



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:41 PM EDT

PDB ID : 3UFH / pdb_00003ufh
Title : Crystal structure of UndA with Iron Citrate bound
Authors : Edwards, M.J.; Clarke, T.A.
Deposited on : 2011-11-01
Resolution : 2.23 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

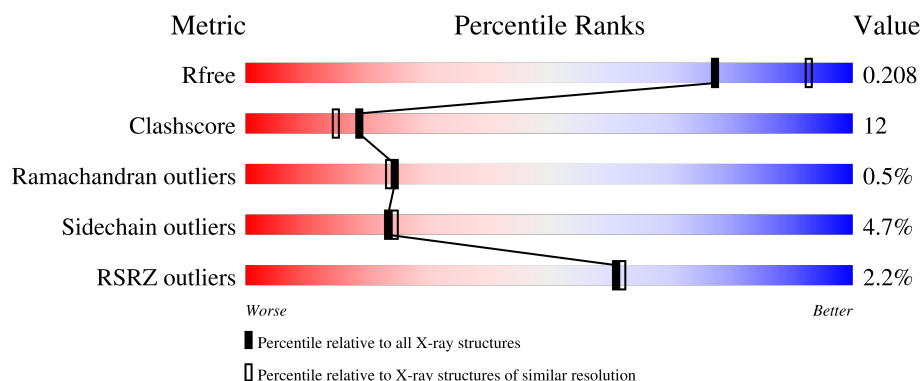
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

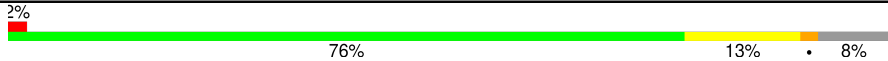
The reported resolution of this entry is 2.23 Å.

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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	874	

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	901	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	902	X	-	-	-
2	HEC	A	903	X	-	-	-
2	HEC	A	904	X	-	-	-
2	HEC	A	905	X	-	-	-
2	HEC	A	906	X	-	-	-
2	HEC	A	907	X	-	-	-
2	HEC	A	908	X	-	-	-
2	HEC	A	909	X	-	-	-
2	HEC	A	910	X	-	-	-
2	HEC	A	911	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7309 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UndA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	800	Total	C	N	O	S	0	1	0
			5956	3695	1030	1196	35			

There are 58 discrepancies between the modelled and reference sequences:

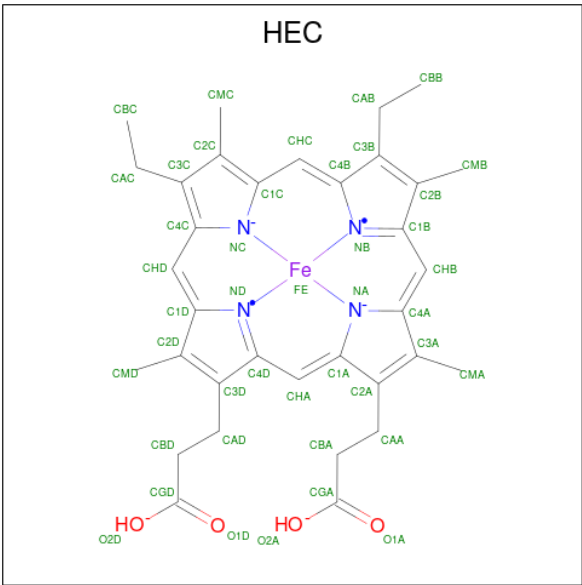
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP F8UWD6
A	1	SER	-	expression tag	UNP F8UWD6
A	2	LYS	-	expression tag	UNP F8UWD6
A	3	LYS	-	expression tag	UNP F8UWD6
A	4	LEU	-	expression tag	UNP F8UWD6
A	5	LEU	-	expression tag	UNP F8UWD6
A	6	SER	-	expression tag	UNP F8UWD6
A	7	VAL	-	expression tag	UNP F8UWD6
A	8	LEU	-	expression tag	UNP F8UWD6
A	9	PHE	-	expression tag	UNP F8UWD6
A	10	GLY	-	expression tag	UNP F8UWD6
A	11	ALA	-	expression tag	UNP F8UWD6
A	12	SER	-	expression tag	UNP F8UWD6
A	13	LEU	-	expression tag	UNP F8UWD6
A	14	ALA	-	expression tag	UNP F8UWD6
A	15	ALA	-	expression tag	UNP F8UWD6
A	16	LEU	-	expression tag	UNP F8UWD6
A	17	ALA	-	expression tag	UNP F8UWD6
A	18	LEU	-	expression tag	UNP F8UWD6
A	19	SER	-	expression tag	UNP F8UWD6
A	20	PRO	-	expression tag	UNP F8UWD6
A	21	THR	-	expression tag	UNP F8UWD6
A	22	ALA	-	expression tag	UNP F8UWD6
A	23	PHE	-	expression tag	UNP F8UWD6
A	24	ALA	-	expression tag	UNP F8UWD6
A	25	ALA	-	expression tag	UNP F8UWD6
A	26	ASP	-	expression tag	UNP F8UWD6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	-	expression tag	UNP F8UWD6
A	844	LYS	-	expression tag	UNP F8UWD6
A	845	GLY	-	expression tag	UNP F8UWD6
A	846	GLU	-	expression tag	UNP F8UWD6
A	847	LEU	-	expression tag	UNP F8UWD6
A	848	LYS	-	expression tag	UNP F8UWD6
A	849	LEU	-	expression tag	UNP F8UWD6
A	850	GLU	-	expression tag	UNP F8UWD6
A	851	GLY	-	expression tag	UNP F8UWD6
A	852	LYS	-	expression tag	UNP F8UWD6
A	853	PRO	-	expression tag	UNP F8UWD6
A	854	ILE	-	expression tag	UNP F8UWD6
A	855	PRO	-	expression tag	UNP F8UWD6
A	856	ASN	-	expression tag	UNP F8UWD6
A	857	PRO	-	expression tag	UNP F8UWD6
A	858	LEU	-	expression tag	UNP F8UWD6
A	859	LEU	-	expression tag	UNP F8UWD6
A	860	GLY	-	expression tag	UNP F8UWD6
A	861	LEU	-	expression tag	UNP F8UWD6
A	862	ASP	-	expression tag	UNP F8UWD6
A	863	SER	-	expression tag	UNP F8UWD6
A	864	THR	-	expression tag	UNP F8UWD6
A	865	ARG	-	expression tag	UNP F8UWD6
A	866	THR	-	expression tag	UNP F8UWD6
A	867	GLY	-	expression tag	UNP F8UWD6
A	868	HIS	-	expression tag	UNP F8UWD6
A	869	HIS	-	expression tag	UNP F8UWD6
A	870	HIS	-	expression tag	UNP F8UWD6
A	871	HIS	-	expression tag	UNP F8UWD6
A	872	HIS	-	expression tag	UNP F8UWD6
A	873	HIS	-	expression tag	UNP F8UWD6

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

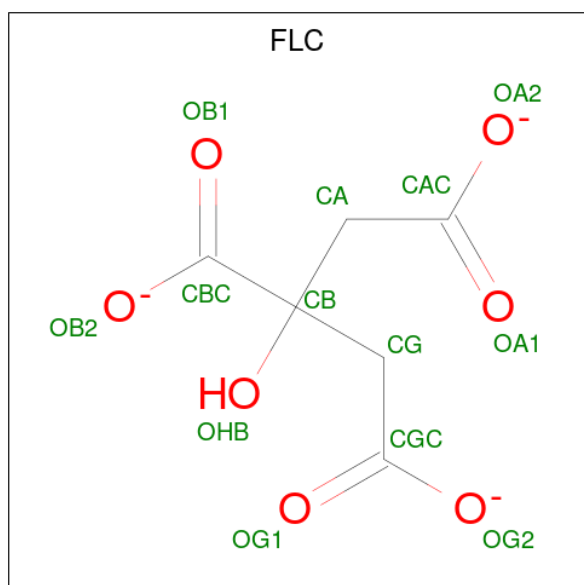
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Fe	0	0
			3	3		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).

