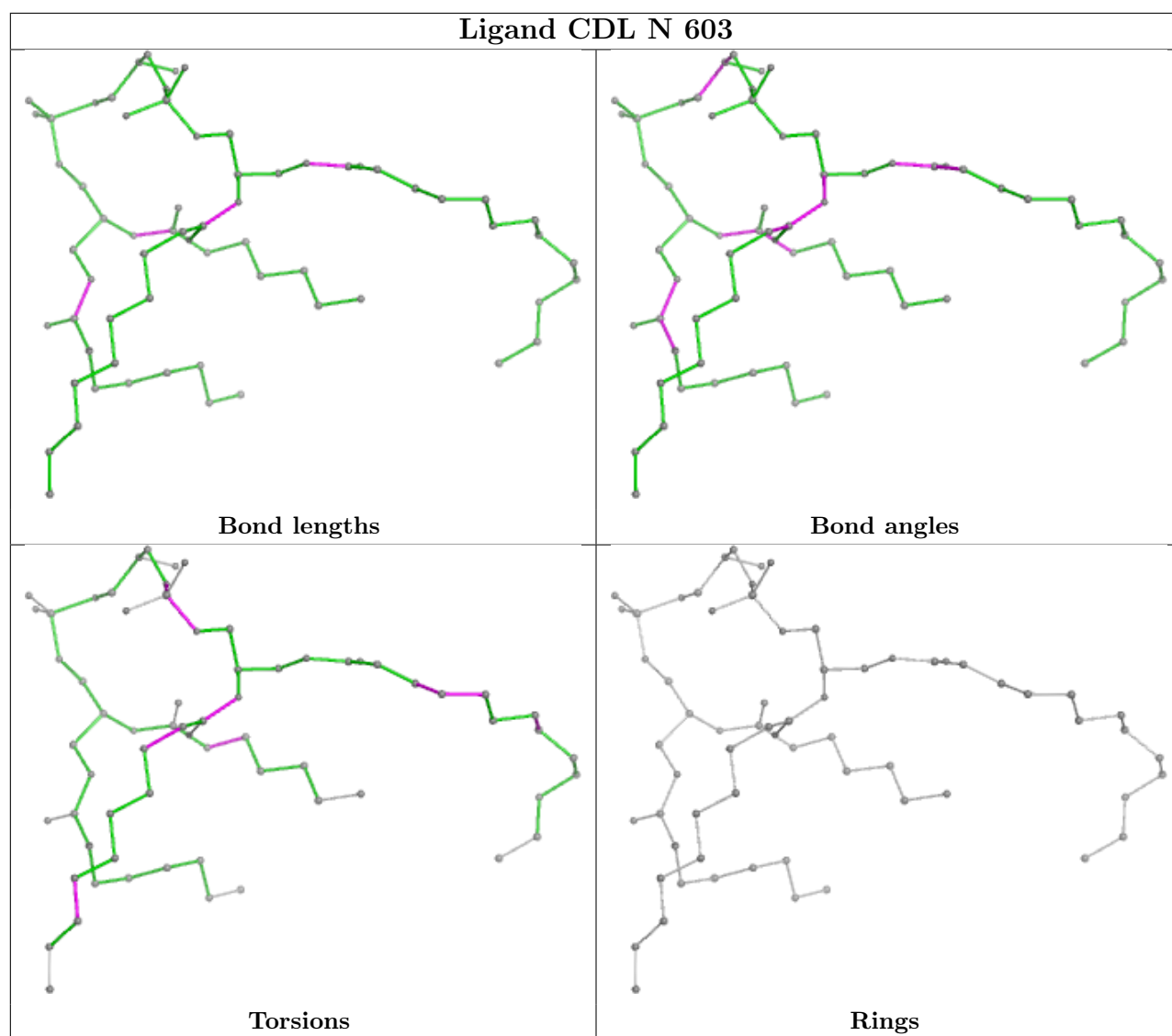


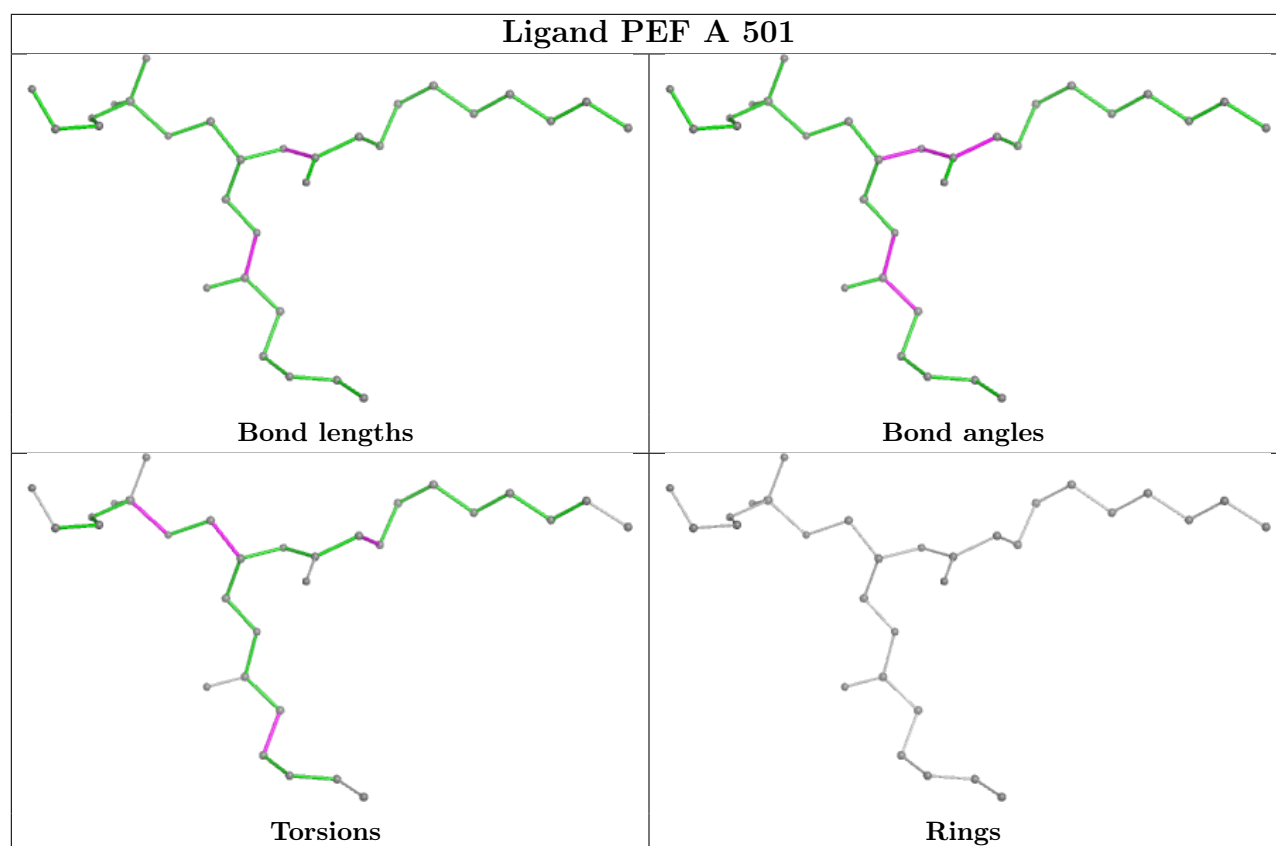




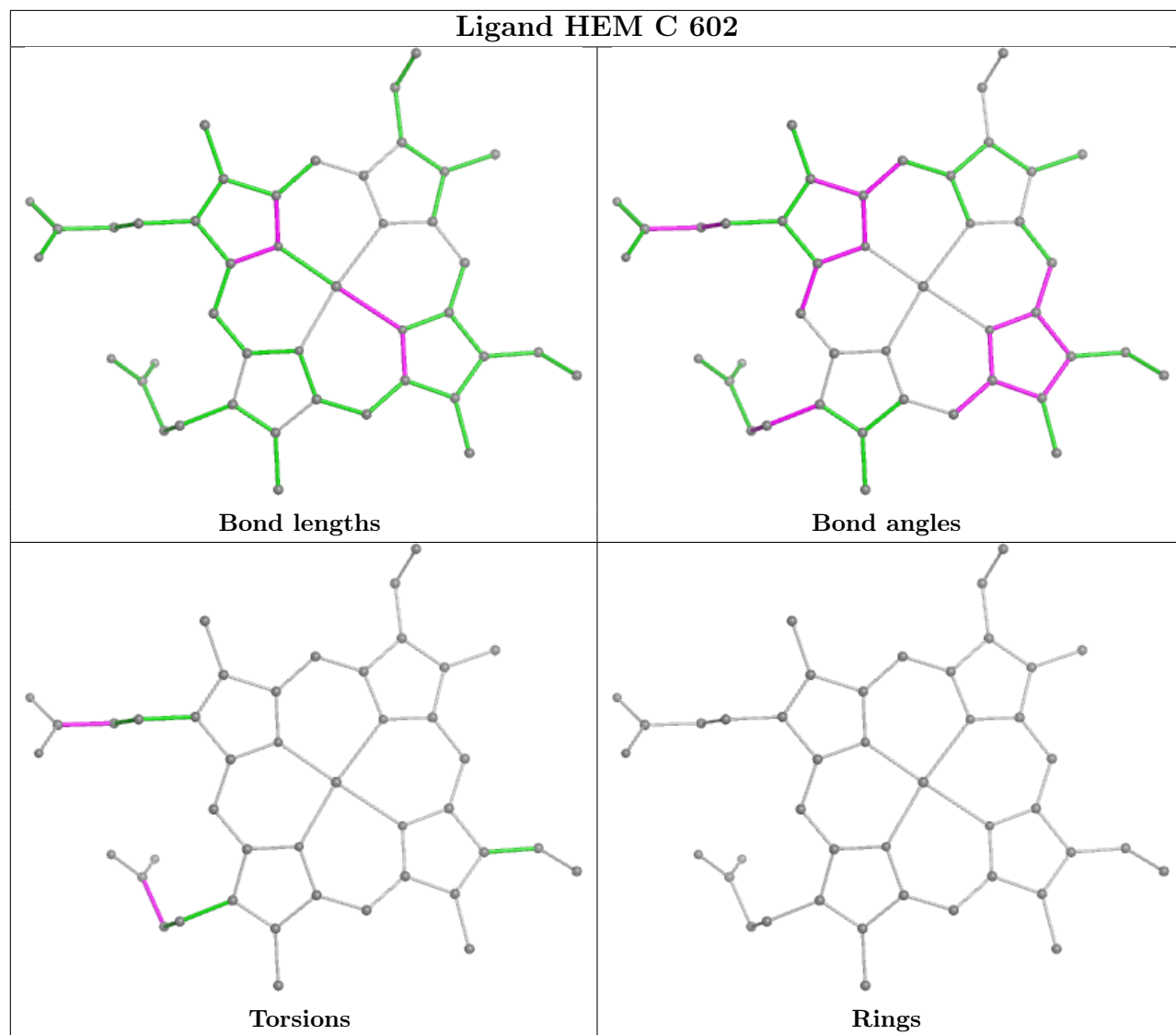


