



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:46 PM EDT

PDB ID : 8DVX / pdb_00008dvx
Title : Structure of acetylated Pig somatic Cytochrome c (Aly39) at 1.5Å
Authors : Edwards, B.F.P.; Huettemann, M.; Vaishnav, A.; Brunzelle, J.; Morse, P.;
Wan, J.
Deposited on : 2022-07-30
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

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) : 2.0
EDS : **FAILED**
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) : 2.50

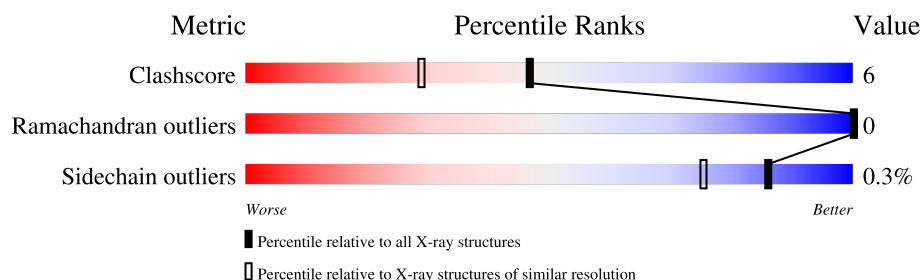
1 Overall quality at a glance

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	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (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 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	104	88% 12%
1	B	104	87% 13%
1	C	104	93% 7%
1	D	104	88% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	201	X	-	-	-
2	HEC	B	201	X	-	-	-
2	HEC	C	201	X	-	-	-
2	HEC	D	201	X	-	-	-

2 Entry composition [i](#)

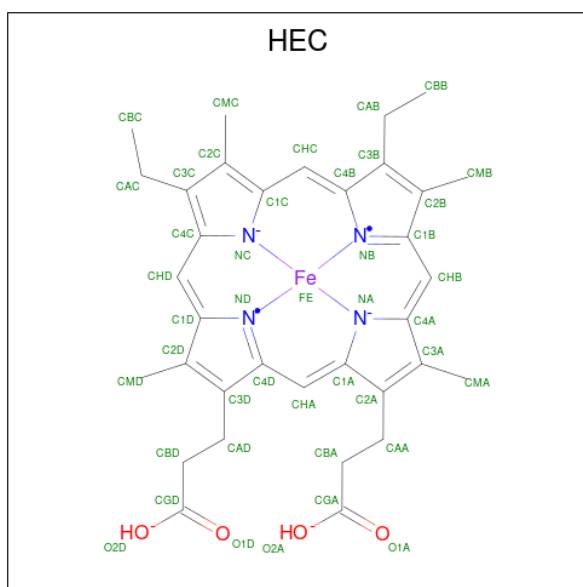
There are 4 unique types of molecules in this entry. The entry contains 3836 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			817	519	143	151	4			
1	B	104	Total	C	N	O	S	0	0	0
			817	519	143	151	4			
1	C	104	Total	C	N	O	S	0	0	0
			817	519	143	151	4			
1	D	104	Total	C	N	O	S	0	0	0
			817	519	143	151	4			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



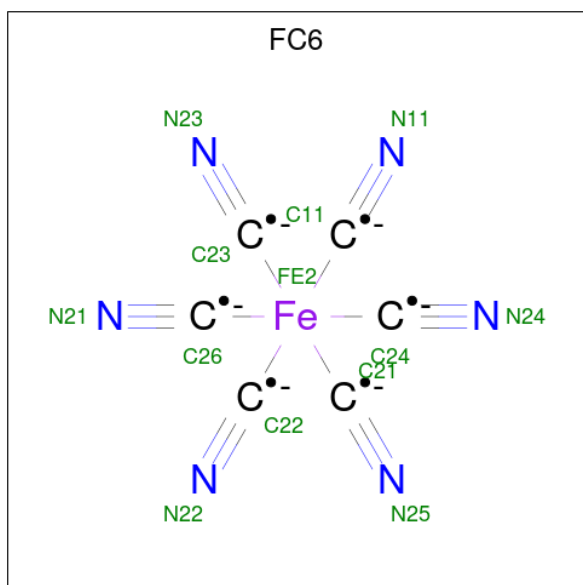
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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

- Molecule 3 is HEXACYANOFERRATE(3-) (CCD ID: FC6) (formula: C_6FeN_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	0	0
			13	6	1	6		
3	A	1	Total	C	Fe	N	0	0
			13	6	1	6		
3	B	1	Total	C	Fe	N	0	0
			13	6	1	6		
3	B	1	Total	C	Fe	N	0	0
			13	6	1	6		
3	B	1	Total	C	Fe	N	0	0
			13	6	1	6		
3	C	1	Total	C	Fe	N	0	0
			13	6	1	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total 87	O 87	0	0
4	B	93	Total 93	O 93	0	0
4	C	64	Total 64	O 64	0	0
4	D	61	Total 61	O 61	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 failed to run properly.

