wwPDB X-ray Structure Validation Summary Report (i)

Dec 14, 2024 – 11:56 PM EST

PDB ID	:	1Z1N
Title	:	Crystal Structure of the sixteen heme cytochrome from Desulfovibrio gigas
Authors	:	Santos-Silva, T.; Dias, J.M.; Romao, M.J.
Deposited on	:	2005-03-04
Resolution	:	2.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

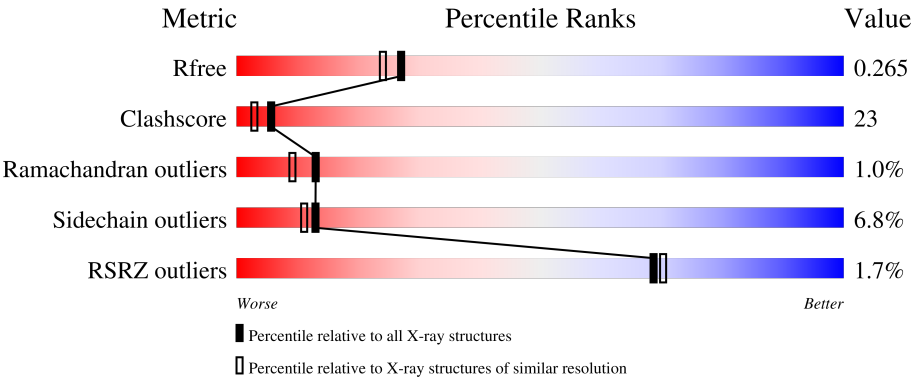
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	560	2%, 68%, 21%, ·, 8%
2	A	2	50%, 50%

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
2	NAG	A	1	X	-	-	-
5	GOL	X	722	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4998 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 sixteen heme cytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	516	3837	2355	703	739	40	0	0	0

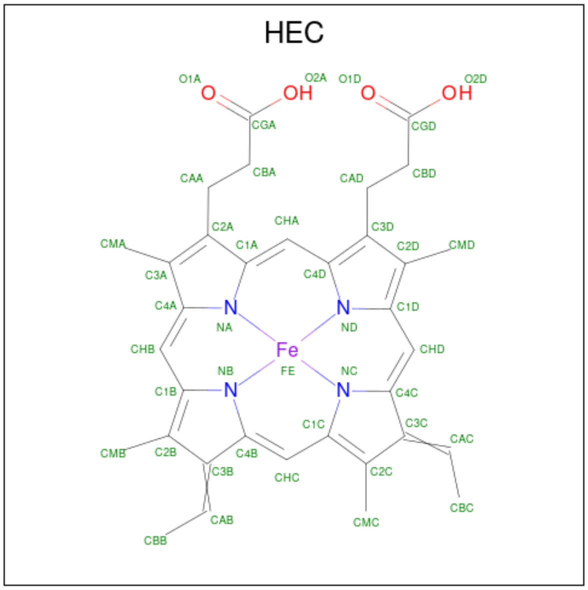
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	X	3	3	3	0	0

- Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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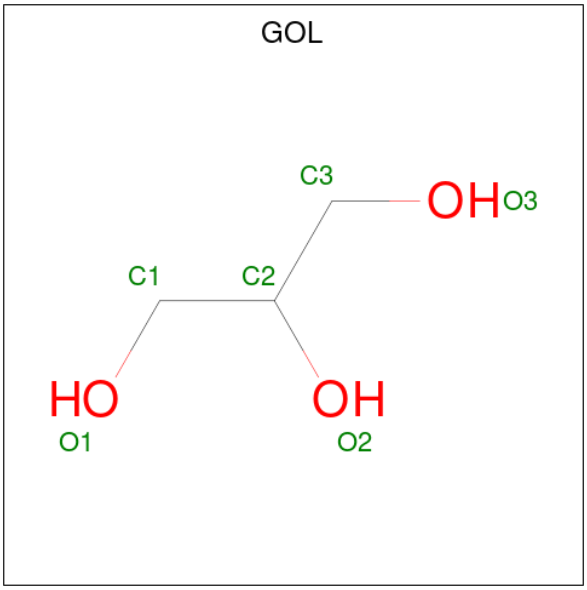
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	X	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

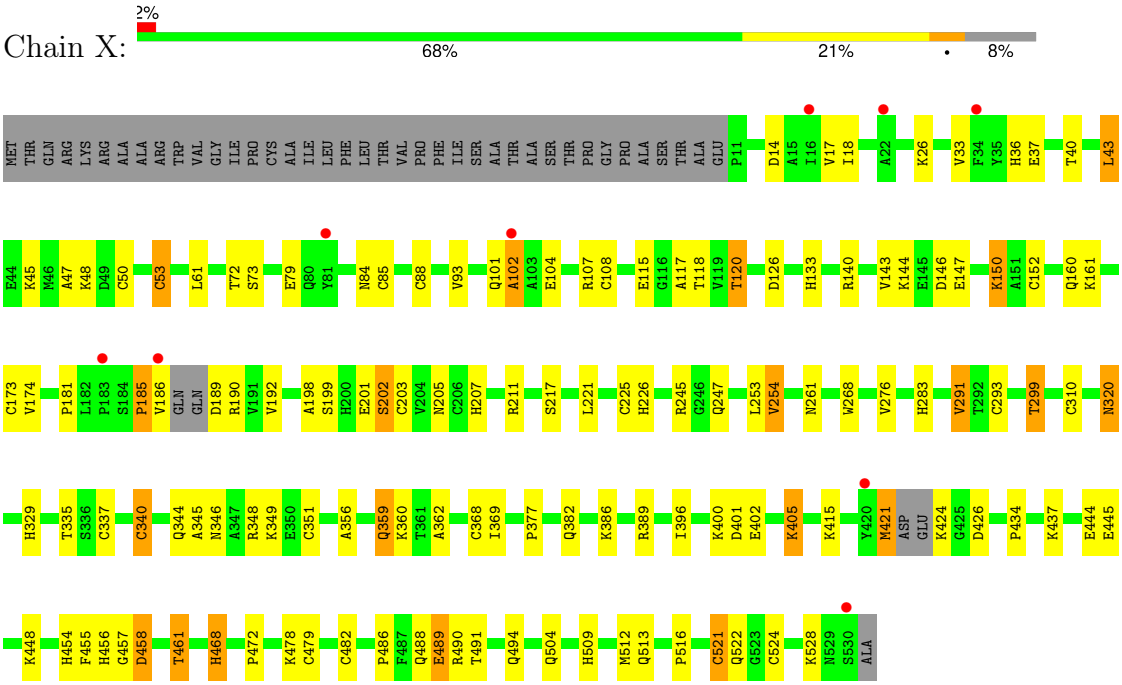
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	412	Total	O	0	0
			412	412		

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: sixteen heme cytochrome

Chain X:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.89Å 90.80Å 83.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.00-2.10) 98.1 (25.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.260 0.204 , 0.265	Depositor DCC
R_{free} test set	1979 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, GOL, NAA, ZN, NAG

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	X	1.00	6/3925 (0.2%)	0.98	8/5326 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	479	CYS	CB-SG	6.77	1.93	1.82
1	X	276	VAL	CB-CG2	6.29	1.66	1.52
1	X	53	CYS	CB-SG	-5.78	1.72	1.81
1	X	340	CYS	CB-SG	5.38	1.91	1.82
1	X	455	PHE	CE1-CZ	5.08	1.47	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	389	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	X	389	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	X	448	LYS	CD-CE-NZ	-7.46	94.53	111.70
1	X	291	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	X	291	VAL	CB-CA-C	-7.21	97.70	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	424	LYS	Peptide

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	X	3837	0	3662	161	1
2	A	28	0	25	1	0
3	X	3	0	0	0	0
4	X	688	0	495	115	1
5	X	30	0	40	6	0
6	X	412	0	0	26	1
All	All	4998	0	4222	190	2

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 23.

The worst 5 of 190 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:X:50:CYS:SG	4:X:704:HEC:HAB	1.37	1.63
1:X:152:CYS:SG	4:X:707:HEC:HAC	1.54	1.44
1:X:310:CYS:SG	4:X:712:HEC:CBC	2.04	1.44
1:X:524:CYS:SG	4:X:719:HEC:CAC	2.12	1.36
1:X:85:CYS:SG	4:X:705:HEC:CAB	2.14	1.35

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:815:HOH:O	6:X:912:HOH:O[3_546]	2.14	0.06
1:X:437:LYS:NZ	4:X:718:HEC:O2D[2_565]	2.15	0.05

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	X	510/560 (91%)	484 (95%)	21 (4%)	5 (1%)	13 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	102	ALA
1	X	160	GLN
1	X	150	LYS
1	X	161	LYS
1	X	185	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	410/450 (91%)	382 (93%)	28 (7%)	13 11

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	299	THR
1	X	522	GLN
1	X	405	LYS
1	X	478	LYS
1	X	359	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such

sidechains are listed below:

Mol	Chain	Res	Type
1	X	494	GLN
1	X	513	GLN
1	X	330	GLN
1	X	346	ASN
1	X	359	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)

2 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	A	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	2.82	6 (35%)
2	NAA	A	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.15	1 (5%)

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
2	NAG	A	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAA	A	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAA	C8-C7	2.72	1.56	1.50
2	A	1	NAG	C3-C2	2.33	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	O3-C3-C2	6.75	123.43	109.40
2	A	1	NAG	C1-O5-C5	5.58	119.66	112.19
2	A	1	NAG	C3-C4-C5	-4.61	101.87	110.23
2	A	1	NAG	O4-C4-C5	2.95	116.59	109.32
2	A	1	NAG	C1-C2-N2	-2.89	105.88	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	NAG	C1

5 of 6 torsion outliers are listed below:

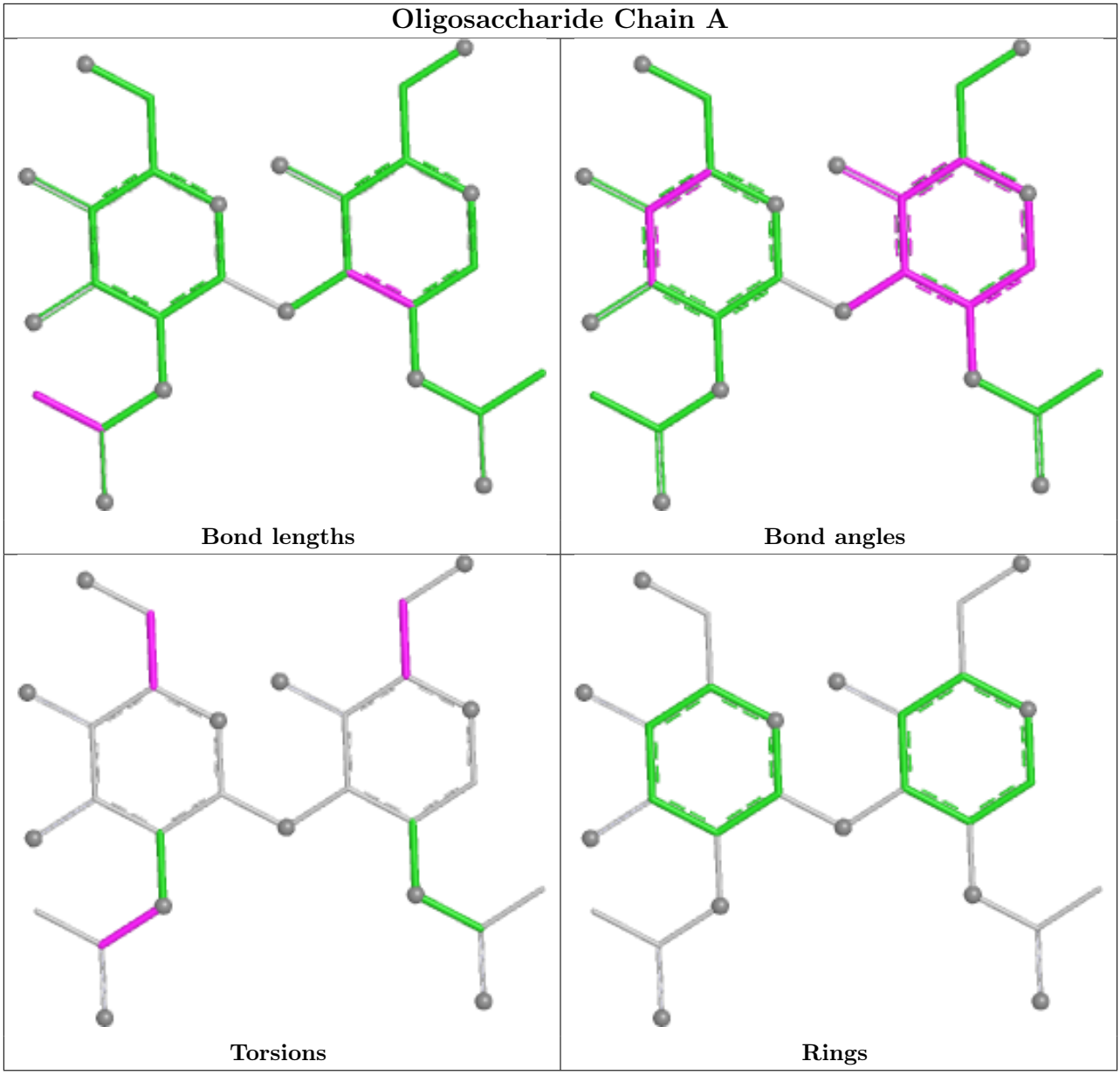
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NAA	C8-C7-N2-C2
2	A	2	NAA	O7-C7-N2-C2
2	A	2	NAA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	X	721	-	5,5,5	0.36	0	5,5,5	0.34	0
4	HEC	X	712	1	32,50,50	1.83	6 (18%)	30,82,82	2.35	9 (30%)
4	HEC	X	708	1	32,50,50	1.90	7 (21%)	30,82,82	2.61	13 (43%)
4	HEC	X	714	1	32,50,50	1.78	8 (25%)	30,82,82	3.51	16 (53%)
4	HEC	X	718	1	32,50,50	2.07	9 (28%)	30,82,82	3.82	14 (46%)
4	HEC	X	713	1	32,50,50	1.97	10 (31%)	30,82,82	2.84	12 (40%)
4	HEC	X	709	1	32,50,50	2.11	6 (18%)	30,82,82	2.38	9 (30%)
5	GOL	X	720	-	5,5,5	0.49	0	5,5,5	0.26	0
4	HEC	X	704	1	32,50,50	1.78	5 (15%)	30,82,82	2.89	11 (36%)
4	HEC	X	715	1	32,50,50	1.76	8 (25%)	30,82,82	3.37	16 (53%)
5	GOL	X	722	4	5,5,5	0.63	0	5,5,5	0.50	0
4	HEC	X	705	1	32,50,50	2.22	10 (31%)	30,82,82	2.42	9 (30%)
4	HEC	X	717	5,1	32,50,50	2.68	11 (34%)	30,82,82	2.80	15 (50%)
4	HEC	X	706	1	32,50,50	1.95	3 (9%)	30,82,82	2.71	10 (33%)
5	GOL	X	724	-	5,5,5	0.55	0	5,5,5	2.14	2 (40%)
4	HEC	X	710	1	32,50,50	1.89	4 (12%)	30,82,82	2.41	12 (40%)
4	HEC	X	716	1	32,50,50	2.02	9 (28%)	30,82,82	3.41	15 (50%)
4	HEC	X	707	1	32,50,50	2.03	10 (31%)	30,82,82	2.63	8 (26%)
5	GOL	X	723	-	5,5,5	0.45	0	5,5,5	0.52	0
4	HEC	X	711	1	32,50,50	2.14	9 (28%)	30,82,82	3.29	11 (36%)
4	HEC	X	719	3,1	32,50,50	2.32	10 (31%)	30,82,82	3.03	12 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	X	721	-	-	3/4/4/4	-
4	HEC	X	712	1	-	6/10/54/54	-
4	HEC	X	708	1	-	4/10/54/54	-
4	HEC	X	714	1	-	2/10/54/54	-
4	HEC	X	718	1	-	3/10/54/54	-
4	HEC	X	713	1	-	6/10/54/54	-
4	HEC	X	709	1	-	2/10/54/54	-
5	GOL	X	720	-	-	2/4/4/4	-
4	HEC	X	704	1	-	1/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	X	715	1	-	4/10/54/54	-
5	GOL	X	722	4	-	4/4/4/4	-
4	HEC	X	705	1	-	1/10/54/54	-
4	HEC	X	717	5,1	-	4/10/54/54	-
4	HEC	X	706	1	-	2/10/54/54	-
5	GOL	X	724	-	-	2/4/4/4	-
4	HEC	X	710	1	-	2/10/54/54	-
4	HEC	X	716	1	-	2/10/54/54	-
4	HEC	X	707	1	-	0/10/54/54	-
5	GOL	X	723	-	-	2/4/4/4	-
4	HEC	X	711	1	-	2/10/54/54	-
4	HEC	X	719	3,1	-	3/10/54/54	-

