



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 09:50 AM EDT

PDB ID : 1QDB  
Title : CYTOCHROME C NITRITE REDUCTASE  
Authors : Einsle, O.; Messerschmidt, A.; Stach, P.; Huber, R.; Kroneck, P.M.H.  
Deposited on : 1999-05-19  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

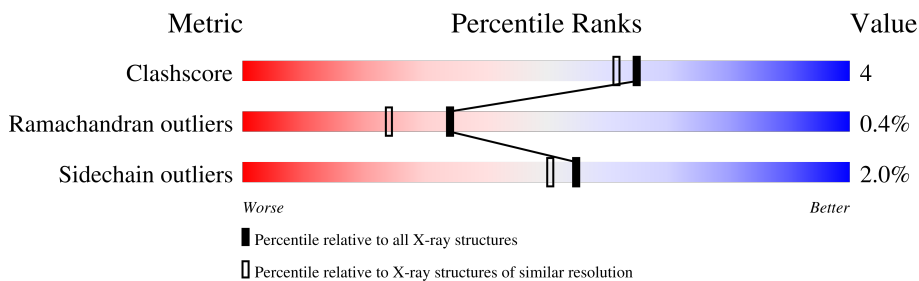
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	
1	C	473	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13431 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 C NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	93	0	0
			3751	2367	654	710	20			
1	B	473	Total	C	N	O	S	14	0	0
			3751	2367	654	710	20			
1	C	473	Total	C	N	O	S	17	0	0
			3751	2367	654	710	20			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

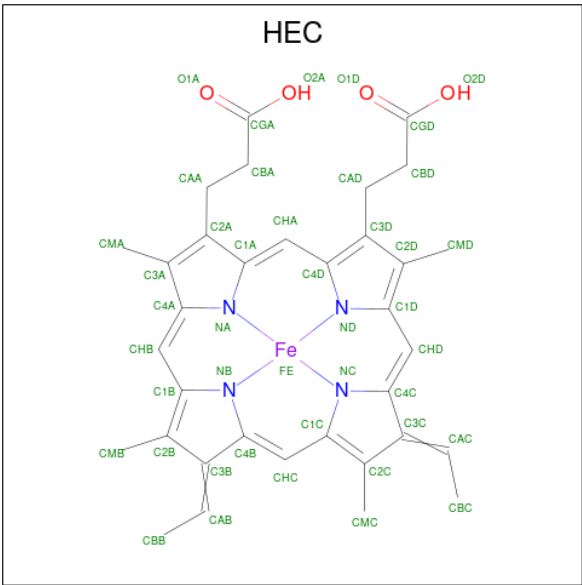
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 5 is water.

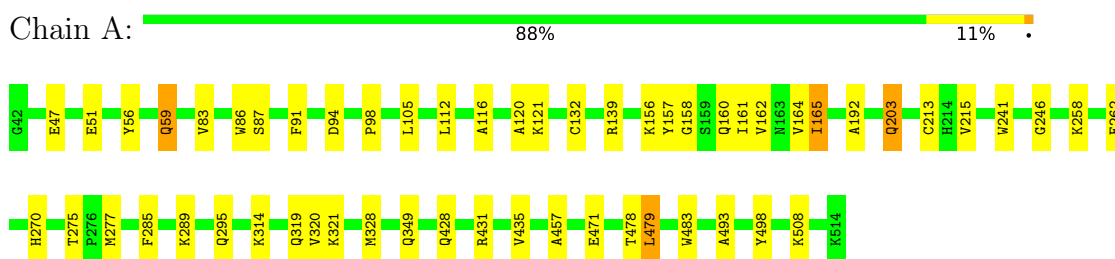
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total 371	O 371	0	0
5	B	505	Total 505	O 505	0	0
5	C	609	Total 609	O 609	0	0

### 3 Residue-property plots

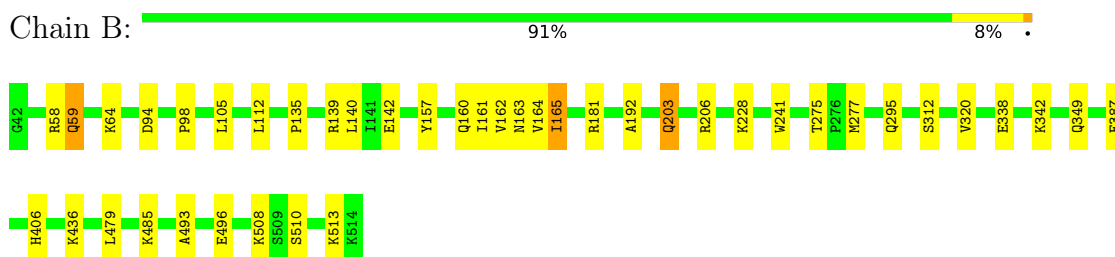
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

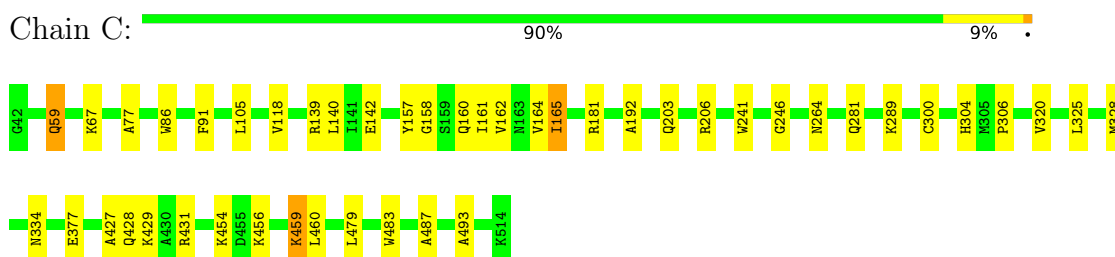
#### • Molecule 1: CYTOCHROME C NITRITE REDUCTASE



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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.48Å 185.34Å 92.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90	Depositor
% Data completeness (in resolution range)	100.0 (25.00-1.90)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.184 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP



## 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: SO4, CA, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/3840	0.60	0/5173
1	B	0.42	0/3840	0.63	0/5173
1	C	0.47	0/3840	0.66	0/5173
All	All	0.42	0/11520	0.63	0/15519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3751	0	3658	36	0
1	B	3751	0	3658	25	0
1	C	3751	0	3658	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	1	0
4	A	215	0	150	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	215	0	150	4	0
4	C	215	0	150	4	0
5	A	371	0	0	3	0
5	B	505	0	0	1	0
5	C	609	0	0	3	0
All	All	13431	0	11424	95	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 4.

The worst 5 of 95 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)
1:A:349:GLN:HE22	1:B:295:GLN:HE22	1.29	0.78
1:A:319:GLN:O	1:A:321:LYS:HD2	1.86	0.75
1:C:456:LYS:O	1:C:459:LYS:HD3	1.87	0.74
1:A:295:GLN:HE22	1:B:349:GLN:HE22	1.34	0.73
1:B:140:LEU:HD12	1:B:161:ILE:HD11	1.71	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	471/473 (100%)	454 (96%)	15 (3%)	2 (0%)	34	24
1	B	471/473 (100%)	465 (99%)	4 (1%)	2 (0%)	34	24
1	C	471/473 (100%)	462 (98%)	7 (2%)	2 (0%)	34	24
All	All	1413/1419 (100%)	1381 (98%)	26 (2%)	6 (0%)	34	24

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ILE
1	B	165	ILE
1	C	165	ILE
1	A	320	VAL
1	C	320	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 X-ray entries followed by that with respect to entries of similar resolution.

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	392/392 (100%)	385 (98%)	7 (2%)	59	55
1	B	392/392 (100%)	383 (98%)	9 (2%)	50	45
1	C	392/392 (100%)	385 (98%)	7 (2%)	59	55
All	All	1176/1176 (100%)	1153 (98%)	23 (2%)	55	51

