



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 AM UTC

PDB ID : 1OFY / pdb_00001ofy
Title : three dimensional structure of the reduced 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 : 2.00 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

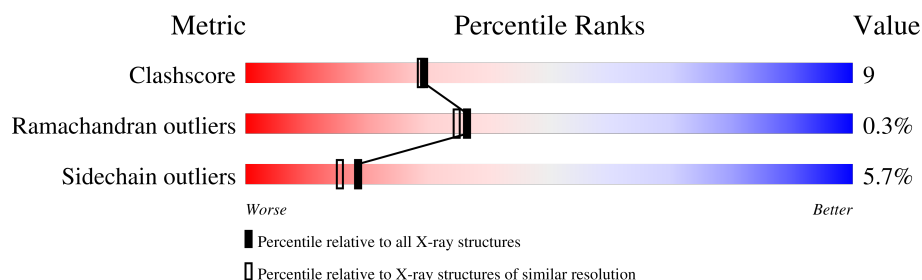
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 ≥ 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

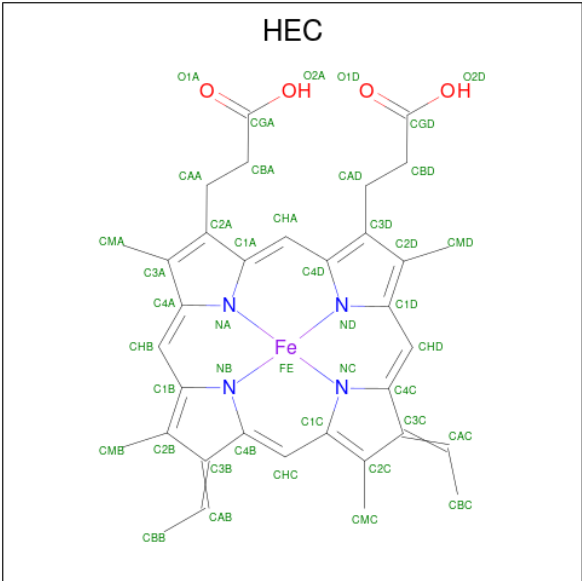
There are 5 unique types of molecules in this entry. The entry contains 5755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	22	4	1
			2223	1363	412	420	28			
1	B	293	Total	C	N	O	S	21	5	1
			2237	1371	413	425	28			

- Molecule 2 is HEME C (CCD ID: 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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	263	Total 263	O 263	0	0
5	B	242	Total 242	O 242	0	0

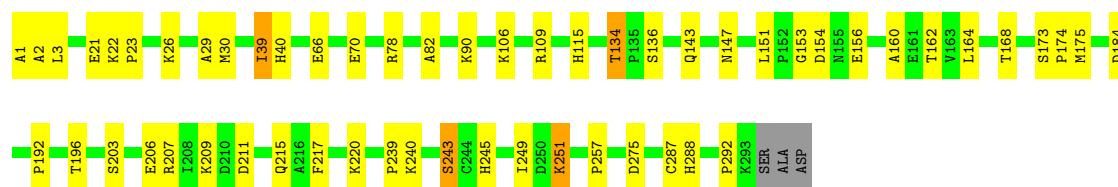
3 Residue-property plots

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.

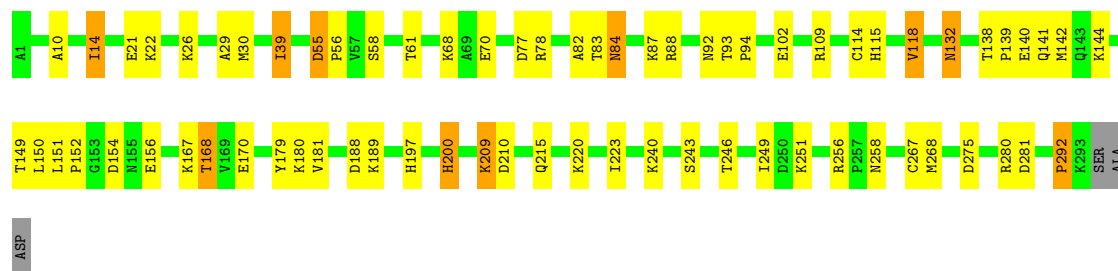
• Molecule 1: NINE HEME CYTOCHROME C

Chain A: 



• Molecule 1: NINE HEME CYTOCHROME C

Chain B: 



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, α , β , γ	60.40Å 105.66Å 80.94Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.7 (25.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.242 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ACT, GOL, 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	0.46	2/2297 (0.1%)	1.25	5/3117 (0.2%)
1	B	0.41	1/2304 (0.0%)	1.24	6/3127 (0.2%)
All	All	0.44	3/4601 (0.1%)	1.24	11/6244 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	PRO	C-N	-5.68	1.25	1.33
1	B	292	PRO	C-N	-5.46	1.25	1.33
1	A	2	ALA	N-CA	5.22	1.53	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	HIS	CA-CB-CG	-7.60	106.20	113.80
1	B	132	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	115	HIS	CA-CB-CG	-5.96	107.84	113.80
1	B	200	HIS	CA-CB-CG	5.62	119.42	113.80
1	A	217	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	1	ALA	O-C-N	5.53	131.85	123.00
1	A	196	THR	CA-C-N	5.53	128.47	120.79
1	A	196	THR	C-N-CA	5.53	128.47	120.79
1	B	83	THR	CA-C-N	-5.14	114.92	122.06
1	B	83	THR	C-N-CA	-5.14	114.92	122.06
1	B	14	ILE	N-CA-C	5.12	115.50	108.12

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	2223	0	2163	34	0
1	B	2237	0	2170	45	0
2	A	387	0	270	11	0
2	B	387	0	270	13	0
3	A	4	0	3	1	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	263	0	0	9	0
5	B	242	0	0	8	0
All	All	5755	0	4892	86	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.

All (86) 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:109:ARG:HH21	1:A:275:ASP:HB2	1.45	0.80
1:B:138:THR:OG1	1:B:141:GLN:HG3	1.84	0.78
1:B:68:LYS:HG3	1:B:70:GLU:OE1	1.85	0.76
1:A:39:ILE:HD12	2:A:1295:HEC:HBD1	1.70	0.74
1:B:152:PRO:O	1:B:156:GLU:HG3	1.90	0.71
1:A:109:ARG:NH2	1:A:275:ASP:HB2	2.08	0.68
1:B:21:GLU:HG2	5:B:2028:HOH:O	1.96	0.66
1:B:240:LYS:HG2	5:B:2231:HOH:O	1.97	0.64
1:B:144:LYS:HG2	1:B:149:THR:OG1	1.97	0.64
1:A:160:ALA:O	1:A:164:LEU:HG	1.98	0.63
1:A:211:ASP:O	1:A:215:GLN:HG3	1.98	0.62
1:A:175:MET:HE1	5:A:2168:HOH:O	1.99	0.61
1:B:151:LEU:HB2	1:B:154:ASP:OD2	1.99	0.61
1:B:92:ASN:O	1:B:94:PRO:HD3	2.01	0.60
1:A:39:ILE:CD1	2:A:1295:HEC:HBD1	2.33	0.58
2:A:1300:HEC:HMB1	2:A:1300:HEC:HBB3	1.84	0.58
1:B:88:ARG:HG2	1:B:93:THR:HA	1.87	0.57
2:A:1300:HEC:HBA2	5:A:2259:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:HG2	1:A:209:LYS:HE2	1.86	0.56
1:B:77:ASP:OD1	4:B:1302:GOL:H11	2.06	0.56
1:B:109:ARG:HD3	5:B:2109:HOH:O	2.05	0.56
2:B:1300:HEC:HMC1	2:B:1300:HEC:HBC3	1.88	0.55
1:A:70:GLU:HG2	5:A:2051:HOH:O	2.06	0.55
1:A:153:GLY:HA2	1:A:156:GLU:OE2	2.06	0.55
1:A:287:CYS:HB2	5:A:2240:HOH:O	2.05	0.55
1:B:246:THR:O	1:B:258:ASN:HB2	2.09	0.52
2:A:1293:HEC:HMB3	2:A:1293:HEC:HBB3	1.91	0.52
1:B:58:SER:OG	1:B:61:THR:HG23	2.11	0.51
1:B:78:ARG:O	1:B:82:ALA:HB2	2.10	0.51
2:A:1298:HEC:O2A	1:B:26:LYS:HD2	2.10	0.51
1:A:143:GLN:O	1:A:147:ASN:OD1	2.30	0.50
1:A:245:HIS:CE1	1:A:257:PRO:HD2	2.46	0.50
1:B:209[B]:LYS:O	1:B:210[B]:ASP:HB2	2.12	0.50
1:A:288:HIS:CD2	2:A:1301:HEC:ND	2.80	0.49
1:B:168:THR:CG2	1:B:215:GLN:HB3	2.42	0.49
1:A:184:ASP:HB3	1:A:192:PRO:HB3	1.94	0.48
1:B:179:TYR:CE2	1:B:180:LYS:HD3	2.49	0.48
1:B:102:GLU:OE1	2:B:1296:HEC:O2A	2.32	0.48
1:B:268:MET:HB3	1:B:281:ASP:OD1	2.14	0.48
5:A:2147:HOH:O	1:B:26:LYS:HE3	2.14	0.47
1:B:138:THR:HB	1:B:140:GLU:OE1	2.13	0.47
1:A:22:LYS:HA	1:A:23:PRO:HD3	1.85	0.46
1:B:200:HIS:HD2	2:B:1300:HEC:NC	2.07	0.46
1:A:239:PRO:HA	1:B:29:ALA:HA	1.98	0.46
1:A:173:SER:OG	1:A:175:MET:HB2	2.16	0.45
2:B:1296:HEC:HMB1	2:B:1296:HEC:HBB3	1.99	0.45
1:B:114:CYS:O	1:B:118:VAL:HG13	2.17	0.45
1:B:144:LYS:HB3	1:B:150:LEU:HB2	1.99	0.45
3:A:1302:ACT:H1	5:A:2263:HOH:O	2.16	0.45
1:A:70:GLU:OE1	1:A:70:GLU:N	2.49	0.44
1:B:156:GLU:HG2	5:B:2023:HOH:O	2.16	0.44
1:B:249:ILE:HD11	5:B:2098:HOH:O	2.16	0.44
1:B:84:ASN:OD1	1:B:84:ASN:N	2.50	0.44
1:A:203:SER:OG	1:A:207:ARG:NH2	2.50	0.44
1:A:40:HIS:CE1	2:A:1295:HEC:NA	2.86	0.44
1:A:106:LYS:NZ	5:A:2091:HOH:O	2.50	0.44
1:A:3:LEU:HD13	5:A:2029:HOH:O	2.18	0.44
1:B:30:MET:HG3	2:B:1297:HEC:C4A	2.48	0.43
1:B:197:HIS:CE1	2:B:1298:HEC:NB	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASP:HA	1:B:56:PRO:HD3	1.92	0.43
1:B:220:LYS:NZ	1:B:223:ILE:HD12	2.33	0.43
1:A:240:LYS:O	1:A:243:SER:HB2	2.19	0.43
1:B:88:ARG:HH21	2:B:1294:HEC:CGD	2.31	0.43
1:A:78:ARG:O	1:A:82:ALA:HB2	2.19	0.43
1:A:29:ALA:HB1	2:A:1297:HEC:O2A	2.18	0.42
1:A:245:HIS:HE1	1:A:257:PRO:HD2	1.83	0.42
1:B:30:MET:HE2	2:B:1297:HEC:C1B	2.50	0.42
1:B:181:VAL:HG11	2:B:1298:HEC:HAD1	2.02	0.42
1:B:39:ILE:HD12	2:B:1295:HEC:HBD1	2.01	0.41
1:A:251:LYS:HB2	5:A:2211:HOH:O	2.18	0.41
1:B:132:ASN:HB2	5:B:2126:HOH:O	2.20	0.41
1:A:151:LEU:O	1:A:154:ASP:N	2.51	0.41
1:B:267:CYS:HA	2:B:1300:HEC:HHC	2.03	0.41
1:A:134:THR:HG22	1:A:162:THR:OG1	2.20	0.41
1:B:68:LYS:HE3	5:B:2078:HOH:O	2.20	0.41
2:A:1300:HEC:HMC3	2:A:1300:HEC:HBC3	2.03	0.41
1:B:10:ALA:HB2	2:B:1293:HEC:C4A	2.51	0.41
1:B:58:SER:O	1:B:61:THR:HG23	2.20	0.41
1:A:245:HIS:CE1	2:A:1299:HEC:NA	2.89	0.40
1:A:30:MET:HE3	1:A:30:MET:HB3	1.95	0.40
1:A:168:THR:CG2	1:A:215:GLN:HB3	2.51	0.40
1:A:173:SER:HA	1:A:174:PRO:HD3	1.98	0.40
1:B:139:PRO:O	1:B:142:MET:HB3	2.21	0.40
2:B:1298:HEC:HBD2	5:B:2231:HOH:O	2.21	0.40

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 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	295/296 (100%)	288 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	296/296 (100%)	281 (95%)	13 (4%)	2 (1%)	18	14
All	All	591/592 (100%)	569 (96%)	20 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP
1	B	292	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	250/249 (100%)	239 (96%)	11 (4%)	25	24
1	B	251/249 (101%)	233 (93%)	18 (7%)	13	10
All	All	501/498 (101%)	472 (94%)	29 (6%)	18	15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	26	LYS
1	A	39	ILE
1	A	66	GLU
1	A	90	LYS
1	A	134	THR
1	A	136	SER
1	A	220	LYS
1	A	243	SER
1	A	249	ILE
1	A	251	LYS
1	B	14	ILE
1	B	22	LYS
1	B	39	ILE

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Mol	Chain	Res	Type
1	B	55	ASP
1	B	84	ASN
1	B	87	LYS
1	B	118	VAL
1	B	167	LYS
1	B	168	THR
1	B	170	GLU
1	B	189	LYS
1	B	209[A]	LYS
1	B	209[B]	LYS
1	B	243	SER
1	B	251	LYS
1	B	256	ARG
1	B	275	ASP
1	B	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	103	GLN
1	B	72	ASN
1	B	143	GLN
1	B	194	ASN
1	B	266	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 oligosaccharides in this entry.

