



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:29 AM UTC

PDB ID : 6M0Q / pdb_00006m0q
Title : Hydroxylamine oxidoreductase from Nitrosomonas europaea
Authors : Fujiwara, T.; Fujimoto, Z.; Nishigaya, Y.; Yamazaki, T.
Deposited on : 2020-02-22
Resolution : 1.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

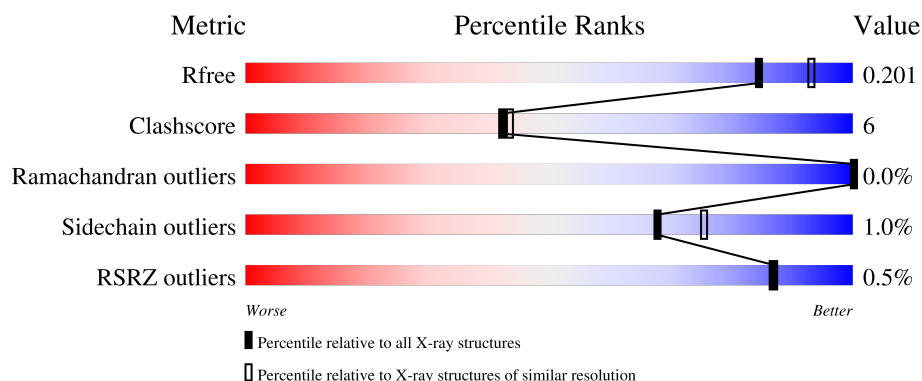
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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.



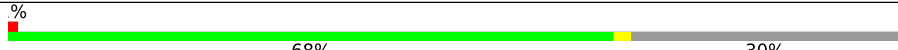
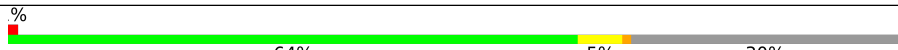
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	570	79% 9% 12%
1	C	570	% 79% 9% 12%
1	E	570	79% 10% 12%
1	G	570	81% 8% 12%
1	I	570	% 78% 10% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	570	
2	B	91	
2	D	91	
2	F	91	
2	H	91	
2	J	91	
2	L	91	

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
6	PGE	G	611	-	-	X	-
6	PGE	I	609	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31763 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.

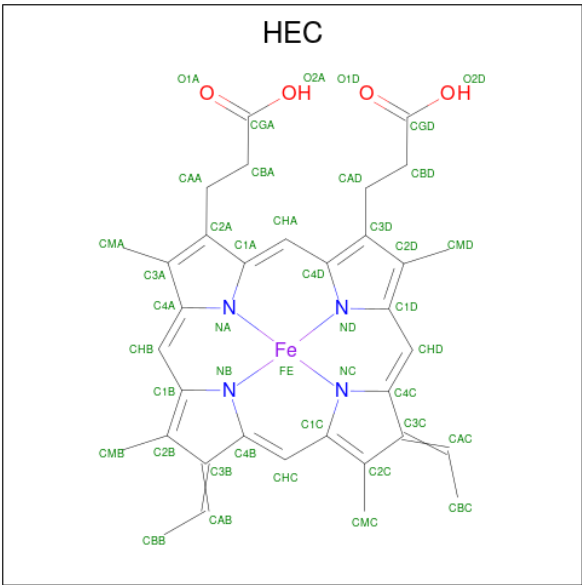
- Molecule 1 is a protein called Aerobic hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	E	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	G	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	I	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	K	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	D	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	F	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	H	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	J	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	L	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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	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	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
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

Continued on next page...

Continued from previous page...

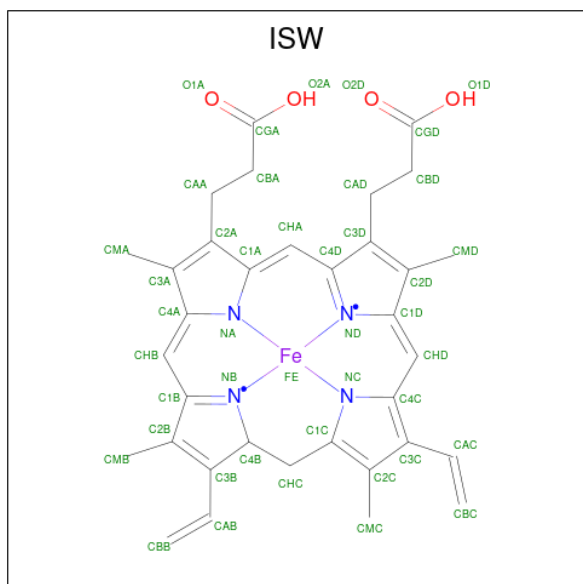
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is {3,3'-[(9S)-8,13-diethenyl-3,7,12,17-tetramethyl-9,10-dihydroporphyrin-2,18-diyl-kappa 4 N 21 ,N 22 ,N 23 ,N 24]dipropanoato(2-)}iron (CCD ID: ISW) (formula: C₃₄H₃₄FeN₄O₄).



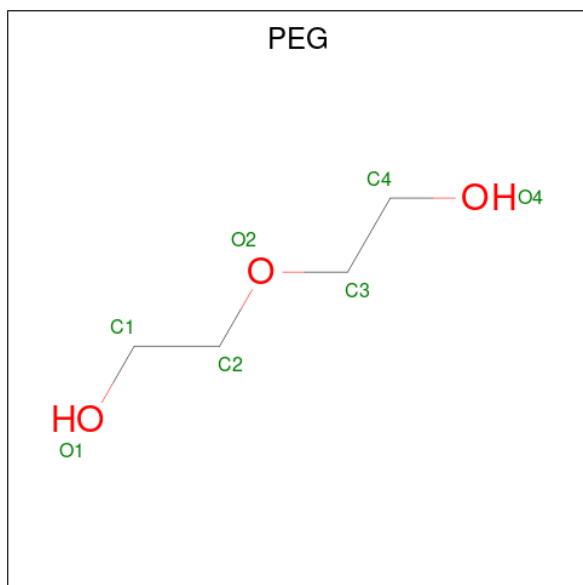
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

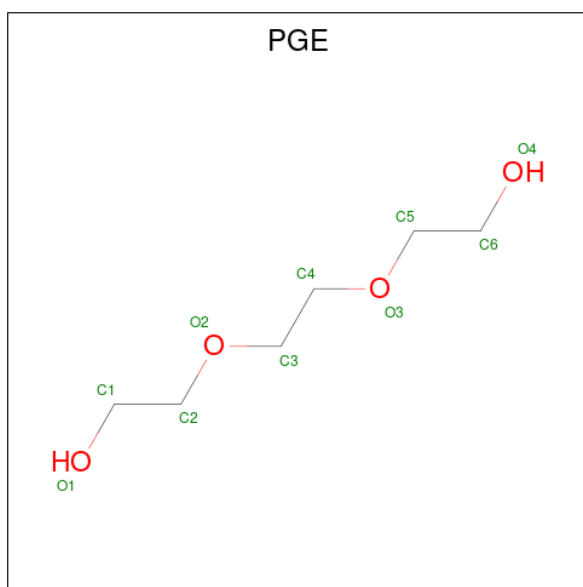
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	I	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



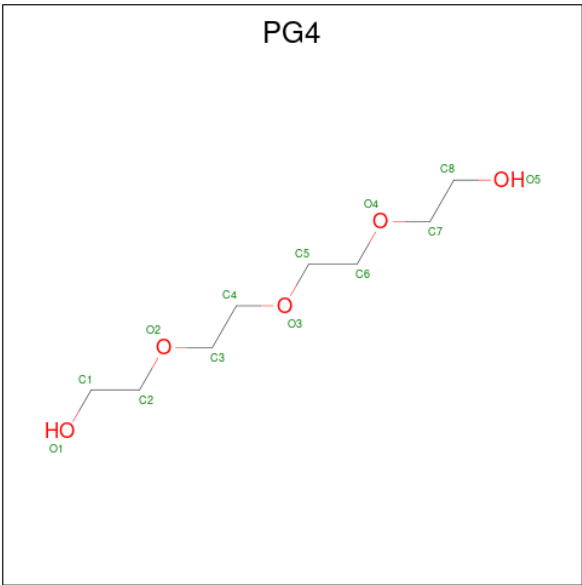
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			7	4	3		
5	C	1	Total	C	O		
			7	4	3		
5	G	1	Total	C	O		
			7	4	3		
5	J	1	Total	C	O		
			7	4	3		
5	K	1	Total	C	O		
			7	4	3		
5	K	1	Total	C	O		
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	K	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	422	Total	O	0	0
			422	422		
8	B	49	Total	O	0	0
			49	49		
8	C	383	Total	O	0	0
			383	383		
8	D	66	Total	O	0	0
			66	66		
8	E	393	Total	O	0	0
			393	393		
8	F	42	Total	O	0	0
			42	42		
8	G	351	Total	O	0	0
			351	351		
8	H	40	Total	O	0	0
			40	40		

Continued on next page...

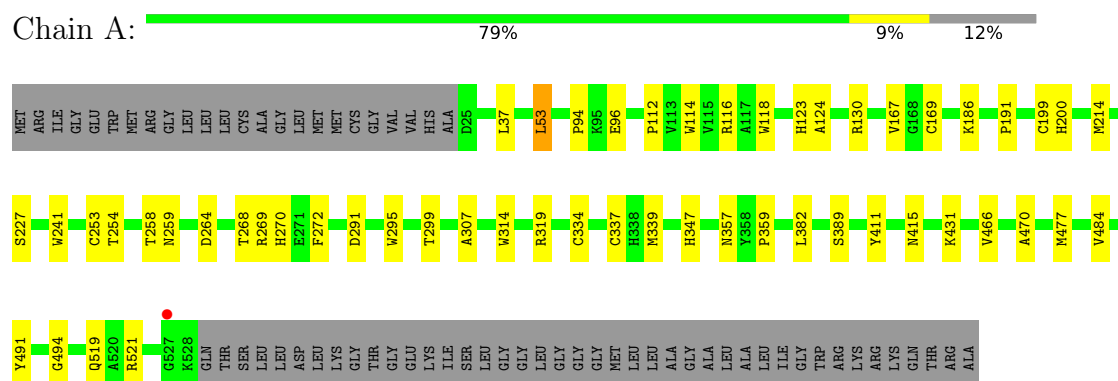
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	313	Total 313	O 313	0	0
8	J	58	Total 58	O 58	0	0
8	K	351	Total 351	O 351	0	0
8	L	33	Total 33	O 33	0	0

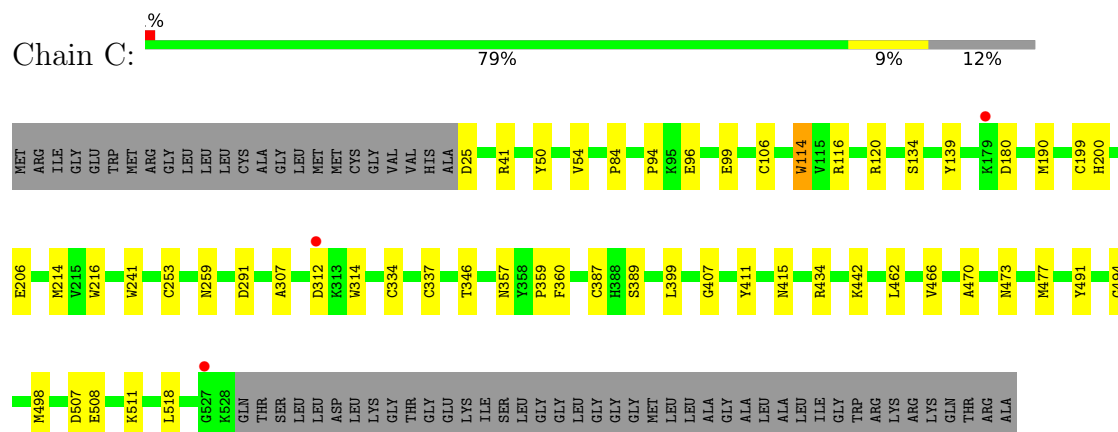
3 Residue-property plots

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.

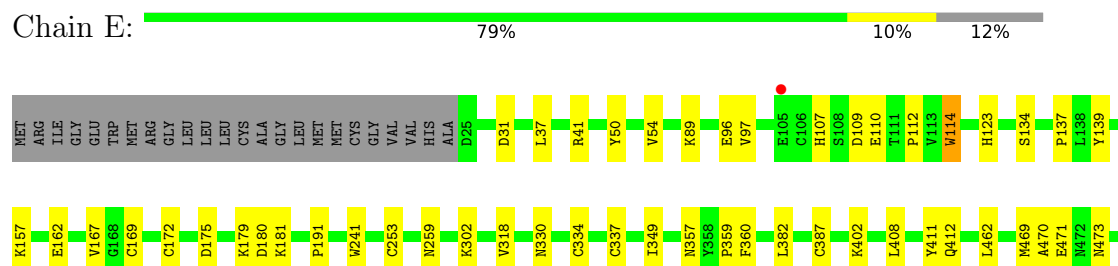
- Molecule 1: Aerobic hydroxylamine oxidoreductase

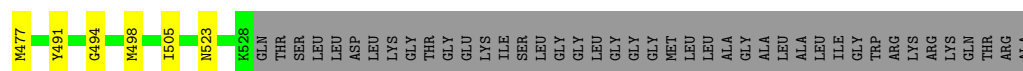


- Molecule 1: Aerobic hydroxylamine oxidoreductase



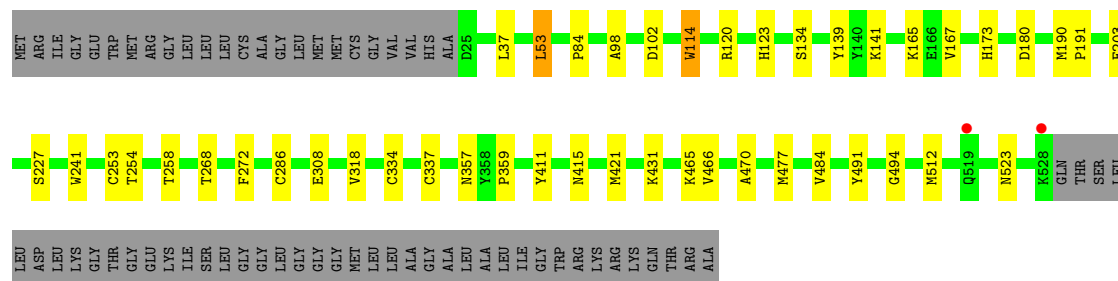
- Molecule 1: Aerobic hydroxylamine oxidoreductase





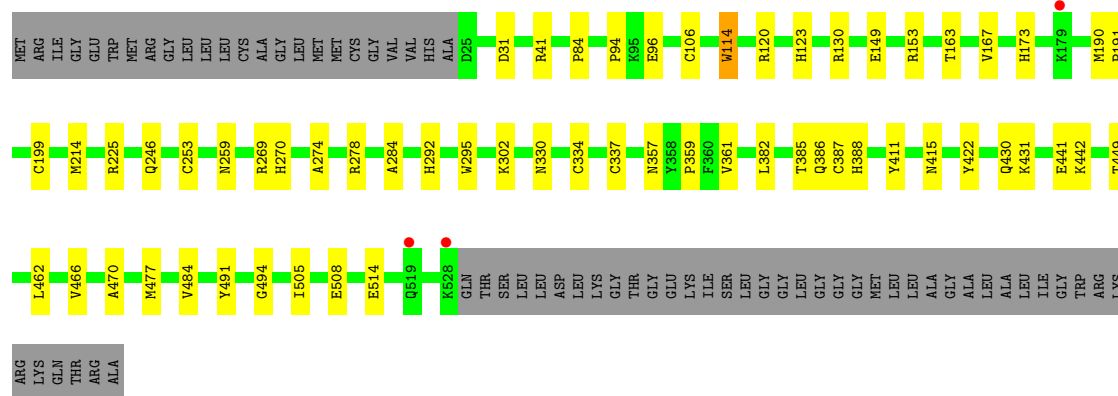
- Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain G: 81% 8% 12%



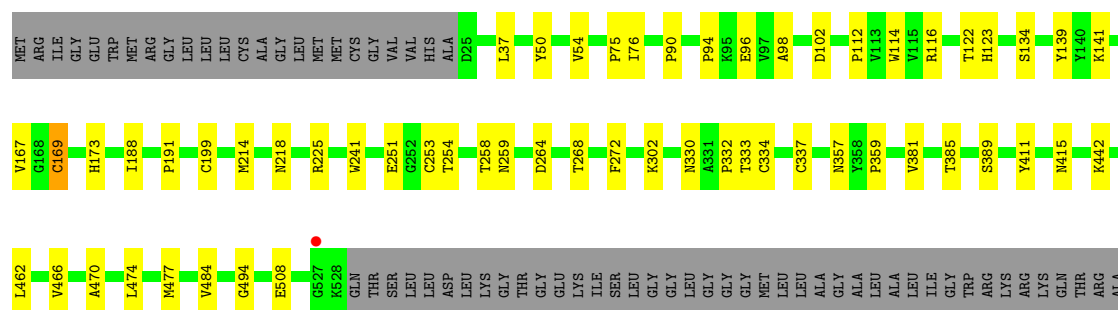
- Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain I: 78% 10% 12%



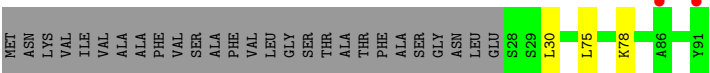
- Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain K: 78% 10% 12%

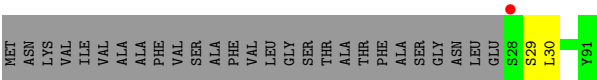


- Molecule 2: Uncharacterized protein

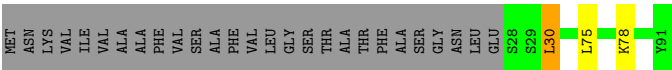
Chain B: 67% 30% 2%



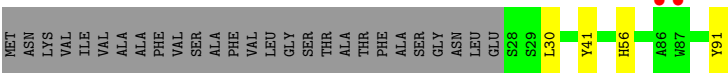
● Molecule 2: Uncharacterized protein



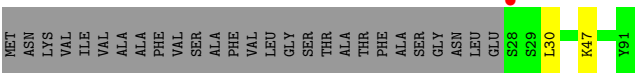
● Molecule 2: Uncharacterized protein



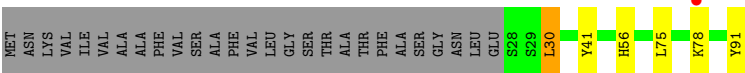
● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.23Å 141.91Å 213.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 1.99 46.18 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.18-1.99) 99.9 (46.18-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.163 , 0.200 0.164 , 0.201	Depositor DCC
R_{free} test set	14603 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31763	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.43% 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: HEC, PGE, ISW, PG4, PEG

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	0.42	0/4121	0.60	0/5583
1	C	0.42	0/4121	0.61	0/5583
1	E	0.43	0/4121	0.62	0/5583
1	G	0.40	0/4121	0.59	0/5583
1	I	0.39	0/4121	0.57	0/5583
1	K	0.41	0/4121	0.59	0/5583
2	B	0.37	0/492	0.52	0/660
2	D	0.36	0/492	0.56	0/660
2	F	0.32	0/492	0.50	0/660
2	H	0.33	0/492	0.49	0/660
2	J	0.35	0/492	0.53	0/660
2	L	0.26	0/492	0.45	0/660
All	All	0.41	0/27678	0.59	0/37458

There are no bond length outliers.

There are no bond angle outliers.

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	4018	0	3822	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4018	0	3823	52	0
1	E	4018	0	3822	46	0
1	G	4018	0	3822	41	0
1	I	4018	0	3824	61	0
1	K	4018	0	3822	47	0
2	B	486	0	491	1	0
2	D	486	0	491	0	0
2	F	486	0	491	2	0
2	H	486	0	491	2	0
2	J	486	0	491	1	0
2	L	486	0	491	4	0
3	A	301	0	212	13	0
3	C	301	0	212	17	0
3	E	301	0	211	20	0
3	G	301	0	211	16	0
3	I	301	0	214	22	0
3	K	301	0	211	20	0
4	A	86	0	56	14	0
4	C	43	0	28	8	0
4	G	86	0	56	18	0
4	I	43	0	28	5	0
5	A	7	0	10	0	0
5	C	7	0	10	1	0
5	G	7	0	10	0	0
5	J	7	0	10	2	0
5	K	14	0	20	2	0
6	A	10	0	14	1	0
6	C	10	0	14	2	0
6	E	20	0	28	2	0
6	G	20	0	28	10	0
6	I	20	0	28	12	0
7	A	13	0	18	3	0
7	C	13	0	18	3	0
7	E	13	0	18	1	0
7	K	13	0	18	0	0
8	A	422	0	0	5	0
8	B	49	0	0	0	0
8	C	383	0	0	5	0
8	D	66	0	0	0	0
8	E	393	0	0	3	0
8	F	42	0	0	0	0
8	G	351	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	40	0	0	0	0
8	I	313	0	0	6	0
8	J	58	0	0	1	0
8	K	351	0	0	2	0
8	L	33	0	0	0	0
All	All	31763	0	27564	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 336 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)
4:G:608:ISW:C4B	1:I:491:TYR:OH	1.74	1.21
1:I:337:CYS:SG	3:I:605:HEC:HAC	1.81	1.18
4:A:608:ISW:C4B	1:C:491:TYR:OH	1.75	1.15
1:C:337:CYS:SG	3:C:605:HEC:HAC	1.87	1.09
1:G:337:CYS:SG	3:G:605:HEC:HAC	1.82	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/570 (88%)	487 (97%)	15 (3%)	0	100	100
1	C	502/570 (88%)	489 (97%)	13 (3%)	0	100	100
1	E	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
1	G	502/570 (88%)	486 (97%)	16 (3%)	0	100	100
1	I	502/570 (88%)	489 (97%)	12 (2%)	1 (0%)	43	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
2	B	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	D	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	F	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	H	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	J	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	L	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
All	All	3384/3966 (85%)	3293 (97%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	292	HIS

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	430/477 (90%)	425 (99%)	5 (1%)	63	70
1	C	430/477 (90%)	429 (100%)	1 (0%)	87	92
1	E	430/477 (90%)	426 (99%)	4 (1%)	70	78
1	G	430/477 (90%)	425 (99%)	5 (1%)	63	70
1	I	430/477 (90%)	427 (99%)	3 (1%)	76	82
1	K	430/477 (90%)	426 (99%)	4 (1%)	70	78
2	B	53/73 (73%)	52 (98%)	1 (2%)	50	56
2	D	53/73 (73%)	51 (96%)	2 (4%)	29	29
2	F	53/73 (73%)	52 (98%)	1 (2%)	50	56
2	H	53/73 (73%)	52 (98%)	1 (2%)	50	56
2	J	53/73 (73%)	52 (98%)	1 (2%)	50	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	53/73 (73%)	52 (98%)	1 (2%)	50 56
All	All	2898/3300 (88%)	2869 (99%)	29 (1%)	68 75

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	53	LEU
1	K	484	VAL
1	G	484	VAL
1	K	37	LEU
1	G	318	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	415	ASN
2	L	61	ASN
1	E	419	HIS
2	F	61	ASN
1	G	513	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](#)

66 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ISW	G	608	1	47,50,50	5.59	20 (42%)	53,82,82	5.17	32 (60%)
5	PEG	K	608	-	6,6,6	0.43	0	5,5,5	0.32	0
5	PEG	K	609	-	6,6,6	0.48	0	5,5,5	0.40	0
3	HEC	C	606	1	46,50,50	1.88	6 (13%)	58,82,82	1.65	8 (13%)
3	HEC	G	604	1	46,50,50	1.80	7 (15%)	58,82,82	1.77	11 (18%)
6	PGE	G	611	-	9,9,9	0.35	0	8,8,8	0.40	0
3	HEC	G	601	1	46,50,50	1.77	5 (10%)	58,82,82	2.06	8 (13%)
3	HEC	A	605	1	46,50,50	1.93	5 (10%)	58,82,82	1.58	6 (10%)
3	HEC	C	603	1	46,50,50	1.82	5 (10%)	58,82,82	1.97	10 (17%)
3	HEC	E	602	1	46,50,50	1.88	4 (8%)	58,82,82	1.57	7 (12%)
3	HEC	G	605	1	46,50,50	1.92	7 (15%)	58,82,82	1.73	6 (10%)
3	HEC	I	601	1	46,50,50	1.90	6 (13%)	58,82,82	1.72	6 (10%)
4	ISW	C	608	8,1	47,50,50	5.71	20 (42%)	53,82,82	4.91	31 (58%)
6	PGE	I	609	-	9,9,9	0.33	0	8,8,8	0.25	0
3	HEC	A	606	1	46,50,50	1.86	8 (17%)	58,82,82	1.60	7 (12%)
3	HEC	E	607	1	46,50,50	1.82	6 (13%)	58,82,82	1.78	10 (17%)
3	HEC	I	603	1	46,50,50	1.96	7 (15%)	58,82,82	1.69	7 (12%)
3	HEC	E	601	1	46,50,50	1.91	7 (15%)	58,82,82	1.93	9 (15%)
4	ISW	I	608	8,1	47,50,50	5.70	22 (46%)	53,82,82	4.80	31 (58%)
3	HEC	I	604	1	46,50,50	1.87	7 (15%)	58,82,82	1.67	7 (12%)
3	HEC	E	603	1	46,50,50	1.87	5 (10%)	58,82,82	1.82	10 (17%)
3	HEC	I	605	1	46,50,50	1.80	7 (15%)	58,82,82	1.65	6 (10%)
3	HEC	E	604	1	46,50,50	1.84	6 (13%)	58,82,82	1.69	7 (12%)
3	HEC	K	602	1	46,50,50	1.93	5 (10%)	58,82,82	1.77	9 (15%)
3	HEC	A	603	1	46,50,50	1.87	9 (19%)	58,82,82	1.75	10 (17%)
3	HEC	K	607	1	46,50,50	1.89	8 (17%)	58,82,82	1.83	11 (18%)
5	PEG	A	610	-	6,6,6	0.52	0	5,5,5	0.41	0
3	HEC	G	602	1	46,50,50	1.86	5 (10%)	58,82,82	1.83	9 (15%)
5	PEG	C	609	-	6,6,6	0.49	0	5,5,5	0.38	0
7	PG4	A	612	-	12,12,12	0.54	0	11,11,11	0.31	0
3	HEC	C	605	1	46,50,50	1.92	8 (17%)	58,82,82	1.66	6 (10%)
3	HEC	K	604	1	46,50,50	1.91	7 (15%)	58,82,82	1.77	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ISW	A	609	8,1	47,50,50	5.58	21 (44%)	53,82,82	4.85	27 (50%)
7	PG4	K	610	-	12,12,12	0.57	0	11,11,11	0.33	0
6	PGE	E	609	-	9,9,9	0.32	0	8,8,8	0.50	0
3	HEC	I	606	1	46,50,50	1.89	7 (15%)	58,82,82	1.79	11 (18%)
5	PEG	G	610	-	6,6,6	0.52	0	5,5,5	0.25	0
7	PG4	C	611	-	12,12,12	0.53	0	11,11,11	0.28	0
3	HEC	E	606	1	46,50,50	1.89	8 (17%)	58,82,82	1.69	6 (10%)
3	HEC	G	603	1	46,50,50	1.85	6 (13%)	58,82,82	2.16	10 (17%)
3	HEC	G	606	1	46,50,50	1.78	6 (13%)	58,82,82	1.86	11 (18%)
6	PGE	C	610	-	9,9,9	0.37	0	8,8,8	0.31	0
6	PGE	G	612	-	9,9,9	0.40	0	8,8,8	0.41	0
3	HEC	I	602	1	46,50,50	1.83	6 (13%)	58,82,82	1.87	10 (17%)
6	PGE	A	611	-	9,9,9	0.35	0	8,8,8	0.35	0
6	PGE	I	610	-	9,9,9	0.29	0	8,8,8	0.24	0
3	HEC	G	607	1	46,50,50	1.88	7 (15%)	58,82,82	1.51	7 (12%)
4	ISW	A	608	8,1	47,50,50	5.55	22 (46%)	53,82,82	5.06	34 (64%)
3	HEC	C	602	1	46,50,50	1.85	7 (15%)	58,82,82	2.03	11 (18%)
3	HEC	A	602	1	46,50,50	1.85	6 (13%)	58,82,82	1.91	11 (18%)
3	HEC	K	606	1	46,50,50	1.86	8 (17%)	58,82,82	1.99	13 (22%)
3	HEC	C	604	1	46,50,50	1.92	8 (17%)	58,82,82	1.73	9 (15%)
3	HEC	I	607	1	46,50,50	1.88	6 (13%)	58,82,82	1.96	11 (18%)
5	PEG	J	101	-	6,6,6	0.49	0	5,5,5	0.51	0
3	HEC	C	601	1	46,50,50	1.80	5 (10%)	58,82,82	1.95	7 (12%)
7	PG4	E	610	-	12,12,12	0.53	0	11,11,11	0.32	0
3	HEC	K	601	1	46,50,50	1.84	5 (10%)	58,82,82	2.08	13 (22%)
3	HEC	C	607	1	46,50,50	1.90	7 (15%)	58,82,82	1.86	10 (17%)
3	HEC	A	607	1	46,50,50	1.86	6 (13%)	58,82,82	1.75	9 (15%)
3	HEC	A	601	1	46,50,50	1.83	4 (8%)	58,82,82	2.19	8 (13%)
3	HEC	K	603	1	46,50,50	1.92	7 (15%)	58,82,82	1.65	8 (13%)
6	PGE	E	608	-	9,9,9	0.37	0	8,8,8	0.30	0
3	HEC	E	605	1	46,50,50	1.91	6 (13%)	58,82,82	1.55	6 (10%)
4	ISW	G	609	8,1	47,50,50	5.62	22 (46%)	53,82,82	4.82	28 (52%)
3	HEC	A	604	1	46,50,50	1.80	5 (10%)	58,82,82	1.95	6 (10%)
3	HEC	K	605	1	46,50,50	1.89	7 (15%)	58,82,82	1.66	8 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ISW	G	608	1	-	4/14/74/74	-
5	PEG	K	608	-	-	2/4/4/4	-
5	PEG	K	609	-	-	2/4/4/4	-
3	HEC	C	606	1	-	8/14/54/54	-
3	HEC	G	604	1	-	7/14/54/54	-
6	PGE	G	611	-	-	6/7/7/7	-
3	HEC	G	601	1	-	8/14/54/54	-
3	HEC	A	605	1	-	9/14/54/54	-
3	HEC	C	603	1	-	5/14/54/54	-
3	HEC	E	602	1	-	8/14/54/54	-
3	HEC	G	605	1	-	9/14/54/54	-
3	HEC	I	601	1	-	6/14/54/54	-
4	ISW	C	608	8,1	-	3/14/74/74	-
6	PGE	I	609	-	-	5/7/7/7	-
3	HEC	A	606	1	-	6/14/54/54	-
3	HEC	E	607	1	-	7/14/54/54	-
3	HEC	I	603	1	-	2/14/54/54	-
3	HEC	E	601	1	-	9/14/54/54	-
4	ISW	I	608	8,1	-	5/14/74/74	-
3	HEC	I	604	1	-	8/14/54/54	-
3	HEC	E	603	1	-	5/14/54/54	-
3	HEC	I	605	1	-	9/14/54/54	-
3	HEC	E	604	1	-	6/14/54/54	-
3	HEC	K	602	1	-	8/14/54/54	-
3	HEC	A	603	1	-	3/14/54/54	-
3	HEC	K	607	1	-	8/14/54/54	-
5	PEG	A	610	-	-	3/4/4/4	-
3	HEC	G	602	1	-	8/14/54/54	-
5	PEG	C	609	-	-	2/4/4/4	-
7	PG4	A	612	-	-	7/10/10/10	-
3	HEC	C	605	1	-	9/14/54/54	-
3	HEC	K	604	1	-	6/14/54/54	-
4	ISW	A	609	8,1	-	3/14/74/74	-
7	PG4	K	610	-	-	5/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	E	609	-	-	3/7/7/7	-
3	HEC	I	606	1	-	6/14/54/54	-
5	PEG	G	610	-	-	3/4/4/4	-
7	PG4	C	611	-	-	5/10/10/10	-
3	HEC	E	606	1	-	6/14/54/54	-
3	HEC	G	603	1	-	5/14/54/54	-
3	HEC	G	606	1	-	7/14/54/54	-
6	PGE	C	610	-	-	4/7/7/7	-
6	PGE	G	612	-	-	5/7/7/7	-
3	HEC	I	602	1	-	8/14/54/54	-
6	PGE	A	611	-	-	3/7/7/7	-
6	PGE	I	610	-	-	6/7/7/7	-
3	HEC	G	607	1	-	7/14/54/54	-
4	ISW	A	608	8,1	-	3/14/74/74	-
3	HEC	C	602	1	-	8/14/54/54	-
3	HEC	A	602	1	-	8/14/54/54	-
3	HEC	K	606	1	-	6/14/54/54	-
3	HEC	C	604	1	-	7/14/54/54	-
3	HEC	I	607	1	-	8/14/54/54	-
5	PEG	J	101	-	-	2/4/4/4	-
3	HEC	C	601	1	-	7/14/54/54	-
7	PG4	E	610	-	-	3/10/10/10	-
3	HEC	K	601	1	-	7/14/54/54	-
3	HEC	C	607	1	-	9/14/54/54	-
3	HEC	A	607	1	-	6/14/54/54	-
3	HEC	A	601	1	-	6/14/54/54	-
3	HEC	K	603	1	-	4/14/54/54	-
6	PGE	E	608	-	-	4/7/7/7	-
3	HEC	E	605	1	-	9/14/54/54	-
4	ISW	G	609	8,1	-	4/14/74/74	-
3	HEC	A	604	1	-	6/14/54/54	-
3	HEC	K	605	1	-	9/14/54/54	-

The worst 5 of 394 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	608	ISW	CHA-C1A	15.86	1.69	1.38
4	I	608	ISW	CHA-C1A	15.70	1.69	1.38
4	A	609	ISW	CHA-C1A	15.65	1.69	1.38
4	G	608	ISW	CHA-C1A	15.47	1.68	1.38
4	G	609	ISW	CHA-C1A	15.07	1.68	1.38

The worst 5 of 542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	608	ISW	CHB-C1B-C2B	-14.45	102.22	125.03
4	A	608	ISW	C1A-CHA-C4D	-13.77	96.76	126.02
4	C	608	ISW	C1A-CHA-C4D	-13.60	97.11	126.02
4	G	608	ISW	C1A-CHA-C4D	-13.50	97.32	126.02
4	A	609	ISW	C1A-CHA-C4D	-12.84	98.73	126.02

There are no chirality outliers.

5 of 385 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	HEC	C2B-C3B-CAB-CBB
3	A	601	HEC	C4B-C3B-CAB-CBB
3	A	601	HEC	C2C-C3C-CAC-CBC
3	A	601	HEC	C4C-C3C-CAC-CBC
3	A	602	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

54 monomers are involved in 184 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	608	ISW	10	0
5	K	609	PEG	2	0
3	C	606	HEC	2	0
3	G	604	HEC	2	0
6	G	611	PGE	6	0
3	G	601	HEC	3	0
3	A	605	HEC	3	0
3	C	603	HEC	4	0
3	E	602	HEC	1	0
3	G	605	HEC	5	0
4	C	608	ISW	8	0
6	I	609	PGE	7	0
3	A	606	HEC	2	0

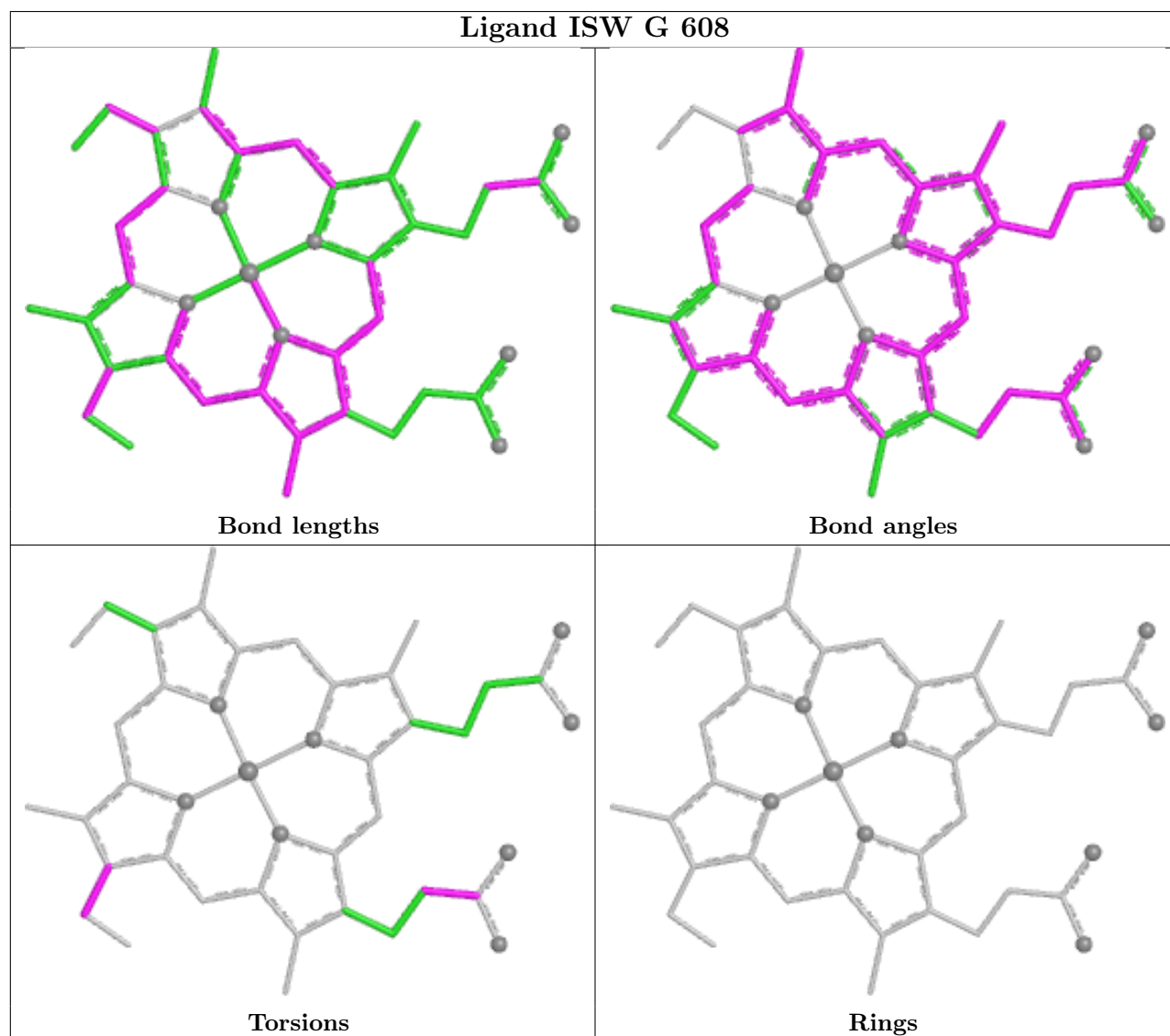
Continued on next page...

Continued from previous page...

