wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2026 – 12:43 PM JST

PDB ID	:	9WTC / pdb_00009wtc
Title	:	Crystal structure of a selenate-soaked multiheme cytochrome c selenoprotein mutant (MccSep U325A)
Authors	:	Mihara, H.; Yoshizawa, T.; Izu, Y.; Inoue, M.; Aono, R.; Zhang, W.; Shibamoto, N.; Tobe, R.; Kurihara, T.; Matsumura, H.
Deposited on	:	2025-09-16
Resolution	:	2.20 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:

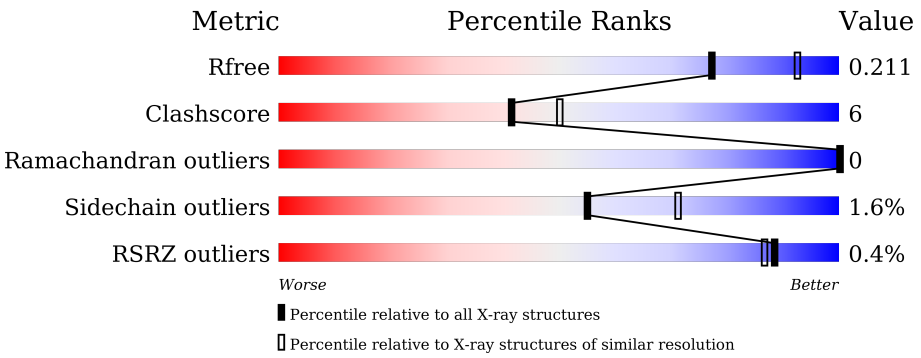
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	450	83% 10% 6%
1	B	450	79% 15% 6%
1	C	450	% 80% 13% 6%
1	D	450	82% 12% 6%

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	HEC	A	501	X	-	-	-
2	HEC	A	502	X	-	-	-
2	HEC	A	503	X	-	-	-
2	HEC	A	504	X	-	-	-
2	HEC	B	501	X	-	-	-
2	HEC	B	502	X	-	-	-
2	HEC	B	503	X	-	-	-
2	HEC	B	504	X	-	-	-
2	HEC	C	502	X	-	-	-
2	HEC	C	503	X	-	-	-
2	HEC	C	504	X	-	-	-
2	HEC	C	505	X	-	-	-
2	HEC	D	503	X	-	-	-
2	HEC	D	504	X	-	-	-
2	HEC	D	506	X	-	-	-
4	EDO	D	515	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c,Multiheme cytochrome c selenoprotein (MccSep).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3322	2084	573	637	28	0	9	0
1	B	422	3325	2091	572	634	28	0	9	0
1	C	422	3318	2079	574	637	28	0	6	0
1	D	422	3300	2070	571	631	28	0	5	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	linker	UNP Q748R4
A	326	PRO	-	linker	UNP Q748R4
A	327	THR	-	linker	UNP Q748R4
A	328	PRO	-	linker	UNP Q748R4
A	329	ASN	-	linker	UNP Q748R4
A	330	ARG	-	linker	UNP Q748R4
A	331	LEU	-	linker	UNP Q748R4
A	332	VAL	-	linker	UNP Q748R4
A	333	LEU	-	linker	UNP Q748R4
A	334	SER	-	linker	UNP Q748R4
A	335	VAL	-	linker	UNP Q748R4
A	336	ILE	-	linker	UNP Q748R4
A	337	ALA	-	linker	UNP Q748R4
A	338	LYS	-	linker	UNP Q748R4
A	339	THR	-	linker	UNP Q748R4
A	340	LYS	-	linker	UNP Q748R4
A	341	ASP	-	linker	UNP Q748R4
A	342	GLY	-	linker	UNP Q748R4
A	343	GLU	-	linker	UNP Q748R4
A	344	GLU	-	linker	UNP Q748R4
A	345	VAL	-	linker	UNP Q748R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	346	PHE	-	linker	UNP Q748R4
A	347	ASN	-	linker	UNP Q748R4
A	348	GLN	-	linker	UNP Q748R4
A	349	GLU	-	linker	UNP Q748R4
A	350	LYS	-	linker	UNP Q748R4
A	351	ILE	-	linker	UNP Q748R4
A	352	TYR	-	linker	UNP Q748R4
B	325	ALA	-	linker	UNP Q748R4
B	326	PRO	-	linker	UNP Q748R4
B	327	THR	-	linker	UNP Q748R4
B	328	PRO	-	linker	UNP Q748R4
B	329	ASN	-	linker	UNP Q748R4
B	330	ARG	-	linker	UNP Q748R4
B	331	LEU	-	linker	UNP Q748R4
B	332	VAL	-	linker	UNP Q748R4
B	333	LEU	-	linker	UNP Q748R4
B	334	SER	-	linker	UNP Q748R4
B	335	VAL	-	linker	UNP Q748R4
B	336	ILE	-	linker	UNP Q748R4
B	337	ALA	-	linker	UNP Q748R4
B	338	LYS	-	linker	UNP Q748R4
B	339	THR	-	linker	UNP Q748R4
B	340	LYS	-	linker	UNP Q748R4
B	341	ASP	-	linker	UNP Q748R4
B	342	GLY	-	linker	UNP Q748R4
B	343	GLU	-	linker	UNP Q748R4
B	344	GLU	-	linker	UNP Q748R4
B	345	VAL	-	linker	UNP Q748R4
B	346	PHE	-	linker	UNP Q748R4
B	347	ASN	-	linker	UNP Q748R4
B	348	GLN	-	linker	UNP Q748R4
B	349	GLU	-	linker	UNP Q748R4
B	350	LYS	-	linker	UNP Q748R4
B	351	ILE	-	linker	UNP Q748R4
B	352	TYR	-	linker	UNP Q748R4
C	325	ALA	-	linker	UNP Q748R4
C	326	PRO	-	linker	UNP Q748R4
C	327	THR	-	linker	UNP Q748R4
C	328	PRO	-	linker	UNP Q748R4
C	329	ASN	-	linker	UNP Q748R4
C	330	ARG	-	linker	UNP Q748R4
C	331	LEU	-	linker	UNP Q748R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	VAL	-	linker	UNP Q748R4
C	333	LEU	-	linker	UNP Q748R4
C	334	SER	-	linker	UNP Q748R4
C	335	VAL	-	linker	UNP Q748R4
C	336	ILE	-	linker	UNP Q748R4
C	337	ALA	-	linker	UNP Q748R4
C	338	LYS	-	linker	UNP Q748R4
C	339	THR	-	linker	UNP Q748R4
C	340	LYS	-	linker	UNP Q748R4
C	341	ASP	-	linker	UNP Q748R4
C	342	GLY	-	linker	UNP Q748R4
C	343	GLU	-	linker	UNP Q748R4
C	344	GLU	-	linker	UNP Q748R4
C	345	VAL	-	linker	UNP Q748R4
C	346	PHE	-	linker	UNP Q748R4
C	347	ASN	-	linker	UNP Q748R4
C	348	GLN	-	linker	UNP Q748R4
C	349	GLU	-	linker	UNP Q748R4
C	350	LYS	-	linker	UNP Q748R4
C	351	ILE	-	linker	UNP Q748R4
C	352	TYR	-	linker	UNP Q748R4
D	325	ALA	-	linker	UNP Q748R4
D	326	PRO	-	linker	UNP Q748R4
D	327	THR	-	linker	UNP Q748R4
D	328	PRO	-	linker	UNP Q748R4
D	329	ASN	-	linker	UNP Q748R4
D	330	ARG	-	linker	UNP Q748R4
D	331	LEU	-	linker	UNP Q748R4
D	332	VAL	-	linker	UNP Q748R4
D	333	LEU	-	linker	UNP Q748R4
D	334	SER	-	linker	UNP Q748R4
D	335	VAL	-	linker	UNP Q748R4
D	336	ILE	-	linker	UNP Q748R4
D	337	ALA	-	linker	UNP Q748R4
D	338	LYS	-	linker	UNP Q748R4
D	339	THR	-	linker	UNP Q748R4
D	340	LYS	-	linker	UNP Q748R4
D	341	ASP	-	linker	UNP Q748R4
D	342	GLY	-	linker	UNP Q748R4
D	343	GLU	-	linker	UNP Q748R4
D	344	GLU	-	linker	UNP Q748R4
D	345	VAL	-	linker	UNP Q748R4

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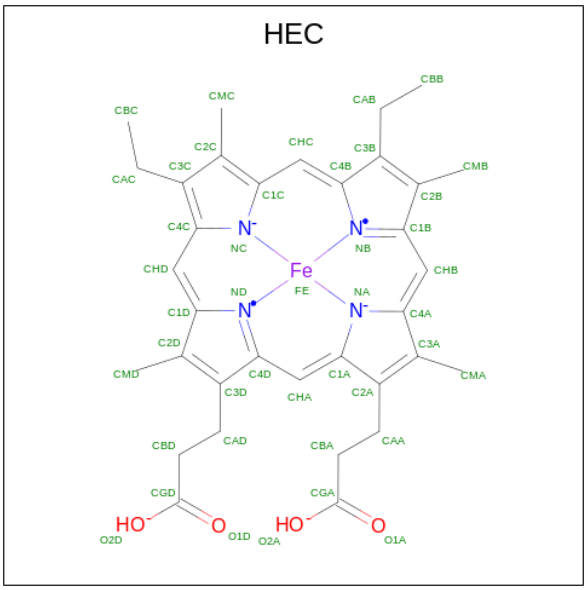
Chain	Residue	Modelled	Actual	Comment	Reference
D	346	PHE	-	linker	UNP Q748R4
D	347	ASN	-	linker	UNP Q748R4
D	348	GLN	-	linker	UNP Q748R4
D	349	GLU	-	linker	UNP Q748R4
D	350	LYS	-	linker	UNP Q748R4
D	351	ILE	-	linker	UNP Q748R4
D	352	TYR	-	linker	UNP Q748R4

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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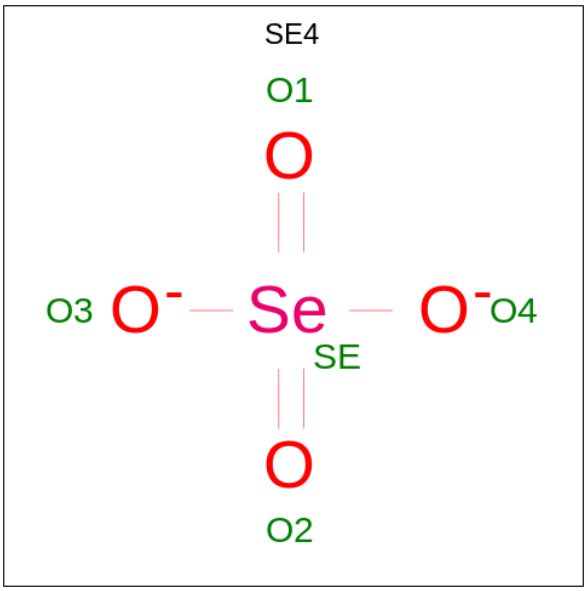
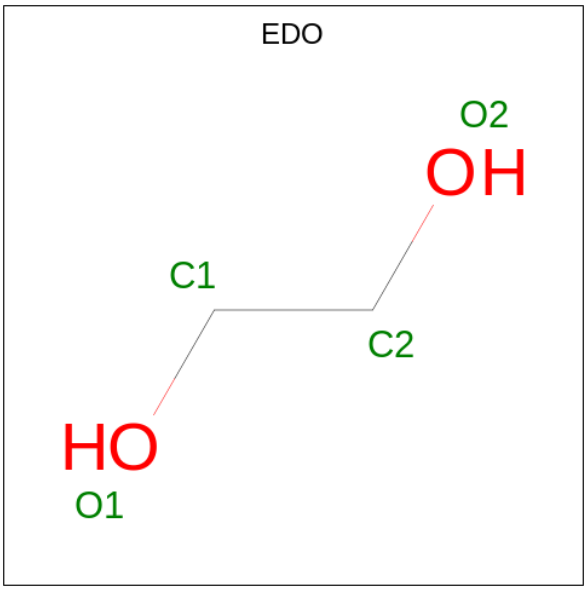
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total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

- Molecule 3 is SELENATE ION (CCD ID: SE4) (formula: O_4Se) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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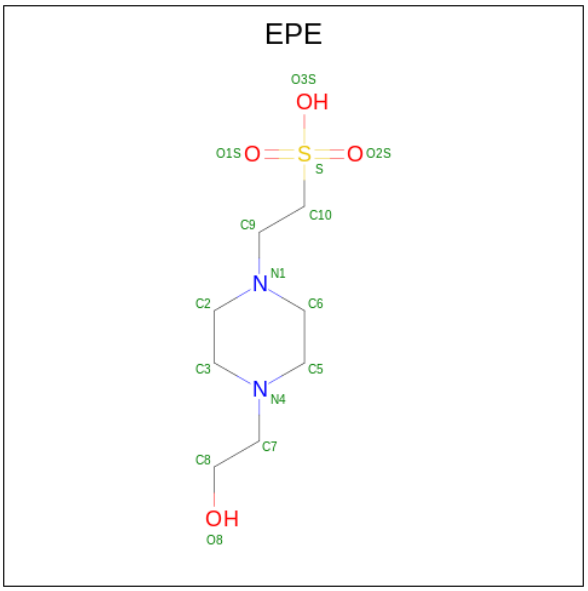
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	15	8	2	4	1	0	0

- Molecule 6 is water.

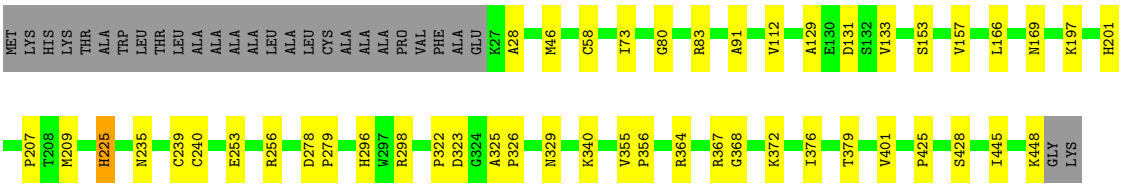
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	254	254	254	0	0
			Total	O		
6	B	253	253	253	0	0
			Total	O		
6	C	162	162	162	0	0
			Total	O		
6	D	247	247	247	0	0

3 Residue-property plots (i)

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

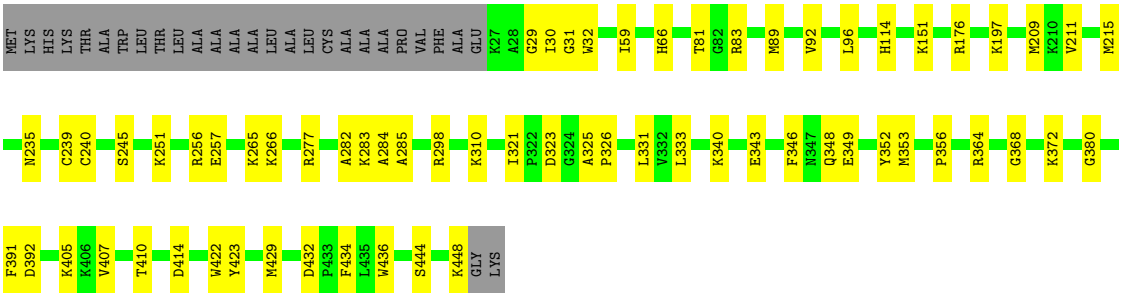
• Molecule 1: Cytochrome c,Multiheme cytochrome c selenoprotein (MccSep)

Chain A:



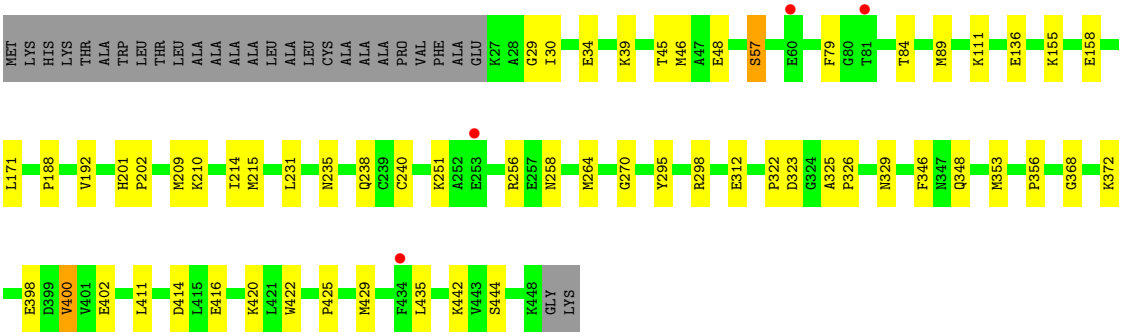
• Molecule 1: Cytochrome c,Multiheme cytochrome c selenoprotein (MccSep)

Chain B:



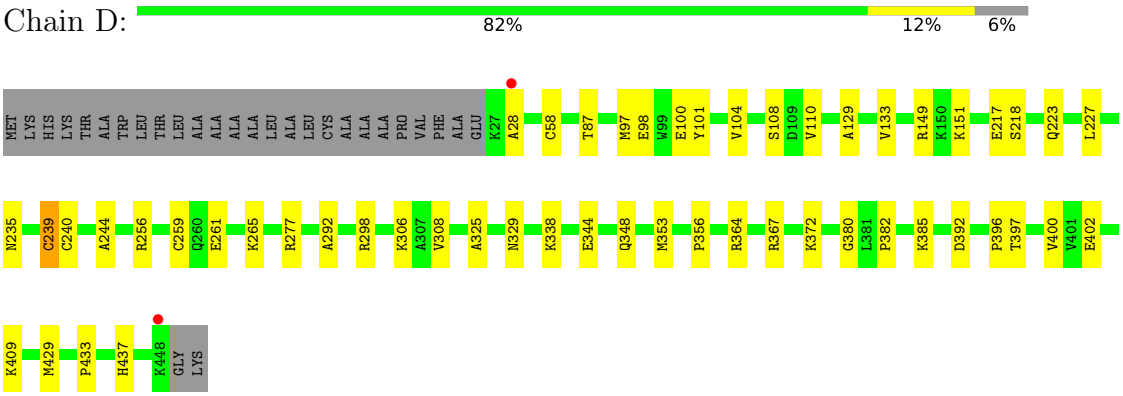
• Molecule 1: Cytochrome c,Multiheme cytochrome c selenoprotein (MccSep)

Chain C:



• Molecule 1: Cytochrome c,Multiheme cytochrome c selenoprotein (MccSep)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.39Å 123.62Å 116.64Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	44.06 – 2.20 44.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.06-2.20) 99.9 (44.06-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.214 0.166 , 0.211	Depositor DCC
R_{free} test set	5986 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15244	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CSD, SE4, EDO, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.32	0/3413	0.49	0/4611
1	B	0.32	0/3421	0.52	0/4623
1	C	0.30	0/3394	0.49	0/4585
1	D	0.33	0/3382	0.49	0/4569
All	All	0.32	0/13610	0.50	0/18388

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	HIS	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	A	3322	0	3243	36	0
1	B	3325	0	3250	56	0
1	C	3318	0	3222	45	0
1	D	3300	0	3218	40	0
2	A	215	0	150	4	0
2	B	215	0	151	1	0
2	C	215	0	150	7	0
2	D	215	0	150	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	32	0	48	8	0
4	B	48	0	72	11	0
4	C	40	0	60	5	0
4	D	48	0	72	14	0
5	B	15	0	17	3	0
6	A	254	0	0	8	0
6	B	253	0	0	13	0
6	C	162	0	0	6	0
6	D	247	0	0	9	0
All	All	15244	0	13803	180	0

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

The worst 5 of 180 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240[B]:CYS:SG	6:B:606:HOH:O	2.16	1.04
1:B:176:ARG:HH22	4:B:519:EDO:H11	1.28	0.99
1:C:240[B]:CYS:SG	6:C:606:HOH:O	2.21	0.98
1:D:240[B]:CYS:SG	6:D:605:HOH:O	2.21	0.98
1:D:397:THR:H	4:D:517:EDO:H22	1.40	0.85

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/450 (95%)	407 (95%)	21 (5%)	0	100	100
1	B	428/450 (95%)	410 (96%)	18 (4%)	0	100	100
1	C	425/450 (94%)	407 (96%)	18 (4%)	0	100	100
1	D	424/450 (94%)	408 (96%)	16 (4%)	0	100	100
All	All	1705/1800 (95%)	1632 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/368 (98%)	356 (99%)	4 (1%)	65	79
1	B	360/368 (98%)	353 (98%)	7 (2%)	50	66
1	C	357/368 (97%)	353 (99%)	4 (1%)	65	79
1	D	356/368 (97%)	349 (98%)	7 (2%)	48	64
All	All	1433/1472 (97%)	1411 (98%)	22 (2%)	55	73

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	400	VAL
1	D	110	VAL
1	D	108	SER

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Mol	Chain	Res	Type
1	D	235	ASN
1	B	235	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	189	GLN
1	C	258	ASN
1	C	348	GLN
1	A	441	GLN
1	A	388	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSD	B	239	2,1	3,7,8	1.08	0	1,8,10	0.82	0
1	CSD	D	239	2,1	3,7,8	1.09	0	1,8,10	3.06	1 (100%)
1	CSD	C	239	2,1	3,7,8	1.04	0	1,8,10	0.34	0
1	CSD	A	239	2,1	3,7,8	0.99	0	1,8,10	0.82	0

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
1	CSD	B	239	2,1	-	1/2/6/8	-
1	CSD	D	239	2,1	-	0/2/6/8	-
1	CSD	C	239	2,1	-	1/2/6/8	-
1	CSD	A	239	2,1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	239	CSD	OD1-SG-CB	3.06	111.37	105.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	239	CSD	CA-CB-SG-OD1
1	B	239	CSD	CA-CB-SG-OD1
1	C	239	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	239	CSD	2	0
1	D	239	CSD	2	0
1	A	239	CSD	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

