



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:37 AM EDT

PDB ID : 4N4O / pdb_00004n4o
Title : Nitrosomonas europea HAO soaked in NH₂OH
Authors : Maalcke, W.J.; Dietl, A.; Marritt, S.J.; Butt, J.N.; Jetten, M.S.M.; Keltjens, J.T.; Barends, T.R.M.B.; Kartal, B.
Deposited on : 2013-10-08
Resolution : 2.47 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

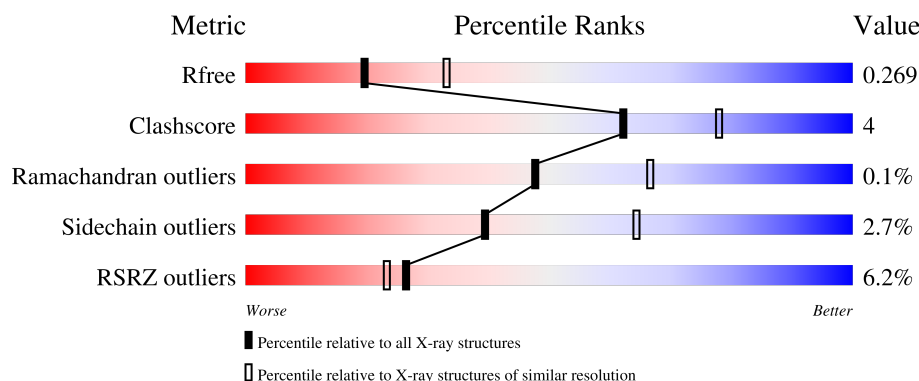
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	546	5% 82% 10% 8%
1	C	546	5% 82% 10% 8%
1	E	546	3% 81% 10% 8%
2	B	57	21% 86% 7% 7%
2	D	57	14% 95% . .

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Mol	Chain	Length	Quality of chain
2	F	57	26% 88% 7%

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
3	HEC	A	601	X	-	-	-
3	HEC	A	602	X	-	-	-
3	HEC	A	603	X	-	-	-
3	HEC	A	604	X	-	-	-
3	HEC	A	605	X	-	-	-
3	HEC	A	606	X	-	-	-
3	HEC	A	607	X	-	-	-
3	HEC	C	602	X	-	-	-
3	HEC	C	603	X	-	-	-
3	HEC	C	604	X	-	-	-
3	HEC	C	605	X	-	-	-
3	HEC	C	606	X	-	-	-
3	HEC	C	607	X	-	-	-
3	HEC	C	608	X	-	-	-
3	HEC	E	602	X	-	-	-
3	HEC	E	603	X	-	-	-
3	HEC	E	604	X	-	-	-
3	HEC	E	605	X	-	-	-
3	HEC	E	606	X	-	-	-
3	HEC	E	607	X	-	-	-
3	HEC	E	608	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15367 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.

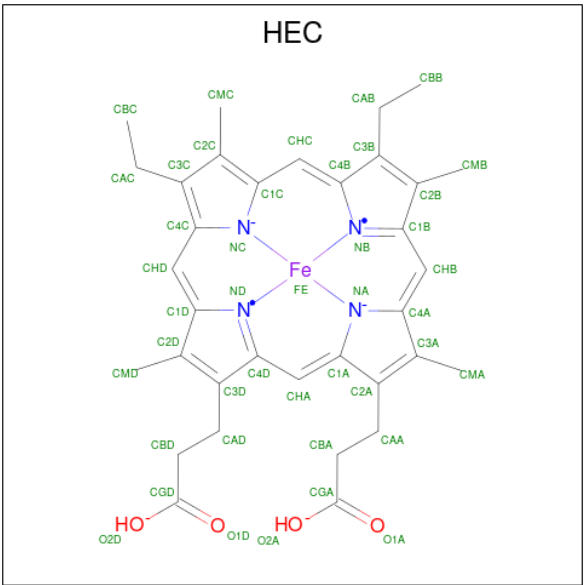
- Molecule 1 is a protein called Hydroxylamine oxidoreductase.

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	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			
1	E	503	Total	C	N	O	S	0	1	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	53	Total	C	N	O	S	0	0	0
			404	253	71	77	3			
2	D	57	Total	C	N	O	S	0	0	0
			429	266	76	84	3			
2	F	55	Total	C	N	O	S	0	0	0
			419	261	74	81	3			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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	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

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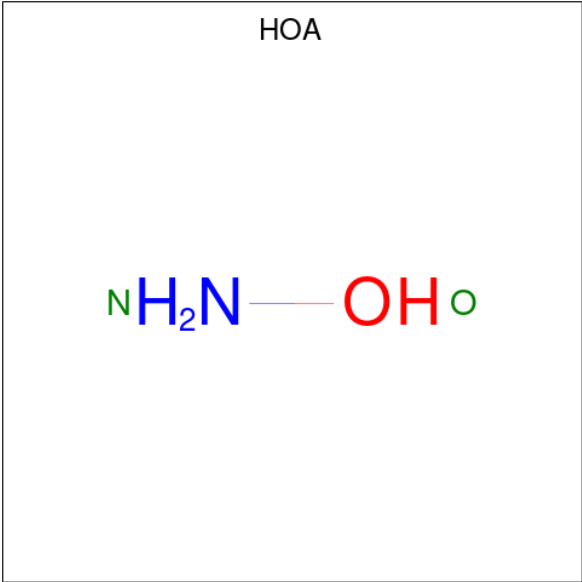
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

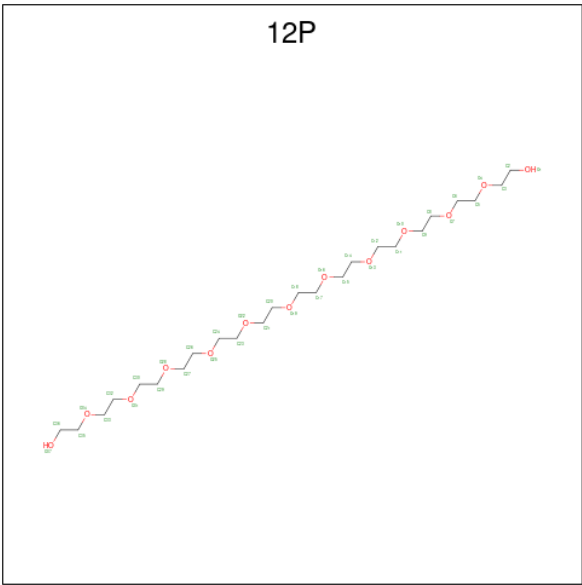
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0

- Molecule 5 is HYDROXYAMINE (CCD ID: HOA) (formula: H₃NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			2	1	1		
5	C	1	Total	N	O	0	0
			2	1	1		
5	E	1	Total	N	O	0	0
			2	1	1		

- Molecule 6 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



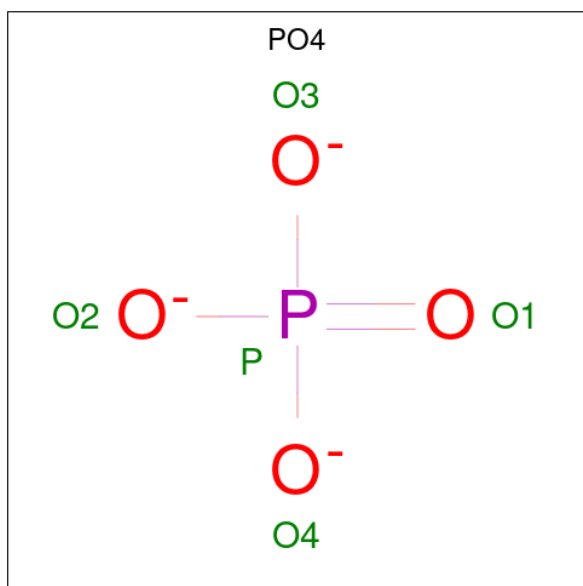
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			25	16	9		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

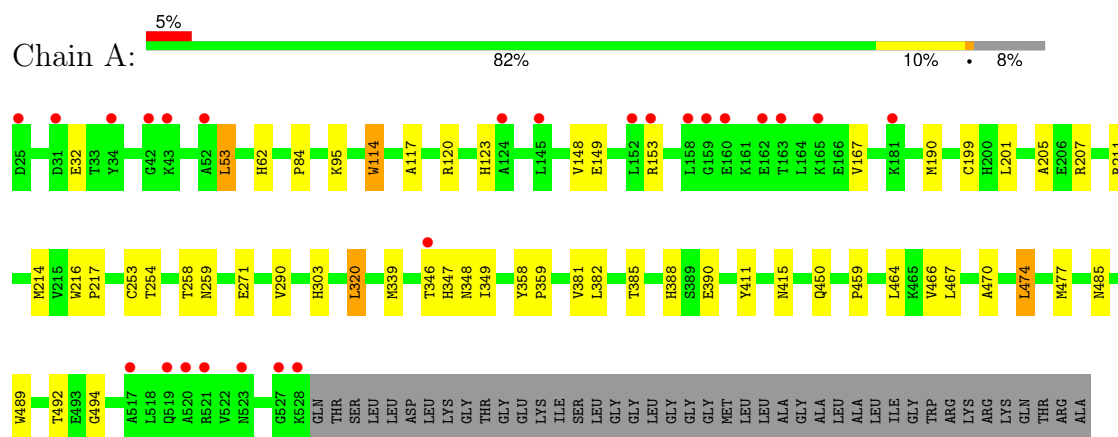
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	295	Total	O	0	0
			295	295		
8	B	37	Total	O	0	0
			37	37		
8	C	284	Total	O	0	0
			284	284		
8	D	41	Total	O	0	0
			41	41		
8	E	301	Total	O	0	0
			301	301		
8	F	35	Total	O	0	0
			35	35		

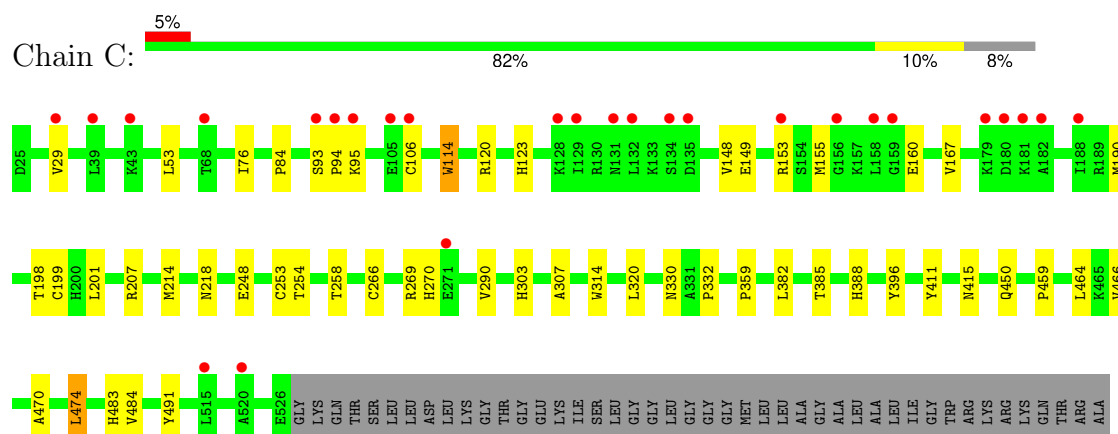
3 Residue-property plots [i](#)

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

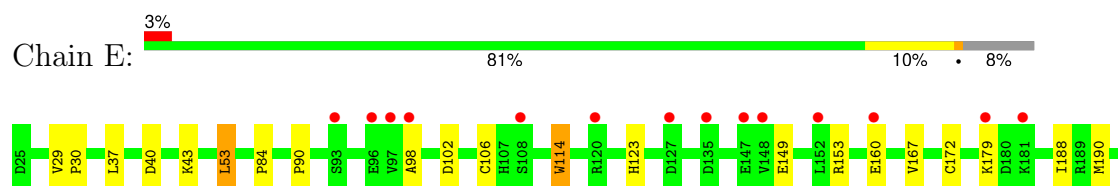
- Molecule 1: Hydroxylamine oxidoreductase

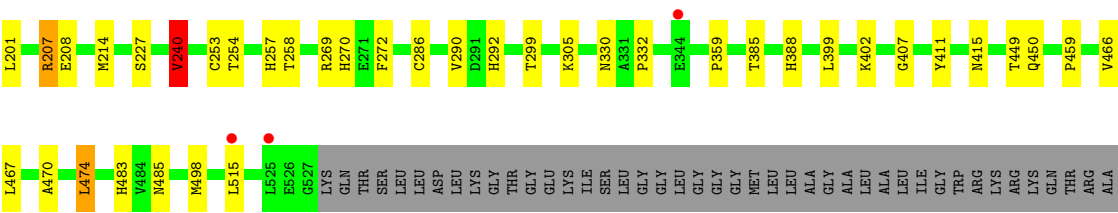


- Molecule 1: Hydroxylamine oxidoreductase

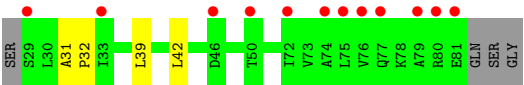
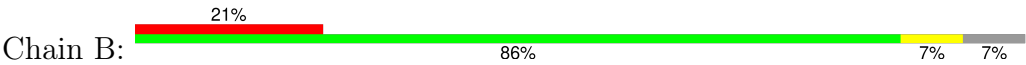


- Molecule 1: Hydroxylamine oxidoreductase

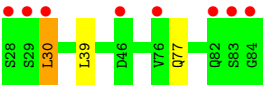




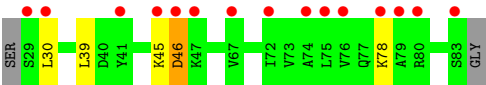
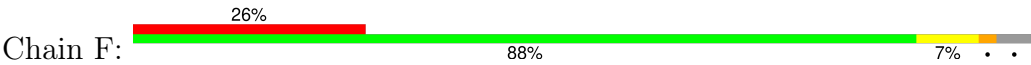
● Molecule 2: hydroxylamine oxidoreductase



● Molecule 2: hydroxylamine oxidoreductase



● Molecule 2: hydroxylamine oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.09Å 141.96Å 106.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.47 49.95 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.95-2.47) 98.1 (49.95-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.010	Depositor
R, R_{free}	0.224 , 0.273 0.221 , 0.269	Depositor DCC
R_{free} test set	7133 reflections (9.32%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15367	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 2.86% 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, PO4, HOA, 12P, K

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	0.41	0/4121	0.81	2/5583 (0.0%)
1	C	0.41	0/4108	0.80	2/5567 (0.0%)
1	E	0.40	0/4121	0.79	3/5583 (0.1%)
2	B	0.43	0/407	0.75	0/546
2	D	0.43	0/432	0.77	0/579
2	F	0.44	0/422	0.77	0/566
All	All	0.41	0/13611	0.80	7/18424 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-C-N	5.88	125.35	119.24
1	A	485	ASN	C-N-CA	5.88	125.35	119.24
1	C	29	VAL	CA-C-N	5.85	125.86	119.89
1	C	29	VAL	C-N-CA	5.85	125.86	119.89
1	E	485	ASN	CA-C-N	5.25	124.71	119.24

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	3821	31	0
1	C	4005	0	3806	32	0
1	E	4018	0	3823	41	0
2	B	404	0	428	1	0
2	D	429	0	449	1	0
2	F	419	0	441	1	0
3	A	344	0	240	9	0
3	C	344	0	240	13	0
3	E	344	0	241	14	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
6	A	12	0	15	1	0
6	C	25	0	33	0	0
7	E	5	0	0	0	0
8	A	295	0	0	0	0
8	B	37	0	0	0	0
8	C	284	0	0	0	0
8	D	41	0	0	0	0
8	E	301	0	0	0	0
8	F	35	0	0	0	0
All	All	15367	0	13537	113	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 4.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:CYS:HA	3:E:601:HEC:HMC3	1.64	0.78
1:E:37:LEU:HD21	1:E:53:LEU:HD13	1.68	0.76
1:A:346:THR:HG22	1:A:348:ASN:H	1.50	0.75
3:E:603:HEC:HBB2	3:E:605:HEC:HAC	1.69	0.72
1:A:253:CYS:HA	3:C:601:HEC:HMC3	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/546 (92%)	484 (96%)	18 (4%)	0	100	100
1	C	500/546 (92%)	482 (96%)	18 (4%)	0	100	100
1	E	502/546 (92%)	484 (96%)	17 (3%)	1 (0%)	43	61
2	B	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
2	D	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
2	F	53/57 (93%)	49 (92%)	3 (6%)	1 (2%)	6	10
All	All	1663/1809 (92%)	1602 (96%)	59 (4%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	46	ASP
1	E	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	430/459 (94%)	418 (97%)	12 (3%)	38	63
1	C	429/459 (94%)	419 (98%)	10 (2%)	44	69
1	E	430/459 (94%)	422 (98%)	8 (2%)	50	73
2	B	46/49 (94%)	44 (96%)	2 (4%)	26	48
2	D	49/49 (100%)	46 (94%)	3 (6%)	17	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	48/49 (98%)	45 (94%)	3 (6%)	16	31
All	All	1432/1524 (94%)	1394 (97%)	38 (3%)	39	64

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	114	TRP
2	F	30	LEU
1	E	201	LEU
1	E	467	LEU
2	F	78	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	386	GLN
1	C	513	GLN
1	E	523	ASN
1	E	450	GLN
1	A	450	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	C	603	1	50,50,50	1.97	10 (20%)	68,82,82	1.40	7 (10%)
3	HEC	C	608	1	50,50,50	1.98	11 (22%)	68,82,82	1.37	7 (10%)
3	HEC	A	602	1	50,50,50	1.97	10 (20%)	68,82,82	1.42	8 (11%)
3	HEC	E	608	1	50,50,50	1.96	11 (22%)	68,82,82	1.40	6 (8%)
6	12P	C	610	-	24,24,36	0.51	0	23,23,35	0.22	0
3	HEC	A	601	1	50,50,50	2.05	9 (18%)	68,82,82	1.42	8 (11%)
3	HEC	C	604	1	50,50,50	2.09	10 (20%)	68,82,82	1.41	6 (8%)
3	HEC	E	605	1	50,50,50	2.05	10 (20%)	68,82,82	1.40	6 (8%)
5	HOA	A	610	3	0,1,1	-	-	-	-	-
3	HEC	C	602	1	50,50,50	2.02	9 (18%)	68,82,82	1.36	8 (11%)
3	HEC	A	604	1	50,50,50	2.01	10 (20%)	68,82,82	1.34	7 (10%)
3	HEC	A	606	1	50,50,50	1.93	10 (20%)	68,82,82	1.37	6 (8%)
3	HEC	C	607	1	50,50,50	1.94	9 (18%)	68,82,82	1.36	7 (10%)
3	HEC	E	607	1	50,50,50	1.92	10 (20%)	68,82,82	1.38	7 (10%)
3	HEC	A	605	1	50,50,50	1.95	9 (18%)	68,82,82	1.41	7 (10%)
3	HEC	C	605	1	50,50,50	2.05	10 (20%)	68,82,82	1.40	8 (11%)
3	HEC	E	603	1	50,50,50	1.93	10 (20%)	68,82,82	1.41	7 (10%)
3	HEC	A	607	1	50,50,50	1.98	11 (22%)	68,82,82	1.42	8 (11%)
7	PO4	E	609	-	4,4,4	0.99	0	6,6,6	0.46	0
3	HEC	E	601	1,5	50,50,50	2.70	17 (34%)	68,82,82	3.09	20 (29%)
3	HEC	C	601	1,5	50,50,50	2.68	16 (32%)	68,82,82	3.07	22 (32%)
3	HEC	E	602	1	50,50,50	2.03	9 (18%)	68,82,82	1.33	8 (11%)
5	HOA	C	609	3	0,1,1	-	-	-	-	-
3	HEC	A	608	1,5	50,50,50	2.71	17 (34%)	68,82,82	3.53	21 (30%)
3	HEC	A	603	1	50,50,50	1.98	10 (20%)	68,82,82	1.42	7 (10%)
3	HEC	C	606	1	50,50,50	1.98	9 (18%)	68,82,82	1.42	7 (10%)
3	HEC	E	606	1	50,50,50	2.01	9 (18%)	68,82,82	1.46	8 (11%)
6	12P	A	611	-	11,11,36	0.52	0	10,10,35	0.17	0
5	HOA	E	610	3	0,1,1	-	-	-	-	-
3	HEC	E	604	1	50,50,50	2.07	10 (20%)	68,82,82	1.39	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	603	1	1/1/3/7	4/14/54/54	-
3	HEC	C	608	1	1/1/3/7	3/14/54/54	-
3	HEC	A	602	1	1/1/3/7	4/14/54/54	-
3	HEC	E	608	1	1/1/3/7	2/14/54/54	-
6	12P	C	610	-	-	16/22/22/34	-
3	HEC	A	601	1	1/1/3/7	2/14/54/54	-
3	HEC	C	604	1	1/1/3/7	2/14/54/54	-
3	HEC	E	605	1	1/1/3/7	3/14/54/54	-
3	HEC	C	602	1	1/1/3/7	2/14/54/54	-
3	HEC	A	604	1	1/1/3/7	2/14/54/54	-
3	HEC	A	606	1	1/1/3/7	5/14/54/54	-
3	HEC	C	607	1	1/1/3/7	3/14/54/54	-
3	HEC	E	607	1	1/1/3/7	2/14/54/54	-
3	HEC	A	605	1	1/1/3/7	7/14/54/54	-
3	HEC	C	605	1	1/1/3/7	2/14/54/54	-
3	HEC	E	603	1	1/1/3/7	4/14/54/54	-
3	HEC	A	607	1	1/1/3/7	4/14/54/54	-
3	HEC	C	601	1,5	-	6/14/54/54	-
3	HEC	E	601	1,5	-	6/14/54/54	-
3	HEC	E	602	1	1/1/3/7	3/14/54/54	-
3	HEC	A	608	1,5	-	7/14/54/54	-
3	HEC	A	603	1	1/1/3/7	6/14/54/54	-
3	HEC	C	606	1	1/1/3/7	7/14/54/54	-
3	HEC	E	606	1	1/1/3/7	7/14/54/54	-
6	12P	A	611	-	-	7/9/9/34	-
3	HEC	E	604	1	1/1/3/7	3/14/54/54	-

The worst 5 of 256 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	608	HEC	CHC-C4B	9.03	1.56	1.38
3	C	601	HEC	CHC-C4B	8.94	1.56	1.38
3	E	601	HEC	CHC-C4B	8.83	1.56	1.38
3	E	606	HEC	C3D-C2D	8.23	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEC	C3D-C2D	8.16	1.54	1.36

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	608	HEC	O2A-CGA-O1A	-14.66	85.63	123.33
3	C	601	HEC	CHA-C1A-NA	-11.96	111.43	124.45
3	A	608	HEC	CHA-C1A-NA	-10.75	112.75	124.45
3	E	601	HEC	CHA-C1A-NA	-10.56	112.95	124.45
3	E	601	HEC	O2A-CGA-O1A	-10.20	97.09	123.33

5 of 21 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	HEC	NA
3	A	602	HEC	NA
3	A	603	HEC	NA
3	A	604	HEC	NA
3	A	605	HEC	NA

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	604	HEC	C2C-C3C-CAC-CBC
3	A	608	HEC	C4C-C3C-CAC-CBC
3	C	604	HEC	C4C-C3C-CAC-CBC
3	A	608	HEC	C2C-C3C-CAC-CBC
3	C	601	HEC	C4B-C3B-CAB-CBB

There are no ring outliers.

