



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:21 am BST

PDB ID : 1OFW  
Title : Three dimensional structure of the oxidized form of nine heme cytochrome c at PH 7.5  
Authors : Bento, I.; Teixeira, V.H.; Baptista, A.M.; Soares, C.M.; Matias, P.M.; Car-rondo, M.A.  
Deposited on : 2003-04-22  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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) : 2.11

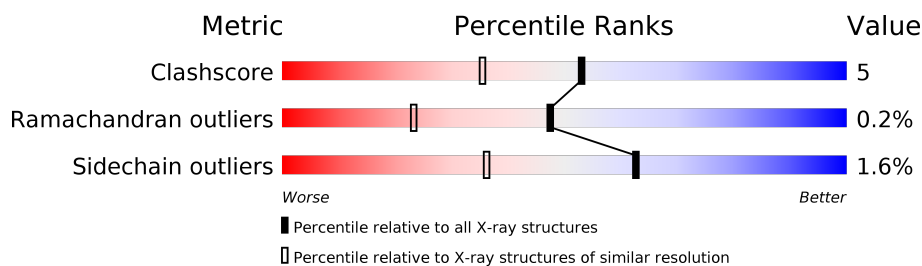
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 on 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	296	
1	B	296	

## 2 Entry composition i

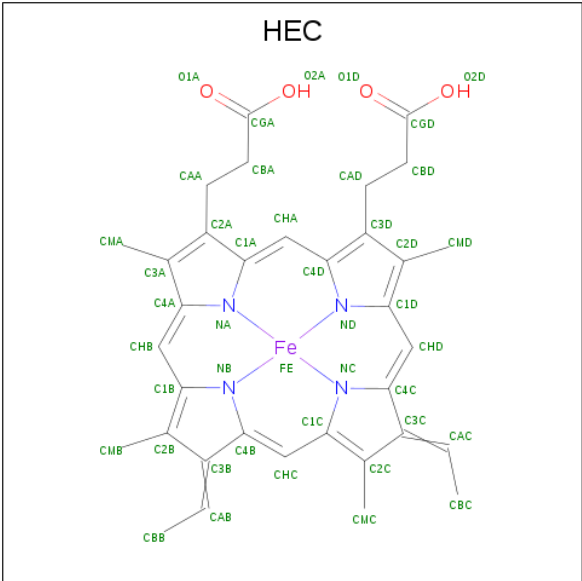
There are 5 unique types of molecules in this entry. The entry contains 5958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NINE-HEME CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	14	12	1
			2261	1389	419	425	28			
1	B	293	Total	C	N	O	S	22	8	1
			2248	1381	416	423	28			

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

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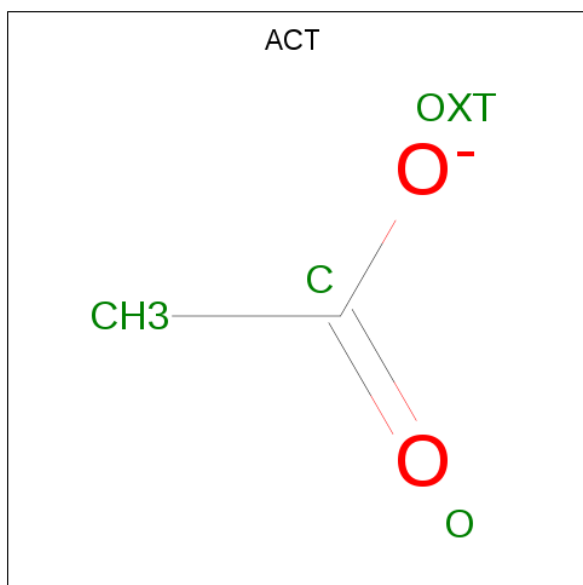
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	324	Total	O	0	0
			324	324		
5	B	317	Total	O	0	0
			317	317		

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

These plots are drawn for all protein, RNA and DNA 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.

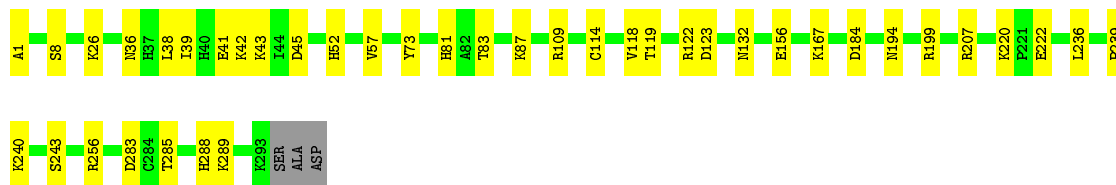
#### • Molecule 1: NINE-HEME CYTOCHROME C

Chain A:  91% 7% ..



#### • Molecule 1: NINE-HEME CYTOCHROME C

Chain B:  85% 14% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.30 Å   105.95 Å   80.37 Å 90.00°   103.18°   90.00°	Depositor
Resolution (Å)	25.00 – 1.50	Depositor
% Data completeness (in resolution range)	98.0 (25.00-1.50)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.171 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEC, ACT

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	0.55	0/2360	1.26	21/3203 (0.7%)
1	B	0.53	0/2326	1.24	17/3156 (0.5%)
All	All	0.54	0/4686	1.25	38/6359 (0.6%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	CD-NE-CZ	10.59	138.43	123.60
1	A	207	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	A	207	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	278	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	199	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	78	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	256	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	87	LYS	C-N-CA	7.54	140.56	121.70
1	B	132	ASN	O-C-N	-6.92	111.64	122.70
1	A	109	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	236	LEU	O-C-N	-6.72	111.94	122.70
1	B	199	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	98	VAL	O-C-N	-6.47	112.34	122.70
1	A	280[A]	ARG	CD-NE-CZ	6.32	132.44	123.60
1	A	280[B]	ARG	CD-NE-CZ	6.32	132.44	123.60
1	A	198	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	B	236	LEU	C-N-CA	6.31	137.47	121.70
1	A	9	GLY	O-C-N	-6.13	112.90	122.70
1	A	231	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	256	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	199	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	122	ARG	NE-CZ-NH1	5.85	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	83	THR	C-N-CA	-5.60	107.69	121.70
1	B	222	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	280[A]	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	280[B]	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	123	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	57	VAL	O-C-N	5.56	131.59	122.70
1	A	207	ARG	CD-NE-CZ	5.42	131.18	123.60
1	B	132	ASN	CA-C-N	5.35	128.97	117.20
1	B	283	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	184	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	103	GLN	CA-CB-CG	5.15	124.72	113.40
1	B	73	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	A	278	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	207	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	7	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2261	0	2199	9	0
1	B	2248	0	2201	19	0
2	A	387	0	270	10	0
2	B	387	0	270	16	0
3	A	6	0	8	0	0
3	B	24	0	32	3	0
4	B	4	0	3	0	0
5	A	324	0	0	6	0
5	B	317	0	0	16	0
All	All	5958	0	4983	55	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 5.

All (55) 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:B:119[B]:THR:CB	5:B:2128:HOH:O	1.72	1.30
1:B:119[B]:THR:N	5:B:2128:HOH:O	1.73	1.09
1:B:119[B]:THR:HB	5:B:2128:HOH:O	1.39	1.03
1:A:45[B]:ASP:HB3	5:A:2049:HOH:O	1.84	0.78
1:A:124:GLU:HG3	5:B:2129:HOH:O	1.87	0.73
1:B:285:THR:O	1:B:289:LYS:HD3	1.95	0.67
1:A:119[B]:THR:OG1	5:A:2121:HOH:O	1.88	0.65
2:B:1294:HEC:HMC1	2:B:1294:HEC:HBC3	1.84	0.58
2:A:1302:HEC:HBC3	2:A:1302:HEC:HMC1	1.84	0.58
1:A:45[B]:ASP:HB2	5:A:2048:HOH:O	2.02	0.58
1:B:36:ASN:ND2	1:B:39:ILE:HD12	2.19	0.58
2:A:1296:HEC:HBC3	2:A:1296:HEC:HMC1	1.86	0.57
2:B:1295:HEC:HMC1	2:B:1295:HEC:HBC3	1.87	0.57
2:A:1300:HEC:HMC1	2:A:1300:HEC:HBC3	1.88	0.56
1:B:1:ALA:HA	5:B:2065:HOH:O	2.05	0.55
2:B:1302:HEC:HBC3	2:B:1302:HEC:HMC1	1.88	0.55
3:B:1305[B]:GOL:H11	5:B:2316:HOH:O	2.06	0.55
2:A:1301:HEC:HMC1	2:A:1301:HEC:HBC3	1.87	0.54
2:B:1296:HEC:HMC1	2:B:1296:HEC:HBC3	1.88	0.54
3:B:1305[B]:GOL:H2	5:B:2316:HOH:O	2.08	0.53
1:B:114:CYS:O	1:B:118[B]:VAL:HG13	2.09	0.52
2:A:1301:HEC:HBB3	2:A:1301:HEC:HMB1	1.92	0.52
2:A:1299:HEC:HBC3	2:A:1299:HEC:HMC1	1.92	0.51
2:B:1301:HEC:HBB3	2:B:1301:HEC:HMB1	1.93	0.51
2:A:1295:HEC:HBB3	2:A:1295:HEC:HMB1	1.93	0.50
2:B:1301:HEC:HBC3	2:B:1301:HEC:HMC1	1.94	0.50
1:A:280[B]:ARG:HD3	5:A:2276:HOH:O	2.11	0.49
1:B:8:SER:OG	1:B:41:GLU:OE1	2.29	0.49
2:B:1299:HEC:HBC1	2:B:1301:HEC:HMC2	1.94	0.49
2:B:1299:HEC:HBC3	2:B:1299:HEC:HMC1	1.94	0.48
1:B:240[B]:LYS:HD2	5:B:2239:HOH:O	2.13	0.48
2:B:1296:HEC:HMB1	2:B:1296:HEC:HBB3	1.96	0.47
2:A:1298:HEC:HMB1	2:A:1298:HEC:HBB3	1.97	0.46
2:B:1298:HEC:HMC1	2:B:1298:HEC:HBC3	1.97	0.46
1:B:81:HIS:HB3	3:B:1305[A]:GOL:H11	1.98	0.46
1:B:156:GLU:HG3	5:B:2156:HOH:O	2.15	0.46
1:A:156:GLU:HG2	5:A:2015:HOH:O	2.15	0.45
1:B:109:ARG:NH2	5:B:2123:HOH:O	2.49	0.45
1:B:109:ARG:NE	5:B:2121:HOH:O	2.49	0.45
2:B:1297:HEC:HBC3	2:B:1297:HEC:HMC1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1302:HEC:HBB3	2:B:1302:HEC:HMB1	1.99	0.45
1:B:43:LYS:HE2	5:B:2292:HOH:O	2.18	0.44
1:B:52:HIS:CE1	2:B:1295:HEC:ND	2.85	0.44
1:A:152:PRO:HD2	5:A:2149:HOH:O	2.18	0.44
2:B:1297:HEC:HBB3	2:B:1297:HEC:HMB1	2.01	0.43
2:A:1296:HEC:HMB1	2:A:1296:HEC:HBB3	2.01	0.42
1:A:243[B]:SER:OG	2:B:1298:HEC:HAA1	2.19	0.42
1:B:38:LEU:CD1	1:B:42:LYS:HE3	2.50	0.42
1:B:288:HIS:CD2	2:B:1302:HEC:ND	2.88	0.42
2:A:1298:HEC:HBC3	2:A:1298:HEC:HMC1	2.01	0.41
1:B:220:LYS:HE3	5:B:2217:HOH:O	2.21	0.41
1:A:203:SER:OG	1:A:207:ARG:NH2	2.54	0.40
1:B:26:LYS:NZ	5:B:2039:HOH:O	2.54	0.40

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	303/296 (102%)	295 (97%)	7 (2%)	1 (0%)	41	18
1	B	299/296 (101%)	292 (98%)	7 (2%)	0	100	100
All	All	602/592 (102%)	587 (98%)	14 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	258/249 (104%)	255 (99%)	3 (1%)	71	48
1	B	254/249 (102%)	248 (98%)	6 (2%)	49	19
All	All	512/498 (103%)	503 (98%)	9 (2%)	62	30

