



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:05 PM EDT

PDB ID : 3D1I / pdb_00003d1i
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase in a complex with nitrite
Authors : Polyakov, K.M.; Boyko, K.M.; Slutsky, A.; Tikhonova, T.V.; Antipov, A.N.; Zvyagilskaya, R.A.; Popov, A.N.; Lamzin, V.S.; Bourenkov, G.P.; Popov, V.O.
Deposited on : 2008-05-06
Resolution : 1.80 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

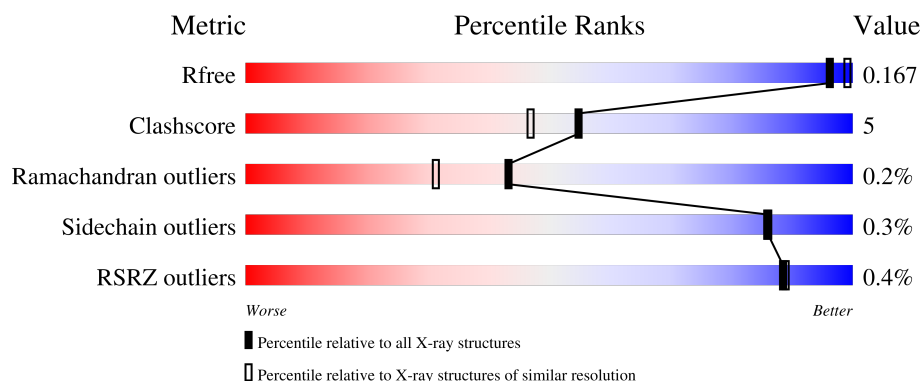
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	
1	B	525	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	1001	X	-	-	-
2	HEC	A	1002	X	-	-	-
2	HEC	A	1003	X	-	-	-
2	HEC	A	1004	X	-	-	-
2	HEC	A	1005	X	-	-	-
2	HEC	A	1006	X	-	-	-
2	HEC	A	1007[A]	X	-	-	-
2	HEC	A	1007[B]	X	-	-	-
2	HEC	B	1001	X	-	-	-
2	HEC	B	1002	X	-	-	-
2	HEC	B	1003	X	-	-	-
2	HEC	B	1004	X	-	-	-
2	HEC	B	1005	X	-	-	-
2	HEC	B	1006	X	-	-	-
2	HEC	B	1007[A]	X	-	-	-
2	HEC	B	1007[B]	X	-	-	-
2	HEC	B	1008	X	-	-	-
6	PG4	B	1011	-	-	-	X
6	PG4	B	1012	-	-	X	-

2 Entry composition [i](#)

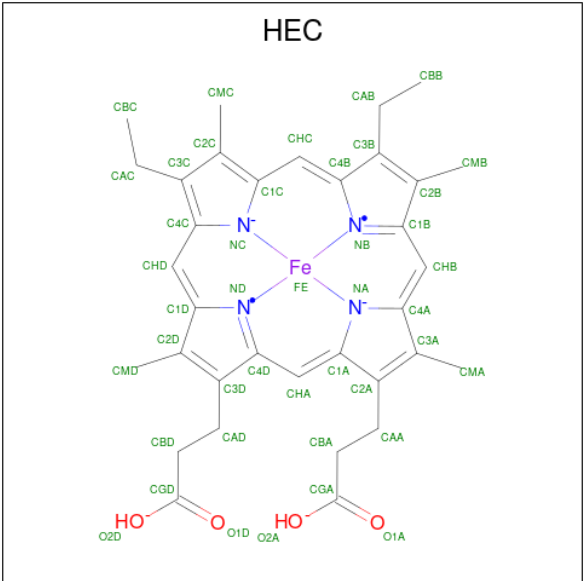
There are 8 unique types of molecules in this entry. The entry contains 18436 atoms, of which 8182 are hydrogens and 0 are deuteriums.

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	1054	23	1
			8034	2591	3856	759	791	37			
1	B	519	Total	C	H	N	O	S	1024	18	0
			8013	2587	3842	762	786	36			

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



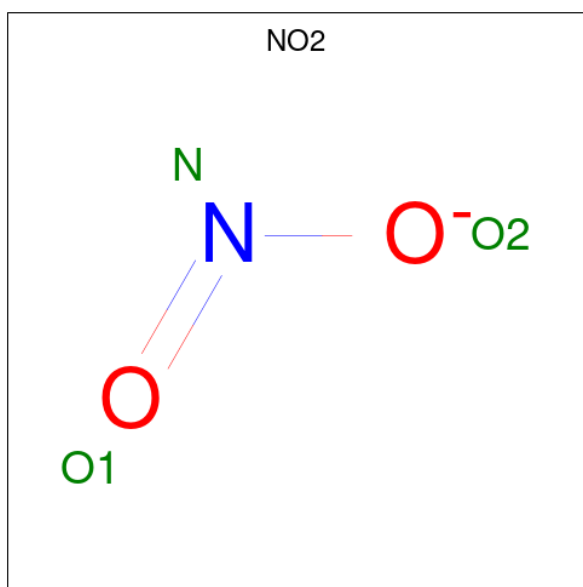
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	18	0
2	B	1	Total 73	C 34	Fe 1	H 30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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is NITRITE ION (CCD ID: NO2) (formula: NO₂).

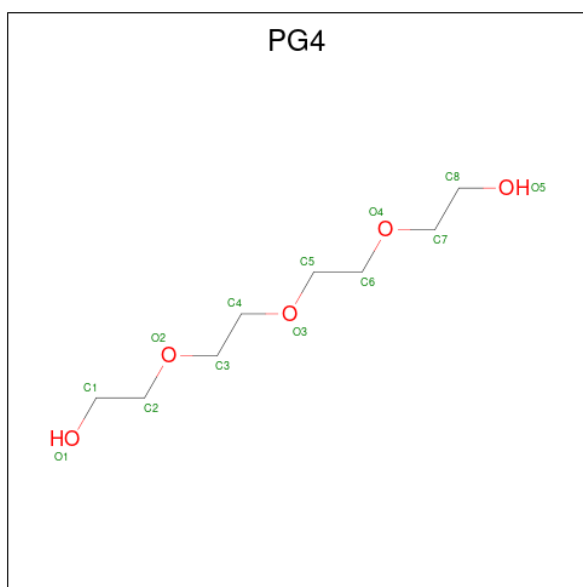


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			3	1	2		
4	B	1	Total	N	O	0	0
			3	1	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

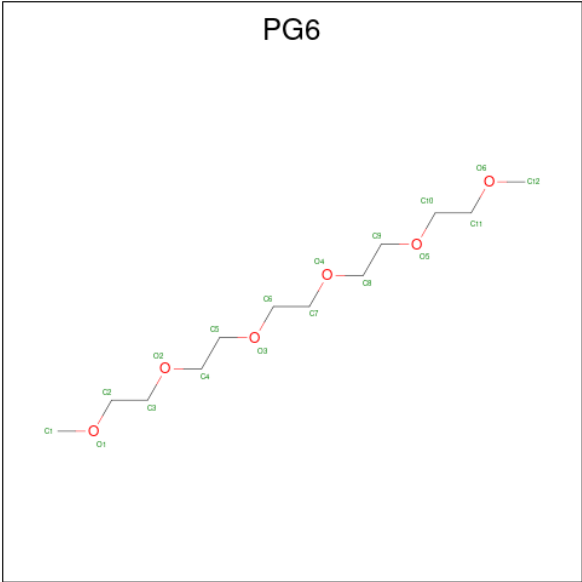
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



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

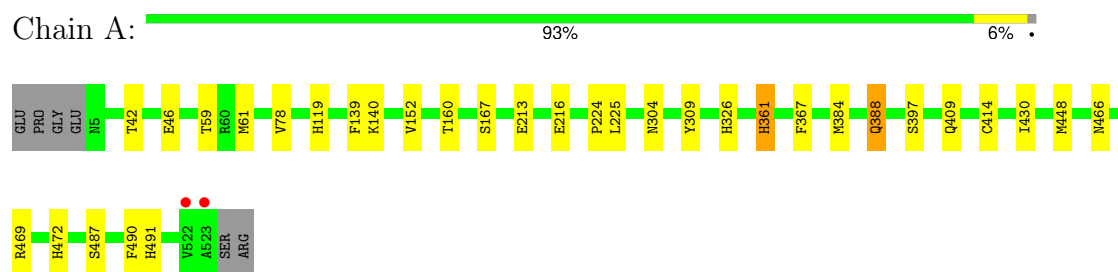
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	557	Total	O	0	0
			557	557		
8	B	573	Total	O	0	0
			573	573		

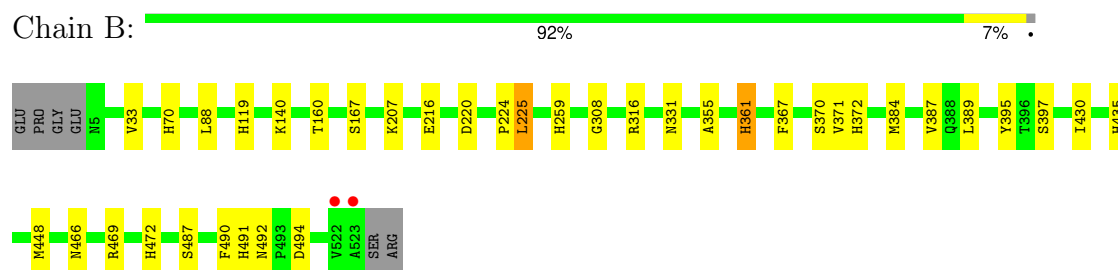
3 Residue-property plots [i](#)

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	193.41Å 193.41Å 193.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 1.80 11.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (11.99-1.80) 99.5 (11.99-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.165 0.151 , 0.167	Depositor DCC
R_{free} test set	11051 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18436	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PG6, NA, HEC, PG4, CA, NO2

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	0.90	0/4415	0.86	0/5986
1	B	0.93	1/4376 (0.0%)	0.88	0/5933
All	All	0.92	1/8791 (0.0%)	0.87	0/11919

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	VAL	CA-CB	5.14	1.59	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4178	3856	3893	26	0
1	B	4171	3842	3900	46	0
2	A	348	242	218	6	0
2	B	348	242	218	6	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	1	0
4	B	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	17	0	16	1	0
6	B	22	0	27	28	0
7	A	14	0	14	3	0
7	B	14	0	14	1	0
8	A	557	0	0	2	0
8	B	573	0	0	0	0
All	All	10254	8182	8300	84	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 5.

All (84) 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:371:VAL:H	6:B:1012:PG4:H51	1.31	0.95
2:A:1008:HEC:HBC3	2:A:1008:HEC:HMC1	1.59	0.84
1:A:139:PHE:HB2	6:A:1011:PG4:H22	1.59	0.84
1:B:372:HIS:H	6:B:1012:PG4:C3	1.98	0.77
1:B:370:SER:HB2	6:B:1012:PG4:H62	1.69	0.75
1:A:213[A]:GLU:OE1	1:A:216[A]:GLU:OE2	2.10	0.69
1:B:494:ASP:CG	6:B:1012:PG4:H82	2.16	0.69
1:B:361:HIS:NE2	4:B:528:NO2:O2	2.26	0.66
1:B:370:SER:CB	6:B:1012:PG4:H62	2.27	0.65
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.77	0.64
1:B:494:ASP:H	6:B:1012:PG4:C7	2.11	0.63
1:B:494:ASP:HB2	6:B:1012:PG4:H72	1.79	0.63
1:B:371:VAL:H	6:B:1012:PG4:C5	2.10	0.63
1:B:371:VAL:N	6:B:1012:PG4:H51	2.09	0.62
1:B:371:VAL:HG23	6:B:1012:PG4:C5	2.32	0.60
1:B:370:SER:CA	6:B:1012:PG4:H62	2.32	0.59
1:B:492:ASN:HA	6:B:1012:PG4:H61	1.85	0.59
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.84	0.59
1:B:370:SER:HA	6:B:1012:PG4:H62	1.86	0.58
1:B:372:HIS:ND1	6:B:1012:PG4:H32	2.20	0.57
1:A:388:GLN:NE2	1:A:409:GLN:OE1	2.38	0.57
1:B:140:LYS:HG2	1:B:160:THR:HG23	1.88	0.55
1:B:308:GLY:O	1:B:316[B]:ARG:HD2	2.07	0.55
7:A:1010:PG6:C10	8:A:1247:HOH:O	2.55	0.54
2:B:1008:HEC:O1A	6:B:1012:PG4:H52	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:HIS:H	6:B:1012:PG4:H32	1.73	0.54
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	1.90	0.54
1:B:371:VAL:CB	6:B:1012:PG4:H51	2.37	0.54
1:B:387[B]:VAL:HG13	1:B:389:LEU:HG	1.91	0.52
1:B:207:LYS:NZ	1:B:220[B]:ASP:OD2	2.40	0.52
2:A:1008:HEC:HMC1	2:A:1008:HEC:CBC	2.36	0.52
1:B:371:VAL:HG23	6:B:1012:PG4:H51	1.91	0.52
1:A:59:THR:HB	1:A:61[C]:MET:HE1	1.92	0.52
1:A:167:SER:HB2	1:A:216[B]:GLU:HG2	1.91	0.52
1:A:59:THR:O	1:A:61[C]:MET:SD	2.69	0.50
1:A:466:ASN:ND2	1:A:469:ARG:HH11	2.09	0.50
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.94	0.49
1:B:371:VAL:HG23	6:B:1012:PG4:H52	1.94	0.49
1:B:372:HIS:HD1	6:B:1012:PG4:H32	1.77	0.49
1:A:430:ILE:HG21	1:A:490:PHE:HA	1.96	0.48
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.12	0.47
1:A:140:LYS:HG2	1:A:160:THR:HG23	1.95	0.47
1:B:371:VAL:N	6:B:1012:PG4:H31	2.29	0.47
1:B:371:VAL:HB	6:B:1012:PG4:H51	1.95	0.47
1:A:384:MET:HB2	1:A:397:SER:O	2.14	0.47
1:B:372:HIS:H	6:B:1012:PG4:H31	1.76	0.47
1:B:355:ALA:HB2	7:B:1010:PG6:H91	1.96	0.47
1:B:259[B]:HIS:HE1	1:B:331:ASN:ND2	2.14	0.46
1:A:78[A]:VAL:HG12	1:A:152:VAL:HG21	1.98	0.46
1:A:361:HIS:NE2	4:A:528:NO2:O2	2.43	0.46
1:B:435:HIS:ND1	6:B:1009:PG4:H31	2.32	0.45
1:B:371:VAL:CG2	6:B:1012:PG4:H51	2.47	0.45
1:B:259[B]:HIS:HE1	1:B:331:ASN:HD22	1.64	0.45
1:B:387[A]:VAL:HG21	1:B:395:TYR:CE1	2.51	0.45
7:A:1010:PG6:O1	8:A:1298:HOH:O	2.21	0.44
1:B:466:ASN:HD22	1:B:469:ARG:HD2	1.82	0.44
1:A:466:ASN:HD22	1:A:469:ARG:HD2	1.83	0.43
1:B:384:MET:HB2	1:B:397:SER:O	2.18	0.43
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.53	0.43
1:A:119:HIS:CD2	2:A:1006:HEC:ND	2.87	0.43
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.99	0.43
1:B:448:MET:HE1	1:B:472:HIS:CD2	2.54	0.43
1:A:167:SER:HB2	1:A:216[A]:GLU:HG3	2.00	0.43
1:B:119:HIS:CD2	2:B:1006:HEC:ND	2.87	0.42
1:A:414[A]:CYS:SG	2:A:1008:HEC:CMC	3.07	0.42
1:B:224:PRO:O	1:B:225:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:HIS:HD1	6:B:1012:PG4:C3	2.33	0.42
1:B:70:HIS:CD2	2:B:1003:HEC:NB	2.87	0.42
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.54	0.42
2:B:1004:HEC:C4D	2:B:1006:HEC:HMD2	2.50	0.42
1:A:224:PRO:O	1:A:225:LEU:C	2.62	0.42
2:A:1008:HEC:HMB1	2:A:1008:HEC:HBB3	2.02	0.42
1:A:448:MET:HE1	1:A:472:HIS:CG	2.56	0.41
1:A:309:TYR:CE1	7:A:1010:PG6:H21	2.55	0.41
1:A:304:ASN:HB2	1:A:326:HIS:HB3	2.01	0.41
1:B:448:MET:HE1	1:B:472:HIS:CG	2.56	0.41
1:A:78[B]:VAL:HG23	1:A:152:VAL:HG21	2.04	0.40
1:A:42:THR:O	1:A:46[A]:GLU:HG3	2.21	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	541/525 (103%)	519 (96%)	21 (4%)	1 (0%)	43	31
1	B	535/525 (102%)	512 (96%)	22 (4%)	1 (0%)	43	31
All	All	1076/1050 (102%)	1031 (96%)	43 (4%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	459/443 (104%)	458 (100%)	1 (0%)	87	87
1	B	454/443 (102%)	451 (99%)	3 (1%)	76	73
All	All	913/886 (103%)	909 (100%)	4 (0%)	86	83

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

Mol	Chain	Res	Type
1	A	388	GLN
1	B	88[A]	LEU
1	B	88[B]	LEU
1	B	225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	190	GLN
1	A	388	GLN
1	A	466	ASN
1	A	467	GLN
1	A	521	GLN
1	B	267	GLN
1	B	275	GLN
1	B	413	ASN
1	B	466	ASN
1	B	521	GLN

5.3.3 RNA ⓘ

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 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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$
2	HEC	B	1005	1	50,50,50	1.33	6 (12%)	68,82,82	1.24	10 (14%)
2	HEC	A	1007[A]	-	50,50,50	1.48	7 (14%)	68,82,82	1.44	11 (16%)
4	NO2	A	528	2	1,2,2	4.61	1 (100%)	0,1,1	-	-
2	HEC	A	1004	4,1,8	50,50,50	1.60	7 (14%)	68,82,82	1.19	7 (10%)
2	HEC	A	1006	1,3	50,50,50	1.65	8 (16%)	68,82,82	1.28	5 (7%)
2	HEC	B	1004	4,1,8	50,50,50	1.70	10 (20%)	68,82,82	1.22	8 (11%)
6	PG4	A	1009	-	5,5,12	0.67	0	4,4,11	0.30	0
6	PG4	A	1011	-	5,5,12	0.81	0	4,4,11	1.35	1 (25%)
4	NO2	B	528	2	1,2,2	4.58	1 (100%)	0,1,1	-	-
7	PG6	B	1010	1	13,13,17	0.54	0	12,12,16	0.71	0
6	PG4	B	1009	-	6,6,12	0.53	0	5,5,11	0.33	0
6	PG4	A	1012	-	4,4,12	0.46	0	3,3,11	0.40	0
2	HEC	B	1006	1,3	50,50,50	1.56	9 (18%)	68,82,82	1.57	14 (20%)
6	PG4	B	1011	-	4,4,12	0.38	0	3,3,11	0.45	0
2	HEC	A	1001	1	50,50,50	1.59	9 (18%)	68,82,82	1.35	12 (17%)
6	PG4	B	1012	-	9,9,12	0.57	0	8,8,11	0.75	0
2	HEC	B	1007[B]	3	50,50,50	1.62	11 (22%)	68,82,82	1.45	15 (22%)
2	HEC	B	1001	1	50,50,50	1.66	9 (18%)	68,82,82	1.48	12 (17%)
2	HEC	A	1002	1	50,50,50	1.59	9 (18%)	68,82,82	1.28	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	1008	1	50,50,50	1.56	6 (12%)	68,82,82	1.23	8 (11%)
7	PG6	A	1010	1	13,13,17	0.51	0	12,12,16	0.45	0
2	HEC	A	1003	1	50,50,50	1.25	2 (4%)	68,82,82	1.19	6 (8%)
2	HEC	A	1007[B]	3	50,50,50	1.47	7 (14%)	68,82,82	1.45	11 (16%)
2	HEC	B	1002	1	50,50,50	1.79	10 (20%)	68,82,82	1.29	6 (8%)
2	HEC	B	1007[A]	-	50,50,50	1.63	11 (22%)	68,82,82	1.44	14 (20%)
2	HEC	A	1005	1	50,50,50	1.43	7 (14%)	68,82,82	1.25	5 (7%)
2	HEC	B	1003	1	50,50,50	1.50	6 (12%)	68,82,82	1.38	9 (13%)
2	HEC	B	1008	1	50,50,50	1.63	12 (24%)	68,82,82	1.53	14 (20%)

