



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 PM UTC

PDB ID : 3FO3 / pdb_00003fo3
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase reduced by sodium dithionite (sulfite complex)
Authors : Trofimov, A.A.; 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 : 2008-12-27
Resolution : 1.40 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

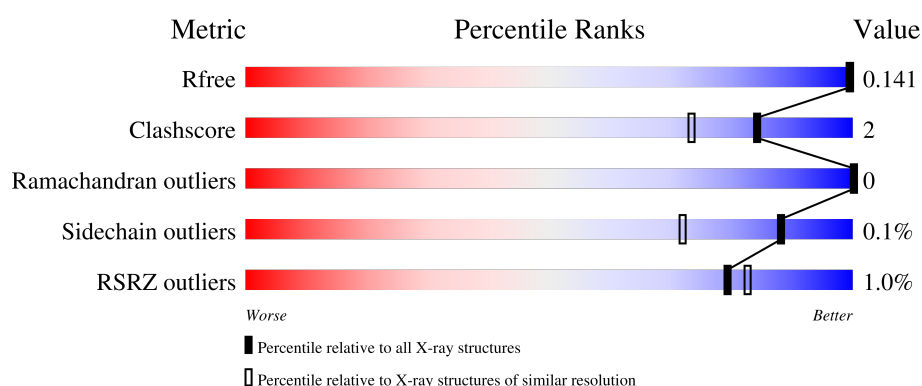
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

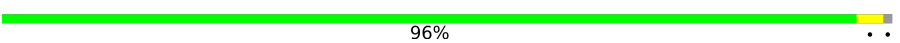
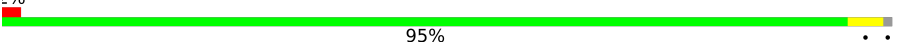
The reported resolution of this entry is 1.40 Å.

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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 $\leq 5\%$. 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	 96%
1	B	525	 95%

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
10	PG4	A	538[A]	-	X	-	-
10	PG4	B	547	-	-	X	-

2 Entry composition i

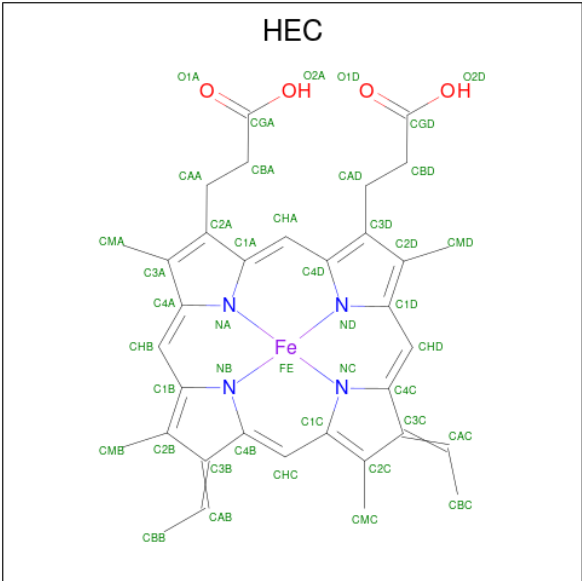
There are 12 unique types of molecules in this entry. The entry contains 16308 atoms, of which 5637 are hydrogens and 0 are deuteriums.

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	H	N	O	S	0	19	1
			6892	2580	2734	754	786	38			
1	B	519	Total	C	H	N	O	S	0	21	1
			6913	2591	2727	762	796	37			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



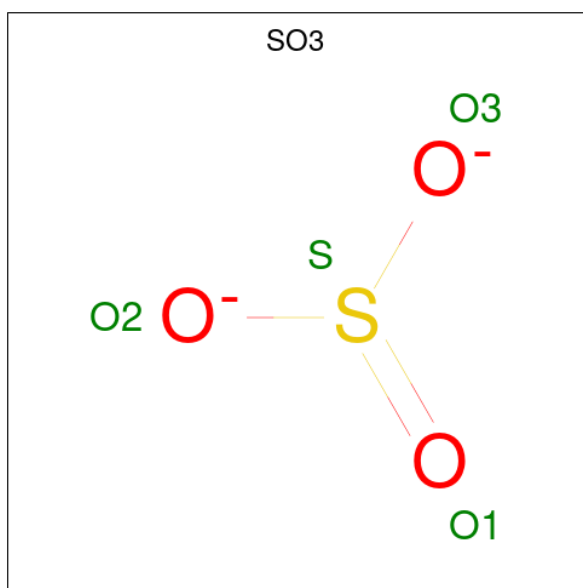
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	A	1	Total	C	Fe	H	N	O	0	1
			55	36	1	8	4	6		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	A	1	Total	C	Fe	H	N	O	0	1
			55	36	1	8	4	6		
2	A	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	1
			55	36	1	8	4	6		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		
2	B	1	Total	C	Fe	H	N	O	0	1
			55	36	1	8	4	6		
2	B	1	Total	C	Fe	H	N	O	0	0
			55	34	1	12	4	4		

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).

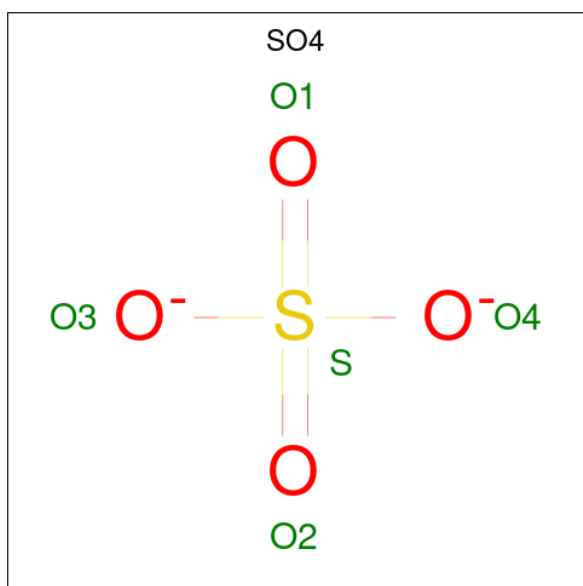


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 4 3 1	0	0
3	B	1	Total O S 4 3 1	0	0
3	B	1	Total O S 6 4 2	0	1

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

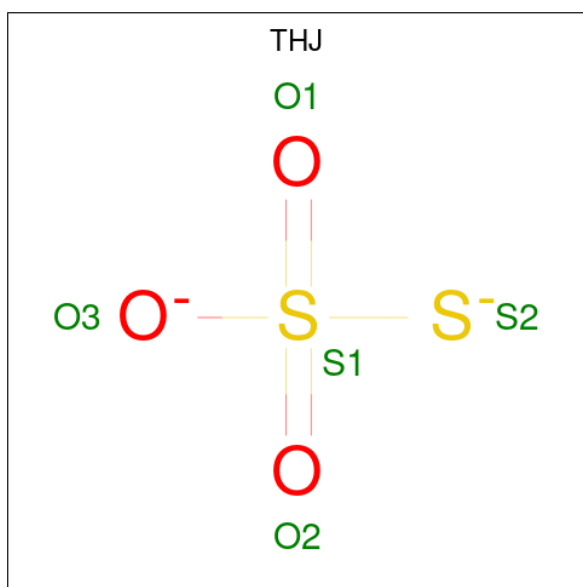
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is THIOSULFATE (CCD ID: THJ) (formula: O₃S₂).

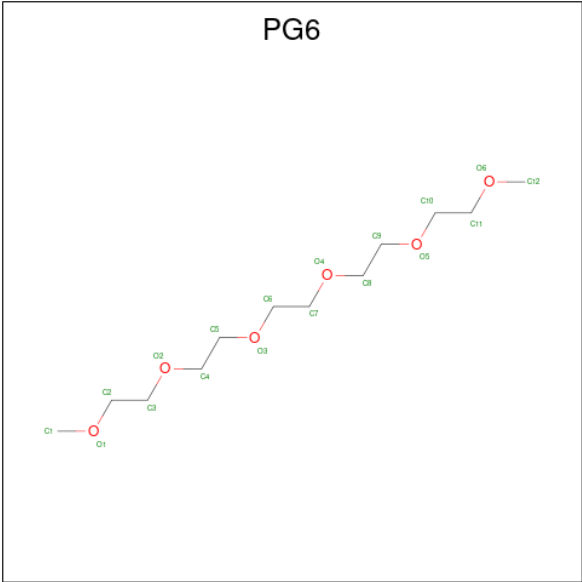


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	3	2		
6	B	1	Total	O	S	0	0
			5	3	2		

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

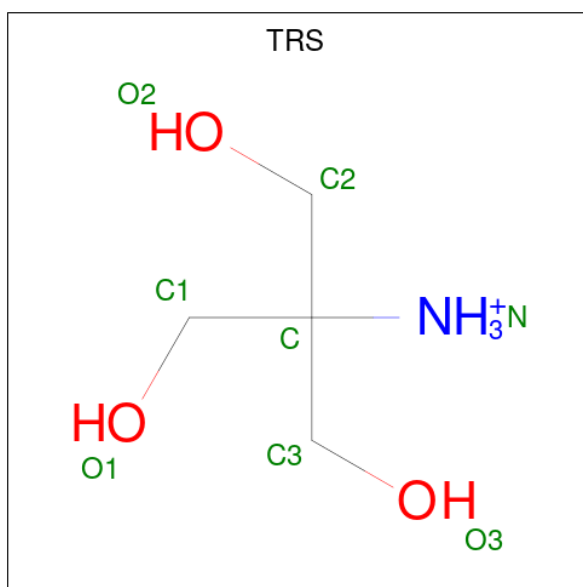
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Na	0	0
			2	2		
7	B	3	Total	Na	0	0
			3	3		

- Molecule 8 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



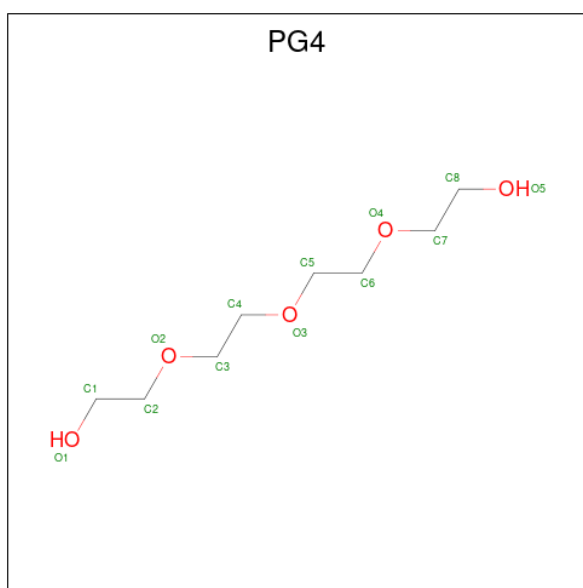
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	11	6		
8	A	1	Total	C	O	0	0
			8	5	3		
8	A	1	Total	C	O	0	0
			9	6	3		
8	A	1	Total	C	O	0	0
			5	3	2		
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			17	11	6		
8	B	1	Total	C	O	0	0
			8	5	3		
8	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



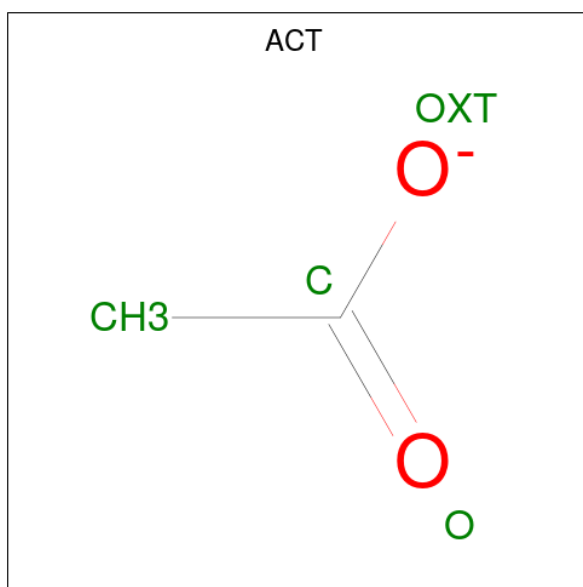
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 11 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

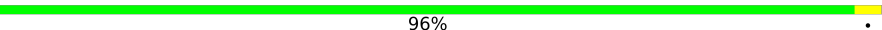
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	701	Total	O	0	0
			701	701		
12	B	684	Total	O	0	0
			684	684		

3 Residue-property plots [i](#)

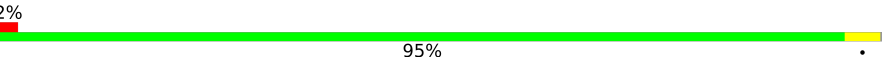
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

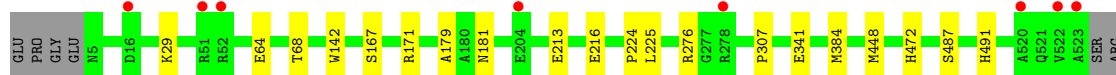
- Molecule 1: Eight-heme nitrite reductase

Chain A:  96%



- Molecule 1: Eight-heme nitrite reductase

Chain B:  95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	193.79Å 193.79Å 193.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.40 12.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (12.00-1.40) 99.4 (12.00-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.126 , 0.139 0.127 , 0.141	Depositor DCC
R_{free} test set	23479 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16308	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 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO3, TRS, NA, ACT, PG6, CA, PG4, SO4, HEC, THJ

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	0.70	0/4368	0.80	0/5922
1	B	0.71	0/4404	0.80	1/5968 (0.0%)
All	All	0.71	0/8772	0.80	1/11890 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	MET	CB-CA-C	-5.67	103.58	111.41

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	4158	2734	3865	10	0
1	B	4186	2727	3886	24	0
2	A	352	88	196	4	0
2	B	352	88	196	2	0
3	A	4	0	0	0	0
3	B	10	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
7	A	2	0	0	0	0
7	B	3	0	0	0	0
8	A	49	0	61	1	0
8	B	30	0	38	1	0
9	A	8	0	12	0	0
9	B	8	0	12	1	0
10	A	37	0	43	2	0
10	B	59	0	69	13	0
11	B	4	0	3	0	0
12	A	701	0	0	4	0
12	B	684	0	0	2	0
All	All	10671	5637	8381	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:B:181:ASN:HD22	10:B:547:PG4:H21	1.17	1.02
1:B:307:PRO:CD	10:B:547:PG4:H22	1.94	0.97
1:B:307:PRO:HD2	10:B:547:PG4:H22	1.48	0.95
1:B:181:ASN:ND2	10:B:547:PG4:H21	1.87	0.89
1:B:213[B]:GLU:OE1	1:B:216[B]:GLU:CD	2.28	0.77
1:B:307:PRO:HD3	10:B:547:PG4:H22	1.71	0.70
1:B:276:ARG:HD2	10:B:539:PG4:H11	1.74	0.70
1:B:171:ARG:NH2	10:B:541:PG4:O1	2.29	0.64
1:B:181:ASN:HD22	10:B:547:PG4:C2	2.04	0.58
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.87	0.57
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.87	0.56
1:A:174:SER:HA	10:A:539:PG4:H22	1.87	0.56
1:B:167:SER:HB2	1:B:216[B]:GLU:HG3	1.88	0.55
1:A:167:SER:HB2	1:A:216:GLU:HG2	1.88	0.55
1:B:213[B]:GLU:OE1	1:B:216[B]:GLU:OE2	2.26	0.54
1:B:142:TRP:CD2	10:B:536:PG4:H21	2.43	0.54
1:A:351:THR:HG23	8:A:543:PG6:H32	1.91	0.53
1:B:213[B]:GLU:OE1	1:B:216[B]:GLU:OE1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TRP:CE2	10:B:536:PG4:H21	2.45	0.52
2:A:1003[B]:HEC:HBA2	12:A:1041:HOH:O	2.09	0.51
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.92	0.51
1:B:307:PRO:HG2	10:B:537:PG4:H32	1.95	0.48
1:A:68[A]:THR:HG21	12:A:809:HOH:O	2.13	0.48
1:B:64:GLU:O	1:B:68[A]:THR:HG23	2.14	0.47
9:B:533:TRS:H22	12:B:659:HOH:O	2.15	0.46
2:A:1003[B]:HEC:CBA	12:A:1041:HOH:O	2.64	0.46
10:A:538[A]:PG4:H31	12:A:1217:HOH:O	2.16	0.45
1:B:29:LYS:HD2	2:B:1003[B]:HEC:HBA2	1.98	0.45
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.52	0.44
1:B:341:GLU:OE2	12:B:782:HOH:O	2.21	0.44
1:B:179:ALA:O	10:B:547:PG4:C1	2.66	0.43
1:A:457:ARG:NH2	6:A:530:THJ:S2	2.85	0.43
1:B:224:PRO:O	1:B:225:LEU:C	2.61	0.43
1:A:448:MET:HE1	1:A:472:HIS:CG	2.54	0.42
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.55	0.42
1:B:448:MET:HE1	1:B:472:HIS:CD2	2.55	0.41
1:A:34:ASN:HB2	8:B:535:PG6:H71	2.02	0.41
1:B:179:ALA:O	10:B:547:PG4:H12	2.21	0.40
1:A:224:PRO:O	1:A:225:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	537/525 (102%)	515 (96%)	22 (4%)	0	100	100
1	B	539/525 (103%)	517 (96%)	22 (4%)	0	100	100
All	All	1076/1050 (102%)	1032 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/443 (102%)	450 (99%)	3 (1%)	76	52
1	B	458/443 (103%)	458 (100%)	0	100	100
All	All	911/886 (103%)	908 (100%)	3 (0%)	88	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	MET
1	A	61[B]	MET
1	A	61[C]	MET

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	388	GLN
1	A	521	GLN
1	B	143	GLN
1	B	388	GLN
1	B	521	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 9 are monoatomic - leaving 56 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
8	PG6	A	543	-	9,9,17	0.52	0	8,8,16	0.43	0
2	HEC	B	1005	1	46,50,50	1.77	6 (13%)	58,82,82	1.84	3 (5%)
10	PG4	A	535	-	4,4,12	0.34	0	3,3,11	0.60	0
8	PG6	B	542	-	4,4,17	0.42	0	3,3,16	0.27	0
2	HEC	A	1004	3,1	46,50,50	1.65	5 (10%)	58,82,82	1.62	3 (5%)
10	PG4	A	538[B]	-	7,7,12	0.46	0	6,6,11	0.43	0
10	PG4	A	538[A]	-	7,4,12	21.50	1 (14%)	6,3,11	5.48	2 (33%)
2	HEC	B	1007[B]	4	46,50,50	1.76	7 (15%)	58,82,82	1.77	7 (12%)
2	HEC	B	1007[A]	-	46,50,50	1.76	7 (15%)	58,82,82	1.75	6 (10%)
10	PG4	A	539	-	5,5,12	0.46	0	4,4,11	0.51	0
6	THJ	A	530	-	3,4,4	0.76	0	2,6,6	0.04	0
2	HEC	A	1006	4,1	46,50,50	1.73	5 (10%)	58,82,82	1.79	3 (5%)
2	HEC	B	1006	4,1	46,50,50	1.72	4 (8%)	58,82,82	1.80	3 (5%)
5	SO4	A	529	-	4,4,4	0.53	0	6,6,6	0.72	0
10	PG4	B	537	-	9,9,12	0.45	0	8,8,11	0.29	0
2	HEC	B	1008	1	46,50,50	1.73	6 (13%)	58,82,82	1.80	4 (6%)
2	HEC	A	1002	1	46,50,50	1.68	3 (6%)	58,82,82	1.75	3 (5%)
6	THJ	B	530	-	3,4,4	0.69	0	2,6,6	0.11	0
9	TRS	A	533	-	7,7,7	0.34	0	9,9,9	1.08	1 (11%)
2	HEC	A	1003[B]	-	46,50,50	1.78	5 (10%)	58,82,82	1.70	7 (12%)
2	HEC	B	1003[B]	-	46,50,50	1.81	7 (15%)	58,82,82	1.69	5 (8%)
2	HEC	A	1003[A]	-	46,50,50	1.78	5 (10%)	58,82,82	1.69	7 (12%)
2	HEC	B	1003[A]	-	46,50,50	1.82	8 (17%)	58,82,82	1.66	6 (10%)
9	TRS	B	533	-	7,7,7	0.31	0	9,9,9	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PG4	B	547	-	6,6,12	0.31	0	5,5,11	0.97	0
10	PG4	A	540	-	5,5,12	0.46	0	4,4,11	0.26	0
10	PG4	B	540	-	3,3,12	0.30	0	2,2,11	0.43	0
10	PG4	B	539	-	4,4,12	0.41	0	3,3,11	0.30	0
2	HEC	A	1005	1	46,50,50	1.71	5 (10%)	58,82,82	1.73	3 (5%)
5	SO4	B	534	-	4,4,4	0.30	0	6,6,6	0.47	0
11	ACT	B	546	-	3,3,3	0.93	0	3,3,3	0.65	0
2	HEC	A	1001	1	46,50,50	1.75	6 (13%)	58,82,82	1.68	2 (3%)
2	HEC	A	1007[B]	4	46,50,50	1.70	6 (13%)	58,82,82	1.74	7 (12%)
10	PG4	B	544	-	4,4,12	0.48	0	3,3,11	0.20	0
10	PG4	B	536	-	7,7,12	0.42	0	6,6,11	0.72	0
3	SO3	B	529[B]	-	1,3,3	0.59	0	0,3,3	-	-
2	HEC	B	1001	1	46,50,50	1.86	6 (13%)	58,82,82	1.83	5 (8%)
3	SO3	B	529[A]	-	1,3,3	0.88	0	0,3,3	-	-
8	PG6	A	532	-	16,16,17	0.52	0	15,15,16	0.35	0
2	HEC	A	1007[A]	-	46,50,50	1.70	6 (13%)	58,82,82	1.73	6 (10%)
8	PG6	A	542	-	4,4,17	0.39	0	3,3,16	0.39	0
8	PG6	B	535	-	7,7,17	0.44	0	6,6,16	0.57	0
8	PG6	B	532	-	16,16,17	0.56	0	15,15,16	0.44	0
8	PG6	A	534	-	7,7,17	0.54	0	6,6,16	0.24	0
8	PG6	A	536	-	8,8,17	0.50	0	7,7,16	0.19	0
10	PG4	B	545	-	3,3,12	0.30	0	2,2,11	0.40	0
2	HEC	A	1008	1	46,50,50	1.78	6 (13%)	58,82,82	1.83	3 (5%)
2	HEC	B	1002	1	46,50,50	1.69	4 (8%)	58,82,82	1.81	4 (6%)
10	PG4	A	541	-	5,5,12	0.52	0	4,4,11	0.39	0
10	PG4	B	541	-	4,4,12	0.38	0	3,3,11	0.32	0
10	PG4	B	543	-	3,3,12	0.37	0	2,2,11	0.22	0
10	PG4	B	538	-	6,6,12	0.43	0	5,5,11	0.40	0
2	HEC	B	1004	3,1	46,50,50	1.74	6 (13%)	58,82,82	1.65	3 (5%)
10	PG4	A	537	-	3,3,12	0.36	0	2,2,11	0.39	0
3	SO3	A	526	2	1,3,3	1.97	0	0,3,3	-	-
3	SO3	B	526	2	1,3,3	2.19	1 (100%)	0,3,3	-	-

