Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 11:02 PM EDT

PDB ID	:	3L1T
Title	:	E. coli NrfA sulfite ocmplex
Authors	:	Clarke, T.A.; Hemmings, A.M.; Butt, J.N.
Deposited on	:	2009-12-14
Resolution	:	2.30 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:

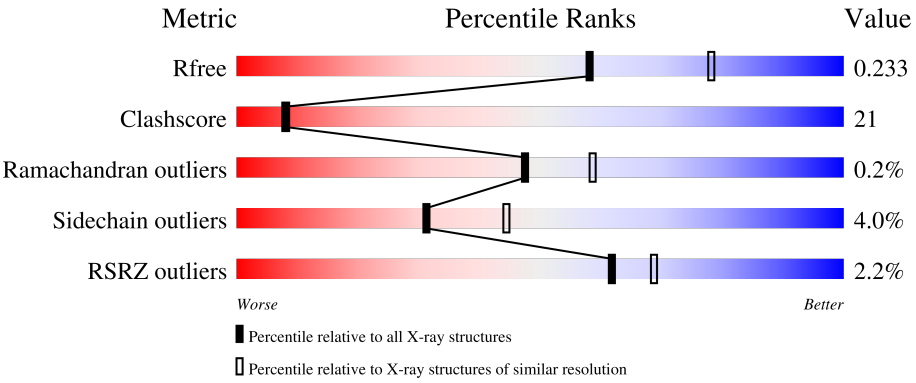
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	452	4% 71% 23%
1	B	452	78% 18%
1	C	452	77% 19%
1	D	452	4% 61% 33%

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
5	EDO	B	483	-	-	X	-
5	EDO	C	9	-	-	X	-
5	EDO	D	482	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15858 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.

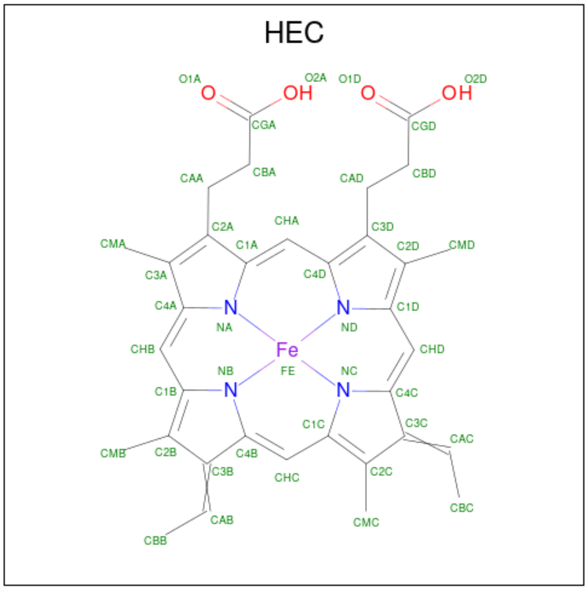
- Molecule 1 is a protein called Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	1	1	0
			3485	2183	620	660	22			
1	B	441	Total	C	N	O	S	0	2	0
			3491	2188	622	659	22			
1	C	441	Total	C	N	O	S	1	4	0
			3502	2195	621	664	22			
1	D	441	Total	C	N	O	S	0	2	0
			3487	2185	619	661	22			

- Molecule 2 is CALCIUM ION (three-letter code: 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 (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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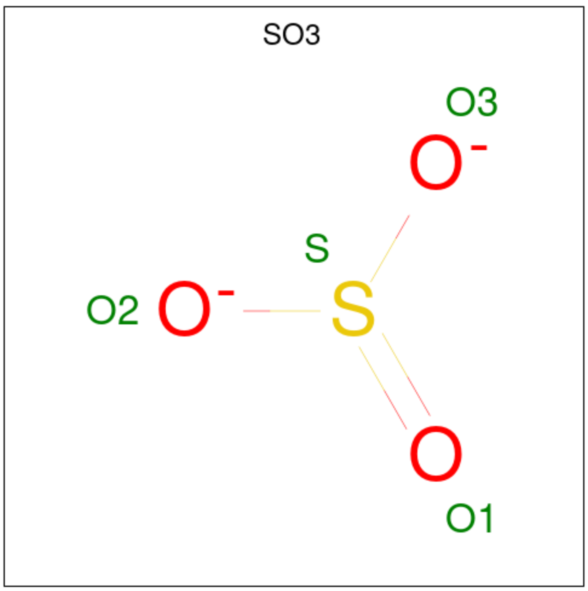
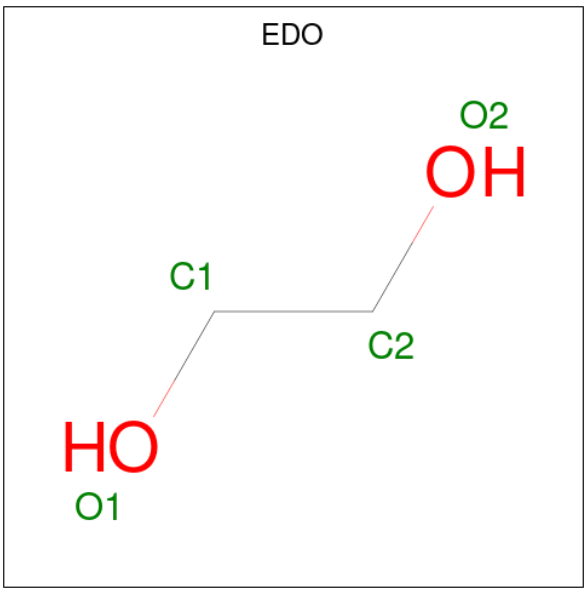
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

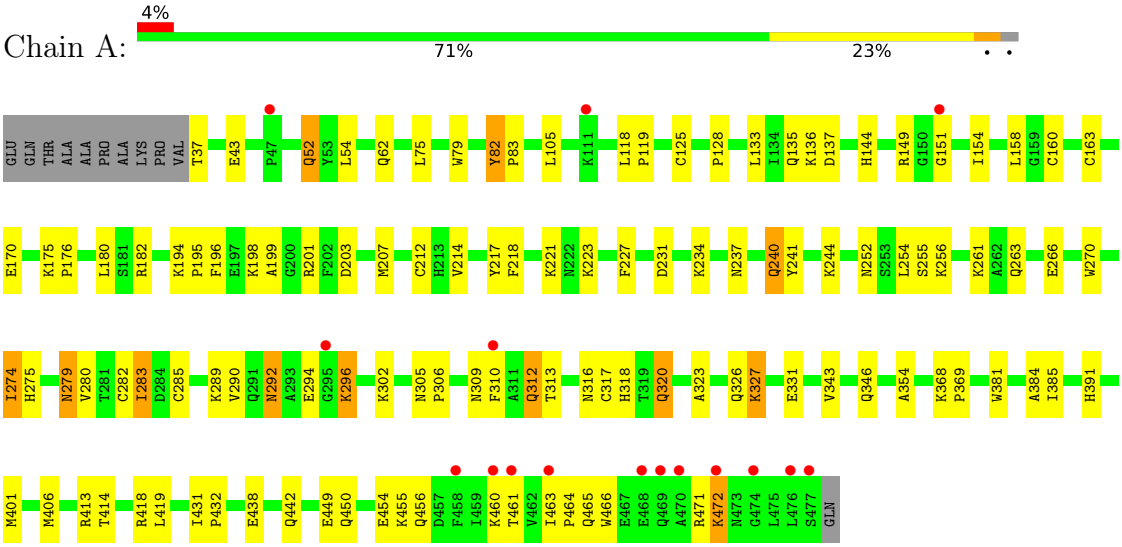
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	222	Total O 222 222	0	0
6	B	291	Total O 291 291	0	0
6	C	292	Total O 292 292	0	0
6	D	152	Total O 152 152	0	0

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.

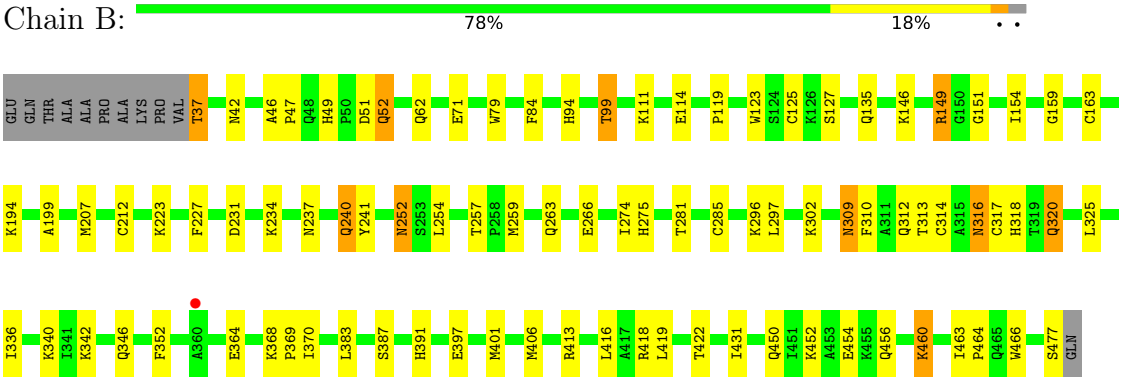
• Molecule 1: Cytochrome c-552

Chain A:



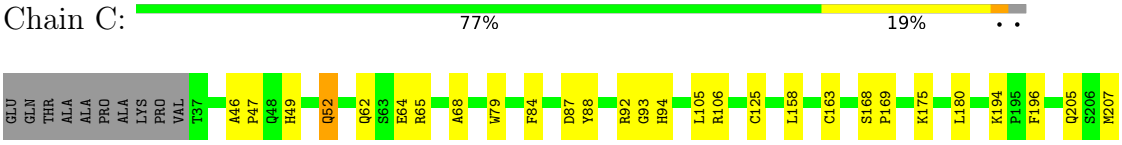
• Molecule 1: Cytochrome c-552

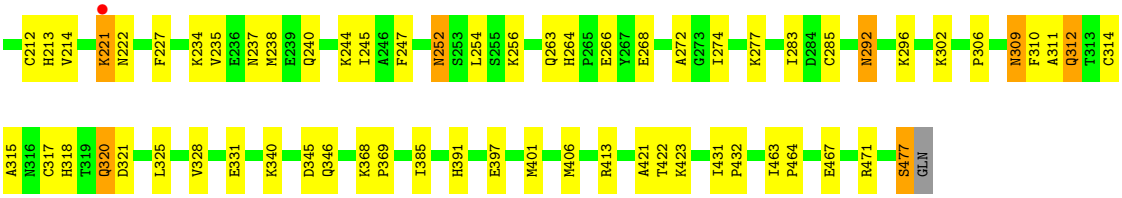
Chain B:



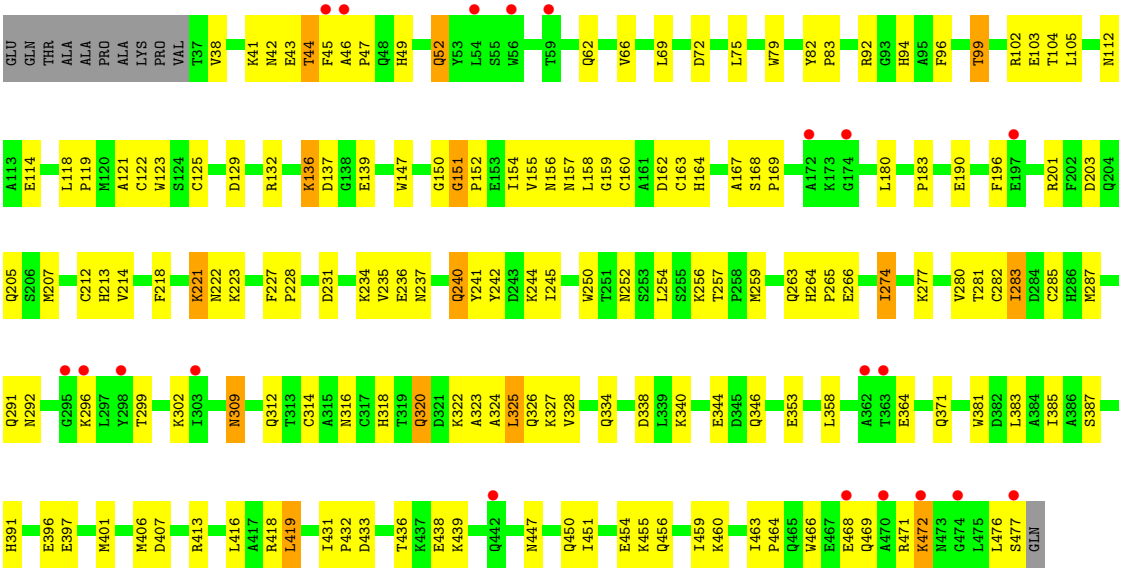
• Molecule 1: Cytochrome c-552

Chain C:





• Molecule 1: Cytochrome c-552



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.52Å 82.23Å 142.17Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	50.36 – 2.30 50.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.36-2.30) 99.7 (50.36-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.177 , 0.238 0.176 , 0.233	Depositor DCC
R_{free} test set	4553 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15858	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, HEC, SO3, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	1/3569 (0.0%)	0.58	0/4827
1	B	0.52	0/3578	0.60	0/4838
1	C	0.53	0/3595	0.59	0/4861
1	D	0.41	0/3577	0.52	0/4838
All	All	0.49	1/14319 (0.0%)	0.57	0/19364

