Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2026 – 05:10 PM EDT

PDB ID	:	2CTH / pdb_00002cth
Title	:	CYTOCHROME C3 FROM DESULFOVIBRIO VULGARIS HILDENBOROUGH
Authors	:	Simoes, P.; Matias, P.M.; Morais, J.; Wilson, K.; Dauter, Z.; Carrondo, M.A.
Deposited on	:	1997-06-18
Resolution	:	1.67 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

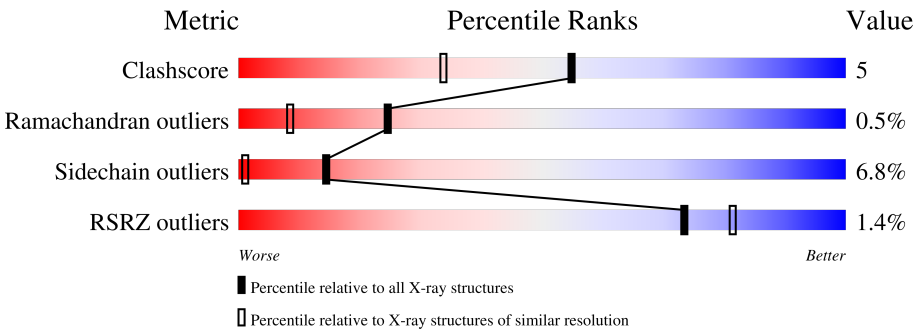
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.67 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	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	107	% 86% 10% •
1	B	107	2% 86% 9% 5%

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	109	X	-	-	-
2	HEC	A	110	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	111	X	-	-	-
2	HEC	A	112	X	-	-	-
2	HEC	B	109	X	-	-	-
2	HEC	B	110	X	-	-	-
2	HEC	B	111	X	-	-	-
2	HEC	B	112	X	-	-	-

2 Entry composition (i)

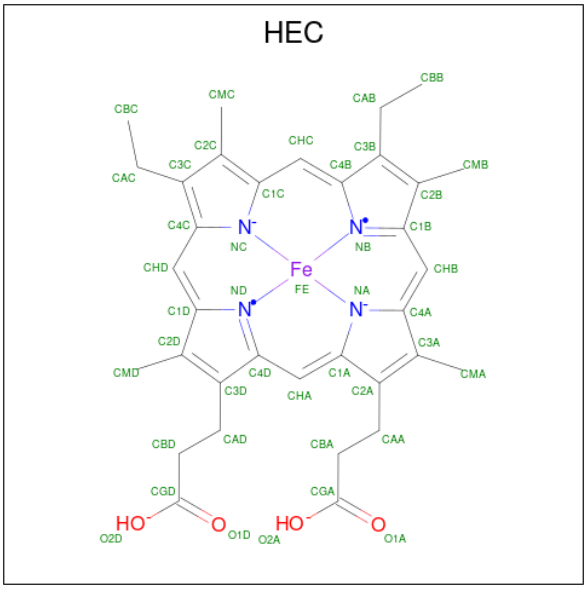
There are 3 unique types of molecules in this entry. The entry contains 2088 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	107	810	495	152	152	11	38	0	0
1	B	107	810	495	152	152	11	46	0	0

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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

- Molecule 3 is water.

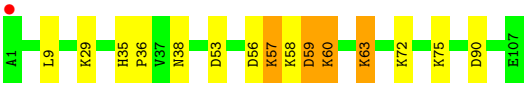
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	56	56	56	0	0
3	B	68	68	68	0	0

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 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.

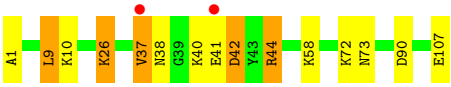
- Molecule 1: CYTOCHROME C3

Chain A:



- Molecule 1: CYTOCHROME C3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	77.30Å 77.30Å 77.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.67 8.00 – 1.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.67) 84.7 (8.00-1.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	SHELXL-93	Depositor
R, R_{free}	0.161 , 0.190 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 91.0	EDS
L-test for twinning[1]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2088	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	1.17	0/827	1.44	3/1101 (0.3%)
1	B	1.48	6/827 (0.7%)	1.58	7/1101 (0.6%)
All	All	1.33	6/1654 (0.4%)	1.51	10/2202 (0.5%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	VAL	C-N	-21.51	1.03	1.33
1	B	73	ASN	N-CA	8.55	1.57	1.46
1	B	72	LYS	CA-C	-6.37	1.44	1.52
1	B	42	ASP	N-CA	5.74	1.53	1.46
1	B	41	GLU	CA-C	5.44	1.59	1.52
1	B	10	LYS	N-CA	5.43	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	VAL	O-C-N	-15.10	108.06	122.71
1	B	72	LYS	O-C-N	-8.49	111.11	122.49
1	B	72	LYS	CA-C-N	-8.39	105.52	121.54
1	B	72	LYS	C-N-CA	-8.39	105.52	121.54
1	A	59	ASP	CA-CB-CG	6.77	119.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	LEU	CA-C-N	-5.26	115.46	122.72
1	B	9	LEU	C-N-CA	-5.26	115.46	122.72
1	A	72	LYS	CA-C-N	-5.08	114.46	122.08
1	A	72	LYS	C-N-CA	-5.08	114.46	122.08
1	B	72	LYS	N-CA-C	5.01	119.67	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	44	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	810	0	792	9	0
1	B	810	0	791	5	1
2	A	172	0	120	1	0
2	B	172	0	120	3	0
3	A	56	0	0	0	0
3	B	68	0	0	0	0
All	All	2088	0	1823	17	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (17) 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:53:ASP:OD1	1:A:63:LYS:HE3	1.88	0.73
1:A:53:ASP:OD1	1:A:63:LYS:CE	2.44	0.66
2:B:112:HEC:HBC3	2:B:112:HEC:HMC1	1.80	0.63
1:B:37:VAL:HG21	2:B:110:HEC:HBC2	1.82	0.61
2:A:112:HEC:HBC3	2:A:112:HEC:HMC1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:OD2	1:B:44:ARG:NH2	2.38	0.55
1:A:56:ASP:C	1:A:56:ASP:OD1	2.52	0.50
1:A:35:HIS:HB2	1:A:36:PRO:HD2	1.97	0.47
1:A:53:ASP:OD1	1:A:63:LYS:HE2	2.16	0.46
2:B:112:HEC:HBC3	2:B:112:HEC:CMC	2.47	0.45
1:A:9:LEU:HD23	1:A:9:LEU:C	2.42	0.45
1:B:37:VAL:HG12	1:B:42:ASP:HB2	1.99	0.43
1:B:26:LYS:HE2	1:B:26:LYS:HB2	1.46	0.43
1:A:59:ASP:O	1:A:60:LYS:HD3	2.20	0.42
1:B:90:ASP:OD1	1:B:90:ASP:C	2.63	0.41
1:A:57:LYS:HB3	1:A:57:LYS:HE3	1.87	0.41
1:A:90:ASP:OD1	1:A:90:ASP:C	2.64	0.41

All (1) 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)
1:B:1:ALA:CB	1:B:90:ASP:OD2[3_654]	2.17	0.03

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	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
1	B	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	12 2
All	All	210/214 (98%)	204 (97%)	5 (2%)	1 (0%)	24 8

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	ASN

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	88/88 (100%)	81 (92%)	7 (8%)	11 1
1	B	88/88 (100%)	83 (94%)	5 (6%)	18 2
All	All	176/176 (100%)	164 (93%)	12 (7%)	14 1

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	38	ASN
1	A	57	LYS
1	A	58	LYS
1	A	60	LYS
1	A	63	LYS
1	A	75	LYS
1	B	9	LEU
1	B	26	LYS
1	B	40	LYS
1	B	58	LYS
1	B	107	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	A	111	1	50,50,50	1.29	7 (14%)	68,82,82	1.05	5 (7%)
2	HEC	A	109	1	50,50,50	1.32	7 (14%)	68,82,82	1.24	8 (11%)
2	HEC	A	110	1	50,50,50	1.38	7 (14%)	68,82,82	1.13	7 (10%)
2	HEC	B	111	1	50,50,50	1.37	9 (18%)	68,82,82	1.14	8 (11%)
2	HEC	B	109	1	50,50,50	1.32	8 (16%)	68,82,82	1.00	4 (5%)
2	HEC	A	112	1	50,50,50	1.33	7 (14%)	68,82,82	1.11	7 (10%)
2	HEC	B	110	1	50,50,50	1.36	6 (12%)	68,82,82	1.28	7 (10%)
2	HEC	B	112	1	50,50,50	1.41	10 (20%)	68,82,82	1.25	9 (13%)