23 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	HEC	2	0
3	C	608	HEC	1	0
3	A	602	HEC	1	0
3	E	608	HEC	2	0
3	A	601	HEC	1	0
3	C	604	HEC	2	0
3	E	605	HEC	2	0
3	C	602	HEC	1	0

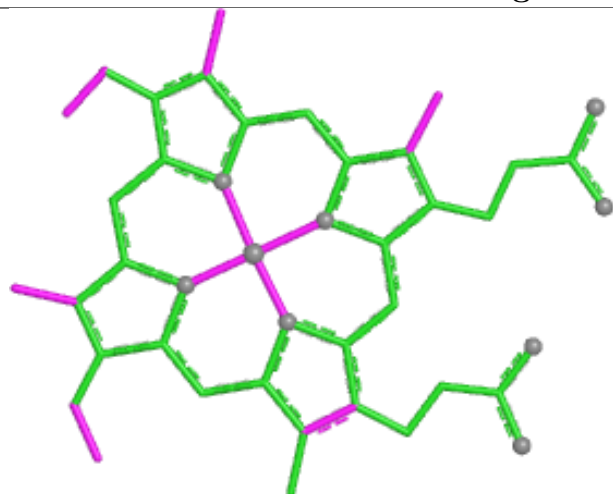
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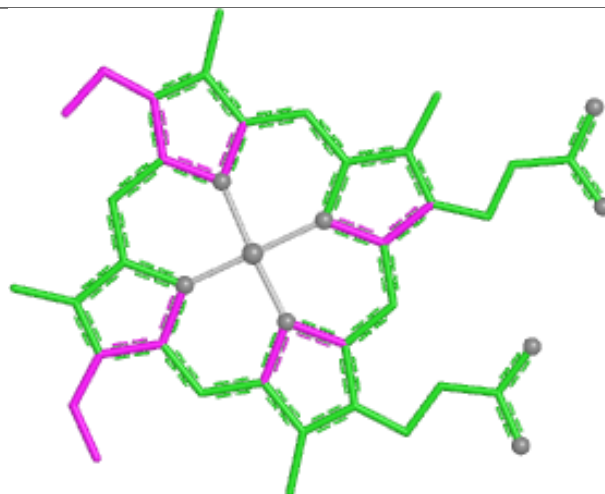
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	HEC	1	0
3	A	606	HEC	2	0
3	C	607	HEC	3	0
3	E	607	HEC	3	0
3	A	605	HEC	1	0
3	C	605	HEC	1	0
3	E	603	HEC	3	0
3	A	607	HEC	1	0
3	E	601	HEC	2	0
3	C	601	HEC	3	0
3	A	608	HEC	3	0
3	C	606	HEC	3	0
3	E	606	HEC	3	0
6	A	611	12P	1	0
3	E	604	HEC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

