wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 07:53 PM EDT

PDB ID	:	2ZO5
Title	:	Structure of the Thioalkalivibrio nitratireducens cytochrome c nitrite reductase in a complex with azide
Authors	:	Polyakov, K.M.; Boyko, K.M.; Slutsky, A.; Tikhonova, T.V.; Antipov, A.N.; Zvyagilskaya, R.A.; Popov, A.N.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.
Deposited on	:	2008-05-05
Resolution	:	1.70 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 (1)) were used in the production of this report:

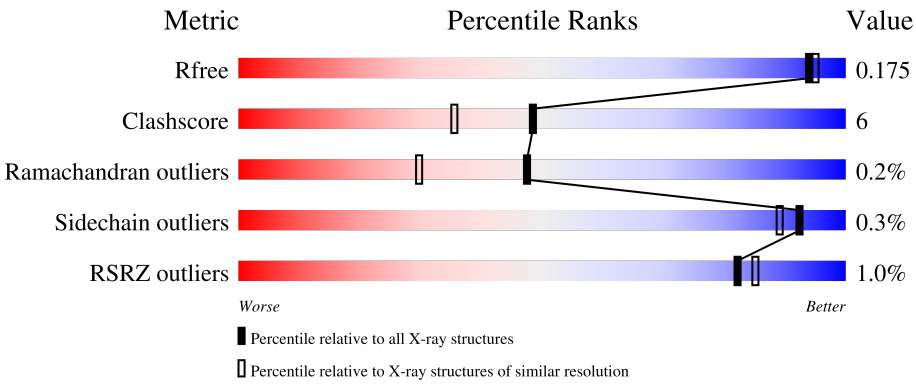
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	525	% 92% 6% •
1	B	525	% 91% 8% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PG4	B	1014	-	-	X	-
7	PG6	B	1011	-	-	X	-
8	TRS	B	1012	-	X	-	-

2 Entry composition (i)

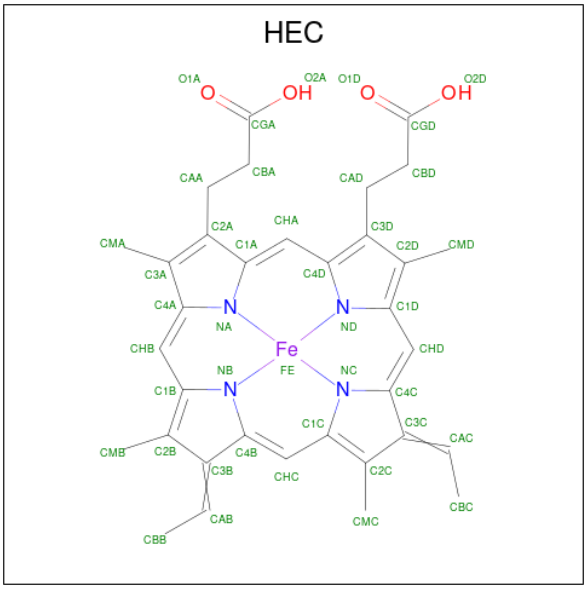
There are 9 unique types of molecules in this entry. The entry contains 18499 atoms, of which 8191 are hydrogens and 0 are deuteriums.

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 Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	519	8029	2592	3850	760	790	37	1054	23	1
1	B	519	8037	2591	3857	763	790	36	1036	19	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	18	0
2	A	1	73	34	1	30	4	4	18	0
2	A	1	73	34	1	30	4	4	18	0
2	A	1	79	36	1	32	4	6	18	1

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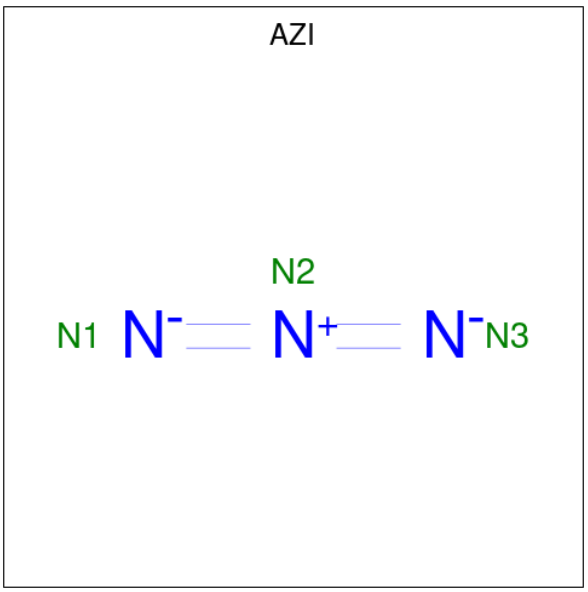
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	79	36	1	32	4	6	18	1
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	18	0

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0

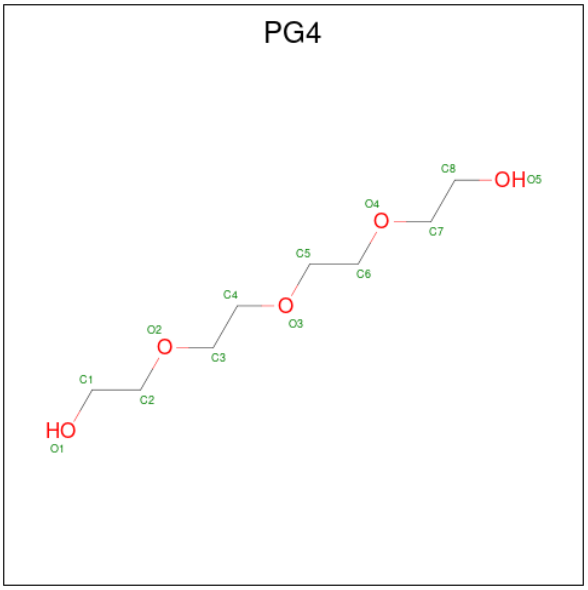
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

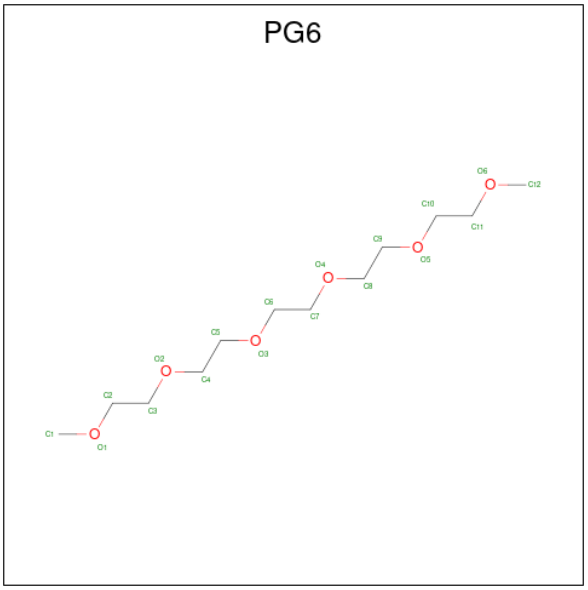
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	8	5	3	0	0
			Total	C	O		
6	A	1	6	4	2	0	0
			Total	C	O		
6	A	1	8	5	3	0	0
			Total	C	O		
6	B	1	7	4	3	0	0
			Total	C	O		
6	B	1	7	4	3	0	0
			Total	C	O		
6	B	1	5	3	2	0	0
			Total	C	O		
6	B	1	9	6	3	0	0
			Total	C	O		
6	B	1	5	3	2	0	0
			Total	C	O		
6	B	1	5	3	2	0	0
			Total	C	O		
6	B	1	7	5	2	0	0

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	14	9	5	0	0

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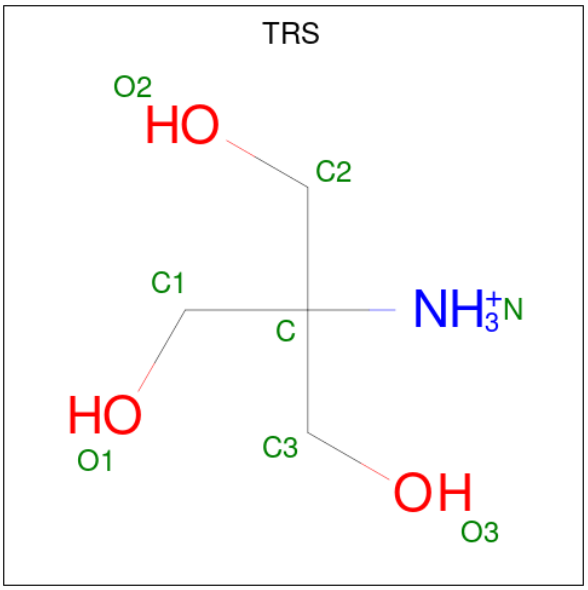
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	14	9	5	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	8	4	1	3	0	0
			Total	C	N	O		
8	B	1	8	4	1	3	0	0

- Molecule 9 is water.

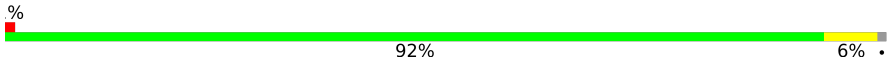
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	549	549	549	0	0
			Total	O		
9	B	575	575	575	0	0

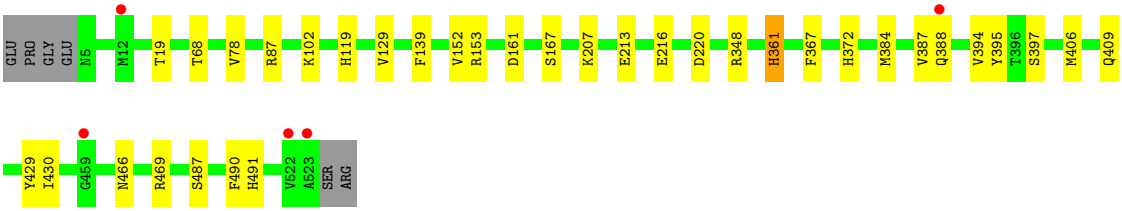
3 Residue-property plots (i)

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: Eight-heme nitrite reductase

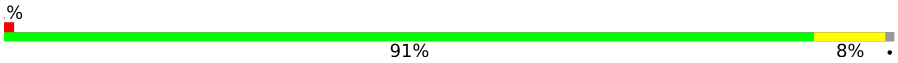
Chain A:

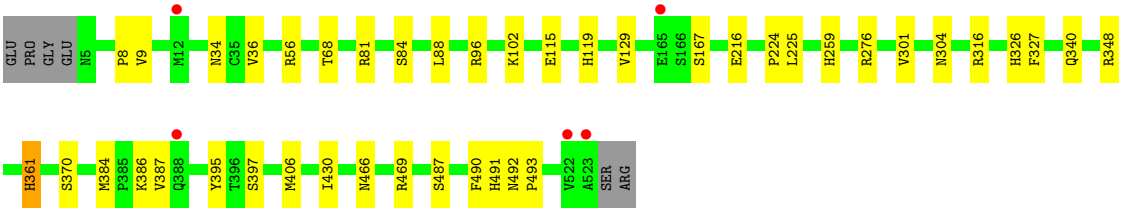




• Molecule 1: Eight-heme nitrite reductase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	193.03Å 193.03Å 193.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 1.70 11.99 – 1.67	Depositor EDS
% Data completeness (in resolution range)	98.4 (11.99-1.70) 98.6 (11.99-1.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.151 , 0.168 0.161 , 0.175	Depositor DCC
R_{free} test set	13645 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18499	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: PG6, TRS, CA, HEC, NA, AZI, PG4

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	0.65	0/4415	0.73	3/5986 (0.1%)
1	B	0.69	1/4388 (0.0%)	0.77	3/5949 (0.1%)
All	All	0.67	1/8803 (0.0%)	0.75	6/11935 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	ARG	CB-CG	-5.09	1.38	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	161	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	153[A]	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	153[B]	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	276	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4179	3850	3897	26	2
1	B	4180	3857	3906	48	0
2	A	348	242	218	11	0
2	B	348	242	218	12	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	0	25	2	0
6	B	45	0	49	21	0
7	A	14	0	14	4	0
7	B	14	0	14	12	0
8	A	8	0	12	0	0
8	B	8	0	9	0	0
9	A	549	0	0	10	0
9	B	575	0	0	15	1
All	All	10308	8191	8362	102	2

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

The worst 5 of 102 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:A:348[A]:ARG:HD2	7:A:1010:PG6:O1	1.49	1.12
1:B:348[B]:ARG:CD	7:B:1011:PG6:O1	1.88	1.07
1:B:348[B]:ARG:HD2	7:B:1011:PG6:O1	1.26	1.05
1:A:348[A]:ARG:CD	7:A:1010:PG6:O1	2.09	0.99
1:B:348[A]:ARG:NH2	7:B:1011:PG6:O4	1.96	0.98

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH12	1:A:429:TYR:HH[12_565]	1.32	0.28
1:A:388:GLN:OE1	9:B:1317:HOH:O[6_456]	2.12	0.08

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	541/525 (103%)	520 (96%)	20 (4%)	1 (0%)	47	30
1	B	536/525 (102%)	514 (96%)	21 (4%)	1 (0%)	47	30
All	All	1077/1050 (103%)	1034 (96%)	41 (4%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS
1	B	361	HIS

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	459/443 (104%)	458 (100%)	1 (0%)	93	90
1	B	456/443 (103%)	453 (99%)	3 (1%)	84	77
All	All	915/886 (103%)	911 (100%)	4 (0%)	92	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	MET
1	B	88[A]	LEU
1	B	88[B]	LEU
1	B	406	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	GLN
1	B	340	GLN
1	B	466	ASN
1	B	413	ASN
1	B	138	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 6 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AZI	B	530	-	0,2,2	-	-	0,1,1	-	-
6	PG4	B	1015	-	4,4,12	0.45	0	3,3,11	0.08	0
6	PG4	B	1016	-	4,4,12	0.65	0	3,3,11	0.50	0
2	HEC	A	1004	1,3,9	32,50,50	2.01	4 (12%)	24,82,82	1.76	4 (16%)
2	HEC	B	1005	1	32,50,50	2.23	7 (21%)	24,82,82	1.81	6 (25%)
2	HEC	A	1002	1	32,50,50	1.81	7 (21%)	24,82,82	1.59	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	B	1003	1	32,50,50	2.01	6 (18%)	24,82,82	2.11	7 (29%)
2	HEC	A	1007[B]	4	32,50,50	2.15	5 (15%)	24,82,82	2.05	7 (29%)
8	TRS	B	1012	-	7,7,7	3.10	1 (14%)	9,9,9	2.20	3 (33%)
2	HEC	A	1007[A]	-	32,50,50	2.16	5 (15%)	24,82,82	2.09	6 (25%)
2	HEC	B	1007[B]	4	32,50,50	2.24	5 (15%)	24,82,82	1.78	4 (16%)
2	HEC	B	1001	1	32,50,50	1.99	7 (21%)	24,82,82	1.77	7 (29%)
6	PG4	B	1017	-	6,6,12	0.42	0	5,5,11	0.21	0
2	HEC	B	1007[A]	-	32,50,50	2.24	5 (15%)	24,82,82	1.82	5 (20%)
6	PG4	A	1011	-	5,5,12	0.56	0	4,4,11	0.69	0
2	HEC	A	1006	1,4	32,50,50	2.11	6 (18%)	24,82,82	1.69	5 (20%)
6	PG4	A	1009	-	7,7,12	0.56	0	6,6,11	0.53	0
3	AZI	A	526	2	0,2,2	-	-	0,1,1	-	-
2	HEC	A	1003	1	32,50,50	1.99	5 (15%)	24,82,82	1.85	7 (29%)
2	HEC	B	1004	1,3,9	32,50,50	2.00	7 (21%)	24,82,82	2.00	6 (25%)
2	HEC	A	1008	1	32,50,50	2.17	5 (15%)	24,82,82	1.84	6 (25%)
3	AZI	A	530	-	0,2,2	-	-	0,1,1	-	-
7	PG6	A	1010	-	13,13,17	0.43	0	12,12,16	0.40	0
6	PG4	B	1009	-	6,6,12	0.52	0	5,5,11	0.62	0
3	AZI	B	526	2	0,2,2	-	-	0,1,1	-	-
6	PG4	B	1014	4	8,8,12	0.45	0	7,7,11	0.76	0
2	HEC	B	1008	1	32,50,50	2.31	5 (15%)	24,82,82	2.51	12 (50%)
2	HEC	B	1002	1	32,50,50	1.89	6 (18%)	24,82,82	1.52	5 (20%)
2	HEC	A	1001	1	32,50,50	2.16	7 (21%)	24,82,82	1.73	6 (25%)
6	PG4	B	1010	-	6,6,12	0.38	0	5,5,11	0.71	0
6	PG4	A	1013	-	7,7,12	0.45	0	6,6,11	0.27	0
8	TRS	A	1012	-	7,7,7	0.12	0	9,9,9	0.78	0
7	PG6	B	1011	-	13,13,17	0.49	0	12,12,16	0.28	0
2	HEC	B	1006	1,4	32,50,50	2.02	7 (21%)	24,82,82	1.91	8 (33%)
6	PG4	B	1013	-	4,4,12	0.42	0	3,3,11	0.35	0
2	HEC	A	1005	1	32,50,50	2.31	8 (25%)	24,82,82	2.02	7 (29%)

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
6	PG4	B	1015	-	-	1/2/2/10	-
6	PG4	B	1016	-	-	2/2/2/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1004	1,3,9	-	2/10/54/54	-
2	HEC	B	1005	1	-	4/10/54/54	-
2	HEC	A	1002	1	-	2/10/54/54	-
2	HEC	B	1003	1	-	2/10/54/54	-
2	HEC	A	1007[B]	4	-	2/10/54/54	-
8	TRS	B	1012	-	-	8/9/9/9	-
2	HEC	A	1007[A]	-	-	2/10/54/54	-
2	HEC	B	1007[B]	4	-	0/10/54/54	-
2	HEC	B	1001	1	-	3/10/54/54	-
6	PG4	B	1017	-	-	1/4/4/10	-
2	HEC	B	1007[A]	-	-	2/10/54/54	-
6	PG4	A	1011	-	-	1/3/3/10	-
2	HEC	A	1006	1,4	-	0/10/54/54	-
6	PG4	A	1009	-	-	2/5/5/10	-
2	HEC	A	1003	1	-	2/10/54/54	-
2	HEC	B	1004	1,3,9	-	2/10/54/54	-
2	HEC	A	1008	1	-	2/10/54/54	-
7	PG6	A	1010	-	-	3/11/11/15	-
6	PG4	B	1009	-	-	4/4/4/10	-
6	PG4	B	1014	4	-	3/6/6/10	-
2	HEC	B	1008	1	-	2/10/54/54	-
2	HEC	B	1002	1	-	2/10/54/54	-
2	HEC	A	1001	1	-	4/10/54/54	-
6	PG4	B	1010	-	-	3/4/4/10	-
6	PG4	A	1013	-	-	2/5/5/10	-
8	TRS	A	1012	-	-	6/9/9/9	-
7	PG6	B	1011	-	-	1/11/11/15	-
2	HEC	B	1006	1,4	-	0/10/54/54	-
6	PG4	B	1013	-	-	2/2/2/10	-
2	HEC	A	1005	1	-	3/10/54/54	-

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1008	HEC	C2B-C3B	-8.55	1.31	1.40
8	B	1012	TRS	C-N	-8.08	1.22	1.49
2	A	1005	HEC	C2B-C3B	-7.57	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1007[A]	HEC	C2B-C3B	-7.45	1.33	1.40
2	A	1007[B]	HEC	C2B-C3B	-7.45	1.33	1.40

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	HEC	C1D-C2D-C3D	-6.12	102.73	107.00
2	B	1008	HEC	CMC-C2C-C1C	-5.96	119.30	128.46
2	A	1007[A]	HEC	CMB-C2B-C1B	-5.95	119.32	128.46
2	A	1007[B]	HEC	CMB-C2B-C1B	-5.95	119.32	128.46
2	B	1007[A]	HEC	CMB-C2B-C1B	-5.17	120.52	128.46

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1012	TRS	C2-C-C1-O1
8	A	1012	TRS	C3-C-C1-O1
8	A	1012	TRS	N-C-C1-O1
8	A	1012	TRS	C1-C-C2-O2
8	A	1012	TRS	C3-C-C2-O2

There are no ring outliers.