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
8	PG6	A	543	-	-	6/7/7/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1005	1	-	8/14/54/54	-
10	PG4	A	535	-	-	0/2/2/10	-
8	PG6	B	542	-	-	2/2/2/15	-
2	HEC	A	1004	3,1	-	6/14/54/54	-
10	PG4	A	538[B]	-	-	2/5/5/10	-
10	PG4	A	538[A]	-	-	4/5/2/10	-
2	HEC	B	1007[B]	4	-	5/14/54/54	-
2	HEC	B	1007[A]	-	-	4/14/54/54	-
10	PG4	A	539	-	-	1/3/3/10	-
2	HEC	A	1006	4,1	-	4/14/54/54	-
2	HEC	B	1006	4,1	-	4/14/54/54	-
10	PG4	B	537	-	-	3/7/7/10	-
2	HEC	B	1008	1	-	8/14/54/54	-
2	HEC	A	1002	1	-	6/14/54/54	-
9	TRS	A	533	-	-	6/9/9/9	-
2	HEC	A	1003[B]	-	-	8/14/54/54	-
2	HEC	B	1003[B]	-	-	6/14/54/54	-
2	HEC	A	1003[A]	-	-	6/14/54/54	-
2	HEC	B	1003[A]	-	-	6/14/54/54	-
9	TRS	B	533	-	-	9/9/9/9	-
10	PG4	B	547	-	-	3/4/4/10	-
10	PG4	A	540	-	-	2/3/3/10	-
10	PG4	B	540	-	-	0/1/1/10	-
10	PG4	B	539	-	-	1/2/2/10	-
2	HEC	A	1005	1	-	8/14/54/54	-
2	HEC	A	1001	1	-	8/14/54/54	-
2	HEC	A	1007[B]	4	-	4/14/54/54	-
10	PG4	B	544	-	-	1/2/2/10	-
10	PG4	B	536	-	-	4/5/5/10	-
2	HEC	B	1001	1	-	7/14/54/54	-
8	PG6	A	532	-	-	0/14/14/15	-
2	HEC	A	1007[A]	-	-	4/14/54/54	-
8	PG6	A	542	-	-	2/2/2/15	-
8	PG6	B	535	-	-	1/5/5/15	-
8	PG6	B	532	-	-	0/14/14/15	-
8	PG6	A	534	-	-	1/5/5/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PG6	A	536	-	-	4/6/6/15	-
10	PG4	B	545	-	-	1/1/1/10	-
2	HEC	A	1008	1	-	8/14/54/54	-
2	HEC	B	1002	1	-	6/14/54/54	-
10	PG4	A	541	-	-	1/3/3/10	-
10	PG4	B	541	-	-	0/2/2/10	-
10	PG4	B	543	-	-	1/1/1/10	-
10	PG4	B	538	-	-	4/4/4/10	-
2	HEC	B	1004	3,1	-	6/14/54/54	-
10	PG4	A	537	-	-	0/1/1/10	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	538[A]	PG4	O3-C5	56.88	3.88	1.42
2	B	1001	HEC	CAC-C3C	6.77	1.57	1.35
2	B	1008	HEC	CAC-C3C	6.76	1.57	1.35
2	B	1004	HEC	CAB-C3B	6.70	1.56	1.35
2	B	1005	HEC	CAC-C3C	6.63	1.56	1.35
2	B	1001	HEC	CAB-C3B	6.58	1.56	1.35
2	B	1006	HEC	CAB-C3B	6.56	1.56	1.35
2	B	1003[A]	HEC	CAB-C3B	6.53	1.56	1.35
2	B	1003[B]	HEC	CAB-C3B	6.53	1.56	1.35
2	A	1003[A]	HEC	CAB-C3B	6.51	1.56	1.35
2	A	1003[B]	HEC	CAB-C3B	6.51	1.56	1.35
2	A	1006	HEC	CAB-C3B	6.47	1.56	1.35
2	A	1008	HEC	CAC-C3C	6.46	1.56	1.35
2	A	1001	HEC	CAB-C3B	6.41	1.55	1.35
2	A	1004	HEC	CAB-C3B	6.41	1.55	1.35
2	A	1001	HEC	CAC-C3C	6.38	1.55	1.35
2	A	1005	HEC	CAB-C3B	6.35	1.55	1.35
2	B	1002	HEC	CAC-C3C	6.34	1.55	1.35
2	A	1005	HEC	CAC-C3C	6.31	1.55	1.35
2	A	1002	HEC	CAB-C3B	6.29	1.55	1.35
2	A	1002	HEC	CAC-C3C	6.29	1.55	1.35
2	A	1007[A]	HEC	CAC-C3C	6.28	1.55	1.35
2	A	1007[B]	HEC	CAC-C3C	6.28	1.55	1.35
2	B	1003[A]	HEC	CAC-C3C	6.22	1.55	1.35
2	B	1003[B]	HEC	CAC-C3C	6.22	1.55	1.35
2	B	1007[A]	HEC	CAC-C3C	6.21	1.55	1.35
2	B	1007[B]	HEC	CAC-C3C	6.21	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	HEC	CAB-C3B	6.20	1.55	1.35
2	A	1007[A]	HEC	CAB-C3B	6.19	1.55	1.35
2	A	1007[B]	HEC	CAB-C3B	6.19	1.55	1.35
2	B	1007[A]	HEC	CAB-C3B	6.11	1.54	1.35
2	B	1007[B]	HEC	CAB-C3B	6.11	1.54	1.35
2	A	1008	HEC	CAB-C3B	6.11	1.54	1.35
2	A	1006	HEC	CAC-C3C	6.09	1.54	1.35
2	B	1005	HEC	CAB-C3B	6.06	1.54	1.35
2	B	1006	HEC	CAC-C3C	5.91	1.54	1.35
2	A	1003[A]	HEC	CAC-C3C	5.77	1.53	1.35
2	A	1003[B]	HEC	CAC-C3C	5.77	1.53	1.35
2	B	1008	HEC	CAB-C3B	5.75	1.53	1.35
2	B	1004	HEC	CAC-C3C	5.72	1.53	1.35
2	A	1004	HEC	CAC-C3C	5.45	1.52	1.35
2	B	1001	HEC	C3D-C2D	4.35	1.50	1.38
2	A	1003[A]	HEC	C3D-C2D	3.97	1.49	1.38
2	A	1003[B]	HEC	C3D-C2D	3.97	1.49	1.38
2	B	1008	HEC	C3D-C2D	3.81	1.48	1.38
2	B	1003[A]	HEC	C3D-C2D	3.72	1.48	1.38
2	B	1003[B]	HEC	C3D-C2D	3.72	1.48	1.38
2	A	1008	HEC	C3D-C2D	3.28	1.47	1.38
2	A	1001	HEC	C3D-C2D	3.23	1.47	1.38
2	A	1002	HEC	C3D-C2D	3.12	1.47	1.38
2	A	1006	HEC	C3D-C2D	3.05	1.46	1.38
2	B	1002	HEC	C3D-C2D	3.04	1.46	1.38
2	B	1004	HEC	CMB-C2B	2.98	1.56	1.50
2	B	1006	HEC	C3D-C2D	2.97	1.46	1.38
2	A	1004	HEC	C3D-C2D	2.87	1.46	1.38
2	B	1001	HEC	CMC-C2C	2.73	1.56	1.50
2	A	1005	HEC	C3D-C2D	2.70	1.45	1.38
2	B	1005	HEC	C3D-C2D	2.70	1.45	1.38
2	B	1003[A]	HEC	CMB-C2B	2.69	1.56	1.50
2	B	1003[B]	HEC	CMB-C2B	2.69	1.56	1.50
2	A	1007[A]	HEC	C3D-C2D	2.68	1.45	1.38
2	A	1007[B]	HEC	C3D-C2D	2.68	1.45	1.38
2	A	1003[A]	HEC	CMB-C2B	2.63	1.56	1.50
2	A	1003[B]	HEC	CMB-C2B	2.63	1.56	1.50
2	B	1007[A]	HEC	CMB-C2B	2.58	1.56	1.50
2	B	1007[B]	HEC	CMB-C2B	2.58	1.56	1.50
2	A	1008	HEC	CMC-C2C	2.55	1.56	1.50
2	B	1004	HEC	C3D-C2D	2.54	1.45	1.38
2	B	1007[A]	HEC	C3D-C2D	2.51	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1007[B]	HEC	C3D-C2D	2.51	1.45	1.38
2	B	1002	HEC	CMB-C2B	2.51	1.55	1.50
2	A	1006	HEC	CMC-C2C	2.50	1.55	1.50
2	A	1001	HEC	CMB-C2B	2.45	1.55	1.50
2	B	1004	HEC	CMC-C2C	2.44	1.55	1.50
2	B	1005	HEC	CMA-C3A	2.40	1.55	1.50
2	B	1008	HEC	CMB-C2B	2.35	1.55	1.50
2	A	1004	HEC	CMB-C2B	2.35	1.55	1.50
2	B	1007[A]	HEC	CBB-CAB	2.34	1.58	1.49
2	B	1007[B]	HEC	CBB-CAB	2.34	1.58	1.49
2	B	1004	HEC	C1B-C2B	2.33	1.48	1.43
2	A	1006	HEC	CBB-CAB	2.33	1.58	1.49
2	A	1007[A]	HEC	C3B-C2B	-2.31	1.33	1.41
2	A	1007[B]	HEC	C3B-C2B	-2.31	1.33	1.41
2	A	1005	HEC	CMB-C2B	2.29	1.55	1.50
2	A	1008	HEC	C3B-C2B	-2.22	1.33	1.41
2	B	1005	HEC	CMB-C2B	2.20	1.55	1.50
3	B	526	SO3	O1-S	2.19	1.53	1.44
2	A	1004	HEC	CMC-C2C	2.15	1.55	1.50
2	B	1005	HEC	CBB-CAB	2.15	1.57	1.49
2	A	1001	HEC	O2A-CGA	-2.14	1.23	1.30
2	B	1007[A]	HEC	C1B-C2B	2.12	1.48	1.43
2	B	1007[B]	HEC	C1B-C2B	2.12	1.48	1.43
2	A	1003[A]	HEC	C3C-C2C	-2.11	1.34	1.41
2	A	1003[B]	HEC	C3C-C2C	-2.11	1.34	1.41
2	B	1003[A]	HEC	O1A-CGA	2.09	1.28	1.22
2	B	1003[A]	HEC	CBB-CAB	2.04	1.57	1.49
2	B	1003[B]	HEC	CBB-CAB	2.04	1.57	1.49
2	B	1007[A]	HEC	C3B-C2B	-2.04	1.34	1.41
2	B	1007[B]	HEC	C3B-C2B	-2.04	1.34	1.41
2	B	1001	HEC	C3C-C2C	-2.04	1.34	1.41
2	A	1005	HEC	CBB-CAB	2.03	1.57	1.49
2	B	1003[A]	HEC	CMD-C2D	2.03	1.54	1.50
2	B	1003[B]	HEC	CMD-C2D	2.03	1.54	1.50
2	A	1007[A]	HEC	CBB-CAB	2.02	1.57	1.49
2	A	1007[B]	HEC	CBB-CAB	2.02	1.57	1.49
2	A	1008	HEC	CBB-CAB	2.01	1.56	1.49
2	B	1008	HEC	C3B-C2B	-2.01	1.34	1.41
2	B	1001	HEC	CMA-C3A	2.01	1.54	1.50
2	A	1001	HEC	C3B-C2B	-2.01	1.34	1.41
2	A	1007[A]	HEC	CMB-C2B	2.01	1.54	1.50
2	A	1007[B]	HEC	CMB-C2B	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003[A]	HEC	C3B-C2B	-2.01	1.34	1.41
2	B	1003[B]	HEC	C3B-C2B	-2.01	1.34	1.41
2	B	1008	HEC	CBB-CAB	2.00	1.56	1.49
2	B	1006	HEC	C2A-C3A	-2.00	1.32	1.36

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	538[A]	PG4	C5-O3-C4	-12.94	56.63	113.26
2	A	1008	HEC	CBB-CAB-C3B	-10.80	105.84	127.43
2	B	1008	HEC	CBB-CAB-C3B	-10.65	106.16	127.43
2	B	1005	HEC	CBB-CAB-C3B	-10.19	107.07	127.43
2	B	1006	HEC	CBB-CAB-C3B	-9.63	108.18	127.43
2	A	1005	HEC	CBB-CAB-C3B	-9.47	108.51	127.43
2	B	1001	HEC	CBB-CAB-C3B	-9.39	108.66	127.43
2	A	1006	HEC	CBB-CAB-C3B	-9.30	108.84	127.43
2	A	1003[A]	HEC	CBB-CAB-C3B	-9.23	109.00	127.43
2	A	1003[B]	HEC	CBB-CAB-C3B	-9.23	109.00	127.43
2	B	1007[A]	HEC	CBB-CAB-C3B	-9.14	109.17	127.43
2	B	1007[B]	HEC	CBB-CAB-C3B	-9.14	109.17	127.43
2	A	1004	HEC	CBB-CAB-C3B	-8.98	109.48	127.43
2	B	1004	HEC	CBB-CAB-C3B	-8.92	109.61	127.43
2	B	1003[A]	HEC	CBB-CAB-C3B	-8.82	109.80	127.43
2	B	1003[B]	HEC	CBB-CAB-C3B	-8.82	109.80	127.43
2	B	1002	HEC	CBB-CAB-C3B	-8.80	109.84	127.43
2	A	1007[A]	HEC	CBB-CAB-C3B	-8.68	110.08	127.43
2	A	1007[B]	HEC	CBB-CAB-C3B	-8.68	110.08	127.43
2	A	1002	HEC	CBB-CAB-C3B	-8.67	110.10	127.43
2	A	1001	HEC	CBB-CAB-C3B	-8.66	110.13	127.43
2	B	1002	HEC	CBC-CAC-C3C	-7.46	112.53	127.43
2	A	1002	HEC	CBC-CAC-C3C	-7.33	112.78	127.43
2	A	1006	HEC	CBC-CAC-C3C	-6.92	113.60	127.43
2	B	1006	HEC	CBC-CAC-C3C	-6.64	114.17	127.43
2	B	1004	HEC	CBC-CAC-C3C	-6.60	114.25	127.43
2	A	1001	HEC	CBC-CAC-C3C	-6.50	114.43	127.43
2	B	1005	HEC	CBC-CAC-C3C	-6.46	114.52	127.43
2	A	1007[A]	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
2	A	1007[B]	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
2	B	1001	HEC	CBC-CAC-C3C	-6.15	115.14	127.43
2	A	1005	HEC	CBC-CAC-C3C	-5.84	115.75	127.43
2	A	1004	HEC	CBC-CAC-C3C	-5.79	115.85	127.43
2	B	1007[A]	HEC	CBC-CAC-C3C	-5.61	116.23	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1007[B]	HEC	CBC-CAC-C3C	-5.61	116.23	127.43
2	B	1008	HEC	CBC-CAC-C3C	-5.10	117.25	127.43
2	A	1008	HEC	CBC-CAC-C3C	-4.69	118.05	127.43
2	A	1003[A]	HEC	CBC-CAC-C3C	-4.31	118.81	127.43
2	A	1003[B]	HEC	CBC-CAC-C3C	-4.31	118.81	127.43
2	B	1003[B]	HEC	CAA-CBA-CGA	-4.27	102.33	113.67
2	B	1003[A]	HEC	CBC-CAC-C3C	-4.18	119.08	127.43
2	B	1003[B]	HEC	CBC-CAC-C3C	-4.18	119.08	127.43
2	A	1003[B]	HEC	CBA-CAA-C2A	3.59	122.45	112.53
10	A	538[A]	PG4	O3-C5-C6	3.51	125.58	110.11
2	A	1007[A]	HEC	CMB-C2B-C1B	-3.37	120.29	125.42
2	A	1007[B]	HEC	CMB-C2B-C1B	-3.37	120.29	125.42
2	B	1003[A]	HEC	CBA-CAA-C2A	-3.08	104.02	112.53
2	A	1003[A]	HEC	O2A-CGA-CBA	3.08	123.72	114.00
2	B	1007[A]	HEC	CMB-C2B-C1B	-3.05	120.77	125.42
2	B	1007[B]	HEC	CMB-C2B-C1B	-3.05	120.77	125.42
2	A	1005	HEC	CMB-C2B-C1B	-3.03	120.81	125.42
2	B	1002	HEC	CAA-CBA-CGA	-2.87	106.06	113.67
2	B	1003[A]	HEC	CMB-C2B-C1B	-2.74	121.25	125.42
2	B	1003[B]	HEC	CMB-C2B-C1B	-2.74	121.25	125.42
2	A	1003[A]	HEC	CMB-C2B-C1B	-2.61	121.45	125.42
2	A	1003[B]	HEC	CMB-C2B-C1B	-2.61	121.45	125.42
2	B	1001	HEC	C4D-C3D-C2D	-2.61	102.83	106.87
2	A	1002	HEC	CAA-CBA-CGA	-2.59	106.79	113.67
2	B	1006	HEC	CAD-C3D-C4D	2.52	129.86	124.94
2	A	1008	HEC	CMB-C2B-C1B	-2.52	121.58	125.42
2	A	1003[B]	HEC	CAA-CBA-CGA	-2.49	107.05	113.67
2	B	1007[A]	HEC	CMD-C2D-C1D	2.49	129.21	125.42
2	B	1007[B]	HEC	CMD-C2D-C1D	2.49	129.21	125.42
2	A	1007[B]	HEC	O2A-CGA-CBA	2.46	121.78	114.00
2	A	1006	HEC	CAD-C3D-C4D	2.44	129.70	124.94
2	B	1008	HEC	C4D-ND-C1D	2.42	109.77	105.82
2	B	1007[B]	HEC	O2A-CGA-CBA	2.42	121.63	114.00
9	A	533	TRS	O2-C2-C	2.35	117.42	110.88
2	A	1007[A]	HEC	O2A-CGA-CBA	2.34	121.40	114.00
2	B	1008	HEC	CMB-C2B-C1B	-2.31	121.91	125.42
2	A	1007[A]	HEC	CAD-C3D-C4D	2.31	129.44	124.94
2	A	1007[B]	HEC	CAD-C3D-C4D	2.31	129.44	124.94
2	B	1003[A]	HEC	O1A-CGA-CBA	-2.25	115.97	123.09
2	A	1003[A]	HEC	O1A-CGA-CBA	-2.22	116.06	123.09
2	A	1003[A]	HEC	CBA-CAA-C2A	-2.22	106.40	112.53
2	A	1003[A]	HEC	O2D-CGD-CBD	2.17	120.84	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003[B]	HEC	O2D-CGD-CBD	2.17	120.84	114.00
2	B	1002	HEC	CAD-C3D-C4D	2.16	129.16	124.94
2	B	1005	HEC	CMB-C2B-C1B	-2.14	122.15	125.42
2	B	1007[B]	HEC	O1A-CGA-CBA	-2.13	116.34	123.09
2	A	1004	HEC	CAD-C3D-C4D	2.12	129.08	124.94
2	B	1001	HEC	CAD-C3D-C4D	2.11	129.06	124.94
2	B	1004	HEC	CAD-C3D-C4D	2.11	129.06	124.94
2	B	1003[A]	HEC	O2D-CGD-CBD	2.10	120.64	114.00
2	B	1003[B]	HEC	O2D-CGD-CBD	2.10	120.64	114.00
2	B	1001	HEC	CMC-C2C-C1C	-2.09	122.24	125.42
2	A	1007[A]	HEC	CMD-C2D-C1D	2.08	128.59	125.42
2	A	1007[B]	HEC	CMD-C2D-C1D	2.08	128.59	125.42
2	A	1007[B]	HEC	O1A-CGA-CBA	-2.03	116.67	123.09
2	B	1007[A]	HEC	O2A-CGA-CBA	2.03	120.40	114.00
2	A	1003[B]	HEC	O2A-CGA-CBA	2.02	120.40	114.00
2	B	1007[A]	HEC	CAD-C3D-C4D	2.02	128.88	124.94
2	B	1007[B]	HEC	CAD-C3D-C4D	2.02	128.88	124.94

There are no chirality outliers.

All (181) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	A	1004	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C2C-C3C-CAC-CBC
2	A	1004	HEC	C4C-C3C-CAC-CBC
2	A	1005	HEC	C2B-C3B-CAB-CBB
2	A	1005	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	C2C-C3C-CAC-CBC
2	A	1005	HEC	C4C-C3C-CAC-CBC
2	A	1006	HEC	C2B-C3B-CAB-CBB
2	A	1006	HEC	C4B-C3B-CAB-CBB
2	A	1006	HEC	C2C-C3C-CAC-CBC
2	A	1006	HEC	C4C-C3C-CAC-CBC
2	A	1007[A]	HEC	C2B-C3B-CAB-CBB
2	A	1007[A]	HEC	C4B-C3B-CAB-CBB
2	A	1007[A]	HEC	C2C-C3C-CAC-CBC
2	A	1007[A]	HEC	C4C-C3C-CAC-CBC
2	A	1007[B]	HEC	C2B-C3B-CAB-CBB
2	A	1007[B]	HEC	C4B-C3B-CAB-CBB
2	A	1007[B]	HEC	C2C-C3C-CAC-CBC
2	A	1007[B]	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	A	1008	HEC	C2B-C3B-CAB-CBB
2	A	1008	HEC	C4B-C3B-CAB-CBB
2	A	1008	HEC	C2C-C3C-CAC-CBC
2	A	1008	HEC	C4C-C3C-CAC-CBC
2	A	1002	HEC	C2B-C3B-CAB-CBB
2	A	1002	HEC	C4B-C3B-CAB-CBB
2	A	1002	HEC	C2C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	A	1003[A]	HEC	C2B-C3B-CAB-CBB
2	A	1003[A]	HEC	C4B-C3B-CAB-CBB
2	A	1003[A]	HEC	C2C-C3C-CAC-CBC
2	A	1003[A]	HEC	C4C-C3C-CAC-CBC
2	A	1003[B]	HEC	C2B-C3B-CAB-CBB
2	A	1003[B]	HEC	C4B-C3B-CAB-CBB
2	A	1003[B]	HEC	C2C-C3C-CAC-CBC
2	A	1003[B]	HEC	C4C-C3C-CAC-CBC
2	A	1001	HEC	C2B-C3B-CAB-CBB
2	A	1001	HEC	C4B-C3B-CAB-CBB
2	A	1001	HEC	C2C-C3C-CAC-CBC
2	A	1001	HEC	C4C-C3C-CAC-CBC
2	B	1004	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C4B-C3B-CAB-CBB
2	B	1004	HEC	C2C-C3C-CAC-CBC
2	B	1004	HEC	C4C-C3C-CAC-CBC
2	B	1005	HEC	C2B-C3B-CAB-CBB
2	B	1005	HEC	C4B-C3B-CAB-CBB
2	B	1005	HEC	C2C-C3C-CAC-CBC
2	B	1005	HEC	C4C-C3C-CAC-CBC
2	B	1006	HEC	C2B-C3B-CAB-CBB
2	B	1006	HEC	C4B-C3B-CAB-CBB
2	B	1006	HEC	C2C-C3C-CAC-CBC
2	B	1006	HEC	C4C-C3C-CAC-CBC
2	B	1007[A]	HEC	C2B-C3B-CAB-CBB
2	B	1007[A]	HEC	C4B-C3B-CAB-CBB
2	B	1007[A]	HEC	C2C-C3C-CAC-CBC
2	B	1007[A]	HEC	C4C-C3C-CAC-CBC
2	B	1007[B]	HEC	C2B-C3B-CAB-CBB
2	B	1007[B]	HEC	C4B-C3B-CAB-CBB
2	B	1007[B]	HEC	C2C-C3C-CAC-CBC
2	B	1007[B]	HEC	C4C-C3C-CAC-CBC
2	B	1008	HEC	C2B-C3B-CAB-CBB
2	B	1008	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	1008	HEC	C2C-C3C-CAC-CBC
2	B	1008	HEC	C4C-C3C-CAC-CBC
2	B	1002	HEC	C2B-C3B-CAB-CBB
2	B	1002	HEC	C4B-C3B-CAB-CBB
2	B	1002	HEC	C2C-C3C-CAC-CBC
2	B	1002	HEC	C4C-C3C-CAC-CBC
2	B	1003[A]	HEC	C2B-C3B-CAB-CBB
2	B	1003[A]	HEC	C4B-C3B-CAB-CBB
2	B	1003[A]	HEC	C2C-C3C-CAC-CBC
2	B	1003[A]	HEC	C4C-C3C-CAC-CBC
2	B	1003[B]	HEC	C2B-C3B-CAB-CBB
2	B	1003[B]	HEC	C4B-C3B-CAB-CBB
2	B	1003[B]	HEC	C2C-C3C-CAC-CBC
2	B	1003[B]	HEC	C4C-C3C-CAC-CBC
2	B	1001	HEC	C2B-C3B-CAB-CBB
2	B	1001	HEC	C4B-C3B-CAB-CBB
2	B	1001	HEC	C2C-C3C-CAC-CBC
2	B	1001	HEC	C4C-C3C-CAC-CBC
9	A	533	TRS	C3-C-C2-O2
9	A	533	TRS	N-C-C2-O2
9	B	533	TRS	C2-C-C1-O1
9	B	533	TRS	C3-C-C1-O1
9	B	533	TRS	C1-C-C3-O3
2	A	1003[B]	HEC	C1A-C2A-CAA-CBA
8	A	543	PG6	O2-C4-C5-O3
10	A	538[A]	PG4	O2-C3-C4-O3
10	B	547	PG4	O1-C1-C2-O2
10	B	537	PG4	O2-C3-C4-O3
8	A	536	PG6	O2-C4-C5-O3
8	A	536	PG6	O1-C2-C3-O2
10	B	539	PG4	O1-C1-C2-O2
10	A	538[B]	PG4	O2-C3-C4-O3
8	A	543	PG6	O1-C2-C3-O2
8	A	543	PG6	O3-C6-C7-O4
10	B	536	PG4	O2-C3-C4-O3
2	A	1003[B]	HEC	C3A-C2A-CAA-CBA
8	B	542	PG6	O1-C2-C3-O2
10	A	540	PG4	O1-C1-C2-O2
10	A	538[A]	PG4	C6-C5-O3-C4
9	B	533	TRS	C2-C-C3-O3
10	B	537	PG4	O3-C5-C6-O4
10	B	545	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	542	PG6	O1-C2-C3-O2
10	B	538	PG4	O2-C3-C4-O3
8	B	535	PG6	C4-C5-O3-C6
10	B	536	PG4	C1-C2-O2-C3
10	A	539	PG4	C4-C3-O2-C2
9	A	533	TRS	C1-C-C2-O2
9	A	533	TRS	C2-C-C3-O3
9	B	533	TRS	N-C-C1-O1
9	B	533	TRS	C3-C-C2-O2
9	B	533	TRS	N-C-C3-O3
8	A	536	PG6	C3-C2-O1-C1
10	B	536	PG4	C3-C4-O3-C5
10	B	544	PG4	C4-C3-O2-C2
10	B	538	PG4	C1-C2-O2-C3
10	A	541	PG4	C4-C3-O2-C2
8	A	543	PG6	C7-C6-O3-C5
10	A	538[B]	PG4	C3-C4-O3-C5
10	B	537	PG4	C6-C5-O3-C4
10	A	538[A]	PG4	O3-C5-C6-O4
10	B	547	PG4	C4-C3-O2-C2
9	A	533	TRS	C1-C-C3-O3
9	B	533	TRS	C1-C-C2-O2
10	B	538	PG4	O1-C1-C2-O2
8	A	543	PG6	C2-C3-O2-C4
8	A	534	PG6	C2-C3-O2-C4
10	B	538	PG4	C4-C3-O2-C2
2	B	1004	HEC	CAA-CBA-CGA-O1A
9	A	533	TRS	N-C-C3-O3
9	B	533	TRS	N-C-C2-O2
2	A	1005	HEC	CAA-CBA-CGA-O2A
2	A	1002	HEC	CAA-CBA-CGA-O1A
2	B	1002	HEC	CAA-CBA-CGA-O1A
2	B	1005	HEC	CAA-CBA-CGA-O2A
2	A	1004	HEC	CAA-CBA-CGA-O1A
8	A	543	PG6	C5-C4-O2-C3
2	A	1005	HEC	CAA-CBA-CGA-O1A
8	B	542	PG6	C3-C2-O1-C1
10	A	538[A]	PG4	C4-C3-O2-C2
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O1A
2	B	1004	HEC	CAA-CBA-CGA-O2A
2	B	1005	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	1008	HEC	CAD-CBD-CGD-O1D
8	A	542	PG6	C3-C2-O1-C1
2	A	1002	HEC	CAA-CBA-CGA-O2A
2	B	1002	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAD-CBD-CGD-O1D
2	A	1008	HEC	CAD-CBD-CGD-O2D
2	A	1001	HEC	CAD-CBD-CGD-O2D
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	A	1001	HEC	CAA-CBA-CGA-O2A
2	B	1008	HEC	CAA-CBA-CGA-O2A
2	B	1003[A]	HEC	CAA-CBA-CGA-O1A
2	B	1003[A]	HEC	CAA-CBA-CGA-O2A
10	B	547	PG4	C1-C2-O2-C3
8	A	536	PG6	C2-C3-O2-C4
2	B	1003[B]	HEC	CAA-CBA-CGA-O2A
2	B	1008	HEC	CAD-CBD-CGD-O2D
2	B	1001	HEC	CAD-CBD-CGD-O1D
10	A	540	PG4	C4-C3-O2-C2
2	B	1008	HEC	CAD-CBD-CGD-O1D
2	B	1005	HEC	CAD-CBD-CGD-O2D
2	B	1005	HEC	CAD-CBD-CGD-O1D
2	A	1008	HEC	CAA-CBA-CGA-O2A
2	A	1008	HEC	CAA-CBA-CGA-O1A
2	A	1003[A]	HEC	CAA-CBA-CGA-O2A
10	B	543	PG4	O1-C1-C2-O2
2	A	1003[A]	HEC	CAA-CBA-CGA-O1A
2	A	1005	HEC	CAD-CBD-CGD-O2D
2	B	1003[B]	HEC	CAA-CBA-CGA-O1A
2	A	1005	HEC	CAD-CBD-CGD-O1D
2	B	1008	HEC	CAA-CBA-CGA-O1A
2	A	1003[B]	HEC	CAA-CBA-CGA-O2A
10	B	536	PG4	C4-C3-O2-C2
2	B	1007[B]	HEC	CAA-CBA-CGA-O2A
2	A	1003[B]	HEC	CAA-CBA-CGA-O1A
2	B	1001	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

