Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 07:27 PM EDT

PDB ID	:	3SCE / pdb_00003sce
Title	:	Structure of the Thioalkalivibrio nitratireducens cytochrome c nitrite reductase with a covalent bond between the CE1 atom of Tyr303 and the CG atom of Gln360 (TvNiRb)
Authors	:	Trofimov, A.A.; Polyakov, K.M.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on	:	2011-06-07
Resolution	:	1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

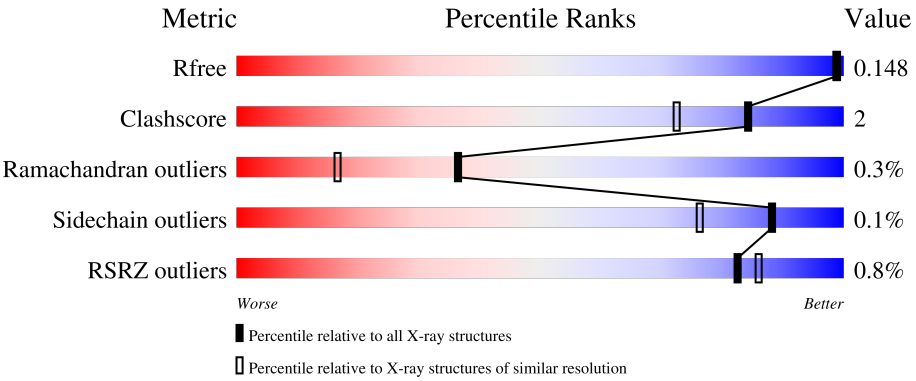
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

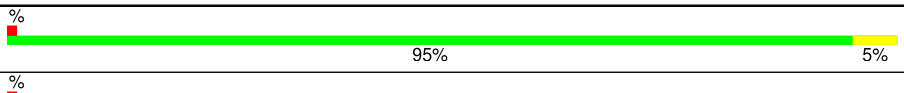
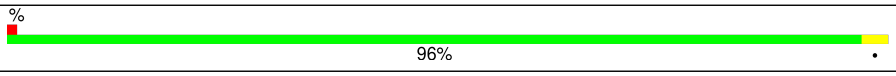
The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	519	
1	B	519	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	1001	X	-	-	-
2	HEC	A	1002	X	-	-	-
2	HEC	A	1003	X	-	-	-
2	HEC	A	1004	X	-	-	-
2	HEC	A	1005[A]	X	-	-	-
2	HEC	A	1005[B]	X	-	-	-
2	HEC	A	1006	X	-	-	-
2	HEC	A	1007[A]	X	-	-	-
2	HEC	A	1007[B]	X	-	-	-
2	HEC	A	1008	X	-	-	-
2	HEC	B	1001	X	-	-	-
2	HEC	B	1002	X	-	-	-
2	HEC	B	1003	X	-	-	-
2	HEC	B	1004	X	-	-	-
2	HEC	B	1005[A]	X	-	-	-
2	HEC	B	1005[B]	X	-	-	-
2	HEC	B	1006	X	-	-	-
2	HEC	B	1007[A]	X	-	-	-
2	HEC	B	1007[B]	X	-	-	-
2	HEC	B	1008	X	-	-	-

2 Entry composition (i)

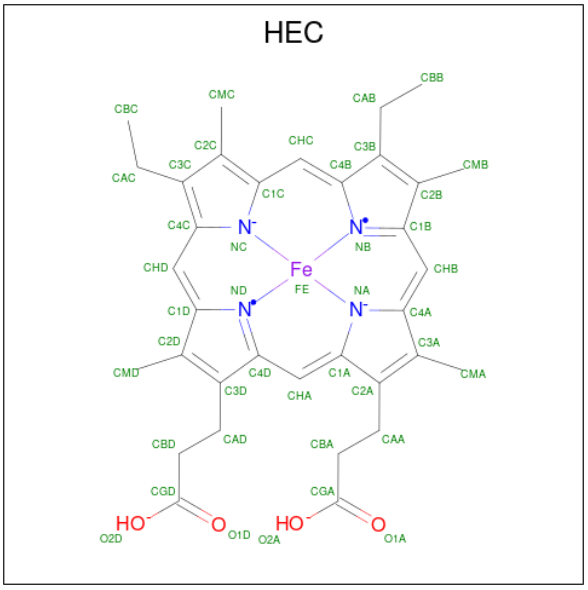
There are 8 unique types of molecules in this entry. The entry contains 10447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	20	0
			4184	2596	758	791	39			
1	B	519	Total	C	N	O	S	0	23	0
			4195	2600	761	795	39			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			46	35	1	4	6		

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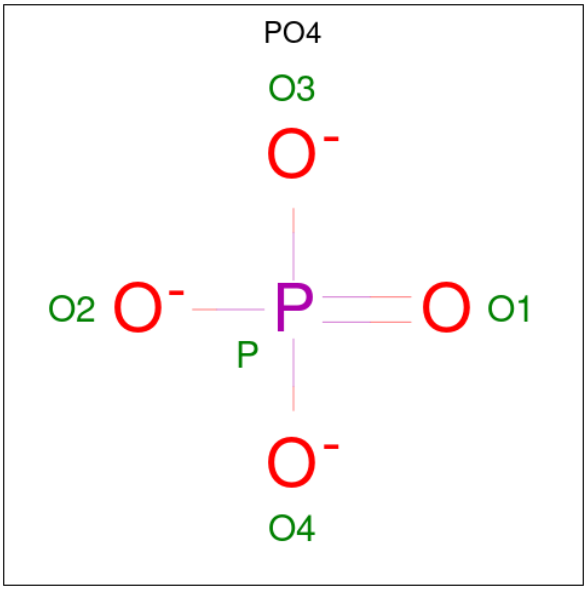
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

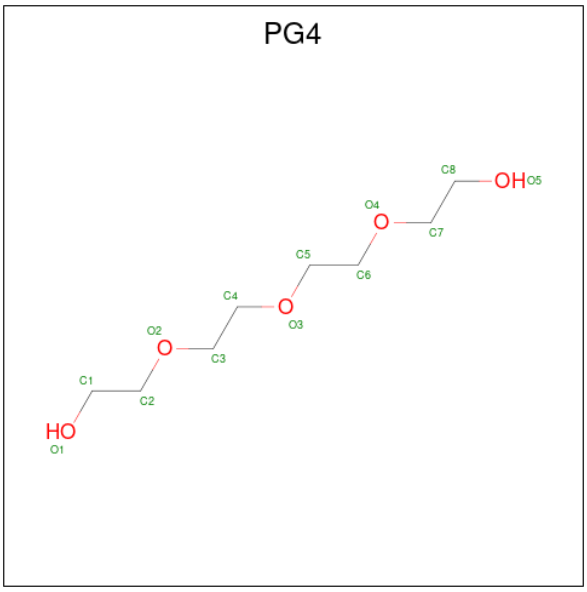


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: 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 TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

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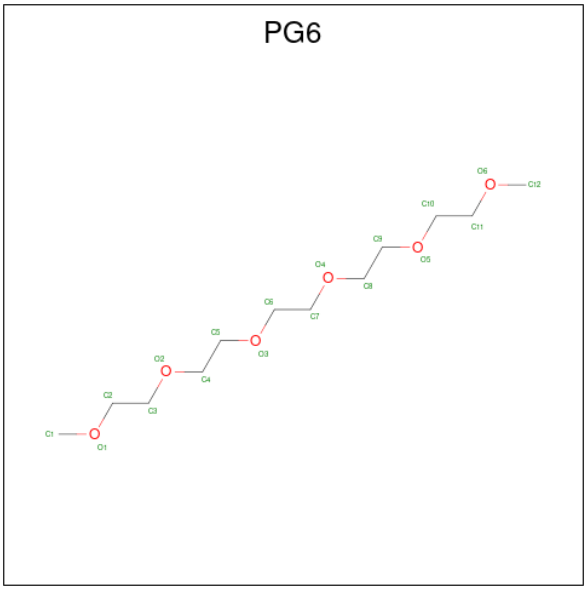
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 5 3 2	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 5 3 2	0	0
5	A	1	Total C O 6 4 2	0	0
5	B	1	Total C O 8 5 3	0	0
5	B	1	Total C O 8 5 3	0	0
5	B	1	Total C O 9 6 3	0	0
5	B	1	Total C O 8 5 3	0	0
5	B	1	Total C O 9 6 3	0	0
5	B	1	Total C O 5 3 2	0	0
5	B	1	Total C O 7 5 2	0	0
5	B	1	Total C O 8 5 3	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (CCD ID: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 10 6 4	0	0
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C O 10 6 4	0	0
6	B	1	Total C O 5 3 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0

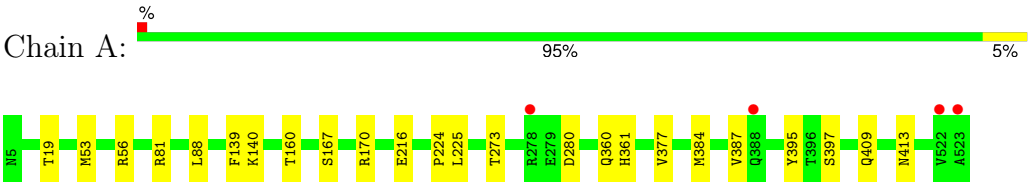
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	601	Total O 601 601	0	0
8	B	585	Total O 585 585	0	0

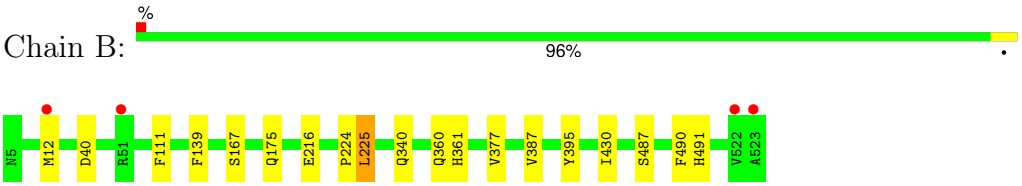
3 Residue-property plots (i)

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



• Molecule 1: Eight-heme nitrite reductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	193.00Å 193.00Å 193.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 1.45 100.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (100.00-1.45) 99.9 (100.00-1.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.124 , 0.140 0.134 , 0.148	Depositor DCC
R_{free} test set	20931 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.053 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: PG6, PG4, PO4, NA, CA, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/4401	0.78	0/5966
1	B	0.62	0/4427	0.78	0/5999
All	All	0.62	0/8828	0.78	0/11965

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	A	4184	0	3911	21	0
1	B	4195	0	3910	13	0
2	A	351	0	192	3	0
2	B	352	0	196	3	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	54	0	64	7	0
5	B	62	0	69	5	0
6	A	17	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	20	0	20	1	0
7	A	2	0	0	0	0
8	A	601	0	0	5	0
8	B	585	0	0	2	0
All	All	10447	0	8382	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (41) 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:409[A]:GLN:NE2	1:A:413[A]:ASN:HD21	1.90	0.69
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.75	0.68
1:B:340:GLN:HE21	5:B:532:PG4:C3	2.12	0.62
1:A:377:VAL:HG22	2:A:1008:HEC:HBC2	1.83	0.60
1:A:167:SER:HB2	1:A:216[A]:GLU:HG2	1.84	0.59
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.84	0.59
5:A:528:PG4:H51	8:A:970:HOH:O	2.03	0.59
1:A:19[B]:THR:HG22	8:A:1103:HOH:O	2.02	0.58
1:B:377:VAL:HG22	2:B:1008:HEC:HBC2	1.86	0.56
1:A:387[A]:VAL:HG21	1:A:395:TYR:CE1	2.42	0.55
1:A:273[A]:THR:HG23	8:A:979:HOH:O	2.07	0.54
1:B:387[B]:VAL:HG21	1:B:395:TYR:CE1	2.43	0.54
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	1.91	0.53
1:A:53:MET:CE	5:A:531:PG4:H21	2.40	0.52
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.92	0.51
1:A:167:SER:HB2	1:A:216[B]:GLU:HG3	1.93	0.51
1:B:40:ASP:HB2	5:B:534:PG4:H21	1.92	0.51
1:A:81:ARG:HH22	5:A:533:PG4:C4	2.25	0.49
1:B:111:PHE:CZ	5:B:529:PG4:H31	2.47	0.49
1:A:53:MET:HE1	5:A:531:PG4:H21	1.94	0.48
1:A:19[A]:THR:HG23	8:A:600:HOH:O	2.15	0.46
1:B:139:PHE:HB2	6:B:524:PG6:H32	1.98	0.45
1:A:384:MET:HB2	1:A:397:SER:O	2.17	0.45
2:A:1008:HEC:HBC3	2:A:1008:HEC:HMC1	1.99	0.45
1:B:224:PRO:O	1:B:225:LEU:C	2.60	0.44
1:B:12[B]:MET:HG3	8:B:1092:HOH:O	2.18	0.44
1:A:409[A]:GLN:HE22	1:A:413[A]:ASN:HD21	1.66	0.43
1:A:56:ARG:CB	5:A:531:PG4:H42	2.48	0.43
1:B:360:GLN:HG3	3:B:1:PO4:O1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HB2	6:A:524:PG6:H32	2.00	0.42
5:B:531:PG4:H21	8:B:861:HOH:O	2.18	0.42
1:A:273[B]:THR:HG21	1:A:280:ASP:CG	2.45	0.42
5:A:528:PG4:H51	5:A:528:PG4:H31	1.82	0.42
1:B:175:GLN:OE1	5:B:529:PG4:H12	2.20	0.41
1:B:430:ILE:HG21	1:B:490:PHE:HA	2.03	0.41
1:A:140:LYS:HG2	1:A:160:THR:HG23	2.01	0.41
1:A:224:PRO:O	1:A:225:LEU:C	2.63	0.41
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.55	0.41
1:A:88[A]:LEU:HD21	8:A:1037:HOH:O	2.21	0.40
1:A:56:ARG:HB2	5:A:531:PG4:H42	2.04	0.40
1:A:360:GLN:HG3	3:A:1:PO4:O2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/519 (104%)	514 (96%)	23 (4%)	1 (0%)	43	21
1	B	541/519 (104%)	517 (96%)	22 (4%)	2 (0%)	30	11
All	All	1079/1038 (104%)	1031 (96%)	45 (4%)	3 (0%)	36	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	LEU
1	A	361	HIS
1	B	361	HIS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	456/438 (104%)	455 (100%)	1 (0%)	87 76
1	B	458/438 (105%)	458 (100%)	0	100 100
All	All	914/876 (104%)	913 (100%)	1 (0%)	88 76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	B	223	HIS
1	B	275	GLN
1	B	340	GLN
1	B	467	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 6 are monoatomic - leaving 45 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	PO4	A	1	2	4,4,4	1.19	0	6,6,6	0.82	0
5	PG4	B	530	-	7,7,12	0.44	0	6,6,11	0.23	0
2	HEC	A	1004	1,8,3	50,50,50	1.38	5 (10%)	68,82,82	1.01	5 (7%)
2	HEC	B	1007[A]	-	50,50,50	1.37	5 (10%)	68,82,82	1.15	5 (7%)
2	HEC	B	1007[B]	4	50,50,50	1.36	5 (10%)	68,82,82	1.18	7 (10%)
5	PG4	A	4	-	5,5,12	0.54	0	4,4,11	0.35	0
2	HEC	A	1006	1,4	50,50,50	1.33	4 (8%)	68,82,82	1.02	4 (5%)
5	PG4	B	532	-	4,4,12	0.41	0	3,3,11	0.34	0
2	HEC	B	1002	1	50,50,50	1.40	7 (14%)	68,82,82	1.05	4 (5%)
5	PG4	B	533	-	6,6,12	0.62	0	5,5,11	0.28	0
2	HEC	A	1003	1	50,50,50	1.38	7 (14%)	68,82,82	1.15	6 (8%)
2	HEC	B	1004	1,8,3	50,50,50	1.45	7 (14%)	68,82,82	1.10	7 (10%)
6	PG6	A	524	-	6,6,17	0.47	0	5,5,16	0.46	0
5	PG4	B	529	-	8,8,12	0.66	0	7,7,11	0.68	0
5	PG4	B	528	-	7,7,12	0.61	0	6,6,11	0.37	0
5	PG4	A	530	-	4,4,12	0.36	0	3,3,11	0.47	0
6	PG6	B	524	-	4,4,17	0.52	0	3,3,16	0.18	0
2	HEC	A	1008	1	50,50,50	1.56	8 (16%)	68,82,82	1.46	9 (13%)
5	PG4	A	526	-	5,5,12	0.51	0	4,4,11	0.34	0
5	PG4	B	534	-	7,7,12	0.64	0	6,6,11	0.69	0
2	HEC	B	1001	1	50,50,50	1.48	6 (12%)	68,82,82	1.04	4 (5%)
2	HEC	B	1006	1,4	50,50,50	1.36	4 (8%)	68,82,82	0.99	3 (4%)
6	PG6	B	526	-	4,4,17	0.31	0	3,3,16	0.30	0
2	HEC	A	1005[A]	-	50,50,50	1.44	4 (8%)	68,82,82	1.19	6 (8%)
5	PG4	A	528	-	8,8,12	0.64	0	7,7,11	0.65	0
2	HEC	B	1008	1	50,50,50	1.61	8 (16%)	68,82,82	1.54	10 (14%)
5	PG4	A	533	-	5,5,12	0.69	0	4,4,11	0.65	0
5	PG4	A	532	-	4,4,12	0.43	0	3,3,11	0.18	0
3	PO4	A	527	-	4,4,4	0.80	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PG6	B	525	1	9,9,17	0.50	0	8,8,16	0.34	0
2	HEC	A	1005[B]	-	50,50,50	1.41	3 (6%)	68,82,82	1.25	8 (11%)
2	HEC	A	1001	1	50,50,50	1.47	6 (12%)	68,82,82	1.15	2 (2%)
5	PG4	A	529	-	6,6,12	0.42	0	5,5,11	0.42	0
3	PO4	B	1	2	4,4,4	0.96	0	6,6,6	1.00	0
2	HEC	A	1002	1	50,50,50	1.36	5 (10%)	68,82,82	1.10	6 (8%)
5	PG4	A	531	-	9,9,12	0.64	0	8,8,11	0.81	0
2	HEC	B	1005[A]	-	50,50,50	1.38	3 (6%)	68,82,82	1.08	3 (4%)
2	HEC	A	1007[A]	-	50,50,50	1.33	6 (12%)	68,82,82	1.16	7 (10%)
5	PG4	B	531	-	8,8,12	0.58	0	7,7,11	0.51	0
6	PG6	A	525	1	9,9,17	0.50	0	8,8,16	0.35	0
2	HEC	B	1005[B]	-	50,50,50	1.36	3 (6%)	68,82,82	1.15	4 (5%)
2	HEC	B	1003	1	50,50,50	1.41	4 (8%)	68,82,82	1.15	6 (8%)
5	PG4	B	4	-	7,7,12	0.46	0	6,6,11	0.35	0
3	PO4	B	527	-	4,4,4	0.78	0	6,6,6	0.45	0
2	HEC	A	1007[B]	4	50,50,50	1.33	6 (12%)	68,82,82	1.17	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	B	530	-	-	3/5/5/10	-
2	HEC	A	1004	1,8,3	1/1/3/7	6/14/54/54	-
2	HEC	B	1007[A]	-	1/1/3/7	6/14/54/54	-
2	HEC	B	1007[B]	4	1/1/3/7	4/14/54/54	-
5	PG4	A	4	-	-	2/3/3/10	-
2	HEC	A	1006	1,4	1/1/3/7	4/14/54/54	-
5	PG4	B	532	-	-	2/2/2/10	-
2	HEC	B	1002	1	1/1/3/7	6/14/54/54	-
5	PG4	B	533	-	-	2/4/4/10	-
2	HEC	A	1003	1	1/1/3/7	6/14/54/54	-
2	HEC	B	1004	1,8,3	1/1/3/7	6/14/54/54	-
6	PG6	A	524	-	-	0/4/4/15	-
5	PG4	B	529	-	-	2/6/6/10	-
5	PG4	B	528	-	-	3/5/5/10	-
5	PG4	A	530	-	-	1/2/2/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG6	B	524	-	-	0/2/2/15	-
2	HEC	A	1008	1	1/1/3/7	7/14/54/54	-
5	PG4	A	526	-	-	1/3/3/10	-
5	PG4	B	534	-	-	5/5/5/10	-
2	HEC	B	1001	1	1/1/3/7	6/14/54/54	-
2	HEC	B	1006	1,4	1/1/3/7	4/14/54/54	-
6	PG6	B	526	-	-	2/2/2/15	-
2	HEC	A	1005[A]	-	1/1/3/7	6/14/54/54	-
5	PG4	A	528	-	-	5/6/6/10	-
2	HEC	B	1008	1	1/1/3/7	5/14/54/54	-
5	PG4	A	533	-	-	2/3/3/10	-
5	PG4	A	532	-	-	1/2/2/10	-
6	PG6	B	525	1	-	1/7/7/15	-
2	HEC	A	1005[B]	-	1/1/3/7	9/14/54/54	-
2	HEC	A	1001	1	1/1/3/7	8/14/54/54	-
5	PG4	A	529	-	-	3/4/4/10	-
2	HEC	A	1002	1	1/1/3/7	6/14/54/54	-
5	PG4	A	531	-	-	4/7/7/10	-
2	HEC	B	1005[A]	-	1/1/3/7	8/14/54/54	-
2	HEC	A	1007[A]	-	1/1/3/7	6/14/54/54	-
5	PG4	B	531	-	-	4/6/6/10	-
6	PG6	A	525	1	-	0/7/7/15	-
2	HEC	B	1005[B]	-	1/1/3/7	9/14/54/54	-
2	HEC	B	1003	1	1/1/3/7	7/14/54/54	-
5	PG4	B	4	-	-	4/5/5/10	-
2	HEC	A	1007[B]	4	1/1/3/7	5/14/54/54	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1008	HEC	C3D-C2D	6.72	1.51	1.36
2	A	1008	HEC	C3D-C2D	6.47	1.50	1.36
2	B	1001	HEC	C3D-C2D	6.16	1.50	1.36
2	A	1005[A]	HEC	C3D-C2D	5.90	1.49	1.36
2	A	1005[B]	HEC	C3D-C2D	5.90	1.49	1.36
2	A	1006	HEC	C3D-C2D	5.90	1.49	1.36
2	A	1003	HEC	C3D-C2D	5.74	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	HEC	C3D-C2D	5.72	1.49	1.36
2	B	1003	HEC	C3D-C2D	5.70	1.49	1.36
2	B	1005[A]	HEC	C3D-C2D	5.55	1.48	1.36
2	B	1005[B]	HEC	C3D-C2D	5.55	1.48	1.36
2	A	1001	HEC	C3D-C2D	5.54	1.48	1.36
2	B	1004	HEC	C3D-C2D	5.43	1.48	1.36
2	B	1002	HEC	C3D-C2D	5.42	1.48	1.36
2	A	1002	HEC	C3D-C2D	5.39	1.48	1.36
2	A	1004	HEC	C3D-C2D	5.16	1.47	1.36
2	B	1007[A]	HEC	C3D-C2D	4.99	1.47	1.36
2	B	1007[B]	HEC	C3D-C2D	4.99	1.47	1.36
2	A	1007[A]	HEC	C3D-C2D	4.79	1.47	1.36
2	A	1007[B]	HEC	C3D-C2D	4.79	1.47	1.36
2	B	1004	HEC	FE-NB	3.93	2.07	1.94
2	A	1001	HEC	FE-NC	3.63	2.07	1.95
2	A	1004	HEC	FE-NB	3.58	2.05	1.94
2	A	1008	HEC	FE-NC	3.26	2.05	1.95
2	A	1001	HEC	FE-NB	2.77	2.03	1.94
2	B	1008	HEC	CMA-C3A	2.76	1.56	1.50
2	B	1001	HEC	FE-NC	2.73	2.04	1.95
2	B	1005[A]	HEC	FE-NB	2.69	2.03	1.94
2	B	1005[B]	HEC	FE-NB	2.69	2.03	1.94
2	B	1003	HEC	FE-ND	2.65	2.03	1.94
2	A	1004	HEC	FE-NC	2.63	2.03	1.95
2	B	1002	HEC	CMB-C2B	2.62	1.56	1.50
2	A	1004	HEC	CAB-C3B	2.58	1.57	1.51
2	A	1002	HEC	FE-ND	2.57	2.02	1.94
2	B	1007[A]	HEC	FE-ND	2.55	2.02	1.94
2	B	1007[B]	HEC	FE-ND	2.55	2.02	1.94
2	A	1007[A]	HEC	FE-NB	2.55	2.02	1.94
2	A	1007[B]	HEC	FE-NB	2.55	2.02	1.94
2	A	1003	HEC	FE-ND	2.50	2.02	1.94
2	B	1003	HEC	FE-NB	2.48	2.02	1.94
2	B	1008	HEC	FE-NA	2.48	2.03	1.95
2	A	1001	HEC	FE-ND	2.45	2.02	1.94
2	A	1002	HEC	FE-NB	2.44	2.02	1.94
2	B	1008	HEC	CMC-C2C	2.44	1.55	1.50
2	A	1006	HEC	FE-NC	2.43	2.03	1.95
2	B	1003	HEC	CMB-C2B	2.43	1.55	1.50
2	B	1008	HEC	FE-NC	2.42	2.03	1.95
2	B	1006	HEC	FE-NB	2.41	2.02	1.94
2	B	1001	HEC	CAC-C3C	2.39	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	FE-NC	2.37	2.03	1.95
2	A	1007[A]	HEC	FE-ND	2.34	2.02	1.94
2	A	1007[B]	HEC	FE-ND	2.34	2.02	1.94
2	A	1003	HEC	CMB-C2B	2.33	1.55	1.50
2	B	1008	HEC	C3C-C2C	-2.33	1.32	1.38
2	B	1008	HEC	CAC-C3C	2.33	1.57	1.51
2	B	1004	HEC	CMA-C3A	2.32	1.55	1.50
2	B	1002	HEC	FE-ND	2.31	2.02	1.94
2	B	1002	HEC	FE-NA	2.31	2.02	1.95
2	A	1008	HEC	CAC-C3C	2.29	1.56	1.51
2	B	1006	HEC	FE-NC	2.28	2.02	1.95
2	A	1007[A]	HEC	FE-NA	2.27	2.02	1.95
2	A	1007[B]	HEC	FE-NA	2.27	2.02	1.95
2	B	1006	HEC	CAB-C3B	2.26	1.56	1.51
2	B	1005[A]	HEC	CMB-C2B	2.26	1.55	1.50
2	B	1005[B]	HEC	CMB-C2B	2.26	1.55	1.50
2	B	1007[A]	HEC	FE-NB	2.25	2.01	1.94
2	B	1007[B]	HEC	FE-NB	2.25	2.01	1.94
2	B	1001	HEC	CMB-C2B	2.22	1.55	1.50
2	B	1004	HEC	CMB-C2B	2.22	1.55	1.50
2	A	1005[A]	HEC	CMB-C2B	2.21	1.55	1.50
2	A	1005[B]	HEC	CMB-C2B	2.21	1.55	1.50
2	A	1001	HEC	CMB-C2B	2.21	1.55	1.50
2	B	1004	HEC	FE-ND	2.20	2.01	1.94
2	A	1006	HEC	CMB-C2B	2.20	1.55	1.50
2	A	1002	HEC	CMB-C2B	2.20	1.55	1.50
2	A	1008	HEC	CMC-C2C	2.19	1.55	1.50
2	A	1005[A]	HEC	O2D-CGD	-2.17	1.23	1.30
2	A	1005[A]	HEC	FE-ND	2.17	2.01	1.94
2	A	1005[B]	HEC	FE-ND	2.17	2.01	1.94
2	A	1008	HEC	FE-ND	2.14	2.01	1.94
2	A	1007[A]	HEC	CMB-C2B	2.14	1.55	1.50
2	A	1007[B]	HEC	CMB-C2B	2.14	1.55	1.50
2	A	1007[A]	HEC	CAC-C3C	2.14	1.56	1.51
2	A	1007[B]	HEC	CAC-C3C	2.14	1.56	1.51
2	B	1002	HEC	CAC-C3C	2.14	1.56	1.51
2	A	1008	HEC	C3C-C2C	-2.13	1.33	1.38
2	B	1004	HEC	CAB-C3B	2.12	1.56	1.51
2	A	1003	HEC	CAC-C3C	2.12	1.56	1.51
2	A	1001	HEC	FE-NA	2.12	2.02	1.95
2	A	1004	HEC	CMC-C2C	2.10	1.55	1.50
2	B	1001	HEC	FE-NB	2.10	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	FE-NB	2.10	2.01	1.94
2	A	1008	HEC	CMA-C3A	2.08	1.55	1.50
2	A	1002	HEC	CMC-C2C	2.07	1.55	1.50
2	B	1007[A]	HEC	CMB-C2B	2.07	1.55	1.50
2	B	1007[B]	HEC	CMB-C2B	2.07	1.55	1.50
2	B	1001	HEC	CAB-C3B	2.06	1.56	1.51
2	B	1002	HEC	FE-NC	2.06	2.01	1.95
2	B	1007[A]	HEC	C3B-C2B	-2.05	1.32	1.36
2	B	1007[B]	HEC	C3B-C2B	-2.05	1.32	1.36
2	B	1008	HEC	CMD-C2D	2.05	1.55	1.50
2	B	1002	HEC	CAB-C3B	2.03	1.56	1.51
2	A	1003	HEC	CMA-C3A	2.03	1.54	1.50
2	B	1004	HEC	FE-NC	2.02	2.01	1.95
2	A	1006	HEC	O1A-CGA	2.02	1.28	1.22
2	A	1008	HEC	C3B-C2B	-2.02	1.32	1.36

