wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 06:53 AM BST

PDB ID	:	6SUV
Title	:	Horse cytochrome c complexed by octa-anionic calixarene
Authors	:	Geremia, S.; Brancatelli, G.
Deposited on	:	2019-09-16
Resolution	:	2.50 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 following versions of software and data (see references (1)) were used in the production of this report:

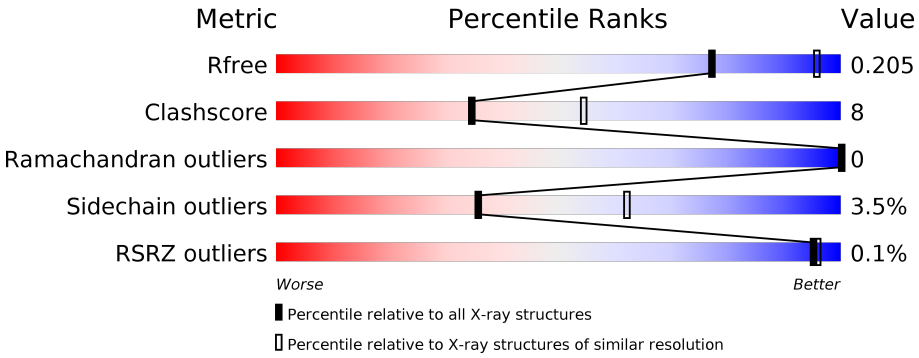
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	AaA	104	96%
1	BaB	104	% 96%
1	CaC	104	99%
1	DaD	104	96%
1	EaE	104	98%
1	FaF	104	97%

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Mol	Chain	Length	Quality of chain
1	GaG	104	97%
1	HaH	104	96%

2 Entry composition (i)

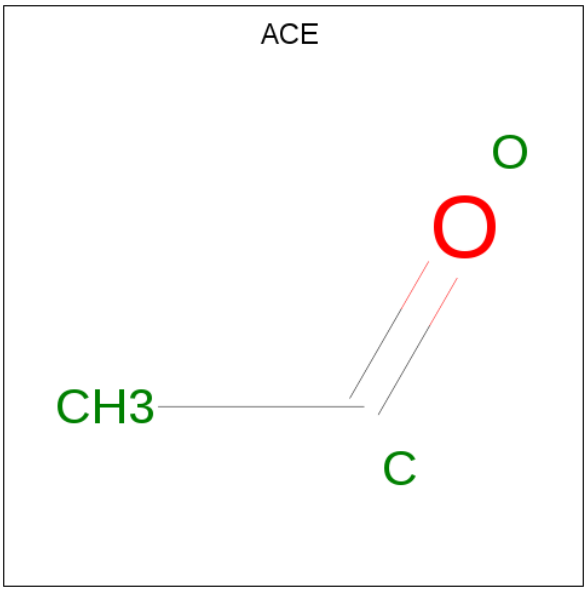
There are 5 unique types of molecules in this entry. The entry contains 7976 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

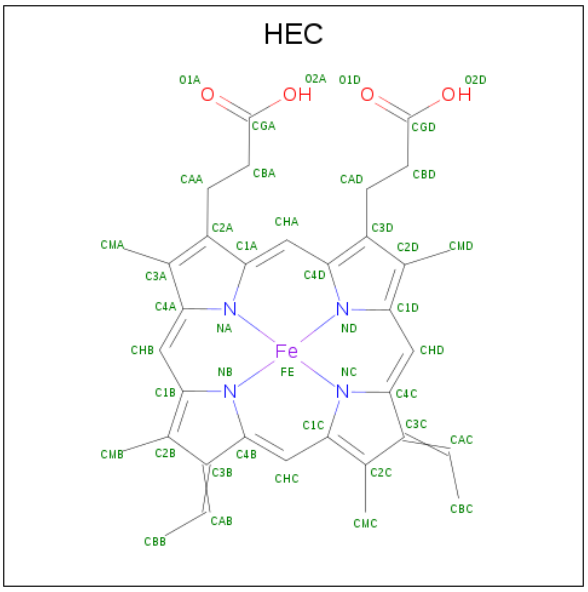
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AaA	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	BaB	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	CaC	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	DaD	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	EaE	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	FaF	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	GaG	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			
1	HaH	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			

- Molecule 2 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).



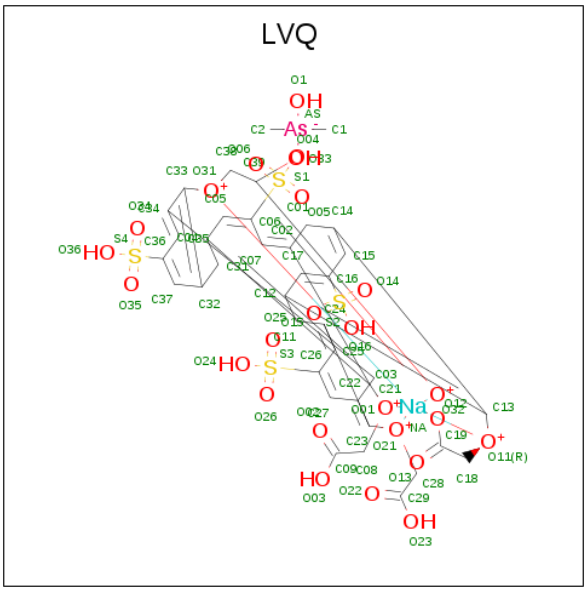
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AaA	1	Total C O 3 2 1	0	0
2	BaB	1	Total C O 3 2 1	0	0
2	CaC	1	Total C O 3 2 1	0	0
2	DaD	1	Total C O 3 2 1	0	0
2	EaE	1	Total C O 3 2 1	0	0
2	FaF	1	Total C O 3 2 1	0	0
2	GaG	1	Total C O 3 2 1	0	0
2	HaH	1	Total C O 3 2 1	0	0

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AaA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	BaB	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	CaC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	DaD	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	EaE	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	FaF	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	GaG	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	HaH	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is octa-anionic calixarene (three-letter code: LVQ) (formula: $C_{38}H_{37}AsNaO_{25}S_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	AaA	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	BaB	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	CaC	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	DaD	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	EaE	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	FaF	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	GaG	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		
4	HaH	1	Total	As	C	Na	O	S	0	0
			69	1	38	1	25	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AaA	52	Total	O	0	0
			52	52		
5	BaB	61	Total	O	0	0
			61	61		
5	CaC	61	Total	O	0	0
			61	61		
5	DaD	64	Total	O	0	0
			64	64		

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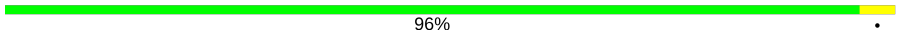
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	EaE	54	Total O 54 54	0	0
5	FaF	61	Total O 61 61	0	0
5	GaG	63	Total O 63 63	0	0
5	HaH	56	Total O 56 56	0	0

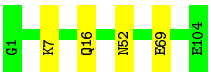
3 Residue-property plots (i)

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

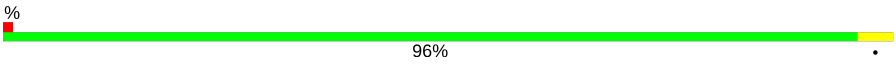
Chain AaA:





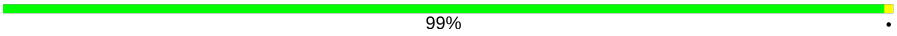
- Molecule 1: Cytochrome c

Chain BaB:



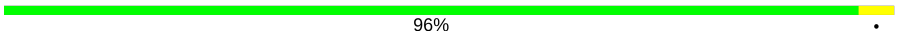
- Molecule 1: Cytochrome c

Chain CaC:



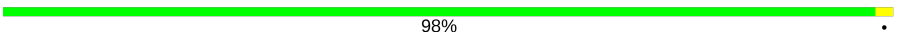
- Molecule 1: Cytochrome c

Chain DaD:



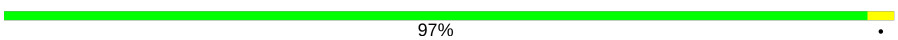
- Molecule 1: Cytochrome c

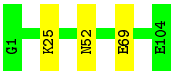
Chain EaE:



- Molecule 1: Cytochrome c

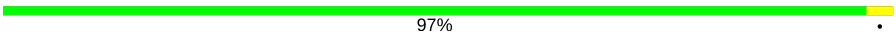
Chain FaF:

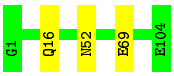




- Molecule 1: Cytochrome c

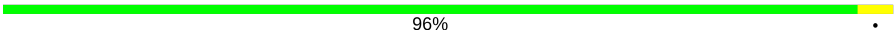
Chain GaG:





- Molecule 1: Cytochrome c

Chain HaH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	65.59Å 65.59Å 250.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 2.50 46.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.38-2.50) 98.0 (46.38-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.170 , 0.237 0.148 , 0.205	Depositor DCC
R_{free} test set	1828 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
Reported twinning fraction	0.499 for H, K, L 0.501 for -K, -H, -L	Depositor
Outliers	0 of 35576 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7976	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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: LVQ, ACE, 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	AaA	0.41	0/839	0.65	0/1118
1	BaB	0.36	0/839	0.63	0/1118
1	CaC	0.41	0/839	0.63	0/1118
1	DaD	0.38	0/839	0.64	0/1118
1	EaE	0.39	0/839	0.66	0/1118
1	FaF	0.39	0/839	0.64	0/1118
1	GaG	0.36	0/839	0.64	0/1118
1	HaH	0.36	0/839	0.61	0/1118
All	All	0.38	0/6712	0.64	0/8944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AaA	823	0	845	0	0
1	BaB	823	0	845	0	0
1	CaC	823	0	845	0	0
1	DaD	823	0	845	0	1
1	EaE	823	0	845	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FaF	823	0	845	0	0
1	GaG	823	0	845	0	0
1	HaH	823	0	844	0	0
2	AaA	3	0	3	0	0
2	BaB	3	0	3	0	0
2	CaC	3	0	3	0	0
2	DaD	3	0	3	0	0
2	EaE	3	0	3	0	0
2	FaF	3	0	3	0	0
2	GaG	3	0	3	0	0
2	HaH	3	0	3	0	0
3	AaA	43	0	30	0	0
3	BaB	43	0	30	0	0
3	CaC	43	0	30	0	0
3	DaD	43	0	30	0	0
3	EaE	43	0	30	0	0
3	FaF	43	0	30	0	0
3	GaG	43	0	30	0	0
3	HaH	43	0	30	0	0
4	AaA	69	0	0	0	0
4	BaB	69	0	0	0	0
4	CaC	69	0	0	0	0
4	DaD	69	0	0	0	0
4	EaE	69	0	0	0	0
4	FaF	69	0	0	0	0
4	GaG	69	0	0	0	1
4	HaH	69	0	0	0	0
5	AaA	52	0	0	0	0
5	BaB	61	0	0	0	0
5	CaC	61	0	0	0	0
5	DaD	64	0	0	0	0
5	EaE	54	0	0	0	0
5	FaF	61	0	0	0	0
5	GaG	63	0	0	0	0
5	HaH	56	0	0	0	0
All	All	7976	0	7023	0	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

There are no clashes within the asymmetric unit.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DaD:72:LYS:NZ	4:GaG:203:LVQ:O05[4_555]	2.01	0.19

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	AaA	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	BaB	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	CaC	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	DaD	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
1	EaE	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	FaF	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
1	GaG	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	HaH	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
All	All	816/832 (98%)	798 (98%)	18 (2%)	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	AaA	86/86 (100%)	82 (95%)	4 (5%)	26	49
1	BaB	86/86 (100%)	82 (95%)	4 (5%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CaC	86/86 (100%)	85 (99%)	1 (1%)	71 88
1	DaD	86/86 (100%)	83 (96%)	3 (4%)	36 62
1	EaE	86/86 (100%)	84 (98%)	2 (2%)	50 76
1	FaF	86/86 (100%)	83 (96%)	3 (4%)	36 62
1	GaG	86/86 (100%)	83 (96%)	3 (4%)	36 62
1	HaH	86/86 (100%)	82 (95%)	4 (5%)	26 49
All	All	688/688 (100%)	664 (96%)	24 (4%)	36 62

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DaD	60	LYS
1	EaE	69	GLU
1	HaH	60	LYS
1	DaD	69	GLU
1	EaE	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	HEC	AaA	202	1	26,50,50	1.19	2 (7%)	18,82,82	1.76	2 (11%)
2	ACE	DaD	201	1	1,2,2	0.20	0	1,1,1	0.51	0
2	ACE	HaH	201	1	1,2,2	0.40	0	1,1,1	0.55	0
2	ACE	CaC	201	1	1,2,2	0.22	0	1,1,1	0.38	0
4	LVQ	CaC	203	-	62,78,78	1.57	11 (17%)	91,136,136	2.48	27 (29%)
3	HEC	BaB	202	1	26,50,50	1.12	2 (7%)	18,82,82	1.98	6 (33%)
4	LVQ	BaB	203	-	62,78,78	1.80	11 (17%)	91,136,136	2.35	28 (30%)
2	ACE	AaA	201	1	1,2,2	0.07	0	1,1,1	0.69	0
4	LVQ	HaH	203	-	62,78,78	1.74	9 (14%)	91,136,136	2.60	33 (36%)
2	ACE	GaG	201	1	1,2,2	0.17	0	1,1,1	0.43	0
2	ACE	BaB	201	1	1,2,2	0.27	0	1,1,1	0.53	0
3	HEC	DaD	202	1	26,50,50	1.27	2 (7%)	18,82,82	1.73	4 (22%)
4	LVQ	DaD	203	-	62,78,78	1.96	13 (20%)	91,136,136	2.61	37 (40%)
3	HEC	FaF	202	1	26,50,50	0.95	1 (3%)	18,82,82	1.90	4 (22%)
3	HEC	GaG	202	1	26,50,50	1.15	2 (7%)	18,82,82	1.95	6 (33%)
4	LVQ	GaG	203	-	62,78,78	1.67	11 (17%)	91,136,136	2.47	33 (36%)
4	LVQ	FaF	203	-	62,78,78	1.98	16 (25%)	91,136,136	2.68	36 (39%)
4	LVQ	EaE	203	-	62,78,78	1.67	7 (11%)	91,136,136	2.50	34 (37%)
2	ACE	FaF	201	1	1,2,2	0.02	0	1,1,1	0.69	0
4	LVQ	AaA	203	-	62,78,78	1.69	9 (14%)	91,136,136	2.05	24 (26%)
2	ACE	EaE	201	1	1,2,2	0.15	0	1,1,1	0.54	0
3	HEC	CaC	202	1	26,50,50	1.03	2 (7%)	18,82,82	1.97	4 (22%)
3	HEC	HaH	202	1	26,50,50	1.23	2 (7%)	18,82,82	2.12	4 (22%)
3	HEC	EaE	202	1	26,50,50	0.86	1 (3%)	18,82,82	1.57	2 (11%)

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	LVQ	BaB	203	-	-	3/26/131/131	-
4	LVQ	EaE	203	-	-	1/26/131/131	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LVQ	HaH	203	-	-	1/26/131/131	-
4	LVQ	DaD	203	-	-	1/26/131/131	-
3	HEC	DaD	202	1	-	0/6/54/54	-
4	LVQ	AaA	203	-	-	2/26/131/131	-
3	HEC	FaF	202	1	-	0/6/54/54	-
3	HEC	AaA	202	1	-	0/6/54/54	-
4	LVQ	GaG	203	-	-	1/26/131/131	-
3	HEC	BaB	202	1	-	1/6/54/54	-
3	HEC	CaC	202	1	-	0/6/54/54	-
4	LVQ	CaC	203	-	-	2/26/131/131	-
4	LVQ	FaF	203	-	-	1/26/131/131	-
3	HEC	GaG	202	1	-	0/6/54/54	-
3	HEC	HaH	202	1	-	0/6/54/54	-
3	HEC	EaE	202	1	-	1/6/54/54	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BaB	203	LVQ	AS-C2	7.55	1.98	1.90
4	FaF	203	LVQ	AS-C2	7.11	1.98	1.90
4	DaD	203	LVQ	AS-C2	7.09	1.98	1.90
4	BaB	203	LVQ	AS-C1	6.74	1.98	1.90
4	EaE	203	LVQ	AS-C2	6.72	1.97	1.90

The worst 5 of 284 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	HaH	203	LVQ	O33-C39-O32	-13.95	116.22	125.68
4	EaE	203	LVQ	O33-C39-O32	-13.52	116.51	125.68
4	DaD	203	LVQ	O33-C39-O32	-13.40	116.59	125.68
4	FaF	203	LVQ	O33-C39-O32	-12.55	117.17	125.68
4	BaB	203	LVQ	O33-C39-O32	-11.17	118.10	125.68

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CaC	203	LVQ	C29-C28-O21-C23
4	AaA	203	LVQ	C09-C08-O01-C03
4	DaD	203	LVQ	C29-C28-O21-C23
4	FaF	203	LVQ	C29-C28-O21-C23

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Mol	Chain	Res	Type	Atoms
4	EaE	203	LVQ	C29-C28-O21-C23

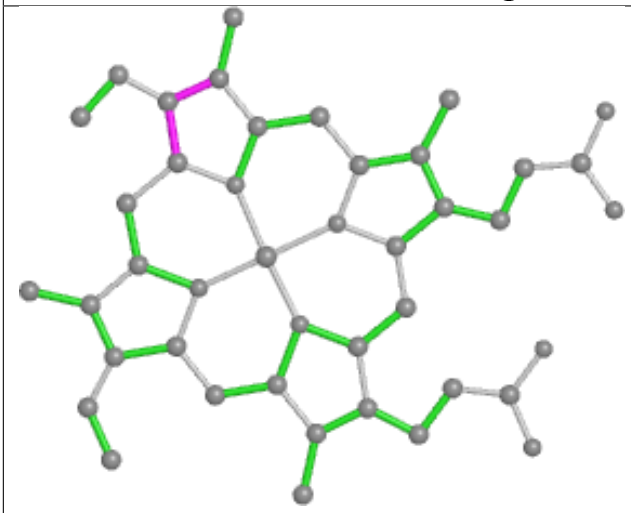
There are no ring outliers.