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	GLN	CD-NE2	-6.21	1.17	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3485	0	3374	139	0
1	B	3491	0	3389	115	0
1	C	3502	0	3396	122	0
1	D	3487	0	3378	189	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	215	0	155	53	0
3	B	215	0	155	42	0
3	C	215	0	155	44	0
3	D	215	0	155	52	0
4	A	4	0	0	0	0
4	B	8	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	10	0
5	C	24	0	36	8	0
5	D	8	0	12	8	0
6	A	222	0	0	16	0
6	B	291	0	0	22	0
6	C	292	0	0	18	0
6	D	152	0	0	25	0
All	All	15858	0	14229	622	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 21.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:HE2	5:B:483:EDO:C1	1.27	1.57
1:B:296:LYS:CE	5:B:483:EDO:H11	1.29	1.53
1:C:125:CYS:SG	3:C:479:HEC:CAC	2.02	1.47
1:A:160:CYS:SG	3:A:480:HEC:CAB	2.02	1.47
1:D:122:CYS:SG	3:D:479:HEC:CAB	2.01	1.47
1:D:212:CYS:SG	3:D:3:HEC:CAC	2.03	1.46
1:A:125:CYS:SG	3:A:479:HEC:CAC	2.08	1.41
1:B:125:CYS:SG	3:B:479:HEC:CAC	2.07	1.40
1:A:198:LYS:HE2	1:C:65:ARG:NH1	1.31	1.40
1:D:52:GLN:H	1:D:52:GLN:NE2	1.21	1.36
1:B:212:CYS:SG	3:B:3:HEC:CAC	2.14	1.35
1:D:125:CYS:SG	3:D:479:HEC:CAC	2.13	1.34
1:A:456:GLN:NE2	1:A:460:LYS:HE3	1.41	1.34
1:B:163:CYS:SG	3:B:480:HEC:CAC	2.18	1.31
1:C:212:CYS:SG	3:C:3:HEC:CAC	2.18	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:CYS:SG	3:D:5:HEC:CAB	2.19	1.31
1:A:317:CYS:SG	3:A:5:HEC:CAC	2.19	1.29
1:B:285:CYS:SG	3:B:4:HEC:CAC	2.19	1.28
1:A:163:CYS:SG	3:A:480:HEC:CAC	2.22	1.27
1:A:212:CYS:SG	3:A:3:HEC:CAC	2.27	1.23
1:C:285:CYS:SG	3:C:4:HEC:CAC	2.29	1.20
1:A:285:CYS:SG	3:A:4:HEC:CAC	2.29	1.20
1:B:317:CYS:SG	3:B:5:HEC:CAC	2.30	1.19
1:A:198:LYS:CE	1:C:65:ARG:NH1	2.07	1.16
1:A:52:GLN:H	1:A:52:GLN:NE2	1.45	1.15
1:A:456:GLN:HE21	1:A:460:LYS:CE	1.61	1.13
1:C:221:LYS:HE3	1:C:221:LYS:N	1.64	1.13
1:D:163:CYS:SG	3:D:480:HEC:CAC	2.37	1.13
1:D:285:CYS:SG	3:D:4:HEC:CAC	2.37	1.13
3:A:5:HEC:HBB3	3:A:5:HEC:HMB1	1.28	1.10
1:C:317:CYS:SG	3:C:5:HEC:CAC	2.39	1.10
1:C:163:CYS:SG	3:C:480:HEC:CAC	2.40	1.09
1:C:221:LYS:HE3	1:C:221:LYS:H	0.97	1.08
3:D:5:HEC:HBB3	3:D:5:HEC:HMB1	1.34	1.05
1:D:52:GLN:NE2	1:D:52:GLN:N	2.05	1.04
1:D:49:HIS:HD2	6:D:643:HOH:O	1.41	1.04
3:D:480:HEC:HMC1	3:D:480:HEC:HBC3	1.42	1.02
1:D:125:CYS:SG	3:D:479:HEC:C3C	2.48	1.01
1:D:52:GLN:N	1:D:52:GLN:HE21	1.59	1.00
1:B:309:ASN:HB3	6:B:543:HOH:O	1.61	0.99
1:C:125:CYS:SG	3:C:479:HEC:C3C	2.50	0.99
1:C:221:LYS:H	1:C:221:LYS:CE	1.76	0.97
1:B:309:ASN:CB	6:B:543:HOH:O	2.12	0.97
3:C:4:HEC:HBC3	3:C:4:HEC:HMC1	1.43	0.97
1:B:212:CYS:SG	3:B:3:HEC:HAC	2.02	0.97
1:C:309:ASN:ND2	1:C:312:GLN:HE22	1.62	0.97
3:D:479:HEC:HMC1	3:D:479:HEC:CBC	1.95	0.96
1:C:345:ASP:OD1	5:C:9:EDO:H11	1.65	0.96
1:D:38:VAL:HG11	1:D:132:ARG:HA	1.45	0.95
3:B:480:HEC:HMC1	3:B:480:HEC:HBC3	1.49	0.94
3:D:480:HEC:HMC1	3:D:480:HEC:CBC	1.99	0.93
3:D:479:HEC:HMC1	3:D:479:HEC:HBC3	1.45	0.93
1:C:320:GLN:HG2	5:C:484:EDO:H22	1.50	0.93
1:A:198:LYS:HE2	1:C:65:ARG:HH12	1.27	0.93
1:A:52:GLN:HE21	1:A:52:GLN:N	1.67	0.92
1:A:125:CYS:SG	3:A:479:HEC:C3C	2.58	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:5:HEC:HMB1	3:B:5:HEC:HBB3	1.52	0.91
1:D:436:THR:OG1	1:D:439:LYS:HG3	1.70	0.91
1:C:125:CYS:SG	3:C:479:HEC:HAC	2.08	0.91
1:C:317:CYS:SG	3:C:5:HEC:HBC3	2.11	0.91
1:A:125:CYS:SG	3:A:479:HEC:HAC	2.11	0.91
3:A:480:HEC:HMB1	3:A:480:HEC:HBB3	1.53	0.91
1:C:317:CYS:SG	3:C:5:HEC:CBC	2.59	0.90
1:B:125:CYS:SG	3:B:479:HEC:CBC	2.58	0.90
1:D:125:CYS:SG	3:D:479:HEC:CBC	2.58	0.90
1:A:198:LYS:HE2	1:C:65:ARG:HH11	1.29	0.89
1:B:37:THR:HA	6:B:924:HOH:O	1.73	0.89
1:B:125:CYS:SG	3:B:479:HEC:C3C	2.60	0.89
1:D:52:GLN:H	1:D:52:GLN:HE21	0.90	0.89
1:C:309:ASN:ND2	1:C:312:GLN:NE2	2.21	0.89
1:A:212:CYS:SG	3:A:3:HEC:CBC	2.60	0.88
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.55	0.88
3:A:479:HEC:HMC1	3:A:479:HEC:HBC3	1.54	0.88
1:D:221:LYS:H	1:D:221:LYS:HZ2	1.17	0.88
3:A:5:HEC:HMB1	3:A:5:HEC:CBB	2.03	0.88
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.56	0.88
3:C:3:HEC:HMC1	3:C:3:HEC:HBC3	1.56	0.88
3:D:5:HEC:HMB1	3:D:5:HEC:CBB	2.05	0.87
1:A:292:ASN:C	1:A:292:ASN:HD22	1.75	0.86
1:A:52:GLN:H	1:A:52:GLN:HE21	0.91	0.86
3:A:3:HEC:HBC3	3:A:3:HEC:HMC1	1.57	0.86
1:D:472:LYS:NZ	1:D:472:LYS:HB3	1.89	0.86
1:B:99:THR:HG22	6:B:506:HOH:O	1.77	0.85
1:A:198:LYS:CE	1:C:65:ARG:HH12	1.80	0.84
3:C:4:HEC:HMC1	3:C:4:HEC:CBC	2.06	0.84
1:B:234:LYS:HE2	6:B:876:HOH:O	1.75	0.84
3:B:4:HEC:HMC1	3:B:4:HEC:HBC3	1.59	0.84
1:A:163:CYS:SG	3:A:480:HEC:CBC	2.65	0.84
1:C:296:LYS:CE	6:C:534:HOH:O	2.26	0.84
1:A:317:CYS:SG	3:A:5:HEC:C3C	2.65	0.83
1:A:317:CYS:SG	3:A:5:HEC:HAC	2.18	0.83
1:B:163:CYS:SG	3:B:480:HEC:HAC	2.18	0.83
1:D:364:GLU:HG2	6:D:531:HOH:O	1.77	0.83
1:A:292:ASN:ND2	1:A:296:LYS:H	1.77	0.83
1:D:212:CYS:SG	3:D:3:HEC:C3C	2.66	0.83
3:A:480:HEC:HMC1	3:A:480:HEC:HBC3	1.60	0.82
3:D:4:HEC:HMC1	3:D:4:HEC:HBC3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLN:HG3	6:B:638:HOH:O	1.80	0.81
1:D:364:GLU:CG	6:D:531:HOH:O	2.26	0.81
1:A:52:GLN:NE2	1:A:52:GLN:N	2.28	0.81
1:C:221:LYS:HD2	6:C:674:HOH:O	1.80	0.80
1:C:296:LYS:HE2	6:C:534:HOH:O	1.82	0.80
1:B:364:GLU:HG3	6:B:981:HOH:O	1.81	0.79
1:D:125:CYS:SG	3:D:479:HEC:HBC3	2.23	0.79
1:D:231:ASP:OD2	1:D:240:GLN:NE2	2.16	0.78
3:A:480:HEC:CBC	3:A:480:HEC:HMC1	2.13	0.78
1:B:37:THR:CA	6:B:924:HOH:O	2.30	0.78
1:B:317:CYS:SG	3:B:5:HEC:CBC	2.72	0.77
1:D:256:LYS:HG3	1:D:358:LEU:HD13	1.67	0.77
1:C:212:CYS:SG	3:C:3:HEC:CBC	2.73	0.77
1:B:163:CYS:SG	3:B:480:HEC:C3C	2.74	0.76
1:B:346:GLN:NE2	1:B:413:ARG:HH11	1.83	0.76
1:B:312:GLN:CD	6:B:638:HOH:O	2.23	0.76
1:D:327:LYS:CE	6:D:1034:HOH:O	2.33	0.76
1:A:212:CYS:SG	3:A:3:HEC:HBC3	2.25	0.76
1:B:52:GLN:H	1:B:52:GLN:NE2	1.84	0.76
3:C:5:HEC:HMB1	3:C:5:HEC:HBB3	1.66	0.75
1:D:334:GLN:HE21	1:D:338[B]:ASP:CG	1.89	0.75
1:A:320:GLN:H	1:A:320:GLN:HE21	1.31	0.75
1:D:314:CYS:SG	3:D:5:HEC:CBB	2.75	0.74
1:B:352:PHE:CD2	1:B:431:ILE:HD12	2.22	0.74
1:C:212:CYS:SG	3:C:3:HEC:C3C	2.75	0.74
1:D:314:CYS:SG	3:D:5:HEC:HAB	2.22	0.74
1:D:256:LYS:HG3	1:D:358:LEU:CD1	2.18	0.74
1:B:296:LYS:CD	5:B:483:EDO:H11	2.17	0.74
1:B:296:LYS:HE2	5:B:483:EDO:C2	2.15	0.74
1:B:391:HIS:HE1	3:B:4:HEC:O2D	1.71	0.74
1:C:163:CYS:SG	3:C:480:HEC:CBC	2.75	0.74
1:D:292:ASN:HD21	1:D:296:LYS:HB2	1.52	0.73
1:A:62:GLN:HE21	1:A:302:LYS:NZ	1.87	0.73
1:B:285:CYS:SG	3:B:4:HEC:CBC	2.76	0.73
3:C:479:HEC:HMC1	3:C:479:HEC:HBC3	1.69	0.73
1:C:328:VAL:HG21	5:C:484:EDO:H12	1.70	0.73
1:D:334:GLN:NE2	1:D:338[B]:ASP:OD1	2.22	0.73
1:A:163:CYS:SG	3:A:480:HEC:C3C	2.77	0.73
1:A:456:GLN:HE21	1:A:460:LYS:HE3	0.67	0.73
3:B:5:HEC:HBC3	3:B:5:HEC:HMC1	1.70	0.72
1:D:221:LYS:H	1:D:221:LYS:NZ	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLN:HB3	6:D:540:HOH:O	1.88	0.72
1:A:198:LYS:CE	1:C:65:ARG:HH11	1.89	0.72
1:B:285:CYS:SG	3:B:4:HEC:HAC	2.27	0.72
1:A:160:CYS:SG	3:A:480:HEC:C3B	2.77	0.71
1:A:449:GLU:HG3	6:A:770:HOH:O	1.90	0.71
1:B:312:GLN:CG	6:B:638:HOH:O	2.37	0.71
1:D:45:PHE:HA	6:D:757:HOH:O	1.90	0.71
5:C:483:EDO:H21	6:C:544:HOH:O	1.90	0.71
1:D:69:LEU:HD12	6:D:499:HOH:O	1.91	0.71
1:B:99:THR:CG2	6:B:506:HOH:O	2.35	0.71
1:D:163:CYS:SG	3:D:480:HEC:CBC	2.78	0.71
1:D:122:CYS:SG	3:D:479:HEC:CBB	2.79	0.71
1:D:201:ARG:O	1:D:205:GLN:HG3	1.89	0.71
1:A:292:ASN:HD21	1:A:296:LYS:H	1.36	0.71
1:D:158:LEU:HG	3:D:3:HEC:HBC2	1.73	0.71
1:D:240:GLN:CB	6:D:540:HOH:O	2.39	0.71
1:B:285:CYS:SG	3:B:4:HEC:C3C	2.79	0.70
1:D:221:LYS:NZ	1:D:221:LYS:N	2.40	0.70
1:B:37:THR:HG22	1:B:135:GLN:OE1	1.92	0.70
3:D:5:HEC:HBC3	3:D:5:HEC:HMC1	1.73	0.70
1:A:231:ASP:OD2	1:A:240:GLN:NE2	2.24	0.70
1:D:92:ARG:NH2	1:D:96:PHE:CD1	2.59	0.70
1:D:163:CYS:SG	3:D:480:HEC:C3C	2.80	0.70
1:B:125:CYS:SG	3:B:479:HEC:HAC	2.28	0.70
1:B:212:CYS:SG	3:B:3:HEC:C3C	2.78	0.70
1:C:175:LYS:HE3	6:C:563:HOH:O	1.91	0.70
1:B:125:CYS:SG	3:B:479:HEC:HBC3	2.31	0.70
1:C:212:CYS:SG	3:C:3:HEC:HAC	2.30	0.70
1:D:456:GLN:HE21	1:D:456:GLN:HA	1.57	0.69
1:C:368:LYS:HB3	1:C:369:PRO:HD3	1.73	0.69
1:D:328:VAL:CG2	5:D:482:EDO:H21	2.22	0.69
1:A:163:CYS:SG	3:A:480:HEC:HBC3	2.32	0.69
1:C:125:CYS:SG	3:C:479:HEC:CBC	2.80	0.69
1:C:62:GLN:HE21	1:C:302:LYS:HZ3	1.39	0.69
3:B:480:HEC:HMC1	3:B:480:HEC:CBC	2.23	0.69
3:B:4:HEC:HMC1	3:B:4:HEC:CBC	2.23	0.69
1:C:52:GLN:H	1:C:52:GLN:NE2	1.91	0.68
3:A:3:HEC:CBC	3:A:3:HEC:HMC1	2.22	0.68
1:D:203:ASP:O	1:D:207:MET:HG3	1.93	0.68
1:B:199:ALA:HA	6:B:600:HOH:O	1.93	0.67
1:A:419:LEU:HA	6:A:648:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:CYS:SG	3:D:4:HEC:HAC	2.34	0.67
1:C:163:CYS:SG	3:C:480:HEC:HBC3	2.34	0.67
1:D:292:ASN:ND2	1:D:296:LYS:HB2	2.10	0.67
1:D:418:ARG:HD3	6:D:490:HOH:O	1.95	0.67
1:D:43:GLU:OE2	1:D:43:GLU:N	2.21	0.66
1:B:146:LYS:O	1:B:149:ARG:HB2	1.94	0.66
1:C:87:ASP:HB2	1:C:105:LEU:HB2	1.76	0.66
1:D:391:HIS:HD2	6:D:804:HOH:O	1.79	0.66
1:C:163:CYS:SG	3:C:480:HEC:C3C	2.84	0.66
1:C:391:HIS:CE1	3:C:4:HEC:O2D	2.45	0.66
1:B:317:CYS:SG	3:B:5:HEC:C3C	2.83	0.66
1:C:345:ASP:CG	5:C:9:EDO:H11	2.16	0.66
1:A:62:GLN:HE21	1:A:302:LYS:HZ3	1.42	0.65
1:C:62:GLN:HE21	1:C:302:LYS:NZ	1.94	0.65
1:A:252:ASN:HD21	1:A:254:LEU:HB2	1.60	0.65
1:B:52:GLN:H	1:B:52:GLN:HE21	1.44	0.65
3:D:479:HEC:CBC	3:D:479:HEC:CMC	2.73	0.65
1:A:320:GLN:H	1:A:320:GLN:NE2	1.95	0.65
1:C:285:CYS:SG	3:C:4:HEC:C3C	2.85	0.65
1:D:328:VAL:CG2	5:D:482:EDO:C2	2.75	0.65
1:A:212:CYS:SG	3:A:3:HEC:C3C	2.84	0.64
1:A:431:ILE:HG22	1:A:432:PRO:O	1.97	0.64
1:D:123:TRP:CG	1:D:154:ILE:HD13	2.33	0.64
3:A:4:HEC:HMB1	3:A:4:HEC:HBB3	1.79	0.64
3:A:5:HEC:HBB3	3:A:5:HEC:CMB	2.17	0.64
1:C:277[B]:LYS:NZ	6:C:629:HOH:O	2.21	0.64
1:B:49:HIS:HE1	6:B:572:HOH:O	1.81	0.64
1:D:324:ALA:HB1	5:D:482:EDO:H11	1.80	0.64
1:A:256:LYS:HD2	6:A:849:HOH:O	1.96	0.64
1:C:49:HIS:HD2	6:C:656:HOH:O	1.81	0.64
3:A:5:HEC:HMC1	3:A:5:HEC:HBC3	1.81	0.63
6:A:581:HOH:O	1:B:342:LYS:HE3	1.98	0.63
1:C:205:GLN:HB3	1:C:283:ILE:HD13	1.79	0.63
1:D:320:GLN:H	1:D:320:GLN:HE21	1.45	0.63
1:C:345:ASP:OD1	5:C:9:EDO:C1	2.43	0.63
3:B:480:HEC:HBB3	3:B:480:HEC:HMB1	1.79	0.63
1:C:309:ASN:HD21	1:C:312:GLN:HE22	1.46	0.63
1:B:320:GLN:H	1:B:320:GLN:HE21	1.47	0.62
1:D:285:CYS:SG	3:D:4:HEC:C3C	2.87	0.62
1:A:285:CYS:SG	3:A:4:HEC:C3C	2.87	0.62
1:A:285:CYS:SG	3:A:4:HEC:CBC	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:480:HEC:HBB3	3:A:480:HEC:CMB	2.28	0.62
1:B:234:LYS:H	1:B:237:ASN:HD22	1.47	0.62
1:D:450:GLN:O	1:D:454:GLU:HG3	1.99	0.62
1:C:318:HIS:HB3	1:C:320:GLN:NE2	2.14	0.62
1:D:235:VAL:HG13	1:D:236:GLU:N	2.15	0.62
1:D:383:LEU:HD23	1:D:401:MET:HE3	1.82	0.62
1:D:455:LYS:O	1:D:459:ILE:HG13	2.00	0.62
1:C:285:CYS:SG	3:C:4:HEC:HAC	2.34	0.62
1:C:317:CYS:SG	3:C:5:HEC:C3C	2.87	0.61
1:A:450:GLN:O	1:A:454:GLU:HG3	2.01	0.61
3:A:479:HEC:HMC1	3:A:479:HEC:CBC	2.27	0.61
3:A:4:HEC:HMC1	3:A:4:HEC:CBC	2.29	0.61
1:B:252:ASN:ND2	1:B:254:LEU:H	1.97	0.61
1:A:125:CYS:SG	3:A:479:HEC:CBC	2.86	0.61
1:B:317:CYS:SG	3:B:5:HEC:HBC3	2.39	0.61
1:C:406:MET:CE	1:D:407:ASP:HB2	2.30	0.61
1:D:472:LYS:HB3	1:D:472:LYS:HZ2	1.61	0.61
1:D:163:CYS:SG	3:D:480:HEC:HBC3	2.40	0.61
1:B:352:PHE:HB2	1:B:431:ILE:HD11	1.83	0.60
1:C:52:GLN:H	1:C:52:GLN:HE21	1.48	0.60
1:A:285:CYS:SG	3:A:4:HEC:HAC	2.36	0.60
1:A:292:ASN:C	1:A:292:ASN:ND2	2.49	0.60
1:B:317:CYS:HG	3:B:5:HEC:CAC	2.12	0.60
3:B:5:HEC:CBC	3:B:5:HEC:HMC1	2.30	0.60
3:C:480:HEC:HBC3	3:C:480:HEC:HMC1	1.82	0.60
1:D:314:CYS:SG	3:D:5:HEC:C3B	2.88	0.60
1:B:123:TRP:CG	1:B:154:ILE:HD13	2.37	0.60
1:D:221:LYS:HZ2	1:D:221:LYS:N	1.92	0.60
1:D:327:LYS:HE3	6:D:1034:HOH:O	2.01	0.60
1:D:456:GLN:HA	1:D:456:GLN:NE2	2.17	0.60
1:A:327:LYS:HE3	1:A:331[B]:GLU:OE2	2.02	0.60
1:D:136:LYS:HG2	1:D:137:ASP:OD1	2.02	0.60
1:A:214:VAL:HG21	1:A:227:PHE:CZ	2.37	0.60
1:D:38:VAL:CG1	1:D:132:ARG:HA	2.25	0.60
1:C:320:GLN:NE2	6:C:933:HOH:O	2.30	0.60
1:C:320:GLN:NE2	1:C:320:GLN:H	1.99	0.59
1:A:346:GLN:NE2	1:A:413:ARG:HH11	2.00	0.59
1:C:285:CYS:SG	3:C:4:HEC:CBC	2.91	0.59
3:C:4:HEC:CBC	3:C:4:HEC:CMC	2.80	0.59
1:B:352:PHE:CB	1:B:431:ILE:HD11	2.31	0.59
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HD2	6:A:513:HOH:O	2.01	0.59
1:B:346:GLN:HE22	1:B:413:ARG:HH11	1.49	0.59
1:D:476:LEU:HG	1:D:477:SER:H	1.68	0.59
3:B:5:HEC:HBB3	3:B:5:HEC:CMB	2.29	0.59
1:D:62:GLN:HE21	1:D:302:LYS:NZ	2.01	0.59
1:C:296:LYS:HD3	6:C:534:HOH:O	2.02	0.59
1:D:433:ASP:OD1	1:D:439:LYS:HD3	2.03	0.58
1:A:252:ASN:ND2	1:A:254:LEU:HB2	2.17	0.58
1:D:320:GLN:H	1:D:320:GLN:NE2	2.01	0.58
1:A:280:VAL:HG13	3:A:5:HEC:HBC2	1.85	0.57
1:D:119:PRO:HG3	1:D:223:LYS:HD2	1.86	0.57
1:B:194:LYS:HB3	1:B:207:MET:HE1	1.86	0.57
1:C:406:MET:HE3	1:D:407:ASP:HB2	1.85	0.57
3:B:5:HEC:HBD2	6:B:627:HOH:O	2.04	0.57
1:A:182:ARG:HG3	6:A:584:HOH:O	2.03	0.57
1:A:201:ARG:HA	6:A:905:HOH:O	2.03	0.57
1:A:406:MET:HG2	1:B:406:MET:HB3	1.86	0.57
1:A:318:HIS:HB3	1:A:320:GLN:NE2	2.19	0.57
3:B:4:HEC:HMB1	3:B:4:HEC:HBB3	1.85	0.57
3:C:3:HEC:HMC1	3:C:3:HEC:CBC	2.31	0.57
1:B:320:GLN:H	1:B:320:GLN:NE2	2.03	0.57
1:D:41:LYS:HA	1:D:156:ASN:OD1	2.05	0.57
1:D:257:THR:O	1:D:259:MET:HG2	2.05	0.56
1:B:364:GLU:N	6:B:895:HOH:O	2.38	0.56
3:C:480:HEC:CBC	3:C:480:HEC:HMC1	2.35	0.56
1:D:235:VAL:HB	1:D:401:MET:HE3	1.87	0.56
3:C:4:HEC:HMB1	3:C:4:HEC:HBB3	1.88	0.56
1:D:312:GLN:HA	1:D:312:GLN:OE1	2.04	0.56
1:A:52:GLN:HG2	3:A:480:HEC:C4A	2.36	0.56
1:A:256:LYS:CD	6:A:849:HOH:O	2.53	0.56
1:A:418:ARG:HD3	6:A:585:HOH:O	2.04	0.56
1:B:391:HIS:CE1	3:B:4:HEC:O2D	2.58	0.56
1:C:296:LYS:CD	6:C:534:HOH:O	2.53	0.56
1:B:163:CYS:SG	3:B:480:HEC:CBC	2.91	0.56
1:C:194:LYS:HB3	1:C:207:MET:HE1	1.87	0.56
1:C:312:GLN:NE2	1:C:312:GLN:H	2.04	0.55
1:A:43:GLU:CD	1:A:43:GLU:H	2.10	0.55
1:D:151:GLY:HA3	1:D:466:TRP:CE2	2.41	0.55
1:C:431:ILE:HG22	1:C:432:PRO:O	2.07	0.55
1:B:212:CYS:SG	3:B:3:HEC:CBC	2.93	0.55
3:A:5:HEC:CBB	3:A:5:HEC:CMB	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HG12	1:A:312:GLN:HG2	1.89	0.55
3:B:3:HEC:HMC1	3:B:3:HEC:HBC3	1.89	0.54
1:A:133:LEU:HD12	1:A:154:ILE:HD11	1.89	0.54
1:A:456:GLN:NE2	1:A:460:LYS:CE	2.37	0.54
1:B:194:LYS:HB3	1:B:207:MET:CE	2.38	0.54
1:B:252:ASN:HD22	1:B:254:LEU:H	1.55	0.54
1:B:296:LYS:NZ	5:B:483:EDO:H22	2.21	0.54
3:B:479:HEC:HBC3	3:B:479:HEC:HMC1	1.89	0.54
1:C:292:ASN:C	1:C:292:ASN:HD22	2.11	0.54
1:D:281:THR:HG22	6:D:500:HOH:O	2.08	0.54
1:C:320:GLN:H	1:C:320:GLN:HE21	1.55	0.54
1:B:383:LEU:HD23	1:B:401:MET:HE3	1.90	0.54
1:C:240:GLN:O	1:C:244:LYS:HG3	2.07	0.54
1:D:43:GLU:O	1:D:45:PHE:N	2.41	0.53
1:A:263:GLN:NE2	6:A:812:HOH:O	2.41	0.53
1:D:456:GLN:O	1:D:460:LYS:HG2	2.08	0.53
1:A:144:HIS:HD2	6:A:597:HOH:O	1.92	0.53
1:C:292:ASN:HD21	1:C:296:LYS:H	1.55	0.53
3:C:5:HEC:CBC	3:C:5:HEC:HMC1	2.39	0.53
1:D:364:GLU:CD	6:D:531:HOH:O	2.46	0.53
3:D:479:HEC:HBB3	3:D:479:HEC:HMB1	1.90	0.53
1:B:309:ASN:HB2	6:B:543:HOH:O	1.95	0.53
1:D:472:LYS:HB3	1:D:472:LYS:HZ3	1.71	0.53
1:A:198:LYS:HD2	6:A:778:HOH:O	2.08	0.53
3:D:479:HEC:HMC1	3:D:479:HEC:HBC2	1.83	0.53
1:D:157:ASN:O	1:D:158:LEU:C	2.47	0.53
1:A:151:GLY:HA3	1:A:466:TRP:CD2	2.44	0.52
1:C:212:CYS:SG	3:C:3:HEC:HBC3	2.49	0.52
1:D:328:VAL:HG21	5:D:482:EDO:H21	1.91	0.52
1:A:343:VAL:HG22	1:A:406:MET:HE2	1.91	0.52
1:A:194:LYS:HB3	1:A:207:MET:CE	2.39	0.52
1:D:381:TRP:O	1:D:385:ILE:HG13	2.10	0.52
1:A:463:ILE:HB	1:A:464:PRO:HD3	1.90	0.52
1:D:94:HIS:CD2	3:D:3:HEC:ND	2.77	0.52
1:C:463:ILE:HB	1:C:464:PRO:HD3	1.92	0.52
1:A:151:GLY:HA3	1:A:466:TRP:CE2	2.44	0.52
1:B:234:LYS:H	1:B:237:ASN:ND2	2.06	0.52
3:D:480:HEC:CBC	3:D:480:HEC:CMC	2.76	0.52
1:D:42:ASN:ND2	6:D:530:HOH:O	2.42	0.51
3:D:5:HEC:HBB3	3:D:5:HEC:CMB	2.23	0.51
1:B:37:THR:HA	1:B:135:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LYS:HB3	1:B:369:PRO:HD3	1.92	0.51
1:A:343:VAL:HG22	1:A:406:MET:CE	2.40	0.51
1:A:461:THR:O	1:A:465:GLN:HG3	2.10	0.51
1:C:49:HIS:HE1	6:C:709:HOH:O	1.93	0.51
1:D:235:VAL:CG1	1:D:236:GLU:N	2.73	0.51
1:C:252:ASN:ND2	1:C:254:LEU:H	2.09	0.51
1:C:346:GLN:NE2	1:C:413:ARG:HH11	2.08	0.51
1:A:218:PHE:HB2	6:A:578:HOH:O	2.11	0.51
3:D:4:HEC:HMC1	3:D:4:HEC:CBC	2.38	0.51
1:D:265:PRO:HD2	1:D:387:SER:HB2	1.93	0.51
1:B:94:HIS:CD2	3:B:3:HEC:ND	2.79	0.51
1:D:346:GLN:NE2	1:D:413:ARG:HH11	2.08	0.51
3:D:479:HEC:HBC3	3:D:479:HEC:CMC	2.31	0.51
1:A:252:ASN:HD22	1:A:255:SER:H	1.57	0.51
1:A:282:CYS:HA	3:A:4:HEC:CHC	2.41	0.51
1:D:46:ALA:N	1:D:47:PRO:CD	2.74	0.51
1:D:252:ASN:ND2	1:D:254:LEU:H	2.08	0.51
1:A:198:LYS:HE3	1:C:65:ARG:NH1	2.15	0.50
1:A:170:GLU:OE1	1:A:175:LYS:HD3	2.11	0.50
1:D:240:GLN:HB2	6:D:540:HOH:O	2.09	0.50
1:D:245:ILE:HD12	6:D:775:HOH:O	2.11	0.50
1:D:323:ALA:HA	1:D:326:GLN:HE21	1.75	0.50
1:D:436:THR:HG1	1:D:439:LYS:HG3	1.75	0.50
1:A:283:ILE:HD11	3:A:3:HEC:HBB1	1.93	0.50
1:D:105:LEU:HD23	1:D:455:LYS:HG2	1.94	0.50
1:D:472:LYS:NZ	1:D:472:LYS:CB	2.69	0.50
3:B:479:HEC:CBC	3:B:479:HEC:HMC1	2.42	0.50
3:C:479:HEC:HMC1	3:C:479:HEC:CBC	2.41	0.50
1:D:256:LYS:HG3	1:D:358:LEU:HD11	1.94	0.50
1:C:175:LYS:CE	6:C:563:HOH:O	2.55	0.50
1:D:125:CYS:SG	3:D:479:HEC:C2C	2.98	0.50
1:D:151:GLY:HA2	1:D:466:TRP:CE3	2.46	0.50
1:C:312:GLN:NE2	1:C:312:GLN:N	2.59	0.49
1:A:323:ALA:HA	1:A:326:GLN:HE21	1.77	0.49
1:B:450:GLN:O	1:B:454:GLU:HG3	2.12	0.49
1:D:252:ASN:HD22	1:D:254:LEU:H	1.59	0.49
1:A:255:SER:HB3	1:A:354:ALA:HB3	1.95	0.49
1:D:312:GLN:O	1:D:316:ASN:ND2	2.46	0.49
3:D:3:HEC:HBC3	3:D:3:HEC:HMC1	1.93	0.49
1:A:62:GLN:NE2	1:A:302:LYS:NZ	2.58	0.49
1:D:371:GLN:NE2	6:D:528:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:HIS:CD2	3:C:3:HEC:ND	2.80	0.49
1:C:397:GLU:OE2	1:C:397:GLU:HA	2.12	0.49
3:C:5:HEC:HBC3	3:C:5:HEC:HMC1	1.95	0.49
1:D:129:ASP:CB	1:D:154:ILE:HA	2.43	0.49
1:D:66:VAL:HG13	6:D:903:HOH:O	2.12	0.49
1:D:151:GLY:CA	1:D:466:TRP:CD2	2.96	0.49
1:D:280:VAL:HG13	3:D:5:HEC:HBC2	1.93	0.49
1:D:291:GLN:HA	1:D:296:LYS:O	2.12	0.48
1:D:397:GLU:O	1:D:401:MET:HG3	2.12	0.48
3:D:5:HEC:CBB	3:D:5:HEC:CMB	2.81	0.48
1:D:282:CYS:HA	3:D:4:HEC:CHC	2.43	0.48
1:C:331[B]:GLU:OE1	1:D:277:LYS:NZ	2.42	0.48
1:D:167:ALA:O	1:D:168:SER:C	2.52	0.48
3:A:3:HEC:CBC	3:A:3:HEC:CMC	2.90	0.48
1:C:68:ALA:HB3	1:C:88:TYR:CD2	2.49	0.48
1:D:235:VAL:HB	1:D:401:MET:CE	2.43	0.48
1:D:309:ASN:OD1	1:D:312:GLN:CG	2.61	0.48
1:D:322:LYS:HE2	6:D:871:HOH:O	2.13	0.48
1:A:234:LYS:H	1:A:237:ASN:ND2	2.11	0.48
1:A:471:ARG:O	1:A:472:LYS:C	2.52	0.48
1:B:285:CYS:SG	3:B:4:HEC:HBC3	2.54	0.48
1:B:418:ARG:O	1:B:422:THR:HG23	2.13	0.48
1:D:419:LEU:HD22	1:D:419:LEU:O	2.14	0.48
1:D:213:HIS:HB3	1:D:266:GLU:HB2	1.96	0.48
1:D:468:GLU:O	1:D:472:LYS:HG2	2.14	0.48
1:A:234:LYS:H	1:A:237:ASN:HD22	1.60	0.47
1:B:352:PHE:CB	1:B:431:ILE:CD1	2.92	0.47
1:C:227:PHE:N	1:C:227:PHE:CD2	2.82	0.47
1:D:328:VAL:CG2	5:D:482:EDO:H22	2.44	0.47
1:D:44:THR:HG22	1:D:44:THR:O	2.14	0.47
1:D:447:ASN:O	1:D:451:ILE:HG13	2.15	0.47
1:A:252:ASN:ND2	1:A:254:LEU:H	2.12	0.47
1:A:414:THR:HG22	1:A:418:ARG:NH1	2.29	0.47
1:C:292:ASN:C	1:C:292:ASN:ND2	2.68	0.47
1:D:99:THR:CG2	6:D:483:HOH:O	2.62	0.47
1:D:328:VAL:HG23	5:D:482:EDO:C2	2.44	0.47
1:A:227:PHE:N	1:A:227:PHE:CD2	2.82	0.47
1:C:274:ILE:HD12	1:C:277[B]:LYS:HD2	1.96	0.47
1:D:328:VAL:HG21	5:D:482:EDO:C2	2.43	0.47
1:A:62:GLN:NE2	1:A:302:LYS:HZ2	2.11	0.47
1:A:256:LYS:CE	6:A:849:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:HB2	6:B:592:HOH:O	2.14	0.47
1:C:194:LYS:HB3	1:C:207:MET:CE	2.44	0.47
1:C:245:ILE:HG13	1:C:247:PHE:HB2	1.97	0.47
1:B:370:ILE:HD13	1:B:416:LEU:HD23	1.95	0.47
1:A:368:LYS:HB3	1:A:369:PRO:HD3	1.97	0.47
1:D:99:THR:HG22	6:D:483:HOH:O	2.16	0.47
1:B:266:GLU:OE1	1:B:387:SER:CB	2.63	0.46
1:C:272:ALA:O	1:C:277[B]:LYS:HE3	2.15	0.46
1:C:421:ALA:C	1:C:423:LYS:H	2.19	0.46
1:D:155:VAL:HB	6:D:533:HOH:O	2.14	0.46
3:D:480:HEC:HMC1	3:D:480:HEC:HBC2	1.94	0.46
1:A:119:PRO:HG3	1:A:223:LYS:HD3	1.97	0.46
1:B:296:LYS:CE	5:B:483:EDO:C2	2.83	0.46
1:B:352:PHE:CG	1:B:431:ILE:CD1	2.98	0.46
1:B:352:PHE:CG	1:B:431:ILE:HD12	2.49	0.46
1:C:309:ASN:HD21	1:C:312:GLN:NE2	2.06	0.46
1:D:383:LEU:HD23	1:D:401:MET:CE	2.44	0.46
1:C:235:VAL:HB	1:C:401:MET:HE3	1.97	0.46
1:B:227:PHE:N	1:B:227:PHE:CD2	2.83	0.46
1:B:391:HIS:H	1:B:391:HIS:CD2	2.33	0.46
1:C:158:LEU:HD11	3:C:3:HEC:C3C	2.45	0.46
1:D:150:GLY:O	1:D:151:GLY:C	2.54	0.46
1:C:318:HIS:HB3	1:C:320:GLN:HE21	1.79	0.46
1:A:195:PRO:HG3	6:A:541:HOH:O	2.15	0.46
1:C:234:LYS:H	1:C:237:ASN:HD22	1.64	0.46
1:C:321:ASP:HB2	6:C:642:HOH:O	2.15	0.46
1:D:160:CYS:O	1:D:164:HIS:HB2	2.16	0.46
1:D:391:HIS:CE1	3:D:4:HEC:O2D	2.67	0.46
1:A:79:TRP:CE2	1:A:261:LYS:HE2	2.51	0.46
1:A:105:LEU:HD23	1:A:455:LYS:HG2	1.97	0.46
1:A:214:VAL:HG21	1:A:227:PHE:CE1	2.51	0.46
1:B:318:HIS:HB3	1:B:320:GLN:NE2	2.31	0.46
1:A:274:ILE:HG13	3:B:5:HEC:HAA2	1.97	0.46
1:B:149:ARG:HG3	6:B:516:HOH:O	2.16	0.46
1:C:309:ASN:CG	1:C:312:GLN:NE2	2.67	0.46
1:D:43:GLU:C	1:D:45:PHE:H	2.19	0.46
1:C:310:PHE:CE2	1:C:314:CYS:HB2	2.51	0.45
1:D:151:GLY:HA3	1:D:466:TRP:CD2	2.52	0.45
1:D:283:ILE:CG2	6:D:519:HOH:O	2.64	0.45
1:B:397:GLU:O	1:B:401:MET:HG3	2.17	0.45
1:C:406:MET:HB3	1:D:406:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:HIS:HB3	1:D:320:GLN:NE2	2.32	0.45
1:B:310:PHE:CE2	1:B:314:CYS:HB2	2.51	0.45
1:C:292:ASN:ND2	1:C:296:LYS:H	2.15	0.45
1:A:163:CYS:SG	3:A:480:HEC:HAC	2.43	0.45
1:B:51:ASP:OD2	5:B:483:EDO:O1	2.35	0.45
1:D:43:GLU:C	1:D:45:PHE:N	2.69	0.45
1:A:391:HIS:HE1	3:A:4:HEC:O2D	1.98	0.45
1:B:42:ASN:OD1	1:B:159:GLY:HA3	2.17	0.45
1:C:477:SER:HB2	6:C:554:HOH:O	2.17	0.45
1:D:227:PHE:N	1:D:227:PHE:CD2	2.85	0.45
1:C:238:MET:CE	1:C:268:GLU:HG2	2.47	0.45
1:A:125:CYS:HG	3:A:479:HEC:CAC	2.22	0.44
1:A:231:ASP:HB3	1:A:240:GLN:HE22	1.82	0.44
1:D:62:GLN:HE21	1:D:302:LYS:HZ1	1.63	0.44
1:D:152:PRO:HG3	1:D:466:TRP:CD1	2.52	0.44
1:A:194:LYS:HE2	6:A:548:HOH:O	2.17	0.44
1:C:194:LYS:HE3	1:C:207:MET:HE3	1.99	0.44
1:C:252:ASN:HD22	1:C:254:LEU:H	1.65	0.44
1:D:158:LEU:CG	3:D:3:HEC:HBC2	2.44	0.44
1:A:217:TYR:HH	1:A:241:TYR:HH	1.58	0.44
1:B:79:TRP:CE3	1:B:84:PHE:HB3	2.53	0.44
1:A:292:ASN:OD1	1:A:296:LYS:CB	2.65	0.44
1:A:381:TRP:CE2	1:A:385:ILE:HD11	2.53	0.44
1:A:472:LYS:HE3	1:A:472:LYS:HA	1.98	0.44
1:D:309:ASN:OD1	1:D:312:GLN:HB2	2.18	0.44
1:B:46:ALA:N	1:B:47:PRO:CD	2.80	0.44
1:B:151:GLY:HA3	1:B:466:TRP:CE2	2.53	0.44
1:C:163:CYS:HG	3:C:480:HEC:CAC	2.26	0.44
5:C:9:EDO:H12	6:C:788:HOH:O	2.17	0.44
1:D:221:LYS:N	1:D:221:LYS:HZ3	2.15	0.44
1:C:180:LEU:HG	1:C:196:PHE:CD1	2.53	0.44
1:D:328:VAL:HG23	5:D:482:EDO:H22	2.00	0.44
1:B:309:ASN:ND2	1:B:312:GLN:HG2	2.33	0.44
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.66	0.44
1:B:383:LEU:HD23	1:B:401:MET:CE	2.48	0.44
1:D:180:LEU:HG	1:D:196:PHE:CD1	2.53	0.44
1:D:228:PRO:HG3	1:D:242:TYR:OH	2.18	0.43
1:B:281:THR:HG22	6:B:493:HOH:O	2.17	0.43
3:A:480:HEC:CBC	3:A:480:HEC:CMC	2.92	0.43
1:C:125:CYS:SG	3:C:479:HEC:C2C	3.04	0.43
1:C:406:MET:HE2	1:D:407:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:OD2	1:D:344:GLU:OE1	2.35	0.43
1:D:121:ALA:HB3	1:D:218:PHE:CZ	2.54	0.43
1:D:476:LEU:O	1:D:477:SER:C	2.57	0.43
1:B:460:LYS:HD3	1:B:460:LYS:HA	1.52	0.43
1:C:213:HIS:HB3	1:C:266:GLU:HB2	2.00	0.43
1:A:310:PHE:HA	1:A:313:THR:OG1	2.19	0.43
1:B:49:HIS:HD2	6:B:706:HOH:O	2.02	0.43
1:C:64:GLU:OE1	6:C:1022:HOH:O	2.22	0.43
1:D:433:ASP:OD1	1:D:439:LYS:CD	2.66	0.43
1:A:384:ALA:N	1:A:401:MET:HE2	2.33	0.43
1:C:397:GLU:O	1:C:401:MET:HG3	2.18	0.43
3:D:480:HEC:HMB1	3:D:480:HEC:HBB3	2.01	0.43
1:A:75:LEU:HB3	1:A:79:TRP:CZ3	2.54	0.43
1:A:199:ALA:HB1	1:A:203:ASP:HB2	2.01	0.43
1:A:317:CYS:SG	3:A:5:HEC:CBC	3.02	0.43
1:B:370:ILE:HD13	1:B:416:LEU:CD2	2.49	0.43
1:C:168:SER:HA	1:C:169:PRO:HD3	1.88	0.43
1:C:467:GLU:O	1:C:471:ARG:HG3	2.19	0.43
1:D:314:CYS:SG	3:D:5:HEC:HBB3	2.56	0.43
1:B:296:LYS:CE	5:B:483:EDO:C1	2.22	0.42
1:B:463:ILE:HB	1:B:464:PRO:HD3	2.01	0.42
1:C:306:PRO:HG2	3:C:4:HEC:CHD	2.49	0.42
1:A:275:HIS:CE1	3:A:5:HEC:NA	2.86	0.42
1:A:305:ASN:HA	1:A:306:PRO:HD3	1.83	0.42
1:D:75:LEU:HB3	1:D:79:TRP:CZ3	2.54	0.42
1:A:289:LYS:NZ	3:A:480:HEC:O1D	2.48	0.42
1:A:313:THR:O	1:A:316:ASN:HB2	2.18	0.42
1:A:320:GLN:HE21	1:A:320:GLN:N	2.09	0.42
1:B:37:THR:CG2	1:B:135:GLN:OE1	2.66	0.42
1:B:452:LYS:O	1:B:456:GLN:HG2	2.19	0.42
1:D:94:HIS:CD2	3:D:3:HEC:C4D	3.03	0.42
1:D:104:THR:HG21	3:D:479:HEC:HMA1	2.02	0.42
1:D:214:VAL:HG21	1:D:227:PHE:CZ	2.54	0.42
1:D:244:LYS:HD2	1:D:244:LYS:HA	1.53	0.42
1:D:263:GLN:O	1:D:264:HIS:C	2.57	0.42
3:A:4:HEC:HBB3	3:A:4:HEC:CMB	2.48	0.42
1:B:240:GLN:HE21	1:B:241:TYR:N	2.17	0.42
1:B:296:LYS:NZ	5:B:483:EDO:C2	2.82	0.42
1:D:102:ARG:HD3	1:D:463:ILE:HD12	2.01	0.42
1:D:139:GLU:OE1	1:D:183:PRO:HB2	2.20	0.42
1:D:221:LYS:HE2	1:D:222:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.85	0.42
1:B:336:ILE:O	1:B:340[A]:LYS:HB3	2.19	0.42
1:D:159:GLY:O	1:D:162:ASP:HB2	2.20	0.42
1:D:391:HIS:CD2	6:D:804:HOH:O	2.62	0.42
1:C:106:ARG:NE	6:C:673:HOH:O	2.36	0.42
1:B:231:ASP:OD2	1:B:240:GLN:NE2	2.53	0.42
1:B:275:HIS:CG	3:B:4:HEC:HBC2	2.54	0.42
1:D:252:ASN:ND2	1:D:254:LEU:HB2	2.34	0.42
1:D:438:GLU:H	1:D:438:GLU:CD	2.22	0.42
1:D:463:ILE:N	1:D:464:PRO:CD	2.83	0.42
3:D:3:HEC:HBB3	3:D:3:HEC:HMB1	2.02	0.42
1:A:118:LEU:HB3	1:A:119:PRO:HD2	2.02	0.41
1:A:180:LEU:HG	1:A:196:PHE:CD1	2.55	0.41
1:B:52:GLN:NE2	1:B:52:GLN:N	2.62	0.41
3:C:3:HEC:CBC	3:C:3:HEC:CMC	2.97	0.41
1:A:158:LEU:HD11	3:A:3:HEC:C3C	2.49	0.41
1:C:346:GLN:HG3	1:C:406:MET:SD	2.60	0.41
1:A:266:GLU:O	1:A:270:TRP:HB3	2.20	0.41
1:B:263:GLN:HA	6:B:1042:HOH:O	2.19	0.41
1:A:37:THR:OG1	1:A:135:GLN:NE2	2.52	0.41
1:B:127:SER:HB3	1:B:154:ILE:HG23	2.03	0.41
1:B:313:THR:O	1:B:316:ASN:HB2	2.20	0.41
1:C:325:LEU:HD23	5:C:484:EDO:H11	2.01	0.41
1:D:123:TRP:CE2	1:D:147:TRP:CD1	3.09	0.41
1:D:340:LYS:CE	6:D:501:HOH:O	2.69	0.41
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.83	0.41
1:A:292:ASN:OD1	1:A:296:LYS:HB3	2.20	0.41
1:B:296:LYS:CE	5:B:483:EDO:H22	2.50	0.41
1:C:65:ARG:NE	6:C:633:HOH:O	2.54	0.41
1:C:311:ALA:O	1:C:315:ALA:HB3	2.21	0.41
1:D:125:CYS:HB3	1:D:212:CYS:HB3	2.03	0.41
1:D:353:GLU:HB2	1:D:416:LEU:HD13	2.02	0.41
1:A:82:TYR:CD1	1:A:83:PRO:HD2	2.55	0.41
1:B:71:GLU:OE2	6:B:636:HOH:O	2.21	0.41
1:C:46:ALA:N	1:C:47:PRO:CD	2.84	0.41
1:D:469:GLN:HA	1:D:469:GLN:NE2	2.36	0.41
1:A:292:ASN:ND2	1:A:294:GLU:H	2.19	0.41
1:D:122:CYS:SG	3:D:479:HEC:C3B	3.00	0.41
1:D:468:GLU:HA	1:D:471:ARG:NH1	2.36	0.41
3:C:5:HEC:HBB3	3:C:5:HEC:CMB	2.44	0.41
1:D:168:SER:HA	1:D:169:PRO:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLN:NE2	1:D:241:TYR:N	2.68	0.41
1:D:274:ILE:HD13	1:D:274:ILE:HA	1.92	0.41
1:D:325:LEU:HD12	1:D:325:LEU:HA	1.72	0.41
1:A:128:PRO:HD3	1:A:158:LEU:HA	2.03	0.41
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.78	0.41
1:A:136:LYS:HE2	1:A:137:ASP:OD1	2.20	0.41
1:A:292:ASN:ND2	1:A:294:GLU:N	2.69	0.41
1:B:352:PHE:CD2	1:B:431:ILE:CD1	3.00	0.41
1:C:79:TRP:CE3	1:C:84:PHE:HB3	2.56	0.41
1:C:92:ARG:HB2	1:C:93:GLY:H	1.77	0.41
1:C:391:HIS:H	1:C:391:HIS:CD2	2.39	0.41
1:D:287:MET:HE1	1:D:299:THR:HG21	2.02	0.41
1:A:283:ILE:HD11	3:A:3:HEC:CBB	2.50	0.41
1:B:119:PRO:HG3	1:B:223:LYS:HD2	2.03	0.41
1:D:82:TYR:CD1	1:D:83:PRO:HD2	2.56	0.41
1:D:118:LEU:HB3	1:D:119:PRO:HD2	2.02	0.41
1:D:151:GLY:HA2	1:D:466:TRP:CZ3	2.56	0.41
1:A:144:HIS:O	1:A:149:ARG:NH2	2.48	0.40
1:A:381:TRP:CZ2	1:A:385:ILE:HD11	2.56	0.40
1:B:62:GLN:HE21	1:B:302:LYS:NZ	2.18	0.40
1:B:123:TRP:CB	1:B:154:ILE:HD13	2.51	0.40
1:D:103:GLU:O	1:D:455:LYS:HE2	2.20	0.40
3:A:480:HEC:HMB1	3:A:480:HEC:CBB	2.35	0.40
1:D:396:GLU:HG2	1:D:397:GLU:N	2.36	0.40
1:A:198:LYS:HE3	1:C:65:ARG:HH11	1.77	0.40
1:A:438:GLU:H	1:A:438:GLU:CD	2.24	0.40
1:C:158:LEU:HD11	3:C:3:HEC:C4C	2.52	0.40
1:D:213:HIS:CE1	3:D:479:HEC:HMD1	2.56	0.40
1:D:431:ILE:HG22	1:D:432:PRO:O	2.21	0.40
1:B:257:THR:O	1:B:259:MET:HG2	2.21	0.40
1:C:214:VAL:HG21	1:C:227:PHE:CZ	2.57	0.40
1:C:263:GLN:O	1:C:264:HIS:C	2.60	0.40
1:D:234:LYS:H	1:D:237:ASN:HD22	1.70	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	440/452 (97%)	423 (96%)	17 (4%)	0	100	100
1	B	441/452 (98%)	427 (97%)	14 (3%)	0	100	100
1	C	443/452 (98%)	434 (98%)	8 (2%)	1 (0%)	47	58
1	D	441/452 (98%)	413 (94%)	25 (6%)	3 (1%)	22	26
All	All	1765/1808 (98%)	1697 (96%)	64 (4%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	THR
1	C	422	THR
1	D	136	LYS
1	D	151	GLY

