



## wwPDB EM Validation Summary Report ⓘ

Jul 16, 2025 – 01:56 AM JST

PDB ID : 8ZNO / pdb\_00008zno  
EMDB ID : EMD-60275  
Title : Cryo-EM structure of Arachis hypogaea bc1 complex  
Authors : Ye, Y.; Dong, J.Q.; Yang, G.F.  
Deposited on : 2024-05-27  
Resolution : 3.02 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

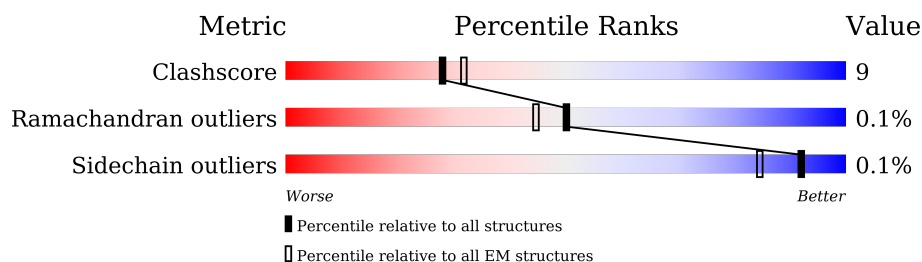
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.02 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)
Clashscore	210492	15764
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	460	86% 14%
1	M	460	77% 23%
2	B	487	78% 22%
2	N	487	82% 18%
3	C	386	84% 15%
3	O	386	79% 20%
4	D	242	80% 19%
4	P	242	81% 19%
5	E	196	67% 33%

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Mol	Chain	Length	Quality of chain
5	Q	196	 65% 34% .
6	F	117	 78% 22%
6	R	117	 71% 26% .
7	G	70	 87% 13%
7	S	70	 84% 16%
8	H	64	 80% 20%
8	T	64	 73% 27%
9	J	60	 82% 18%
9	V	60	 73% 27%
10	K	29	 86% 14%
10	W	29	 97% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	FES	E	301	-	-	X	-
16	FES	Q	301	-	-	X	-

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 34447 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 Mitochondrial-processing peptidase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		
1	M	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		

- Molecule 2 is a protein called Mitochondrial-processing peptidase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		
2	N	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3076	2059	501	502	14		
3	O	385	Total	C	N	O	S	0	0
			3068	2055	500	499	14		

- Molecule 4 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		
4	P	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLN	ASN	conflict	UNP A0A445B1W5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	125	GLU	ASP	conflict	UNP A0A445B1W5
D	186	PRO	ARG	conflict	UNP A0A445B1W5
D	246	SER	ALA	conflict	UNP A0A445B1W5
P	81	GLN	ASN	conflict	UNP A0A445B1W5
P	125	GLU	ASP	conflict	UNP A0A445B1W5
P	186	PRO	ARG	conflict	UNP A0A445B1W5
P	246	SER	ALA	conflict	UNP A0A445B1W5

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		
5	Q	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	117	Total	C	N	O	S	0	0
			986	628	179	174	5		
6	R	117	Total	C	N	O	S	0	0
			986	628	179	174	5		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			573	378	95	98	2		
7	S	70	Total	C	N	O	S	0	0
			573	378	95	98	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	64	Total	C	N	O	S	0	0
			519	330	87	96	6		
8	T	64	Total	C	N	O	S	0	0
			519	330	87	96	6		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			486	312	88	85	1		
9	V	60	Total	C	N	O	S	0	0
			486	312	88	85	1		

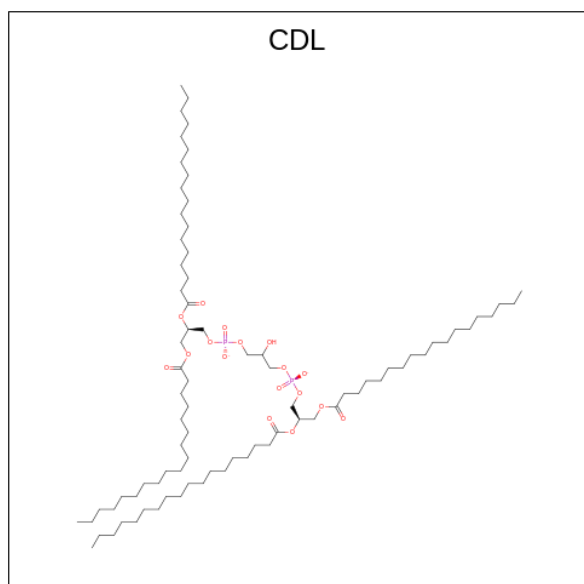
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 6.7 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	29	Total	C	N	O	S	0	0
			218	145	35	37	1		
10	W	29	Total	C	N	O	S	0	0
			218	145	35	37	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Zn	0
			1	1	
11	N	1	Total	Zn	0
			1	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



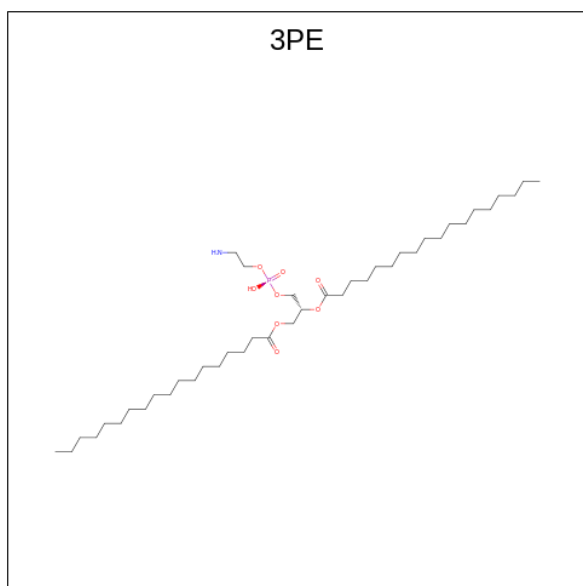
Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	O	P	0
			69	50	17	2	

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Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			30	21	8	1	
12	D	1	Total	C	O	P	0
			64	45	17	2	
12	N	1	Total	C	O	P	0
			70	51	17	2	
12	O	1	Total	C	O	P	0
			81	62	17	2	
12	O	1	Total	C	O	P	0
			58	39	17	2	
12	P	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 13 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
13	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
13	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
13	C	1	Total	C	N	O	P	0
			34	24	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total 36	C 26	N 1	O 8	P 1	0
13	E	1	Total 30	C 20	N 1	O 8	P 1	0
13	G	1	Total 32	C 22	N 1	O 8	P 1	0
13	O	1	Total 38	C 28	N 1	O 8	P 1	0
13	P	1	Total 39	C 29	N 1	O 8	P 1	0
13	R	1	Total 48	C 38	N 1	O 8	P 1	0
13	S	1	Total 33	C 23	N 1	O 8	P 1	0

- # HEM

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



- [illegible]

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

- 
- Diagram illustrating a square planar complex with two iron (Fe) and two sulfur (S) atoms. The atoms are labeled as S1, FE2, FE1, and S2. The bonds are colored: S1-Fe2 is yellow, Fe2-S2 is purple, S2-Fe1 is yellow, and Fe1-S1 is purple.

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

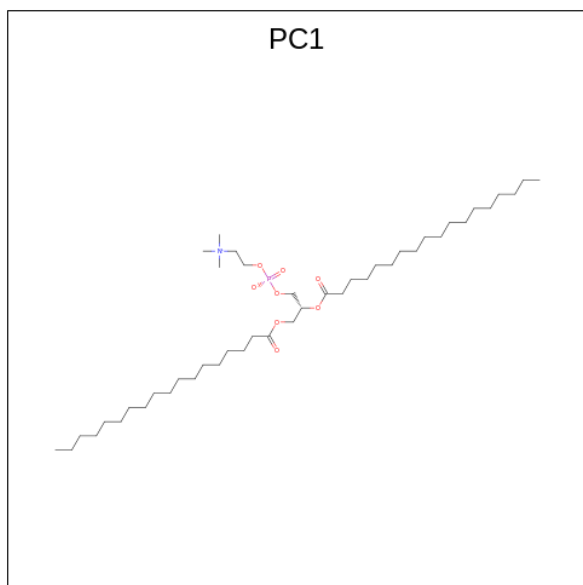


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PDB  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			AltConf
16	Q	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).

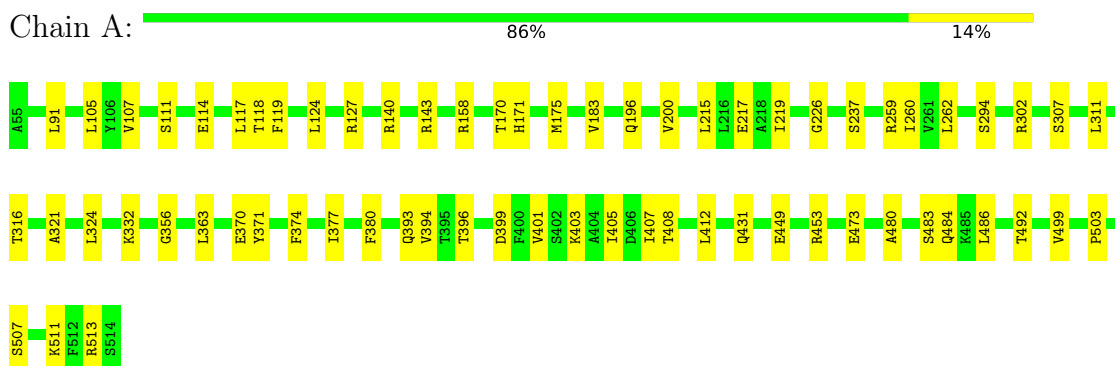


Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			25	17	1	6	1	

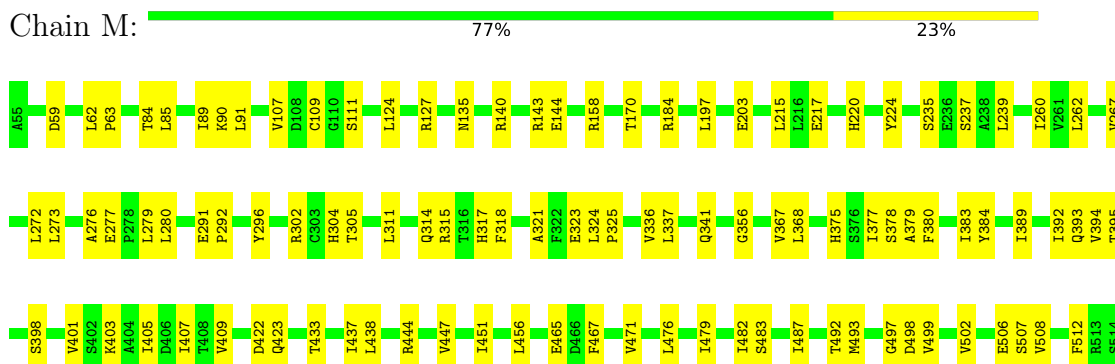
### 3 Residue-property plots

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: Mitochondrial-processing peptidase subunit alpha



- Molecule 1: Mitochondrial-processing peptidase subunit alpha



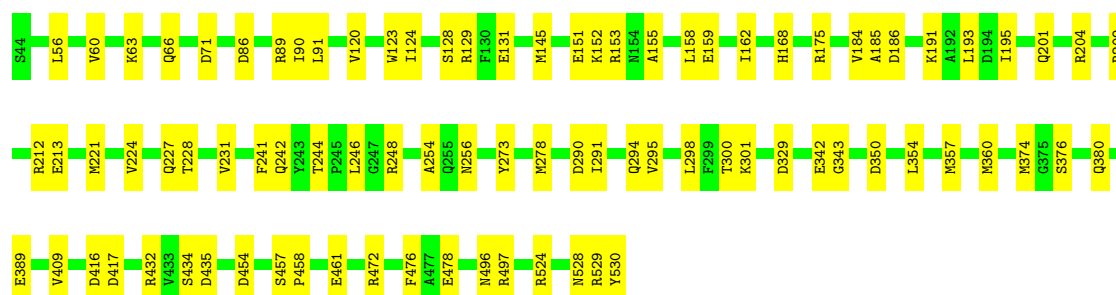
- Molecule 2: Mitochondrial-processing peptidase subunit beta





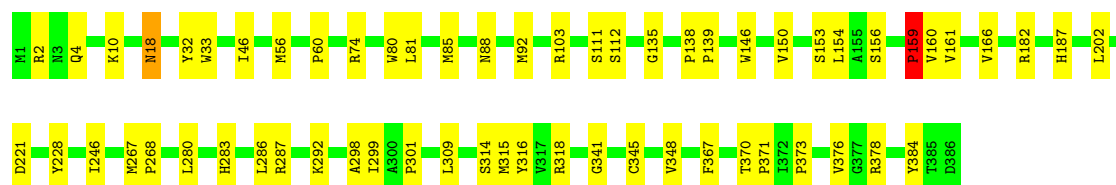
• Molecule 2: Mitochondrial-processing peptidase subunit beta