1 monomer is involved in 1 short contact:

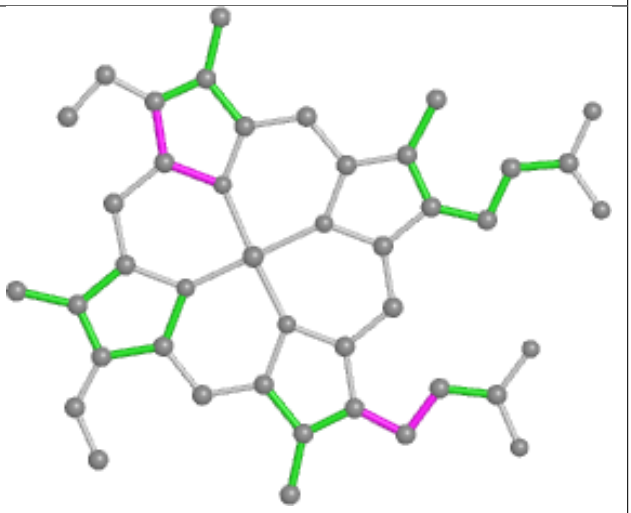
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	GaG	203	LVQ	0	1

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.

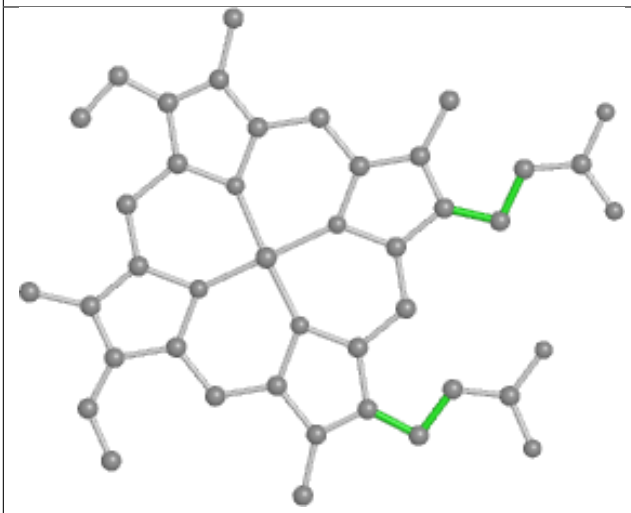
Ligand HEC AaA 202



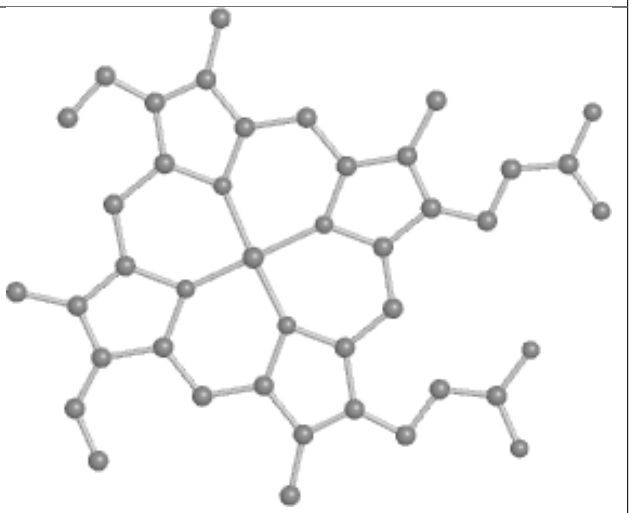
Bond lengths



Bond angles

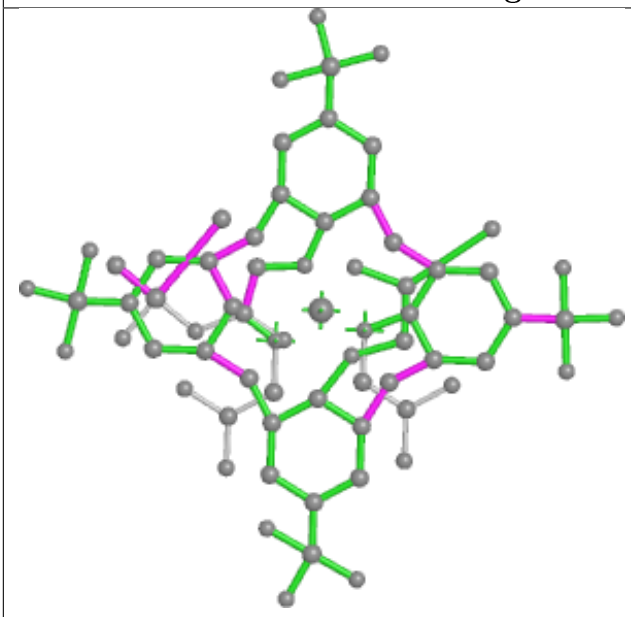


Torsions

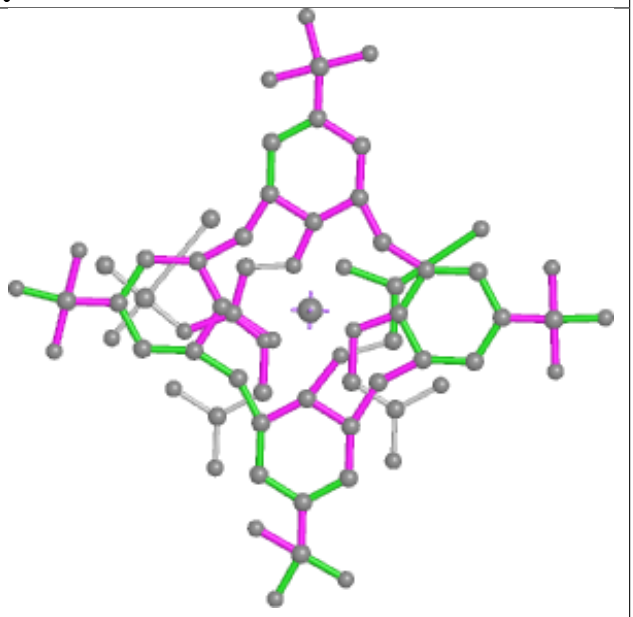


Rings

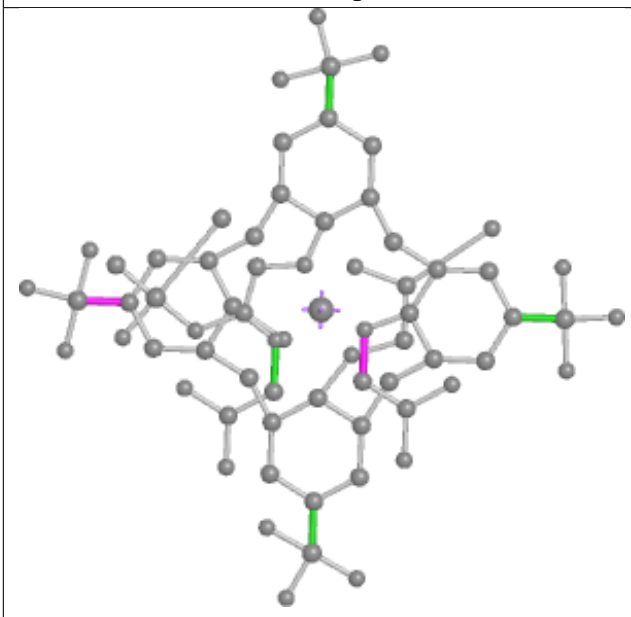
Ligand LVQ CaC 203



Bond lengths



Bond angles



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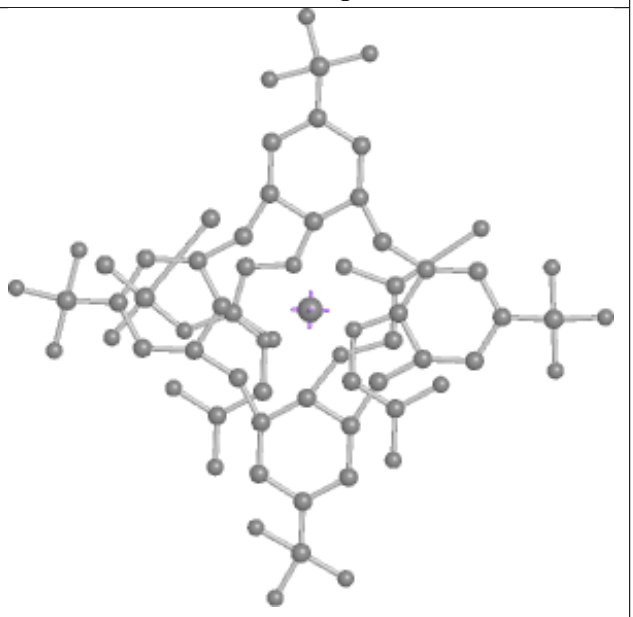
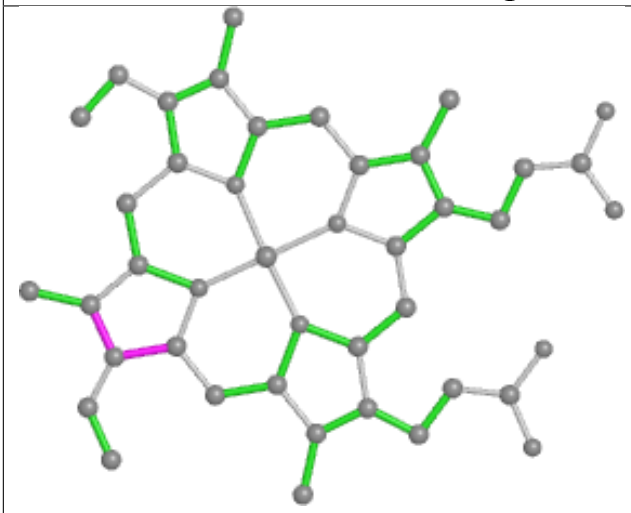
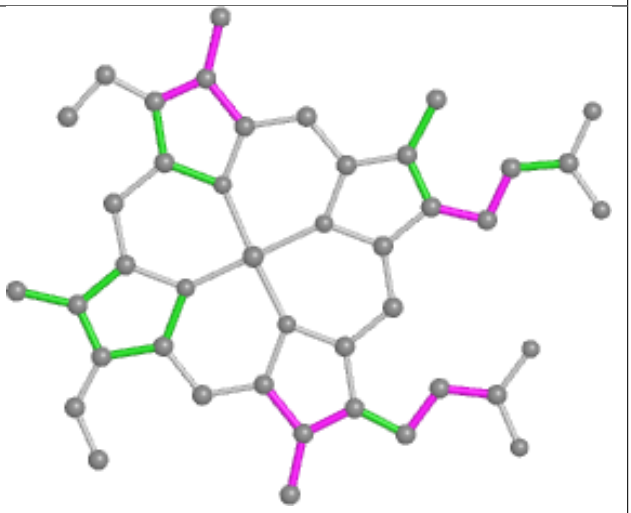


Rings

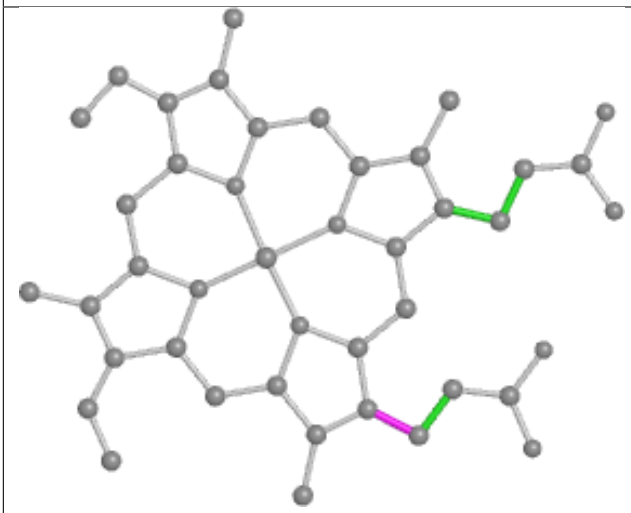
Ligand HEC BaB 202



Bond lengths



Bond angles



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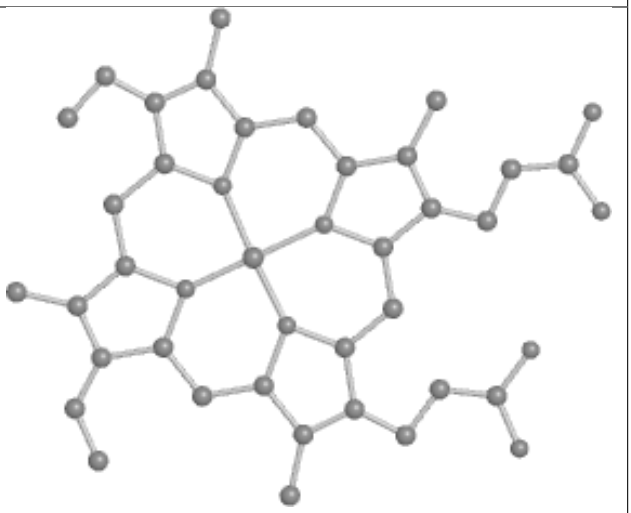
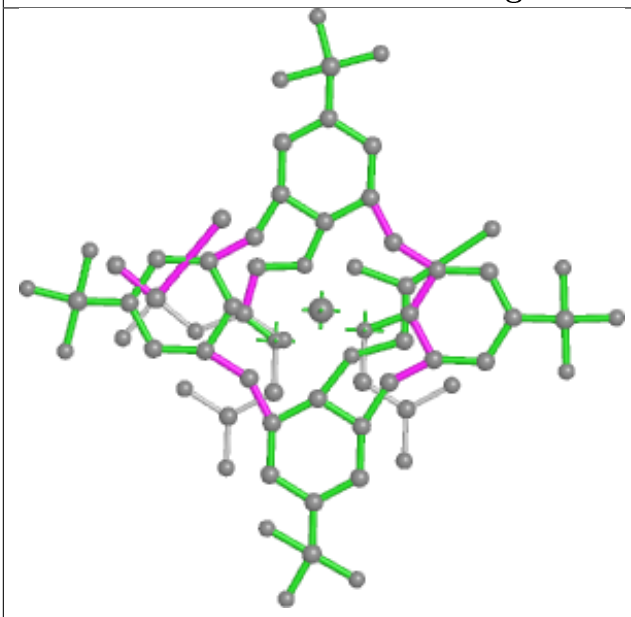
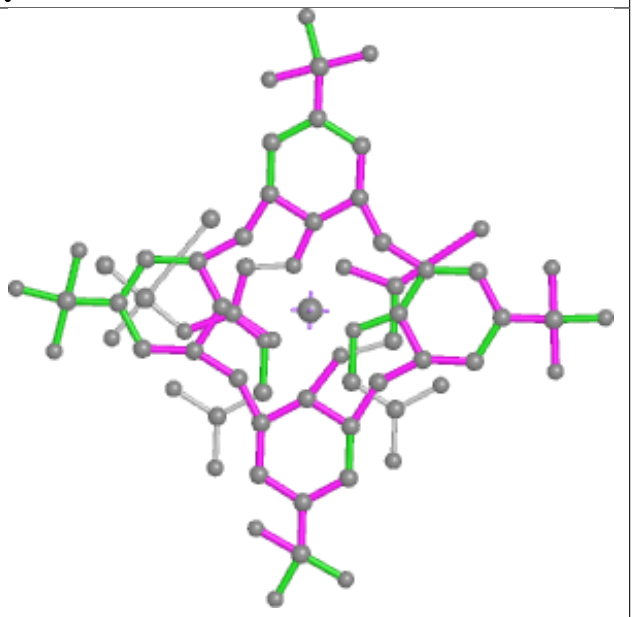