- Molecule 1: Cytochrome c

Chain A:  88% 12%



- Molecule 1: Cytochrome c

Chain B:  87% 13%



- Molecule 1: Cytochrome c

Chain C:  93% 7%



- Molecule 1: Cytochrome c

Chain D:  88% 12%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	34.66Å 54.56Å 61.78Å 65.97° 87.40° 84.07°	Depositor
Resolution (Å)	30.38 – 1.50	Depositor
% Data completeness (in resolution range)	84.8 (30.38-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.171 , 0.204	Depositor
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.016	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,-k+l	Xtriage
Total number of atoms	3836	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: FC6, ALY, 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	0.70	0/820	0.79	0/1091
1	B	0.74	0/820	0.86	0/1091
1	C	0.67	0/820	0.79	0/1091
1	D	0.69	0/820	0.82	0/1091
All	All	0.70	0/3280	0.82	0/4364

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	817	0	832	9	0
1	B	817	0	832	15	0
1	C	817	0	832	6	0
1	D	817	0	832	10	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	1	0
3	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	52	0	0	2	0
3	C	13	0	0	0	0
4	A	87	0	0	2	1
4	B	93	0	0	2	3
4	C	64	0	0	1	0
4	D	61	0	0	3	2
All	All	3836	0	3448	40	3

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 6.

All (40) 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:5:LYS:HA	1:B:8:LYS:HE3	1.48	0.93
1:C:70:ASN:HB3	1:C:73:LYS:HG2	1.72	0.72
1:B:25:LYS:NZ	4:B:302:HOH:O	2.25	0.69
1:B:62:GLU:H	1:B:62:GLU:CD	2.04	0.65
1:A:21:GLU:OE2	4:A:301:HOH:O	2.15	0.64
1:D:72:LYS:HE3	1:D:77:GLY:H	1.63	0.64
1:B:72:LYS:HE3	1:C:16:GLN:OE1	1.99	0.63
1:B:9:ILE:HD13	1:B:90:GLU:HG3	1.82	0.61
2:D:201:HEC:HBC3	2:D:201:HEC:HMC1	1.83	0.60
1:B:21:GLU:OE1	4:B:301:HOH:O	2.17	0.60
1:D:72:LYS:HD2	1:D:76:PRO:HA	1.85	0.58
1:C:42:GLN:HE21	1:C:42:GLN:HA	1.70	0.57
2:B:201:HEC:HMC1	2:B:201:HEC:HBC3	1.86	0.57
1:B:5:LYS:HA	1:B:8:LYS:CE	2.30	0.56
1:C:38:ARG:NH2	4:C:301:HOH:O	2.37	0.55
1:B:4:GLU:O	1:B:8:LYS:HE2	2.07	0.54
1:A:69:GLU:HG2	1:A:86:LYS:HE2	1.91	0.52
1:C:42:GLN:HA	1:C:42:GLN:NE2	2.24	0.52
1:D:5:LYS:NZ	4:D:303:HOH:O	2.43	0.51
1:A:81:ILE:HG23	1:D:16:GLN:NE2	2.28	0.49
1:B:86:LYS:HE2	1:B:86:LYS:H	1.78	0.49
1:B:4:GLU:HG2	1:B:8:LYS:NZ	2.28	0.48
1:B:86:LYS:H	1:B:86:LYS:CE	2.25	0.48
1:D:9:ILE:CD1	1:D:90:GLU:HG3	2.44	0.48
1:D:9:ILE:HD13	1:D:90:GLU:HG3	1.96	0.48
1:B:57:ILE:C	1:B:57:ILE:HD12	2.40	0.47
1:B:40:THR:HG22	1:B:59:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HE2	1:B:86:LYS:HB2	1.78	0.45
1:A:6:GLY:HA2	1:A:9:ILE:HD12	2.00	0.43
1:D:57:ILE:C	1:D:57:ILE:HD12	2.43	0.43
1:D:38:ARG:HD2	4:D:308:HOH:O	2.19	0.43
1:A:52:ASN:ND2	4:A:304:HOH:O	2.51	0.43
1:A:25:LYS:HA	1:A:25:LYS:HD2	1.79	0.42
1:A:81:ILE:HG23	1:D:16:GLN:HE21	1.84	0.42
2:A:201:HEC:HMB1	2:A:201:HEC:HBB3	2.01	0.42
3:B:203:FC6:N11	1:C:90:GLU:OE1	2.53	0.42
1:B:90:GLU:OE1	3:B:203:FC6:N24	2.54	0.41
1:D:8:LYS:NZ	4:D:305:HOH:O	2.50	0.41
1:A:40:THR:HG22	1:A:59:TRP:CE2	2.56	0.40
1:A:57:ILE:HD12	1:A:57:ILE:C	2.47	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:354:HOH:O	4:D:322:HOH:O[1_465]	2.04	0.16
4:B:330:HOH:O	4:D:341:HOH:O[1_465]	2.14	0.06
4:A:345:HOH:O	4:B:308:HOH:O[1_655]	2.15	0.05