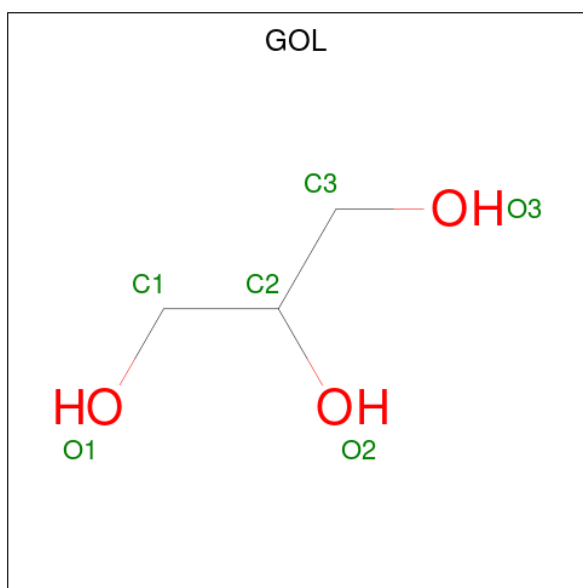


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	6	7		
6	A	1	Total	C	O	0	0
			13	6	7		
6	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

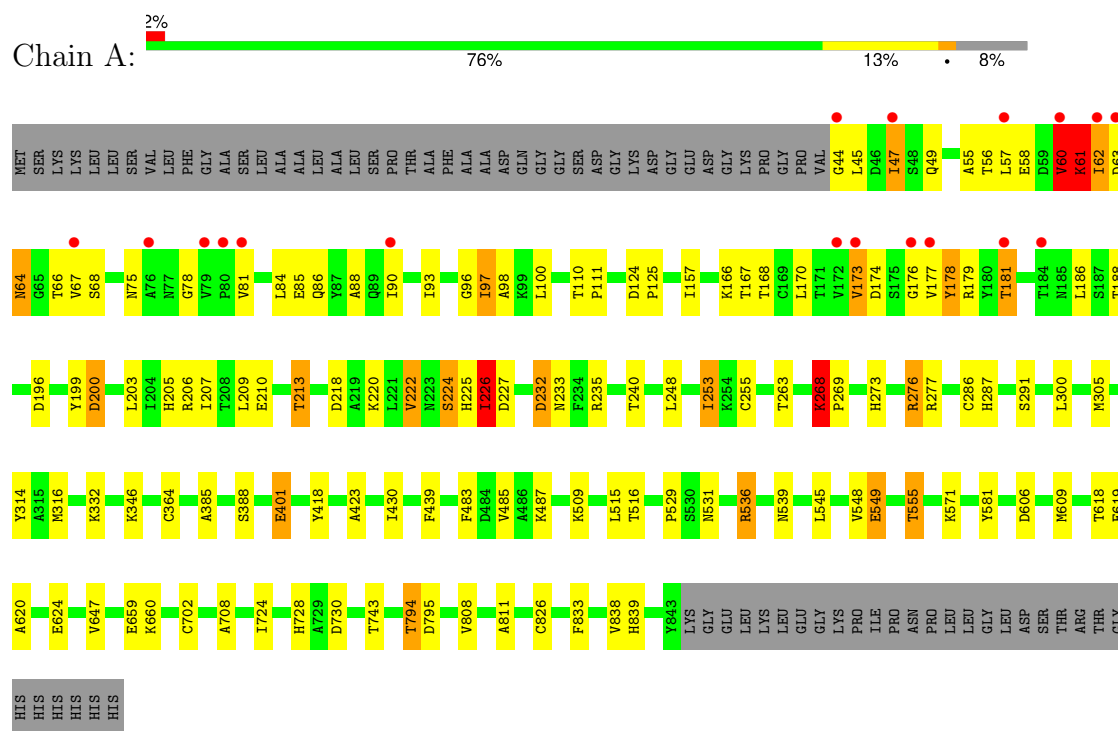
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	828	Total	O	0	0
			828	828		

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: UndA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.88Å 106.53Å 151.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.63 – 2.23 61.63 – 2.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.63-2.23) 98.9 (61.63-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.211 0.161 , 0.208	Depositor DCC
R_{free} test set	2800 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7309	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: CA, FE, MG, FLC, O, HEC, GOL

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	0.94	1/6084 (0.0%)	0.97	14/8279 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ILE	CA-CB	5.08	1.61	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ILE	N-CA-C	10.29	121.09	108.53
1	A	61	LYS	N-CA-C	8.29	119.56	107.88
1	A	708	ALA	N-CA-C	7.69	119.44	111.14
1	A	647	VAL	N-CA-C	6.45	118.36	112.43
1	A	110	THR	CA-C-N	6.34	126.31	120.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	VAL	Peptide

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	5956	0	5724	141	0
2	A	473	0	335	46	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
6	A	39	0	12	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	A	828	0	0	12	0
All	All	7309	0	6079	150	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 12.

The worst 5 of 150 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:286:CYS:SG	2:A:907:HEC:HAC	1.54	1.47
1:A:286:CYS:SG	2:A:907:HEC:CAC	2.06	1.44
1:A:702:CYS:SG	2:A:905:HEC:CAC	2.08	1.42
1:A:364:CYS:SG	2:A:908:HEC:CAC	2.07	1.41
1:A:255:CYS:SG	2:A:906:HEC:CAC	2.08	1.41

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	799/874 (91%)	755 (94%)	40 (5%)	4 (0%)	24 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	168	THR
1	A	218	ASP
1	A	268	LYS

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	645/700 (92%)	615 (95%)	30 (5%)	23 24

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	SER
1	A	581	TYR
1	A	240	THR
1	A	794	THR
1	A	515	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	225	HIS
1	A	437	HIS
1	A	441	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	GOL	A	922	-	5,5,5	0.59	0	5,5,5	0.73	0
2	HEC	A	905	3,1	50,50,50	1.67	8 (16%)	68,82,82	1.50	11 (16%)
6	FLC	A	920	5	12,12,12	1.02	0	17,17,17	1.28	2 (11%)
2	HEC	A	901	1	50,50,50	1.92	8 (16%)	68,82,82	1.55	10 (14%)
2	HEC	A	902	1	50,50,50	1.85	8 (16%)	68,82,82	1.48	9 (13%)
2	HEC	A	903	1	50,50,50	1.72	7 (14%)	68,82,82	1.53	11 (16%)
2	HEC	A	904	1	50,50,50	1.87	10 (20%)	68,82,82	1.41	10 (14%)
2	HEC	A	906	1	50,50,50	1.69	8 (16%)	68,82,82	1.42	15 (22%)
2	HEC	A	909	1	50,50,50	1.71	5 (10%)	68,82,82	1.22	5 (7%)
6	FLC	A	918	5	12,12,12	0.87	0	17,17,17	2.07	7 (41%)
2	HEC	A	907	1,4	50,50,50	1.81	9 (18%)	68,82,82	1.53	11 (16%)
2	HEC	A	911	1	50,50,50	1.89	9 (18%)	68,82,82	1.38	9 (13%)
2	HEC	A	908	1	50,50,50	1.61	10 (20%)	68,82,82	1.42	9 (13%)
6	FLC	A	919	5	12,12,12	1.24	0	17,17,17	1.16	1 (5%)
2	HEC	A	910	1	50,50,50	1.85	7 (14%)	68,82,82	1.44	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	922	-	-	0/4/4/4	-
2	HEC	A	905	3,1	1/1/3/7	9/14/54/54	-
6	FLC	A	920	5	-	7/16/16/16	-
2	HEC	A	901	1	1/1/3/7	6/14/54/54	-
2	HEC	A	902	1	1/1/3/7	5/14/54/54	-
2	HEC	A	903	1	1/1/3/7	5/14/54/54	-
2	HEC	A	904	1	1/1/3/7	7/14/54/54	-
2	HEC	A	906	1	1/1/3/7	8/14/54/54	-
2	HEC	A	909	1	1/1/3/7	3/14/54/54	-
6	FLC	A	918	5	-	1/16/16/16	-
2	HEC	A	907	1,4	1/1/3/7	4/14/54/54	-
2	HEC	A	911	1	1/1/3/7	8/14/54/54	-
2	HEC	A	908	1	1/1/3/7	6/14/54/54	-
6	FLC	A	919	5	-	0/16/16/16	-
2	HEC	A	910	1	1/1/3/7	6/14/54/54	-