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	363/370 (98%)	348 (96%)	15 (4%)	30	43
1	B	364/370 (98%)	348 (96%)	16 (4%)	28	39
1	C	366/370 (99%)	354 (97%)	12 (3%)	38	53
1	D	364/370 (98%)	349 (96%)	15 (4%)	30	43
All	All	1457/1480 (98%)	1399 (96%)	58 (4%)	31	44

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	82	TYR
1	A	221	LYS
1	A	240	GLN
1	A	244	LYS
1	A	274	ILE
1	A	279	ASN
1	A	283	ILE
1	A	292	ASN
1	A	296	LYS
1	A	309	ASN
1	A	312	GLN
1	A	320	GLN
1	A	327	LYS
1	A	472	LYS
1	B	37	THR
1	B	52	GLN
1	B	99	THR
1	B	111	LYS
1	B	114	GLU
1	B	149	ARG
1	B	240	GLN
1	B	252	ASN
1	B	274	ILE
1	B	309	ASN
1	B	316	ASN
1	B	320	GLN
1	B	325	LEU
1	B	419	LEU
1	B	460	LYS
1	B	477	SER
1	C	52	GLN
1	C	221	LYS
1	C	222	ASN
1	C	252	ASN
1	C	256	LYS
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	340	LYS
1	C	385	ILE

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Mol	Chain	Res	Type
1	C	477	SER
1	D	52	GLN
1	D	99	THR
1	D	112	ASN
1	D	114	GLU
1	D	190	GLU
1	D	221	LYS
1	D	240	GLN
1	D	250	TRP
1	D	274	ILE
1	D	283	ILE
1	D	309	ASN
1	D	320	GLN
1	D	325	LEU
1	D	419	LEU
1	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	62	GLN
1	A	135	GLN
1	A	237	ASN
1	A	240	GLN
1	A	252	ASN
1	A	279	ASN
1	A	291	GLN
1	A	292	ASN
1	A	309	ASN
1	A	320	GLN
1	A	326	GLN
1	A	334	GLN
1	A	346	GLN
1	A	371	GLN
1	A	388	HIS
1	A	391	HIS
1	A	427	HIS
1	A	456	GLN
1	A	469	GLN
1	B	49	HIS
1	B	52	GLN

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Mol	Chain	Res	Type
1	B	62	GLN
1	B	222	ASN
1	B	237	ASN
1	B	240	GLN
1	B	252	ASN
1	B	309	ASN
1	B	320	GLN
1	B	337	ASN
1	B	346	GLN
1	B	371	GLN
1	B	388	HIS
1	B	391	HIS
1	B	469	GLN
1	C	48	GLN
1	C	49	HIS
1	C	52	GLN
1	C	62	GLN
1	C	237	ASN
1	C	240	GLN
1	C	252	ASN
1	C	279	ASN
1	C	291	GLN
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	326	GLN
1	C	346	GLN
1	C	371	GLN
1	C	388	HIS
1	C	391	HIS
1	C	427	HIS
1	C	450	GLN
1	C	469	GLN
1	D	42	ASN
1	D	52	GLN
1	D	62	GLN
1	D	144	HIS
1	D	237	ASN
1	D	240	GLN
1	D	252	ASN
1	D	291	GLN

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Mol	Chain	Res	Type
1	D	320	GLN
1	D	326	GLN
1	D	334	GLN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS
1	D	427	HIS
1	D	456	GLN
1	D	469	GLN
1	D	473	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 8 are monoatomic - leaving 37 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	$\#\|Z\| > 2$
3	HEC	A	3	1,2	32,50,50	2.33	4 (12%)	24,82,82	2.02	4 (16%)
3	HEC	C	479	1,4	32,50,50	2.12	4 (12%)	24,82,82	1.47	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	D	480	1	32,50,50	2.22	4 (12%)	24,82,82	1.34	4 (16%)
3	HEC	C	3	1,2	32,50,50	2.03	4 (12%)	24,82,82	1.74	5 (20%)
5	EDO	D	11	-	3,3,3	0.33	0	2,2,2	0.76	0
5	EDO	C	482	-	3,3,3	0.42	0	2,2,2	0.60	0
5	EDO	B	12	-	3,3,3	0.50	0	2,2,2	0.42	0
3	HEC	D	4	1,2	32,50,50	2.12	4 (12%)	24,82,82	1.62	4 (16%)
5	EDO	C	7	-	3,3,3	0.39	0	2,2,2	0.55	0
4	SO3	B	481	-	1,3,3	0.45	0	0,3,3	-	-
3	HEC	B	480	1	32,50,50	2.07	4 (12%)	24,82,82	1.40	3 (12%)
4	SO3	A	481	3	1,3,3	0.78	0	0,3,3	-	-
5	EDO	B	483	-	3,3,3	0.54	0	2,2,2	0.18	0
3	HEC	A	480	1	32,50,50	2.17	3 (9%)	24,82,82	1.50	3 (12%)
4	SO3	D	481	3	1,3,3	0.53	0	0,3,3	-	-
3	HEC	D	479	1,4	32,50,50	2.23	4 (12%)	24,82,82	1.45	5 (20%)
3	HEC	C	5	1	32,50,50	2.08	3 (9%)	24,82,82	1.88	8 (33%)
5	EDO	D	482	-	3,3,3	0.47	0	2,2,2	0.34	0
3	HEC	B	4	1,2	32,50,50	2.14	5 (15%)	24,82,82	2.12	10 (41%)
4	SO3	B	482	3	1,3,3	0.39	0	0,3,3	-	-
5	EDO	A	6	-	3,3,3	0.35	0	2,2,2	0.85	0
3	HEC	A	4	1,2	32,50,50	2.16	3 (9%)	24,82,82	2.02	9 (37%)
3	HEC	B	5	1	32,50,50	2.11	4 (12%)	24,82,82	1.76	4 (16%)
4	SO3	C	481	3	1,3,3	0.25	0	0,3,3	-	-
5	EDO	A	8	-	3,3,3	0.49	0	2,2,2	0.25	0
3	HEC	D	3	1,2	32,50,50	2.18	6 (18%)	24,82,82	1.45	2 (8%)
3	HEC	B	479	1,4	32,50,50	1.96	3 (9%)	24,82,82	1.32	4 (16%)
5	EDO	C	9	-	3,3,3	0.46	0	2,2,2	0.70	0
3	HEC	C	480	1	32,50,50	2.10	3 (9%)	24,82,82	1.51	5 (20%)
5	EDO	C	483	-	3,3,3	0.43	0	2,2,2	0.43	0
3	HEC	A	5	1	32,50,50	2.08	4 (12%)	24,82,82	1.78	4 (16%)
5	EDO	C	484	-	3,3,3	0.47	0	2,2,2	0.26	0
3	HEC	B	3	1,2	32,50,50	2.09	7 (21%)	24,82,82	1.91	6 (25%)
5	EDO	C	10	-	3,3,3	0.44	0	2,2,2	0.43	0
3	HEC	C	4	1,2	32,50,50	2.09	3 (9%)	24,82,82	1.73	5 (20%)
3	HEC	D	5	1	32,50,50	2.03	4 (12%)	24,82,82	1.80	7 (29%)
3	HEC	A	479	1,4	32,50,50	2.17	3 (9%)	24,82,82	1.52	3 (12%)

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
3	HEC	A	3	1,2	-	0/10/54/54	-
3	HEC	C	479	1,4	-	2/10/54/54	-
3	HEC	D	480	1	-	4/10/54/54	-
3	HEC	C	3	1,2	-	0/10/54/54	-
5	EDO	D	11	-	-	1/1/1/1	-
5	EDO	C	482	-	-	0/1/1/1	-
5	EDO	B	12	-	-	0/1/1/1	-
3	HEC	D	4	1,2	-	2/10/54/54	-
5	EDO	C	7	-	-	1/1/1/1	-
3	HEC	B	480	1	-	2/10/54/54	-
5	EDO	B	483	-	-	1/1/1/1	-
3	HEC	A	480	1	-	2/10/54/54	-
3	HEC	D	479	1,4	-	3/10/54/54	-
3	HEC	C	5	1	-	5/10/54/54	-
5	EDO	D	482	-	-	0/1/1/1	-
3	HEC	B	4	1,2	-	2/10/54/54	-
5	EDO	A	6	-	-	0/1/1/1	-
3	HEC	A	4	1,2	-	0/10/54/54	-
3	HEC	B	5	1	-	5/10/54/54	-
5	EDO	A	8	-	-	0/1/1/1	-
3	HEC	D	3	1,2	-	2/10/54/54	-
3	HEC	B	479	1,4	-	2/10/54/54	-
5	EDO	C	9	-	-	1/1/1/1	-
3	HEC	C	480	1	-	2/10/54/54	-
5	EDO	C	483	-	-	0/1/1/1	-
3	HEC	A	5	1	-	5/10/54/54	-
5	EDO	C	484	-	-	1/1/1/1	-
3	HEC	B	3	1,2	-	0/10/54/54	-
5	EDO	C	10	-	-	1/1/1/1	-
3	HEC	C	4	1,2	-	0/10/54/54	-
3	HEC	D	5	1	-	4/10/54/54	-
3	HEC	A	479	1,4	-	3/10/54/54	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3	HEC	C2B-C3B	-8.33	1.32	1.40
3	A	4	HEC	C2B-C3B	-6.66	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	480	HEC	C2B-C3B	-6.56	1.33	1.40
3	D	479	HEC	C3C-C2C	-6.42	1.34	1.40
3	C	5	HEC	C2B-C3B	-6.40	1.34	1.40
3	D	480	HEC	C2B-C3B	-6.38	1.34	1.40
3	C	4	HEC	C2B-C3B	-6.37	1.34	1.40
3	B	4	HEC	C2B-C3B	-6.34	1.34	1.40
3	C	479	HEC	C2B-C3B	-6.31	1.34	1.40
3	D	4	HEC	C2B-C3B	-6.26	1.34	1.40
3	D	3	HEC	C2B-C3B	-6.25	1.34	1.40
3	A	479	HEC	C2B-C3B	-6.24	1.34	1.40
3	A	480	HEC	C3C-C2C	-6.23	1.34	1.40
3	B	480	HEC	C2B-C3B	-6.21	1.34	1.40
3	D	480	HEC	C3C-C2C	-6.18	1.34	1.40
3	B	5	HEC	C2B-C3B	-6.14	1.34	1.40
3	A	480	HEC	C2B-C3B	-6.10	1.34	1.40
3	D	5	HEC	C2B-C3B	-5.96	1.34	1.40
3	C	4	HEC	C3C-C2C	-5.93	1.34	1.40
3	B	5	HEC	C3C-C2C	-5.92	1.34	1.40
3	A	5	HEC	C2B-C3B	-5.88	1.34	1.40
3	A	479	HEC	C3C-C2C	-5.87	1.34	1.40
3	B	3	HEC	C2B-C3B	-5.83	1.34	1.40
3	D	479	HEC	C2B-C3B	-5.71	1.34	1.40
3	D	4	HEC	C3C-C2C	-5.69	1.34	1.40
3	B	479	HEC	C2B-C3B	-5.69	1.34	1.40
3	D	479	HEC	C3D-C2D	5.63	1.54	1.37
3	A	4	HEC	C3D-C2D	5.61	1.54	1.37
3	D	480	HEC	C3D-C2D	5.61	1.54	1.37
3	C	479	HEC	C3C-C2C	-5.58	1.34	1.40
3	D	5	HEC	C3D-C2D	5.54	1.54	1.37
3	A	479	HEC	C3D-C2D	5.52	1.54	1.37
3	B	3	HEC	C3D-C2D	5.50	1.54	1.37
3	C	3	HEC	C2B-C3B	-5.50	1.35	1.40
3	C	3	HEC	C3D-C2D	5.47	1.53	1.37
3	D	3	HEC	C3C-C2C	-5.46	1.35	1.40
3	B	4	HEC	C3C-C2C	-5.43	1.35	1.40
3	D	4	HEC	C3D-C2D	5.43	1.53	1.37
3	B	480	HEC	C3C-C2C	-5.37	1.35	1.40
3	D	3	HEC	C3D-C2D	5.36	1.53	1.37
3	A	480	HEC	C3D-C2D	5.34	1.53	1.37
3	C	480	HEC	C3D-C2D	5.34	1.53	1.37
3	B	5	HEC	C3D-C2D	5.29	1.53	1.37
3	C	5	HEC	C3D-C2D	5.28	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	HEC	C3C-C2C	-5.25	1.35	1.40
3	A	5	HEC	C3C-C2C	-5.23	1.35	1.40
3	B	4	HEC	C3D-C2D	5.21	1.53	1.37
3	C	5	HEC	C3C-C2C	-5.17	1.35	1.40
3	A	3	HEC	C3D-C2D	5.15	1.52	1.37
3	A	5	HEC	C3D-C2D	5.10	1.52	1.37
3	C	3	HEC	C3C-C2C	-5.09	1.35	1.40
3	A	3	HEC	C3C-C2C	-5.06	1.35	1.40
3	C	479	HEC	C3D-C2D	5.01	1.52	1.37
3	B	479	HEC	C3D-C2D	4.99	1.52	1.37
3	C	4	HEC	C3D-C2D	4.94	1.52	1.37
3	C	480	HEC	C3C-C2C	-4.86	1.35	1.40
3	B	480	HEC	C3D-C2D	4.84	1.52	1.37
3	B	479	HEC	C3C-C2C	-4.83	1.35	1.40
3	D	5	HEC	C3C-C2C	-4.66	1.35	1.40
3	B	3	HEC	C3C-C2C	-4.54	1.36	1.40
3	D	3	HEC	CAD-C3D	2.76	1.56	1.52
3	B	3	HEC	CAD-C3D	2.75	1.56	1.52
3	A	5	HEC	CAD-C3D	2.65	1.55	1.52
3	B	5	HEC	CAD-C3D	2.64	1.55	1.52
3	B	4	HEC	CMD-C2D	2.51	1.56	1.51
3	D	479	HEC	CAD-C3D	2.41	1.55	1.52
3	B	480	HEC	CAD-C3D	2.29	1.55	1.52
3	B	4	HEC	CMB-C2B	2.27	1.57	1.51
3	B	3	HEC	C3C-C4C	2.24	1.47	1.43
3	C	3	HEC	CAD-C3D	2.20	1.55	1.52
3	B	3	HEC	C4D-ND	2.10	1.40	1.36
3	D	5	HEC	CAD-C3D	2.09	1.55	1.52
3	D	3	HEC	C1D-ND	2.09	1.40	1.36
3	D	3	HEC	C4D-ND	2.07	1.40	1.36
3	A	3	HEC	CMC-C2C	2.06	1.56	1.51
3	B	3	HEC	C1D-ND	2.03	1.40	1.36
3	D	4	HEC	CAD-C3D	2.03	1.55	1.52
3	C	479	HEC	CAD-C3D	2.03	1.55	1.52
3	D	480	HEC	CAA-C2A	2.02	1.55	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3	HEC	CBD-CAD-C3D	-6.11	102.19	112.62
3	B	5	HEC	CBA-CAA-C2A	-5.42	103.47	112.60
3	A	4	HEC	CBA-CAA-C2A	-5.01	104.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	4	HEC	CBA-CAA-C2A	-4.81	104.50	112.60
3	C	3	HEC	CMC-C2C-C1C	-4.39	121.71	128.46
3	A	3	HEC	CMC-C2C-C1C	-4.25	121.93	128.46
3	A	5	HEC	CBA-CAA-C2A	-4.01	105.84	112.60
3	A	5	HEC	CMC-C2C-C1C	-3.95	122.39	128.46
3	D	4	HEC	CMC-C2C-C1C	-3.75	122.69	128.46
3	B	3	HEC	CBD-CAD-C3D	-3.68	106.35	112.62
3	C	5	HEC	CMC-C2C-C1C	-3.67	122.82	128.46
3	D	3	HEC	CBA-CAA-C2A	-3.66	106.44	112.60
3	B	480	HEC	CMC-C2C-C1C	-3.60	122.93	128.46
3	C	3	HEC	CBA-CAA-C2A	-3.51	106.69	112.60
3	C	4	HEC	CMC-C2C-C1C	-3.48	123.12	128.46
3	D	5	HEC	CMC-C2C-C1C	-3.42	123.20	128.46
3	B	3	HEC	CBA-CAA-C2A	-3.40	106.87	112.60
3	B	4	HEC	CBD-CAD-C3D	-3.39	106.83	112.62
3	A	4	HEC	CMC-C2C-C1C	-3.38	123.28	128.46
3	D	4	HEC	CBA-CAA-C2A	-3.37	106.92	112.60
3	B	4	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
3	B	3	HEC	CMB-C2B-C1B	-3.37	123.29	128.46
3	C	4	HEC	CMB-C2B-C1B	-3.31	123.38	128.46
3	A	479	HEC	C1D-C2D-C3D	-3.28	104.71	107.00
3	A	5	HEC	CAD-CBD-CGD	-3.27	104.60	113.76
3	C	5	HEC	C1D-C2D-C3D	-3.26	104.73	107.00
3	B	3	HEC	CMC-C2C-C1C	-3.26	123.46	128.46
3	B	479	HEC	CMB-C2B-C1B	-3.25	123.47	128.46
3	C	480	HEC	CMC-C2C-C1C	-3.21	123.54	128.46
3	D	5	HEC	CBA-CAA-C2A	-3.13	107.32	112.60
3	A	3	HEC	C1D-C2D-C3D	-3.12	104.83	107.00
3	A	4	HEC	C1D-C2D-C3D	-3.10	104.84	107.00
3	D	3	HEC	CMC-C2C-C1C	-3.05	123.78	128.46
3	C	3	HEC	CBD-CAD-C3D	-3.00	107.49	112.62
3	B	4	HEC	CMB-C2B-C1B	-2.98	123.88	128.46
3	A	3	HEC	CBA-CAA-C2A	-2.98	107.58	112.60
3	C	479	HEC	CMC-C2C-C1C	-2.96	123.91	128.46
3	C	5	HEC	CMD-C2D-C3D	2.92	130.44	124.94
3	D	5	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
3	A	479	HEC	CMC-C2C-C1C	-2.90	124.00	128.46
3	D	5	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
3	A	4	HEC	CMB-C2B-C1B	-2.86	124.07	128.46
3	C	4	HEC	CAD-CBD-CGD	-2.85	105.78	113.76
3	B	4	HEC	CMC-C2C-C1C	-2.82	124.13	128.46
3	A	480	HEC	CAD-CBD-CGD	-2.77	105.99	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4	HEC	CAD-CBD-CGD	-2.77	106.00	113.76
3	C	479	HEC	CMB-C2B-C1B	-2.75	124.24	128.46
3	B	479	HEC	CMC-C2C-C1C	-2.74	124.26	128.46
3	B	3	HEC	CMB-C2B-C3B	2.73	129.03	125.82
3	B	5	HEC	CMC-C2C-C1C	-2.71	124.30	128.46
3	D	479	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
3	C	4	HEC	CBA-CAA-C2A	-2.69	108.07	112.60
3	B	4	HEC	CAD-CBD-CGD	-2.67	106.27	113.76
3	C	4	HEC	C1D-C2D-C3D	-2.65	105.15	107.00
3	A	480	HEC	C1D-C2D-C3D	-2.64	105.16	107.00
3	C	5	HEC	CMB-C2B-C1B	-2.64	124.41	128.46
3	A	5	HEC	CMC-C2C-C3C	2.63	128.91	125.82
3	C	5	HEC	CBA-CAA-C2A	-2.63	108.17	112.60
3	A	479	HEC	CMB-C2B-C1B	-2.57	124.52	128.46
3	D	4	HEC	CMB-C2B-C1B	-2.55	124.55	128.46
3	C	480	HEC	C1D-C2D-C3D	-2.51	105.25	107.00
3	D	5	HEC	CMD-C2D-C3D	2.50	129.65	124.94
3	D	479	HEC	CMD-C2D-C3D	2.47	129.60	124.94
3	D	480	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
3	D	479	HEC	CMB-C2B-C1B	-2.44	124.72	128.46
3	B	5	HEC	C1D-C2D-C3D	-2.43	105.31	107.00
3	D	479	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
3	A	480	HEC	CMC-C2C-C1C	-2.42	124.75	128.46
3	C	480	HEC	CMB-C2B-C1B	-2.41	124.76	128.46
3	C	5	HEC	CAD-CBD-CGD	-2.40	107.04	113.76
3	C	5	HEC	CMD-C2D-C1D	-2.37	124.82	128.46
3	B	3	HEC	CMC-C2C-C3C	2.35	128.58	125.82
3	A	4	HEC	O2A-CGA-CBA	2.33	121.51	114.03
3	C	479	HEC	C1D-C2D-C3D	-2.32	105.38	107.00
3	D	4	HEC	CAA-CBA-CGA	-2.32	107.26	113.76
3	B	4	HEC	O1A-CGA-CBA	-2.28	115.76	123.08
3	B	480	HEC	CMB-C2B-C1B	-2.28	124.97	128.46
3	D	480	HEC	CAD-CBD-CGD	-2.25	107.46	113.76
3	B	479	HEC	CMB-C2B-C3B	2.24	128.46	125.82
3	B	4	HEC	O1D-CGD-CBD	-2.23	115.90	123.08
3	B	479	HEC	C1D-C2D-C3D	-2.23	105.44	107.00
3	C	479	HEC	CBD-CAD-C3D	-2.22	108.83	112.62
3	A	4	HEC	O1D-CGD-CBD	-2.22	115.94	123.08
3	D	479	HEC	CMD-C2D-C1D	-2.20	125.09	128.46
3	D	480	HEC	CMB-C2B-C1B	-2.15	125.15	128.46
3	B	5	HEC	CMD-C2D-C3D	2.14	128.97	124.94
3	C	3	HEC	CMD-C2D-C3D	2.13	128.97	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	479	HEC	CBA-CAA-C2A	-2.11	109.05	112.60
3	B	4	HEC	CMB-C2B-C3B	2.09	128.28	125.82
3	A	4	HEC	O2D-CGD-CBD	2.09	120.74	114.03
3	D	480	HEC	CMC-C2C-C1C	-2.07	125.28	128.46
3	D	5	HEC	CBD-CAD-C3D	-2.07	109.08	112.62
3	C	480	HEC	CBD-CAD-C3D	-2.06	109.11	112.62
3	B	480	HEC	CMC-C2C-C3C	2.05	128.23	125.82
3	C	480	HEC	CBA-CAA-C2A	-2.04	109.16	112.60
3	C	5	HEC	C2B-C3B-C4B	2.03	108.54	106.35
3	A	4	HEC	O1A-CGA-CBA	-2.01	116.62	123.08
3	D	5	HEC	CMD-C2D-C1D	-2.01	125.38	128.46
3	B	4	HEC	O2D-CGD-CBD	2.01	120.48	114.03
3	C	3	HEC	CMD-C2D-C1D	-2.01	125.38	128.46

