



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:59 AM UTC

PDB ID : 6I5B / pdb_00006i5b
Title : Crystal Structure of Outer Cell Wall Cytochrome OcwA
Authors : Hermann, B.; Einsle, O.
Deposited on : 2018-11-13
Resolution : 2.20 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

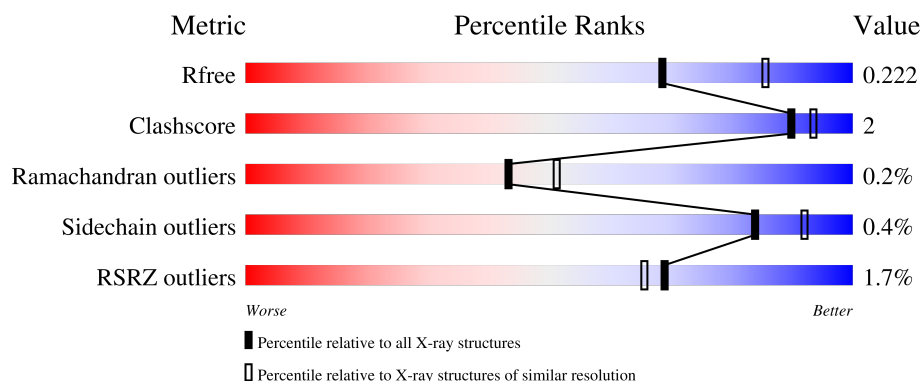
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	526	% 89% 8%
1	B	526	2% 89% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8278 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3667	2298	636	704	29			
1	B	483	Total	C	N	O	S	0	0	0
			3659	2294	634	702	29			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	LYS	-	expression tag	UNP D5XBK3
A	527	GLY	-	expression tag	UNP D5XBK3
A	528	GLU	-	expression tag	UNP D5XBK3
A	529	LEU	-	expression tag	UNP D5XBK3
A	530	LYS	-	expression tag	UNP D5XBK3
A	531	LEU	-	expression tag	UNP D5XBK3
A	532	GLU	-	expression tag	UNP D5XBK3
A	533	GLY	-	expression tag	UNP D5XBK3
A	534	LYS	-	expression tag	UNP D5XBK3
A	535	PRO	-	expression tag	UNP D5XBK3
A	536	ILE	-	expression tag	UNP D5XBK3
A	537	PRO	-	expression tag	UNP D5XBK3
A	538	ASP	-	expression tag	UNP D5XBK3
A	539	PRO	-	expression tag	UNP D5XBK3
A	540	LEU	-	expression tag	UNP D5XBK3
A	541	LEU	-	expression tag	UNP D5XBK3
A	542	GLY	-	expression tag	UNP D5XBK3
A	543	LEU	-	expression tag	UNP D5XBK3
A	544	ASP	-	expression tag	UNP D5XBK3
A	545	SER	-	expression tag	UNP D5XBK3
A	546	THR	-	expression tag	UNP D5XBK3
A	547	ARG	-	expression tag	UNP D5XBK3
A	548	THR	-	expression tag	UNP D5XBK3
A	549	GLY	-	expression tag	UNP D5XBK3
A	550	HIS	-	expression tag	UNP D5XBK3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	551	HIS	-	expression tag	UNP D5XBK3
A	552	HIS	-	expression tag	UNP D5XBK3
A	553	HIS	-	expression tag	UNP D5XBK3
A	554	HIS	-	expression tag	UNP D5XBK3
A	555	HIS	-	expression tag	UNP D5XBK3
B	526	LYS	-	expression tag	UNP D5XBK3
B	527	GLY	-	expression tag	UNP D5XBK3
B	528	GLU	-	expression tag	UNP D5XBK3
B	529	LEU	-	expression tag	UNP D5XBK3
B	530	LYS	-	expression tag	UNP D5XBK3
B	531	LEU	-	expression tag	UNP D5XBK3
B	532	GLU	-	expression tag	UNP D5XBK3
B	533	GLY	-	expression tag	UNP D5XBK3
B	534	LYS	-	expression tag	UNP D5XBK3
B	535	PRO	-	expression tag	UNP D5XBK3
B	536	ILE	-	expression tag	UNP D5XBK3
B	537	PRO	-	expression tag	UNP D5XBK3
B	538	ASP	-	expression tag	UNP D5XBK3
B	539	PRO	-	expression tag	UNP D5XBK3
B	540	LEU	-	expression tag	UNP D5XBK3
B	541	LEU	-	expression tag	UNP D5XBK3
B	542	GLY	-	expression tag	UNP D5XBK3
B	543	LEU	-	expression tag	UNP D5XBK3
B	544	ASP	-	expression tag	UNP D5XBK3
B	545	SER	-	expression tag	UNP D5XBK3
B	546	THR	-	expression tag	UNP D5XBK3
B	547	ARG	-	expression tag	UNP D5XBK3
B	548	THR	-	expression tag	UNP D5XBK3
B	549	GLY	-	expression tag	UNP D5XBK3
B	550	HIS	-	expression tag	UNP D5XBK3
B	551	HIS	-	expression tag	UNP D5XBK3
B	552	HIS	-	expression tag	UNP D5XBK3
B	553	HIS	-	expression tag	UNP D5XBK3
B	554	HIS	-	expression tag	UNP D5XBK3
B	555	HIS	-	expression tag	UNP D5XBK3

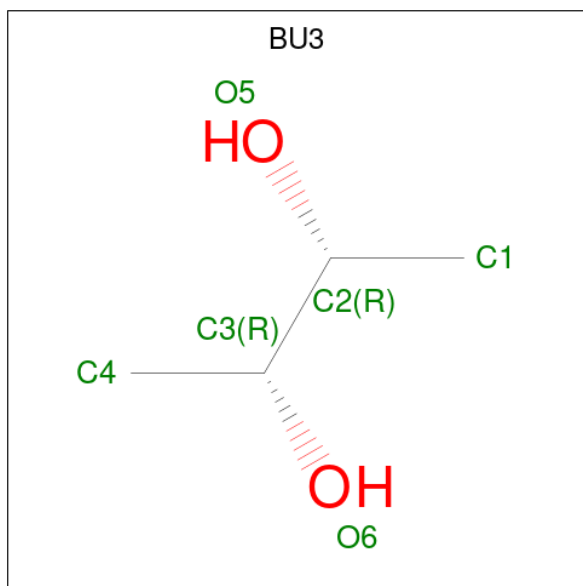
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

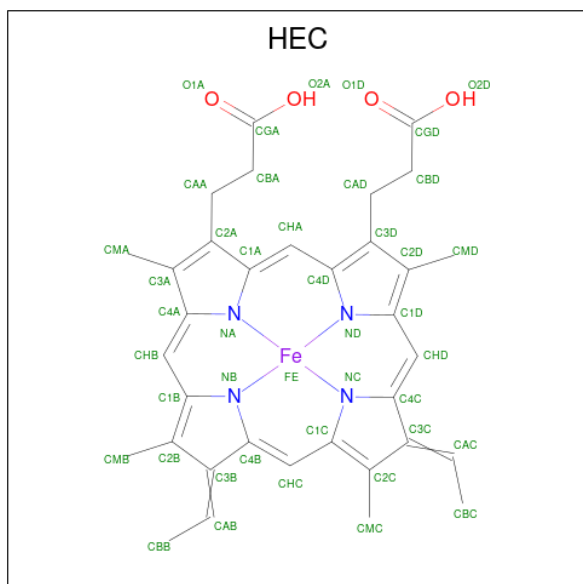
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

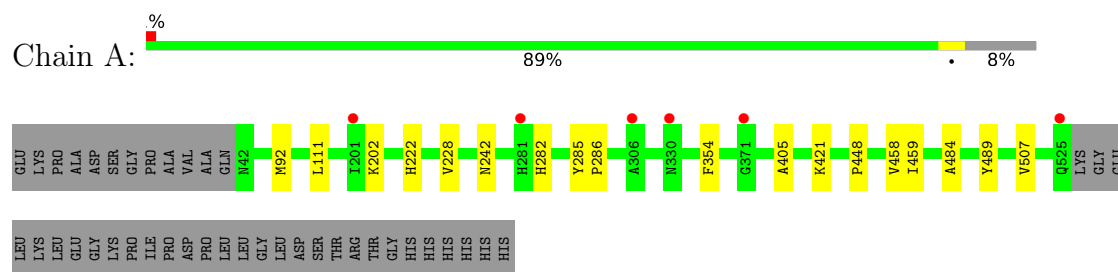
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total 78	O 78	0	0
6	B	92	Total 92	O 92	0	0

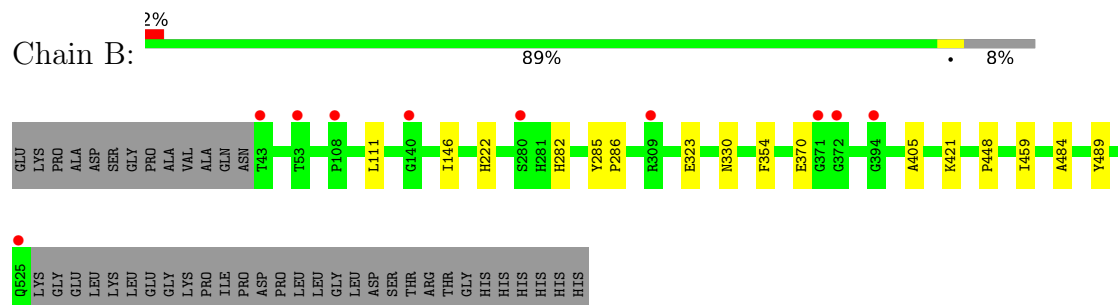
3 Residue-property plots [i](#)

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

- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.85Å 62.97Å 84.21Å 101.54° 99.13° 98.41°	Depositor
Resolution (Å)	80.94 – 2.20 80.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (80.94-2.20) 98.1 (80.94-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.203 , 0.233 (Not available) , 0.222	Depositor DCC
R_{free} test set	2643 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.9	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	0.96	EDS
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: MG, BU3, HEC, CL

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	0.60	0/3760	0.84	0/5092
1	B	0.60	0/3752	0.85	1/5081 (0.0%)
All	All	0.60	0/7512	0.84	1/10173 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLU	N-CA-C	5.46	120.39	111.37

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	3667	0	3536	12	1
1	B	3659	0	3530	8	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	10	0	0
5	A	387	0	271	11	0
5	B	387	0	270	8	0
6	A	78	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	92	0	0	0	0
All	All	8278	0	7617	29	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HD11	5:A:612:HEC:HBB3	1.66	0.76
1:B:459:ILE:HD11	5:B:1009:HEC:HBB3	1.73	0.68
1:A:458:VAL:HG11	5:A:612:HEC:HMA3	1.78	0.65
5:B:1007:HEC:HBC3	5:B:1007:HEC:HMC3	1.89	0.55
5:B:1009:HEC:HBB3	5:B:1009:HEC:HMB3	1.89	0.54
1:A:92:MET:HE3	1:B:146:ILE:HD12	1.90	0.53
1:A:222:HIS:CE1	5:A:605:HEC:HMD1	2.43	0.53
1:A:111:LEU:HD22	1:A:421:LYS:HE2	1.93	0.51
1:B:222:HIS:CE1	5:B:1002:HEC:HMD1	2.46	0.50
5:A:609:HEC:HBC3	5:A:609:HEC:HMC1	1.94	0.48
5:A:606:HEC:HMC3	5:A:606:HEC:HBC3	1.96	0.48
1:B:111:LEU:HD22	1:B:421:LYS:HE2	1.97	0.47
1:B:405:ALA:HB1	5:B:1009:HEC:HMD3	1.99	0.45
5:A:610:HEC:HMC3	5:A:610:HEC:CBC	2.48	0.44
1:A:405:ALA:HB1	5:A:612:HEC:HMD3	1.98	0.44
1:A:507:VAL:HG11	5:A:611:HEC:HMD2	2.00	0.44
1:A:448:PRO:HD2	1:B:448:PRO:HD2	1.99	0.43
5:B:1006:HEC:HMC1	5:B:1006:HEC:HBC3	2.00	0.42
1:A:484:ALA:HA	1:A:489:TYR:CD1	2.55	0.42
1:B:484:ALA:HA	1:B:489:TYR:CD1	2.55	0.42
5:B:1005:HEC:HMC1	5:B:1005:HEC:HBC3	2.02	0.41
5:A:606:HEC:HMC3	5:A:606:HEC:CBC	2.50	0.41
5:A:610:HEC:HMC3	5:A:610:HEC:HBC3	2.02	0.41
1:A:228:VAL:CG2	1:A:242:ASN:HB3	2.50	0.41
1:A:285:TYR:HB3	1:A:286:PRO:HD3	2.03	0.41
5:A:612:HEC:HBB3	5:A:612:HEC:HMB1	2.02	0.41
1:B:285:TYR:HB3	1:B:286:PRO:HD3	2.03	0.40
1:A:228:VAL:CG2	1:A:242:ASN:CB	3.00	0.40
5:B:1001:HEC:HBC3	5:B:1001:HEC:HMC1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:O	1:B:370:GLU:O[1_544]	2.05	0.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/526 (92%)	468 (97%)	13 (3%)	1 (0%)	43	51
1	B	481/526 (91%)	469 (98%)	11 (2%)	1 (0%)	43	51
All	All	963/1052 (92%)	937 (97%)	24 (2%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	HIS
1	B	282	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/421 (92%)	386 (100%)	1 (0%)	86	93
1	B	386/421 (92%)	384 (100%)	2 (0%)	81	90
All	All	773/842 (92%)	770 (100%)	3 (0%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	PHE
1	B	330	ASN
1	B	354	PHE

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

Mol	Chain	Res	Type
1	A	114	GLN
1	A	505	ASN
1	B	84	ASN
1	B	114	GLN
1	B	525	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	HEC	B	1004	1	46,50,50	1.68	6 (13%)	58,82,82	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEC	B	1006	1	46,50,50	1.80	8 (17%)	58,82,82	1.95	12 (20%)
5	HEC	A	609	1	46,50,50	1.58	8 (17%)	58,82,82	1.60	12 (20%)
5	HEC	B	1009	1,2	46,50,50	1.67	9 (19%)	58,82,82	1.57	12 (20%)
5	HEC	A	607	1	46,50,50	1.66	7 (15%)	58,82,82	1.28	8 (13%)
5	HEC	B	1001	1	46,50,50	1.61	9 (19%)	58,82,82	1.53	12 (20%)
5	HEC	B	1007	1	46,50,50	1.70	10 (21%)	58,82,82	1.46	10 (17%)
5	HEC	A	605	1	46,50,50	1.65	6 (13%)	58,82,82	1.71	13 (22%)
5	HEC	B	1003	1	46,50,50	1.71	7 (15%)	58,82,82	1.33	7 (12%)
5	HEC	A	604	1	46,50,50	1.65	8 (17%)	58,82,82	1.39	9 (15%)
5	HEC	A	611	1	46,50,50	1.57	6 (13%)	58,82,82	1.69	10 (17%)
5	HEC	A	608	6,1	46,50,50	1.58	7 (15%)	58,82,82	1.46	10 (17%)
5	HEC	A	610	1	46,50,50	1.49	8 (17%)	58,82,82	1.55	10 (17%)
4	BU3	A	603	-	4,5,5	0.42	0	6,6,6	0.32	0
5	HEC	B	1005	1	46,50,50	1.84	9 (19%)	58,82,82	2.33	18 (31%)
5	HEC	A	606	1	46,50,50	1.63	6 (13%)	58,82,82	1.45	9 (15%)
5	HEC	A	612	1,2	46,50,50	1.64	9 (19%)	58,82,82	1.53	14 (24%)
5	HEC	B	1008	1	46,50,50	1.63	7 (15%)	58,82,82	1.76	11 (18%)
5	HEC	B	1002	1	46,50,50	1.68	9 (19%)	58,82,82	1.59	10 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	B	1004	1	-	9/14/54/54	-
5	HEC	B	1006	1	-	7/14/54/54	-
5	HEC	A	609	1	-	7/14/54/54	-
5	HEC	B	1009	1,2	-	7/14/54/54	-
5	HEC	A	607	1	-	9/14/54/54	-
5	HEC	B	1001	1	-	9/14/54/54	-
5	HEC	B	1007	1	-	6/14/54/54	-
5	HEC	A	605	1	-	7/14/54/54	-
5	HEC	B	1003	1	-	11/14/54/54	-
5	HEC	A	604	1	-	8/14/54/54	-
5	HEC	A	611	1	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	608	6,1	-	10/14/54/54	-
5	HEC	A	610	1	-	6/14/54/54	-
4	BU3	A	603	-	-	4/4/4/4	-
5	HEC	B	1005	1	-	8/14/54/54	-
5	HEC	A	606	1	-	11/14/54/54	-
5	HEC	A	612	1,2	-	10/14/54/54	-
5	HEC	B	1008	1	-	9/14/54/54	-
5	HEC	B	1002	1	-	10/14/54/54	-