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	710	HEC	C2B-C3B	-6.41	1.33	1.40
4	X	705	HEC	C2B-C3B	-6.18	1.33	1.40
4	X	711	HEC	C2B-C3B	-5.92	1.34	1.40
4	X	717	HEC	C3C-C2C	-5.82	1.34	1.40
4	X	709	HEC	C3D-C2D	5.77	1.54	1.37

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	714	HEC	CMC-C2C-C1C	-9.77	114.15	128.46
4	X	711	HEC	CMC-C2C-C1C	-9.47	114.58	128.46
4	X	719	HEC	CMC-C2C-C1C	-8.81	115.54	128.46
4	X	704	HEC	CBB-CAB-C3B	-8.75	107.00	127.49
4	X	719	HEC	CBD-CAD-C3D	-8.06	98.98	112.54

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	704	HEC	C3D-CAD-CBD-CGD
4	X	713	HEC	C2D-C3D-CAD-CBD
4	X	713	HEC	C4D-C3D-CAD-CBD
5	X	720	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	X	721	GOL	C1-C2-C3-O3

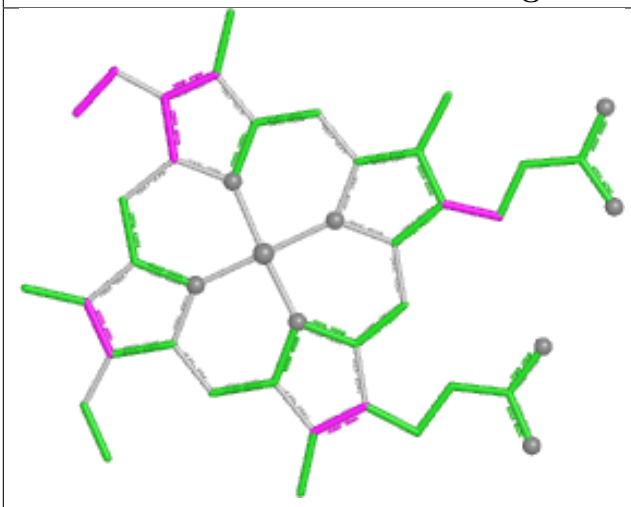
There are no ring outliers.

18 monomers are involved in 117 short contacts:

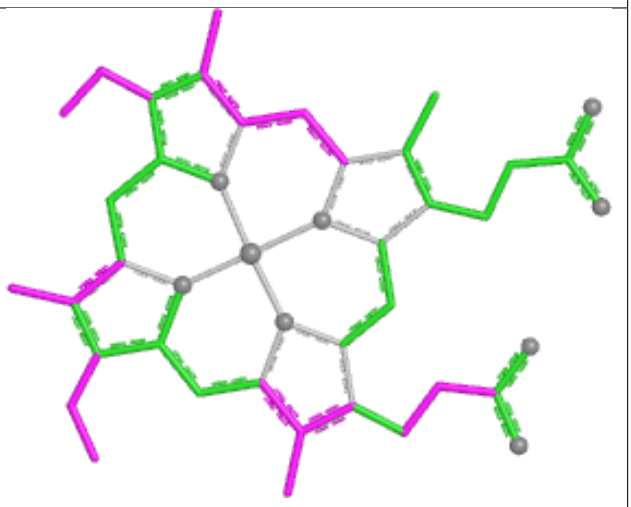
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	712	HEC	5	0
4	X	708	HEC	3	0
4	X	714	HEC	1	0
4	X	718	HEC	8	1
4	X	713	HEC	13	0
4	X	709	HEC	7	0
4	X	704	HEC	14	0
4	X	715	HEC	4	0
5	X	722	GOL	5	0
4	X	705	HEC	12	0
4	X	717	HEC	10	0
4	X	706	HEC	2	0
4	X	710	HEC	6	0
4	X	716	HEC	2	0
4	X	707	HEC	6	0
5	X	723	GOL	1	0
4	X	711	HEC	11	0
4	X	719	HEC	12	0

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

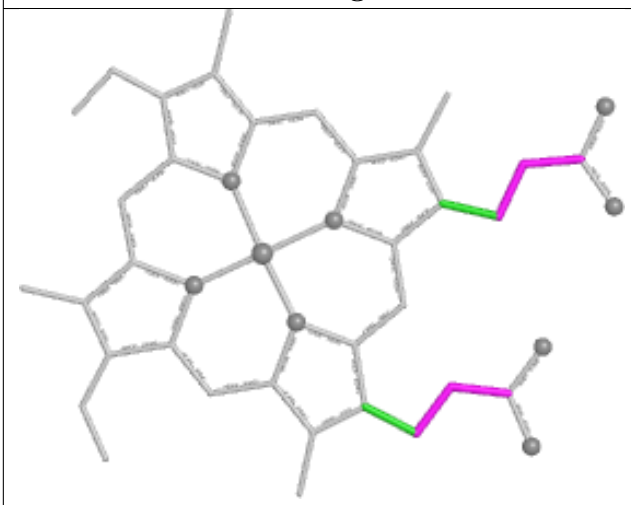
Ligand HEC X 712



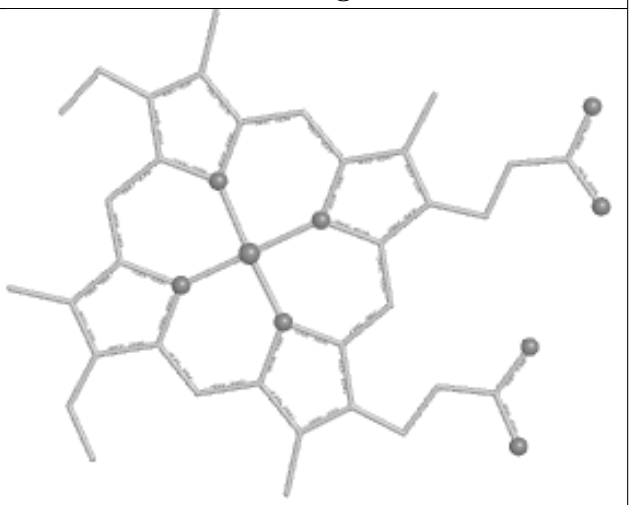
Bond lengths



Bond angles

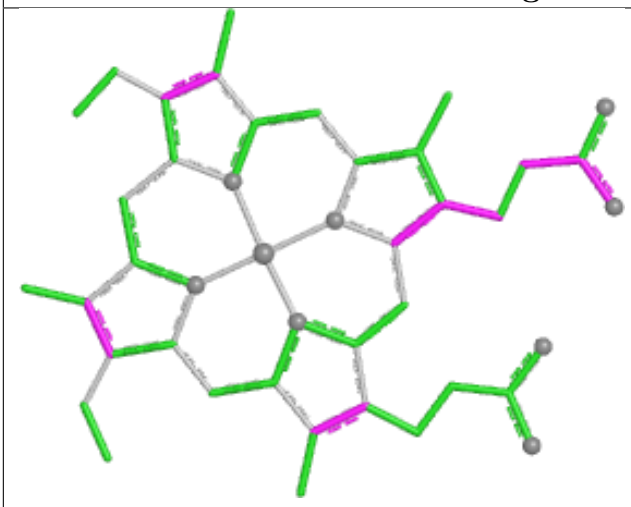


Torsions

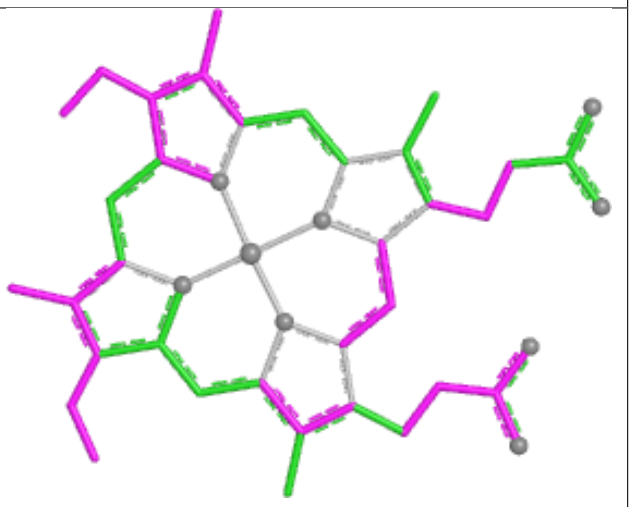


Rings

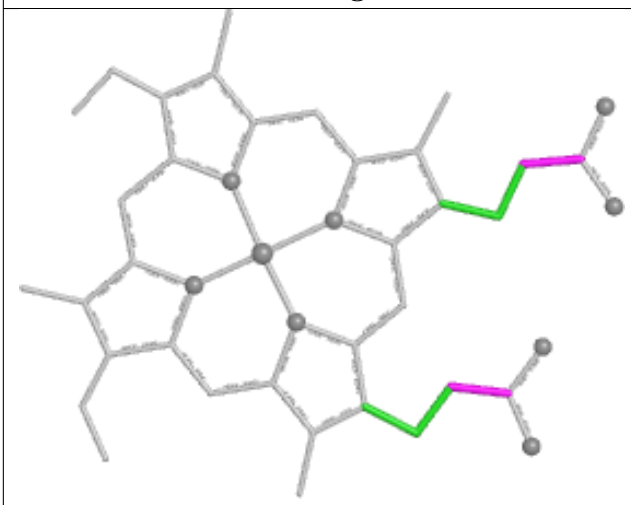
Ligand HEC X 708



Bond lengths



Bond angles



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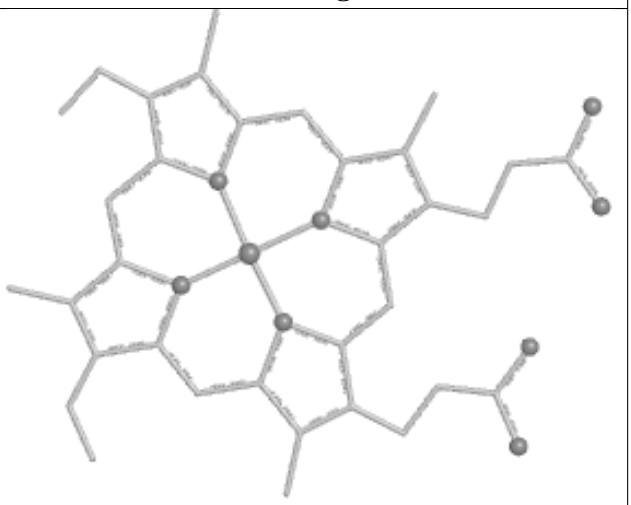
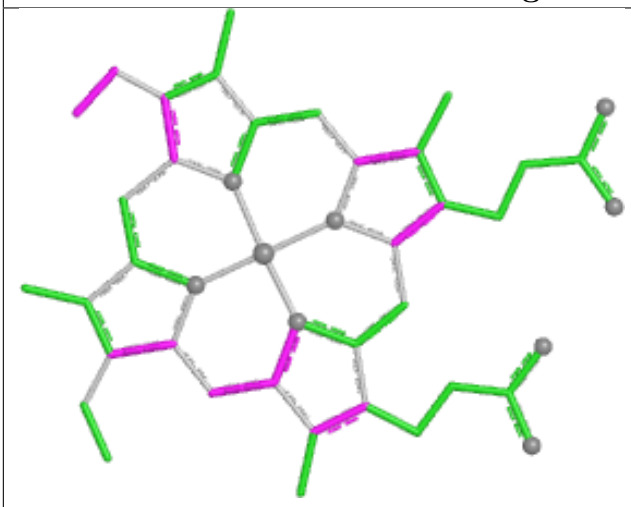
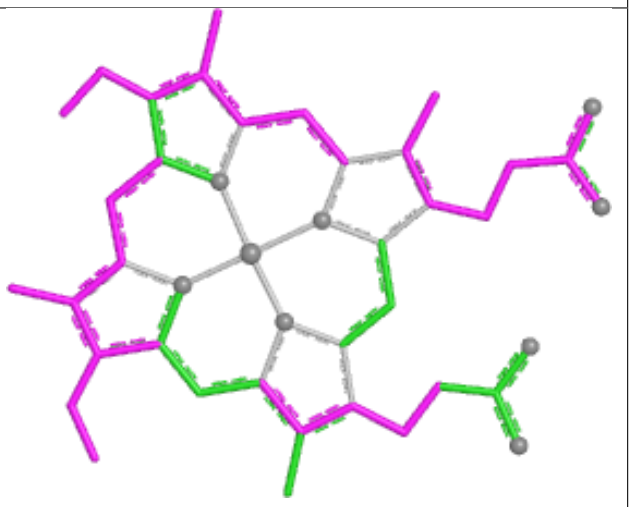


Rings

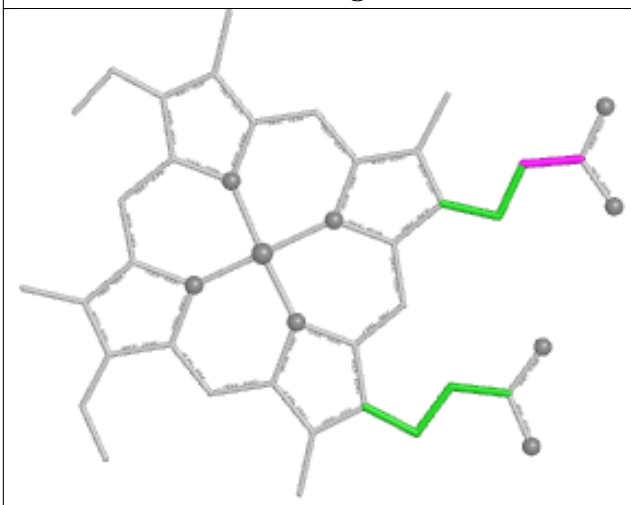
Ligand HEC X 714



Bond lengths



Bond angles



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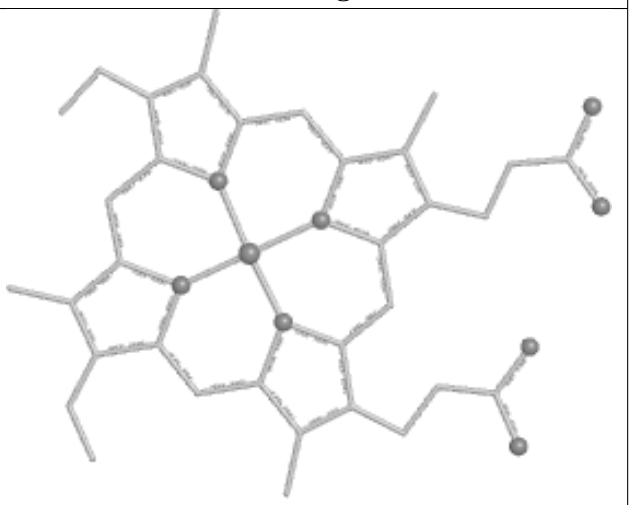
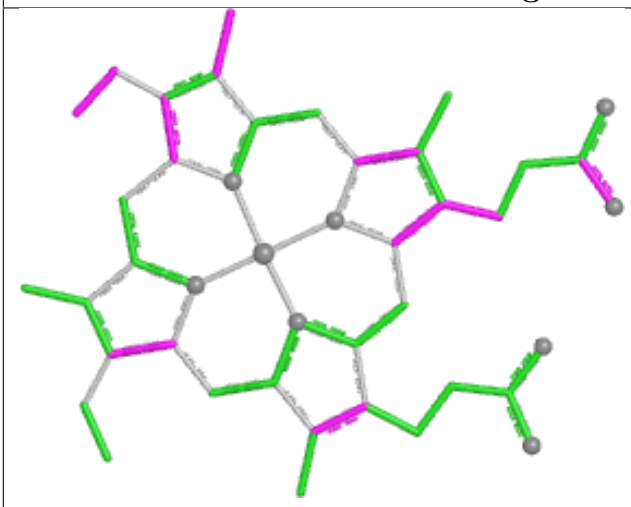