67 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	D	514	-	3,3,3	0.53	0	2,2,2	0.19	0
2	HEC	D	503	1	50,50,50	1.51	7 (14%)	68,82,82	1.55	11 (16%)
4	EDO	C	512	-	3,3,3	0.45	0	2,2,2	0.39	0
3	SE4	B	506	-	4,4,4	0.55	0	1,6,6	2.72	1 (100%)
4	EDO	B	514	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	D	512	-	3,3,3	0.50	0	2,2,2	0.25	0
2	HEC	A	501	1	50,50,50	1.38	9 (18%)	68,82,82	1.31	9 (13%)
4	EDO	D	516	-	3,3,3	0.51	0	2,2,2	0.36	0
4	EDO	D	518	-	3,3,3	0.66	0	2,2,2	0.17	0
2	HEC	B	503	1	50,50,50	1.47	7 (14%)	68,82,82	1.39	9 (13%)
4	EDO	B	511	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	C	515	-	3,3,3	0.60	0	2,2,2	0.15	0
4	EDO	D	515	-	3,3,3	0.46	0	2,2,2	0.19	0
4	EDO	A	510	-	3,3,3	0.67	0	2,2,2	0.07	0
4	EDO	A	512	-	3,3,3	0.41	0	2,2,2	0.43	0
4	EDO	B	518	-	3,3,3	0.45	0	2,2,2	0.14	0
4	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EPE	B	507	-	15,15,15	0.79	1 (6%)	18,20,20	2.10	7 (38%)
4	EDO	D	517	-	3,3,3	0.53	0	2,2,2	0.37	0
2	HEC	C	506	1	50,50,50	1.49	9 (18%)	68,82,82	1.36	9 (13%)
4	EDO	D	509	-	3,3,3	0.56	0	2,2,2	0.18	0
4	EDO	B	515	-	3,3,3	0.46	0	2,2,2	0.48	0
2	HEC	D	504	1	50,50,50	1.35	4 (8%)	68,82,82	1.19	5 (7%)
2	HEC	D	507	1	50,50,50	1.49	8 (16%)	68,82,82	1.39	12 (17%)
2	HEC	D	506	1	50,50,50	1.41	8 (16%)	68,82,82	1.23	8 (11%)
2	HEC	B	502	1	50,50,50	1.35	6 (12%)	68,82,82	1.19	8 (11%)
2	HEC	A	504	1	50,50,50	1.43	7 (14%)	68,82,82	1.21	7 (10%)
2	HEC	A	505	1	50,50,50	1.47	8 (16%)	68,82,82	1.44	10 (14%)
4	EDO	B	517	-	3,3,3	0.77	0	2,2,2	0.20	0
4	EDO	C	514	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	C	508	-	3,3,3	0.52	0	2,2,2	0.32	0
4	EDO	B	510	-	3,3,3	0.52	0	2,2,2	0.37	0
4	EDO	C	513	-	3,3,3	0.53	0	2,2,2	0.29	0
4	EDO	A	508	-	3,3,3	0.51	0	2,2,2	0.51	0
4	EDO	D	510	-	3,3,3	0.54	0	2,2,2	0.47	0
4	EDO	D	513	-	3,3,3	0.54	0	2,2,2	0.20	0
2	HEC	C	504	1	50,50,50	1.41	7 (14%)	68,82,82	1.31	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	C	505	1	50,50,50	1.41	5 (10%)	68,82,82	1.34	9 (13%)
4	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.36	0
2	HEC	C	503	1	50,50,50	1.44	7 (14%)	68,82,82	1.37	10 (14%)
2	HEC	D	505	1	50,50,50	1.49	9 (18%)	68,82,82	1.26	8 (11%)
4	EDO	B	516	-	3,3,3	0.48	0	2,2,2	0.38	0
3	SE4	C	507	-	4,4,4	0.57	0	1,6,6	2.68	1 (100%)
3	SE4	D	508	-	4,4,4	0.55	0	1,6,6	2.04	1 (100%)
4	EDO	A	514	-	3,3,3	0.52	0	2,2,2	0.09	0
4	EDO	B	513	-	3,3,3	0.59	0	2,2,2	0.21	0
4	EDO	C	509	-	3,3,3	0.56	0	2,2,2	0.22	0
2	HEC	B	505	1	50,50,50	1.42	6 (12%)	68,82,82	1.26	9 (13%)
4	EDO	B	512	-	3,3,3	0.49	0	2,2,2	0.60	0
2	HEC	C	502	1	50,50,50	1.53	7 (14%)	68,82,82	1.53	13 (19%)
4	EDO	D	511	-	3,3,3	0.58	0	2,2,2	0.05	0
4	EDO	B	519	-	3,3,3	0.78	0	2,2,2	0.45	0
3	SE4	A	506	-	4,4,4	0.59	0	1,6,6	2.84	1 (100%)
4	EDO	A	513	-	3,3,3	0.54	0	2,2,2	0.14	0
4	EDO	C	510	-	3,3,3	0.45	0	2,2,2	0.27	0
4	EDO	A	507	-	3,3,3	0.52	0	2,2,2	0.39	0
4	EDO	B	509	-	3,3,3	0.36	0	2,2,2	0.51	0
4	EDO	A	511	-	3,3,3	0.60	0	2,2,2	0.38	0
4	EDO	C	501	-	3,3,3	0.51	0	2,2,2	0.36	0
2	HEC	B	504	1	50,50,50	1.36	6 (12%)	68,82,82	1.21	3 (4%)
4	EDO	C	511	-	3,3,3	0.36	0	2,2,2	0.35	0
2	HEC	A	503	1	50,50,50	1.40	8 (16%)	68,82,82	1.16	5 (7%)
4	EDO	C	516	-	3,3,3	0.57	0	2,2,2	0.41	0
2	HEC	A	502	1	50,50,50	1.44	6 (12%)	68,82,82	1.34	7 (10%)
4	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.42	0
4	EDO	D	502	-	3,3,3	0.43	0	2,2,2	0.58	0
2	HEC	B	501	1	50,50,50	1.49	8 (16%)	68,82,82	1.44	10 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	514	-	-	1/1/1/1	-
2	HEC	D	503	1	1/1/3/7	8/14/54/54	-
4	EDO	C	512	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	514	-	-	1/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-
2	HEC	A	501	1	1/1/3/7	6/14/54/54	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	D	518	-	-	1/1/1/1	-
2	HEC	B	503	1	1/1/3/7	4/14/54/54	-
4	EDO	B	511	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
5	EPE	B	507	-	-	4/9/19/19	0/1/1/1
4	EDO	D	517	-	-	1/1/1/1	-
2	HEC	C	506	1	-	7/14/54/54	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-
2	HEC	D	504	1	1/1/3/7	7/14/54/54	-
2	HEC	D	507	1	-	9/14/54/54	-
2	HEC	D	506	1	1/1/3/7	4/14/54/54	-
2	HEC	B	502	1	1/1/3/7	7/14/54/54	-
2	HEC	A	504	1	1/1/3/7	6/14/54/54	-
2	HEC	A	505	1	-	9/14/54/54	-
4	EDO	B	517	-	-	0/1/1/1	-
4	EDO	C	514	-	-	0/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
2	HEC	C	504	1	1/1/3/7	6/14/54/54	-
2	HEC	C	505	1	1/1/3/7	4/14/54/54	-
4	EDO	A	509	-	-	0/1/1/1	-
2	HEC	C	503	1	1/1/3/7	7/14/54/54	-
2	HEC	D	505	1	-	4/14/54/54	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
2	HEC	B	505	1	-	9/14/54/54	-
4	EDO	B	512	-	-	1/1/1/1	-
2	HEC	C	502	1	1/1/3/7	6/14/54/54	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	A	507	-	-	0/1/1/1	-
4	EDO	B	509	-	-	0/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	501	-	-	0/1/1/1	-
2	HEC	B	504	1	1/1/3/7	4/14/54/54	-
4	EDO	C	511	-	-	1/1/1/1	-
2	HEC	A	503	1	1/1/3/7	6/14/54/54	-
4	EDO	C	516	-	-	0/1/1/1	-
2	HEC	A	502	1	1/1/3/7	7/14/54/54	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
2	HEC	B	501	1	1/1/3/7	6/14/54/54	-

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	505	HEC	FE-NC	4.47	2.10	1.95
2	B	503	HEC	FE-ND	4.36	2.08	1.94
2	D	503	HEC	FE-ND	4.17	2.07	1.94
2	B	501	HEC	FE-NB	4.05	2.07	1.94
2	C	502	HEC	CBB-CAB	-4.01	1.33	1.51

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	HEC	CBD-CAD-C3D	-4.33	100.58	112.63
5	B	507	EPE	C5-N4-C3	4.21	118.31	108.83
2	D	505	HEC	CBC-CAC-C3C	3.72	122.68	112.43
5	B	507	EPE	C7-N4-C3	3.66	120.60	111.23
5	B	507	EPE	C7-N4-C5	3.62	120.48	111.23

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA
2	A	502	HEC	NA
2	A	503	HEC	NA
2	A	504	HEC	NA
2	B	501	HEC	NA

5 of 142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	HEC	C2C-C3C-CAC-CBC
2	C	502	HEC	C2C-C3C-CAC-CBC
2	C	503	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C2C-C3C-CAC-CBC
2	B	501	HEC	C2C-C3C-CAC-CBC

There are no ring outliers.

35 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	512	EDO	1	0
4	D	516	EDO	1	0
4	D	515	EDO	4	0
4	A	510	EDO	1	0
4	A	512	EDO	1	0
4	B	518	EDO	1	0
4	B	508	EDO	2	0
5	B	507	EPE	3	0
4	D	517	EDO	3	0
2	C	506	HEC	1	0
4	D	509	EDO	1	0
4	B	515	EDO	2	0
2	D	504	HEC	1	0
2	D	507	HEC	1	0
2	A	505	HEC	1	0
4	C	508	EDO	1	0
4	B	510	EDO	2	0
4	A	508	EDO	1	0
2	C	504	HEC	1	0
2	C	503	HEC	2	0
4	A	514	EDO	1	0
4	B	513	EDO	1	0
4	C	509	EDO	1	0
2	B	505	HEC	1	0

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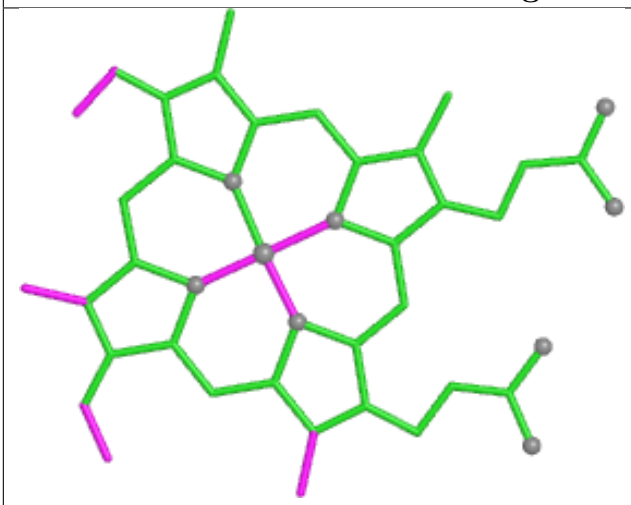
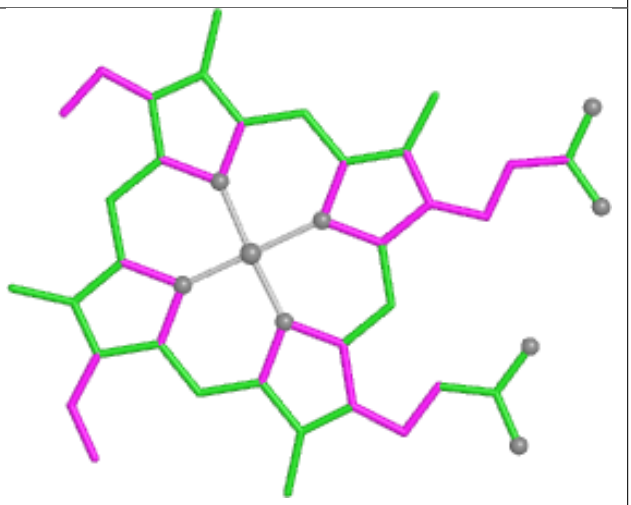
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	HEC	4	0
4	D	511	EDO	1	0
4	B	519	EDO	2	0
4	A	513	EDO	2	0
4	B	509	EDO	1	0
4	A	511	EDO	2	0
4	C	501	EDO	1	0
4	C	511	EDO	1	0
2	A	502	HEC	3	0
4	D	501	EDO	3	0
4	D	502	EDO	1	0

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

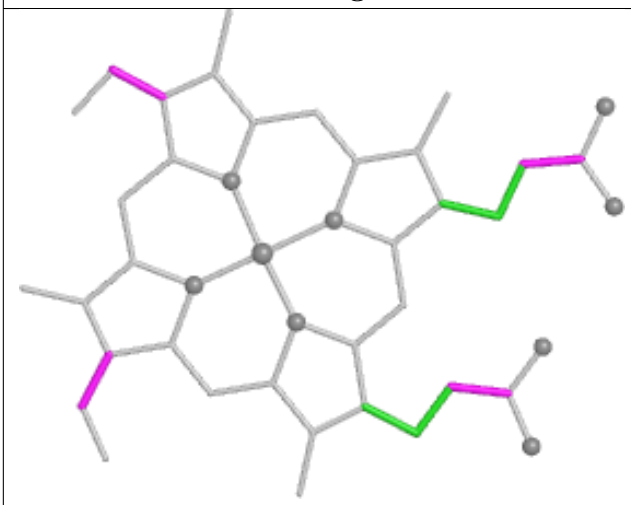
Ligand HEC D 503



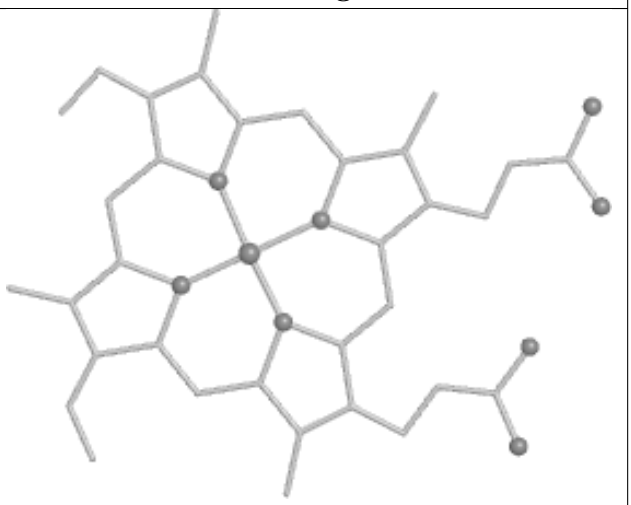
Bond lengths



Bond angles

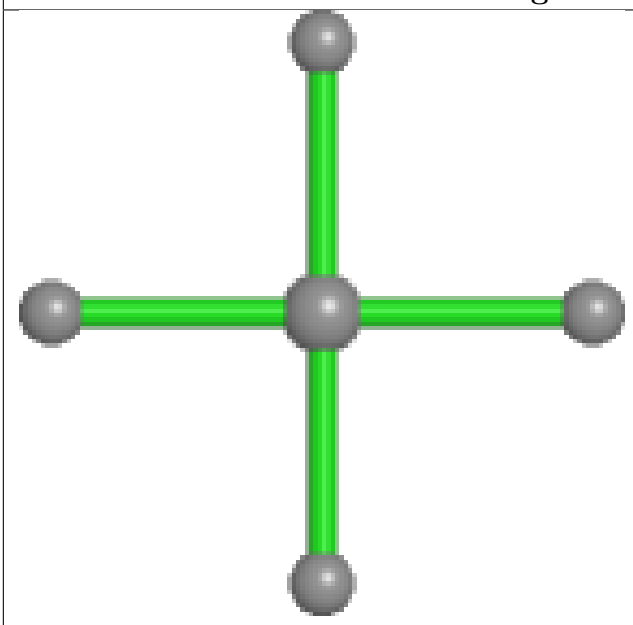


Torsions

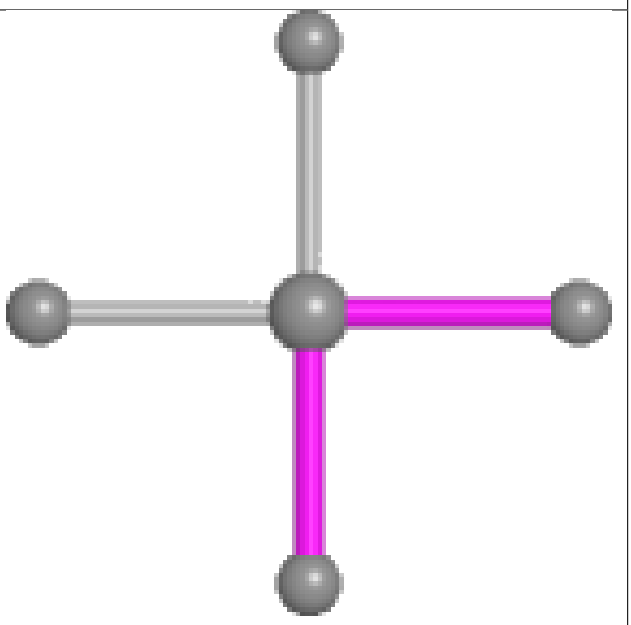


Rings

Ligand SE4 B 506



Bond lengths



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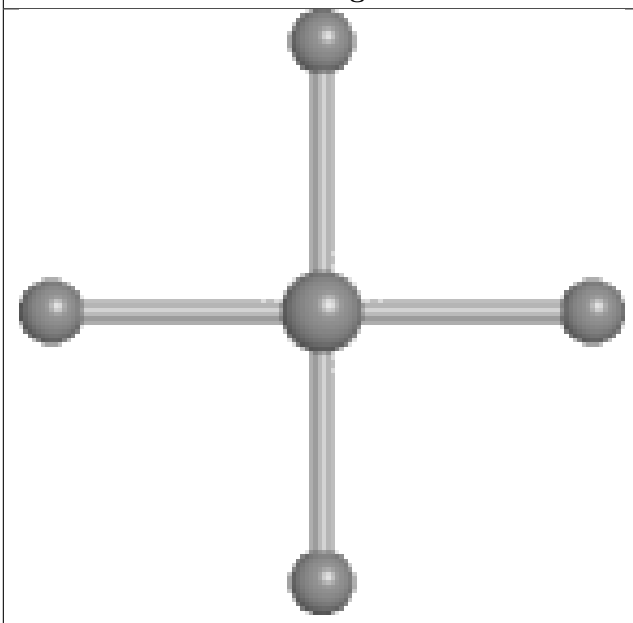
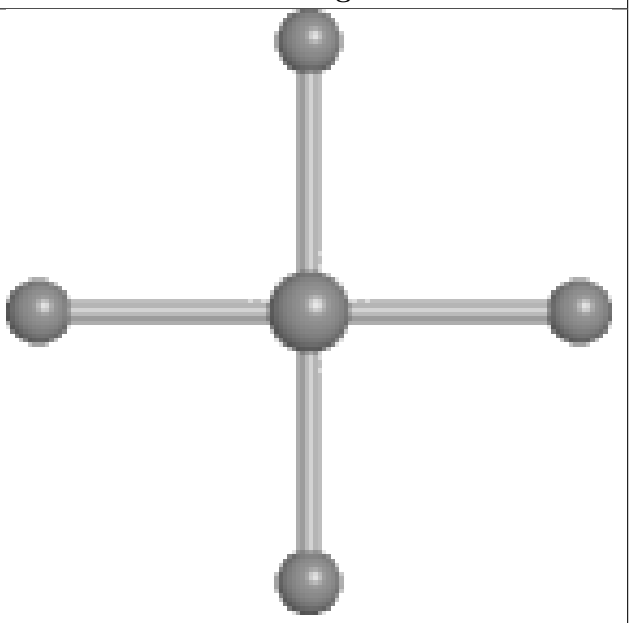
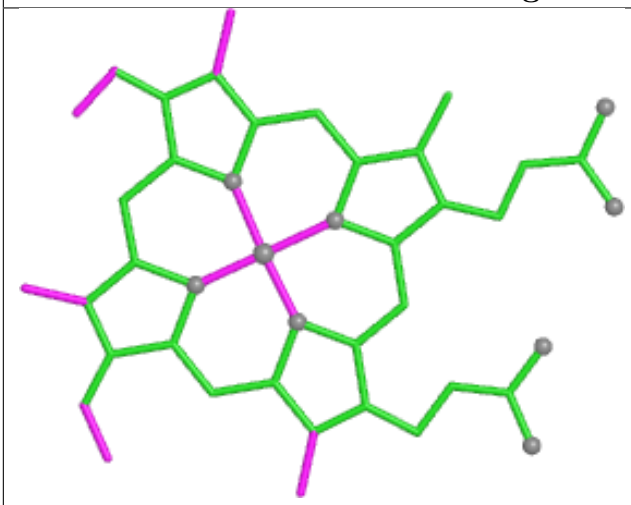


Torsions

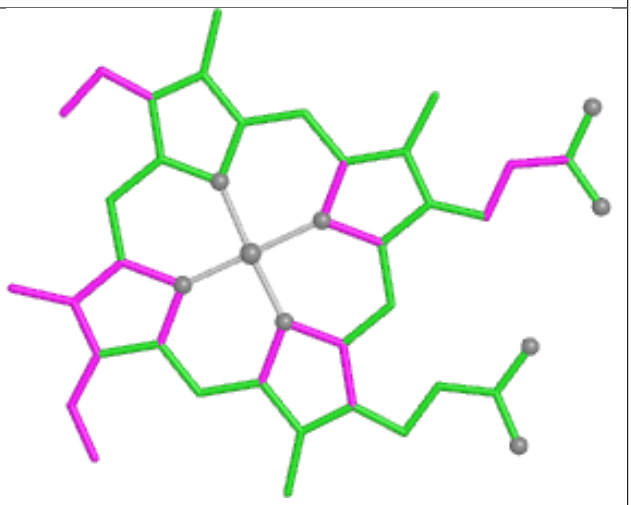


Rings

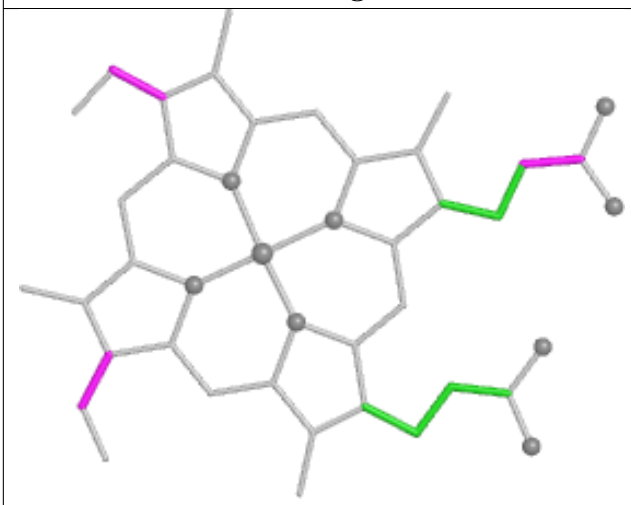
Ligand HEC A 501



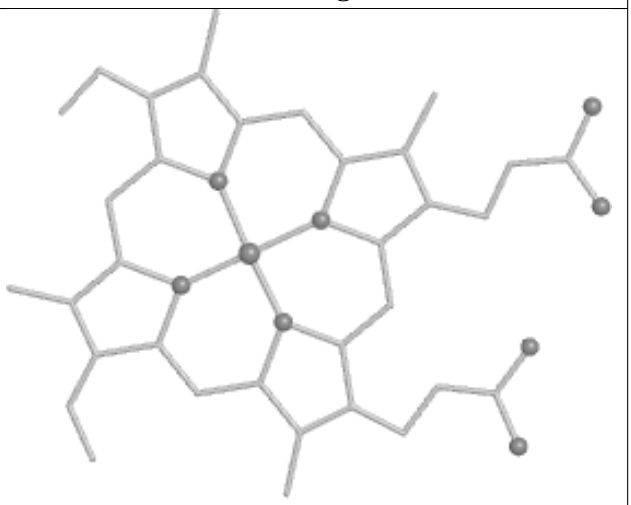
Bond lengths



Bond angles

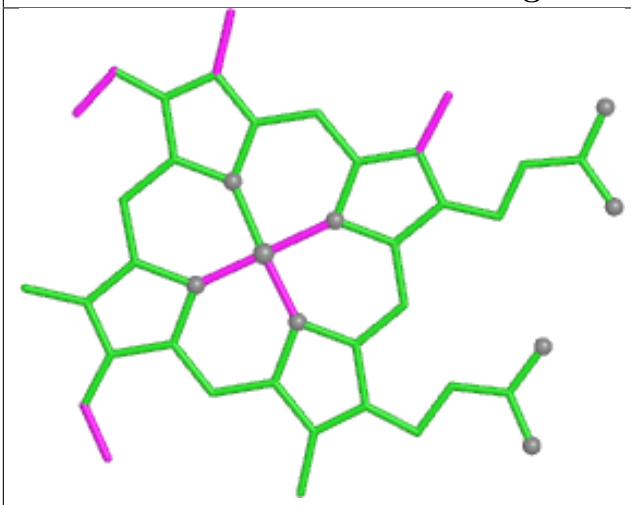


Torsions



Rings

Ligand HEC B 503



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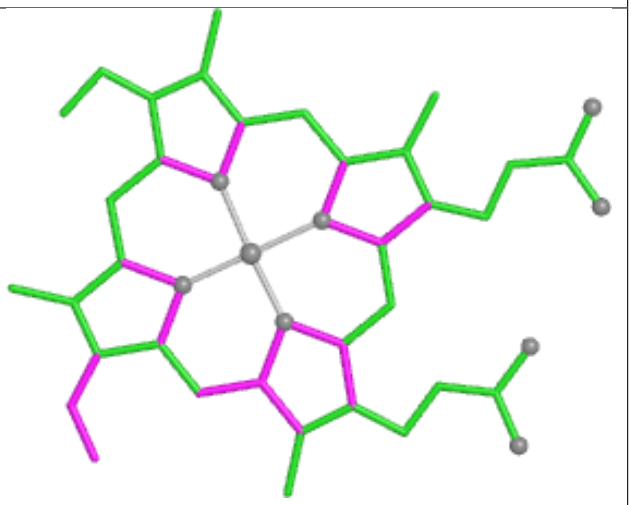
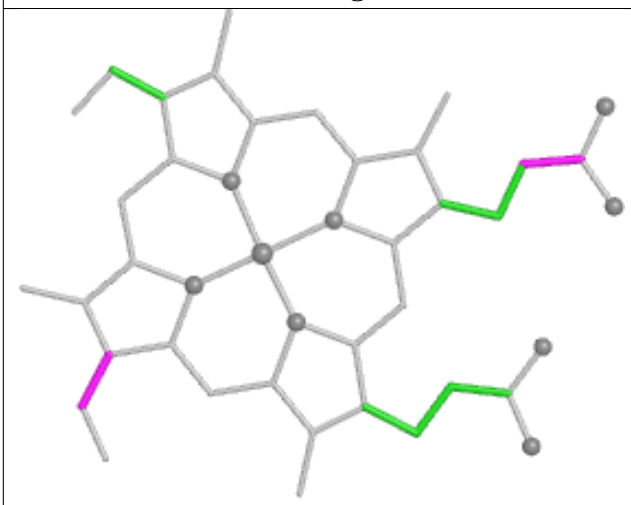
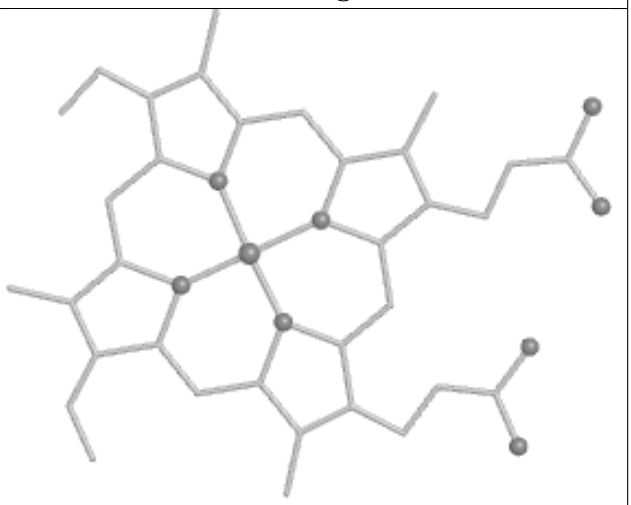