Chain N: 82% 18%



• Molecule 3: Cytochrome b

Chain C: 84% 15%



• Molecule 3: Cytochrome b

Chain O: 79% 20%

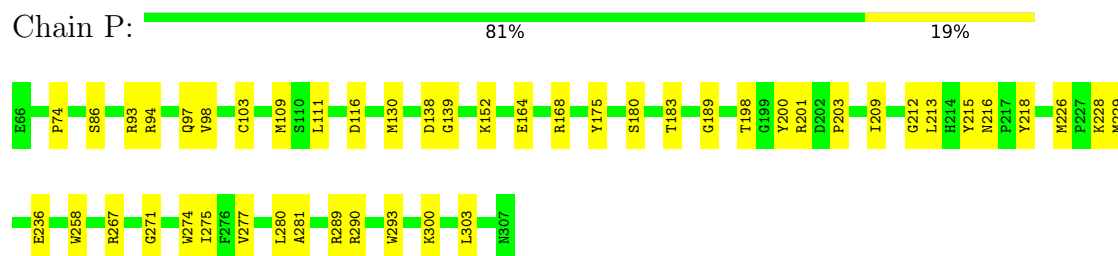


• Molecule 4: Cytochrome c domain-containing protein

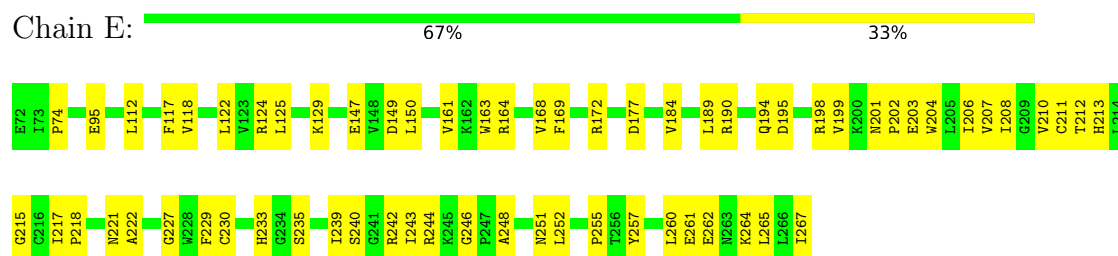
Chain D: 80% 19%



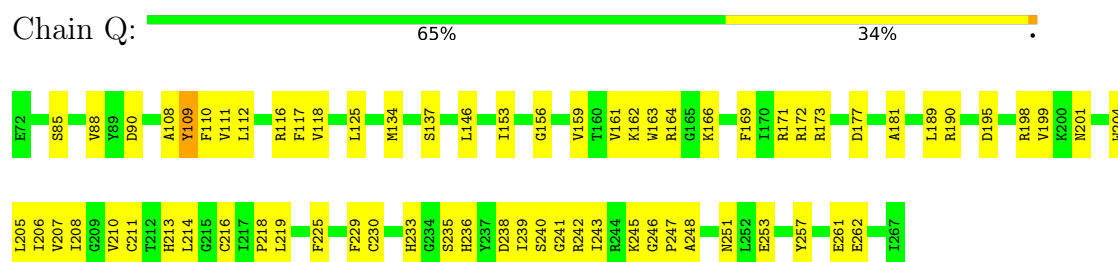
- Molecule 4: Cytochrome c domain-containing protein



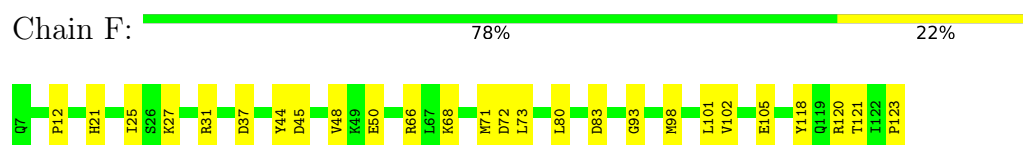
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



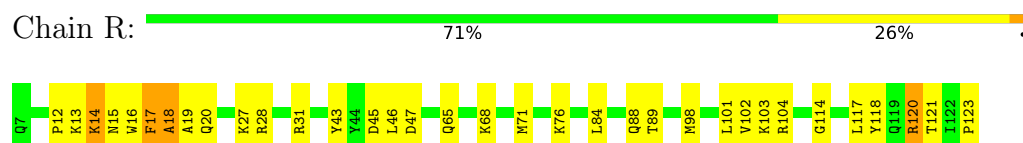
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7

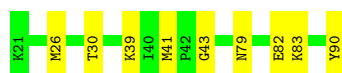


- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 7: Cytochrome b-c1 complex subunit 8





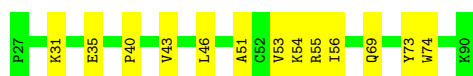
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain S: 84% 16%



- Molecule 8: Cytochrome b-c1 complex subunit 6

Chain H: 80% 20%



- Molecule 8: Cytochrome b-c1 complex subunit 6

Chain T: 73% 27%



- Molecule 9: Complex III subunit 9

Chain J: 82% 18%



- Molecule 9: Complex III subunit 9

Chain V: 73% 27%



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein

Chain K: 86% 14%



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein

Chain W: 97%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53892	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 ( $e^-/\text{\AA}^2$ )	48.42	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (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: HEC, PC1, ZN, 3PE, CDL, HEM, FES

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	0.16	0/3574	0.37	0/4860
1	M	0.17	0/3574	0.41	0/4860
2	B	0.20	0/3933	0.45	0/5332
2	N	0.21	0/3933	0.46	0/5332
3	C	0.26	0/3194	0.47	0/4379
3	O	0.26	0/3186	0.49	0/4368
4	D	0.22	0/1946	0.41	0/2644
4	P	0.22	0/1946	0.44	0/2644
5	E	0.17	0/1576	0.47	0/2144
5	Q	0.49	3/1576 (0.2%)	0.53	0/2144
6	F	0.23	0/1008	0.42	0/1352
6	R	0.66	2/1008 (0.2%)	0.58	1/1352 (0.1%)
7	G	0.19	0/591	0.44	0/799
7	S	0.21	0/591	0.57	0/799
8	H	0.17	0/529	0.40	0/705
8	T	0.27	0/529	0.65	0/705
9	J	0.18	0/496	0.46	0/666
9	V	0.19	0/496	0.47	0/666
10	K	0.13	0/226	0.28	0/310
10	W	0.13	0/226	0.28	0/310
All	All	0.25	5/34138 (0.0%)	0.46	1/46371 (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
3	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	108	ALA	C-O	-7.64	1.14	1.24
5	Q	108	ALA	CA-C	-5.90	1.44	1.52
6	R	17	PHE	N-CA	-5.18	1.41	1.46
6	R	120	ARG	C-O	-5.17	1.17	1.23
5	Q	111	VAL	C-O	-5.04	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	17	PHE	N-CA-C	-9.23	96.73	111.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	159	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3495	48	0
1	M	3502	0	3495	64	0
2	B	3855	0	3817	77	0
2	N	3855	0	3817	64	0
3	C	3076	0	3058	53	0
3	O	3068	0	3054	59	0
4	D	1893	0	1827	43	0
4	P	1893	0	1827	44	0
5	E	1536	0	1539	50	0
5	Q	1536	0	1539	72	0
6	F	986	0	997	18	0
6	R	986	0	997	43	0
7	G	573	0	585	8	0
7	S	573	0	585	14	0
8	H	519	0	517	9	0
8	T	519	0	517	13	0
9	J	486	0	481	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	486	0	481	14	0
10	K	218	0	212	3	0
10	W	218	0	212	1	0
11	B	1	0	0	0	0
11	N	1	0	0	0	0
12	B	69	0	85	1	0
12	C	30	0	33	14	0
12	D	64	0	72	2	0
12	N	70	0	87	10	0
12	O	139	0	172	7	0
12	P	63	0	70	2	0
13	C	219	0	288	7	0
13	E	30	0	34	1	0
13	G	32	0	38	0	0
13	O	38	0	50	2	0
13	P	39	0	52	1	0
13	R	48	0	73	3	0
13	S	33	0	40	0	0
14	C	86	0	60	5	0
14	O	86	0	60	5	0
15	D	43	0	32	5	0
15	P	43	0	32	4	0
16	E	4	0	0	3	0
16	Q	4	0	0	2	0
17	P	25	0	31	3	0
All	All	34447	0	34361	647	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 647 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:13:LYS:O	6:R:14:LYS:HE2	1.37	1.21
4:D:229:MET:SD	15:D:402:HEC:HMC2	1.93	1.09
6:R:17:PHE:O	6:R:19:ALA:N	1.94	1.00
12:C:408:CDL:H112	4:D:289:ARG:NH1	1.81	0.96
4:D:229:MET:SD	15:D:402:HEC:CMC	2.54	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	458/460 (100%)	429 (94%)	29 (6%)	0	100	100
1	M	458/460 (100%)	442 (96%)	16 (4%)	0	100	100
2	B	485/487 (100%)	448 (92%)	37 (8%)	0	100	100
2	N	485/487 (100%)	453 (93%)	32 (7%)	0	100	100
3	C	384/386 (100%)	360 (94%)	22 (6%)	2 (0%)	25	59
3	O	383/386 (99%)	357 (93%)	26 (7%)	0	100	100
4	D	240/242 (99%)	222 (92%)	18 (8%)	0	100	100
4	P	240/242 (99%)	224 (93%)	16 (7%)	0	100	100
5	E	194/196 (99%)	171 (88%)	23 (12%)	0	100	100
5	Q	194/196 (99%)	174 (90%)	19 (10%)	1 (0%)	25	59
6	F	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
6	R	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	14	47
7	G	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
7	S	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
8	H	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
8	T	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
9	J	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
9	V	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
10	K	27/29 (93%)	27 (100%)	0	0	100	100
10	W	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	4181/4222 (99%)	3903 (93%)	274 (7%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	18	ALA

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Mol	Chain	Res	Type
5	Q	109	TYR
3	C	159	PRO
3	C	160	VAL

### 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	384/384 (100%)	384 (100%)	0	100	100
1	M	384/384 (100%)	384 (100%)	0	100	100
2	B	409/409 (100%)	409 (100%)	0	100	100
2	N	409/409 (100%)	409 (100%)	0	100	100
3	C	331/331 (100%)	330 (100%)	1 (0%)	91	96
3	O	330/331 (100%)	330 (100%)	0	100	100
4	D	197/197 (100%)	196 (100%)	1 (0%)	86	94
4	P	197/197 (100%)	197 (100%)	0	100	100
5	E	169/169 (100%)	169 (100%)	0	100	100
5	Q	169/169 (100%)	168 (99%)	1 (1%)	84	92
6	F	104/104 (100%)	104 (100%)	0	100	100
6	R	104/104 (100%)	103 (99%)	1 (1%)	73	88
7	G	63/63 (100%)	63 (100%)	0	100	100
7	S	63/63 (100%)	63 (100%)	0	100	100
8	H	58/58 (100%)	58 (100%)	0	100	100
8	T	58/58 (100%)	58 (100%)	0	100	100
9	J	49/49 (100%)	49 (100%)	0	100	100
9	V	49/49 (100%)	49 (100%)	0	100	100
10	K	19/19 (100%)	19 (100%)	0	100	100
10	W	19/19 (100%)	19 (100%)	0	100	100
All	All	3565/3566 (100%)	3561 (100%)	4 (0%)	92	97

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

Mol	Chain	Res	Type
3	C	18	ASN
4	D	229	MET
5	Q	109	TYR
6	R	14	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	201	GLN
9	V	54	ASN
3	O	4	GLN
5	Q	182	ASN
2	N	397	ASN