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	496	GLU
1	C	67	LYS
1	C	59	GLN
1	C	105	LEU
1	A	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	477	GLN
1	C	160	GLN
1	C	59	GLN
1	C	203	GLN
1	A	494	ASN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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$
4	HEC	B	519	1	32,50,50	1.63	2 (6%)	24,82,82	1.60	5 (20%)
4	HEC	B	515	1,3	32,50,50	1.33	2 (6%)	24,82,82	1.87	6 (25%)
4	HEC	A	518	1	32,50,50	1.64	4 (12%)	24,82,82	1.30	1 (4%)
4	HEC	C	517	1	32,50,50	1.64	6 (18%)	24,82,82	1.85	6 (25%)
3	SO4	B	1507	-	4,4,4	0.49	0	6,6,6	0.31	0
3	SO4	C	1503	4	4,4,4	0.64	0	6,6,6	0.92	0
4	HEC	A	516	1	32,50,50	1.44	4 (12%)	24,82,82	1.10	0
3	SO4	C	1508	-	4,4,4	0.24	0	6,6,6	0.30	0
4	HEC	C	519	1	32,50,50	1.64	6 (18%)	24,82,82	1.80	4 (16%)
3	SO4	C	1509	-	4,4,4	0.41	0	6,6,6	0.41	0
4	HEC	C	515	1,3	32,50,50	1.46	7 (21%)	24,82,82	1.28	3 (12%)
3	SO4	B	1502	4	4,4,4	0.30	0	6,6,6	0.53	0
3	SO4	B	1505	-	4,4,4	0.46	0	6,6,6	0.31	0
4	HEC	B	518	1	32,50,50	1.52	4 (12%)	24,82,82	2.11	7 (29%)
4	HEC	B	516	1	32,50,50	1.50	5 (15%)	24,82,82	1.27	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HEC	A	519	1	32,50,50	1.51	6 (18%)	24,82,82	1.79	6 (25%)
4	HEC	C	518	1	32,50,50	1.57	4 (12%)	24,82,82	1.90	6 (25%)
4	HEC	B	517	1	32,50,50	1.75	5 (15%)	24,82,82	1.33	4 (16%)
3	SO4	A	1501	4	4,4,4	0.46	0	6,6,6	0.67	0
4	HEC	A	517	1	32,50,50	1.45	6 (18%)	24,82,82	1.89	5 (20%)
4	HEC	C	516	1	32,50,50	1.40	3 (9%)	24,82,82	1.41	3 (12%)
3	SO4	A	1506	-	4,4,4	0.38	0	6,6,6	0.15	0
4	HEC	A	515	1,3	32,50,50	1.45	3 (9%)	24,82,82	1.37	3 (12%)
3	SO4	A	1504	-	4,4,4	0.54	0	6,6,6	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	B	518	1	-	0/10/54/54	-
4	HEC	B	516	1	-	2/10/54/54	-
4	HEC	A	515	1,3	-	2/10/54/54	-
4	HEC	B	515	1,3	-	2/10/54/54	-
4	HEC	B	519	1	-	5/10/54/54	-
4	HEC	A	518	1	-	0/10/54/54	-
4	HEC	C	517	1	-	0/10/54/54	-
4	HEC	C	515	1,3	-	2/10/54/54	-
4	HEC	A	516	1	-	4/10/54/54	-
4	HEC	A	519	1	-	4/10/54/54	-
4	HEC	C	518	1	-	0/10/54/54	-
4	HEC	C	519	1	-	4/10/54/54	-
4	HEC	B	517	1	-	0/10/54/54	-
4	HEC	A	517	1	-	2/10/54/54	-
4	HEC	C	516	1	-	2/10/54/54	-

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	517	HEC	C3C-C2C	-6.18	1.34	1.40
4	B	519	HEC	C2B-C3B	-5.19	1.35	1.40
4	C	519	HEC	C3C-C2C	-4.80	1.35	1.40
4	A	518	HEC	C3C-C2C	-4.62	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	517	HEC	C3C-C2C	-4.57	1.36	1.40

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	517	HEC	CMB-C2B-C1B	-5.41	120.15	128.46
4	A	517	HEC	CMB-C2B-C3B	4.94	131.63	125.82
4	C	518	HEC	CMC-C2C-C1C	-4.90	120.94	128.46
4	B	515	HEC	CMB-C2B-C3B	4.86	131.53	125.82
4	C	517	HEC	CMB-C2B-C1B	-4.62	121.36	128.46

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	516	HEC	CAA-CBA-CGA-O1A
4	B	516	HEC	CAA-CBA-CGA-O1A
4	B	516	HEC	CAA-CBA-CGA-O2A
4	C	516	HEC	CAA-CBA-CGA-O2A
4	A	516	HEC	CAA-CBA-CGA-O2A

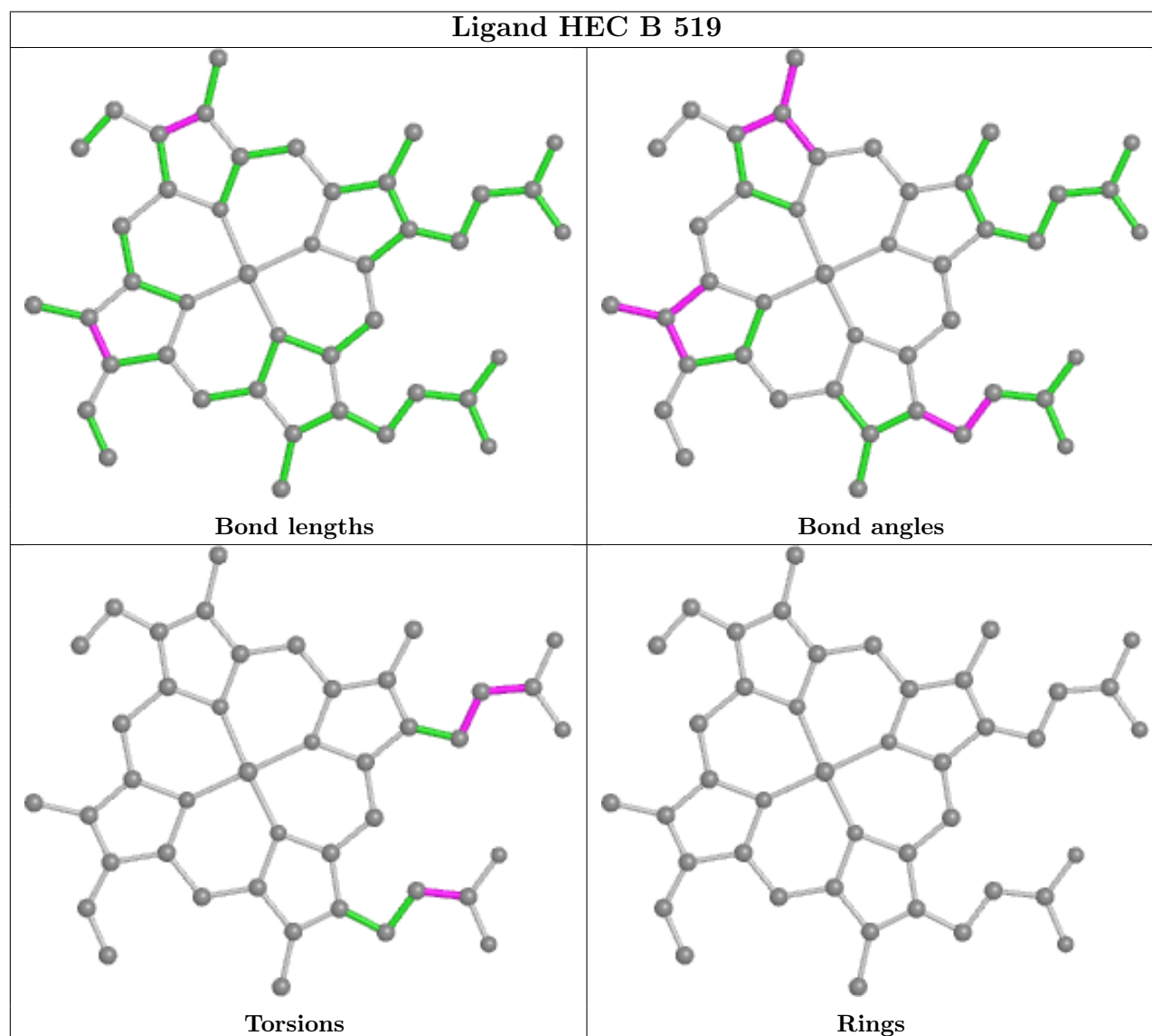
There are no ring outliers.

9 monomers are involved in 13 short contacts:

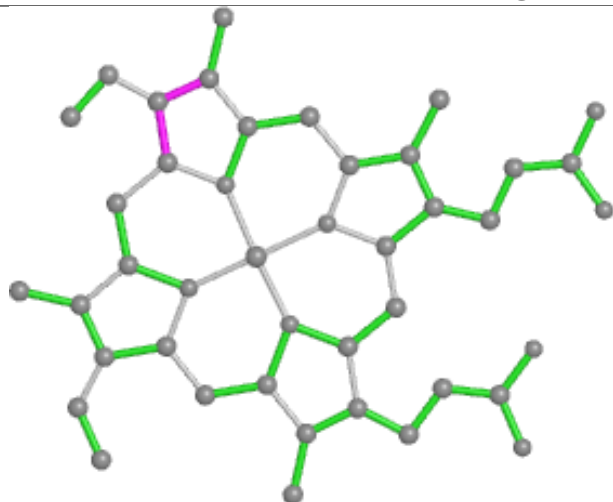
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	515	HEC	1	0
4	A	518	HEC	2	0
4	C	517	HEC	1	0
3	C	1503	SO4	1	0
4	C	515	HEC	1	0
4	B	518	HEC	2	0
4	C	518	HEC	2	0
4	B	517	HEC	1	0
4	A	515	HEC	2	0