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
2	HEC	B	1005	1	1/1/7/7	8/14/54/54	-
2	HEC	A	1007[A]	-	1/1/7/7	5/14/54/54	-
2	HEC	A	1004	4,1,8	1/1/7/7	6/14/54/54	-
2	HEC	A	1006	1,3	1/1/7/7	5/14/54/54	-
2	HEC	B	1004	4,1,8	1/1/7/7	6/14/54/54	-
6	PG4	A	1009	-	-	3/3/3/10	-
6	PG4	A	1011	-	-	2/3/3/10	-
7	PG6	B	1010	1	-	7/11/11/15	-
6	PG4	B	1009	-	-	4/4/4/10	-
6	PG4	A	1012	-	-	0/2/2/10	-
2	HEC	B	1006	1,3	1/1/7/7	4/14/54/54	-
6	PG4	B	1011	-	-	2/2/2/10	-
2	HEC	A	1001	1	1/1/7/7	8/14/54/54	-
6	PG4	B	1012	-	-	5/7/7/10	-
2	HEC	B	1007[B]	3	1/1/7/7	5/14/54/54	-
2	HEC	B	1001	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1002	1	1/1/7/7	6/14/54/54	-
2	HEC	A	1008	1	-	8/14/54/54	-
7	PG6	A	1010	1	-	2/11/11/15	-
2	HEC	A	1003	1	1/1/7/7	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1007[B]	3	1/1/7/7	6/14/54/54	-
2	HEC	B	1002	1	1/1/7/7	6/14/54/54	-
2	HEC	B	1007[A]	-	1/1/7/7	6/14/54/54	-
2	HEC	A	1005	1	1/1/7/7	8/14/54/54	-
2	HEC	B	1003	1	1/1/7/7	6/14/54/54	-
2	HEC	B	1008	1	1/1/7/7	6/14/54/54	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	HEC	C3D-C2D	6.27	1.50	1.36
2	B	1001	HEC	C3D-C2D	6.16	1.50	1.36
2	B	1008	HEC	C3D-C2D	6.07	1.49	1.36
2	A	1008	HEC	C3D-C2D	5.96	1.49	1.36
2	A	1006	HEC	C3D-C2D	5.96	1.49	1.36
2	B	1006	HEC	C3D-C2D	5.74	1.49	1.36
2	A	1001	HEC	C3D-C2D	5.51	1.48	1.36
2	A	1002	HEC	C3D-C2D	5.40	1.48	1.36
2	A	1004	HEC	C3D-C2D	5.29	1.48	1.36
2	B	1007[A]	HEC	C3D-C2D	5.26	1.48	1.36
2	B	1007[B]	HEC	C3D-C2D	5.26	1.48	1.36
2	B	1004	HEC	C3D-C2D	5.23	1.48	1.36
2	B	1003	HEC	C3D-C2D	5.23	1.48	1.36
2	A	1005	HEC	C3D-C2D	5.03	1.47	1.36
2	A	1003	HEC	C3D-C2D	4.94	1.47	1.36
2	A	1007[A]	HEC	C3D-C2D	4.85	1.47	1.36
2	A	1007[B]	HEC	C3D-C2D	4.85	1.47	1.36
4	A	528	NO2	O1-N	4.61	1.45	1.22
4	B	528	NO2	O1-N	4.58	1.45	1.22
2	B	1004	HEC	CMC-C2C	4.21	1.59	1.50
2	A	1004	HEC	CMC-C2C	3.91	1.58	1.50
2	B	1005	HEC	C3D-C2D	3.82	1.45	1.36
2	A	1001	HEC	FE-NC	3.65	2.07	1.95
2	A	1008	HEC	CMD-C2D	3.45	1.57	1.50
2	B	1004	HEC	CMB-C2B	3.37	1.57	1.50
2	B	1002	HEC	CMC-C2C	3.35	1.57	1.50
2	A	1004	HEC	CMB-C2B	3.31	1.57	1.50
2	B	1004	HEC	FE-NB	3.30	2.05	1.94
2	B	1001	HEC	FE-NC	3.28	2.06	1.95
2	B	1003	HEC	CMA-C3A	3.16	1.57	1.50
2	A	1003	HEC	CMB-C2B	3.15	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	HEC	FE-NA	3.14	2.05	1.95
2	B	1002	HEC	FE-ND	3.11	2.04	1.94
2	B	1003	HEC	CMB-C2B	3.09	1.57	1.50
2	B	1002	HEC	CMB-C2B	3.09	1.57	1.50
2	A	1004	HEC	FE-NB	3.03	2.04	1.94
2	A	1006	HEC	CAC-C3C	2.94	1.58	1.51
2	B	1007[A]	HEC	FE-ND	2.93	2.03	1.94
2	B	1007[B]	HEC	FE-ND	2.93	2.03	1.94
2	A	1006	HEC	CMC-C2C	2.92	1.56	1.50
2	A	1005	HEC	CMA-C3A	2.91	1.56	1.50
2	A	1002	HEC	CAC-C3C	2.91	1.58	1.51
2	B	1007[A]	HEC	CMD-C2D	2.90	1.56	1.50
2	B	1007[B]	HEC	CMD-C2D	2.90	1.56	1.50
2	B	1007[A]	HEC	CMB-C2B	2.90	1.56	1.50
2	B	1007[B]	HEC	CMB-C2B	2.90	1.56	1.50
2	B	1007[A]	HEC	CHA-C4D	-2.88	1.32	1.39
2	B	1007[B]	HEC	CHA-C4D	-2.88	1.32	1.39
2	A	1008	HEC	CMA-C3A	2.87	1.56	1.50
2	A	1001	HEC	CAC-C3C	2.87	1.58	1.51
2	A	1002	HEC	CMB-C2B	2.84	1.56	1.50
2	B	1001	HEC	CMA-C3A	2.83	1.56	1.50
2	B	1005	HEC	CMB-C2B	2.81	1.56	1.50
2	B	1002	HEC	C4B-NB	-2.80	1.35	1.40
2	B	1005	HEC	CMA-C3A	2.80	1.56	1.50
2	B	1003	HEC	CMD-C2D	2.78	1.56	1.50
2	B	1001	HEC	CAC-C3C	2.76	1.58	1.51
2	B	1006	HEC	CMC-C2C	2.74	1.56	1.50
2	B	1003	HEC	CMC-C2C	2.71	1.56	1.50
2	B	1006	HEC	CMA-C3A	2.70	1.56	1.50
2	A	1001	HEC	FE-ND	2.68	2.03	1.94
2	A	1006	HEC	FE-NC	2.67	2.04	1.95
2	B	1008	HEC	CAC-C3C	2.66	1.57	1.51
2	A	1006	HEC	FE-NA	2.65	2.03	1.95
2	A	1005	HEC	O2D-CGD	-2.65	1.22	1.30
2	B	1006	HEC	CAC-C3C	2.63	1.57	1.51
2	B	1002	HEC	CAC-C3C	2.62	1.57	1.51
2	B	1005	HEC	O2D-CGD	-2.60	1.22	1.30
2	A	1001	HEC	CMA-C3A	2.60	1.56	1.50
2	B	1002	HEC	CMA-C3A	2.59	1.56	1.50
2	A	1002	HEC	CMA-C3A	2.59	1.56	1.50
2	A	1004	HEC	CAB-C3B	2.59	1.57	1.51
2	B	1008	HEC	CMC-C2C	2.57	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1007[A]	HEC	C4B-NB	-2.56	1.35	1.40
2	B	1007[B]	HEC	C4B-NB	-2.56	1.35	1.40
2	A	1008	HEC	CHA-C4D	-2.52	1.33	1.39
2	B	1008	HEC	C2A-C3A	-2.52	1.31	1.36
2	B	1001	HEC	C1C-NC	-2.51	1.34	1.39
2	A	1002	HEC	CAB-C3B	2.50	1.57	1.51
2	A	1007[A]	HEC	C4B-NB	-2.50	1.35	1.40
2	A	1007[B]	HEC	C4B-NB	-2.50	1.35	1.40
2	A	1001	HEC	FE-NB	2.49	2.02	1.94
2	B	1003	HEC	C1C-C2C	2.48	1.48	1.43
2	B	1007[A]	HEC	FE-NB	2.44	2.02	1.94
2	B	1007[B]	HEC	FE-NB	2.44	2.02	1.94
2	A	1005	HEC	CMB-C2B	2.43	1.55	1.50
2	A	1002	HEC	FE-NC	2.42	2.03	1.95
2	A	1007[A]	HEC	CMA-C3A	2.38	1.55	1.50
2	A	1007[B]	HEC	CMA-C3A	2.38	1.55	1.50
2	B	1006	HEC	CAB-C3B	2.37	1.57	1.51
2	B	1007[A]	HEC	CHD-C1D	-2.37	1.33	1.38
2	B	1007[B]	HEC	CHD-C1D	-2.37	1.33	1.38
2	B	1002	HEC	FE-NB	2.36	2.02	1.94
2	A	1007[A]	HEC	CMB-C2B	2.34	1.55	1.50
2	A	1007[B]	HEC	CMB-C2B	2.34	1.55	1.50
2	B	1005	HEC	CAC-C3C	2.33	1.57	1.51
2	A	1008	HEC	CMB-C2B	2.33	1.55	1.50
2	B	1004	HEC	C1B-C2B	2.32	1.49	1.44
2	A	1002	HEC	CMD-C2D	2.31	1.55	1.50
2	B	1002	HEC	CAB-C3B	2.30	1.57	1.51
2	B	1007[A]	HEC	CMC-C2C	2.29	1.55	1.50
2	B	1007[B]	HEC	CMC-C2C	2.29	1.55	1.50
2	B	1001	HEC	CAB-C3B	2.29	1.56	1.51
2	B	1008	HEC	CMA-C3A	2.28	1.55	1.50
2	B	1004	HEC	O2D-CGD	-2.26	1.23	1.30
2	B	1001	HEC	CMD-C2D	2.26	1.55	1.50
2	B	1008	HEC	C4B-NB	-2.26	1.36	1.40
2	B	1006	HEC	CHB-C4A	-2.23	1.34	1.38
2	B	1004	HEC	C4C-NC	-2.22	1.35	1.39
2	B	1006	HEC	FE-NC	2.22	2.02	1.95
2	A	1007[A]	HEC	FE-NB	2.22	2.01	1.94
2	A	1007[B]	HEC	FE-NB	2.22	2.01	1.94
2	A	1001	HEC	CAB-C3B	2.21	1.56	1.51
2	A	1005	HEC	CHD-C1D	-2.21	1.34	1.38
2	A	1004	HEC	C1B-C2B	2.20	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1008	HEC	CMB-C2B	2.20	1.55	1.50
2	B	1004	HEC	CMA-C3A	2.20	1.55	1.50
2	A	1006	HEC	C1C-NC	-2.19	1.35	1.39
2	A	1001	HEC	CMB-C2B	2.19	1.55	1.50
2	B	1002	HEC	CMD-C2D	2.17	1.55	1.50
2	A	1007[A]	HEC	CHA-C4D	-2.17	1.34	1.39
2	A	1007[B]	HEC	CHA-C4D	-2.17	1.34	1.39
2	A	1001	HEC	CMD-C2D	2.15	1.55	1.50
2	B	1008	HEC	CHB-C4A	-2.15	1.34	1.38
2	B	1008	HEC	CMD-C2D	2.14	1.55	1.50
2	B	1006	HEC	FE-NA	2.14	2.02	1.95
2	A	1005	HEC	CMD-C2D	2.14	1.55	1.50
2	A	1005	HEC	C2A-C3A	-2.13	1.32	1.36
2	B	1008	HEC	C1A-NA	-2.13	1.35	1.39
2	B	1007[A]	HEC	CMA-C3A	2.12	1.55	1.50
2	B	1007[B]	HEC	CMA-C3A	2.12	1.55	1.50
2	B	1005	HEC	CHC-C1C	-2.12	1.34	1.39
2	A	1002	HEC	C4B-C3B	2.11	1.48	1.45
2	A	1006	HEC	C1A-NA	-2.10	1.35	1.39
2	A	1008	HEC	CMC-C2C	2.09	1.55	1.50
2	B	1007[A]	HEC	C1B-NB	-2.08	1.34	1.38
2	B	1007[B]	HEC	C1B-NB	-2.08	1.34	1.38
2	B	1004	HEC	FE-ND	2.08	2.01	1.94
2	B	1008	HEC	CHC-C1C	-2.08	1.34	1.39
2	A	1006	HEC	CMD-C2D	2.07	1.55	1.50
2	A	1007[A]	HEC	CHD-C1D	-2.07	1.34	1.38
2	A	1007[B]	HEC	CHD-C1D	-2.07	1.34	1.38
2	A	1004	HEC	CBA-CGA	2.04	1.55	1.50
2	B	1008	HEC	C3B-C2B	-2.03	1.32	1.36
2	B	1006	HEC	C1A-NA	-2.02	1.35	1.39
2	B	1001	HEC	C1A-NA	-2.01	1.35	1.39
2	B	1004	HEC	C4C-C3C	2.01	1.48	1.44
2	A	1002	HEC	FE-NA	2.00	2.01	1.95

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1008	HEC	C1D-ND-C4D	4.97	111.09	105.21
2	B	1001	HEC	CMC-C2C-C1C	-4.86	118.02	125.42
2	A	1004	HEC	CAD-C3D-C4D	4.19	131.99	124.70
2	A	1001	HEC	C1D-ND-C4D	4.03	109.98	105.21
2	B	1006	HEC	C2D-C1D-ND	4.01	114.45	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1008	HEC	CMC-C2C-C1C	-3.89	119.49	125.42
2	B	1007[A]	HEC	CMB-C2B-C1B	-3.78	119.13	125.03
2	B	1007[B]	HEC	CMB-C2B-C1B	-3.78	119.13	125.03
2	B	1007[A]	HEC	C1D-ND-C4D	3.77	109.67	105.21
2	B	1007[B]	HEC	C1D-ND-C4D	3.77	109.67	105.21
2	A	1008	HEC	O1A-CGA-CBA	-3.73	111.25	123.09
2	B	1002	HEC	CAA-CBA-CGA	-3.69	103.88	113.67
2	B	1006	HEC	C1D-C2D-C3D	-3.67	103.12	106.98
2	A	1007[A]	HEC	CMB-C2B-C1B	-3.64	119.35	125.03
2	A	1007[B]	HEC	CMB-C2B-C1B	-3.64	119.35	125.03
2	A	1007[A]	HEC	CMD-C2D-C1D	3.58	130.63	125.03
2	A	1007[B]	HEC	CMD-C2D-C1D	3.58	130.63	125.03
2	B	1002	HEC	C1D-ND-C4D	3.57	109.43	105.21
2	B	1004	HEC	CHB-C1B-NB	-3.53	120.62	124.42
2	B	1006	HEC	CAD-C3D-C4D	3.44	130.69	124.70
2	A	1004	HEC	CMD-C2D-C1D	3.36	130.29	125.03
2	B	1003	HEC	C3D-C4D-ND	3.33	113.57	110.35
2	B	1004	HEC	CAD-C3D-C4D	3.26	130.37	124.70
2	B	1001	HEC	CHB-C4A-NA	3.17	127.91	124.45
2	B	1001	HEC	C2A-C1A-NA	-3.12	107.32	110.32
2	A	1003	HEC	CMD-C2D-C1D	3.11	129.89	125.03
2	B	1003	HEC	C1D-C2D-C3D	-3.09	103.72	106.98
2	B	1008	HEC	O1A-CGA-CBA	-3.08	113.31	123.09
2	A	1001	HEC	CAD-CBD-CGD	-3.05	105.58	113.67
2	A	1008	HEC	C1D-ND-C4D	3.04	108.81	105.21
2	B	1005	HEC	CHC-C4B-NB	-3.01	120.64	124.37
2	B	1008	HEC	CAD-C3D-C4D	3.00	129.93	124.70
2	B	1004	HEC	C1D-C2D-C3D	-2.96	103.87	106.98
2	A	1003	HEC	CBC-CAC-C3C	2.95	120.43	112.42
2	A	1006	HEC	C4A-NA-C1A	2.95	110.63	105.82
2	B	1006	HEC	CMA-C3A-C4A	-2.91	119.60	124.73
2	B	1007[A]	HEC	CBD-CAD-C3D	-2.89	104.53	112.53
2	B	1007[B]	HEC	CBD-CAD-C3D	-2.89	104.53	112.53
2	A	1008	HEC	O2A-CGA-CBA	2.89	123.12	114.00
2	A	1005	HEC	C1D-C2D-C3D	-2.87	103.97	106.98
2	B	1007[A]	HEC	C4B-NB-C1B	2.82	108.55	105.21
2	B	1007[B]	HEC	C4B-NB-C1B	2.82	108.55	105.21
2	A	1005	HEC	CMB-C2B-C1B	-2.82	120.63	125.03
2	A	1006	HEC	CHB-C4A-NA	2.81	127.52	124.45
2	A	1004	HEC	CBB-CAB-C3B	-2.81	104.80	112.42
2	A	1002	HEC	C2A-C1A-NA	-2.80	107.62	110.32
2	A	1007[A]	HEC	CAD-C3D-C4D	2.80	129.58	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1007[B]	HEC	CAD-C3D-C4D	2.80	129.58	124.70
2	B	1006	HEC	C3B-C4B-NB	2.80	113.24	110.17
2	B	1006	HEC	CMC-C2C-C1C	-2.79	121.17	125.42
2	A	1006	HEC	C2A-C1A-NA	-2.79	107.63	110.32
2	A	1007[A]	HEC	CAC-C3C-C4C	2.78	128.74	124.91
2	A	1007[B]	HEC	CAC-C3C-C4C	2.78	128.74	124.91
2	A	1006	HEC	CAD-C3D-C4D	2.78	129.54	124.70
2	B	1001	HEC	CAC-C3C-C4C	2.78	128.73	124.91
2	A	1005	HEC	CMC-C2C-C1C	-2.78	121.19	125.42
2	B	1006	HEC	CBB-CAB-C3B	-2.77	104.92	112.42
2	A	1001	HEC	CHD-C1D-ND	2.76	127.78	124.37
2	A	1002	HEC	C1B-C2B-C3B	2.75	109.88	106.98
2	B	1005	HEC	C3B-C4B-NB	2.75	113.18	110.17
2	A	1001	HEC	CMC-C2C-C1C	-2.71	121.29	125.42
2	B	1008	HEC	CHD-C1D-ND	2.70	127.71	124.37
2	A	1002	HEC	CAA-CBA-CGA	-2.68	106.56	113.67
2	B	1004	HEC	C1D-ND-C4D	2.67	108.37	105.21
2	B	1007[A]	HEC	CBB-CAB-C3B	-2.66	105.22	112.42
2	B	1007[B]	HEC	CBB-CAB-C3B	-2.66	105.22	112.42
2	A	1002	HEC	CMD-C2D-C1D	2.66	129.19	125.03
2	B	1006	HEC	CMA-C3A-C2A	2.64	133.30	126.15
2	A	1007[A]	HEC	C1D-C2D-C3D	-2.63	104.22	106.98
2	A	1007[B]	HEC	C1D-C2D-C3D	-2.63	104.22	106.98
2	A	1006	HEC	C2D-C1D-ND	2.60	112.83	109.84
2	A	1004	HEC	CAD-C3D-C2D	-2.60	123.00	127.87
2	B	1001	HEC	CMD-C2D-C1D	2.59	129.09	125.03
2	B	1008	HEC	CAC-C3C-C2C	2.59	130.99	126.89
2	B	1005	HEC	O1A-CGA-CBA	-2.57	114.94	123.09
2	B	1002	HEC	O2A-CGA-CBA	2.57	122.12	114.00
2	B	1005	HEC	CMD-C2D-C1D	2.57	129.04	125.03
2	B	1007[A]	HEC	C3C-C4C-NC	2.56	112.99	110.15
2	B	1007[B]	HEC	C3C-C4C-NC	2.56	112.99	110.15
2	B	1004	HEC	CAD-C3D-C2D	-2.54	123.10	127.87
2	B	1003	HEC	CAB-C3B-C4B	2.52	128.07	124.79
2	B	1005	HEC	CAD-C3D-C4D	2.52	129.09	124.70
2	B	1005	HEC	O2A-CGA-CBA	2.51	121.93	114.00
2	B	1001	HEC	C4A-NA-C1A	2.51	109.91	105.82
2	A	1007[A]	HEC	C1D-ND-C4D	2.50	108.17	105.21
2	A	1007[B]	HEC	C1D-ND-C4D	2.50	108.17	105.21
2	A	1008	HEC	CBD-CAD-C3D	-2.48	105.67	112.53
2	A	1001	HEC	CHA-C1A-NA	2.48	127.15	124.45
2	A	1002	HEC	C4B-C3B-C2B	-2.46	103.31	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1007[B]	HEC	O2A-CGA-CBA	2.46	121.78	114.00
2	B	1006	HEC	C4B-NB-C1B	-2.45	102.30	105.21
2	A	1003	HEC	CAD-C3D-C4D	2.45	128.97	124.70
2	B	1008	HEC	CBD-CAD-C3D	-2.44	105.78	112.53
2	B	1008	HEC	O2A-CGA-CBA	2.44	121.70	114.00
2	A	1008	HEC	CHD-C1D-ND	2.42	127.36	124.37
2	B	1007[A]	HEC	C4C-NC-C1C	-2.42	101.88	105.82
2	B	1007[B]	HEC	C4C-NC-C1C	-2.42	101.88	105.82
2	A	1007[A]	HEC	CBD-CAD-C3D	-2.41	105.87	112.53
2	A	1007[B]	HEC	CBD-CAD-C3D	-2.41	105.87	112.53
2	A	1001	HEC	C1B-C2B-C3B	2.39	109.50	106.98
2	A	1007[A]	HEC	CBA-CAA-C2A	-2.39	105.92	112.53
2	B	1003	HEC	CHC-C4B-NB	-2.39	121.41	124.37
2	B	1001	HEC	O2A-CGA-CBA	2.36	121.46	114.00
2	B	1008	HEC	CMB-C2B-C1B	-2.36	121.35	125.03
2	A	1003	HEC	CAD-CBD-CGD	-2.36	107.41	113.67
2	B	1003	HEC	CAD-CBD-CGD	-2.35	107.43	113.67
2	B	1005	HEC	CBB-CAB-C3B	-2.35	106.05	112.42
2	B	1005	HEC	CHD-C1D-ND	2.34	127.26	124.37
2	A	1002	HEC	C1D-C2D-C3D	-2.32	104.54	106.98
2	B	1007[A]	HEC	C2B-C1B-NB	-2.30	107.24	109.90
2	B	1007[B]	HEC	C2B-C1B-NB	-2.30	107.24	109.90
2	B	1008	HEC	CAD-CBD-CGD	-2.30	107.57	113.67
2	B	1008	HEC	CAD-C3D-C2D	-2.29	123.57	127.87
2	B	1003	HEC	C4B-NB-C1B	-2.29	102.49	105.21
2	A	1008	HEC	CAD-C3D-C4D	2.27	128.65	124.70
2	B	1008	HEC	C4C-NC-C1C	-2.27	102.13	105.82
2	A	1007[A]	HEC	C2B-C1B-NB	-2.26	107.29	109.90
2	A	1007[B]	HEC	C2B-C1B-NB	-2.26	107.29	109.90
2	B	1008	HEC	C1D-C2D-C3D	-2.26	104.60	106.98
2	B	1001	HEC	O1A-CGA-CBA	-2.24	115.99	123.09
2	A	1002	HEC	CBB-CAB-C3B	-2.24	106.36	112.42
2	B	1003	HEC	O2A-CGA-CBA	2.23	121.05	114.00
2	A	1001	HEC	C4C-NC-C1C	2.23	109.46	105.82
2	A	1004	HEC	CBC-CAC-C3C	2.22	118.44	112.42
2	A	1005	HEC	CMD-C2D-C1D	2.21	128.49	125.03
2	B	1007[A]	HEC	CBA-CAA-C2A	-2.21	106.42	112.53
2	A	1001	HEC	CHB-C4A-NA	2.20	126.85	124.45
2	B	1004	HEC	CHB-C1B-C2B	2.20	128.50	125.03
2	B	1002	HEC	C1D-C2D-C3D	-2.20	104.66	106.98
2	B	1008	HEC	CMD-C2D-C1D	2.20	128.47	125.03
2	A	1004	HEC	C1D-ND-C4D	2.20	107.81	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	HEC	CAD-C3D-C4D	2.19	128.52	124.70
6	A	1011	PG4	O2-C2-C1	2.19	119.77	110.11
2	B	1007[A]	HEC	C2C-C1C-NC	2.18	113.64	110.14
2	B	1007[B]	HEC	C2C-C1C-NC	2.18	113.64	110.14
2	B	1006	HEC	CAD-C3D-C2D	-2.18	123.78	127.87
2	A	1003	HEC	CBA-CAA-C2A	-2.17	106.53	112.53
2	B	1007[A]	HEC	C1D-C2D-C3D	-2.17	104.70	106.98
2	B	1007[B]	HEC	C1D-C2D-C3D	-2.17	104.70	106.98
2	B	1001	HEC	C3C-C4C-NC	-2.16	107.75	110.15
2	B	1004	HEC	CHD-C1D-ND	2.16	127.03	124.37
2	A	1004	HEC	C1D-C2D-C3D	-2.15	104.72	106.98
2	B	1001	HEC	CBB-CAB-C3B	-2.15	106.61	112.42
2	B	1002	HEC	CMC-C2C-C1C	-2.14	122.15	125.42
2	A	1005	HEC	CAD-CBD-CGD	-2.14	107.98	113.67
2	B	1006	HEC	C1C-C2C-C3C	2.13	109.26	106.82
2	A	1001	HEC	O2A-CGA-CBA	2.13	120.73	114.00
2	A	1001	HEC	C2A-C1A-NA	-2.13	108.27	110.32
2	B	1006	HEC	C4A-NA-C1A	2.13	109.29	105.82
2	A	1003	HEC	O1D-CGD-CBD	-2.12	116.37	123.09
2	A	1001	HEC	O1A-CGA-CBA	-2.11	116.40	123.09
2	B	1007[B]	HEC	O2A-CGA-CBA	2.10	120.65	114.00
2	B	1002	HEC	CAD-C3D-C4D	2.08	128.32	124.70
2	A	1007[A]	HEC	CAD-C3D-C2D	-2.08	123.98	127.87
2	A	1007[B]	HEC	CAD-C3D-C2D	-2.08	123.98	127.87
2	B	1001	HEC	CAA-C2A-C1A	-2.08	120.63	124.85
2	A	1007[A]	HEC	CBC-CAC-C3C	2.07	118.04	112.42
2	A	1007[B]	HEC	CBC-CAC-C3C	2.07	118.04	112.42
2	B	1007[A]	HEC	CAD-C3D-C4D	2.07	128.31	124.70
2	B	1007[B]	HEC	CAD-C3D-C4D	2.07	128.31	124.70
2	B	1006	HEC	C3D-C4D-ND	2.06	112.34	110.35
2	B	1004	HEC	CMD-C2D-C1D	2.05	128.24	125.03
2	B	1001	HEC	C1D-ND-C4D	2.05	107.64	105.21
2	B	1007[A]	HEC	CMD-C2D-C1D	2.05	128.24	125.03
2	B	1007[B]	HEC	CMD-C2D-C1D	2.05	128.24	125.03
2	B	1007[B]	HEC	O1A-CGA-CBA	-2.04	116.61	123.09
2	A	1008	HEC	CMB-C2B-C1B	-2.04	121.84	125.03
2	B	1006	HEC	O1A-CGA-CBA	-2.03	116.64	123.09
2	B	1005	HEC	CAD-CBD-CGD	-2.03	108.28	113.67
2	A	1008	HEC	CMC-C2C-C1C	-2.03	122.33	125.42
2	B	1005	HEC	CAA-CBA-CGA	-2.03	108.29	113.67
2	B	1003	HEC	O1A-CGA-CBA	-2.02	116.69	123.09
2	B	1007[A]	HEC	C4B-C3B-C2B	-2.01	103.96	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1007[B]	HEC	C4B-C3B-C2B	-2.01	103.96	106.89
2	B	1003	HEC	CHA-C4D-ND	-2.01	122.26	124.42
2	A	1002	HEC	C1D-ND-C4D	2.00	107.58	105.21