23 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1015	PG4	1	0
6	B	1016	PG4	4	0
2	A	1004	HEC	2	0
2	B	1005	HEC	1	0
2	A	1002	HEC	1	0
2	B	1003	HEC	2	0
2	B	1001	HEC	2	0
6	A	1011	PG4	1	0
2	A	1006	HEC	1	0
3	A	526	AZI	1	0
2	A	1003	HEC	2	0
2	B	1004	HEC	2	0
2	A	1008	HEC	3	0
7	A	1010	PG6	4	0
6	B	1009	PG4	5	0

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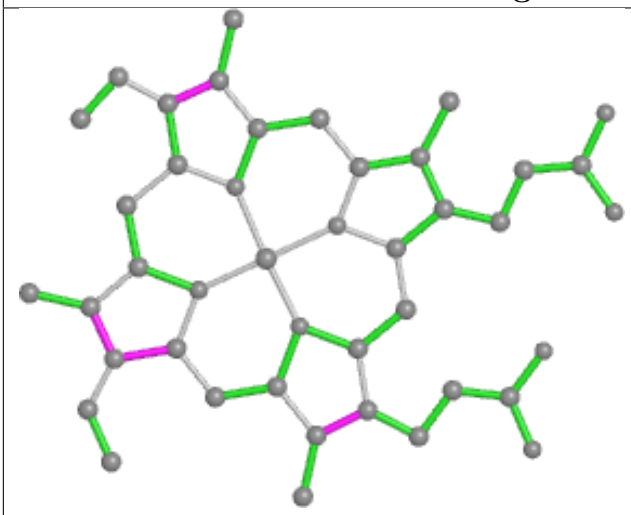
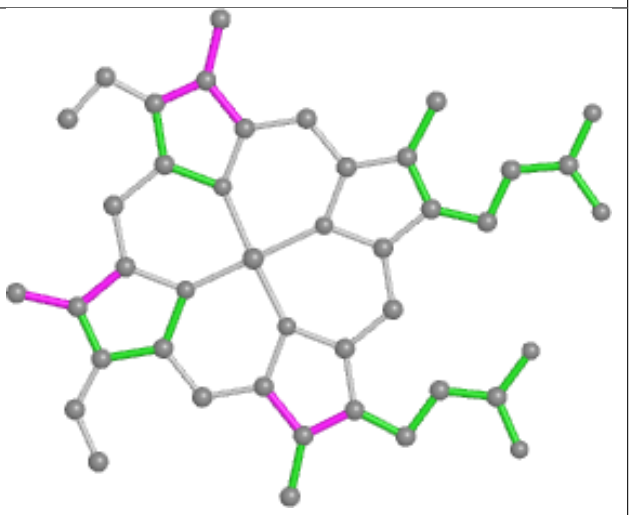
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	526	AZI	1	0
6	B	1014	PG4	11	0
2	B	1008	HEC	2	0
2	B	1002	HEC	2	0
2	A	1001	HEC	2	0
6	A	1013	PG4	1	0
7	B	1011	PG6	12	0
2	B	1006	HEC	1	0

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.