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEC	C3D-C2D	7.89	1.53	1.36
2	A	910	HEC	C3D-C2D	7.52	1.53	1.36
2	A	911	HEC	C3D-C2D	7.48	1.52	1.36
2	A	902	HEC	FE-ND	7.42	2.17	1.94
2	A	906	HEC	C3D-C2D	7.39	1.52	1.36

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	HEC	C1D-ND-C4D	5.98	112.29	105.21
2	A	903	HEC	C1D-ND-C4D	5.63	111.87	105.21
2	A	910	HEC	C1D-ND-C4D	5.57	111.81	105.21
2	A	901	HEC	C1D-ND-C4D	5.31	111.49	105.21
2	A	907	HEC	C1D-ND-C4D	5.14	111.29	105.21

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	HEC	NA
2	A	902	HEC	NA
2	A	903	HEC	NA
2	A	904	HEC	NA
2	A	905	HEC	NA

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	905	HEC	C1A-C2A-CAA-CBA
2	A	905	HEC	C3A-C2A-CAA-CBA
2	A	908	HEC	C2C-C3C-CAC-CBC
2	A	909	HEC	C2C-C3C-CAC-CBC
2	A	911	HEC	C1A-C2A-CAA-CBA

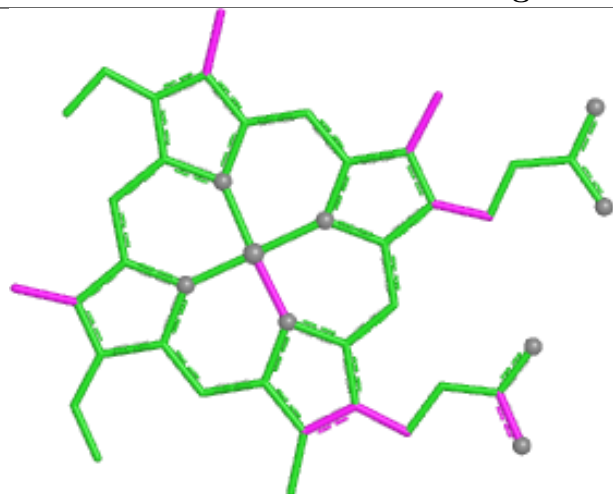
There are no ring outliers.

10 monomers are involved in 46 short contacts:

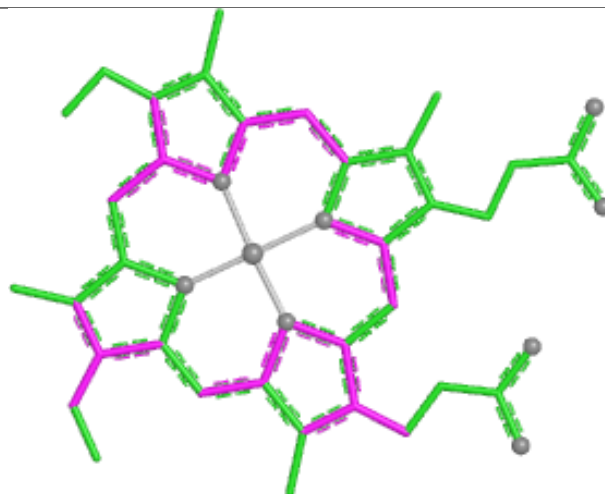
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	HEC	6	0
2	A	901	HEC	7	0
2	A	902	HEC	1	0
2	A	903	HEC	1	0
2	A	906	HEC	6	0
2	A	909	HEC	1	0
2	A	907	HEC	9	0
2	A	911	HEC	9	0
2	A	908	HEC	5	0
2	A	910	HEC	1	0