5.6 Ligand geometry

21 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
2	HEC	B	1299	1	46,50,50	1.53	2 (4%)	58,82,82	1.57	3 (5%)
2	HEC	A	1293	1	46,50,50	1.52	2 (4%)	58,82,82	1.39	2 (3%)
2	HEC	A	1294	1	46,50,50	1.52	2 (4%)	58,82,82	1.54	2 (3%)
2	HEC	A	1300	1	46,50,50	1.50	3 (6%)	58,82,82	1.40	6 (10%)
2	HEC	A	1297	1	46,50,50	1.50	2 (4%)	58,82,82	1.47	5 (8%)
2	HEC	B	1300	1	46,50,50	1.50	2 (4%)	58,82,82	1.28	2 (3%)
2	HEC	A	1301	1	46,50,50	1.53	2 (4%)	58,82,82	1.80	7 (12%)
3	ACT	A	1302	-	3,3,3	1.25	1 (33%)	3,3,3	0.71	0
2	HEC	B	1301	1	46,50,50	1.50	2 (4%)	58,82,82	1.52	3 (5%)
2	HEC	B	1294	1	46,50,50	1.49	2 (4%)	58,82,82	1.49	3 (5%)
4	GOL	A	1303	-	5,5,5	0.16	0	5,5,5	0.37	0
2	HEC	A	1296	1	46,50,50	1.52	2 (4%)	58,82,82	1.47	5 (8%)
2	HEC	A	1299	1	46,50,50	1.52	2 (4%)	58,82,82	1.55	3 (5%)
2	HEC	B	1293	1	46,50,50	1.51	2 (4%)	58,82,82	1.61	6 (10%)
2	HEC	B	1296	1	46,50,50	1.53	2 (4%)	58,82,82	1.36	2 (3%)
2	HEC	B	1295	1	46,50,50	1.49	3 (6%)	58,82,82	1.43	4 (6%)
2	HEC	B	1298	1	46,50,50	1.53	2 (4%)	58,82,82	1.61	4 (6%)
4	GOL	B	1302	-	5,5,5	0.21	0	5,5,5	0.55	0
2	HEC	A	1298	1	46,50,50	1.50	2 (4%)	58,82,82	1.46	2 (3%)
2	HEC	B	1297	1	46,50,50	1.53	3 (6%)	58,82,82	1.60	3 (5%)
2	HEC	A	1295	1	46,50,50	1.51	2 (4%)	58,82,82	1.33	3 (5%)

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
2	HEC	B	1299	1	-	6/14/54/54	-
2	HEC	A	1293	1	-	6/14/54/54	-
2	HEC	A	1294	1	-	4/14/54/54	-
2	HEC	A	1300	1	-	8/14/54/54	-
2	HEC	A	1297	1	-	7/14/54/54	-
2	HEC	B	1300	1	-	9/14/54/54	-
2	HEC	A	1301	1	-	4/14/54/54	-
2	HEC	B	1301	1	-	5/14/54/54	-
2	HEC	B	1294	1	-	7/14/54/54	-
4	GOL	A	1303	-	-	2/4/4/4	-
2	HEC	A	1296	1	-	8/14/54/54	-
2	HEC	A	1299	1	-	8/14/54/54	-
2	HEC	B	1293	1	-	7/14/54/54	-
2	HEC	B	1296	1	-	8/14/54/54	-
2	HEC	B	1295	1	-	8/14/54/54	-
2	HEC	B	1298	1	-	4/14/54/54	-
4	GOL	B	1302	-	-	2/4/4/4	-
2	HEC	A	1298	1	-	4/14/54/54	-
2	HEC	B	1297	1	-	8/14/54/54	-
2	HEC	A	1295	1	-	8/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1299	HEC	CAC-C3C	6.01	1.54	1.35
2	A	1299	HEC	CAC-C3C	6.00	1.54	1.35
2	A	1294	HEC	CAC-C3C	6.00	1.54	1.35
2	B	1297	HEC	CAC-C3C	5.99	1.54	1.35
2	B	1298	HEC	CAB-C3B	5.99	1.54	1.35
2	A	1296	HEC	CAC-C3C	5.94	1.54	1.35
2	B	1296	HEC	CAC-C3C	5.85	1.54	1.35
2	A	1300	HEC	CAC-C3C	5.85	1.54	1.35
2	A	1301	HEC	CAB-C3B	5.83	1.53	1.35
2	A	1293	HEC	CAC-C3C	5.77	1.53	1.35
2	B	1296	HEC	CAB-C3B	5.77	1.53	1.35
2	B	1300	HEC	CAB-C3B	5.75	1.53	1.35
2	B	1293	HEC	CAC-C3C	5.74	1.53	1.35
2	A	1297	HEC	CAB-C3B	5.72	1.53	1.35
2	B	1301	HEC	CAC-C3C	5.72	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1293	HEC	CAB-C3B	5.70	1.53	1.35
2	B	1295	HEC	CAB-C3B	5.69	1.53	1.35
2	B	1294	HEC	CAC-C3C	5.68	1.53	1.35
2	A	1295	HEC	CAC-C3C	5.67	1.53	1.35
2	B	1301	HEC	CAB-C3B	5.67	1.53	1.35
2	B	1297	HEC	CAB-C3B	5.65	1.53	1.35
2	A	1298	HEC	CAC-C3C	5.63	1.53	1.35
2	B	1300	HEC	CAC-C3C	5.63	1.53	1.35
2	B	1293	HEC	CAB-C3B	5.61	1.53	1.35
2	A	1296	HEC	CAB-C3B	5.61	1.53	1.35
2	A	1298	HEC	CAB-C3B	5.60	1.53	1.35
2	A	1297	HEC	CAC-C3C	5.56	1.53	1.35
2	A	1294	HEC	CAB-C3B	5.56	1.53	1.35
2	B	1294	HEC	CAB-C3B	5.56	1.53	1.35
2	A	1299	HEC	CAB-C3B	5.55	1.53	1.35
2	A	1295	HEC	CAB-C3B	5.54	1.53	1.35
2	B	1298	HEC	CAC-C3C	5.49	1.52	1.35
2	B	1299	HEC	CAB-C3B	5.47	1.52	1.35
2	A	1301	HEC	CAC-C3C	5.46	1.52	1.35
2	A	1300	HEC	CAB-C3B	5.37	1.52	1.35
2	B	1295	HEC	CAC-C3C	5.35	1.52	1.35
3	A	1302	ACT	O-C	2.10	1.31	1.22
2	A	1300	HEC	C3C-C2C	-2.06	1.34	1.41
2	B	1295	HEC	C3C-C2C	-2.05	1.34	1.41
2	B	1297	HEC	C3B-C2B	-2.04	1.34	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	HEC	CBB-CAB-C3B	-8.80	109.85	127.43
2	B	1297	HEC	CBB-CAB-C3B	-8.33	110.79	127.43
2	B	1298	HEC	CBB-CAB-C3B	-8.30	110.84	127.43
2	A	1294	HEC	CBC-CAC-C3C	-7.51	112.43	127.43
2	A	1299	HEC	CBB-CAB-C3B	-7.45	112.54	127.43
2	B	1301	HEC	CBC-CAC-C3C	-7.35	112.74	127.43
2	A	1298	HEC	CBB-CAB-C3B	-7.18	113.09	127.43
2	B	1299	HEC	CBB-CAB-C3B	-7.11	113.21	127.43
2	B	1295	HEC	CBB-CAB-C3B	-7.11	113.22	127.43
2	A	1297	HEC	CBB-CAB-C3B	-7.09	113.27	127.43
2	A	1293	HEC	CBB-CAB-C3B	-7.05	113.34	127.43
2	A	1299	HEC	CBC-CAC-C3C	-6.90	113.64	127.43
2	B	1294	HEC	CBB-CAB-C3B	-6.87	113.69	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1294	HEC	CBC-CAC-C3C	-6.87	113.70	127.43
2	A	1294	HEC	CBB-CAB-C3B	-6.85	113.75	127.43
2	A	1298	HEC	CBC-CAC-C3C	-6.83	113.79	127.43
2	B	1297	HEC	CBC-CAC-C3C	-6.75	113.95	127.43
2	B	1299	HEC	CBC-CAC-C3C	-6.71	114.02	127.43
2	A	1296	HEC	CBB-CAB-C3B	-6.67	114.10	127.43
2	B	1293	HEC	CBB-CAB-C3B	-6.59	114.27	127.43
2	B	1301	HEC	CBB-CAB-C3B	-6.56	114.32	127.43
2	B	1298	HEC	CBC-CAC-C3C	-6.54	114.37	127.43
2	A	1296	HEC	CBC-CAC-C3C	-6.51	114.41	127.43
2	B	1300	HEC	CBB-CAB-C3B	-6.37	114.71	127.43
2	B	1296	HEC	CBB-CAB-C3B	-6.19	115.06	127.43
2	B	1293	HEC	CBC-CAC-C3C	-6.12	115.21	127.43
2	A	1293	HEC	CBC-CAC-C3C	-6.11	115.21	127.43
2	B	1296	HEC	CBC-CAC-C3C	-6.05	115.33	127.43
2	A	1300	HEC	CBC-CAC-C3C	-5.98	115.48	127.43
2	A	1300	HEC	CBB-CAB-C3B	-5.87	115.71	127.43
2	A	1301	HEC	CBC-CAC-C3C	-5.73	115.98	127.43
2	A	1297	HEC	CBC-CAC-C3C	-5.69	116.07	127.43
2	A	1295	HEC	CBB-CAB-C3B	-5.67	116.10	127.43
2	A	1295	HEC	CBC-CAC-C3C	-5.26	116.91	127.43
2	B	1300	HEC	CBC-CAC-C3C	-4.73	117.98	127.43
2	B	1295	HEC	CBC-CAC-C3C	-4.16	119.12	127.43
2	A	1301	HEC	CMD-C2D-C3D	2.87	131.71	125.62
2	B	1293	HEC	CMB-C2B-C1B	-2.84	121.09	125.42
2	B	1293	HEC	O1A-CGA-CBA	-2.79	114.25	123.09
2	A	1301	HEC	CMD-C2D-C1D	-2.61	121.45	125.42
2	A	1297	HEC	CHA-C1A-NA	-2.57	121.66	124.45
2	A	1299	HEC	O1A-CGA-CBA	-2.51	115.12	123.09
2	A	1296	HEC	O1A-CGA-CBA	-2.49	115.20	123.09
2	A	1301	HEC	O1A-CGA-CBA	-2.44	115.36	123.09
2	A	1295	HEC	CMC-C2C-C1C	-2.37	121.81	125.42
2	B	1294	HEC	O1D-CGD-CBD	-2.33	115.70	123.09
2	A	1300	HEC	O1A-CGA-CBA	-2.31	115.77	123.09
2	B	1293	HEC	CMB-C2B-C3B	2.30	131.95	126.55
2	B	1293	HEC	CAA-CBA-CGA	-2.29	107.58	113.67
2	B	1299	HEC	O1D-CGD-CBD	-2.28	115.86	123.09
2	A	1297	HEC	O1A-CGA-CBA	-2.26	115.91	123.09
2	B	1298	HEC	CMD-C2D-C3D	2.26	130.41	125.62
2	A	1300	HEC	CMC-C2C-C1C	-2.26	121.98	125.42
2	A	1301	HEC	C4D-CHA-C1A	2.25	131.59	124.66
2	A	1300	HEC	CMC-C2C-C3C	2.24	131.83	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1295	HEC	CAA-C2A-C3A	-2.17	123.80	127.87
2	A	1296	HEC	O2A-CGA-O1A	2.15	128.85	123.33
2	B	1298	HEC	O1A-CGA-CBA	-2.15	116.29	123.09
2	B	1297	HEC	CHA-C1A-NA	-2.11	122.16	124.45
2	A	1300	HEC	O1D-CGD-CBD	-2.10	116.44	123.09
2	A	1301	HEC	O1D-CGD-CBD	-2.08	116.50	123.09
2	A	1296	HEC	O1D-CGD-CBD	-2.06	116.55	123.09
2	B	1301	HEC	CMC-C2C-C3C	2.05	131.38	126.55
2	A	1297	HEC	O2A-CGA-O1A	2.03	128.56	123.33
2	B	1295	HEC	O1D-CGD-CBD	-2.02	116.69	123.09

