



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 05:19 PM EDT

PDB ID : 2OT4 / pdb_00002ot4
Title : Structure of a hexameric multiheme c nitrite reductase from the extremophile bacterium *Thiobacillus denitrificans*
Authors : Polyakov, K.M.; Boyko, K.M.; Slutsky, A.; Tikhonova, T.V.; Antipov, A.N.; Zvyagilskaya, R.A.; Popov, A.N.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.
Deposited on : 2007-02-07
Resolution : 1.50 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

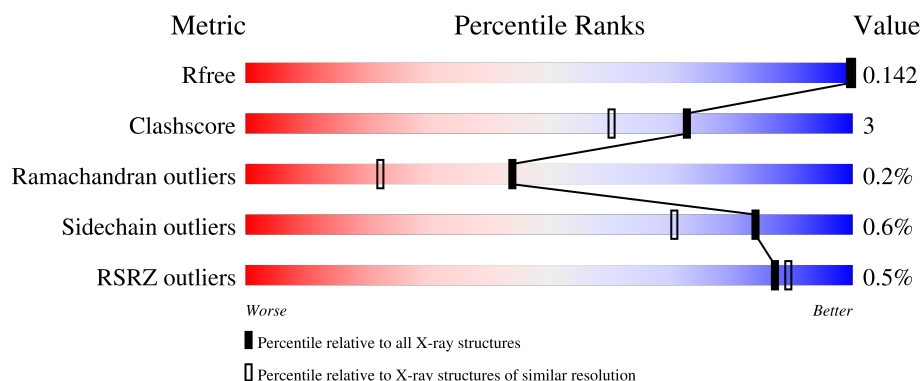
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5% .</div> </div> </div>
1	B	525	<div> <div></div> <div>94%</div> <div>5% ..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19040 atoms, of which 8559 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	520	Total	C	H	N	O	S	1099	32	0
			8158	2605	3946	766	801	40			
1	B	520	Total	C	H	N	O	S	1095	27	0
			8146	2602	3939	764	802	39			

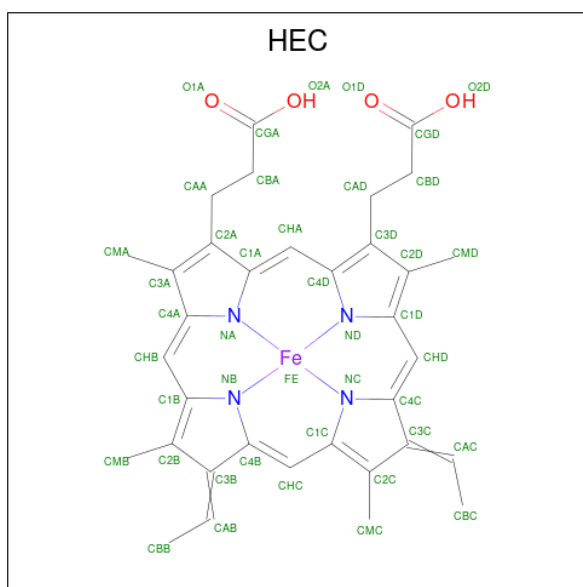
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	GLU	GLN	conflict	UNP Q5F2I3
B	467	GLU	GLN	conflict	UNP Q5F2I3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



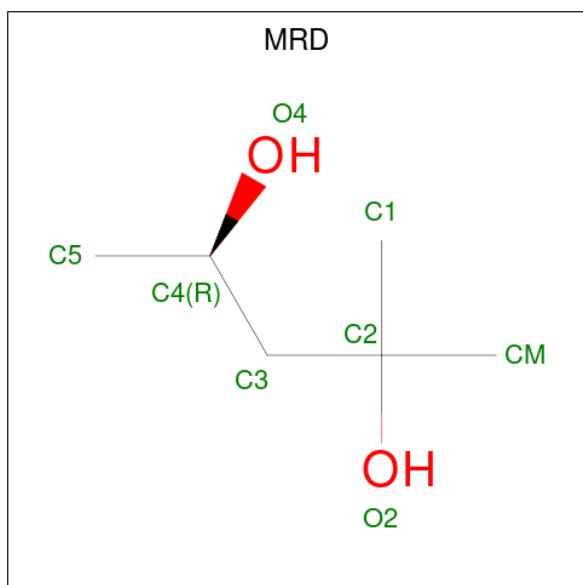
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 150	C 68	Fe 2	H 64	N 8	O 8	36	1
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	A	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0
3	B	1	Total 150	C 68	Fe 2	H 64	N 8	O 8	36	1
3	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	18	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		
3	B	1	Total	C	Fe	H	N	O	18	0
			75	34	1	32	4	4		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



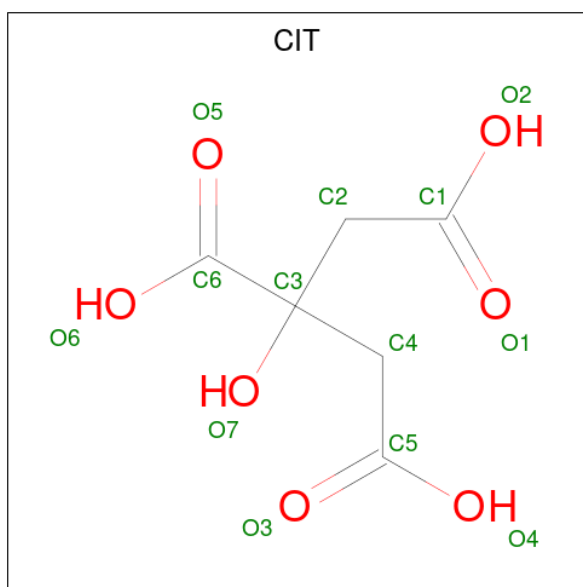
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	10	0
			22	6	14	2		
4	A	1	Total	C	H	O	10	0
			22	6	14	2		
4	B	1	Total	C	H	O	9	0
			21	6	13	2		
4	B	1	Total	C	H	O	10	0
			22	6	14	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	10	0
			22	6	14	2		
5	B	1	Total	C	H	O	10	0
			22	6	14	2		
5	B	1	Total	C	H	O	6	0
			18	6	10	2		

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	1	0
			18	6	5	7		

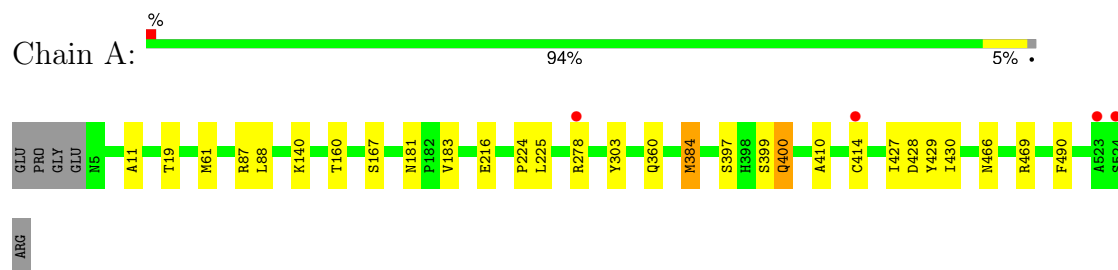
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	601	Total 601	O 601	0	0
7	B	616	Total 616	O 616	0	0

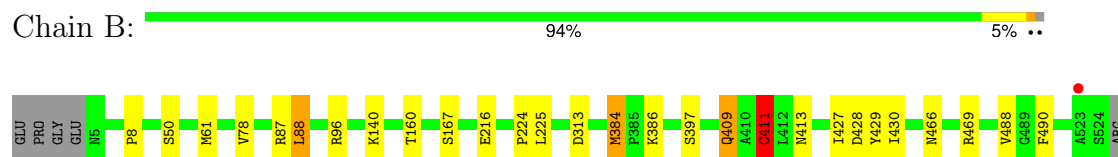
3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	193.92Å 193.92Å 193.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.04 – 1.50 24.04 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.04-1.50) 97.3 (24.04-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.126 , 0.141 0.128 , 0.142	Depositor DCC
R_{free} test set	11295 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19040	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 2.12% 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: MPD, CA, MRD, HEC, CIT

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	0.73	0/4477	0.81	1/6068 (0.0%)
1	B	0.74	4/4435 (0.1%)	0.83	1/6013 (0.0%)
All	All	0.73	4/8912 (0.0%)	0.82	2/12081 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411[A]	CYS	CA-C	5.63	1.60	1.52
1	B	411[B]	CYS	CA-C	5.63	1.60	1.52
1	B	409[A]	GLN	CA-C	5.41	1.59	1.52
1	B	409[B]	GLN	CA-C	5.41	1.59	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	MET	CB-CA-C	5.79	118.34	111.15
1	B	384	MET	CB-CA-C	5.19	117.58	111.15

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	4212	3946	3859	20	1
1	B	4207	3939	3897	22	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	387	288	270	11	0
3	B	387	288	270	7	0
4	A	16	28	28	2	0
4	B	16	27	28	1	0
5	A	8	14	14	0	0
5	B	16	24	28	0	0
6	B	13	5	5	1	1
7	A	601	0	0	5	1
7	B	616	0	0	9	0
All	All	10481	8559	8399	55	4

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 3.

All (55) 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:410[B]:ALA:O	3:A:1008[B]:HEC:HMC2	1.64	0.98
1:A:410[B]:ALA:O	3:A:1008[B]:HEC:CMC	2.15	0.94
3:A:1008[A]:HEC:HBC3	3:A:1008[A]:HEC:HMC1	1.57	0.85
3:A:1008[A]:HEC:HMC1	3:A:1008[A]:HEC:CBC	2.14	0.78
1:B:386:LYS:NZ	7:B:2672:HOH:O	2.13	0.77
3:A:1008[B]:HEC:HMC1	3:A:1008[B]:HEC:HBC3	1.71	0.72
6:B:2010:CIT:O3	7:B:2877:HOH:O	2.08	0.71
1:A:410[B]:ALA:O	3:A:1008[B]:HEC:HMC3	1.92	0.69
1:A:399[B]:SER:O	1:A:400[B]:GLN:C	2.40	0.65
1:B:428:ASP:HB3	7:B:2881:HOH:O	1.98	0.62
3:B:1008[B]:HEC:HMC1	3:B:1008[B]:HEC:HBC3	1.82	0.61
1:B:88[A]:LEU:HD13	7:B:2847:HOH:O	2.00	0.60
1:A:384:MET:HB2	1:A:397:SER:O	2.01	0.60
1:A:181:ASN:HD22	1:A:183:VAL:H	1.50	0.59
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.04	0.56
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.03	0.56
3:A:1002:HEC:HMC1	3:A:1002:HEC:HBC3	1.87	0.56
1:B:413:ASN:ND2	7:B:2942:HOH:O	2.40	0.55
3:B:1002:HEC:HMC1	3:B:1002:HEC:HBC3	1.89	0.55
1:B:384:MET:HB2	1:B:397:SER:O	2.07	0.54
1:A:11:ALA:HB3	4:A:2005:MRD:H5C2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:HG2	1:A:160[A]:THR:HG23	1.89	0.54
1:B:88[A]:LEU:CD1	7:B:2847:HOH:O	2.55	0.54
1:A:19:THR:HG22	7:A:2870:HOH:O	2.07	0.54
1:A:399[B]:SER:O	1:A:400[B]:GLN:O	2.27	0.53
1:B:427:ILE:HD11	3:B:1008[B]:HEC:HBB3	1.92	0.52
1:A:427:ILE:HD11	3:A:1008[B]:HEC:HBB3	1.91	0.52
1:B:167:SER:HB2	1:B:216[A]:GLU:HG2	1.93	0.51
3:B:1008[B]:HEC:HBB3	3:B:1008[B]:HEC:CMB	2.40	0.51
1:B:140:LYS:HG2	1:B:160[A]:THR:HG23	1.92	0.51
3:B:1008[A]:HEC:CBC	3:B:1008[A]:HEC:HMC1	2.40	0.50
1:B:167:SER:HB2	1:B:216[B]:GLU:HG3	1.94	0.49
1:A:303:TYR:OH	1:A:360[B]:GLN:NE2	2.45	0.48
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.96	0.48
3:A:1008[B]:HEC:HBD2	3:A:1008[B]:HEC:HMD3	1.96	0.47
1:A:430:ILE:HG21	1:A:490:PHE:HA	1.97	0.47
1:B:411[B]:CYS:HA	3:B:1008[B]:HEC:HHC	1.97	0.47
1:A:88[B]:LEU:HD21	7:A:2949:HOH:O	2.16	0.46
1:B:313:ASP:C	4:B:2288:MRD:H5C3	2.41	0.46
3:B:1008[B]:HEC:HBB3	3:B:1008[B]:HEC:HMB1	1.97	0.45
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.82	0.45
1:A:428:ASP:HB3	7:A:3337:HOH:O	2.16	0.44
3:A:1008[B]:HEC:HBD2	3:A:1008[B]:HEC:CMD	2.48	0.44
1:A:140:LYS:NZ	7:A:3293:HOH:O	2.50	0.43
4:A:2005:MRD:H1C1	1:B:8:PRO:HG3	1.99	0.43
1:B:413:ASN:HB2	7:B:2936:HOH:O	2.18	0.43
1:A:88[B]:LEU:CD2	7:A:2949:HOH:O	2.67	0.42
1:B:160[B]:THR:HG23	7:B:2457:HOH:O	2.19	0.41
1:A:167:SER:HB2	1:A:216[A]:GLU:HG2	2.02	0.41
1:B:224:PRO:O	1:B:225:LEU:C	2.63	0.41
1:B:409[B]:GLN:OE1	7:B:2675:HOH:O	2.22	0.41
3:A:1002:HEC:HBC3	3:A:1002:HEC:CMC	2.51	0.41
1:A:224:PRO:O	1:A:225:LEU:C	2.63	0.40
1:B:96[B]:ARG:CZ	1:B:488:VAL:HG22	2.50	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH11	1:A:429:TYR:HH[12_565]	1.31	0.29
1:B:87:ARG:HH11	1:B:429:TYR:HH[6_456]	1.32	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:OG	6:B:2010:CIT:O6[7_555]	2.12	0.08
7:A:3162:HOH:O	7:A:3164:HOH:O[12_565]	2.18	0.02

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	551/525 (105%)	523 (95%)	26 (5%)	2 (0%)	30	12
1	B	545/525 (104%)	521 (96%)	22 (4%)	2 (0%)	30	12
All	All	1096/1050 (104%)	1044 (95%)	48 (4%)	4 (0%)	44	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411[A]	CYS
1	B	411[B]	CYS
1	A	400[A]	GLN
1	A	400[B]	GLN

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	462/443 (104%)	455 (98%)	7 (2%)	60	35
1	B	459/443 (104%)	455 (99%)	4 (1%)	75	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	921/886 (104%)	910 (99%)	11 (1%)	84	44

All (11) 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
1	A	278[A]	ARG
1	A	278[B]	ARG
1	A	414[A]	CYS
1	A	414[B]	CYS
1	B	61[A]	MET
1	B	61[B]	MET
1	B	88[A]	LEU
1	B	88[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	190	GLN
1	A	340	GLN
1	A	466	ASN
1	B	190	GLN
1	B	340	GLN
1	B	413	ASN
1	B	466	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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$
5	MPD	B	2040	-	7,7,7	0.27	0	9,10,10	0.71	0
3	HEC	B	1008[A]	1	32,50,50	2.18	4 (12%)	30,82,82	2.58	9 (30%)
3	HEC	A	1001	1	32,50,50	1.91	6 (18%)	30,82,82	2.13	7 (23%)
3	HEC	A	1008[A]	1	32,50,50	2.26	3 (9%)	30,82,82	2.30	9 (30%)
3	HEC	B	1004	1	32,50,50	1.78	4 (12%)	30,82,82	2.11	6 (20%)
3	HEC	B	1002	1	32,50,50	1.63	3 (9%)	30,82,82	2.23	7 (23%)
3	HEC	A	1004	1	32,50,50	1.89	3 (9%)	30,82,82	2.12	6 (20%)
3	HEC	A	1007	1	32,50,50	2.01	3 (9%)	30,82,82	2.39	7 (23%)
3	HEC	A	1003	1	32,50,50	1.78	3 (9%)	30,82,82	2.13	9 (30%)
3	HEC	B	1003	1	32,50,50	1.79	5 (15%)	30,82,82	2.28	9 (30%)
5	MPD	A	2001	-	7,7,7	0.31	0	9,10,10	0.97	1 (11%)
3	HEC	A	1006	1	32,50,50	1.77	5 (15%)	30,82,82	2.34	8 (26%)
3	HEC	B	1006	1	32,50,50	1.62	6 (18%)	30,82,82	2.26	8 (26%)
5	MPD	B	2002	-	7,7,7	0.33	0	9,10,10	0.80	0
4	MRD	B	2288	-	7,7,7	0.28	0	9,10,10	0.70	0
6	CIT	B	2010	-	12,12,12	1.21	0	17,17,17	1.59	3 (17%)
3	HEC	B	1008[B]	1	32,50,50	2.27	7 (21%)	30,82,82	2.33	8 (26%)
3	HEC	A	1008[B]	1	32,50,50	2.23	4 (12%)	30,82,82	2.24	9 (30%)
4	MRD	A	2270	-	7,7,7	0.37	0	9,10,10	0.70	0
3	HEC	B	1001	1	32,50,50	1.80	4 (12%)	30,82,82	2.26	10 (33%)
4	MRD	B	2004	-	7,7,7	0.40	0	9,10,10	0.78	0
4	MRD	A	2005	-	7,7,7	0.37	0	9,10,10	0.72	0
3	HEC	B	1007	1	32,50,50	1.97	4 (12%)	30,82,82	2.36	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	A	1002	1	32,50,50	1.76	4 (12%)	30,82,82	2.05	5 (16%)
3	HEC	A	1005	1	32,50,50	1.97	8 (25%)	30,82,82	2.36	8 (26%)
3	HEC	B	1005	1	32,50,50	1.79	5 (15%)	30,82,82	2.29	7 (23%)

