wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 07:06 AM EST

PDB ID	:	1IQC
Title	:	Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors	:	Shimizu, H.
Deposited on	:	2001-07-20
Resolution	:	1.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

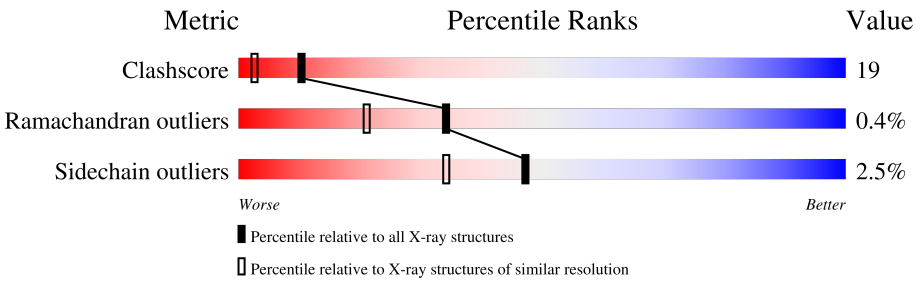
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	83% 16% •
1	B	308	74% 24% •
1	C	308	88% 11% •
1	D	308	52% 44% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10767 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2388	1497	411	467	13	0	0	0
1	B	308	2388	1497	411	467	13	0	0	0
1	C	308	2388	1497	411	467	13	0	0	0
1	D	308	2388	1497	411	467	13	0	0	0

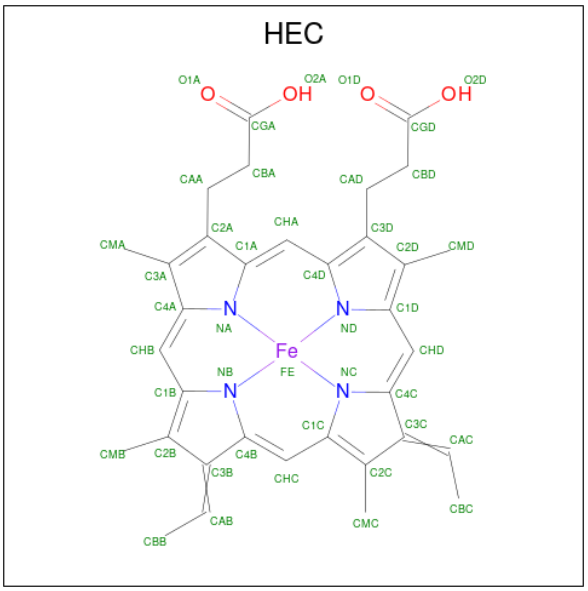
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

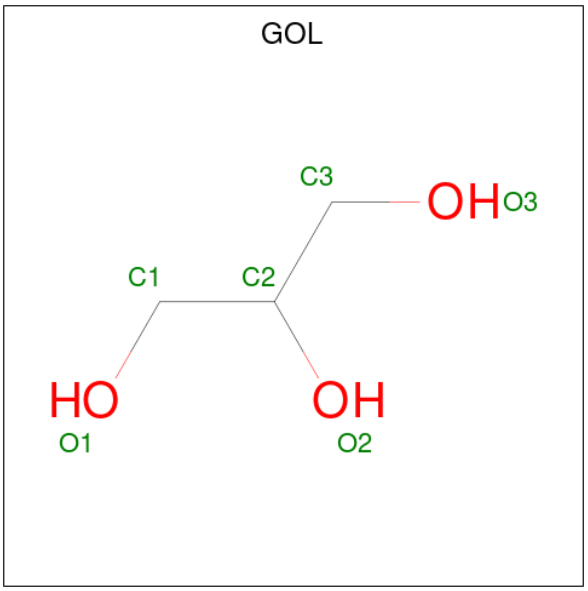
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	D	1	1	1	0	0

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	260	260	260	0	0
			Total	O		
6	B	199	199	199	0	0
			Total	O		
6	C	279	279	279	0	0
			Total	O		
6	D	120	120	120	0	0

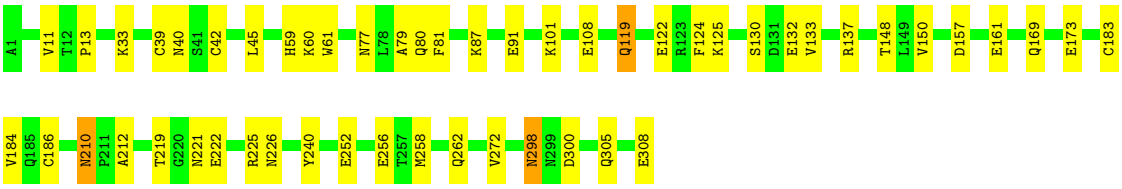
3 Residue-property plots (i)

