



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:53 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 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

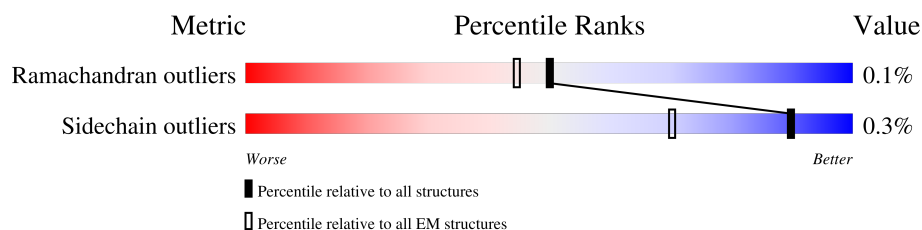
1 Overall quality at a glance

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.





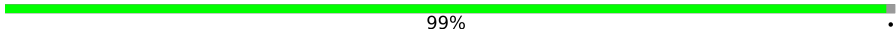
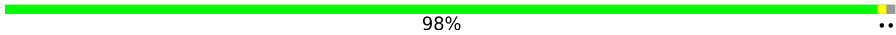
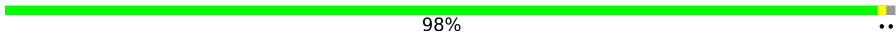
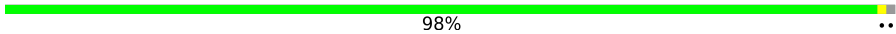


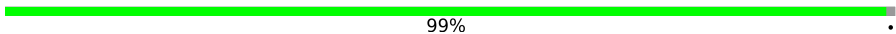
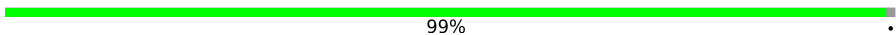
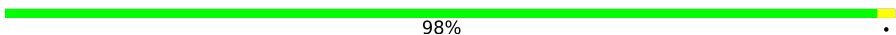




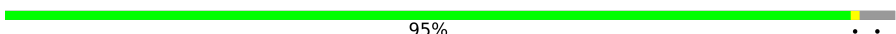
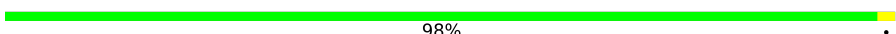
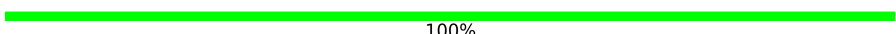
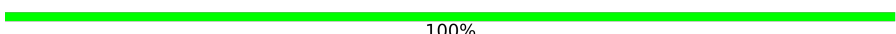




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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 [i](#)

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

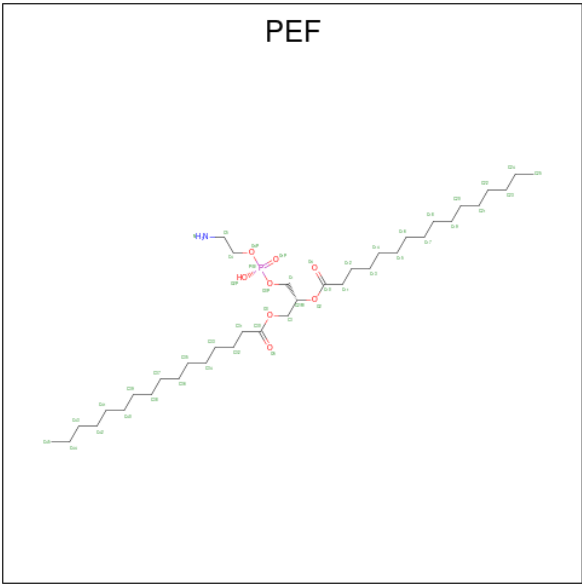
- Molecule 22 is a protein called COX26; SYNONYM: Uncharacterized protein YDR119W-A.

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: C₃₇H₇₄NO₈P).



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	

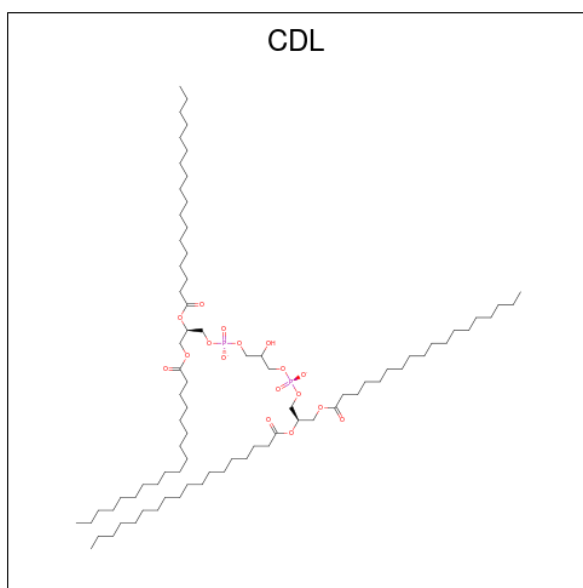
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Mol	Chain	Residues	Atoms					AltConf
24	a	1	Total 33	C 23	N 1	O 8	P 1	0
24	b	1	Total 40	C 30	N 1	O 8	P 1	0
24	b	1	Total 33	C 23	N 1	O 8	P 1	0
24	c	1	Total 36	C 26	N 1	O 8	P 1	0
24	c	1	Total 41	C 31	N 1	O 8	P 1	0
24	e	1	Total 42	C 32	N 1	O 8	P 1	0

- # HEM

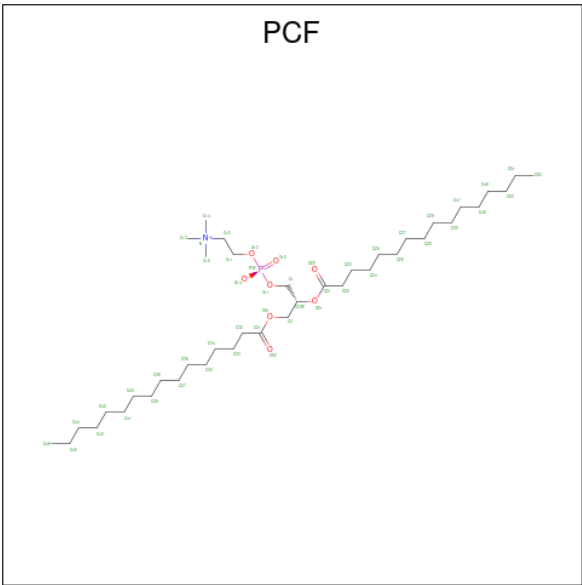
- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand

of Interest" by depositor).



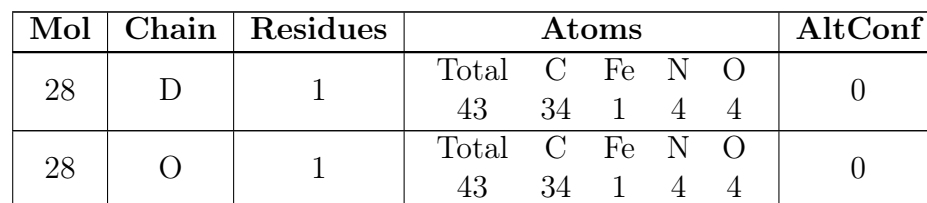
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			55	36	17	2	
26	D	1	Total	C	O	P	0
			67	48	17	2	
26	H	1	Total	C	O	P	0
			53	34	17	2	
26	L	1	Total	C	O	P	0
			58	39	17	2	
26	N	1	Total	C	O	P	0
			66	47	17	2	
26	O	1	Total	C	O	P	0
			71	52	17	2	
26	S	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



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: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



-
- FES
- S1 — S — Fe — Fe2
- | |
- Fe1 — S — S2

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



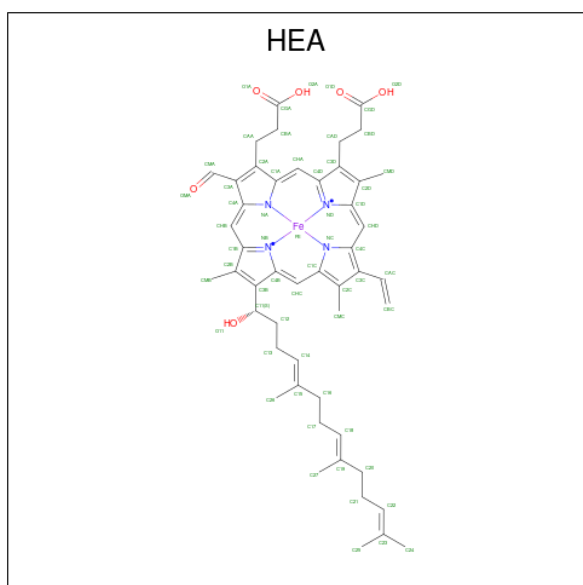
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Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			4	2	2	

- 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: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).

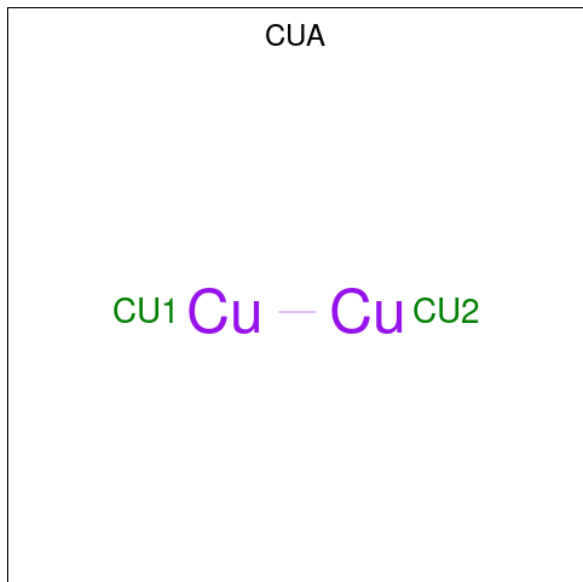


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- 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: 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: 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.

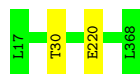
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

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%



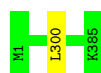
- Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

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%





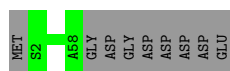
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S: 98% ..



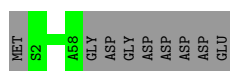
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

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%



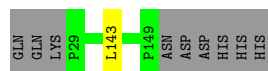
- Molecule 13: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

Chain c:  99%



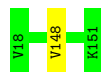
- Molecule 14: CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4

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.

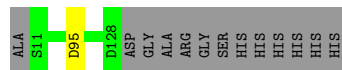
- Molecule 20: Cytochrome c oxidase subunit 6B

Chain j:  91% 6%



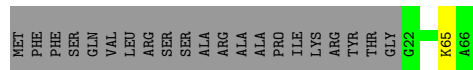
- Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13

Chain k:  89% 10%



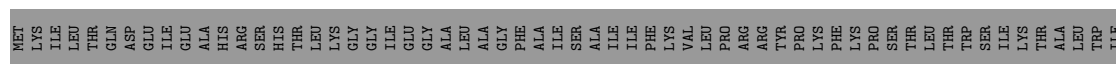
- Molecule 22: COX26; SYNONYM: Uncharacterized protein YDR119W-A

Chain l:  67% 32%



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

Chain m:  44% 56%





WORLD WIDE
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

5.1 Standard geometry

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

All (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
6	F	123	CYS	CA-CB-SG	6.04	124.87	114.00
11	a	213	ASP	CB-CG-OD1	6.00	123.70	118.30
5	P	198	LEU	CA-CB-CG	5.99	129.07	115.30
13	c	137	LEU	CA-CB-CG	5.78	128.60	115.30
17	g	19	LEU	CB-CG-CD2	5.70	120.69	111.00
11	a	21	LEU	CA-CB-CG	5.67	128.35	115.30
3	N	300	LEU	CA-CB-CG	5.54	128.04	115.30
11	a	48	LEU	CA-CB-CG	5.33	127.57	115.30
12	b	161	LEU	CA-CB-CG	5.28	127.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	528	ASN	C-N-CA	5.24	134.79	121.70
11	a	197	LEU	CA-CB-CG	5.12	127.07	115.30
7	R	83	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (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
3	N	345	GLU	Peptide
5	P	125	GLU	Peptide
11	a	120	GLU	Peptide
11	a	442	ASP	Peptide
11	a	520	SER	Peptide
11	a	91	THR	Peptide
13	c	22	TRP	Peptide
14	d	143	LEU	Peptide
21	k	95	ASP	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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
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

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

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	30	THR
5	E	124	HIS
6	F	123	CYS
8	H	7	LYS
3	N	184	TYR
3	N	213	THR
6	Q	101	CYS
8	S	7	LYS
11	a	244	VAL
13	c	18	MET
15	e	148	VAL
16	f	106	ARG
20	j	27	CYS
20	j	41	LYS
22	l	65	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	126	GLN
1	A	200	HIS
1	A	271	ASN
1	A	317	HIS
1	A	345	HIS
1	A	352	ASN
1	A	376	GLN
1	A	385	ASN
1	A	388	ASN
2	B	157	ASN
2	B	252	GLN
2	B	292	GLN
3	C	7	ASN
3	C	338	GLN
3	C	384	ASN
4	D	78	HIS
4	D	122	ASN
4	D	246	GLN
5	E	97	ASN
5	E	112	GLN
7	G	79	HIS
7	G	86	HIS
8	H	34	GLN
8	H	43	ASN
10	J	29	ASN
10	J	52	GLN
1	L	42	HIS
1	L	121	ASN
1	L	126	GLN
1	L	205	ASN
1	L	271	ASN
1	L	298	GLN
1	L	307	GLN
1	L	310	GLN
1	L	317	HIS
1	L	345	HIS
1	L	376	GLN
1	L	388	ASN
2	M	49	HIS
2	M	58	ASN
2	M	191	ASN
2	M	258	ASN

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Mol	Chain	Res	Type
2	M	325	ASN
2	M	352	ASN
3	N	138	GLN
3	N	202	HIS
3	N	338	GLN
3	N	384	ASN
4	O	127	ASN
4	O	246	GLN
5	P	130	ASN
5	P	141	GLN
5	P	151	GLN
6	Q	131	GLN
9	T	44	ASN
10	U	14	HIS
10	U	29	ASN
10	U	52	GLN
11	a	99	ASN
11	a	175	ASN
11	a	257	HIS
11	a	475	GLN
11	a	478	ASN
11	a	481	ASN
11	a	482	ASN
11	a	505	ASN
11	a	533	GLN
12	b	26	GLN
12	b	77	HIS
13	c	10	GLN
13	c	47	ASN
14	d	119	HIS
16	f	44	HIS
19	i	42	ASN
23	m	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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
31	a	603	HEA	C3B-C2B	5.35	1.46	1.34
31	a	602	HEA	C3A-C2A	5.03	1.47	1.40
31	a	603	HEA	C3A-C2A	5.01	1.47	1.40
31	a	603	HEA	C3D-C2D	4.91	1.47	1.36
31	a	602	HEA	CHC-C4B	4.83	1.47	1.35
31	a	602	HEA	C3D-C2D	4.72	1.46	1.36
31	a	602	HEA	CHD-C1D	4.62	1.46	1.35
24	N	605	PEF	O2-C10	4.53	1.47	1.34
31	a	603	HEA	C3C-C2C	4.50	1.46	1.40
24	e	201	PEF	O2-C10	4.37	1.46	1.34
31	a	603	HEA	CHC-C4B	4.36	1.46	1.35
24	C	605	PEF	O2-C10	4.33	1.46	1.34
26	O	402	CDL	OB8-CB7	4.33	1.46	1.33
26	C	603	CDL	OB6-CB5	4.30	1.46	1.34
24	a	605	PEF	O2-C10	4.29	1.46	1.34
26	D	402	CDL	OB8-CB7	4.29	1.45	1.33
24	e	201	PEF	O3-C30	4.28	1.45	1.33
24	A	501	PEF	O3-C30	4.27	1.45	1.33
26	L	501	CDL	OB8-CB7	4.26	1.45	1.33
24	U	101	PEF	O3-C30	4.26	1.45	1.33
24	J	101	PEF	O3-C30	4.26	1.45	1.33
26	S	101	CDL	OB8-CB7	4.24	1.45	1.33
26	S	101	CDL	OA8-CA7	4.24	1.45	1.33
24	E	302	PEF	O3-C30	4.24	1.45	1.33
27	C	606	PCF	O31-C31	4.24	1.45	1.33
24	C	604	PEF	O3-C30	4.23	1.45	1.33
26	H	601	CDL	OB8-CB7	4.23	1.45	1.33
27	e	202	PCF	O31-C31	4.23	1.45	1.33
24	H	602	PEF	O3-C30	4.22	1.45	1.33
24	c	301	PEF	O3-C30	4.22	1.45	1.33
27	N	606	PCF	O21-C21	4.22	1.46	1.34
24	b	302	PEF	O3-C30	4.21	1.45	1.33
24	S	102	PEF	O2-C10	4.21	1.46	1.34
27	N	606	PCF	O31-C31	4.21	1.45	1.33
26	D	402	CDL	OA8-CA7	4.21	1.45	1.33
26	L	501	CDL	OA8-CA7	4.21	1.45	1.33
26	N	603	CDL	OA8-CA7	4.21	1.45	1.33
24	a	605	PEF	O3-C30	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	601	CDL	OA6-CA5	4.20	1.46	1.34
26	O	402	CDL	OA8-CA7	4.20	1.45	1.33
24	b	303	PEF	O3-C30	4.20	1.45	1.33
26	H	601	CDL	OA8-CA7	4.20	1.45	1.33
27	S	103	PCF	O21-C21	4.20	1.46	1.34
26	L	501	CDL	OB6-CB5	4.19	1.46	1.34
27	T	101	PCF	O21-C21	4.18	1.46	1.34
31	a	603	HEA	CHD-C1D	4.18	1.45	1.35
24	E	302	PEF	O2-C10	4.18	1.46	1.34
27	T	101	PCF	O31-C31	4.18	1.45	1.33
26	N	603	CDL	OB6-CB5	4.17	1.46	1.34
24	b	302	PEF	O2-C10	4.17	1.46	1.34
24	N	604	PEF	O3-C30	4.17	1.45	1.33
27	S	103	PCF	O31-C31	4.17	1.45	1.33
24	N	605	PEF	O3-C30	4.16	1.45	1.33
24	H	602	PEF	O2-C10	4.16	1.46	1.34
24	J	101	PEF	O2-C10	4.16	1.46	1.34
26	C	603	CDL	OB8-CB7	4.16	1.45	1.33
26	N	603	CDL	OB8-CB7	4.16	1.45	1.33
24	c	302	PEF	O3-C30	4.15	1.45	1.33
24	C	605	PEF	O3-C30	4.14	1.45	1.33
24	c	302	PEF	O2-C10	4.13	1.46	1.34
26	S	101	CDL	OB6-CB5	4.13	1.46	1.34
31	a	602	HEA	C3C-C2C	4.13	1.46	1.40
24	P	302	PEF	O2-C10	4.13	1.45	1.34
26	L	501	CDL	OA6-CA5	4.11	1.45	1.34
27	I	101	PCF	O31-C31	4.11	1.45	1.33
24	L	502	PEF	O2-C10	4.10	1.45	1.34
24	P	302	PEF	O3-C30	4.09	1.45	1.33
24	L	502	PEF	O3-C30	4.09	1.45	1.33
26	D	402	CDL	OA6-CA5	4.08	1.45	1.34
27	C	606	PCF	O21-C21	4.08	1.45	1.34
26	N	603	CDL	OA6-CA5	4.08	1.45	1.34
24	C	604	PEF	O2-C10	4.08	1.45	1.34
26	H	601	CDL	OB6-CB5	4.07	1.45	1.34
26	O	402	CDL	OA6-CA5	4.07	1.45	1.34
26	C	603	CDL	OA6-CA5	4.07	1.45	1.34
24	U	101	PEF	O2-C10	4.07	1.45	1.34
26	S	101	CDL	OA6-CA5	4.07	1.45	1.34
24	A	501	PEF	O2-C10	4.06	1.45	1.34
24	S	102	PEF	O3-C30	4.06	1.45	1.33
27	e	202	PCF	O21-C21	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	301	PEF	O2-C10	4.04	1.45	1.34
26	O	402	CDL	OB6-CB5	4.03	1.45	1.34
24	N	604	PEF	O2-C10	4.03	1.45	1.34
26	D	402	CDL	OB6-CB5	4.02	1.45	1.34
27	I	101	PCF	O21-C21	4.00	1.45	1.34
24	b	303	PEF	O2-C10	3.95	1.45	1.34
28	O	401	HEC	C4B-C3B	3.71	1.49	1.43
28	D	401	HEC	C4B-C3B	3.64	1.49	1.43
25	C	602	HEM	C1B-NB	-3.62	1.34	1.40
31	a	603	HEA	C1D-ND	-3.57	1.34	1.40
25	N	602	HEM	C1B-NB	-3.54	1.34	1.40
28	D	401	HEC	C3C-C4C	3.51	1.49	1.43
25	C	601	HEM	C1B-NB	-3.40	1.34	1.40
25	C	602	HEM	C4D-ND	-3.38	1.34	1.40
25	N	601	HEM	C1B-NB	-3.37	1.34	1.40
25	N	602	HEM	C4D-ND	-3.35	1.34	1.40
28	O	401	HEC	C3C-C4C	3.30	1.49	1.43
28	O	401	HEC	C3D-C2D	3.25	1.47	1.37
28	D	401	HEC	C3D-C2D	3.23	1.47	1.37
28	O	401	HEC	C2A-C3A	3.18	1.47	1.37
28	D	401	HEC	C2A-C3A	3.16	1.47	1.37
31	a	602	HEA	FE-NB	3.05	2.11	1.96
25	N	601	HEM	C4D-ND	-3.03	1.35	1.40
31	a	603	HEA	FE-NB	3.02	2.11	1.96
31	a	602	HEA	C1D-ND	-3.01	1.35	1.40
25	C	601	HEM	C4D-ND	-3.00	1.35	1.40
31	a	603	HEA	FE-ND	2.97	2.11	1.96
31	a	603	HEA	C4B-NB	-2.94	1.35	1.40
31	a	602	HEA	C4B-C3B	2.93	1.49	1.44
31	a	602	HEA	FE-ND	2.92	2.11	1.96
31	a	602	HEA	C4B-NB	-2.91	1.35	1.40
25	C	601	HEM	FE-NB	2.87	2.11	1.96
25	N	601	HEM	FE-NB	2.86	2.11	1.96
25	C	602	HEM	FE-NB	2.85	2.11	1.96
25	N	602	HEM	FE-NB	2.84	2.10	1.96
28	O	401	HEC	C3A-C4A	2.64	1.48	1.42
28	D	401	HEC	C2A-C1A	2.60	1.48	1.42
26	C	603	CDL	OA8-CA7	2.53	1.45	1.33
28	D	401	HEC	C3A-C4A	2.51	1.48	1.42
31	a	603	HEA	C4D-C3D	2.48	1.49	1.45
31	a	602	HEA	C2A-C1A	2.48	1.48	1.42
28	O	401	HEC	C2A-C1A	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C1D-CHD	2.44	1.47	1.41
31	a	603	HEA	C2A-C1A	2.43	1.48	1.42
31	a	603	HEA	C4B-C3B	2.41	1.48	1.44
28	D	401	HEC	C1D-CHD	2.40	1.47	1.41
28	D	401	HEC	C1B-CHB	2.39	1.47	1.41
28	O	401	HEC	C1B-CHB	2.38	1.47	1.41
28	D	401	HEC	C4D-CHA	2.37	1.47	1.41
31	a	602	HEA	C1C-CHC	2.35	1.47	1.41
28	O	401	HEC	C1C-CHC	2.35	1.47	1.41
28	D	401	HEC	C1C-CHC	2.34	1.47	1.41
31	a	603	HEA	C1B-C2B	2.34	1.49	1.44
28	O	401	HEC	C4D-CHA	2.34	1.47	1.41
31	a	603	HEA	C4C-CHD	2.29	1.47	1.41
25	C	601	HEM	C1D-ND	-2.16	1.34	1.38
31	a	602	HEA	C4C-CHD	2.16	1.47	1.41
25	N	601	HEM	C1D-ND	-2.16	1.34	1.38
31	a	602	HEA	C4D-C3D	2.16	1.48	1.45
25	C	602	HEM	C1D-ND	-2.13	1.34	1.38
25	N	602	HEM	C1D-ND	-2.08	1.34	1.38
25	C	601	HEM	C4B-NB	-2.03	1.34	1.38
31	a	602	HEA	C1D-C2D	2.03	1.48	1.44
31	a	603	HEA	CHB-C1B	2.01	1.46	1.41