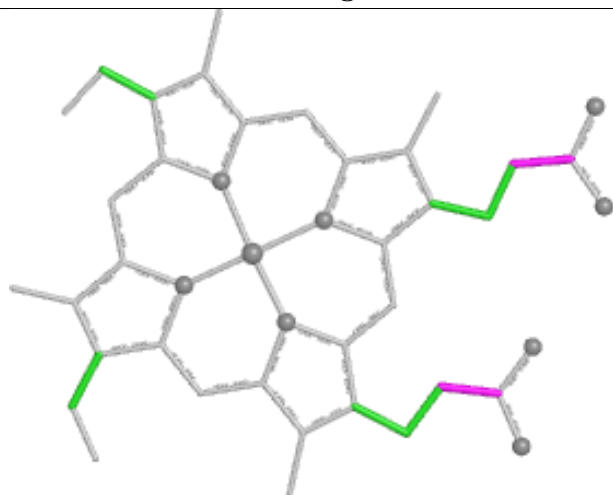
Ligand HEC C 603



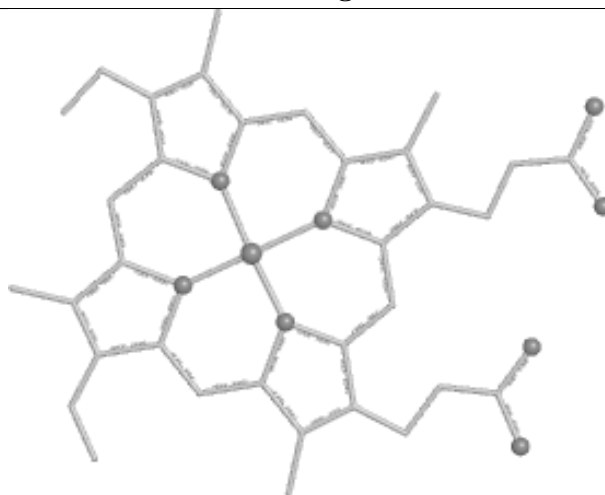
Bond lengths



Bond angles

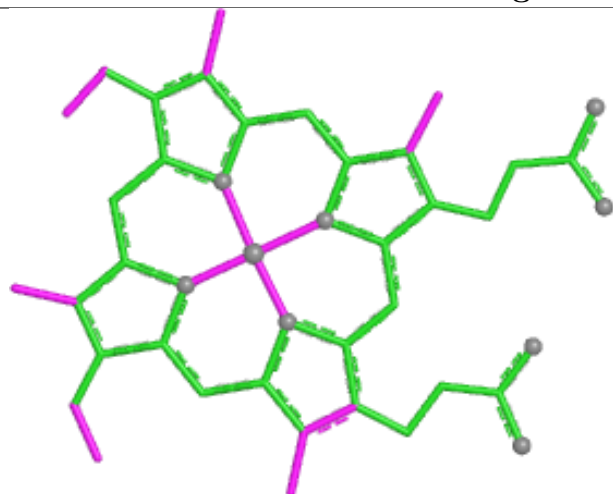


Torsions

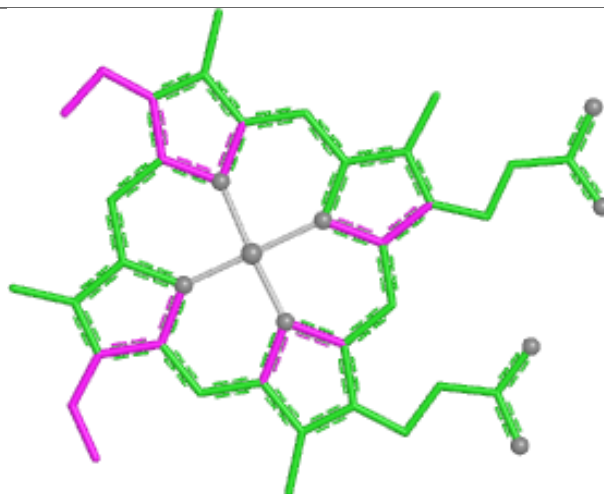


Rings

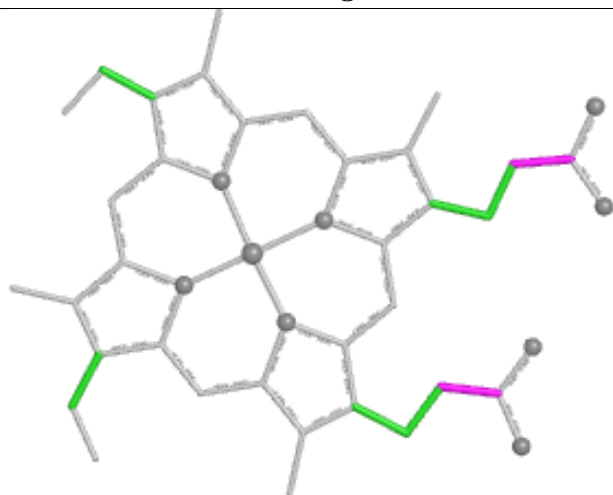
Ligand HEC C 608



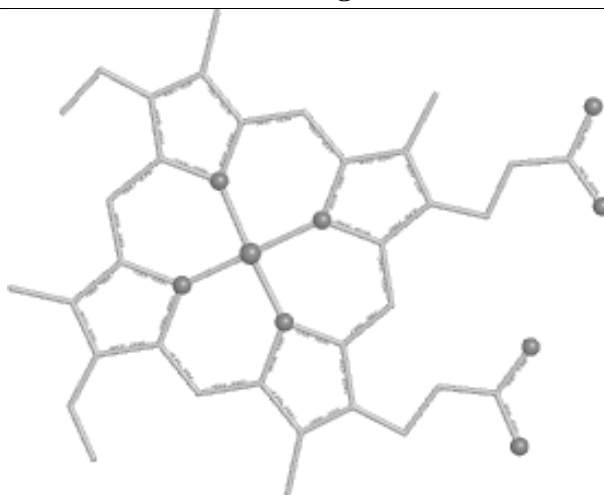
Bond lengths



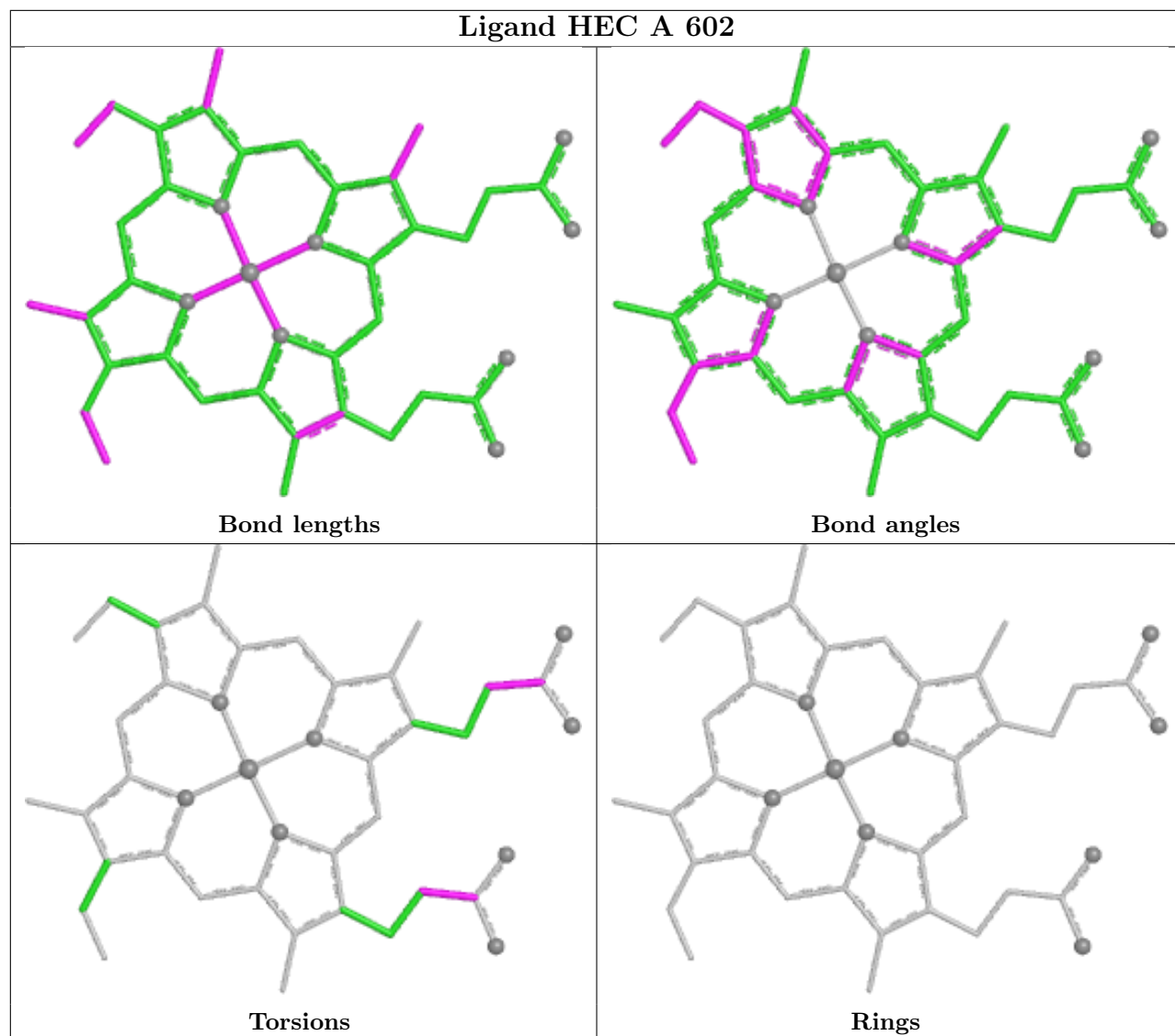
Bond angles



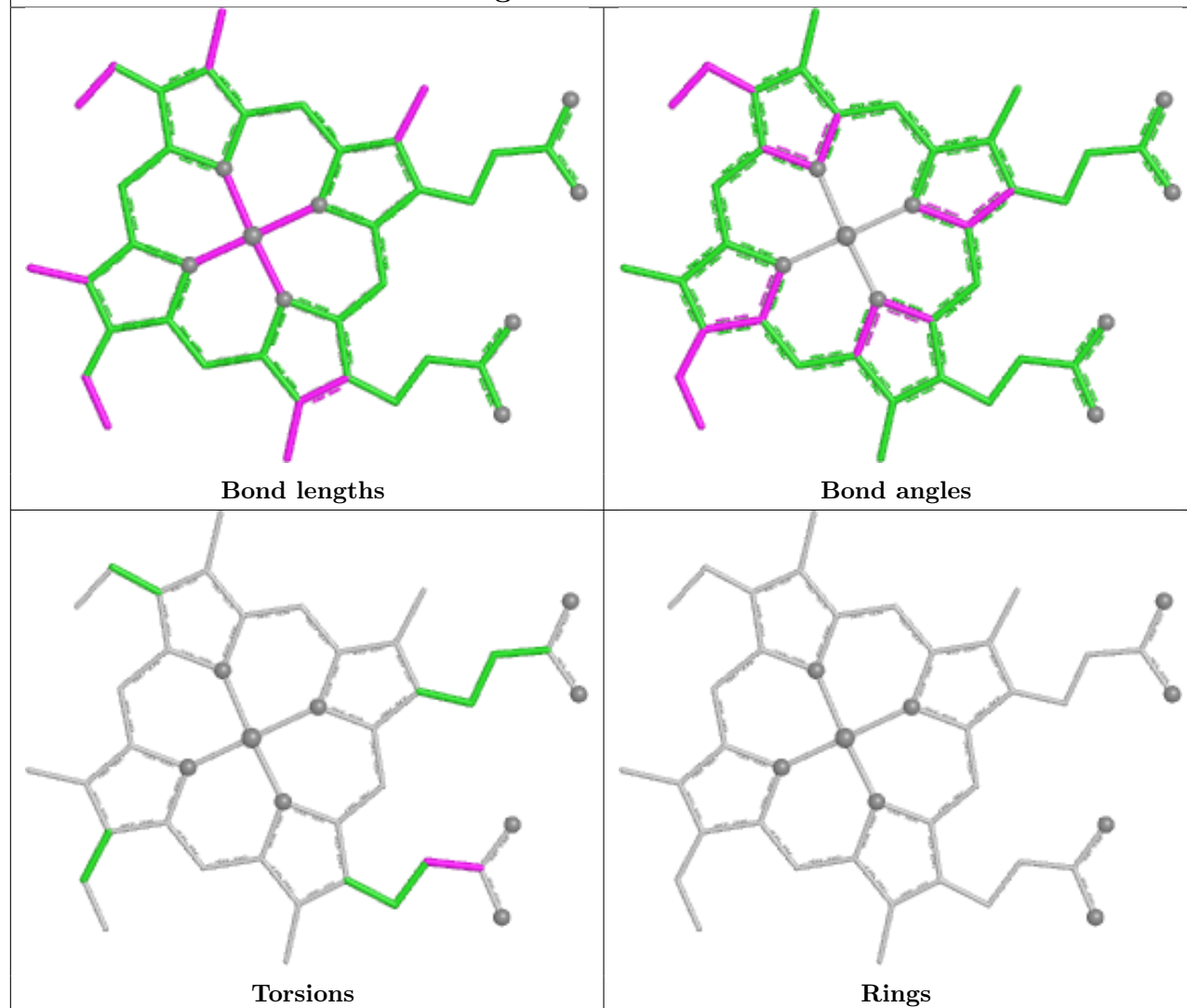
Torsions



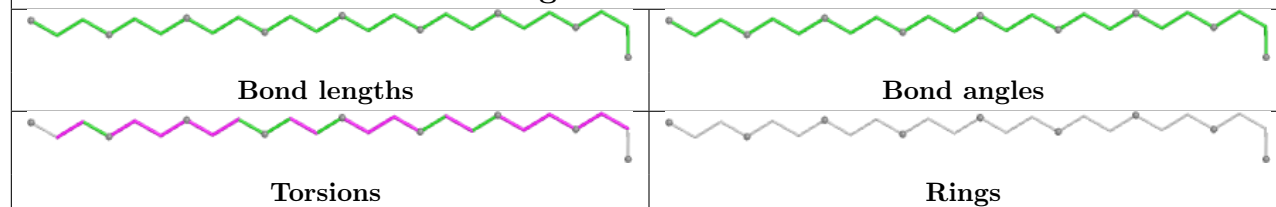
Rings

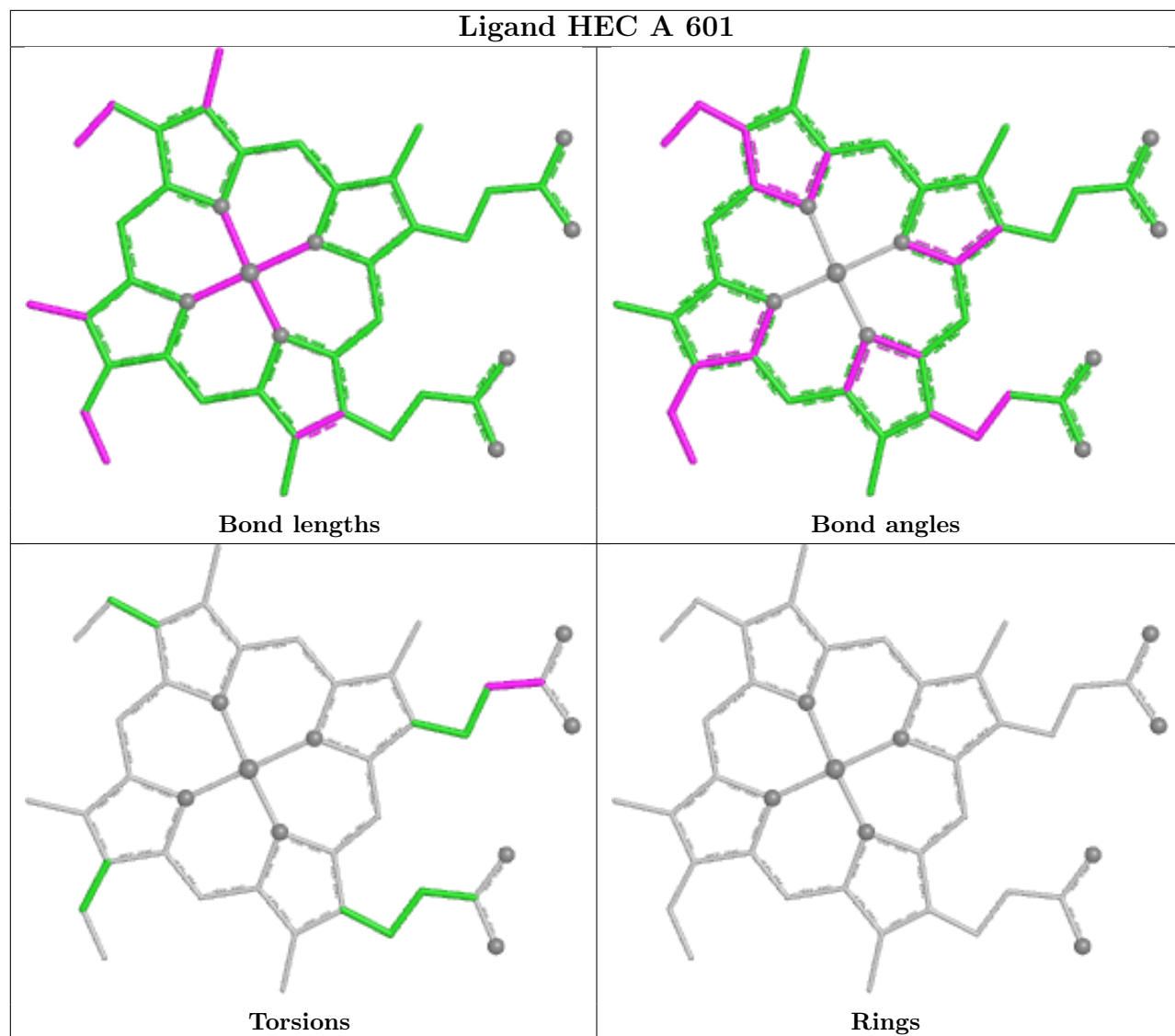


Ligand HEC E 608

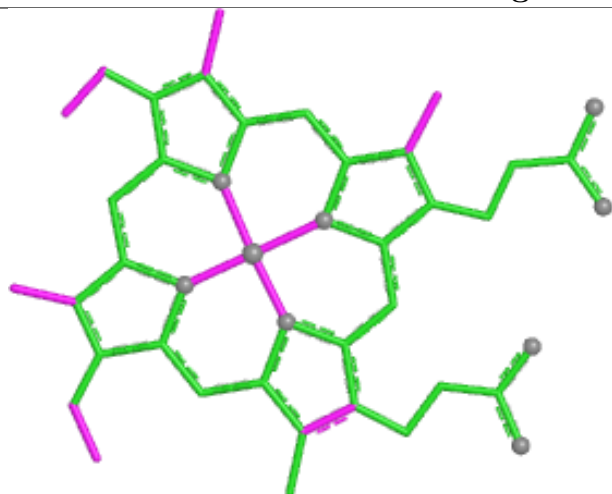


Ligand 12P C 610

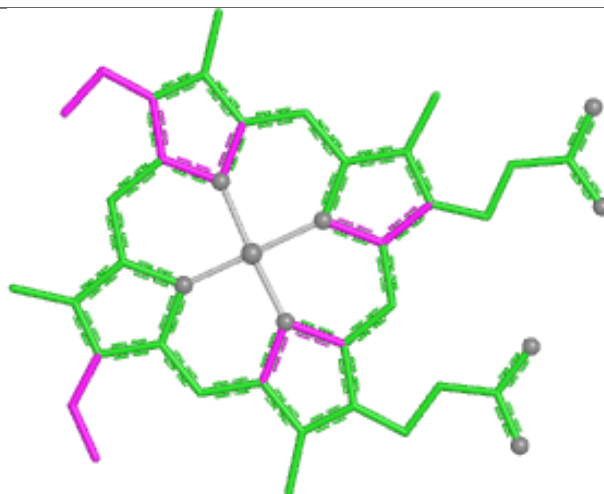




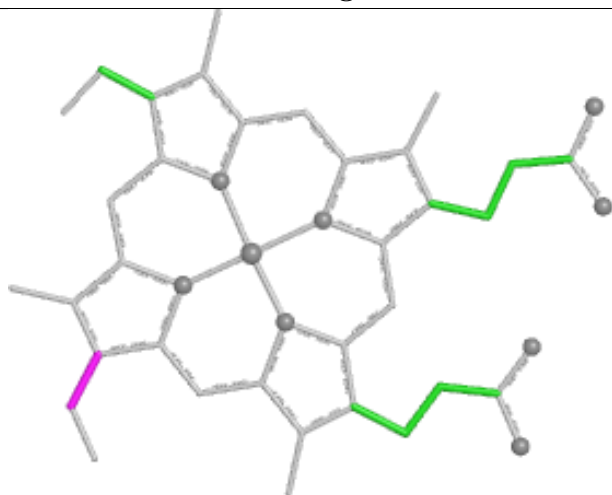
Ligand HEC C 604



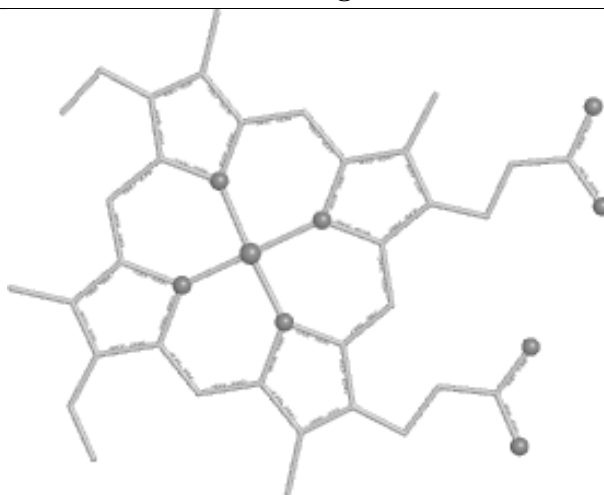
Bond lengths



Bond angles

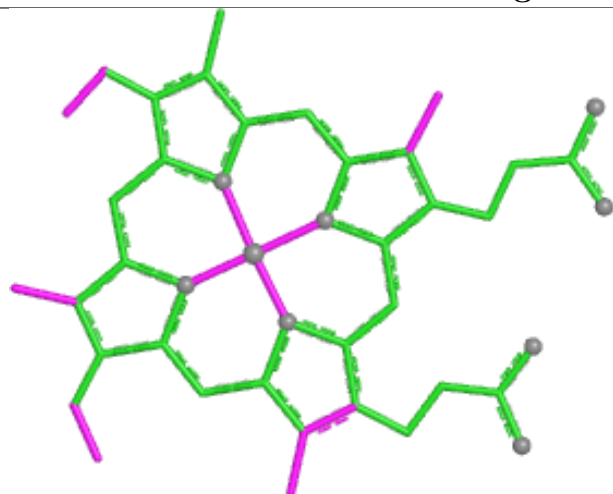


Torsions

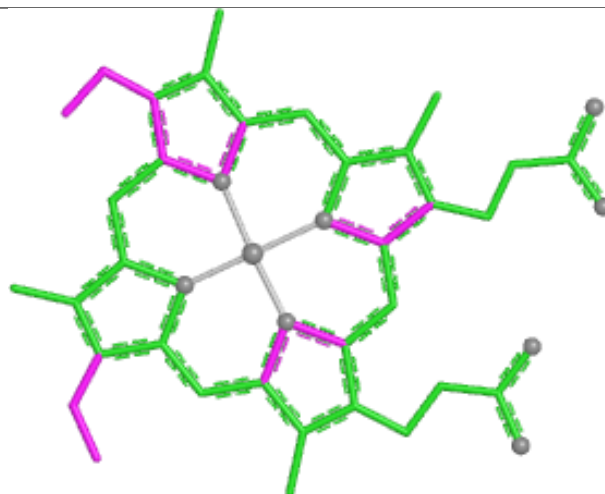


Rings

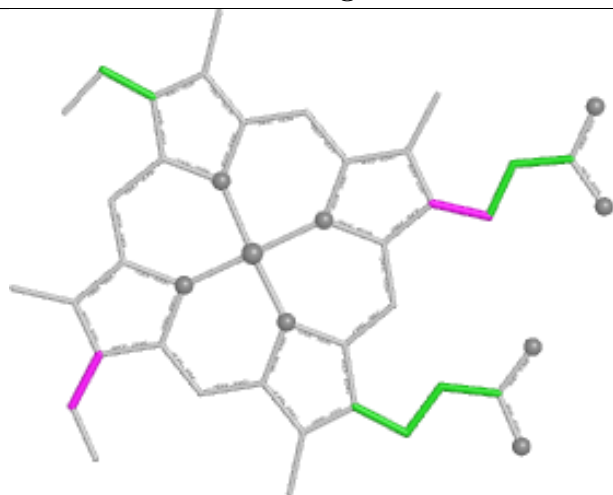
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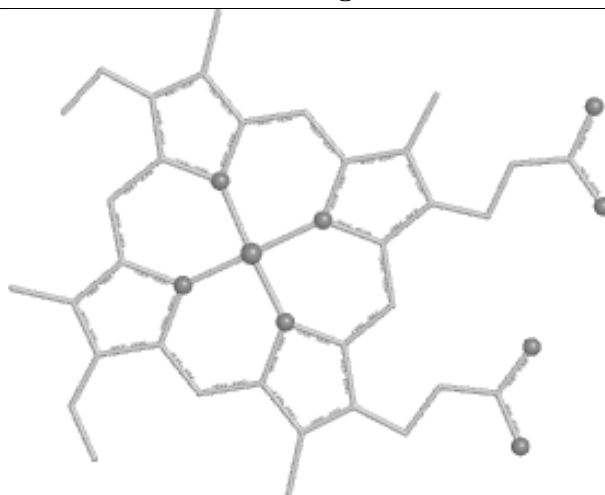
Bond lengths



Bond angles

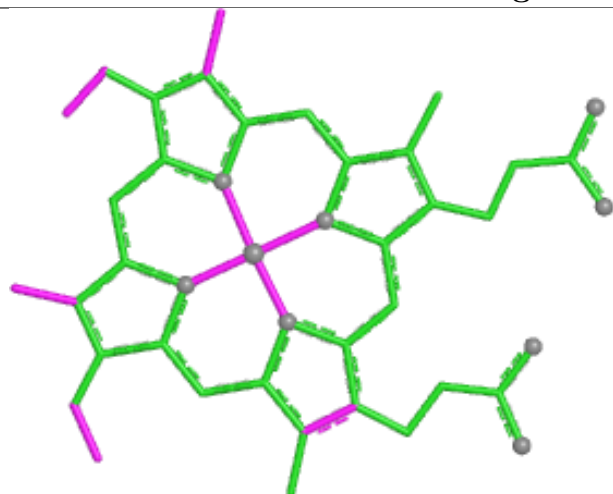


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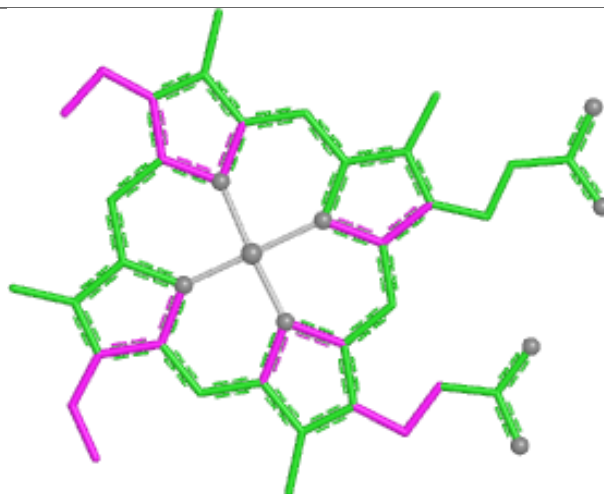


Rings

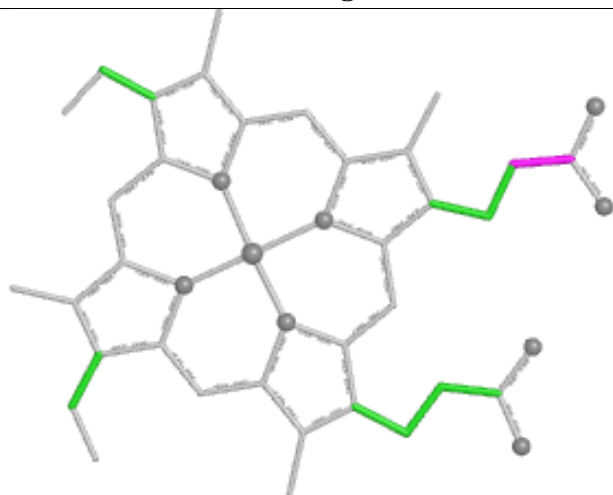
Ligand HEC C 602



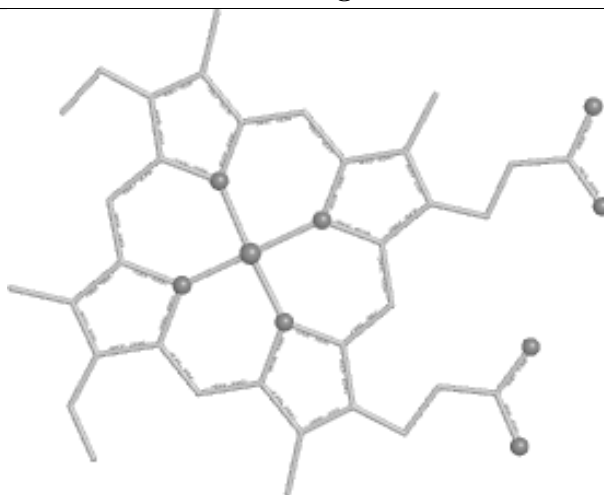
Bond lengths



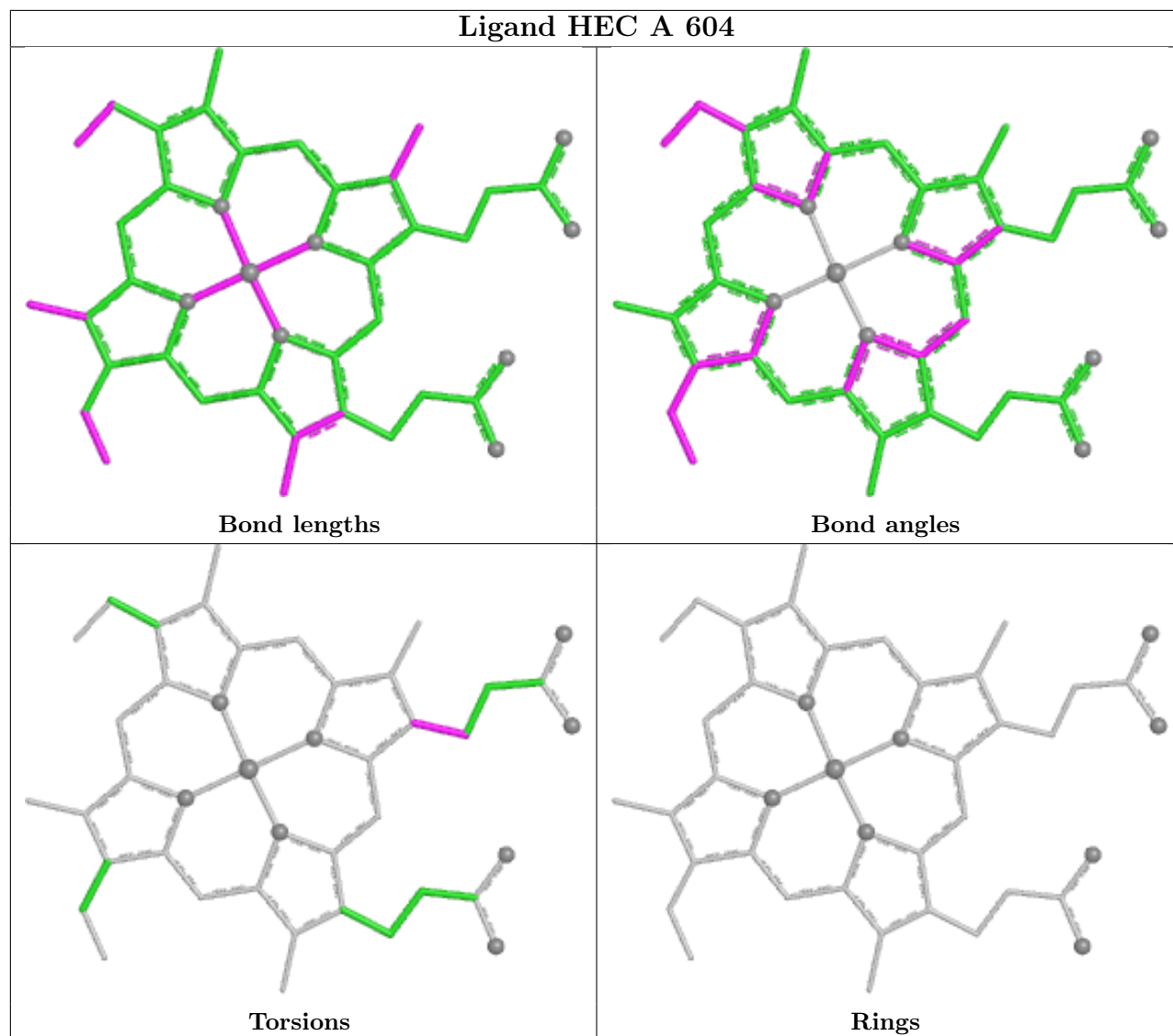
Bond angles

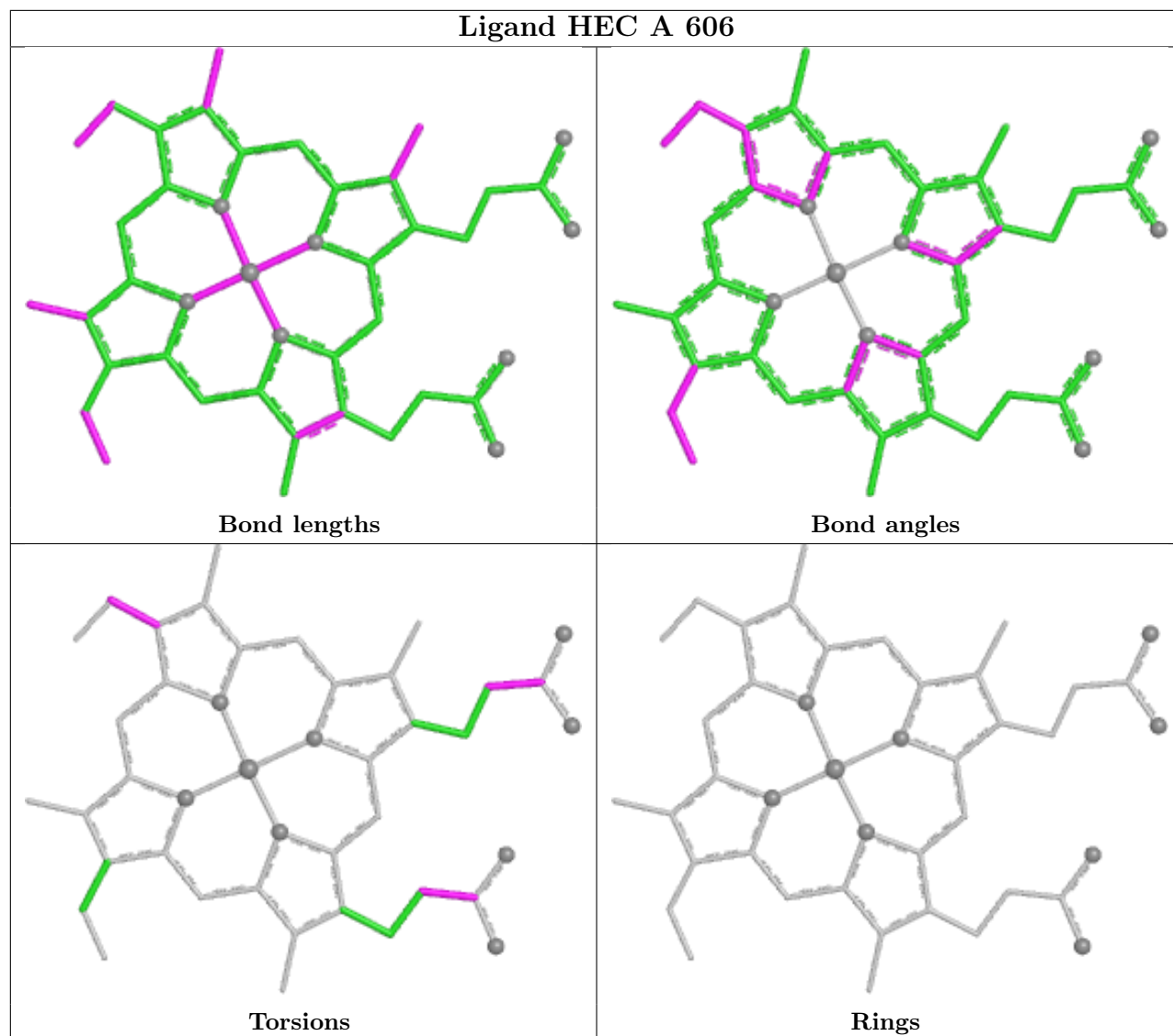


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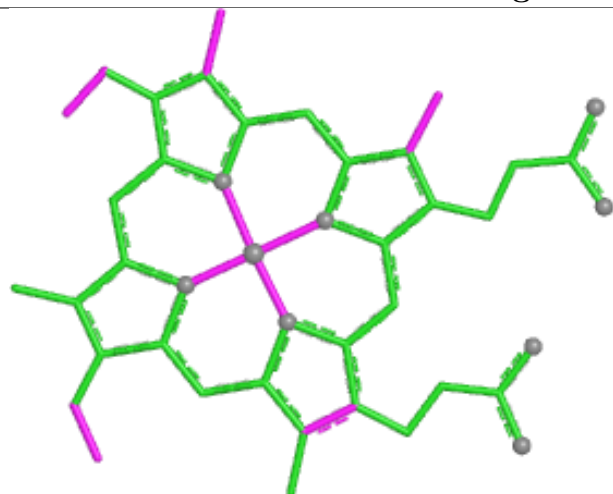