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	MPD	B	2040	-	-	1/5/5/5	-
3	HEC	B	1008[A]	1	-	2/10/54/54	-
3	HEC	A	1001	1	-	4/10/54/54	-
3	HEC	A	1008[A]	1	-	6/10/54/54	-
3	HEC	B	1004	1	-	2/10/54/54	-
3	HEC	B	1002	1	-	2/10/54/54	-
3	HEC	A	1004	1	-	2/10/54/54	-
3	HEC	A	1007	1	-	0/10/54/54	-
3	HEC	A	1003	1	-	2/10/54/54	-
3	HEC	B	1003	1	-	3/10/54/54	-
5	MPD	A	2001	-	-	0/5/5/5	-
3	HEC	A	1006	1	-	2/10/54/54	-
3	HEC	B	1006	1	-	0/10/54/54	-
5	MPD	B	2002	-	-	0/5/5/5	-
4	MRD	B	2288	-	-	0/5/5/5	-
6	CIT	B	2010	-	-	2/16/16/16	-
3	HEC	B	1008[B]	1	-	0/10/54/54	-
3	HEC	A	1008[B]	1	-	6/10/54/54	-
4	MRD	A	2270	-	-	0/5/5/5	-
3	HEC	B	1001	1	-	4/10/54/54	-
4	MRD	B	2004	-	-	5/5/5/5	-
4	MRD	A	2005	-	-	3/5/5/5	-
3	HEC	B	1007	1	-	1/10/54/54	-
3	HEC	A	1002	1	-	2/10/54/54	-
3	HEC	A	1005	1	-	4/10/54/54	-
3	HEC	B	1005	1	-	4/10/54/54	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	HEC	C2B-C3B	-7.58	1.32	1.40
3	B	1008[A]	HEC	C2B-C3B	-7.45	1.32	1.40
3	B	1008[B]	HEC	C2B-C3B	-7.17	1.32	1.40
3	A	1008[B]	HEC	C2B-C3B	-7.09	1.32	1.40
3	A	1008[A]	HEC	C2B-C3B	-7.01	1.32	1.40
3	A	1008[A]	HEC	C3C-C2C	-6.95	1.33	1.40
3	A	1005	HEC	C2B-C3B	-6.75	1.33	1.40
3	B	1007	HEC	C2B-C3B	-6.67	1.33	1.40
3	A	1004	HEC	C3C-C2C	-5.91	1.34	1.40
3	A	1004	HEC	C2B-C3B	-5.79	1.34	1.40
3	A	1008[B]	HEC	C3D-C2D	5.74	1.54	1.37
3	A	1001	HEC	C2B-C3B	-5.71	1.34	1.40
3	B	1007	HEC	C3C-C2C	-5.71	1.34	1.40
3	B	1001	HEC	C3C-C2C	-5.69	1.34	1.40
3	A	1003	HEC	C3C-C2C	-5.63	1.34	1.40
3	B	1008[A]	HEC	C3C-C2C	-5.56	1.34	1.40
3	B	1008[B]	HEC	C3D-C2D	5.55	1.54	1.37
3	B	1008[B]	HEC	C3C-C2C	-5.44	1.34	1.40
3	A	1002	HEC	C3C-C2C	-5.38	1.34	1.40
3	A	1001	HEC	C3C-C2C	-5.25	1.34	1.40
3	A	1008[B]	HEC	C3C-C2C	-5.18	1.34	1.40
3	A	1008[A]	HEC	C3D-C2D	5.09	1.52	1.37
3	A	1006	HEC	C2B-C3B	-5.03	1.35	1.40
3	B	1003	HEC	C2B-C3B	-5.02	1.35	1.40
3	B	1008[A]	HEC	C3D-C2D	4.93	1.52	1.37
3	B	1004	HEC	C2B-C3B	-4.88	1.35	1.40
3	B	1002	HEC	C3C-C2C	-4.69	1.35	1.40
3	B	1005	HEC	C2B-C3B	-4.46	1.35	1.40
3	B	1006	HEC	C3C-C2C	-4.46	1.35	1.40
3	B	1005	HEC	C3C-C2C	-4.42	1.35	1.40
3	A	1006	HEC	C3C-C2C	-4.36	1.35	1.40
3	A	1007	HEC	C3C-C2C	-4.29	1.35	1.40
3	B	1004	HEC	C3C-C2C	-4.27	1.35	1.40
3	B	1003	HEC	C3C-C2C	-4.25	1.36	1.40
3	A	1002	HEC	C2B-C3B	-4.08	1.36	1.40
3	A	1005	HEC	C3C-C2C	-3.98	1.36	1.40
3	A	1003	HEC	C2B-C3B	-3.96	1.36	1.40
3	B	1006	HEC	C2B-C3B	-3.80	1.36	1.40
3	B	1001	HEC	C3D-C2D	3.69	1.48	1.37
3	A	1003	HEC	C3D-C2D	3.56	1.48	1.37
3	B	1001	HEC	C2B-C3B	-3.44	1.36	1.40
3	A	1006	HEC	C3D-C2D	3.43	1.47	1.37
3	B	1006	HEC	C3D-C2D	3.39	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005	HEC	C3D-C2D	3.39	1.47	1.37
3	A	1007	HEC	C3D-C2D	3.35	1.47	1.37
3	B	1003	HEC	C3D-C2D	3.31	1.47	1.37
3	A	1001	HEC	C3D-C2D	3.26	1.47	1.37
3	B	1005	HEC	C3D-C2D	3.25	1.47	1.37
3	B	1004	HEC	C3D-C2D	3.13	1.47	1.37
3	B	1002	HEC	C3D-C2D	3.08	1.46	1.37
3	A	1004	HEC	C3D-C2D	3.05	1.46	1.37
3	B	1007	HEC	C3D-C2D	2.96	1.46	1.37
3	A	1002	HEC	C3D-C2D	2.83	1.46	1.37
3	A	1005	HEC	C3C-C4C	2.54	1.47	1.43
3	A	1005	HEC	O2D-CGD	-2.41	1.22	1.30
3	A	1005	HEC	C4B-C3B	2.39	1.47	1.43
3	B	1002	HEC	C2B-C3B	-2.37	1.38	1.40
3	B	1005	HEC	O2D-CGD	-2.33	1.23	1.30
3	A	1005	HEC	C1D-ND	2.29	1.41	1.36
3	B	1006	HEC	C3C-C4C	2.27	1.47	1.43
3	A	1008[B]	HEC	C4D-ND	2.25	1.40	1.36
3	B	1003	HEC	C4D-CHA	-2.23	1.34	1.41
3	B	1004	HEC	C4D-ND	2.22	1.40	1.36
3	A	1001	HEC	CBB-CAB	2.20	1.57	1.49
3	B	1003	HEC	C3C-C4C	2.20	1.47	1.43
3	A	1002	HEC	C1B-NB	2.19	1.40	1.36
3	A	1001	HEC	C1D-ND	2.18	1.40	1.36
3	A	1006	HEC	C3C-C4C	2.15	1.47	1.43
3	A	1006	HEC	CBB-CAB	2.13	1.57	1.49
3	B	1008[B]	HEC	C4D-ND	2.12	1.40	1.36
3	B	1006	HEC	C4D-ND	2.11	1.40	1.36
3	A	1001	HEC	C4D-ND	2.06	1.40	1.36
3	A	1005	HEC	CBB-CAB	2.05	1.57	1.49
3	B	1007	HEC	C4B-C3B	2.05	1.46	1.43
3	B	1008[B]	HEC	C2A-C1A	2.03	1.47	1.42
3	B	1008[B]	HEC	C3C-C4C	2.02	1.46	1.43
3	B	1005	HEC	C2A-C1A	2.01	1.47	1.42
3	B	1006	HEC	C1D-CHD	-2.01	1.35	1.41
3	B	1008[B]	HEC	C1D-ND	2.01	1.40	1.36
3	B	1001	HEC	C4D-ND	2.01	1.40	1.36
3	B	1008[A]	HEC	C1D-CHD	-2.00	1.35	1.41

All (145) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1008[A]	HEC	CBB-CAB-C3B	-8.34	107.98	127.49
3	B	1001	HEC	CBB-CAB-C3B	-8.25	108.18	127.49
3	A	1008[A]	HEC	CBB-CAB-C3B	-7.97	108.83	127.49
3	B	1005	HEC	CBB-CAB-C3B	-7.97	108.83	127.49
3	B	1007	HEC	CBB-CAB-C3B	-7.62	109.65	127.49
3	A	1004	HEC	CBB-CAB-C3B	-7.57	109.78	127.49
3	A	1001	HEC	CBB-CAB-C3B	-7.56	109.79	127.49
3	A	1003	HEC	CBB-CAB-C3B	-7.55	109.81	127.49
3	B	1002	HEC	CBB-CAB-C3B	-7.54	109.85	127.49
3	B	1006	HEC	CBB-CAB-C3B	-7.52	109.89	127.49
3	A	1005	HEC	CBB-CAB-C3B	-7.46	110.03	127.49
3	A	1006	HEC	CBB-CAB-C3B	-7.45	110.06	127.49
3	B	1003	HEC	CBB-CAB-C3B	-7.44	110.08	127.49
3	A	1002	HEC	CBB-CAB-C3B	-7.08	110.92	127.49
3	B	1008[B]	HEC	CBB-CAB-C3B	-7.07	110.94	127.49
3	B	1004	HEC	CBB-CAB-C3B	-6.81	111.54	127.49
3	A	1007	HEC	CBB-CAB-C3B	-6.70	111.81	127.49
3	A	1008[B]	HEC	CBB-CAB-C3B	-6.57	112.12	127.49
3	A	1007	HEC	CMB-C2B-C1B	-6.54	118.88	128.46
3	A	1008[B]	HEC	CBC-CAC-C3C	-5.60	114.38	127.49
3	B	1002	HEC	CBC-CAC-C3C	-5.48	114.66	127.49
3	A	1005	HEC	CBC-CAC-C3C	-5.48	114.67	127.49
3	B	1007	HEC	CMB-C2B-C1B	-5.47	120.44	128.46
3	A	1008[A]	HEC	CBC-CAC-C3C	-5.43	114.78	127.49
3	A	1006	HEC	CBC-CAC-C3C	-5.41	114.84	127.49
3	A	1002	HEC	CBC-CAC-C3C	-5.36	114.96	127.49
3	B	1008[B]	HEC	CBC-CAC-C3C	-5.29	115.12	127.49
3	B	1008[A]	HEC	CBC-CAC-C3C	-5.24	115.23	127.49
3	A	1007	HEC	CBC-CAC-C3C	-5.03	115.71	127.49
3	A	1001	HEC	CBC-CAC-C3C	-4.93	115.95	127.49
3	B	1006	HEC	CBC-CAC-C3C	-4.83	116.18	127.49
3	B	1003	HEC	CMB-C2B-C1B	-4.81	121.41	128.46
3	B	1005	HEC	CBC-CAC-C3C	-4.79	116.28	127.49
3	A	1008[B]	HEC	CMC-C2C-C1C	-4.78	121.45	128.46
3	B	1004	HEC	CBC-CAC-C3C	-4.66	116.59	127.49
3	A	1005	HEC	CMB-C2B-C1B	-4.53	121.81	128.46
3	B	1001	HEC	CBC-CAC-C3C	-4.50	116.97	127.49
3	B	1008[B]	HEC	CMC-C2C-C1C	-4.44	121.95	128.46
3	B	1006	HEC	CMC-C2C-C1C	-4.39	122.02	128.46
3	B	1005	HEC	CMB-C2B-C1B	-4.38	122.04	128.46
3	A	1002	HEC	CMB-C2B-C1B	-4.24	122.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	HEC	CBC-CAC-C3C	-4.20	117.67	127.49
3	A	1004	HEC	CMB-C2B-C1B	-4.07	122.49	128.46
3	B	1005	HEC	CMB-C2B-C3B	4.04	130.57	125.82
3	B	1008[B]	HEC	CBD-CAD-C3D	-3.96	105.88	112.54
3	A	1004	HEC	CBC-CAC-C3C	-3.93	118.30	127.49
3	A	1003	HEC	CMB-C2B-C1B	-3.90	122.74	128.46
3	A	1008[A]	HEC	CBA-CAA-C2A	-3.87	106.17	112.55
3	B	1008[A]	HEC	CMC-C2C-C1C	-3.86	122.81	128.46
3	B	1007	HEC	CBD-CAD-C3D	-3.85	106.07	112.54
3	A	1007	HEC	CMB-C2B-C3B	3.83	130.32	125.82
3	B	1007	HEC	CBC-CAC-C3C	-3.82	118.55	127.49
3	B	1008[A]	HEC	C1D-C2D-C3D	-3.80	104.35	107.00
3	B	1008[A]	HEC	CBD-CAD-C3D	-3.80	106.16	112.54
3	A	1007	HEC	CBD-CAD-C3D	-3.79	106.17	112.54
3	A	1006	HEC	CMC-C2C-C1C	-3.76	122.95	128.46
3	B	1004	HEC	CMB-C2B-C1B	-3.69	123.05	128.46
6	B	2010	CIT	O6-C6-C3	3.69	120.22	113.14
3	B	1008[A]	HEC	CMC-C2C-C3C	3.62	130.07	125.82
3	B	1004	HEC	CMC-C2C-C1C	-3.61	123.17	128.46
3	B	1008[A]	HEC	CBA-CAA-C2A	-3.60	106.62	112.55
3	A	1006	HEC	CMB-C2B-C1B	-3.58	123.21	128.46
3	A	1001	HEC	CMB-C2B-C1B	-3.58	123.21	128.46
3	B	1002	HEC	CMB-C2B-C1B	-3.43	123.43	128.46
3	B	1006	HEC	CMB-C2B-C1B	-3.40	123.47	128.46
3	A	1005	HEC	CMB-C2B-C3B	3.38	129.80	125.82
3	B	1007	HEC	CMB-C2B-C3B	3.32	129.73	125.82
3	B	1002	HEC	CMC-C2C-C1C	-3.32	123.59	128.46
3	A	1005	HEC	CMC-C2C-C1C	-3.32	123.59	128.46
3	B	1007	HEC	CMC-C2C-C1C	-3.31	123.61	128.46
3	B	1004	HEC	CMB-C2B-C3B	3.25	129.65	125.82
3	A	1007	HEC	C1D-C2D-C3D	-3.13	104.82	107.00
3	A	1003	HEC	CBC-CAC-C3C	-3.12	120.18	127.49
3	A	1003	HEC	CMC-C2C-C1C	-3.08	123.95	128.46
3	B	1005	HEC	CMC-C2C-C1C	-3.07	123.96	128.46
3	B	1001	HEC	CMC-C2C-C1C	-3.06	123.97	128.46
3	A	1008[A]	HEC	C1D-C2D-C3D	-3.04	104.88	107.00
3	B	1001	HEC	CMB-C2B-C1B	-2.96	124.12	128.46
3	A	1006	HEC	CMB-C2B-C3B	2.96	129.30	125.82
3	A	1004	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
3	A	1004	HEC	CMC-C2C-C1C	-2.94	124.16	128.46
3	B	1001	HEC	CBD-CAD-C3D	-2.91	107.65	112.54
3	B	1003	HEC	CMB-C2B-C3B	2.90	129.23	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	HEC	CBA-CAA-C2A	-2.88	107.80	112.55
3	A	1004	HEC	CMB-C2B-C3B	2.87	129.19	125.82
3	B	1007	HEC	C1D-C2D-C3D	-2.86	105.00	107.00
3	A	1006	HEC	CMC-C2C-C3C	2.86	129.18	125.82
3	B	1002	HEC	CAA-CBA-CGA	-2.84	106.18	113.83
3	A	1001	HEC	CMC-C2C-C1C	-2.81	124.34	128.46
3	B	1003	HEC	CBA-CAA-C2A	-2.80	107.93	112.55
3	B	1008[B]	HEC	CMC-C2C-C3C	-2.80	122.53	125.82
3	A	1002	HEC	CMB-C2B-C3B	2.80	129.11	125.82
3	A	1008[B]	HEC	CBA-CAA-C2A	-2.79	107.95	112.55
3	B	1008[B]	HEC	CMB-C2B-C1B	-2.74	124.44	128.46
3	B	1008[A]	HEC	O1A-CGA-CBA	-2.69	114.57	123.09
3	B	1003	HEC	CMC-C2C-C1C	-2.66	124.56	128.46
3	B	1008[A]	HEC	O2A-CGA-CBA	2.65	122.37	114.00
3	A	1008[A]	HEC	O1A-CGA-CBA	-2.60	114.84	123.09
3	B	1003	HEC	C1D-C2D-C3D	-2.56	105.21	107.00
3	B	1006	HEC	CMA-C3A-C2A	2.56	129.76	124.94
3	A	1005	HEC	CMC-C2C-C3C	2.55	128.82	125.82
3	B	1006	HEC	CMC-C2C-C3C	2.55	128.82	125.82
3	B	1005	HEC	CMA-C3A-C2A	2.55	129.74	124.94
3	A	1006	HEC	CBD-CAD-C3D	-2.53	108.28	112.54
3	B	1004	HEC	C1D-C2D-C3D	-2.52	105.24	107.00
3	A	1008[B]	HEC	CMD-C2D-C1D	-2.52	124.77	128.46
5	A	2001	MPD	CM-C2-C1	-2.50	105.02	110.63
3	A	1003	HEC	CMC-C2C-C3C	2.49	128.75	125.82
3	A	1006	HEC	CMA-C3A-C2A	2.44	129.55	124.94
3	B	1006	HEC	CBD-CAD-C3D	-2.39	108.53	112.54
3	A	1007	HEC	CBA-CAA-C2A	-2.36	108.67	112.55
3	B	1002	HEC	CMC-C2C-C3C	2.36	128.59	125.82
3	A	1003	HEC	O2D-CGD-CBD	2.35	121.44	114.00
3	B	1002	HEC	CMB-C2B-C3B	2.35	128.59	125.82
3	A	1008[A]	HEC	O2A-CGA-CBA	2.31	121.31	114.00
3	A	1008[B]	HEC	O1A-CGA-CBA	-2.30	115.81	123.09
3	B	1007	HEC	CBA-CAA-C2A	-2.28	108.80	112.55
3	B	1007	HEC	CMA-C3A-C2A	2.27	129.21	124.94
3	B	1008[B]	HEC	O1A-CGA-CBA	-2.26	115.93	123.09
3	A	1008[A]	HEC	C2B-C3B-C4B	2.25	108.78	106.35
3	A	1003	HEC	O1D-CGD-CBD	-2.25	115.95	123.09
3	B	1003	HEC	O2D-CGD-CBD	2.25	121.09	114.00
3	B	1008[B]	HEC	O2A-CGA-CBA	2.24	121.08	114.00
3	B	1001	HEC	C3C-C4C-NC	-2.22	106.75	110.94
3	B	1003	HEC	O2A-CGA-CBA	2.19	120.91	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1008[B]	HEC	O2A-CGA-CBA	2.17	120.87	114.00
3	B	1001	HEC	O1D-CGD-CBD	-2.16	116.23	123.09
3	A	1005	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
3	A	1001	HEC	CAD-CBD-CGD	-2.15	108.03	113.83
3	A	1001	HEC	CMC-C2C-C3C	2.14	128.34	125.82
3	B	1005	HEC	O1A-CGA-CBA	-2.14	116.29	123.09
3	A	1008[A]	HEC	CMD-C2D-C3D	2.14	128.97	124.94
3	B	1001	HEC	CBA-CAA-C2A	-2.12	109.06	112.55
3	A	1008[B]	HEC	CMB-C2B-C1B	-2.11	125.36	128.46
6	B	2010	CIT	O4-C5-C4	2.11	121.02	114.35
3	A	1003	HEC	CMA-C3A-C2A	2.10	128.90	124.94
3	B	1001	HEC	C4C-C3C-C2C	2.10	108.62	106.35
3	A	1002	HEC	CAA-CBA-CGA	-2.07	108.25	113.83
3	A	1001	HEC	O1A-CGA-CBA	-2.07	116.53	123.09
6	B	2010	CIT	O2-C1-C2	2.07	120.89	114.35
3	A	1005	HEC	CMA-C3A-C2A	2.05	128.81	124.94
3	A	1008[B]	HEC	CMD-C2D-C3D	2.05	128.81	124.94
3	B	1001	HEC	CMD-C2D-C1D	-2.01	125.51	128.46
3	B	1006	HEC	CBA-CAA-C2A	-2.01	109.24	112.55
3	A	1008[A]	HEC	CMB-C2B-C1B	-2.00	125.52	128.46