Rings

Ligand HEC X 718



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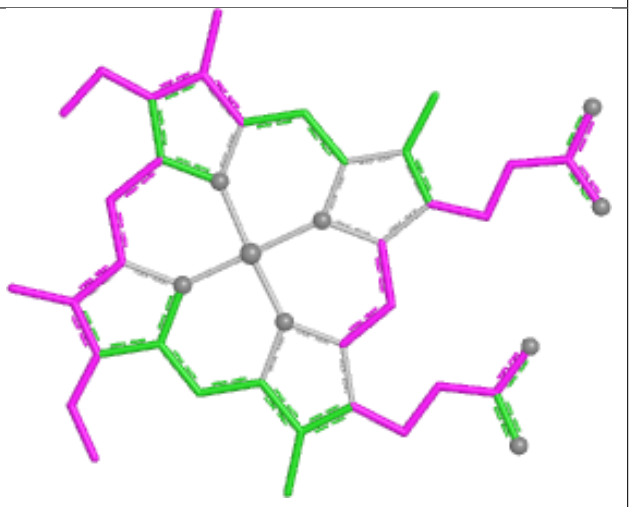
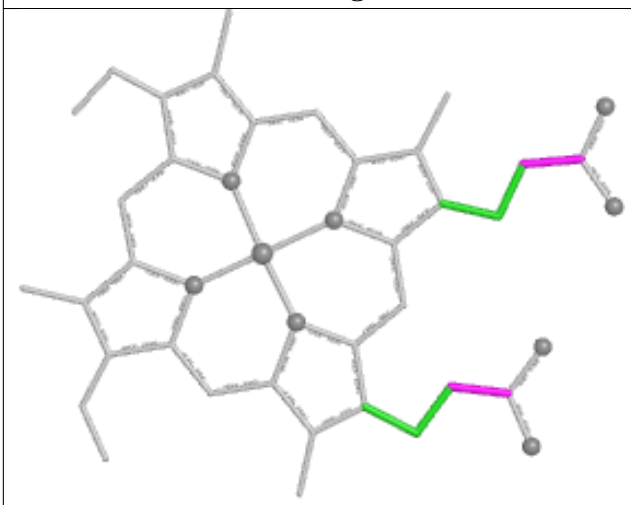


Bond angles



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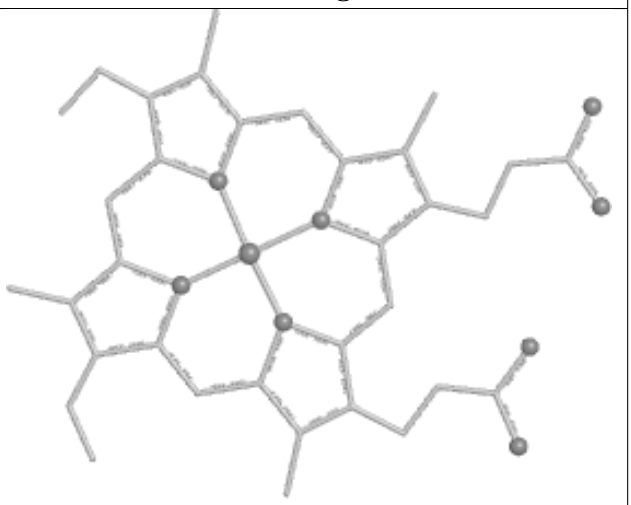
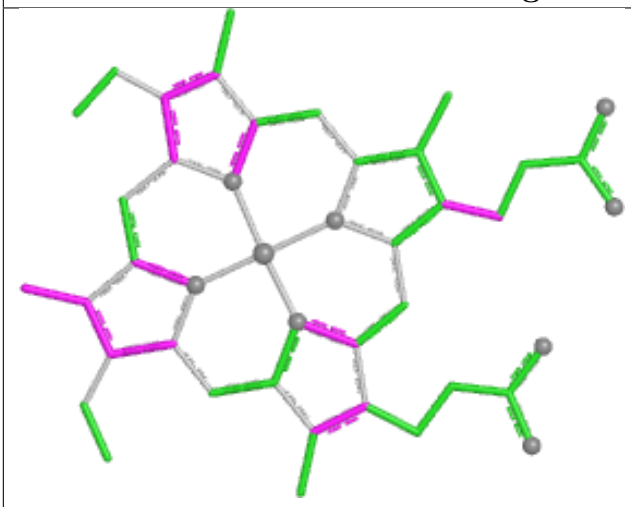


Rings

Ligand HEC X 713



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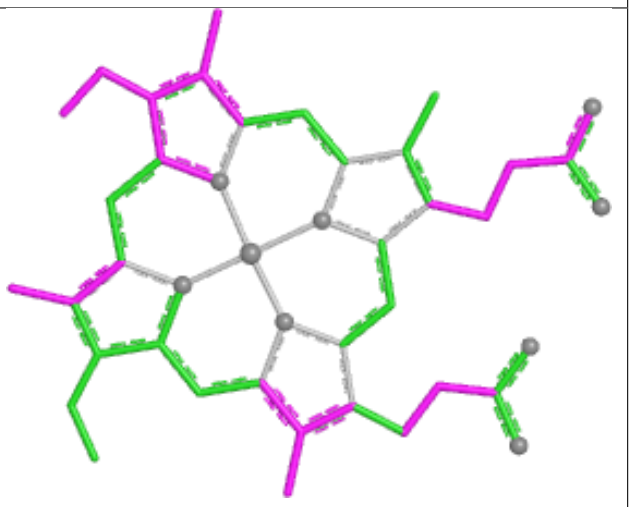

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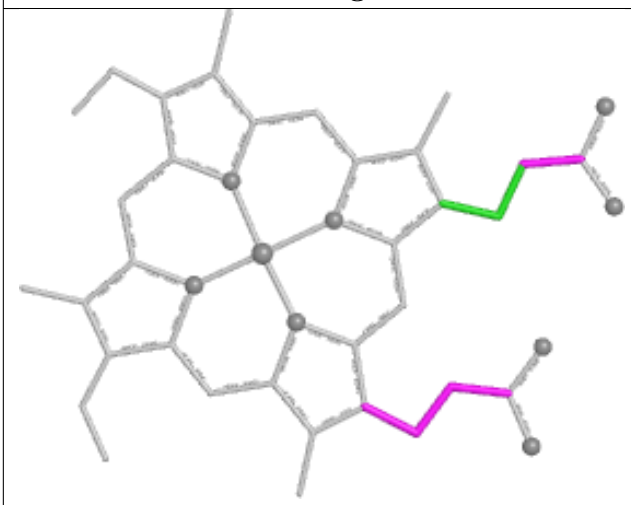

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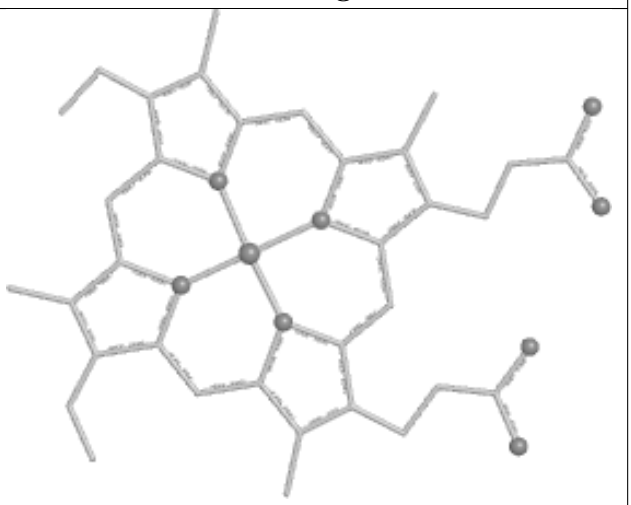

Rings

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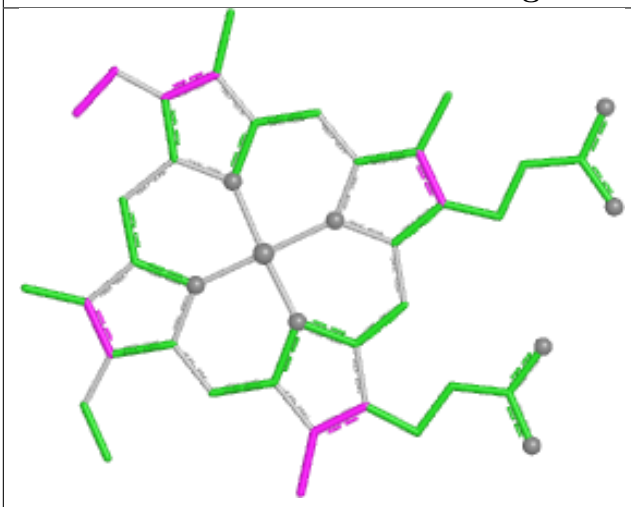

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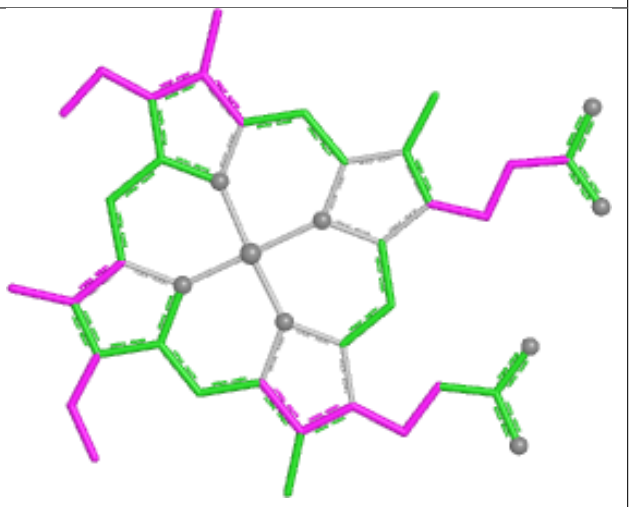

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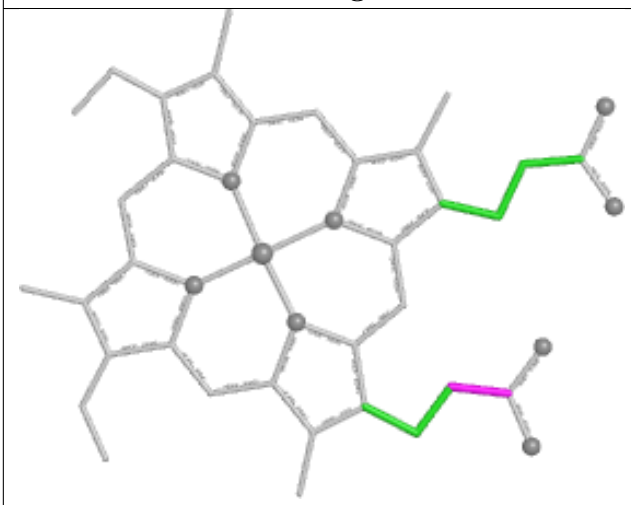

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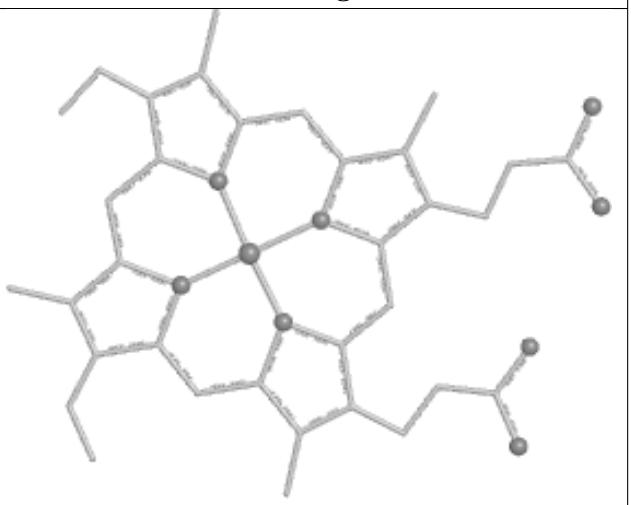

Rings

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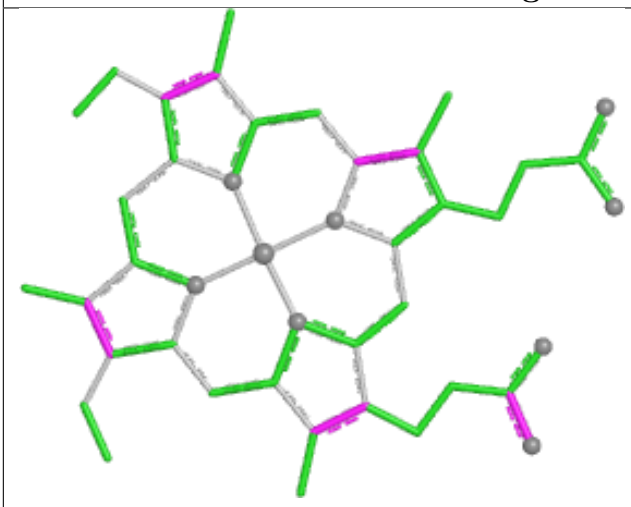

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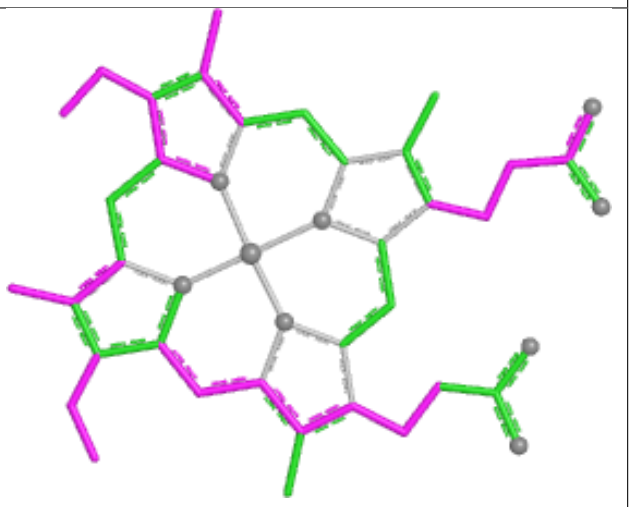

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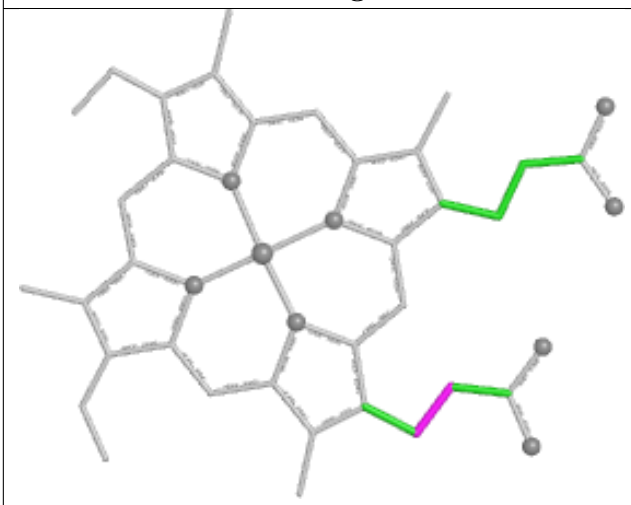