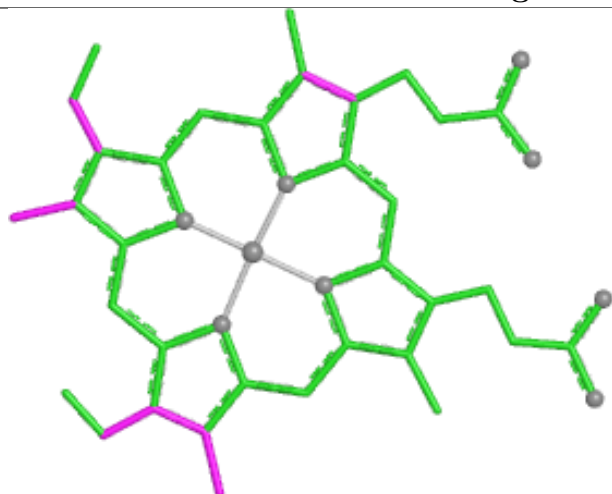
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	607	HEC	2	0
3	I	603	HEC	3	0
3	E	601	HEC	2	0
4	I	608	ISW	5	0
3	I	604	HEC	4	0
3	E	603	HEC	1	0
3	I	605	HEC	6	0
3	E	604	HEC	7	0
3	K	602	HEC	4	0
3	G	602	HEC	3	0
5	C	609	PEG	1	0
7	A	612	PG4	3	0
3	C	605	HEC	6	0
3	K	604	HEC	3	0
4	A	609	ISW	6	0
6	E	609	PGE	1	0
3	I	606	HEC	2	0
7	C	611	PG4	3	0
3	E	606	HEC	3	0
3	G	606	HEC	4	0
6	C	610	PGE	2	0
6	G	612	PGE	4	0
3	I	602	HEC	5	0
6	A	611	PGE	1	0
6	I	610	PGE	5	0
4	A	608	ISW	8	0
3	C	602	HEC	4	0
3	A	602	HEC	6	0
3	K	606	HEC	4	0
3	I	607	HEC	3	0
5	J	101	PEG	2	0
3	C	601	HEC	1	0
7	E	610	PG4	1	0
3	K	601	HEC	3	0
3	C	607	HEC	2	0
3	K	603	HEC	1	0
6	E	608	PGE	1	0
3	E	605	HEC	6	0
4	G	609	ISW	8	0
3	A	604	HEC	2	0
3	K	605	HEC	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

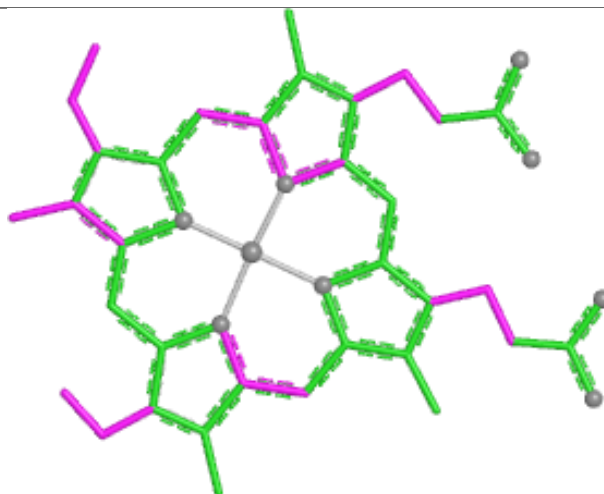
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