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	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
1	B	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
1	C	101/104 (97%)	96 (95%)	5 (5%)	0	100	100
1	D	101/104 (97%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	404/416 (97%)	390 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	83/83 (100%)	83 (100%)	0	100	100
1	B	83/83 (100%)	83 (100%)	0	100	100
1	C	83/83 (100%)	83 (100%)	0	100	100
1	D	83/83 (100%)	82 (99%)	1 (1%)	63	38
All	All	332/332 (100%)	331 (100%)	1 (0%)	86	75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	42	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	B	12	GLN
1	C	42	GLN
1	C	52	ASN
1	D	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	ALY	D	39	1	10,11,12	1.00	1 (10%)	7,12,14	1.10	1 (14%)
1	ALY	B	39	1	10,11,12	0.91	1 (10%)	7,12,14	1.07	0
1	ALY	C	39	1	10,11,12	1.01	1 (10%)	7,12,14	1.24	1 (14%)
1	ALY	A	39	1	10,11,12	1.04	1 (10%)	7,12,14	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	D	39	1	-	3/9/10/12	-
1	ALY	B	39	1	-	2/9/10/12	-
1	ALY	C	39	1	-	2/9/10/12	-
1	ALY	A	39	1	-	2/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ALY	CH-NZ	2.20	1.40	1.34
1	C	39	ALY	CH-NZ	2.19	1.40	1.34
1	D	39	ALY	CH-NZ	2.18	1.40	1.34
1	B	39	ALY	CH-NZ	2.18	1.39	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ALY	CE-NZ-CH	2.74	126.61	122.56
1	D	39	ALY	CE-NZ-CH	2.21	125.83	122.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	39	ALY	CG-CD-CE-NZ
1	D	39	ALY	CG-CD-CE-NZ
1	A	39	ALY	CG-CD-CE-NZ
1	C	39	ALY	CE-CD-CG-CB
1	D	39	ALY	CA-CB-CG-CD
1	D	39	ALY	CE-CD-CG-CB
1	A	39	ALY	CA-CB-CG-CD
1	B	39	ALY	CA-CB-CG-CD
1	B	39	ALY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	FC6	A	202	-	12,12,12	2.78	6 (50%)	-		
3	FC6	A	203	-	12,12,12	2.65	8 (66%)	-		
3	FC6	B	205	-	12,12,12	2.72	6 (50%)	-		
3	FC6	B	202	-	12,12,12	2.84	8 (66%)	-		
3	FC6	B	203	-	12,12,12	2.85	7 (58%)	-		
3	FC6	C	202	-	12,12,12	3.32	9 (75%)	-		
2	HEC	A	201	1	50,50,50	1.43	7 (14%)	68,82,82	1.92	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FC6	B	204	-	12,12,12	2.58	6 (50%)	-		
2	HEC	B	201	1	50,50,50	1.50	7 (14%)	68,82,82	1.97	21 (30%)
2	HEC	C	201	1	50,50,50	1.58	8 (16%)	68,82,82	1.71	20 (29%)
2	HEC	D	201	1	50,50,50	1.48	6 (12%)	68,82,82	1.67	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	C	201	1	1/1/3/7	8/14/54/54	-
2	HEC	B	201	1	1/1/3/7	8/14/54/54	-
2	HEC	A	201	1	1/1/3/7	8/14/54/54	-
2	HEC	D	201	1	1/1/3/7	6/14/54/54	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	FC6	C23-FE2	-5.93	1.76	1.93
2	D	201	HEC	C3D-C2D	5.31	1.48	1.36
2	A	201	HEC	C3D-C2D	5.21	1.48	1.36
3	C	202	FC6	C21-FE2	-5.18	1.78	1.93
3	B	203	FC6	C21-FE2	-4.66	1.80	1.93