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5	HEC	C2A-CAA-CBA-CGA
3	A	479	HEC	C3D-CAD-CBD-CGD
3	B	5	HEC	C2A-CAA-CBA-CGA
3	C	5	HEC	C2A-CAA-CBA-CGA
5	C	484	EDO	O1-C1-C2-O2
5	C	7	EDO	O1-C1-C2-O2
3	D	479	HEC	C3D-CAD-CBD-CGD
5	B	483	EDO	O1-C1-C2-O2
5	C	9	EDO	O1-C1-C2-O2
5	D	11	EDO	O1-C1-C2-O2
3	A	5	HEC	CAA-CBA-CGA-O1A
3	B	5	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAA-CBA-CGA-O1A
3	A	480	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAA-CBA-CGA-O1A
3	C	5	HEC	CAA-CBA-CGA-O1A
3	B	480	HEC	CAA-CBA-CGA-O1A
3	A	480	HEC	CAA-CBA-CGA-O1A
3	B	479	HEC	CAA-CBA-CGA-O2A
3	C	480	HEC	CAA-CBA-CGA-O1A
3	B	480	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAD-CBD-CGD-O1D
3	B	479	HEC	CAA-CBA-CGA-O1A
3	A	479	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	479	HEC	CAA-CBA-CGA-O1A
3	D	479	HEC	CAA-CBA-CGA-O1A
3	C	5	HEC	CAA-CBA-CGA-O2A
3	A	479	HEC	CAA-CBA-CGA-O2A
3	C	479	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAD-CBD-CGD-O2D
3	D	479	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAD-CBD-CGD-O1D
3	D	5	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAD-CBD-CGD-O2D
5	C	10	EDO	O1-C1-C2-O2
3	C	5	HEC	CAD-CBD-CGD-O2D
3	C	480	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAD-CBD-CGD-O2D
3	D	480	HEC	CAD-CBD-CGD-O2D
3	C	5	HEC	CAD-CBD-CGD-O1D
3	D	480	HEC	CAA-CBA-CGA-O2A
3	D	480	HEC	CAA-CBA-CGA-O1A
3	D	5	HEC	CAD-CBD-CGD-O1D
3	D	480	HEC	CAD-CBD-CGD-O1D
3	D	3	HEC	CAD-CBD-CGD-O2D
3	B	4	HEC	CAA-CBA-CGA-O1A
3	B	4	HEC	CAA-CBA-CGA-O2A
3	D	4	HEC	CAA-CBA-CGA-O1A
3	D	4	HEC	CAA-CBA-CGA-O2A
3	D	3	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

25 monomers are involved in 217 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	HEC	10	0
3	C	479	HEC	7	0
3	D	480	HEC	9	0
3	C	3	HEC	11	0
3	D	4	HEC	8	0
3	B	480	HEC	7	0
5	B	483	EDO	10	0
3	A	480	HEC	15	0
3	D	479	HEC	16	0
3	C	5	HEC	8	0

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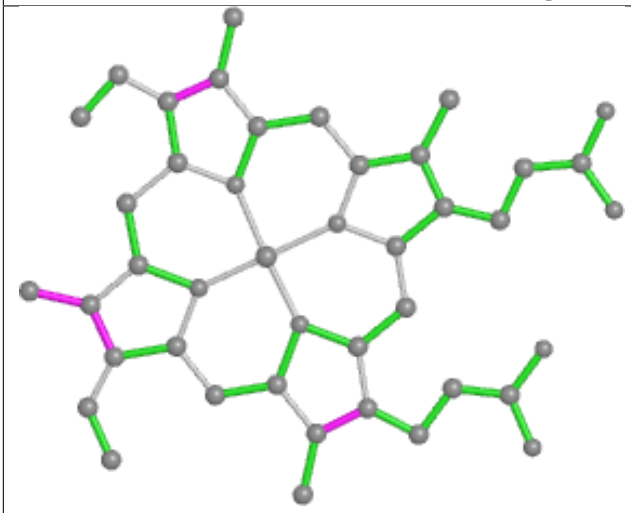
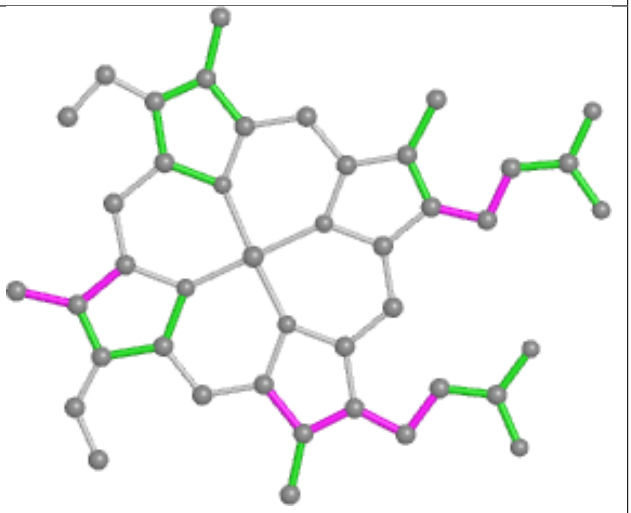
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	482	EDO	8	0
3	B	4	HEC	11	0
3	A	4	HEC	10	0
3	B	5	HEC	11	0
3	D	3	HEC	8	0
3	B	479	HEC	7	0
5	C	9	EDO	4	0
3	C	480	HEC	7	0
5	C	483	EDO	1	0
3	A	5	HEC	11	0
5	C	484	EDO	3	0
3	B	3	HEC	6	0
3	C	4	HEC	11	0
3	D	5	HEC	11	0
3	A	479	HEC	7	0

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.

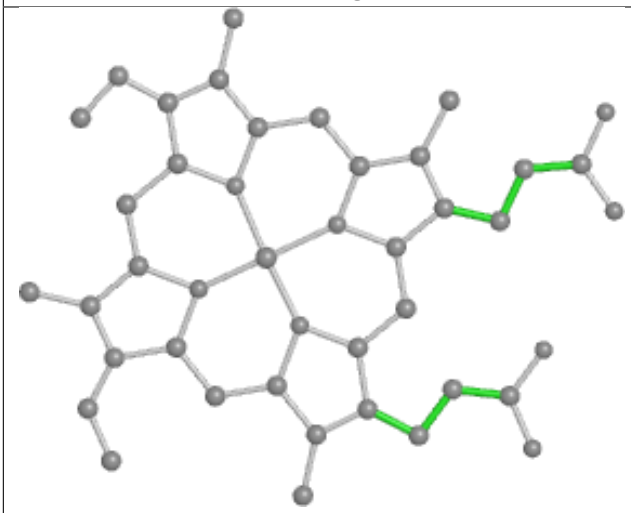
Ligand HEC A 3



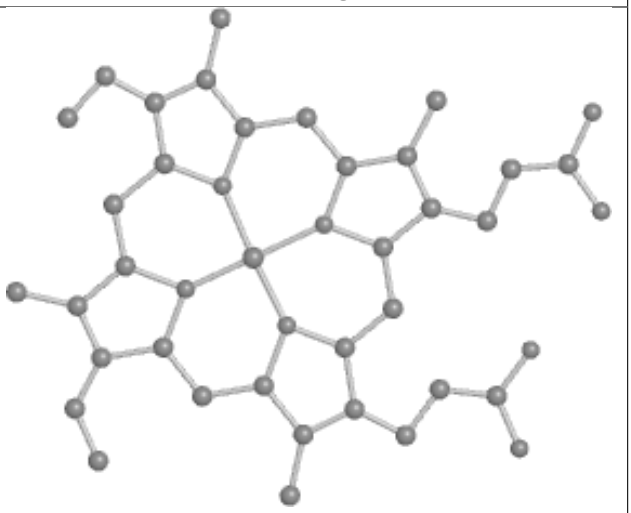
Bond lengths



Bond angles

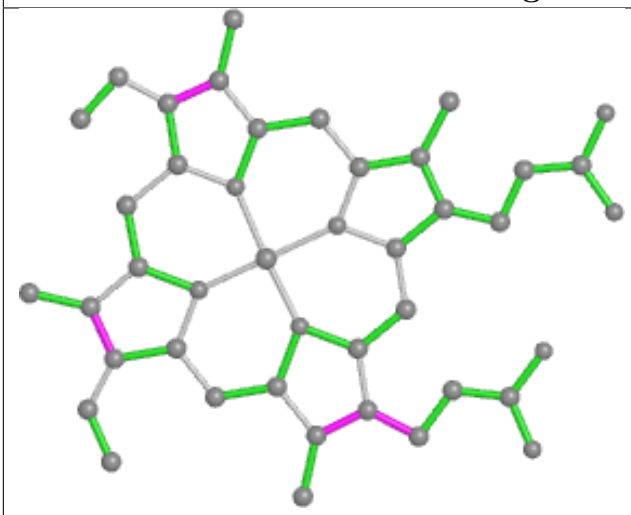


Torsions

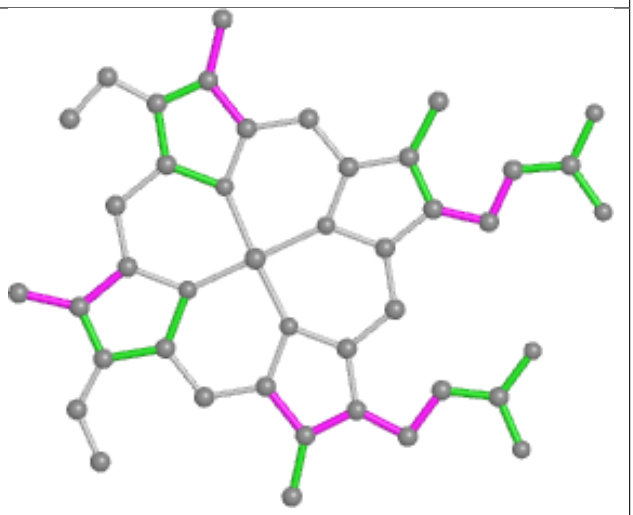


Rings

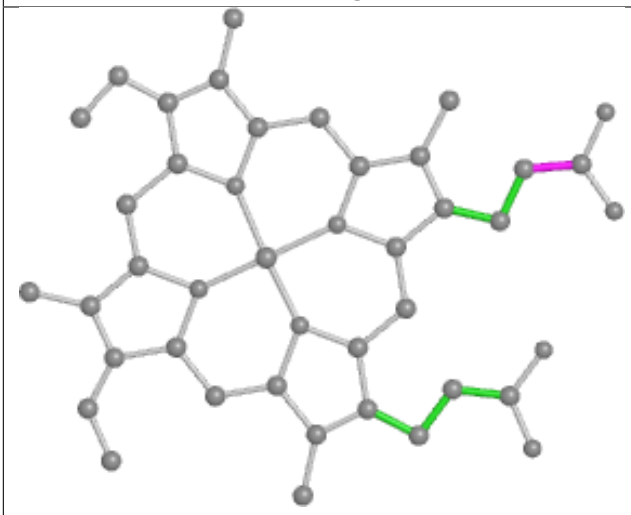
Ligand HEC C 479



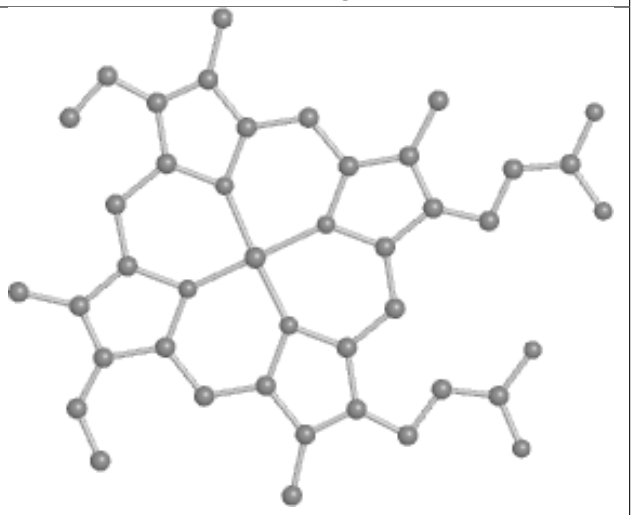
Bond lengths



Bond angles

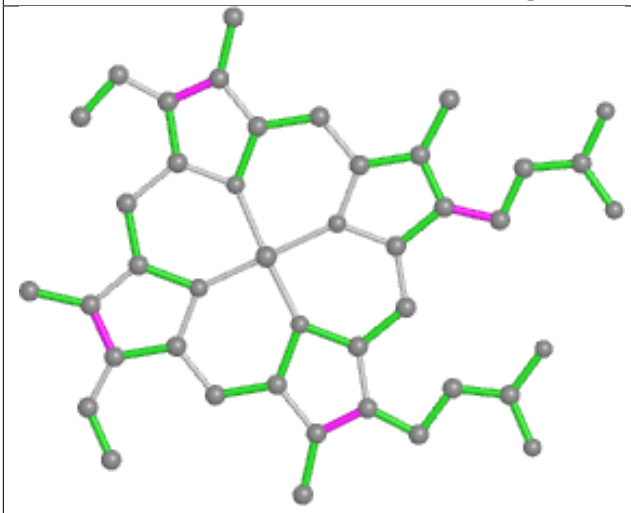


Torsions

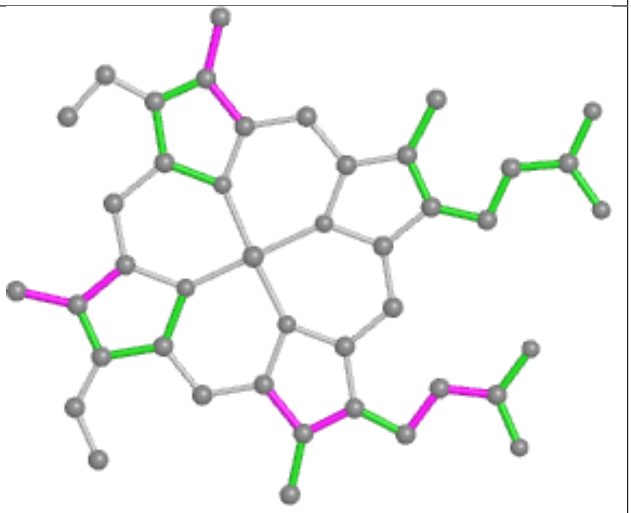


Rings

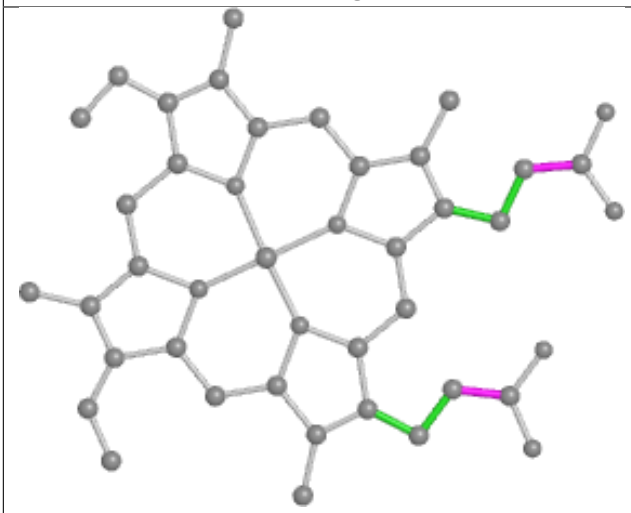
Ligand HEC D 480



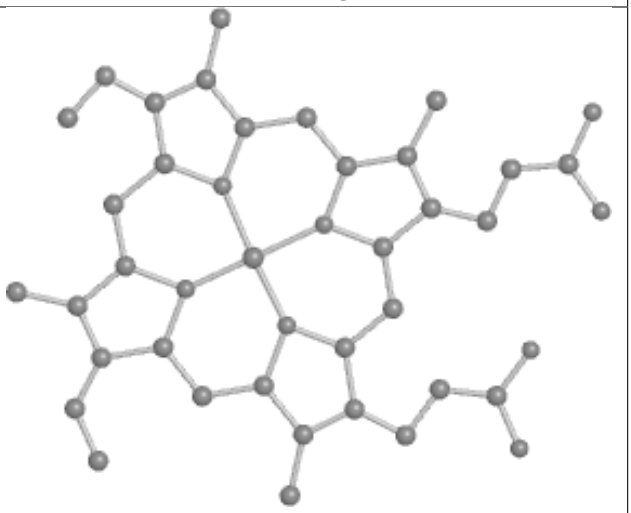
Bond lengths



Bond angles

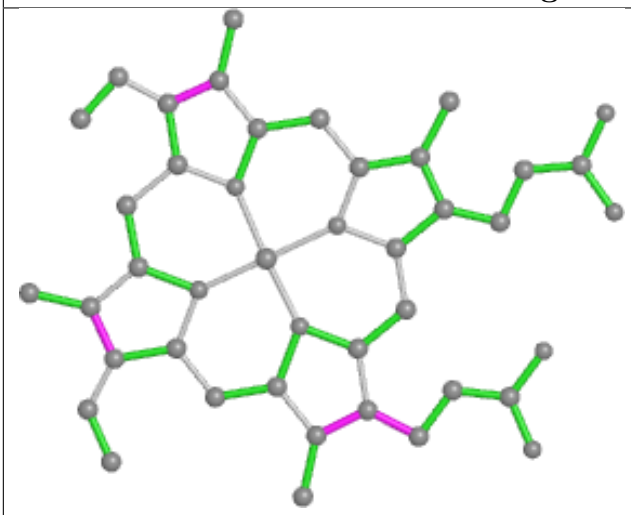


Torsions

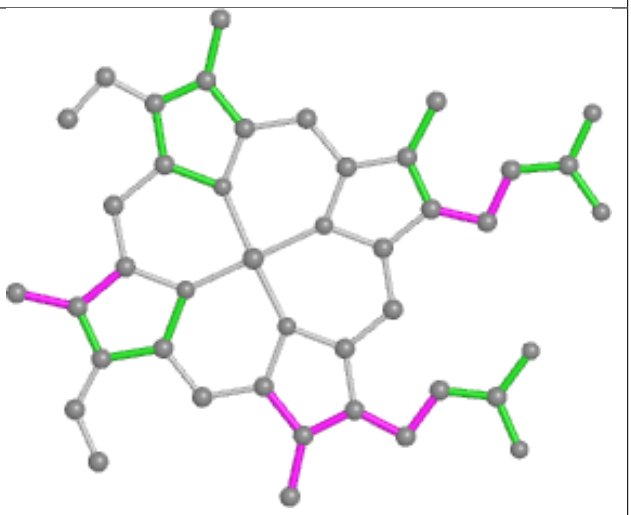


Rings

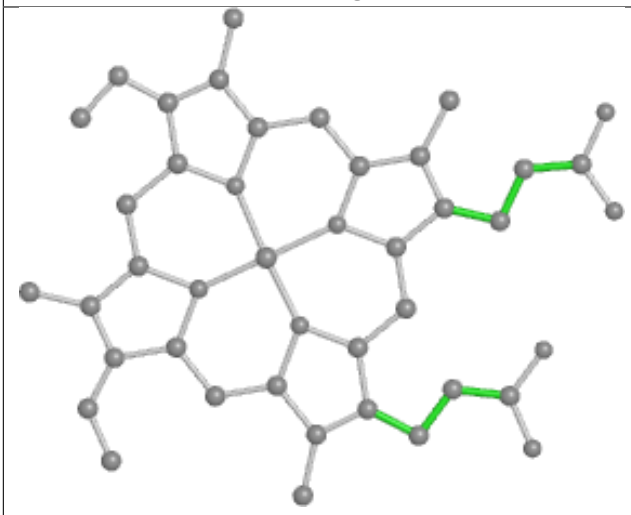
Ligand HEC C 3



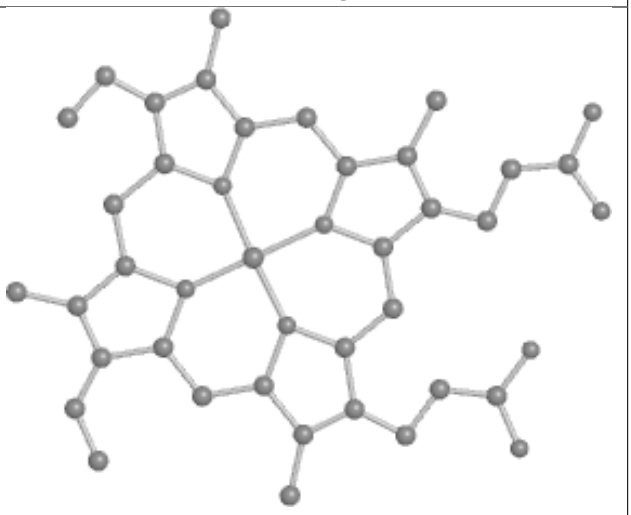
Bond lengths



Bond angles

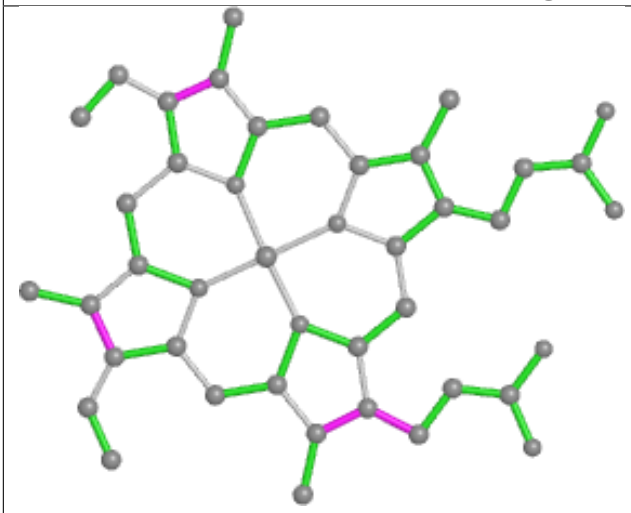


Torsions



Rings

Ligand HEC D 4



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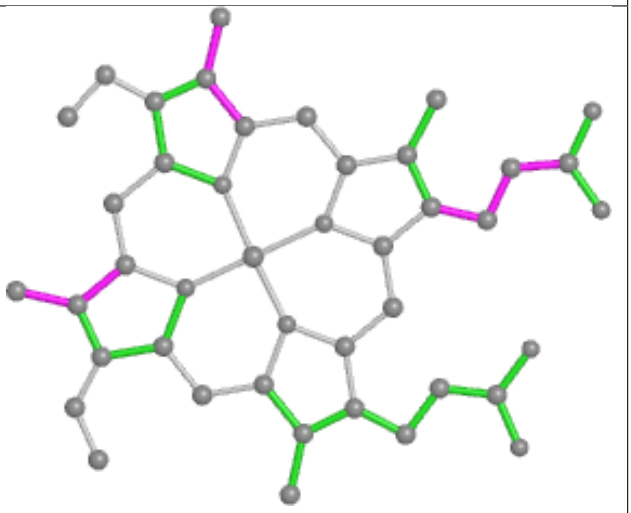

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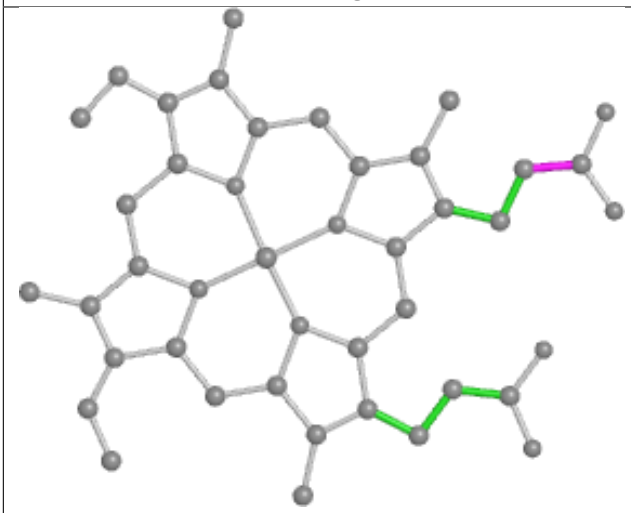

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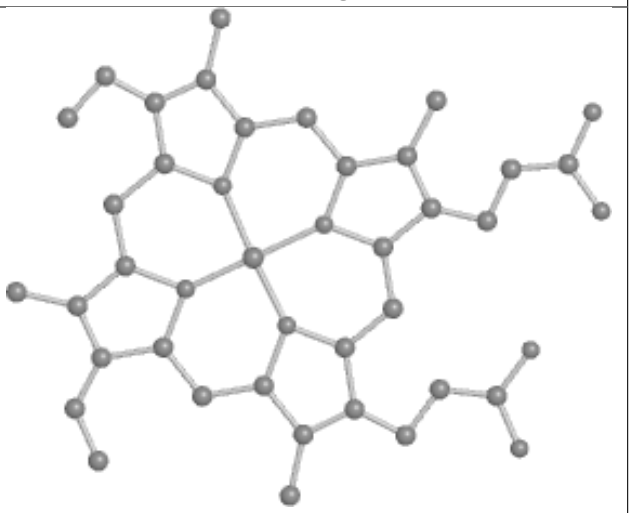
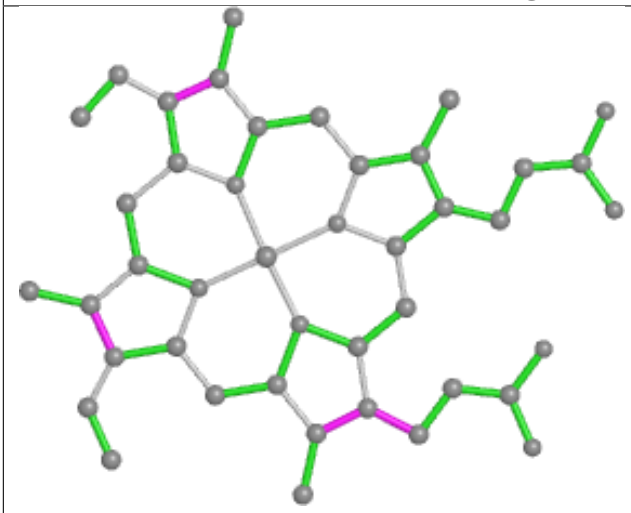


Rings

Ligand HEC B 480



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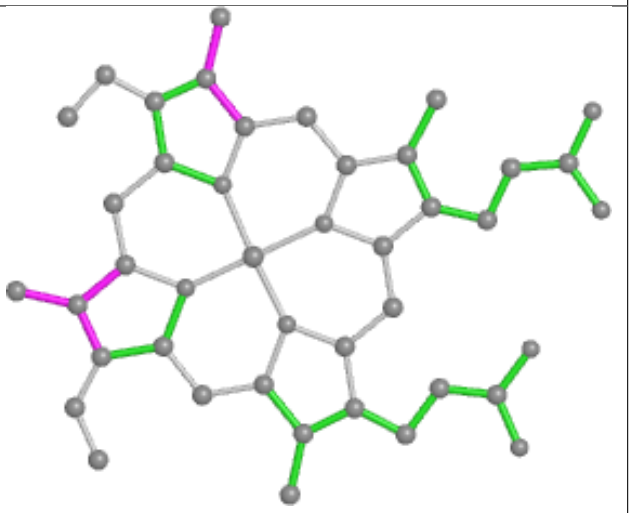
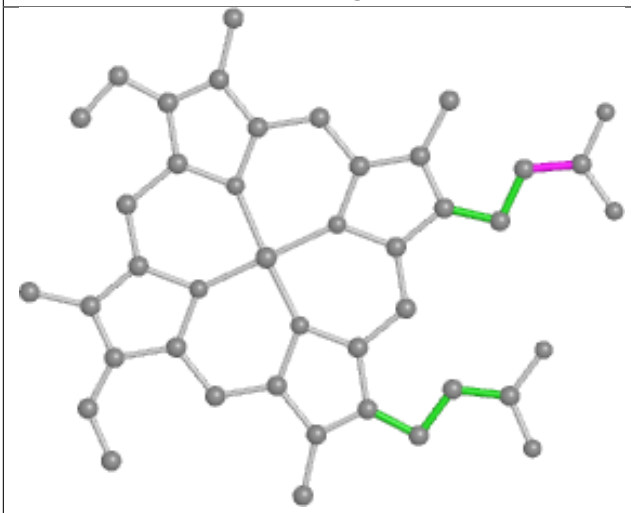