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	A	170	GLU
1	A	251	LYS
1	B	45	ASP
1	B	167	LYS
1	B	194	ASN
1	B	239	PRO
1	B	243[A]	SER
1	B	243[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	B	103	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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$
3	GOL	B	1305[A]	-	5,5,5	0.37	0	5,5,5	0.70	0
3	GOL	B	1304	-	5,5,5	0.55	0	5,5,5	1.71	2 (40%)
3	GOL	B	1305[B]	-	5,5,5	0.33	0	5,5,5	0.97	0
2	HEC	B	1296	1	26,50,50	1.93	2 (7%)	18,82,82	2.36	6 (33%)
2	HEC	B	1294	1	26,50,50	2.17	5 (19%)	18,82,82	2.03	7 (38%)
2	HEC	A	1299	1	26,50,50	1.59	2 (7%)	18,82,82	1.55	5 (27%)
2	HEC	A	1302	1	26,50,50	1.93	3 (11%)	18,82,82	1.92	5 (27%)
2	HEC	A	1300	1	26,50,50	2.00	2 (7%)	18,82,82	2.21	10 (55%)
2	HEC	A	1298	1	26,50,50	1.79	3 (11%)	18,82,82	1.90	5 (27%)
2	HEC	A	1295	1	26,50,50	1.95	4 (15%)	18,82,82	2.40	7 (38%)
2	HEC	A	1297	1	26,50,50	1.92	4 (15%)	18,82,82	2.21	7 (38%)
2	HEC	A	1294	1	26,50,50	1.97	4 (15%)	18,82,82	2.20	10 (55%)
2	HEC	B	1298	1	26,50,50	2.04	3 (11%)	18,82,82	2.18	7 (38%)
2	HEC	B	1299	1	26,50,50	1.76	2 (7%)	18,82,82	1.99	6 (33%)
2	HEC	A	1301	1	26,50,50	1.89	2 (7%)	18,82,82	2.67	9 (50%)
2	HEC	A	1296	1	26,50,50	1.89	2 (7%)	18,82,82	2.22	8 (44%)
2	HEC	B	1297	1	26,50,50	2.16	3 (11%)	18,82,82	1.91	6 (33%)
4	ACT	B	1303	-	1,3,3	1.08	0	0,3,3	0.00	-
3	GOL	A	1303	-	5,5,5	0.26	0	5,5,5	0.99	0
2	HEC	B	1295	1	26,50,50	1.74	3 (11%)	18,82,82	2.41	5 (27%)
2	HEC	B	1300	1	26,50,50	2.08	3 (11%)	18,82,82	2.02	7 (38%)
2	HEC	B	1302	1	26,50,50	1.83	3 (11%)	18,82,82	1.82	5 (27%)
3	GOL	B	1306	-	5,5,5	0.17	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	B	1301	1	26,50,50	1.92	4 (15%)	18,82,82	2.58	7 (38%)

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
3	GOL	B	1305[A]	-	-	2/4/4/4	-
3	GOL	B	1304	-	-	3/4/4/4	-
3	GOL	B	1305[B]	-	-	4/4/4/4	-
2	HEC	B	1296	1	-	0/6/54/54	-
2	HEC	B	1294	1	-	0/6/54/54	-
2	HEC	A	1299	1	-	0/6/54/54	-
2	HEC	A	1302	1	-	0/6/54/54	-
2	HEC	A	1300	1	-	0/6/54/54	-
2	HEC	A	1298	1	-	0/6/54/54	-
2	HEC	A	1295	1	-	0/6/54/54	-
2	HEC	A	1297	1	-	0/6/54/54	-
2	HEC	A	1294	1	-	0/6/54/54	-
2	HEC	B	1298	1	-	0/6/54/54	-
2	HEC	B	1299	1	-	0/6/54/54	-
2	HEC	A	1301	1	-	0/6/54/54	-
2	HEC	A	1296	1	-	0/6/54/54	-
2	HEC	B	1297	1	-	0/6/54/54	-
3	GOL	A	1303	-	-	2/4/4/4	-
2	HEC	B	1295	1	-	0/6/54/54	-
2	HEC	B	1300	1	-	0/6/54/54	-
2	HEC	B	1302	1	-	0/6/54/54	-
3	GOL	B	1306	-	-	0/4/4/4	-
2	HEC	B	1301	1	-	1/6/54/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1294	HEC	C3B-C2B	-8.02	1.32	1.40
2	B	1297	HEC	C3B-C2B	-7.15	1.33	1.40
2	A	1300	HEC	C3C-C2C	-6.70	1.33	1.40
2	B	1296	HEC	C3C-C2C	-6.69	1.33	1.40
2	B	1300	HEC	C3C-C2C	-6.55	1.33	1.40
2	B	1298	HEC	C3B-C2B	-6.41	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1295	HEC	C3B-C2B	-6.27	1.34	1.40
2	A	1302	HEC	C3B-C2B	-6.20	1.34	1.40
2	B	1297	HEC	C3C-C2C	-6.17	1.34	1.40
2	A	1296	HEC	C3C-C2C	-6.15	1.34	1.40
2	A	1301	HEC	C3C-C2C	-5.97	1.34	1.40
2	B	1300	HEC	C3B-C2B	-5.85	1.34	1.40
2	A	1300	HEC	C3B-C2B	-5.79	1.34	1.40
2	B	1298	HEC	C3C-C2C	-5.79	1.34	1.40
2	A	1294	HEC	C3C-C2C	-5.71	1.34	1.40
2	B	1301	HEC	C3B-C2B	-5.70	1.34	1.40
2	B	1295	HEC	C3B-C2B	-5.69	1.34	1.40
2	A	1294	HEC	C3B-C2B	-5.60	1.34	1.40
2	B	1302	HEC	C3B-C2B	-5.56	1.34	1.40
2	A	1297	HEC	C3B-C2B	-5.48	1.35	1.40
2	B	1299	HEC	C3B-C2B	-5.41	1.35	1.40
2	A	1297	HEC	C3C-C2C	-5.35	1.35	1.40
2	B	1301	HEC	C3C-C2C	-5.14	1.35	1.40
2	A	1301	HEC	C3B-C2B	-4.97	1.35	1.40
2	A	1298	HEC	C3C-C2C	-4.92	1.35	1.40
2	B	1294	HEC	C3C-C2C	-4.83	1.35	1.40
2	A	1298	HEC	C3B-C2B	-4.77	1.35	1.40
2	B	1302	HEC	C3C-C2C	-4.77	1.35	1.40
2	A	1295	HEC	C3C-C2C	-4.75	1.35	1.40
2	B	1299	HEC	C3C-C2C	-4.60	1.35	1.40
2	A	1299	HEC	C3C-C2C	-4.58	1.36	1.40
2	A	1296	HEC	C3B-C2B	-4.53	1.36	1.40
2	A	1299	HEC	C3B-C2B	-4.45	1.36	1.40
2	B	1296	HEC	C3B-C2B	-4.25	1.36	1.40
2	B	1295	HEC	C3C-C2C	-4.03	1.36	1.40
2	A	1302	HEC	C3C-C2C	-3.92	1.36	1.40
2	B	1301	HEC	CAD-C3D	2.63	1.55	1.52
2	A	1302	HEC	CAD-C3D	2.61	1.55	1.52
2	A	1295	HEC	CAD-C3D	2.54	1.55	1.52
2	B	1300	HEC	CAD-C3D	2.42	1.55	1.52
2	A	1297	HEC	C1D-ND	2.36	1.41	1.36
2	A	1294	HEC	C3B-C4B	2.33	1.47	1.43
2	B	1294	HEC	C3B-C4B	2.26	1.47	1.43
2	B	1302	HEC	C1B-NB	2.24	1.40	1.36
2	B	1294	HEC	CAD-C3D	2.21	1.55	1.52
2	B	1294	HEC	CMD-C2D	2.20	1.56	1.51
2	A	1294	HEC	CMD-C2D	2.17	1.56	1.51
2	B	1297	HEC	CAD-C3D	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1297	HEC	C3B-C4B	2.16	1.47	1.43
2	B	1301	HEC	C3C-C4C	2.13	1.46	1.43
2	B	1295	HEC	C3B-C4B	2.12	1.46	1.43
2	A	1295	HEC	C3B-C4B	2.06	1.46	1.43
2	A	1298	HEC	CAD-C3D	2.03	1.55	1.52
2	B	1298	HEC	C3B-C4B	2.01	1.46	1.43