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

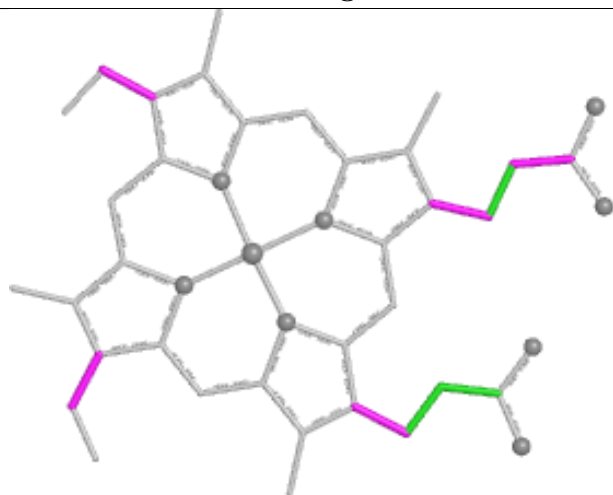
Ligand HEC A 905



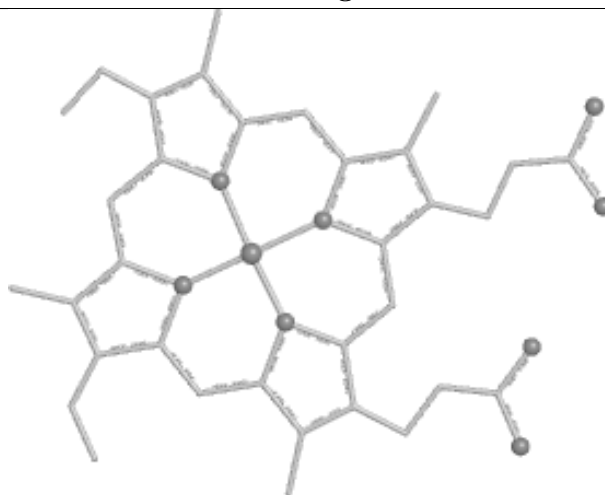
Bond lengths



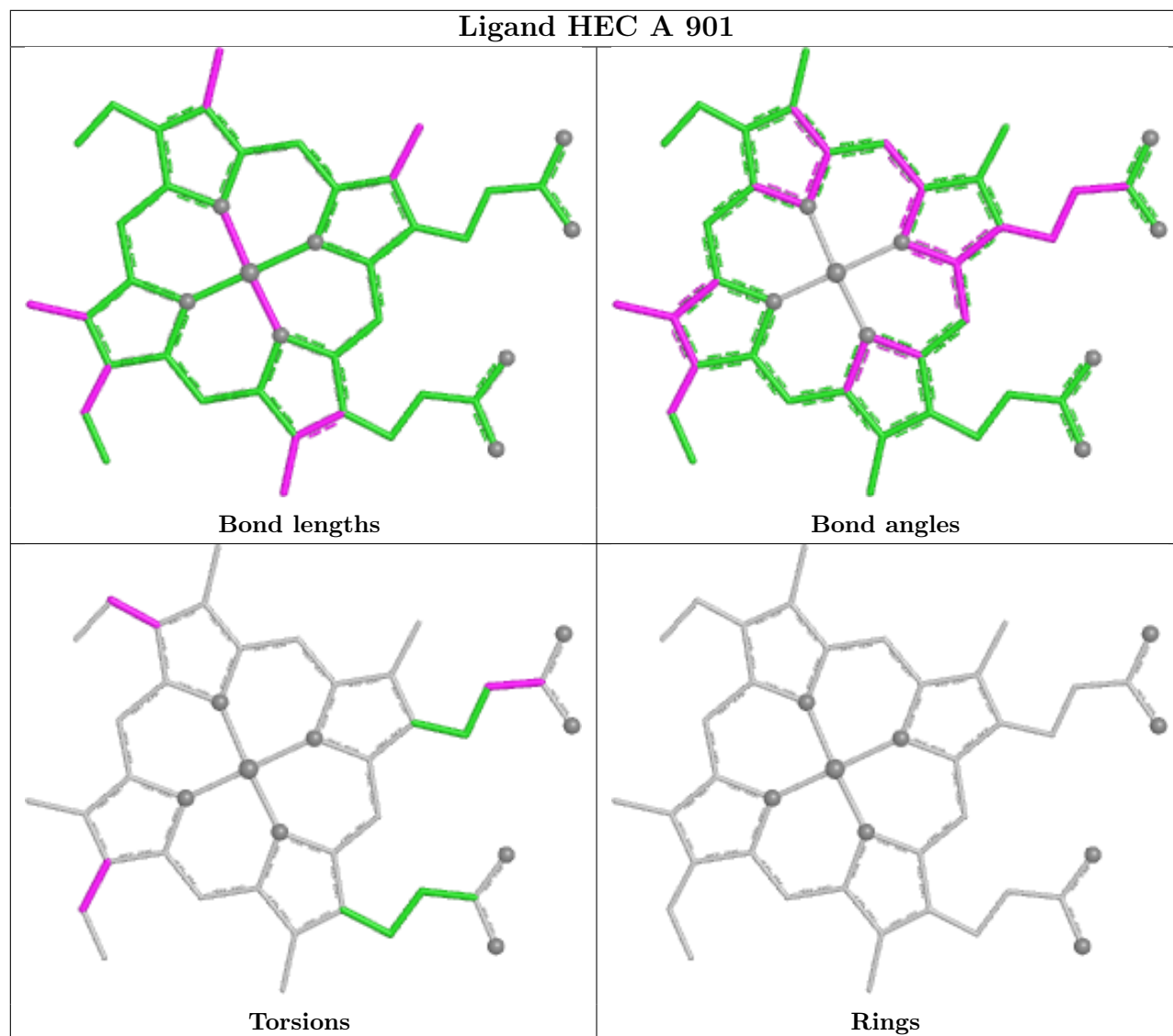
Bond angles



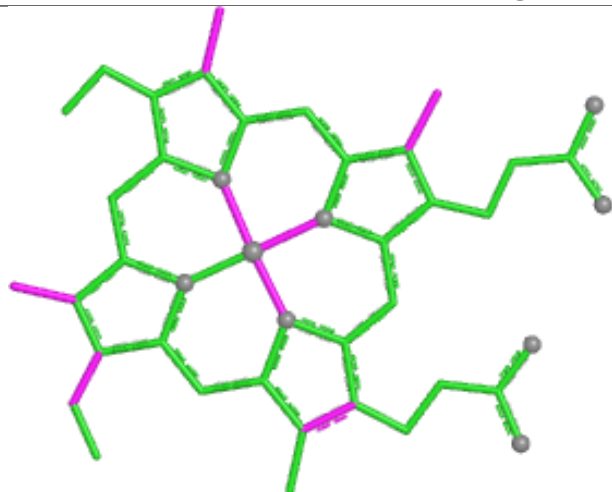
Torsions



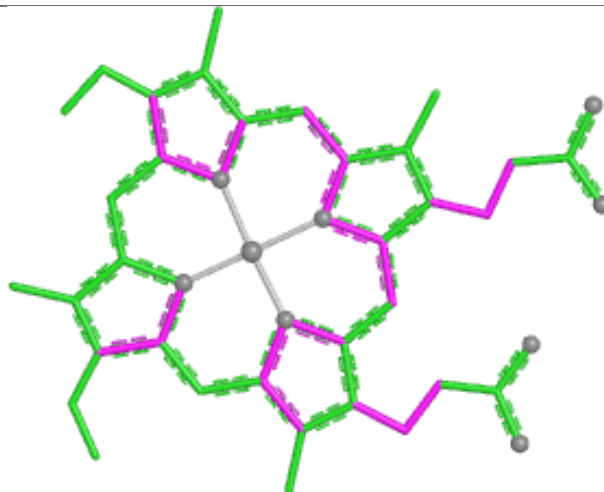
Rings



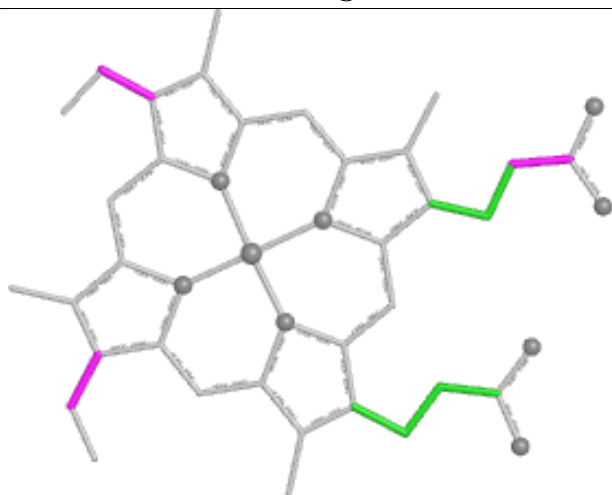
Ligand HEC A 902



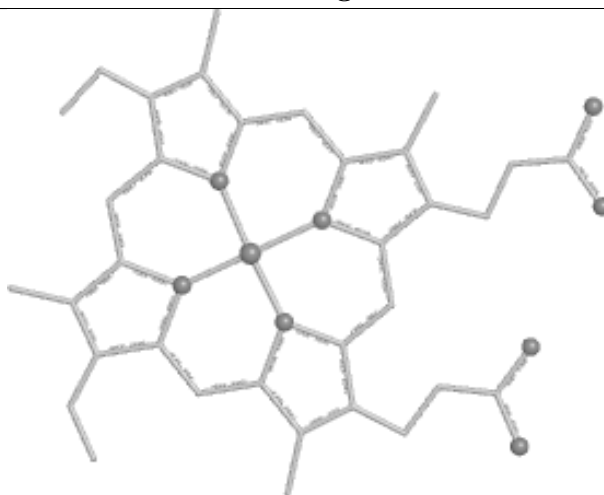
Bond lengths



Bond angles

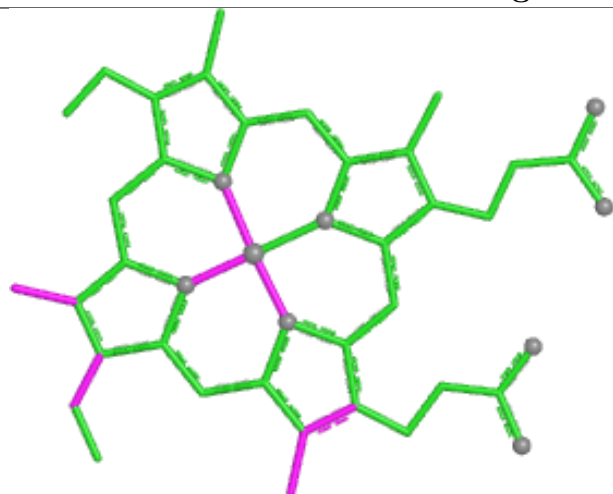


Torsions

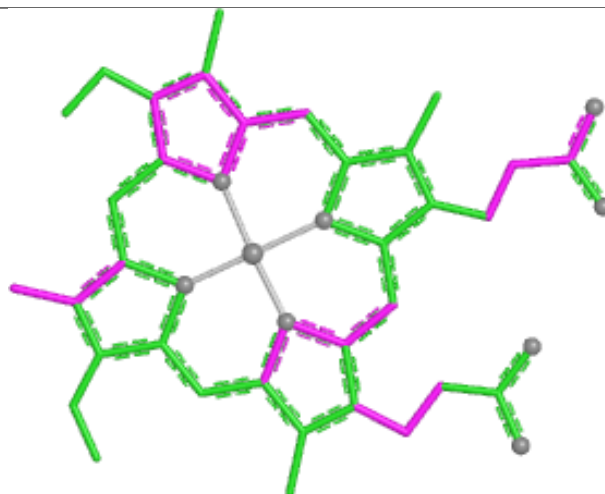