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: di-heme peroxidase

Chain A: 83% 16%

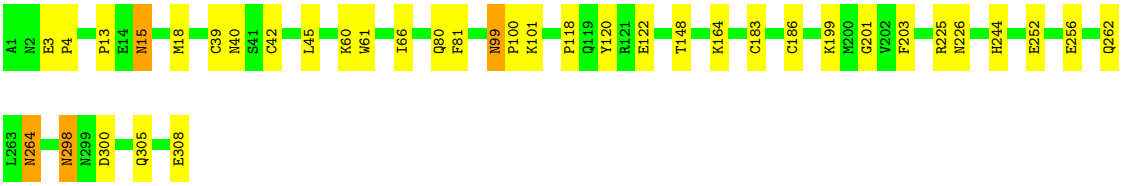


• Molecule 1: di-heme peroxidase

Chain B: 74% 24%

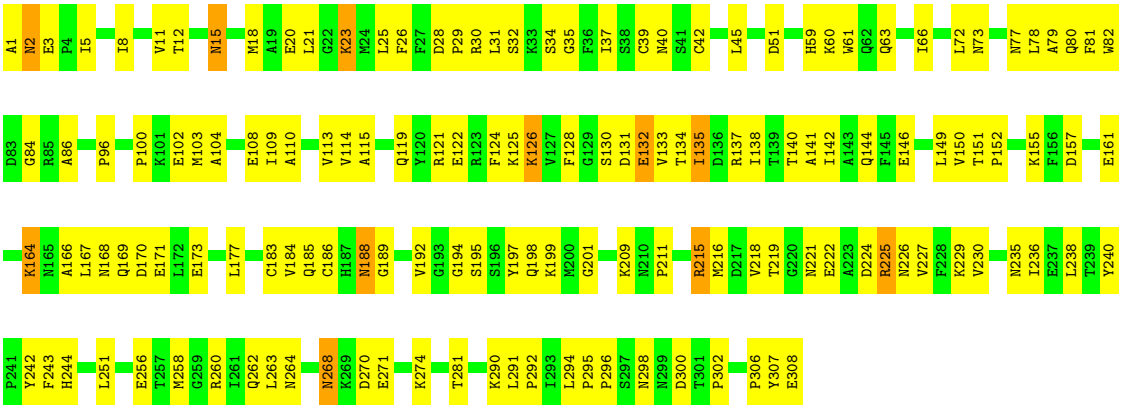
• Molecule 1: di-heme peroxidase

Chain C: 88% 11%



• Molecule 1: di-heme peroxidase

Chain D: 52% 44%


A1 N2 E3 P4 I5 I8 V11 T12 N15 M18 A19 E20 L21 G22 K23 M24 L25 F26 F27 D28 P29 R30 L31 S32 K33 S34 G35 F36 I37 S38 C39 N40 S41 C42 L45 D51 H59 K60 W61 Q62 Q63 I66 L72 N73 N77 L78 A79 Q80 F81 W82
D83 G84 R85 A86 P96 P100 K101 E102 M103 A104 E108 I109 A110 V113 V114 A115 Q119 Y120 R121 E122 R123 F124 K125 K126 V127 F128 G129 S130 D131 E132 V133 T134 I135 D136 R137 I138 T139 T140 A141 I142 A143 Q144 F145 E146 L149 V150 T151 P152 K155 F156 D157 E161
K164 N165 A166 L167 N168 Q169 D170 E171 L172 E173 L177 C183 V184 Q185 C186 H187 N188 G189 V192 G193 G194 S195 S196 Y197 Q198 K199 M200 G201 K209 N210 P211 R215 M216 D217 V218 T219 G220 N221 E222 A223 D224 R225 N226 V227 F228 K229 V230 N235 I236 E237 L238 T239 Y240
P241 Y242 F243 H244 L251 E256 T257 M258 G259 R260 I261 Q262 L263 N264 N268 K269 D270 E271 K274 T281 K290 L291 P292 I293 L294 P295 P296 S297 N298 N299 D300 T301 P302 P306 Y307 E308

4 Data and refinement statistics (i)

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	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms ($Å^2$)	30.0	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: HEC, MG, GOL, CA

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	0.32	0/2441	0.58	0/3304
1	B	0.29	0/2441	0.56	0/3304
1	C	0.32	0/2441	0.58	0/3304
1	D	0.29	0/2441	0.52	0/3304
All	All	0.30	0/9764	0.56	0/13216

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

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	2388	0	2331	53	0
1	B	2388	0	2331	81	0
1	C	2388	0	2331	40	0
1	D	2388	0	2331	179	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	64	15	0
4	B	86	0	64	15	0
4	C	86	0	64	14	0
4	D	86	0	64	17	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9588	348	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 19.

The worst 5 of 348 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:186:CYS:SG	4:B:402:HEC:HAC	1.50	1.50
1:D:42:CYS:SG	4:D:401:HEC:HAC	1.70	1.31
1:C:39:CYS:SG	4:C:401:HEC:HAB	1.72	1.25
1:A:183:CYS:SG	4:A:402:HEC:HAB	1.75	1.21
1:A:39:CYS:SG	4:A:401:HEC:HAB	1.77	1.15

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	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	15	5
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100	100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	22	10
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	34	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	GLU

5.3.2 Protein sidechains (i)

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	260/260 (100%)	255 (98%)	5 (2%)	57	46
1	B	260/260 (100%)	254 (98%)	6 (2%)	50	37
1	C	260/260 (100%)	255 (98%)	5 (2%)	57	46
1	D	260/260 (100%)	250 (96%)	10 (4%)	33	18
All	All	1040/1040 (100%)	1014 (98%)	26 (2%)	47	34

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	264	ASN
1	D	23	LYS
1	D	268	ASN

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Mol	Chain	Res	Type
1	D	15	ASN
1	D	126	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	15	ASN
1	D	299	ASN
1	C	176	ASN
1	D	298	ASN
1	D	144	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	C	402	1	32,50,50	1.44	3 (9%)	24,82,82	1.30	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	1410	-	5,5,5	0.29	0	5,5,5	0.27	0
4	HEC	A	401	1,6	32,50,50	1.24	3 (9%)	24,82,82	1.13	1 (4%)
4	HEC	B	402	1	32,50,50	1.40	3 (9%)	24,82,82	0.90	0
4	HEC	B	401	1,6	32,50,50	1.36	6 (18%)	24,82,82	0.97	1 (4%)
4	HEC	A	402	1	32,50,50	1.49	2 (6%)	24,82,82	1.26	1 (4%)
4	HEC	C	401	1,6	32,50,50	1.44	4 (12%)	24,82,82	1.15	2 (8%)
4	HEC	D	401	1,6	32,50,50	1.40	4 (12%)	24,82,82	0.91	0
4	HEC	D	402	1	32,50,50	1.43	4 (12%)	24,82,82	1.75	1 (4%)

