



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:51 AM EDT

PDB ID : 2RDZ / pdb_00002rdz
Title : High Resolution Crystal Structure of the Escherichia coli Cytochrome c Nitrite Reductase.
Authors : Clarke, T.A.; Hemmings, A.M.; Richardson, D.J.
Deposited on : 2007-09-25
Resolution : 1.74 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	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

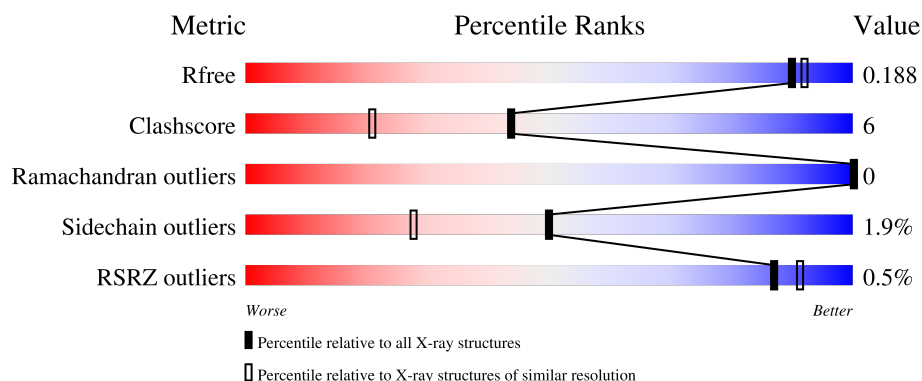
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	 88% 8% ..
1	B	452	 86% 10% ..
1	C	452	 87% 10% ..
1	D	452	 86% 11% ..

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
3	HEC	A	1	X	-	-	-
3	HEC	A	2	X	-	-	-
3	HEC	A	3	X	-	-	-
3	HEC	A	4	X	-	-	-
3	HEC	A	5	X	-	-	-
3	HEC	B	1	X	-	-	-
3	HEC	B	2	X	-	-	-
3	HEC	B	3	X	-	-	-
3	HEC	B	4	X	-	-	-
3	HEC	B	5	X	-	-	-
3	HEC	C	1	X	-	-	-
3	HEC	C	2	X	-	-	-
3	HEC	C	3	X	-	-	-
3	HEC	C	4	X	-	-	-
3	HEC	C	5	X	-	-	-
3	HEC	D	1	X	-	-	-
3	HEC	D	2	X	-	-	-
3	HEC	D	3	X	-	-	-
3	HEC	D	4	X	-	-	-
3	HEC	D	5	X	-	-	-
5	EDO	C	21	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17176 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.

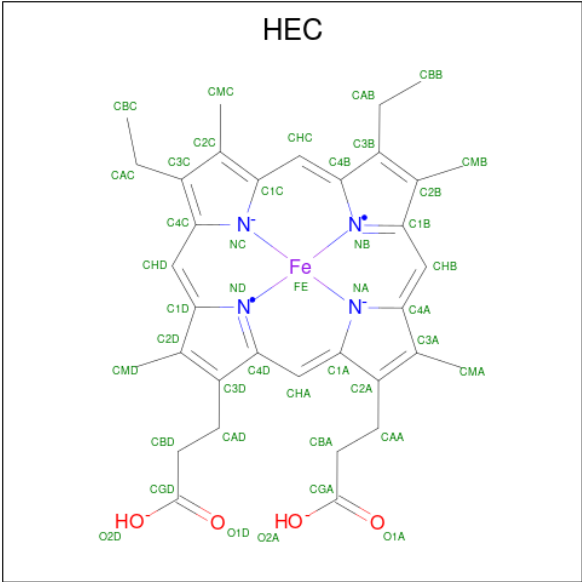
- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	2	0
			3487	2187	619	659	22			
1	B	441	Total	C	N	O	S	0	8	0
			3520	2209	622	667	22			
1	C	441	Total	C	N	O	S	0	5	0
			3502	2197	620	662	23			
1	D	441	Total	C	N	O	S	0	7	0
			3514	2203	623	666	22			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

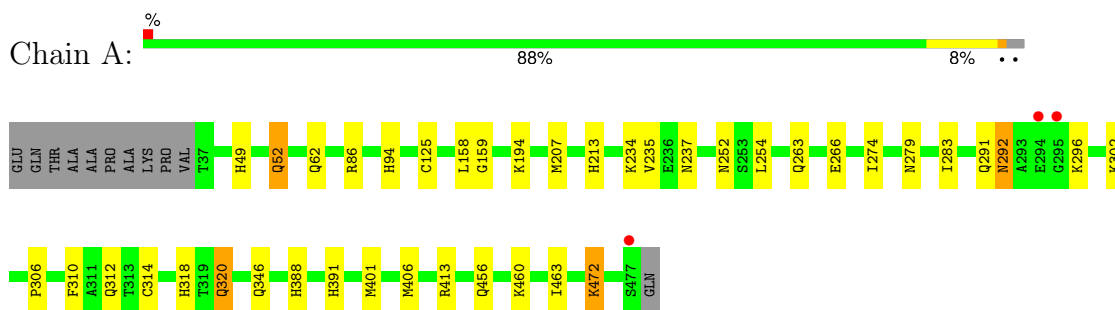
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	547	Total O 548 548	0	1
6	B	553	Total O 554 554	0	1
6	C	490	Total O 491 491	0	1
6	D	559	Total O 560 560	0	1

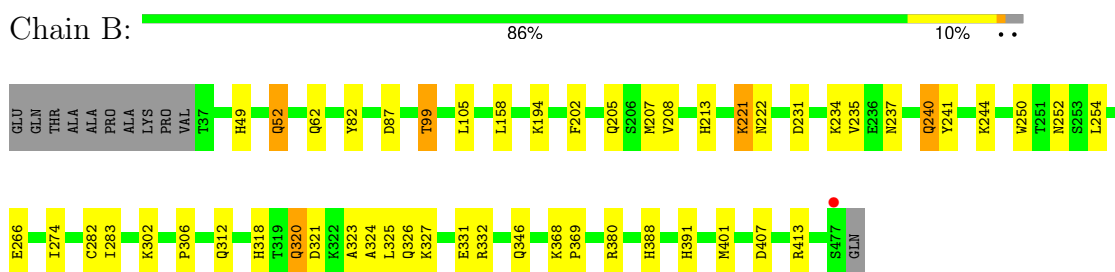
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

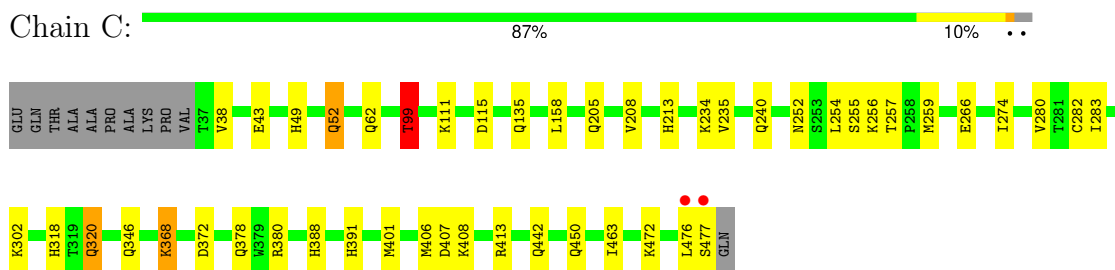
• Molecule 1: Cytochrome c-552



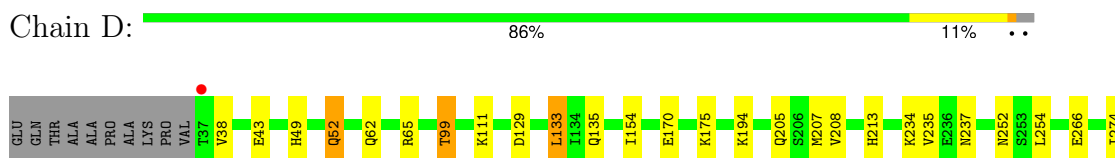
• Molecule 1: Cytochrome c-552



• Molecule 1: Cytochrome c-552



• Molecule 1: Cytochrome c-552





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.46Å 79.30Å 137.58Å 90.00° 101.57° 90.00°	Depositor
Resolution (Å)	39.65 – 1.74 39.65 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.65-1.74) 99.1 (39.65-1.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.154 , 0.189 0.154 , 0.188	Depositor DCC
R_{free} test set	9756 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17176	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: CA, SO4, HEC, EDO

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	1/3577 (0.0%)	0.81	0/4839
1	B	0.72	0/3628	0.82	0/4906
1	C	0.67	1/3601 (0.0%)	0.81	1/4870 (0.0%)
1	D	0.73	1/3619 (0.0%)	0.83	0/4895
All	All	0.70	3/14425 (0.0%)	0.81	1/19510 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	ILE	CA-CB	6.74	1.57	1.54
1	D	463	ILE	CA-CB	6.43	1.57	1.54
1	C	463	ILE	CA-CB	5.45	1.56	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	THR	N-CA-CB	5.10	117.62	110.12

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	3487	0	3382	35	0
1	B	3520	0	3422	43	0
1	C	3502	0	3400	44	0
1	D	3514	0	3411	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	215	0	151	15	0
3	B	215	0	150	9	0
3	C	215	0	150	9	0
3	D	215	0	150	6	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	32	0	48	4	0
5	B	24	0	36	0	0
5	C	24	0	36	4	0
5	D	32	0	48	2	0
6	A	548	0	0	5	0
6	B	554	0	0	10	0
6	C	491	0	0	10	0
6	D	560	0	0	13	0
All	All	17176	0	14384	180	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 6.

All (180) 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:125:CYS:SG	3:A:1:HEC:CAC	2.28	1.20
1:C:476:LEU:HB3	1:C:477:SER:HA	1.20	1.12
5:A:11:EDO:H22	1:B:332:ARG:HH12	1.27	0.99
1:C:476:LEU:HB3	1:C:477:SER:CA	2.00	0.92
1:B:99:THR:HG21	6:B:882:HOH:O	1.70	0.90
1:D:99:THR:HG21	6:D:809:HOH:O	1.76	0.85
3:A:2:HEC:HMC1	3:A:2:HEC:HBC3	1.64	0.77
5:A:11:EDO:H22	1:B:332:ARG:NH1	2.00	0.76
1:D:65:ARG:NH1	6:D:840:HOH:O	2.19	0.75
1:C:442:GLN:HB3	6:C:920:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLN:HE21	1:B:302:LYS:HZ3	1.36	0.73
1:A:86:ARG:HE	5:A:21:EDO:H21	1.53	0.72
1:A:125:CYS:SG	3:A:1:HEC:C3C	2.78	0.71
3:B:2:HEC:HMC1	3:B:2:HEC:HBC3	1.72	0.71
1:C:99:THR:HG23	6:C:490:HOH:O	1.90	0.71
1:C:476:LEU:CB	1:C:477:SER:HA	2.09	0.71
1:D:65:ARG:HG3	5:D:481:EDO:H21	1.73	0.70
1:A:320:GLN:HE21	1:A:320:GLN:H	1.40	0.70
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.77	0.68
1:B:62:GLN:HE21	1:B:302:LYS:NZ	1.91	0.67
1:B:99:THR:HG23	6:B:516:HOH:O	1.93	0.67
1:D:133:LEU:CD2	1:D:154:ILE:HD11	2.24	0.66
1:C:49:HIS:HD2	6:C:612:HOH:O	1.78	0.66
1:C:320:GLN:HE21	1:C:320:GLN:H	1.44	0.65
3:D:2:HEC:HMC1	3:D:2:HEC:HBC3	1.78	0.65
1:B:221:LYS:HZ3	1:B:222:ASN:H	1.44	0.65
1:B:391:HIS:HE1	3:B:4:HEC:O2D	1.80	0.64
3:B:4:HEC:HMC1	3:B:4:HEC:HBC3	1.79	0.64
1:A:391:HIS:HE1	3:A:4:HEC:O2D	1.81	0.64
1:D:320:GLN:HE21	1:D:320:GLN:H	1.45	0.64
1:A:125:CYS:SG	3:A:1:HEC:HAC	2.33	0.63
1:D:309:ASN:HD21	1:D:312[A]:GLN:NE2	1.97	0.63
1:D:252:ASN:ND2	1:D:254:LEU:H	1.97	0.62
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.83	0.61
1:D:49:HIS:HD2	6:D:688:HOH:O	1.83	0.61
1:A:292:ASN:C	1:A:292:ASN:HD22	2.07	0.61
1:D:62:GLN:HE21	1:D:302:LYS:NZ	1.98	0.61
1:D:320:GLN:H	1:D:320:GLN:NE2	1.99	0.61
1:D:309:ASN:HD21	1:D:312[A]:GLN:HE21	1.50	0.60
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.00	0.59
1:C:320:GLN:H	1:C:320:GLN:NE2	2.01	0.59
1:B:346:GLN:NE2	1:B:413:ARG:HH11	2.01	0.58
1:C:52:GLN:NE2	1:C:52:GLN:H	2.01	0.58
1:D:99:THR:HG23	6:D:493:HOH:O	2.02	0.58
1:C:388:HIS:HE1	6:C:518:HOH:O	1.84	0.58
1:D:346:GLN:NE2	1:D:413:ARG:HH11	2.02	0.57
1:B:312[B]:GLN:NE2	6:B:1028:HOH:O	2.38	0.57
1:A:320:GLN:H	1:A:320:GLN:NE2	2.03	0.57
1:A:252:ASN:ND2	1:A:254:LEU:H	2.03	0.57
1:D:133:LEU:HD23	1:D:154:ILE:HD11	1.84	0.57
1:B:252:ASN:ND2	1:B:254:LEU:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:ND2	1:A:296:LYS:H	2.04	0.56
1:C:49:HIS:HE1	6:C:634:HOH:O	1.89	0.56
1:B:320:GLN:HE21	1:B:320:GLN:H	1.52	0.56
1:A:49:HIS:HD2	6:A:688:HOH:O	1.88	0.55
1:C:274:ILE:CG2	3:C:5:HEC:HAD1	2.36	0.55
1:D:43:GLU:H	1:D:43:GLU:CD	2.14	0.55
1:B:49:HIS:HD2	6:B:653:HOH:O	1.88	0.55
1:D:170:GLU:HB3	1:D:175[B]:LYS:HD3	1.88	0.55
1:A:125:CYS:SG	3:A:1:HEC:CBC	2.94	0.55
1:B:320:GLN:H	1:B:320:GLN:NE2	2.04	0.55
1:C:346:GLN:NE2	1:C:413:ARG:HH11	2.05	0.55
1:A:388:HIS:HE1	6:A:483:HOH:O	1.90	0.55
1:B:221:LYS:HZ2	1:B:221:LYS:H	1.55	0.54
1:C:111:LYS:HG2	1:C:115:ASP:OD2	2.07	0.54
1:D:274:ILE:CG2	3:D:5:HEC:HAD1	2.37	0.54
1:A:52:GLN:NE2	1:A:52:GLN:H	2.06	0.54
3:C:1:HEC:HMC1	3:C:1:HEC:HBC3	1.90	0.54
1:C:408:LYS:HZ2	5:C:21:EDO:H12	1.72	0.54
1:D:252:ASN:HD22	1:D:254:LEU:H	1.56	0.54
1:A:213:HIS:HB3	1:A:266:GLU:HB2	1.89	0.54
1:B:52:GLN:NE2	1:B:52:GLN:H	2.06	0.53
1:A:274:ILE:CG2	3:A:5:HEC:HAD1	2.39	0.53
1:C:240:GLN:HB3	6:C:692:HOH:O	2.08	0.53
1:C:407:ASP:OD2	5:C:21:EDO:H11	2.08	0.53
1:D:52:GLN:H	1:D:52:GLN:NE2	2.06	0.53
1:B:240:GLN:HE21	1:B:241:TYR:N	2.07	0.52
1:C:252:ASN:ND2	1:C:254:LEU:H	2.07	0.52
1:D:459:ILE:HA	1:D:463:ILE:HD12	1.91	0.52
1:C:476:LEU:CB	1:C:477:SER:CA	2.80	0.52
1:D:472:LYS:HG3	6:D:664:HOH:O	2.10	0.51
1:B:274:ILE:CG2	3:B:5:HEC:HAD1	2.41	0.51
1:C:235:VAL:HB	1:C:401:MET:HE3	1.92	0.51
1:A:292:ASN:HD21	1:A:296:LYS:H	1.57	0.50
1:C:368:LYS:HE3	1:C:372:ASP:OD2	2.11	0.50
5:A:11:EDO:C2	1:B:332:ARG:HH12	2.12	0.50
1:D:280:VAL:HG13	3:D:5:HEC:HBC2	1.93	0.50
1:D:234:LYS:HE2	6:D:1039:HOH:O	2.10	0.50
1:D:274:ILE:HG21	3:D:5:HEC:HAD1	1.93	0.50
1:A:49:HIS:HE1	6:A:648:HOH:O	1.94	0.50
1:C:408:LYS:NZ	5:C:21:EDO:H12	2.25	0.50
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259[B]:MET:HE1	1:C:378:GLN:CD	2.37	0.49
1:C:213:HIS:HB3	1:C:266:GLU:HB2	1.95	0.49
1:D:279[A]:ASN:ND2	6:D:836:HOH:O	2.46	0.49
3:C:4:HEC:HMC1	3:C:4:HEC:HBC3	1.93	0.49
1:D:235:VAL:HB	1:D:401:MET:HE3	1.95	0.48
1:B:221:LYS:NZ	6:B:821:HOH:O	2.46	0.48
1:A:234:LYS:H	1:A:237:ASN:HD22	1.60	0.48
1:B:235:VAL:HB	1:B:401:MET:HE3	1.95	0.48
1:C:280:VAL:HG13	3:C:5:HEC:HBC2	1.95	0.48
1:A:406:MET:HE3	1:B:407:ASP:HB2	1.96	0.48
1:D:318:HIS:HB3	1:D:320:GLN:NE2	2.29	0.48
1:B:306:PRO:HB2	3:B:5:HEC:HBB1	1.97	0.47
1:D:49:HIS:HE1	6:D:662:HOH:O	1.97	0.47
1:D:472:LYS:CG	6:D:664:HOH:O	2.62	0.47
1:C:205:GLN:HB3	1:C:283:ILE:HD13	1.97	0.47
1:B:49:HIS:HE1	6:B:583:HOH:O	1.98	0.46
1:C:282:CYS:HA	3:C:4:HEC:CHC	2.46	0.46
1:B:321[B]:ASP:OD1	1:B:324:ALA:HB2	2.15	0.46
1:B:380:ARG:NH1	6:B:597:HOH:O	2.47	0.46
1:C:256:LYS:HE2	6:C:772:HOH:O	2.14	0.46
1:D:62:GLN:HE21	1:D:302:LYS:HZ1	1.62	0.46
1:D:38:VAL:HG23	1:D:135:GLN:CD	2.41	0.46
1:B:202:PHE:HE1	6:B:958:HOH:O	1.99	0.46
1:B:213:HIS:HB3	1:B:266:GLU:HB2	1.97	0.46
1:D:133:LEU:HD22	1:D:154:ILE:HD11	1.97	0.46
1:C:257:THR:O	1:C:259[B]:MET:HG2	2.15	0.45
1:D:388:HIS:HE1	6:D:555:HOH:O	1.99	0.45
1:A:283:ILE:HG12	3:A:2:HEC:HMD2	1.97	0.45
1:B:327[A]:LYS:HG3	6:B:851:HOH:O	2.15	0.45
1:C:252:ASN:HD22	1:C:255:SER:H	1.65	0.45
1:C:318:HIS:HB3	1:C:320:GLN:NE2	2.31	0.45
1:B:283:ILE:HG12	3:B:2:HEC:HMD2	1.98	0.45
1:B:323:ALA:HA	1:B:326:GLN:HE21	1.81	0.45
1:D:213:HIS:HB3	1:D:266:GLU:HB2	1.97	0.45
1:D:234:LYS:H	1:D:237:ASN:HD22	1.65	0.45
1:C:205:GLN:O	1:C:208[B]:VAL:HG12	2.17	0.45
1:B:234:LYS:H	1:B:237:ASN:HD22	1.64	0.44
1:D:474:GLY:HA2	6:D:641:HOH:O	2.18	0.44
1:C:257:THR:HB	1:C:259[A]:MET:SD	2.58	0.44
1:D:205:GLN:O	1:D:208:VAL:HG22	2.18	0.44
1:B:205:GLN:O	1:B:208[B]:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:VAL:HG23	1:C:135:GLN:OE1	2.17	0.43
1:C:43:GLU:CD	1:C:43:GLU:H	2.26	0.43
1:B:388:HIS:HE1	6:B:484:HOH:O	2.01	0.43
1:D:467:GLU:O	1:D:471:ARG:HG3	2.18	0.43
1:C:259[B]:MET:CE	1:C:378:GLN:NE2	2.82	0.43
1:B:87:ASP:HB2	1:B:105:LEU:HB2	1.99	0.43
1:B:158:LEU:HG	3:B:3:HEC:HBC2	1.99	0.43
1:B:194:LYS:HE3	1:B:207:MET:CE	2.49	0.43
1:D:52:GLN:H	1:D:52:GLN:HE21	1.65	0.43
1:A:159:GLY:O	3:A:2:HEC:HMC3	2.19	0.42
1:C:274:ILE:HG21	3:C:5:HEC:HAD1	2.01	0.42
1:C:450:GLN:HG3	6:C:854:HOH:O	2.18	0.42
1:B:82:TYR:CD1	1:B:250:TRP:HB3	2.54	0.42
1:D:431:ILE:HG22	1:D:432:PRO:O	2.19	0.42
6:C:646:HOH:O	5:D:25:EDO:H22	2.20	0.42
1:C:62:GLN:HE21	1:C:302:LYS:NZ	2.18	0.42
1:D:194:LYS:HB3	1:D:207:MET:HE1	2.02	0.42
1:B:282:CYS:HA	3:B:4:HEC:CHC	2.50	0.42
1:A:263:GLN:NE2	6:A:1005:HOH:O	2.53	0.41
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.35	0.41
3:A:1:HEC:HMC1	3:A:1:HEC:HBC3	2.01	0.41
1:B:318:HIS:HB3	1:B:320:GLN:NE2	2.35	0.41
1:C:407:ASP:OD2	5:C:21:EDO:C1	2.68	0.41
1:D:408:LYS:NZ	6:D:873:HOH:O	2.53	0.41
1:C:380:ARG:NH1	6:C:600:HOH:O	2.53	0.41
3:C:2:HEC:HMC1	3:C:2:HEC:HBC3	2.02	0.41
1:A:62:GLN:HE21	1:A:302:LYS:NZ	2.17	0.41
3:A:2:HEC:HMC1	3:A:2:HEC:CBC	2.44	0.41
1:D:129:ASP:HB3	1:D:154:ILE:HD13	2.02	0.41
1:C:406:MET:HE3	1:D:407:ASP:HB2	2.02	0.41
1:D:234:LYS:HD3	6:D:1011:HOH:O	2.20	0.41
1:A:94:HIS:CD2	3:A:3:HEC:ND	2.88	0.41
1:C:158:LEU:HG	3:C:3:HEC:HBC2	2.03	0.41
1:A:158:LEU:HG	3:A:3:HEC:HBC2	2.02	0.41
1:A:456:GLN:HE21	1:A:460:LYS:HE3	1.85	0.41
1:B:368:LYS:HB3	1:B:369:PRO:HD3	2.02	0.41
1:A:235:VAL:HB	1:A:401:MET:HE3	2.03	0.40
1:A:306:PRO:HG2	3:A:4:HEC:CHD	2.51	0.40
1:D:456:GLN:NE2	1:D:460:LYS:HE3	2.36	0.40
3:D:4:HEC:HMC1	3:D:4:HEC:HBC3	2.03	0.40
1:A:291:GLN:NE2	6:A:913:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASP:CB	1:B:240:GLN:HE22	2.34	0.40
3:B:2:HEC:HMC1	3:B:2:HEC:CBC	2.47	0.40
1:A:194:LYS:HB3	1:A:207:MET:HE1	2.03	0.40
1:A:310:PHE:CE2	1:A:314:CYS:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/452 (98%)	432 (98%)	9 (2%)	0	100	100
1	B	447/452 (99%)	437 (98%)	10 (2%)	0	100	100
1	C	444/452 (98%)	432 (97%)	12 (3%)	0	100	100
1	D	446/452 (99%)	436 (98%)	10 (2%)	0	100	100
All	All	1778/1808 (98%)	1737 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	364/370 (98%)	358 (98%)	6 (2%)	55	35
1	B	370/370 (100%)	363 (98%)	7 (2%)	50	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	367/370 (99%)	361 (98%)	6 (2%)	55	35
1	D	369/370 (100%)	359 (97%)	10 (3%)	39	16
All	All	1470/1480 (99%)	1441 (98%)	29 (2%)	50	26