3	B	202	FC6	C22-FE2	-4.34	1.81	1.93
2	B	201	HEC	C3D-C2D	4.22	1.45	1.36
3	A	202	FC6	C21-FE2	-4.19	1.81	1.93
3	B	203	FC6	C22-FE2	-4.00	1.82	1.93
3	A	202	FC6	C22-FE2	-3.99	1.82	1.93
3	A	202	FC6	C26-FE2	-3.98	1.82	1.93
2	C	201	HEC	C3D-C2D	3.98	1.45	1.36
2	C	201	HEC	FE-NA	3.97	2.08	1.95
3	A	202	FC6	C23-FE2	-3.94	1.82	1.93
3	B	205	FC6	C11-FE2	-3.94	1.82	1.93
2	C	201	HEC	FE-NC	3.90	2.08	1.95
3	B	202	FC6	C21-FE2	-3.84	1.82	1.93
3	B	203	FC6	C23-FE2	-3.83	1.82	1.93
3	C	202	FC6	C24-FE2	-3.80	1.82	1.93
3	B	202	FC6	C26-FE2	-3.80	1.82	1.93
3	B	203	FC6	C26-FE2	-3.67	1.83	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	205	FC6	C23-FE2	-3.67	1.83	1.93
3	A	203	FC6	C22-FE2	-3.60	1.83	1.93
3	B	204	FC6	C21-FE2	-3.55	1.83	1.93
3	A	203	FC6	C11-FE2	-3.53	1.83	1.93
3	B	202	FC6	C11-FE2	-3.49	1.83	1.93
3	A	203	FC6	C21-FE2	-3.49	1.83	1.93
3	B	204	FC6	C24-FE2	-3.43	1.83	1.93
3	B	205	FC6	C26-FE2	-3.41	1.83	1.93
3	B	205	FC6	C21-FE2	-3.40	1.83	1.93
3	B	204	FC6	C23-FE2	-3.40	1.83	1.93
3	B	202	FC6	C23-FE2	-3.36	1.84	1.93
3	B	205	FC6	C22-FE2	-3.35	1.84	1.93
2	B	201	HEC	FE-NA	3.33	2.06	1.95
3	C	202	FC6	C21-N25	3.32	1.22	1.15
3	B	205	FC6	C24-FE2	-3.31	1.84	1.93
3	C	202	FC6	C23-N23	3.29	1.22	1.15
3	A	202	FC6	C11-FE2	-3.27	1.84	1.93
2	C	201	HEC	C4C-NC	-3.24	1.33	1.39
2	C	201	HEC	C1A-NA	-3.19	1.33	1.39
3	A	202	FC6	C24-FE2	-3.18	1.84	1.93
3	B	204	FC6	C11-FE2	-3.18	1.84	1.93
3	A	203	FC6	C26-FE2	-3.17	1.84	1.93
3	C	202	FC6	C22-N22	3.16	1.22	1.15
3	A	203	FC6	C24-FE2	-3.12	1.84	1.93
3	B	202	FC6	C24-FE2	-3.11	1.84	1.93
2	B	201	HEC	FE-NC	3.09	2.05	1.95
3	B	204	FC6	C22-FE2	-3.06	1.84	1.93
3	B	203	FC6	C11-FE2	-3.03	1.85	1.93
2	B	201	HEC	C1A-NA	-2.99	1.34	1.39
3	A	203	FC6	C23-FE2	-2.98	1.85	1.93
3	B	204	FC6	C26-FE2	-2.98	1.85	1.93
3	B	203	FC6	C24-FE2	-2.87	1.85	1.93
3	C	202	FC6	C26-FE2	-2.85	1.85	1.93
2	D	201	HEC	CAB-C3B	2.66	1.57	1.51
2	A	201	HEC	CMB-C2B	2.65	1.56	1.50
2	B	201	HEC	CMB-C2B	2.59	1.56	1.50
2	A	201	HEC	CAB-C3B	2.56	1.57	1.51
2	D	201	HEC	CMB-C2B	2.54	1.56	1.50
2	A	201	HEC	FE-NA	2.51	2.03	1.95
2	D	201	HEC	CMD-C2D	2.48	1.55	1.50
2	C	201	HEC	CMC-C2C	2.48	1.55	1.50
2	B	201	HEC	O1D-CGD	2.46	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	FC6	C26-N21	2.45	1.20	1.15
2	B	201	HEC	CHA-C4D	-2.43	1.33	1.39
3	B	202	FC6	C24-N24	2.43	1.20	1.15
2	A	201	HEC	FE-ND	2.42	2.02	1.94
2	C	201	HEC	CMB-C2B	2.41	1.55	1.50
3	C	202	FC6	C22-FE2	-2.39	1.86	1.93
2	C	201	HEC	C4A-NA	-2.33	1.35	1.39
2	D	201	HEC	C4B-NB	-2.32	1.36	1.40
3	C	202	FC6	C11-FE2	-2.28	1.87	1.93
2	A	201	HEC	CMD-C2D	2.17	1.55	1.50
2	D	201	HEC	FE-NA	2.16	2.02	1.95
3	B	203	FC6	C23-N23	2.09	1.19	1.15
3	A	203	FC6	C23-N23	2.08	1.19	1.15
2	A	201	HEC	O1D-CGD	2.07	1.28	1.22
3	A	203	FC6	C24-N24	2.03	1.19	1.15