Rings

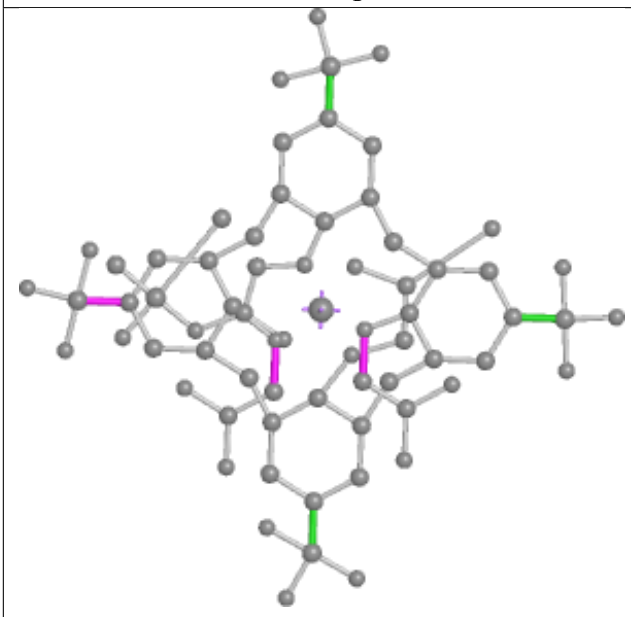
Ligand LVQ BaB 203



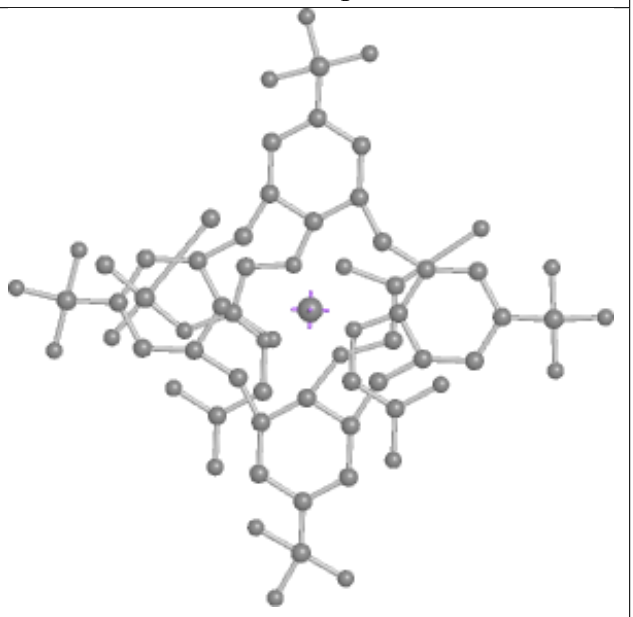
Bond lengths



Bond angles

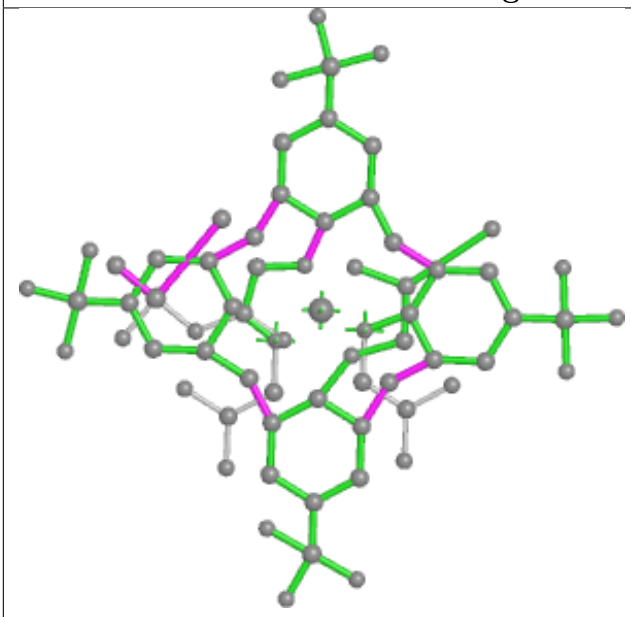


Torsions

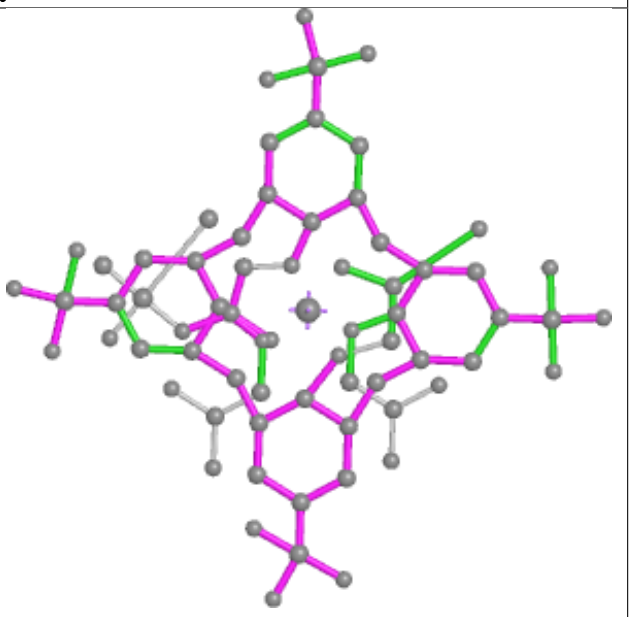


Rings

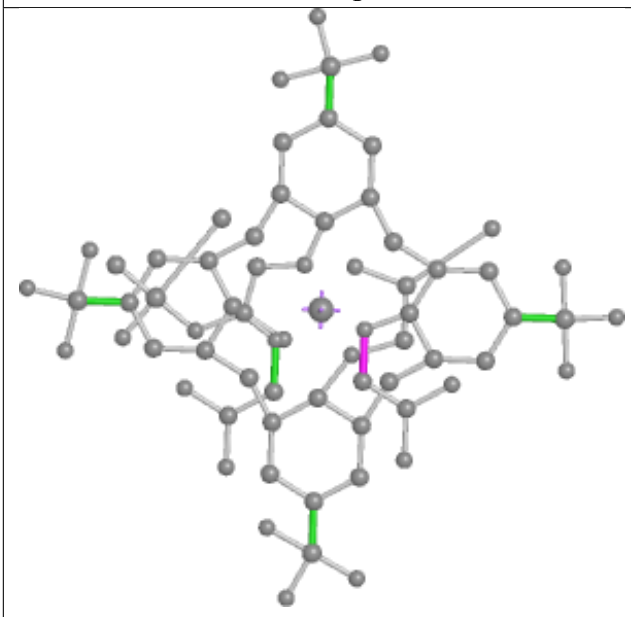
Ligand LVQ HaH 203



Bond lengths



Bond angles



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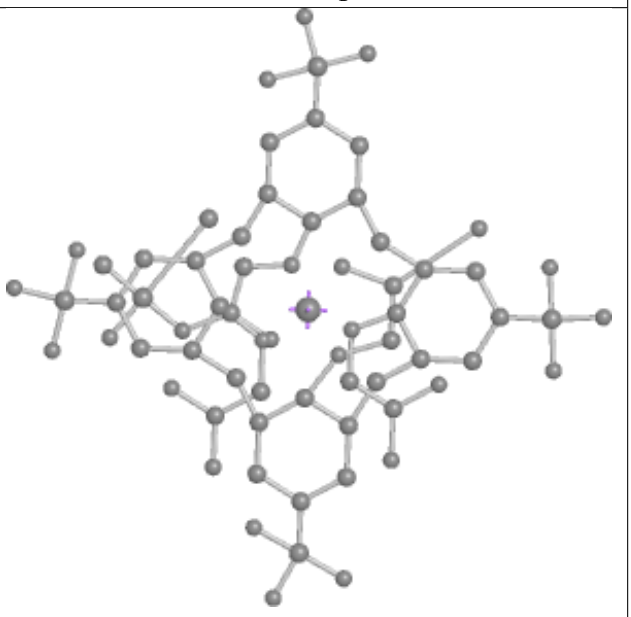
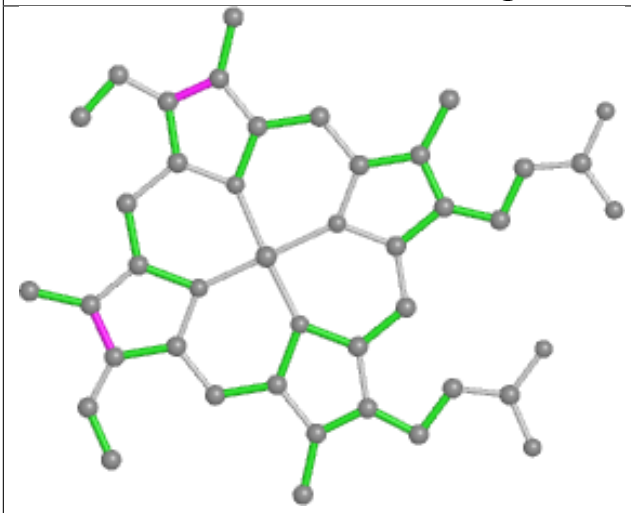
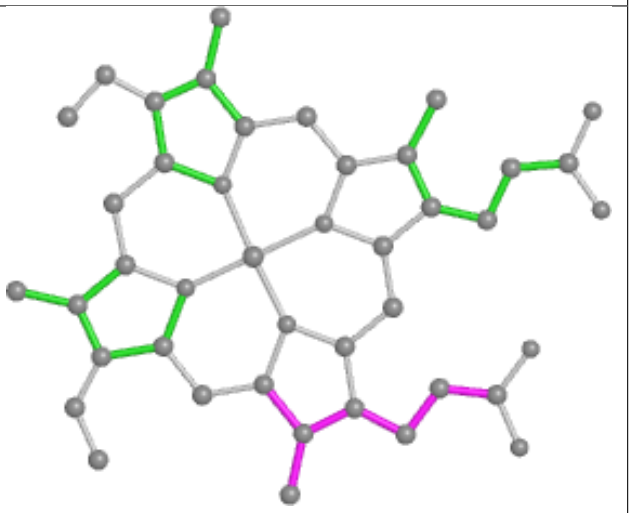


Rings

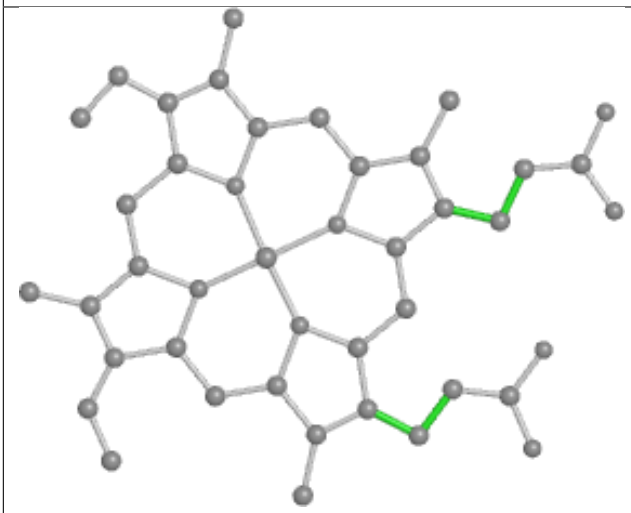
Ligand HEC DaD 202



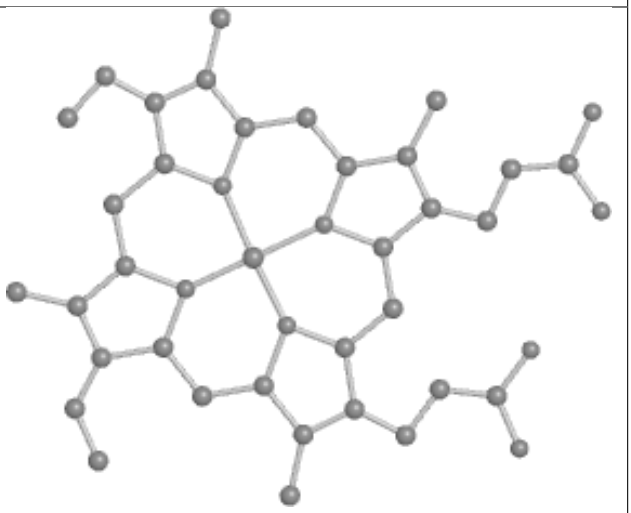
Bond lengths



Bond angles

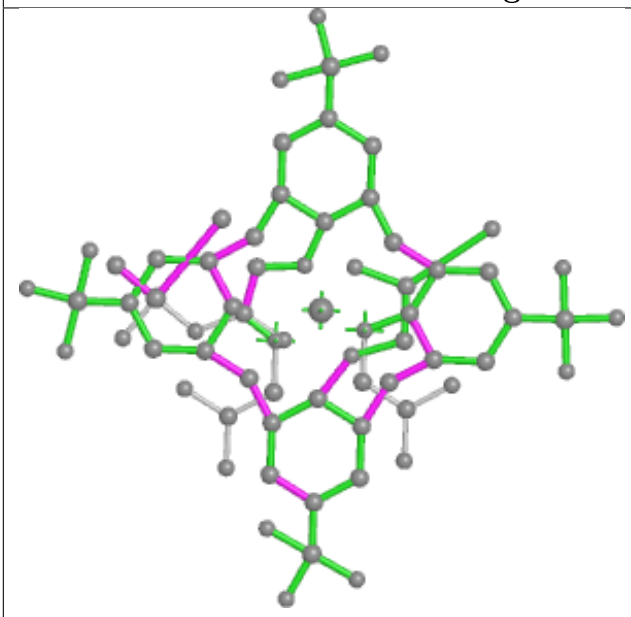


Torsions



Rings

Ligand LVQ DaD 203



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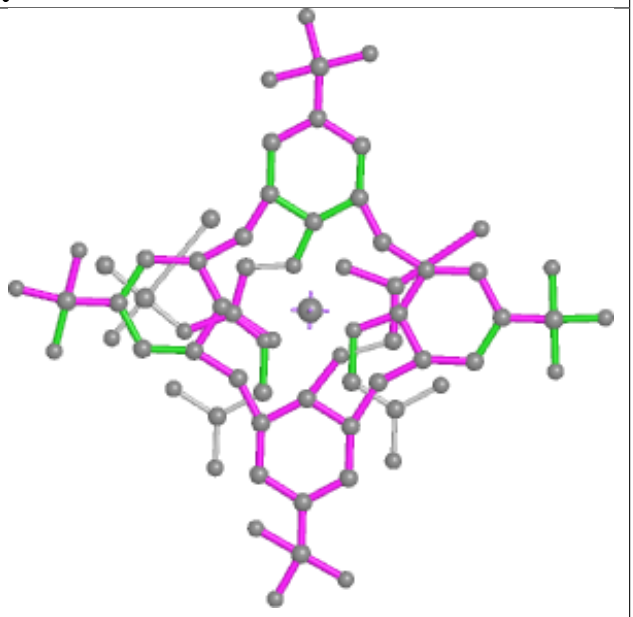
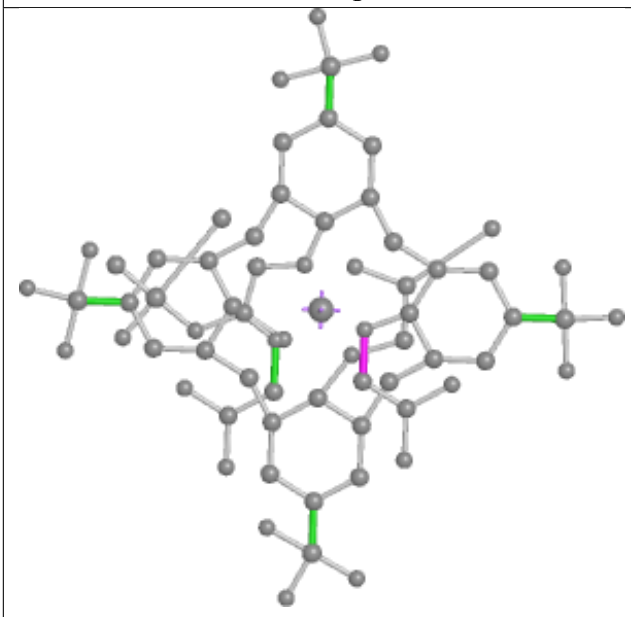


Bond angles



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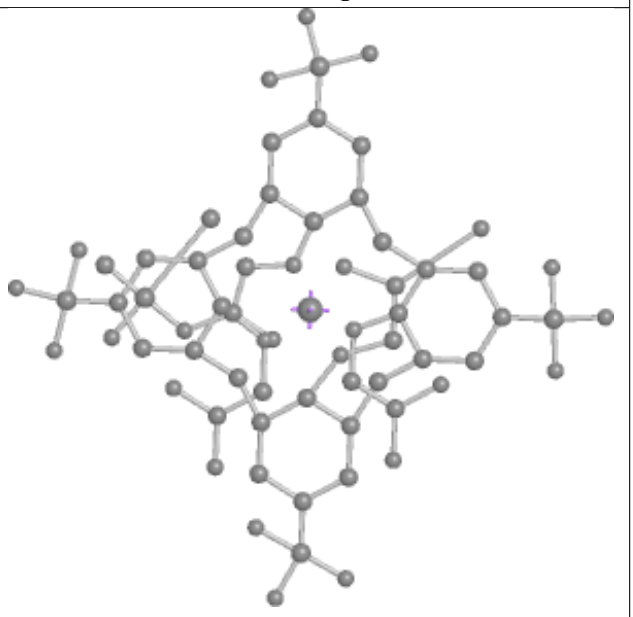
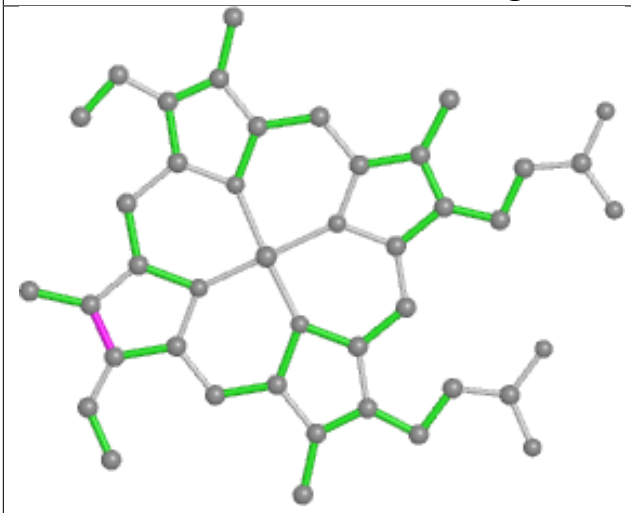
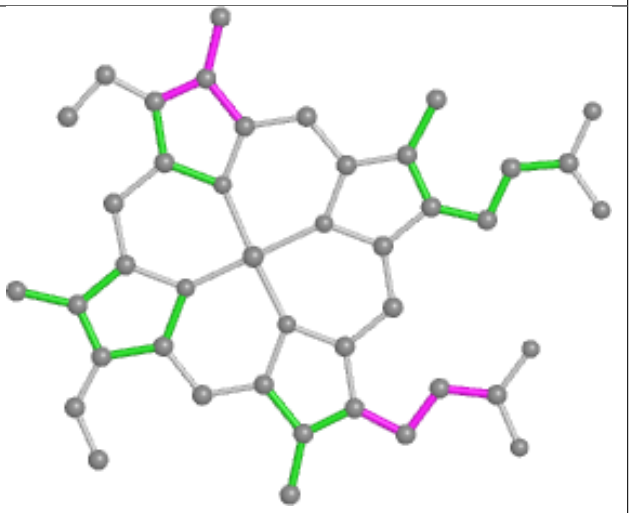