15 monomers are involved in 25 short contacts:

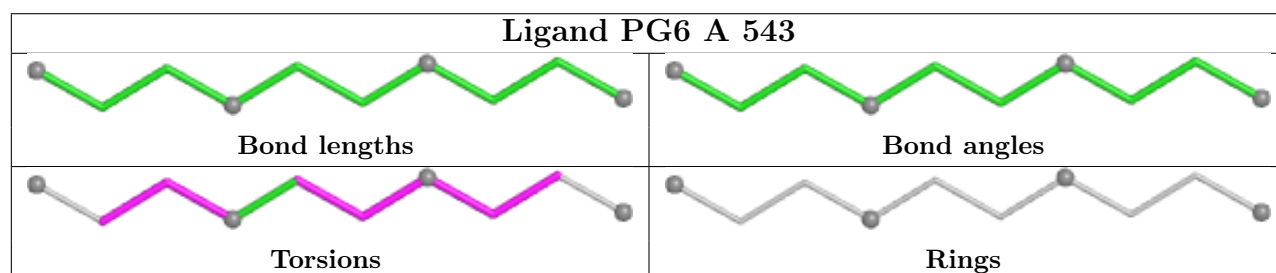
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	543	PG6	1	0
10	A	538[A]	PG4	1	0

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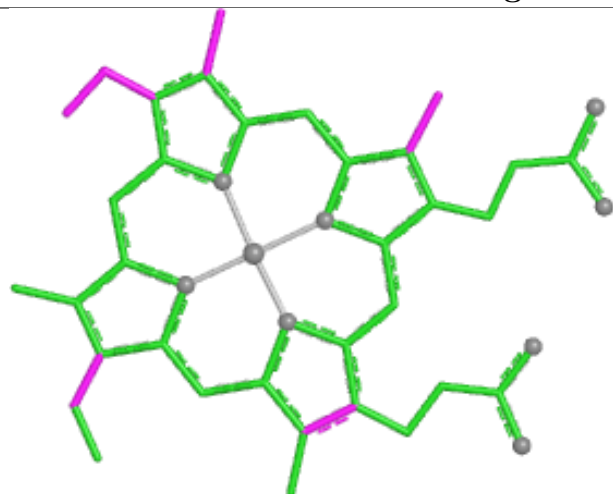
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	539	PG4	1	0
6	A	530	THJ	1	0
10	B	537	PG4	1	0
2	A	1002	HEC	1	0
2	A	1003[B]	HEC	3	0
2	B	1003[B]	HEC	1	0
9	B	533	TRS	1	0
10	B	547	PG4	8	0
10	B	539	PG4	1	0
10	B	536	PG4	2	0
8	B	535	PG6	1	0
2	B	1002	HEC	1	0
10	B	541	PG4	1	0

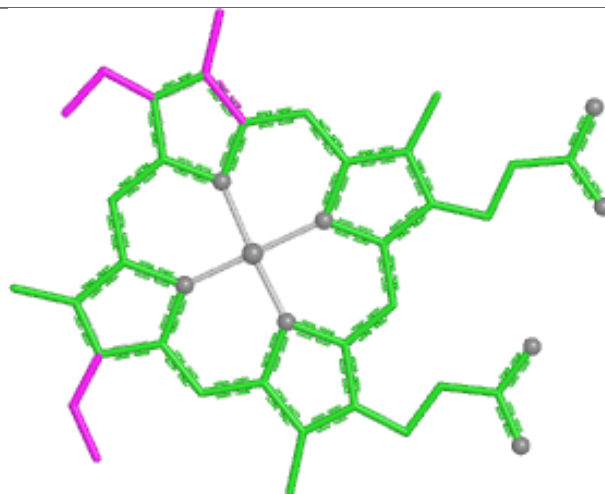
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



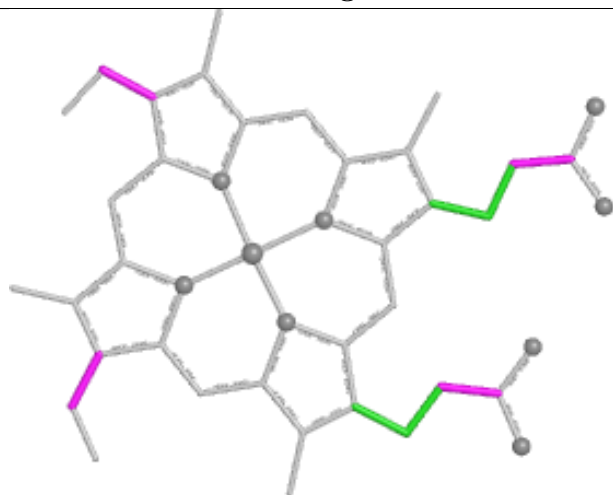
Ligand HEC B 1005



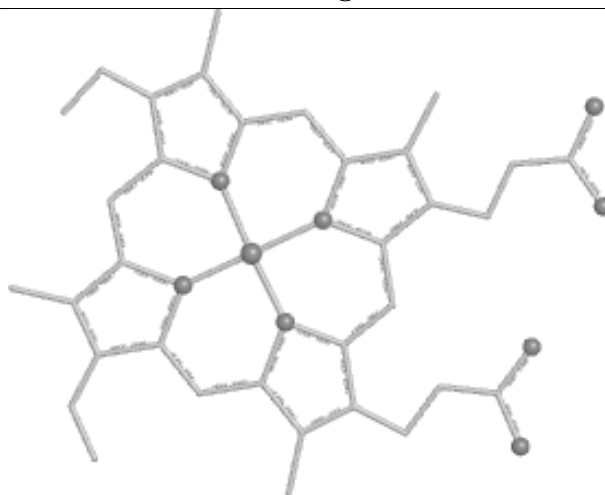
Bond lengths



Bond angles

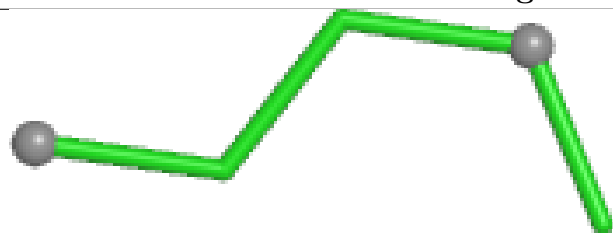


Torsions

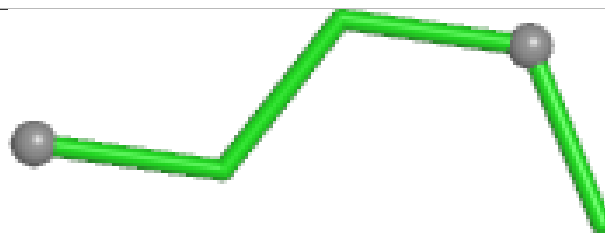


Rings

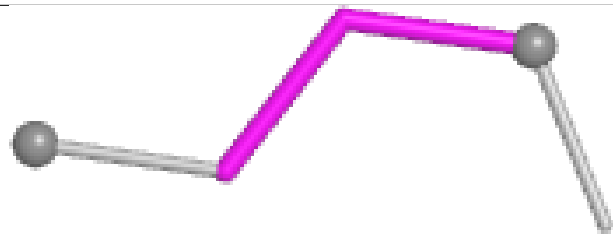
Ligand PG6 B 542



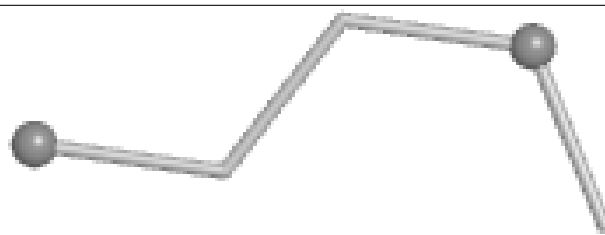
Bond lengths



Bond angles

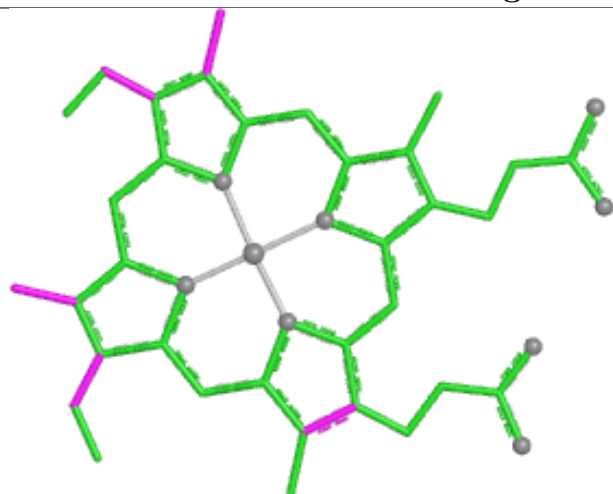


Torsions

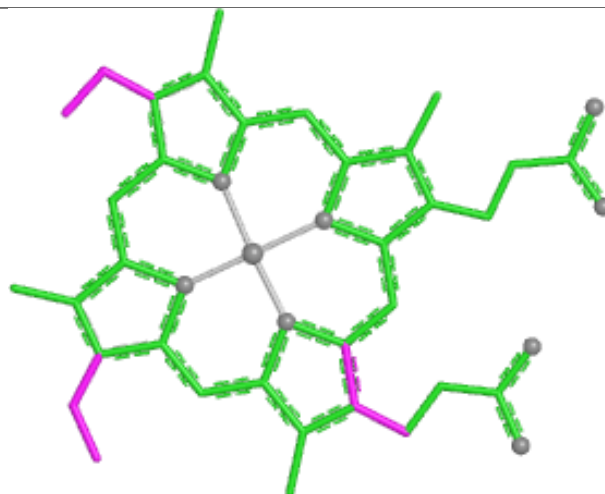


Rings

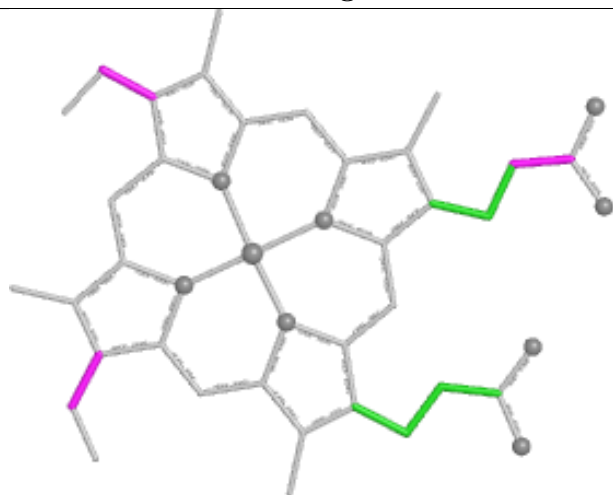
Ligand HEC A 1004



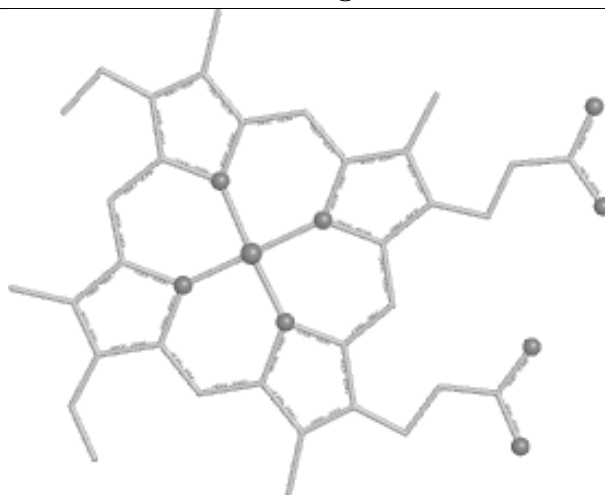
Bond lengths



Bond angles

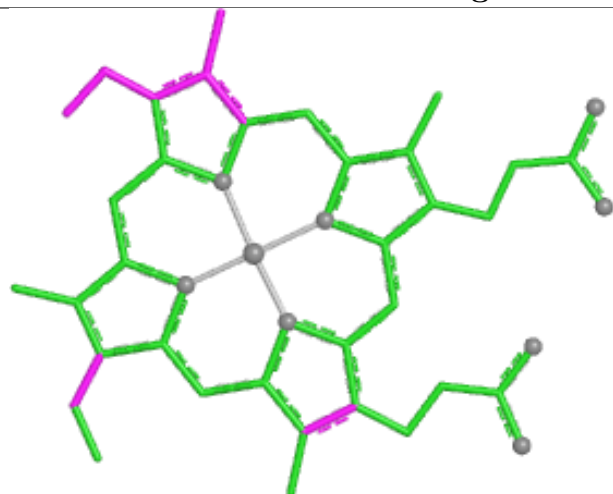


Torsions

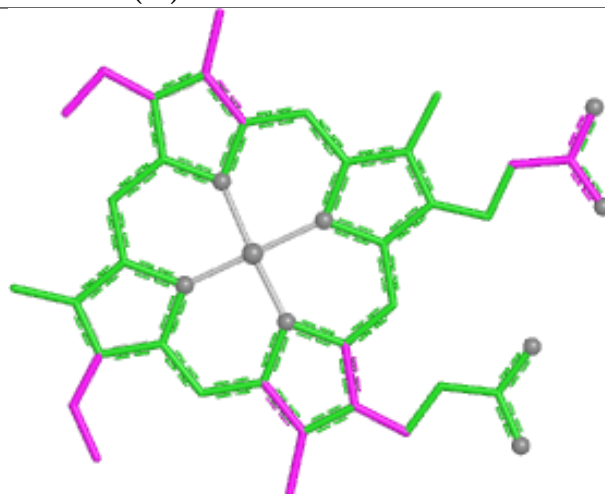


Rings

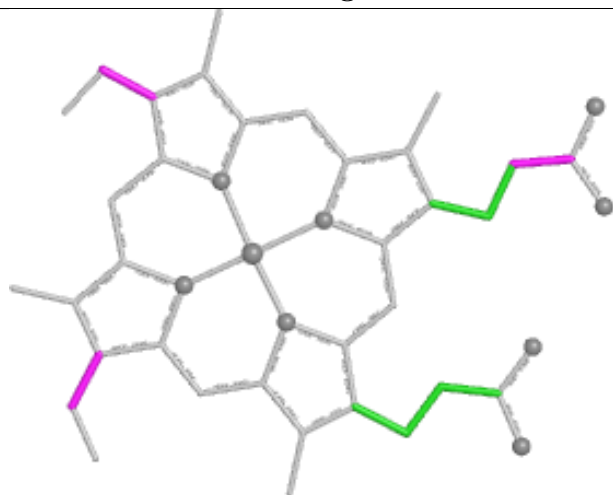
Ligand HEC B 1007 (B)



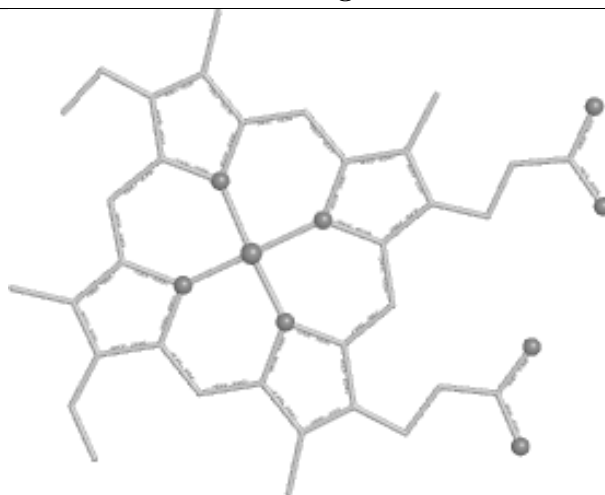
Bond lengths



Bond angles

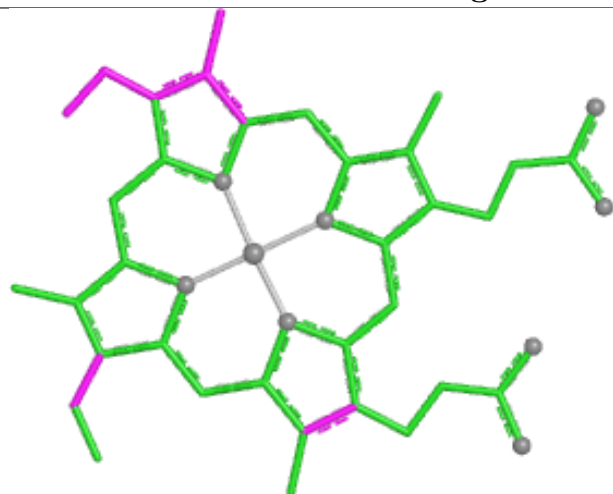


Torsions

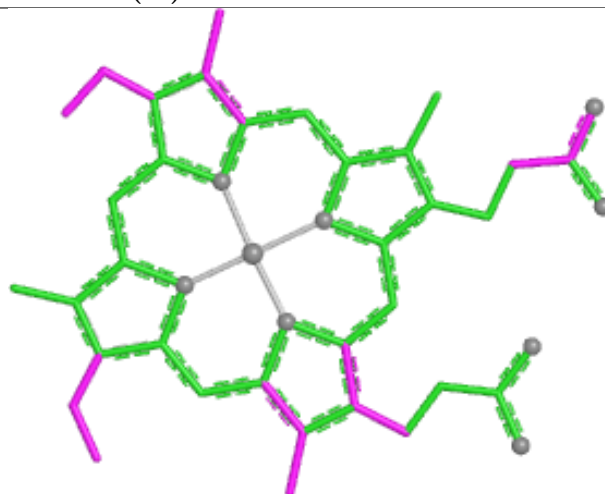


Rings

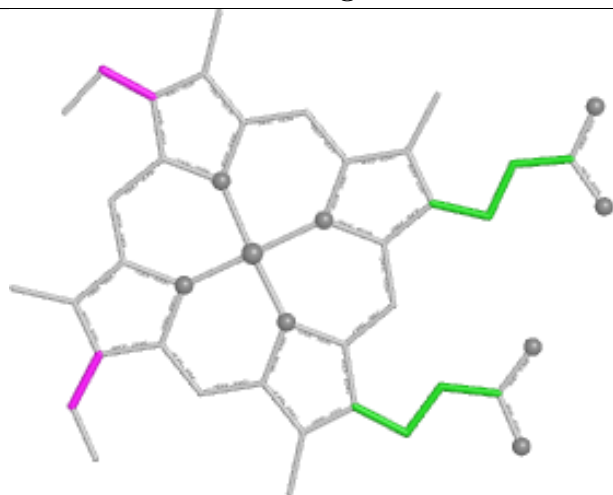
Ligand HEC B 1007 (A)