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	HEC	CMC-C2C-C1C	-5.97	119.29	128.46
2	B	1296	HEC	CMC-C2C-C3C	5.96	132.83	125.82
2	B	1295	HEC	CMB-C2B-C1B	-5.55	119.93	128.46
2	A	1301	HEC	CMC-C2C-C3C	5.51	132.30	125.82
2	B	1295	HEC	CMB-C2B-C3B	5.31	132.06	125.82
2	B	1301	HEC	CMC-C2C-C3C	5.20	131.94	125.82
2	A	1301	HEC	CAA-CBA-CGA	5.19	121.39	112.67
2	B	1296	HEC	CMC-C2C-C1C	-5.05	120.70	128.46
2	B	1295	HEC	CMD-C2D-C1D	-4.65	121.32	128.46
2	A	1296	HEC	CMC-C2C-C3C	4.60	131.22	125.82
2	A	1295	HEC	CMD-C2D-C1D	-4.48	121.58	128.46
2	B	1294	HEC	CMB-C2B-C1B	-4.46	121.61	128.46
2	A	1296	HEC	CMC-C2C-C1C	-4.41	121.69	128.46
2	B	1298	HEC	CMC-C2C-C3C	4.29	130.86	125.82
2	A	1297	HEC	CMB-C2B-C3B	4.20	130.76	125.82
2	A	1295	HEC	CMC-C2C-C3C	4.12	130.67	125.82
2	A	1297	HEC	CMB-C2B-C1B	-4.12	122.13	128.46
2	A	1298	HEC	CMC-C2C-C1C	-4.09	122.18	128.46
2	B	1301	HEC	CMB-C2B-C1B	-3.83	122.58	128.46
2	A	1301	HEC	CMC-C2C-C1C	-3.82	122.59	128.46
2	A	1294	HEC	CMD-C2D-C1D	-3.77	122.66	128.46
2	A	1295	HEC	CMB-C2B-C1B	-3.77	122.68	128.46
2	B	1301	HEC	CMB-C2B-C3B	3.76	130.24	125.82
2	B	1298	HEC	CMC-C2C-C1C	-3.76	122.69	128.46
2	A	1301	HEC	CMB-C2B-C1B	-3.74	122.71	128.46
2	A	1302	HEC	CMD-C2D-C1D	-3.70	122.78	128.46
2	B	1298	HEC	CMB-C2B-C1B	-3.68	122.81	128.46
2	A	1300	HEC	CMD-C2D-C1D	-3.66	122.84	128.46
2	B	1299	HEC	CMC-C2C-C3C	3.63	130.08	125.82
2	A	1294	HEC	CBA-CAA-C2A	-3.59	105.86	112.48
2	B	1302	HEC	CMC-C2C-C3C	3.59	130.04	125.82
2	A	1295	HEC	CBD-CAD-C3D	-3.57	105.90	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1299	HEC	CMB-C2B-C1B	-3.57	122.98	128.46
2	A	1300	HEC	CMB-C2B-C1B	-3.55	123.00	128.46
2	A	1297	HEC	CMD-C2D-C1D	-3.51	123.07	128.46
2	A	1298	HEC	CMC-C2C-C3C	3.50	129.94	125.82
2	B	1299	HEC	CMC-C2C-C1C	-3.50	123.09	128.46
2	A	1295	HEC	CMC-C2C-C1C	-3.45	123.16	128.46
2	B	1300	HEC	CMC-C2C-C3C	3.39	129.80	125.82
2	A	1296	HEC	CMB-C2B-C1B	-3.38	123.26	128.46
2	B	1295	HEC	CMD-C2D-C3D	3.37	131.30	124.94
2	B	1297	HEC	CMB-C2B-C1B	-3.36	123.29	128.46
2	A	1302	HEC	CMB-C2B-C1B	-3.36	123.30	128.46
2	A	1294	HEC	CMB-C2B-C1B	-3.34	123.34	128.46
2	B	1294	HEC	CMB-C2B-C3B	3.34	129.74	125.82
2	B	1297	HEC	CMB-C2B-C3B	3.33	129.73	125.82
2	B	1300	HEC	CAA-CBA-CGA	3.30	118.21	112.67
2	B	1298	HEC	CMB-C2B-C3B	3.29	129.69	125.82
2	A	1301	HEC	CMA-C3A-C2A	3.27	131.10	124.94
2	B	1298	HEC	C1D-C2D-C3D	3.22	109.23	107.00
2	A	1302	HEC	CBD-CAD-C3D	-3.21	106.56	112.49
2	B	1300	HEC	CMC-C2C-C1C	-3.19	123.55	128.46
2	A	1299	HEC	CMC-C2C-C1C	-3.19	123.56	128.46
2	A	1295	HEC	CMB-C2B-C3B	3.16	129.54	125.82
2	A	1300	HEC	CBA-CAA-C2A	-3.16	106.66	112.48
2	A	1298	HEC	CMB-C2B-C1B	-3.15	123.62	128.46
3	B	1304	GOL	O2-C2-C1	3.10	122.78	109.12
2	A	1300	HEC	CMB-C2B-C3B	3.10	129.47	125.82
2	B	1294	HEC	CMD-C2D-C1D	-3.06	123.76	128.46
2	A	1295	HEC	CMD-C2D-C3D	3.01	130.61	124.94
2	B	1302	HEC	CMC-C2C-C1C	-3.00	123.86	128.46
2	B	1297	HEC	CMC-C2C-C3C	2.98	129.33	125.82
2	B	1297	HEC	C1D-C2D-C3D	2.97	109.06	107.00
2	B	1302	HEC	CMD-C2D-C1D	-2.97	123.90	128.46
2	A	1298	HEC	CMB-C2B-C3B	2.95	129.29	125.82
2	A	1296	HEC	CMD-C2D-C1D	-2.95	123.93	128.46
2	A	1302	HEC	CMB-C2B-C3B	2.95	129.29	125.82
2	A	1301	HEC	CMB-C2B-C3B	2.87	129.19	125.82
2	A	1294	HEC	CAA-CBA-CGA	2.86	117.47	112.67
2	A	1299	HEC	CMB-C2B-C1B	-2.83	124.11	128.46
2	B	1299	HEC	CMB-C2B-C3B	2.81	129.12	125.82
2	B	1300	HEC	CMB-C2B-C1B	-2.81	124.14	128.46
2	A	1296	HEC	CMB-C2B-C3B	2.79	129.10	125.82
2	A	1297	HEC	CMC-C2C-C3C	2.78	129.09	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	HEC	CAD-CBD-CGD	-2.78	108.01	112.67
2	A	1294	HEC	CMA-C3A-C2A	2.77	130.17	124.94
2	A	1297	HEC	CMC-C2C-C1C	-2.76	124.22	128.46
2	A	1294	HEC	CMC-C2C-C1C	-2.76	124.22	128.46
2	A	1299	HEC	CMC-C2C-C3C	2.75	129.06	125.82
2	A	1296	HEC	CAA-CBA-CGA	-2.69	108.16	112.67
2	B	1299	HEC	CBD-CAD-C3D	-2.68	107.55	112.49
2	A	1299	HEC	CBD-CAD-C3D	-2.67	107.55	112.49
2	B	1296	HEC	CMB-C2B-C3B	2.67	128.96	125.82
2	B	1294	HEC	CBD-CAD-C3D	-2.66	107.59	112.49
2	B	1300	HEC	CBA-CAA-C2A	-2.65	107.60	112.48
2	B	1296	HEC	C4C-C3C-C2C	2.60	109.16	106.35
2	A	1300	HEC	CMC-C2C-C1C	-2.60	124.47	128.46
2	B	1300	HEC	CMB-C2B-C3B	2.58	128.86	125.82
2	A	1300	HEC	CMC-C2C-C3C	2.54	128.81	125.82
2	B	1296	HEC	CMB-C2B-C1B	-2.53	124.58	128.46
2	B	1301	HEC	CMD-C2D-C1D	-2.52	124.58	128.46
2	A	1301	HEC	CMD-C2D-C1D	-2.50	124.62	128.46
2	A	1297	HEC	CAD-CBD-CGD	-2.45	108.56	112.67
2	B	1297	HEC	CMC-C2C-C1C	-2.45	124.70	128.46
2	B	1302	HEC	CMB-C2B-C1B	-2.45	124.70	128.46
2	A	1300	HEC	C4C-C3C-C2C	2.41	108.95	106.35
2	A	1298	HEC	CMD-C2D-C1D	-2.40	124.78	128.46
2	B	1297	HEC	CMD-C2D-C1D	-2.40	124.78	128.46
2	B	1299	HEC	CMD-C2D-C1D	-2.38	124.80	128.46
2	B	1295	HEC	CBD-CAD-C3D	-2.38	108.10	112.49
2	B	1300	HEC	CMD-C2D-C1D	-2.38	124.81	128.46
2	A	1302	HEC	CMD-C2D-C3D	2.34	129.35	124.94
2	B	1294	HEC	CBA-CAA-C2A	-2.34	108.17	112.48
2	B	1301	HEC	CMD-C2D-C3D	2.34	129.35	124.94
2	A	1301	HEC	C4C-C3C-C2C	2.30	108.84	106.35
2	A	1301	HEC	CBD-CAD-C3D	-2.30	108.25	112.49
2	B	1294	HEC	CMA-C3A-C2A	2.29	129.25	124.94
2	A	1294	HEC	CMD-C2D-C3D	2.28	129.24	124.94
2	A	1294	HEC	CMB-C2B-C3B	2.25	128.47	125.82
2	B	1298	HEC	CMD-C2D-C1D	-2.23	125.03	128.46
2	A	1294	HEC	CMC-C2C-C3C	2.19	128.40	125.82
2	A	1294	HEC	CAD-CBD-CGD	-2.19	108.99	112.67
2	A	1299	HEC	CMB-C2B-C3B	2.18	128.39	125.82
2	A	1296	HEC	CMD-C2D-C3D	2.17	129.04	124.94
2	A	1297	HEC	C1D-C2D-C3D	2.14	108.49	107.00
2	B	1302	HEC	C4C-C3C-C2C	2.13	108.66	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1298	HEC	CMA-C3A-C2A	2.11	128.91	124.94
2	A	1296	HEC	CMA-C3A-C2A	2.10	128.90	124.94
2	B	1301	HEC	CAD-CBD-CGD	-2.09	109.16	112.67
2	B	1294	HEC	C1D-C2D-C3D	2.07	108.44	107.00
2	B	1296	HEC	CMA-C3A-C2A	2.07	128.84	124.94
3	B	1304	GOL	O2-C2-C3	2.05	118.17	109.12
2	A	1300	HEC	C1D-C2D-C3D	2.05	108.42	107.00
2	A	1300	HEC	CMD-C2D-C3D	2.01	128.74	124.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1304	GOL	O1-C1-C2-C3
3	B	1304	GOL	C1-C2-C3-O3
3	B	1305[B]	GOL	O1-C1-C2-C3
3	B	1305[B]	GOL	C1-C2-C3-O3
3	B	1304	GOL	O1-C1-C2-O2
3	B	1305[B]	GOL	O2-C2-C3-O3
3	B	1305[B]	GOL	O1-C1-C2-O2
3	A	1303	GOL	O1-C1-C2-O2
2	B	1301	HEC	C2A-CAA-CBA-CGA
3	B	1305[A]	GOL	C1-C2-C3-O3
3	A	1303	GOL	O1-C1-C2-C3
3	B	1305[A]	GOL	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1305[A]	GOL	1	0
3	B	1305[B]	GOL	2	0
2	B	1296	HEC	2	0
2	B	1294	HEC	1	0
2	A	1299	HEC	1	0
2	A	1302	HEC	1	0
2	A	1300	HEC	1	0
2	A	1298	HEC	2	0
2	A	1295	HEC	1	0
2	B	1298	HEC	2	0
2	B	1299	HEC	2	0

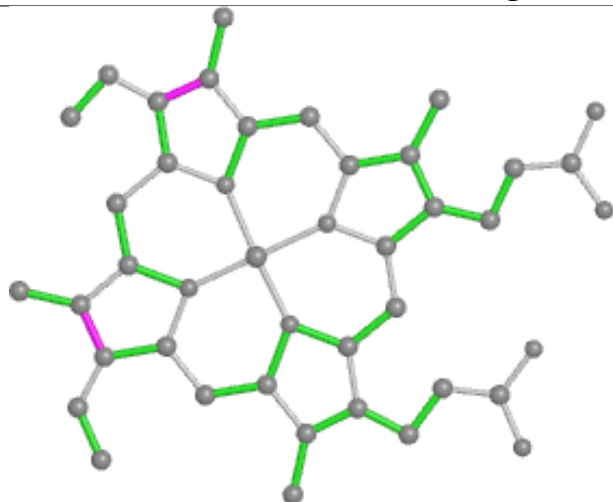
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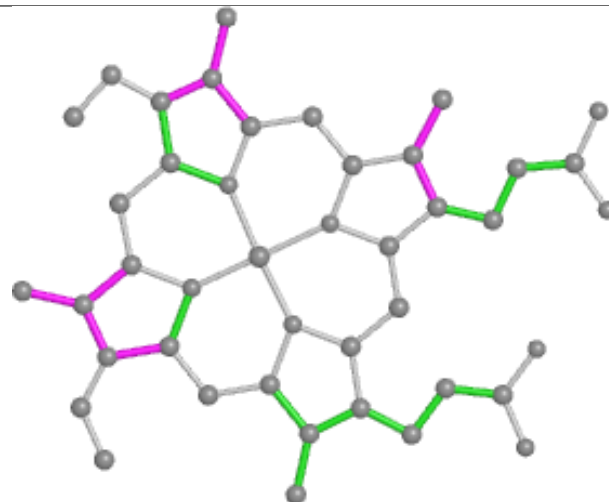
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	HEC	2	0
2	A	1296	HEC	2	0
2	B	1297	HEC	2	0
2	B	1295	HEC	2	0
2	B	1302	HEC	3	0
2	B	1301	HEC	3	0

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.

