



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:52 AM UTC

PDB ID : 3L1T / pdb_00003l1t
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

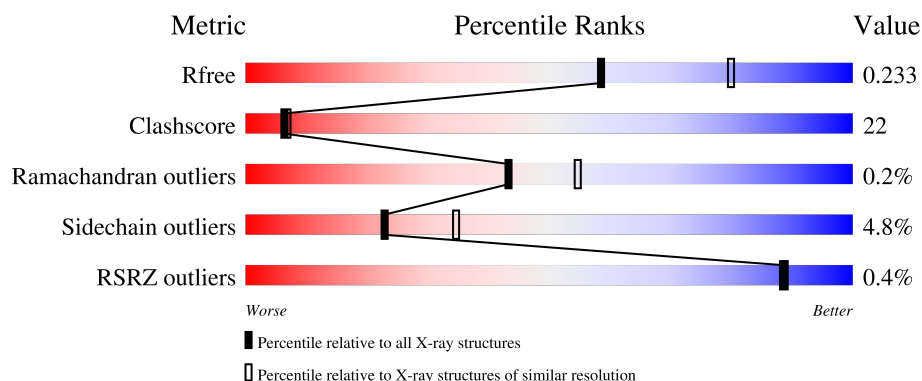
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

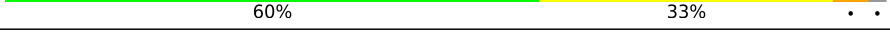
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	
1	B	452	
1	C	452	
1	D	452	

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

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.

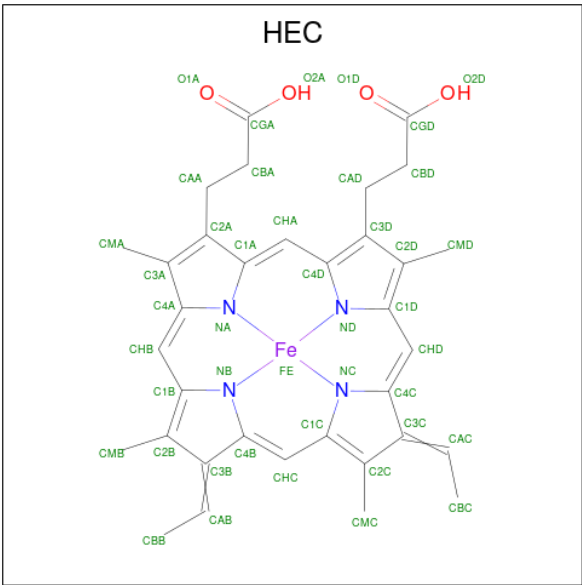
- Molecule 1 is a protein called Cytochrome c-552.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



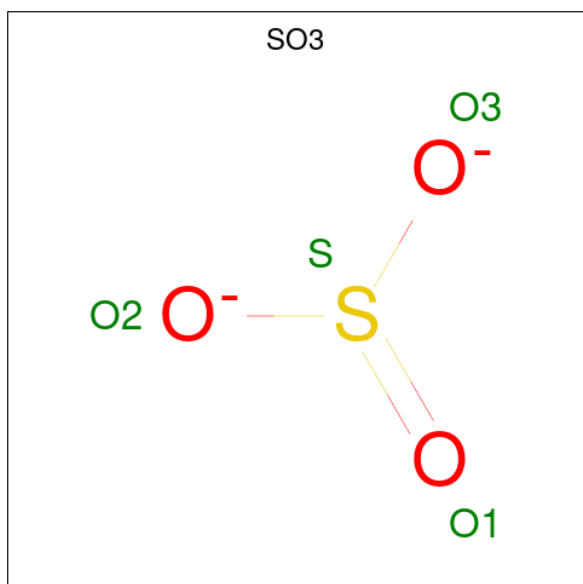
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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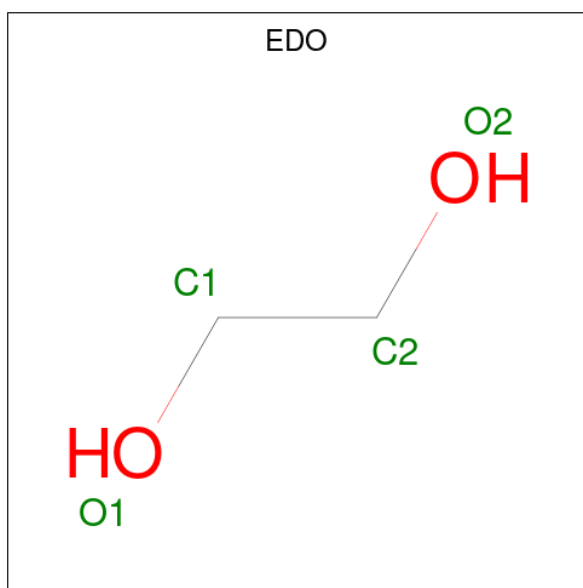
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

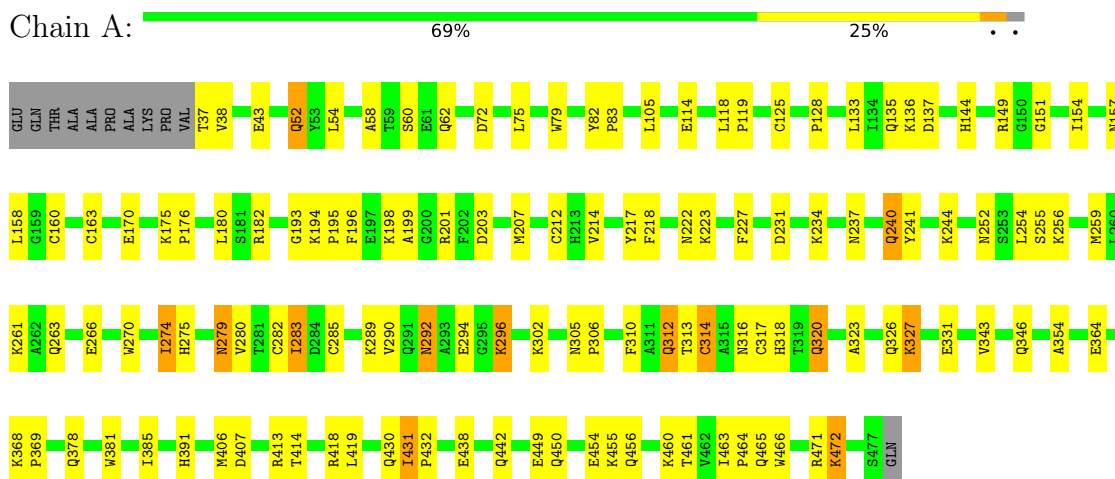
- Molecule 6 is water.

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

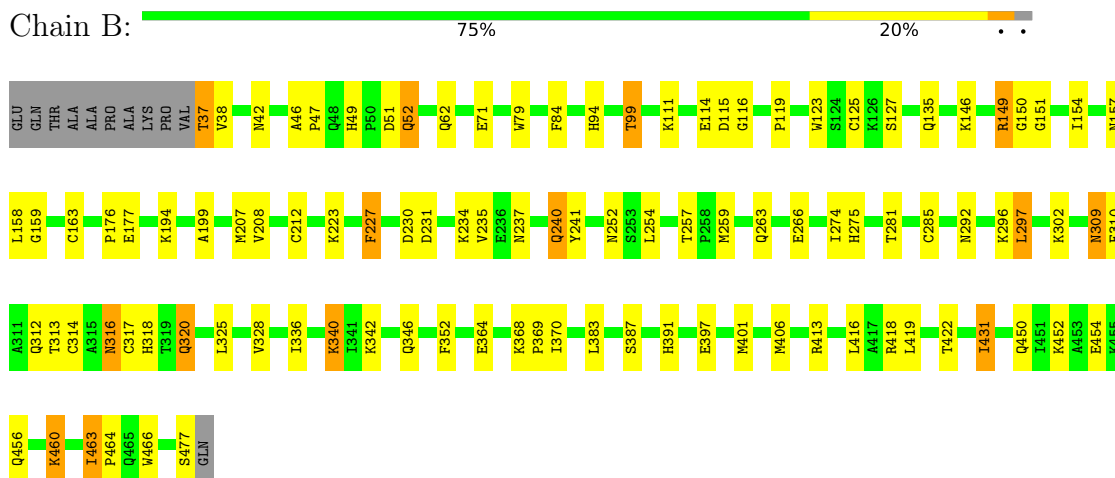
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

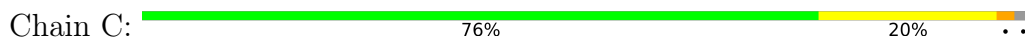
• Molecule 1: Cytochrome c-552

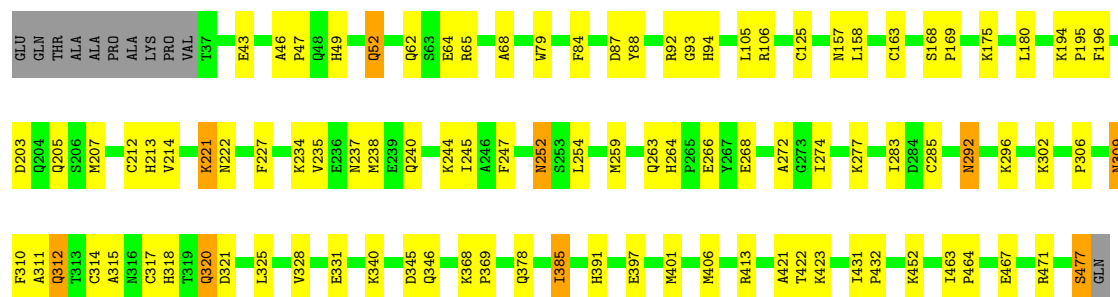


• Molecule 1: Cytochrome c-552

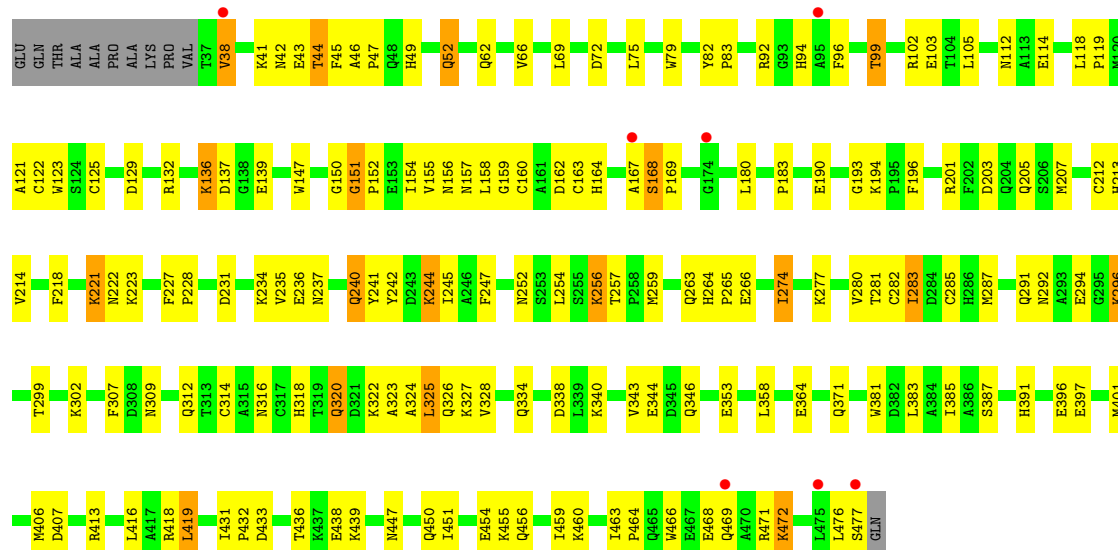


• Molecule 1: Cytochrome c-552





● Molecule 1: Cytochrome c-552



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.52Å 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
$\langle I/\sigma(I) \rangle$ 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 (4.99%)	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)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/3569 (0.0%)	0.86	4/4827 (0.1%)
1	B	0.66	1/3578 (0.0%)	0.85	0/4838
1	C	0.65	0/3595	0.84	0/4861
1	D	0.53	0/3577	0.79	2/4838 (0.0%)
All	All	0.62	2/14319 (0.0%)	0.84	6/19364 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	GLN	CD-NE2	-7.58	1.17	1.33
1	B	463	ILE	CA-CB	5.73	1.56	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	D	168	SER	CA-C-N	5.58	124.93	118.85
1	D	168	SER	C-N-CA	5.58	124.93	118.85
1	A	72	ASP	CA-C-N	5.27	124.89	119.56
1	A	72	ASP	C-N-CA	5.27	124.89	119.56
1	A	314	CYS	N-CA-C	5.08	117.47	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3485	0	3374	145	0
1	B	3491	0	3389	124	0
1	C	3502	0	3396	128	0
1	D	3487	0	3378	200	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	215	0	155	50	0
3	B	215	0	155	37	0
3	C	215	0	155	40	0
3	D	215	0	155	47	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	23	0
6	C	292	0	0	18	0
6	D	152	0	0	25	0
All	All	15858	0	14229	640	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 22.

All (640) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:C:406:MET:HE3	1:D:407:ASP:HB2	1.39	1.01
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
3:A:5:HEC:HBB3	3:A:5:HEC:HMB1	1.45	0.98
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
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
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:D:5:HEC:HBB3	3:D:5:HEC:HMB1	1.49	0.94
1:C:320:GLN:HG2	5:C:484:EDO:H22	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:292:ASN:C	1:A:292:ASN:HD22	1.75	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
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:235:VAL:HB	1:D:401:MET:HE3	1.50	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
3:D:479:HEC:HBC3	3:D:479:HEC:HMC1	1.53	0.88
1:C:391:HIS:HE1	3:C:4:HEC:O2D	1.55	0.88
1:D:221:LYS:H	1:D:221:LYS:HZ2	1.17	0.88
3:C:3:HEC:HMC1	3:C:3:HEC:HBC3	1.56	0.88
3:D:480:HEC:HMC1	3:D:480:HEC:HBC3	1.55	0.87
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:D:472:LYS:HB3	1:D:472:LYS:HZ2	1.40	0.85
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
1:B:234:LYS:HE2	6:B:876:HOH:O	1.75	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
1:B:235:VAL:HB	1:B:401:MET:HE3	1.62	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:NE2	1:A:52:GLN:N	2.28	0.81
1:B:312:GLN:CD	6:B:638:HOH:O	2.23	0.80
1:A:62:GLN:HE21	1:A:302:LYS:HZ3	1.29	0.80
1:D:334:GLN:HE21	1:D:338[B]:ASP:CG	1.89	0.80
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
3:C:4:HEC:HBC3	3:C:4:HEC:HMC1	1.64	0.79
1:D:231:ASP:OD2	1:D:240:GLN:NE2	2.16	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:A:343:VAL:HG22	1:A:406:MET:HE2	1.65	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
3:A:480:HEC:HMC1	3:A:480:HEC:HBC3	1.67	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
1:A:320:GLN:H	1:A:320:GLN:HE21	1.31	0.75
3:A:5:HEC:HBB3	3:A:5:HEC:CMB	2.17	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:194:LYS:HB3	1:B:207:MET:HE1	1.69	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
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
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: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
1:A:231:ASP:OD2	1:A:240:GLN:NE2	2.24	0.70
1:C:345:ASP:CG	5:C:9:EDO:H11	2.16	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
3:D:479:HEC:CBC	3:D:479:HEC:HMC1	2.21	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
3:B:480:HEC:HMC1	3:B:480:HEC:HBC3	1.73	0.69
1:C:125:CYS:SG	3:C:479:HEC:CBC	2.80	0.69
3:D:5:HEC:HBB3	3:D:5:HEC:CMB	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:287:MET:HE2	1:D:299:THR:CG2	2.24	0.68
1:D:203:ASP:O	1:D:207:MET:HG3	1.93	0.68
3:D:479:HEC:HMB3	3:D:479:HEC:HBB3	1.74	0.68
1:B:199:ALA:HA	6:B:600:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HA	6:A:648:HOH:O	1.94	0.67
1:D:285:CYS:SG	3:D:4:HEC:HAC	2.34	0.67
1:B:312:GLN:CG	6:B:638:HOH:O	2.37	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:C:62:GLN:HE21	1:C:302:LYS:HZ3	1.41	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
3:D:479:HEC:CBC	3:D:479:HEC:CMC	2.73	0.66
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:480:HEC:HMC1	3:D:480:HEC:CBC	2.27	0.65
1:A:320:GLN:H	1:A:320:GLN:NE2	1.95	0.65
1:C:194:LYS:HE3	1:C:207:MET:HE3	1.78	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
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
3:A:480:HEC:HBB3	3:A:480:HEC:CMB	2.28	0.64
1:C:49:HIS:HD2	6:C:656:HOH:O	1.81	0.64
3:D:480:HEC:CBC	3:D:480:HEC:CMC	2.76	0.64
3:A:479:HEC:HMC1	3:A:479:HEC:HBC3	1.79	0.63
1:C:194:LYS:HB3	1:C:207:MET:HE1	1.80	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
3:B:4:HEC:HMC1	3:B:4:HEC:HBC3	1.78	0.63
1:C:345:ASP:OD1	5:C:9:EDO:C1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:5:HEC:HBB3	3:B:5:HEC:CMB	2.29	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:CBC	2.87	0.62
1:A:285:CYS:SG	3:A:4:HEC:C3C	2.87	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: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:D:125:CYS:HG	3:D:479:HEC:CAC	2.09	0.62
1:C:317:CYS:SG	3:C:5:HEC:C3C	2.87	0.61
1:D:383:LEU:HD23	1:D:401:MET:HE1	1.81	0.61
1:A:450:GLN:O	1:A:454:GLU:HG3	2.01	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: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:D:235:VAL:HG13	1:D:236:GLU:N	2.15	0.60
1:A:285:CYS:SG	3:A:4:HEC:HAC	2.36	0.60
1:D:314:CYS:SG	3:D:5:HEC:C3B	2.88	0.60
3:A:5:HEC:CMB	3:A:5:HEC:CBB	2.79	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:43:GLU:CD	1:A:43:GLU:H	2.10	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:A:343:VAL:CG2	1:A:406:MET:HE2	2.32	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:D:287:MET:HE2	1:D:299:THR:HG22	1.84	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:HBC3	3:C:4:HEC:CMC	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:HE1	3:D:4:HEC:O2D	1.85	0.59
3:A:4:HEC:HMC1	3:A:4:HEC:HBC3	1.84	0.59
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:HBC3	3:B:5:HEC:HMC1	1.83	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
3:D:5:HEC:CBB	3:D:5:HEC:CMB	2.81	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
3:A:480:HEC:CBC	3:A:480:HEC:HMC1	2.34	0.58
1:C:292:ASN:C	1:C:292:ASN:HD22	2.11	0.58
1:D:320:GLN:H	1:D:320:GLN:NE2	2.01	0.58
1:D:364:GLU:CD	6:D:531:HOH:O	2.46	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
3:B:5:HEC:HBD2	6:B:627:HOH:O	2.04	0.57
1:D:157:ASN:O	1:D:158:LEU:C	2.47	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: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
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:312:GLN:NE2	1:C:312:GLN:H	2.04	0.55
3:D:5:HEC:HMB1	3:D:5:HEC:CBB	2.30	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:B:5:HEC:HBB3	3:B:5:HEC:HMB1	1.88	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
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: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
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: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:167:ALA:O	1:D:168:SER:C	2.52	0.53
1:B:309:ASN:HB2	6:B:543:HOH:O	1.95	0.53
1:D:287:MET:HE2	1:D:299:THR:HG21	1.90	0.53
1:A:198:LYS:HD2	6:A:778:HOH:O	2.08	0.53
1:A:471:ARG:O	1:A:472:LYS:C	2.52	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:235:VAL:CB	1:D:401:MET:HE3	2.33	0.52
1:C:292:ASN:C	1:C:292:ASN:ND2	2.68	0.52
1:D:328:VAL:HG21	5:D:482:EDO:H21	1.91	0.52
3:B:480:HEC:HBC3	3:B:480:HEC:CMC	2.37	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
1:C:309:ASN:CG	1:C:312:GLN:NE2	2.67	0.52
3:A:5:HEC:HMB1	3:A:5:HEC:CBB	2.28	0.51
1:D:42:ASN:ND2	6:D:530:HOH:O	2.42	0.51
1:B:37:THR:HA	1:B:135:GLN:HE22	1.76	0.51
1:B:368:LYS:HB3	1:B:369:PRO:HD3	1.92	0.51
1:C:421:ALA:C	1:C:423:LYS:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:480:HEC:HBB3	3:A:480:HEC:HMB1	1.91	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
1:D:150:GLY:O	1:D:151:GLY:C	2.54	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
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:C:235:VAL:HB	1:C:401:MET:HE3	1.93	0.50
1:A:170:GLU:OE1	1:A:175:LYS:HD3	2.11	0.50
1:D:43:GLU:C	1:D:45:PHE:H	2.19	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:B:194:LYS:HB3	1:B:207:MET:CE	2.38	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
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:D:43:GLU:C	1:D:45:PHE:N	2.69	0.49
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:4:HEC:HMC1	3:D:4:HEC:HBC3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ASP:CB	1:D:154:ILE:HA	2.43	0.49
1:A:343:VAL:HG22	1:A:406:MET:CE	2.40	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
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
3:A:3:HEC:CBC	3:A:3:HEC:CMC	2.90	0.48
3:A:4:HEC:HBC3	3:A:4:HEC:CMC	2.44	0.48
1:C:68:ALA:HB3	1:C:88:TYR:CD2	2.49	0.48
1:A:292:ASN:C	1:A:292:ASN:ND2	2.49	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: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:476:LEU:O	1:D:477:SER:C	2.57	0.48
3:C:5:HEC:CMB	3:C:5:HEC:HBB3	2.44	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
3:C:480:HEC:HBC3	3:C:480:HEC:HMC1	1.96	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
3:A:480:HEC:CBC	3:A:480:HEC:CMC	2.92	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:D:99:THR:CG2	6:D:483:HOH:O	2.62	0.47
1:D:263:GLN:O	1:D:264:HIS:C	2.57	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:256:LYS:CE	6:A:849:HOH:O	2.62	0.47
3:A:479:HEC:HBC3	3:A:479:HEC:CMC	2.43	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:D:438:GLU:H	1:D:438:GLU:CD	2.22	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:D:155:VAL:HB	6:D:533:HOH:O	2.14	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: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:A:407:ASP:HB2	1:B:406:MET:HE3	1.98	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
3:D:4:HEC:HBC3	3:D:4:HEC:CMC	2.46	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:A:217:TYR:HH	1:A:241:TYR:HH	1.58	0.45
3:B:480:HEC:CBC	3:B:480:HEC:CMC	2.94	0.45
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
1:D:318:HIS:HB3	1:D:320:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:CD	1:A:438:GLU:H	2.24	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:C:263:GLN:O	1:C:264:HIS:C	2.60	0.45
3:C:479:HEC:HMC1	3:C:479:HEC:HBC3	1.98	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: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:B:230:ASP:CG	6:B:766:HOH:O	2.60	0.45
1:C:238:MET:CE	1:C:268:GLU:HG2	2.47	0.45
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: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: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:B:266:GLU:OE1	1:B:387:SER:OG	2.33	0.44
1:C:157:ASN:O	1:C:158:LEU:C	2.61	0.44
1:D:292:ASN:C	1:D:294:GLU:H	2.25	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
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:B:115:ASP:CG	1:B:116:GLY:H	2.26	0.44
1:C:180:LEU:HG	1:C:196:PHE:CD1	2.53	0.44
1:C:259:MET:CE	1:C:378:GLN:CD	2.90	0.44
1:D:52:GLN:N	1:D:52:GLN:CD	2.73	0.44
1:D:328:VAL:HG23	5:D:482:EDO:H22	2.00	0.44
1:A:193:GLY:C	1:A:195:PRO:HD3	2.42	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:C:385:ILE:CD1	1:C:385:ILE:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:385:ILE:C	1:D:385:ILE:HD12	2.43	0.43
1:B:281:THR:HG22	6:B:493:HOH:O	2.17	0.43
1:C:406:MET:HE3	1:D:407:ASP:CB	2.28	0.43
1:D:334:GLN:NE2	1:D:338[B]:ASP:CG	2.65	0.43
1:A:194:LYS:O	1:A:207:MET:HE1	2.19	0.43
1:B:37:THR:HG22	1:B:135:GLN:CD	2.42	0.43
1:C:125:CYS:SG	3:C:479:HEC:C2C	3.04	0.43
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:266:GLU:HB3	3:D:4:HEC:HMB2	2.01	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:42:ASN:O	1:D:43:GLU:C	2.61	0.43
1:D:433:ASP:OD1	1:D:439:LYS:CD	2.66	0.43
1:B:150:GLY:O	1:B:151:GLY:C	2.62	0.43
1:C:238:MET:HE1	1:C:268:GLU:HG2	2.01	0.43
1:C:397:GLU:O	1:C:401:MET:HG3	2.18	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
3:B:4:HEC:CBC	3:B:4:HEC:CMC	2.97	0.42
1:C:43:GLU:CD	6:C:590:HOH:O	2.62	0.42
1:C:306:PRO:HG2	3:C:4:HEC:CHD	2.49	0.42
3:D:5:HEC:HBC3	3:D:5:HEC:HMC1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:CG2	1:B:135:GLN:OE1	2.66	0.42
1:B:292:ASN:OD1	1:B:292:ASN:C	2.63	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: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:A:430:GLN:C	1:A:431:ILE:HD13	2.44	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
3:C:5:HEC:HBB3	3:C:5:HEC:HMB1	2.02	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
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.85	0.42
1:A:157:ASN:O	1:A:158:LEU:C	2.62	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:307:PHE:O	1:D:322:LYS:NZ	2.49	0.42
1:D:391:HIS:CD2	6:D:804:HOH:O	2.62	0.42
1:D:247:PHE:CD2	1:D:247:PHE:C	2.98	0.42
3:B:479:HEC:CBC	3:B:479:HEC:HMC3	2.50	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:463:ILE:N	1:D:464:PRO:CD	2.83	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:D:292:ASN:C	1:D:294:GLU:N	2.78	0.41
1:A:158:LEU:HD11	3:A:3:HEC:C3C	2.49	0.41
1:B:194:LYS:O	1:B:207:MET:HE1	2.19	0.41
1:C:346:GLN:HG3	1:C:406:MET:SD	2.60	0.41
1:D:343:VAL:HG22	1:D:406:MET:HE2	2.02	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:A:58:ALA:C	1:A:60:SER:N	2.78	0.41
1:B:127:SER:HB3	1:B:154:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASN:O	1:B:158:LEU:C	2.63	0.41
1:B:313:THR:O	1:B:316:ASN:HB2	2.20	0.41
1:C:194:LYS:O	1:C:195:PRO:C	2.63	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:194:LYS:NZ	1:C:203:ASP:OD2	2.53	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
1:B:176:PRO:O	1:B:177:GLU:C	2.64	0.41
1:C:194:LYS:O	1:C:207:MET:HE1	2.21	0.41
1:D:168:SER:HA	1:D:169:PRO:HD3	1.81	0.41
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:A:259:MET:CE	1:A:378:GLN:CD	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLY:C	1:D:194:LYS:HG3	2.45	0.41
1:D:419:LEU:HD22	1:D:419:LEU:C	2.46	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
1:C:385:ILE:C	1:C:385:ILE:HD12	2.46	0.40
1:D:396:GLU:HG2	1:D:397:GLU:N	2.36	0.40
1:A:194:LYS:HB3	1:A:207:MET:HE1	2.03	0.40
1:A:198:LYS:HE3	1:C:65:ARG:HH11	1.77	0.40
1:C:158:LEU:HD11	3:C:3:HEC:C4C	2.52	0.40
1:D:431:ILE:HG22	1:D:432:PRO:O	2.21	0.40
3:A:479:HEC:CBC	3:A:479:HEC:CMC	3.00	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:D:234:LYS:H	1:D:237:ASN:HD22	1.70	0.40
3:D:479:HEC:CMC	3:D:479:HEC:HBC2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	43	55
1	D	441/452 (98%)	413 (94%)	25 (6%)	3 (1%)	18	23
All	All	1765/1808 (98%)	1697 (96%)	64 (4%)	4 (0%)	43	55