Bond angles

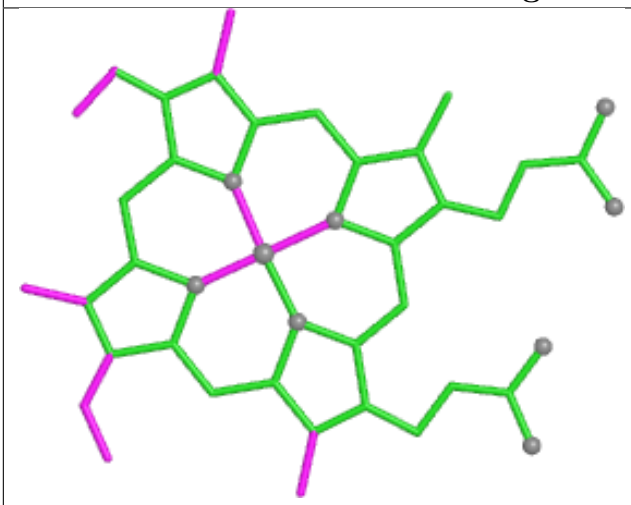


Torsions



Rings

Ligand HEC C 506



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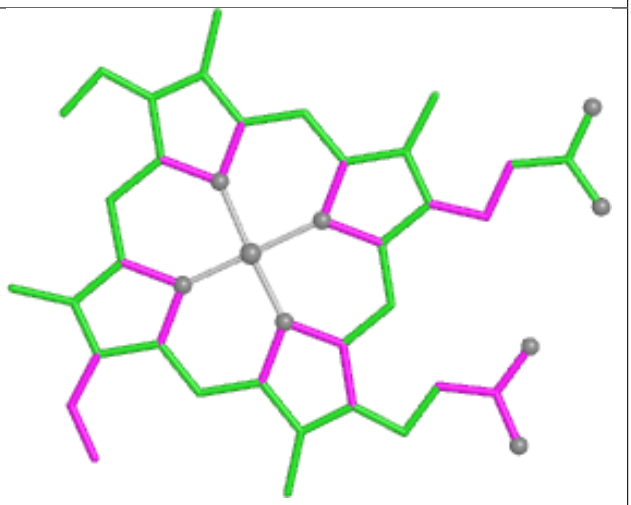

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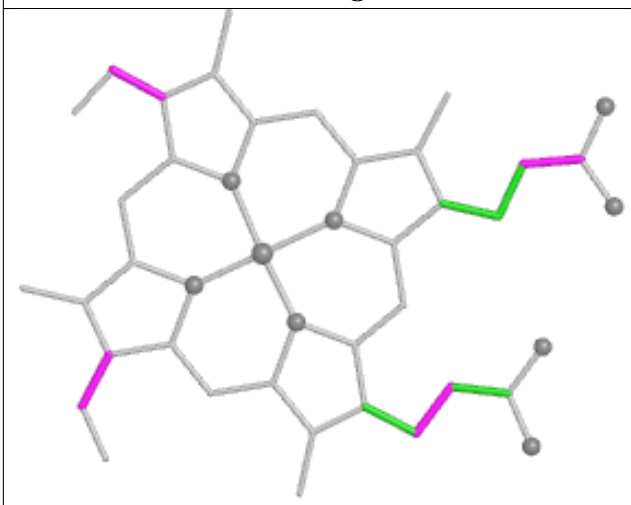

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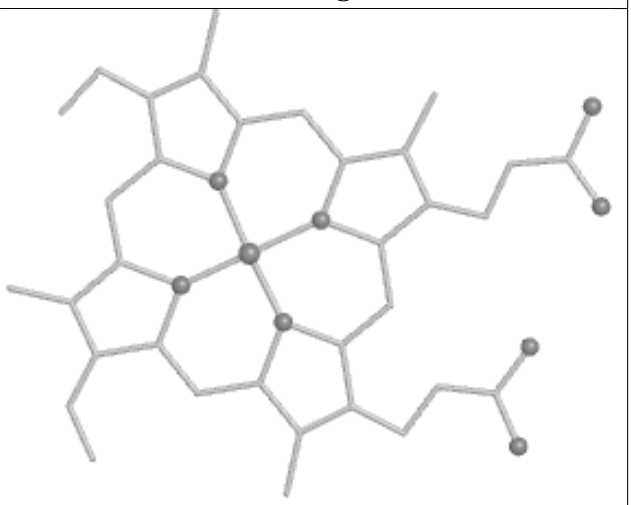

Rings

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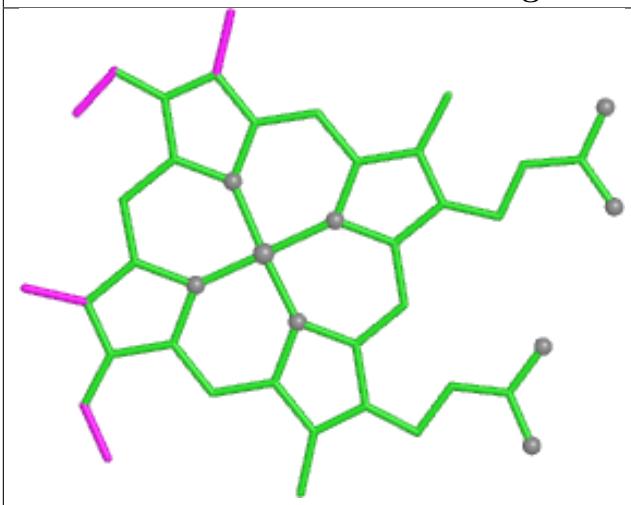

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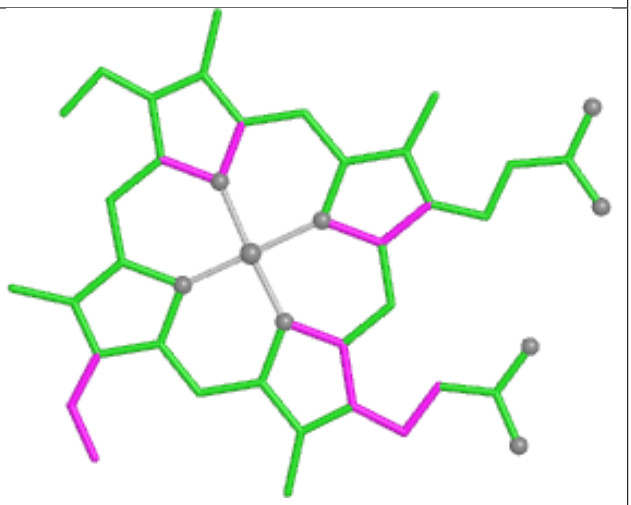

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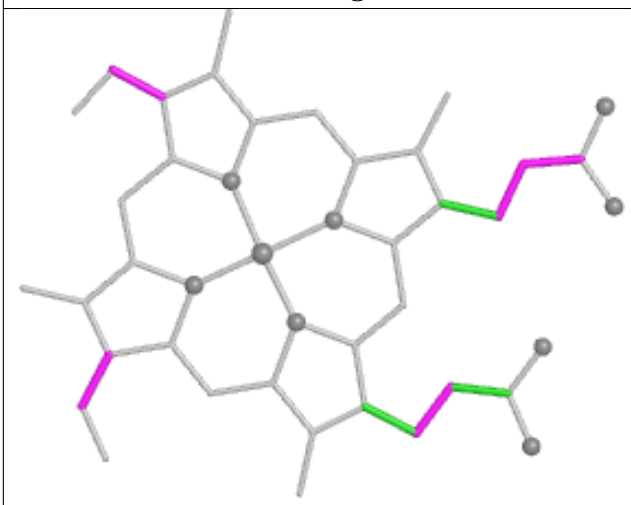

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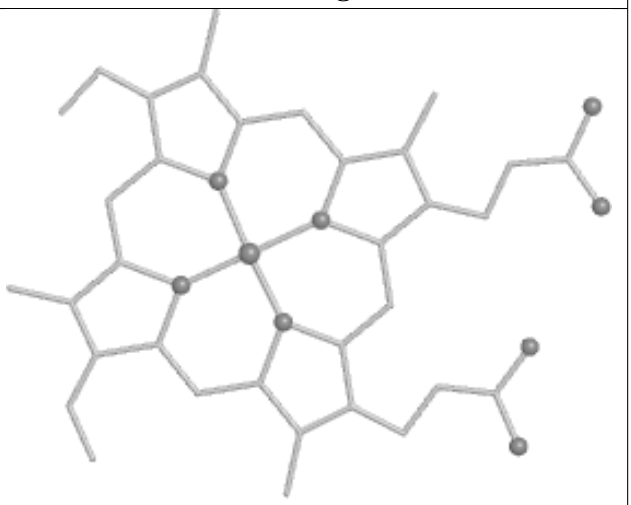

Rings

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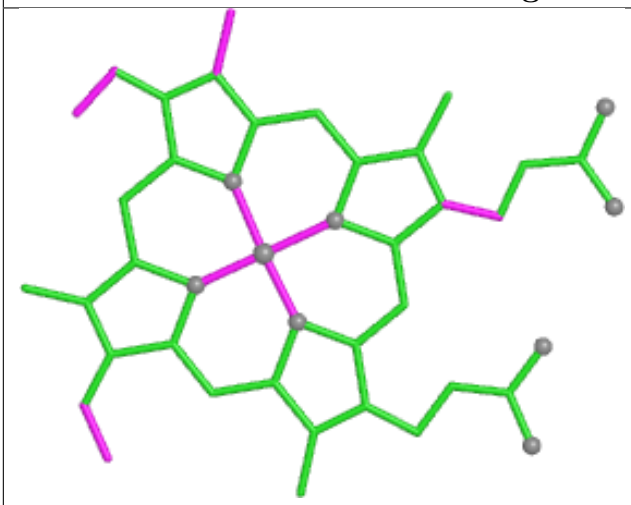

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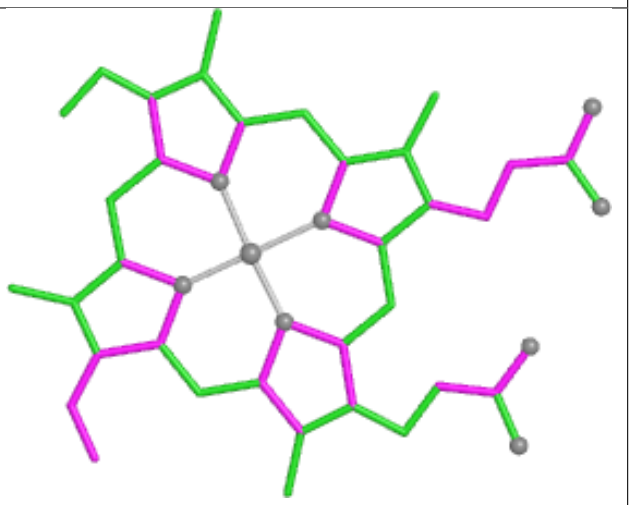

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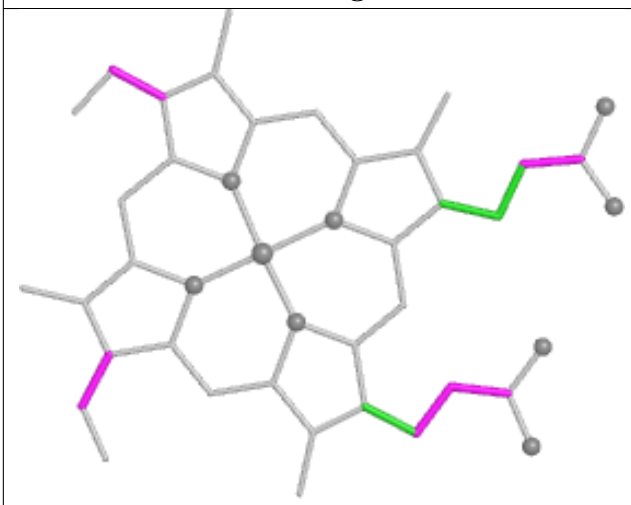

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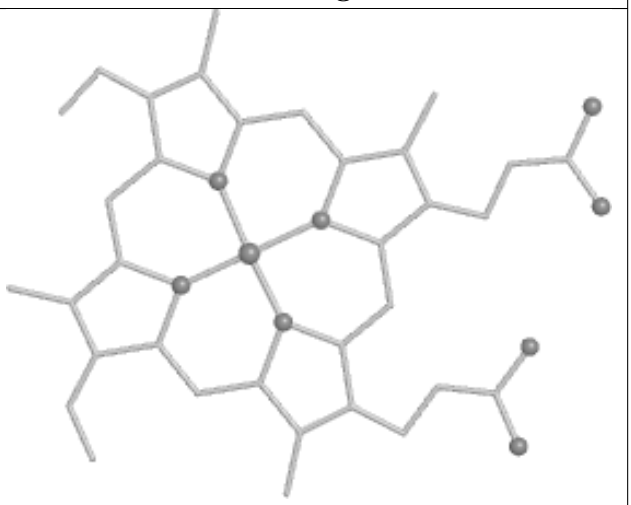

Rings

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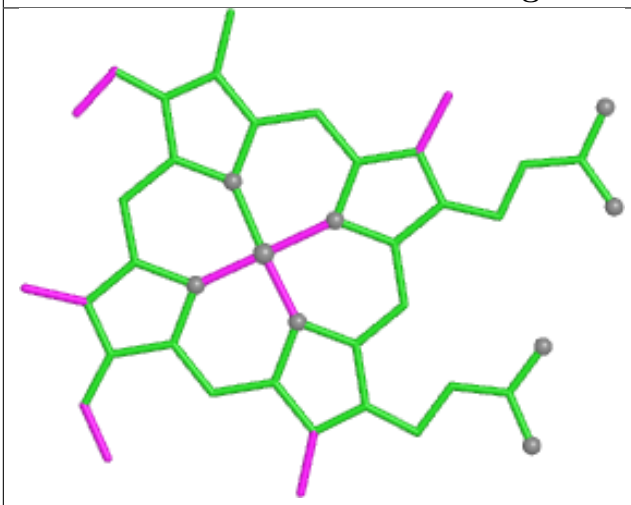

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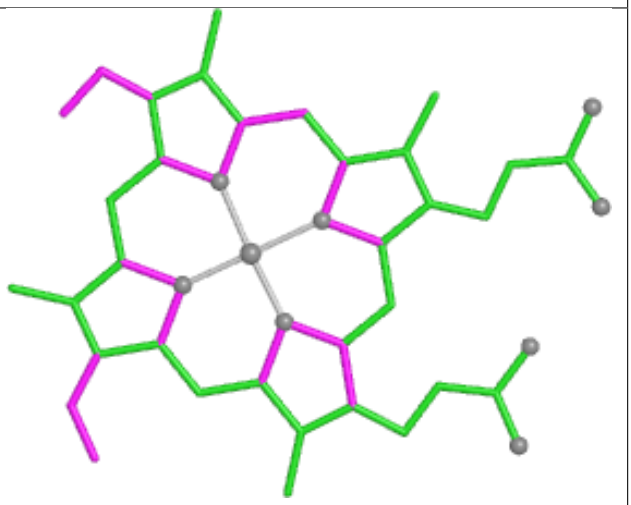

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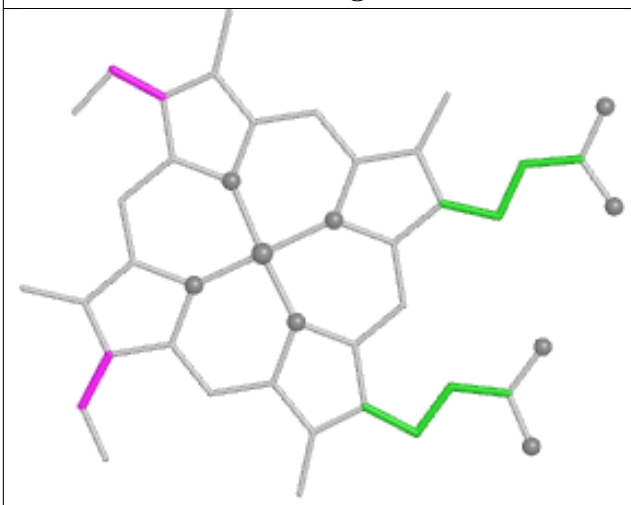

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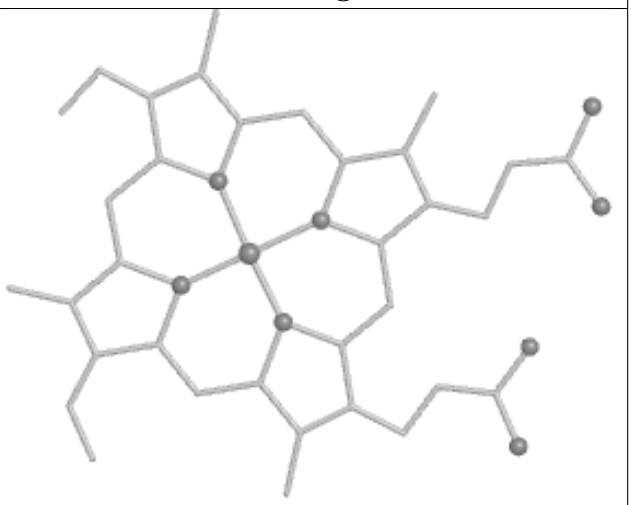
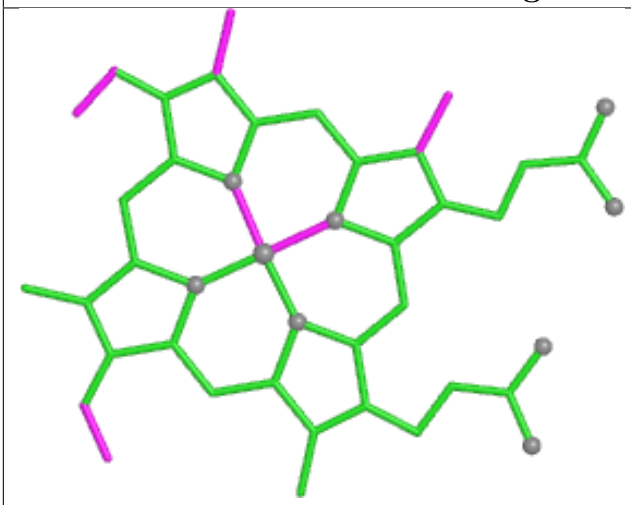


Rings

Ligand HEC B 502



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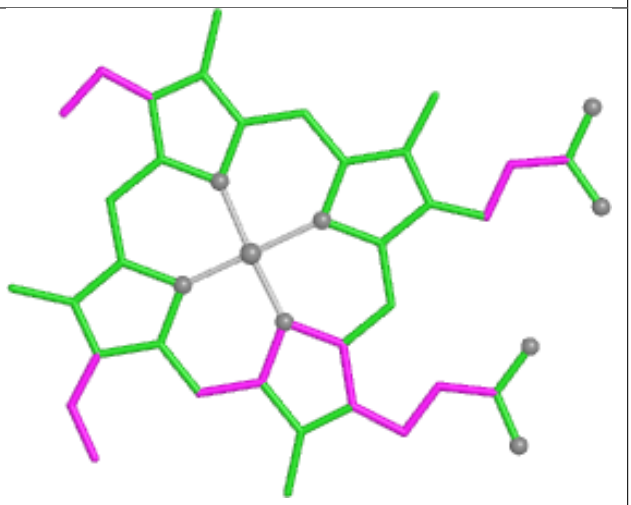
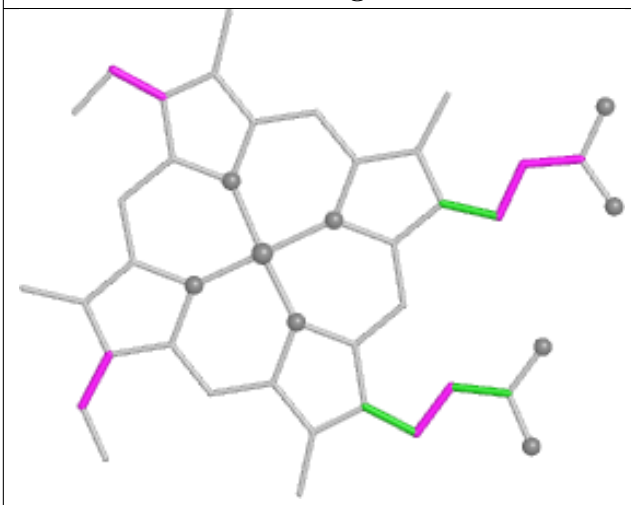


Bond angles



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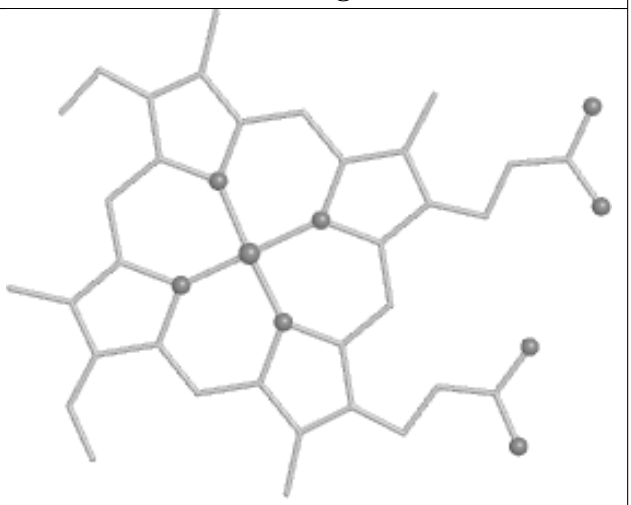
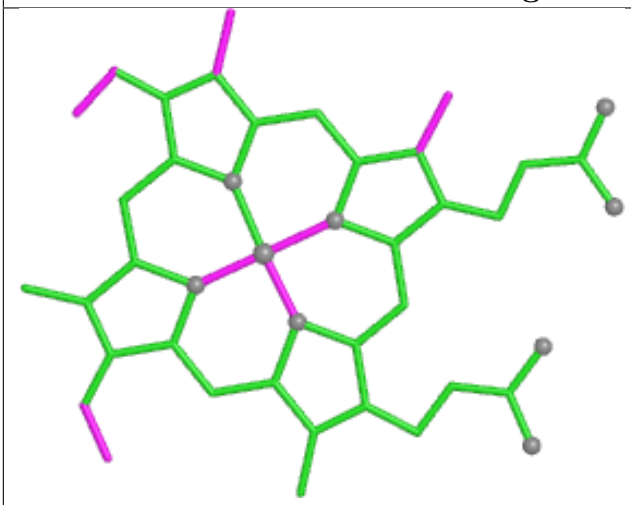


Rings

Ligand HEC A 504



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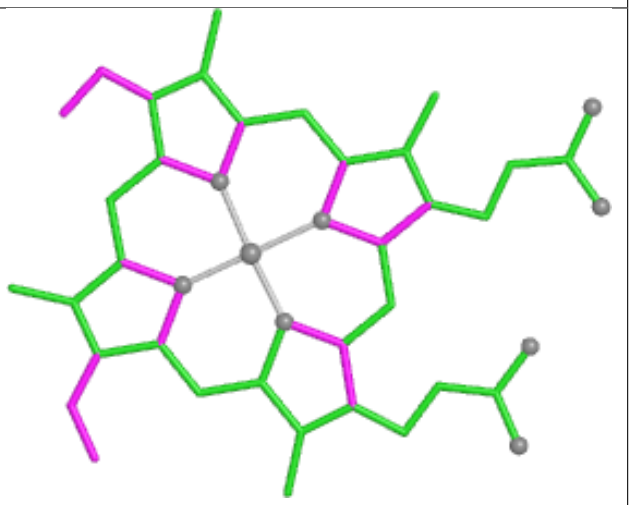
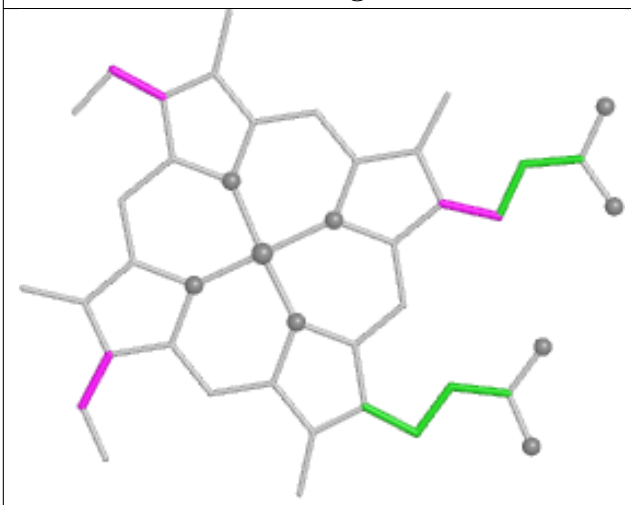