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1005	HEC	CBB-CAB	-6.32	1.26	1.49
5	B	1009	HEC	CAC-C3C	5.07	1.51	1.35
5	B	1008	HEC	CAC-C3C	5.03	1.51	1.35
5	B	1004	HEC	CAC-C3C	4.84	1.50	1.35
5	A	607	HEC	CAC-C3C	4.80	1.50	1.35
5	A	611	HEC	CAC-C3C	4.75	1.50	1.35
5	A	605	HEC	CAC-C3C	4.73	1.50	1.35
5	B	1007	HEC	CAC-C3C	4.72	1.50	1.35
5	B	1002	HEC	CAB-C3B	4.71	1.50	1.35
5	A	608	HEC	CAC-C3C	4.70	1.50	1.35
5	A	605	HEC	CAB-C3B	4.70	1.50	1.35
5	A	606	HEC	CAC-C3C	4.68	1.50	1.35
5	A	612	HEC	CAC-C3C	4.66	1.50	1.35
5	B	1005	HEC	CAC-C3C	4.64	1.50	1.35
5	A	609	HEC	CAB-C3B	4.59	1.49	1.35
5	A	607	HEC	CAB-C3B	4.57	1.49	1.35
5	A	604	HEC	CAC-C3C	4.55	1.49	1.35
5	B	1005	HEC	CAB-C3B	4.55	1.49	1.35
5	A	604	HEC	CAB-C3B	4.53	1.49	1.35
5	B	1001	HEC	CAB-C3B	4.53	1.49	1.35
5	B	1001	HEC	CAC-C3C	4.53	1.49	1.35
5	B	1002	HEC	CAC-C3C	4.52	1.49	1.35
5	A	606	HEC	CAB-C3B	4.52	1.49	1.35
5	B	1006	HEC	CAC-C3C	4.50	1.49	1.35
5	B	1003	HEC	CAC-C3C	4.49	1.49	1.35
5	A	610	HEC	CAC-C3C	4.49	1.49	1.35
5	B	1009	HEC	CAB-C3B	4.48	1.49	1.35
5	B	1006	HEC	CBB-CAB	4.47	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	HEC	CAB-C3B	4.37	1.49	1.35
5	A	612	HEC	CAB-C3B	4.35	1.49	1.35
5	B	1003	HEC	CAB-C3B	4.34	1.49	1.35
5	A	609	HEC	CAC-C3C	4.27	1.48	1.35
5	B	1007	HEC	CAB-C3B	4.25	1.48	1.35
5	A	608	HEC	CAB-C3B	4.25	1.48	1.35
5	B	1003	HEC	CBC-CAC	-4.23	1.33	1.49
5	B	1006	HEC	CAB-C3B	4.17	1.48	1.35
5	B	1006	HEC	C1D-ND	-4.17	1.31	1.39
5	A	611	HEC	CAB-C3B	4.16	1.48	1.35
5	A	610	HEC	CAB-C3B	4.04	1.48	1.35
5	B	1006	HEC	C1B-NB	-3.93	1.32	1.39
5	B	1008	HEC	CAB-C3B	3.88	1.47	1.35
5	B	1002	HEC	C1D-ND	-3.85	1.32	1.39
5	A	611	HEC	C4D-ND	-3.80	1.32	1.39
5	B	1007	HEC	CBB-CAB	-3.79	1.35	1.49
5	B	1008	HEC	C4D-ND	-3.78	1.32	1.39
5	B	1009	HEC	C1D-ND	-3.72	1.32	1.39
5	B	1006	HEC	C4B-NB	-3.67	1.32	1.39
5	A	611	HEC	C1D-ND	-3.64	1.32	1.39
5	A	608	HEC	C4B-NB	-3.61	1.32	1.39
5	A	612	HEC	C1D-ND	-3.60	1.32	1.39
5	A	606	HEC	C1D-ND	-3.57	1.32	1.39
5	A	609	HEC	C1D-ND	-3.55	1.32	1.39
5	A	605	HEC	C1D-ND	-3.54	1.32	1.39
5	A	604	HEC	C1D-ND	-3.49	1.33	1.39
5	B	1001	HEC	C1D-ND	-3.45	1.33	1.39
5	B	1004	HEC	C1D-ND	-3.44	1.33	1.39
5	A	606	HEC	C4D-ND	-3.41	1.33	1.39
5	B	1007	HEC	C4B-NB	-3.40	1.33	1.39
5	A	608	HEC	C1D-ND	-3.38	1.33	1.39
5	A	607	HEC	C1B-NB	-3.35	1.33	1.39
5	A	607	HEC	C1D-ND	-3.34	1.33	1.39
5	A	606	HEC	C1B-NB	-3.32	1.33	1.39
5	A	612	HEC	C1B-NB	-3.31	1.33	1.39
5	A	604	HEC	C4B-NB	-3.25	1.33	1.39
5	A	604	HEC	C4D-ND	-3.25	1.33	1.39
5	B	1004	HEC	C1B-NB	-3.25	1.33	1.39
5	B	1003	HEC	C1D-ND	-3.24	1.33	1.39
5	B	1003	HEC	C4D-ND	-3.22	1.33	1.39
5	A	610	HEC	C1D-ND	-3.22	1.33	1.39
5	B	1003	HEC	C1B-NB	-3.22	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	HEC	C4D-ND	-3.21	1.33	1.39
5	A	607	HEC	C4B-NB	-3.20	1.33	1.39
5	B	1003	HEC	C4B-NB	-3.19	1.33	1.39
5	B	1004	HEC	C4B-NB	-3.18	1.33	1.39
5	B	1001	HEC	C4B-NB	-3.17	1.33	1.39
5	A	611	HEC	C4B-NB	-3.16	1.33	1.39
5	B	1005	HEC	C1D-ND	-3.16	1.33	1.39
5	B	1001	HEC	C4D-ND	-3.15	1.33	1.39
5	B	1006	HEC	C4D-ND	-3.15	1.33	1.39
5	B	1009	HEC	C1B-NB	-3.13	1.33	1.39
5	B	1007	HEC	C1D-ND	-3.11	1.33	1.39
5	B	1001	HEC	C1B-NB	-3.05	1.33	1.39
5	B	1009	HEC	C4B-NB	-3.03	1.33	1.39
5	A	609	HEC	C1B-NB	-3.02	1.33	1.39
5	B	1004	HEC	C4D-ND	-2.96	1.34	1.39
5	B	1008	HEC	C1B-NB	-2.96	1.34	1.39
5	A	606	HEC	C4B-NB	-2.93	1.34	1.39
5	A	610	HEC	C4B-NB	-2.93	1.34	1.39
5	A	604	HEC	C1B-NB	-2.88	1.34	1.39
5	B	1007	HEC	C1B-NB	-2.85	1.34	1.39
5	B	1007	HEC	C4D-ND	-2.85	1.34	1.39
5	A	605	HEC	C4D-ND	-2.84	1.34	1.39
5	A	612	HEC	C4D-ND	-2.83	1.34	1.39
5	A	607	HEC	C4D-ND	-2.80	1.34	1.39
5	B	1008	HEC	C1D-ND	-2.80	1.34	1.39
5	B	1005	HEC	C4B-NB	-2.80	1.34	1.39
5	A	605	HEC	C4B-NB	-2.75	1.34	1.39
5	A	608	HEC	C4D-ND	-2.75	1.34	1.39
5	A	605	HEC	C1B-NB	-2.73	1.34	1.39
5	B	1005	HEC	C1B-NB	-2.72	1.34	1.39
5	A	609	HEC	C4B-NB	-2.69	1.34	1.39
5	B	1002	HEC	C1B-NB	-2.68	1.34	1.39
5	A	611	HEC	C1B-NB	-2.66	1.34	1.39
5	B	1008	HEC	C4B-NB	-2.66	1.34	1.39
5	B	1008	HEC	C4A-C3A	-2.65	1.40	1.45
5	B	1002	HEC	C4B-NB	-2.58	1.34	1.39
5	B	1009	HEC	C4D-ND	-2.51	1.34	1.39
5	B	1005	HEC	C4D-ND	-2.51	1.34	1.39
5	B	1007	HEC	C3B-C4B	2.48	1.50	1.46
5	A	608	HEC	C1B-NB	-2.47	1.35	1.39
5	A	604	HEC	C1D-C2D	2.44	1.48	1.43
5	A	612	HEC	C4B-NB	-2.43	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	HEC	C1B-NB	-2.42	1.35	1.39
5	A	609	HEC	C4D-ND	-2.41	1.35	1.39
5	B	1009	HEC	C3B-C4B	2.40	1.50	1.46
5	A	610	HEC	C4D-ND	-2.37	1.35	1.39
5	A	612	HEC	C3B-C4B	2.33	1.50	1.46
5	B	1001	HEC	C4A-C3A	-2.24	1.40	1.45
5	B	1006	HEC	C4A-C3A	-2.23	1.40	1.45
5	A	607	HEC	C4A-C3A	-2.22	1.40	1.45
5	B	1005	HEC	C1D-C2D	2.19	1.48	1.43
5	B	1009	HEC	C1C-NC	-2.16	1.35	1.39
5	A	609	HEC	C4A-C3A	-2.13	1.41	1.45
5	B	1005	HEC	C3B-C4B	2.13	1.49	1.46
5	B	1001	HEC	C3B-C4B	2.13	1.49	1.46
5	A	612	HEC	C4A-C3A	-2.12	1.41	1.45
5	A	610	HEC	C3B-C4B	2.11	1.49	1.46
5	B	1007	HEC	C1A-C2A	-2.11	1.41	1.45
5	B	1002	HEC	C1D-C2D	2.10	1.48	1.43
5	B	1001	HEC	C1D-C2D	2.10	1.48	1.43
5	B	1009	HEC	C4A-C3A	-2.08	1.41	1.45
5	B	1007	HEC	C1D-C2D	2.07	1.48	1.43
5	B	1002	HEC	C1A-C2A	-2.06	1.41	1.45
5	B	1002	HEC	CHC-C4B	2.05	1.42	1.38
5	A	608	HEC	C3B-C4B	2.05	1.49	1.46
5	A	610	HEC	C1D-C2D	2.04	1.47	1.43
5	A	609	HEC	C3B-C4B	2.03	1.49	1.46
5	A	604	HEC	C4A-C3A	-2.03	1.41	1.45
5	A	612	HEC	CHC-C4B	2.01	1.42	1.38

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1005	HEC	CBB-CAB-C3B	12.59	152.60	127.43
5	B	1006	HEC	CBB-CAB-C3B	-9.46	108.53	127.43
5	B	1008	HEC	CHC-C4B-NB	5.41	130.35	124.45
5	A	611	HEC	CHC-C4B-NB	5.03	129.93	124.45
5	A	610	HEC	CBB-CAB-C3B	-4.93	117.58	127.43
5	B	1008	HEC	CBB-CAB-C3B	-4.75	117.94	127.43
5	A	605	HEC	C4B-NB-C1B	4.52	113.19	105.82
5	A	609	HEC	CHC-C4B-NB	4.48	129.34	124.45
5	B	1008	HEC	C2A-C1A-NA	-4.43	106.05	110.32
5	B	1002	HEC	C4B-NB-C1B	4.32	112.87	105.82
5	A	611	HEC	CBB-CAB-C3B	-4.32	118.80	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	609	HEC	CBB-CAB-C3B	-4.28	118.87	127.43
5	B	1009	HEC	CBA-CAA-C2A	-4.16	101.03	112.53
5	B	1006	HEC	CHC-C4B-NB	3.91	128.71	124.45
5	A	605	HEC	CHC-C4B-NB	3.85	128.65	124.45
5	B	1005	HEC	C4D-ND-C1D	3.81	112.04	105.82
5	A	604	HEC	CHA-C1A-NA	3.80	128.59	124.45
5	A	609	HEC	C2A-C1A-NA	-3.77	106.68	110.32
5	A	606	HEC	CHC-C4B-NB	3.77	128.55	124.45
5	B	1005	HEC	CHC-C4B-NB	3.75	128.54	124.45
5	B	1005	HEC	C2A-C1A-NA	-3.75	106.70	110.32
5	A	605	HEC	C2A-C1A-NA	-3.68	106.77	110.32
5	B	1006	HEC	C2A-C1A-NA	-3.65	106.80	110.32
5	B	1002	HEC	CHA-C1A-NA	3.62	128.39	124.45
5	A	610	HEC	CHC-C4B-NB	3.61	128.39	124.45
5	A	611	HEC	C2A-C1A-NA	-3.57	106.88	110.32
5	B	1001	HEC	CHA-C1A-NA	3.52	128.29	124.45
5	B	1008	HEC	C4B-NB-C1B	3.52	111.56	105.82
5	B	1009	HEC	O2D-CGD-CBD	3.46	124.93	114.00
5	B	1001	HEC	C2A-C1A-NA	-3.46	106.99	110.32
5	A	605	HEC	CHA-C1A-NA	3.45	128.21	124.45
5	B	1005	HEC	C4B-NB-C1B	3.44	111.42	105.82
5	B	1001	HEC	CHD-C4C-NC	3.43	128.19	124.45
5	B	1002	HEC	CHC-C4B-NB	3.40	128.16	124.45
5	A	609	HEC	CHA-C1A-NA	3.39	128.14	124.45
5	A	604	HEC	CHD-C4C-NC	3.38	128.13	124.45
5	A	608	HEC	CHD-C4C-NC	3.37	128.13	124.45
5	A	605	HEC	C4D-ND-C1D	3.37	111.32	105.82
5	B	1007	HEC	C4D-ND-C1D	3.36	111.31	105.82
5	B	1002	HEC	CHD-C4C-NC	3.35	128.10	124.45
5	B	1003	HEC	CHC-C4B-NB	3.31	128.05	124.45
5	B	1001	HEC	CHC-C4B-NB	3.28	128.02	124.45
5	A	611	HEC	C4B-NB-C1B	3.27	111.16	105.82
5	A	612	HEC	CHC-C4B-NB	3.26	128.01	124.45
5	A	611	HEC	C4D-ND-C1D	3.24	111.11	105.82
5	B	1008	HEC	C4D-ND-C1D	3.22	111.07	105.82
5	A	611	HEC	CBA-CAA-C2A	-3.20	103.67	112.53
5	A	608	HEC	C4B-NB-C1B	3.20	111.04	105.82
5	A	607	HEC	CHC-C4B-NB	3.18	127.92	124.45
5	A	608	HEC	CHA-C1A-NA	3.17	127.90	124.45
5	A	610	HEC	CHA-C4D-ND	3.16	129.60	123.86
5	A	612	HEC	CBB-CAB-C3B	-3.15	121.13	127.43
5	A	612	HEC	C4B-NB-C1B	3.14	110.94	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	HEC	CHC-C4B-NB	3.11	127.84	124.45
5	A	612	HEC	CHA-C1A-NA	3.11	127.84	124.45
5	B	1007	HEC	C4B-NB-C1B	3.11	110.89	105.82
5	A	606	HEC	CHD-C4C-NC	3.10	127.83	124.45
5	A	606	HEC	C2A-C1A-NA	-3.10	107.33	110.32
5	A	605	HEC	C4C-NC-C1C	3.07	110.83	105.82
5	B	1008	HEC	CHA-C1A-NA	3.05	127.77	124.45
5	B	1003	HEC	C4B-NB-C1B	3.02	110.74	105.82
5	B	1001	HEC	CBC-CAC-C3C	-2.98	121.48	127.43
5	B	1007	HEC	CHA-C4D-ND	2.96	129.23	123.86
5	B	1003	HEC	C2A-C1A-NA	-2.96	107.47	110.32
5	B	1006	HEC	CHA-C1A-NA	2.96	127.67	124.45
5	A	610	HEC	C2A-C1A-NA	-2.96	107.47	110.32
5	A	606	HEC	C4B-NB-C1B	2.95	110.63	105.82
5	A	605	HEC	CHD-C4C-NC	2.95	127.67	124.45
5	A	608	HEC	C4D-ND-C1D	2.94	110.62	105.82
5	B	1004	HEC	CHC-C4B-NB	2.91	127.62	124.45
5	B	1009	HEC	CBB-CAB-C3B	-2.90	121.64	127.43
5	B	1009	HEC	C4B-NB-C1B	2.89	110.54	105.82
5	B	1001	HEC	C4D-ND-C1D	2.88	110.52	105.82
5	A	604	HEC	C4B-NB-C1B	2.86	110.49	105.82
5	A	607	HEC	C2A-C1A-NA	-2.85	107.57	110.32
5	B	1002	HEC	C4C-NC-C1C	2.85	110.47	105.82
5	B	1006	HEC	C4B-NB-C1B	2.85	110.46	105.82
5	A	610	HEC	C4D-ND-C1D	2.83	110.43	105.82
5	B	1007	HEC	CHA-C1A-NA	2.82	127.52	124.45
5	A	609	HEC	C4D-ND-C1D	2.80	110.39	105.82
5	B	1006	HEC	O2D-CGD-CBD	2.80	122.84	114.00
5	A	612	HEC	C2A-C1A-NA	-2.78	107.64	110.32
5	B	1001	HEC	C4B-NB-C1B	2.77	110.34	105.82
5	A	604	HEC	C2A-C1A-NA	-2.77	107.65	110.32
5	A	605	HEC	C4A-NA-C1A	2.77	110.34	105.82
5	B	1009	HEC	C2A-C1A-NA	-2.77	107.65	110.32
5	A	608	HEC	CHA-C4D-ND	2.76	128.86	123.86
5	A	608	HEC	C2A-C1A-NA	-2.75	107.67	110.32
5	A	606	HEC	C4D-ND-C1D	2.74	110.29	105.82
5	B	1005	HEC	CHD-C4C-NC	2.72	127.42	124.45
5	B	1007	HEC	CHC-C4B-NB	2.72	127.41	124.45
5	B	1009	HEC	CHA-C1A-NA	2.70	127.39	124.45
5	B	1005	HEC	CHA-C4D-ND	2.69	128.74	123.86
5	B	1004	HEC	C4B-NB-C1B	2.68	110.19	105.82
5	B	1006	HEC	CHB-C4A-NA	2.67	127.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	HEC	CBC-CAC-C3C	-2.64	122.16	127.43
5	A	611	HEC	CHA-C1A-NA	2.64	127.32	124.45
5	B	1003	HEC	C4D-ND-C1D	2.63	110.11	105.82
5	A	607	HEC	CHA-C4D-ND	2.63	128.63	123.86
5	B	1004	HEC	C2A-C1A-NA	-2.63	107.79	110.32
5	B	1003	HEC	CHD-C4C-NC	2.61	127.29	124.45
5	B	1008	HEC	CHD-C1D-ND	2.59	128.56	123.86
5	A	612	HEC	O2D-CGD-CBD	2.58	122.15	114.00
5	B	1007	HEC	C2A-C1A-NA	-2.57	107.84	110.32
5	B	1008	HEC	O2D-CGD-CBD	2.56	122.10	114.00
5	A	608	HEC	CHC-C4B-NB	2.56	127.24	124.45
5	A	611	HEC	CHD-C4C-NC	2.55	127.23	124.45
5	B	1002	HEC	O2D-CGD-CBD	2.55	122.06	114.00
5	B	1005	HEC	C3D-C4D-ND	-2.54	107.33	110.15
5	B	1009	HEC	CHC-C4B-NB	2.54	127.22	124.45
5	B	1005	HEC	C4C-NC-C1C	2.54	109.96	105.82
5	B	1005	HEC	CAA-C2A-C3A	-2.53	123.14	127.87
5	B	1006	HEC	C4D-ND-C1D	2.52	109.94	105.82
5	B	1005	HEC	CBD-CAD-C3D	-2.51	105.60	112.53
5	B	1002	HEC	C4D-ND-C1D	2.51	109.91	105.82
5	A	609	HEC	C4B-NB-C1B	2.49	109.89	105.82
5	B	1004	HEC	CBB-CAB-C3B	-2.49	122.45	127.43
5	B	1003	HEC	CHA-C4D-ND	2.49	128.38	123.86
5	A	610	HEC	C4B-NB-C1B	2.49	109.88	105.82
5	A	606	HEC	CHA-C1A-NA	2.48	127.15	124.45
5	A	611	HEC	O2D-CGD-CBD	2.47	121.82	114.00
5	A	607	HEC	CAD-CBD-CGD	-2.46	107.15	113.67
5	B	1005	HEC	CHB-C4A-NA	2.44	127.11	124.45
5	B	1001	HEC	C4C-NC-C1C	2.43	109.78	105.82
5	B	1008	HEC	C4C-NC-C1C	2.42	109.76	105.82
5	A	604	HEC	C4C-NC-C1C	2.41	109.75	105.82
5	A	612	HEC	CHD-C1D-ND	2.41	128.23	123.86
5	A	609	HEC	CHA-C4D-ND	2.41	128.23	123.86
5	A	609	HEC	CHD-C4C-NC	2.40	127.07	124.45
5	B	1009	HEC	CHD-C4C-NC	2.40	127.06	124.45
5	A	604	HEC	C4D-ND-C1D	2.40	109.73	105.82
5	B	1006	HEC	CHD-C4C-NC	2.39	127.05	124.45
5	B	1002	HEC	O2D-CGD-O1D	-2.38	117.22	123.33
5	A	612	HEC	C4D-ND-C1D	2.36	109.68	105.82
5	B	1006	HEC	O2D-CGD-O1D	-2.35	117.28	123.33
5	A	612	HEC	CHD-C4C-NC	2.35	127.01	124.45
5	B	1007	HEC	CHB-C4A-NA	2.34	127.00	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	610	HEC	CHB-C1B-NB	2.34	128.10	123.86
5	A	611	HEC	CHA-C4D-ND	2.33	128.09	123.86
5	A	609	HEC	O2D-CGD-CBD	2.31	121.31	114.00
5	A	606	HEC	C4A-NA-C1A	2.30	109.58	105.82
5	B	1002	HEC	C4A-NA-C1A	2.29	109.56	105.82
5	A	608	HEC	CHB-C1B-NB	2.29	128.02	123.86
5	B	1007	HEC	CMD-C2D-C1D	2.28	128.89	125.42
5	B	1004	HEC	CHA-C1A-NA	2.26	126.92	124.45
5	B	1005	HEC	CAA-C2A-C1A	2.26	129.44	124.85
5	A	607	HEC	C4B-NB-C1B	2.26	109.50	105.82
5	B	1007	HEC	CBD-CAD-C3D	-2.26	106.29	112.53
5	A	608	HEC	C4C-NC-C1C	2.25	109.50	105.82
5	B	1008	HEC	C4A-NA-C1A	2.25	109.48	105.82
5	B	1002	HEC	C2A-C1A-NA	-2.24	108.16	110.32
5	A	604	HEC	CHB-C1B-NB	2.24	127.93	123.86
5	A	605	HEC	CHB-C1B-NB	2.23	127.90	123.86
5	B	1005	HEC	CHB-C1B-NB	2.23	127.90	123.86
5	A	607	HEC	CMD-C2D-C1D	2.23	128.81	125.42
5	A	608	HEC	O2D-CGD-CBD	2.22	121.00	114.00
5	B	1007	HEC	CHD-C4C-NC	2.21	126.86	124.45
5	A	607	HEC	CHD-C1D-ND	2.21	127.87	123.86
5	A	605	HEC	O2A-CGA-CBA	2.21	120.97	114.00
5	A	612	HEC	C4C-NC-C1C	2.21	109.42	105.82
5	A	604	HEC	CBD-CAD-C3D	2.20	118.60	112.53
5	A	612	HEC	CHA-C4D-ND	2.19	127.82	123.86
5	A	610	HEC	CHA-C1A-NA	2.18	126.83	124.45
5	A	605	HEC	C2B-C1B-NB	-2.16	106.67	110.14
5	A	610	HEC	CHD-C1D-ND	2.15	127.75	123.86
5	B	1009	HEC	CHA-C4D-ND	2.14	127.74	123.86
5	A	609	HEC	C4A-NA-C1A	2.13	109.30	105.82
5	B	1004	HEC	O2A-CGA-CBA	2.13	120.72	114.00
5	B	1005	HEC	C4A-NA-C1A	2.12	109.28	105.82
5	B	1005	HEC	O2A-CGA-CBA	2.12	120.69	114.00
5	A	609	HEC	O2D-CGD-O1D	-2.12	117.88	123.33
5	A	605	HEC	CHA-C4D-ND	2.12	127.70	123.86
5	A	612	HEC	O2A-CGA-CBA	2.12	120.68	114.00
5	B	1001	HEC	CHB-C4A-NA	2.11	126.75	124.45
5	B	1001	HEC	O2D-CGD-CBD	2.11	120.66	114.00
5	A	612	HEC	CBA-CAA-C2A	-2.10	106.73	112.53
5	B	1008	HEC	C3D-C4D-ND	-2.09	107.83	110.15
5	B	1009	HEC	C4D-ND-C1D	2.08	109.21	105.82
5	A	609	HEC	CHD-C1D-ND	2.08	127.62	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1009	HEC	CAD-C3D-C4D	2.07	128.99	124.94
5	A	610	HEC	O2A-CGA-CBA	2.06	120.52	114.00
5	B	1009	HEC	O1D-CGD-CBD	-2.06	116.55	123.09
5	B	1006	HEC	CBC-CAC-C3C	-2.06	123.31	127.43
5	A	605	HEC	C2D-C1D-ND	-2.06	106.84	110.14
5	B	1001	HEC	CMD-C2D-C1D	2.05	128.54	125.42
5	B	1005	HEC	C2D-C1D-ND	-2.04	106.86	110.14
5	A	607	HEC	CBB-CAB-C3B	-2.04	123.35	127.43
5	B	1006	HEC	CHA-C4D-ND	2.04	127.55	123.86
5	A	612	HEC	O2A-CGA-O1A	-2.03	118.11	123.33
5	B	1003	HEC	C4C-NC-C1C	2.03	109.13	105.82
5	A	606	HEC	C4C-NC-C1C	2.02	109.12	105.82
5	B	1001	HEC	O2A-CGA-CBA	2.01	120.35	114.00
5	B	1004	HEC	C4C-NC-C1C	2.00	109.08	105.82
5	B	1005	HEC	CBA-CAA-C2A	2.00	118.07	112.53