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1008	HEC	CAC-C3C-C4C	5.39	132.32	124.91
2	A	1008	HEC	CAC-C3C-C4C	5.00	131.79	124.91
2	B	1008	HEC	C1D-ND-C4D	4.81	110.91	105.21
2	A	1008	HEC	C1D-ND-C4D	4.66	110.72	105.21
2	A	1001	HEC	C1D-ND-C4D	4.31	110.31	105.21
2	A	1005[A]	HEC	C1D-ND-C4D	4.29	110.29	105.21
2	A	1005[B]	HEC	C1D-ND-C4D	4.29	110.29	105.21
2	B	1007[A]	HEC	CMB-C2B-C1B	-4.03	118.73	125.03
2	B	1007[B]	HEC	CMB-C2B-C1B	-4.03	118.73	125.03
2	B	1001	HEC	C1D-ND-C4D	3.77	109.68	105.21
2	A	1007[A]	HEC	C1D-ND-C4D	3.71	109.60	105.21
2	A	1007[B]	HEC	C1D-ND-C4D	3.71	109.60	105.21
2	B	1008	HEC	CAC-C3C-C2C	-3.67	121.09	126.89
2	B	1007[A]	HEC	C1D-ND-C4D	3.58	109.45	105.21
2	B	1007[B]	HEC	C1D-ND-C4D	3.58	109.45	105.21
2	B	1003	HEC	C1D-ND-C4D	3.53	109.39	105.21
2	A	1008	HEC	CAC-C3C-C2C	-3.30	121.67	126.89
2	B	1002	HEC	C1D-ND-C4D	3.22	109.03	105.21
2	B	1004	HEC	C1D-ND-C4D	3.03	108.80	105.21
2	A	1007[A]	HEC	CMB-C2B-C1B	-3.02	120.32	125.03
2	A	1007[B]	HEC	CMB-C2B-C1B	-3.02	120.32	125.03
2	A	1002	HEC	C1D-ND-C4D	2.99	108.74	105.21
2	B	1005[A]	HEC	C1D-ND-C4D	2.91	108.65	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1005[B]	HEC	C1D-ND-C4D	2.91	108.65	105.21
2	B	1002	HEC	CAA-CBA-CGA	-2.86	106.08	113.67
2	A	1003	HEC	C1D-ND-C4D	2.77	108.48	105.21
2	A	1005[A]	HEC	CMB-C2B-C1B	-2.75	120.74	125.03
2	A	1005[B]	HEC	CMB-C2B-C1B	-2.75	120.74	125.03
2	A	1004	HEC	CAD-C3D-C4D	2.73	129.45	124.70
2	A	1003	HEC	CAB-C3B-C4B	2.71	128.32	124.79
2	A	1002	HEC	CAD-C3D-C4D	2.71	129.41	124.70
2	B	1004	HEC	CAD-C3D-C4D	2.66	129.33	124.70
2	B	1008	HEC	CHA-C4D-ND	2.65	127.27	124.42
2	A	1006	HEC	C1D-ND-C4D	2.61	108.30	105.21
2	B	1007[B]	HEC	O2A-CGA-CBA	2.61	122.24	114.00
2	B	1008	HEC	O1A-CGA-CBA	-2.58	114.91	123.09
2	B	1003	HEC	CBC-CAC-C3C	2.56	119.35	112.42
2	B	1006	HEC	C1D-ND-C4D	2.54	108.21	105.21
2	A	1008	HEC	O1A-CGA-CBA	-2.53	115.06	123.09
2	A	1007[A]	HEC	CMD-C2D-C1D	2.53	128.98	125.03
2	A	1007[B]	HEC	CMD-C2D-C1D	2.53	128.98	125.03
2	A	1001	HEC	CAD-C3D-C4D	2.51	129.07	124.70
2	B	1005[A]	HEC	C2A-C1A-NA	-2.50	107.91	110.32
2	B	1005[B]	HEC	C2A-C1A-NA	-2.50	107.91	110.32
2	A	1005[A]	HEC	CAB-C3B-C4B	2.48	128.02	124.79
2	A	1005[B]	HEC	CAB-C3B-C4B	2.48	128.02	124.79
2	B	1006	HEC	CAD-C3D-C4D	2.47	129.00	124.70
2	B	1007[A]	HEC	C1B-C2B-C3B	2.46	109.57	106.98
2	B	1007[B]	HEC	C1B-C2B-C3B	2.46	109.57	106.98
2	B	1002	HEC	CMD-C2D-C1D	2.45	128.86	125.03
2	A	1008	HEC	O2A-CGA-CBA	2.43	121.68	114.00
2	B	1005[B]	HEC	O2D-CGD-CBD	2.43	121.68	114.00
2	A	1004	HEC	C1D-C2D-C3D	-2.42	104.43	106.98
2	A	1004	HEC	CAD-C3D-C2D	-2.42	123.34	127.87
2	A	1002	HEC	CMB-C2B-C1B	-2.41	121.26	125.03
2	B	1008	HEC	CHD-C1D-ND	2.41	127.35	124.37
2	A	1003	HEC	CAD-C3D-C4D	2.41	128.90	124.70
2	A	1004	HEC	C1D-ND-C4D	2.40	108.05	105.21
2	A	1002	HEC	CAA-CBA-CGA	-2.40	107.30	113.67
2	B	1002	HEC	CAD-C3D-C4D	2.39	128.86	124.70
2	B	1001	HEC	CHD-C1D-ND	2.35	127.28	124.37
2	A	1003	HEC	CMB-C2B-C1B	-2.34	121.38	125.03
2	B	1003	HEC	CMB-C2B-C1B	-2.33	121.39	125.03
2	B	1003	HEC	O2D-CGD-CBD	2.32	121.34	114.00
2	B	1005[A]	HEC	CAB-C3B-C4B	2.32	127.81	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1005[B]	HEC	CAB-C3B-C4B	2.32	127.81	124.79
2	A	1004	HEC	CMD-C2D-C1D	2.32	128.66	125.03
2	A	1003	HEC	O2A-CGA-CBA	2.32	121.32	114.00
2	A	1006	HEC	O1A-CGA-CBA	-2.31	115.77	123.09
2	A	1005[A]	HEC	CAD-C3D-C4D	2.29	128.70	124.70
2	A	1005[B]	HEC	CAD-C3D-C4D	2.29	128.70	124.70
2	B	1007[A]	HEC	CAD-C3D-C4D	2.26	128.63	124.70
2	B	1007[B]	HEC	CAD-C3D-C4D	2.26	128.63	124.70
2	B	1004	HEC	CMB-C2B-C1B	-2.24	121.54	125.03
2	A	1006	HEC	C2A-C1A-NA	-2.23	108.18	110.32
2	B	1004	HEC	C4B-NB-C1B	2.22	107.83	105.21
2	A	1008	HEC	CMB-C2B-C1B	-2.21	121.58	125.03
2	B	1008	HEC	O2A-CGA-CBA	2.20	120.96	114.00
2	A	1005[A]	HEC	CMC-C2C-C1C	-2.20	122.08	125.42
2	A	1005[B]	HEC	CMC-C2C-C1C	-2.20	122.08	125.42
2	B	1003	HEC	CHD-C1D-ND	2.19	127.08	124.37
2	A	1005[A]	HEC	CMD-C2D-C1D	2.18	128.44	125.03
2	A	1005[B]	HEC	CMD-C2D-C1D	2.18	128.44	125.03
2	A	1008	HEC	CHD-C1D-ND	2.18	127.06	124.37
2	A	1003	HEC	CBC-CAC-C3C	2.18	118.33	112.42
2	A	1002	HEC	C2A-C1A-NA	-2.18	108.22	110.32
2	A	1007[A]	HEC	C1B-C2B-C3B	2.18	109.27	106.98
2	A	1007[B]	HEC	C1B-C2B-C3B	2.18	109.27	106.98
2	B	1001	HEC	CMC-C2C-C1C	-2.18	122.10	125.42
2	A	1008	HEC	CAD-C3D-C4D	2.16	128.47	124.70
2	A	1007[A]	HEC	CAD-C3D-C4D	2.16	128.47	124.70
2	A	1007[B]	HEC	CAD-C3D-C4D	2.16	128.47	124.70
2	B	1007[B]	HEC	O1A-CGA-CBA	-2.16	116.25	123.09
2	B	1004	HEC	C2A-C1A-NA	-2.14	108.25	110.32
2	A	1007[A]	HEC	C2B-C1B-NB	-2.14	107.43	109.90
2	A	1007[B]	HEC	C2B-C1B-NB	-2.14	107.43	109.90
2	B	1004	HEC	CMD-C2D-C1D	2.13	128.37	125.03
2	B	1001	HEC	CBA-CAA-C2A	-2.13	106.65	112.53
2	A	1005[B]	HEC	O2D-CGD-CBD	2.13	120.72	114.00
2	B	1008	HEC	CHD-C4C-C3C	2.11	129.91	125.30
2	A	1006	HEC	C1D-C2D-C3D	-2.11	104.76	106.98
2	B	1006	HEC	C2A-C1A-NA	-2.06	108.33	110.32
2	B	1008	HEC	C1B-C2B-C3B	2.06	109.15	106.98
2	A	1005[B]	HEC	CBD-CAD-C3D	-2.06	106.84	112.53
2	B	1007[A]	HEC	CBD-CAD-C3D	-2.05	106.87	112.53
2	B	1007[B]	HEC	CBD-CAD-C3D	-2.05	106.87	112.53
2	A	1007[A]	HEC	CHD-C1D-ND	2.05	126.90	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1007[B]	HEC	CHD-C1D-ND	2.05	126.90	124.37
2	B	1003	HEC	O1D-CGD-CBD	-2.05	116.61	123.09
2	B	1008	HEC	C2B-C1B-NB	-2.04	107.54	109.90
2	B	1004	HEC	C1D-C2D-C3D	-2.04	104.83	106.98
2	A	1002	HEC	C1B-C2B-C3B	2.04	109.13	106.98
2	A	1008	HEC	CBD-CAD-C3D	-2.04	106.89	112.53

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1004	HEC	NA
2	A	1005[A]	HEC	NA
2	A	1005[B]	HEC	NA
2	A	1006	HEC	NA
2	A	1007[A]	HEC	NA
2	A	1007[B]	HEC	NA
2	A	1008	HEC	NA
2	A	1002	HEC	NA
2	A	1003	HEC	NA
2	A	1001	HEC	NA
2	B	1004	HEC	NA
2	B	1005[A]	HEC	NA
2	B	1005[B]	HEC	NA
2	B	1006	HEC	NA
2	B	1007[A]	HEC	NA
2	B	1007[B]	HEC	NA
2	B	1008	HEC	NA
2	B	1002	HEC	NA
2	B	1003	HEC	NA
2	B	1001	HEC	NA

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1002	HEC	C2C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	B	1002	HEC	C4C-C3C-CAC-CBC
2	A	1002	HEC	C2C-C3C-CAC-CBC
5	A	531	PG4	C6-C5-O3-C4
5	B	531	PG4	C1-C2-O2-C3
2	A	1001	HEC	C2B-C3B-CAB-CBB
5	A	529	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C2B-C3B-CAB-CBB
2	B	1007[A]	HEC	C2B-C3B-CAB-CBB
2	B	1007[B]	HEC	C2B-C3B-CAB-CBB
5	A	528	PG4	O2-C3-C4-O3
5	B	534	PG4	O2-C3-C4-O3
5	B	4	PG4	O2-C3-C4-O3
5	B	531	PG4	O2-C3-C4-O3
2	A	1001	HEC	C2C-C3C-CAC-CBC
2	A	1001	HEC	C4C-C3C-CAC-CBC
2	A	1007[A]	HEC	C2B-C3B-CAB-CBB
2	A	1007[B]	HEC	C2B-C3B-CAB-CBB
5	B	530	PG4	O2-C3-C4-O3
5	A	528	PG4	C3-C4-O3-C5
2	B	1007[A]	HEC	C4C-C3C-CAC-CBC
2	B	1007[B]	HEC	C4C-C3C-CAC-CBC
2	A	1003	HEC	C4C-C3C-CAC-CBC
5	A	526	PG4	O1-C1-C2-O2
5	A	531	PG4	O3-C5-C6-O4
5	B	528	PG4	O1-C1-C2-O2
2	B	1007[A]	HEC	C2C-C3C-CAC-CBC
2	B	1007[B]	HEC	C2C-C3C-CAC-CBC
2	A	1007[A]	HEC	C4C-C3C-CAC-CBC
2	A	1007[B]	HEC	C4C-C3C-CAC-CBC
5	B	530	PG4	O1-C1-C2-O2
2	A	1008	HEC	C2B-C3B-CAB-CBB
2	B	1001	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C4C-C3C-CAC-CBC
5	A	4	PG4	C4-C3-O2-C2
5	A	532	PG4	O1-C1-C2-O2
2	A	1007[A]	HEC	C2C-C3C-CAC-CBC
2	A	1007[B]	HEC	C2C-C3C-CAC-CBC
5	B	534	PG4	C3-C4-O3-C5
2	A	1001	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C4C-C3C-CAC-CBC
2	A	1005[A]	HEC	C2B-C3B-CAB-CBB
2	A	1005[B]	HEC	C2B-C3B-CAB-CBB
5	A	530	PG4	O1-C1-C2-O2
5	B	4	PG4	O1-C1-C2-O2
6	B	526	PG6	O2-C4-C5-O3
2	B	1008	HEC	C4C-C3C-CAC-CBC
2	A	1006	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	1005[A]	HEC	C2B-C3B-CAB-CBB
2	B	1005[B]	HEC	C2B-C3B-CAB-CBB
2	B	1002	HEC	C2B-C3B-CAB-CBB
2	A	1004	HEC	C4B-C3B-CAB-CBB
2	B	1008	HEC	C2C-C3C-CAC-CBC
2	B	1003	HEC	C2C-C3C-CAC-CBC
2	B	1004	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C2B-C3B-CAB-CBB
2	A	1003	HEC	C2C-C3C-CAC-CBC
5	A	529	PG4	O1-C1-C2-O2
5	A	533	PG4	O1-C1-C2-O2
2	A	1002	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C4C-C3C-CAC-CBC
2	A	1005[A]	HEC	C4C-C3C-CAC-CBC
2	A	1005[B]	HEC	C4C-C3C-CAC-CBC
2	B	1001	HEC	C2C-C3C-CAC-CBC
5	B	529	PG4	O2-C3-C4-O3
2	B	1008	HEC	C2B-C3B-CAB-CBB
2	B	1005[A]	HEC	C4C-C3C-CAC-CBC
2	B	1005[B]	HEC	C4C-C3C-CAC-CBC
2	A	1007[A]	HEC	C4B-C3B-CAB-CBB
2	A	1007[B]	HEC	C4B-C3B-CAB-CBB
2	B	1006	HEC	C4C-C3C-CAC-CBC
5	A	528	PG4	C6-C5-O3-C4
2	A	1006	HEC	C4C-C3C-CAC-CBC
2	B	1001	HEC	C4B-C3B-CAB-CBB
2	B	1001	HEC	C4C-C3C-CAC-CBC
2	B	1004	HEC	C2C-C3C-CAC-CBC
2	B	1007[A]	HEC	C4B-C3B-CAB-CBB
2	B	1007[B]	HEC	C4B-C3B-CAB-CBB
5	A	4	PG4	O1-C1-C2-O2
2	B	1006	HEC	C2B-C3B-CAB-CBB
5	B	4	PG4	C4-C3-O2-C2
5	A	533	PG4	C4-C3-O2-C2
5	A	528	PG4	C4-C3-O2-C2
5	B	529	PG4	C1-C2-O2-C3
5	B	534	PG4	C4-C3-O2-C2
2	A	1008	HEC	C2C-C3C-CAC-CBC
5	A	531	PG4	C1-C2-O2-C3
2	B	1005[B]	HEC	C3D-CAD-CBD-CGD
2	B	1002	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	A	531	PG4	O2-C3-C4-O3
5	B	528	PG4	C1-C2-O2-C3
2	A	1008	HEC	C4C-C3C-CAC-CBC
2	A	1005[A]	HEC	C4B-C3B-CAB-CBB
2	A	1005[B]	HEC	C4B-C3B-CAB-CBB
2	A	1006	HEC	C2C-C3C-CAC-CBC
5	B	4	PG4	C1-C2-O2-C3
5	B	530	PG4	C4-C3-O2-C2
5	B	531	PG4	C6-C5-O3-C4
2	A	1002	HEC	C4B-C3B-CAB-CBB
5	B	534	PG4	O1-C1-C2-O2
2	A	1005[B]	HEC	C3D-CAD-CBD-CGD
2	B	1006	HEC	C2C-C3C-CAC-CBC
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	A	1006	HEC	C4B-C3B-CAB-CBB
5	B	533	PG4	C4-C3-O2-C2
2	B	1004	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O2A
2	A	1004	HEC	CAA-CBA-CGA-O1A
2	A	1001	HEC	CAA-CBA-CGA-O1A
2	B	1002	HEC	CAA-CBA-CGA-O1A
2	B	1004	HEC	CAA-CBA-CGA-O1A
2	A	1005[A]	HEC	C2C-C3C-CAC-CBC
2	A	1005[B]	HEC	C2C-C3C-CAC-CBC
2	B	1005[A]	HEC	C2C-C3C-CAC-CBC
2	B	1005[B]	HEC	C2C-C3C-CAC-CBC
2	B	1005[A]	HEC	CAA-CBA-CGA-O1A
2	B	1005[B]	HEC	CAA-CBA-CGA-O1A
2	A	1005[A]	HEC	CAA-CBA-CGA-O1A
2	A	1005[B]	HEC	CAA-CBA-CGA-O1A
2	B	1005[A]	HEC	CAA-CBA-CGA-O2A
2	B	1005[B]	HEC	CAA-CBA-CGA-O2A
5	B	532	PG4	C1-C2-O2-C3
2	A	1005[A]	HEC	CAA-CBA-CGA-O2A
2	A	1005[B]	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAD-CBD-CGD-O1D
2	B	1005[A]	HEC	C4B-C3B-CAB-CBB
2	B	1005[B]	HEC	C4B-C3B-CAB-CBB
2	A	1002	HEC	CAA-CBA-CGA-O1A
2	A	1002	HEC	CAA-CBA-CGA-O2A
2	B	1002	HEC	CAA-CBA-CGA-O2A
5	B	534	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	A	529	PG4	C4-C3-O2-C2
2	A	1001	HEC	CAD-CBD-CGD-O2D
2	A	1004	HEC	C2C-C3C-CAC-CBC
2	B	1005[B]	HEC	CAD-CBD-CGD-O2D
2	B	1003	HEC	CAD-CBD-CGD-O2D
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	A	1008	HEC	CAA-CBA-CGA-O2A
5	B	532	PG4	O1-C1-C2-O2
6	B	526	PG6	C4-C5-O3-C6
2	A	1003	HEC	CAD-CBD-CGD-O2D
2	B	1008	HEC	CAA-CBA-CGA-O2A
2	A	1005[B]	HEC	CAD-CBD-CGD-O2D
2	B	1005[B]	HEC	CAD-CBD-CGD-O1D
2	B	1001	HEC	CAD-CBD-CGD-O1D
2	B	1003	HEC	CAD-CBD-CGD-O1D
2	A	1008	HEC	CAA-CBA-CGA-O1A
2	A	1005[B]	HEC	CAD-CBD-CGD-O1D
2	B	1006	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	CAD-CBD-CGD-O1D
5	B	531	PG4	C3-C4-O3-C5
2	B	1008	HEC	CAA-CBA-CGA-O1A
2	A	1008	HEC	CAD-CBD-CGD-O1D
5	A	528	PG4	O1-C1-C2-O2
6	B	525	PG6	O3-C6-C7-O4
2	B	1007[A]	HEC	CAA-CBA-CGA-O1A
5	B	533	PG4	O2-C3-C4-O3
2	A	1007[A]	HEC	CAA-CBA-CGA-O1A
2	B	1003	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	C4B-C3B-CAB-CBB
2	B	1007[A]	HEC	CAA-CBA-CGA-O2A
5	B	528	PG4	C4-C3-O2-C2
2	A	1007[A]	HEC	CAA-CBA-CGA-O2A
2	A	1008	HEC	CAD-CBD-CGD-O2D
2	B	1005[A]	HEC	CAD-CBD-CGD-O2D
2	B	1003	HEC	CAA-CBA-CGA-O2A
2	A	1007[B]	HEC	CAA-CBA-CGA-O2A
2	B	1005[A]	HEC	CAD-CBD-CGD-O1D

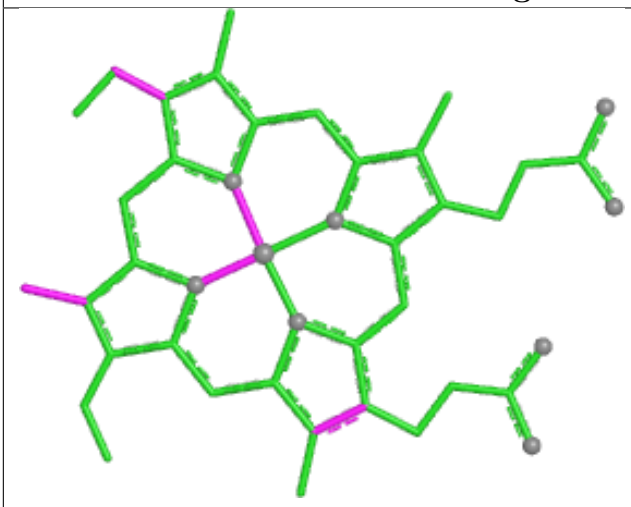
There are no ring outliers.