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1008[A]	HEC	C2D-C3D-CAD-CBD
3	A	1008[A]	HEC	C4D-C3D-CAD-CBD
3	A	1008[B]	HEC	C2D-C3D-CAD-CBD
3	A	1008[B]	HEC	C4D-C3D-CAD-CBD
4	A	2005	MRD	C1-C2-C3-C4
4	A	2005	MRD	O2-C2-C3-C4
4	B	2004	MRD	C1-C2-C3-C4
4	B	2004	MRD	O2-C2-C3-C4
4	B	2004	MRD	C2-C3-C4-O4
4	B	2004	MRD	C2-C3-C4-C5
4	B	2004	MRD	CM-C2-C3-C4
3	A	1004	HEC	CAA-CBA-CGA-O2A
3	B	1005	HEC	CAA-CBA-CGA-O2A
3	B	1002	HEC	CAA-CBA-CGA-O1A
3	B	1004	HEC	CAA-CBA-CGA-O1A
3	A	1004	HEC	CAA-CBA-CGA-O1A
3	A	1005	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	1002	HEC	CAA-CBA-CGA-O1A
3	B	1005	HEC	CAA-CBA-CGA-O1A
3	B	1004	HEC	CAA-CBA-CGA-O2A
3	A	1001	HEC	CAD-CBD-CGD-O1D
3	A	1005	HEC	CAA-CBA-CGA-O2A
3	A	1002	HEC	CAA-CBA-CGA-O2A
3	A	1001	HEC	CAA-CBA-CGA-O2A
3	B	1002	HEC	CAA-CBA-CGA-O2A
3	A	1001	HEC	CAA-CBA-CGA-O1A
3	A	1008[B]	HEC	CAD-CBD-CGD-O2D
3	B	1008[A]	HEC	CAA-CBA-CGA-O2A
3	A	1001	HEC	CAD-CBD-CGD-O2D
3	B	1001	HEC	CAD-CBD-CGD-O2D
3	B	1003	HEC	CAD-CBD-CGD-O2D
3	A	1008[B]	HEC	CAD-CBD-CGD-O1D
3	A	1008[B]	HEC	CAA-CBA-CGA-O2A
3	B	1008[A]	HEC	CAA-CBA-CGA-O1A
3	A	1003	HEC	CAD-CBD-CGD-O2D
3	B	1003	HEC	CAD-CBD-CGD-O1D
3	A	1008[A]	HEC	CAD-CBD-CGD-O2D
3	A	1008[A]	HEC	CAD-CBD-CGD-O1D
3	A	1003	HEC	CAD-CBD-CGD-O1D
3	B	1001	HEC	CAD-CBD-CGD-O1D
3	A	1005	HEC	CAD-CBD-CGD-O1D
6	B	2010	CIT	C3-C4-C5-O3
3	A	1005	HEC	CAD-CBD-CGD-O2D
3	A	1008[B]	HEC	CAA-CBA-CGA-O1A
3	B	1005	HEC	CAD-CBD-CGD-O2D
3	A	1006	HEC	CAA-CBA-CGA-O1A
3	A	1008[A]	HEC	CAA-CBA-CGA-O2A
5	B	2040	MPD	C2-C3-C4-O4
3	B	1001	HEC	CAA-CBA-CGA-O1A
3	A	1008[A]	HEC	CAA-CBA-CGA-O1A
4	A	2005	MRD	CM-C2-C3-C4
6	B	2010	CIT	C3-C4-C5-O4
3	B	1005	HEC	CAD-CBD-CGD-O1D
3	A	1006	HEC	CAA-CBA-CGA-O2A
3	B	1003	HEC	CAA-CBA-CGA-O2A
3	B	1007	HEC	CAA-CBA-CGA-O2A
3	B	1001	HEC	CAA-CBA-CGA-O2A

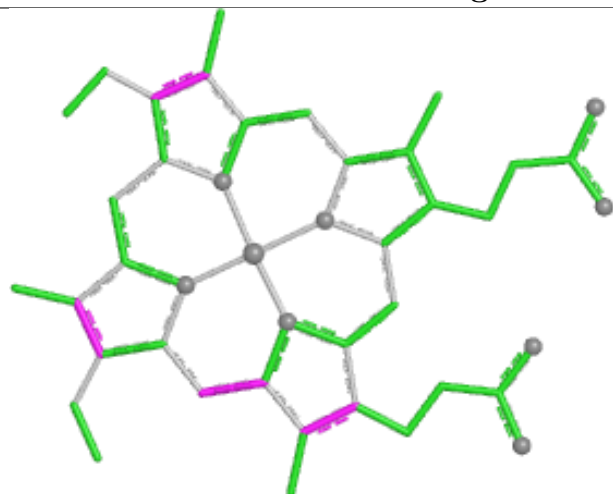
There are no ring outliers.

9 monomers are involved in 23 short contacts:

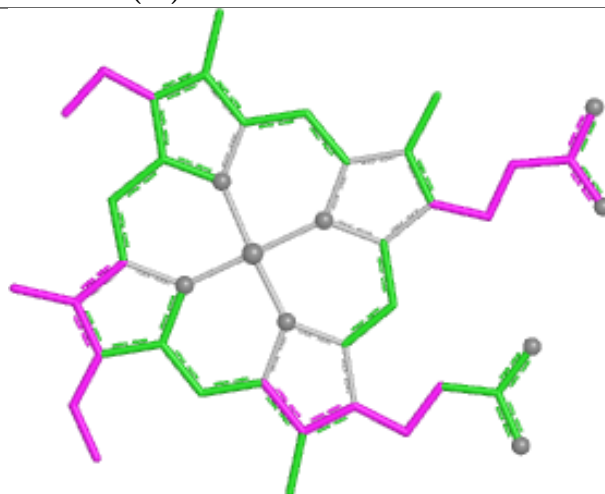
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1008[A]	HEC	1	0
3	A	1008[A]	HEC	2	0
3	B	1002	HEC	1	0
4	B	2288	MRD	1	0
6	B	2010	CIT	1	1
3	B	1008[B]	HEC	5	0
3	A	1008[B]	HEC	7	0
4	A	2005	MRD	2	0
3	A	1002	HEC	2	0

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.

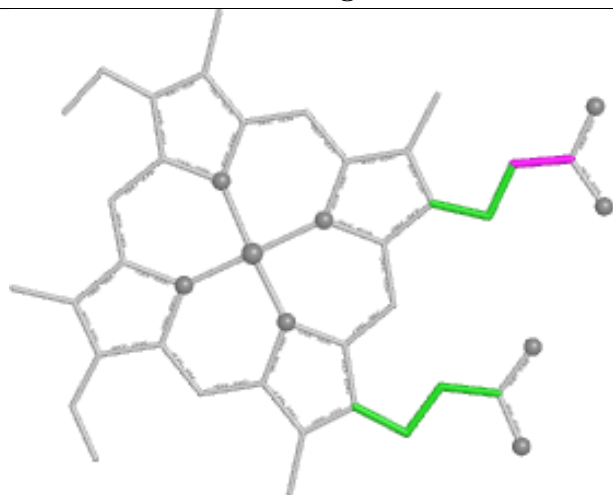
Ligand HEC B 1008 (A)



Bond lengths



Bond angles

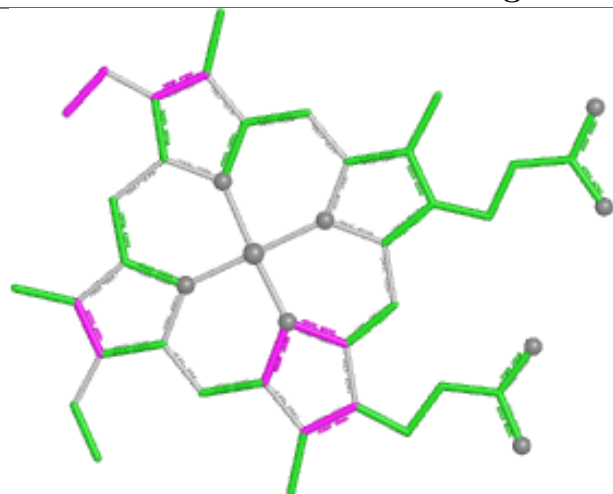


Torsions

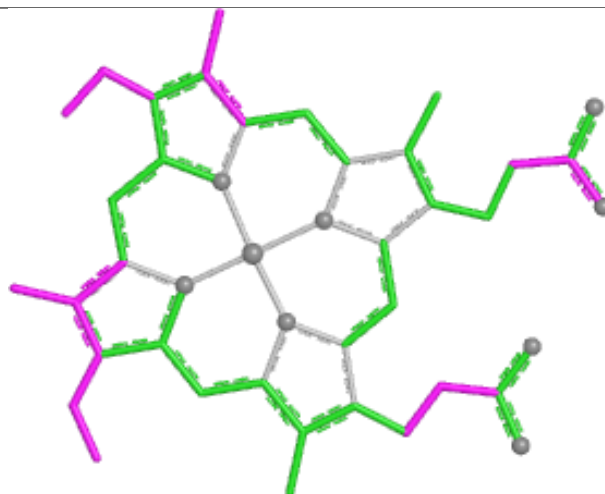


Rings

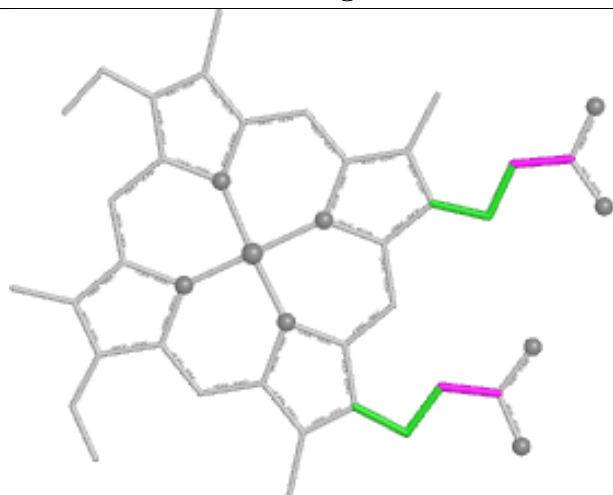
Ligand HEC A 1001



Bond lengths



Bond angles

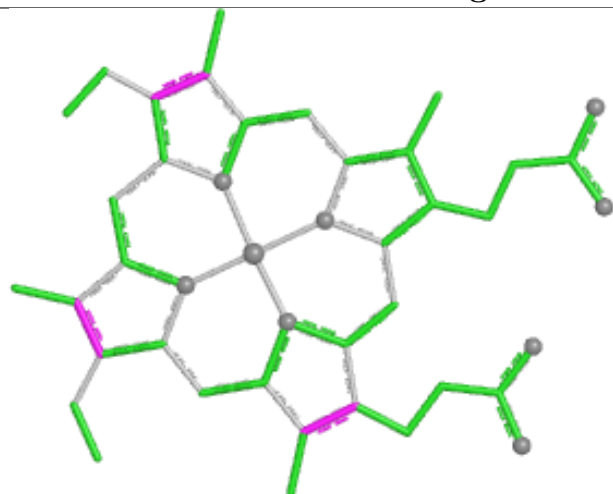


Torsions

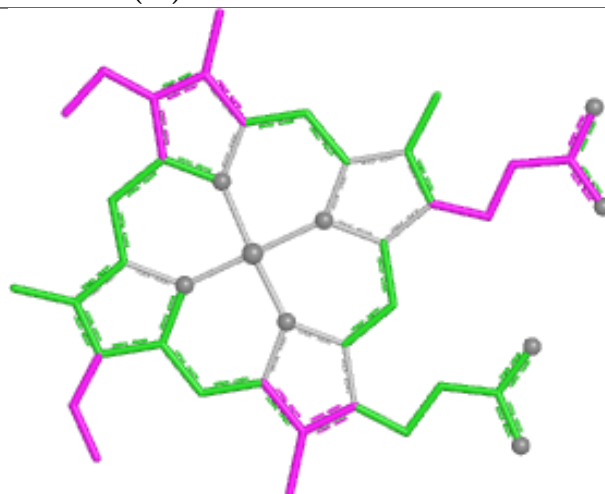


Rings

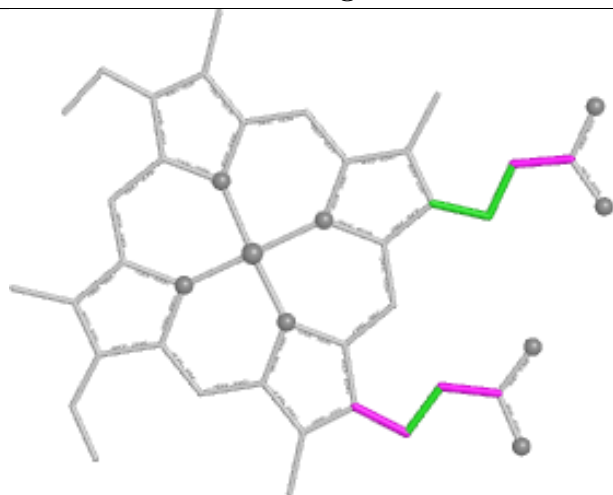
Ligand HEC A 1008 (A)



Bond lengths



Bond angles

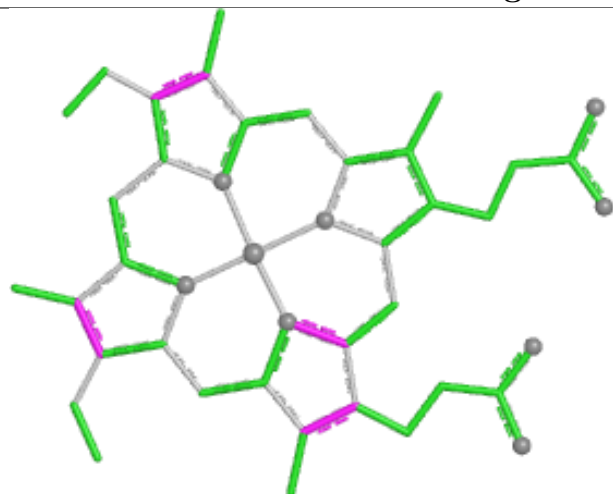


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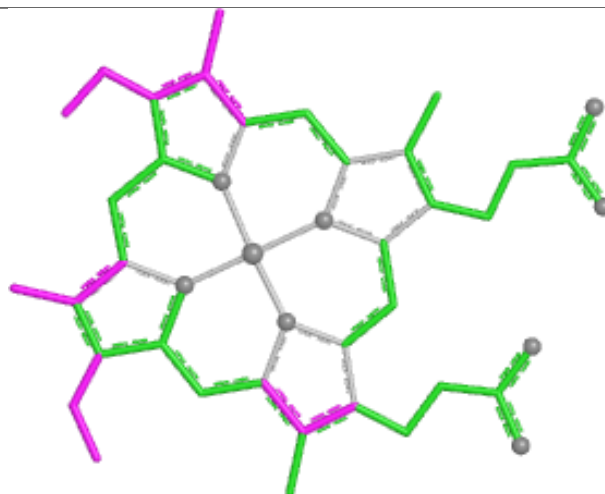