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	BU3	C1-C2-C3-O6
4	A	603	BU3	O5-C2-C3-C4
4	A	603	BU3	C1-C2-C3-C4
5	A	604	HEC	C4B-C3B-CAB-CBB
5	A	604	HEC	C2D-C3D-CAD-CBD
5	A	604	HEC	C4D-C3D-CAD-CBD
5	A	605	HEC	C2B-C3B-CAB-CBB
5	A	605	HEC	C4B-C3B-CAB-CBB
5	A	605	HEC	C2C-C3C-CAC-CBC
5	A	605	HEC	C4C-C3C-CAC-CBC
5	A	606	HEC	C2B-C3B-CAB-CBB
5	A	606	HEC	C4B-C3B-CAB-CBB
5	A	606	HEC	C2C-C3C-CAC-CBC
5	A	606	HEC	C4C-C3C-CAC-CBC
5	A	607	HEC	C2B-C3B-CAB-CBB
5	A	607	HEC	C4B-C3B-CAB-CBB
5	A	607	HEC	C2C-C3C-CAC-CBC
5	A	607	HEC	C4C-C3C-CAC-CBC
5	A	608	HEC	C2B-C3B-CAB-CBB
5	A	608	HEC	C4B-C3B-CAB-CBB
5	A	608	HEC	C2C-C3C-CAC-CBC
5	A	608	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	A	609	HEC	C2B-C3B-CAB-CBB
5	A	609	HEC	C4B-C3B-CAB-CBB
5	A	609	HEC	C2C-C3C-CAC-CBC
5	A	609	HEC	C4C-C3C-CAC-CBC
5	A	610	HEC	C2B-C3B-CAB-CBB
5	A	610	HEC	C4B-C3B-CAB-CBB
5	A	610	HEC	C2C-C3C-CAC-CBC
5	A	610	HEC	C4C-C3C-CAC-CBC
5	A	611	HEC	C2B-C3B-CAB-CBB
5	A	611	HEC	C4B-C3B-CAB-CBB
5	A	611	HEC	C2C-C3C-CAC-CBC
5	A	611	HEC	C4C-C3C-CAC-CBC
5	A	612	HEC	C2B-C3B-CAB-CBB
5	A	612	HEC	C4B-C3B-CAB-CBB
5	A	612	HEC	C2C-C3C-CAC-CBC
5	A	612	HEC	C4C-C3C-CAC-CBC
5	B	1001	HEC	C2B-C3B-CAB-CBB
5	B	1001	HEC	C4B-C3B-CAB-CBB
5	B	1001	HEC	C2C-C3C-CAC-CBC
5	B	1001	HEC	C4C-C3C-CAC-CBC
5	B	1002	HEC	C2B-C3B-CAB-CBB
5	B	1002	HEC	C4B-C3B-CAB-CBB
5	B	1002	HEC	C2C-C3C-CAC-CBC
5	B	1002	HEC	C4C-C3C-CAC-CBC
5	B	1003	HEC	C2B-C3B-CAB-CBB
5	B	1003	HEC	C4B-C3B-CAB-CBB
5	B	1003	HEC	C2C-C3C-CAC-CBC
5	B	1003	HEC	C4C-C3C-CAC-CBC
5	B	1004	HEC	C2B-C3B-CAB-CBB
5	B	1004	HEC	C4B-C3B-CAB-CBB
5	B	1004	HEC	C2C-C3C-CAC-CBC
5	B	1004	HEC	C4C-C3C-CAC-CBC
5	B	1005	HEC	C2C-C3C-CAC-CBC
5	B	1005	HEC	C4C-C3C-CAC-CBC
5	B	1006	HEC	C2B-C3B-CAB-CBB
5	B	1006	HEC	C4B-C3B-CAB-CBB
5	B	1006	HEC	C2C-C3C-CAC-CBC
5	B	1006	HEC	C4C-C3C-CAC-CBC
5	B	1007	HEC	C2B-C3B-CAB-CBB
5	B	1007	HEC	C4B-C3B-CAB-CBB
5	B	1007	HEC	C2C-C3C-CAC-CBC
5	B	1007	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	B	1008	HEC	C2B-C3B-CAB-CBB
5	B	1008	HEC	C4B-C3B-CAB-CBB
5	B	1008	HEC	C2C-C3C-CAC-CBC
5	B	1008	HEC	C4C-C3C-CAC-CBC
5	B	1009	HEC	C2B-C3B-CAB-CBB
5	B	1009	HEC	C4B-C3B-CAB-CBB
5	B	1009	HEC	C2C-C3C-CAC-CBC
5	B	1009	HEC	C4C-C3C-CAC-CBC
5	A	608	HEC	C3D-CAD-CBD-CGD
5	A	609	HEC	C2A-CAA-CBA-CGA
5	B	1005	HEC	C2A-CAA-CBA-CGA
5	B	1006	HEC	C2A-CAA-CBA-CGA
5	A	606	HEC	C1A-C2A-CAA-CBA
5	A	606	HEC	C3A-C2A-CAA-CBA
5	B	1003	HEC	C3A-C2A-CAA-CBA
5	B	1003	HEC	C1A-C2A-CAA-CBA
5	B	1005	HEC	C1A-C2A-CAA-CBA
5	A	612	HEC	C2A-CAA-CBA-CGA
5	B	1005	HEC	C3A-C2A-CAA-CBA
5	A	605	HEC	C2A-CAA-CBA-CGA
5	B	1002	HEC	C2A-CAA-CBA-CGA
5	A	607	HEC	C3D-CAD-CBD-CGD
5	A	612	HEC	C3D-CAD-CBD-CGD
5	B	1004	HEC	C3D-CAD-CBD-CGD
5	B	1005	HEC	C4B-C3B-CAB-CBB
5	B	1009	HEC	C3D-CAD-CBD-CGD
5	A	604	HEC	C2B-C3B-CAB-CBB
5	A	608	HEC	C2A-CAA-CBA-CGA
5	B	1008	HEC	C2A-CAA-CBA-CGA
5	A	607	HEC	CAD-CBD-CGD-O2D
5	B	1009	HEC	CAD-CBD-CGD-O1D
5	B	1002	HEC	CAA-CBA-CGA-O1A
5	A	612	HEC	CAD-CBD-CGD-O1D
5	A	612	HEC	CAD-CBD-CGD-O2D
5	A	604	HEC	CAA-CBA-CGA-O1A
5	B	1001	HEC	CAA-CBA-CGA-O1A
5	B	1002	HEC	CAA-CBA-CGA-O2A
5	A	605	HEC	CAA-CBA-CGA-O1A
5	B	1004	HEC	CAD-CBD-CGD-O2D
5	B	1009	HEC	CAD-CBD-CGD-O2D
5	A	607	HEC	CAD-CBD-CGD-O1D
5	A	608	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	B	1001	HEC	CAA-CBA-CGA-O2A
5	B	1004	HEC	CAA-CBA-CGA-O1A
5	A	604	HEC	CAA-CBA-CGA-O2A
5	B	1003	HEC	CAD-CBD-CGD-O1D
5	B	1003	HEC	CAD-CBD-CGD-O2D
5	B	1003	HEC	CAA-CBA-CGA-O1A
5	B	1004	HEC	CAA-CBA-CGA-O2A
5	B	1001	HEC	CAD-CBD-CGD-O1D
5	B	1006	HEC	CAA-CBA-CGA-O2A
5	A	608	HEC	CAD-CBD-CGD-O2D
5	A	604	HEC	CAD-CBD-CGD-O2D
5	B	1003	HEC	CAA-CBA-CGA-O2A
5	B	1008	HEC	CAD-CBD-CGD-O2D
5	A	606	HEC	CAD-CBD-CGD-O2D
5	A	605	HEC	CAA-CBA-CGA-O2A
5	B	1004	HEC	CAD-CBD-CGD-O1D
5	B	1007	HEC	CAA-CBA-CGA-O2A
5	A	604	HEC	CAD-CBD-CGD-O1D
5	A	607	HEC	CAA-CBA-CGA-O2A
5	A	612	HEC	CAA-CBA-CGA-O2A
5	B	1006	HEC	CAA-CBA-CGA-O1A
5	A	610	HEC	CAA-CBA-CGA-O2A
5	B	1005	HEC	CAA-CBA-CGA-O2A
5	A	610	HEC	CAA-CBA-CGA-O1A
5	A	612	HEC	CAA-CBA-CGA-O1A
5	A	606	HEC	CAA-CBA-CGA-O1A
5	A	607	HEC	CAA-CBA-CGA-O1A
5	B	1005	HEC	CAA-CBA-CGA-O1A
5	B	1007	HEC	CAA-CBA-CGA-O1A
5	A	606	HEC	CAA-CBA-CGA-O2A
5	A	606	HEC	CAD-CBD-CGD-O1D
5	A	608	HEC	CAA-CBA-CGA-O2A
5	B	1008	HEC	CAD-CBD-CGD-O1D
5	A	609	HEC	CAD-CBD-CGD-O2D
5	B	1001	HEC	CAD-CBD-CGD-O2D
5	B	1008	HEC	CAA-CBA-CGA-O2A
5	A	606	HEC	C2A-CAA-CBA-CGA
5	A	608	HEC	CAA-CBA-CGA-O1A
5	A	609	HEC	CAD-CBD-CGD-O1D
4	A	603	BU3	O5-C2-C3-O6
5	B	1002	HEC	C1A-C2A-CAA-CBA
5	B	1001	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
5	B	1002	HEC	CAD-CBD-CGD-O2D
5	B	1008	HEC	CAA-CBA-CGA-O1A
5	B	1003	HEC	C2A-CAA-CBA-CGA
5	A	611	HEC	CAD-CBD-CGD-O2D
5	B	1002	HEC	CAD-CBD-CGD-O1D

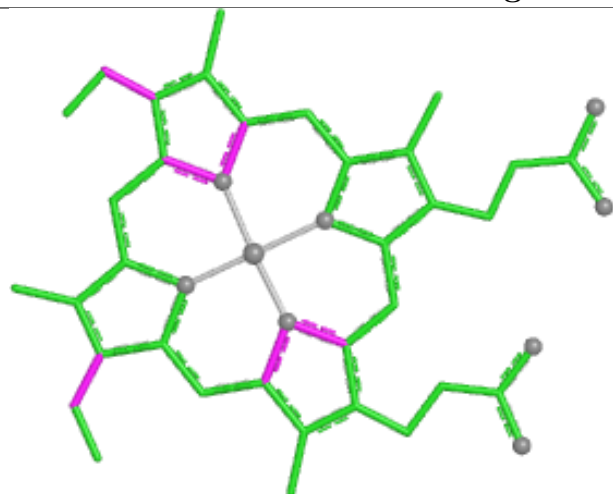
There are no ring outliers.

12 monomers are involved in 19 short contacts:

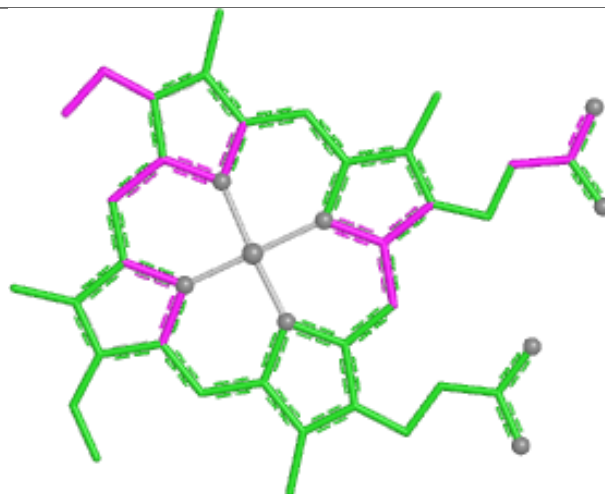
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1006	HEC	1	0
5	A	609	HEC	1	0
5	B	1009	HEC	3	0
5	B	1001	HEC	1	0
5	B	1007	HEC	1	0
5	A	605	HEC	1	0
5	A	611	HEC	1	0
5	A	610	HEC	2	0
5	B	1005	HEC	1	0
5	A	606	HEC	2	0
5	A	612	HEC	4	0
5	B	1002	HEC	1	0