All (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
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
28	O	401	HEC	CMC-C2C-C3C	6.24	133.15	125.82
31	a	602	HEA	C3D-C4D-ND	6.08	116.24	110.36
31	a	602	HEA	C2B-C1B-NB	6.02	117.09	109.88
31	a	603	HEA	C3B-C4B-NB	5.97	116.91	109.84
31	a	603	HEA	CHA-C4D-ND	-5.61	118.34	124.43
31	a	602	HEA	C2D-C1D-ND	5.59	116.46	109.84
28	O	401	HEC	C1D-C2D-C3D	-5.57	103.12	107.00
28	D	401	HEC	C1D-C2D-C3D	-5.50	103.17	107.00
31	a	603	HEA	C4D-CHA-C1A	-5.41	115.42	122.56
31	a	602	HEA	CBA-CAA-C2A	-5.20	103.85	112.60
25	C	601	HEM	CHC-C4B-NB	5.16	130.03	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C3B-C4B-NB	5.07	115.85	109.84
24	C	605	PEF	O2-C10-C11	5.03	122.35	111.50
25	N	602	HEM	CHC-C4B-NB	4.86	129.71	124.43
25	N	601	HEM	CHC-C4B-NB	4.76	129.61	124.43
26	O	402	CDL	OB6-CB5-C51	4.75	121.73	111.50
26	D	402	CDL	OB6-CB5-C51	4.66	121.55	111.50
25	C	602	HEM	CHC-C4B-NB	4.66	129.50	124.43
31	a	603	HEA	C2B-C1B-NB	4.62	115.42	109.88
25	C	601	HEM	CHD-C1D-ND	4.51	129.33	124.43
25	N	602	HEM	CHD-C1D-ND	4.47	129.29	124.43
31	a	602	HEA	C1D-C2D-C3D	-4.46	102.27	106.96
25	C	601	HEM	CAD-C3D-C4D	4.46	132.45	124.66
24	J	101	PEF	O2-C10-C11	4.38	120.94	111.50
25	N	601	HEM	CAD-C3D-C4D	4.36	132.28	124.66
31	a	603	HEA	C1D-C2D-C3D	-4.34	102.39	106.96
25	N	601	HEM	CHD-C1D-ND	4.33	129.14	124.43
27	T	101	PCF	O21-C21-C22	4.26	120.67	111.50
25	C	602	HEM	CHD-C1D-ND	4.21	129.00	124.43
31	a	602	HEA	CHB-C1B-NB	-4.17	119.90	124.43
26	C	603	CDL	OA6-CA5-C11	4.09	120.32	111.50
31	a	602	HEA	C1B-C2B-C3B	-4.06	101.95	106.80
24	b	303	PEF	O2-C10-C11	4.05	120.24	111.50
26	S	101	CDL	OA6-CA5-C11	4.04	120.21	111.50
26	C	603	CDL	OB6-CB5-C51	4.03	120.19	111.50
24	C	604	PEF	O2-C10-C11	3.99	120.09	111.50
24	H	602	PEF	O2-C10-C11	3.98	120.09	111.50
26	L	501	CDL	OA6-CA5-C11	3.98	120.07	111.50
24	a	605	PEF	O2-C10-C11	3.98	120.07	111.50
27	N	606	PCF	O21-C21-C22	3.97	120.06	111.50
24	c	301	PEF	O2-C10-C11	3.95	120.01	111.50
24	P	302	PEF	O2-C10-C11	3.95	120.01	111.50
24	c	302	PEF	O2-C10-C11	3.95	120.01	111.50
24	S	102	PEF	O2-C10-C11	3.93	119.98	111.50
24	b	302	PEF	O2-C10-C11	3.93	119.96	111.50
24	E	302	PEF	O2-C10-C11	3.88	119.87	111.50
24	A	501	PEF	O2-C10-C11	3.88	119.87	111.50
26	H	601	CDL	OA6-CA5-C11	3.87	119.84	111.50
24	L	502	PEF	O2-C10-C11	3.86	119.82	111.50
27	e	202	PCF	O21-C21-C22	3.86	119.81	111.50
31	a	602	HEA	C13-C12-C11	-3.84	108.58	114.35
26	S	101	CDL	OB6-CB5-C51	3.81	119.71	111.50
31	a	602	HEA	C3C-C4C-NC	3.80	114.12	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	603	CDL	OB6-CB5-C51	3.75	119.58	111.50
24	N	604	PEF	O2-C10-C11	3.75	119.58	111.50
31	a	602	HEA	C26-C15-C16	3.75	121.58	115.27
31	a	603	HEA	CMC-C2C-C3C	3.73	131.66	124.68
31	a	603	HEA	C3C-C4C-NC	3.72	114.01	109.21
27	C	606	PCF	O21-C21-C22	3.66	119.39	111.50
24	U	101	PEF	O2-C10-C11	3.65	119.37	111.50
31	a	603	HEA	CMB-C2B-C1B	3.65	130.60	125.04
31	a	603	HEA	C4D-C3D-C2D	-3.63	101.61	106.90
26	H	601	CDL	OB6-CB5-C51	3.62	119.31	111.50
27	I	101	PCF	O21-C21-C22	3.60	119.26	111.50
26	L	501	CDL	OB6-CB5-C51	3.59	119.23	111.50
25	N	601	HEM	CHB-C1B-NB	3.59	128.81	124.38
26	O	402	CDL	OA6-CA5-C11	3.58	119.22	111.50
25	C	601	HEM	C1B-NB-C4B	3.56	108.75	105.07
25	N	601	HEM	C1B-NB-C4B	3.56	108.75	105.07
25	C	602	HEM	CHB-C1B-NB	3.53	128.74	124.38
25	N	602	HEM	C1B-NB-C4B	3.49	108.68	105.07
31	a	603	HEA	C4B-C3B-C2B	-3.47	101.49	107.41
25	N	602	HEM	CHB-C1B-NB	3.43	128.62	124.38
31	a	603	HEA	CHB-C1B-NB	-3.42	120.72	124.43
25	C	601	HEM	CHB-C1B-NB	3.41	128.59	124.38
31	a	602	HEA	CMB-C2B-C1B	3.40	130.22	125.04
26	O	402	CDL	OB8-CB7-C71	3.40	120.29	111.38
26	N	603	CDL	OA6-CA5-C11	3.40	118.82	111.50
25	C	602	HEM	C1B-NB-C4B	3.39	108.57	105.07
26	D	402	CDL	CB4-OB6-CB5	-3.37	109.50	117.79
25	N	602	HEM	CHA-C4D-ND	3.35	128.52	124.38
26	D	402	CDL	OA6-CA5-C11	3.34	118.70	111.50
25	C	602	HEM	CHA-C4D-ND	3.33	128.50	124.38
31	a	602	HEA	CHA-C4D-ND	-3.29	120.86	124.43
27	S	103	PCF	O21-C21-C22	3.17	118.34	111.50
31	a	603	HEA	C1D-ND-C4D	-3.14	101.83	105.07
24	N	605	PEF	O2-C10-C11	3.14	118.26	111.50
24	H	602	PEF	O3-C30-C31	3.10	121.65	111.91
31	a	602	HEA	C27-C19-C20	3.09	120.47	115.27
27	C	606	PCF	O31-C31-C32	3.08	121.58	111.91
24	U	101	PEF	O3-C30-C31	3.07	121.55	111.91
25	N	601	HEM	CBD-CAD-C3D	3.03	121.05	112.63
31	a	603	HEA	C13-C12-C11	-3.03	109.80	114.35
25	C	601	HEM	CBD-CAD-C3D	3.03	121.03	112.63
31	a	602	HEA	C4D-C3D-C2D	-3.01	102.50	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	603	CDL	OB8-CB7-C71	3.00	121.32	111.91
24	b	303	PEF	C2-O2-C10	-2.99	110.42	117.79
28	O	401	HEC	CMB-C2B-C1B	-2.96	123.92	128.46
24	e	201	PEF	O2-C10-C11	2.94	117.83	111.50
26	H	601	CDL	OA8-CA7-C31	2.91	121.05	111.91
25	N	601	HEM	CAD-C3D-C2D	-2.88	122.52	127.88
25	C	601	HEM	CAD-C3D-C2D	-2.87	122.54	127.88
27	S	103	PCF	C3-C2-C1	-2.86	105.02	111.79
24	E	302	PEF	C2-O2-C10	-2.85	110.78	117.79
26	L	501	CDL	OB8-CB7-C71	2.84	120.83	111.91
31	a	603	HEA	CAD-C3D-C4D	2.84	129.63	124.66
26	O	402	CDL	OA8-CA7-C31	2.84	120.82	111.91
31	a	603	HEA	C27-C19-C20	2.84	120.04	115.27
27	I	101	PCF	O31-C31-C32	2.83	120.80	111.91
26	O	402	CDL	CB4-OB6-CB5	-2.82	110.84	117.79
31	a	603	HEA	C1B-C2B-C3B	-2.81	103.44	106.80
24	E	302	PEF	O3-C30-C31	2.81	120.74	111.91
24	b	302	PEF	O3-C30-C31	2.81	120.73	111.91
26	S	101	CDL	OA8-CA7-C31	2.81	120.71	111.91
26	S	101	CDL	OB8-CB7-C71	2.80	120.70	111.91
31	a	602	HEA	CMD-C2D-C1D	2.79	129.29	125.04
25	N	602	HEM	CAD-CBD-CGD	-2.79	107.60	113.60
25	C	601	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
31	a	602	HEA	CMC-C2C-C3C	2.76	129.84	124.68
26	H	601	CDL	OB8-CB7-C71	2.76	120.55	111.91
31	a	602	HEA	CAD-C3D-C4D	2.75	129.46	124.66
25	N	601	HEM	CHD-C1D-C2D	-2.75	120.69	124.98
31	a	602	HEA	C4B-C3B-C2B	-2.73	102.74	107.41
24	b	303	PEF	O3-C30-C31	2.73	120.46	111.91
31	a	602	HEA	CAD-CBD-CGD	-2.72	107.74	113.60
31	a	603	HEA	CBA-CAA-C2A	-2.71	108.04	112.60
27	S	103	PCF	O31-C31-C32	2.71	120.41	111.91
24	P	302	PEF	O3-C30-C31	2.70	120.39	111.91
27	N	606	PCF	O31-C31-C32	2.69	120.36	111.91
28	D	401	HEC	CMB-C2B-C1B	-2.68	124.34	128.46
25	C	602	HEM	CAD-CBD-CGD	-2.67	107.85	113.60
31	a	602	HEA	C4B-NB-C1B	-2.66	102.33	105.07
28	O	401	HEC	C4C-C3C-C2C	-2.64	103.50	106.35
24	C	604	PEF	O3-C30-C31	2.64	120.19	111.91
26	C	603	CDL	OB8-CB7-C71	2.63	120.18	111.91
24	L	502	PEF	O3-C30-C31	2.63	120.16	111.91
26	D	402	CDL	OB8-CB7-C71	2.62	120.12	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	602	HEM	C4D-ND-C1D	2.61	107.77	105.07
24	N	604	PEF	C2-O2-C10	-2.58	111.44	117.79
31	a	602	HEA	CHC-C4B-NB	-2.57	121.21	124.38
25	N	602	HEM	CHD-C1D-C2D	-2.56	120.98	124.98
26	S	101	CDL	CA4-OA6-CA5	-2.55	111.50	117.79
27	e	202	PCF	O31-C31-C32	2.55	119.90	111.91
28	D	401	HEC	C4C-C3C-C2C	-2.55	103.60	106.35
24	a	605	PEF	O3-C30-C31	2.53	119.86	111.91
24	e	201	PEF	O3-C30-C31	2.53	119.84	111.91
31	a	603	HEA	CHC-C4B-NB	-2.52	121.26	124.38
24	N	604	PEF	O3-C30-C31	2.52	119.82	111.91
28	O	401	HEC	CAA-CBA-CGA	-2.49	106.77	113.76
24	S	102	PEF	O3-C30-C31	2.49	119.73	111.91
24	c	301	PEF	C2-O2-C10	-2.48	111.68	117.79
26	L	501	CDL	OA8-CA7-C31	2.48	119.68	111.91
24	C	604	PEF	C2-O2-C10	-2.47	111.71	117.79
26	N	603	CDL	CB2-C1-CA2	-2.47	105.52	112.79
31	a	602	HEA	C1D-ND-C4D	-2.47	102.52	105.07
25	C	602	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
26	D	402	CDL	OA8-CA7-C31	2.46	119.64	111.91
31	a	603	HEA	CHD-C1D-C2D	-2.44	119.97	126.72
24	C	605	PEF	O3-C30-C31	2.43	119.53	111.91
31	a	602	HEA	C25-C23-C24	2.42	119.95	114.60
26	N	603	CDL	OA8-CA7-C31	2.38	119.39	111.91
24	J	101	PEF	O3-C30-C31	2.38	119.37	111.91
31	a	603	HEA	C13-C14-C15	-2.38	121.94	127.66
24	A	501	PEF	O3-C30-C31	2.37	119.34	111.91
31	a	603	HEA	C25-C23-C24	2.36	119.81	114.60
24	N	605	PEF	O3-C30-C31	2.35	119.28	111.91
25	C	602	HEM	CHB-C1B-C2B	-2.34	120.25	126.72
24	L	502	PEF	C2-O2-C10	-2.34	112.04	117.79
26	C	603	CDL	CA4-OA6-CA5	-2.34	112.04	117.79
25	C	602	HEM	C4D-ND-C1D	2.31	107.46	105.07
31	a	602	HEA	C17-C18-C19	-2.31	122.11	127.66
27	C	606	PCF	O31-C31-O32	-2.30	117.78	123.59
27	T	101	PCF	C2-O21-C21	-2.30	112.12	117.79
25	N	602	HEM	CMC-C2C-C3C	2.30	128.98	124.68
31	a	603	HEA	CMB-C2B-C3B	-2.30	125.97	130.34
25	C	601	HEM	CMC-C2C-C3C	2.29	128.96	124.68
28	D	401	HEC	CAA-CBA-CGA	-2.29	107.34	113.76
31	a	603	HEA	C4B-NB-C1B	-2.28	102.72	105.07
31	a	603	HEA	CAA-CBA-CGA	-2.25	107.45	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	HEC	CAD-CBD-CGD	-2.25	107.45	113.76
26	O	402	CDL	OB6-CB5-OB7	-2.25	118.27	123.70
31	a	603	HEA	C26-C15-C16	2.24	119.03	115.27
25	N	602	HEM	CHB-C1B-C2B	-2.23	120.54	126.72
27	I	101	PCF	C2-O21-C21	-2.22	112.32	117.79
24	S	102	PEF	C2-O2-C10	-2.22	112.33	117.79
27	T	101	PCF	O31-C31-C32	2.22	118.86	111.91
25	C	602	HEM	CBA-CAA-C2A	-2.21	108.84	112.62
24	c	301	PEF	O3-C30-C31	2.21	118.83	111.91
24	a	605	PEF	O2-C2-C1	2.19	116.31	108.40
27	C	606	PCF	C2-O21-C21	-2.17	112.44	117.79
24	H	602	PEF	O3-C30-O5	-2.15	118.16	123.59
27	e	202	PCF	C2-O21-C21	-2.15	112.51	117.79
27	I	101	PCF	O31-C31-O32	-2.14	118.19	123.59
24	H	602	PEF	C2-O2-C10	-2.14	112.53	117.79
28	D	401	HEC	CMC-C2C-C1C	-2.14	125.18	128.46
27	N	606	PCF	C2-O21-C21	-2.13	112.53	117.79
26	H	601	CDL	CB4-OB6-CB5	-2.13	112.54	117.79
25	N	601	HEM	CHB-C1B-C2B	-2.13	120.83	126.72
25	N	601	HEM	CAA-CBA-CGA	-2.12	107.81	113.76
24	A	501	PEF	C2-O2-C10	-2.12	112.57	117.79
28	O	401	HEC	CMA-C3A-C2A	2.11	128.91	124.94
24	C	605	PEF	O2-C10-O4	-2.10	118.62	123.70
25	C	601	HEM	CAA-CBA-CGA	-2.09	107.89	113.76
26	D	402	CDL	OB6-CB5-OB7	-2.09	118.66	123.70
26	S	101	CDL	CB4-OB6-CB5	-2.09	112.66	117.79
25	C	602	HEM	C4B-C3B-C2B	-2.07	105.47	107.11
28	D	401	HEC	CMA-C3A-C2A	2.07	128.84	124.94
26	C	603	CDL	OB8-CB7-OB9	-2.06	118.40	123.59
25	N	601	HEM	CMC-C2C-C3C	2.05	128.52	124.68
27	S	103	PCF	O31-C31-O32	-2.04	118.44	123.59
25	C	601	HEM	C4D-ND-C1D	2.04	107.18	105.07
24	L	502	PEF	O3-C30-O5	-2.04	118.45	123.59
31	a	602	HEA	C13-C14-C15	-2.03	122.76	127.66
26	N	603	CDL	CA4-OA6-CA5	-2.03	112.79	117.79
25	N	602	HEM	O2A-CGA-CBA	2.02	120.53	114.03
25	C	601	HEM	CHB-C1B-C2B	-2.02	121.13	126.72
31	a	602	HEA	OMA-CMA-C3A	-2.02	120.52	124.91
24	P	302	PEF	O3-C30-O5	-2.01	118.52	123.59
24	b	303	PEF	O2-C10-O4	-2.01	118.85	123.70
26	S	101	CDL	OB8-CB7-OB9	-2.01	118.53	123.59
28	D	401	HEC	C2B-C3B-C4B	-2.01	104.19	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	HEC	C3C-C4C-NC	2.00	114.72	110.94

There are no chirality outliers.