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 ⓘ

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%)	345 (95%)	18 (5%)	22	33
1	B	364/370 (98%)	341 (94%)	23 (6%)	16	23
1	C	366/370 (99%)	354 (97%)	12 (3%)	33	50
1	D	364/370 (98%)	347 (95%)	17 (5%)	23	35
All	All	1457/1480 (98%)	1387 (95%)	70 (5%)	23	35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	52	GLN
1	A	114	GLU
1	A	222	ASN
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	312	GLN
1	A	314	CYS
1	A	320	GLN
1	A	327	LYS
1	A	364	GLU
1	A	431	ILE
1	A	472	LYS

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Mol	Chain	Res	Type
1	B	37	THR
1	B	38	VAL
1	B	52	GLN
1	B	99	THR
1	B	111	LYS
1	B	114	GLU
1	B	149	ARG
1	B	208	VAL
1	B	227	PHE
1	B	240	GLN
1	B	274	ILE
1	B	297	LEU
1	B	309	ASN
1	B	316	ASN
1	B	320	GLN
1	B	325	LEU
1	B	328	VAL
1	B	340[A]	LYS
1	B	340[B]	LYS
1	B	419	LEU
1	B	431	ILE
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	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	340	LYS
1	C	385	ILE
1	C	452	LYS
1	C	477	SER
1	D	38	VAL
1	D	52	GLN
1	D	99	THR
1	D	112	ASN
1	D	114	GLU
1	D	190	GLU
1	D	221	LYS

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Mol	Chain	Res	Type
1	D	240	GLN
1	D	244	LYS
1	D	256	LYS
1	D	274	ILE
1	D	283	ILE
1	D	296	LYS
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 (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	62	GLN
1	A	135	GLN
1	A	156	ASN
1	A	205	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	337	ASN
1	A	346	GLN
1	A	388	HIS
1	A	391	HIS
1	A	456	GLN
1	A	469	GLN
1	B	49	HIS
1	B	52	GLN
1	B	62	GLN
1	B	237	ASN
1	B	240	GLN
1	B	252	ASN
1	B	320	GLN

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Mol	Chain	Res	Type
1	B	346	GLN
1	B	349	HIS
1	B	371	GLN
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	156	ASN
1	C	237	ASN
1	C	240	GLN
1	C	252	ASN
1	C	291	GLN
1	C	292	ASN
1	C	309	ASN
1	C	312	GLN
1	C	320	GLN
1	C	334	GLN
1	C	346	GLN
1	C	371	GLN
1	C	391	HIS
1	C	427	HIS
1	C	450	GLN
1	C	456	GLN
1	C	469	GLN
1	D	42	ASN
1	D	52	GLN
1	D	62	GLN
1	D	135	GLN
1	D	237	ASN
1	D	240	GLN
1	D	252	ASN
1	D	291	GLN
1	D	320	GLN
1	D	326	GLN
1	D	334	GLN
1	D	337	ASN
1	D	346	GLN
1	D	371	GLN
1	D	388	HIS
1	D	391	HIS

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Mol	Chain	Res	Type
1	D	427	HIS
1	D	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	SO3	D	481	3	1,3,3	0.53	0	0,3,3	-	-
3	HEC	D	479	4,1	46,50,50	1.89	7 (15%)	58,82,82	2.10	6 (10%)
3	HEC	C	3	1,2	46,50,50	1.90	6 (13%)	58,82,82	1.98	7 (12%)
5	EDO	C	482	-	3,3,3	0.39	0	2,2,2	0.63	0
5	EDO	C	7	-	3,3,3	0.36	0	2,2,2	0.58	0
3	HEC	B	480	1	46,50,50	1.80	6 (13%)	58,82,82	1.90	6 (10%)
3	HEC	B	4	1,2	46,50,50	1.87	6 (13%)	58,82,82	2.02	13 (22%)
5	EDO	A	8	-	3,3,3	0.46	0	2,2,2	0.30	0
3	HEC	B	479	4,1	46,50,50	1.85	3 (6%)	58,82,82	1.75	4 (6%)
4	SO3	A	481	3	1,3,3	0.77	0	0,3,3	-	-
5	EDO	C	9	-	3,3,3	0.43	0	2,2,2	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	D	5	1	46,50,50	1.89	5 (10%)	58,82,82	1.83	5 (8%)
3	HEC	C	5	1	46,50,50	1.92	5 (10%)	58,82,82	1.74	6 (10%)
3	HEC	D	4	1,2	46,50,50	1.85	5 (10%)	58,82,82	1.87	5 (8%)
4	SO3	B	482	3	1,3,3	0.39	0	0,3,3	-	-
5	EDO	B	12	-	3,3,3	0.47	0	2,2,2	0.46	0
5	EDO	C	484	-	3,3,3	0.44	0	2,2,2	0.30	0
5	EDO	C	10	-	3,3,3	0.42	0	2,2,2	0.47	0
4	SO3	B	481	-	1,3,3	0.45	0	0,3,3	-	-
4	SO3	C	481	3	1,3,3	0.25	0	0,3,3	-	-
3	HEC	A	4	1,2	46,50,50	1.94	6 (13%)	58,82,82	2.03	10 (17%)
5	EDO	C	483	-	3,3,3	0.40	0	2,2,2	0.47	0
5	EDO	A	6	-	3,3,3	0.33	0	2,2,2	0.86	0
3	HEC	C	480	1	46,50,50	1.89	6 (13%)	58,82,82	1.79	4 (6%)
3	HEC	D	480	1	46,50,50	1.88	7 (15%)	58,82,82	1.86	5 (8%)
3	HEC	A	3	1,2	46,50,50	1.91	8 (17%)	58,82,82	2.01	7 (12%)
5	EDO	D	482	-	3,3,3	0.44	0	2,2,2	0.39	0
3	HEC	C	4	1,2	46,50,50	1.83	5 (10%)	58,82,82	2.01	4 (6%)
5	EDO	D	11	-	3,3,3	0.31	0	2,2,2	0.78	0
5	EDO	B	483	-	3,3,3	0.51	0	2,2,2	0.23	0
3	HEC	D	3	1,2	46,50,50	1.88	8 (17%)	58,82,82	1.96	6 (10%)
3	HEC	A	479	4,1	46,50,50	1.86	7 (15%)	58,82,82	1.78	4 (6%)
3	HEC	B	3	1,2	46,50,50	1.93	5 (10%)	58,82,82	1.68	7 (12%)
3	HEC	A	480	1	46,50,50	1.86	6 (13%)	58,82,82	1.88	5 (8%)
3	HEC	B	5	1	46,50,50	1.88	7 (15%)	58,82,82	1.99	7 (12%)
3	HEC	C	479	4,1	46,50,50	1.91	7 (15%)	58,82,82	1.76	4 (6%)
3	HEC	A	5	1	46,50,50	1.87	5 (10%)	58,82,82	1.83	7 (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	D	479	4,1	-	5/14/54/54	-
3	HEC	C	3	1,2	-	4/14/54/54	-
5	EDO	C	482	-	-	0/1/1/1	-
5	EDO	C	7	-	-	1/1/1/1	-
3	HEC	B	480	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	4	1,2	-	6/14/54/54	-
5	EDO	A	8	-	-	0/1/1/1	-
3	HEC	B	479	4,1	-	5/14/54/54	-
5	EDO	C	9	-	-	1/1/1/1	-
3	HEC	D	5	1	-	9/14/54/54	-
3	HEC	C	5	1	-	7/14/54/54	-
3	HEC	D	4	1,2	-	4/14/54/54	-
5	EDO	B	12	-	-	0/1/1/1	-
5	EDO	C	484	-	-	1/1/1/1	-
5	EDO	C	10	-	-	1/1/1/1	-
3	HEC	A	4	1,2	-	4/14/54/54	-
5	EDO	C	483	-	-	0/1/1/1	-
5	EDO	A	6	-	-	0/1/1/1	-
3	HEC	C	480	1	-	5/14/54/54	-
3	HEC	D	480	1	-	7/14/54/54	-
3	HEC	A	3	1,2	-	3/14/54/54	-
5	EDO	D	482	-	-	0/1/1/1	-
3	HEC	C	4	1,2	-	3/14/54/54	-
5	EDO	D	11	-	-	1/1/1/1	-
5	EDO	B	483	-	-	1/1/1/1	-
3	HEC	D	3	1,2	-	5/14/54/54	-
3	HEC	A	479	4,1	-	7/14/54/54	-
3	HEC	B	3	1,2	-	4/14/54/54	-
3	HEC	A	480	1	-	4/14/54/54	-
3	HEC	B	5	1	-	9/14/54/54	-
3	HEC	C	479	4,1	-	6/14/54/54	-
3	HEC	A	5	1	-	9/14/54/54	-

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	HEC	CAC-C3C	7.01	1.57	1.35
3	A	4	HEC	CAC-C3C	6.88	1.57	1.35
3	D	5	HEC	CAC-C3C	6.69	1.56	1.35
3	A	5	HEC	CAC-C3C	6.65	1.56	1.35
3	B	479	HEC	CAC-C3C	6.56	1.56	1.35
3	B	3	HEC	CAC-C3C	6.55	1.56	1.35
3	B	5	HEC	CAC-C3C	6.54	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	480	HEC	CAC-C3C	6.49	1.56	1.35
3	C	479	HEC	CAC-C3C	6.46	1.56	1.35
3	A	3	HEC	CAC-C3C	6.43	1.55	1.35
3	D	4	HEC	CAC-C3C	6.43	1.55	1.35
3	C	480	HEC	CAC-C3C	6.42	1.55	1.35
3	C	479	HEC	CAB-C3B	6.41	1.55	1.35
3	B	4	HEC	CAB-C3B	6.37	1.55	1.35
3	B	479	HEC	CAB-C3B	6.35	1.55	1.35
3	C	4	HEC	CAB-C3B	6.33	1.55	1.35
3	C	480	HEC	CAB-C3B	6.31	1.55	1.35
3	C	5	HEC	CAB-C3B	6.29	1.55	1.35
3	C	3	HEC	CAC-C3C	6.29	1.55	1.35
3	C	4	HEC	CAC-C3C	6.29	1.55	1.35
3	D	3	HEC	CAC-C3C	6.28	1.55	1.35
3	A	4	HEC	CAB-C3B	6.27	1.55	1.35
3	C	3	HEC	CAB-C3B	6.26	1.55	1.35
3	D	480	HEC	CAC-C3C	6.24	1.55	1.35
3	D	479	HEC	CAB-C3B	6.23	1.55	1.35
3	B	480	HEC	CAC-C3C	6.18	1.55	1.35
3	D	480	HEC	CAB-C3B	6.18	1.55	1.35
3	D	479	HEC	CAC-C3C	6.16	1.55	1.35
3	B	4	HEC	CAC-C3C	6.14	1.54	1.35
3	A	479	HEC	CAB-C3B	6.14	1.54	1.35
3	B	480	HEC	CAB-C3B	6.13	1.54	1.35
3	D	3	HEC	CAB-C3B	6.09	1.54	1.35
3	B	3	HEC	CAB-C3B	6.07	1.54	1.35
3	A	479	HEC	CAC-C3C	6.06	1.54	1.35
3	B	5	HEC	CAB-C3B	5.99	1.54	1.35
3	D	5	HEC	CAB-C3B	5.95	1.54	1.35
3	D	479	HEC	C3D-C2D	5.93	1.54	1.38
3	A	4	HEC	C3D-C2D	5.91	1.54	1.38
3	D	480	HEC	C3D-C2D	5.91	1.54	1.38
3	A	480	HEC	CAB-C3B	5.86	1.54	1.35
3	A	5	HEC	CAB-C3B	5.86	1.54	1.35
3	D	5	HEC	C3D-C2D	5.82	1.54	1.38
3	A	479	HEC	C3D-C2D	5.80	1.54	1.38
3	B	3	HEC	C3D-C2D	5.78	1.54	1.38
3	A	3	HEC	CAB-C3B	5.78	1.53	1.35
3	D	4	HEC	CAB-C3B	5.77	1.53	1.35
3	C	3	HEC	C3D-C2D	5.74	1.53	1.38
3	D	4	HEC	C3D-C2D	5.69	1.53	1.38
3	D	3	HEC	C3D-C2D	5.62	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	480	HEC	C3D-C2D	5.60	1.53	1.38
3	C	480	HEC	C3D-C2D	5.59	1.53	1.38
3	B	5	HEC	C3D-C2D	5.54	1.53	1.38
3	C	5	HEC	C3D-C2D	5.53	1.53	1.38
3	B	4	HEC	C3D-C2D	5.45	1.53	1.38
3	A	3	HEC	C3D-C2D	5.38	1.52	1.38
3	A	5	HEC	C3D-C2D	5.32	1.52	1.38
3	C	479	HEC	C3D-C2D	5.22	1.52	1.38
3	B	479	HEC	C3D-C2D	5.20	1.52	1.38
3	C	4	HEC	C3D-C2D	5.14	1.52	1.38
3	B	480	HEC	C3D-C2D	5.03	1.52	1.38
3	B	4	HEC	CMB-C2B	3.02	1.57	1.50
3	B	4	HEC	CMD-C2D	2.97	1.56	1.50
3	A	3	HEC	CMC-C2C	2.79	1.56	1.50
3	A	3	HEC	C3B-C2B	-2.70	1.32	1.41
3	C	480	HEC	CMC-C2C	2.57	1.56	1.50
3	A	4	HEC	CMA-C3A	2.51	1.55	1.50
3	A	4	HEC	CMD-C2D	2.40	1.55	1.50
3	D	3	HEC	CMC-C2C	2.38	1.55	1.50
3	C	3	HEC	CMD-C2D	2.34	1.55	1.50
3	A	3	HEC	CMA-C3A	2.34	1.55	1.50
3	D	3	HEC	CMB-C2B	2.30	1.55	1.50
3	B	3	HEC	CMC-C2C	2.30	1.55	1.50
3	C	3	HEC	CMC-C2C	2.27	1.55	1.50
3	D	3	HEC	CMA-C3A	2.25	1.55	1.50
3	A	5	HEC	CMC-C2C	2.25	1.55	1.50
3	B	480	HEC	CMC-C2C	2.23	1.55	1.50
3	A	480	HEC	CMA-C3A	2.22	1.55	1.50
3	B	3	HEC	CMB-C2B	2.19	1.55	1.50
3	A	3	HEC	CMB-C2B	2.19	1.55	1.50
3	A	4	HEC	C3B-C2B	-2.18	1.33	1.41
3	C	479	HEC	CMB-C2B	2.17	1.55	1.50
3	C	4	HEC	CMC-C2C	2.17	1.55	1.50
3	D	479	HEC	CMC-C2C	2.17	1.55	1.50
3	B	5	HEC	CMC-C2C	2.16	1.55	1.50
3	A	479	HEC	CMD-C2D	2.16	1.55	1.50
3	D	5	HEC	CMD-C2D	2.15	1.55	1.50
3	C	480	HEC	C3B-C2B	-2.15	1.33	1.41
3	A	479	HEC	CMC-C2C	2.13	1.55	1.50
3	D	5	HEC	CMB-C2B	2.12	1.55	1.50
3	D	479	HEC	C3C-C2C	-2.11	1.34	1.41
3	D	480	HEC	CMC-C2C	2.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	HEC	CMD-C2D	2.10	1.55	1.50
3	C	5	HEC	C3B-C2B	-2.10	1.34	1.41
3	C	479	HEC	CMA-C3A	2.10	1.55	1.50
3	D	480	HEC	C3B-C2B	-2.09	1.34	1.41
3	C	4	HEC	C3B-C2B	-2.09	1.34	1.41
3	B	4	HEC	C3B-C2B	-2.08	1.34	1.41
3	C	479	HEC	CMD-C2D	2.08	1.55	1.50
3	C	479	HEC	C3B-C2B	-2.07	1.34	1.41
3	B	5	HEC	CMA-C3A	2.07	1.55	1.50
3	C	3	HEC	CMB-C2B	2.07	1.55	1.50
3	D	4	HEC	CMB-C2B	2.07	1.55	1.50
3	A	479	HEC	CMA-C3A	2.06	1.55	1.50
3	D	4	HEC	C3B-C2B	-2.06	1.34	1.41
3	D	3	HEC	C3B-C2B	-2.06	1.34	1.41
3	D	479	HEC	CMD-C2D	2.05	1.55	1.50
3	A	479	HEC	C3B-C2B	-2.05	1.34	1.41
3	A	480	HEC	C3C-C2C	-2.05	1.34	1.41
3	C	5	HEC	CMA-C3A	2.05	1.55	1.50
3	B	480	HEC	C3B-C2B	-2.04	1.34	1.41
3	A	3	HEC	CMD-C2D	2.04	1.55	1.50
3	D	479	HEC	CMA-C3A	2.04	1.55	1.50
3	C	480	HEC	CMB-C2B	2.04	1.54	1.50
3	D	480	HEC	CMA-C3A	2.04	1.54	1.50
3	D	480	HEC	C3C-C2C	-2.03	1.34	1.41
3	B	5	HEC	CMB-C2B	2.03	1.54	1.50
3	B	480	HEC	CMA-C3A	2.03	1.54	1.50
3	B	5	HEC	C3B-C2B	-2.02	1.34	1.41
3	A	5	HEC	CMD-C2D	2.01	1.54	1.50
3	A	480	HEC	C3B-C2B	-2.01	1.34	1.41