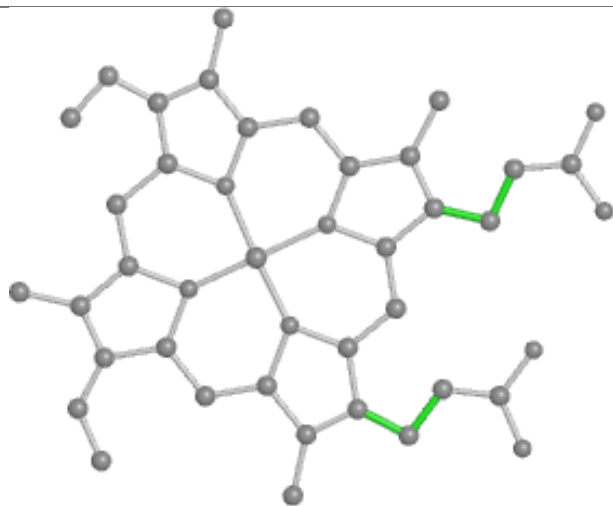
## Ligand HEC B 1296



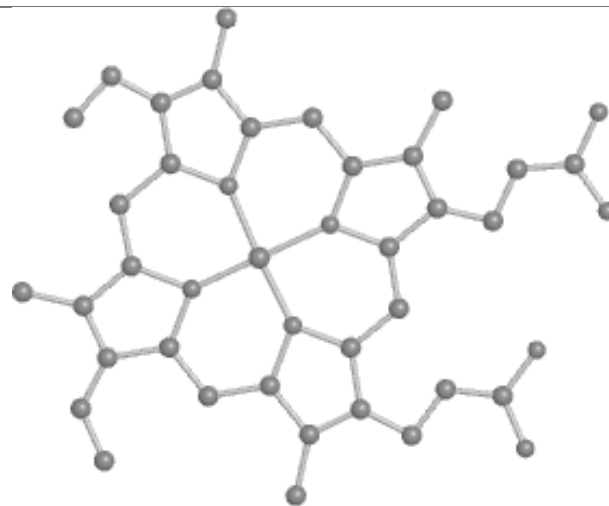
Bond lengths



Bond angles

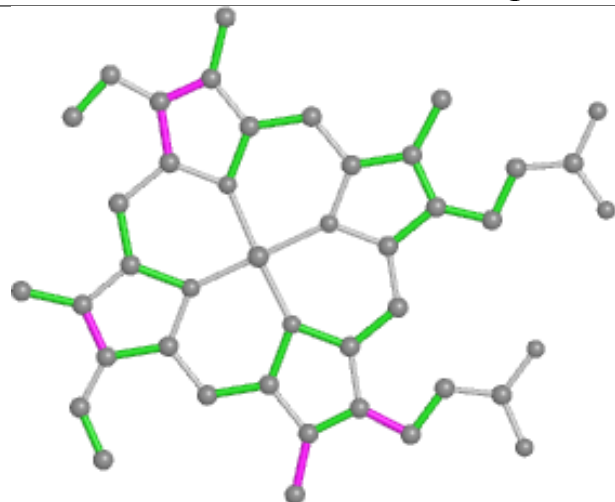


Torsions

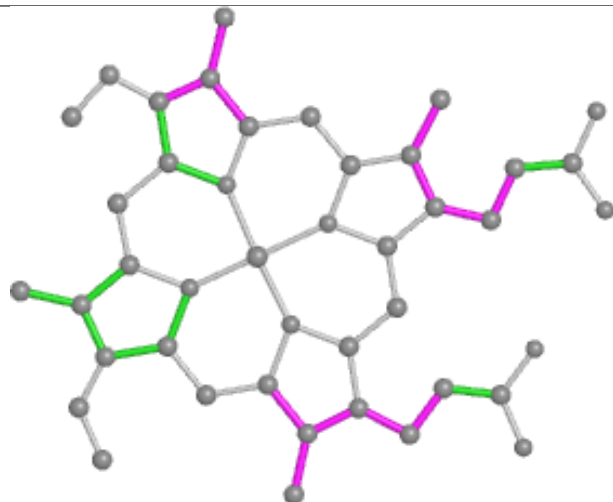


Rings

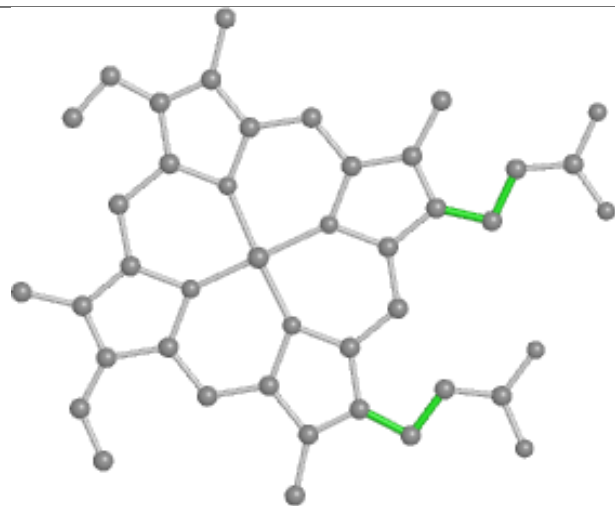