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1293	HEC	C2B-C3B-CAB-CBB
2	A	1293	HEC	C4B-C3B-CAB-CBB
2	A	1293	HEC	C2C-C3C-CAC-CBC
2	A	1293	HEC	C4C-C3C-CAC-CBC
2	A	1294	HEC	C2B-C3B-CAB-CBB
2	A	1294	HEC	C4B-C3B-CAB-CBB
2	A	1294	HEC	C2C-C3C-CAC-CBC
2	A	1294	HEC	C4C-C3C-CAC-CBC
2	A	1295	HEC	C2B-C3B-CAB-CBB
2	A	1295	HEC	C4B-C3B-CAB-CBB
2	A	1295	HEC	C2C-C3C-CAC-CBC
2	A	1295	HEC	C4C-C3C-CAC-CBC
2	A	1296	HEC	C2B-C3B-CAB-CBB
2	A	1296	HEC	C4B-C3B-CAB-CBB
2	A	1296	HEC	C2C-C3C-CAC-CBC
2	A	1296	HEC	C4C-C3C-CAC-CBC
2	A	1297	HEC	C2B-C3B-CAB-CBB
2	A	1297	HEC	C4B-C3B-CAB-CBB
2	A	1297	HEC	C2C-C3C-CAC-CBC
2	A	1297	HEC	C4C-C3C-CAC-CBC
2	A	1298	HEC	C2B-C3B-CAB-CBB
2	A	1298	HEC	C4B-C3B-CAB-CBB
2	A	1298	HEC	C2C-C3C-CAC-CBC
2	A	1298	HEC	C4C-C3C-CAC-CBC
2	A	1299	HEC	C2B-C3B-CAB-CBB
2	A	1299	HEC	C4B-C3B-CAB-CBB
2	A	1299	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	A	1299	HEC	C4C-C3C-CAC-CBC
2	A	1300	HEC	C2B-C3B-CAB-CBB
2	A	1300	HEC	C4B-C3B-CAB-CBB
2	A	1300	HEC	C2C-C3C-CAC-CBC
2	A	1300	HEC	C4C-C3C-CAC-CBC
2	A	1301	HEC	C2B-C3B-CAB-CBB
2	A	1301	HEC	C4B-C3B-CAB-CBB
2	A	1301	HEC	C2C-C3C-CAC-CBC
2	A	1301	HEC	C4C-C3C-CAC-CBC
2	B	1293	HEC	C2B-C3B-CAB-CBB
2	B	1293	HEC	C4B-C3B-CAB-CBB
2	B	1293	HEC	C2C-C3C-CAC-CBC
2	B	1293	HEC	C4C-C3C-CAC-CBC
2	B	1294	HEC	C2B-C3B-CAB-CBB
2	B	1294	HEC	C4B-C3B-CAB-CBB
2	B	1294	HEC	C2C-C3C-CAC-CBC
2	B	1294	HEC	C4C-C3C-CAC-CBC
2	B	1295	HEC	C2B-C3B-CAB-CBB
2	B	1295	HEC	C4B-C3B-CAB-CBB
2	B	1295	HEC	C2C-C3C-CAC-CBC
2	B	1295	HEC	C4C-C3C-CAC-CBC
2	B	1296	HEC	C2B-C3B-CAB-CBB
2	B	1296	HEC	C4B-C3B-CAB-CBB
2	B	1296	HEC	C2C-C3C-CAC-CBC
2	B	1296	HEC	C4C-C3C-CAC-CBC
2	B	1297	HEC	C2B-C3B-CAB-CBB
2	B	1297	HEC	C4B-C3B-CAB-CBB
2	B	1297	HEC	C2C-C3C-CAC-CBC
2	B	1297	HEC	C4C-C3C-CAC-CBC
2	B	1298	HEC	C2B-C3B-CAB-CBB
2	B	1298	HEC	C4B-C3B-CAB-CBB
2	B	1298	HEC	C2C-C3C-CAC-CBC
2	B	1298	HEC	C4C-C3C-CAC-CBC
2	B	1299	HEC	C2B-C3B-CAB-CBB
2	B	1299	HEC	C4B-C3B-CAB-CBB
2	B	1299	HEC	C2C-C3C-CAC-CBC
2	B	1299	HEC	C4C-C3C-CAC-CBC
2	B	1300	HEC	C2B-C3B-CAB-CBB
2	B	1300	HEC	C4B-C3B-CAB-CBB
2	B	1300	HEC	C2C-C3C-CAC-CBC
2	B	1300	HEC	C4C-C3C-CAC-CBC
2	B	1301	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	1301	HEC	C4B-C3B-CAB-CBB
2	B	1301	HEC	C2C-C3C-CAC-CBC
2	B	1301	HEC	C4C-C3C-CAC-CBC
4	A	1303	GOL	O1-C1-C2-C3
2	B	1294	HEC	C3D-CAD-CBD-CGD
2	B	1300	HEC	C2A-CAA-CBA-CGA
4	B	1302	GOL	O1-C1-C2-C3
4	A	1303	GOL	O1-C1-C2-O2
4	B	1302	GOL	O1-C1-C2-O2
2	B	1296	HEC	CAD-CBD-CGD-O2D
2	A	1300	HEC	CAA-CBA-CGA-O1A
2	B	1295	HEC	CAA-CBA-CGA-O2A
2	B	1300	HEC	CAA-CBA-CGA-O1A
2	A	1300	HEC	CAD-CBD-CGD-O1D
2	B	1296	HEC	CAA-CBA-CGA-O2A
2	B	1296	HEC	CAD-CBD-CGD-O1D
2	A	1300	HEC	CAD-CBD-CGD-O2D
2	B	1295	HEC	CAD-CBD-CGD-O1D
2	B	1296	HEC	CAA-CBA-CGA-O1A
2	A	1296	HEC	CAD-CBD-CGD-O2D
2	B	1300	HEC	CAA-CBA-CGA-O2A
2	B	1295	HEC	CAA-CBA-CGA-O1A
2	A	1297	HEC	CAD-CBD-CGD-O1D
2	B	1294	HEC	CAD-CBD-CGD-O2D
2	A	1300	HEC	CAA-CBA-CGA-O2A
2	B	1294	HEC	CAD-CBD-CGD-O1D
2	B	1297	HEC	CAD-CBD-CGD-O1D
2	B	1300	HEC	CAD-CBD-CGD-O1D
2	A	1299	HEC	CAA-CBA-CGA-O2A
2	A	1296	HEC	CAD-CBD-CGD-O1D
2	B	1297	HEC	CAD-CBD-CGD-O2D
2	A	1297	HEC	CAD-CBD-CGD-O2D
2	A	1296	HEC	CAA-CBA-CGA-O2A
2	B	1297	HEC	CAA-CBA-CGA-O2A
2	B	1295	HEC	CAD-CBD-CGD-O2D
2	B	1300	HEC	CAD-CBD-CGD-O2D
2	A	1295	HEC	CAA-CBA-CGA-O2A
2	A	1299	HEC	CAA-CBA-CGA-O1A
2	A	1293	HEC	CAD-CBD-CGD-O2D
2	A	1299	HEC	CAD-CBD-CGD-O2D
2	B	1297	HEC	CAA-CBA-CGA-O1A
2	A	1296	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	1293	HEC	C2D-C3D-CAD-CBD
2	A	1295	HEC	CAA-CBA-CGA-O1A
2	A	1299	HEC	CAD-CBD-CGD-O1D
2	B	1299	HEC	CAA-CBA-CGA-O1A
2	B	1299	HEC	CAA-CBA-CGA-O2A
2	B	1293	HEC	CAA-CBA-CGA-O2A
2	A	1293	HEC	CAD-CBD-CGD-O1D
2	A	1295	HEC	CAD-CBD-CGD-O2D
2	A	1297	HEC	CAA-CBA-CGA-O2A
2	B	1293	HEC	CAA-CBA-CGA-O1A
2	B	1301	HEC	CAD-CBD-CGD-O2D
2	A	1295	HEC	CAD-CBD-CGD-O1D

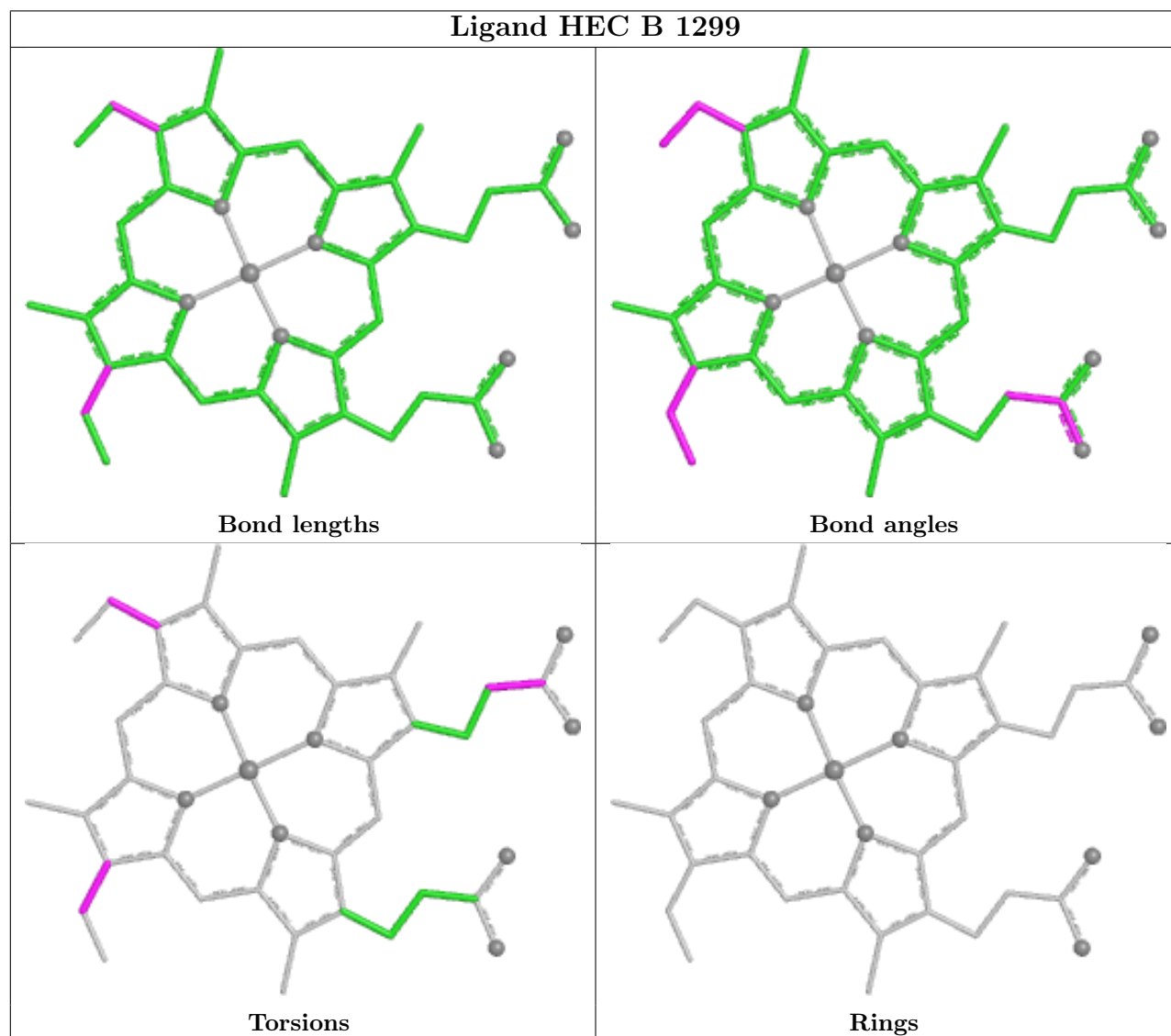
There are no ring outliers.