15 monomers are involved in 22 short contacts:

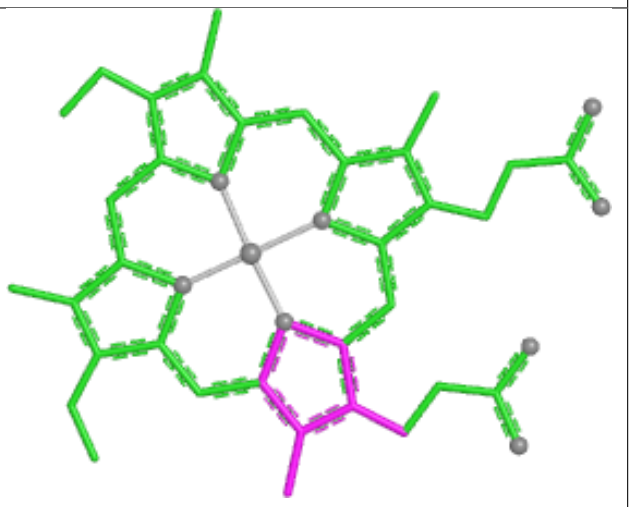
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PO4	1	0
5	B	532	PG4	1	0
2	B	1002	HEC	1	0
6	A	524	PG6	1	0
5	B	529	PG4	2	0
6	B	524	PG6	1	0
2	A	1008	HEC	2	0
5	B	534	PG4	1	0
5	A	528	PG4	2	0
2	B	1008	HEC	2	0
5	A	533	PG4	1	0
3	B	1	PO4	1	0
2	A	1002	HEC	1	0
5	A	531	PG4	4	0
5	B	531	PG4	1	0

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.

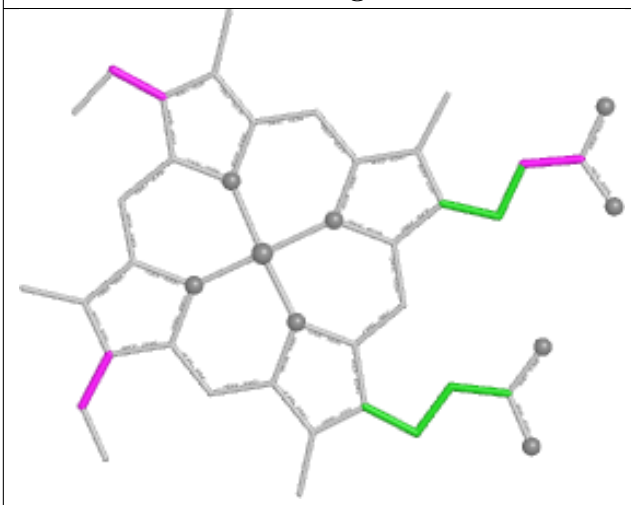
Ligand HEC A 1004



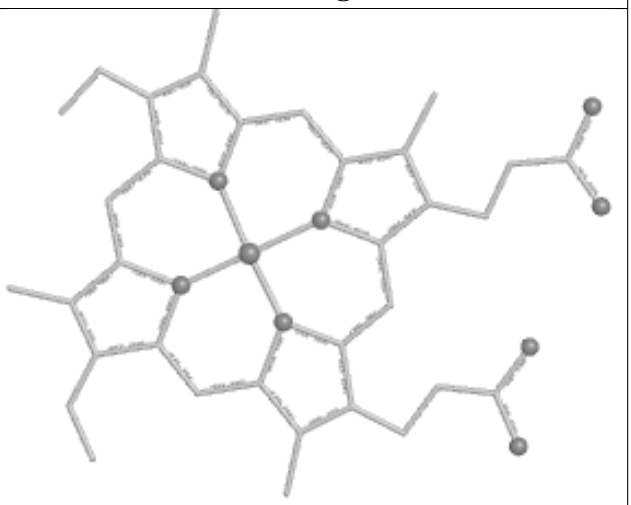
Bond lengths



Bond angles

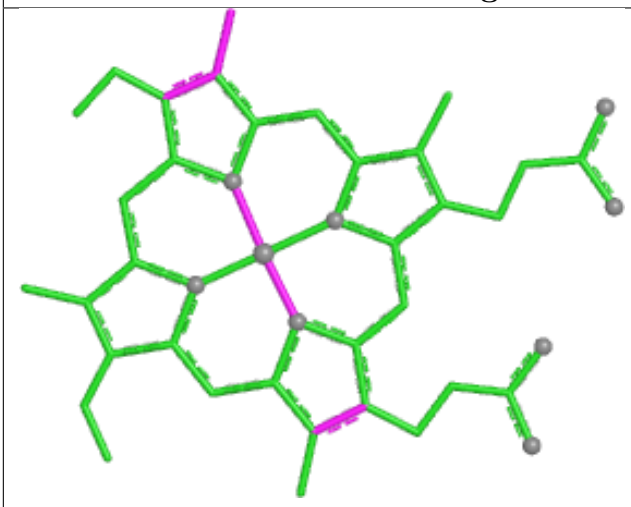


Torsions

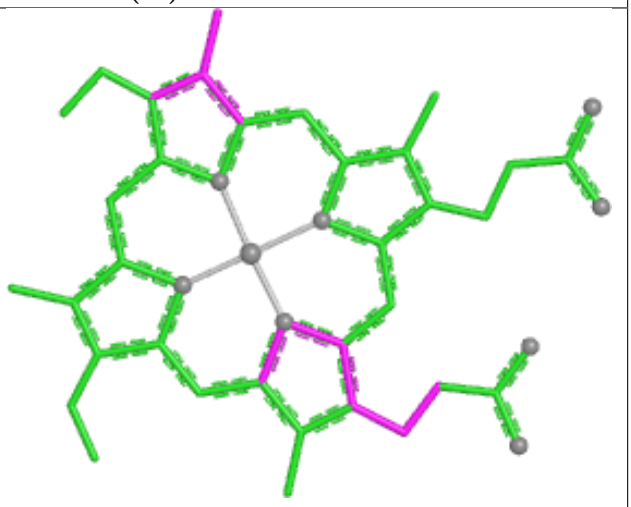


Rings

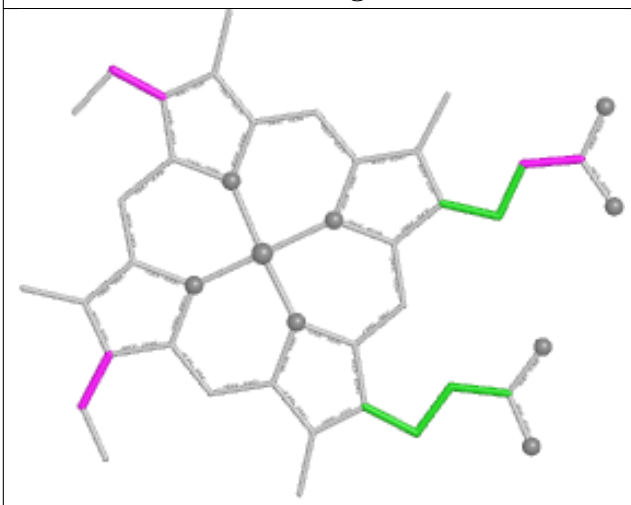
Ligand HEC B 1007 (A)



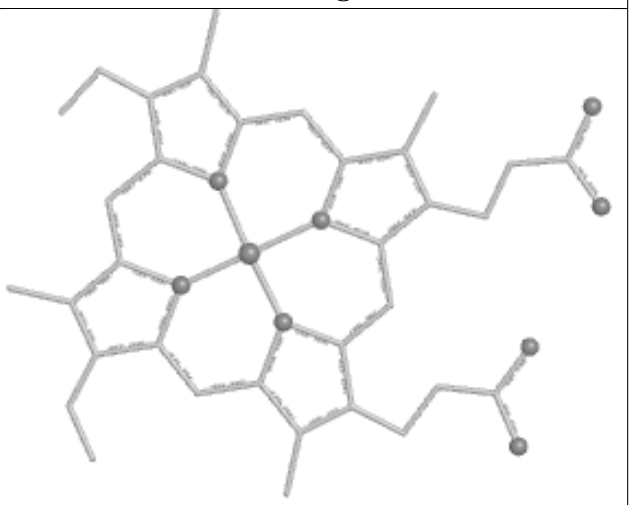
Bond lengths



Bond angles

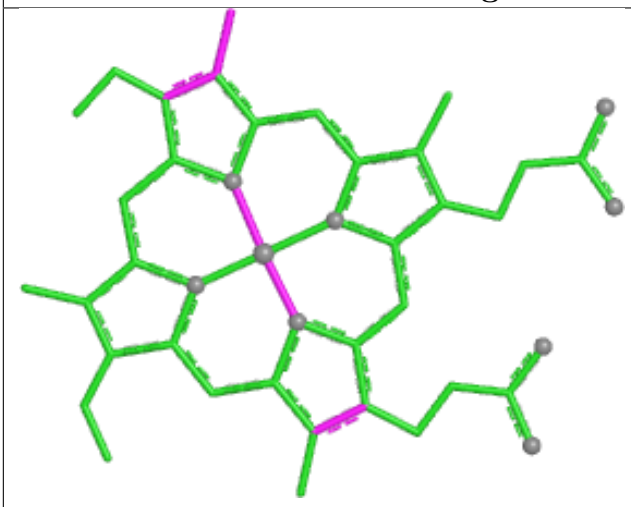


Torsions

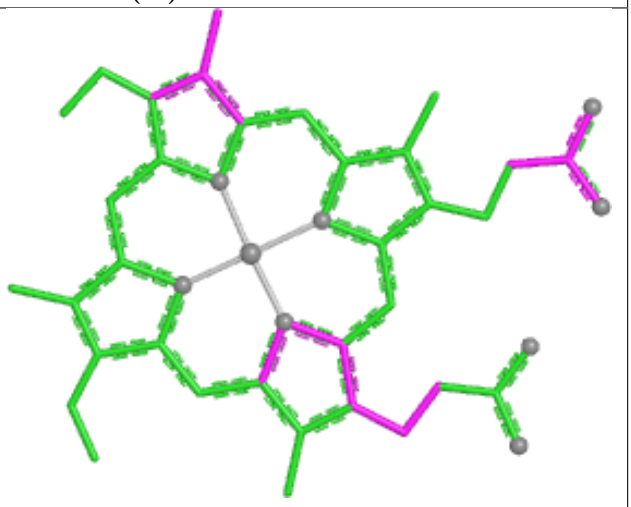


Rings

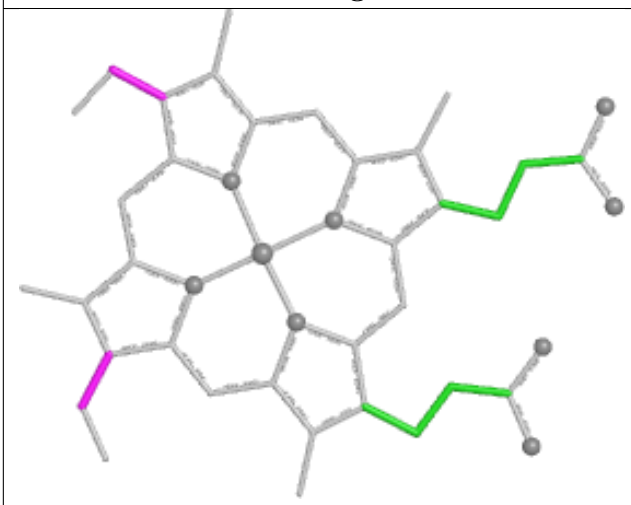
Ligand HEC B 1007 (B)



Bond lengths



Bond angles



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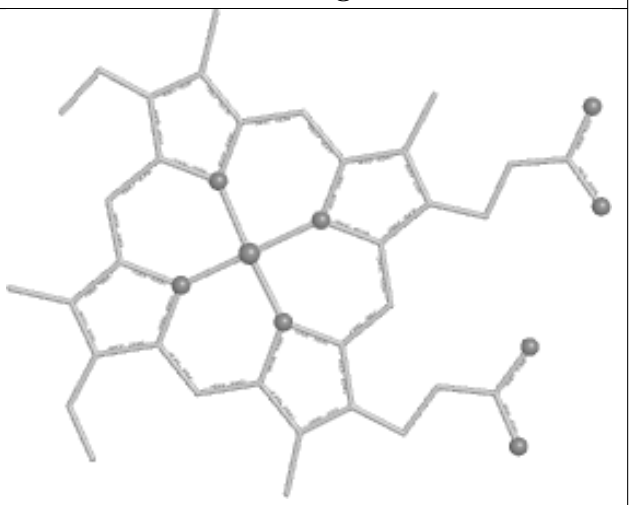
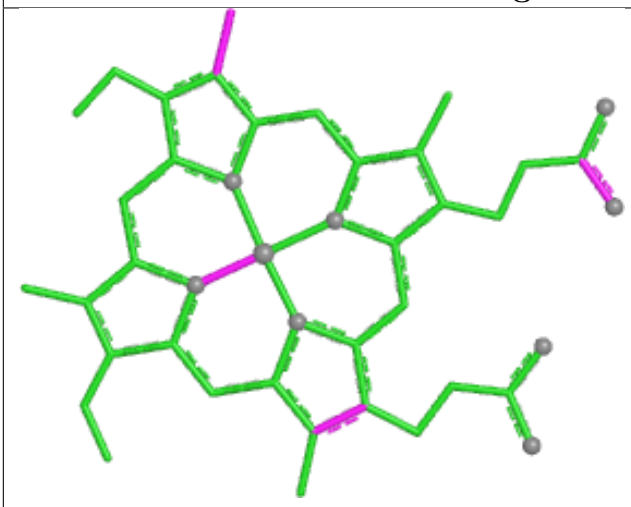


Rings

Ligand HEC A 1006



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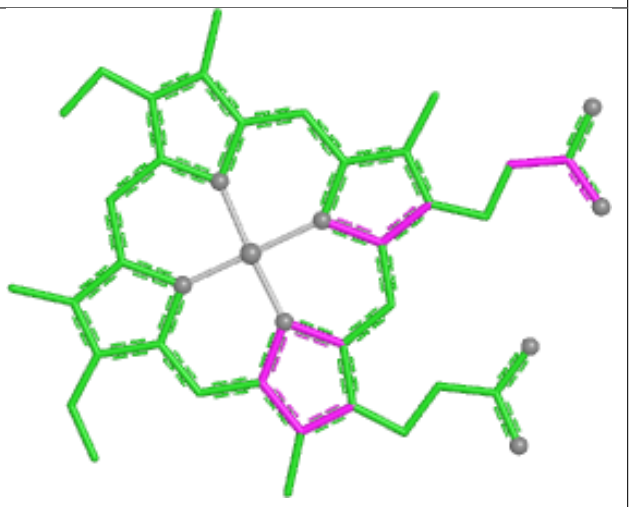
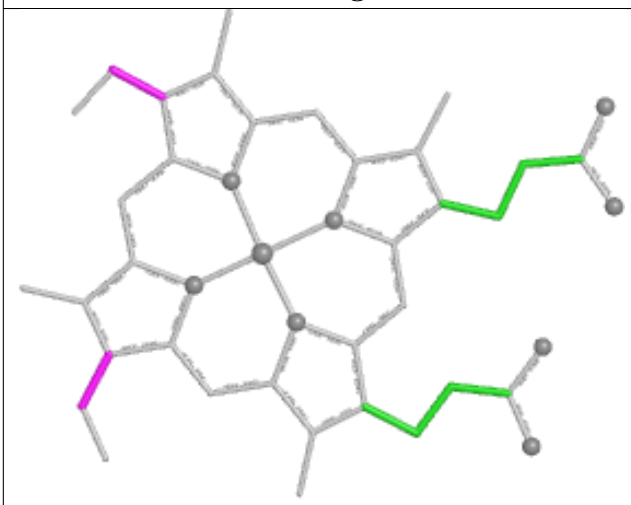


Bond angles



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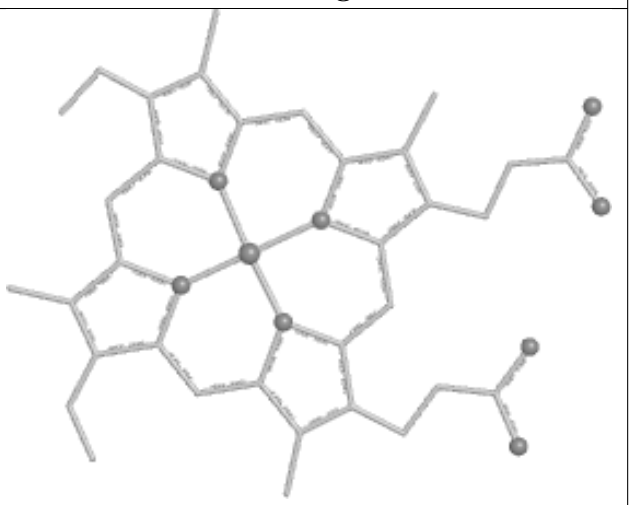
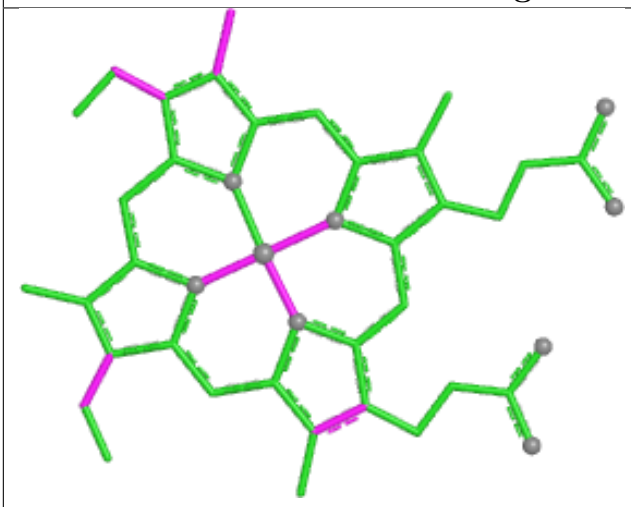


Rings

Ligand HEC B 1002



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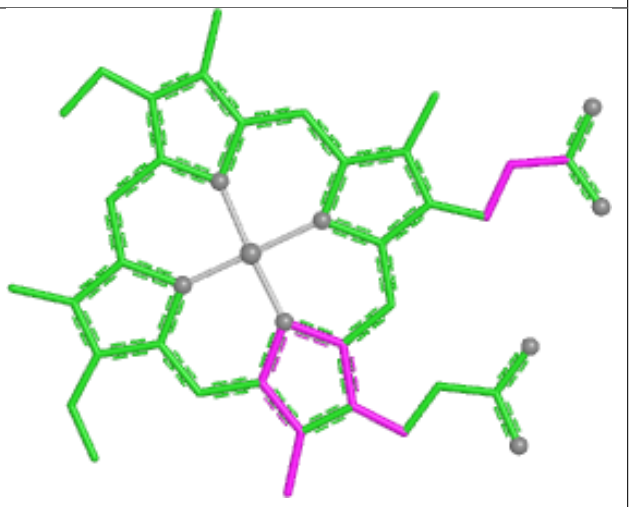
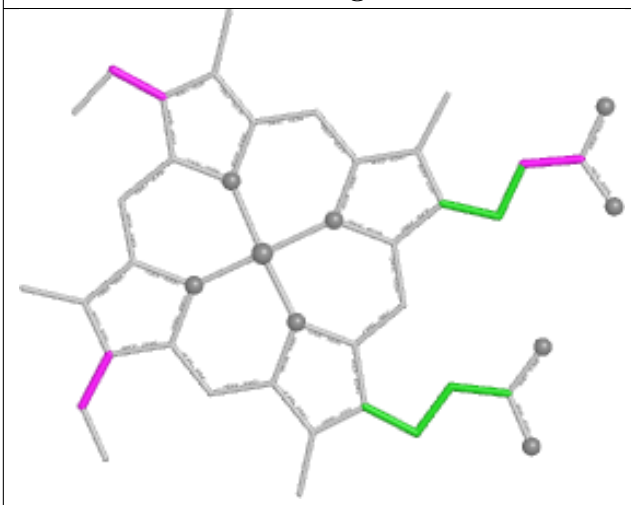


Bond angles



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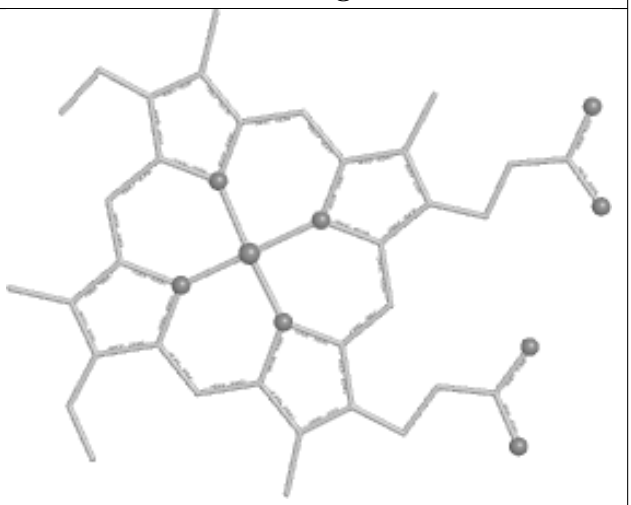
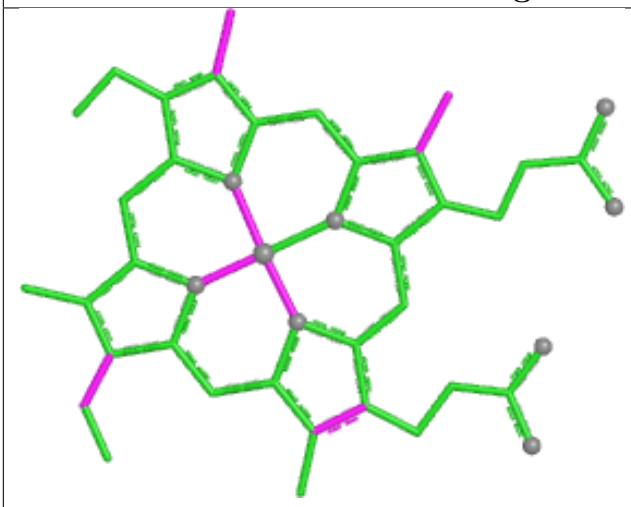


Rings

Ligand HEC A 1003



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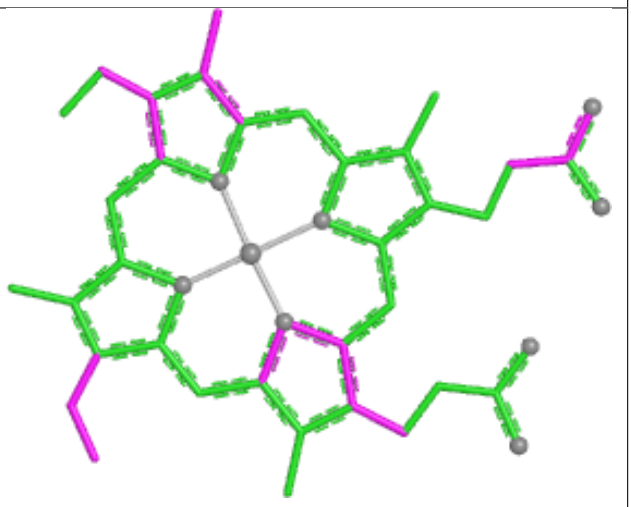
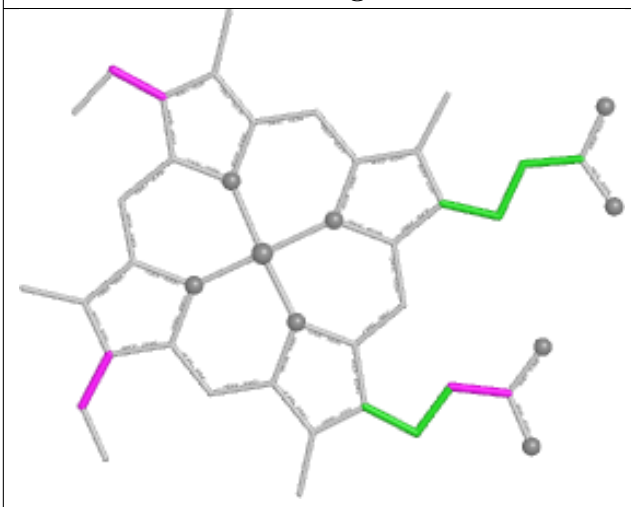


Bond angles



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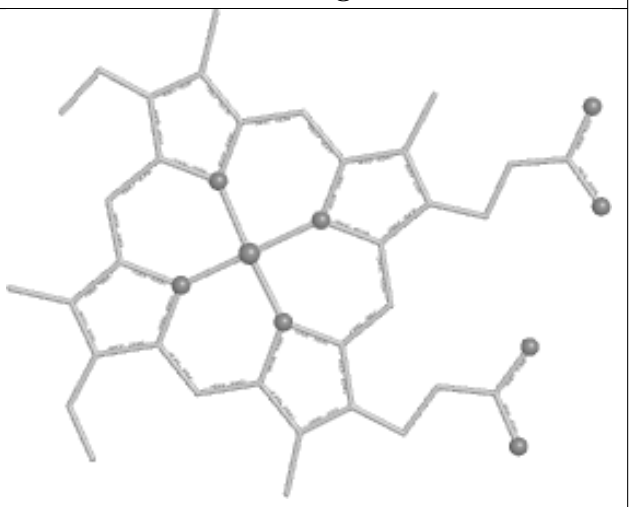
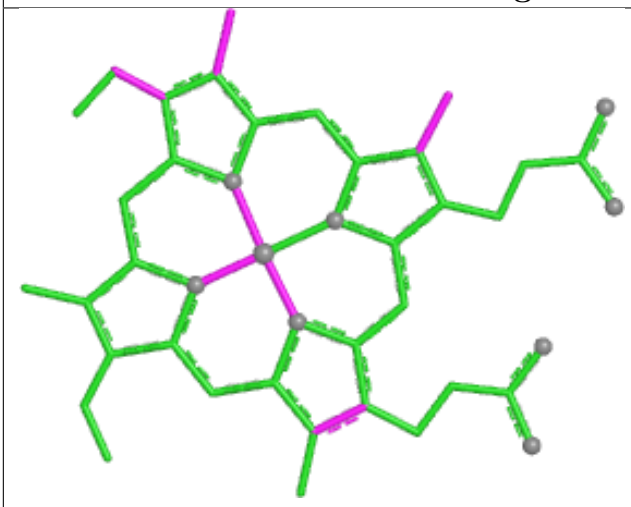