Bond angles



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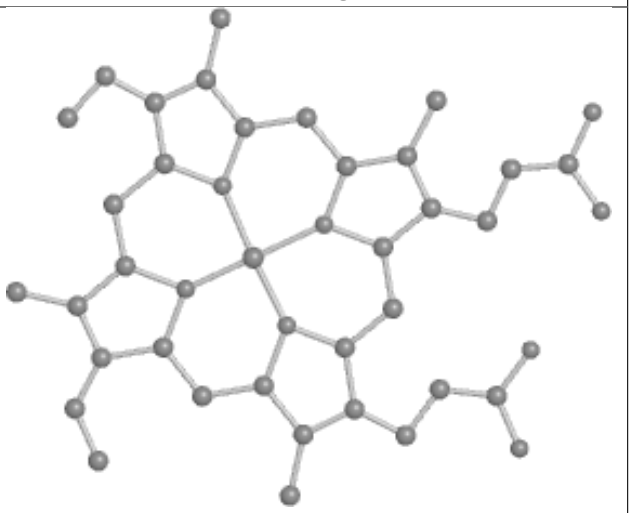
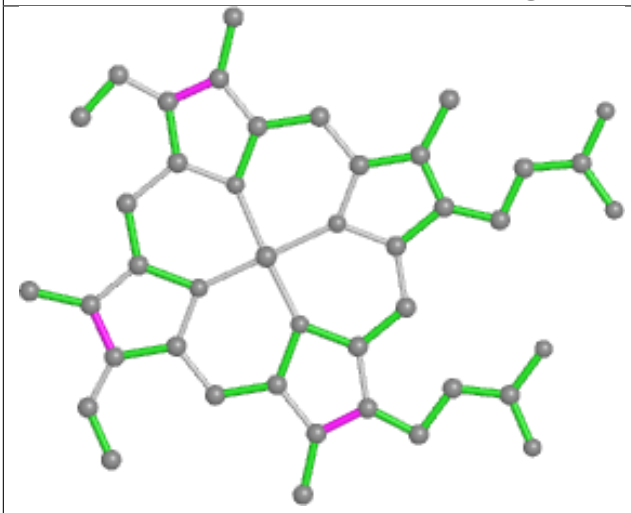


Rings

Ligand HEC A 480



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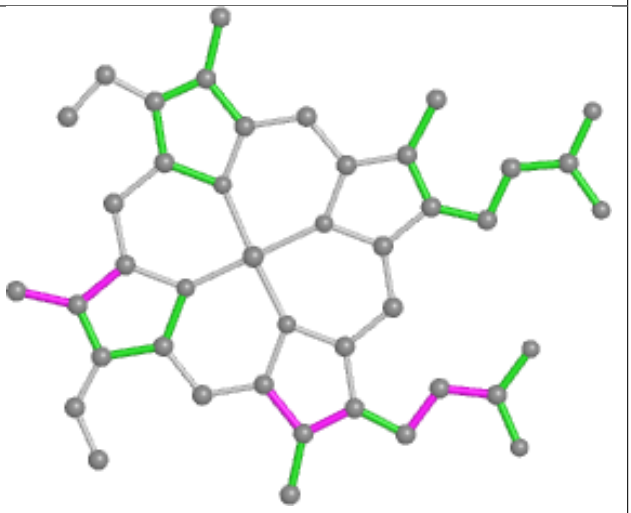

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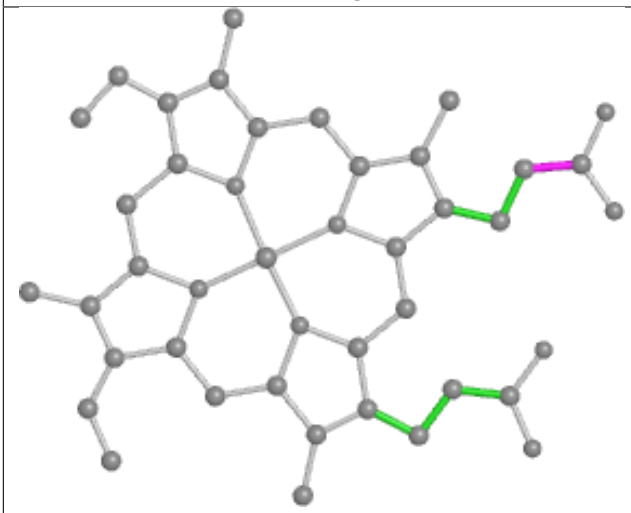

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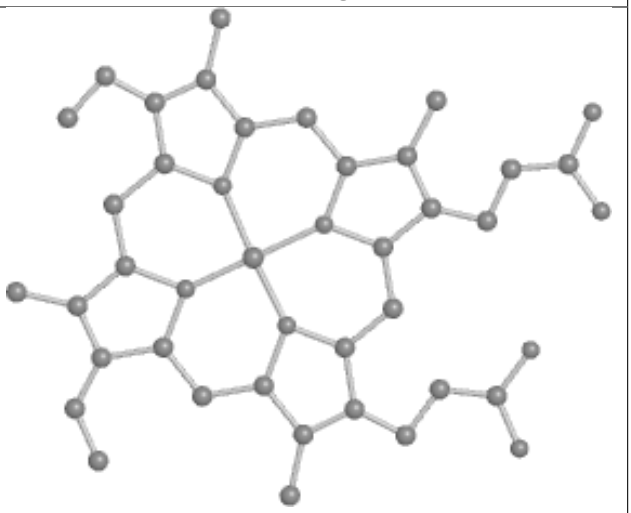
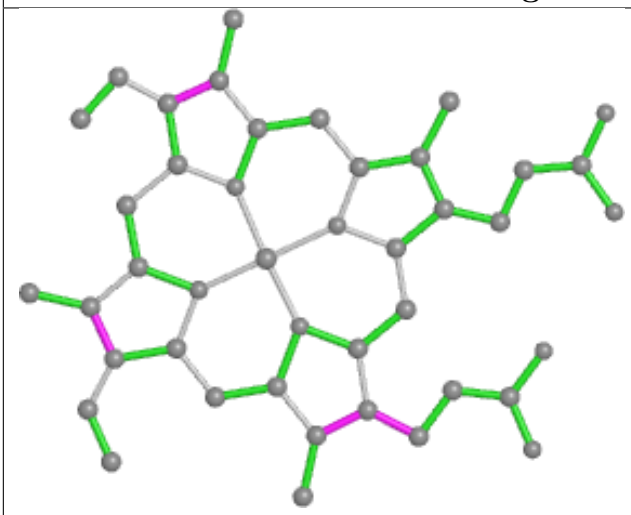


Rings

Ligand HEC D 479



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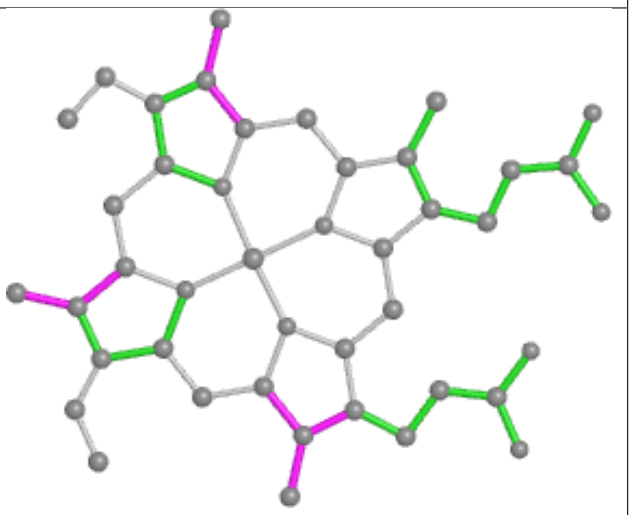

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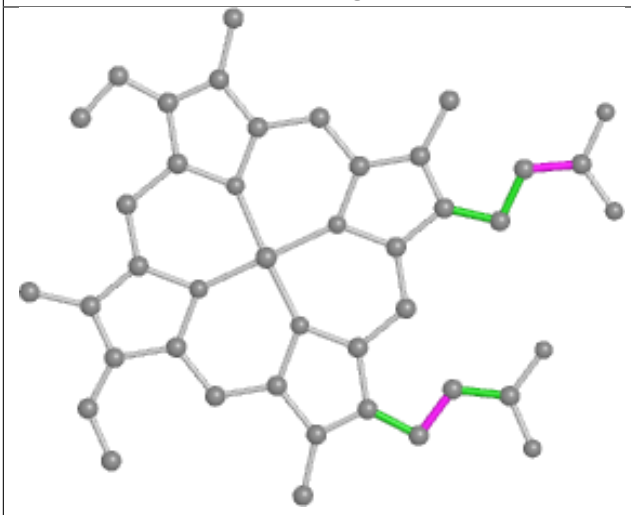

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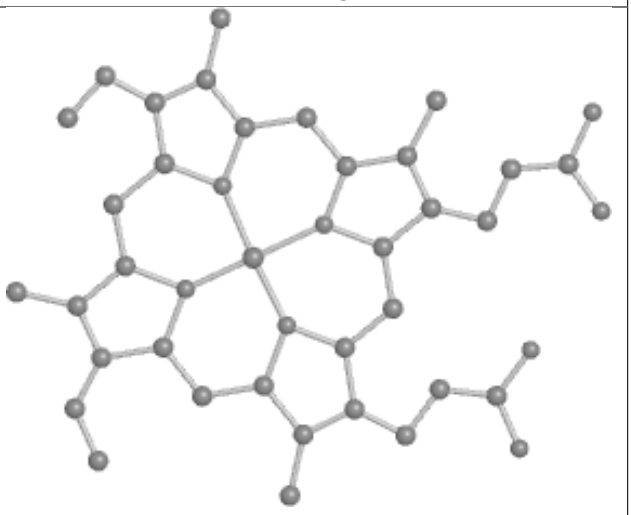
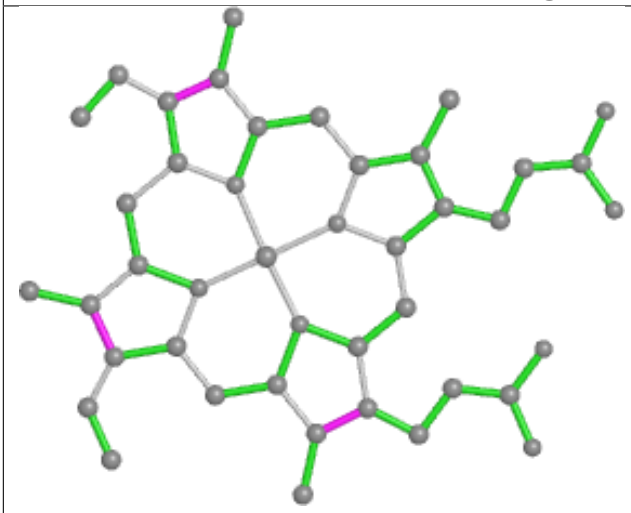


Rings

Ligand HEC C 5



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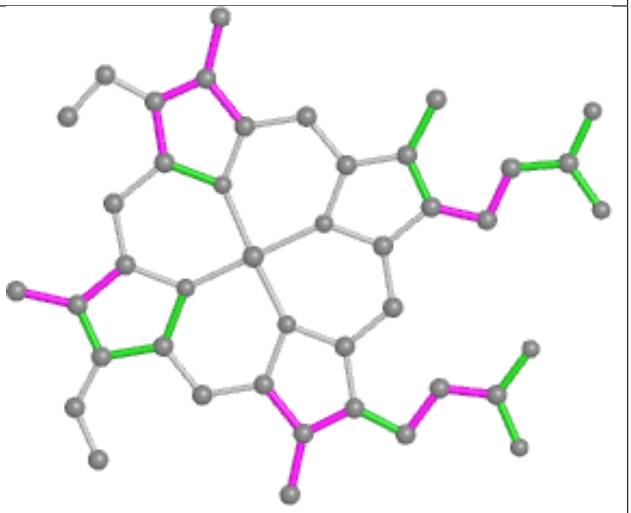

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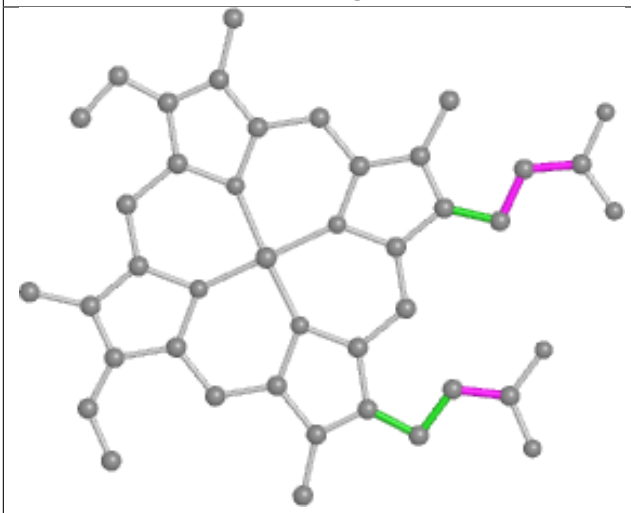

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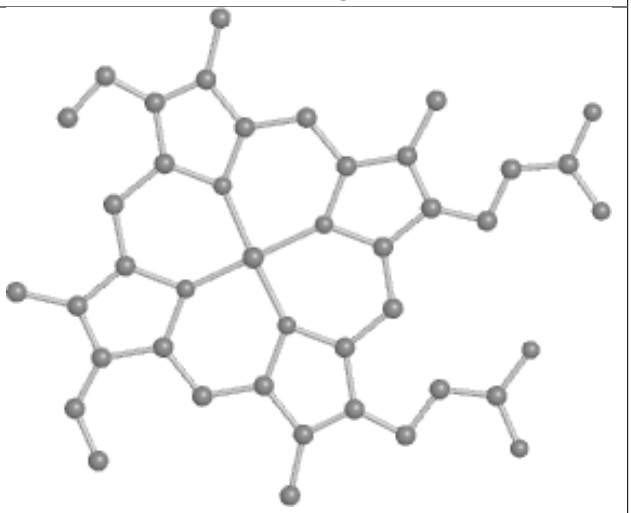
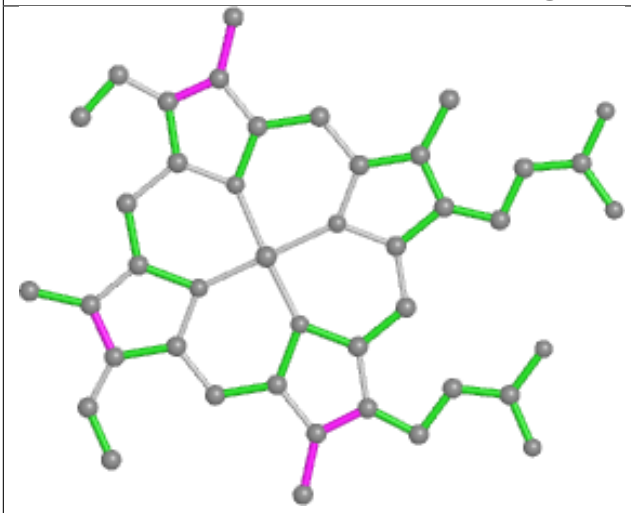


Rings

Ligand HEC B 4



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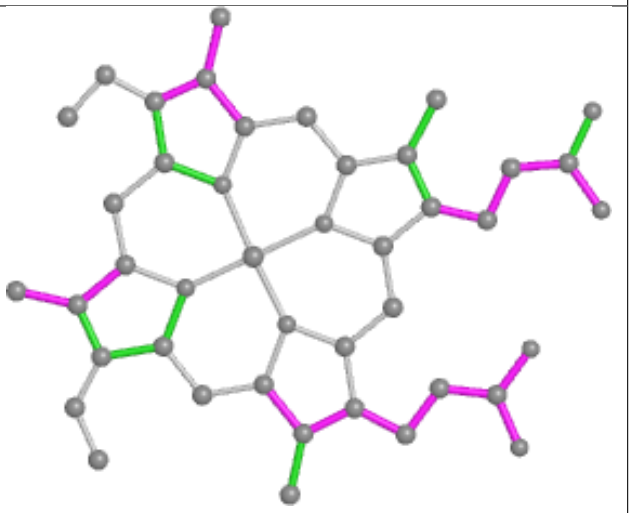
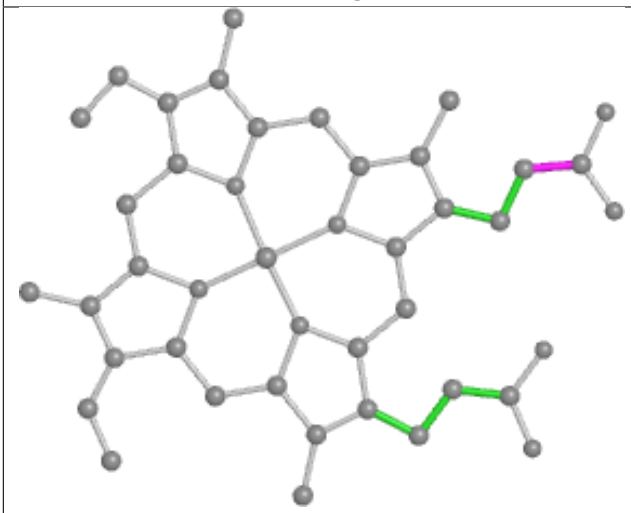


Bond angles



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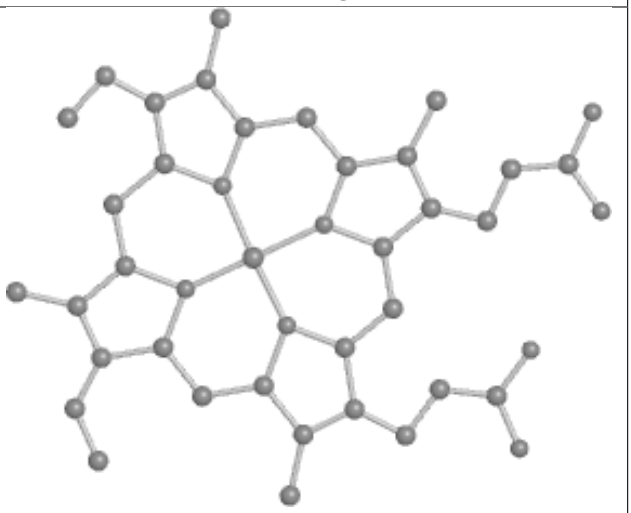
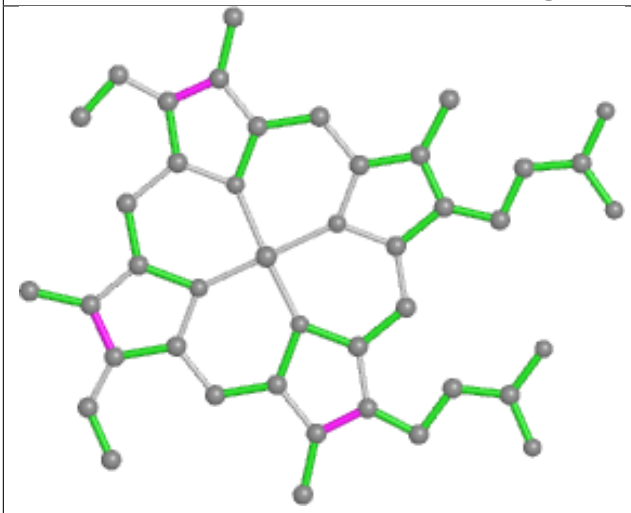


Rings

Ligand HEC A 4



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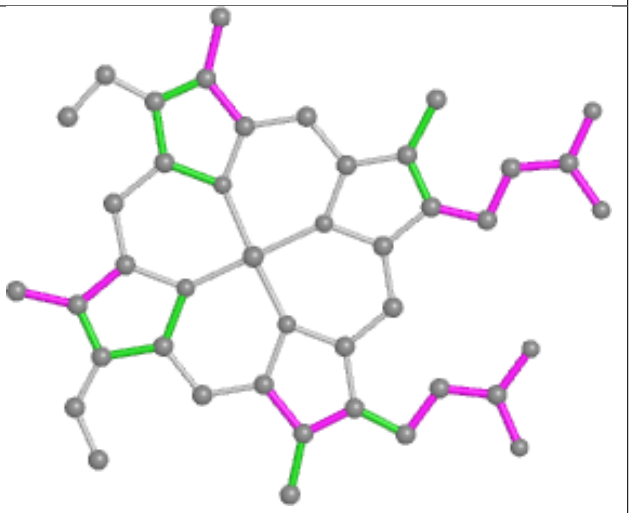

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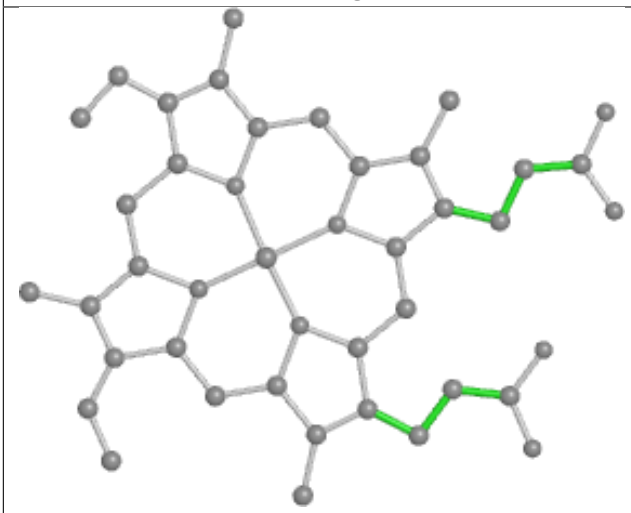

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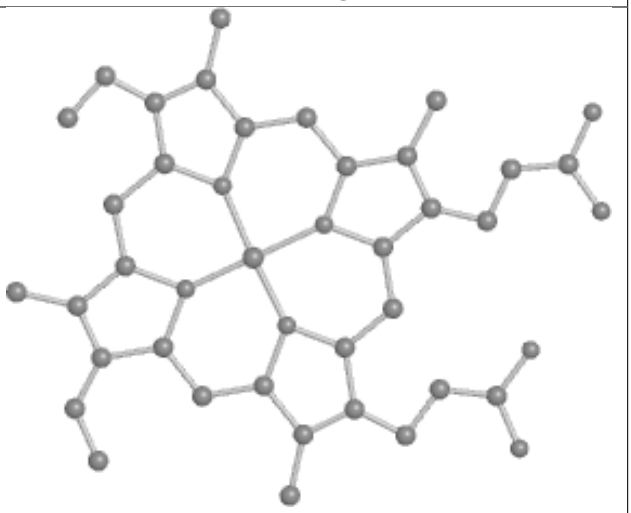
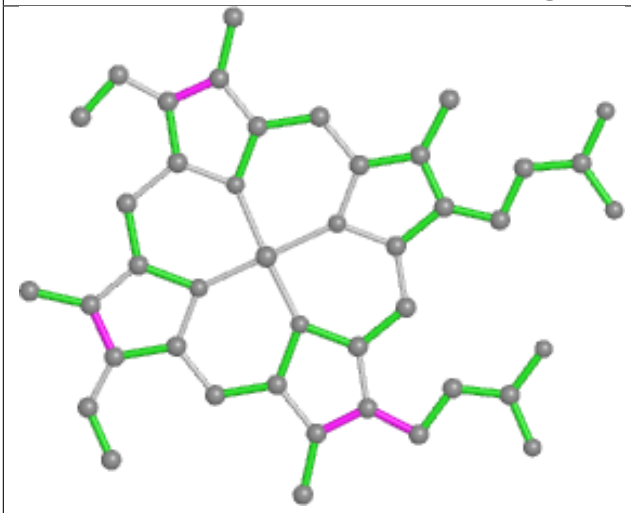


Rings

Ligand HEC B 5



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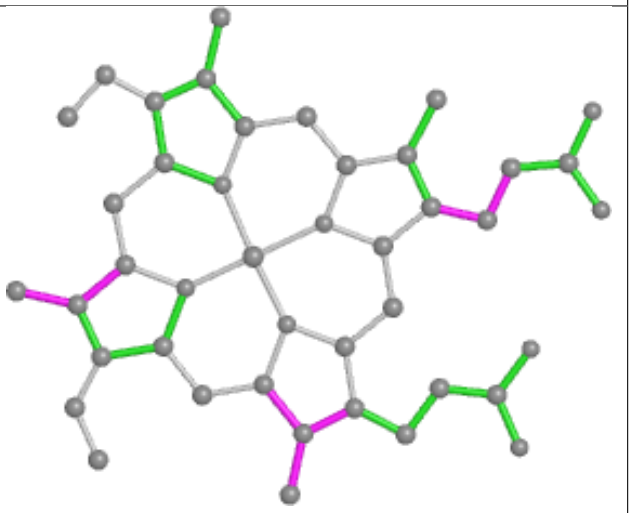
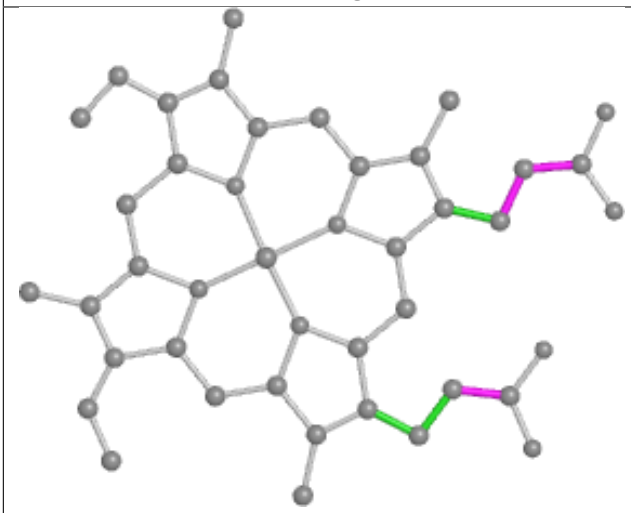


Bond angles



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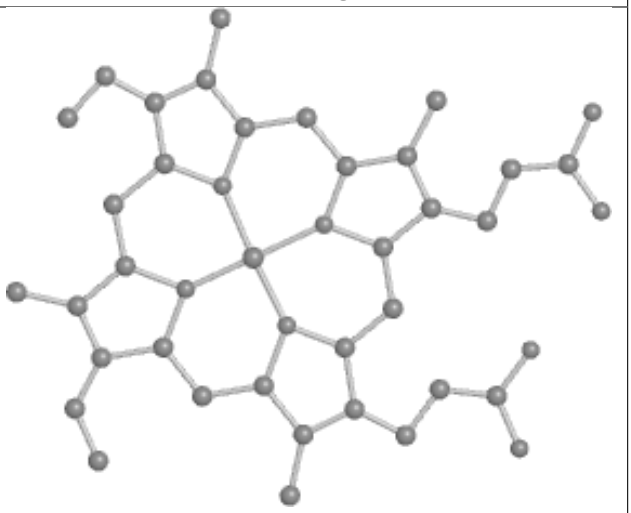
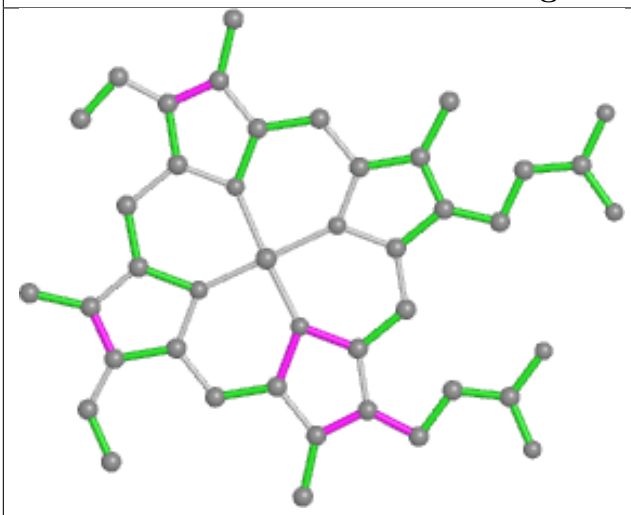