16 monomers are involved in 26 short contacts:

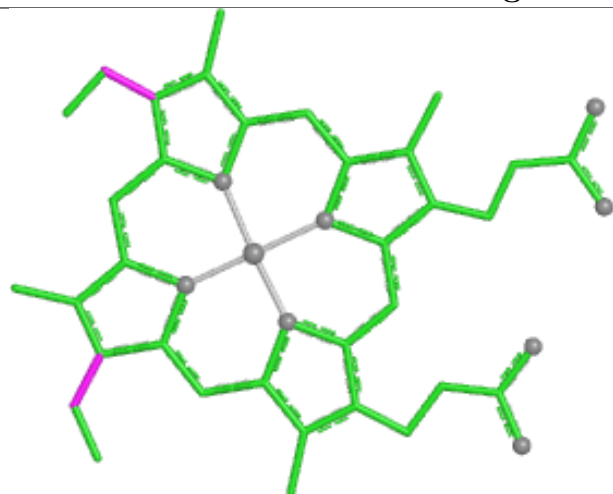
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1293	HEC	1	0
2	A	1300	HEC	3	0
2	A	1297	HEC	1	0
2	B	1300	HEC	3	0
2	A	1301	HEC	1	0
3	A	1302	ACT	1	0
2	B	1294	HEC	1	0
2	A	1299	HEC	1	0
2	B	1293	HEC	1	0
2	B	1296	HEC	2	0
2	B	1295	HEC	1	0
2	B	1298	HEC	3	0
4	B	1302	GOL	1	0
2	A	1298	HEC	1	0
2	B	1297	HEC	2	0
2	A	1295	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

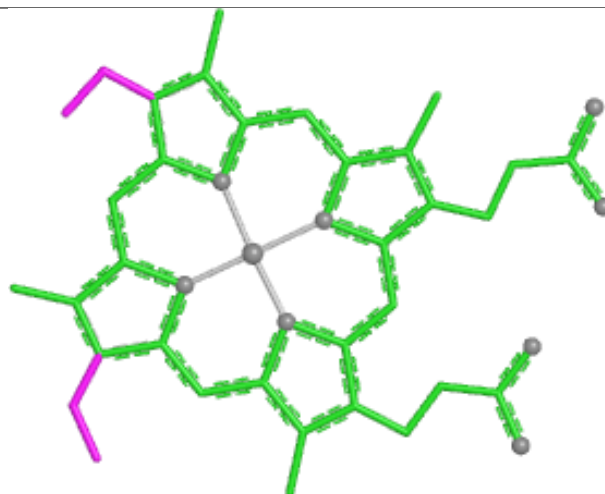
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



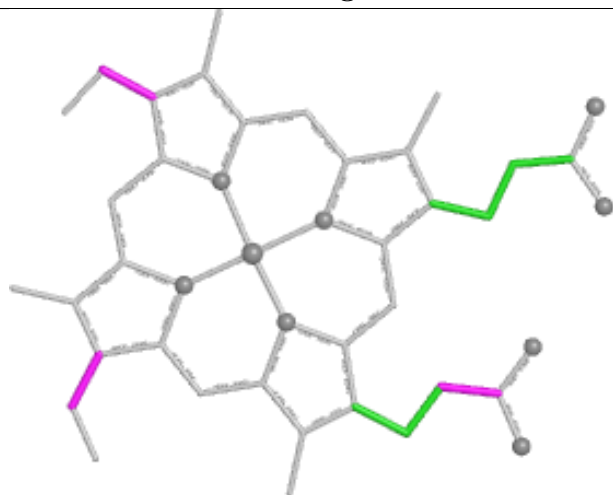
Ligand HEC A 1293



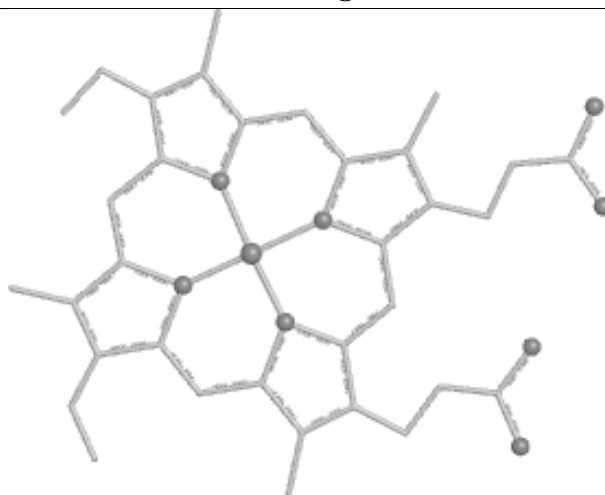
Bond lengths



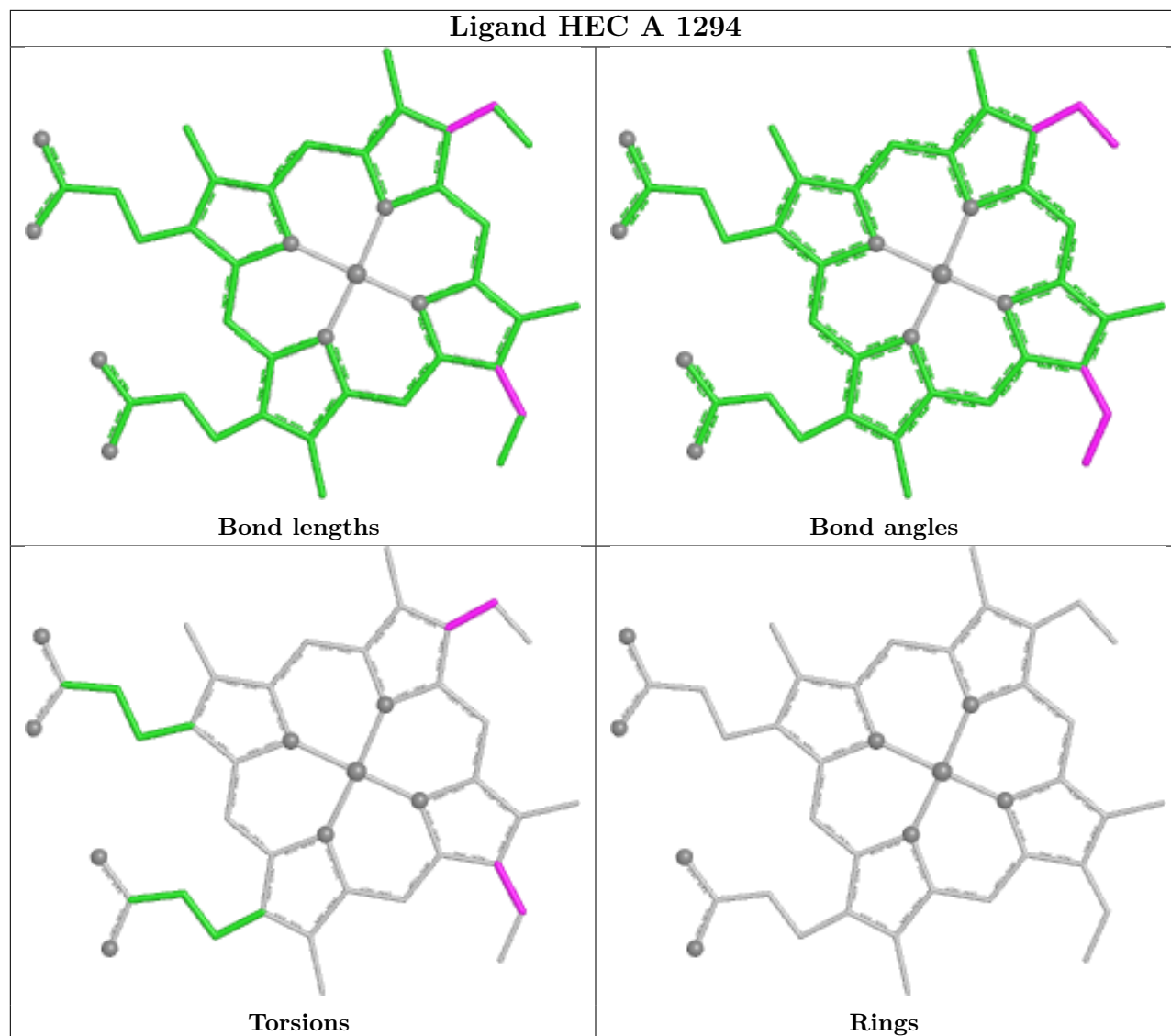
Bond angles



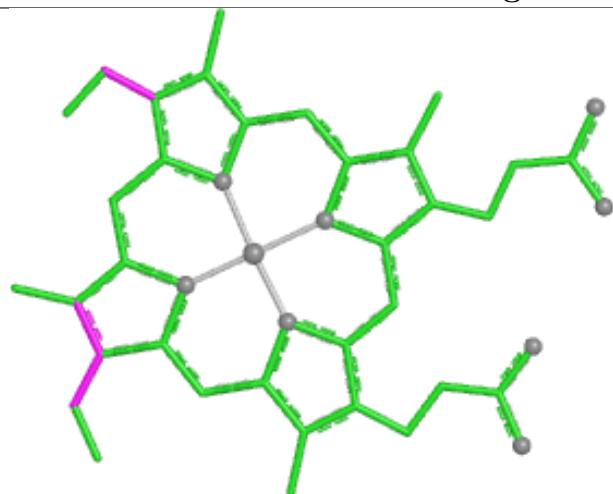
Torsions



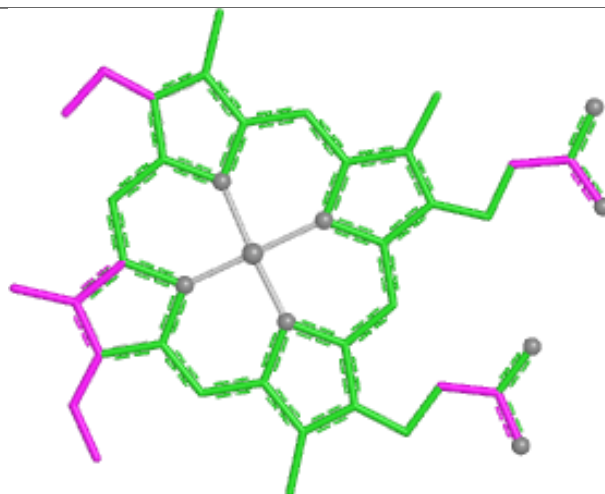
Rings



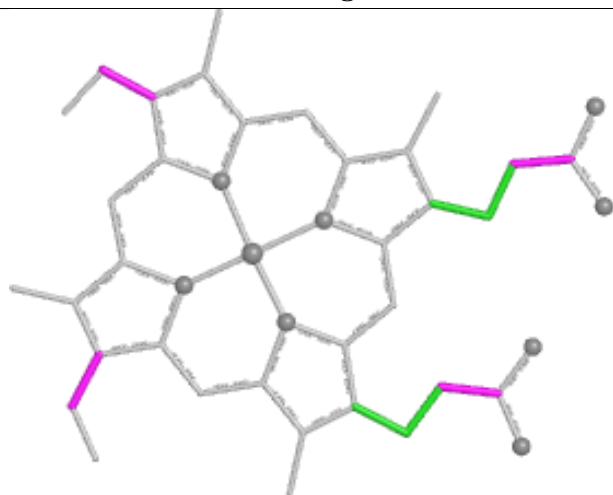
Ligand HEC A 1300



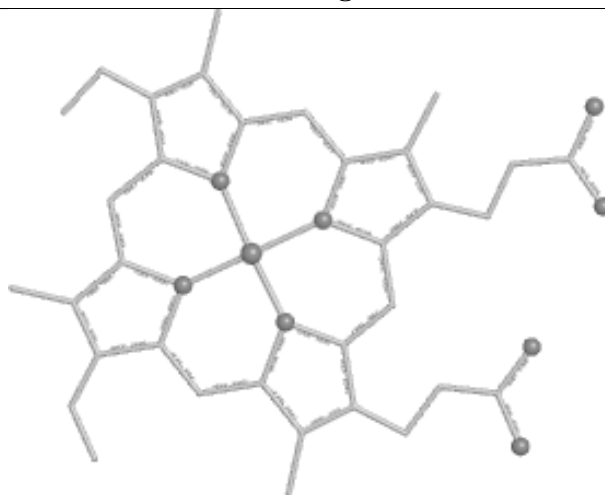
Bond lengths



Bond angles

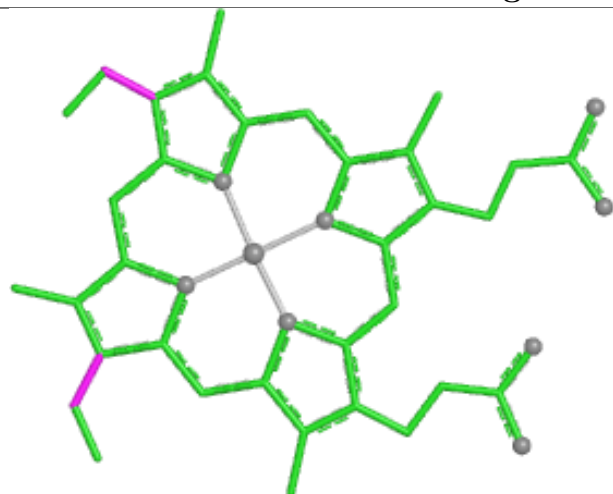


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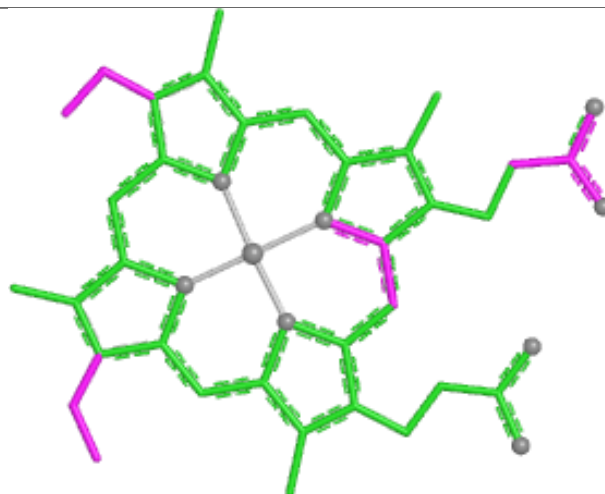