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	HEC	CMC-C2C-C1C	-7.01	114.75	125.42
2	D	201	HEC	CHB-C1B-NB	4.69	129.47	124.42
2	C	201	HEC	CHC-C4B-NB	4.54	129.99	124.37
2	A	201	HEC	CHD-C1D-ND	4.52	129.95	124.37
2	B	201	HEC	CHA-C4D-ND	4.49	129.26	124.42
2	A	201	HEC	CHB-C4A-NA	4.36	129.20	124.45
2	B	201	HEC	CAD-C3D-C4D	4.31	132.21	124.70
2	B	201	HEC	CHB-C4A-NA	4.25	129.08	124.45
2	B	201	HEC	CMB-C2B-C1B	-4.12	118.60	125.03
2	B	201	HEC	C1D-ND-C4D	4.04	109.99	105.21
2	A	201	HEC	C1D-ND-C4D	3.77	109.67	105.21
2	A	201	HEC	CHB-C1B-NB	3.66	128.36	124.42
2	B	201	HEC	CHC-C4B-NB	3.63	128.85	124.37
2	B	201	HEC	CBD-CAD-C3D	-3.57	102.65	112.53
2	A	201	HEC	CMD-C2D-C1D	3.44	130.41	125.03
2	B	201	HEC	CHD-C1D-ND	3.41	128.58	124.37
2	D	201	HEC	CMC-C2C-C1C	-3.38	120.27	125.42
2	A	201	HEC	CBD-CAD-C3D	-3.37	103.22	112.53
2	D	201	HEC	CBD-CAD-C3D	-3.31	103.38	112.53
2	D	201	HEC	C1D-ND-C4D	3.24	109.05	105.21
2	D	201	HEC	CAD-C3D-C4D	3.18	130.25	124.70
2	D	201	HEC	CMD-C2D-C1D	3.08	129.84	125.03
2	C	201	HEC	C2A-C1A-NA	-3.07	107.36	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	HEC	C1D-ND-C4D	3.00	108.76	105.21
2	C	201	HEC	C4A-NA-C1A	2.88	110.51	105.82
2	D	201	HEC	CAD-C3D-C2D	-2.82	122.59	127.87
2	C	201	HEC	C3C-C4C-NC	-2.72	107.13	110.15
2	D	201	HEC	CHD-C1D-ND	2.71	127.72	124.37
2	C	201	HEC	C4C-NC-C1C	2.64	110.12	105.82
2	C	201	HEC	CHA-C1A-NA	2.64	127.33	124.45
2	D	201	HEC	O1A-CGA-CBA	-2.58	114.92	123.09
2	B	201	HEC	CBB-CAB-C3B	-2.57	105.46	112.42
2	C	201	HEC	CHD-C4C-NC	2.54	128.47	123.86
2	C	201	HEC	O2D-CGD-CBD	2.54	122.03	114.00
2	C	201	HEC	CHB-C4A-NA	2.54	127.22	124.45
2	A	201	HEC	CHA-C1A-C2A	2.53	128.85	124.86
2	A	201	HEC	O1A-CGA-CBA	-2.50	115.18	123.09
2	B	201	HEC	C1B-C2B-C3B	2.49	109.60	106.98
2	D	201	HEC	CBB-CAB-C3B	-2.48	105.68	112.42
2	C	201	HEC	O2A-CGA-CBA	2.48	121.84	114.00
2	C	201	HEC	CBD-CAD-C3D	-2.47	105.70	112.53
2	B	201	HEC	CAD-C3D-C2D	-2.46	123.26	127.87
2	C	201	HEC	O1A-CGA-CBA	-2.45	115.31	123.09
2	B	201	HEC	C4A-NA-C1A	2.44	109.80	105.82
2	A	201	HEC	CBA-CAA-C2A	-2.39	105.92	112.53
2	B	201	HEC	CBA-CAA-C2A	-2.38	105.94	112.53
2	C	201	HEC	CHA-C4D-ND	2.38	126.98	124.42
2	B	201	HEC	C4C-CHD-C1D	-2.37	120.67	126.25
2	B	201	HEC	C2B-C1B-NB	-2.36	107.18	109.90
2	A	201	HEC	C3D-C4D-ND	-2.29	108.14	110.35
2	D	201	HEC	O2D-CGD-CBD	2.27	121.18	114.00
2	B	201	HEC	C3D-C4D-ND	-2.26	108.16	110.35
2	A	201	HEC	CAC-C3C-C4C	2.26	128.02	124.91
2	B	201	HEC	C1D-C2D-C3D	2.25	109.34	106.98
2	B	201	HEC	O1D-CGD-CBD	-2.25	115.96	123.09
2	C	201	HEC	CBA-CAA-C2A	-2.23	106.38	112.53
2	D	201	HEC	CBA-CAA-C2A	-2.21	106.43	112.53
2	B	201	HEC	O2D-CGD-CBD	2.20	120.94	114.00
2	C	201	HEC	CAC-C3C-C4C	-2.19	121.89	124.91
2	B	201	HEC	CMA-C3A-C4A	-2.19	120.87	124.73
2	A	201	HEC	CMC-C2C-C3C	2.16	130.21	125.62
2	C	201	HEC	CMA-C3A-C4A	-2.15	120.94	124.73
2	C	201	HEC	CMA-C3A-C2A	2.15	131.95	126.15
2	D	201	HEC	C3D-C4D-ND	-2.13	108.30	110.35
2	A	201	HEC	CAD-C3D-C4D	2.10	128.36	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	HEC	CMC-C2C-C3C	2.08	130.04	125.62
2	C	201	HEC	CHC-C4B-C3B	-2.08	121.40	125.23
2	D	201	HEC	CAB-C3B-C2B	2.07	131.36	127.56
2	A	201	HEC	CAD-C3D-C2D	-2.06	124.01	127.87
2	A	201	HEC	O1D-CGD-CBD	-2.05	116.60	123.09
2	C	201	HEC	CMD-C2D-C1D	2.04	128.22	125.03
2	B	201	HEC	CHD-C4C-NC	2.02	127.52	123.86
2	A	201	HEC	CHD-C1D-C2D	-2.01	121.25	126.95