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

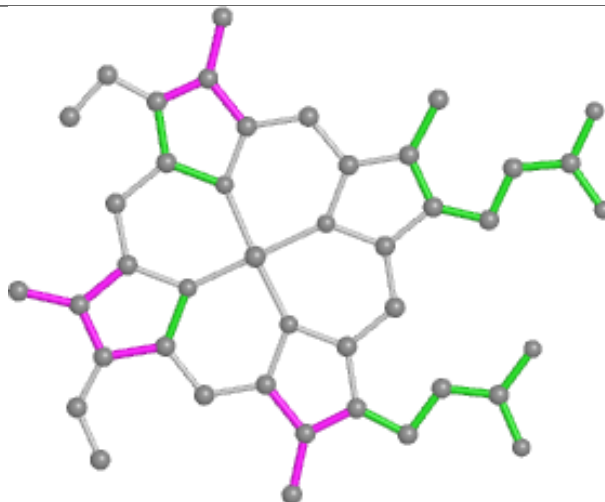
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



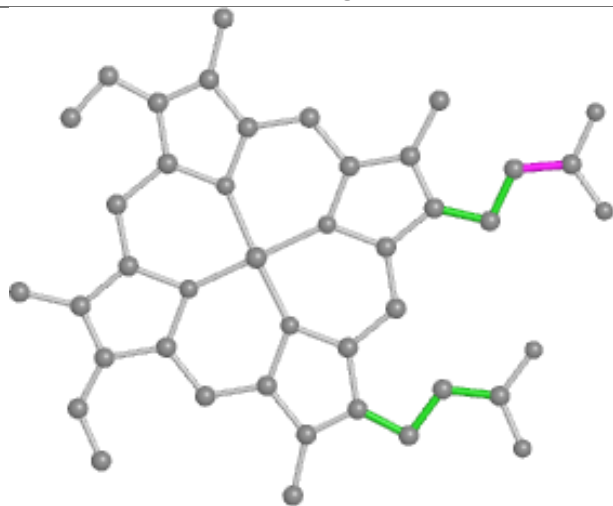
## Ligand HEC B 515



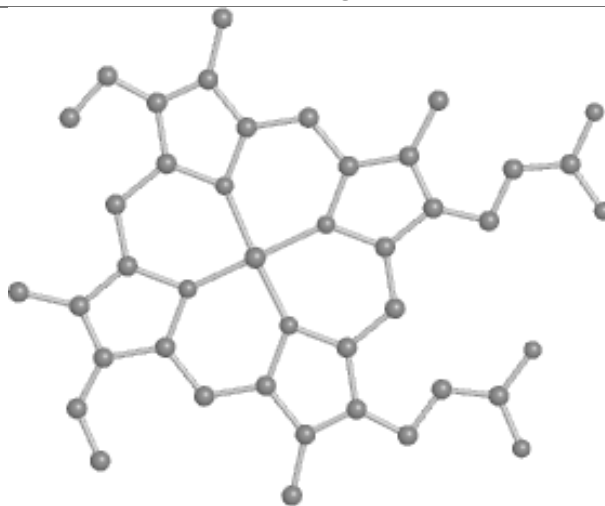
Bond lengths



Bond angles



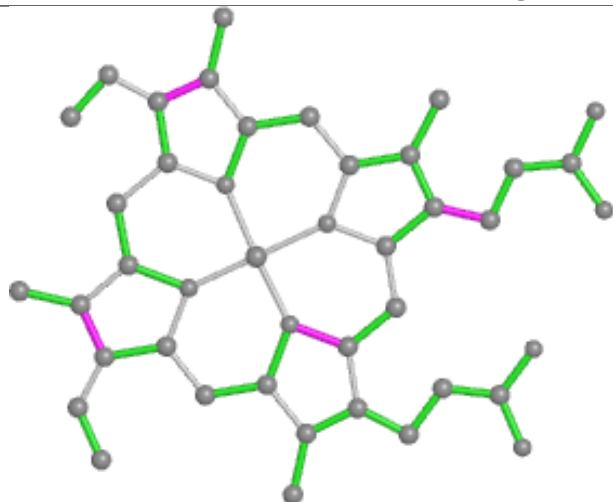
Torsions