Rings

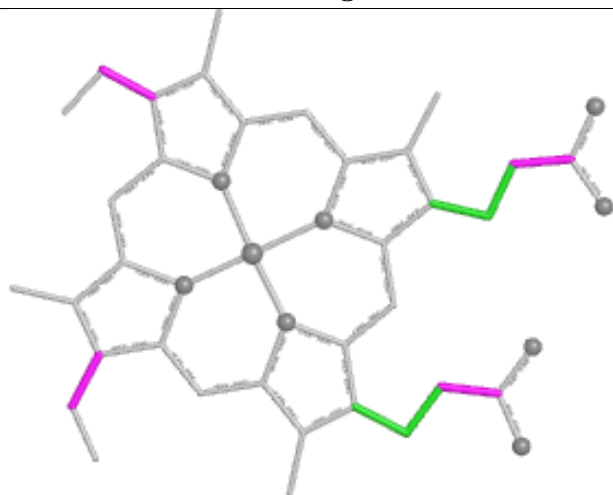
Ligand HEC A 1297



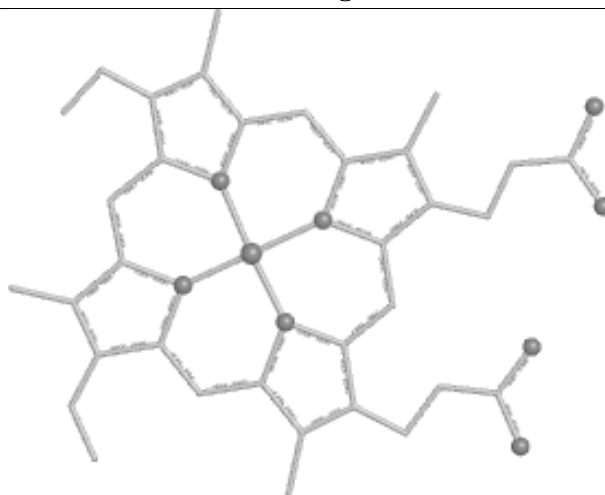
Bond lengths



Bond angles

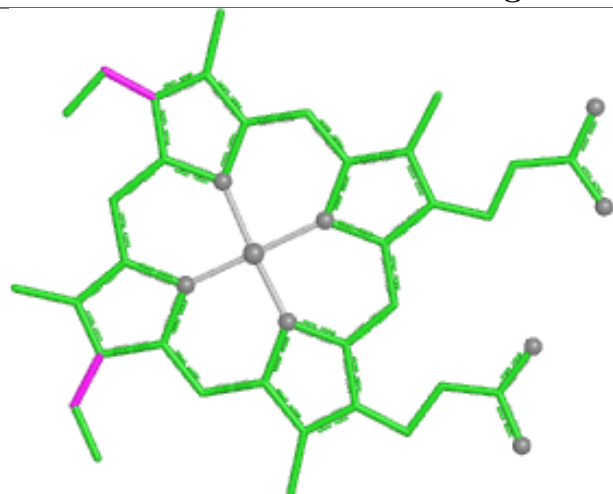


Torsions

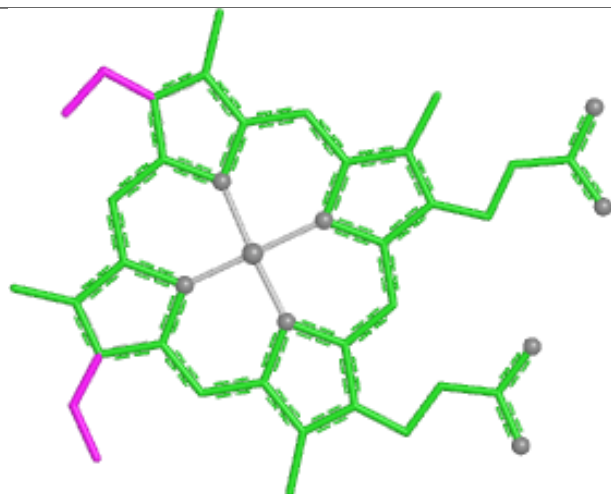


Rings

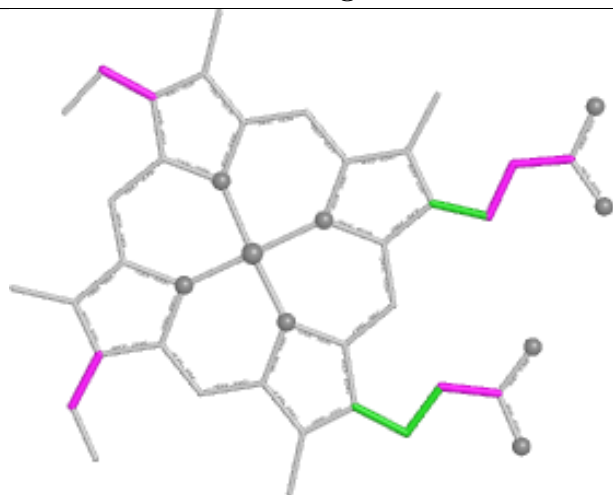
Ligand HEC B 1300



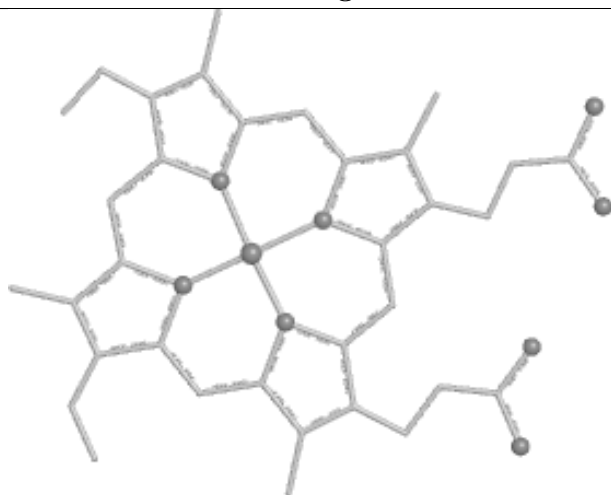
Bond lengths



Bond angles

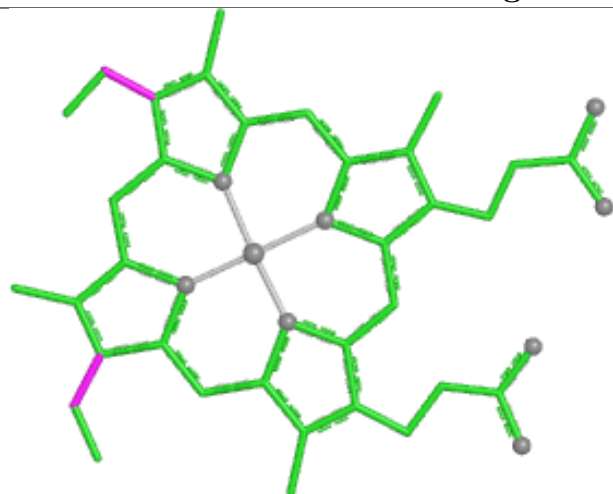


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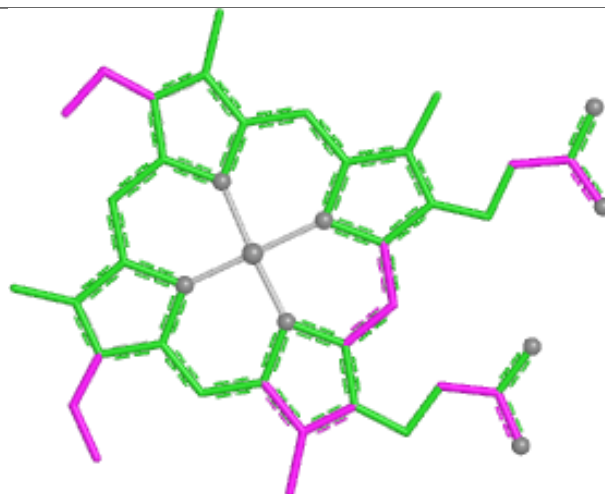