All (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
24	C	605	PEF	C4-O4P-P-O2P
24	E	302	PEF	C11-C10-O2-C2
24	J	101	PEF	O2-C2-C3-O3
24	J	101	PEF	C11-C10-O2-C2
24	L	502	PEF	C1-O3P-P-O2P
24	L	502	PEF	C4-O4P-P-O3P
24	N	604	PEF	C1-O3P-P-O4P
24	S	102	PEF	C4-O4P-P-O1P
24	b	302	PEF	C1-O3P-P-O1P
24	b	302	PEF	C1-O3P-P-O2P
24	b	303	PEF	O4P-C4-C5-N
24	b	303	PEF	C1-O3P-P-O2P
24	b	303	PEF	C4-O4P-P-O2P
24	c	301	PEF	C1-O3P-P-O2P
24	c	301	PEF	C4-O4P-P-O2P
24	e	201	PEF	C1-O3P-P-O1P
24	e	201	PEF	C1-O3P-P-O2P
24	e	201	PEF	C1-O3P-P-O4P
25	C	601	HEM	C2B-C3B-CAB-CBB
25	C	601	HEM	C4B-C3B-CAB-CBB
25	N	601	HEM	C2B-C3B-CAB-CBB
25	N	601	HEM	C4B-C3B-CAB-CBB
26	C	603	CDL	CA2-OA2-PA1-OA3
26	C	603	CDL	CA2-OA2-PA1-OA4
26	C	603	CDL	CA2-OA2-PA1-OA5
26	C	603	CDL	CA3-OA5-PA1-OA3
26	C	603	CDL	CA3-OA5-PA1-OA4
26	C	603	CDL	CB3-OB5-PB2-OB2
26	C	603	CDL	CB3-OB5-PB2-OB3
26	C	603	CDL	CB3-OB5-PB2-OB4
26	C	603	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
26	D	402	CDL	CA2-OA2-PA1-OA4
26	D	402	CDL	CA3-OA5-PA1-OA3
26	D	402	CDL	CB2-OB2-PB2-OB3
26	D	402	CDL	CB2-OB2-PB2-OB4
26	D	402	CDL	CB2-OB2-PB2-OB5
26	H	601	CDL	O1-C1-CB2-OB2
26	L	501	CDL	CA3-OA5-PA1-OA3
26	L	501	CDL	CB2-OB2-PB2-OB3
26	L	501	CDL	CB2-OB2-PB2-OB4
26	N	603	CDL	CA3-OA5-PA1-OA3
26	O	402	CDL	O1-C1-CB2-OB2
26	O	402	CDL	CA2-OA2-PA1-OA3
26	O	402	CDL	CB2-OB2-PB2-OB3
26	O	402	CDL	CB3-OB5-PB2-OB3
26	S	101	CDL	CA2-OA2-PA1-OA3
26	S	101	CDL	CB2-OB2-PB2-OB3
26	S	101	CDL	CB2-OB2-PB2-OB4
26	S	101	CDL	CB3-OB5-PB2-OB2
26	S	101	CDL	CB3-OB5-PB2-OB3
26	S	101	CDL	CB3-OB5-PB2-OB4
27	C	606	PCF	C1-O11-P-O12
27	N	606	PCF	C11-O13-P-O12
27	N	606	PCF	C11-O13-P-O14
27	N	606	PCF	O13-C11-C12-N
27	S	103	PCF	O13-C11-C12-N
27	S	103	PCF	O11-C1-C2-O21
31	a	602	HEA	C11-C12-C13-C14
31	a	602	HEA	C14-C15-C16-C17
31	a	602	HEA	C26-C15-C16-C17
27	S	103	PCF	O32-C31-O31-C3
24	E	302	PEF	O4-C10-O2-C2
24	J	101	PEF	O4-C10-O2-C2
26	C	603	CDL	OB7-CB5-OB6-CB4
27	S	103	PCF	C32-C31-O31-C3
24	U	101	PEF	C31-C30-O3-C3
26	D	402	CDL	O1-C1-CB2-OB2
26	S	101	CDL	O1-C1-CB2-OB2
31	a	602	HEA	C27-C19-C20-C21
31	a	602	HEA	C18-C19-C20-C21
24	U	101	PEF	O5-C30-O3-C3
26	H	601	CDL	CA2-C1-CB2-OB2
26	O	402	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
26	S	101	CDL	CA2-C1-CB2-OB2
24	J	101	PEF	C12-C13-C14-C15
24	A	501	PEF	C30-C31-C32-C33
26	D	402	CDL	OB5-CB3-CB4-OB6
24	a	605	PEF	O4-C10-O2-C2
24	a	605	PEF	C11-C10-O2-C2
24	L	502	PEF	C10-C11-C12-C13
24	A	501	PEF	C10-C11-C12-C13
24	U	101	PEF	C30-C31-C32-C33
27	N	606	PCF	C21-C22-C23-C24
26	N	603	CDL	CB5-C51-C52-C53
24	c	302	PEF	C11-C10-O2-C2
24	C	604	PEF	C4-O4P-P-O3P
24	E	302	PEF	C1-O3P-P-O4P
24	E	302	PEF	C4-O4P-P-O3P
24	J	101	PEF	C1-O3P-P-O4P
24	L	502	PEF	C1-O3P-P-O4P
24	N	605	PEF	C1-O3P-P-O4P
24	P	302	PEF	C1-O3P-P-O4P
24	b	302	PEF	C1-O3P-P-O4P
24	b	302	PEF	C4-O4P-P-O3P
24	b	303	PEF	C1-O3P-P-O4P
24	b	303	PEF	C4-O4P-P-O3P
24	c	301	PEF	C1-O3P-P-O4P
24	c	301	PEF	C4-O4P-P-O3P
24	c	302	PEF	C1-O3P-P-O4P
24	c	302	PEF	C4-O4P-P-O3P
24	e	201	PEF	C4-O4P-P-O3P
26	C	603	CDL	CA3-OA5-PA1-OA2
26	D	402	CDL	CA2-OA2-PA1-OA5
26	D	402	CDL	CA3-OA5-PA1-OA2
26	H	601	CDL	CA2-OA2-PA1-OA5
26	H	601	CDL	CB2-OB2-PB2-OB5
26	L	501	CDL	CA3-OA5-PA1-OA2
26	L	501	CDL	CB2-OB2-PB2-OB5
26	O	402	CDL	CA2-OA2-PA1-OA5
26	O	402	CDL	CA3-OA5-PA1-OA2
26	S	101	CDL	CB2-OB2-PB2-OB5
27	N	606	PCF	C11-O13-P-O11
26	D	402	CDL	CA7-C31-C32-C33
26	D	402	CDL	CA2-C1-CB2-OB2
24	c	302	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
24	C	605	PEF	C16-C17-C18-C19
24	E	302	PEF	C11-C12-C13-C14
24	P	302	PEF	C33-C34-C35-C36
26	H	601	CDL	C31-C32-C33-C34
27	e	202	PCF	C26-C27-C28-C29
25	C	601	HEM	C2D-C3D-CAD-CBD
25	N	601	HEM	C2D-C3D-CAD-CBD
24	E	302	PEF	C37-C38-C39-C40
24	U	101	PEF	C19-C20-C21-C22
24	c	301	PEF	C31-C32-C33-C34
25	C	601	HEM	C4D-C3D-CAD-CBD
24	a	605	PEF	C30-C31-C32-C33
24	C	605	PEF	C31-C32-C33-C34
24	P	302	PEF	C12-C13-C14-C15
26	D	402	CDL	C11-CA5-OA6-CA4
26	N	603	CDL	C11-CA5-OA6-CA4
26	O	402	CDL	C51-CB5-OB6-CB4
24	N	605	PEF	C14-C15-C16-C17
26	L	501	CDL	C12-C13-C14-C15
24	b	302	PEF	C17-C18-C19-C20
24	e	201	PEF	C20-C21-C22-C23
24	U	101	PEF	C11-C12-C13-C14
24	N	604	PEF	C34-C35-C36-C37
24	b	302	PEF	C13-C14-C15-C16
26	S	101	CDL	C71-C72-C73-C74
24	b	303	PEF	C31-C30-O3-C3
24	c	302	PEF	C38-C39-C40-C41
26	D	402	CDL	C73-C74-C75-C76
27	I	101	PCF	C27-C28-C29-C30
27	e	202	PCF	C24-C25-C26-C27
24	C	604	PEF	C1-C2-C3-O3
24	N	605	PEF	C32-C33-C34-C35
26	D	402	CDL	C58-C59-C60-C61
24	C	605	PEF	C19-C20-C21-C22
26	N	603	CDL	C35-C36-C37-C38
27	C	606	PCF	C35-C36-C37-C38
24	N	605	PEF	C21-C22-C23-C24
24	b	302	PEF	C10-C11-C12-C13
26	D	402	CDL	OA7-CA5-OA6-CA4
26	N	603	CDL	OA7-CA5-OA6-CA4
24	U	101	PEF	C38-C39-C40-C41
24	C	604	PEF	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
24	b	303	PEF	O5-C30-O3-C3
25	N	601	HEM	C4D-C3D-CAD-CBD
24	N	604	PEF	O4-C10-O2-C2
24	e	201	PEF	O4-C10-O2-C2
26	H	601	CDL	OB7-CB5-OB6-CB4
26	O	402	CDL	OB7-CB5-OB6-CB4
26	L	501	CDL	C71-CB7-OB8-CB6
27	C	606	PCF	C32-C31-O31-C3
24	C	604	PEF	C31-C32-C33-C34
26	C	603	CDL	CB7-C71-C72-C73
26	S	101	CDL	CB5-C51-C52-C53
24	N	604	PEF	C11-C10-O2-C2
24	N	605	PEF	C11-C10-O2-C2
24	e	201	PEF	C11-C10-O2-C2
26	D	402	CDL	C51-CB5-OB6-CB4
26	H	601	CDL	C11-CA5-OA6-CA4
26	H	601	CDL	C51-CB5-OB6-CB4
26	S	101	CDL	C11-CA5-OA6-CA4
27	I	101	PCF	C35-C36-C37-C38
24	N	605	PEF	O4-C10-O2-C2
26	L	501	CDL	OB6-CB4-CB6-OB8
26	L	501	CDL	CA5-C11-C12-C13
27	N	606	PCF	C25-C26-C27-C28
27	C	606	PCF	O32-C31-O31-C3
24	C	604	PEF	O4-C10-O2-C2
26	H	601	CDL	OA7-CA5-OA6-CA4
26	S	101	CDL	OA7-CA5-OA6-CA4
24	c	301	PEF	C11-C10-O2-C2
26	O	402	CDL	CB3-OB5-PB2-OB2
24	b	302	PEF	C19-C20-C21-C22
24	b	302	PEF	O3P-C1-C2-C3
26	D	402	CDL	OB5-CB3-CB4-CB6
27	S	103	PCF	O11-C1-C2-C3
27	N	606	PCF	C22-C23-C24-C25
27	T	101	PCF	C24-C25-C26-C27
26	O	402	CDL	CA7-C31-C32-C33
24	b	302	PEF	C11-C10-O2-C2
24	C	605	PEF	C1-C2-C3-O3
24	N	605	PEF	C13-C14-C15-C16
26	D	402	CDL	CA3-CA4-CA6-OA8
27	N	606	PCF	C1-C2-C3-O31
26	L	501	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
24	a	605	PEF	C1-C2-O2-C10
24	E	302	PEF	C14-C15-C16-C17
26	D	402	CDL	OA6-CA4-CA6-OA8
27	N	606	PCF	O21-C2-C3-O31
27	T	101	PCF	C47-C48-C49-C50
26	D	402	CDL	OB7-CB5-OB6-CB4
24	L	502	PEF	C20-C21-C22-C23
24	C	605	PEF	C20-C21-C22-C23
26	L	501	CDL	C52-C53-C54-C55
27	C	606	PCF	C47-C48-C49-C50
24	C	605	PEF	C13-C14-C15-C16
24	b	302	PEF	O2-C10-C11-C12
24	e	201	PEF	O3P-C1-C2-C3
27	e	202	PCF	O11-C1-C2-C3
27	e	202	PCF	C21-C22-C23-C24
24	E	302	PEF	C35-C36-C37-C38
24	J	101	PEF	C10-C11-C12-C13
26	D	402	CDL	CB5-C51-C52-C53
26	D	402	CDL	O1-C1-CA2-OA2
24	b	302	PEF	O4-C10-O2-C2
24	L	502	PEF	C31-C30-O3-C3
24	N	604	PEF	C10-C11-C12-C13
24	J	101	PEF	C1-C2-C3-O3
24	U	101	PEF	C1-C2-C3-O3
26	C	603	CDL	CB3-CB4-CB6-OB8
26	L	501	CDL	CB3-CB4-CB6-OB8
24	c	301	PEF	O4-C10-O2-C2
26	N	603	CDL	C15-C16-C17-C18
24	c	302	PEF	C34-C35-C36-C37
26	L	501	CDL	C53-C54-C55-C56
24	U	101	PEF	C14-C15-C16-C17
26	N	603	CDL	CA3-OA5-PA1-OA2
26	S	101	CDL	CA3-OA5-PA1-OA2
26	C	603	CDL	CB5-C51-C52-C53
27	T	101	PCF	C23-C24-C25-C26
24	b	303	PEF	O3P-C1-C2-O2
27	e	202	PCF	O11-C1-C2-O21
26	N	603	CDL	CA5-C11-C12-C13
24	L	502	PEF	C11-C12-C13-C14
24	S	102	PEF	O2-C2-C3-O3
24	e	201	PEF	O2-C2-C3-O3
26	C	603	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
27	C	606	PCF	C41-C42-C43-C44
27	T	101	PCF	C21-C22-C23-C24
31	a	602	HEA	C19-C20-C21-C22
24	J	101	PEF	C13-C14-C15-C16
24	S	102	PEF	C40-C41-C42-C43
26	D	402	CDL	C61-C62-C63-C64
24	c	302	PEF	C31-C32-C33-C34
24	P	302	PEF	C11-C10-O2-C2
27	S	103	PCF	C22-C21-O21-C2
24	A	501	PEF	O3P-C1-C2-C3
24	N	604	PEF	O3P-C1-C2-C3
26	L	501	CDL	OA5-CA3-CA4-CA6
27	C	606	PCF	O11-C1-C2-C3
24	N	605	PEF	C17-C18-C19-C20
24	C	605	PEF	C3-C2-O2-C10
24	e	201	PEF	C1-C2-O2-C10
24	P	302	PEF	O4-C10-O2-C2
27	N	606	PCF	C24-C25-C26-C27
26	S	101	CDL	CB3-CB4-CB6-OB8
24	c	301	PEF	O3P-C1-C2-O2
26	O	402	CDL	OA5-CA3-CA4-OA6
26	S	101	CDL	OB5-CB3-CB4-OB6
27	C	606	PCF	O11-C1-C2-O21
27	S	103	PCF	O22-C21-O21-C2
24	U	101	PEF	O2-C2-C3-O3
24	L	502	PEF	O5-C30-O3-C3
24	b	303	PEF	O4-C10-O2-C2
24	E	302	PEF	C30-C31-C32-C33
24	b	303	PEF	C11-C10-O2-C2
27	C	606	PCF	C22-C21-O21-C2
24	C	605	PEF	C4-O4P-P-O3P
24	a	605	PEF	C1-O3P-P-O4P
24	a	605	PEF	C4-O4P-P-O3P
26	O	402	CDL	CB2-OB2-PB2-OB5
26	H	601	CDL	O1-C1-CA2-OA2
26	C	603	CDL	C1-CB2-OB2-PB2
24	P	302	PEF	C32-C33-C34-C35
24	C	604	PEF	C4-O4P-P-O1P
24	C	605	PEF	C4-O4P-P-O1P
24	E	302	PEF	C1-O3P-P-O1P
24	E	302	PEF	C4-O4P-P-O1P
24	E	302	PEF	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
24	J	101	PEF	C1-O3P-P-O1P
24	J	101	PEF	C1-O3P-P-O2P
24	L	502	PEF	C4-O4P-P-O2P
24	N	604	PEF	C1-O3P-P-O2P
24	N	605	PEF	C1-O3P-P-O1P
24	P	302	PEF	C1-O3P-P-O1P
24	b	302	PEF	C4-O4P-P-O1P
24	c	302	PEF	C1-O3P-P-O1P
24	c	302	PEF	C4-O4P-P-O1P
24	e	201	PEF	C4-O4P-P-O1P
26	D	402	CDL	CA3-OA5-PA1-OA4
26	H	601	CDL	CA2-OA2-PA1-OA3
26	H	601	CDL	CB2-OB2-PB2-OB3
26	L	501	CDL	CA3-OA5-PA1-OA4
26	O	402	CDL	CA2-OA2-PA1-OA4
26	O	402	CDL	CA3-OA5-PA1-OA3
26	C	603	CDL	OA5-CA3-CA4-CA6
24	L	502	PEF	O2-C10-C11-C12
24	A	501	PEF	O3P-C1-C2-O2
24	b	302	PEF	O3P-C1-C2-O2
26	C	603	CDL	OA5-CA3-CA4-OA6
26	L	501	CDL	OA5-CA3-CA4-OA6
28	O	401	HEC	C3D-CAD-CBD-CGD
31	a	602	HEA	C2A-CAA-CBA-CGA
27	T	101	PCF	C25-C26-C27-C28
24	S	102	PEF	C1-C2-C3-O3
24	U	101	PEF	C39-C40-C41-C42
27	I	101	PCF	O13-C11-C12-N
27	T	101	PCF	O13-C11-C12-N
27	e	202	PCF	O13-C11-C12-N
24	C	604	PEF	O2-C2-C3-O3
24	C	605	PEF	O2-C2-C3-O3
24	b	303	PEF	C31-C32-C33-C34
24	L	502	PEF	C17-C18-C19-C20
26	O	402	CDL	C32-C33-C34-C35
24	N	605	PEF	C3-C2-O2-C10
24	c	301	PEF	O3P-C1-C2-C3
26	O	402	CDL	OA5-CA3-CA4-CA6
26	S	101	CDL	OB5-CB3-CB4-CB6
27	C	606	PCF	O22-C21-O21-C2
24	N	604	PEF	O3P-C1-C2-O2
24	C	604	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
24	H	602	PEF	C1-O3P-P-O4P
24	H	602	PEF	C4-O4P-P-O3P
24	S	102	PEF	C4-O4P-P-O3P
24	U	101	PEF	C1-O3P-P-O4P
24	U	101	PEF	C4-O4P-P-O3P
26	D	402	CDL	CB3-OB5-PB2-OB2
26	H	601	CDL	CB3-OB5-PB2-OB2
26	L	501	CDL	CA2-OA2-PA1-OA5
26	L	501	CDL	CB3-OB5-PB2-OB2
26	N	603	CDL	CA2-OA2-PA1-OA5
26	S	101	CDL	CA2-OA2-PA1-OA5
27	C	606	PCF	C40-C41-C42-C43
24	J	101	PEF	C31-C30-O3-C3
24	J	101	PEF	O5-C30-O3-C3
24	b	302	PEF	C32-C33-C34-C35
24	C	604	PEF	O3P-C1-C2-O2
24	P	302	PEF	O3P-C1-C2-O2
26	O	402	CDL	C31-C32-C33-C34
24	b	302	PEF	C11-C12-C13-C14
25	C	601	HEM	CAA-CBA-CGA-O2A
31	a	602	HEA	CAA-CBA-CGA-O1A
25	C	602	HEM	CAD-CBD-CGD-O1D
31	a	602	HEA	CAA-CBA-CGA-O2A
26	C	603	CDL	OA7-CA5-OA6-CA4
25	C	601	HEM	CAA-CBA-CGA-O1A
25	N	601	HEM	CAD-CBD-CGD-O1D
26	D	402	CDL	CA6-CA4-OA6-CA5
24	P	302	PEF	C34-C35-C36-C37
26	O	402	CDL	C72-C71-CB7-OB8
26	H	601	CDL	OB5-CB3-CB4-CB6
26	C	603	CDL	C11-CA5-OA6-CA4
25	N	601	HEM	CAA-CBA-CGA-O1A
25	N	601	HEM	CAA-CBA-CGA-O2A
26	N	603	CDL	C31-C32-C33-C34
25	N	601	HEM	CAD-CBD-CGD-O2D
26	S	101	CDL	OB6-CB4-CB6-OB8
27	T	101	PCF	C34-C35-C36-C37
26	S	101	CDL	C1-CB2-OB2-PB2
24	b	302	PEF	O4-C10-C11-C12
31	a	603	HEA	CAA-CBA-CGA-O1A
25	N	602	HEM	CAD-CBD-CGD-O1D
24	S	102	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	S	103	PCF	C33-C34-C35-C36
25	C	601	HEM	CAD-CBD-CGD-O2D
24	U	101	PEF	C33-C34-C35-C36
24	c	302	PEF	C15-C16-C17-C18
24	P	302	PEF	O3P-C1-C2-C3
24	b	303	PEF	O3P-C1-C2-C3
24	c	302	PEF	C35-C36-C37-C38
24	H	602	PEF	C11-C12-C13-C14
26	H	601	CDL	CB4-CB3-OB5-PB2
27	N	606	PCF	C2-C1-O11-P
24	e	201	PEF	O2-C10-C11-C12
27	I	101	PCF	O31-C31-C32-C33
24	L	502	PEF	C12-C13-C14-C15
27	C	606	PCF	O31-C31-C32-C33
24	E	302	PEF	C32-C33-C34-C35
31	a	603	HEA	CAD-CBD-CGD-O2D
25	C	601	HEM	CAD-CBD-CGD-O1D
25	C	602	HEM	CAD-CBD-CGD-O2D
26	H	601	CDL	C72-C71-CB7-OB8
26	N	603	CDL	C32-C33-C34-C35
25	N	602	HEM	CAA-CBA-CGA-O2A
31	a	603	HEA	CAD-CBD-CGD-O1D
24	J	101	PEF	C14-C15-C16-C17
24	N	604	PEF	C32-C33-C34-C35
24	b	302	PEF	O3-C30-C31-C32
27	I	101	PCF	C24-C25-C26-C27
28	O	401	HEC	CAD-CBD-CGD-O2D
24	H	602	PEF	C33-C34-C35-C36
31	a	602	HEA	C15-C16-C17-C18
24	b	303	PEF	O3-C30-C31-C32
25	N	602	HEM	CAA-CBA-CGA-O1A
24	S	102	PEF	O3P-C1-C2-C3
28	O	401	HEC	CAD-CBD-CGD-O1D
24	L	502	PEF	O3-C30-C31-C32
24	L	502	PEF	C30-C31-C32-C33
27	C	606	PCF	C11-C12-N-C14
26	D	402	CDL	C71-CB7-OB8-CB6
24	P	302	PEF	O3-C30-C31-C32
26	C	603	CDL	C11-C12-C13-C14
25	N	602	HEM	CAD-CBD-CGD-O2D
26	S	101	CDL	C72-C71-CB7-OB8
31	a	603	HEA	CAA-CBA-CGA-O2A

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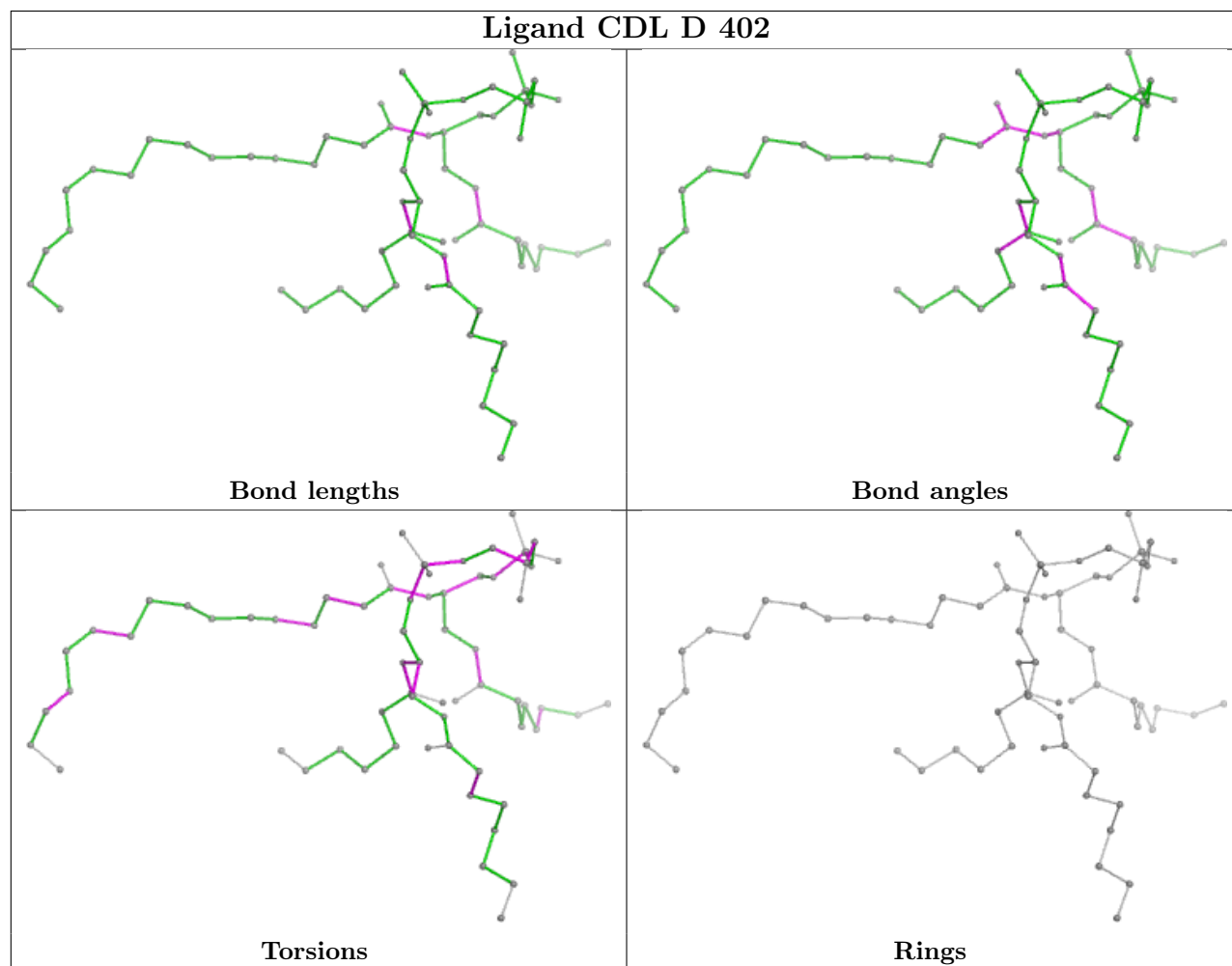
Mol	Chain	Res	Type	Atoms
26	H	601	CDL	CA7-C31-C32-C33
26	H	601	CDL	C72-C71-CB7-OB9
24	e	201	PEF	O4-C10-C11-C12
27	C	606	PCF	O32-C31-C32-C33
25	C	602	HEM	CAA-CBA-CGA-O2A
24	S	102	PEF	O2-C10-C11-C12
24	P	302	PEF	O5-C30-C31-C32
24	b	302	PEF	O5-C30-C31-C32
27	I	101	PCF	O32-C31-C32-C33
24	H	602	PEF	C1-O3P-P-O1P
24	H	602	PEF	C4-O4P-P-O1P
24	J	101	PEF	C4-O4P-P-O1P
24	U	101	PEF	C1-O3P-P-O1P
26	H	601	CDL	CB3-OB5-PB2-OB3
26	L	501	CDL	CB3-OB5-PB2-OB3
26	S	101	CDL	CA3-OA5-PA1-OA4
24	b	303	PEF	O5-C30-C31-C32
26	S	101	CDL	C72-C71-CB7-OB9
26	D	402	CDL	C52-C53-C54-C55
24	J	101	PEF	C11-C12-C13-C14
24	P	302	PEF	C38-C39-C40-C41
27	C	606	PCF	C11-C12-N-C13
24	c	301	PEF	O2-C10-C11-C12
24	E	302	PEF	O2-C10-C11-C12
27	T	101	PCF	O21-C21-C22-C23
24	S	102	PEF	C35-C36-C37-C38
27	e	202	PCF	O22-C21-O21-C2
24	L	502	PEF	O5-C30-C31-C32
27	T	101	PCF	O22-C21-C22-C23
26	D	402	CDL	OB9-CB7-OB8-CB6
24	S	102	PEF	O4-C10-C11-C12
25	C	602	HEM	CAA-CBA-CGA-O1A

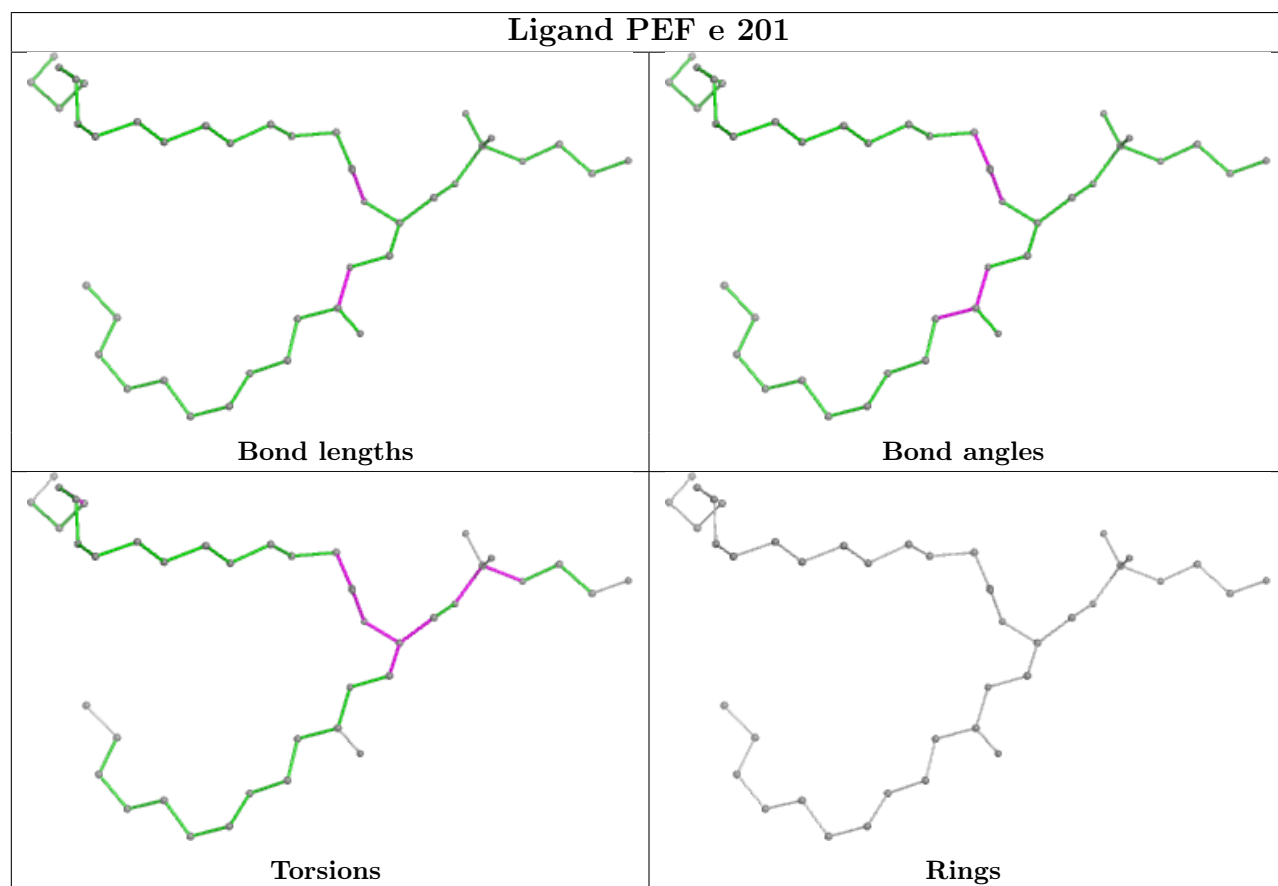
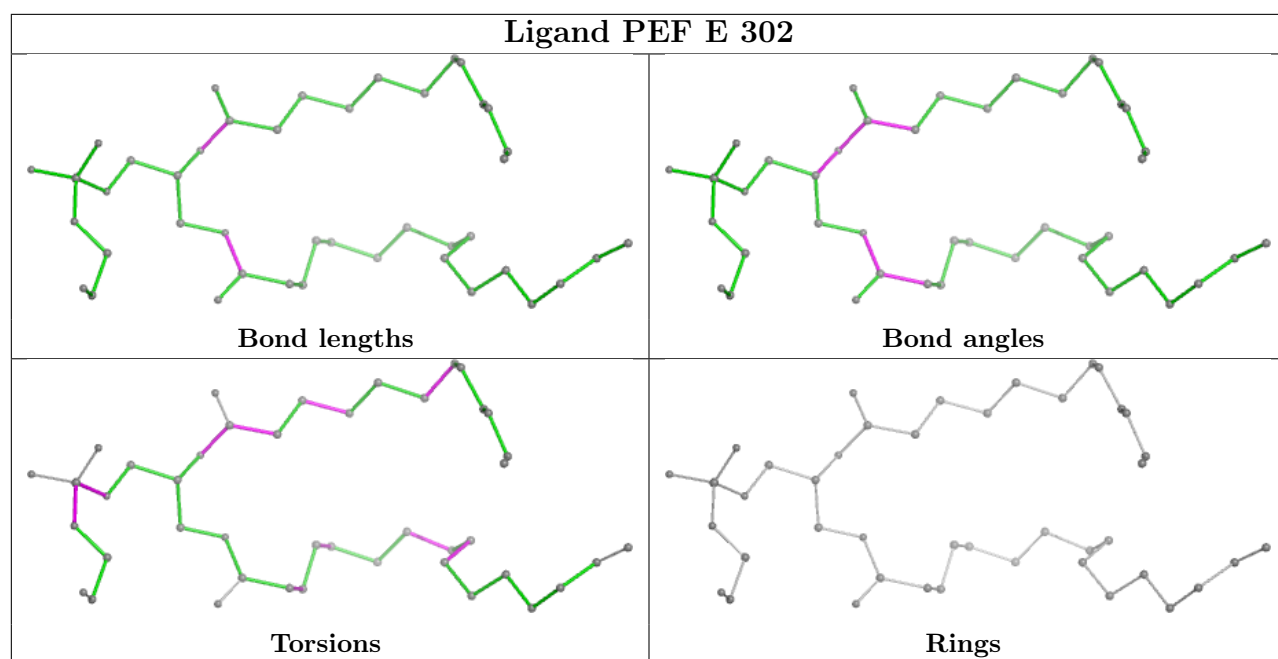
There are no ring outliers.