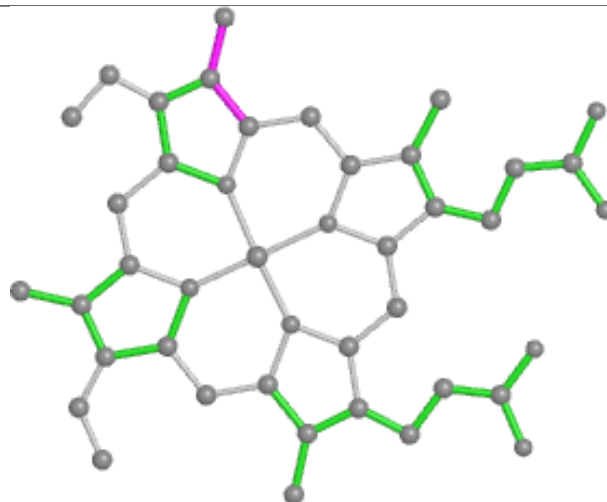
Rings



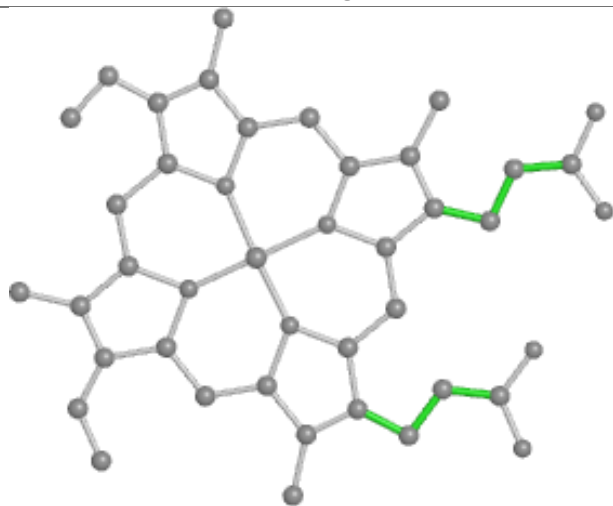
## Ligand HEC A 518



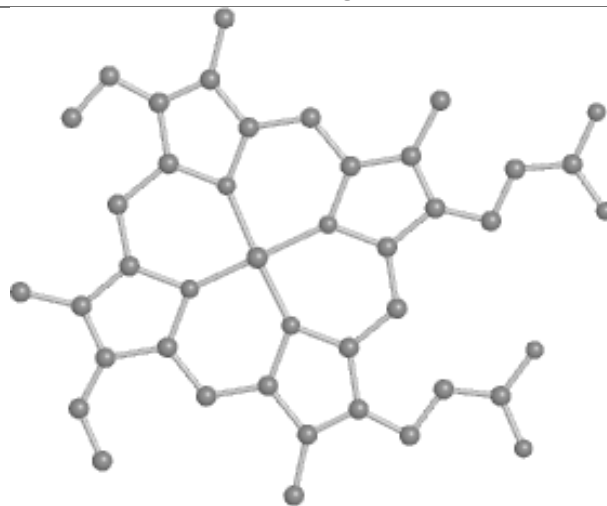
Bond lengths



Bond angles

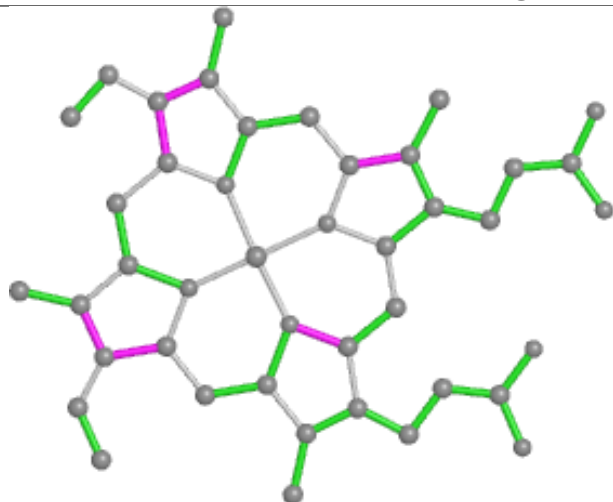


Torsions

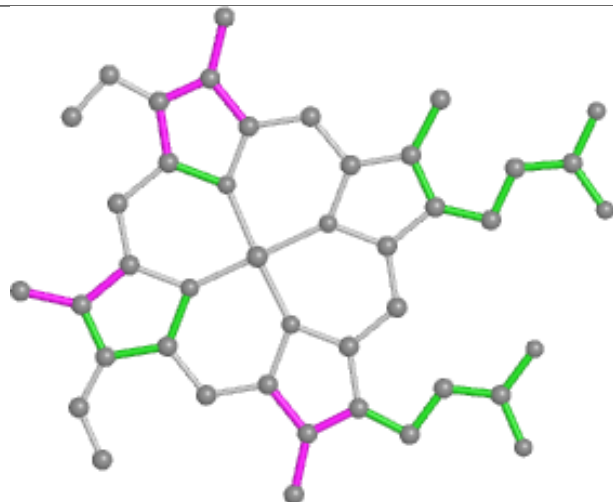


Rings

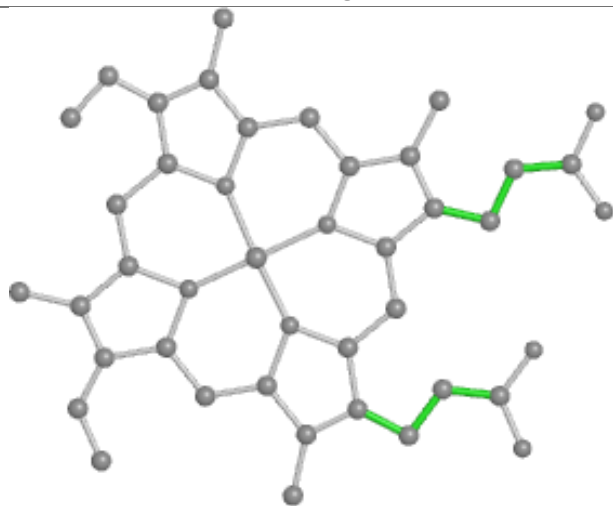
## Ligand HEC C 517



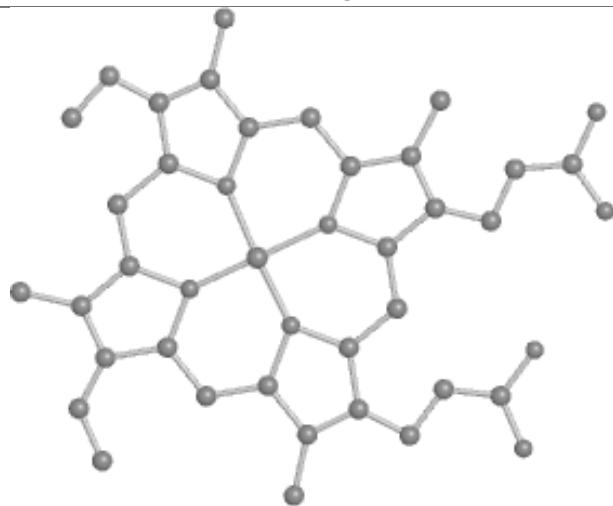