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

Mol	Chain	Res	Type
1	A	52	GLN
1	A	279	ASN
1	A	292	ASN
1	A	312	GLN
1	A	320	GLN
1	A	472	LYS
1	B	52	GLN
1	B	99	THR
1	B	221	LYS
1	B	240	GLN
1	B	244	LYS
1	B	320	GLN
1	B	325	LEU
1	C	52	GLN
1	C	99	THR
1	C	234	LYS
1	C	320	GLN
1	C	368	LYS
1	C	472	LYS
1	D	52	GLN
1	D	99	THR
1	D	111	LYS
1	D	133	LEU
1	D	297	LEU
1	D	316	ASN
1	D	320	GLN
1	D	325	LEU
1	D	442[A]	GLN
1	D	442[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	HIS
1	A	52	GLN
1	A	62	GLN
1	A	237	ASN
1	A	240	GLN
1	A	252	ASN
1	A	279	ASN
1	A	292	ASN
1	A	320	GLN
1	A	346	GLN
1	A	371	GLN
1	A	388	HIS
1	A	391	HIS
1	A	456	GLN
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	237	ASN
1	B	240	GLN
1	B	252	ASN
1	B	309	ASN
1	B	320	GLN
1	B	326	GLN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	C	49	HIS
1	C	52	GLN
1	C	62	GLN
1	C	252	ASN
1	C	291	GLN
1	C	309	ASN
1	C	320	GLN
1	C	346	GLN
1	C	388	HIS
1	C	391	HIS
1	C	442	GLN
1	C	469	GLN
1	D	49	HIS
1	D	52	GLN
1	D	62	GLN

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Mol	Chain	Res	Type
1	D	156	ASN
1	D	237	ASN
1	D	252	ASN
1	D	316	ASN
1	D	320	GLN
1	D	346	GLN
1	D	388	HIS
1	D	391	HIS
1	D	469	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 8 are monoatomic - leaving 52 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	$\# Z > 2$
5	EDO	D	25	-	3,3,3	0.49	0	2,2,2	0.17	0
5	EDO	C	25	-	3,3,3	0.36	0	2,2,2	0.53	0
5	EDO	A	20	-	3,3,3	0.46	0	2,2,2	0.04	0
5	EDO	D	21	-	3,3,3	0.47	0	2,2,2	0.50	0
5	EDO	D	6	-	3,3,3	0.52	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	C	2	1	50,50,50	1.93	8 (16%)	68,82,82	1.38	8 (11%)
5	EDO	B	19	-	3,3,3	0.45	0	2,2,2	0.21	0
5	EDO	B	16	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	B	481	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	C	21	-	3,3,3	0.34	0	2,2,2	0.63	0
5	EDO	C	22	-	3,3,3	0.43	0	2,2,2	0.26	0
3	HEC	D	3	2,1	50,50,50	1.66	8 (16%)	68,82,82	1.27	6 (8%)
3	HEC	A	4	2,1	50,50,50	1.75	8 (16%)	68,82,82	1.35	7 (10%)
3	HEC	D	2	1	50,50,50	1.83	7 (14%)	68,82,82	1.31	7 (10%)
4	SO4	B	2001	-	4,4,4	0.36	0	6,6,6	0.26	0
5	EDO	B	20	-	3,3,3	0.42	0	2,2,2	0.56	0
3	HEC	B	2	1	50,50,50	2.91	10 (20%)	68,82,82	2.42	11 (16%)
3	HEC	C	4	2,1	50,50,50	1.71	8 (16%)	68,82,82	1.38	6 (8%)
5	EDO	A	15	-	3,3,3	0.37	0	2,2,2	0.40	0
5	EDO	A	13	-	3,3,3	0.36	0	2,2,2	0.67	0
5	EDO	C	23	-	3,3,3	0.40	0	2,2,2	0.45	0
5	EDO	B	18	-	3,3,3	0.40	0	2,2,2	0.38	0
3	HEC	B	4	2,1	50,50,50	1.75	7 (14%)	68,82,82	1.41	9 (13%)
3	HEC	C	3	2,1	50,50,50	1.75	9 (18%)	68,82,82	1.38	8 (11%)
3	HEC	A	2	1	50,50,50	1.74	9 (18%)	68,82,82	1.29	7 (10%)
3	HEC	A	1	6,1	50,50,50	1.82	7 (14%)	68,82,82	1.33	8 (11%)
3	HEC	C	1	6,1	50,50,50	1.86	7 (14%)	68,82,82	1.20	6 (8%)
4	SO4	D	2001	-	4,4,4	0.19	0	6,6,6	0.32	0
3	HEC	B	3	2,1	50,50,50	1.74	8 (16%)	68,82,82	1.32	4 (5%)
3	HEC	C	5	1	50,50,50	1.80	7 (14%)	68,82,82	1.17	3 (4%)
3	HEC	D	1	6,1	50,50,50	1.84	7 (14%)	68,82,82	1.38	8 (11%)
4	SO4	C	2001	-	4,4,4	0.27	0	6,6,6	0.37	0
5	EDO	A	14	-	3,3,3	0.37	0	2,2,2	0.41	0
5	EDO	A	22	-	3,3,3	0.40	0	2,2,2	0.43	0
3	HEC	A	3	2,1	50,50,50	1.83	8 (16%)	68,82,82	1.33	5 (7%)
3	HEC	A	5	1	50,50,50	1.70	6 (12%)	68,82,82	1.25	6 (8%)
5	EDO	D	22	-	3,3,3	0.41	0	2,2,2	0.72	0
3	HEC	B	1	6,1	50,50,50	1.86	9 (18%)	68,82,82	1.26	4 (5%)
3	HEC	D	5	1	50,50,50	1.70	8 (16%)	68,82,82	1.07	4 (5%)
5	EDO	A	11	-	3,3,3	0.35	0	2,2,2	0.76	0
5	EDO	D	24	-	3,3,3	0.44	0	2,2,2	0.41	0
3	HEC	D	4	1	50,50,50	1.67	7 (14%)	68,82,82	1.44	7 (10%)
5	EDO	D	23	-	3,3,3	0.44	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	21	-	3,3,3	0.39	0	2,2,2	0.46	0
3	HEC	B	5	1	50,50,50	1.70	10 (20%)	68,82,82	1.18	5 (7%)
4	SO4	A	2001	-	4,4,4	0.20	0	6,6,6	0.34	0
5	EDO	A	481	-	3,3,3	0.37	0	2,2,2	0.31	0
5	EDO	B	17	-	3,3,3	0.42	0	2,2,2	0.46	0
5	EDO	D	481	-	3,3,3	0.30	0	2,2,2	0.40	0
5	EDO	D	482	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	C	481	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	C	12	-	3,3,3	0.41	0	2,2,2	0.75	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
5	EDO	D	25	-	-	1/1/1/1	-
5	EDO	C	25	-	-	0/1/1/1	-
5	EDO	A	20	-	-	1/1/1/1	-
5	EDO	D	21	-	-	1/1/1/1	-
5	EDO	D	6	-	-	0/1/1/1	-
3	HEC	C	2	1	1/1/3/7	6/14/54/54	-
5	EDO	B	19	-	-	0/1/1/1	-
5	EDO	B	16	-	-	0/1/1/1	-
5	EDO	B	481	-	-	0/1/1/1	-
5	EDO	C	21	-	-	1/1/1/1	-
5	EDO	C	22	-	-	0/1/1/1	-
3	HEC	D	3	2,1	1/1/3/7	4/14/54/54	-
3	HEC	A	4	2,1	1/1/3/7	4/14/54/54	-
3	HEC	D	2	1	1/1/3/7	6/14/54/54	-
5	EDO	B	20	-	-	0/1/1/1	-
3	HEC	B	2	1	1/1/3/7	6/14/54/54	-
3	HEC	C	4	2,1	1/1/3/7	4/14/54/54	-
5	EDO	A	15	-	-	1/1/1/1	-
5	EDO	A	13	-	-	0/1/1/1	-
5	EDO	C	23	-	-	1/1/1/1	-
5	EDO	B	18	-	-	0/1/1/1	-
3	HEC	B	4	2,1	1/1/3/7	4/14/54/54	-
3	HEC	C	3	2,1	1/1/3/7	4/14/54/54	-
3	HEC	A	2	1	1/1/3/7	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	1	6,1	1/1/3/7	4/14/54/54	-
3	HEC	C	1	6,1	1/1/3/7	4/14/54/54	-
3	HEC	B	3	2,1	1/1/3/7	3/14/54/54	-
3	HEC	C	5	1	1/1/3/7	8/14/54/54	-
3	HEC	D	1	6,1	1/1/3/7	4/14/54/54	-
5	EDO	A	14	-	-	0/1/1/1	-
5	EDO	A	22	-	-	1/1/1/1	-
3	HEC	A	3	2,1	1/1/3/7	4/14/54/54	-
3	HEC	A	5	1	1/1/3/7	9/14/54/54	-
5	EDO	D	22	-	-	1/1/1/1	-
3	HEC	B	1	6,1	1/1/3/7	5/14/54/54	-
3	HEC	D	5	1	1/1/3/7	8/14/54/54	-
5	EDO	A	11	-	-	0/1/1/1	-
5	EDO	D	24	-	-	1/1/1/1	-
3	HEC	D	4	1	1/1/3/7	5/14/54/54	-
5	EDO	D	23	-	-	1/1/1/1	-
5	EDO	A	21	-	-	1/1/1/1	-
3	HEC	B	5	1	1/1/3/7	8/14/54/54	-
5	EDO	A	481	-	-	0/1/1/1	-
5	EDO	B	17	-	-	0/1/1/1	-
5	EDO	D	481	-	-	0/1/1/1	-
5	EDO	D	482	-	-	0/1/1/1	-
5	EDO	C	481	-	-	0/1/1/1	-
5	EDO	C	12	-	-	0/1/1/1	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	HEC	C1D-ND	14.49	1.65	1.40
3	C	1	HEC	C3D-C2D	7.93	1.53	1.36
3	C	2	HEC	C3D-C2D	7.71	1.53	1.36
3	C	3	HEC	C3D-C2D	7.54	1.53	1.36
3	C	5	HEC	C3D-C2D	7.50	1.52	1.36
3	B	4	HEC	C3D-C2D	7.49	1.52	1.36
3	A	4	HEC	C3D-C2D	7.46	1.52	1.36
3	D	1	HEC	C3D-C2D	7.38	1.52	1.36
3	A	3	HEC	C3D-C2D	7.32	1.52	1.36
3	A	1	HEC	C3D-C2D	7.29	1.52	1.36
3	D	4	HEC	C3D-C2D	7.26	1.52	1.36
3	B	3	HEC	C3D-C2D	7.19	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	HEC	C3D-C2D	7.15	1.52	1.36
3	D	5	HEC	C3D-C2D	7.10	1.52	1.36
3	C	4	HEC	C3D-C2D	7.10	1.52	1.36
3	A	5	HEC	C3D-C2D	7.05	1.52	1.36
3	D	2	HEC	C3D-C2D	7.01	1.51	1.36
3	B	2	HEC	C3D-C2D	7.00	1.51	1.36
3	D	3	HEC	C3D-C2D	6.88	1.51	1.36
3	A	2	HEC	C3D-C2D	6.77	1.51	1.36
3	B	5	HEC	C3D-C2D	6.76	1.51	1.36
3	B	2	HEC	CHD-C1D	-6.51	1.25	1.38
3	D	1	HEC	FE-ND	5.52	2.11	1.94
3	C	1	HEC	FE-ND	5.33	2.11	1.94
3	A	3	HEC	FE-NC	4.96	2.11	1.95
3	B	1	HEC	FE-ND	4.93	2.10	1.94
3	D	2	HEC	FE-ND	4.92	2.10	1.94
3	C	2	HEC	FE-ND	4.90	2.10	1.94
3	C	2	HEC	FE-NA	4.73	2.10	1.95
3	A	1	HEC	FE-ND	4.68	2.09	1.94
3	A	5	HEC	FE-ND	4.66	2.09	1.94
3	C	1	HEC	FE-NB	4.60	2.09	1.94
3	B	1	HEC	FE-NB	4.37	2.08	1.94
3	A	2	HEC	FE-NB	4.27	2.08	1.94
3	B	2	HEC	FE-ND	4.25	2.08	1.94
3	B	2	HEC	FE-NA	4.16	2.08	1.95
3	C	2	HEC	FE-NC	4.15	2.08	1.95
3	B	3	HEC	FE-NC	4.12	2.08	1.95
3	B	2	HEC	FE-NC	4.09	2.08	1.95
3	A	2	HEC	FE-NC	4.09	2.08	1.95
3	C	3	HEC	FE-NB	4.04	2.07	1.94
3	D	2	HEC	FE-NC	4.00	2.08	1.95
3	D	3	HEC	FE-NC	3.94	2.08	1.95
3	B	5	HEC	FE-ND	3.90	2.06	1.94
3	D	2	HEC	FE-NA	3.87	2.07	1.95
3	A	1	HEC	FE-NB	3.83	2.06	1.94
3	C	4	HEC	FE-NC	3.80	2.07	1.95
3	C	3	HEC	FE-NC	3.76	2.07	1.95
3	C	4	HEC	FE-ND	3.74	2.06	1.94
3	C	5	HEC	FE-NB	3.72	2.06	1.94
3	C	5	HEC	FE-NC	3.69	2.07	1.95
3	D	1	HEC	FE-NA	3.66	2.07	1.95
3	A	3	HEC	FE-NA	3.66	2.07	1.95
3	B	4	HEC	FE-ND	3.66	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	HEC	FE-NC	3.66	2.07	1.95
3	D	5	HEC	FE-ND	3.54	2.05	1.94
3	A	4	HEC	FE-NA	3.50	2.06	1.95
3	D	3	HEC	FE-NB	3.42	2.05	1.94
3	B	3	HEC	FE-NB	3.35	2.05	1.94
3	B	2	HEC	FE-NB	3.32	2.05	1.94
3	A	2	HEC	FE-NA	3.27	2.05	1.95
3	A	3	HEC	FE-NB	3.27	2.05	1.94
3	C	2	HEC	FE-NB	3.26	2.04	1.94
3	C	5	HEC	FE-NA	3.26	2.05	1.95
3	A	5	HEC	FE-NB	3.25	2.04	1.94
3	B	4	HEC	FE-NC	3.25	2.05	1.95
3	D	2	HEC	FE-NB	3.24	2.04	1.94
3	C	5	HEC	FE-ND	3.19	2.04	1.94
3	D	4	HEC	FE-ND	3.18	2.04	1.94
3	A	4	HEC	FE-NB	3.18	2.04	1.94
3	A	1	HEC	FE-NC	3.14	2.05	1.95
3	A	4	HEC	FE-ND	3.14	2.04	1.94
3	C	3	HEC	FE-ND	3.10	2.04	1.94
3	D	5	HEC	FE-NC	3.09	2.05	1.95
3	B	1	HEC	FE-NA	3.07	2.05	1.95
3	B	3	HEC	FE-ND	2.98	2.04	1.94
3	A	2	HEC	FE-ND	2.97	2.04	1.94
3	C	3	HEC	FE-NA	2.96	2.04	1.95
3	B	3	HEC	FE-NA	2.92	2.04	1.95
3	B	4	HEC	FE-NB	2.87	2.03	1.94
3	B	5	HEC	FE-NC	2.82	2.04	1.95
3	B	4	HEC	FE-NA	2.82	2.04	1.95
3	C	4	HEC	FE-NB	2.80	2.03	1.94
3	D	3	HEC	FE-ND	2.78	2.03	1.94
3	A	3	HEC	FE-ND	2.76	2.03	1.94
3	D	1	HEC	FE-NB	2.69	2.03	1.94
3	A	1	HEC	CMA-C3A	2.65	1.56	1.50
3	D	4	HEC	FE-NB	2.64	2.03	1.94
3	B	5	HEC	FE-NB	2.62	2.03	1.94
3	B	1	HEC	FE-NC	2.58	2.03	1.95
3	C	5	HEC	CMC-C2C	2.57	1.56	1.50
3	D	1	HEC	CMB-C2B	2.56	1.56	1.50
3	B	4	HEC	CMD-C2D	2.56	1.56	1.50
3	C	4	HEC	FE-NA	2.54	2.03	1.95
3	D	1	HEC	FE-NC	2.53	2.03	1.95
3	D	3	HEC	CMD-C2D	2.50	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	HEC	CMB-C2B	2.50	1.55	1.50
3	A	1	HEC	FE-NA	2.47	2.03	1.95
3	C	5	HEC	CAC-C3C	2.46	1.57	1.51
3	A	5	HEC	FE-NA	2.46	2.03	1.95
3	B	5	HEC	CMB-C2B	2.46	1.55	1.50
3	A	3	HEC	CMB-C2B	2.45	1.55	1.50
3	B	5	HEC	CMA-C3A	2.43	1.55	1.50
3	B	1	HEC	CMA-C3A	2.41	1.55	1.50
3	D	3	HEC	CMA-C3A	2.41	1.55	1.50
3	B	1	HEC	CMC-C2C	2.40	1.55	1.50
3	A	4	HEC	CMD-C2D	2.40	1.55	1.50
3	B	3	HEC	CMC-C2C	2.38	1.55	1.50
3	A	3	HEC	CMC-C2C	2.36	1.55	1.50
3	A	3	HEC	CMD-C2D	2.35	1.55	1.50
3	D	5	HEC	CMC-C2C	2.35	1.55	1.50
3	A	4	HEC	CMA-C3A	2.35	1.55	1.50
3	D	4	HEC	CMD-C2D	2.34	1.55	1.50
3	C	2	HEC	CMB-C2B	2.34	1.55	1.50
3	C	1	HEC	CMA-C3A	2.34	1.55	1.50
3	C	2	HEC	CMC-C2C	2.34	1.55	1.50
3	B	2	HEC	CMB-C2B	2.33	1.55	1.50
3	D	5	HEC	CMB-C2B	2.30	1.55	1.50
3	D	4	HEC	FE-NA	2.30	2.02	1.95
3	D	2	HEC	CMB-C2B	2.29	1.55	1.50
3	C	2	HEC	CMA-C3A	2.29	1.55	1.50
3	B	1	HEC	CMB-C2B	2.28	1.55	1.50
3	B	3	HEC	CMD-C2D	2.25	1.55	1.50
3	C	1	HEC	CMB-C2B	2.25	1.55	1.50
3	D	4	HEC	CMA-C3A	2.24	1.55	1.50
3	A	2	HEC	CMA-C3A	2.24	1.55	1.50
3	C	4	HEC	CMD-C2D	2.24	1.55	1.50
3	B	5	HEC	FE-NA	2.23	2.02	1.95
3	B	4	HEC	CMC-C2C	2.23	1.55	1.50
3	A	1	HEC	CAC-C3C	2.20	1.56	1.51
3	C	4	HEC	CMB-C2B	2.20	1.55	1.50
3	D	3	HEC	CMC-C2C	2.19	1.55	1.50
3	B	5	HEC	CAC-C3C	2.18	1.56	1.51
3	D	5	HEC	CMD-C2D	2.16	1.55	1.50
3	D	1	HEC	CMC-C2C	2.16	1.55	1.50
3	C	4	HEC	CMA-C3A	2.16	1.55	1.50
3	C	3	HEC	CMC-C2C	2.15	1.55	1.50
3	C	3	HEC	CMD-C2D	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	HEC	CMB-C2B	2.15	1.55	1.50
3	C	3	HEC	CAC-C3C	2.14	1.56	1.51
3	B	2	HEC	CMC-C2C	2.11	1.55	1.50
3	D	5	HEC	FE-NA	2.10	2.02	1.95
3	A	2	HEC	CAC-C3C	2.10	1.56	1.51
3	B	1	HEC	C4B-NB	-2.10	1.36	1.40
3	A	5	HEC	CMA-C3A	2.09	1.55	1.50
3	A	5	HEC	CMB-C2B	2.09	1.55	1.50
3	D	2	HEC	CAC-C3C	2.09	1.56	1.51
3	D	3	HEC	FE-NA	2.08	2.02	1.95
3	A	2	HEC	CAB-C3B	2.08	1.56	1.51
3	A	4	HEC	FE-NC	2.08	2.02	1.95
3	D	5	HEC	CAC-C3C	2.07	1.56	1.51
3	B	5	HEC	C4B-NB	-2.04	1.36	1.40
3	B	5	HEC	CMD-C2D	2.04	1.55	1.50
3	C	1	HEC	CMC-C2C	2.04	1.54	1.50
3	C	1	HEC	CMD-C2D	2.03	1.54	1.50
3	A	4	HEC	CMB-C2B	2.02	1.54	1.50
3	B	2	HEC	CAC-C3C	2.02	1.56	1.51
3	B	3	HEC	CAC-C3C	2.01	1.56	1.51