All (17) chirality outliers are listed below:

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

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	HEC	C2C-C3C-CAC-CBC
2	B	1002	HEC	C2C-C3C-CAC-CBC
2	A	1008	HEC	C2C-C3C-CAC-CBC
2	B	1008	HEC	C2C-C3C-CAC-CBC
2	B	1002	HEC	C4C-C3C-CAC-CBC
6	A	1011	PG4	C1-C2-O2-C3
2	A	1008	HEC	C4C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	B	1008	HEC	C4C-C3C-CAC-CBC
2	B	1003	HEC	C4C-C3C-CAC-CBC
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	A	1001	HEC	C2B-C3B-CAB-CBB
2	B	1007[A]	HEC	C2C-C3C-CAC-CBC
2	B	1007[B]	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	A	1007[A]	HEC	C2B-C3B-CAB-CBB
2	A	1007[B]	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C2C-C3C-CAC-CBC
2	B	1007[A]	HEC	C4C-C3C-CAC-CBC
2	B	1007[B]	HEC	C4C-C3C-CAC-CBC
6	B	1012	PG4	C3-C4-O3-C5
2	B	1001	HEC	C2B-C3B-CAB-CBB
2	A	1008	HEC	C2B-C3B-CAB-CBB
6	B	1012	PG4	O3-C5-C6-O4
2	A	1003	HEC	C2C-C3C-CAC-CBC
2	A	1001	HEC	C2C-C3C-CAC-CBC
2	A	1005	HEC	C2C-C3C-CAC-CBC
2	A	1006	HEC	C2C-C3C-CAC-CBC
2	A	1007[A]	HEC	C4C-C3C-CAC-CBC
2	A	1007[B]	HEC	C4C-C3C-CAC-CBC
2	A	1001	HEC	C4B-C3B-CAB-CBB
2	B	1007[A]	HEC	C2B-C3B-CAB-CBB
2	B	1007[B]	HEC	C2B-C3B-CAB-CBB
6	B	1009	PG4	C4-C3-O2-C2
7	B	1010	PG6	C8-C9-O5-C10
2	A	1003	HEC	C4C-C3C-CAC-CBC
2	B	1008	HEC	C2B-C3B-CAB-CBB
2	A	1005	HEC	C4C-C3C-CAC-CBC
2	A	1001	HEC	C4C-C3C-CAC-CBC
2	A	1007[A]	HEC	C2C-C3C-CAC-CBC
2	A	1007[B]	HEC	C2C-C3C-CAC-CBC
2	A	1006	HEC	C2B-C3B-CAB-CBB
2	B	1005	HEC	C2C-C3C-CAC-CBC
6	B	1009	PG4	O1-C1-C2-O2
2	A	1005	HEC	C2B-C3B-CAB-CBB
6	B	1009	PG4	O2-C3-C4-O3
7	B	1010	PG6	O1-C2-C3-O2
2	A	1004	HEC	C4C-C3C-CAC-CBC
2	A	1004	HEC	C4B-C3B-CAB-CBB
2	B	1004	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	C2B-C3B-CAB-CBB
2	B	1005	HEC	C4C-C3C-CAC-CBC
2	B	1002	HEC	C2B-C3B-CAB-CBB
2	B	1003	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C4C-C3C-CAC-CBC
6	B	1011	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	B	1001	HEC	C2C-C3C-CAC-CBC
2	A	1004	HEC	C2C-C3C-CAC-CBC
2	B	1006	HEC	C2B-C3B-CAB-CBB
7	B	1010	PG6	O3-C6-C7-O4
6	B	1012	PG4	O2-C3-C4-O3
2	B	1005	HEC	C2B-C3B-CAB-CBB
7	A	1010	PG6	O4-C8-C9-O5
2	B	1001	HEC	C4B-C3B-CAB-CBB
2	A	1007[A]	HEC	C4B-C3B-CAB-CBB
2	A	1007[B]	HEC	C4B-C3B-CAB-CBB
6	B	1011	PG4	O1-C1-C2-O2
7	B	1010	PG6	O4-C8-C9-O5
2	B	1007[A]	HEC	C4B-C3B-CAB-CBB
2	B	1007[B]	HEC	C4B-C3B-CAB-CBB
2	B	1006	HEC	C2C-C3C-CAC-CBC
2	A	1006	HEC	C4C-C3C-CAC-CBC
6	A	1011	PG4	O1-C1-C2-O2
2	B	1006	HEC	C4C-C3C-CAC-CBC
6	A	1009	PG4	C4-C3-O2-C2
7	B	1010	PG6	C2-C3-O2-C4
6	B	1009	PG4	C1-C2-O2-C3
7	B	1010	PG6	C4-C5-O3-C6
6	B	1012	PG4	O4-C7-C8-O5
2	A	1006	HEC	C4B-C3B-CAB-CBB
2	A	1002	HEC	C2B-C3B-CAB-CBB
6	A	1009	PG4	C3-C4-O3-C5
2	A	1003	HEC	C4B-C3B-CAB-CBB
7	B	1010	PG6	C9-C8-O4-C7
2	B	1005	HEC	C4B-C3B-CAB-CBB
2	B	1004	HEC	C2C-C3C-CAC-CBC
2	B	1008	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	B	1006	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	CAA-CBA-CGA-O1A
6	A	1009	PG4	O2-C3-C4-O3
2	B	1002	HEC	CAA-CBA-CGA-O1A
2	B	1003	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	CAA-CBA-CGA-O1A
6	B	1012	PG4	C6-C5-O3-C4
2	A	1002	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	1003	HEC	CAD-CBD-CGD-O2D
2	A	1005	HEC	CAA-CBA-CGA-O2A
2	A	1002	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAD-CBD-CGD-O1D
2	B	1005	HEC	CAA-CBA-CGA-O2A
2	A	1008	HEC	C4B-C3B-CAB-CBB
2	B	1004	HEC	CAA-CBA-CGA-O1A
2	B	1002	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O1A
2	A	1001	HEC	CAD-CBD-CGD-O2D
2	A	1005	HEC	CAD-CBD-CGD-O2D
2	A	1003	HEC	CAD-CBD-CGD-O1D
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	B	1003	HEC	CAD-CBD-CGD-O2D
2	A	1005	HEC	C4B-C3B-CAB-CBB
2	A	1008	HEC	CAD-CBD-CGD-O1D
2	B	1001	HEC	CAD-CBD-CGD-O1D
2	B	1008	HEC	CAD-CBD-CGD-O2D
2	A	1005	HEC	CAD-CBD-CGD-O1D
2	B	1003	HEC	CAD-CBD-CGD-O1D
2	A	1002	HEC	C4B-C3B-CAB-CBB
2	B	1002	HEC	C4B-C3B-CAB-CBB
2	B	1008	HEC	CAD-CBD-CGD-O1D
2	B	1001	HEC	C4C-C3C-CAC-CBC
7	A	1010	PG6	C8-C9-O5-C10
2	B	1007[A]	HEC	CAA-CBA-CGA-O1A
2	A	1007[A]	HEC	CAA-CBA-CGA-O1A
2	B	1007[A]	HEC	CAA-CBA-CGA-O2A
2	A	1008	HEC	CAA-CBA-CGA-O2A
2	B	1005	HEC	CAD-CBD-CGD-O1D
2	A	1008	HEC	CAD-CBD-CGD-O2D
2	B	1005	HEC	CAD-CBD-CGD-O2D
2	A	1008	HEC	CAA-CBA-CGA-O1A
2	A	1006	HEC	CAA-CBA-CGA-O2A
2	B	1007[B]	HEC	CAA-CBA-CGA-O2A
2	A	1007[B]	HEC	CAA-CBA-CGA-O2A
2	A	1007[B]	HEC	CAA-CBA-CGA-O1A

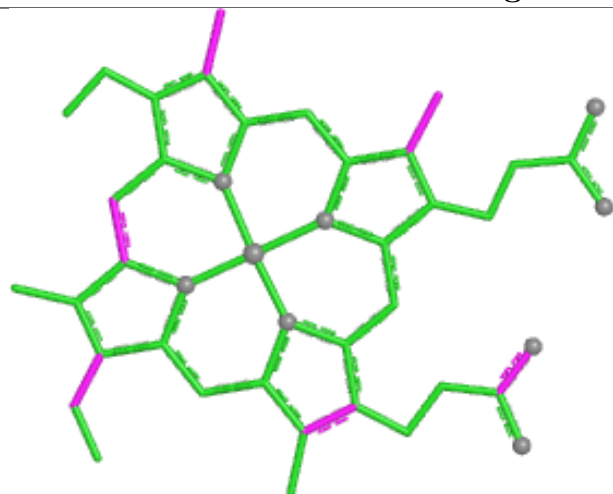
There are no ring outliers.

15 monomers are involved in 46 short contacts:

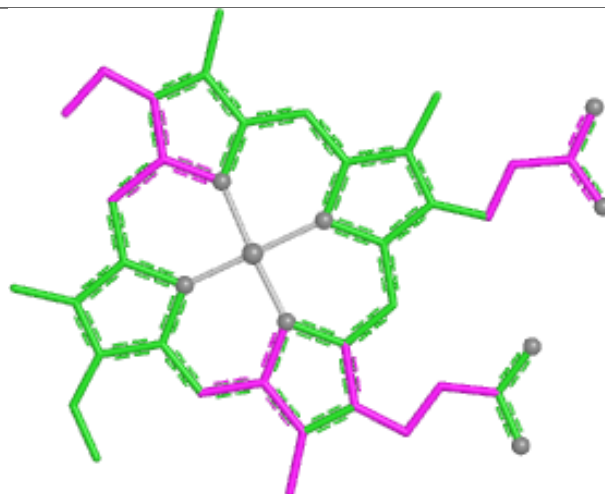
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	528	NO2	1	0
2	A	1006	HEC	1	0
2	B	1004	HEC	1	0
6	A	1011	PG4	1	0
4	B	528	NO2	1	0
7	B	1010	PG6	1	0
6	B	1009	PG4	1	0
2	B	1006	HEC	2	0
6	B	1012	PG4	27	0
2	A	1002	HEC	1	0
2	A	1008	HEC	4	0
7	A	1010	PG6	3	0
2	B	1002	HEC	1	0
2	B	1003	HEC	1	0
2	B	1008	HEC	2	0

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.

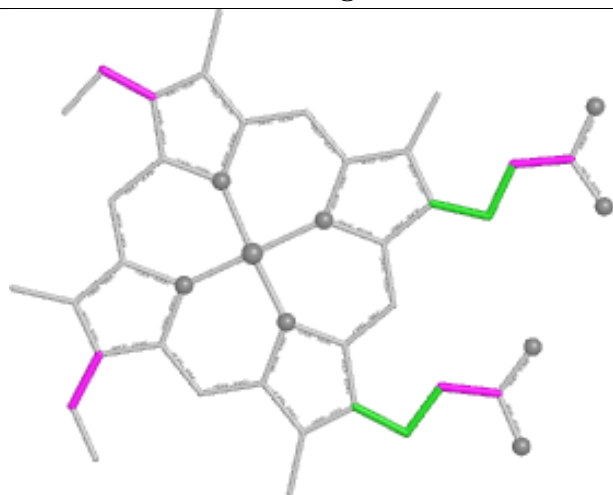
Ligand HEC B 1005



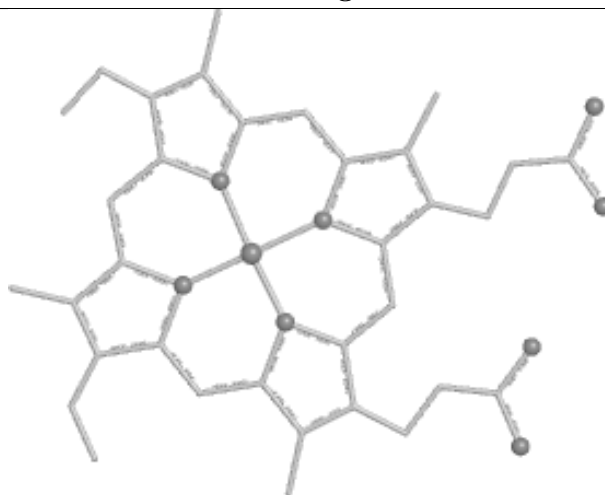
Bond lengths



Bond angles

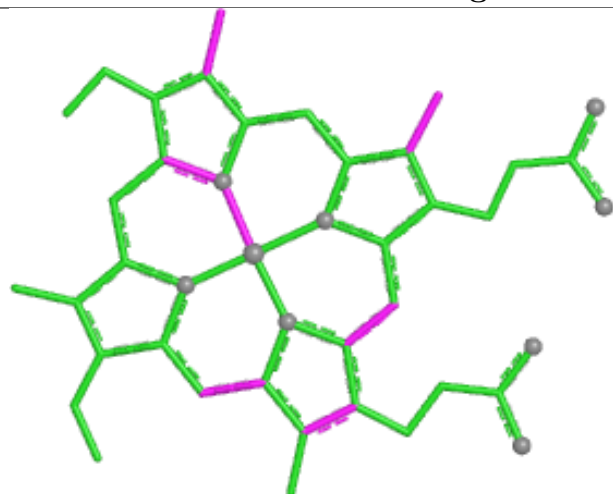


Torsions

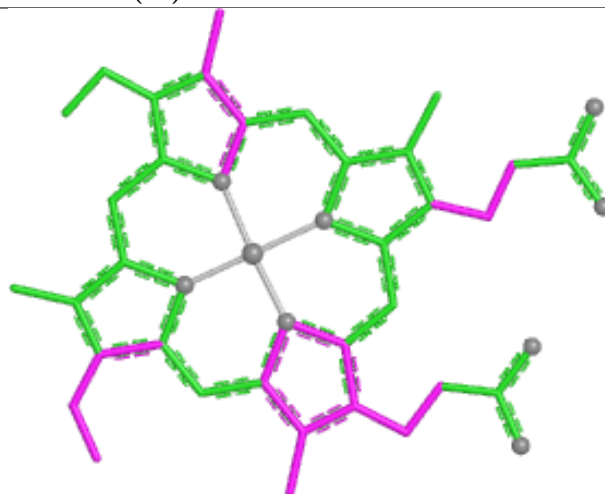


Rings

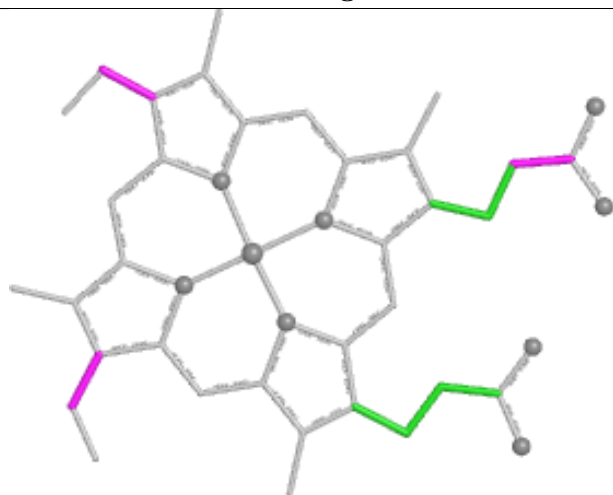
Ligand HEC A 1007 (A)