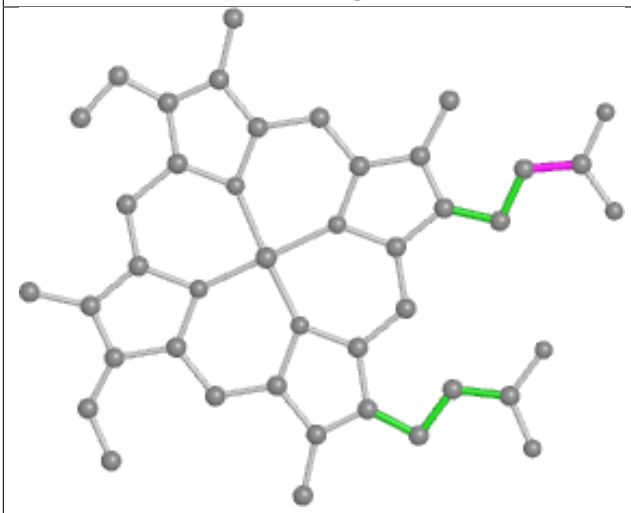
Ligand HEC A 1004



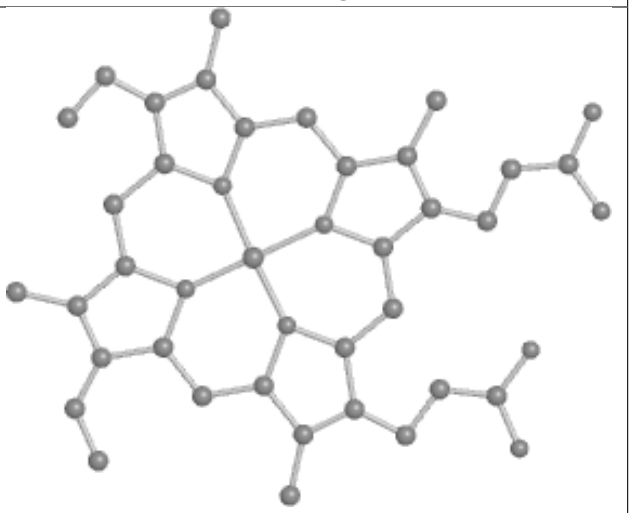
Bond lengths



Bond angles

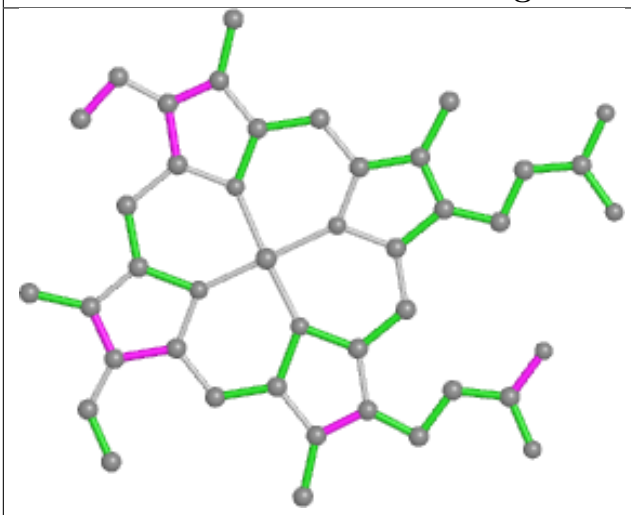


Torsions

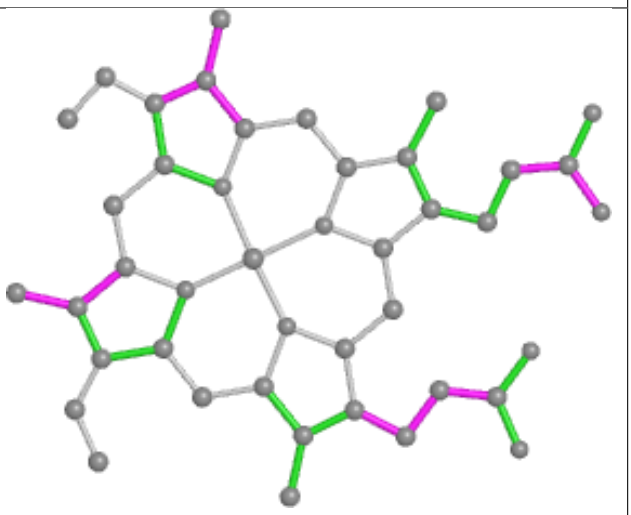


Rings

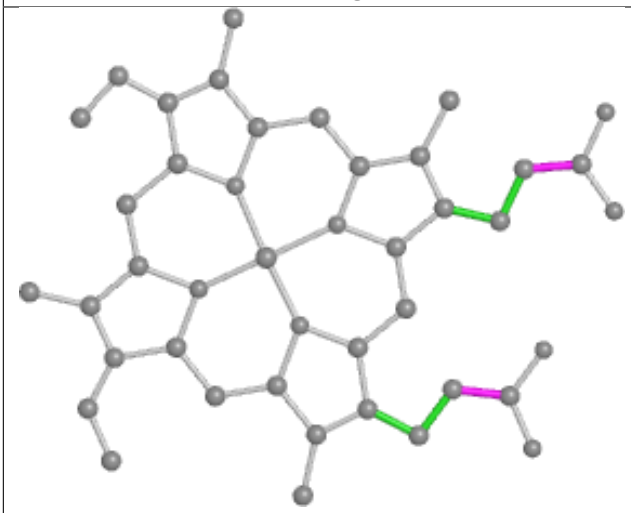
Ligand HEC B 1005



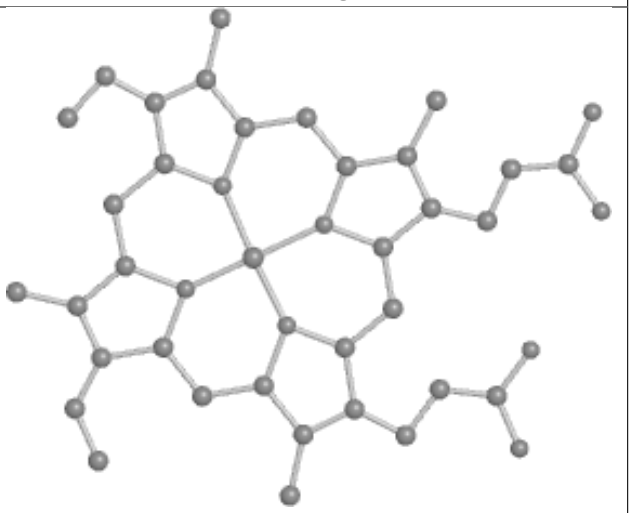
Bond lengths



Bond angles

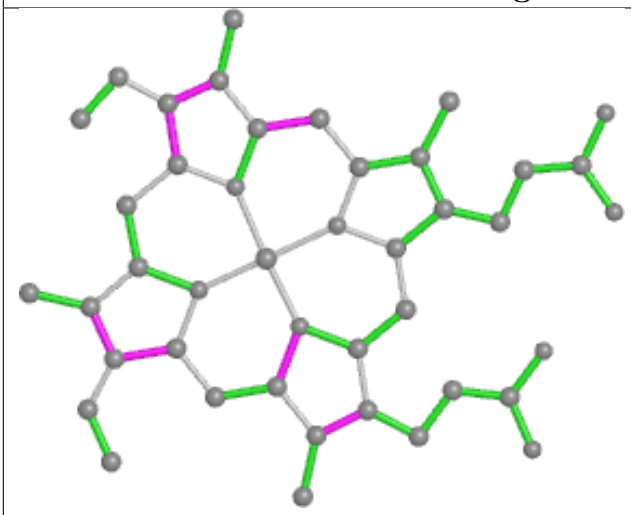


Torsions

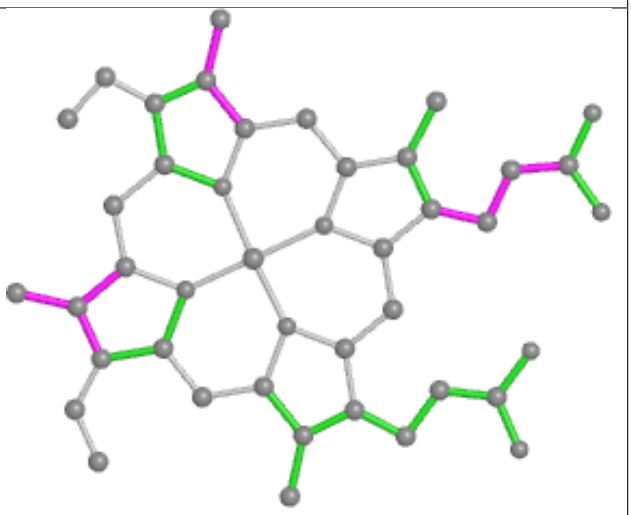


Rings

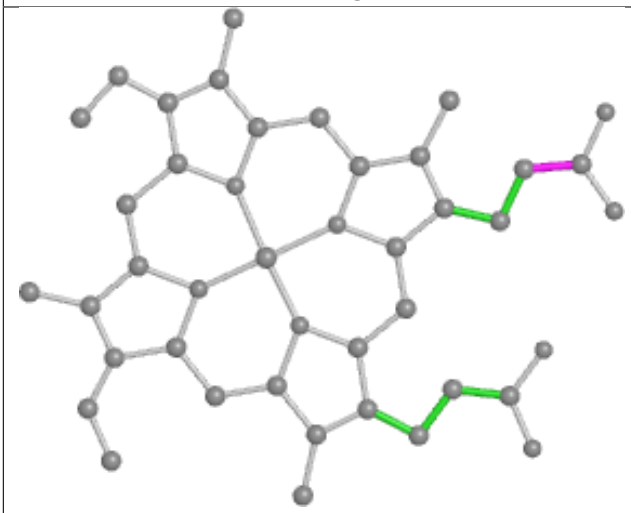
Ligand HEC A 1002



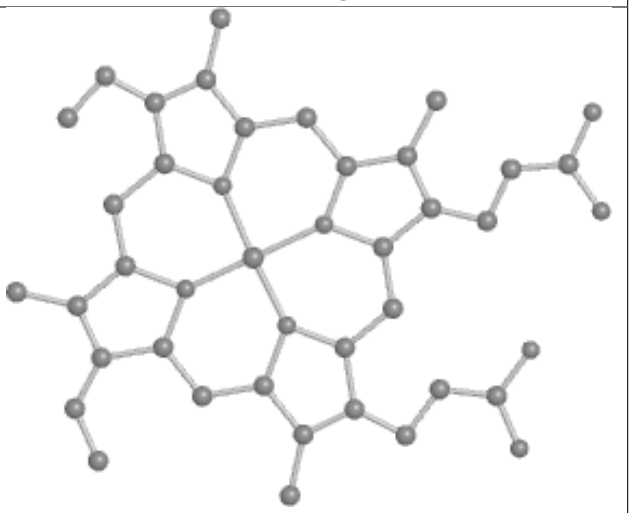
Bond lengths



Bond angles

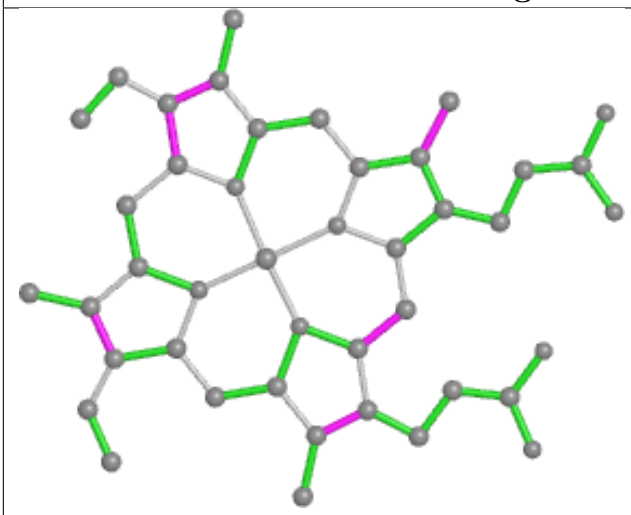


Torsions

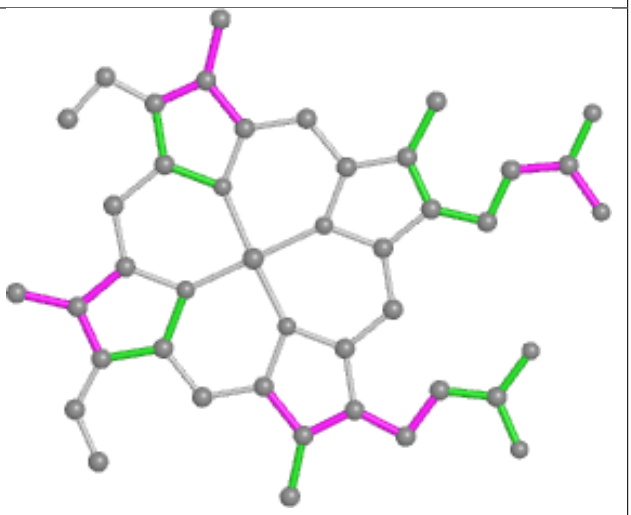


Rings

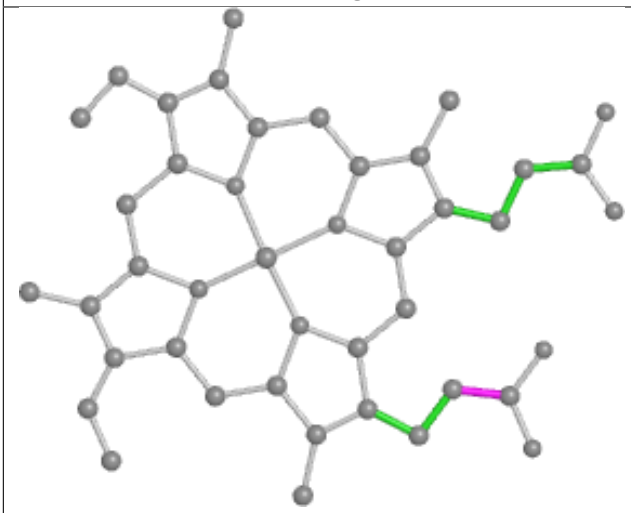
Ligand HEC B 1003



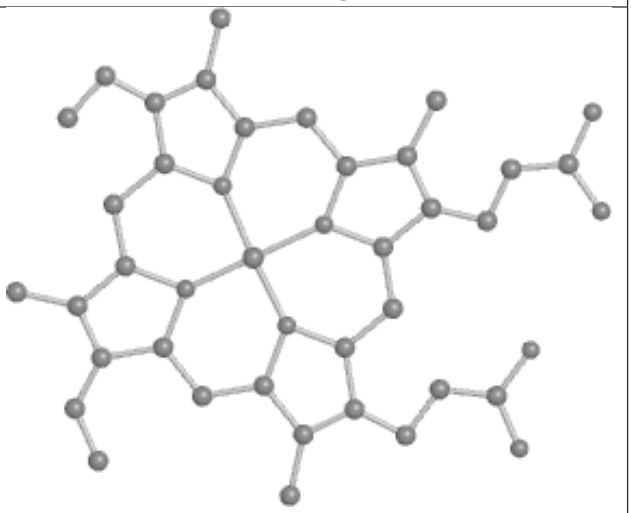
Bond lengths



Bond angles

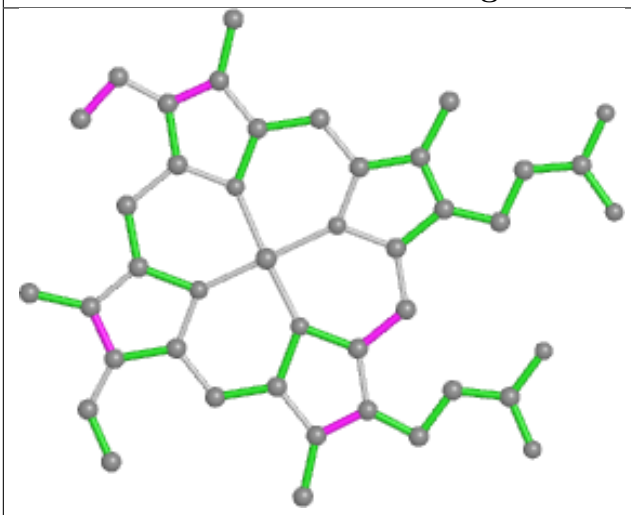


Torsions



Rings

Ligand HEC A 1007 (B)



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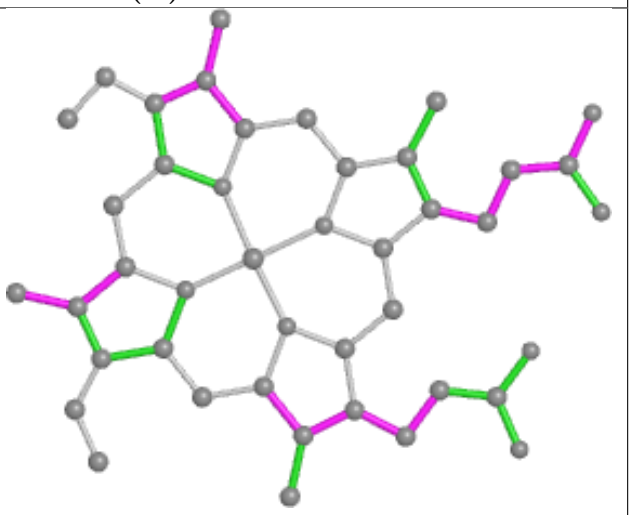
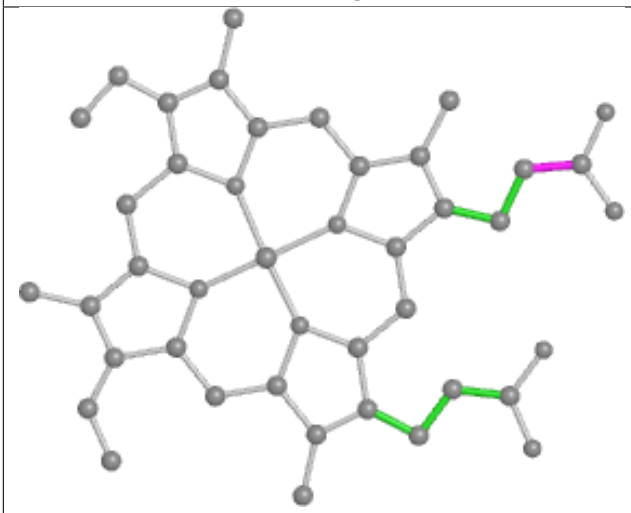
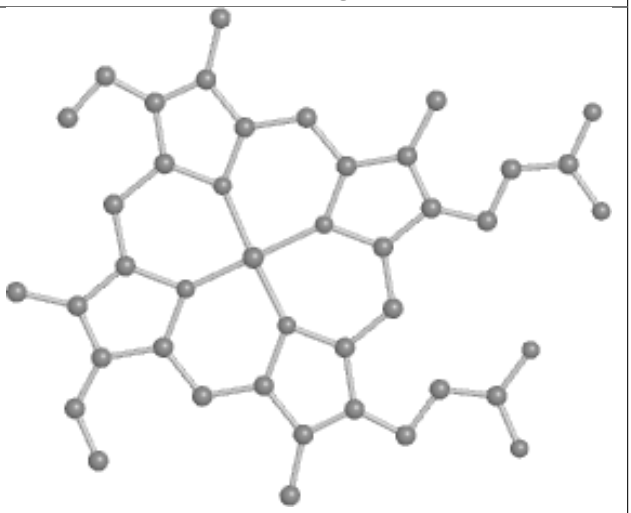


Bond angles

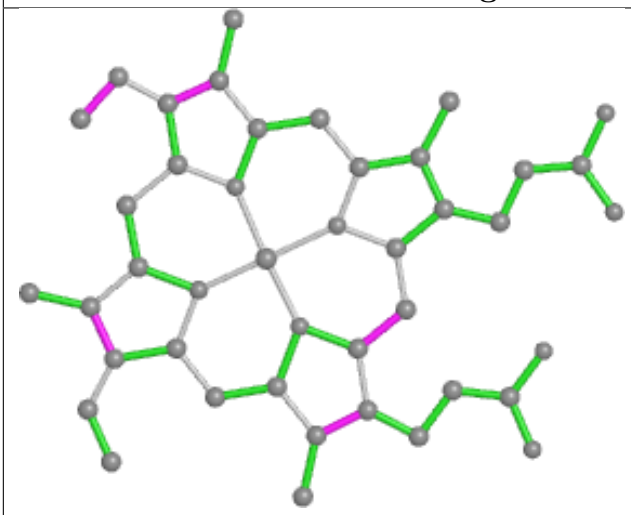


Torsions



Rings

Ligand HEC A 1007 (A)



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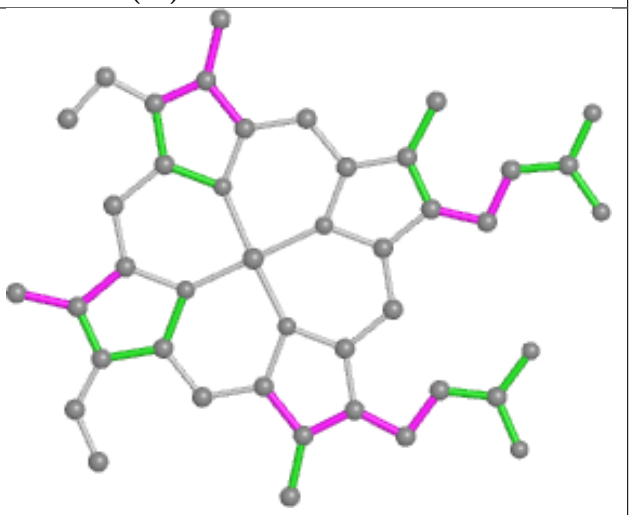
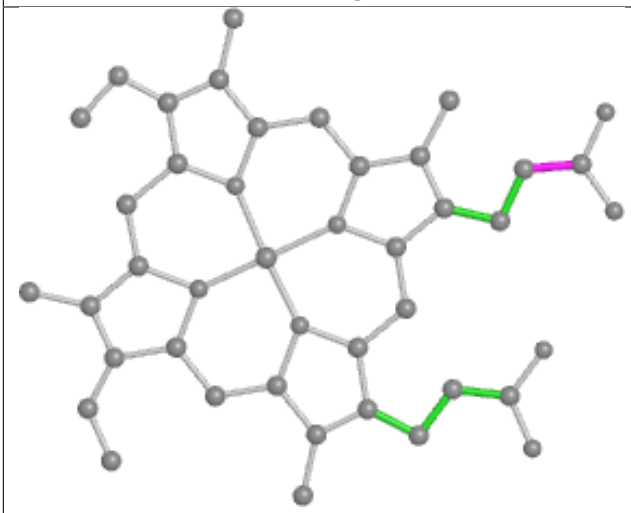


Bond angles



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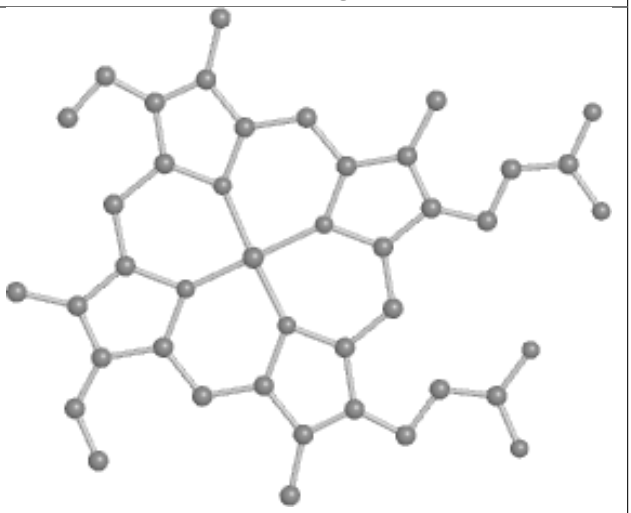
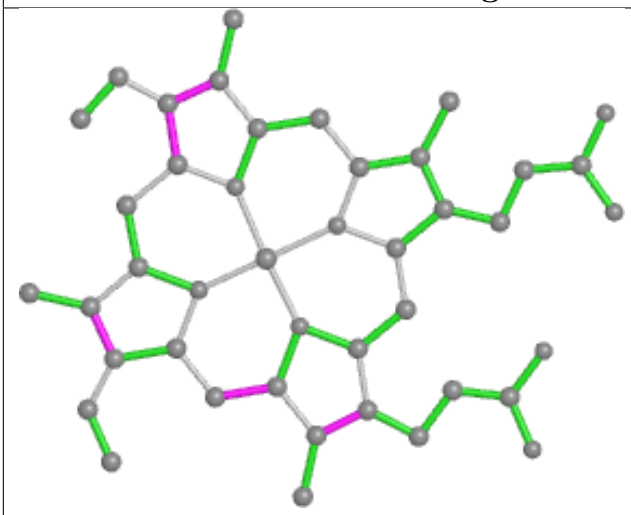


Rings

Ligand HEC B 1007 (B)



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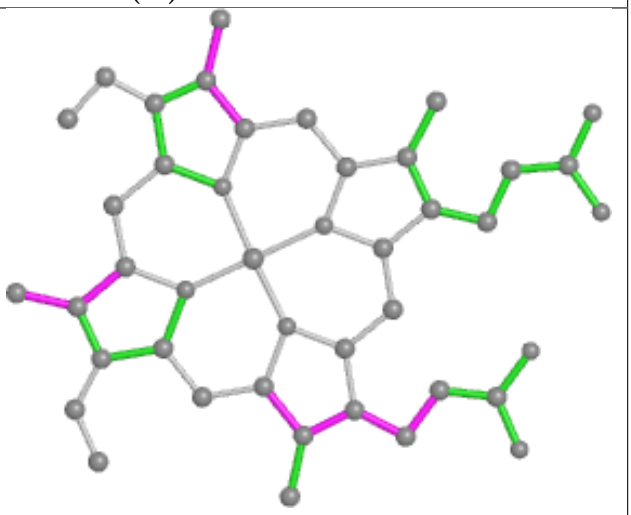
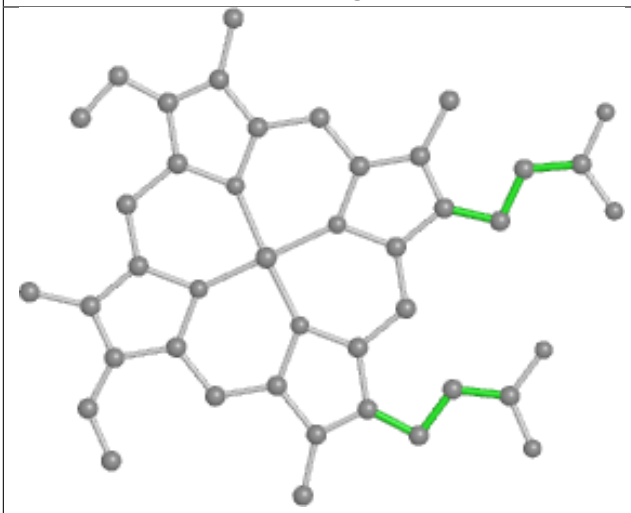


Bond angles



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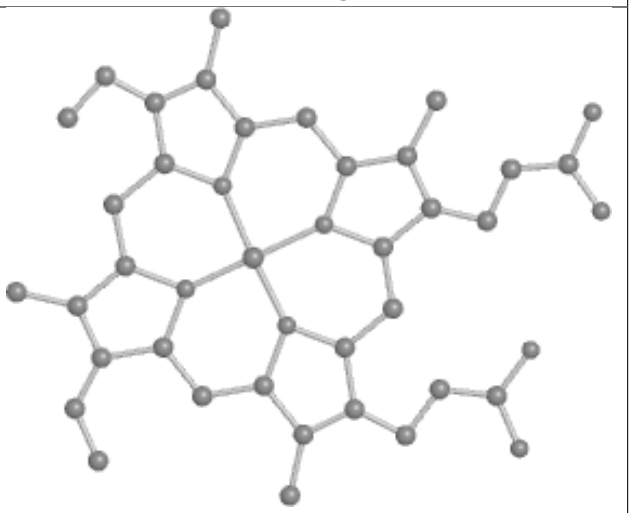
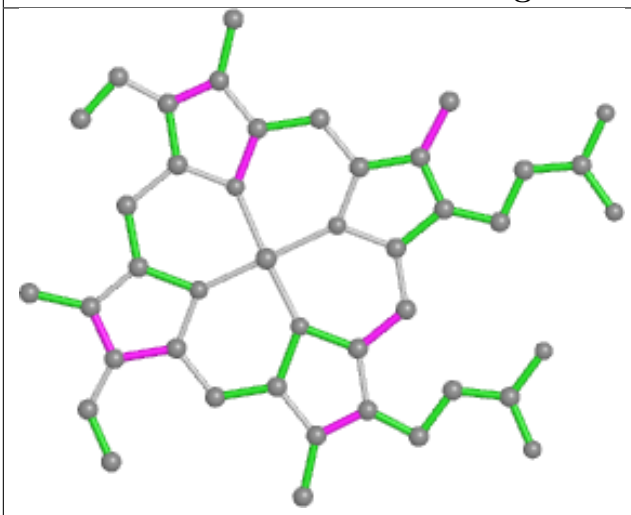
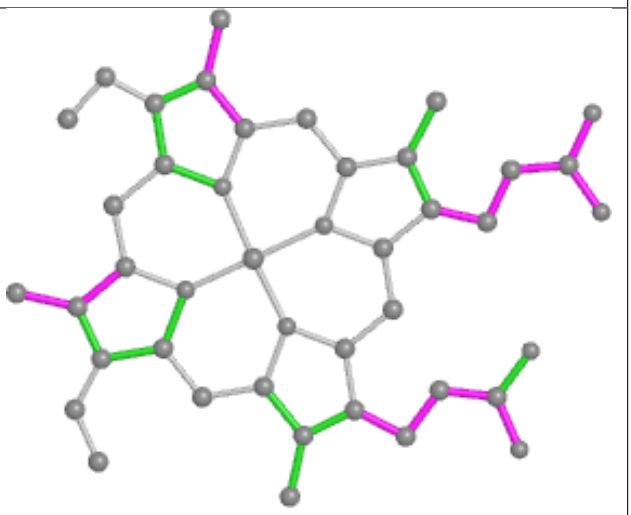