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	HEC	NA
2	B	201	HEC	NA
2	C	201	HEC	NA
2	D	201	HEC	NA

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	HEC	C4C-C3C-CAC-CBC
2	D	201	HEC	C2C-C3C-CAC-CBC
2	C	201	HEC	C4C-C3C-CAC-CBC
2	A	201	HEC	C2B-C3B-CAB-CBB
2	D	201	HEC	C2B-C3B-CAB-CBB
2	B	201	HEC	C2B-C3B-CAB-CBB
2	B	201	HEC	C4C-C3C-CAC-CBC
2	A	201	HEC	C2C-C3C-CAC-CBC
2	B	201	HEC	C2C-C3C-CAC-CBC
2	A	201	HEC	C4C-C3C-CAC-CBC
2	C	201	HEC	C2C-C3C-CAC-CBC
2	C	201	HEC	C2B-C3B-CAB-CBB
2	A	201	HEC	C4B-C3B-CAB-CBB
2	C	201	HEC	C4B-C3B-CAB-CBB
2	B	201	HEC	C4B-C3B-CAB-CBB
2	D	201	HEC	C4B-C3B-CAB-CBB
2	C	201	HEC	CAD-CBD-CGD-O2D
2	A	201	HEC	CAD-CBD-CGD-O2D
2	C	201	HEC	CAA-CBA-CGA-O2A
2	A	201	HEC	CAA-CBA-CGA-O2A
2	C	201	HEC	CAD-CBD-CGD-O1D
2	A	201	HEC	CAA-CBA-CGA-O1A

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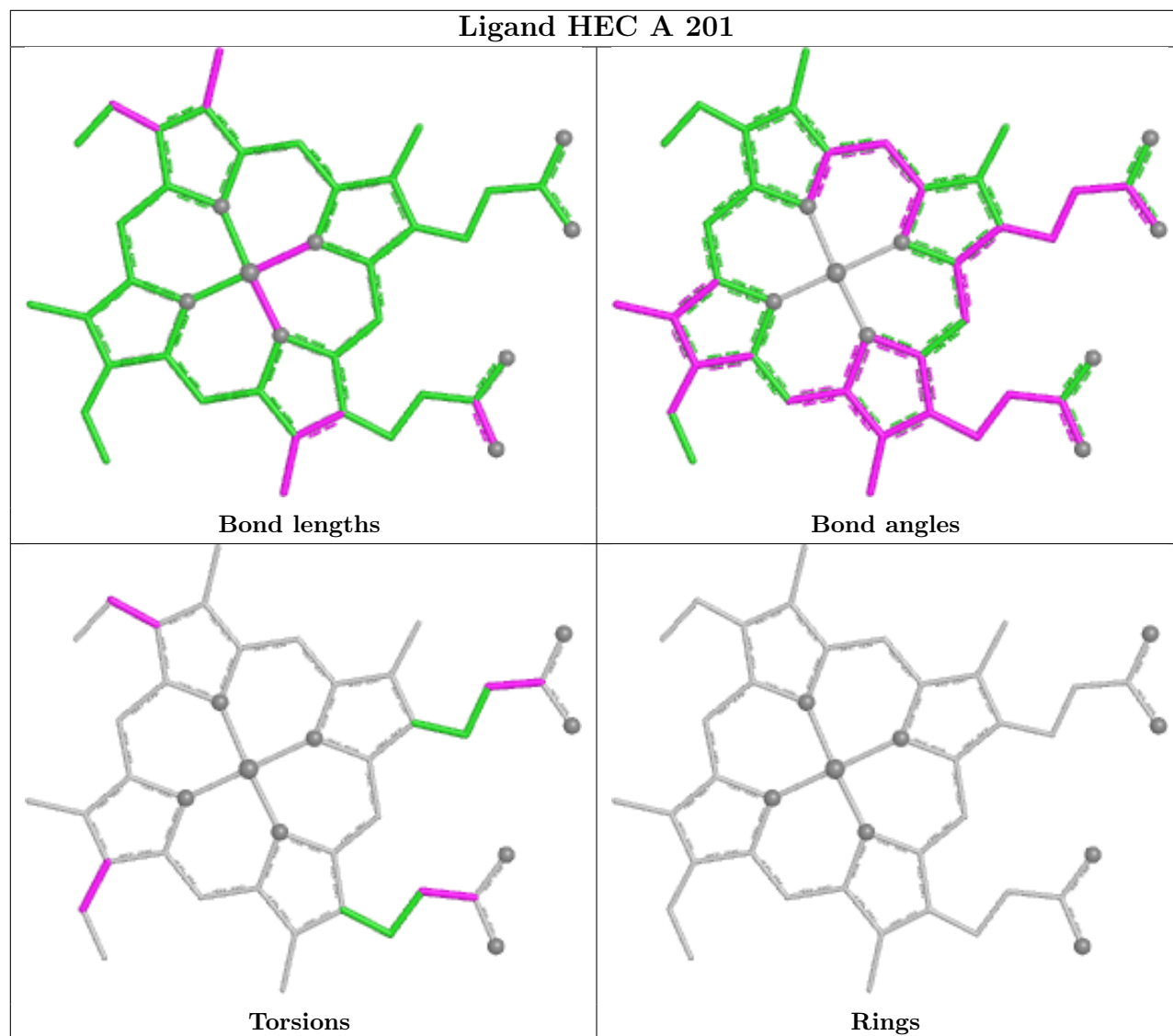
Mol	Chain	Res	Type	Atoms
2	D	201	HEC	CAD-CBD-CGD-O2D
2	B	201	HEC	CAA-CBA-CGA-O2A
2	D	201	HEC	CAA-CBA-CGA-O2A
2	B	201	HEC	CAA-CBA-CGA-O1A
2	B	201	HEC	CAD-CBD-CGD-O1D
2	B	201	HEC	CAD-CBD-CGD-O2D
2	A	201	HEC	CAD-CBD-CGD-O1D
2	C	201	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