Rings

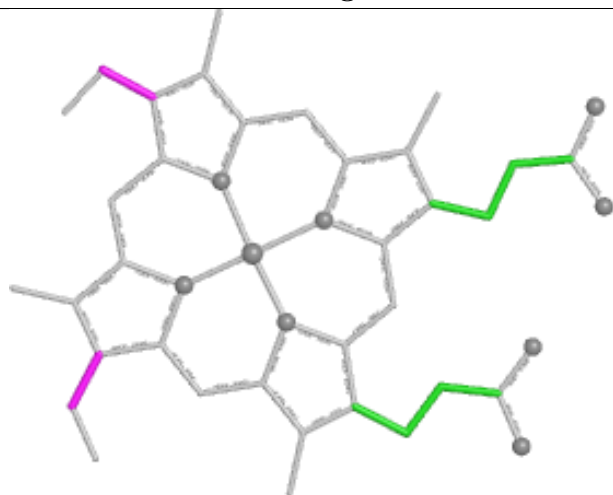
Ligand HEC A 1301



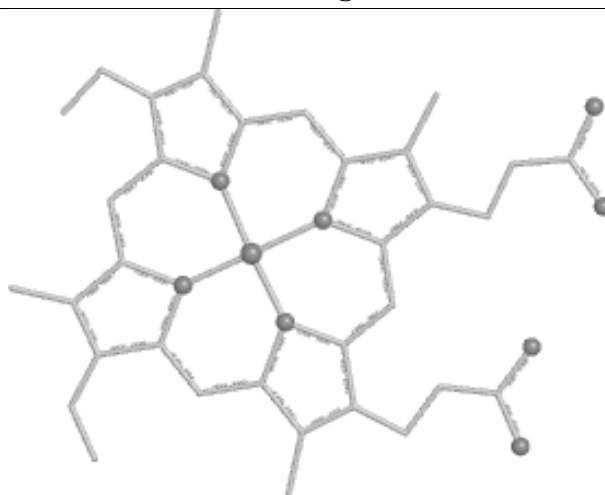
Bond lengths



Bond angles

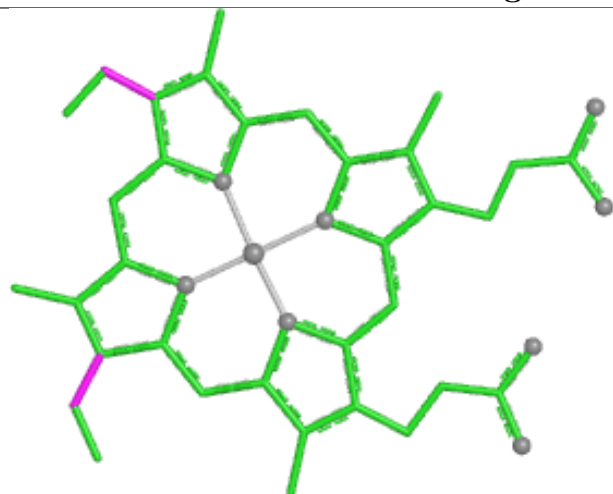


Torsions

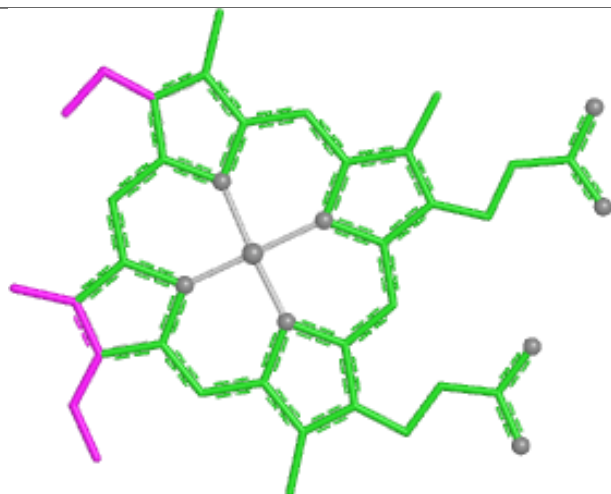


Rings

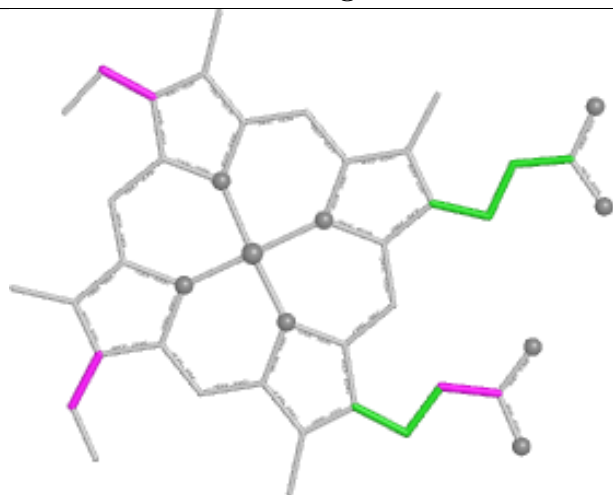
Ligand HEC B 1301



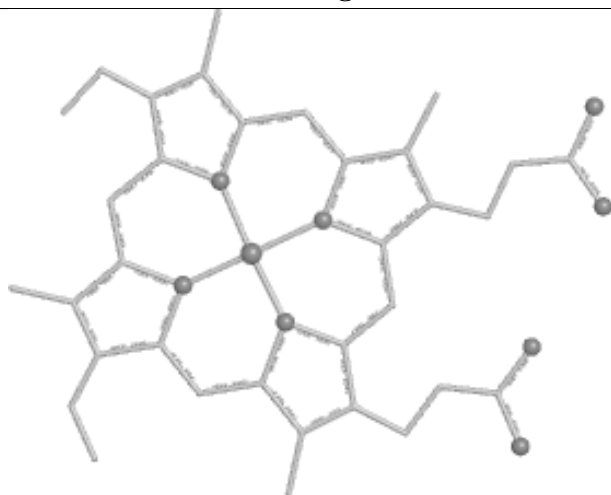
Bond lengths



Bond angles

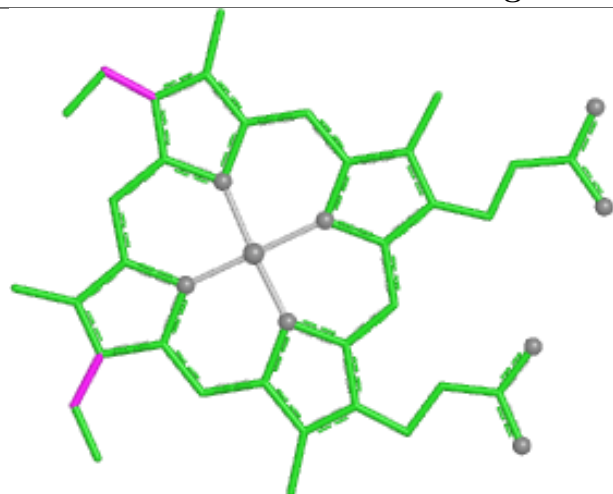


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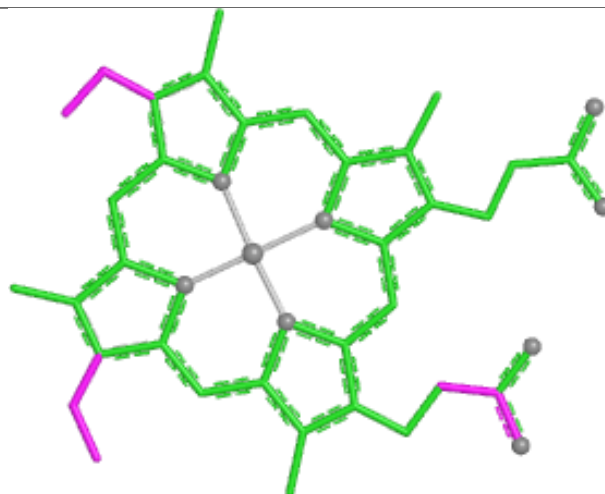


Rings

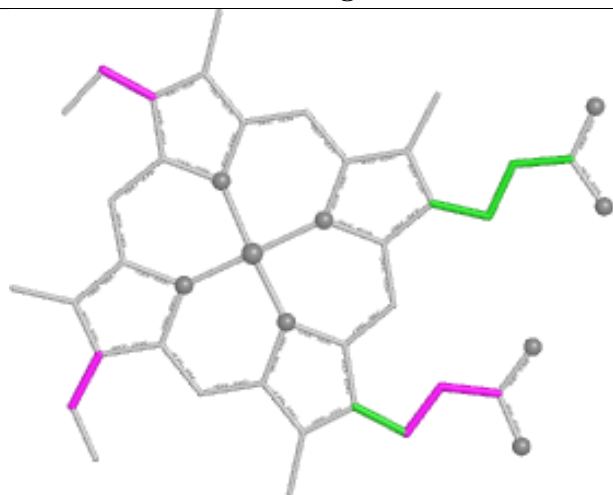
Ligand HEC B 1294



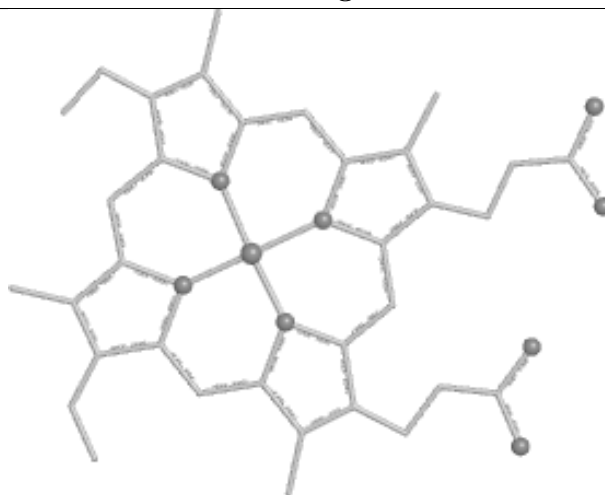
Bond lengths



Bond angles

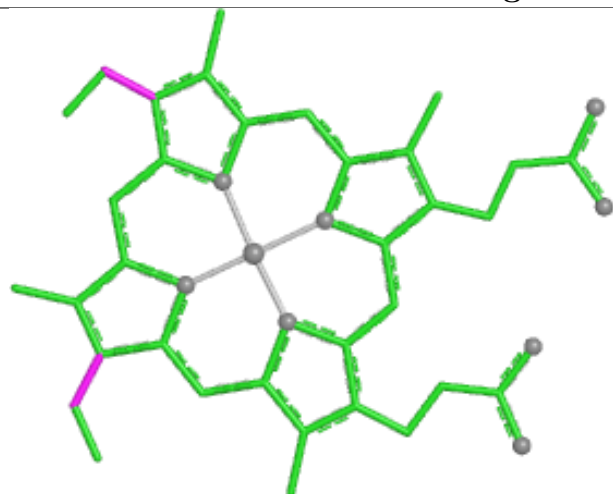


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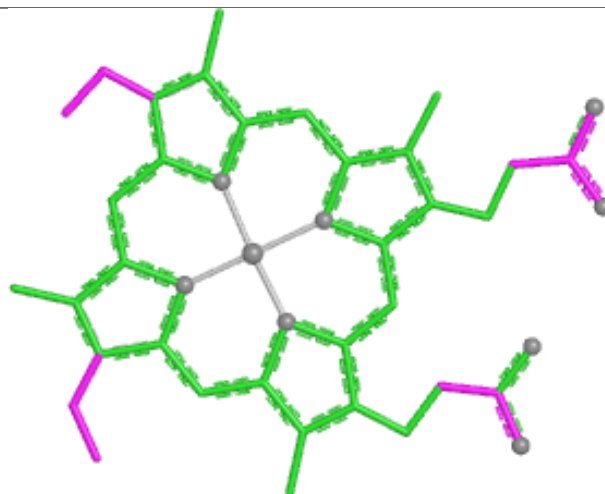


Rings

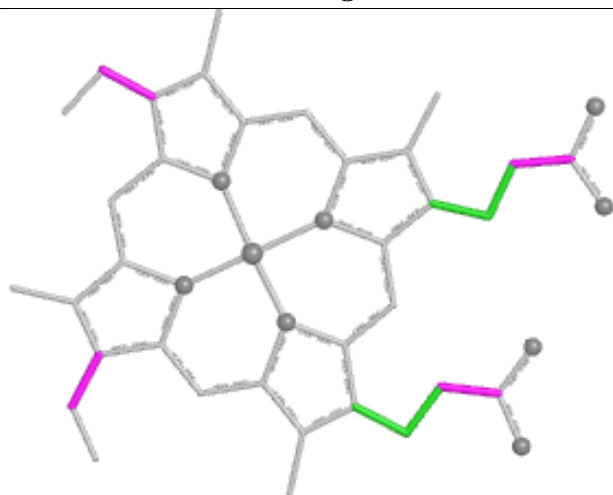
Ligand HEC A 1296



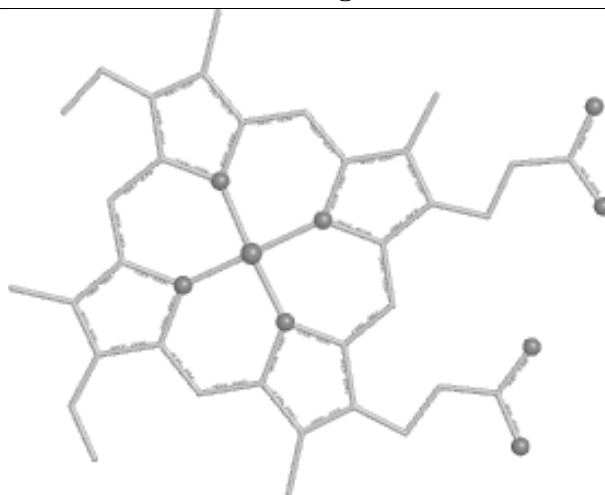
Bond lengths



Bond angles

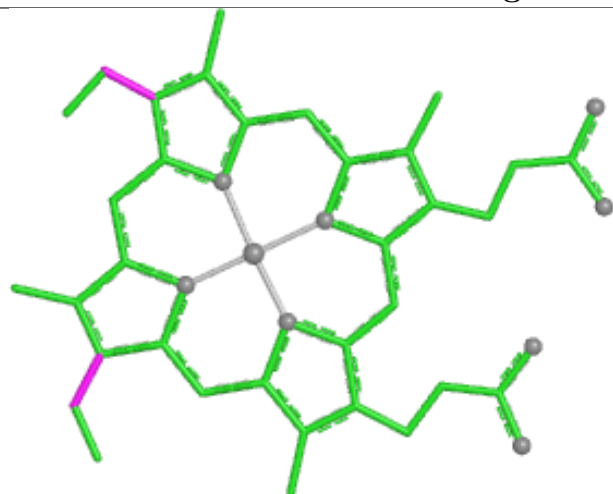


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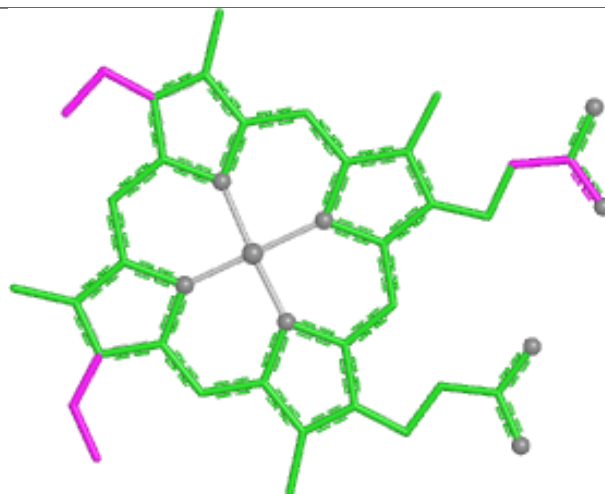


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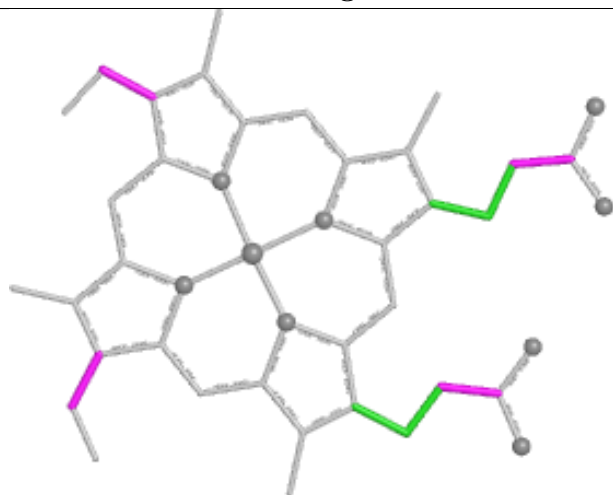
Ligand HEC A 1299



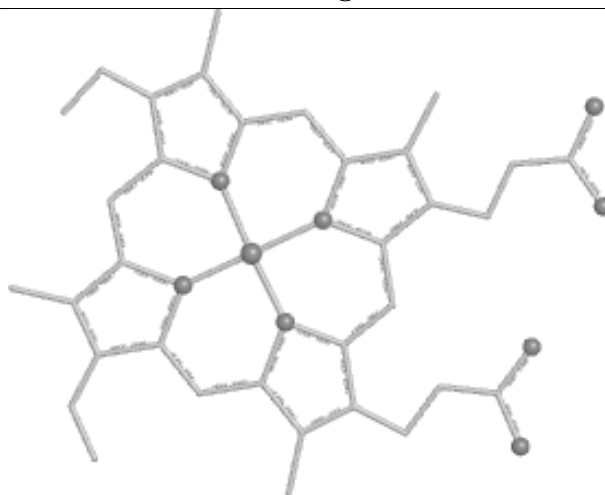
Bond lengths



Bond angles

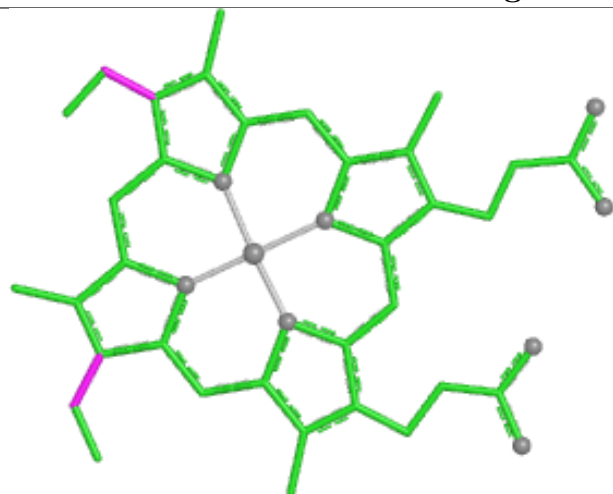


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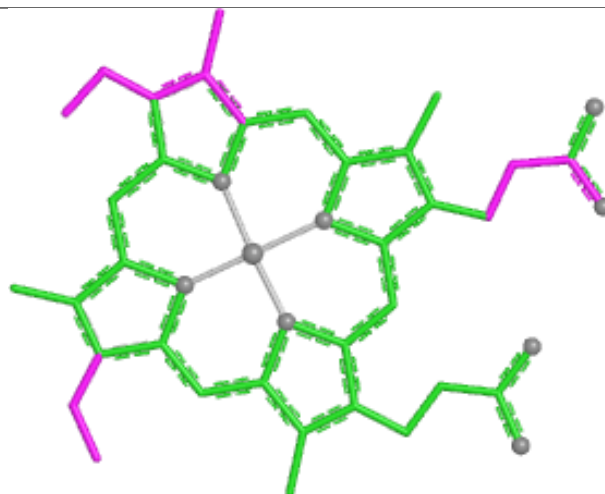