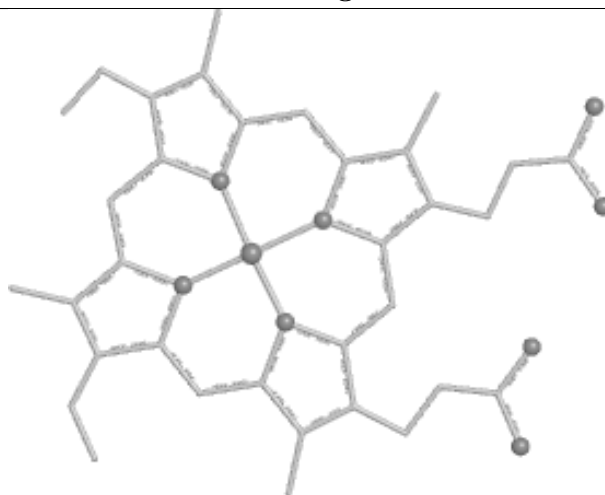
Bond lengths



Bond angles

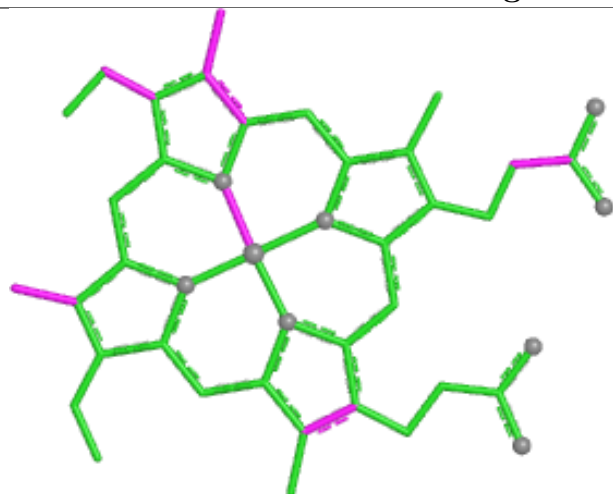


Torsions

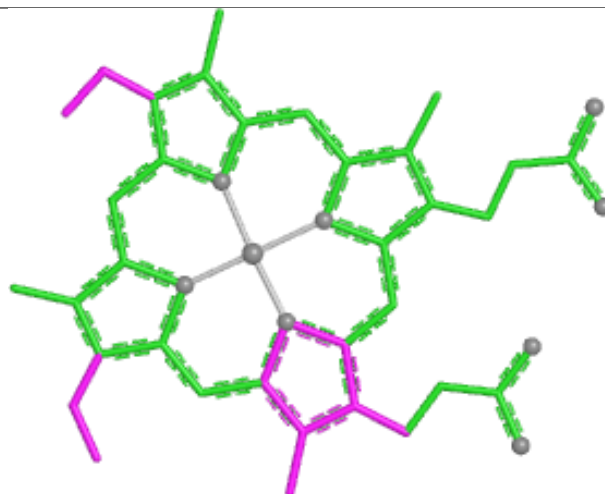


Rings

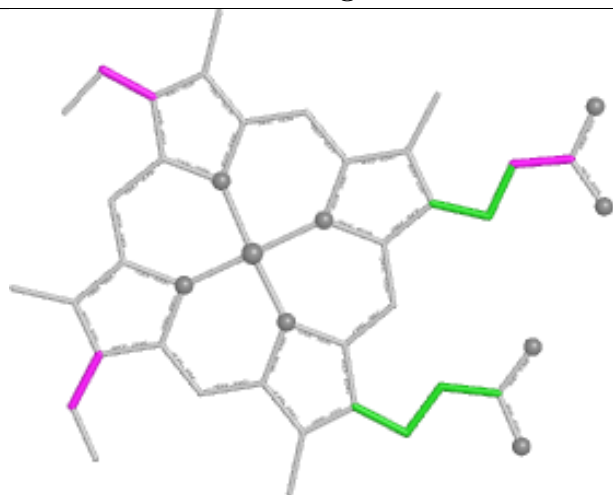
Ligand HEC A 1004



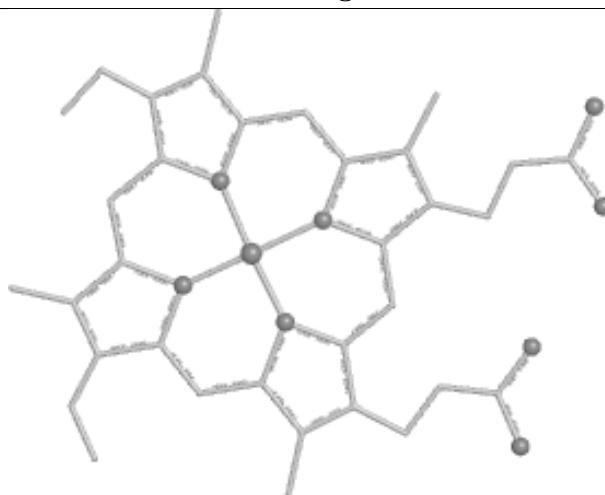
Bond lengths



Bond angles

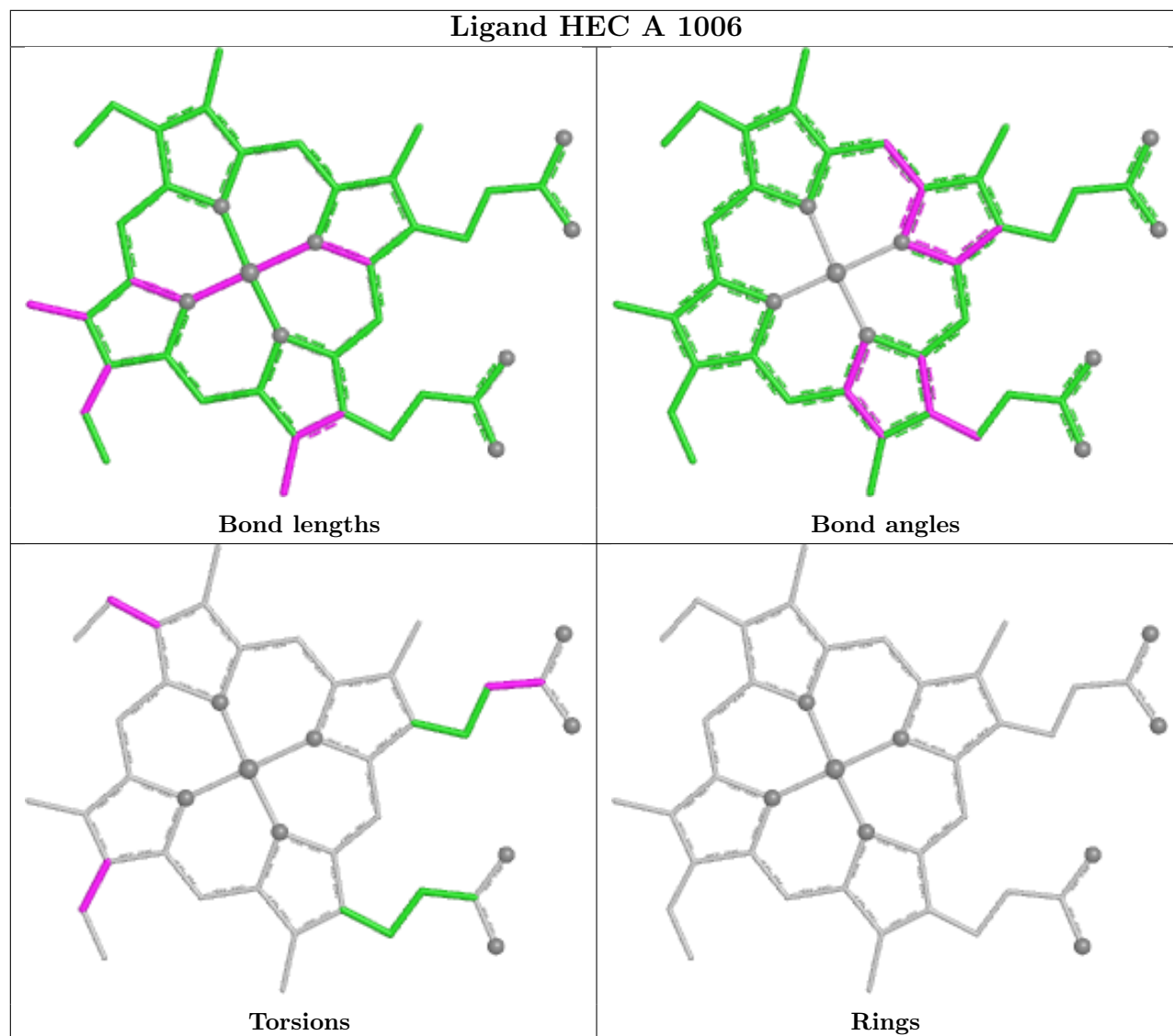


Torsions

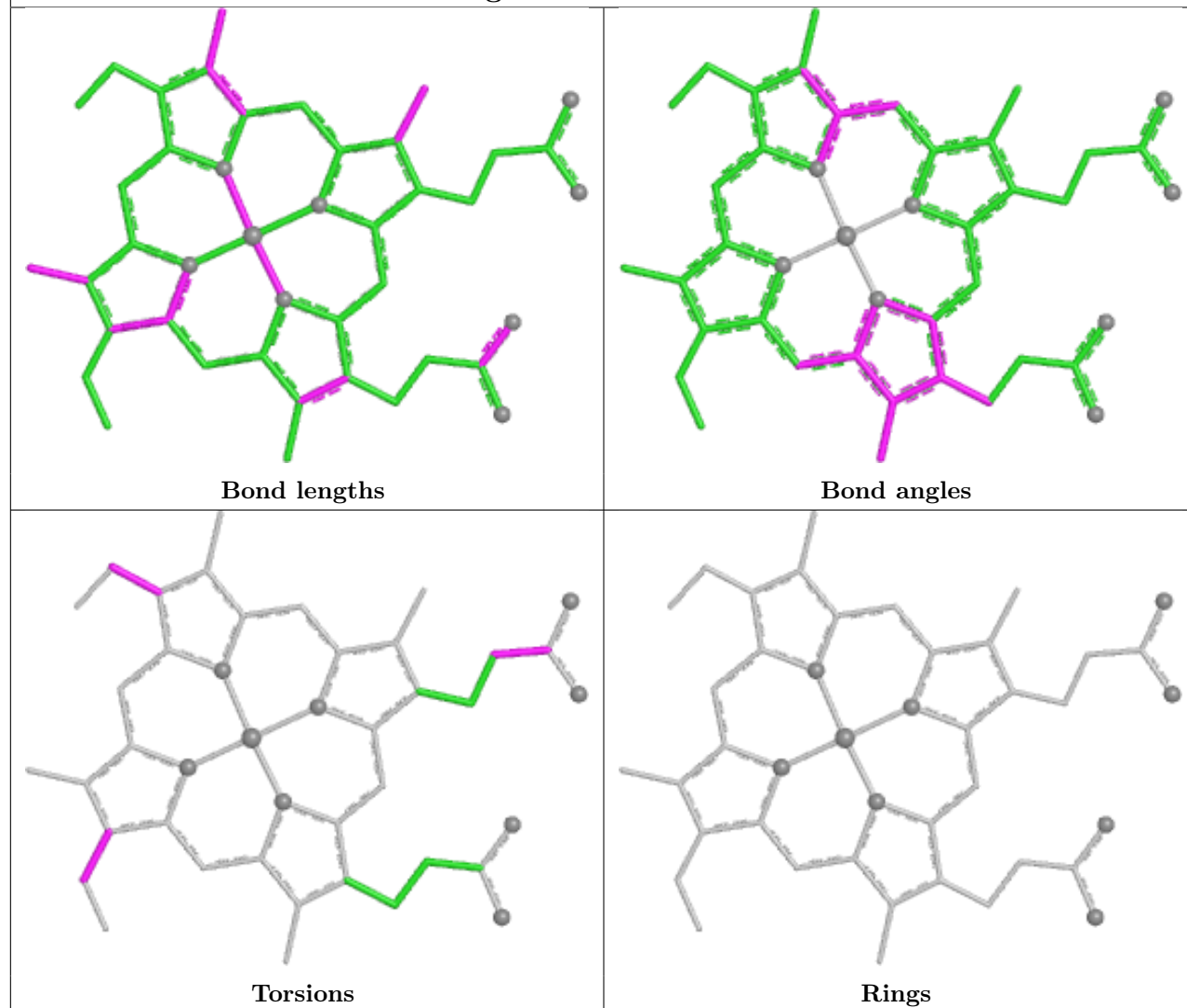


Rings

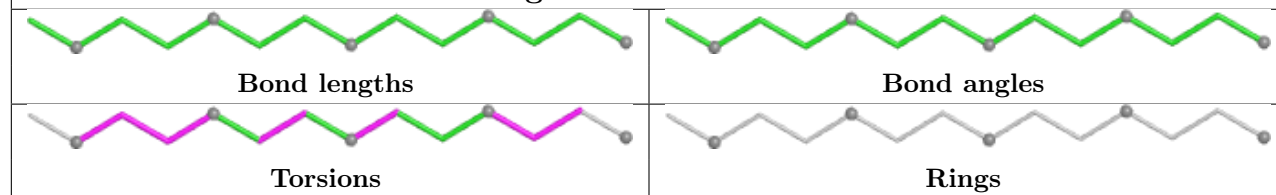
Ligand HEC A 1006



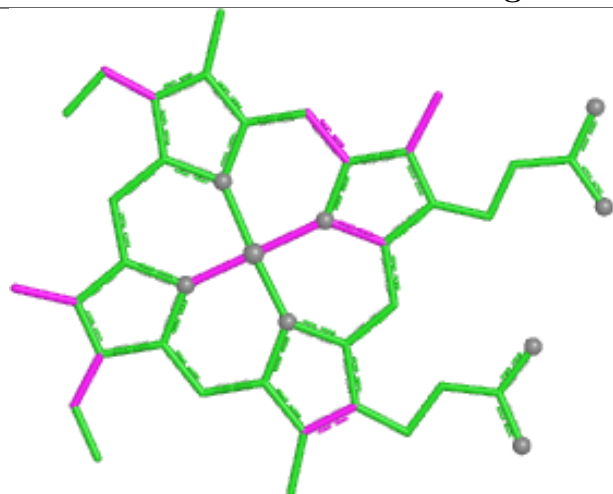
Ligand HEC B 1004



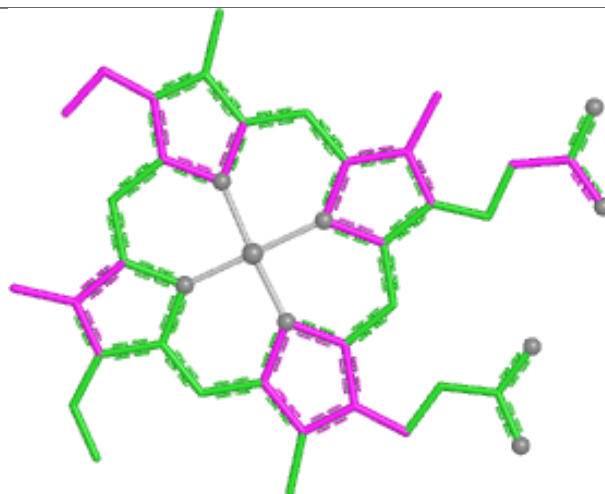
Ligand PG6 B 1010



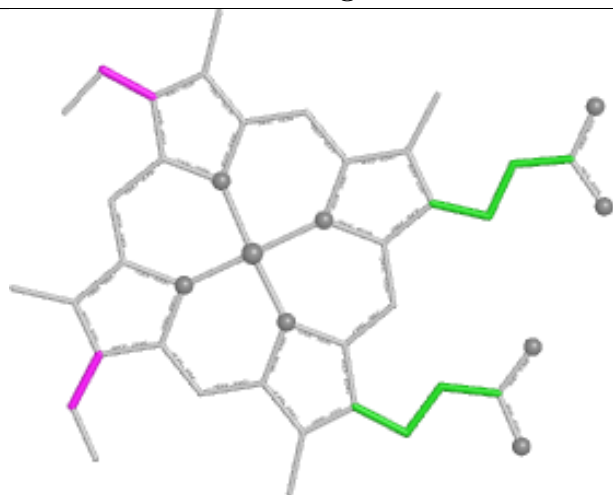
Ligand HEC B 1006



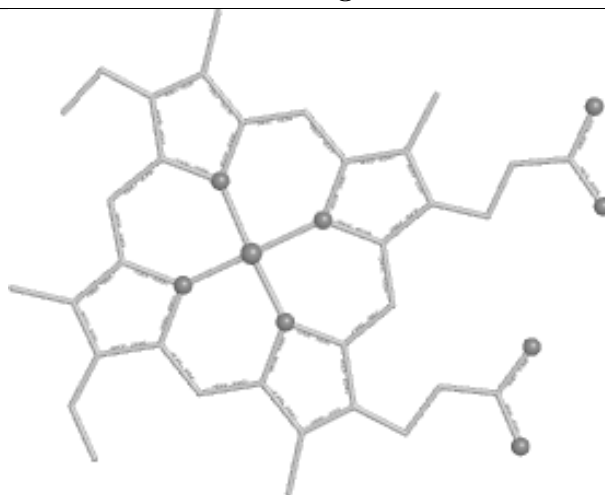
Bond lengths



Bond angles

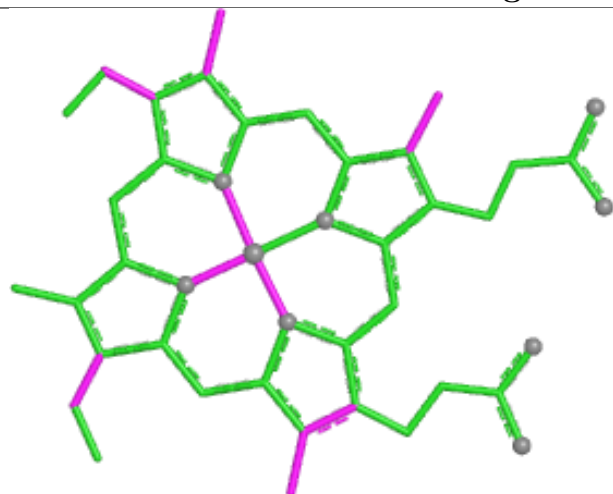


Torsions

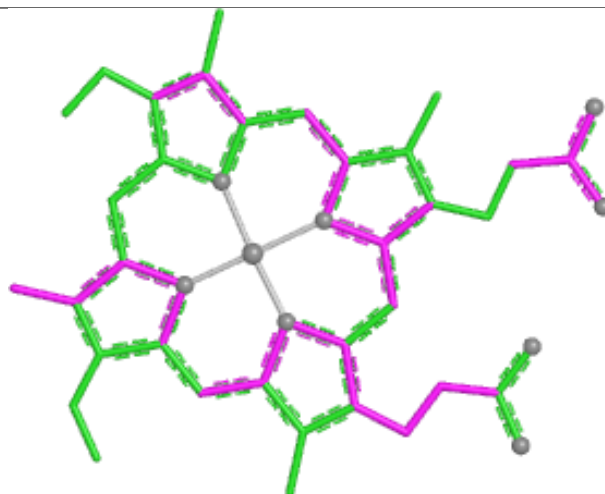


Rings

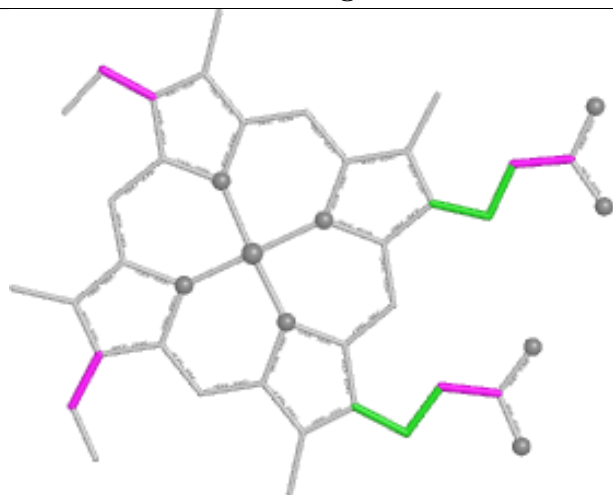
Ligand HEC A 1001



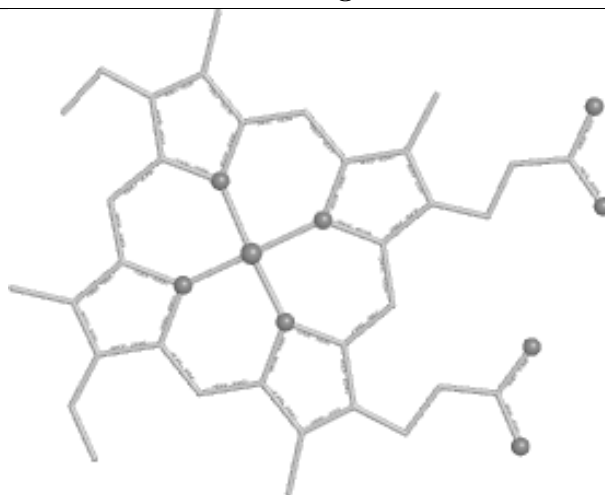
Bond lengths



Bond angles

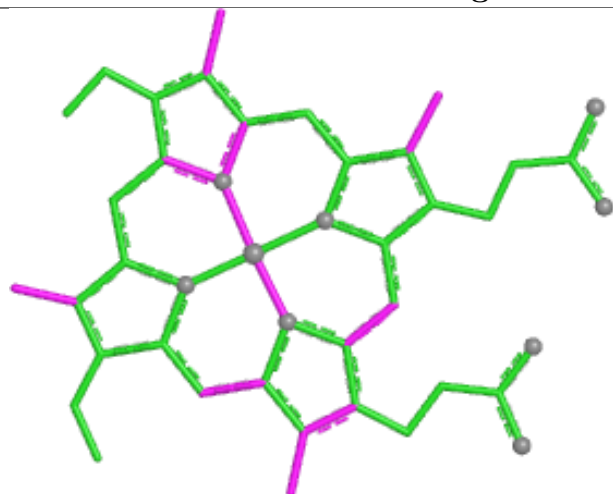


Torsions

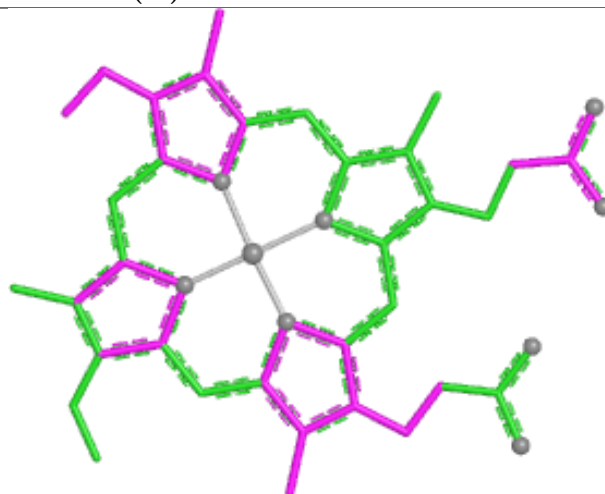


Rings

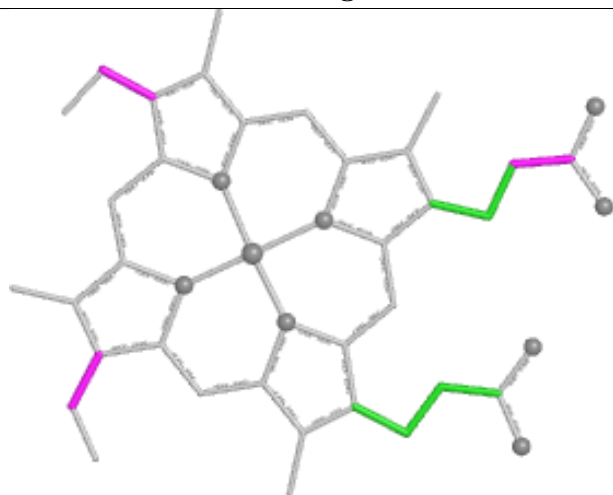
Ligand HEC B 1007 (B)