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	A	111	1	1/1/3/7	6/14/54/54	-
2	HEC	A	109	1	1/1/3/7	4/14/54/54	-
2	HEC	A	110	1	1/1/3/7	5/14/54/54	-
2	HEC	B	111	1	1/1/3/7	4/14/54/54	-
2	HEC	B	109	1	1/1/3/7	4/14/54/54	-
2	HEC	A	112	1	1/1/3/7	6/14/54/54	-
2	HEC	B	110	1	1/1/3/7	3/14/54/54	-
2	HEC	B	112	1	1/1/3/7	8/14/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	110	HEC	FE-NB	3.27	2.05	1.94
2	B	111	HEC	FE-NB	3.16	2.04	1.94
2	A	110	HEC	CBC-CAC	-2.96	1.38	1.51
2	B	109	HEC	FE-NB	2.95	2.04	1.94
2	B	110	HEC	FE-NB	2.90	2.03	1.94
2	B	111	HEC	CMB-C2B	2.87	1.56	1.50
2	A	109	HEC	FE-NB	2.84	2.03	1.94
2	B	110	HEC	CBC-CAC	-2.83	1.39	1.51
2	B	112	HEC	CAC-C3C	2.80	1.58	1.51
2	A	109	HEC	CMB-C2B	2.72	1.56	1.50
2	A	112	HEC	CMD-C2D	2.71	1.56	1.50
2	B	109	HEC	CBB-CAB	-2.69	1.40	1.51
2	A	111	HEC	FE-NB	2.66	2.03	1.94
2	A	109	HEC	C4B-C3B	2.62	1.49	1.45
2	B	112	HEC	CMB-C2B	2.58	1.56	1.50
2	B	112	HEC	CBC-CAC	-2.57	1.40	1.51
2	A	111	HEC	FE-NC	2.55	2.03	1.95
2	B	109	HEC	C4A-NA	-2.55	1.34	1.39
2	A	111	HEC	CBB-CAB	-2.53	1.40	1.51
2	A	112	HEC	CBC-CAC	-2.51	1.40	1.51
2	A	110	HEC	CMB-C2B	2.51	1.55	1.50
2	B	109	HEC	CMC-C2C	2.50	1.55	1.50
2	A	112	HEC	FE-NB	2.50	2.02	1.94
2	B	112	HEC	FE-NB	2.49	2.02	1.94
2	B	109	HEC	CMA-C3A	2.49	1.55	1.50
2	A	111	HEC	CMB-C2B	2.42	1.55	1.50
2	B	111	HEC	C4B-C3B	2.37	1.49	1.45
2	B	109	HEC	CMB-C2B	2.37	1.55	1.50
2	B	111	HEC	CMC-C2C	2.35	1.55	1.50
2	A	112	HEC	C3D-C2D	-2.33	1.31	1.36
2	A	111	HEC	CBC-CAC	-2.33	1.41	1.51
2	B	110	HEC	CBB-CAB	-2.31	1.41	1.51
2	B	110	HEC	CMA-C3A	2.28	1.55	1.50
2	A	110	HEC	CMC-C2C	2.28	1.55	1.50
2	B	111	HEC	FE-ND	2.26	2.01	1.94
2	B	112	HEC	FE-ND	2.25	2.01	1.94
2	B	109	HEC	CMD-C2D	2.25	1.55	1.50
2	A	110	HEC	CMA-C3A	2.22	1.55	1.50
2	A	112	HEC	FE-NC	2.21	2.02	1.95
2	B	109	HEC	FE-NC	2.20	2.02	1.95
2	A	111	HEC	CMC-C2C	2.20	1.55	1.50
2	B	110	HEC	CAA-C2A	2.20	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	HEC	CAA-C2A	2.18	1.56	1.51
2	A	112	HEC	CMC-C2C	2.17	1.55	1.50
2	A	112	HEC	C3C-C2C	-2.17	1.33	1.38
2	A	109	HEC	CMD-C2D	2.17	1.55	1.50
2	A	110	HEC	FE-ND	2.12	2.01	1.94
2	B	112	HEC	CMD-C2D	2.12	1.55	1.50
2	B	111	HEC	CAD-C3D	2.11	1.56	1.51
2	A	111	HEC	CMA-C3A	2.11	1.55	1.50
2	A	109	HEC	FE-ND	2.11	2.01	1.94
2	B	111	HEC	CMA-C3A	2.11	1.55	1.50
2	B	110	HEC	CMB-C2B	2.10	1.55	1.50
2	B	111	HEC	CMD-C2D	2.09	1.55	1.50
2	A	109	HEC	CMC-C2C	2.07	1.55	1.50
2	A	110	HEC	C3C-C2C	-2.06	1.33	1.38
2	B	112	HEC	CMA-C3A	2.05	1.55	1.50
2	B	112	HEC	C4B-C3B	2.03	1.48	1.45
2	B	112	HEC	FE-NA	2.02	2.01	1.95
2	A	109	HEC	CBB-CAB	-2.02	1.43	1.51
2	B	111	HEC	C1D-ND	-2.01	1.36	1.40

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	109	HEC	CAB-C3B-C2B	3.47	133.93	127.56
2	A	109	HEC	CAB-C3B-C4B	-3.30	120.50	124.79
2	A	109	HEC	CMB-C2B-C1B	-3.17	120.08	125.03
2	B	111	HEC	C1B-C2B-C3B	3.15	110.29	106.98
2	B	110	HEC	O2A-CGA-O1A	3.04	131.15	123.33
2	B	110	HEC	O1A-CGA-CBA	-3.04	113.46	123.09
2	B	112	HEC	C1D-ND-C4D	2.88	108.62	105.21
2	B	112	HEC	CHD-C1D-ND	2.87	127.92	124.37
2	B	112	HEC	C3D-C4D-ND	-2.70	107.74	110.35
2	B	112	HEC	CMB-C2B-C1B	-2.67	120.85	125.03
2	A	109	HEC	C1B-C2B-C3B	2.65	109.77	106.98
2	B	110	HEC	C3D-C4D-ND	-2.62	107.82	110.35
2	B	109	HEC	CMB-C2B-C1B	-2.57	121.02	125.03
2	A	112	HEC	CAB-C3B-C2B	2.55	132.25	127.56
2	A	109	HEC	CAC-C3C-C2C	2.55	130.93	126.89
2	A	109	HEC	O1A-CGA-CBA	-2.53	115.06	123.09
2	A	111	HEC	C3D-C4D-ND	-2.52	107.91	110.35
2	B	110	HEC	C1D-ND-C4D	2.52	108.19	105.21
2	A	111	HEC	O1A-CGA-CBA	-2.47	115.27	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	110	HEC	CMC-C2C-C1C	-2.46	121.67	125.42
2	A	112	HEC	CMC-C2C-C1C	-2.44	121.70	125.42
2	A	110	HEC	O1A-CGA-CBA	-2.39	115.50	123.09
2	A	110	HEC	CMB-C2B-C1B	-2.39	121.31	125.03
2	B	109	HEC	C1B-C2B-C3B	2.37	109.47	106.98
2	B	110	HEC	CAC-C3C-C2C	2.36	130.62	126.89
2	A	111	HEC	CHD-C1D-ND	2.31	127.22	124.37
2	B	112	HEC	C2D-C1D-ND	-2.27	107.23	109.84
2	B	111	HEC	CAB-C3B-C2B	2.25	131.68	127.56
2	A	112	HEC	CMC-C2C-C3C	2.24	130.38	125.62
2	A	109	HEC	O2D-CGD-O1D	2.22	129.03	123.33
2	B	110	HEC	O1D-CGD-CBD	-2.21	116.07	123.09
2	B	112	HEC	O1D-CGD-CBD	-2.20	116.12	123.09
2	B	112	HEC	CAB-C3B-C4B	-2.20	121.93	124.79
2	A	112	HEC	CAB-C3B-C4B	-2.18	121.95	124.79
2	B	111	HEC	O1A-CGA-CBA	-2.18	116.18	123.09
2	B	111	HEC	CHD-C1D-ND	2.17	127.06	124.37
2	B	112	HEC	CAB-C3B-C2B	2.17	131.55	127.56
2	A	110	HEC	CMC-C2C-C3C	2.17	130.23	125.62
2	A	110	HEC	O2A-CGA-O1A	2.17	128.91	123.33
2	B	112	HEC	CHA-C4D-ND	2.16	126.75	124.42
2	A	111	HEC	O2A-CGA-O1A	2.12	128.80	123.33
2	A	110	HEC	C1B-C2B-C3B	2.12	109.21	106.98
2	B	111	HEC	C3D-C4D-ND	-2.11	108.31	110.35
2	B	111	HEC	C1D-ND-C4D	2.11	107.70	105.21
2	A	110	HEC	C3D-C4D-ND	-2.07	108.35	110.35
2	B	109	HEC	C2A-C1A-NA	-2.06	108.33	110.32
2	B	111	HEC	O2A-CGA-O1A	2.04	128.59	123.33
2	A	112	HEC	C3D-C4D-ND	-2.03	108.39	110.35
2	A	112	HEC	O1A-CGA-CBA	-2.03	116.65	123.09
2	A	111	HEC	C1D-ND-C4D	2.03	107.61	105.21
2	B	110	HEC	CHC-C4B-NB	-2.03	121.86	124.37
2	A	109	HEC	O1D-CGD-CBD	-2.02	116.69	123.09
2	B	109	HEC	C1C-C2C-C3C	2.02	109.13	106.82
2	A	112	HEC	O1D-CGD-CBD	-2.02	116.69	123.09
2	B	111	HEC	CBA-CAA-C2A	2.01	118.09	112.53

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	109	HEC	NA
2	A	110	HEC	NA

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Mol	Chain	Res	Type	Atom
2	A	111	HEC	NA
2	A	112	HEC	NA
2	B	109	HEC	NA
2	B	110	HEC	NA
2	B	111	HEC	NA
2	B	112	HEC	NA