Rings

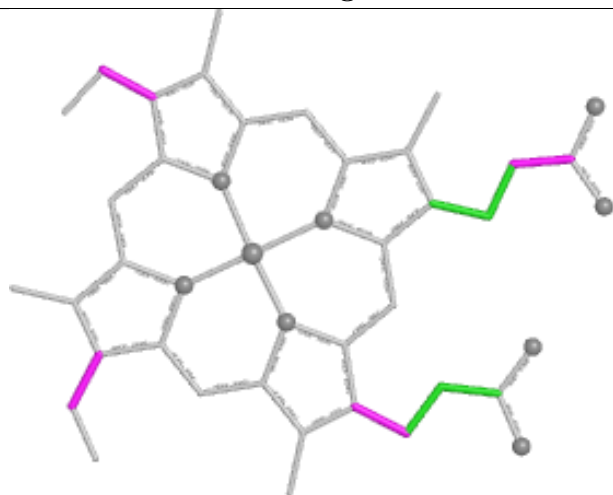
Ligand HEC B 1293



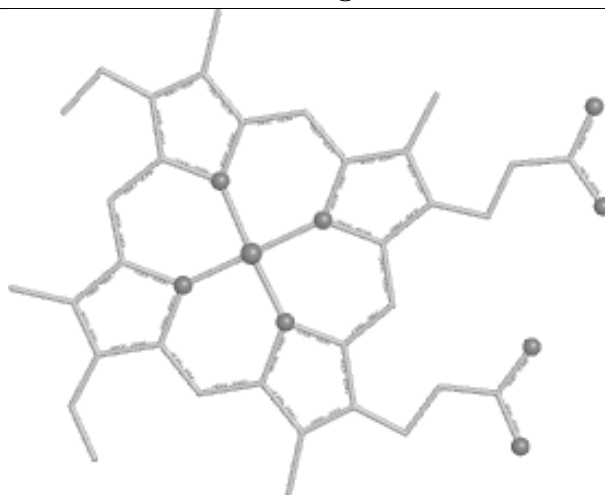
Bond lengths



Bond angles

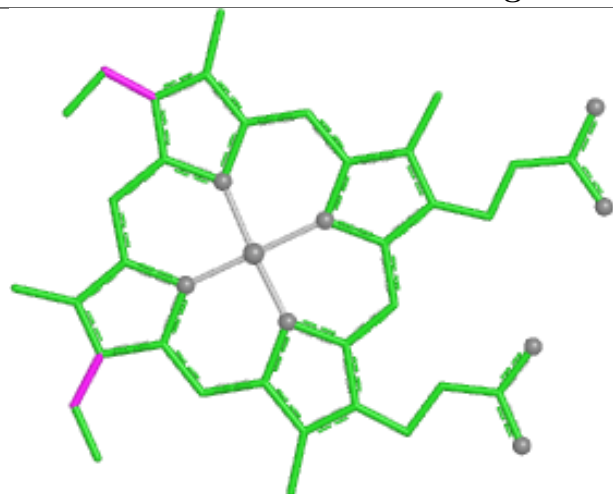


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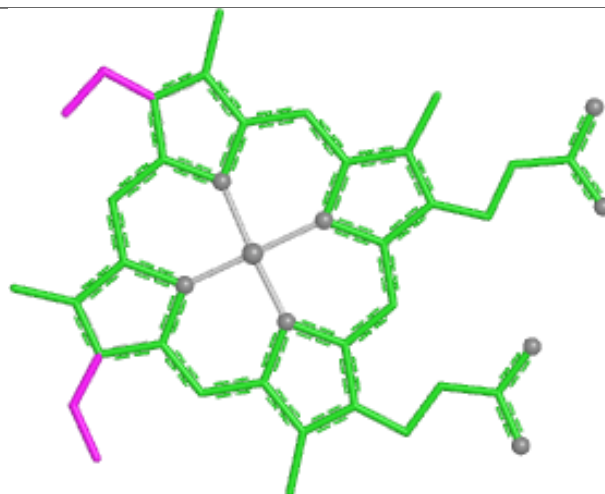


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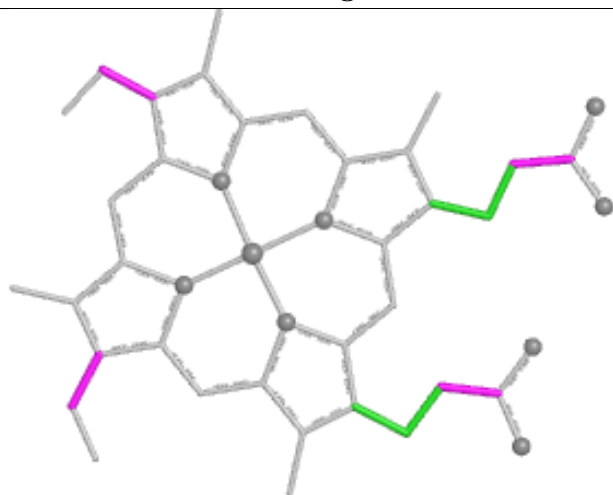
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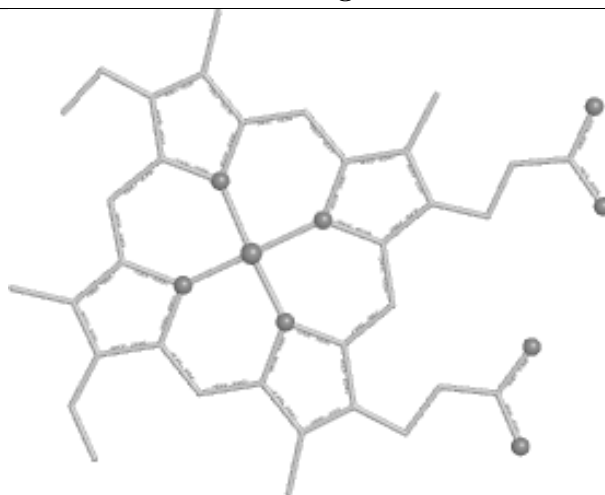
Bond lengths



Bond angles

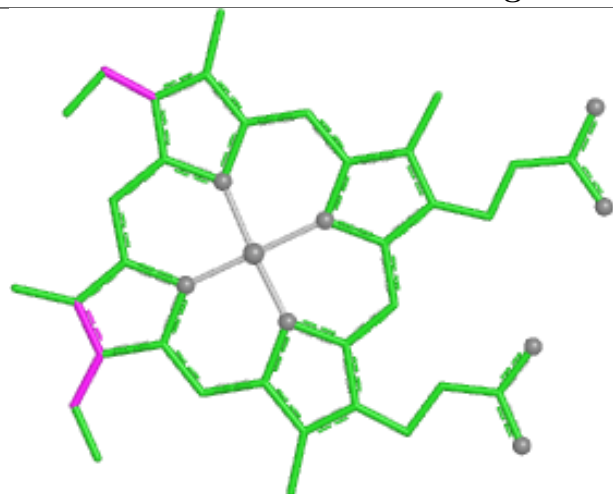


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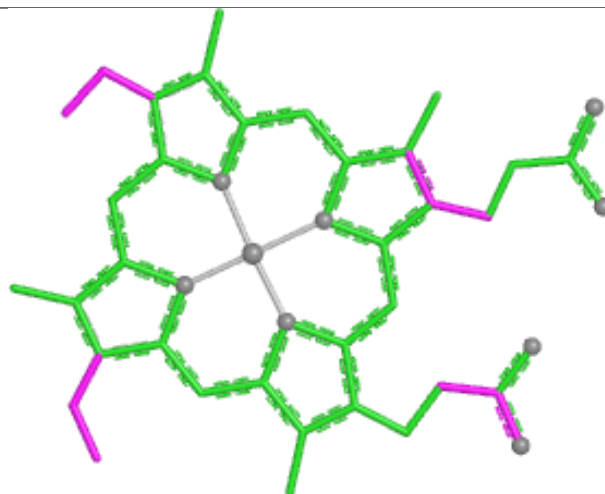


Rings

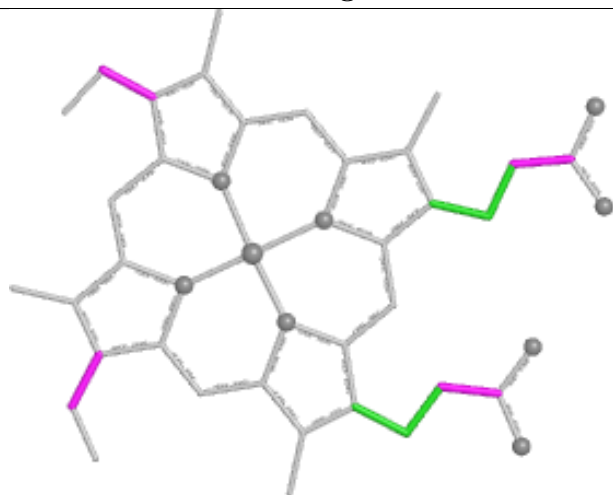
Ligand HEC B 1295



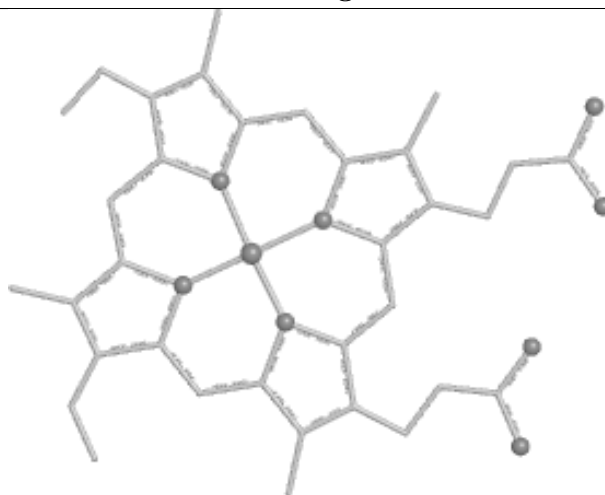
Bond lengths



Bond angles

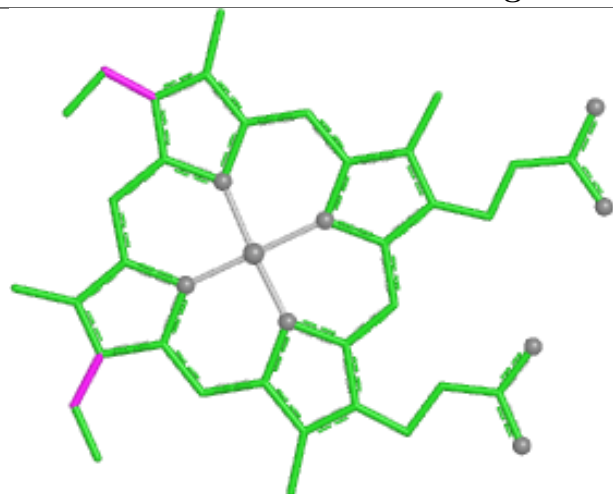


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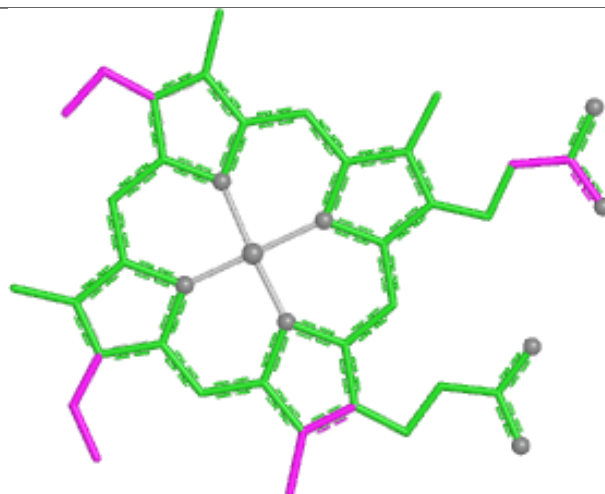