Rings

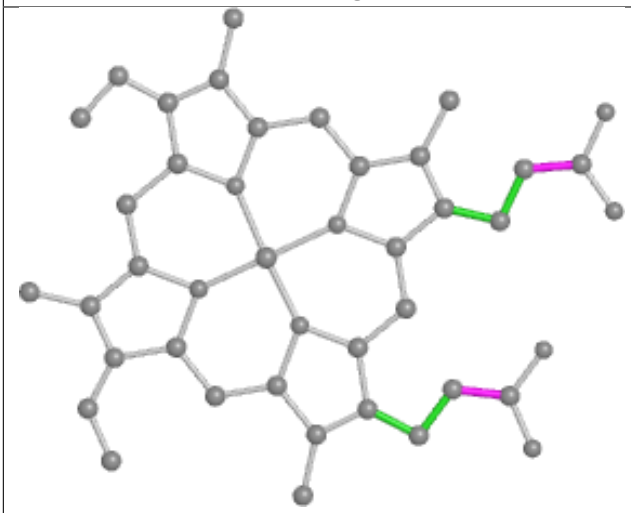
Ligand HEC B 1001



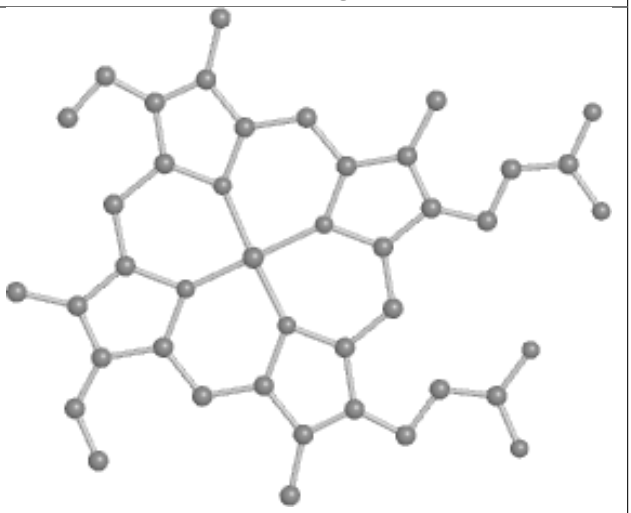
Bond lengths



Bond angles

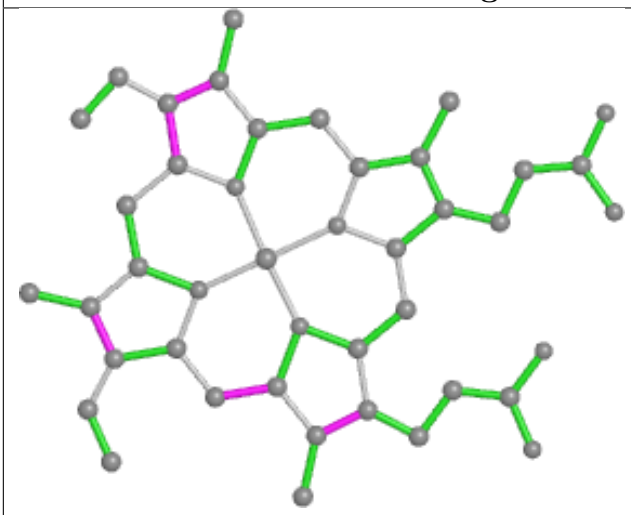


Torsions

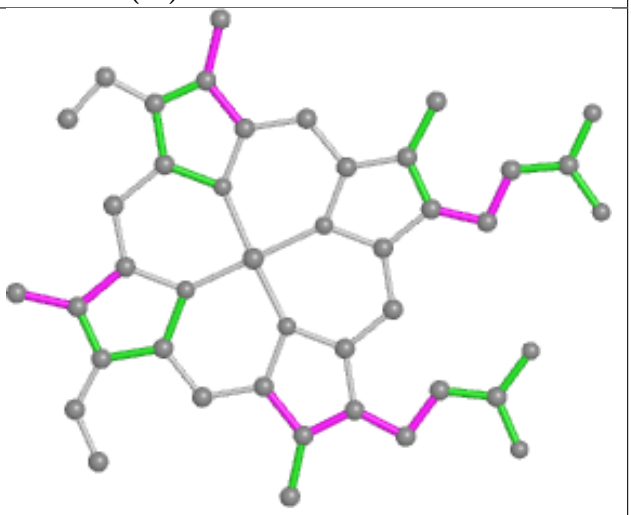


Rings

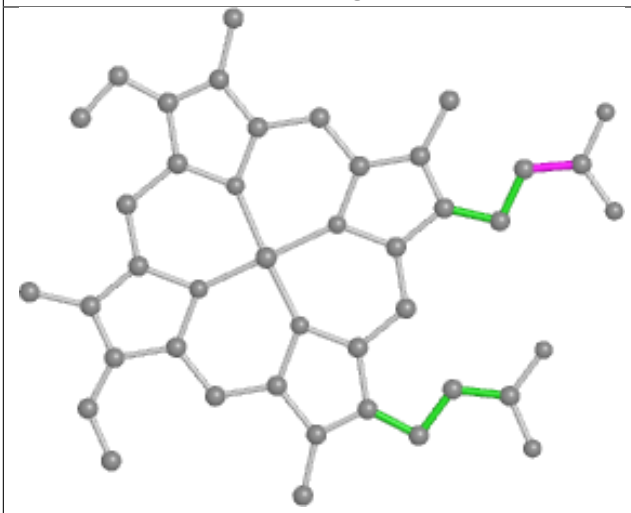
Ligand HEC B 1007 (A)



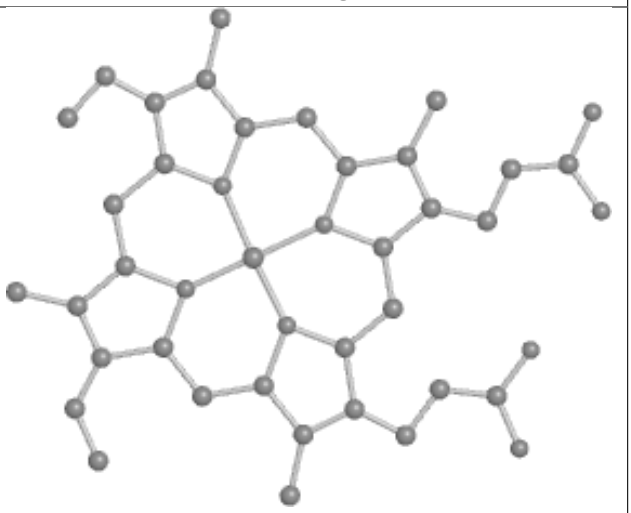
Bond lengths



Bond angles

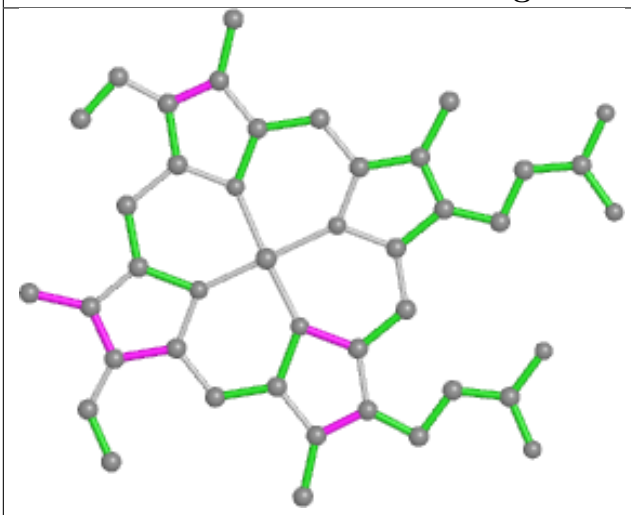


Torsions

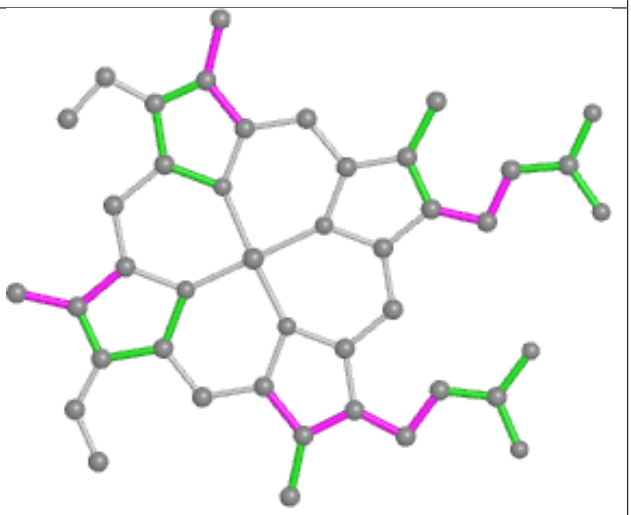


Rings

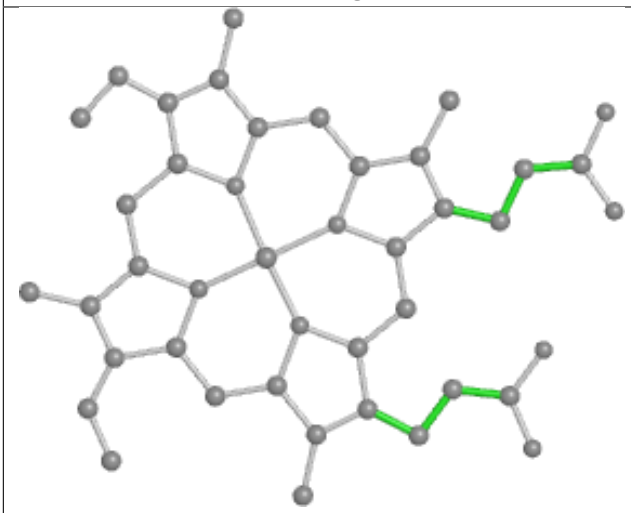
Ligand HEC A 1006



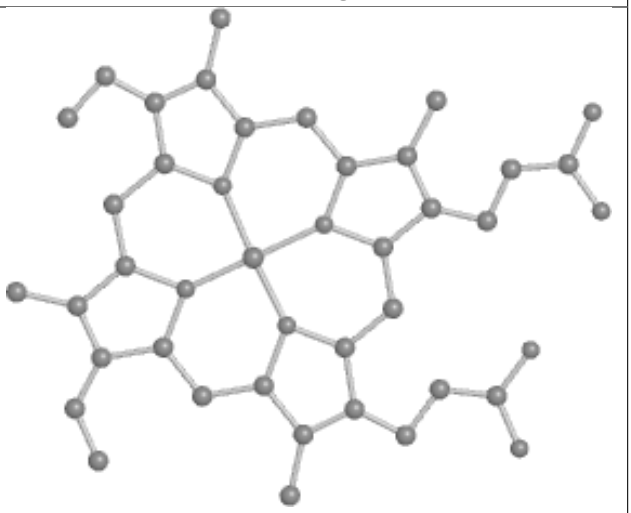
Bond lengths



Bond angles

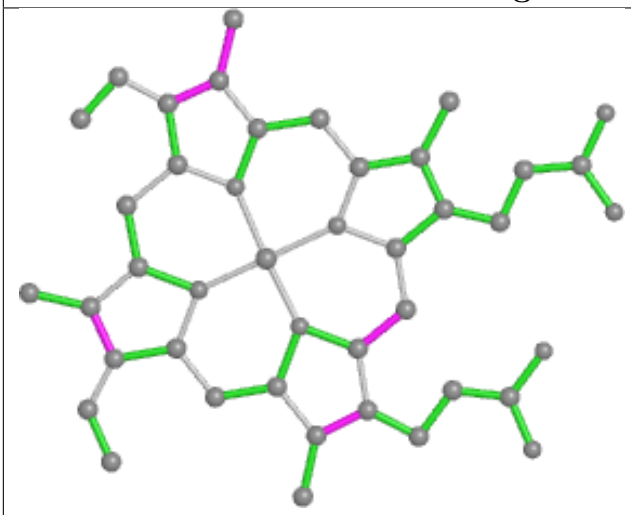


Torsions

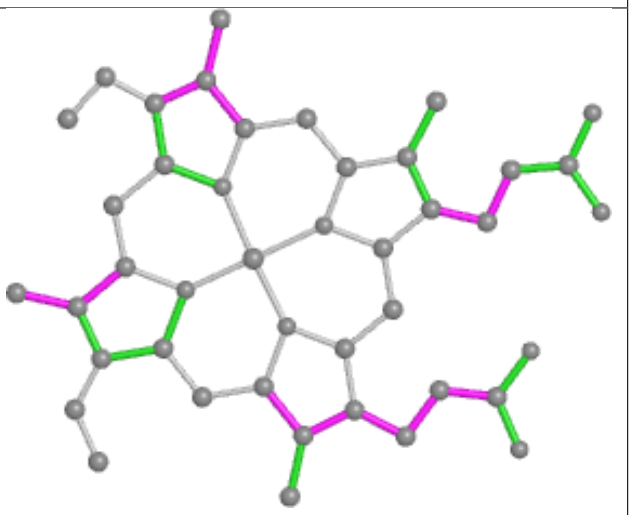


Rings

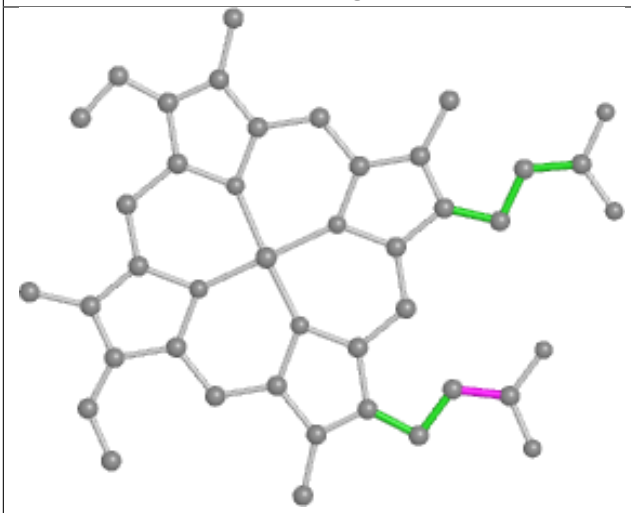
Ligand HEC A 1003



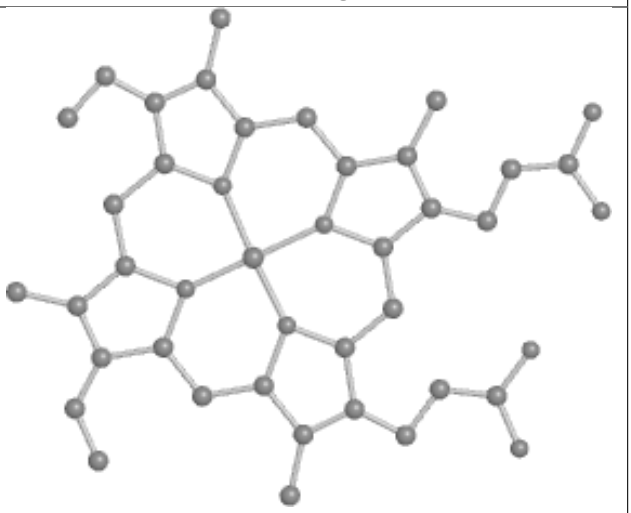
Bond lengths



Bond angles

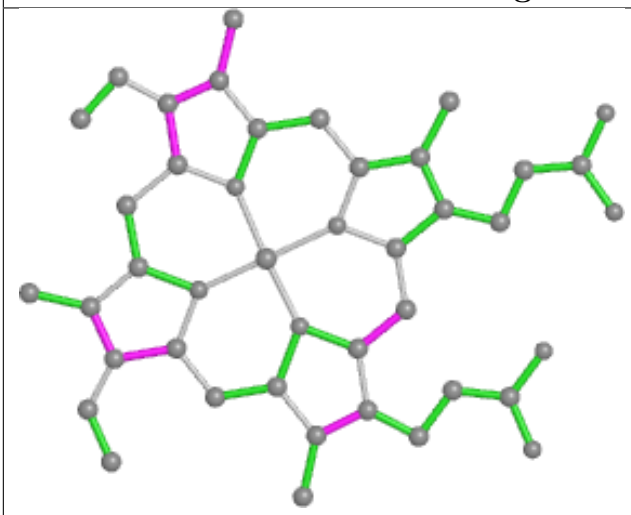


Torsions



Rings

Ligand HEC B 1004



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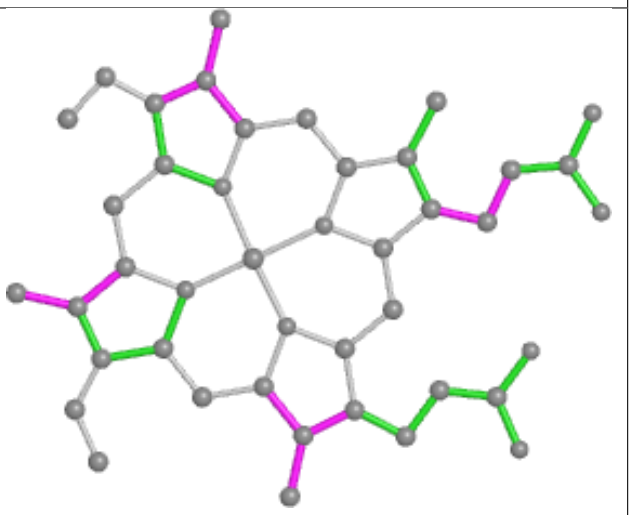
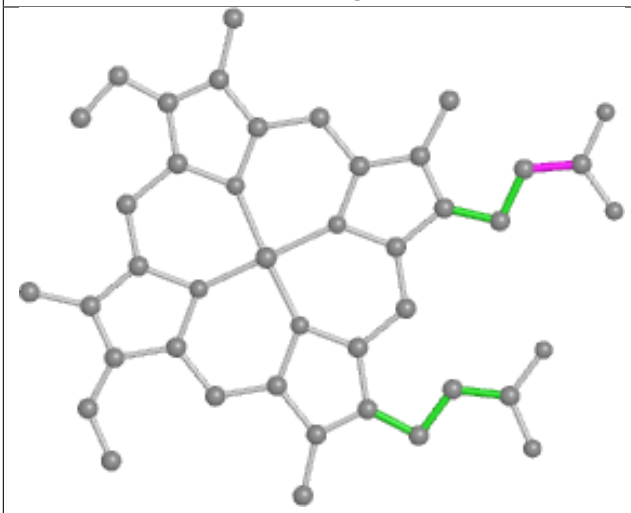