### 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 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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
13	3PE	C	401	-	27,27,50	1.13	4 (14%)	30,32,55	1.14	2 (6%)
13	3PE	C	407	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
12	CDL	D	401	-	63,63,99	1.07	8 (12%)	69,75,111	1.22	4 (5%)
13	3PE	C	409	-	35,35,50	1.02	4 (11%)	38,40,55	1.09	2 (5%)
13	3PE	O	401	-	37,37,50	1.00	4 (10%)	40,42,55	1.11	2 (5%)
13	3PE	C	402	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
13	3PE	G	201	-	31,31,50	1.06	4 (12%)	34,36,55	1.14	2 (5%)
14	HEM	C	403	3	41,50,50	1.43	3 (7%)	45,82,82	1.52	12 (26%)
13	3PE	E	302	-	29,29,50	1.10	4 (13%)	32,34,55	1.19	2 (6%)
14	HEM	O	404	3	41,50,50	1.44	4 (9%)	45,82,82	1.58	10 (22%)
12	CDL	P	404	-	62,62,99	1.09	8 (12%)	68,74,111	1.15	4 (5%)
14	HEM	O	403	3	41,50,50	1.48	3 (7%)	45,82,82	1.42	7 (15%)
12	CDL	N	602	-	69,69,99	0.42	0	75,81,111	0.74	3 (4%)
13	3PE	C	405	-	36,36,50	1.00	4 (11%)	39,41,55	1.17	2 (5%)
16	FES	E	301	5	0,4,4	-	-	-	-	-
13	3PE	P	402	-	38,38,50	0.97	3 (7%)	41,43,55	1.11	2 (4%)
13	3PE	S	101	-	32,32,50	1.08	4 (12%)	35,37,55	1.10	2 (5%)
13	3PE	R	201	-	47,47,50	0.89	4 (8%)	50,52,55	1.05	2 (4%)
12	CDL	B	602	-	68,68,99	1.05	8 (11%)	74,80,111	1.16	4 (5%)
12	CDL	O	402	-	80,80,99	0.96	7 (8%)	86,92,111	1.13	4 (4%)
12	CDL	C	408	-	29,29,99	0.55	0	33,34,111	0.97	3 (9%)
17	PC1	P	401	-	24,24,53	0.53	0	29,30,61	0.65	1 (3%)
13	3PE	C	406	-	32,32,50	1.05	4 (12%)	35,37,55	1.16	2 (5%)
15	HEC	D	402	4	32,50,50	2.19	3 (9%)	24,82,82	1.78	5 (20%)
15	HEC	P	403	4	32,50,50	2.24	3 (9%)	24,82,82	1.46	4 (16%)
16	FES	Q	301	5	0,4,4	-	-	-	-	-
12	CDL	O	405	-	57,57,99	1.13	8 (14%)	63,69,111	1.20	4 (6%)
14	HEM	C	404	3	41,50,50	1.44	3 (7%)	45,82,82	1.57	10 (22%)

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
13	3PE	C	401	-	-	13/31/31/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	3PE	C	407	-	-	14/37/37/54	-
12	CDL	D	401	-	-	33/74/74/110	-
13	3PE	C	409	-	-	22/39/39/54	-
13	3PE	O	401	-	-	18/41/41/54	-
13	3PE	C	402	-	-	20/54/54/54	-
13	3PE	G	201	-	-	20/35/35/54	-
14	HEM	C	403	3	-	3/12/54/54	-
13	3PE	E	302	-	-	11/33/33/54	-
14	HEM	O	404	3	-	4/12/54/54	-
12	CDL	P	404	-	-	42/73/73/110	-
14	HEM	O	403	3	-	5/12/54/54	-
12	CDL	N	602	-	-	46/80/80/110	-
13	3PE	C	405	-	-	22/40/40/54	-
16	FES	E	301	5	-	-	0/1/1/1
13	3PE	P	402	-	-	16/42/42/54	-
13	3PE	S	101	-	-	15/36/36/54	-
13	3PE	R	201	-	-	23/51/51/54	-
12	CDL	B	602	-	-	45/79/79/110	-
12	CDL	O	402	-	-	43/91/91/110	-
12	CDL	C	408	-	-	14/31/31/110	-
17	PC1	P	401	-	-	12/25/25/57	-
13	3PE	C	406	-	-	10/36/36/54	-
15	HEC	D	402	4	-	2/10/54/54	-
15	HEC	P	403	4	-	0/10/54/54	-
16	FES	Q	301	5	-	-	0/1/1/1
12	CDL	O	405	-	-	40/68/68/110	-
14	HEM	C	404	3	-	4/12/54/54	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	403	HEC	C2B-C3B	-6.93	1.33	1.40
15	P	403	HEC	C3C-C2C	-6.67	1.33	1.40
15	D	402	HEC	C2B-C3B	-6.60	1.33	1.40
15	D	402	HEC	C3C-C2C	-6.41	1.34	1.40
15	D	402	HEC	C3D-C2D	5.28	1.53	1.37



The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	405	CDL	OA6-CA5-C11	4.38	120.94	111.50
12	D	401	CDL	OA6-CA5-C11	4.36	120.89	111.50
13	C	405	3PE	O21-C21-C22	4.33	120.83	111.50
12	B	602	CDL	OA6-CA5-C11	4.23	120.63	111.50
13	E	302	3PE	O21-C21-C22	4.23	120.61	111.50

There are no chirality outliers.

5 of 497 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	602	CDL	O1-C1-CA2-OA2
12	B	602	CDL	CB2-C1-CA2-OA2
12	B	602	CDL	CA2-C1-CB2-OB2
12	B	602	CDL	CA2-OA2-PA1-OA3
12	B	602	CDL	CA2-OA2-PA1-OA4

There are no ring outliers.

23 monomers are involved in 75 short contacts:

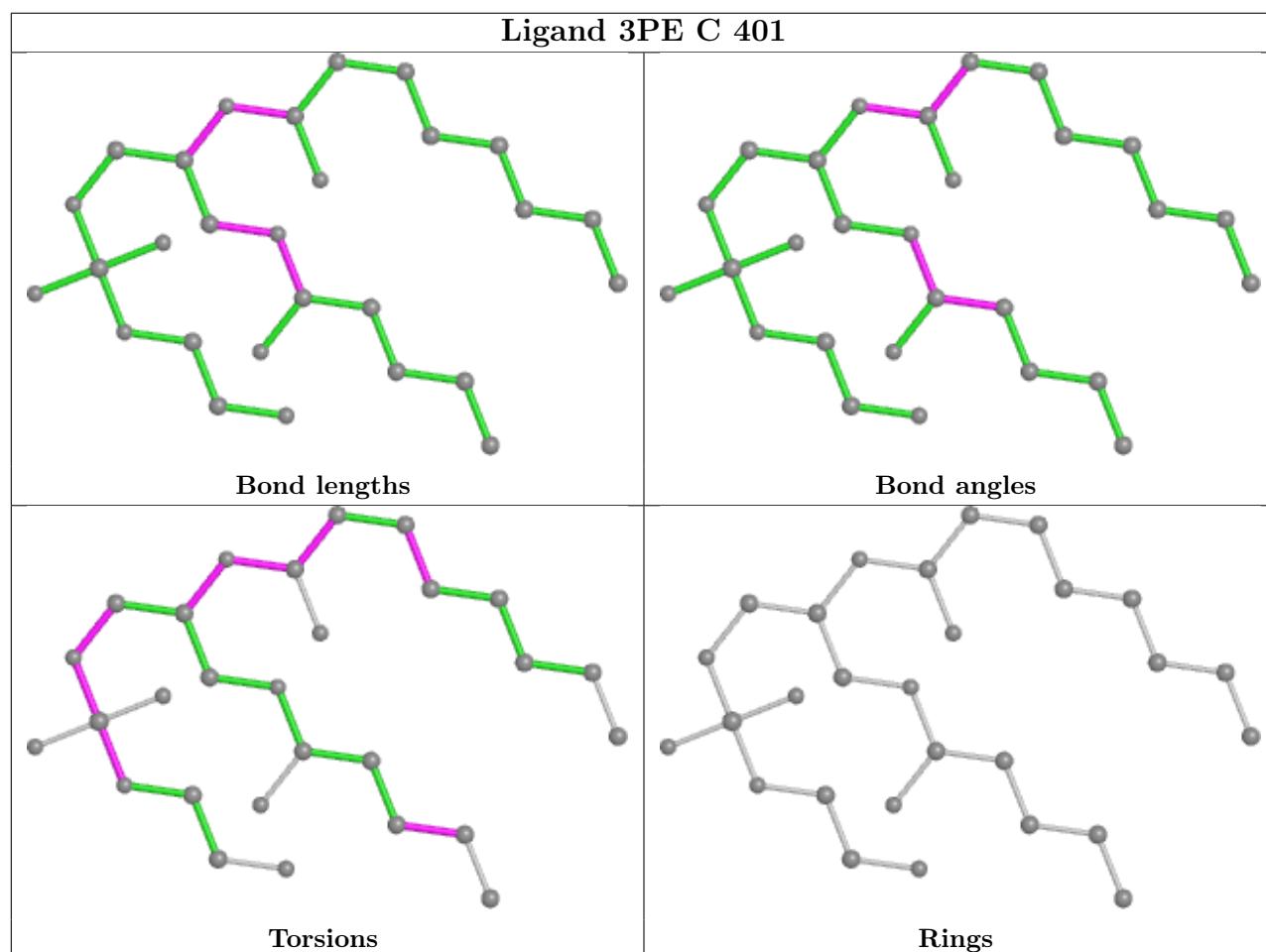
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	401	CDL	2	0
13	O	401	3PE	2	0
13	C	402	3PE	3	0
14	C	403	HEM	2	0
13	E	302	3PE	1	0
14	O	404	HEM	3	0
12	P	404	CDL	2	0
14	O	403	HEM	2	0
12	N	602	CDL	10	0
13	C	405	3PE	3	0
16	E	301	FES	3	0
13	P	402	3PE	1	0
13	R	201	3PE	3	0
12	B	602	CDL	1	0
12	O	402	CDL	4	0
12	C	408	CDL	14	0
17	P	401	PC1	3	0
13	C	406	3PE	1	0
15	D	402	HEC	5	0
15	P	403	HEC	4	0
16	Q	301	FES	2	0