Rings

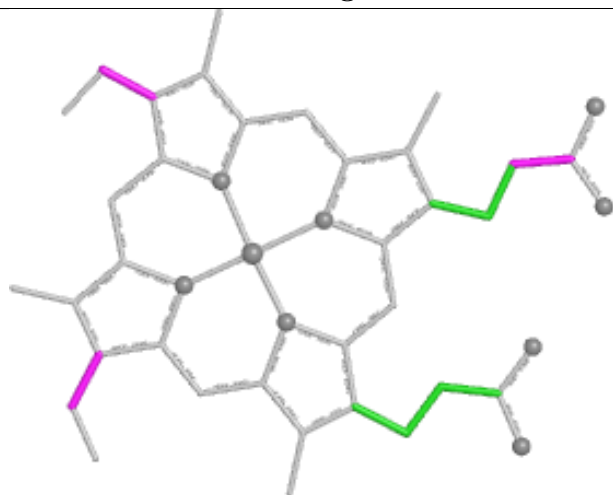
Ligand HEC A 903



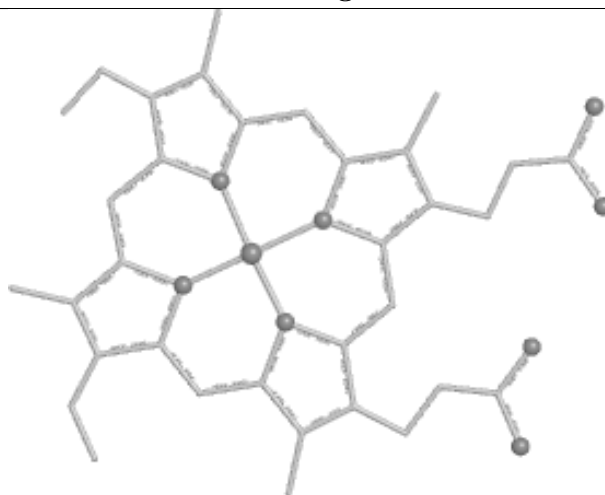
Bond lengths



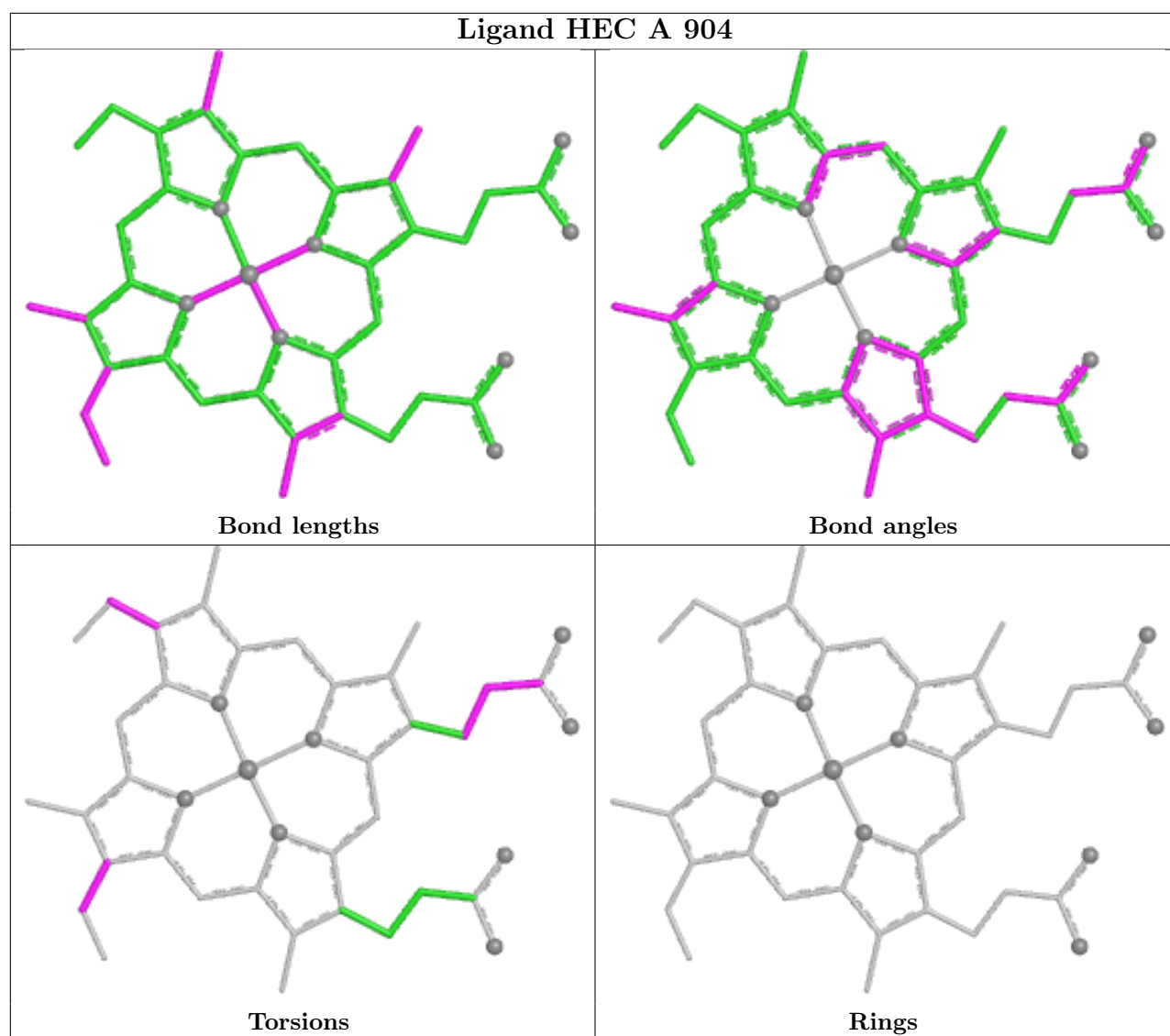
Bond angles

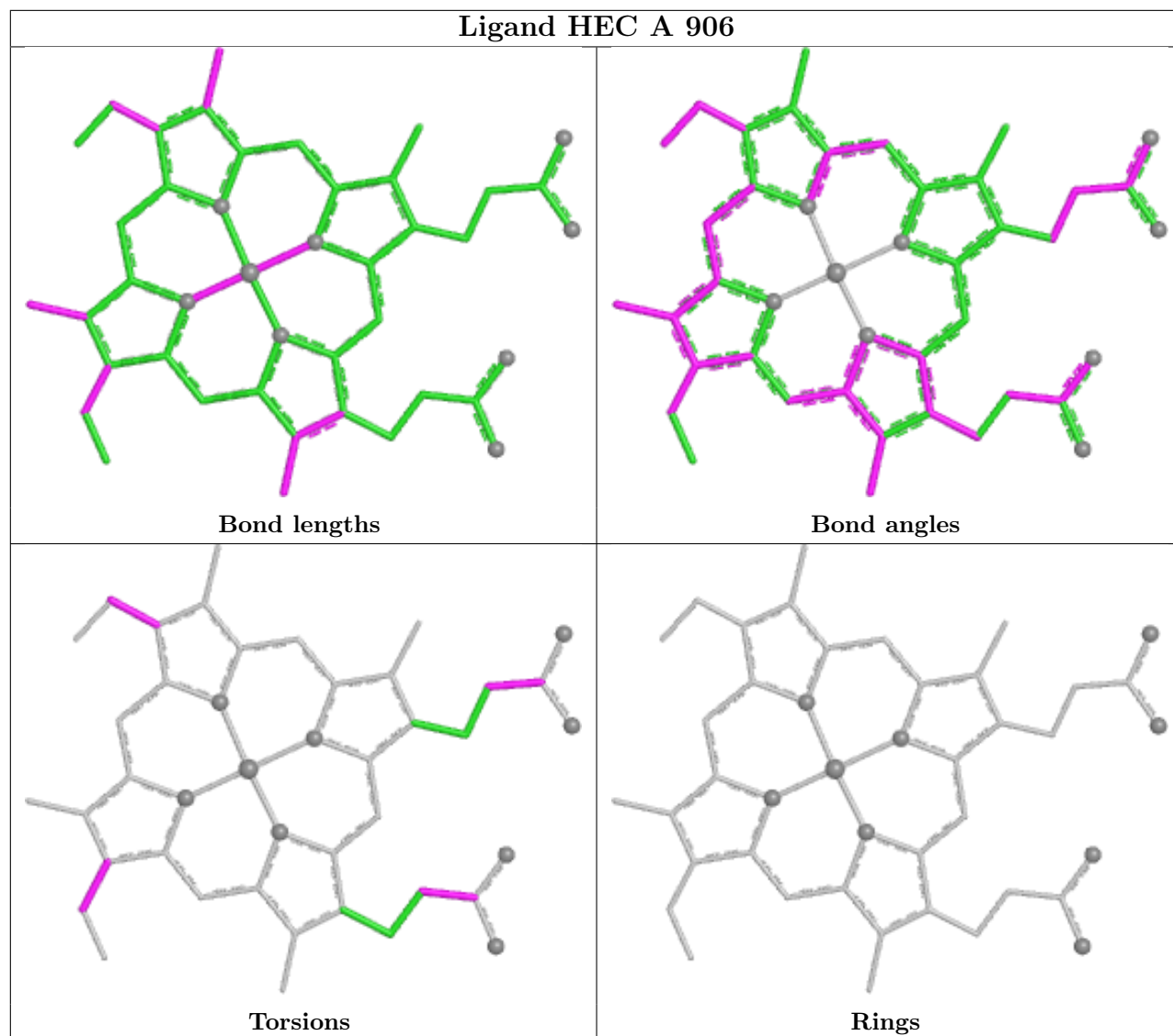


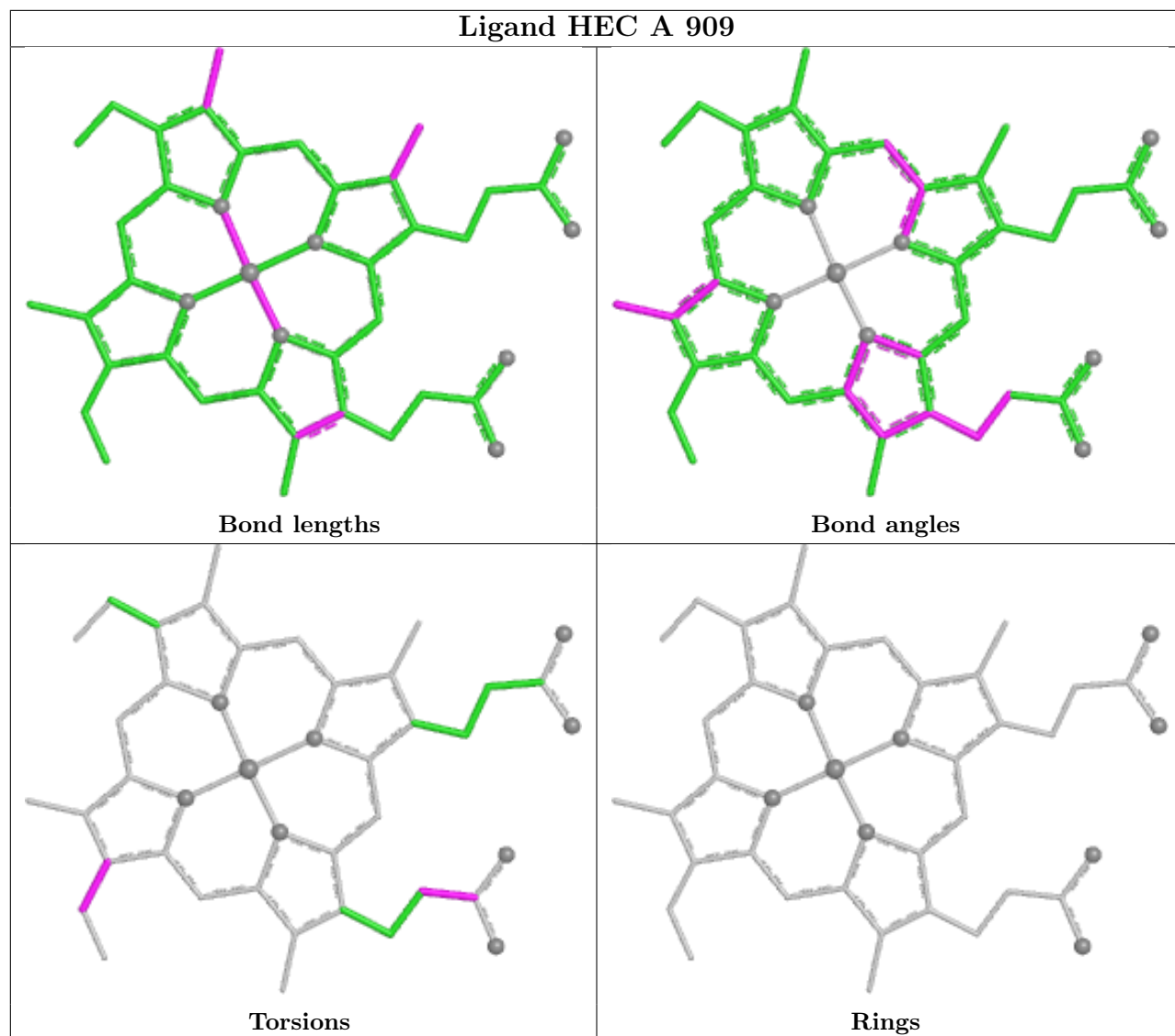
Torsions



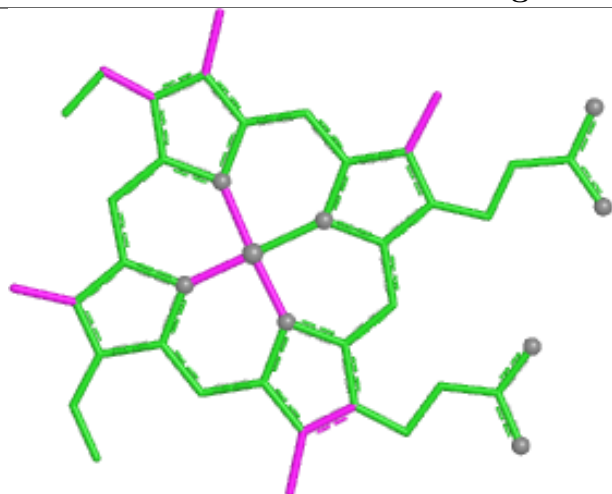
Rings



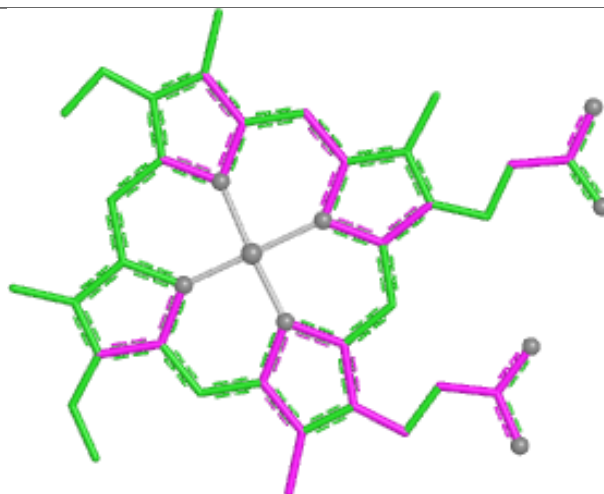




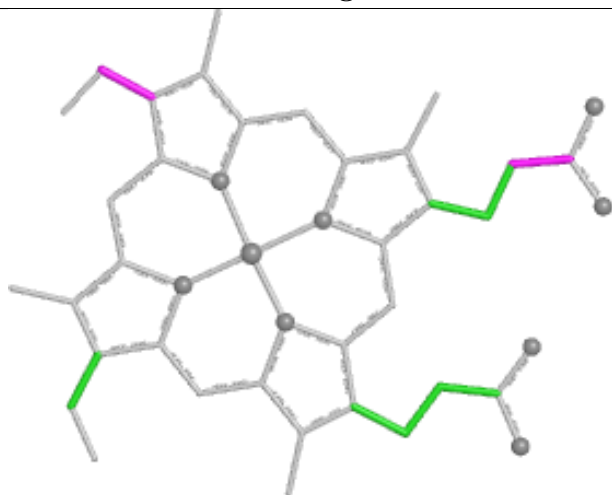
Ligand HEC A 907



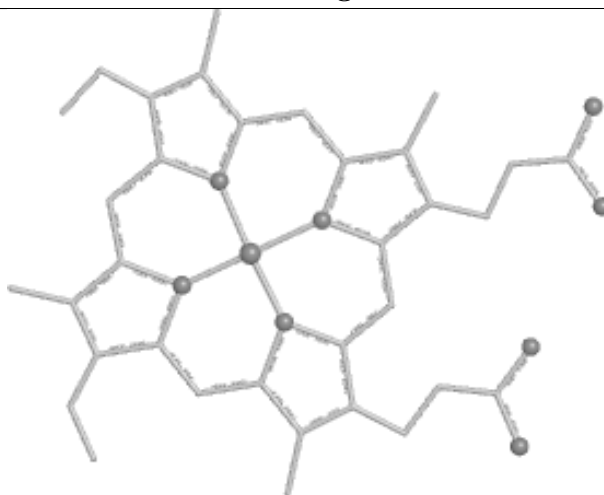
Bond lengths



Bond angles

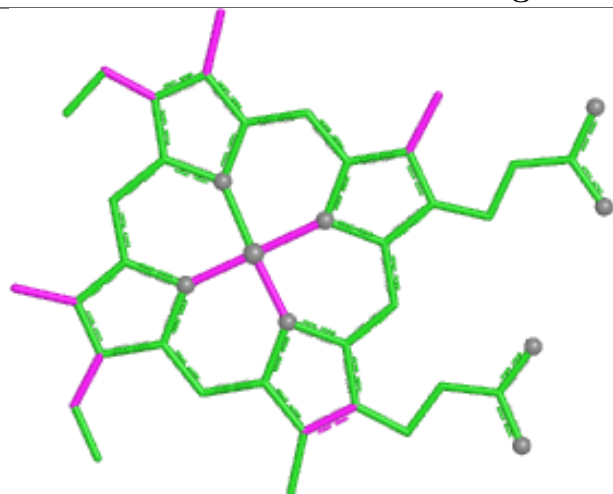