## Ligand HEC B 1294



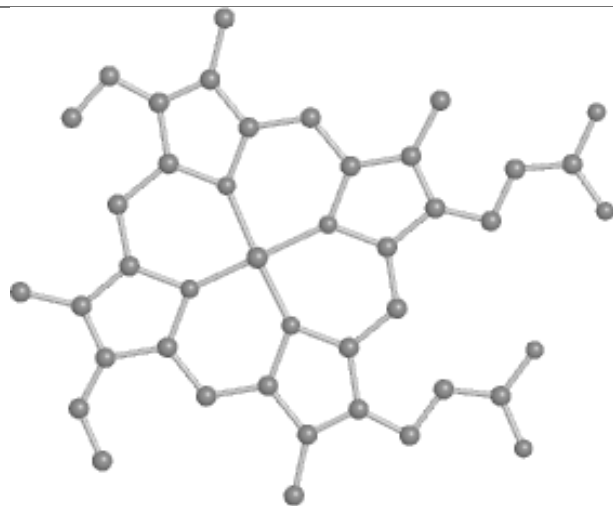
Bond lengths



Bond angles

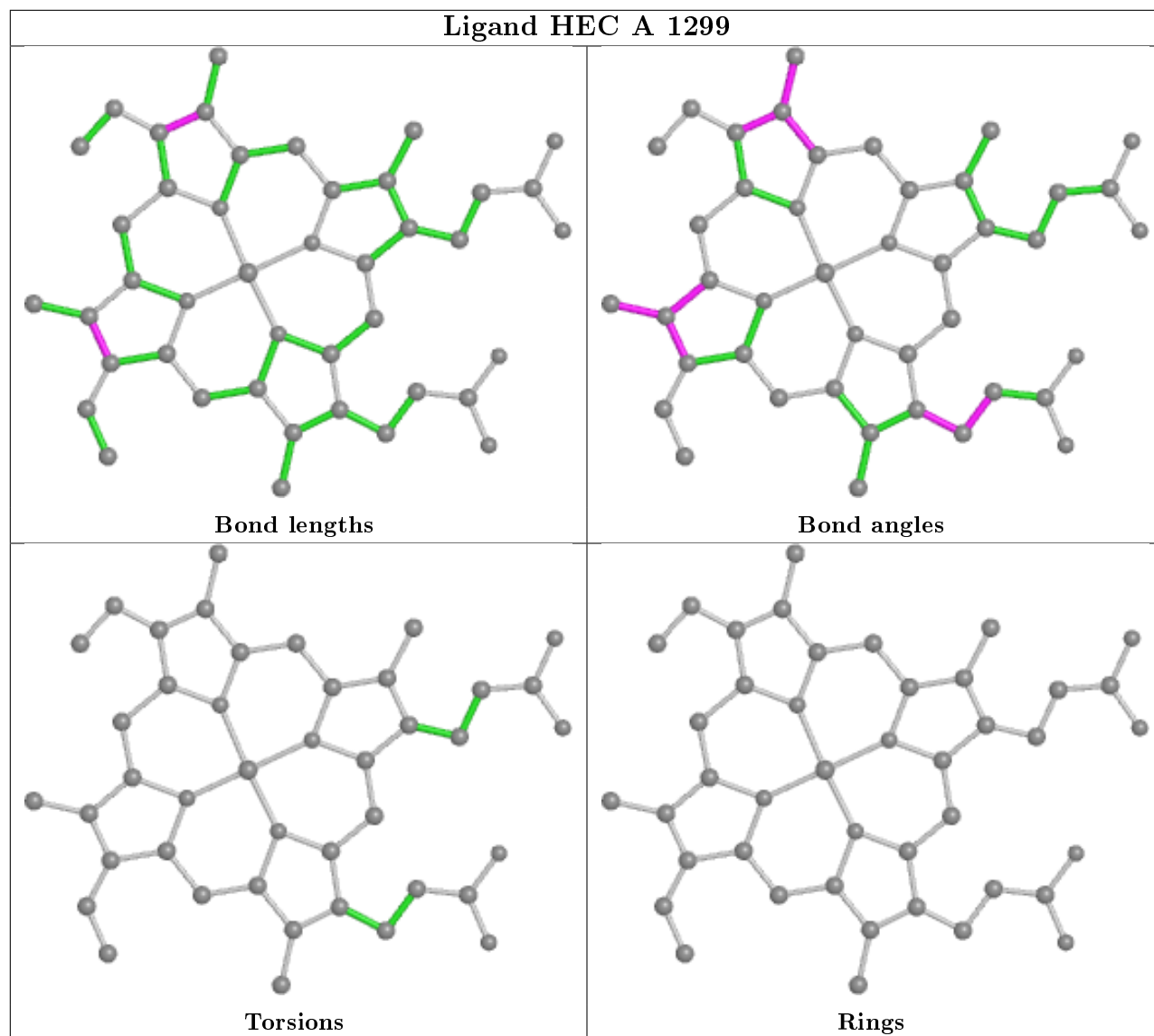


Torsions

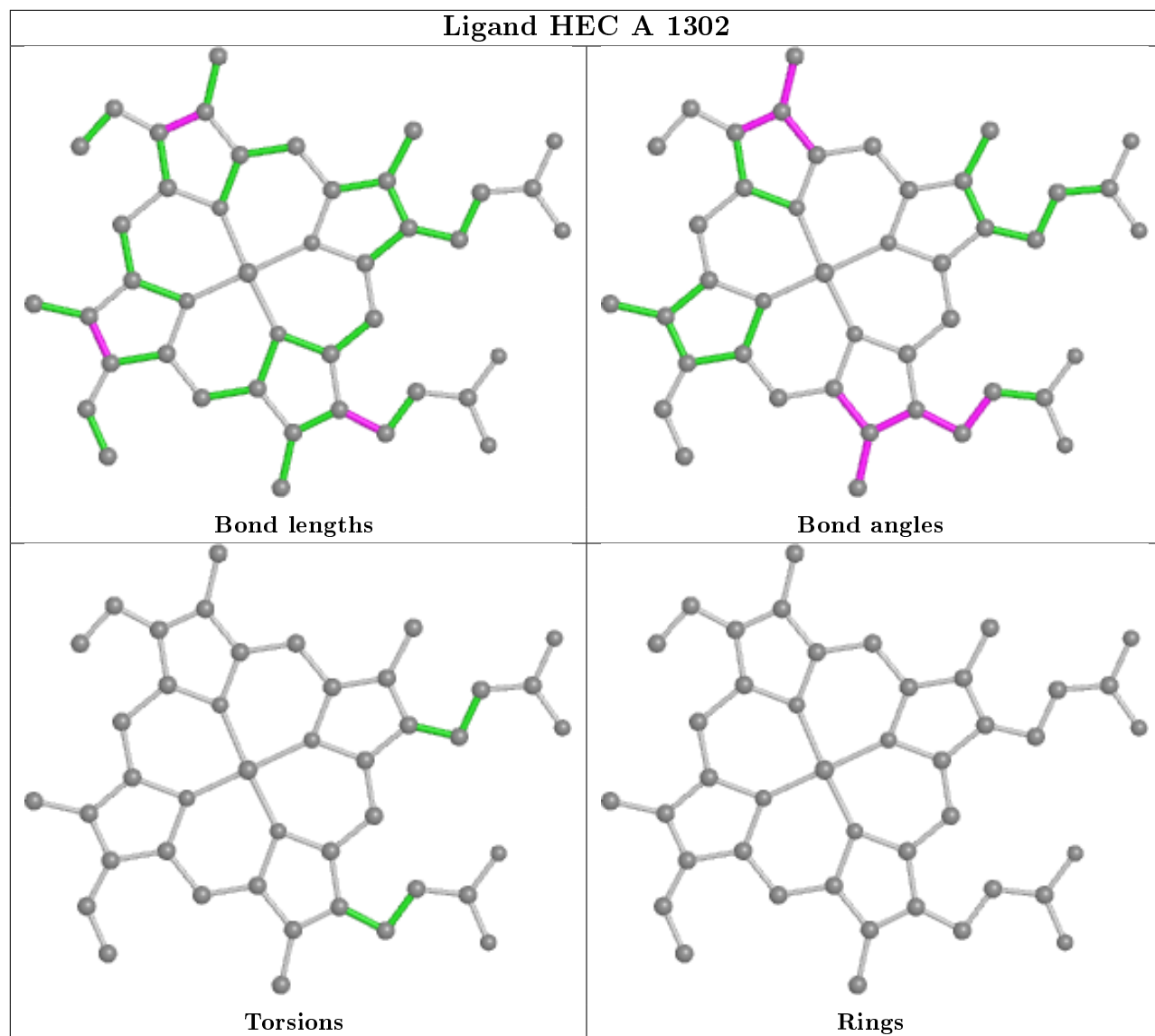


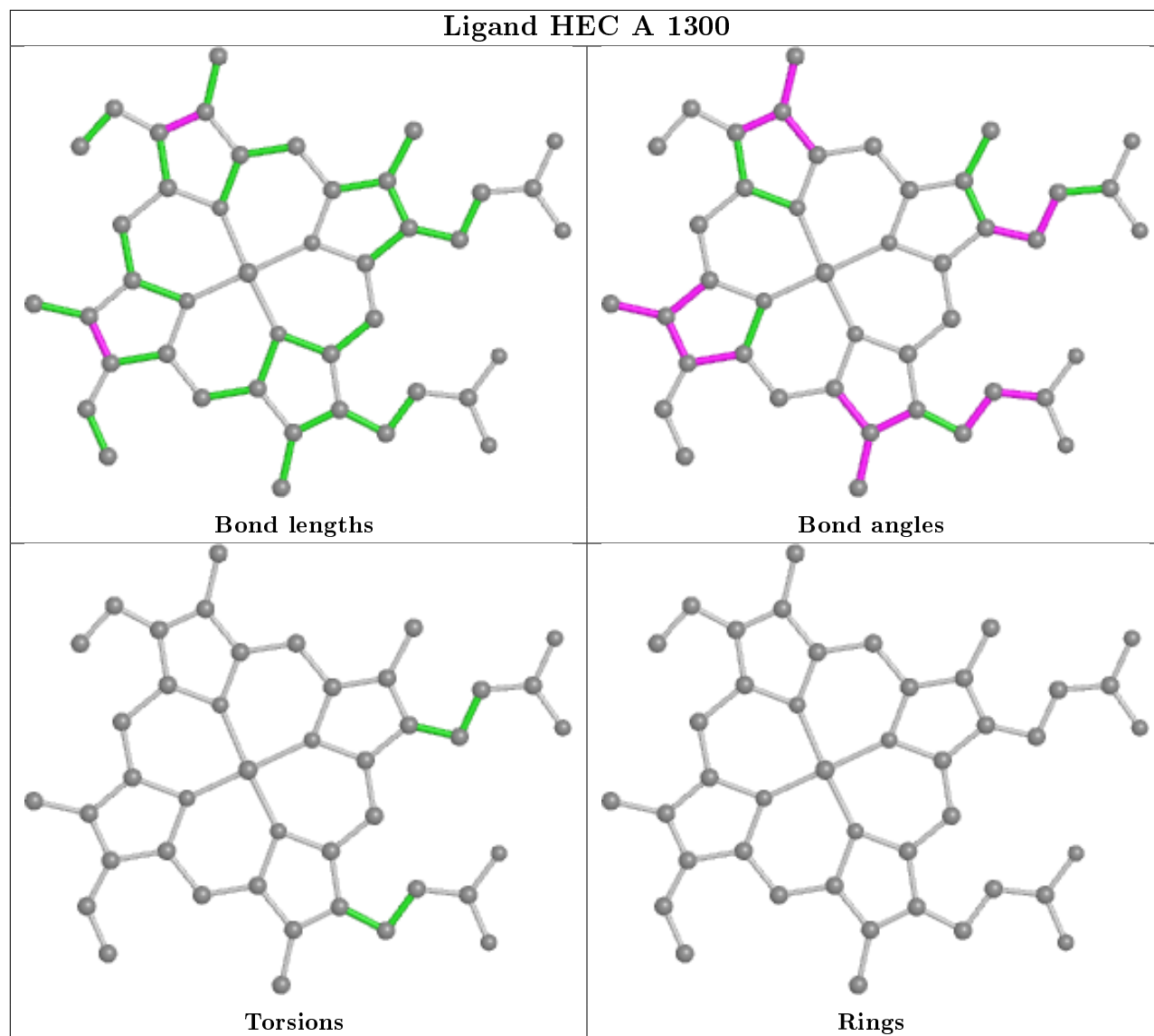
Rings

## Ligand HEC A 1299

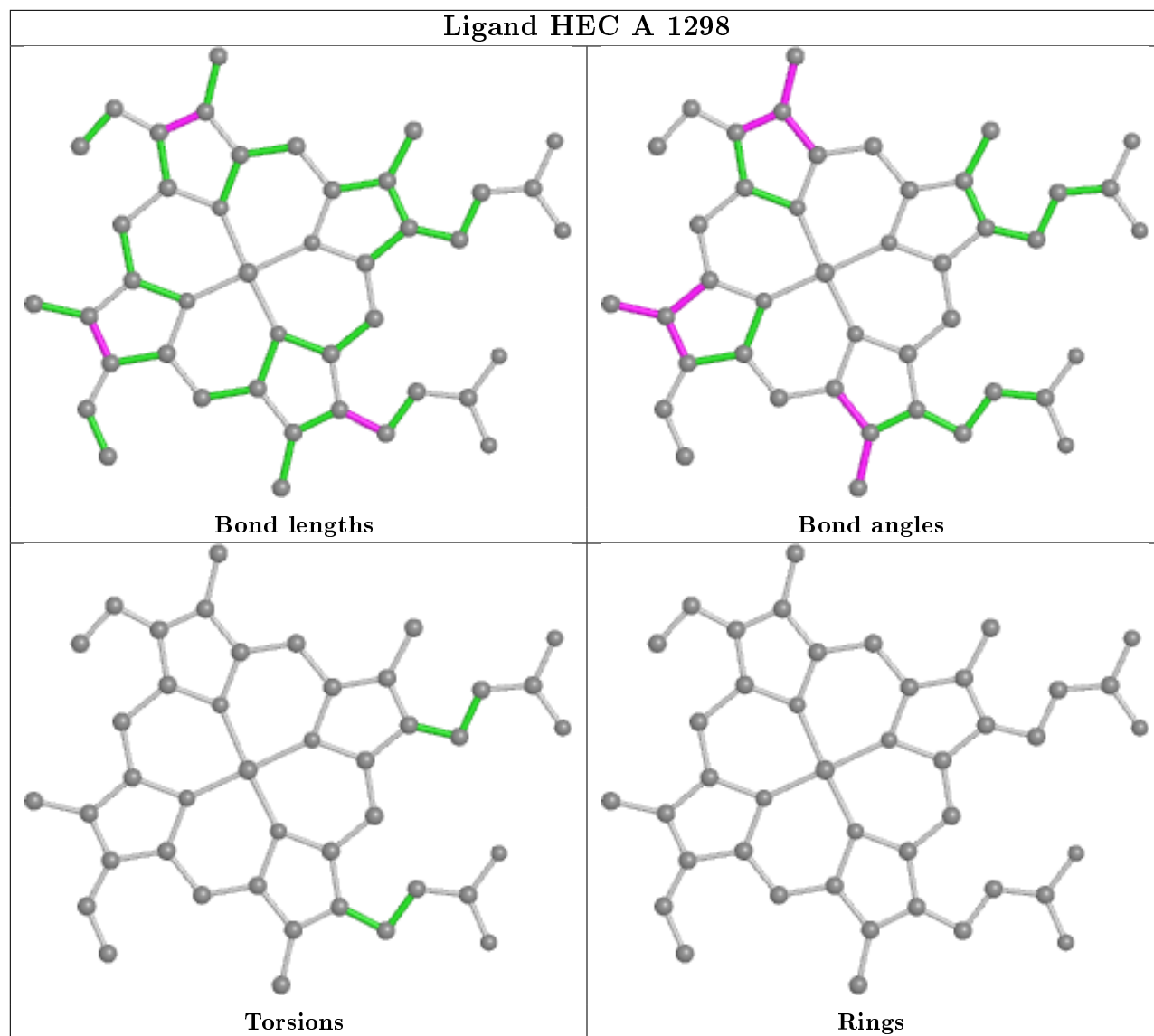