Rings

Ligand HEC B 1004



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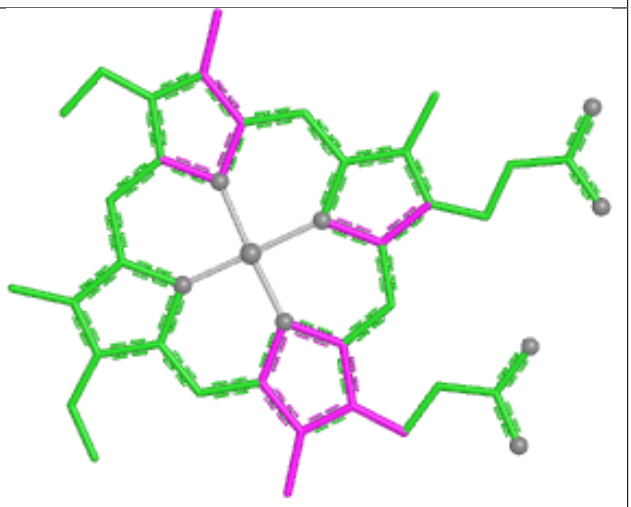
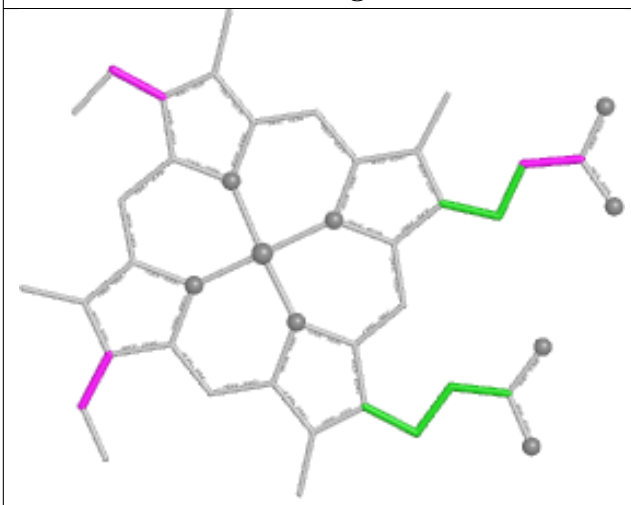


Bond angles



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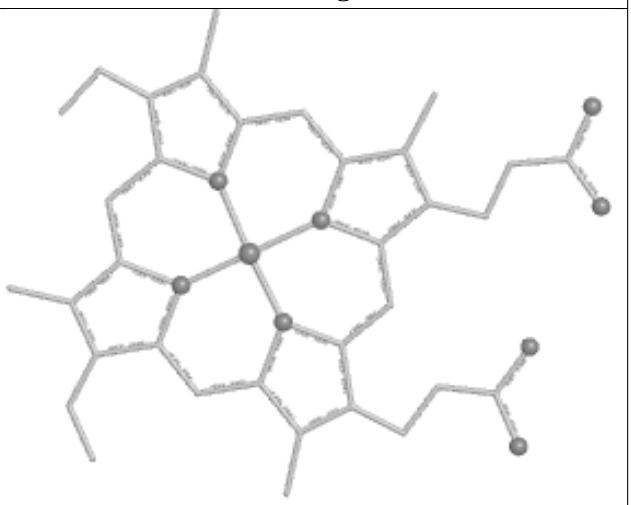
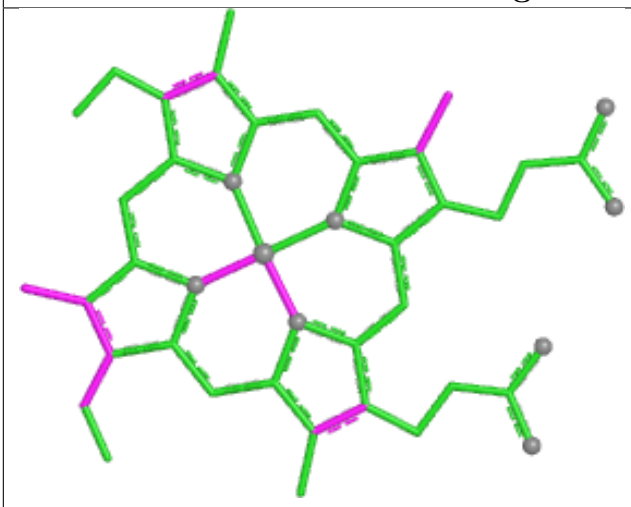


Rings

Ligand HEC A 1008



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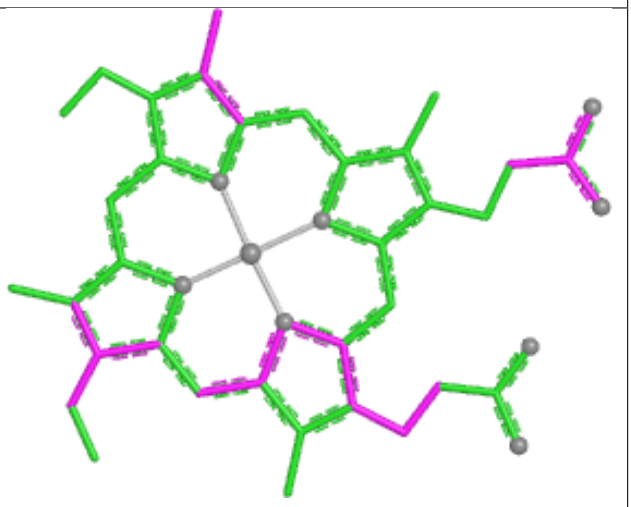
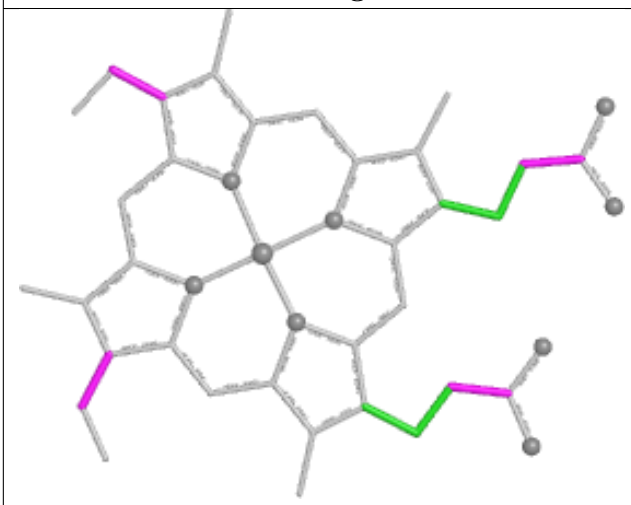


Bond angles



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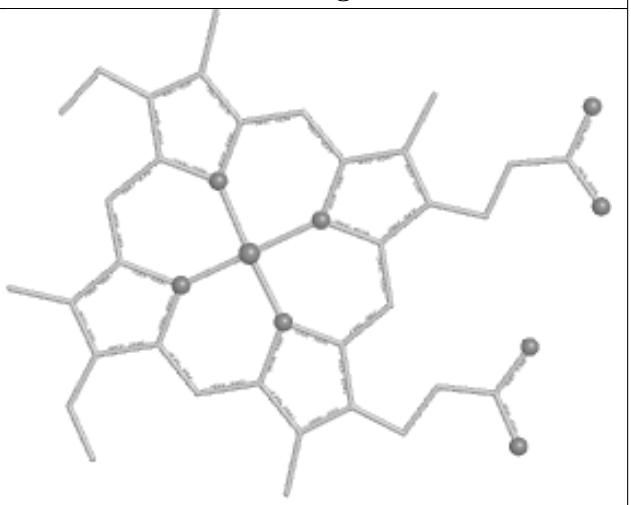
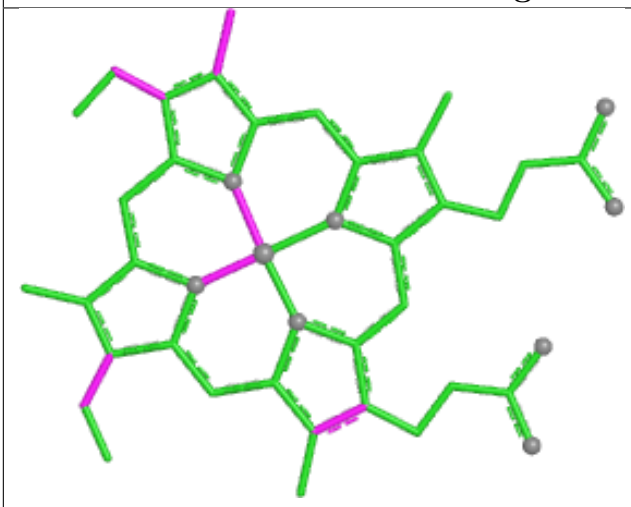


Rings

Ligand HEC B 1001



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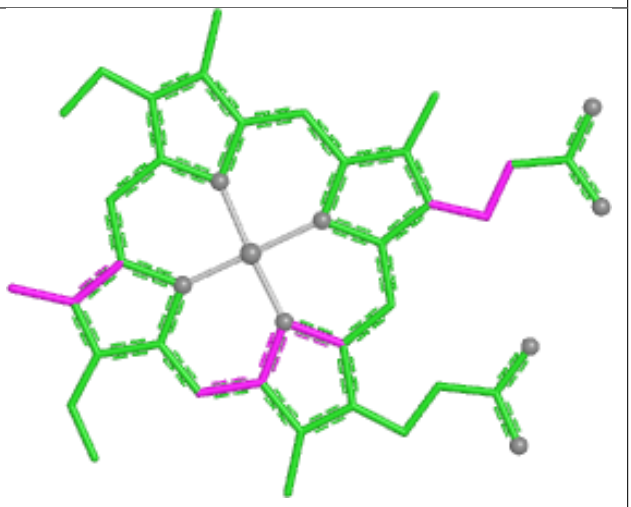
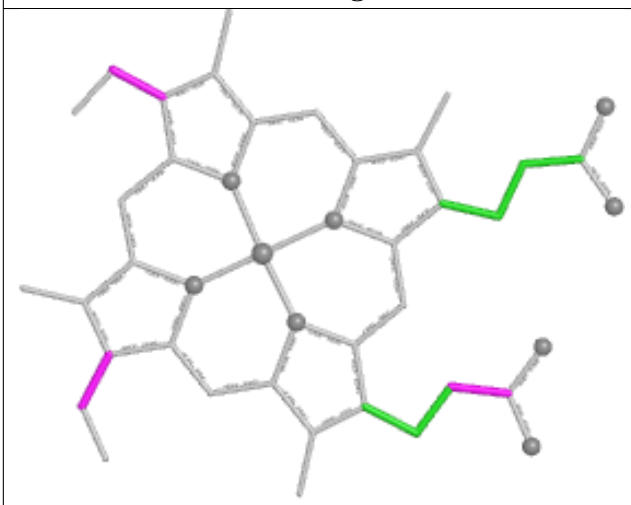


Bond angles



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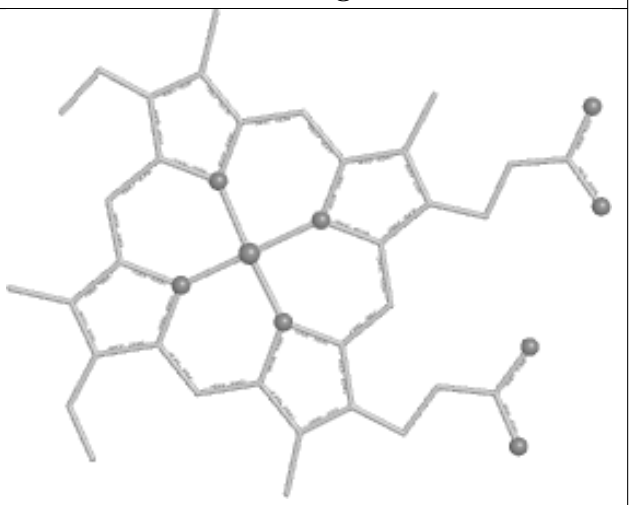
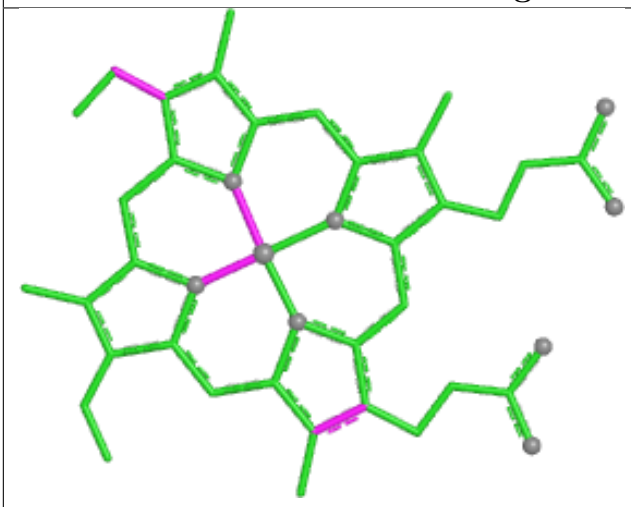


Rings

Ligand HEC B 1006



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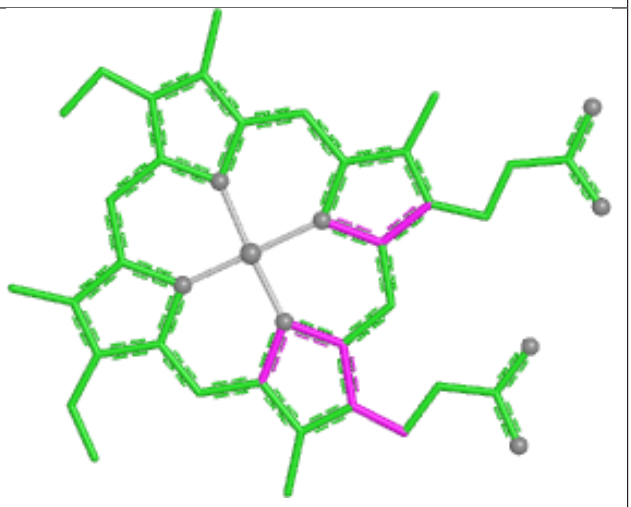
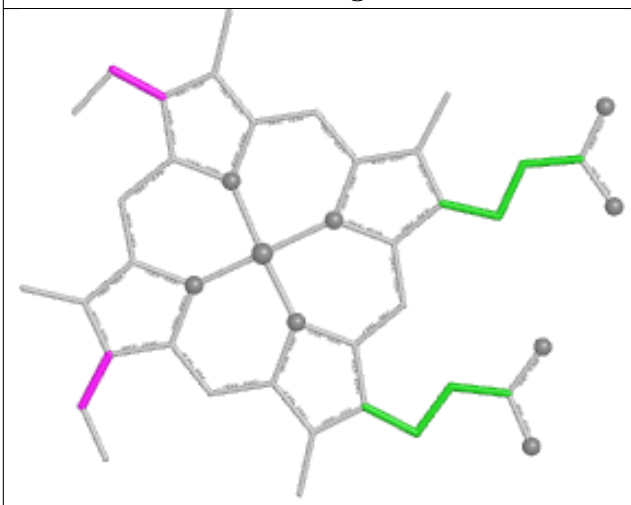
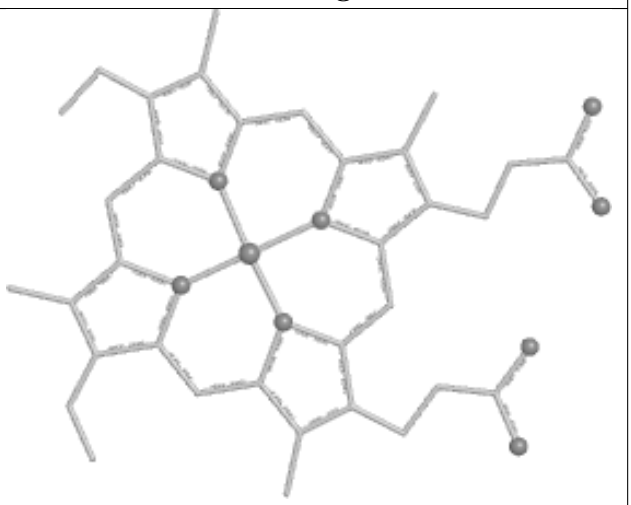


Bond angles

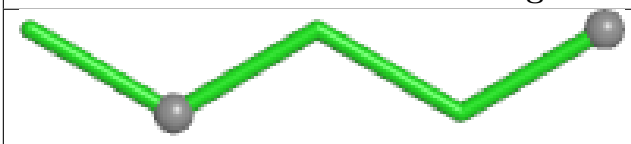


Torsions



Rings

Ligand PG6 B 526



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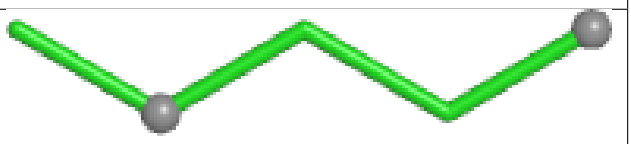
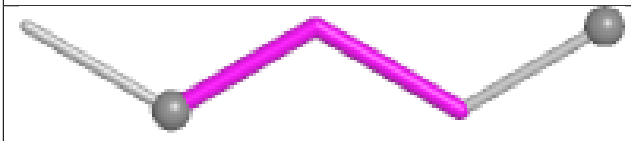


Bond angles



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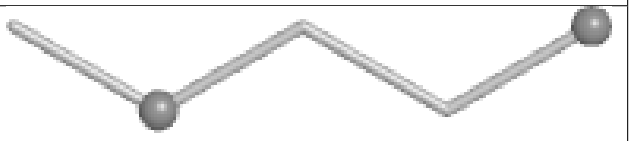
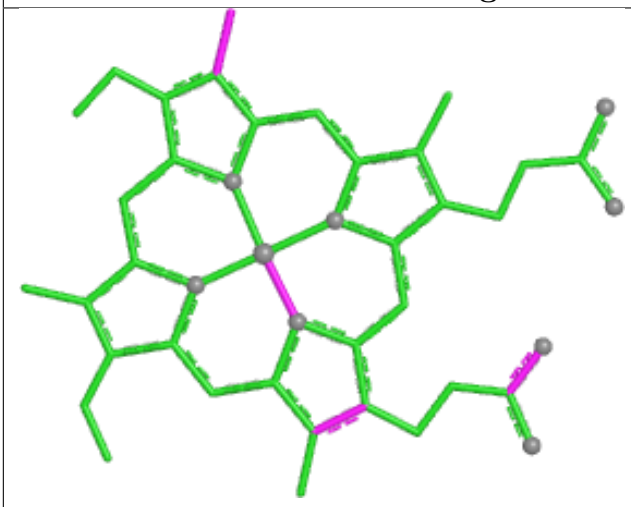


Rings

Ligand HEC A 1005 (A)



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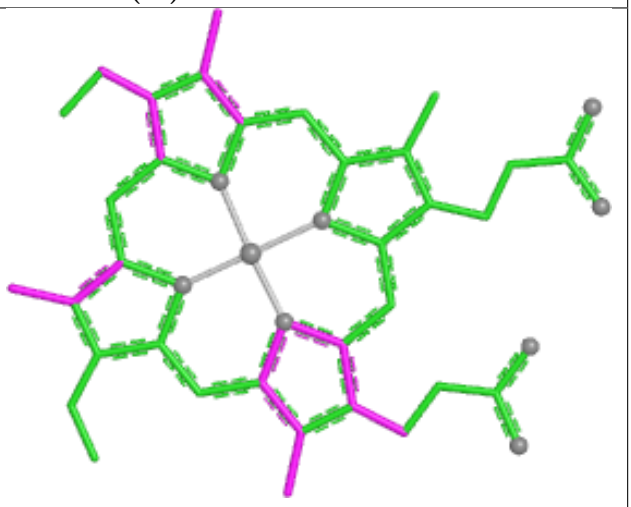
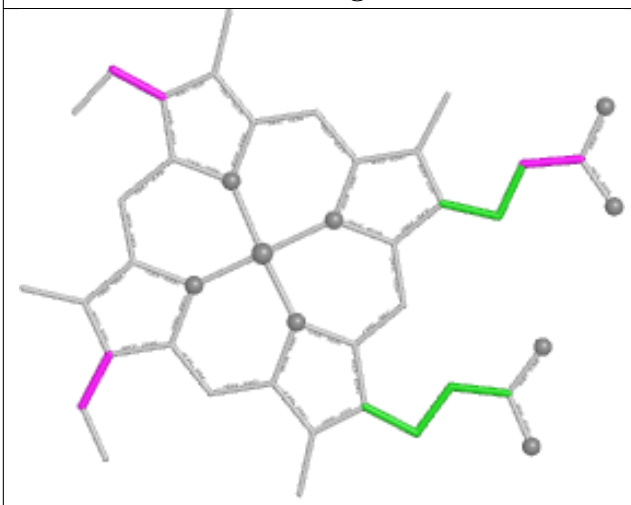


Bond angles



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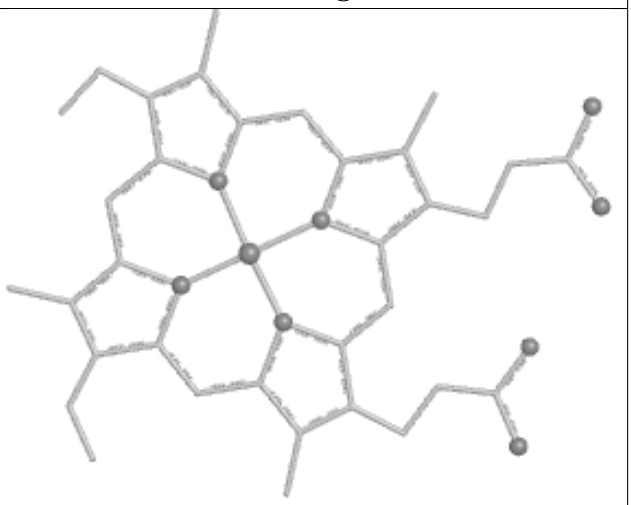
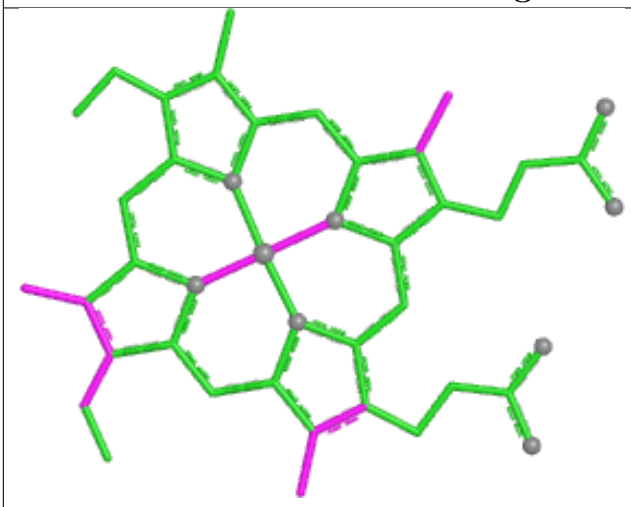


Rings

Ligand HEC B 1008



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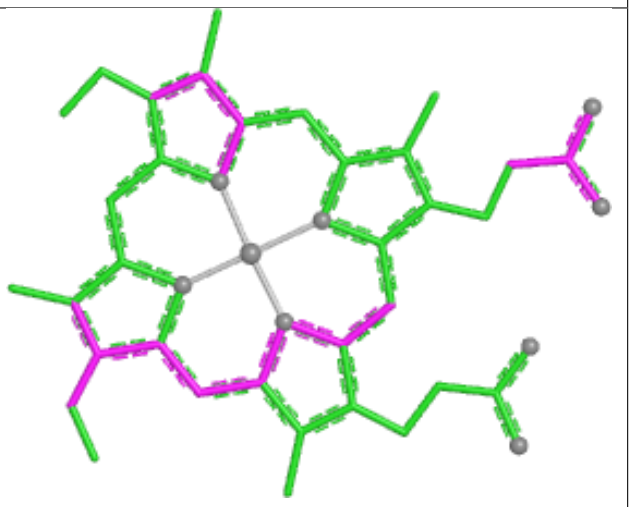
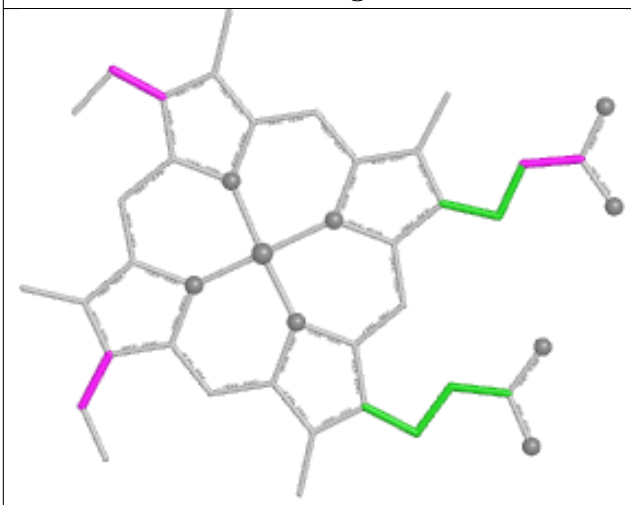