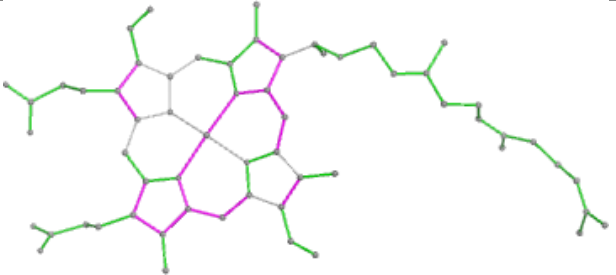
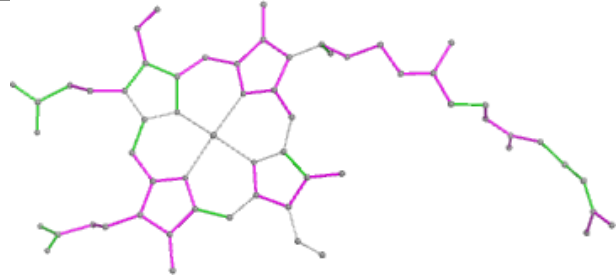
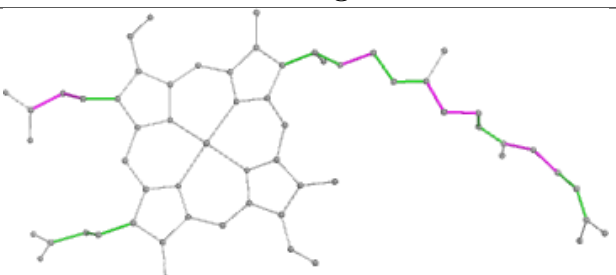
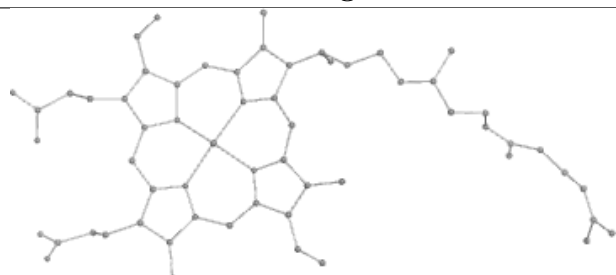