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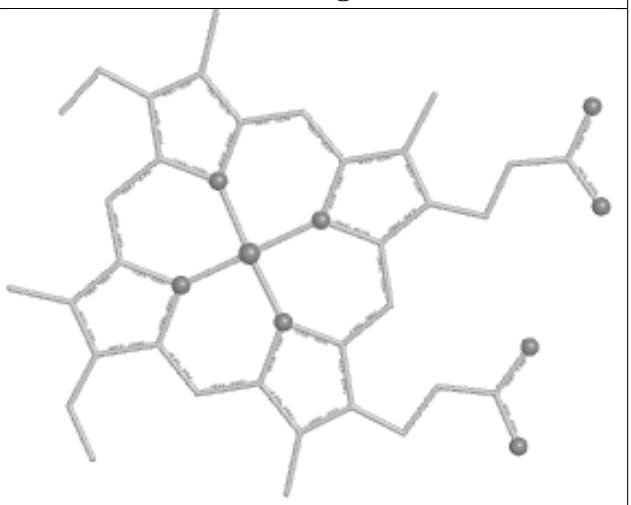
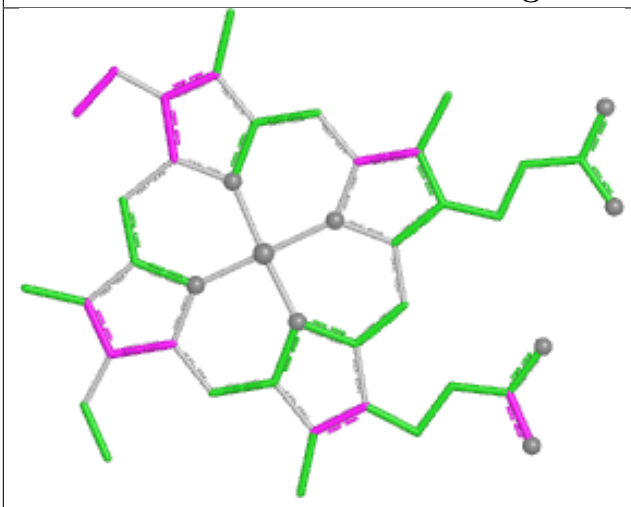


Rings

Ligand HEC X 715



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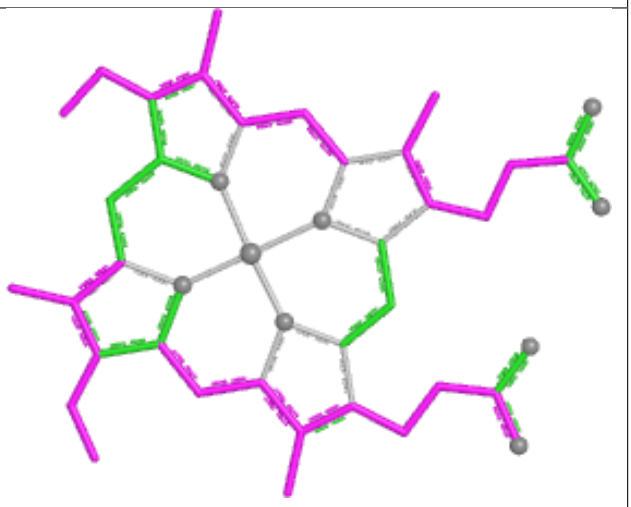

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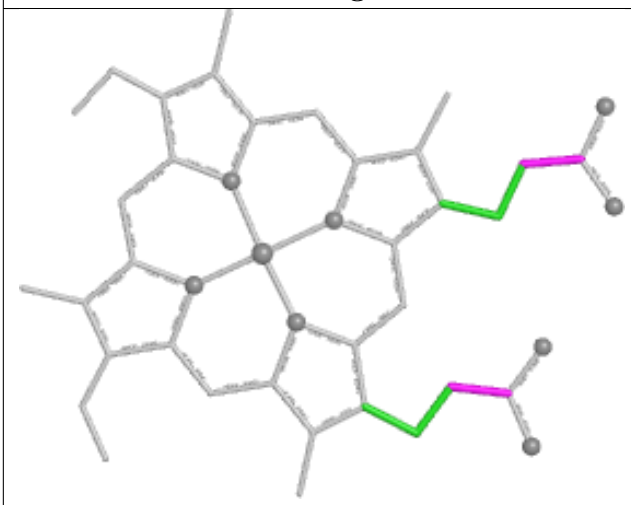

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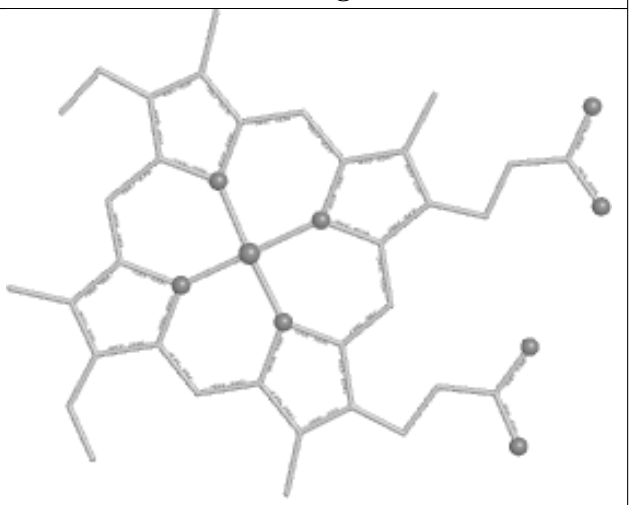
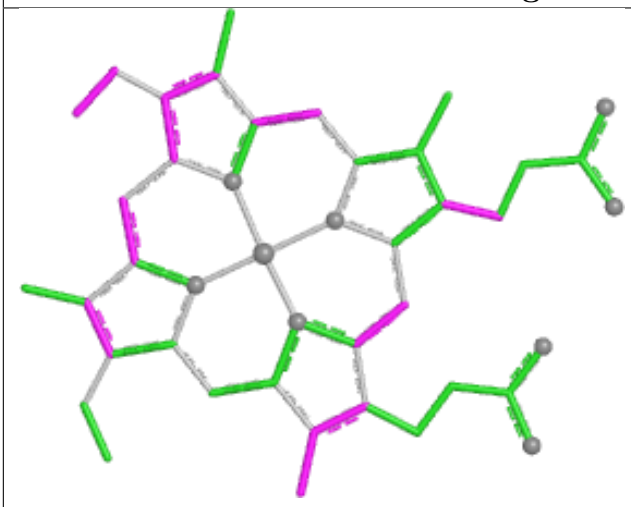


Rings

Ligand HEC X 705



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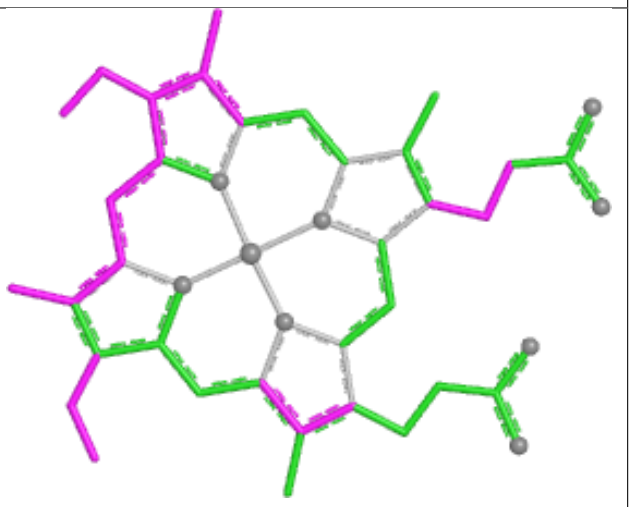

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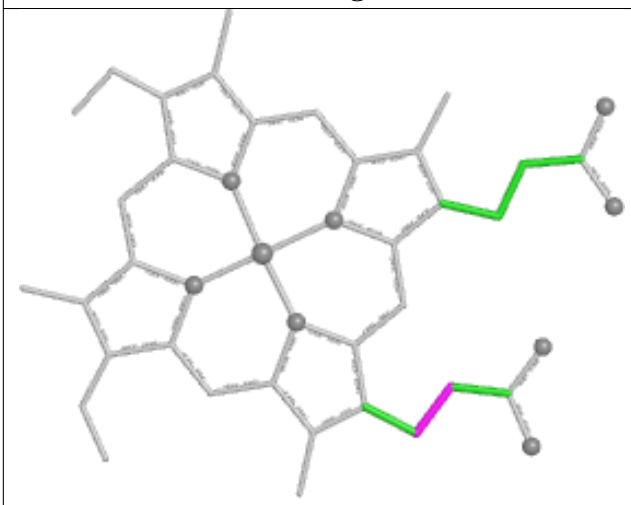

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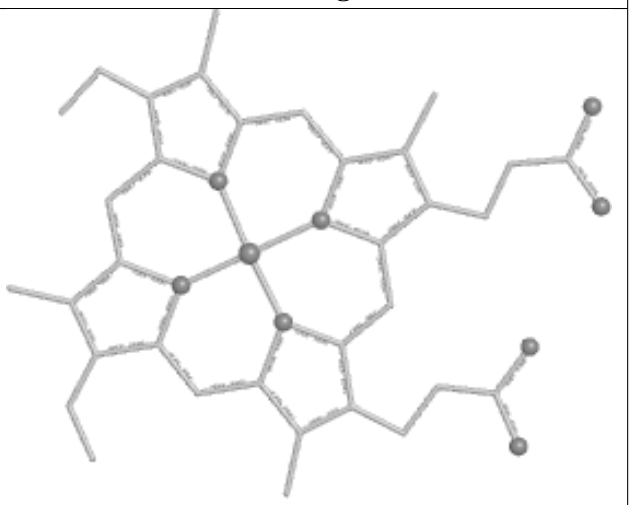
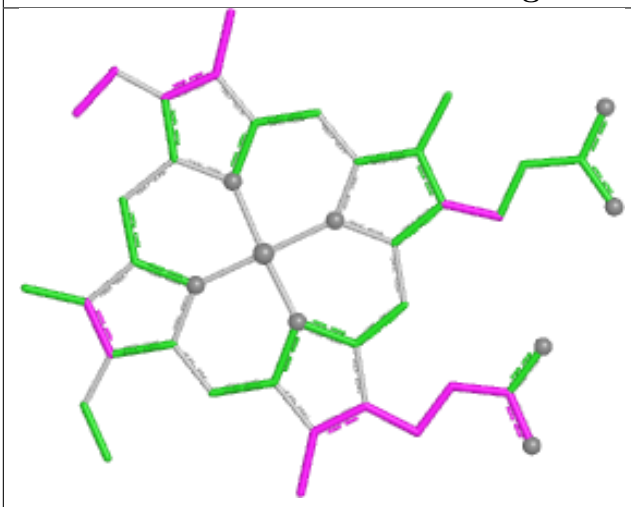


Rings

Ligand HEC X 717



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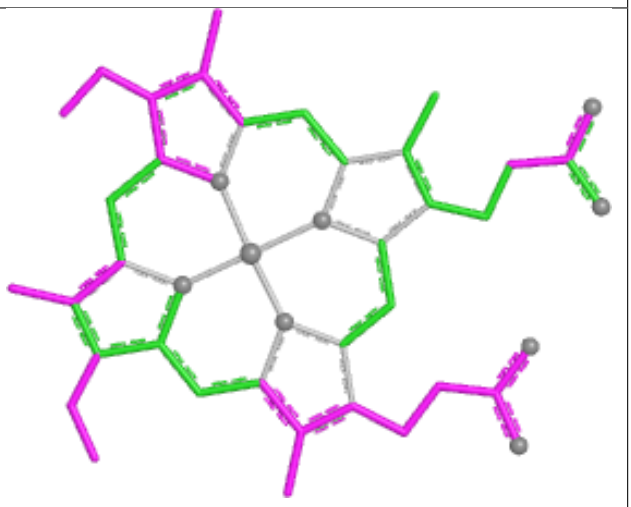

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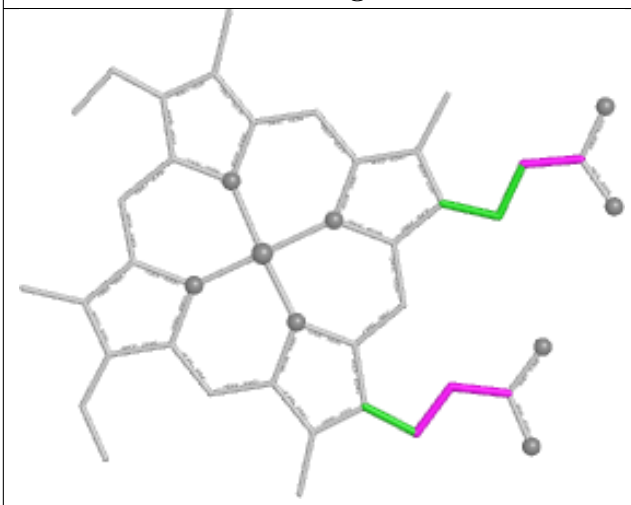

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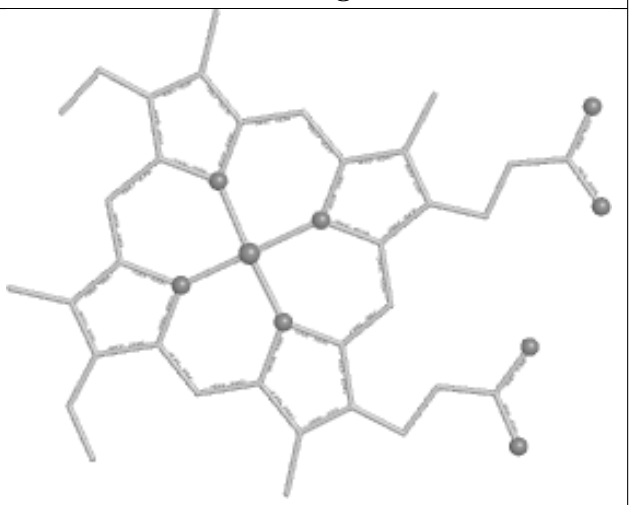
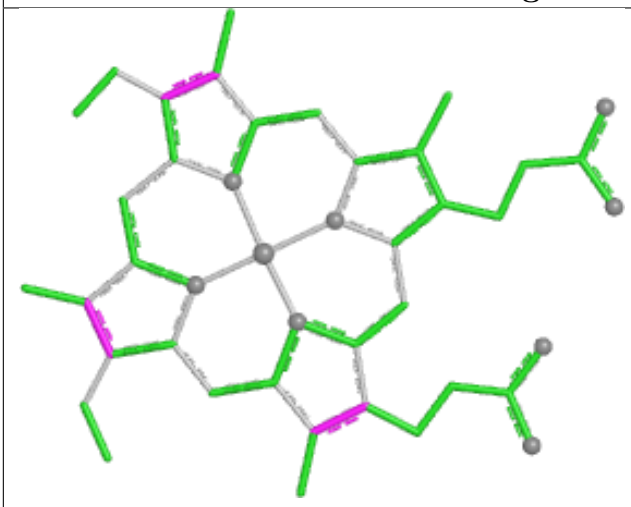