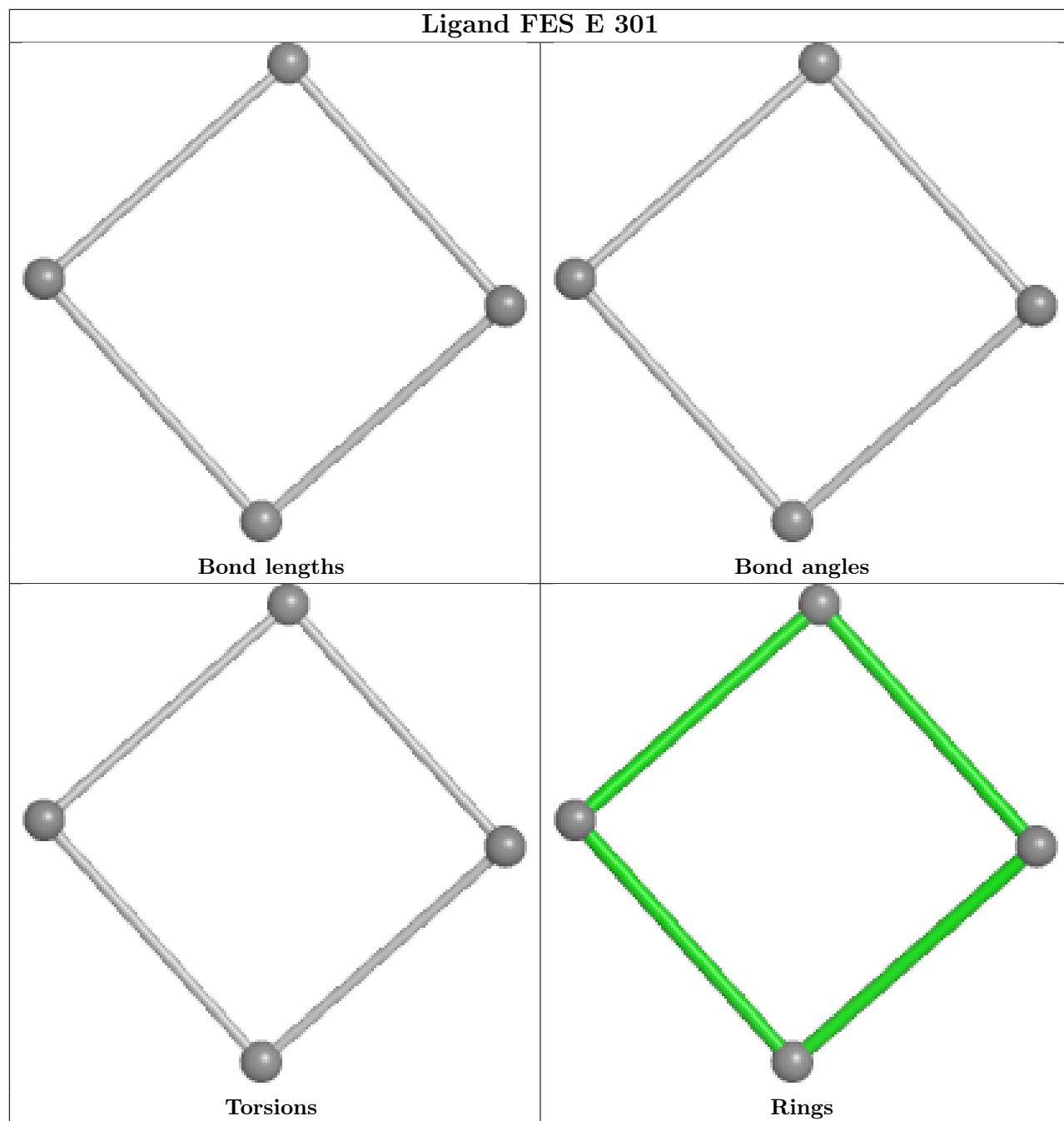
No monomer is involved in short contacts.

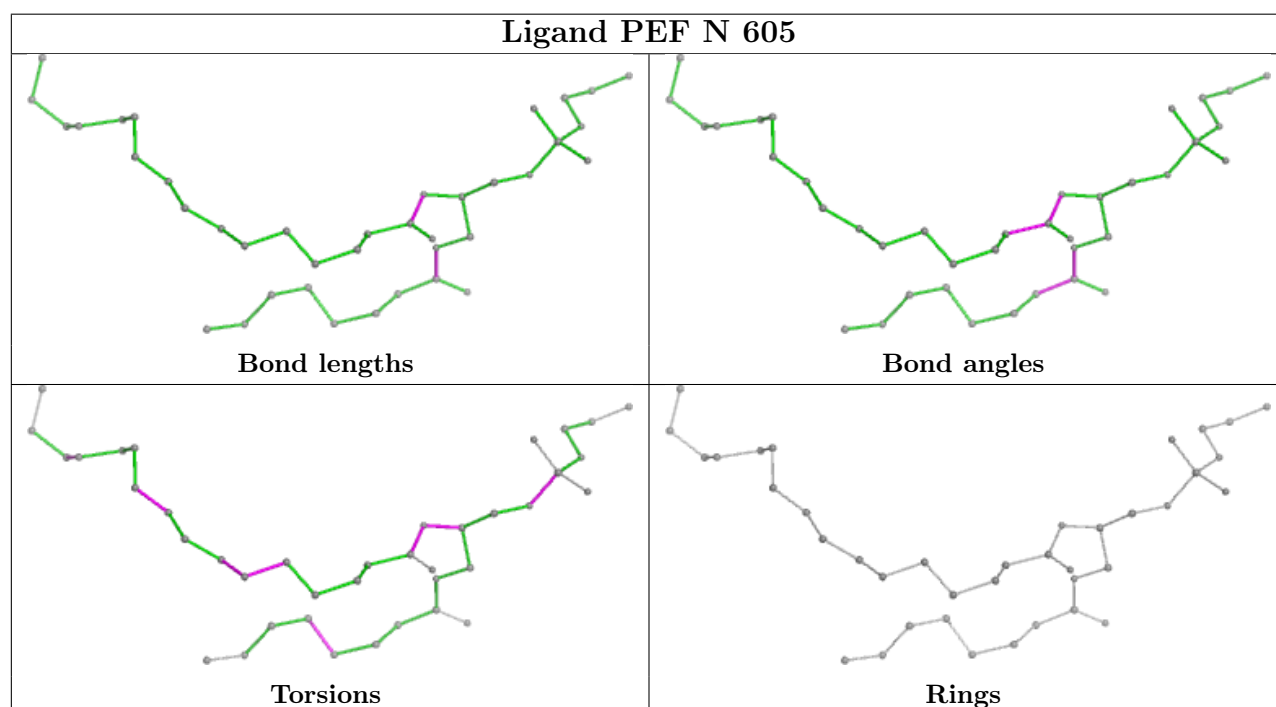
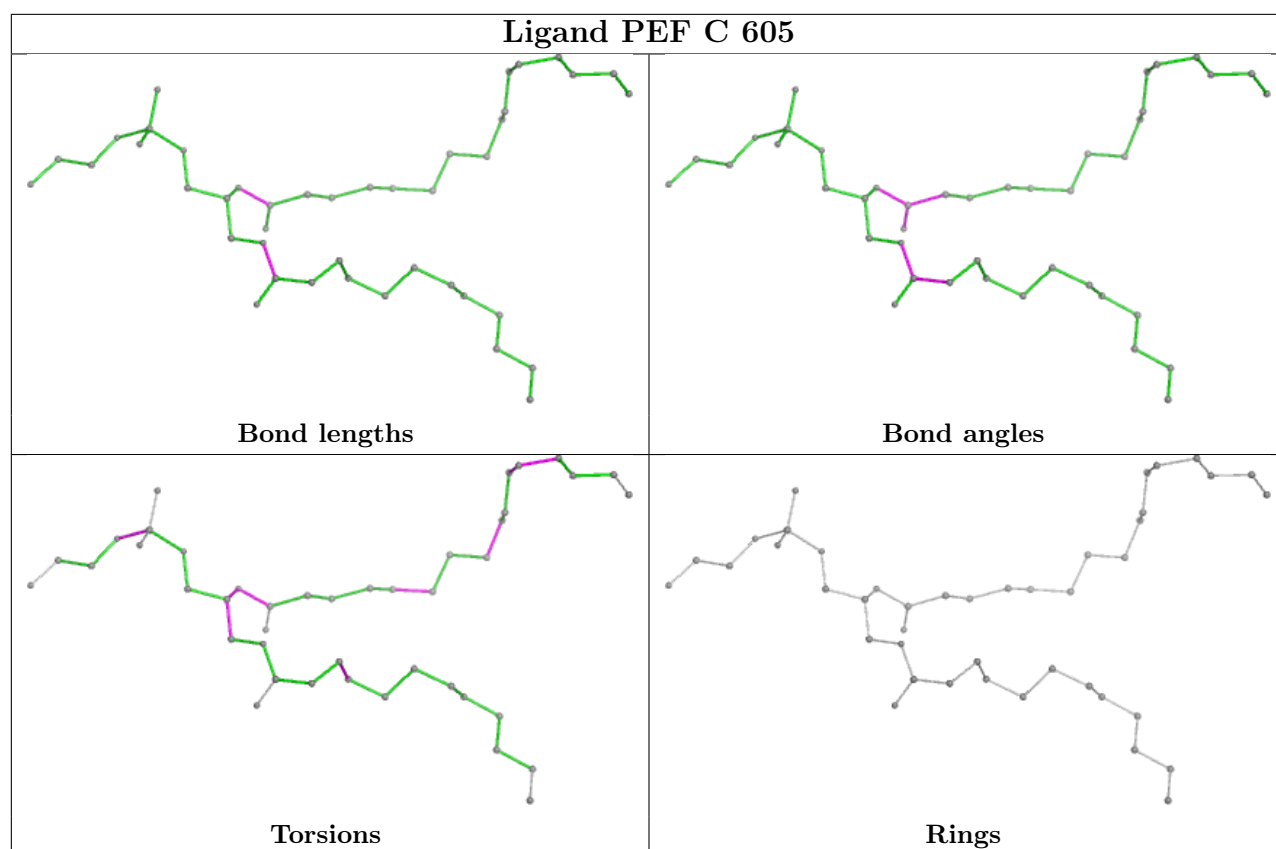
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

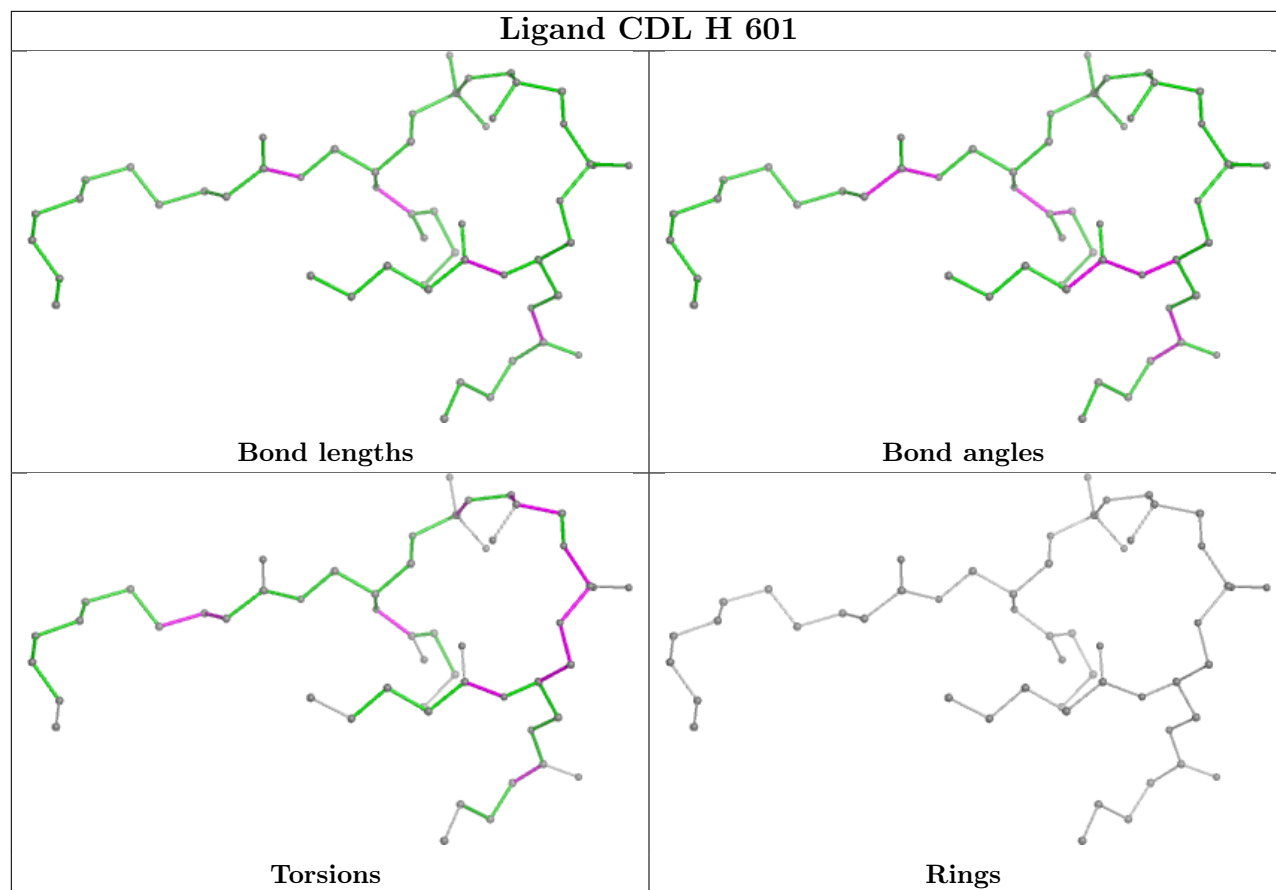
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