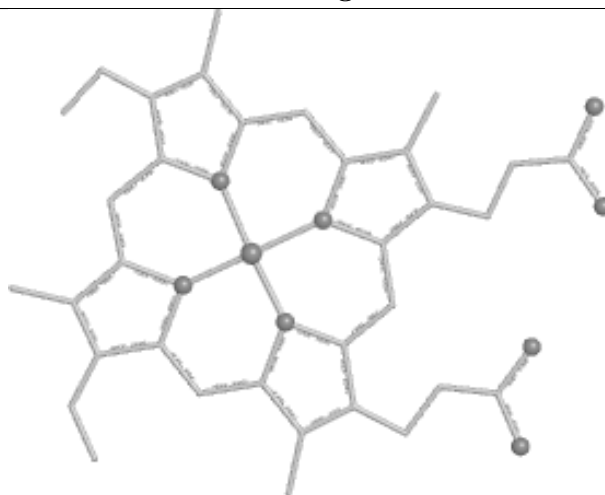
Bond lengths



Bond angles

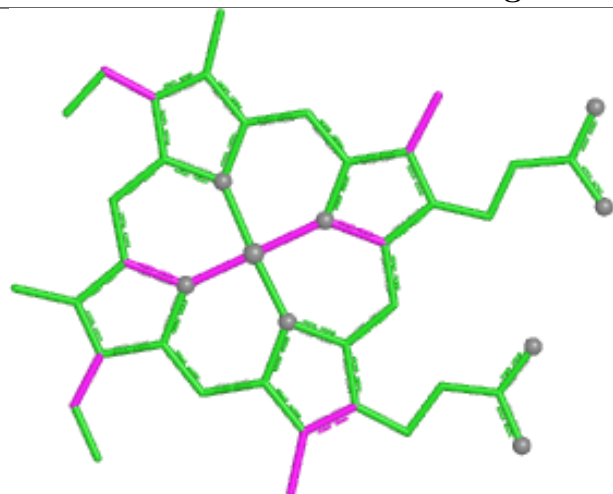


Torsions

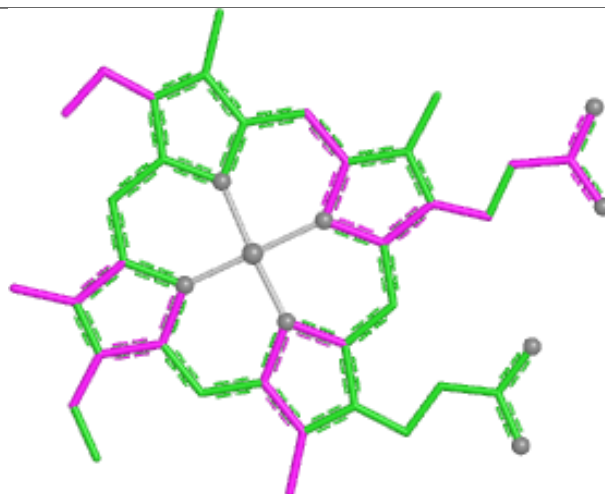


Rings

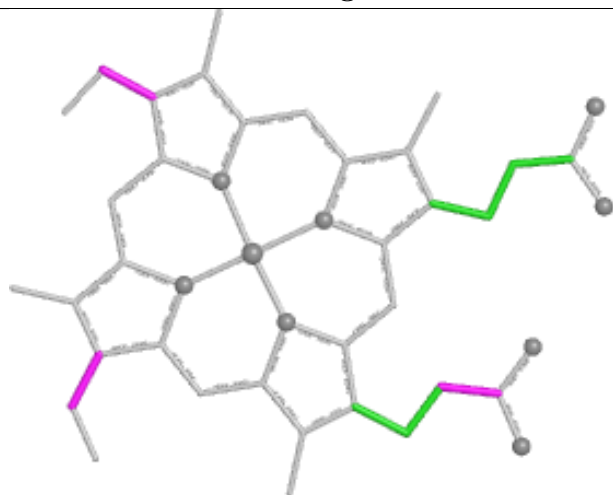
Ligand HEC B 1001



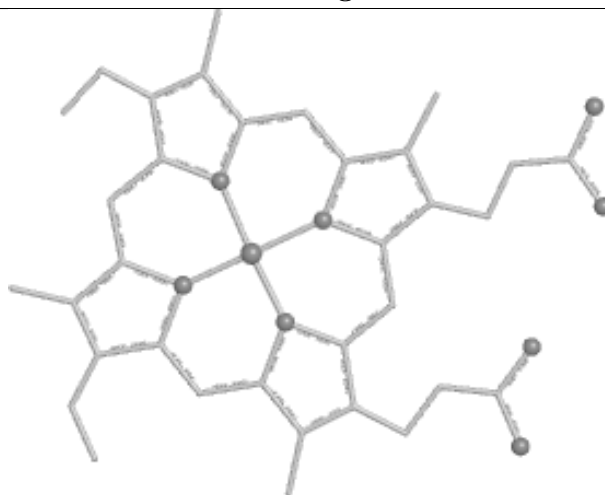
Bond lengths



Bond angles

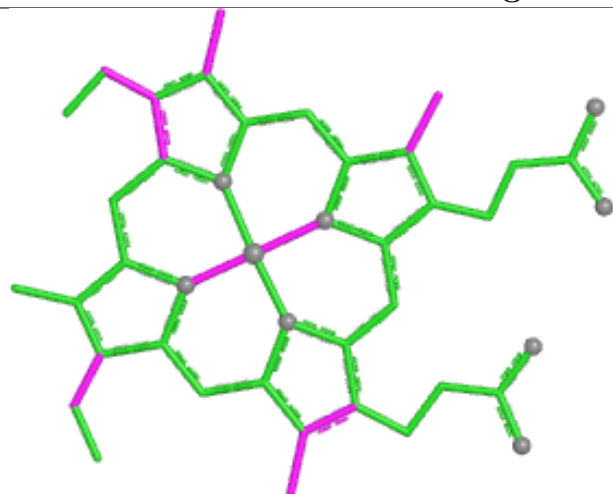


Torsions

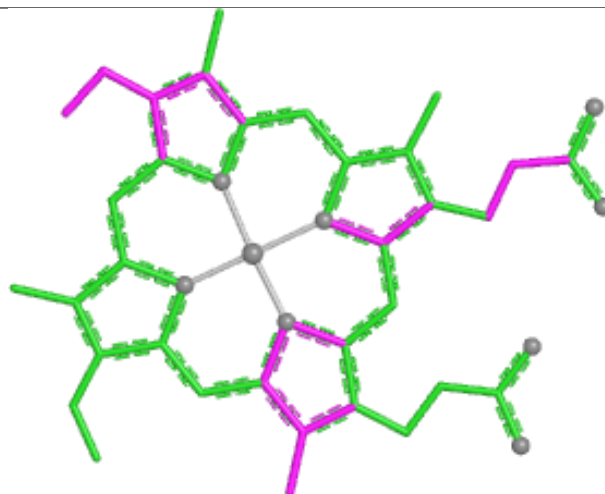


Rings

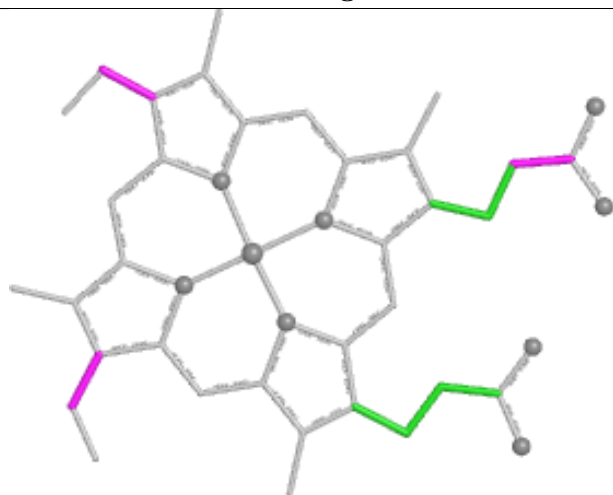
Ligand HEC A 1002



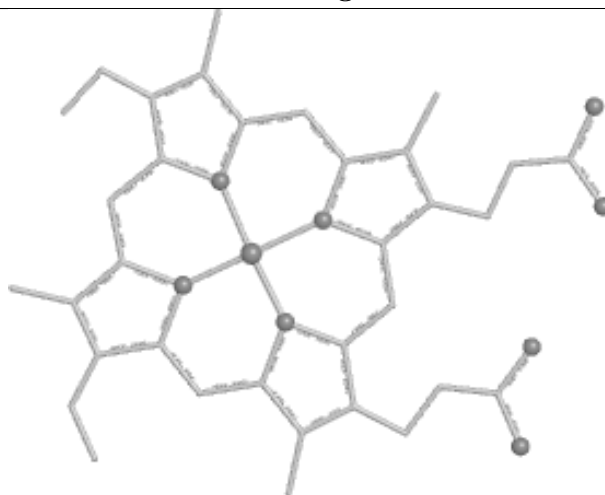
Bond lengths



Bond angles

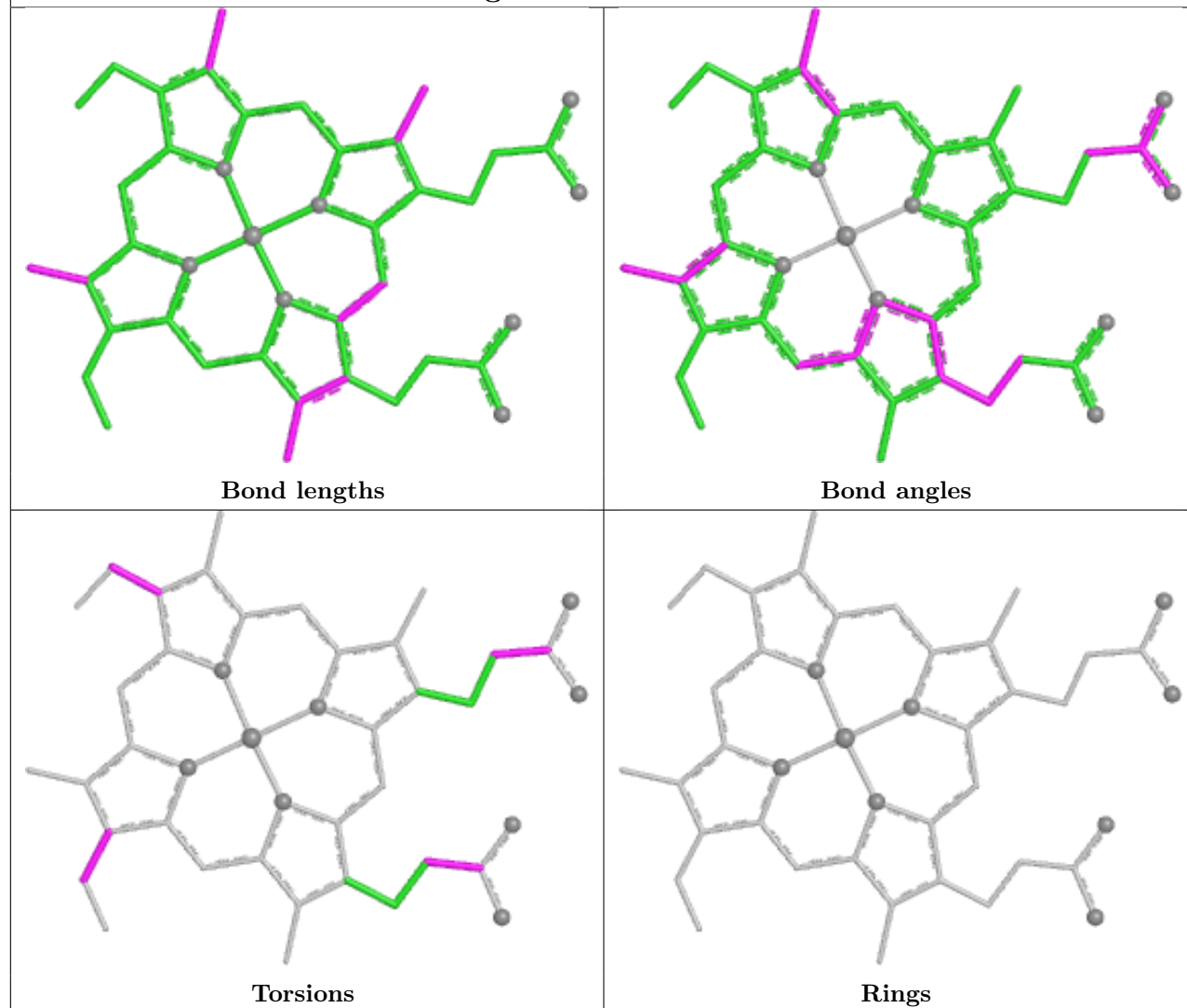


Torsions

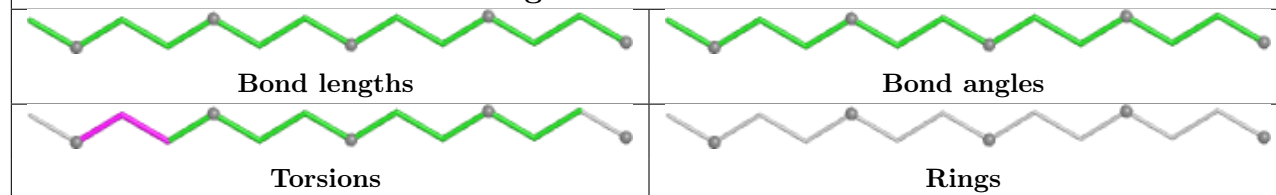


Rings

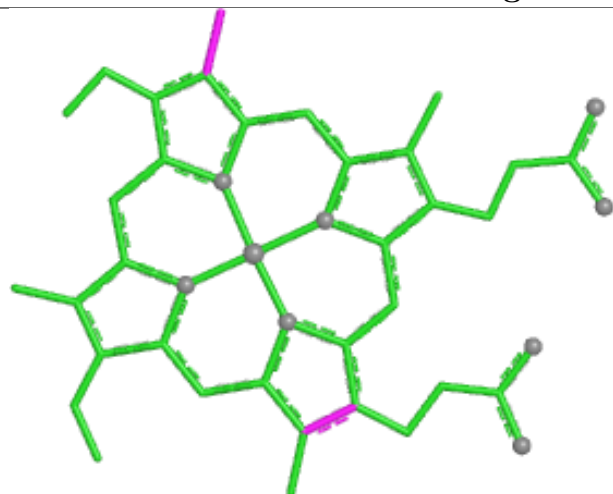
Ligand HEC A 1008



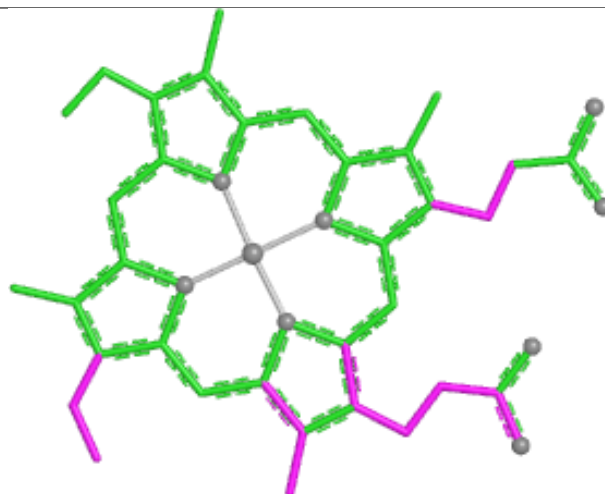
Ligand PG6 A 1010



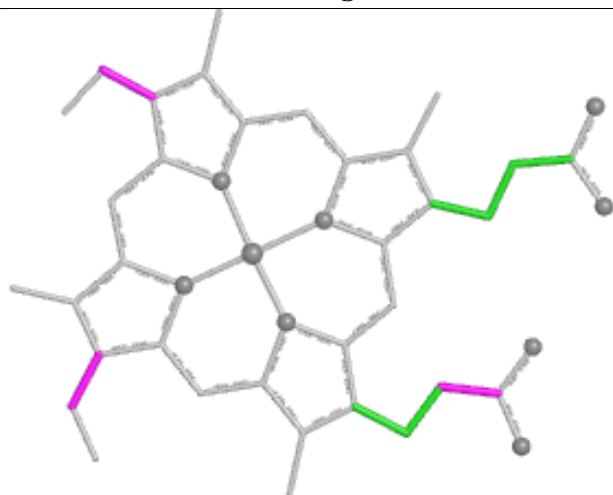
Ligand HEC A 1003



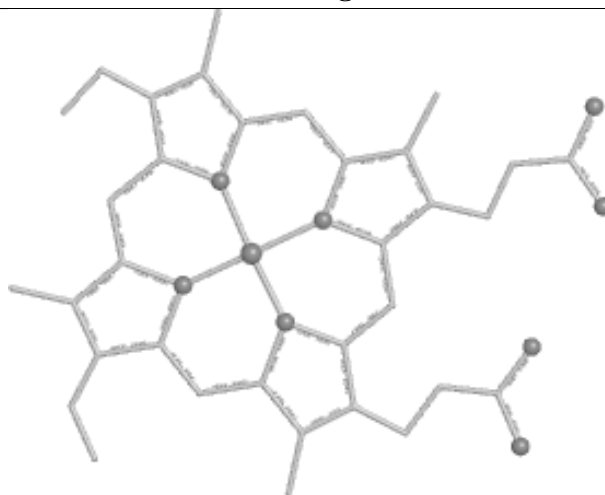
Bond lengths



Bond angles

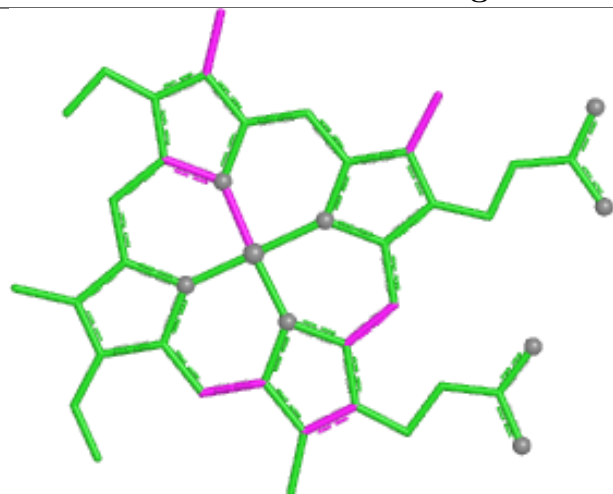


Torsions

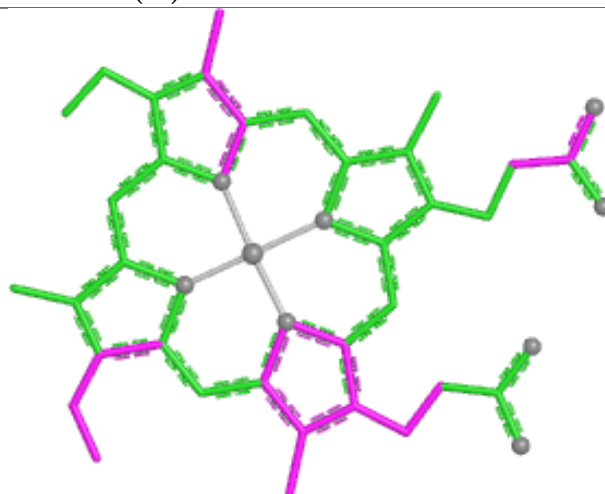


Rings

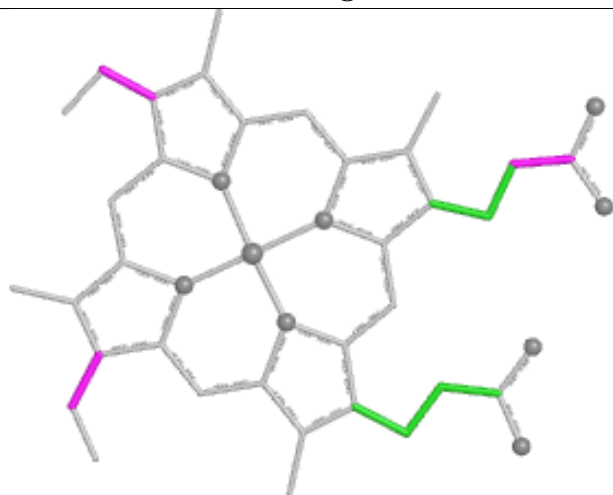
Ligand HEC A 1007 (B)