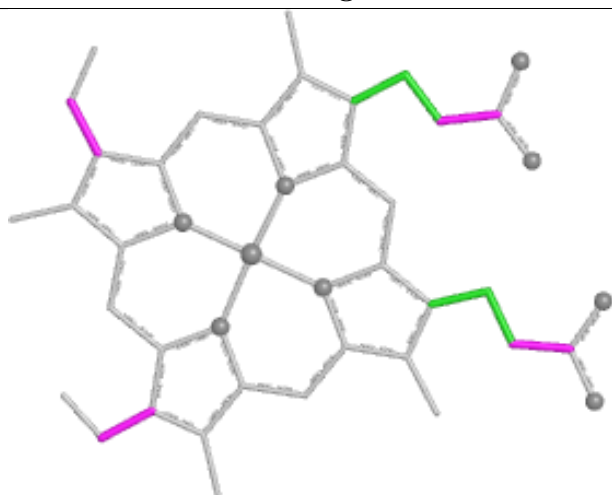
Ligand HEC C 606



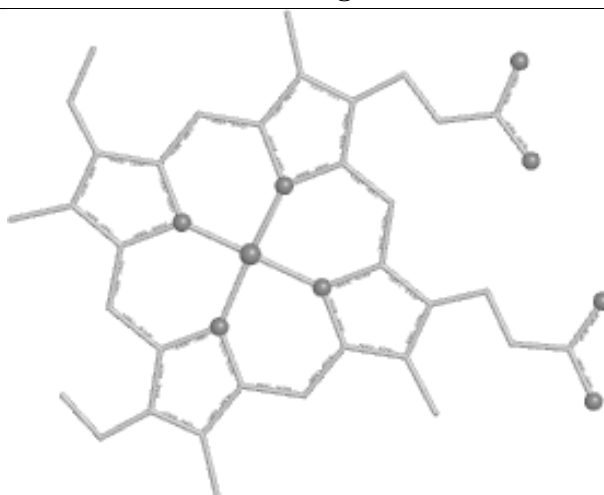
Bond lengths



Bond angles

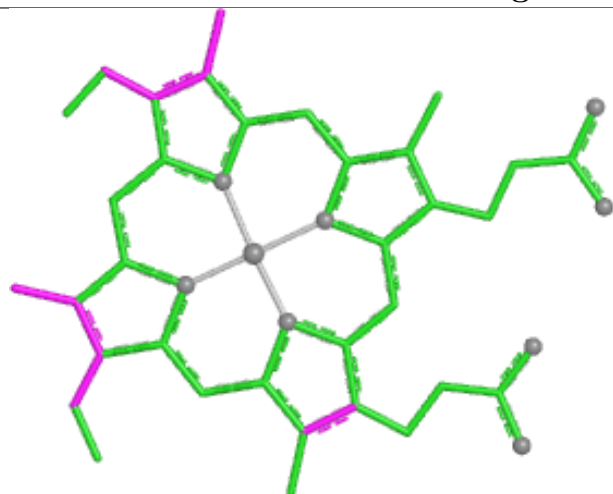


Torsions

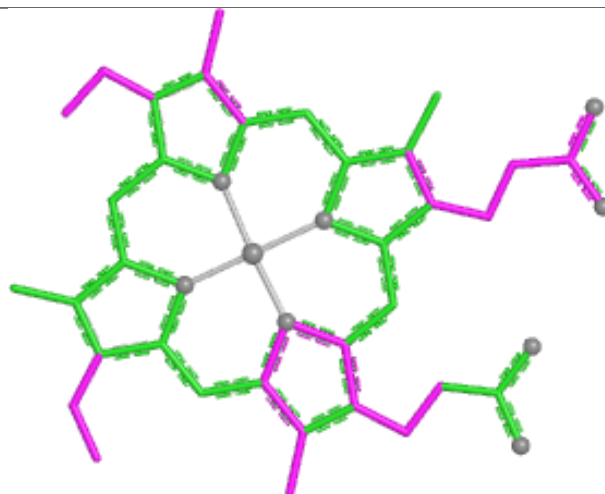


Rings

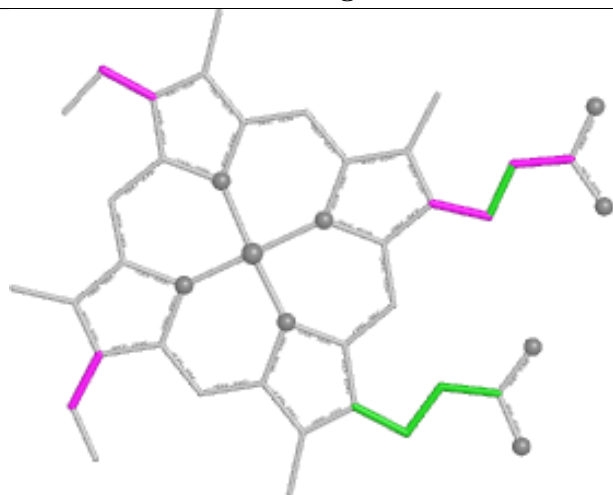
Ligand HEC G 604



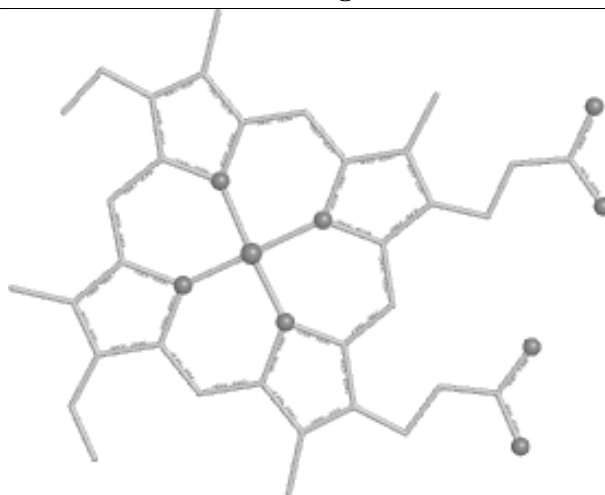
Bond lengths



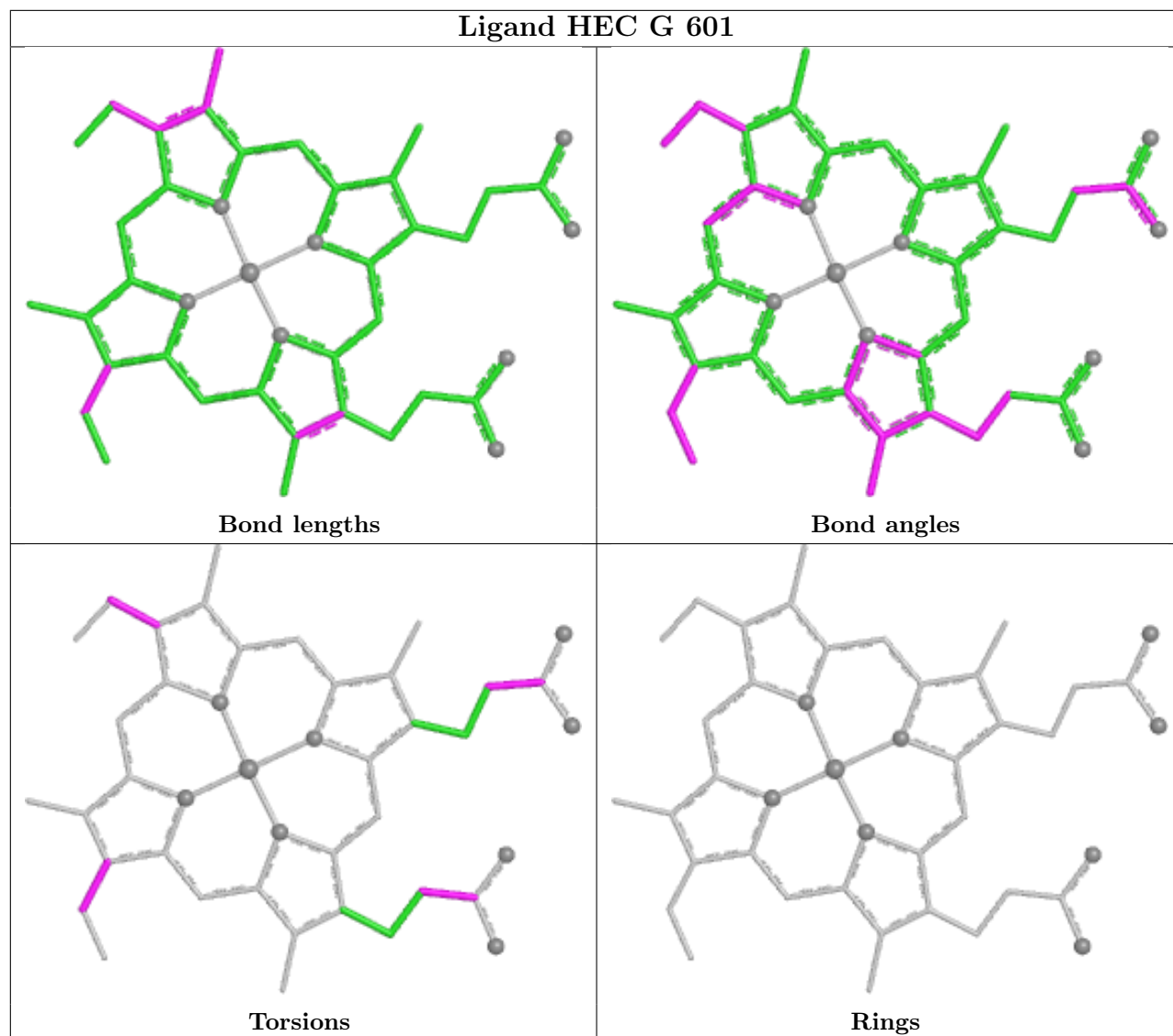
Bond angles

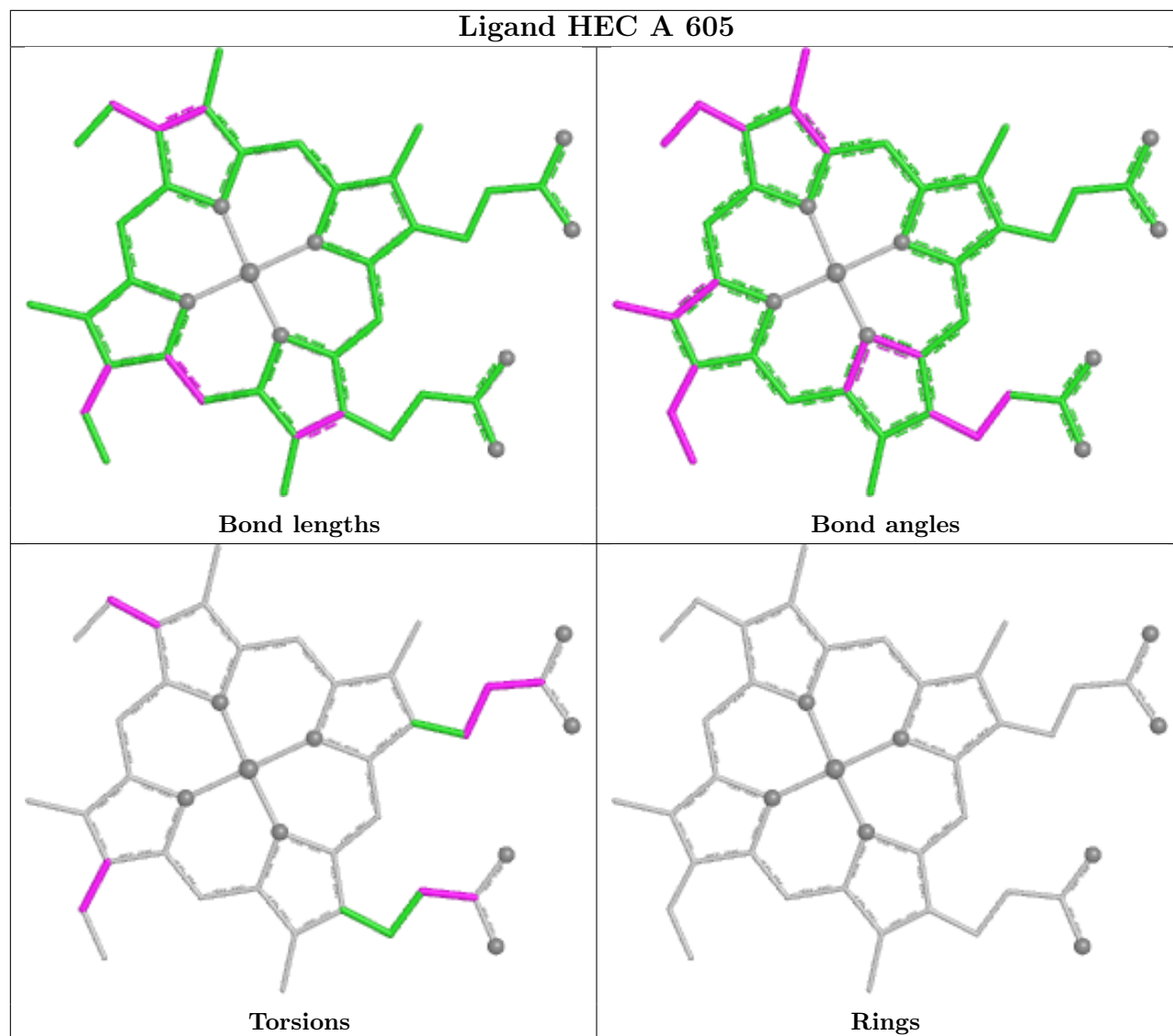


Torsions

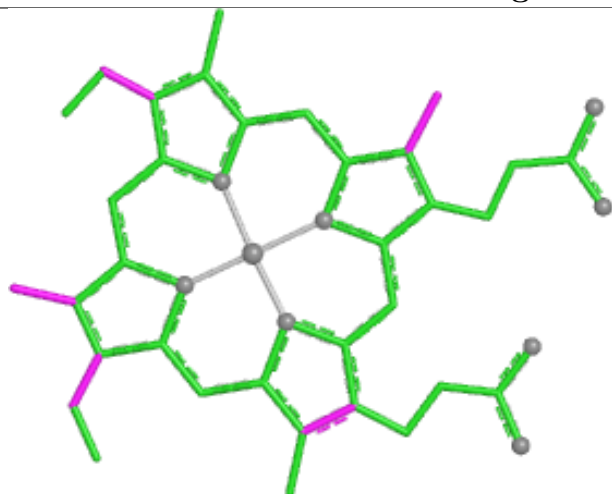


Rings

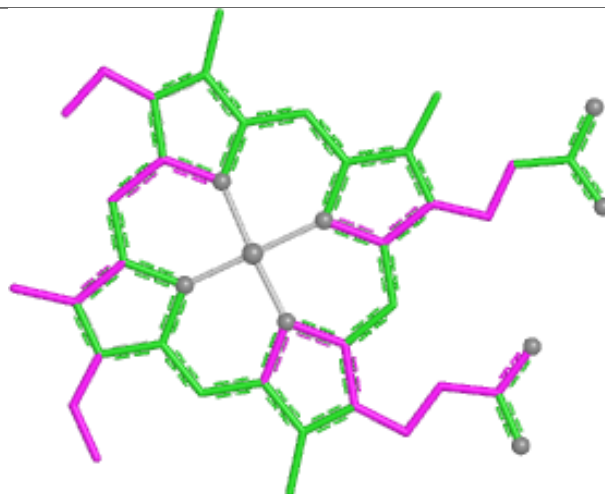




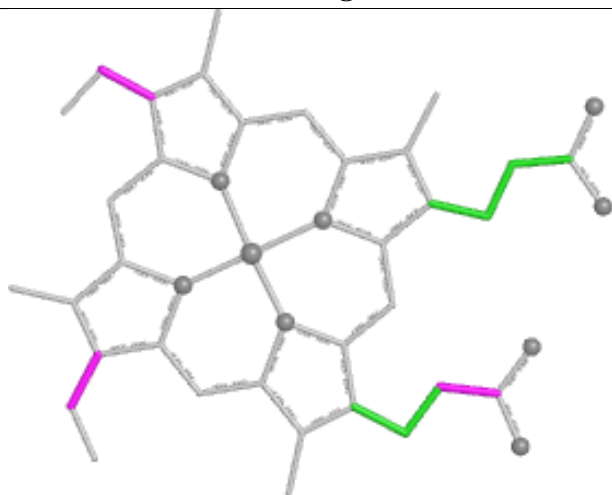
Ligand HEC C 603



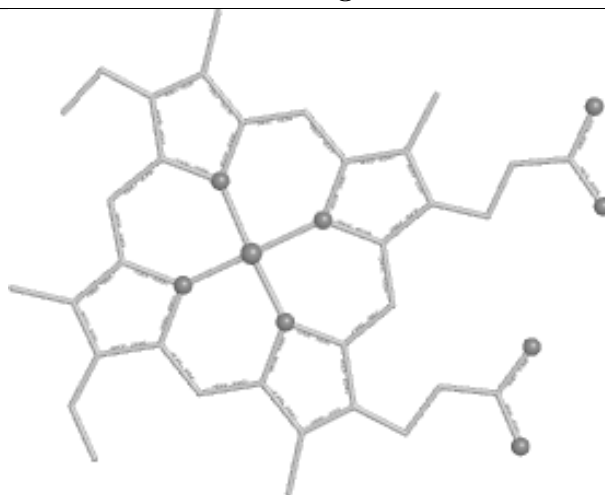
Bond lengths



Bond angles

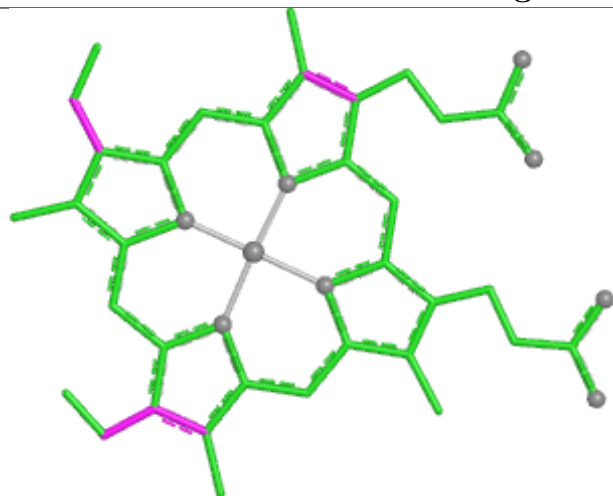


Torsions

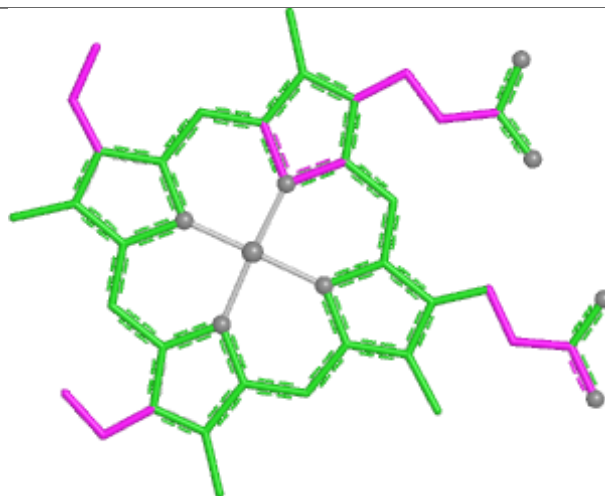


Rings

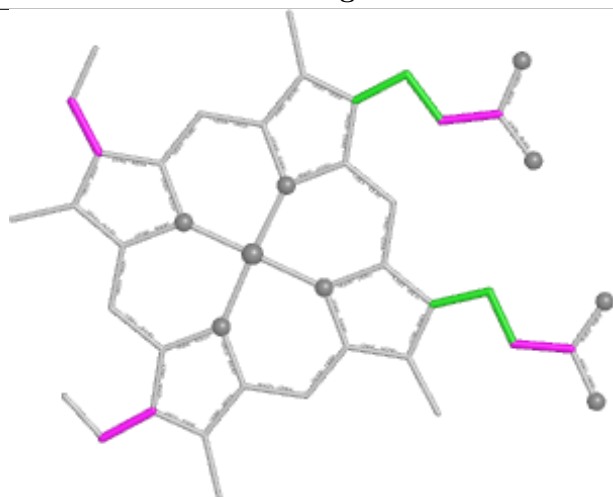
Ligand HEC E 602



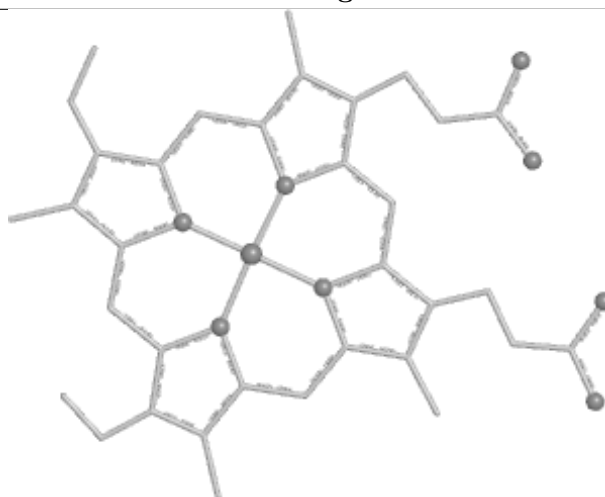
Bond lengths



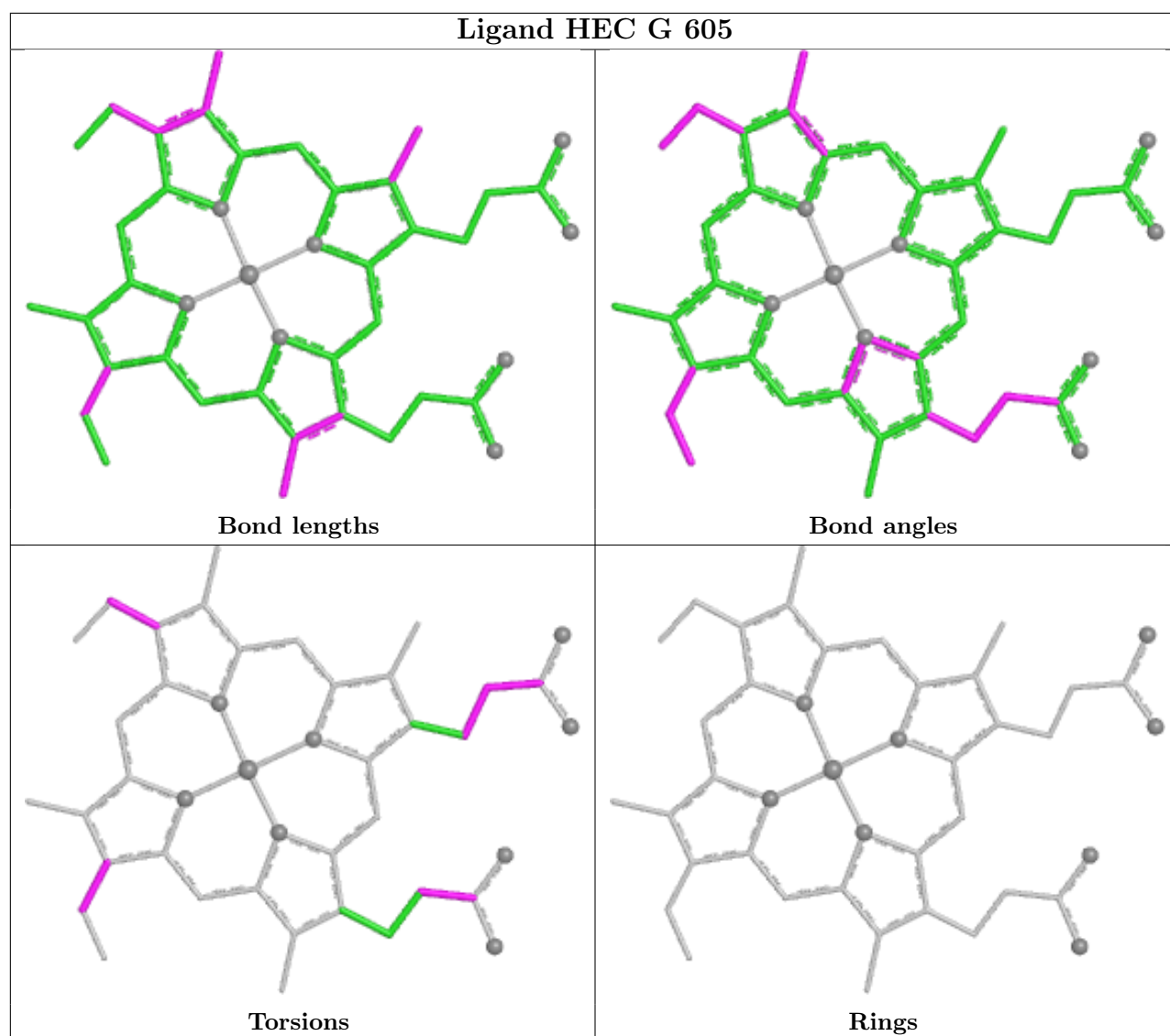
Bond angles



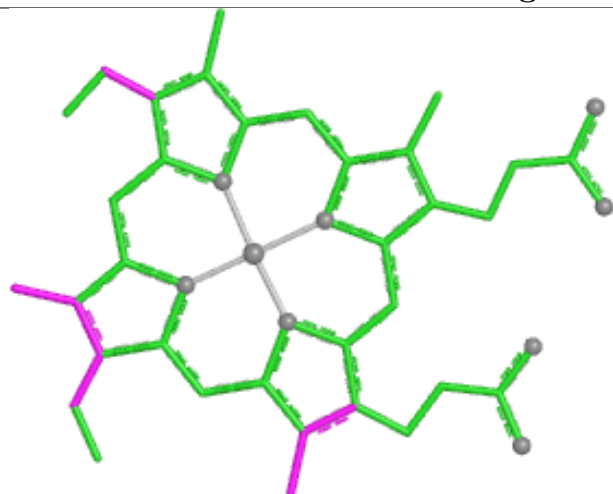
Torsions



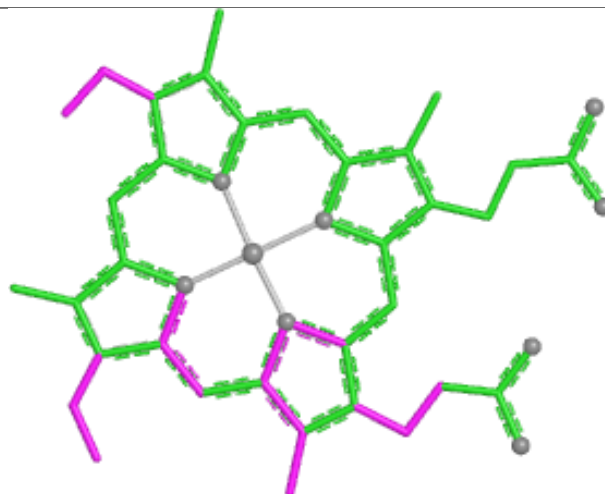
Rings



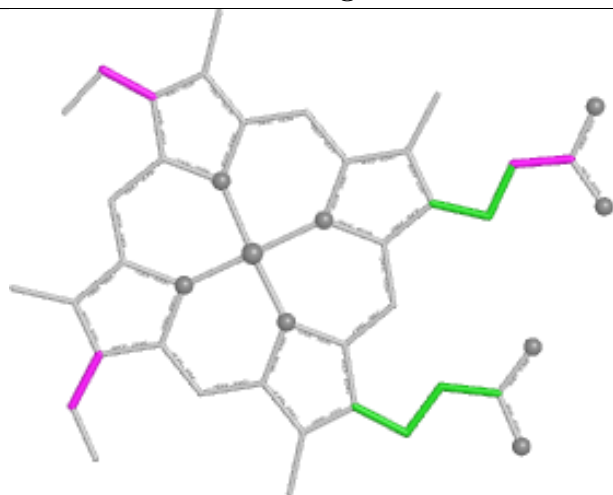
Ligand HEC I 601



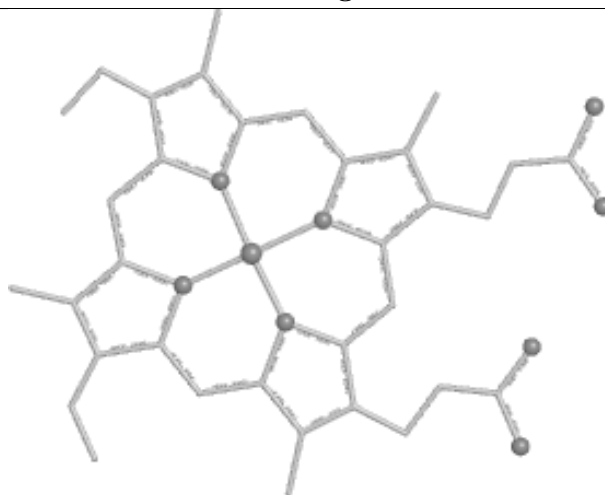
Bond lengths



Bond angles

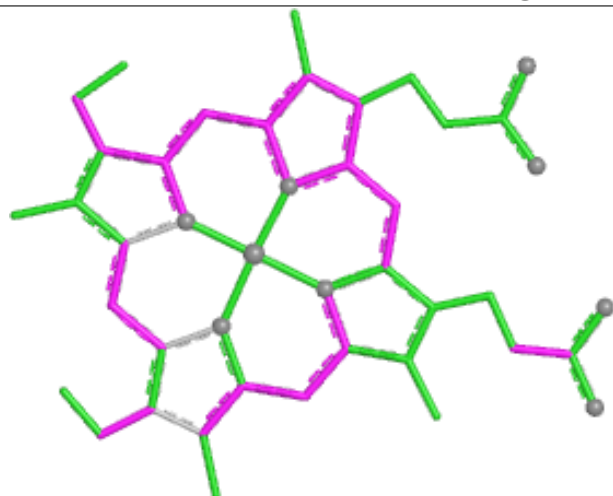


Torsions

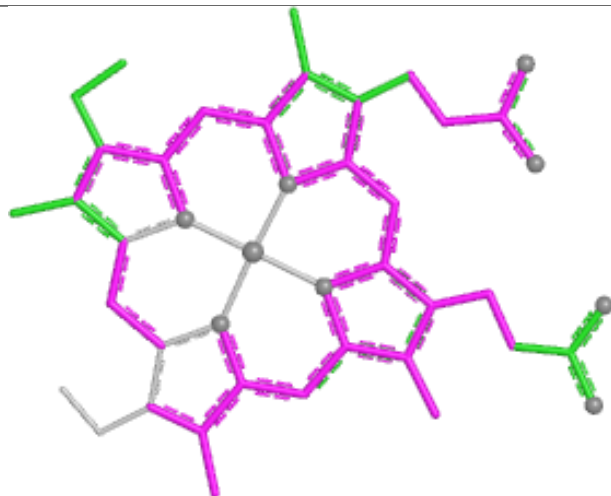


Rings

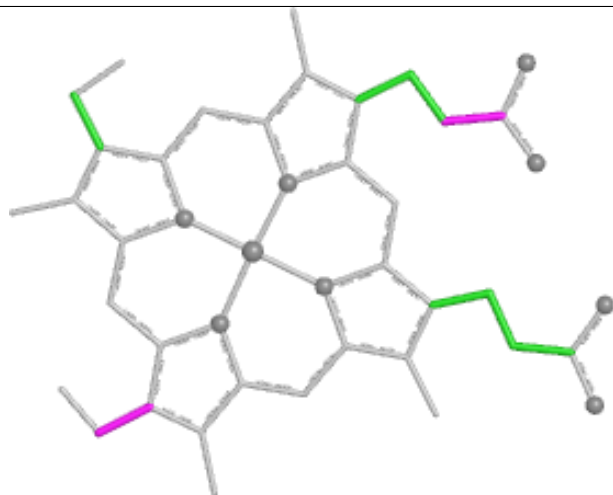
Ligand ISW C 608



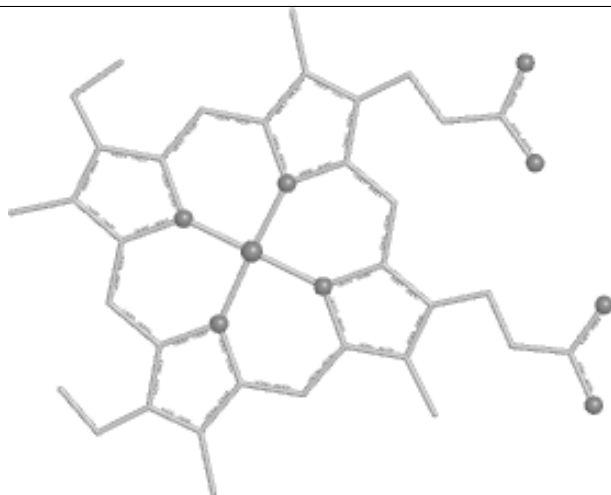
Bond lengths



Bond angles

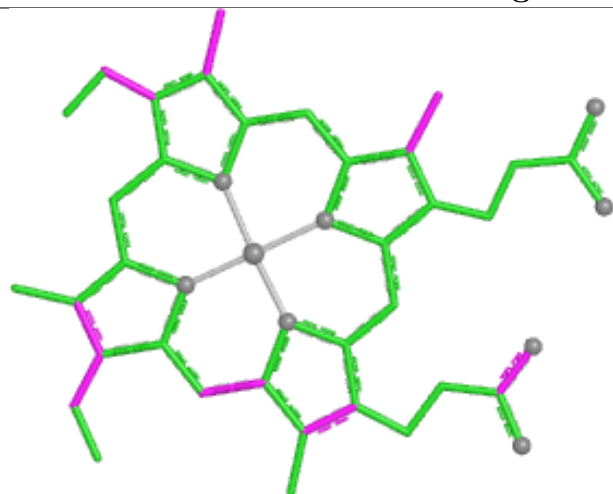


Torsions

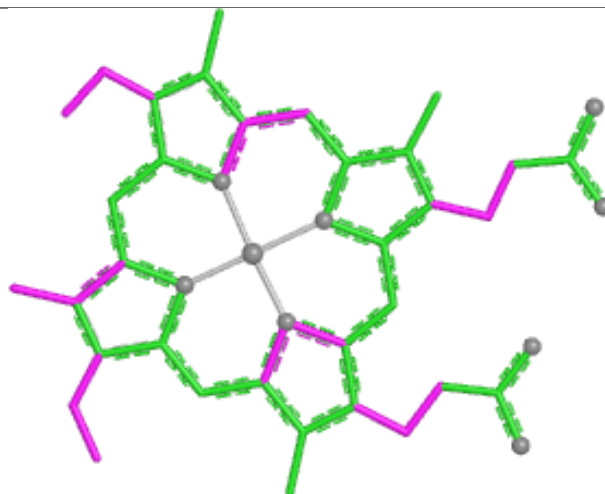


Rings

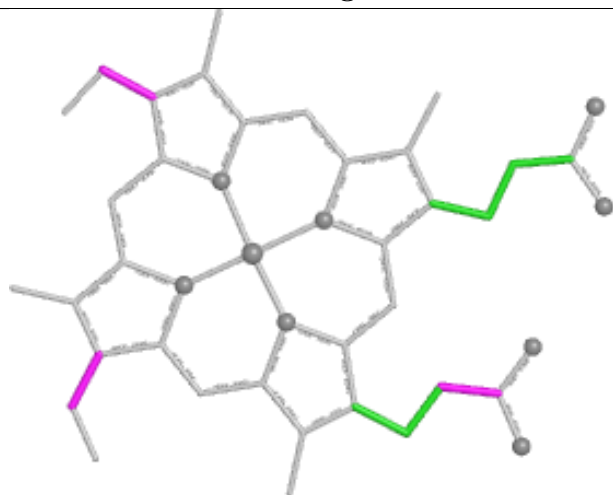
Ligand HEC A 606



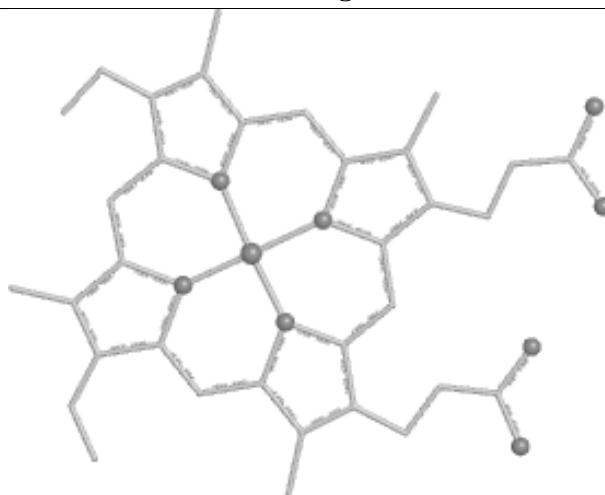
Bond lengths



Bond angles

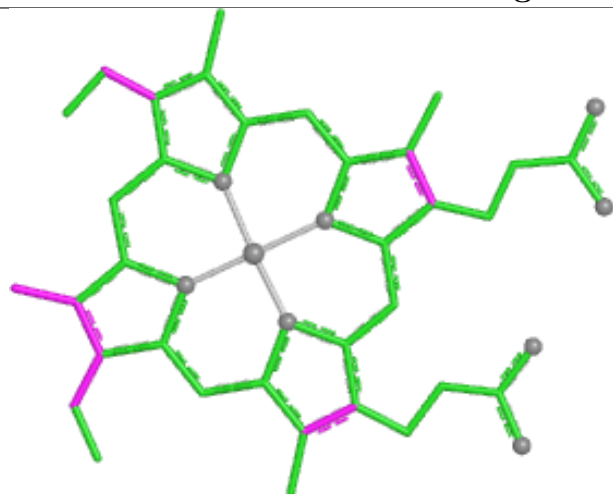


Torsions

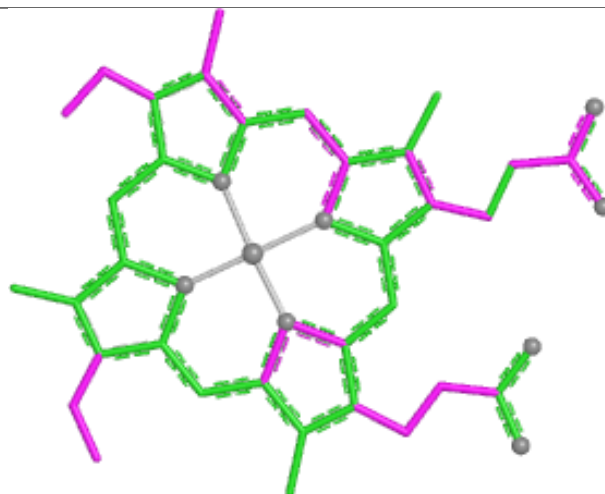


Rings

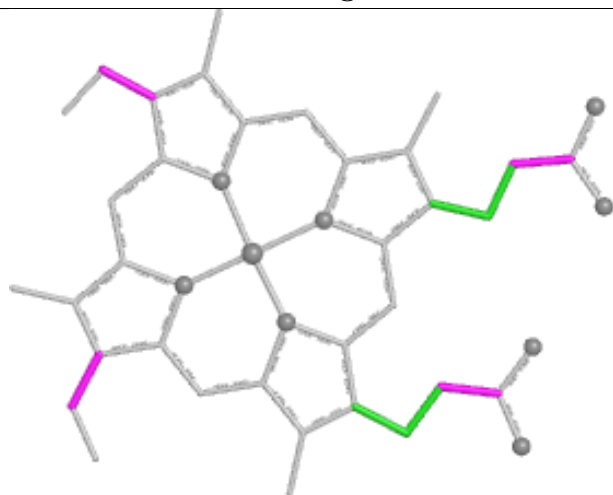
Ligand HEC E 607



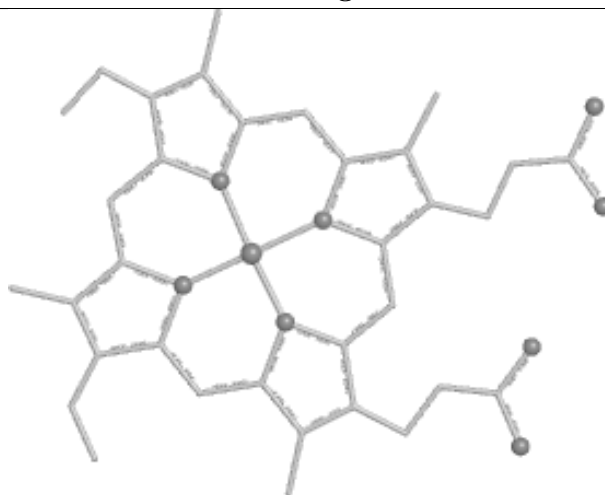
Bond lengths



Bond angles

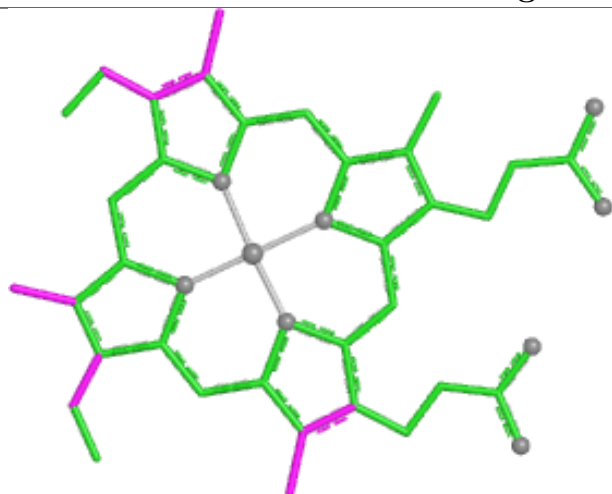


Torsions

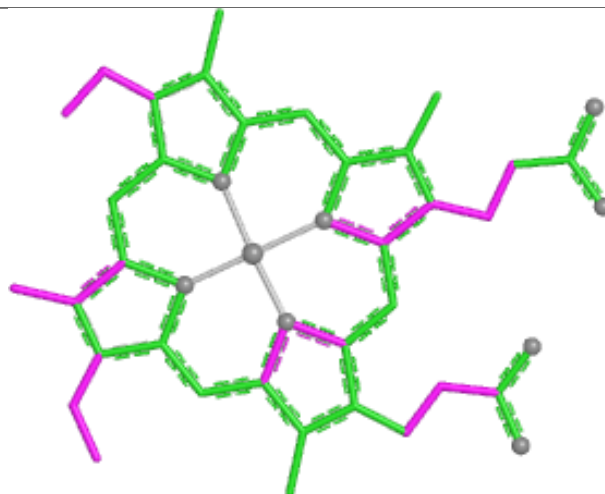


Rings

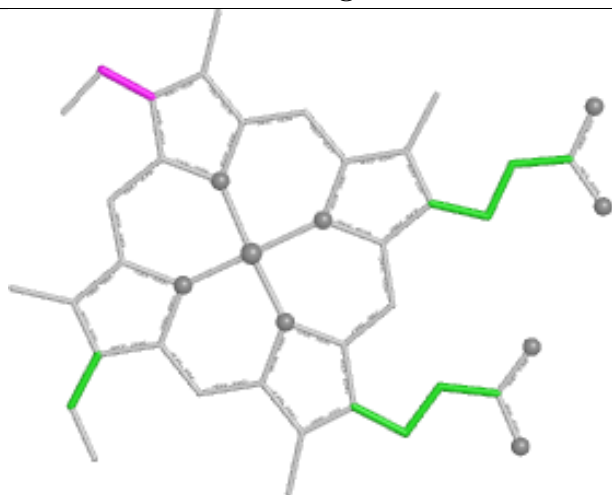
Ligand HEC I 603



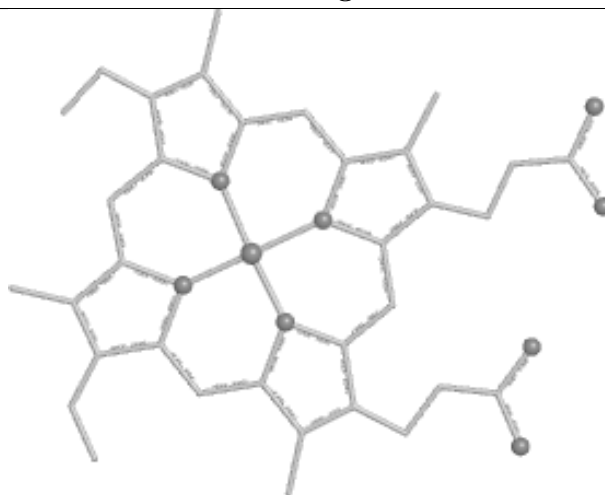
Bond lengths



Bond angles

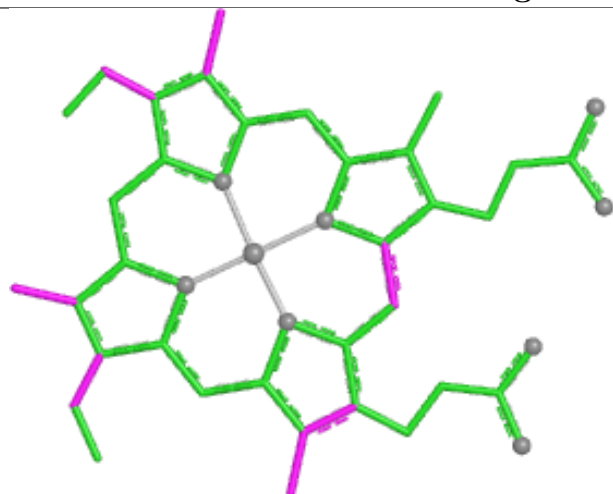


Torsions

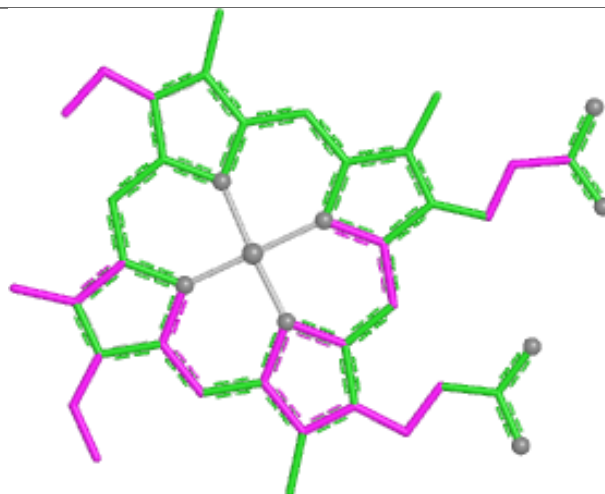


Rings

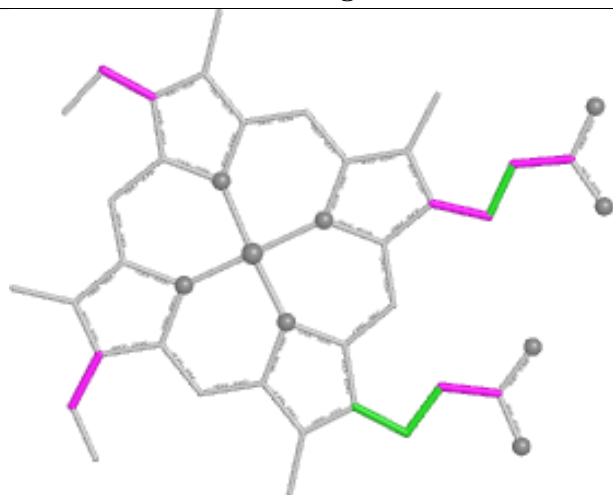
Ligand HEC E 601



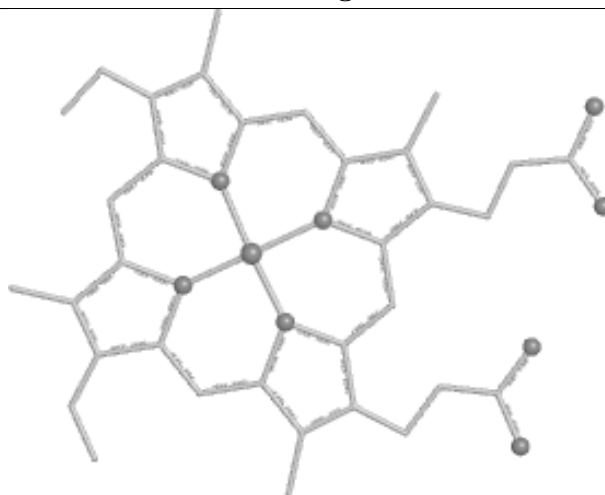
Bond lengths



Bond angles

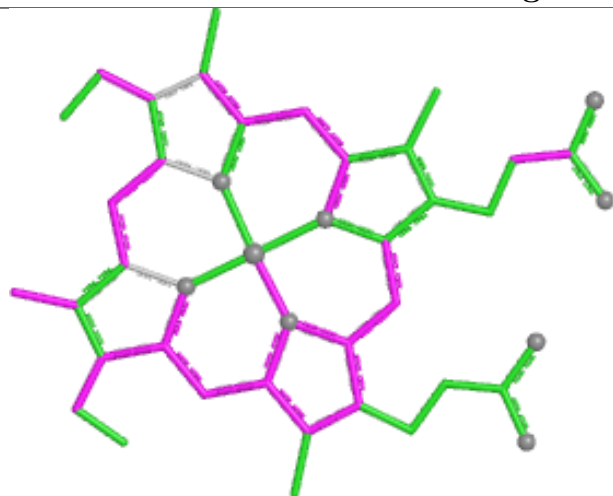


Torsions

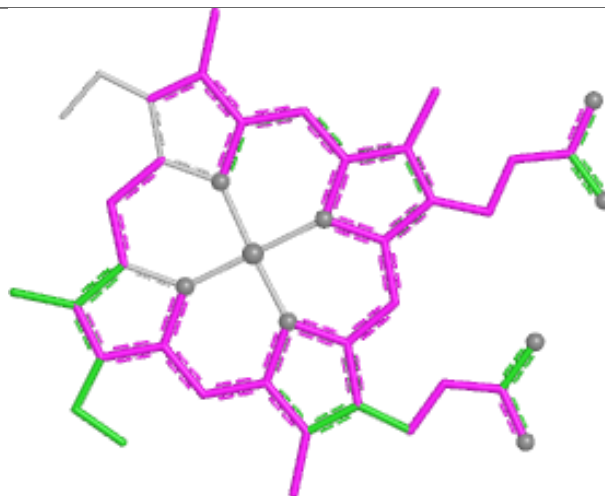


Rings

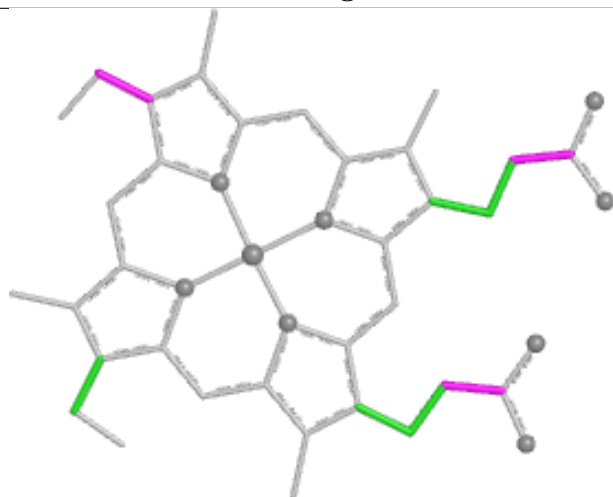
Ligand ISW I 608



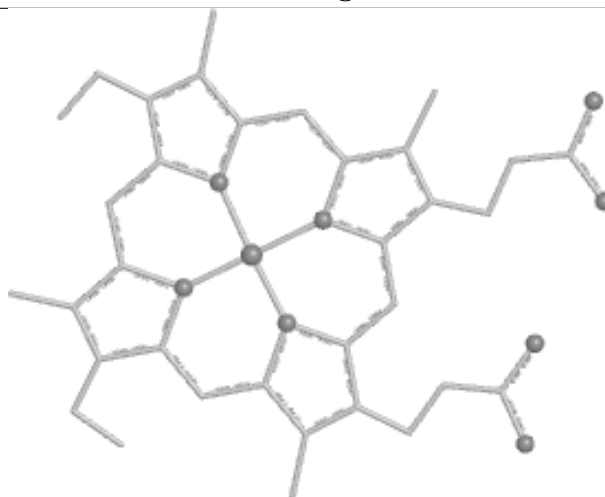
Bond lengths



Bond angles

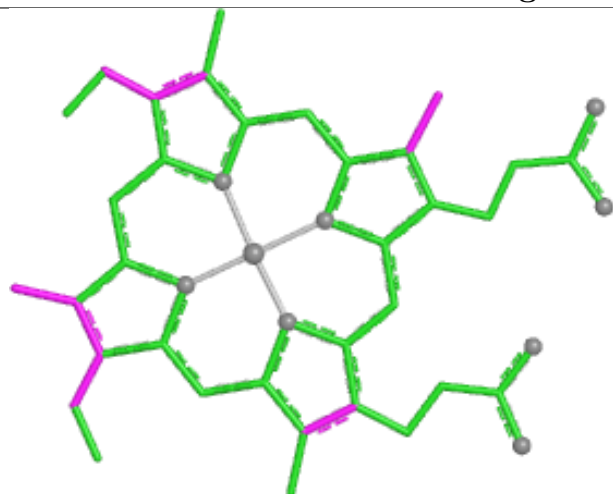


Torsions

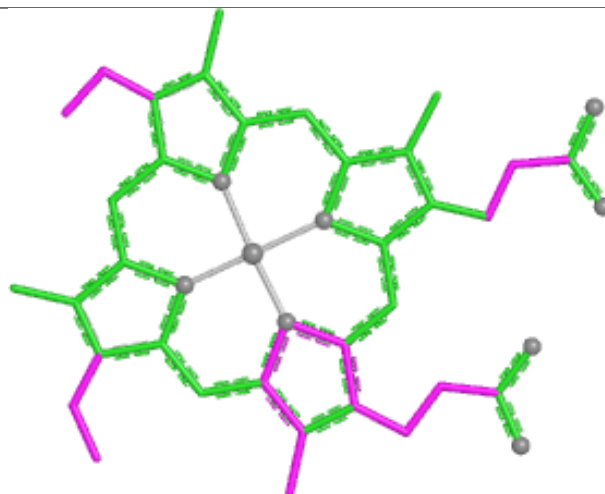


Rings

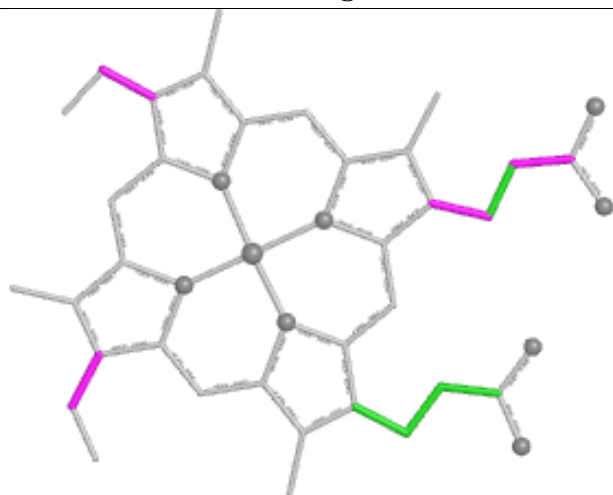
Ligand HEC I 604



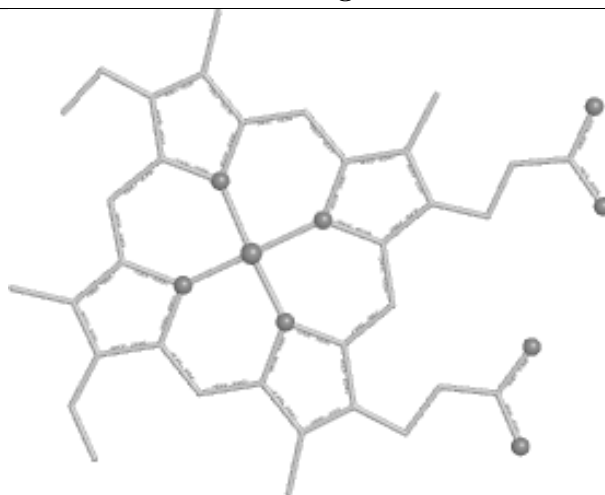
Bond lengths



Bond angles

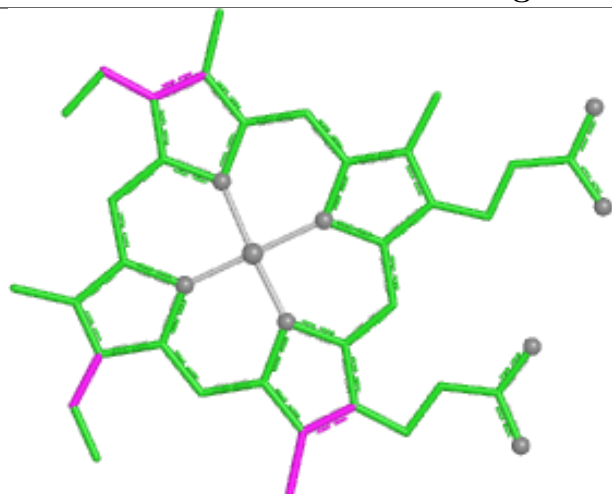


Torsions

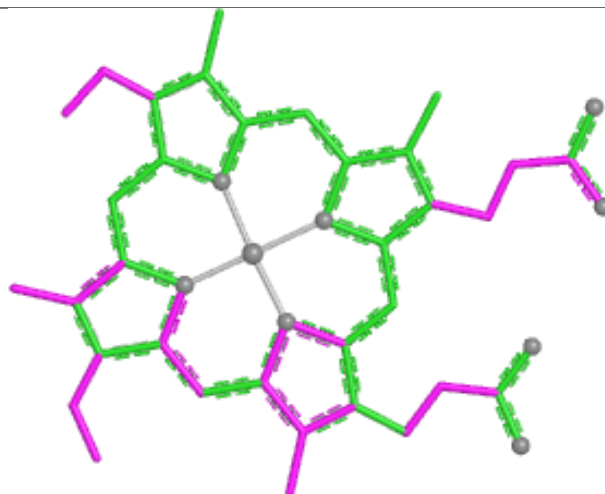


Rings

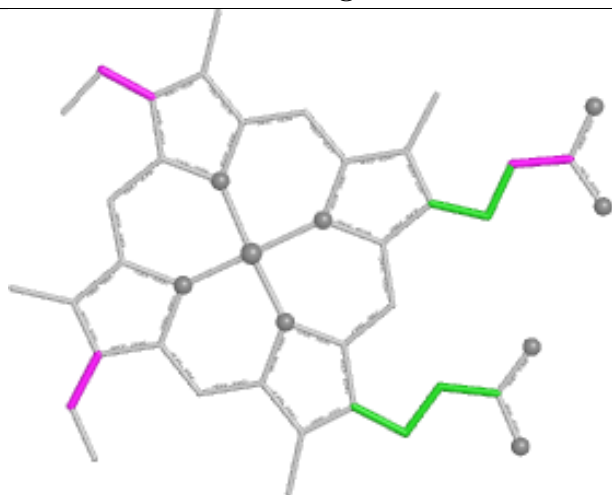
Ligand HEC E 603



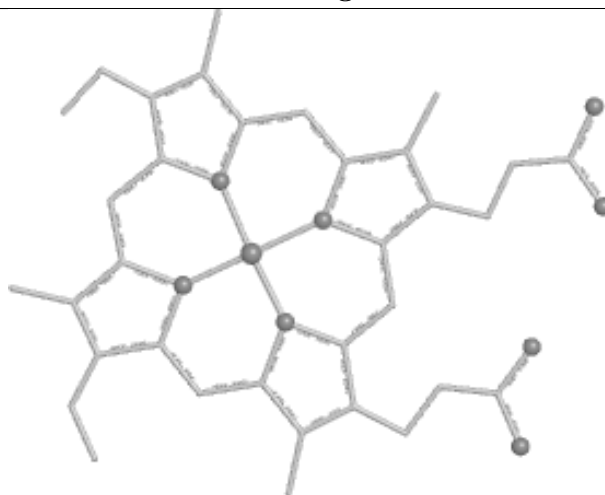
Bond lengths



Bond angles

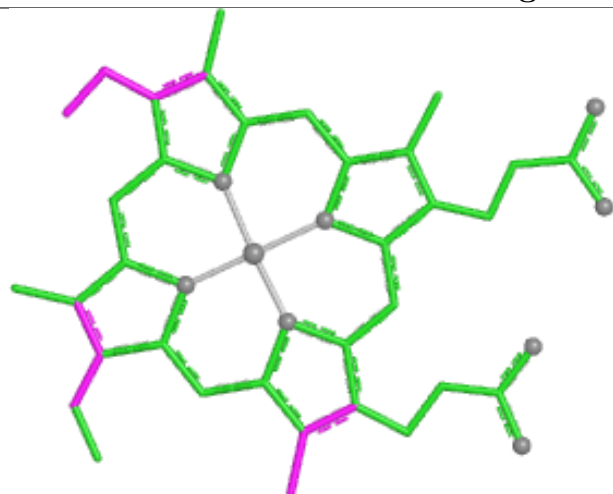


Torsions

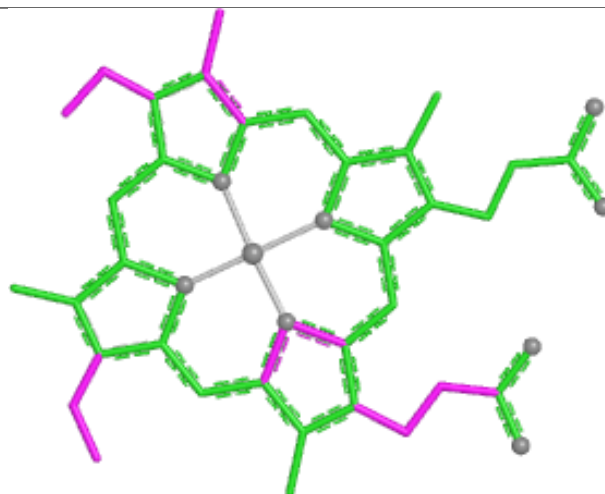


Rings

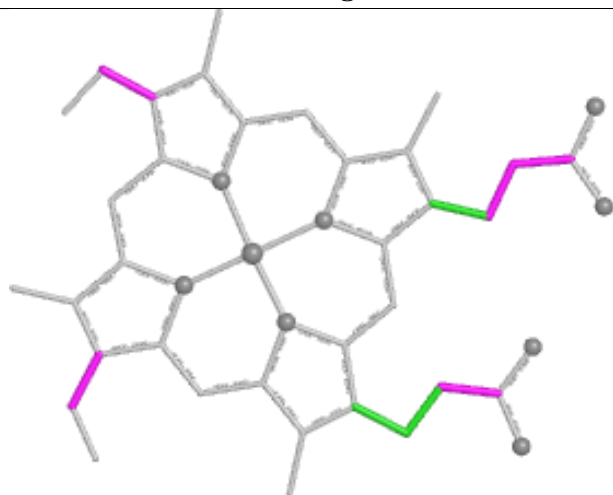
Ligand HEC I 605



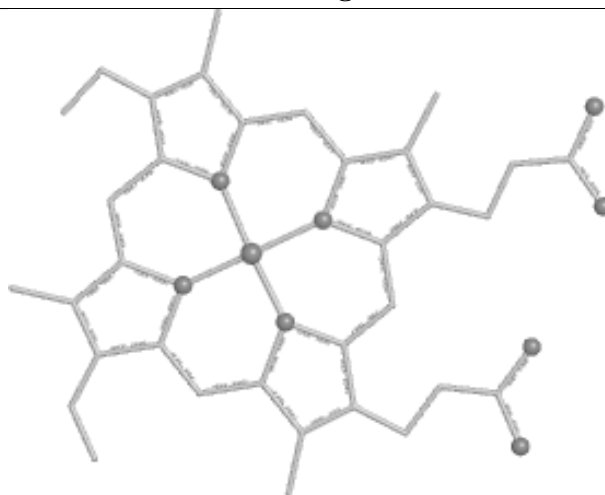
Bond lengths



Bond angles

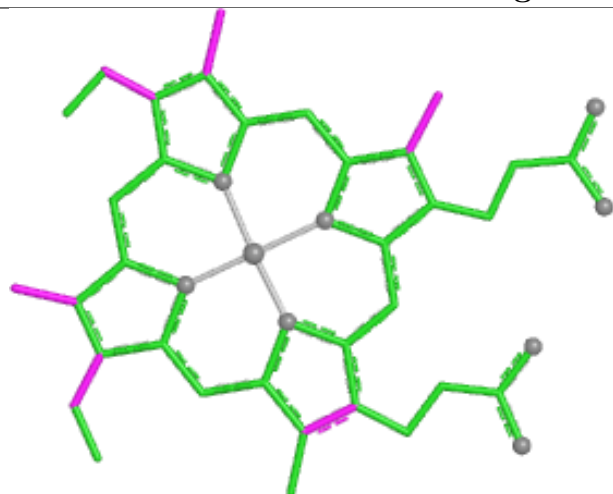


Torsions

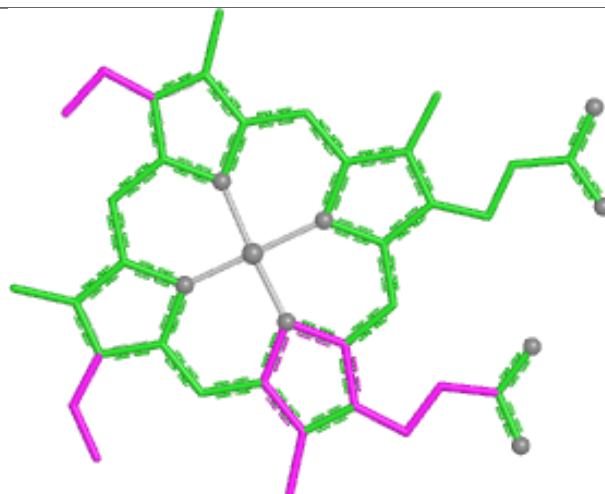


Rings

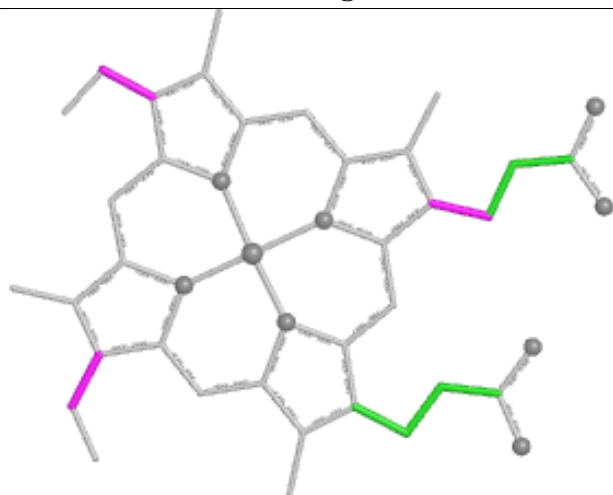