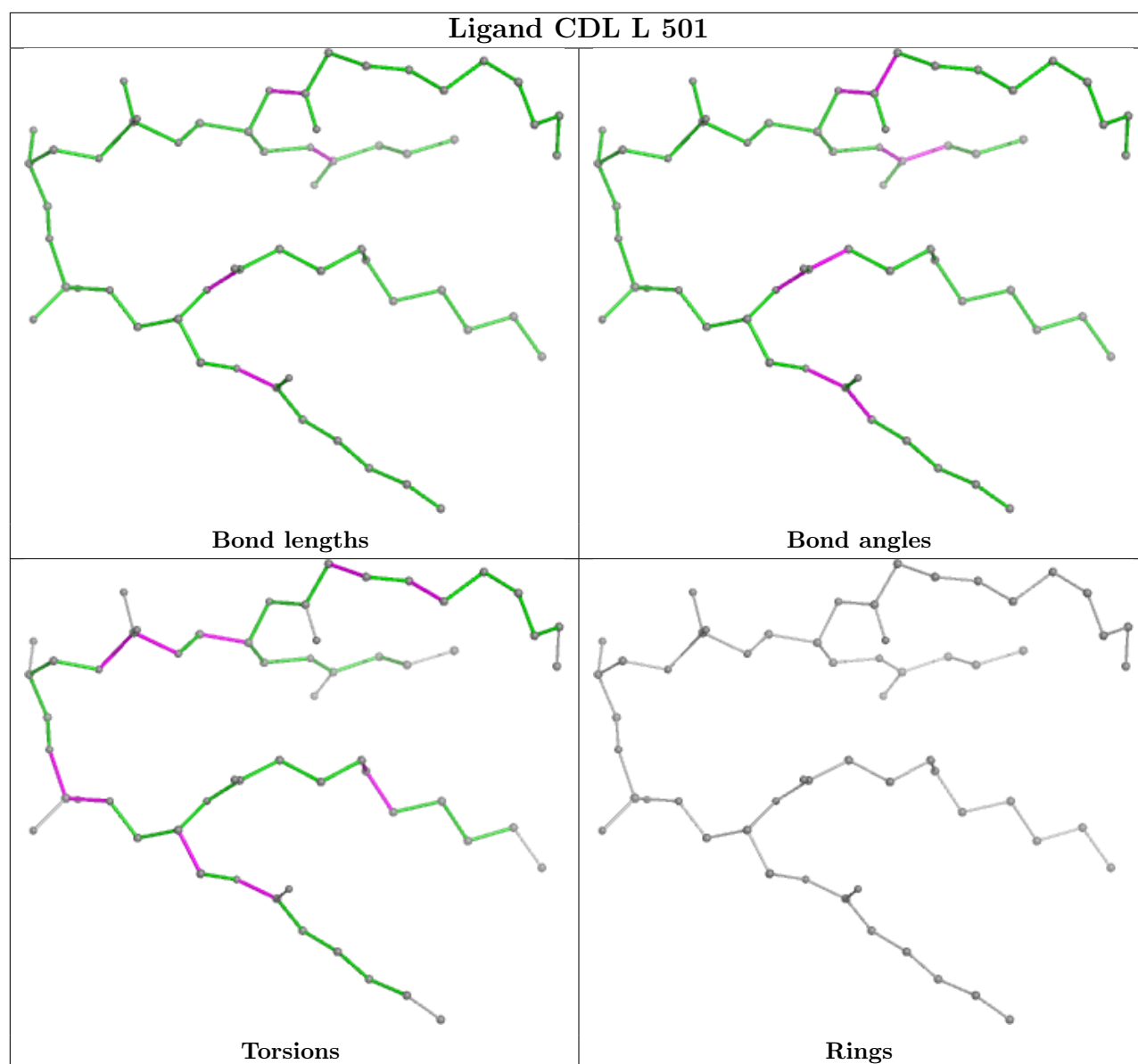


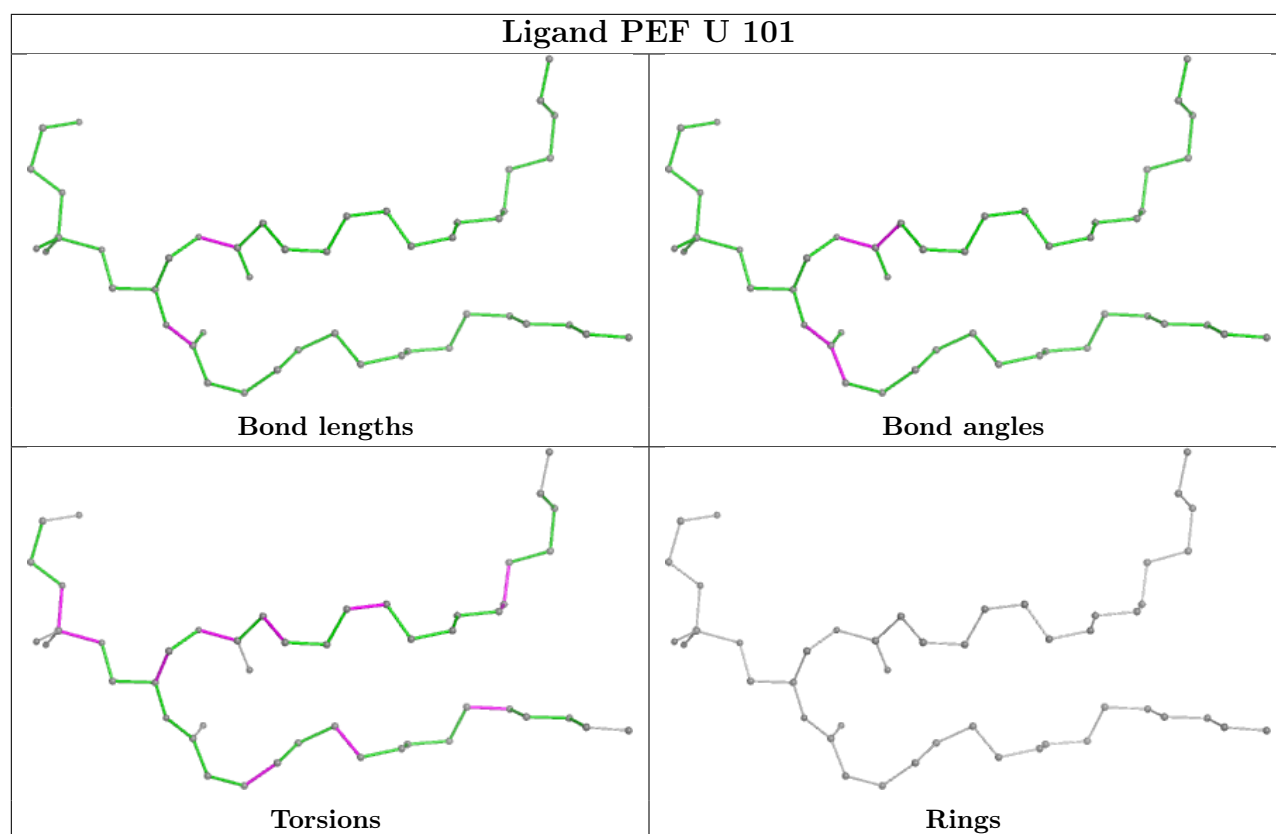


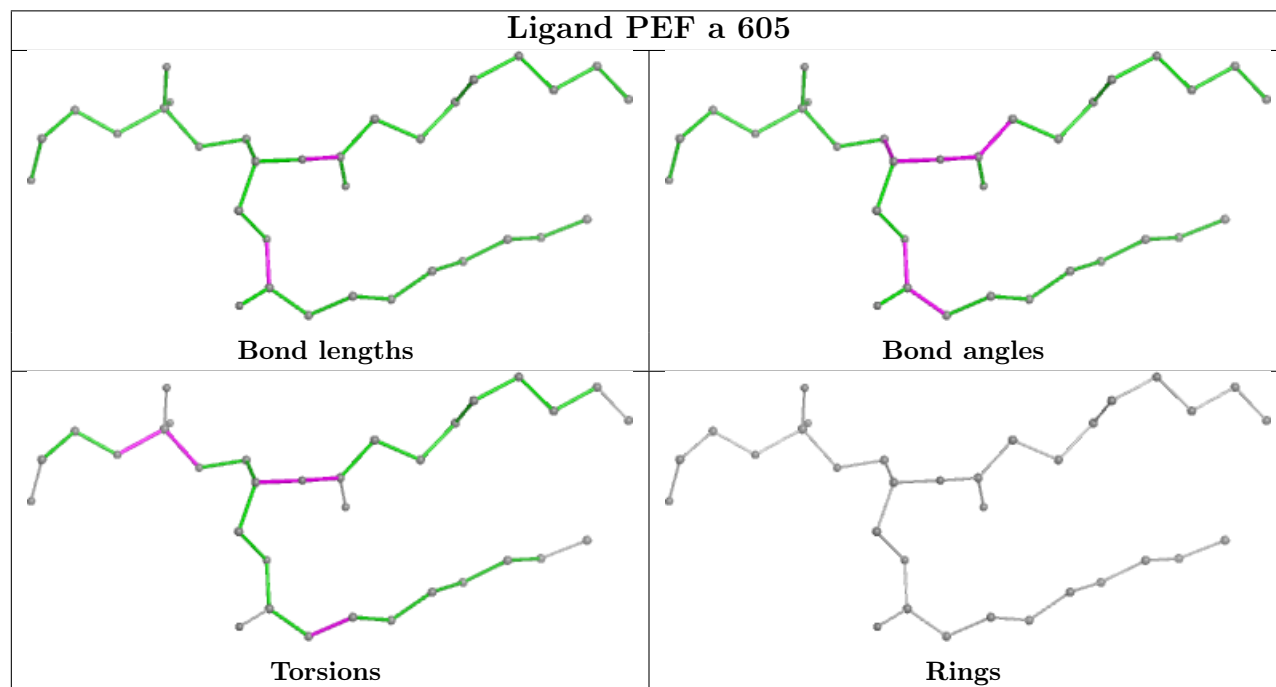
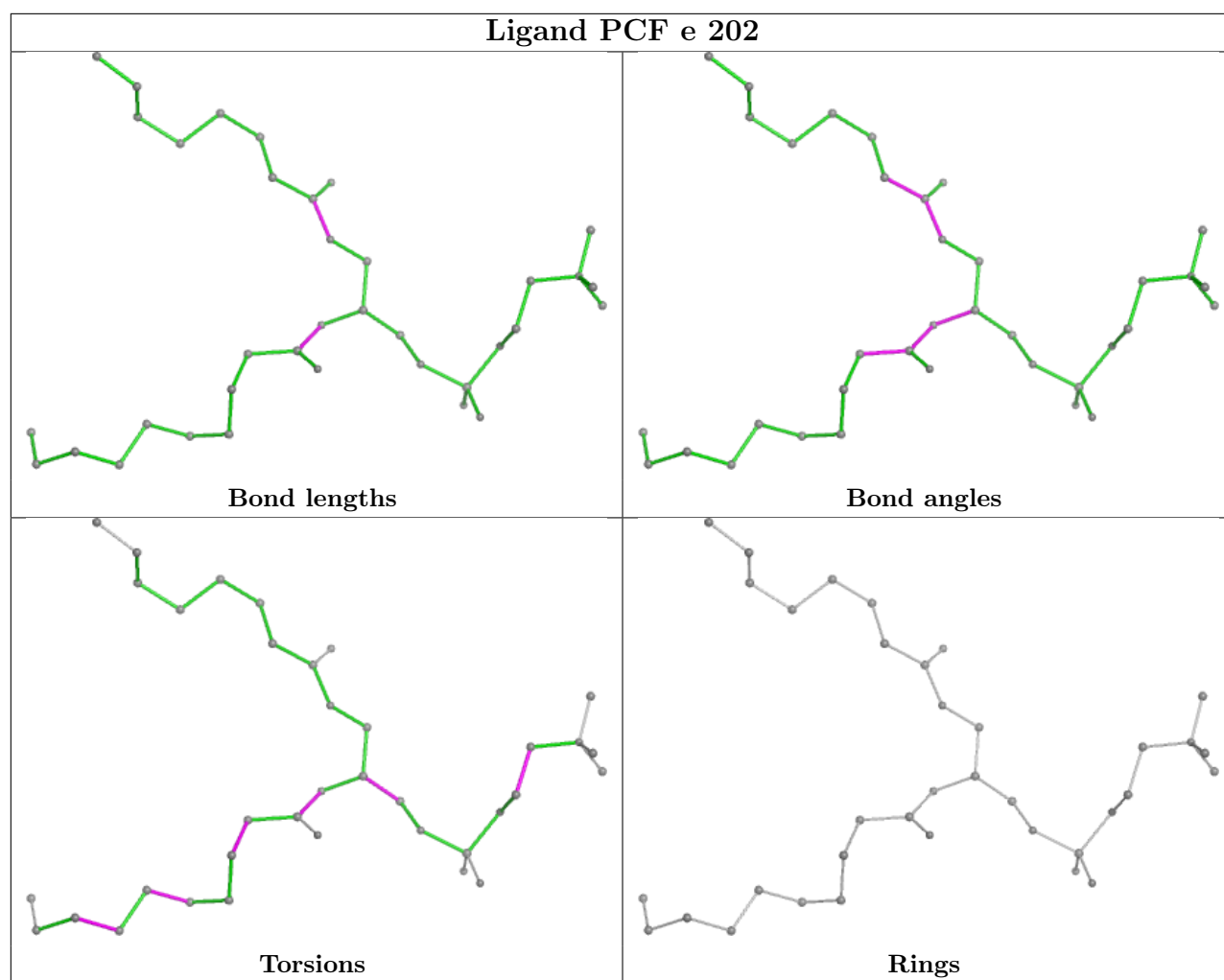


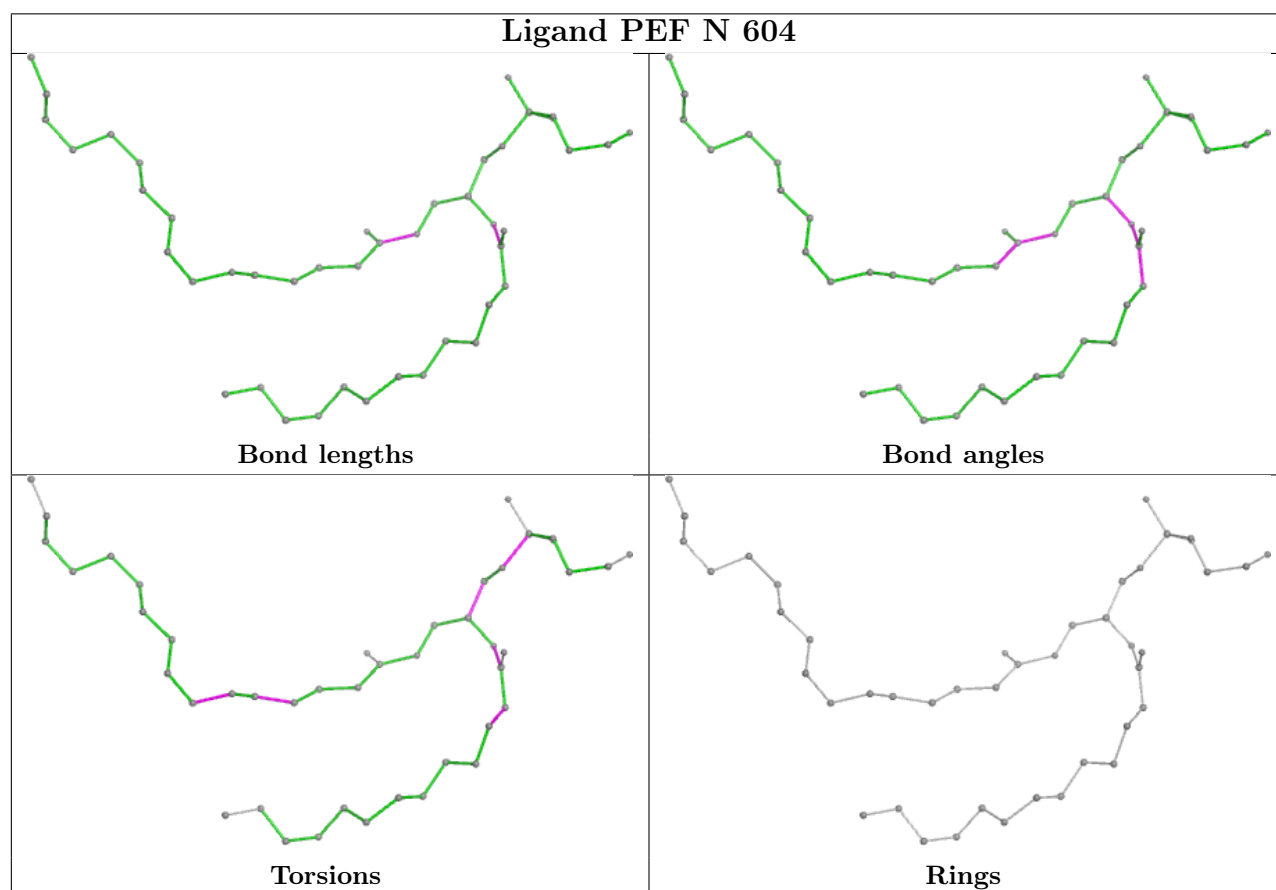
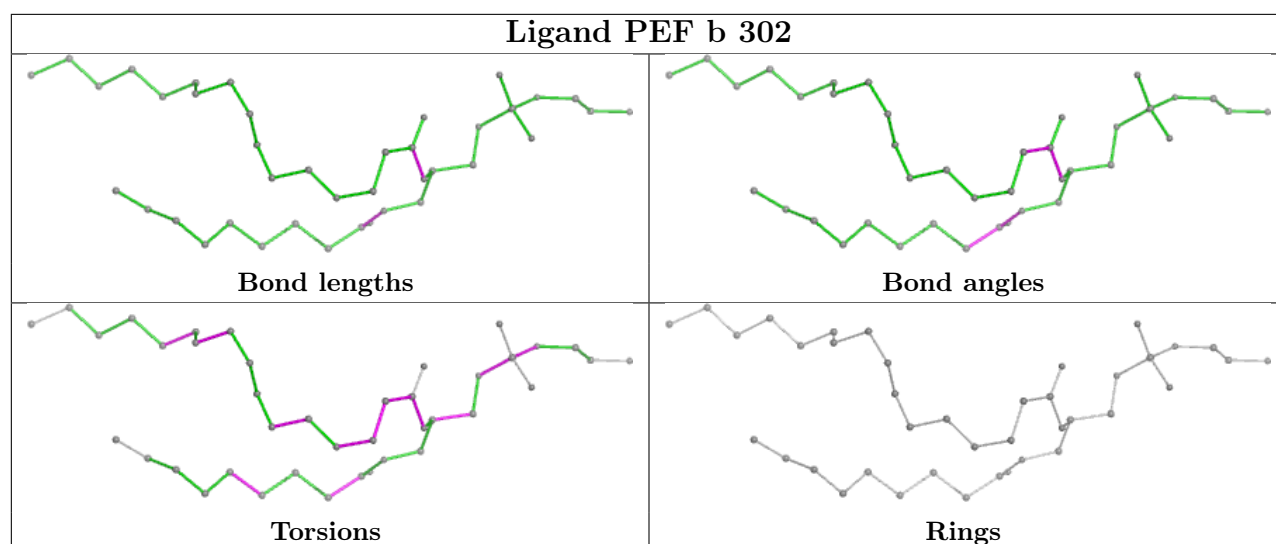


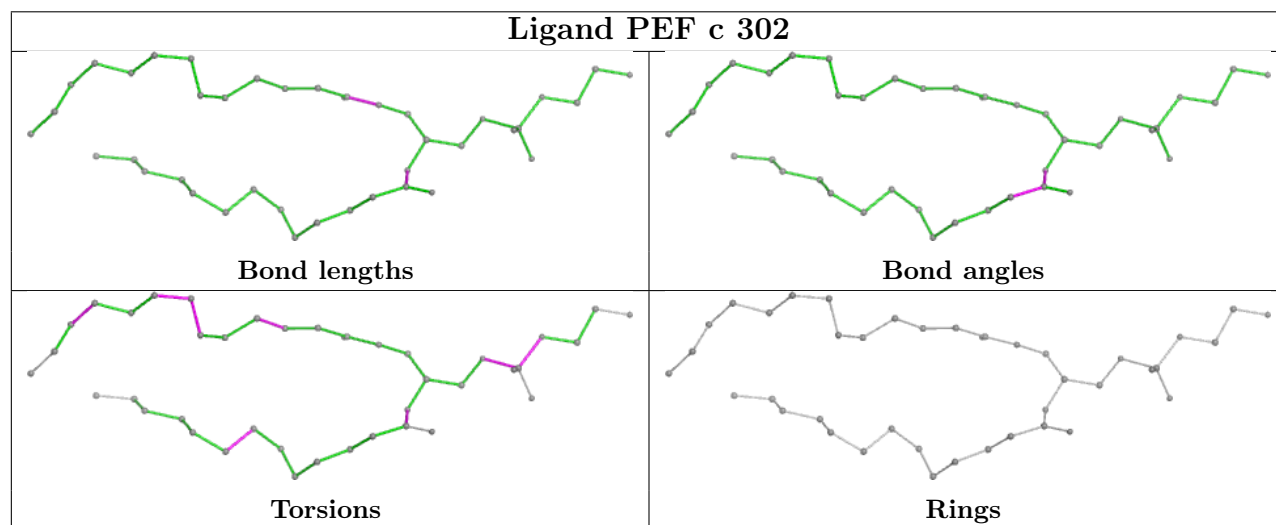
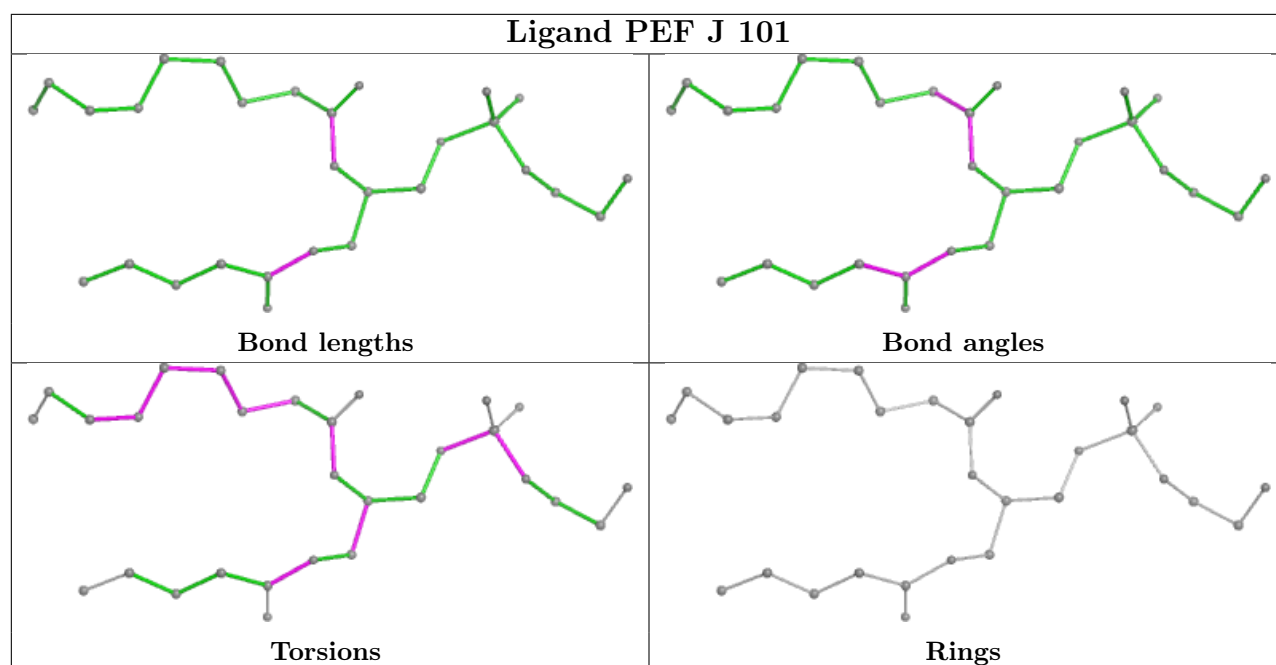


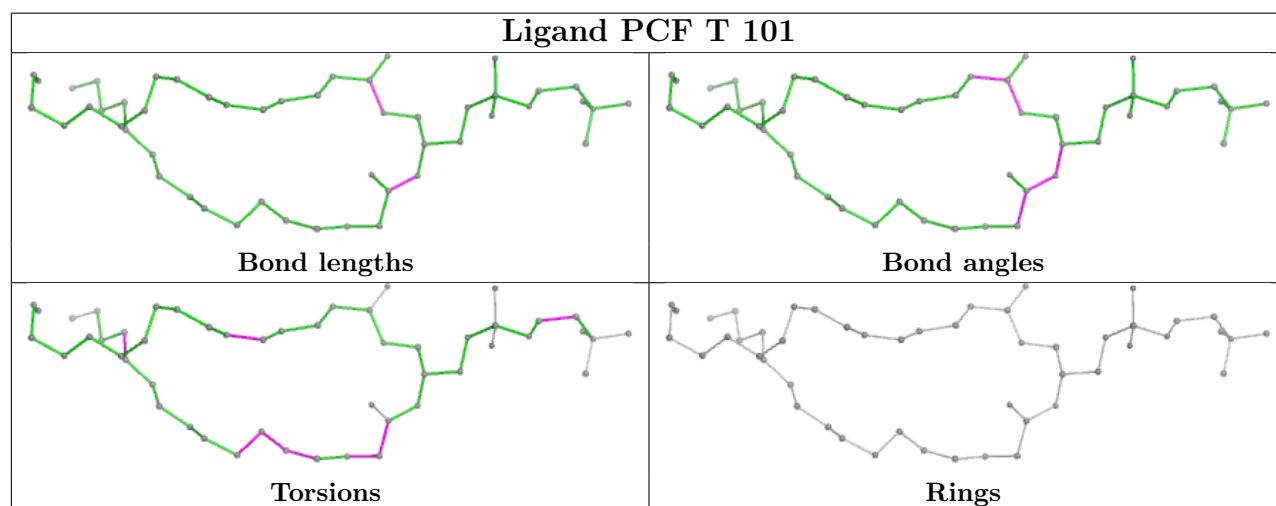
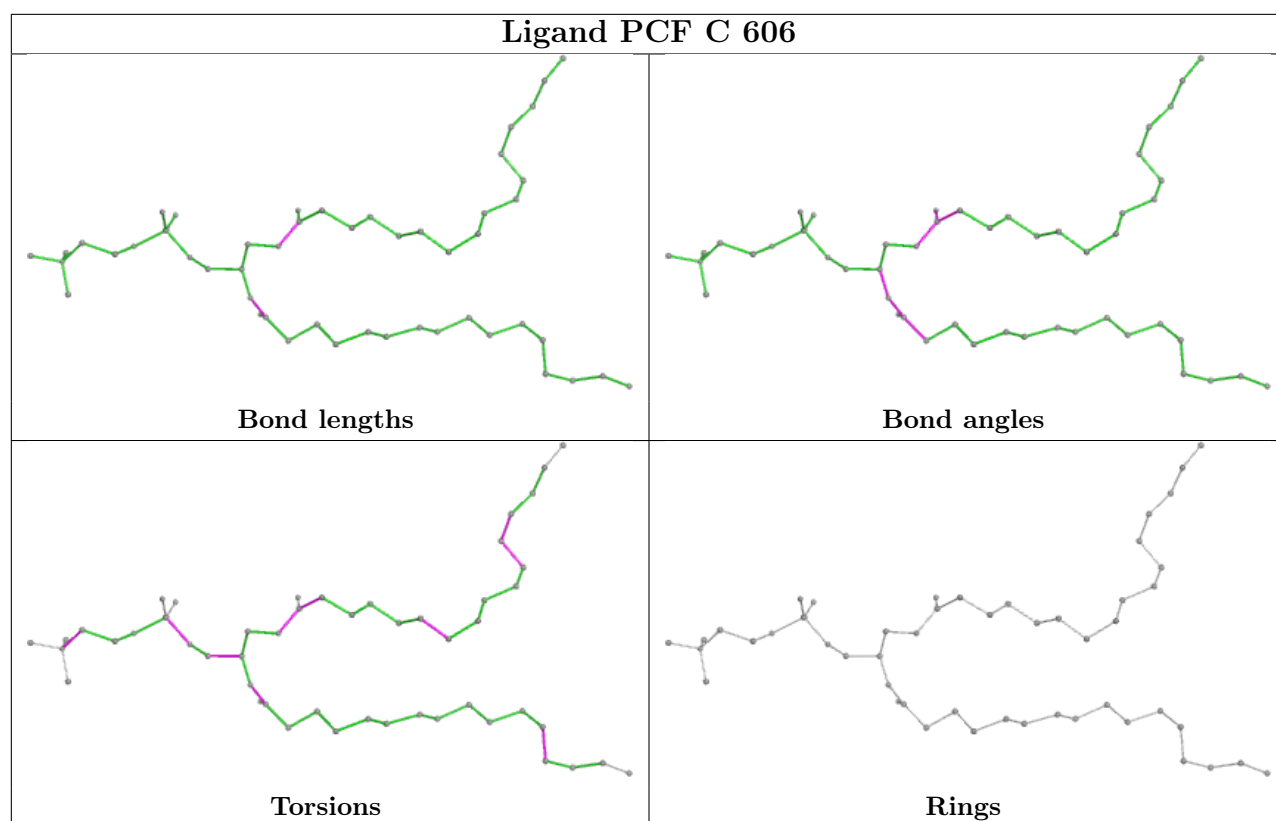