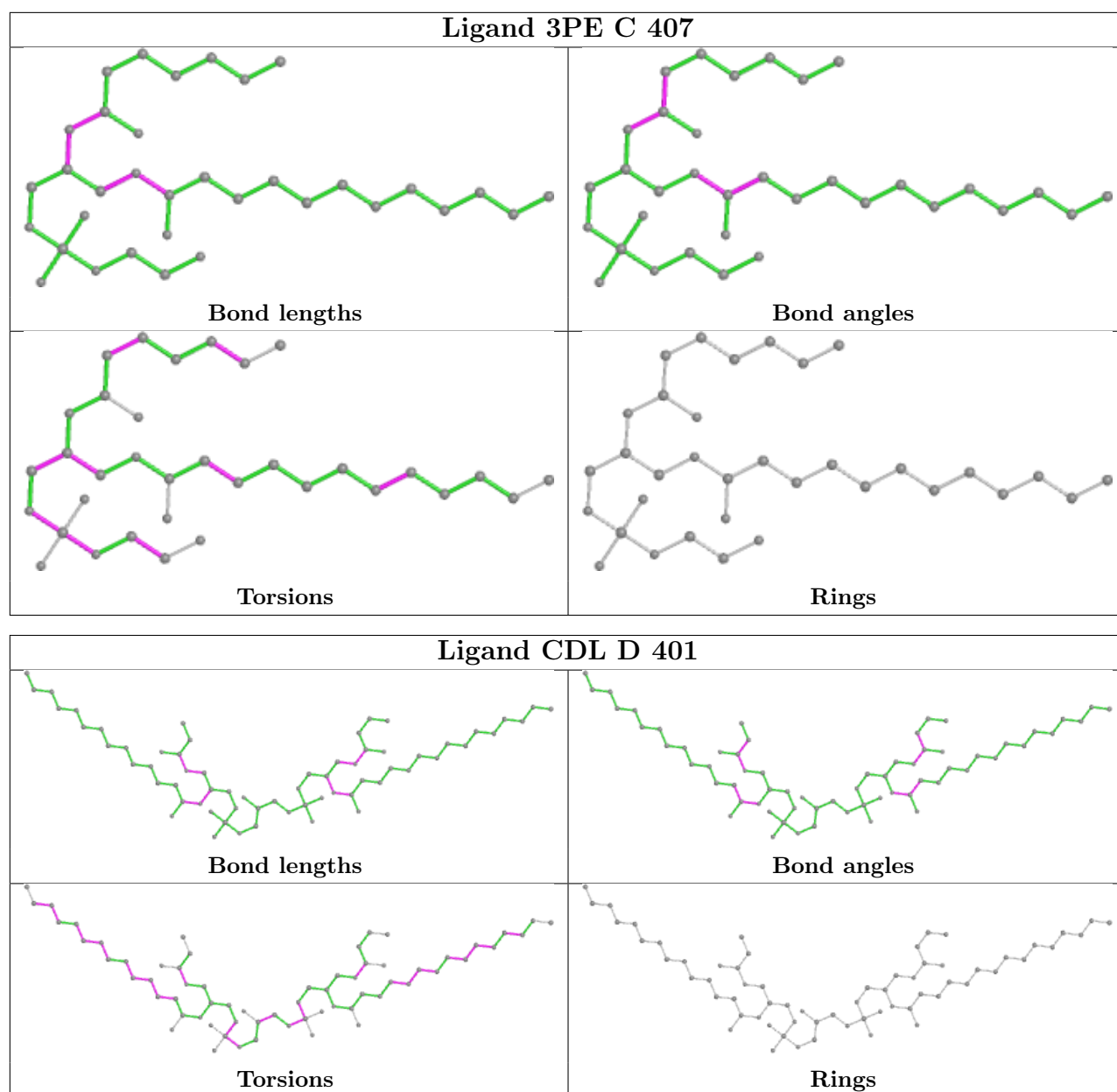
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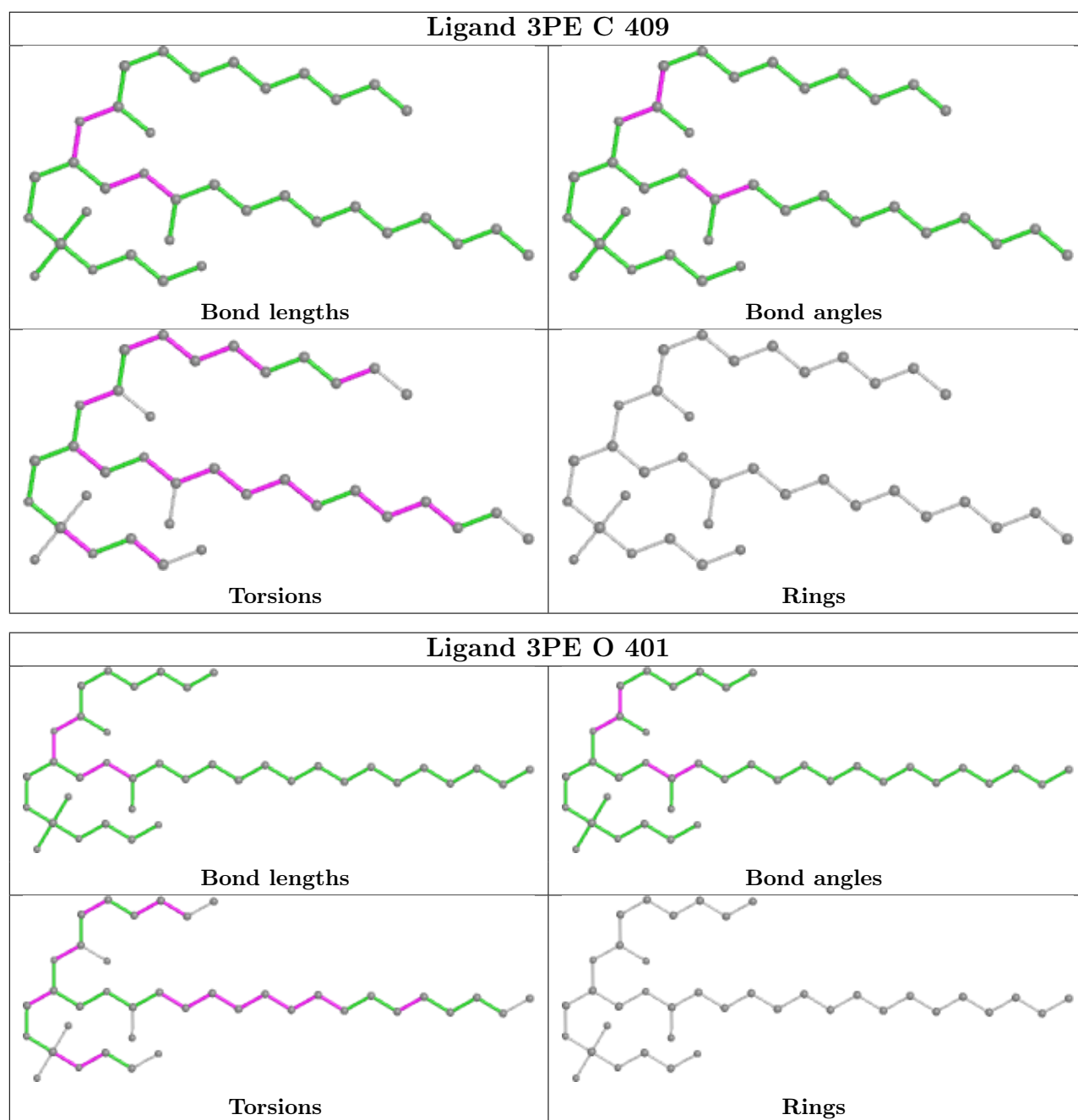
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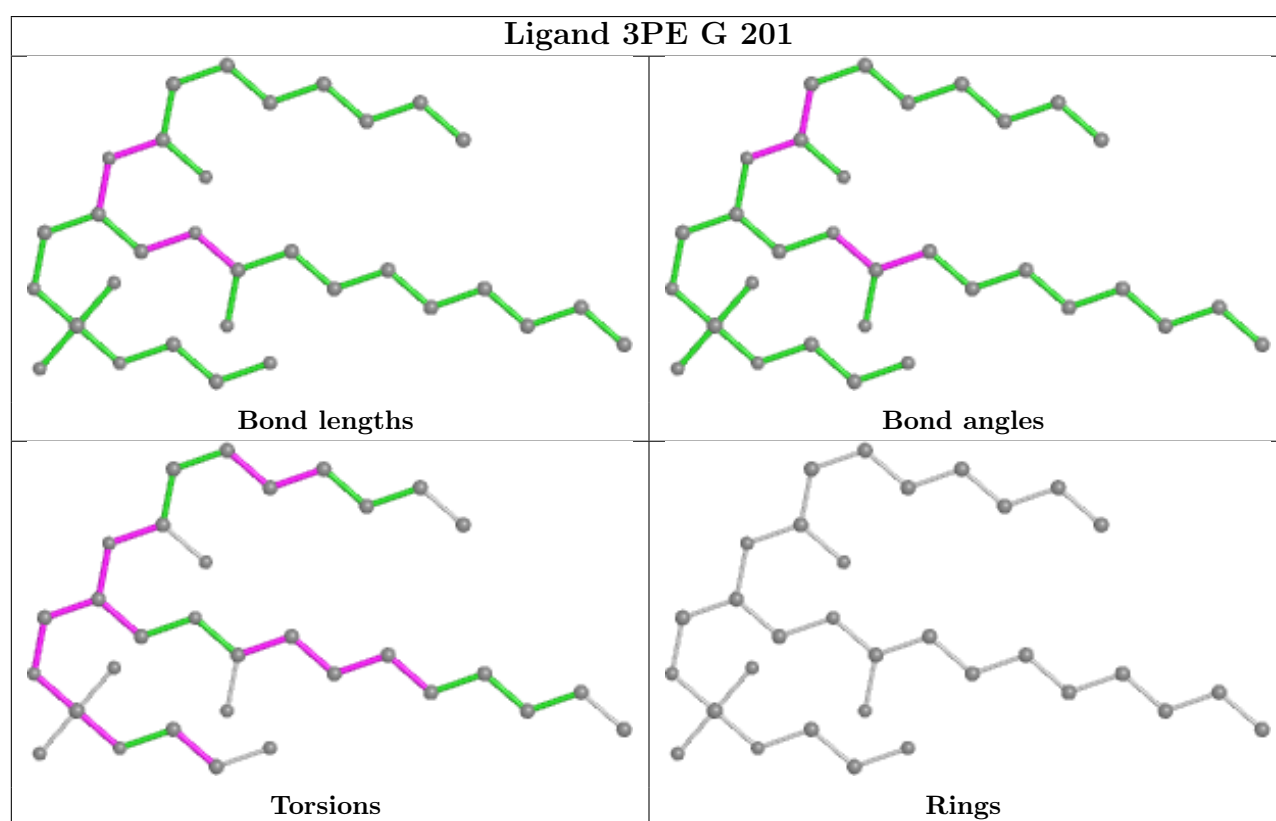
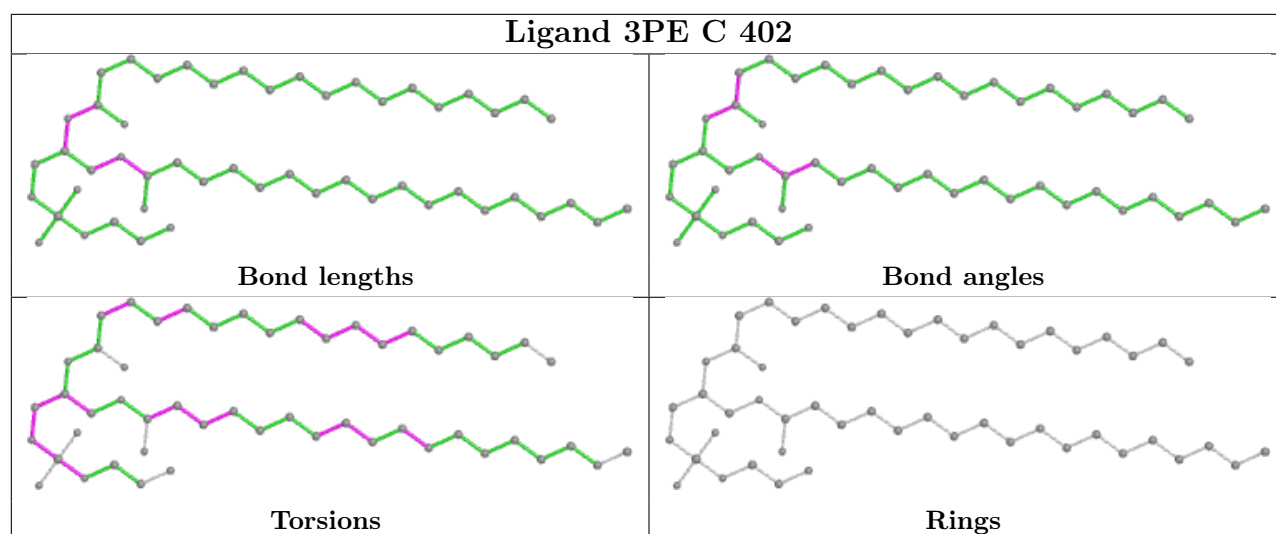
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	O	405	CDL	3	0
14	C	404	HEM	3	0

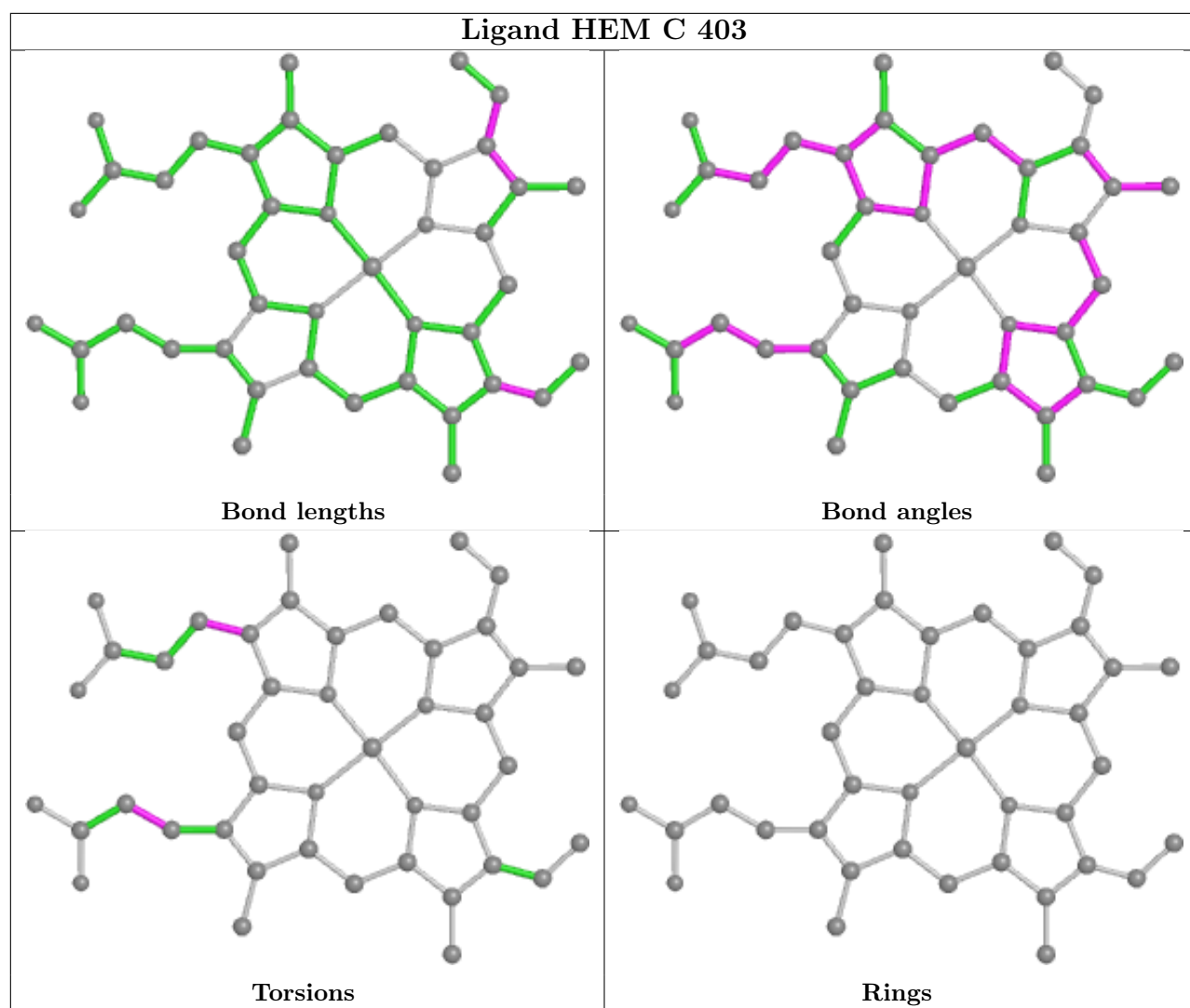
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