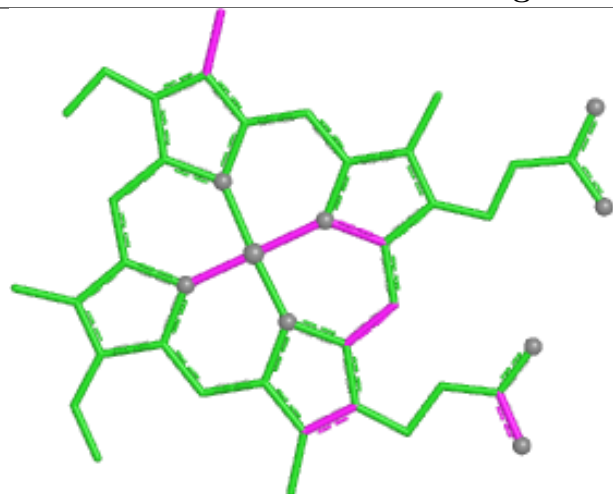
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	FC6	2	0
2	A	201	HEC	1	0
2	B	201	HEC	1	0
2	D	201	HEC	1	0

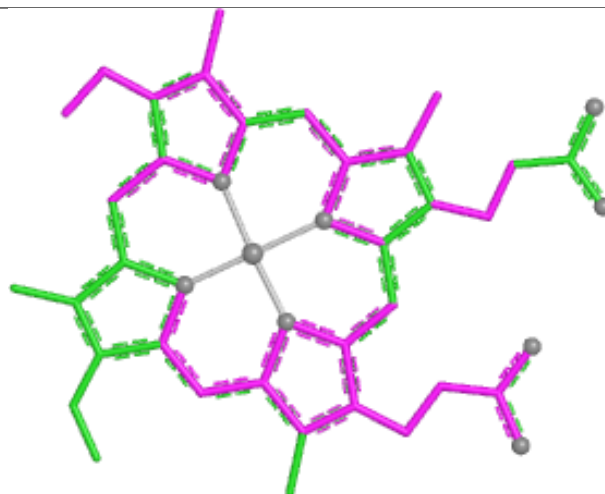
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