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	CBB-CAB-C3B	-10.00	107.44	127.43
3	B	479	HEC	CBB-CAB-C3B	-10.00	107.45	127.43
3	A	4	HEC	CBB-CAB-C3B	-9.93	107.59	127.43
3	D	479	HEC	CBB-CAB-C3B	-9.91	107.63	127.43
3	C	479	HEC	CBB-CAB-C3B	-9.59	108.26	127.43
3	A	480	HEC	CBB-CAB-C3B	-9.53	108.39	127.43
3	A	5	HEC	CBB-CAB-C3B	-9.44	108.57	127.43
3	C	4	HEC	CBB-CAB-C3B	-9.42	108.61	127.43
3	C	3	HEC	CBB-CAB-C3B	-9.14	109.16	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	HEC	CBB-CAB-C3B	-9.07	109.30	127.43
3	D	5	HEC	CBB-CAB-C3B	-8.96	109.53	127.43
3	D	4	HEC	CBB-CAB-C3B	-8.91	109.63	127.43
3	D	3	HEC	CBB-CAB-C3B	-8.91	109.63	127.43
3	B	4	HEC	CBB-CAB-C3B	-8.84	109.76	127.43
3	B	480	HEC	CBB-CAB-C3B	-8.80	109.85	127.43
3	D	479	HEC	CBC-CAC-C3C	-8.63	110.18	127.43
3	A	3	HEC	CBC-CAC-C3C	-8.53	110.38	127.43
3	D	3	HEC	CBC-CAC-C3C	-8.49	110.47	127.43
3	C	480	HEC	CBB-CAB-C3B	-8.47	110.51	127.43
3	C	5	HEC	CBB-CAB-C3B	-8.43	110.58	127.43
3	D	480	HEC	CBC-CAC-C3C	-8.15	111.15	127.43
3	D	480	HEC	CBB-CAB-C3B	-8.15	111.15	127.43
3	C	3	HEC	CBC-CAC-C3C	-8.13	111.18	127.43
3	A	479	HEC	CBB-CAB-C3B	-8.12	111.21	127.43
3	C	4	HEC	CBC-CAC-C3C	-8.05	111.34	127.43
3	B	3	HEC	CBB-CAB-C3B	-7.84	111.76	127.43
3	B	480	HEC	CBC-CAC-C3C	-7.72	112.00	127.43
3	A	4	HEC	CBC-CAC-C3C	-7.25	112.95	127.43
3	D	4	HEC	CBC-CAC-C3C	-7.15	113.14	127.43
3	A	480	HEC	CBC-CAC-C3C	-7.07	113.30	127.43
3	A	479	HEC	CBC-CAC-C3C	-6.72	114.01	127.43
3	B	4	HEC	CBC-CAC-C3C	-6.46	114.53	127.43
3	B	5	HEC	CBC-CAC-C3C	-6.36	114.72	127.43
3	C	480	HEC	CBC-CAC-C3C	-6.32	114.80	127.43
3	D	5	HEC	CBC-CAC-C3C	-6.23	114.98	127.43
3	A	5	HEC	CBC-CAC-C3C	-5.87	115.70	127.43
3	C	479	HEC	CBC-CAC-C3C	-5.35	116.74	127.43
3	C	5	HEC	CBC-CAC-C3C	-5.26	116.92	127.43
3	B	3	HEC	CBC-CAC-C3C	-5.14	117.16	127.43
3	B	479	HEC	CBC-CAC-C3C	-4.58	118.28	127.43
3	B	4	HEC	C4D-ND-C1D	4.07	112.46	105.82
3	A	3	HEC	CBD-CAD-C3D	-3.74	102.19	112.53
3	A	4	HEC	C4D-ND-C1D	3.69	111.84	105.82
3	A	479	HEC	C4D-ND-C1D	3.65	111.77	105.82
3	D	479	HEC	C4D-ND-C1D	3.63	111.74	105.82
3	C	4	HEC	C4D-ND-C1D	3.59	111.67	105.82
3	A	5	HEC	CAD-CBD-CGD	-3.42	104.60	113.67
3	C	480	HEC	C4D-ND-C1D	3.37	111.32	105.82
3	D	480	HEC	C4D-ND-C1D	3.36	111.30	105.82
3	A	479	HEC	C2A-C1A-NA	-3.35	107.09	110.32
3	C	3	HEC	C4D-ND-C1D	3.30	111.21	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	HEC	CBA-CAA-C2A	-3.28	103.47	112.53
3	B	5	HEC	CHA-C1A-NA	3.25	128.00	124.45
3	B	480	HEC	C4D-ND-C1D	3.25	111.11	105.82
3	B	3	HEC	C4D-ND-C1D	3.21	111.05	105.82
3	A	480	HEC	C4D-ND-C1D	3.19	111.02	105.82
3	D	5	HEC	C4D-ND-C1D	3.18	111.01	105.82
3	D	479	HEC	C2A-C1A-NA	-3.16	107.28	110.32
3	D	4	HEC	C4D-ND-C1D	3.07	110.83	105.82
3	C	479	HEC	C4D-ND-C1D	3.04	110.77	105.82
3	A	4	HEC	CBA-CAA-C2A	-3.03	104.15	112.53
3	B	479	HEC	C4D-ND-C1D	2.99	110.70	105.82
3	C	4	HEC	CAD-CBD-CGD	-2.97	105.78	113.67
3	B	4	HEC	CBA-CAA-C2A	-2.91	104.50	112.53
3	A	480	HEC	CAD-CBD-CGD	-2.90	105.99	113.67
3	A	4	HEC	CAD-CBD-CGD	-2.89	106.00	113.67
3	B	5	HEC	C2A-C1A-NA	-2.81	107.61	110.32
3	B	4	HEC	C2A-C1A-NA	-2.81	107.61	110.32
3	B	4	HEC	CAD-CBD-CGD	-2.79	106.27	113.67
3	A	3	HEC	C4D-ND-C1D	2.77	110.34	105.82
3	B	4	HEC	C3D-C4D-ND	-2.70	107.16	110.15
3	D	3	HEC	C4D-ND-C1D	2.69	110.20	105.82
3	B	5	HEC	C4D-ND-C1D	2.66	110.16	105.82
3	C	480	HEC	CHD-C4C-NC	2.56	127.24	124.45
3	D	3	HEC	CAD-C3D-C4D	2.55	129.92	124.94
3	A	5	HEC	CHC-C4B-NB	2.54	127.22	124.45
3	C	5	HEC	C4D-ND-C1D	2.50	109.89	105.82
3	C	5	HEC	CAD-CBD-CGD	-2.50	107.04	113.67
3	A	3	HEC	CMD-C2D-C1D	2.49	129.22	125.42
3	C	3	HEC	CHD-C1D-ND	2.47	128.34	123.86
3	C	3	HEC	CMC-C2C-C1C	-2.43	121.71	125.42
3	A	5	HEC	CBA-CAA-C2A	-2.42	105.84	112.53
3	D	4	HEC	CAA-CBA-CGA	-2.42	107.26	113.67
3	D	479	HEC	CAA-C2A-C3A	-2.41	123.36	127.87
3	A	4	HEC	O2A-CGA-CBA	2.38	121.51	114.00
3	D	480	HEC	CAD-CBD-CGD	-2.34	107.46	113.67
3	D	3	HEC	C2A-C1A-NA	-2.33	108.07	110.32
3	D	5	HEC	C2A-C1A-NA	-2.33	108.08	110.32
3	B	5	HEC	CHD-C4C-NC	2.32	126.98	124.45
3	B	480	HEC	C2A-C1A-NA	-2.32	108.09	110.32
3	B	4	HEC	O1A-CGA-CBA	-2.31	115.76	123.09
3	C	3	HEC	C2A-C1A-NA	-2.30	108.10	110.32
3	A	3	HEC	CHD-C4C-NC	2.30	126.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	HEC	CMC-C2C-C1C	-2.29	121.93	125.42
3	A	5	HEC	C4D-ND-C1D	2.28	109.53	105.82
3	B	4	HEC	CMD-C2D-C1D	2.27	128.88	125.42
3	C	5	HEC	CMD-C2D-C3D	2.27	130.44	125.62
3	B	4	HEC	O1D-CGD-CBD	-2.27	115.90	123.09
3	A	4	HEC	O1D-CGD-CBD	-2.25	115.94	123.09
3	B	3	HEC	CBD-CAD-C3D	-2.24	106.35	112.53
3	D	5	HEC	CHC-C4B-NB	2.23	126.88	124.45
3	D	3	HEC	CBA-CAA-C2A	-2.20	106.44	112.53
3	A	4	HEC	CHD-C4C-NC	2.20	126.85	124.45
3	D	480	HEC	CHD-C4C-NC	2.20	126.85	124.45
3	B	480	HEC	CAD-C3D-C4D	2.14	129.12	124.94
3	A	4	HEC	O2D-CGD-CBD	2.13	120.74	114.00
3	B	479	HEC	C2A-C1A-NA	-2.13	108.27	110.32
3	D	479	HEC	CHC-C4B-NB	2.12	126.76	124.45
3	C	3	HEC	CBA-CAA-C2A	-2.11	106.69	112.53
3	B	3	HEC	C2A-C1A-NA	-2.10	108.29	110.32
3	B	3	HEC	CHC-C4B-NB	2.10	126.74	124.45
3	C	5	HEC	C2A-C1A-NA	-2.10	108.30	110.32
3	B	4	HEC	CBD-CAD-C3D	-2.06	106.83	112.53
3	B	4	HEC	O2D-CGD-CBD	2.05	120.48	114.00
3	B	3	HEC	CBA-CAA-C2A	-2.05	106.87	112.53
3	A	4	HEC	O1A-CGA-CBA	-2.04	116.62	123.09
3	B	4	HEC	O2A-CGA-CBA	2.03	120.42	114.00
3	D	4	HEC	CBA-CAA-C2A	-2.03	106.92	112.53
3	B	480	HEC	O2A-CGA-CBA	2.03	120.40	114.00
3	C	479	HEC	C2A-C1A-NA	-2.02	108.38	110.32
3	A	5	HEC	CAA-CBA-CGA	-2.01	108.34	113.67
3	A	480	HEC	O1D-CGD-CBD	-2.00	116.73	123.09

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	479	HEC	C2B-C3B-CAB-CBB
3	A	479	HEC	C4B-C3B-CAB-CBB
3	A	479	HEC	C2C-C3C-CAC-CBC
3	A	479	HEC	C4C-C3C-CAC-CBC
3	A	480	HEC	C2B-C3B-CAB-CBB
3	A	480	HEC	C4B-C3B-CAB-CBB
3	A	3	HEC	C2B-C3B-CAB-CBB
3	A	3	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	A	3	HEC	C2C-C3C-CAC-CBC
3	A	4	HEC	C2B-C3B-CAB-CBB
3	A	4	HEC	C4B-C3B-CAB-CBB
3	A	4	HEC	C2C-C3C-CAC-CBC
3	A	4	HEC	C4C-C3C-CAC-CBC
3	A	5	HEC	C2B-C3B-CAB-CBB
3	A	5	HEC	C4B-C3B-CAB-CBB
3	A	5	HEC	C2C-C3C-CAC-CBC
3	A	5	HEC	C4C-C3C-CAC-CBC
3	B	479	HEC	C2C-C3C-CAC-CBC
3	B	480	HEC	C2B-C3B-CAB-CBB
3	B	480	HEC	C4B-C3B-CAB-CBB
3	B	480	HEC	C2C-C3C-CAC-CBC
3	B	480	HEC	C4C-C3C-CAC-CBC
3	B	3	HEC	C2B-C3B-CAB-CBB
3	B	3	HEC	C2C-C3C-CAC-CBC
3	B	3	HEC	C4C-C3C-CAC-CBC
3	B	4	HEC	C2B-C3B-CAB-CBB
3	B	4	HEC	C4B-C3B-CAB-CBB
3	B	4	HEC	C2C-C3C-CAC-CBC
3	B	5	HEC	C2B-C3B-CAB-CBB
3	B	5	HEC	C4B-C3B-CAB-CBB
3	B	5	HEC	C2C-C3C-CAC-CBC
3	C	479	HEC	C2B-C3B-CAB-CBB
3	C	479	HEC	C2C-C3C-CAC-CBC
3	C	479	HEC	C4C-C3C-CAC-CBC
3	C	480	HEC	C2B-C3B-CAB-CBB
3	C	480	HEC	C4B-C3B-CAB-CBB
3	C	480	HEC	C2C-C3C-CAC-CBC
3	C	3	HEC	C2B-C3B-CAB-CBB
3	C	3	HEC	C2C-C3C-CAC-CBC
3	C	3	HEC	C4C-C3C-CAC-CBC
3	C	4	HEC	C2B-C3B-CAB-CBB
3	C	4	HEC	C4B-C3B-CAB-CBB
3	C	4	HEC	C2C-C3C-CAC-CBC
3	C	5	HEC	C2B-C3B-CAB-CBB
3	C	5	HEC	C4B-C3B-CAB-CBB
3	D	479	HEC	C2B-C3B-CAB-CBB
3	D	479	HEC	C4B-C3B-CAB-CBB
3	D	480	HEC	C2B-C3B-CAB-CBB
3	D	480	HEC	C4B-C3B-CAB-CBB
3	D	480	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	D	3	HEC	C2B-C3B-CAB-CBB
3	D	3	HEC	C4B-C3B-CAB-CBB
3	D	3	HEC	C2C-C3C-CAC-CBC
3	D	3	HEC	C4C-C3C-CAC-CBC
3	D	4	HEC	C2B-C3B-CAB-CBB
3	D	4	HEC	C4B-C3B-CAB-CBB
3	D	4	HEC	C2C-C3C-CAC-CBC
3	D	4	HEC	C4C-C3C-CAC-CBC
3	D	5	HEC	C2B-C3B-CAB-CBB
3	D	5	HEC	C4B-C3B-CAB-CBB
3	D	5	HEC	C2C-C3C-CAC-CBC
3	D	5	HEC	C4C-C3C-CAC-CBC
5	C	484	EDO	O1-C1-C2-O2
3	A	479	HEC	C3D-CAD-CBD-CGD
3	A	5	HEC	C2A-CAA-CBA-CGA
3	C	5	HEC	C2A-CAA-CBA-CGA
5	C	7	EDO	O1-C1-C2-O2
3	B	5	HEC	C2A-CAA-CBA-CGA
3	D	479	HEC	C3D-CAD-CBD-CGD
3	B	479	HEC	C4B-C3B-CAB-CBB
3	B	3	HEC	C4B-C3B-CAB-CBB
3	B	4	HEC	C4C-C3C-CAC-CBC
3	B	5	HEC	C4C-C3C-CAC-CBC
3	C	479	HEC	C4B-C3B-CAB-CBB
3	C	3	HEC	C4B-C3B-CAB-CBB
5	B	483	EDO	O1-C1-C2-O2
3	B	479	HEC	C2B-C3B-CAB-CBB
3	B	479	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
3	A	479	HEC	CAA-CBA-CGA-O2A
3	C	479	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAA-CBA-CGA-O1A
3	D	479	HEC	CAA-CBA-CGA-O1A
3	B	5	HEC	CAD-CBD-CGD-O2D
3	C	479	HEC	CAA-CBA-CGA-O1A
3	D	479	HEC	CAA-CBA-CGA-O2A
3	B	5	HEC	CAA-CBA-CGA-O1A
3	D	5	HEC	CAA-CBA-CGA-O1A
5	C	9	EDO	O1-C1-C2-O2
5	D	11	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	5	HEC	CAA-CBA-CGA-O2A
3	A	480	HEC	CAA-CBA-CGA-O1A
3	A	480	HEC	CAA-CBA-CGA-O2A
3	C	480	HEC	CAA-CBA-CGA-O1A
3	B	480	HEC	CAA-CBA-CGA-O1A
3	B	480	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAA-CBA-CGA-O1A
3	B	5	HEC	CAD-CBD-CGD-O1D
3	A	5	HEC	CAD-CBD-CGD-O2D
3	C	5	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	CAA-CBA-CGA-O2A
3	A	5	HEC	CAA-CBA-CGA-O2A
3	C	5	HEC	CAD-CBD-CGD-O2D
5	C	10	EDO	O1-C1-C2-O2
3	D	5	HEC	CAD-CBD-CGD-O2D
3	C	480	HEC	CAA-CBA-CGA-O2A
3	D	480	HEC	CAD-CBD-CGD-O2D
3	D	5	HEC	CAD-CBD-CGD-O1D
3	C	5	HEC	CAD-CBD-CGD-O1D
3	D	480	HEC	CAA-CBA-CGA-O1A
3	D	480	HEC	CAD-CBD-CGD-O1D
3	D	480	HEC	CAA-CBA-CGA-O2A
3	D	5	HEC	C2A-CAA-CBA-CGA
3	D	3	HEC	CAD-CBD-CGD-O2D
3	B	4	HEC	CAA-CBA-CGA-O1A
3	B	4	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

25 monomers are involved in 200 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	479	HEC	14	0
3	C	3	HEC	11	0
3	B	480	HEC	7	0
3	B	4	HEC	10	0
3	B	479	HEC	6	0
5	C	9	EDO	4	0
3	D	5	HEC	11	0
3	C	5	HEC	8	0
3	D	4	HEC	9	0
5	C	484	EDO	3	0
3	A	4	HEC	9	0

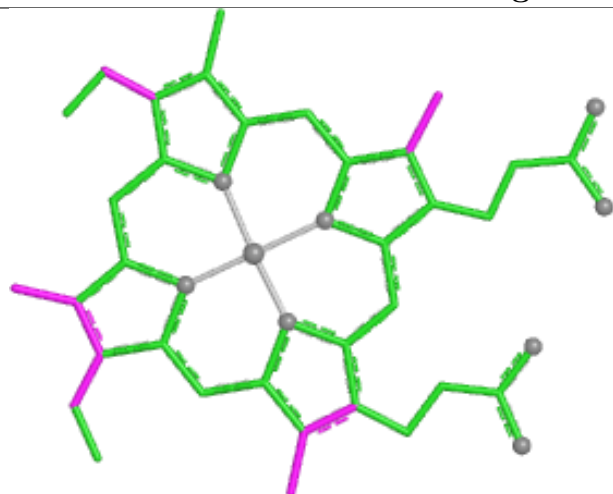
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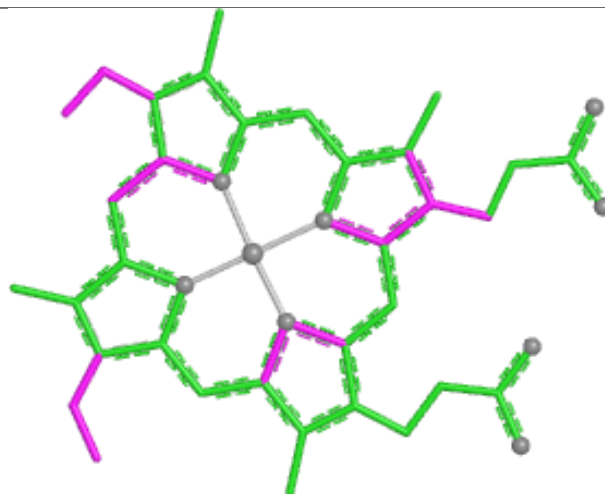
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	483	EDO	1	0
3	C	480	HEC	5	0
3	D	480	HEC	7	0
3	A	3	HEC	10	0
5	D	482	EDO	8	0
3	C	4	HEC	10	0
5	B	483	EDO	10	0
3	D	3	HEC	6	0
3	A	479	HEC	7	0
3	B	3	HEC	5	0
3	A	480	HEC	14	0
3	B	5	HEC	9	0
3	C	479	HEC	6	0
3	A	5	HEC	10	0

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

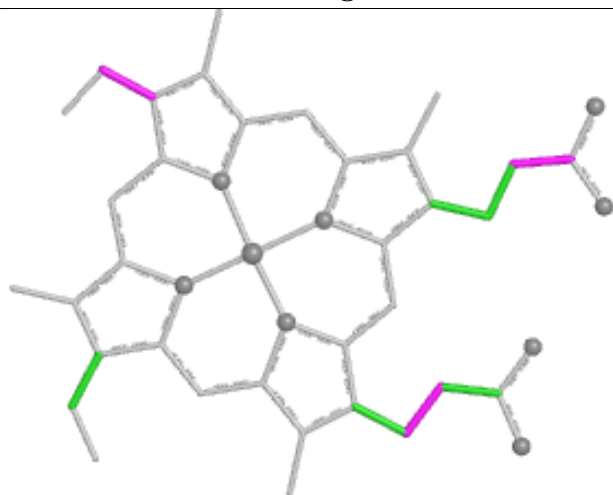
Ligand HEC D 479



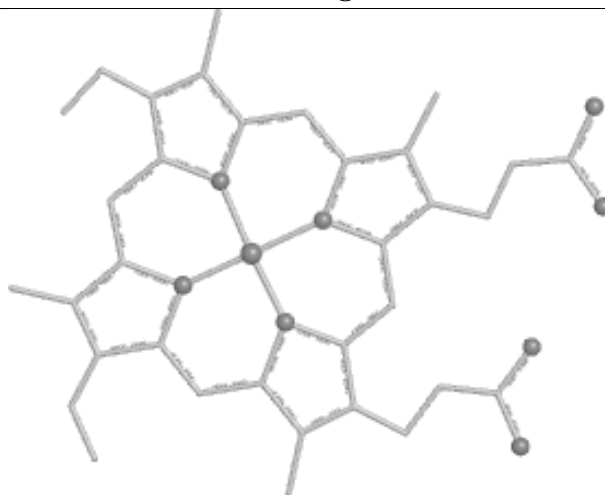
Bond lengths



Bond angles

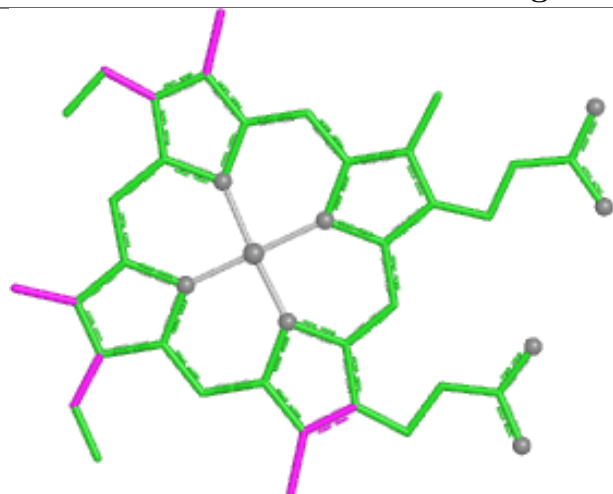


Torsions

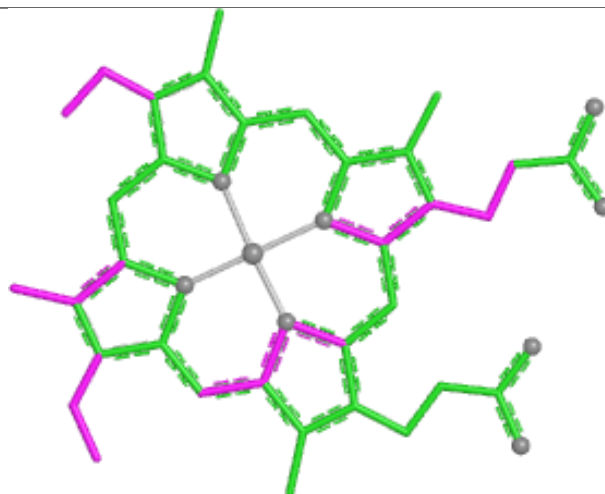


Rings

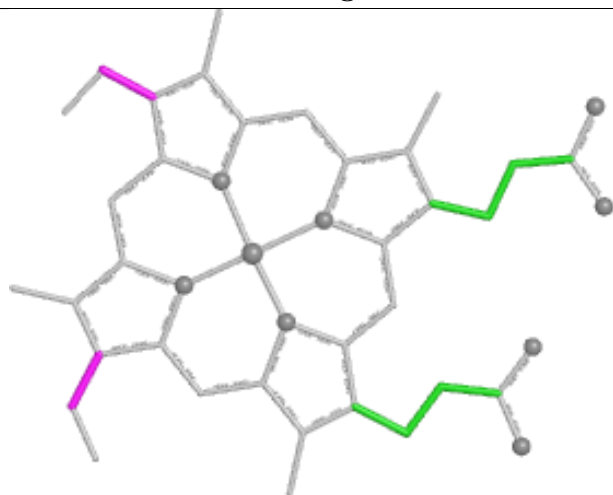
Ligand HEC C 3



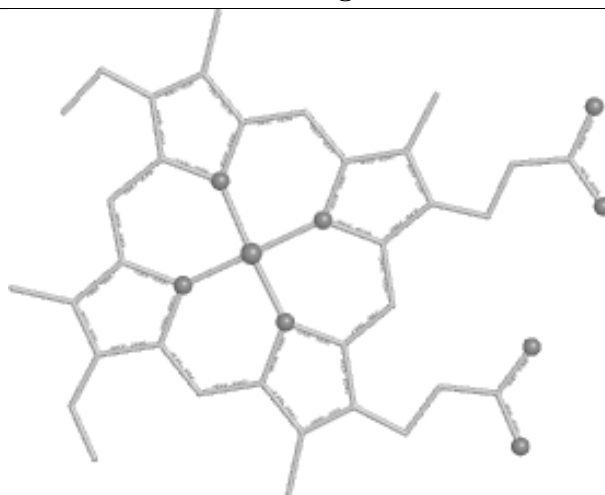
Bond lengths



Bond angles

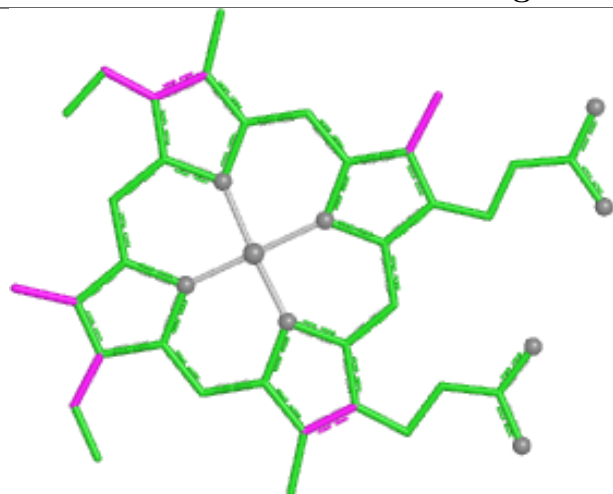


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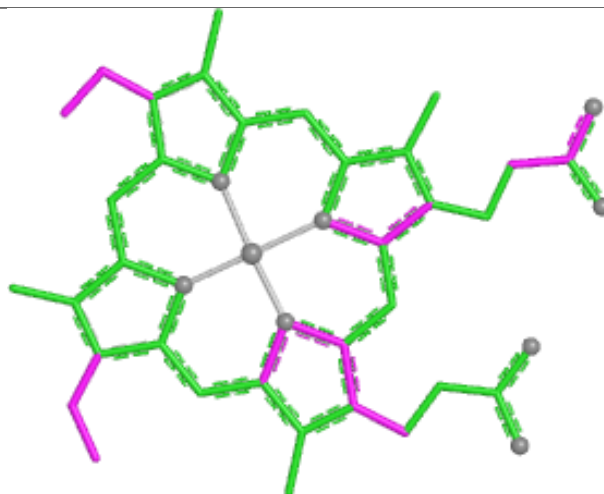