Bond angles



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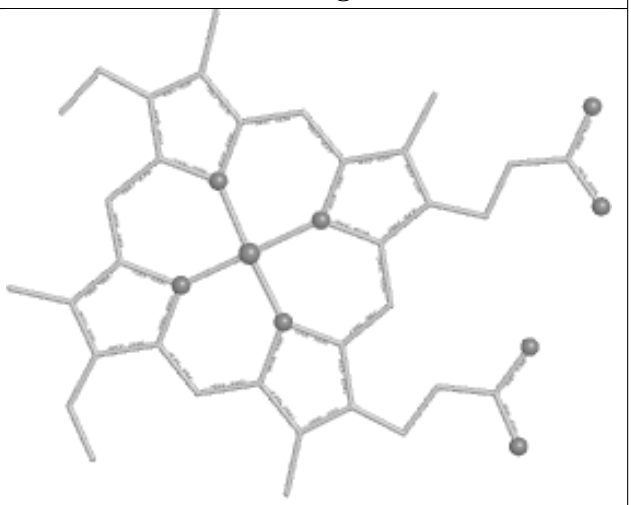
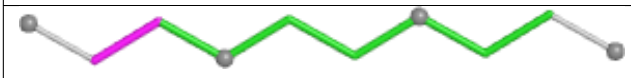


Rings

Ligand PG6 B 525

Bond lengths

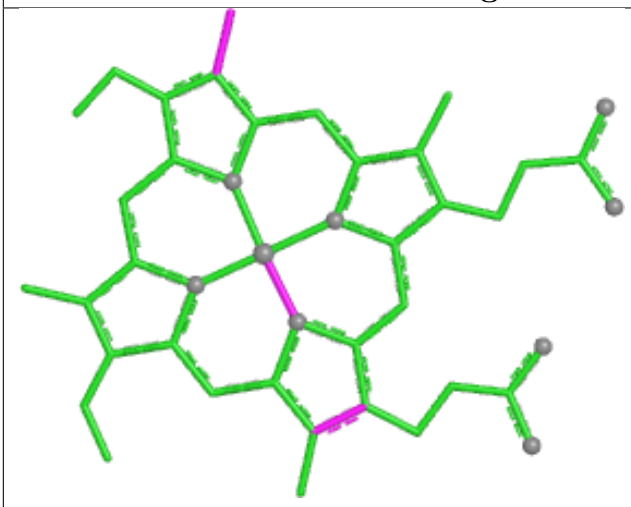
Bond angles



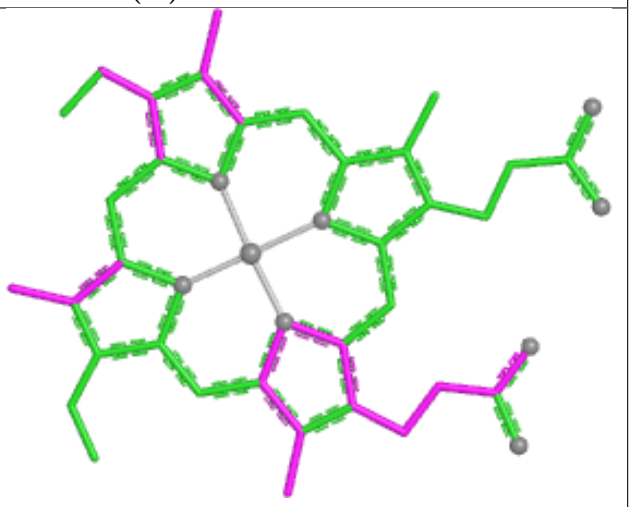
Torsions

Rings

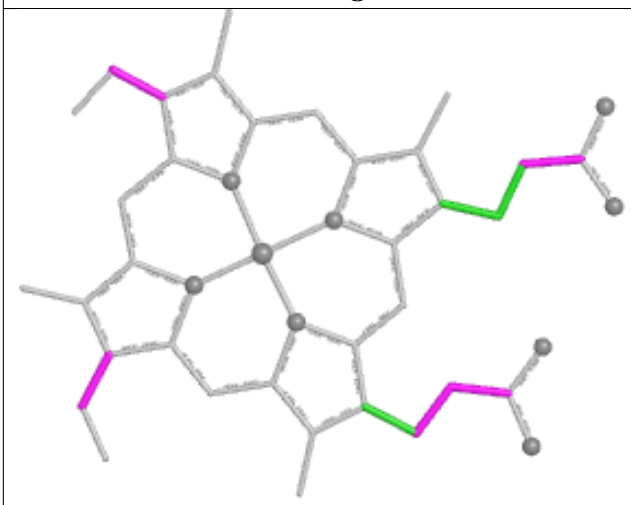
Ligand HEC A 1005 (B)



Bond lengths



Bond angles



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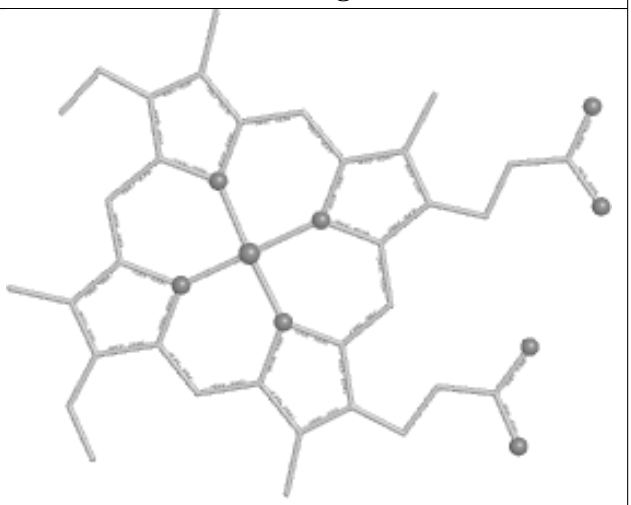
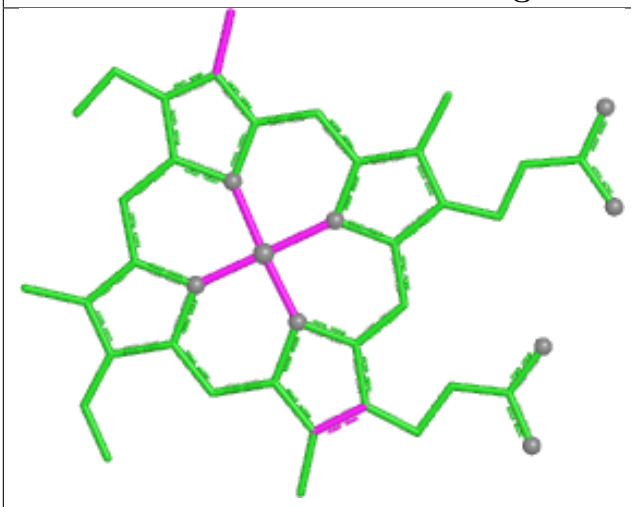
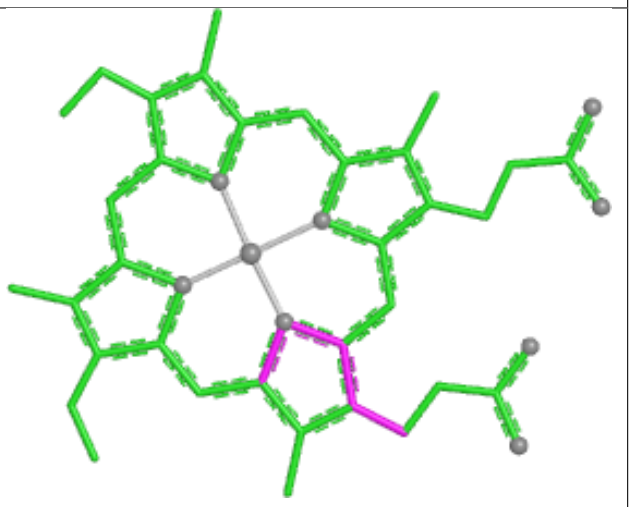


Rings

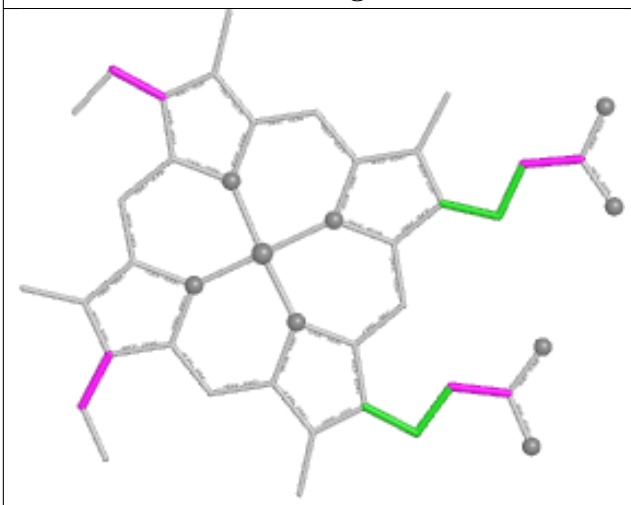
Ligand HEC A 1001



Bond lengths



Bond angles



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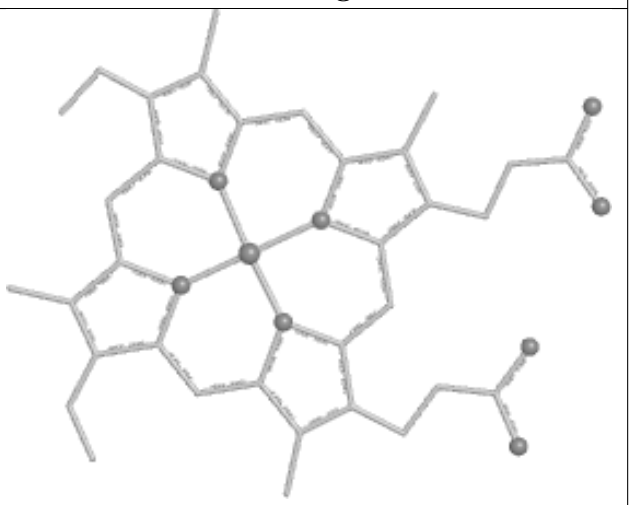
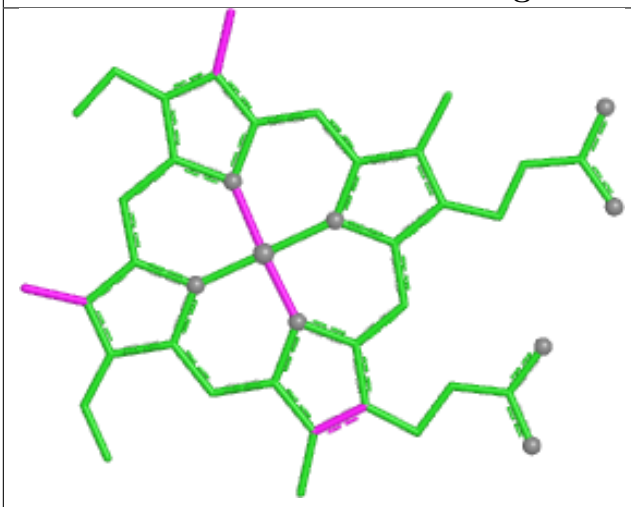
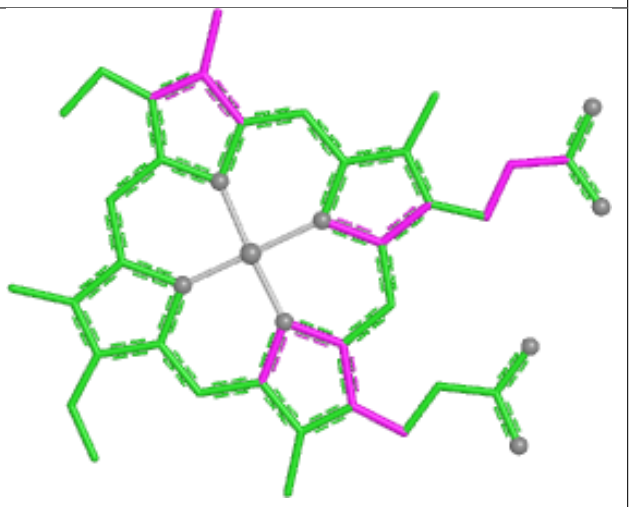


Rings

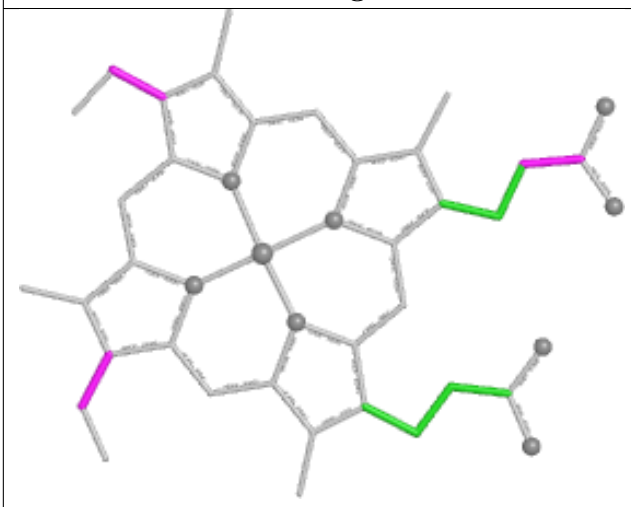
Ligand HEC A 1002



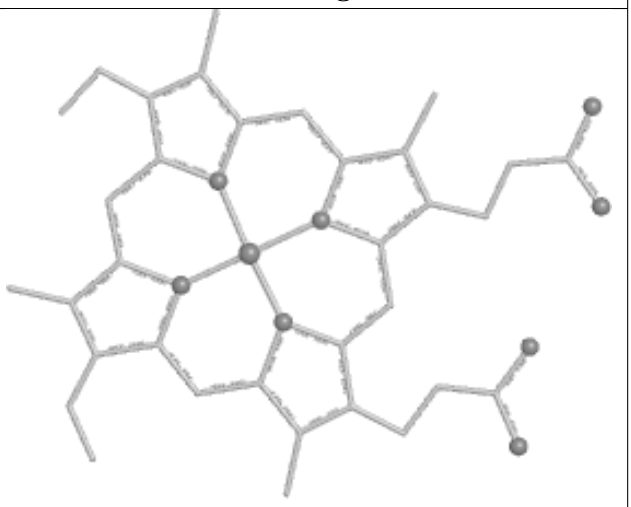
Bond lengths



Bond angles

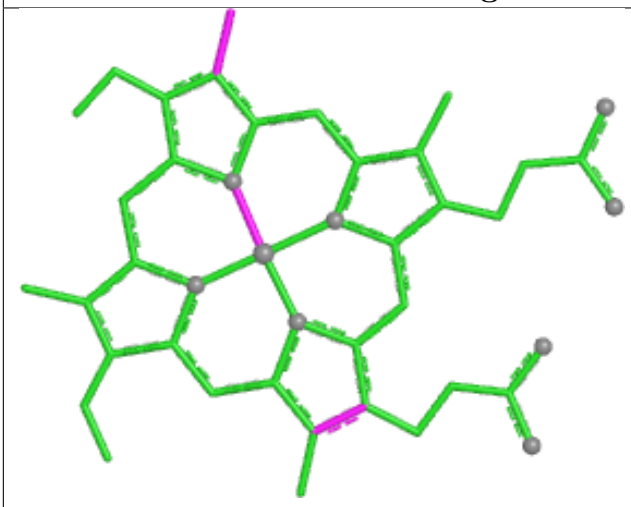


Torsions

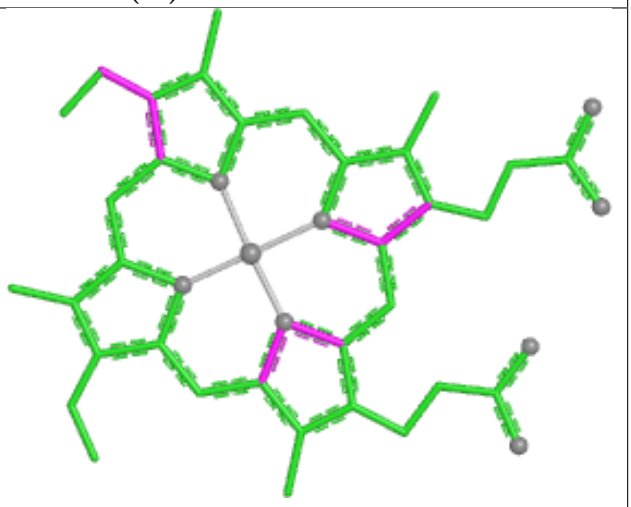


Rings

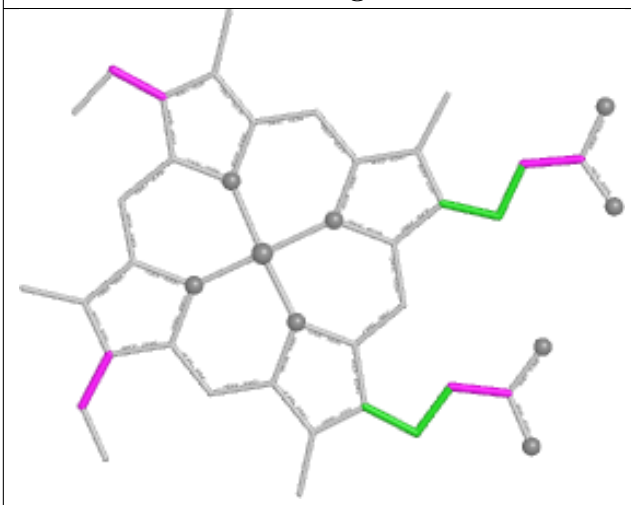
Ligand HEC B 1005 (A)



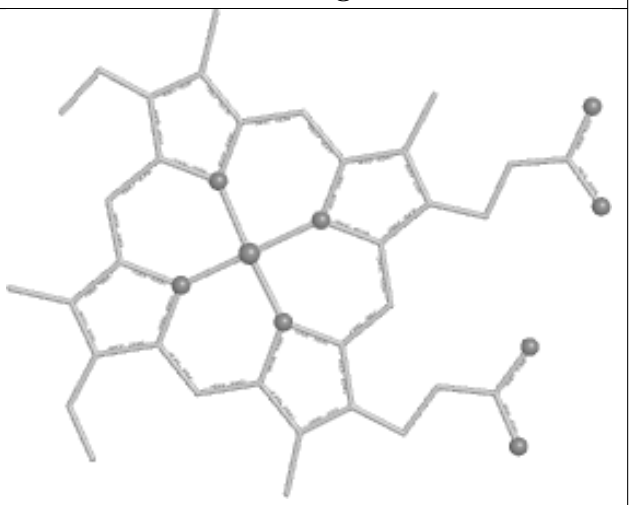
Bond lengths



Bond angles

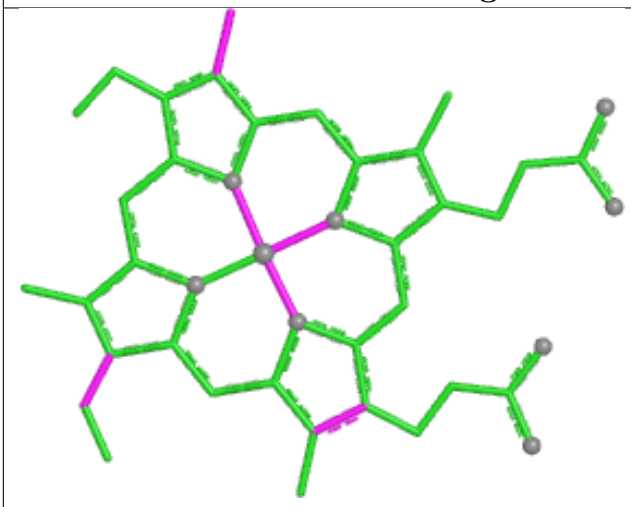


Torsions

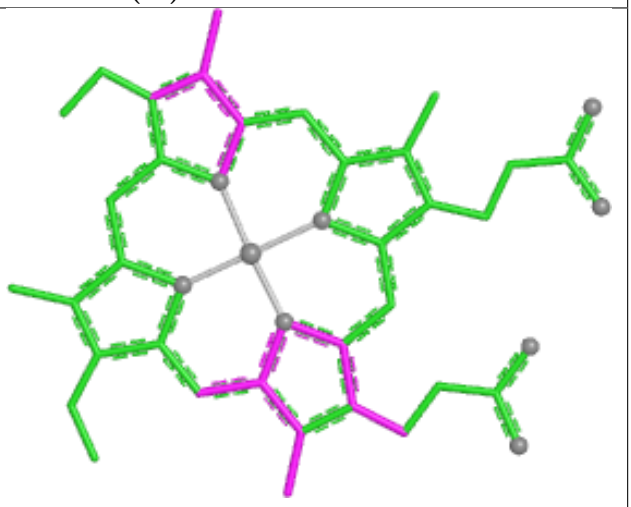


Rings

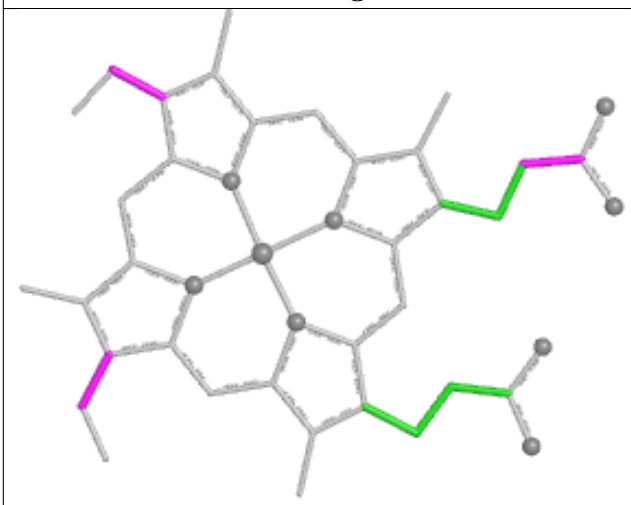
Ligand HEC A 1007 (A)



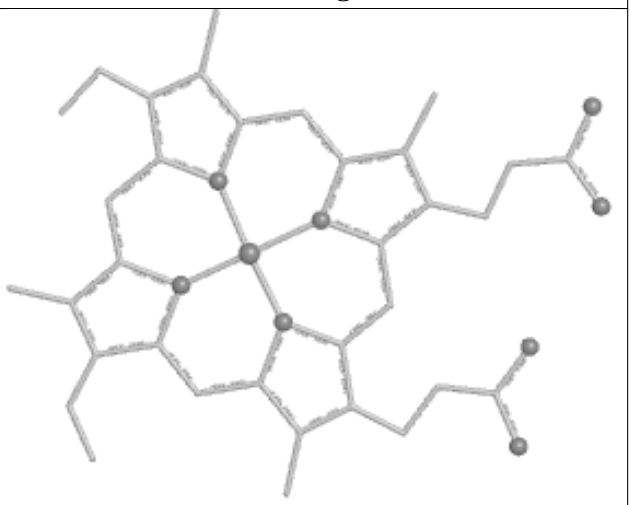
Bond lengths



Bond angles

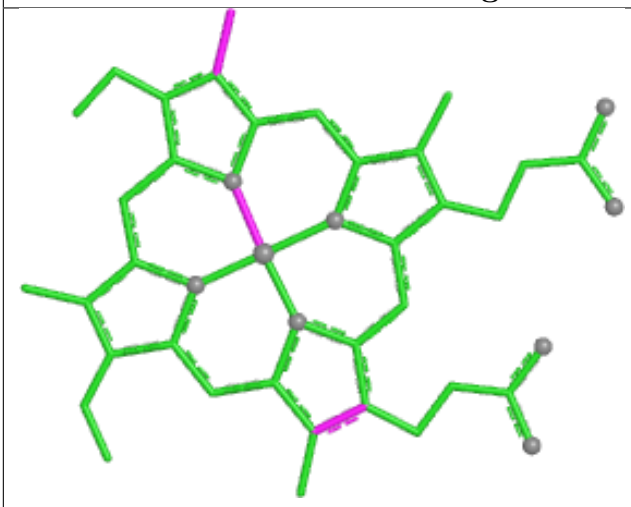


Torsions

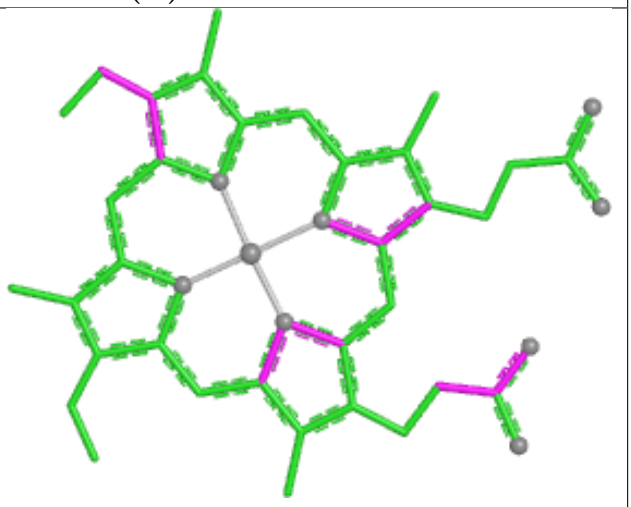


Rings

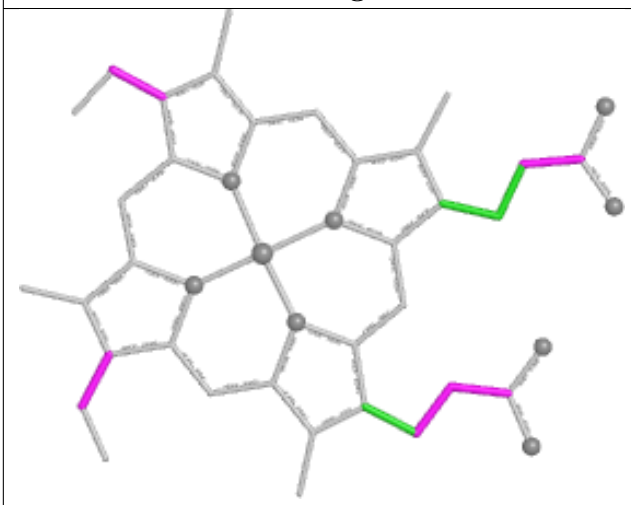
Ligand HEC B 1005 (B)