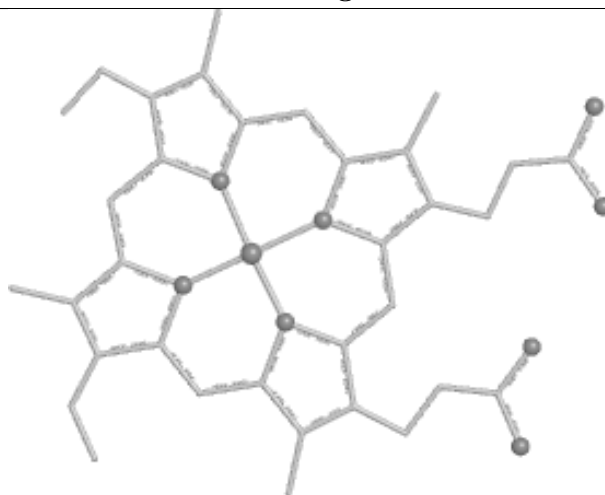
Bond lengths



Bond angles

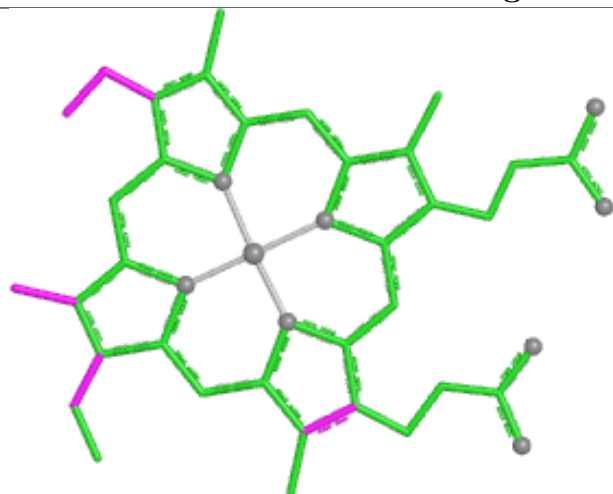


Torsions

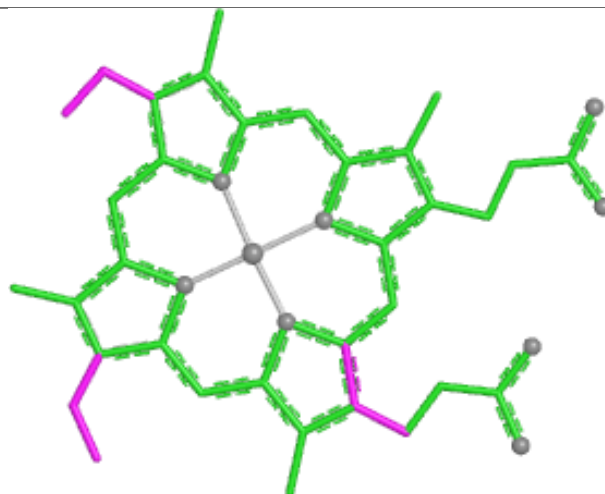


Rings

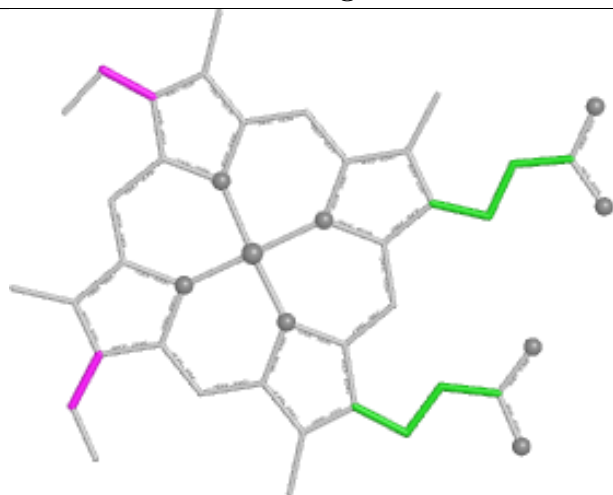
Ligand HEC A 1006



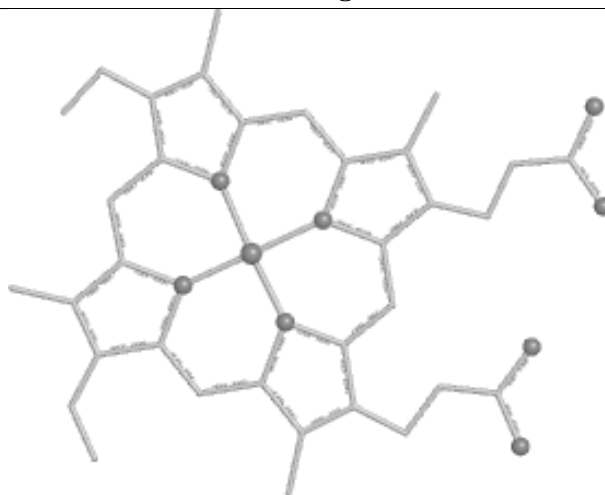
Bond lengths



Bond angles

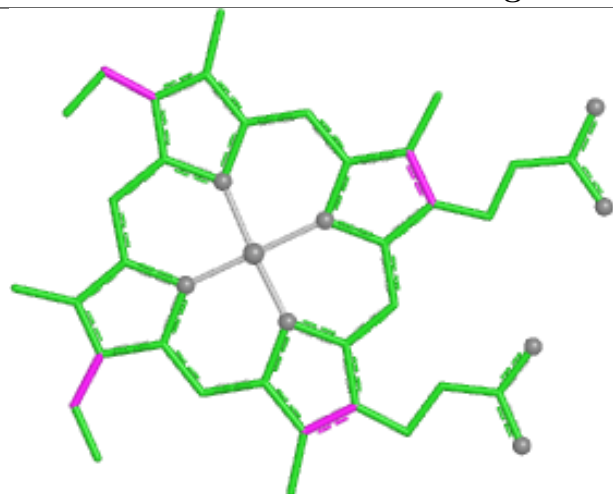


Torsions

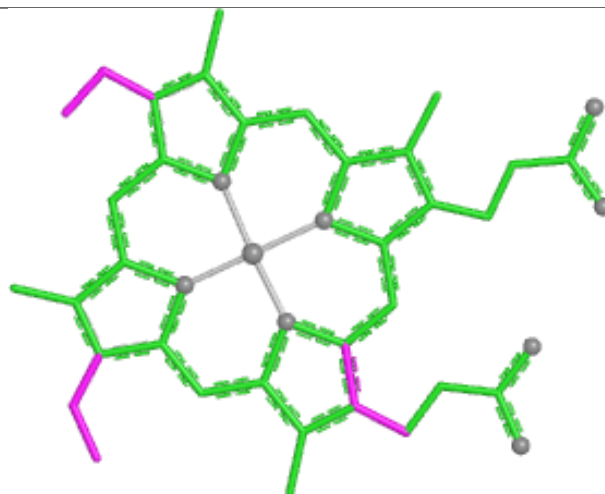


Rings

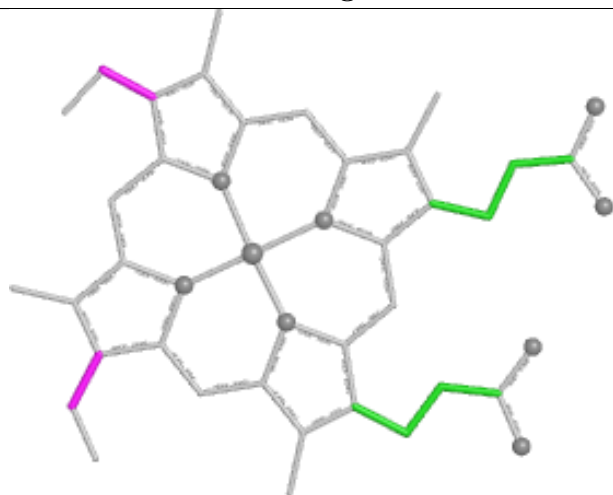
Ligand HEC B 1006



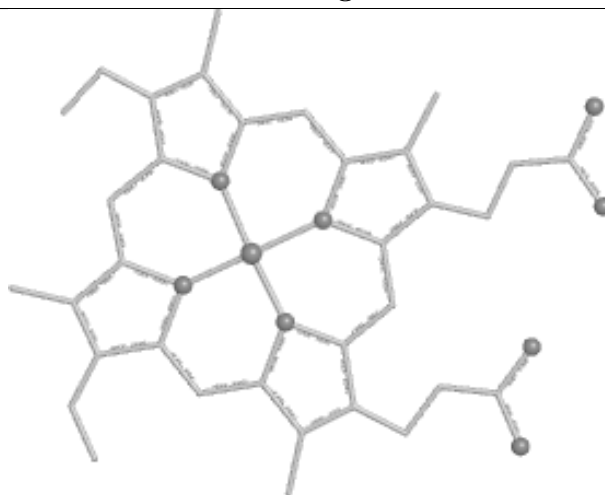
Bond lengths



Bond angles

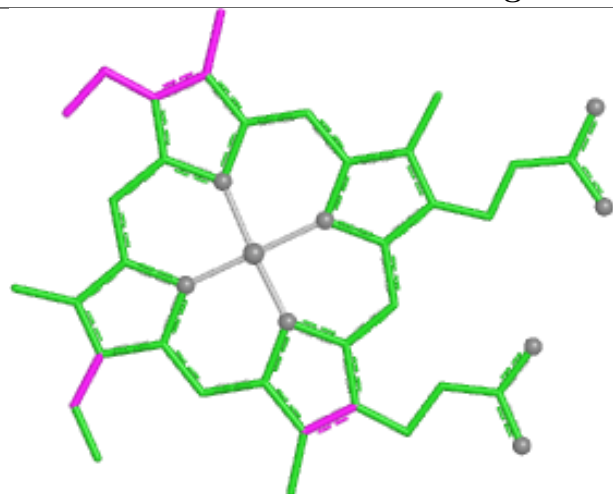


Torsions

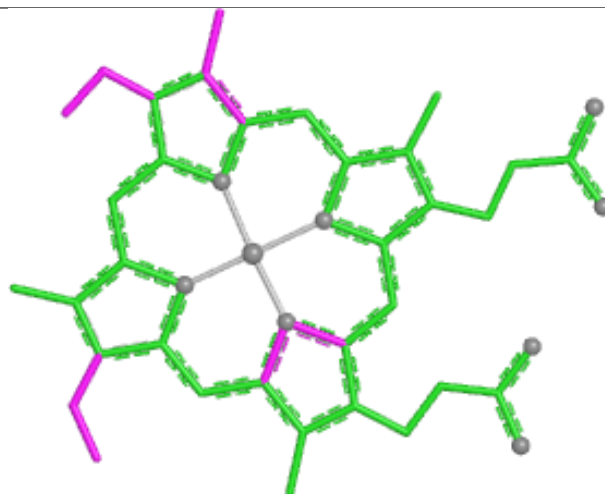


Rings

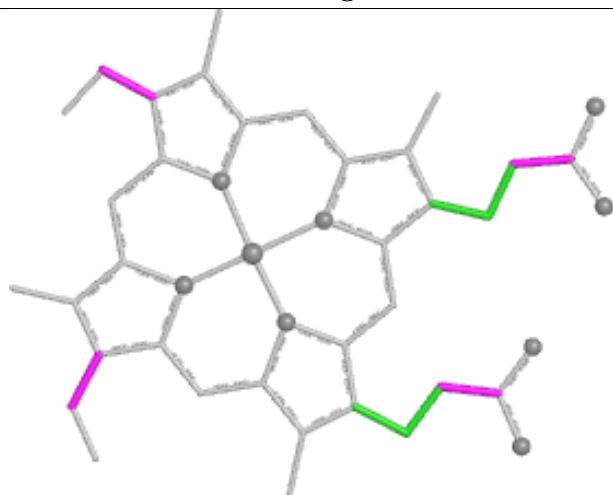
Ligand HEC B 1008



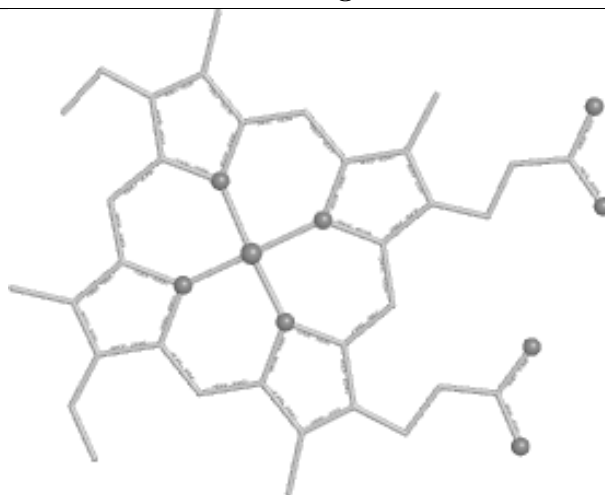
Bond lengths



Bond angles

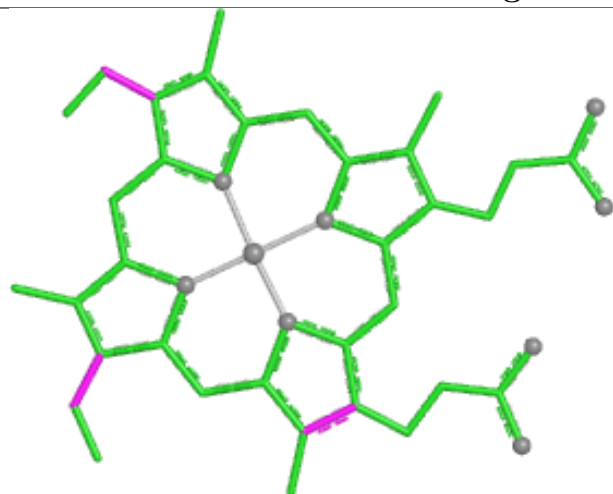


Torsions

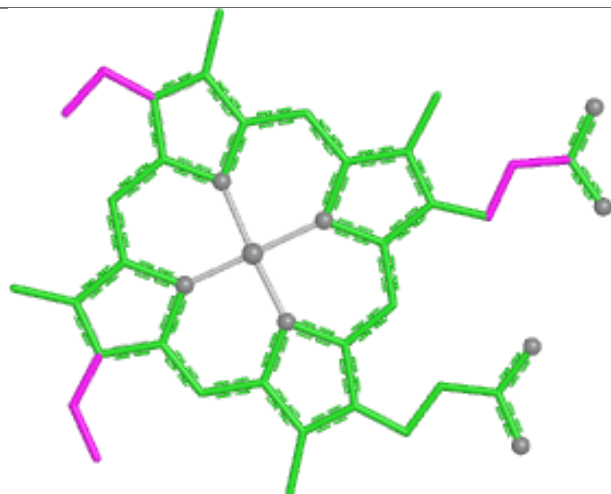


Rings

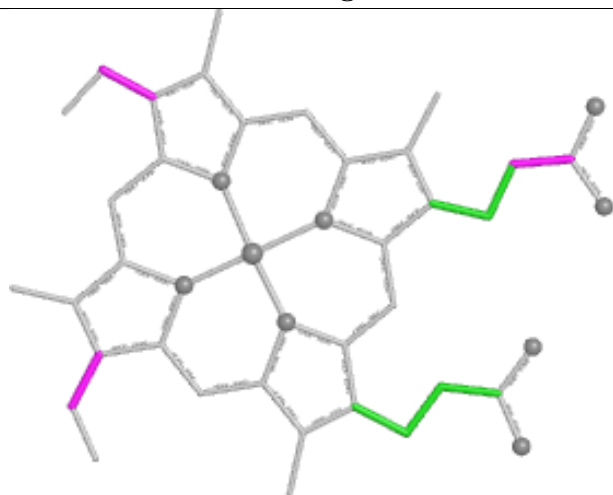
Ligand HEC A 1002



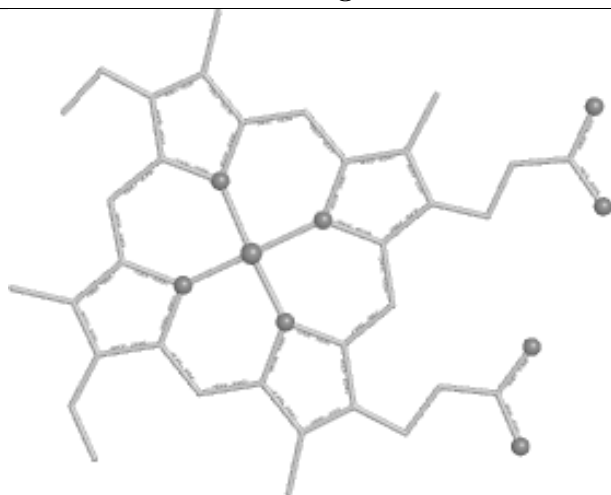
Bond lengths



Bond angles

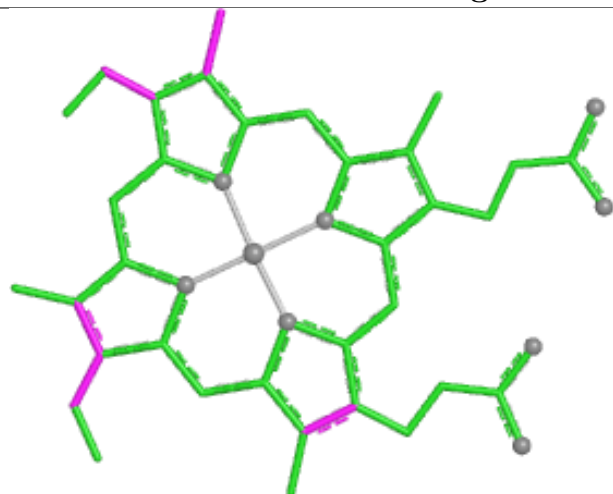


Torsions

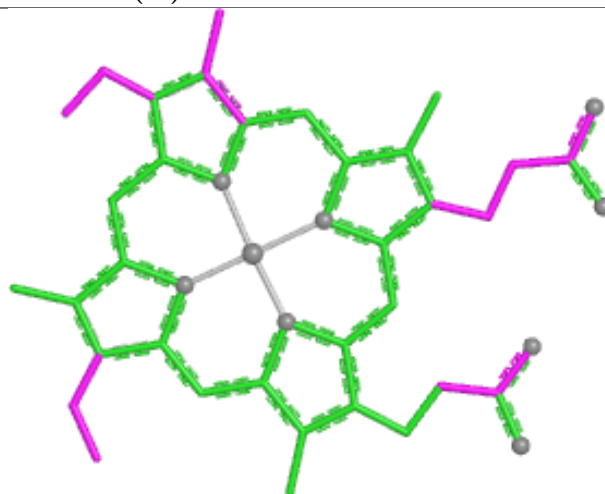


Rings

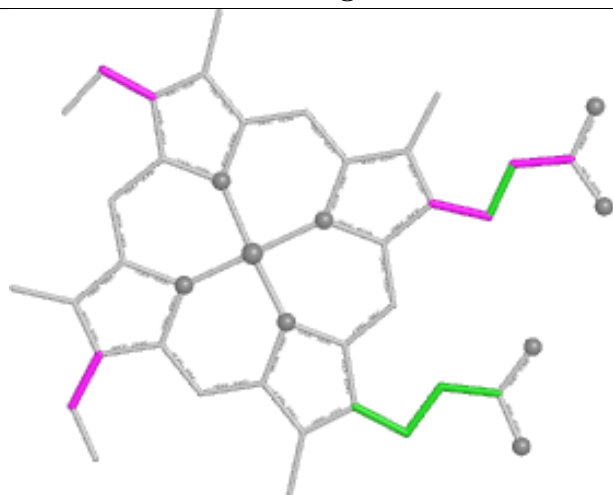
Ligand HEC A 1003 (B)



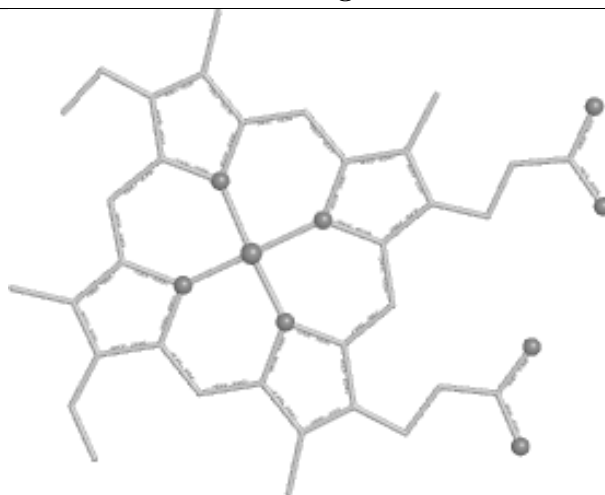
Bond lengths



Bond angles

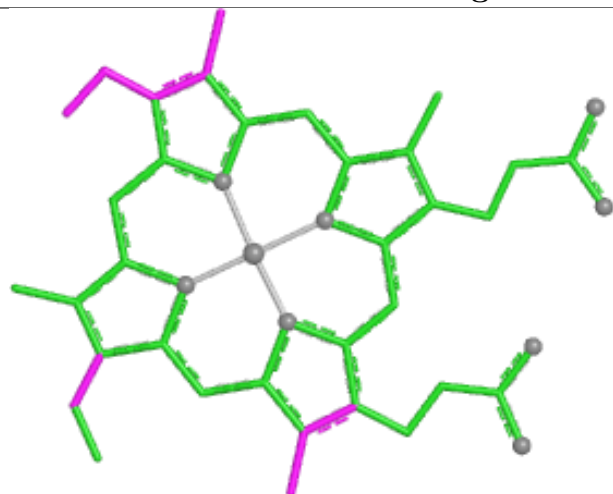


Torsions

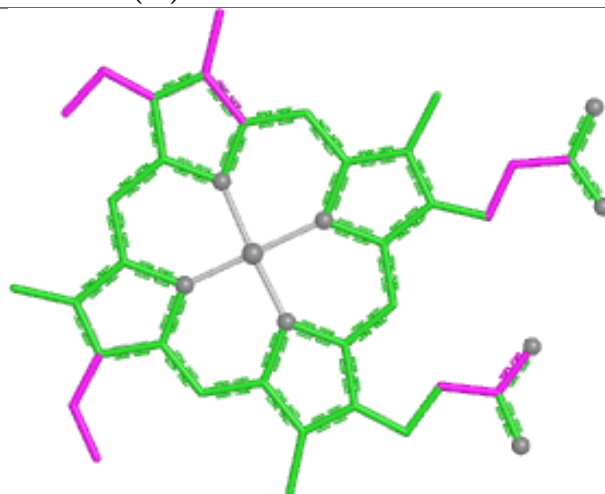


Rings

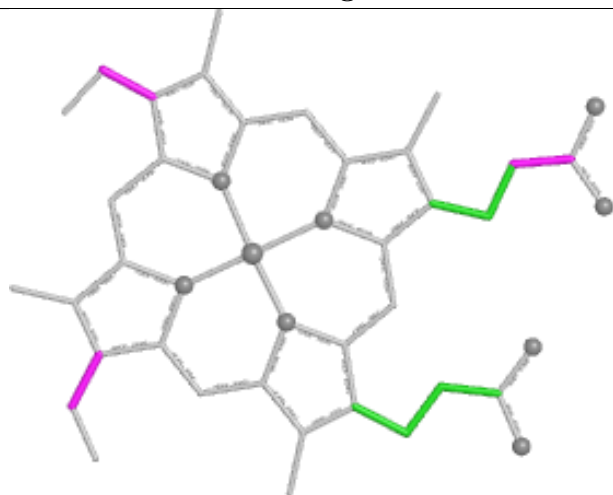
Ligand HEC B 1003 (B)



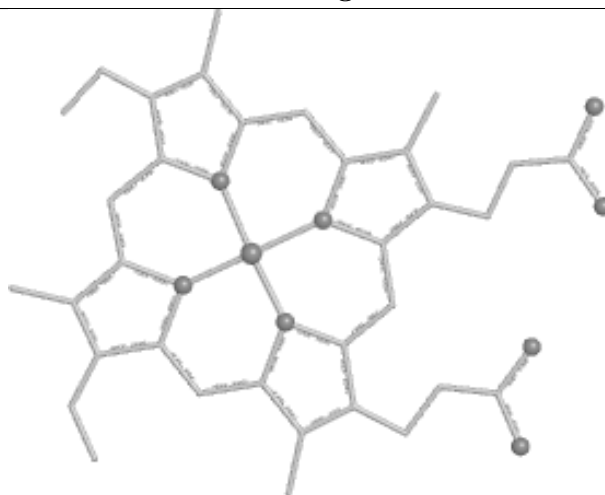
Bond lengths



Bond angles

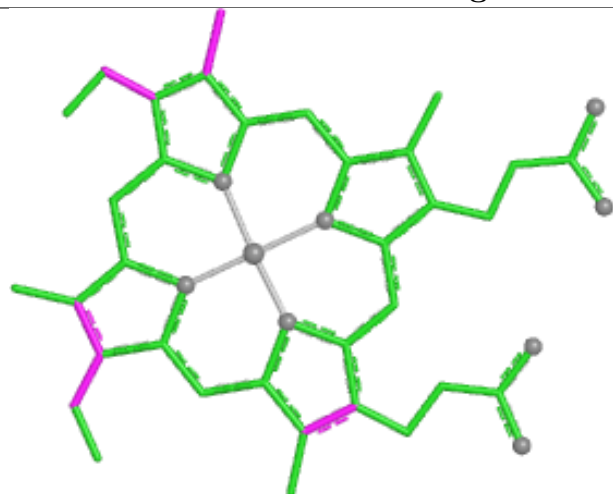


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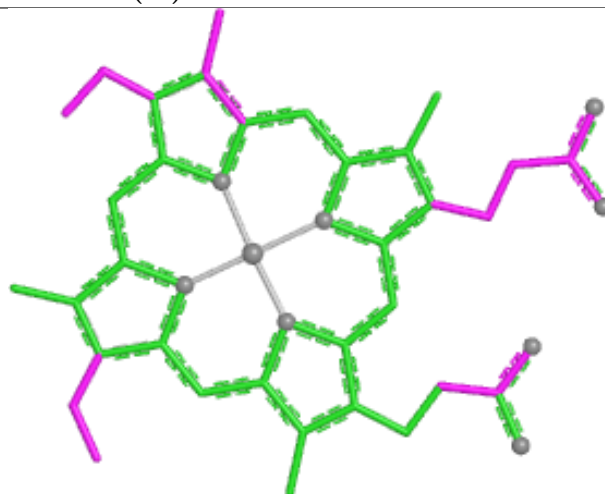


Rings

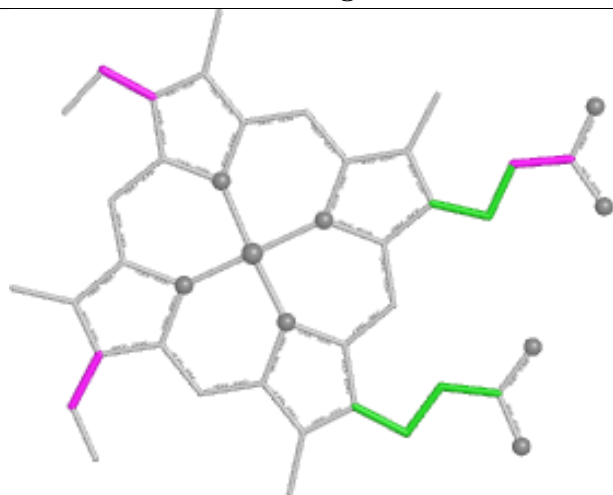
Ligand HEC A 1003 (A)



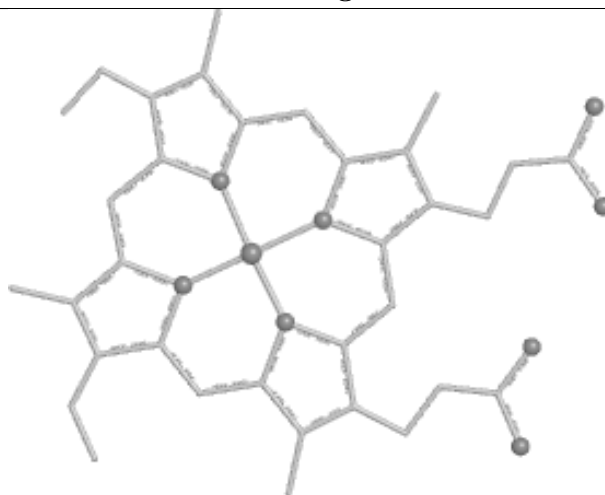
Bond lengths



Bond angles

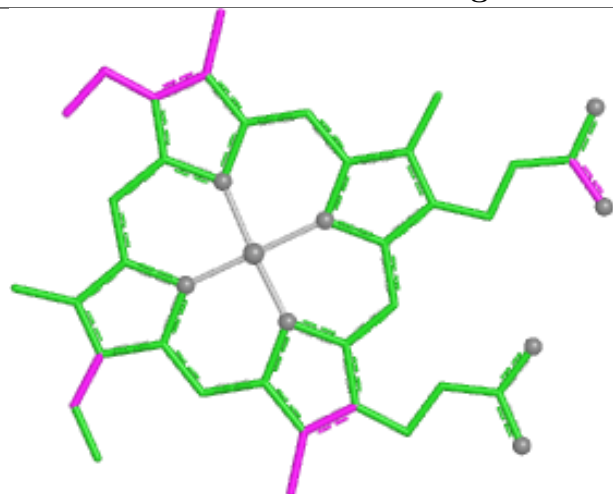


Torsions

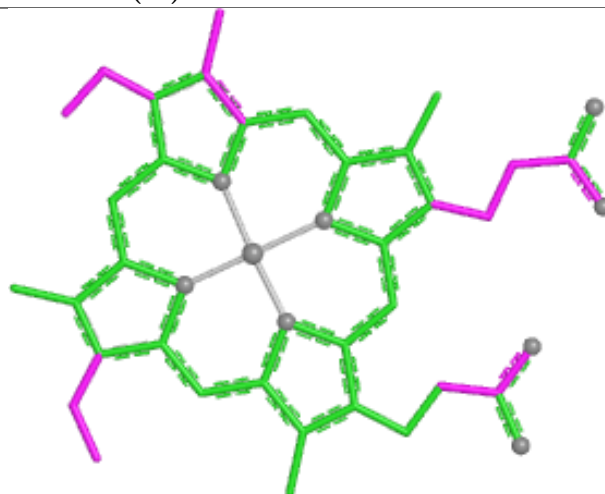


Rings

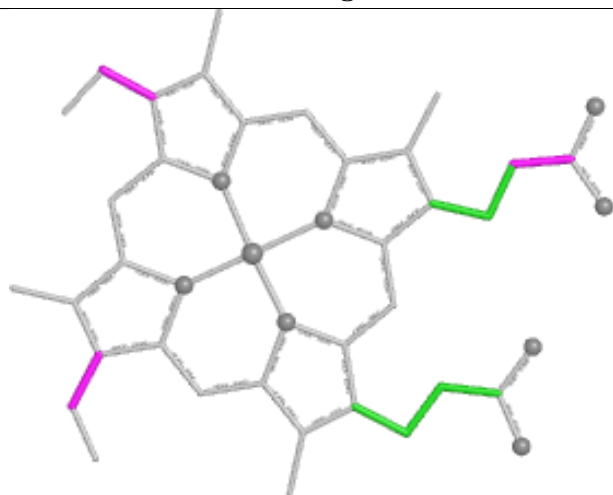
Ligand HEC B 1003 (A)