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	C	402	1	-	2/10/54/54	-
5	GOL	B	1410	-	-	0/4/4/4	-
4	HEC	A	401	1,6	-	1/10/54/54	-
4	HEC	B	402	1	-	2/10/54/54	-
4	HEC	B	401	1,6	-	2/10/54/54	-
4	HEC	A	402	1	-	2/10/54/54	-
4	HEC	C	401	1,6	-	2/10/54/54	-
4	HEC	D	401	1,6	-	5/10/54/54	-
4	HEC	D	402	1	-	3/10/54/54	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	HEC	C3C-C2C	-4.63	1.35	1.40
4	A	402	HEC	C2B-C3B	-4.60	1.35	1.40
4	A	402	HEC	C3C-C2C	-4.48	1.36	1.40
4	C	401	HEC	C2B-C3B	-4.30	1.36	1.40
4	D	402	HEC	C3C-C2C	-4.05	1.36	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	402	HEC	CBD-CAD-C3D	6.97	124.51	112.62
4	C	401	HEC	CBD-CAD-C3D	-2.99	107.52	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	HEC	CBD-CAD-C3D	-2.97	107.56	112.62
4	A	401	HEC	CBD-CAD-C3D	-2.90	107.66	112.62
4	C	402	HEC	CMB-C2B-C1B	-2.52	124.58	128.46

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	HEC	C4D-C3D-CAD-CBD
4	D	401	HEC	C3A-C2A-CAA-CBA
4	C	401	HEC	CAA-CBA-CGA-O2A
4	D	401	HEC	CAA-CBA-CGA-O2A
4	D	402	HEC	CAD-CBD-CGD-O2D

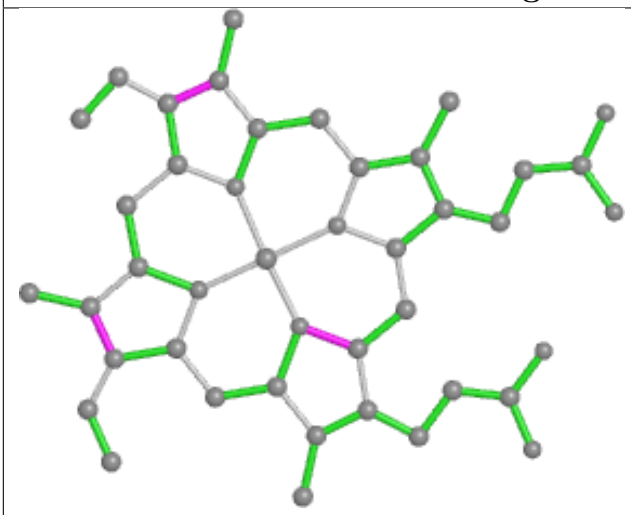
There are no ring outliers.

8 monomers are involved in 61 short contacts:

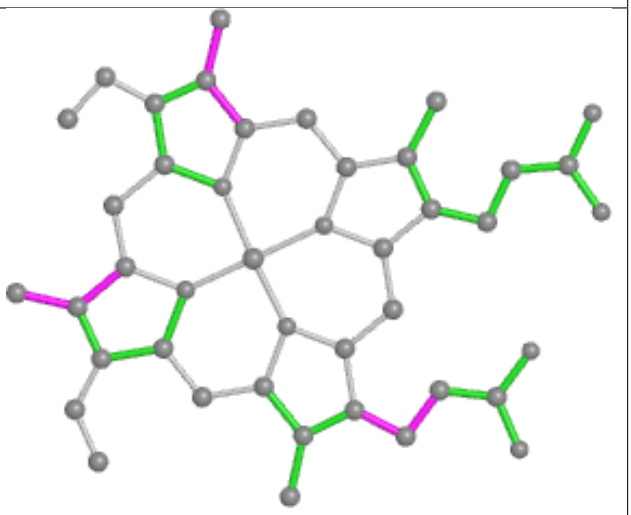
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	HEC	7	0
4	A	401	HEC	7	0
4	B	402	HEC	6	0
4	B	401	HEC	9	0
4	A	402	HEC	8	0
4	C	401	HEC	7	0
4	D	401	HEC	6	0
4	D	402	HEC	11	0

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 then 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.