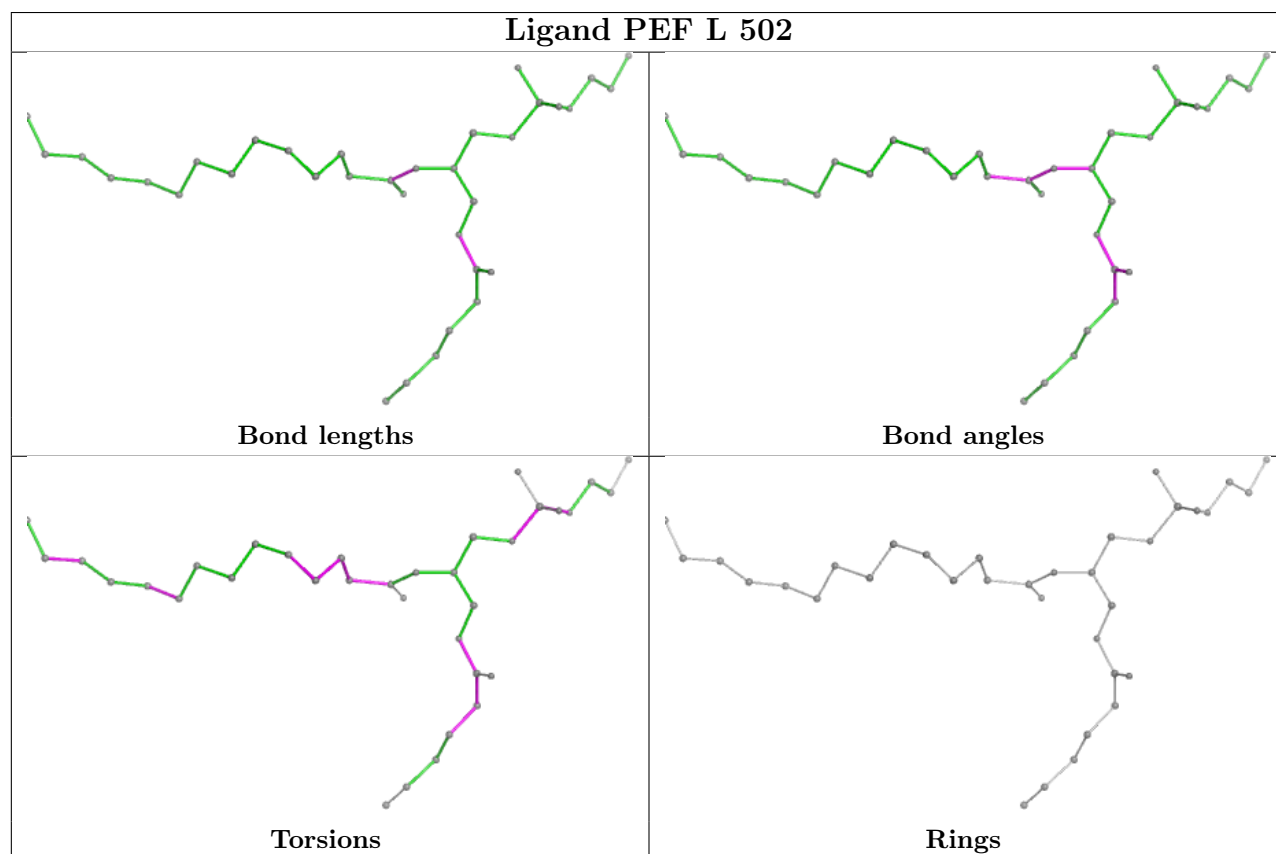
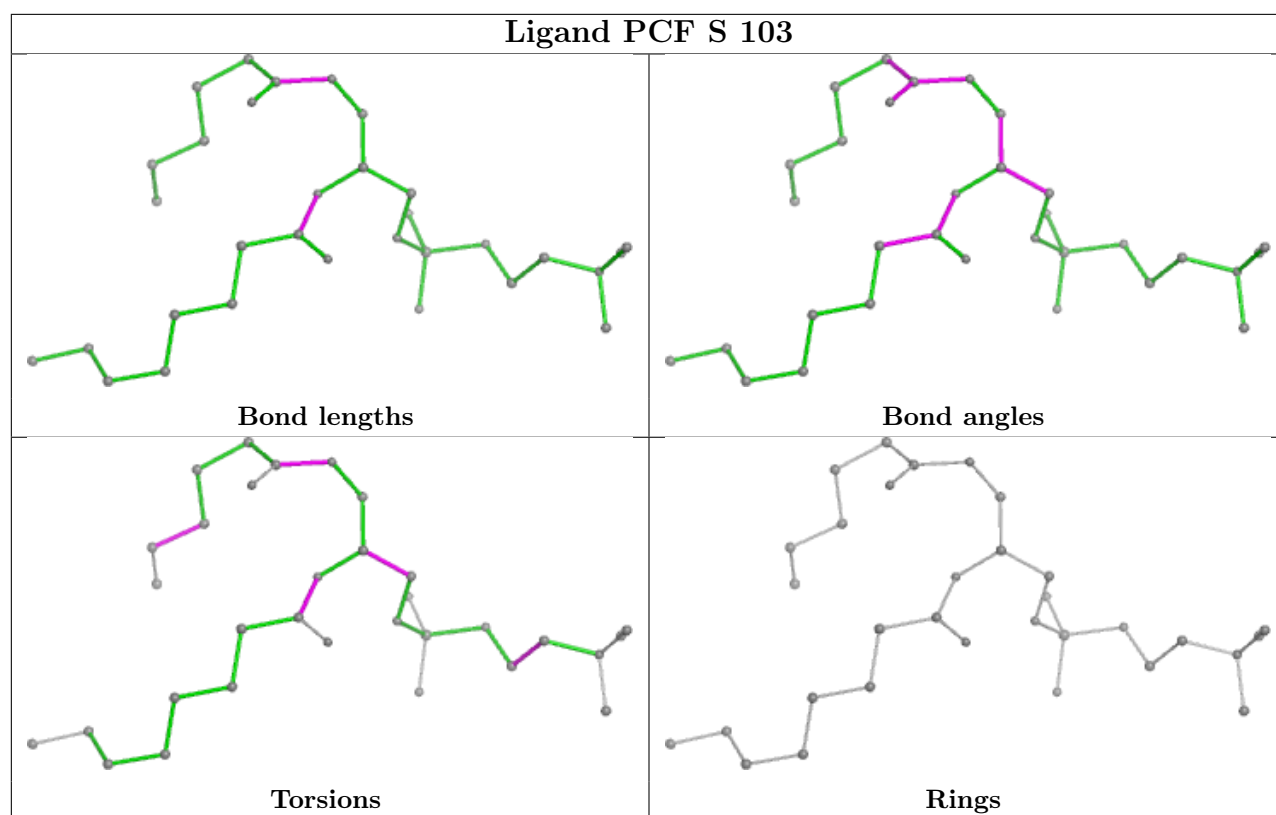


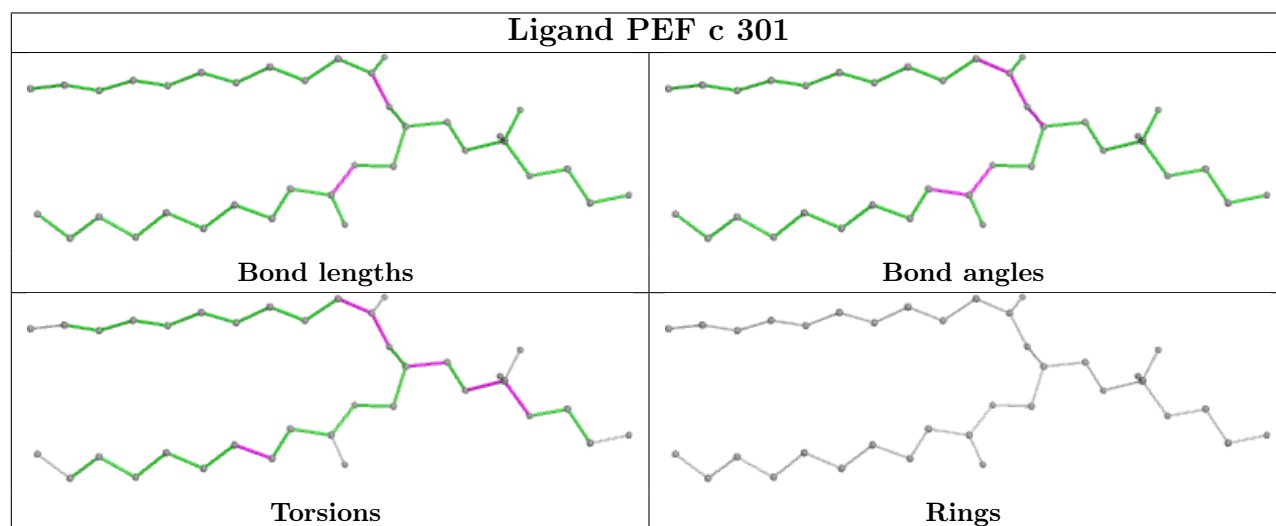
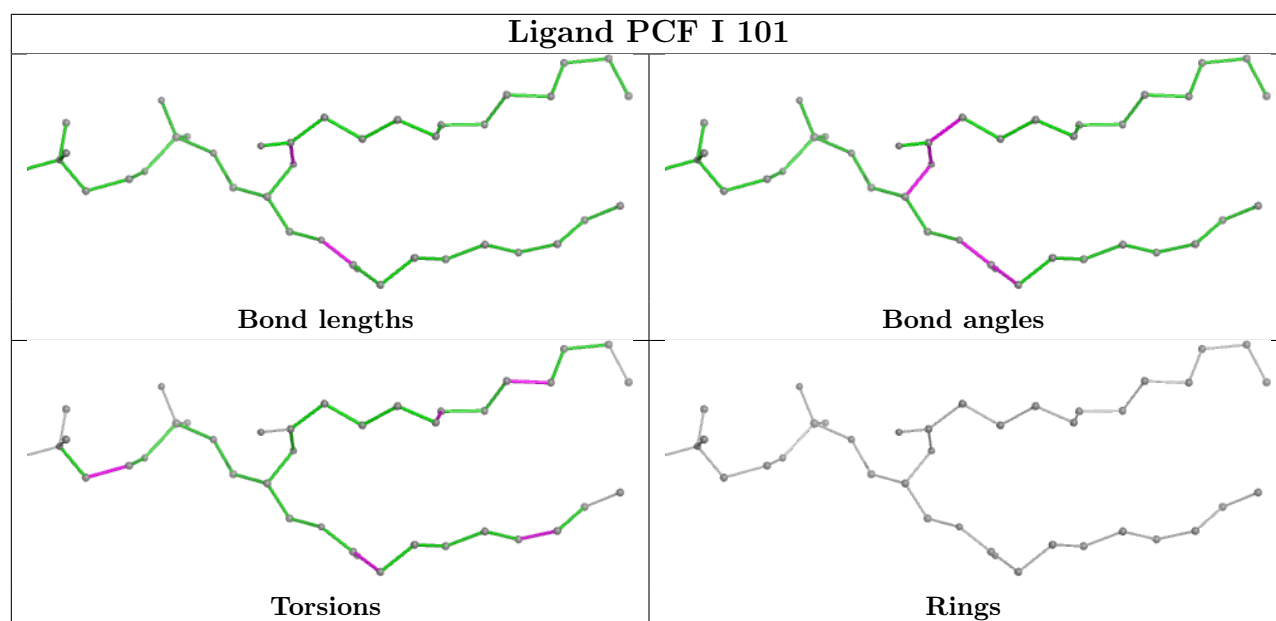


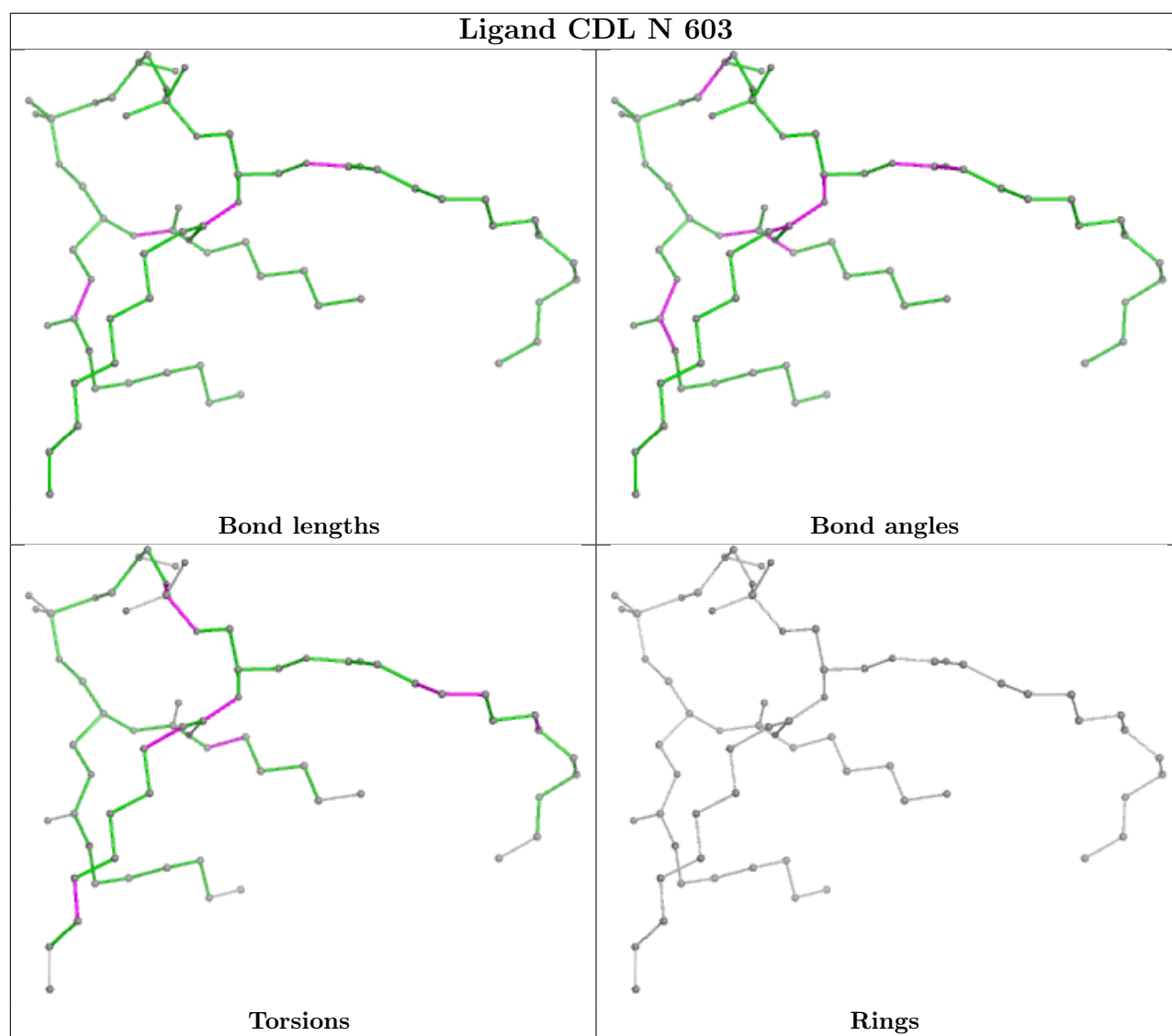


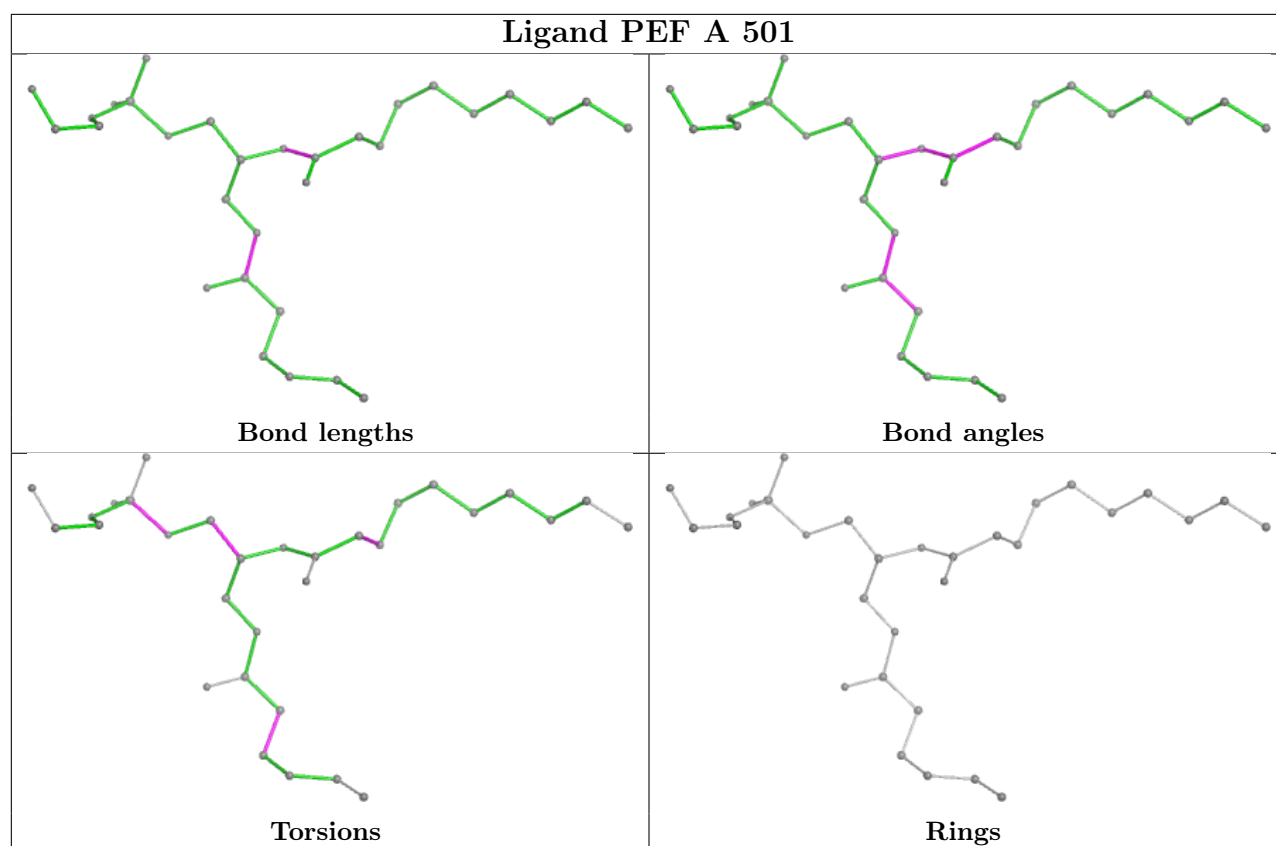


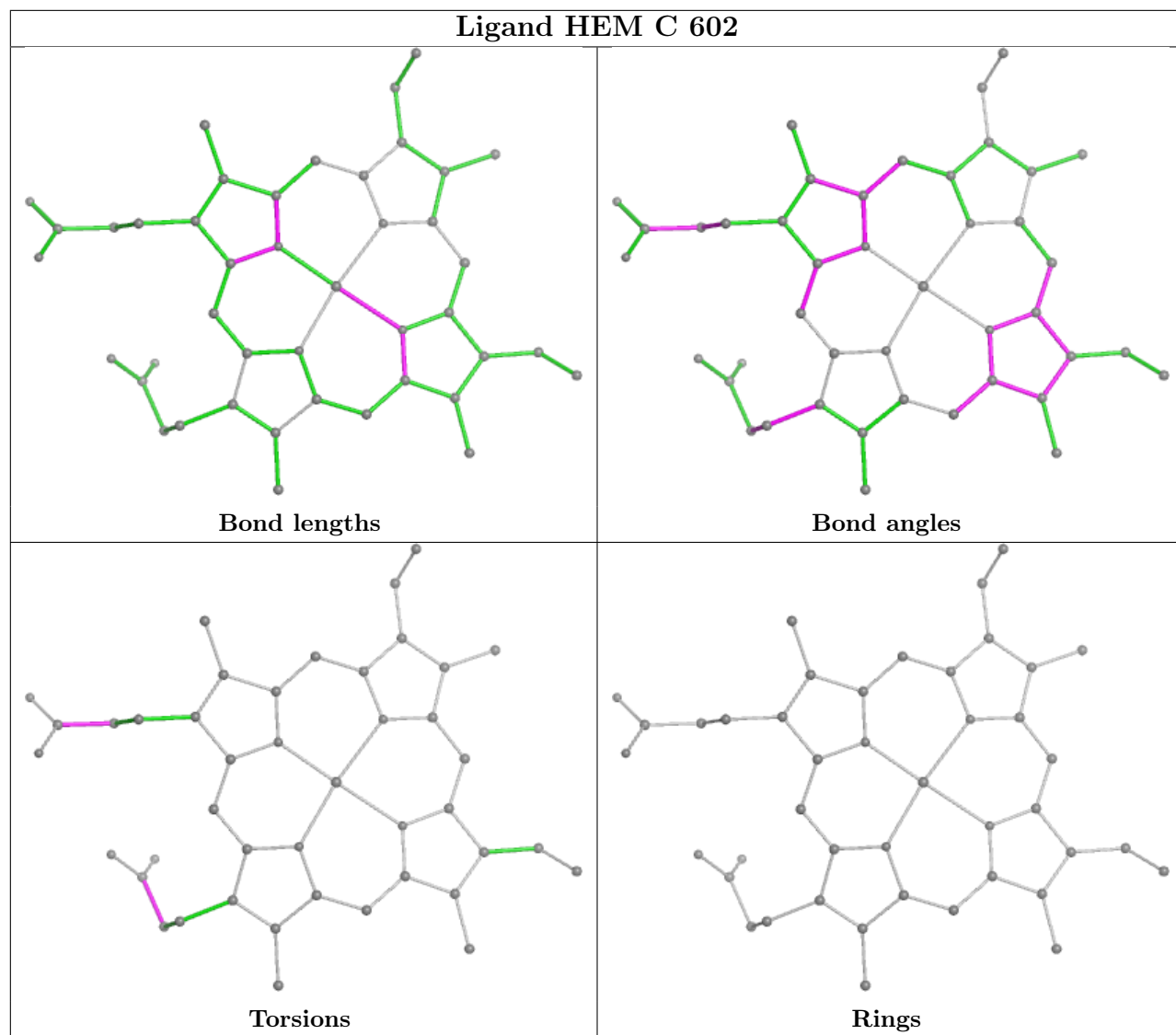


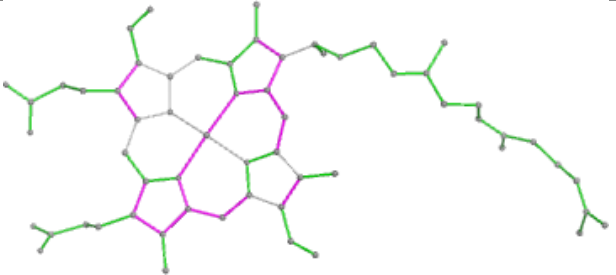
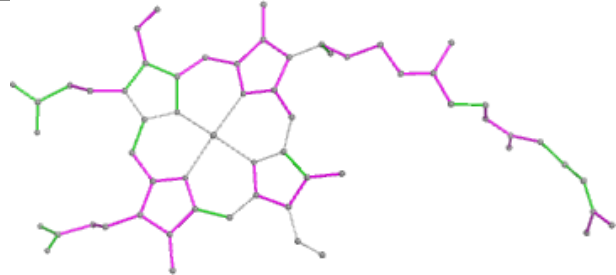
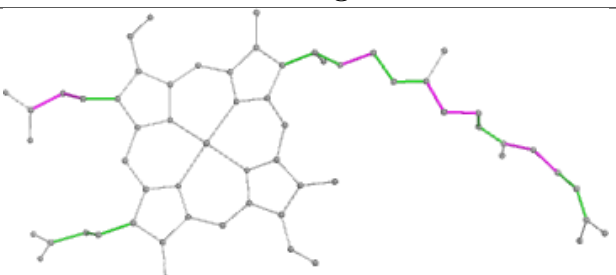
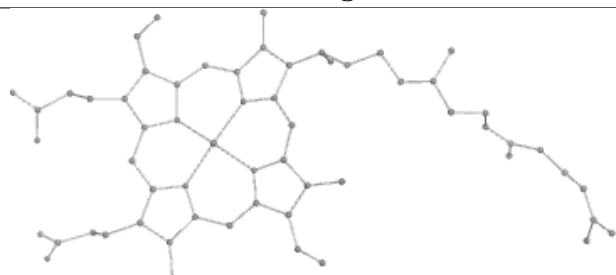