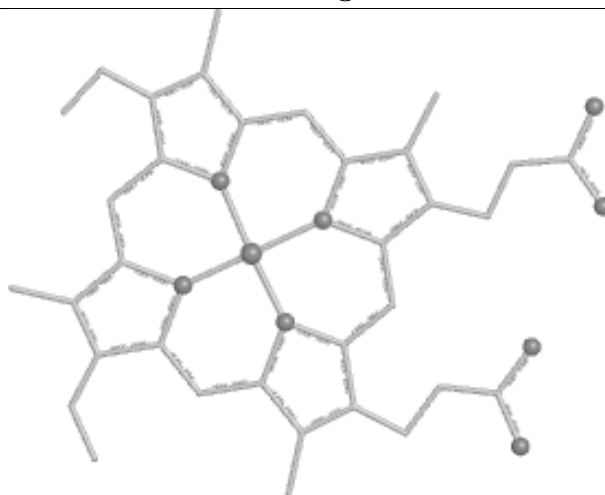
Bond lengths



Bond angles

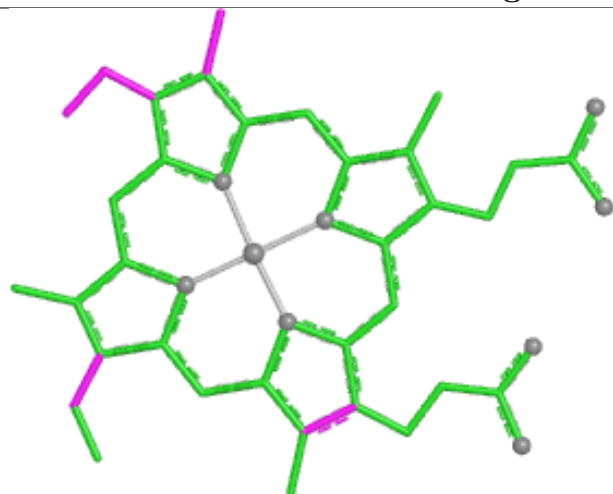


Torsions

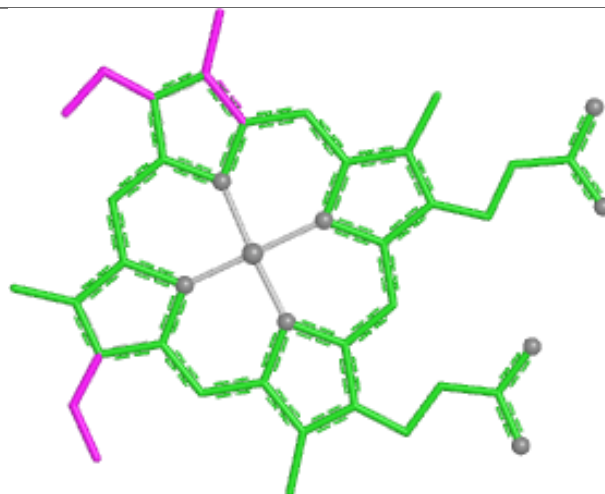


Rings

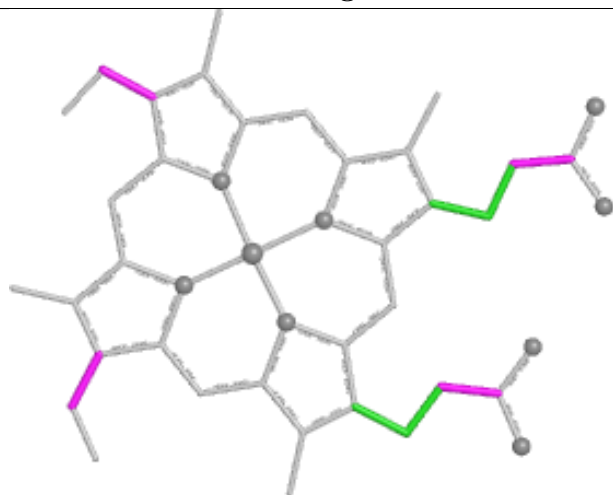
Ligand HEC A 1005



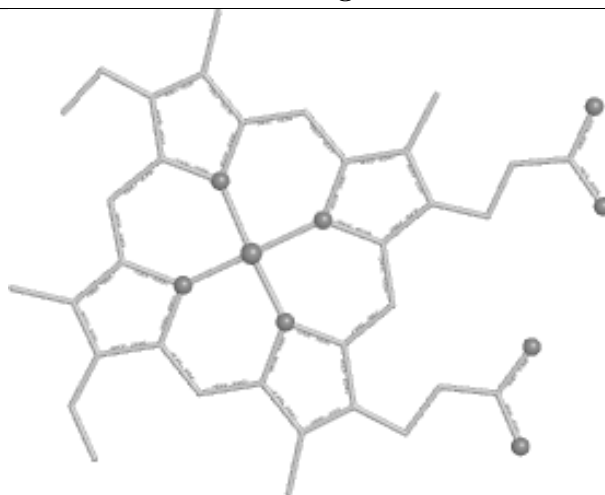
Bond lengths



Bond angles

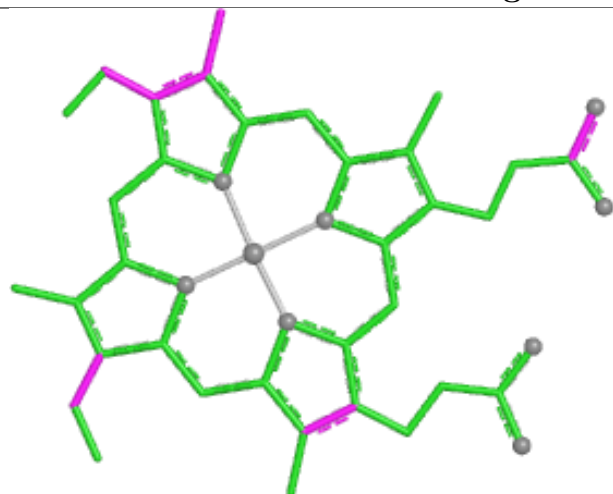


Torsions

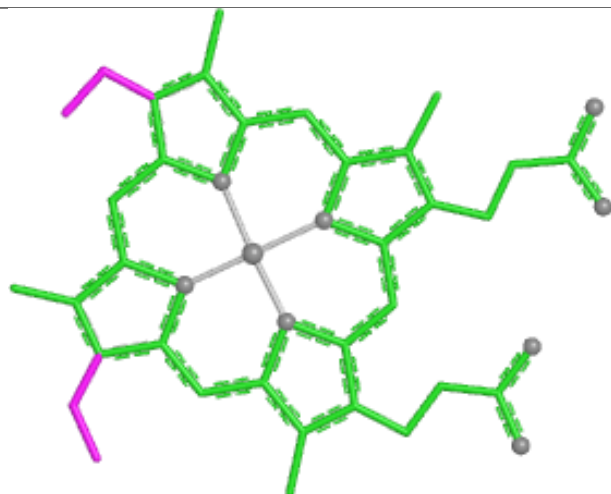


Rings

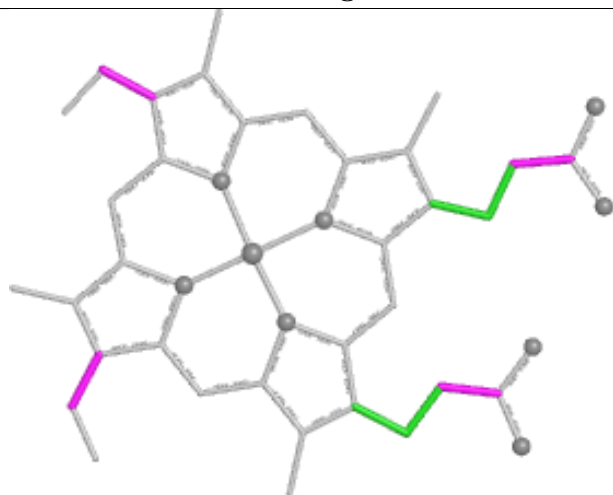
Ligand HEC A 1001



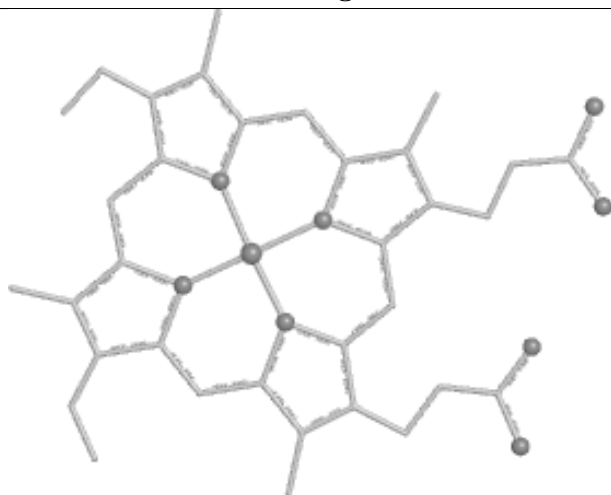
Bond lengths



Bond angles

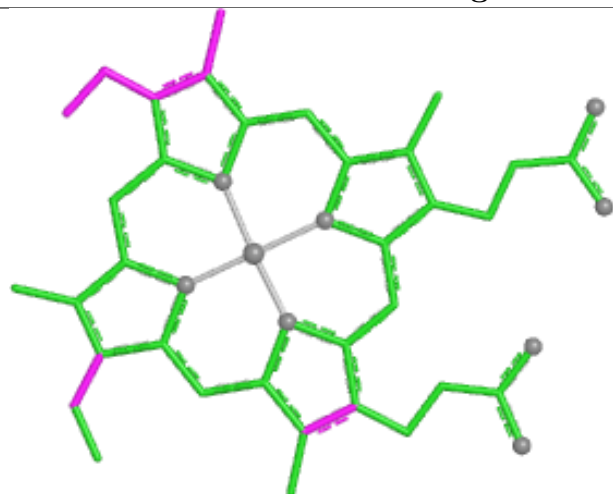


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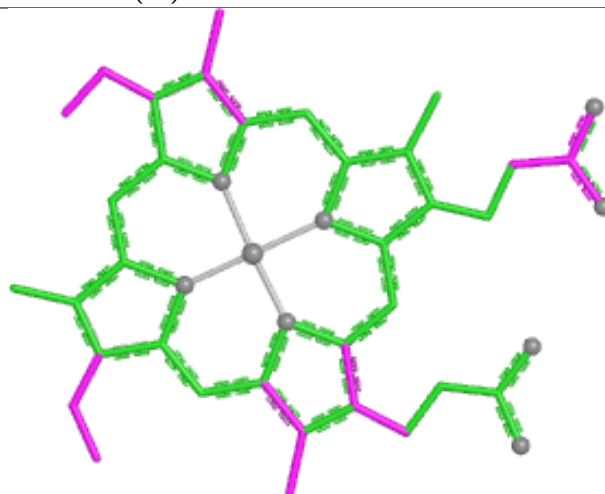


Rings

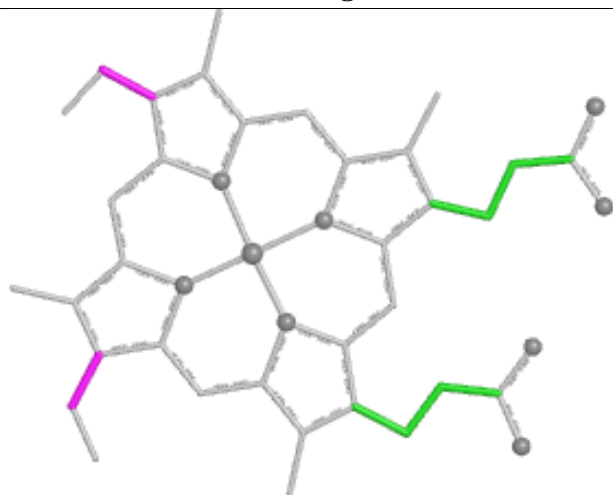
Ligand HEC A 1007 (B)



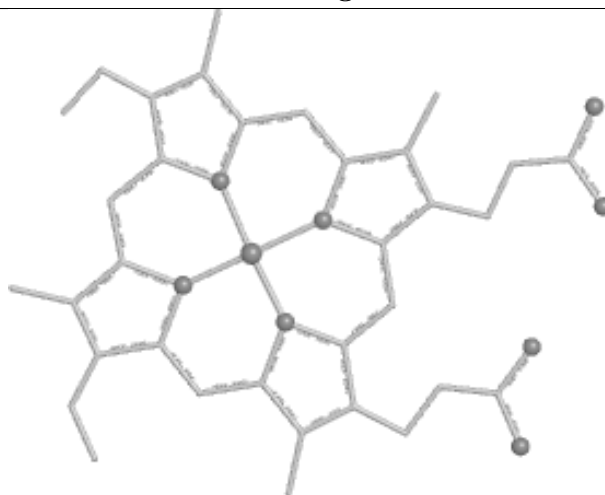
Bond lengths



Bond angles

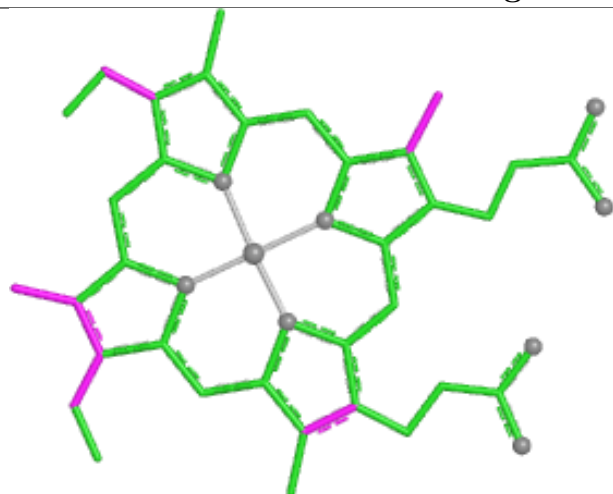


Torsions

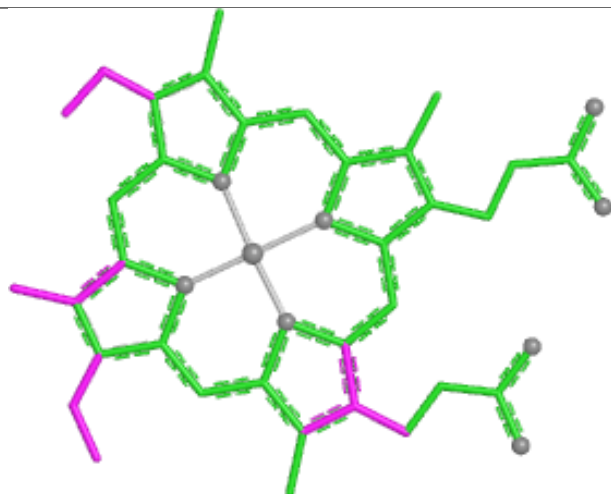


Rings

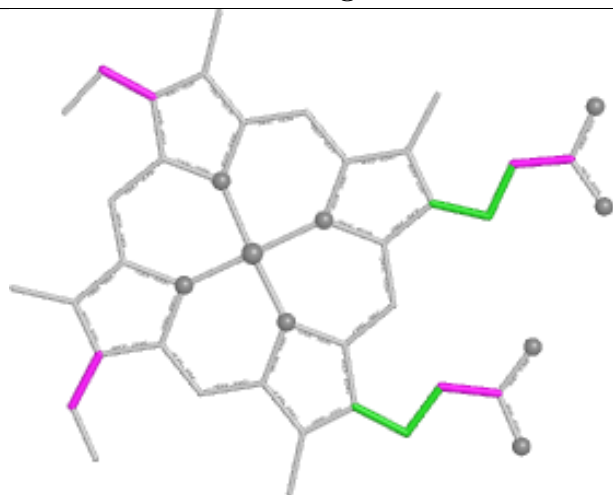
Ligand HEC B 1001



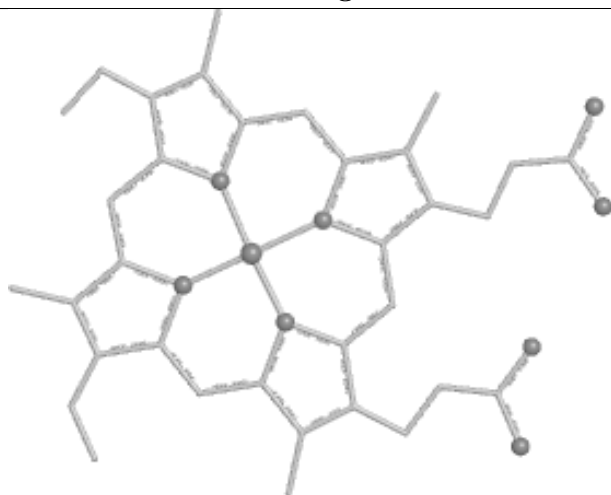
Bond lengths



Bond angles

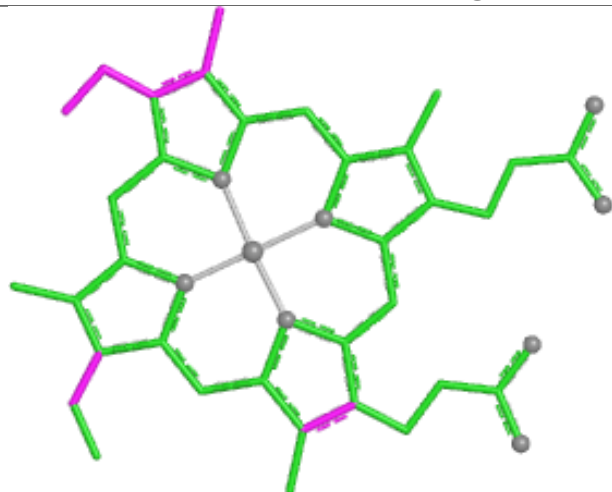


Torsions

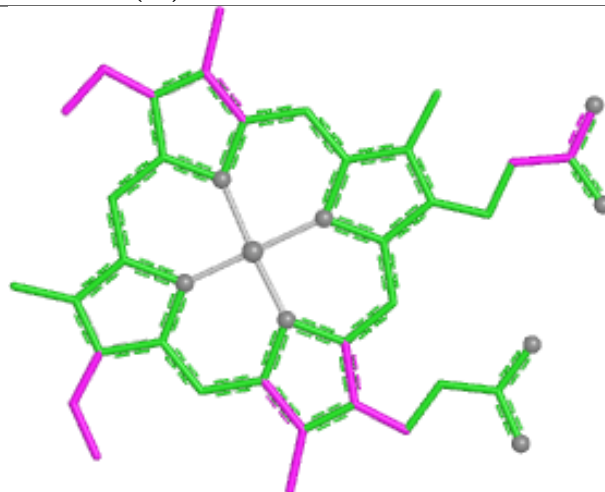


Rings

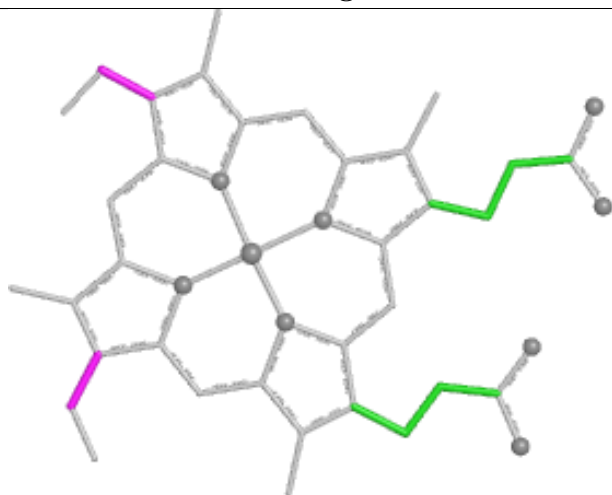
Ligand HEC A 1007 (A)