## Ligand HEC A 1302

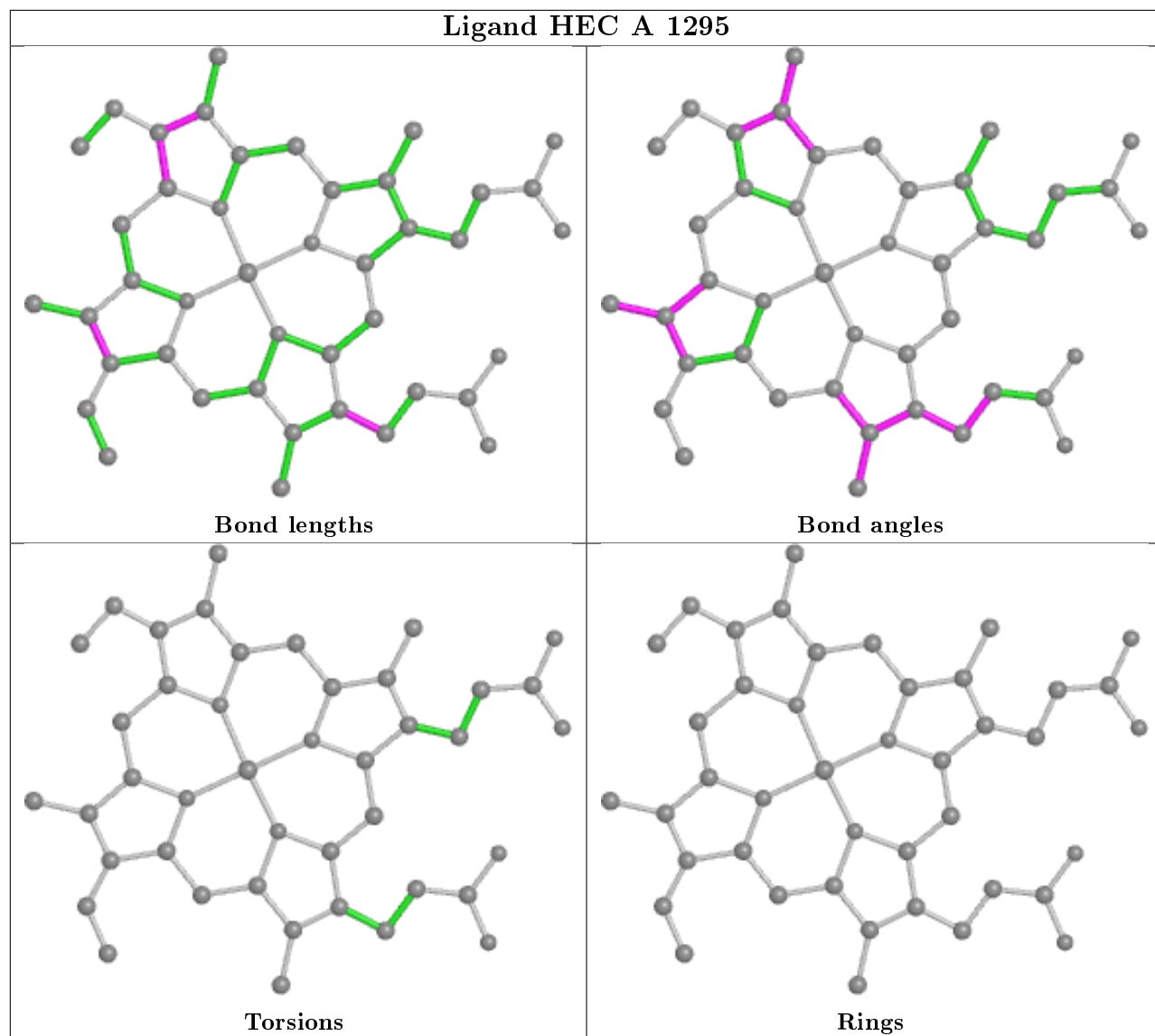




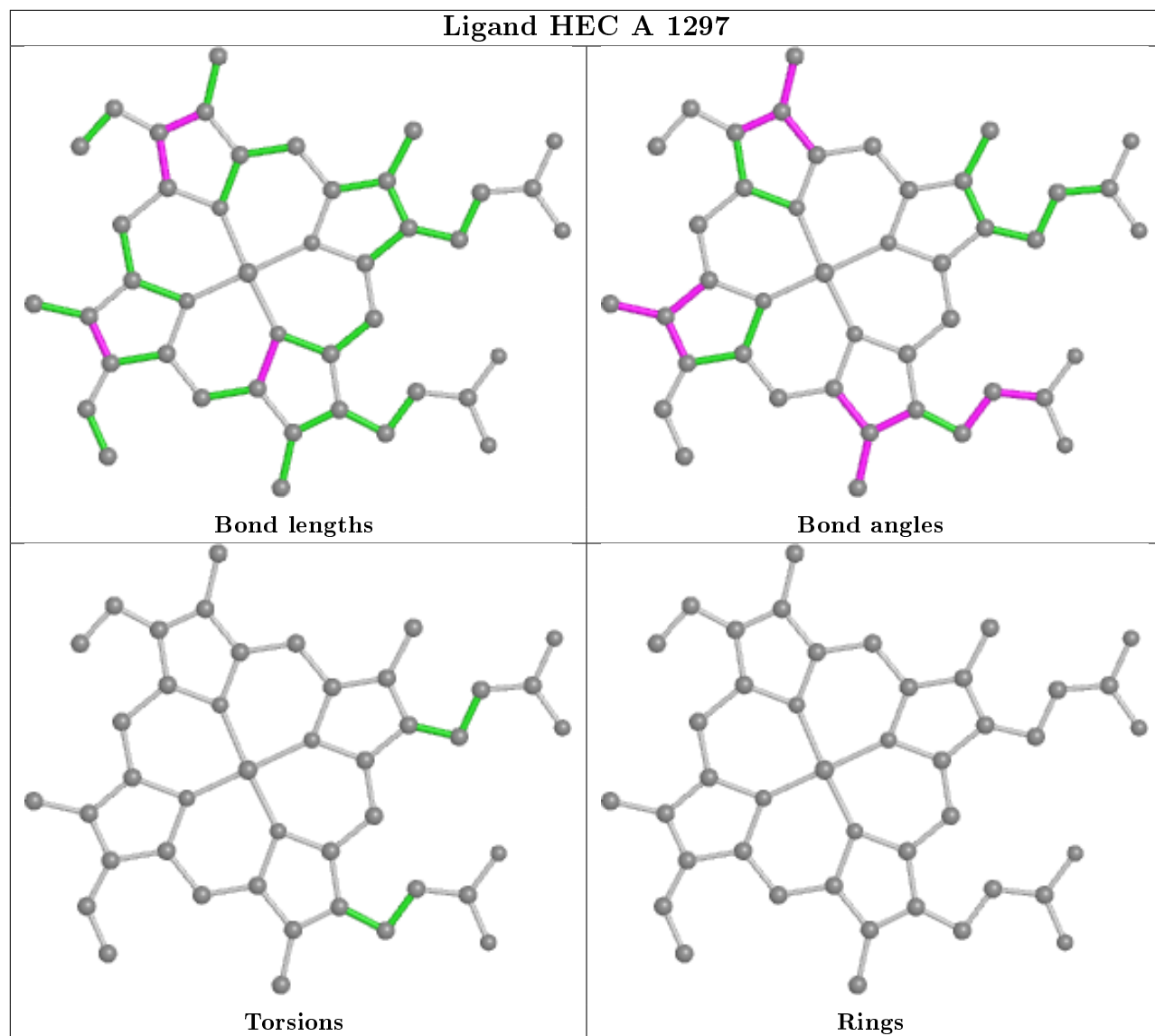
## Ligand HEC A 1298



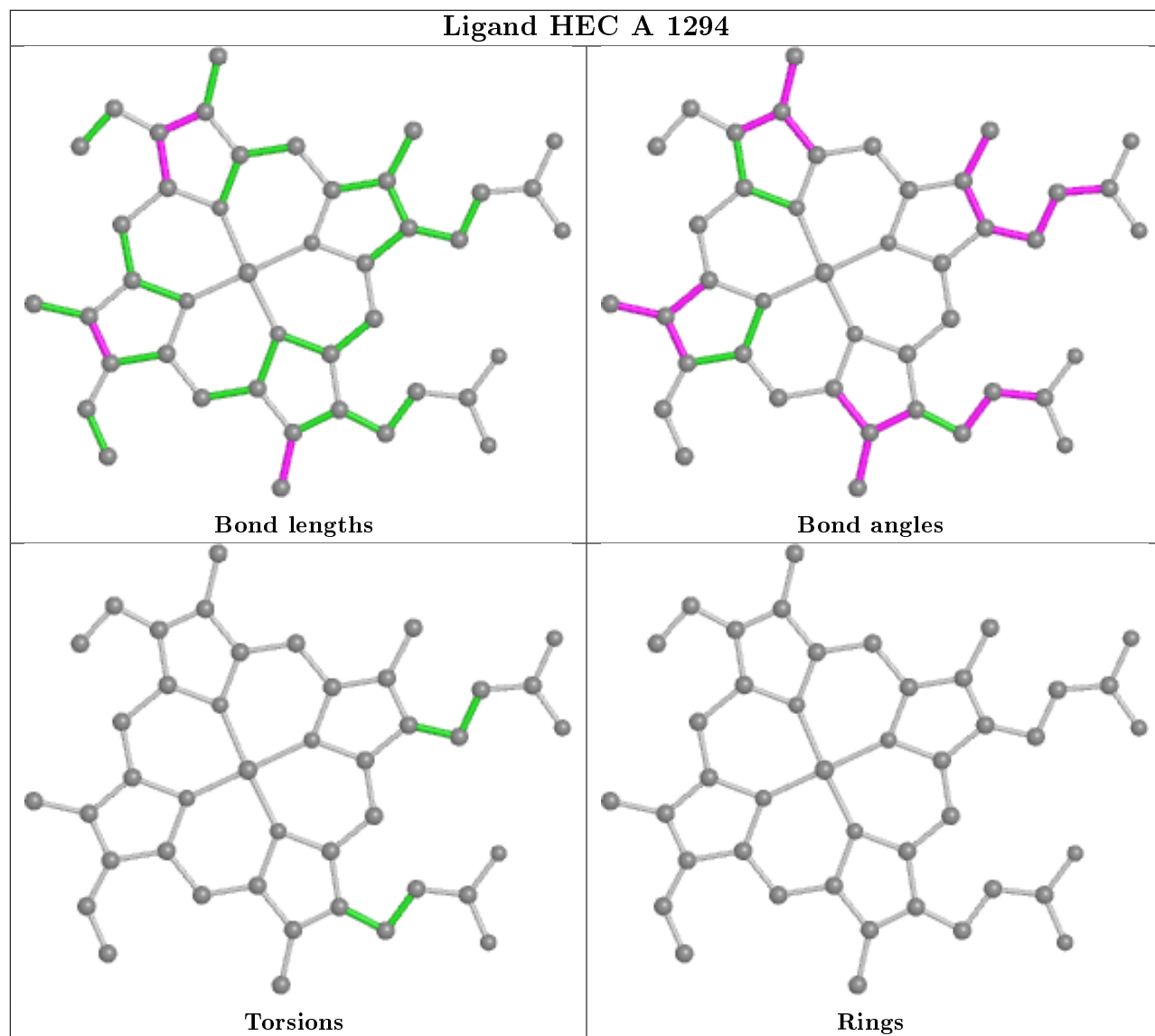
## Ligand HEC A 1295

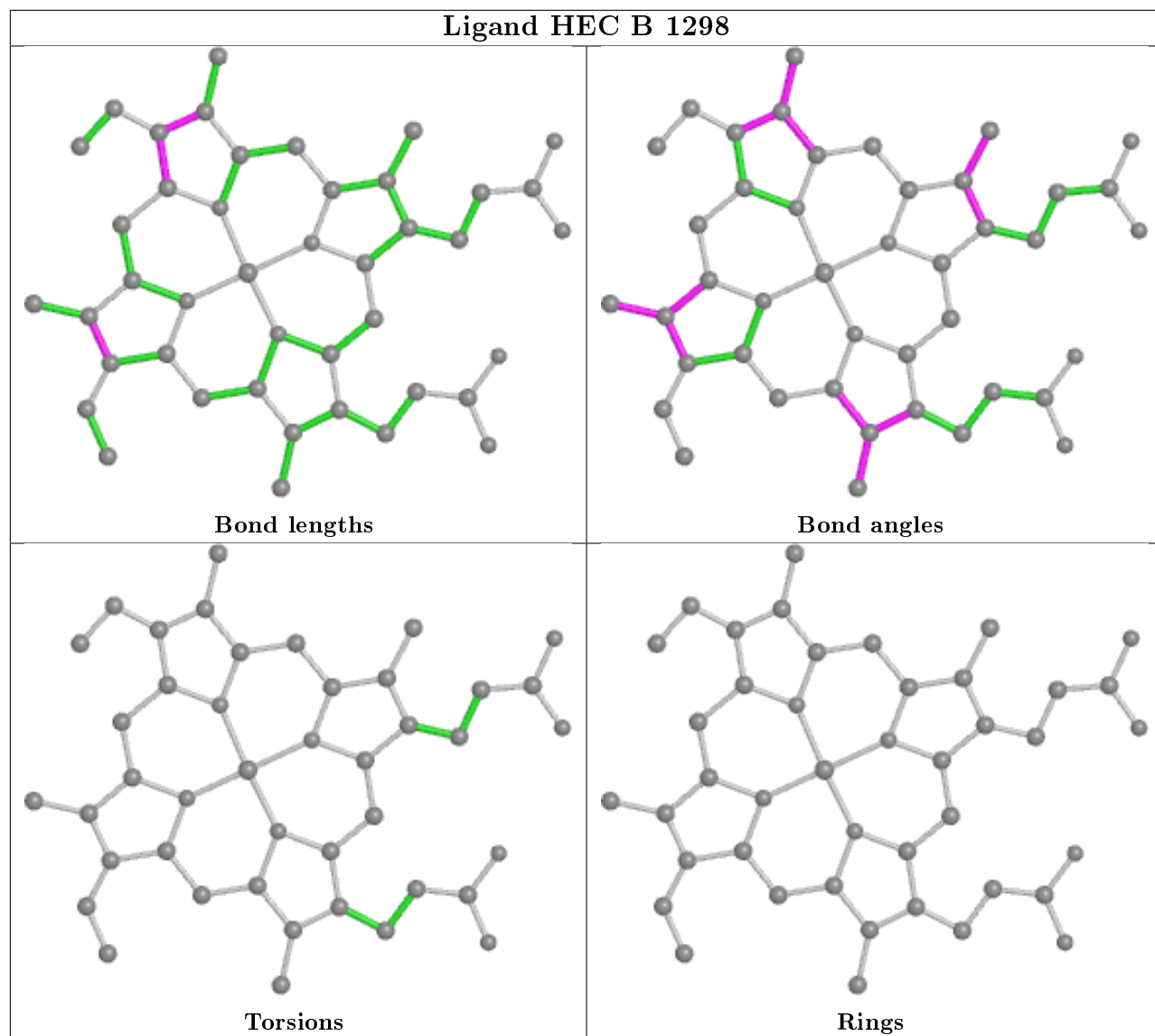


## Ligand HEC A 1297

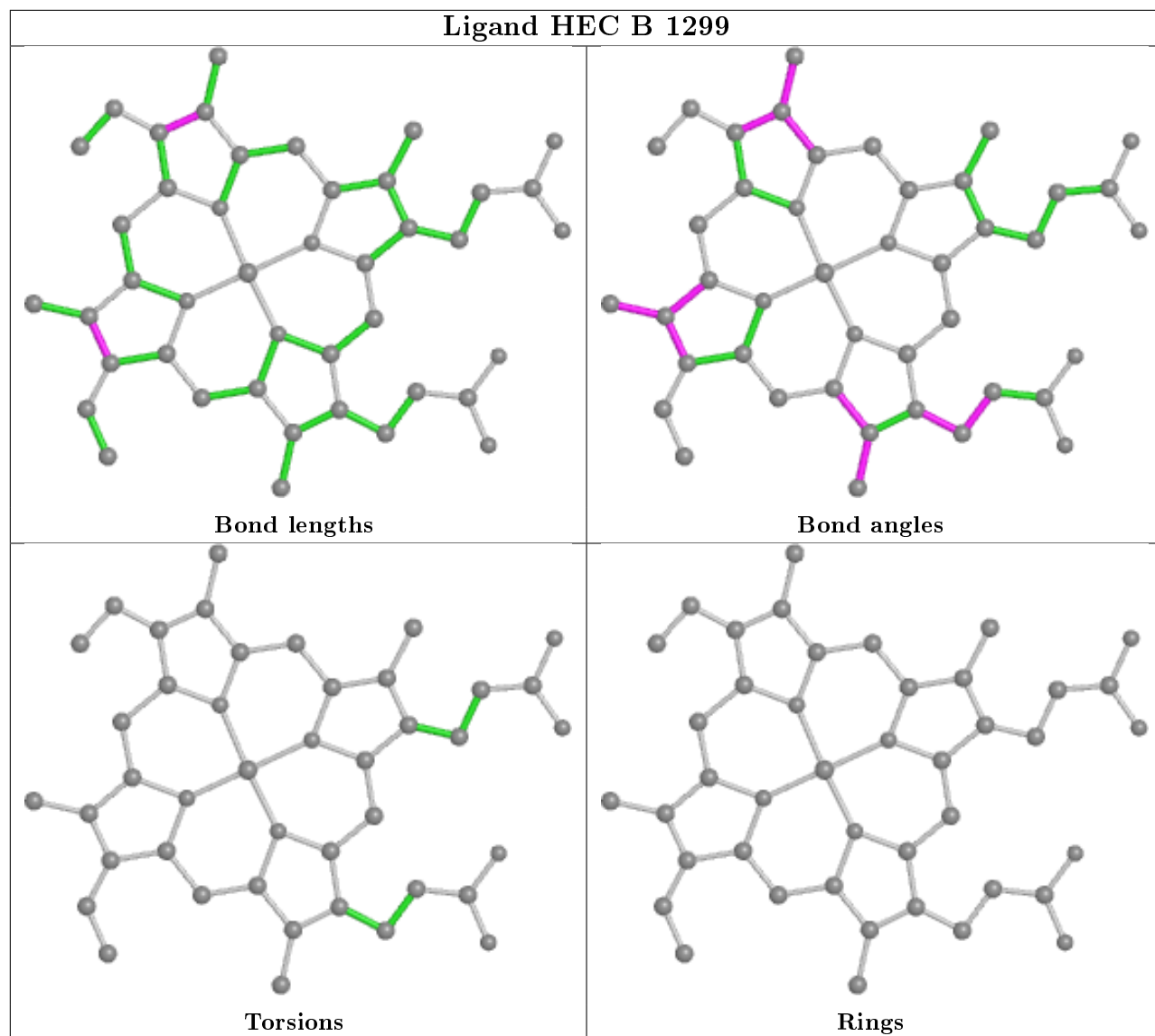