Bond lengths



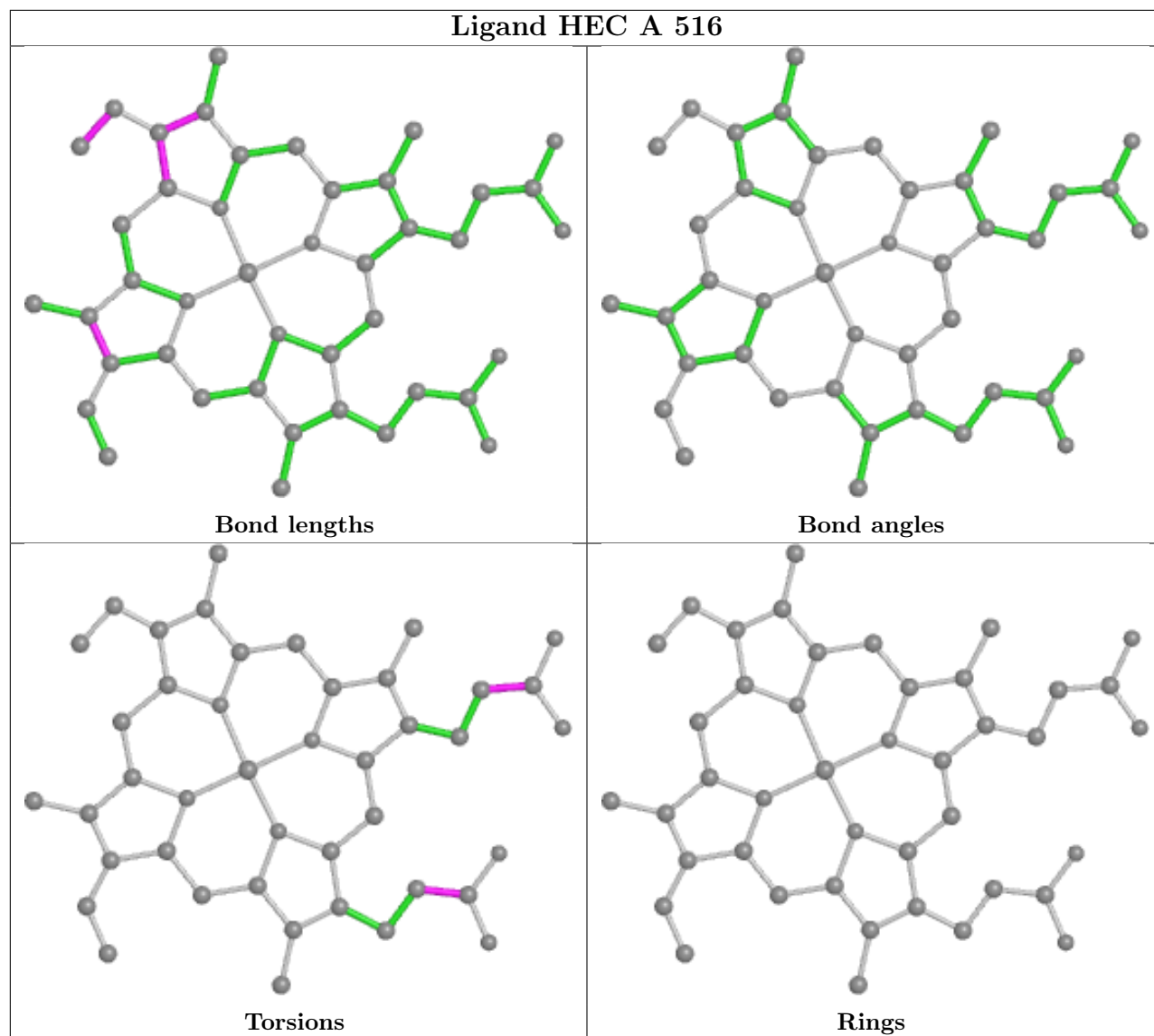
Bond angles



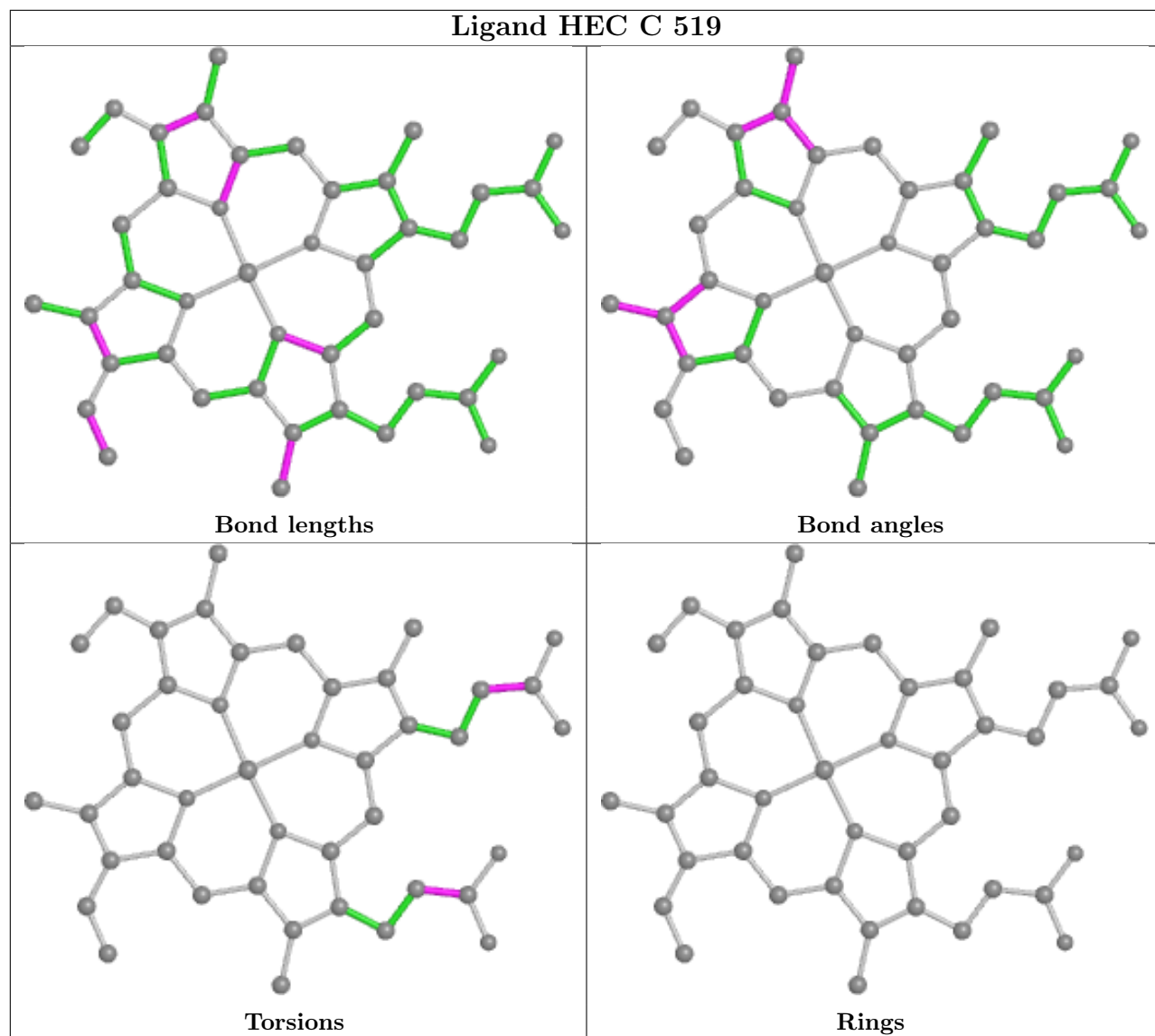
Torsions

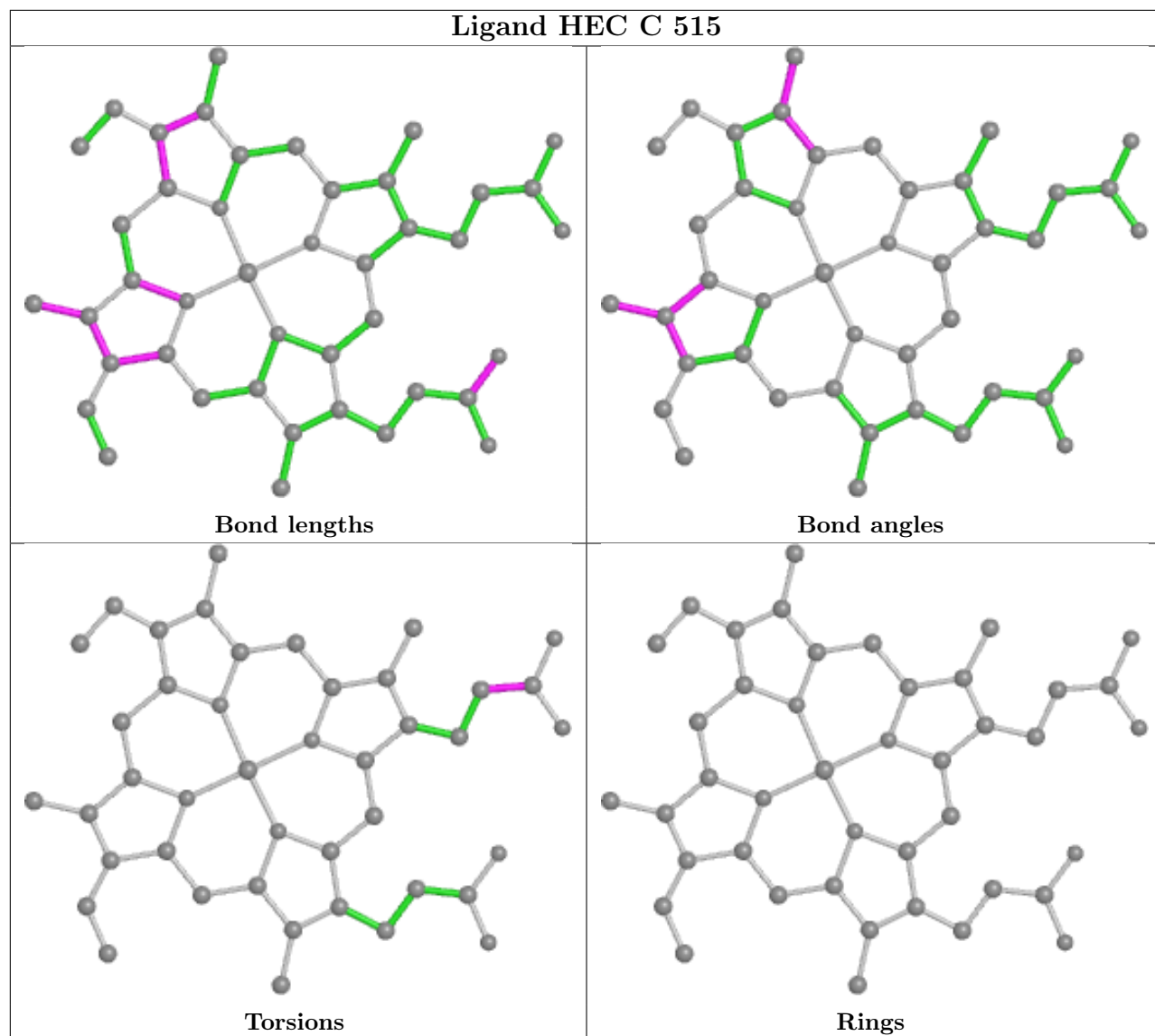


Rings

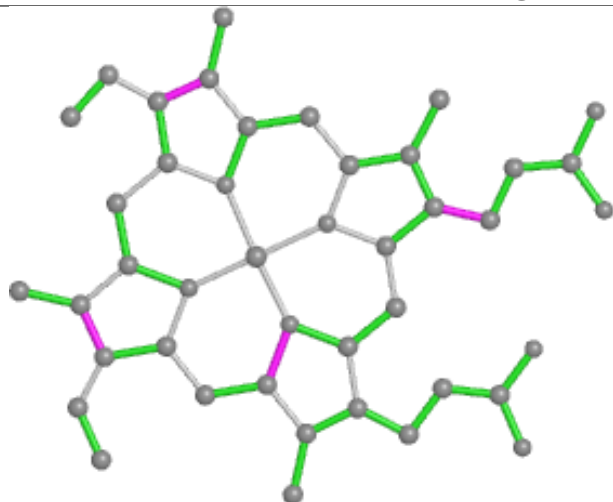


## Ligand HEC C 519

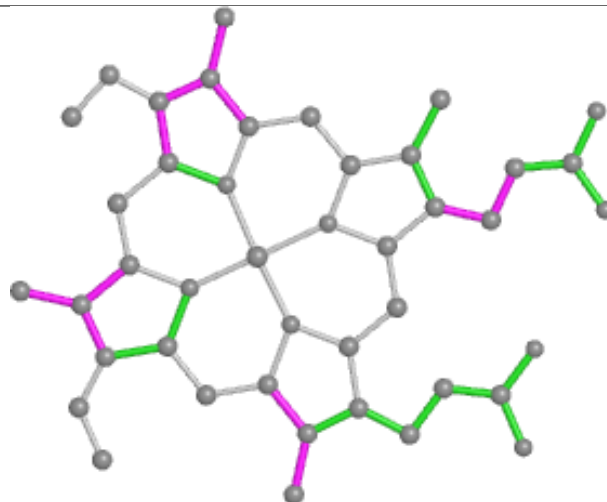




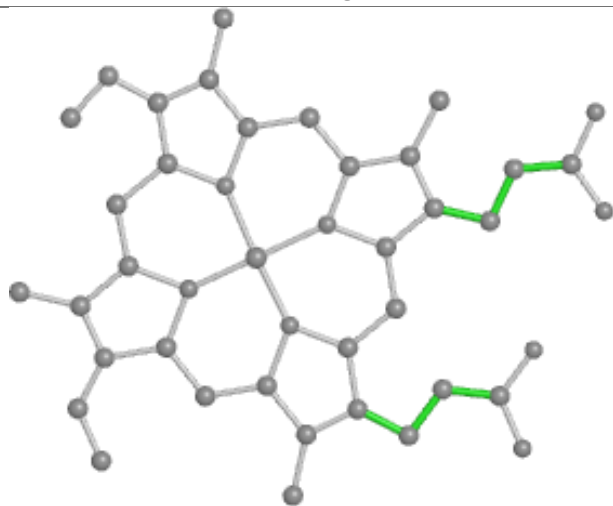