Torsions

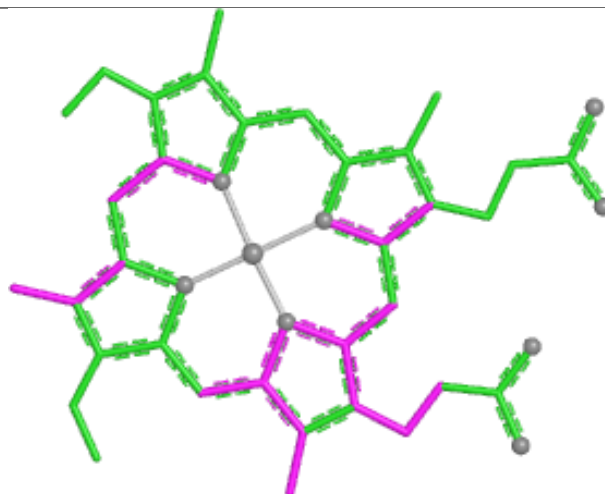


Rings

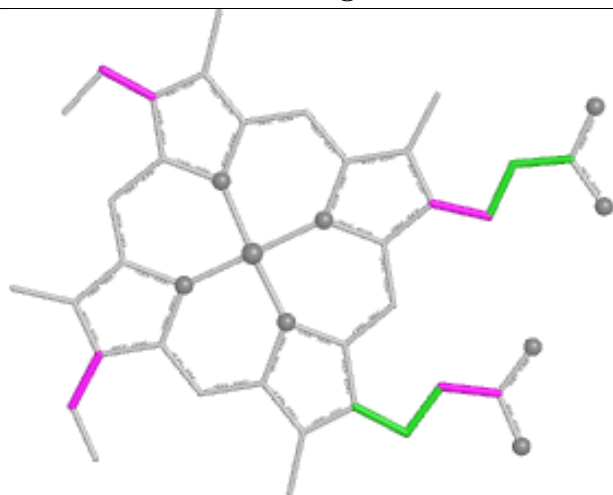
Ligand HEC A 911



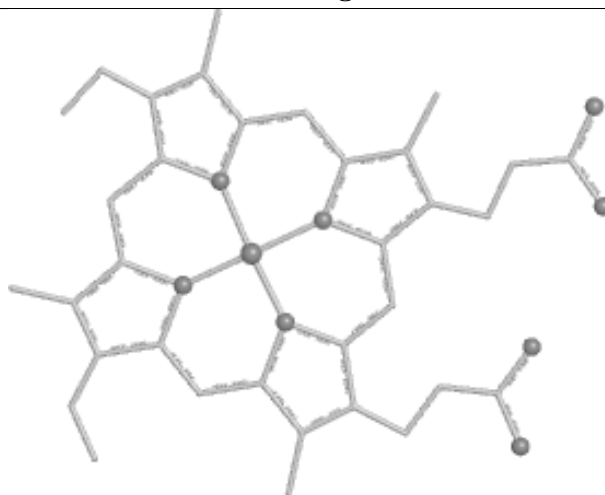
Bond lengths



Bond angles

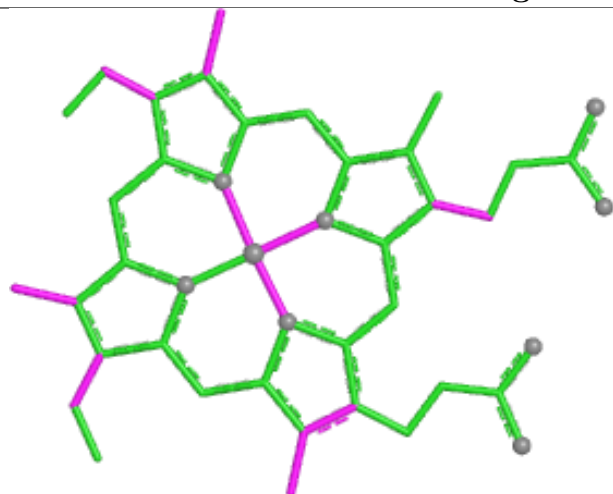


Torsions

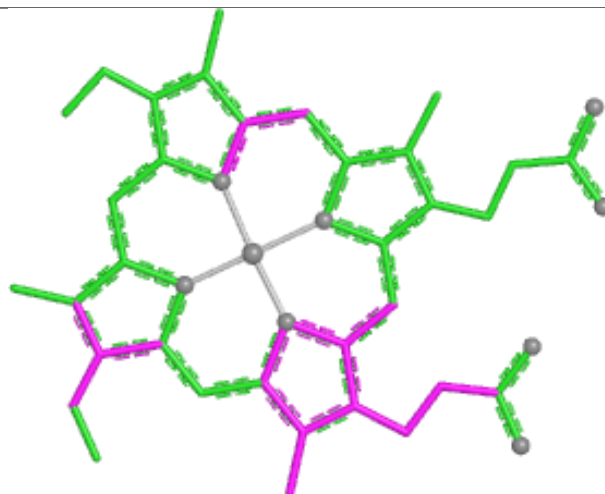


Rings

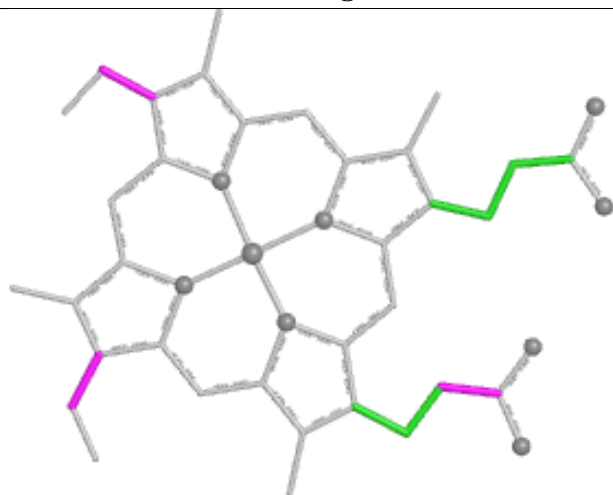
Ligand HEC A 908



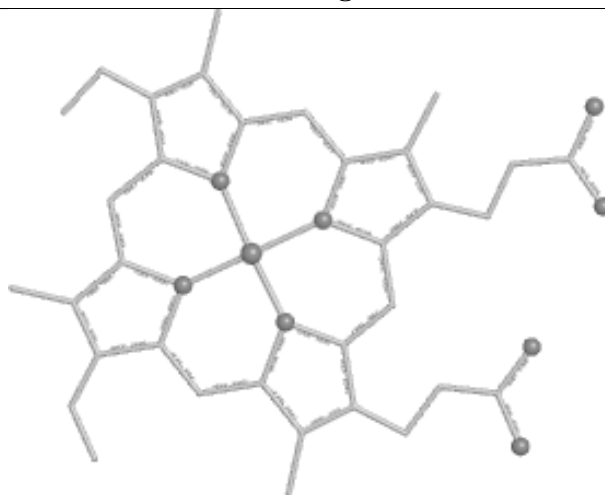
Bond lengths



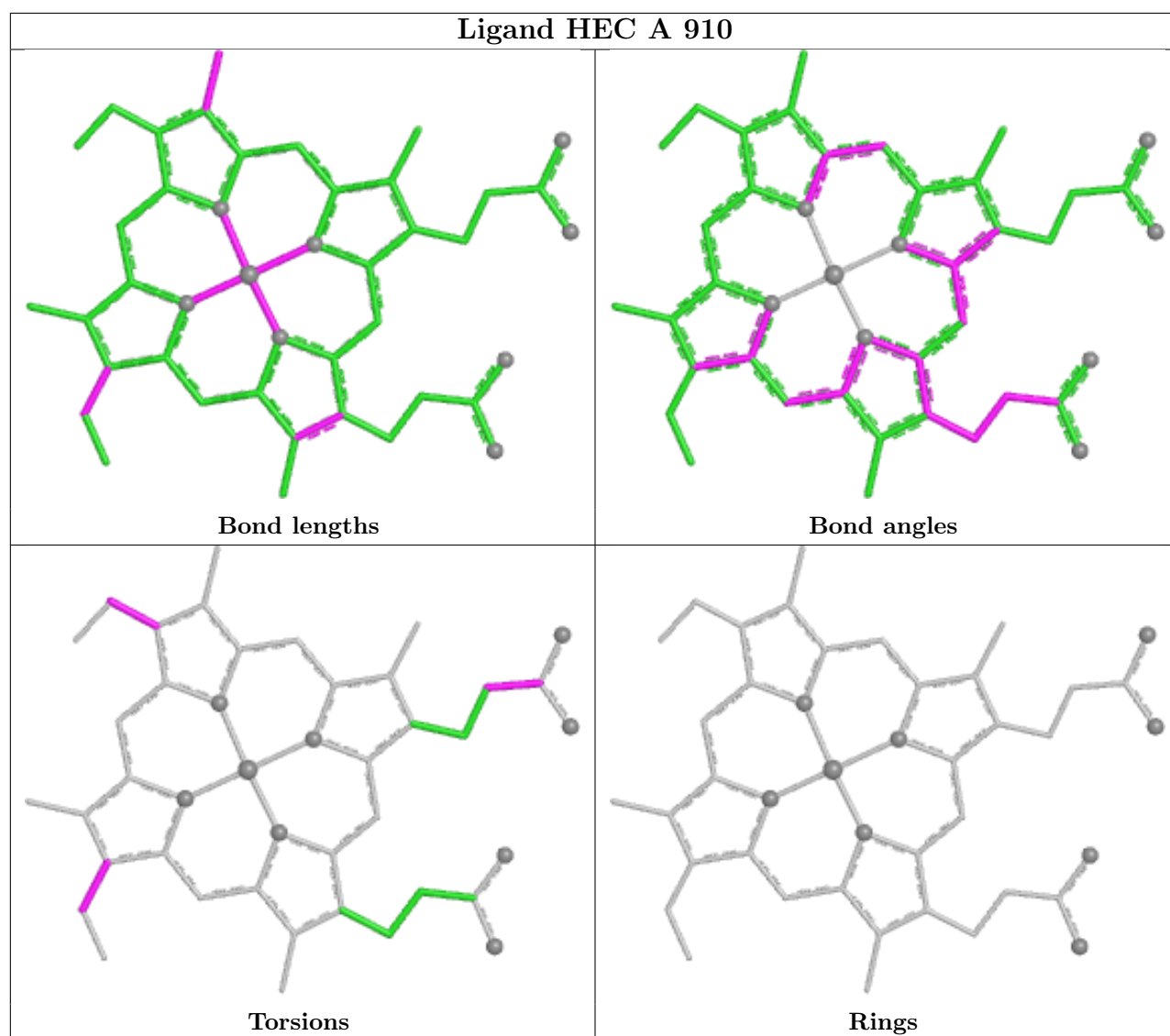
Bond angles



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	800/874 (91%)	-0.25	18 (2%) 61 62	11, 31, 67, 88	1 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	ILE	4.0