Bond angles



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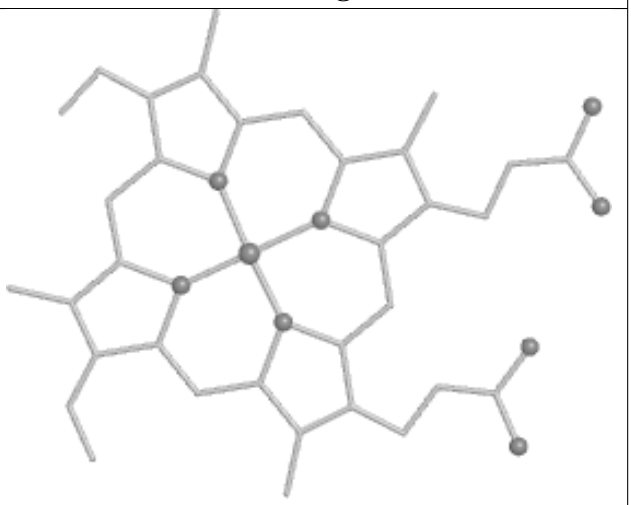
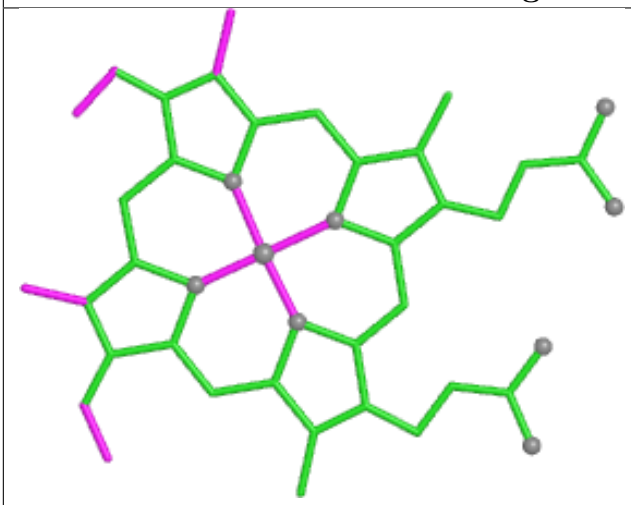


Rings

Ligand HEC A 505



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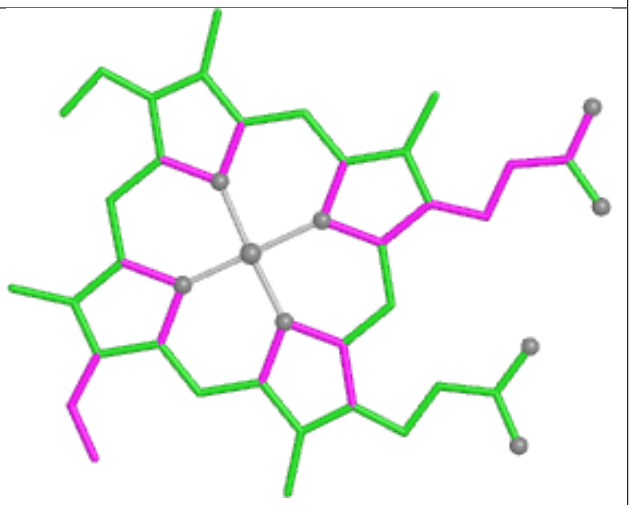
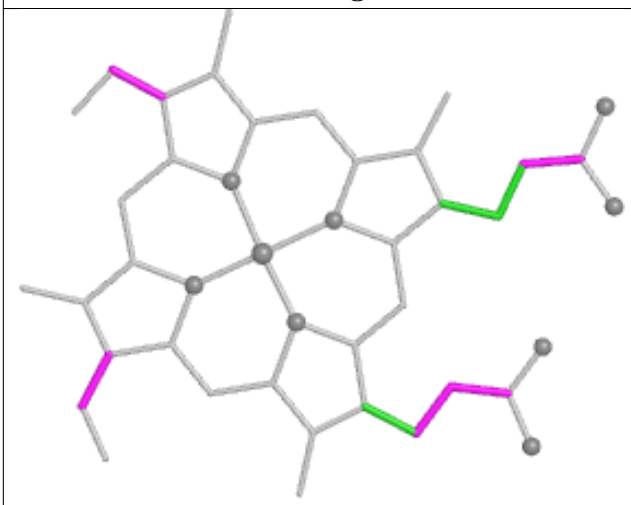


Bond angles



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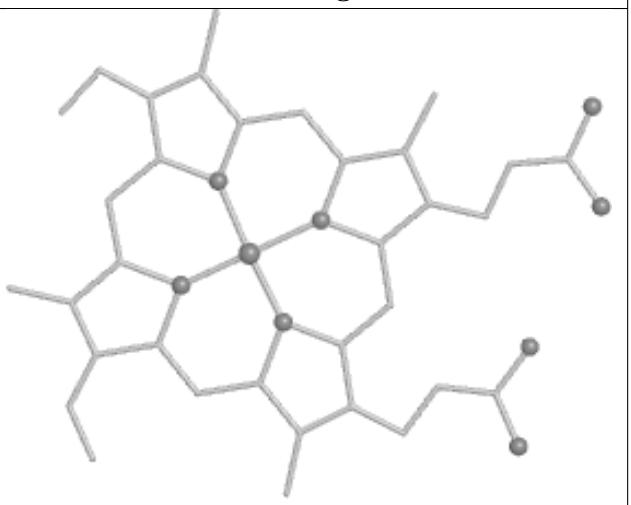
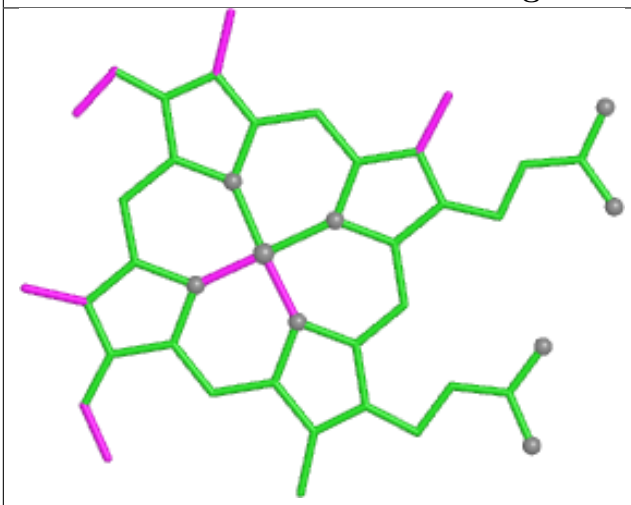


Rings

Ligand HEC C 504



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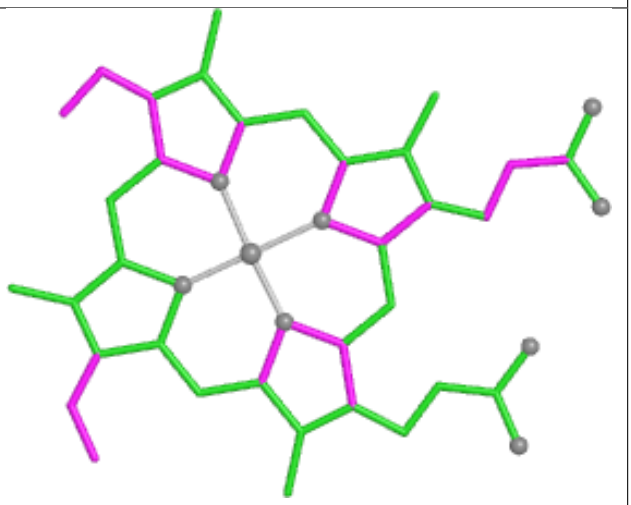
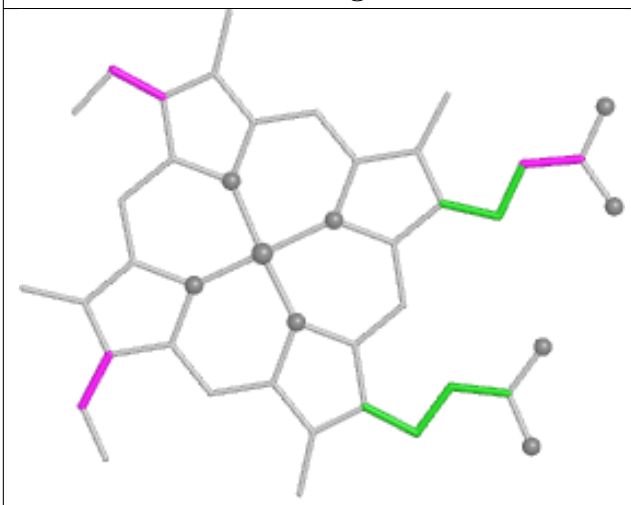
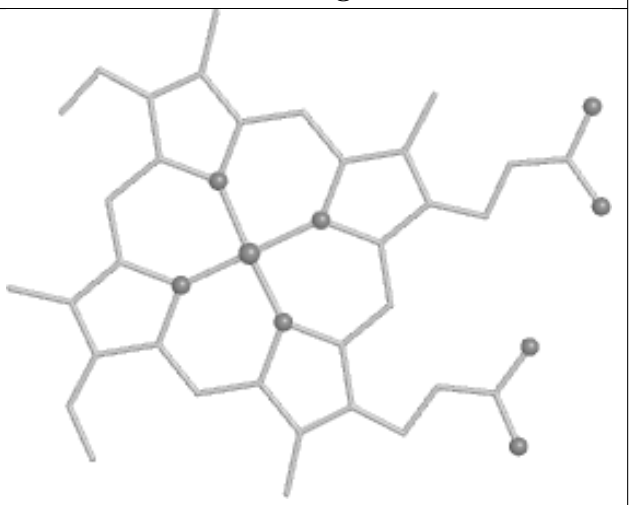


Bond angles

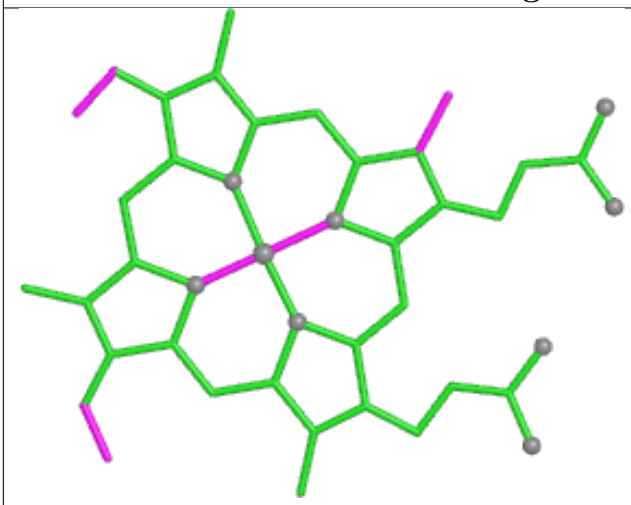


Torsions



Rings

Ligand HEC C 505



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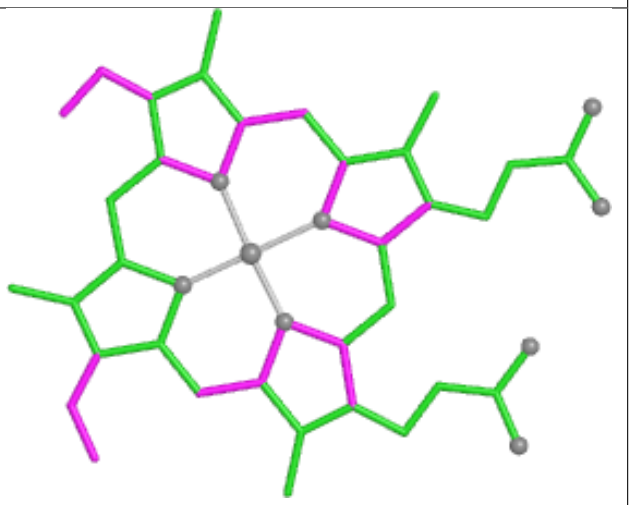
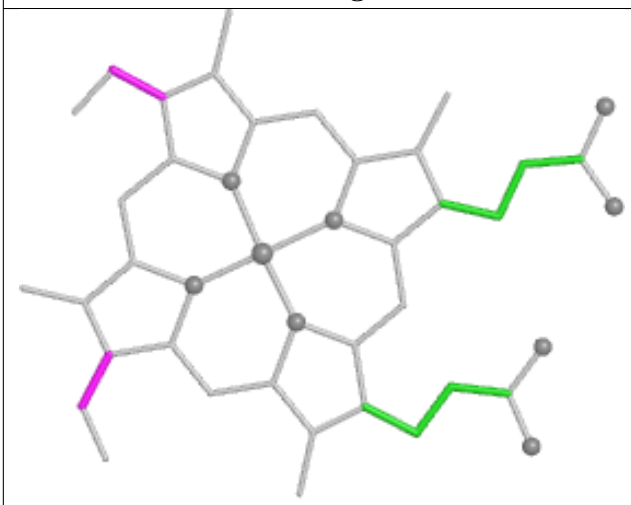
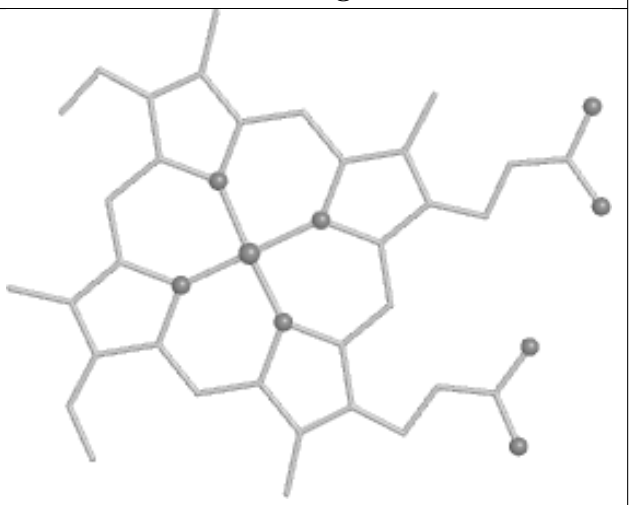


Bond angles

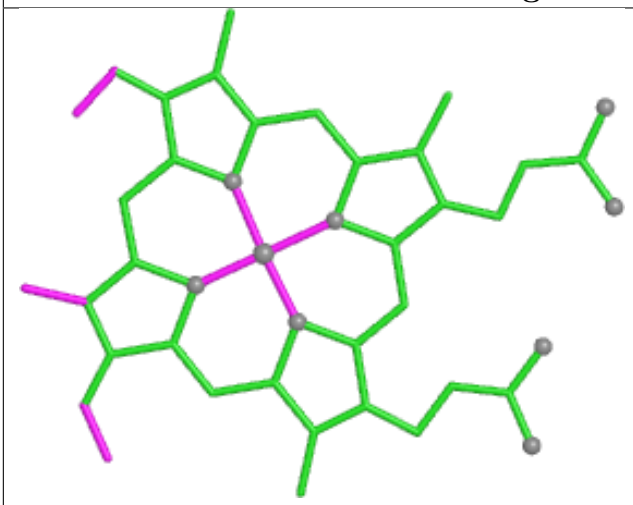


Torsions



Rings

Ligand HEC C 503



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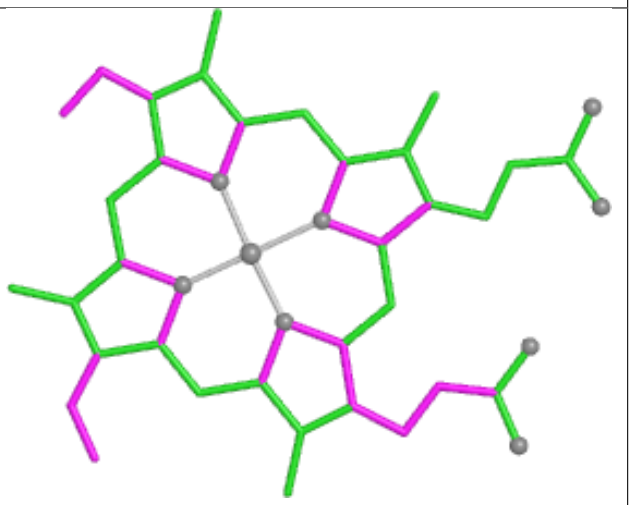

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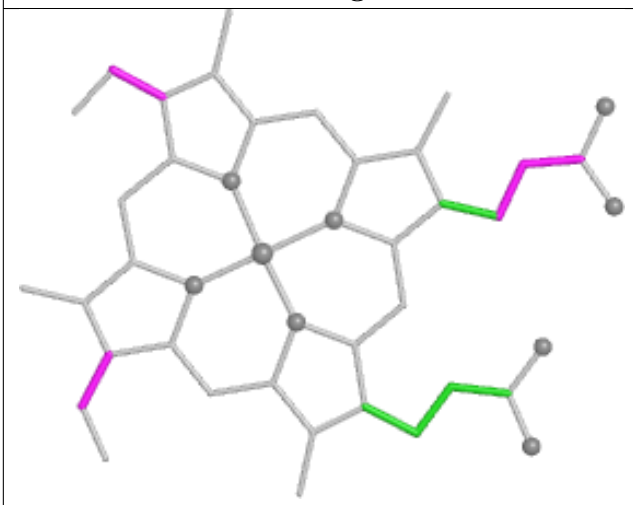

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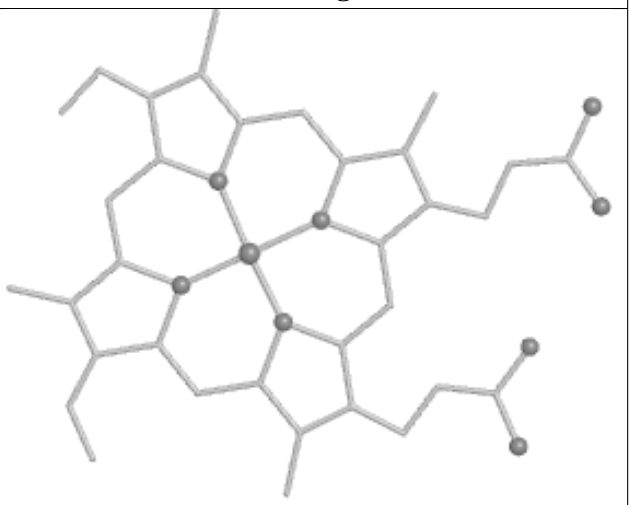
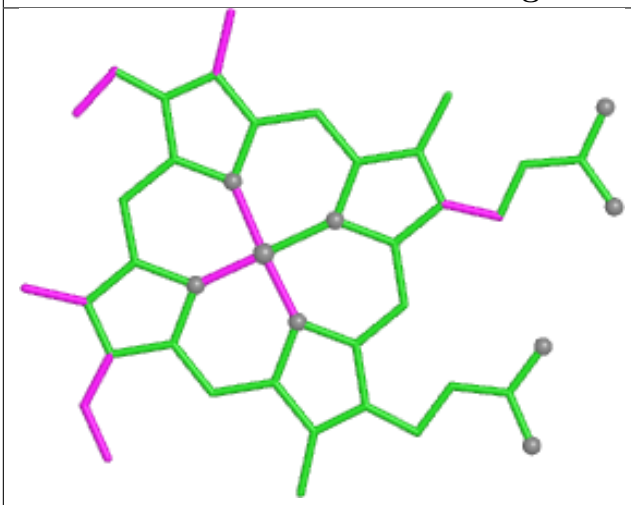


Rings

Ligand HEC D 505



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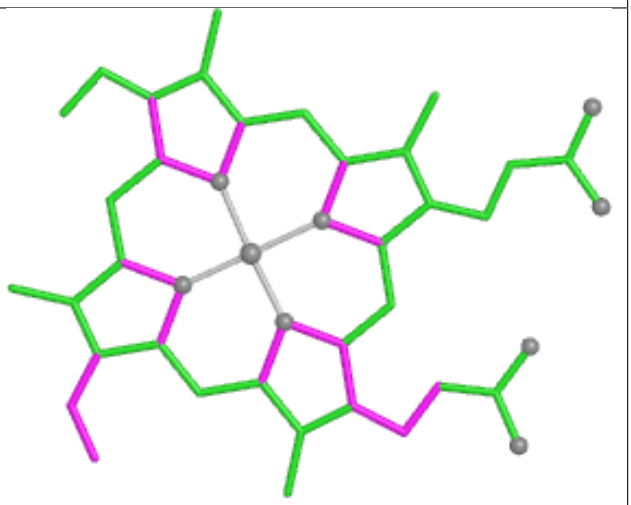
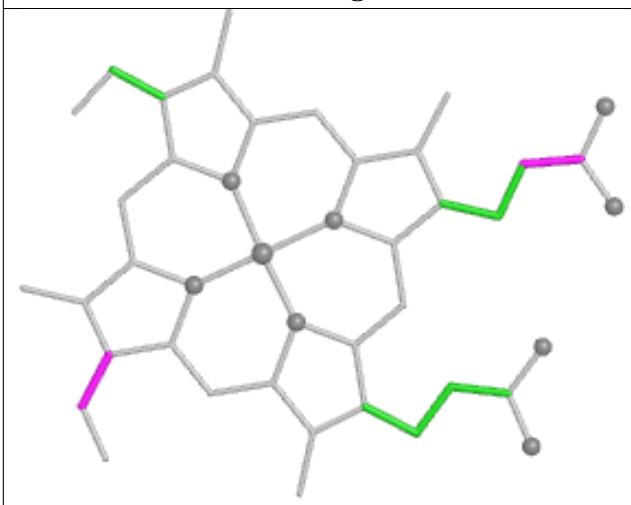


Bond angles



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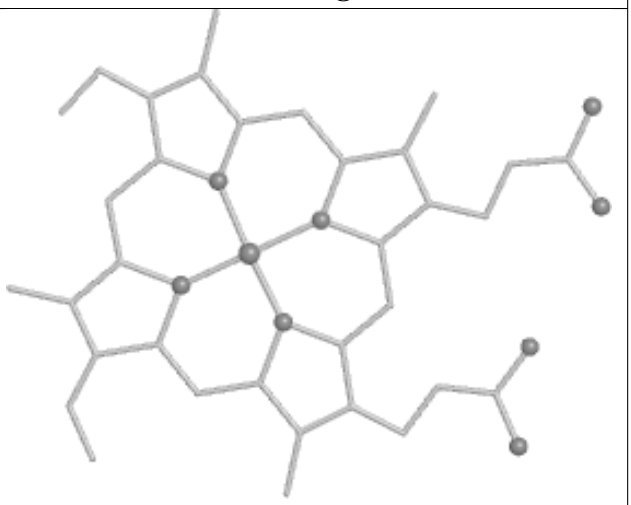
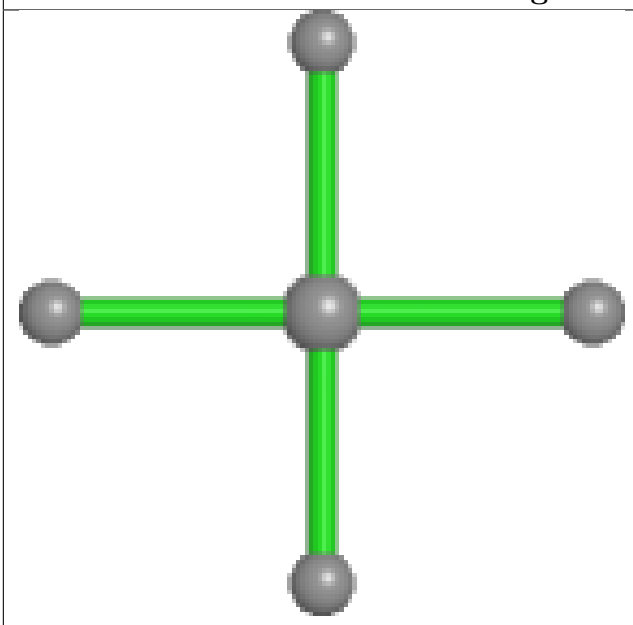