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

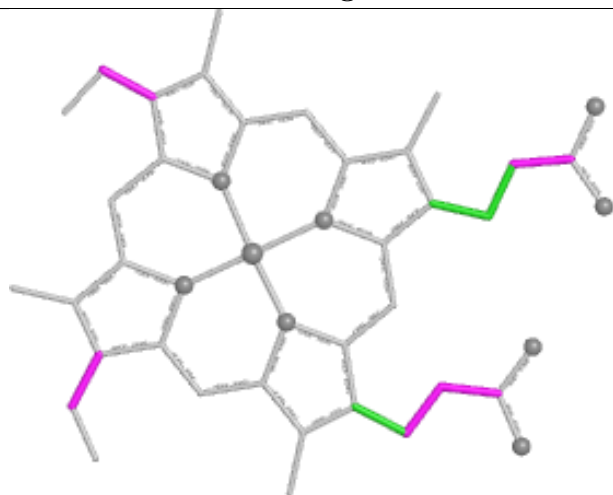
Ligand HEC B 1004



Bond lengths



Bond angles

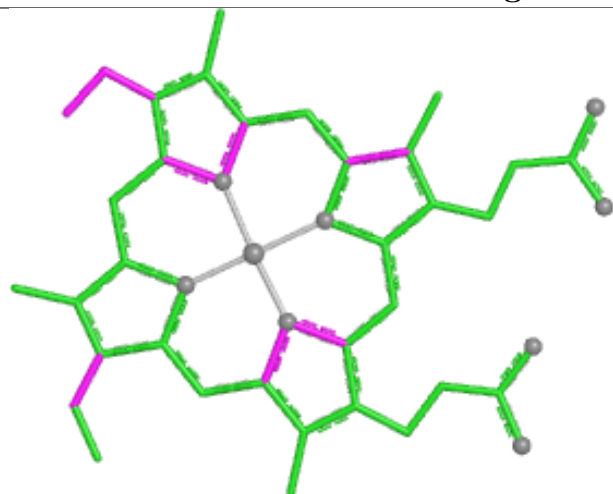


Torsions

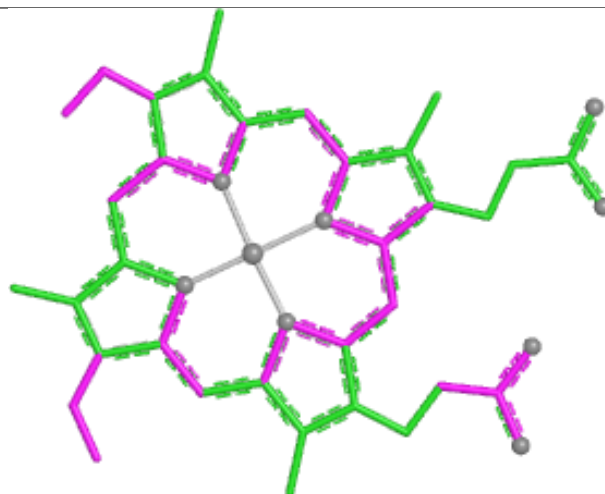


Rings

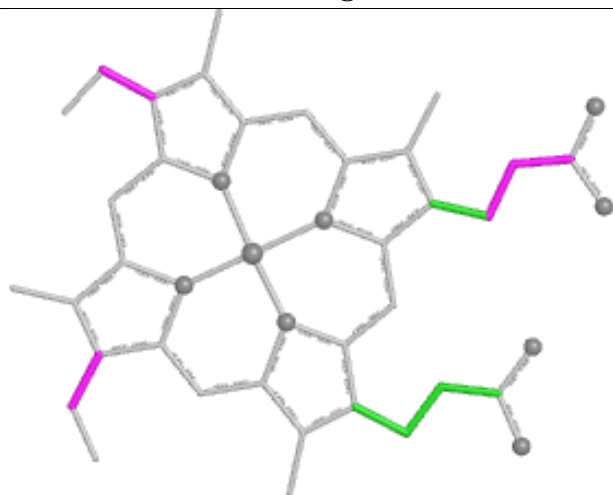
Ligand HEC B 1006



Bond lengths



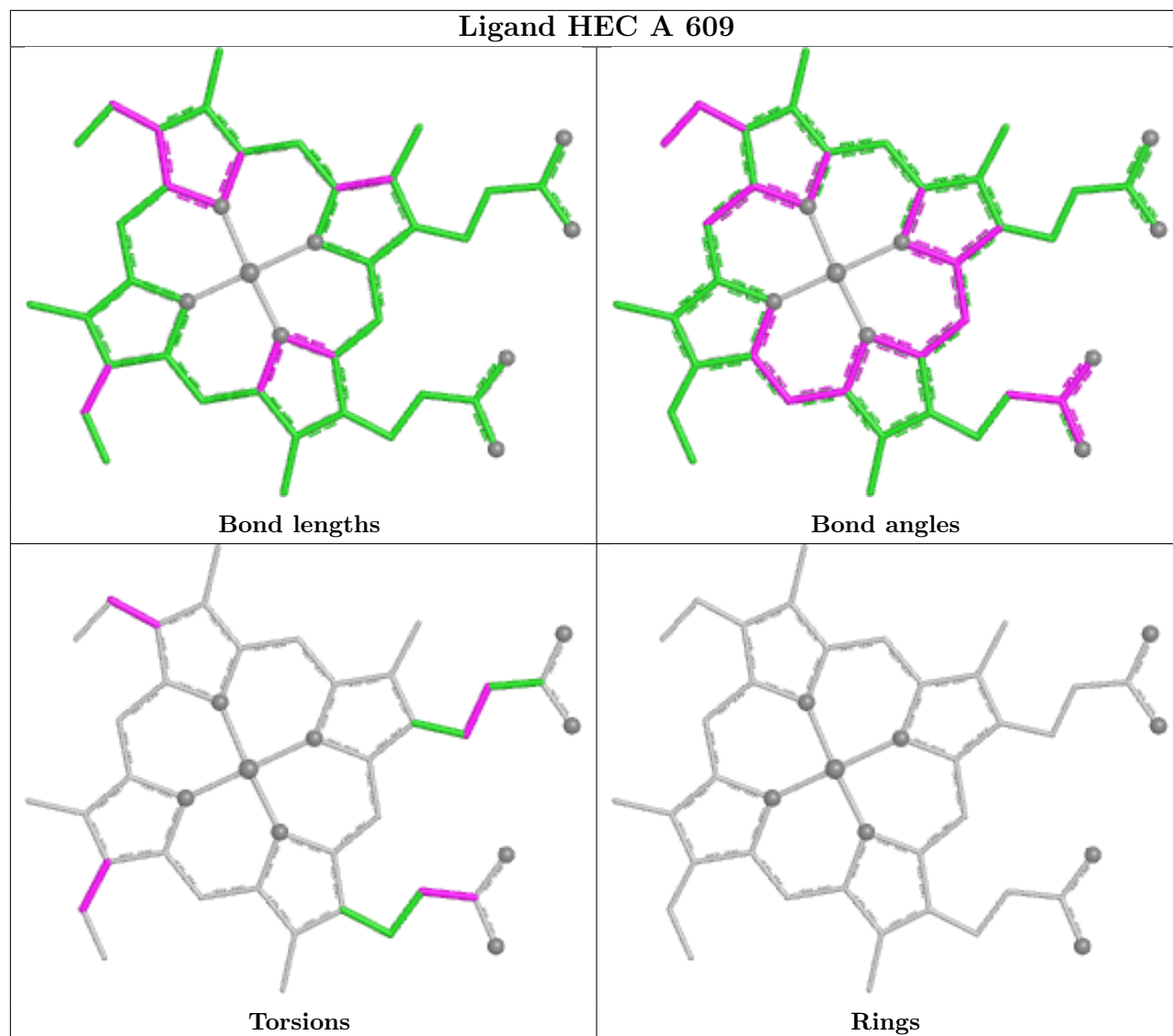
Bond angles



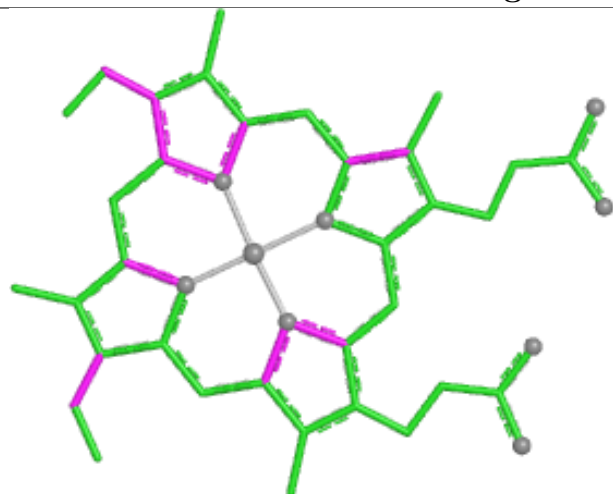
Torsions



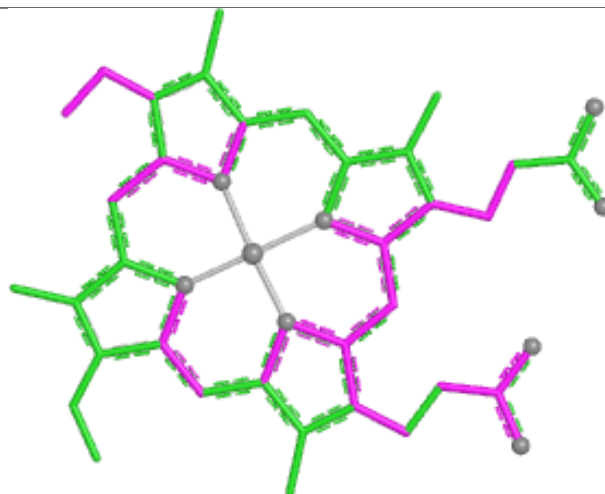
Rings



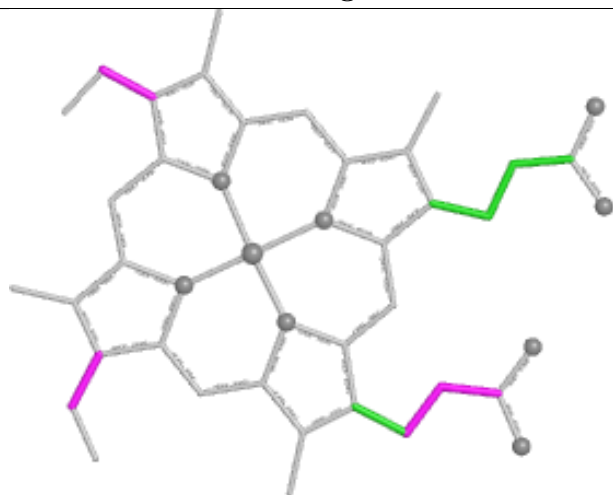
Ligand HEC B 1009



Bond lengths



Bond angles

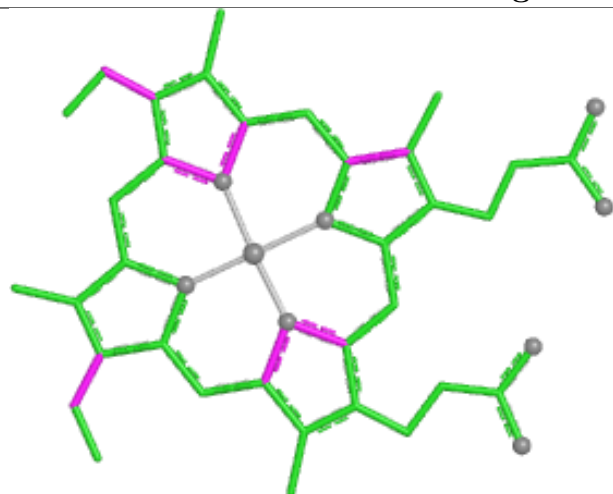


Torsions

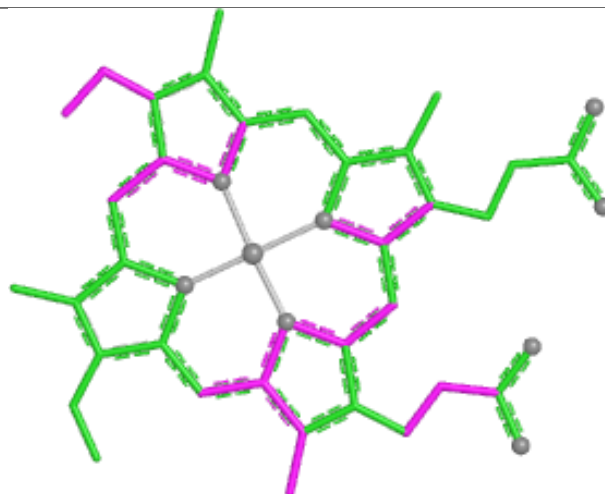


Rings

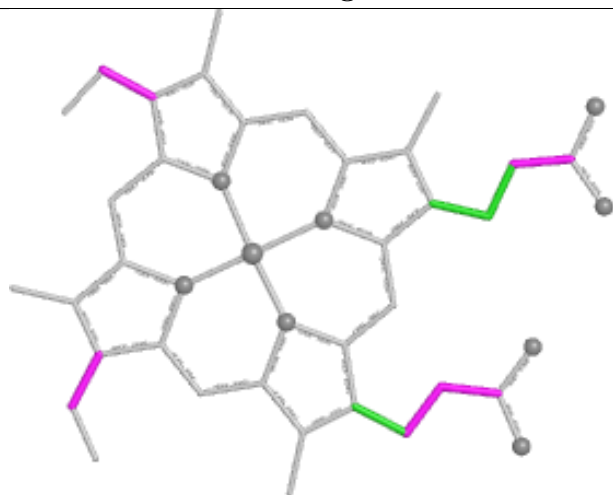
Ligand HEC A 607



Bond lengths



Bond angles

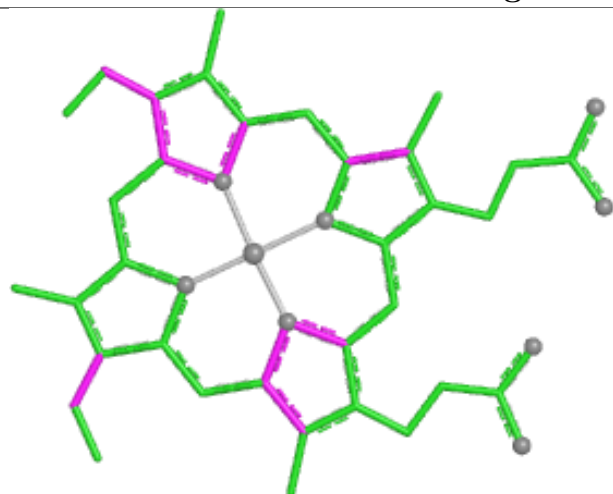


Torsions

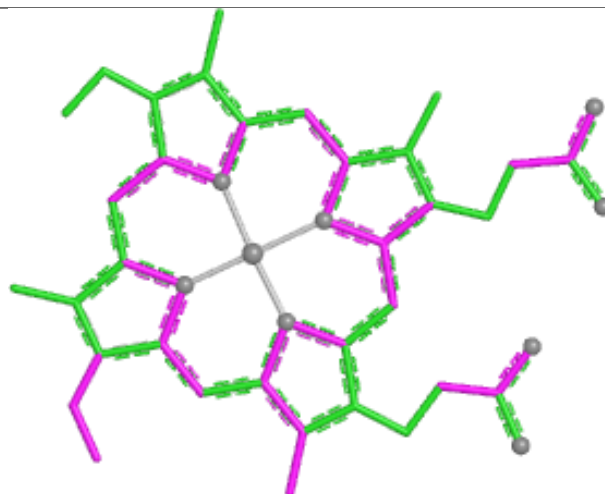


Rings

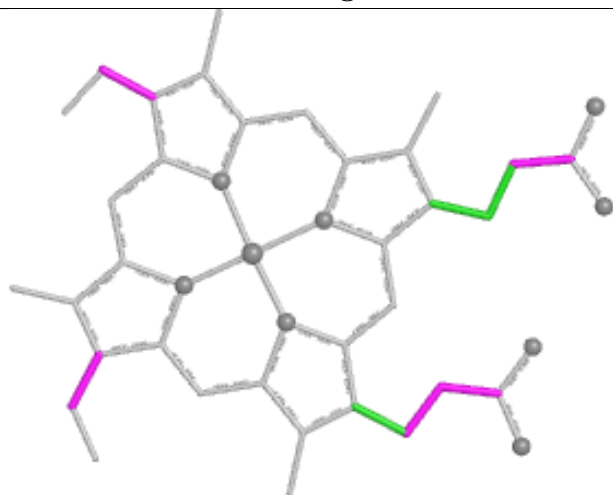
Ligand HEC B 1001



Bond lengths



Bond angles

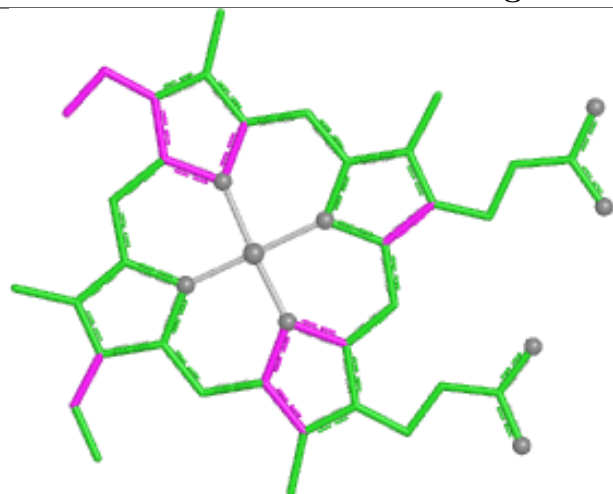