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	HEC	C2D-C1D-ND	-10.16	98.16	109.84
3	B	2	HEC	C1D-C2D-C3D	7.95	115.35	106.98
3	B	2	HEC	CHD-C1D-ND	-7.26	115.39	124.37
3	B	4	HEC	C1D-ND-C4D	6.18	112.52	105.21
3	B	2	HEC	CHD-C1D-C2D	6.09	144.26	126.95
3	C	2	HEC	C1D-ND-C4D	5.95	112.25	105.21
3	D	4	HEC	C1D-ND-C4D	5.89	112.19	105.21
3	D	2	HEC	C1D-ND-C4D	5.61	111.85	105.21
3	C	4	HEC	C1D-ND-C4D	5.53	111.75	105.21
3	A	3	HEC	C1D-ND-C4D	5.45	111.66	105.21
3	D	1	HEC	C1D-ND-C4D	5.40	111.60	105.21
3	C	3	HEC	C1D-ND-C4D	5.30	111.49	105.21
3	B	2	HEC	C1D-ND-C4D	5.29	111.48	105.21
3	A	4	HEC	C1D-ND-C4D	5.28	111.46	105.21
3	B	3	HEC	C1D-ND-C4D	5.14	111.29	105.21
3	A	2	HEC	C1D-ND-C4D	4.80	110.89	105.21
3	B	1	HEC	C1D-ND-C4D	4.73	110.81	105.21
3	A	1	HEC	C1D-ND-C4D	4.70	110.78	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	HEC	C1D-ND-C4D	4.69	110.76	105.21
3	B	2	HEC	CMD-C2D-C1D	-4.57	117.89	125.03
3	B	2	HEC	C4C-CHD-C1D	4.42	136.65	126.25
3	D	3	HEC	C1D-ND-C4D	4.31	110.31	105.21
3	A	5	HEC	C1D-ND-C4D	4.18	110.16	105.21
3	C	5	HEC	C1D-ND-C4D	3.75	109.64	105.21
3	B	5	HEC	C1D-ND-C4D	3.72	109.62	105.21
3	D	5	HEC	C1D-ND-C4D	3.51	109.36	105.21
3	A	2	HEC	C2A-C1A-NA	-3.40	107.04	110.32
3	A	5	HEC	C4B-NB-C1B	3.11	108.89	105.21
3	D	2	HEC	C2A-C1A-NA	-3.11	107.33	110.32
3	A	1	HEC	C4B-NB-C1B	3.10	108.88	105.21
3	D	1	HEC	C2A-C1A-NA	-3.06	107.38	110.32
3	C	2	HEC	C2A-C1A-NA	-3.04	107.39	110.32
3	C	4	HEC	C2A-C1A-NA	-3.02	107.41	110.32
3	C	1	HEC	C4B-NB-C1B	3.00	108.76	105.21
3	C	3	HEC	C4B-NB-C1B	2.97	108.73	105.21
3	C	5	HEC	C4B-NB-C1B	2.92	108.67	105.21
3	A	4	HEC	C4B-NB-C1B	2.87	108.60	105.21
3	D	4	HEC	C4B-NB-C1B	2.83	108.56	105.21
3	D	4	HEC	O1A-CGA-CBA	-2.80	114.20	123.09
3	C	4	HEC	CAD-C3D-C4D	2.79	129.55	124.70
3	D	1	HEC	CAD-C3D-C4D	2.74	129.47	124.70
3	A	4	HEC	CAD-C3D-C4D	2.72	129.43	124.70
3	B	5	HEC	CBC-CAC-C3C	2.71	119.77	112.42
3	A	1	HEC	CAC-C3C-C2C	2.65	131.09	126.89
3	A	1	HEC	C2A-C1A-NA	-2.65	107.77	110.32
3	A	3	HEC	C4B-NB-C1B	2.63	108.32	105.21
3	A	5	HEC	CAC-C3C-C2C	2.63	131.05	126.89
3	A	3	HEC	C2A-C1A-NA	-2.63	107.79	110.32
3	B	4	HEC	CBA-CAA-C2A	-2.63	105.27	112.53
3	D	4	HEC	CAC-C3C-C2C	2.62	131.03	126.89
3	C	1	HEC	CBC-CAC-C3C	2.57	119.39	112.42
3	B	4	HEC	CMC-C2C-C1C	-2.56	121.53	125.42
3	B	4	HEC	C3D-C4D-ND	-2.55	107.88	110.35
3	B	1	HEC	C4B-NB-C1B	2.55	108.23	105.21
3	C	2	HEC	C3C-C4C-NC	-2.53	107.34	110.15
3	D	3	HEC	CMD-C2D-C1D	2.53	128.99	125.03
3	B	3	HEC	C4B-NB-C1B	2.52	108.19	105.21
3	D	3	HEC	CAD-C3D-C4D	2.51	129.07	124.70
3	B	3	HEC	CHD-C1D-ND	2.51	127.47	124.37
3	C	2	HEC	C4B-NB-C1B	2.50	108.17	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	C4B-NB-C1B	2.49	108.15	105.21
3	A	3	HEC	CHD-C1D-ND	2.49	127.44	124.37
3	B	2	HEC	C2A-C1A-NA	-2.48	107.93	110.32
3	D	1	HEC	CHB-C4A-NA	2.47	127.14	124.45
3	A	1	HEC	CBC-CAC-C3C	2.45	119.06	112.42
3	C	4	HEC	CAD-CBD-CGD	-2.44	107.19	113.67
3	D	4	HEC	C2B-C1B-NB	-2.44	107.08	109.90
3	D	5	HEC	CAD-CBD-CGD	-2.40	107.31	113.67
3	C	2	HEC	CHD-C1D-ND	2.39	127.32	124.37
3	B	4	HEC	C4B-NB-C1B	2.38	108.03	105.21
3	C	3	HEC	CHD-C1D-ND	2.38	127.31	124.37
3	A	2	HEC	CHA-C1A-C2A	2.37	128.61	124.86
3	D	1	HEC	C4B-NB-C1B	2.37	108.01	105.21
3	C	3	HEC	C2A-C1A-NA	-2.37	108.04	110.32
3	D	3	HEC	CBC-CAC-C3C	2.36	118.81	112.42
3	D	5	HEC	CAD-C3D-C4D	2.34	128.77	124.70
3	B	4	HEC	CAB-C3B-C4B	-2.34	121.75	124.79
3	B	4	HEC	O1A-CGA-CBA	-2.32	115.75	123.09
3	D	3	HEC	C4B-NB-C1B	2.30	107.93	105.21
3	A	4	HEC	CHD-C1D-ND	2.29	127.20	124.37
3	D	4	HEC	O2A-CGA-CBA	2.28	121.22	114.00
3	B	2	HEC	C4B-NB-C1B	2.28	107.91	105.21
3	B	2	HEC	CAD-CBD-CGD	-2.27	107.64	113.67
3	A	4	HEC	CBA-CAA-C2A	-2.26	106.29	112.53
3	D	4	HEC	CAD-C3D-C4D	2.26	128.63	124.70
3	B	1	HEC	C2B-C1B-NB	-2.24	107.32	109.90
3	C	2	HEC	C4C-NC-C1C	2.23	109.45	105.82
3	C	2	HEC	C3D-C4D-ND	-2.22	108.20	110.35
3	A	5	HEC	CBC-CAC-C3C	2.22	118.44	112.42
3	D	5	HEC	C1D-C2D-C3D	-2.21	104.65	106.98
3	A	1	HEC	CAB-C3B-C4B	-2.21	121.91	124.79
3	C	3	HEC	C3B-C4B-NB	-2.21	107.75	110.17
3	A	2	HEC	CHD-C1D-ND	2.21	127.10	124.37
3	A	4	HEC	CAC-C3C-C2C	2.20	130.38	126.89
3	C	3	HEC	O2A-CGA-CBA	2.19	120.92	114.00
3	A	2	HEC	C4B-NB-C1B	2.19	107.80	105.21
3	A	5	HEC	C3B-C4B-NB	-2.19	107.77	110.17
3	D	2	HEC	C3D-C4D-ND	-2.18	108.25	110.35
3	A	1	HEC	CHA-C1A-NA	2.17	126.81	124.45
3	A	1	HEC	CAC-C3C-C4C	-2.13	121.99	124.91
3	B	5	HEC	CAD-C3D-C4D	2.12	128.40	124.70
3	A	2	HEC	C4A-NA-C1A	2.12	109.27	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	HEC	CHA-C1A-NA	2.12	126.76	124.45
3	C	1	HEC	C1D-C2D-C3D	-2.11	104.76	106.98
3	B	4	HEC	O2A-CGA-CBA	2.10	120.63	114.00
3	B	5	HEC	CMC-C2C-C1C	-2.09	122.23	125.42
3	D	3	HEC	C2A-C1A-NA	-2.09	108.31	110.32
3	D	2	HEC	C1D-C2D-C3D	-2.08	104.79	106.98
3	A	5	HEC	C1D-C2D-C3D	-2.08	104.79	106.98
3	D	2	HEC	C4A-NA-C1A	2.08	109.21	105.82
3	A	2	HEC	CAD-C3D-C4D	2.07	128.31	124.70
3	D	2	HEC	CHA-C1A-C2A	2.07	128.13	124.86
3	A	4	HEC	C2A-C1A-NA	-2.07	108.33	110.32
3	C	3	HEC	C2B-C1B-NB	-2.06	107.52	109.90
3	B	3	HEC	CBC-CAC-C3C	2.06	118.00	112.42
3	D	1	HEC	CAC-C3C-C2C	2.05	130.14	126.89
3	B	1	HEC	CAD-C3D-C4D	2.05	128.27	124.70
3	C	4	HEC	CHA-C4D-C3D	2.05	127.76	124.77
3	B	4	HEC	CAD-CBD-CGD	-2.05	108.24	113.67
3	B	2	HEC	CBC-CAC-C3C	2.04	117.96	112.42
3	D	1	HEC	CBC-CAC-C3C	2.04	117.95	112.42
3	C	1	HEC	C2B-C1B-NB	-2.04	107.55	109.90
3	C	5	HEC	CHA-C1A-NA	2.04	126.67	124.45
3	C	4	HEC	CHA-C1A-NA	2.03	126.66	124.45
3	C	2	HEC	CHA-C1A-C2A	2.03	128.06	124.86
3	D	2	HEC	CAD-CBD-CGD	-2.03	108.29	113.67
3	A	3	HEC	C2B-C1B-NB	-2.02	107.57	109.90
3	D	1	HEC	C4A-NA-C1A	2.02	109.11	105.82
3	C	3	HEC	CAD-CBD-CGD	-2.01	108.34	113.67

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	HEC	NA
3	A	2	HEC	NA
3	A	3	HEC	NA
3	A	4	HEC	NA
3	A	5	HEC	NA
3	B	1	HEC	NA
3	B	2	HEC	NA
3	B	3	HEC	NA
3	B	4	HEC	NA
3	B	5	HEC	NA
3	C	1	HEC	NA

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Mol	Chain	Res	Type	Atom
3	C	2	HEC	NA
3	C	3	HEC	NA
3	C	4	HEC	NA
3	C	5	HEC	NA
3	D	1	HEC	NA
3	D	2	HEC	NA
3	D	3	HEC	NA
3	D	4	HEC	NA
3	D	5	HEC	NA

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	HEC	C2C-C3C-CAC-CBC
3	A	4	HEC	C2C-C3C-CAC-CBC
3	A	5	HEC	C2C-C3C-CAC-CBC
3	B	2	HEC	C2C-C3C-CAC-CBC
3	B	4	HEC	C2C-C3C-CAC-CBC
3	C	1	HEC	C2C-C3C-CAC-CBC
3	C	4	HEC	C2C-C3C-CAC-CBC
3	C	5	HEC	C2C-C3C-CAC-CBC
3	D	4	HEC	C2C-C3C-CAC-CBC
3	A	1	HEC	C2C-C3C-CAC-CBC
3	A	2	HEC	C4C-C3C-CAC-CBC
3	A	5	HEC	C4C-C3C-CAC-CBC
3	B	2	HEC	C4C-C3C-CAC-CBC
3	B	4	HEC	C4C-C3C-CAC-CBC
3	C	4	HEC	C4C-C3C-CAC-CBC
3	C	5	HEC	C4C-C3C-CAC-CBC
3	D	4	HEC	C4C-C3C-CAC-CBC
3	A	4	HEC	C4C-C3C-CAC-CBC
3	D	1	HEC	C4C-C3C-CAC-CBC
3	A	1	HEC	C4C-C3C-CAC-CBC
3	C	1	HEC	C4C-C3C-CAC-CBC
3	D	4	HEC	C2B-C3B-CAB-CBB
3	B	1	HEC	C2C-C3C-CAC-CBC
3	D	1	HEC	C2C-C3C-CAC-CBC
3	B	1	HEC	C4C-C3C-CAC-CBC
3	A	4	HEC	C2B-C3B-CAB-CBB
3	C	2	HEC	C2C-C3C-CAC-CBC
3	B	4	HEC	C2B-C3B-CAB-CBB
3	C	4	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	D	5	HEC	C2B-C3B-CAB-CBB
3	D	2	HEC	C2C-C3C-CAC-CBC
3	D	5	HEC	C2C-C3C-CAC-CBC
3	A	5	HEC	C2B-C3B-CAB-CBB
3	B	2	HEC	C2B-C3B-CAB-CBB
3	C	5	HEC	C2B-C3B-CAB-CBB
3	B	5	HEC	C2C-C3C-CAC-CBC
3	C	3	HEC	C2C-C3C-CAC-CBC
3	C	2	HEC	C4C-C3C-CAC-CBC
3	B	5	HEC	C2B-C3B-CAB-CBB
3	D	2	HEC	C2B-C3B-CAB-CBB
3	D	4	HEC	C4B-C3B-CAB-CBB
3	B	3	HEC	C2C-C3C-CAC-CBC
3	C	3	HEC	C4C-C3C-CAC-CBC
3	B	5	HEC	C4C-C3C-CAC-CBC
3	D	5	HEC	C4C-C3C-CAC-CBC
3	D	3	HEC	C2C-C3C-CAC-CBC
3	D	5	HEC	C4B-C3B-CAB-CBB
3	A	2	HEC	C2B-C3B-CAB-CBB
3	C	4	HEC	C4B-C3B-CAB-CBB
3	B	3	HEC	C4C-C3C-CAC-CBC
3	D	2	HEC	C4C-C3C-CAC-CBC
3	D	3	HEC	C4C-C3C-CAC-CBC
3	B	4	HEC	C4B-C3B-CAB-CBB
3	C	2	HEC	C2B-C3B-CAB-CBB
3	A	4	HEC	C4B-C3B-CAB-CBB
3	D	4	HEC	C2A-CAA-CBA-CGA
3	D	3	HEC	C2B-C3B-CAB-CBB
3	A	5	HEC	C4B-C3B-CAB-CBB
3	C	5	HEC	C4B-C3B-CAB-CBB
3	A	3	HEC	C2B-C3B-CAB-CBB
5	C	21	EDO	O1-C1-C2-O2
3	B	2	HEC	C4B-C3B-CAB-CBB
3	D	2	HEC	C4B-C3B-CAB-CBB
3	B	5	HEC	C4B-C3B-CAB-CBB
3	A	3	HEC	C2C-C3C-CAC-CBC
3	C	3	HEC	C2B-C3B-CAB-CBB
3	C	2	HEC	C4B-C3B-CAB-CBB
3	A	2	HEC	C4B-C3B-CAB-CBB
3	A	3	HEC	C4C-C3C-CAC-CBC
5	A	22	EDO	O1-C1-C2-O2
3	C	3	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	D	3	HEC	C4B-C3B-CAB-CBB
3	D	1	HEC	CAA-CBA-CGA-O1A
3	B	3	HEC	C2B-C3B-CAB-CBB
3	A	1	HEC	CAA-CBA-CGA-O1A
3	A	5	HEC	CAD-CBD-CGD-O2D
3	A	1	HEC	CAA-CBA-CGA-O2A
3	B	1	HEC	CAA-CBA-CGA-O1A
3	B	2	HEC	CAA-CBA-CGA-O1A
3	B	2	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAD-CBD-CGD-O1D
3	D	1	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAD-CBD-CGD-O1D
5	A	21	EDO	O1-C1-C2-O2
3	A	5	HEC	CAD-CBD-CGD-O1D
3	D	2	HEC	CAA-CBA-CGA-O1A
3	D	5	HEC	CAD-CBD-CGD-O2D
3	C	1	HEC	CAA-CBA-CGA-O1A
3	C	2	HEC	CAA-CBA-CGA-O2A
3	A	3	HEC	C4B-C3B-CAB-CBB
3	B	1	HEC	C2B-C3B-CAB-CBB
3	B	1	HEC	CAA-CBA-CGA-O2A
3	A	2	HEC	CAA-CBA-CGA-O1A
3	C	2	HEC	CAA-CBA-CGA-O1A
3	C	1	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAD-CBD-CGD-O2D
3	A	5	HEC	C3D-CAD-CBD-CGD
3	D	2	HEC	CAA-CBA-CGA-O2A
5	D	24	EDO	O1-C1-C2-O2
5	D	23	EDO	O1-C1-C2-O2
5	D	25	EDO	O1-C1-C2-O2
3	A	2	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAD-CBD-CGD-O2D
3	B	5	HEC	CAD-CBD-CGD-O1D
3	C	5	HEC	CAA-CBA-CGA-O1A
5	A	20	EDO	O1-C1-C2-O2
5	D	21	EDO	O1-C1-C2-O2
5	D	22	EDO	O1-C1-C2-O2
3	A	5	HEC	CAA-CBA-CGA-O1A
3	B	5	HEC	CAA-CBA-CGA-O1A
3	D	5	HEC	CAA-CBA-CGA-O1A
3	C	5	HEC	CAA-CBA-CGA-O2A
5	A	15	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	23	EDO	O1-C1-C2-O2
3	D	5	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAA-CBA-CGA-O2A

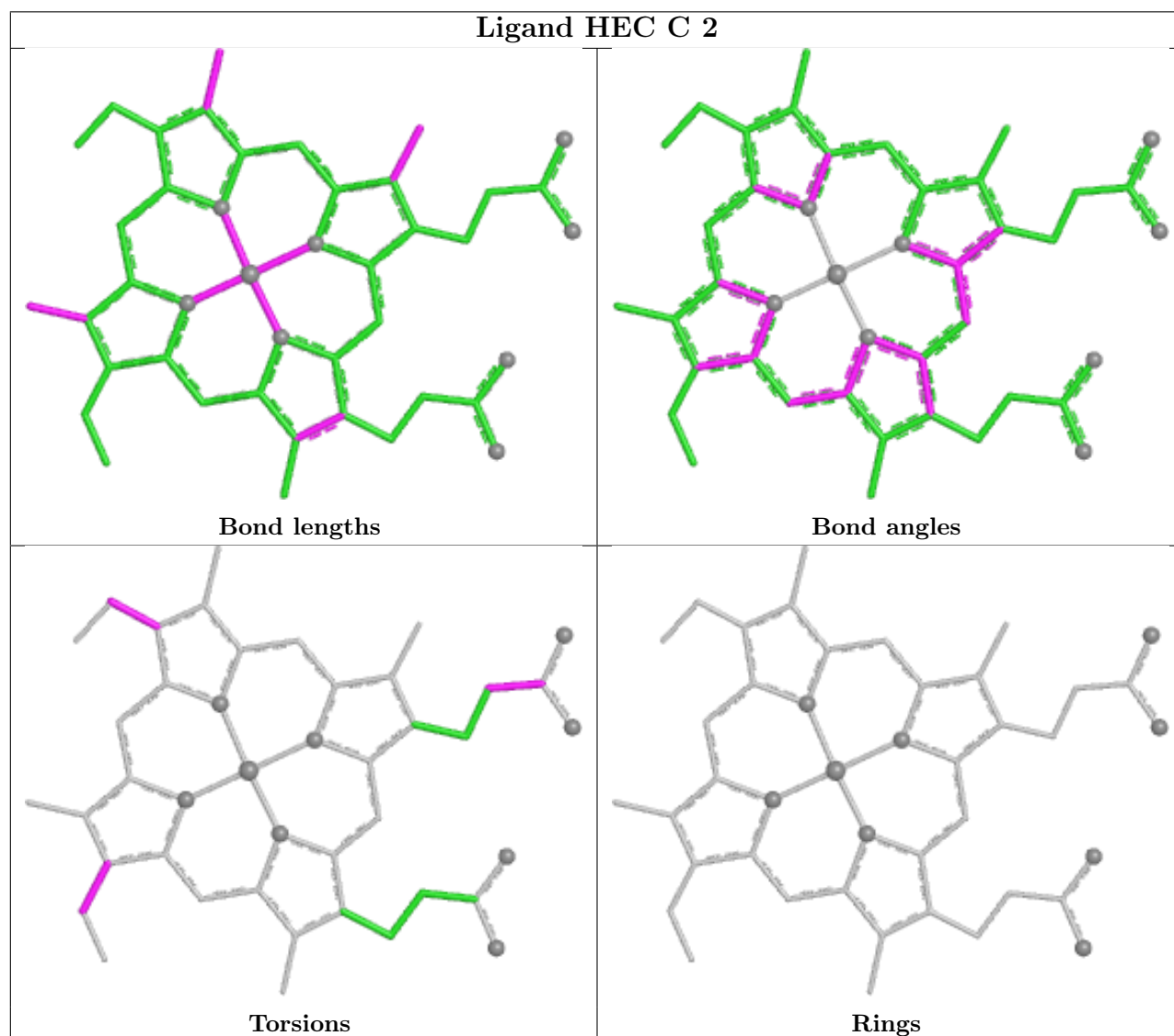
There are no ring outliers.

22 monomers are involved in 49 short contacts:

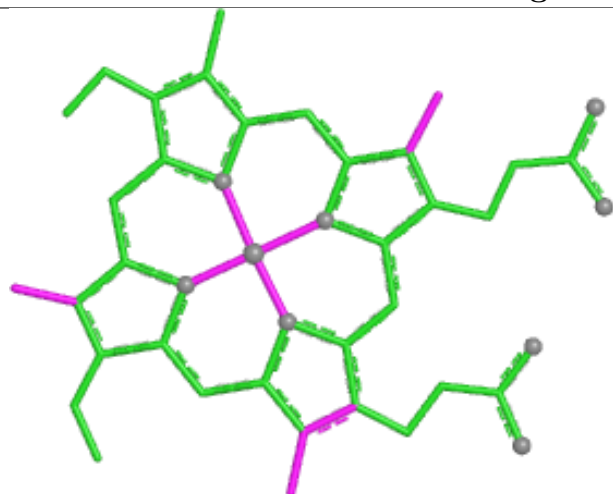
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	25	EDO	1	0
3	C	2	HEC	1	0
5	C	21	EDO	4	0
3	A	4	HEC	3	0
3	D	2	HEC	1	0
3	B	2	HEC	3	0
3	C	4	HEC	3	0
3	B	4	HEC	3	0
3	C	3	HEC	1	0
3	A	2	HEC	4	0
3	A	1	HEC	5	0
3	C	1	HEC	1	0
3	B	3	HEC	1	0
3	C	5	HEC	3	0
3	A	3	HEC	2	0
3	A	5	HEC	1	0
3	D	5	HEC	3	0
5	A	11	EDO	3	0
3	D	4	HEC	2	0
5	A	21	EDO	1	0
3	B	5	HEC	2	0
5	D	481	EDO	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.