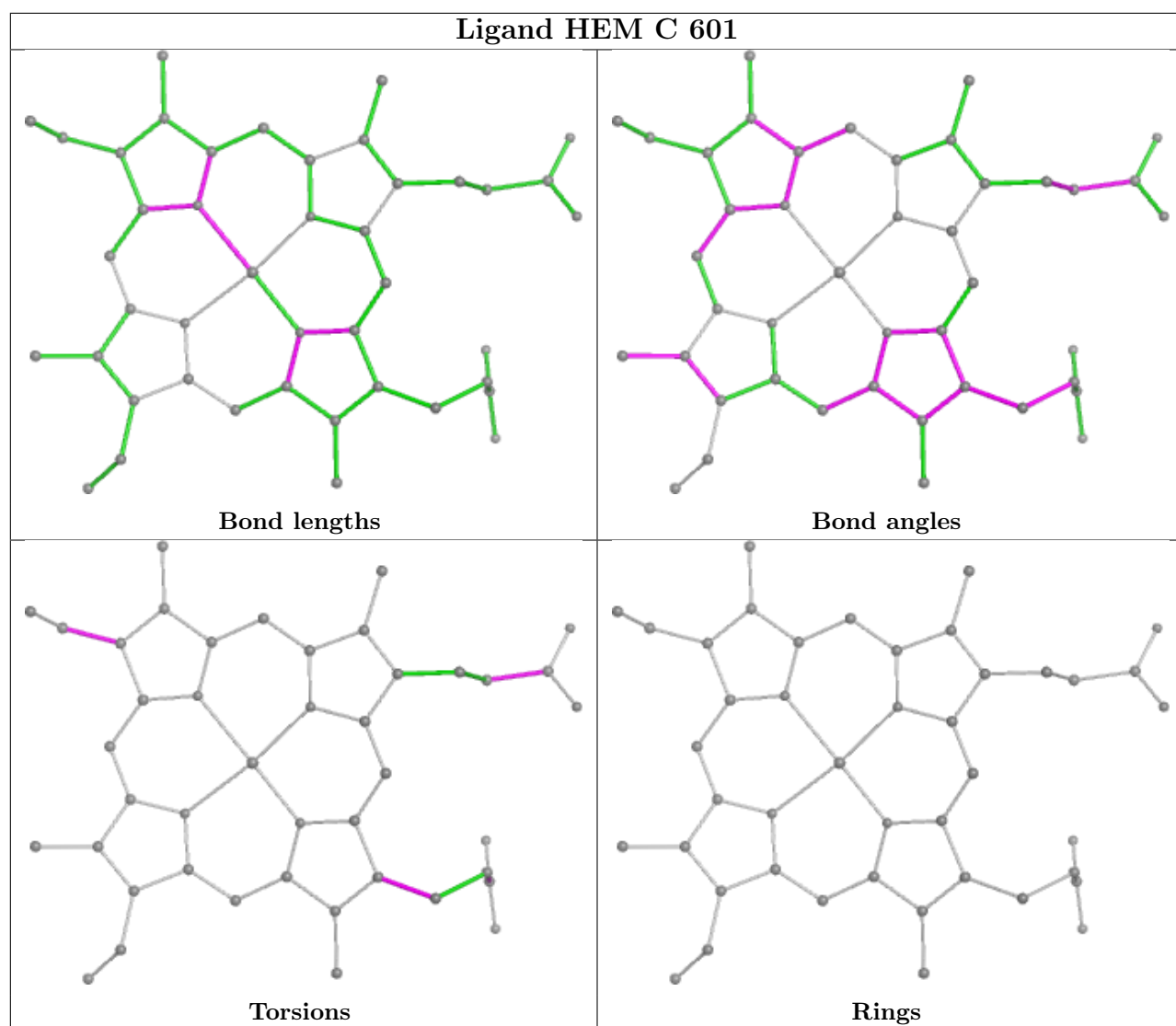


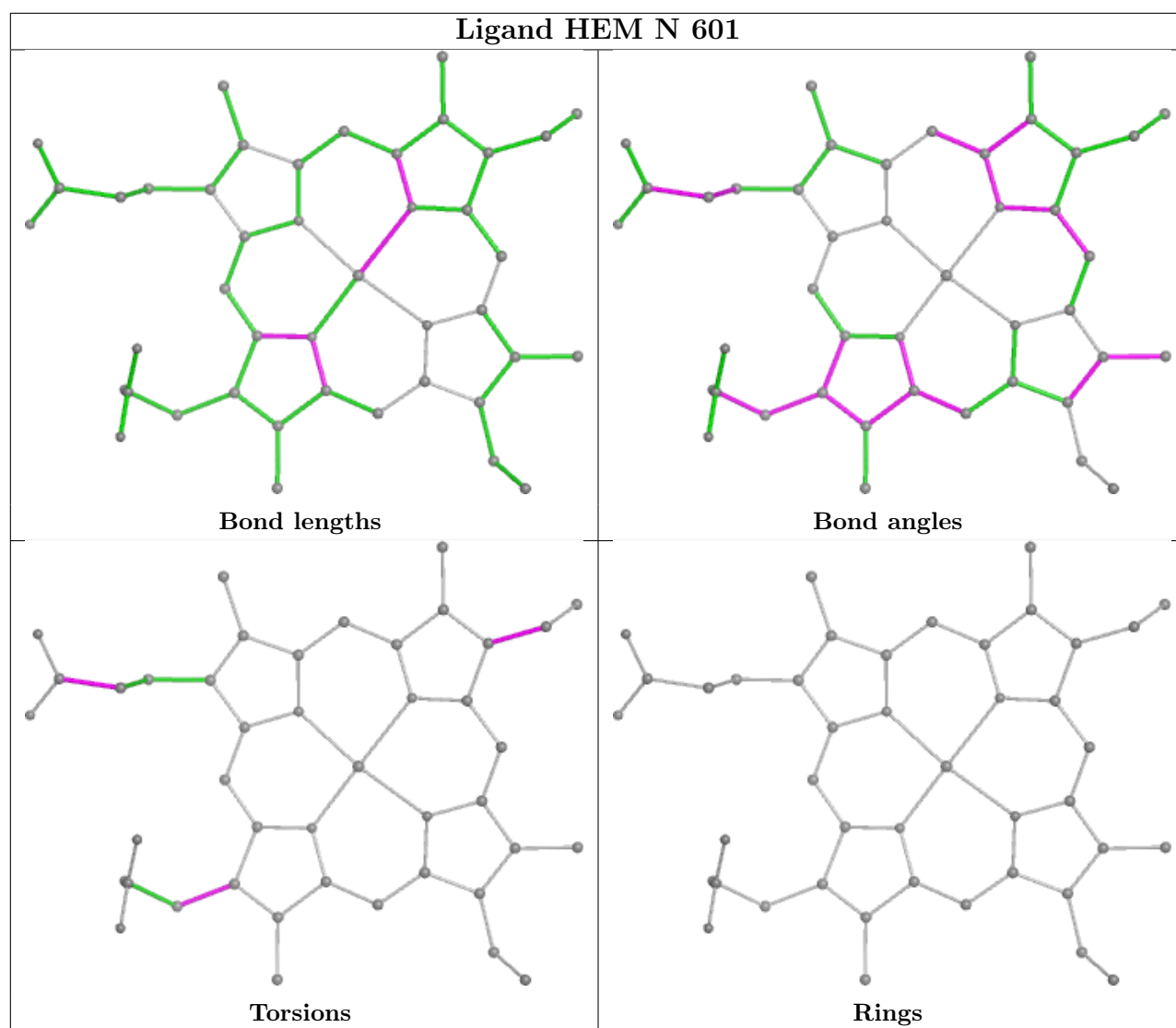


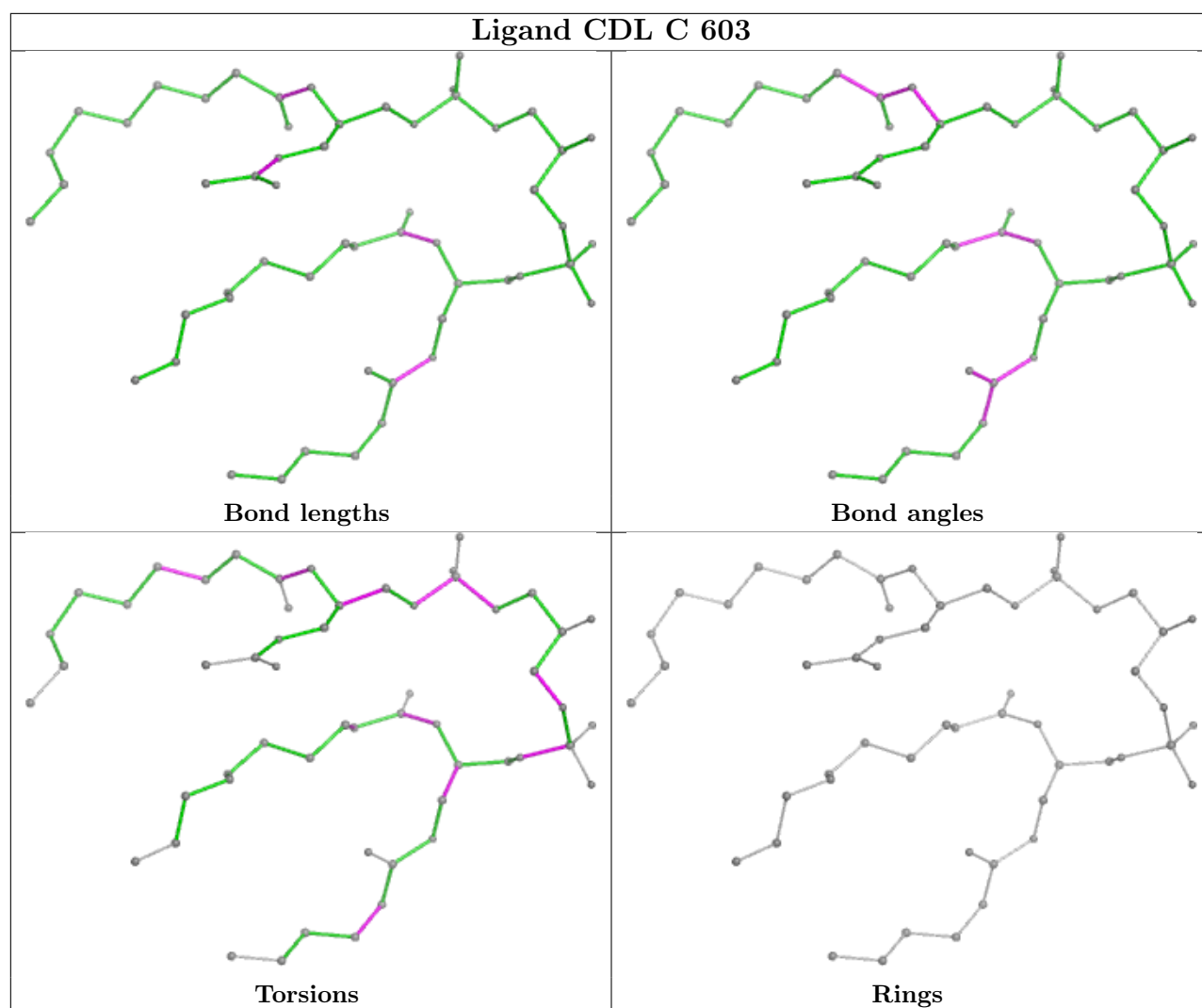


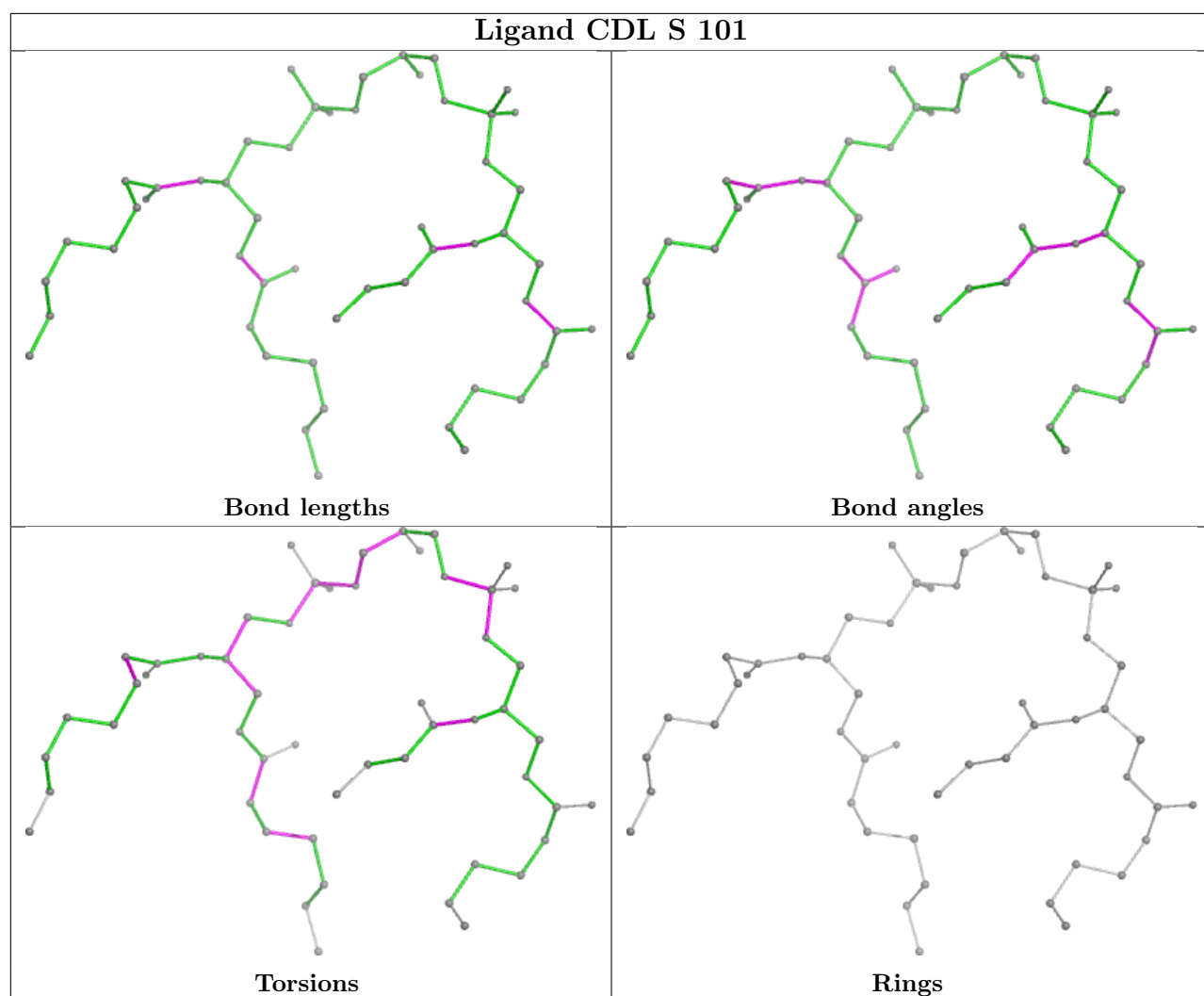
Ligand HEA a 602	
	Bond lengths
	Bond angles
	Torsions
	Rings

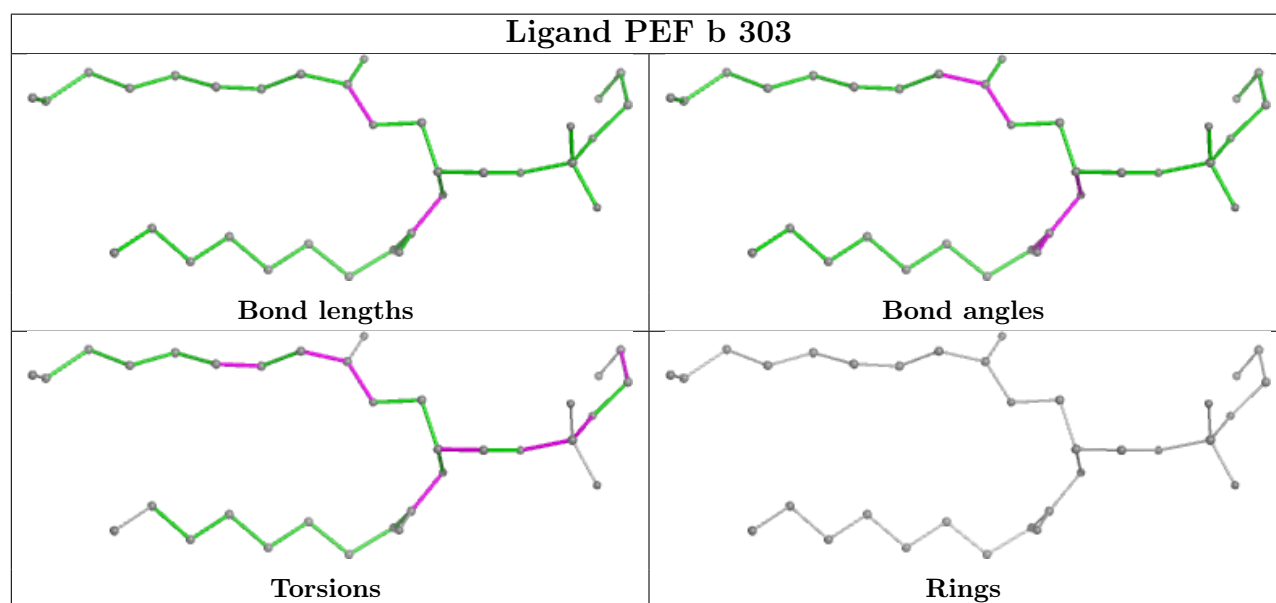
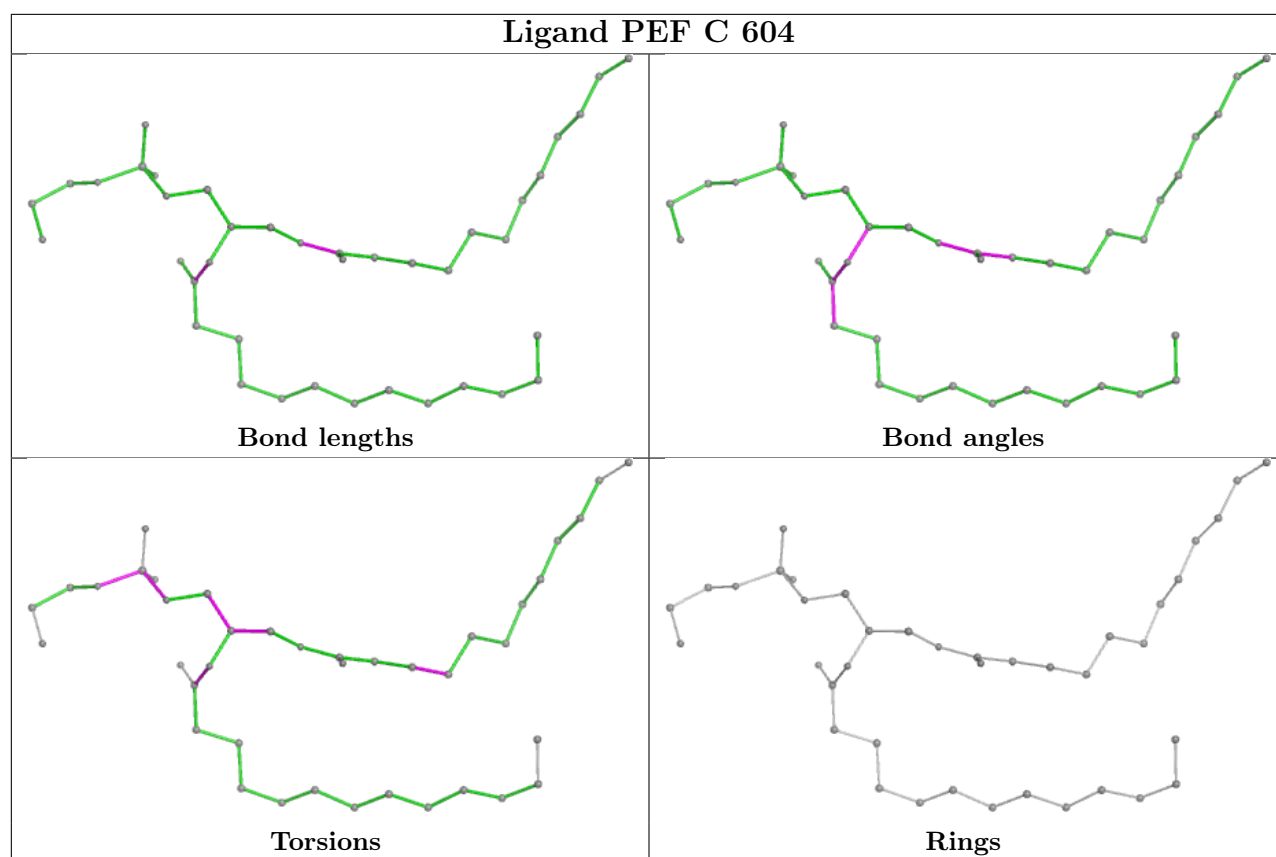
Ligand CUA b 301	
	Bond lengths
	Bond angles
	Torsions
	Rings