Torsions

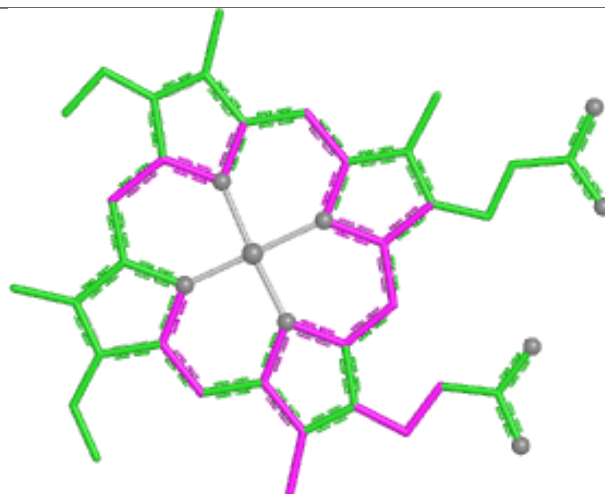


Rings

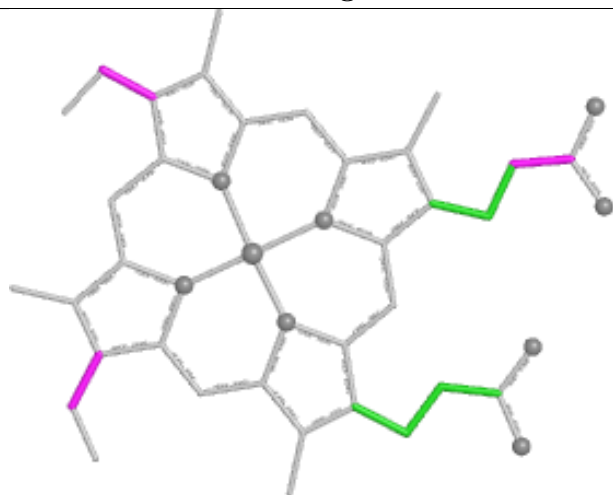
Ligand HEC B 1007



Bond lengths



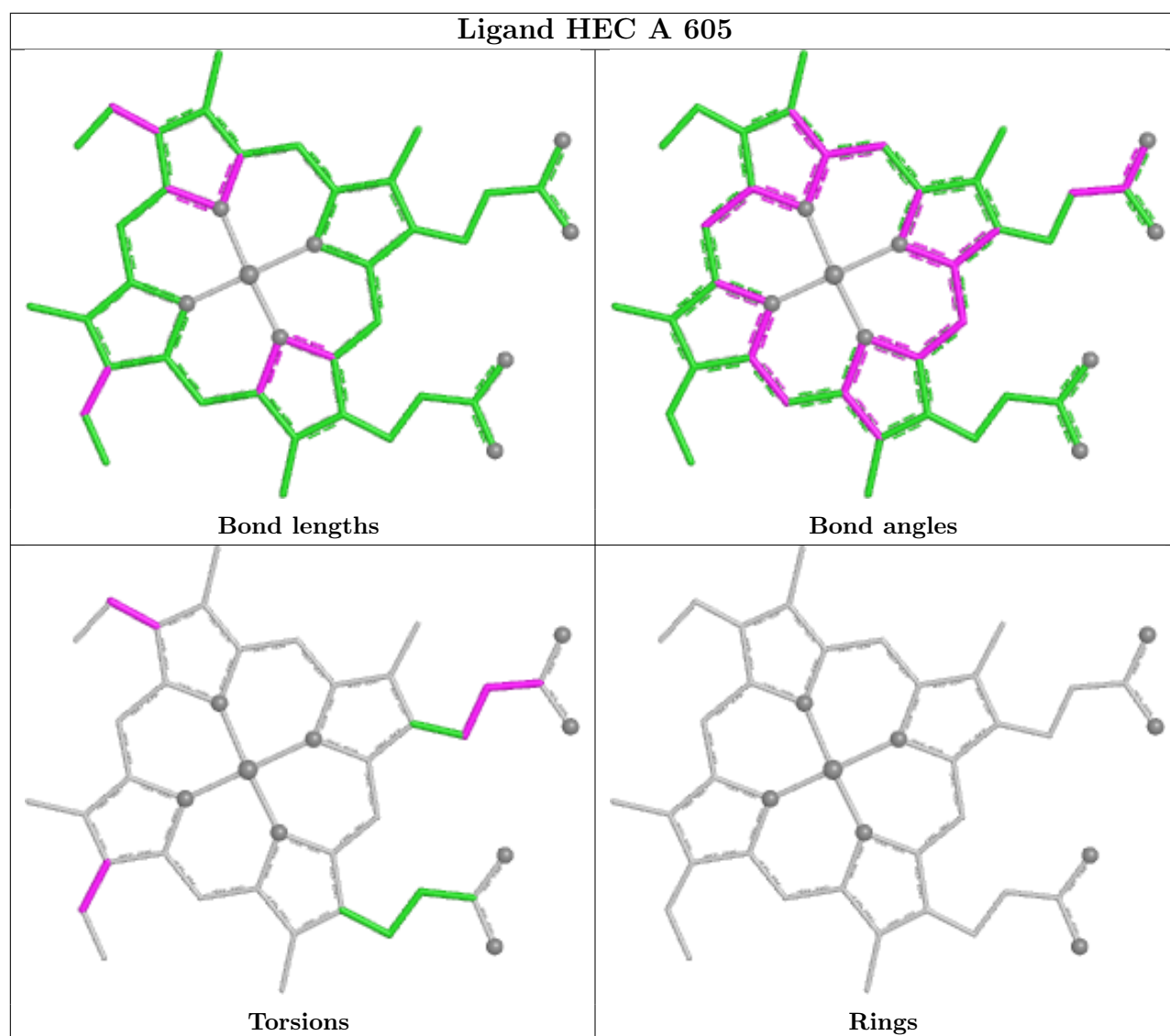
Bond angles



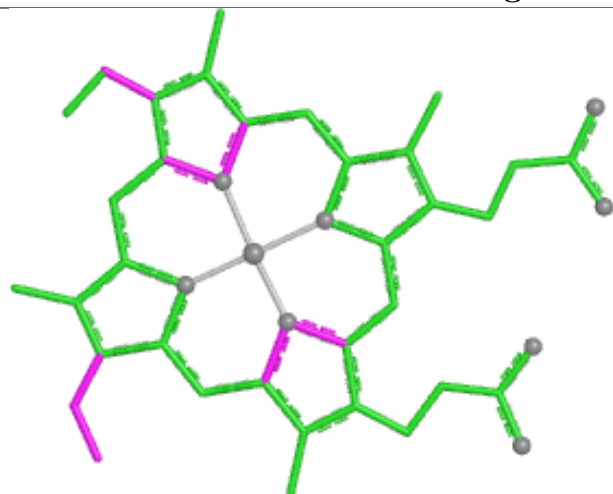
Torsions



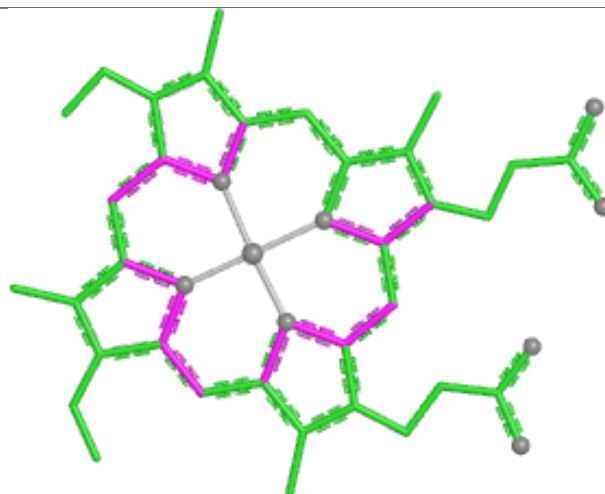
Rings



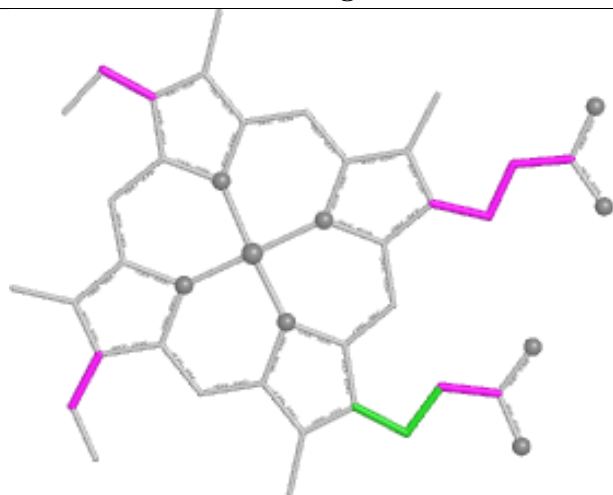
Ligand HEC B 1003



Bond lengths



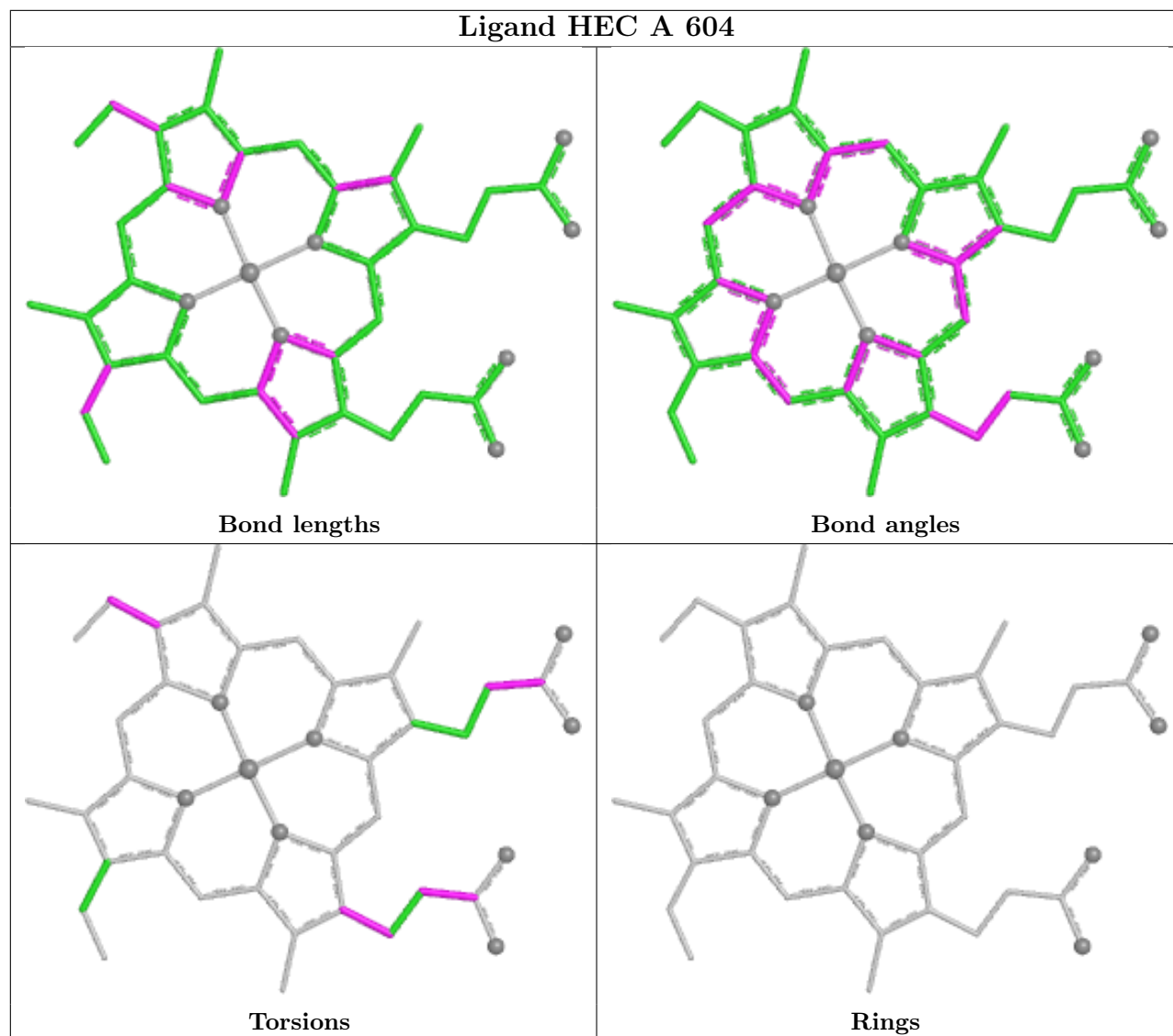
Bond angles

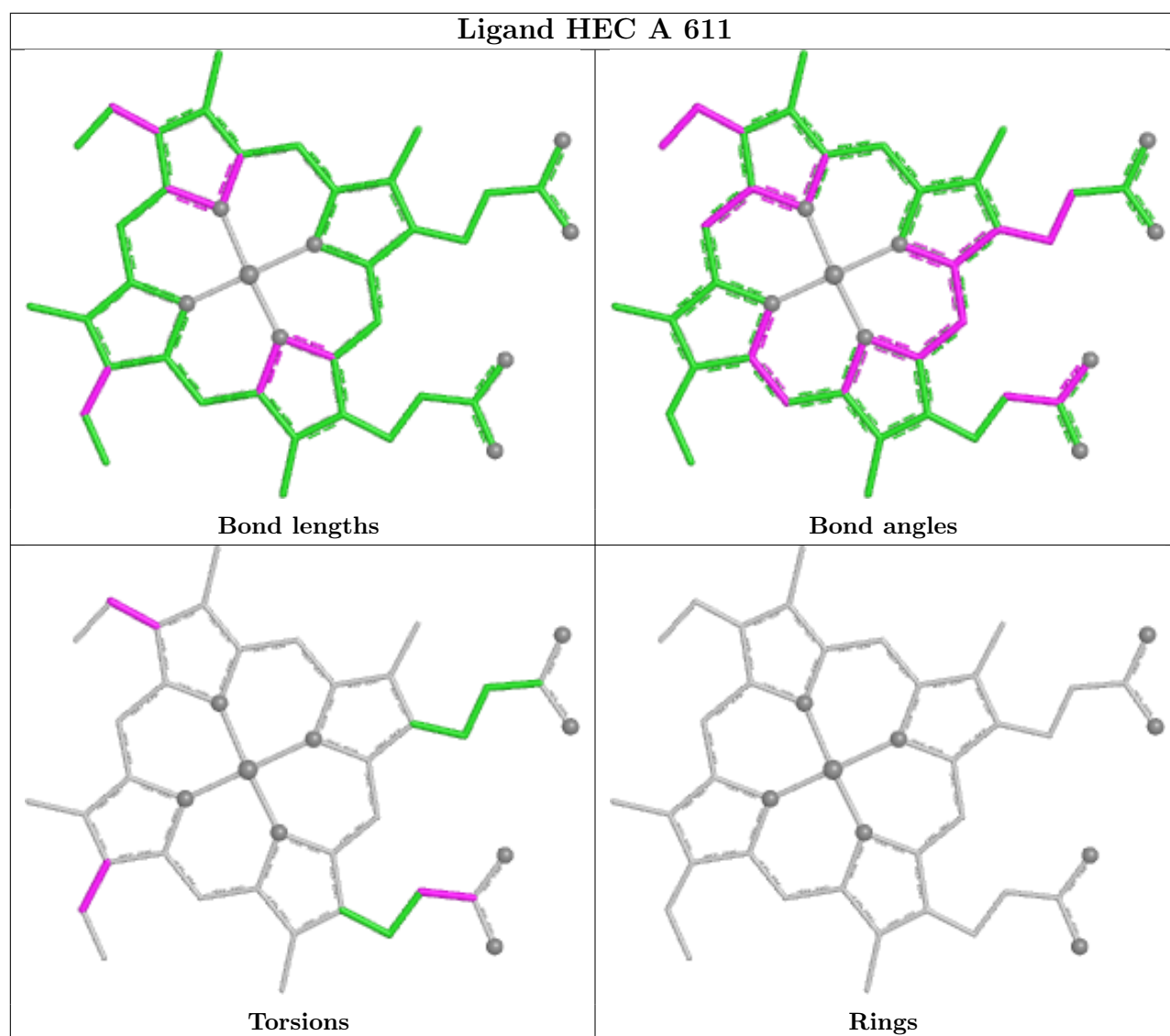


Torsions

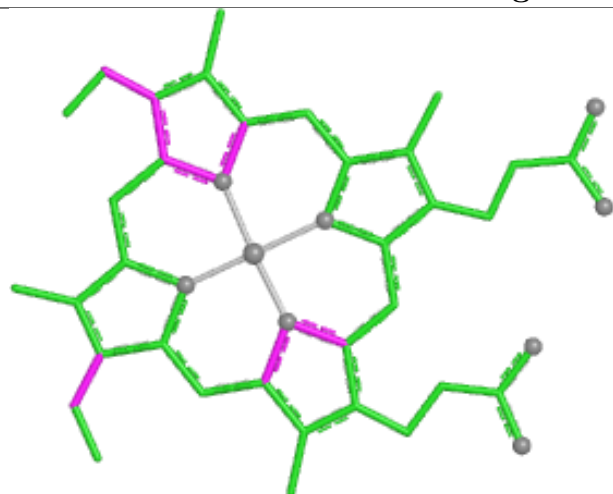


Rings

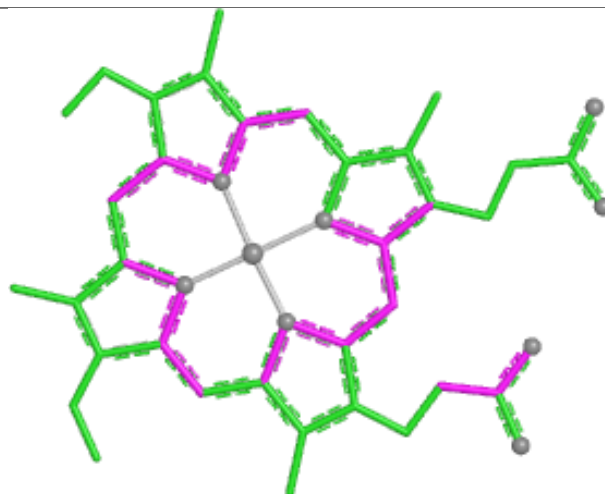




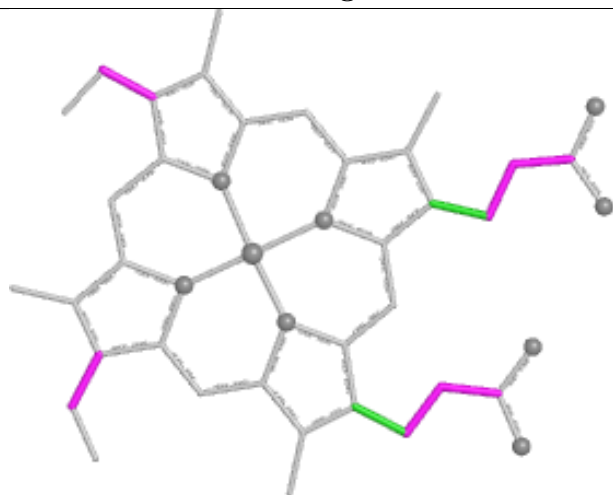
Ligand HEC A 608



Bond lengths



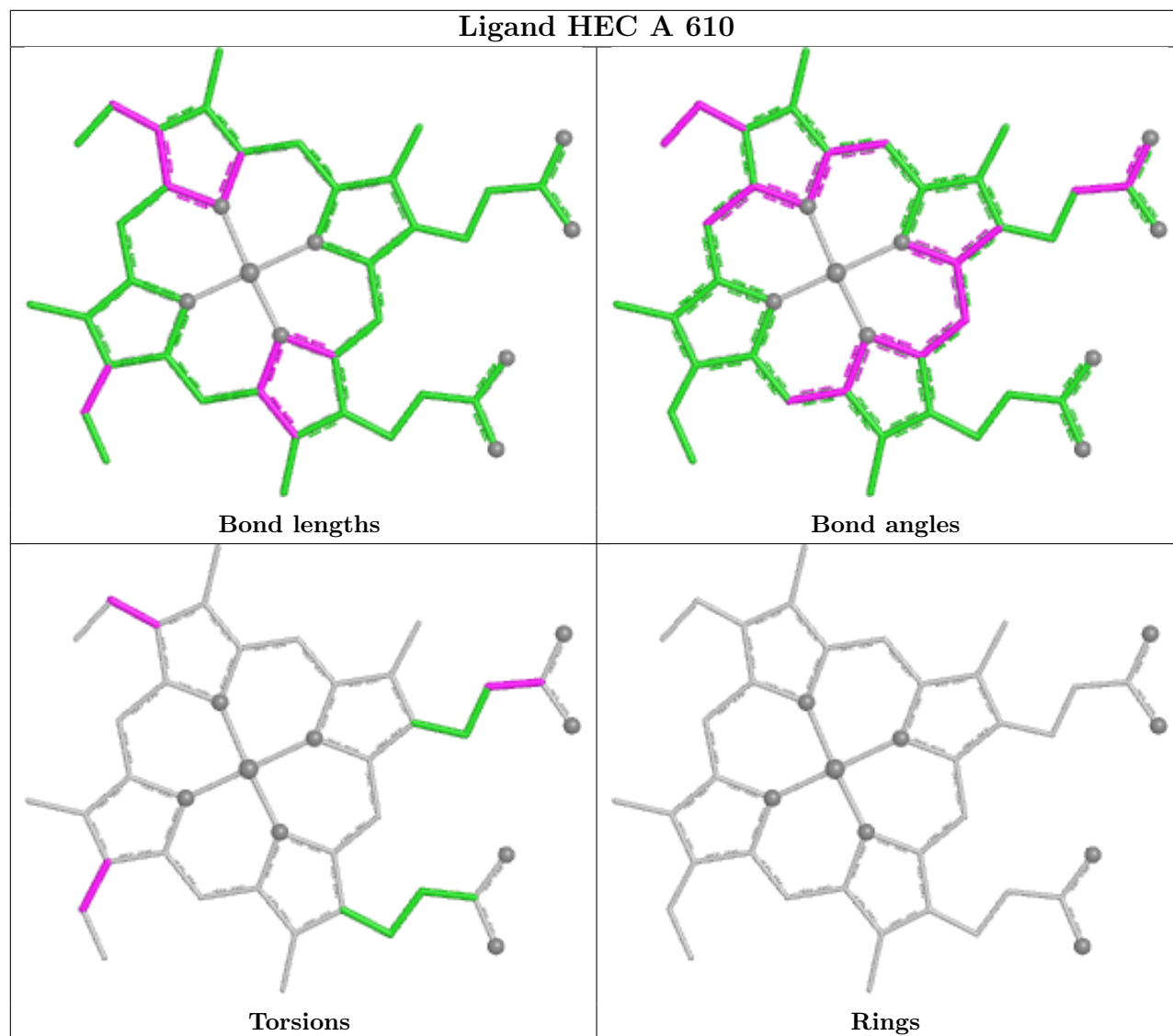
Bond angles



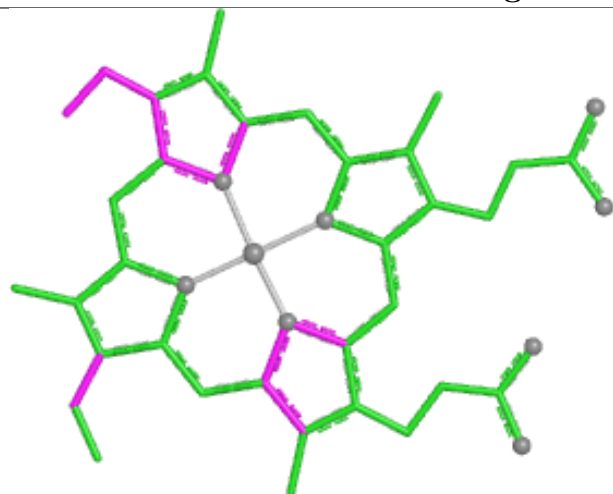
Torsions



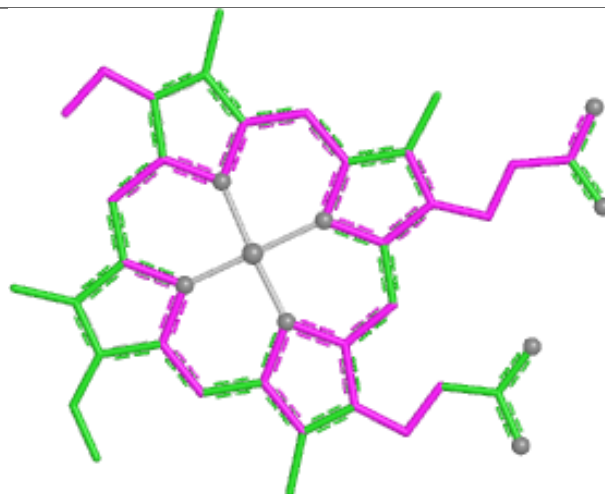
Rings



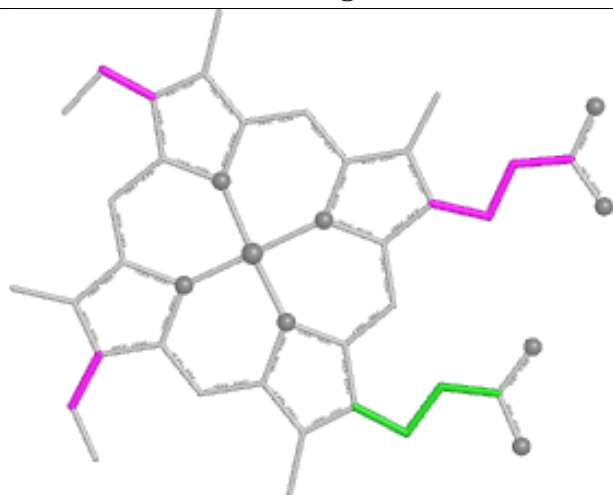
Ligand HEC B 1005



Bond lengths



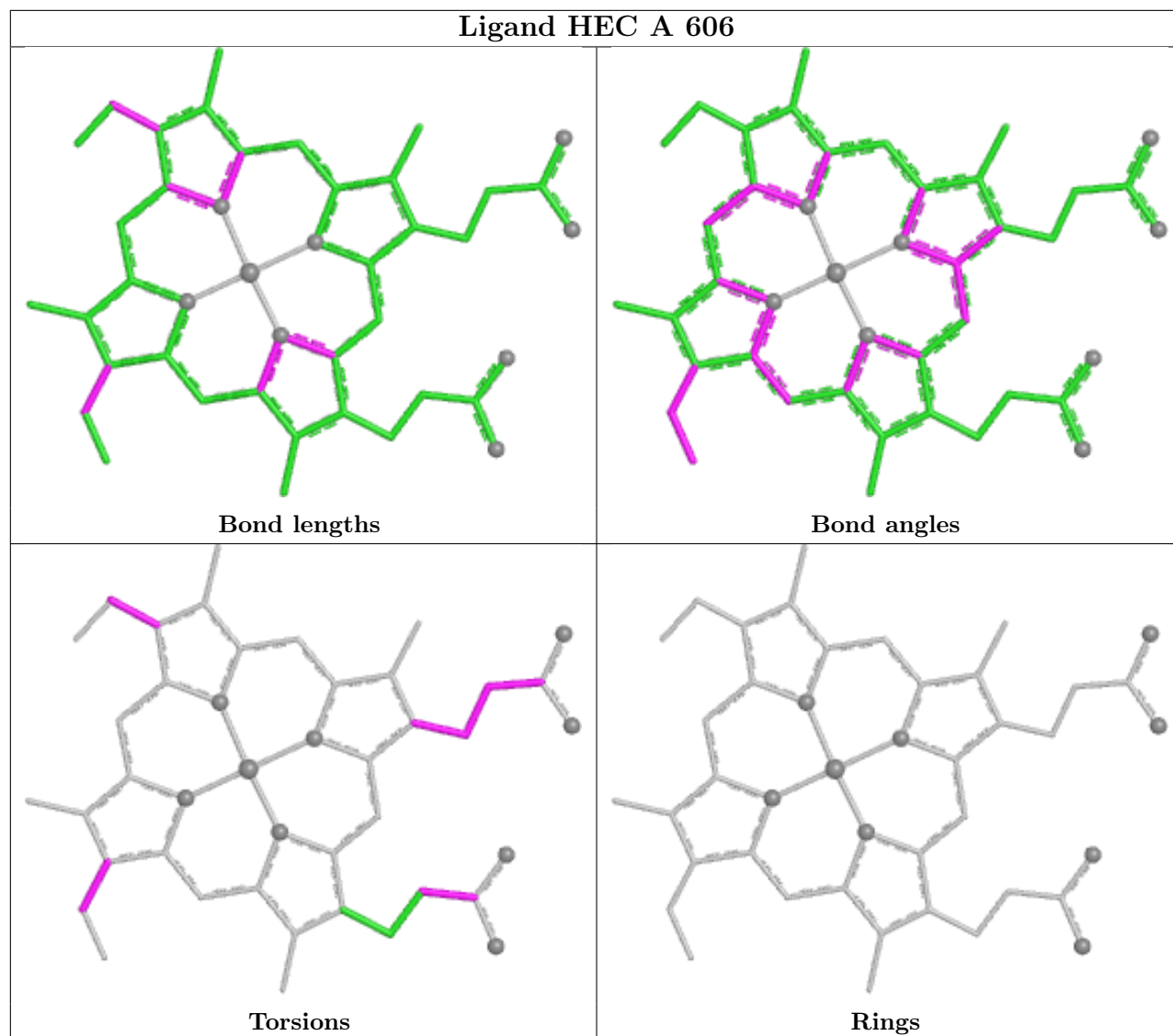
Bond angles



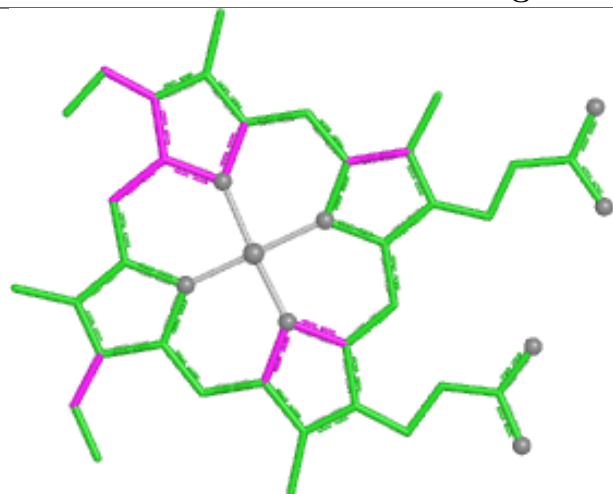