Rings

Ligand HEC D 3



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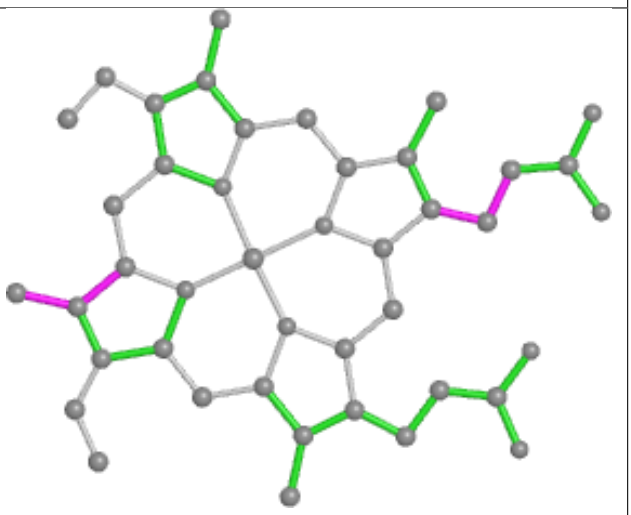
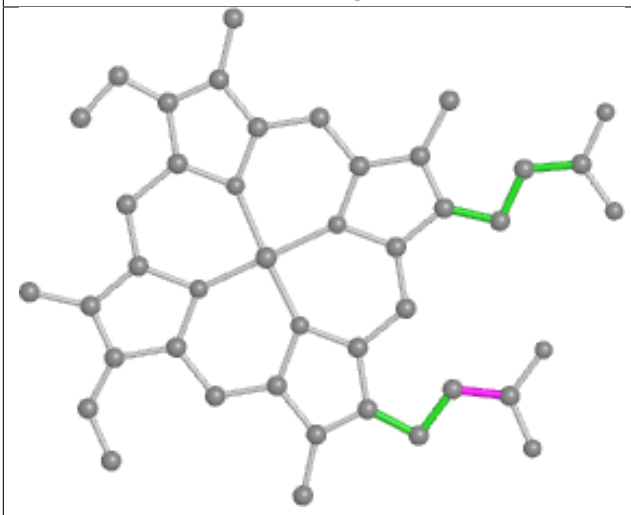


Bond angles



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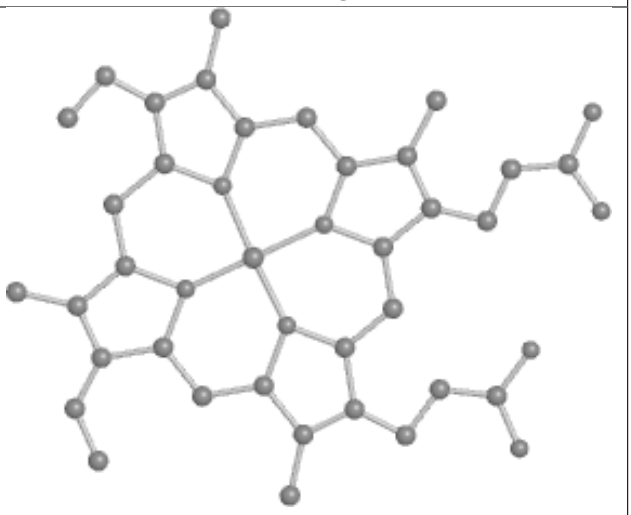
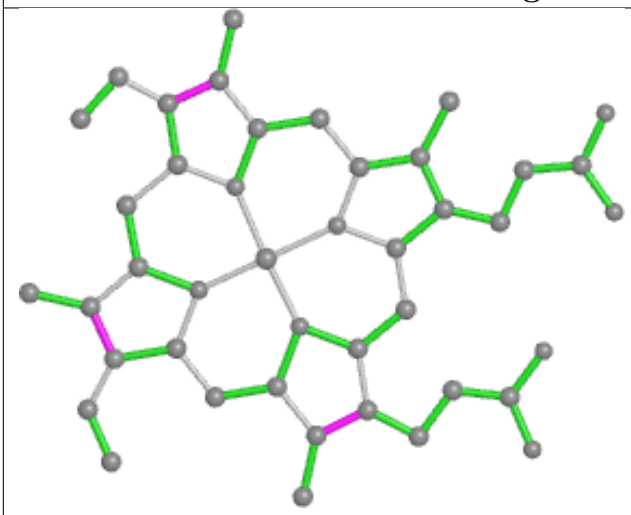


Rings

Ligand HEC B 479



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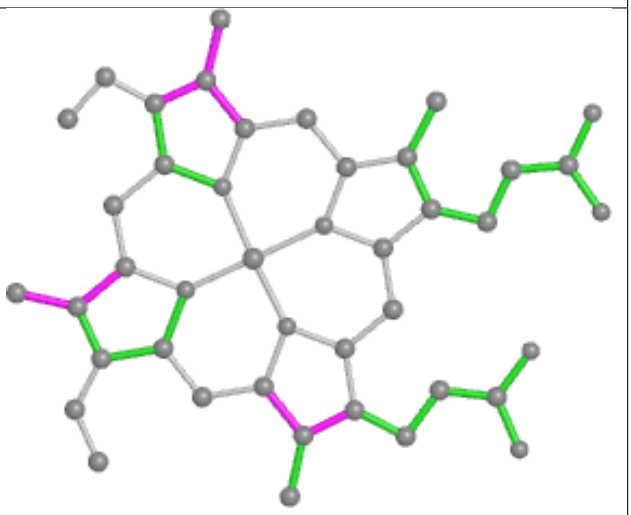

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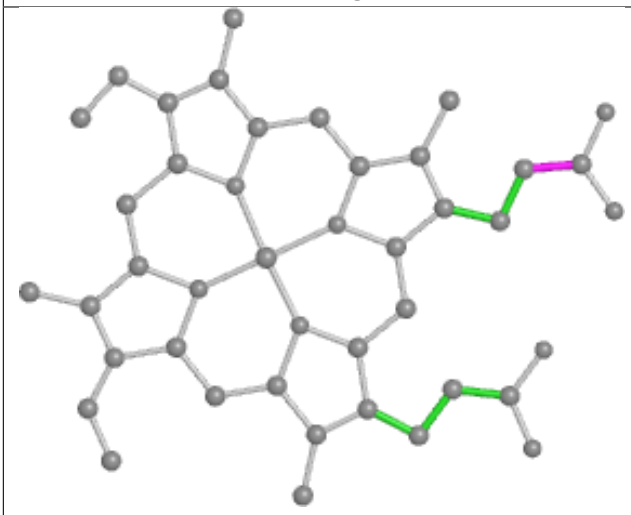

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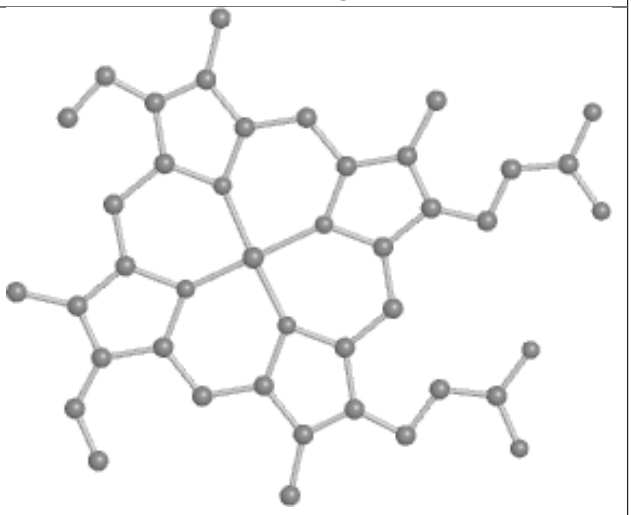
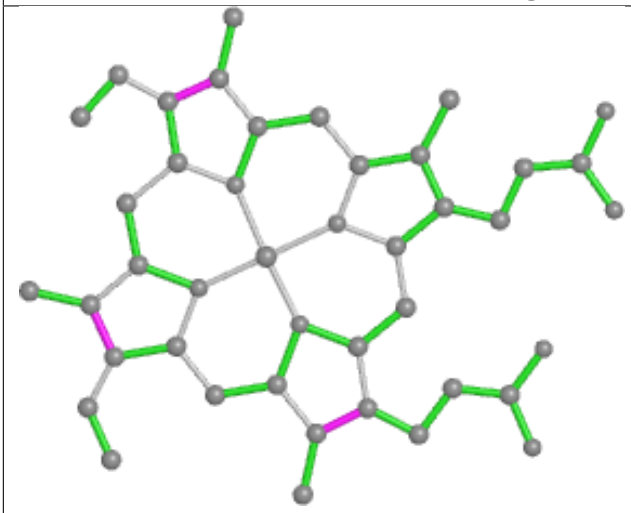


Rings

Ligand HEC C 480



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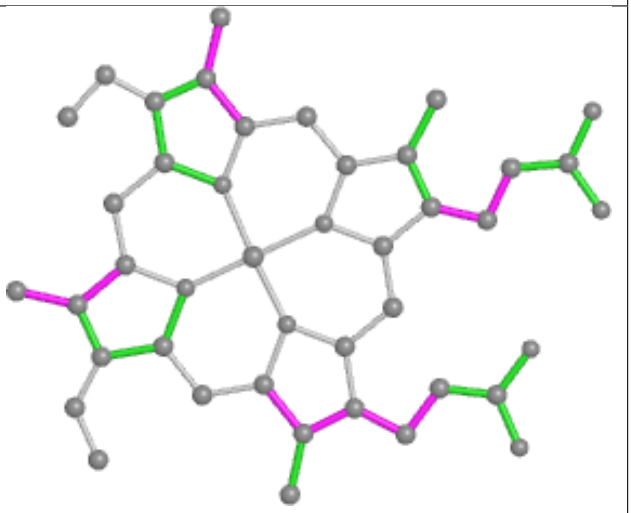

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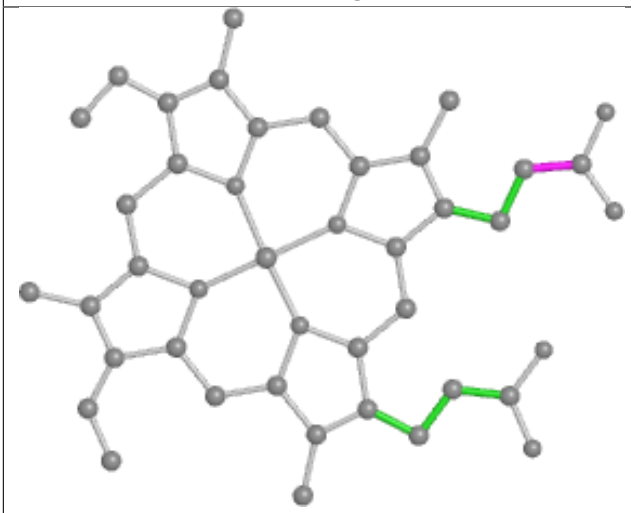

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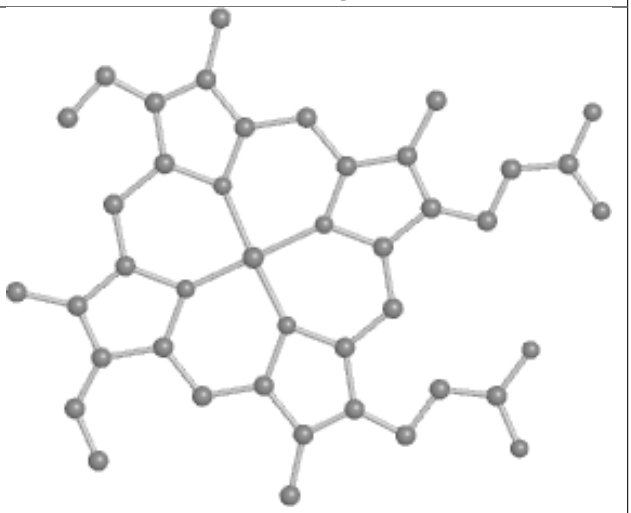
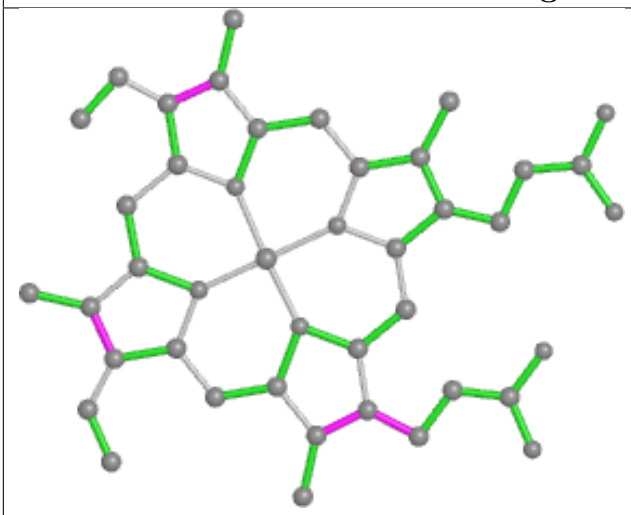


Rings

Ligand HEC A 5



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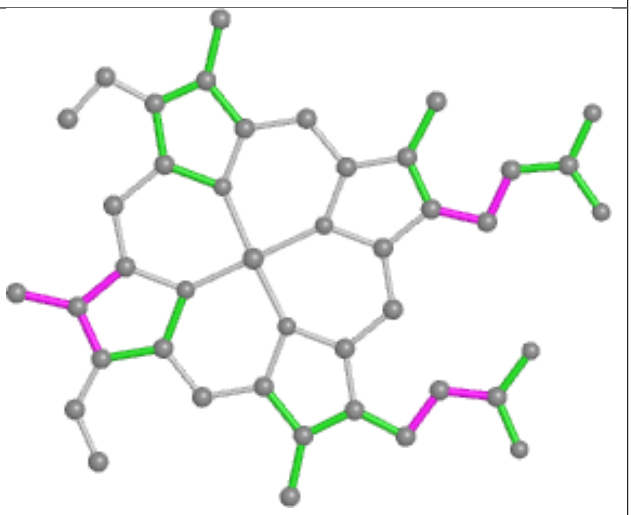
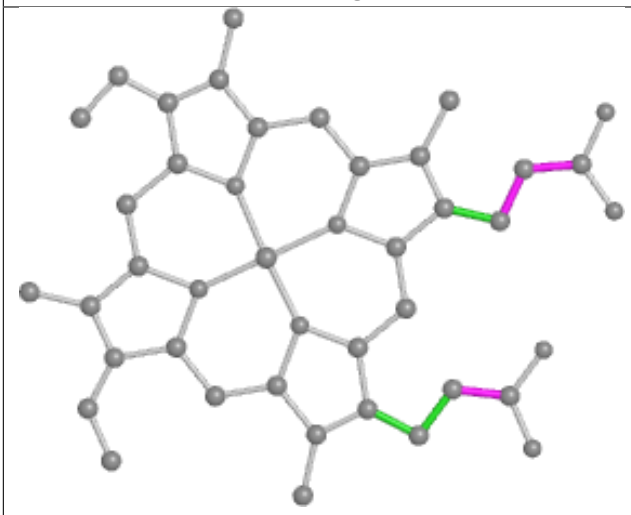
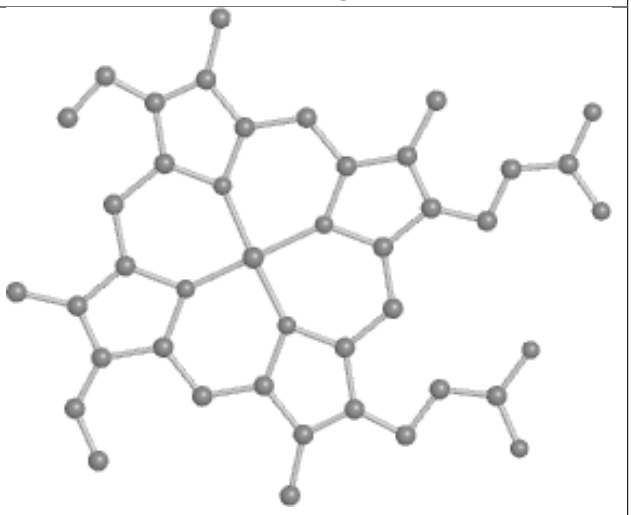


Bond angles

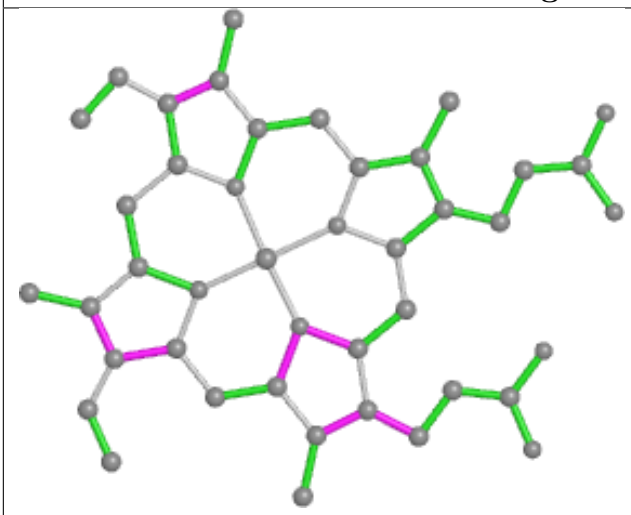


Torsions



Rings

Ligand HEC B 3



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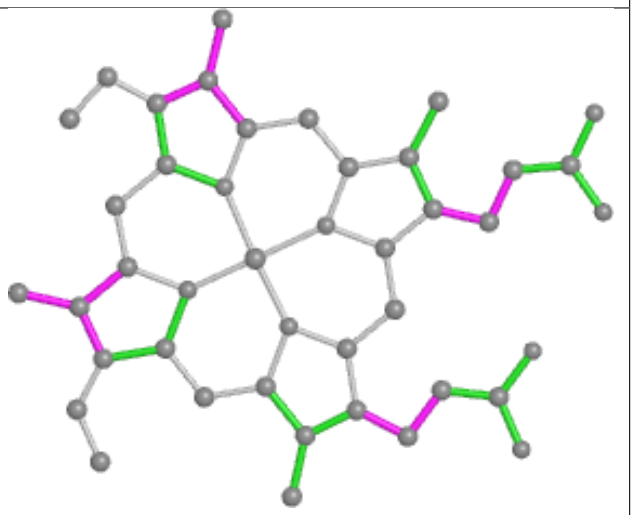
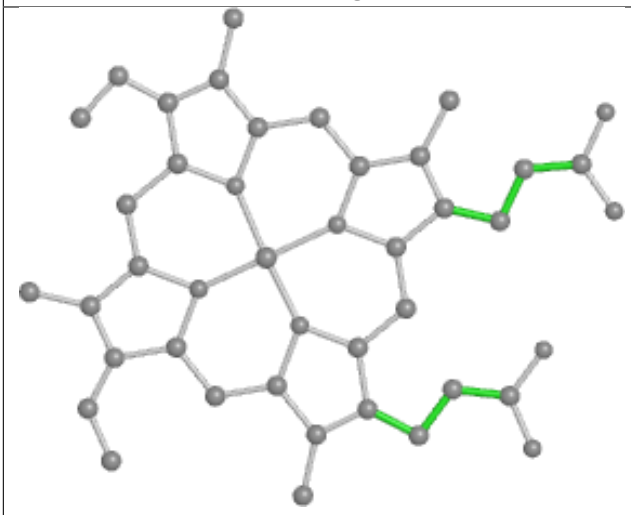
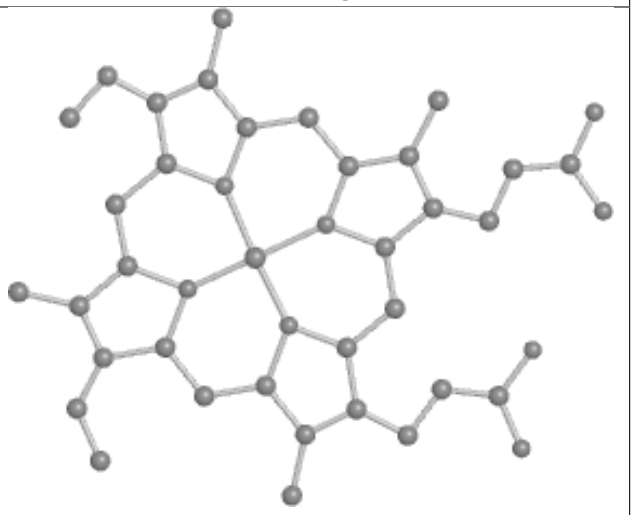