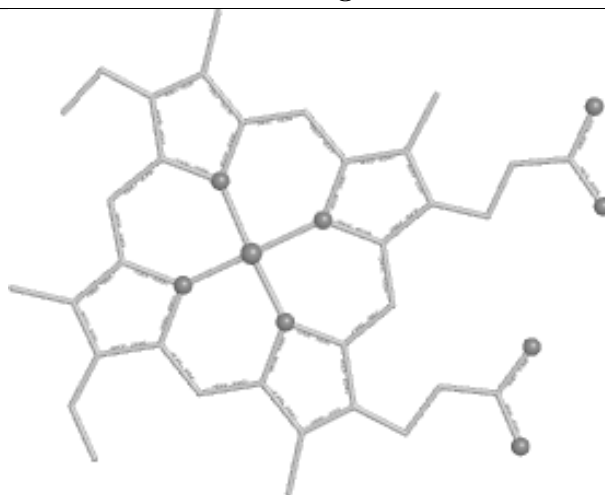
Bond lengths



Bond angles

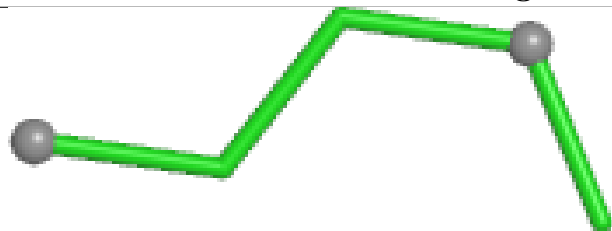


Torsions

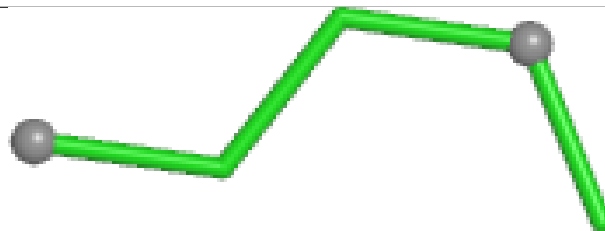


Rings

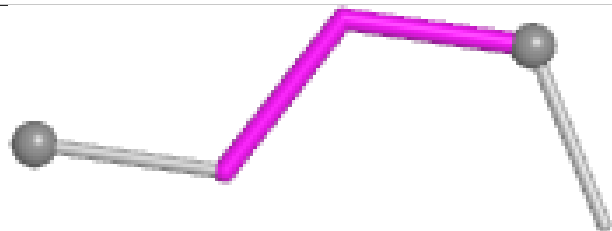
Ligand PG6 A 542



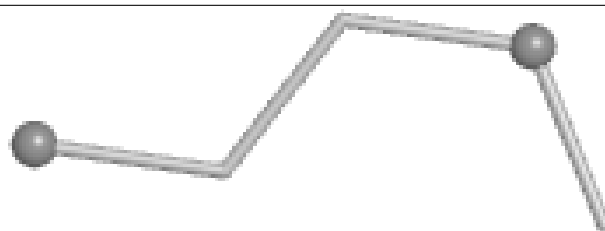
Bond lengths



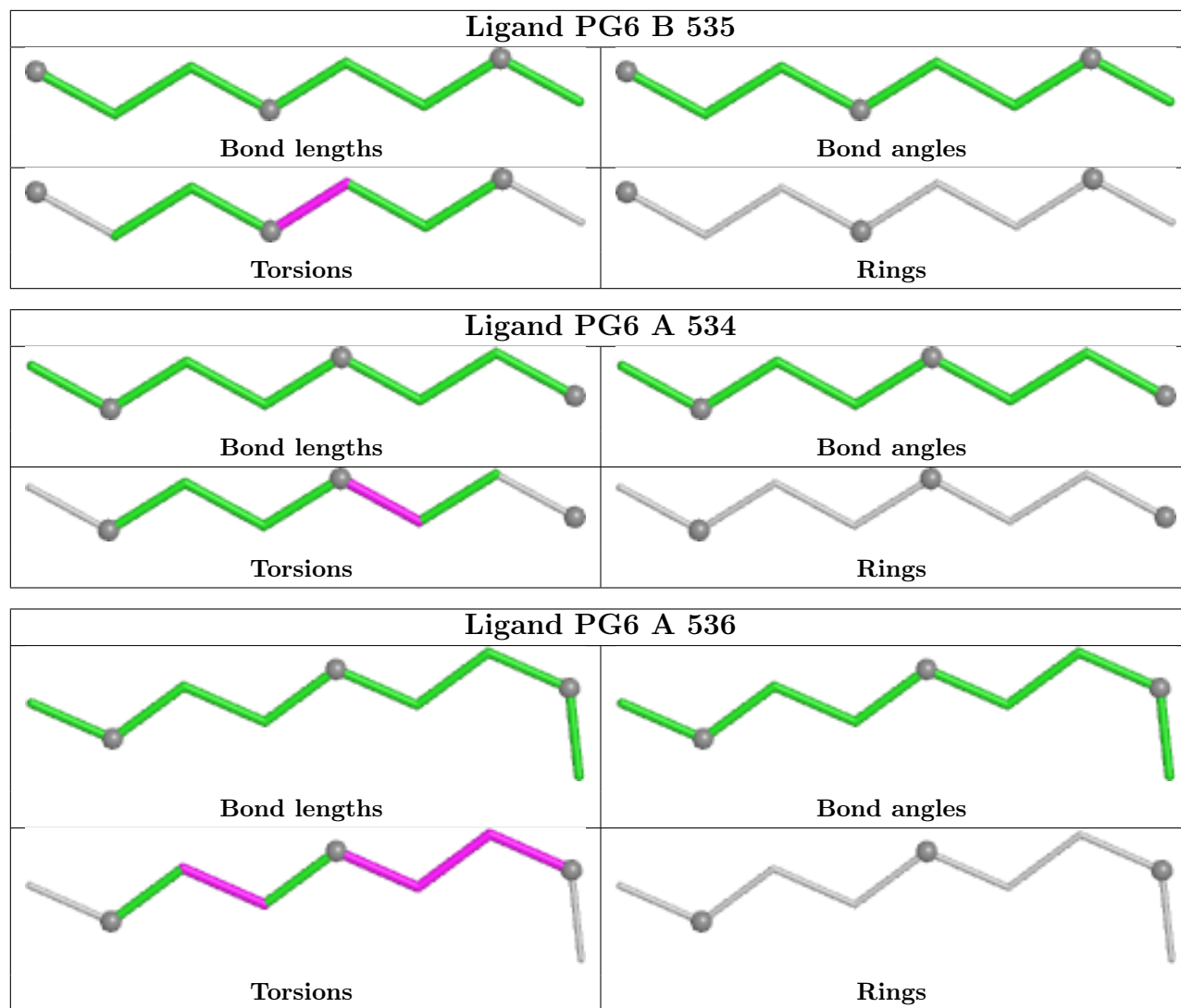
Bond angles



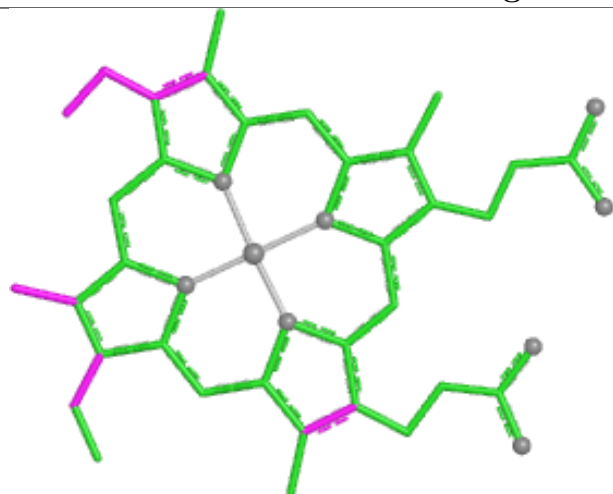
Torsions



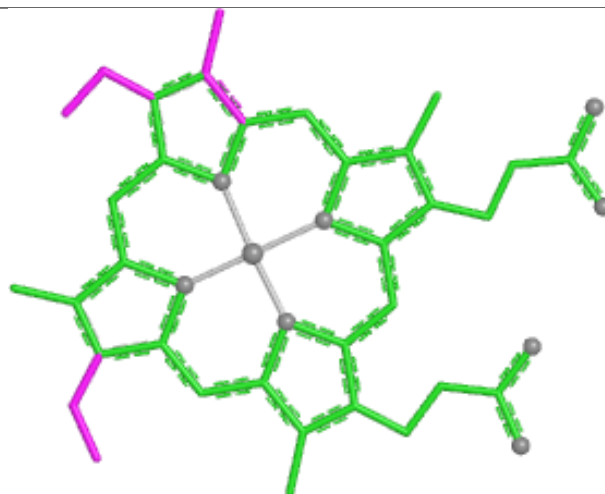
Rings



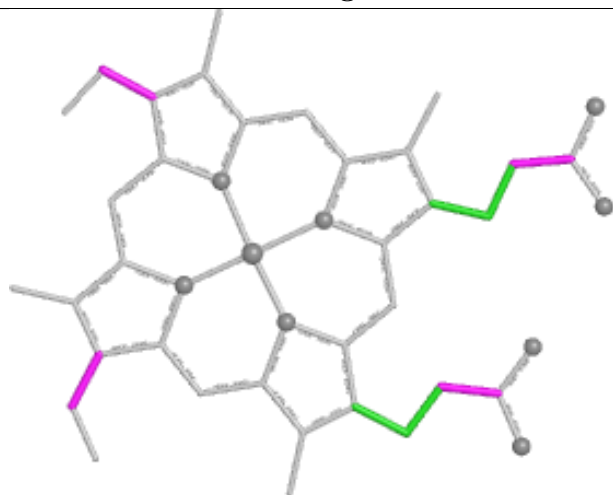
Ligand HEC A 1008



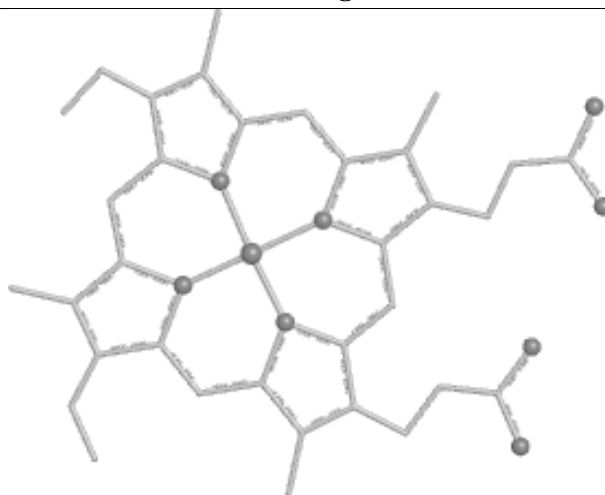
Bond lengths



Bond angles

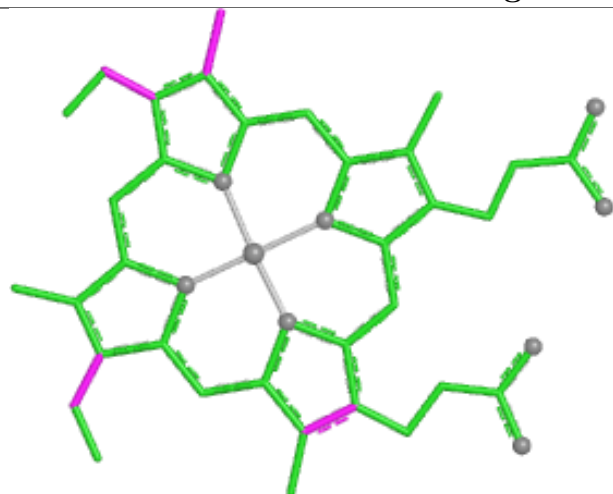


Torsions

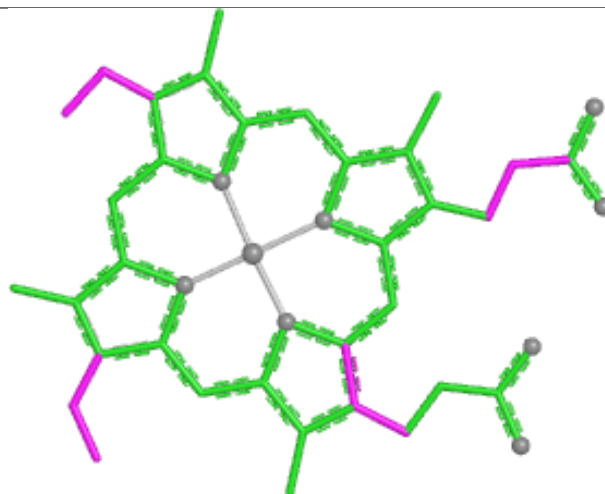


Rings

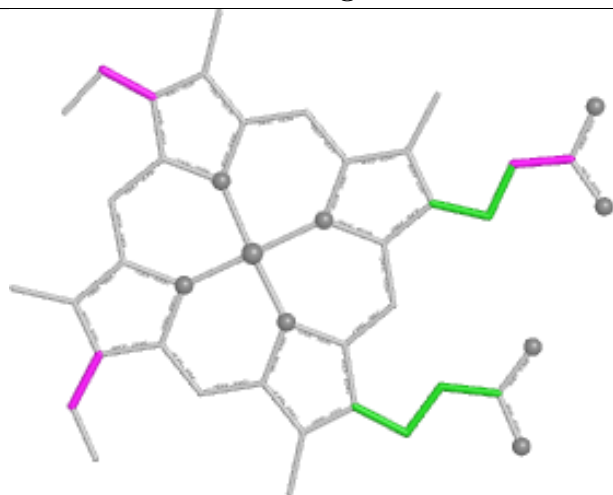
Ligand HEC B 1002



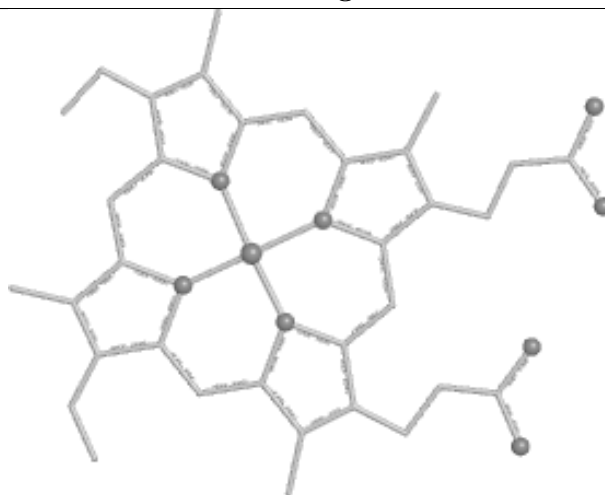
Bond lengths



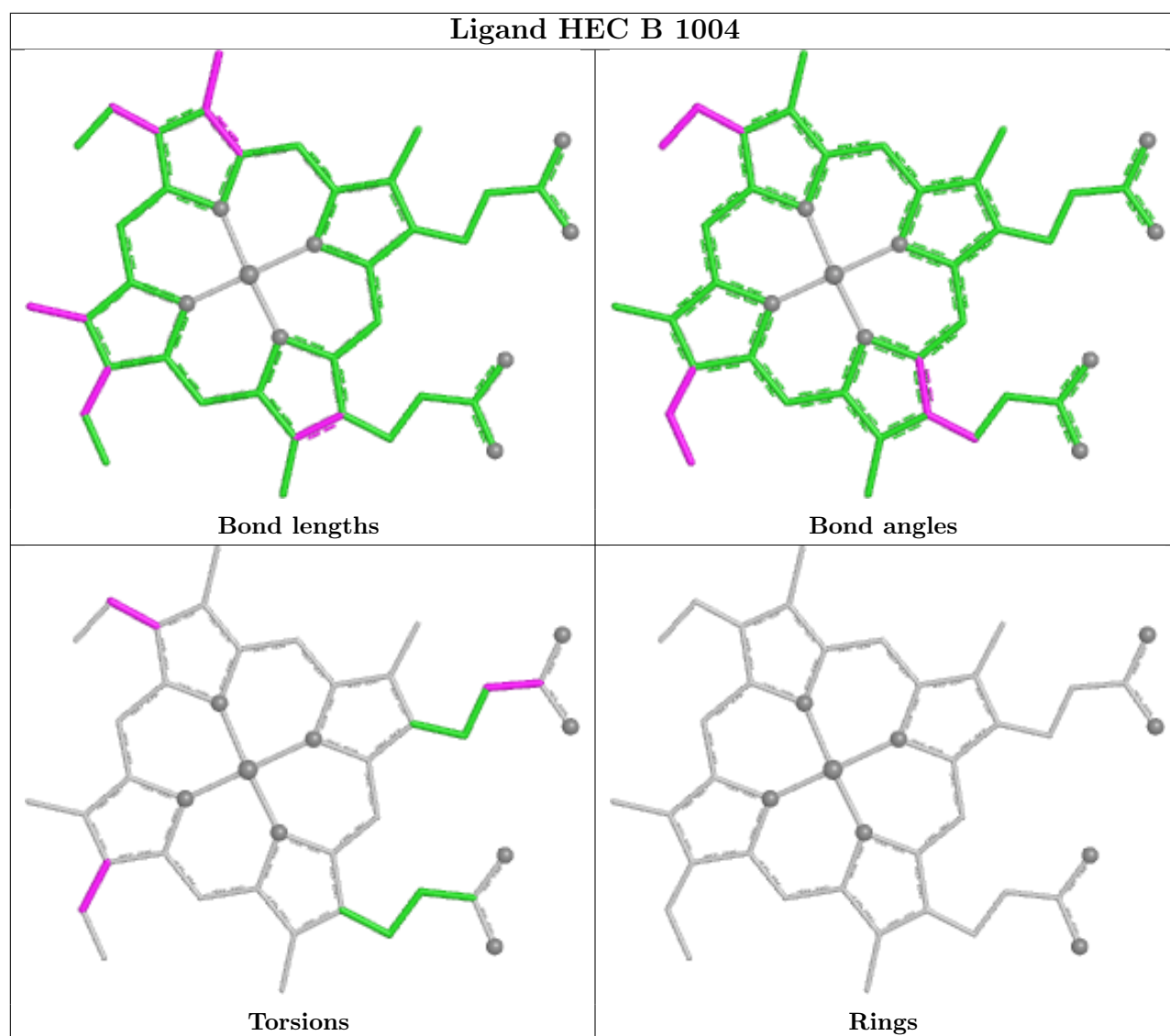
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.88	2 (0%) 88 91	9, 15, 25, 44	20 (3%)
1	B	519/525 (98%)	-0.83	8 (1%) 72 75	9, 15, 26, 44	23 (4%)
All	All	1038/1050 (98%)	-0.86	10 (0%) 79 83	9, 15, 25, 44	43 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	9.2
1	B	523	ALA	9.1
1	B	522	VAL	5.0
1	A	522	VAL	4.9
1	B	51	ARG	2.3
1	B	204	GLU	2.2
1	B	52	ARG	2.2
1	B	278	ARG	2.1
1	B	16	ASP	2.1
1	B	520	ALA	2.0

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 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, 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
8	PG6	A	536	9/18	0.56	0.30	40,42,42,42	9
11	ACT	B	546	4/4	0.59	0.26	34,35,36,36	0
10	PG4	B	544	5/13	0.67	0.19	25,26,28,29	5
10	PG4	B	537	10/13	0.70	0.22	39,42,44,44	10
10	PG4	B	540	4/13	0.70	0.27	29,31,31,31	4
10	PG4	A	541	6/13	0.76	0.23	36,36,37,38	6
10	PG4	B	541	5/13	0.76	0.19	47,47,48,49	0
10	PG4	A	538[A]	5/13	0.77	0.21	36,38,40,41	2
10	PG4	A	538[B]	8/13	0.77	0.21	39,40,41,41	5
8	PG6	A	542	5/18	0.79	0.34	52,52,52,53	5
8	PG6	A	543	10/18	0.79	0.19	29,31,33,34	10
10	PG4	A	537	4/13	0.80	0.21	35,36,36,36	4
9	TRS	B	533	8/8	0.81	0.16	15,15,16,16	8
10	PG4	B	545	4/13	0.81	0.44	35,35,36,36	4
10	PG4	A	539	6/13	0.81	0.17	47,48,48,48	0
10	PG4	B	538	7/13	0.84	0.13	31,31,32,33	7
8	PG6	B	542	5/18	0.85	0.17	45,45,45,45	5
10	PG4	B	536	8/13	0.85	0.18	18,25,29,29	8
8	PG6	B	535	8/18	0.85	0.13	34,36,38,38	0
10	PG4	B	543	4/13	0.86	0.14	47,48,48,48	0
8	PG6	B	532	17/18	0.86	0.14	16,19,22,25	17
8	PG6	A	532	17/18	0.87	0.12	17,21,27,29	17
10	PG4	A	540	6/13	0.87	0.12	50,50,51,51	0
9	TRS	A	533	8/8	0.88	0.13	12,13,14,14	8
10	PG4	B	547	7/13	0.89	0.14	18,22,24,26	7
8	PG6	A	534	8/18	0.89	0.12	28,33,40,40	0
10	PG4	B	539	5/13	0.91	0.14	23,27,27,27	5
3	SO3	B	529[A]	4/4	0.92	0.22	17,18,20,22	4
3	SO3	B	529[B]	4/4	0.92	0.22	17,18,22,22	4
5	SO4	A	529	5/5	0.92	0.16	19,21,26,26	5
10	PG4	A	535	5/13	0.94	0.12	14,17,20,22	5
5	SO4	B	534	5/5	0.96	0.13	14,18,23,25	5
6	THJ	A	530	5/5	0.96	0.08	24,24,24,28	5
7	NA	B	548	1/1	0.97	0.09	24,24,24,24	1
7	NA	B	549	1/1	0.97	0.07	30,30,30,30	1
6	THJ	B	530	5/5	0.98	0.07	23,23,23,25	5
2	HEC	B	1003[B]	43/43	0.99	0.05	12,13,23,33	4

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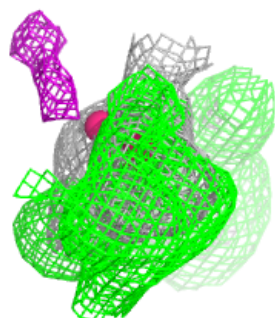
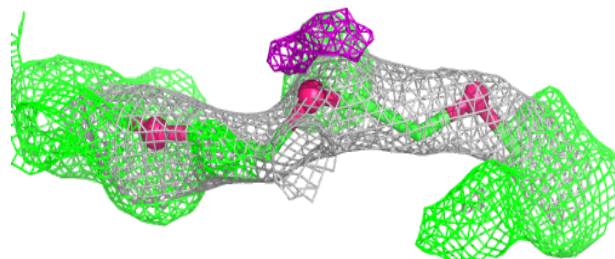
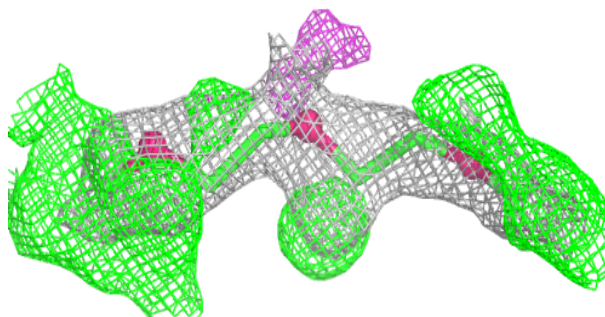
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	B	1001	43/43	0.99	0.05	17,19,24,26	0
2	HEC	A	1004	43/43	0.99	0.04	11,12,14,17	0
2	HEC	A	1005	43/43	0.99	0.03	11,12,16,19	0
4	CA	A	528	1/1	0.99	0.03	18,18,18,18	1
2	HEC	A	1006	43/43	0.99	0.04	10,11,12,14	0
2	HEC	A	1007[A]	43/43	0.99	0.04	10,11,13,14	4
2	HEC	A	1007[B]	43/43	0.99	0.04	10,11,13,14	4
2	HEC	A	1008	43/43	0.99	0.05	12,14,22,34	0
7	NA	A	544	1/1	0.99	0.03	23,23,23,23	1
2	HEC	A	1002	43/43	0.99	0.03	12,13,15,17	0
2	HEC	A	1003[A]	43/43	0.99	0.05	11,13,21,29	4
2	HEC	A	1003[B]	43/43	0.99	0.05	11,13,23,29	4
2	HEC	A	1001	43/43	0.99	0.04	13,14,20,21	0
2	HEC	B	1004	43/43	0.99	0.04	10,12,14,16	0
2	HEC	B	1007[A]	43/43	0.99	0.04	10,11,13,14	4
2	HEC	B	1007[B]	43/43	0.99	0.04	10,11,13,14	4
2	HEC	B	1008	43/43	0.99	0.04	11,14,21,32	0
2	HEC	B	1002	43/43	0.99	0.04	13,15,17,19	0
2	HEC	B	1003[A]	43/43	0.99	0.05	12,13,23,33	4
2	HEC	B	1006	43/43	1.00	0.03	9,11,12,13	0
2	HEC	B	1005	43/43	1.00	0.03	10,12,15,19	0
4	CA	A	527	1/1	1.00	0.01	13,13,13,13	0
7	NA	A	531	1/1	1.00	0.02	23,23,23,23	1
3	SO3	A	526	4/4	1.00	0.05	14,15,17,18	0
7	NA	B	531	1/1	1.00	0.08	23,23,23,23	1
4	CA	B	527	1/1	1.00	0.01	13,13,13,13	0
4	CA	B	528	1/1	1.00	0.02	18,18,18,18	1
3	SO3	B	526	4/4	1.00	0.05	14,14,16,17	0

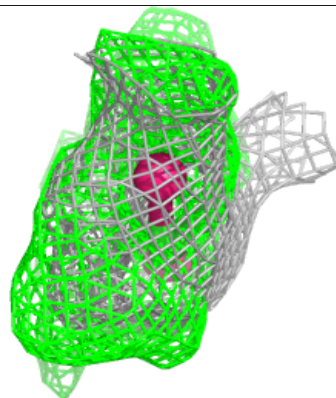
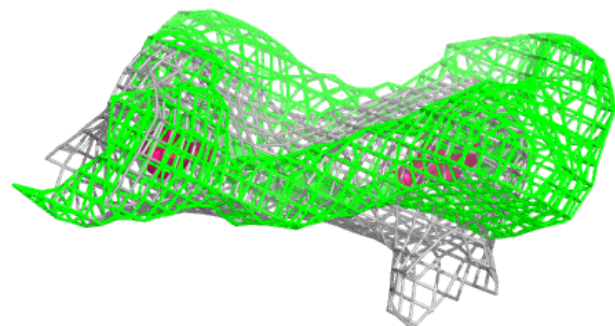
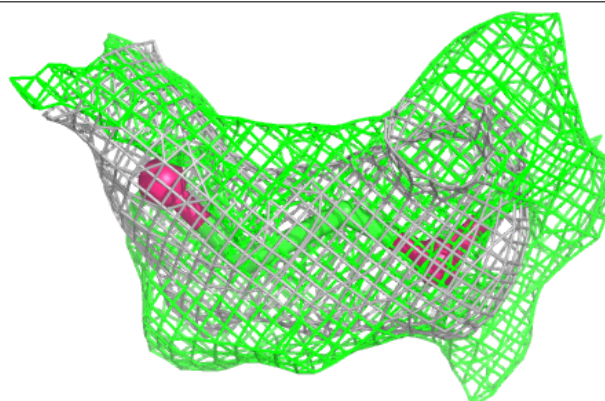
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PG6 A 536:

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

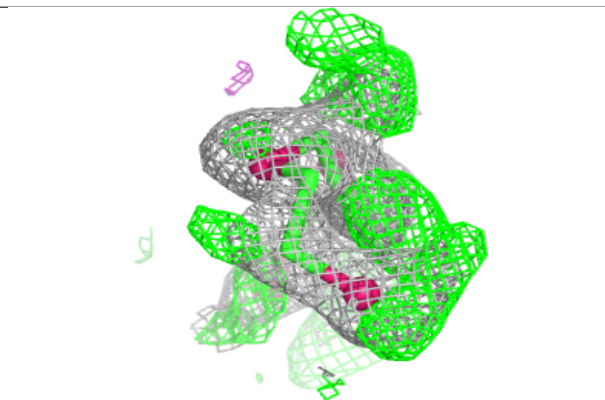
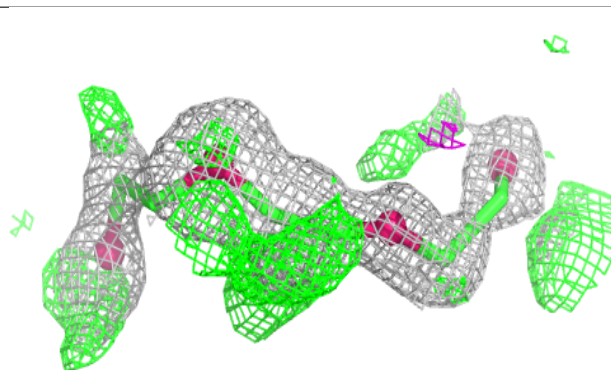
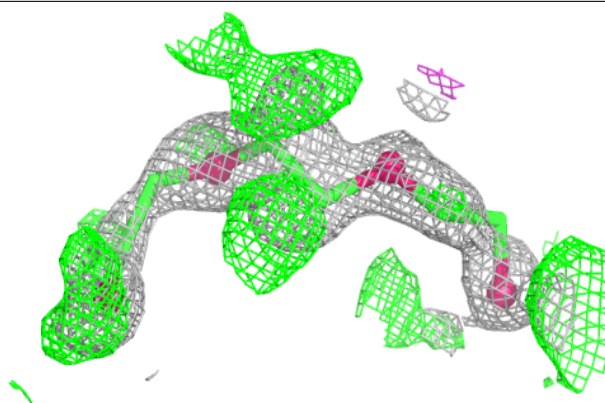
**Electron density around PG6 A 542:**