Rings

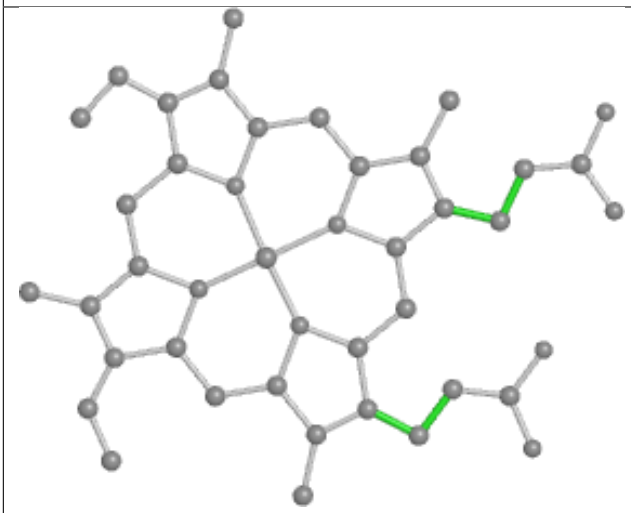
Ligand HEC FaF 202



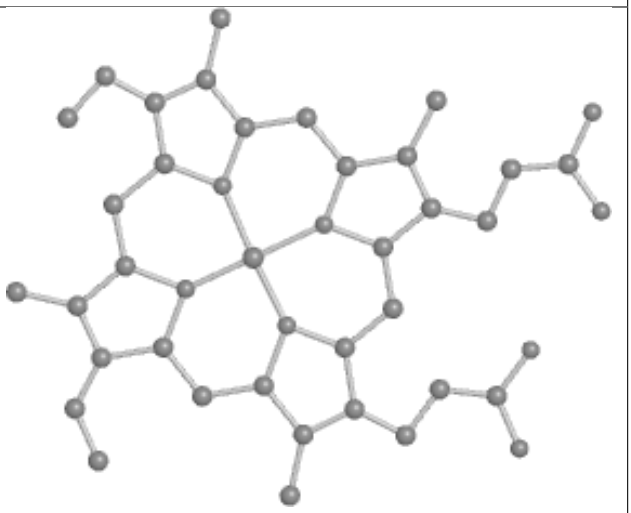
Bond lengths



Bond angles

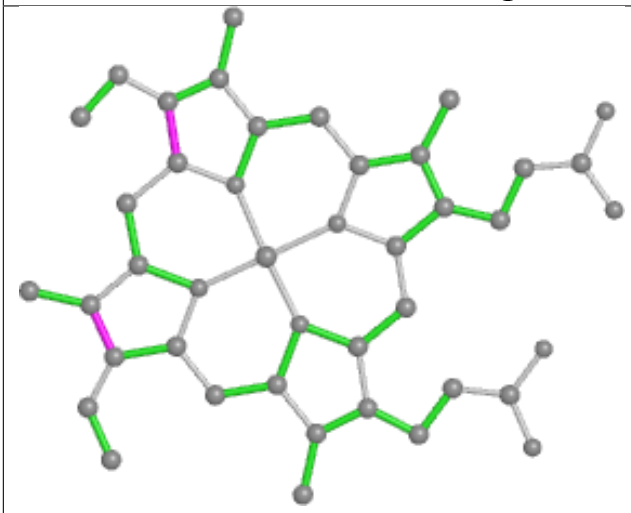


Torsions

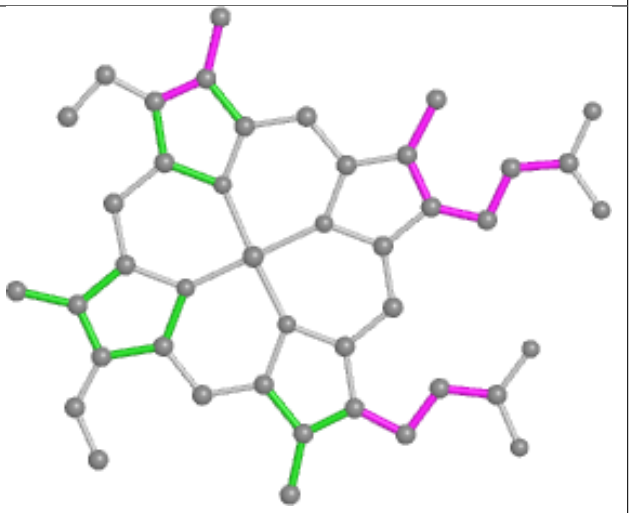


Rings

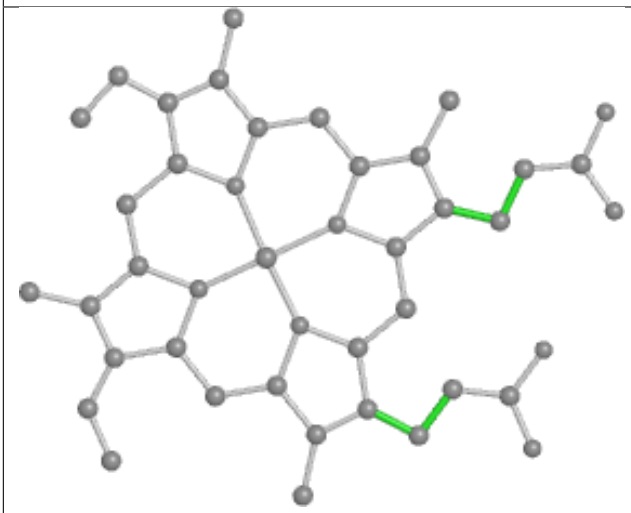
Ligand HEC GaG 202



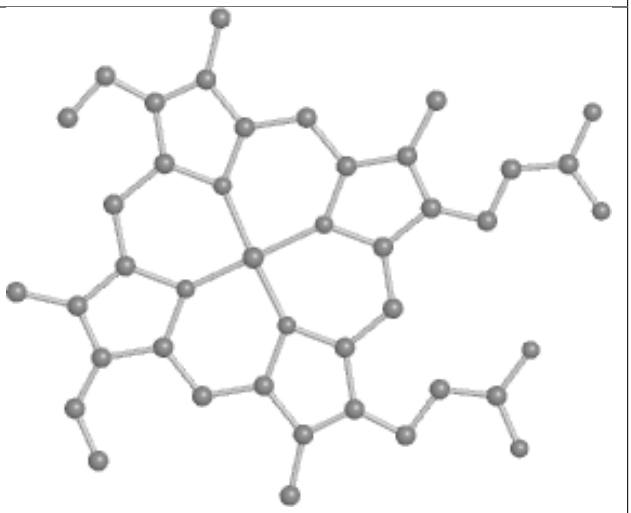
Bond lengths



Bond angles

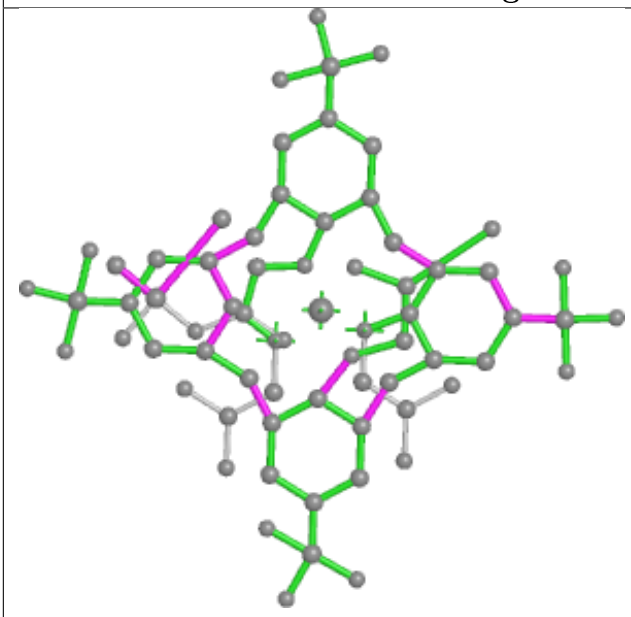


Torsions



Rings

Ligand LVQ GaG 203



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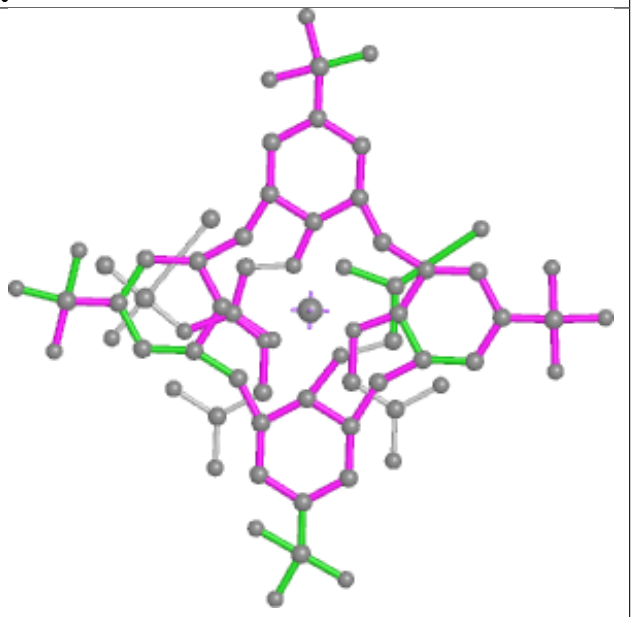
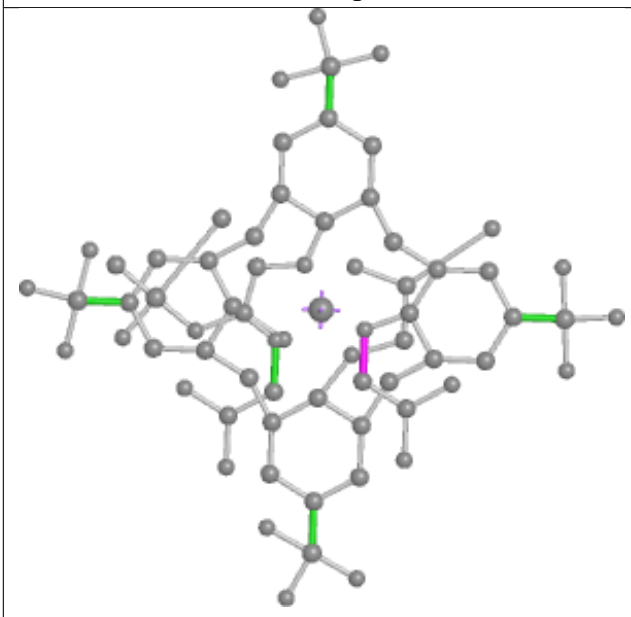
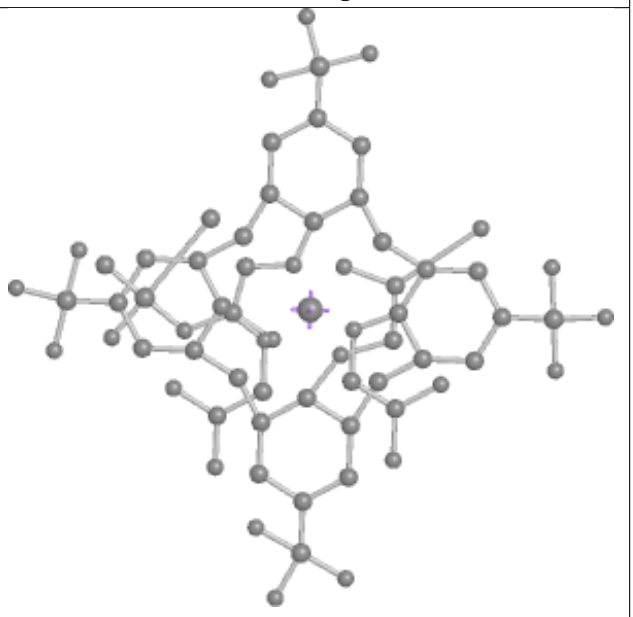