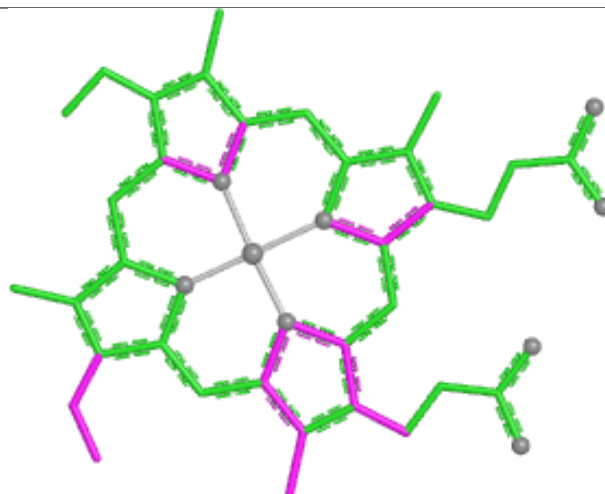
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



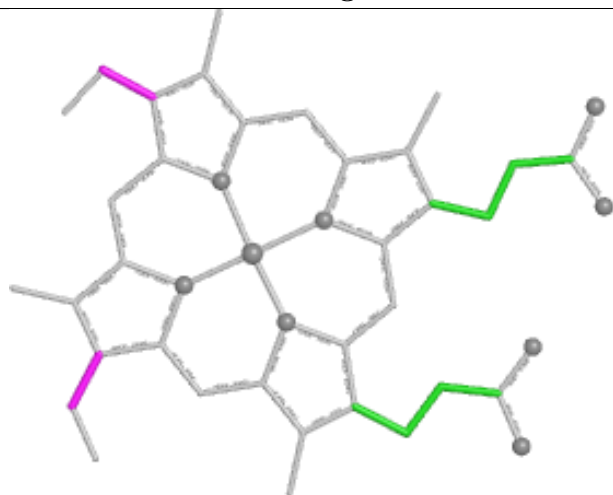
Ligand HEC D 3



Bond lengths



Bond angles

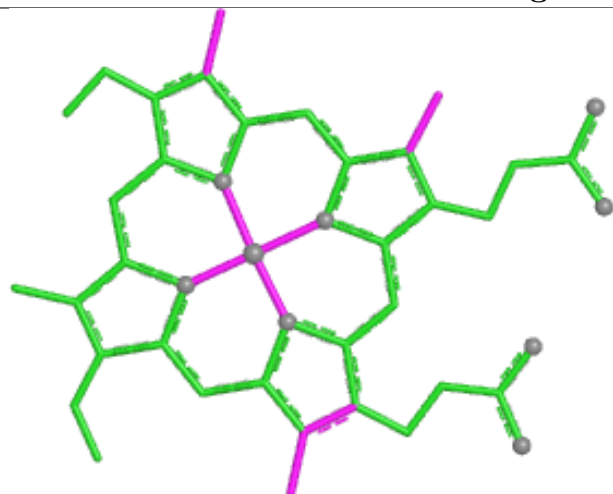


Torsions

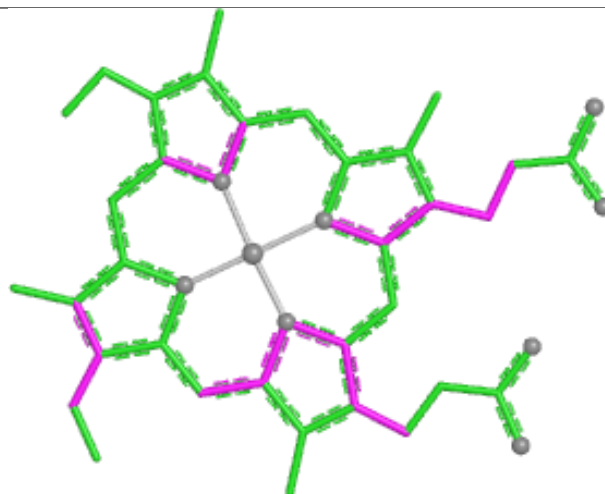


Rings

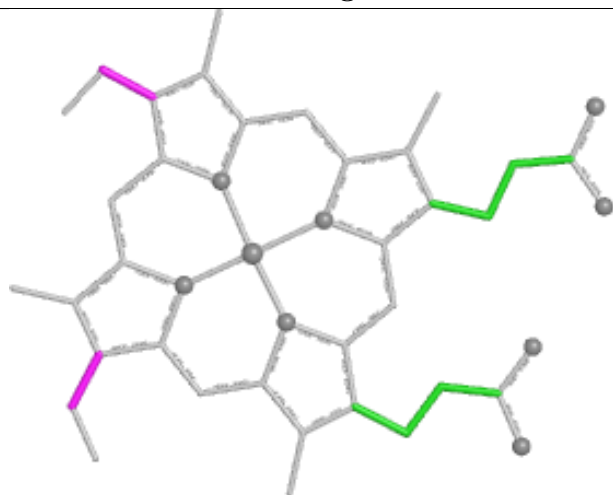
Ligand HEC A 4



Bond lengths



Bond angles

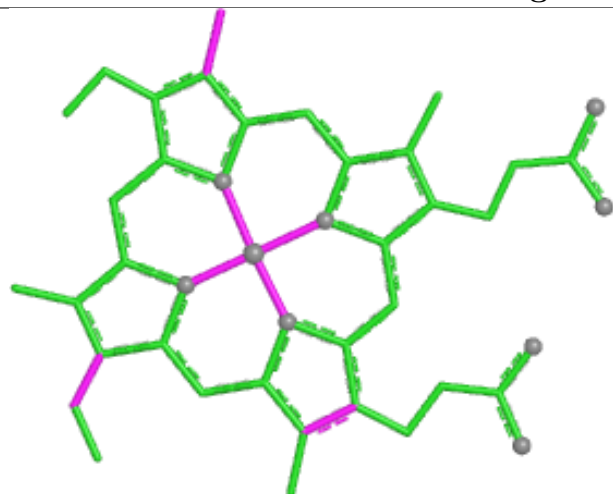


Torsions

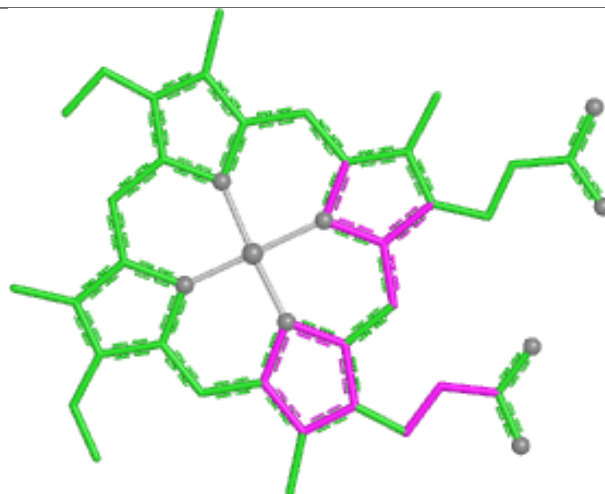


Rings

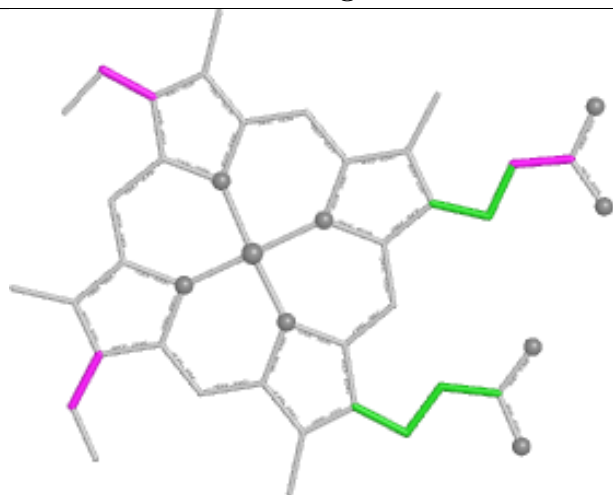
Ligand HEC D 2



Bond lengths



Bond angles

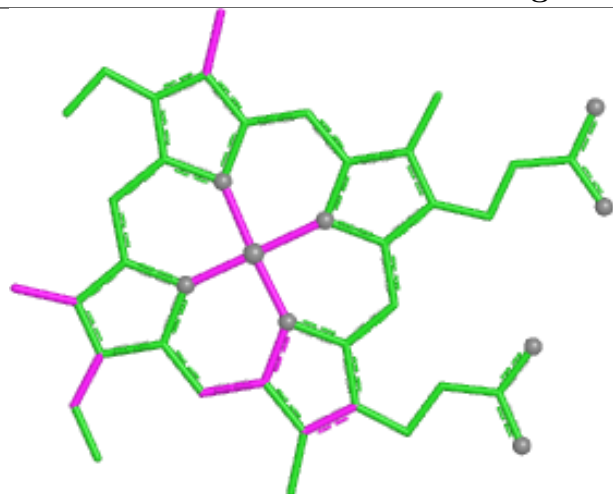


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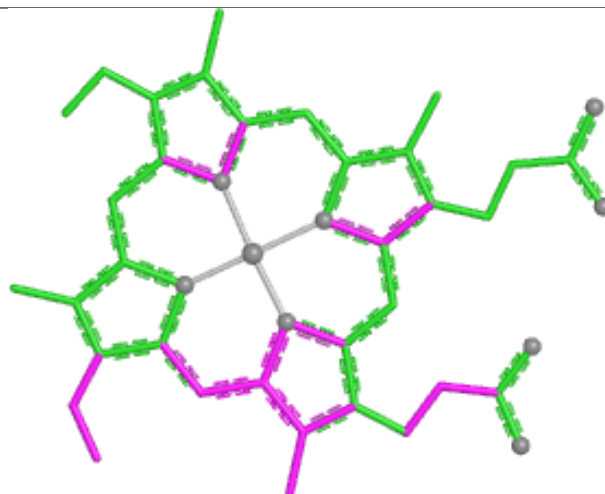


Rings

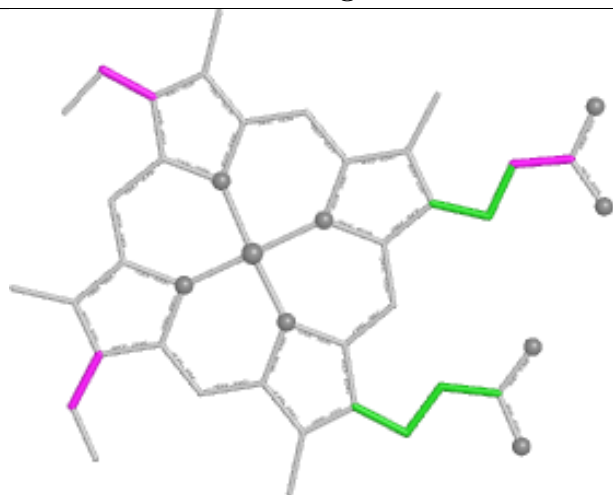
Ligand HEC B 2



Bond lengths



Bond angles

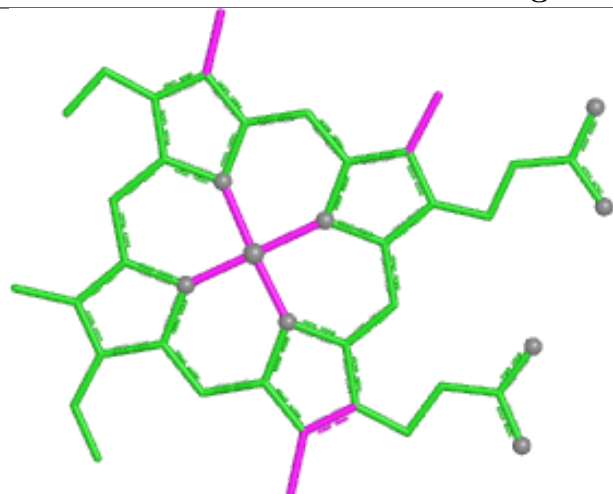


Torsions

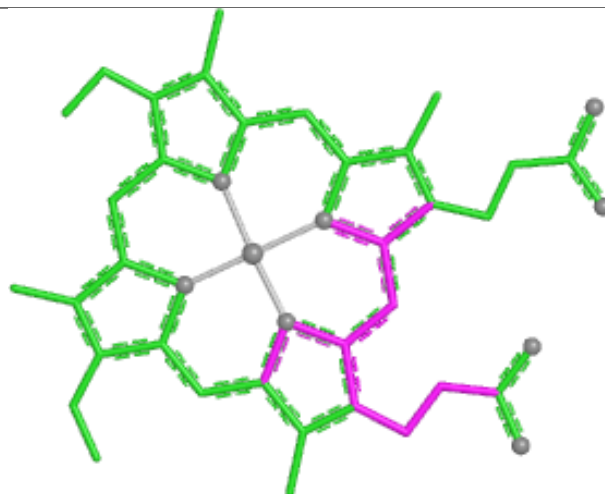


Rings

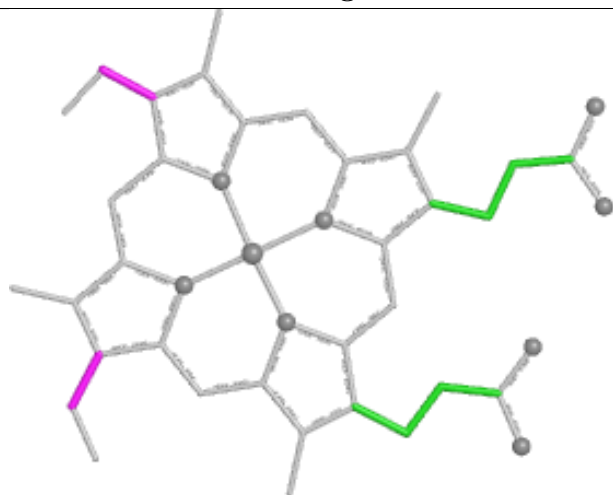
Ligand HEC C 4



Bond lengths



Bond angles

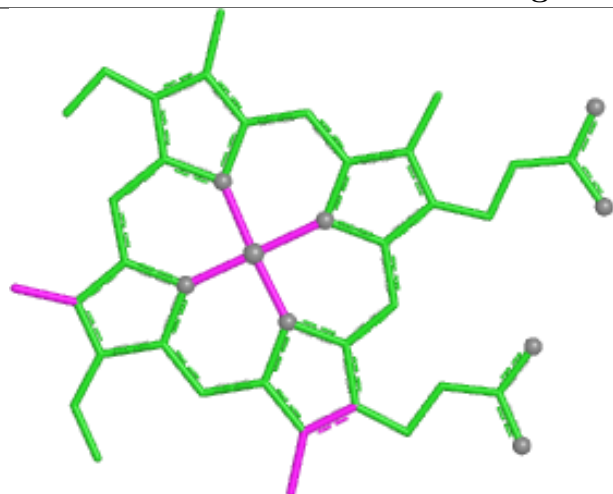


Torsions

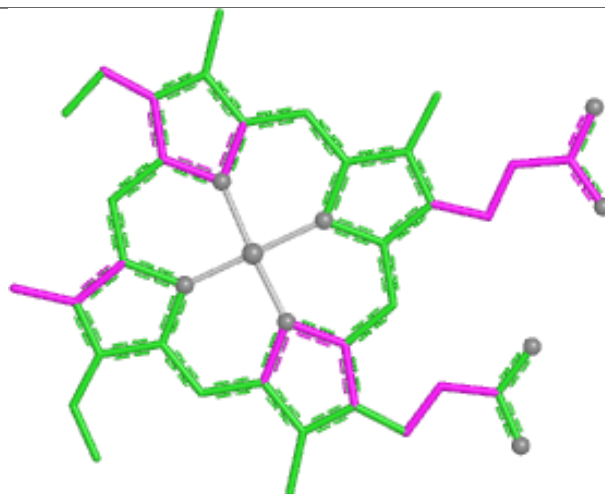


Rings

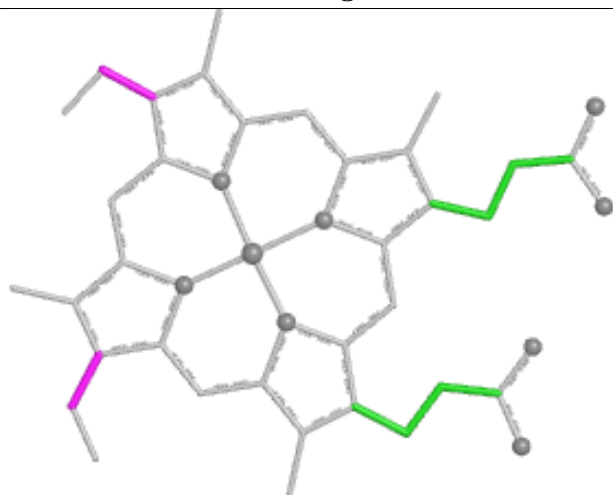
Ligand HEC B 4



Bond lengths



Bond angles

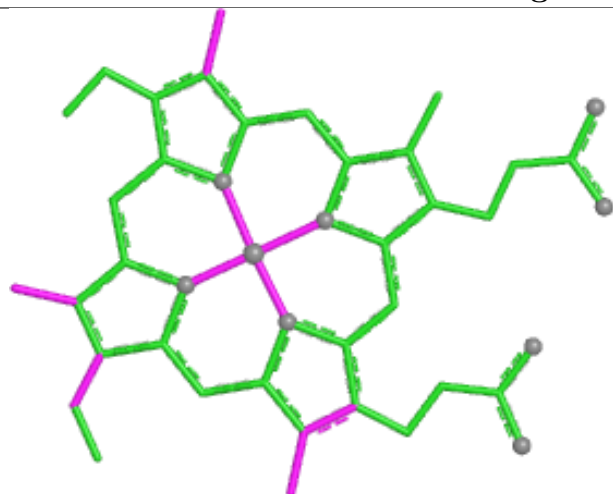


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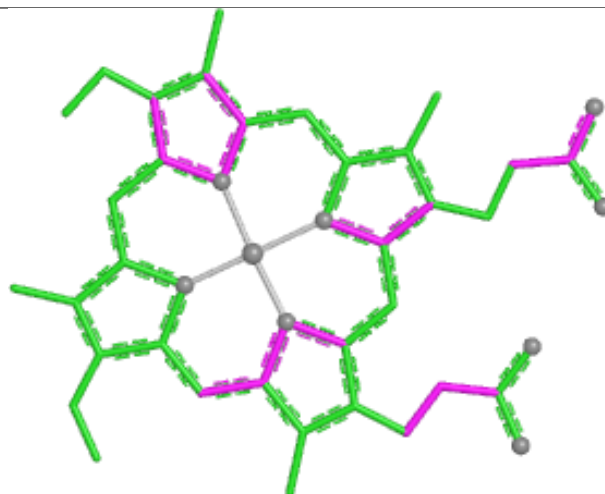


Rings

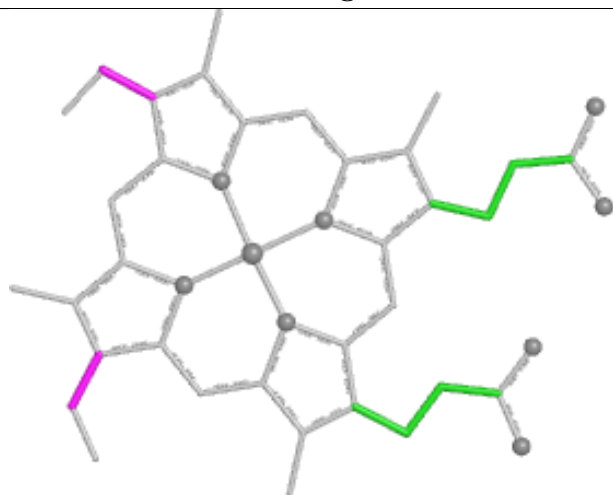
Ligand HEC C 3



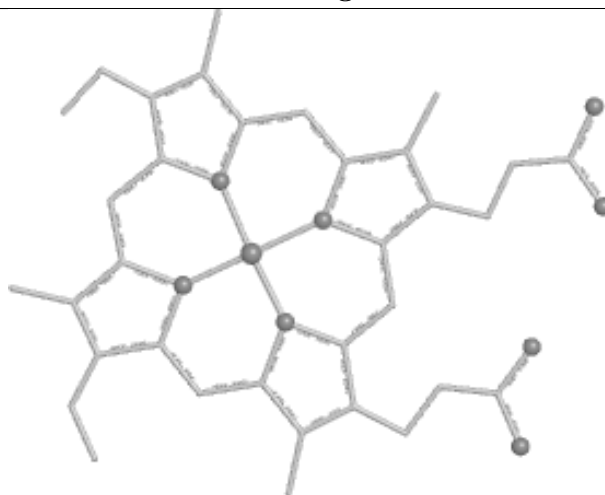
Bond lengths



Bond angles

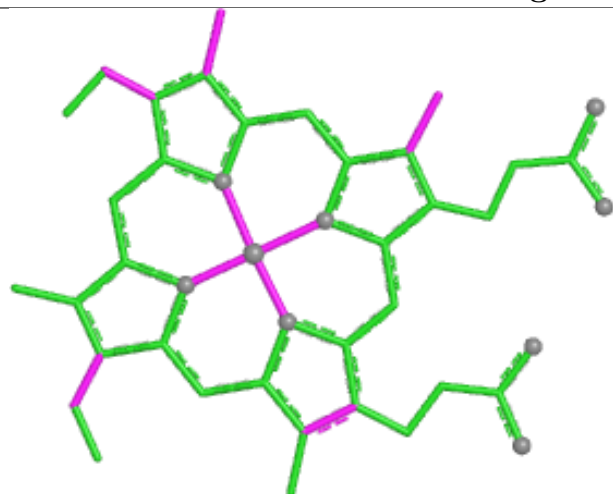


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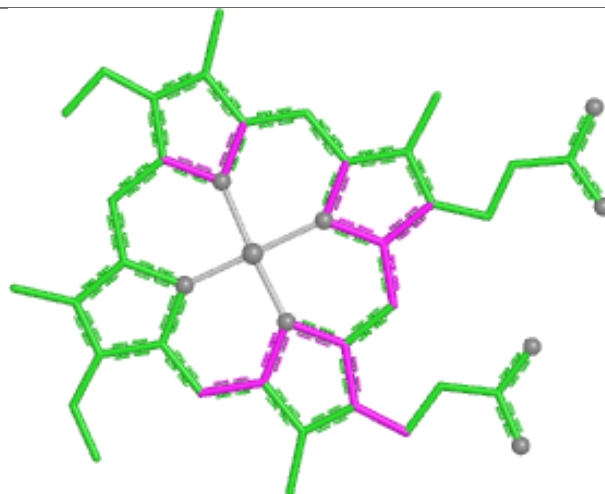