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

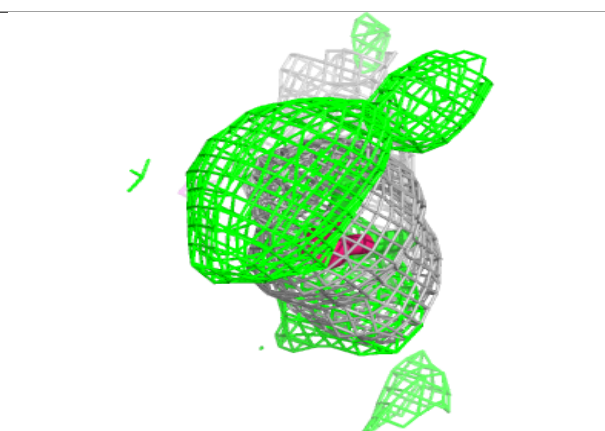
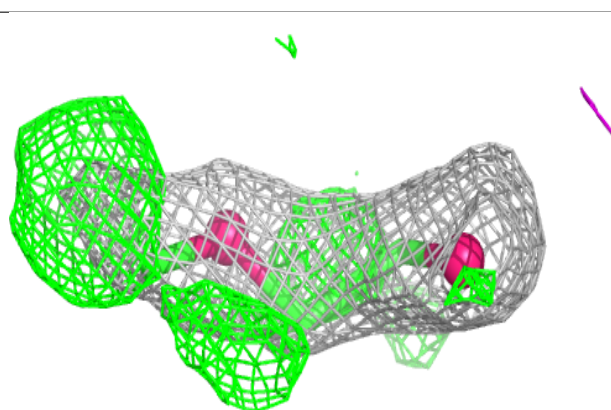
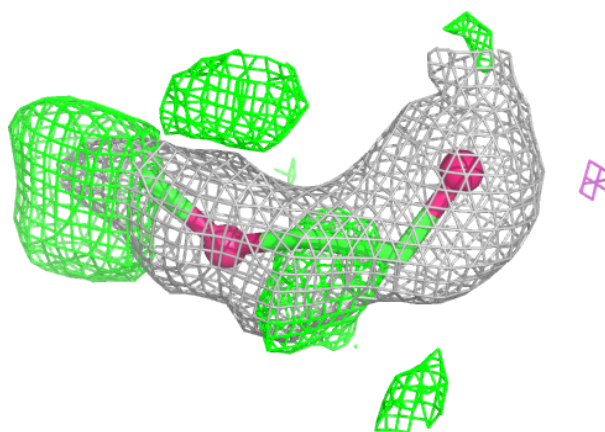


Electron density around PG6 A 543:

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

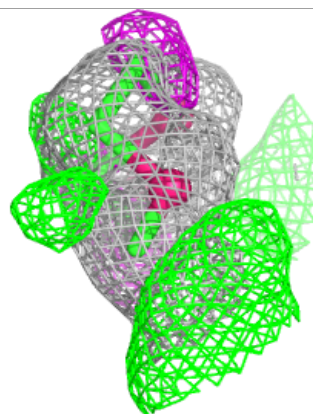
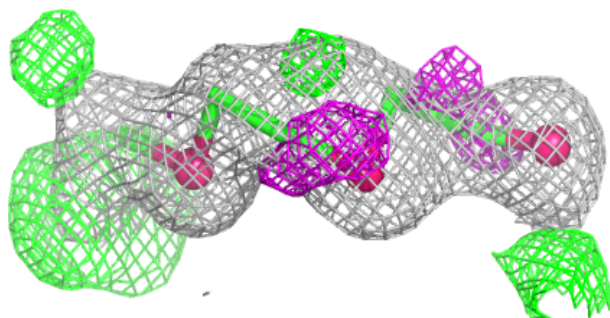
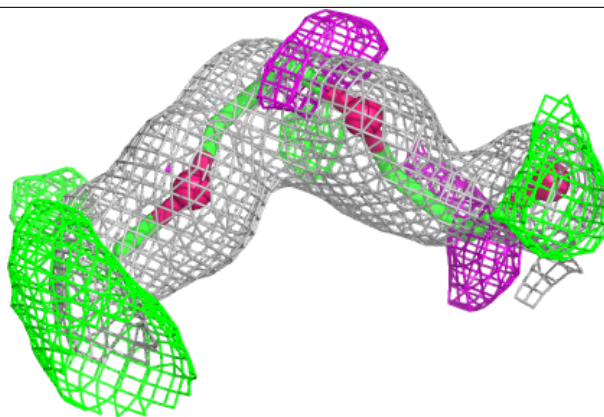
**Electron density around PG6 B 542:**

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



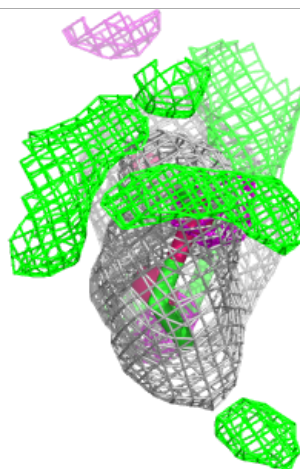
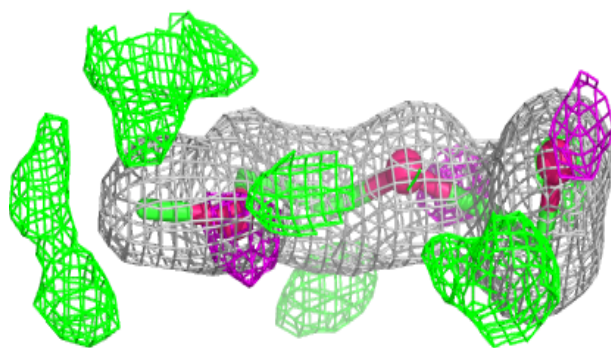
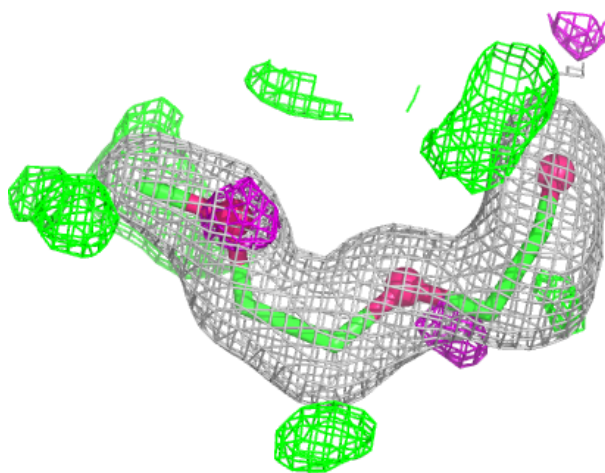
Electron density around PG6 B 535:

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



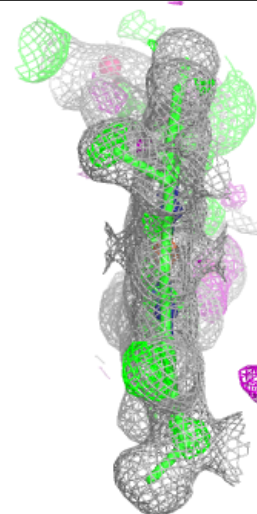
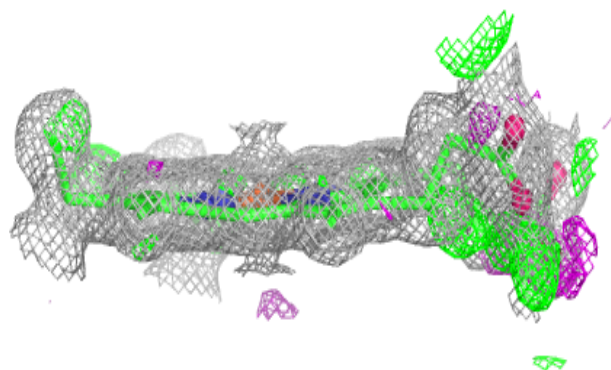
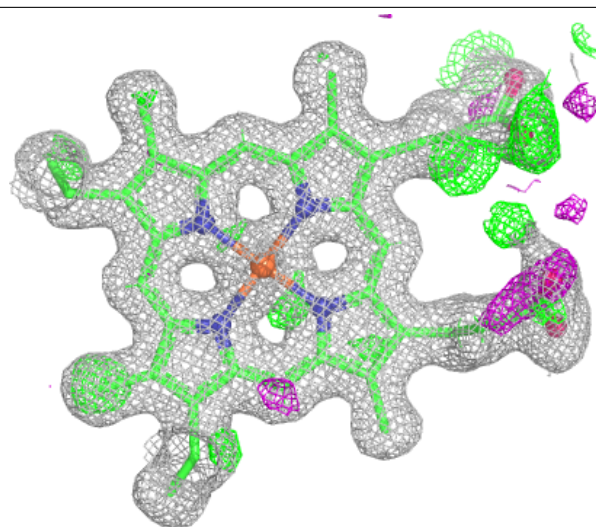
Electron density around PG6 A 534:

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



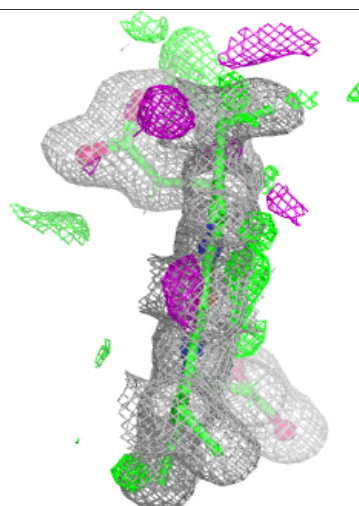
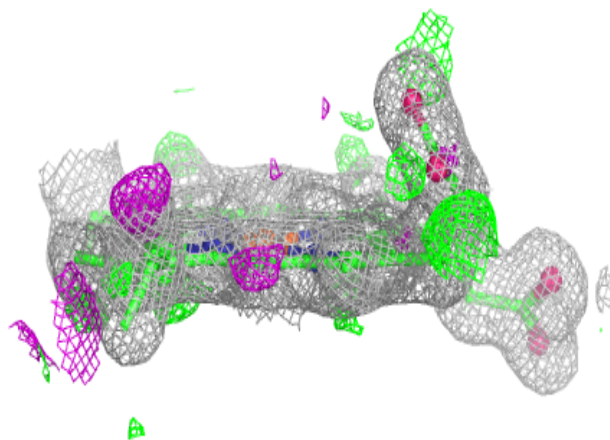
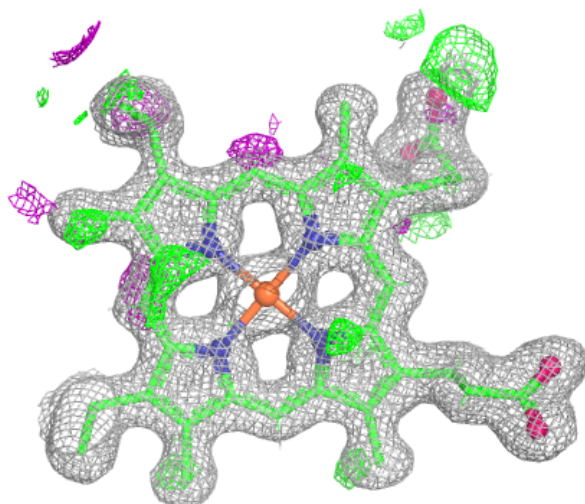
Electron density around HEC B 1003 (B):

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



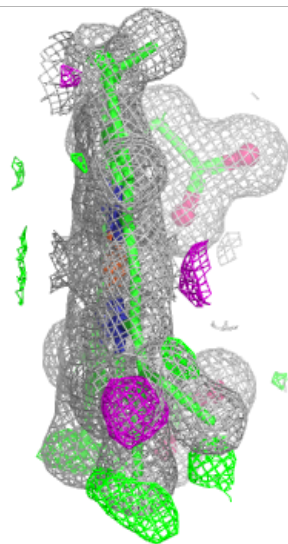
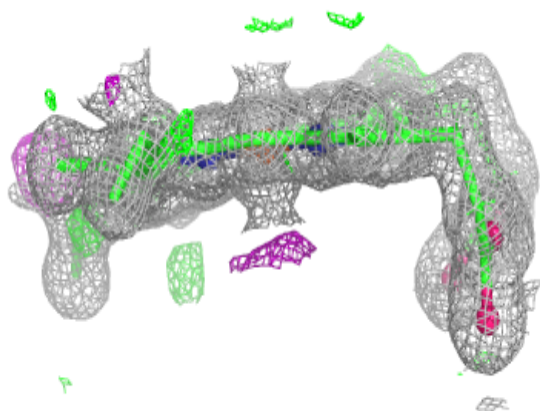
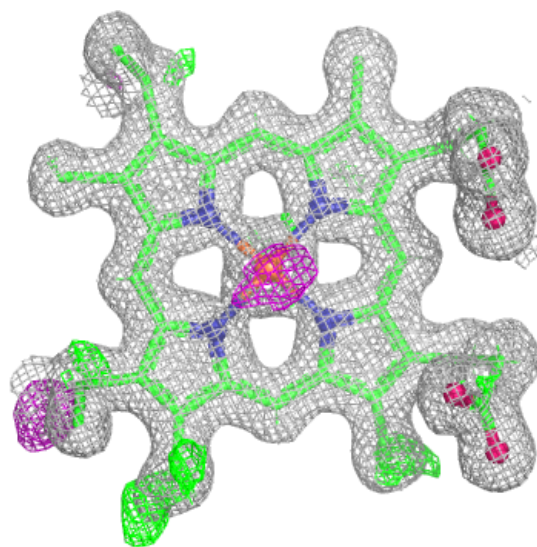
Electron density around HEC B 1001:

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



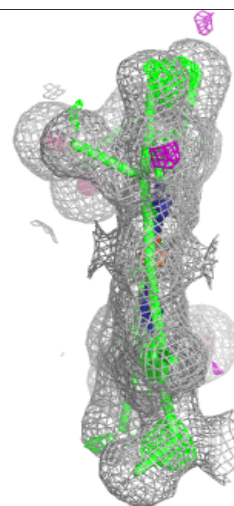
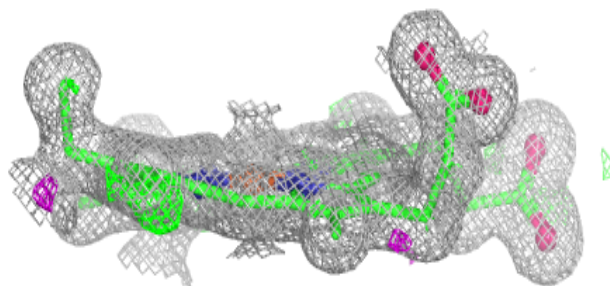
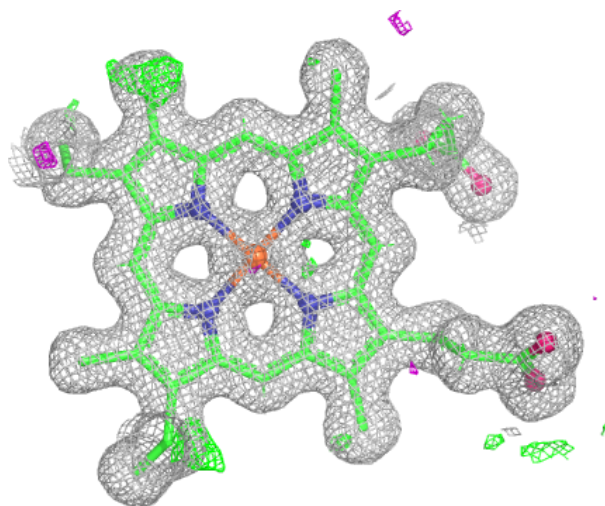
Electron density around HEC A 1004:

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and green (positive)



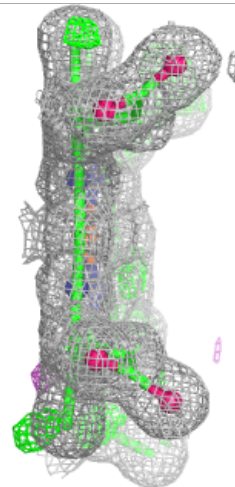
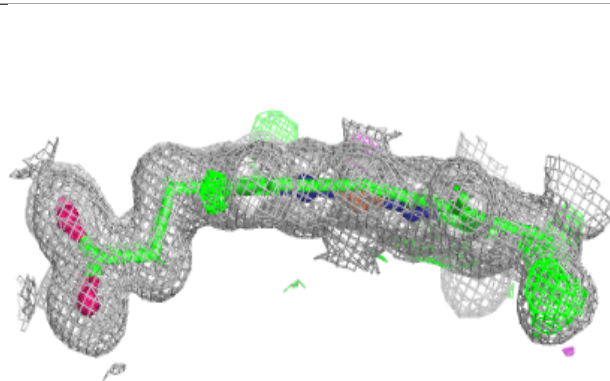
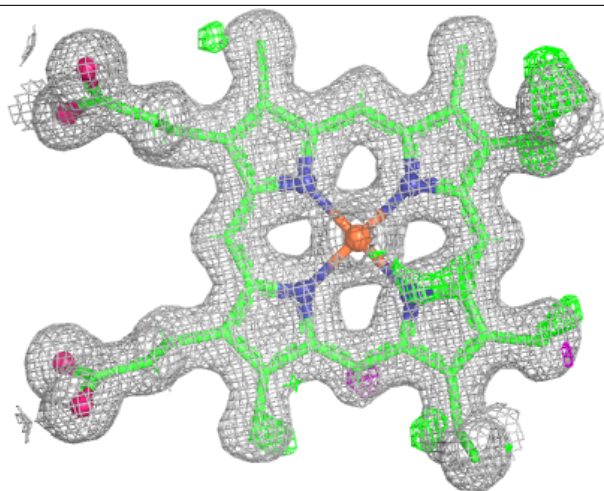
Electron density around HEC A 1005:

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



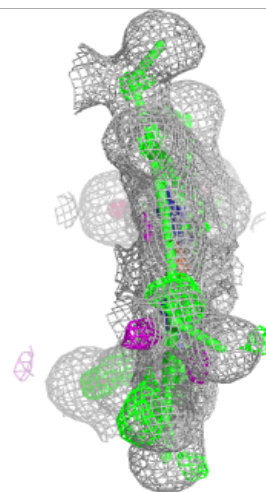
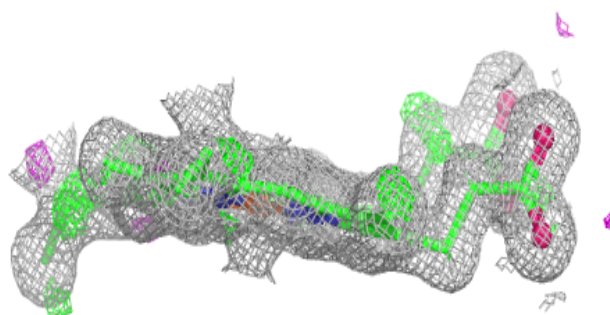
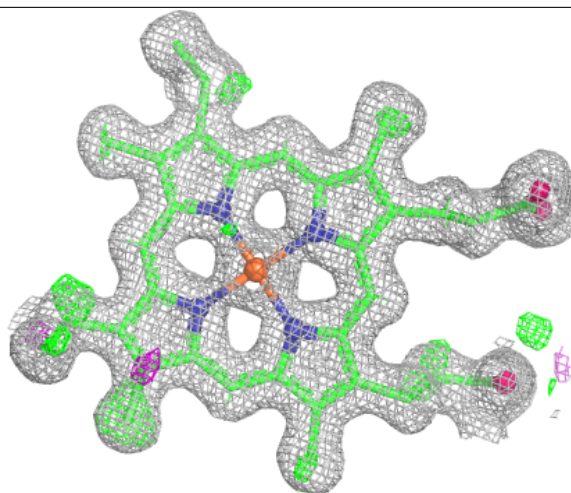
Electron density around HEC A 1006:

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



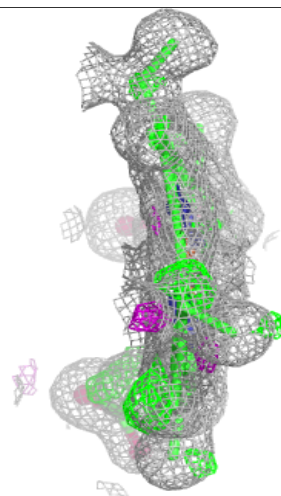
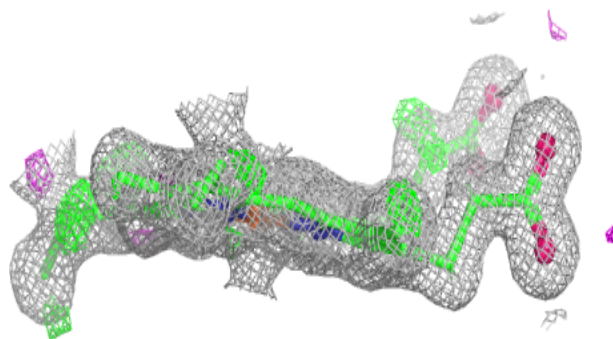
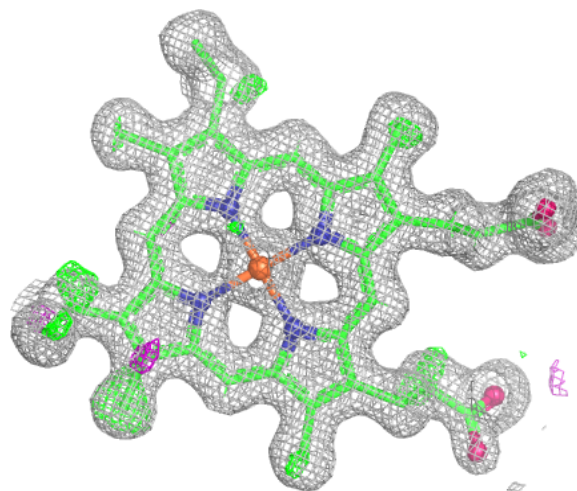
Electron density around HEC A 1007 (A):

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and green (positive)



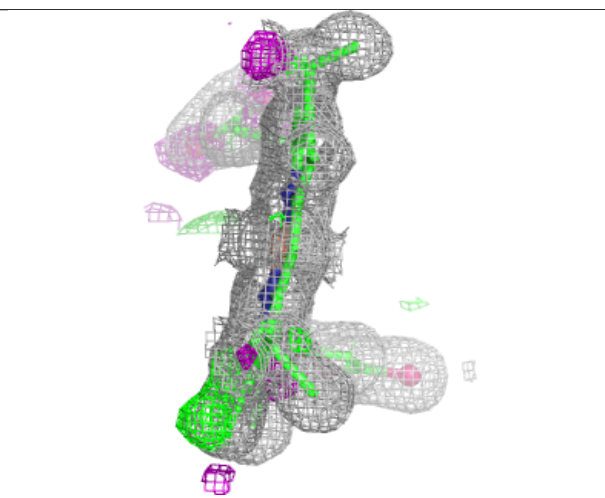
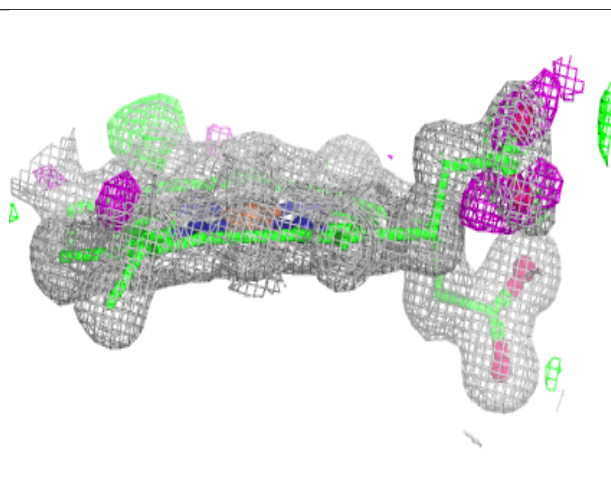
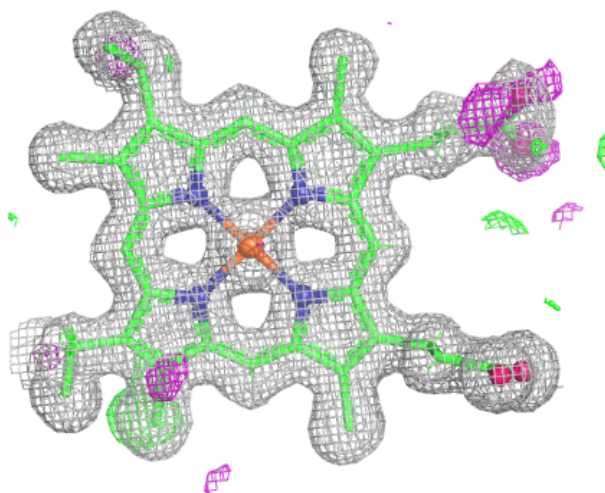
Electron density around HEC A 1007 (B):

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and green (positive)