Bond angles

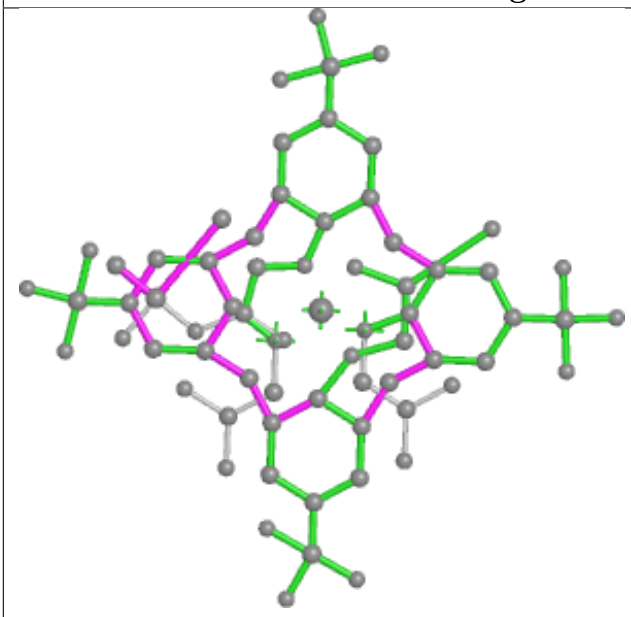


Torsions

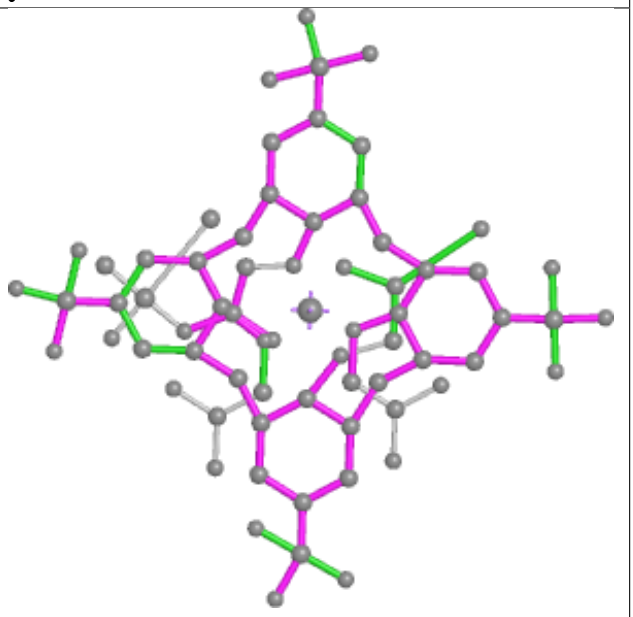


Rings

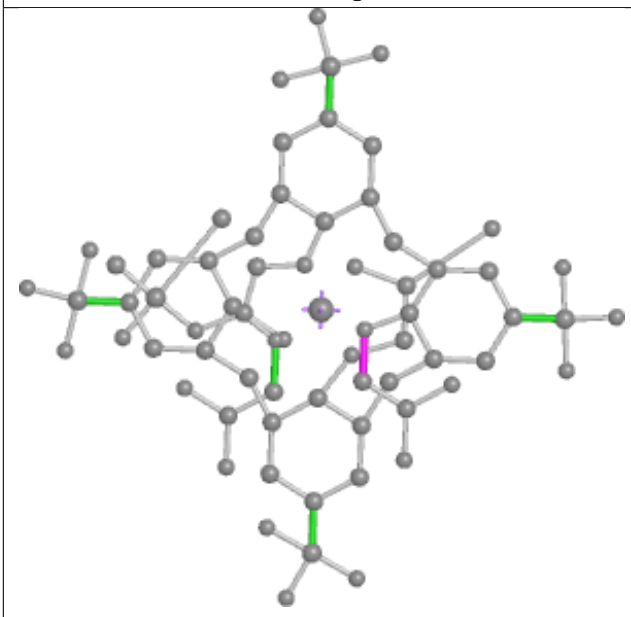
Ligand LVQ FaF 203



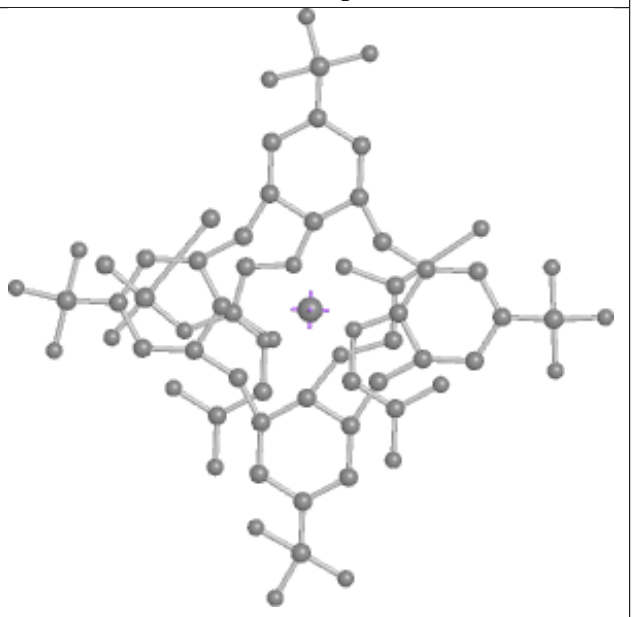
Bond lengths



Bond angles

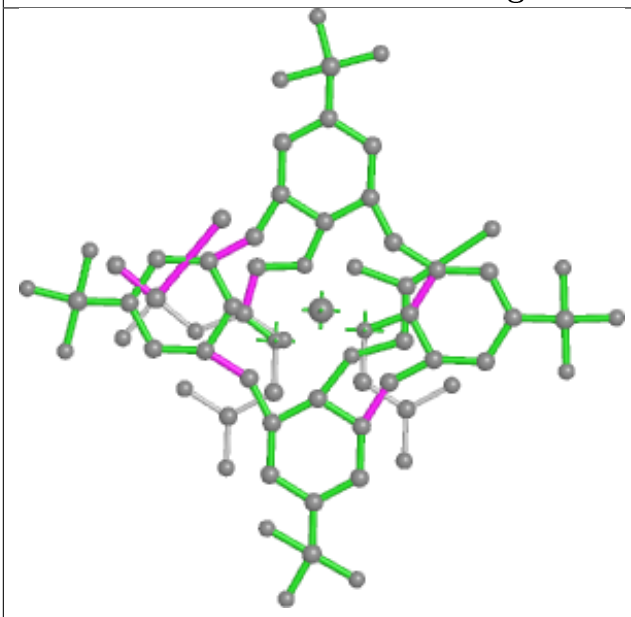


Torsions

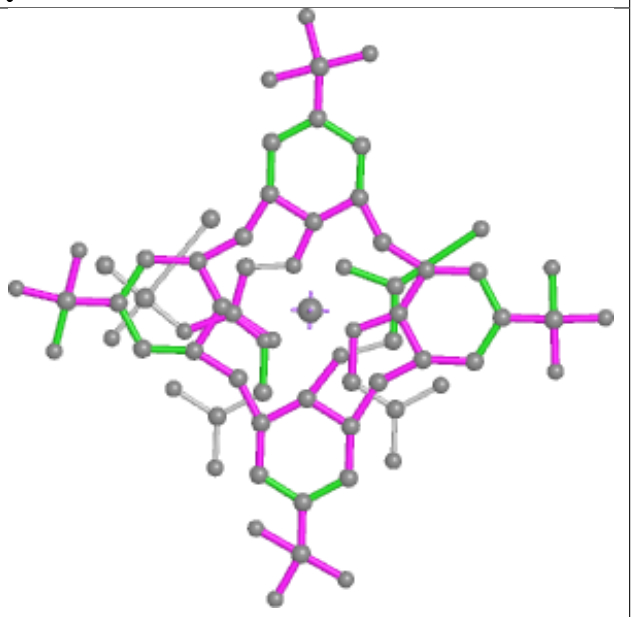


Rings

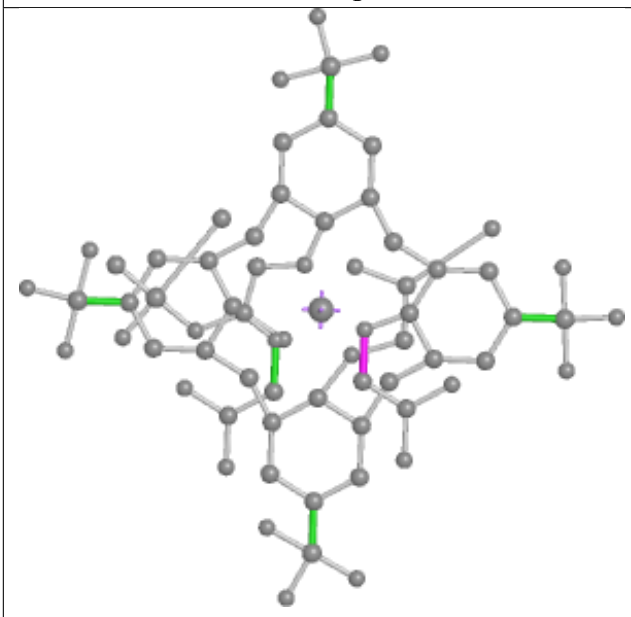
Ligand LVQ EaE 203



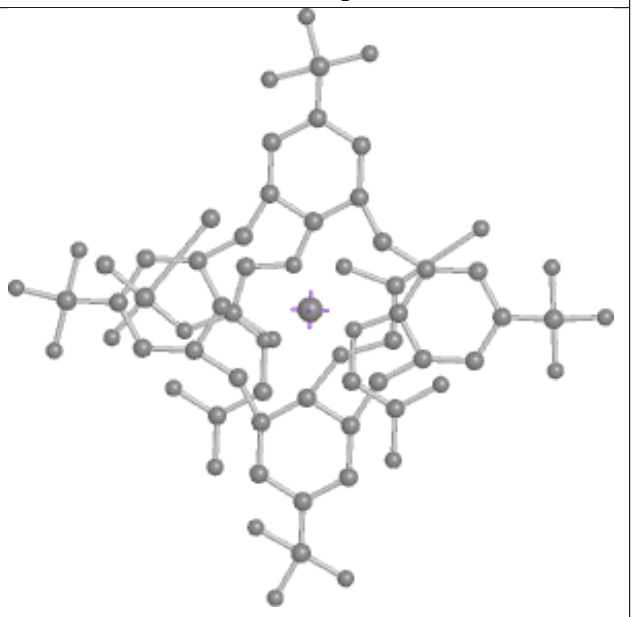
Bond lengths



Bond angles

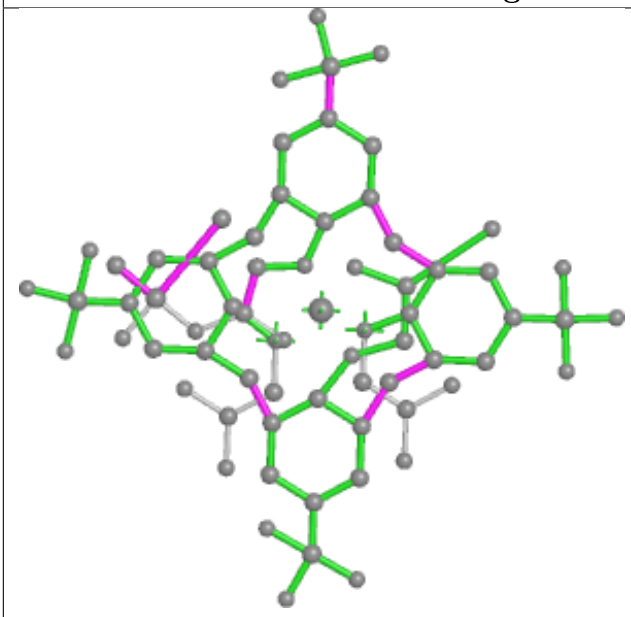


Torsions

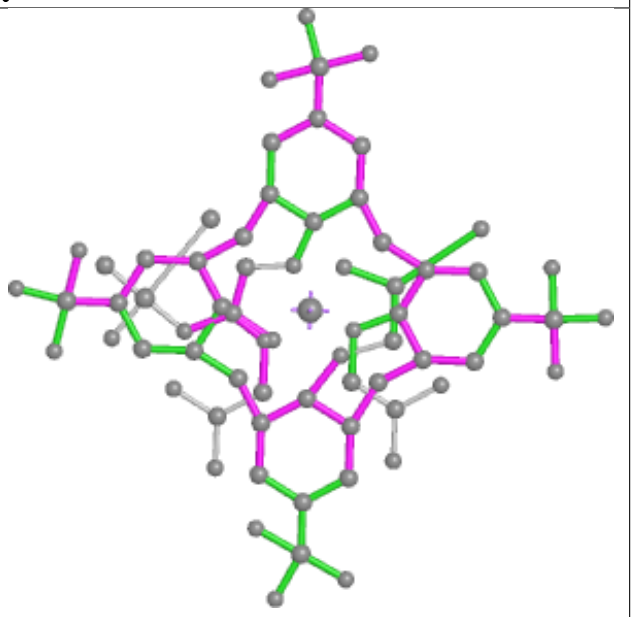


Rings

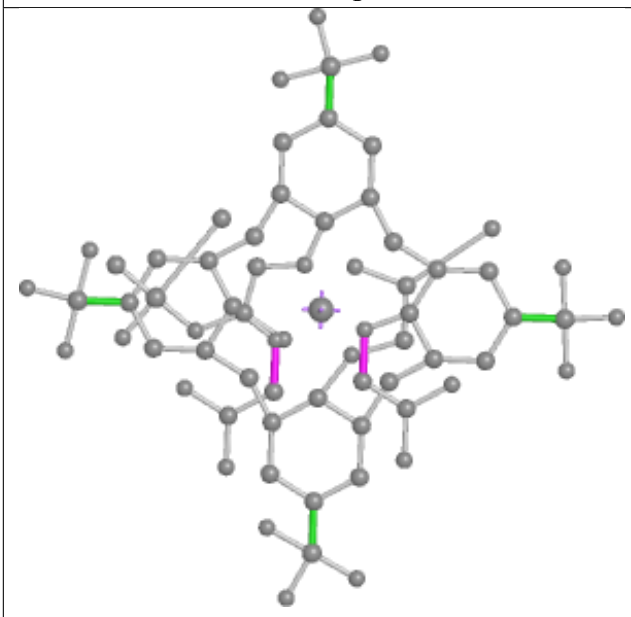
Ligand LVQ AaA 203



Bond lengths



Bond angles



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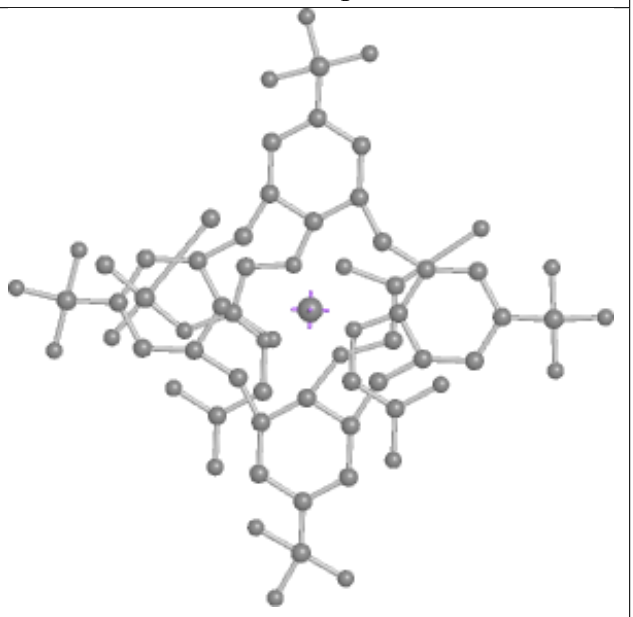
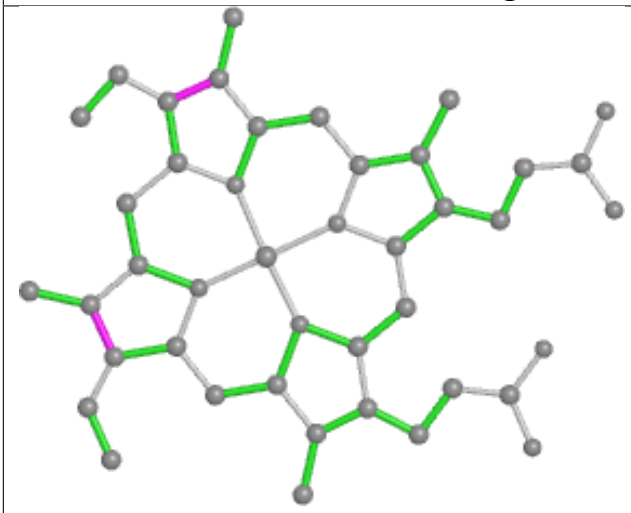
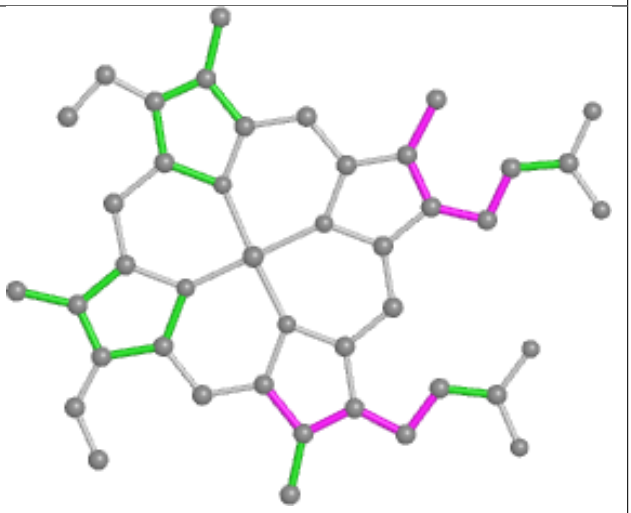