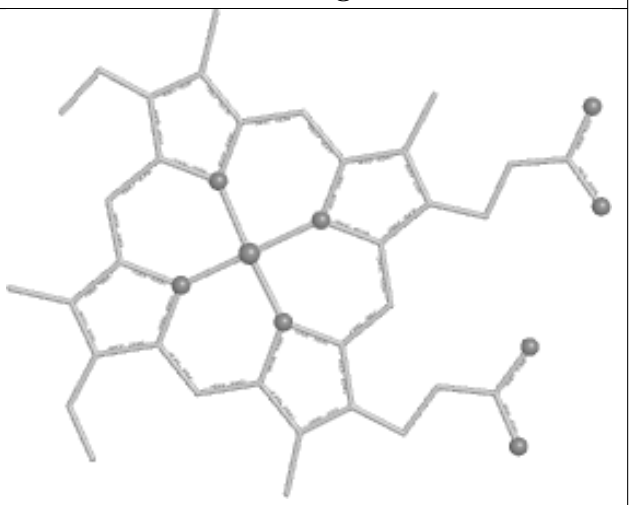
Bond lengths



Bond angles

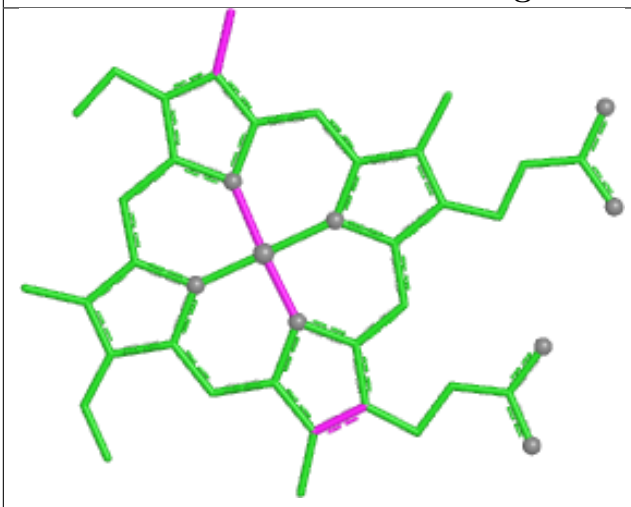


Torsions

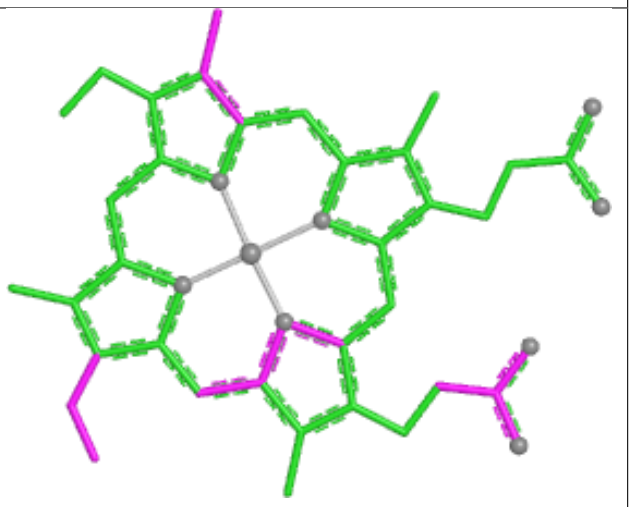


Rings

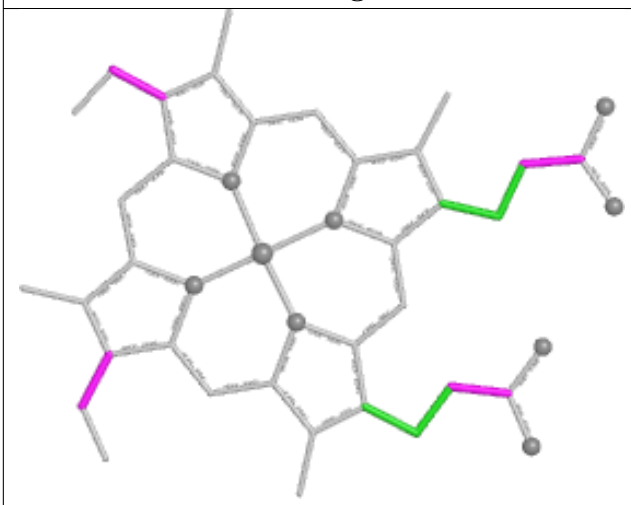
Ligand HEC B 1003



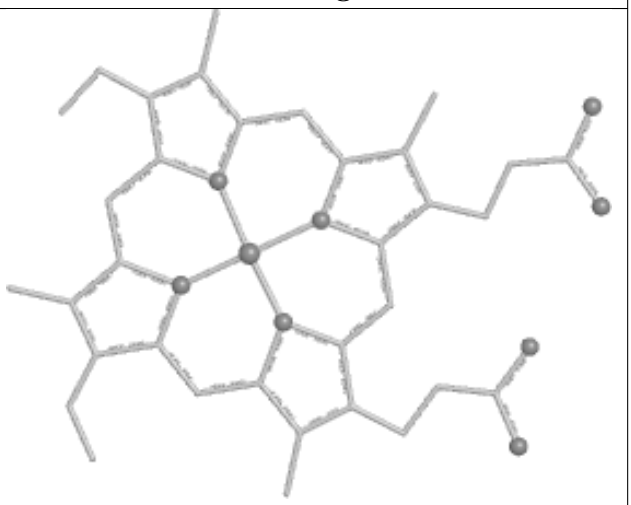
Bond lengths



Bond angles

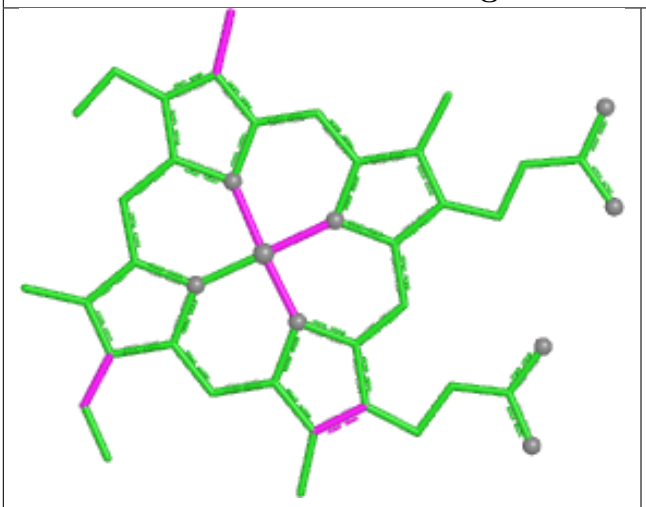


Torsions

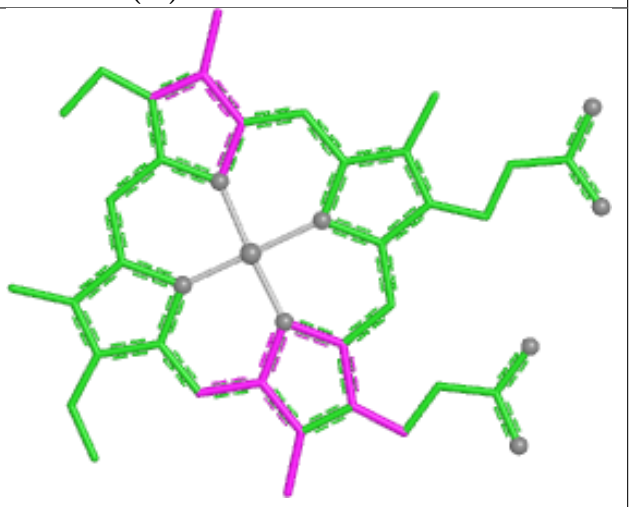


Rings

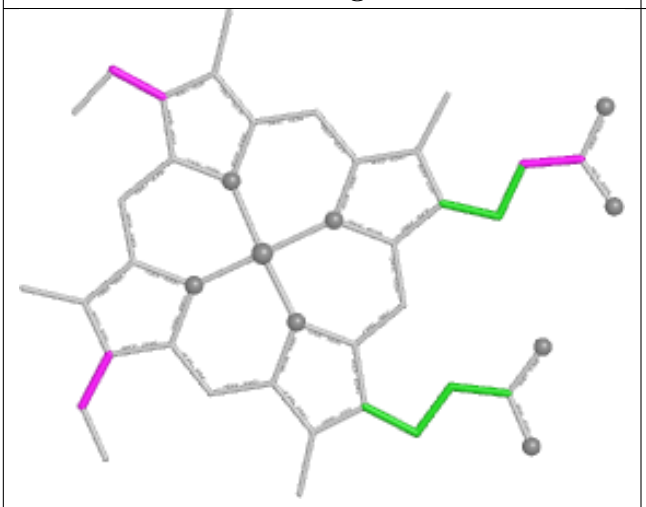
Ligand HEC A 1007 (B)



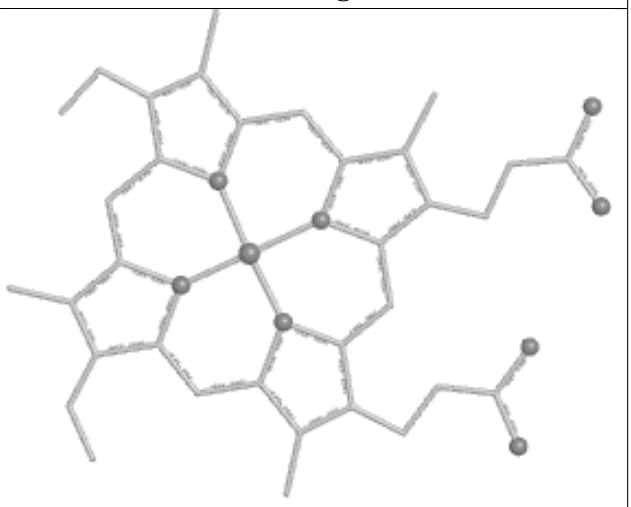
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	519/519 (100%)	-0.55	4 (0%)	82	86	8, 14, 25, 52	23 (4%)
1	B	519/519 (100%)	-0.61	4 (0%)	82	86	8, 14, 24, 50	25 (4%)
All	All	1038/1038 (100%)	-0.58	8 (0%)	82	86	8, 14, 24, 52	48 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	4.9
1	B	523	ALA	4.6
1	B	522	VAL	4.3
1	A	522	VAL	3.8
1	A	388	GLN	3.2
1	A	278	ARG	2.4
1	B	12[A]	MET	2.3
1	B	51	ARG	2.3

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 oligosaccharides in this entry.

6.4 Ligands

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PG4	A	533	6/13	0.58	0.26	25,38,41,47	0
5	PG4	B	534	8/13	0.64	0.24	38,42,45,47	0
5	PG4	A	529	7/13	0.68	0.26	50,51,54,56	0
5	PG4	A	528	9/13	0.70	0.24	34,43,49,50	0
5	PG4	B	530	8/13	0.71	0.24	44,49,50,51	0
5	PG4	A	531	10/13	0.72	0.23	35,44,50,50	0
5	PG4	A	526	6/13	0.74	0.26	38,47,50,51	0
5	PG4	B	532	5/13	0.74	0.23	41,43,46,46	0
5	PG4	B	528	8/13	0.74	0.24	37,48,50,52	0
5	PG4	B	533	7/13	0.75	0.23	42,44,47,49	0
5	PG4	A	530	5/13	0.76	0.25	45,45,49,51	0
5	PG4	B	531	9/13	0.78	0.21	41,46,48,53	0
5	PG4	A	4	6/13	0.78	0.22	45,46,49,56	0
5	PG4	A	532	5/13	0.81	0.21	46,47,50,51	0
6	PG6	A	525	10/18	0.81	0.25	20,21,26,28	10
6	PG6	B	526	5/18	0.81	0.23	41,44,48,51	0
6	PG6	B	525	10/18	0.82	0.23	19,23,26,29	10
5	PG4	B	4	8/13	0.82	0.22	45,48,52,53	0
5	PG4	B	529	9/13	0.88	0.25	15,22,28,28	9
3	PO4	A	527	5/5	0.91	0.10	16,17,19,19	5
7	NA	A	534	1/1	0.92	0.09	25,25,25,25	1
6	PG6	B	524	5/18	0.93	0.13	19,28,35,38	0
6	PG6	A	524	7/18	0.94	0.13	19,31,49,53	0
3	PO4	B	527	5/5	0.95	0.10	12,15,16,17	5
3	PO4	B	1	5/5	0.97	0.10	9,9,11,12	5
2	HEC	A	1008	43/43	0.98	0.07	11,17,28,44	0
7	NA	A	535	1/1	0.98	0.15	31,31,31,31	0
2	HEC	A	1004	43/43	0.99	0.04	9,11,13,14	0
2	HEC	A	1002	43/43	0.99	0.04	10,11,13,15	0
2	HEC	A	1003	43/43	0.99	0.04	9,11,20,31	0
2	HEC	A	1001	43/43	0.99	0.05	11,13,16,19	0
2	HEC	B	1005[A]	43/43	0.99	0.04	9,11,14,18	4
2	HEC	B	1005[B]	43/43	0.99	0.04	9,11,21,27	4
2	HEC	B	1006	43/43	0.99	0.04	8,10,11,13	0
2	HEC	B	1007[A]	43/43	0.99	0.04	9,11,13,17	4
2	HEC	B	1007[B]	43/43	0.99	0.04	9,11,12,14	4
2	HEC	B	1008	43/43	0.99	0.07	12,17,30,43	0
2	HEC	B	1002	43/43	0.99	0.05	11,13,15,17	0
2	HEC	B	1003	43/43	0.99	0.05	10,12,21,32	0
2	HEC	B	1001	43/43	0.99	0.05	12,15,19,23	0
3	PO4	A	1	5/5	0.99	0.07	8,9,12,14	5

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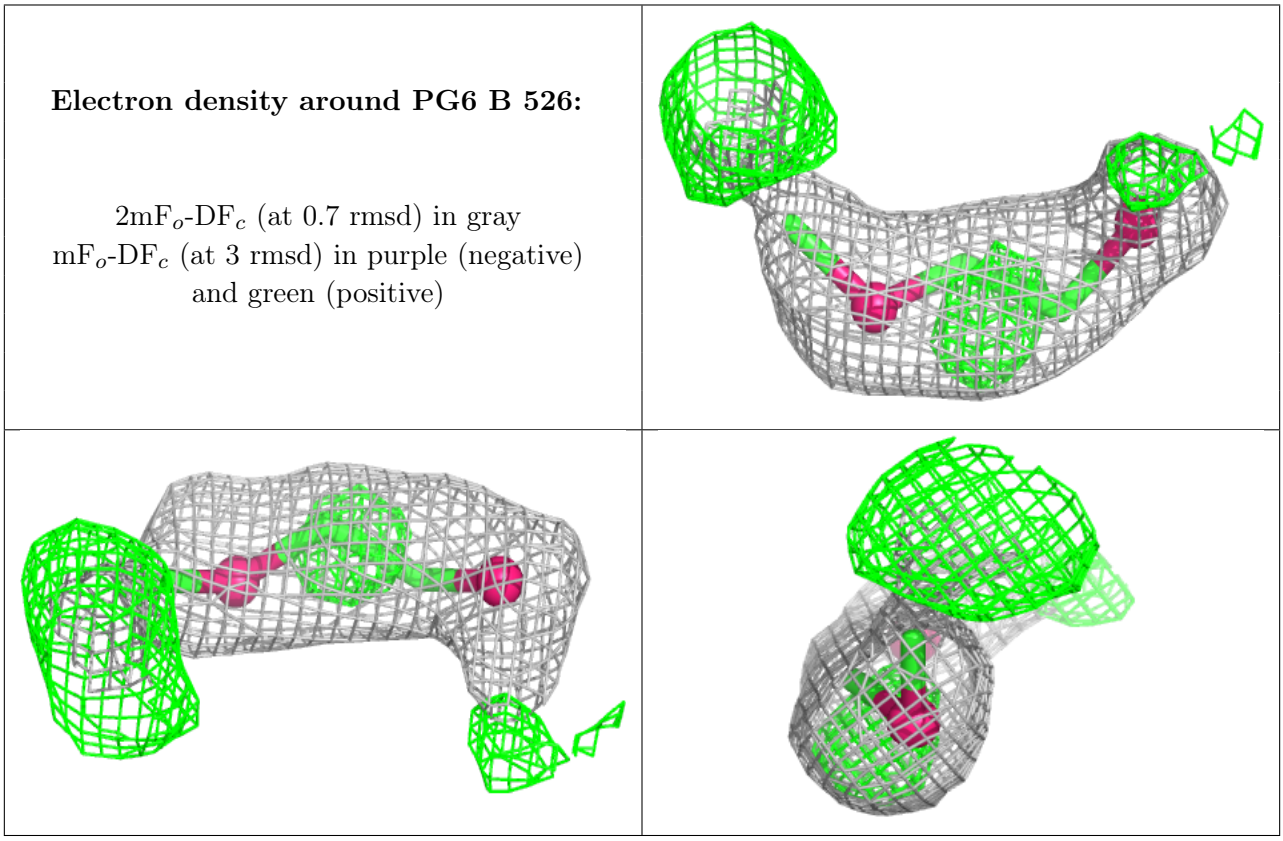
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	1005[A]	43/43	0.99	0.04	9,10,13,16	4
2	HEC	A	1005[B]	43/43	0.99	0.04	9,10,18,31	4
2	HEC	A	1006	43/43	0.99	0.04	8,10,11,12	0
4	CA	A	3	1/1	0.99	0.05	14,14,14,14	1
4	CA	B	3	1/1	0.99	0.06	14,14,14,14	1
2	HEC	A	1007[A]	43/43	0.99	0.04	9,11,13,15	3
2	HEC	A	1007[B]	43/43	0.99	0.04	9,11,12,13	3
4	CA	A	2	1/1	1.00	0.05	14,14,14,14	0
2	HEC	B	1004	43/43	1.00	0.03	10,11,13,13	0
4	CA	B	2	1/1	1.00	0.04	13,13,13,13	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.

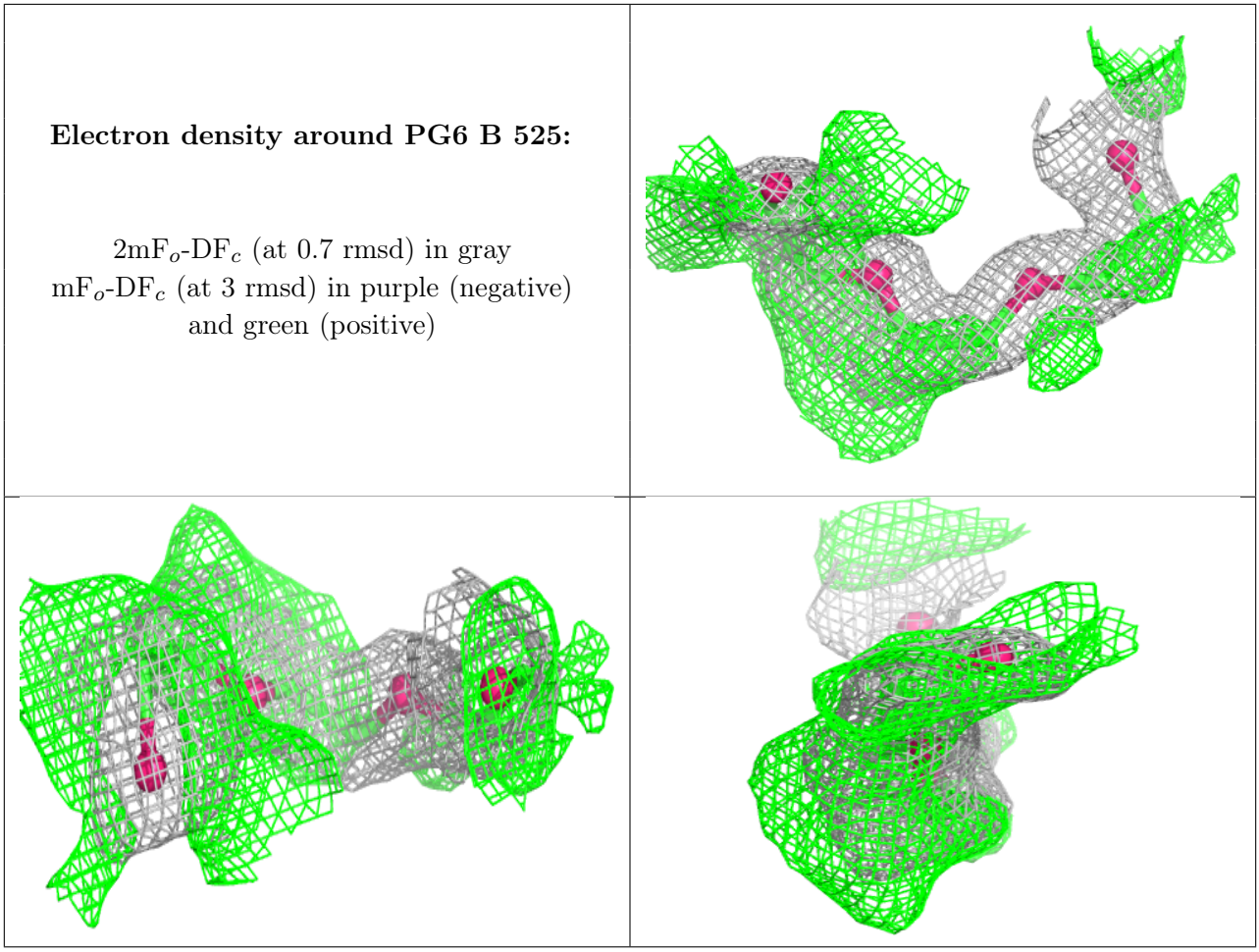
Electron density around PG6 B 526:

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



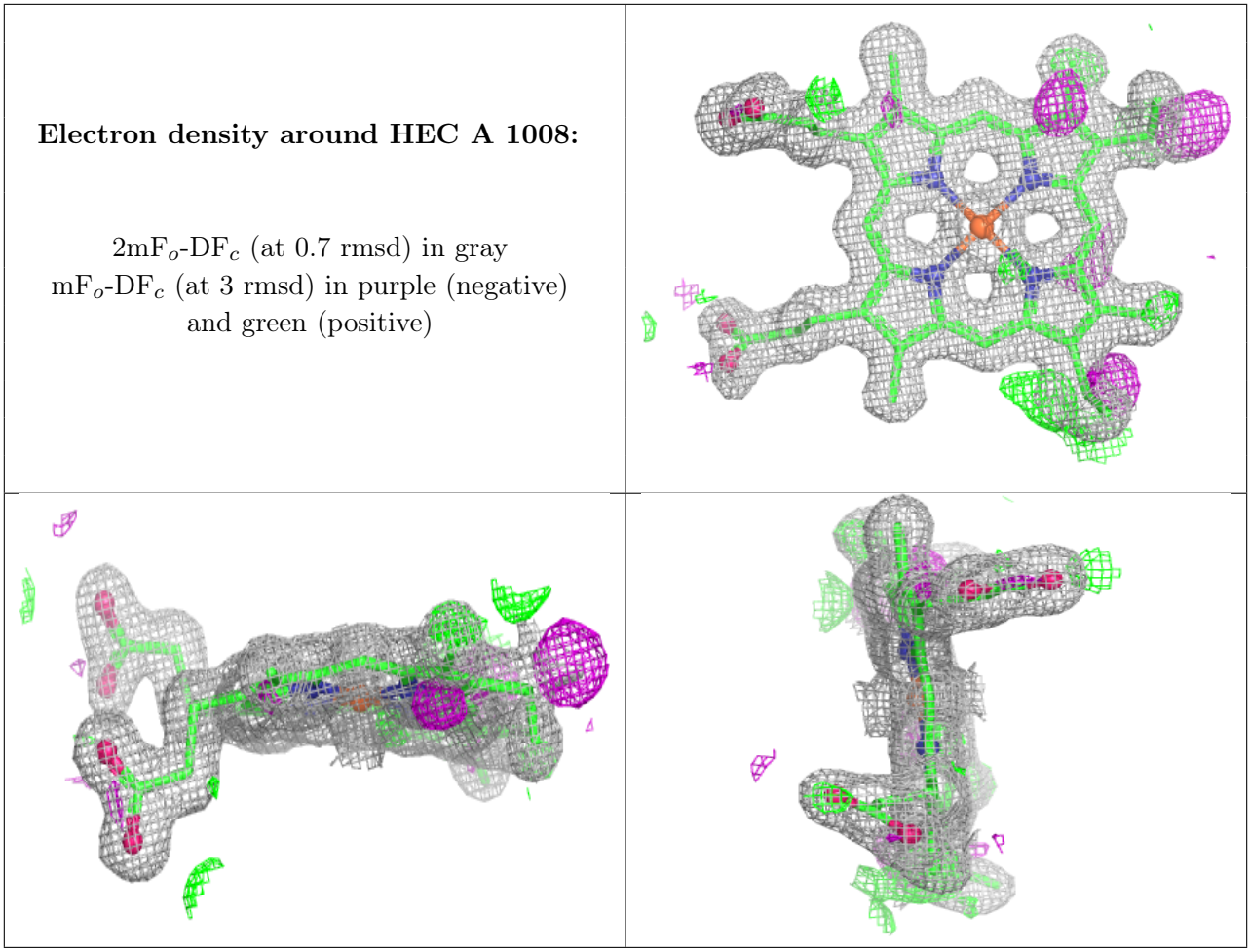
Electron density around PG6 B 525:

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



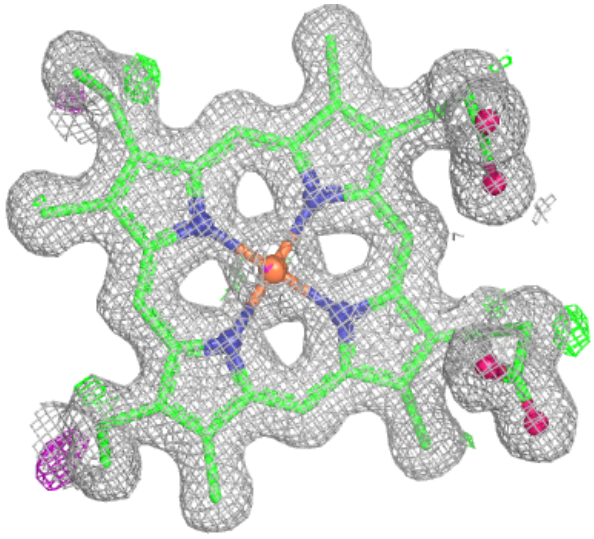
Electron density around HEC A 1008:

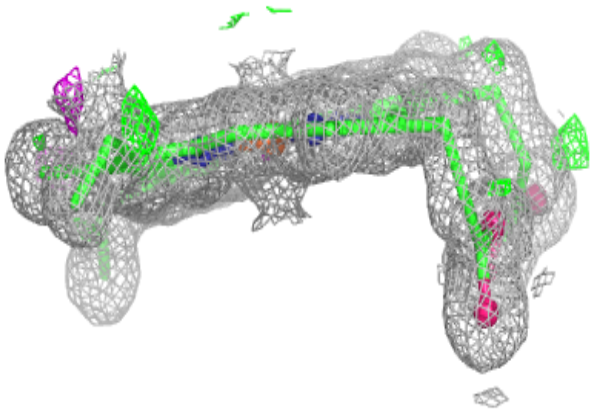
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

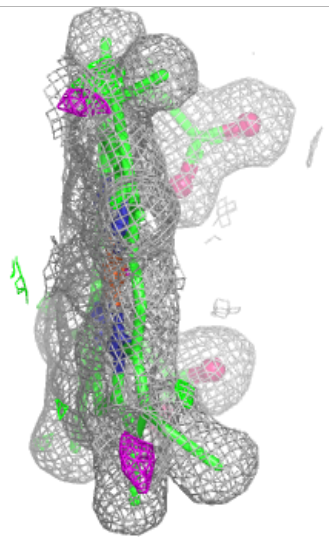


Electron density around HEC A 1004:

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

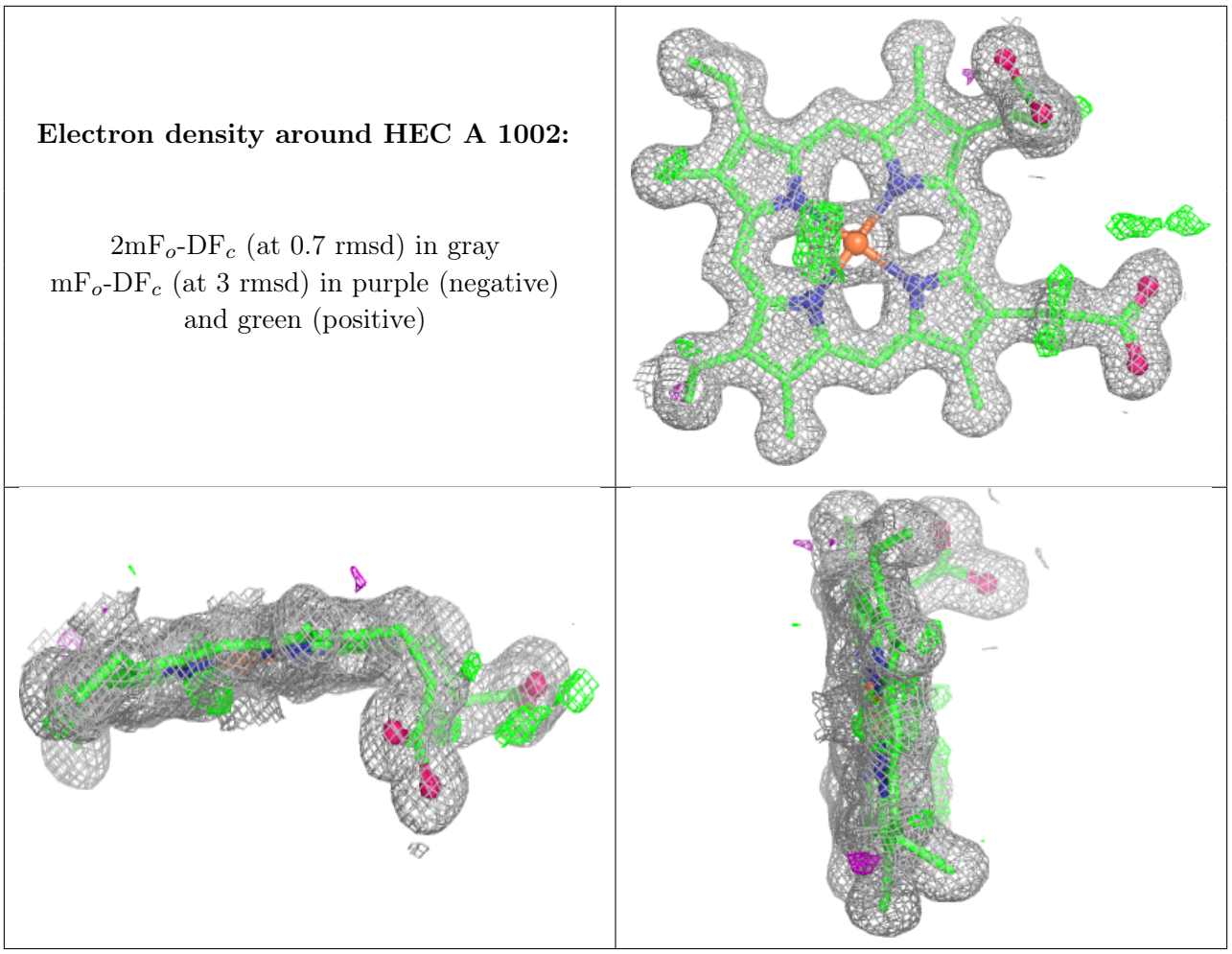






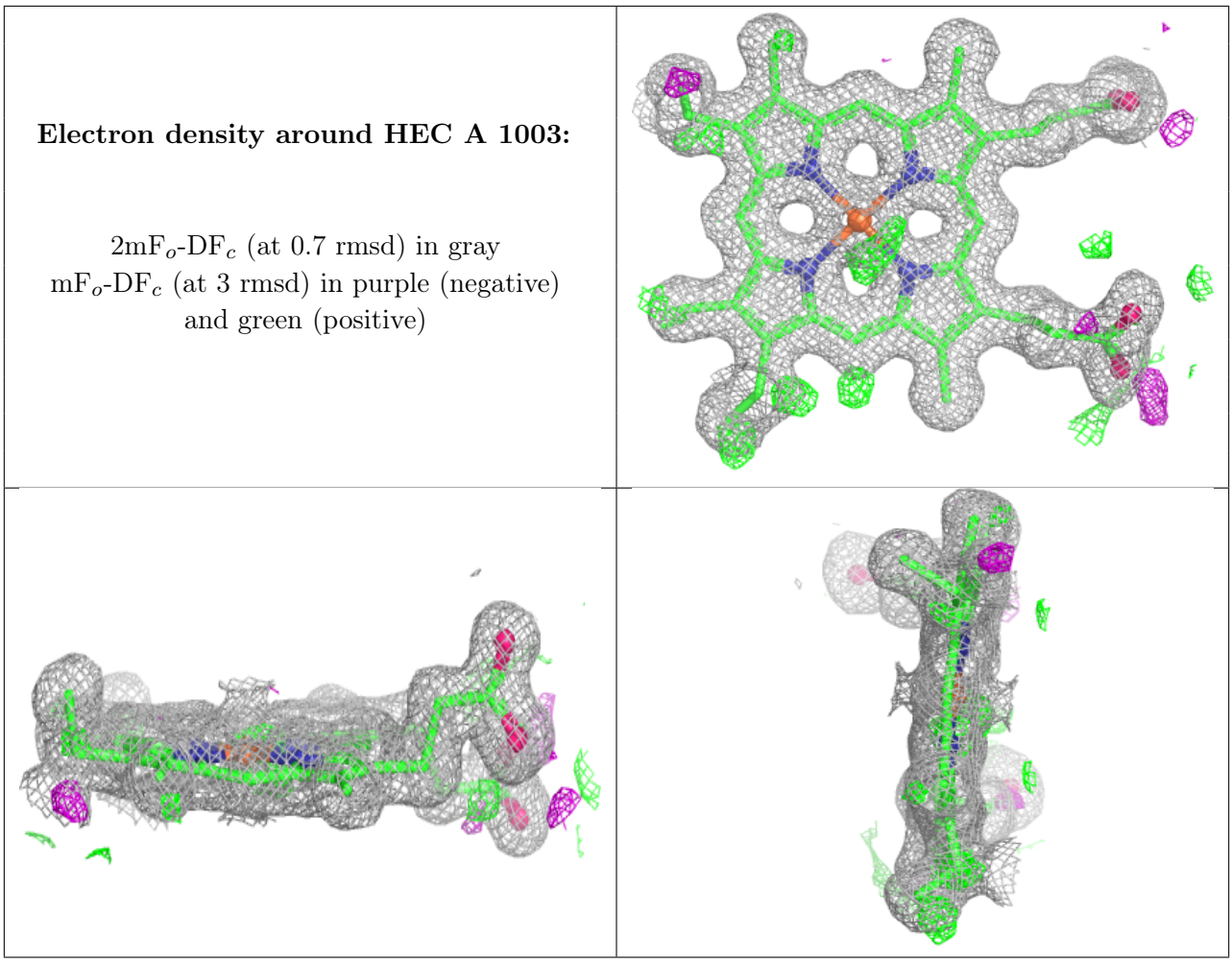
Electron density around HEC A 1002:

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



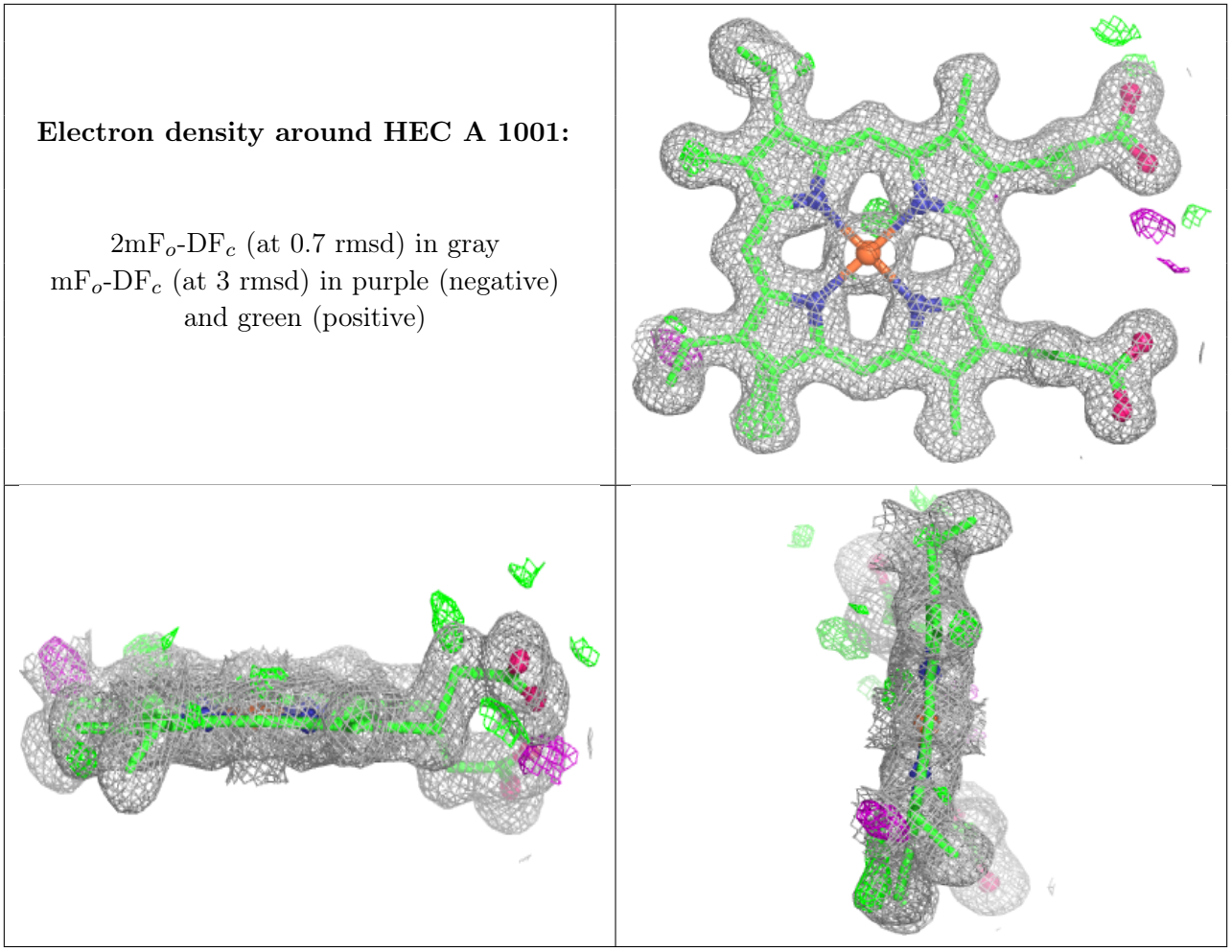
Electron density around HEC A 1003:

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



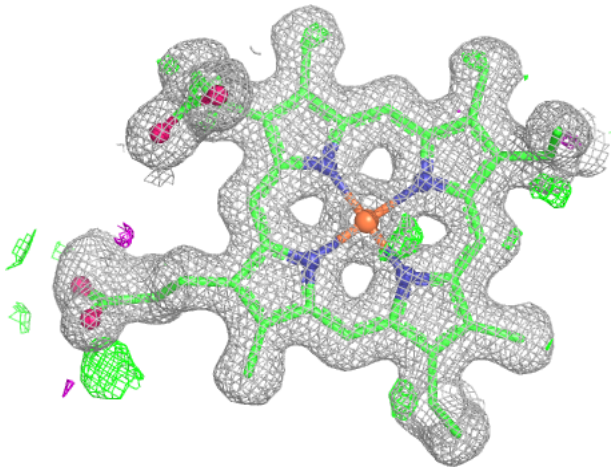
Electron density around HEC A 1001:

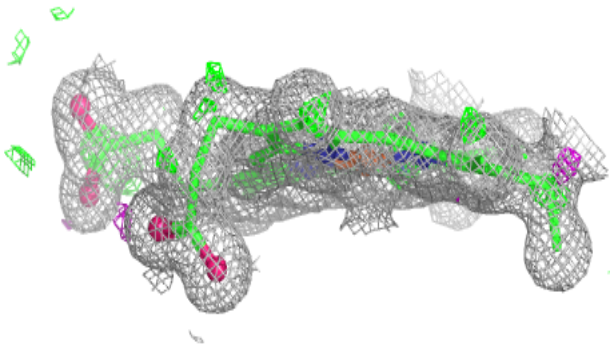
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

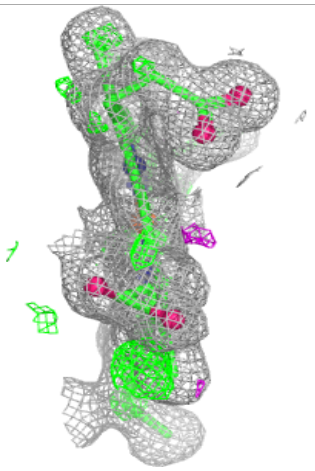


Electron density around HEC B 1005 (A):

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

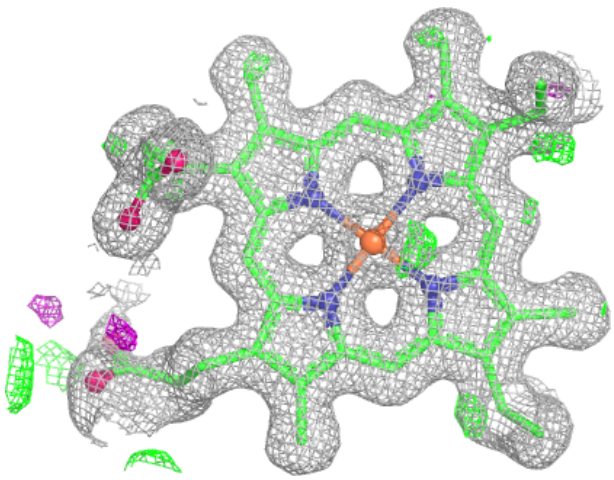


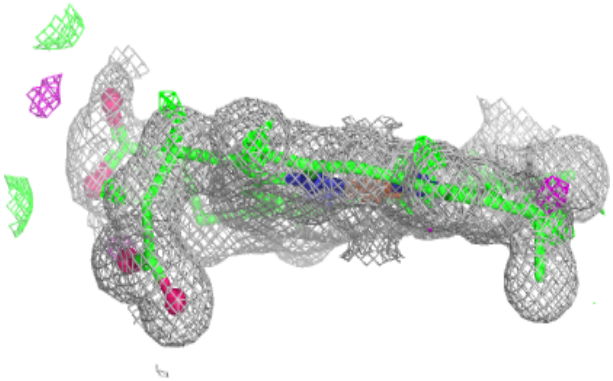


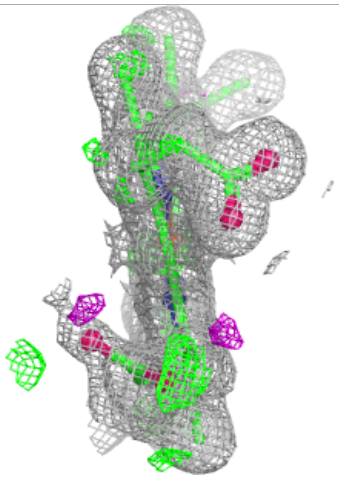


Electron density around HEC B 1005 (B):

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

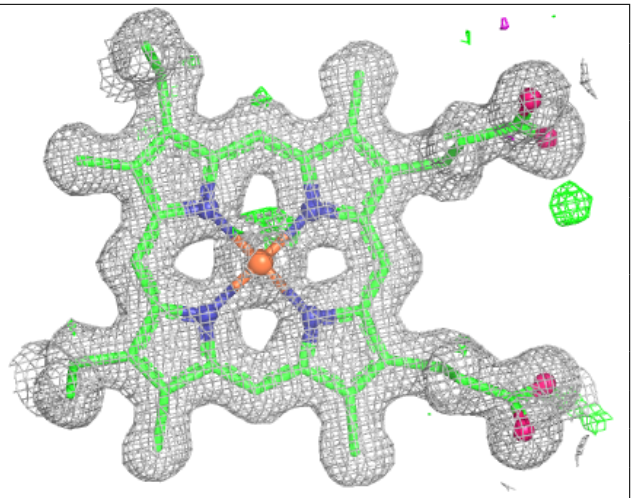


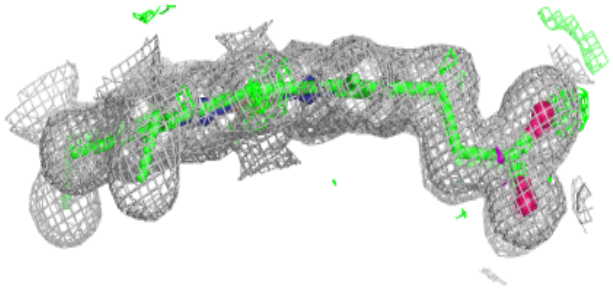


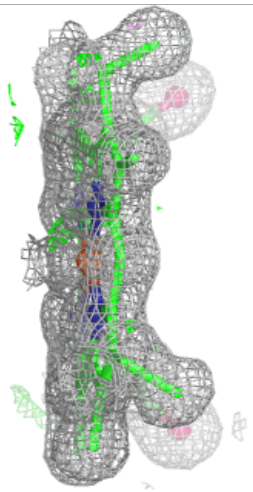


Electron density around HEC B 1006:

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

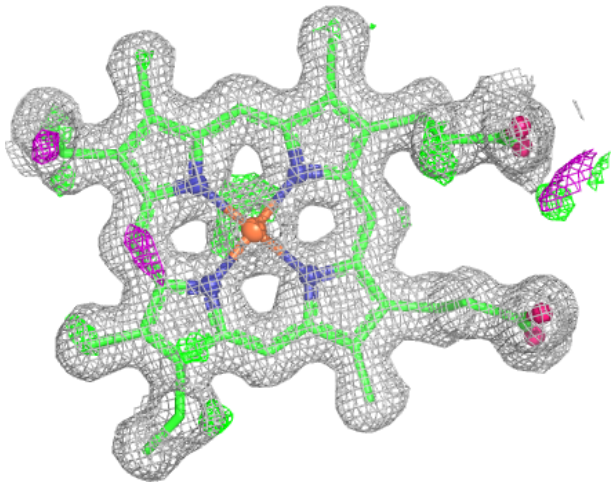


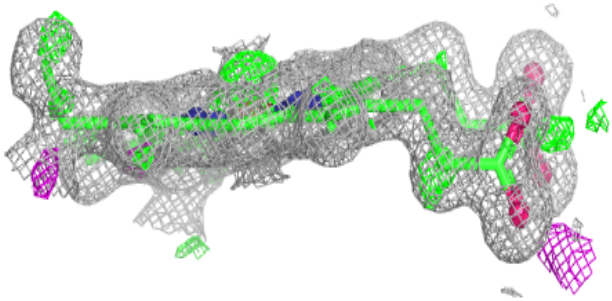


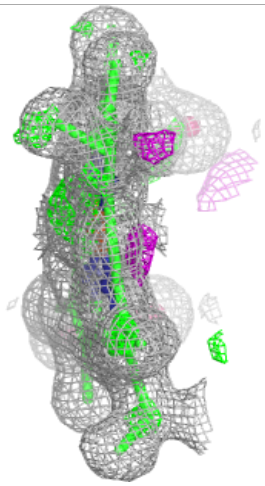


Electron density around HEC B 1007 (A):

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

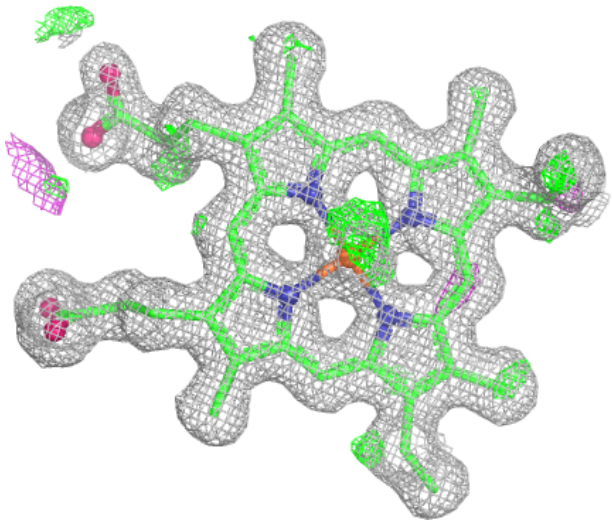


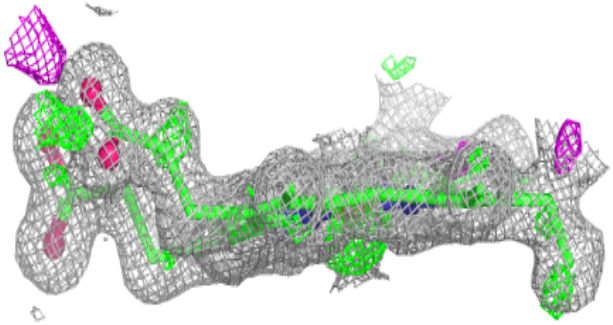


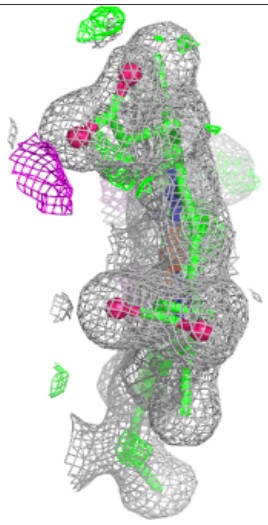


Electron density around HEC B 1007 (B):