## Ligand HEC A 1294

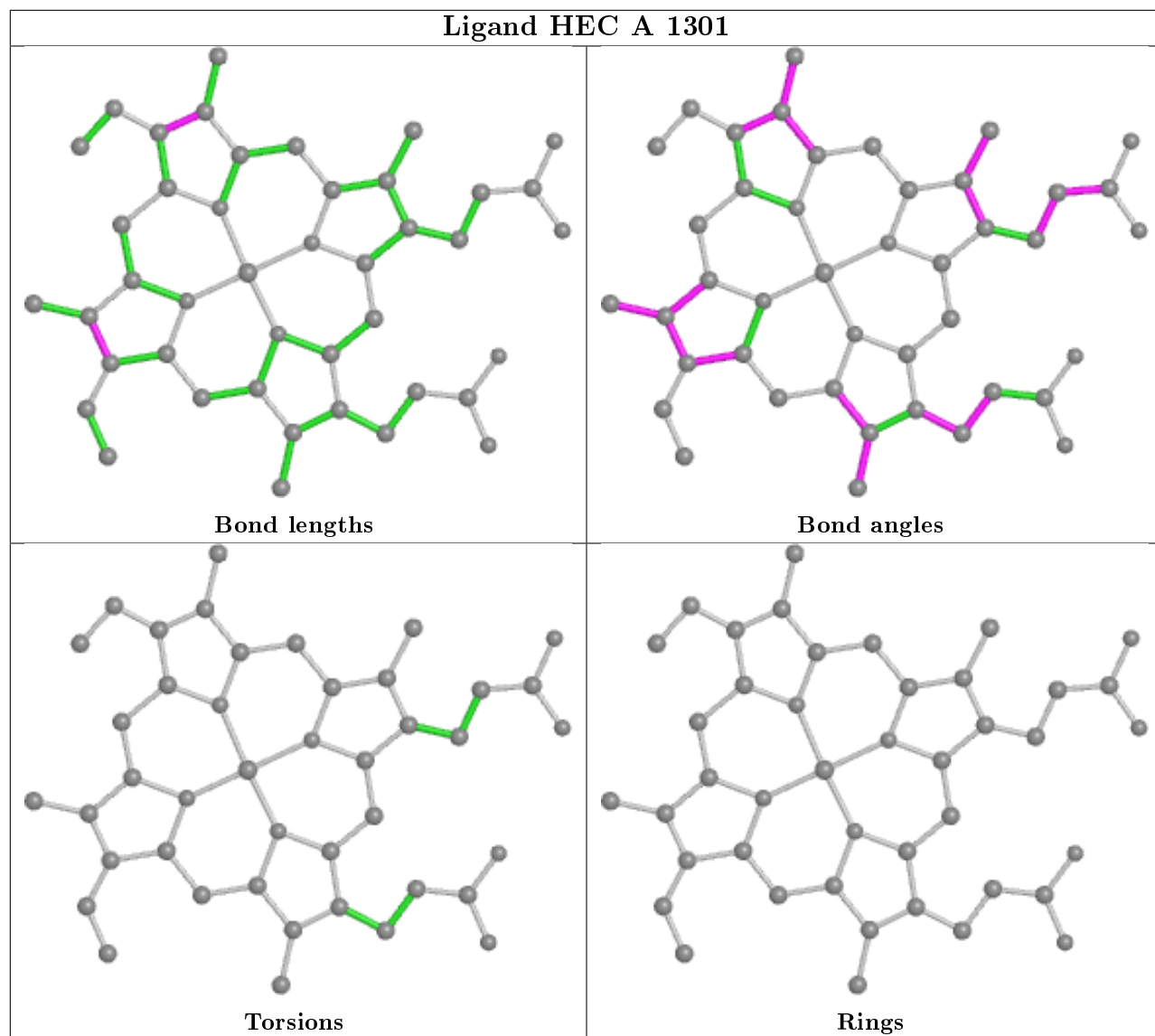




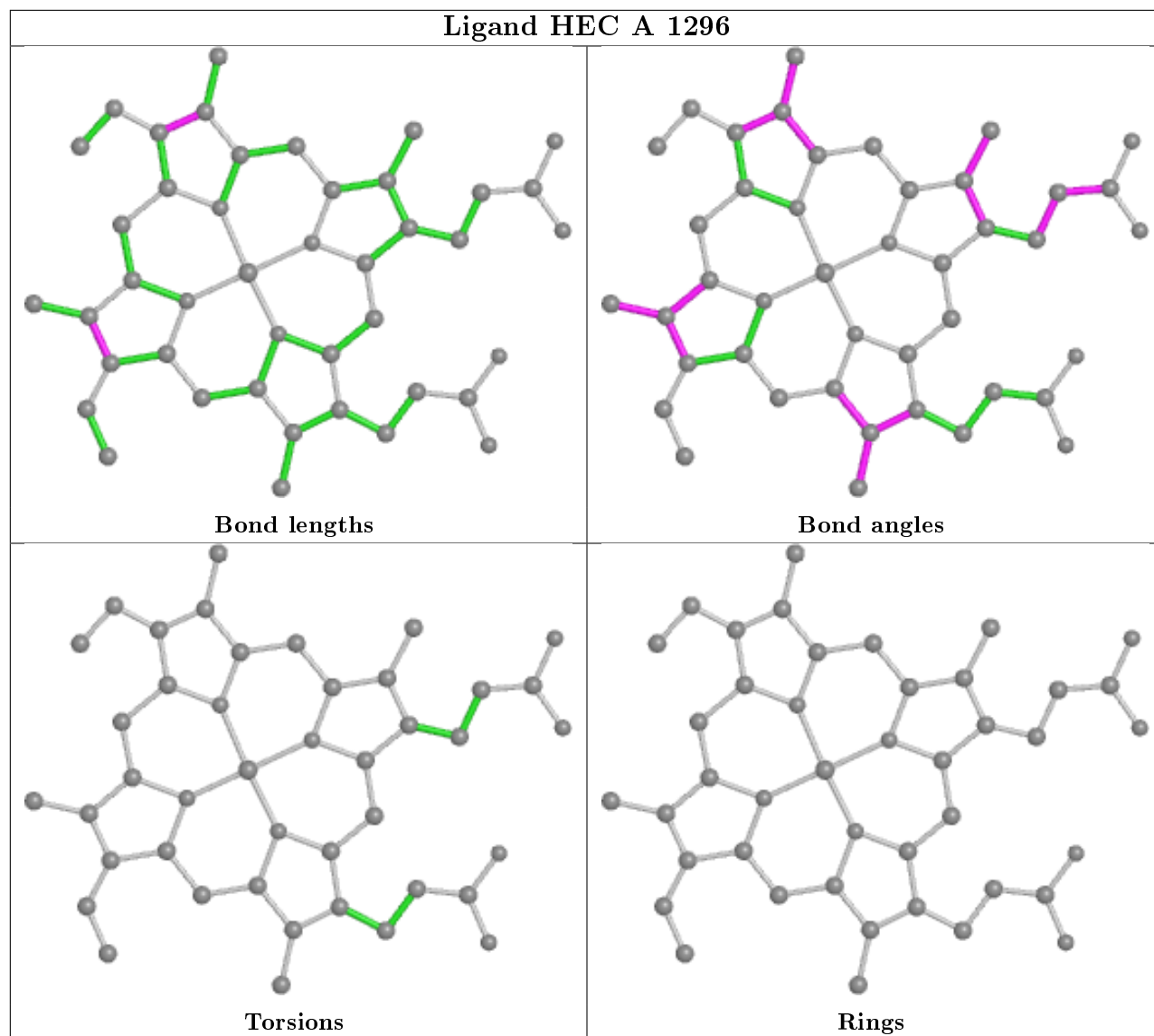
## Ligand HEC B 1299



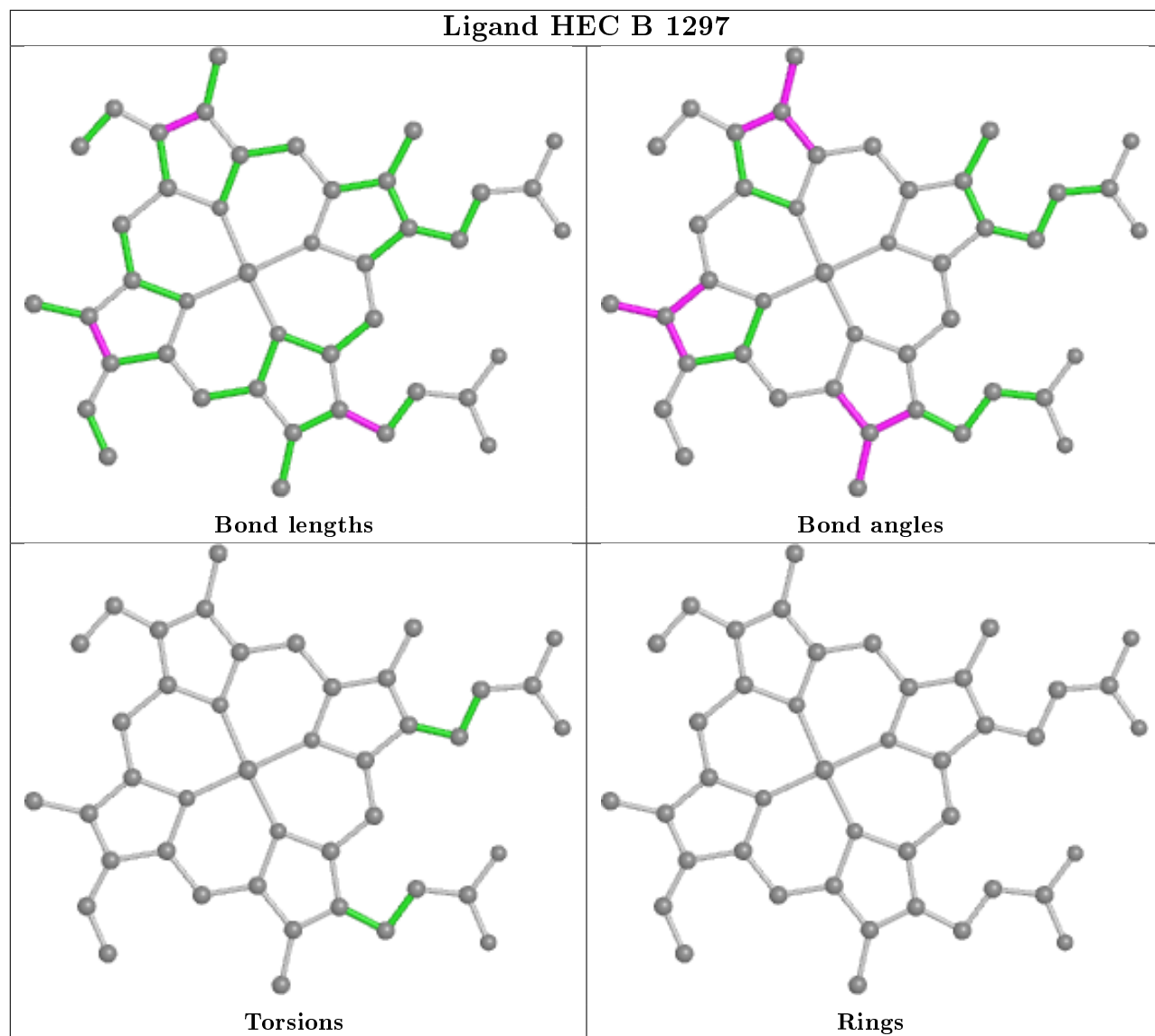
## Ligand HEC A 1301



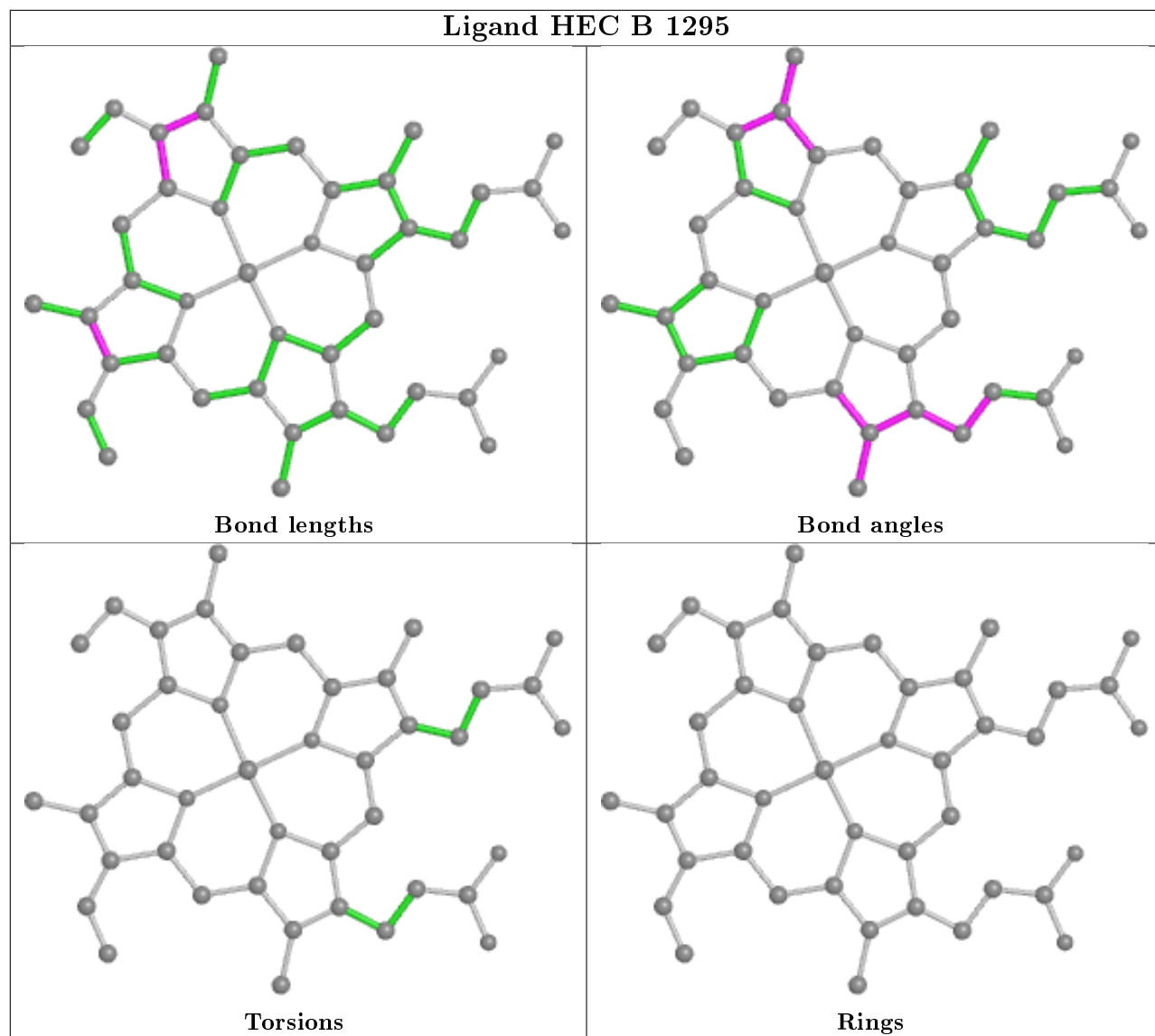