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	112	HEC	C2C-C3C-CAC-CBC
2	A	112	HEC	C2C-C3C-CAC-CBC
2	A	112	HEC	C4C-C3C-CAC-CBC
2	B	112	HEC	C4C-C3C-CAC-CBC
2	A	111	HEC	C2B-C3B-CAB-CBB
2	B	112	HEC	C2B-C3B-CAB-CBB
2	B	111	HEC	C2B-C3B-CAB-CBB
2	A	112	HEC	C2B-C3B-CAB-CBB
2	B	109	HEC	C2C-C3C-CAC-CBC
2	A	109	HEC	C2C-C3C-CAC-CBC
2	B	111	HEC	C2C-C3C-CAC-CBC
2	A	111	HEC	C2C-C3C-CAC-CBC
2	A	110	HEC	C3D-CAD-CBD-CGD
2	A	110	HEC	C2B-C3B-CAB-CBB
2	B	110	HEC	C2B-C3B-CAB-CBB
2	A	111	HEC	C4C-C3C-CAC-CBC
2	B	111	HEC	C4C-C3C-CAC-CBC
2	B	112	HEC	C4B-C3B-CAB-CBB
2	A	112	HEC	C4B-C3B-CAB-CBB
2	B	109	HEC	CAD-CBD-CGD-O2D
2	B	109	HEC	CAD-CBD-CGD-O1D
2	B	109	HEC	C4C-C3C-CAC-CBC
2	A	112	HEC	CAA-CBA-CGA-O2A
2	A	112	HEC	CAA-CBA-CGA-O1A
2	A	109	HEC	C4C-C3C-CAC-CBC
2	B	112	HEC	CAA-CBA-CGA-O2A
2	A	109	HEC	CAD-CBD-CGD-O2D
2	A	110	HEC	CAD-CBD-CGD-O2D
2	B	112	HEC	CAD-CBD-CGD-O2D
2	A	110	HEC	CAD-CBD-CGD-O1D
2	A	111	HEC	CAA-CBA-CGA-O2A
2	A	111	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	110	HEC	C2C-C3C-CAC-CBC
2	A	109	HEC	CAD-CBD-CGD-O1D
2	B	112	HEC	CAA-CBA-CGA-O1A
2	B	112	HEC	CAD-CBD-CGD-O1D
2	B	110	HEC	CAD-CBD-CGD-O2D
2	A	111	HEC	CAA-CBA-CGA-O1A
2	A	110	HEC	C4B-C3B-CAB-CBB
2	B	111	HEC	C4B-C3B-CAB-CBB

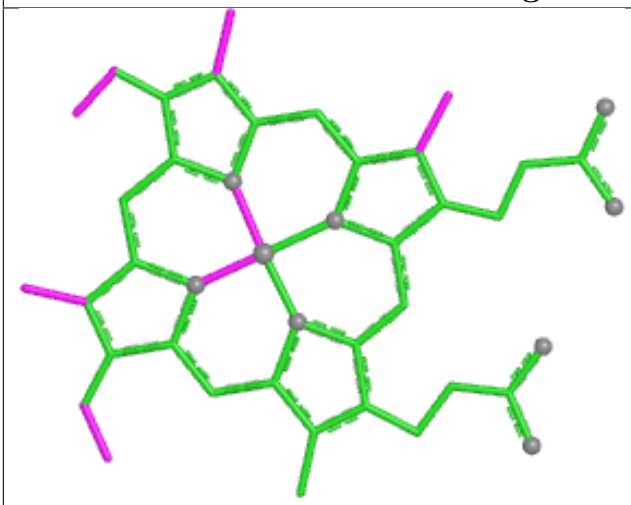
There are no ring outliers.

3 monomers are involved in 4 short contacts:

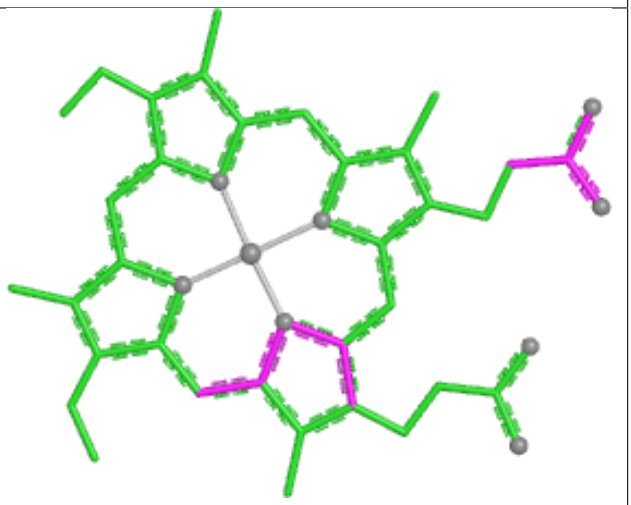
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	112	HEC	1	0
2	B	110	HEC	1	0
2	B	112	HEC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

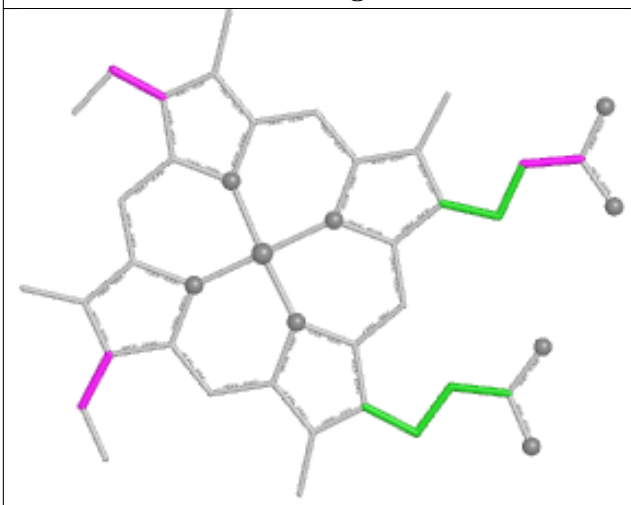
Ligand HEC A 111



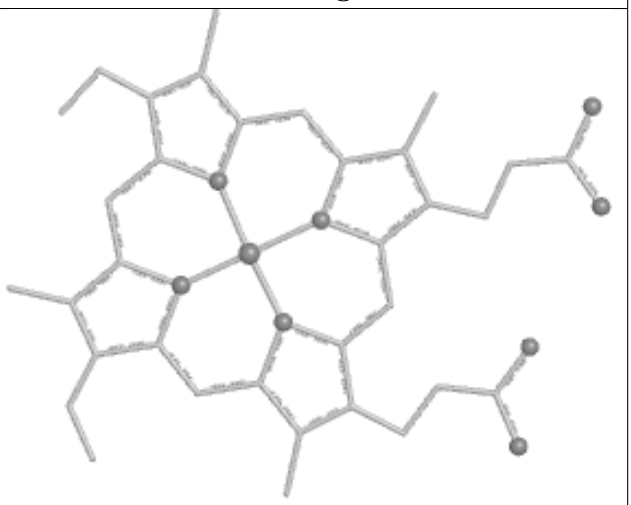
Bond lengths



Bond angles

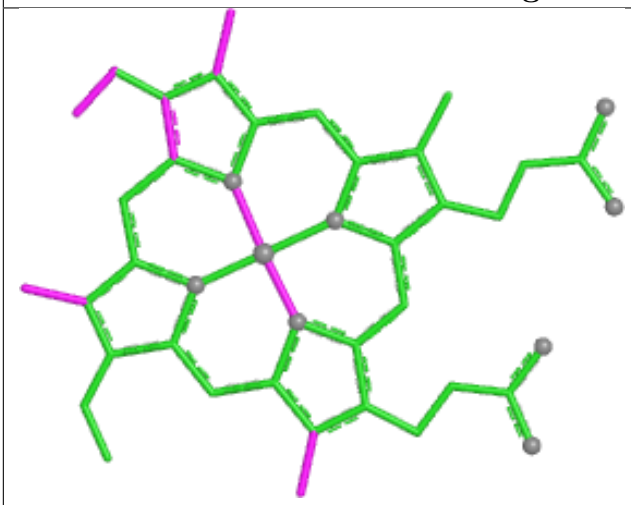


Torsions



Rings

Ligand HEC A 109



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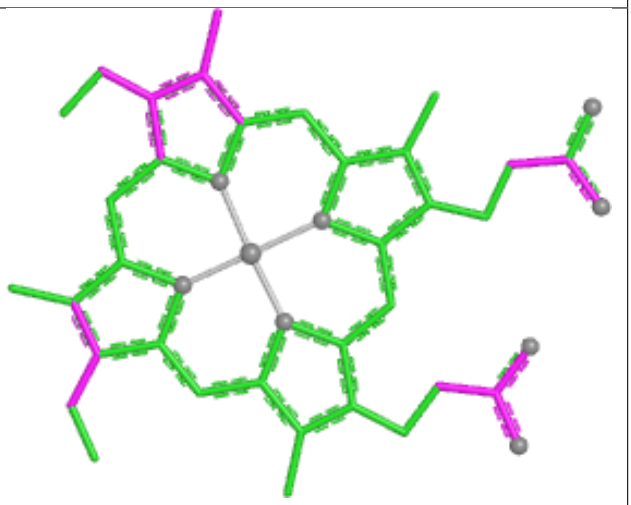