Rings

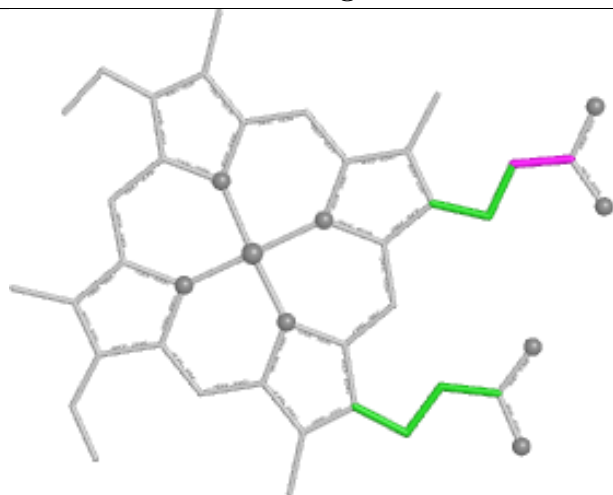
Ligand HEC B 1004



Bond lengths



Bond angles

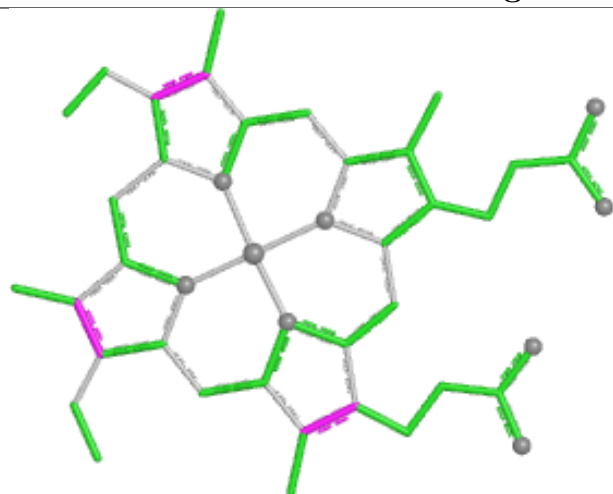


Torsions

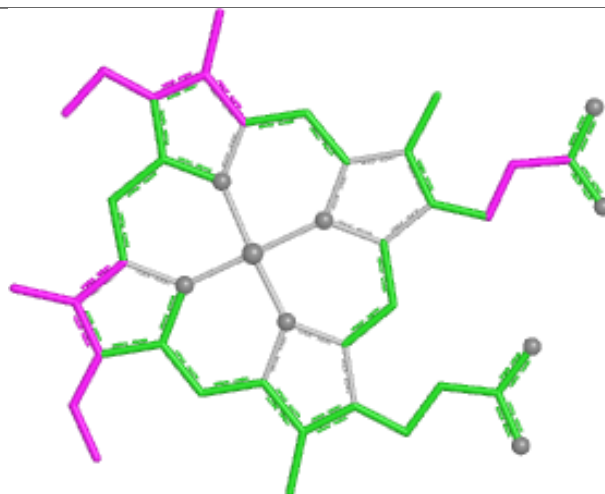


Rings

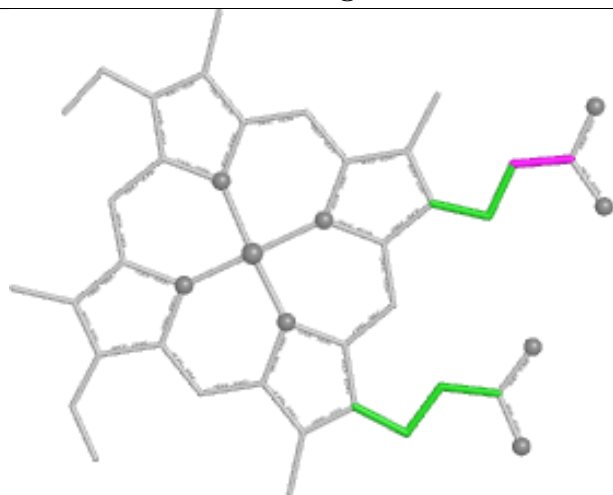
Ligand HEC B 1002



Bond lengths



Bond angles

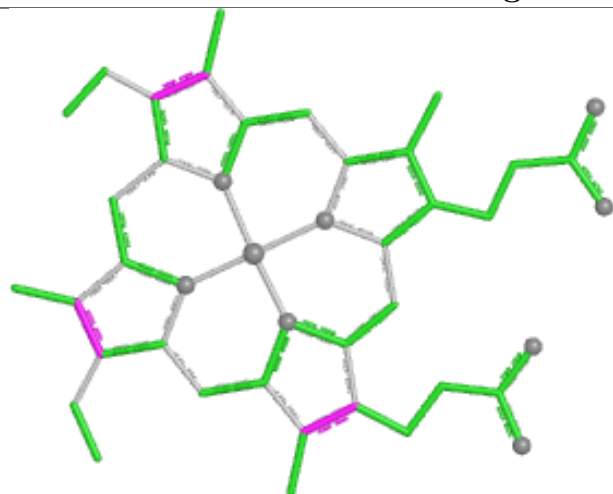


Torsions

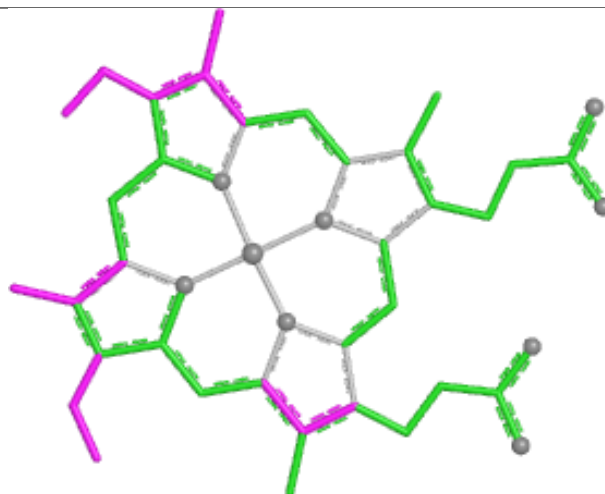


Rings

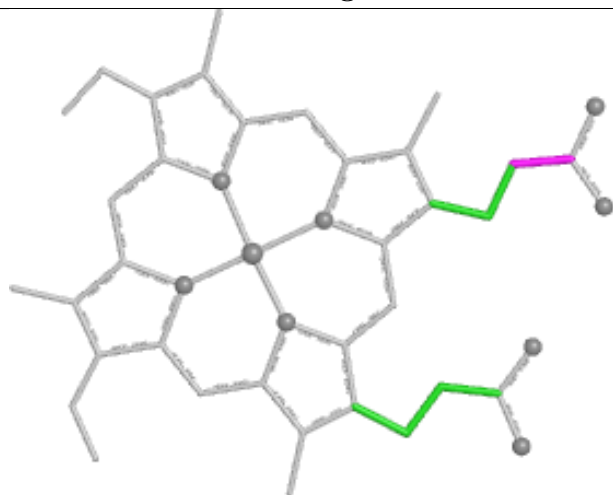
Ligand HEC A 1004



Bond lengths



Bond angles

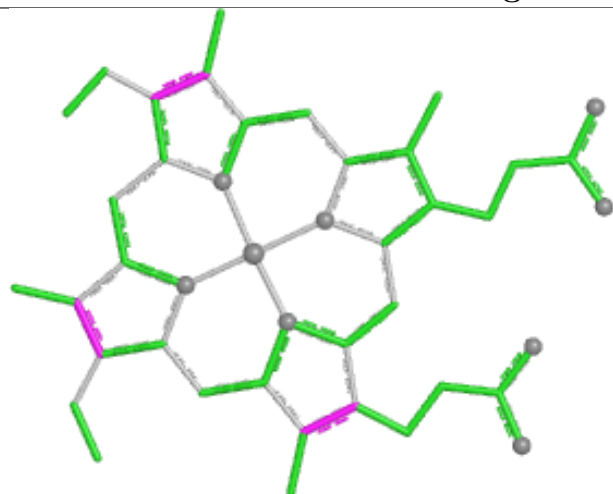


Torsions

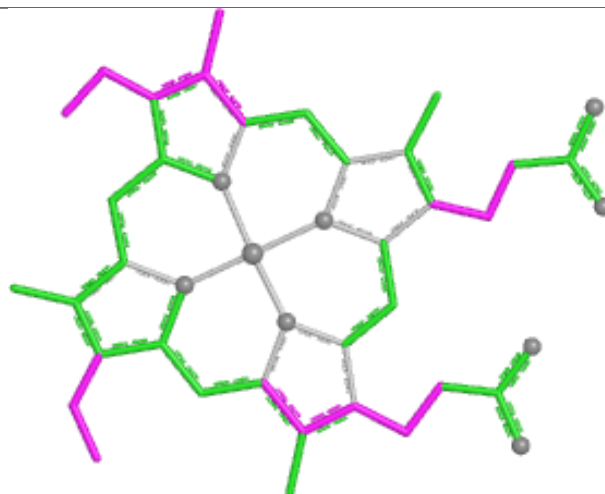


Rings

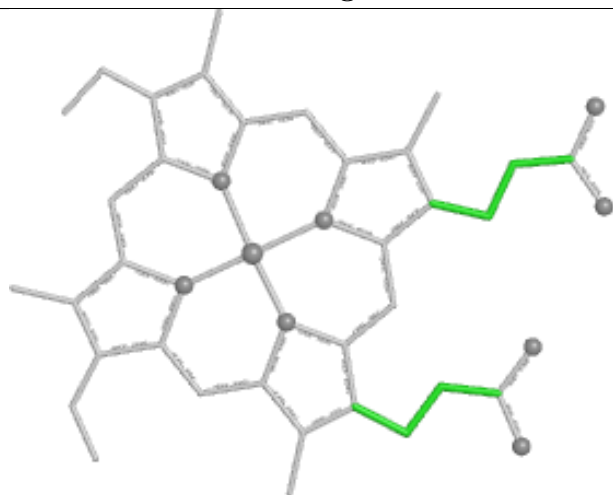
Ligand HEC A 1007



Bond lengths



Bond angles

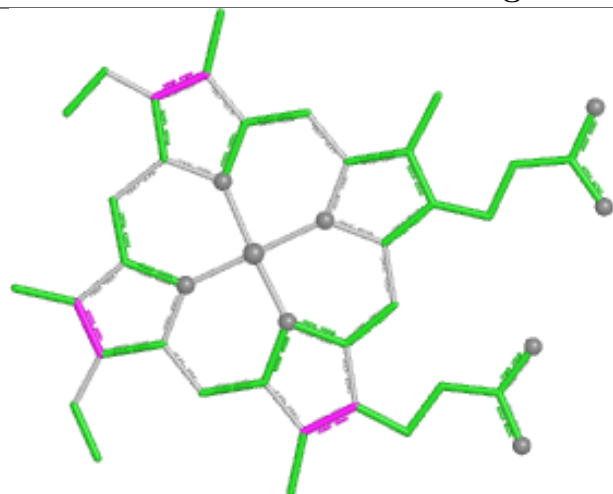


Torsions

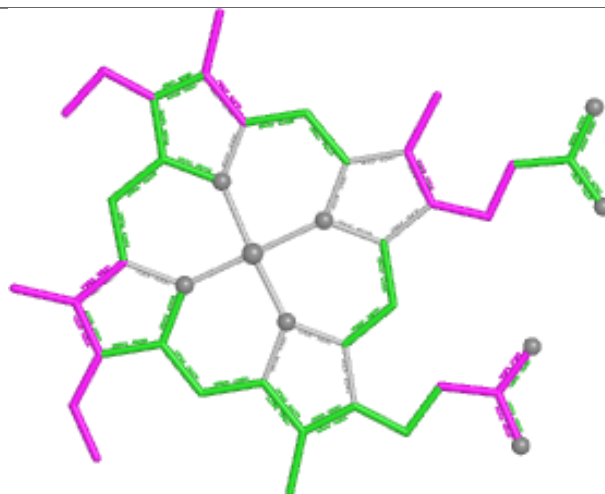


Rings

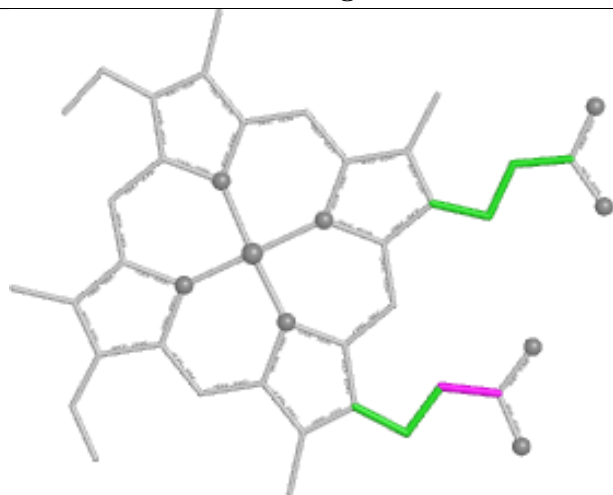
Ligand HEC A 1003



Bond lengths



Bond angles

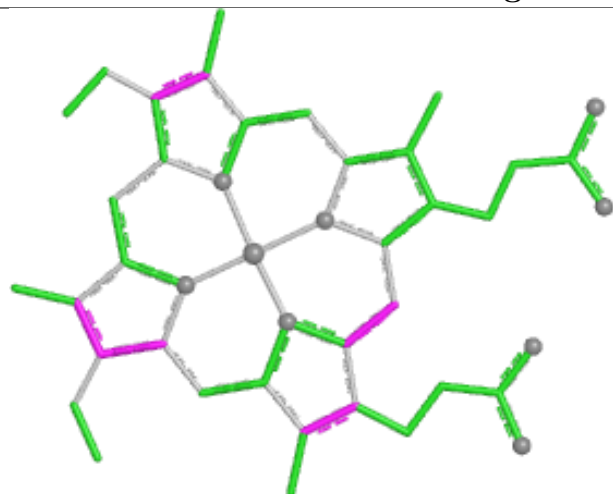


Torsions

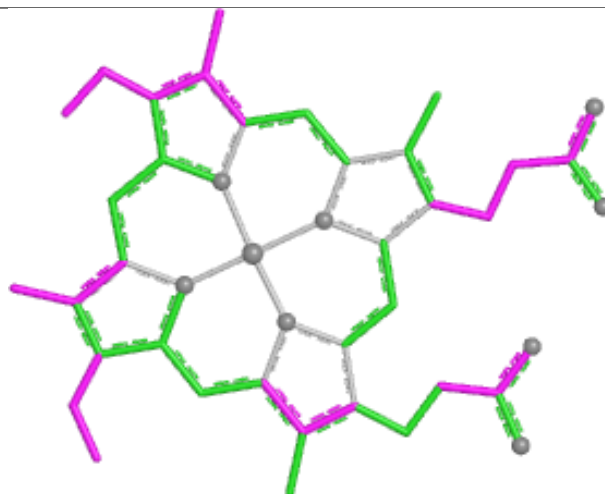


Rings

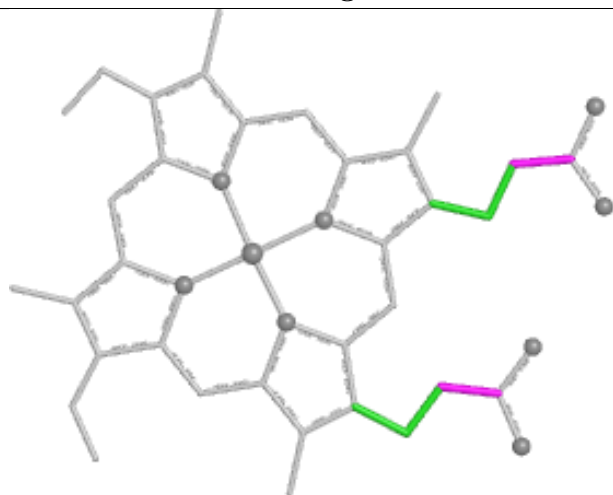
Ligand HEC B 1003



Bond lengths



Bond angles

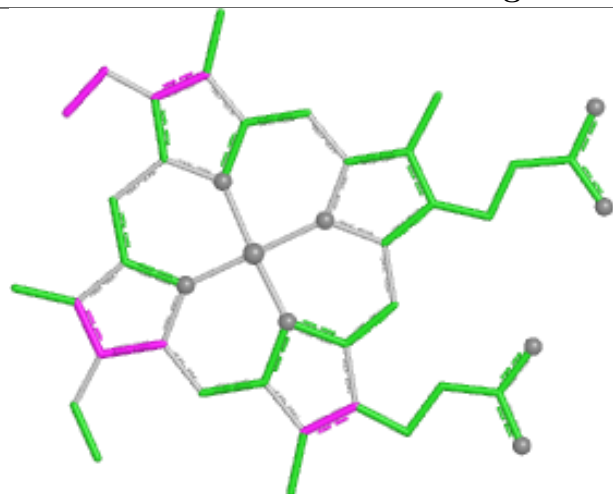


Torsions

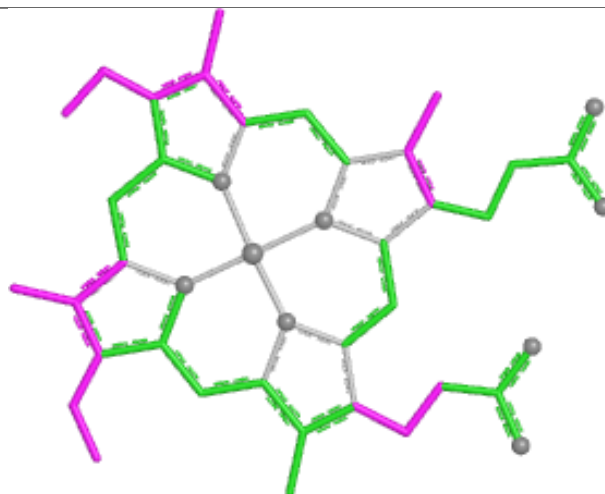


Rings

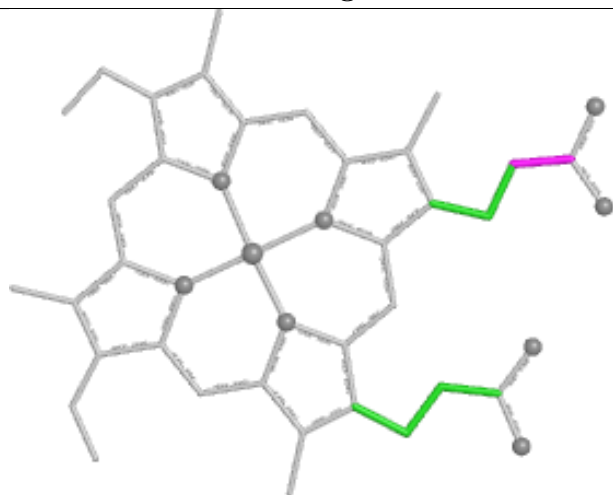
Ligand HEC A 1006