Rings

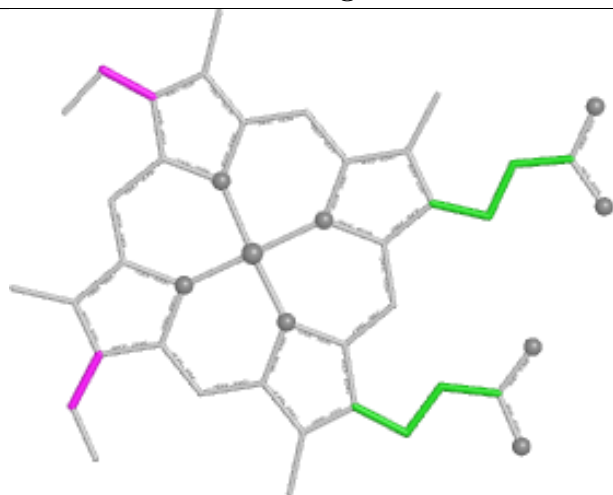
Ligand HEC B 1298



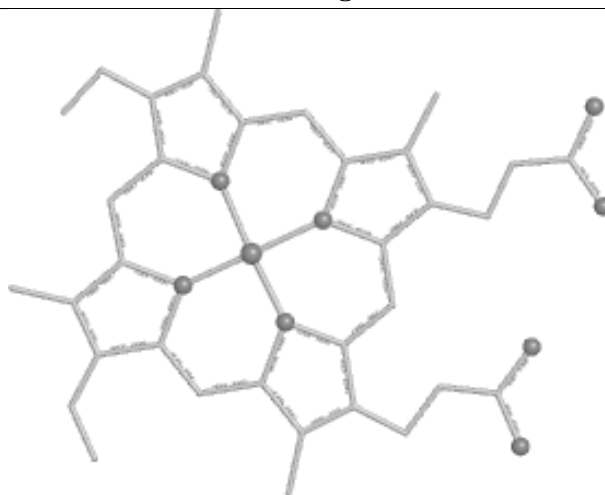
Bond lengths



Bond angles

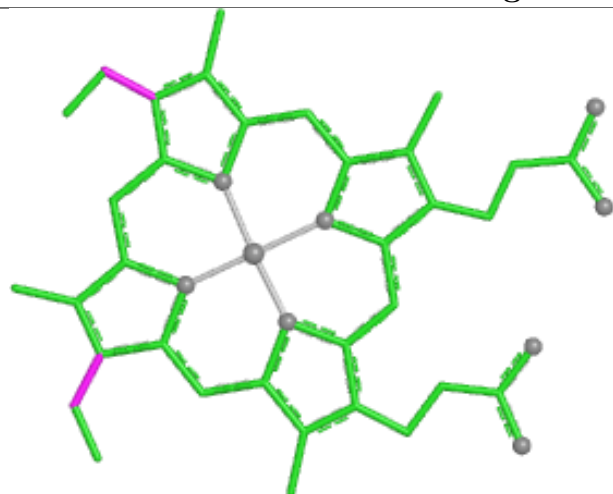


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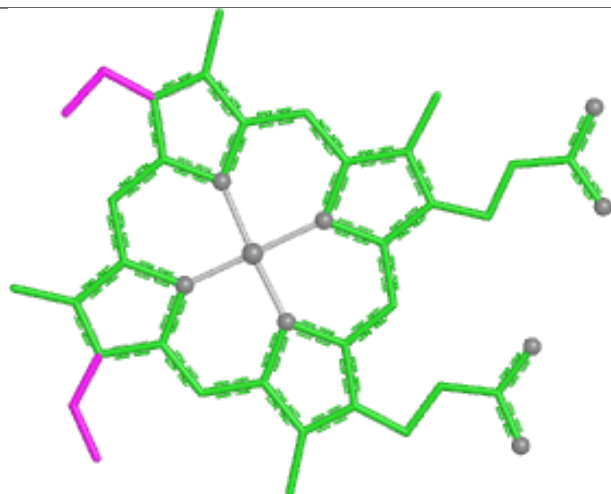


Rings

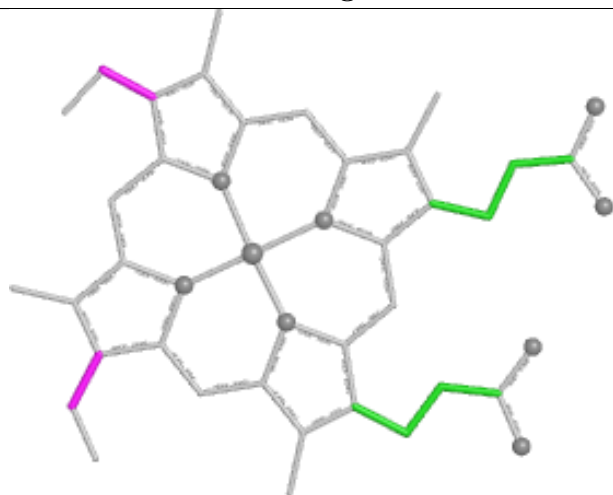
Ligand HEC A 1298



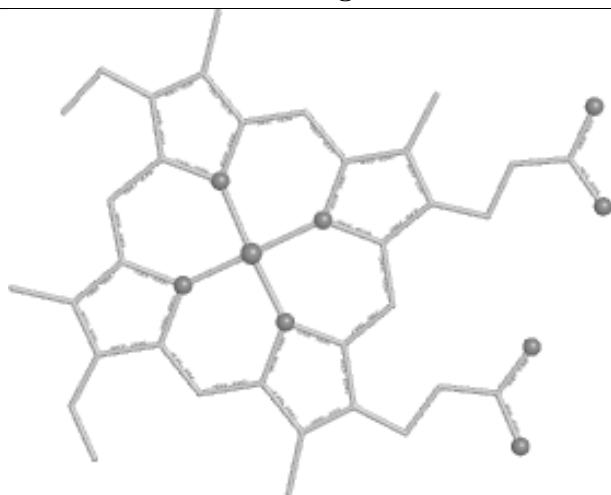
Bond lengths



Bond angles

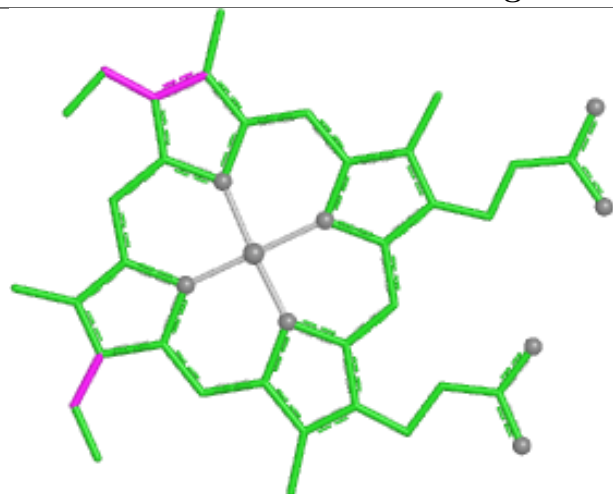


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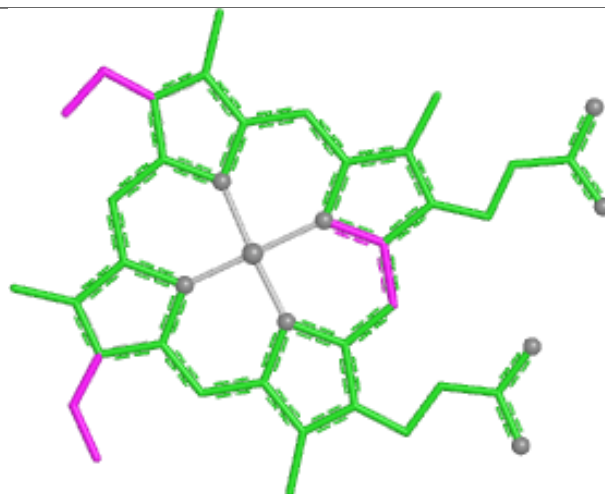


Rings

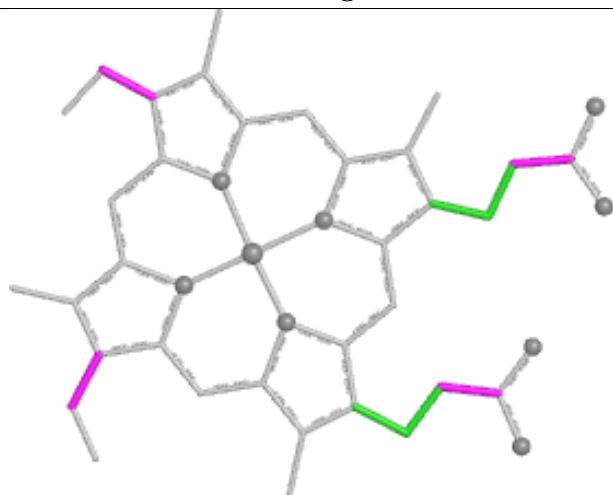
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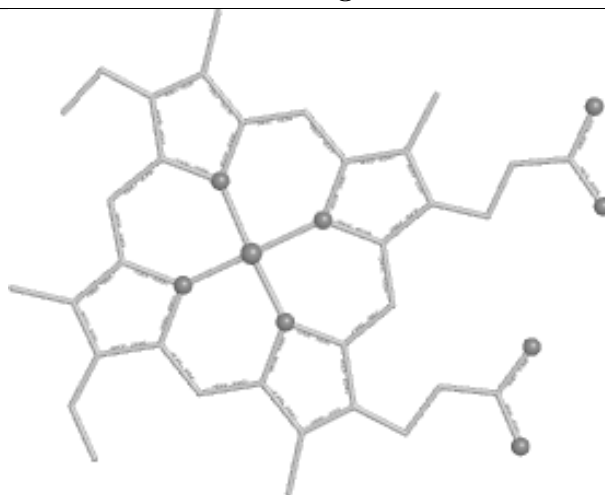
Bond lengths



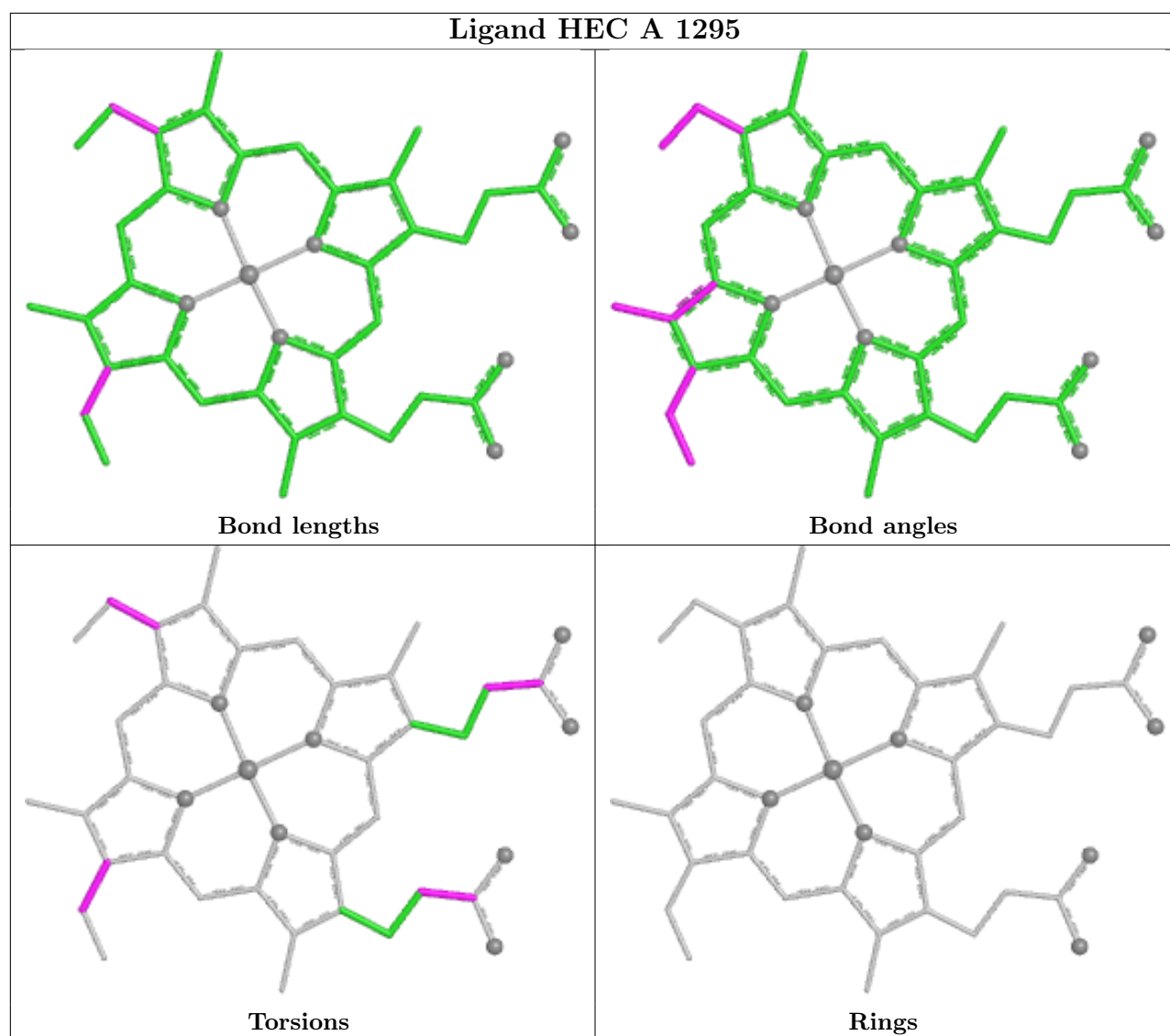
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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.