Rings

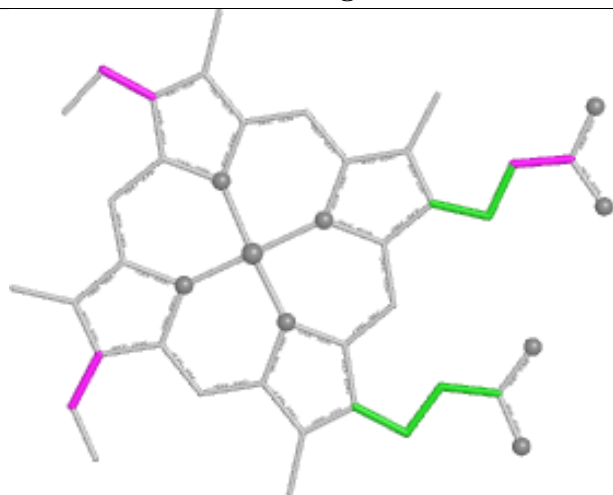
Ligand HEC A 2



Bond lengths



Bond angles

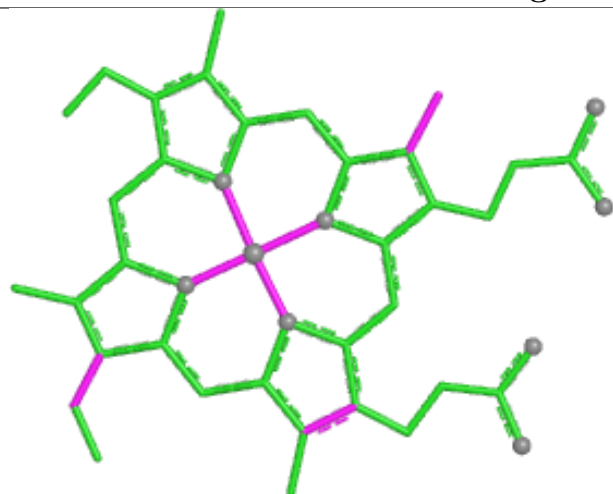


Torsions

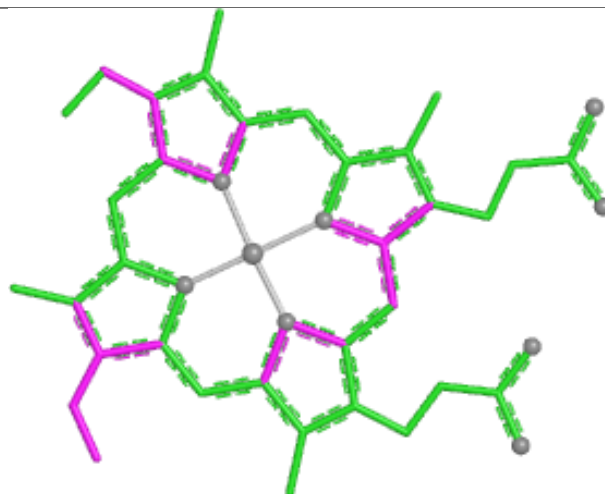


Rings

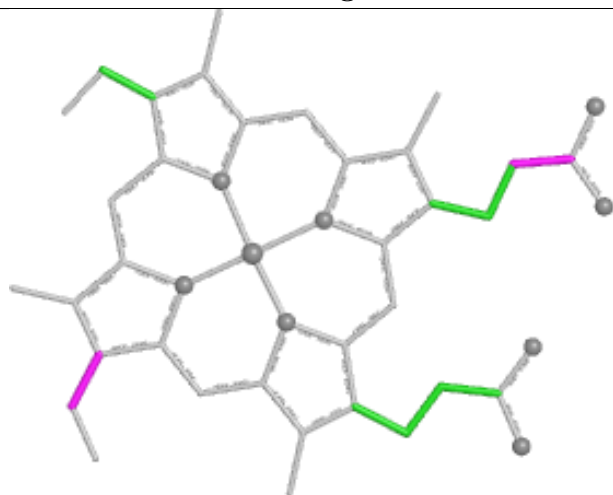
Ligand HEC A 1



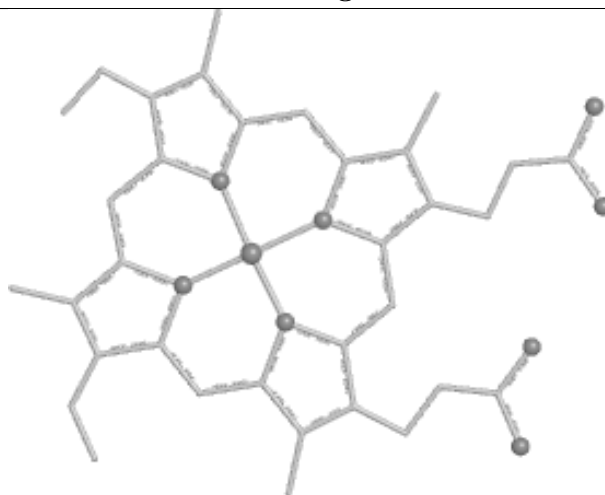
Bond lengths



Bond angles

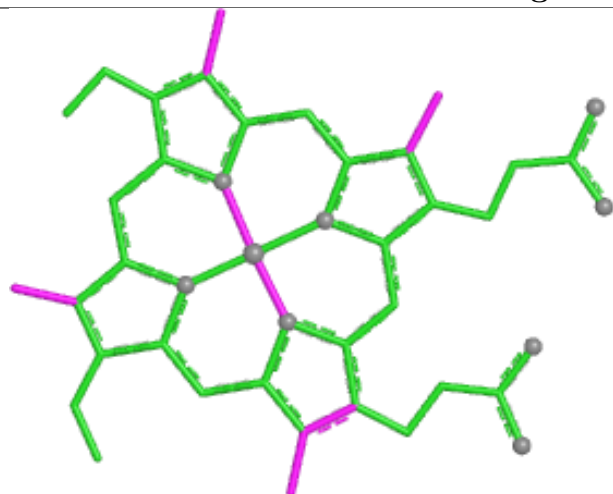


Torsions

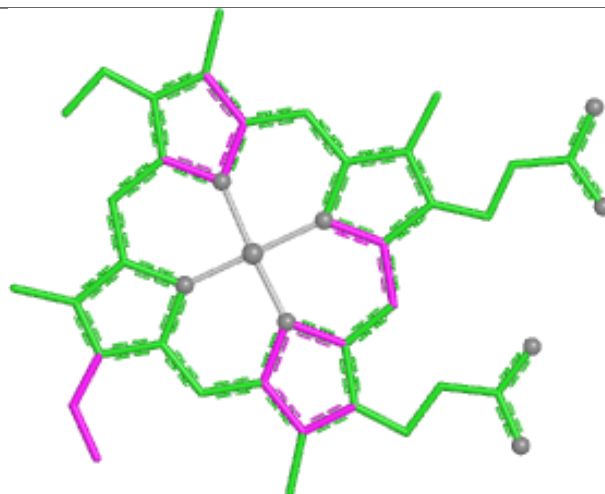


Rings

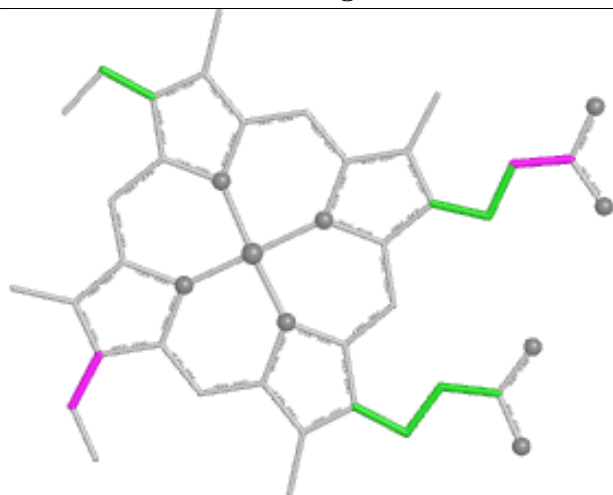
Ligand HEC C 1



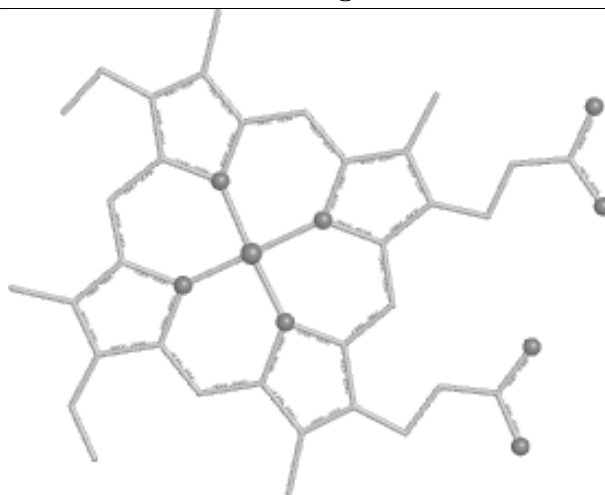
Bond lengths



Bond angles

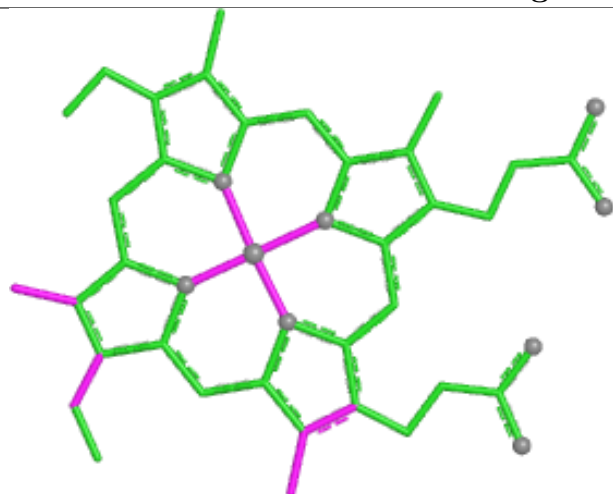


Torsions

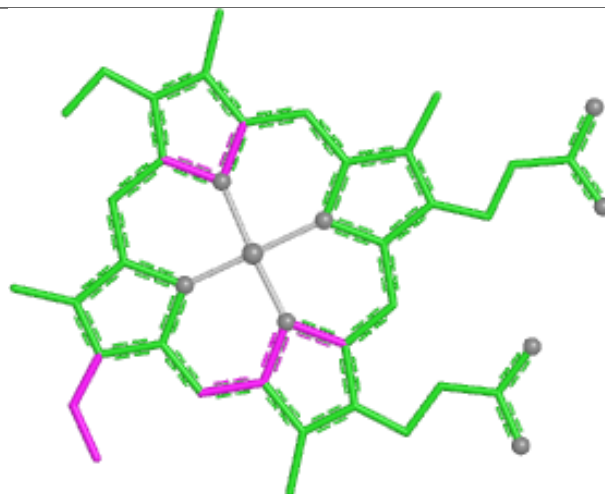


Rings

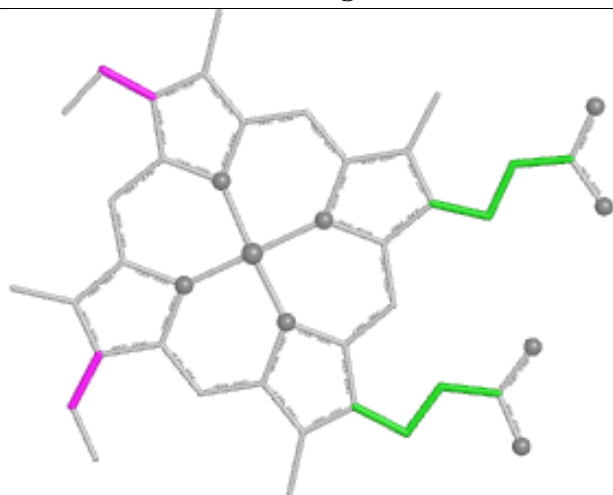
Ligand HEC B 3



Bond lengths



Bond angles

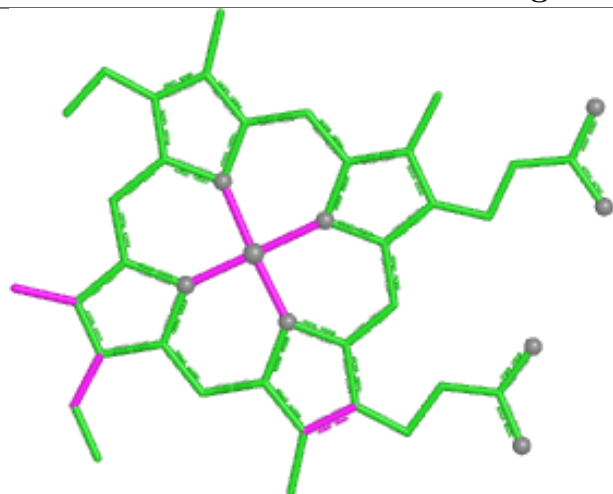


Torsions

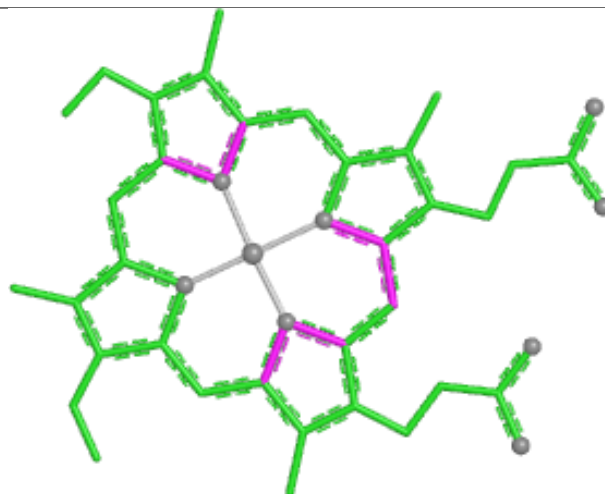


Rings

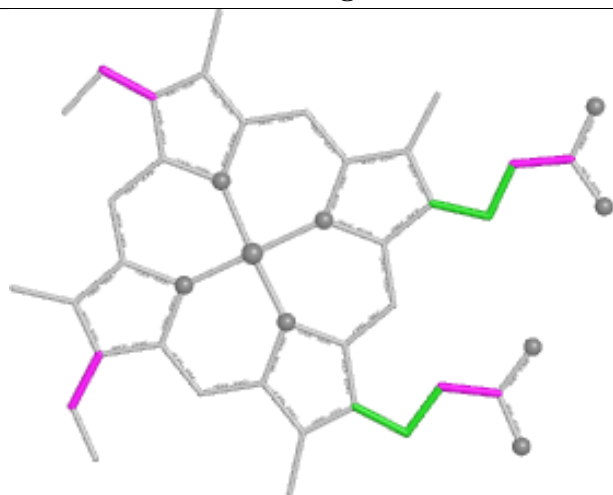
Ligand HEC C 5



Bond lengths



Bond angles

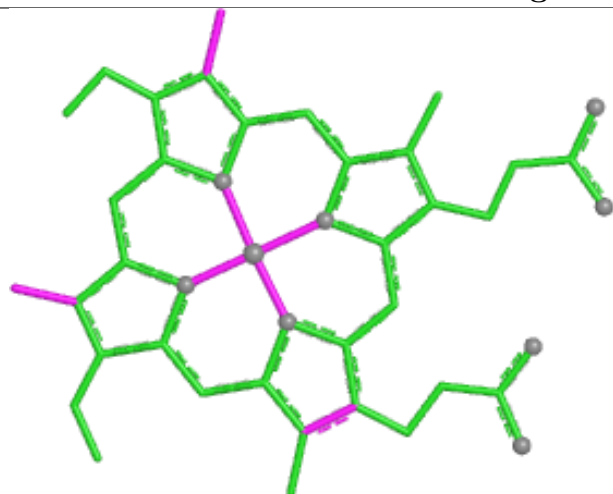


Torsions

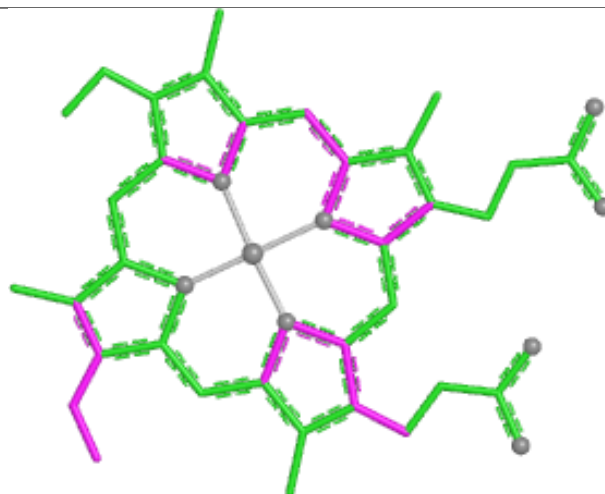


Rings

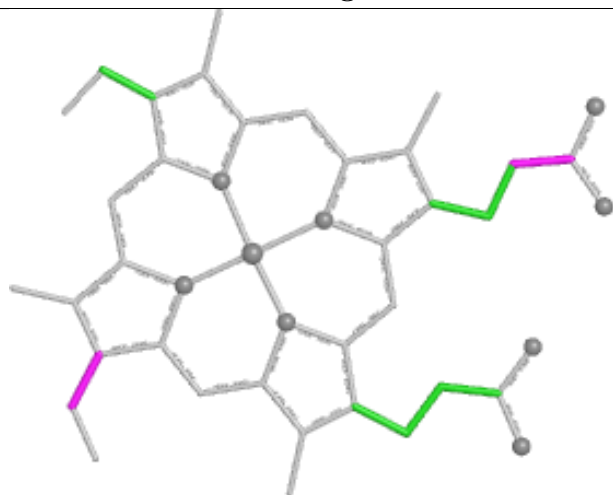
Ligand HEC D 1



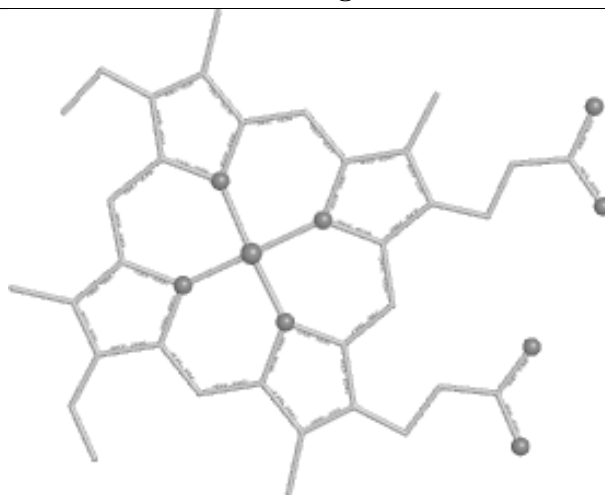
Bond lengths



Bond angles

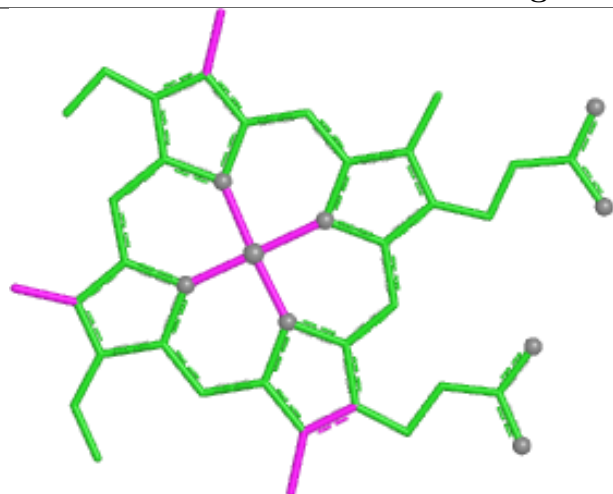


Torsions

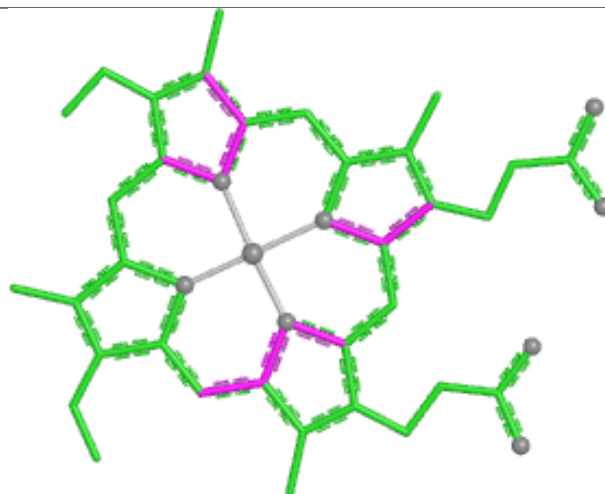


Rings

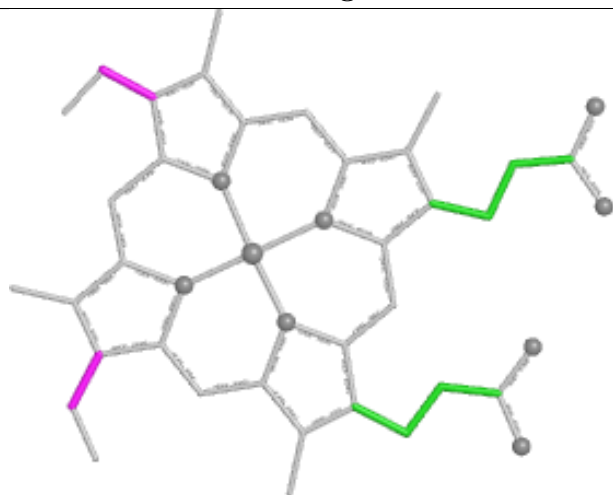
Ligand HEC A 3



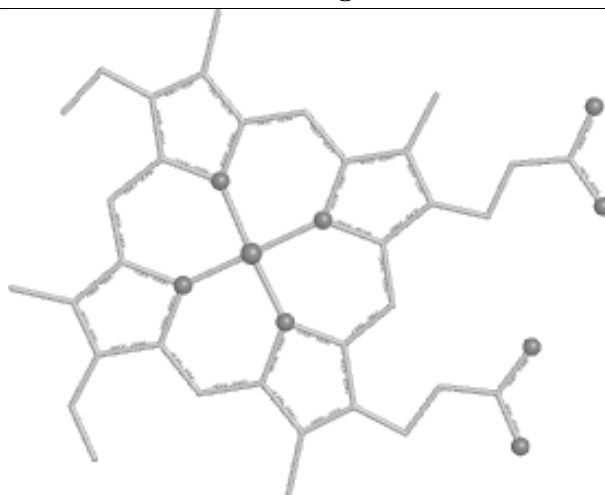
Bond lengths



Bond angles

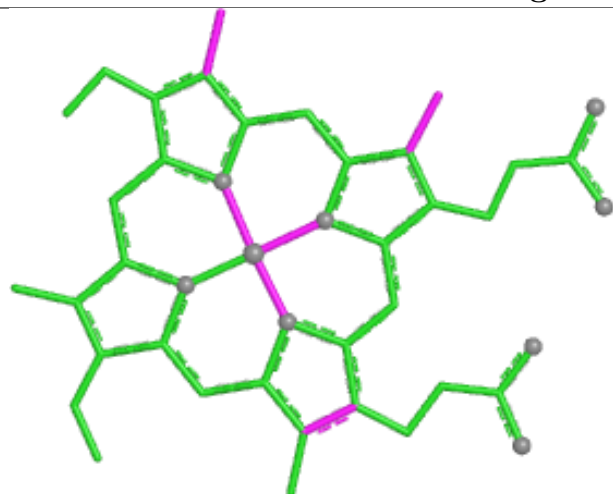


Torsions

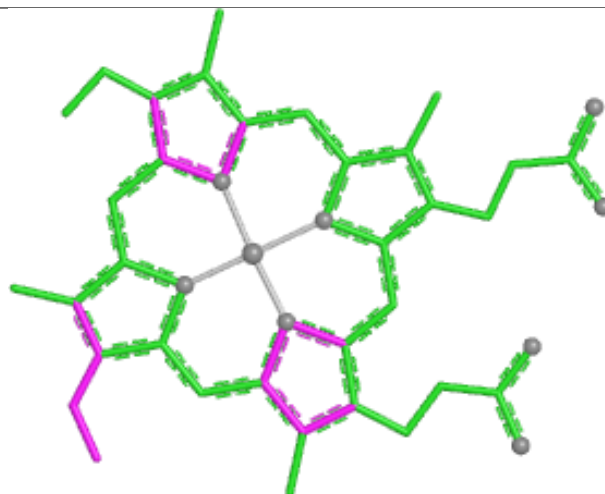


Rings

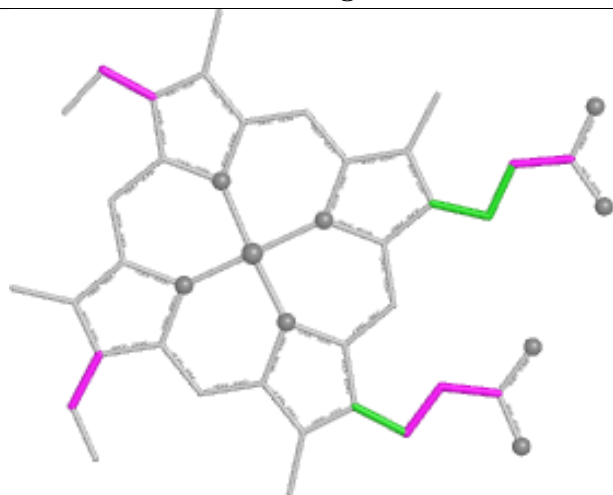
Ligand HEC A 5



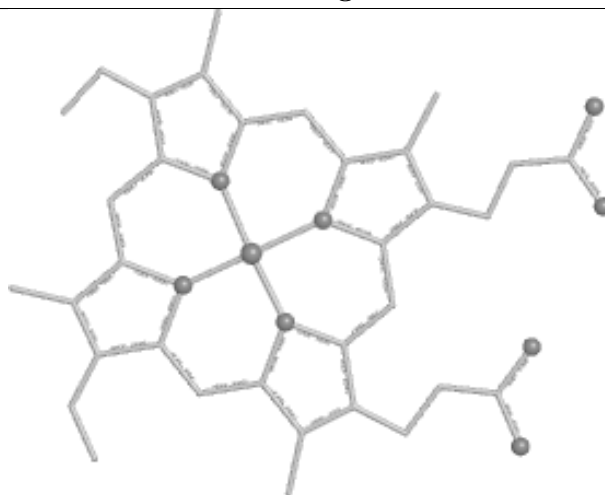
Bond lengths



Bond angles

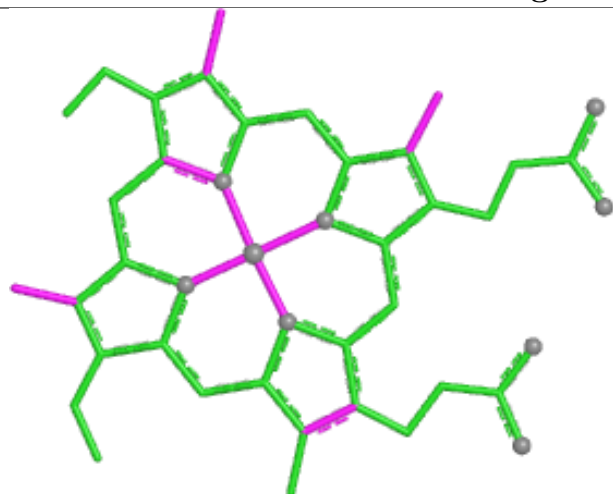


Torsions

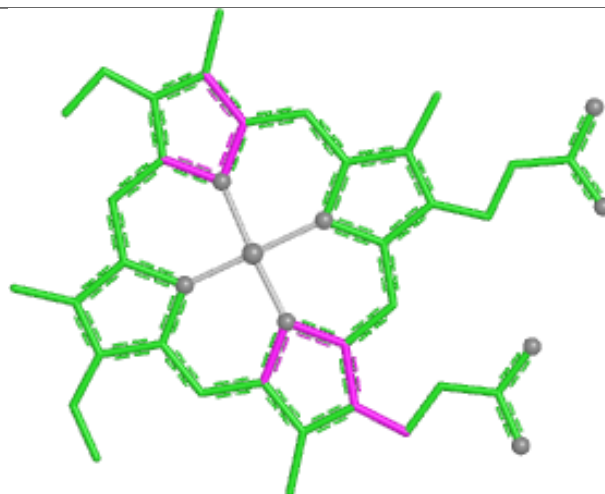


Rings

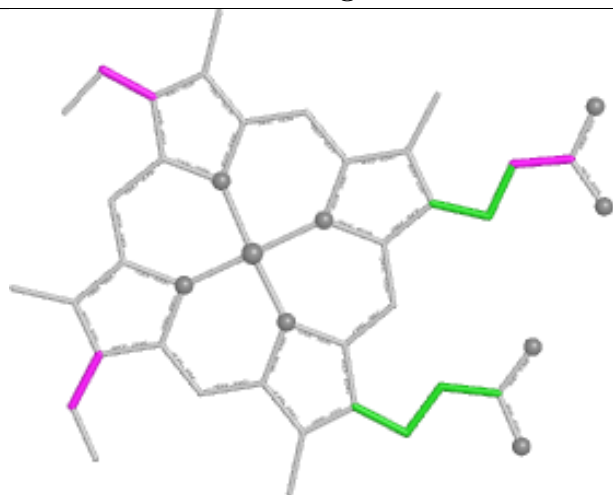
Ligand HEC B 1



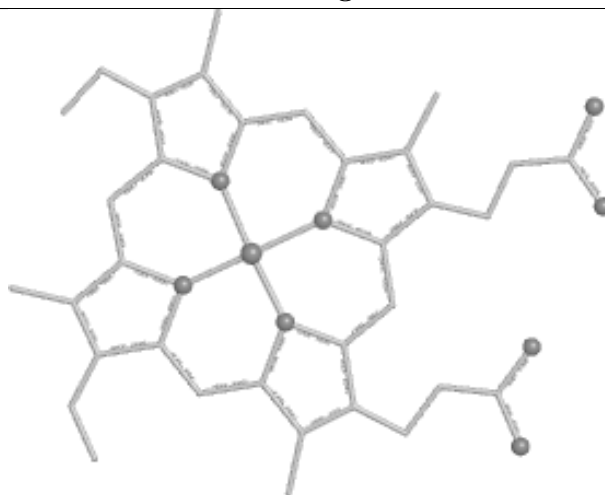
Bond lengths



Bond angles

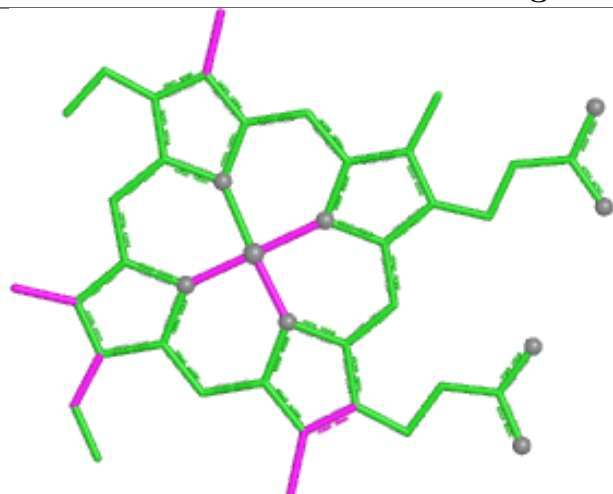


Torsions

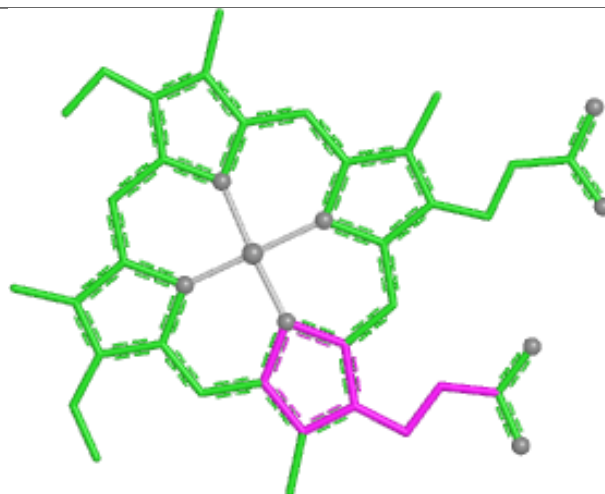


Rings

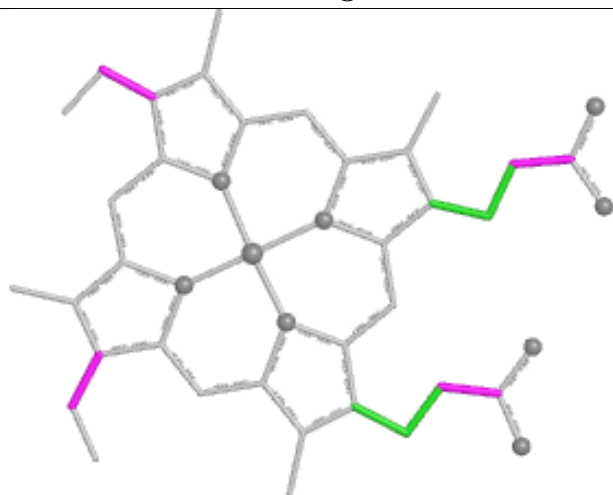
Ligand HEC D 5



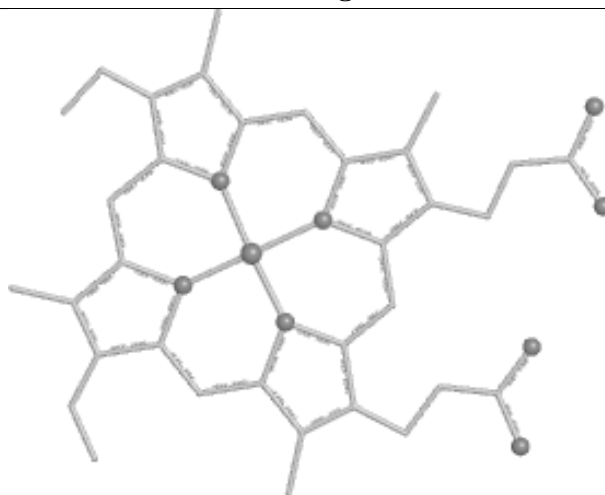
Bond lengths



Bond angles

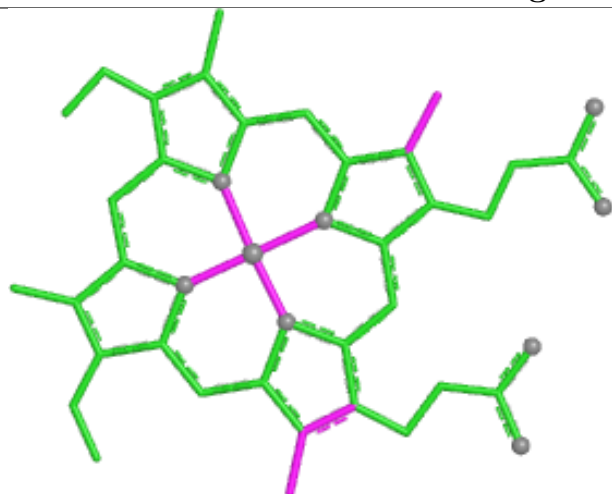


Torsions

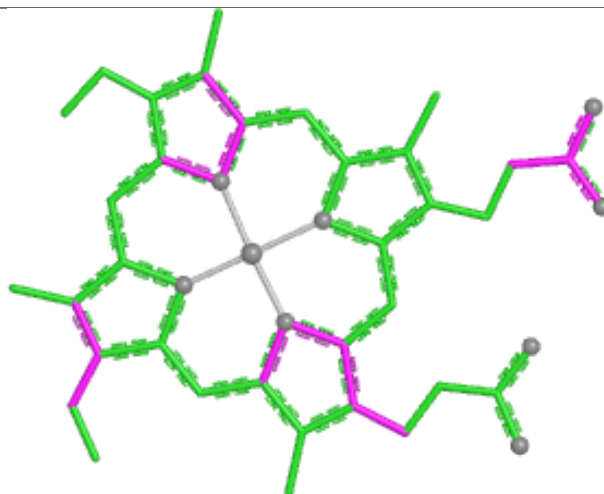


Rings