Torsions



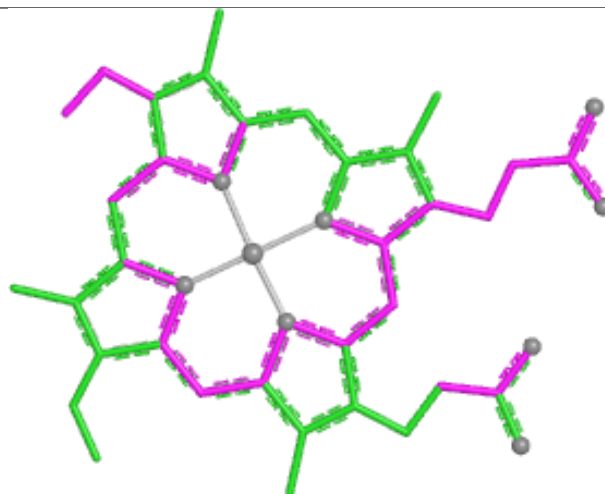
Rings



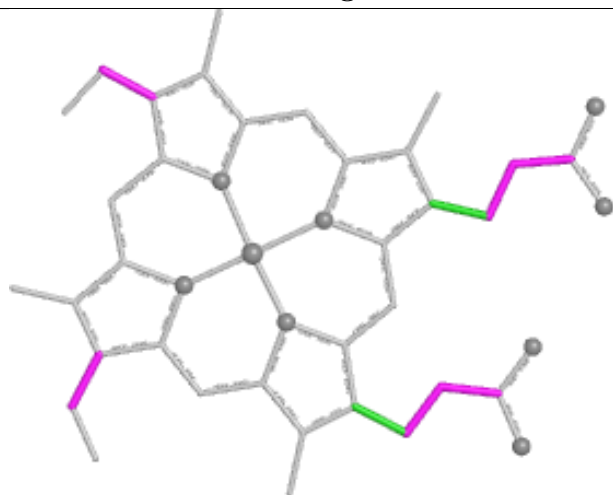
Ligand HEC A 612



Bond lengths



Bond angles

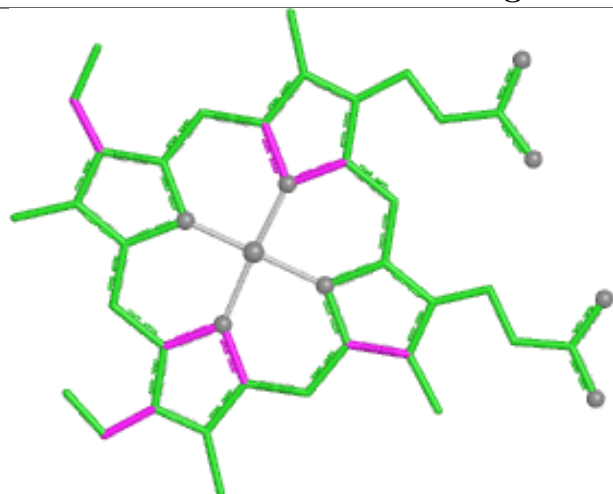


Torsions

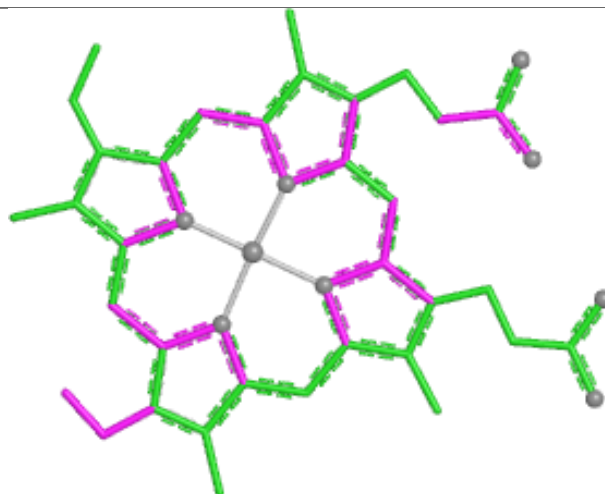


Rings

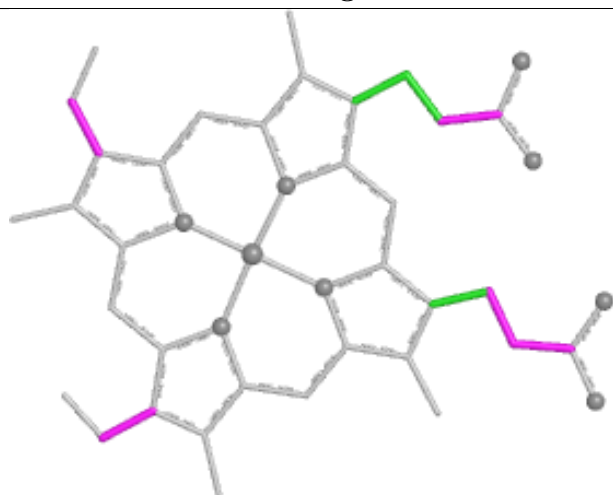
Ligand HEC B 1008



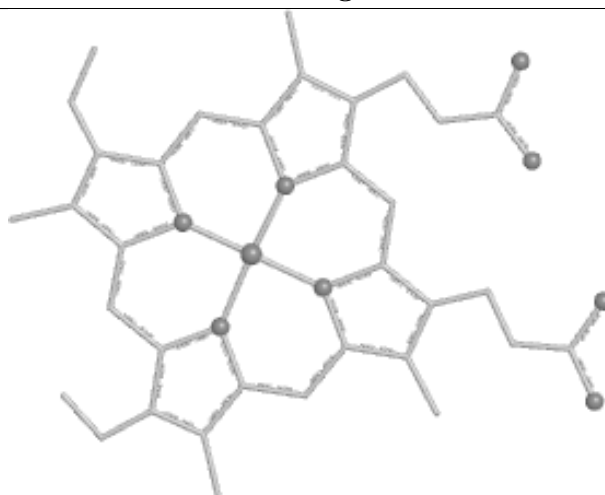
Bond lengths



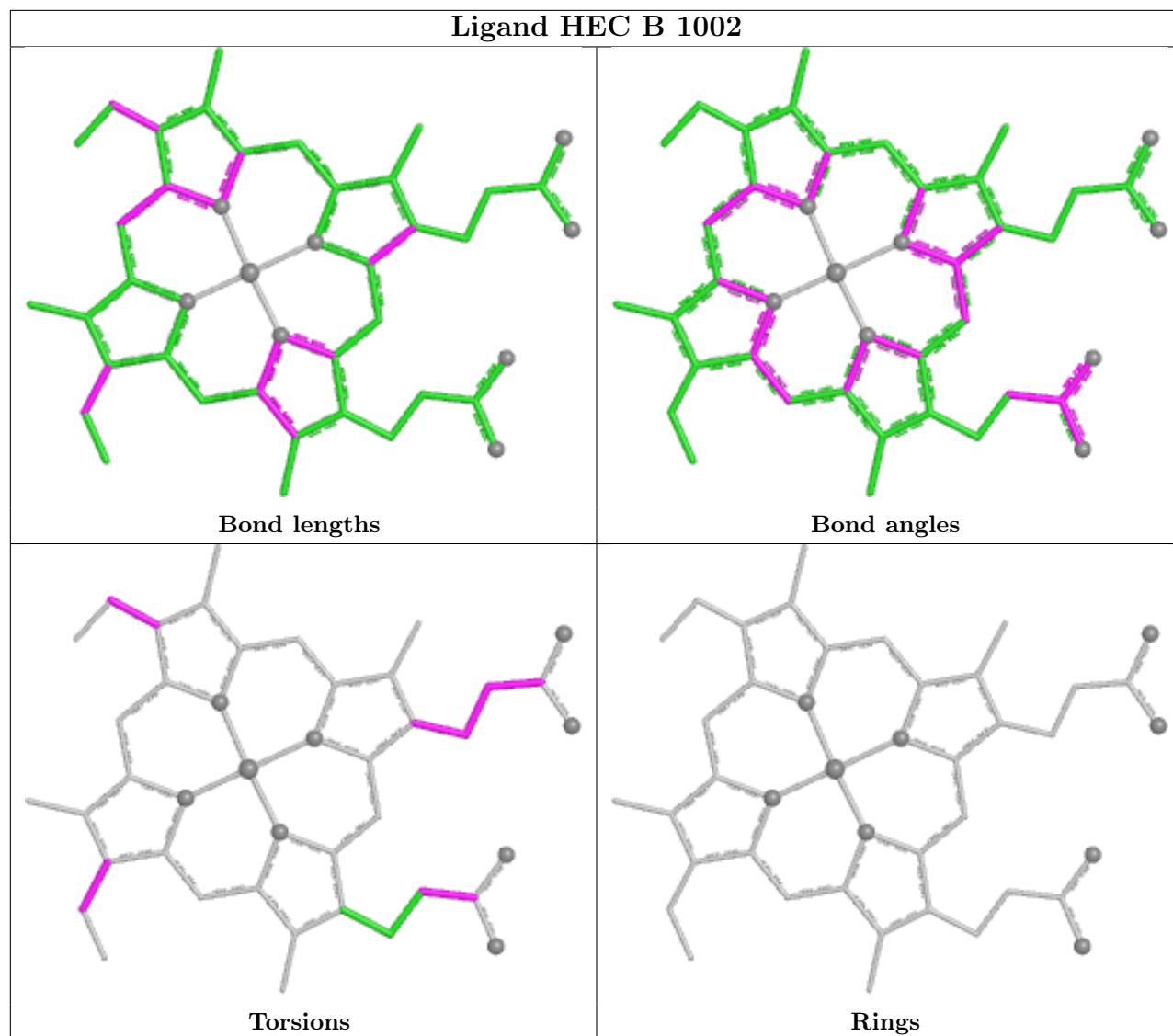
Bond angles



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	484/526 (92%)	0.13	6 (1%) 76 74	33, 56, 84, 107	0
1	B	483/526 (91%)	0.19	10 (2%) 63 60	35, 59, 94, 118	0
All	All	967/1052 (91%)	0.16	16 (1%) 69 66	33, 57, 89, 118	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	GLN	4.5
1	A	525	GLN	4.3
1	B	371	GLY	3.8
1	B	309	ARG	2.9
1	B	280	SER	2.7
1	B	394	GLY	2.6
1	A	371	GLY	2.4
1	B	43	THR	2.3
1	A	330	ASN	2.2
1	A	281	HIS	2.2
1	B	53	THR	2.2
1	B	140	GLY	2.1
1	A	306	ALA	2.1
1	B	108	PRO	2.1
1	A	201	ILE	2.0
1	B	372	GLY	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