Bond lengths



Bond angles

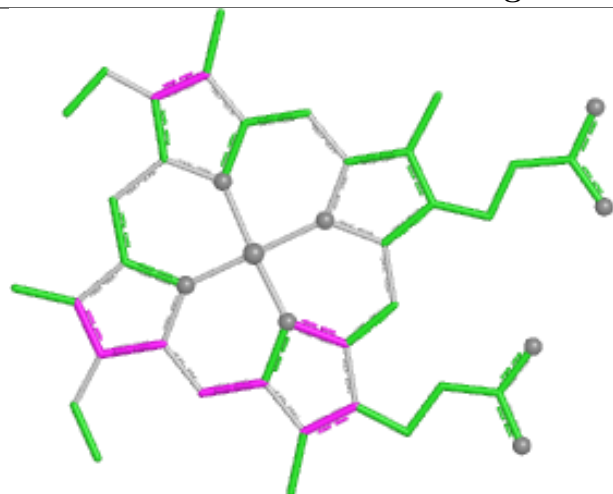


Torsions

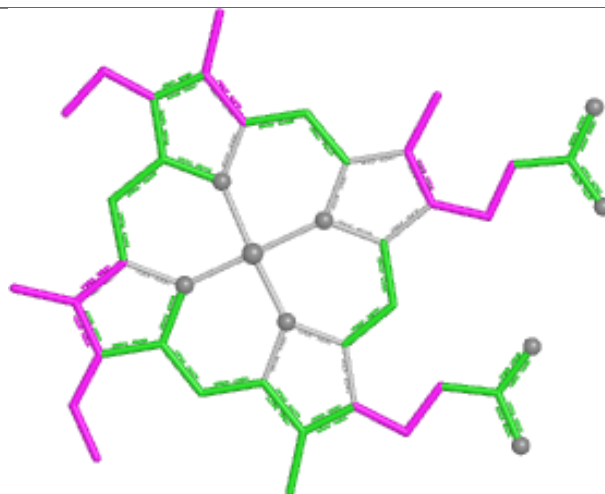


Rings

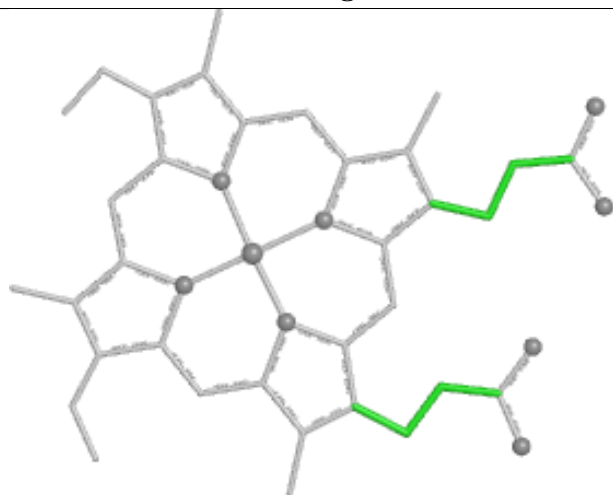
Ligand HEC B 1006



Bond lengths



Bond angles

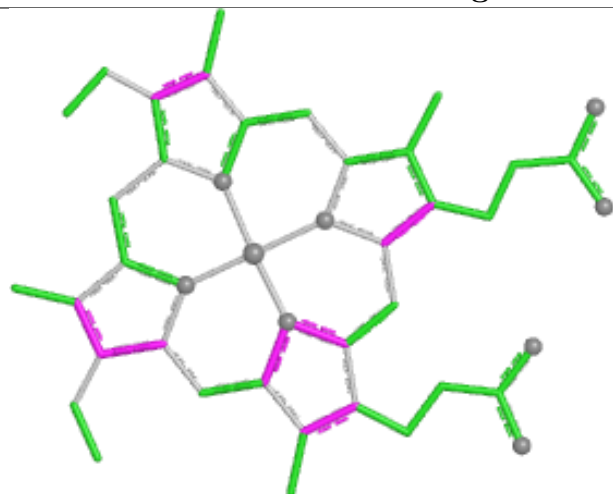


Torsions

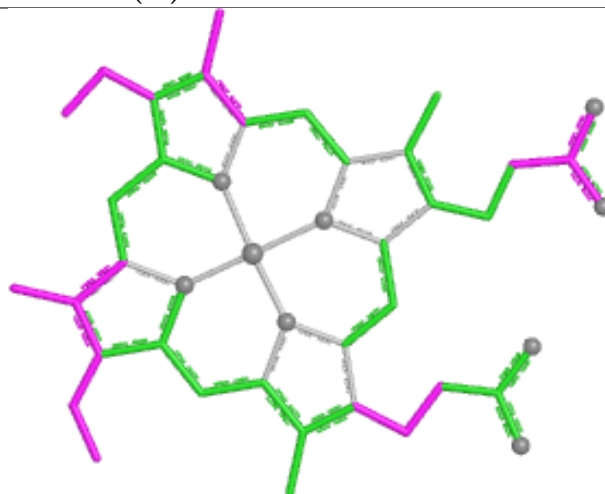


Rings

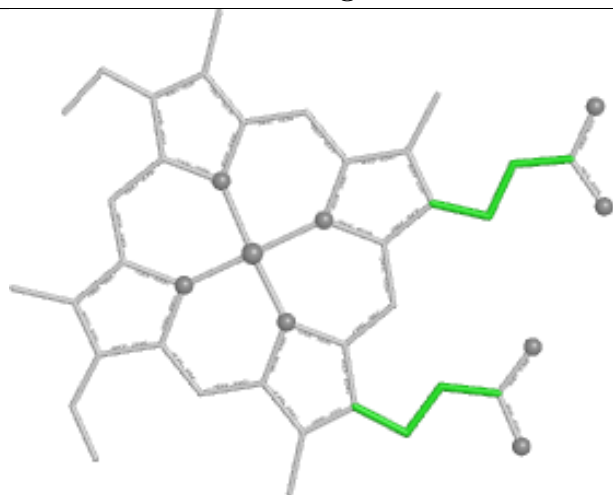
Ligand HEC B 1008 (B)



Bond lengths



Bond angles

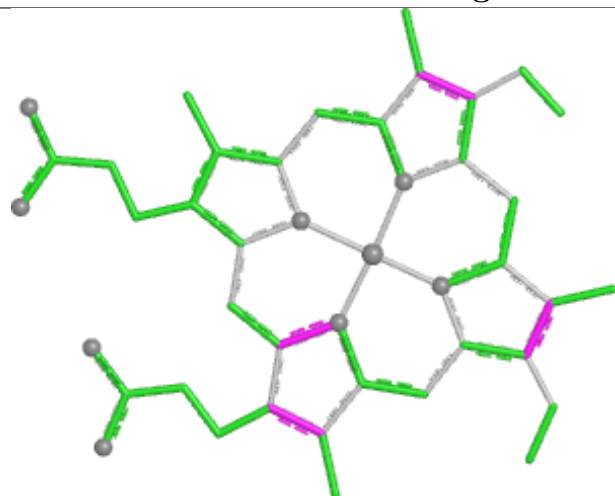


Torsions

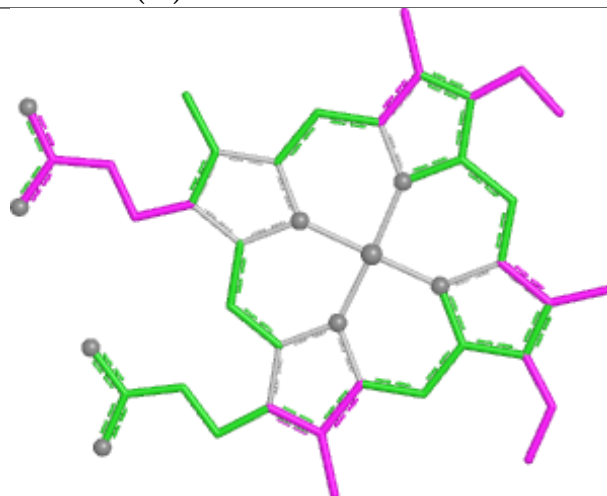


Rings

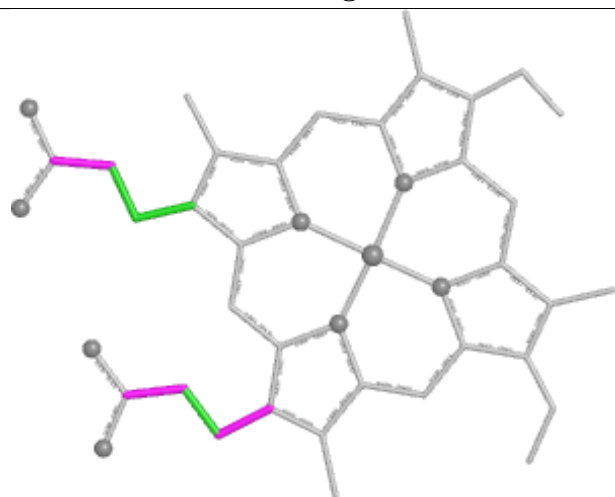
Ligand HEC A 1008 (B)



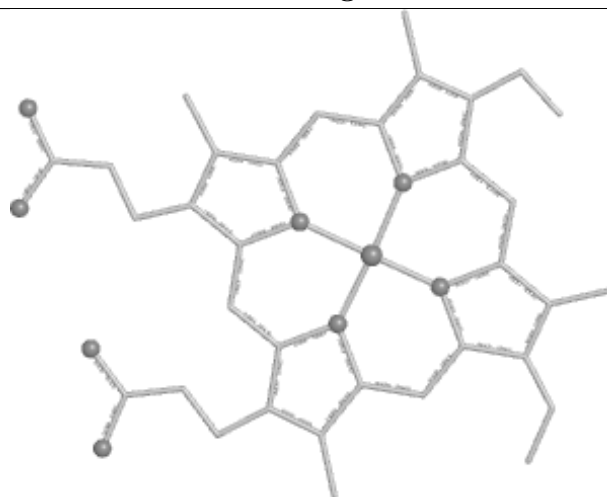
Bond lengths



Bond angles

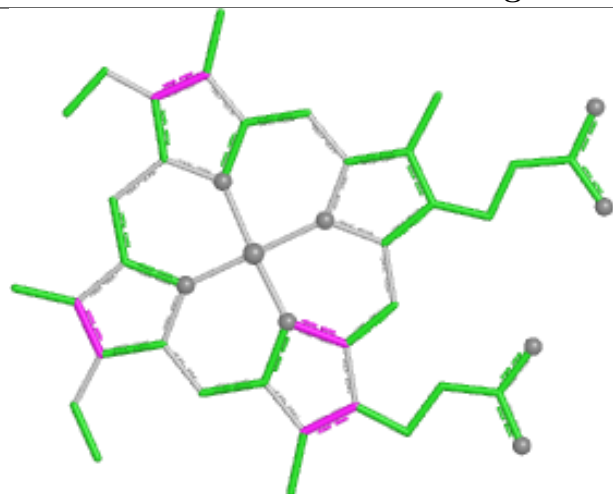


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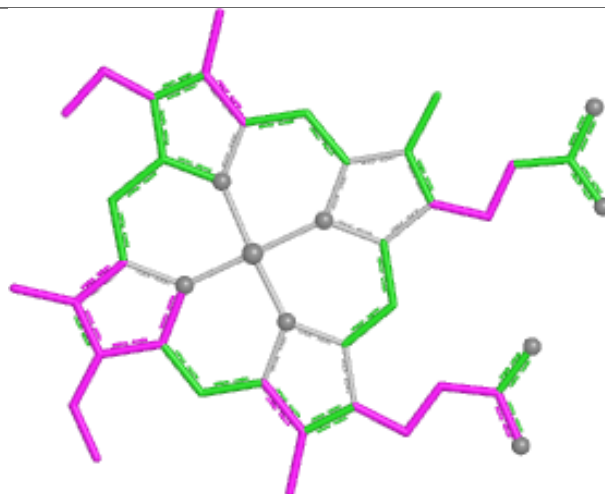


Rings

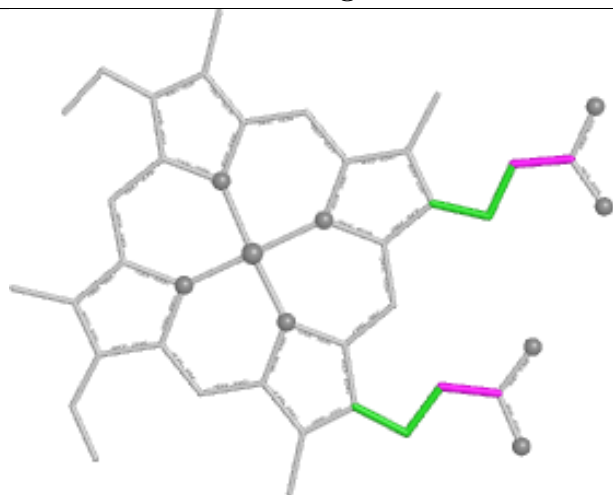
Ligand HEC B 1001



Bond lengths



Bond angles

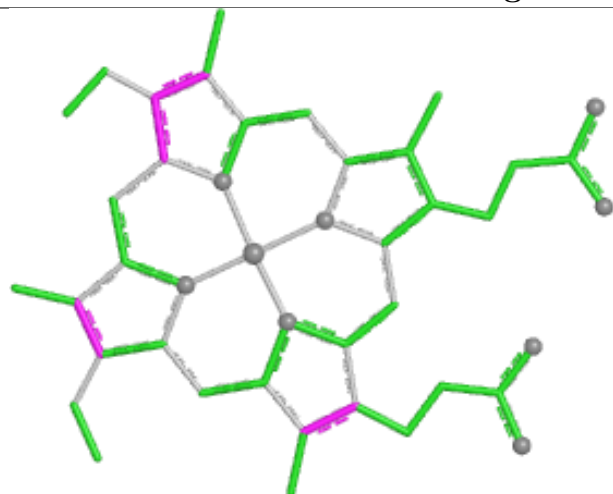


Torsions

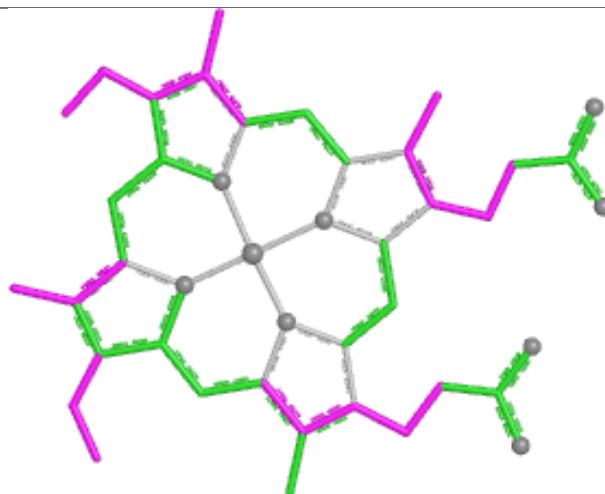


Rings

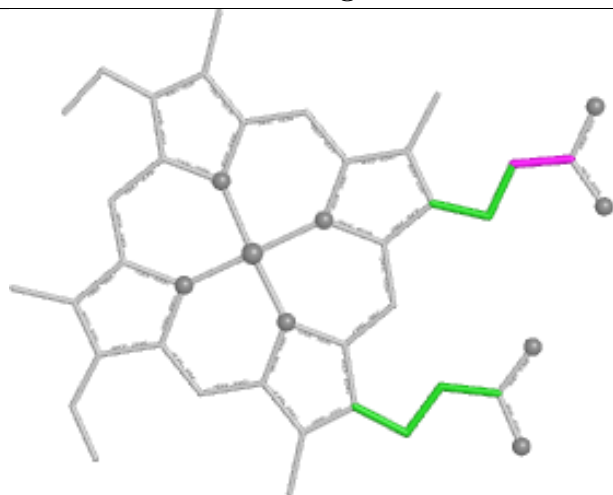
Ligand HEC B 1007



Bond lengths



Bond angles

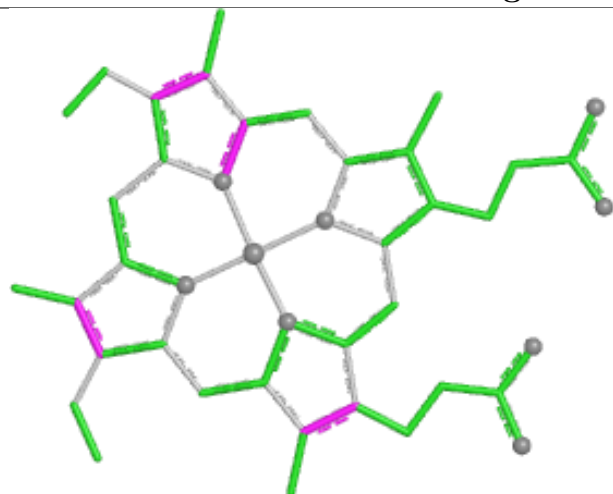


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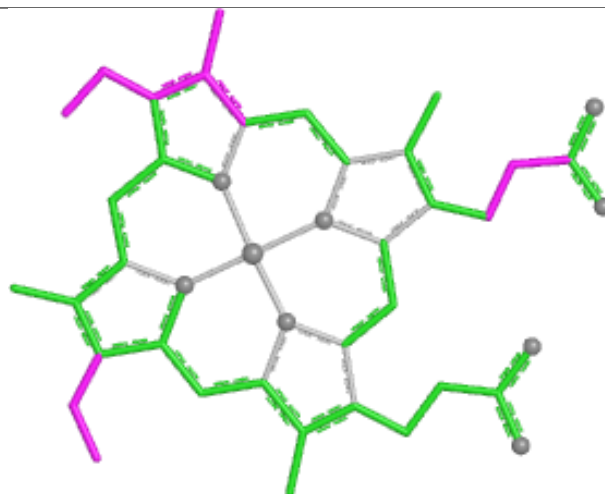