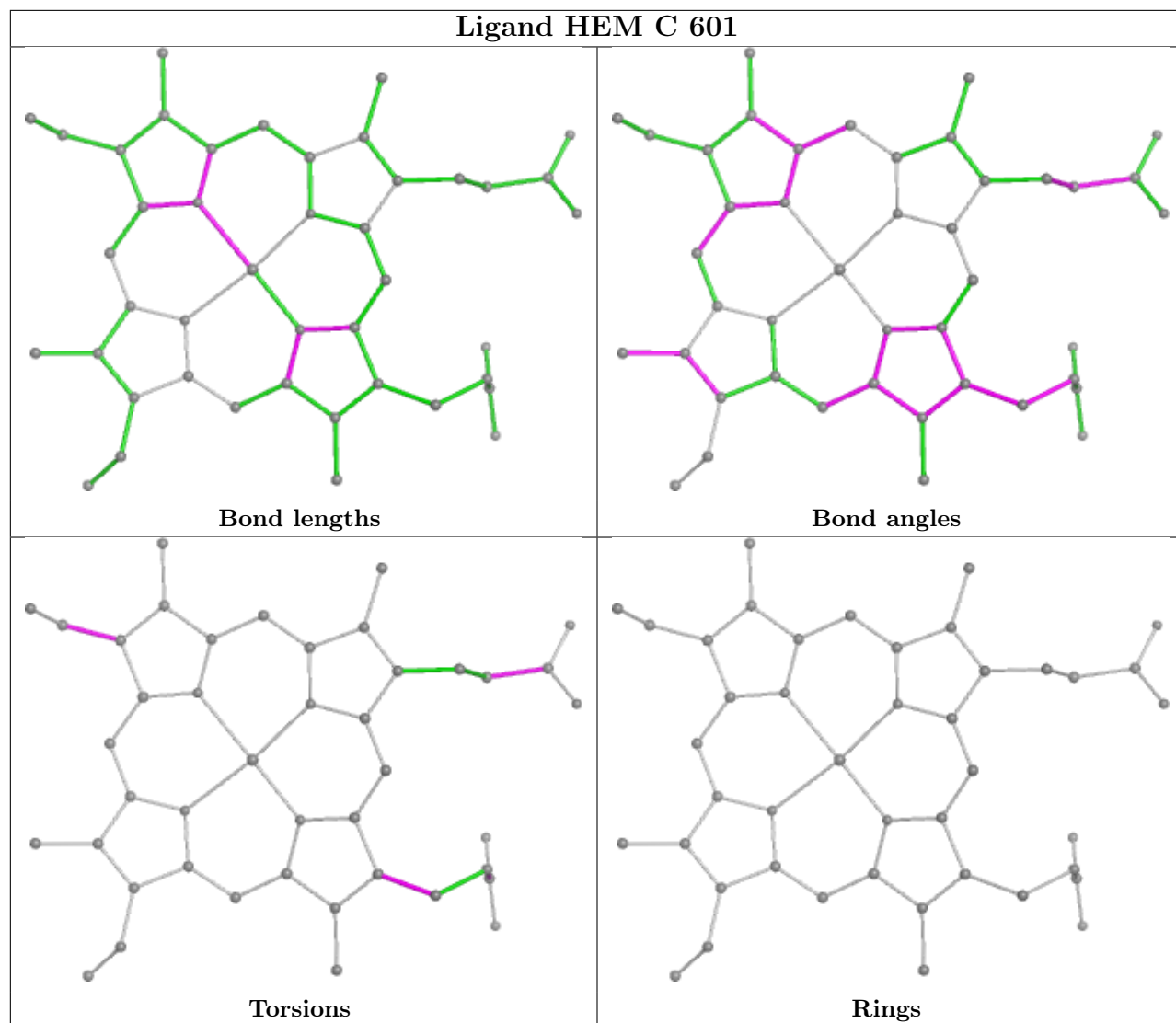


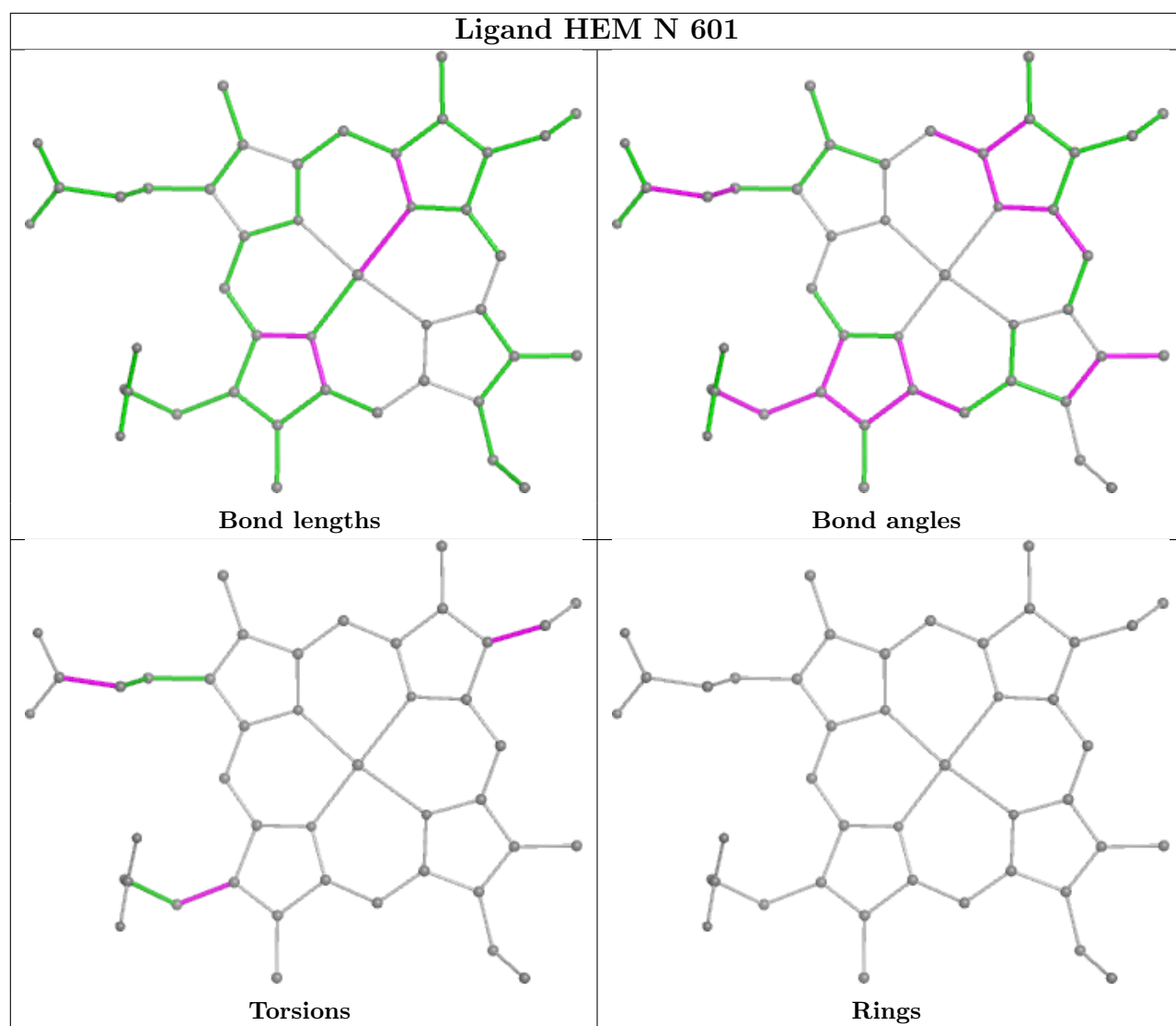


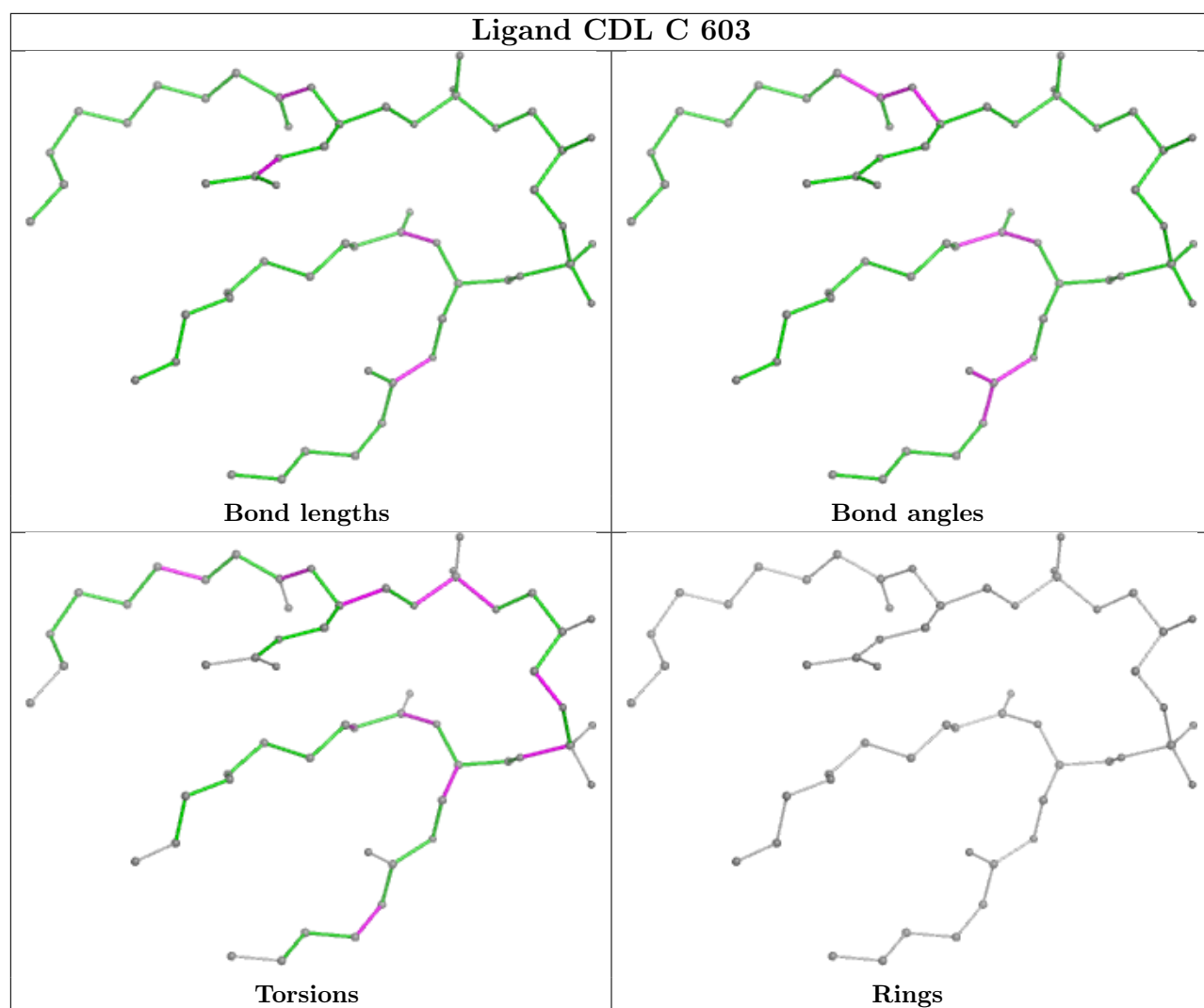


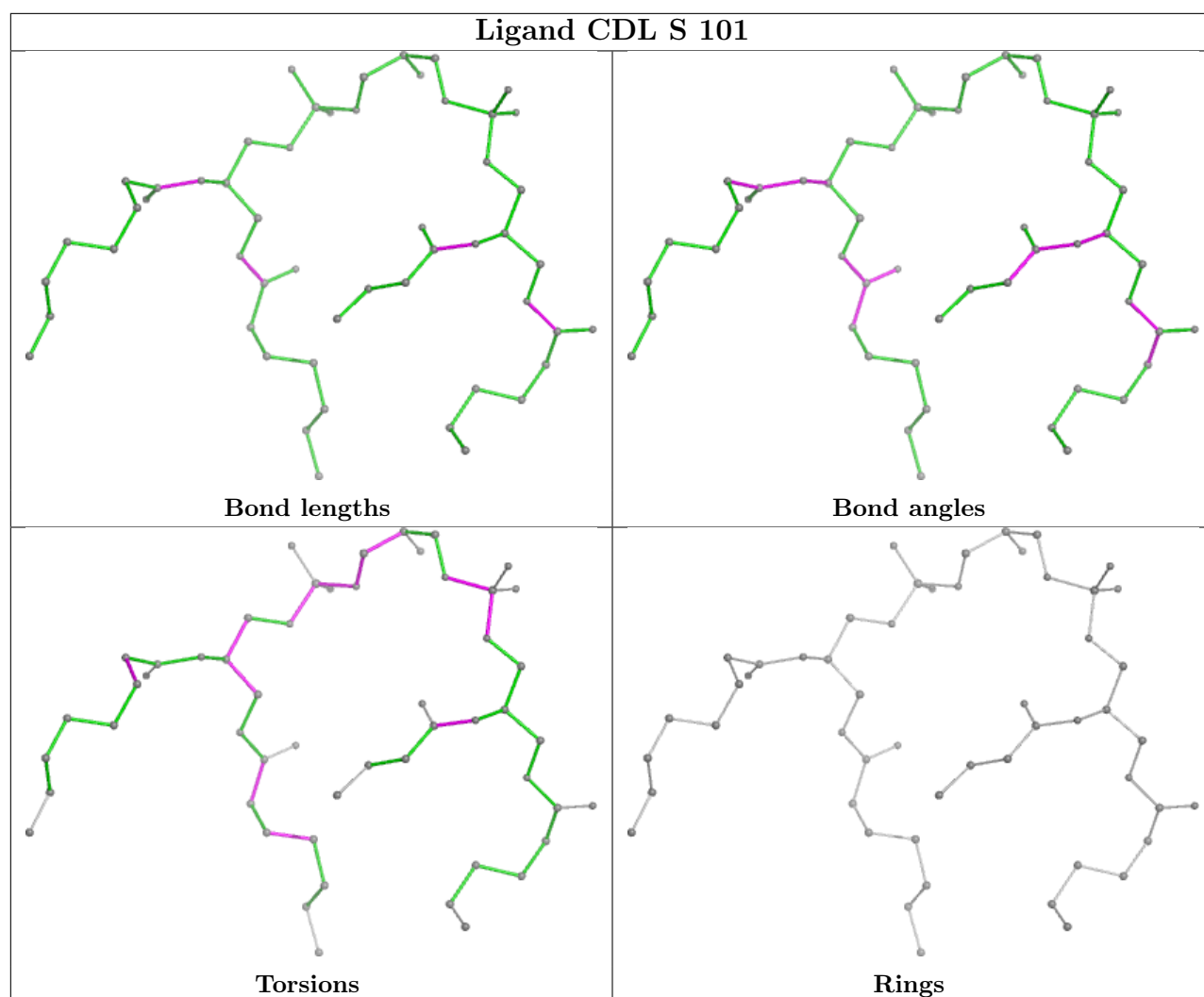