Rings

Ligand HEC X 706



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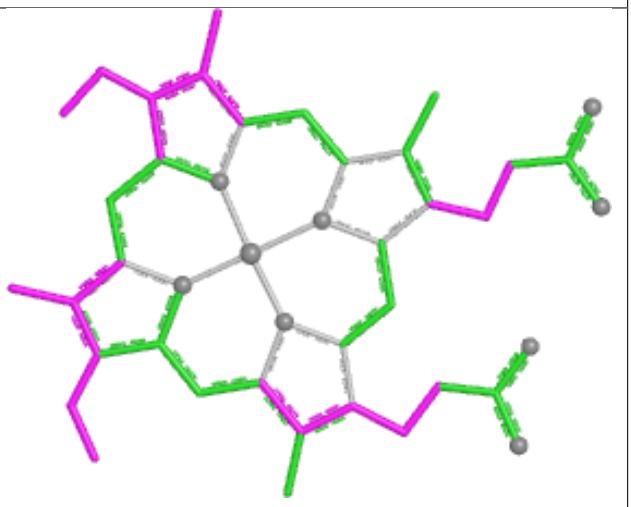

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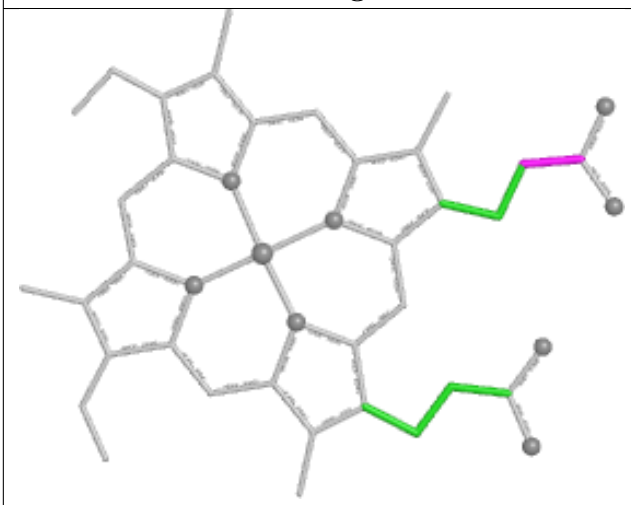

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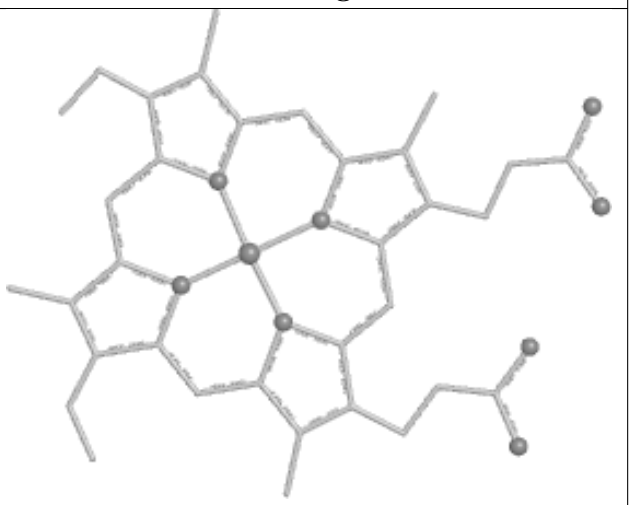
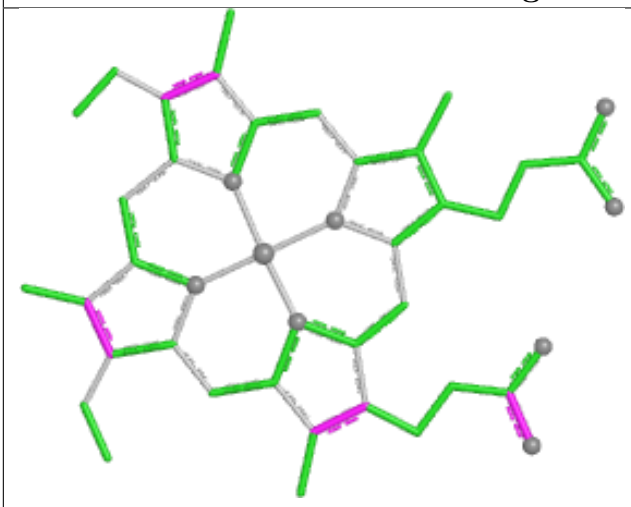


Rings

Ligand HEC X 710



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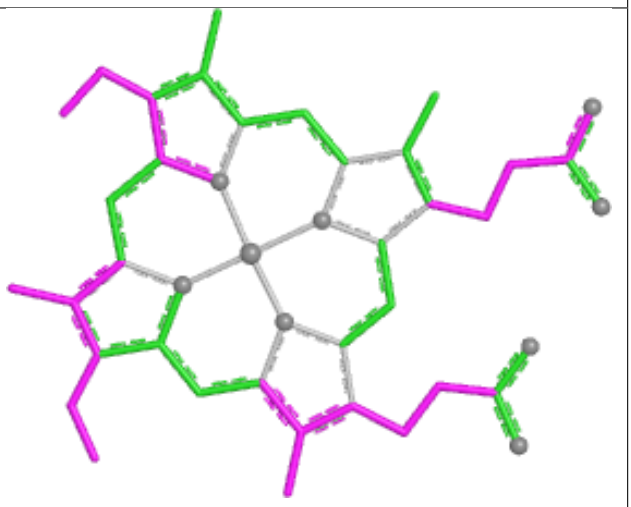
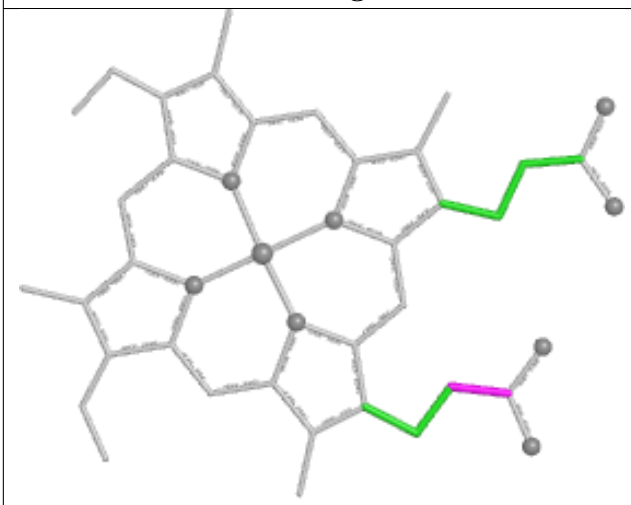


Bond angles



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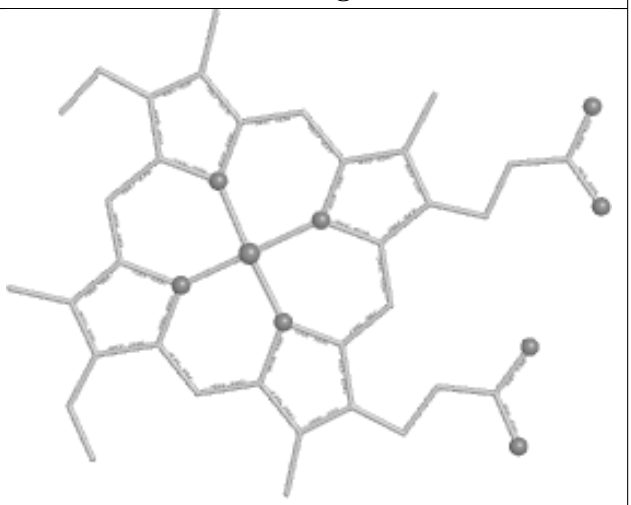
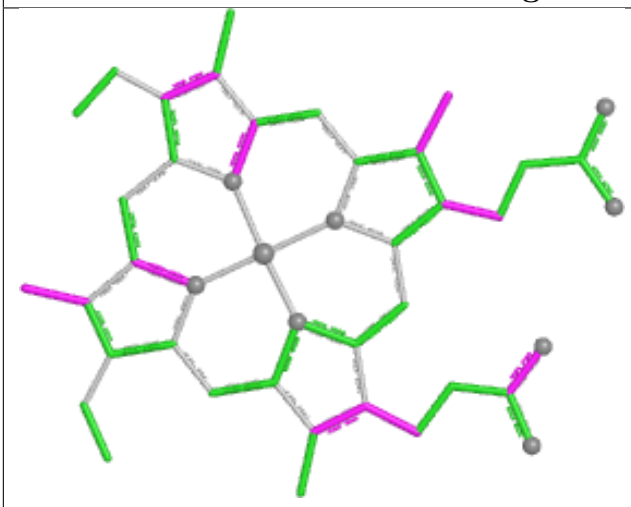
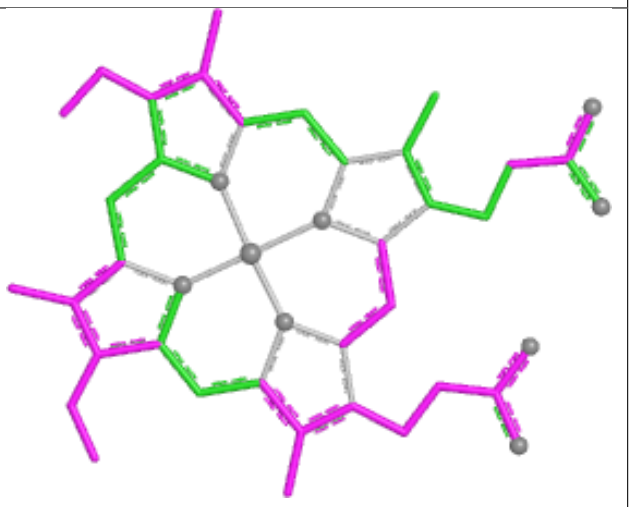