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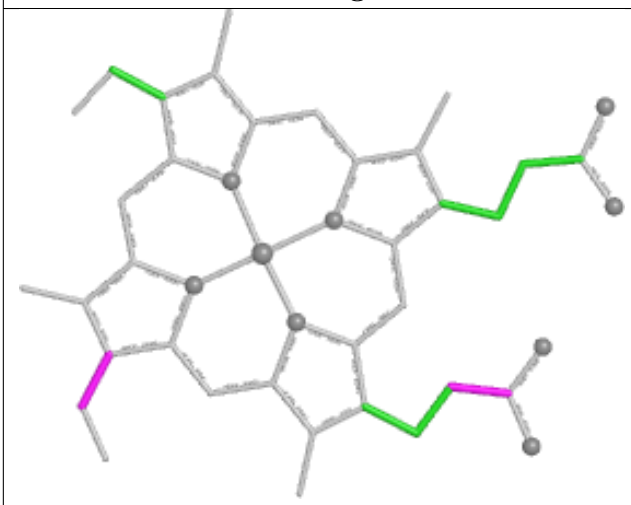

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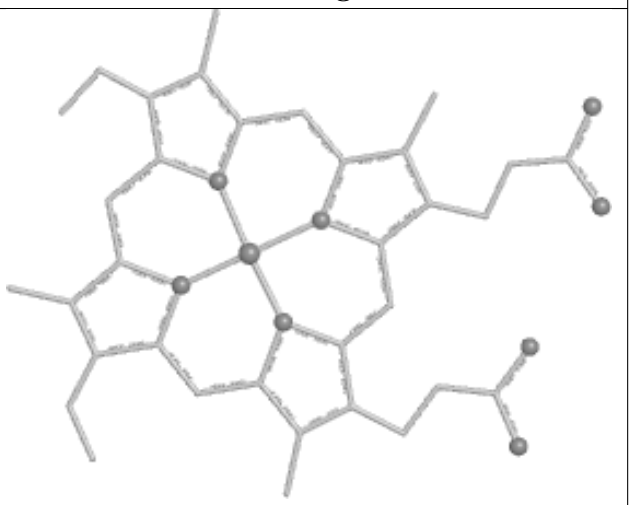
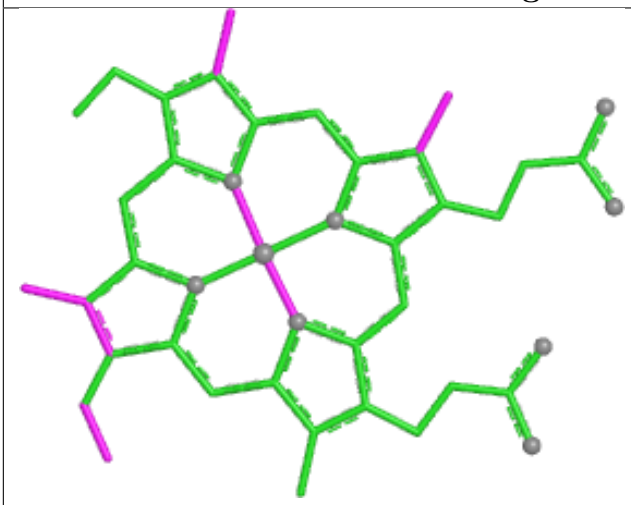
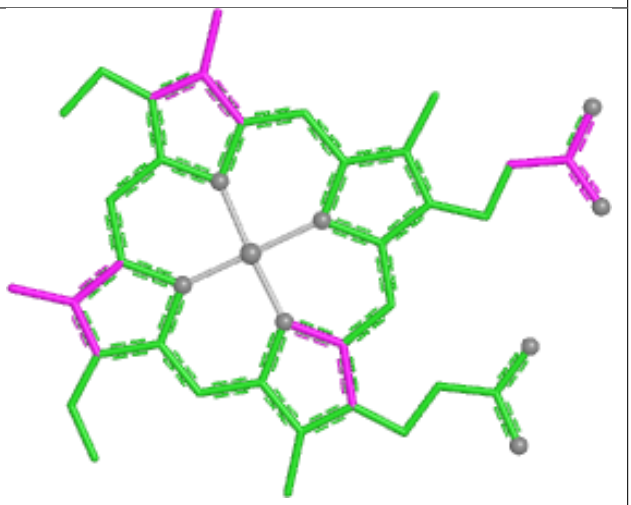