Ligand HEA a 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

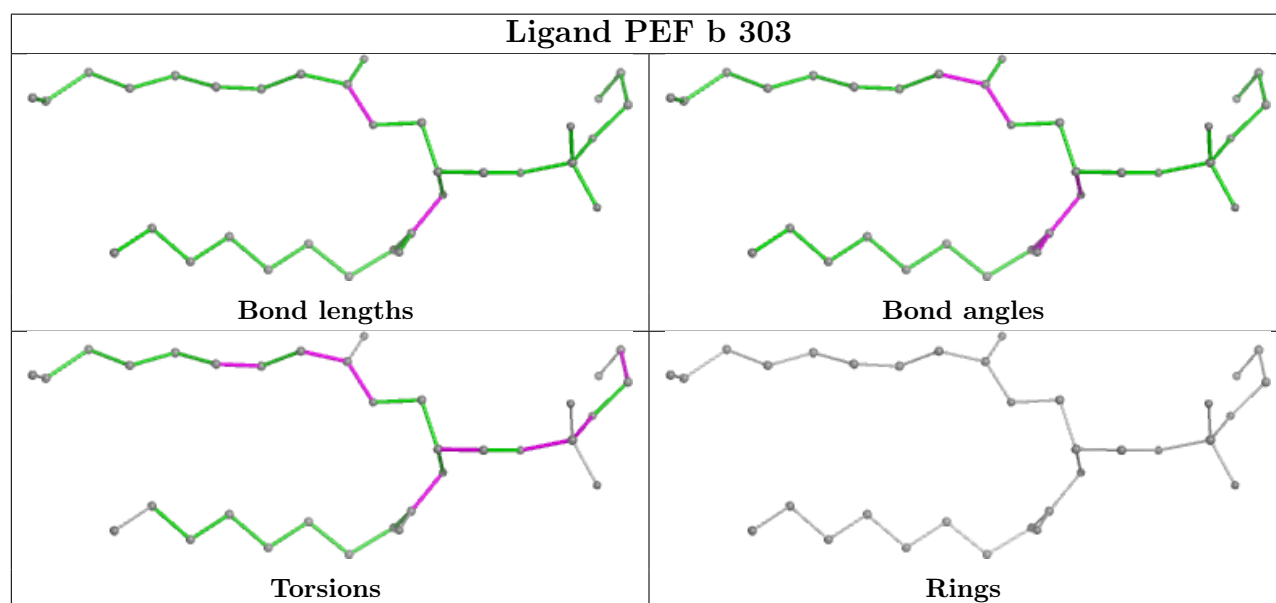
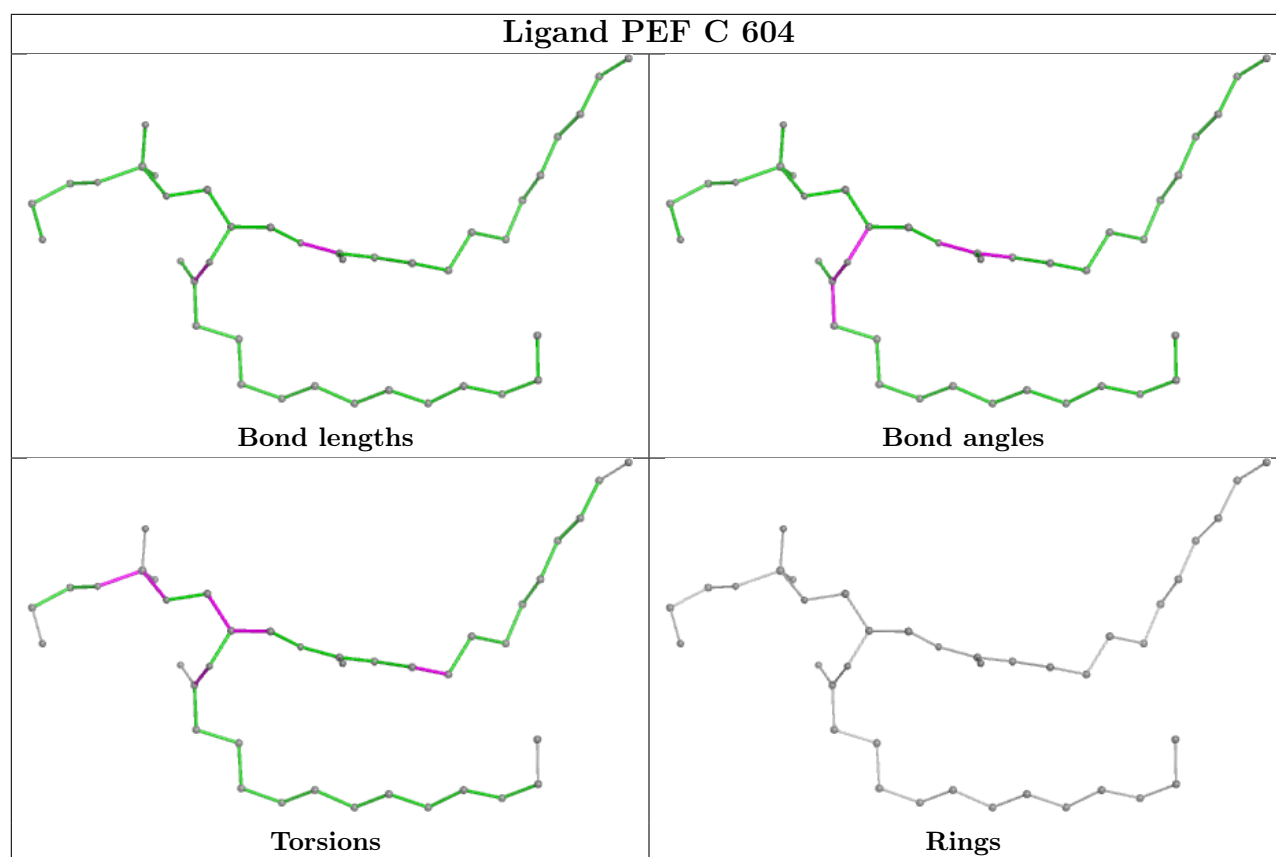
Ligand CUA b 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