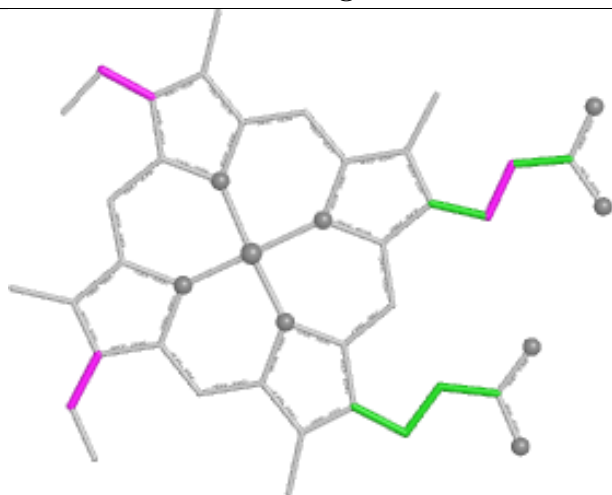
Ligand HEC D 4



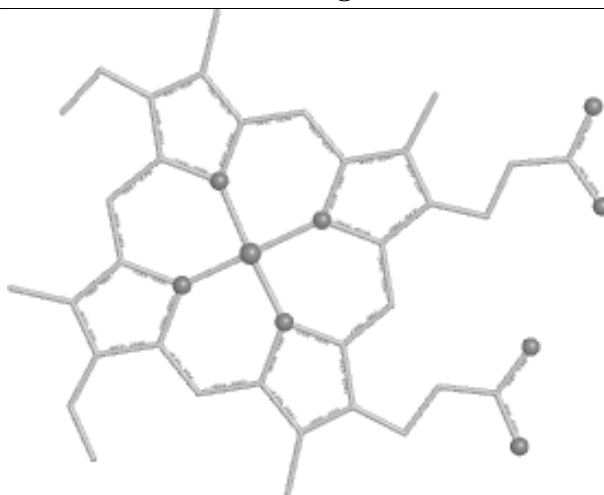
Bond lengths



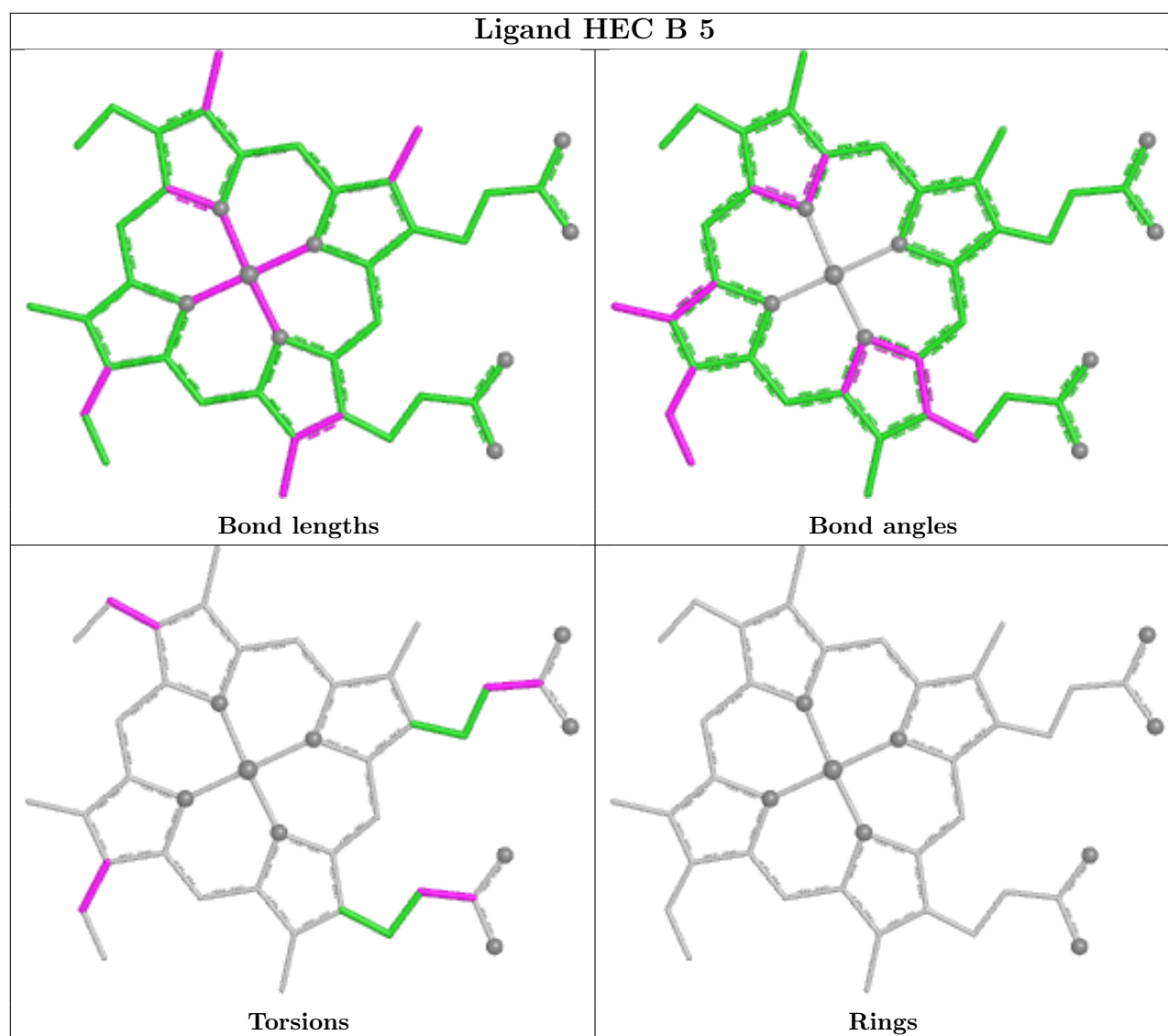
Bond angles



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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/452 (97%)	-0.45	3 (0%) 84 89	7, 13, 24, 34	10 (2%)
1	B	441/452 (97%)	-0.52	1 (0%) 91 93	6, 12, 22, 28	17 (3%)
1	C	441/452 (97%)	-0.24	2 (0%) 87 91	8, 16, 27, 38	14 (3%)
1	D	441/452 (97%)	-0.49	2 (0%) 87 91	6, 12, 21, 27	15 (3%)
All	All	1764/1808 (97%)	-0.43	8 (0%) 87 91	6, 13, 24, 38	56 (3%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	SER	6.4
1	C	477	SER	5.5
1	D	37	THR	5.0
1	C	476	LEU	2.5
1	A	295	GLY	2.5
1	A	294	GLU	2.4
1	A	477	SER	2.2
1	D	477	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	11	4/4	0.78	0.15	26,26,29,30	0
5	EDO	D	22	4/4	0.79	0.16	33,33,33,35	0
5	EDO	C	21	4/4	0.82	0.15	34,35,35,36	0
5	EDO	C	25	4/4	0.84	0.13	23,23,26,28	0
5	EDO	D	25	4/4	0.84	0.17	27,27,30,30	0
5	EDO	C	12	4/4	0.85	0.14	28,29,30,32	0
5	EDO	D	481	4/4	0.87	0.16	34,34,35,35	0
5	EDO	B	20	4/4	0.87	0.12	23,28,30,35	0
5	EDO	A	21	4/4	0.87	0.11	32,32,32,34	0
5	EDO	D	21	4/4	0.88	0.13	23,29,32,35	0
5	EDO	B	18	4/4	0.88	0.12	27,28,28,28	0
5	EDO	C	23	4/4	0.88	0.14	35,35,35,36	0
5	EDO	D	23	4/4	0.90	0.10	24,28,30,34	0
5	EDO	A	22	4/4	0.90	0.12	20,25,28,31	0
5	EDO	B	17	4/4	0.91	0.09	28,29,30,31	0
2	CA	D	1502	1/1	0.91	0.06	16,16,16,16	1
5	EDO	A	13	4/4	0.91	0.09	22,23,25,28	0
4	SO4	C	2001	5/5	0.92	0.11	36,36,38,39	0
4	SO4	D	2001	5/5	0.93	0.13	33,33,34,37	0
5	EDO	B	19	4/4	0.93	0.10	20,25,25,25	0
5	EDO	A	14	4/4	0.93	0.09	30,31,31,33	0
5	EDO	A	15	4/4	0.93	0.08	27,27,27,27	0
2	CA	C	1502	1/1	0.94	0.10	31,31,31,31	0
4	SO4	A	2001	5/5	0.94	0.09	23,25,27,31	0
5	EDO	D	24	4/4	0.94	0.08	20,21,22,22	0
2	CA	A	1502	1/1	0.95	0.13	28,28,28,28	0
2	CA	B	1502	1/1	0.96	0.07	25,25,25,25	0
5	EDO	A	481	4/4	0.97	0.06	11,12,14,17	0
3	HEC	C	4	43/43	0.97	0.07	9,12,20,28	0
5	EDO	C	481	4/4	0.97	0.06	13,16,18,19	0
4	SO4	B	2001	5/5	0.97	0.08	21,21,25,27	0
5	EDO	D	482	4/4	0.97	0.05	17,18,18,19	0
3	HEC	C	1	43/43	0.98	0.05	9,12,13,13	0
3	HEC	C	2	43/43	0.98	0.06	12,16,17,19	0
3	HEC	A	1	43/43	0.98	0.05	7,9,10,11	0
3	HEC	C	5	43/43	0.98	0.07	11,14,22,30	0
5	EDO	C	22	4/4	0.98	0.05	18,18,20,21	0