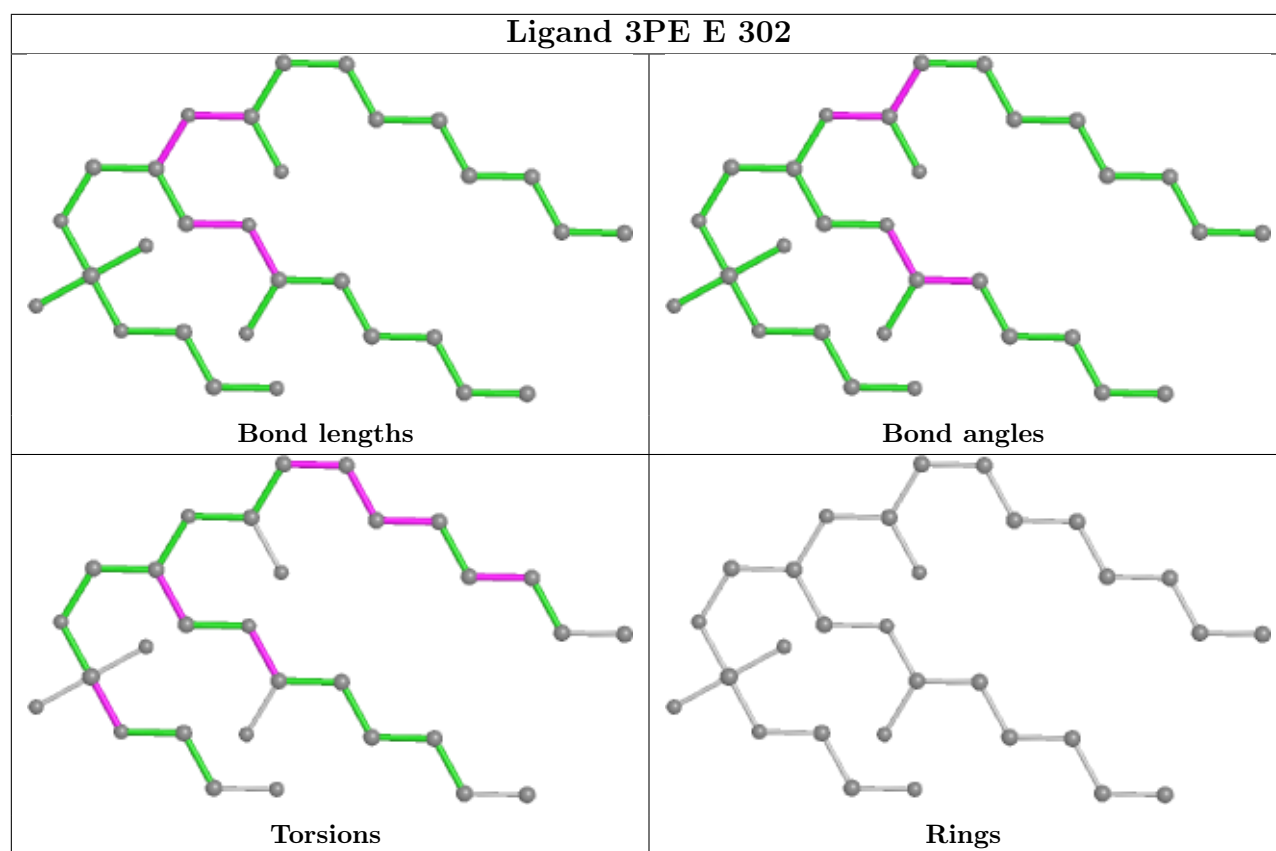


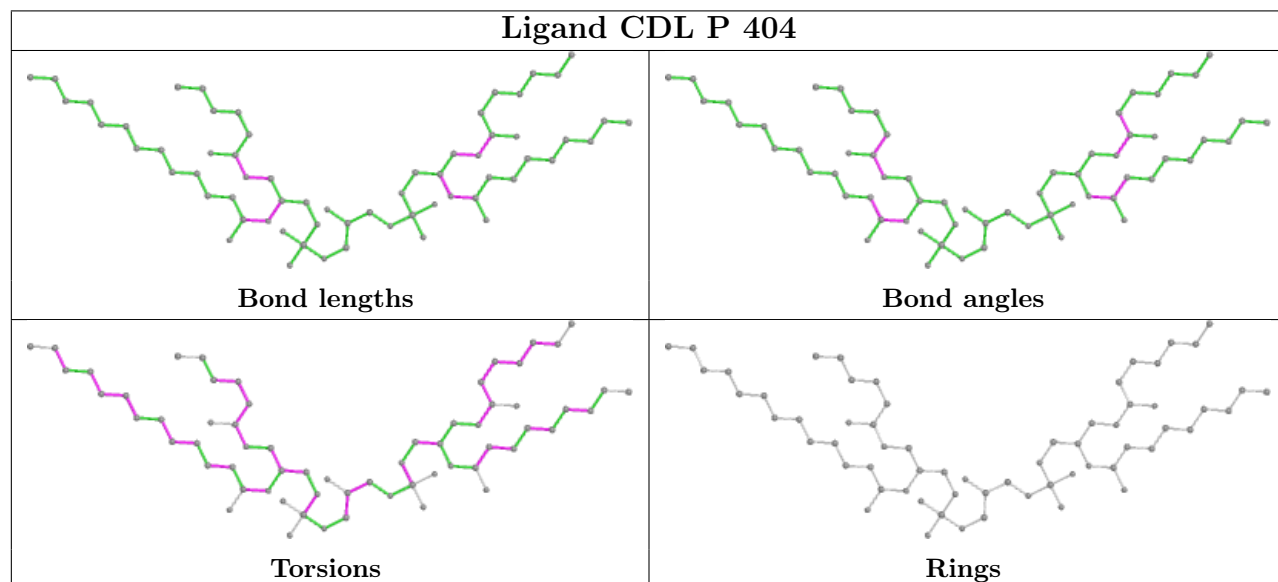
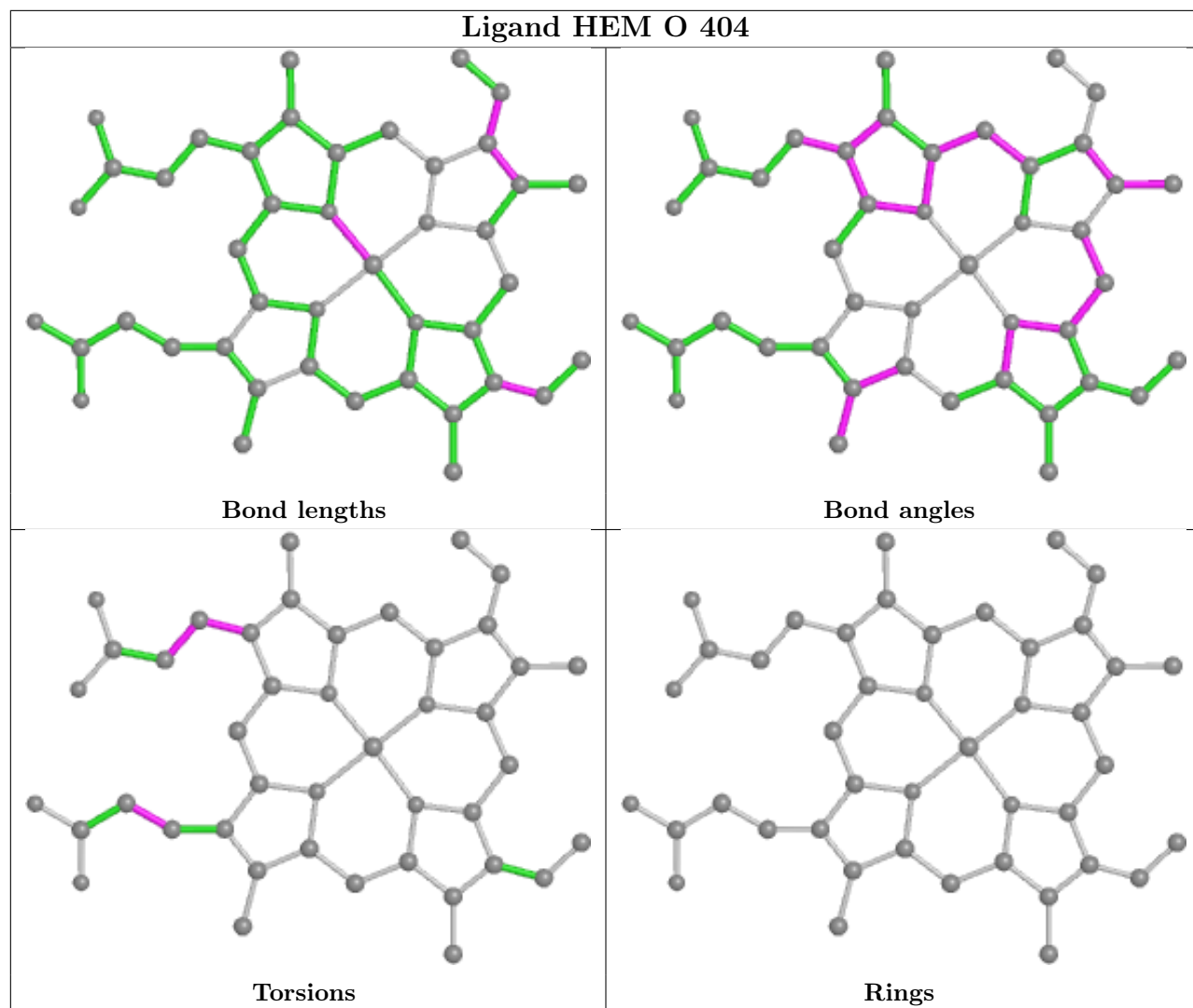