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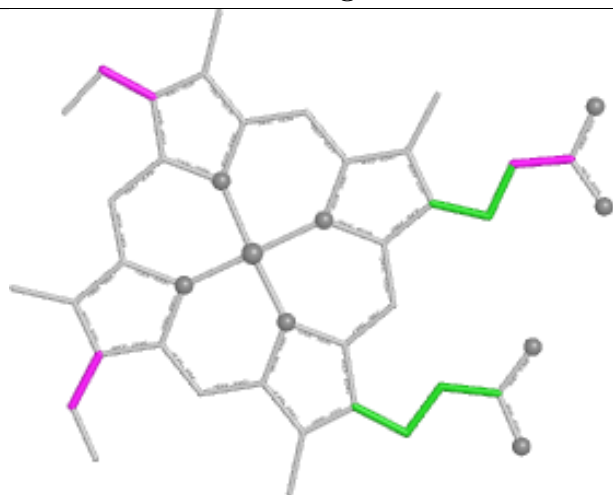
Ligand HEC B 480



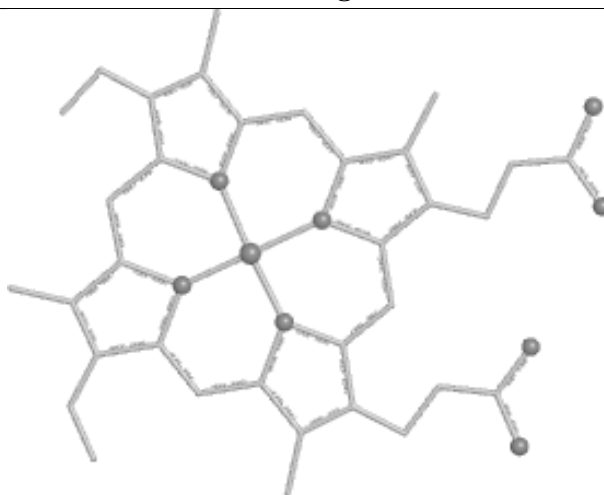
Bond lengths



Bond angles

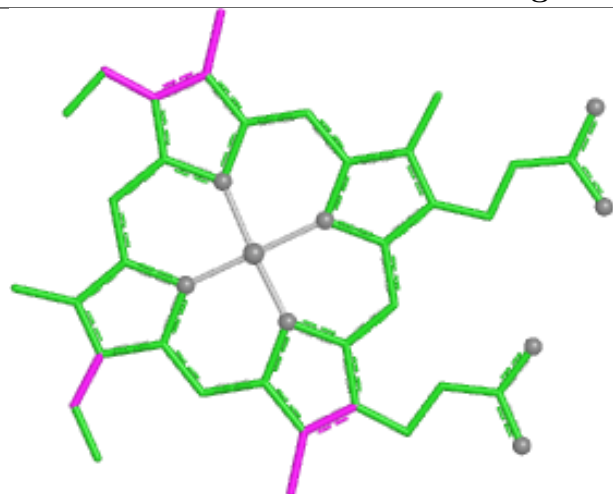


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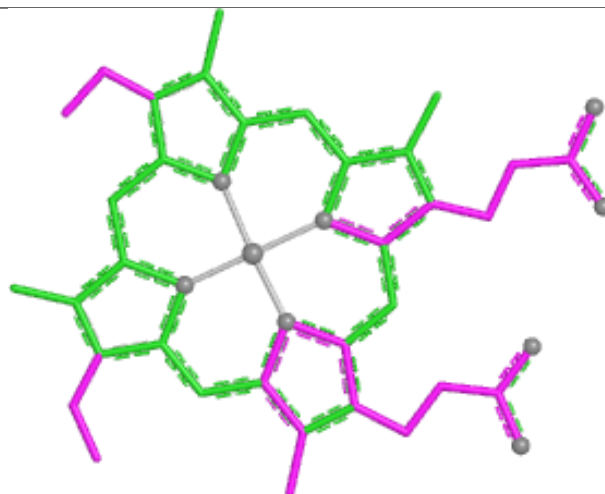


Rings

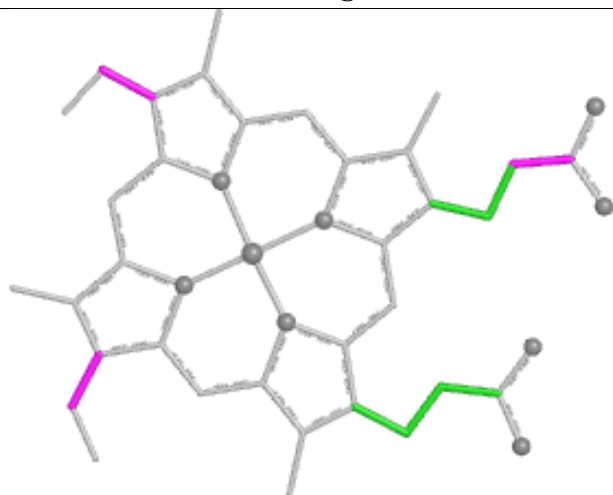
Ligand HEC B 4



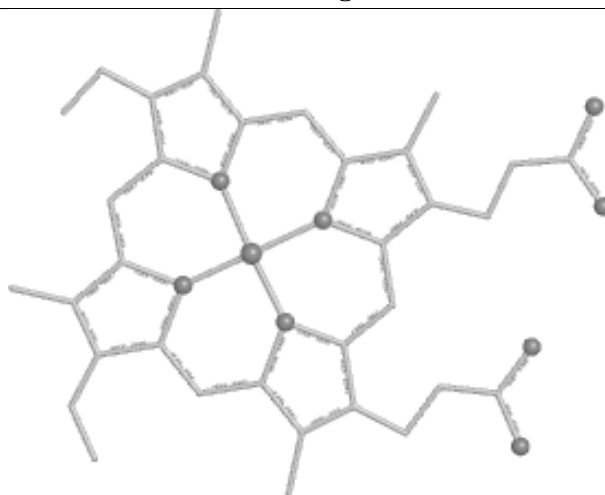
Bond lengths



Bond angles

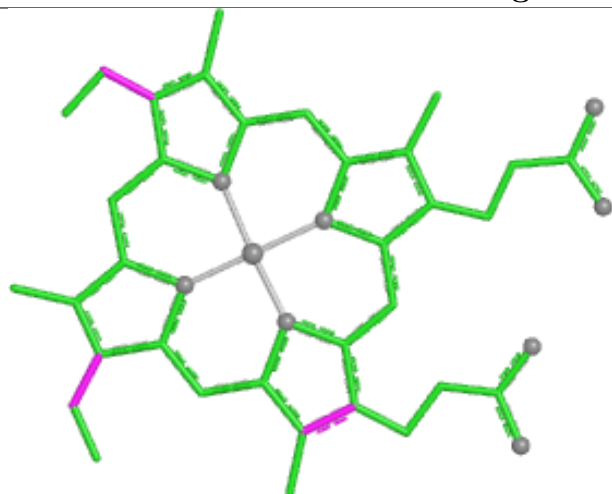


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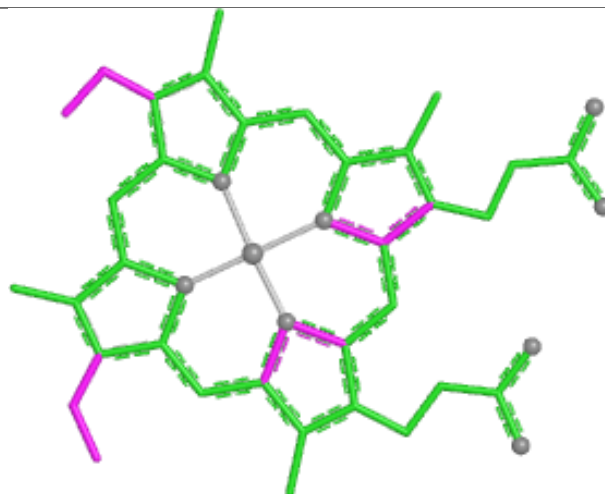


Rings

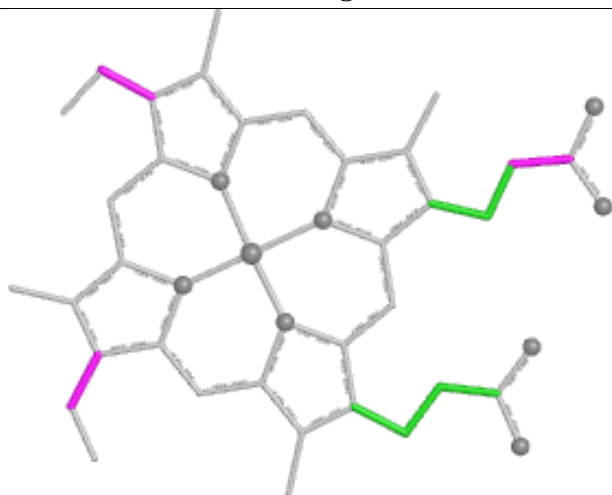
Ligand HEC B 479



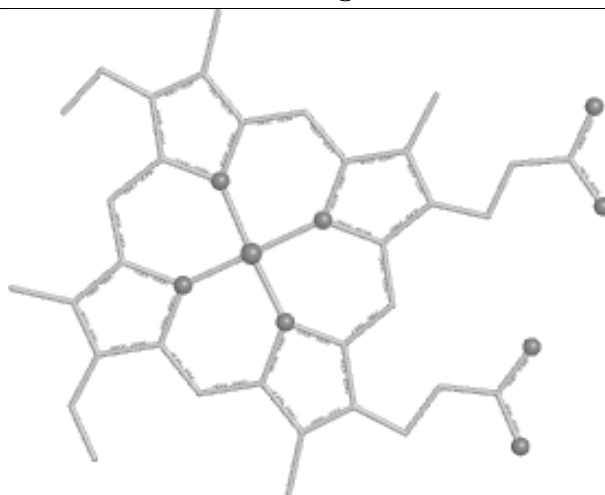
Bond lengths



Bond angles

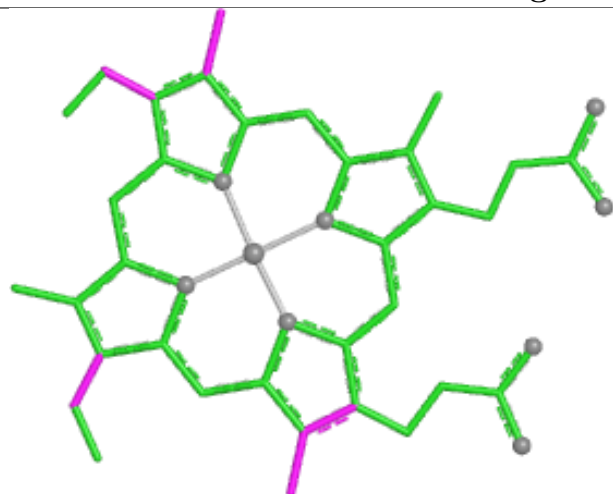


Torsions

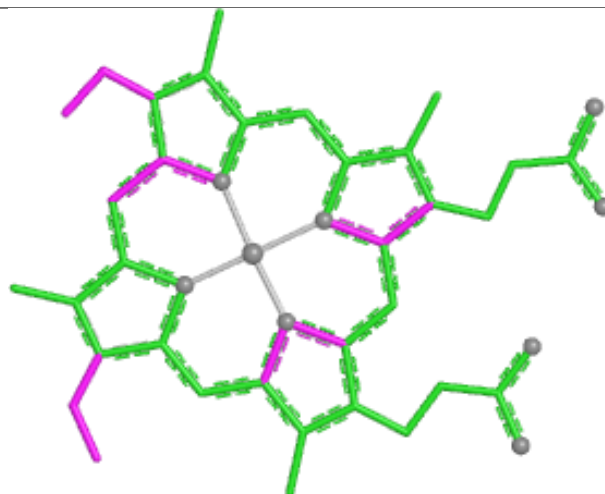


Rings

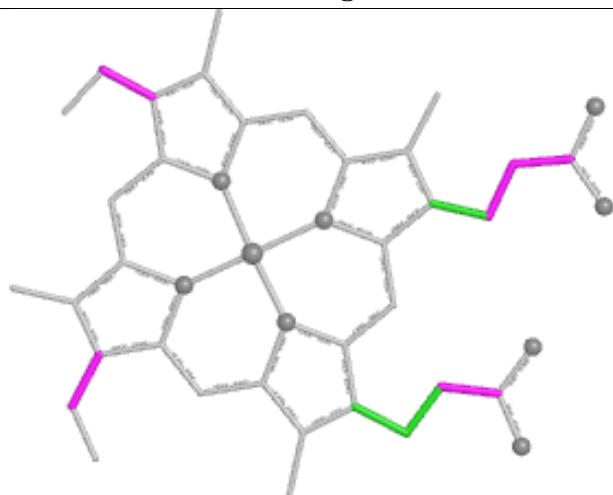
Ligand HEC D 5



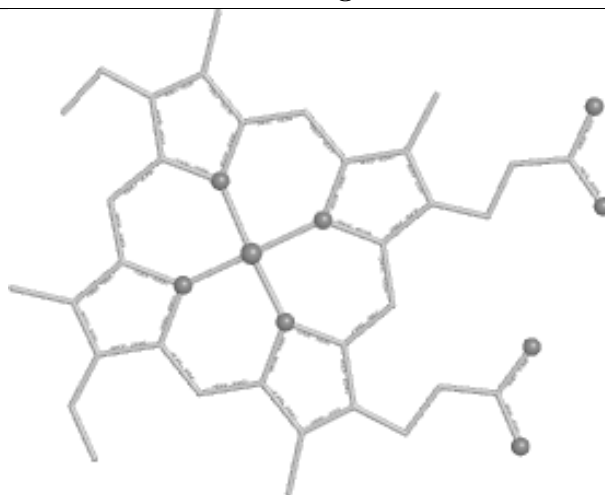
Bond lengths



Bond angles

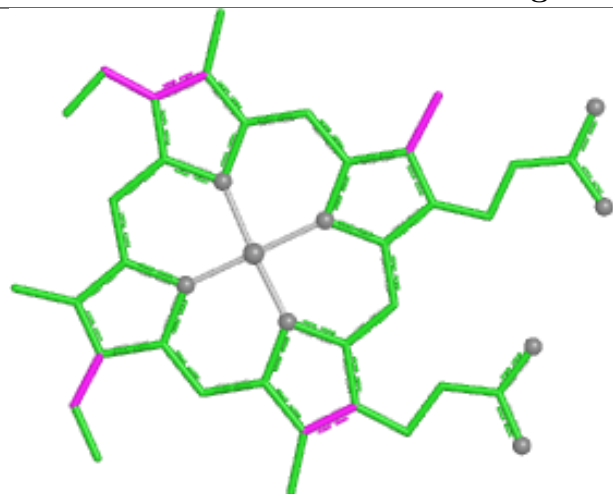


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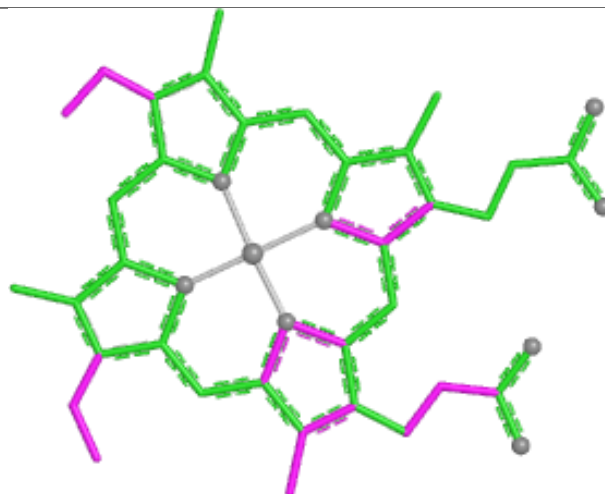


Rings

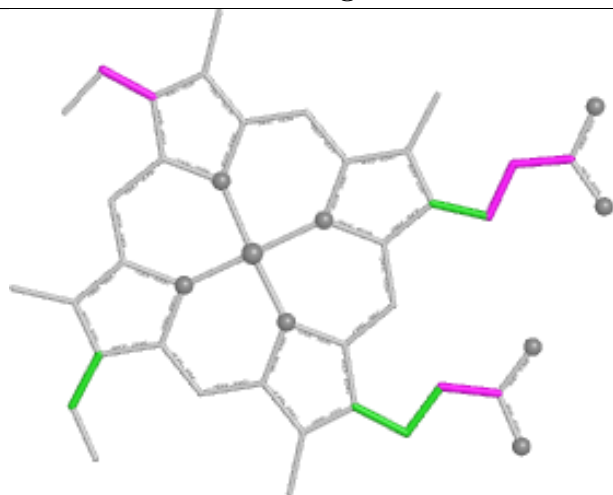
Ligand HEC C 5



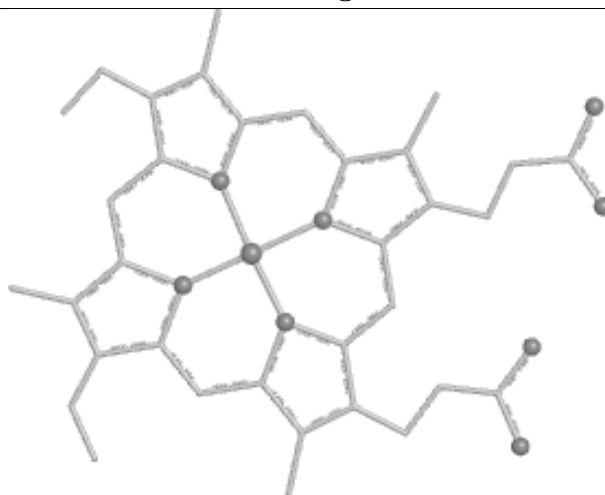
Bond lengths



Bond angles

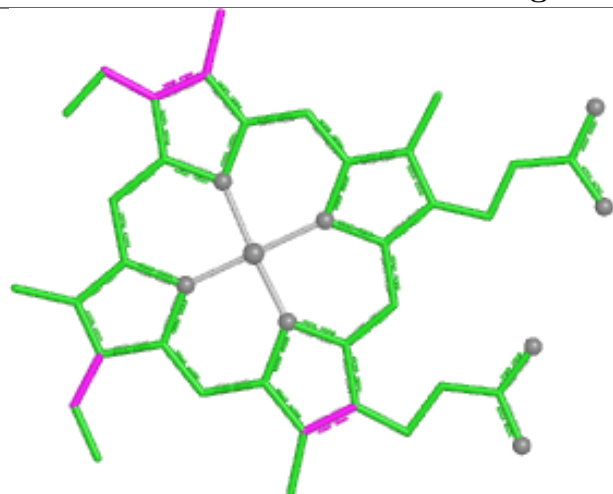


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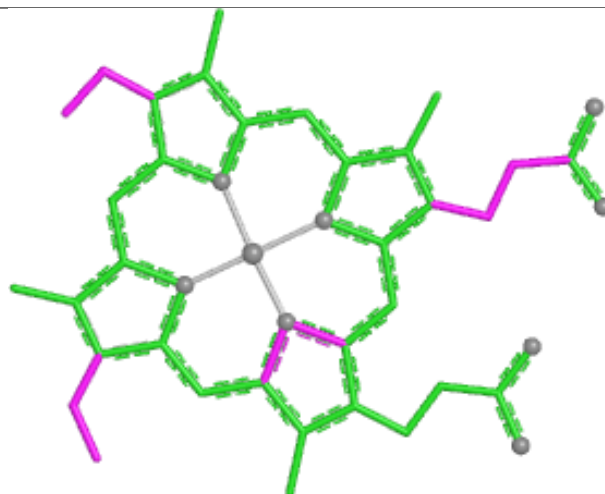


Rings

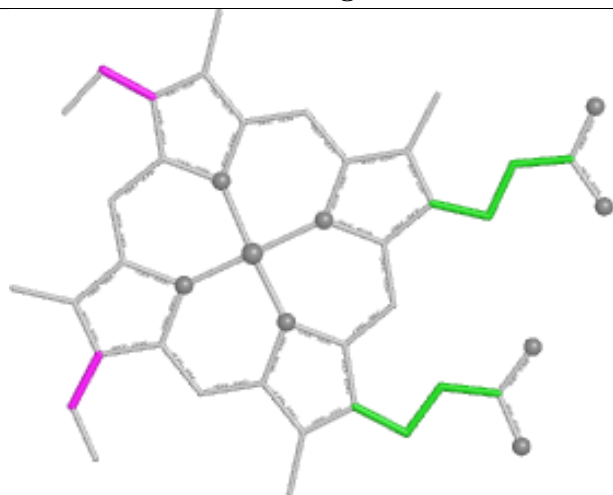
Ligand HEC D 4



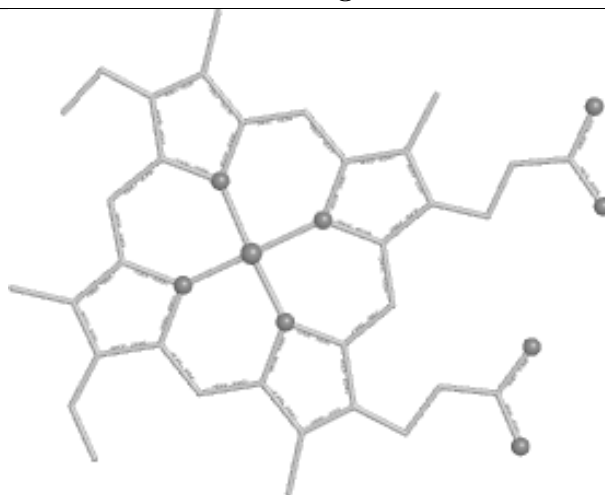
Bond lengths



Bond angles

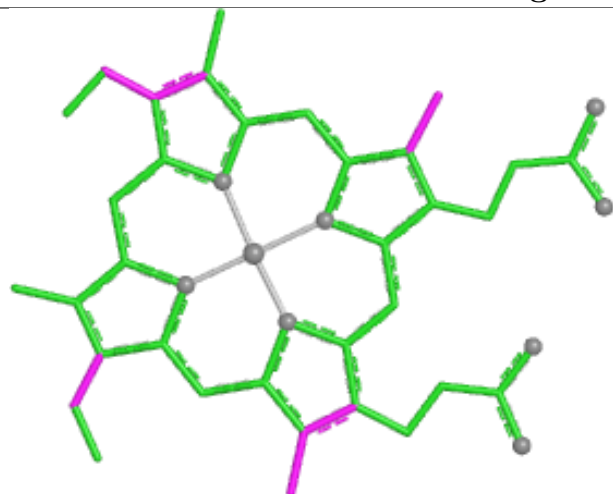


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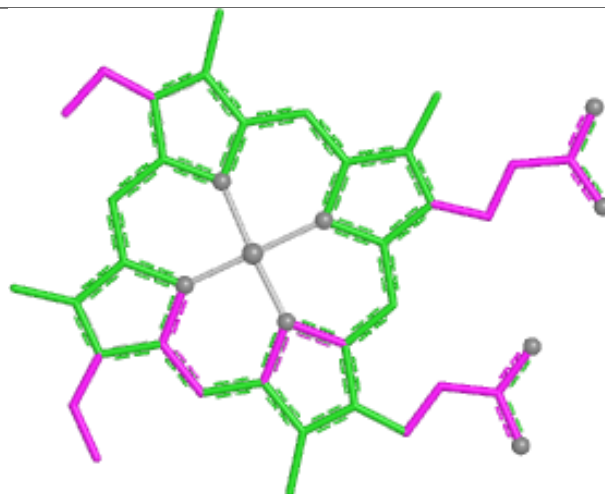