Rings

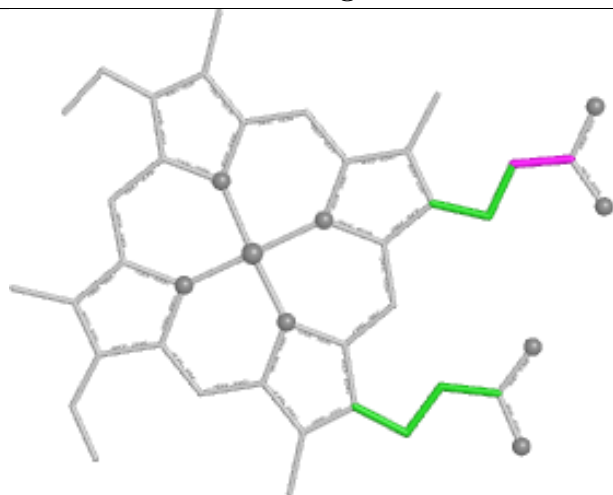
Ligand HEC A 1002



Bond lengths



Bond angles

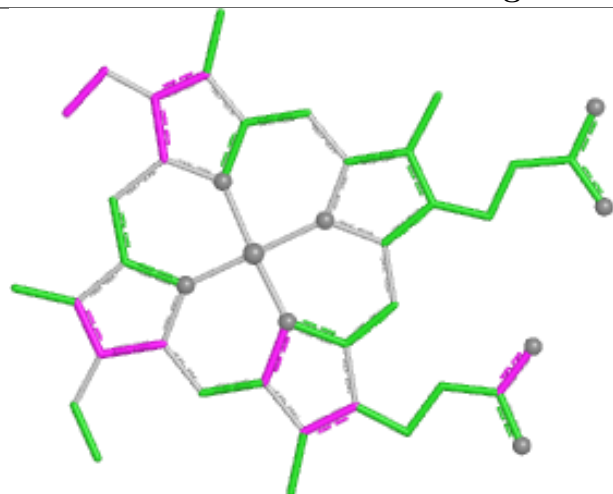


Torsions

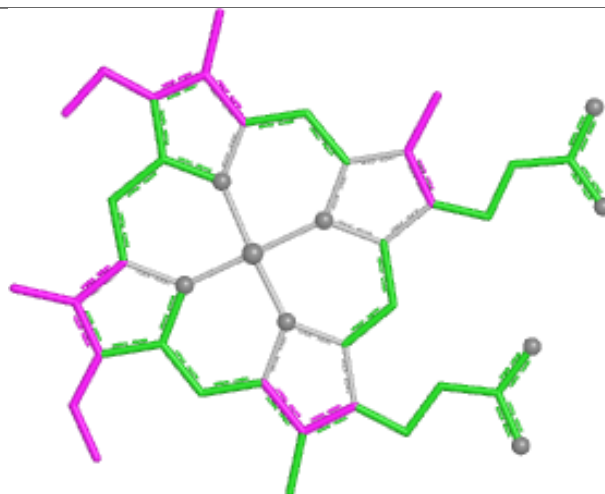


Rings

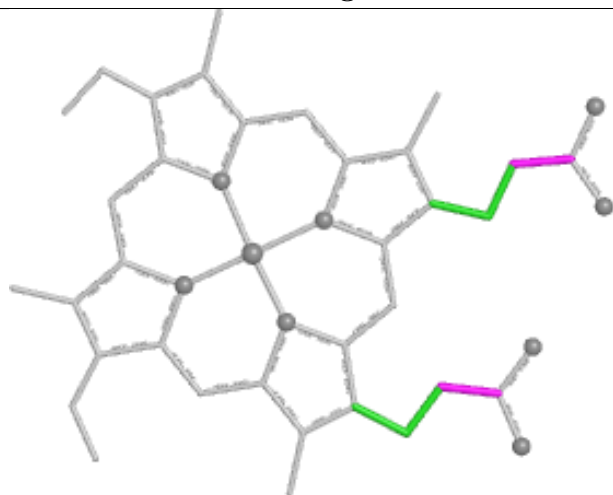
Ligand HEC A 1005



Bond lengths



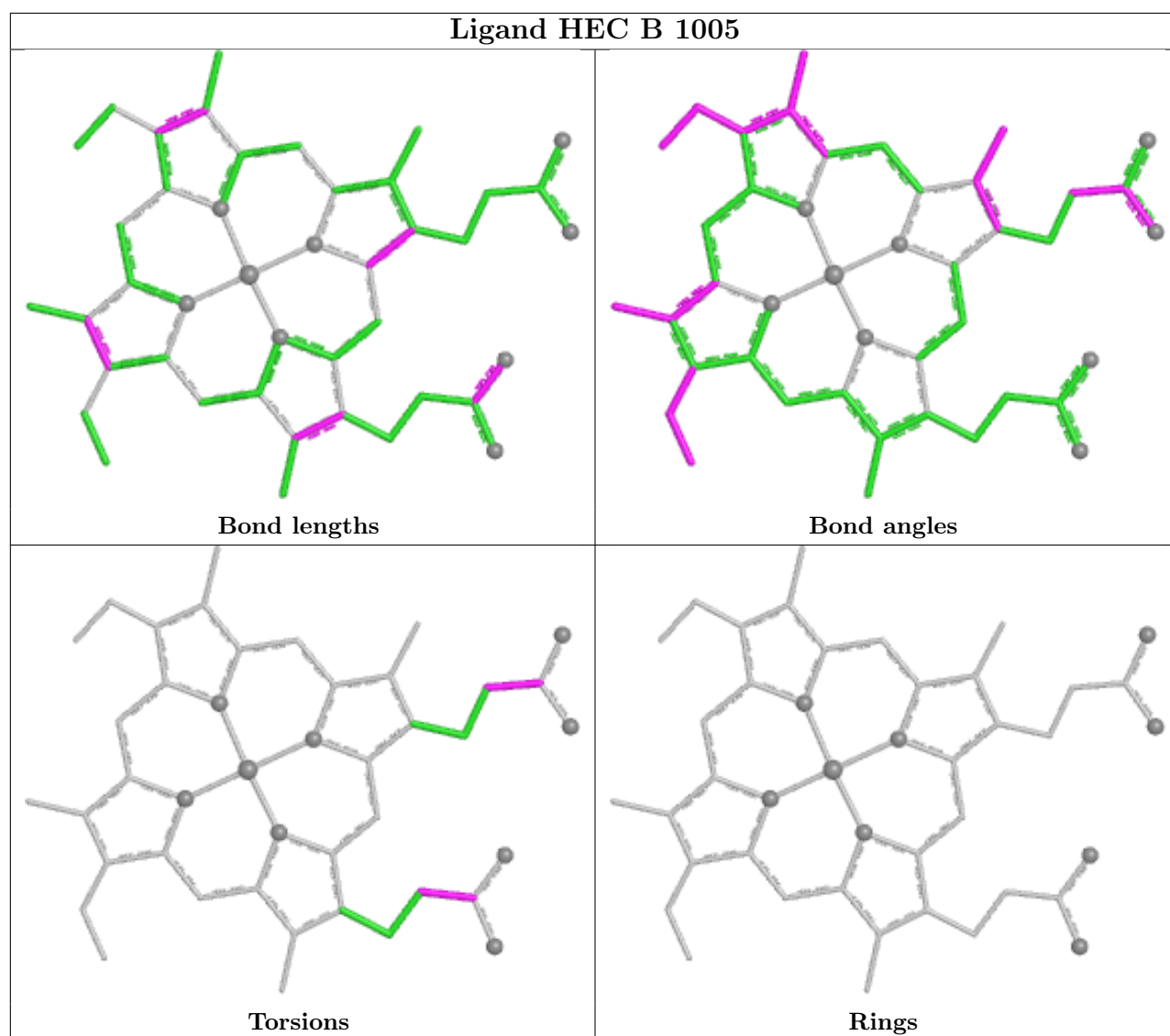
Bond angles



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	520/525 (99%)	-0.76	4 (0%)	82 86	6, 14, 23, 40	31 (5%)
1	B	520/525 (99%)	-0.82	1 (0%)	92 92	5, 13, 23, 39	26 (5%)
All	All	1040/1050 (99%)	-0.79	5 (0%)	87 89	5, 14, 23, 40	57 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278[A]	ARG	3.9
1	A	523	ALA	3.4
1	B	523	ALA	2.8
1	A	524	SER	2.2
1	A	414[A]	CYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

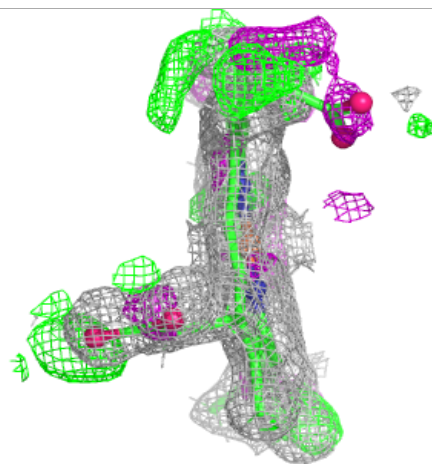
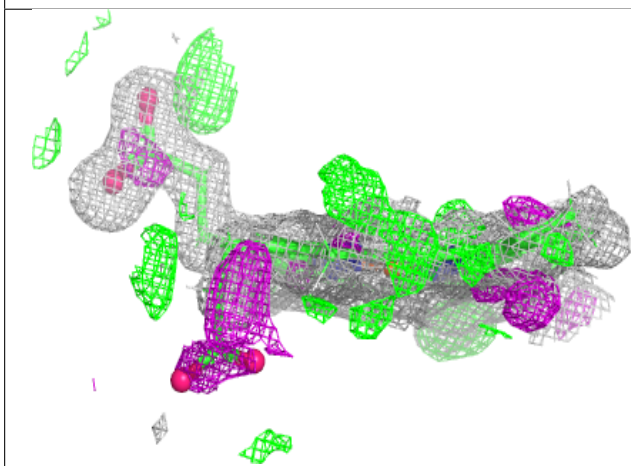
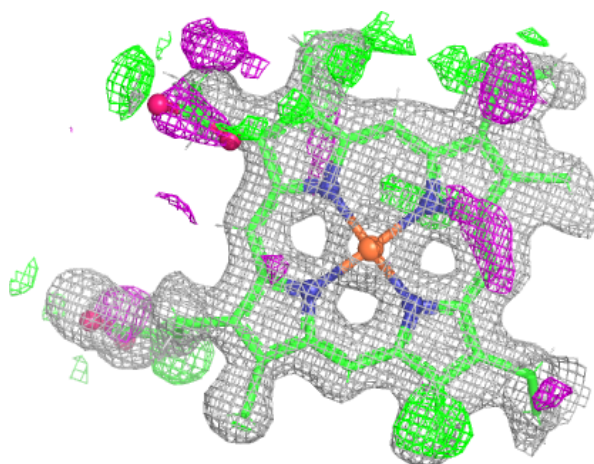
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MRD	A	2005	8/8	0.80	0.24	24,26,30,32	22
5	MPD	B	2040	8/8	0.80	0.34	29,33,36,36	18
4	MRD	B	2288	8/8	0.85	0.35	28,31,35,35	22
4	MRD	B	2004	8/8	0.89	0.25	21,26,31,31	21
4	MRD	A	2270	8/8	0.91	0.18	22,24,26,26	22
6	CIT	B	2010	13/13	0.93	0.11	23,28,31,31	18
5	MPD	A	2001	8/8	0.94	0.10	17,20,21,21	10
5	MPD	B	2002	8/8	0.95	0.08	16,19,22,22	10
3	HEC	A	1008[A]	43/43	0.96	0.11	12,17,29,37	75
3	HEC	A	1008[B]	43/43	0.96	0.11	20,23,34,40	75
3	HEC	B	1008[A]	43/43	0.97	0.09	10,15,26,34	75
3	HEC	B	1008[B]	43/43	0.97	0.09	19,22,32,38	75
3	HEC	B	1007	43/43	0.99	0.03	10,12,13,17	18
3	HEC	A	1006	43/43	0.99	0.04	10,12,13,13	18
3	HEC	A	1007	43/43	0.99	0.04	11,13,15,18	18
3	HEC	B	1002	43/43	0.99	0.04	11,14,17,17	18
3	HEC	B	1003	43/43	0.99	0.05	11,13,21,33	18
3	HEC	B	1001	43/43	0.99	0.05	14,17,20,22	18
3	HEC	A	1004	43/43	0.99	0.04	11,13,16,16	18
3	HEC	A	1005	43/43	0.99	0.04	11,13,18,26	18
3	HEC	A	1002	43/43	0.99	0.04	12,14,15,17	18
3	HEC	A	1003	43/43	0.99	0.05	11,13,22,33	18
3	HEC	A	1001	43/43	0.99	0.04	12,15,19,23	18
3	HEC	B	1004	43/43	0.99	0.04	10,11,14,15	18
3	HEC	B	1005	43/43	0.99	0.04	10,12,18,26	18
3	HEC	B	1006	43/43	0.99	0.04	9,11,12,13	18
2	CA	A	2744	1/1	1.00	0.09	18,18,18,18	0
2	CA	B	2333	1/1	1.00	0.09	17,17,17,17	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.