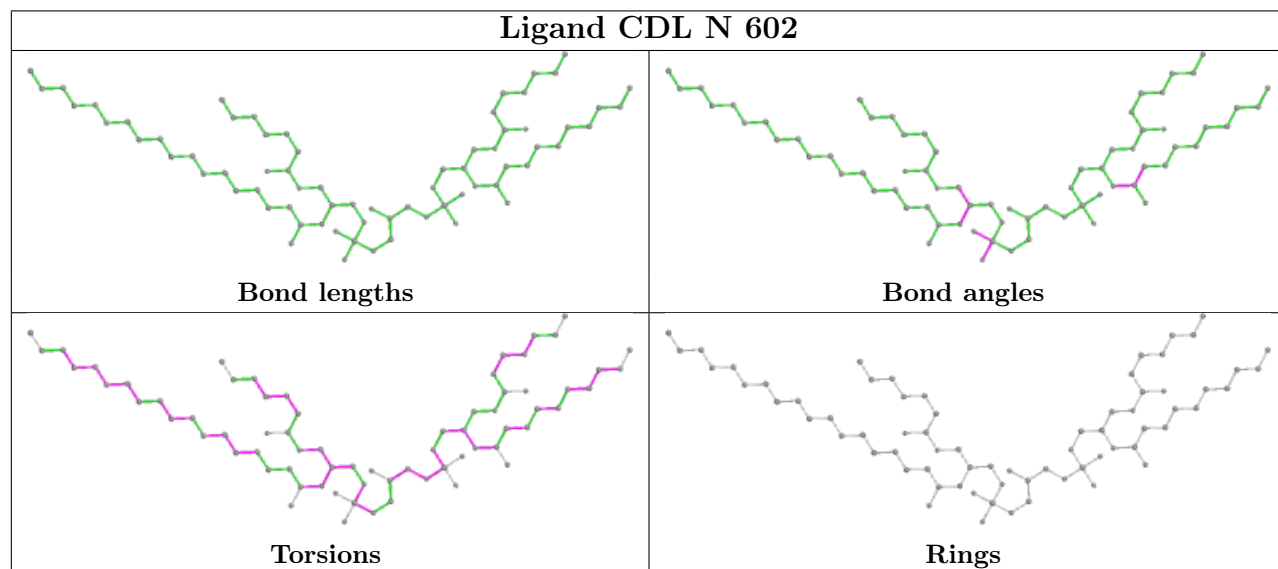
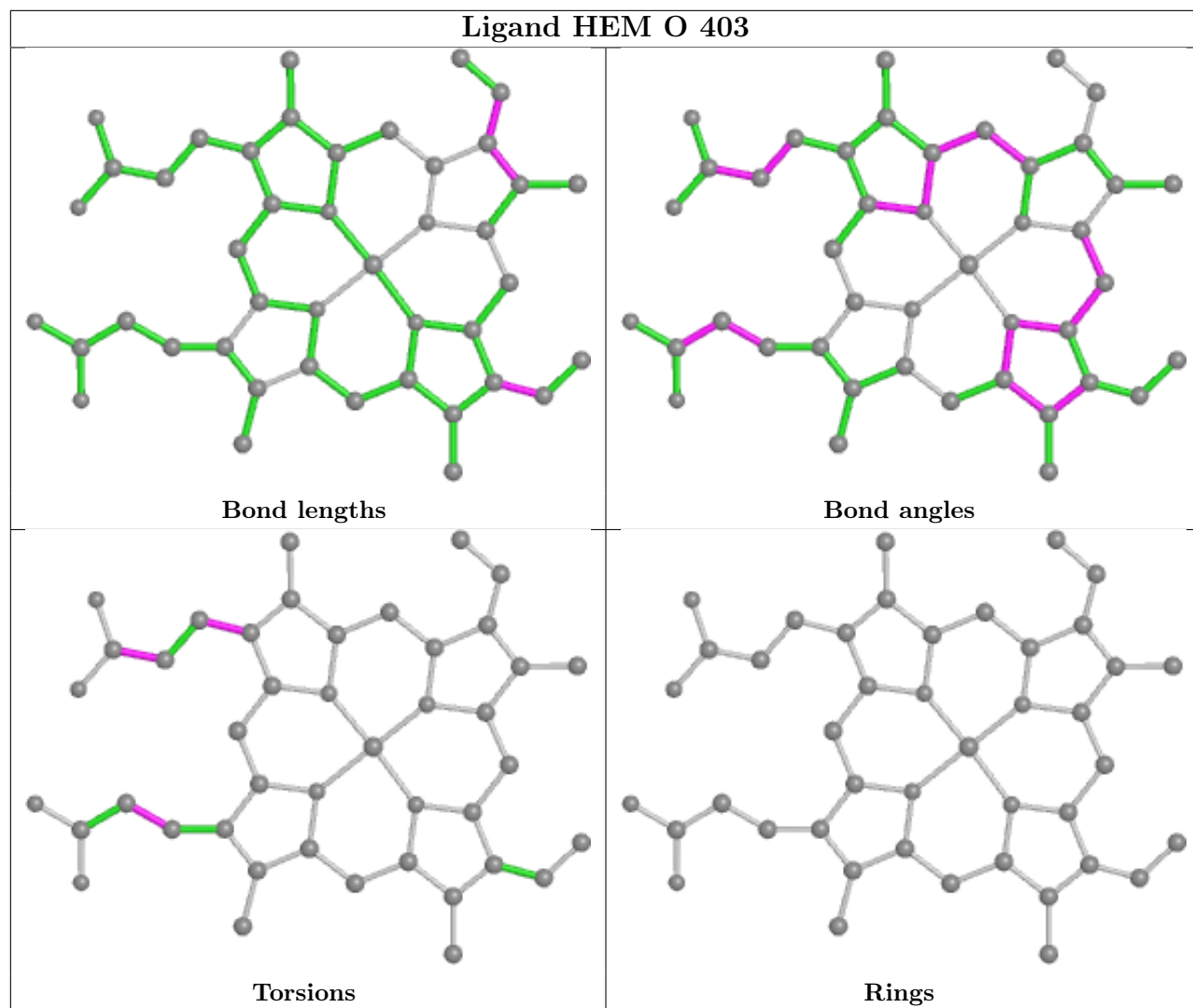


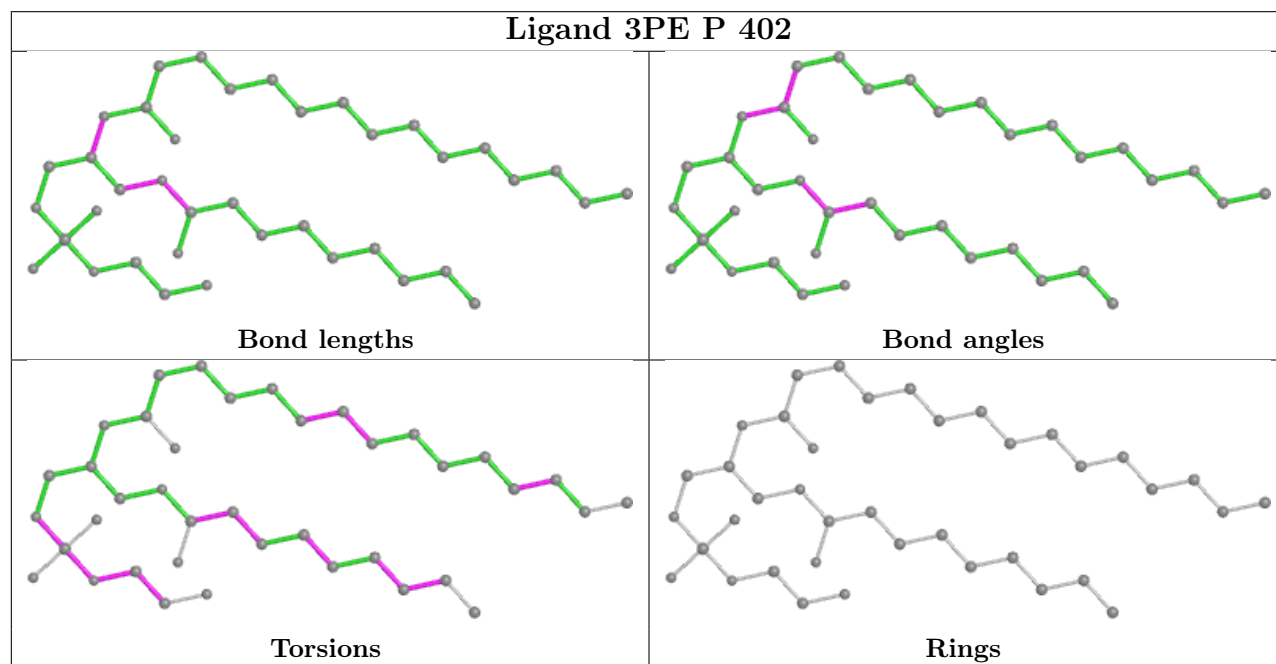
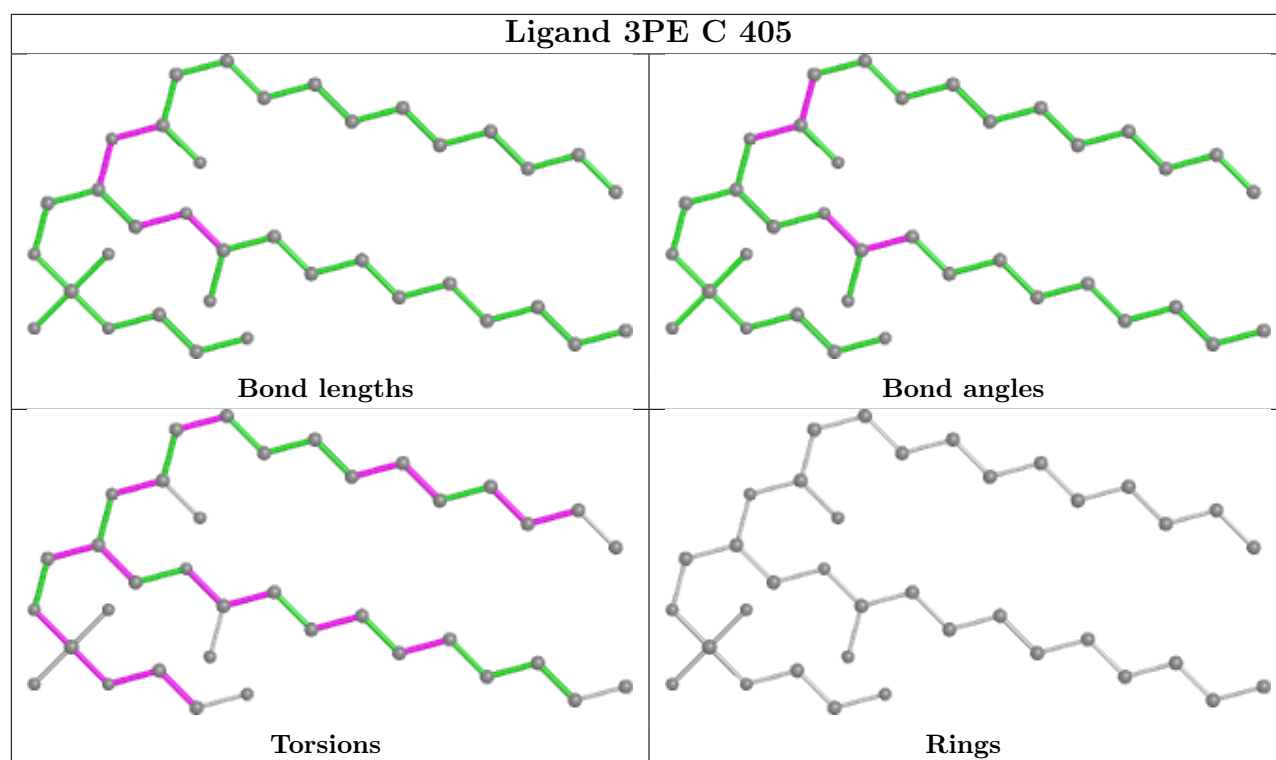