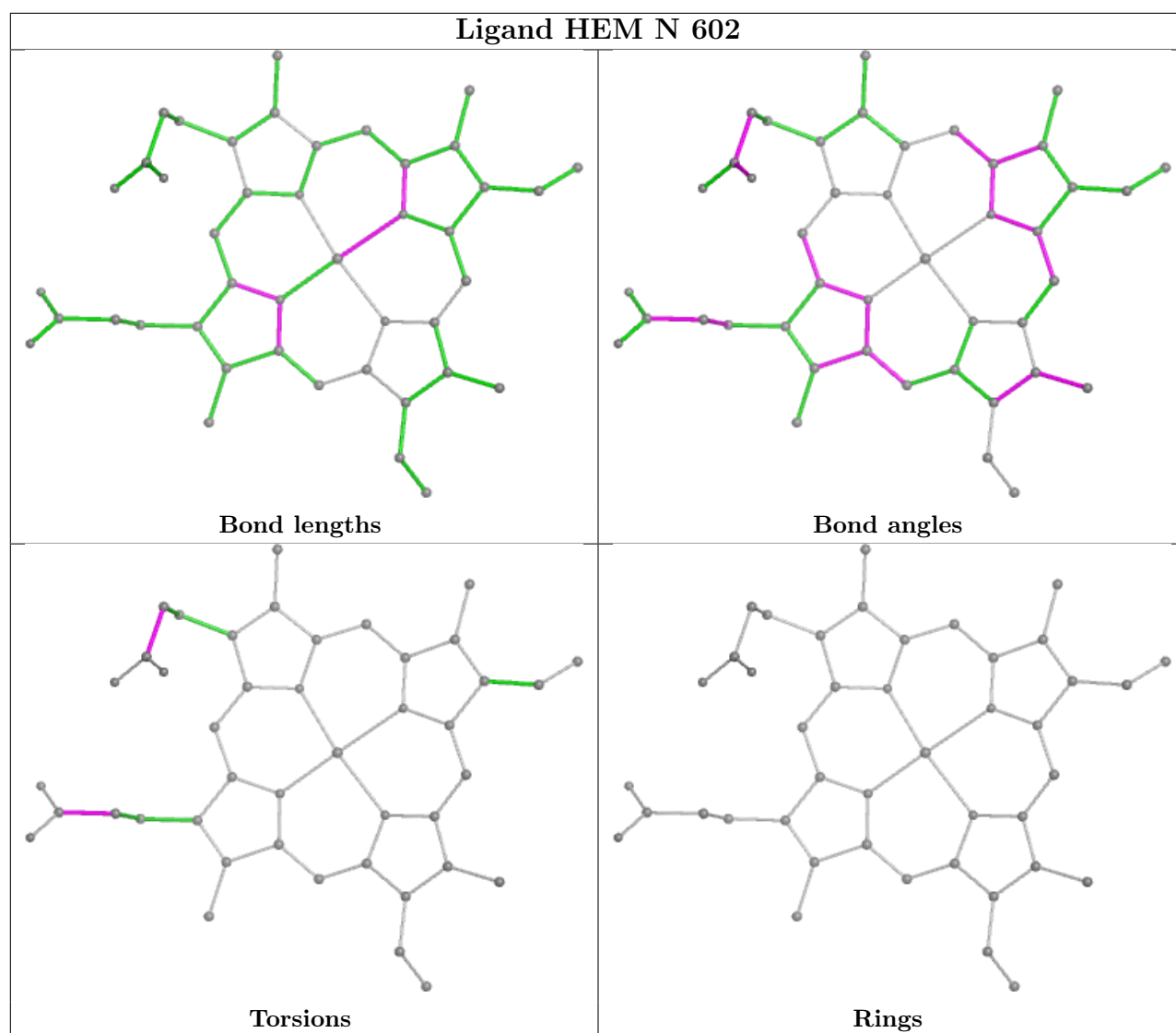




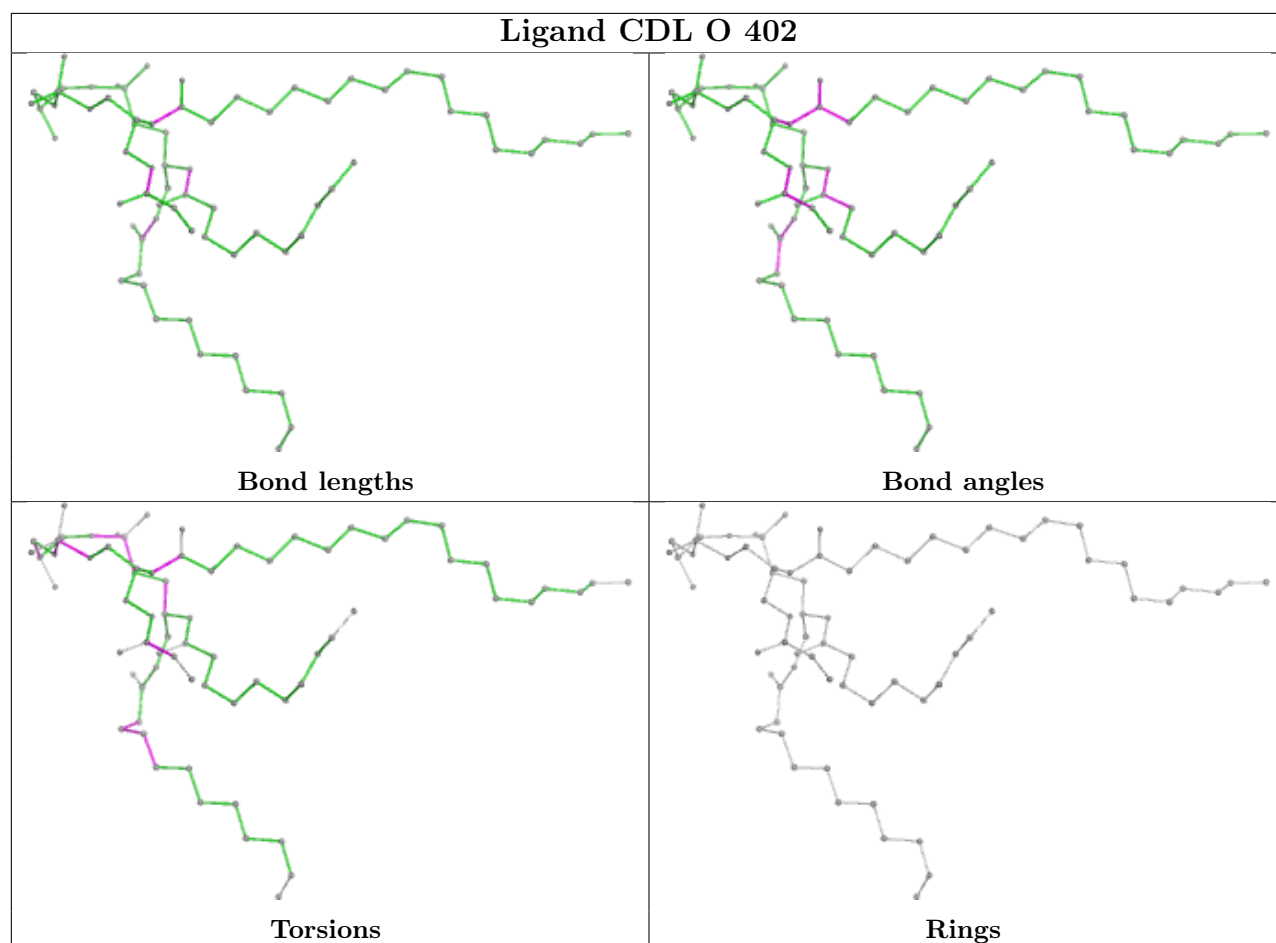
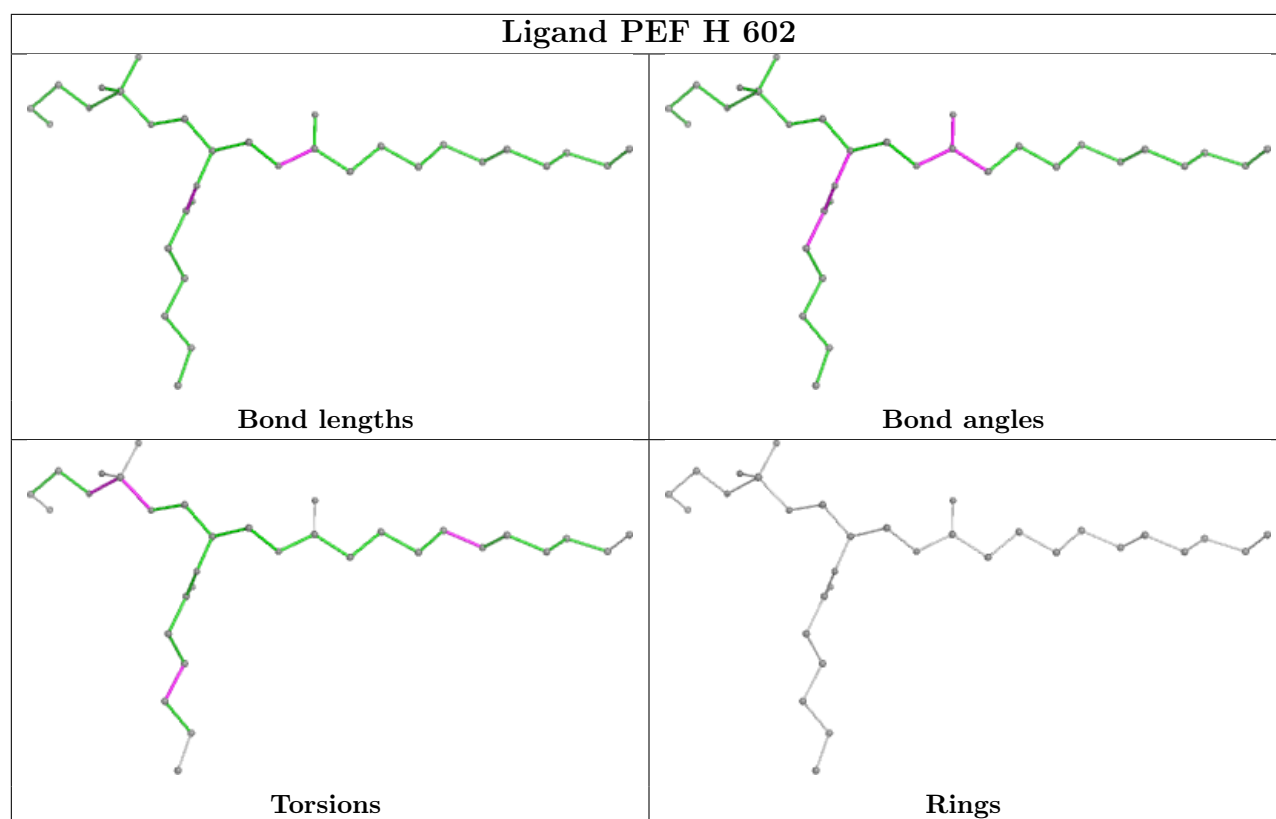