Rings

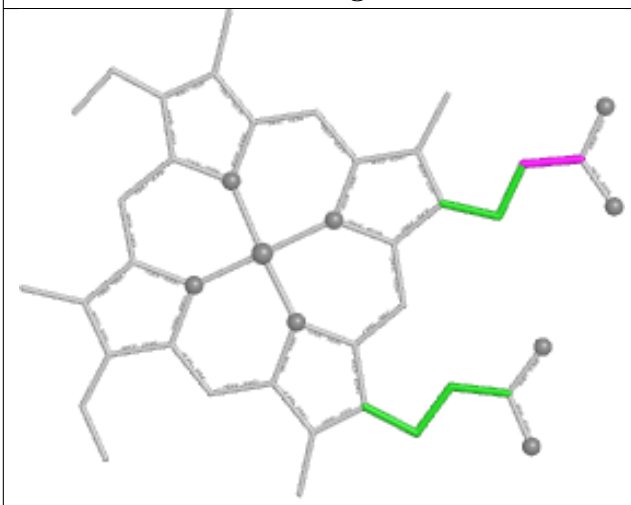
Ligand HEC X 716



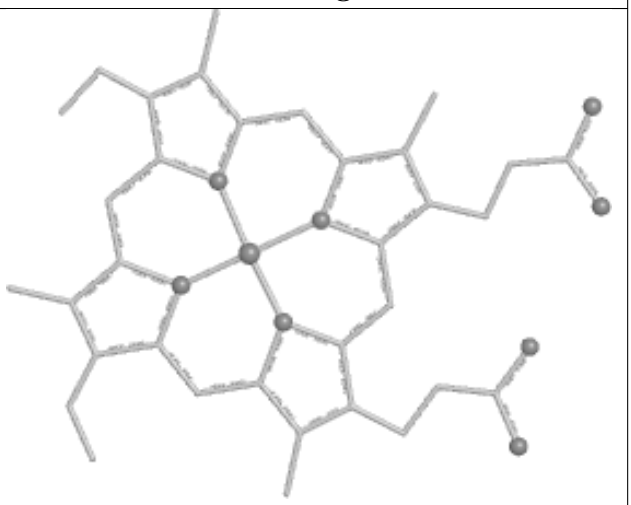
Bond lengths



Bond angles

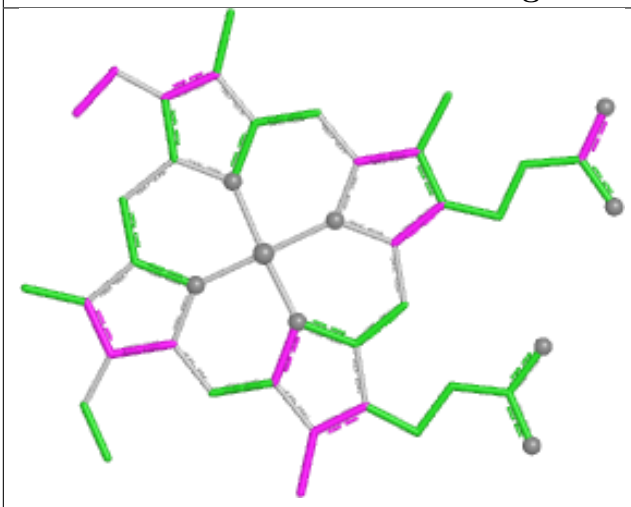


Torsions

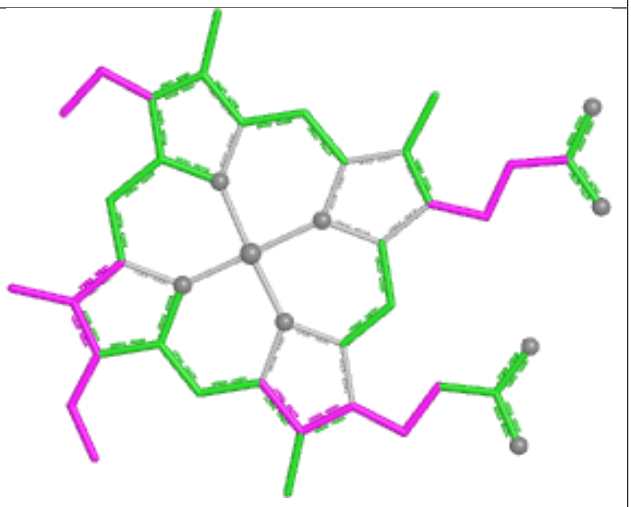


Rings

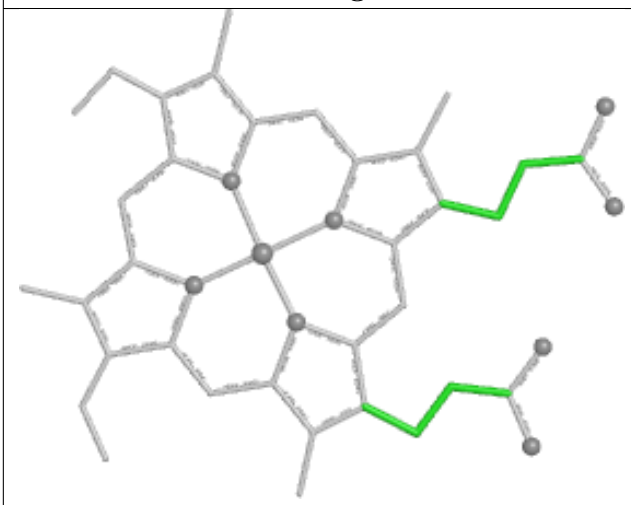
Ligand HEC X 707



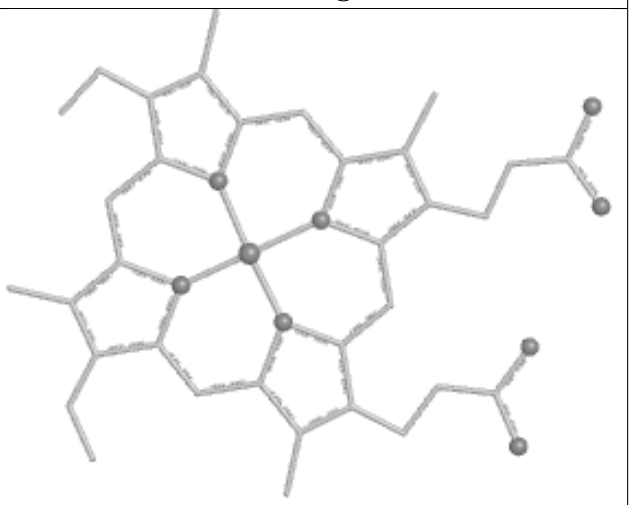
Bond lengths



Bond angles

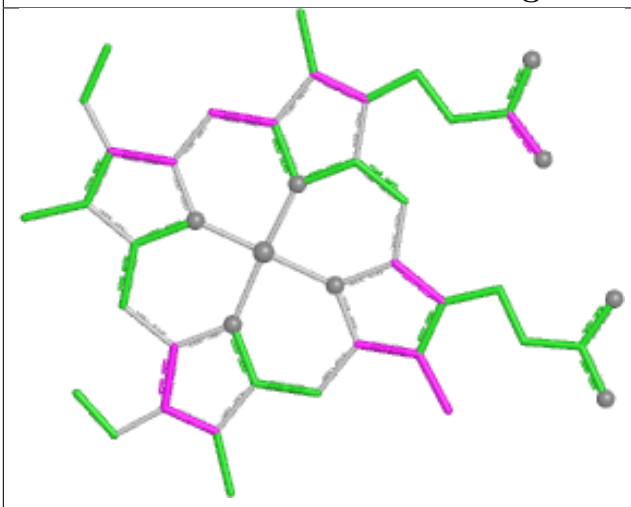


Torsions

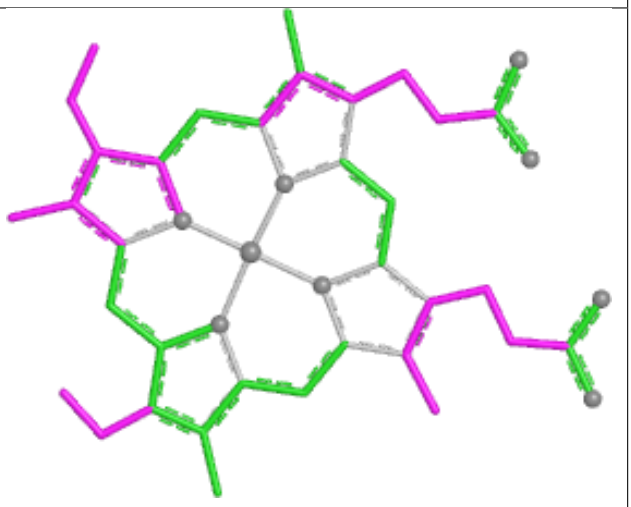


Rings

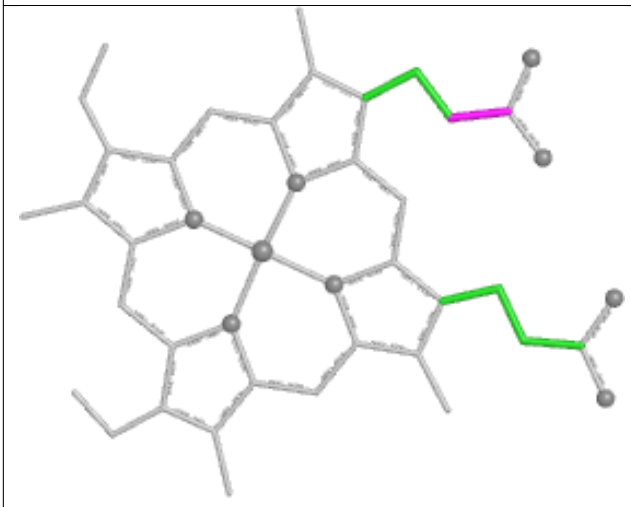
Ligand HEC X 711



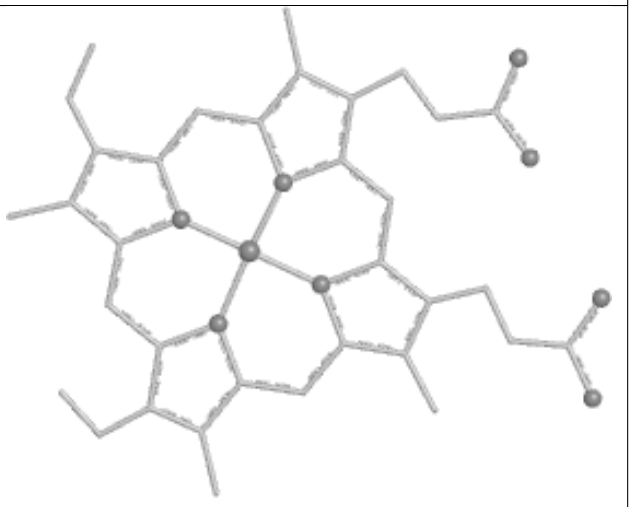
Bond lengths



Bond angles

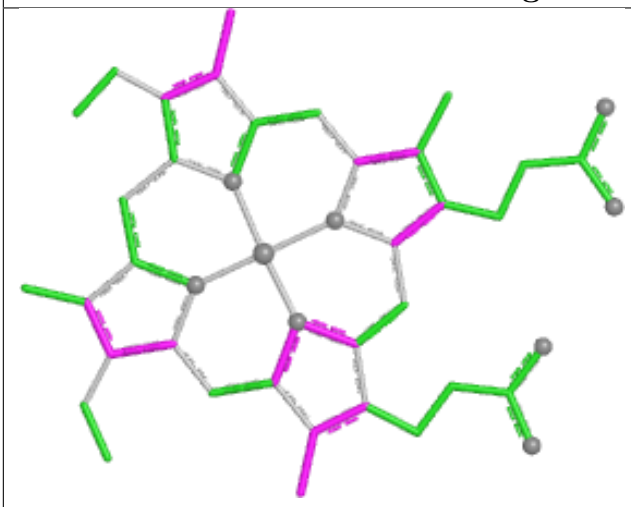


Torsions

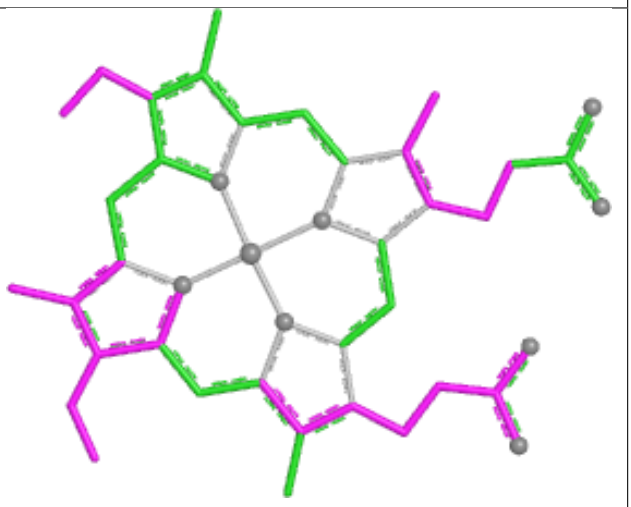


Rings

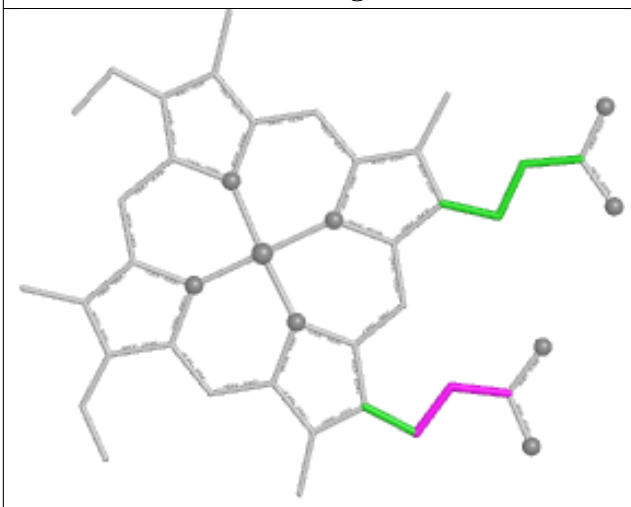
Ligand HEC X 719



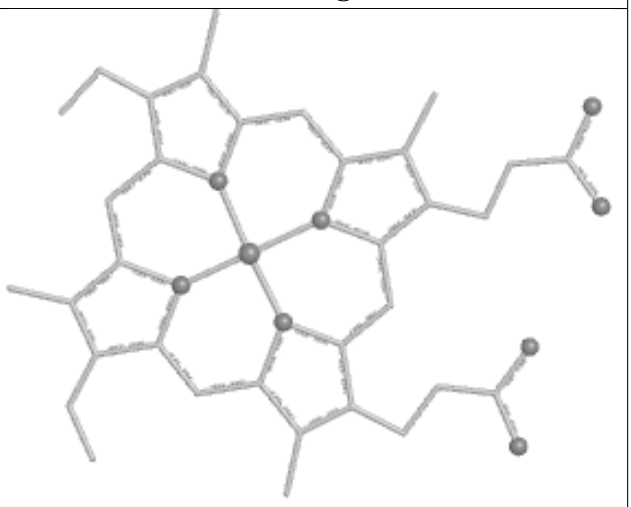
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	X	516/560 (92%)	0.12	9 (1%)	69	70	28, 55, 82, 91	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	530	SER	5.2
1	X	22	ALA	3.1
1	X	16	ILE	2.9
1	X	102	ALA	2.8
1	X	186	VAL	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

SUGAR-RSR INFOmissingINFO

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	X	724	6/6	0.73	0.17	57,62,66,73	0
5	GOL	X	720	6/6	0.79	0.10	86,88,89,90	0

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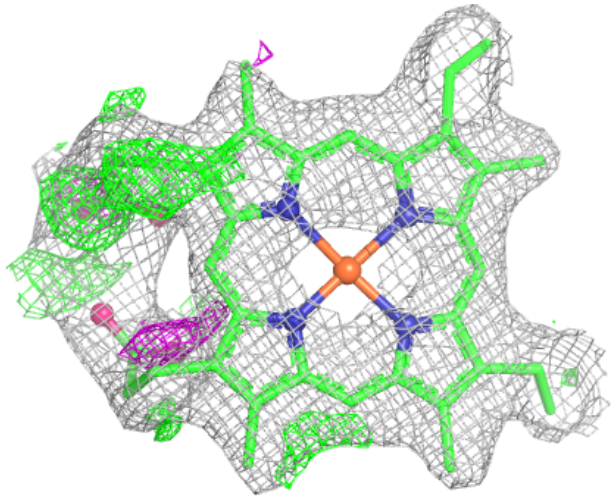
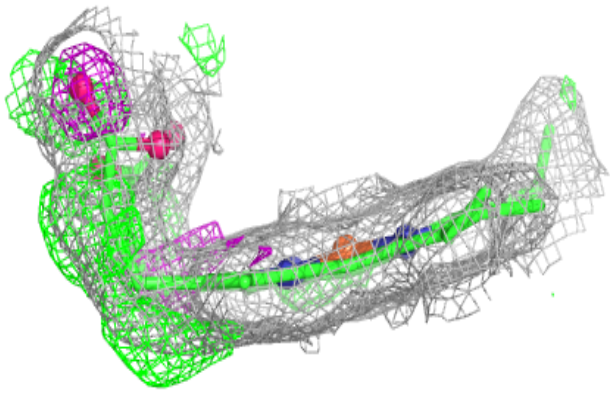
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	X	723	6/6	0.82	0.13	53,61,66,70	0
5	GOL	X	721	6/6	0.85	0.11	62,69,71,73	0
3	ZN	X	702	1/1	0.88	0.07	72,72,72,72	0
5	GOL	X	722	6/6	0.92	0.13	28,54,59,60	0
4	HEC	X	717	43/43	0.93	0.10	20,31,41,50	0
3	ZN	X	703	1/1	0.93	0.11	69,69,69,69	0
4	HEC	X	706	43/43	0.93	0.11	58,73,75,77	0
4	HEC	X	704	43/43	0.95	0.10	52,59,63,65	0
4	HEC	X	708	43/43	0.95	0.09	48,58,73,78	0
4	HEC	X	709	43/43	0.95	0.09	45,49,65,71	0
4	HEC	X	710	43/43	0.95	0.09	49,55,65,72	0
4	HEC	X	705	43/43	0.95	0.09	45,51,75,80	0
4	HEC	X	719	43/43	0.96	0.08	29,38,50,64	0
4	HEC	X	712	43/43	0.96	0.09	40,50,61,67	0
4	HEC	X	714	43/43	0.97	0.07	28,33,52,58	0
4	HEC	X	715	43/43	0.97	0.07	30,38,56,65	0
4	HEC	X	711	43/43	0.97	0.07	27,37,52,61	0
4	HEC	X	718	43/43	0.97	0.06	25,31,49,56	0
4	HEC	X	707	43/43	0.97	0.07	38,48,54,57	0
4	HEC	X	713	43/43	0.98	0.06	20,26,41,47	0
4	HEC	X	716	43/43	0.98	0.06	28,31,43,53	0
3	ZN	X	701	1/1	1.00	0.01	42,42,42,42	0

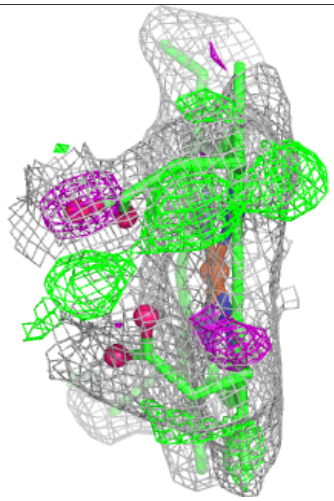
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC X 717:

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

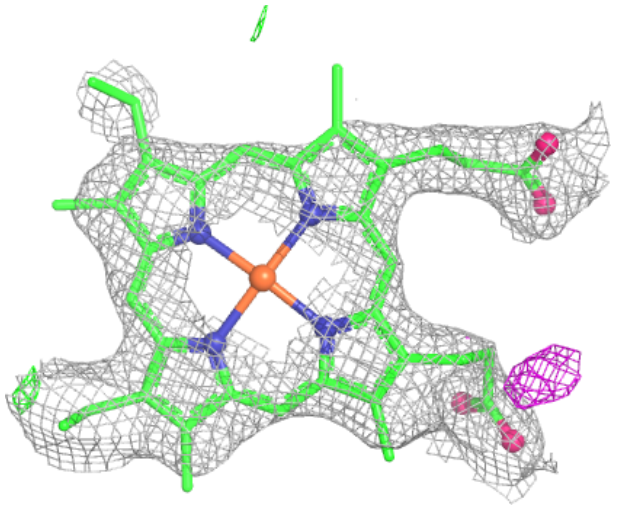


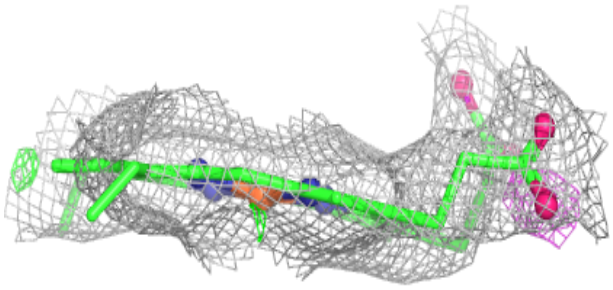


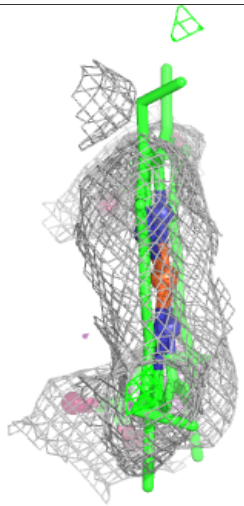


Electron density around HEC X 706:

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

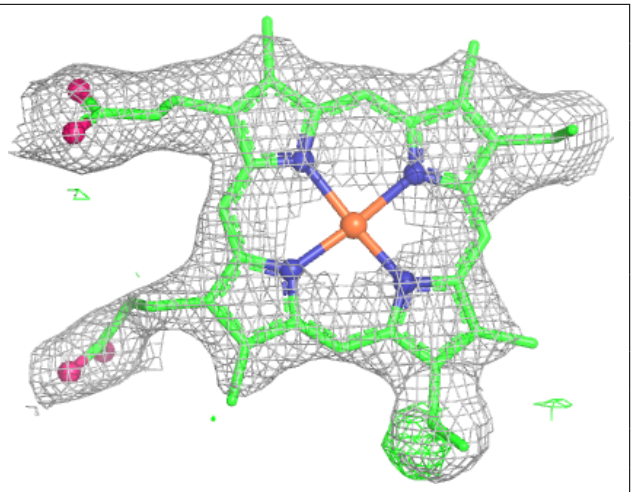


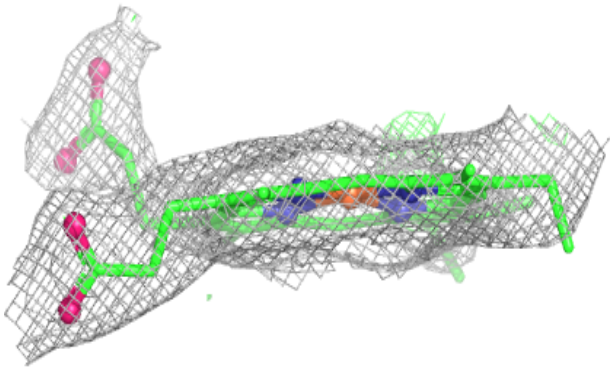


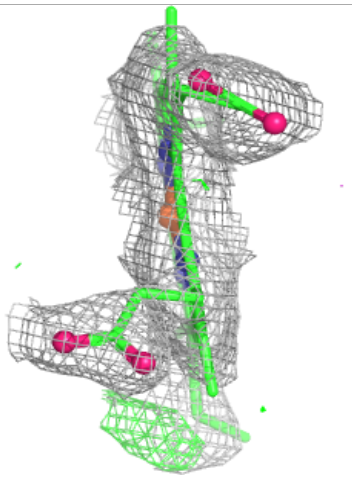


Electron density around HEC X 704:

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

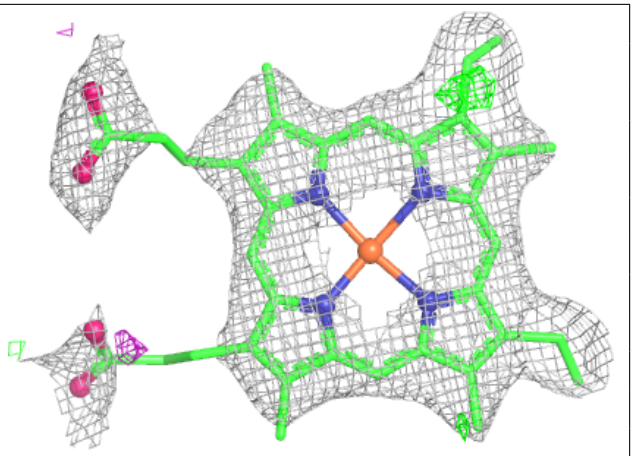


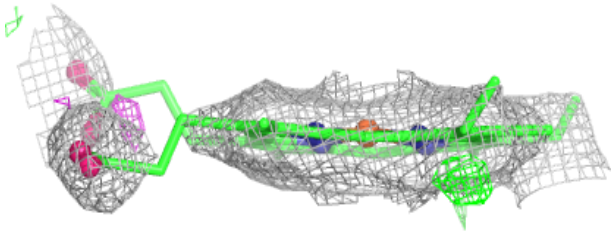


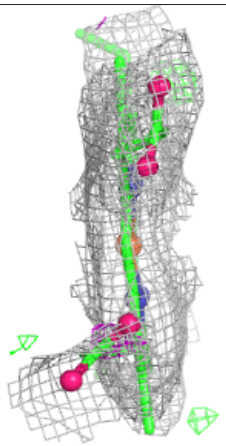


Electron density around HEC X 708:

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

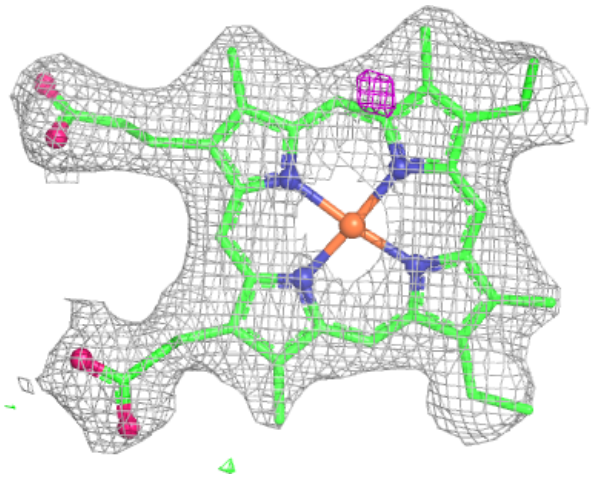


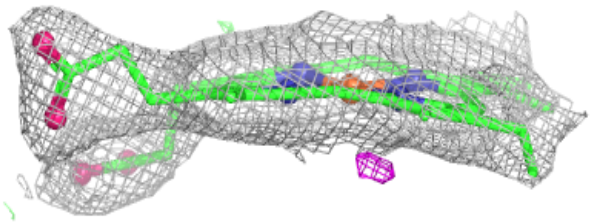


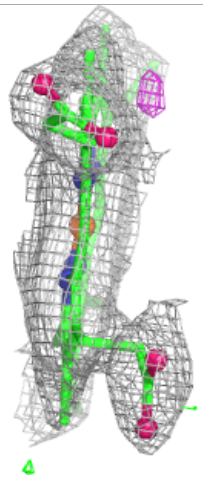


Electron density around HEC X 709:

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

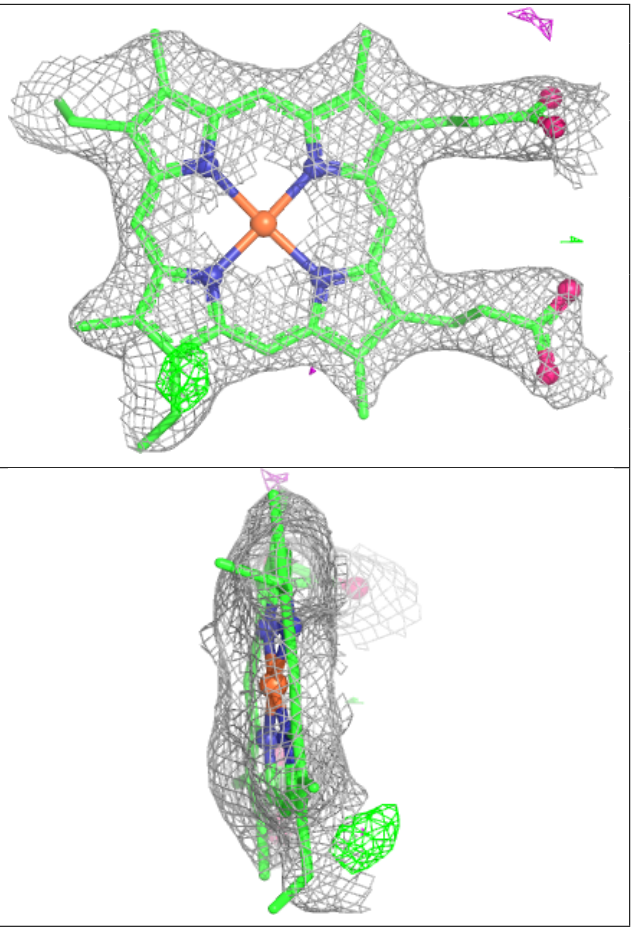


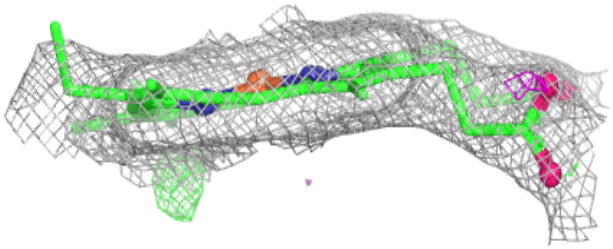




Electron density around HEC X 710:

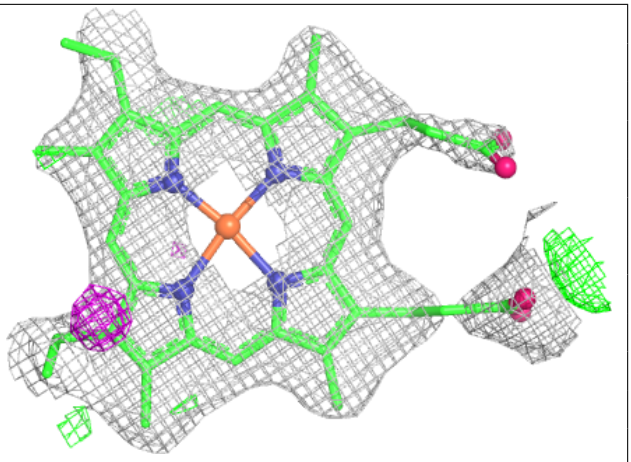
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

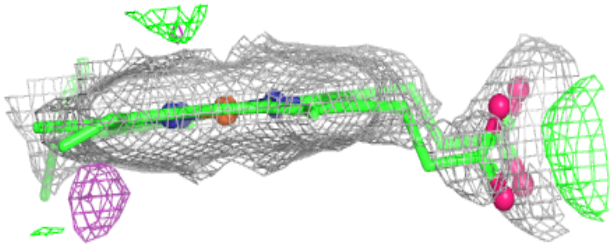


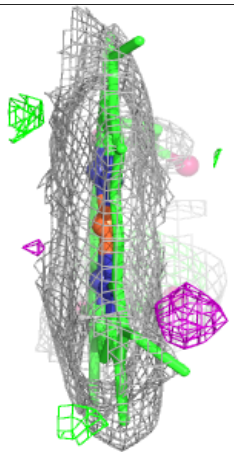


Electron density around HEC X 705:

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

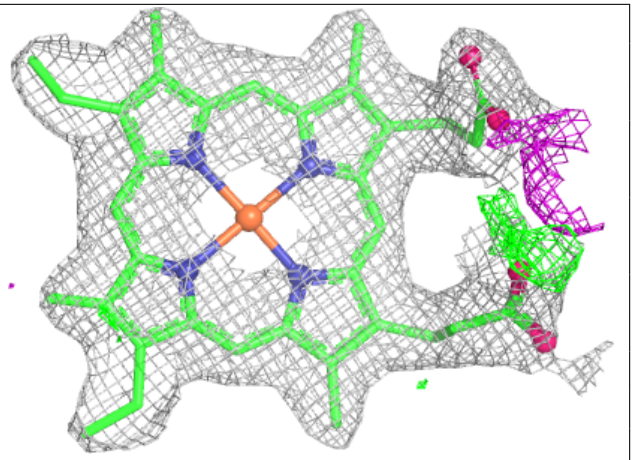


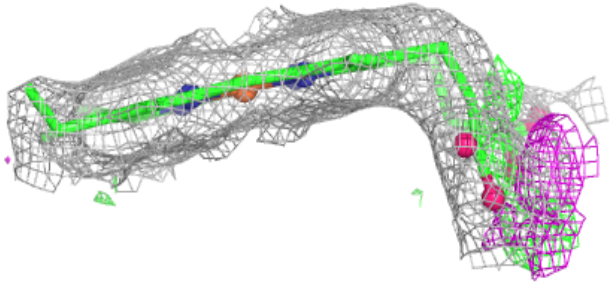


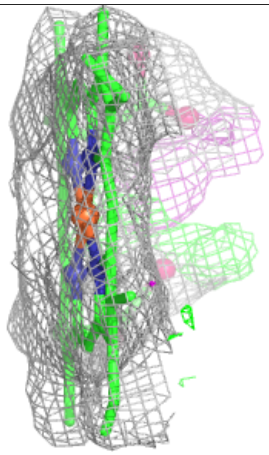


Electron density around HEC X 719:

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

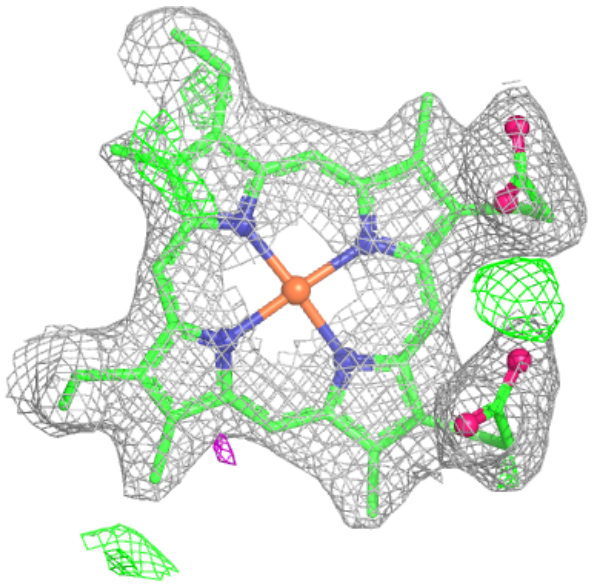


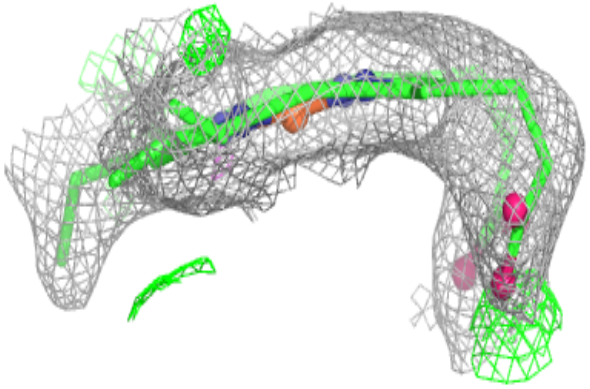


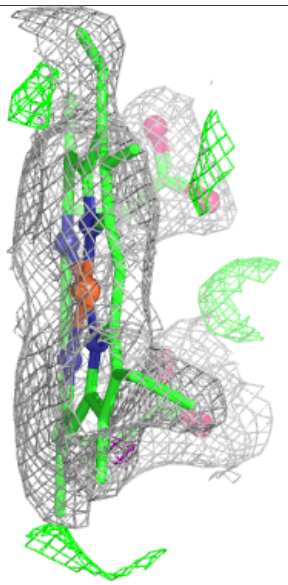


Electron density around HEC X 712:

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

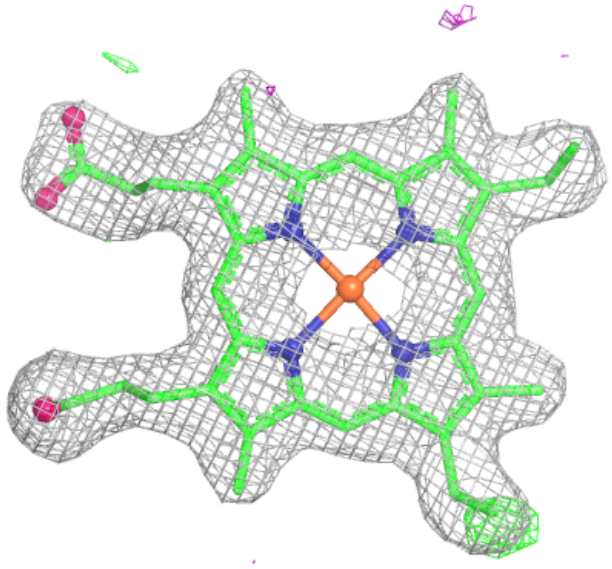


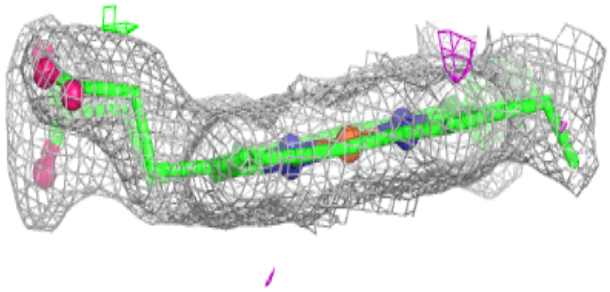


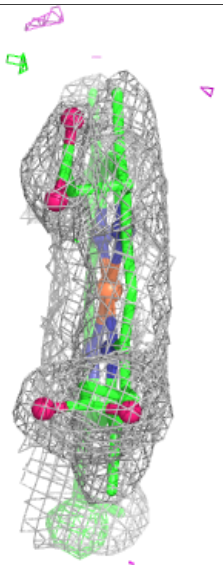


Electron density around HEC X 714:

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

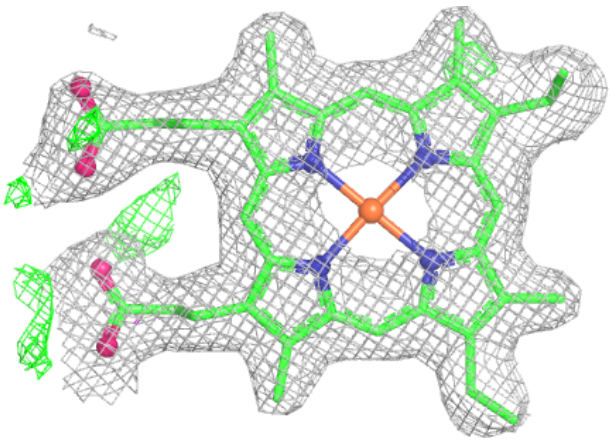


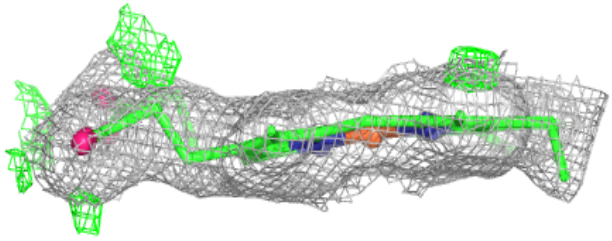


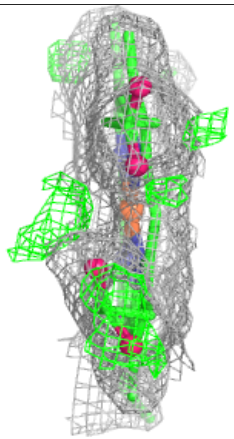


Electron density around HEC X 715:

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

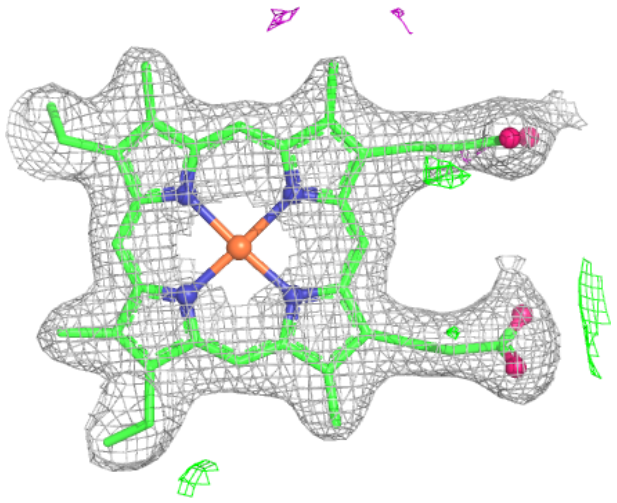


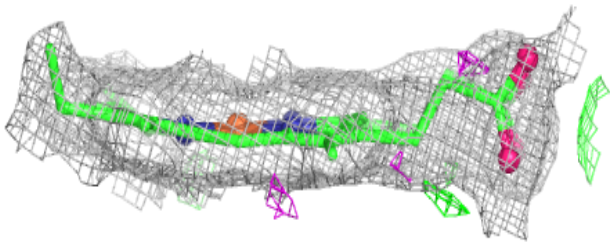


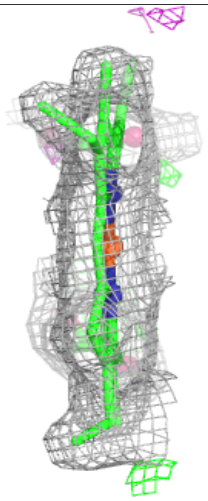


Electron density around HEC X 711:

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

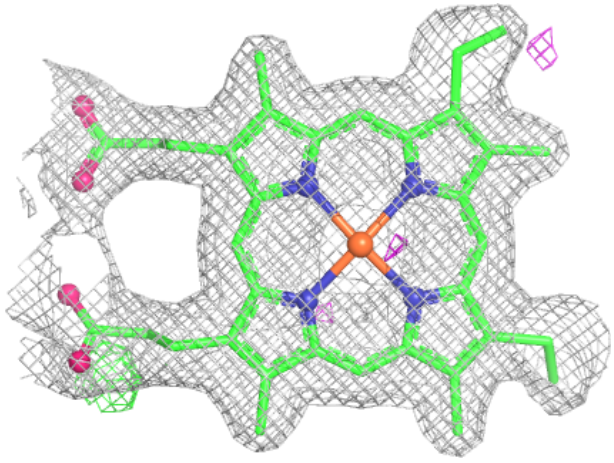


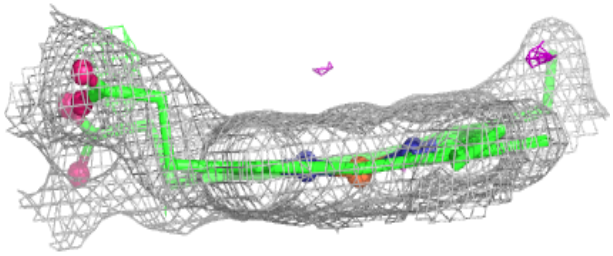


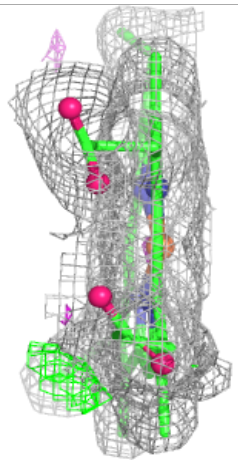


Electron density around HEC X 718:

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

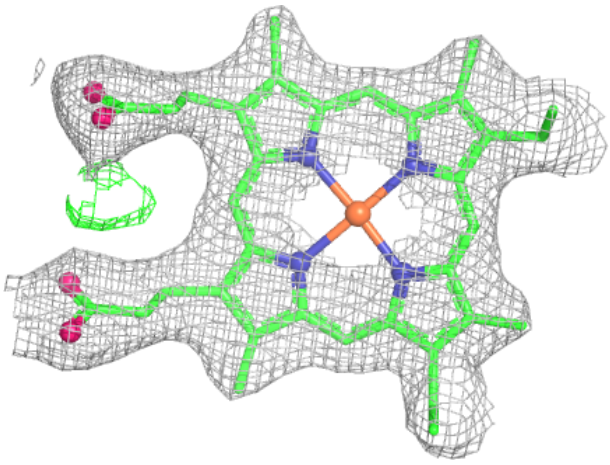


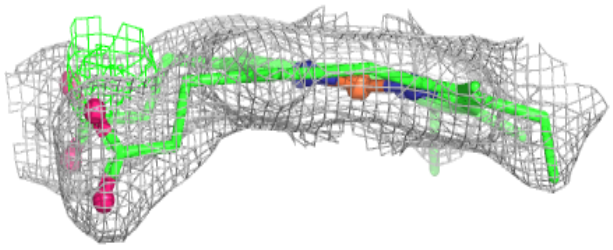


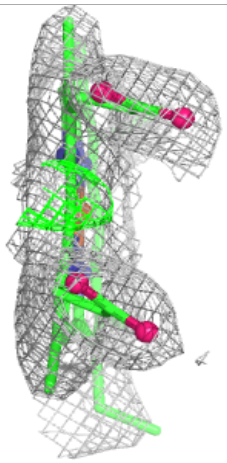


Electron density around HEC X 707:

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

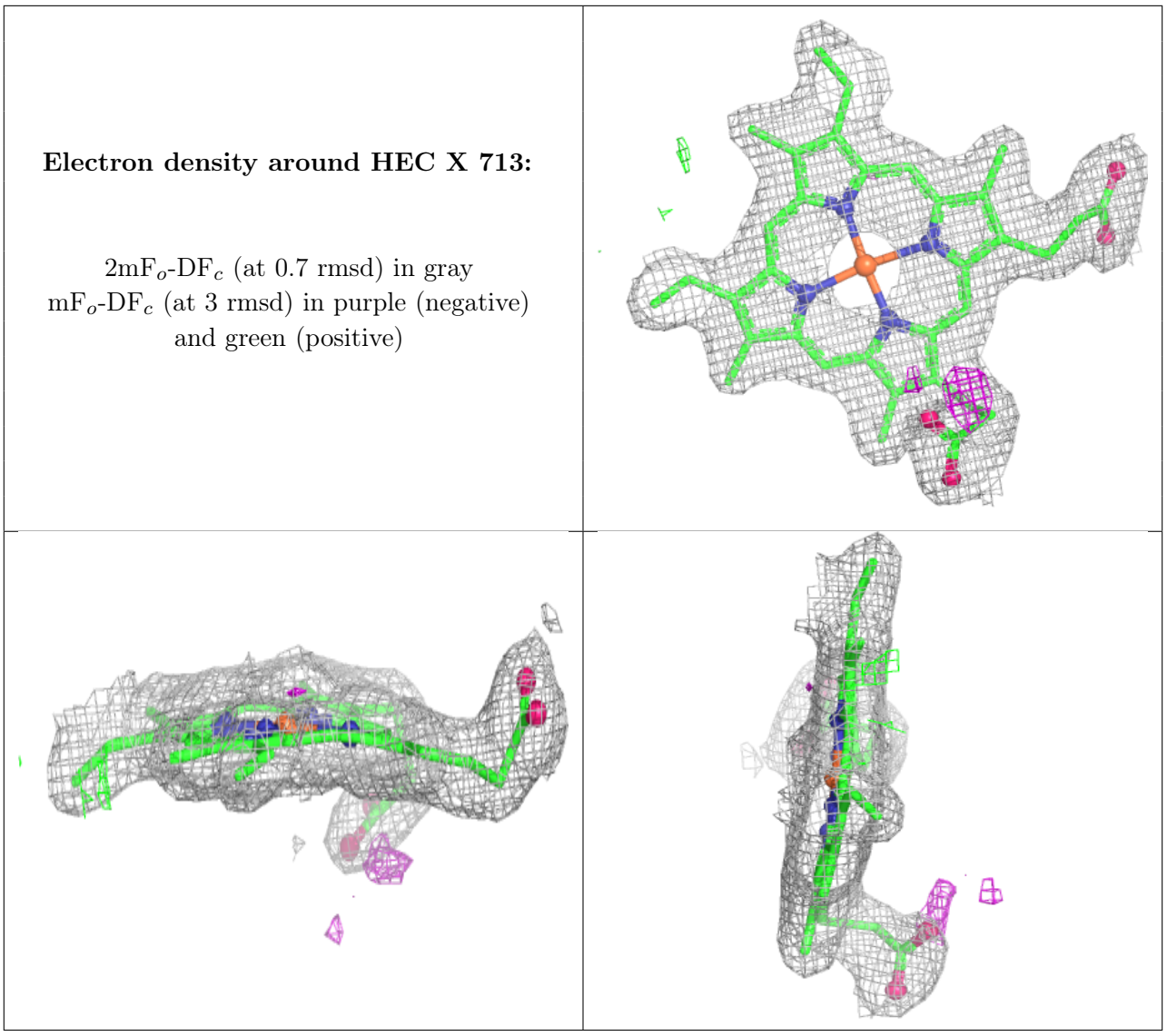






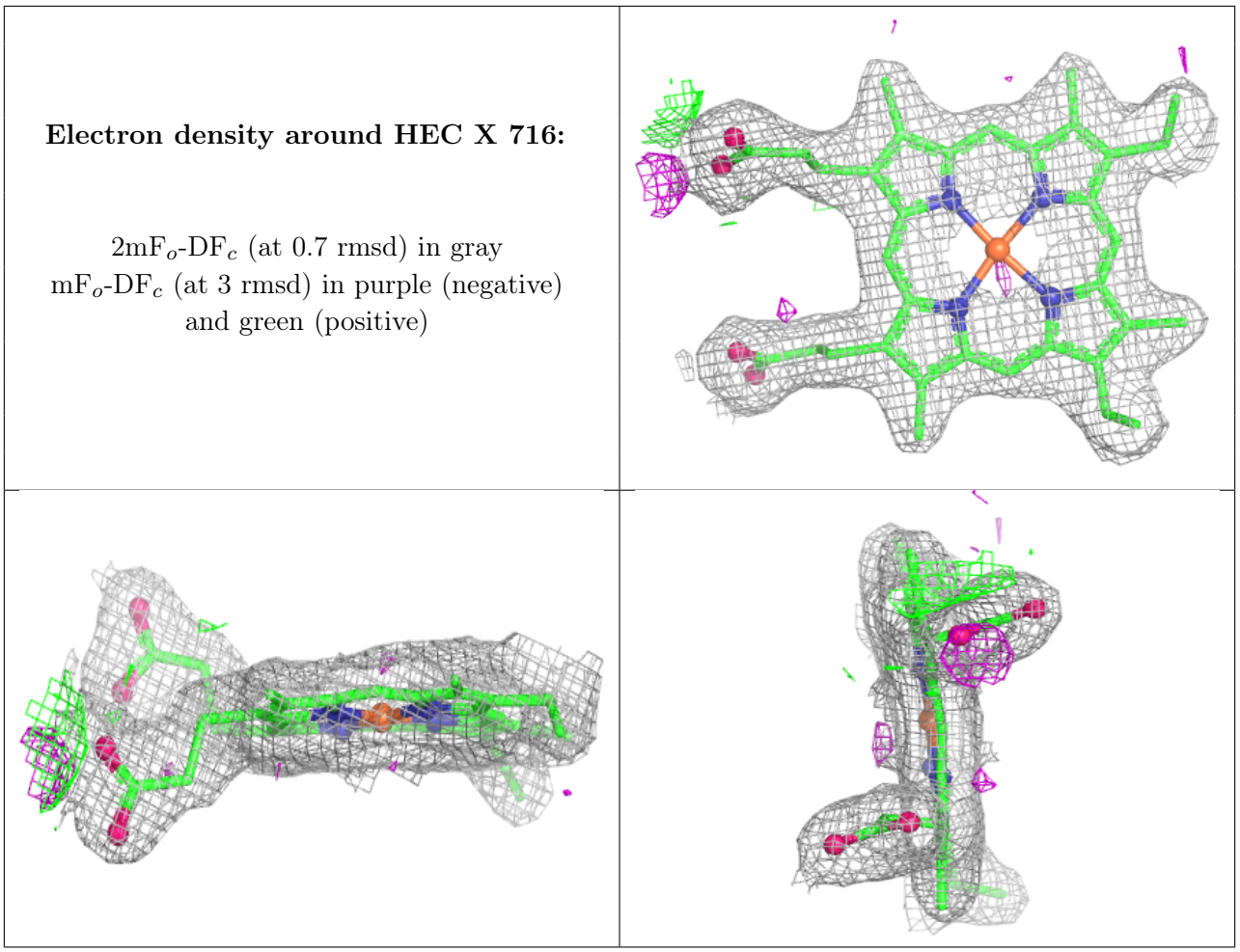
Electron density around HEC X 713:

$2mF_o$-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 X 716:

$2mF_o$-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.