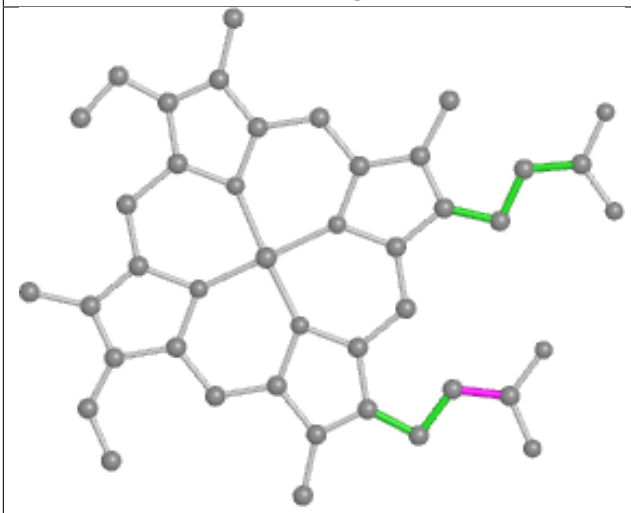
Ligand HEC C 402



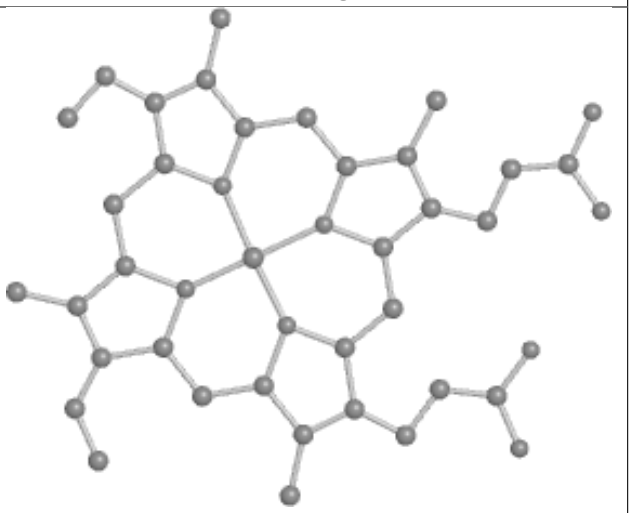
Bond lengths



Bond angles

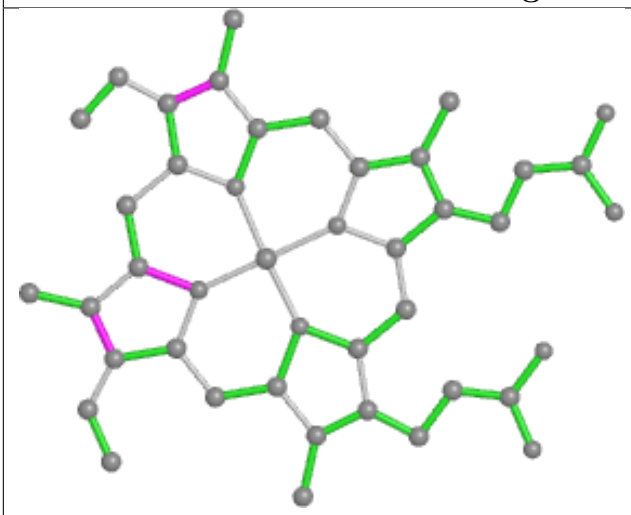


Torsions

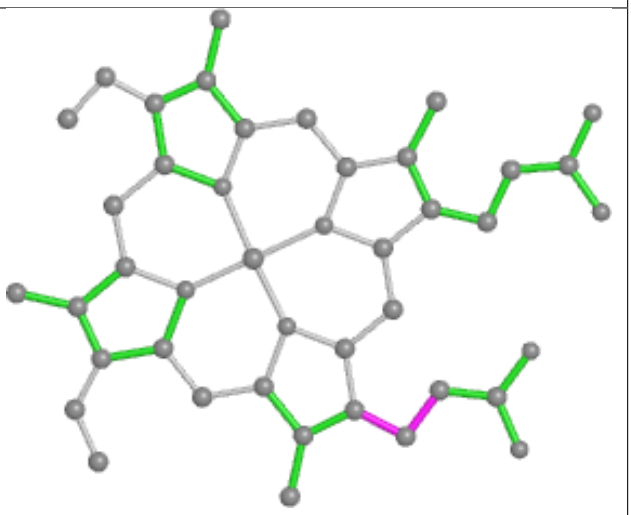


Rings

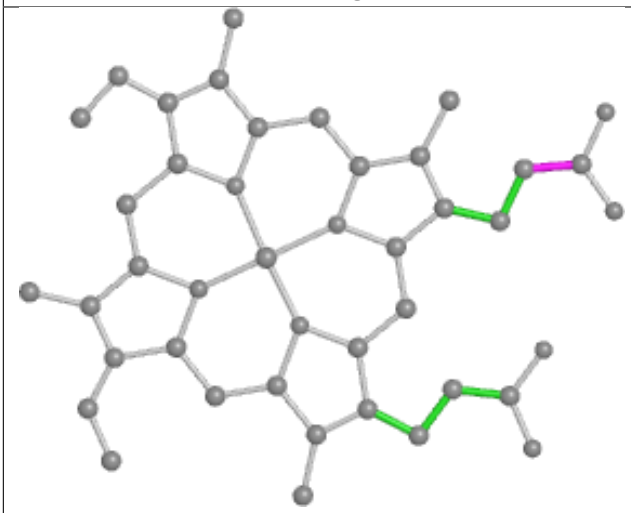
Ligand HEC A 401



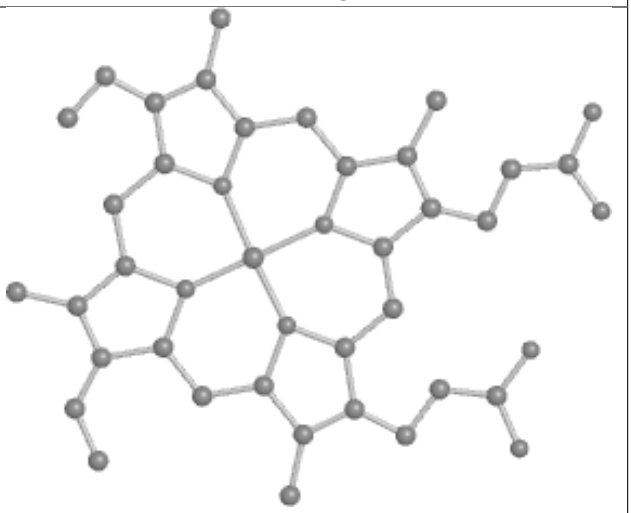
Bond lengths



Bond angles

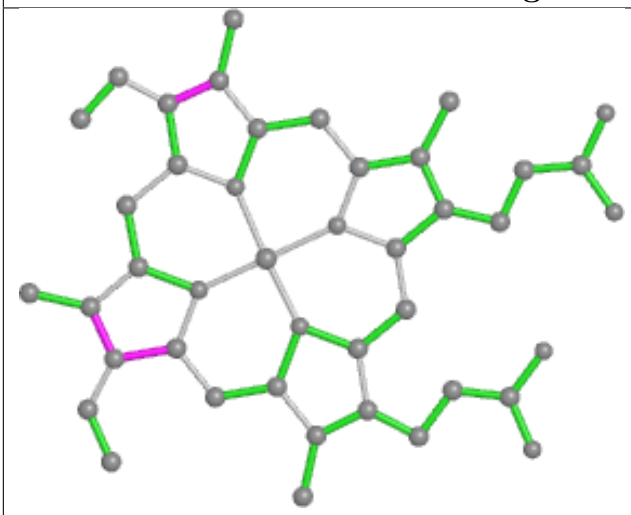


Torsions



Rings

Ligand HEC B 402