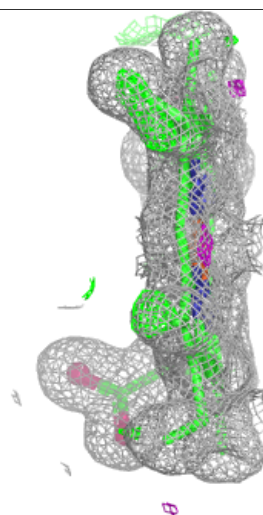
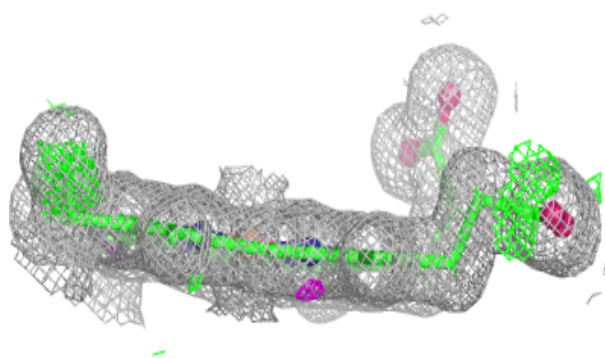
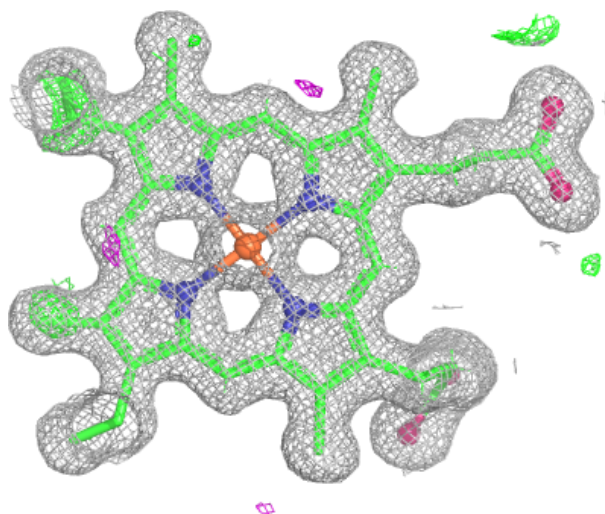
Electron density around HEC A 1008:

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



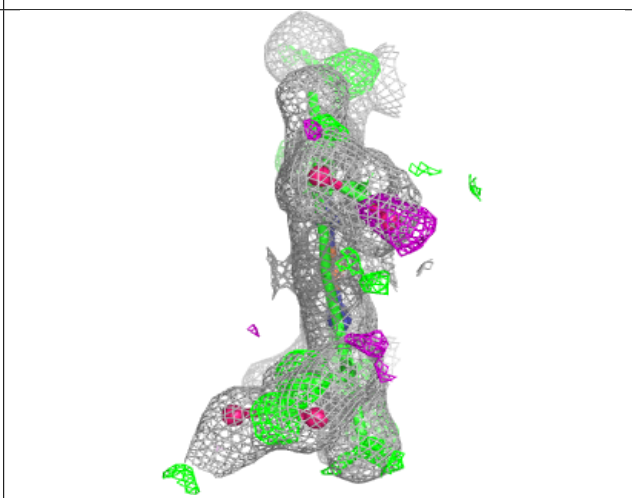
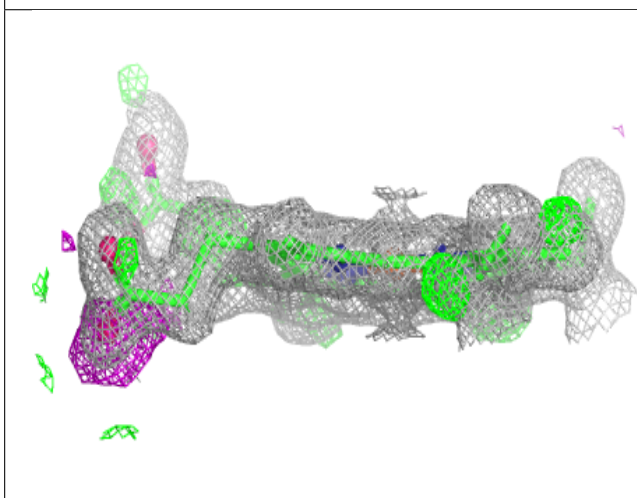
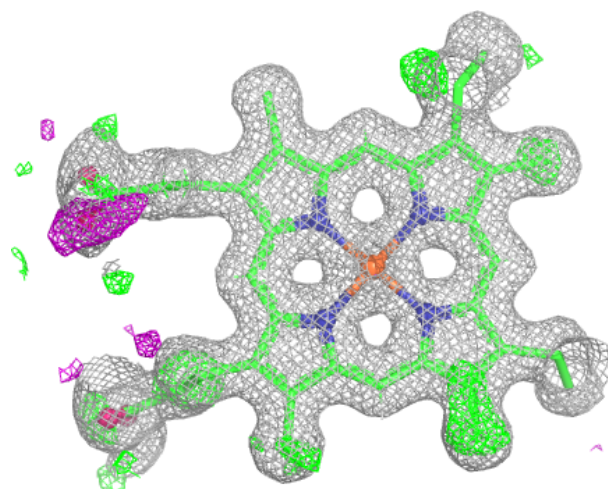
Electron density around HEC A 1002:

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



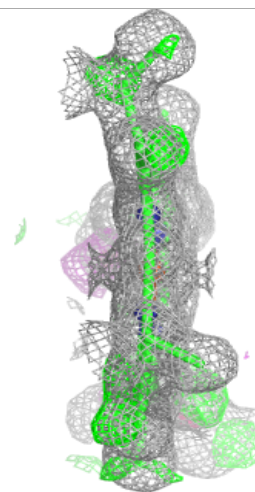
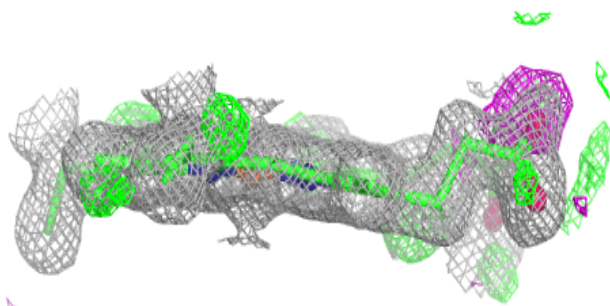
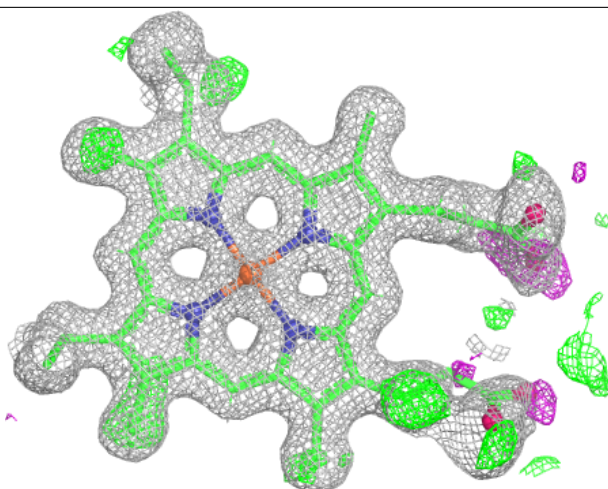
Electron density around HEC A 1003 (A):

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



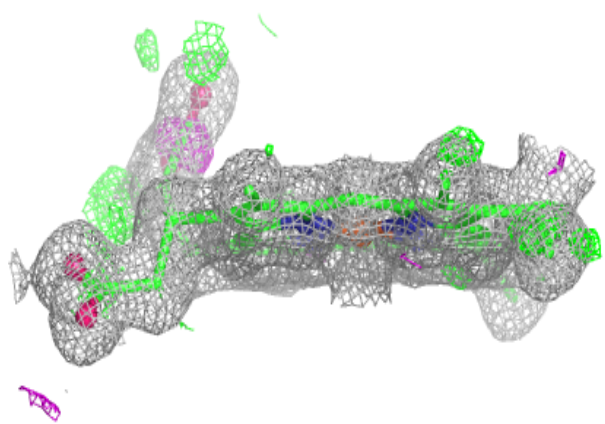
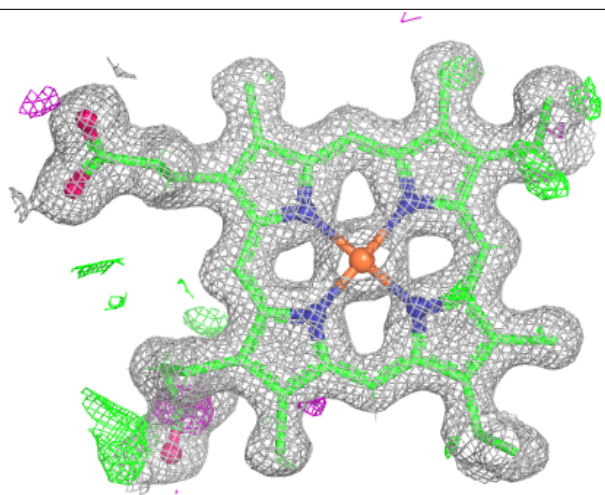
Electron density around HEC A 1003 (B):

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



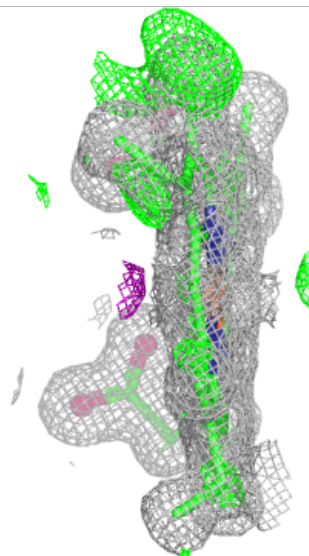
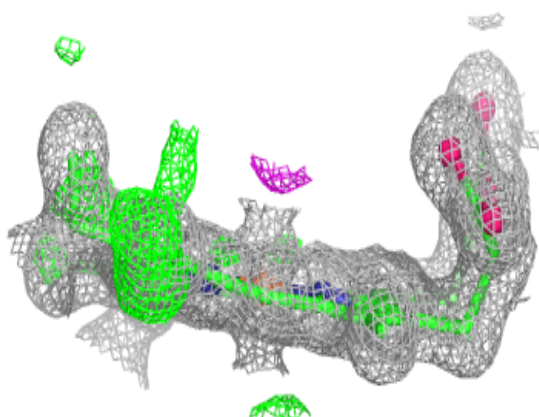
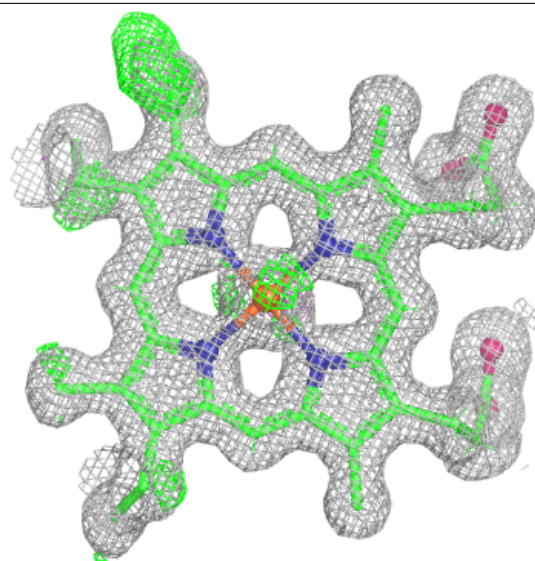
Electron density around HEC A 1001:

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



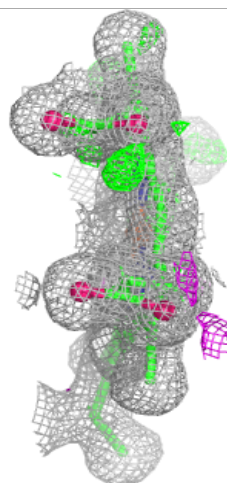
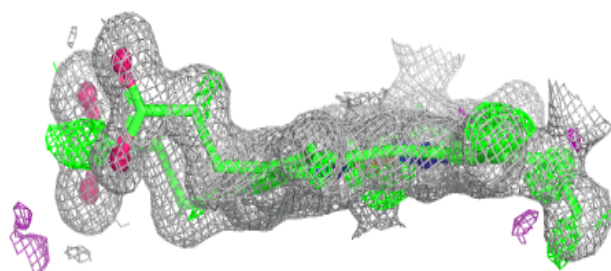
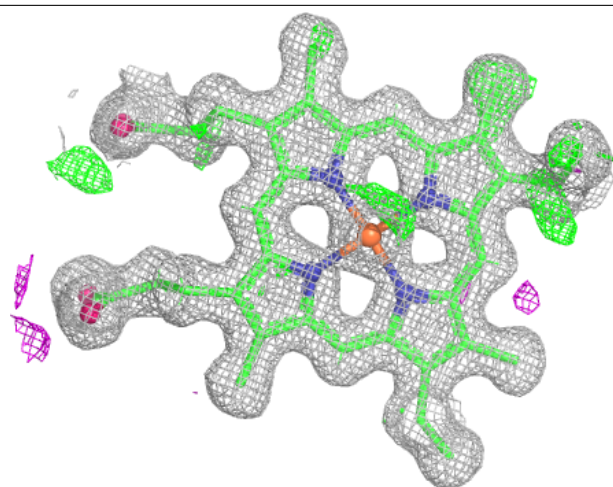
Electron density around HEC B 1004:

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



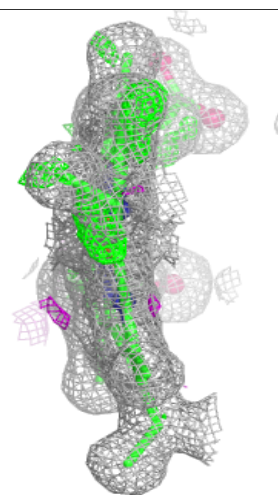
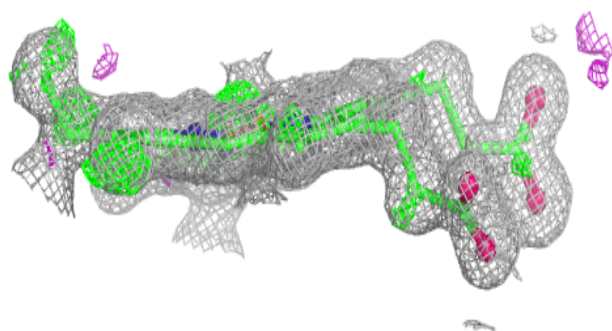
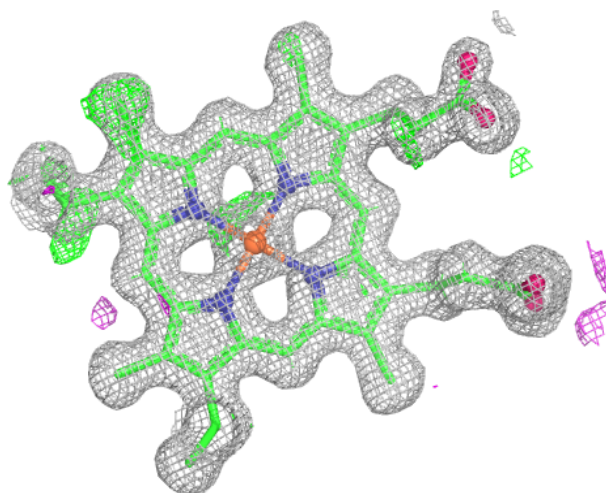
Electron density around HEC B 1007 (A):

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



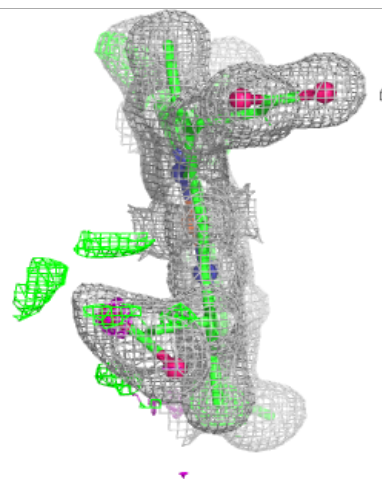
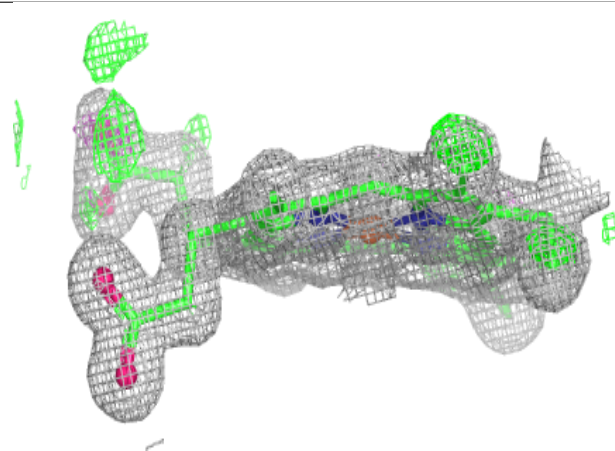
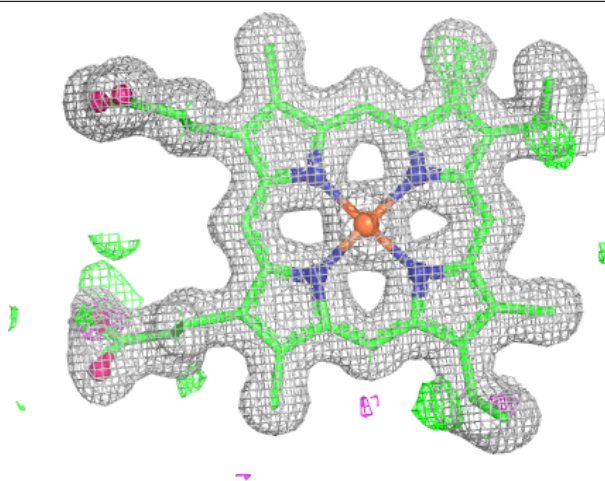
Electron density around HEC B 1007 (B):

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



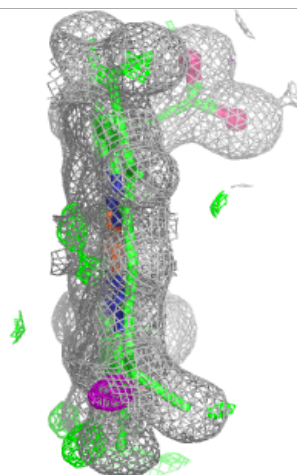
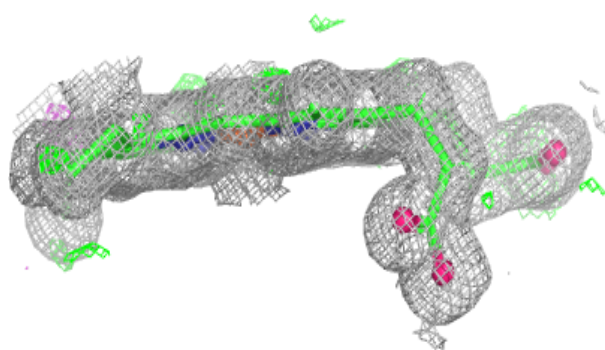
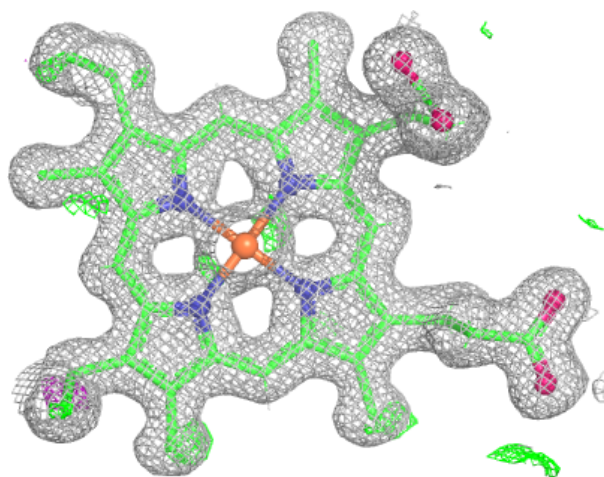
Electron density around HEC B 1008:

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



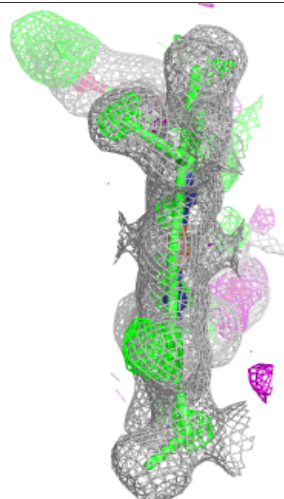
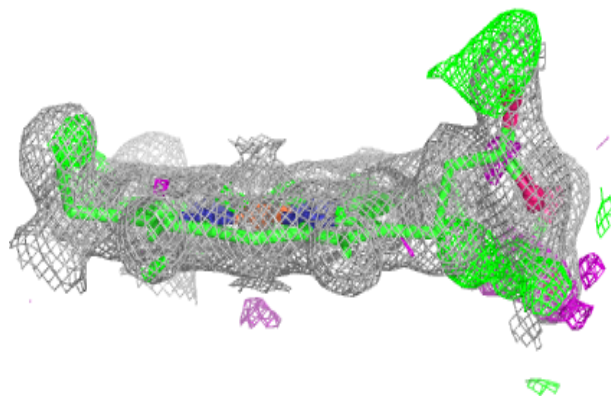
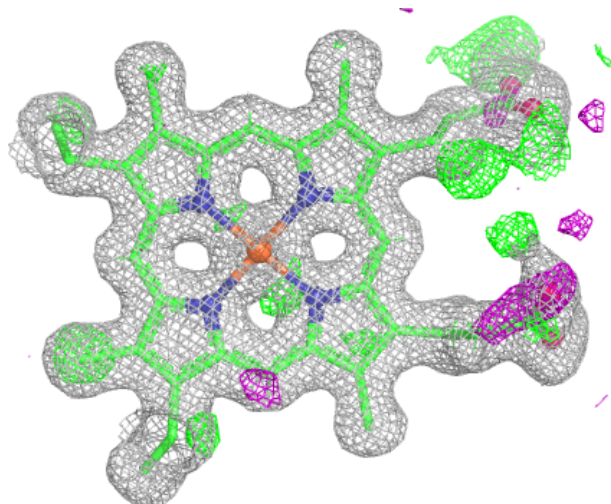
Electron density around HEC B 1002:

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



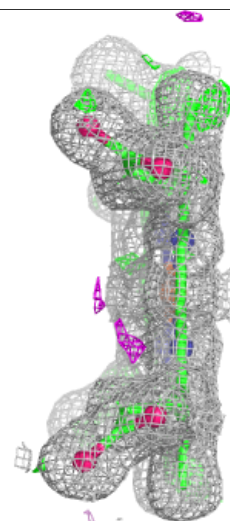
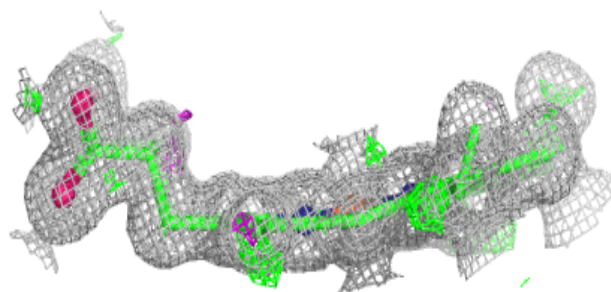
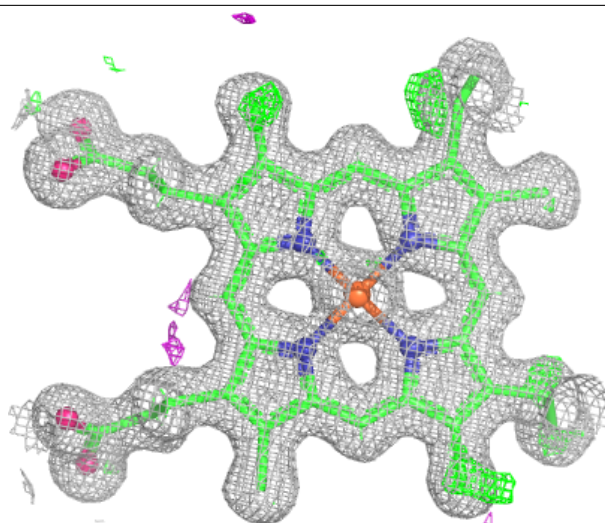
Electron density around HEC B 1003 (A):

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



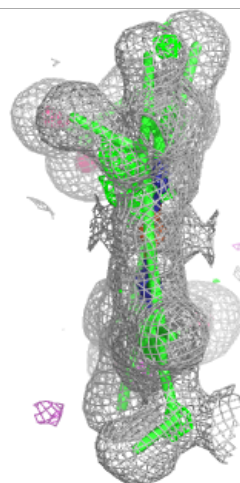
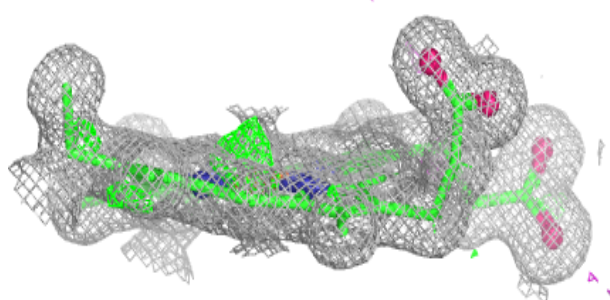
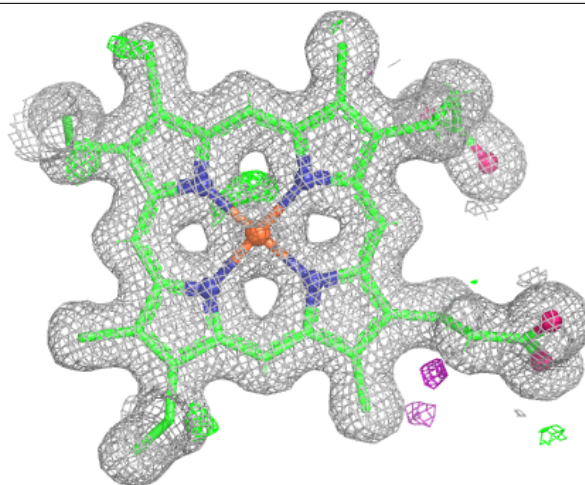
Electron density around HEC B 1006:

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



Electron density around HEC B 1005:

$2mF_o-DF_c$ (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.