Rings

Ligand SE4 C 507



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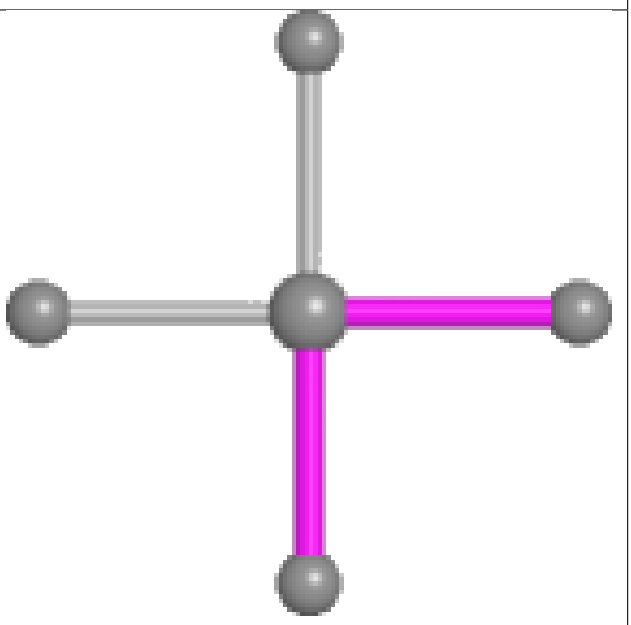
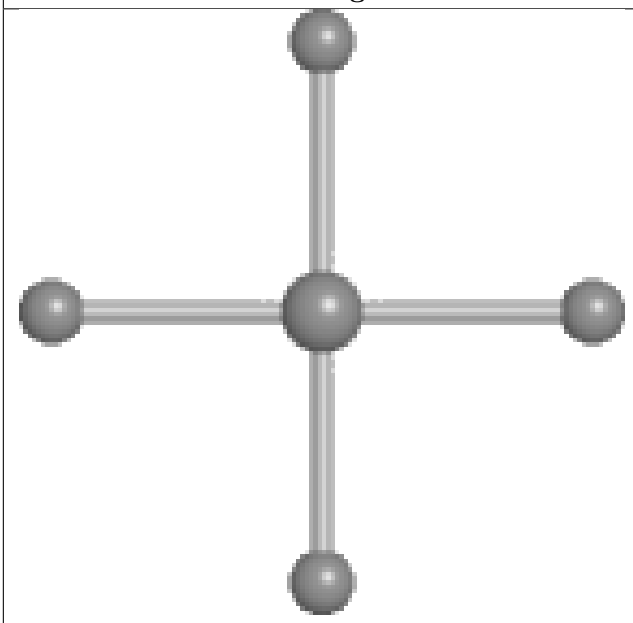
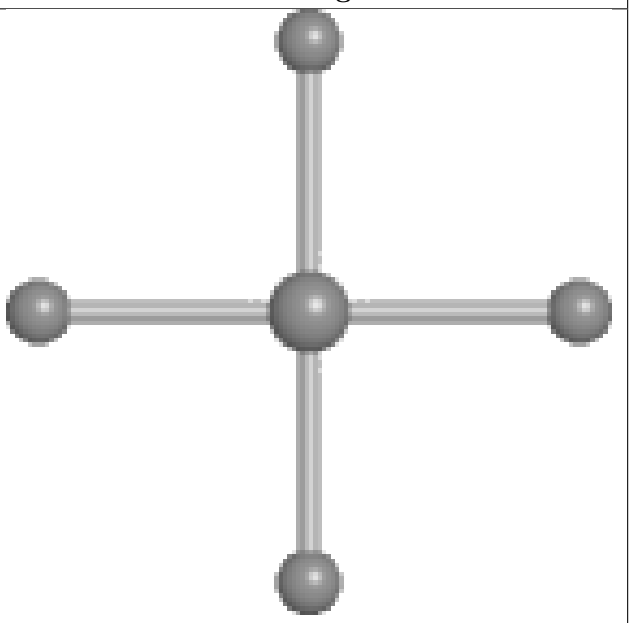


Bond angles

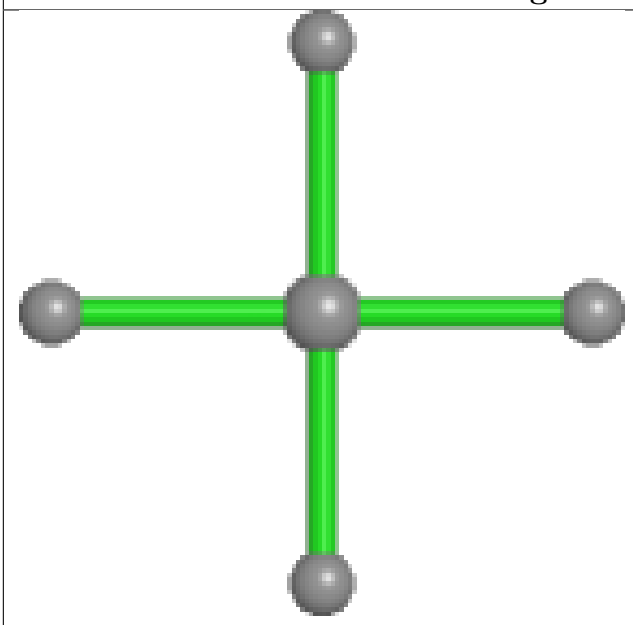


Torsions

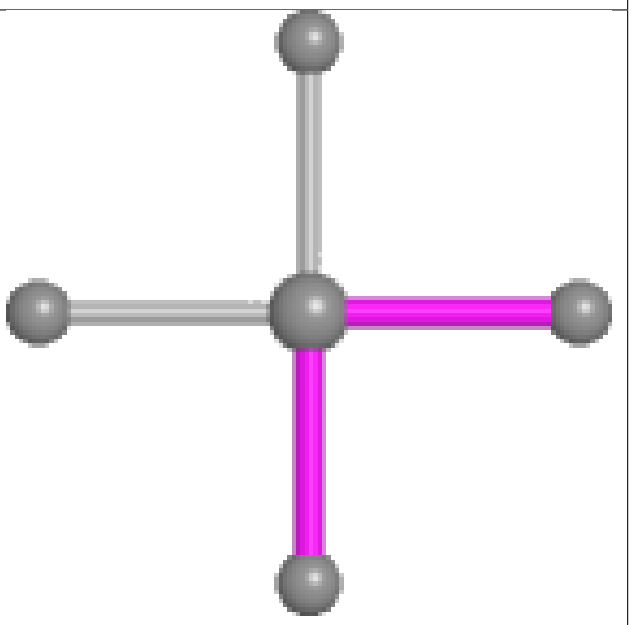


Rings

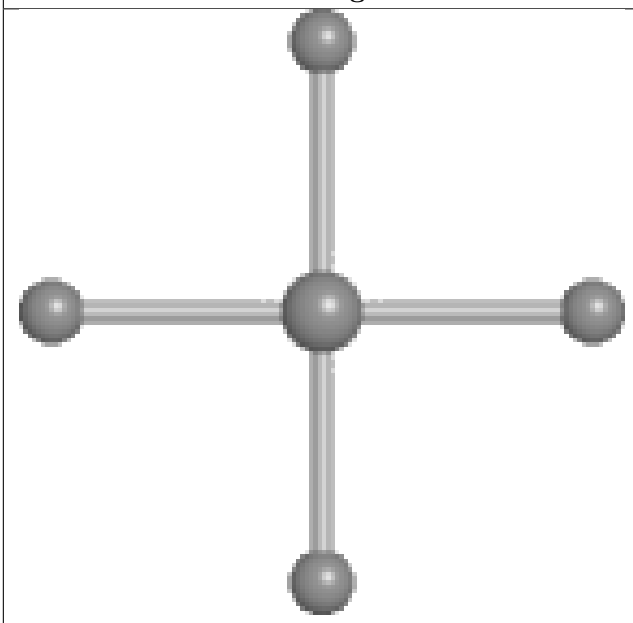
Ligand SE4 D 508



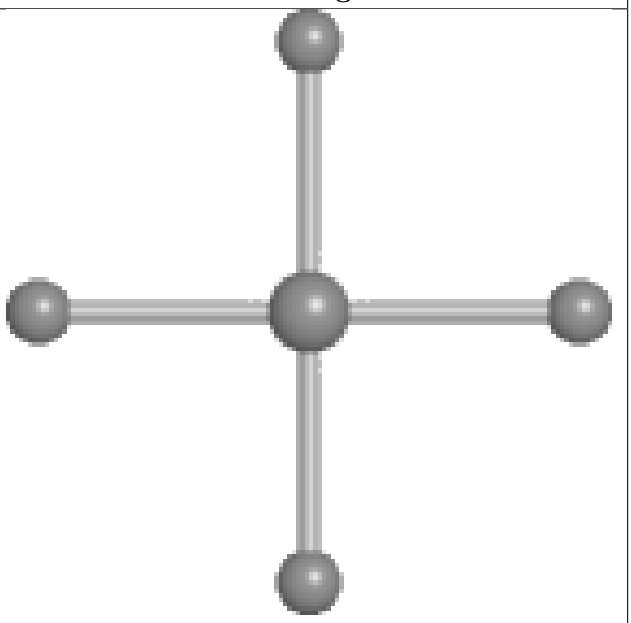
Bond lengths



Bond angles

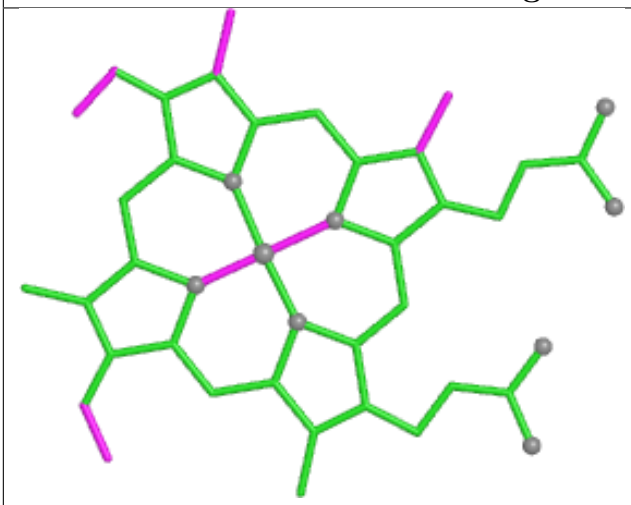


Torsions



Rings

Ligand HEC B 505



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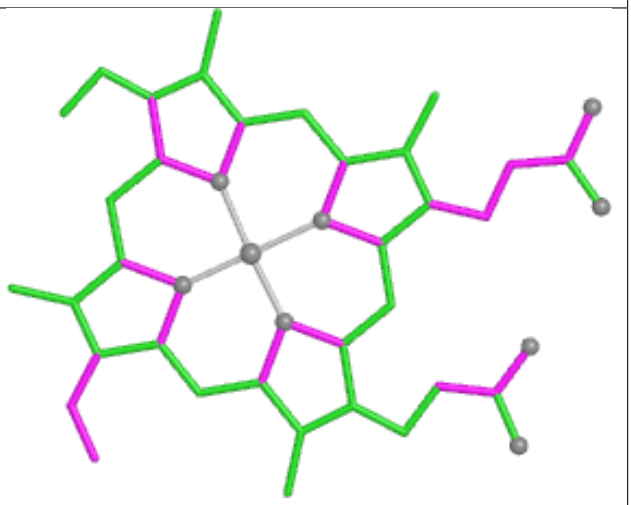
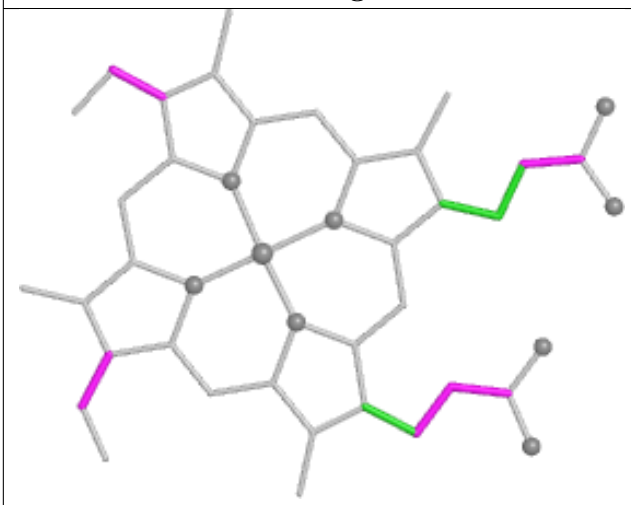


Bond angles



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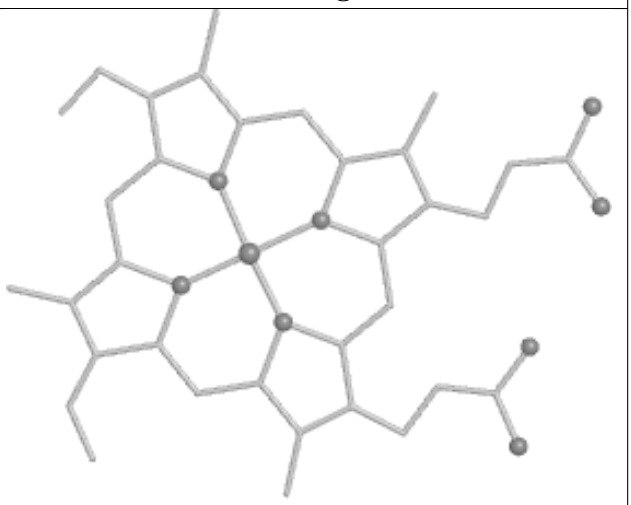
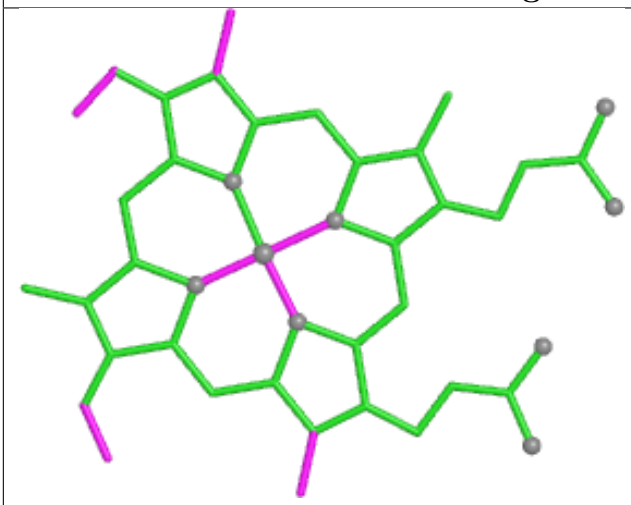


Rings

Ligand HEC C 502



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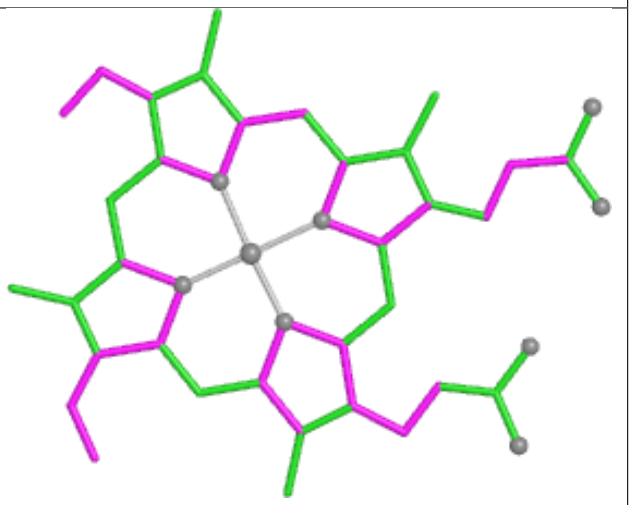
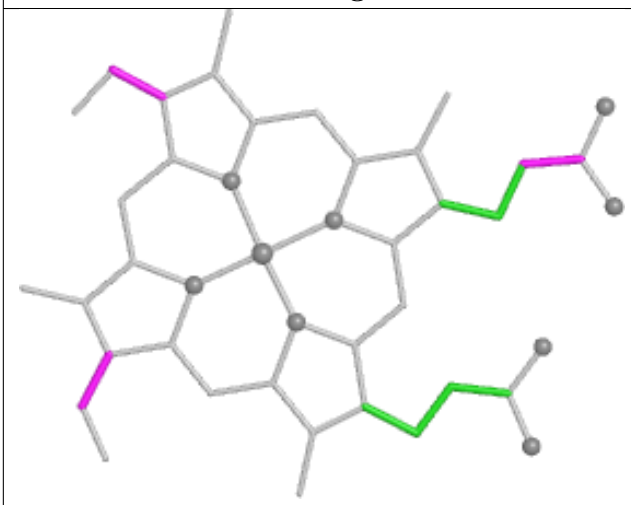


Bond angles



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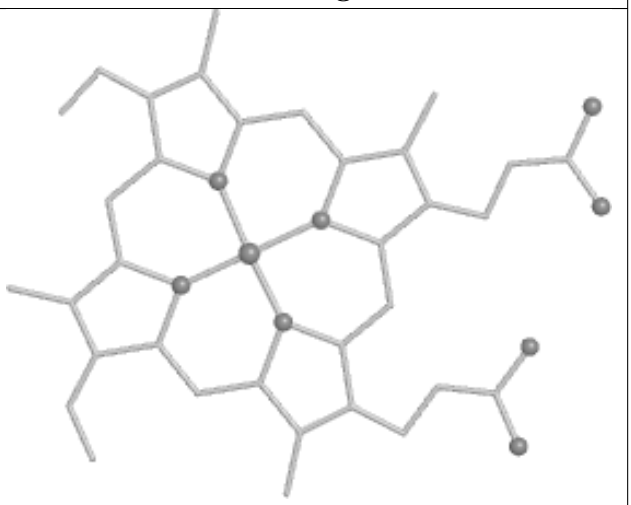
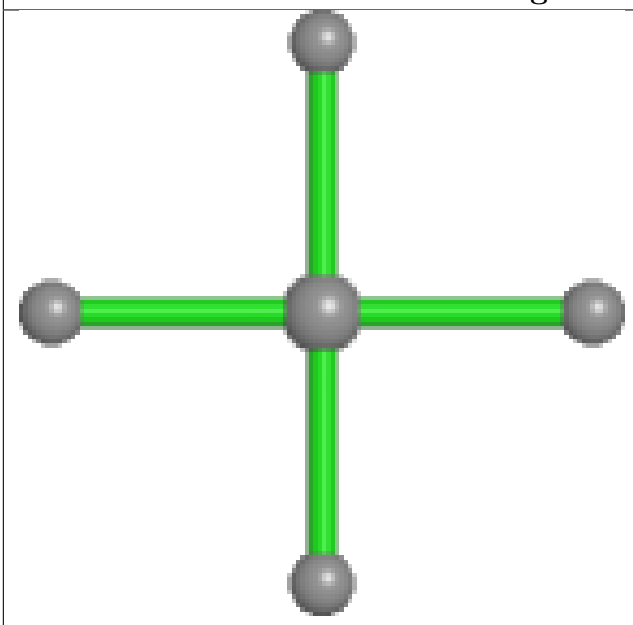


Rings

Ligand SE4 A 506



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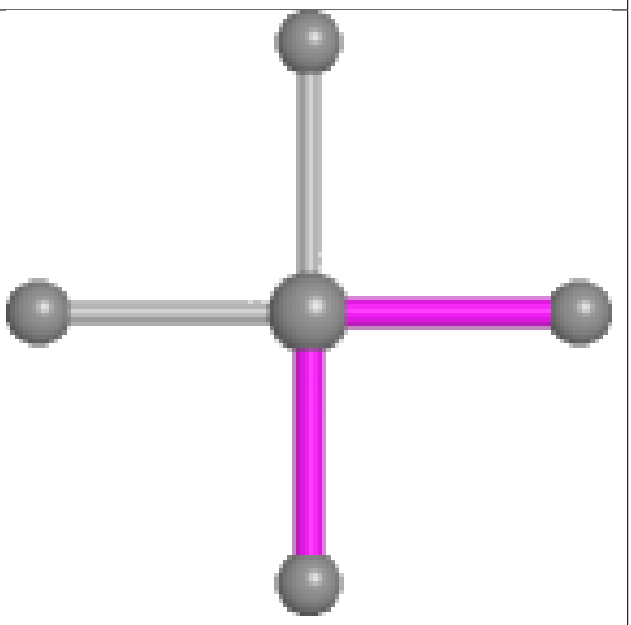
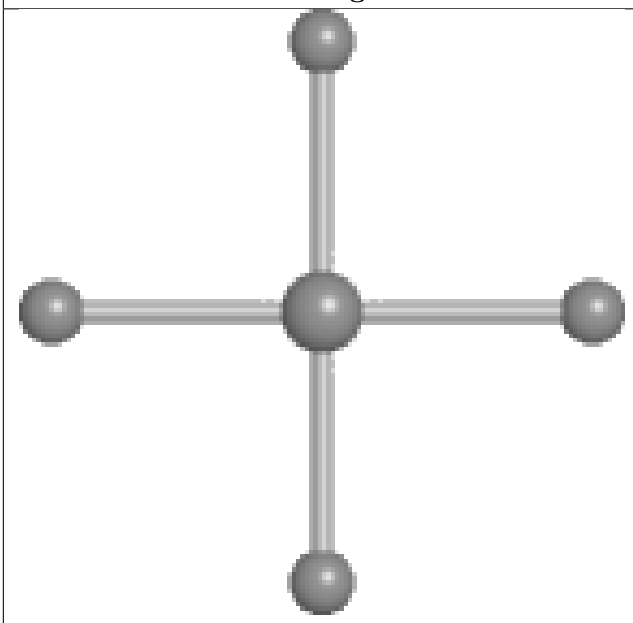
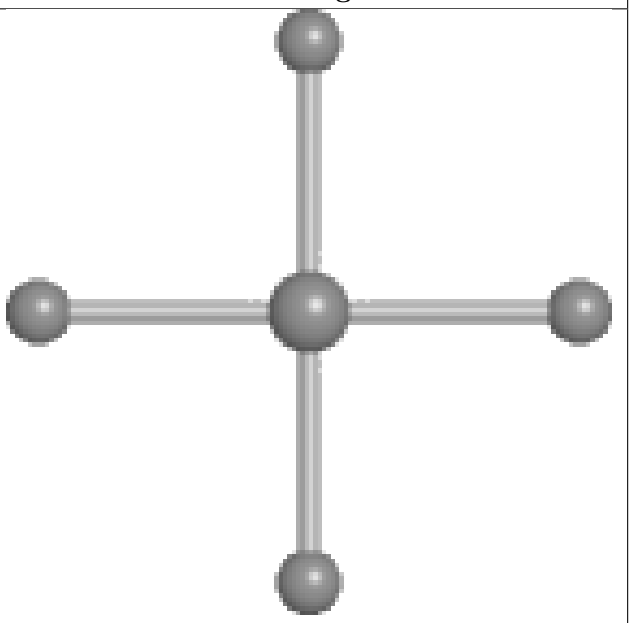


Bond angles



Torsions



Rings

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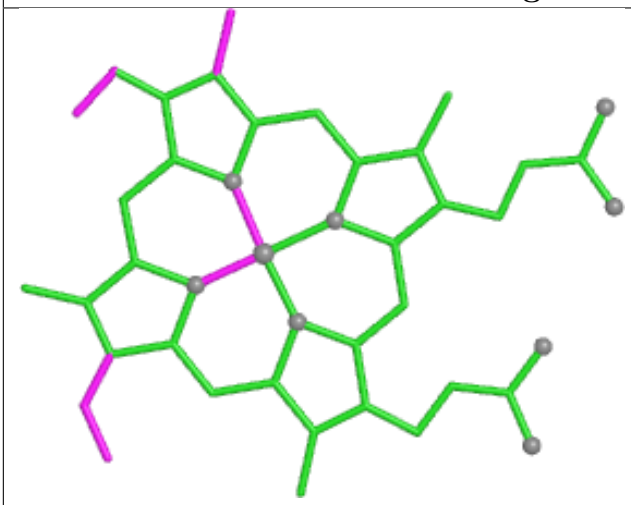