Bond angles

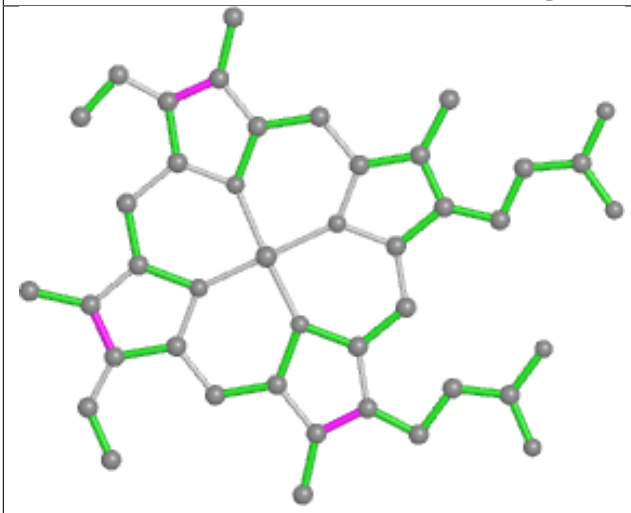


Torsions

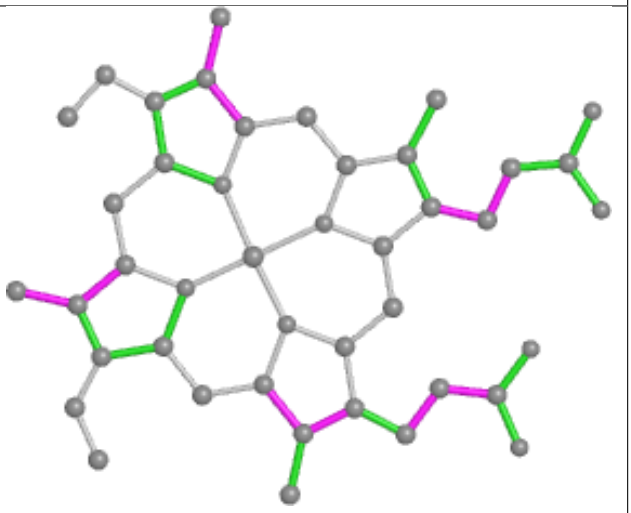


Rings

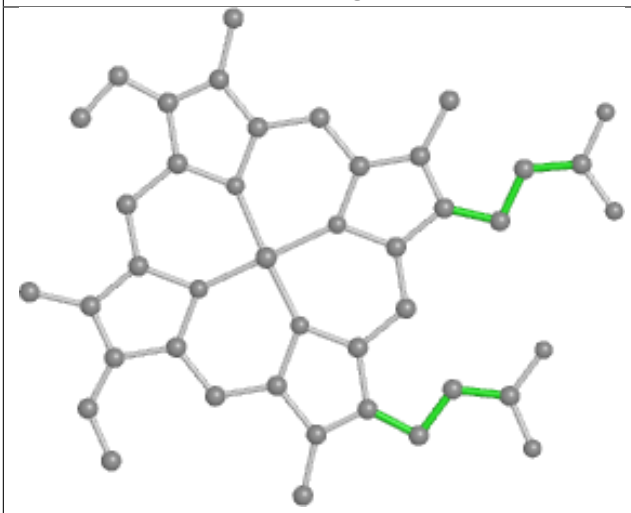
Ligand HEC C 4



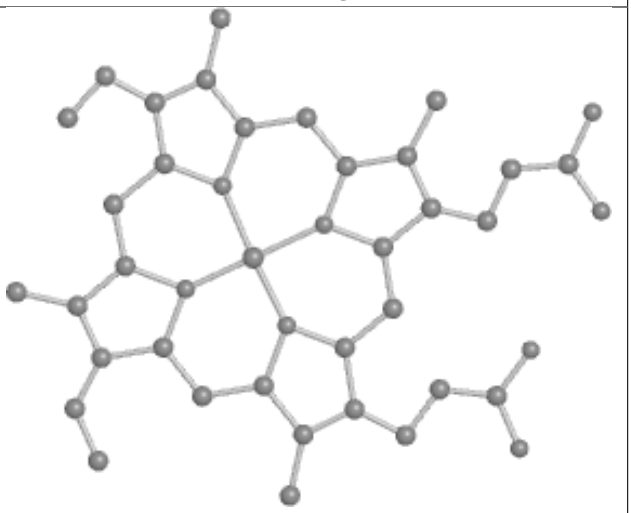
Bond lengths



Bond angles

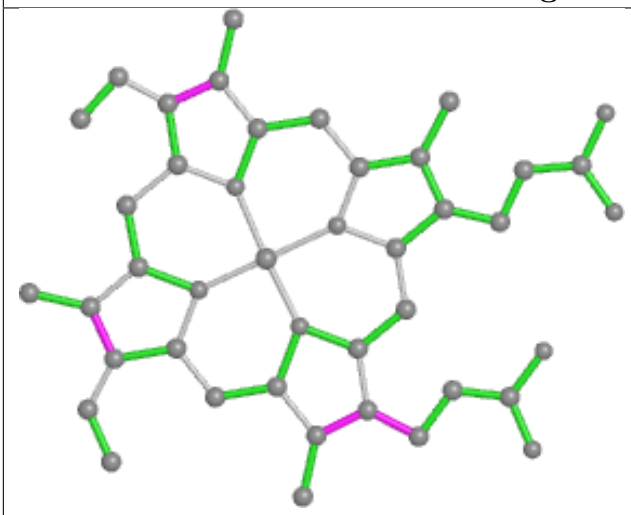


Torsions

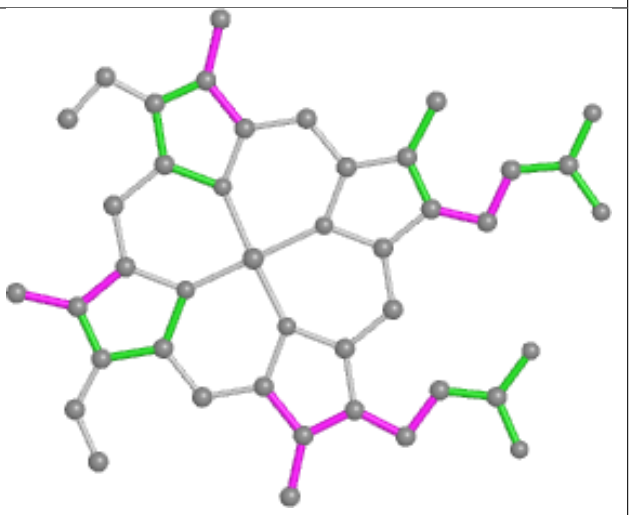


Rings

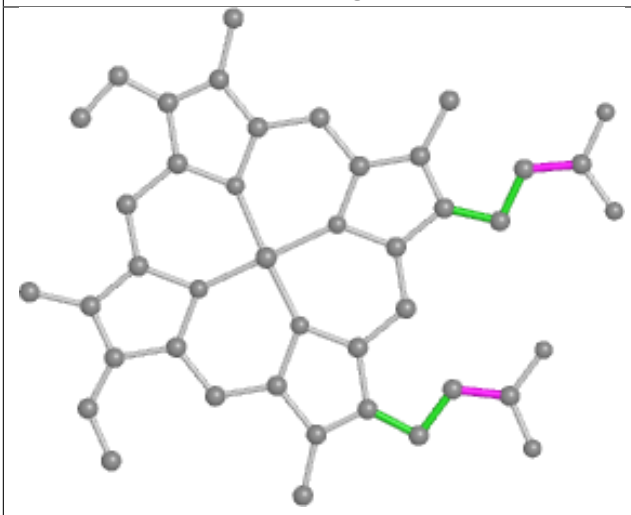
Ligand HEC D 5



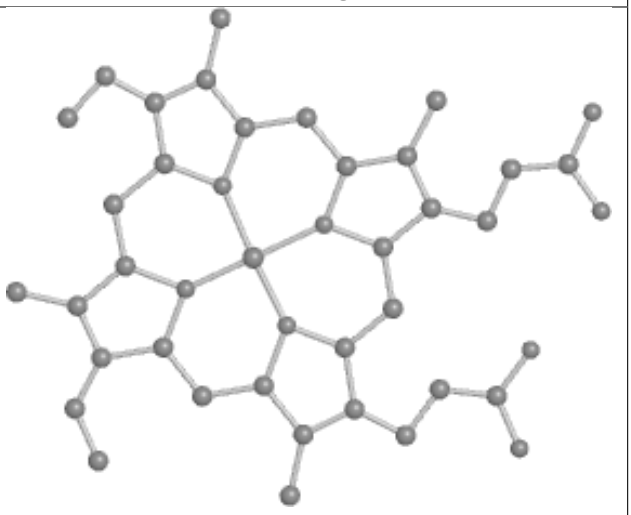
Bond lengths



Bond angles

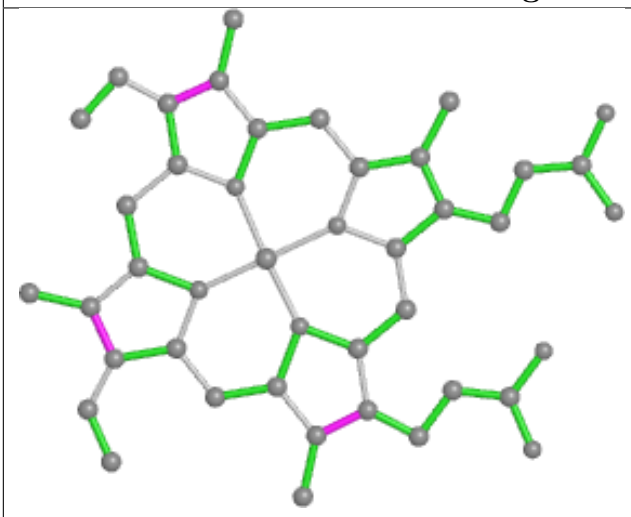


Torsions

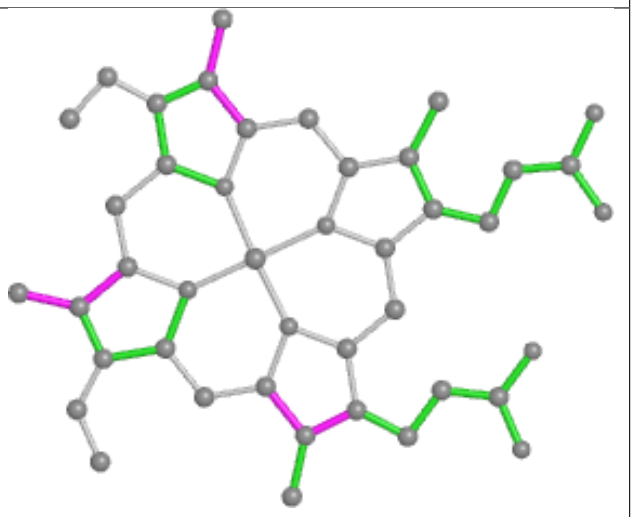


Rings

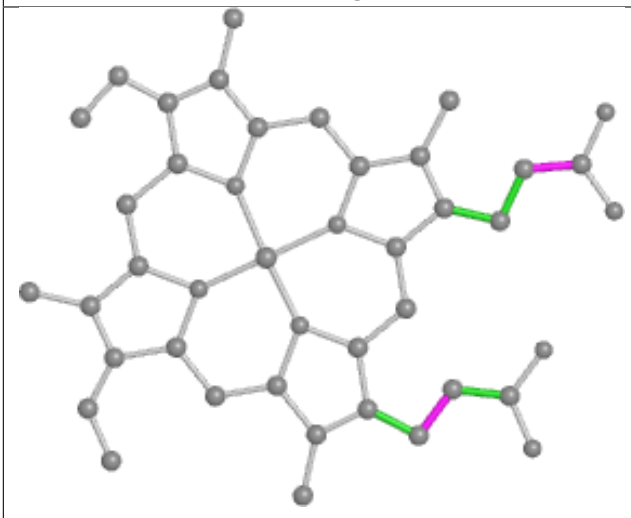
Ligand HEC A 479



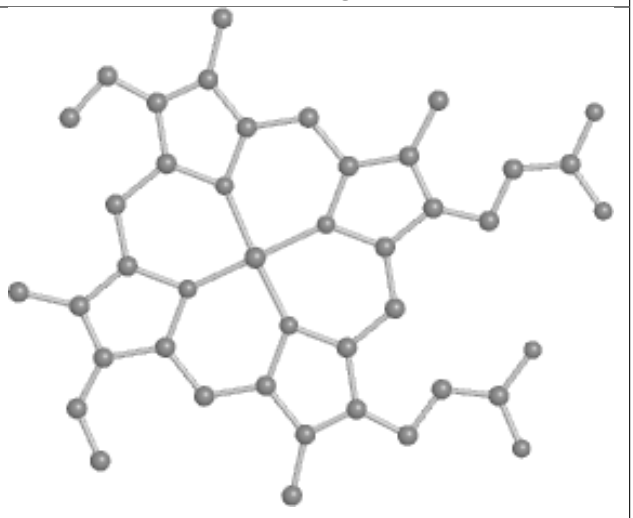
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.23	16 (3%) 42 49	15, 27, 42, 53	2 (0%)
1	B	441/452 (97%)	-0.06	1 (0%) 95 96	12, 23, 35, 41	2 (0%)
1	C	441/452 (97%)	-0.09	1 (0%) 95 96	14, 24, 34, 41	3 (0%)
1	D	441/452 (97%)	0.42	20 (4%) 33 40	23, 39, 56, 62	0
All	All	1764/1808 (97%)	0.13	38 (2%) 62 69	12, 27, 48, 62	7 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	LYS	3.8
1	A	476	LEU	3.7
1	A	477	SER	3.7
1	D	295	GLY	3.5
1	D	296	LYS	3.3
1	D	362	ALA	3.1
1	A	461	THR	2.9
1	D	174	GLY	2.9
1	D	468	GLU	2.9
1	C	221	LYS	2.8
1	D	477	SER	2.7
1	A	460	LYS	2.6
1	A	468	GLU	2.6
1	D	45	PHE	2.6
1	D	442	GLN	2.5
1	D	472	LYS	2.5
1	D	474	GLY	2.5
1	D	197	GLU	2.4
1	A	310	PHE	2.4
1	B	360	ALA	2.4
1	D	363	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	303	ILE	2.3
1	A	458	PHE	2.3
1	A	463	ILE	2.2
1	A	151	GLY	2.2
1	D	56	TRP	2.2
1	A	470	ALA	2.2
1	D	298	TYR	2.2
1	D	54	LEU	2.2
1	D	172	ALA	2.1
1	A	295	GLY	2.1
1	D	46	ALA	2.1
1	D	59	THR	2.1
1	A	47	PRO	2.1
1	A	469	GLN	2.0
1	A	474	GLY	2.0
1	A	111	LYS	2.0
1	D	470	ALA	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 monosaccharides 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, 95^{th} 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	CA	C	2	1/1	0.38	0.21	81,81,81,81	0
2	CA	A	2	1/1	0.64	0.12	93,93,93,93	0
5	EDO	B	483	4/4	0.88	0.55	44,45,46,47	0
2	CA	B	2	1/1	0.89	0.17	62,62,62,62	0
5	EDO	C	482	4/4	0.90	0.21	40,40,42,45	0
2	CA	D	2	1/1	0.91	0.07	82,82,82,82	0

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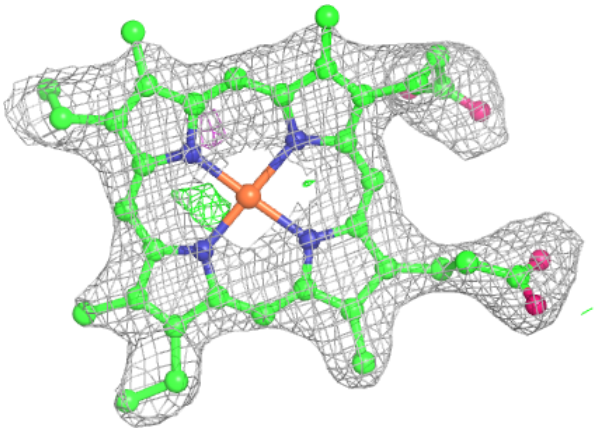
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	9	4/4	0.91	0.18	42,44,44,44	0
5	EDO	D	482	4/4	0.91	0.14	52,53,53,54	0
5	EDO	C	484	4/4	0.92	0.23	51,51,51,53	0
5	EDO	C	7	4/4	0.92	0.22	50,50,50,51	0
5	EDO	A	6	4/4	0.94	0.18	37,37,37,37	0
3	HEC	D	480	43/43	0.94	0.21	42,45,47,49	0
4	SO3	D	481	4/4	0.94	0.15	45,46,46,47	0
5	EDO	C	483	4/4	0.94	0.22	38,39,39,39	0
5	EDO	D	11	4/4	0.94	0.14	43,44,45,46	0
5	EDO	B	12	4/4	0.95	0.12	33,35,36,38	0
3	HEC	A	480	43/43	0.96	0.19	24,30,32,35	0
4	SO3	B	481	4/4	0.96	0.13	48,49,49,50	0
5	EDO	A	8	4/4	0.96	0.11	37,37,38,38	0
3	HEC	D	5	43/43	0.97	0.17	28,30,38,43	0
3	HEC	A	5	43/43	0.97	0.14	18,23,32,40	0
3	HEC	C	4	43/43	0.97	0.15	13,17,25,27	0
3	HEC	D	479	43/43	0.97	0.16	25,32,36,37	0
3	HEC	A	4	43/43	0.97	0.13	16,21,30,32	0
5	EDO	C	10	4/4	0.97	0.14	23,26,27,29	0
3	HEC	D	3	43/43	0.97	0.17	25,30,33,35	0
3	HEC	D	4	43/43	0.97	0.15	24,27,35,41	0
3	HEC	C	479	43/43	0.98	0.14	12,15,18,21	0
3	HEC	C	480	43/43	0.98	0.14	14,17,21,22	0
3	HEC	A	3	43/43	0.98	0.15	16,21,27,30	0
3	HEC	C	5	43/43	0.98	0.15	16,20,30,32	0
3	HEC	A	479	43/43	0.98	0.14	15,23,26,27	0
2	CA	C	1	1/1	0.98	0.11	19,19,19,19	0
3	HEC	B	480	43/43	0.98	0.14	13,16,19,20	0
3	HEC	B	3	43/43	0.98	0.14	9,14,20,23	0
3	HEC	B	4	43/43	0.98	0.14	10,16,21,27	0
4	SO3	A	481	4/4	0.98	0.13	28,29,30,31	0
3	HEC	B	5	43/43	0.98	0.15	14,18,28,33	0
4	SO3	B	482	4/4	0.98	0.15	28,28,30,33	0
4	SO3	C	481	4/4	0.98	0.11	23,23,27,27	0
3	HEC	C	3	43/43	0.99	0.14	9,13,17,19	0
2	CA	D	1	1/1	0.99	0.09	29,29,29,29	0
3	HEC	B	479	43/43	0.99	0.13	10,15,17,18	0
2	CA	B	1	1/1	0.99	0.10	19,19,19,19	0
2	CA	A	1	1/1	0.99	0.12	18,18,18,18	0

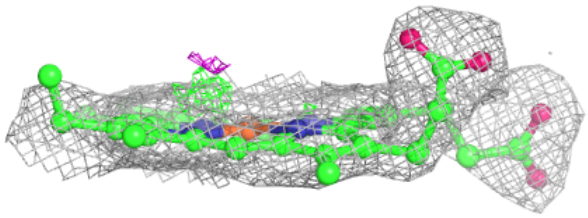
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

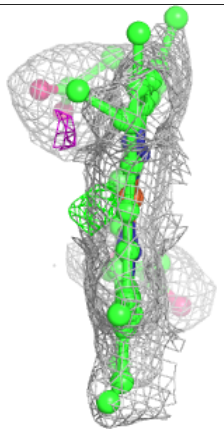
orientation to approximate a three-dimensional view.

Electron density around HEC D 480:

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

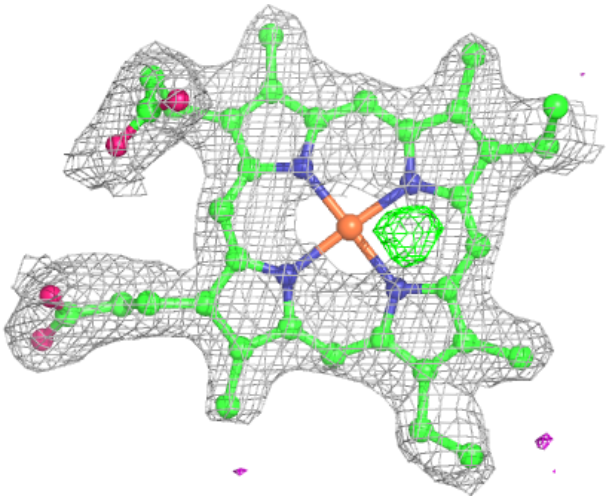


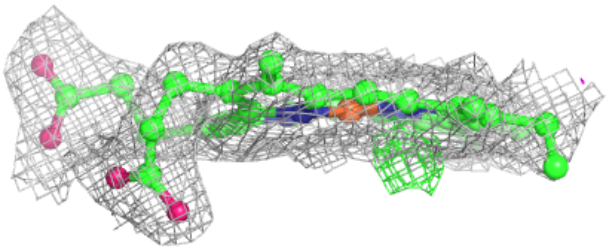


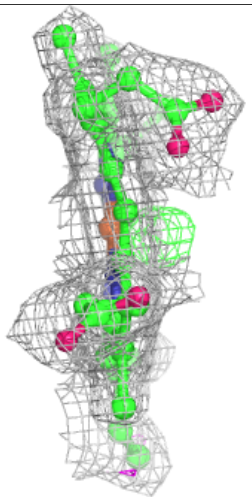


Electron density around HEC A 480:

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

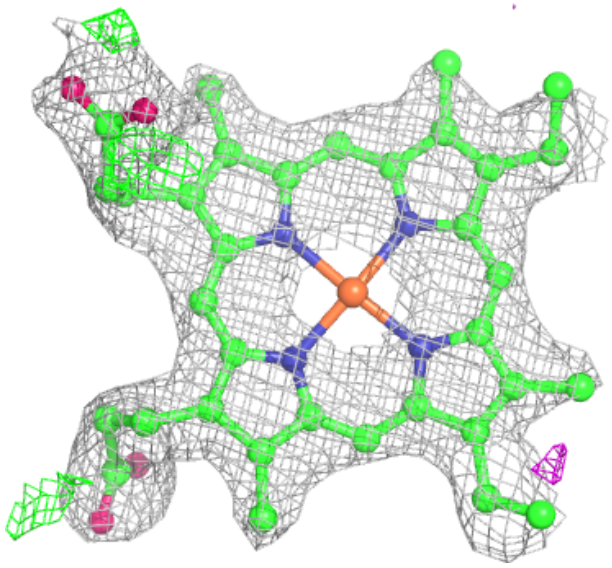


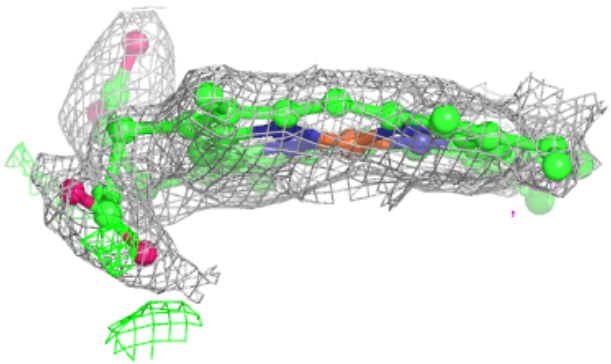


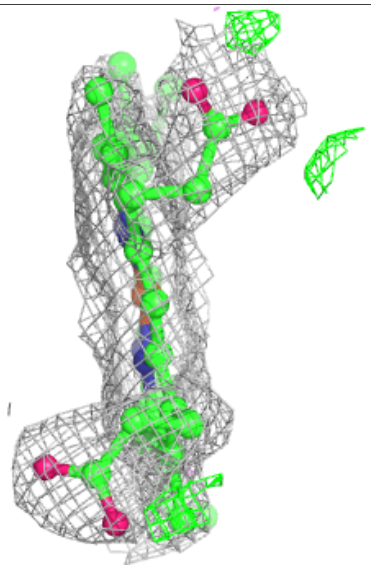


Electron density around HEC D 5:

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

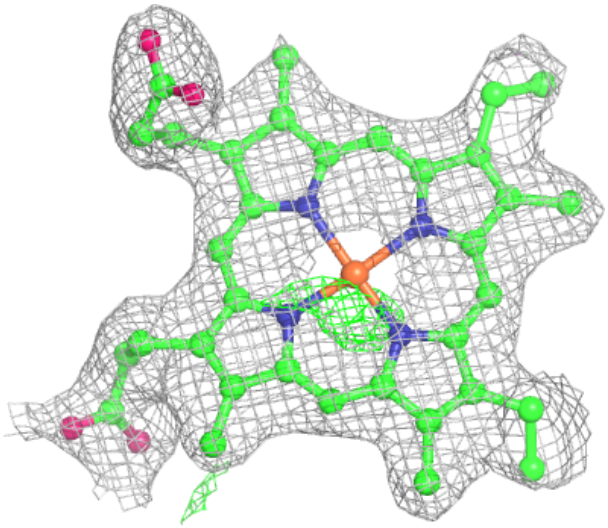


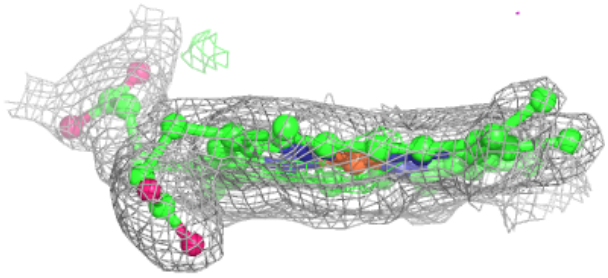


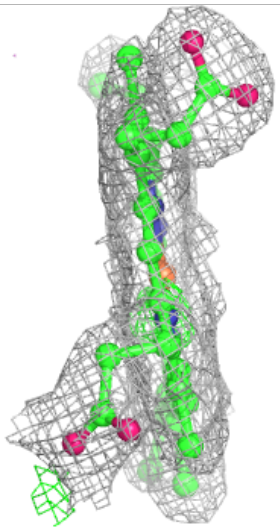


Electron density around HEC A 5:

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

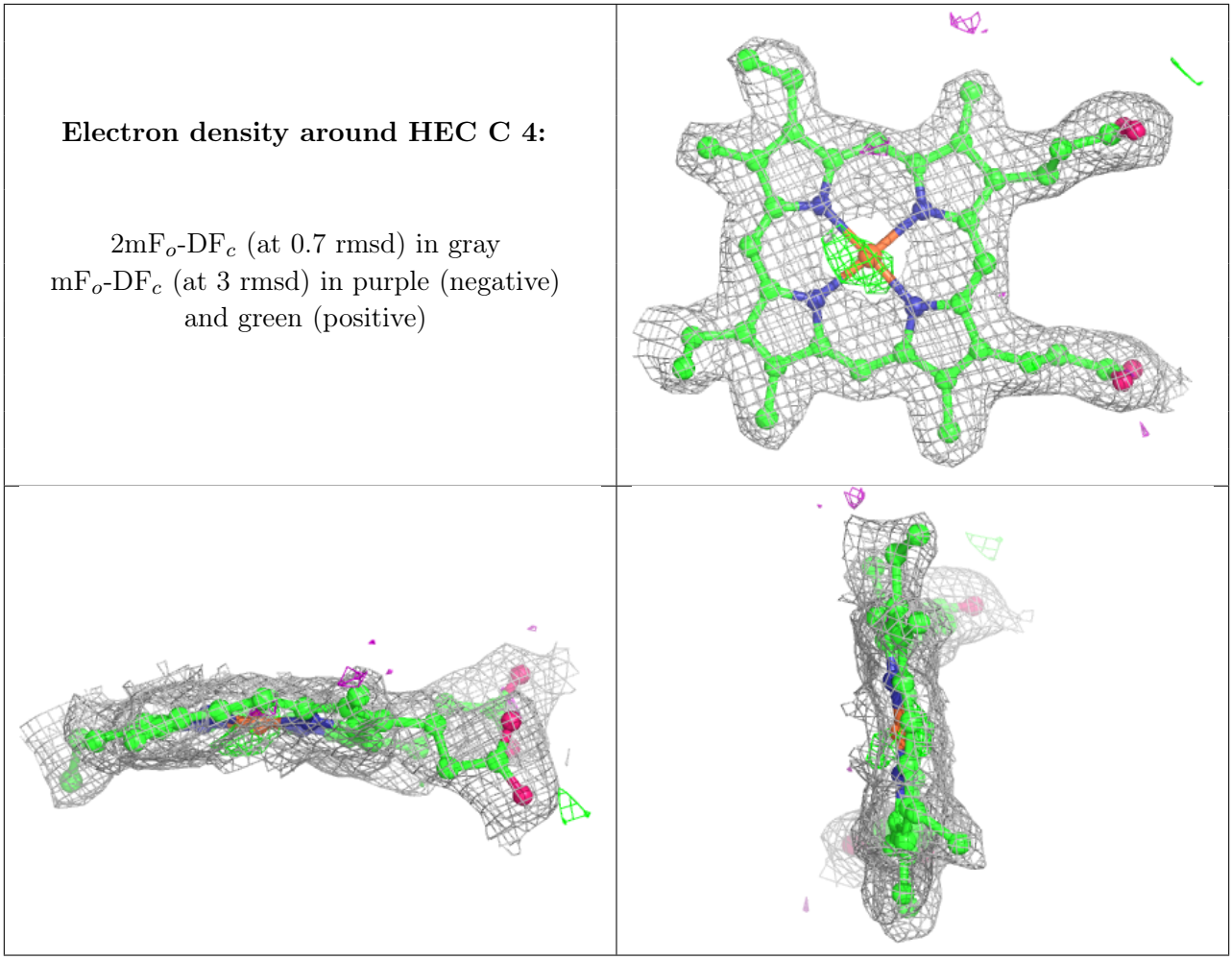






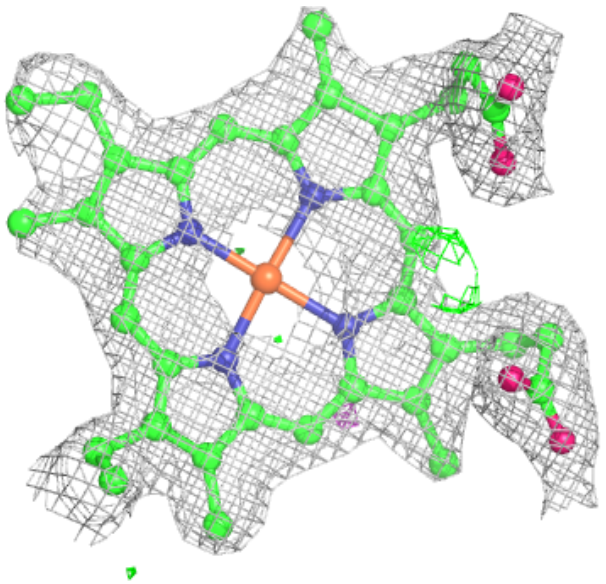
Electron density around HEC C 4:

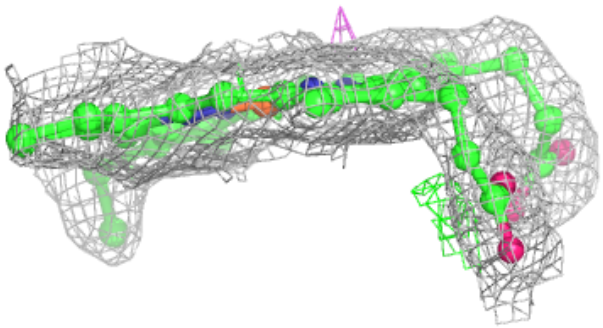
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

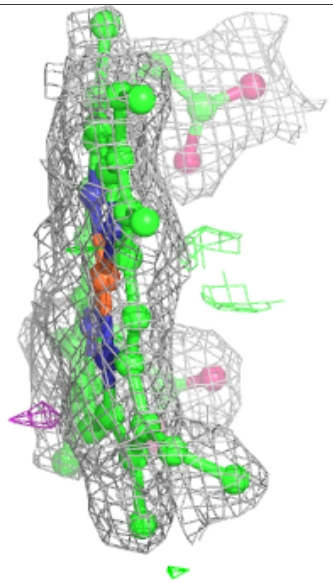


Electron density around HEC D 479:

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

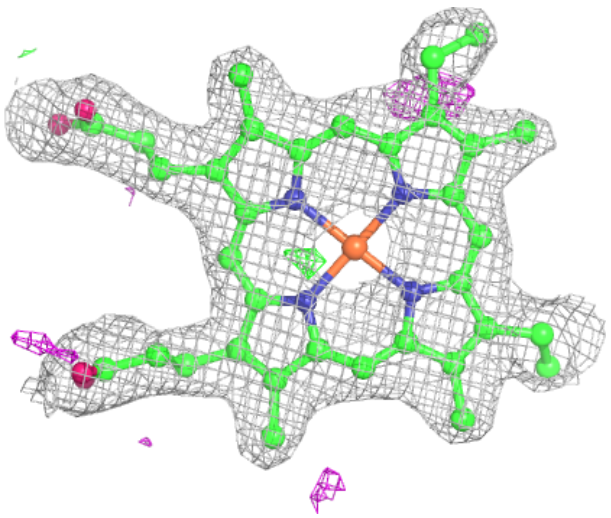


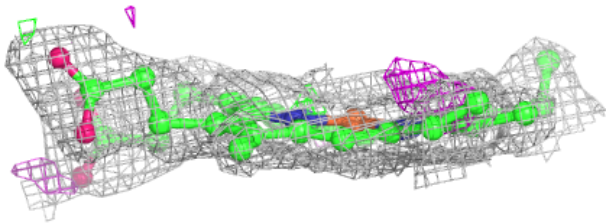


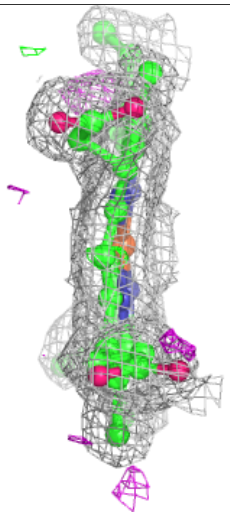


Electron density around HEC A 4:

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

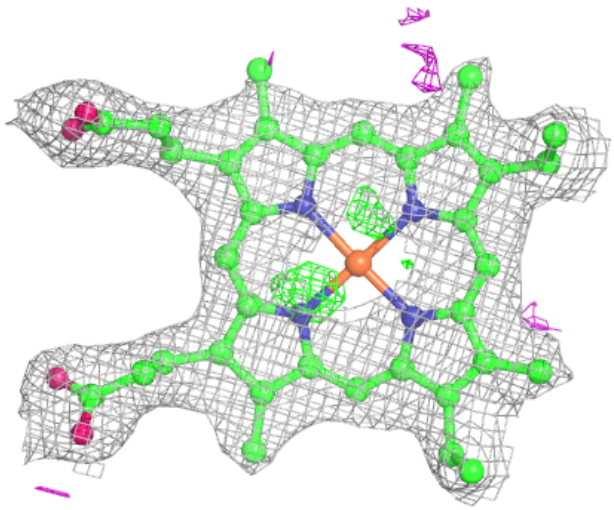


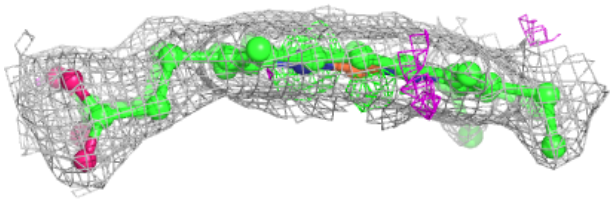


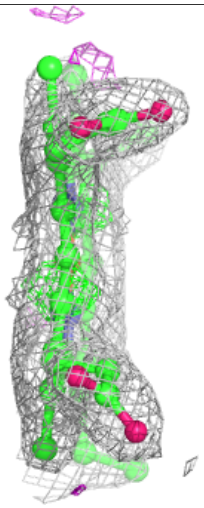


Electron density around HEC D 3:

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

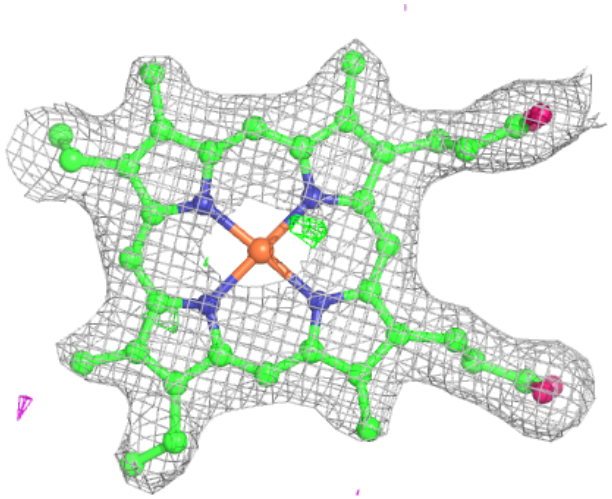


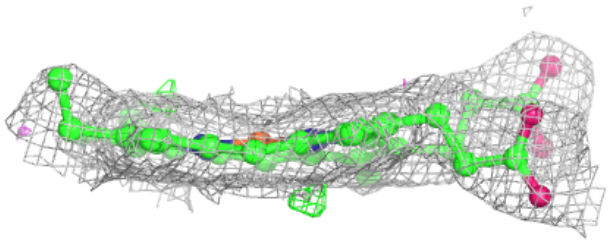


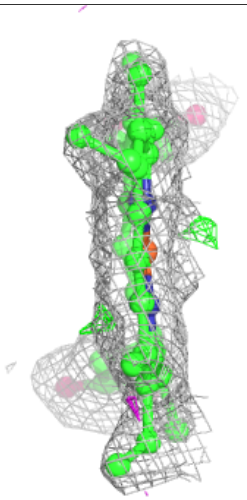


Electron density around HEC D 4:

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

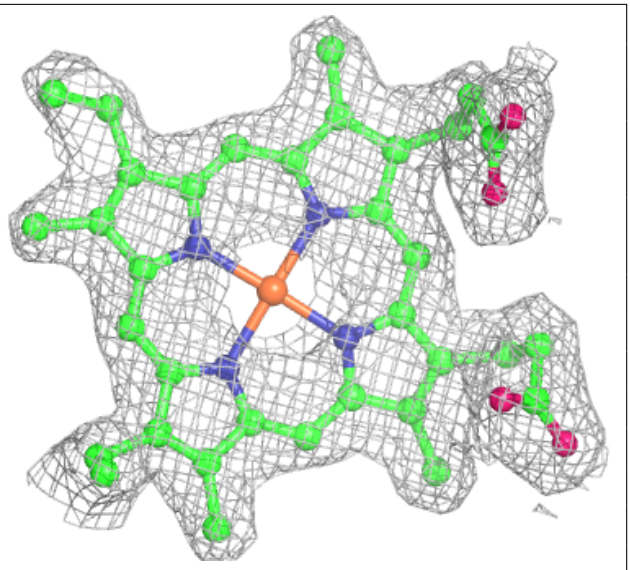


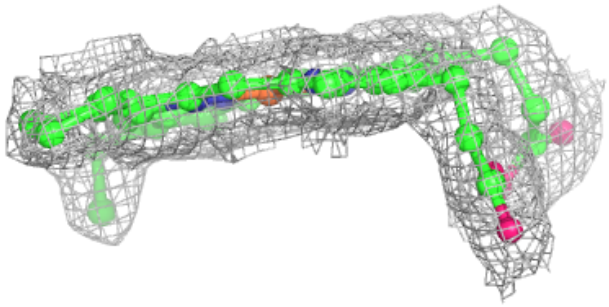


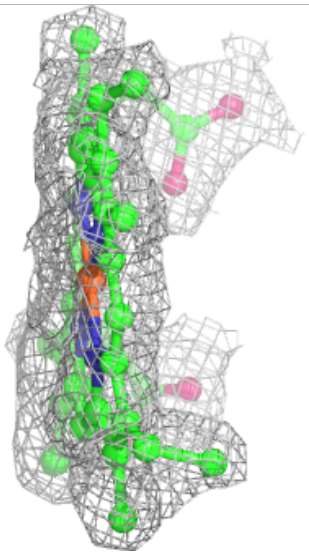


Electron density around HEC C 479:

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

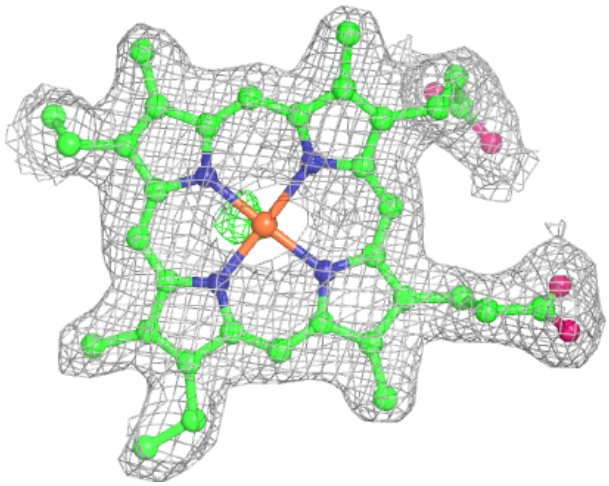


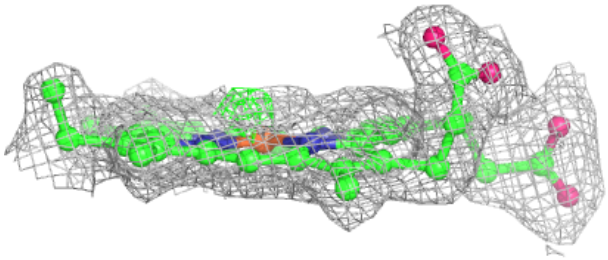




Electron density around HEC C 480:

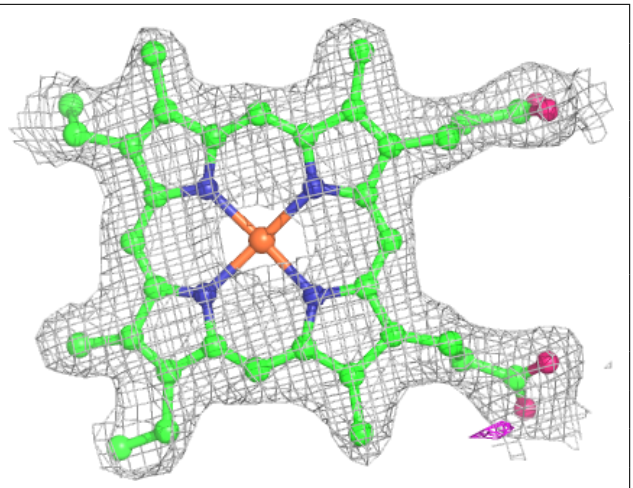
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

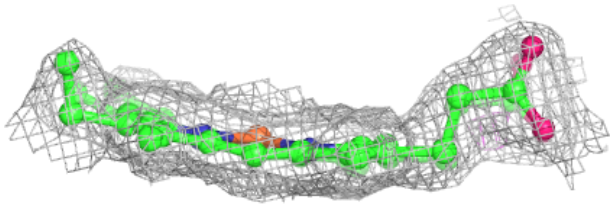


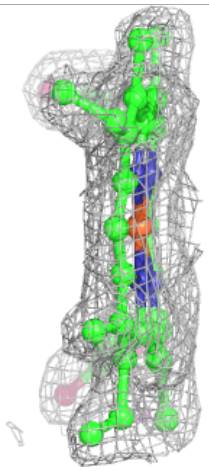


Electron density around HEC A 3:

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

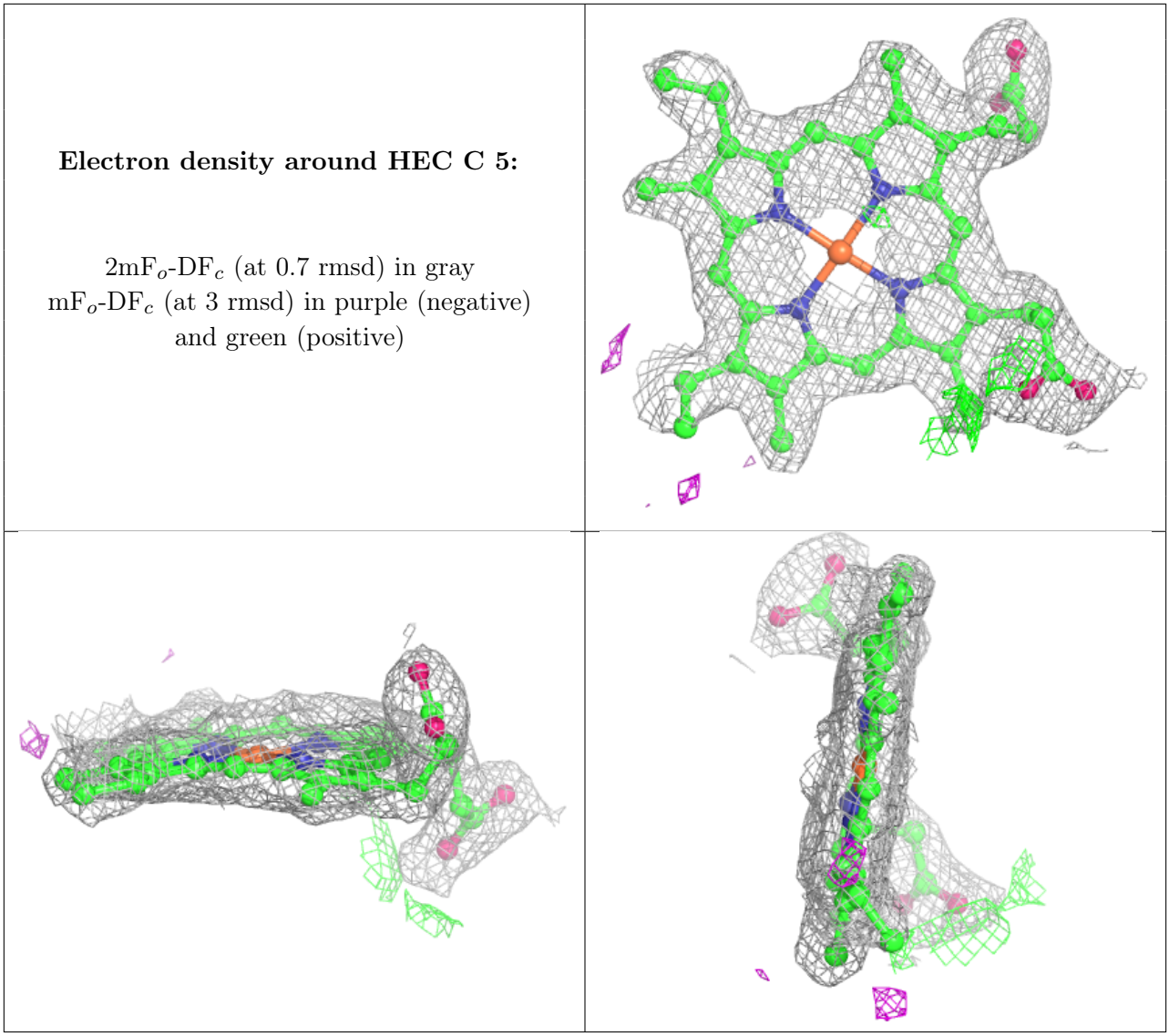






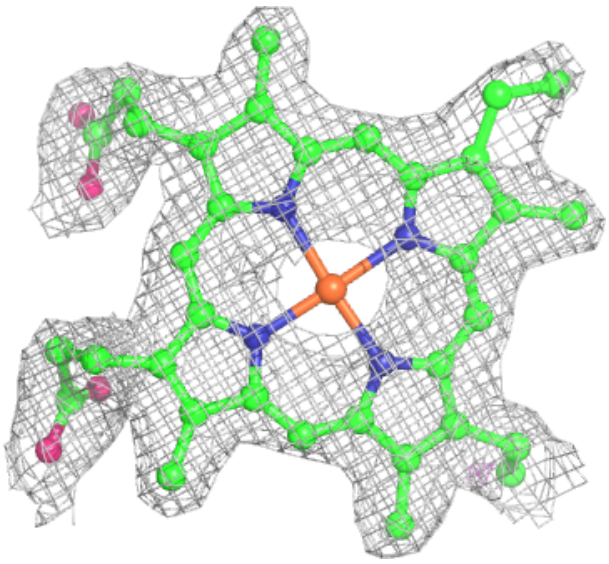
Electron density around HEC C 5:

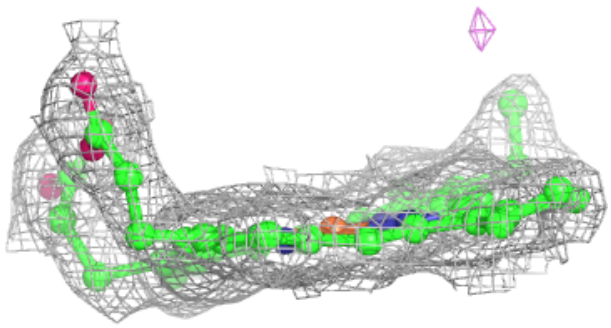
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

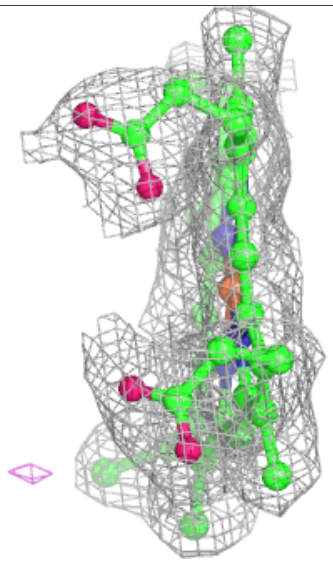


Electron density around HEC A 479:

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

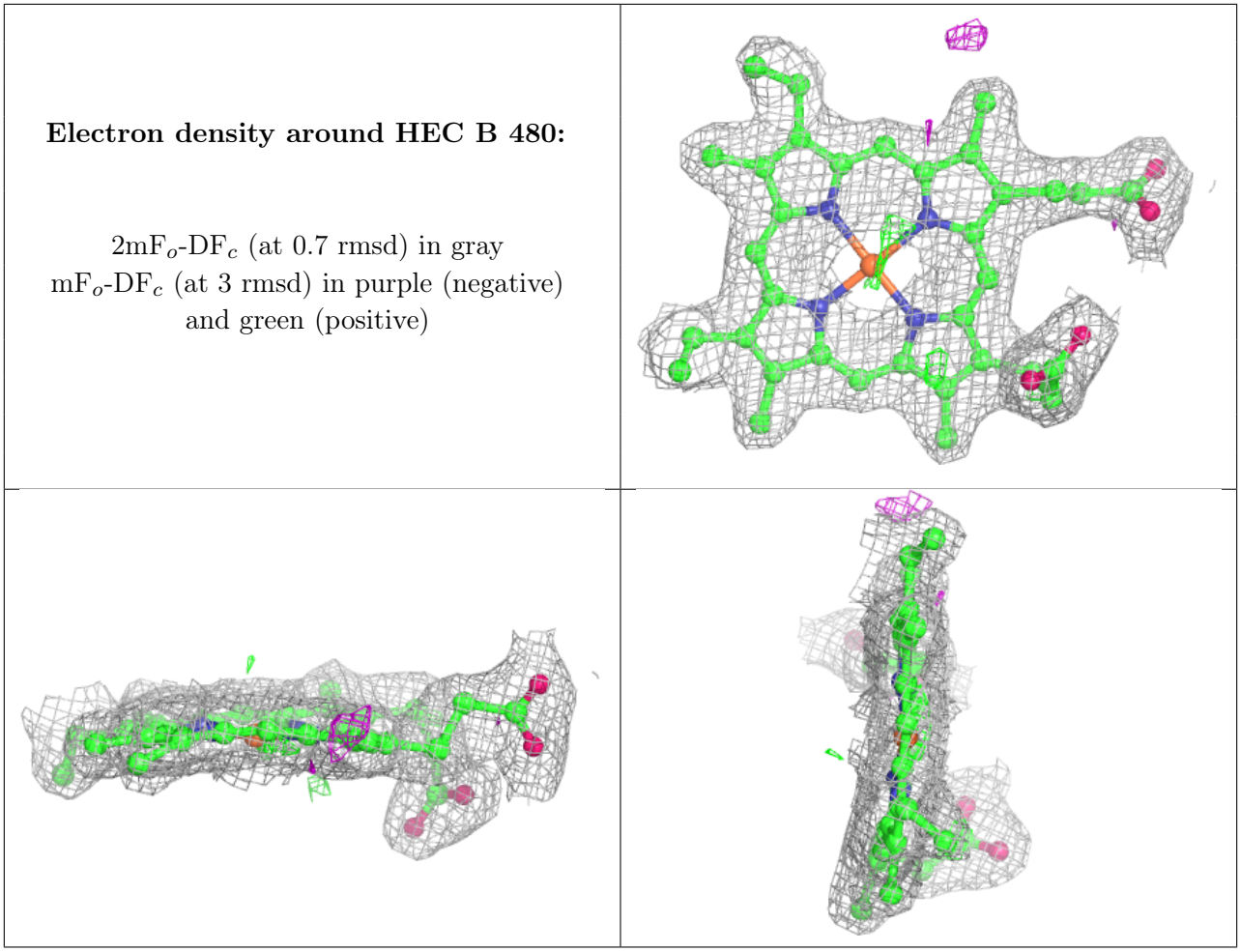






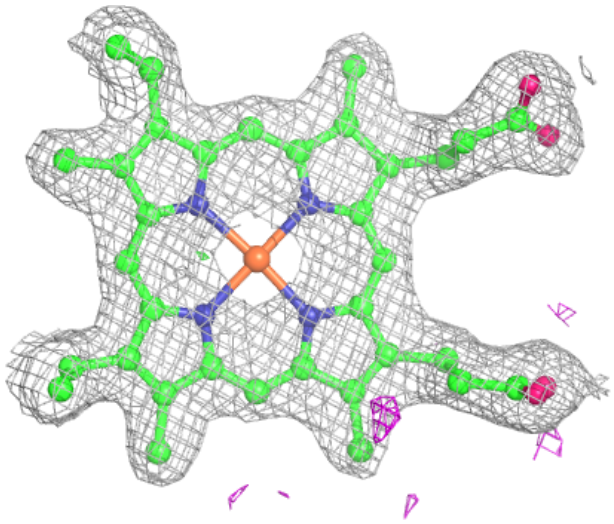
Electron density around HEC B 480:

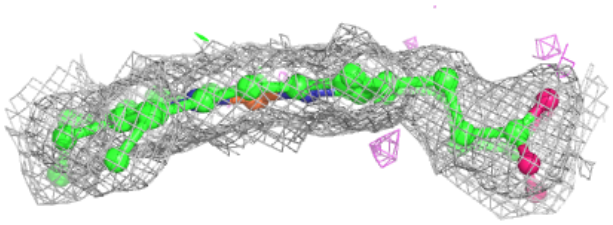
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

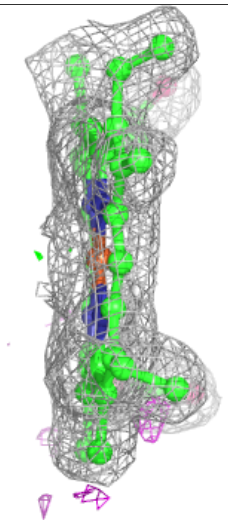


Electron density around HEC B 3:

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

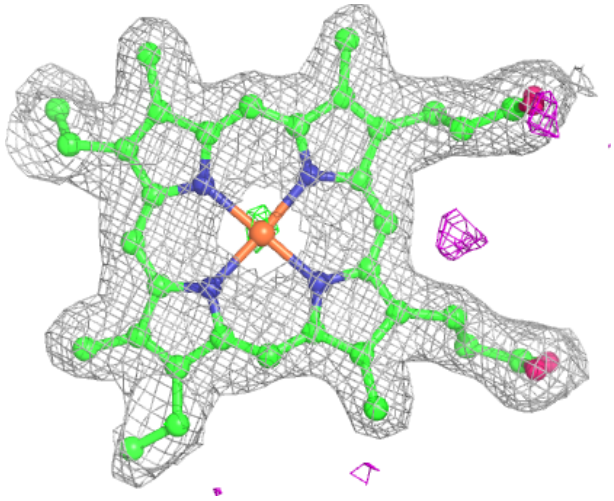


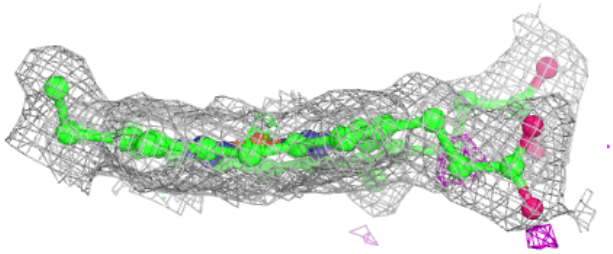


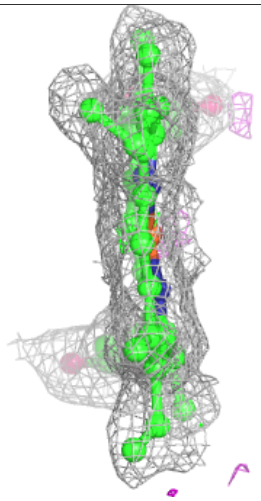


Electron density around HEC B 4:

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

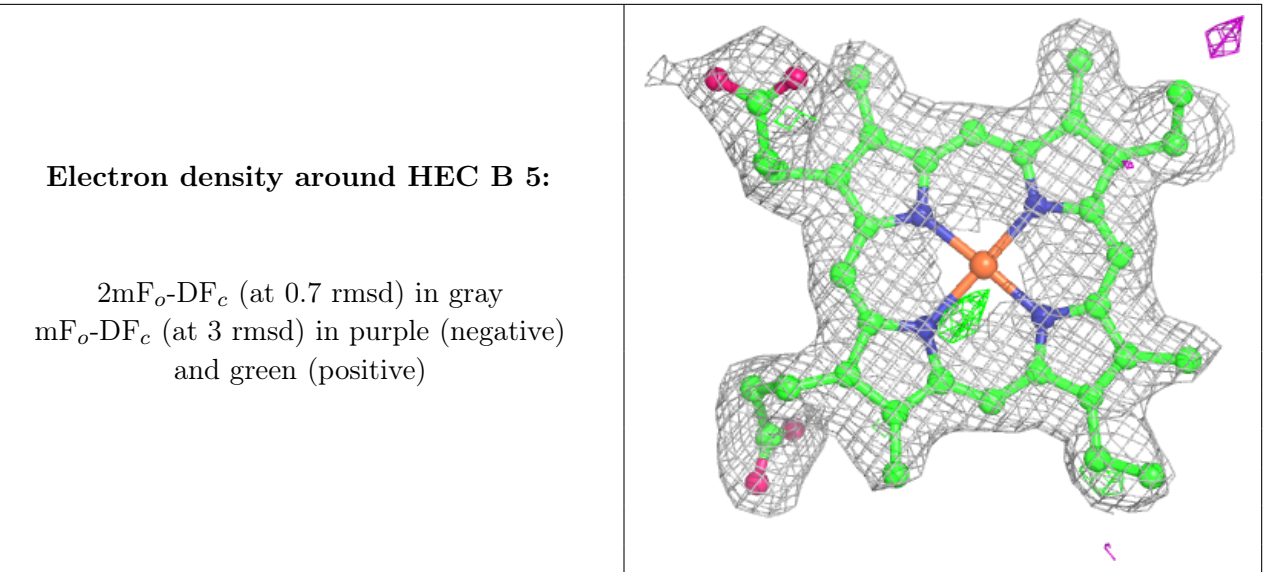


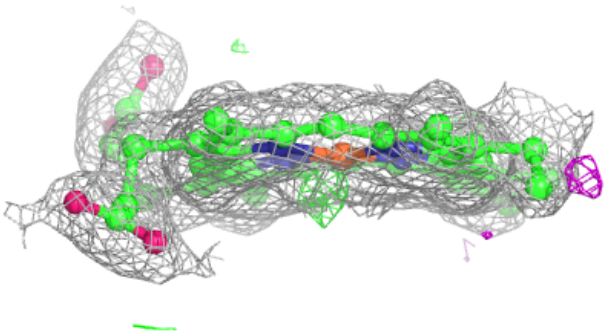


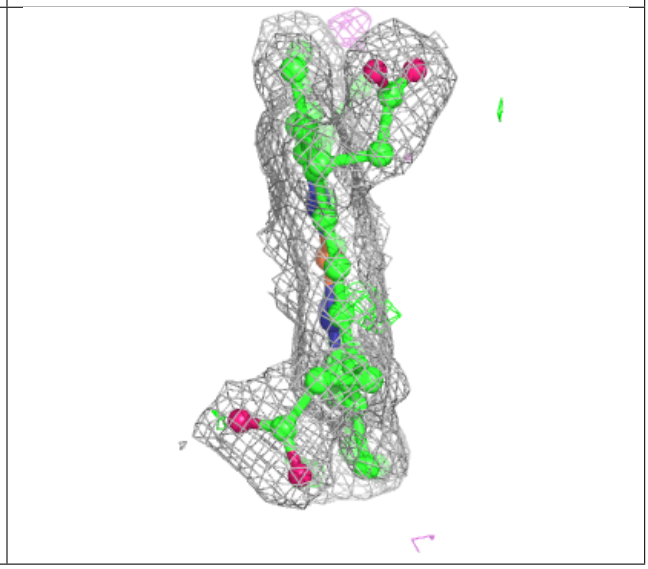


Electron density around HEC B 5:

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

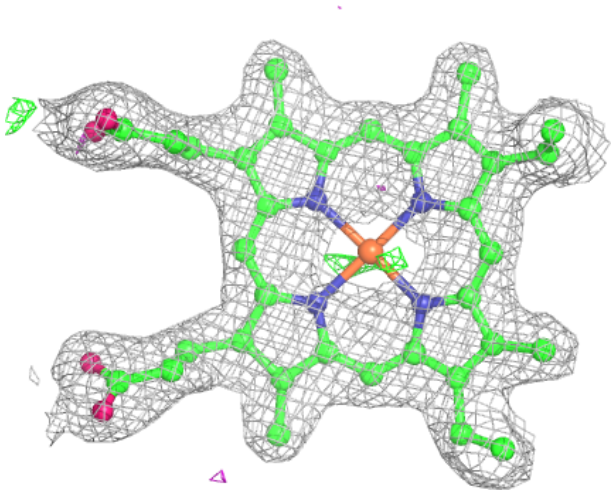


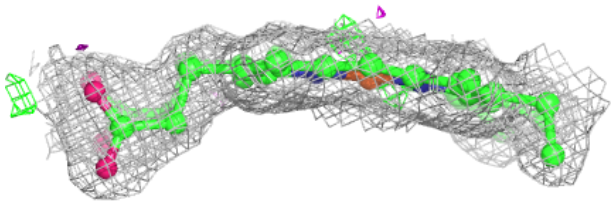


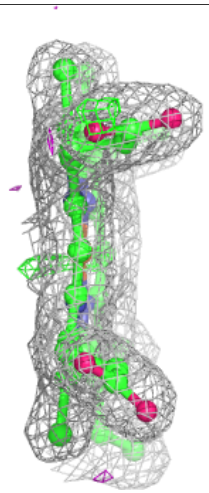


Electron density around HEC C 3:

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

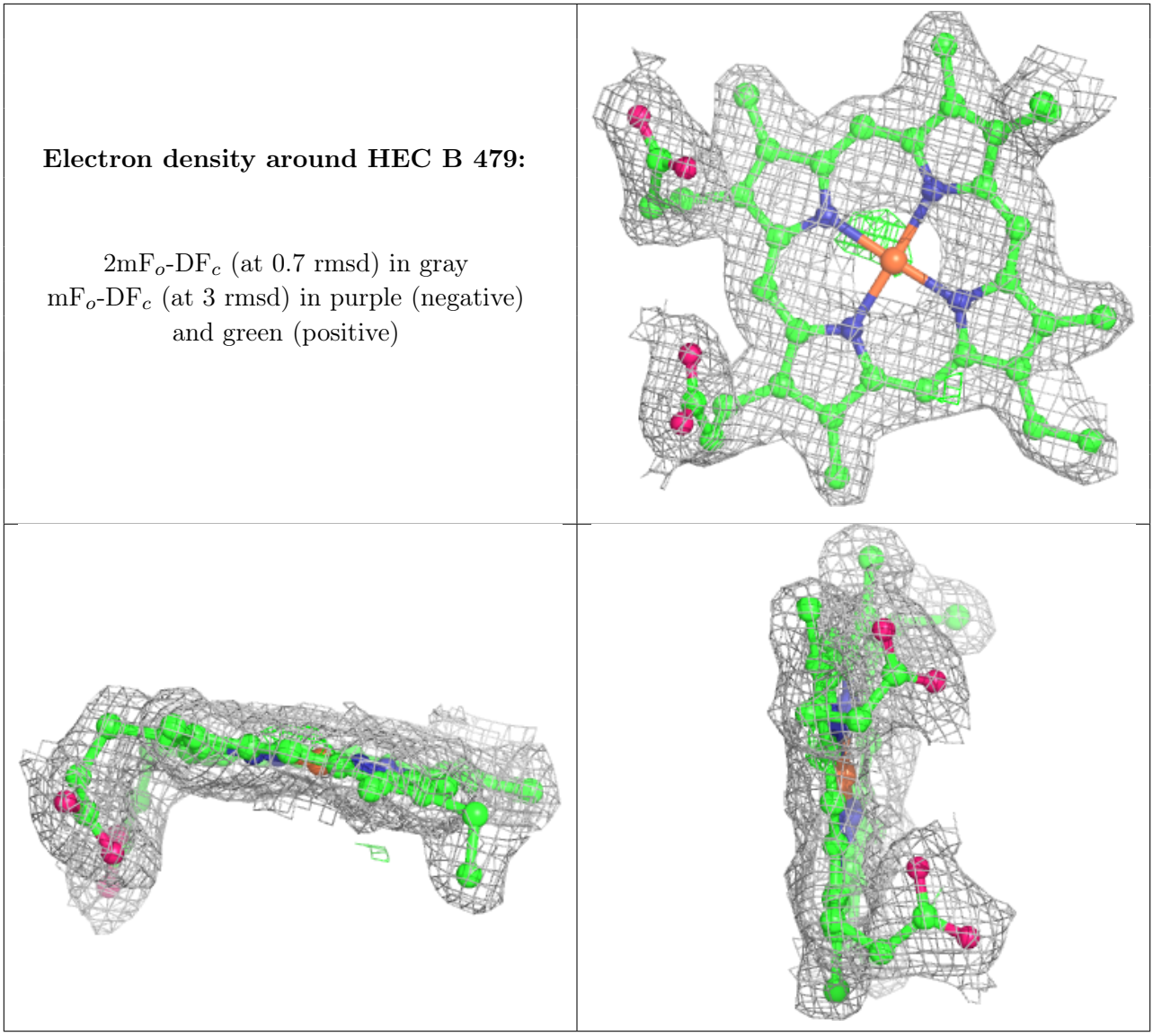






Electron density around HEC B 479:

$2mF_o$-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.