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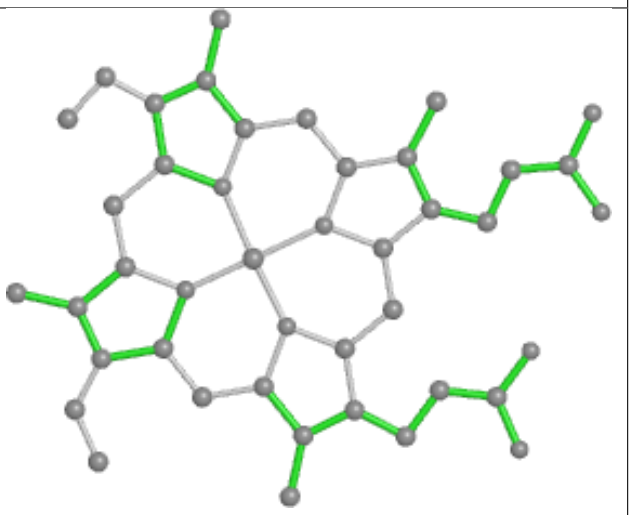
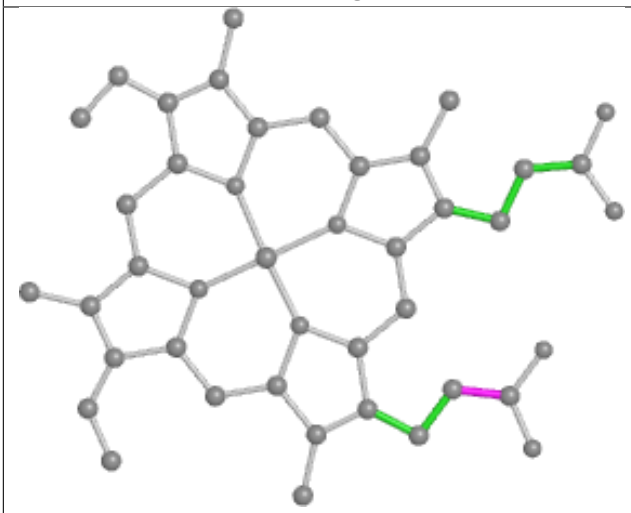


Bond angles



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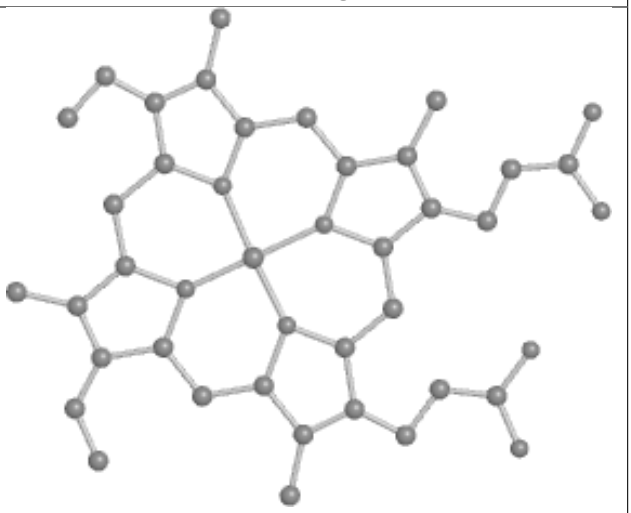
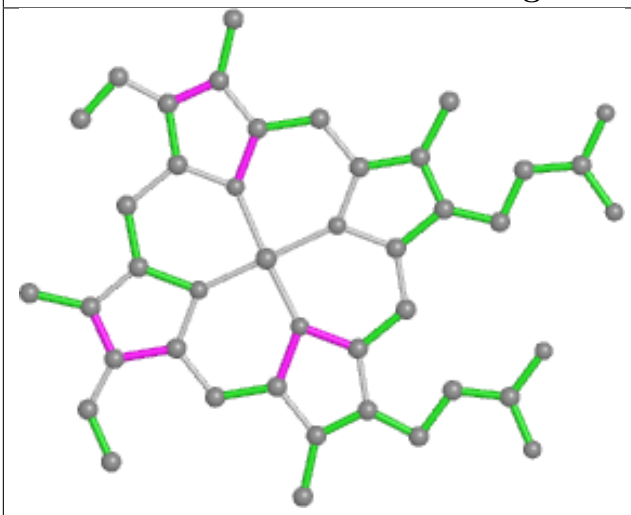


Rings

Ligand HEC B 401



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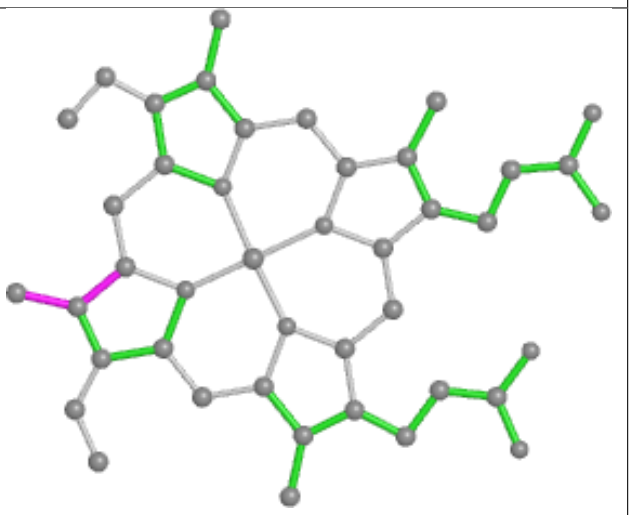
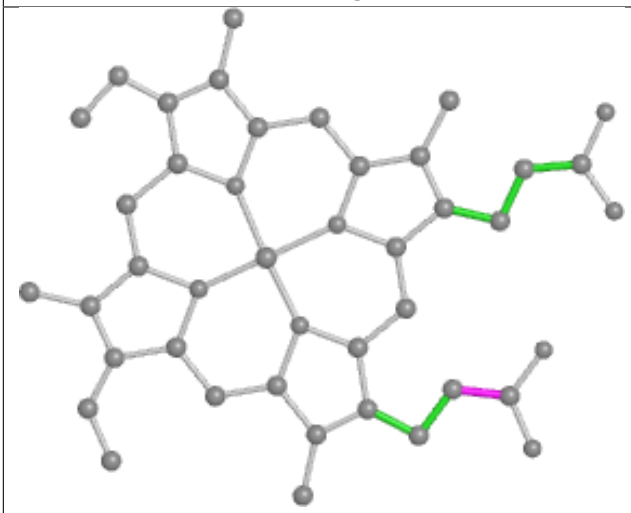