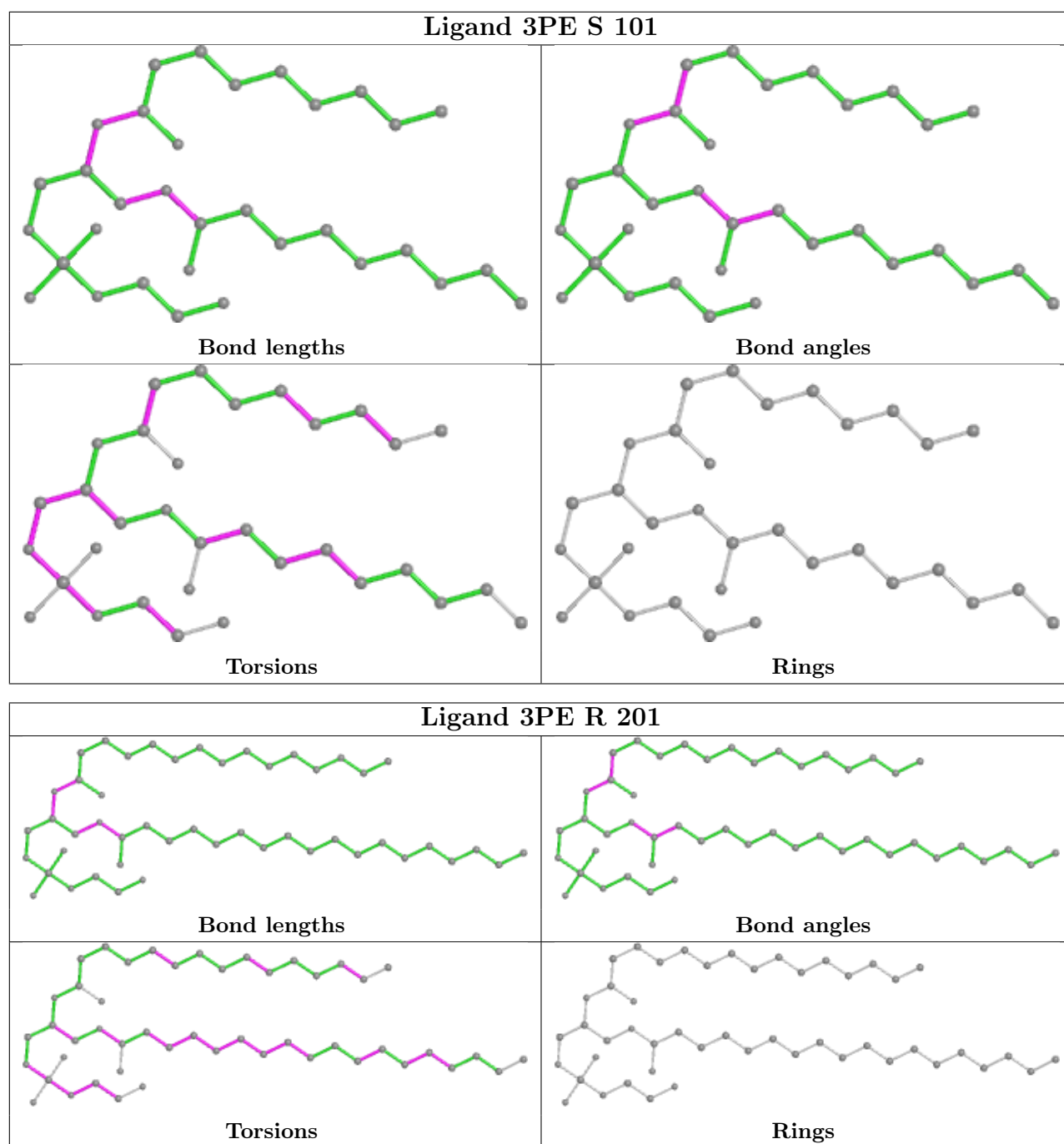


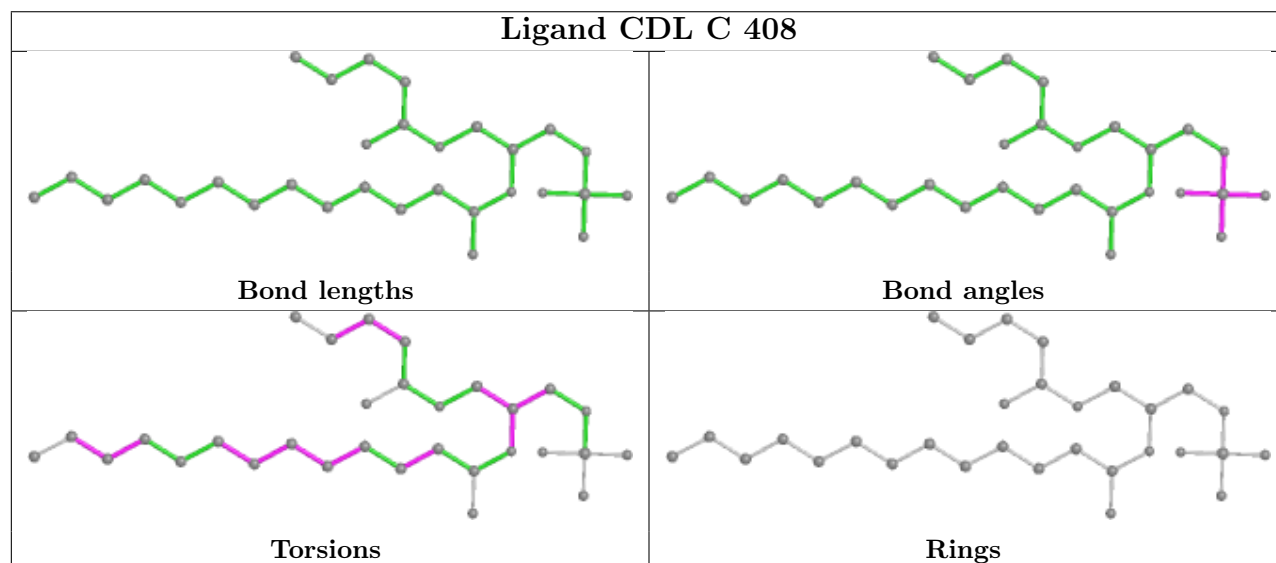
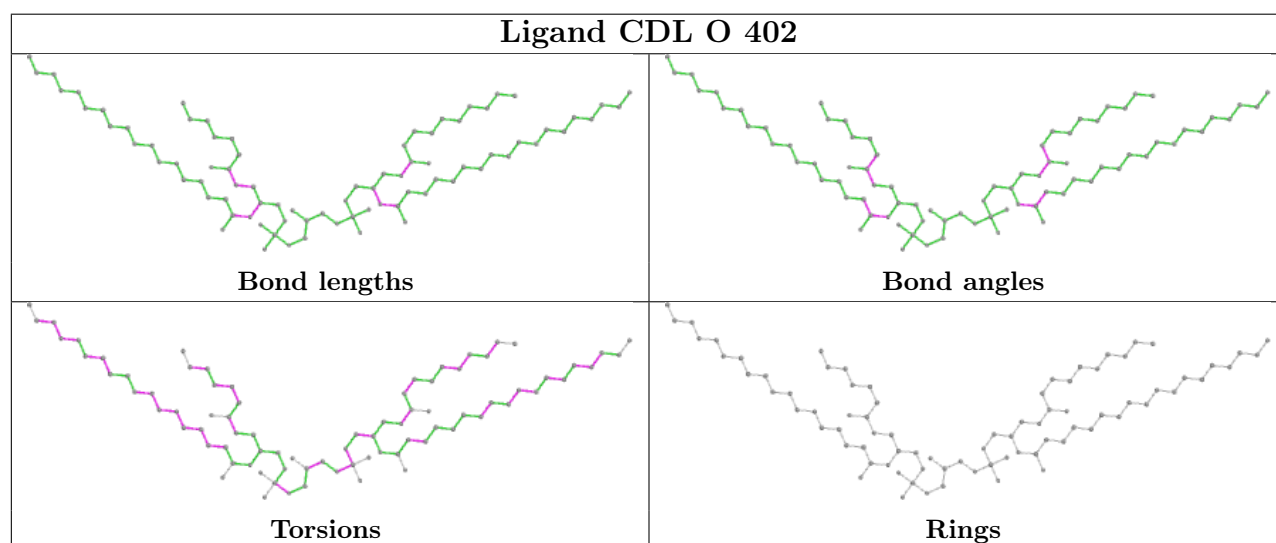
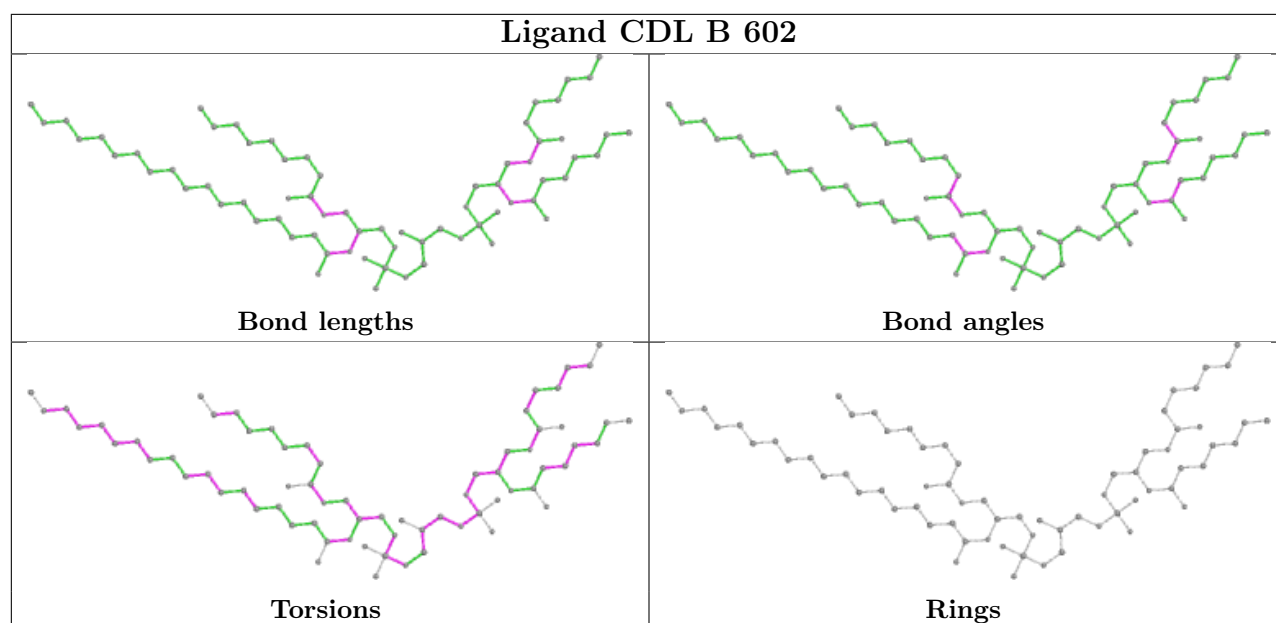


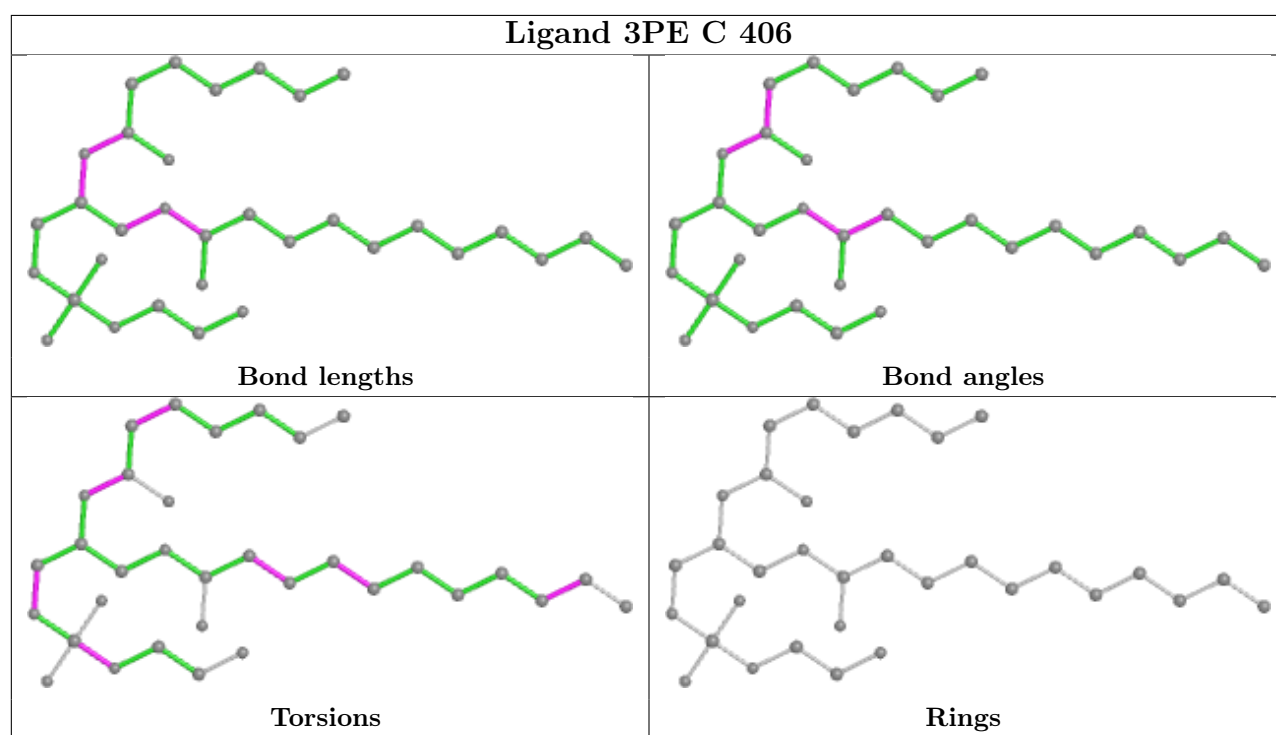
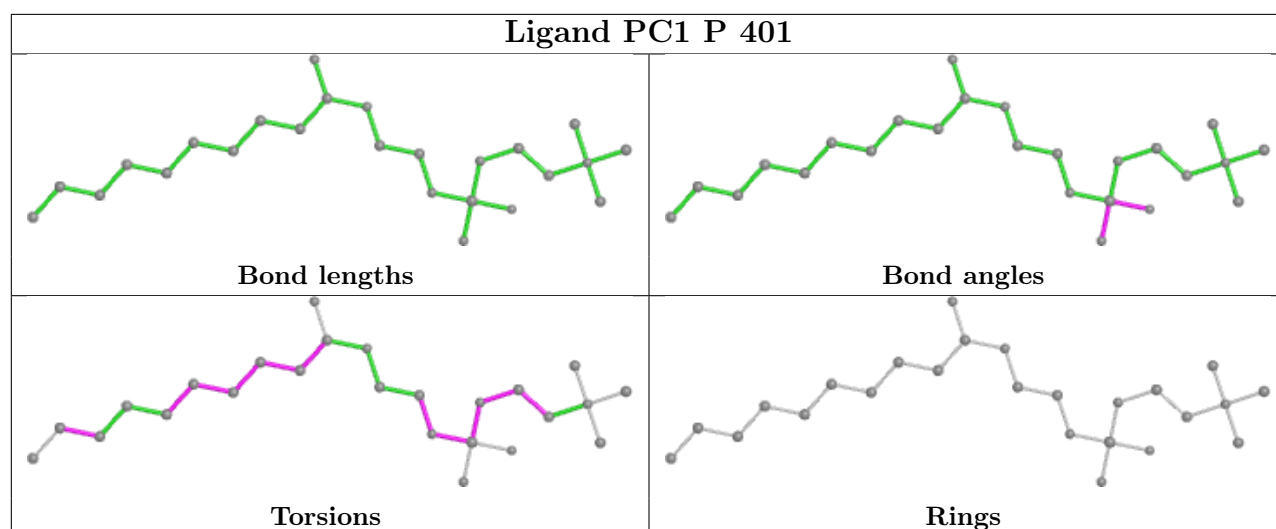