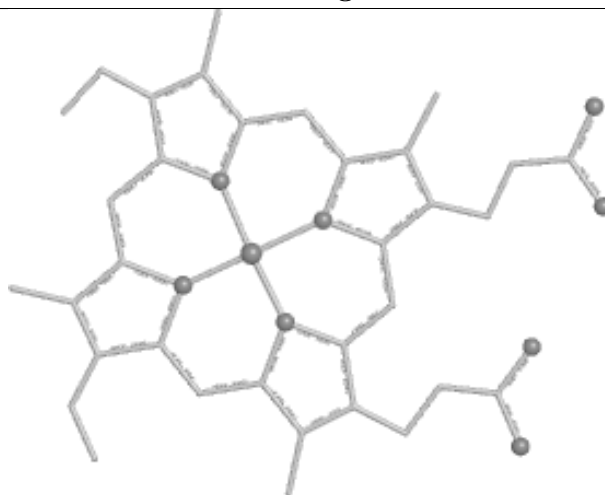
Bond lengths



Bond angles

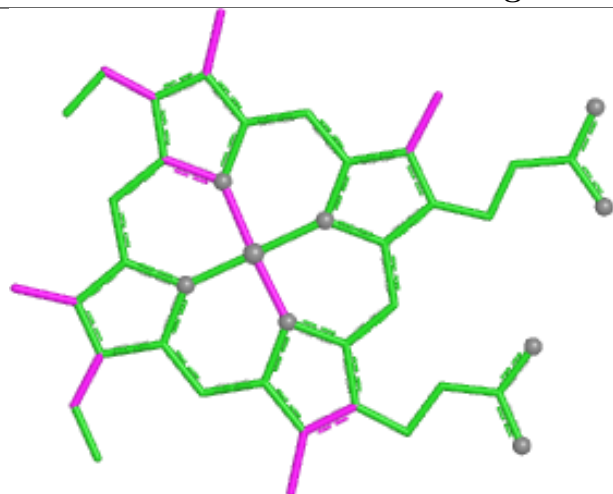


Torsions

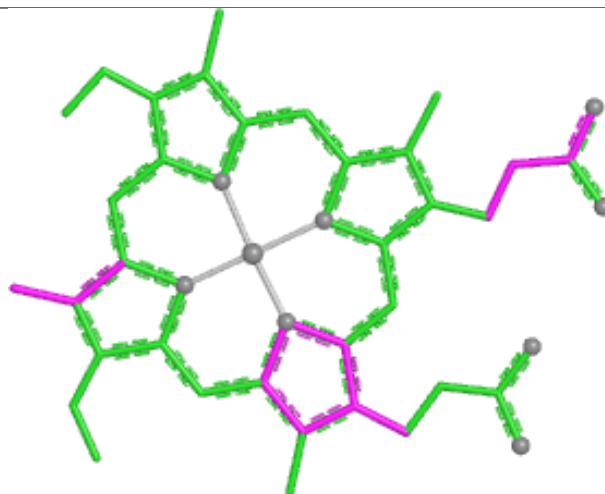


Rings

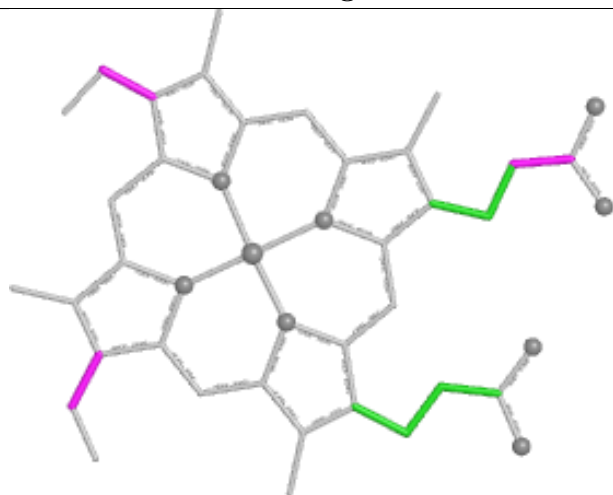
Ligand HEC B 1002



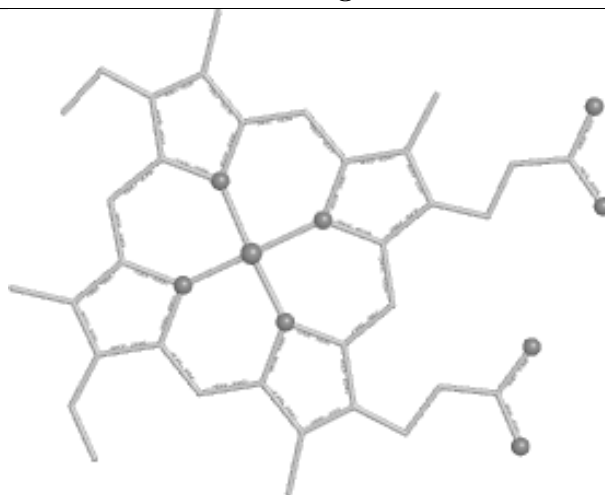
Bond lengths



Bond angles

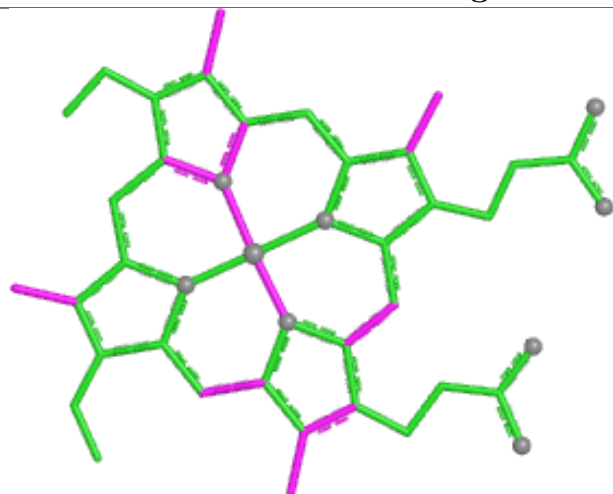


Torsions

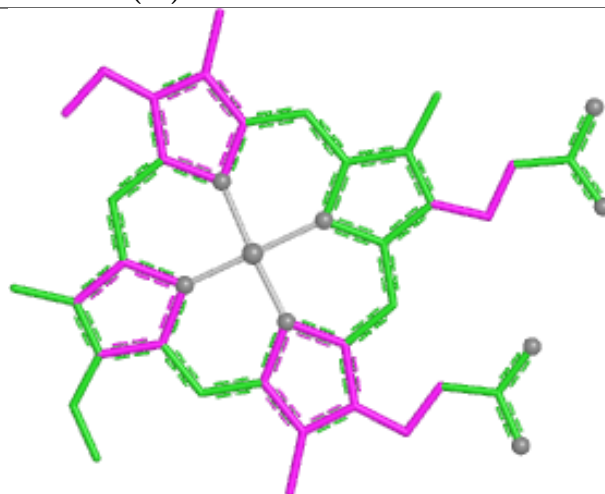


Rings

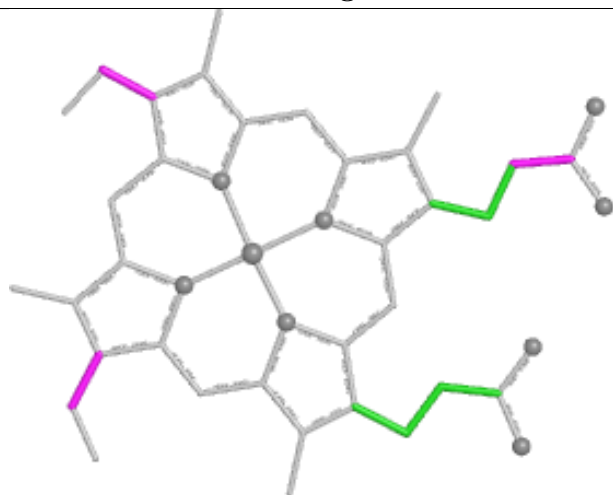
Ligand HEC B 1007 (A)



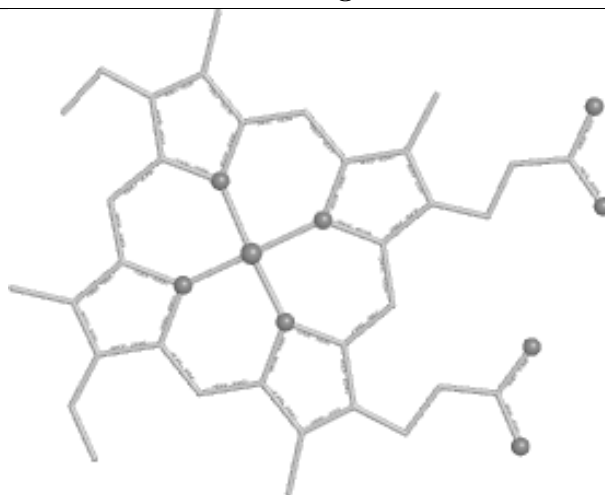
Bond lengths



Bond angles

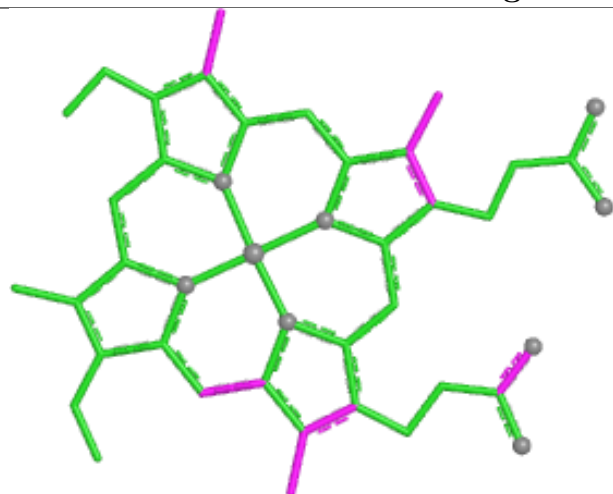


Torsions

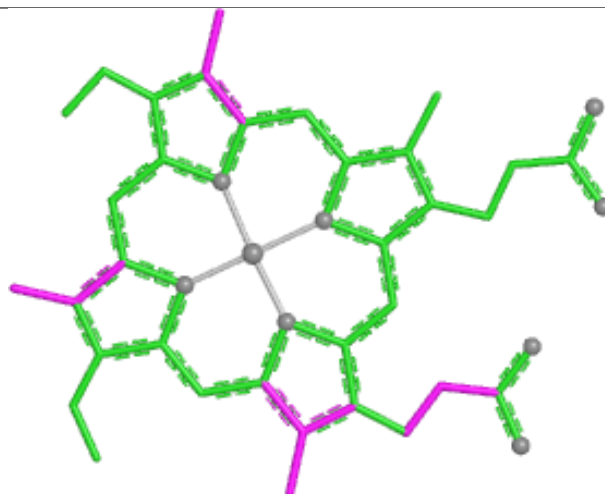


Rings

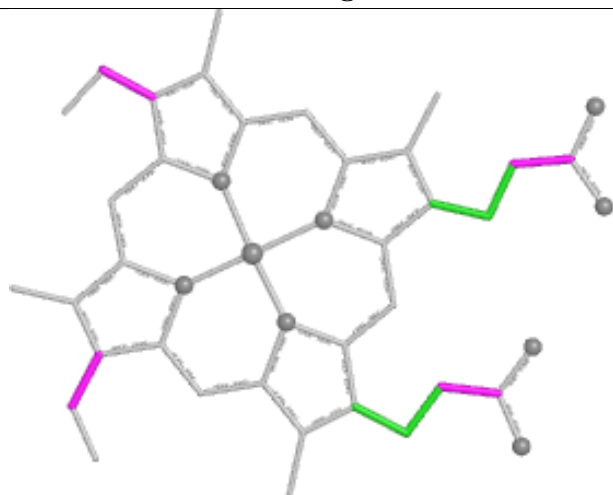
Ligand HEC A 1005



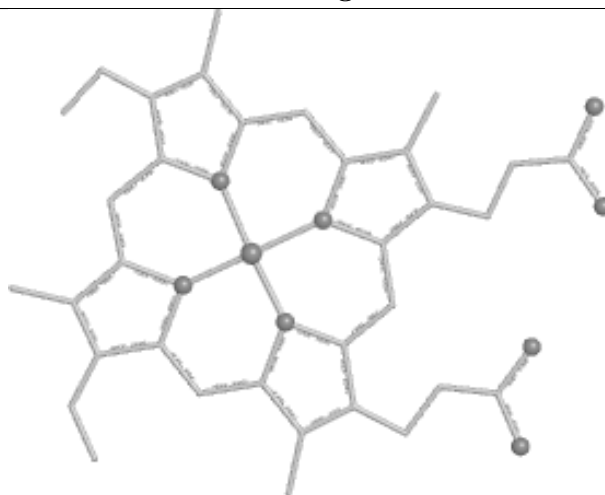
Bond lengths



Bond angles

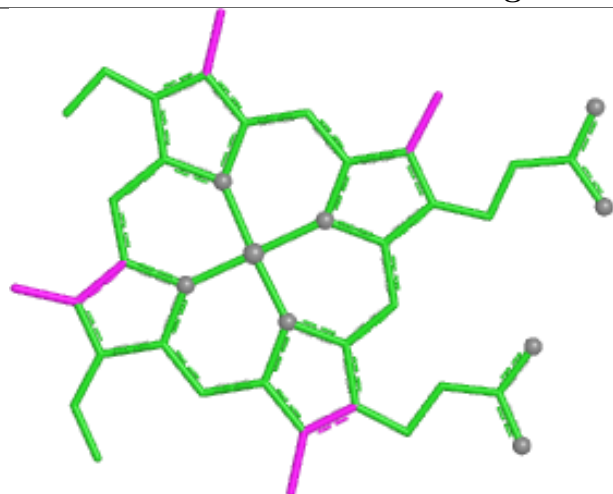


Torsions

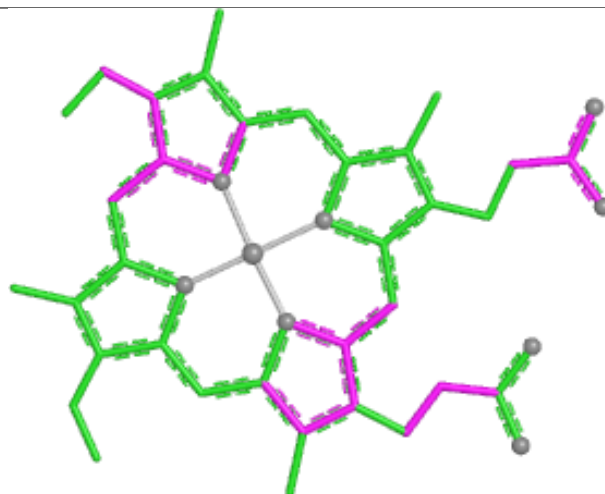


Rings

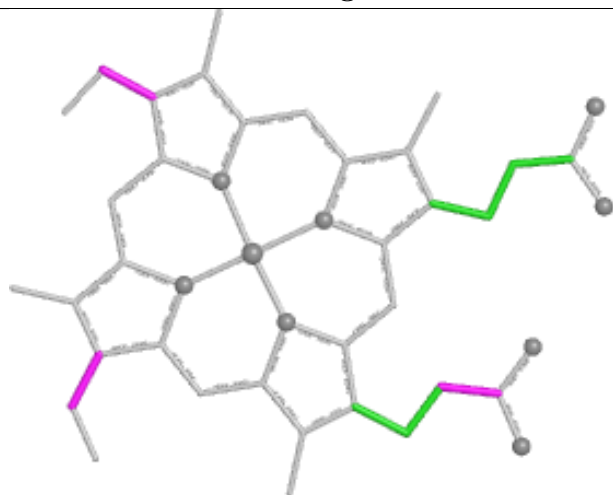
Ligand HEC B 1003



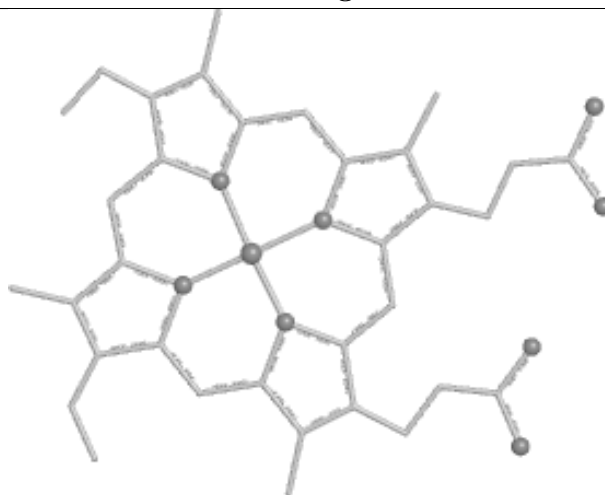
Bond lengths



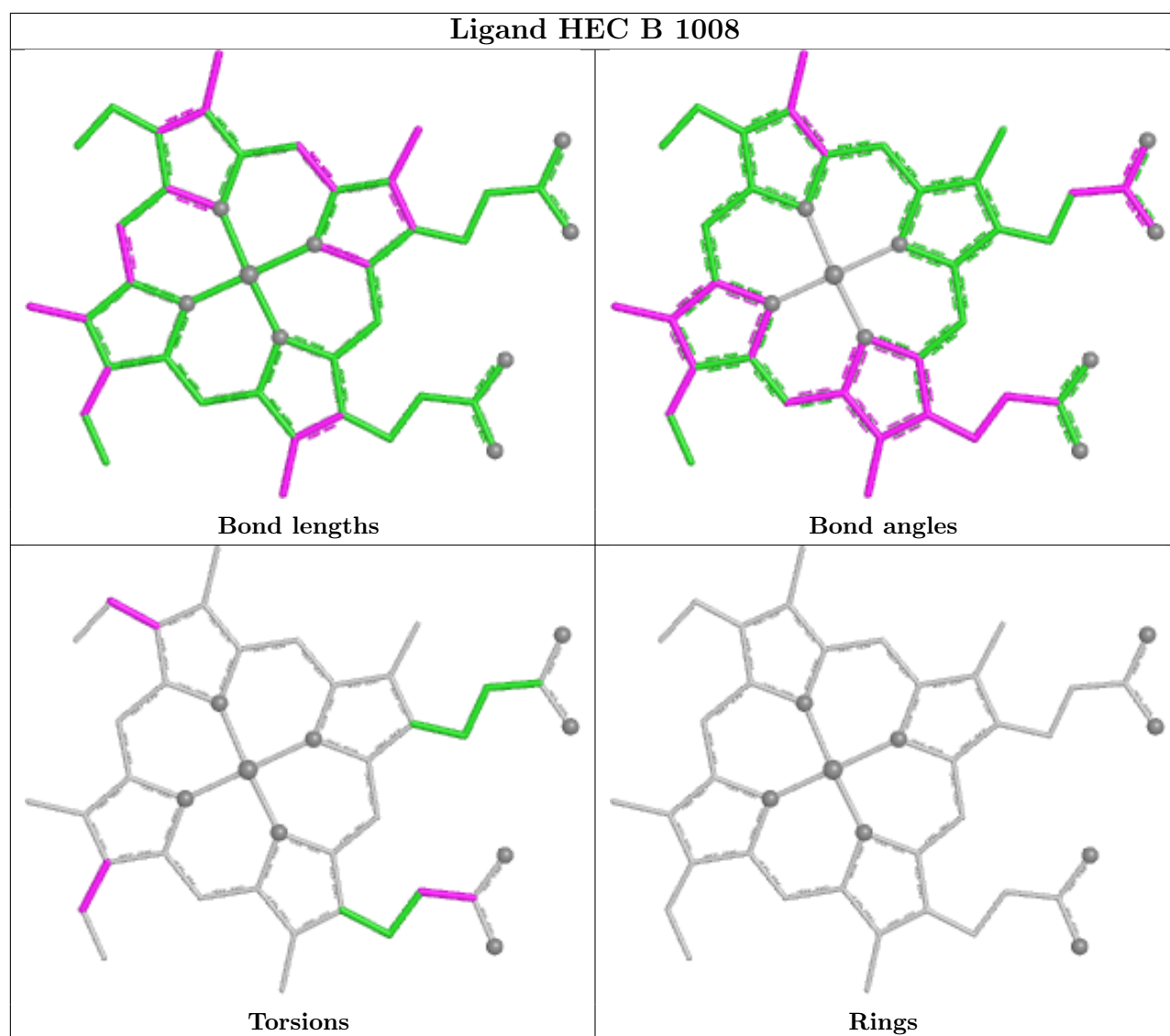
Bond angles



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%)	-0.91	2 (0%) 88 89	6, 16, 25, 49	22 (4%)
1	B	519/525 (98%)	-0.96	2 (0%) 88 89	6, 14, 26, 53	17 (3%)
All	All	1038/1050 (98%)	-0.93	4 (0%) 88 89	6, 15, 26, 53	39 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	8.4
1	B	523	ALA	4.3
1	A	522	VAL	3.6
1	B	522	VAL	3.3

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PG4	A	1009	6/13	0.47	0.30	22,28,31,33	6

Continued on next page...