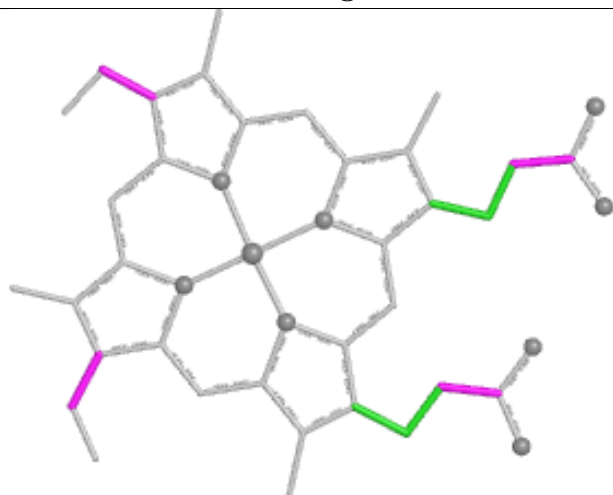
Ligand HEC B 201



Bond lengths



Bond angles

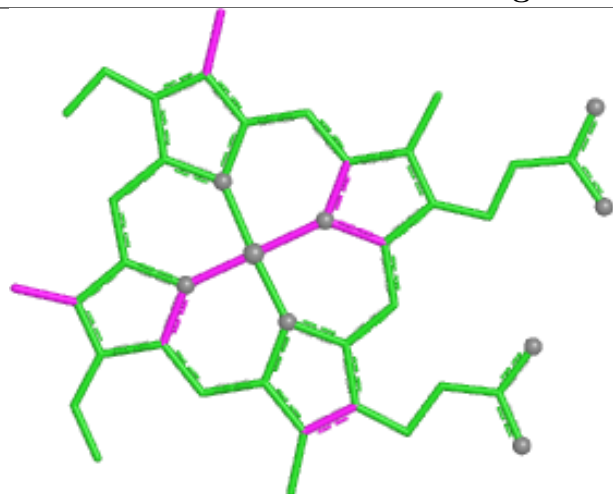


Torsions

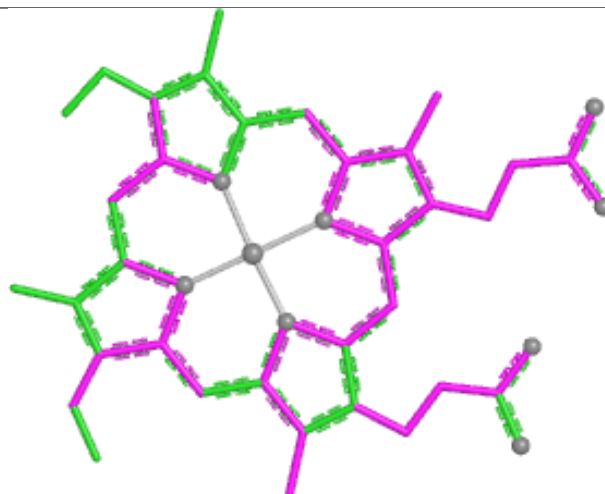


Rings

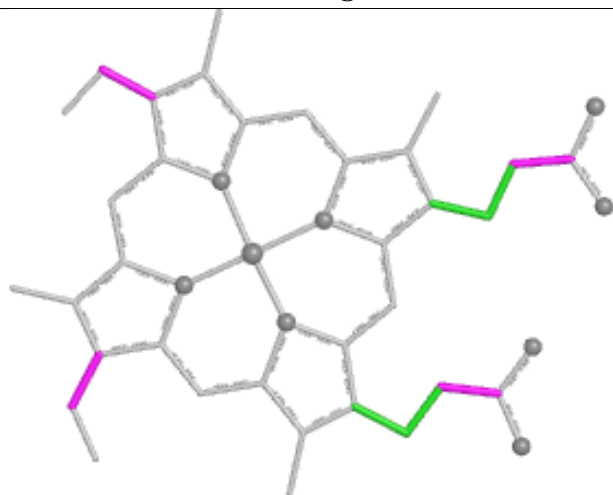
Ligand HEC C 201



Bond lengths



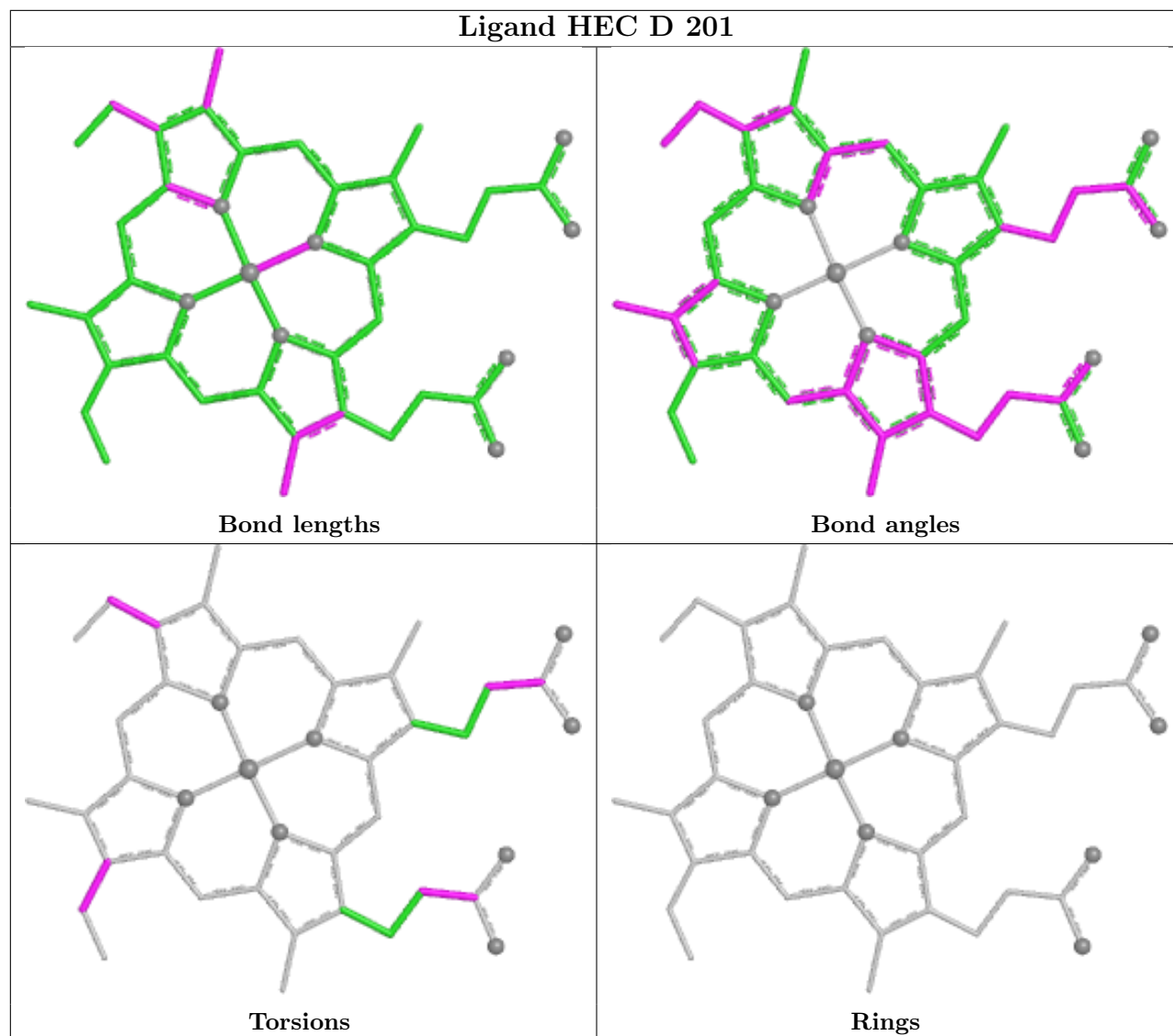
Bond angles



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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.