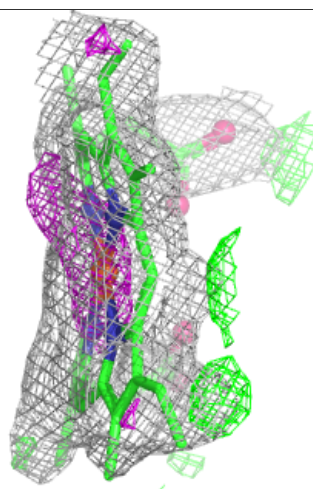
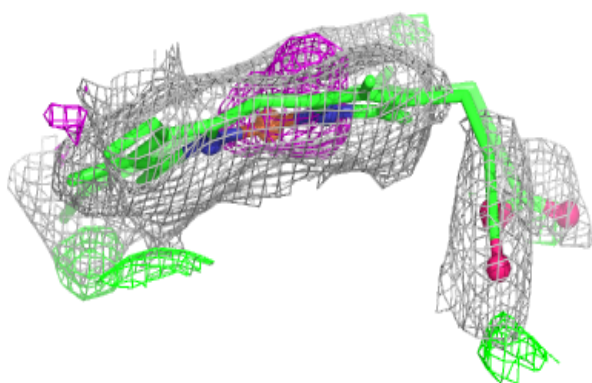
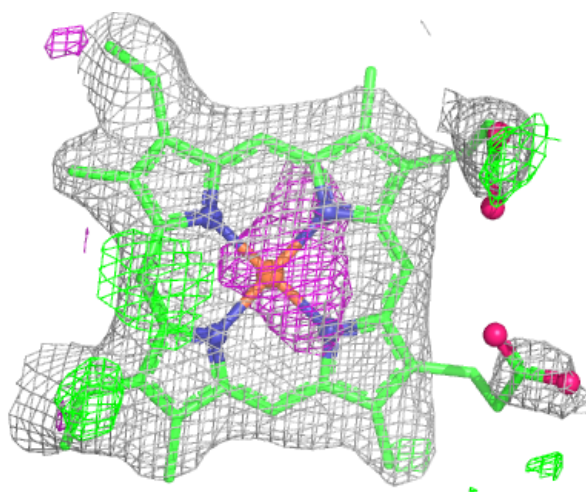
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BU3	A	603	6/6	0.83	0.18	76,79,81,84	0
2	MG	A	601	1/1	0.89	0.12	69,69,69,69	0
5	HEC	A	605	43/43	0.89	0.13	51,71,98,101	0
5	HEC	B	1002	43/43	0.91	0.13	62,81,100,104	0
5	HEC	B	1005	43/43	0.94	0.10	50,58,90,99	0
5	HEC	A	604	43/43	0.95	0.11	58,63,81,89	0
5	HEC	A	608	43/43	0.96	0.09	43,54,90,113	0
5	HEC	B	1001	43/43	0.96	0.10	61,70,93,109	0
5	HEC	A	606	43/43	0.97	0.08	43,48,68,79	0
5	HEC	A	609	43/43	0.97	0.07	30,34,52,64	0
5	HEC	A	612	43/43	0.97	0.07	37,40,53,59	0
5	HEC	B	1009	43/43	0.97	0.07	37,40,50,52	0
5	HEC	A	607	43/43	0.98	0.07	37,42,57,69	0
5	HEC	A	610	43/43	0.98	0.06	29,33,46,52	0
5	HEC	B	1003	43/43	0.98	0.07	48,52,64,75	0
5	HEC	B	1004	43/43	0.98	0.07	40,43,57,71	0
5	HEC	A	611	43/43	0.98	0.07	33,35,45,58	0
5	HEC	B	1006	43/43	0.98	0.08	34,38,57,63	0
5	HEC	B	1007	43/43	0.98	0.06	36,40,49,52	0
5	HEC	B	1008	43/43	0.98	0.07	35,39,52,69	0
3	CL	A	602	1/1	0.98	0.06	51,51,51,51	0

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

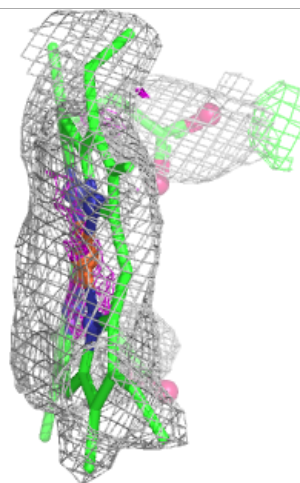
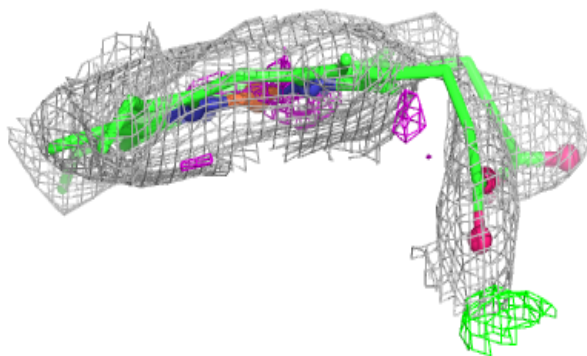
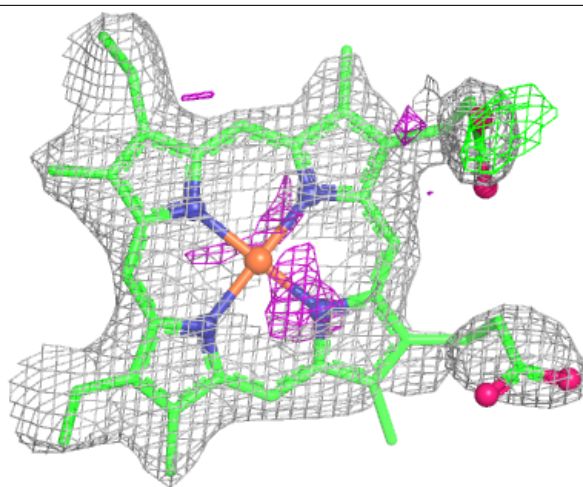
Electron density around HEC A 605:

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



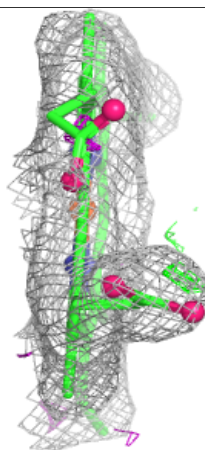
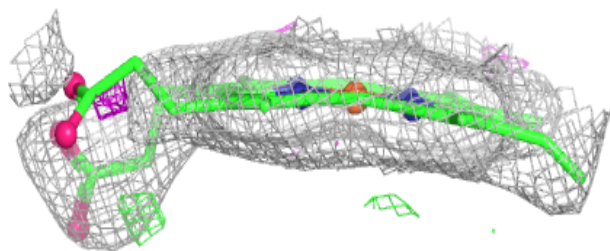
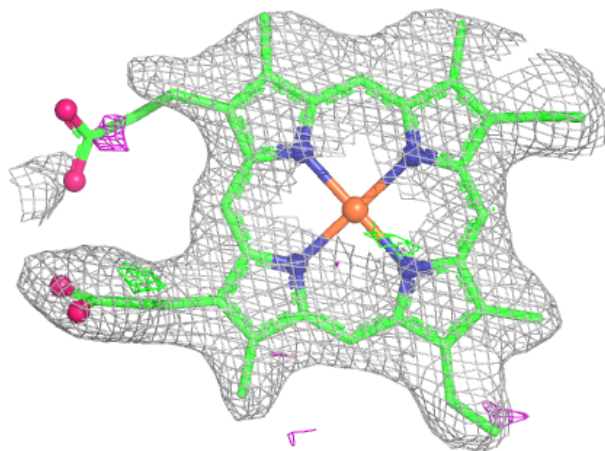
Electron density around HEC B 1002:

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



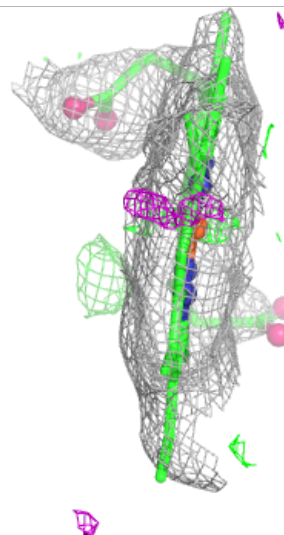
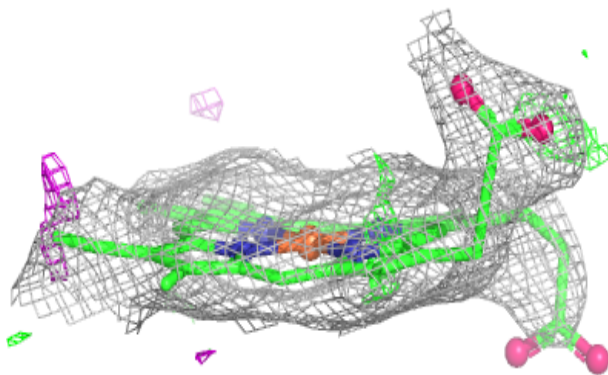
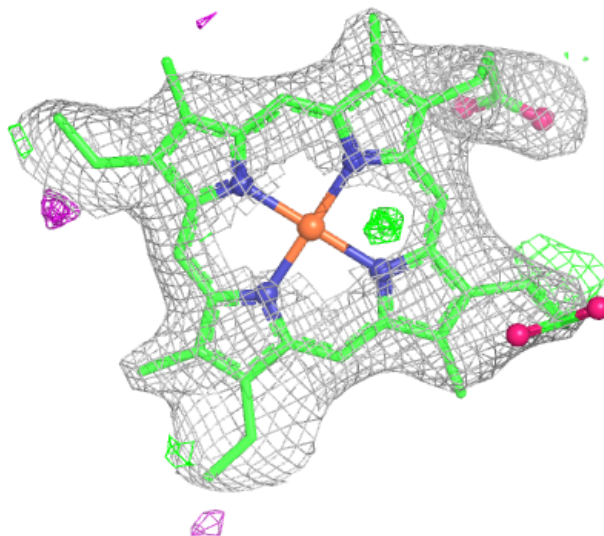
Electron density around HEC B 1005:

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and green (positive)



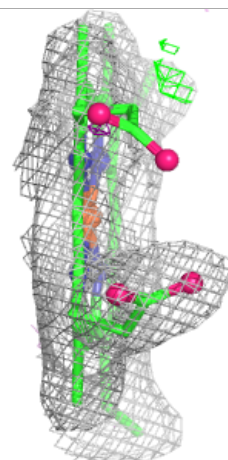
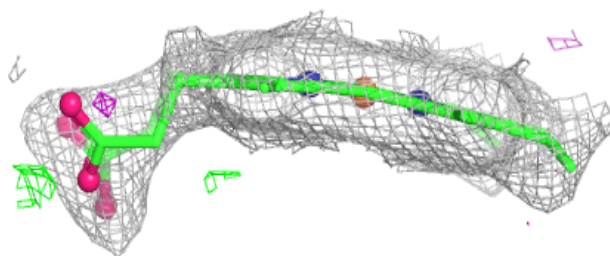
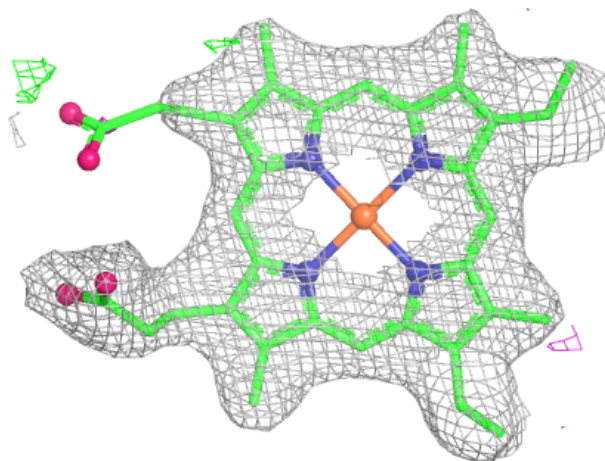
Electron density around HEC A 604:

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and green (positive)



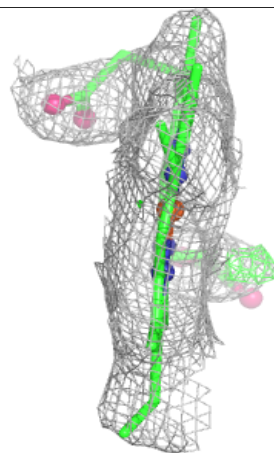
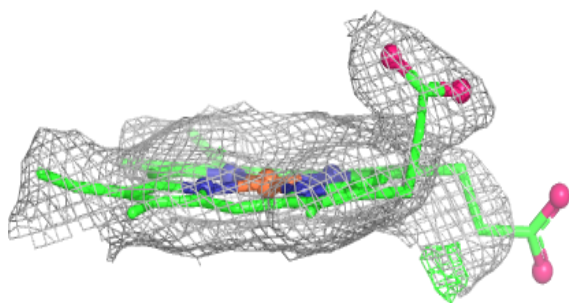
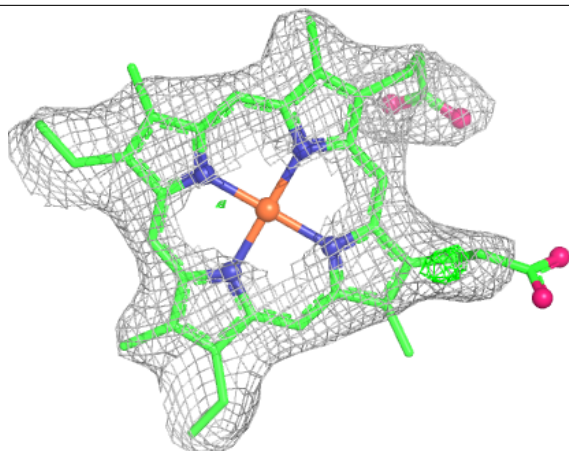
Electron density around HEC A 608:

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and green (positive)



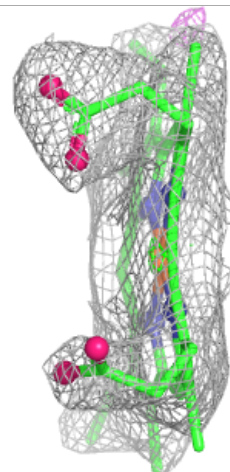
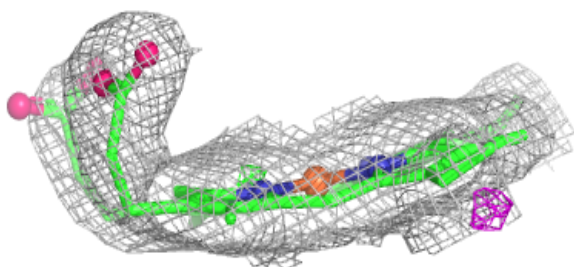
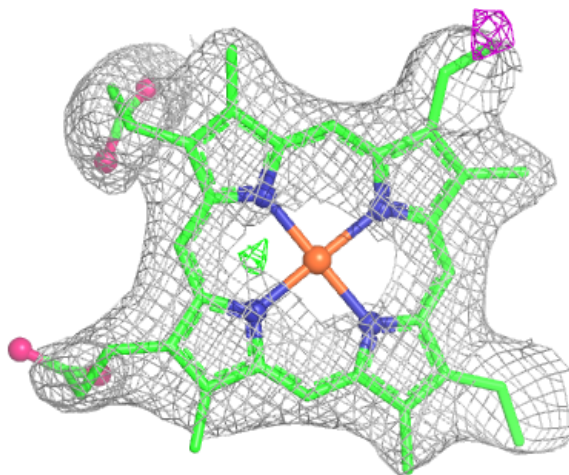
Electron density around HEC B 1001:

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and green (positive)



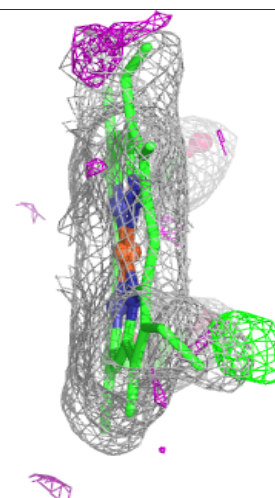
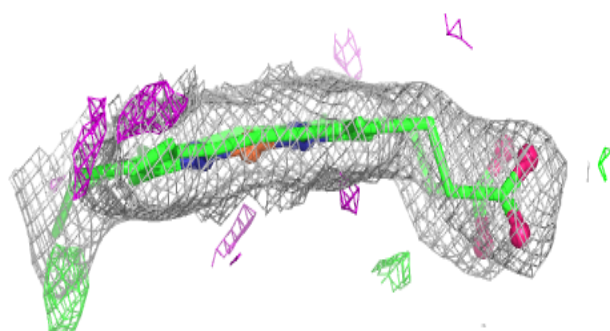
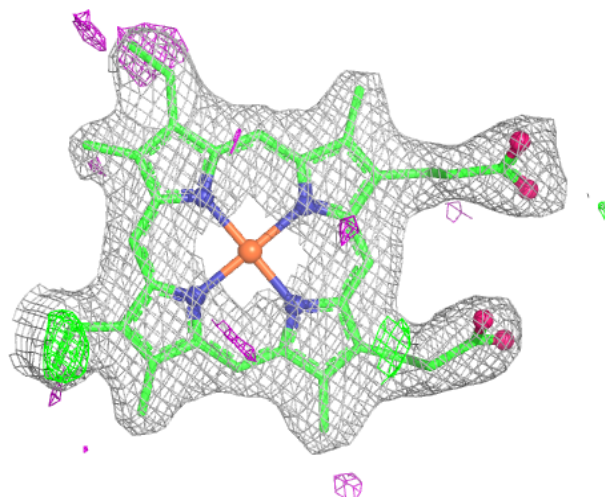
Electron density around HEC A 606:

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



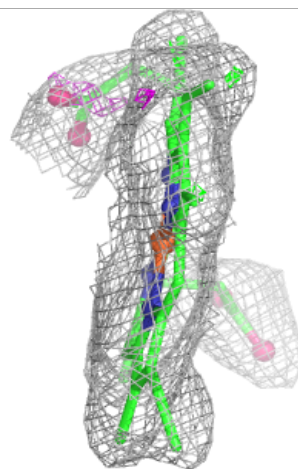
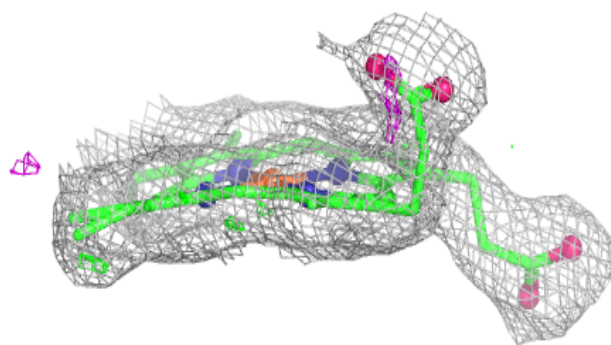
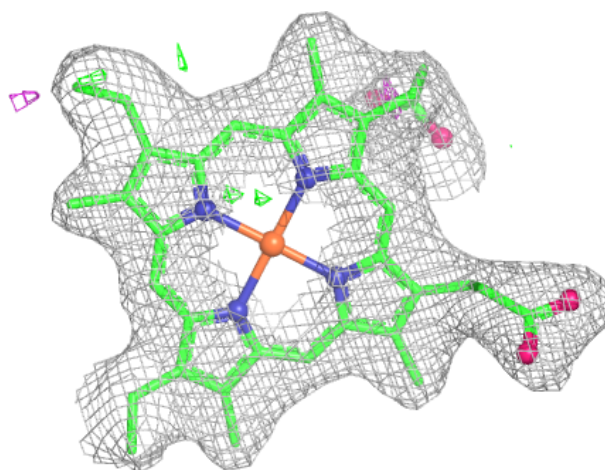
Electron density around HEC A 609:

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and green (positive)