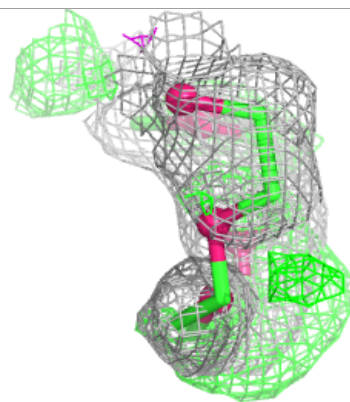
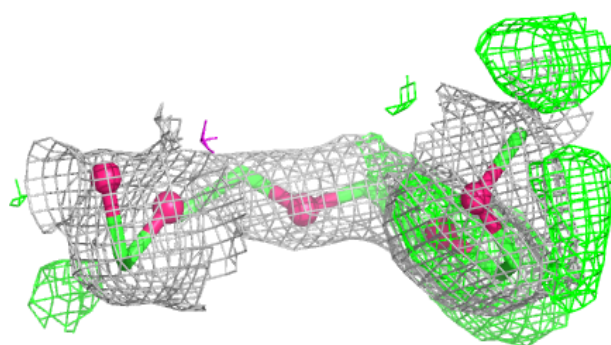
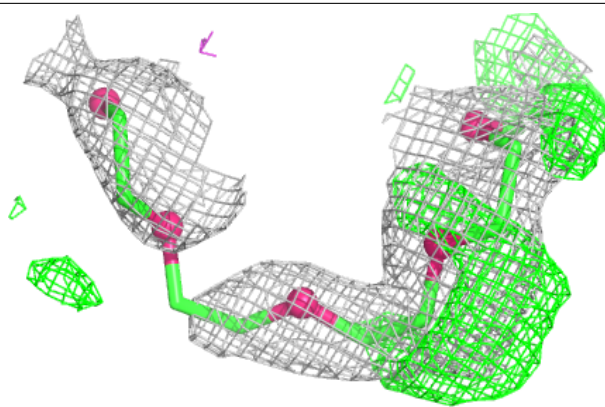
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PG4	B	1011	5/13	0.66	0.42	26,27,29,30	5
6	PG4	A	1012	5/13	0.71	0.32	23,26,30,33	5
7	PG6	A	1010	14/18	0.77	0.20	27,30,35,35	14
7	PG6	B	1010	14/18	0.80	0.17	28,31,36,37	14
6	PG4	B	1012	10/13	0.81	0.20	14,16,24,29	10
6	PG4	B	1009	7/13	0.85	0.24	23,26,28,29	7
6	PG4	A	1011	6/13	0.88	0.19	11,22,22,24	6
3	CA	A	527	1/1	0.92	0.08	20,20,20,20	1
2	HEC	A	1008	43/43	0.98	0.06	15,21,33,41	18
2	HEC	B	1005	43/43	0.99	0.04	11,13,20,27	18
2	HEC	B	1006	43/43	0.99	0.04	9,11,13,14	18
2	HEC	B	1007[A]	43/43	0.99	0.04	10,12,13,16	24
2	HEC	B	1007[B]	43/43	0.99	0.04	10,12,15,21	24
2	HEC	B	1008	43/43	0.99	0.05	14,18,26,35	18
2	HEC	B	1002	43/43	0.99	0.04	13,15,18,19	18
2	HEC	B	1003	43/43	0.99	0.05	12,14,26,35	18
2	HEC	B	1001	43/43	0.99	0.05	14,20,24,24	18
3	CA	A	526	1/1	0.99	0.02	15,15,15,15	0
2	HEC	A	1005	43/43	0.99	0.04	11,13,21,29	18
3	CA	B	527	1/1	0.99	0.03	18,18,18,18	1
4	NO2	A	528	3/3	0.99	0.09	16,16,16,16	3
4	NO2	B	528	3/3	0.99	0.06	16,16,16,17	3
5	NA	A	529	1/1	0.99	0.07	24,24,24,24	1
5	NA	B	529	1/1	0.99	0.10	26,26,26,26	1
2	HEC	A	1006	43/43	0.99	0.04	11,13,15,16	18
2	HEC	A	1007[A]	43/43	0.99	0.04	12,13,16,16	24
2	HEC	A	1007[B]	43/43	0.99	0.04	12,13,16,23	24
2	HEC	A	1004	43/43	0.99	0.04	12,15,18,18	18
2	HEC	A	1002	43/43	0.99	0.04	11,15,17,18	18
2	HEC	A	1003	43/43	0.99	0.05	11,15,25,35	18
2	HEC	A	1001	43/43	0.99	0.05	14,17,21,26	18
2	HEC	B	1004	43/43	0.99	0.04	11,13,16,16	18
3	CA	B	526	1/1	1.00	0.02	14,14,14,14	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.

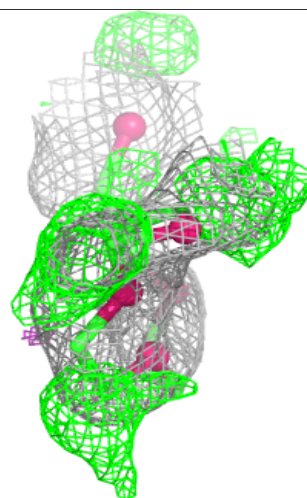
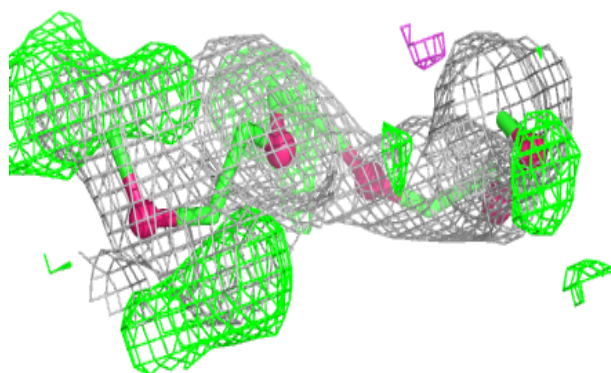
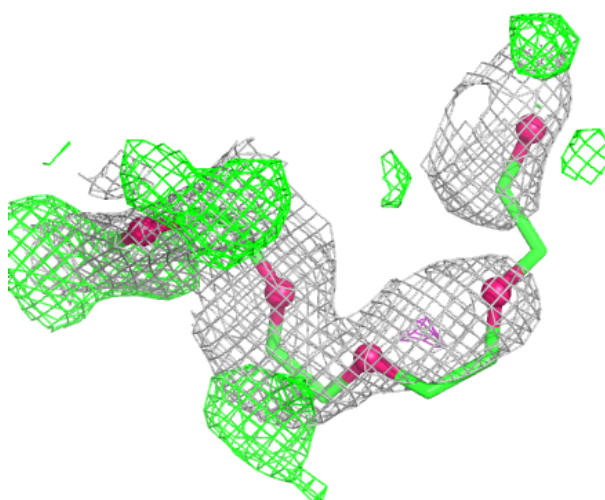
Electron density around PG6 A 1010:

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



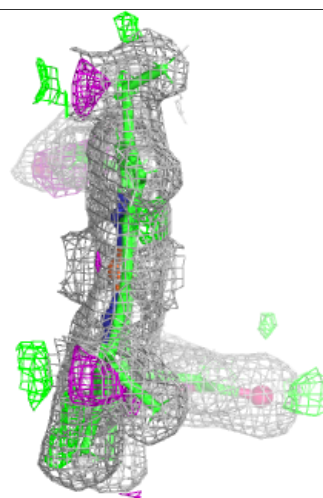
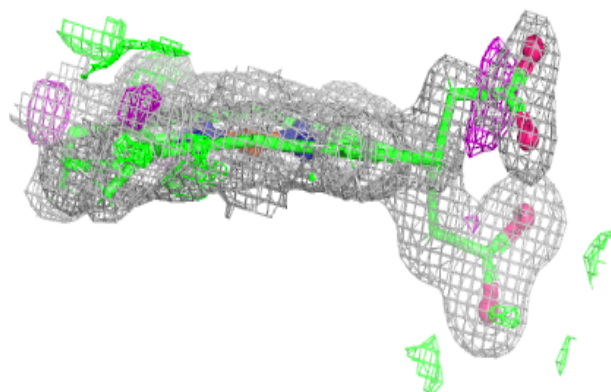
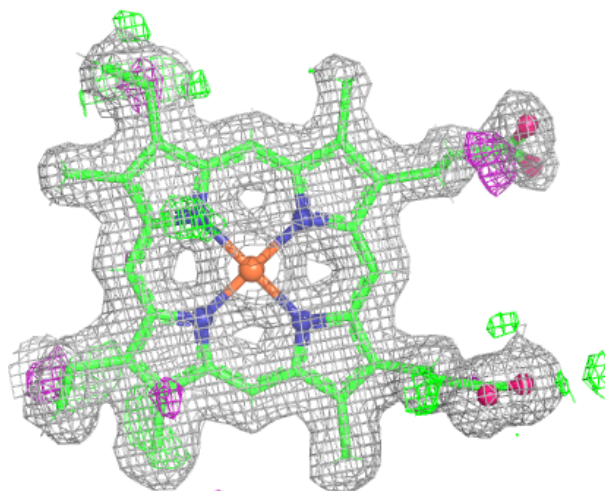
Electron density around PG6 B 1010:

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



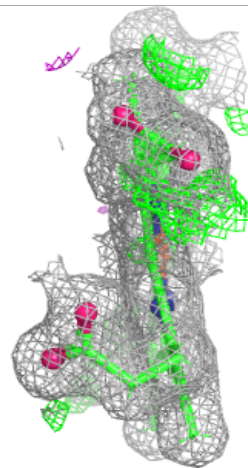
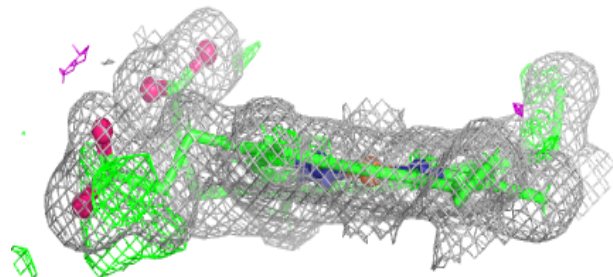
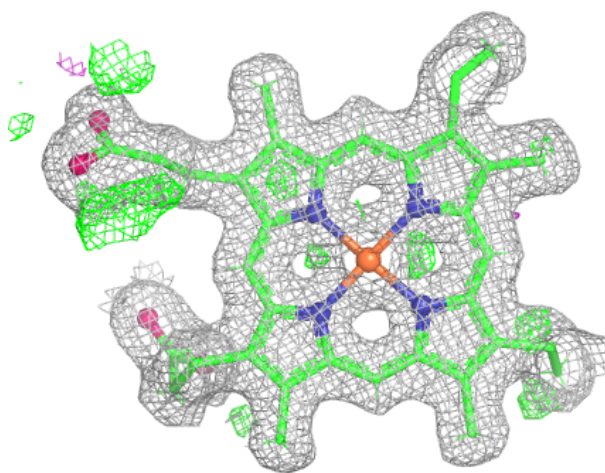
Electron density around HEC A 1008:

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



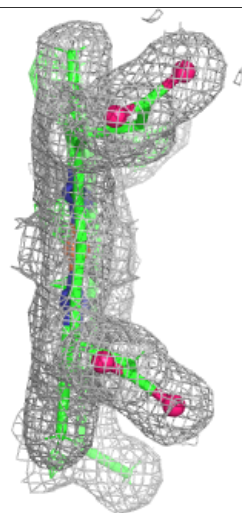
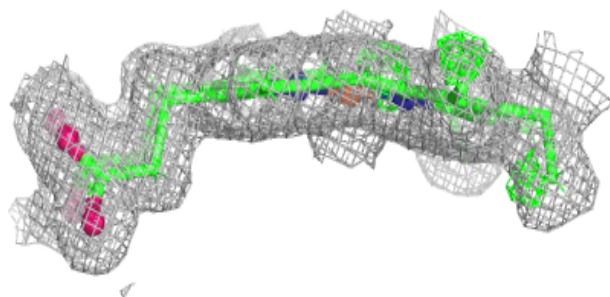
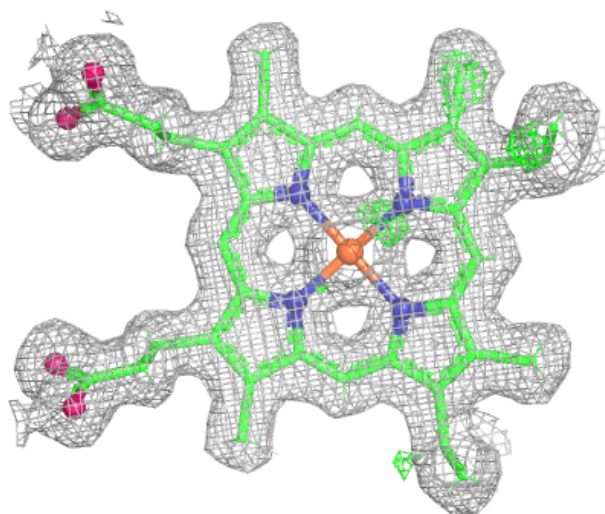
Electron density around HEC B 1005:

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and green (positive)



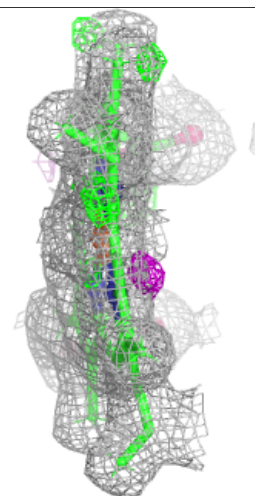
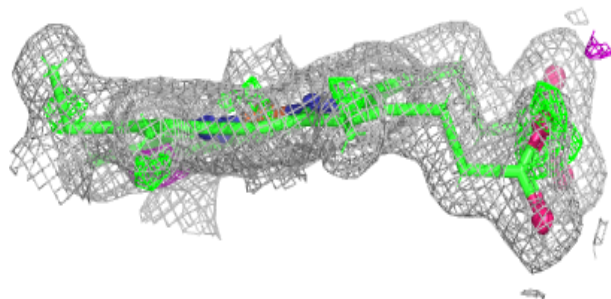
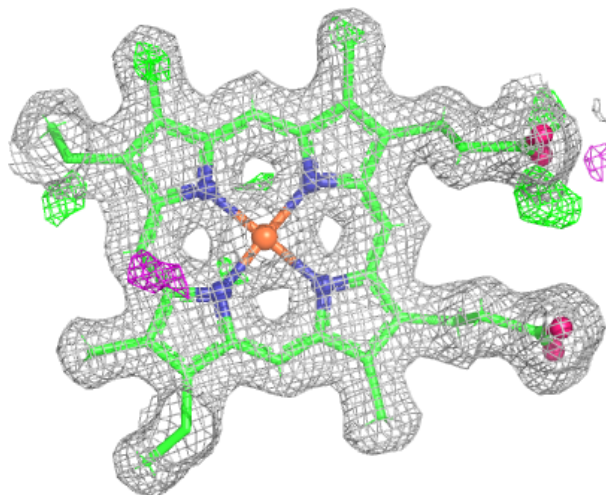
Electron density around HEC B 1006:

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and green (positive)



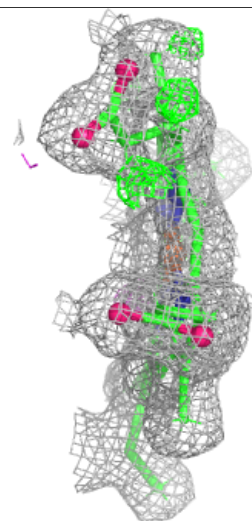
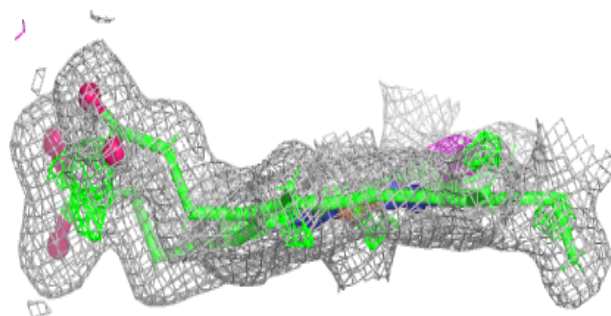
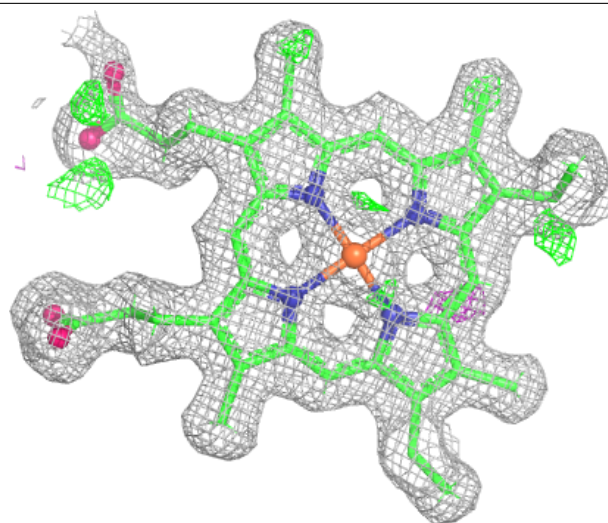
Electron density around HEC B 1007 (A):

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



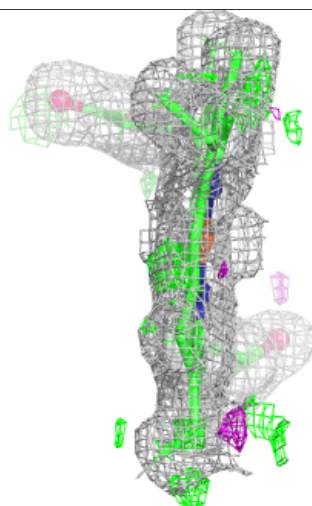
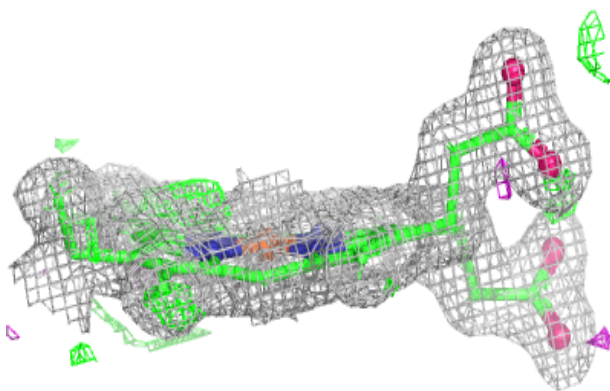
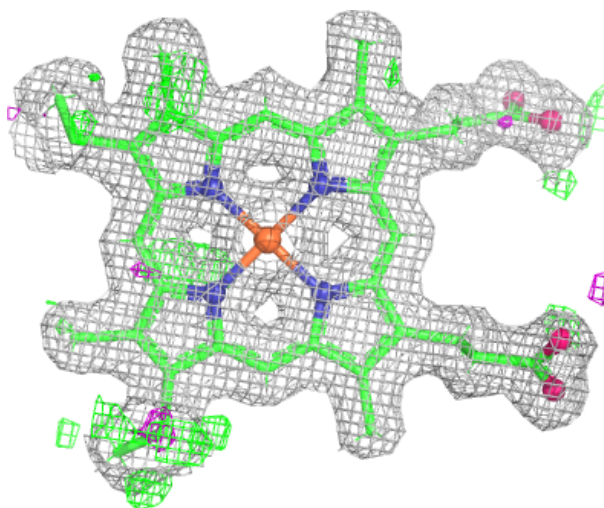
Electron density around HEC B 1007 (B):

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



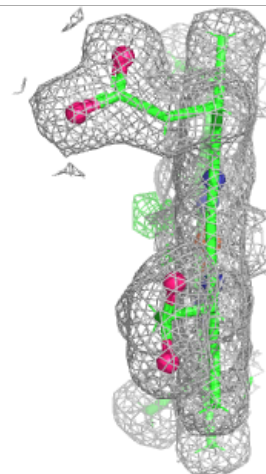
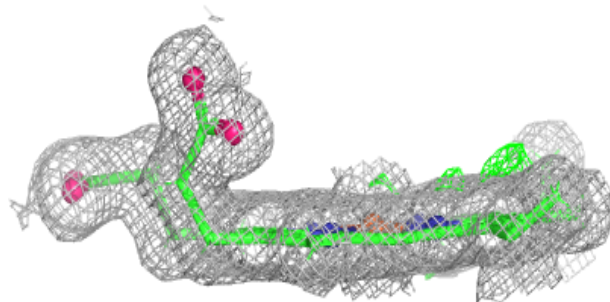
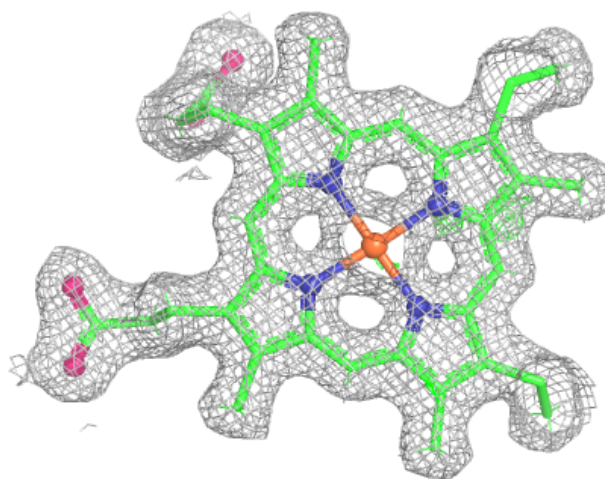
Electron density around HEC B 1008:

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



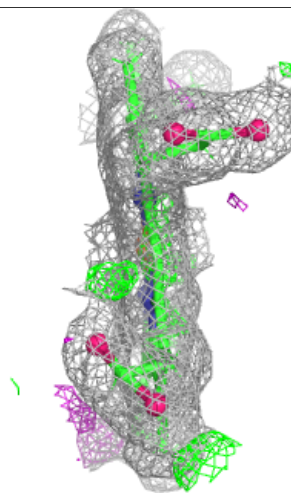
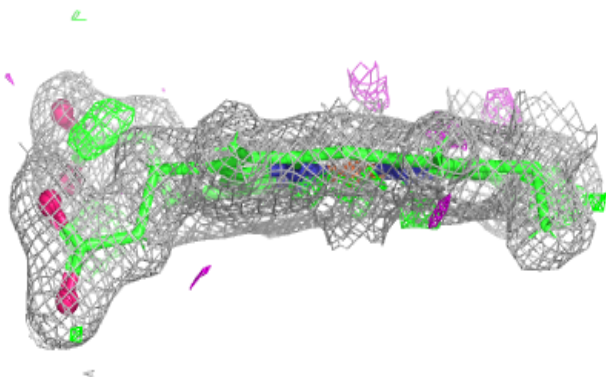
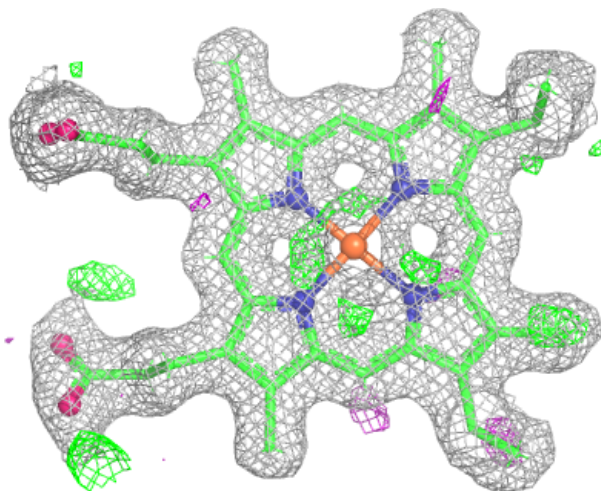
Electron density around HEC B 1002:

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



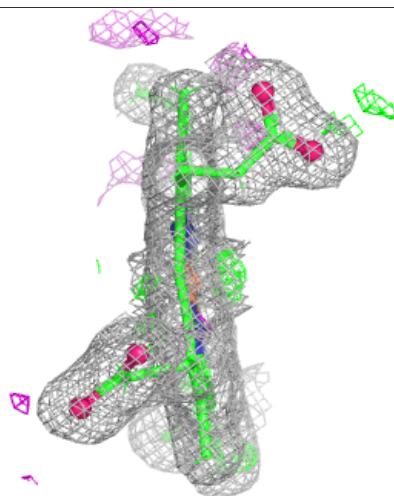
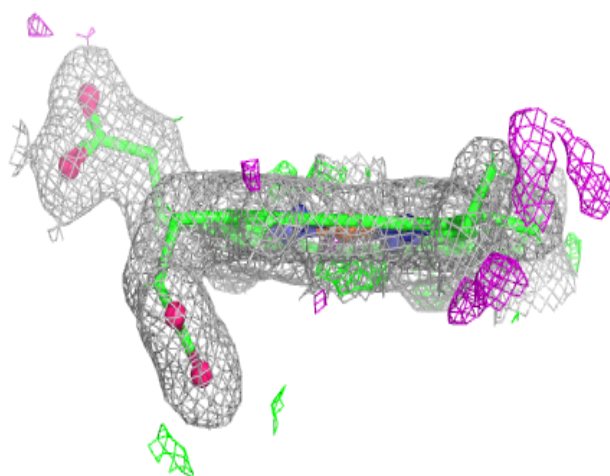
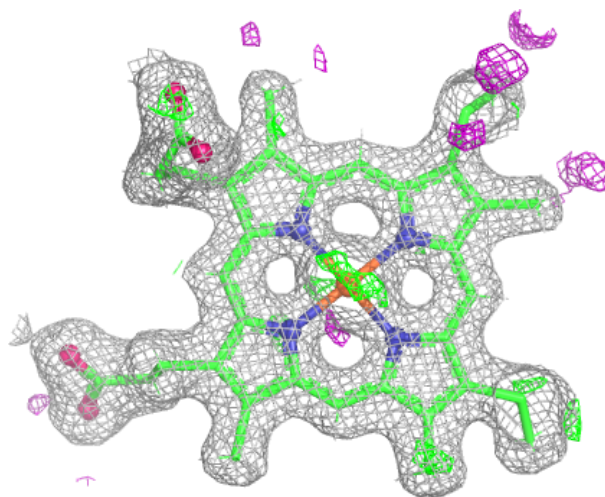
Electron density around HEC B 1003:

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



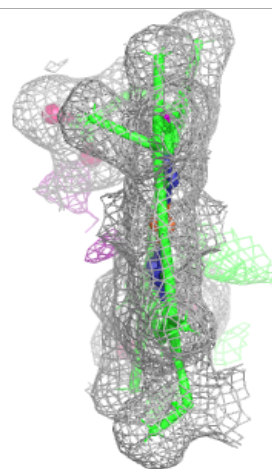
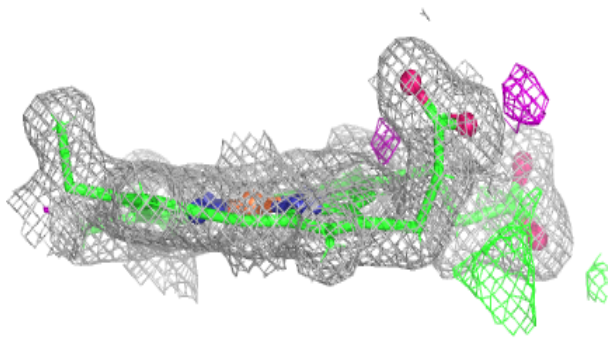
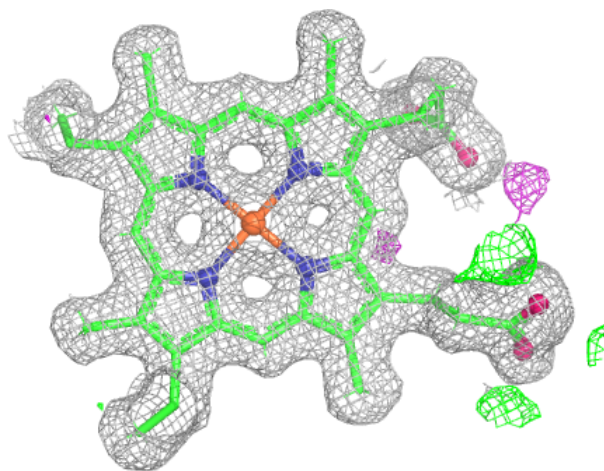
Electron density around HEC B 1001:

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and green (positive)



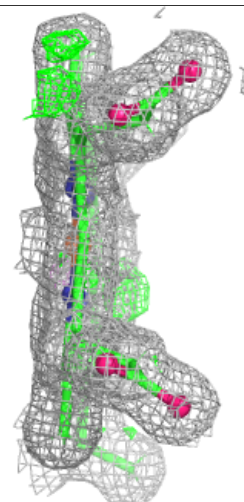
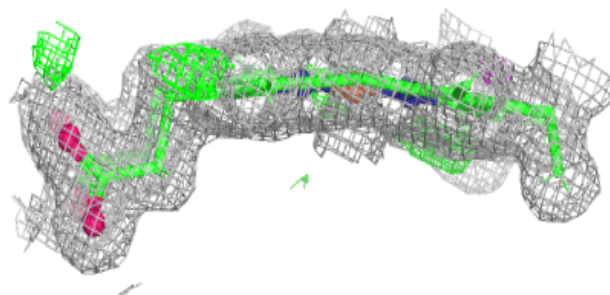
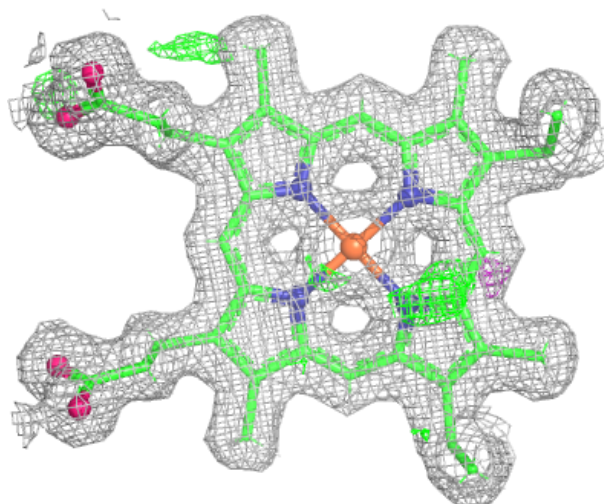
Electron density around HEC A 1005:

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and green (positive)



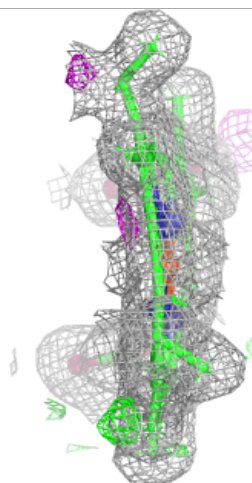
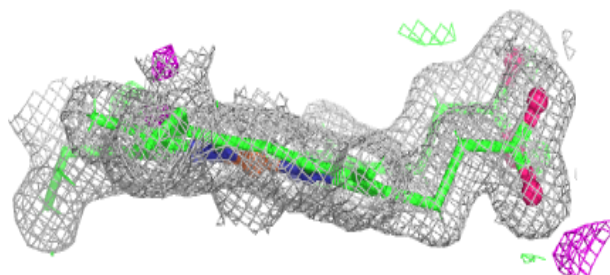
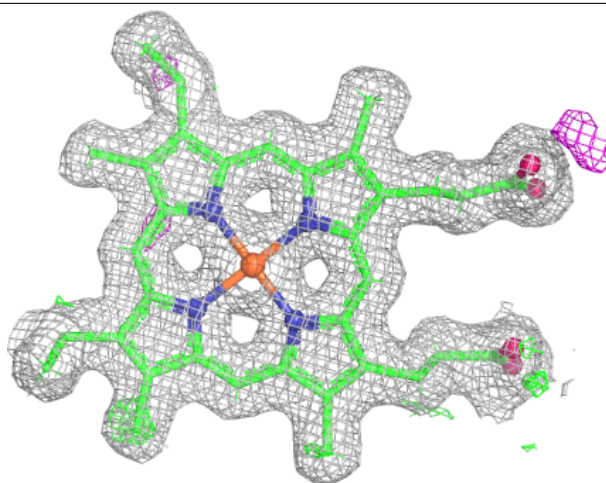
Electron density around HEC A 1006:

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



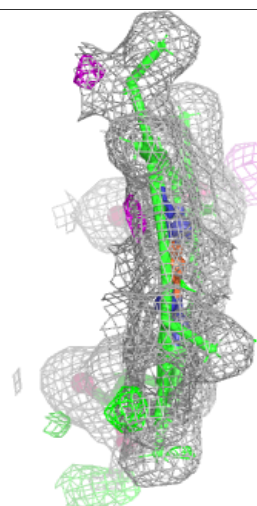
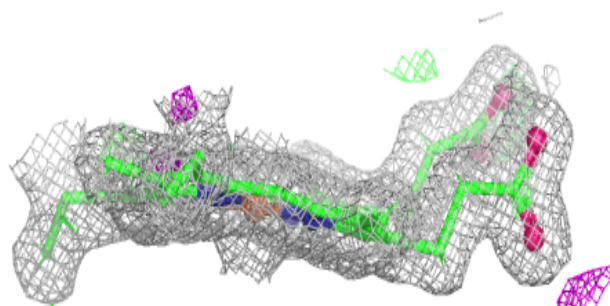
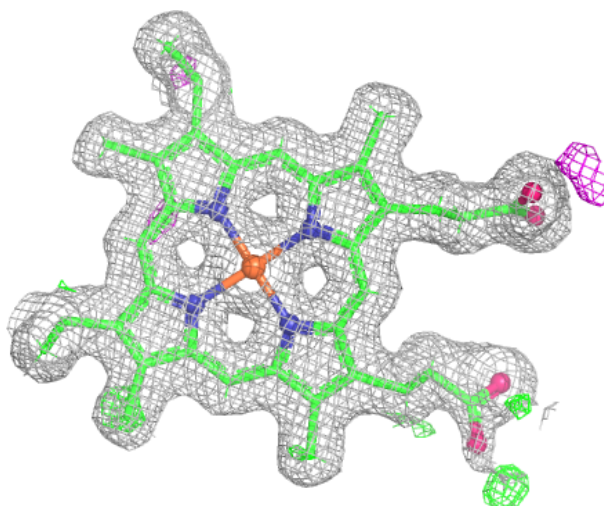
Electron density around HEC A 1007 (A):

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



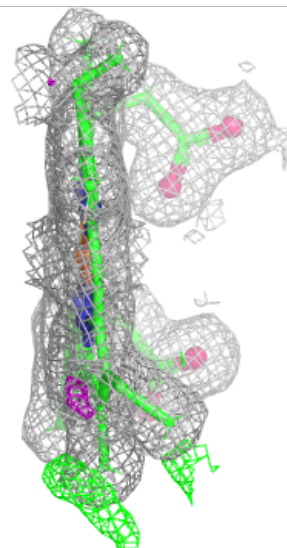
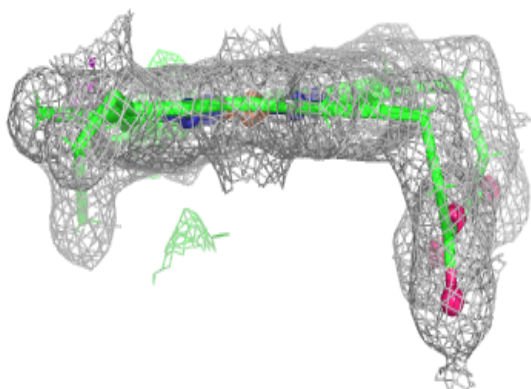
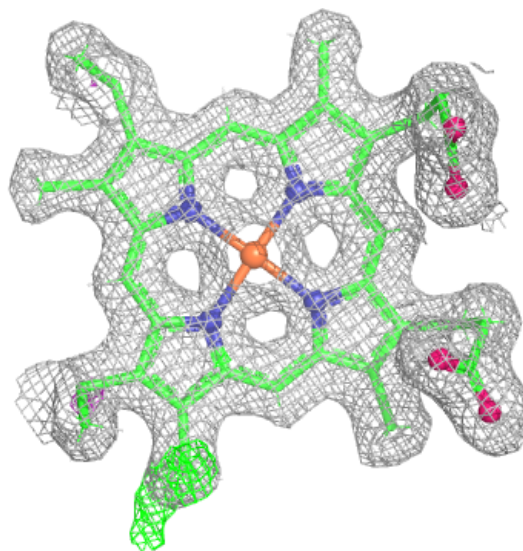
Electron density around HEC A 1007 (B):

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



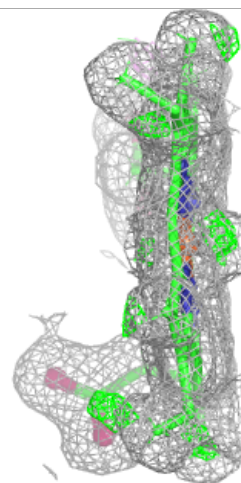
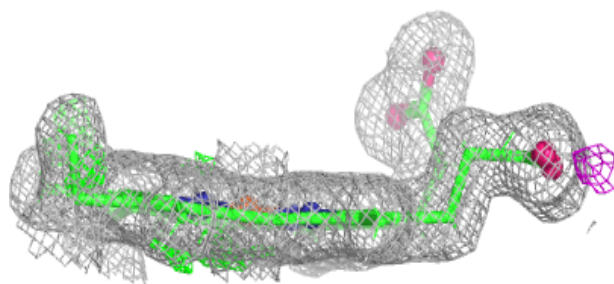
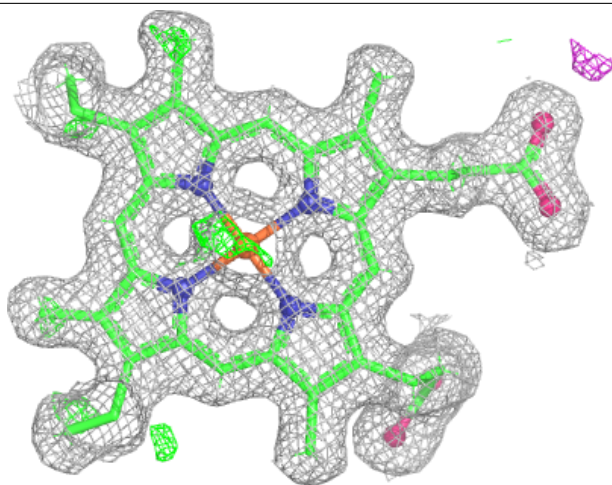
Electron density around HEC A 1004:

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



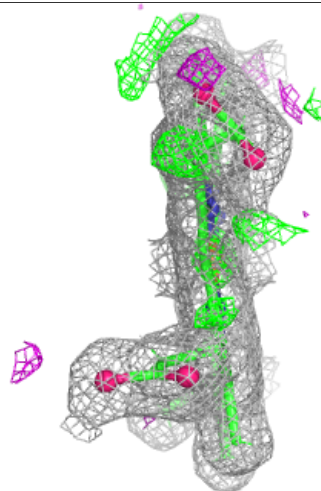
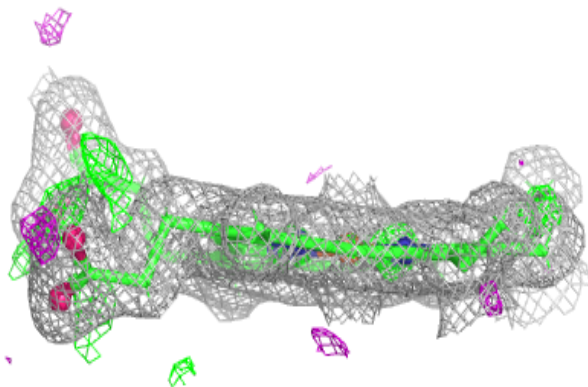
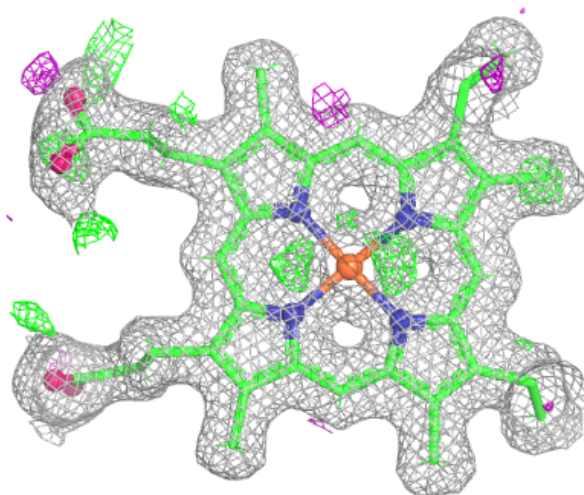
Electron density around HEC A 1002:

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



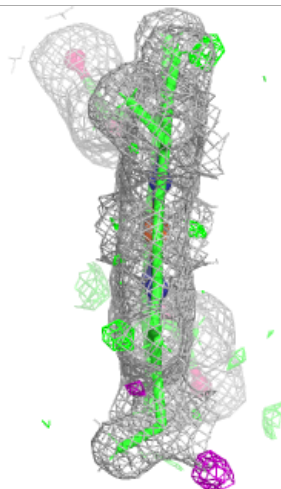
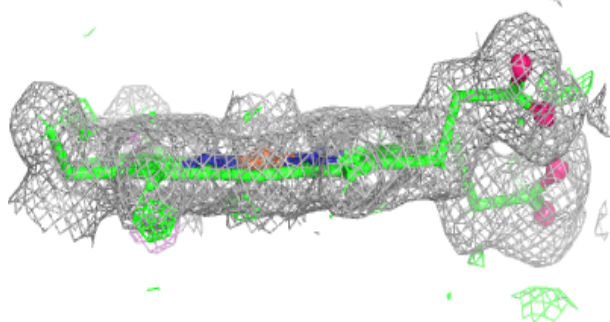
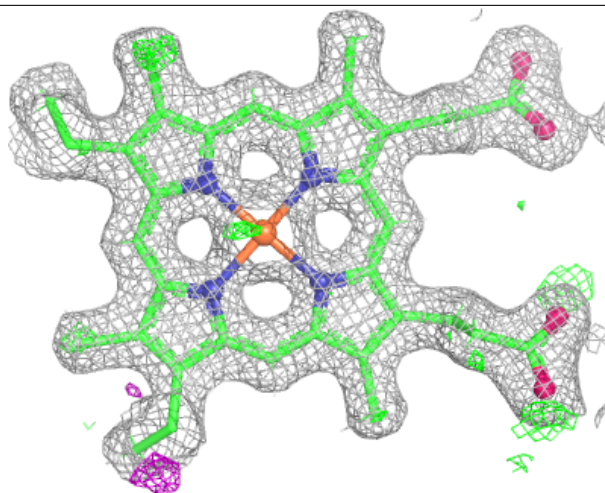
Electron density around HEC A 1003:

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



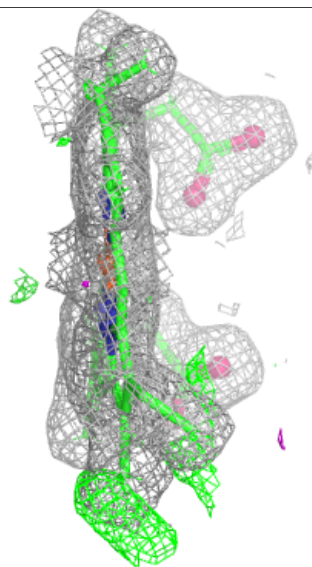
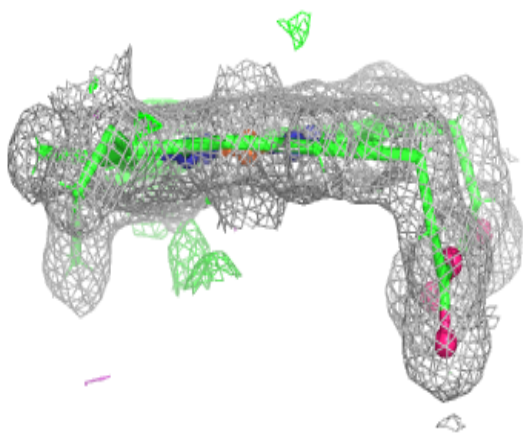
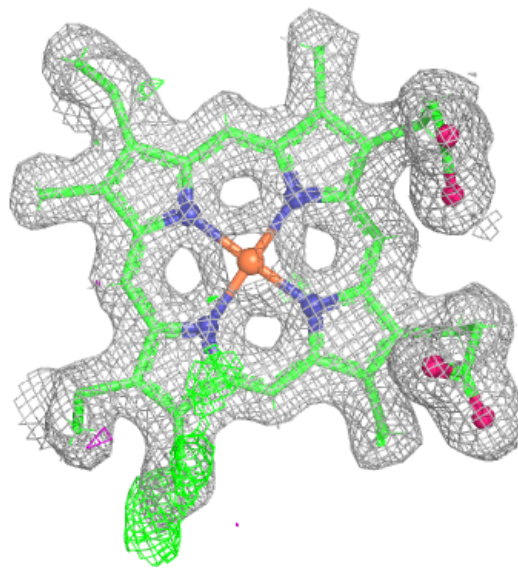
Electron density around HEC A 1001:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.