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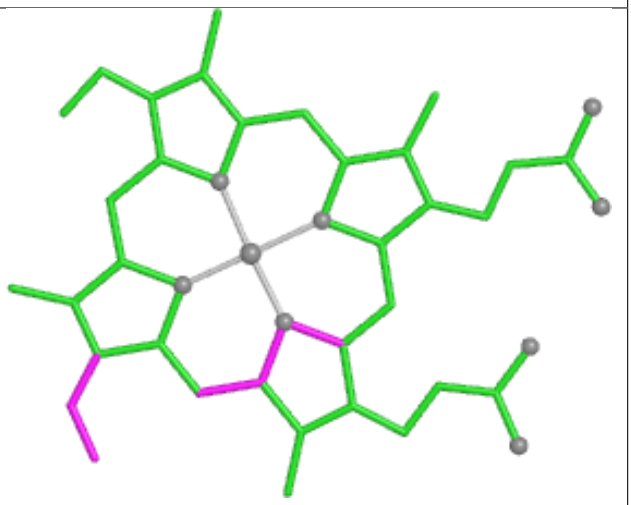

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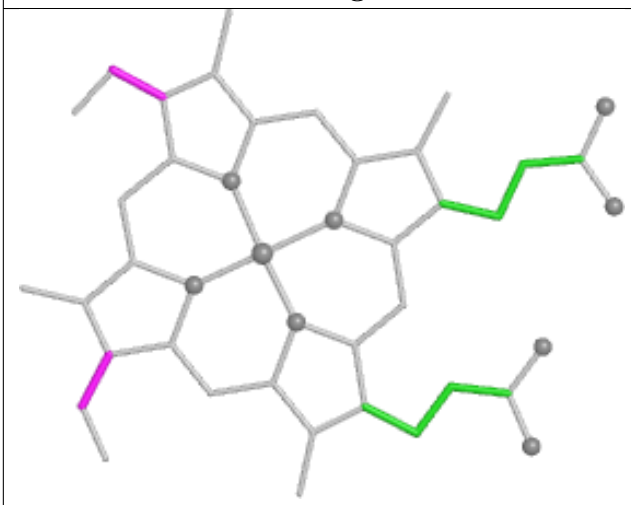
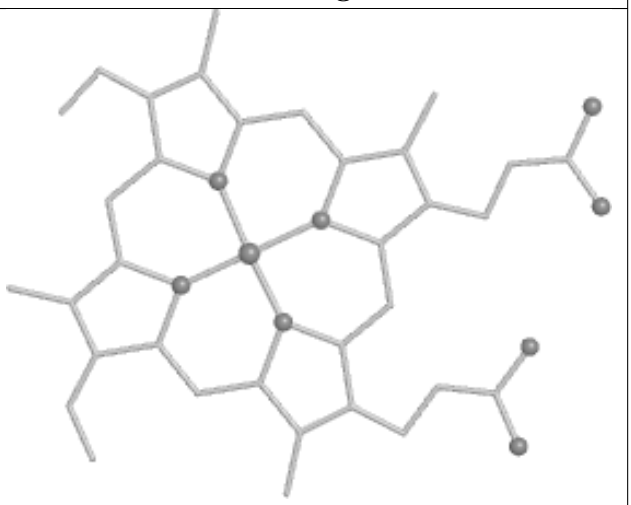


Torsions



Rings

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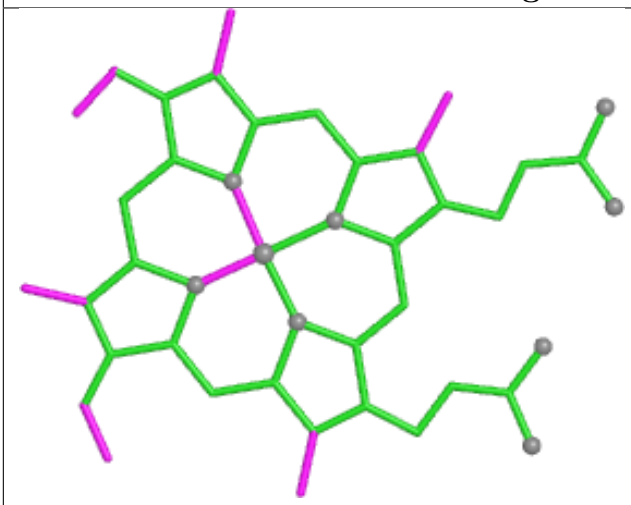

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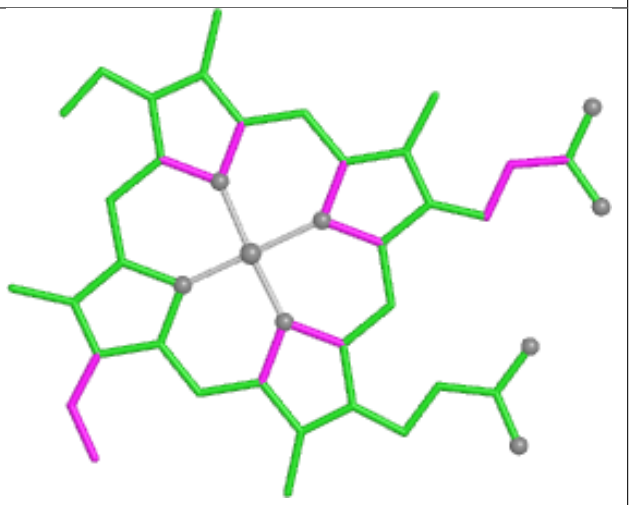
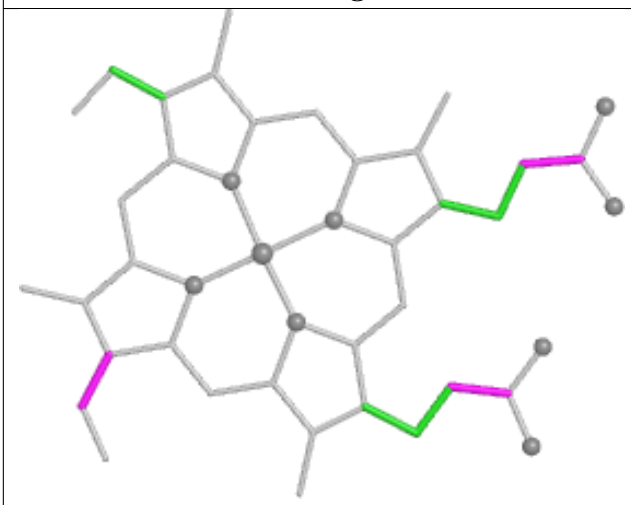


Bond angles



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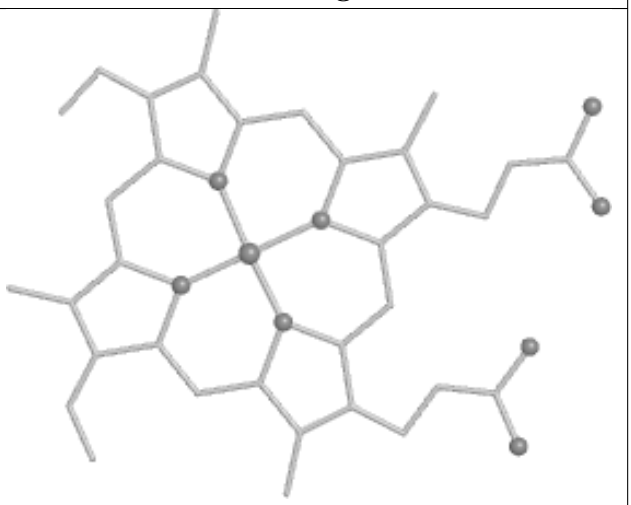
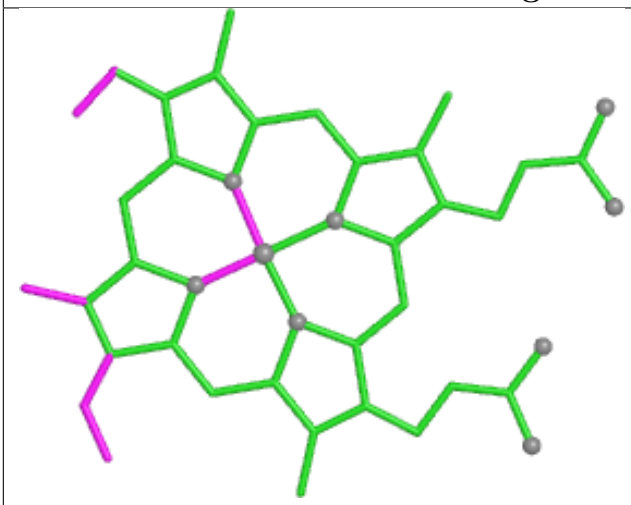
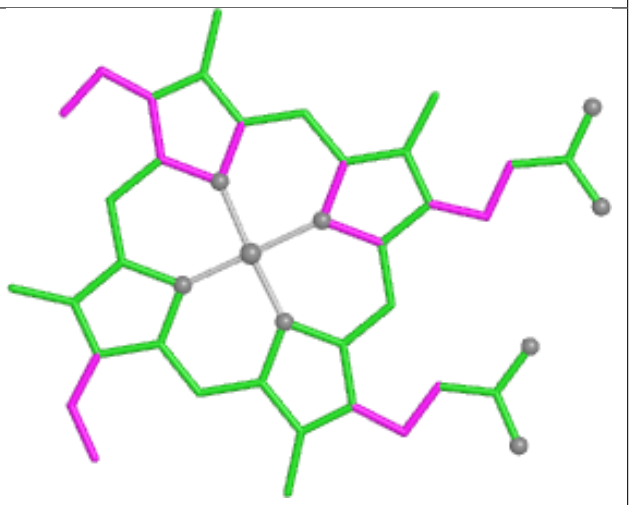


Rings

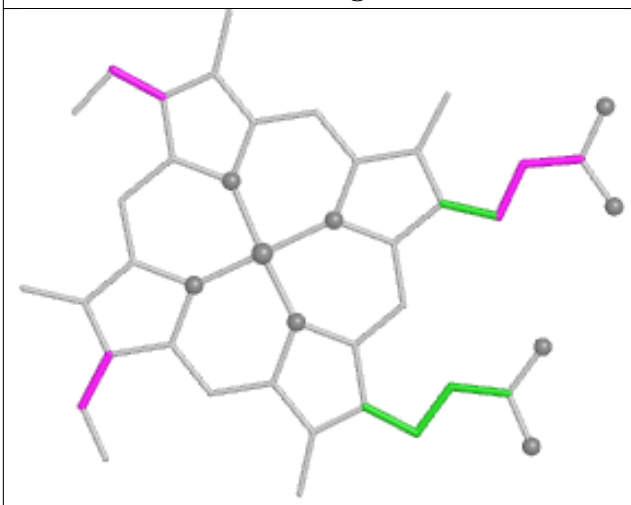
Ligand HEC A 502



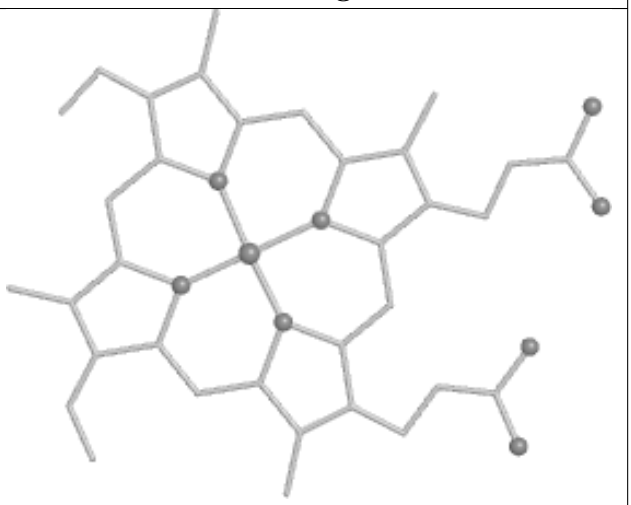
Bond lengths



Bond angles

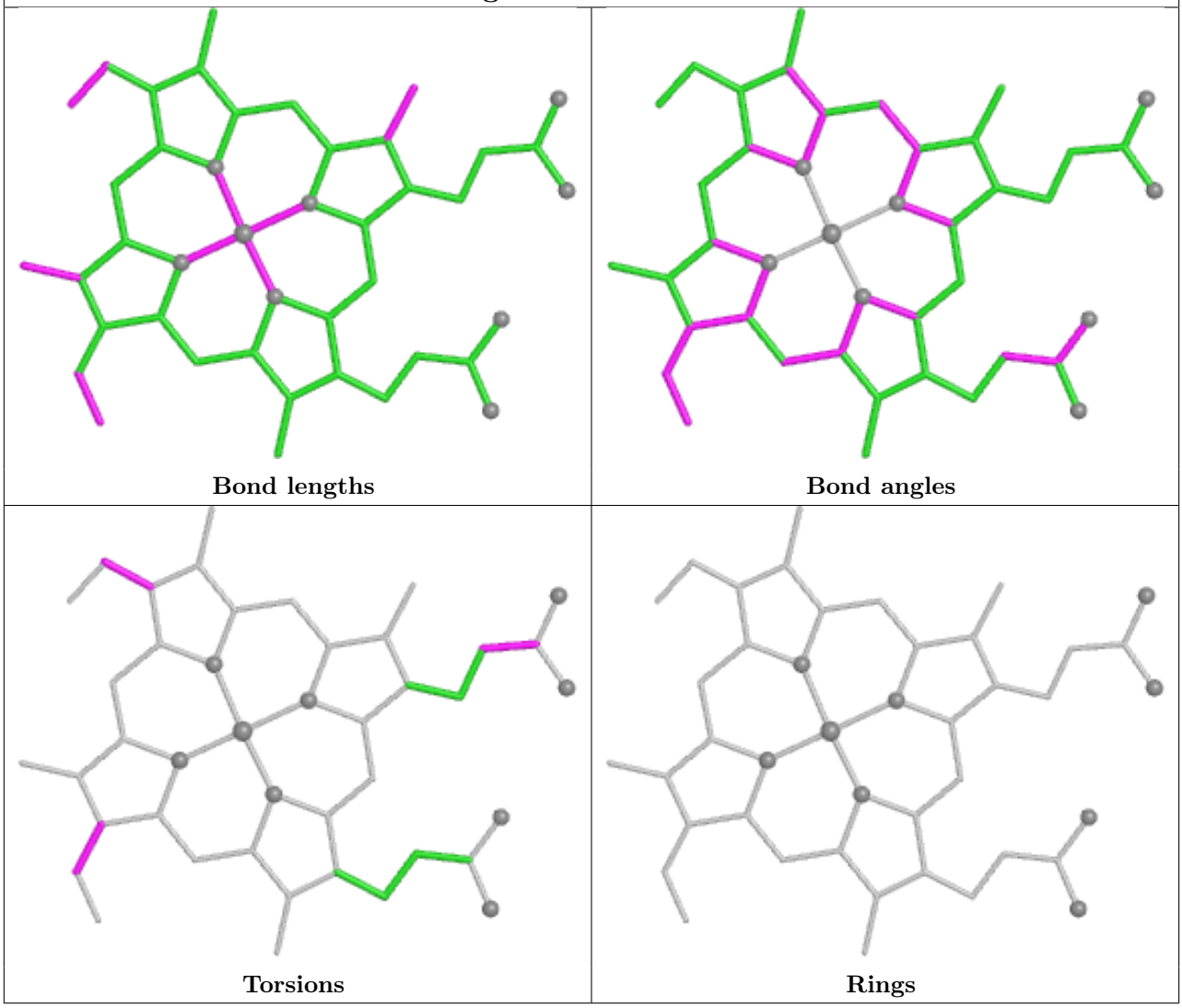


Torsions



Rings

Ligand HEC B 501



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	421/450 (93%)	-0.32	0	100	100	17, 43, 66, 88	9 (2%)
1	B	421/450 (93%)	-0.38	0	100	100	20, 42, 62, 76	9 (2%)
1	C	421/450 (93%)	-0.15	4 (0%)	79	77	23, 48, 68, 100	6 (1%)
1	D	421/450 (93%)	-0.34	2 (0%)	87	85	21, 43, 62, 79	5 (1%)
All	All	1684/1800 (93%)	-0.30	6 (0%)	88	87	17, 44, 65, 100	29 (1%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60[A]	GLU	3.0
1	D	28	ALA	2.6
1	D	448	LYS	2.2
1	C	434	PHE	2.1
1	C	253[A]	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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
1	CSD	B	239	8/9	0.97	0.07	33,37,45,46	0
1	CSD	C	239	8/9	0.97	0.07	39,42,47,51	0
1	CSD	D	239	8/9	0.97	0.07	34,39,40,50	0
1	CSD	A	239	8/9	0.98	0.06	37,39,47,50	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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
4	EDO	D	501	4/4	0.65	0.19	61,63,64,70	0
4	EDO	C	515	4/4	0.67	0.23	64,67,71,72	0
4	EDO	A	513	4/4	0.67	0.25	67,67,71,73	0
4	EDO	D	516	4/4	0.73	0.16	55,59,71,81	0
4	EDO	D	518	4/4	0.78	0.21	42,58,73,75	0
4	EDO	D	513	4/4	0.80	0.23	64,65,65,65	0
4	EDO	C	514	4/4	0.81	0.15	58,64,66,70	0
4	EDO	B	519	4/4	0.81	0.22	40,41,54,59	0
4	EDO	D	517	4/4	0.82	0.14	50,51,52,62	4
4	EDO	A	511	4/4	0.83	0.19	50,56,58,59	0
4	EDO	C	513	4/4	0.84	0.19	51,54,55,56	4
4	EDO	B	517	4/4	0.85	0.17	51,54,60,64	0
4	EDO	B	513	4/4	0.86	0.16	40,40,43,44	4
4	EDO	B	516	4/4	0.86	0.14	50,55,56,59	4
4	EDO	D	511	4/4	0.86	0.13	47,53,59,65	0
4	EDO	D	512	4/4	0.86	0.15	45,49,59,60	0
5	EPE	B	507	15/15	0.86	0.16	56,60,68,70	15
4	EDO	A	509	4/4	0.87	0.12	48,59,60,66	0
4	EDO	D	509	4/4	0.88	0.14	49,52,52,60	0
4	EDO	A	514	4/4	0.88	0.27	42,51,54,62	0
4	EDO	B	510	4/4	0.89	0.15	50,52,56,59	0
4	EDO	C	512	4/4	0.89	0.16	43,43,46,51	4
4	EDO	C	508	4/4	0.90	0.17	49,59,59,61	0
4	EDO	D	510	4/4	0.90	0.18	50,52,53,65	0
4	EDO	C	510	4/4	0.90	0.12	43,46,48,52	4
4	EDO	B	514	4/4	0.90	0.12	46,49,56,56	4
4	EDO	B	509	4/4	0.90	0.13	44,44,56,56	0
4	EDO	D	514	4/4	0.90	0.14	42,42,43,48	4
4	EDO	A	508	4/4	0.90	0.17	44,45,53,53	4
4	EDO	B	508	4/4	0.90	0.15	42,63,66,71	0
4	EDO	C	501	4/4	0.90	0.10	41,42,47,61	0
4	EDO	D	502	4/4	0.90	0.12	40,41,44,45	4

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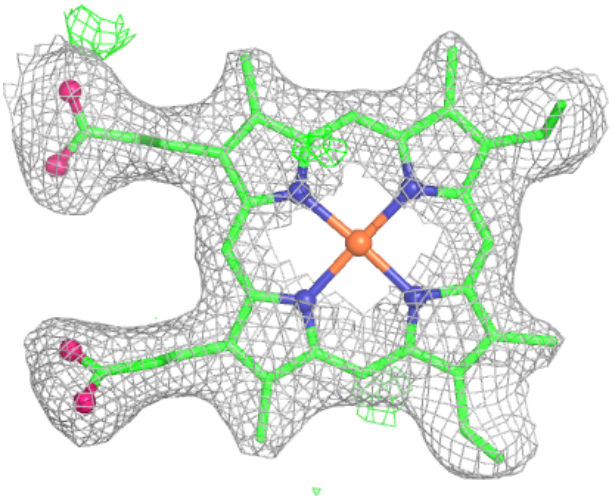
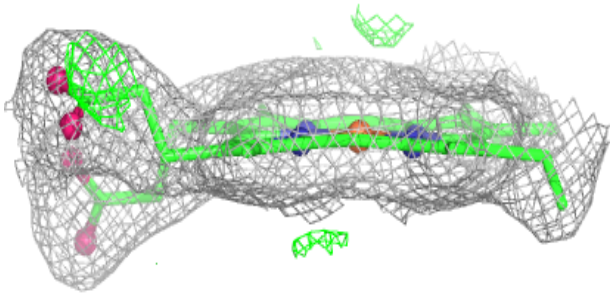
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	511	4/4	0.91	0.10	56,63,63,71	0
4	EDO	C	516	4/4	0.91	0.17	50,58,61,63	0
4	EDO	C	509	4/4	0.92	0.13	53,55,58,58	0
4	EDO	B	515	4/4	0.92	0.09	44,52,61,70	0
4	EDO	A	510	4/4	0.92	0.15	38,45,48,48	0
4	EDO	D	515	4/4	0.92	0.16	29,32,39,43	4
4	EDO	B	512	4/4	0.93	0.15	44,49,51,64	0
4	EDO	B	518	4/4	0.94	0.14	35,42,46,48	4
4	EDO	A	507	4/4	0.94	0.13	38,45,50,57	0
4	EDO	A	512	4/4	0.94	0.09	45,45,54,55	0
4	EDO	C	511	4/4	0.95	0.15	32,37,39,41	4
2	HEC	D	503	43/43	0.97	0.07	41,51,57,66	0
2	HEC	C	502	43/43	0.97	0.08	47,56,67,68	0
2	HEC	B	501	43/43	0.98	0.07	40,49,58,64	0
2	HEC	B	502	43/43	0.98	0.07	31,36,50,60	0
2	HEC	B	503	43/43	0.98	0.06	31,42,55,59	0
2	HEC	B	504	43/43	0.98	0.06	28,34,42,50	0
2	HEC	A	501	43/43	0.98	0.07	33,41,54,59	0
2	HEC	C	503	43/43	0.98	0.08	36,43,62,63	0
2	HEC	C	504	43/43	0.98	0.08	36,45,57,65	0
2	HEC	C	505	43/43	0.98	0.08	33,39,52,57	0
2	HEC	A	502	43/43	0.98	0.07	30,38,53,56	0
2	HEC	D	504	43/43	0.98	0.06	29,36,47,54	0
2	HEC	D	505	43/43	0.98	0.06	34,43,56,60	0
3	SE4	A	506	5/5	0.98	0.14	40,42,51,55	5
3	SE4	C	507	5/5	0.98	0.13	46,47,54,54	5
2	HEC	A	503	43/43	0.98	0.07	29,35,49,55	0
2	HEC	D	507	43/43	0.99	0.05	28,35,40,45	0
2	HEC	C	506	43/43	0.99	0.06	33,39,45,52	0
3	SE4	B	506	5/5	0.99	0.15	34,34,38,44	5
2	HEC	A	505	43/43	0.99	0.06	28,34,41,48	0
3	SE4	D	508	5/5	0.99	0.11	39,41,44,51	5
2	HEC	B	505	43/43	0.99	0.06	29,35,41,52	0
2	HEC	A	504	43/43	0.99	0.06	30,34,45,52	0
2	HEC	D	506	43/43	0.99	0.06	29,35,43,49	0

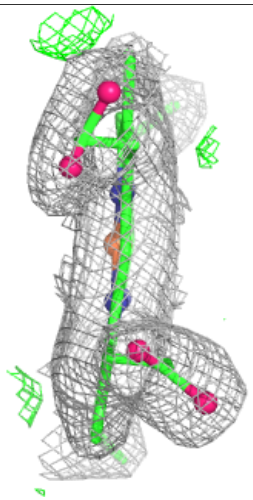
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC D 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