## Ligand HEC B 518



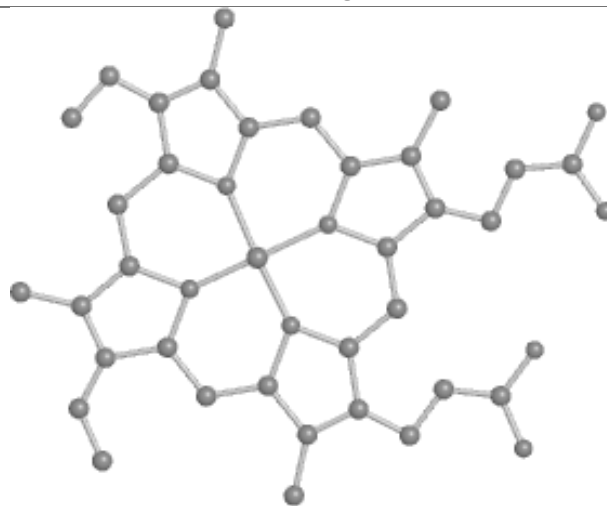
Bond lengths



Bond angles

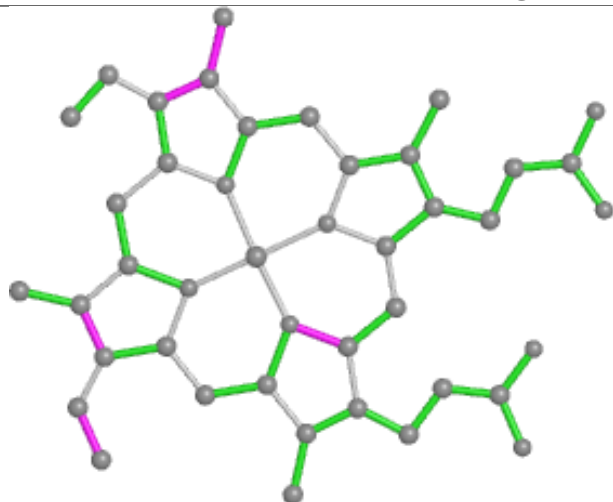


Torsions

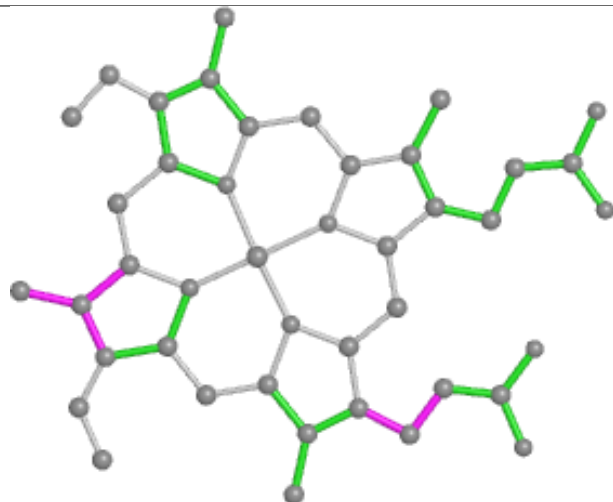


Rings

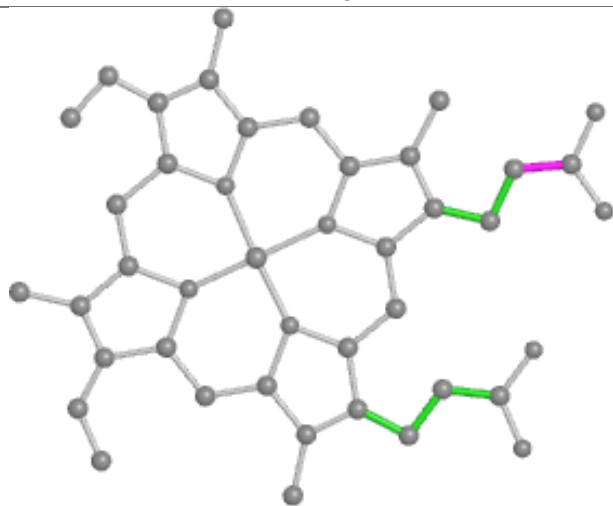
## Ligand HEC B 516



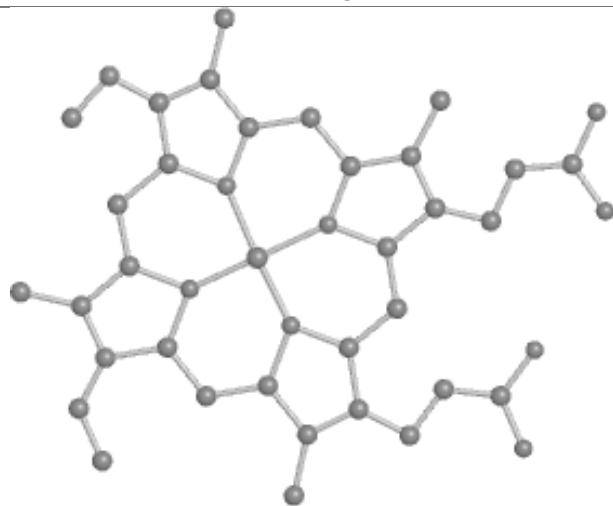
Bond lengths



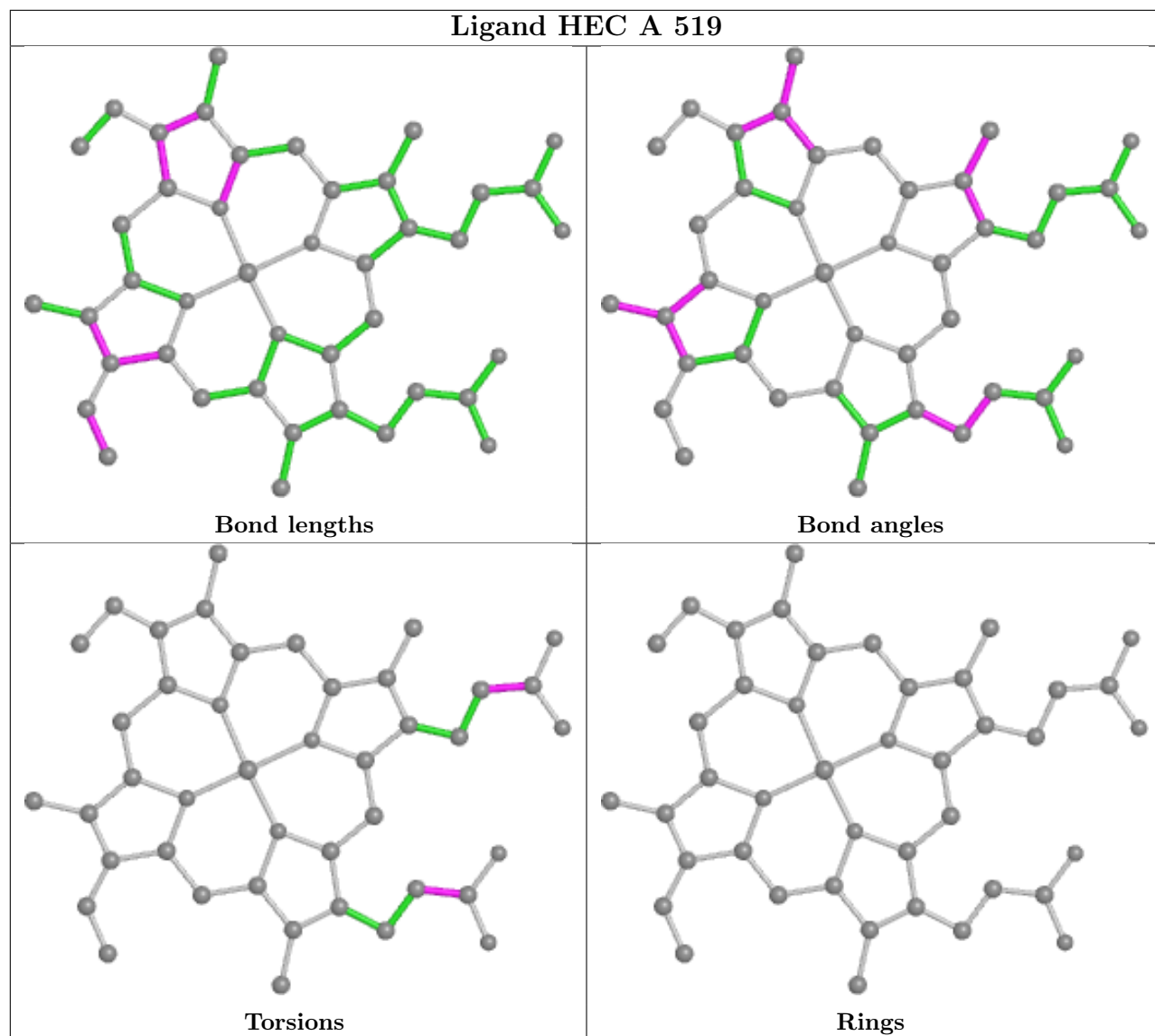