## Ligand HEC A 1296



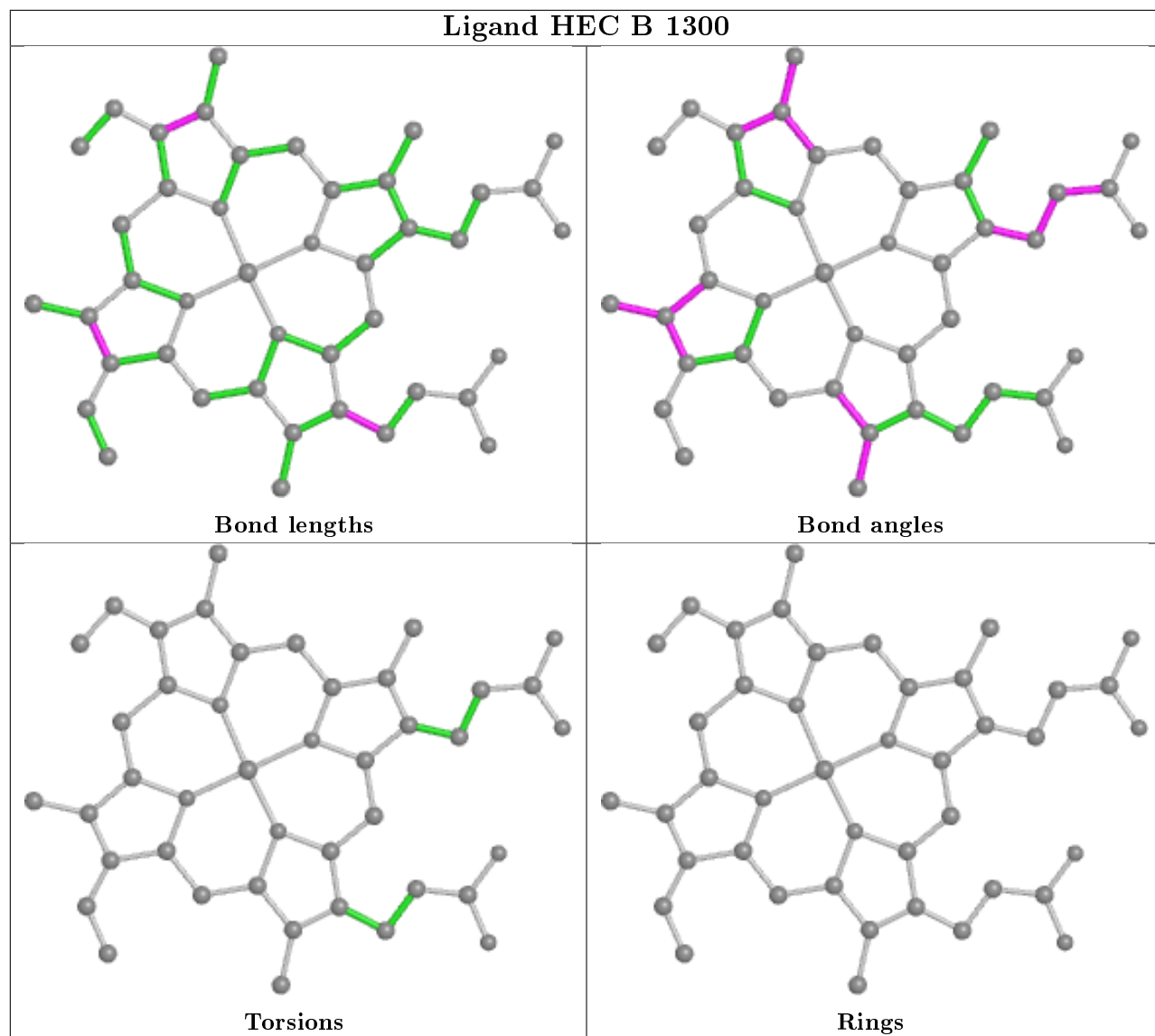
## Ligand HEC B 1297



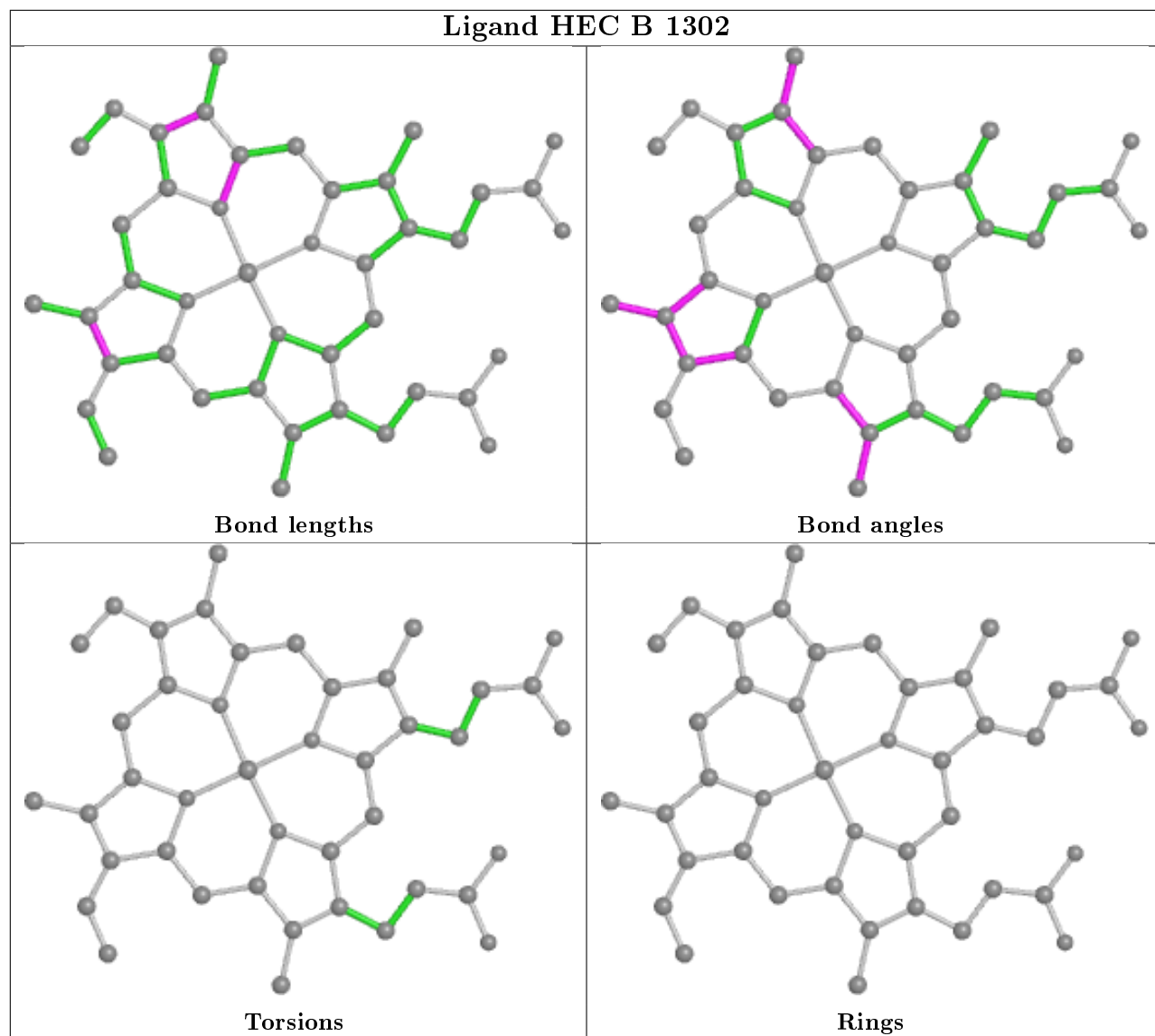
## Ligand HEC B 1295

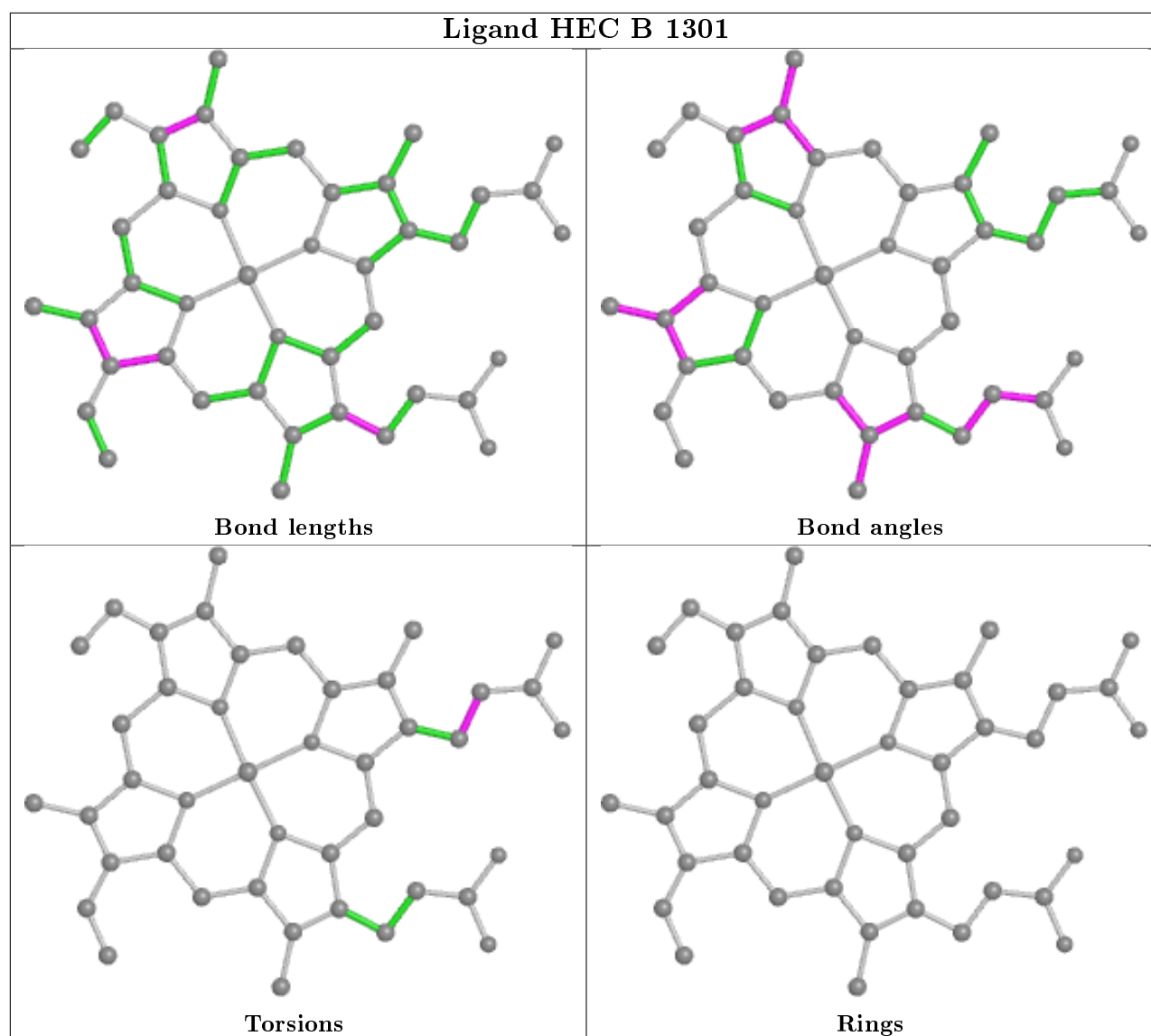


## Ligand HEC B 1300



## Ligand HEC B 1302





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.