Rings

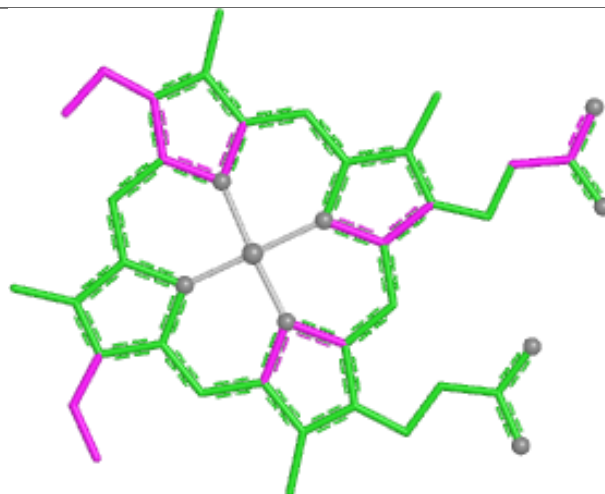




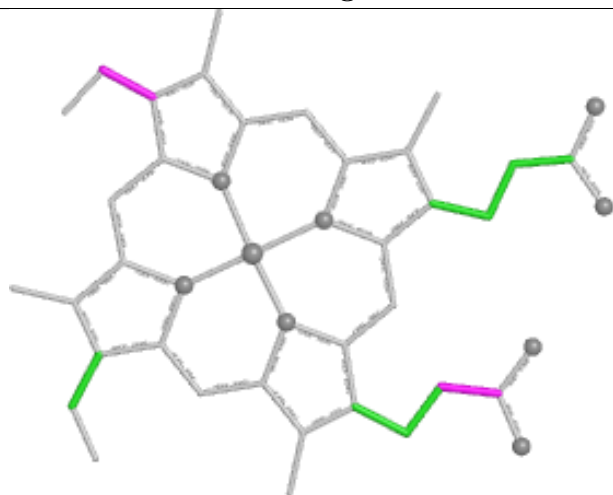
Ligand HEC C 607



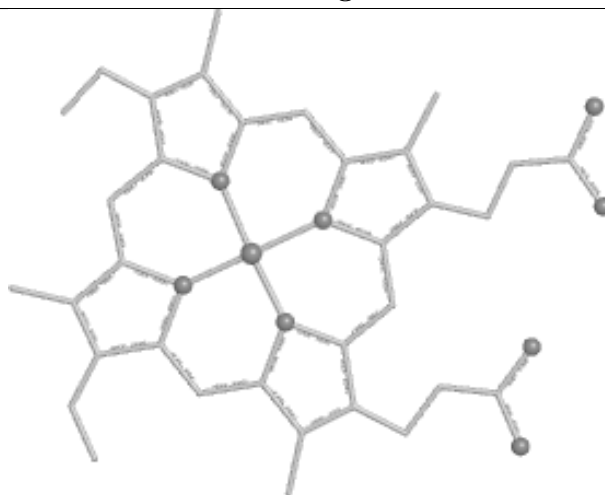
Bond lengths



Bond angles

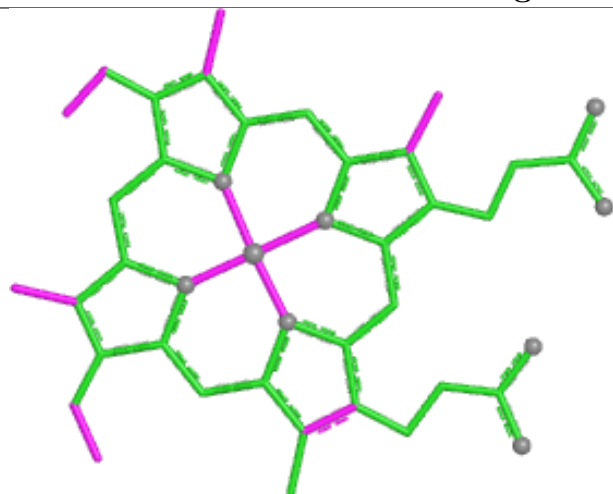


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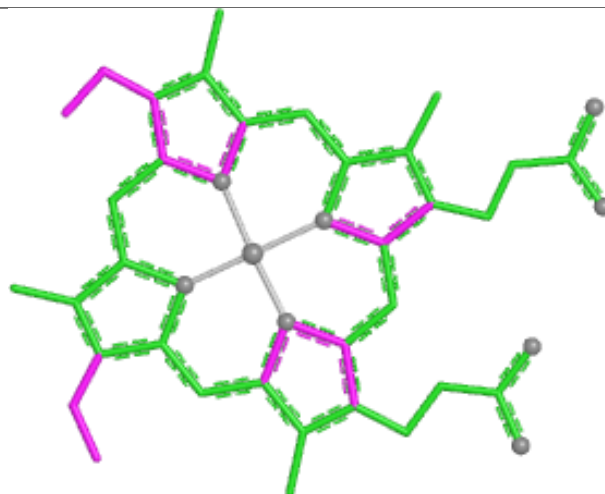


Rings

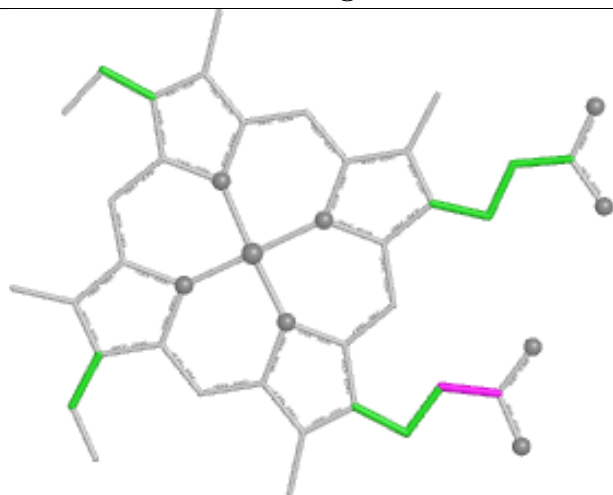
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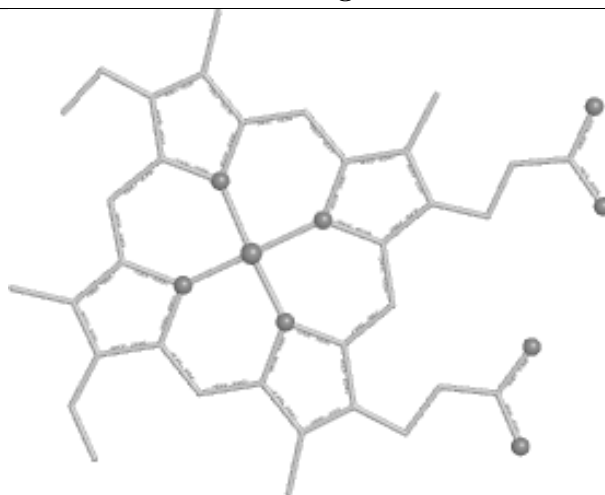
Bond lengths



Bond angles

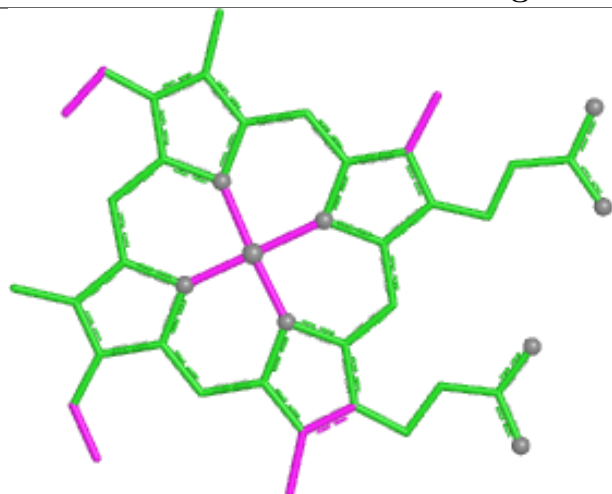


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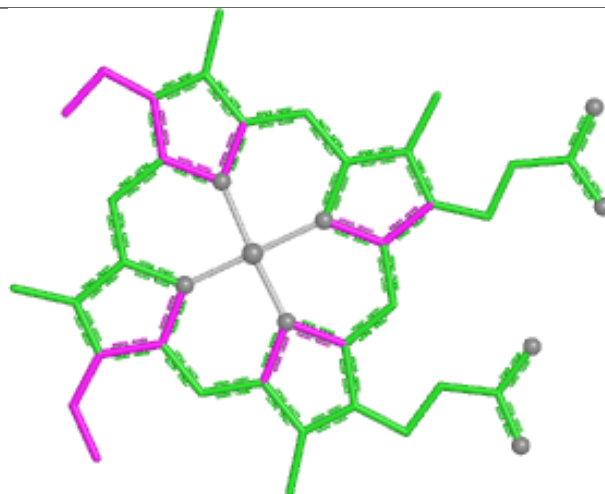


Rings

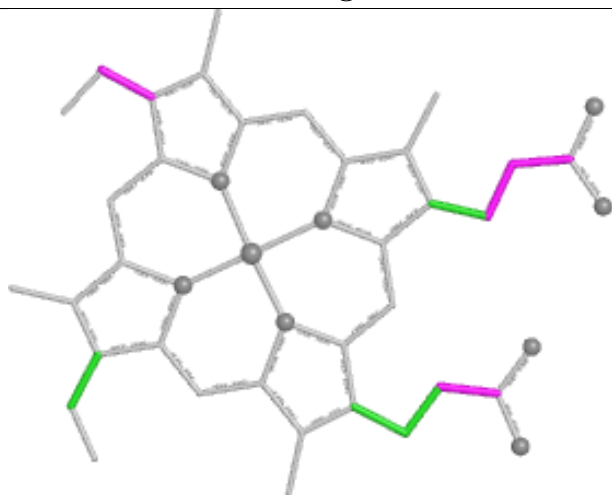
Ligand HEC A 605



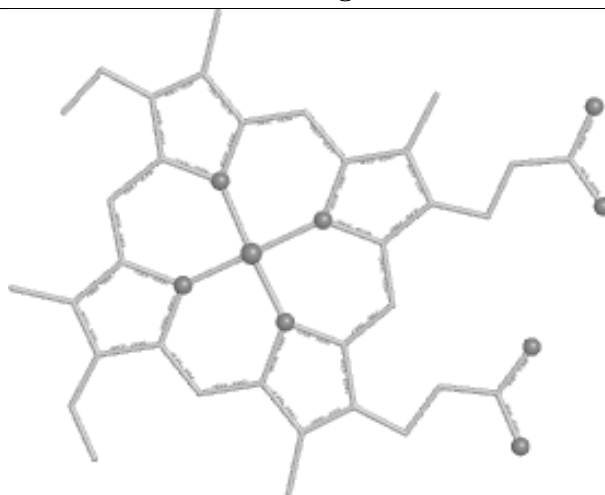
Bond lengths



Bond angles

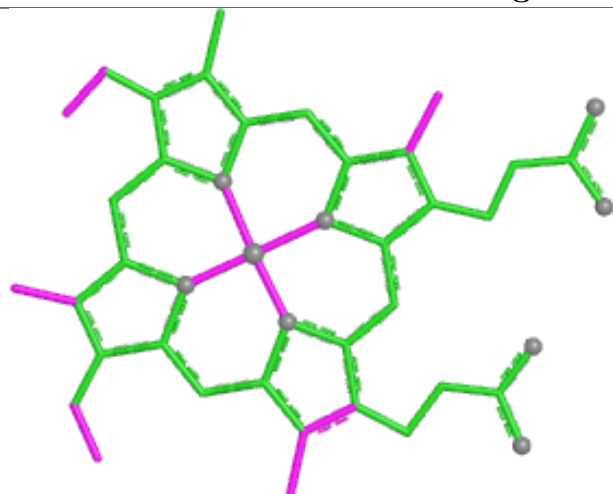


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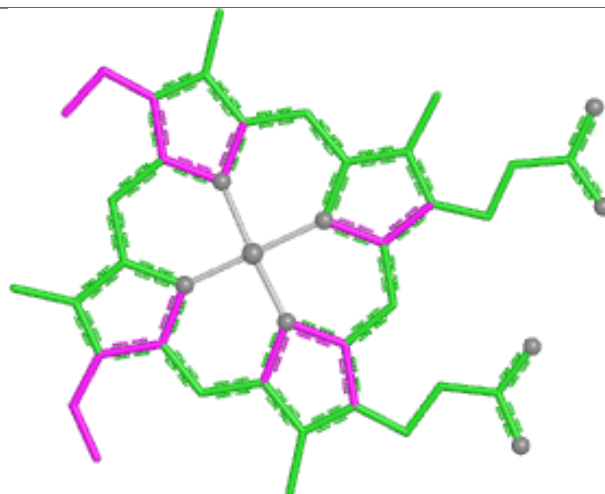


Rings

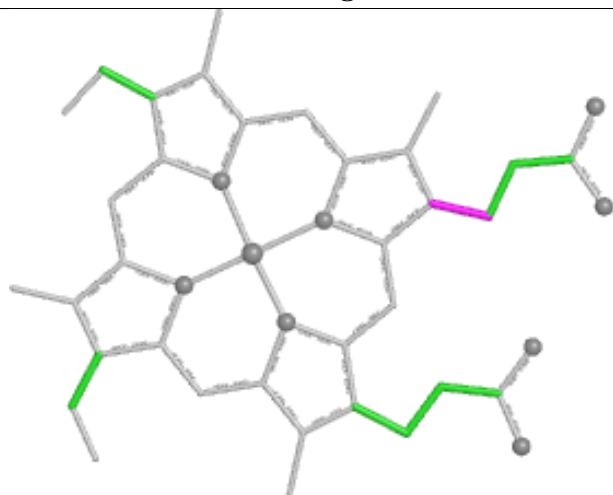
Ligand HEC C 605



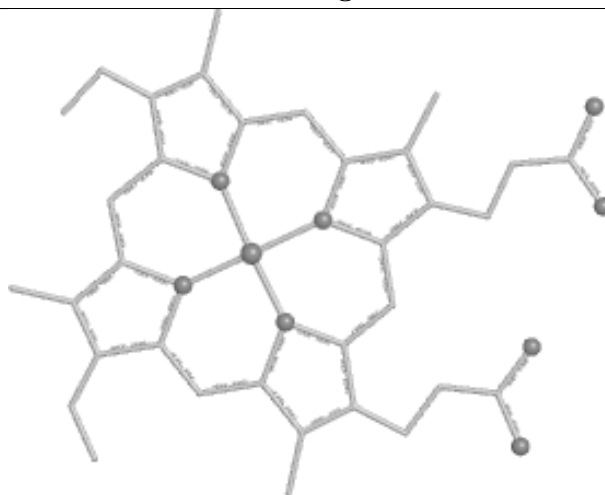
Bond lengths



Bond angles

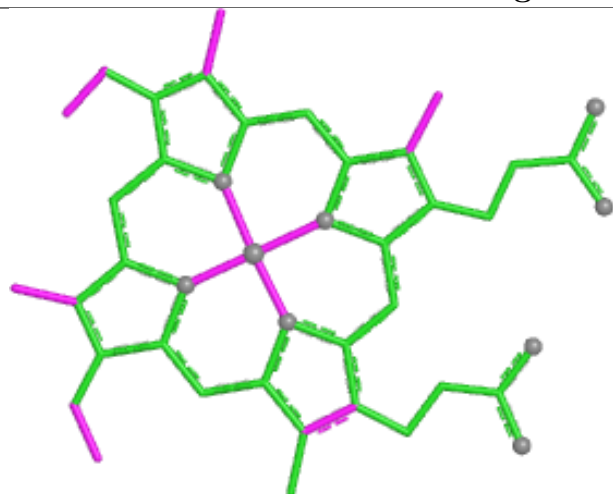


Torsions

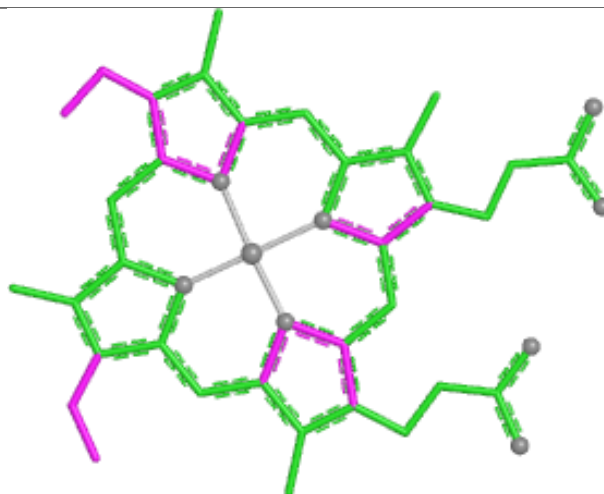


Rings

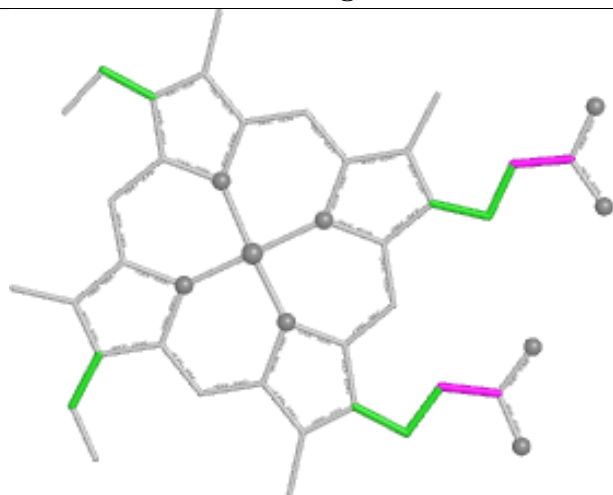
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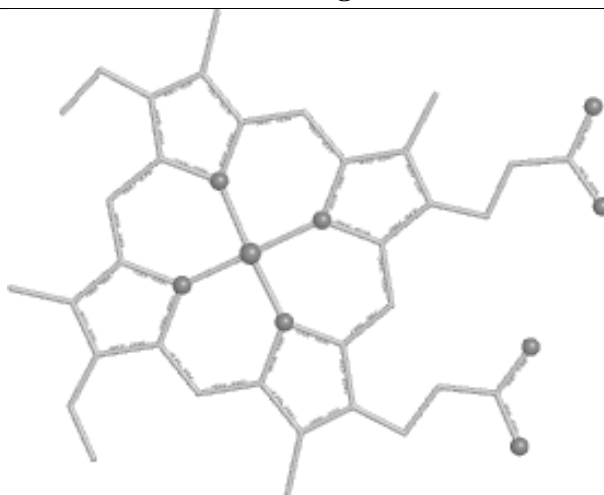
Bond lengths



Bond angles

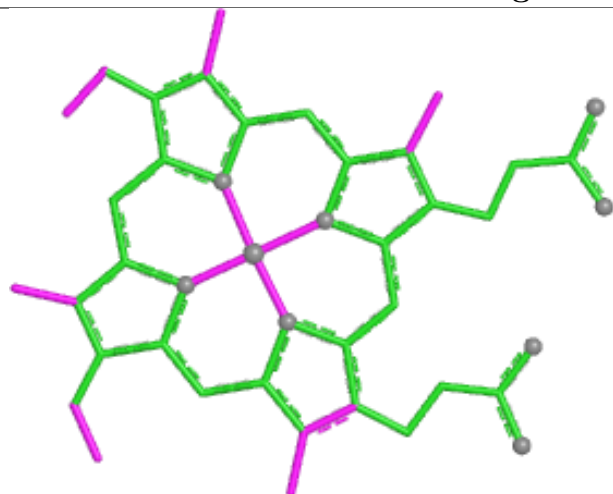


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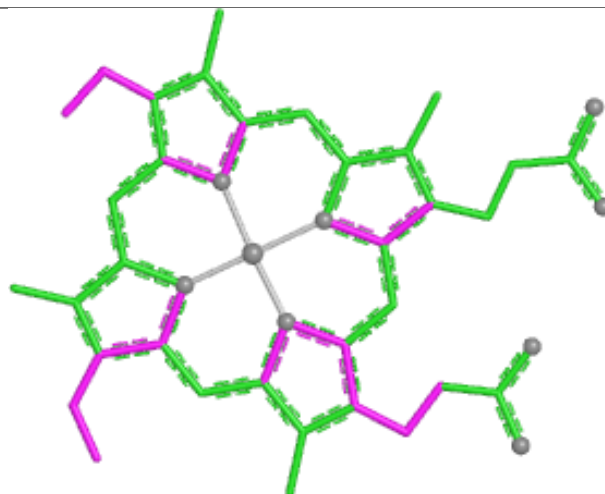


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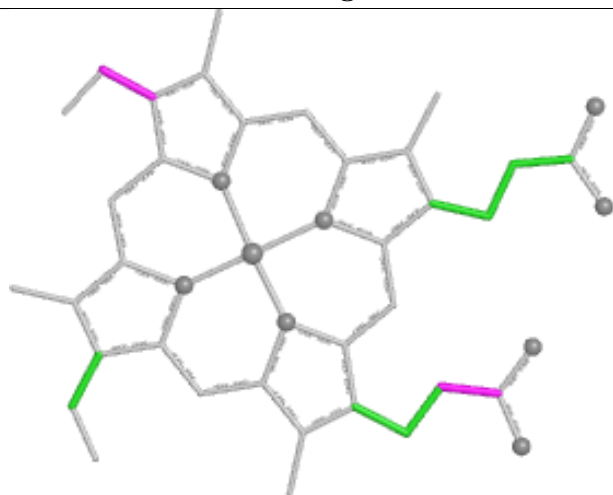
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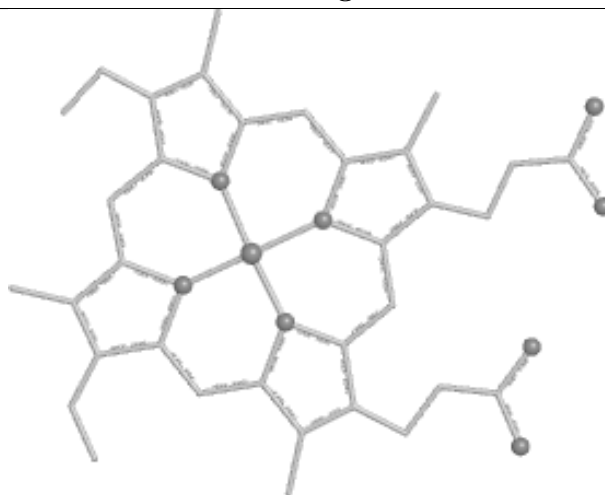
Bond lengths