Rings

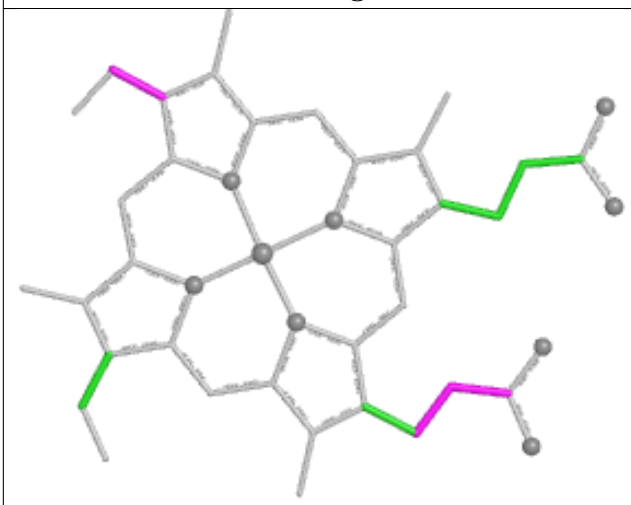
Ligand HEC A 110



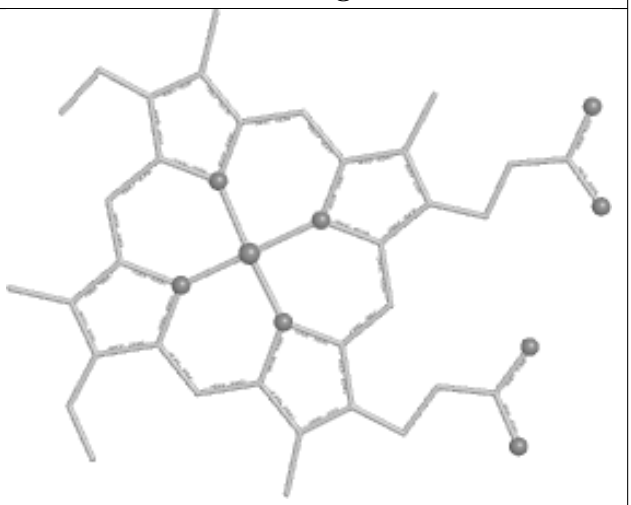
Bond lengths



Bond angles

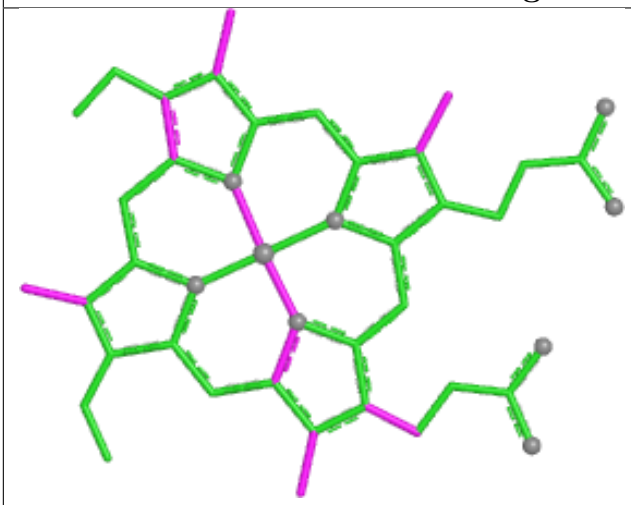


Torsions

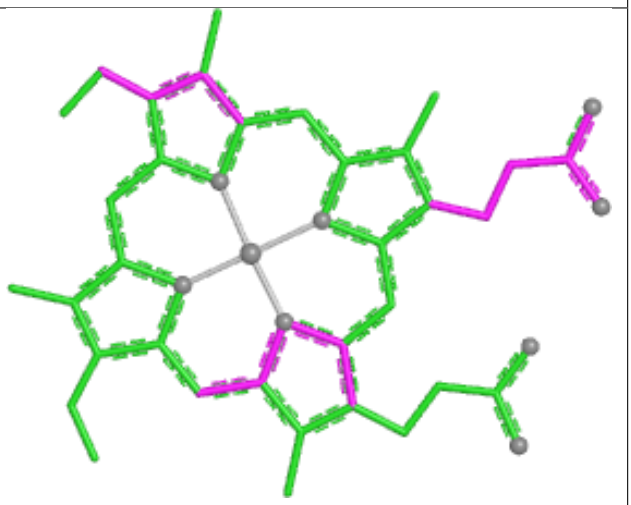


Rings

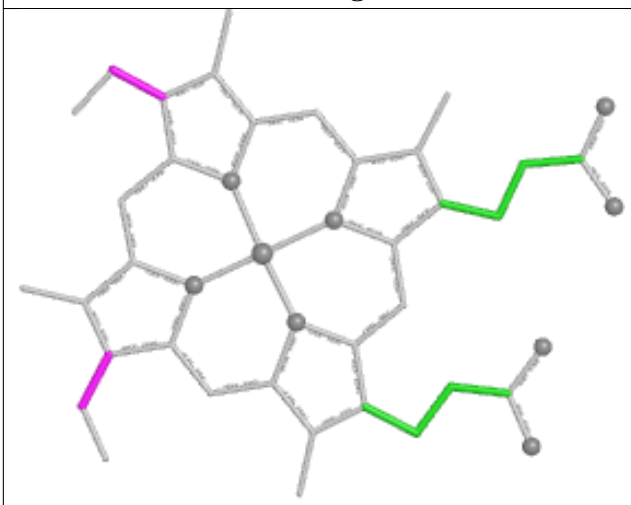
Ligand HEC B 111



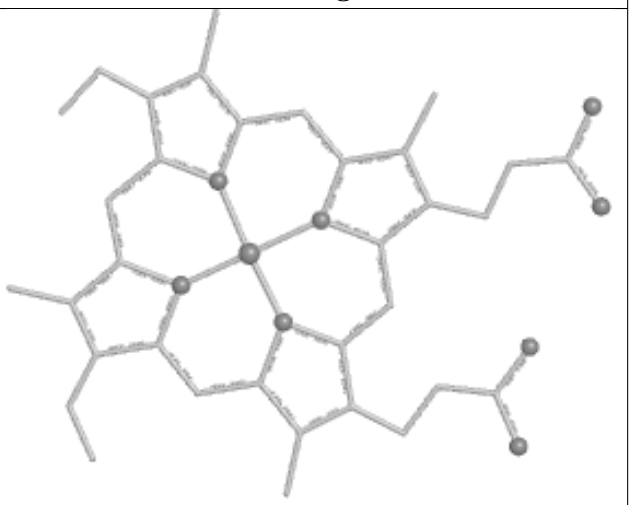
Bond lengths



Bond angles

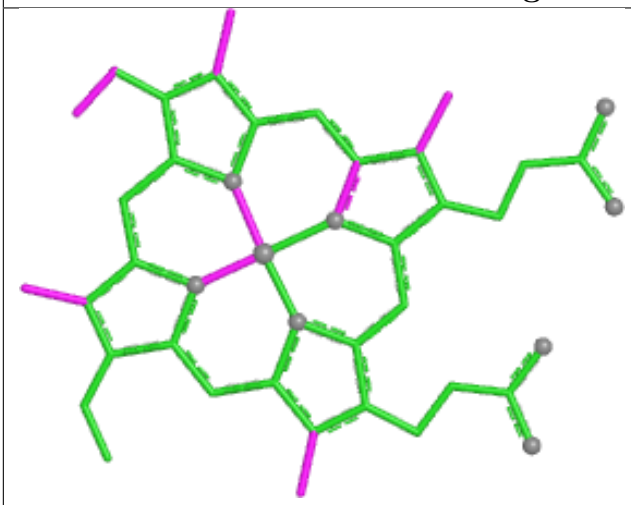


Torsions

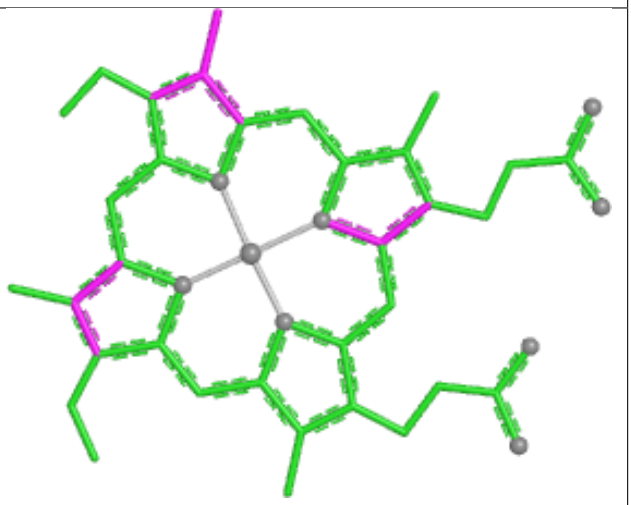


Rings

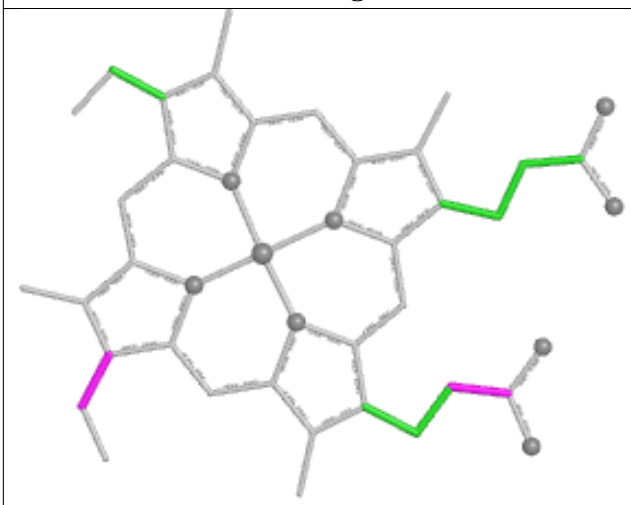
Ligand HEC B 109



Bond lengths



Bond angles



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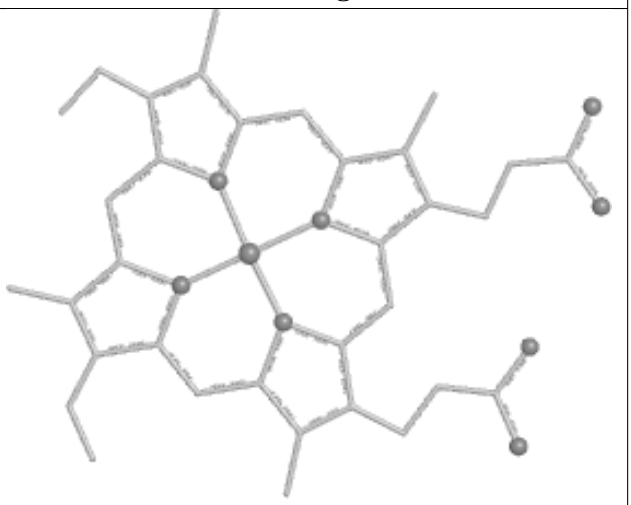
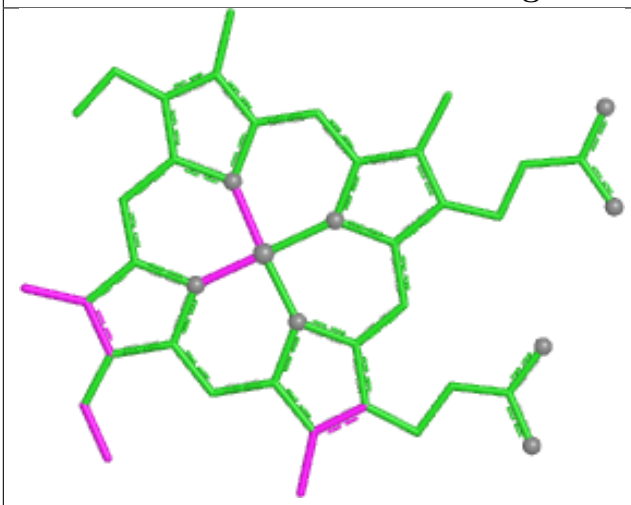
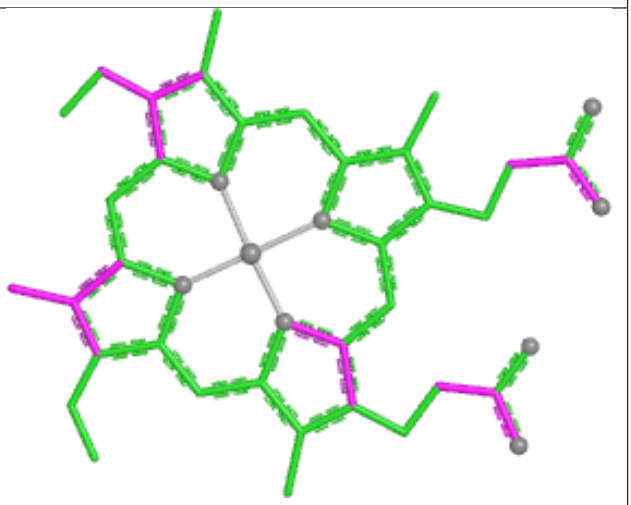