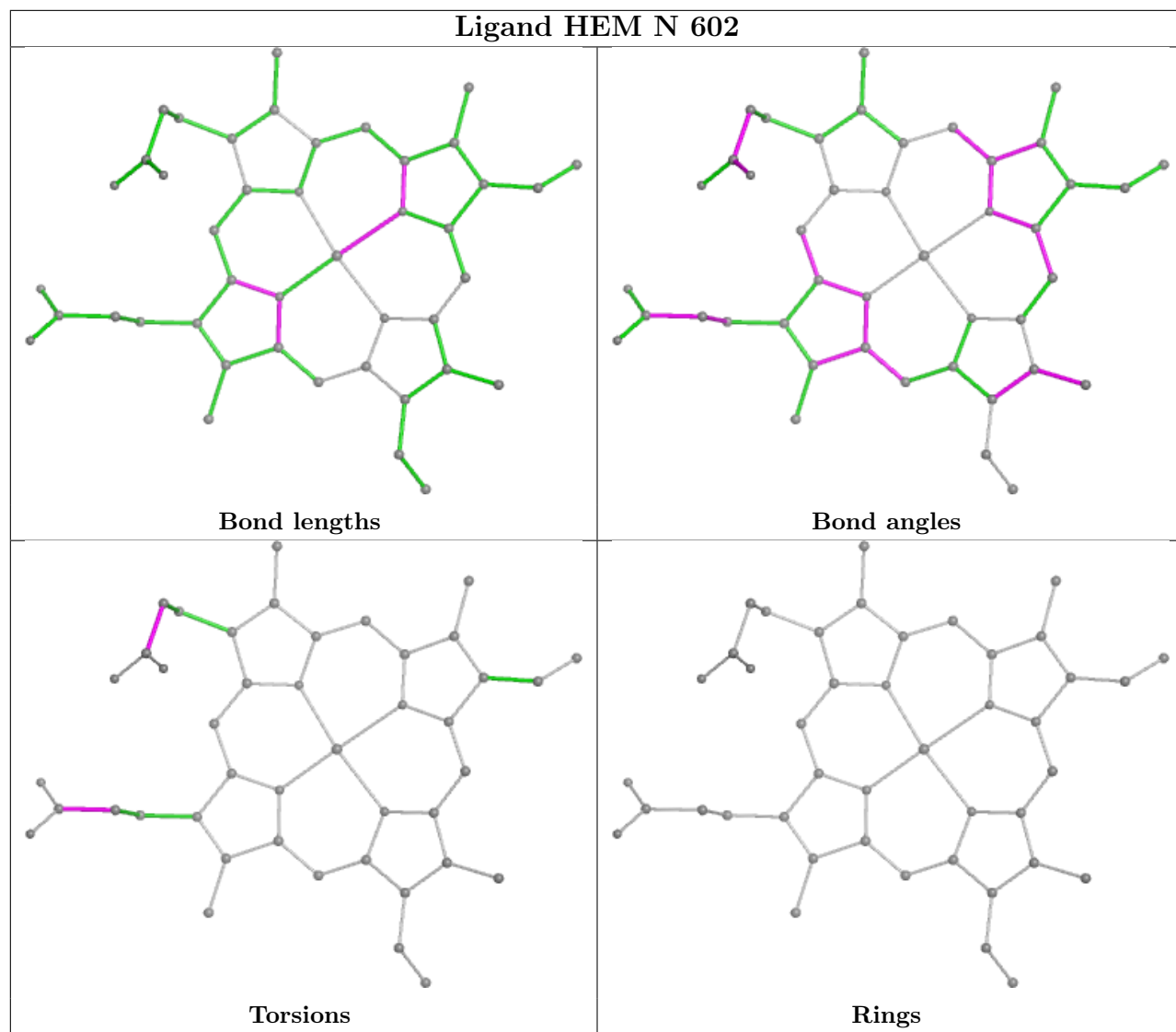


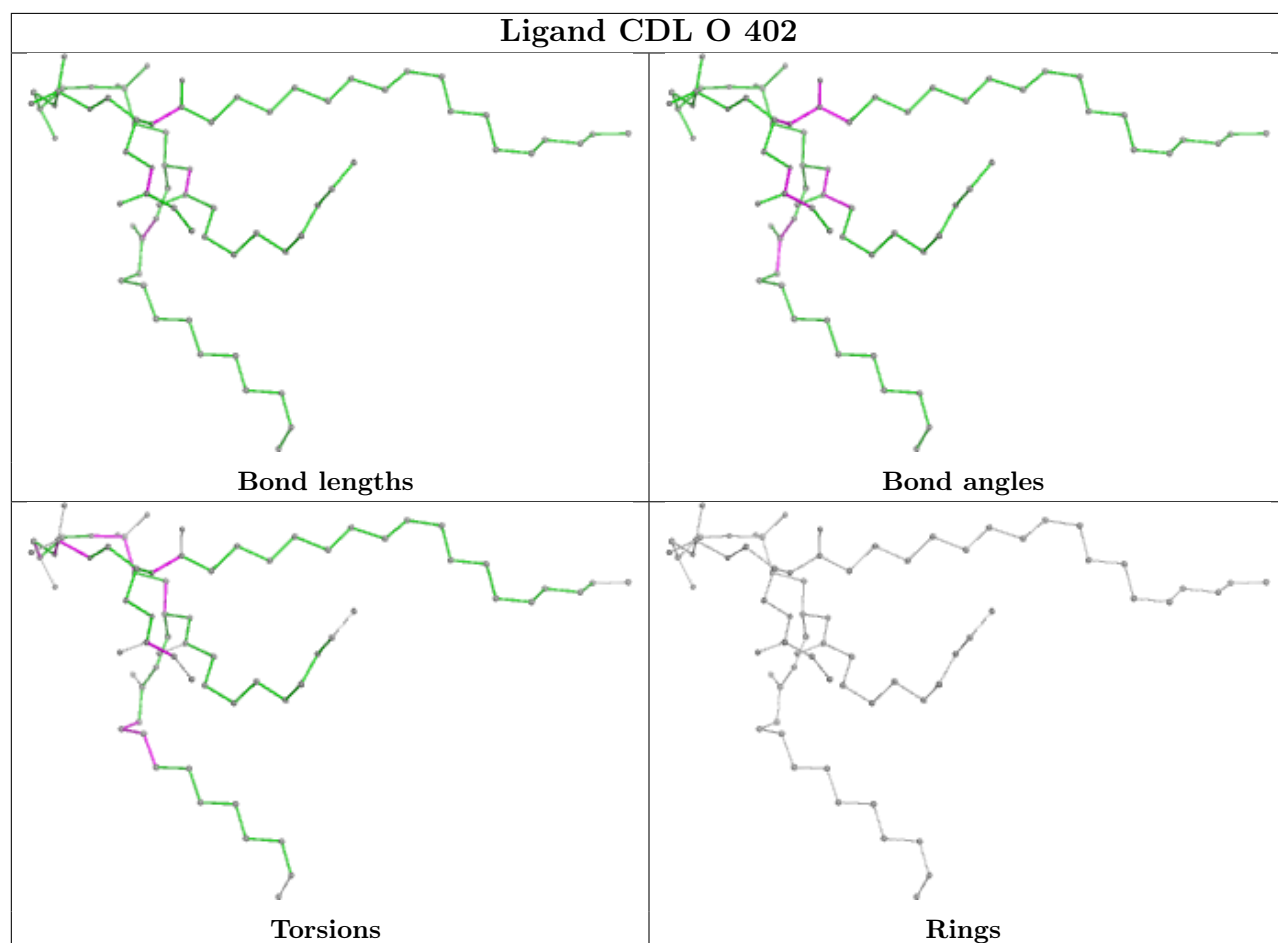
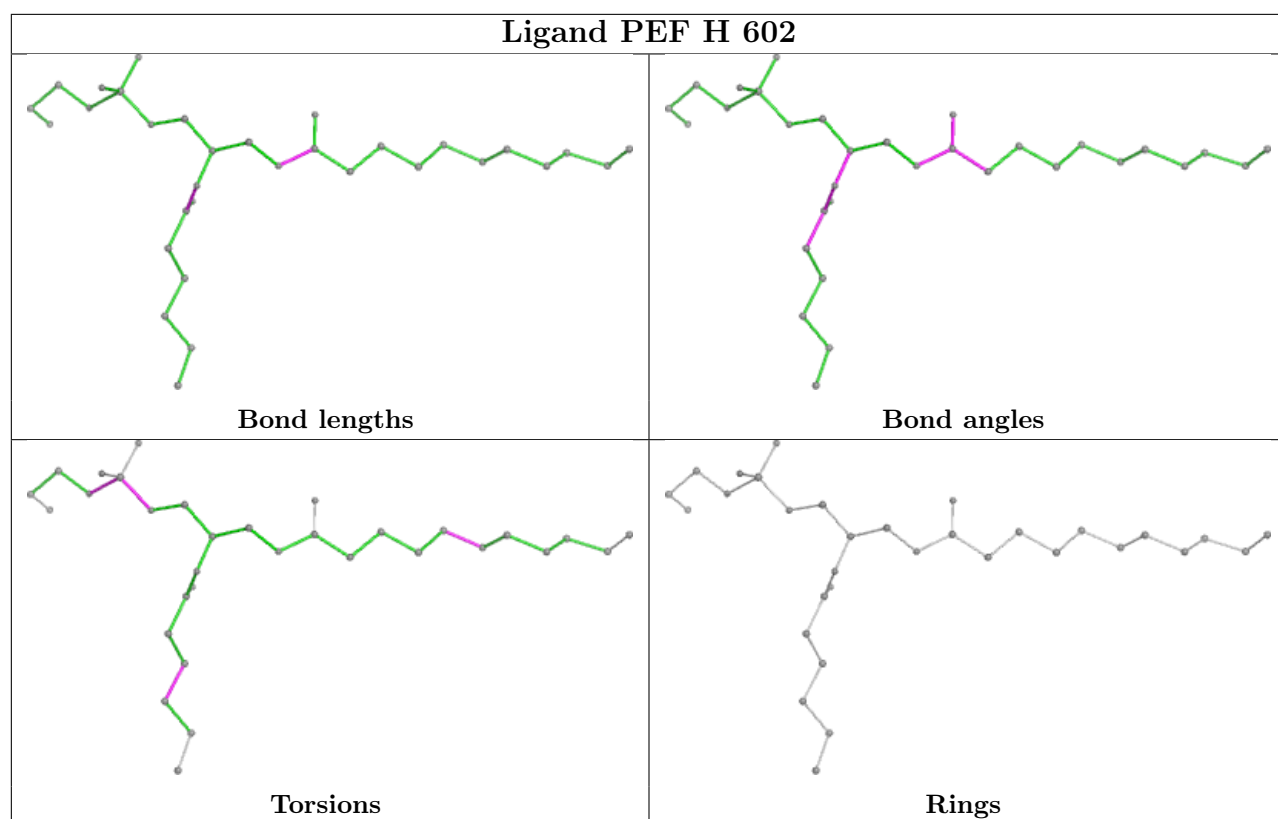


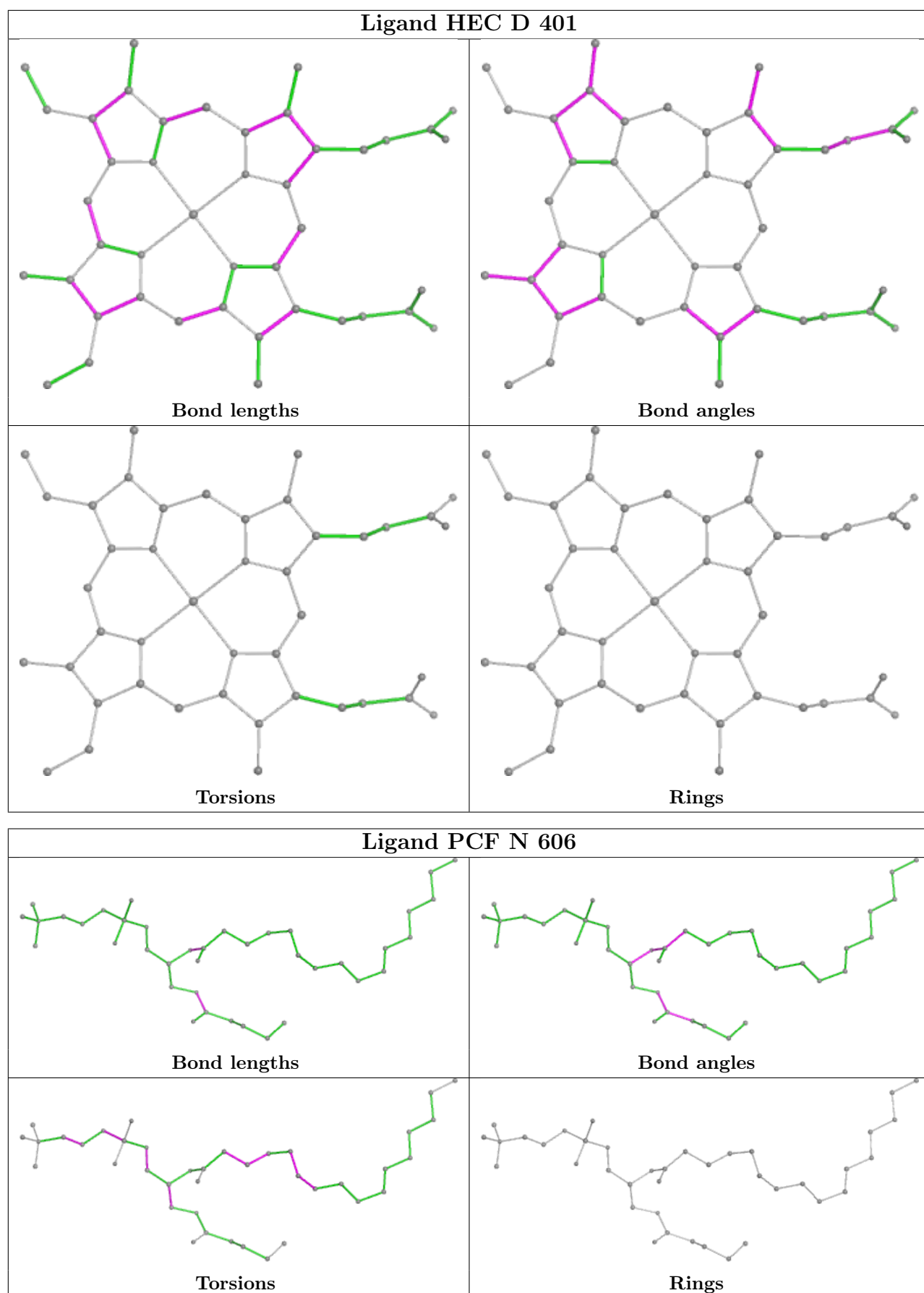


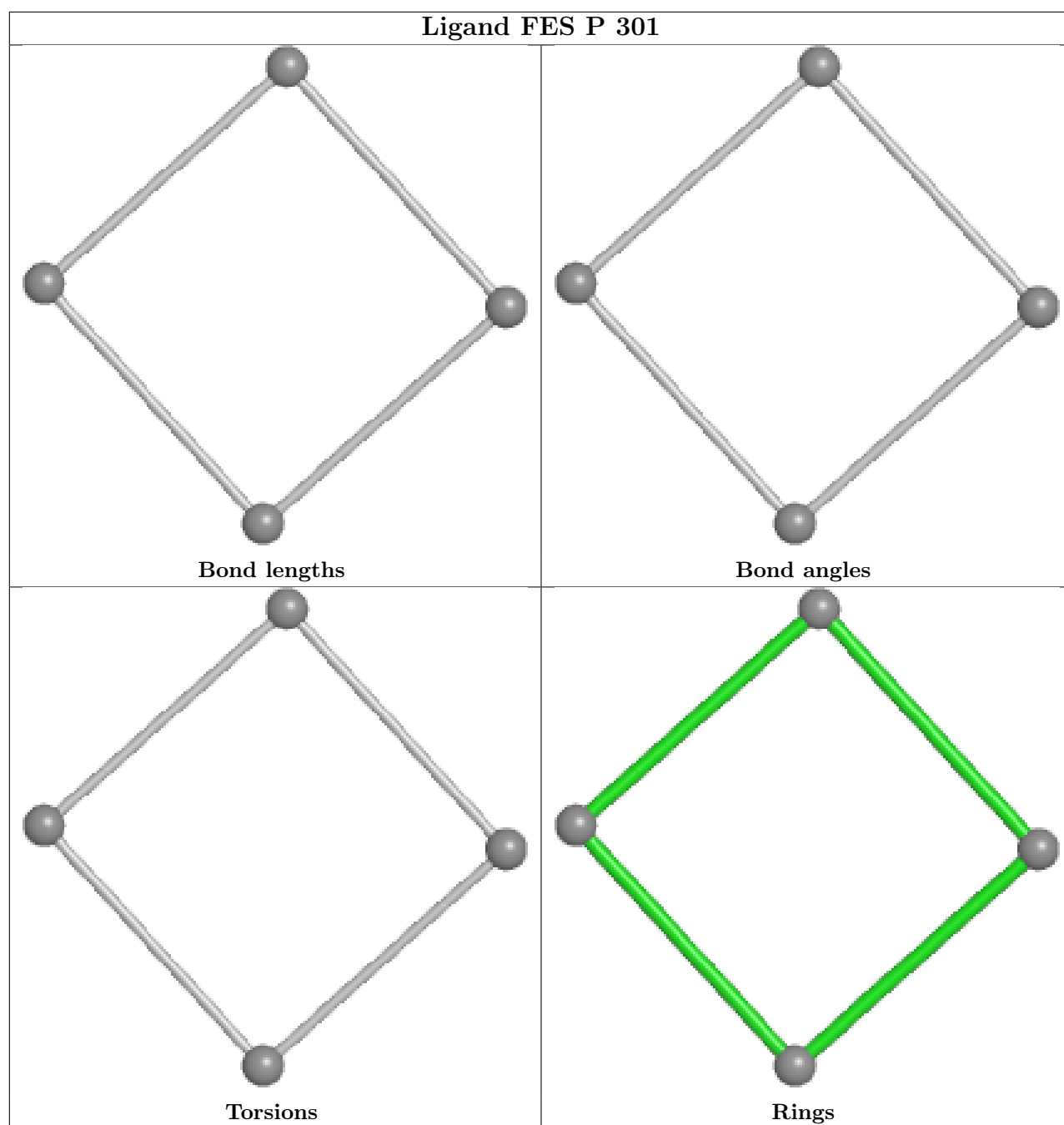


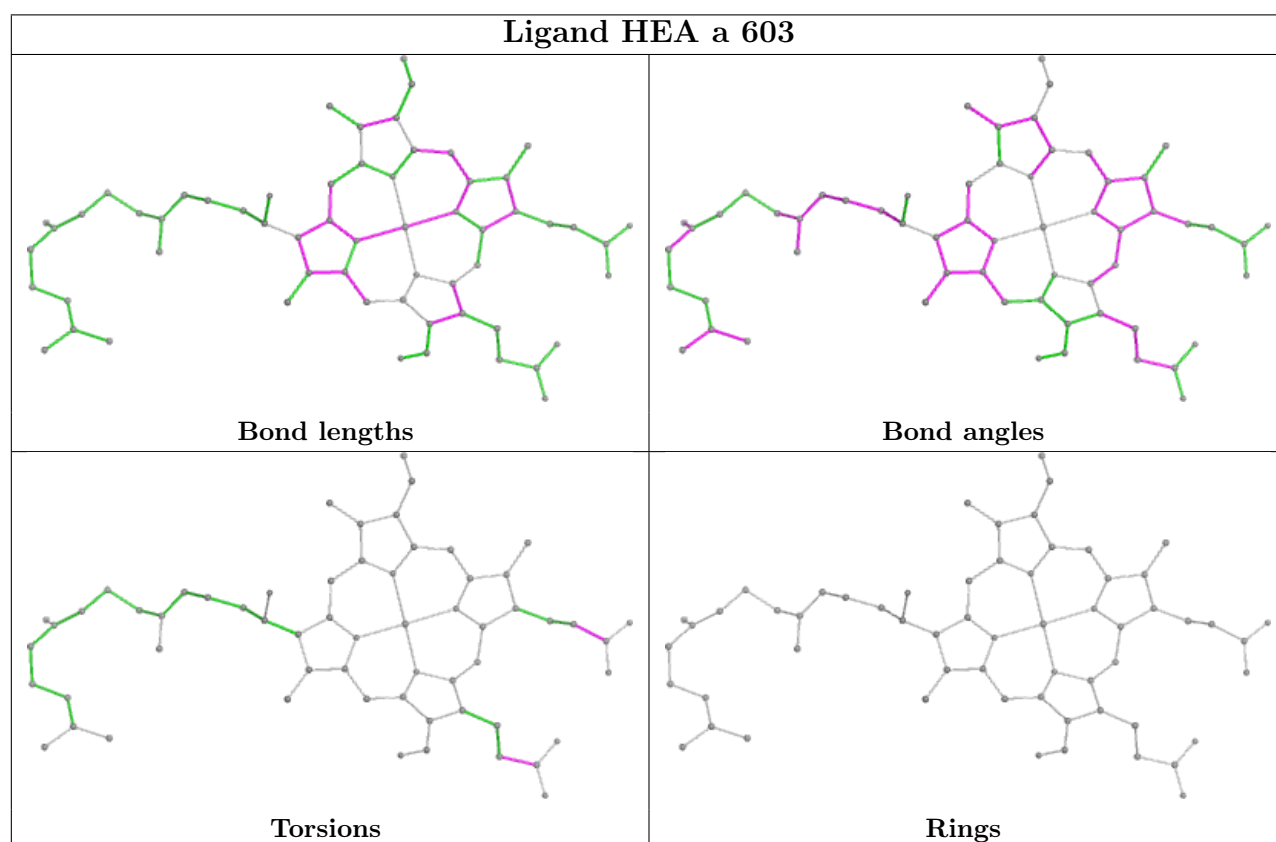
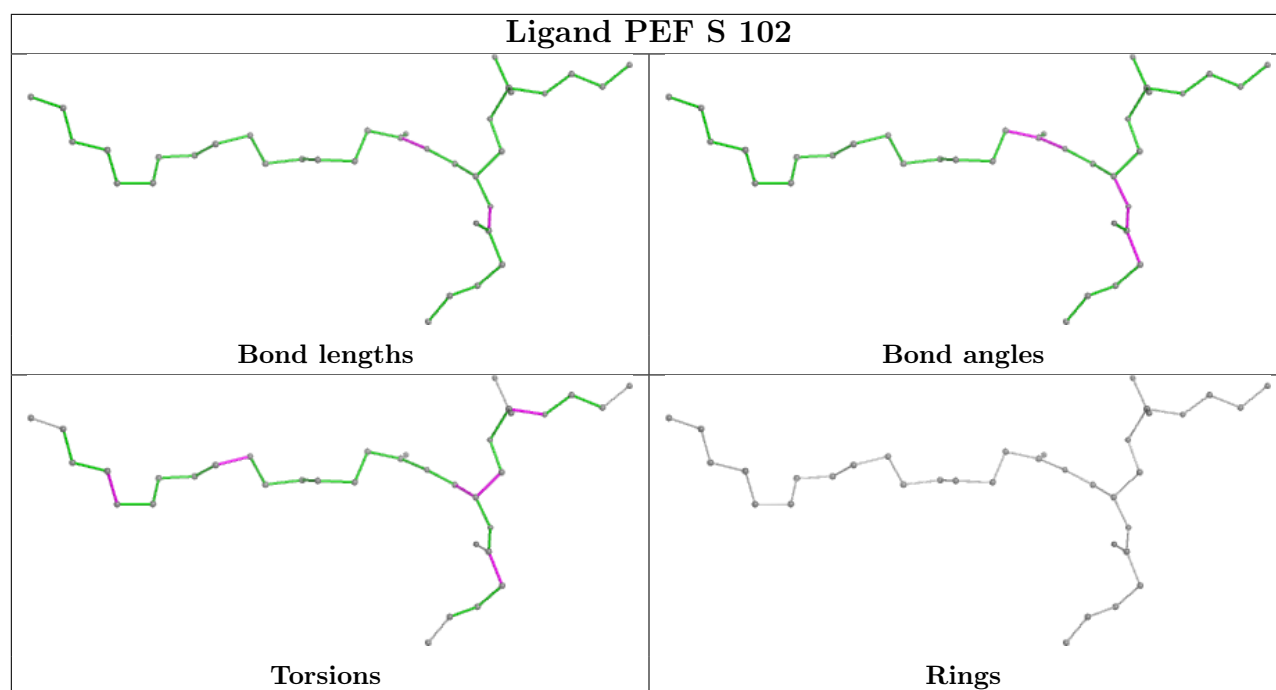


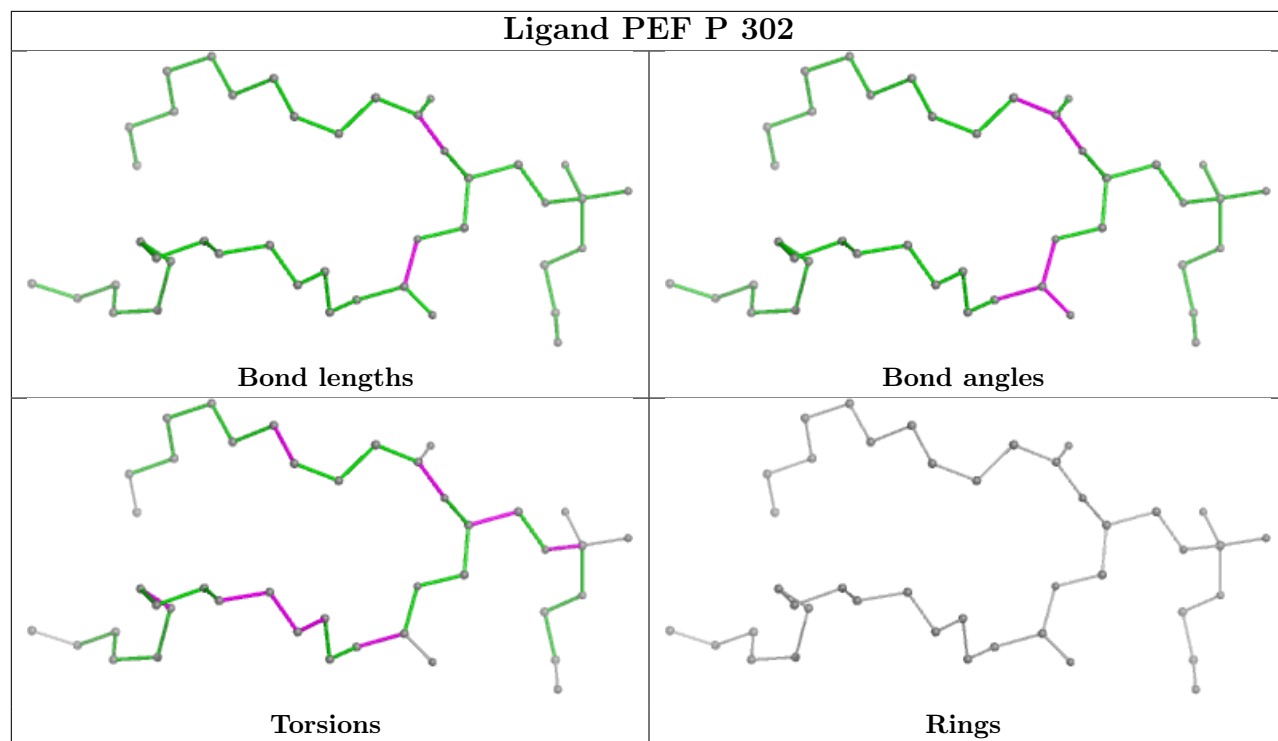


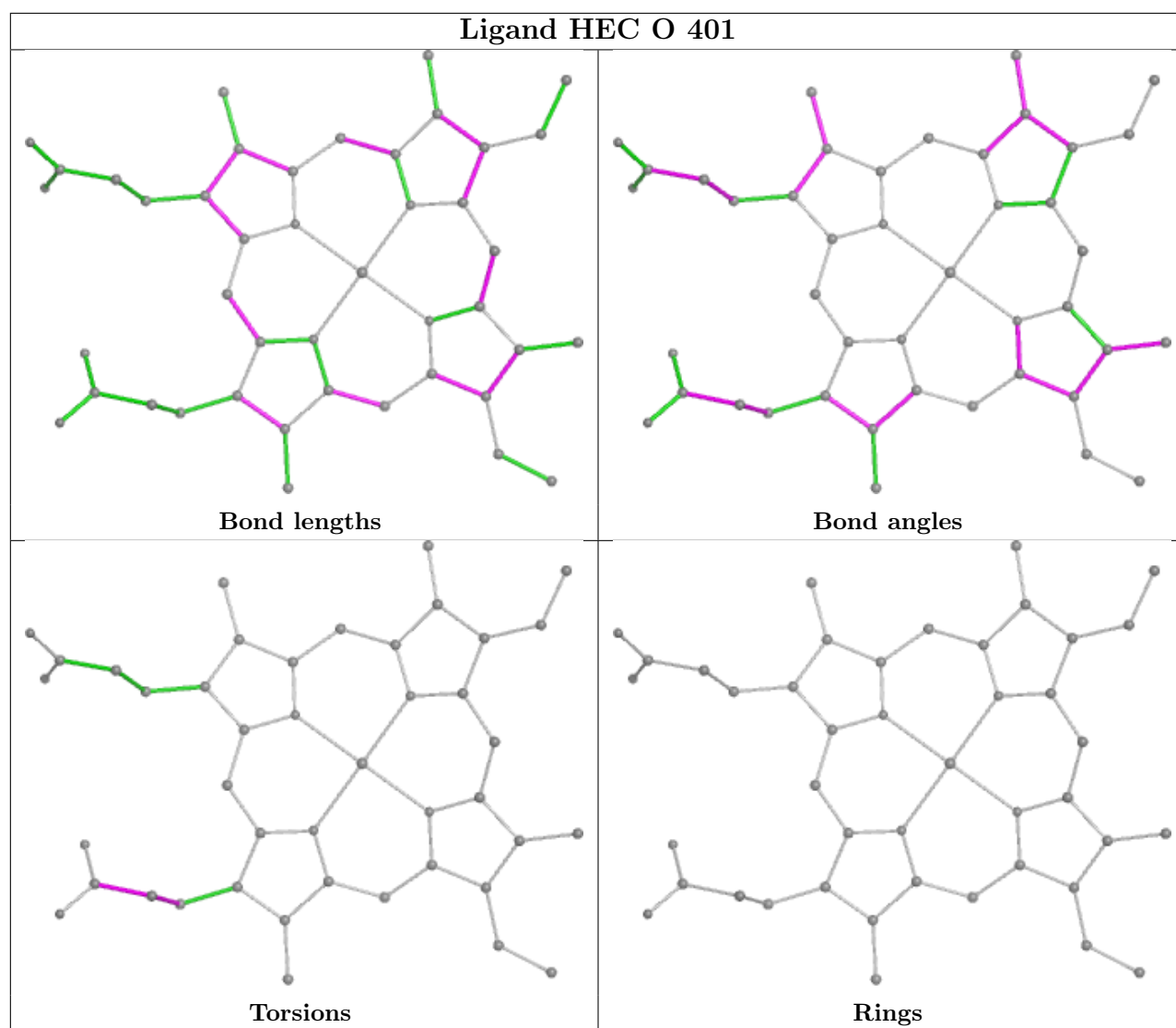












5.7 Other polymers [i](#)

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.