Bond angles

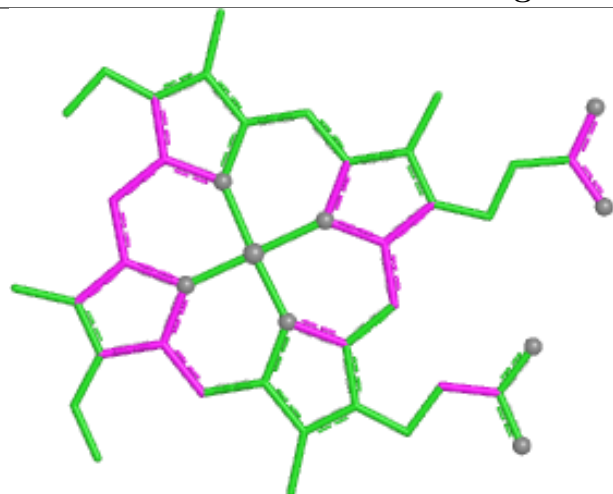


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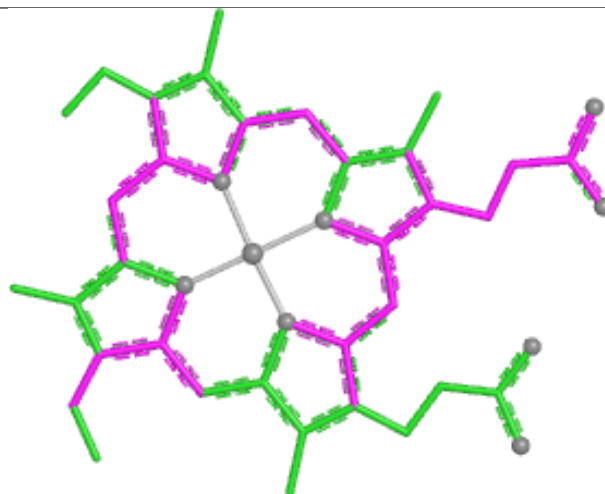


Rings

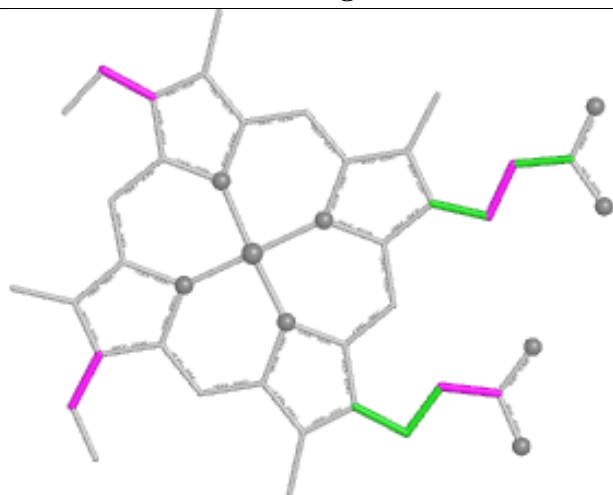
Ligand HEC E 601



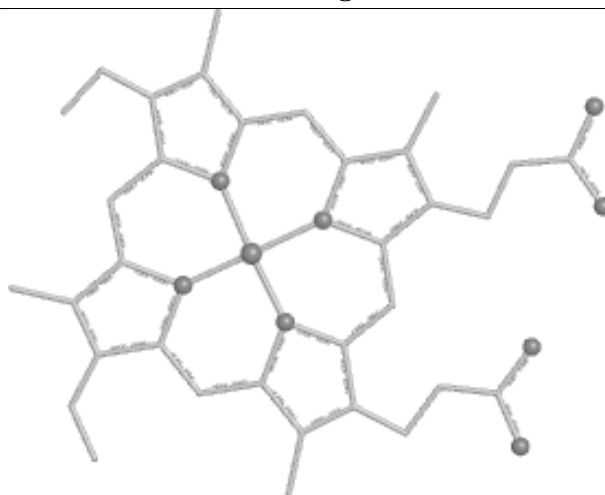
Bond lengths



Bond angles

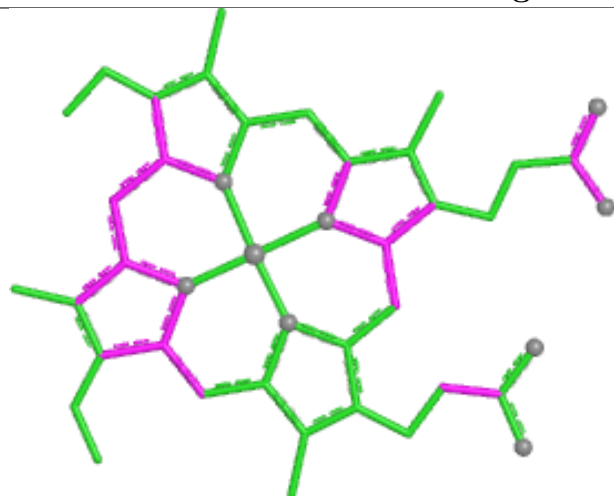


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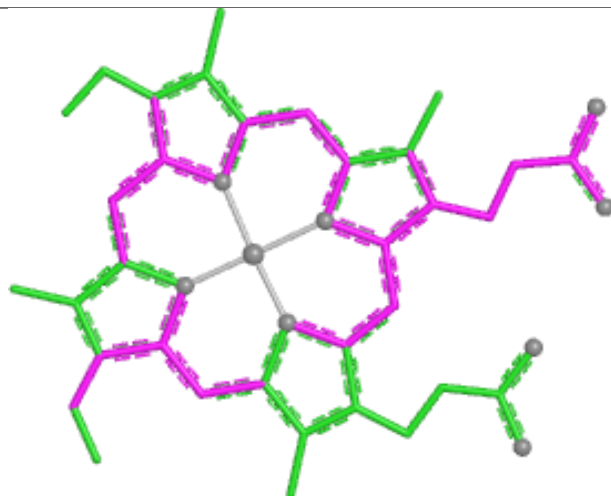


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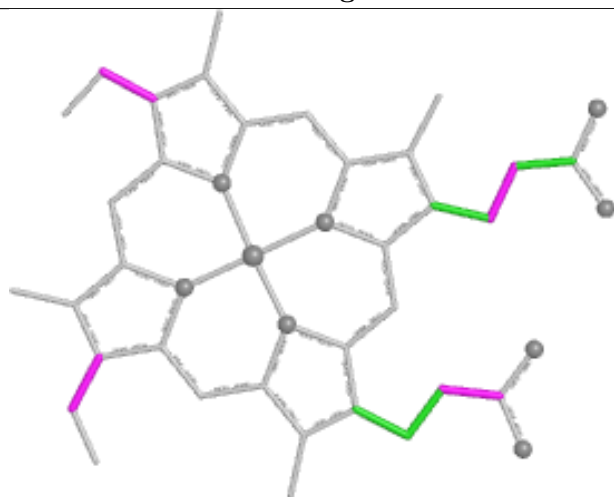
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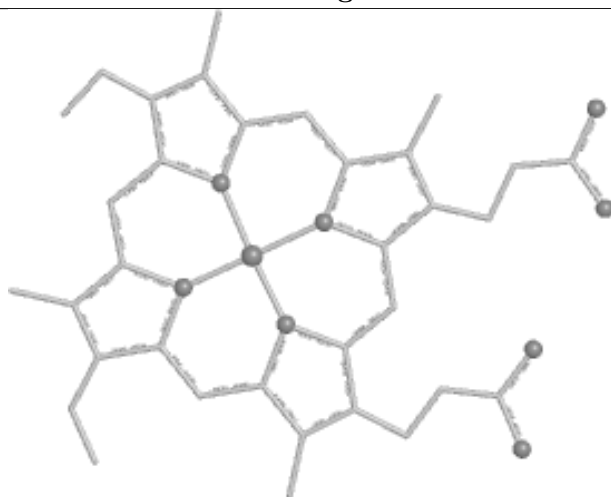
Bond lengths