Bond angles



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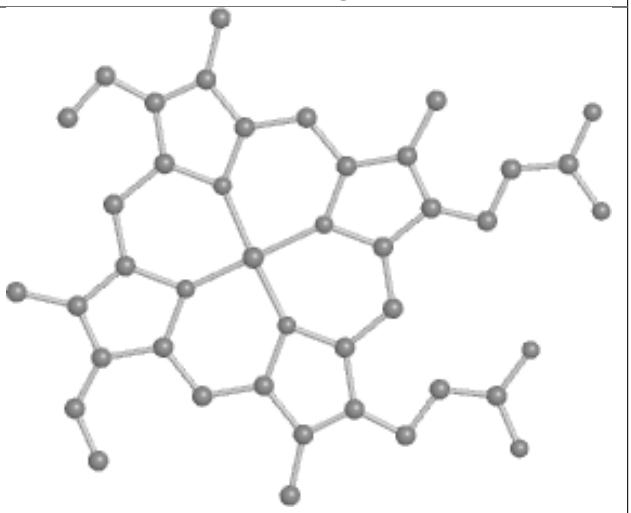
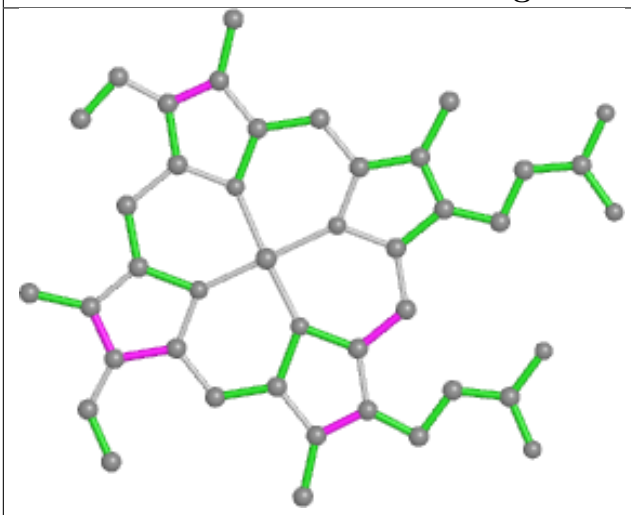
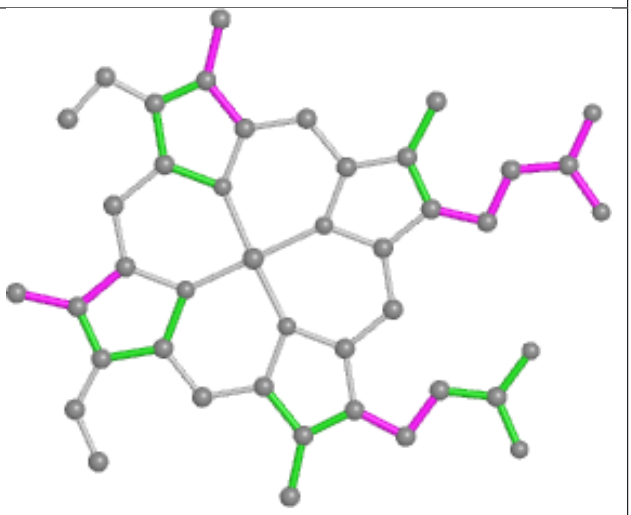


Rings

Ligand HEC A 1008



Bond lengths



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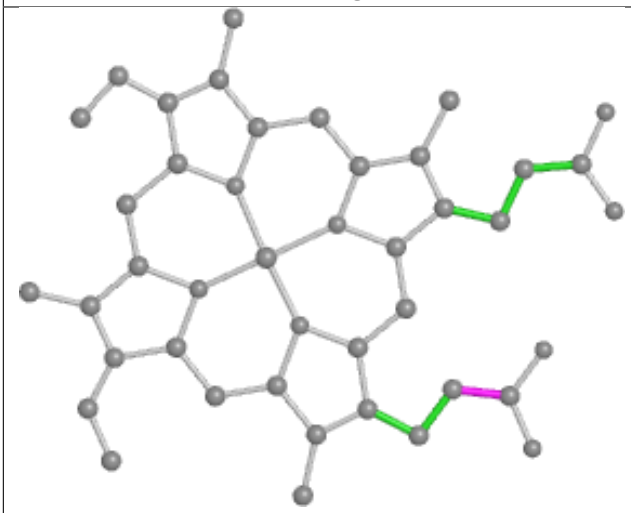

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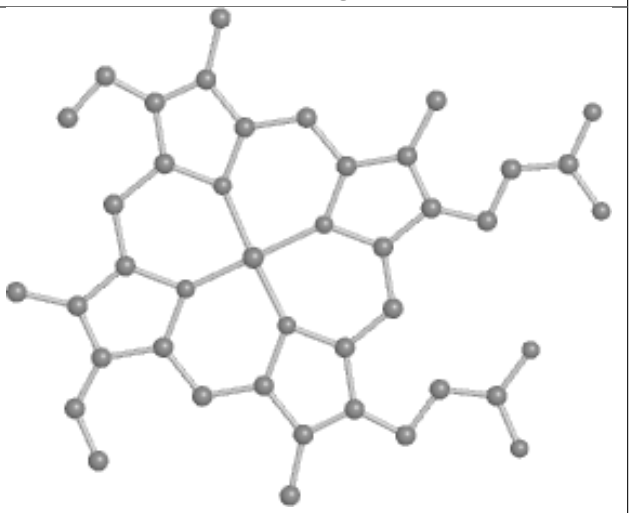
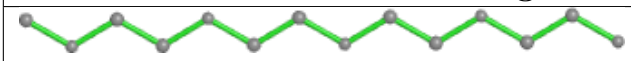


Rings

Ligand PG6 A 1010



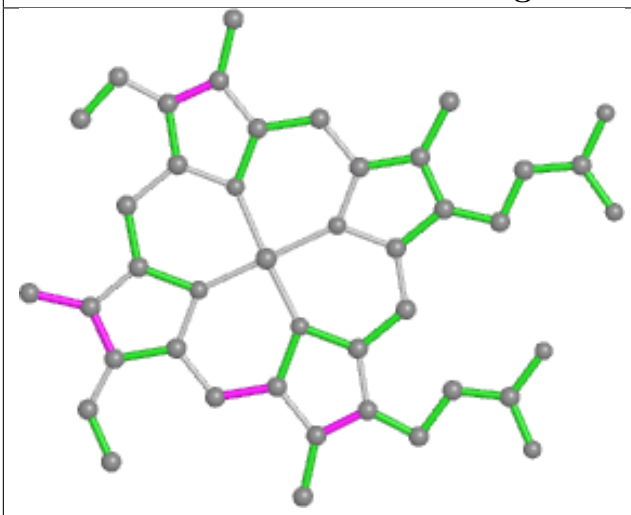
Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 1008



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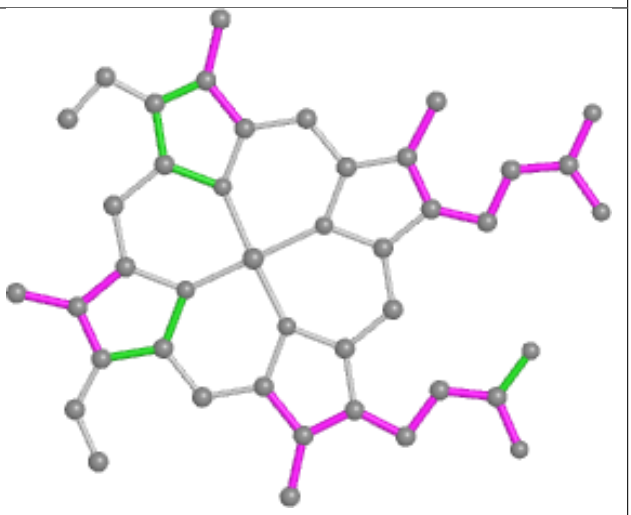

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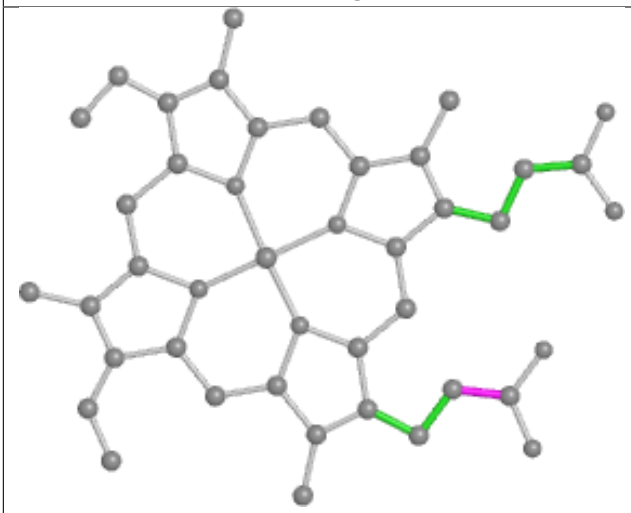

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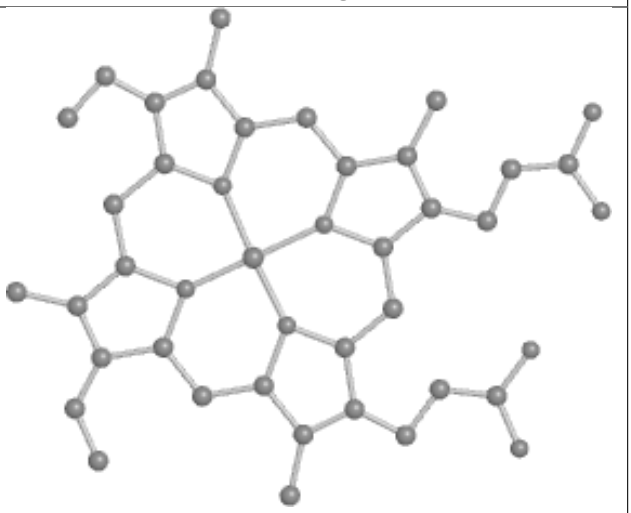
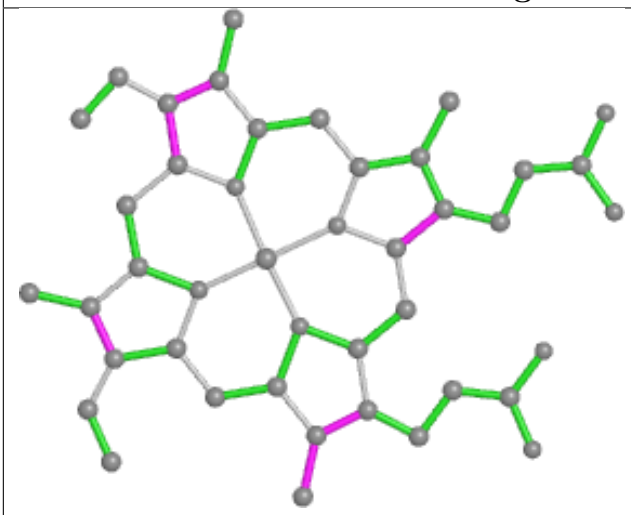


Rings

Ligand HEC B 1002



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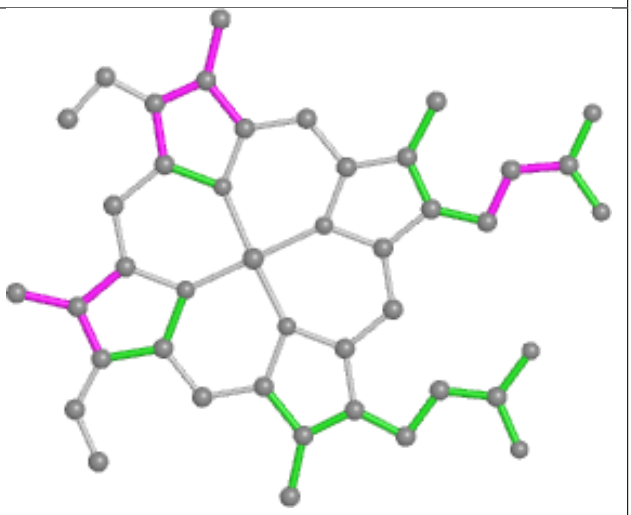
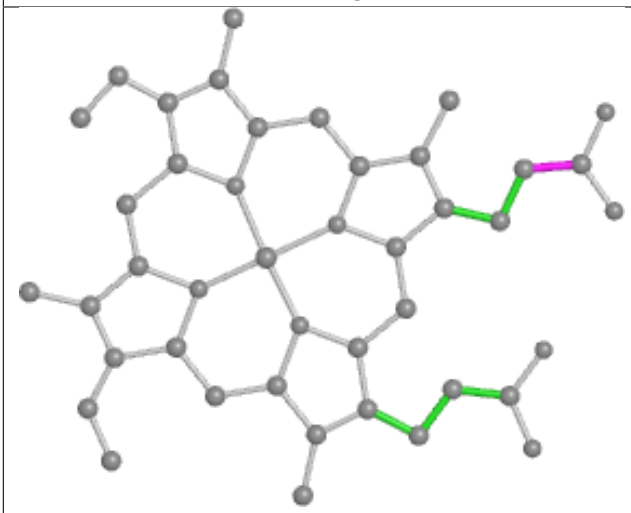
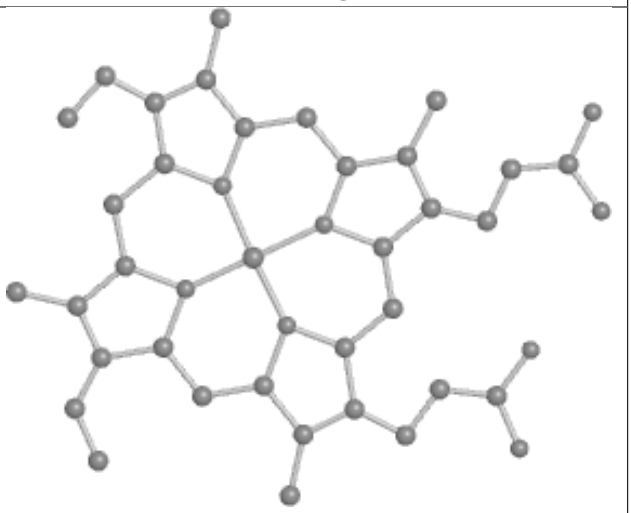