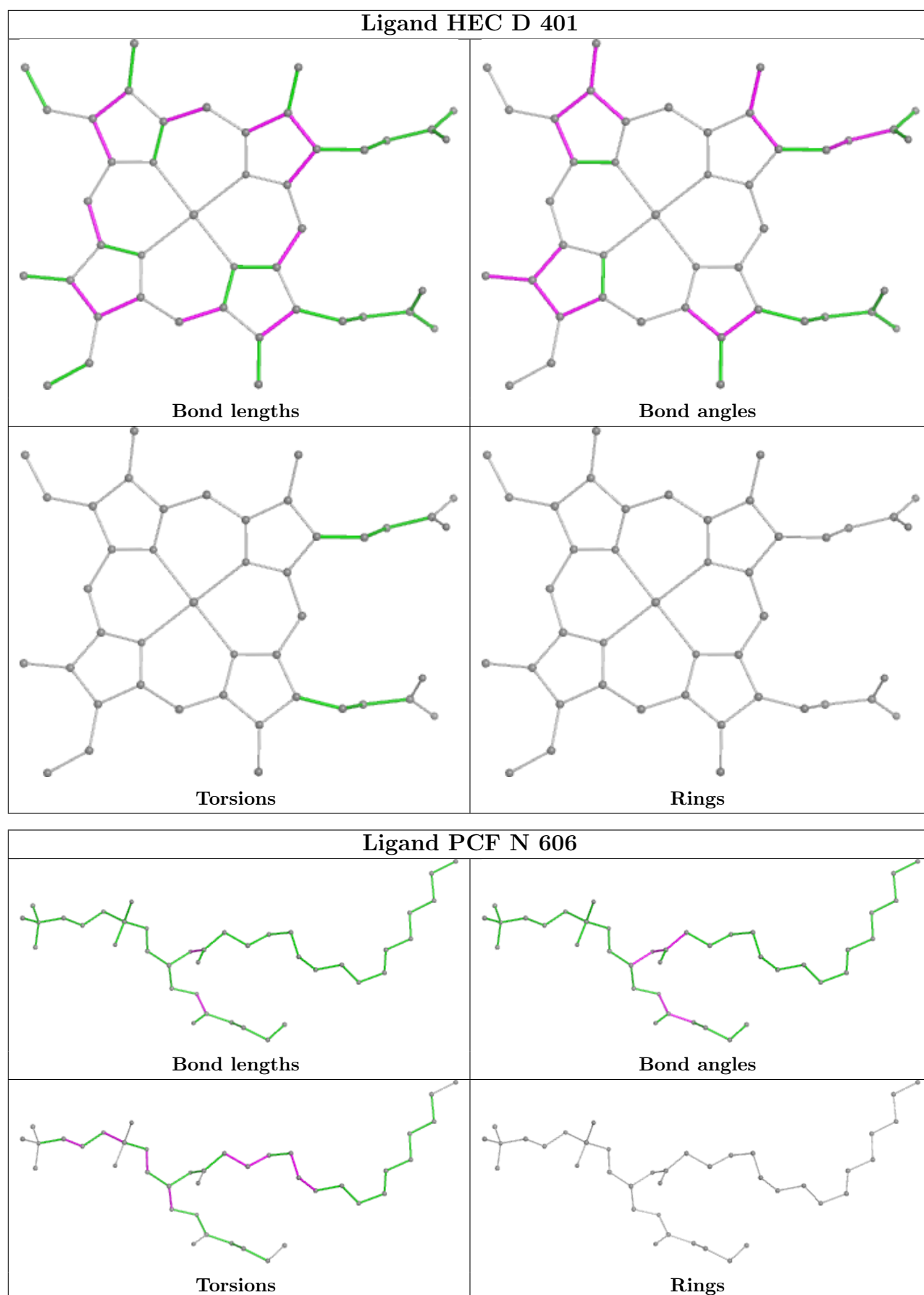


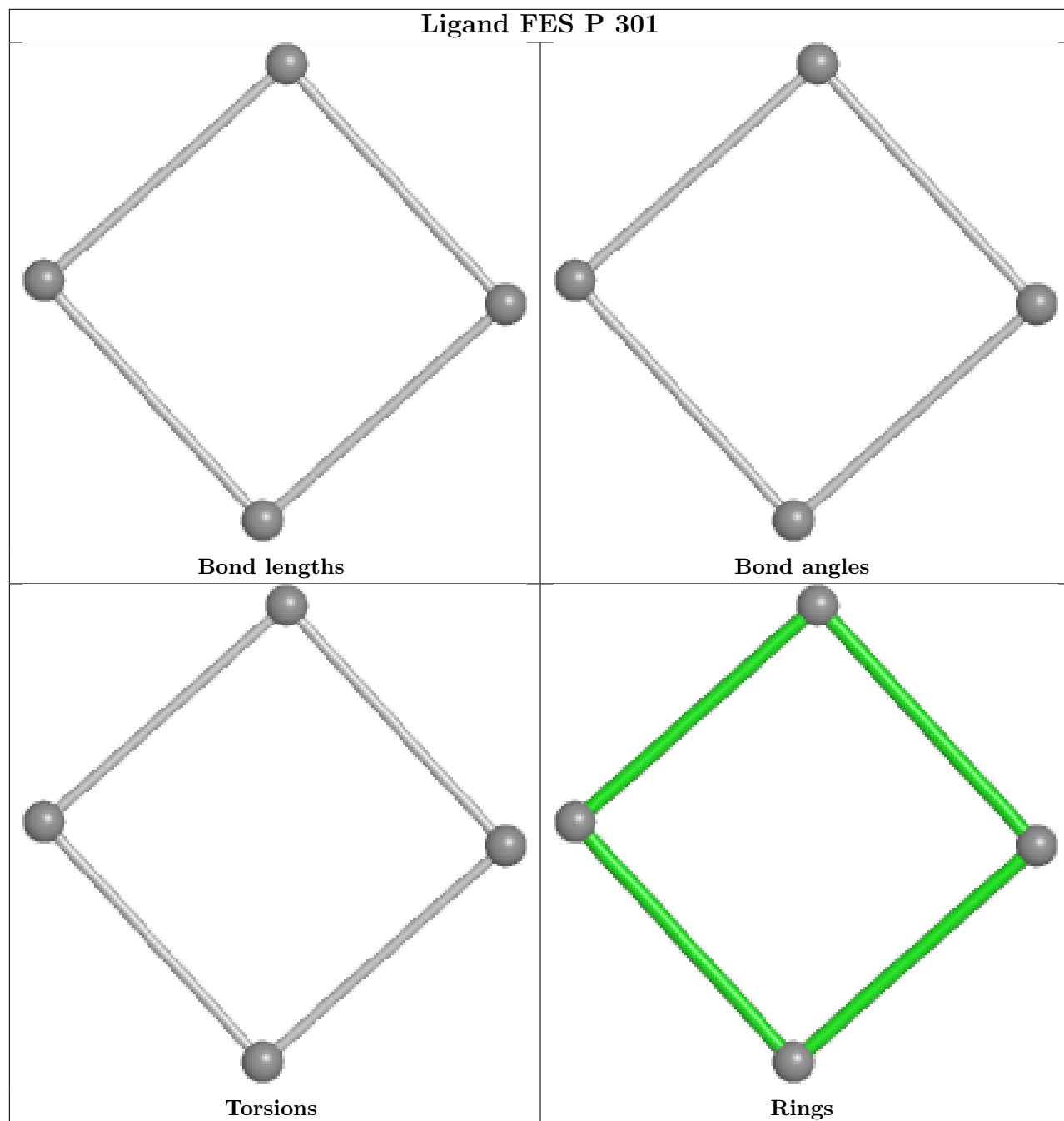