Rings

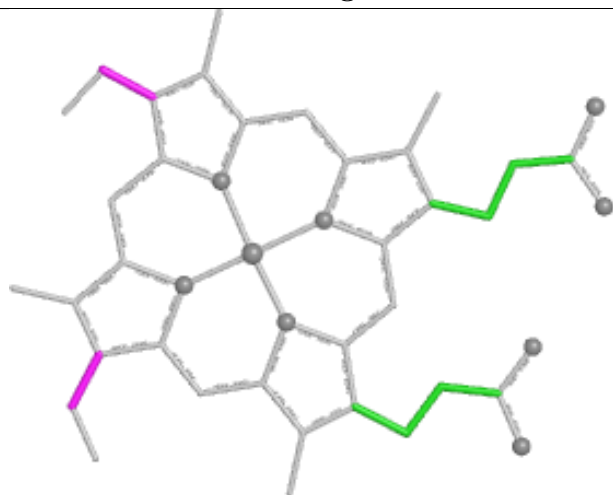
Ligand HEC A 4



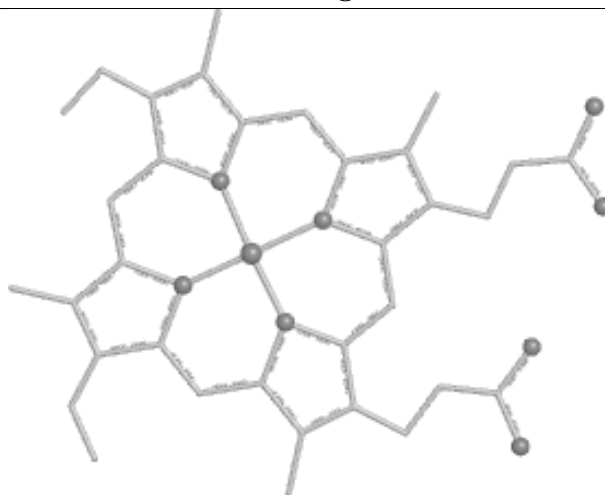
Bond lengths



Bond angles

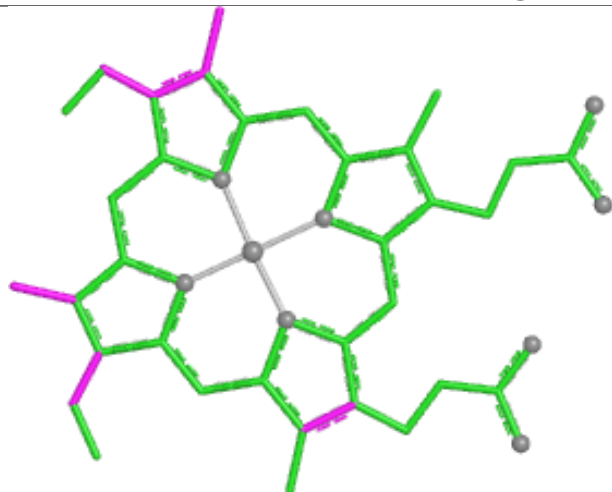


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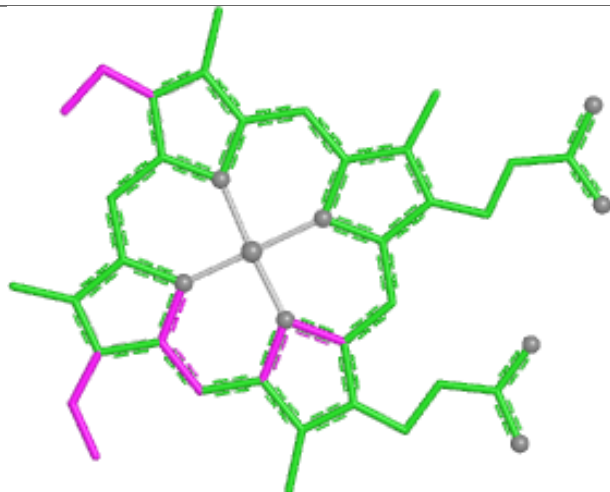


Rings

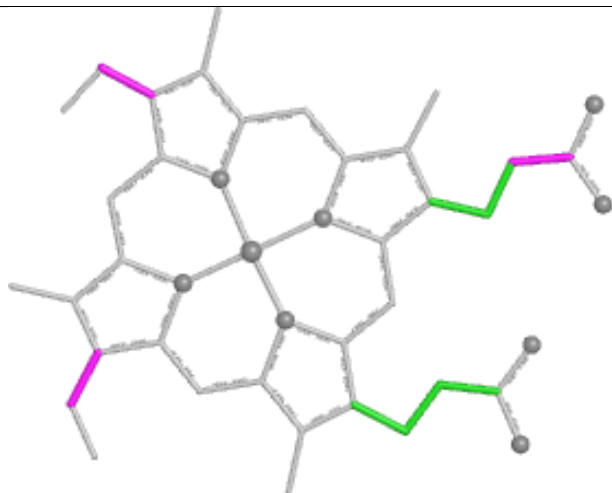
Ligand HEC C 480



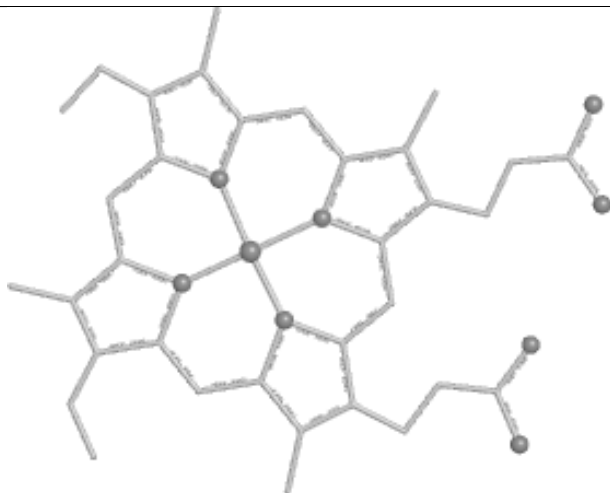
Bond lengths



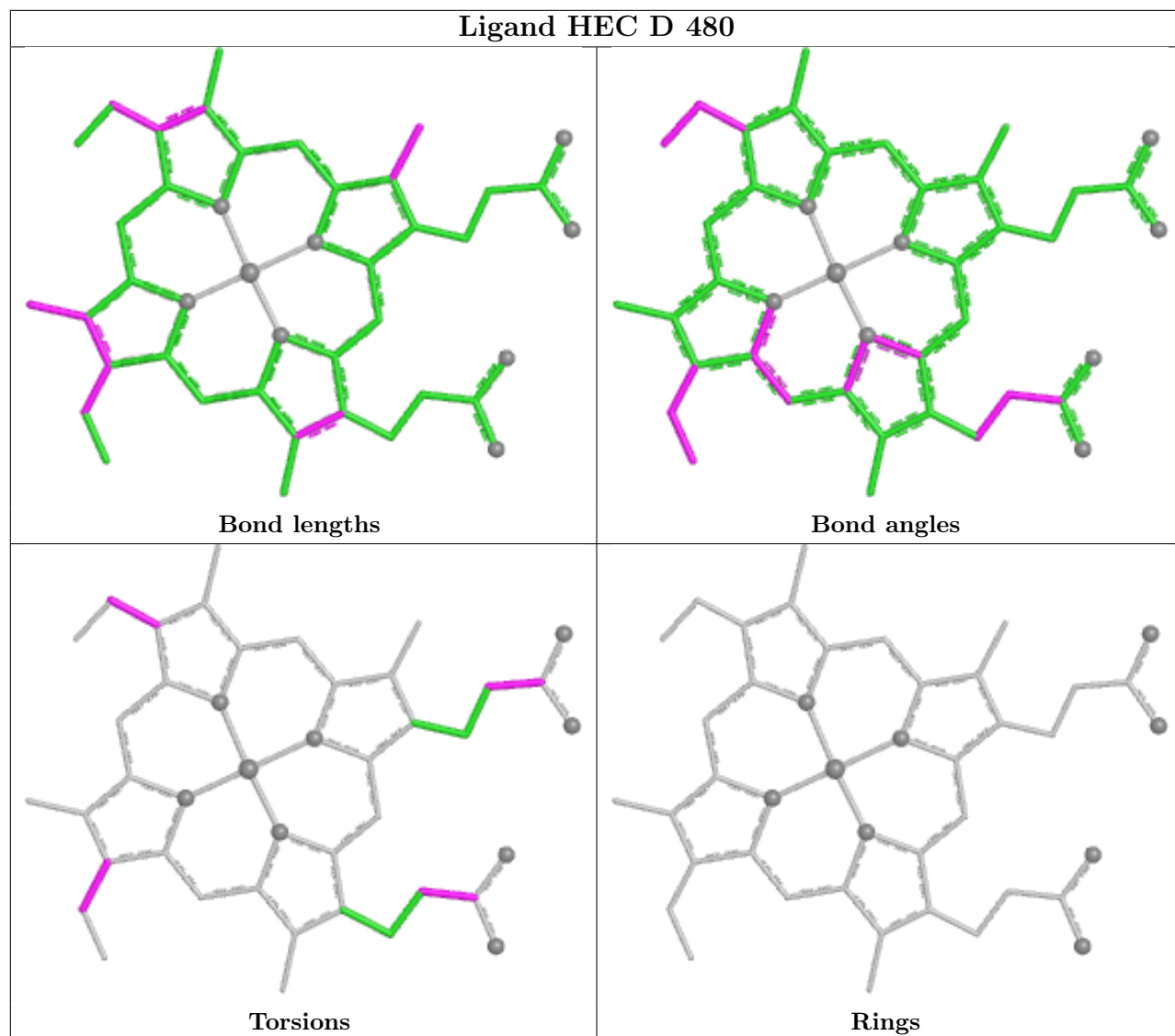
Bond angles



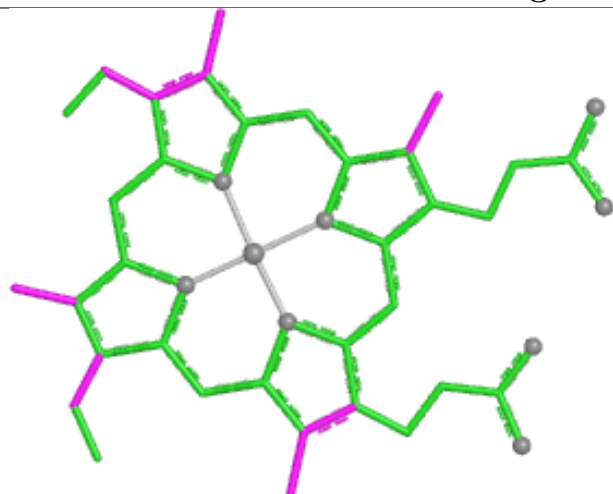
Torsions



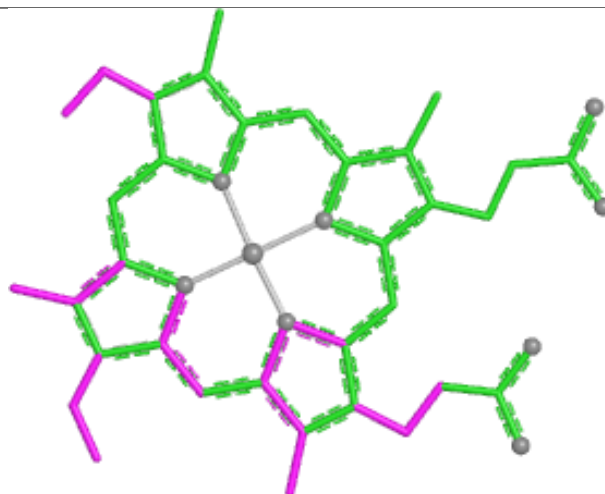
Rings



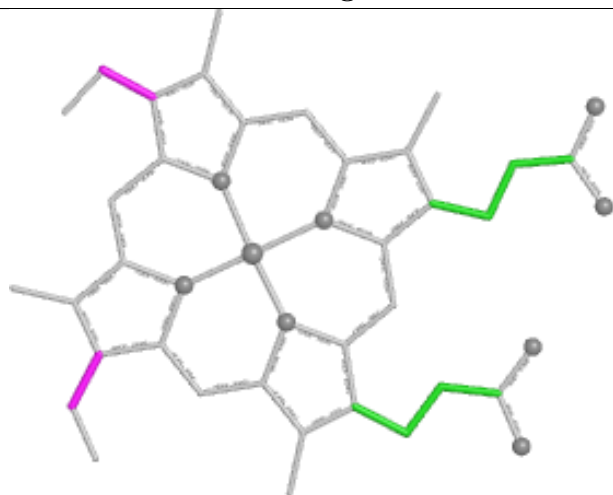
Ligand HEC A 3



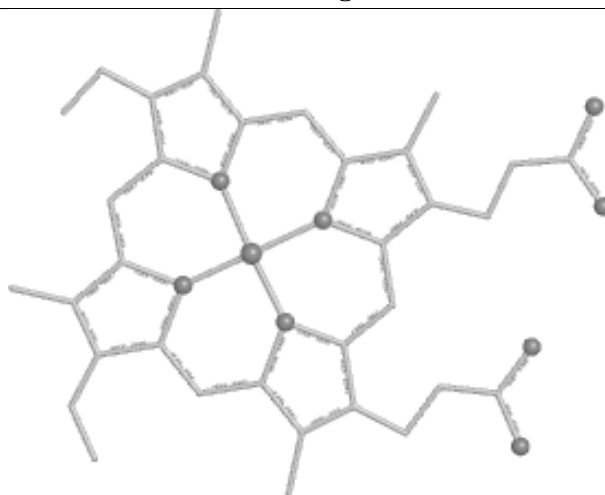
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Bond angles

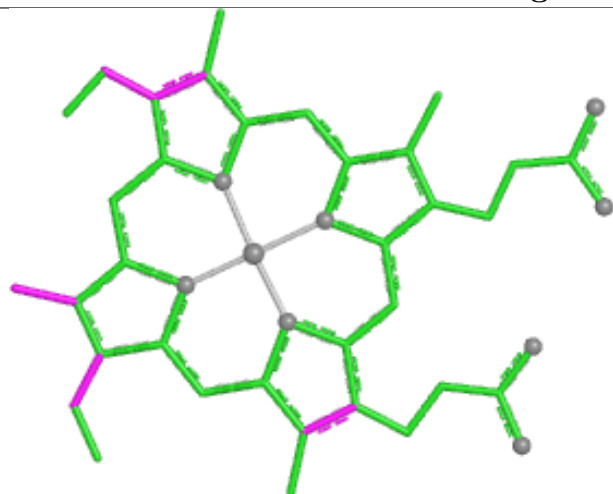


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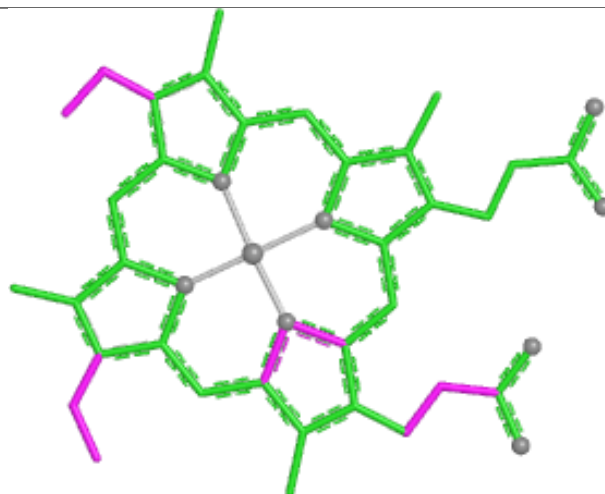


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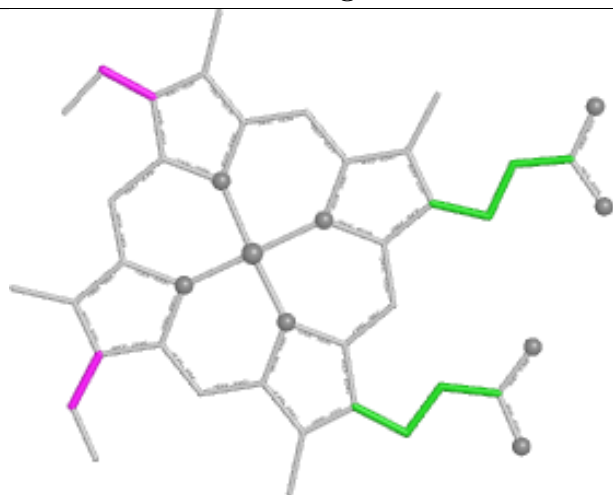
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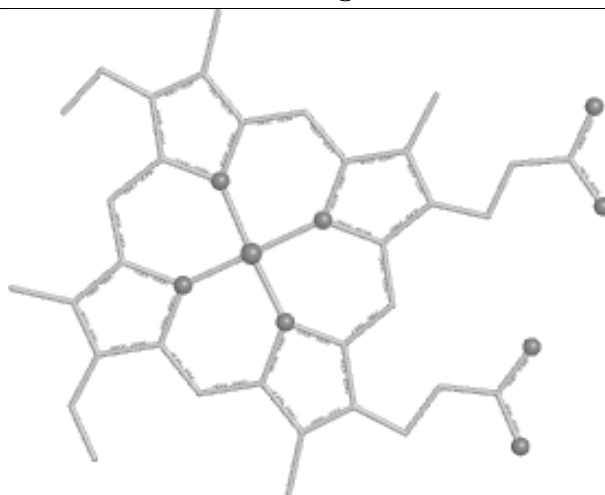
Bond lengths



Bond angles

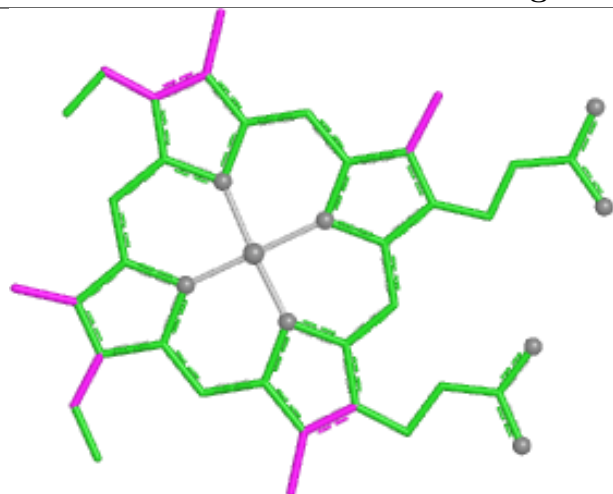


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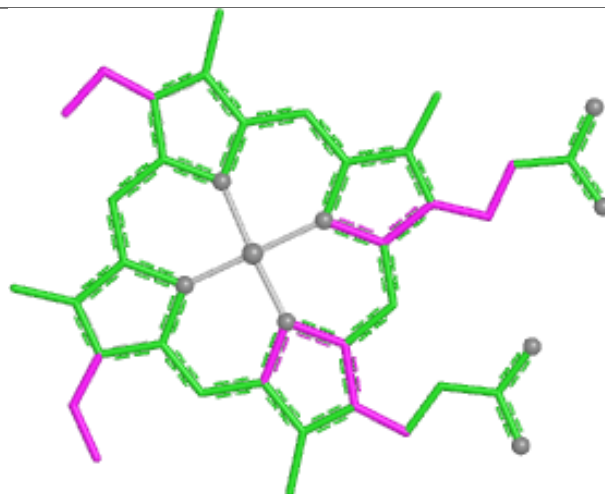