Bond angles

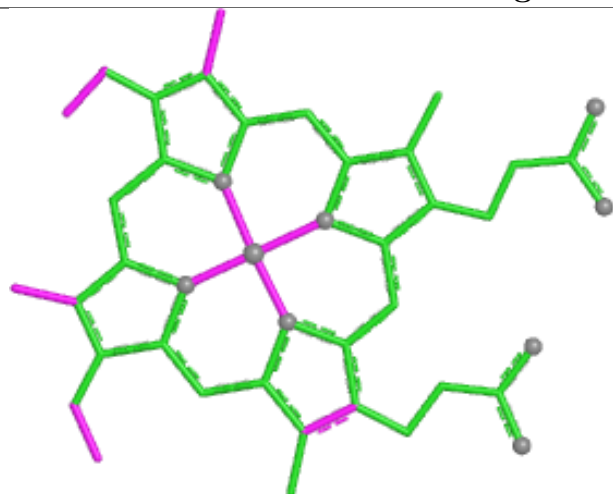


Torsions

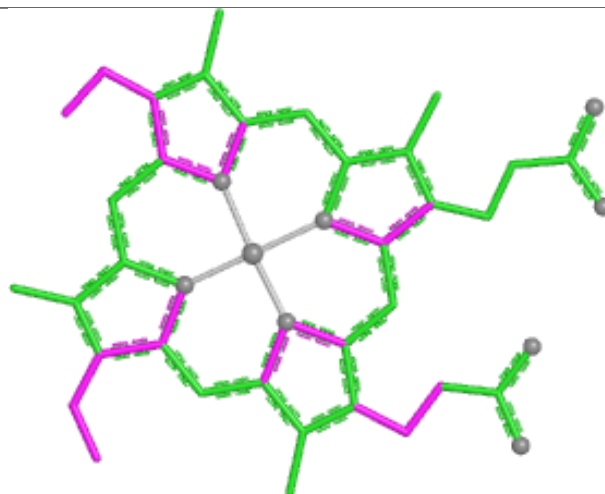


Rings

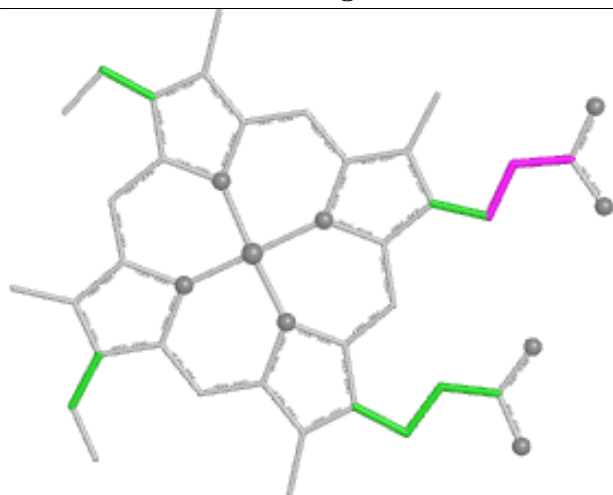
Ligand HEC E 602



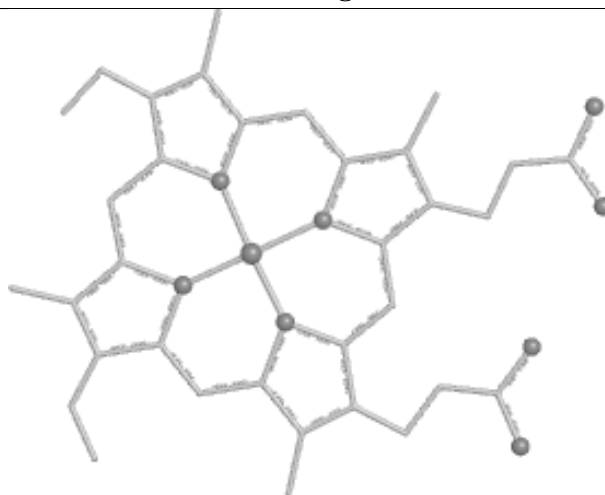
Bond lengths



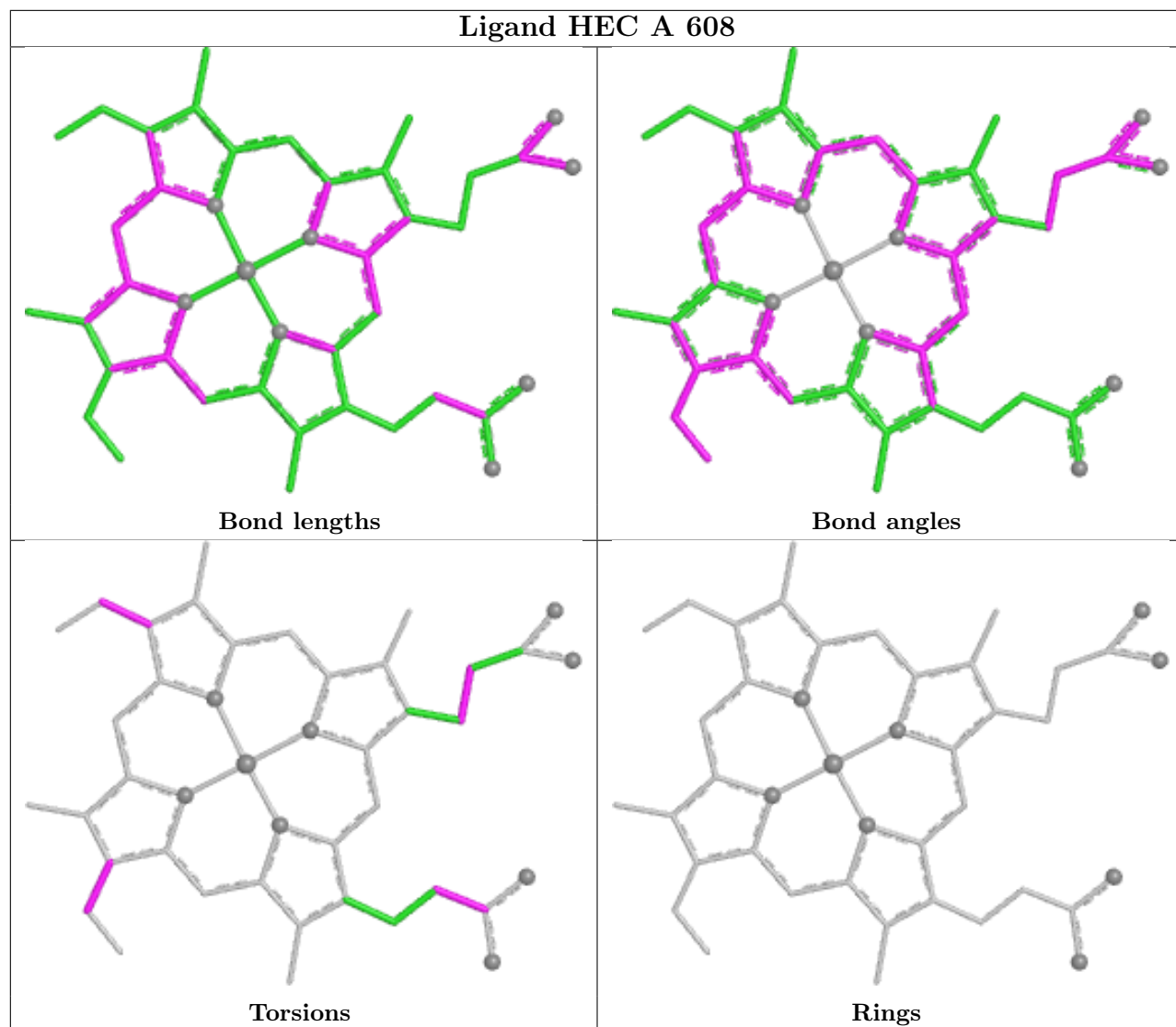
Bond angles



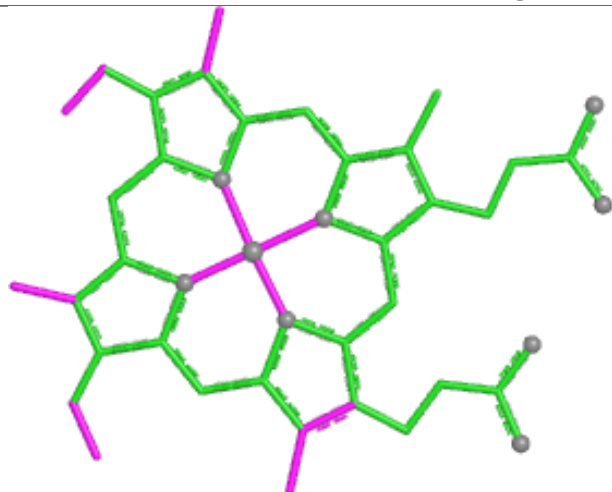
Torsions



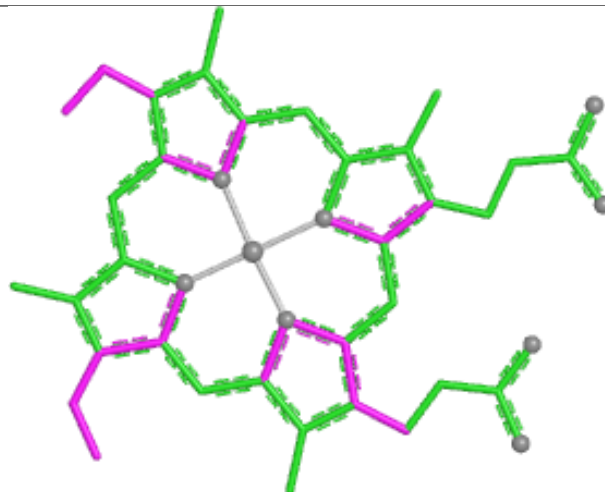
Rings



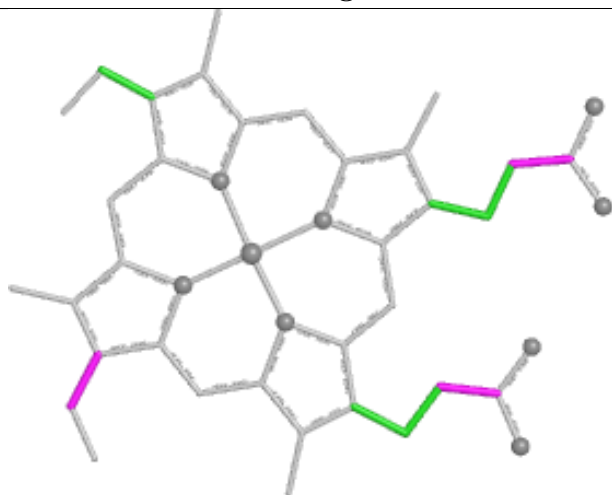
Ligand HEC A 603



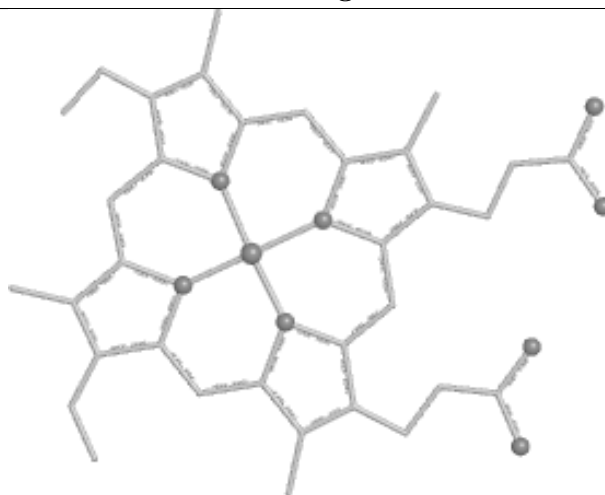
Bond lengths



Bond angles

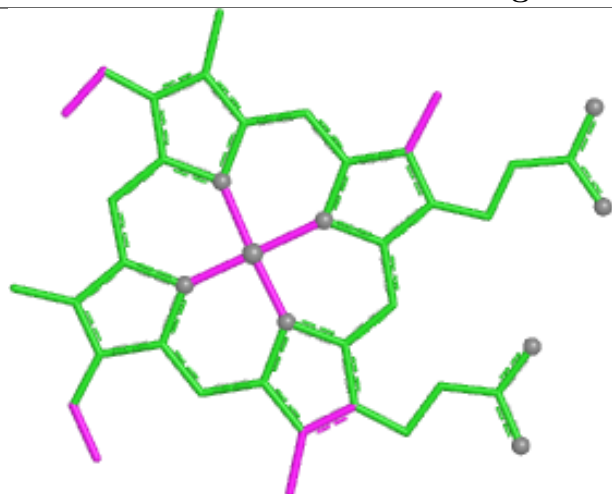


Torsions

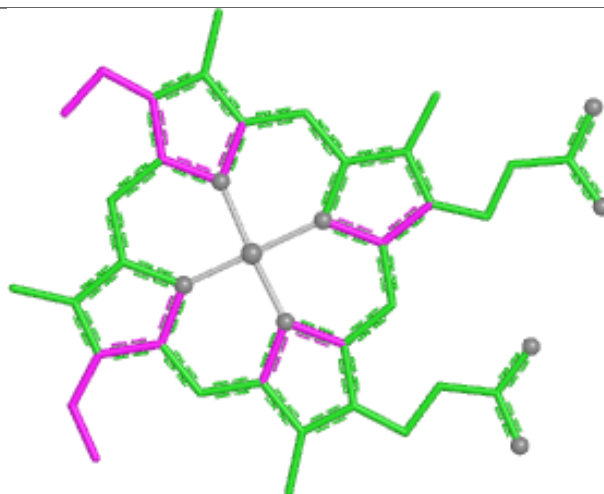


Rings

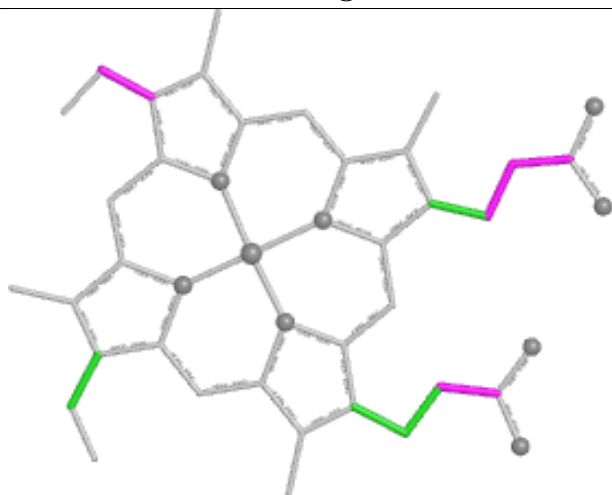
Ligand HEC C 606



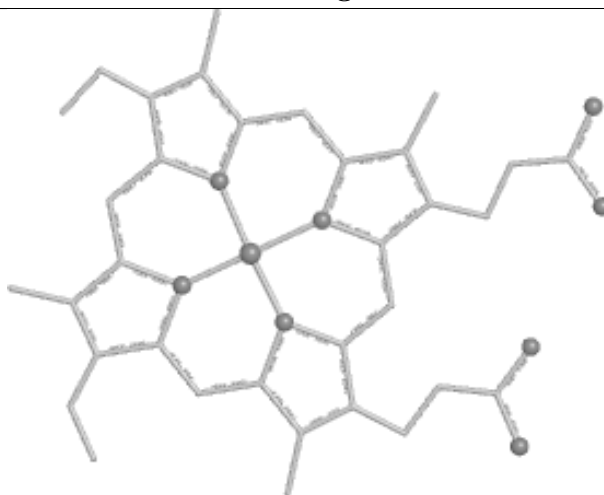
Bond lengths



Bond angles

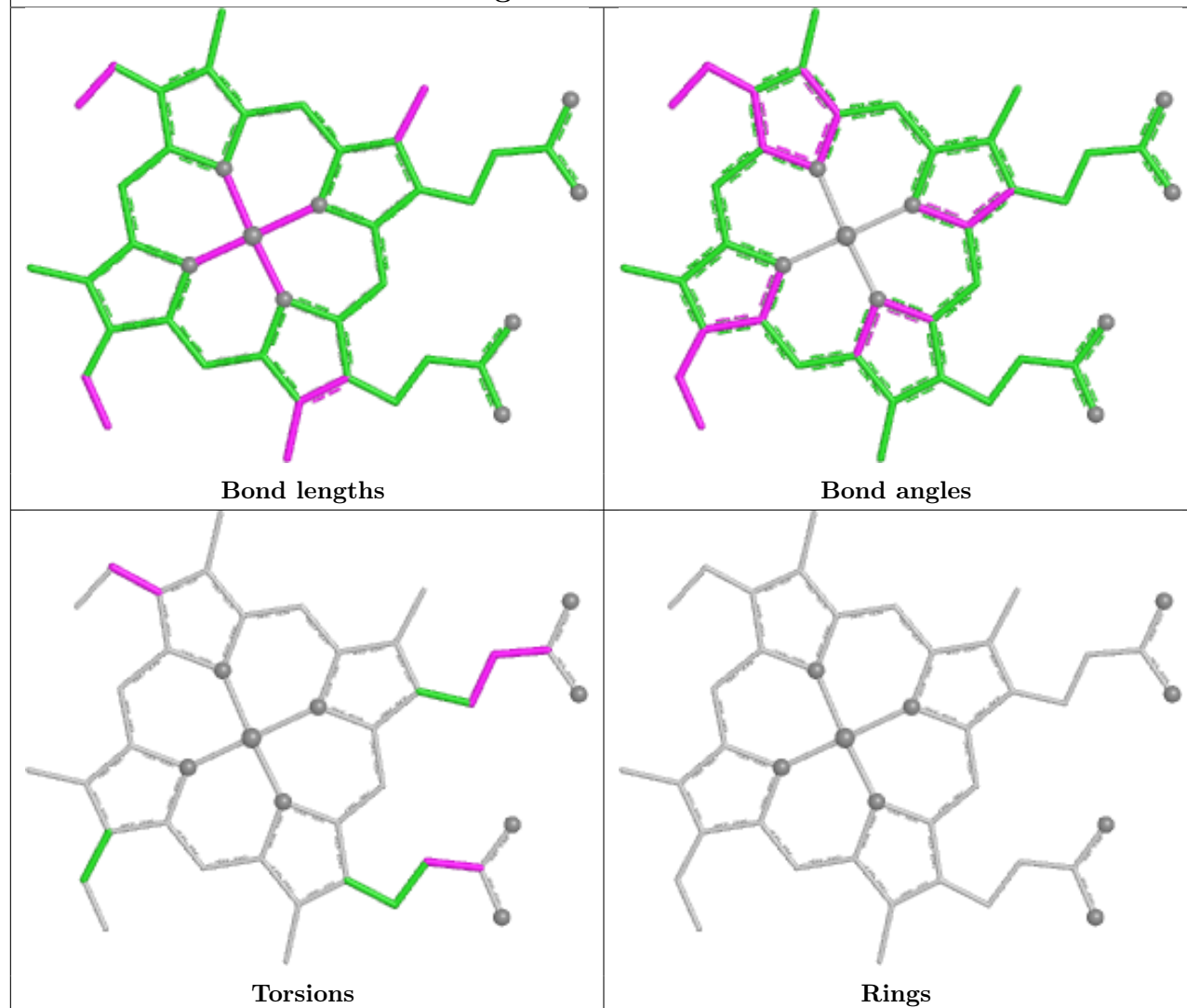


Torsions

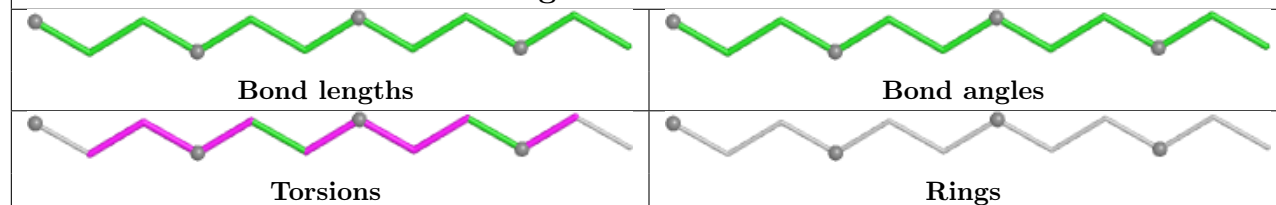


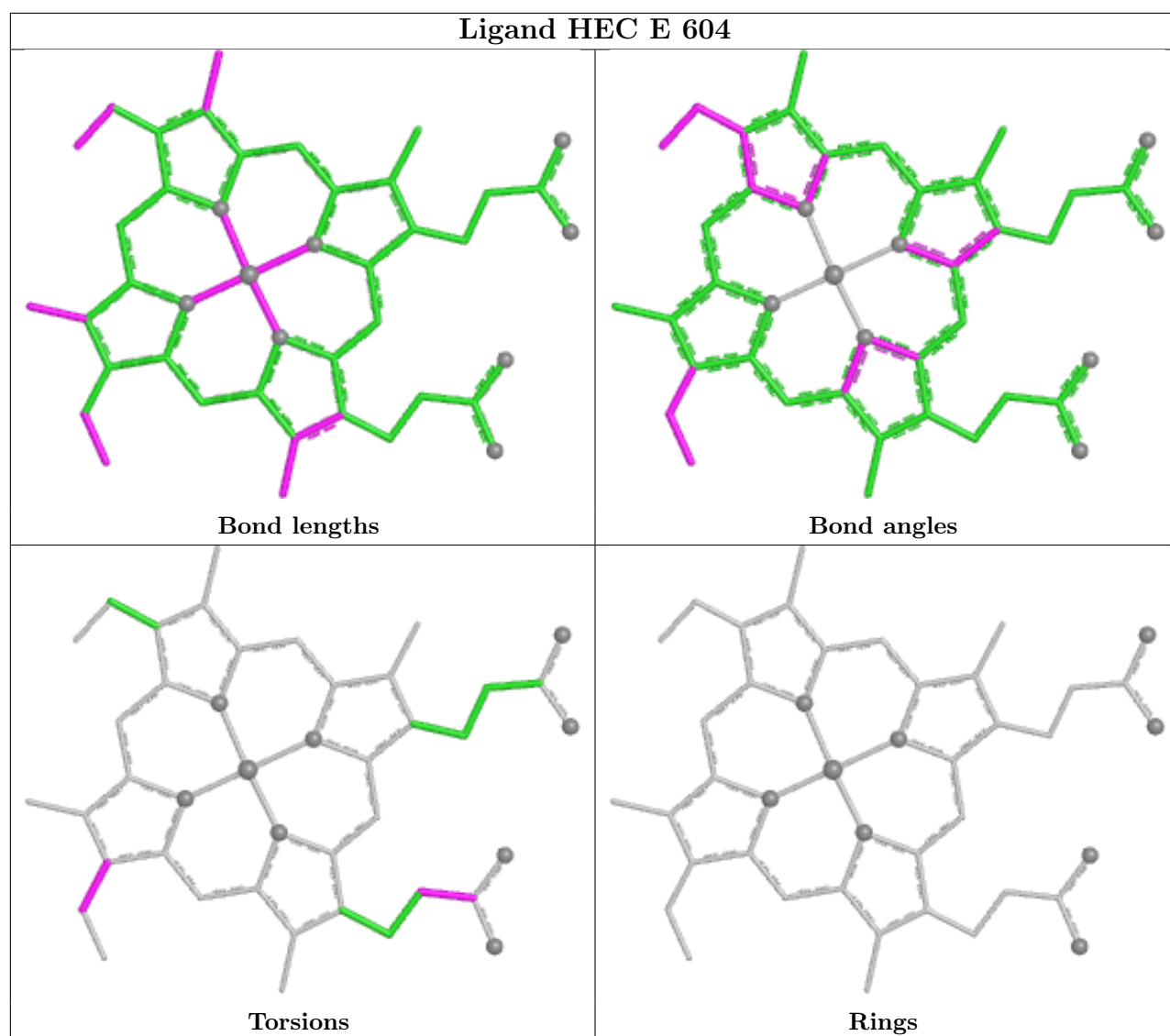
Rings

Ligand HEC E 606



Ligand 12P A 611





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	504/546 (92%)	0.57	25 (4%) 34 30	18, 31, 50, 60	0
1	C	502/546 (91%)	0.57	27 (5%) 31 28	18, 32, 48, 51	0
1	E	503/546 (92%)	0.42	17 (3%) 48 44	18, 29, 45, 56	1 (0%)
2	B	53/57 (92%)	1.20	12 (22%) 2 2	32, 43, 62, 64	0
2	D	57/57 (100%)	0.82	8 (14%) 6 5	25, 33, 58, 59	0
2	F	55/57 (96%)	1.53	15 (27%) 1 1	40, 46, 68, 68	0
All	All	1674/1809 (92%)	0.59	104 (6%) 26 23	18, 32, 50, 68	1 (0%)

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	SER	5.6
1	A	527	GLY	4.8
1	E	179[A]	LYS	4.5
2	F	79	ALA	4.4
1	A	528	LYS	3.9

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

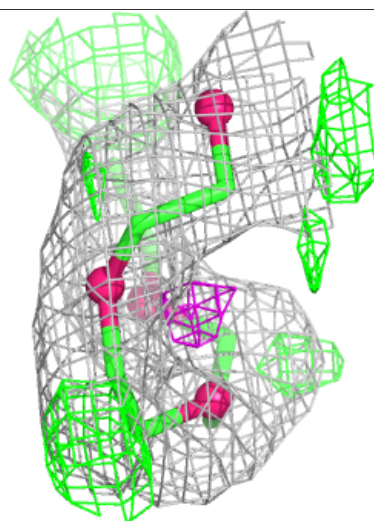
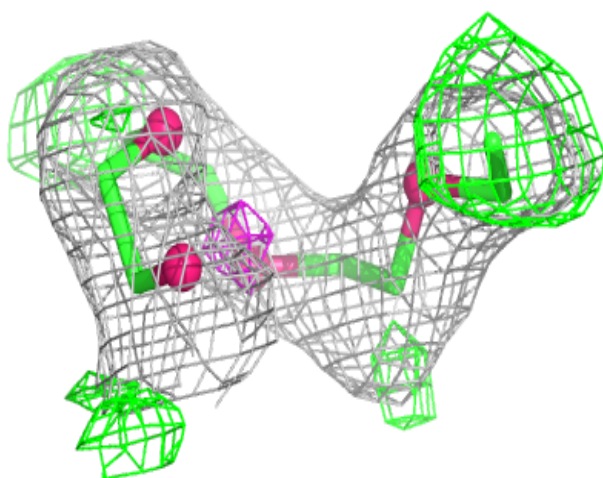
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	12P	A	611	12/37	0.65	0.26	50,51,51,51	0
6	12P	C	610	25/37	0.73	0.23	57,58,59,59	0
4	K	A	609	1/1	0.80	0.22	31,31,31,31	0
3	HEC	C	604	43/43	0.90	0.16	39,42,43,43	0
3	HEC	E	604	43/43	0.91	0.14	38,40,41,42	0
5	HOA	E	610	2/2	0.91	0.12	23,23,23,24	0
7	PO4	E	609	5/5	0.91	0.11	51,51,52,52	0
5	HOA	A	610	2/2	0.93	0.13	21,21,21,22	0
5	HOA	C	609	2/2	0.93	0.09	26,26,26,26	0
3	HEC	A	608	43/43	0.94	0.10	22,24,27,28	0
3	HEC	E	605	43/43	0.94	0.11	29,30,32,34	0
3	HEC	A	602	43/43	0.94	0.11	34,36,37,37	0
3	HEC	C	605	43/43	0.95	0.10	34,36,37,37	0
3	HEC	E	601	43/43	0.95	0.09	23,25,27,28	0
3	HEC	E	603	43/43	0.95	0.11	31,32,33,35	0
3	HEC	A	601	43/43	0.95	0.10	27,28,29,29	0
3	HEC	C	601	43/43	0.95	0.10	20,21,23,23	0
3	HEC	A	605	43/43	0.95	0.10	22,23,24,25	0
3	HEC	E	606	43/43	0.96	0.08	19,20,21,22	0
3	HEC	A	603	43/43	0.96	0.10	27,30,31,32	0
3	HEC	C	607	43/43	0.96	0.09	18,19,21,22	0
3	HEC	A	606	43/43	0.96	0.09	21,23,25,26	0
3	HEC	E	602	43/43	0.96	0.09	26,26,27,27	0
3	HEC	C	602	43/43	0.96	0.09	25,26,28,29	0
3	HEC	C	603	43/43	0.96	0.10	31,32,33,33	0
3	HEC	A	607	43/43	0.96	0.09	26,27,27,28	0
3	HEC	C	608	43/43	0.97	0.09	19,21,23,23	0
3	HEC	E	607	43/43	0.97	0.08	19,19,20,21	0
3	HEC	E	608	43/43	0.97	0.08	24,24,27,28	0
3	HEC	C	606	43/43	0.97	0.08	19,20,21,22	0
3	HEC	A	604	43/43	0.97	0.09	25,27,30,31	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.

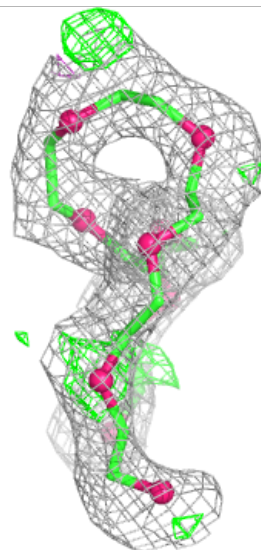
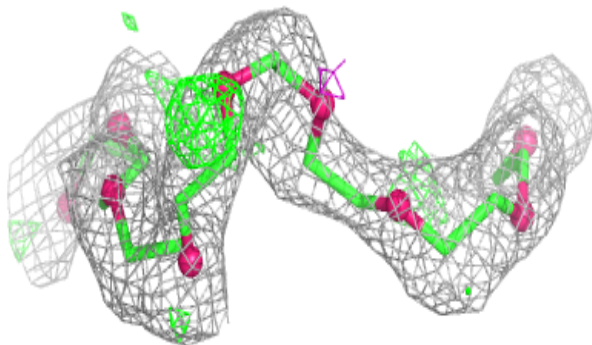
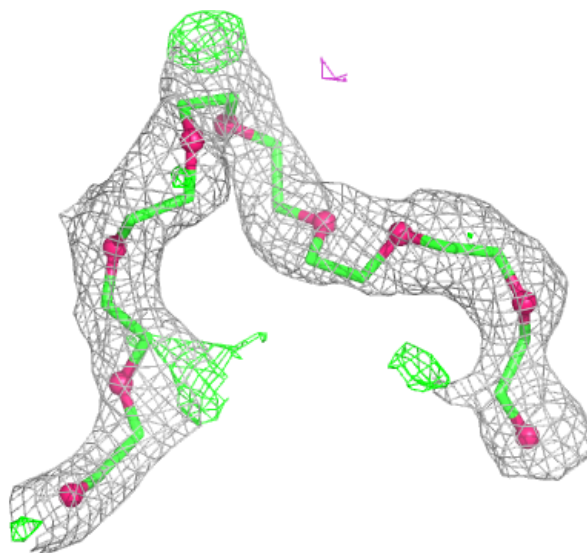
Electron density around 12P A 611:

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



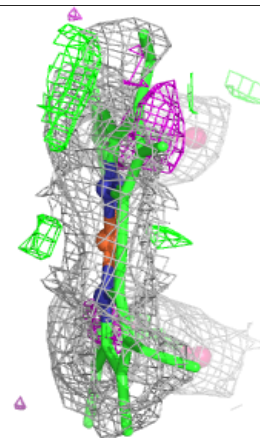
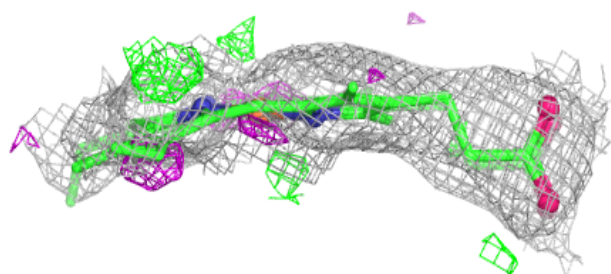
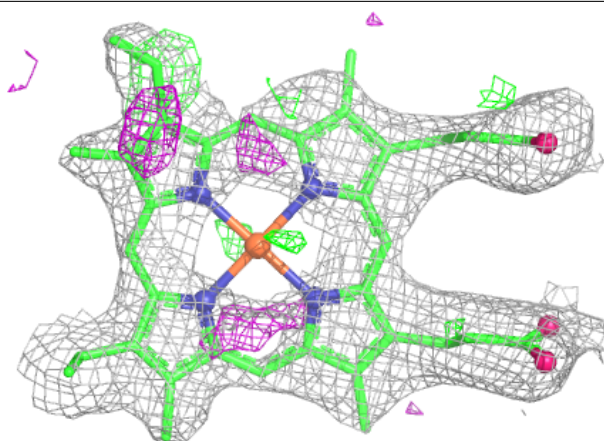
Electron density around 12P C 610:

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and green (positive)



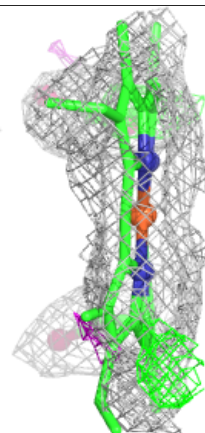
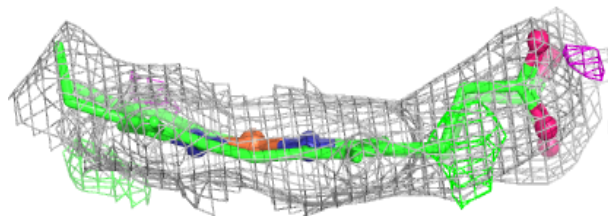
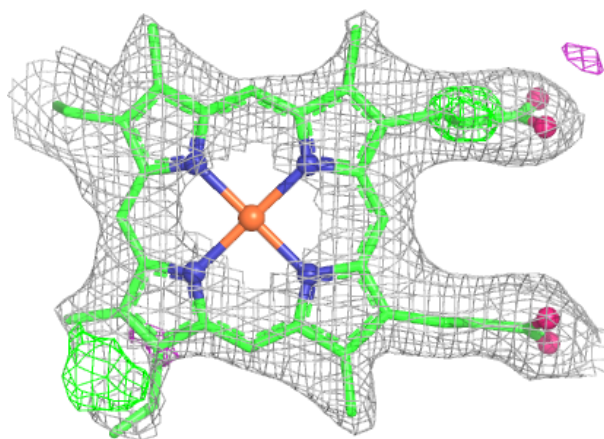
Electron density around HEC C 604:

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and green (positive)



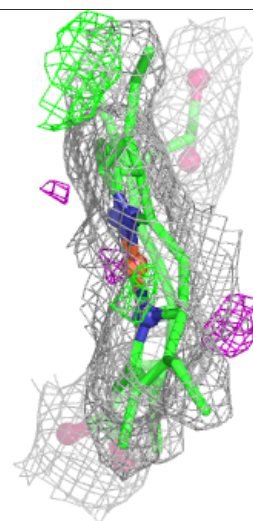
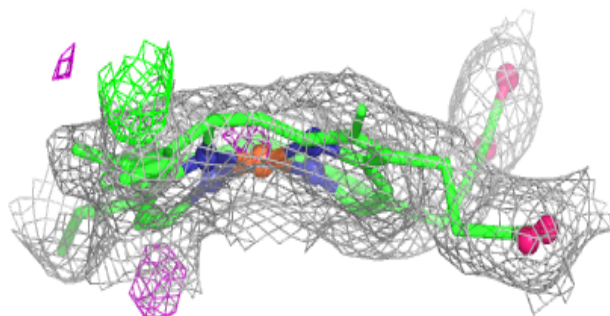
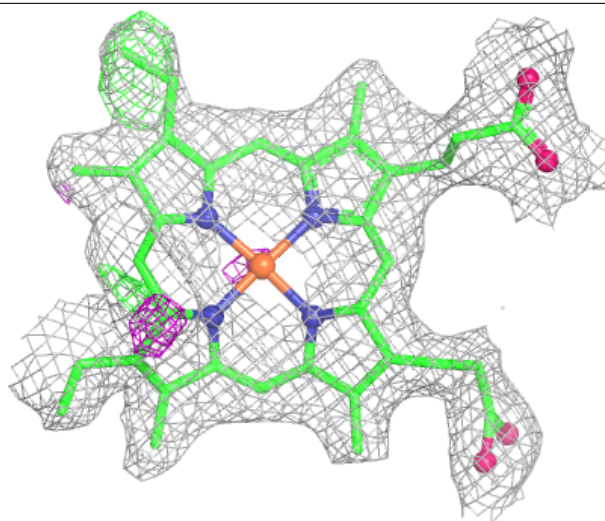
Electron density around HEC E 604:

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and green (positive)



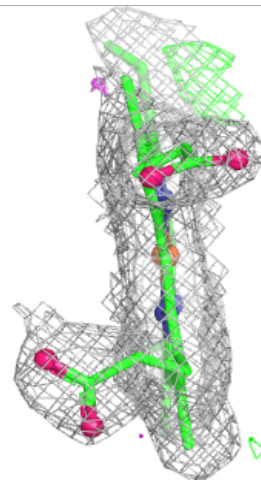
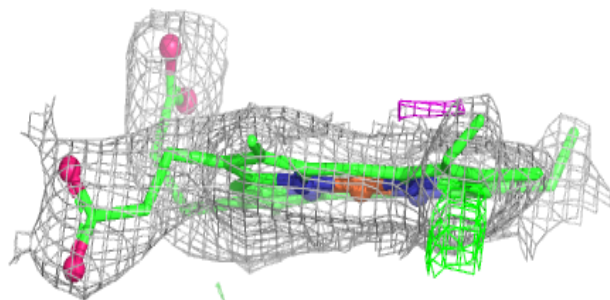
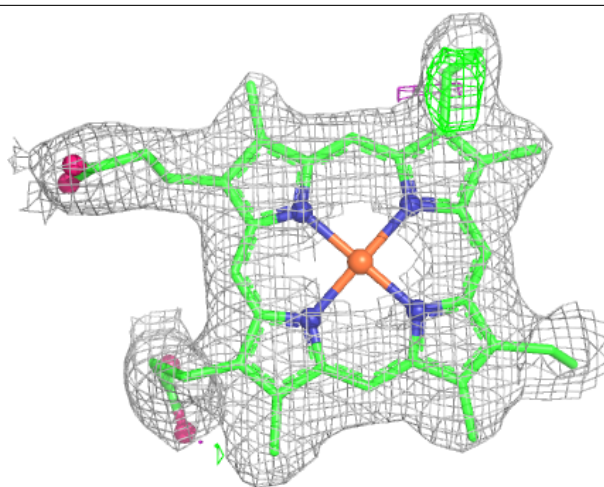
Electron density around HEC A 608:

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and green (positive)



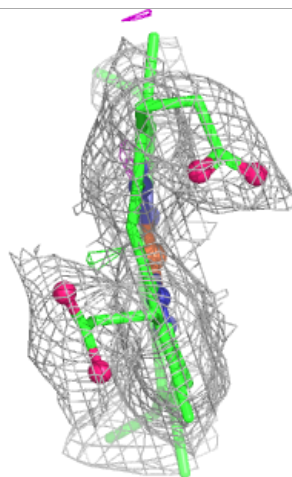
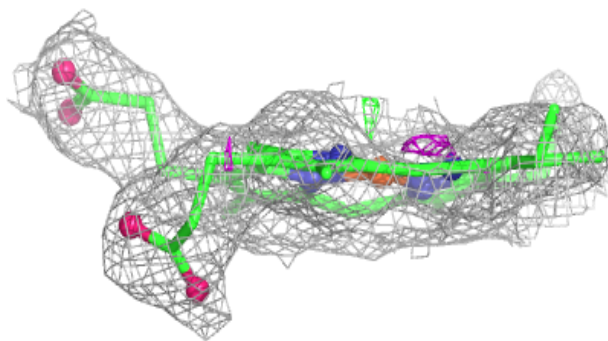
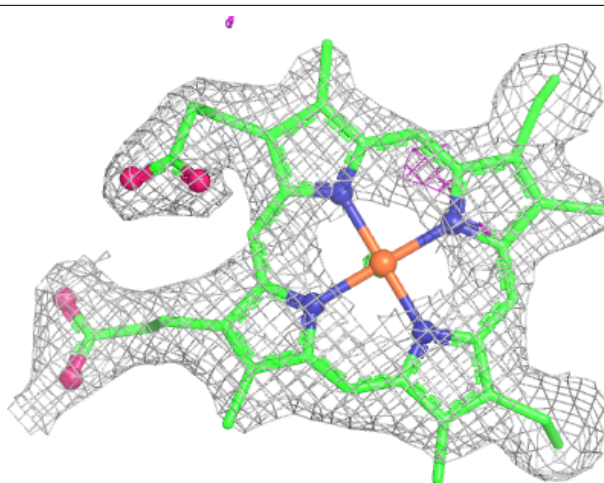
Electron density around HEC E 605:

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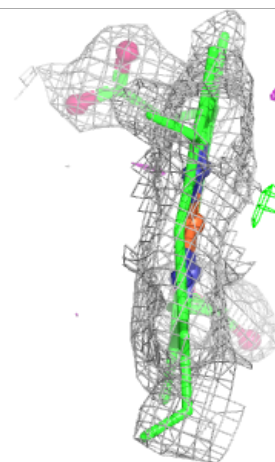
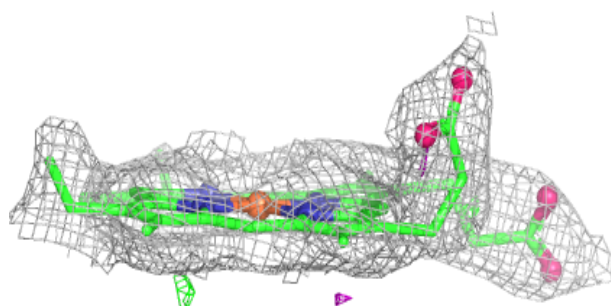
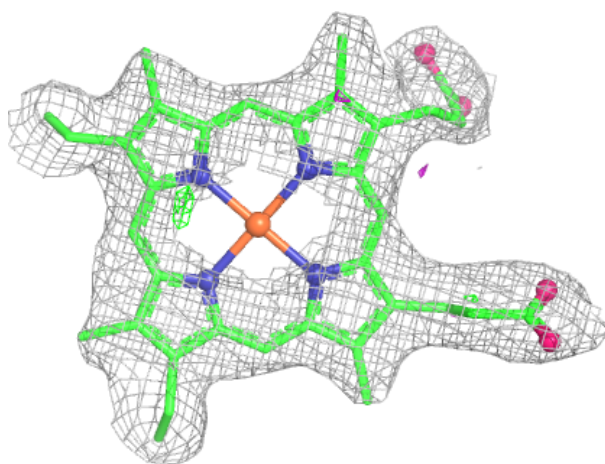
Electron density around HEC A 602:

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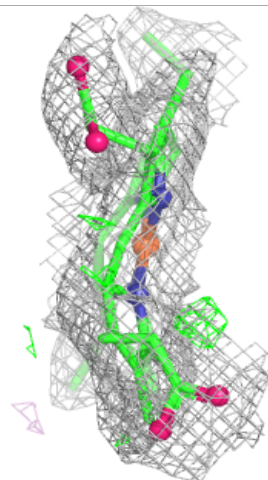
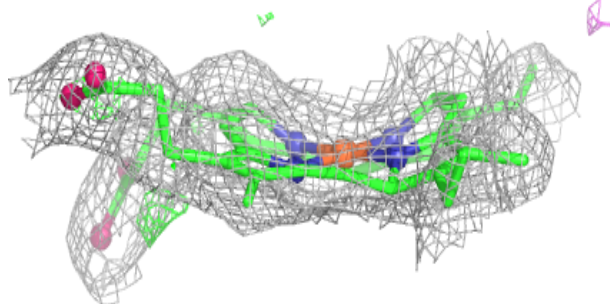
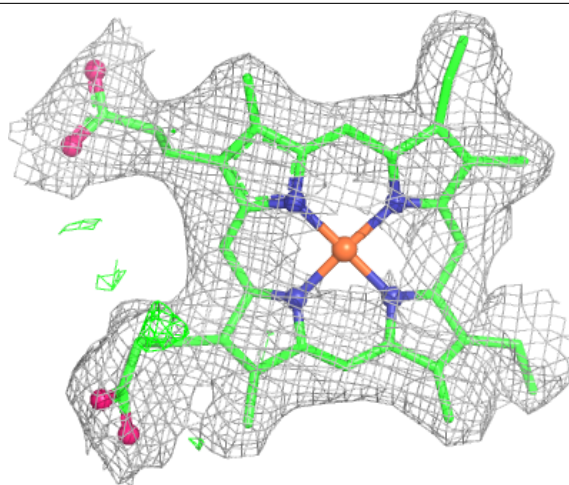
Electron density around HEC C 605:

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and green (positive)



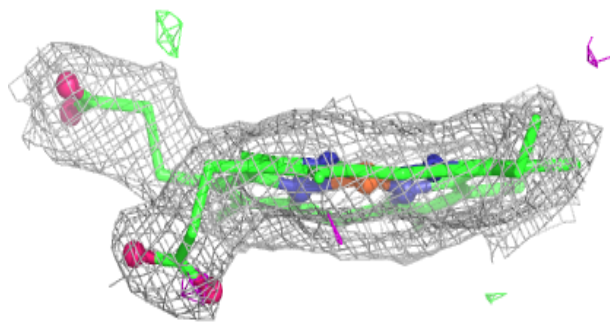
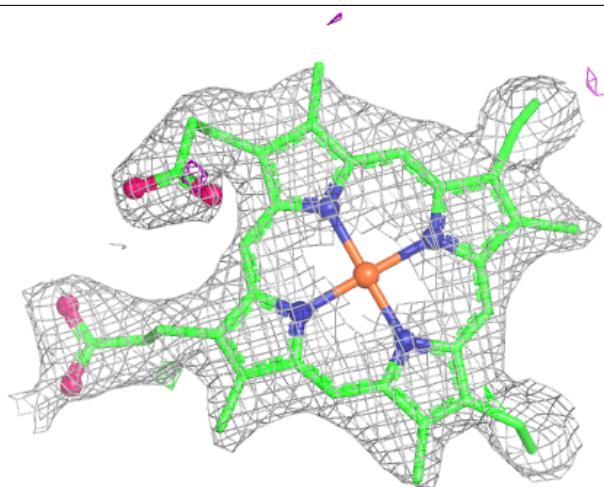
Electron density around HEC E 601:

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and green (positive)



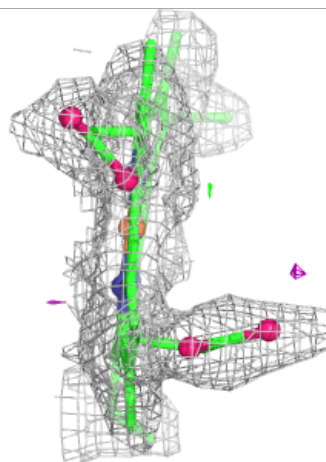
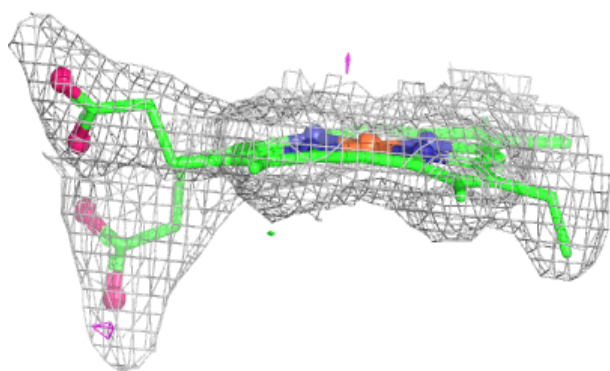
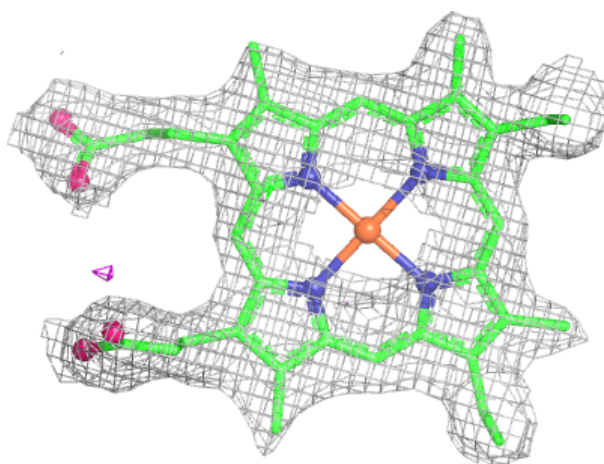
Electron density around HEC E 603:

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and green (positive)



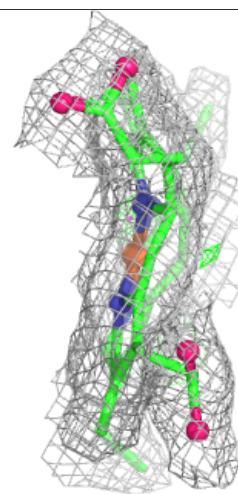
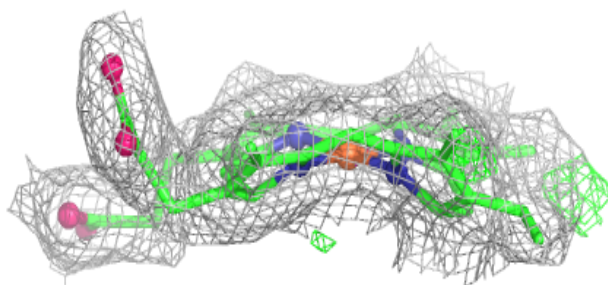
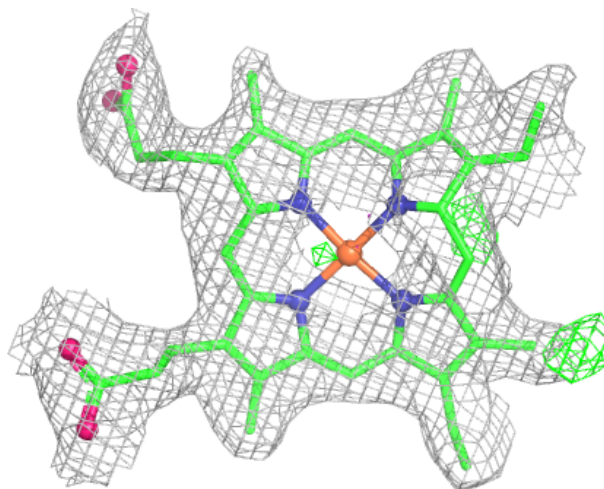
Electron density around HEC A 601:

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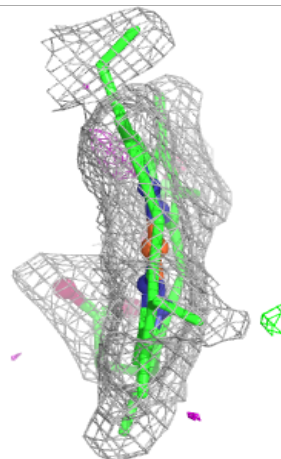
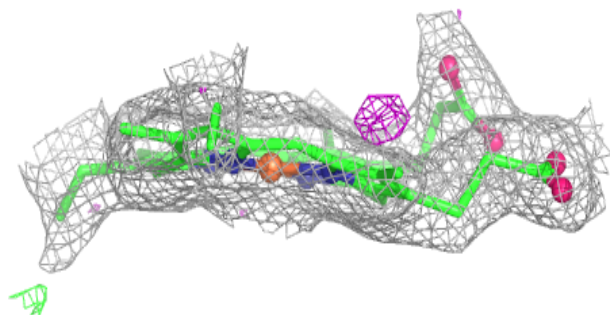
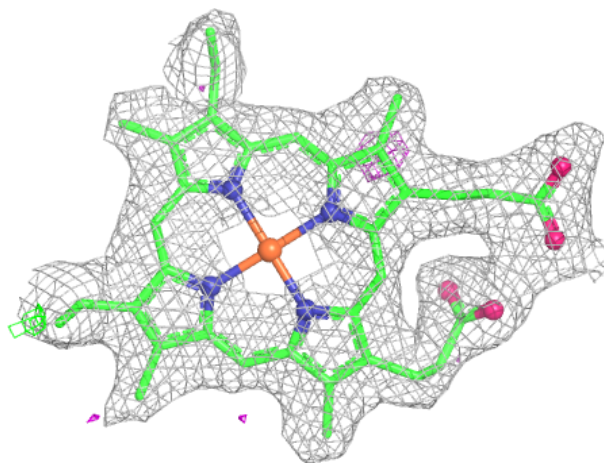
Electron density around HEC C 601:

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and green (positive)



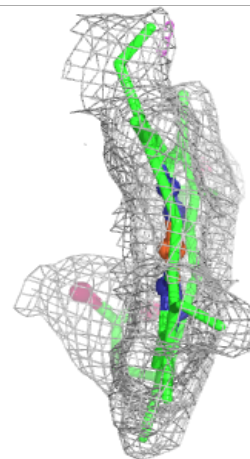
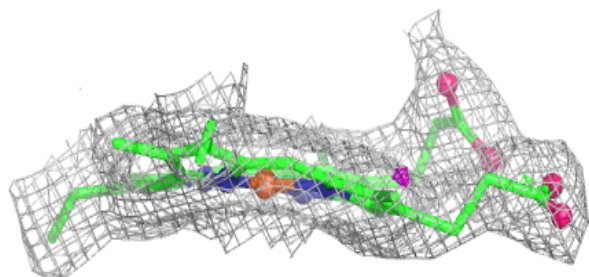
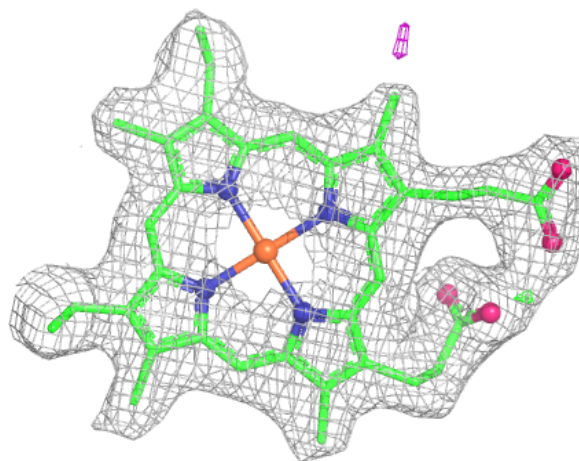
Electron density around HEC A 605:

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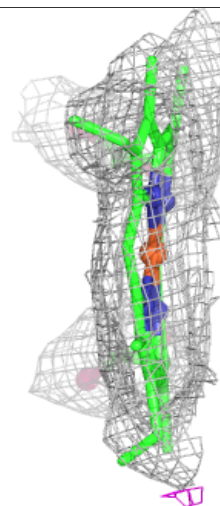
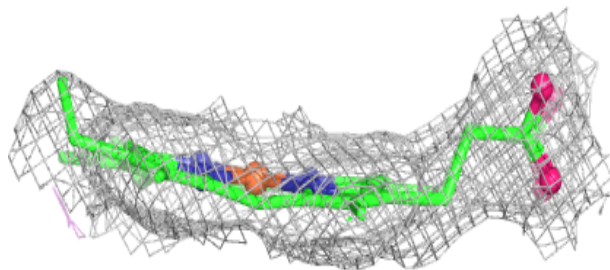
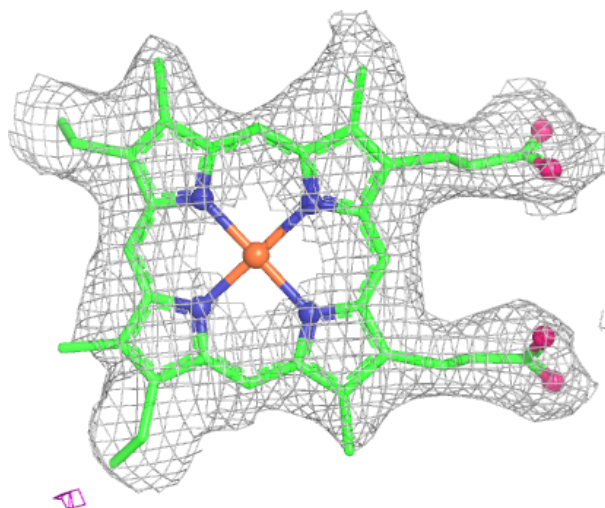
Electron density around HEC E 606:

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and green (positive)



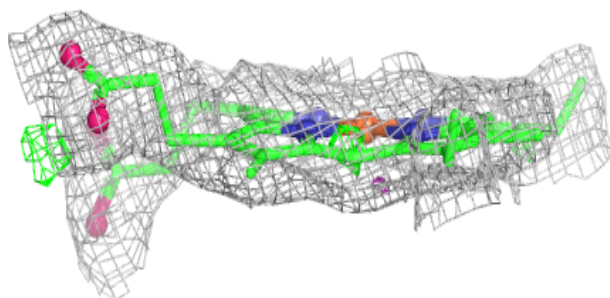
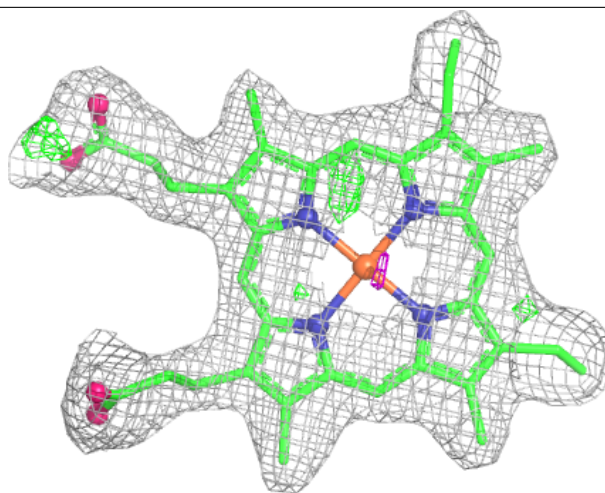
Electron density around HEC A 603:

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and green (positive)



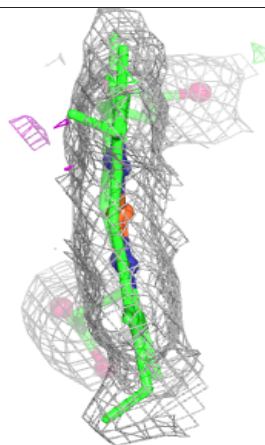
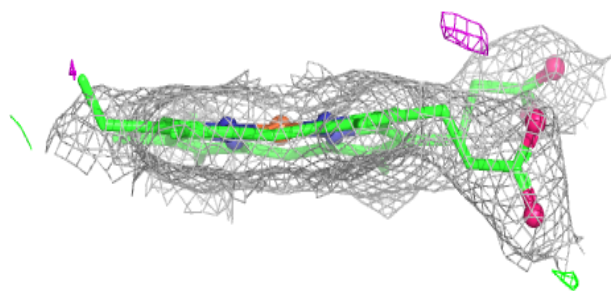
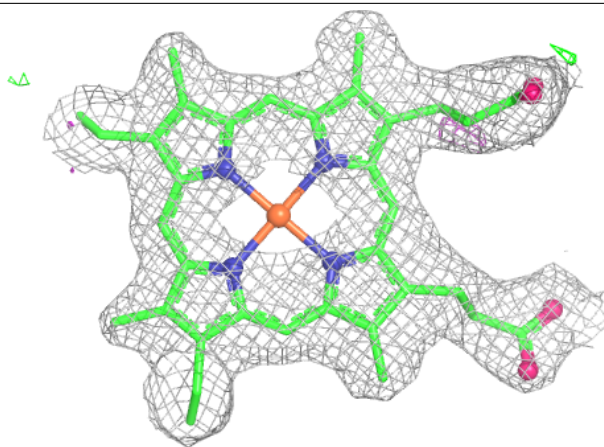
Electron density around HEC C 607:

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and green (positive)



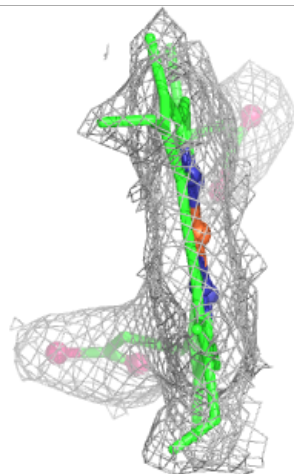
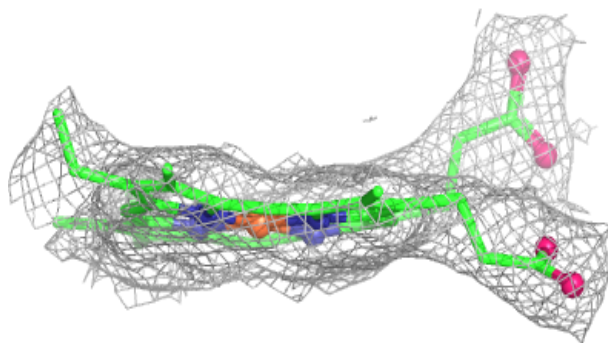
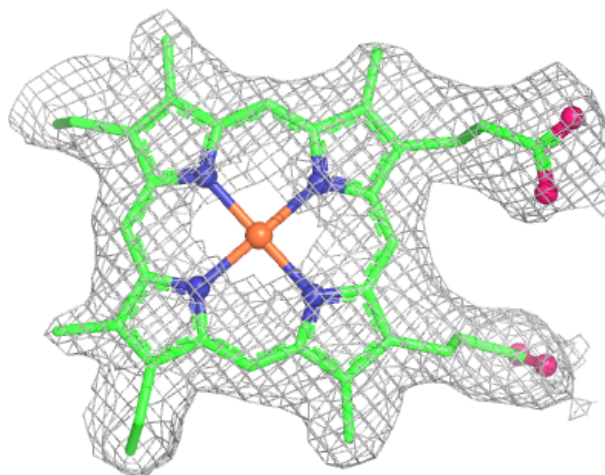
Electron density around HEC A 606:

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



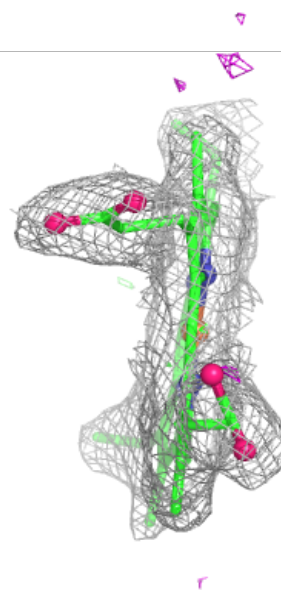
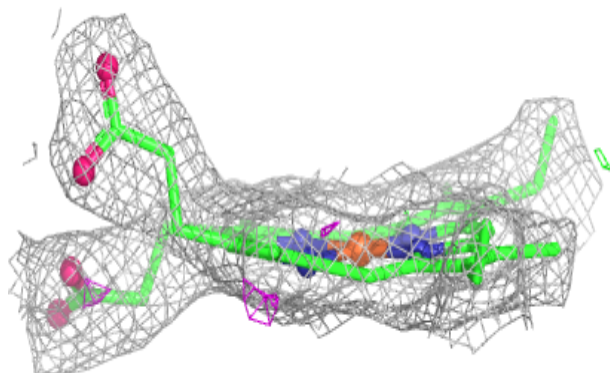
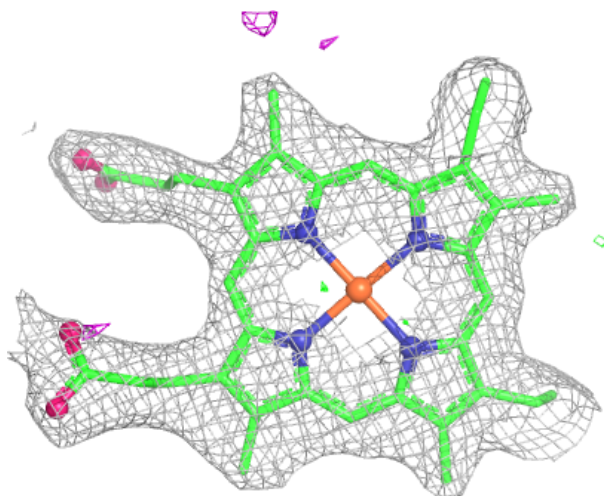
Electron density around HEC E 602:

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



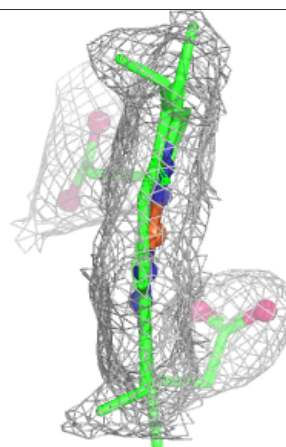
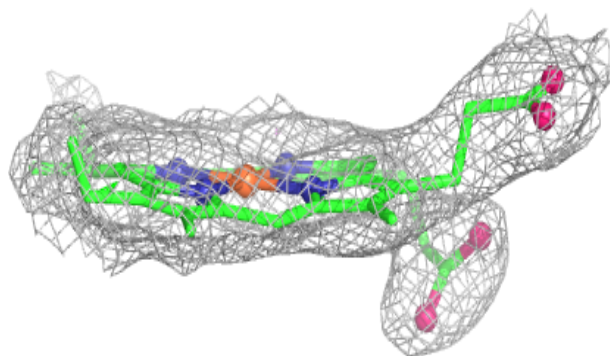
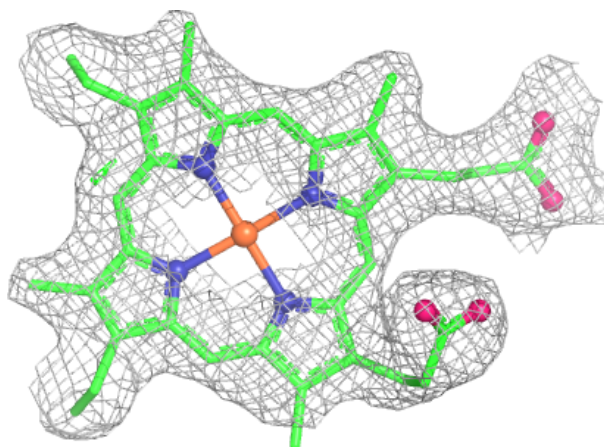
Electron density around HEC C 602:

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



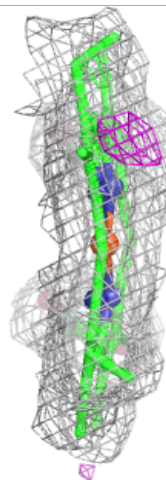
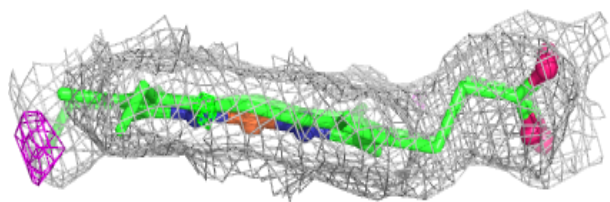
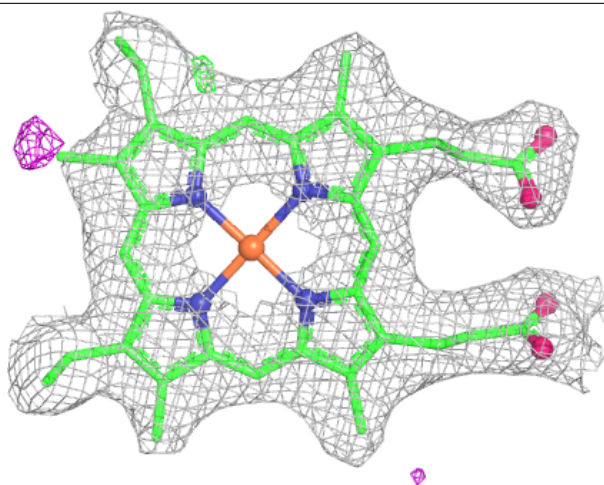
Electron density around HEC C 603:

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



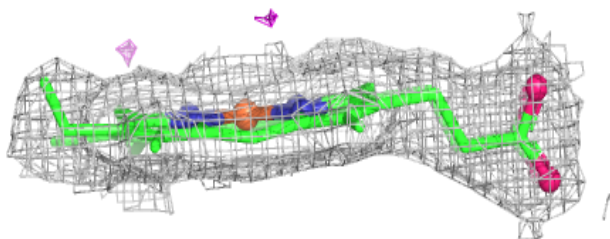
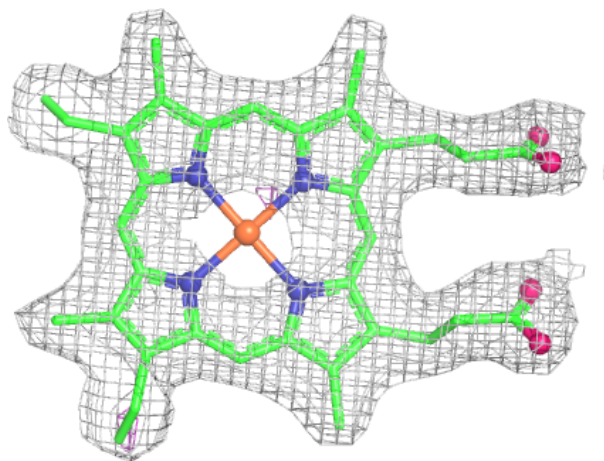
Electron density around HEC A 607:

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



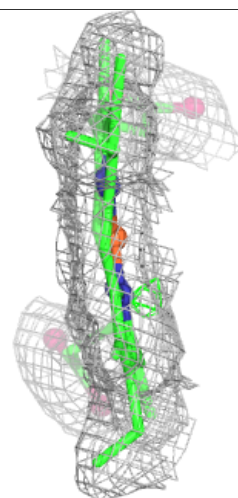
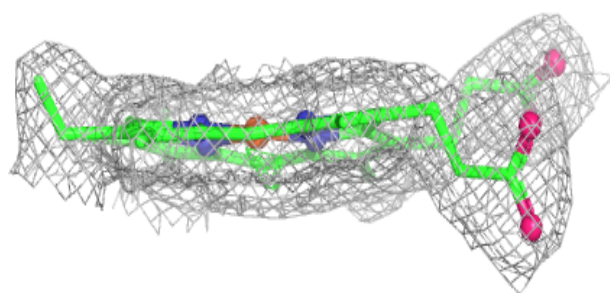
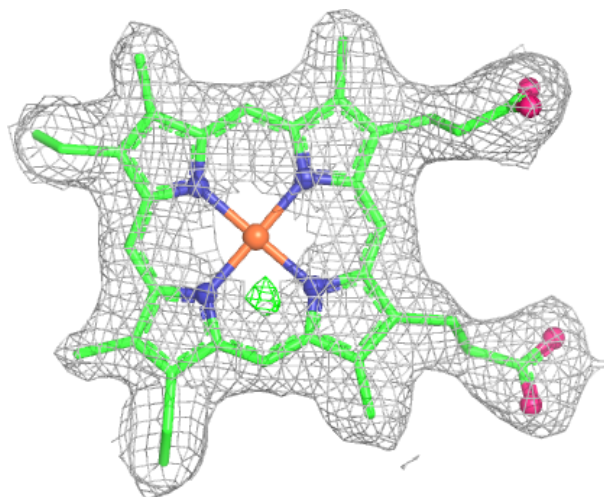
Electron density around HEC C 608:

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



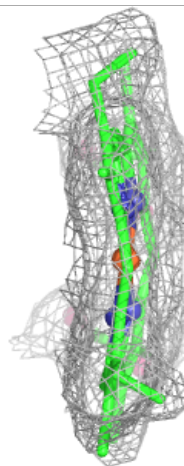
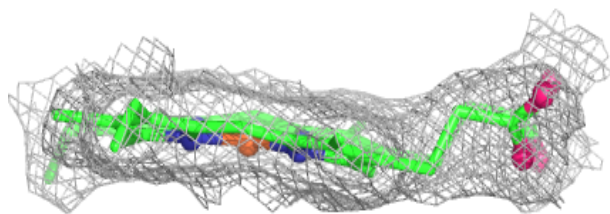
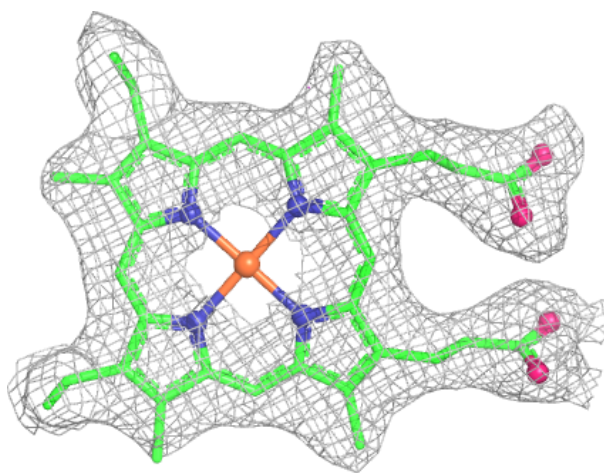
Electron density around HEC E 607:

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



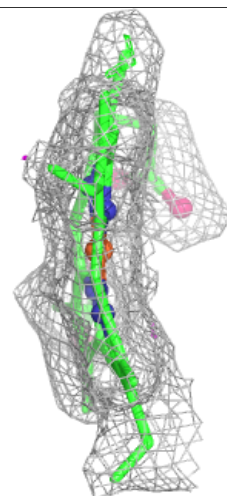
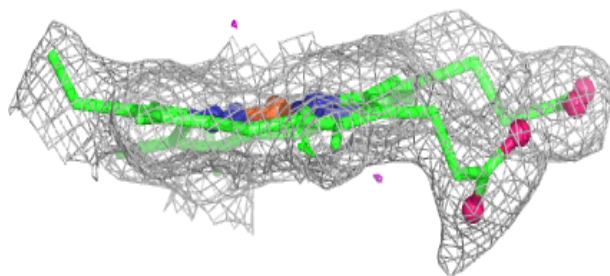
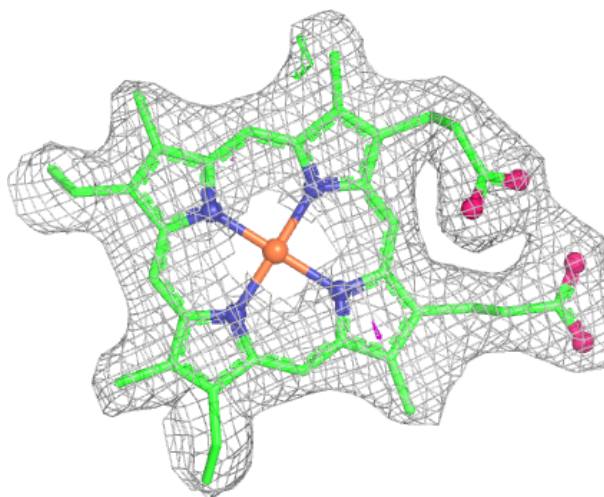
Electron density around HEC E 608:

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



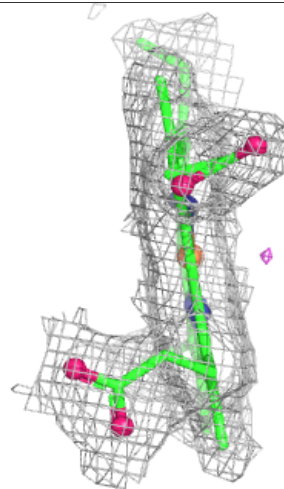
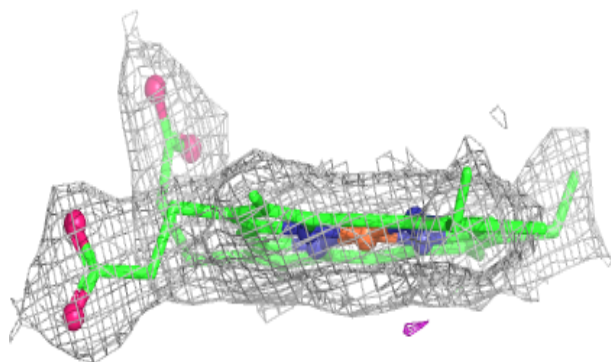
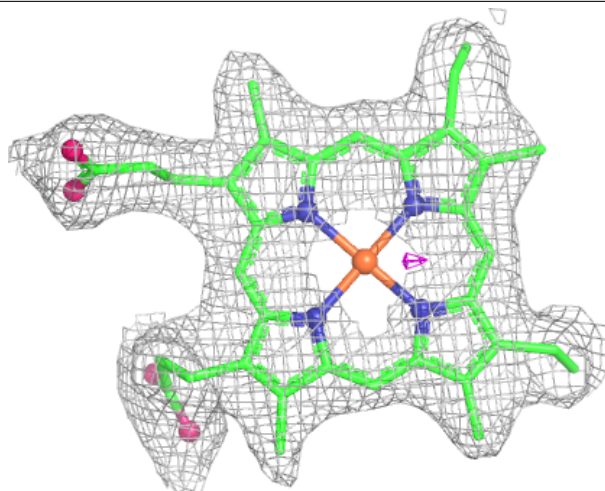
Electron density around HEC C 606:

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



Electron density around HEC A 604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.