Bond angles



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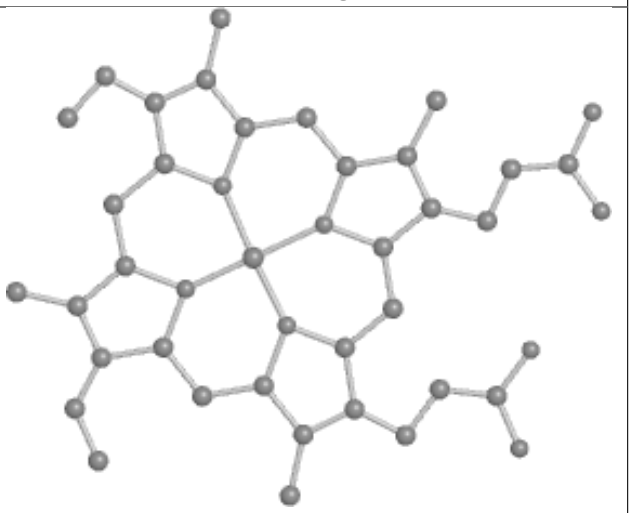
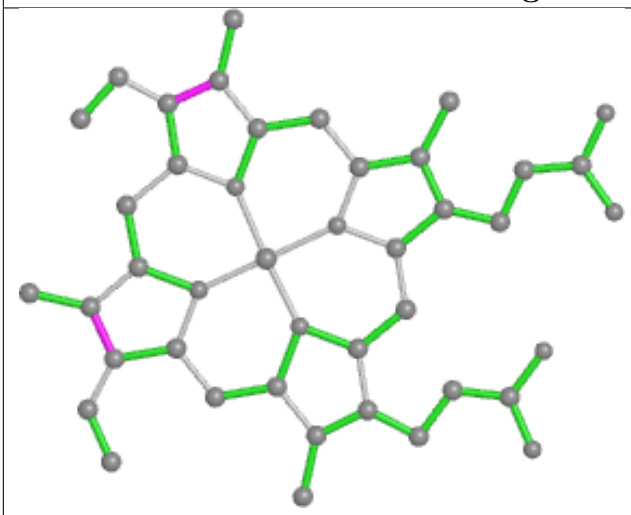
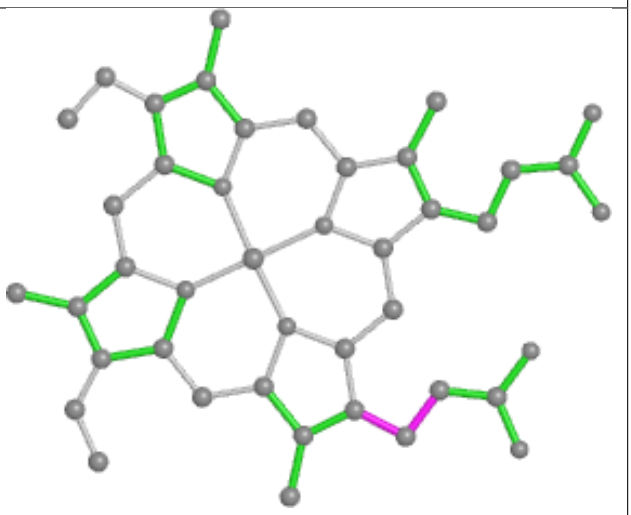