Rings

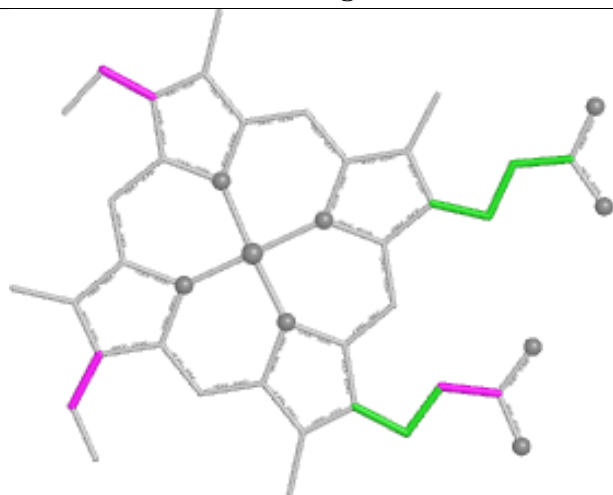
Ligand HEC D 3



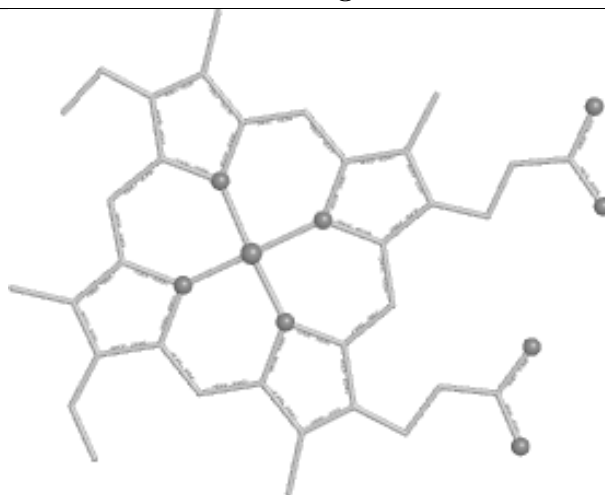
Bond lengths



Bond angles

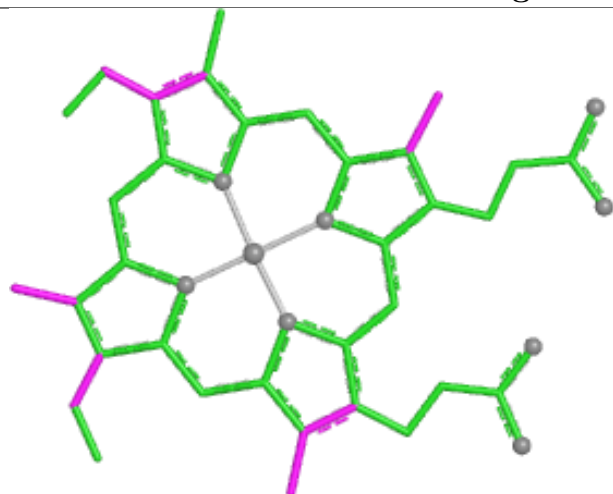


Torsions

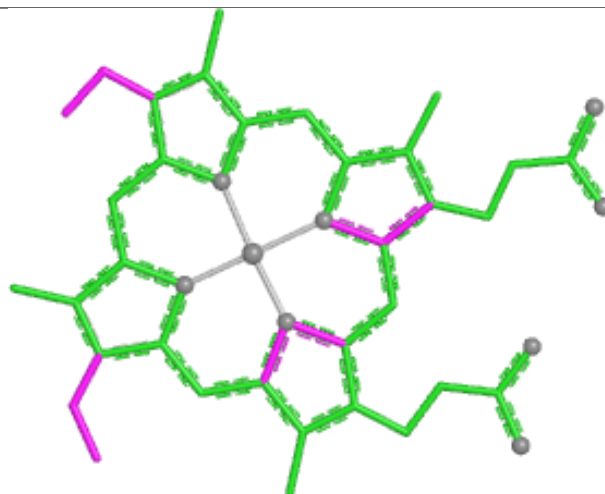


Rings

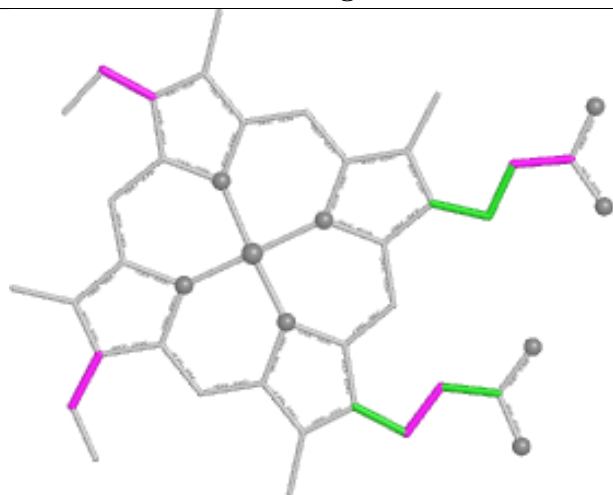
Ligand HEC A 479



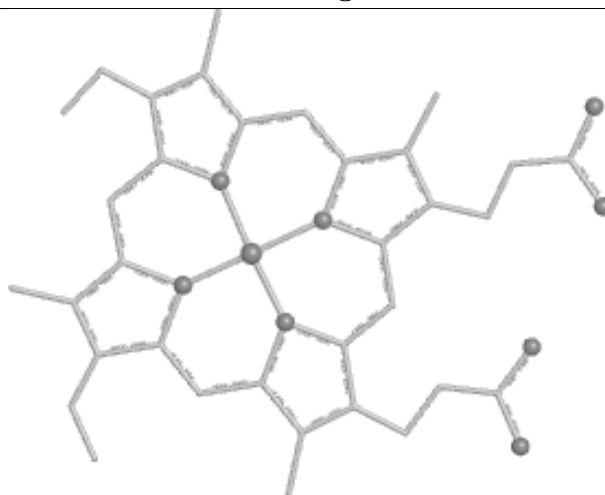
Bond lengths



Bond angles

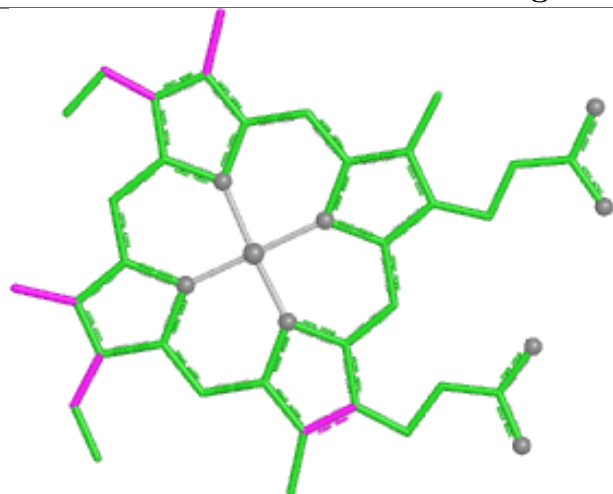


Torsions

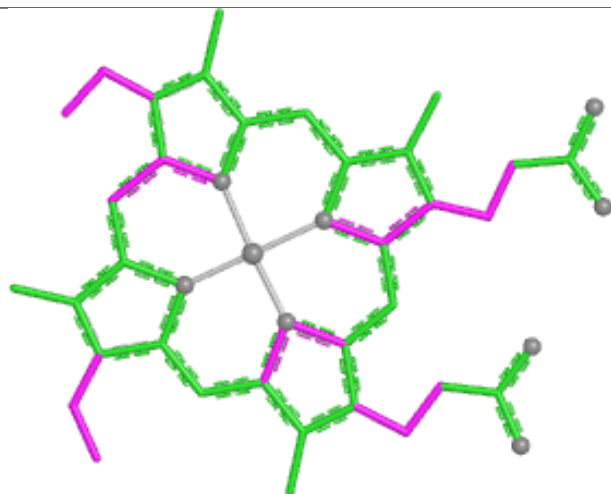


Rings

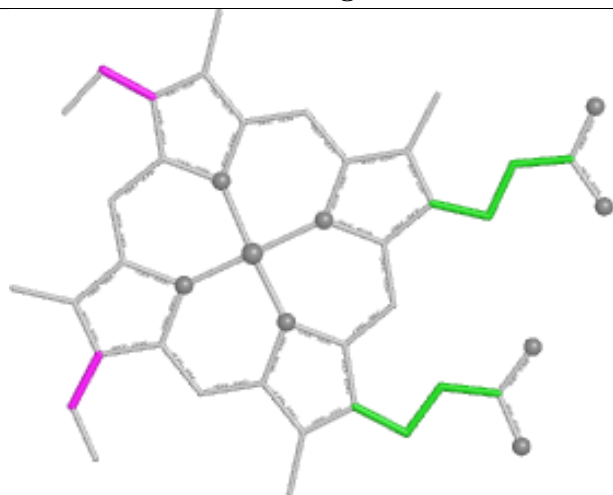
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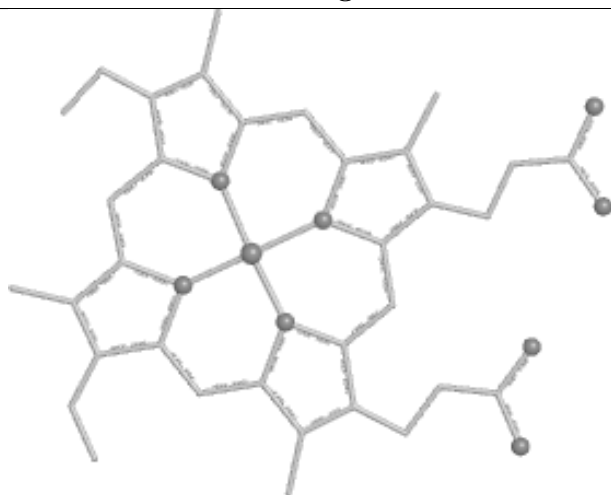
Bond lengths



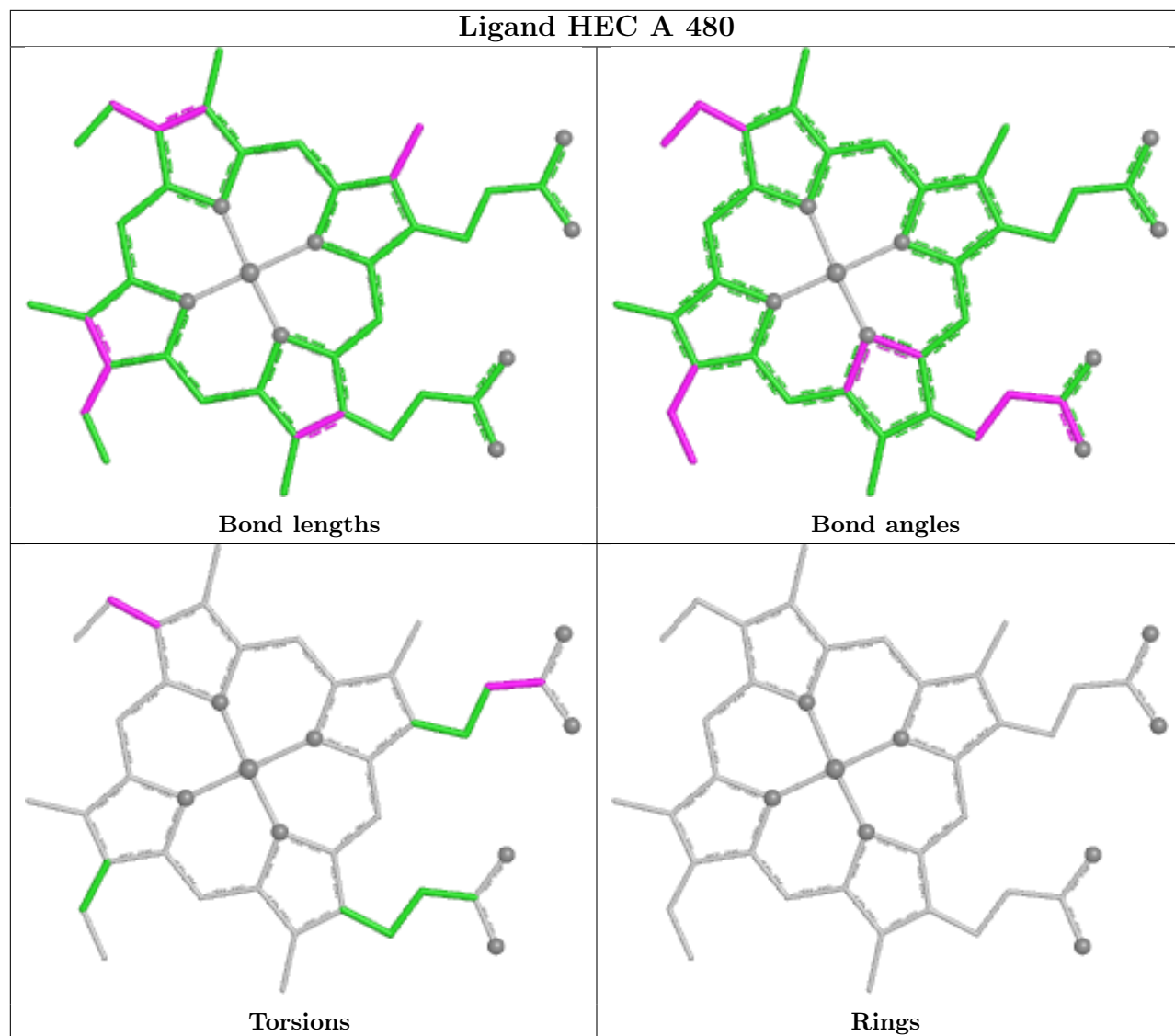
Bond angles



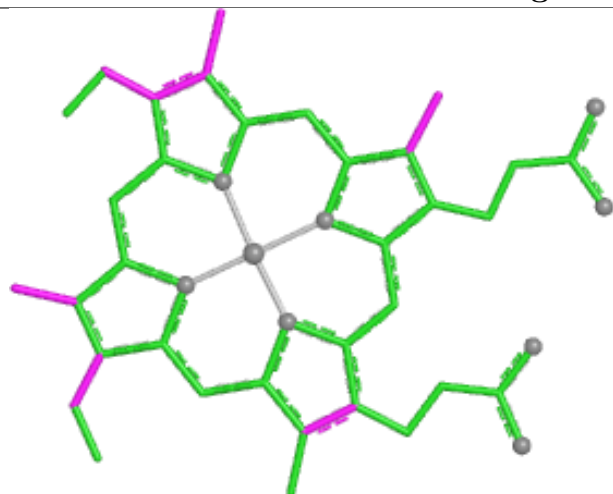
Torsions



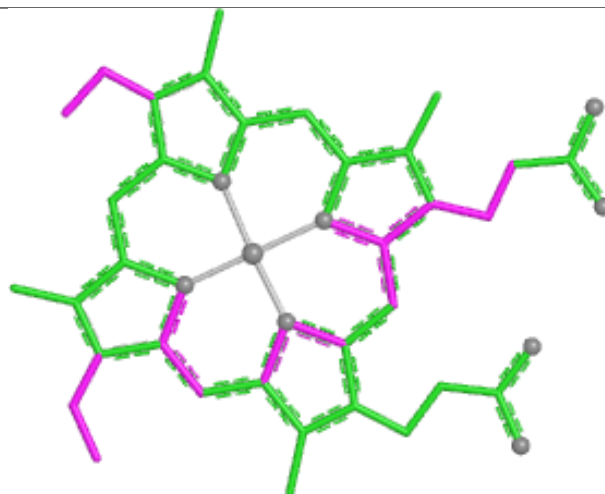
Rings



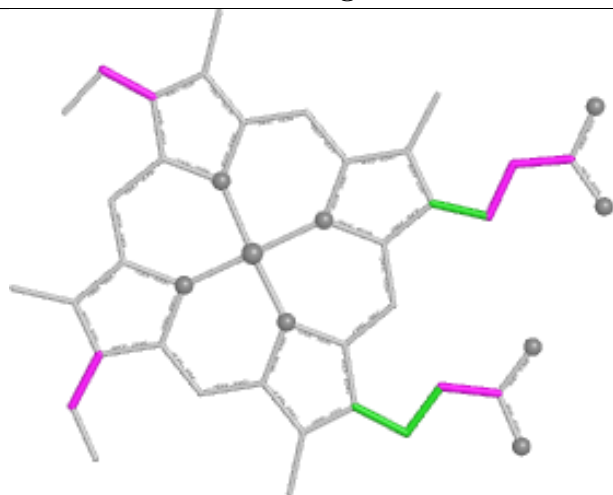
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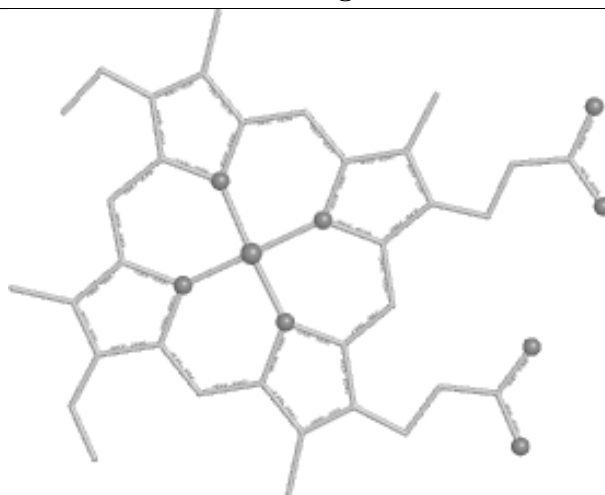
Bond lengths



Bond angles

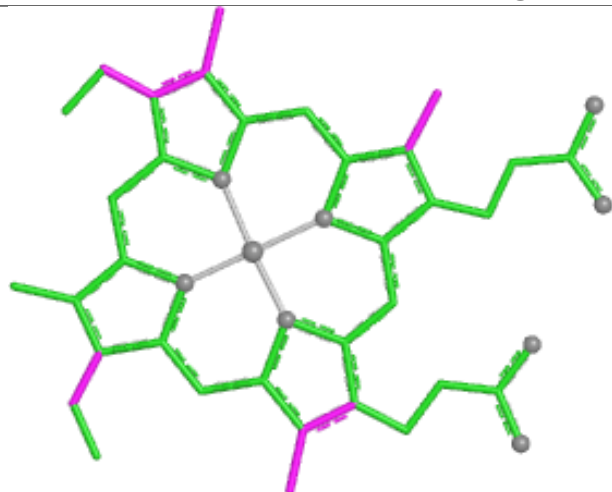


Torsions

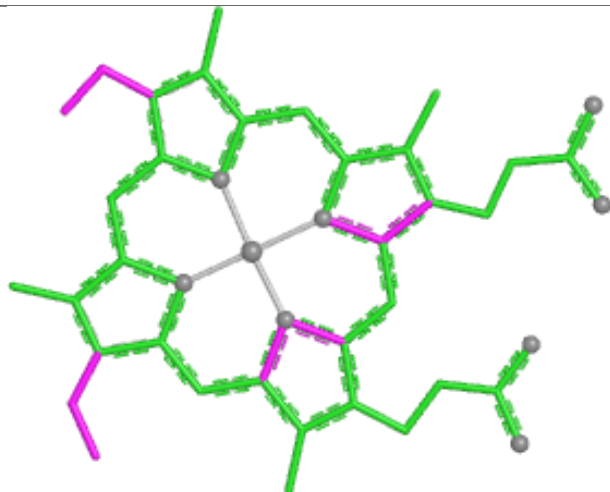


Rings

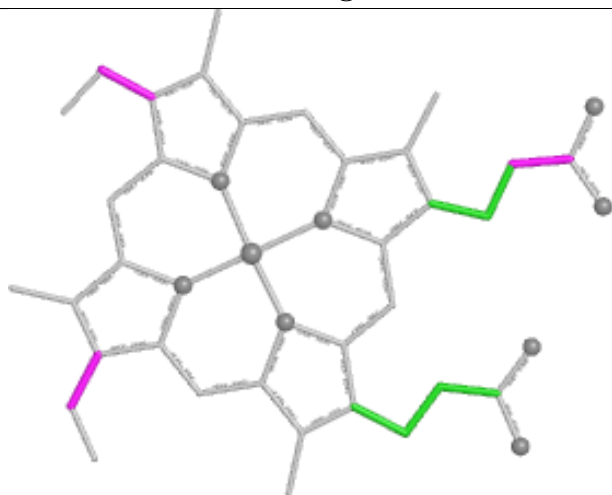
Ligand HEC C 479



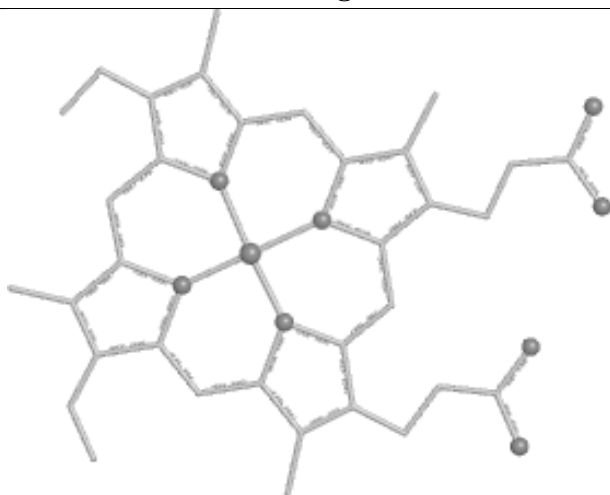
Bond lengths



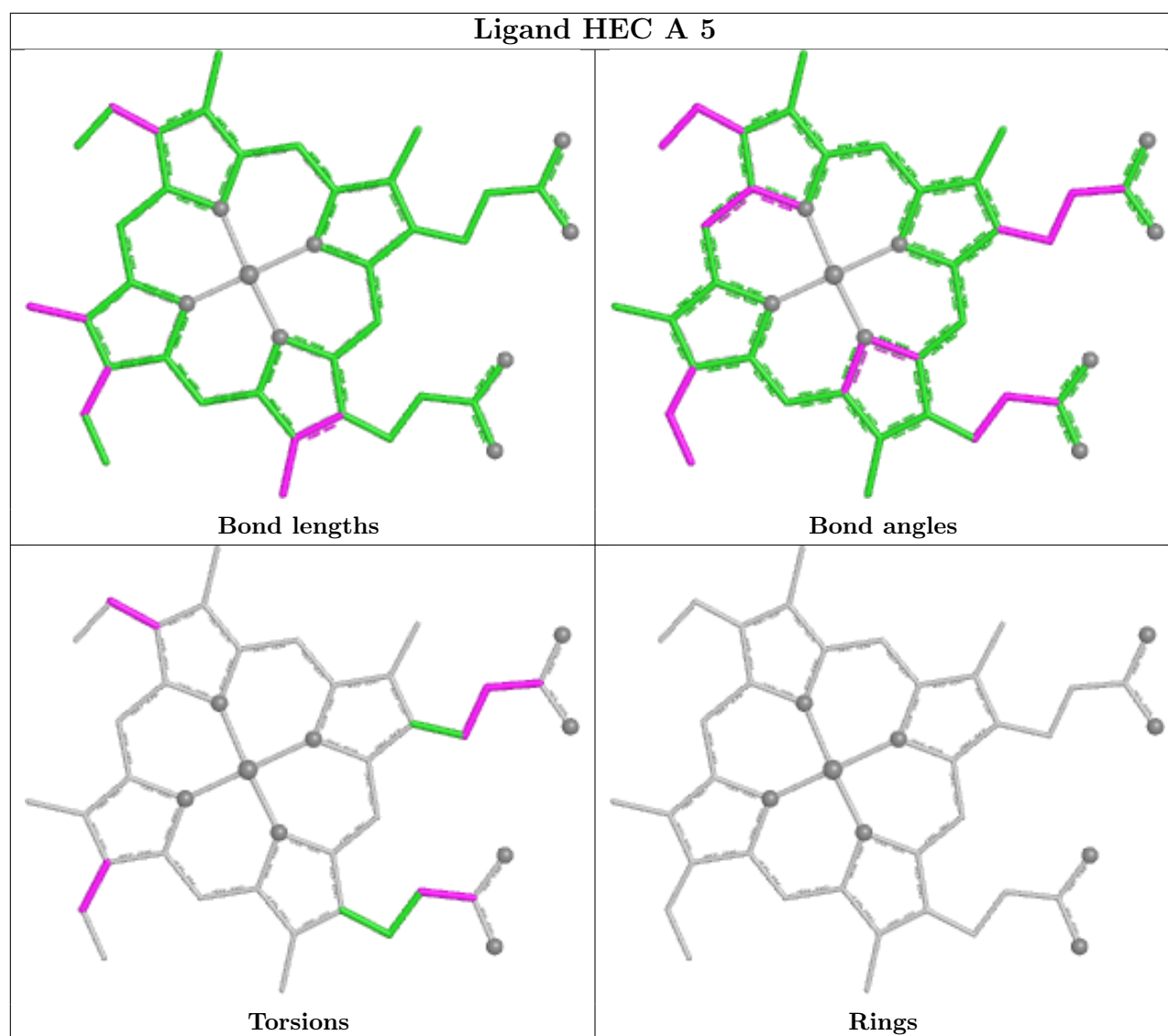
Bond angles



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	441/452 (97%)	-0.30	0	100	100	11, 27, 42, 53	3 (0%)
1	B	441/452 (97%)	-0.55	0	100	100	8, 23, 35, 41	3 (0%)
1	C	441/452 (97%)	-0.50	0	100	100	11, 24, 34, 41	7 (1%)
1	D	441/452 (97%)	0.20	7 (1%)	70	72	17, 39, 56, 62	2 (0%)
All	All	1764/1808 (97%)	-0.29	7 (0%)	88	89	8, 27, 48, 62	15 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	SER	3.3
1	D	167	ALA	2.8
1	D	475	LEU	2.4
1	D	469	GLN	2.2
1	D	38	VAL	2.2
1	D	174	GLY	2.1
1	D	95	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 oligosaccharides in this entry.