Ligand HEC E 604



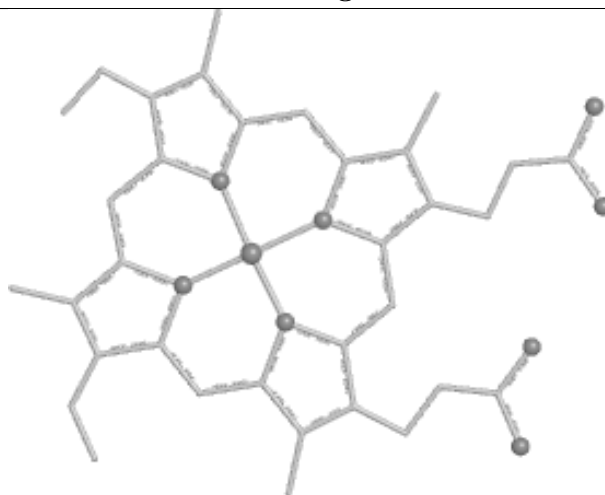
Bond lengths



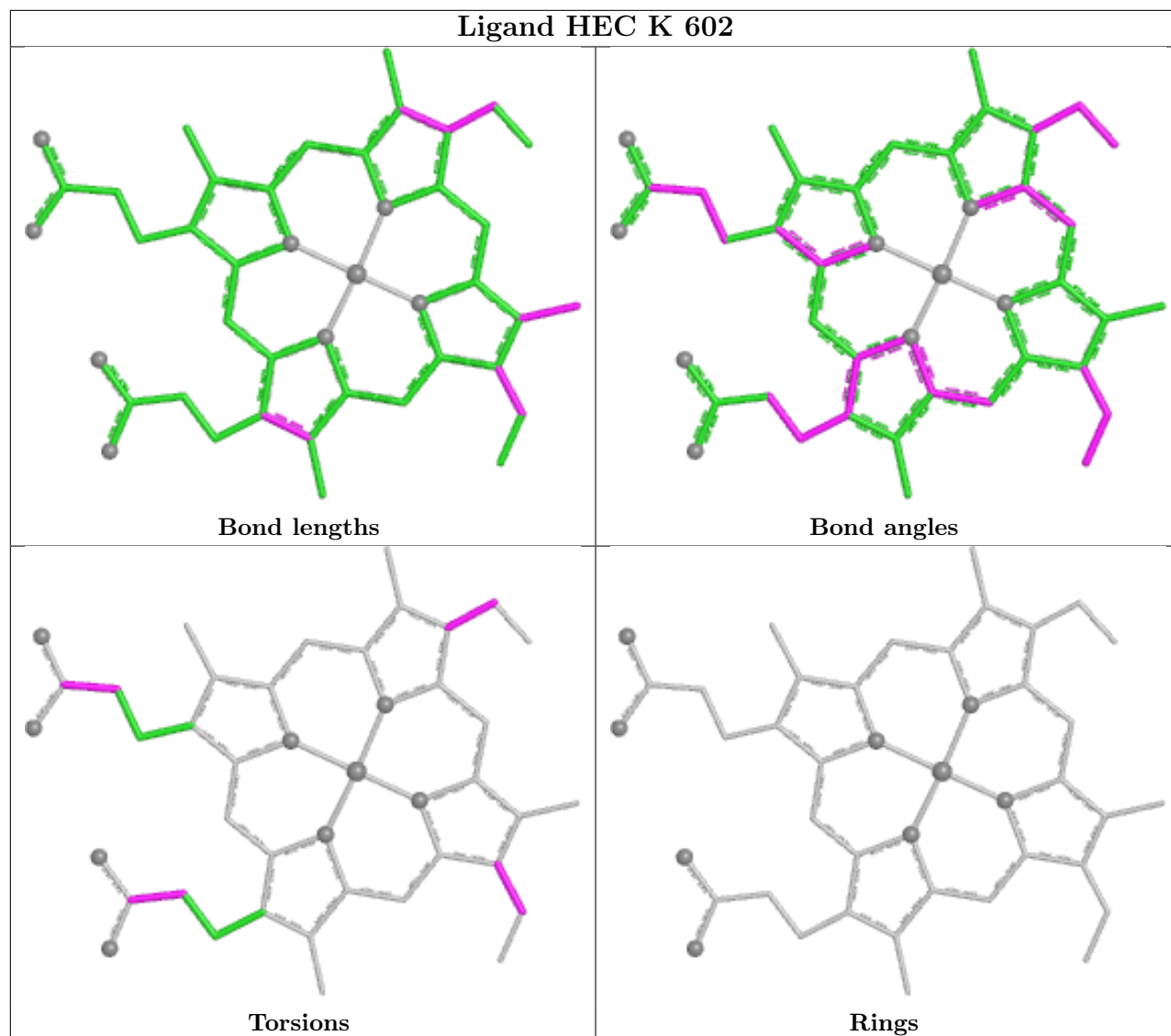
Bond angles



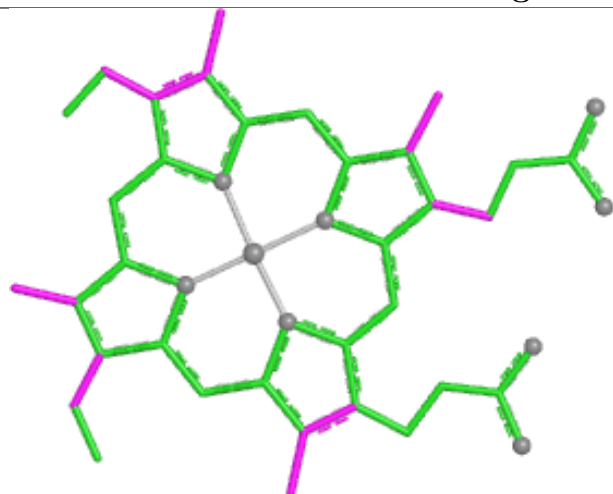
Torsions



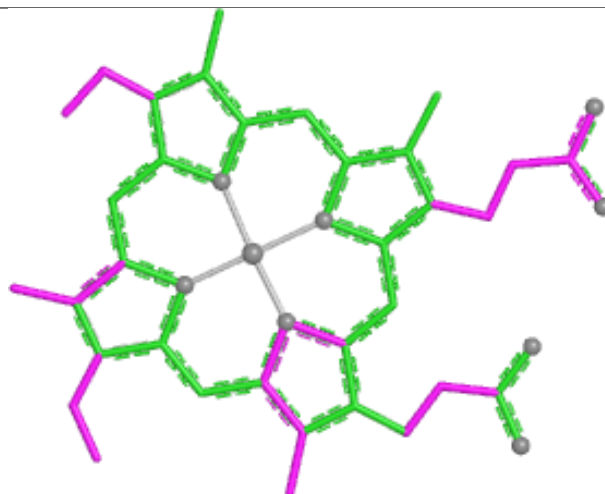
Rings



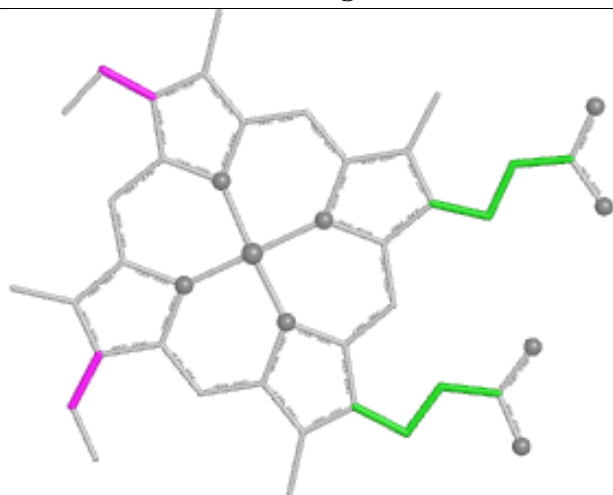
Ligand HEC A 603



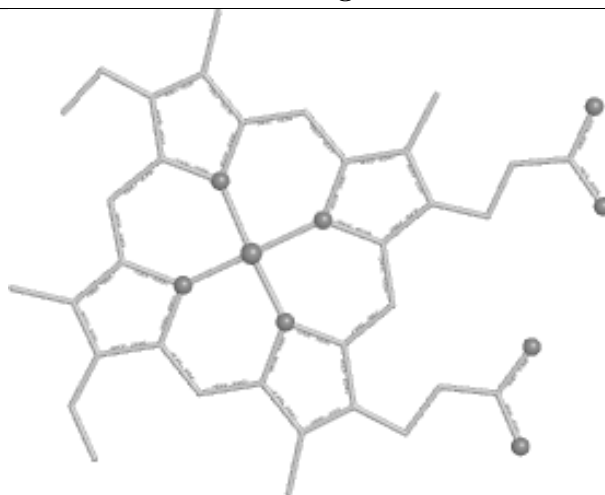
Bond lengths



Bond angles

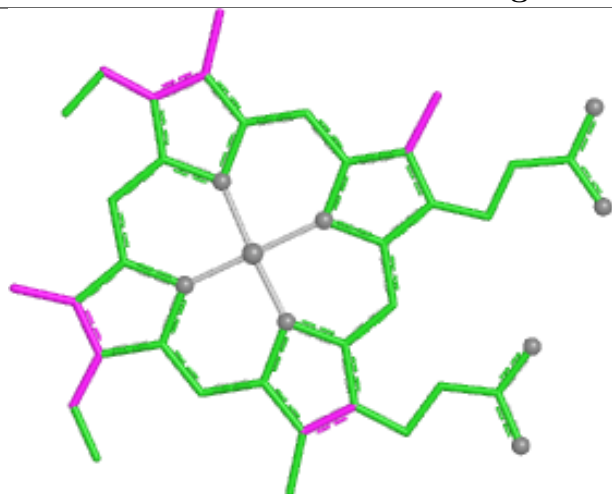


Torsions

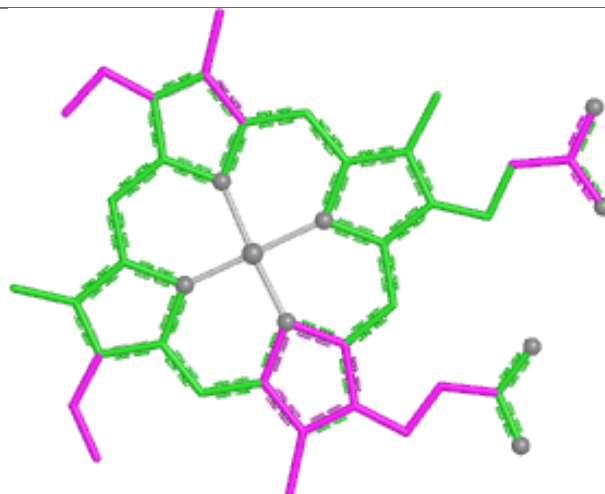


Rings

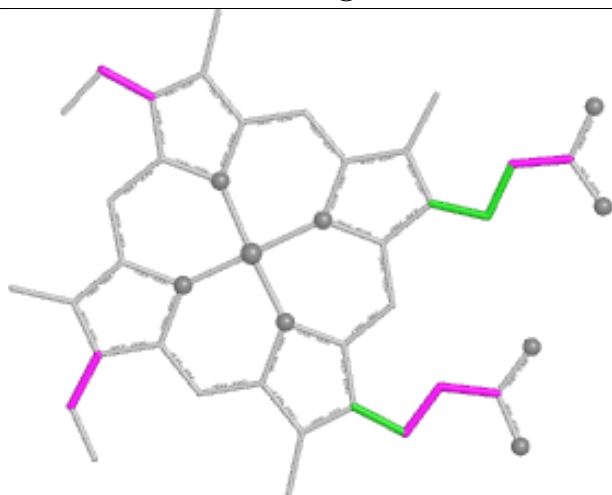
Ligand HEC K 607



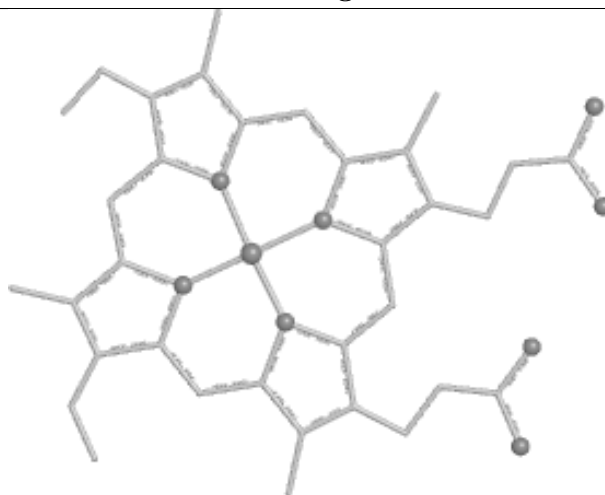
Bond lengths



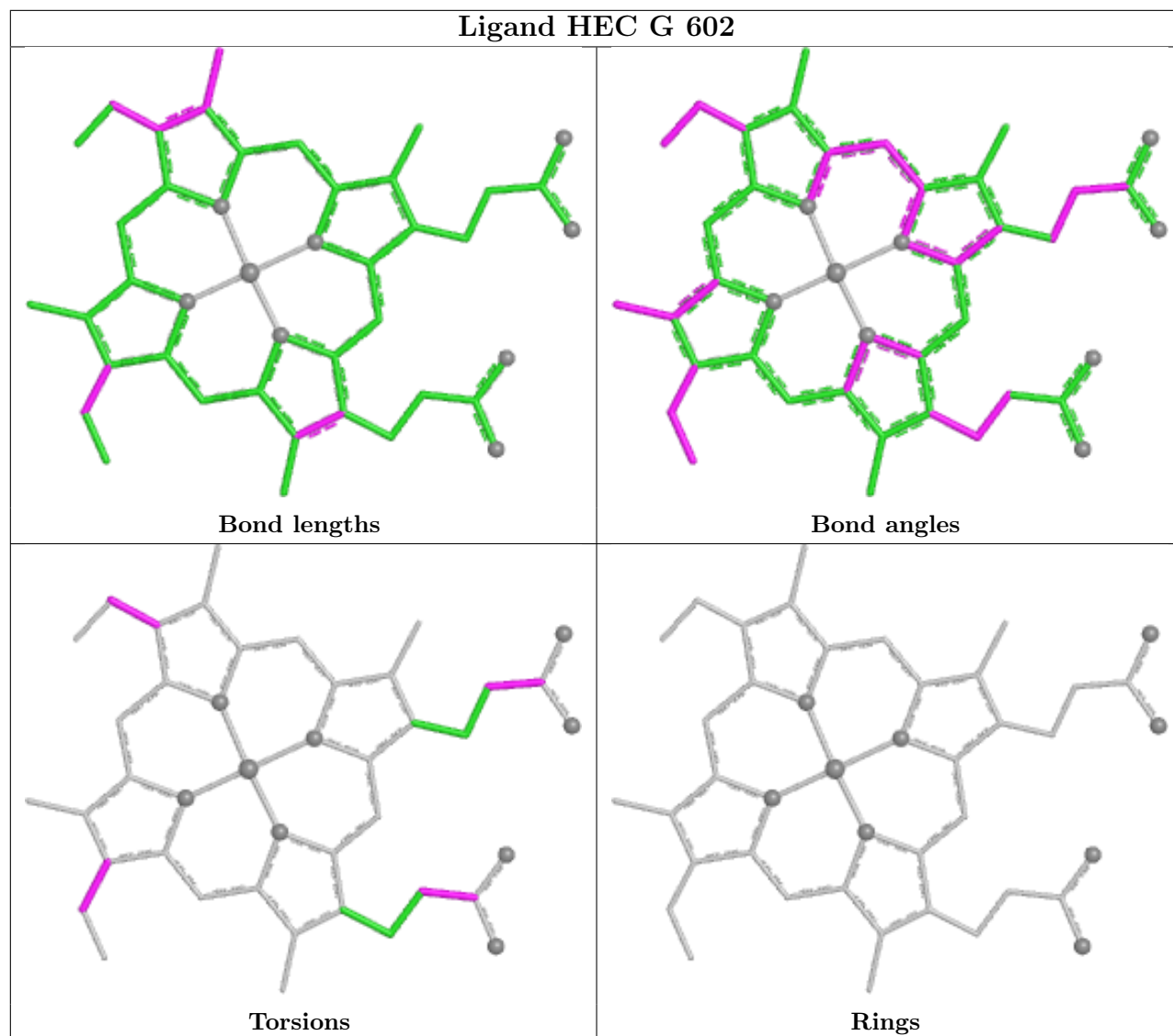
Bond angles



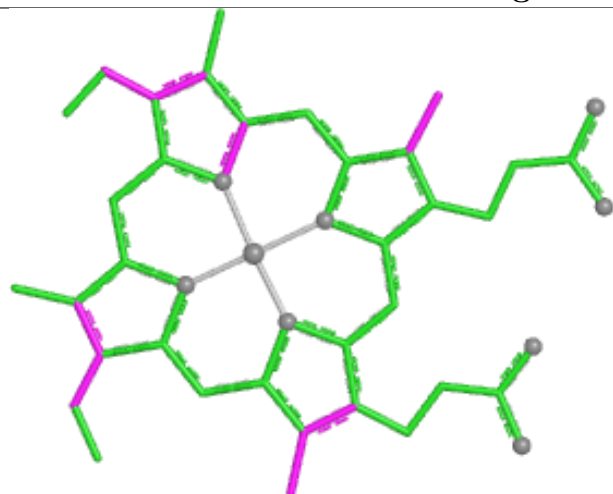
Torsions



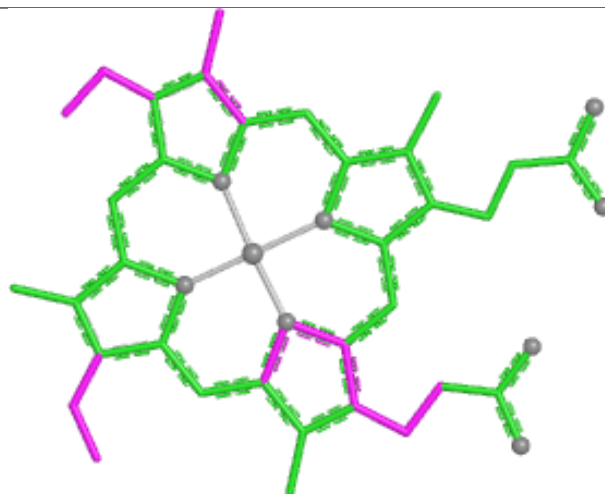
Rings



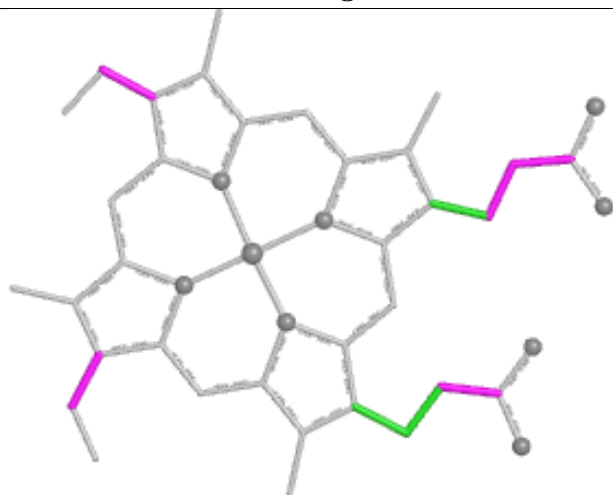
Ligand HEC C 605



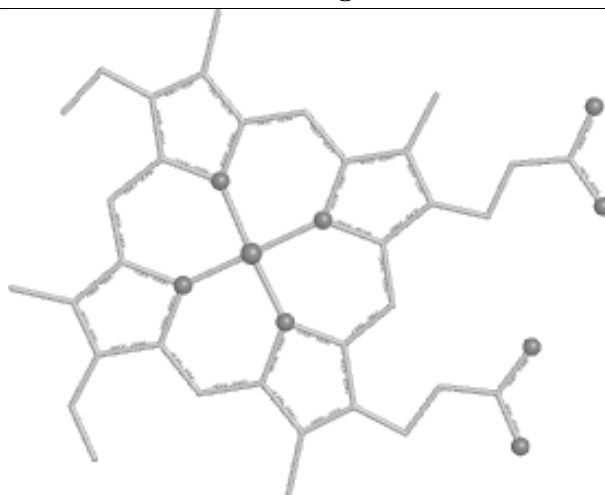
Bond lengths



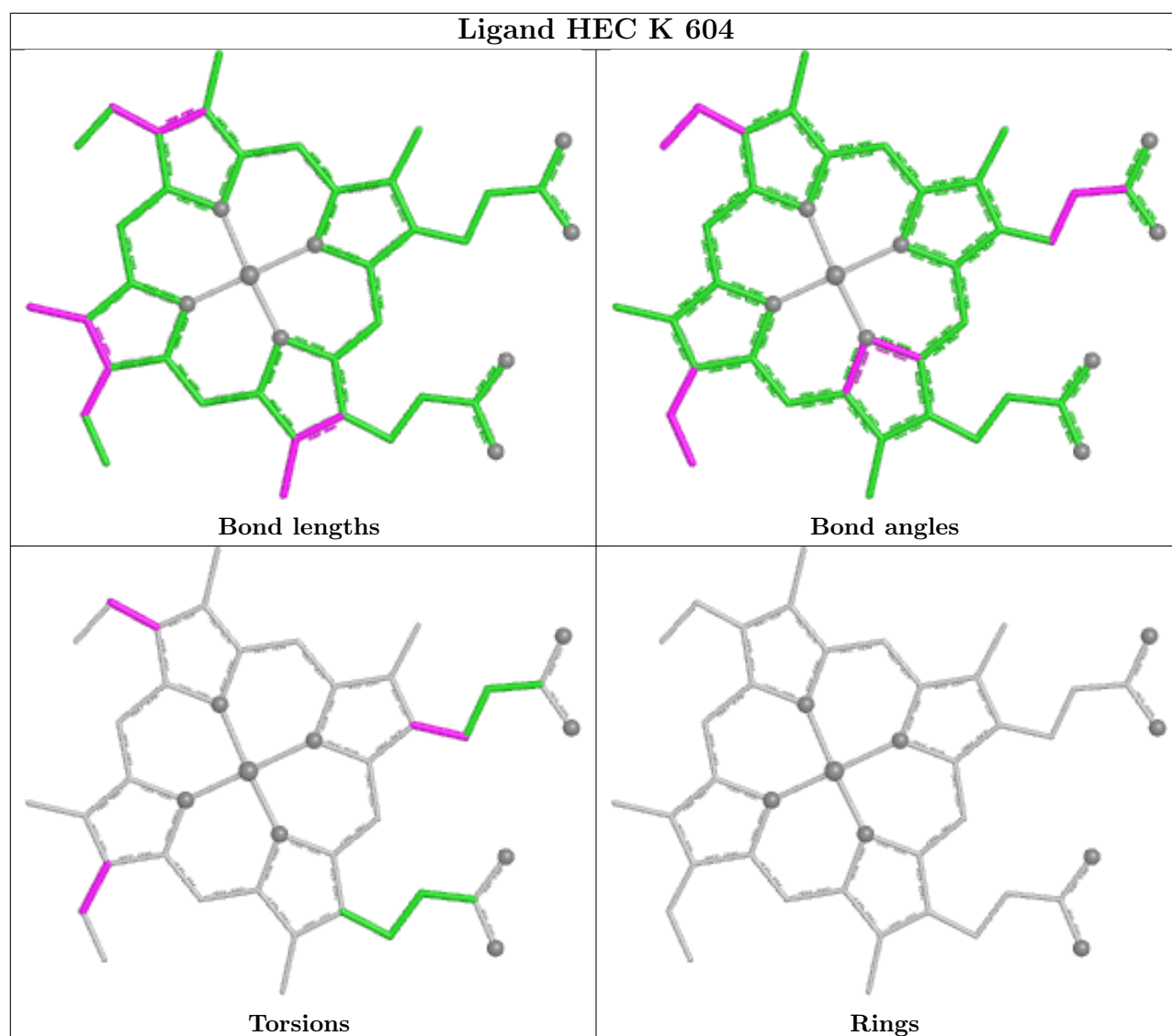
Bond angles



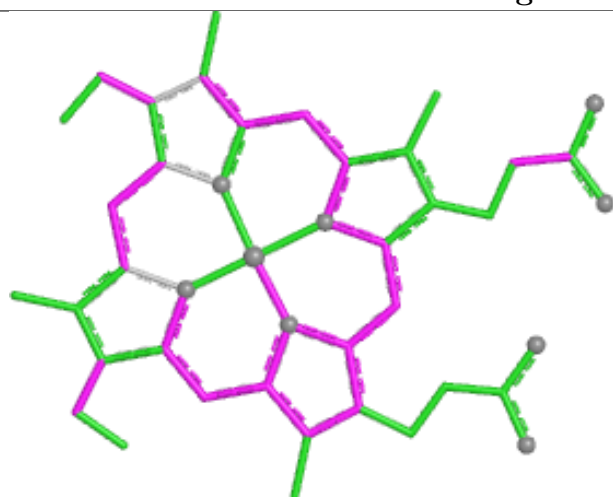
Torsions



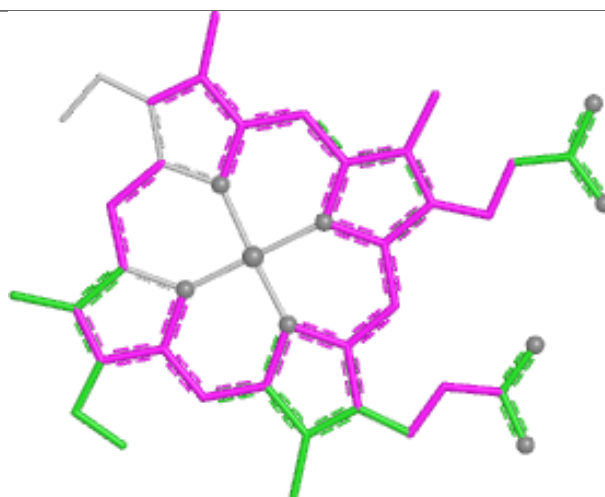
Rings



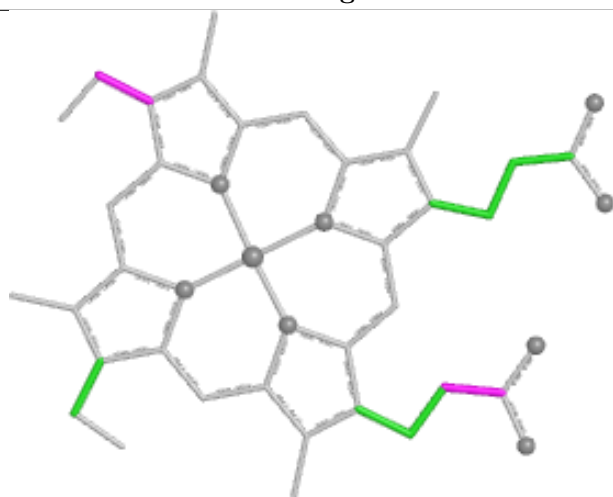
Ligand ISW A 609



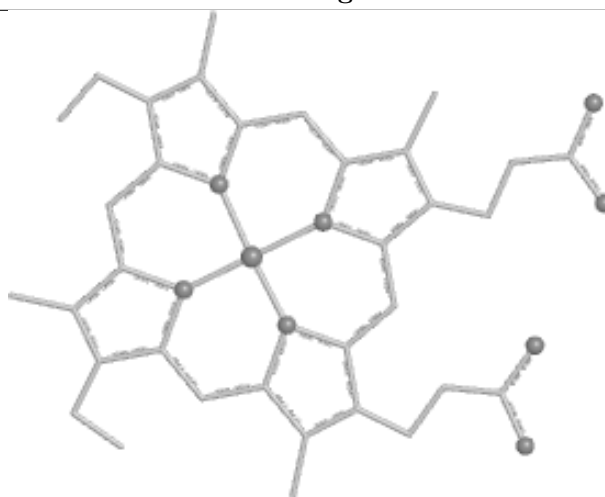
Bond lengths



Bond angles

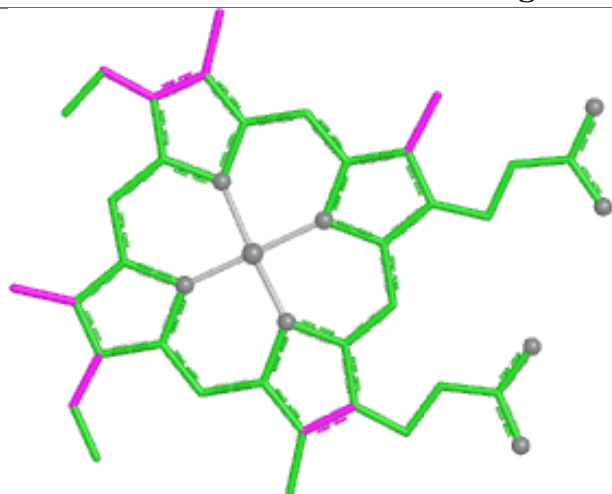


Torsions

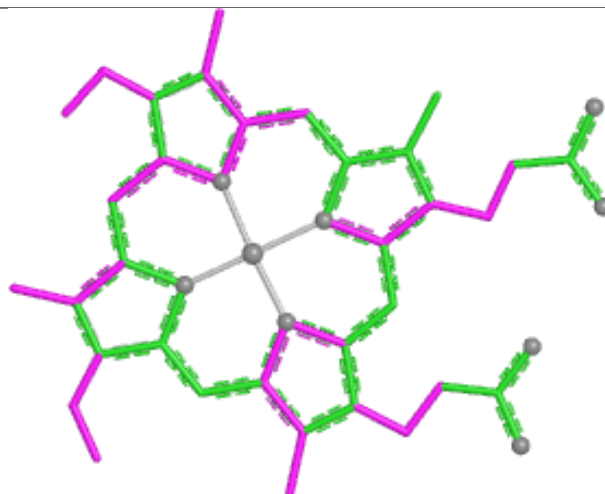


Rings

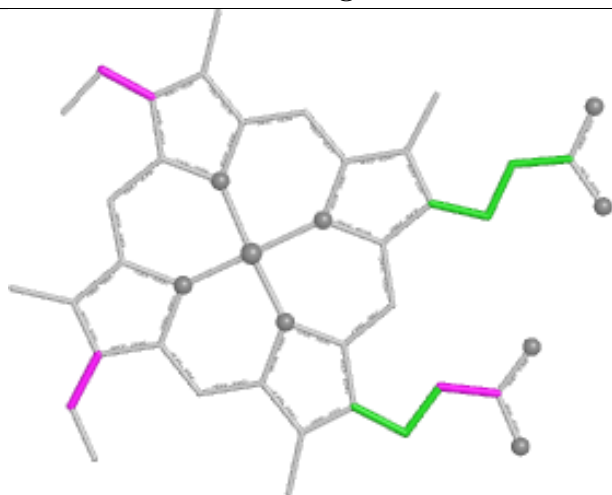
Ligand HEC I 606



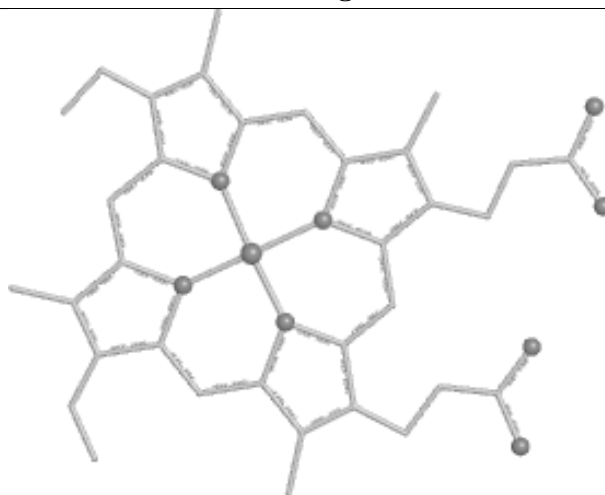
Bond lengths



Bond angles

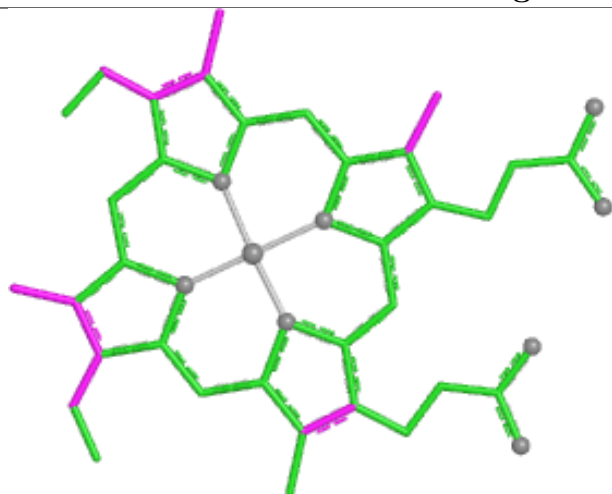


Torsions

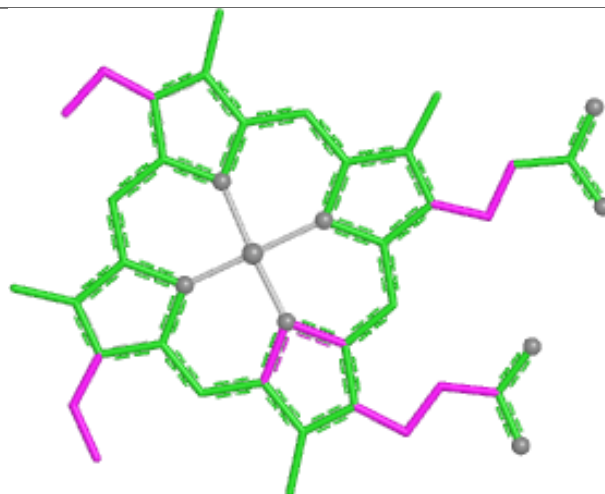


Rings

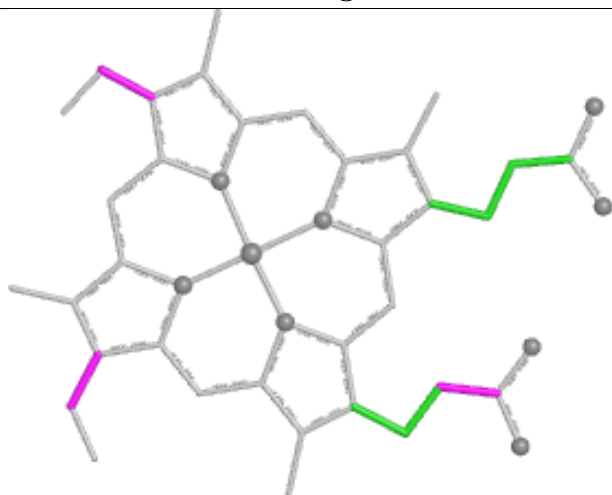
Ligand HEC E 606



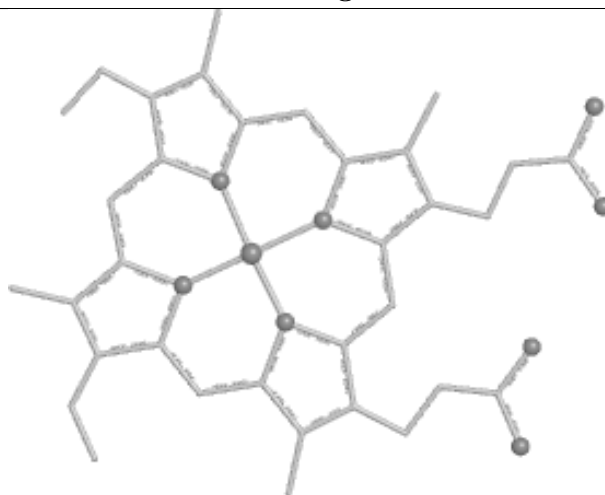
Bond lengths



Bond angles

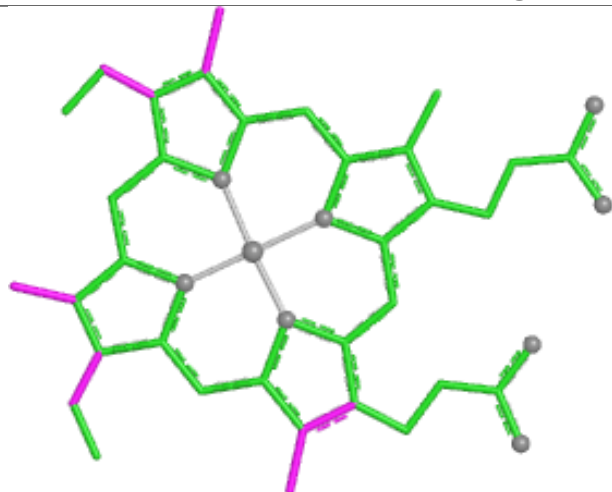


Torsions

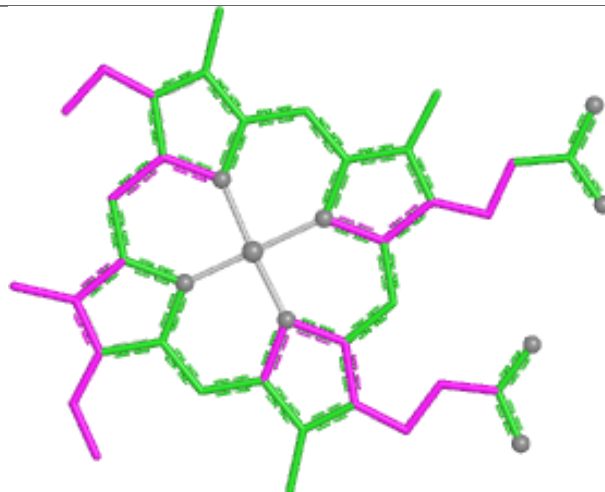


Rings

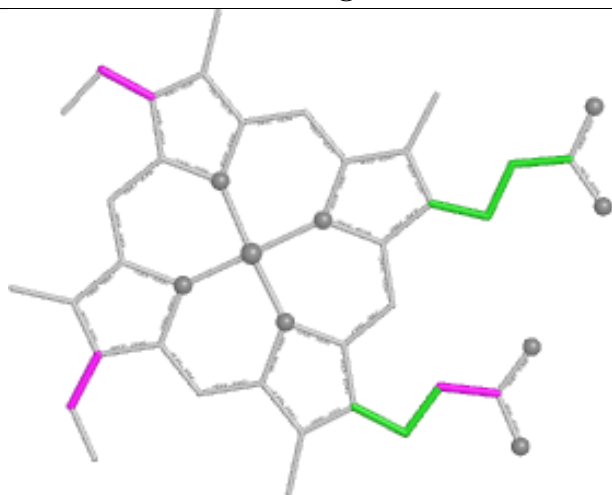
Ligand HEC G 603



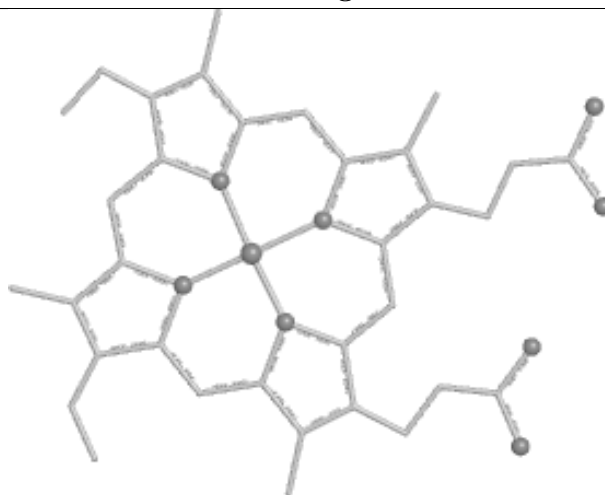
Bond lengths



Bond angles

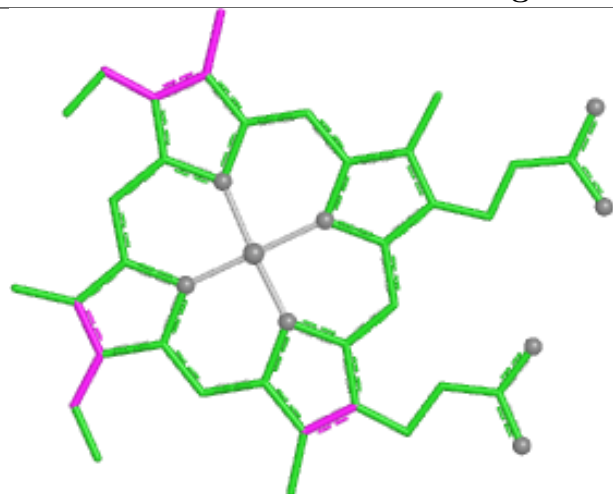


Torsions

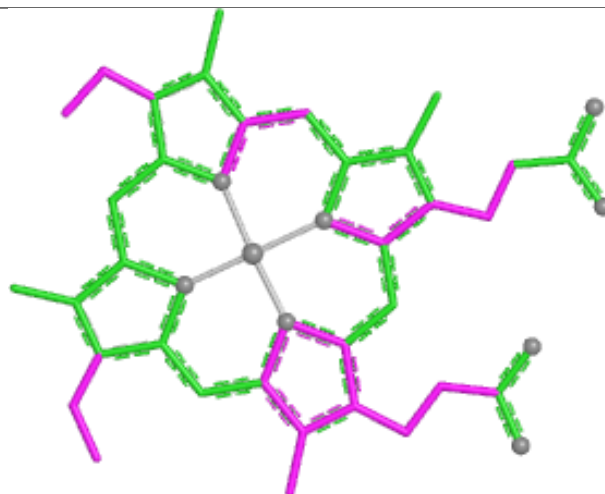


Rings

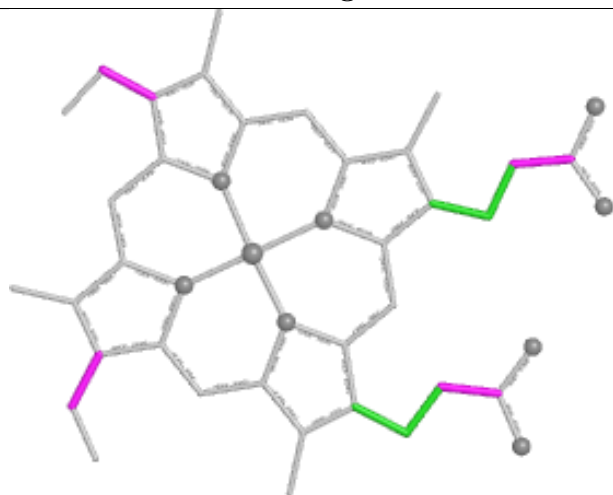
Ligand HEC G 606



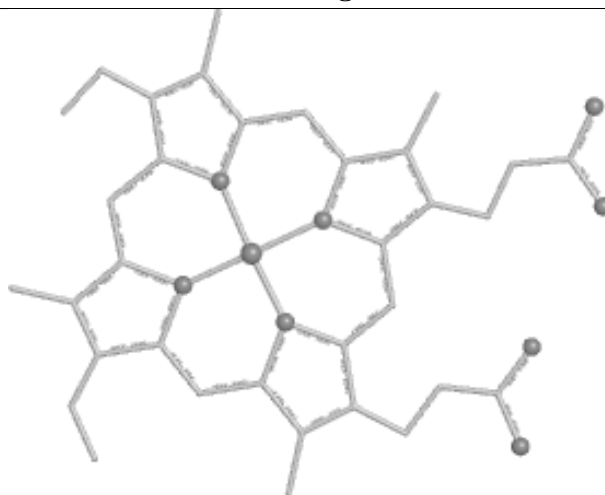
Bond lengths



Bond angles

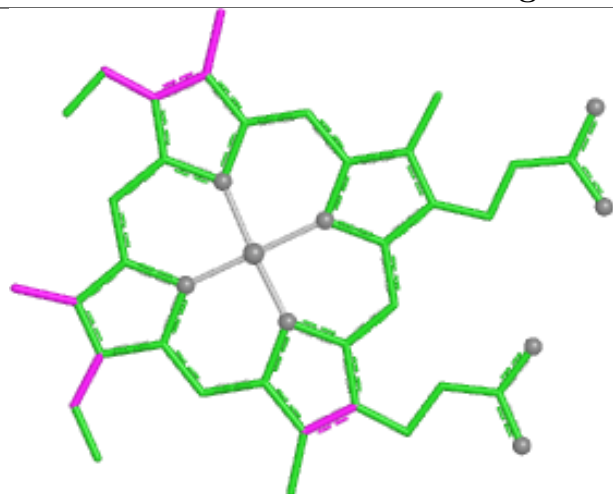


Torsions

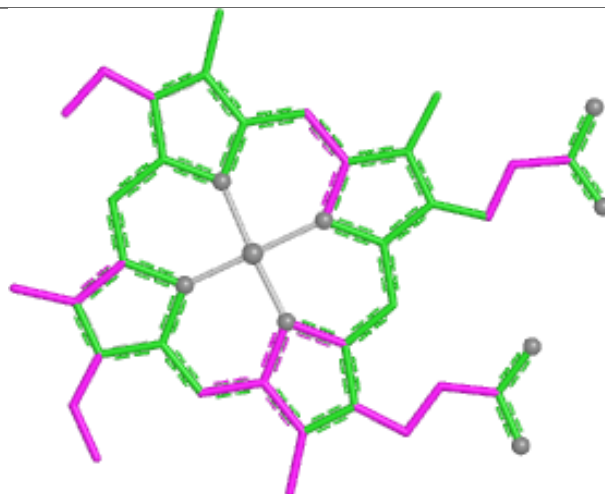


Rings

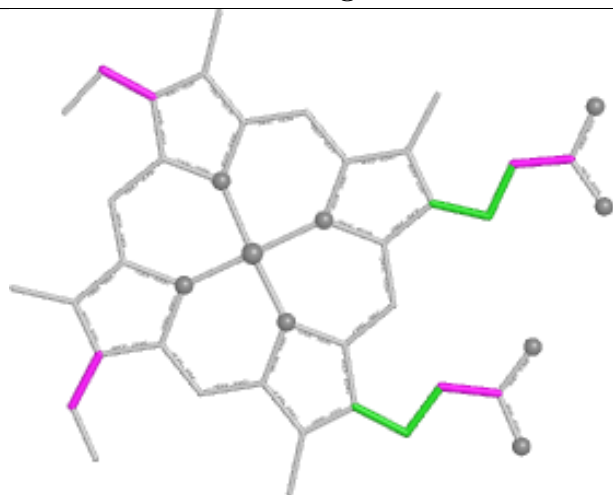
Ligand HEC I 602



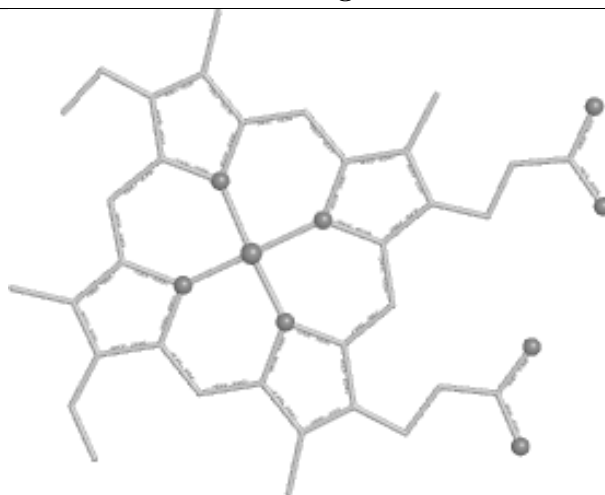
Bond lengths



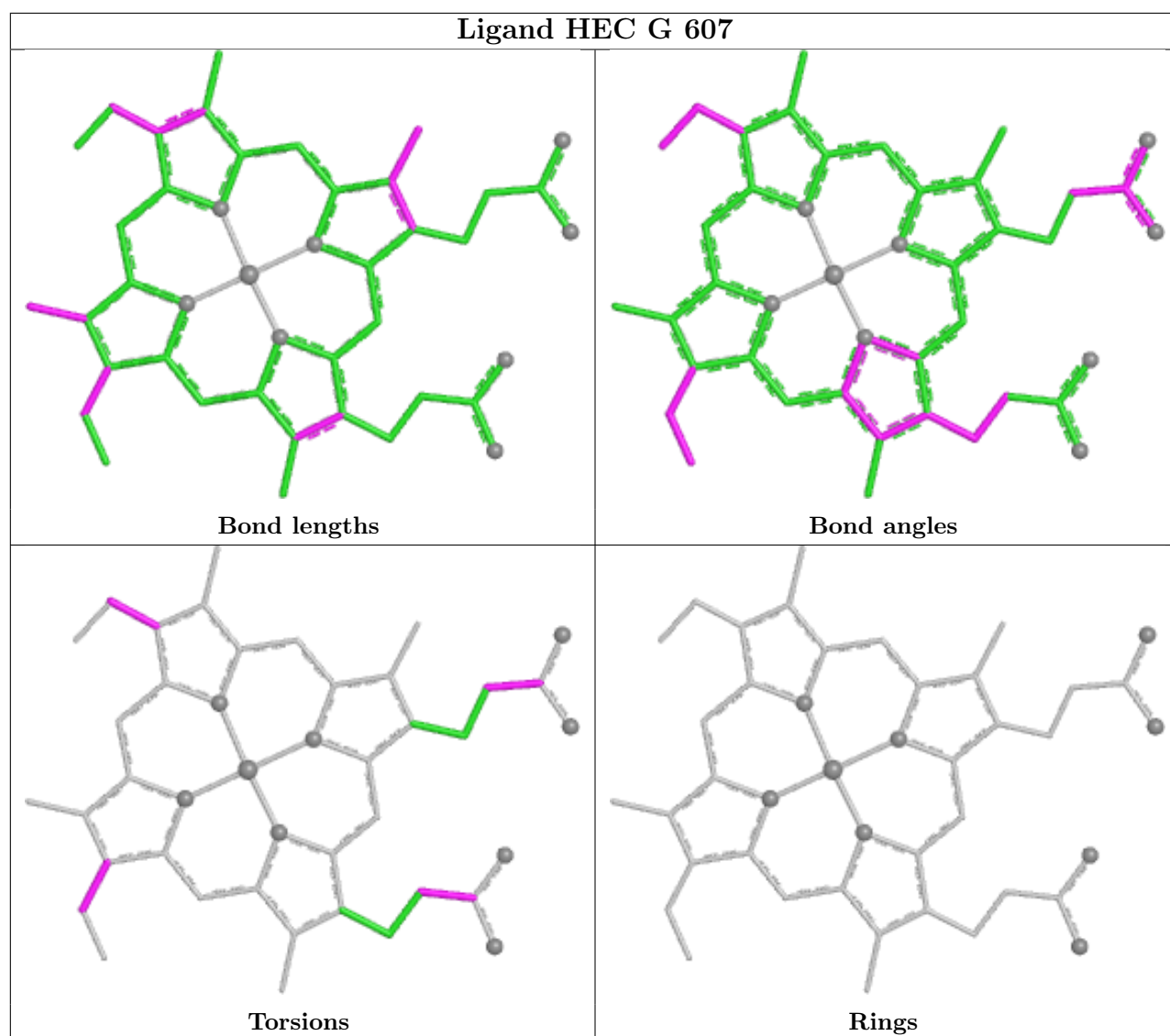
Bond angles



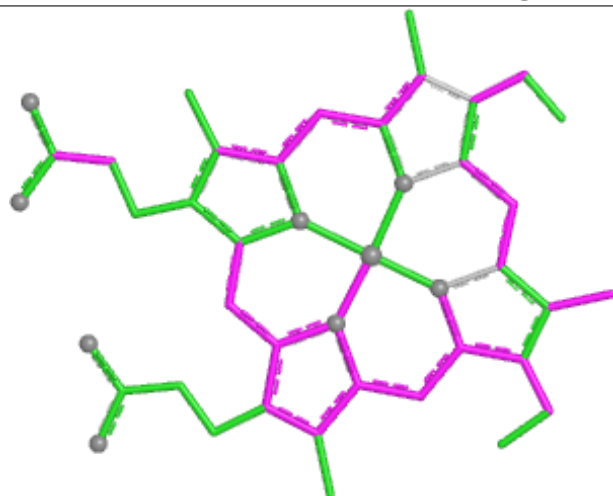
Torsions



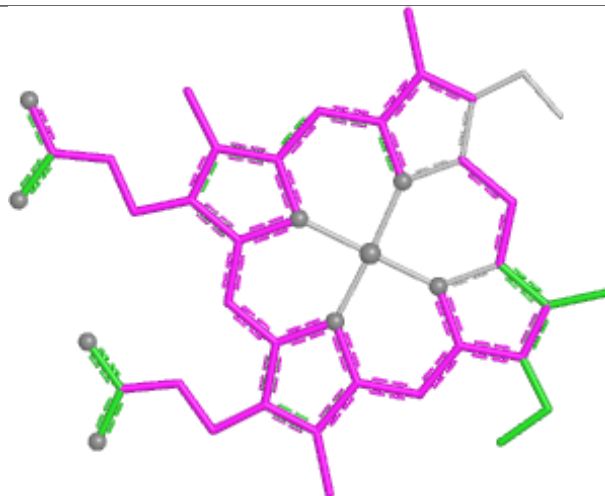
Rings



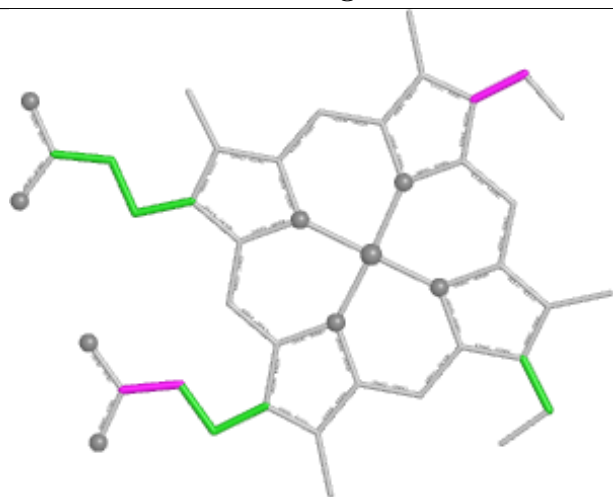
Ligand ISW A 608



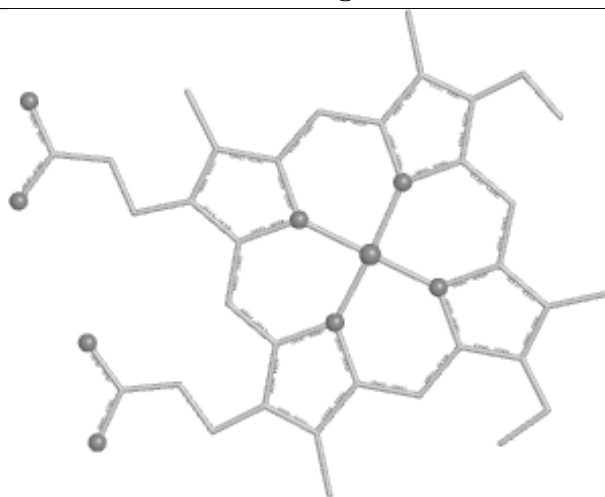
Bond lengths



Bond angles

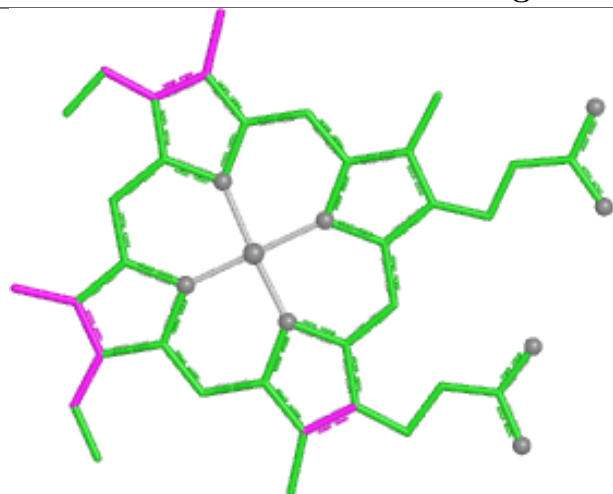


Torsions

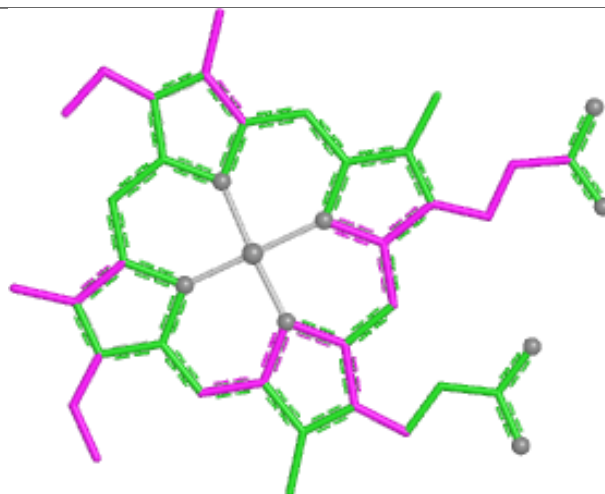


Rings

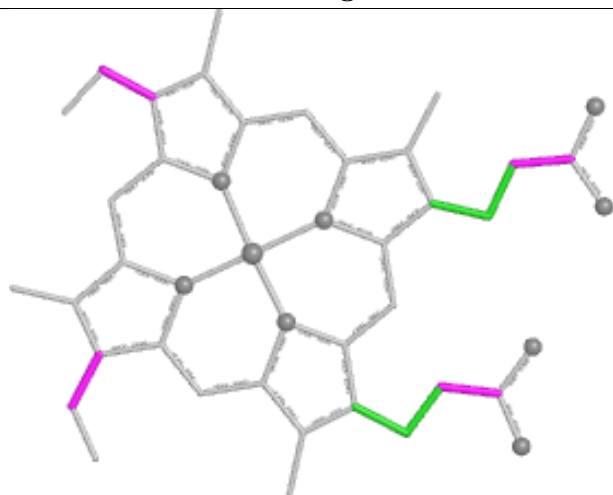
Ligand HEC C 602



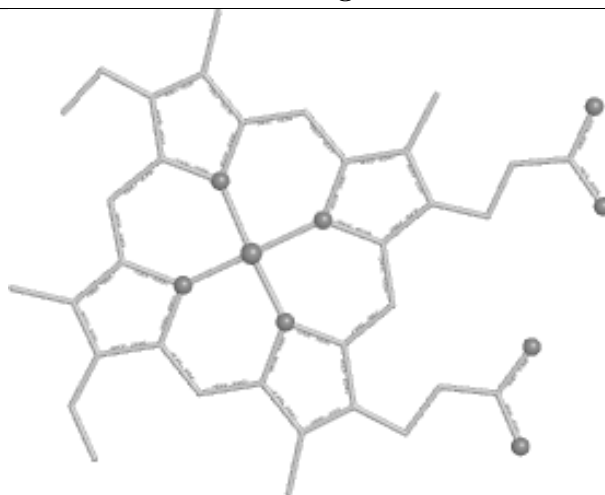
Bond lengths



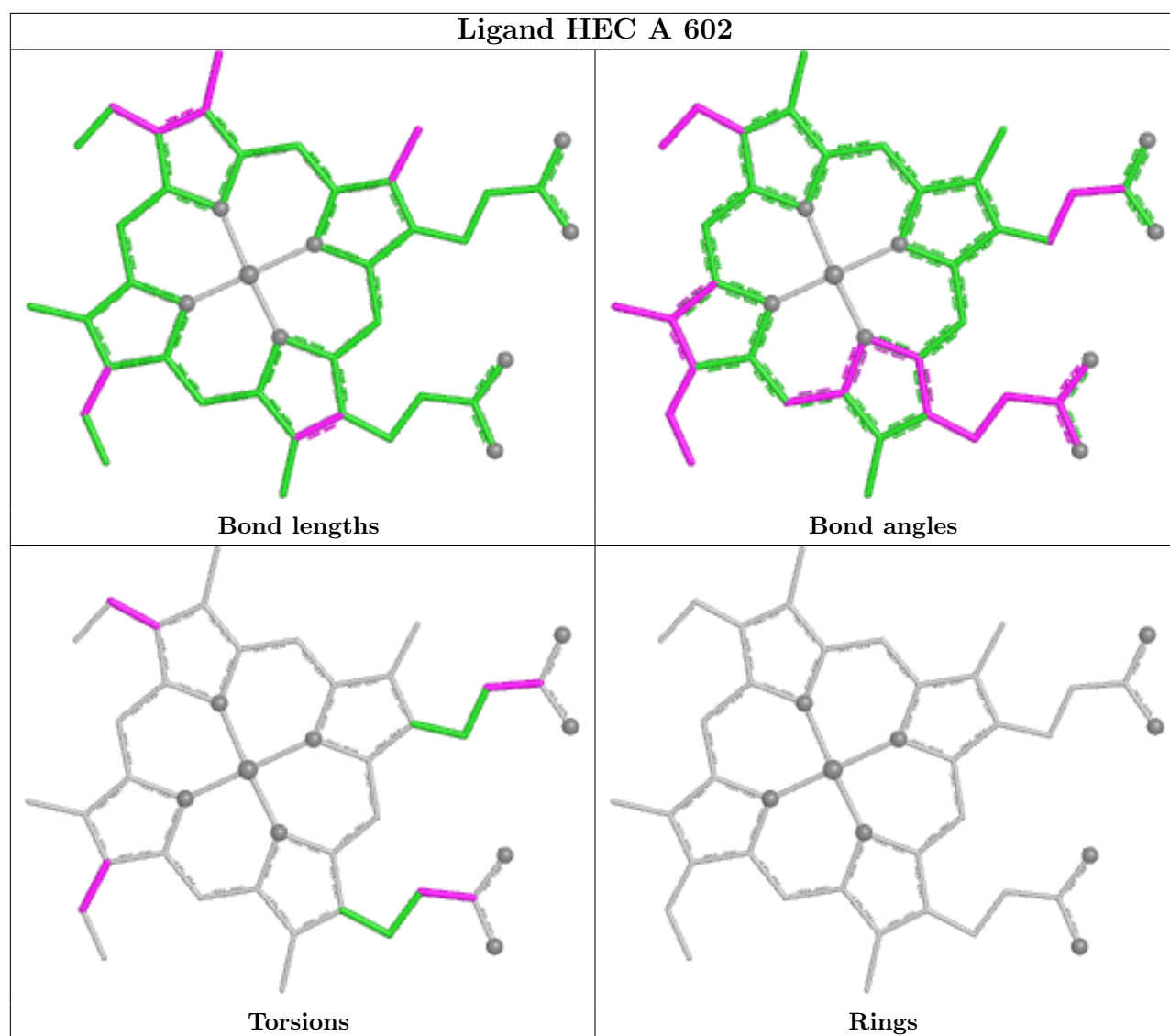
Bond angles



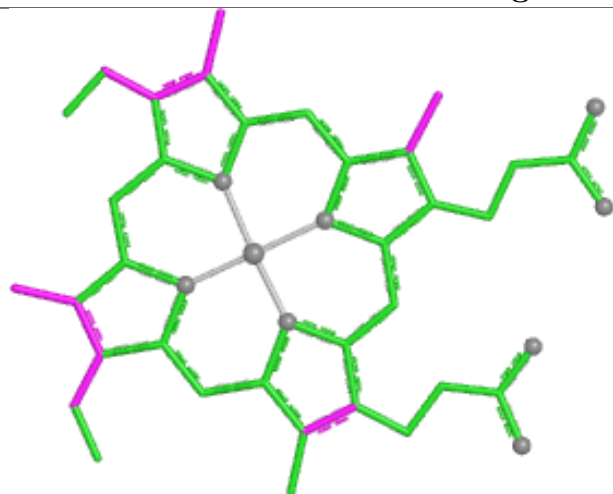
Torsions



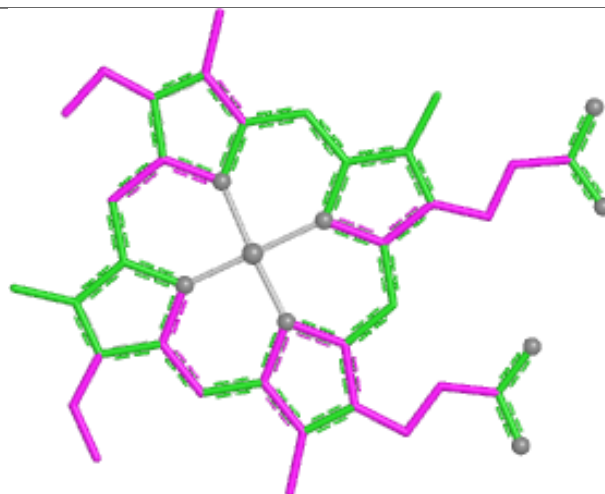
Rings



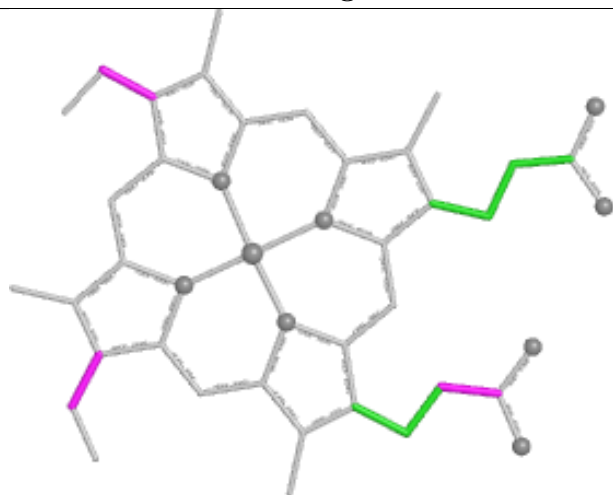
Ligand HEC K 606



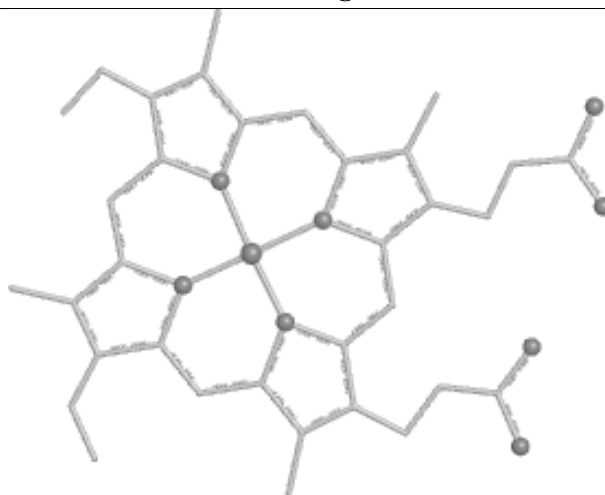
Bond lengths



Bond angles

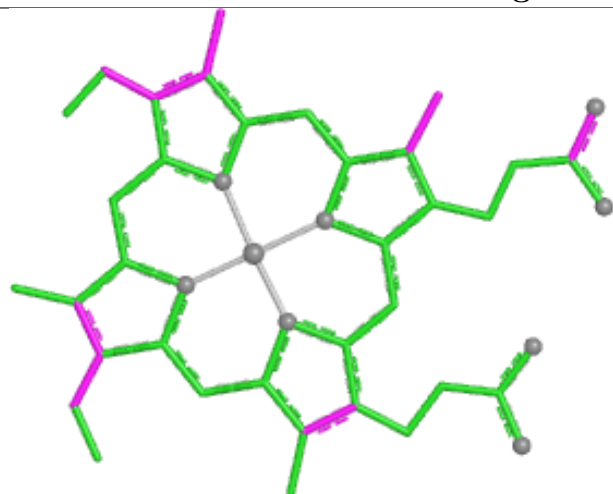


Torsions

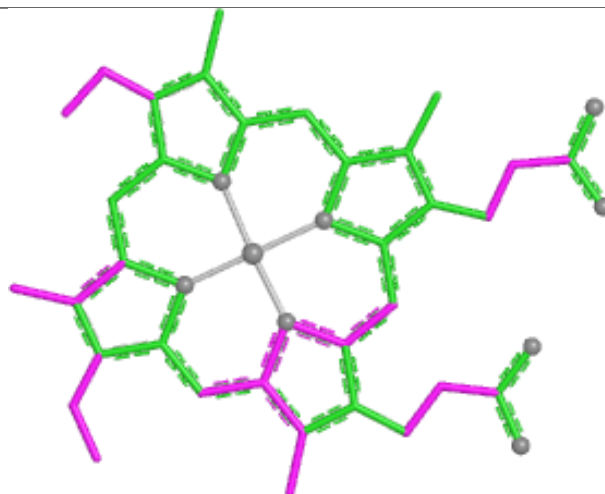


Rings

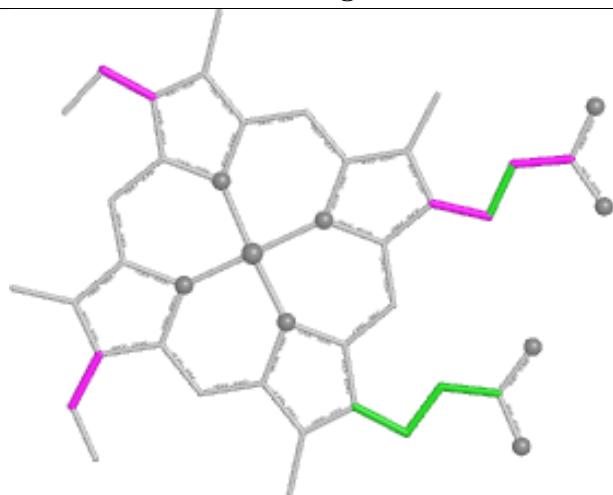
Ligand HEC C 604



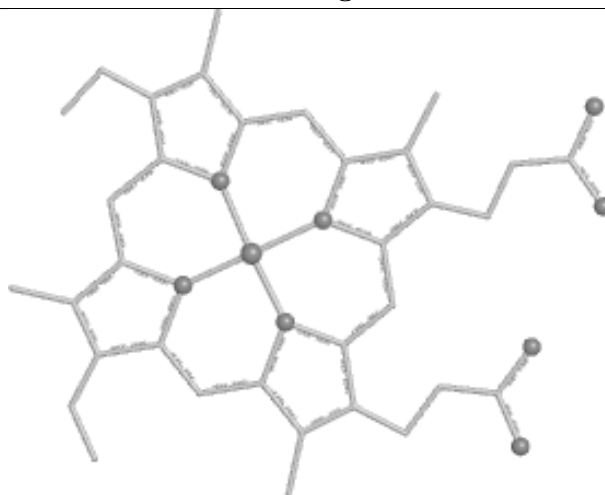
Bond lengths



Bond angles

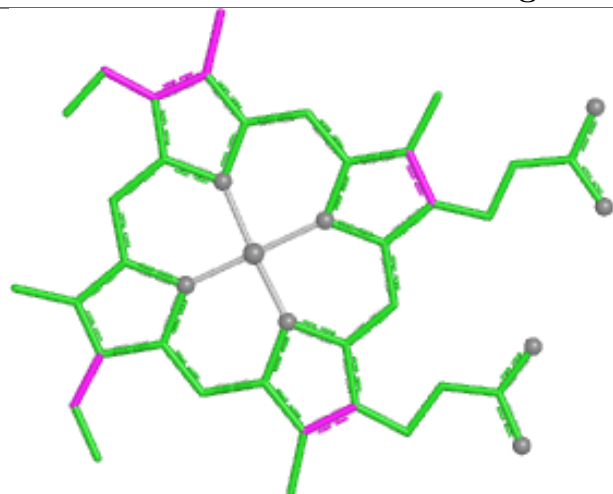


Torsions

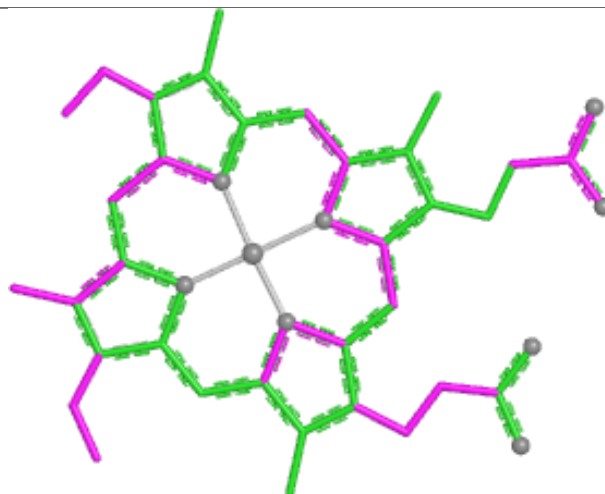


Rings