Rings

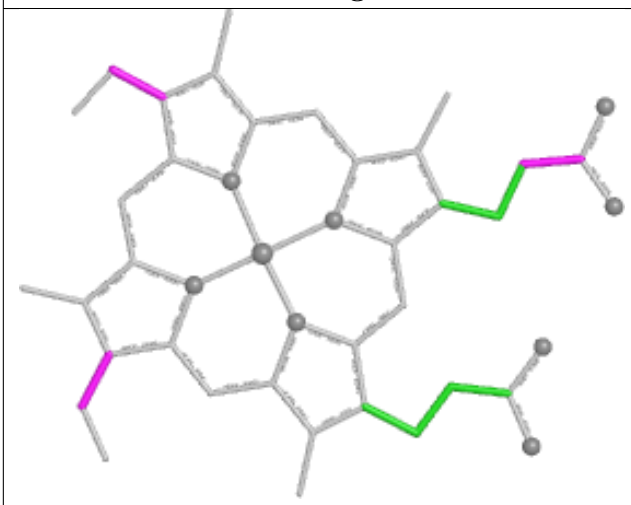
Ligand HEC A 112



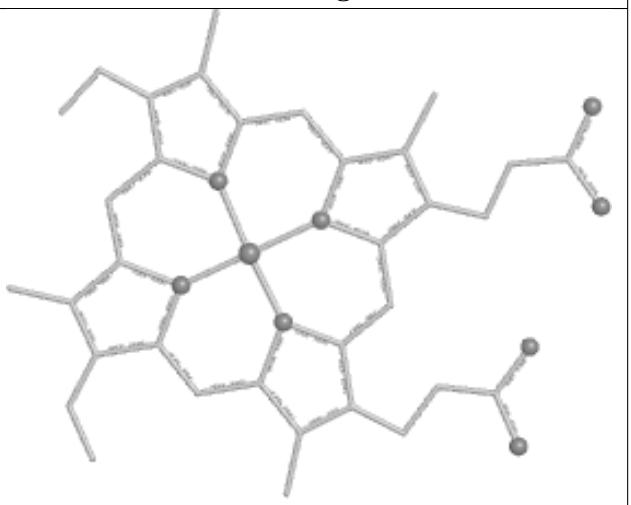
Bond lengths



Bond angles

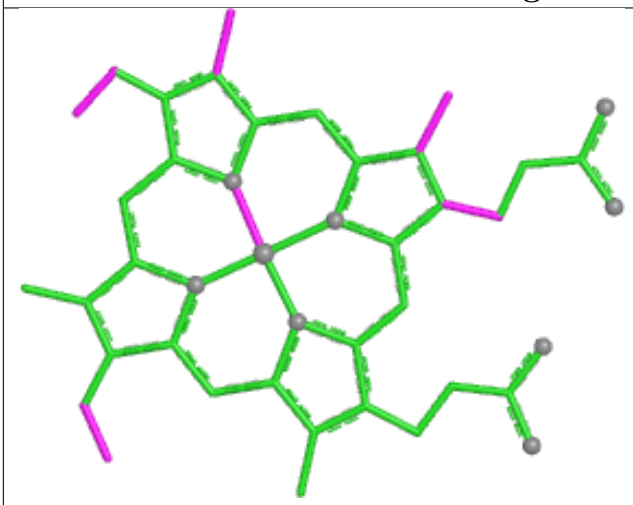


Torsions

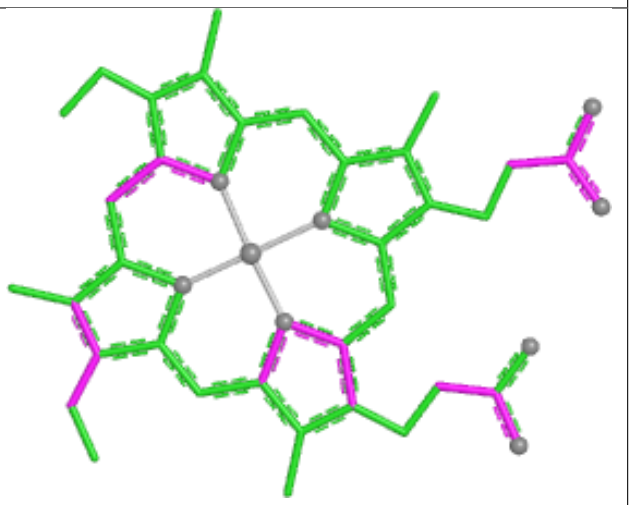


Rings

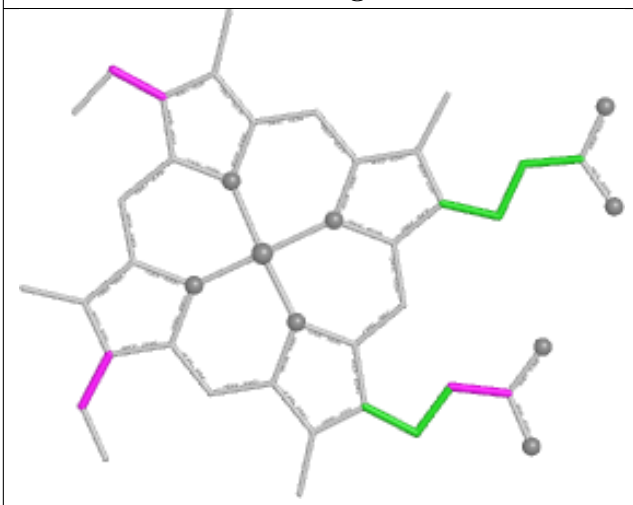
Ligand HEC B 110



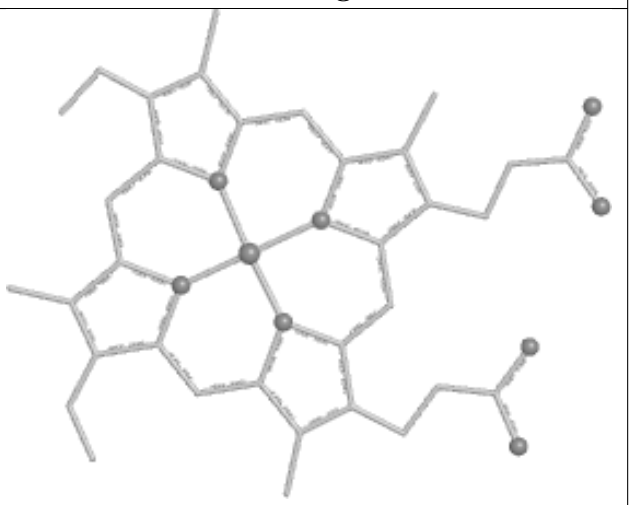
Bond lengths



Bond angles

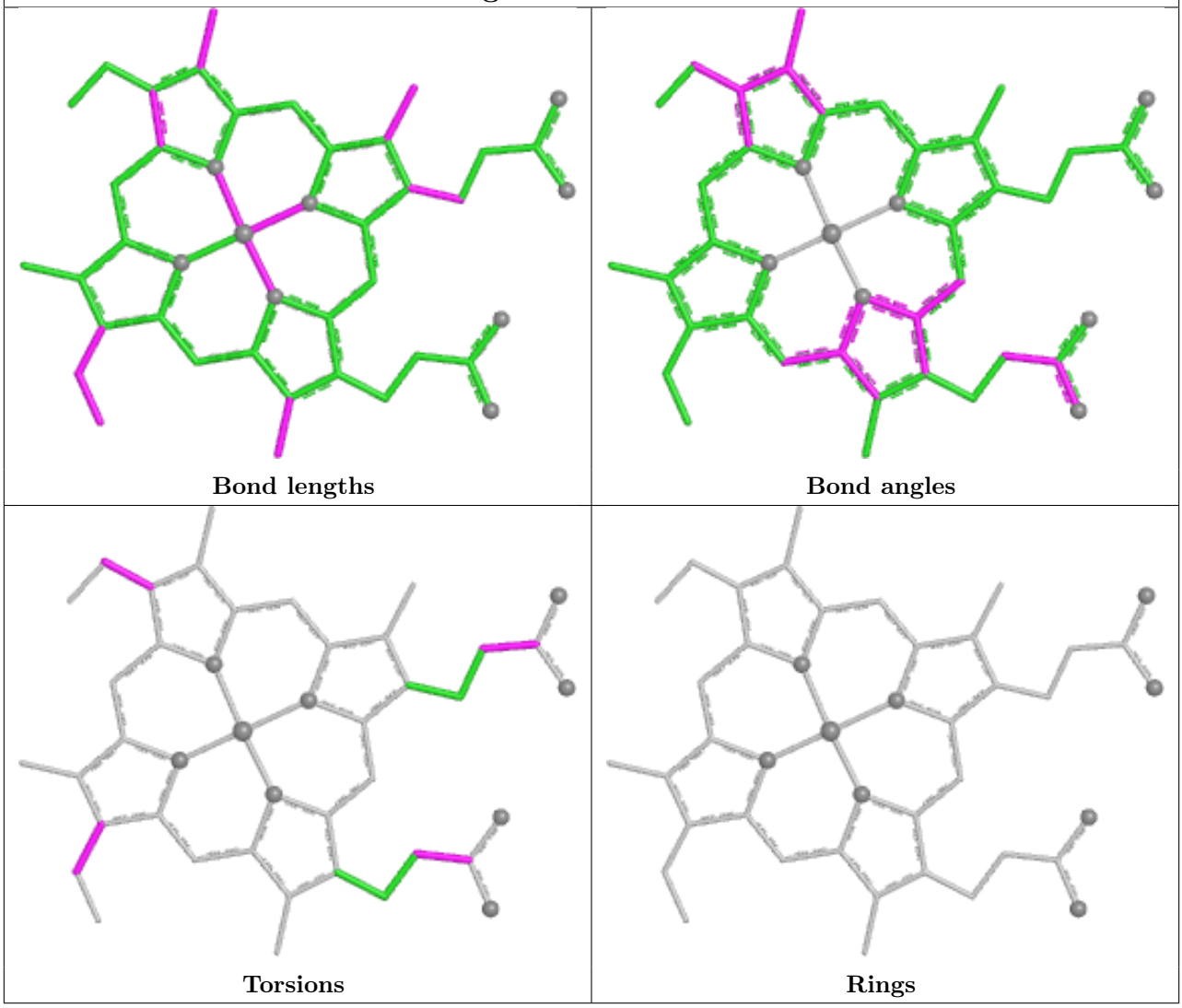


Torsions



Rings

Ligand HEC B 112



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	37:VAL	C	38:ASN	N	1.03

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	107/107 (100%)	-0.57	1 (0%)	81	88	14, 21, 37, 43	13 (12%)
1	B	107/107 (100%)	-0.38	2 (1%)	66	74	14, 23, 39, 58	16 (14%)
All	All	214/214 (100%)	-0.47	3 (1%)	73	81	14, 22, 39, 58	29 (13%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	GLU	2.3
1	A	1	ALA	2.2
1	B	37	VAL	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 (i)