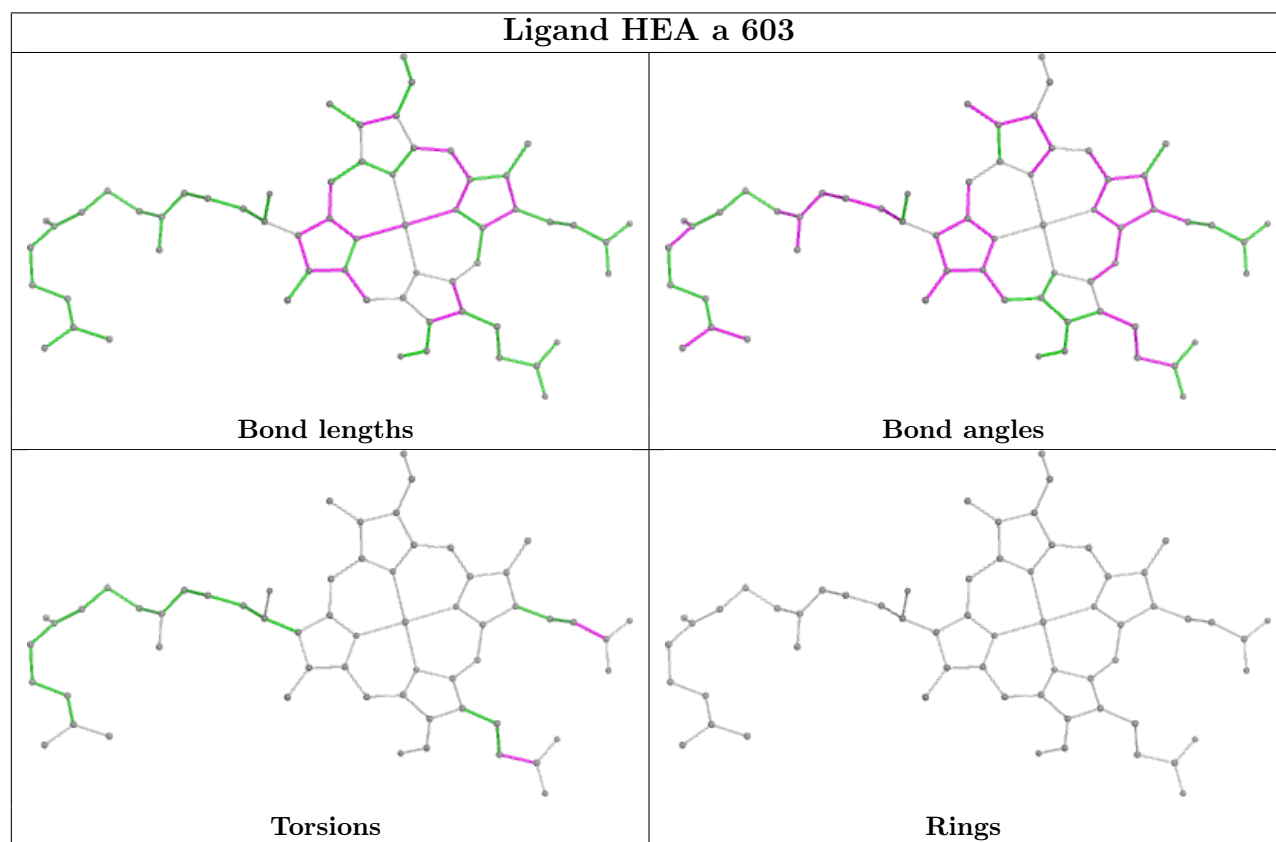
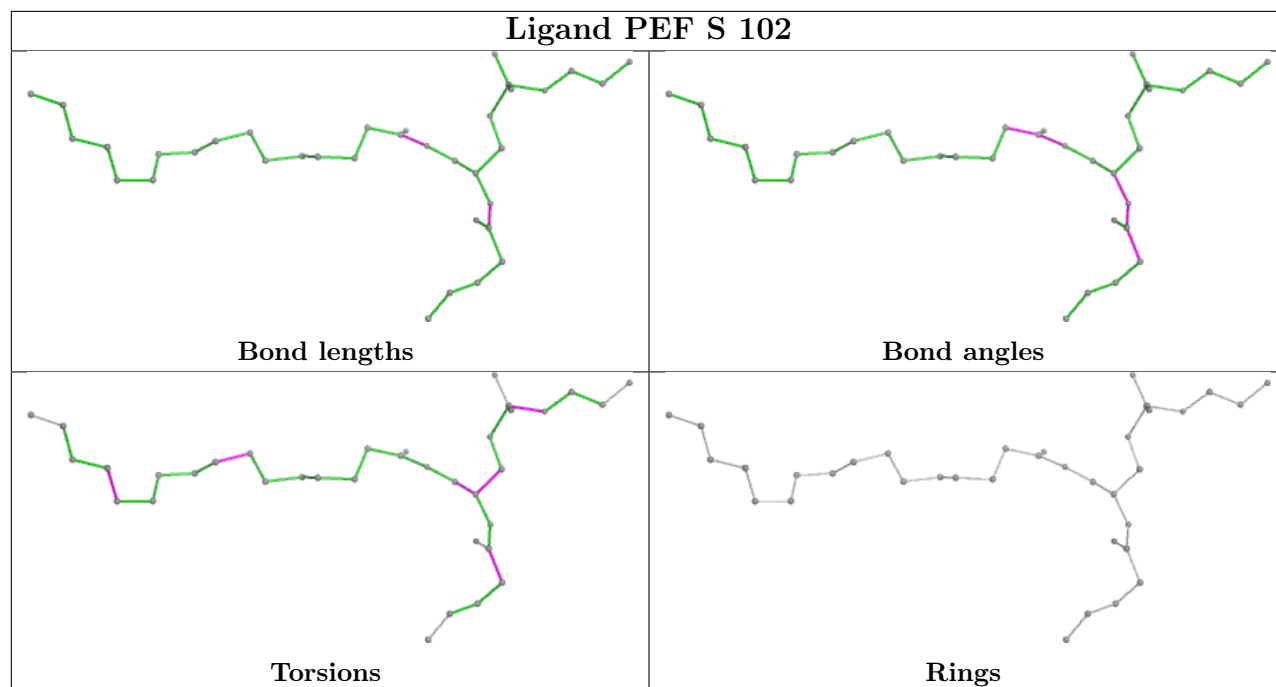