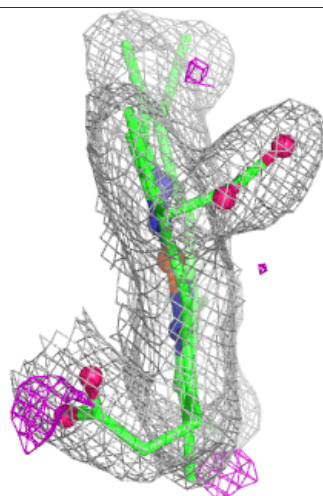
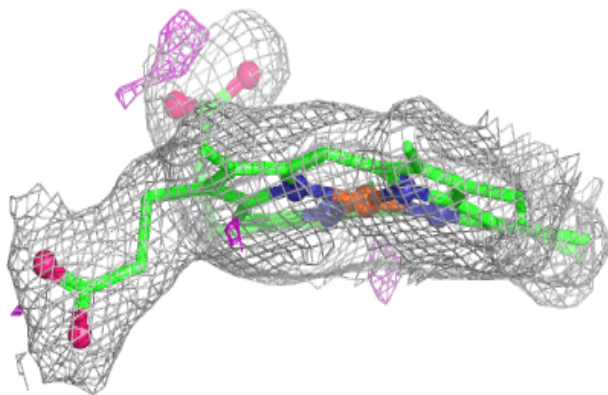
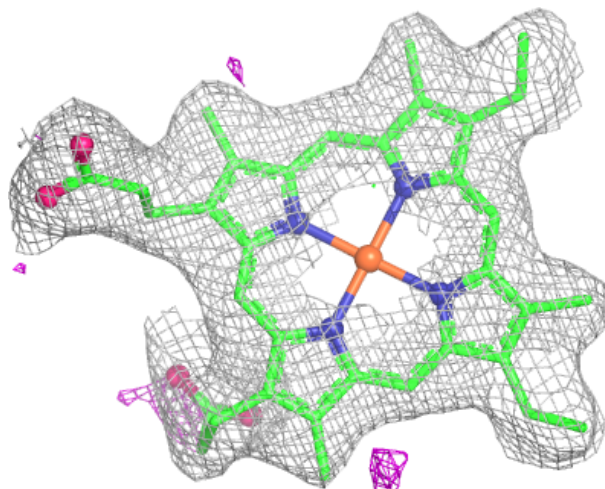
Electron density around HEC A 612:

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and green (positive)



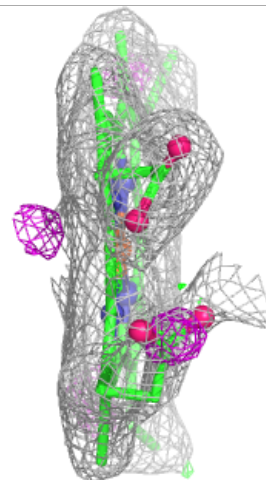
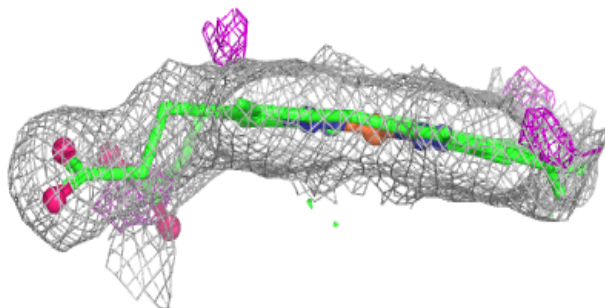
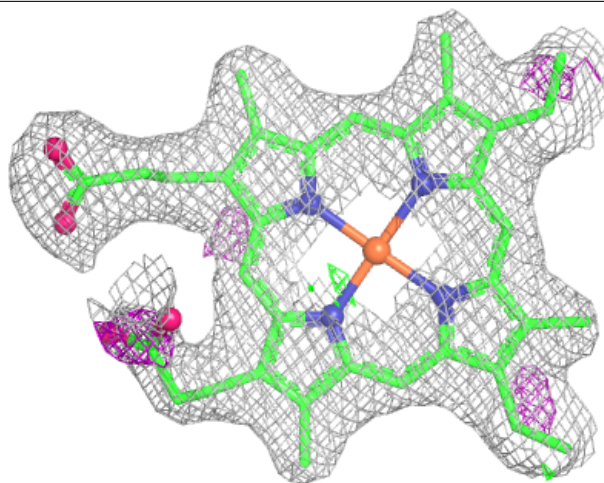
Electron density around HEC B 1009:

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



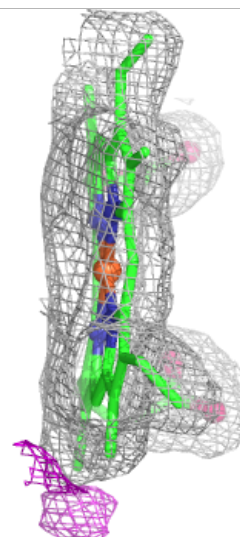
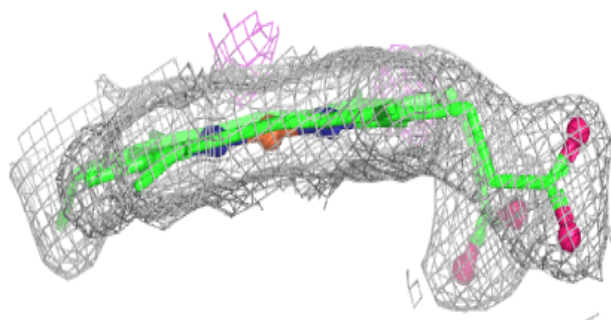
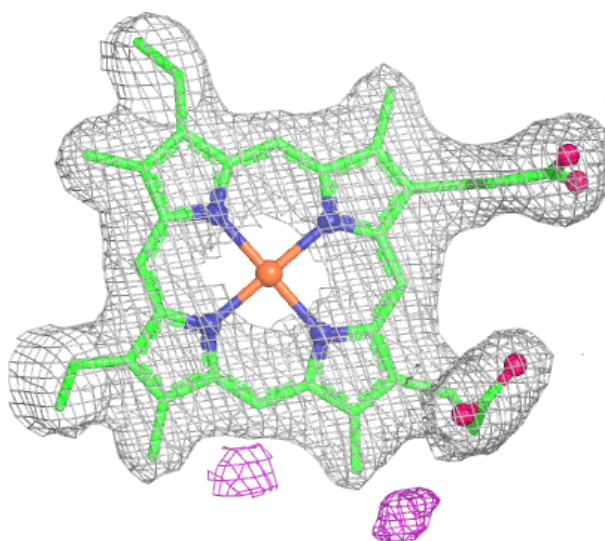
Electron density around HEC A 607:

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and green (positive)



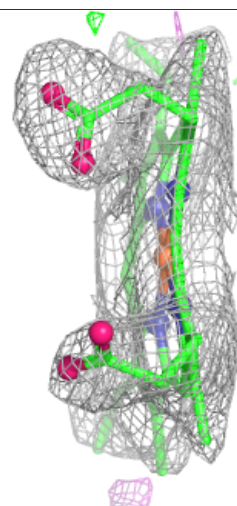
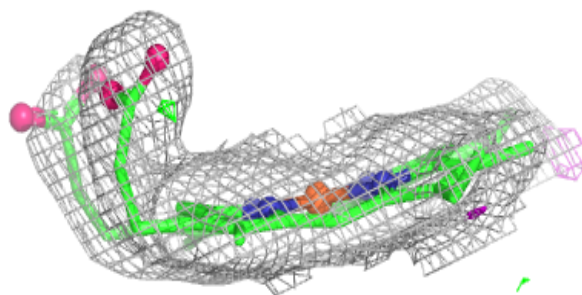
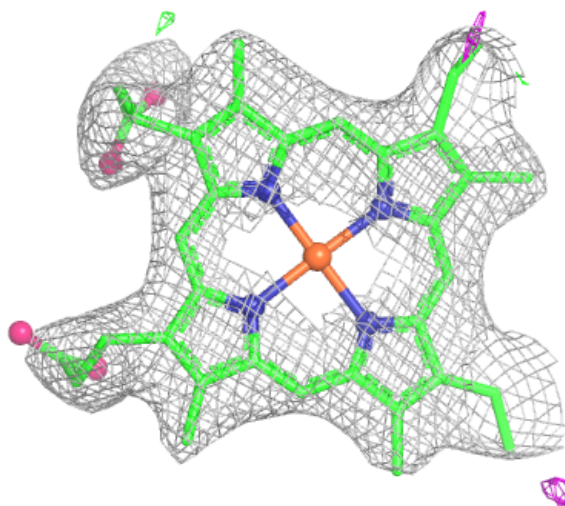
Electron density around HEC A 610:

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



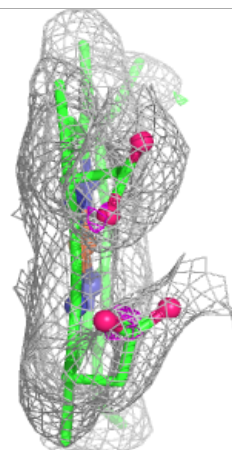
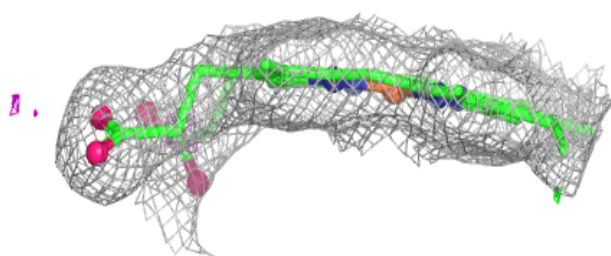
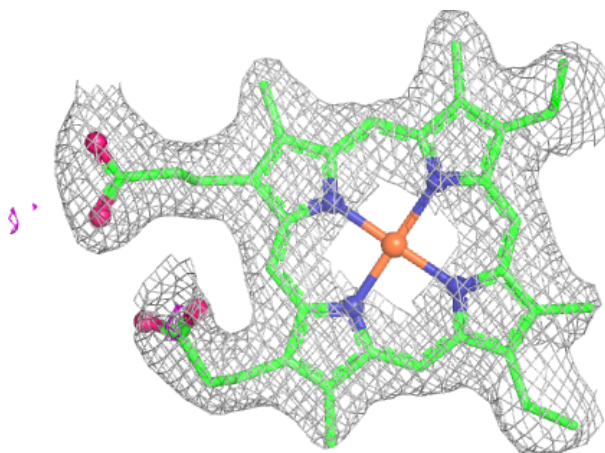
Electron density around HEC B 1003:

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



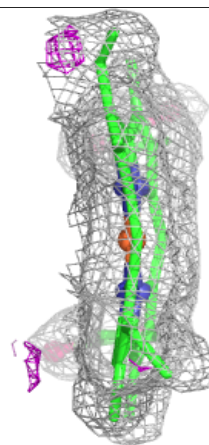
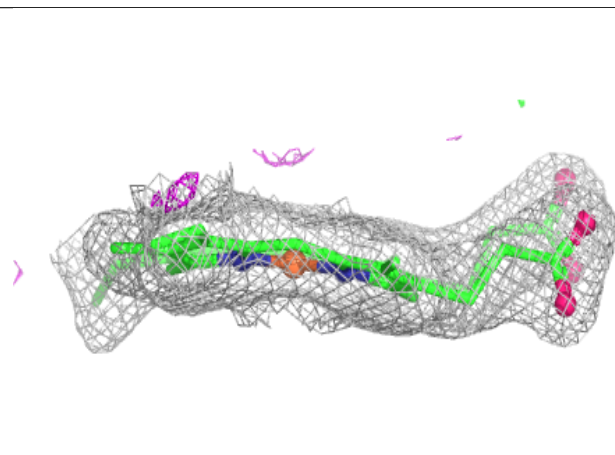
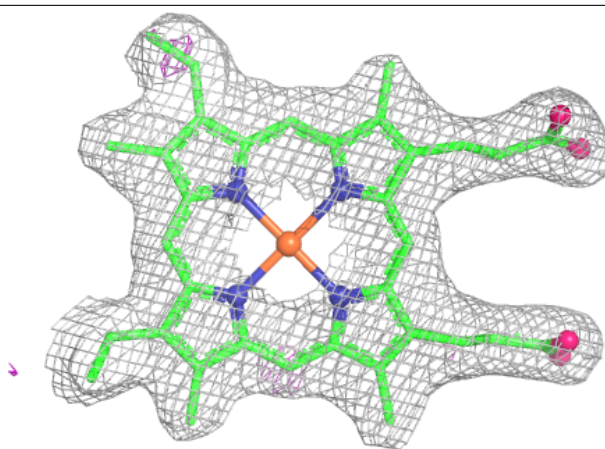
Electron density around HEC B 1004:

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



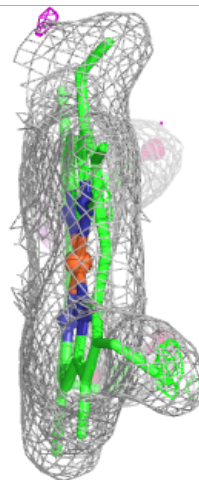
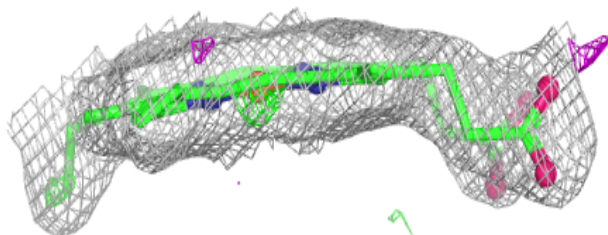
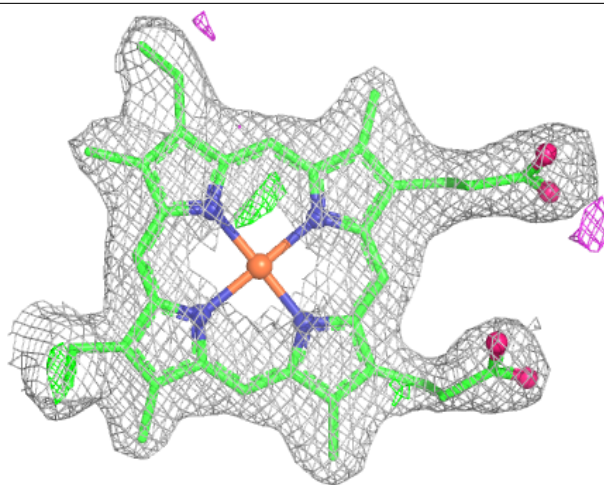
Electron density around HEC A 611:

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



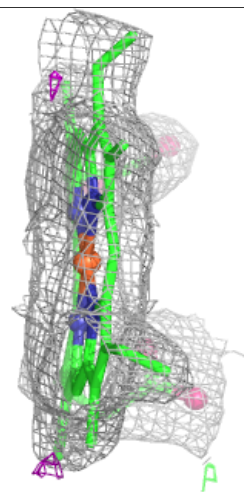
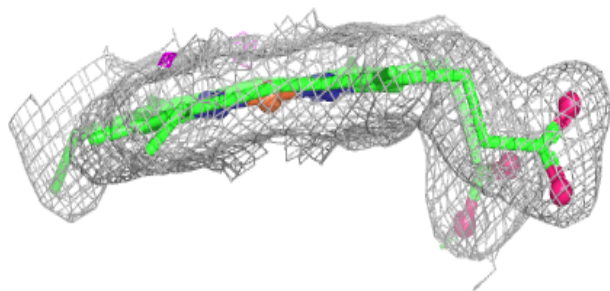
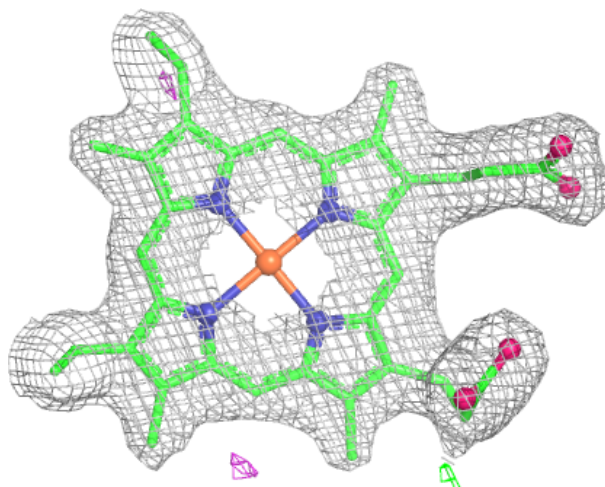
Electron density around HEC B 1006:

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



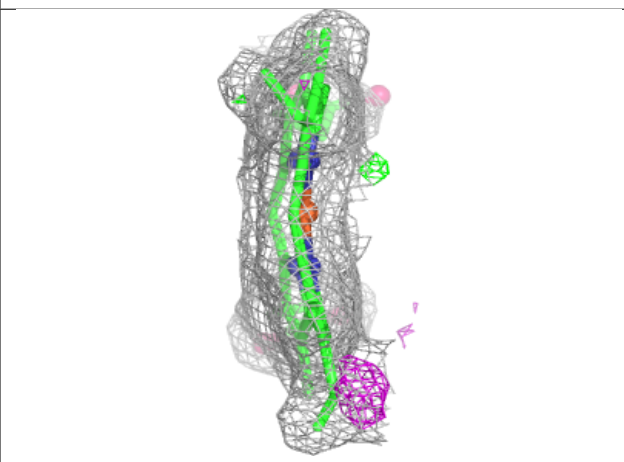
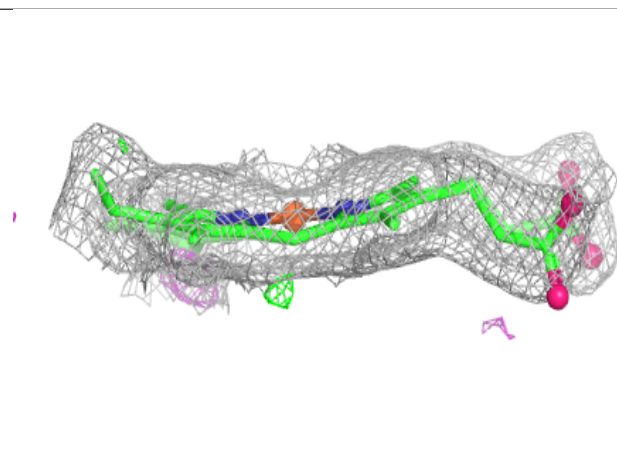
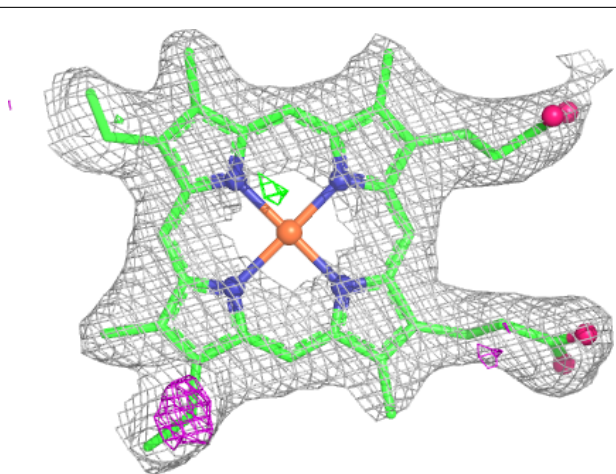
Electron density around HEC B 1007:

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



Electron density around HEC B 1008:

$2mF_o-DF_c$ (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.