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
2	HEC	A	110	43/43	0.98	0.05	16,21,32,32	3
2	HEC	A	111	43/43	0.98	0.05	11,18,32,42	0

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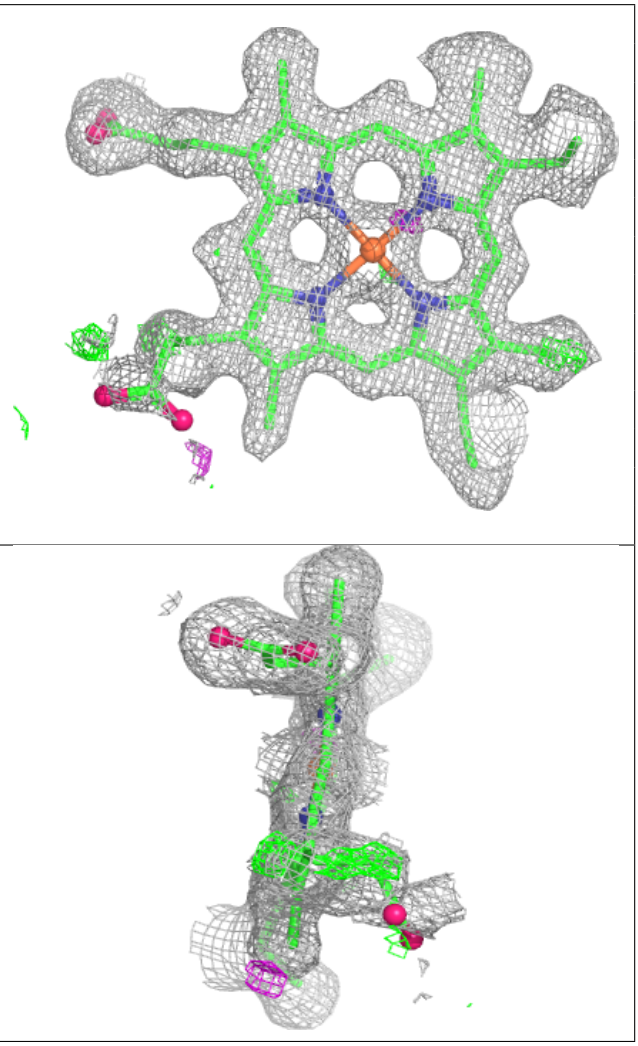
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	B	110	43/43	0.98	0.05	15,20,38,45	0
2	HEC	B	111	43/43	0.98	0.05	12,17,37,53	0
2	HEC	B	112	43/43	0.98	0.05	13,18,34,60	0
2	HEC	A	109	43/43	0.99	0.05	11,14,22,29	0
2	HEC	A	112	43/43	0.99	0.05	11,16,38,68	0
2	HEC	B	109	43/43	0.99	0.04	10,14,22,33	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.

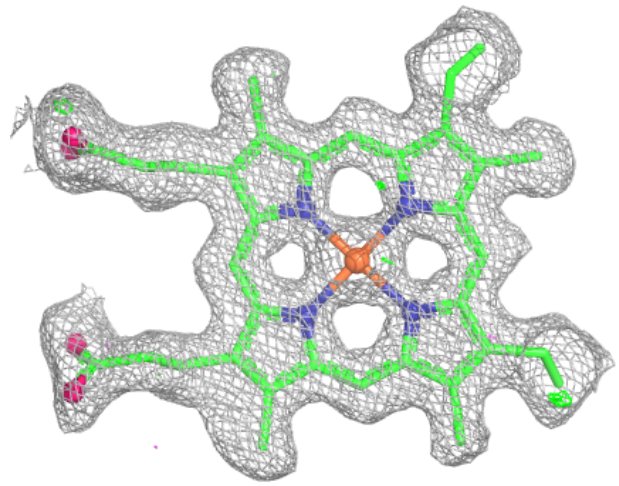
Electron density around HEC A 110:

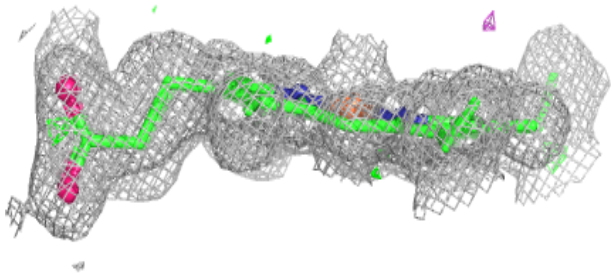
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

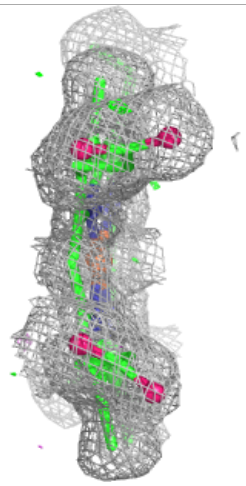


Electron density around HEC A 111:

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

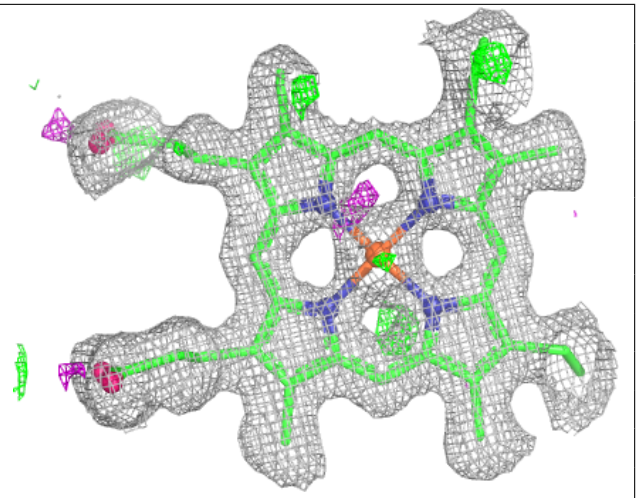


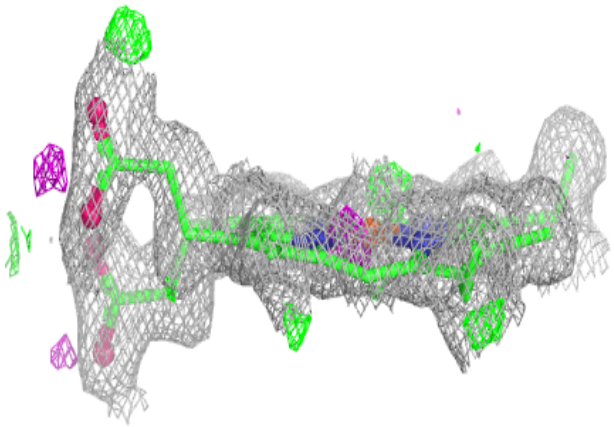




Electron density around HEC B 110:

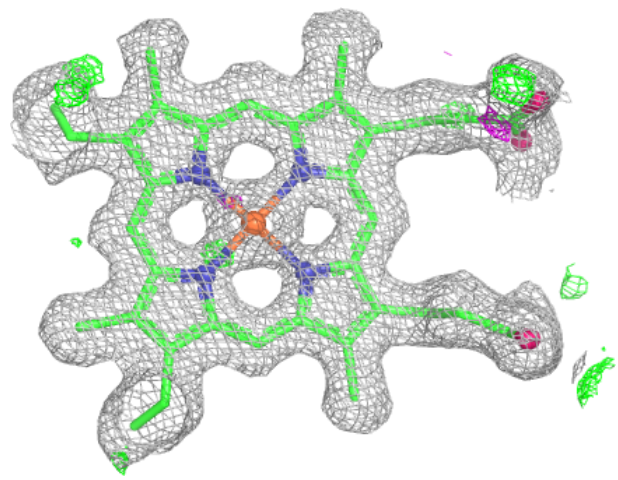
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