Bond angles



Torsions

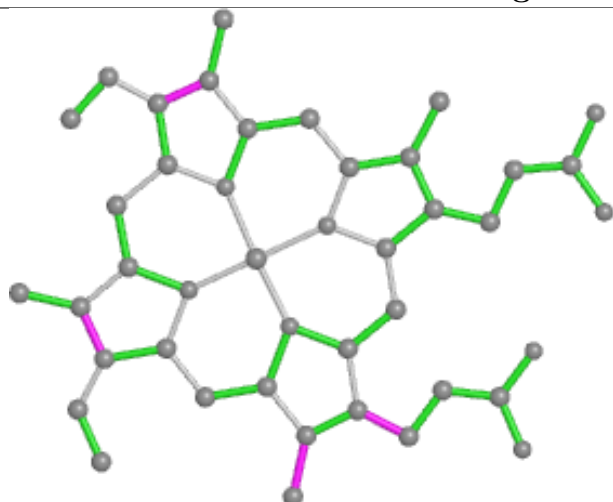


Rings

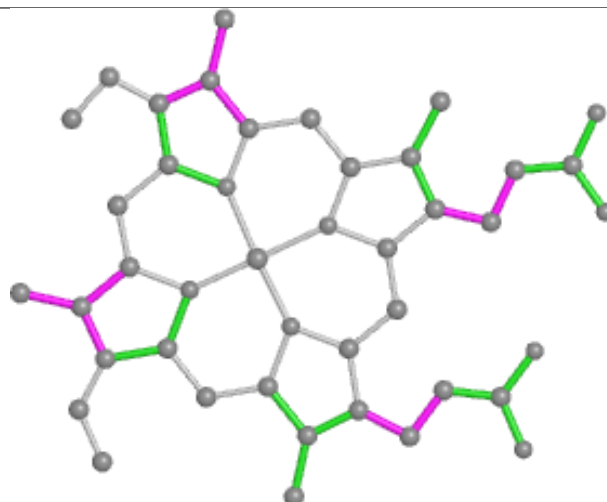




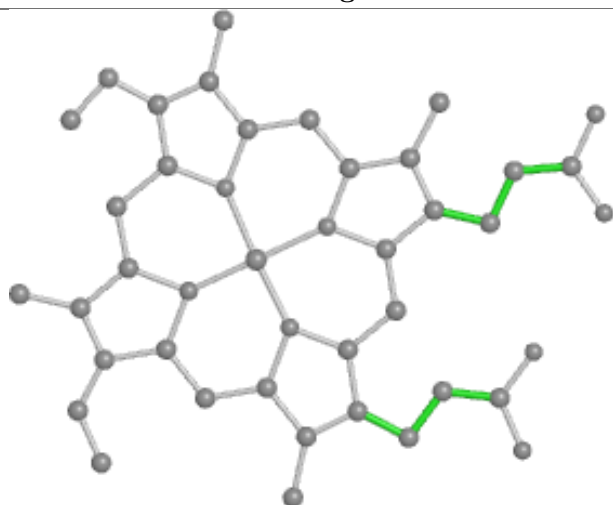
## Ligand HEC C 518



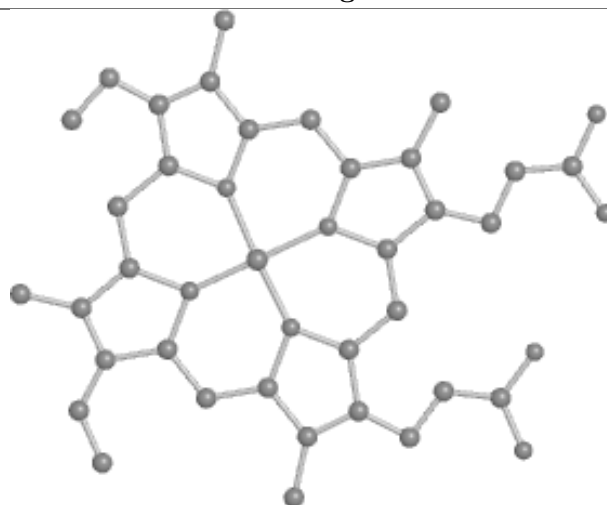
Bond lengths



Bond angles

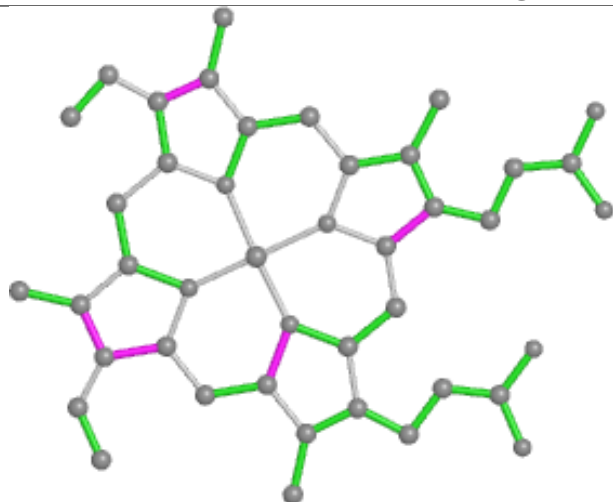


Torsions

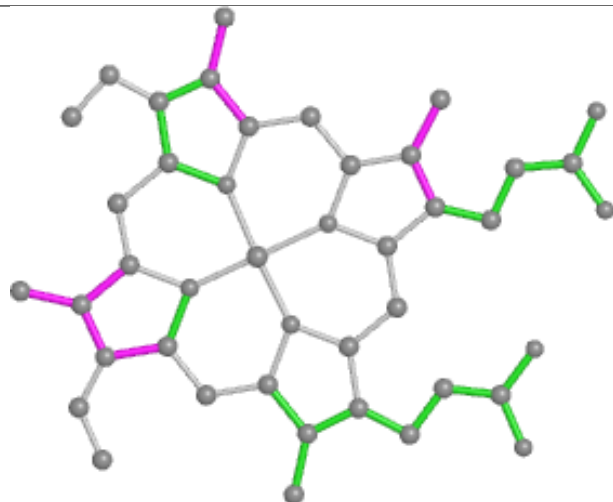


Rings