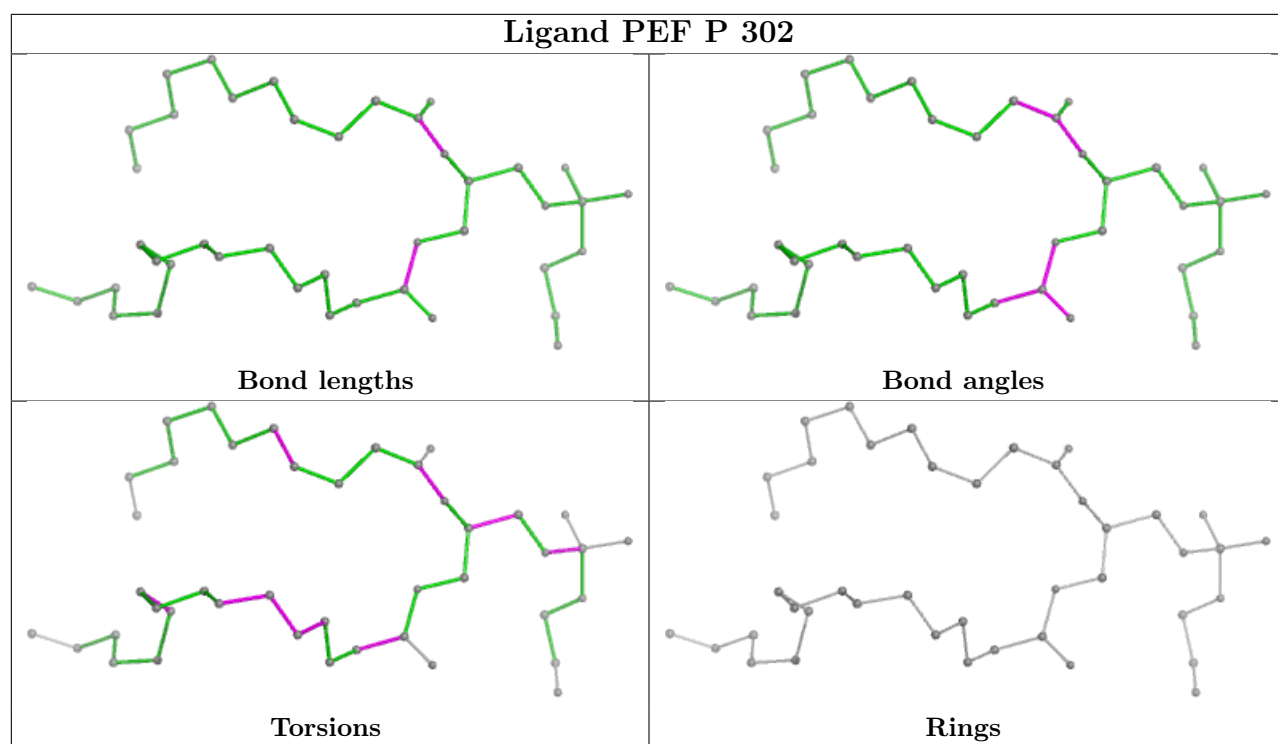


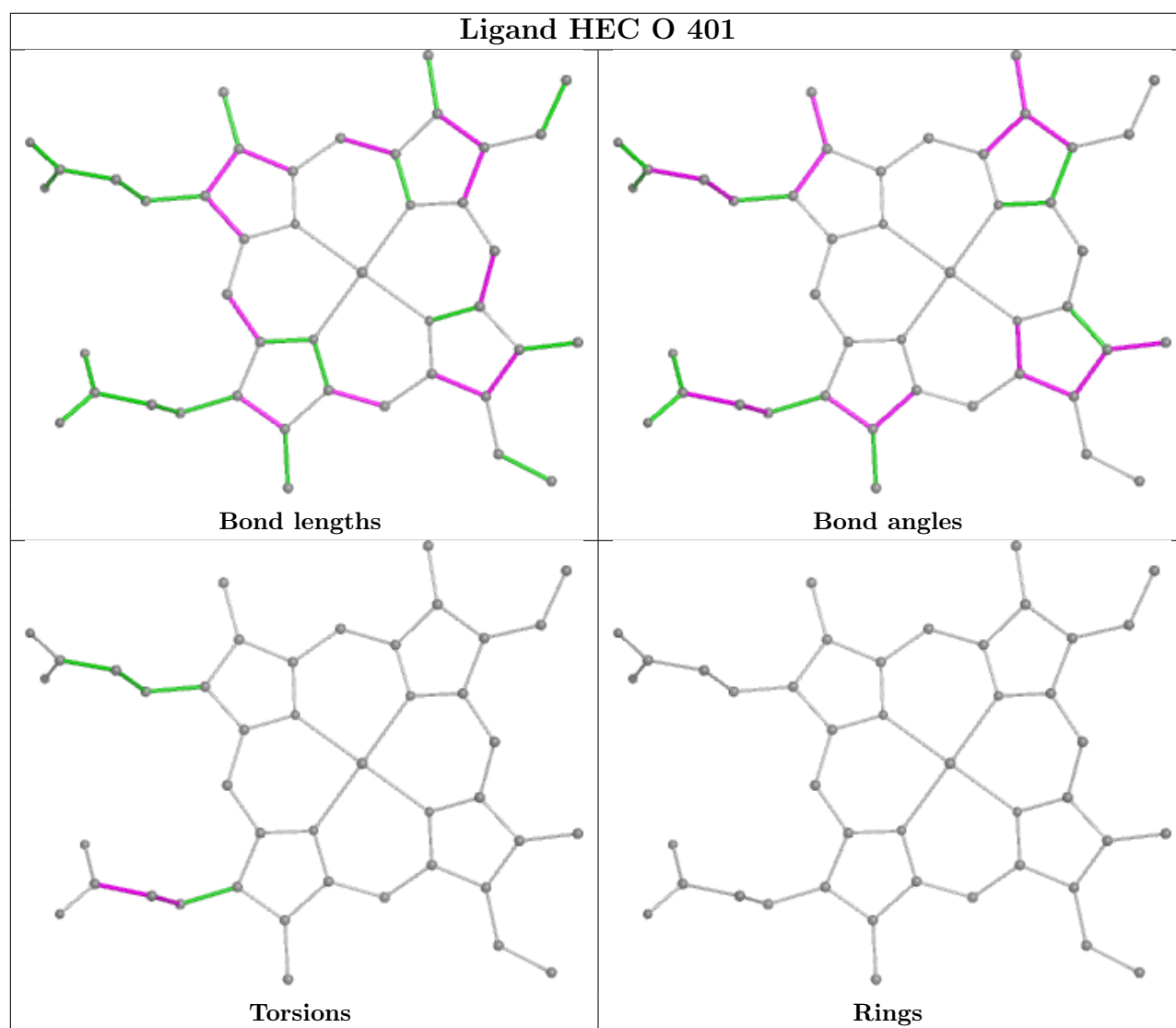












## 5.7 Other polymers [i](#)

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-10318. 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.