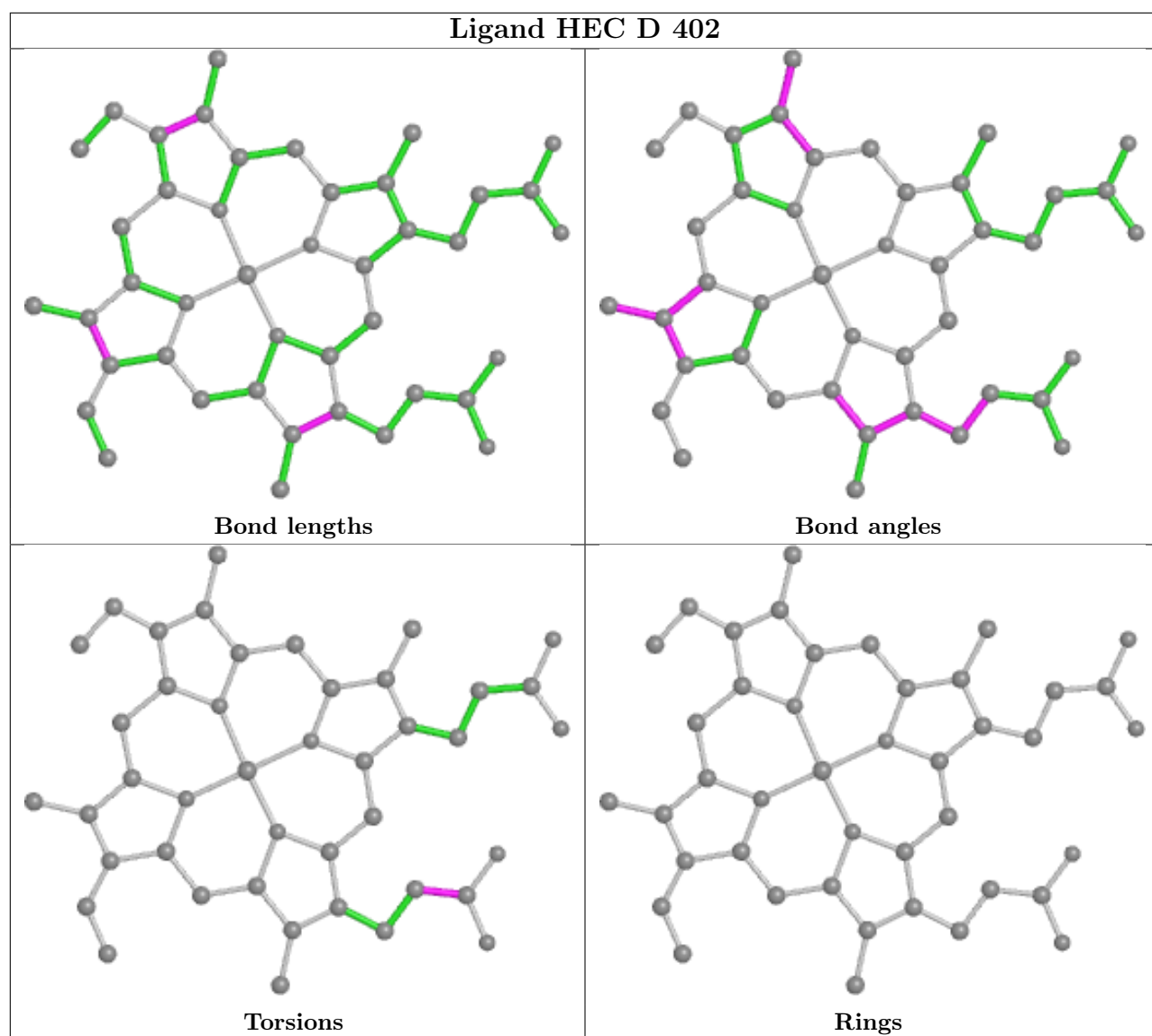


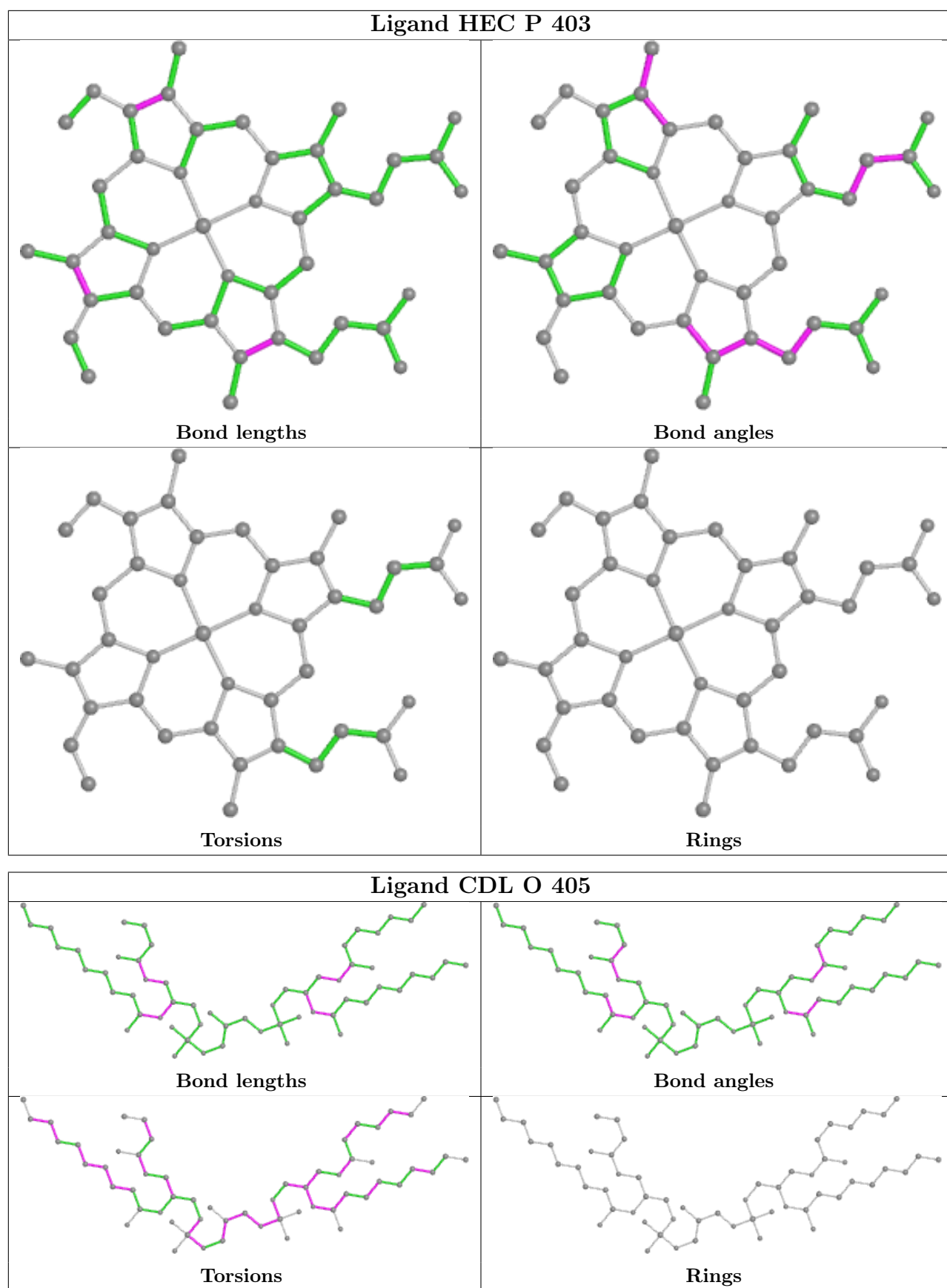


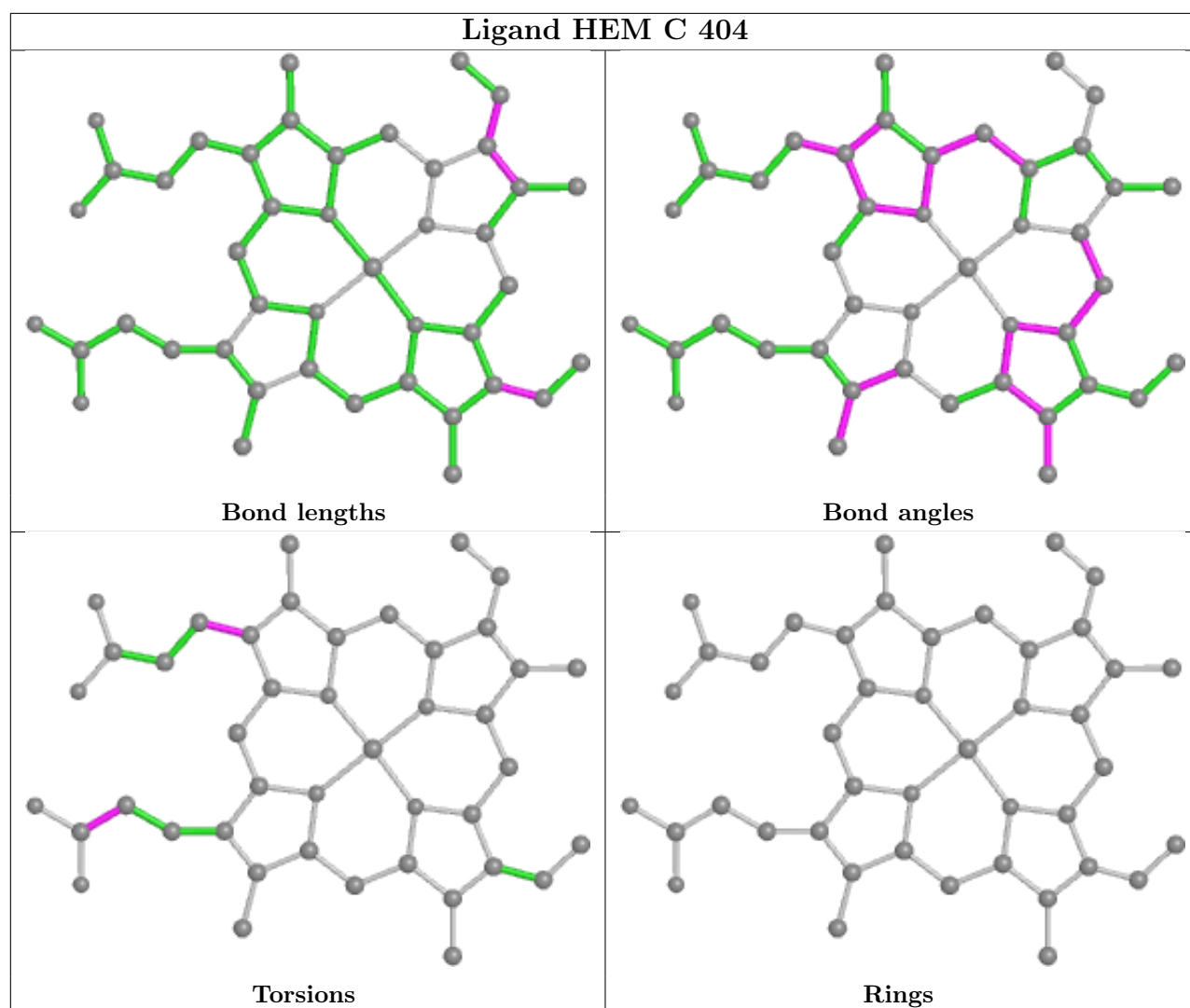












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.