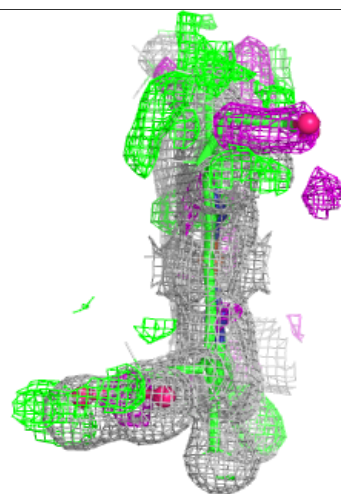
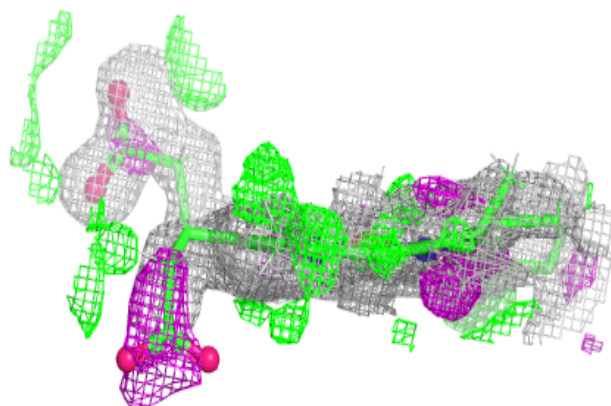
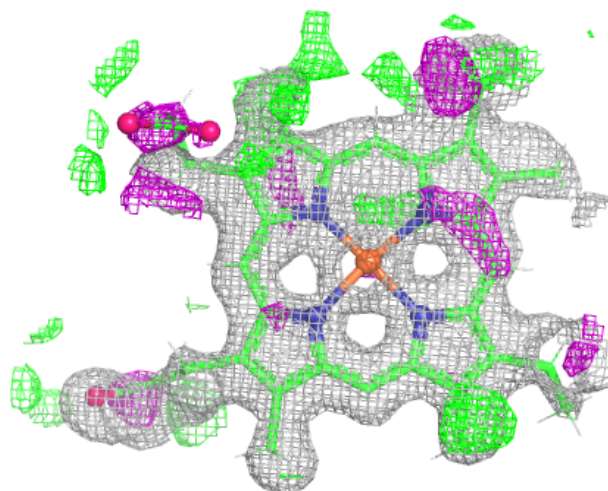
Electron density around HEC A 1008 (A):

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



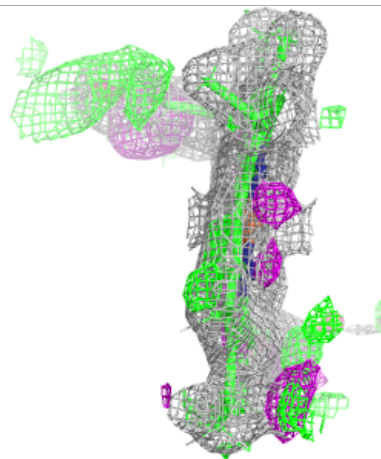
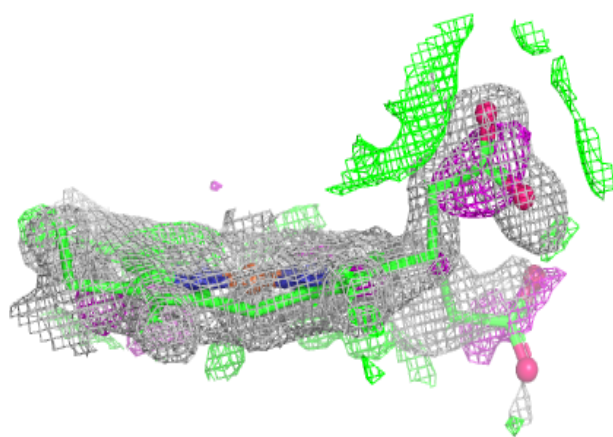
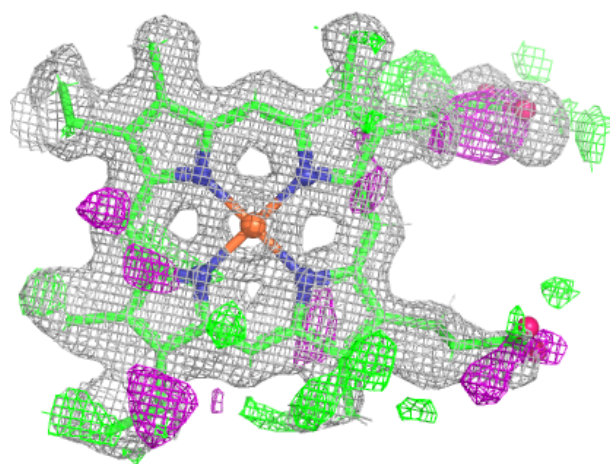
Electron density around HEC A 1008 (B):

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



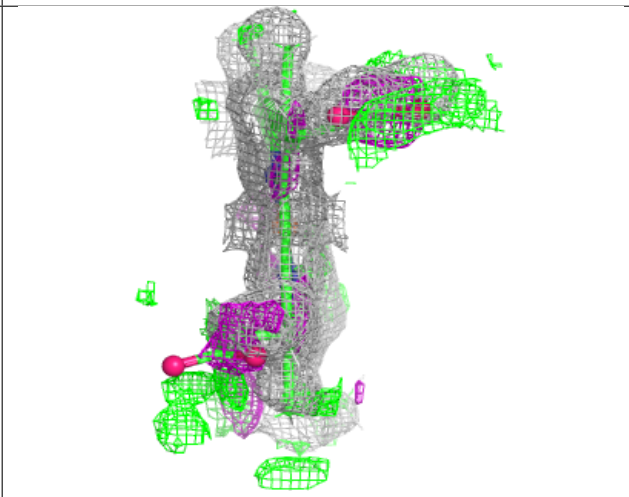
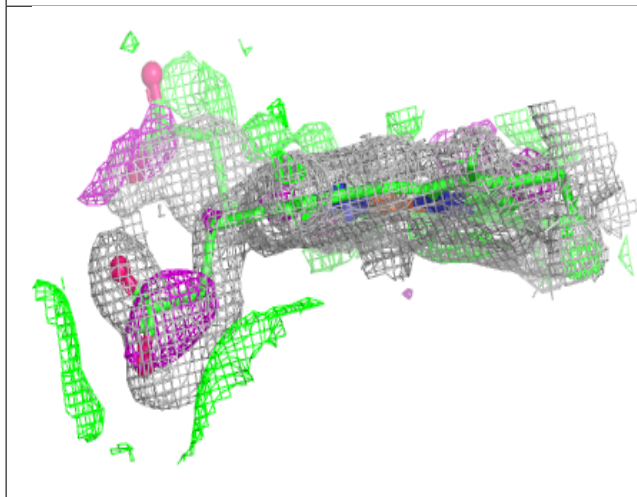
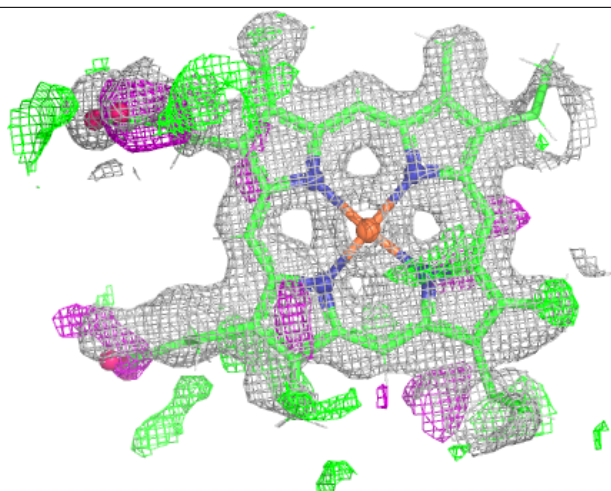
Electron density around HEC B 1008 (A):

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



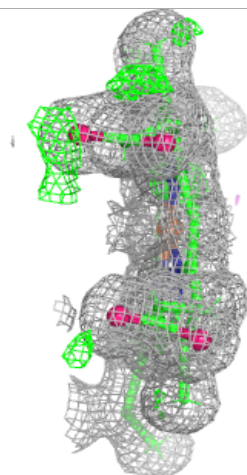
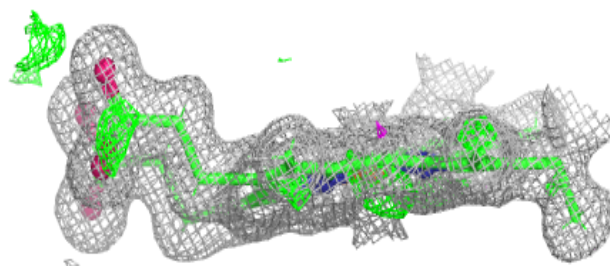
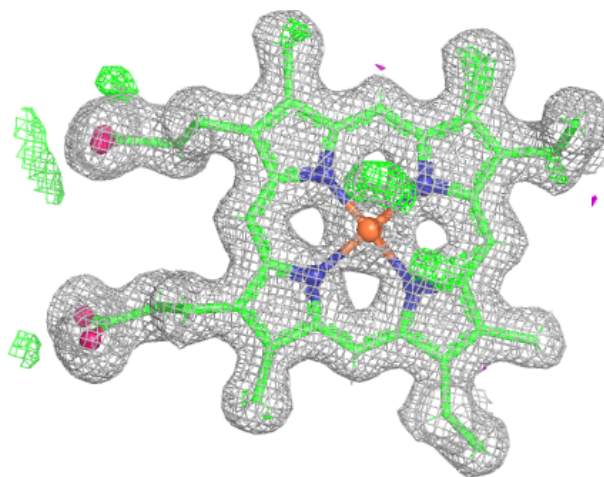
Electron density around HEC B 1008 (B):

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and green (positive)



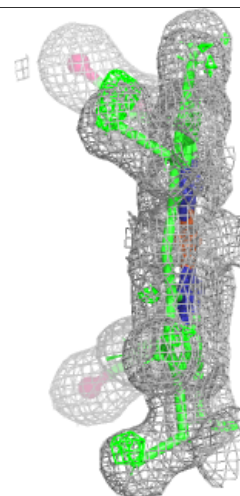
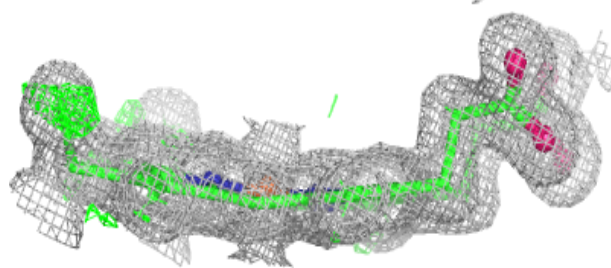
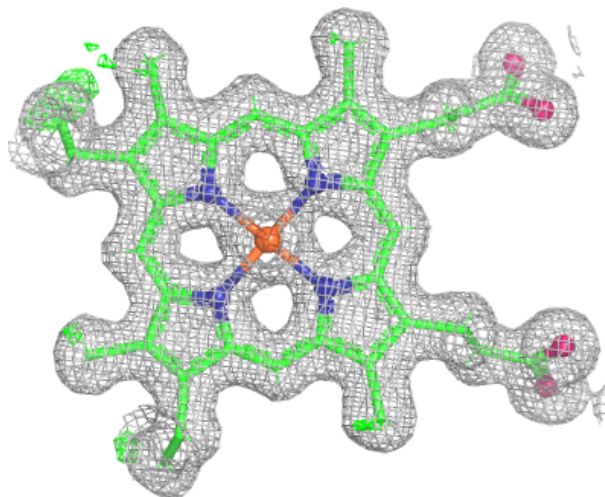
Electron density around HEC B 1007:

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



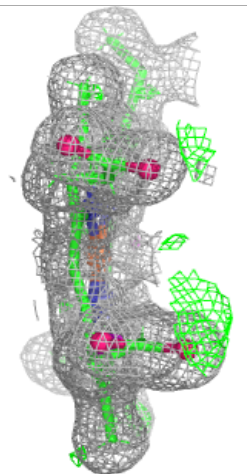
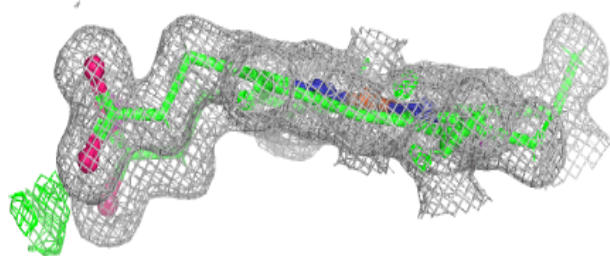
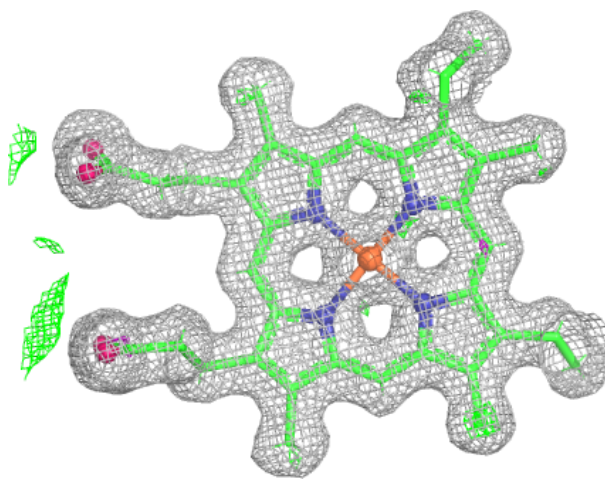
Electron density around HEC A 1006:

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



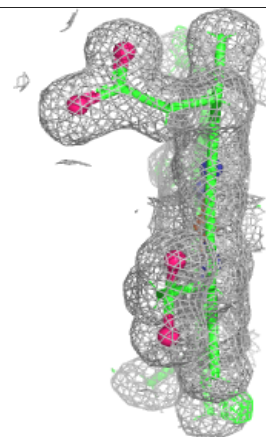
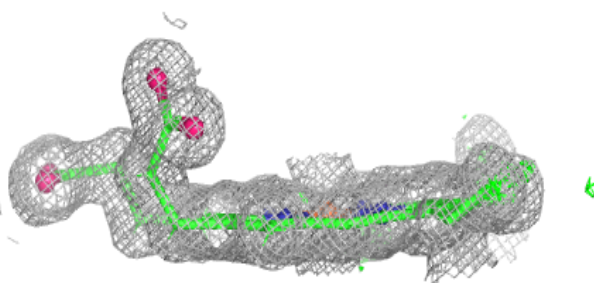
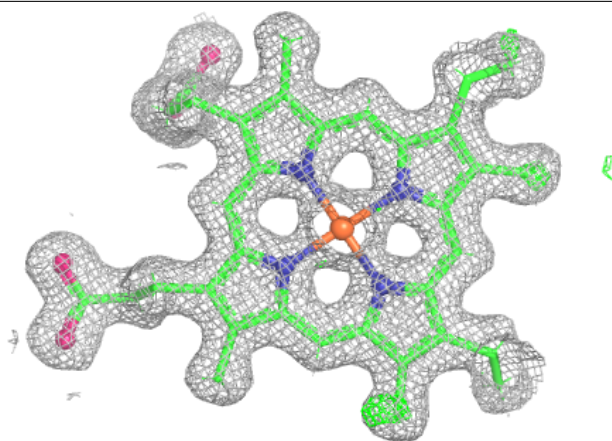
Electron density around HEC A 1007:

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



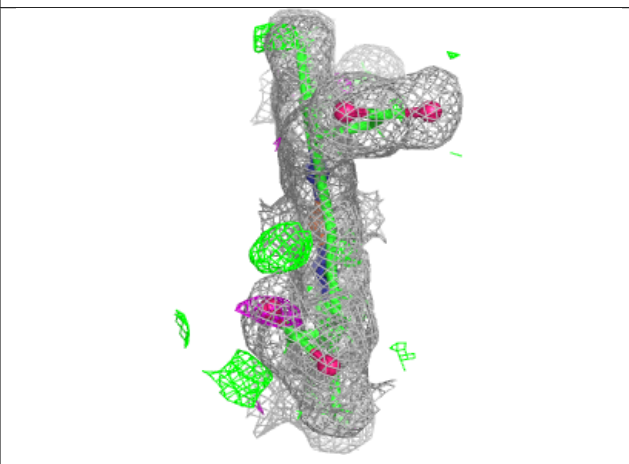
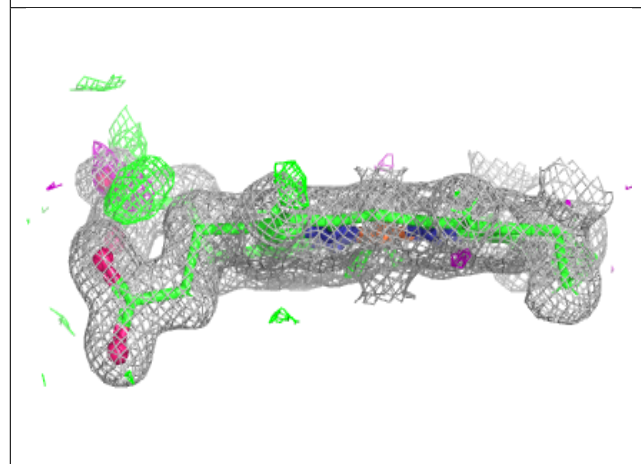
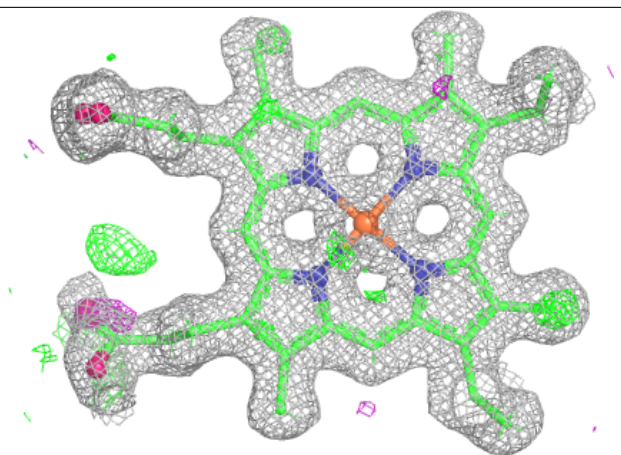
Electron density around HEC B 1002:

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



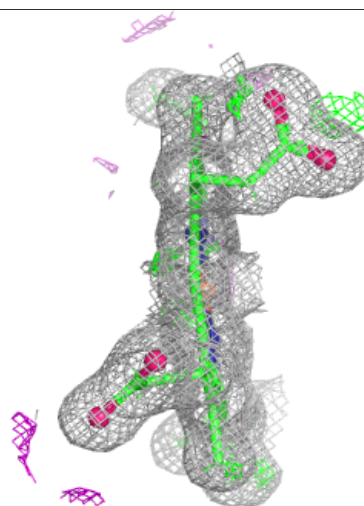
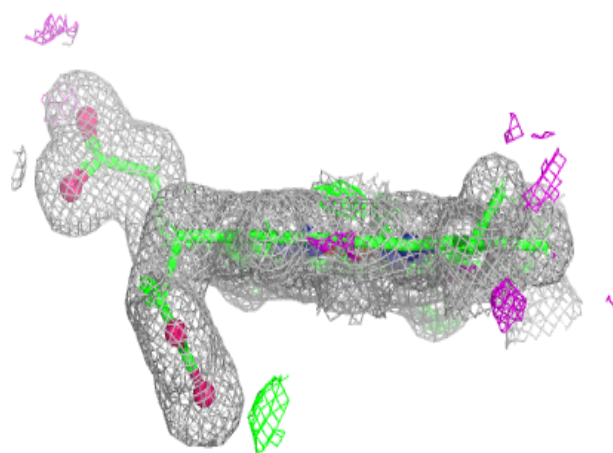
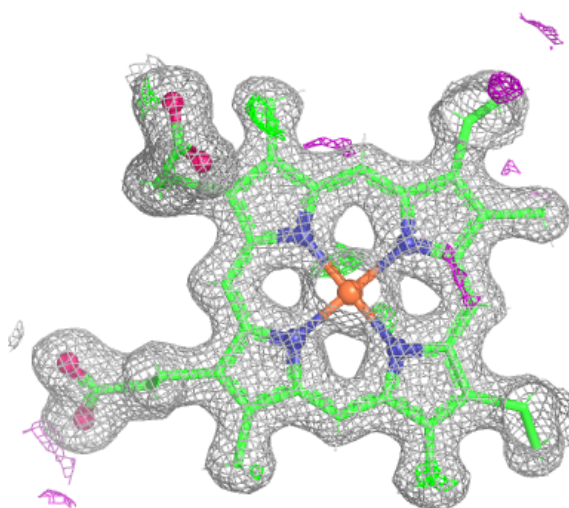
Electron density around HEC B 1003:

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



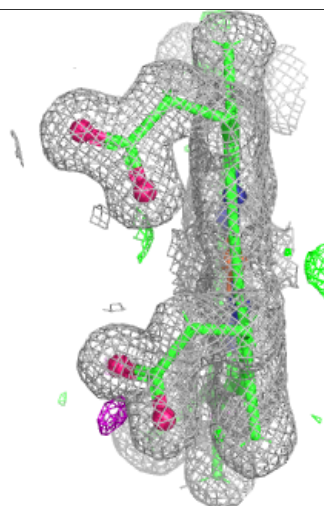
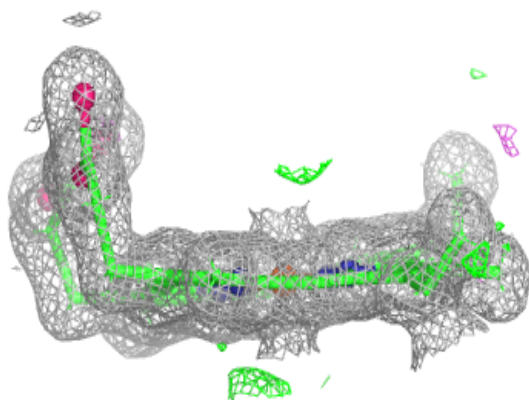
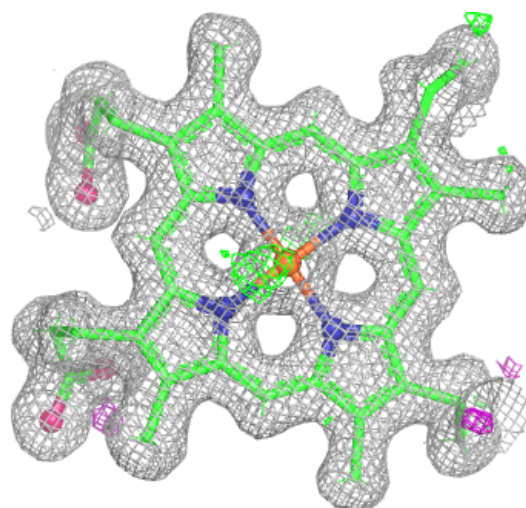
Electron density around HEC B 1001:

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



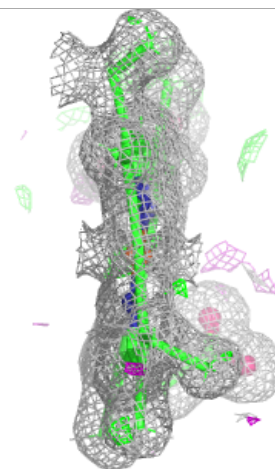
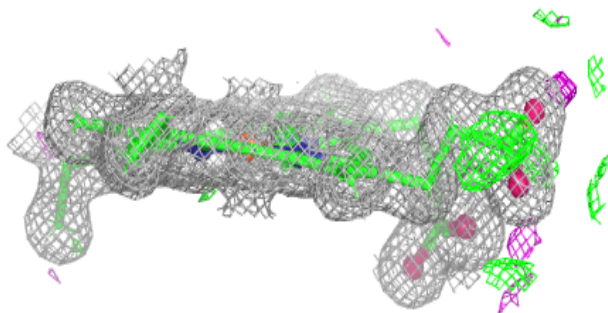
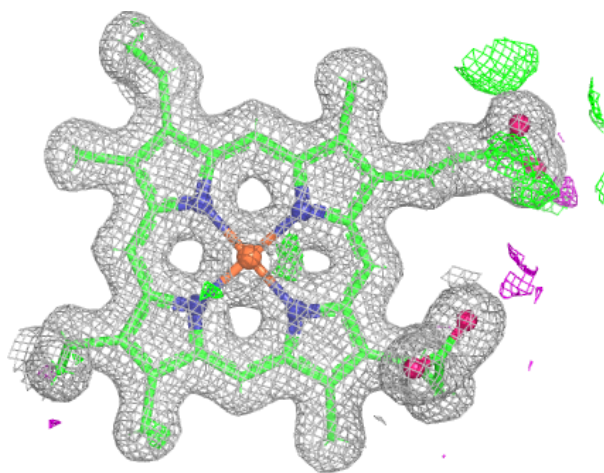
Electron density around HEC A 1004:

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



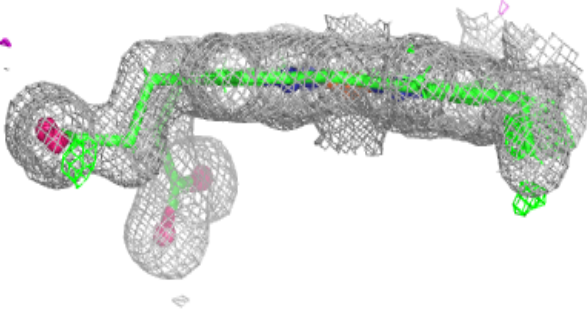
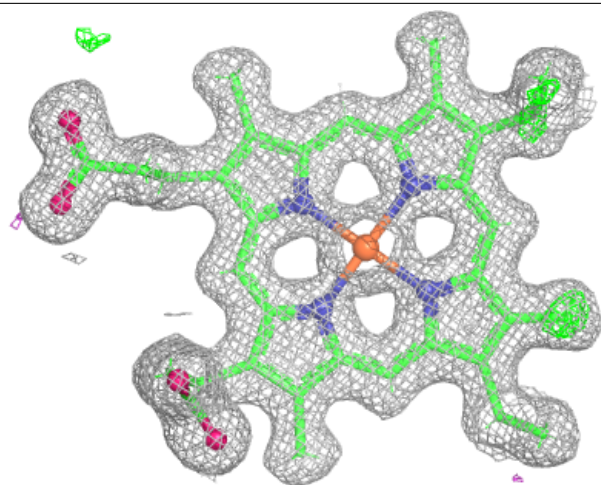
Electron density around HEC A 1005:

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



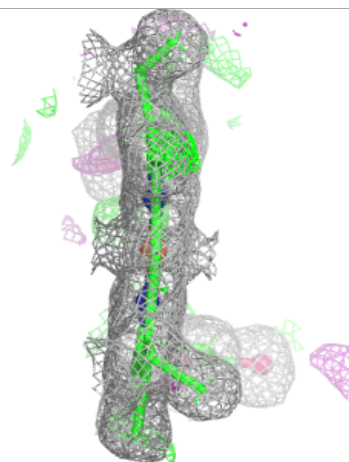
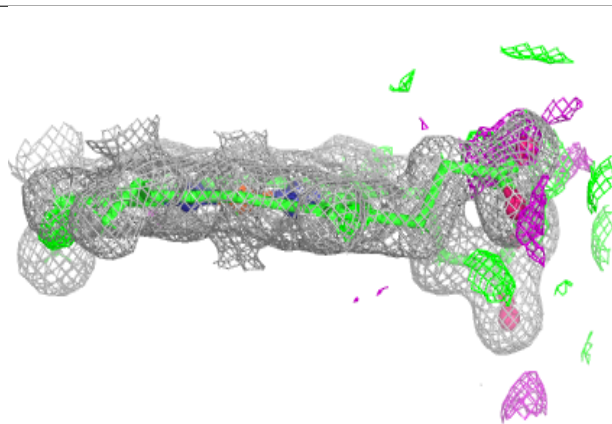
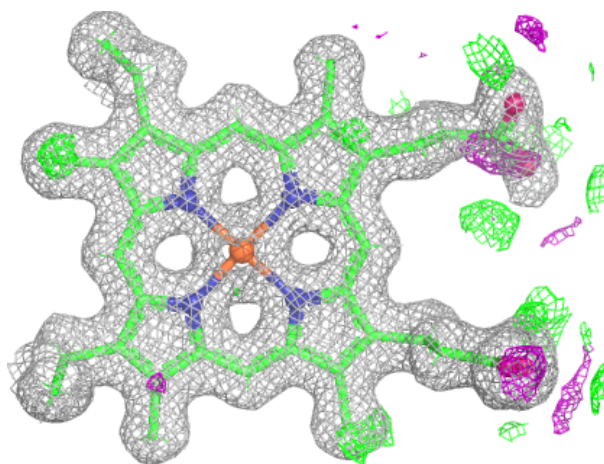
Electron density around HEC A 1002:

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



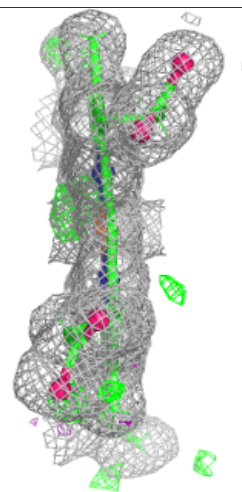
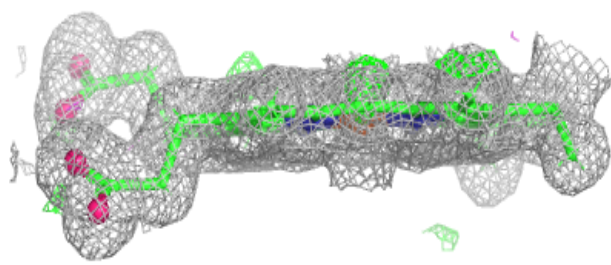
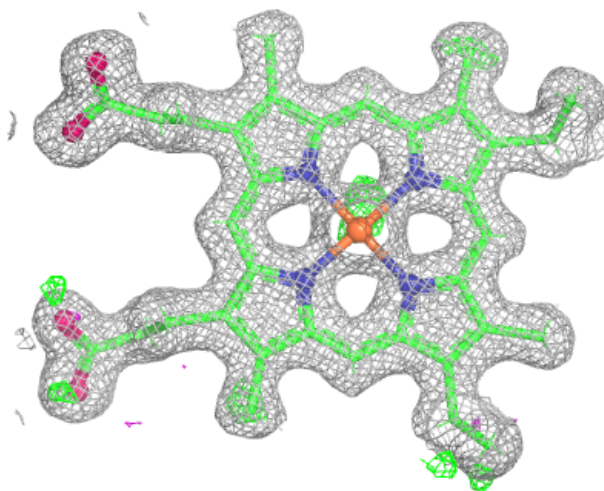
Electron density around HEC A 1003:

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



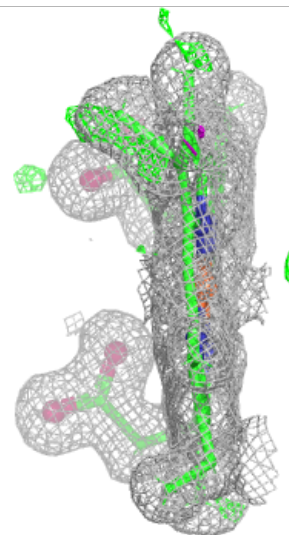
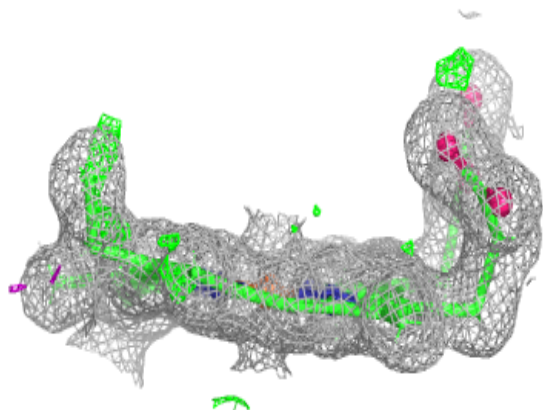
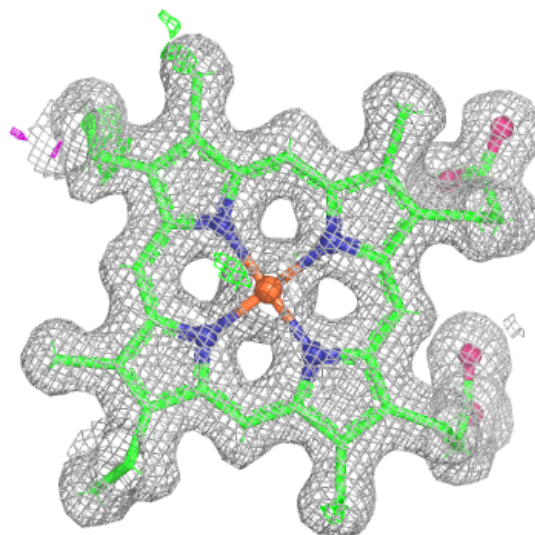
Electron density around HEC A 1001:

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



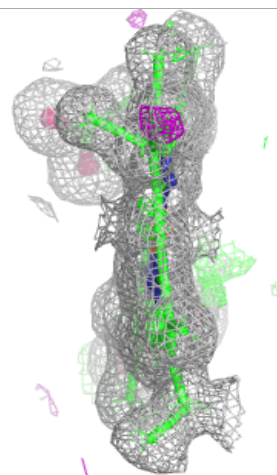
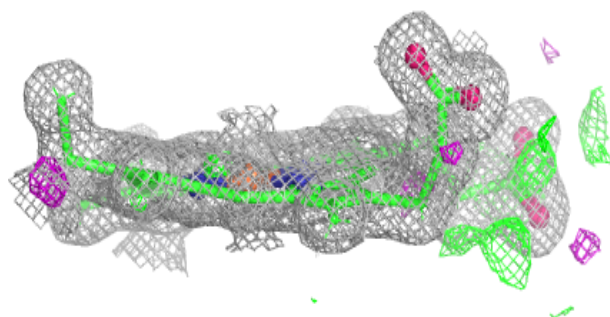
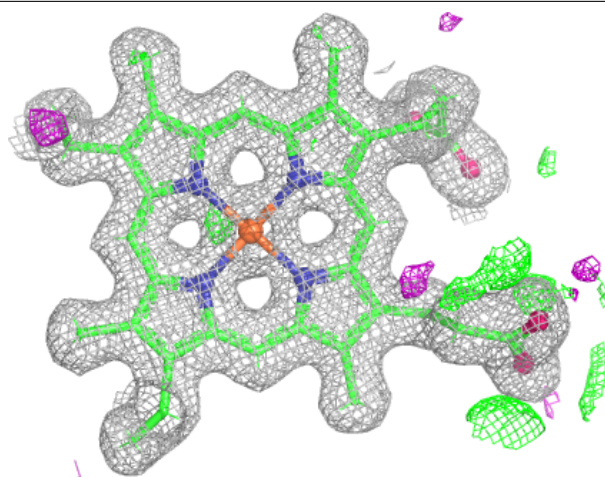
Electron density around HEC B 1004:

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



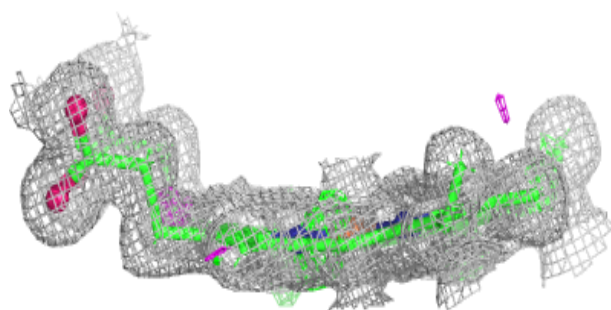
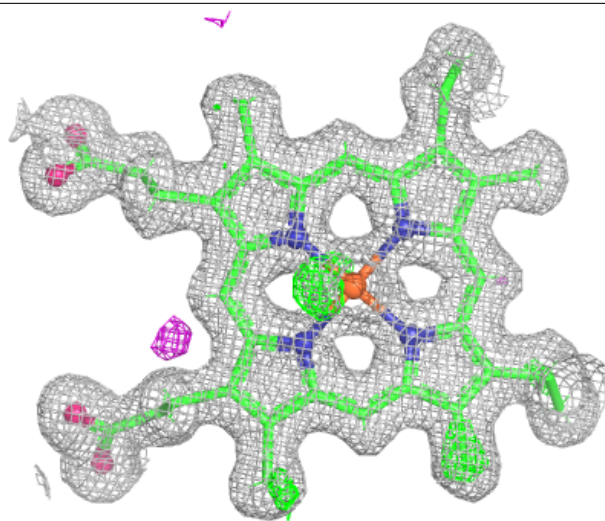
Electron density around HEC B 1005:

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



Electron density around HEC B 1006:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.