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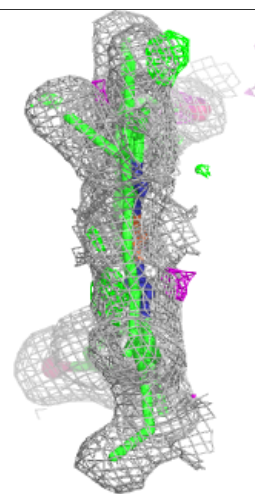
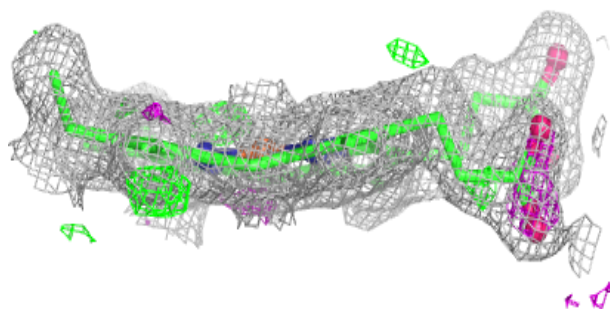
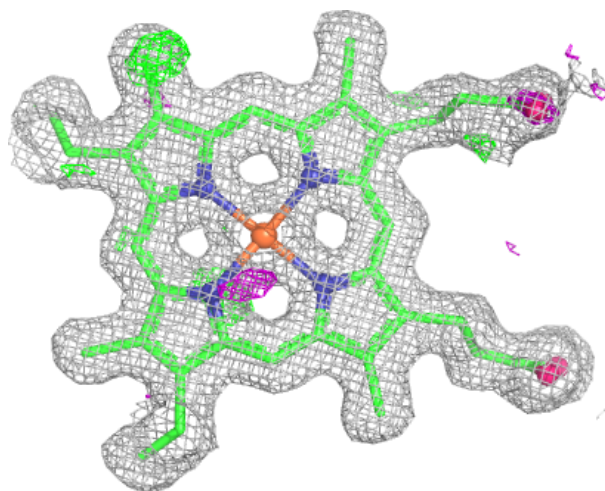
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	D	4	43/43	0.98	0.05	5,8,16,26	0
5	EDO	A	20	4/4	0.98	0.05	18,19,19,20	0
3	HEC	D	5	43/43	0.98	0.06	7,11,22,24	0
3	HEC	A	2	43/43	0.98	0.06	10,12,15,16	0
5	EDO	D	6	4/4	0.98	0.04	12,13,15,18	0
5	EDO	B	481	4/4	0.98	0.05	12,14,16,18	0
5	EDO	B	16	4/4	0.98	0.05	16,17,17,19	0
3	HEC	A	4	43/43	0.98	0.06	5,9,18,26	0
3	HEC	A	5	43/43	0.98	0.06	8,10,19,24	0
3	HEC	B	4	43/43	0.98	0.06	6,8,17,25	0
3	HEC	D	2	43/43	0.99	0.05	7,10,12,14	0
3	HEC	D	3	43/43	0.99	0.05	4,7,9,12	0
3	HEC	B	5	43/43	0.99	0.06	7,10,19,23	0
3	HEC	B	1	43/43	0.99	0.04	6,8,10,11	0
3	HEC	B	2	43/43	0.99	0.05	7,9,12,12	0
3	HEC	C	3	43/43	0.99	0.05	9,11,14,15	0
3	HEC	B	3	43/43	0.99	0.04	5,7,10,11	0
3	HEC	A	3	43/43	0.99	0.05	7,9,11,13	0
3	HEC	D	1	43/43	0.99	0.04	5,7,9,10	0
2	CA	C	1501	1/1	1.00	0.01	11,11,11,11	0
2	CA	B	1501	1/1	1.00	0.02	10,10,10,10	0
2	CA	D	1501	1/1	1.00	0.01	8,8,8,8	0
2	CA	A	1501	1/1	1.00	0.01	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

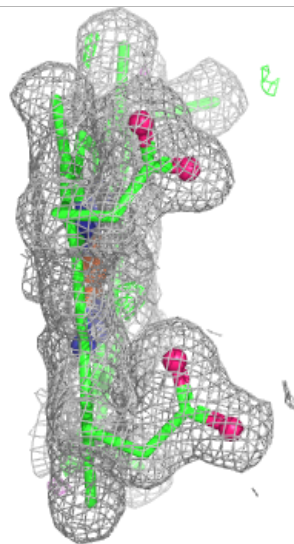
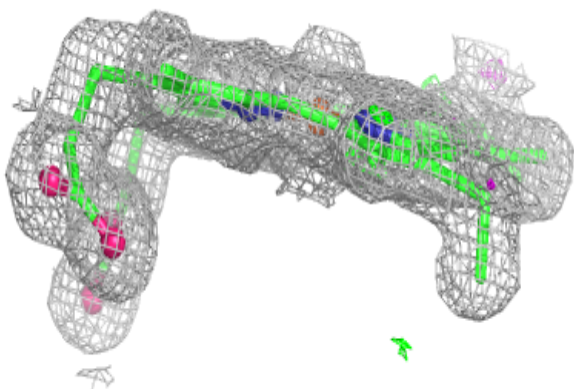
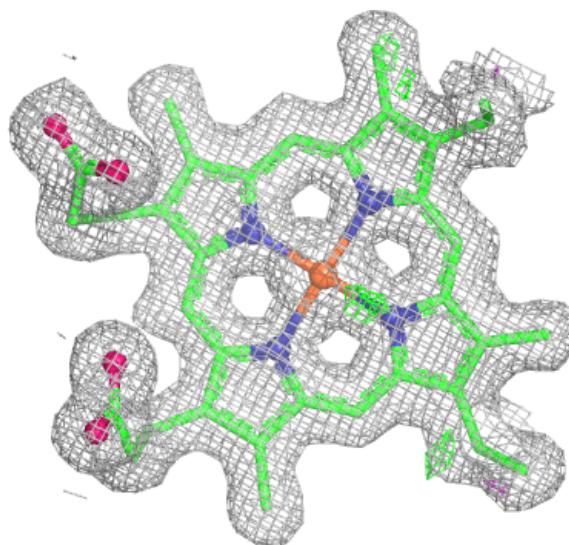
Electron density around HEC C 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



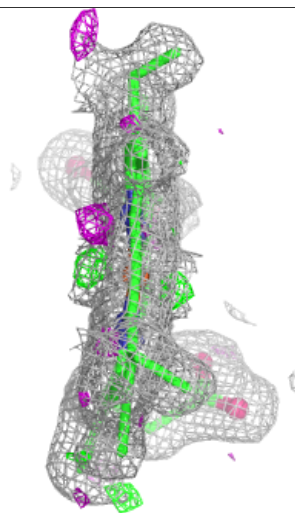
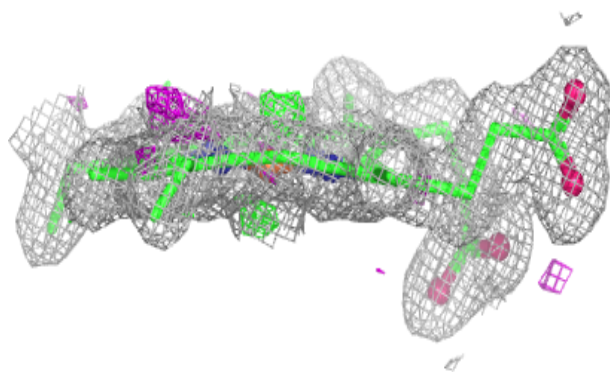
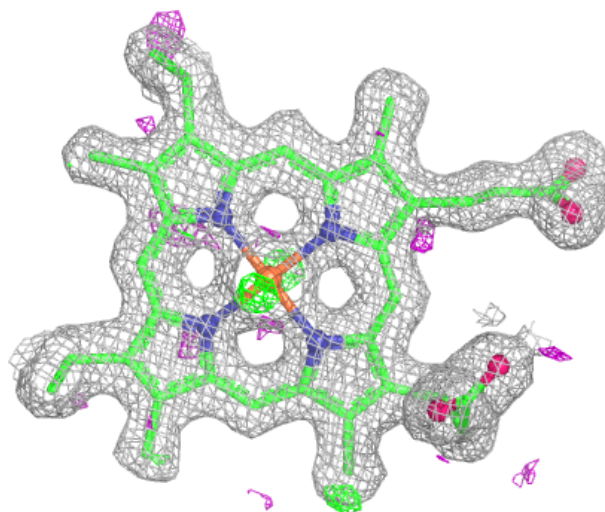
Electron density around HEC C 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



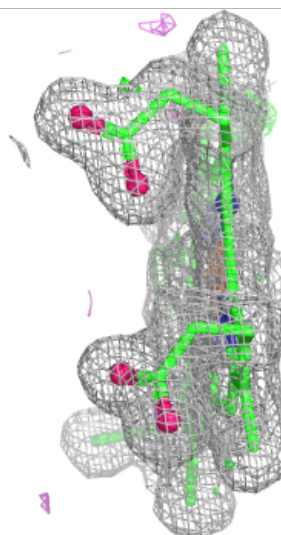
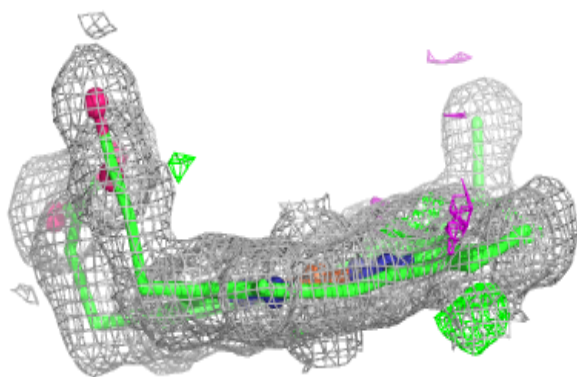
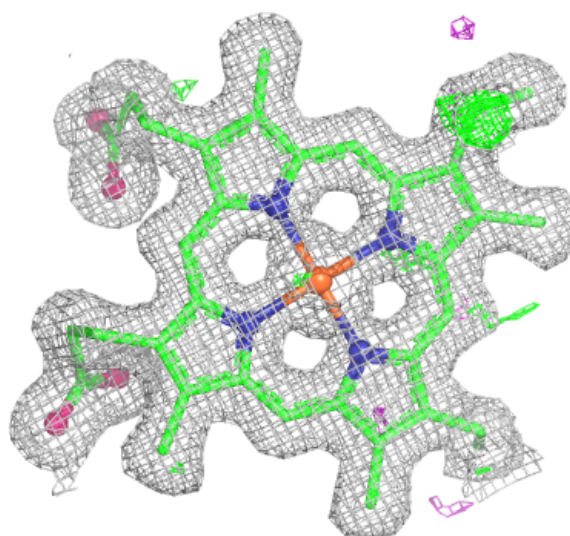
Electron density around HEC C 2:

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and green (positive)



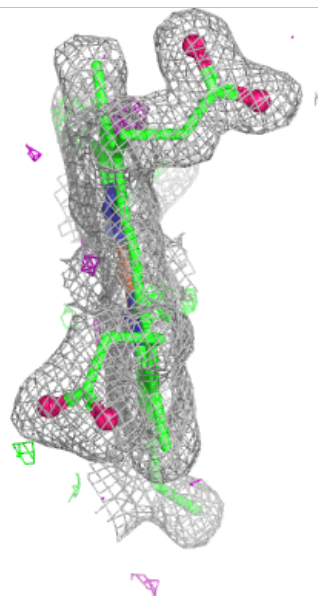
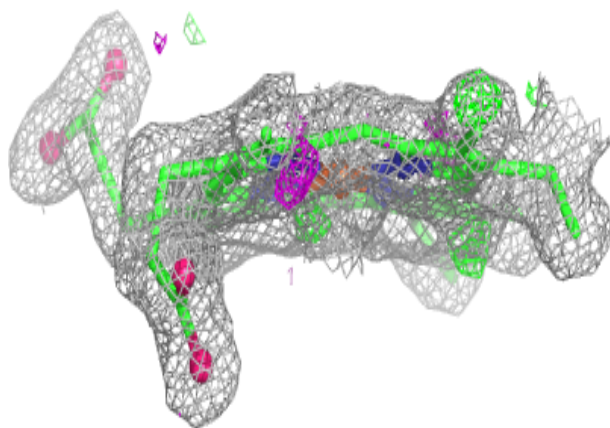
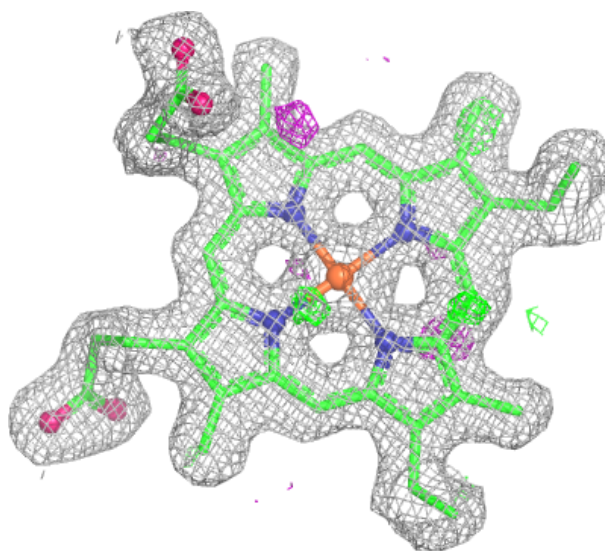
Electron density around HEC A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



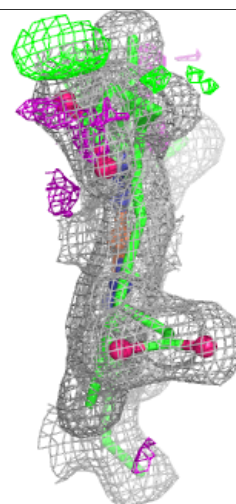
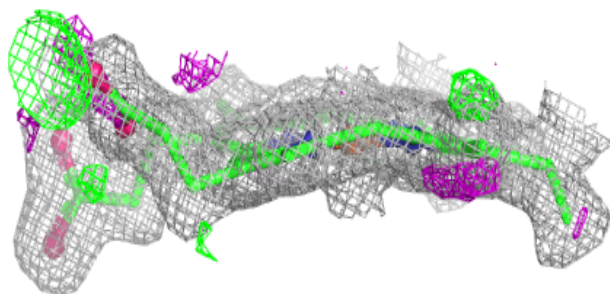
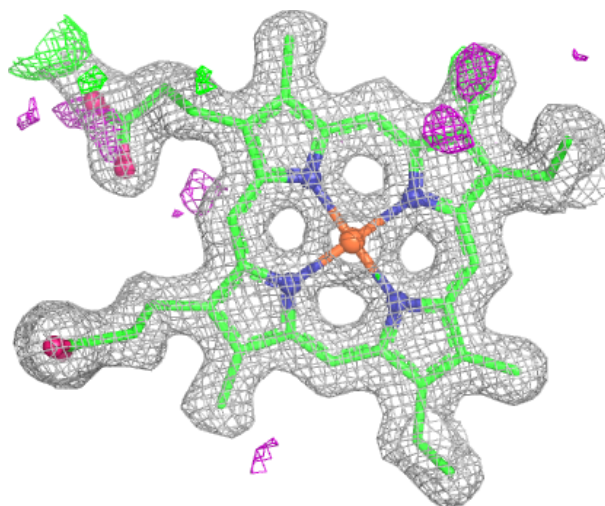
Electron density around HEC C 5:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



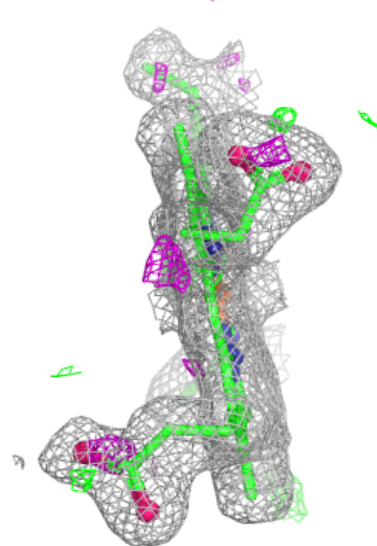
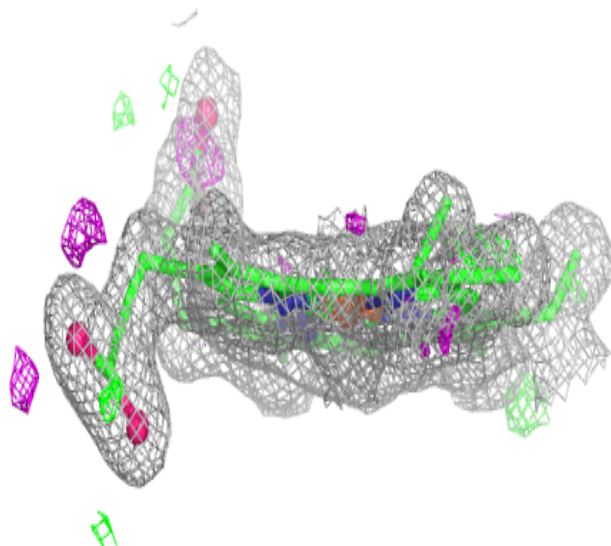
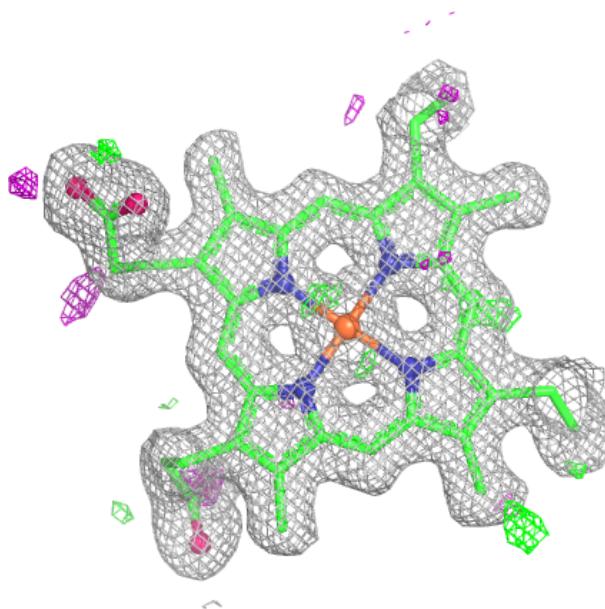
Electron density around HEC D 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



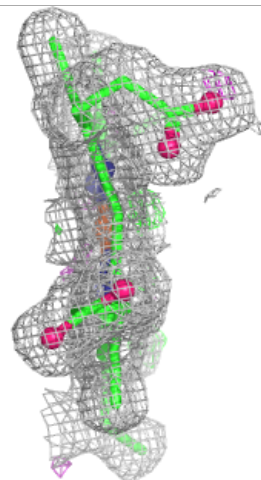
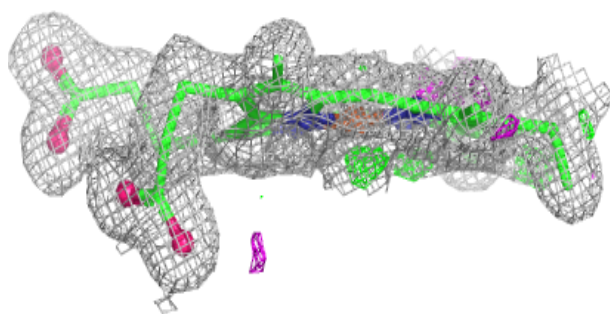
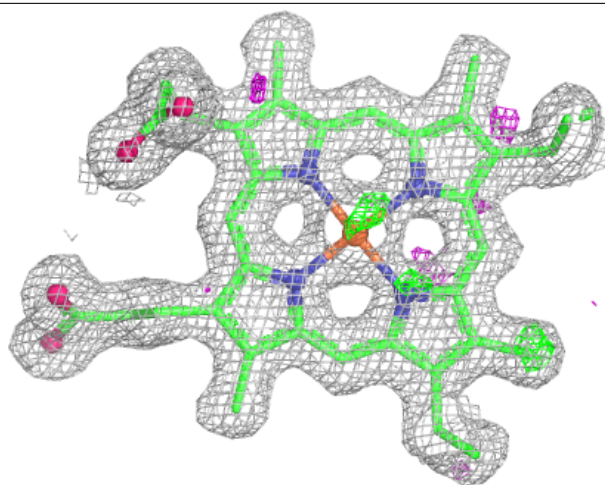
Electron density around HEC D 5:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



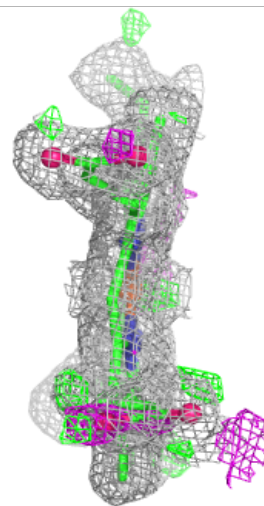
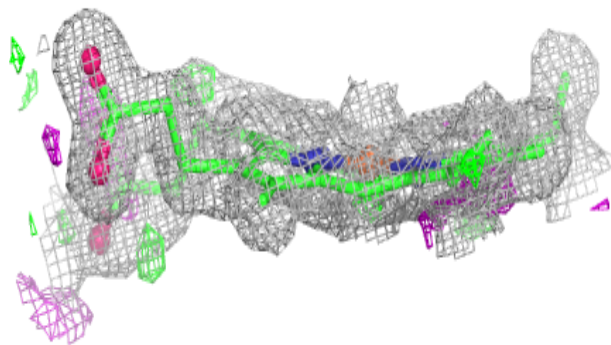
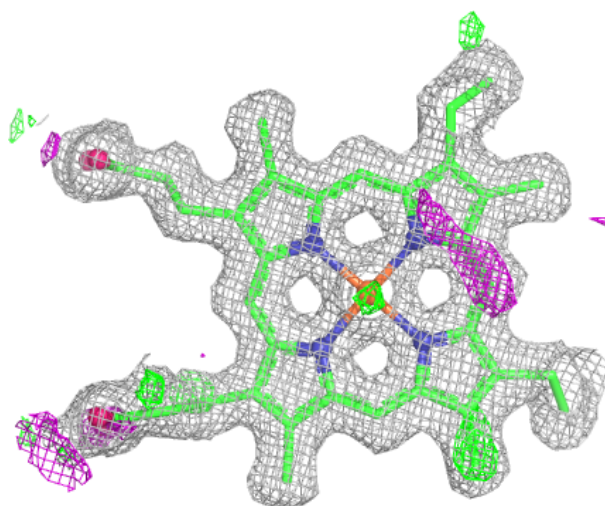
Electron density around HEC A 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