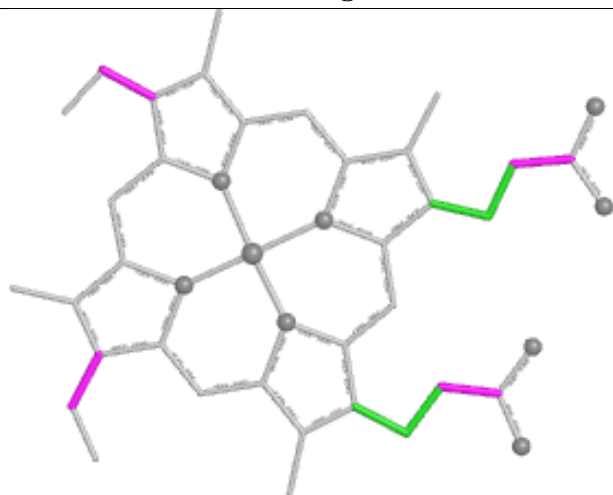
Ligand HEC I 607



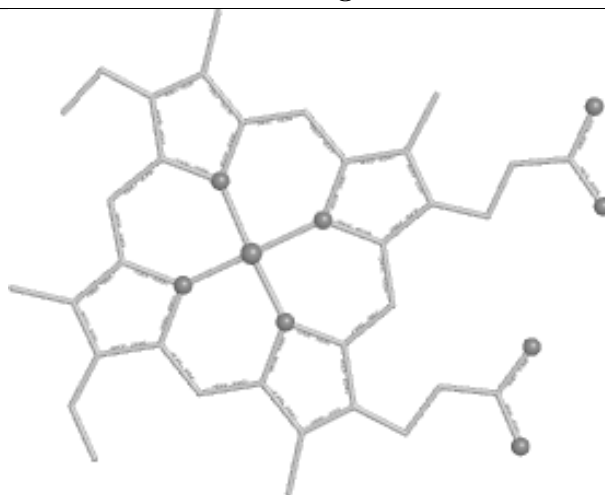
Bond lengths



Bond angles

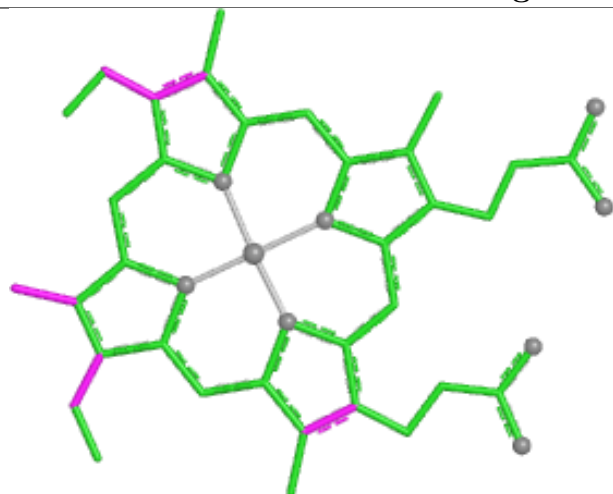


Torsions

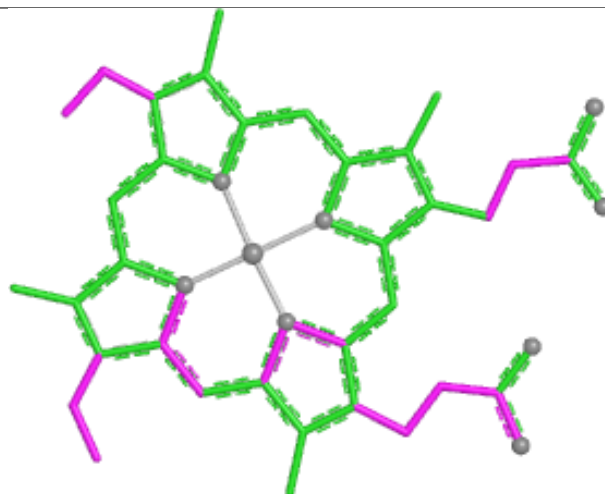


Rings

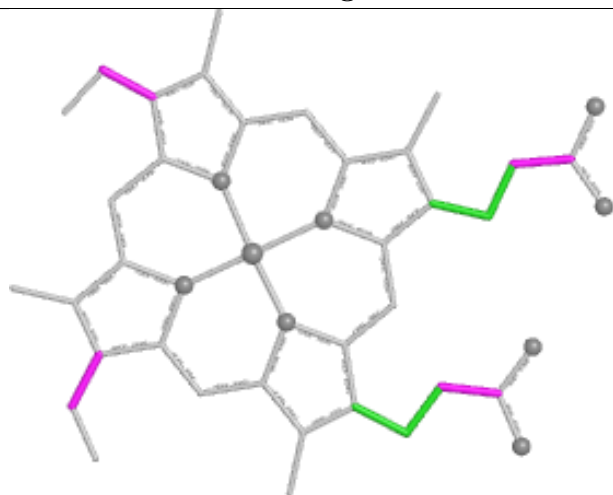
Ligand HEC C 601



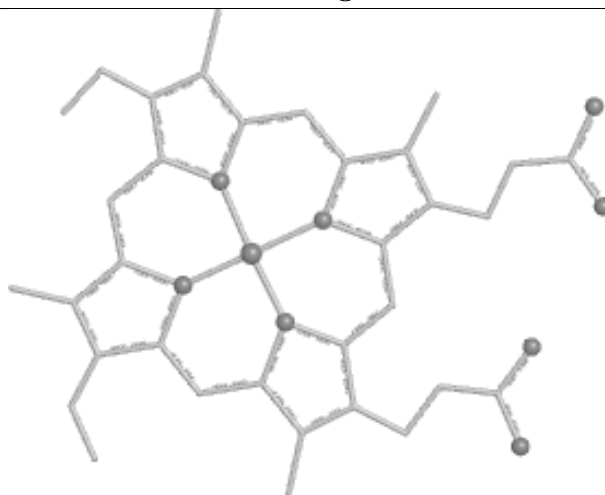
Bond lengths



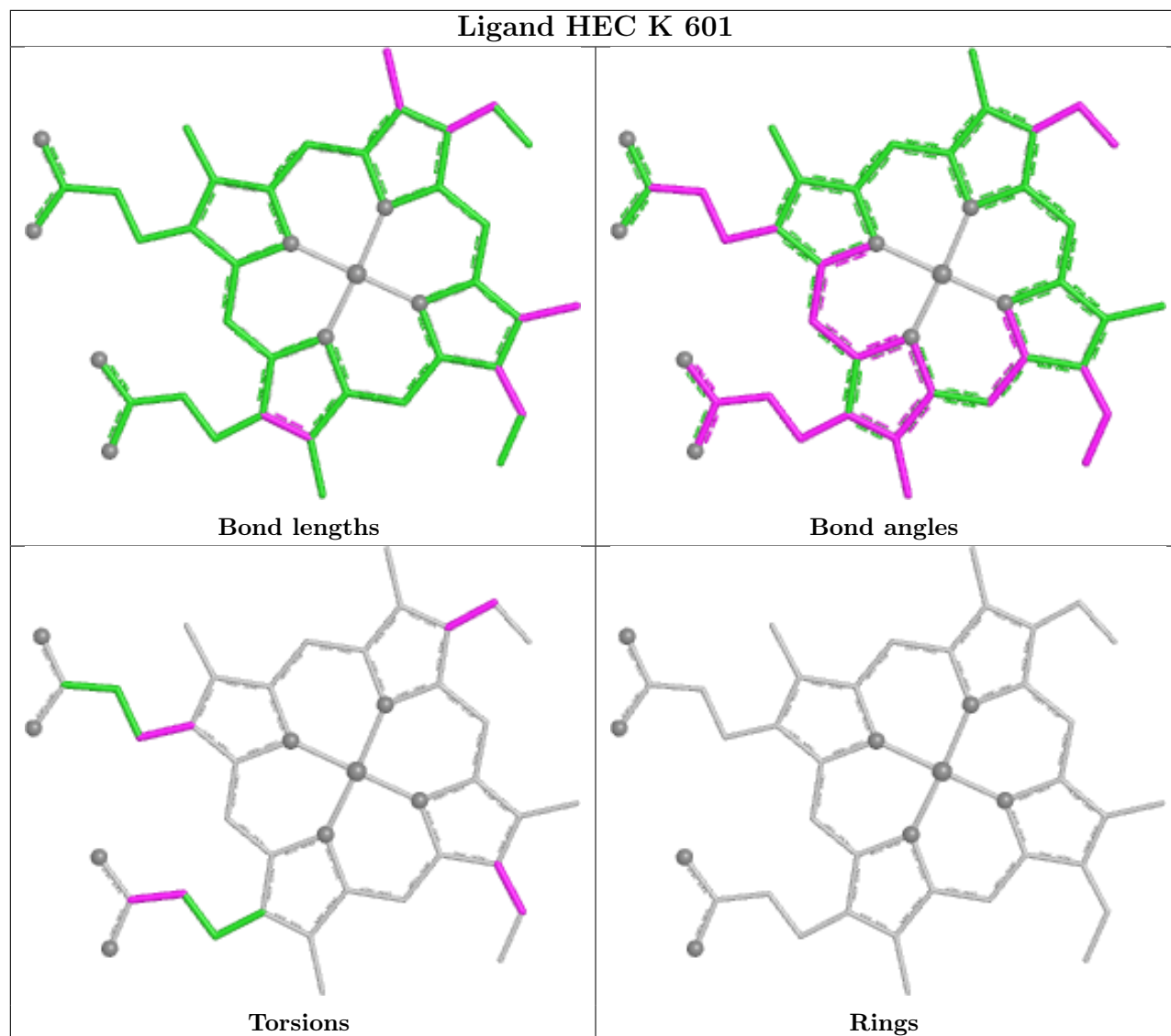
Bond angles



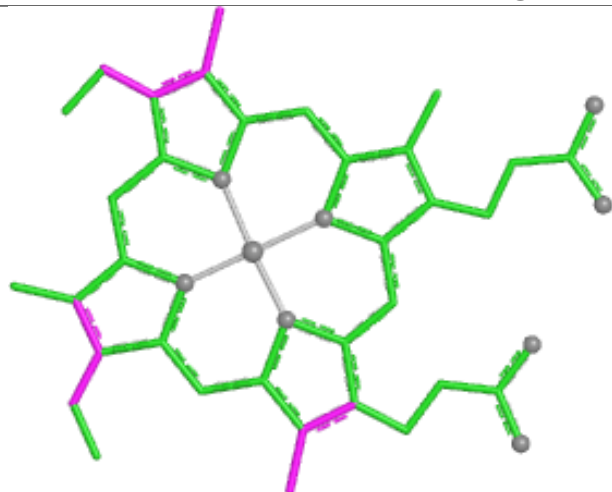
Torsions



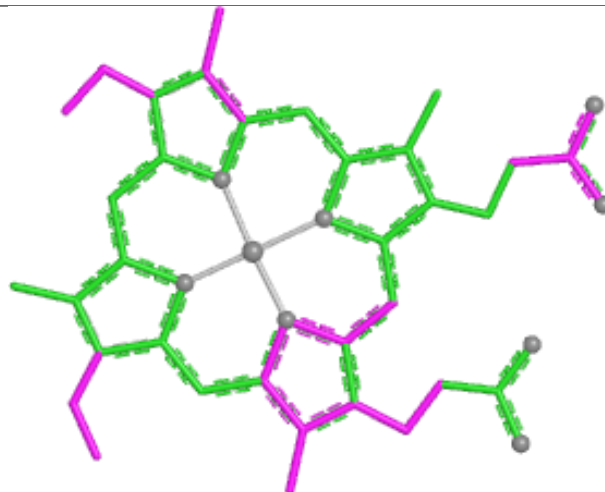
Rings



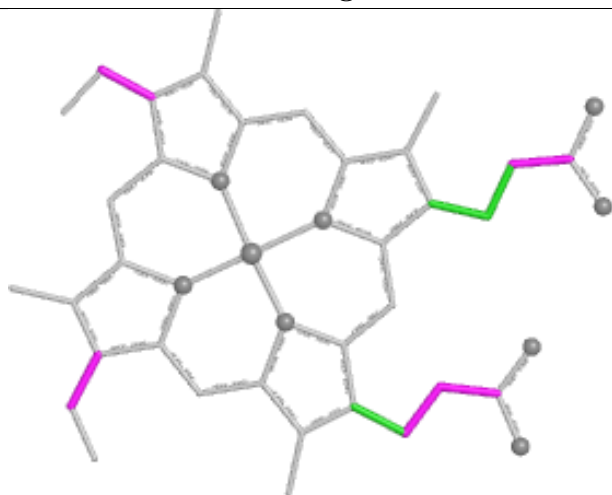
Ligand HEC C 607



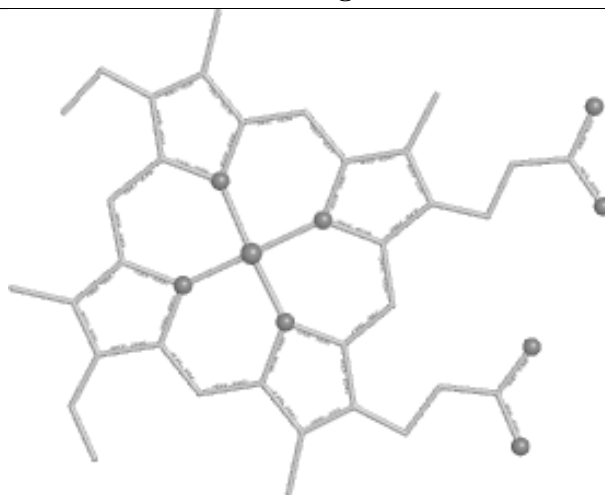
Bond lengths



Bond angles

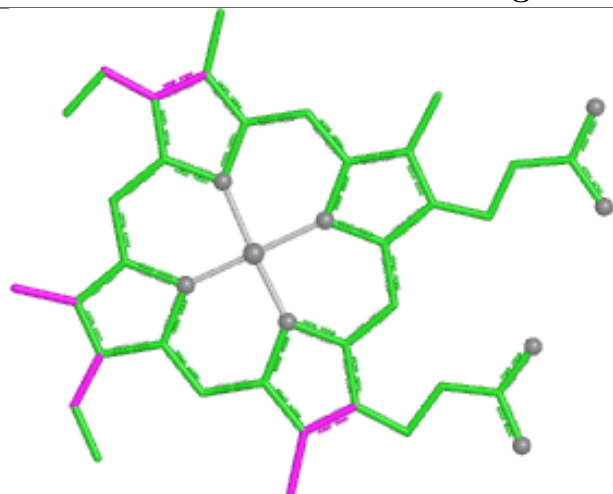


Torsions

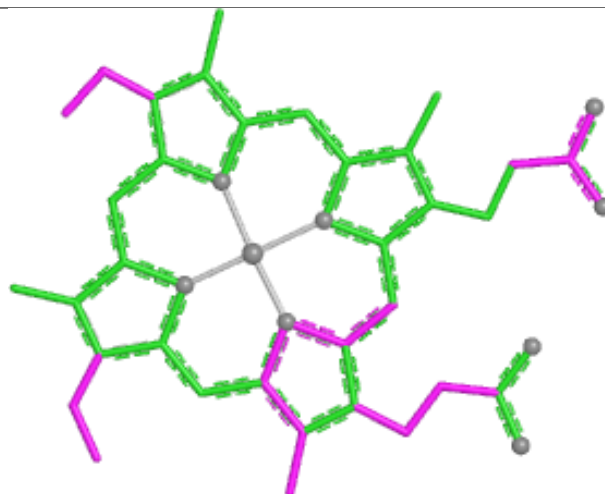


Rings

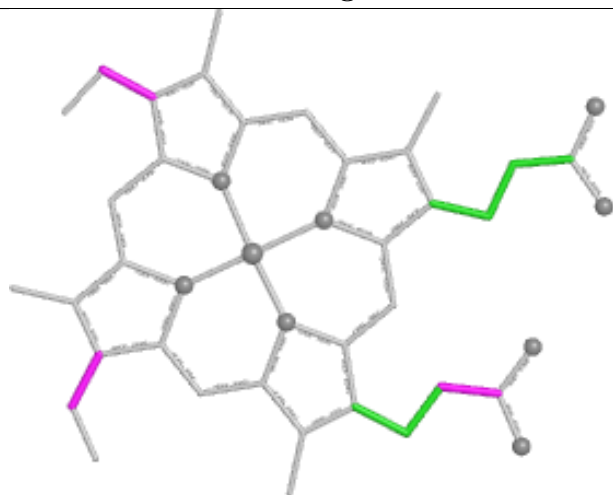
Ligand HEC A 607



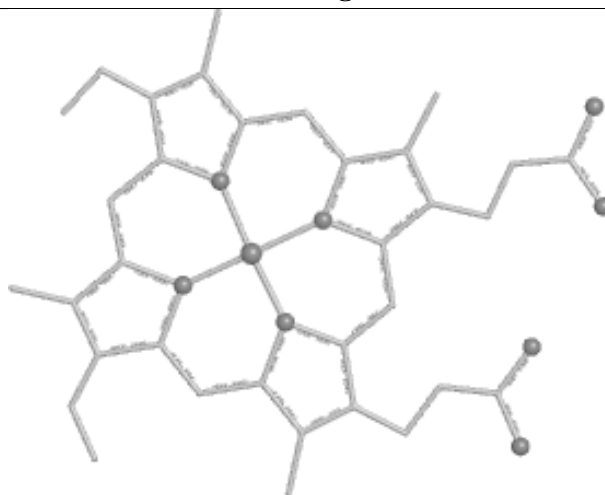
Bond lengths



Bond angles

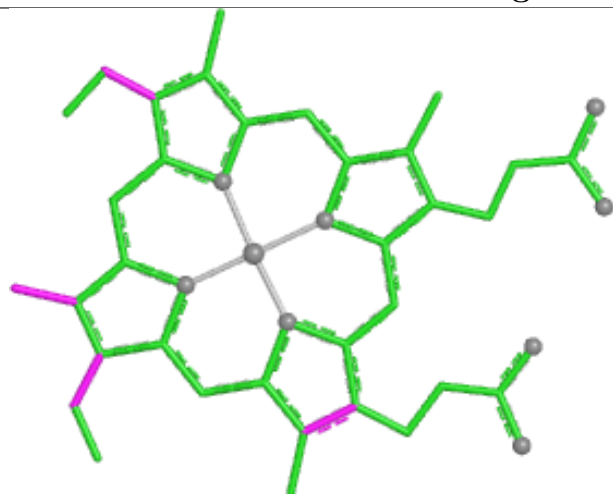


Torsions

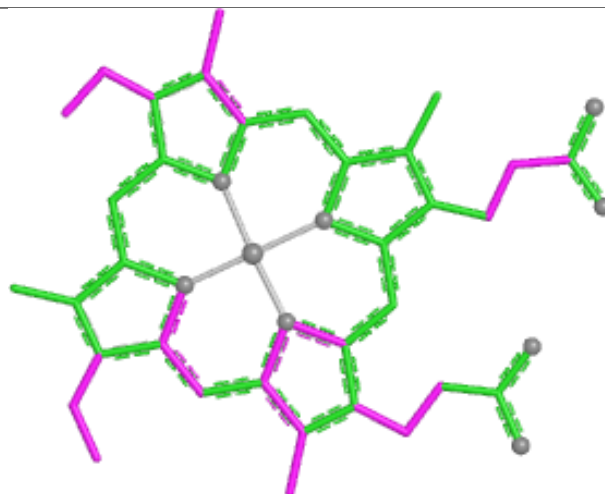


Rings

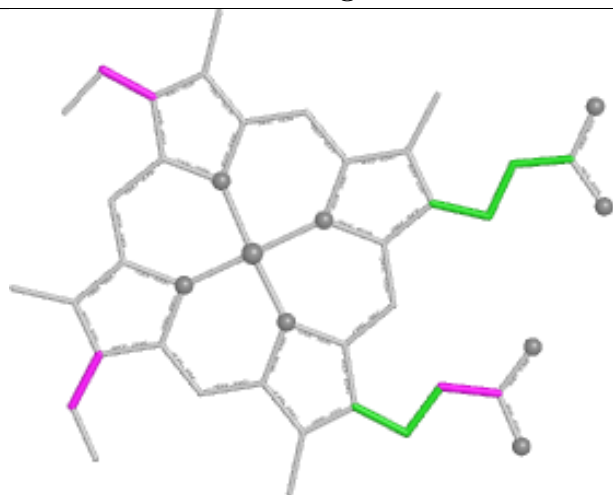
Ligand HEC A 601



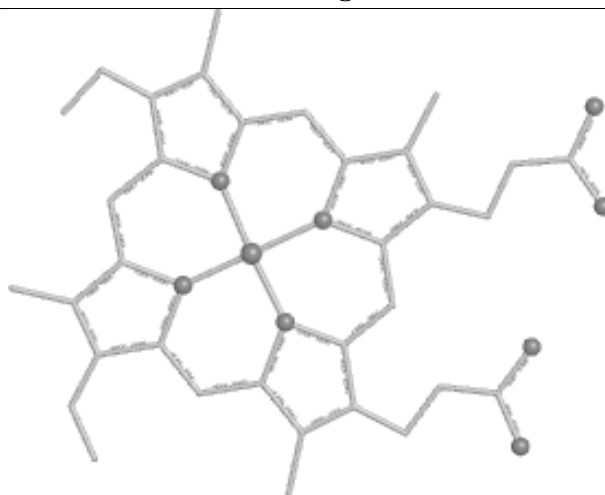
Bond lengths



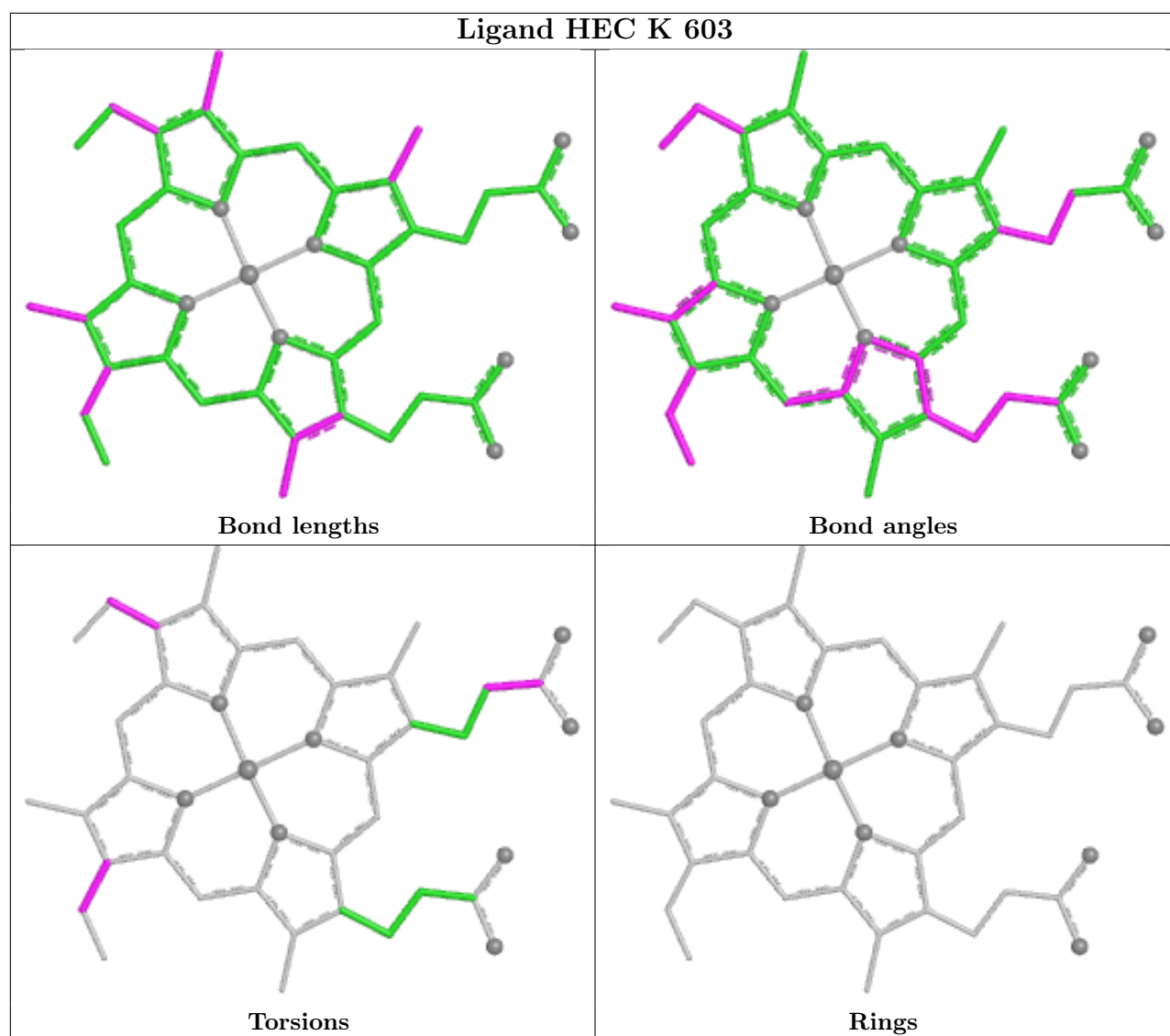
Bond angles



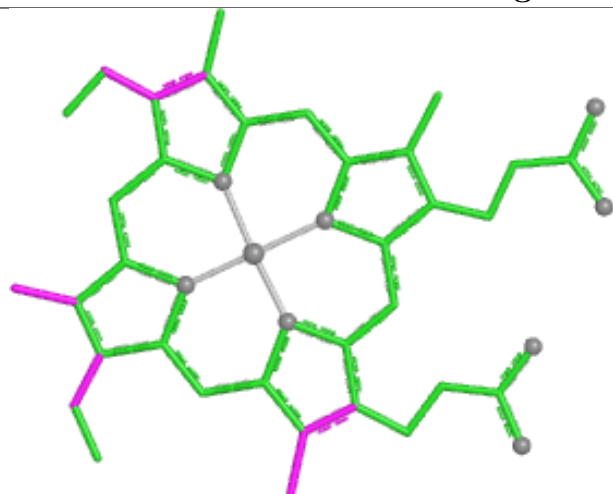
Torsions



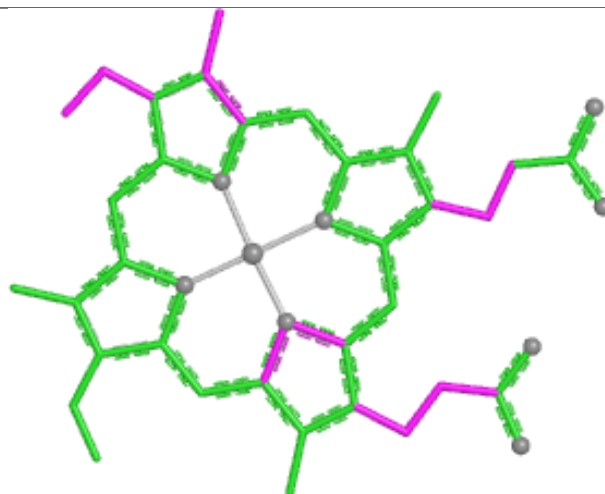
Rings



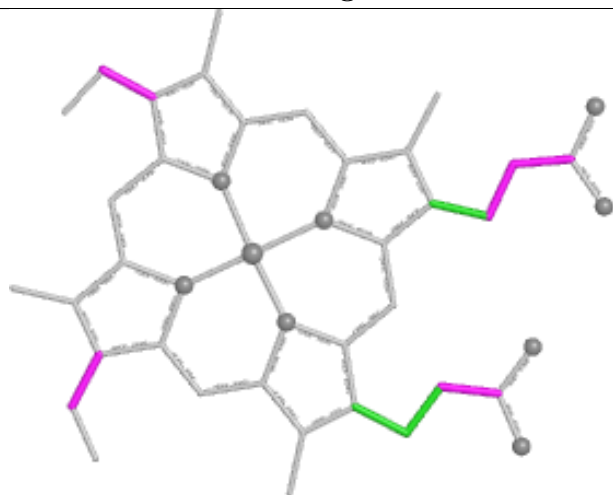
Ligand HEC E 605



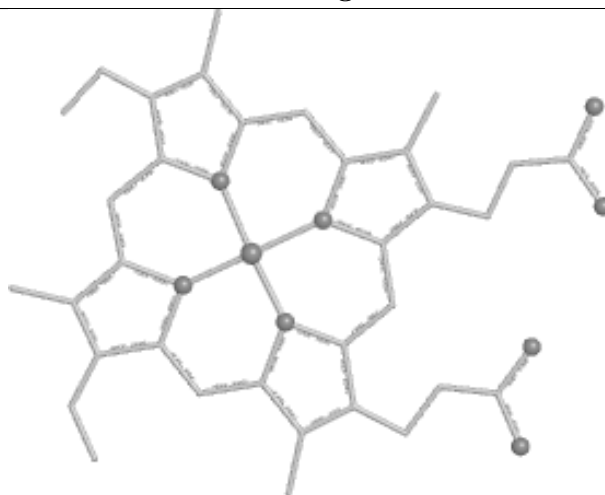
Bond lengths



Bond angles

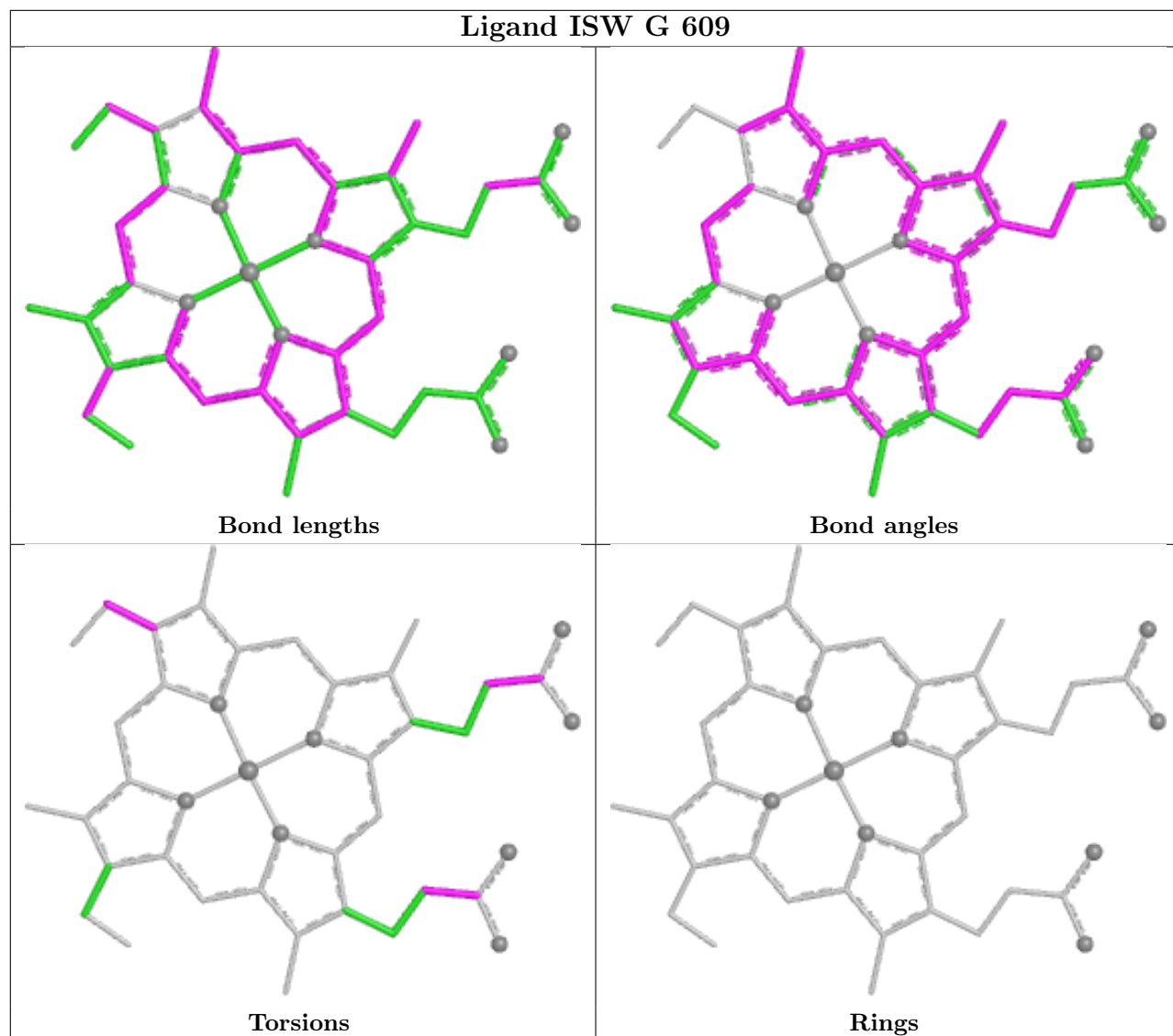


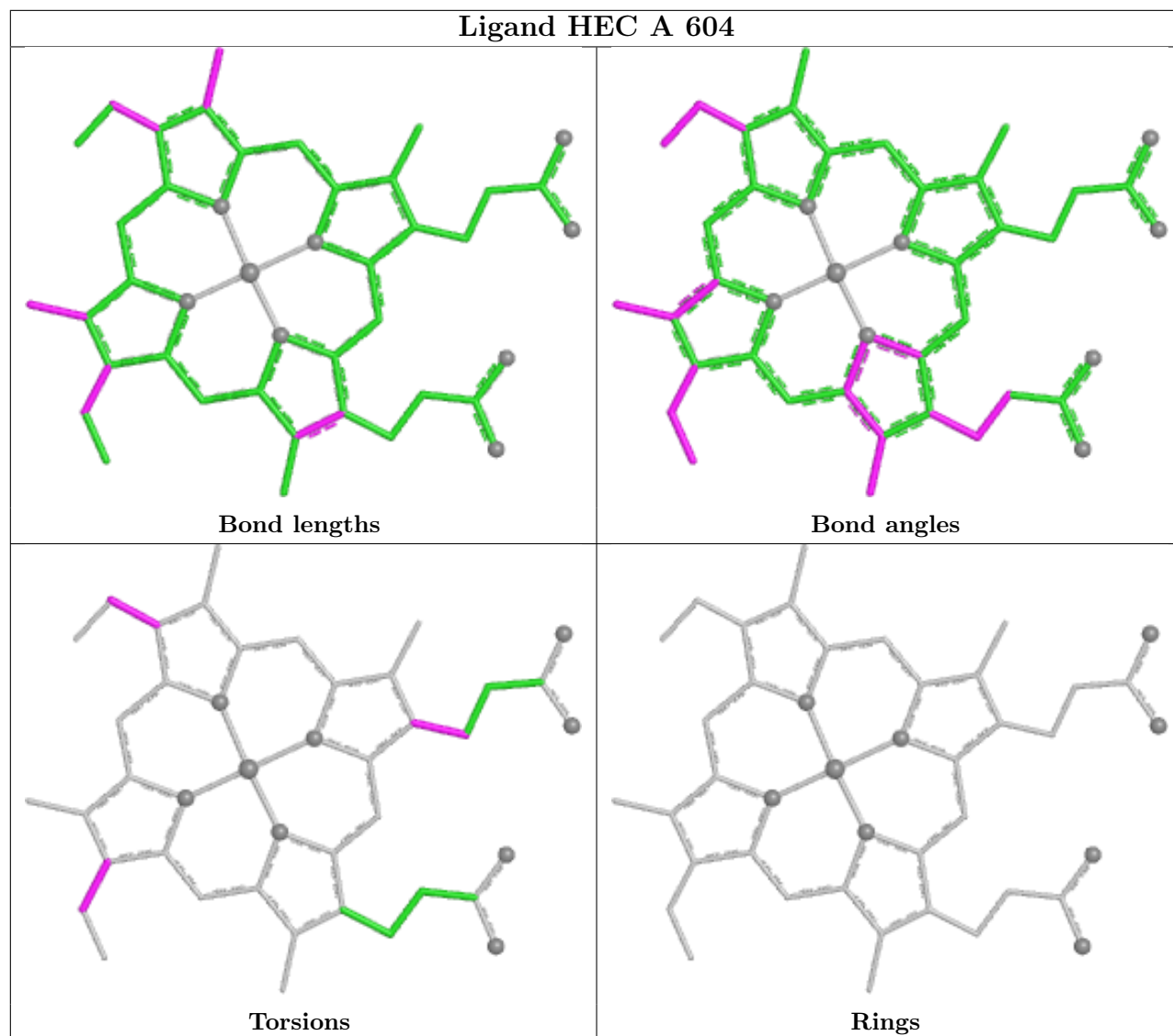
Torsions

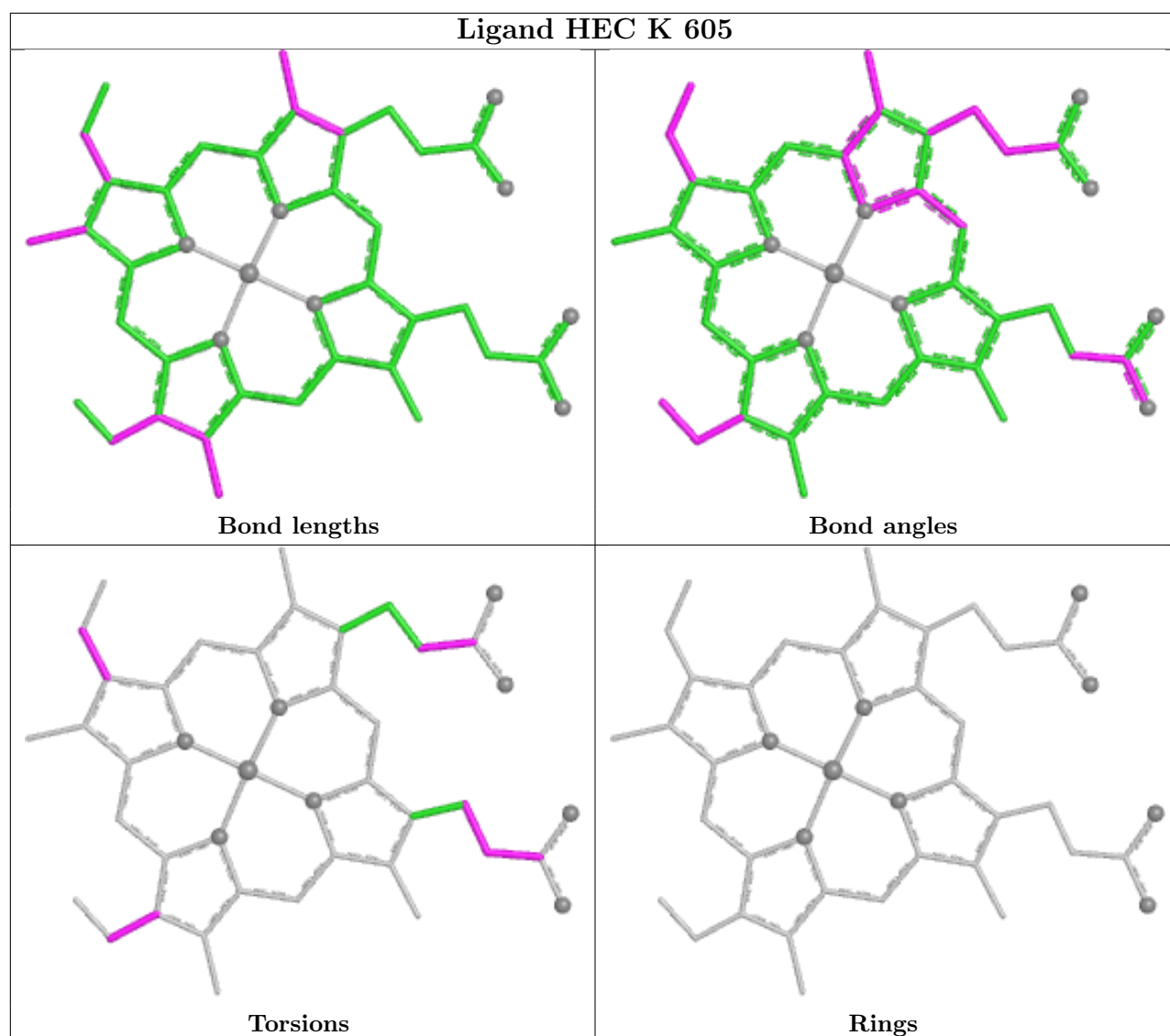


Rings

Ligand ISW G 609







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	504/570 (88%)	-0.51	1 (0%) 91 90	19, 27, 46, 69	0
1	C	504/570 (88%)	-0.43	3 (0%) 85 85	18, 29, 46, 82	0
1	E	504/570 (88%)	-0.45	1 (0%) 91 90	19, 27, 46, 76	0
1	G	504/570 (88%)	-0.36	2 (0%) 88 88	20, 30, 52, 81	0
1	I	504/570 (88%)	-0.33	3 (0%) 85 85	19, 32, 53, 90	0
1	K	504/570 (88%)	-0.36	1 (0%) 91 90	21, 30, 50, 87	0
2	B	64/91 (70%)	0.21	2 (3%) 51 50	23, 43, 77, 85	0
2	D	64/91 (70%)	0.06	1 (1%) 70 70	25, 34, 69, 85	0
2	F	64/91 (70%)	0.23	0 100 100	26, 45, 70, 87	0
2	H	64/91 (70%)	0.23	2 (3%) 51 50	25, 44, 73, 80	0
2	J	64/91 (70%)	0.11	1 (1%) 70 70	26, 37, 69, 90	0
2	L	64/91 (70%)	0.43	1 (1%) 70 70	30, 50, 81, 91	0
All	All	3408/3966 (85%)	-0.34	18 (0%) 87 87	18, 30, 56, 91	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	91	TYR	3.2
1	E	105	GLU	3.1
2	H	86	ALA	3.0
1	K	527	GLY	2.9
1	I	528	LYS	2.9

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(Å ²)	Q<0.9
6	PGE	E	608	10/10	0.78	0.16	60,62,65,66	0
7	PG4	E	610	13/13	0.83	0.16	61,63,64,65	0
5	PEG	J	101	7/7	0.84	0.13	58,59,61,61	0
6	PGE	E	609	10/10	0.86	0.15	52,52,55,56	0
7	PG4	K	610	13/13	0.88	0.13	48,55,61,63	0
6	PGE	I	609	10/10	0.89	0.11	56,58,60,60	0
7	PG4	A	612	13/13	0.89	0.14	50,56,60,60	0
6	PGE	A	611	10/10	0.89	0.11	46,50,61,63	0
6	PGE	G	612	10/10	0.89	0.13	49,52,56,58	0
7	PG4	C	611	13/13	0.90	0.14	60,64,67,67	0
6	PGE	G	611	10/10	0.90	0.10	52,53,55,55	0
5	PEG	K	608	7/7	0.90	0.13	49,51,54,55	0
6	PGE	C	610	10/10	0.91	0.10	53,55,57,57	0
5	PEG	K	609	7/7	0.91	0.11	49,51,55,56	0
5	PEG	A	610	7/7	0.91	0.10	43,46,50,51	0
6	PGE	I	610	10/10	0.91	0.12	49,53,55,55	0
5	PEG	C	609	7/7	0.94	0.08	42,44,52,54	0
5	PEG	G	610	7/7	0.95	0.09	50,51,52,53	0
4	ISW	G	608	43/43	0.96	0.08	21,27,36,38	0
4	ISW	I	608	43/43	0.96	0.08	20,28,40,41	0
4	ISW	A	609	43/43	0.96	0.09	16,25,34,37	0
4	ISW	C	608	43/43	0.96	0.08	14,27,37,38	0
4	ISW	G	609	43/43	0.97	0.08	19,28,35,37	0