Bond angles

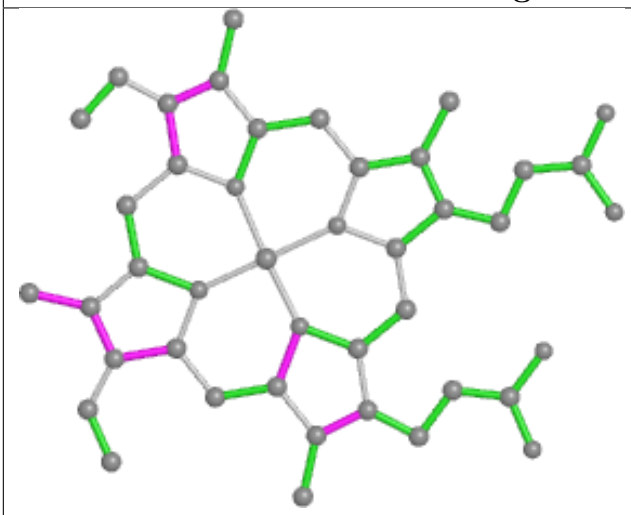


Torsions

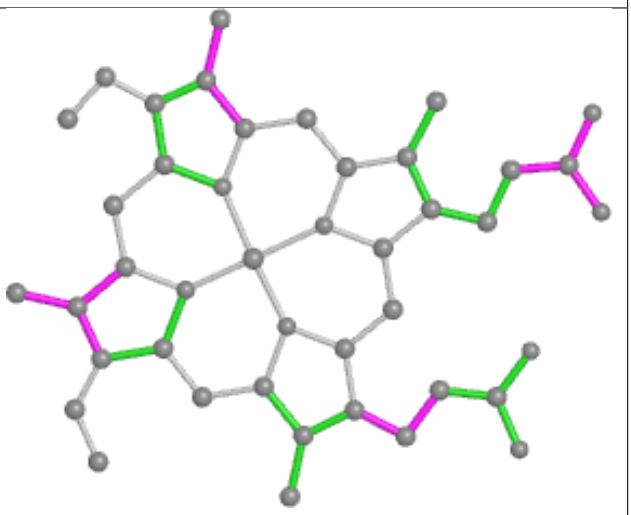


Rings

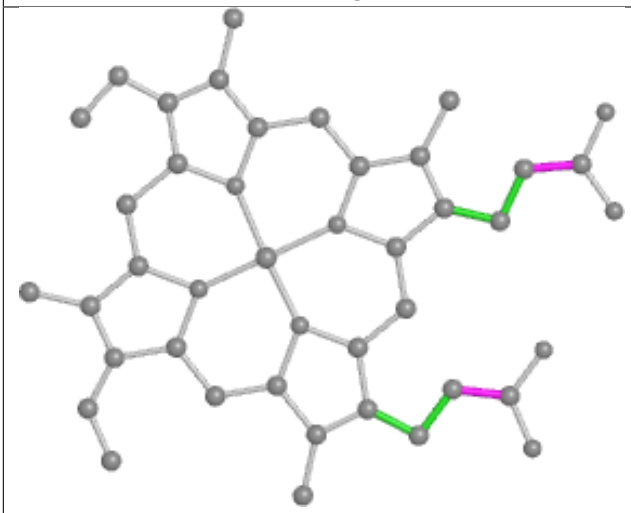
Ligand HEC A 1001



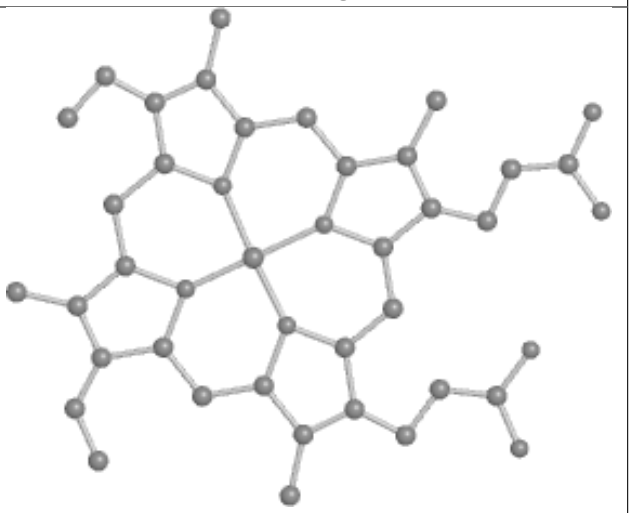
Bond lengths



Bond angles

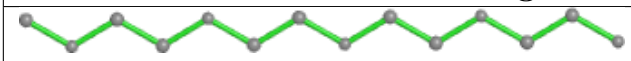


Torsions



Rings

Ligand PG6 B 1011



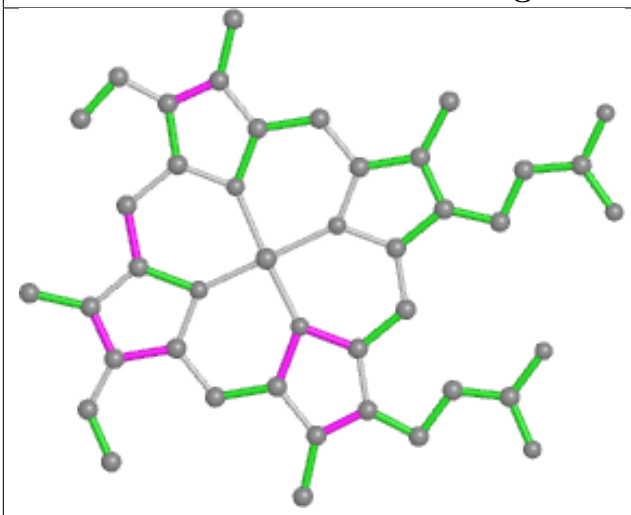
Bond lengths

Bond angles

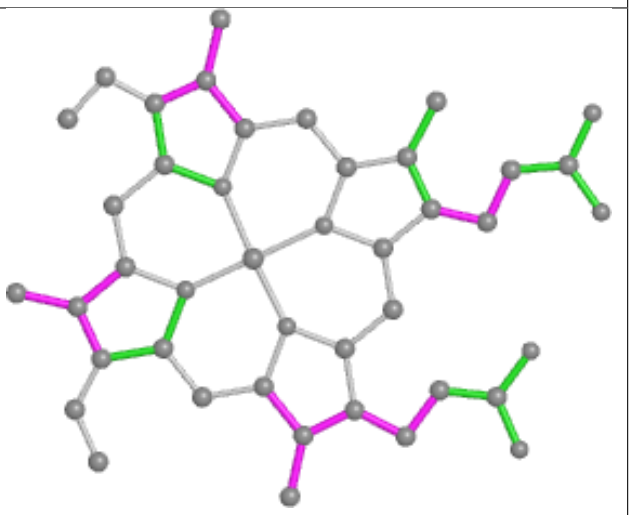
Torsions

Rings

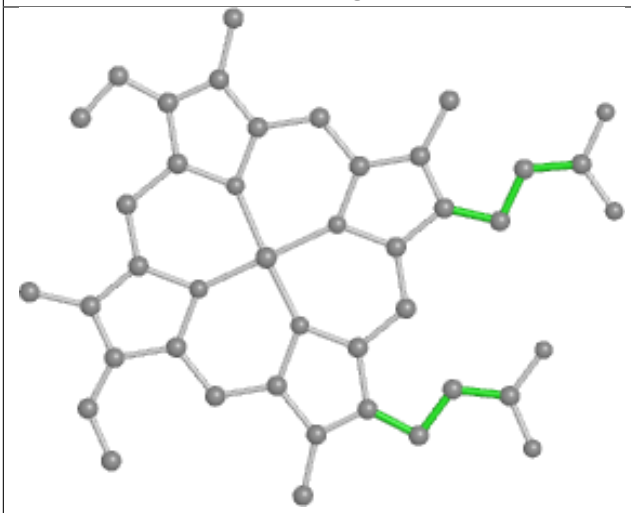
Ligand HEC B 1006



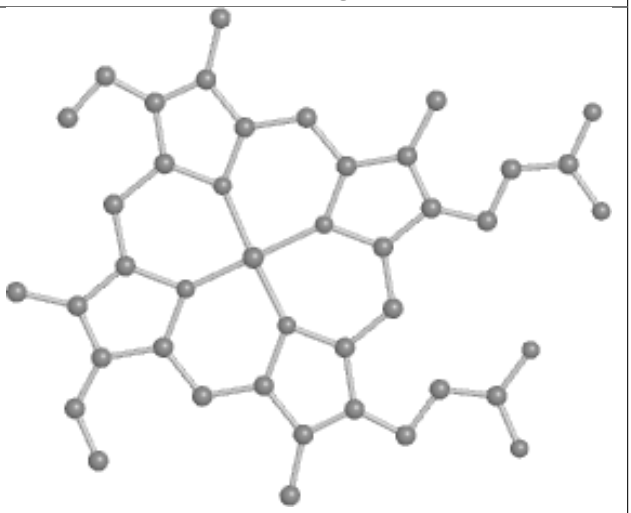
Bond lengths



Bond angles

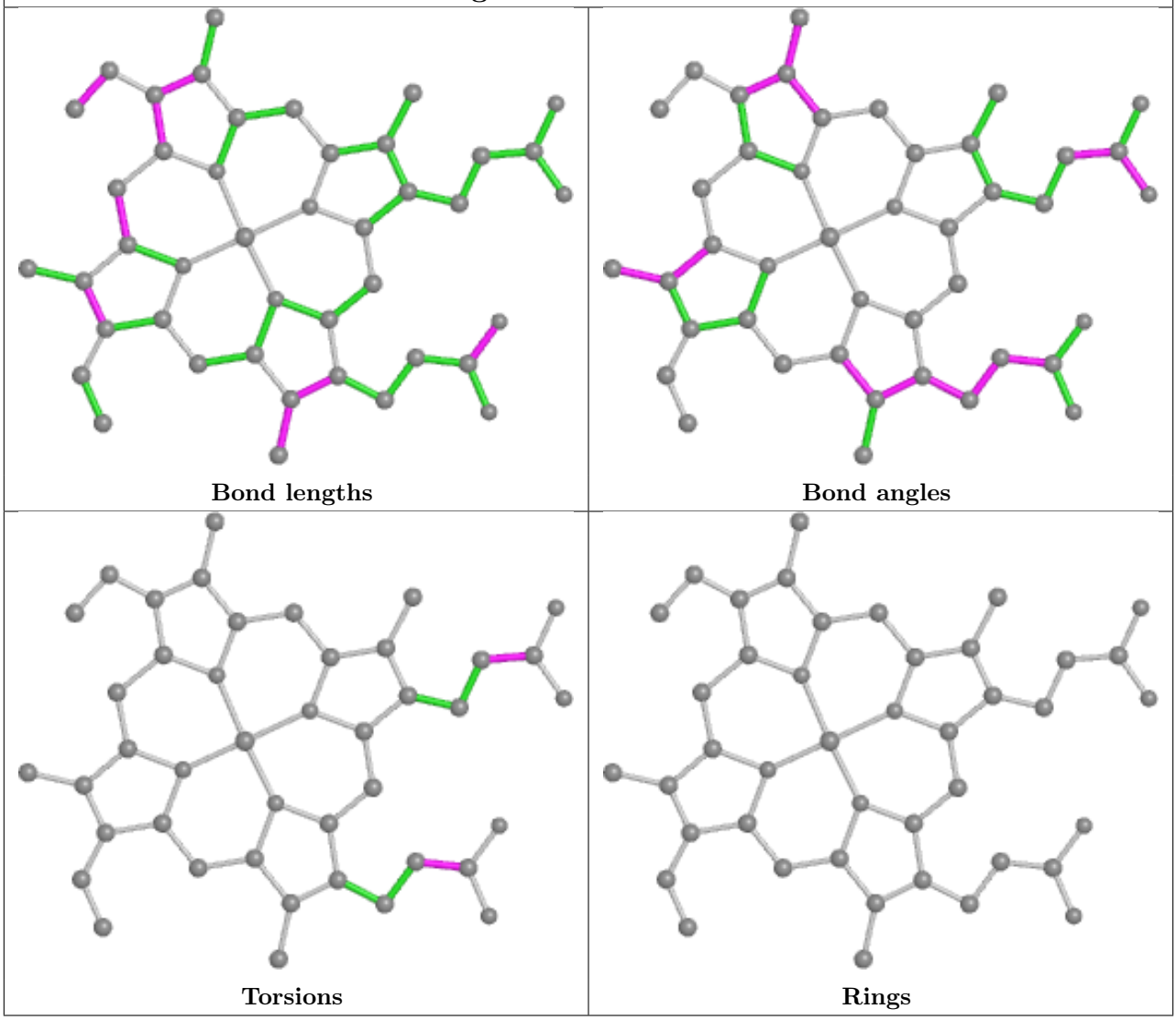


Torsions



Rings

Ligand HEC A 1005



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	519/525 (98%)	-0.54	5 (0%)	82	85	13, 18, 28, 47	0
1	B	519/525 (98%)	-0.59	5 (0%)	82	85	11, 16, 27, 49	0
All	All	1038/1050 (98%)	-0.57	10 (0%)	82	85	11, 17, 28, 49	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	VAL	6.9
1	B	523	ALA	5.6
1	A	523	ALA	5.6
1	B	522	VAL	4.9
1	B	388	GLN	2.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

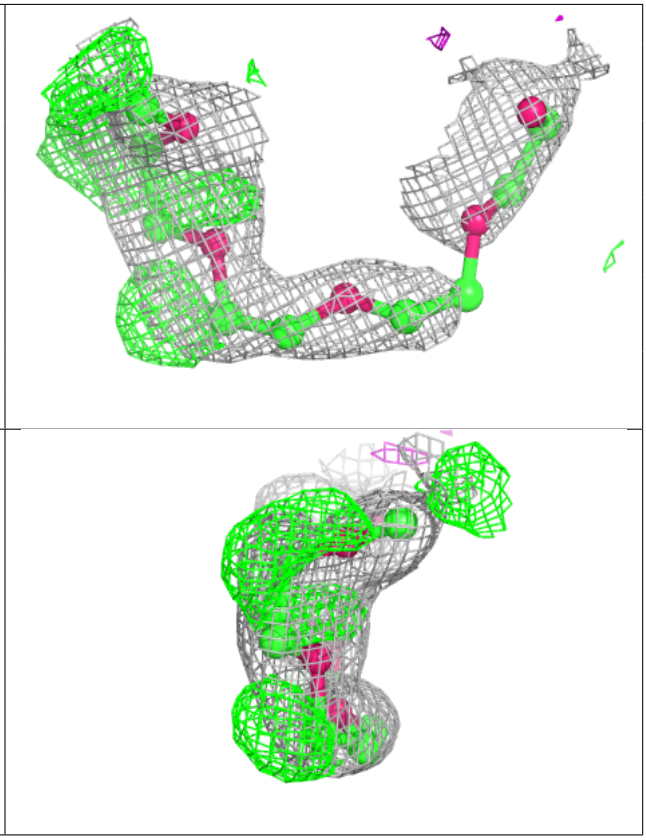
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PG4	B	1017	7/13	0.74	0.27	30,30,33,33	7
6	PG4	B	1010	7/13	0.75	0.20	27,29,31,32	7
6	PG4	B	1016	5/13	0.76	0.33	17,18,22,23	5
6	PG4	A	1009	8/13	0.76	0.18	29,33,34,35	8
6	PG4	B	1013	5/13	0.79	0.23	26,26,28,28	5
7	PG6	A	1010	14/18	0.80	0.14	21,27,31,32	14
8	TRS	B	1012	8/8	0.81	0.24	22,25,26,27	8
8	TRS	A	1012	8/8	0.83	0.20	27,28,28,28	8
7	PG6	B	1011	14/18	0.83	0.17	27,31,33,35	14
6	PG4	B	1015	5/13	0.86	0.20	23,24,25,27	5
6	PG4	A	1011	6/13	0.87	0.34	14,23,26,27	6
3	AZI	A	530	3/3	0.87	0.14	33,33,35,38	0
6	PG4	B	1014	9/13	0.88	0.22	15,19,24,25	9
6	PG4	B	1009	7/13	0.88	0.30	18,22,26,26	7
6	PG4	A	1013	8/13	0.89	0.15	35,43,50,51	0
3	AZI	B	530	3/3	0.90	0.12	31,31,35,36	0
3	AZI	A	526	3/3	0.94	0.18	20,20,22,23	3
2	HEC	A	1008	43/43	0.96	0.10	15,20,31,40	18
4	CA	B	528	1/1	0.96	0.08	19,19,19,19	1
2	HEC	B	1003	43/43	0.97	0.08	11,14,25,34	18
4	CA	A	528	1/1	0.97	0.09	19,19,19,19	1
2	HEC	A	1003	43/43	0.97	0.08	12,14,23,34	18
5	NA	B	529	1/1	0.97	0.12	18,18,18,18	1
2	HEC	B	1008	43/43	0.97	0.09	13,17,25,35	18
3	AZI	B	526	3/3	0.97	0.12	18,18,18,21	3
2	HEC	B	1007[A]	43/43	0.98	0.07	11,12,14,15	24
2	HEC	B	1007[B]	43/43	0.98	0.07	11,12,14,19	24
2	HEC	A	1006	43/43	0.98	0.07	11,13,15,16	18
2	HEC	B	1002	43/43	0.98	0.07	13,16,17,19	18
2	HEC	A	1007[A]	43/43	0.98	0.07	12,14,15,15	24
2	HEC	B	1001	43/43	0.98	0.07	16,19,23,25	18
2	HEC	A	1007[B]	43/43	0.98	0.07	12,14,16,19	24
2	HEC	A	1004	43/43	0.98	0.07	13,15,20,21	18
2	HEC	A	1002	43/43	0.98	0.07	13,15,17,19	18
2	HEC	A	1005	43/43	0.98	0.07	11,14,21,27	18
2	HEC	A	1001	43/43	0.98	0.08	14,17,19,23	18
2	HEC	B	1005	43/43	0.98	0.07	10,13,21,27	18
5	NA	A	529	1/1	0.98	0.22	25,25,25,25	1
2	HEC	B	1006	43/43	0.98	0.07	9,12,13,14	18
4	CA	B	527	1/1	0.99	0.03	14,14,14,14	0
4	CA	A	527	1/1	0.99	0.04	16,16,16,16	0
2	HEC	B	1004	43/43	0.99	0.07	12,14,18,18	18

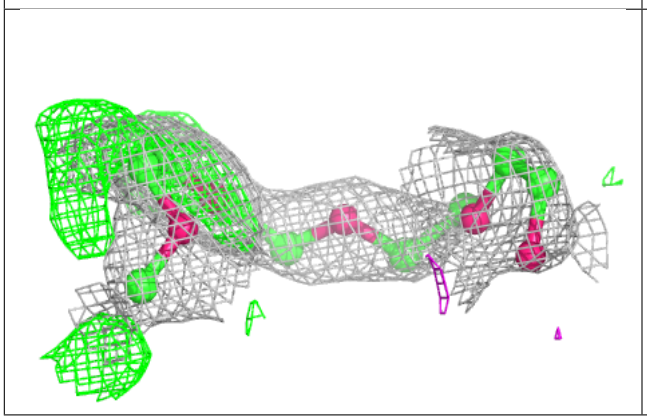
The following is a graphical depiction of the model fit to experimental electron density of all

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 PG6 A 1010:

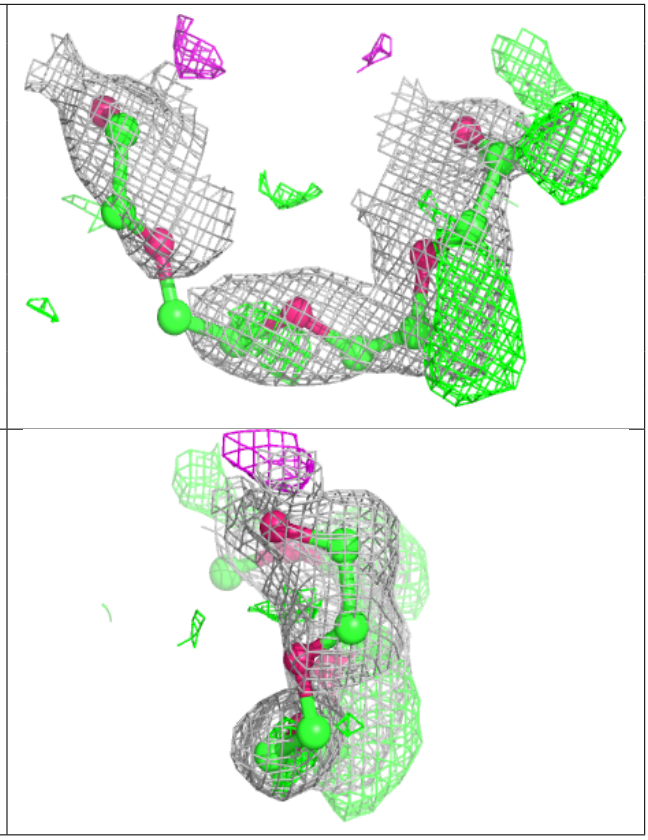
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





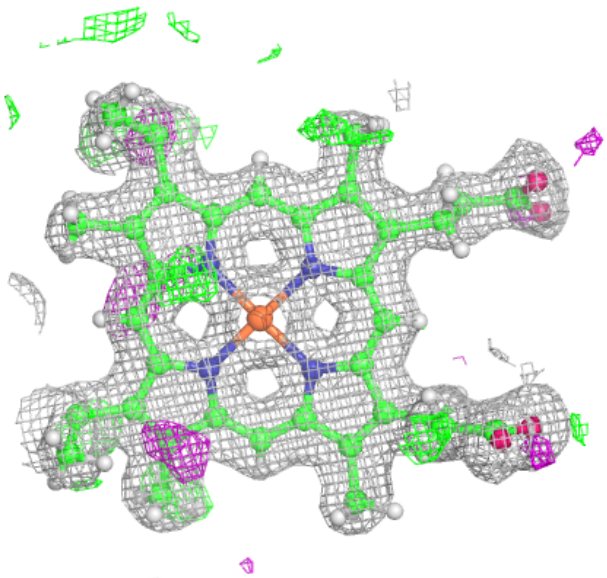
Electron density around PG6 B 1011:

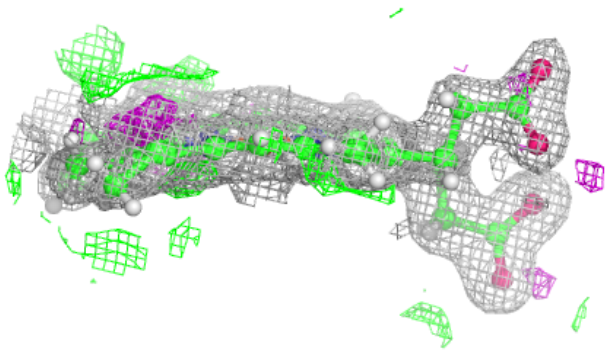
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

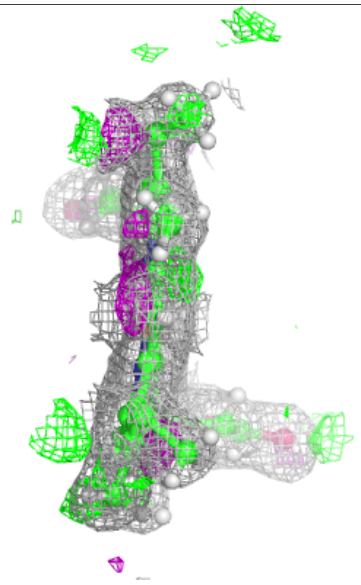


Electron density around HEC A 1008:

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

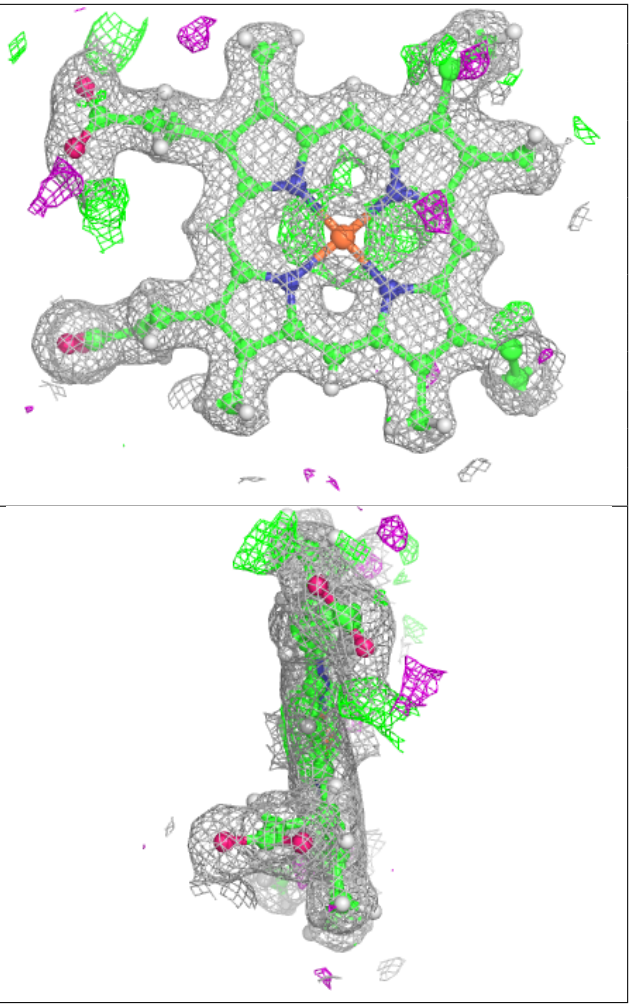






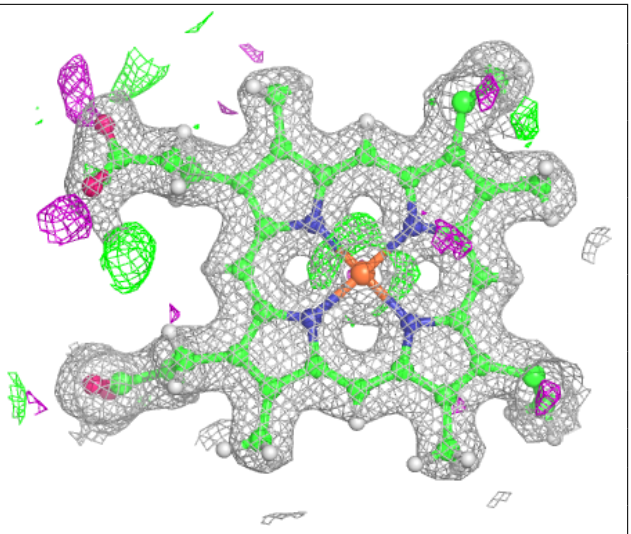
Electron density around HEC B 1003:

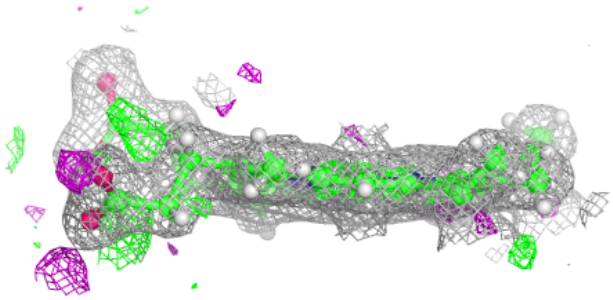
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

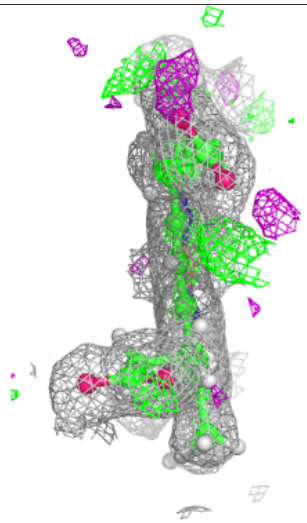


Electron density around HEC A 1003:

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

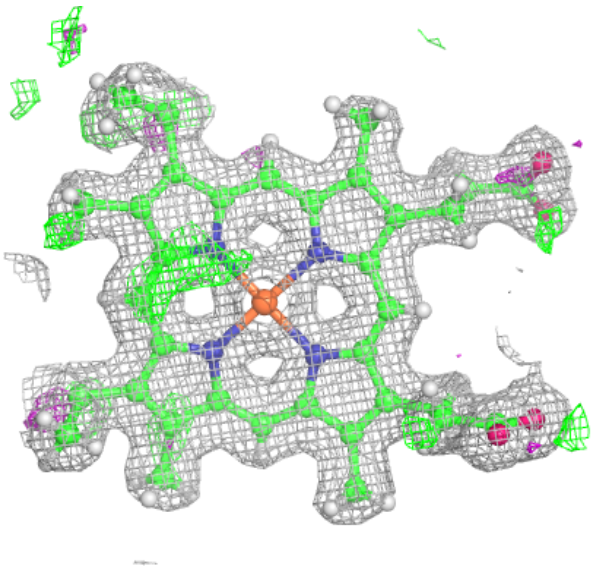


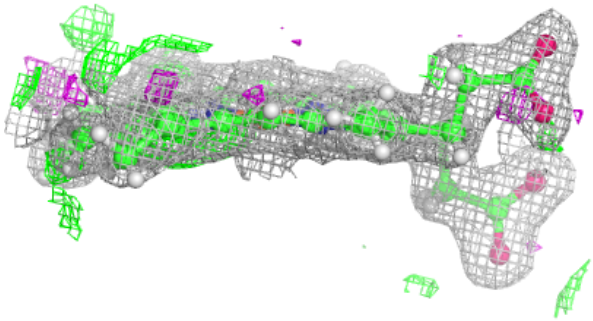


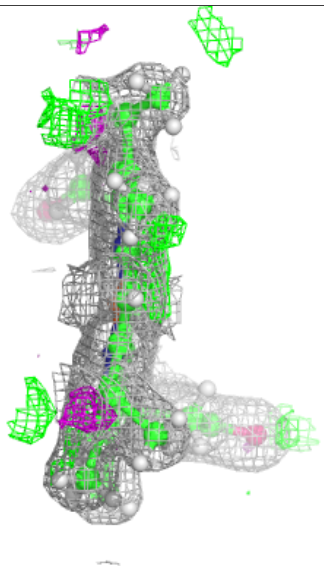


Electron density around HEC B 1008:

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

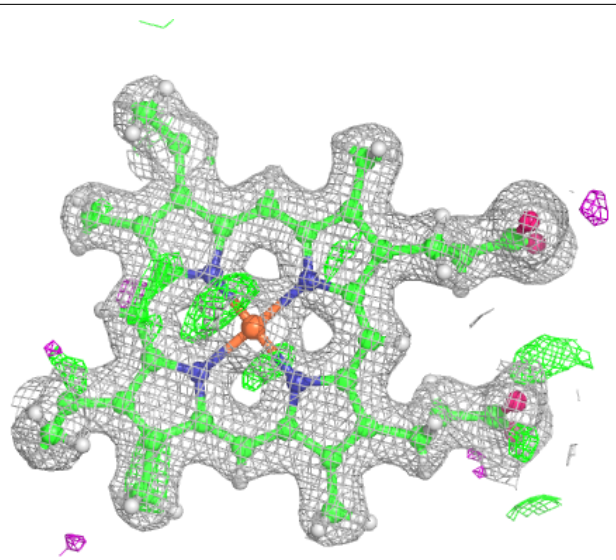


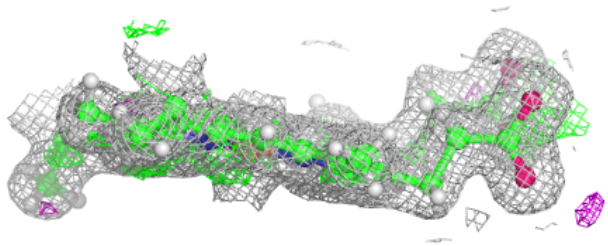


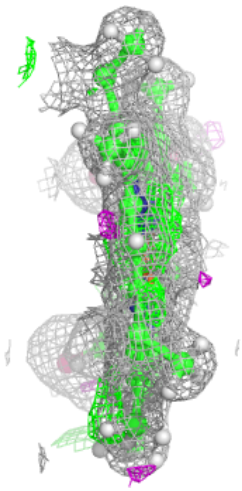


Electron density around HEC B 1007 (A):

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

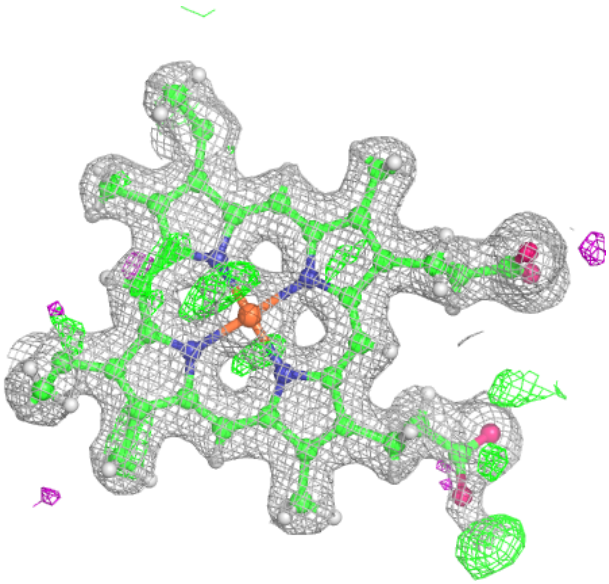


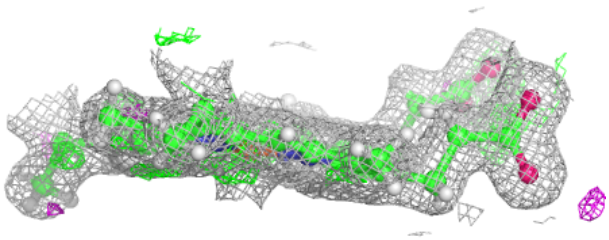


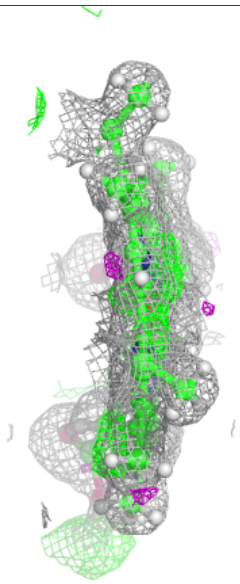


Electron density around HEC B 1007 (B):

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

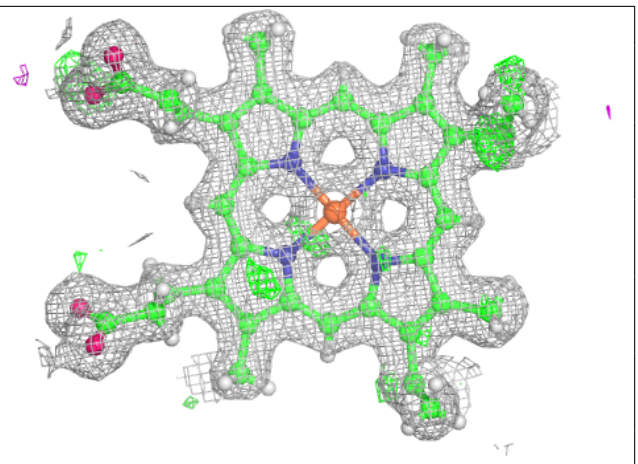


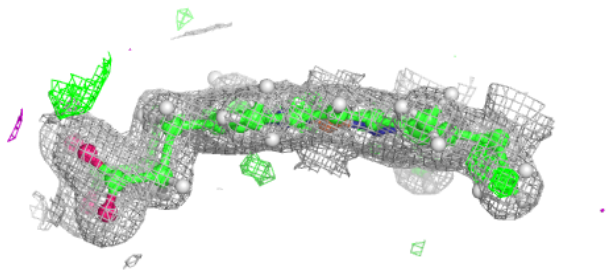


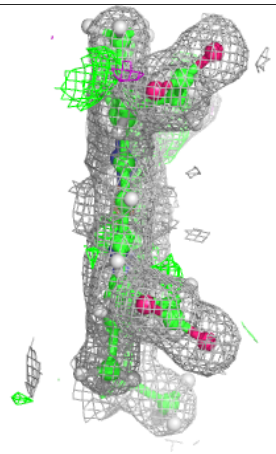


Electron density around HEC A 1006:

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

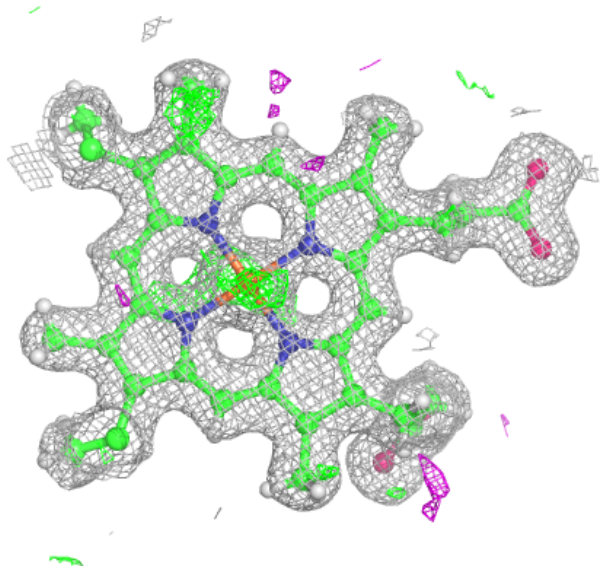


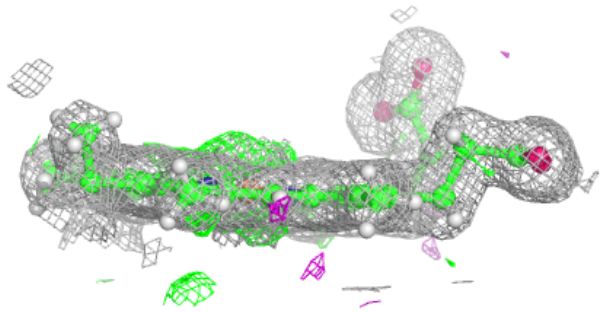


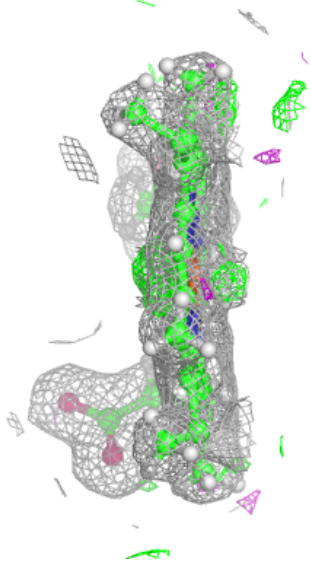


Electron density around HEC B 1002:

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

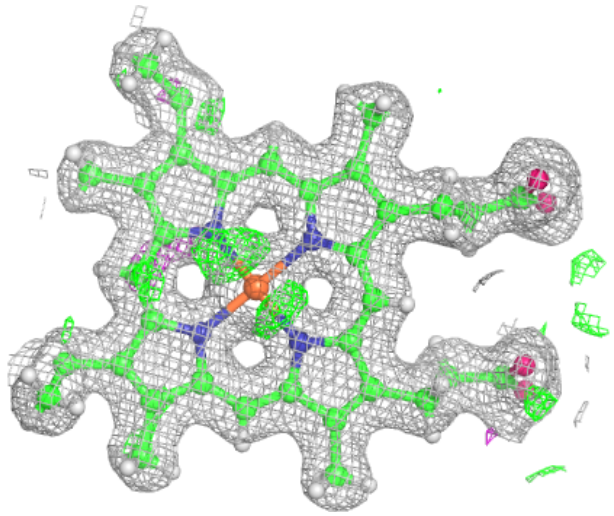


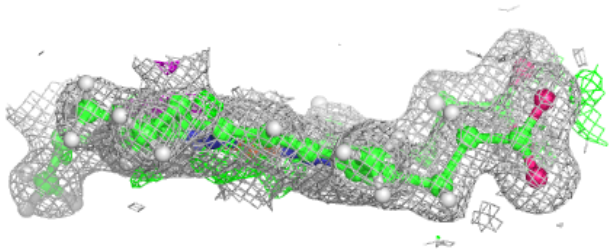


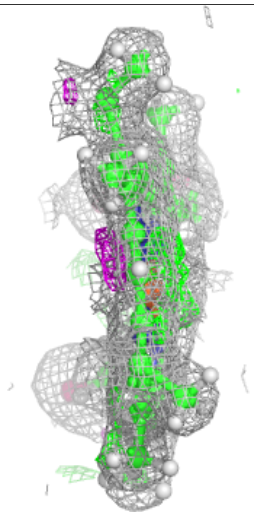


Electron density around HEC A 1007 (A):

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

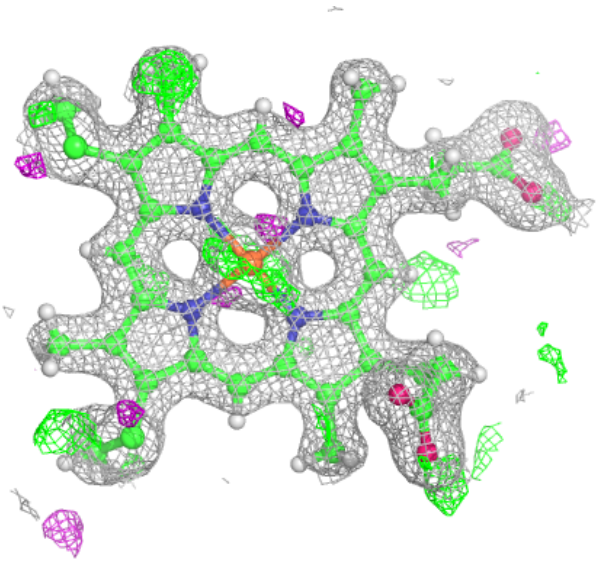


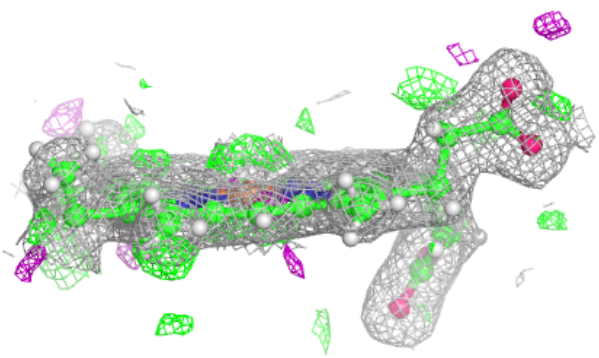


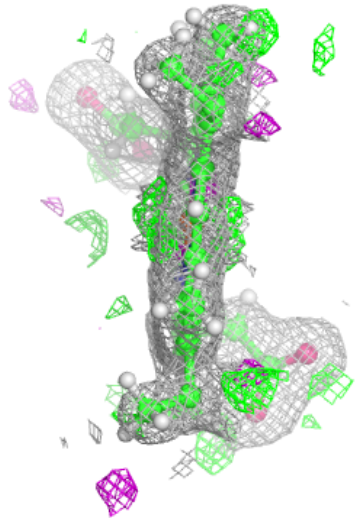


Electron density around HEC B 1001:

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

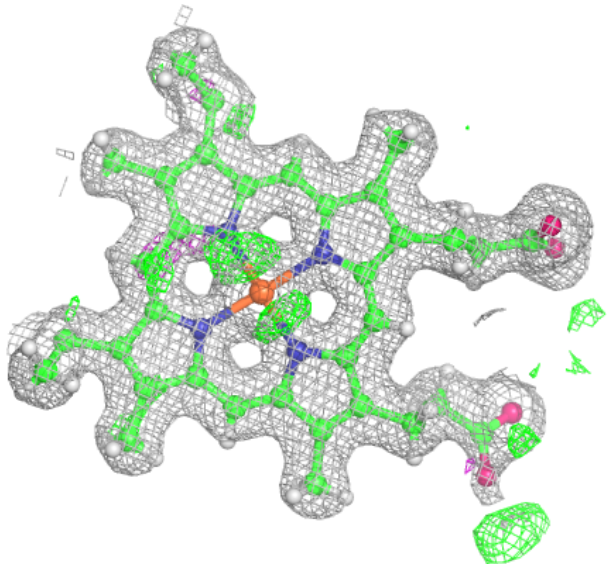


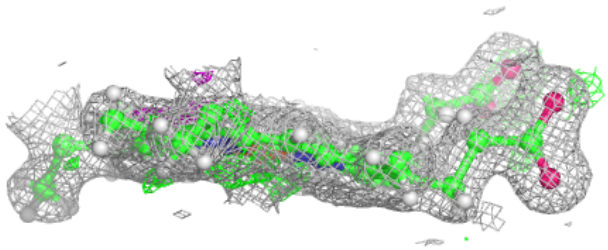


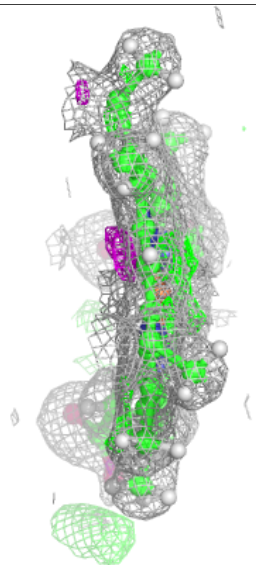


Electron density around HEC A 1007 (B):

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

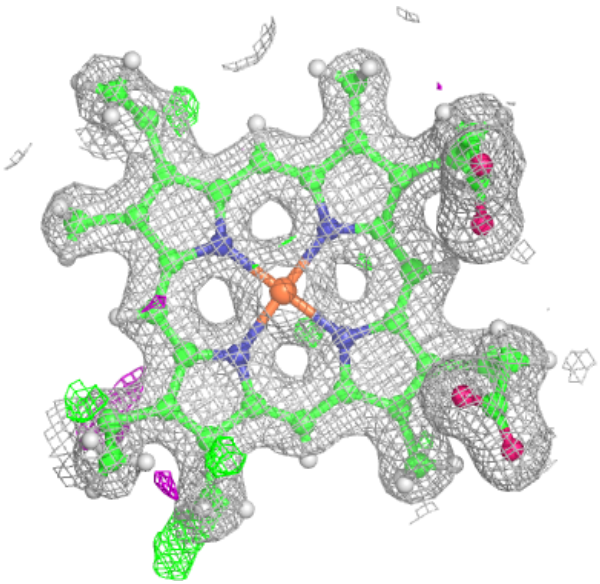


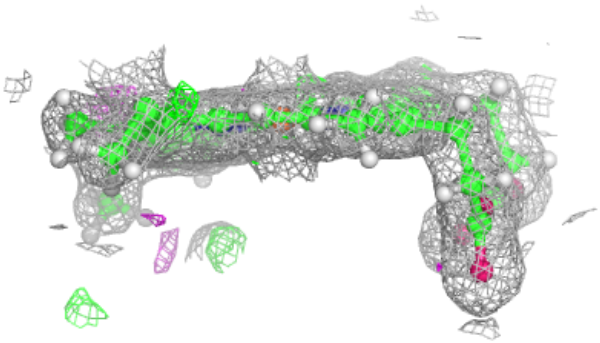


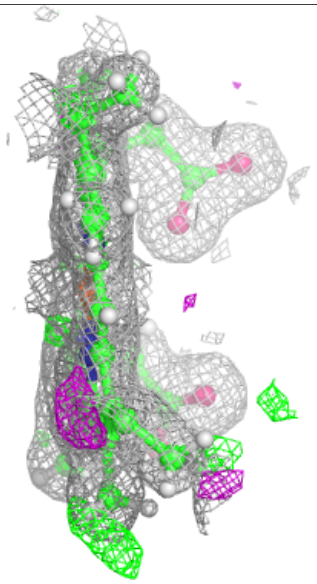


Electron density around HEC A 1004:

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

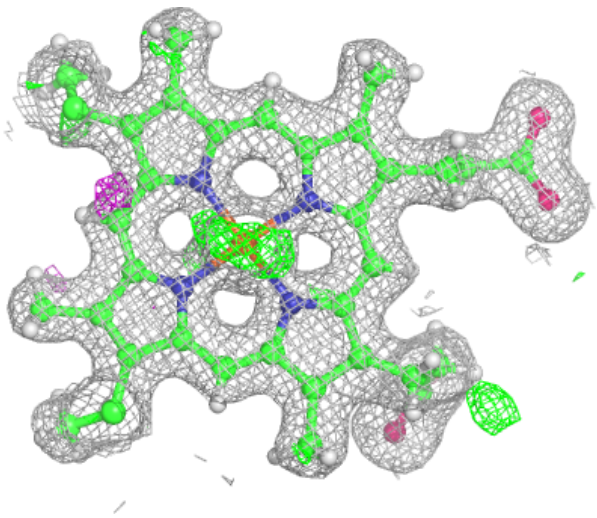


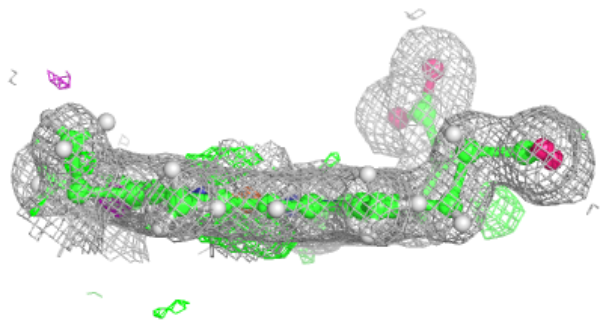




Electron density around HEC A 1002:

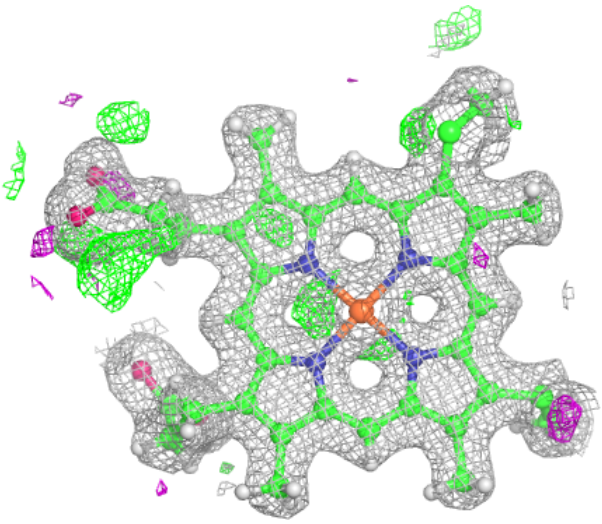
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

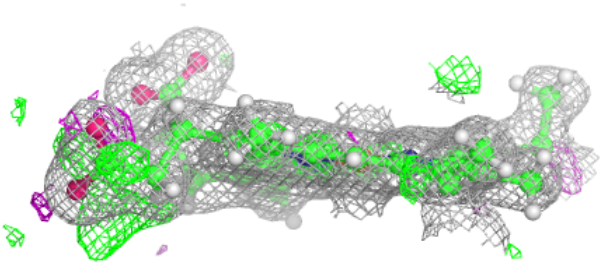


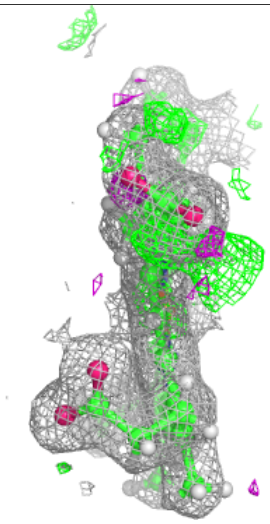


Electron density around HEC A 1005:

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

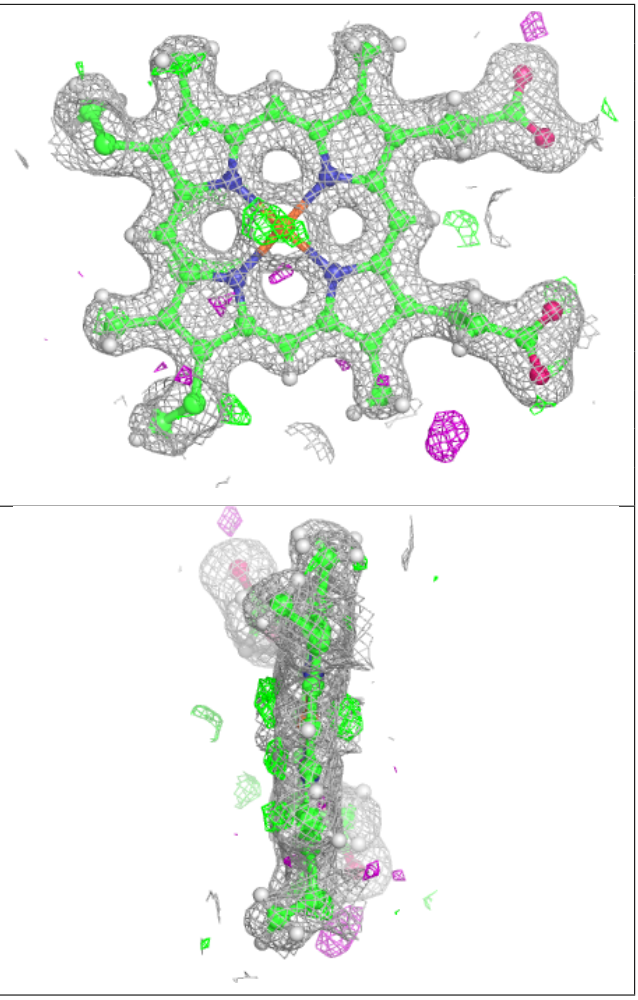






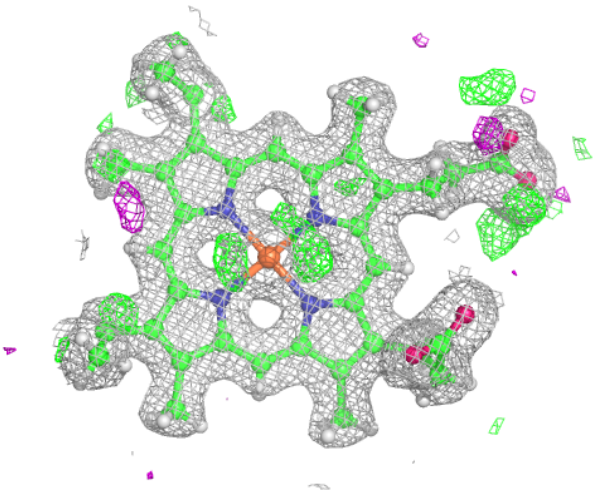
Electron density around HEC A 1001:

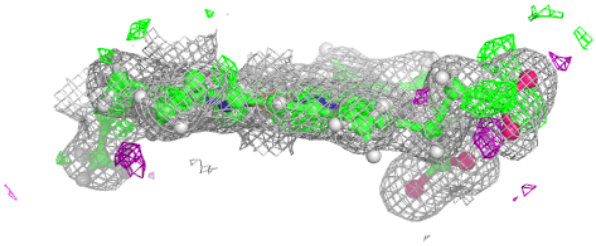
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

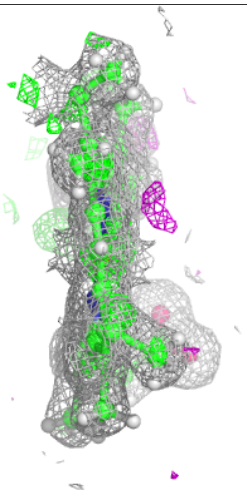


Electron density around HEC B 1005:

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

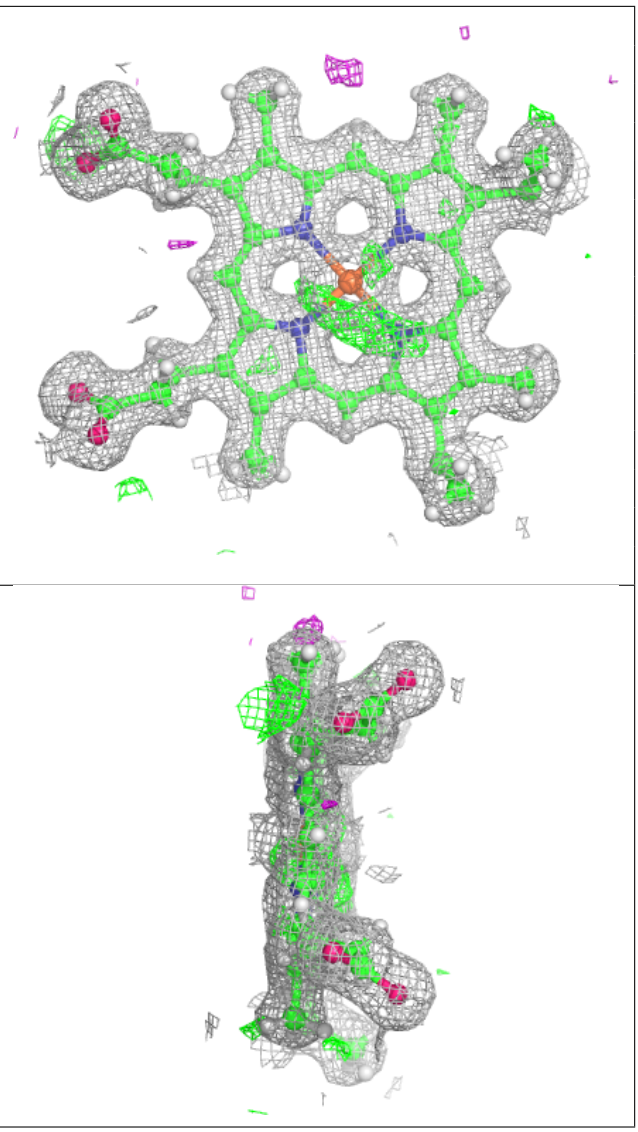






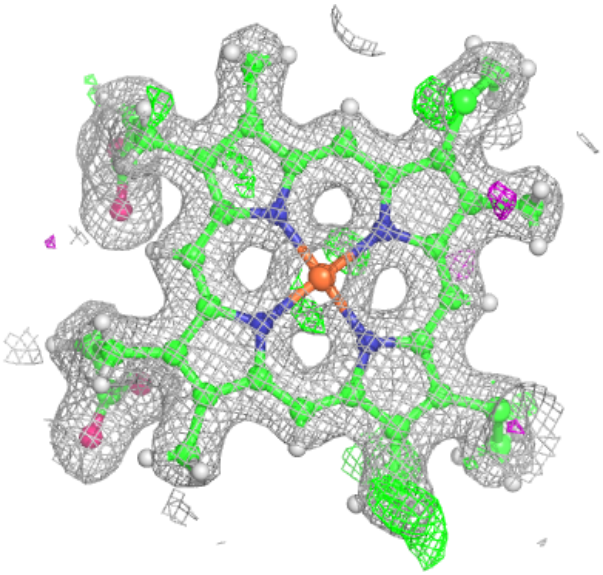
Electron density around HEC B 1006:

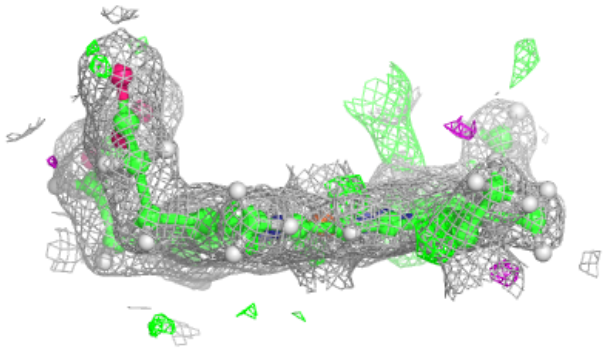
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

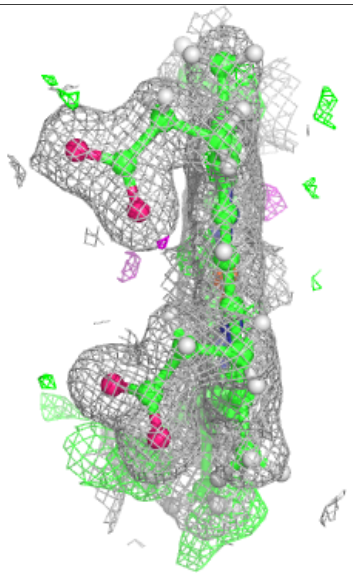


Electron density around HEC B 1004:

$2mF_o$-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.