Rings

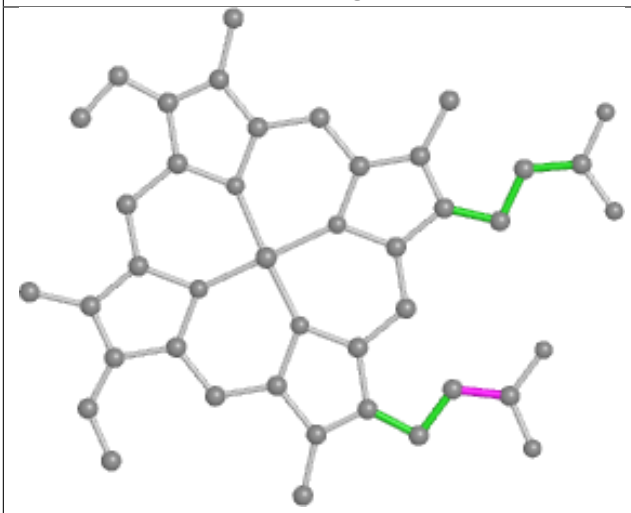
Ligand HEC A 402



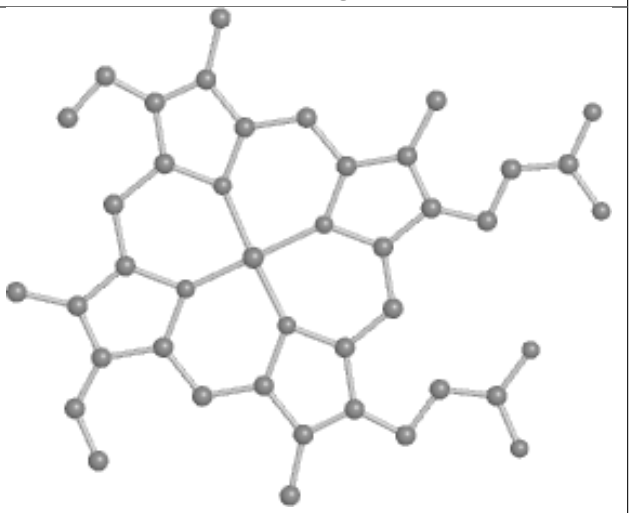
Bond lengths



Bond angles

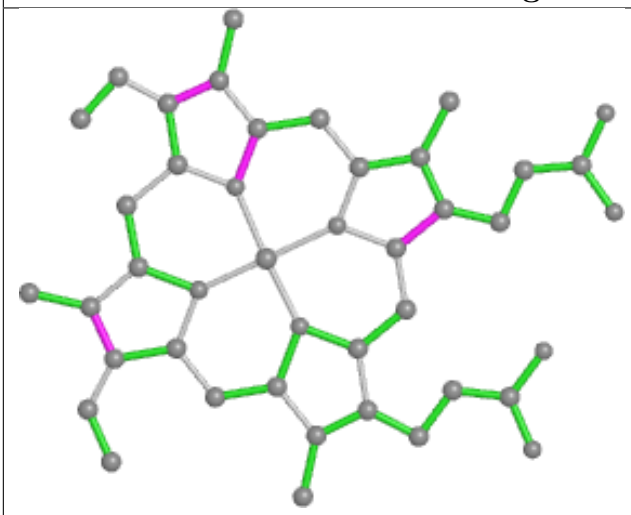


Torsions



Rings

Ligand HEC C 401



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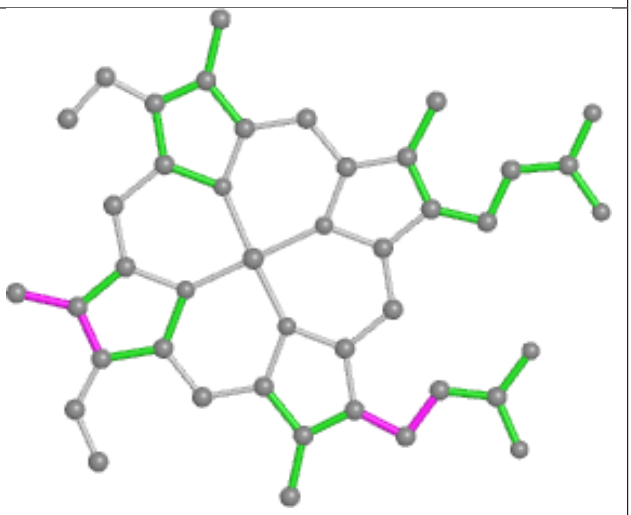
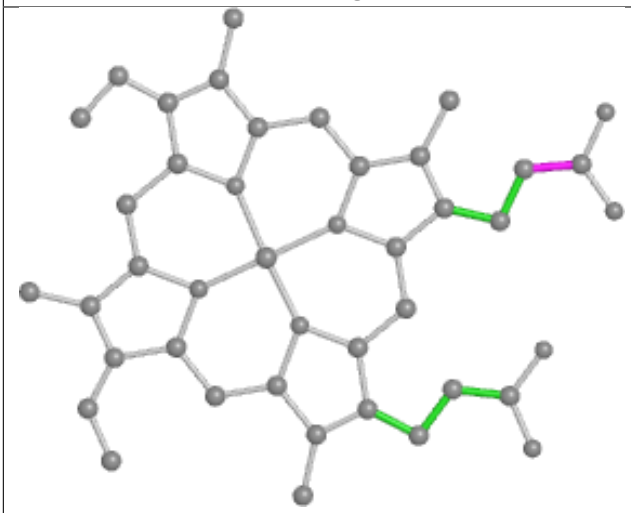


Bond angles



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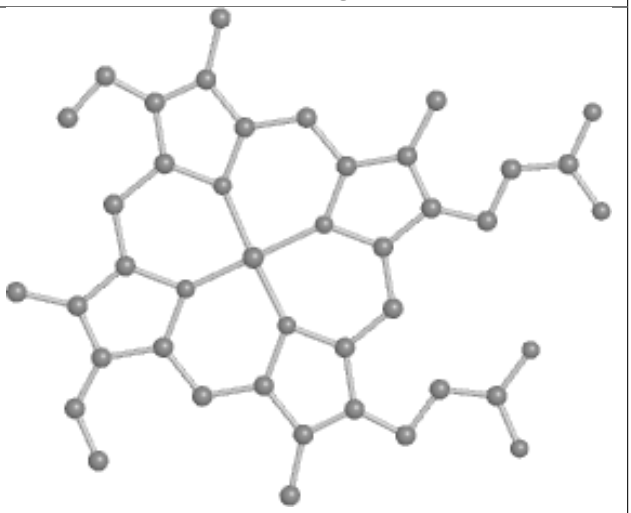
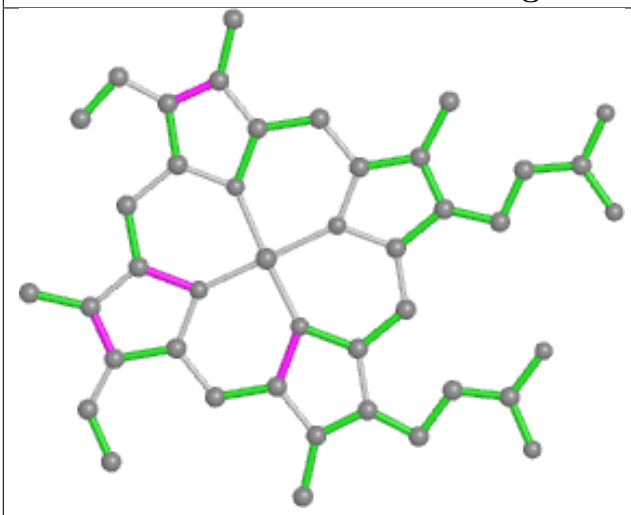