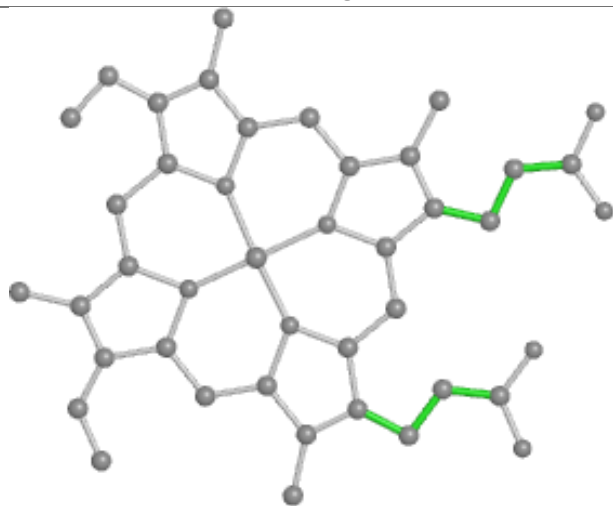
## Ligand HEC B 517



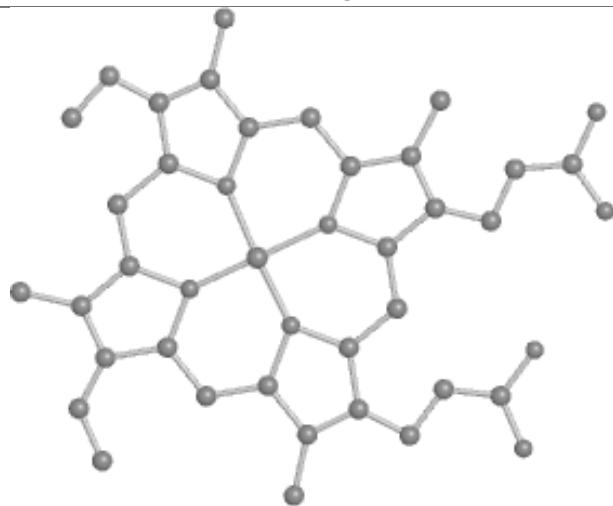
Bond lengths



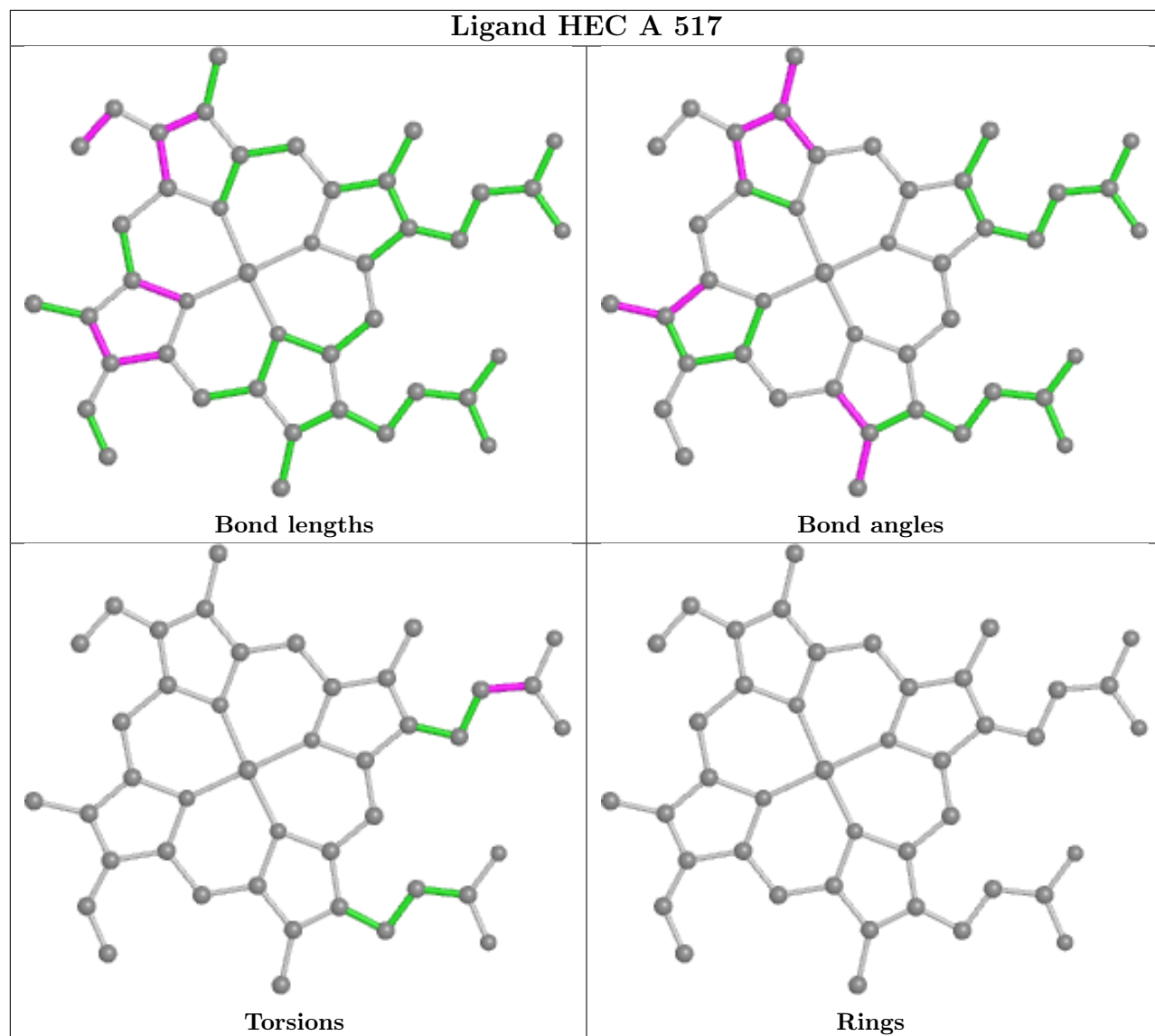
Bond angles



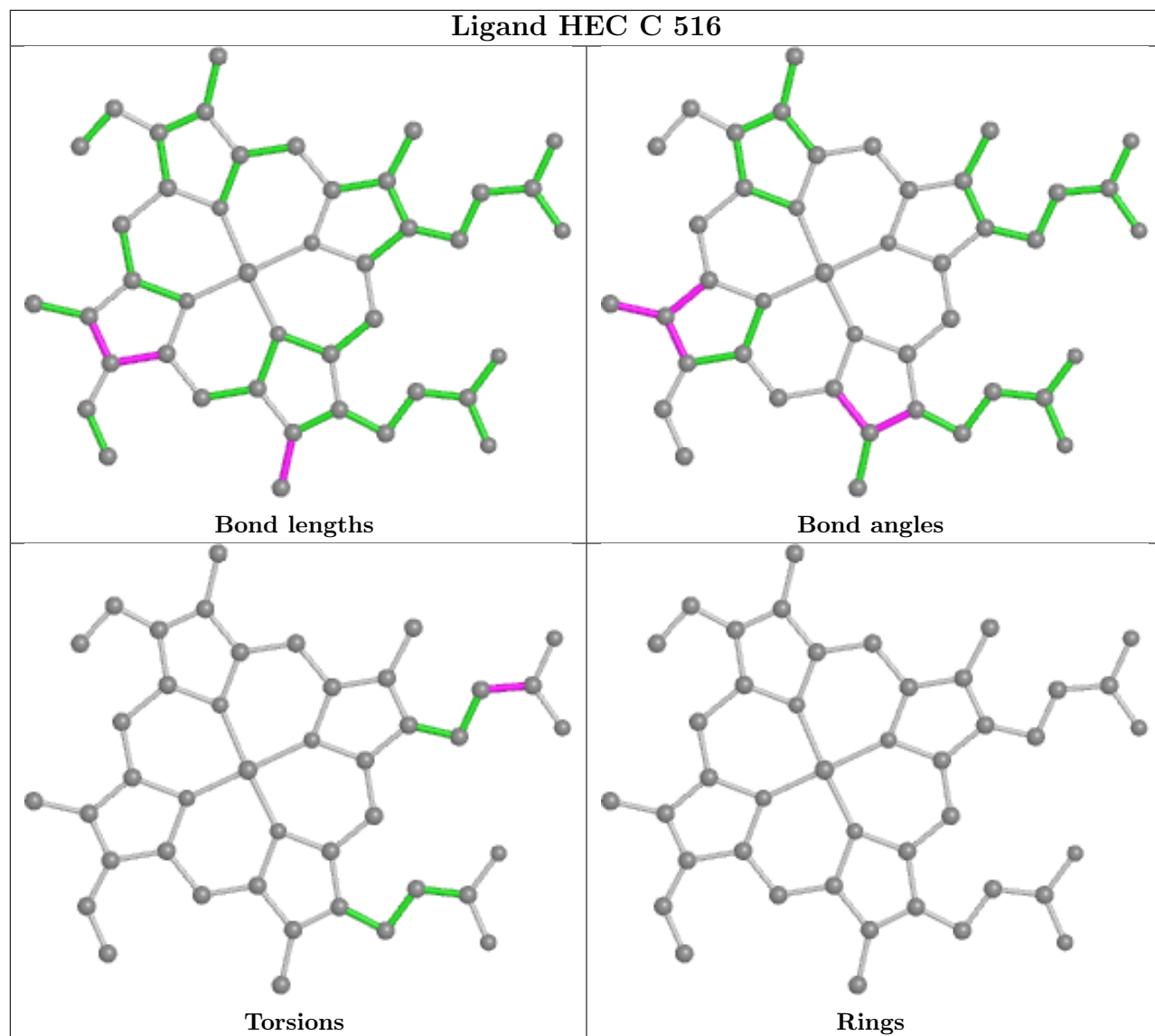
Torsions

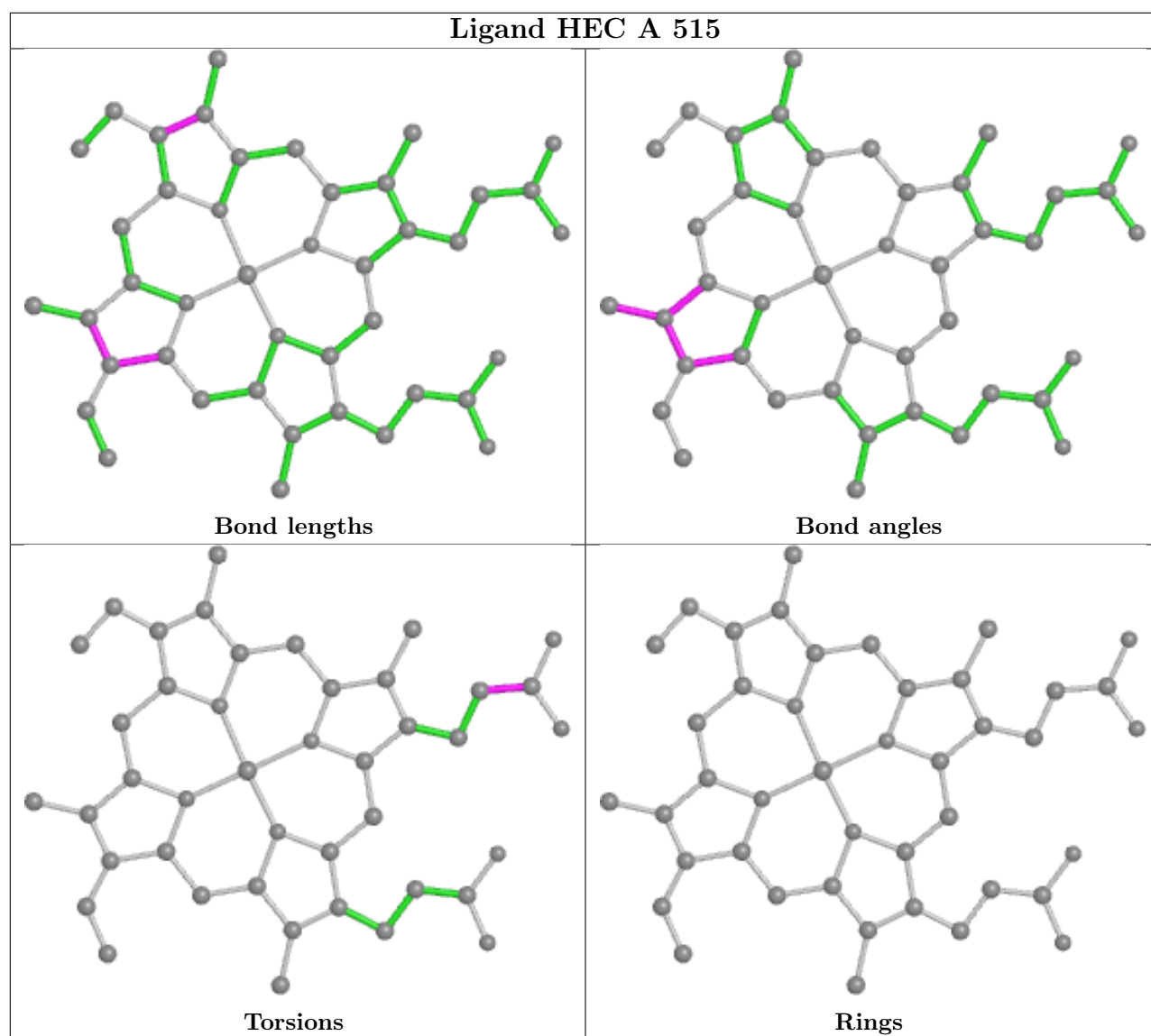


Rings



## Ligand HEC C 516





## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.