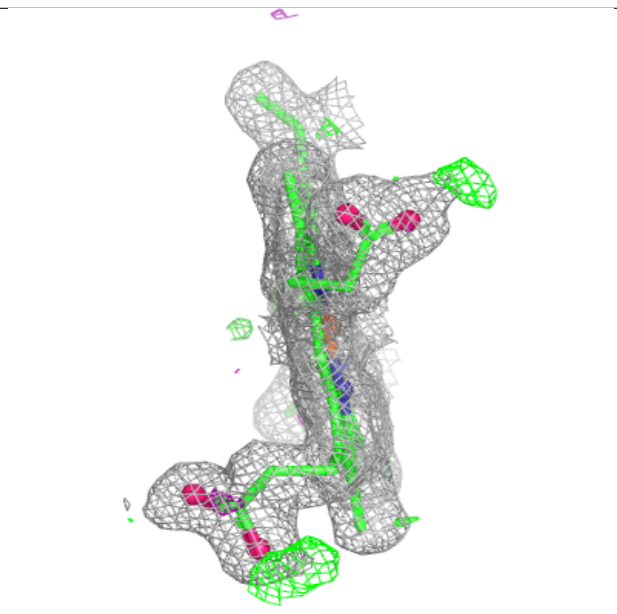
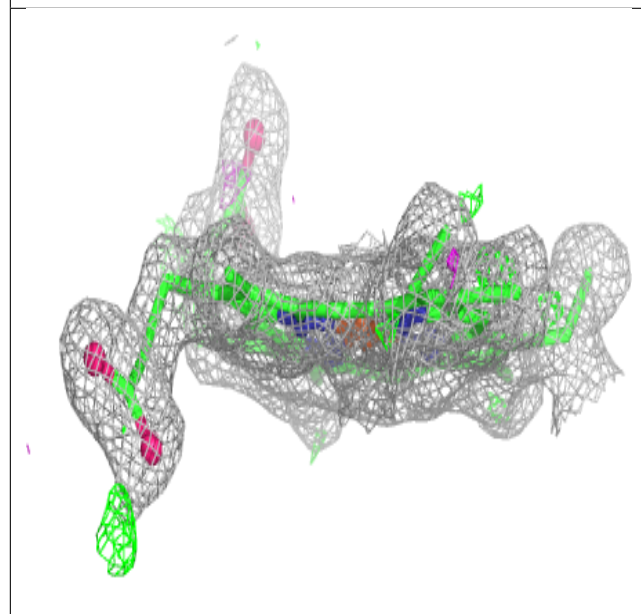
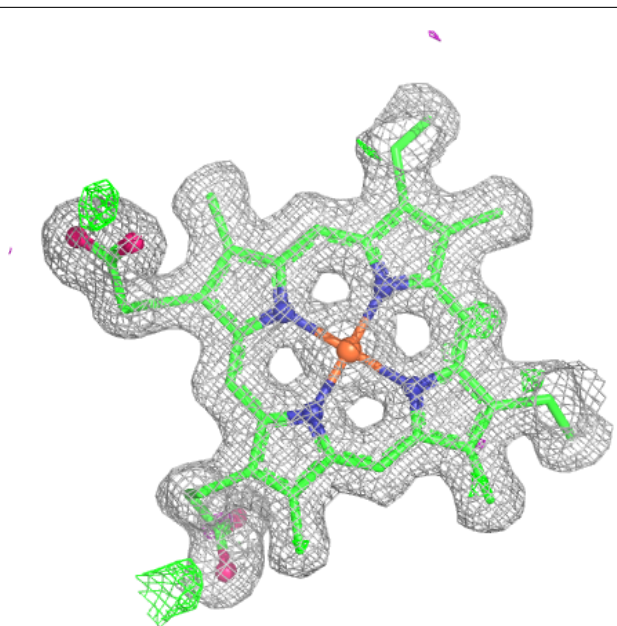
Electron density around HEC A 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



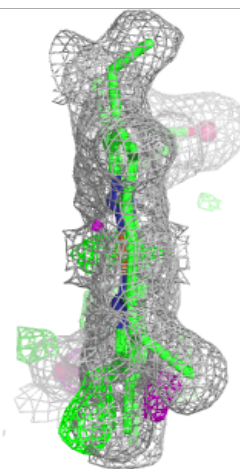
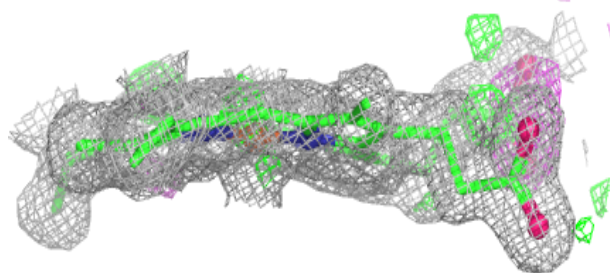
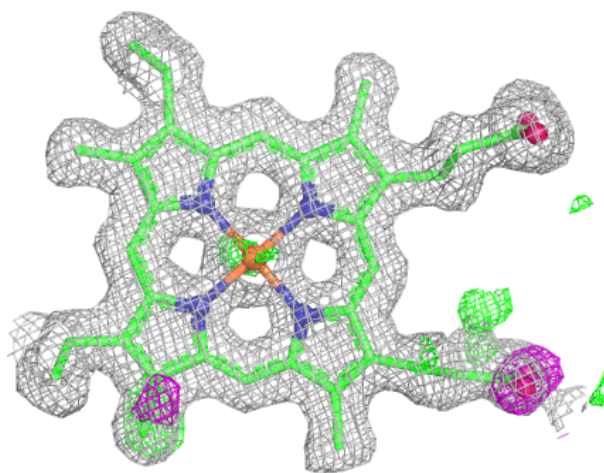
Electron density around HEC A 5:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



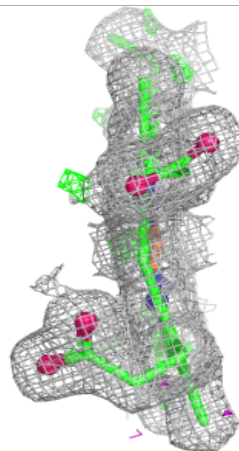
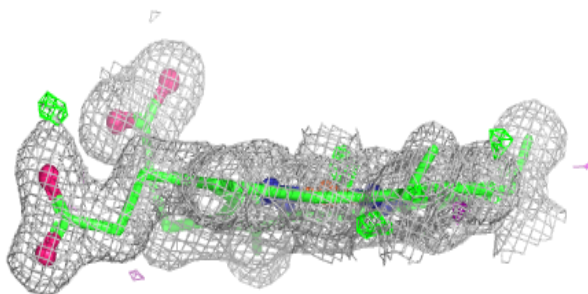
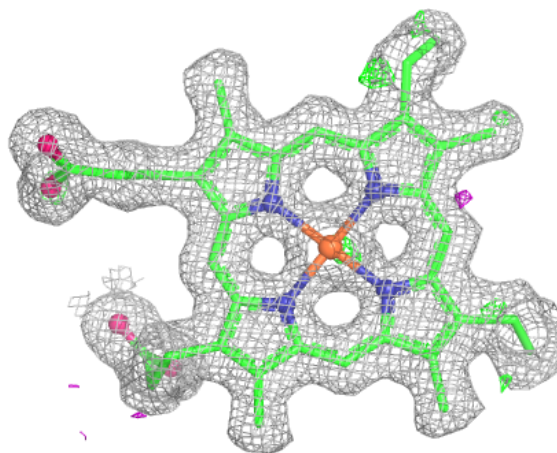
Electron density around HEC B 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



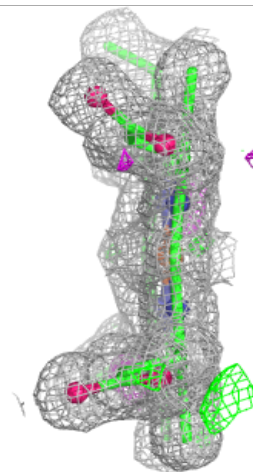
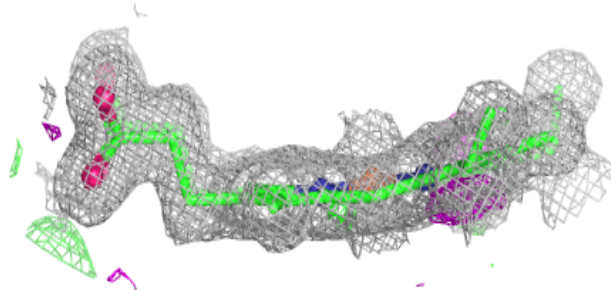
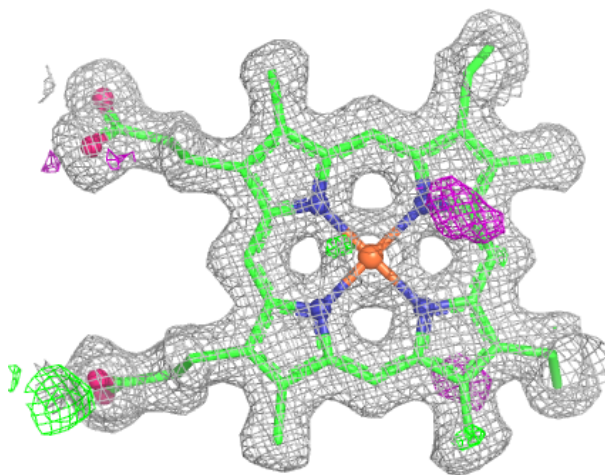
Electron density around HEC D 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



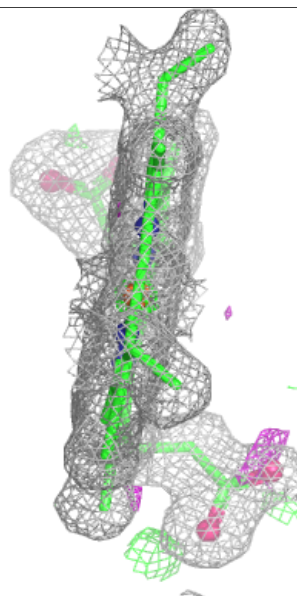
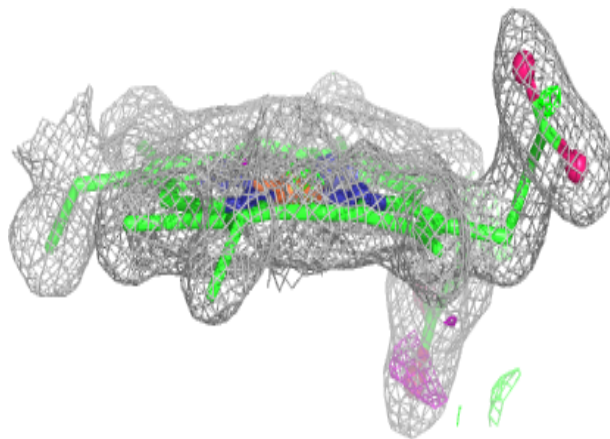
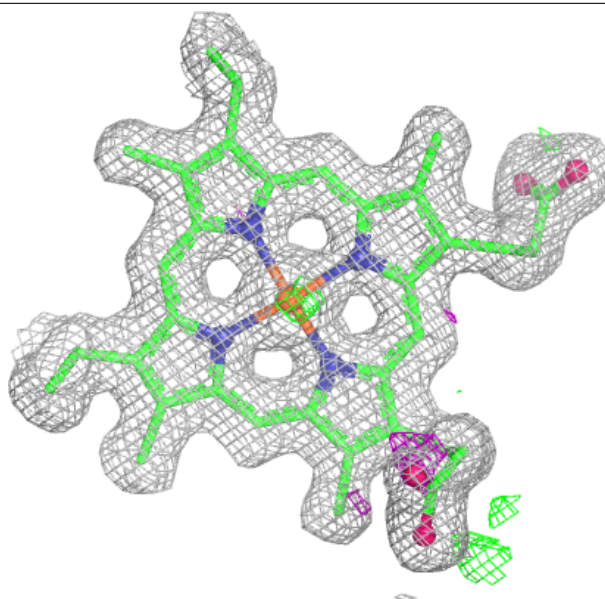
Electron density around HEC D 3:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



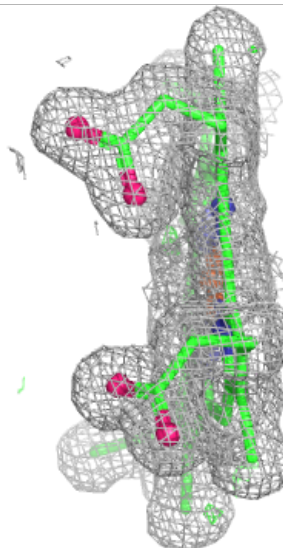
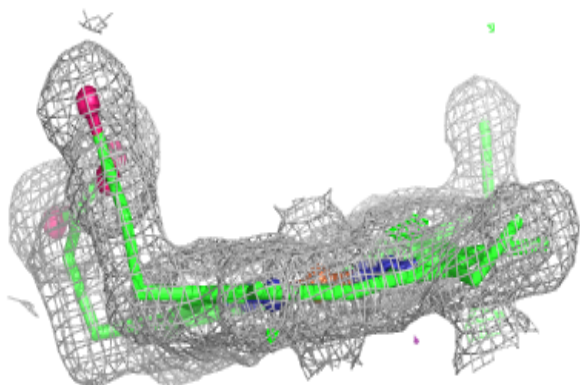
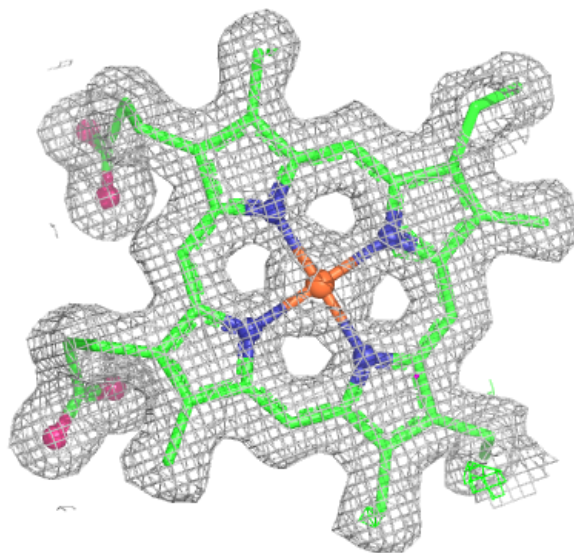
Electron density around HEC B 5:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



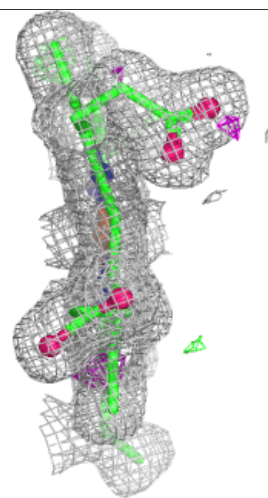
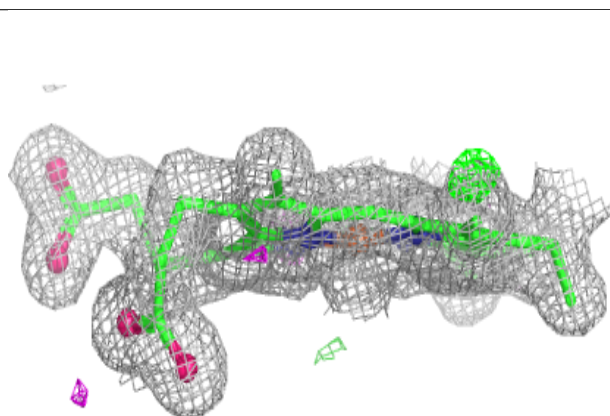
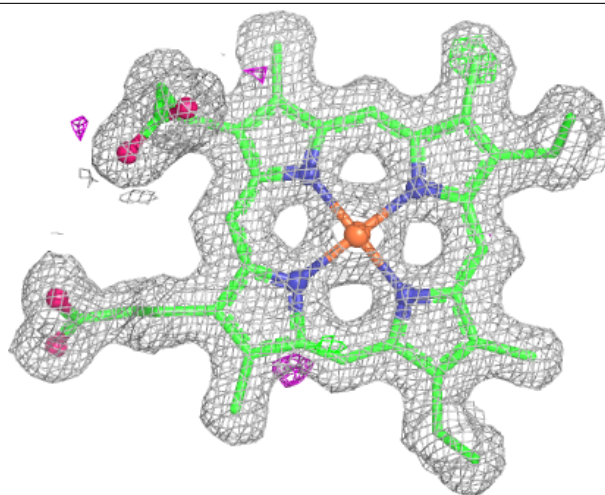
Electron density around HEC B 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



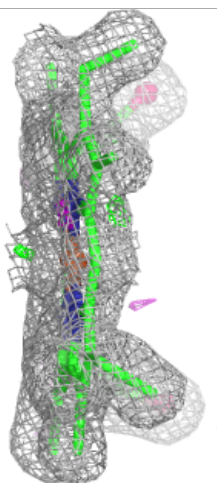
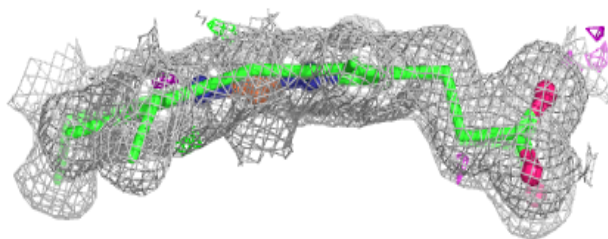
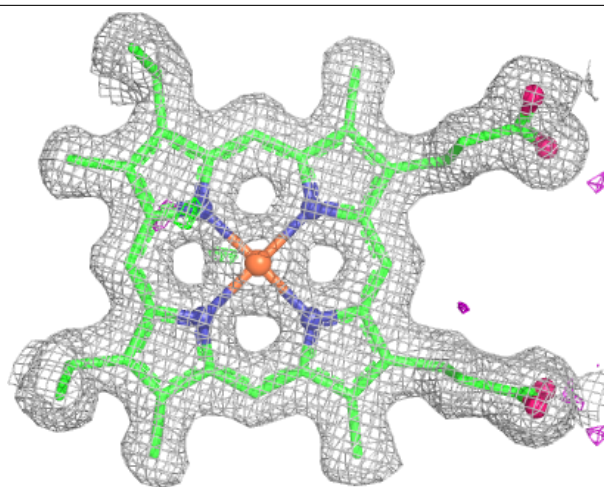
Electron density around HEC B 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



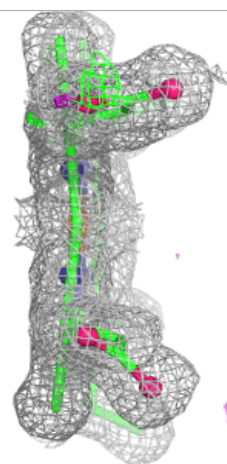
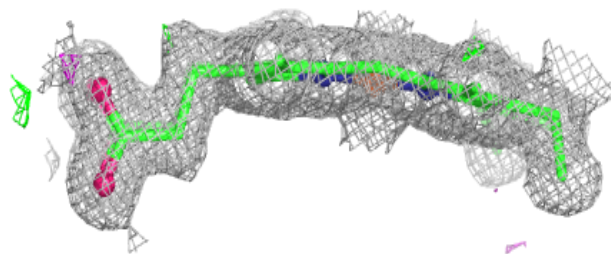
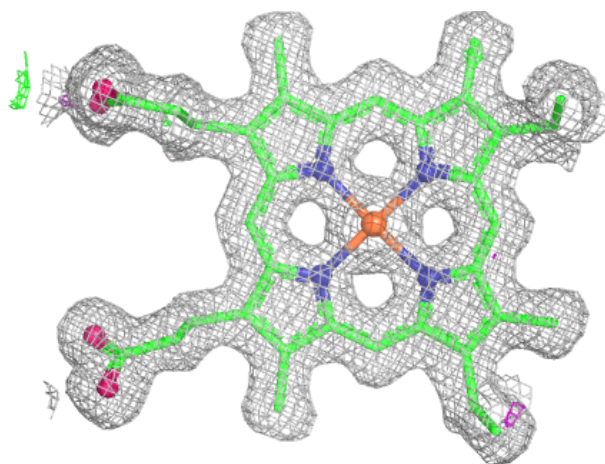
Electron density around HEC C 3:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



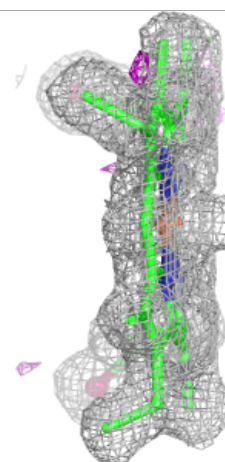
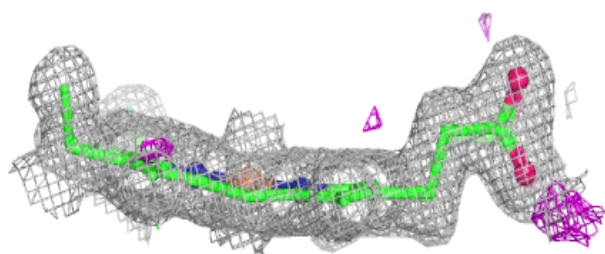
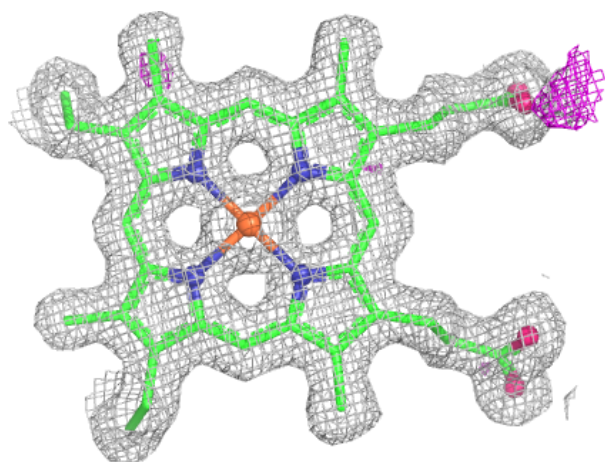
Electron density around HEC B 3:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



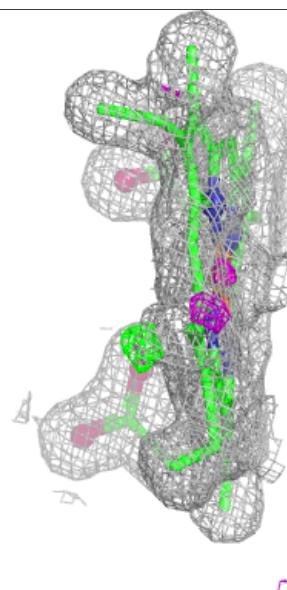
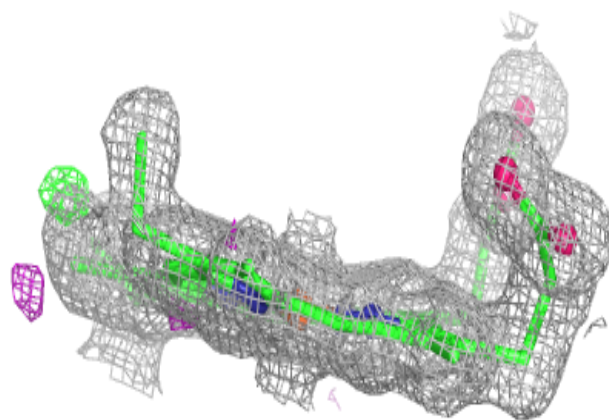
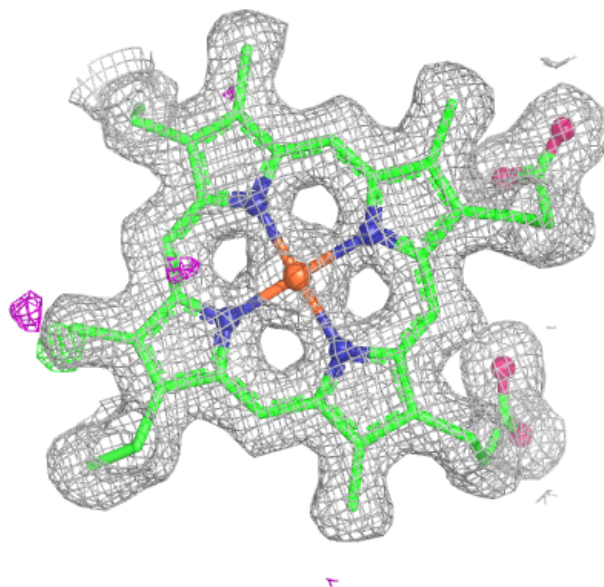
Electron density around HEC A 3:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.