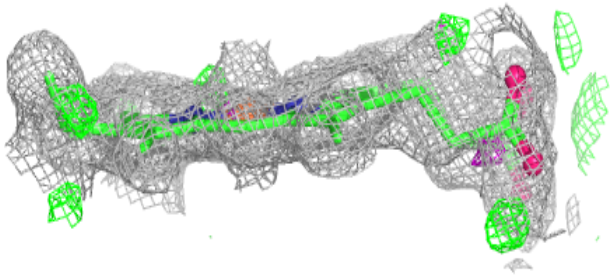


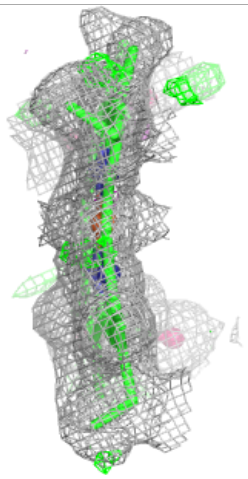


Electron density around HEC B 111:

$2mF_o$-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 112:

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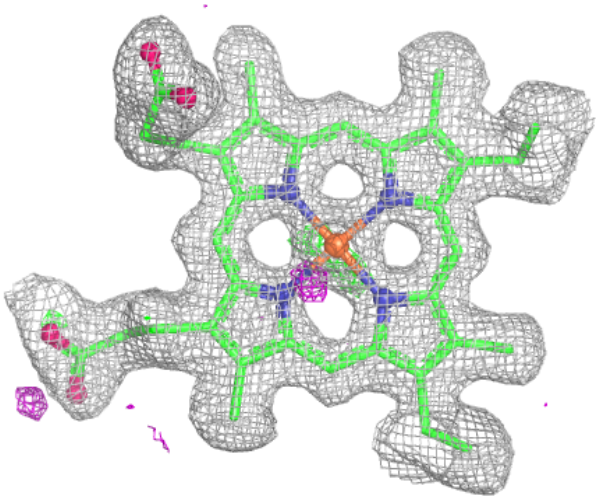
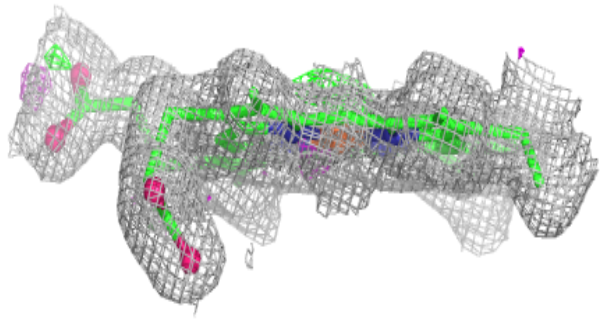
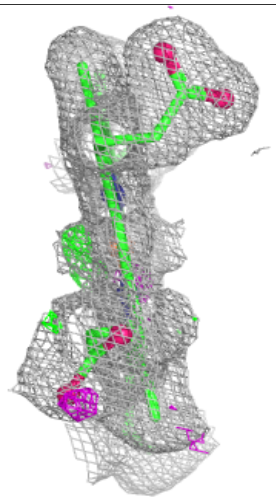
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

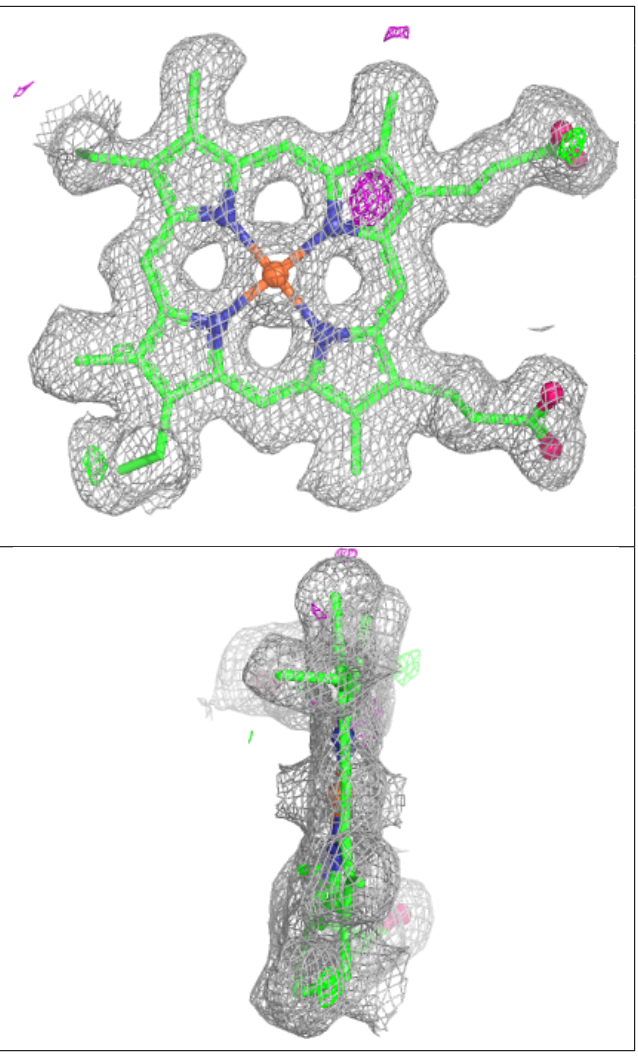






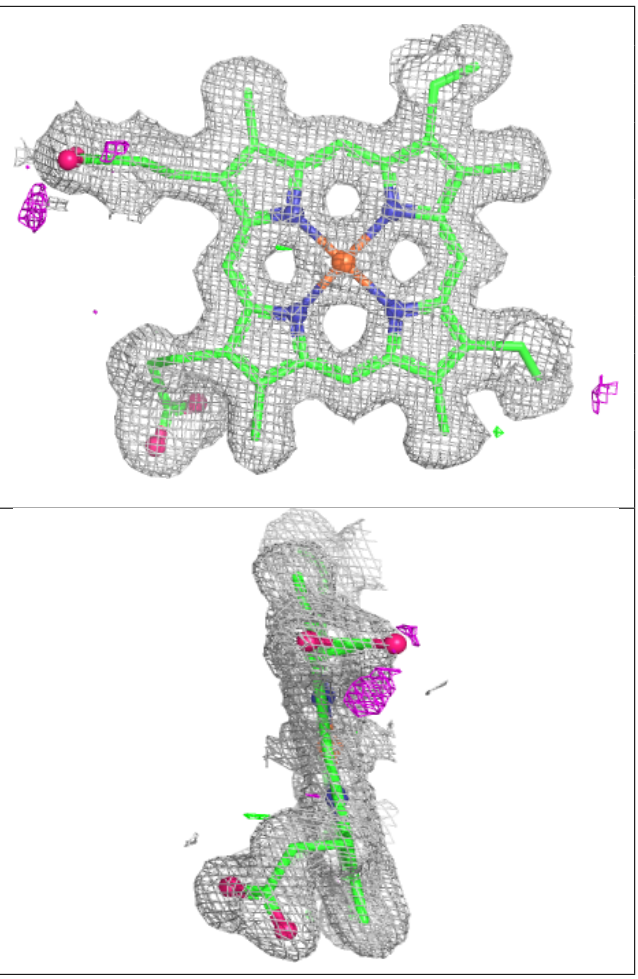
Electron density around HEC A 109:

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



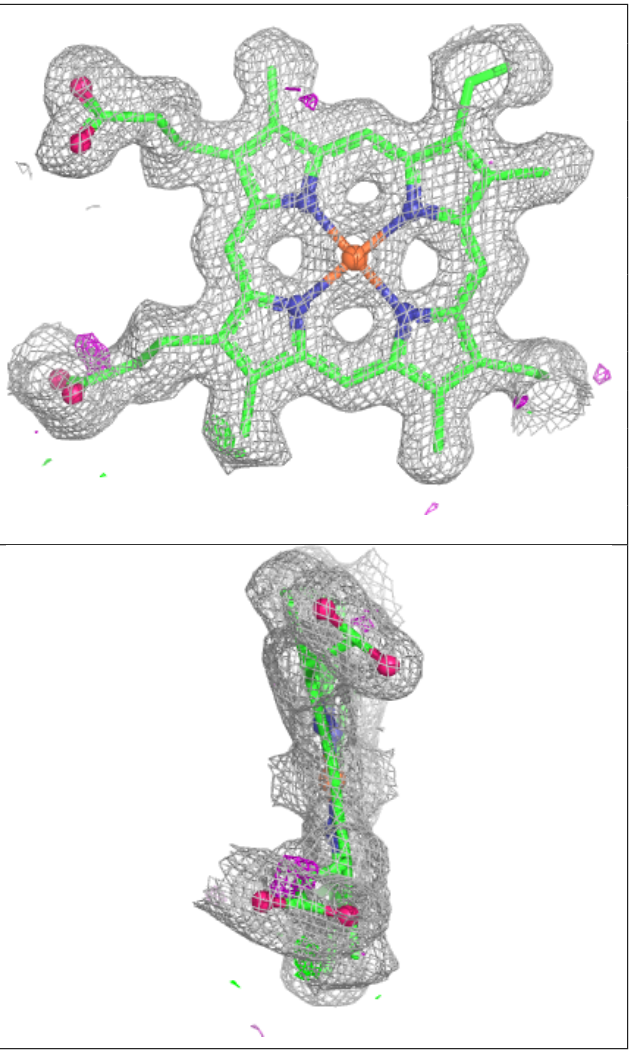
Electron density around HEC A 112:

$2mF_o$-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 109:

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 (i)

There are no such residues in this entry.