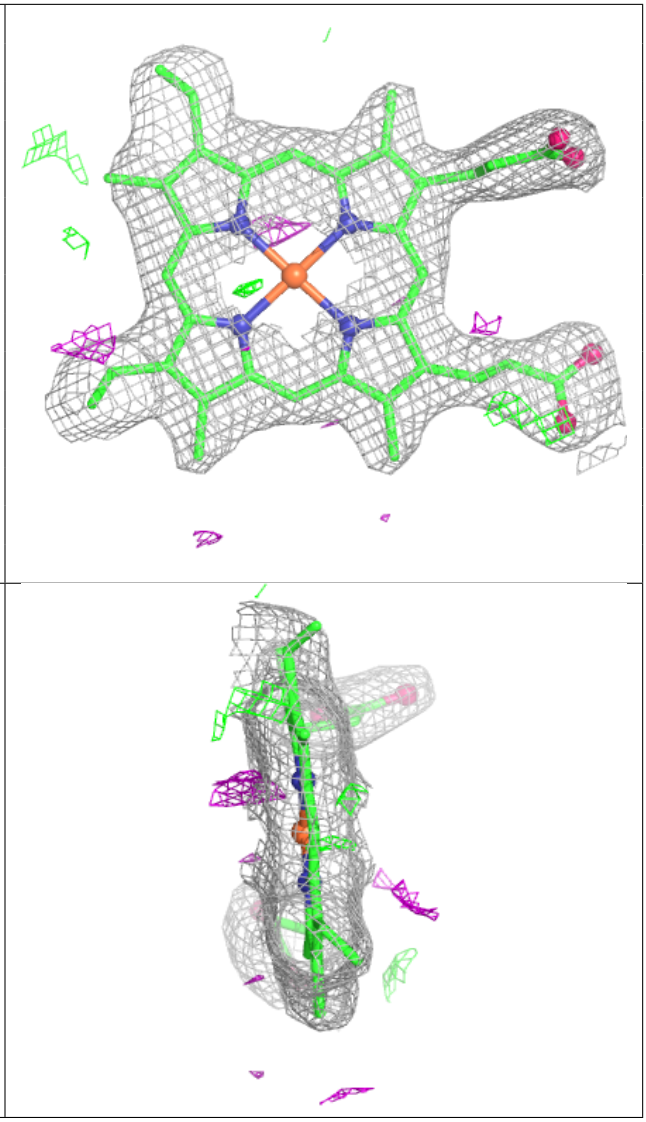






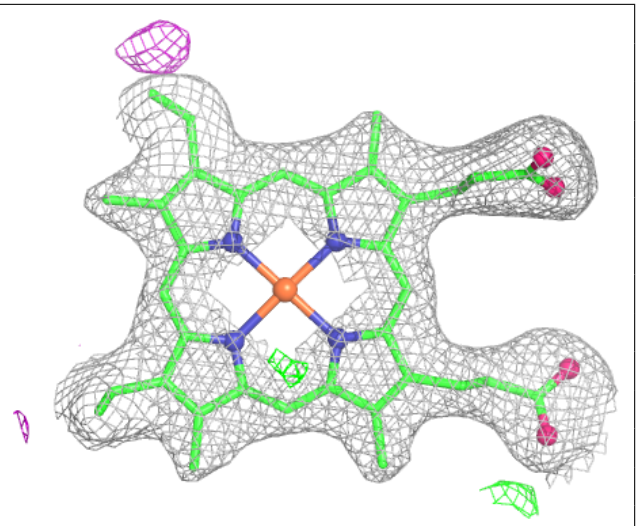
Electron density around HEC C 502:

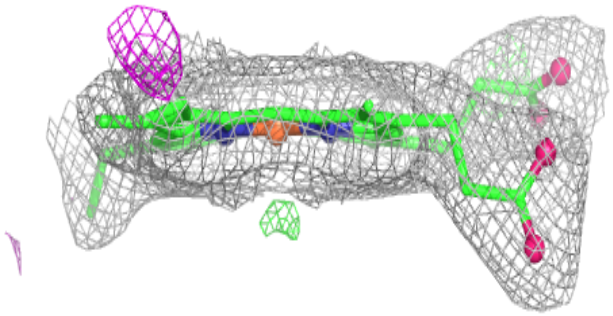
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

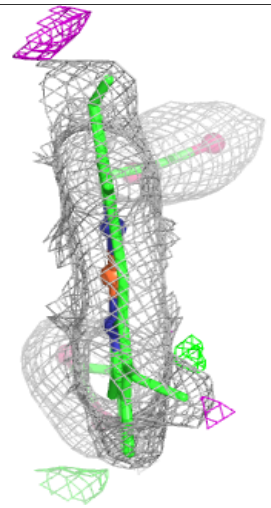


Electron density around HEC B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

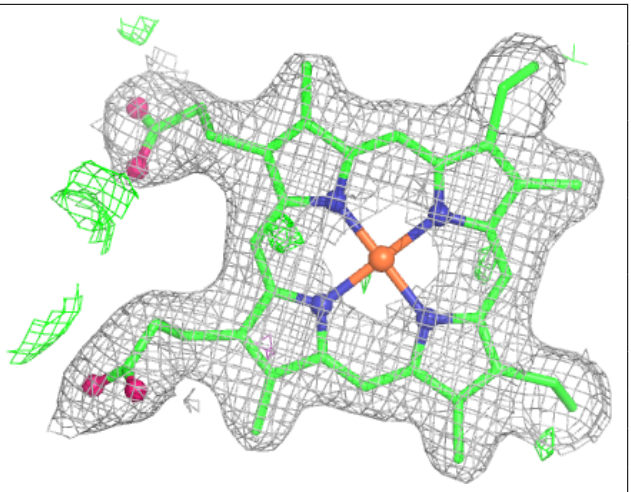


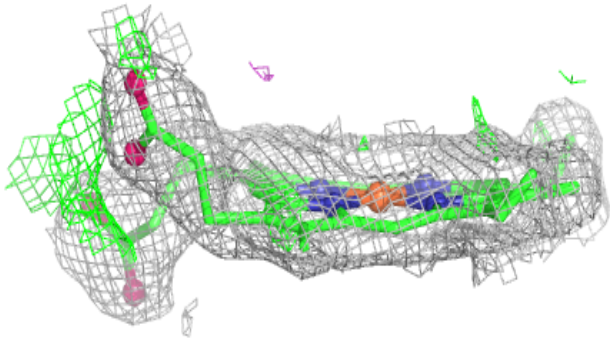


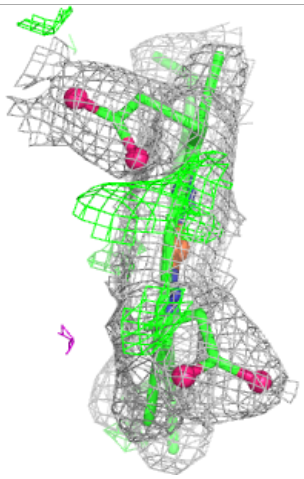


Electron density around HEC B 502:

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

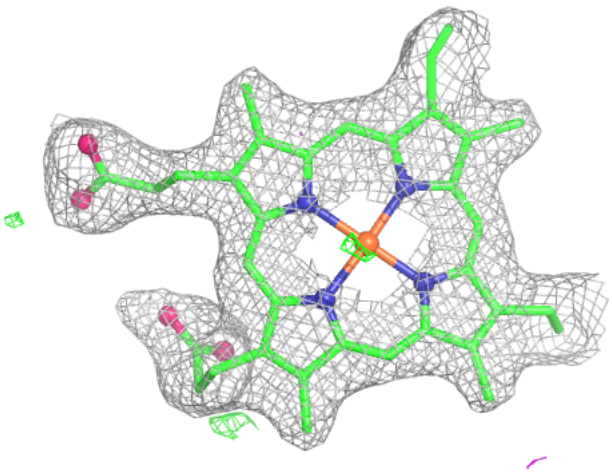


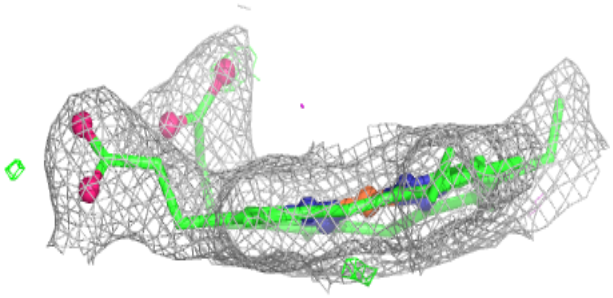


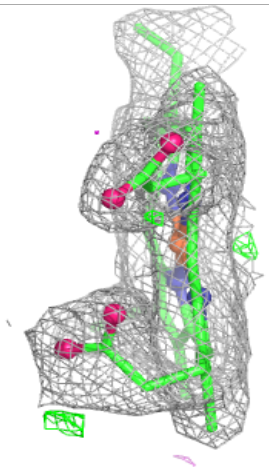


Electron density around HEC B 503:

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

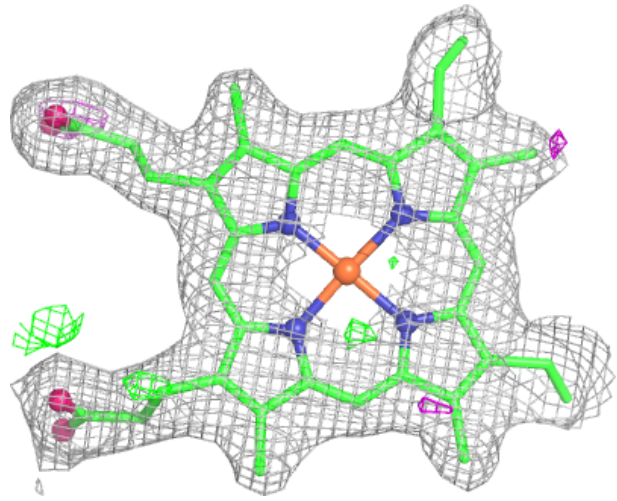


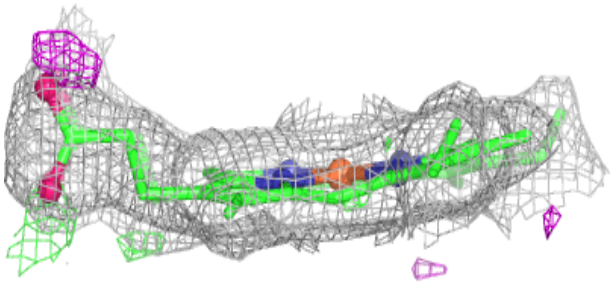


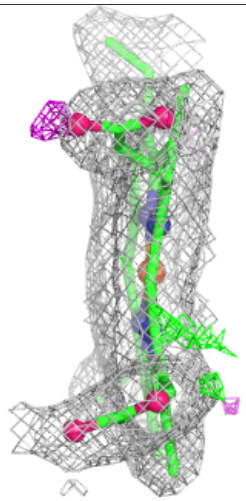


Electron density around HEC B 504:

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

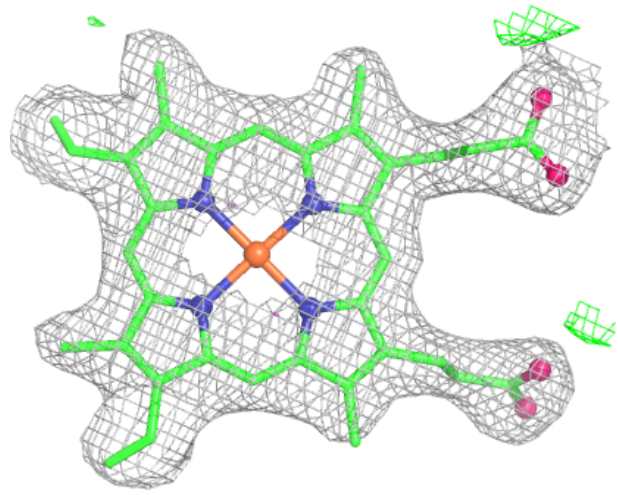


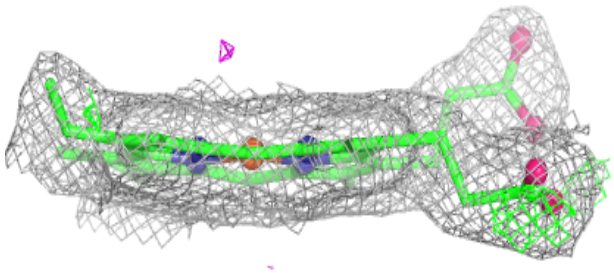


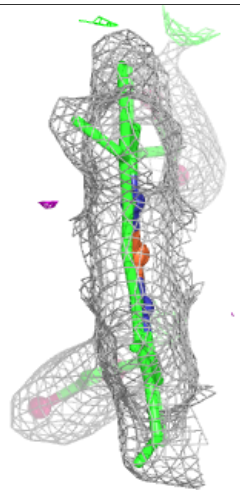


Electron density around HEC A 501:

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

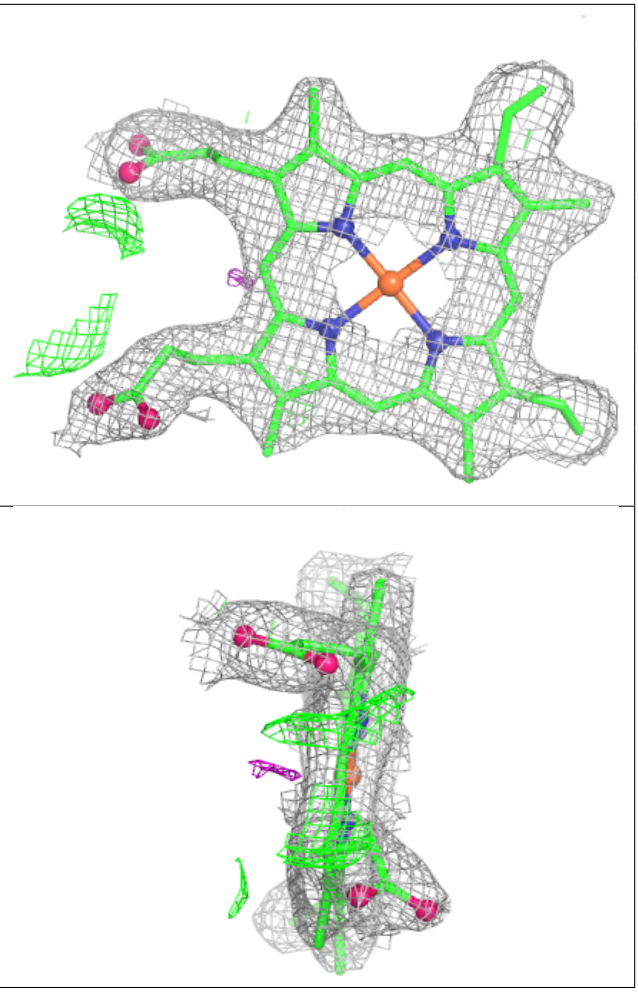






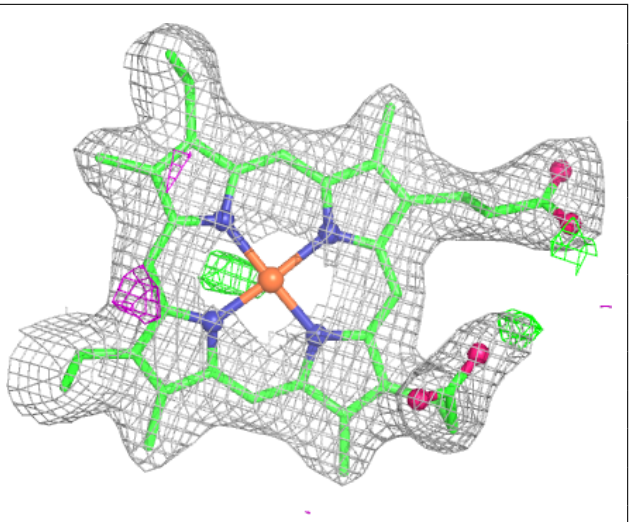
Electron density around HEC C 503:

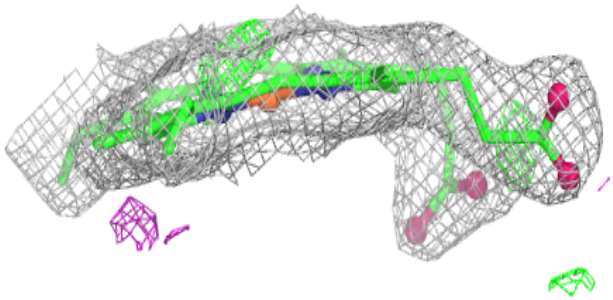
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

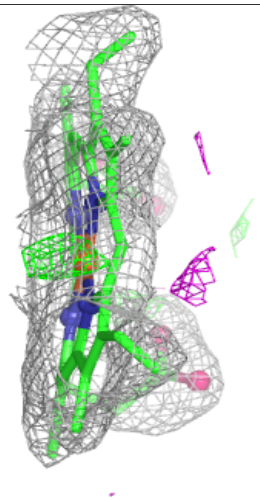


Electron density around HEC C 504:

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

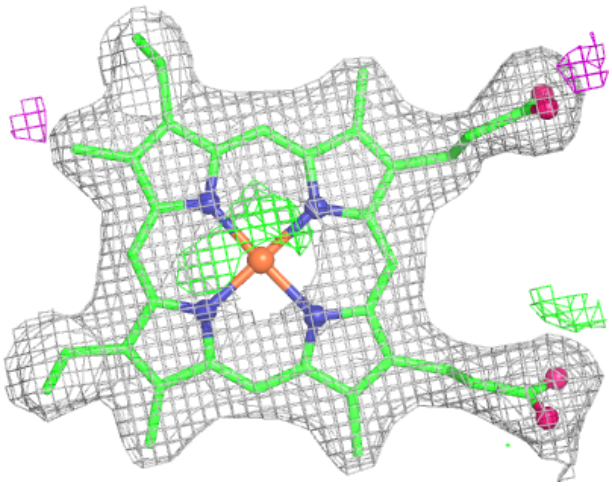


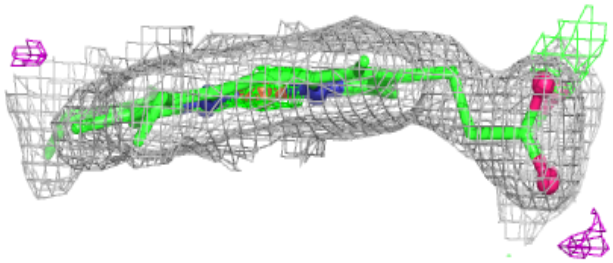


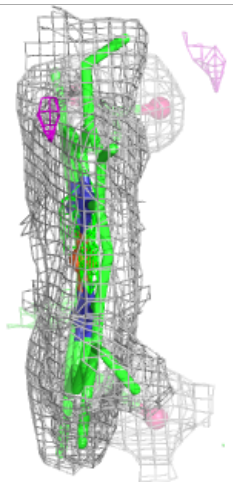


Electron density around HEC C 505:

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

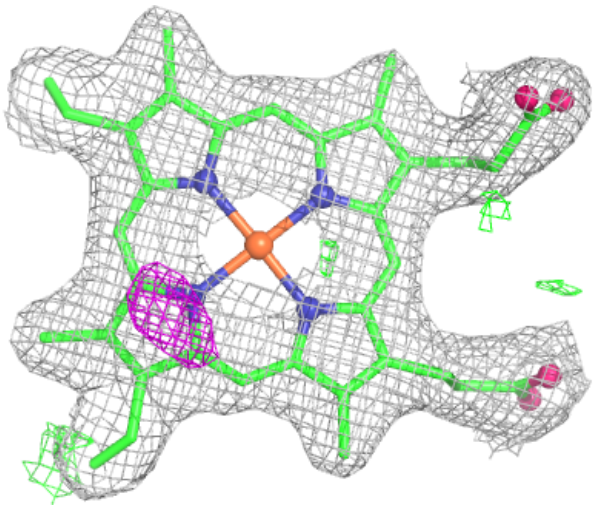


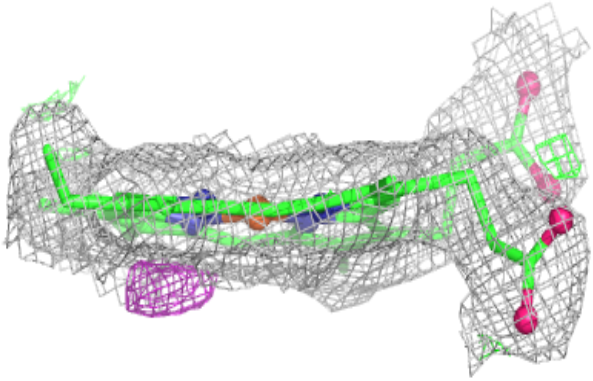


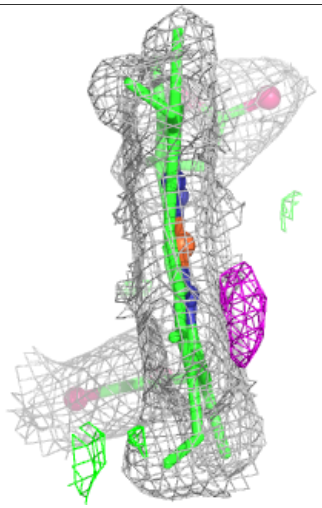


Electron density around HEC A 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

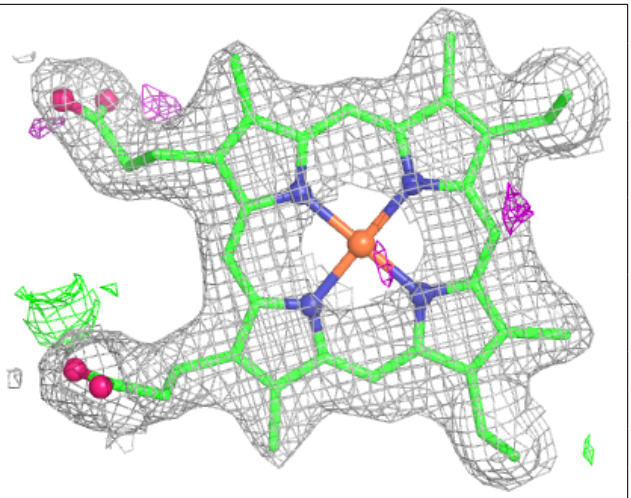


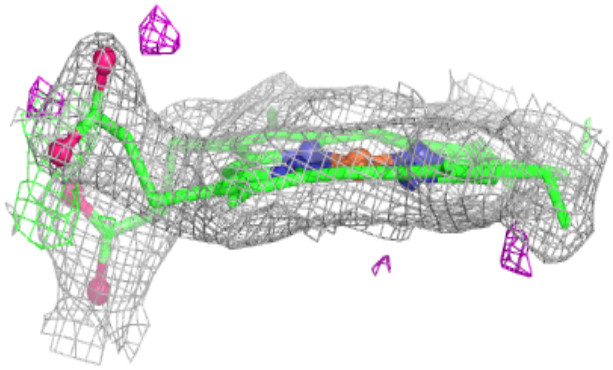


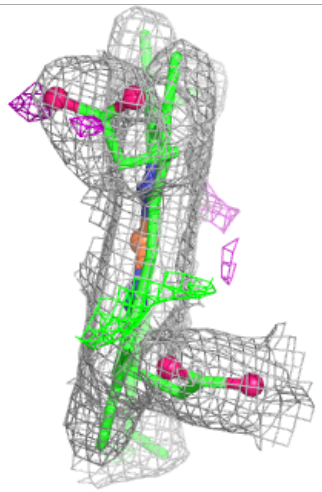


Electron density around HEC D 504:

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

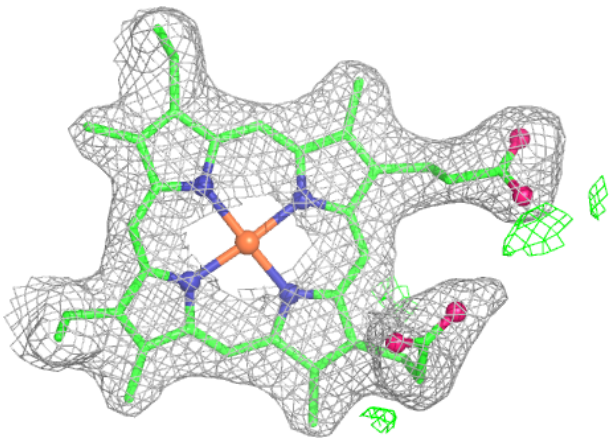


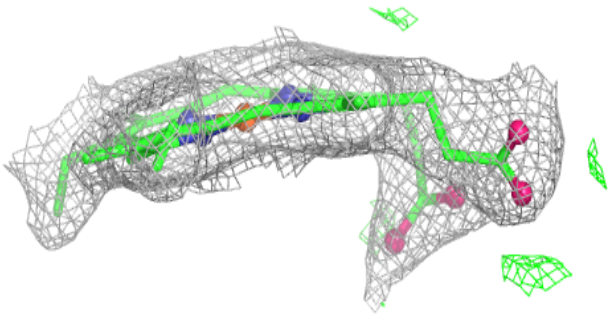


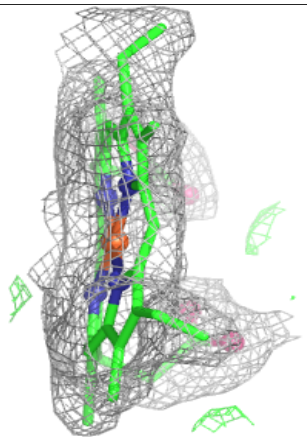


Electron density around HEC D 505:

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







Electron density around SE4 A 506:

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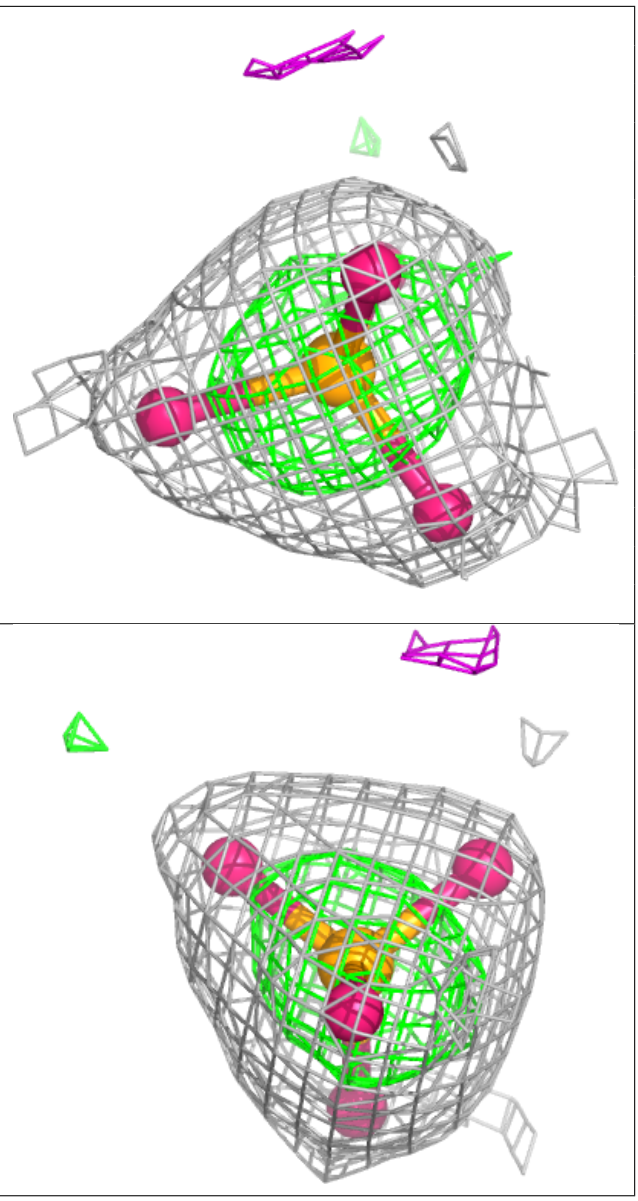
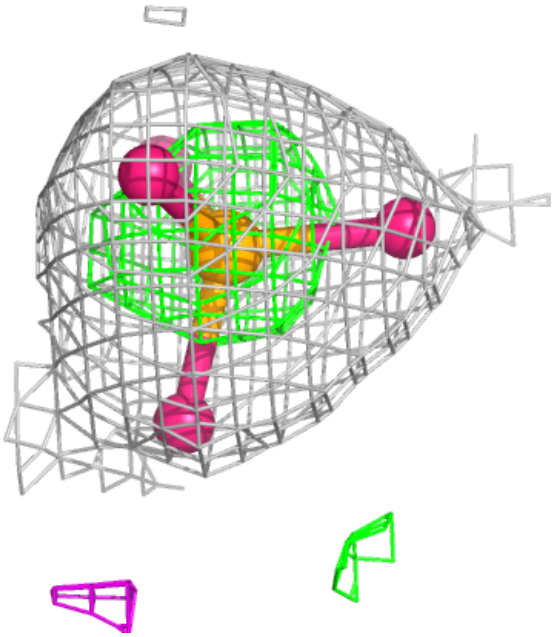
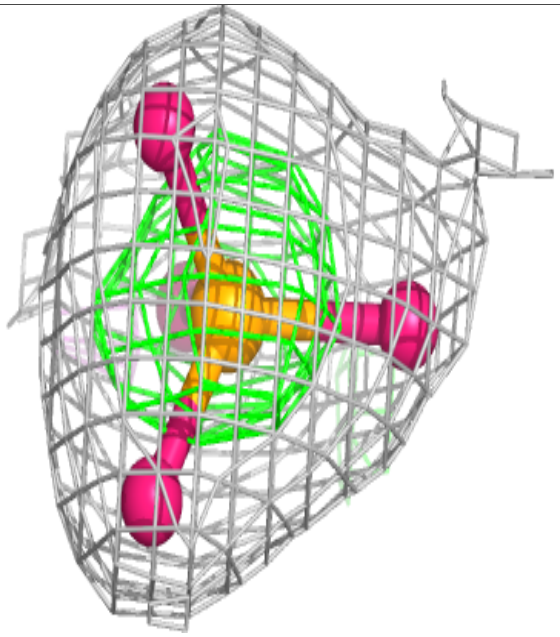
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

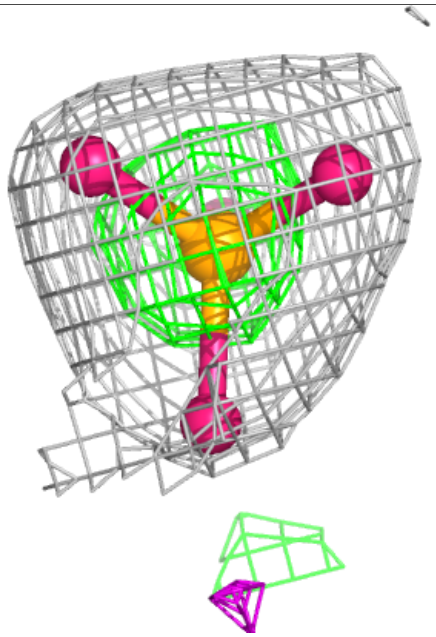


Electron density around SE4 C 507:

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

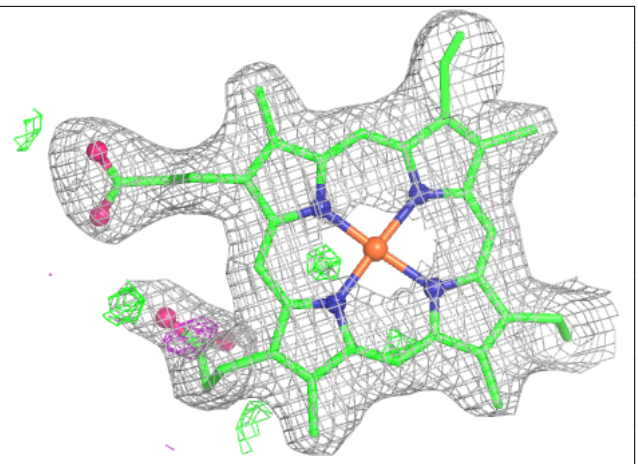


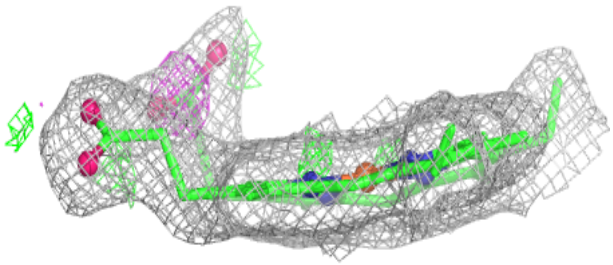


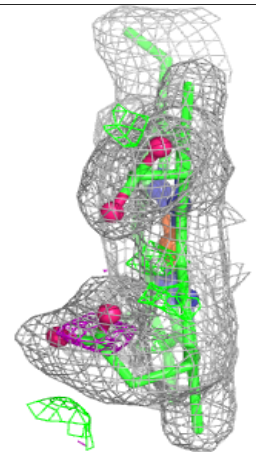


Electron density around HEC A 503:

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

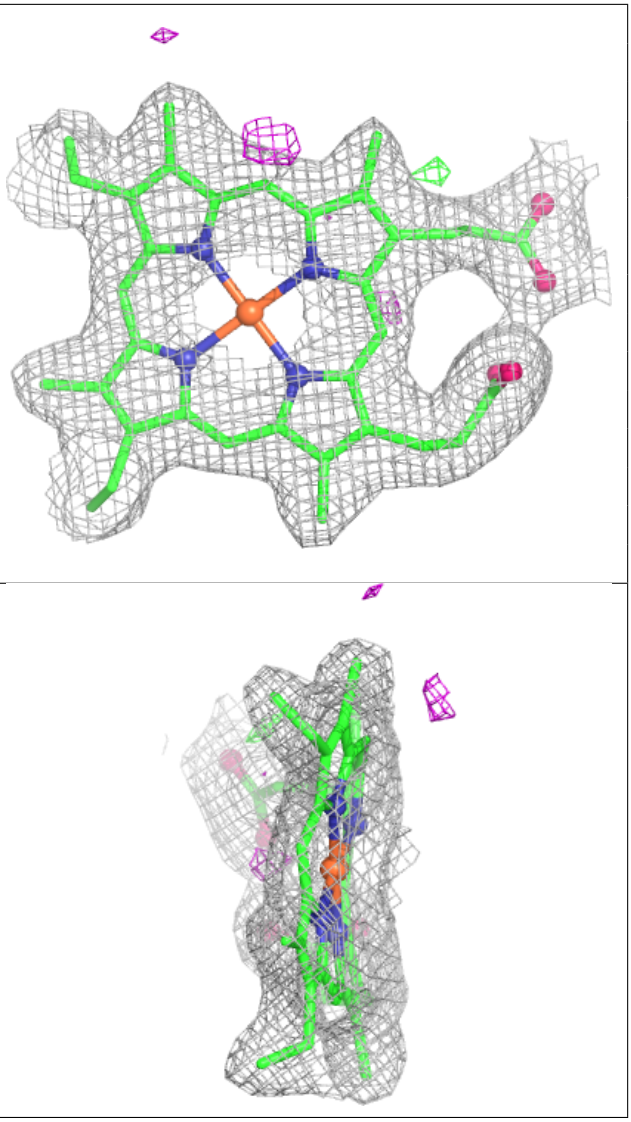






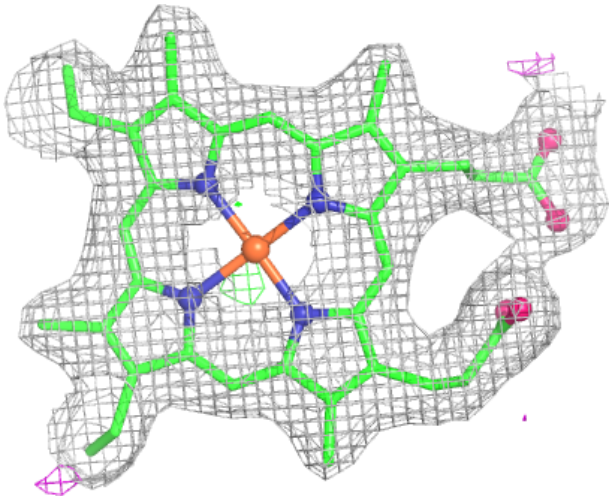
Electron density around HEC D 507:

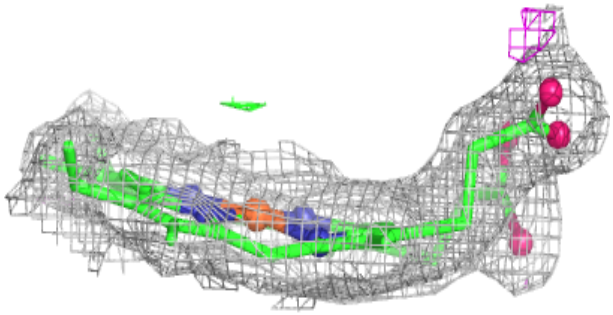
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

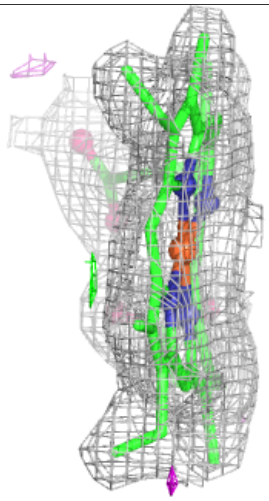


Electron density around HEC C 506:

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

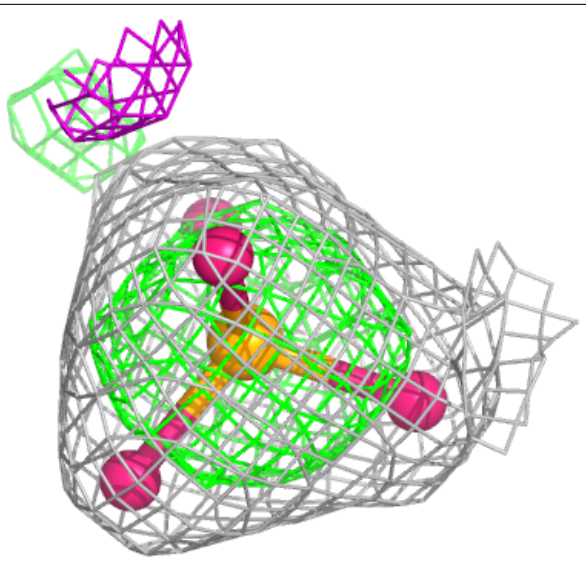


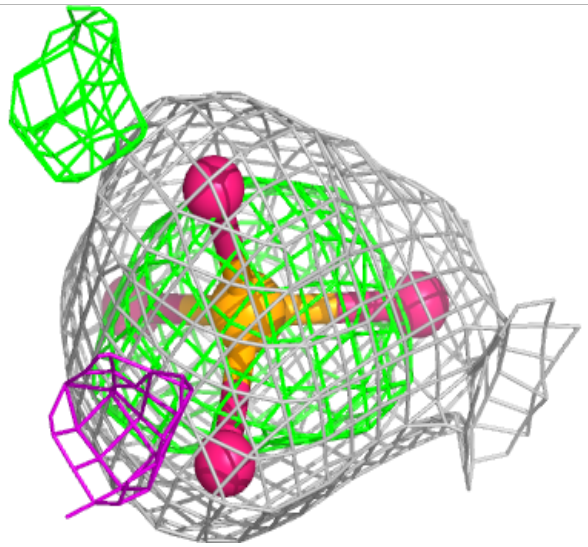


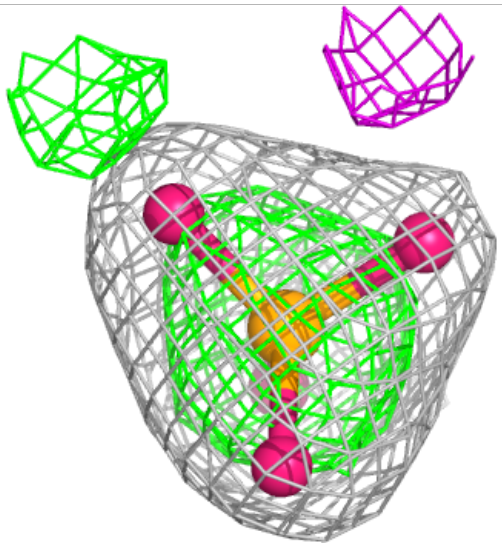


Electron density around SE4 B 506:

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

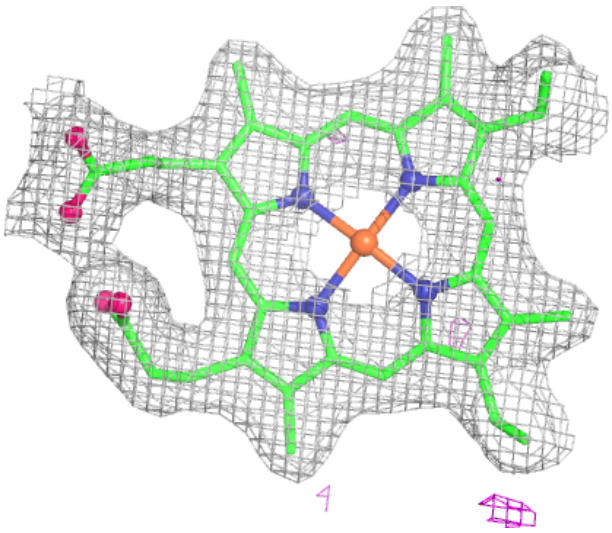


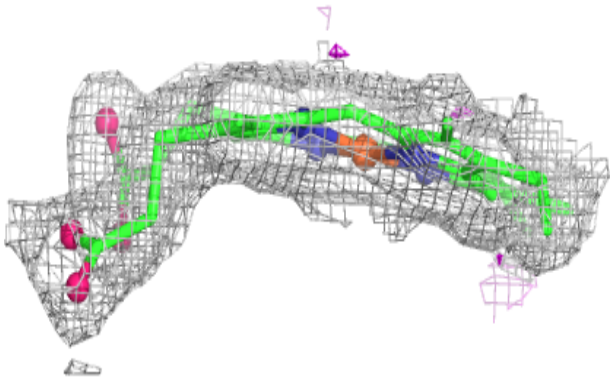




Electron density around HEC A 505:

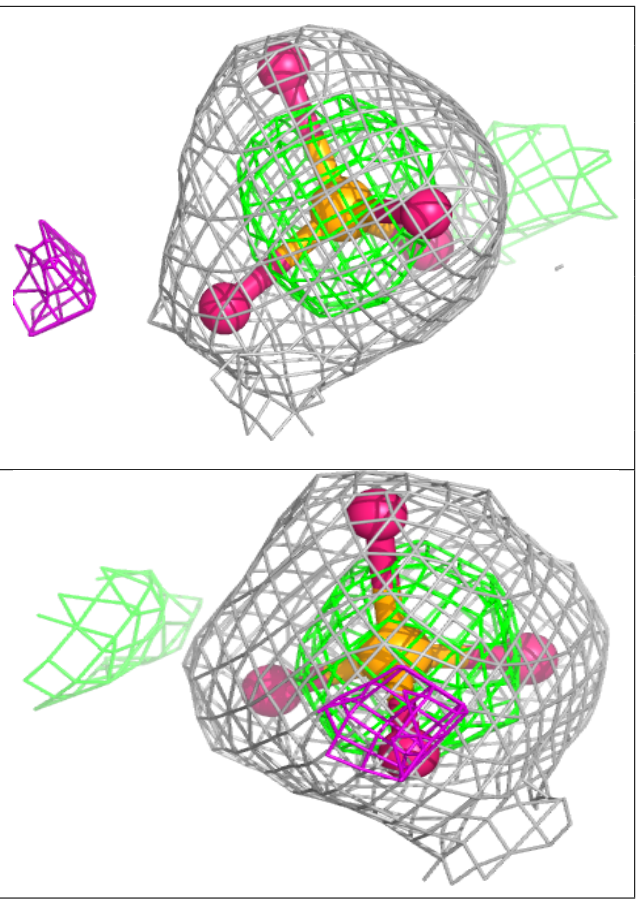
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





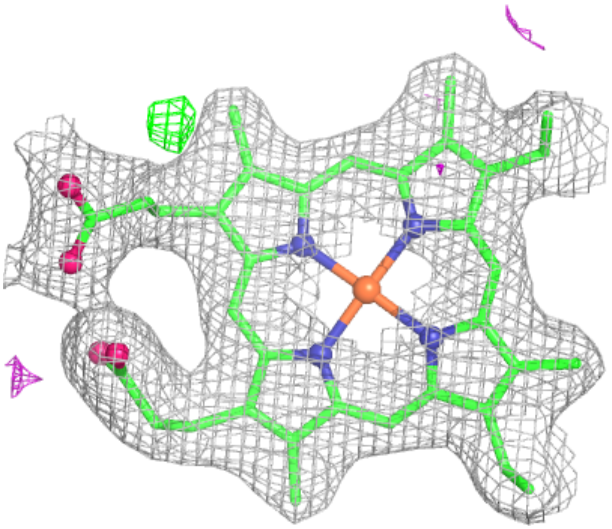
Electron density around SE4 D 508:

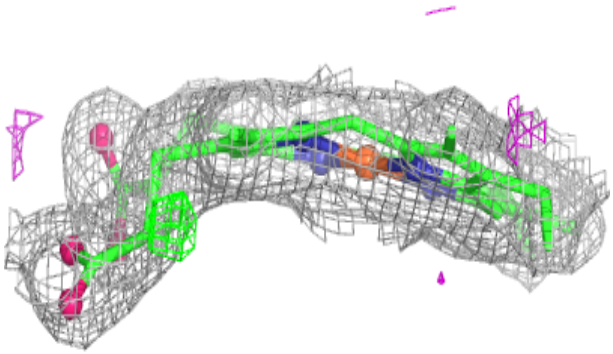
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

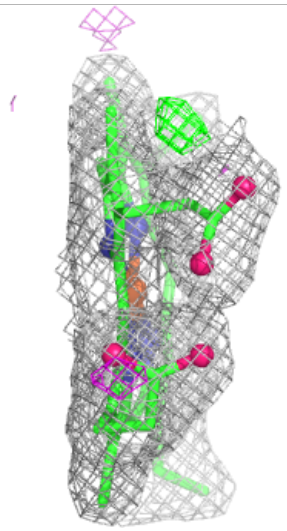


Electron density around HEC B 505:

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

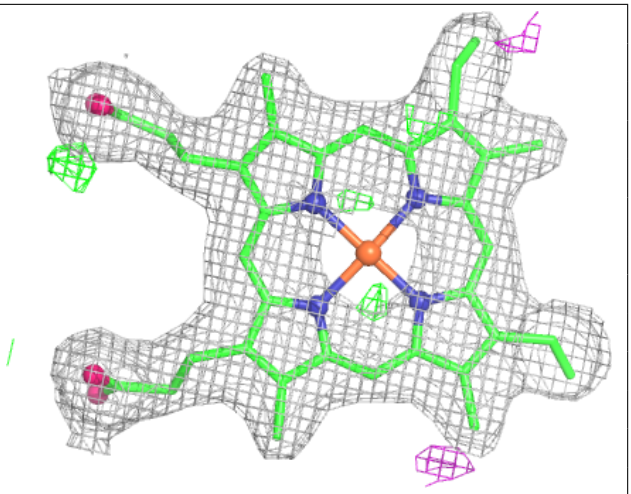


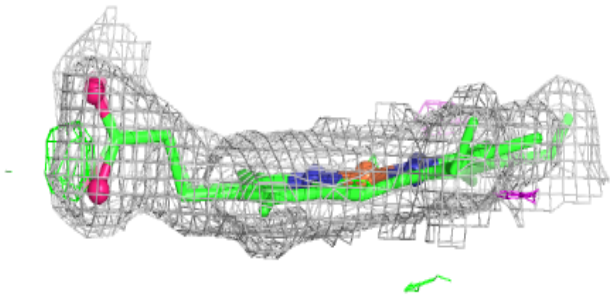




Electron density around HEC A 504:

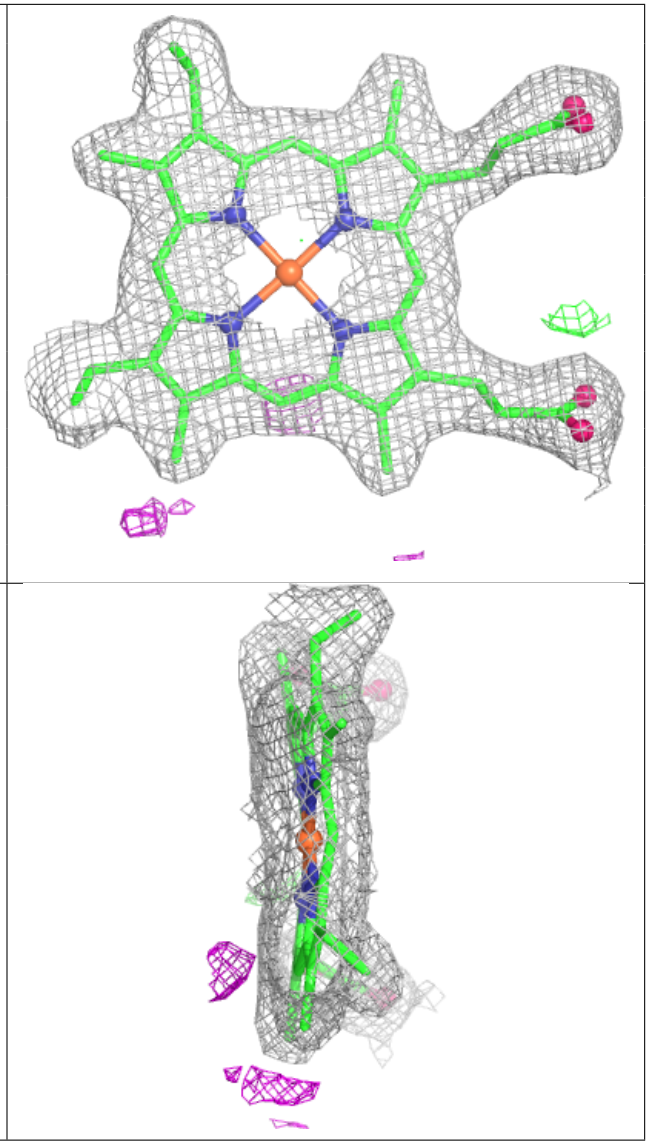
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC D 506:

$2mF_o$-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.