4	ISW	A	608	43/43	0.97	0.08	16,25,36,39	0
3	HEC	C	607	43/43	0.98	0.06	14,17,28,33	0
3	HEC	E	602	43/43	0.98	0.05	17,23,28,30	0
3	HEC	E	607	43/43	0.98	0.06	16,21,32,37	0
3	HEC	G	604	43/43	0.98	0.05	19,24,28,30	0
3	HEC	G	605	43/43	0.98	0.06	16,20,25,27	0
3	HEC	G	607	43/43	0.98	0.06	16,22,31,36	0
3	HEC	I	601	43/43	0.98	0.05	19,25,31,33	0
3	HEC	I	602	43/43	0.98	0.06	19,26,33,36	0

Continued on next page...

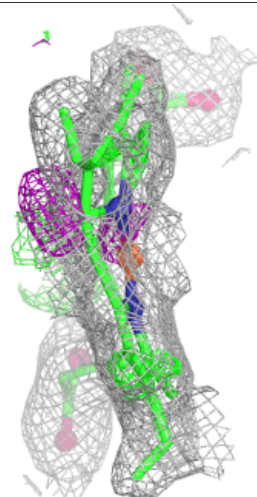
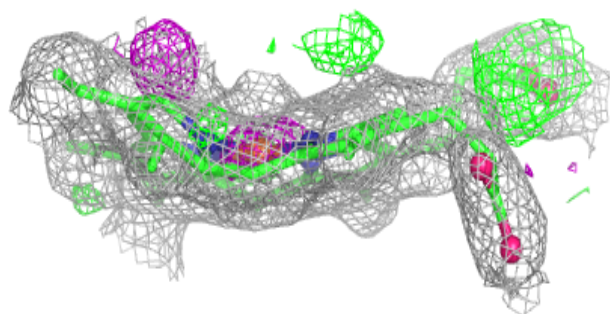
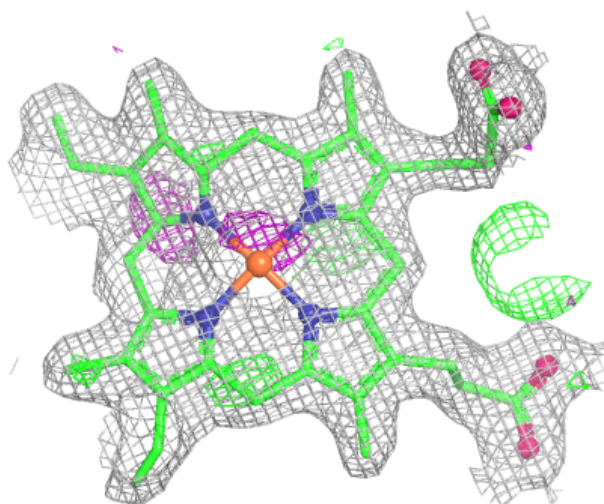
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	I	603	43/43	0.98	0.06	25,31,35,39	0
3	HEC	I	605	43/43	0.98	0.05	15,21,25,26	0
3	HEC	K	602	43/43	0.98	0.06	22,27,33,35	0
3	HEC	K	603	43/43	0.98	0.06	23,27,33,42	0
3	HEC	K	605	43/43	0.98	0.06	14,21,25,27	0
3	HEC	K	607	43/43	0.98	0.06	16,21,35,36	0
3	HEC	A	603	43/43	0.98	0.06	19,27,31,33	0
3	HEC	A	605	43/43	0.98	0.06	15,19,22,24	0
3	HEC	C	602	43/43	0.98	0.05	17,23,28,32	0
3	HEC	C	603	43/43	0.98	0.06	22,26,29,36	0
3	HEC	C	604	43/43	0.98	0.05	18,21,25,27	0
3	HEC	C	601	43/43	0.99	0.05	17,23,26,29	0
3	HEC	G	601	43/43	0.99	0.05	14,22,29,33	0
3	HEC	G	602	43/43	0.99	0.05	18,27,31,32	0
3	HEC	G	603	43/43	0.99	0.05	22,28,34,38	0
3	HEC	A	601	43/43	0.99	0.05	14,21,28,29	0
3	HEC	A	604	43/43	0.99	0.05	17,22,26,30	0
3	HEC	G	606	43/43	0.99	0.06	17,23,33,36	0
3	HEC	A	602	43/43	0.99	0.05	18,22,28,35	0
3	HEC	C	605	43/43	0.99	0.05	16,21,23,25	0
3	HEC	C	606	43/43	0.99	0.05	15,21,32,36	0
3	HEC	A	606	43/43	0.99	0.06	14,20,28,32	0
3	HEC	I	604	43/43	0.99	0.05	20,26,29,31	0
3	HEC	E	601	43/43	0.99	0.05	16,21,27,30	0
3	HEC	I	606	43/43	0.99	0.05	14,22,34,39	0
3	HEC	I	607	43/43	0.99	0.05	16,20,30,36	0
3	HEC	K	601	43/43	0.99	0.05	16,27,31,37	0
3	HEC	A	607	43/43	0.99	0.05	16,20,28,31	0
3	HEC	E	603	43/43	0.99	0.05	21,26,30,34	0
3	HEC	K	604	43/43	0.99	0.05	19,23,27,29	0
3	HEC	E	604	43/43	0.99	0.05	17,22,25,27	0
3	HEC	K	606	43/43	0.99	0.05	17,22,34,37	0
3	HEC	E	605	43/43	0.99	0.05	15,20,22,23	0
3	HEC	E	606	43/43	0.99	0.05	15,19,29,32	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.

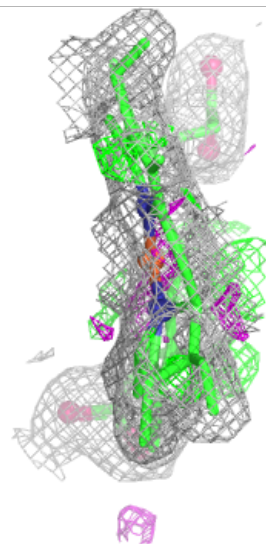
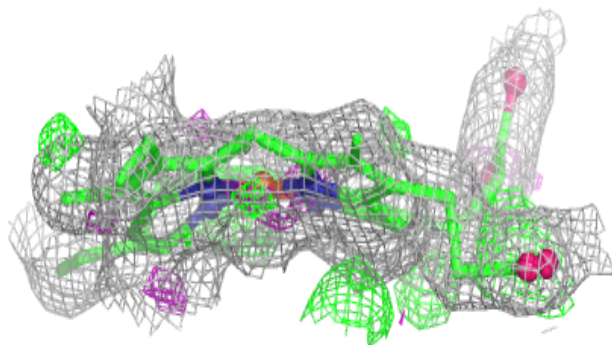
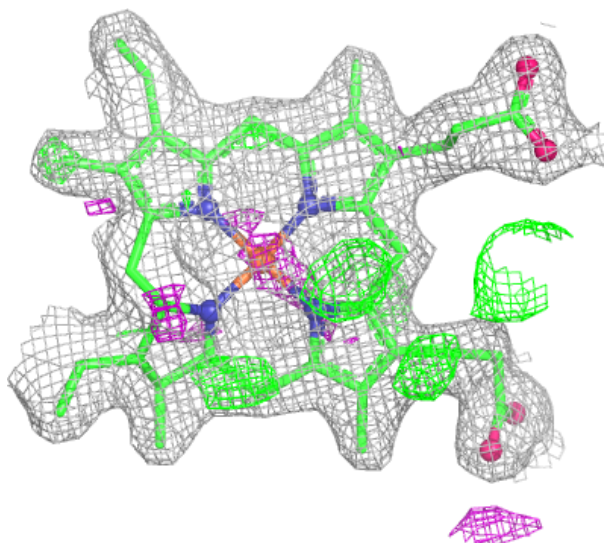
Electron density around ISW G 608:

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



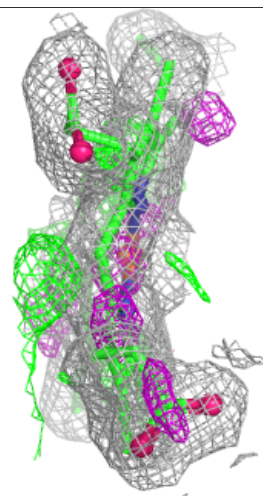
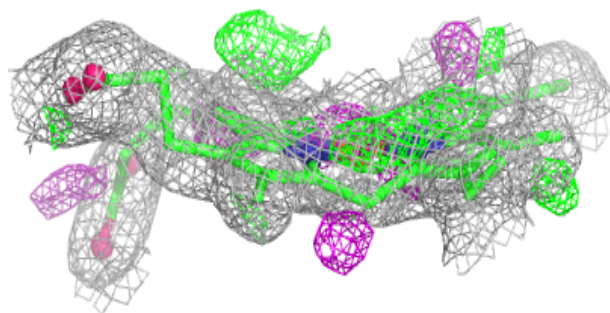
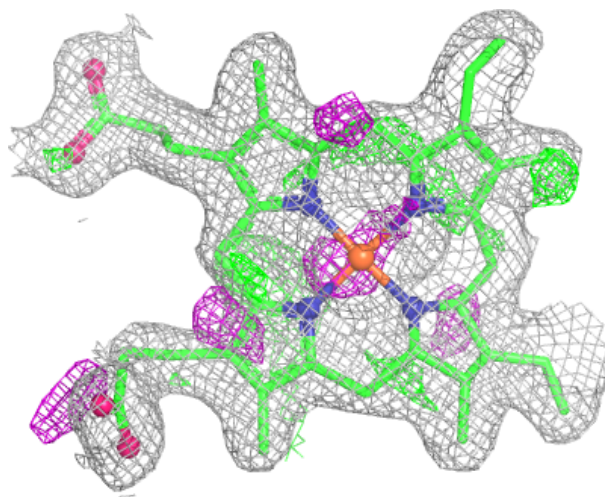
Electron density around ISW I 608:

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



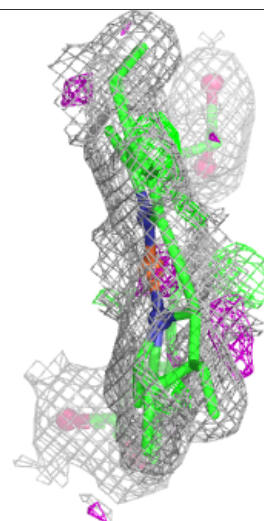
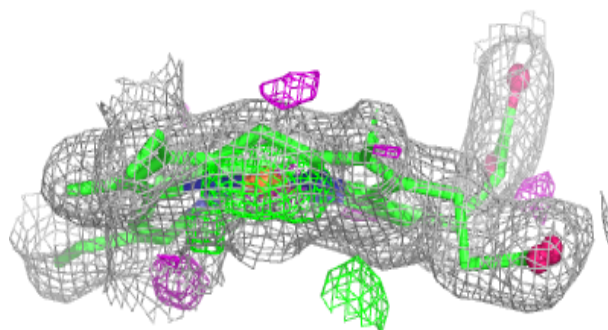
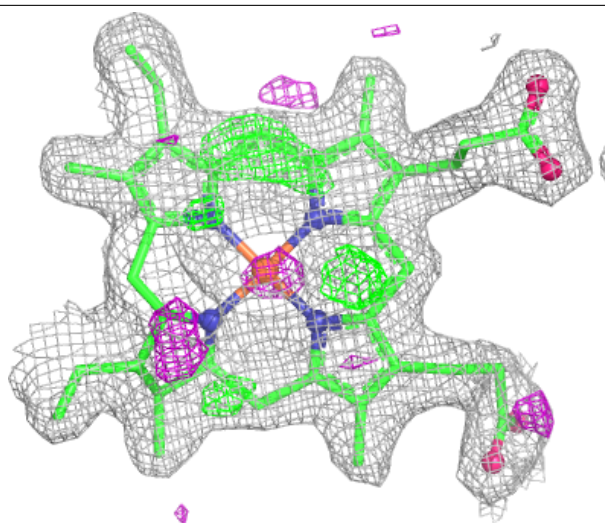
Electron density around ISW A 609:

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



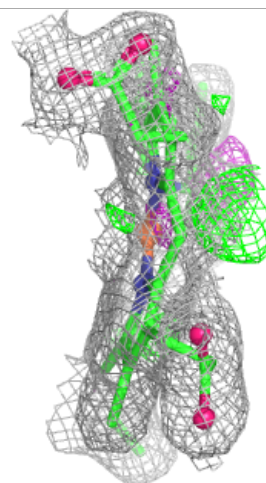
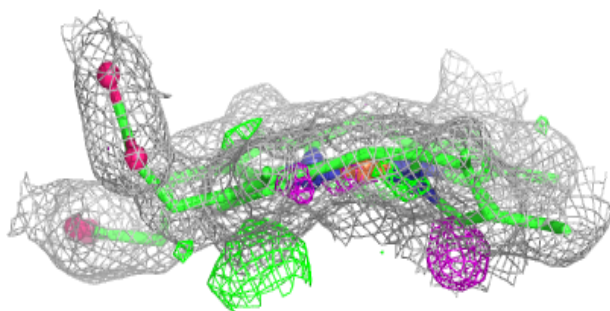
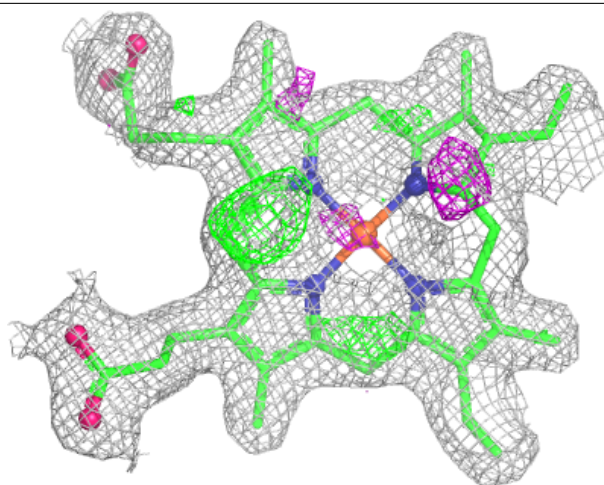
Electron density around ISW C 608:

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



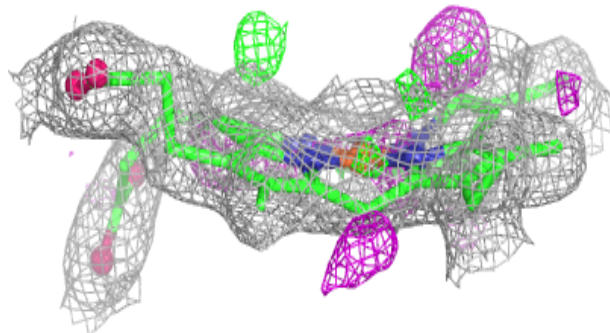
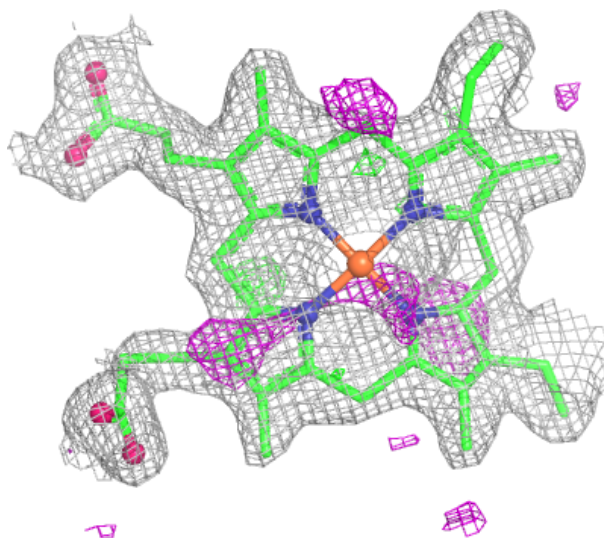
Electron density around ISW G 609:

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



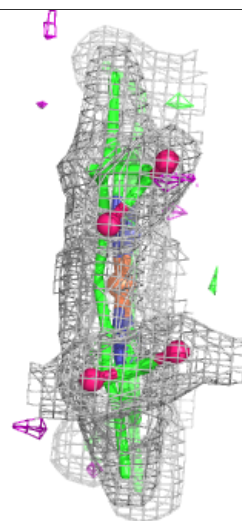
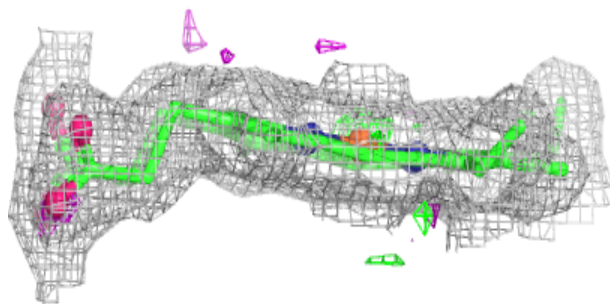
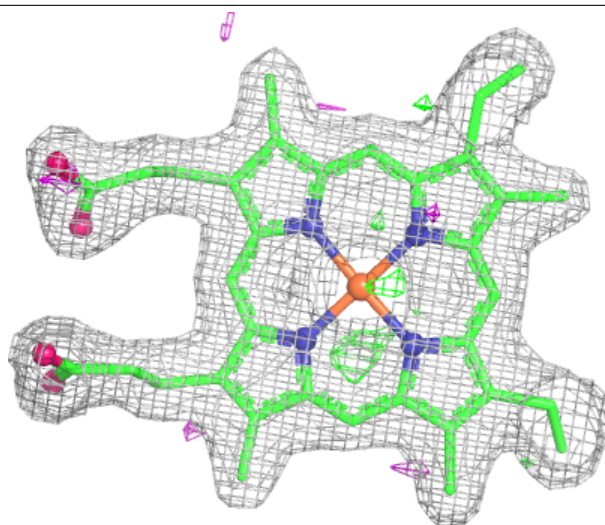
Electron density around ISW A 608:

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



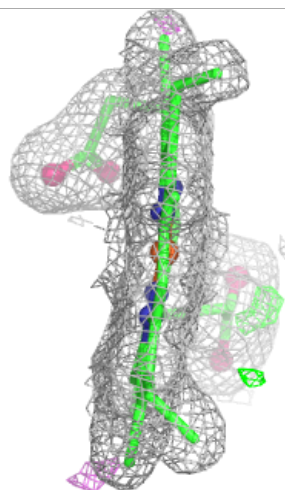
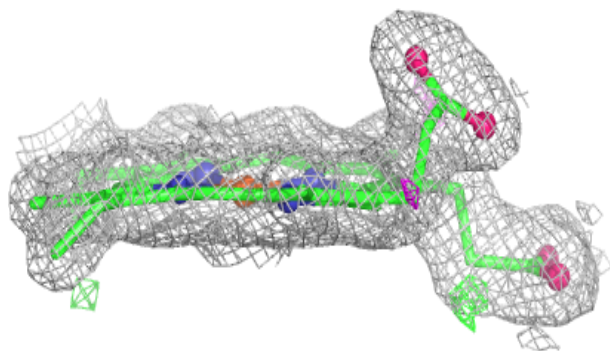
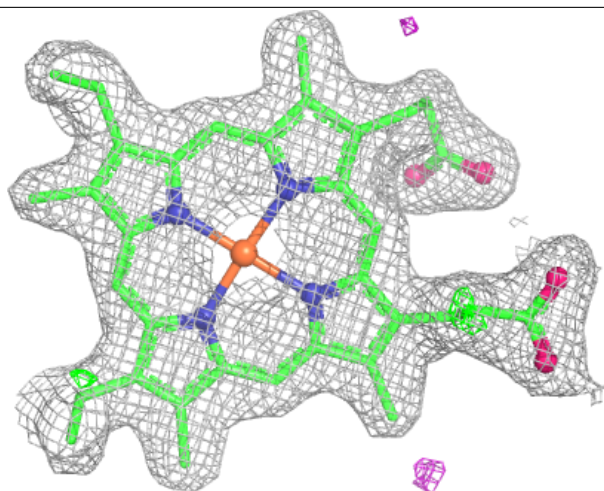
Electron density around HEC C 607:

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



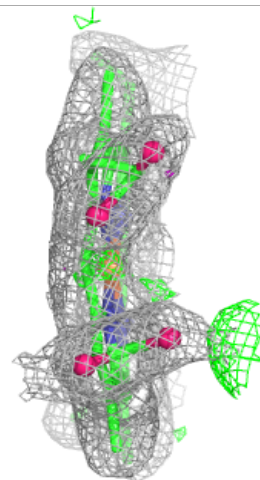
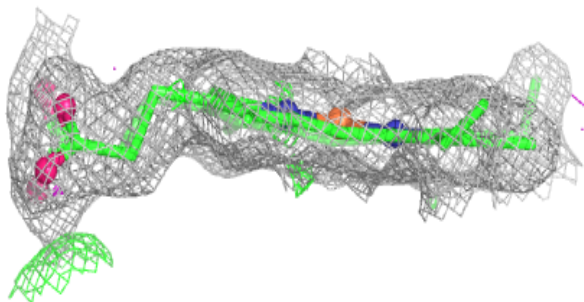
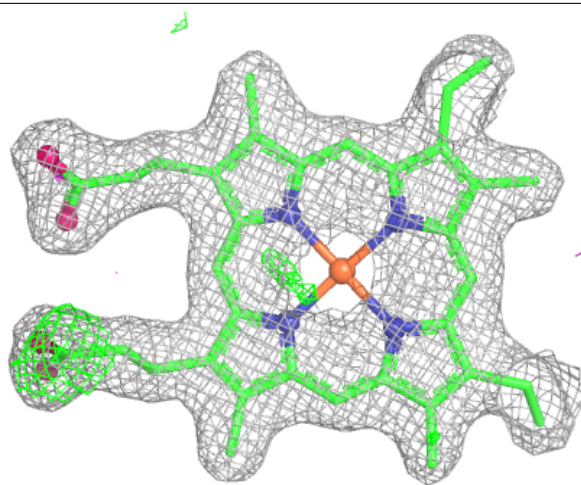
Electron density around HEC E 602:

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



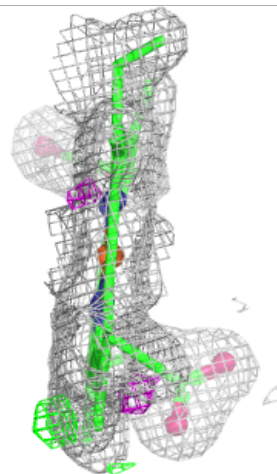
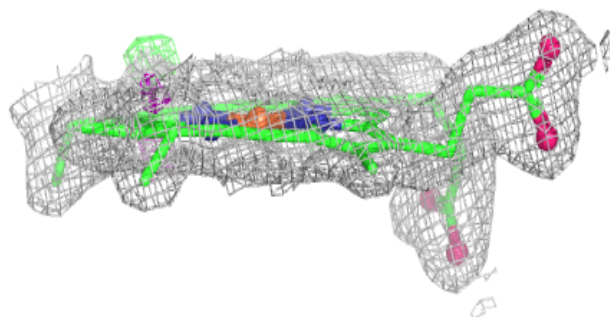
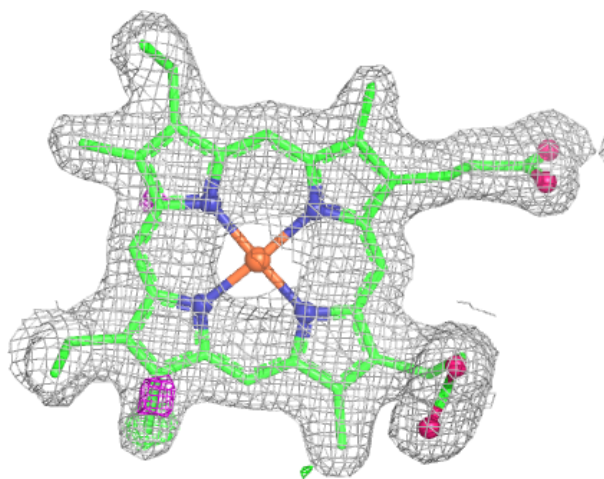
Electron density around HEC E 607:

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



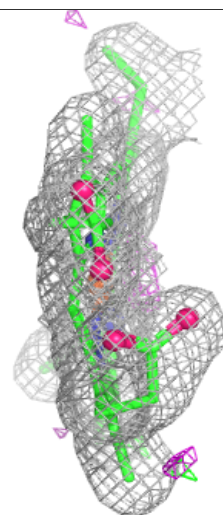
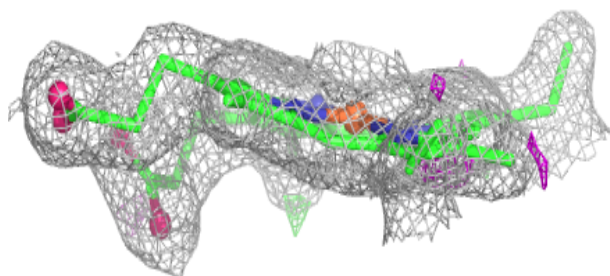
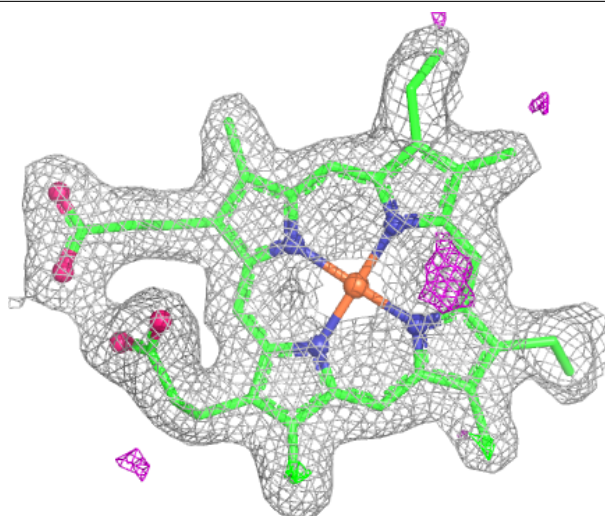
Electron density around HEC G 604:

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



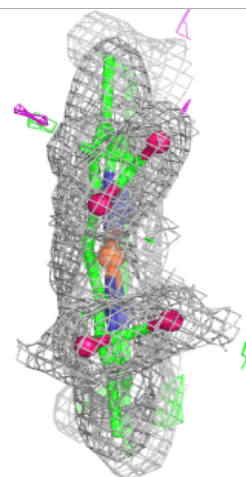
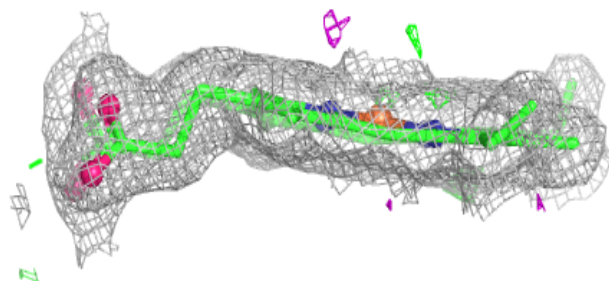
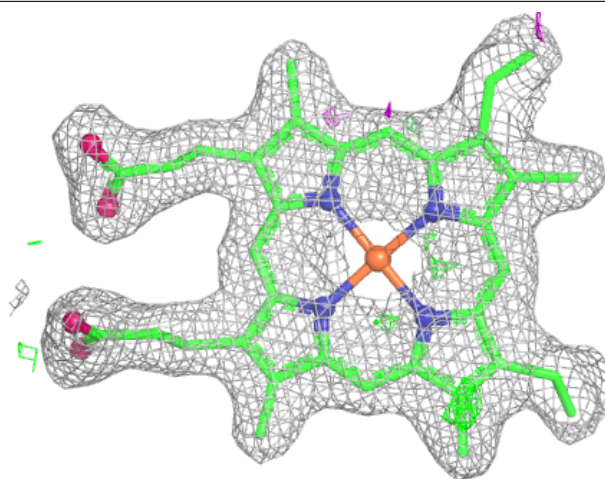
Electron density around HEC G 605:

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



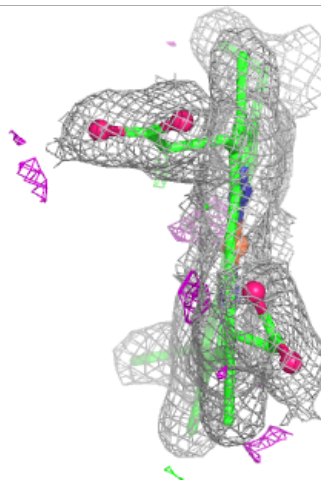
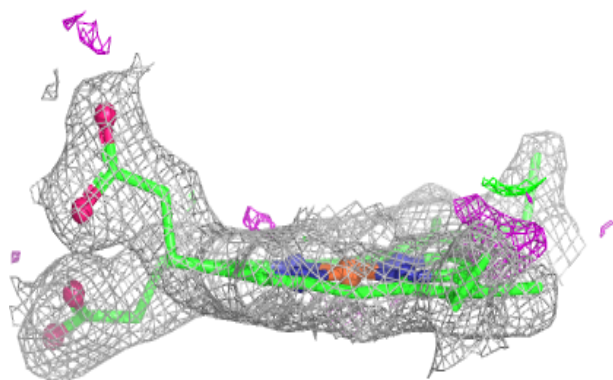
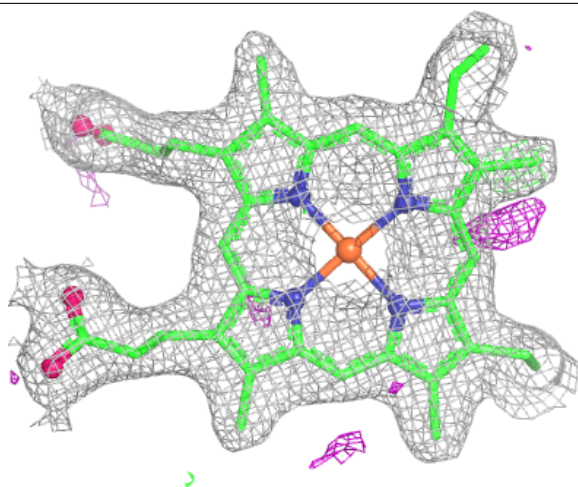
Electron density around HEC G 607:

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



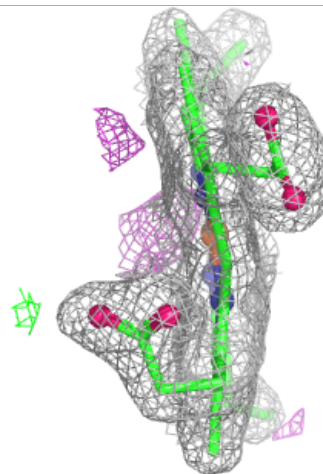
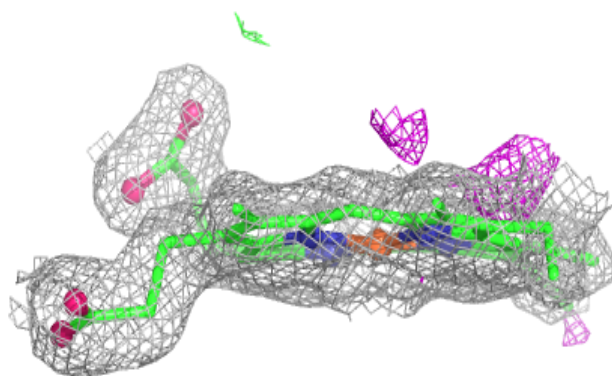
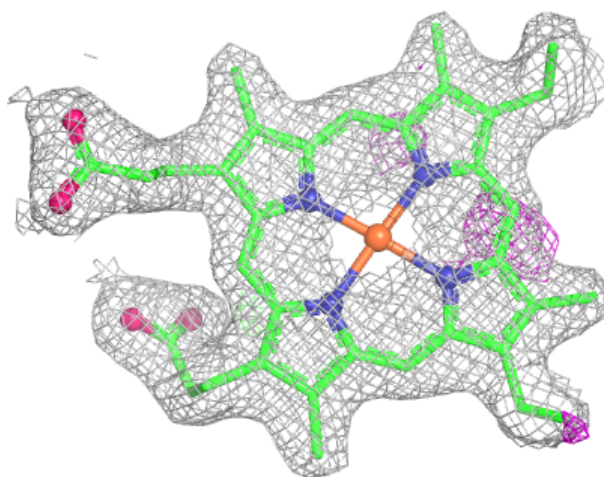
Electron density around HEC I 601:

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



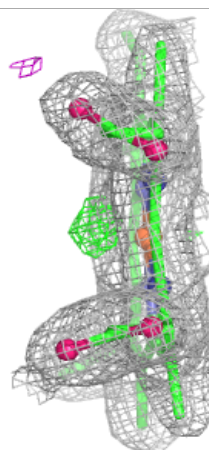
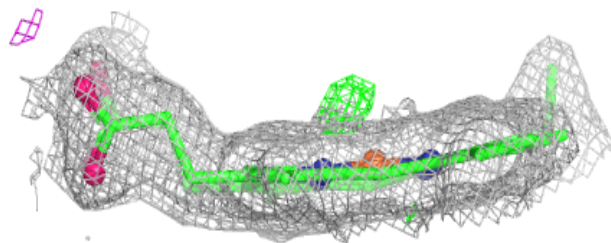
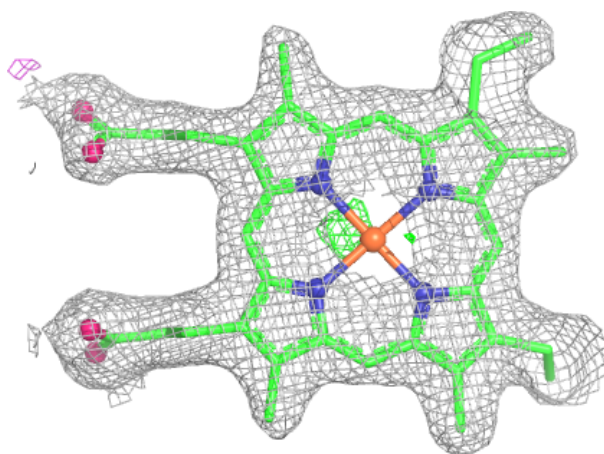
Electron density around HEC I 602:

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



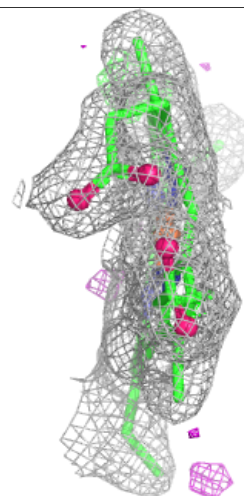
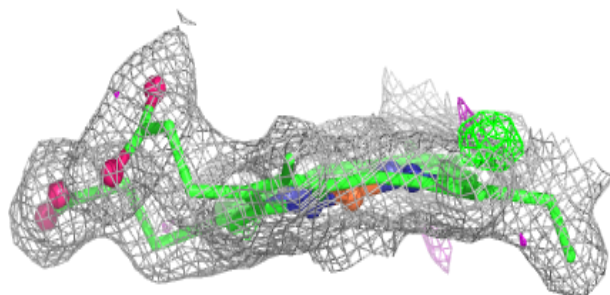
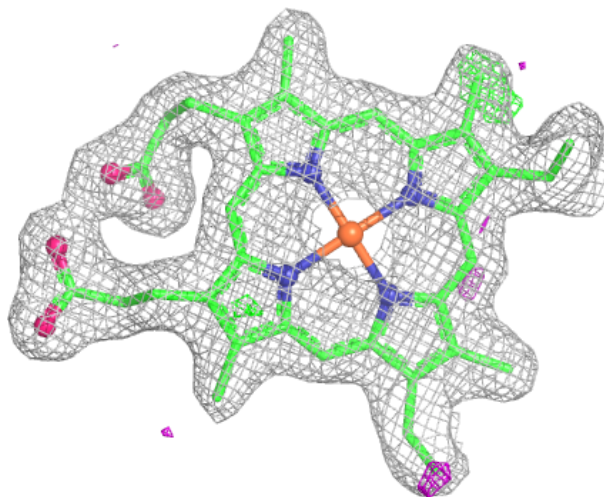
Electron density around HEC I 603:

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



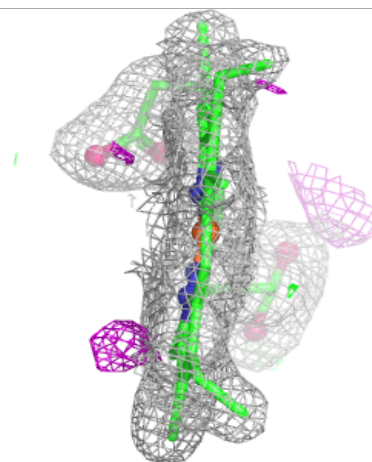
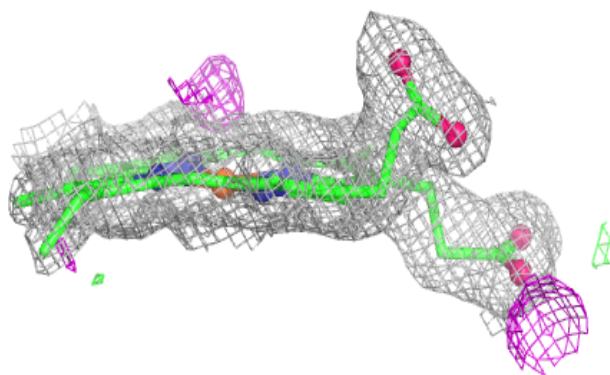
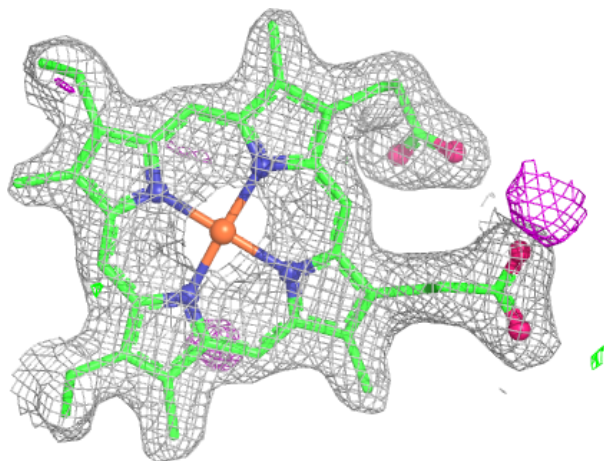
Electron density around HEC I 605:

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



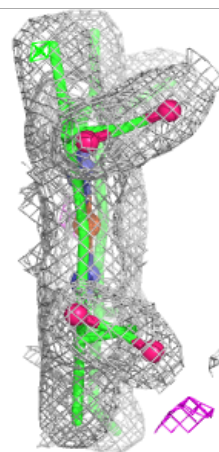
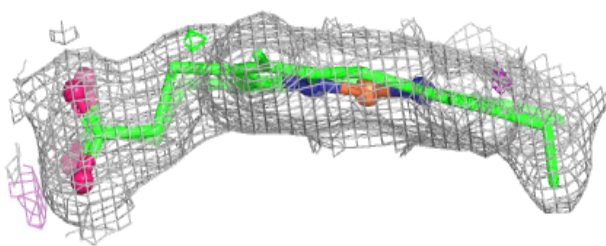
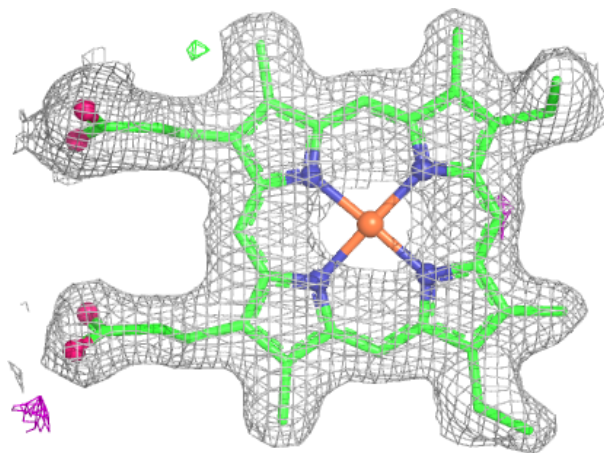
Electron density around HEC K 602:

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



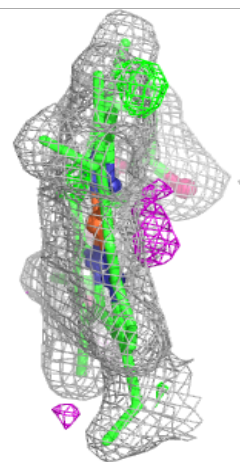
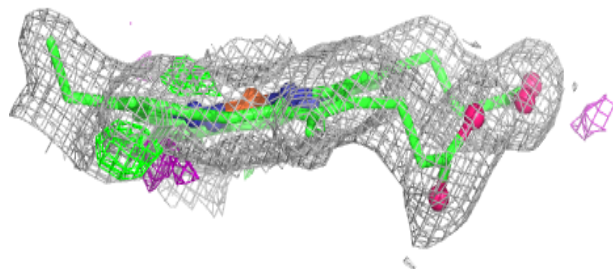
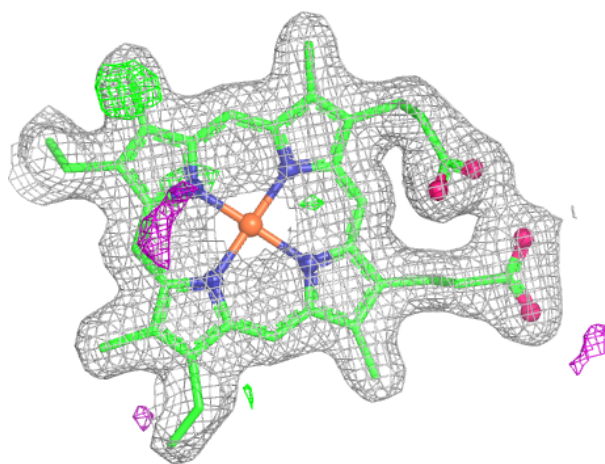
Electron density around HEC K 603:

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



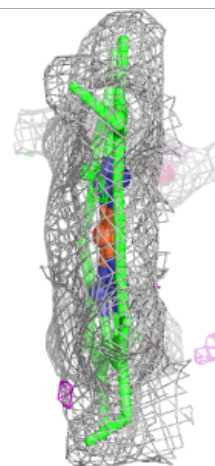
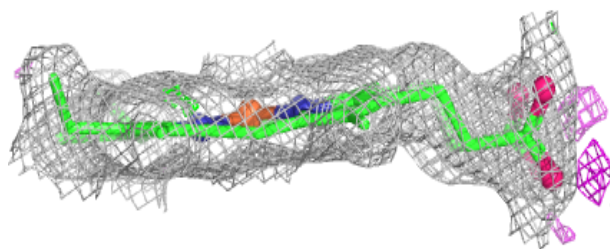
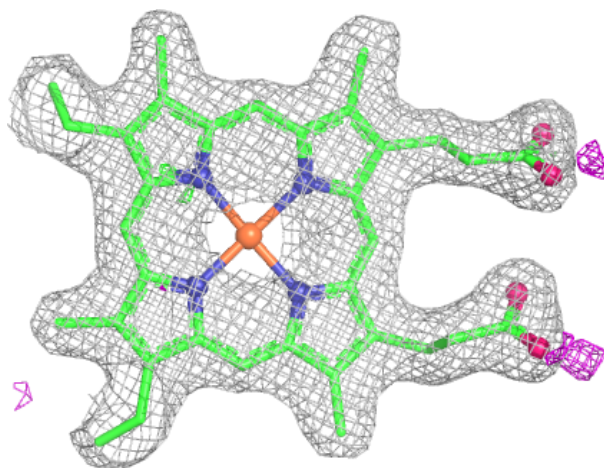
Electron density around HEC K 605:

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



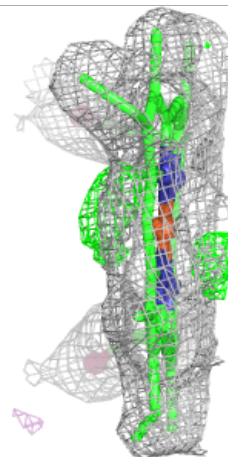
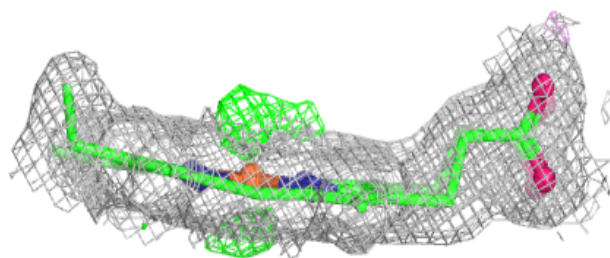
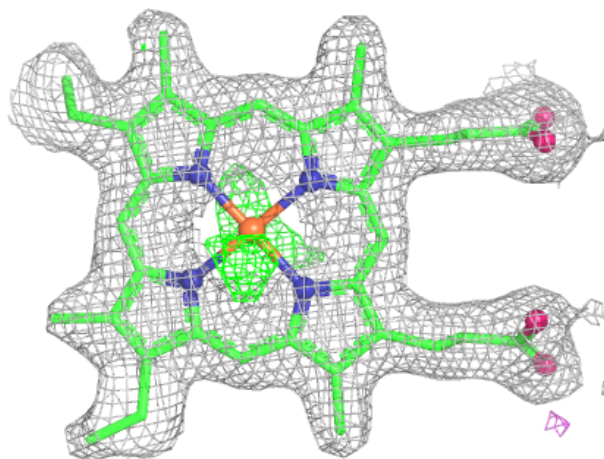
Electron density around HEC K 607:

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



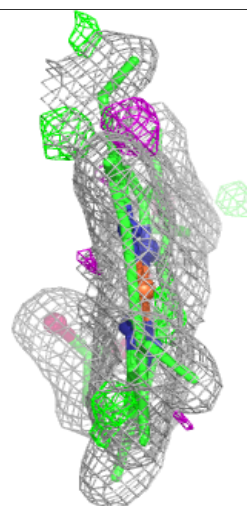
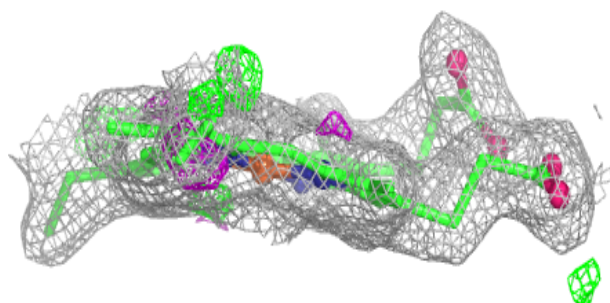
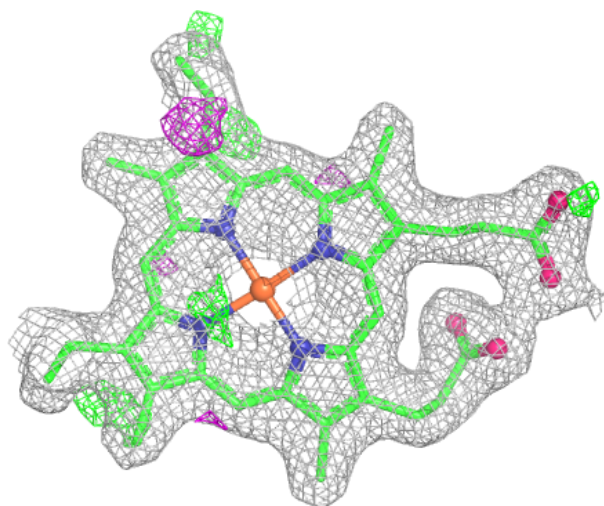
Electron density around HEC A 603:

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



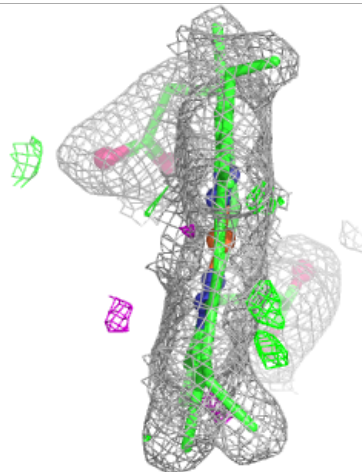
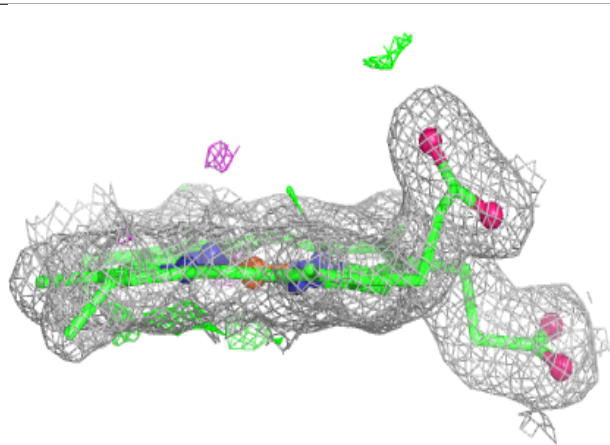
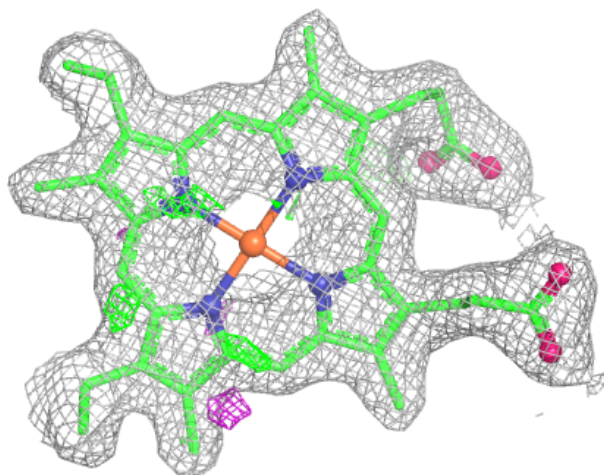
Electron density around HEC A 605:

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



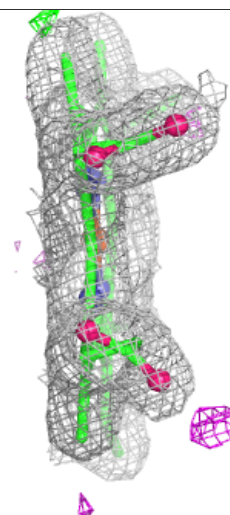
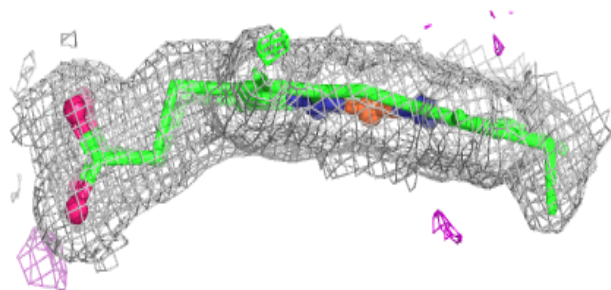
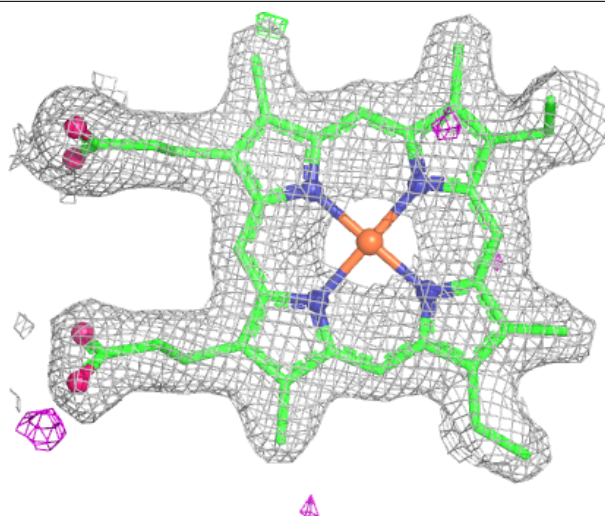
Electron density around HEC C 602:

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



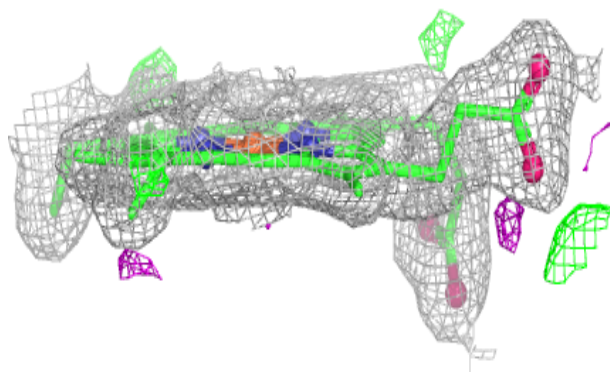
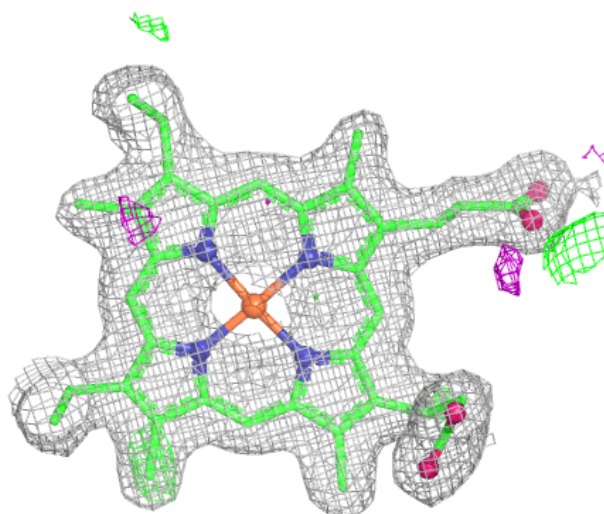
Electron density around HEC C 603:

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



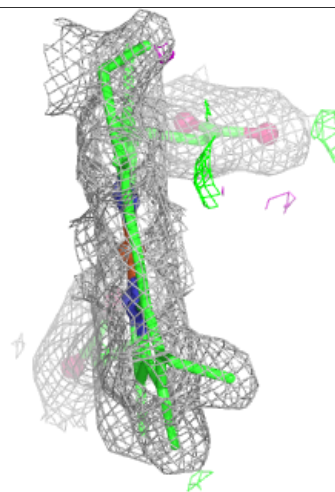
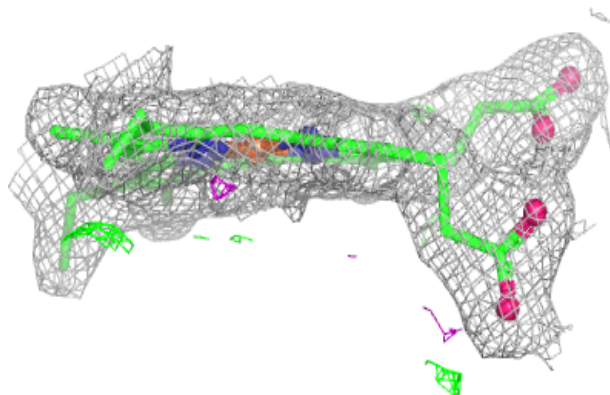
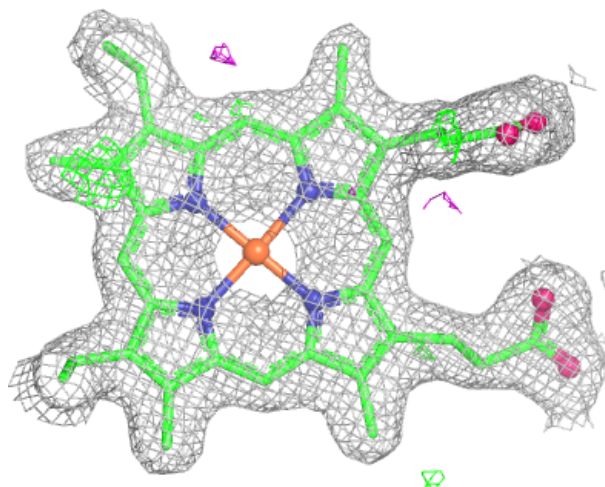
Electron density around HEC C 604:

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



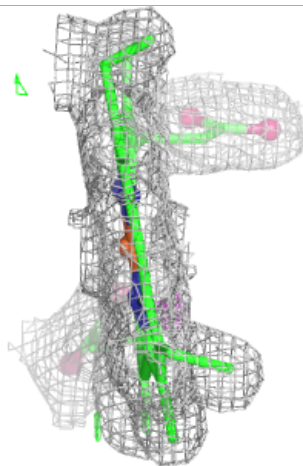
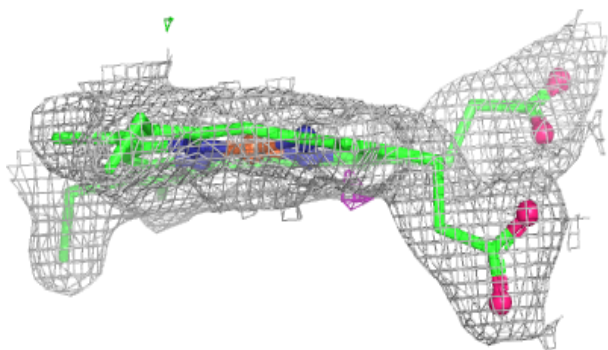
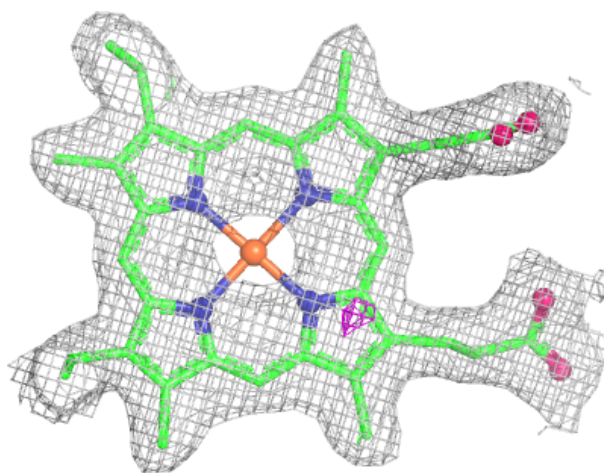
Electron density around HEC C 601:

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



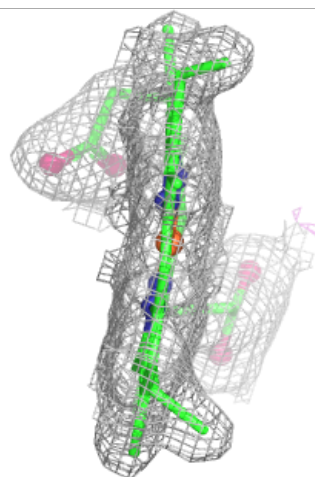
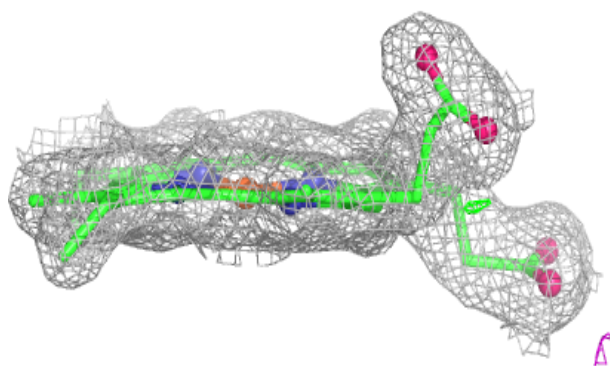
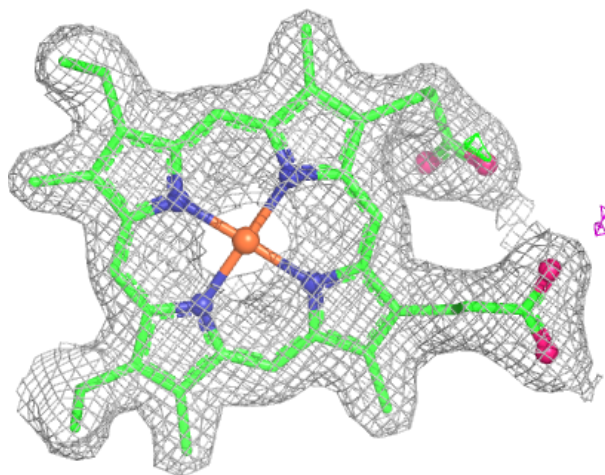
Electron density around HEC G 601:

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



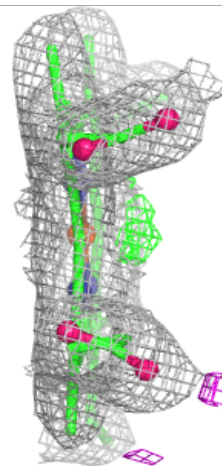
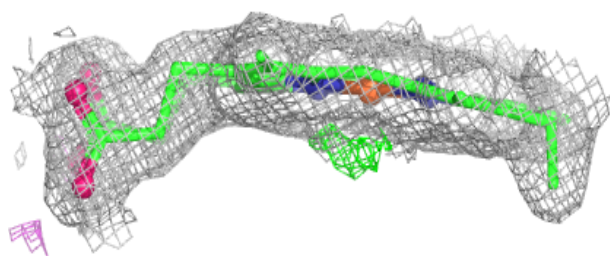
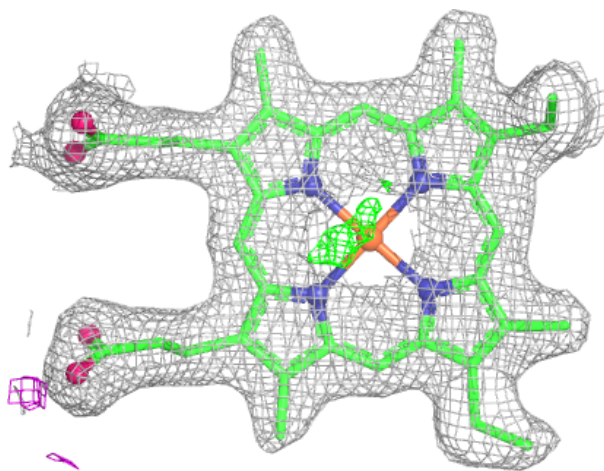
Electron density around HEC G 602:

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



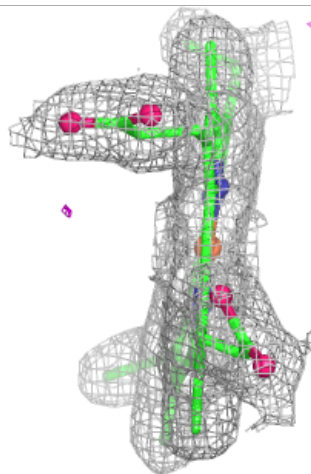
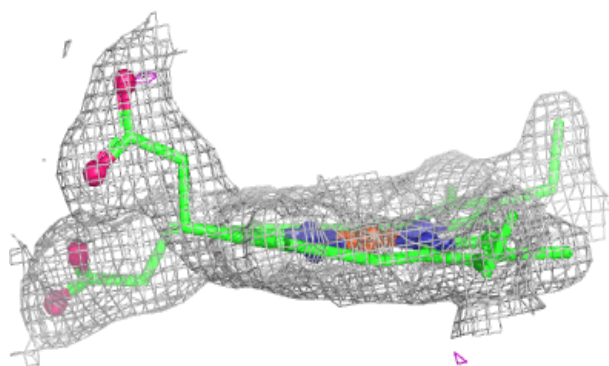
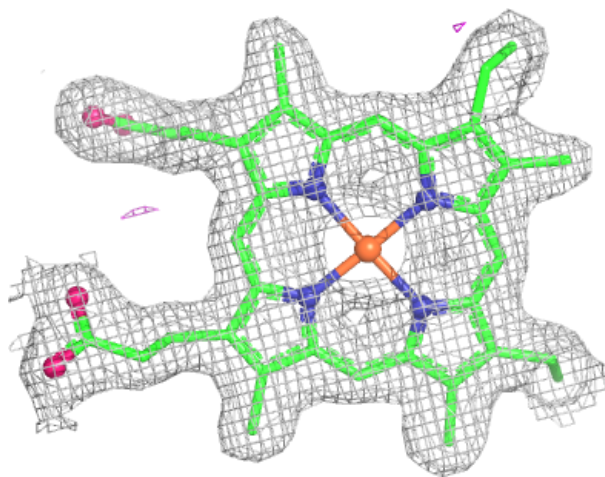
Electron density around HEC G 603:

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



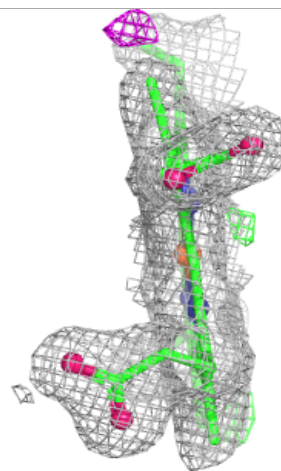
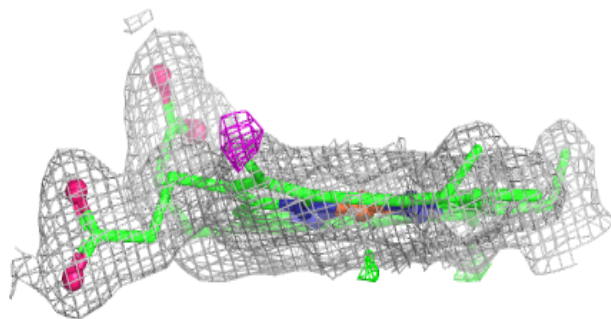
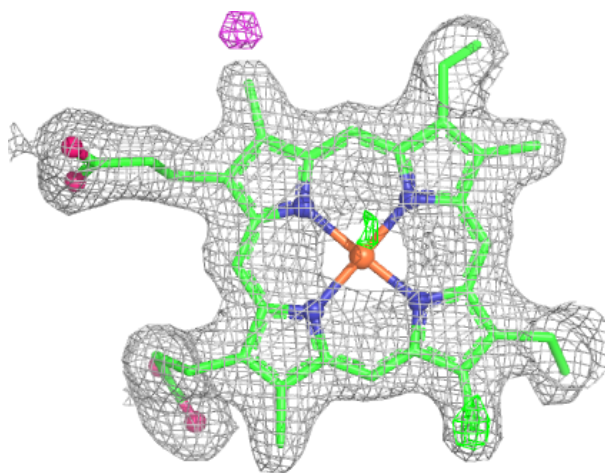
Electron density around HEC A 601:

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



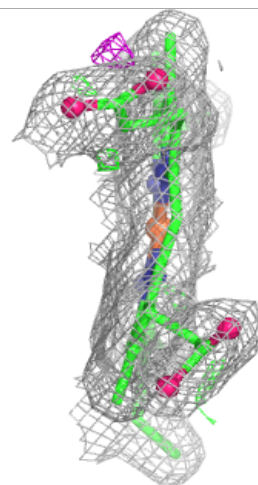
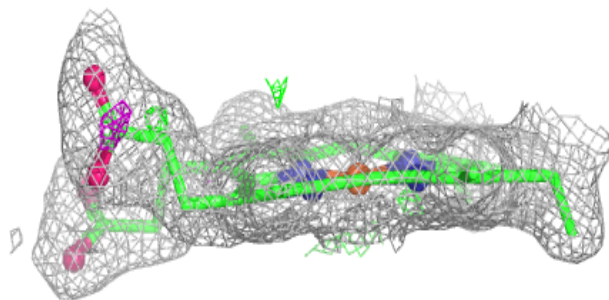
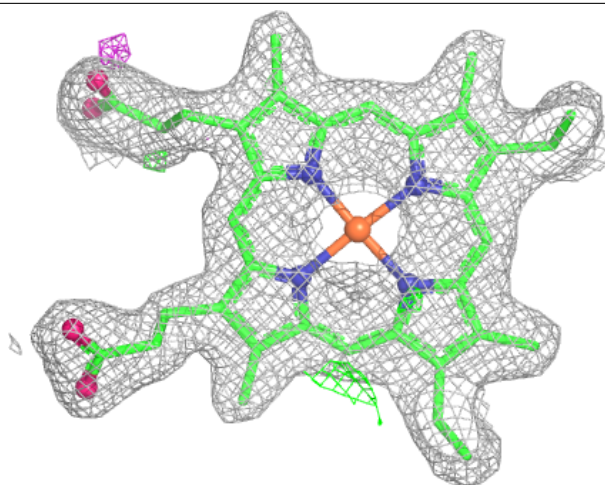
Electron density around HEC A 604:

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



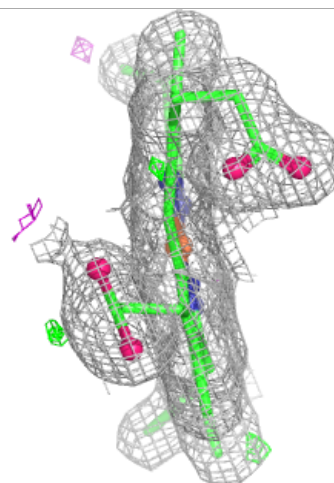
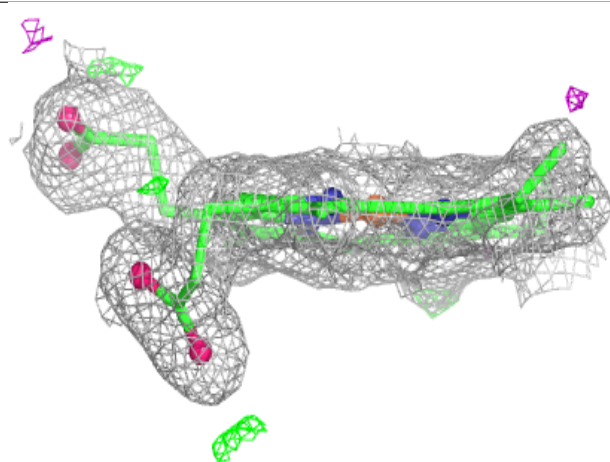
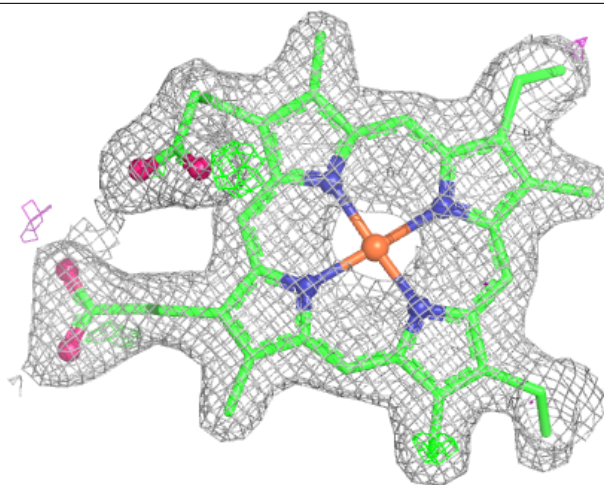
Electron density around HEC G 606:

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



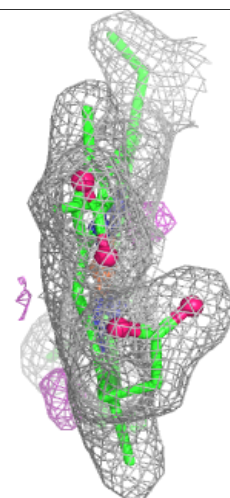
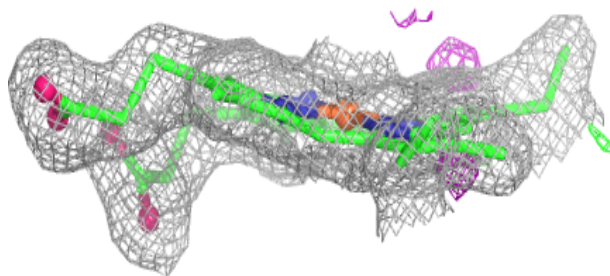
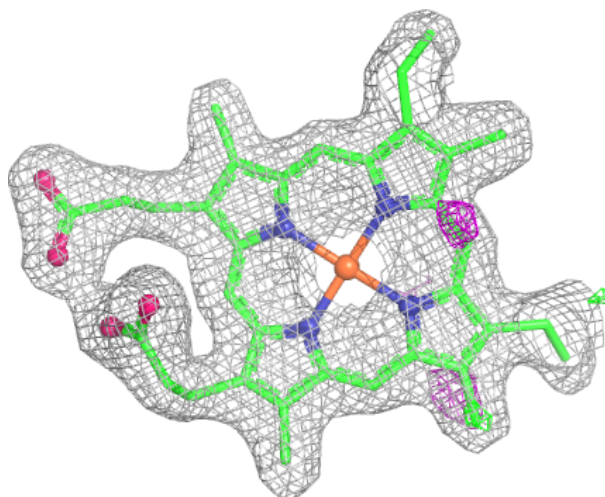
Electron density around HEC A 602:

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



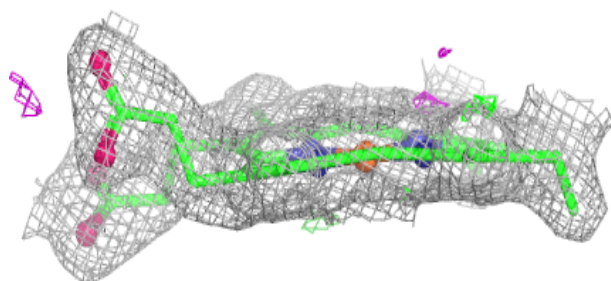
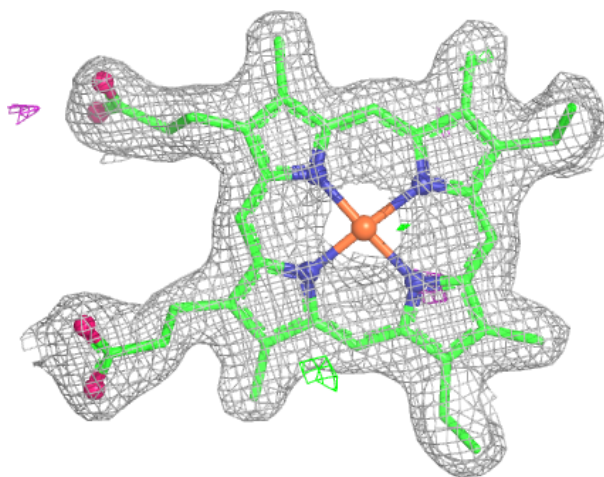
Electron density around HEC C 605:

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



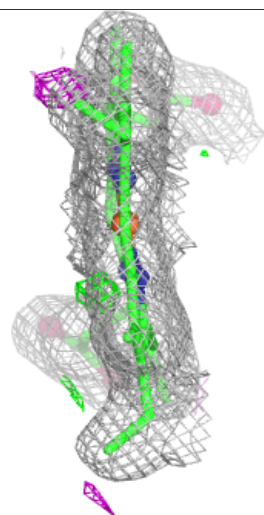
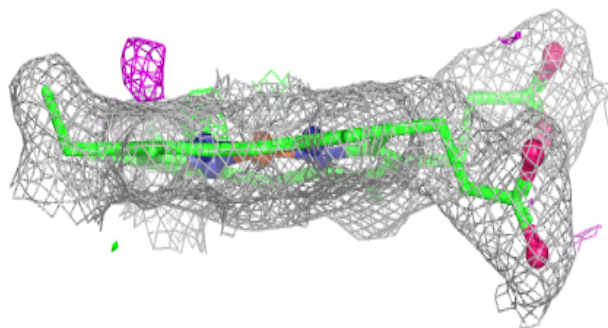
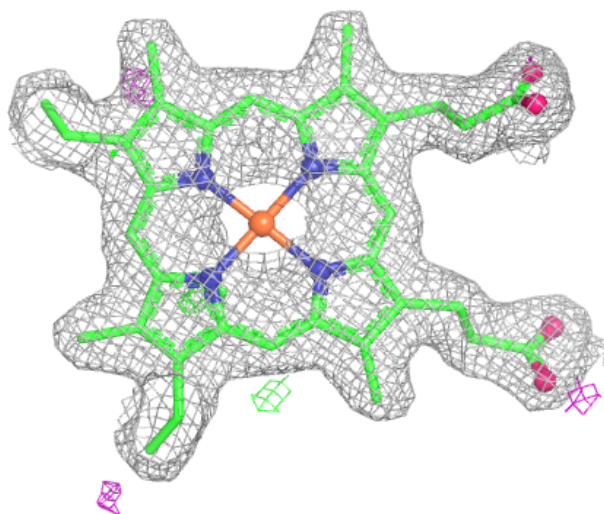
Electron density around HEC C 606:

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



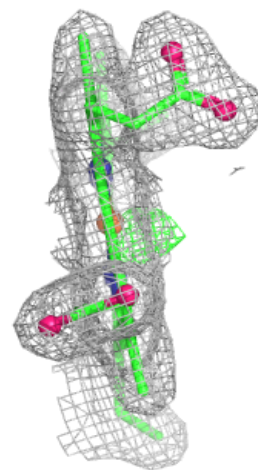
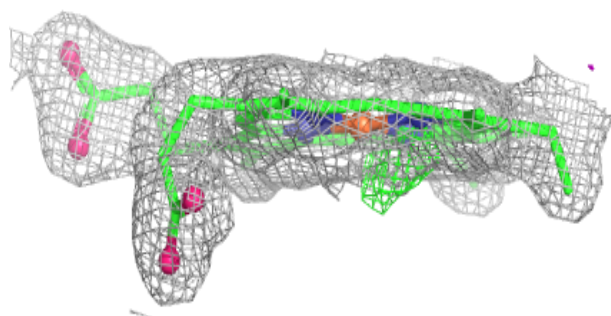
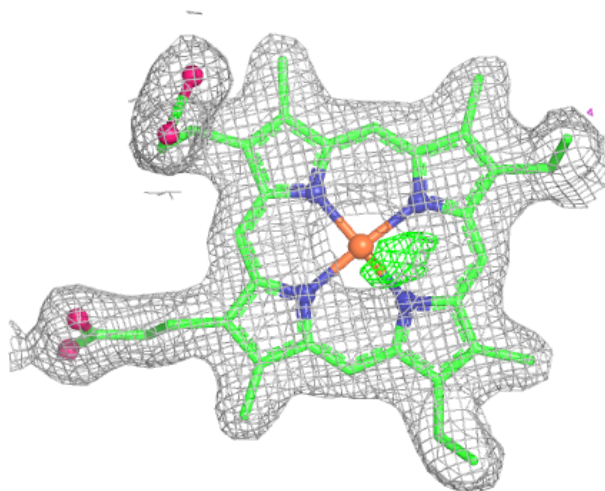
Electron density around HEC A 606:

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



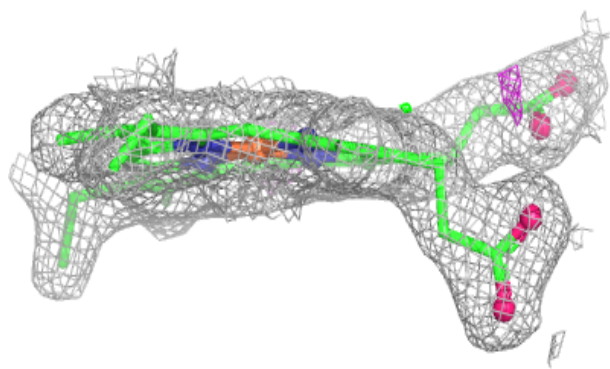
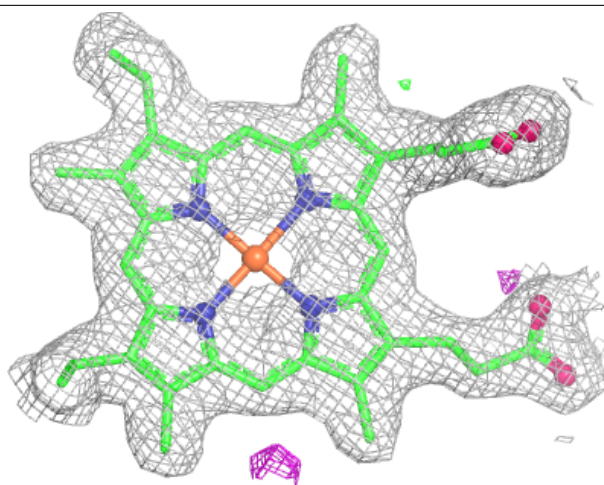
Electron density around HEC I 604:

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



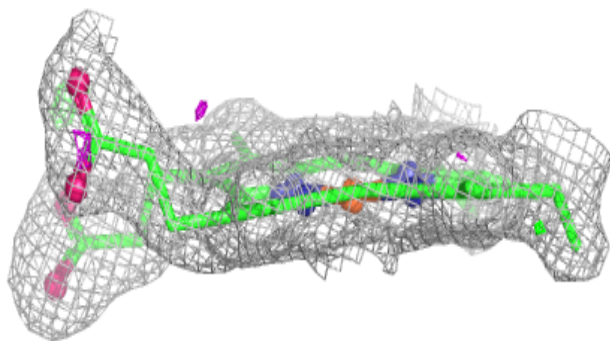
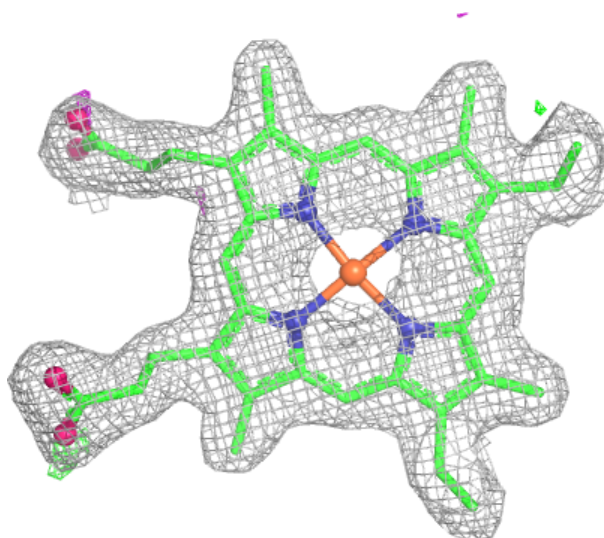
Electron density around HEC E 601:

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



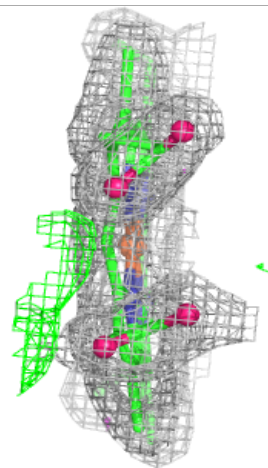
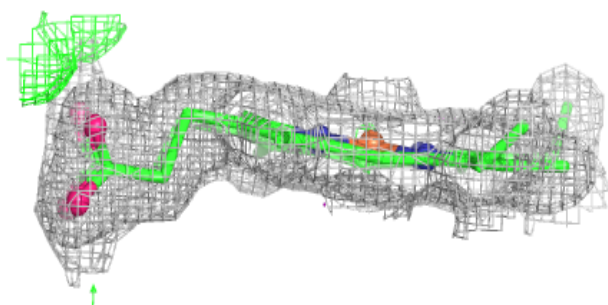
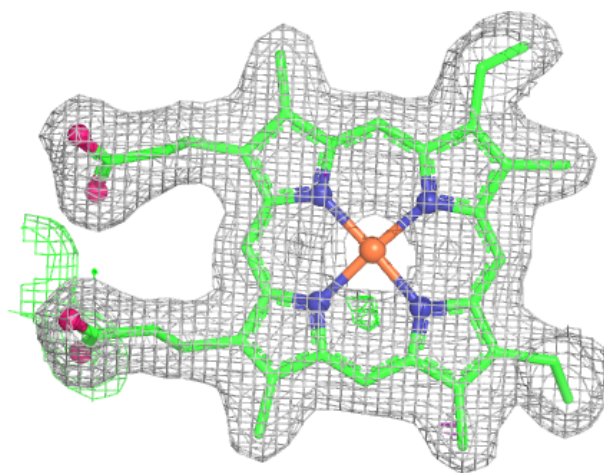
Electron density around HEC I 606:

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



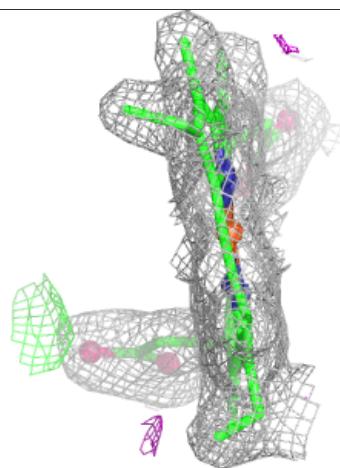
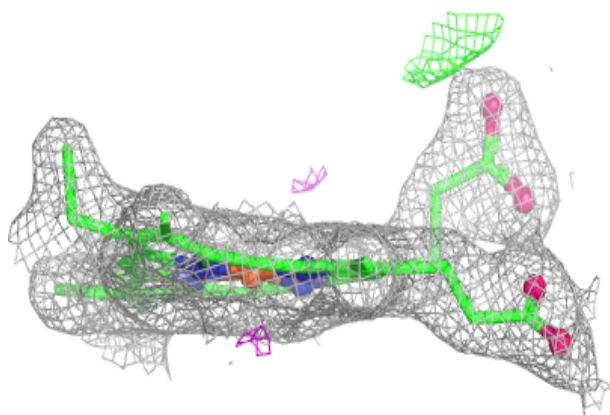
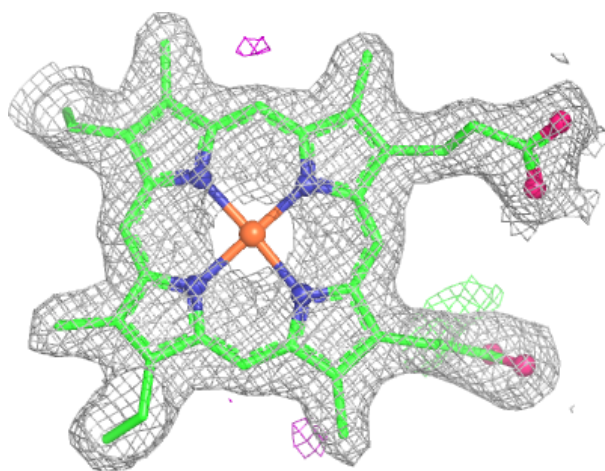
Electron density around HEC I 607:

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



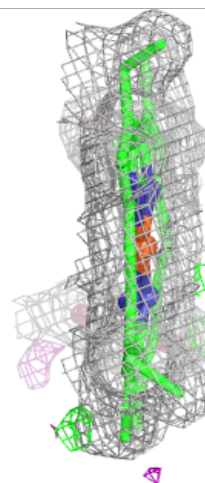
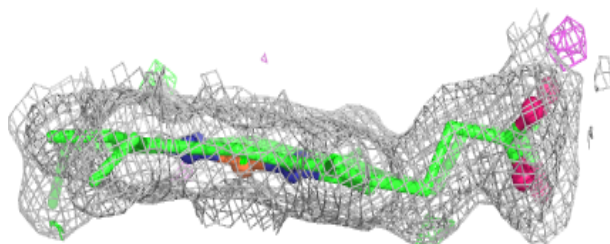
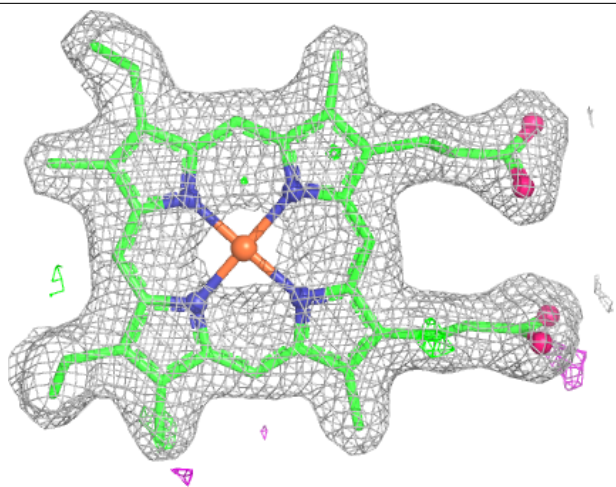
Electron density around HEC K 601:

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



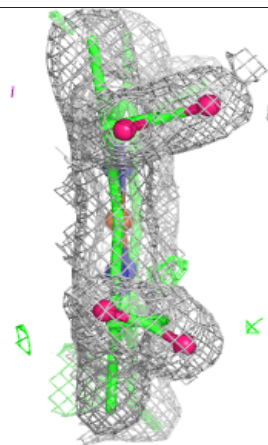
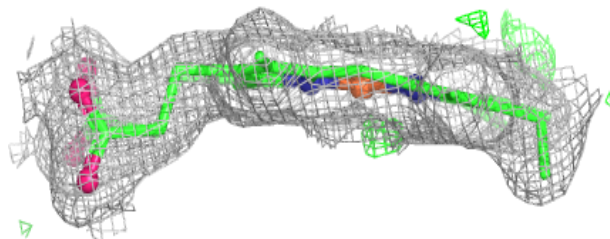
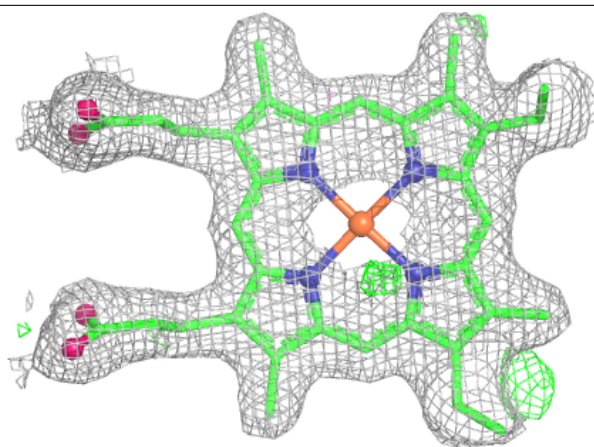
Electron density around HEC A 607:

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



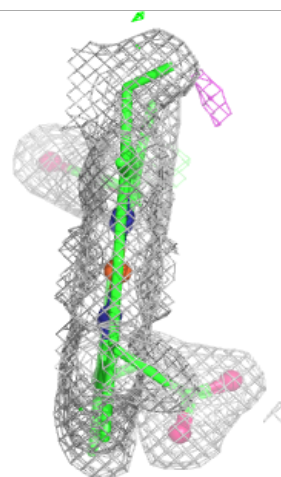
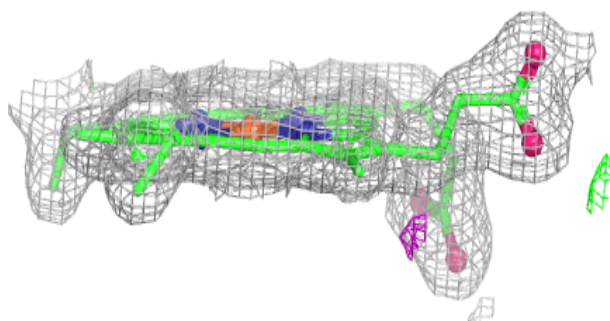
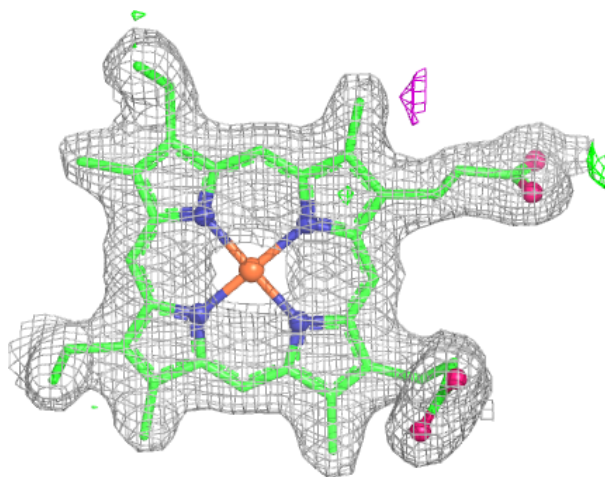
Electron density around HEC E 603:

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



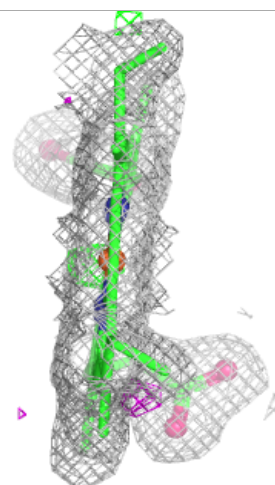
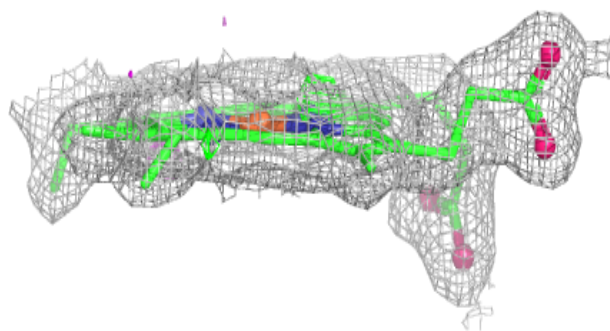
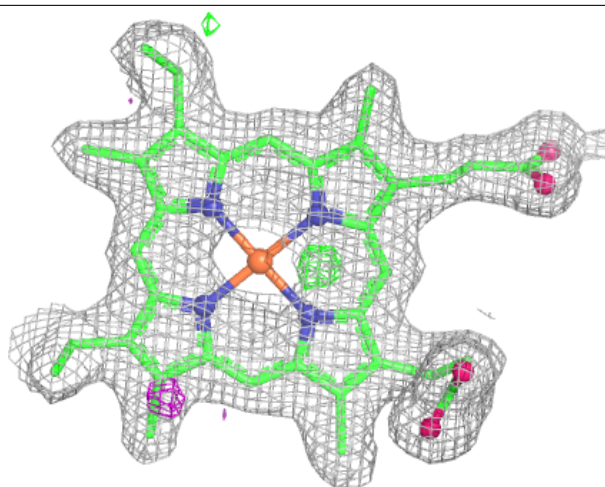
Electron density around HEC K 604:

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



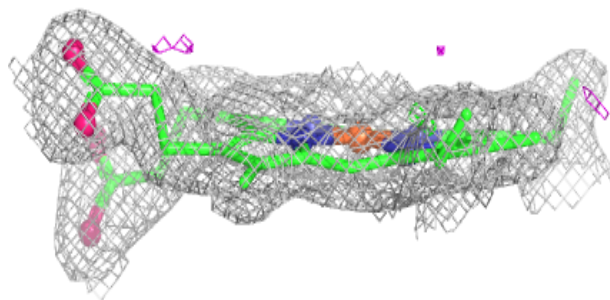
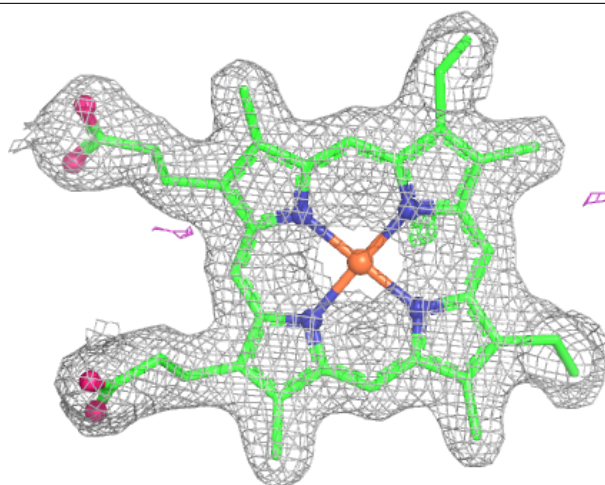
Electron density around HEC E 604:

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



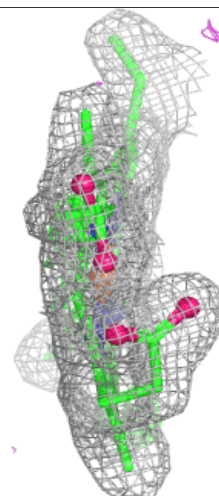
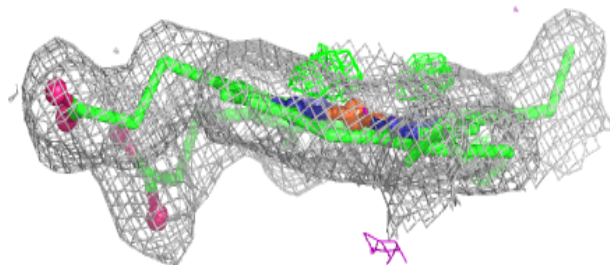
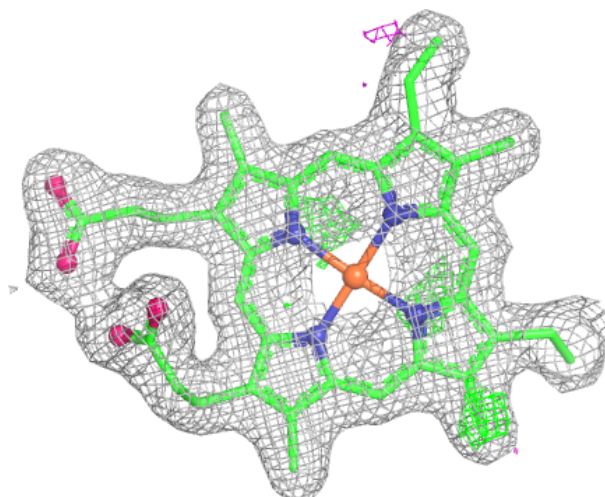
Electron density around HEC K 606:

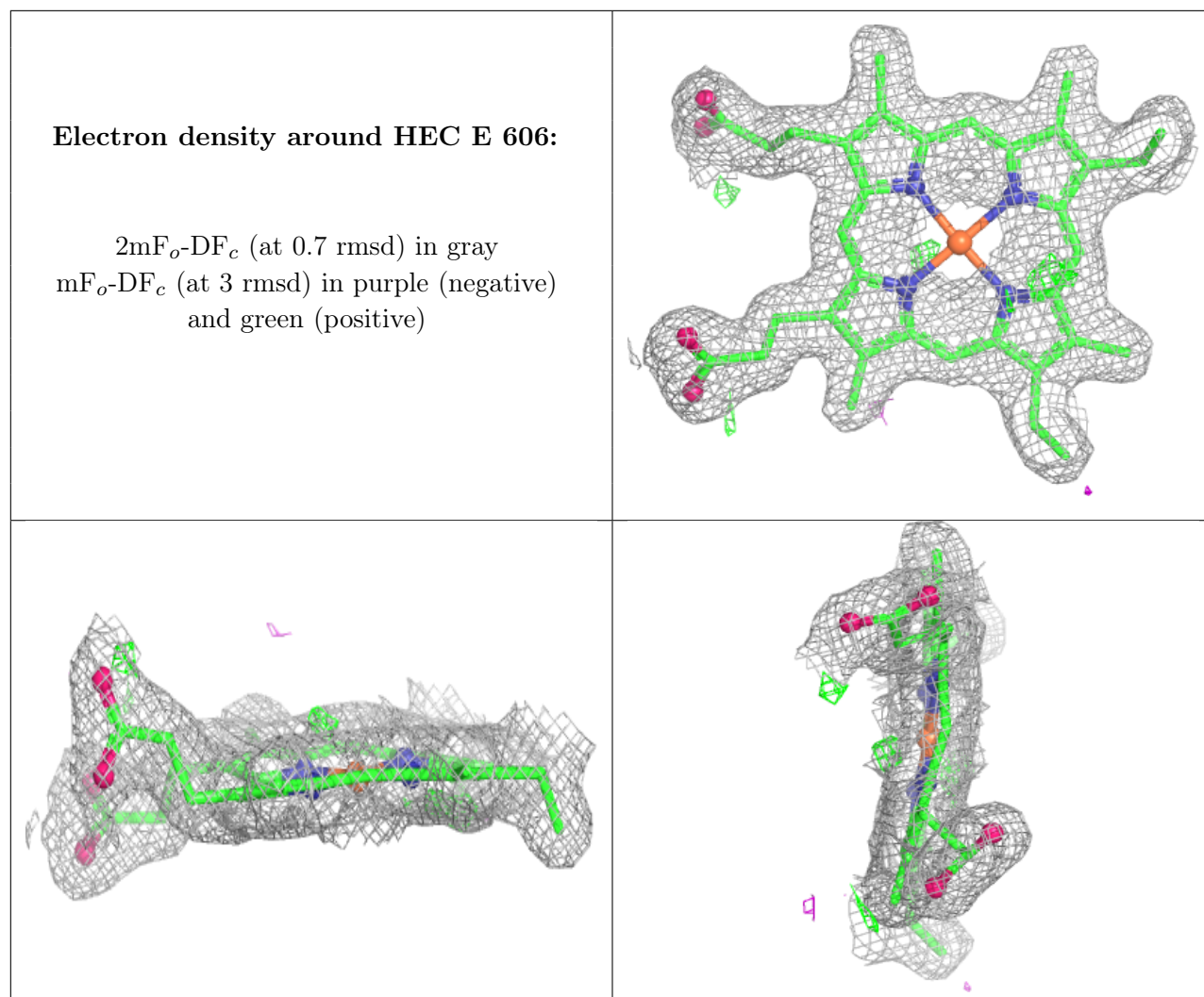
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC E 605:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.