Rings

Ligand HEC D 401



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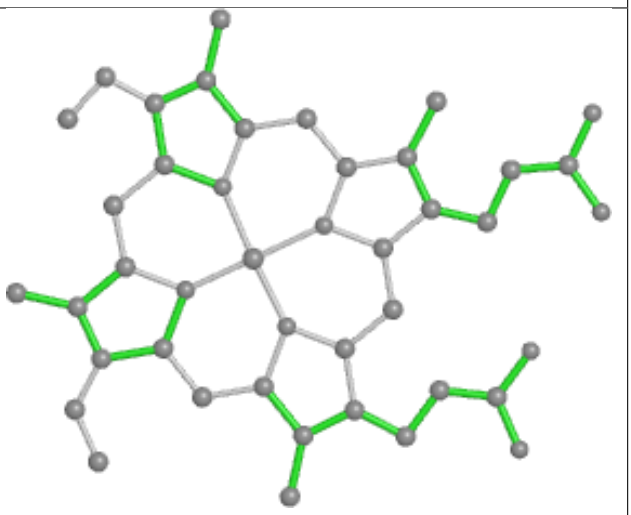
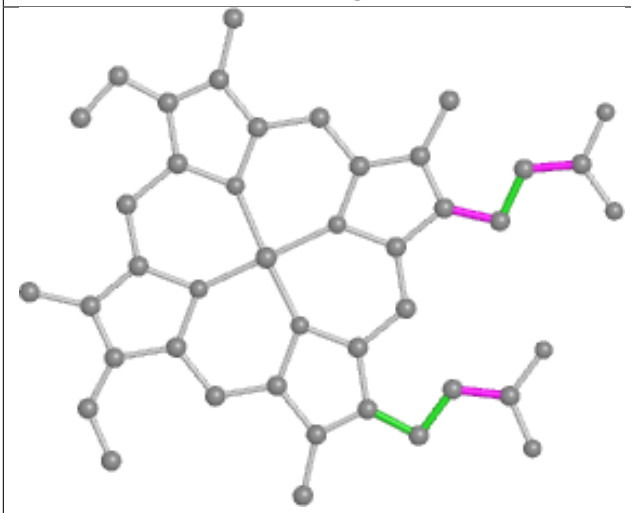
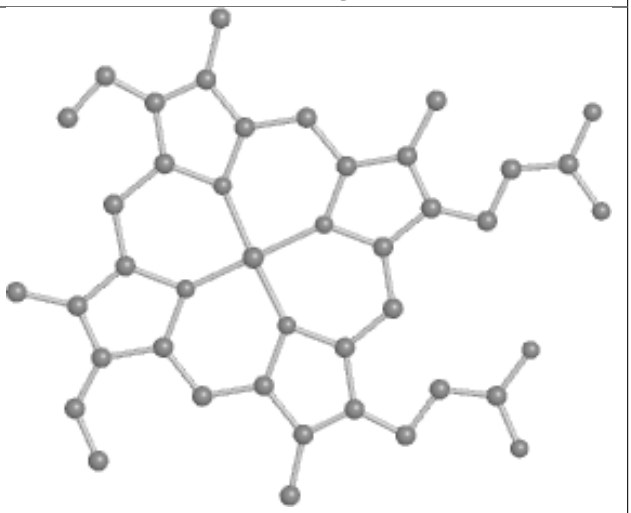


Bond angles

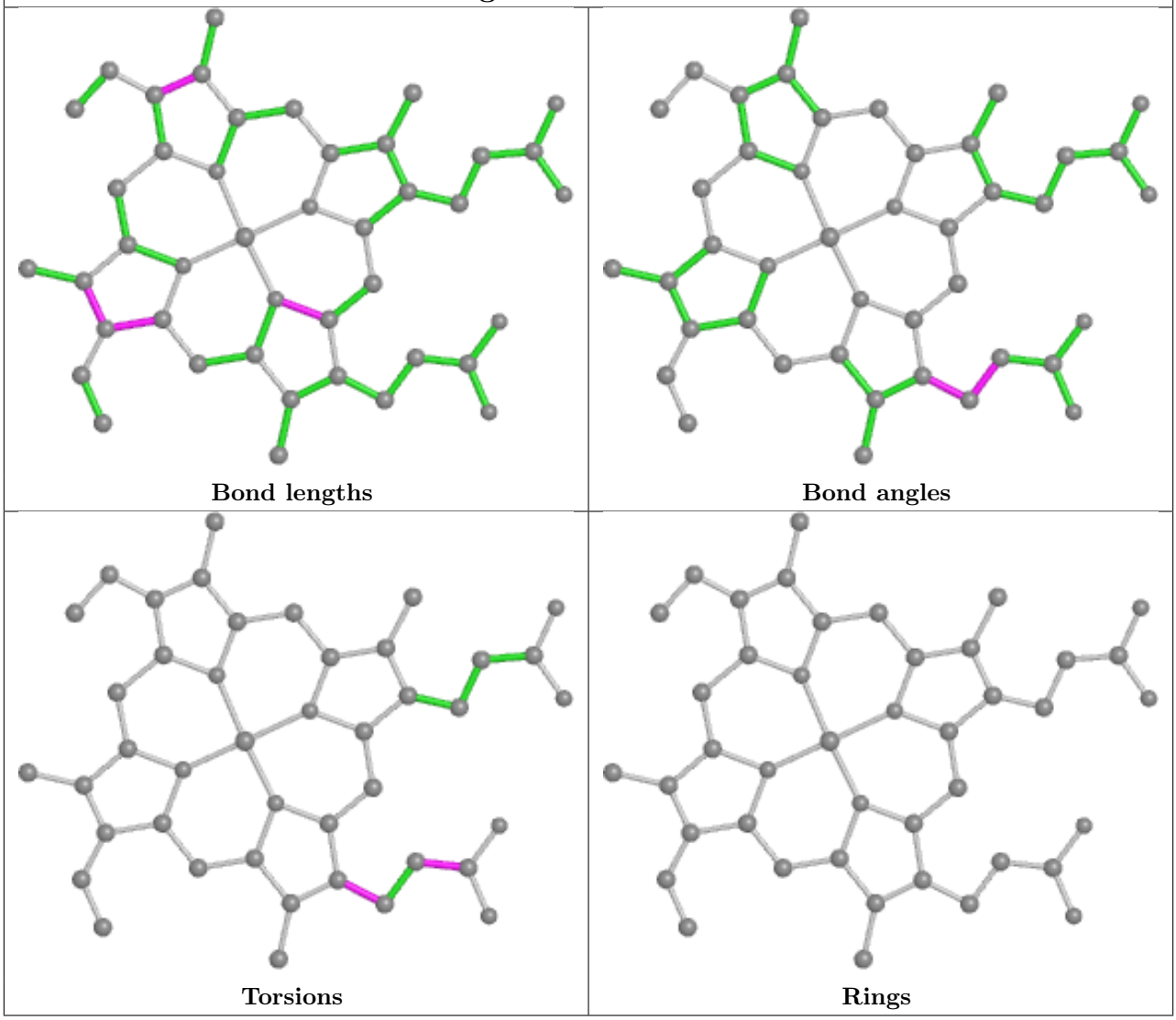


Torsions



Rings

Ligand HEC D 402



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.