6.4 Ligands

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

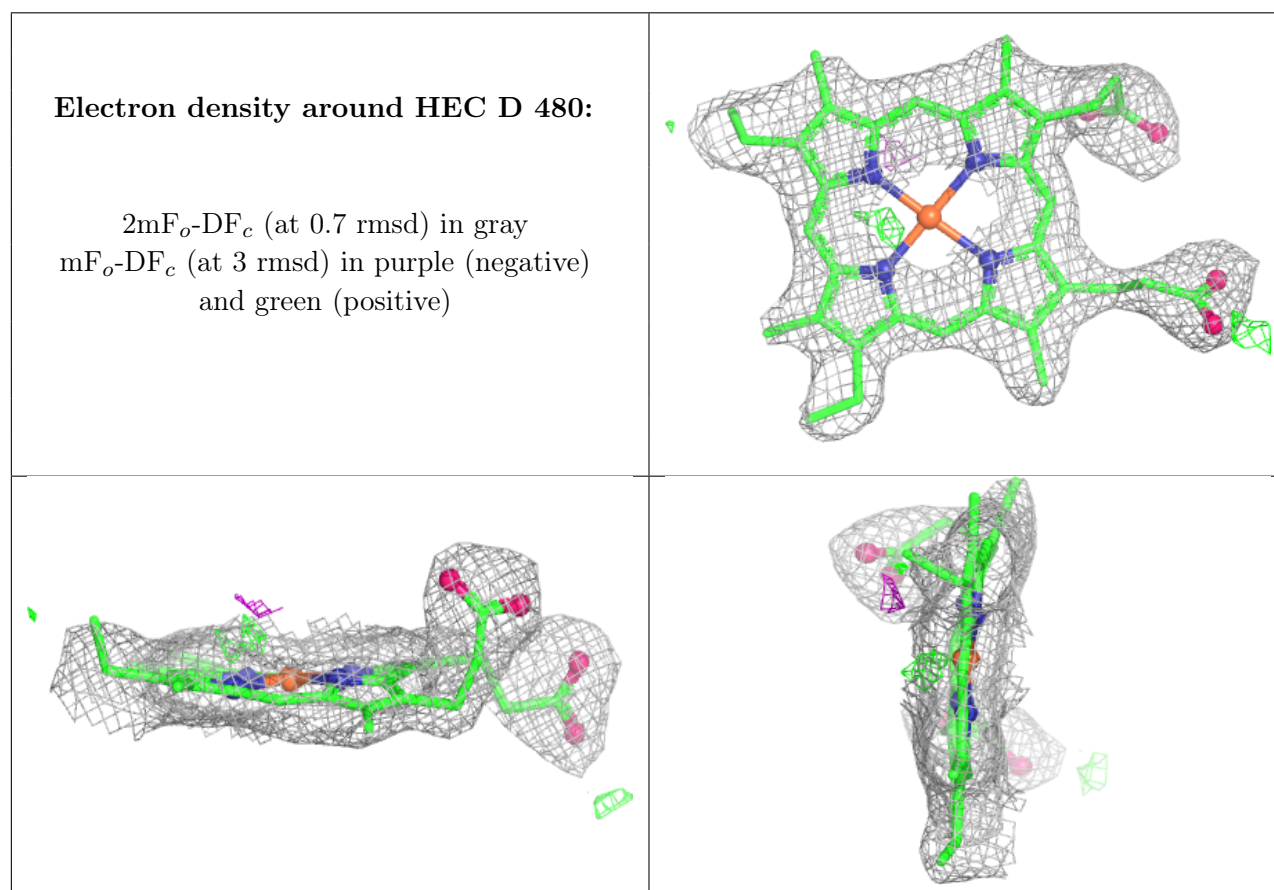
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	C	2	1/1	0.57	0.20	81,81,81,81	0
2	CA	A	2	1/1	0.68	0.16	93,93,93,93	0
5	EDO	C	482	4/4	0.82	0.16	40,40,42,45	0
2	CA	B	2	1/1	0.87	0.10	62,62,62,62	0
5	EDO	C	484	4/4	0.87	0.12	51,51,51,53	0
5	EDO	A	6	4/4	0.88	0.14	37,37,37,37	0
5	EDO	B	483	4/4	0.88	0.15	44,45,46,47	0
5	EDO	C	7	4/4	0.88	0.15	50,50,50,51	0
2	CA	D	2	1/1	0.89	0.12	82,82,82,82	0
5	EDO	D	11	4/4	0.90	0.14	43,44,45,46	0
5	EDO	C	9	4/4	0.91	0.12	42,44,44,44	0
5	EDO	D	482	4/4	0.91	0.12	52,53,53,54	0
5	EDO	B	12	4/4	0.91	0.08	33,35,36,38	0
5	EDO	C	483	4/4	0.93	0.10	38,39,39,39	0
5	EDO	A	8	4/4	0.94	0.09	37,37,38,38	0
4	SO3	B	481	4/4	0.94	0.10	48,49,49,50	0
4	SO3	D	481	4/4	0.96	0.07	45,46,46,47	0
3	HEC	D	480	43/43	0.96	0.10	42,45,47,49	0
3	HEC	D	479	43/43	0.97	0.08	25,32,36,37	0
3	HEC	A	480	43/43	0.97	0.07	24,30,32,35	0
3	HEC	D	3	43/43	0.97	0.08	25,30,33,35	0
3	HEC	D	4	43/43	0.97	0.07	24,27,35,41	0
5	EDO	C	10	4/4	0.97	0.08	23,26,27,29	0
3	HEC	D	5	43/43	0.97	0.07	28,30,38,43	0
3	HEC	A	5	43/43	0.97	0.08	18,23,32,40	0
3	HEC	A	3	43/43	0.98	0.06	16,21,27,30	0
3	HEC	A	4	43/43	0.98	0.06	16,21,30,32	0
3	HEC	A	479	43/43	0.98	0.06	15,23,26,27	0
3	HEC	B	479	43/43	0.98	0.05	10,15,17,18	0
3	HEC	B	480	43/43	0.98	0.05	13,16,19,20	0
4	SO3	A	481	4/4	0.98	0.06	28,29,30,31	0
3	HEC	B	4	43/43	0.98	0.06	10,16,21,27	0
3	HEC	B	5	43/43	0.98	0.07	14,18,28,33	0
3	HEC	C	4	43/43	0.98	0.06	13,17,25,27	0
3	HEC	C	5	43/43	0.98	0.06	16,20,30,32	0
3	HEC	C	3	43/43	0.99	0.05	9,13,17,19	0
2	CA	A	1	1/1	0.99	0.02	18,18,18,18	0

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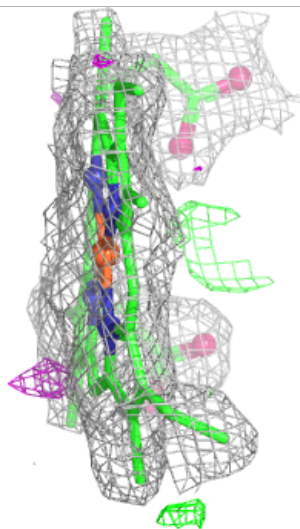
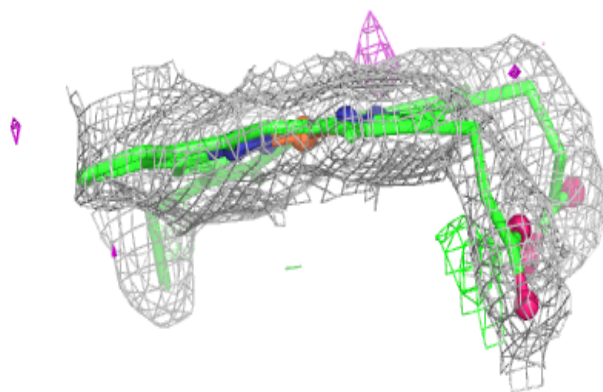
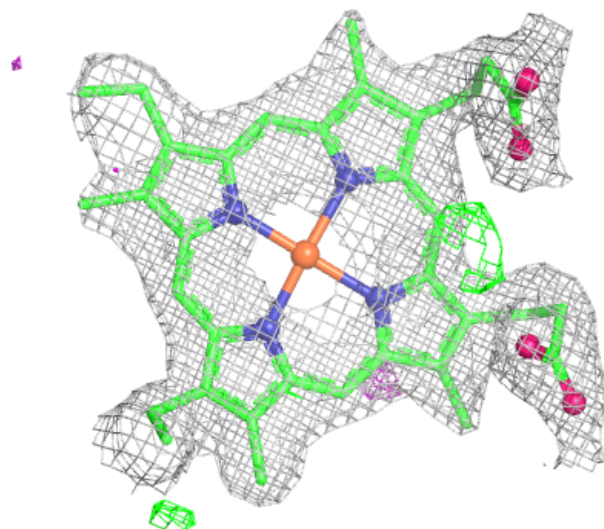
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	B	3	43/43	0.99	0.05	9,14,20,23	0
4	SO3	B	482	4/4	0.99	0.05	28,28,30,33	0
4	SO3	C	481	4/4	0.99	0.05	23,23,27,27	0
2	CA	D	1	1/1	0.99	0.02	29,29,29,29	0
2	CA	C	1	1/1	0.99	0.02	19,19,19,19	0
3	HEC	C	479	43/43	0.99	0.05	12,15,18,21	0
3	HEC	C	480	43/43	0.99	0.05	14,17,21,22	0
2	CA	B	1	1/1	1.00	0.01	19,19,19,19	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.



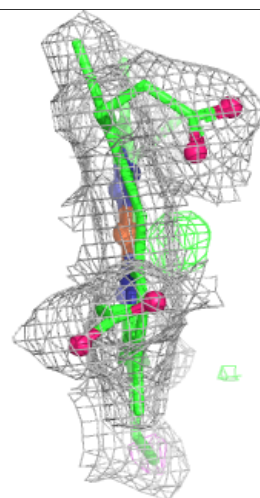
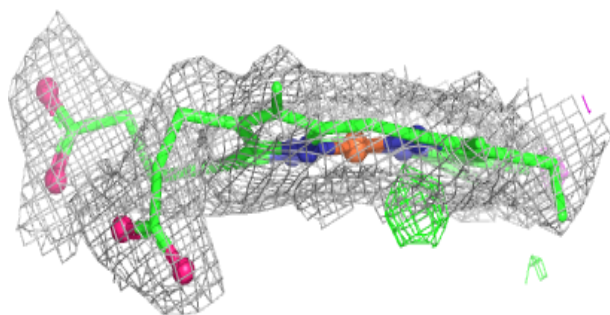
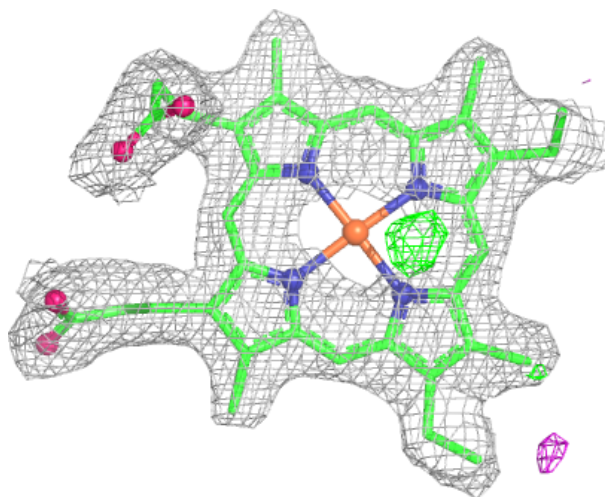
Electron density around HEC D 479:

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



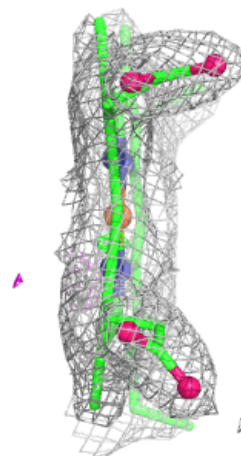
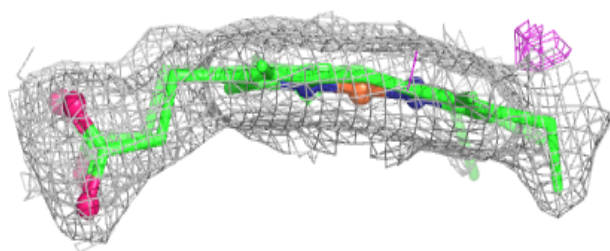
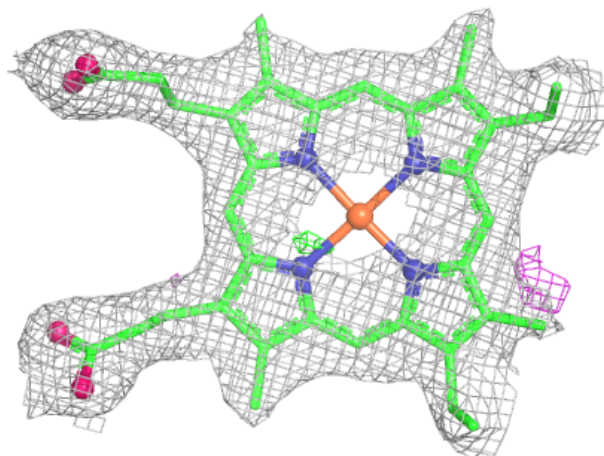
Electron density around HEC A 480:

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and green (positive)



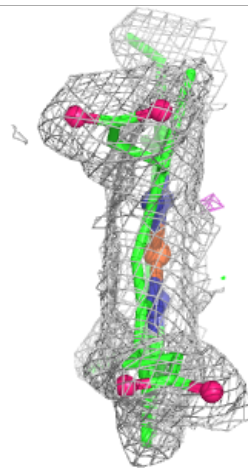
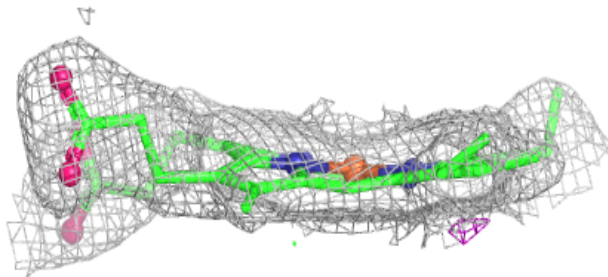
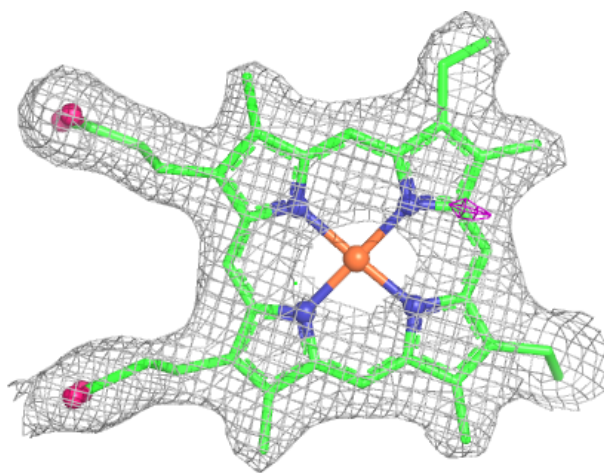
Electron density around HEC D 3:

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and green (positive)



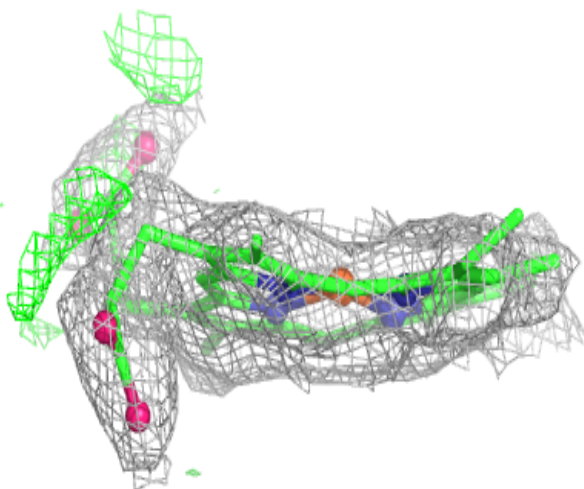
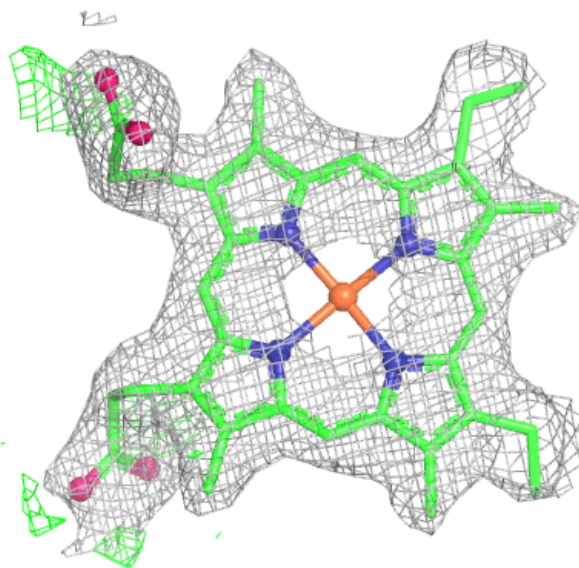
Electron density around HEC D 4:

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and green (positive)



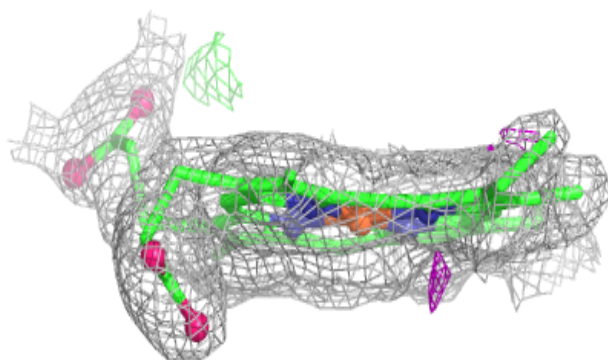
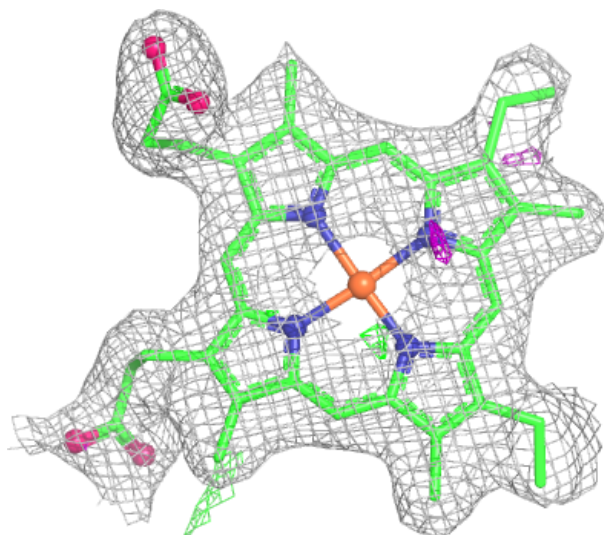
Electron density around HEC D 5:

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and green (positive)



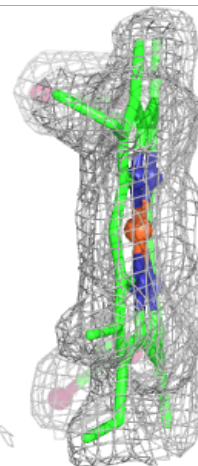
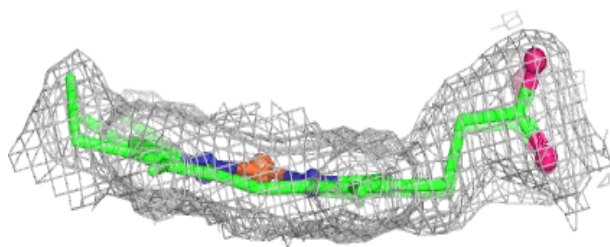
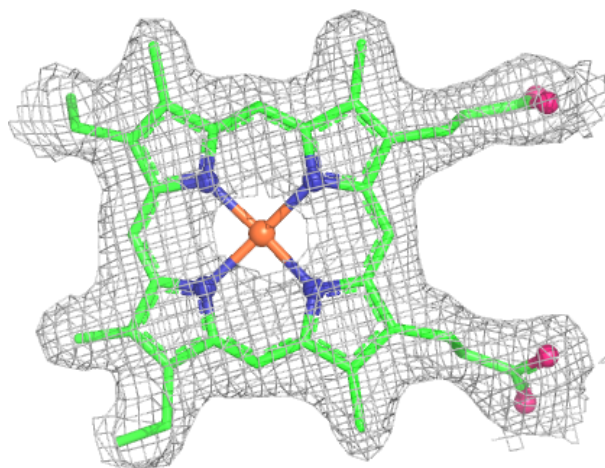
Electron density around HEC A 5:

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and green (positive)



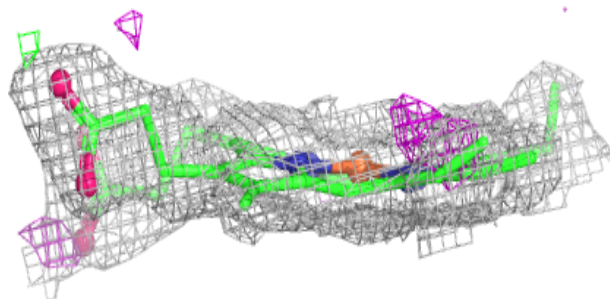
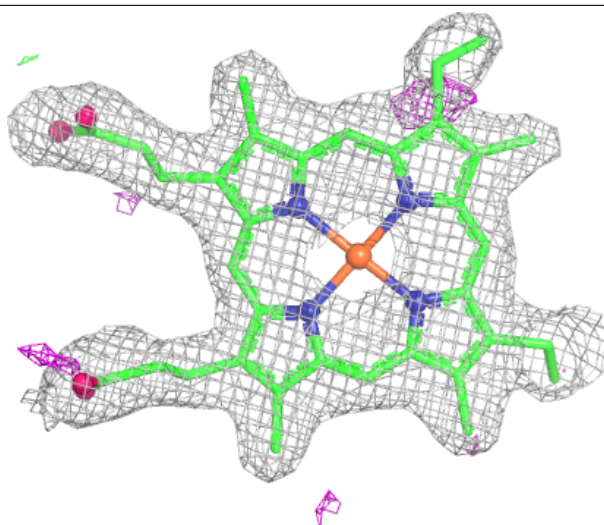
Electron density around HEC A 3:

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and green (positive)



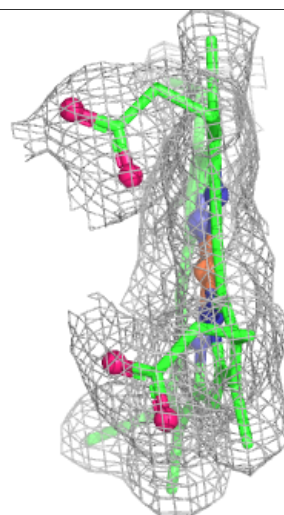
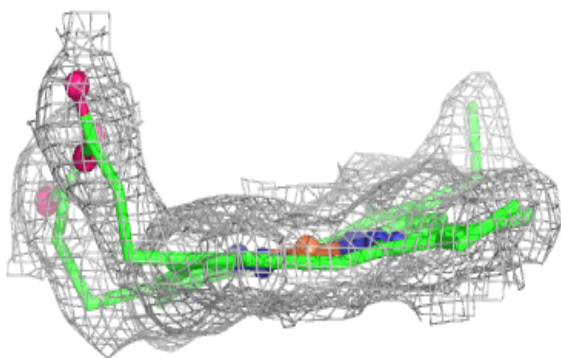
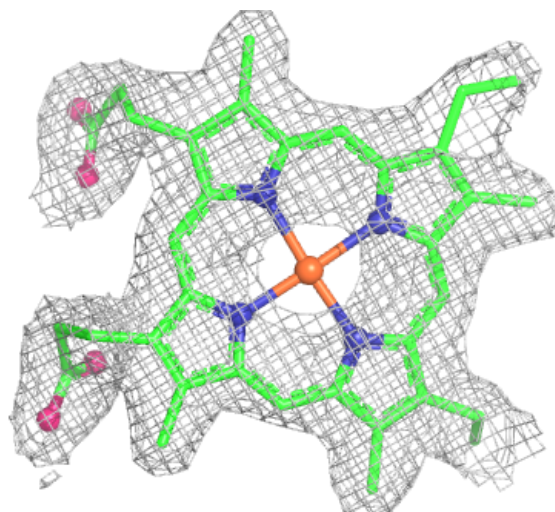
Electron density around HEC A 4:

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and green (positive)



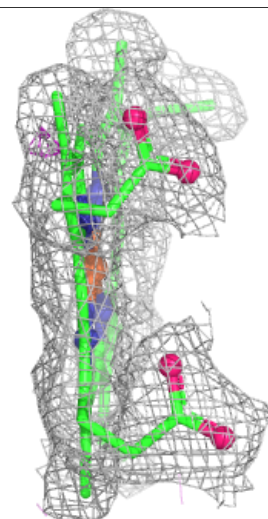
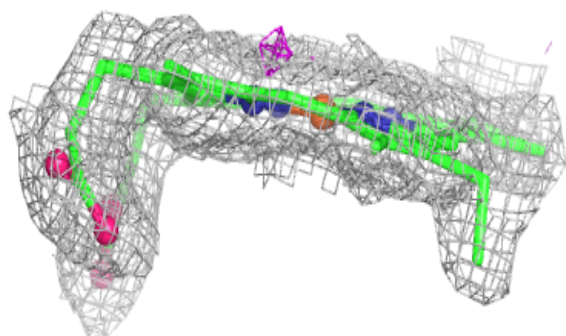
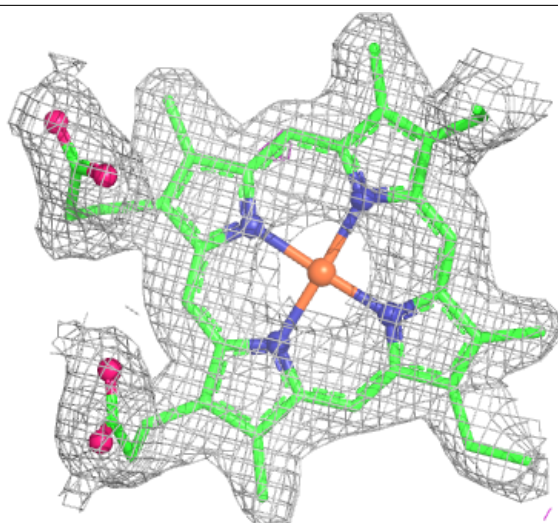
Electron density around HEC A 479:

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and green (positive)



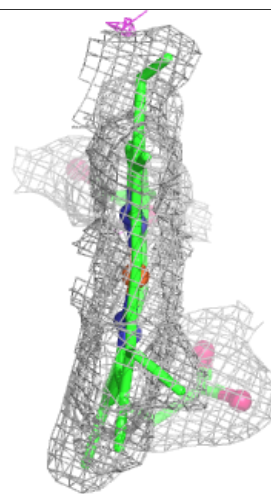
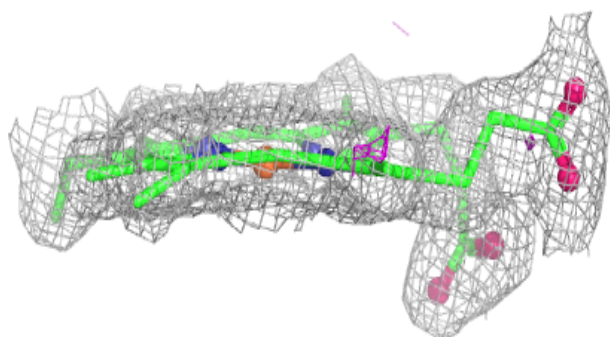
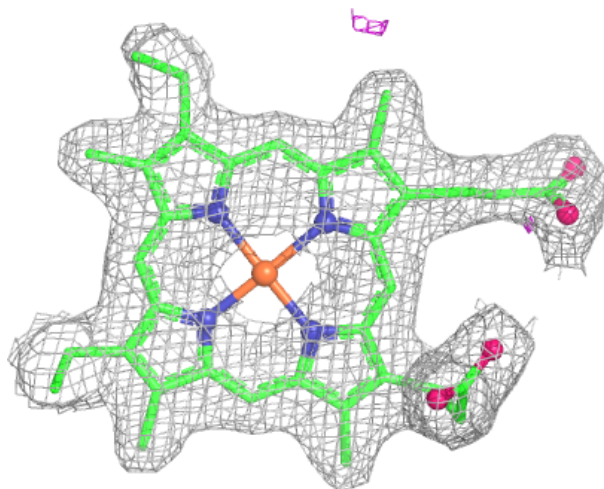
Electron density around HEC B 479:

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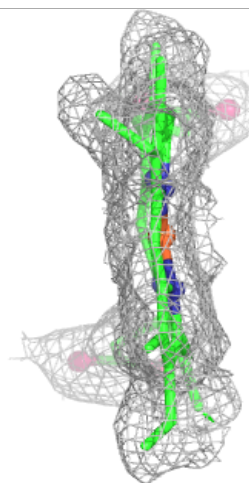
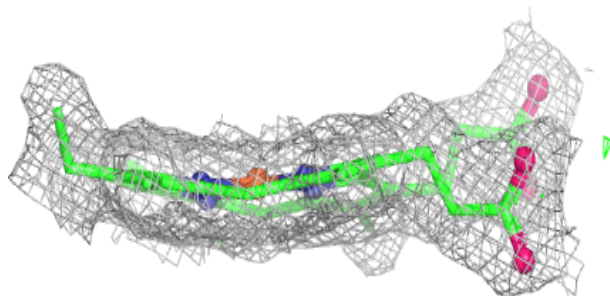
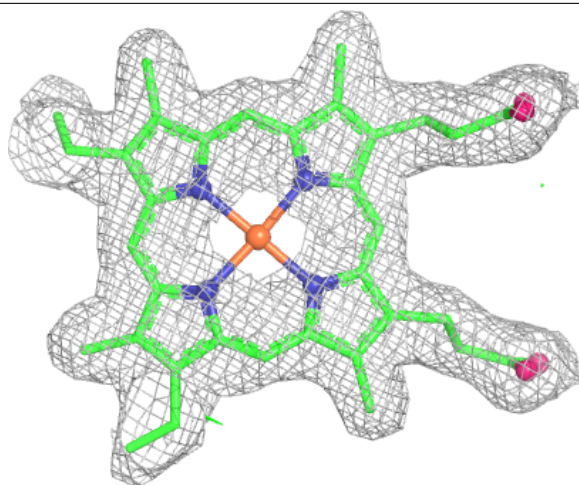
Electron density around HEC B 480:

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and green (positive)



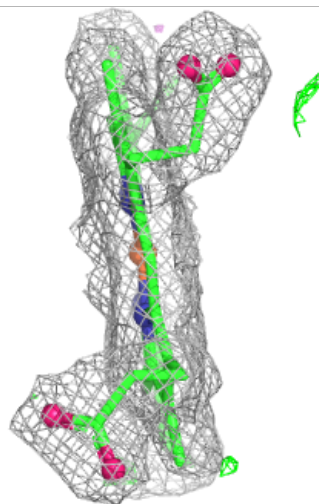
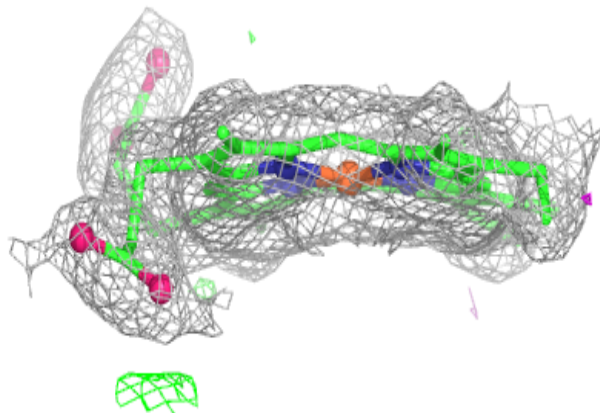
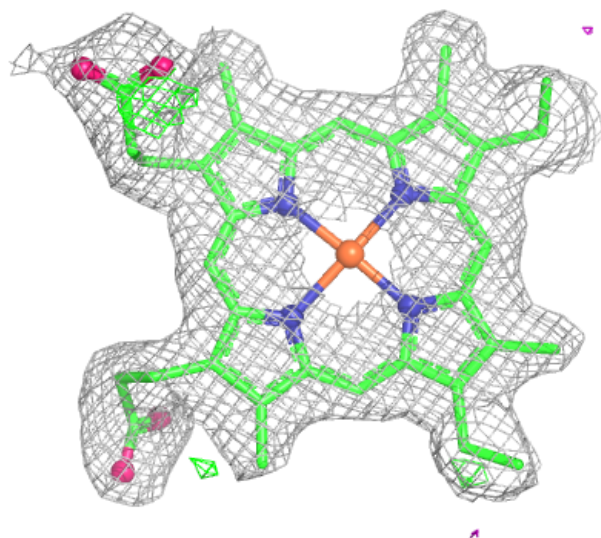
Electron density around HEC B 4:

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and green (positive)



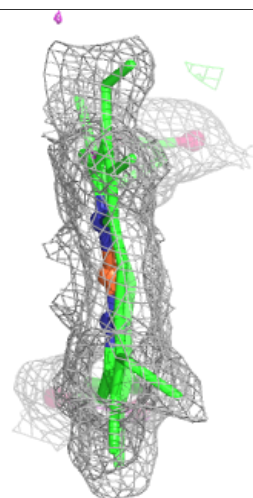
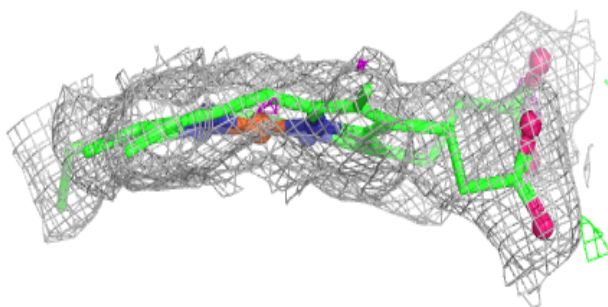
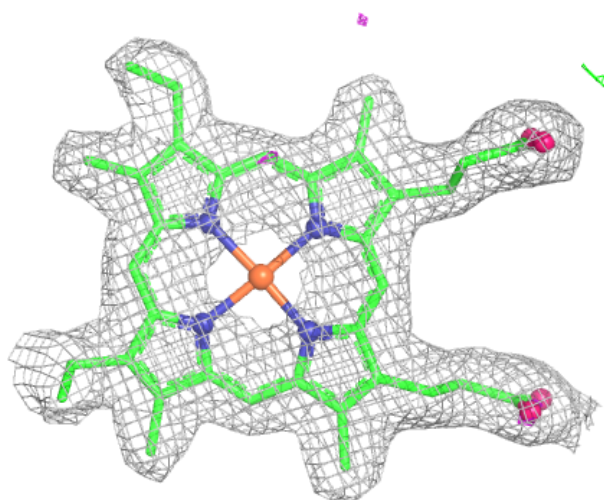
Electron density around HEC B 5:

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and green (positive)



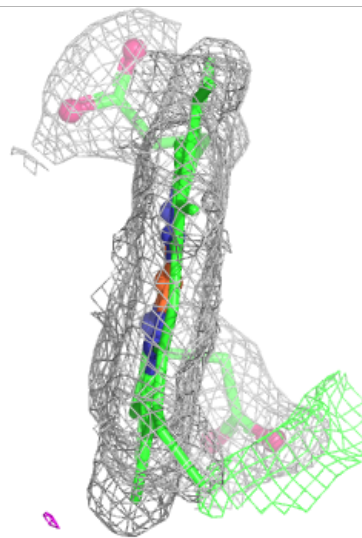
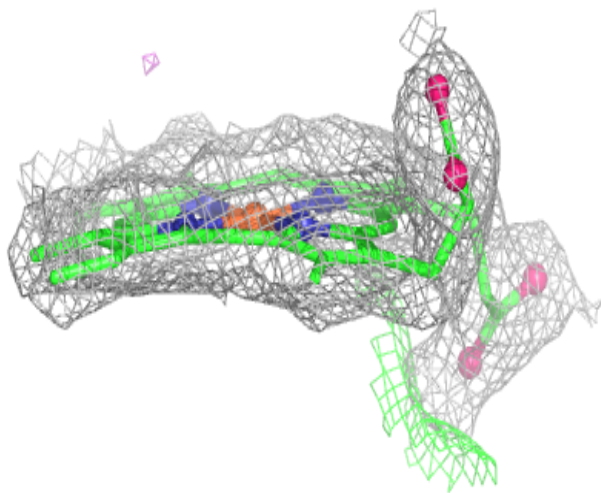
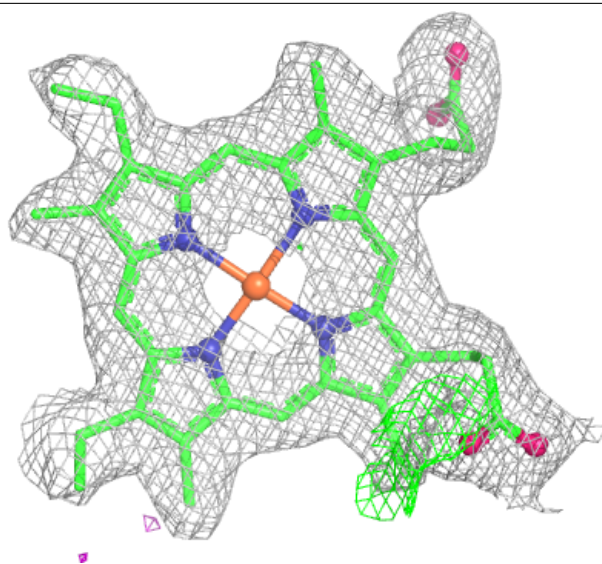
Electron density around HEC C 4:

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and green (positive)



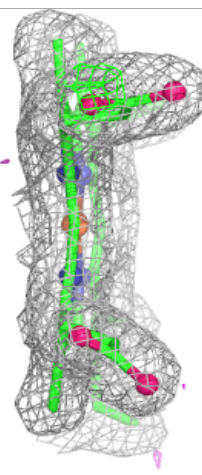
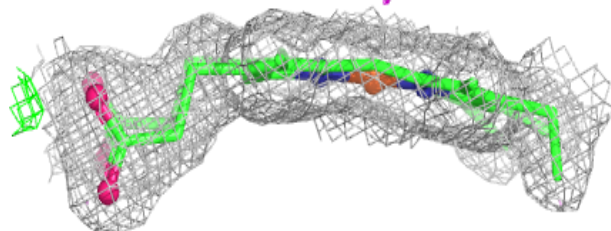
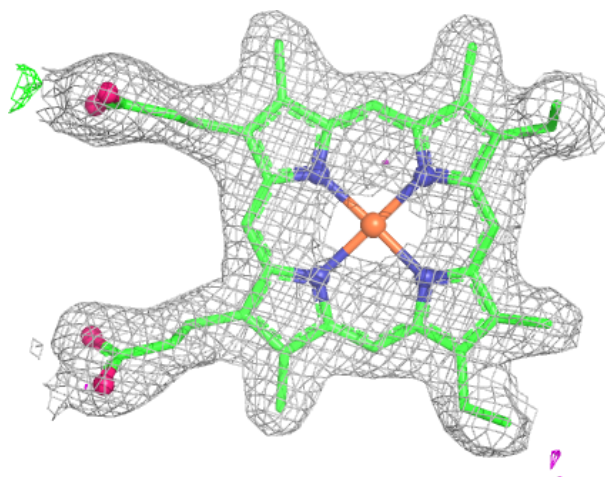
Electron density around HEC C 5:

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and green (positive)



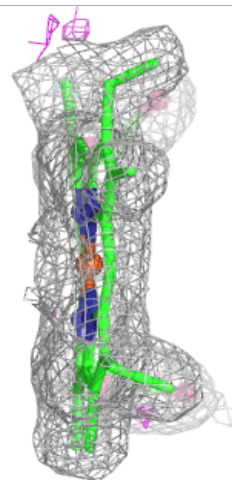
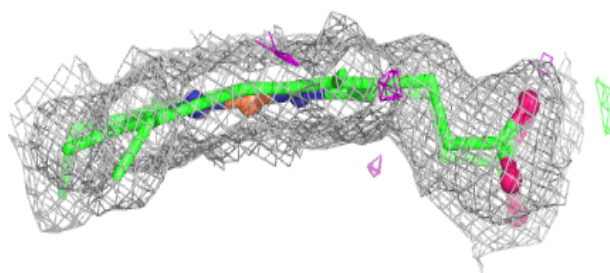
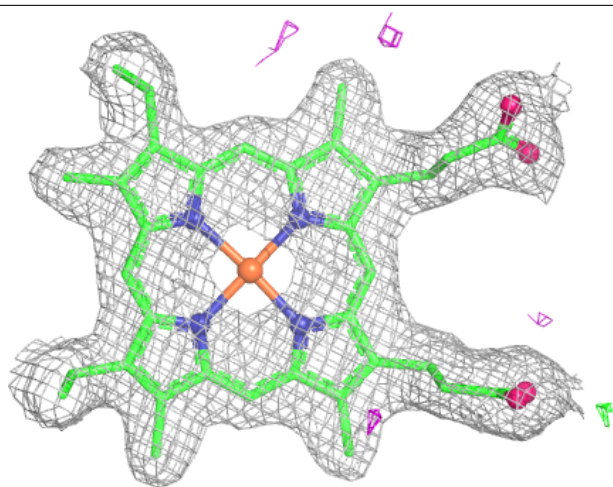
Electron density around HEC C 3:

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and green (positive)



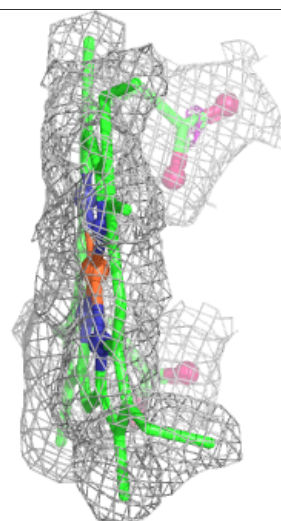
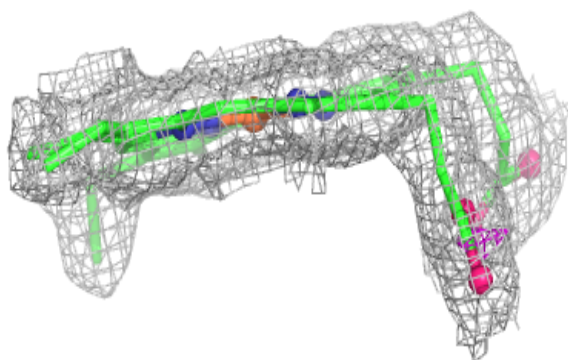
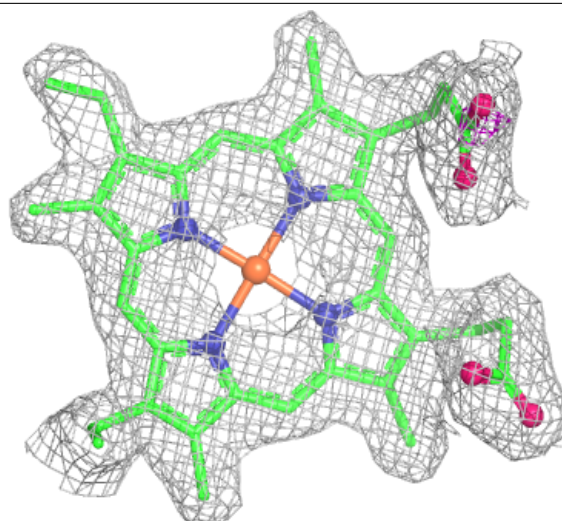
Electron density around HEC B 3:

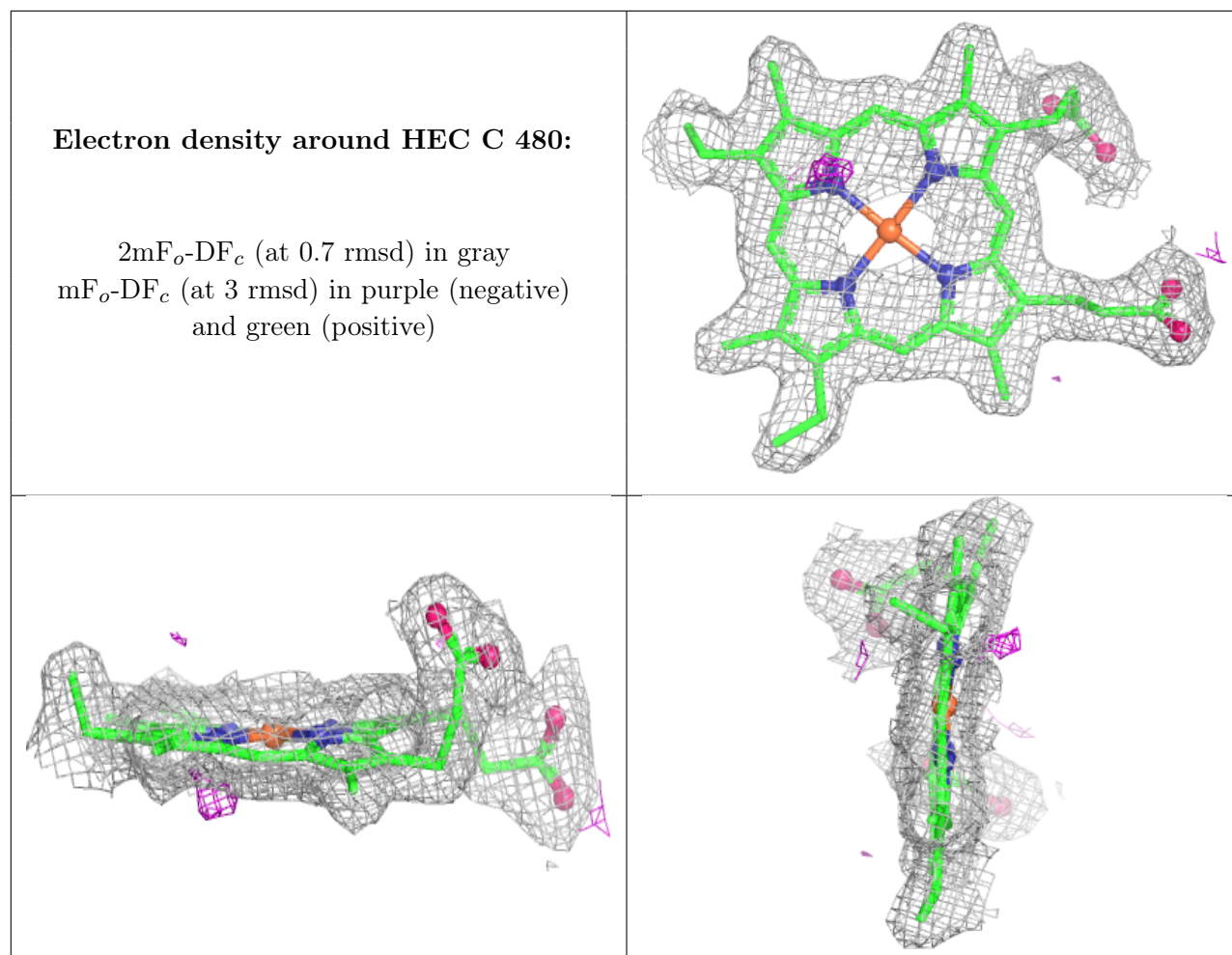
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.