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

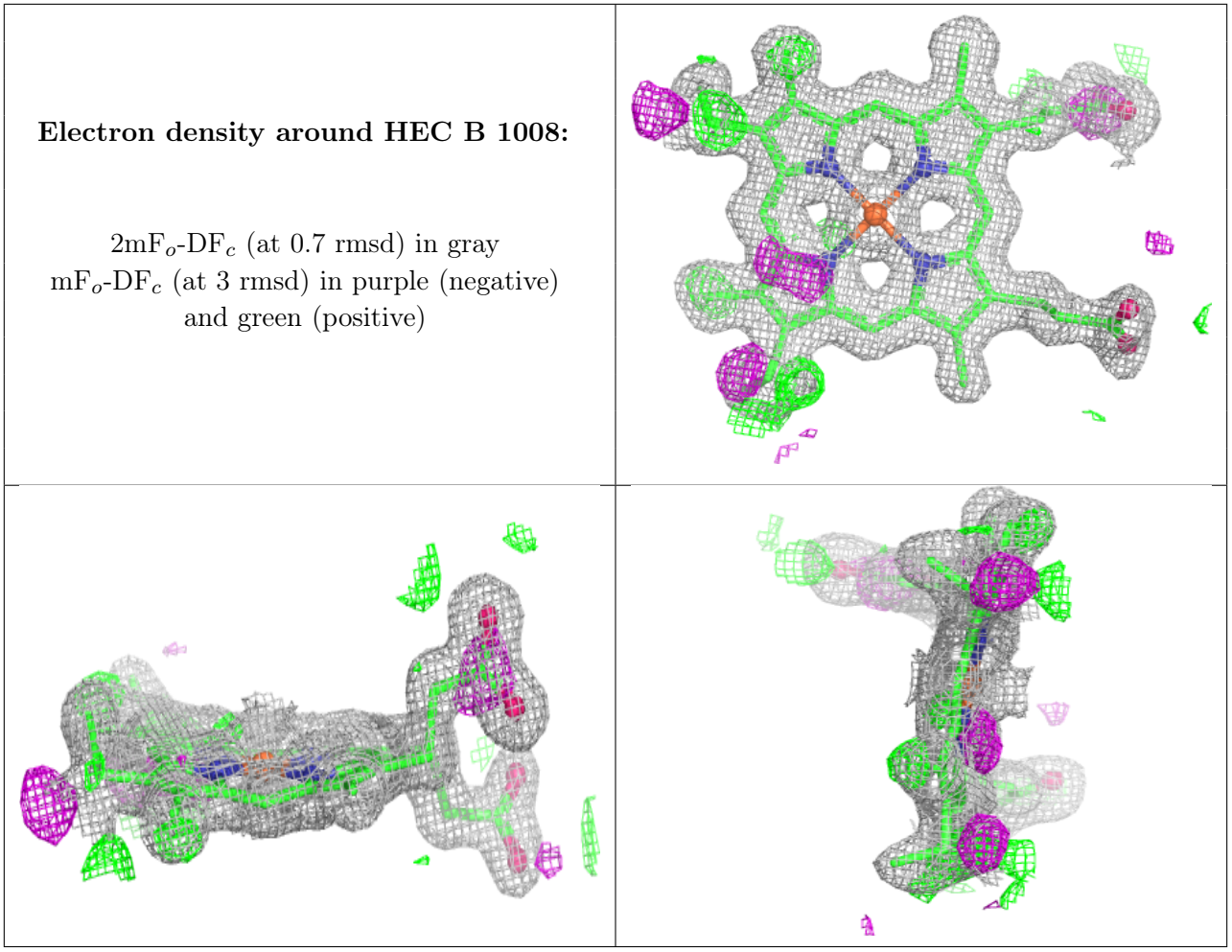






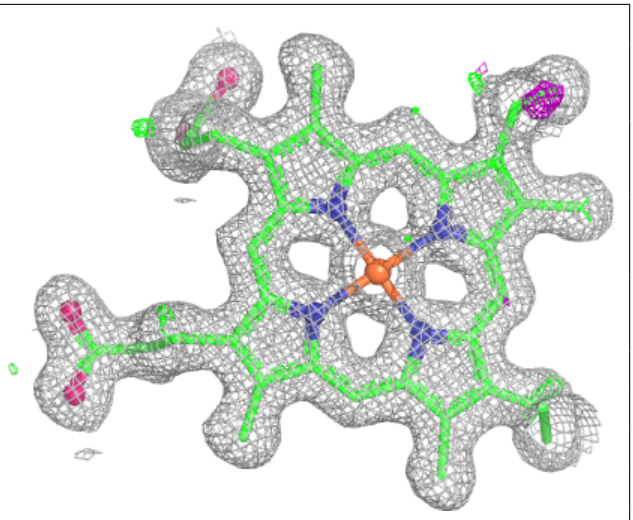
Electron density around HEC B 1008:

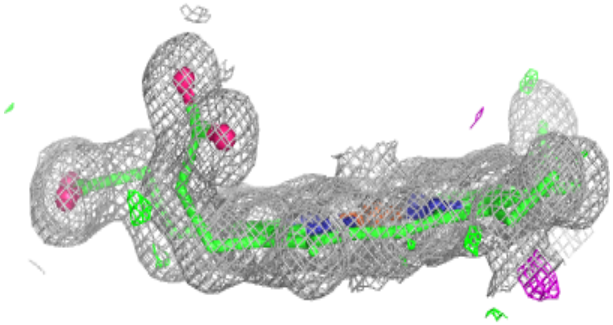
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

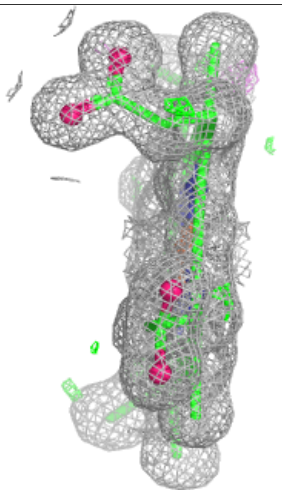


Electron density around HEC B 1002:

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

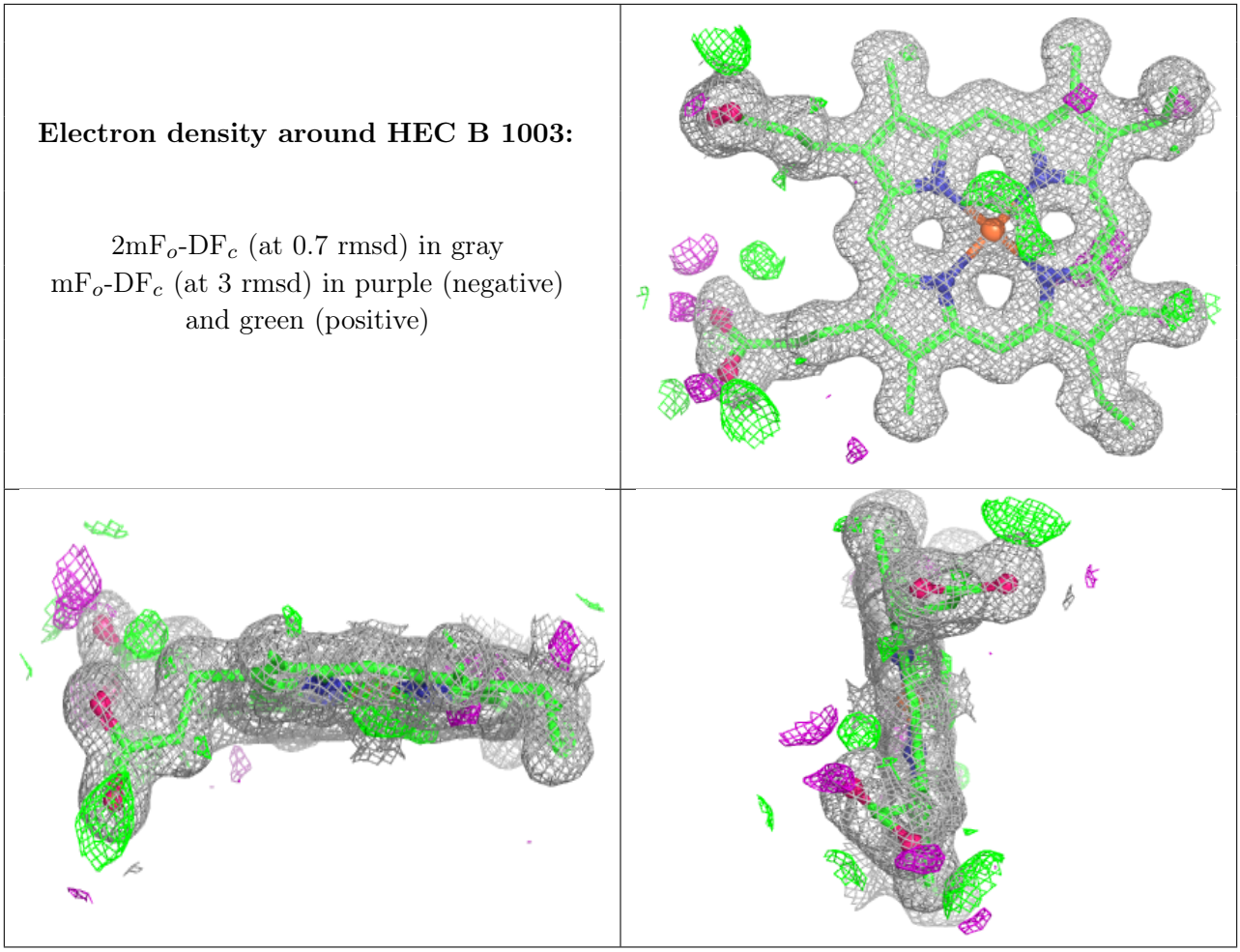






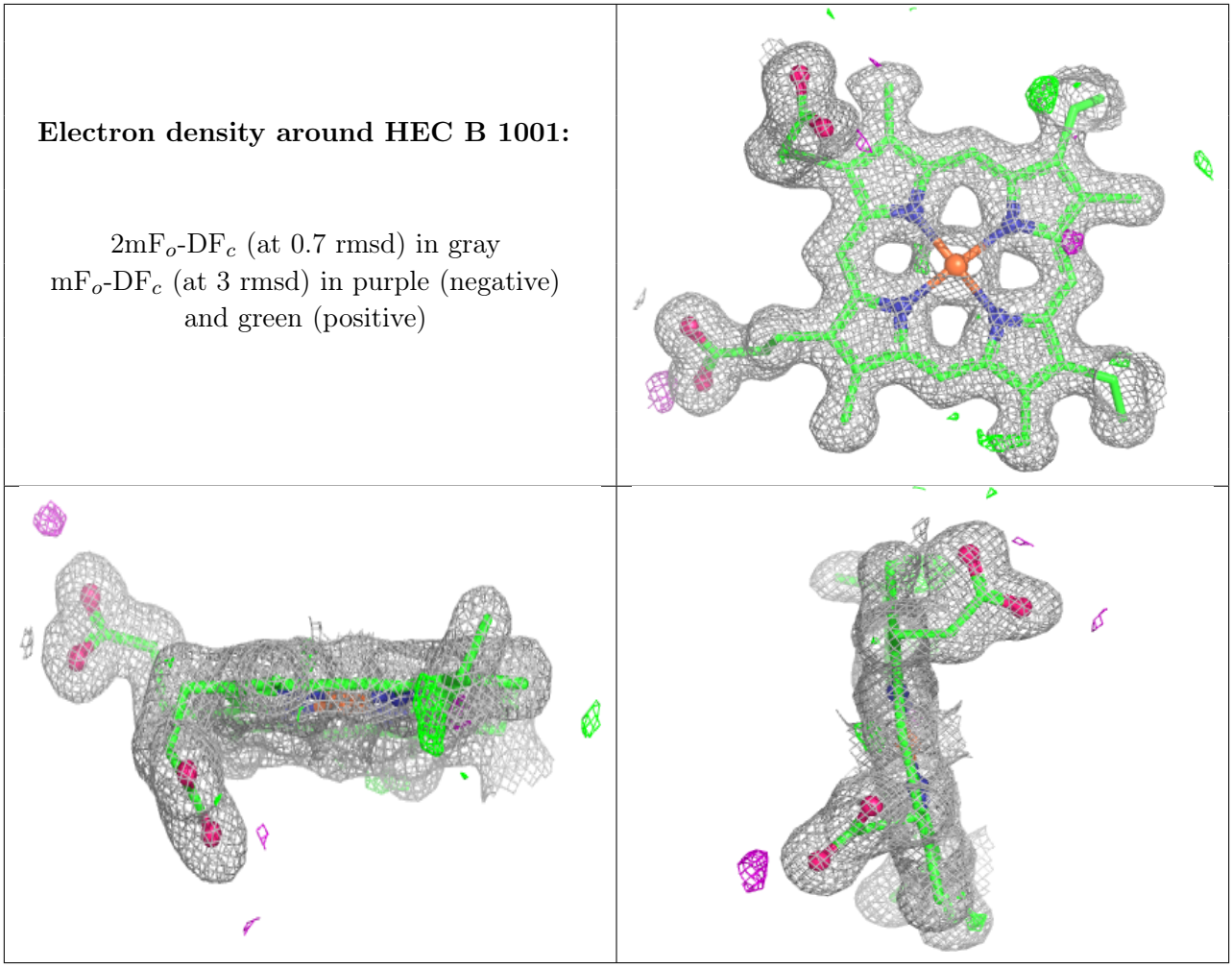
Electron density around HEC B 1003:

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



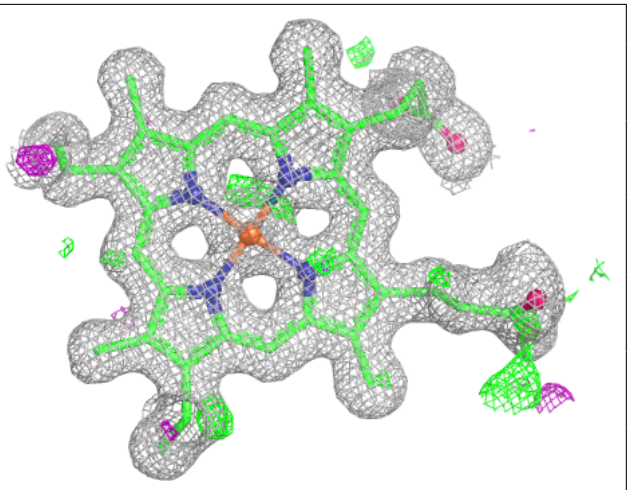
Electron density around HEC B 1001:

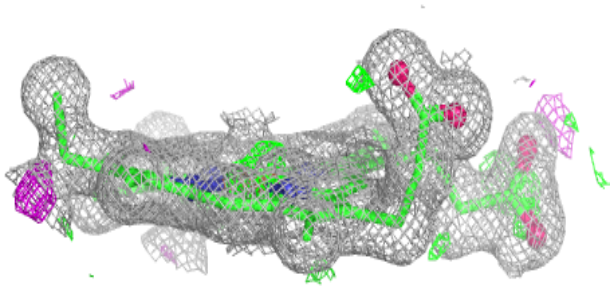
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

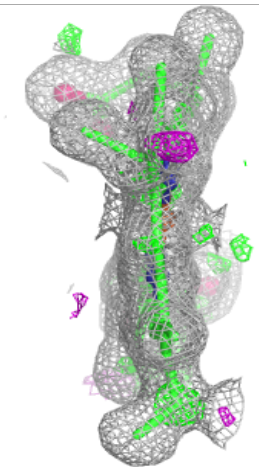


Electron density around HEC A 1005 (A):

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

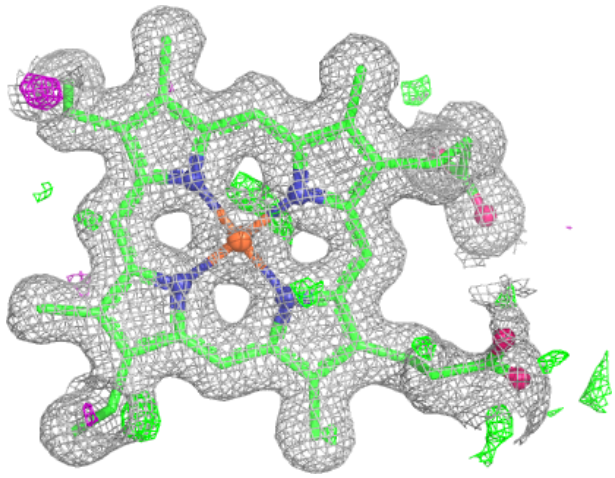


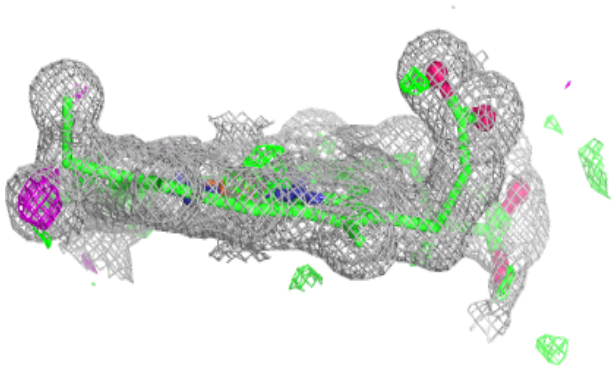


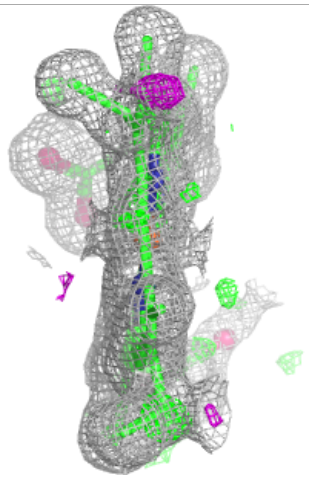


Electron density around HEC A 1005 (B):

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

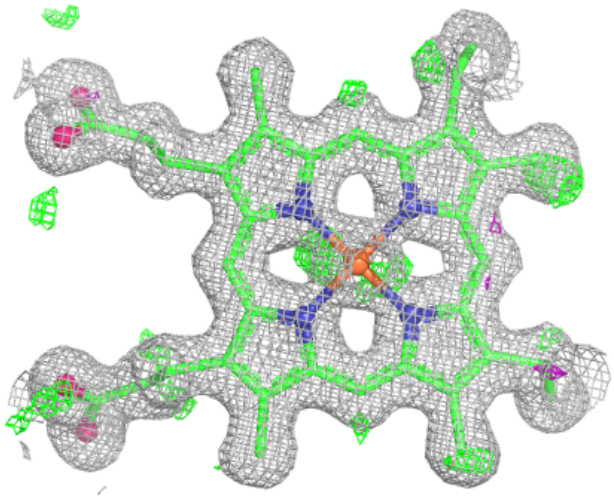


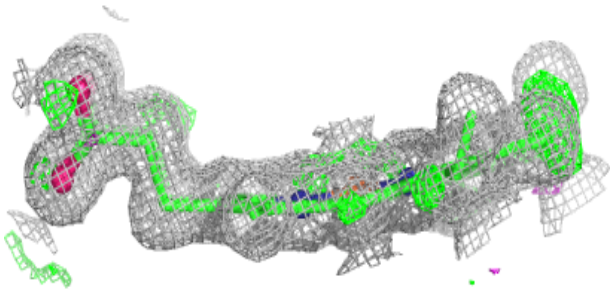


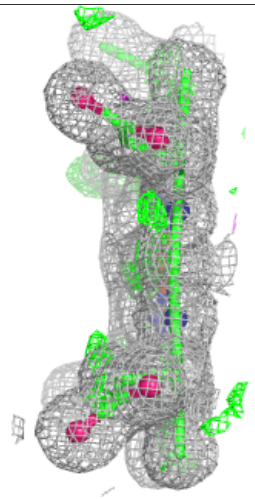


Electron density around HEC A 1006:

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

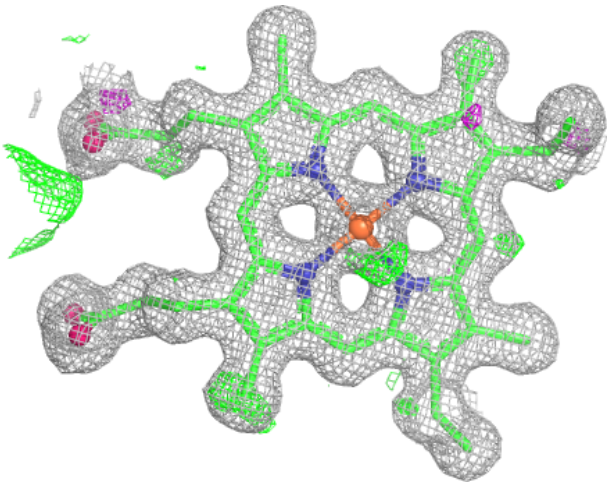


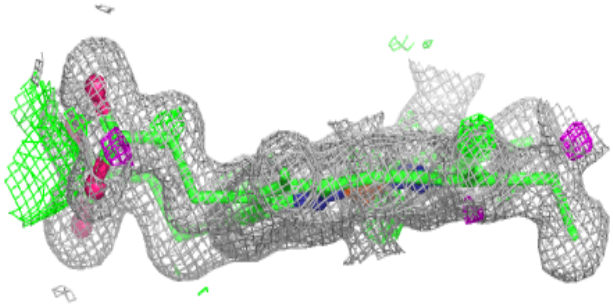


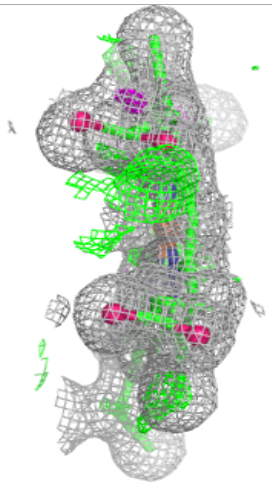


Electron density around HEC A 1007 (A):

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

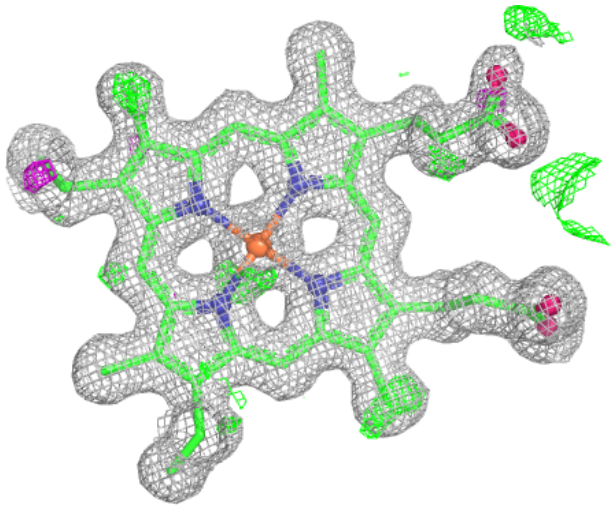


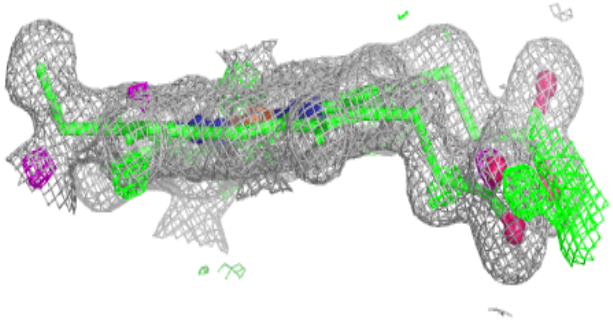


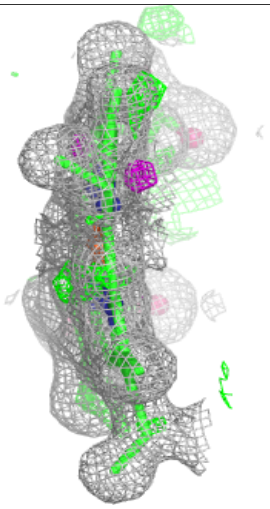


Electron density around HEC A 1007 (B):

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

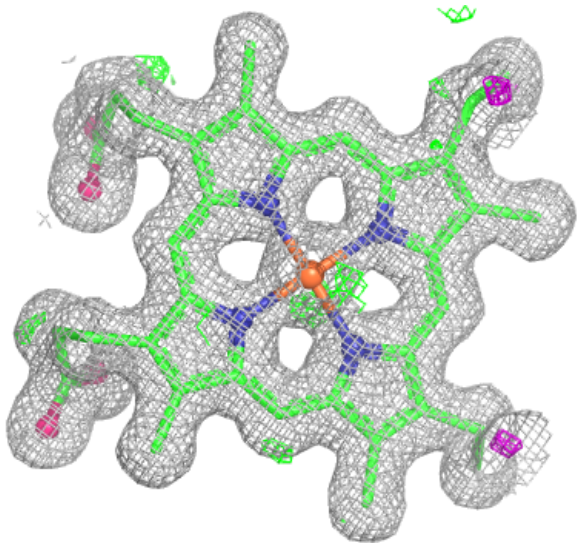


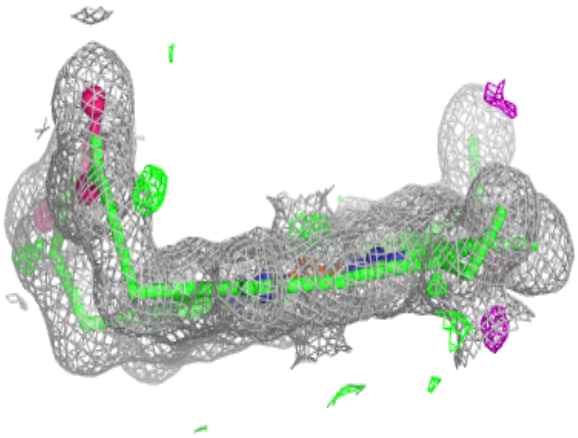


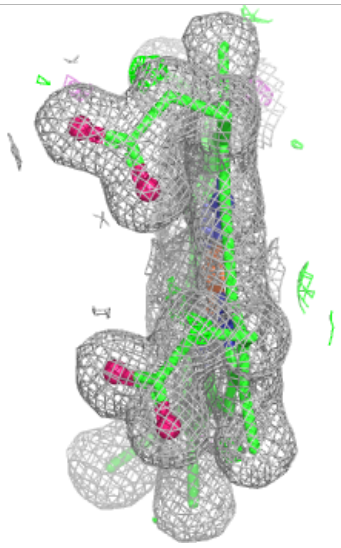


Electron density around HEC B 1004:

$2mF_o$-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

There are no such residues in this entry.