Rings

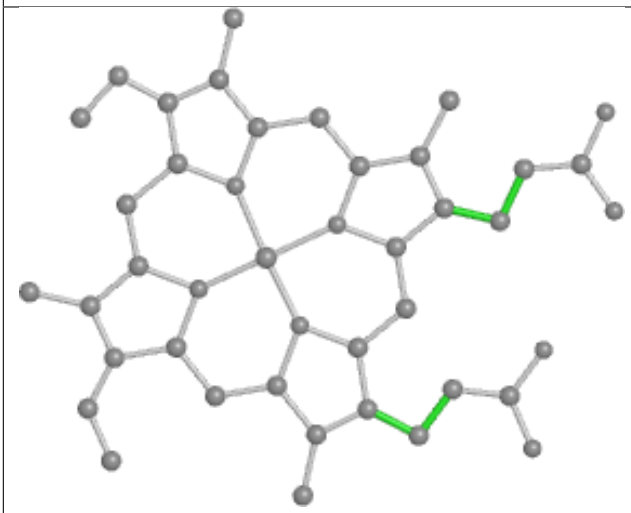
Ligand HEC CaC 202



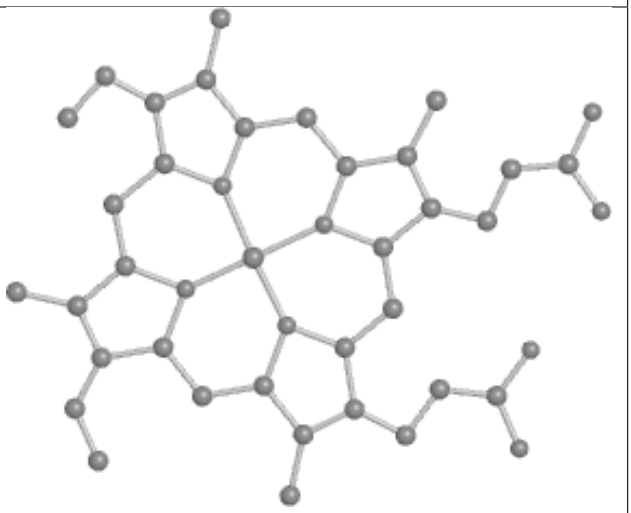
Bond lengths



Bond angles

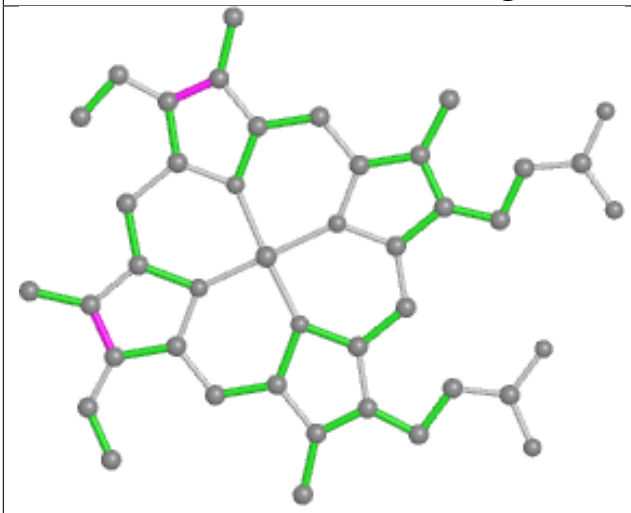


Torsions

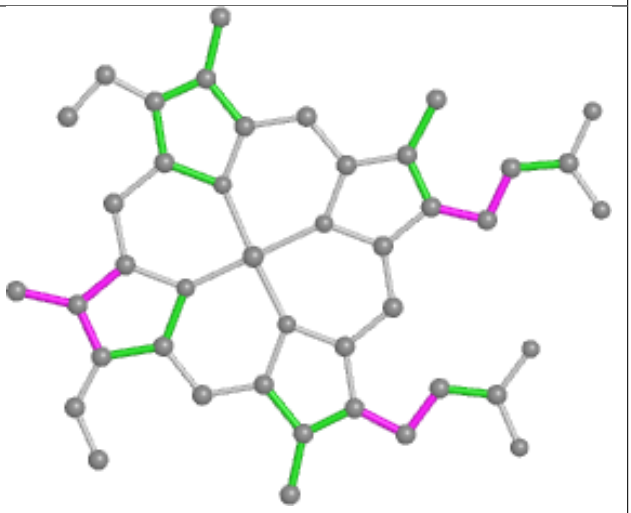


Rings

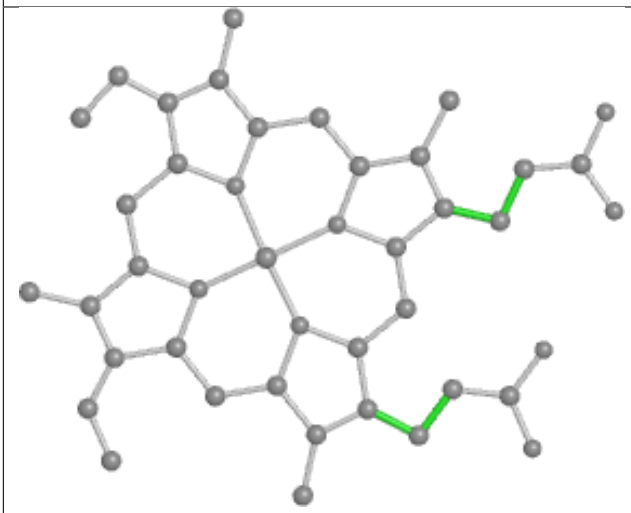
Ligand HEC HaH 202



Bond lengths



Bond angles



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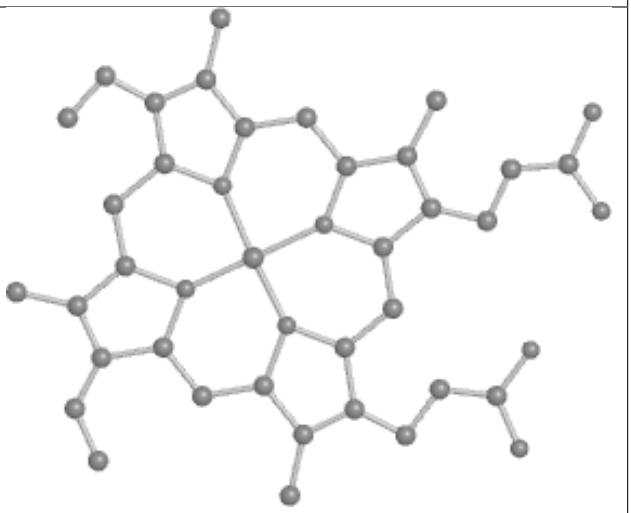
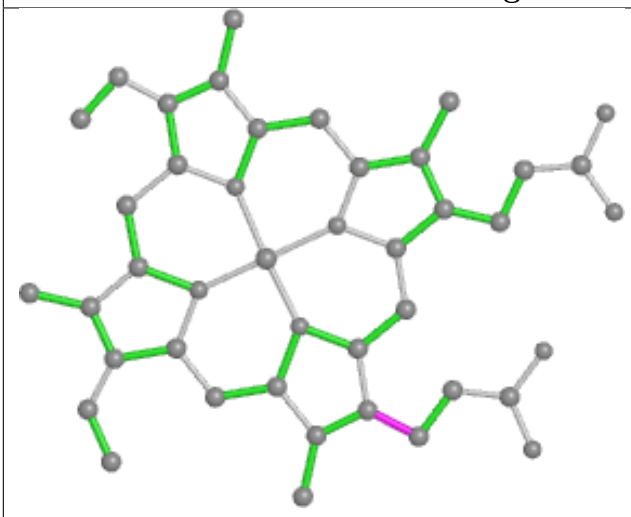
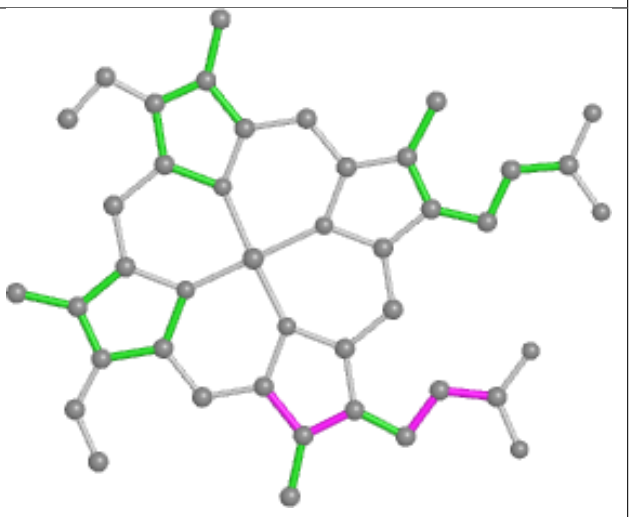


Rings

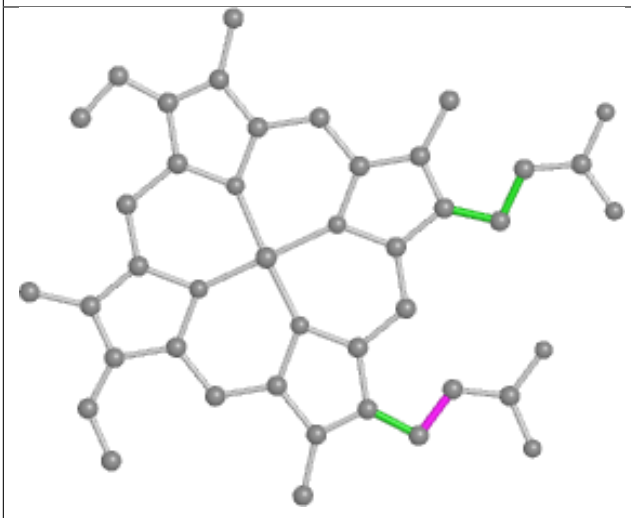
Ligand HEC EaE 202



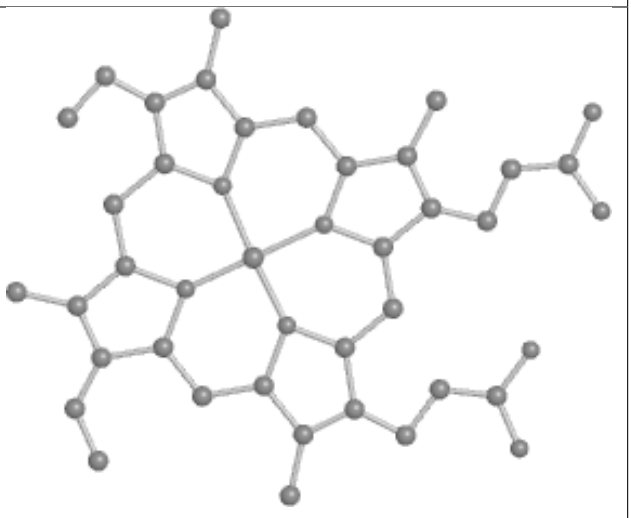
Bond lengths



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	AaA	104/104 (100%)	-0.34	0 100 100	16, 23, 38, 62	0
1	BaB	104/104 (100%)	-0.18	1 (0%) 82 84	15, 29, 42, 88	0
1	CaC	104/104 (100%)	-0.35	0 100 100	14, 23, 40, 51	0
1	DaD	104/104 (100%)	-0.29	0 100 100	13, 23, 37, 62	0
1	EaE	104/104 (100%)	-0.36	0 100 100	14, 24, 39, 64	0
1	FaF	104/104 (100%)	-0.23	0 100 100	14, 27, 42, 64	0
1	GaG	104/104 (100%)	-0.41	0 100 100	12, 21, 33, 71	0
1	HaH	104/104 (100%)	-0.24	0 100 100	17, 27, 38, 49	0
All	All	832/832 (100%)	-0.30	1 (0%) 95 96	12, 24, 41, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BaB	104	GLU	2.0

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

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

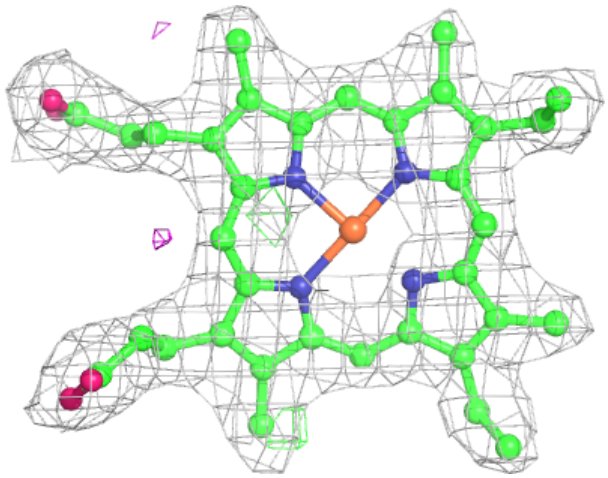
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

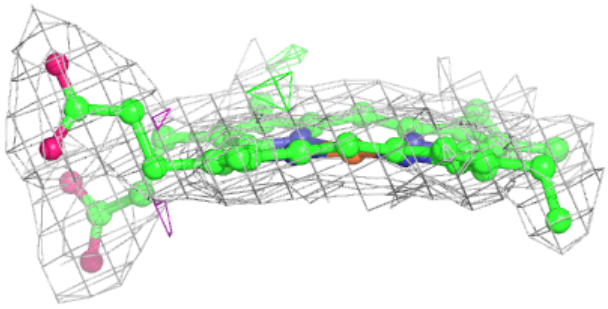
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACE	HaH	201	3/3	0.92	0.10	30,30,34,34	0
2	ACE	CaC	201	3/3	0.94	0.16	34,34,36,37	0
2	ACE	GaG	201	3/3	0.95	0.25	39,39,40,42	0
2	ACE	FaF	201	3/3	0.96	0.15	33,33,35,37	0
2	ACE	BaB	201	3/3	0.96	0.15	26,26,28,29	0
3	HEC	BaB	202	43/43	0.97	0.13	15,17,21,27	0
2	ACE	DaD	201	3/3	0.97	0.16	30,30,31,32	0
3	HEC	AaA	202	43/43	0.97	0.13	12,16,18,20	0
3	HEC	FaF	202	43/43	0.97	0.13	14,17,22,24	0
4	LVQ	FaF	203	69/69	0.97	0.14	18,23,36,45	0
4	LVQ	EaE	203	69/69	0.97	0.13	15,25,47,58	0
4	LVQ	CaC	203	69/69	0.97	0.13	16,25,37,43	0
4	LVQ	AaA	203	69/69	0.97	0.13	17,27,52,65	0
3	HEC	EaE	202	43/43	0.97	0.14	15,17,22,29	0
3	HEC	GaG	202	43/43	0.98	0.13	12,17,22,26	0
4	LVQ	GaG	203	69/69	0.98	0.12	11,18,26,32	0
4	LVQ	BaB	203	69/69	0.98	0.12	16,24,38,48	0
2	ACE	AaA	201	3/3	0.98	0.13	29,29,34,36	0
3	HEC	DaD	202	43/43	0.98	0.13	13,19,21,23	0
4	LVQ	DaD	203	69/69	0.98	0.14	13,18,27,32	0
3	HEC	CaC	202	43/43	0.98	0.14	14,16,19,21	0
3	HEC	HaH	202	43/43	0.98	0.13	15,19,26,34	0
4	LVQ	HaH	203	69/69	0.98	0.12	18,25,42,49	0
2	ACE	EaE	201	3/3	0.99	0.13	17,17,18,18	0

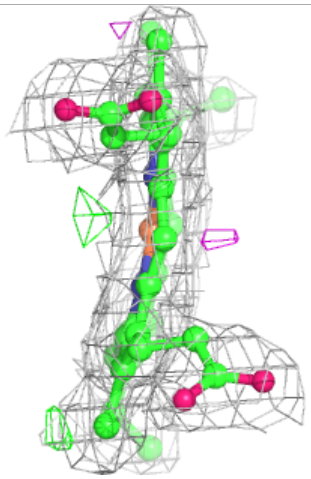
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC BaB 202:

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

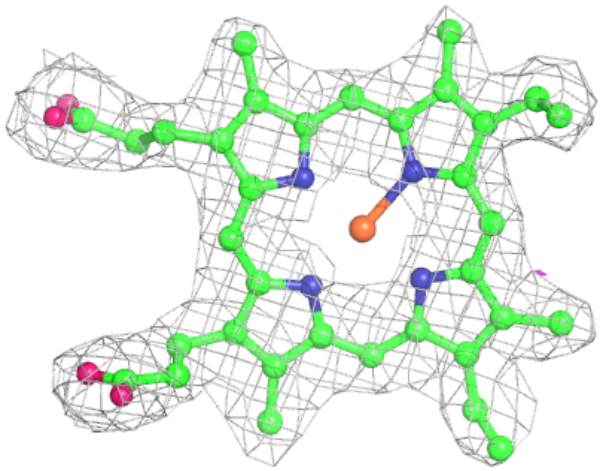


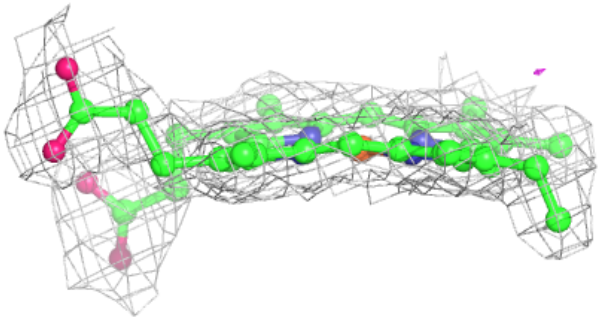


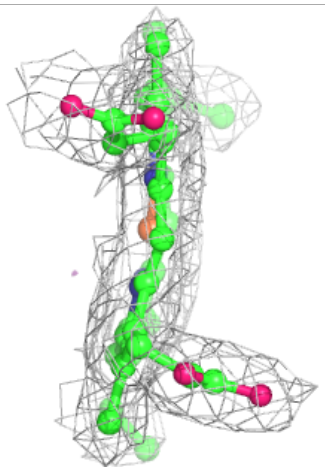


Electron density around HEC AaA 202:

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

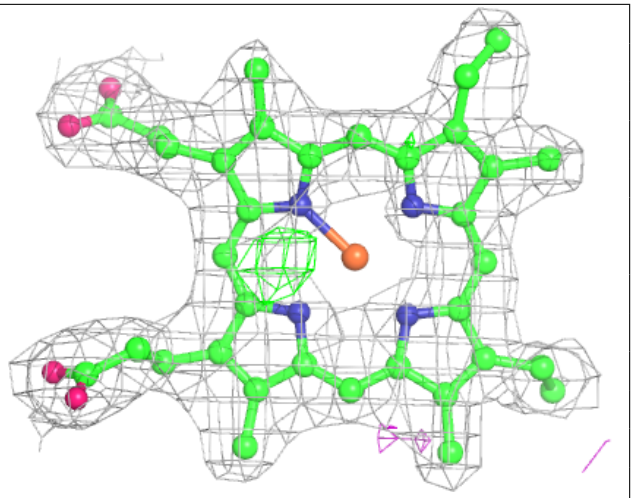


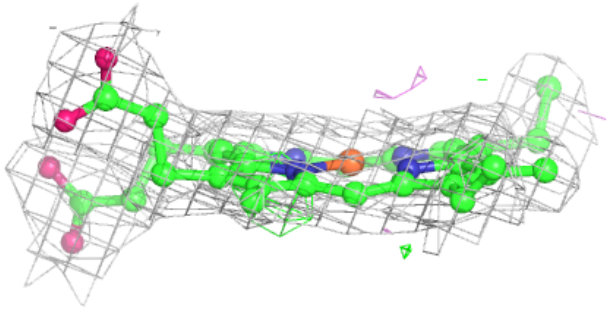


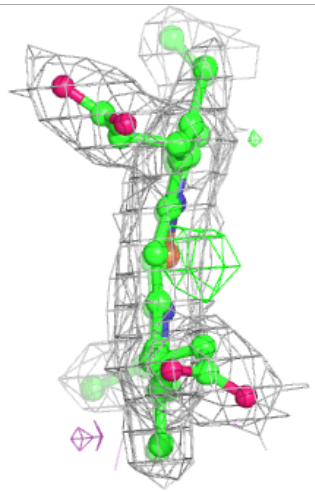


Electron density around HEC FaF 202:

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

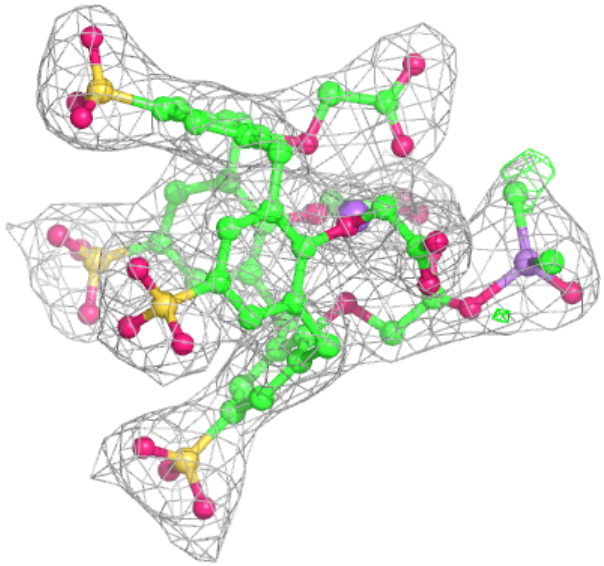


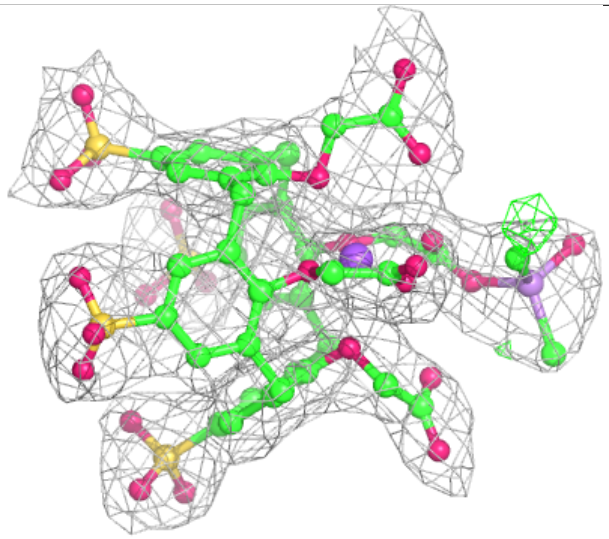


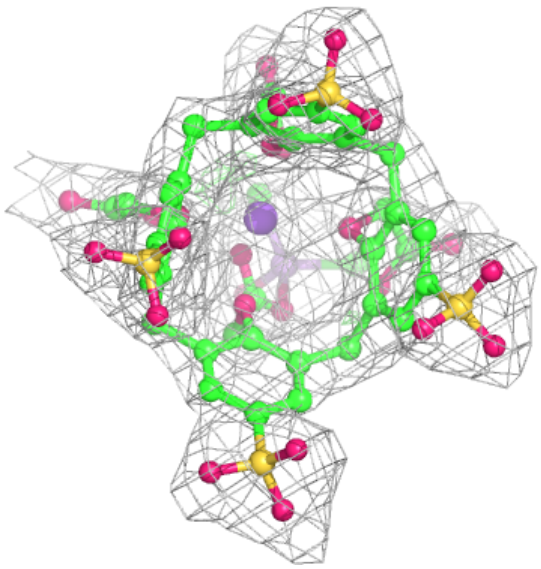


Electron density around LVQ FaF 203:

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

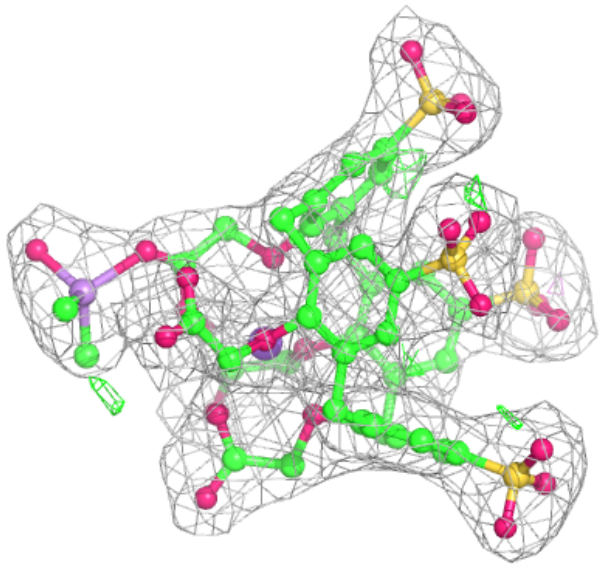


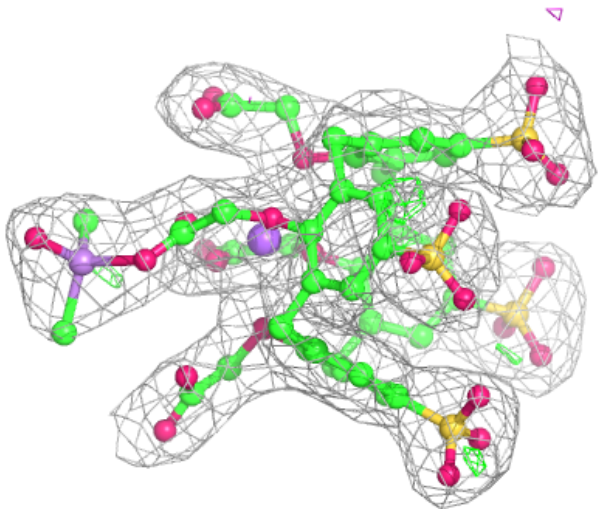


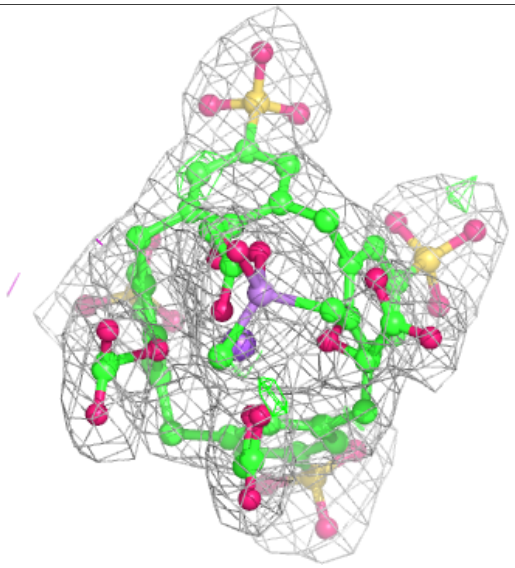


Electron density around LVQ EaE 203:

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

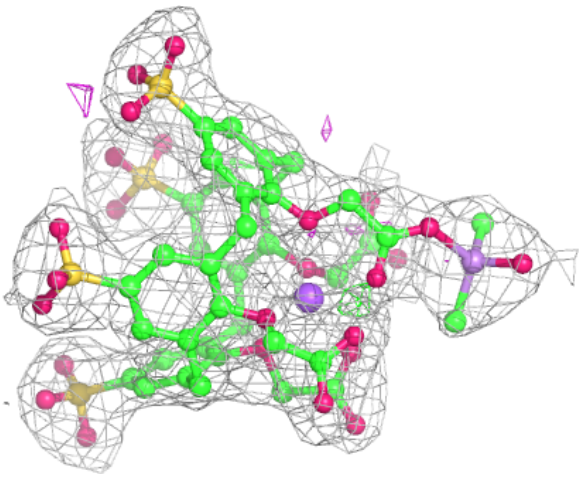


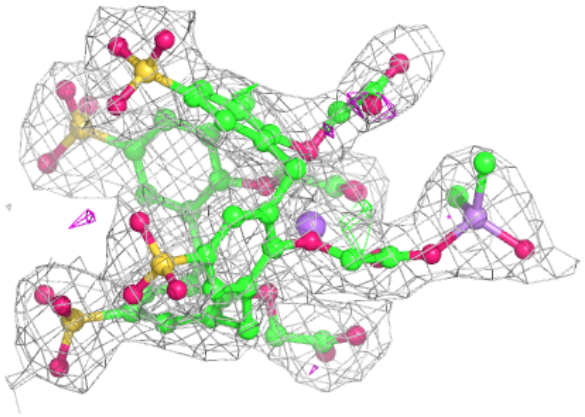


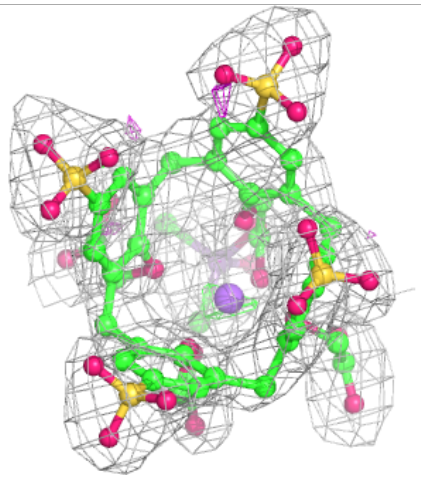


Electron density around LVQ CaC 203:

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

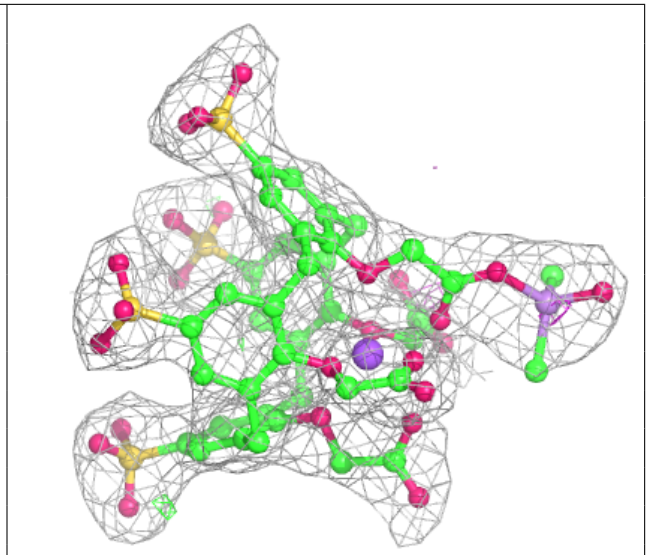


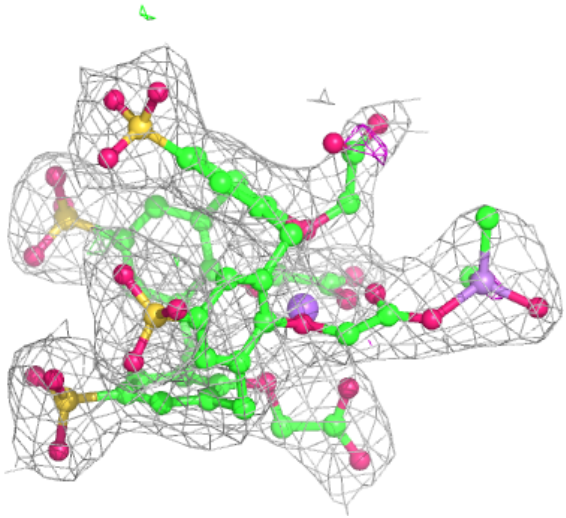


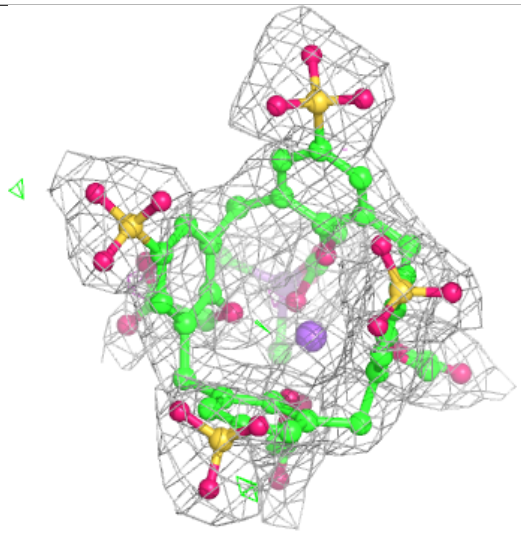


Electron density around LVQ AaA 203:

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

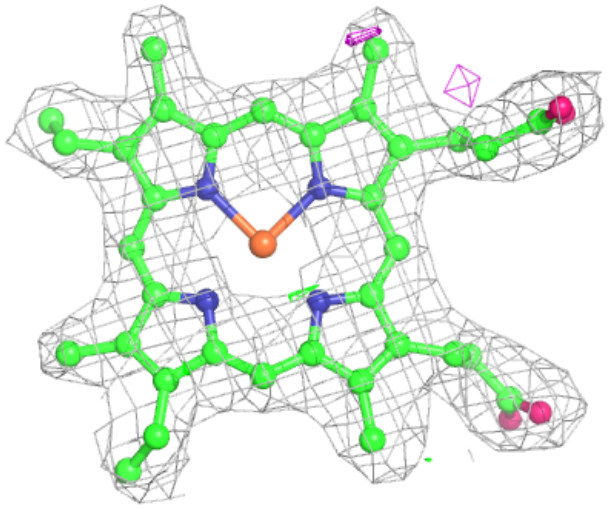


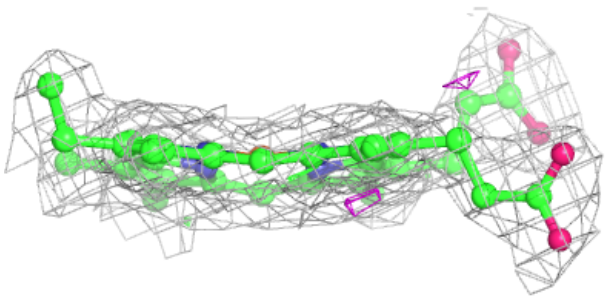


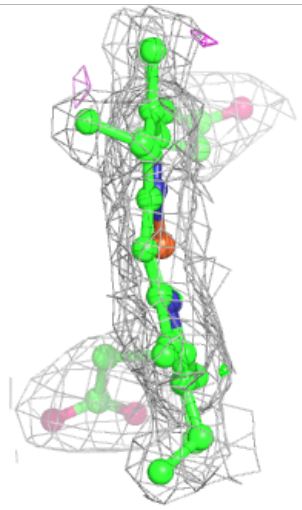


Electron density around HEC EaE 202:

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

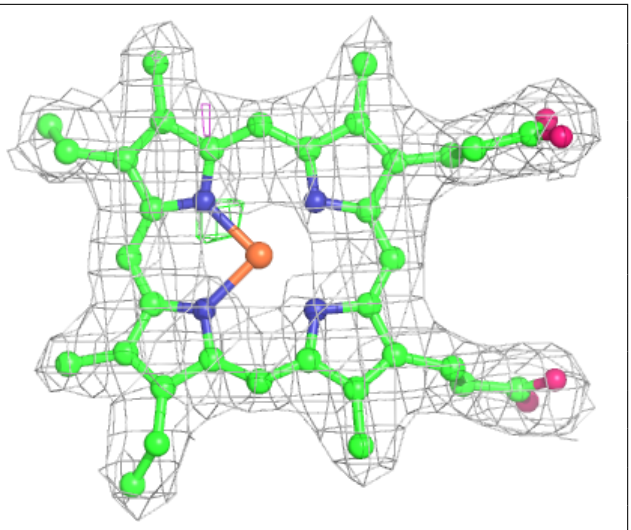


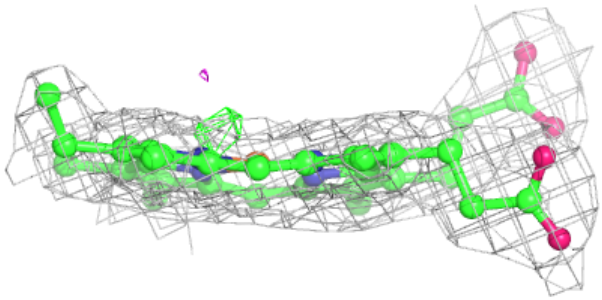


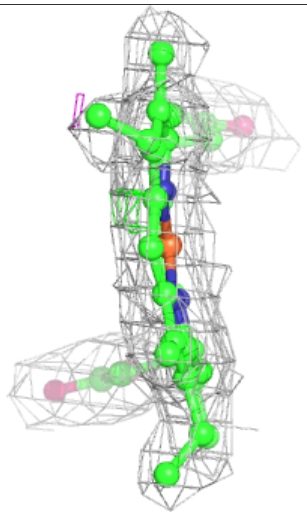


Electron density around HEC GaG 202:

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

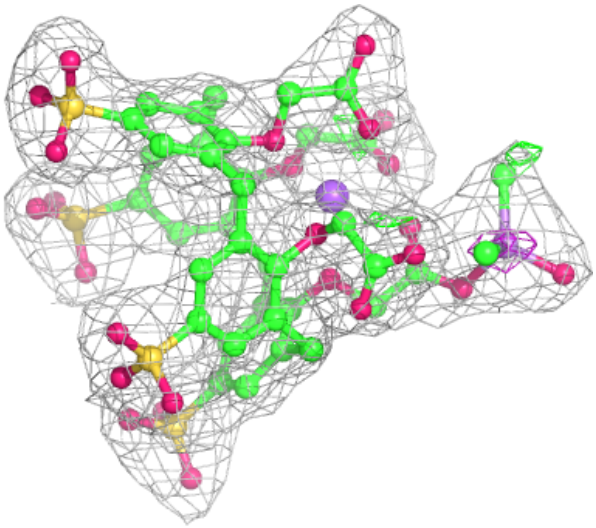


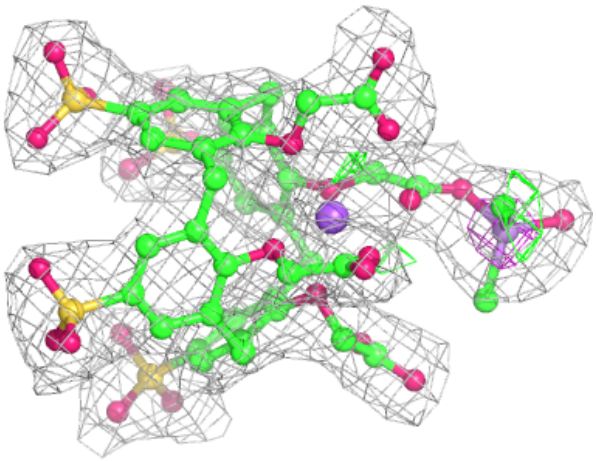


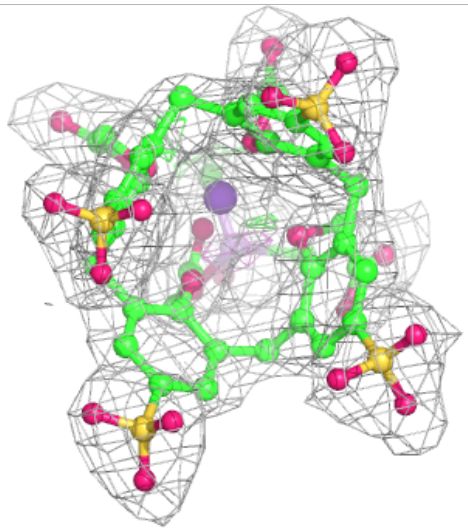


Electron density around LVQ GaG 203:

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

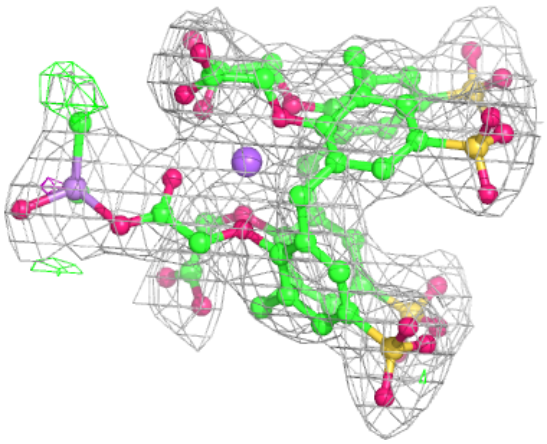


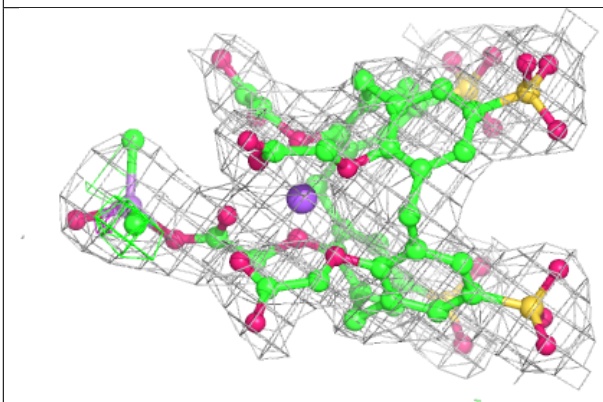


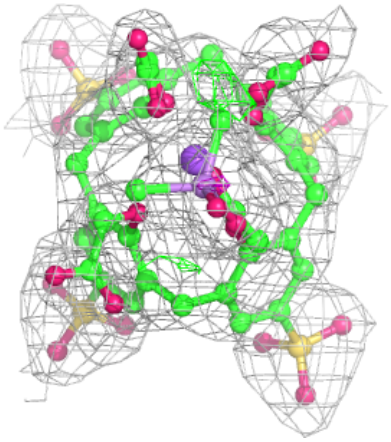


Electron density around LVQ BaB 203:

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

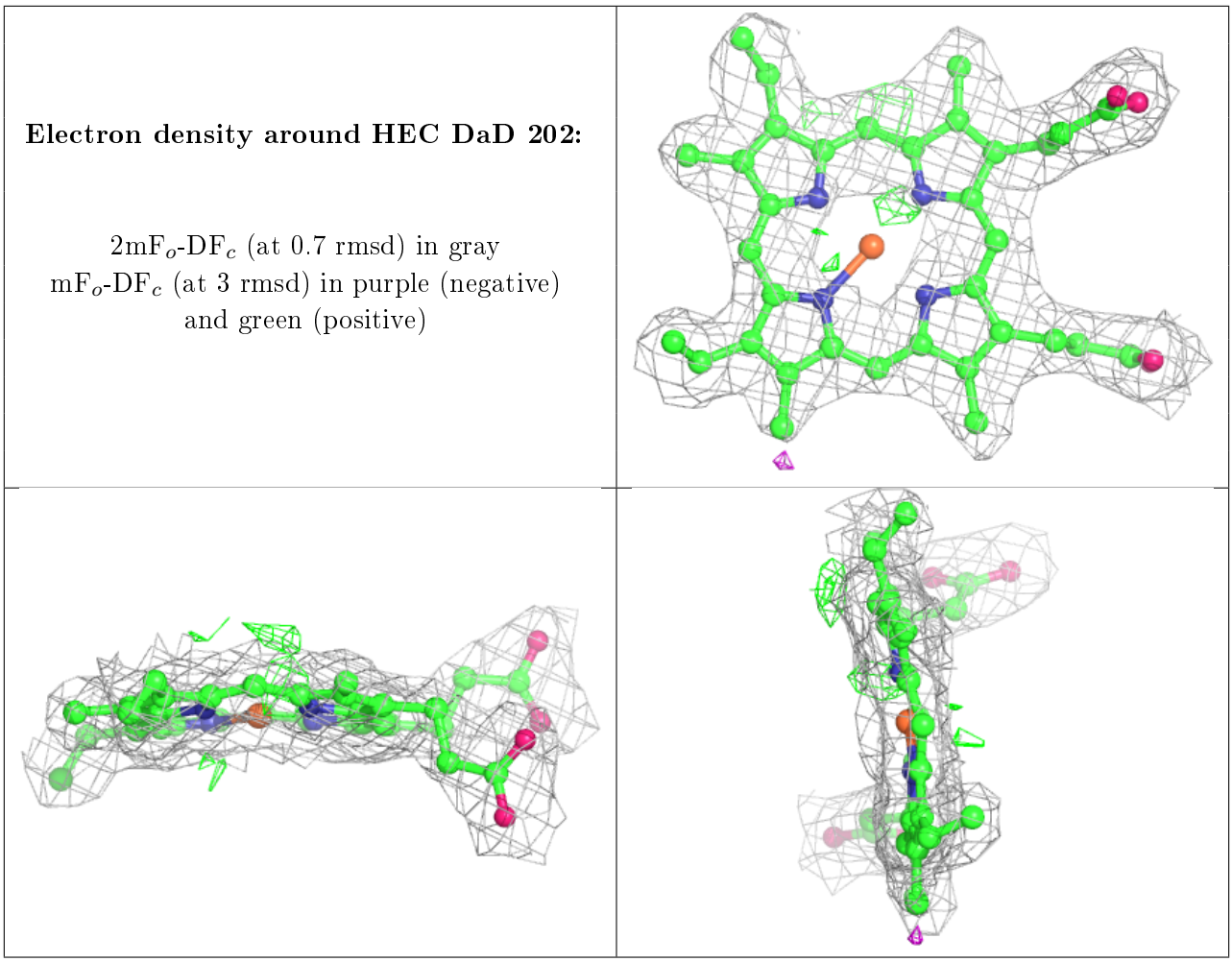






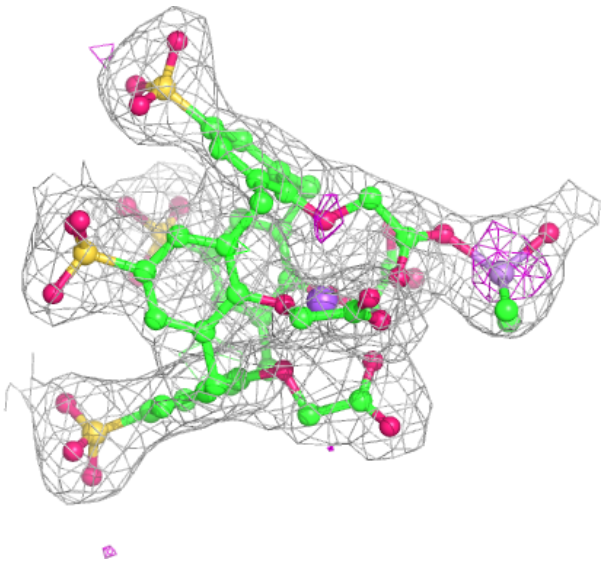
Electron density around HEC DaD 202:

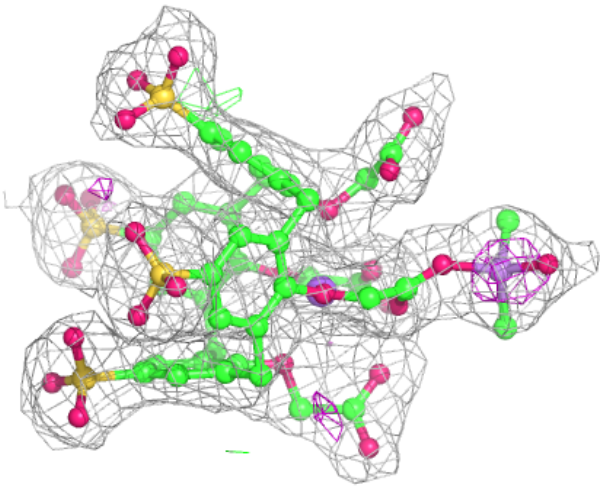
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

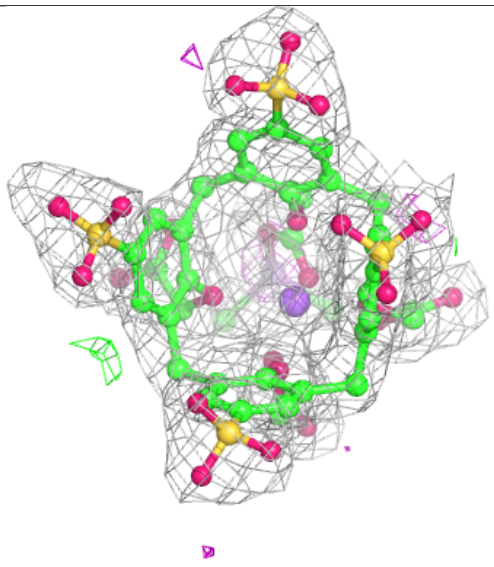


Electron density around LVQ DaD 203:

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

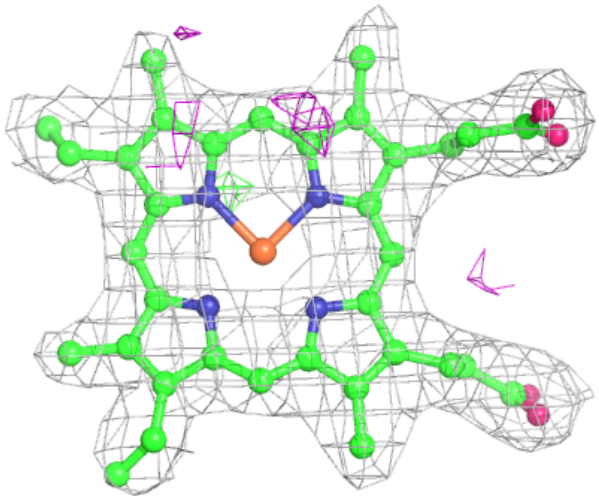


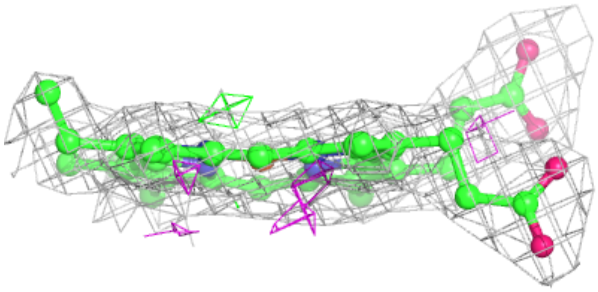


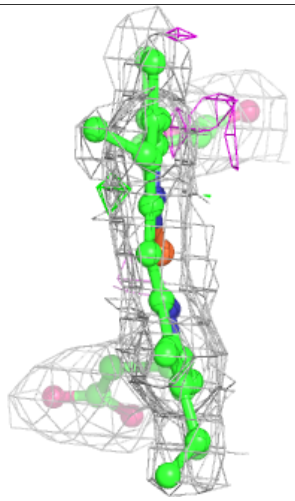


Electron density around HEC CaC 202:

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

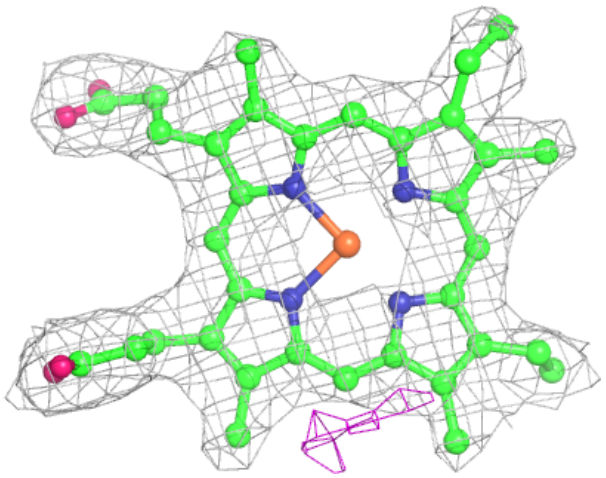


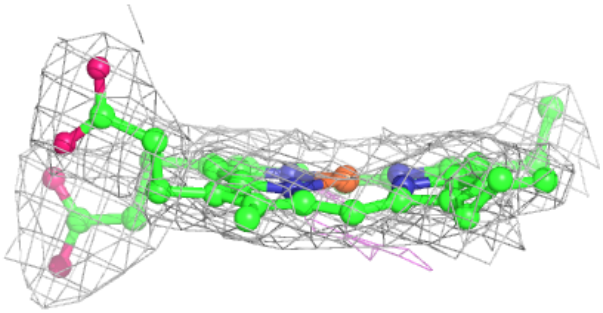


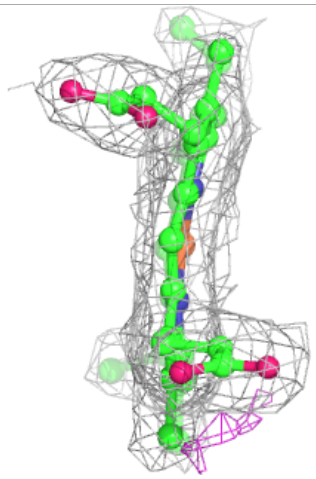


Electron density around HEC HaH 202:

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

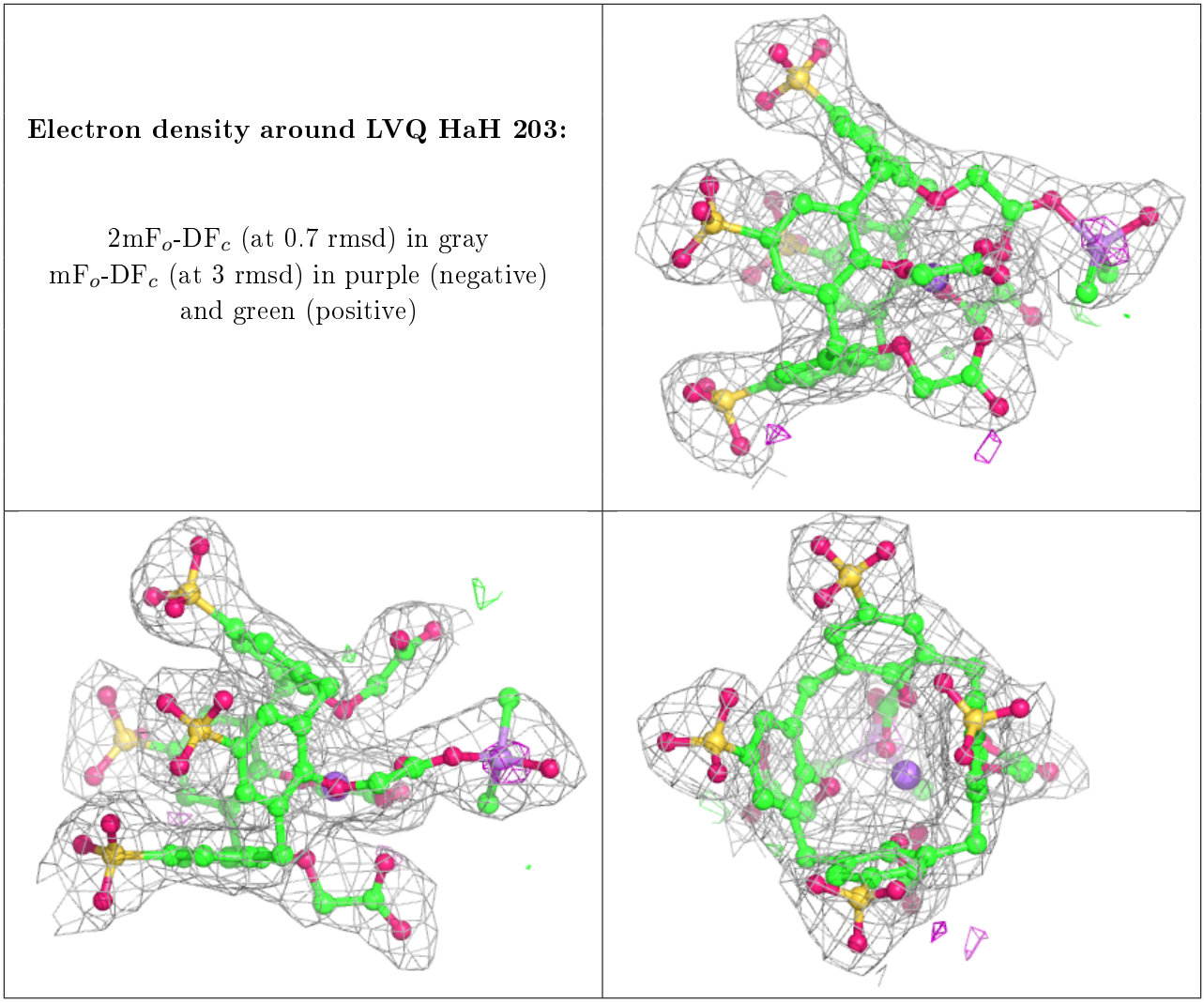






Electron density around LVQ HaH 203:

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



6.5 Other polymers

There are no such residues in this entry.