1	A	60	VAL	3.9
1	A	173	VAL	3.3
1	A	57	LEU	3.2
1	A	177	VAL	3.1

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 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	FLC	A	920	13/13	0.86	0.12	55,65,67,70	0
7	O	A	921	1/1	0.86	0.19	61,61,61,61	0

Continued on next page...

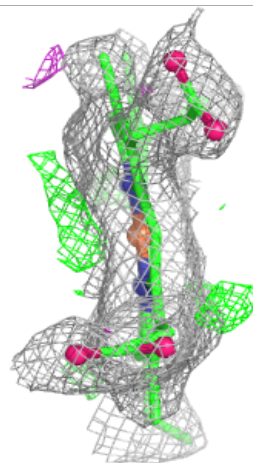
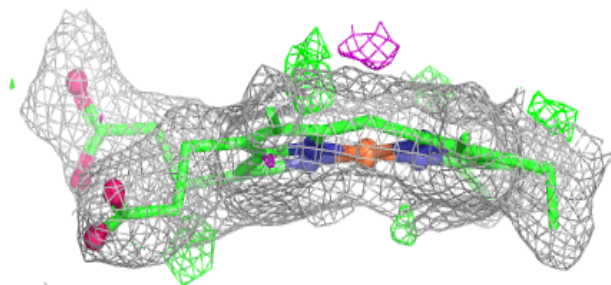
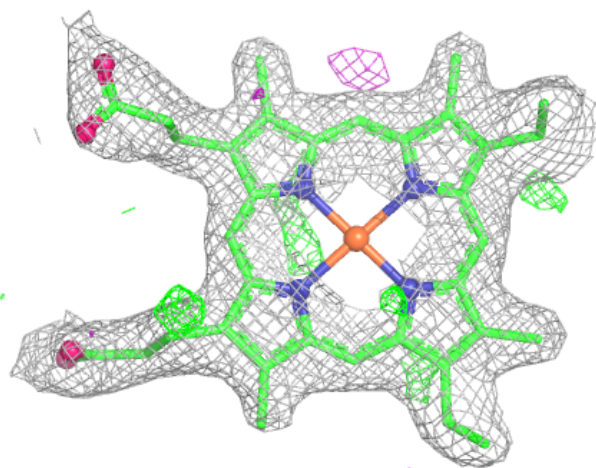
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FLC	A	919	13/13	0.91	0.09	39,40,48,48	0
6	FLC	A	918	13/13	0.92	0.08	39,40,50,50	0
8	GOL	A	922	6/6	0.93	0.15	26,32,42,43	0
3	MG	A	912	1/1	0.96	0.04	23,23,23,23	0
2	HEC	A	901	43/43	0.97	0.09	25,42,54,64	0
2	HEC	A	910	43/43	0.98	0.06	23,32,40,43	0
2	HEC	A	911	43/43	0.98	0.07	18,33,61,69	0
2	HEC	A	907	43/43	0.98	0.07	21,31,39,43	0
5	FE	A	915	1/1	0.98	0.04	53,53,53,53	0
5	FE	A	917	1/1	0.98	0.07	44,44,44,44	0
4	CA	A	913	1/1	0.99	0.02	33,33,33,33	0
2	HEC	A	906	43/43	0.99	0.06	14,22,42,46	0
5	FE	A	916	1/1	0.99	0.10	43,43,43,43	0
2	HEC	A	902	43/43	0.99	0.04	11,21,28,34	0
2	HEC	A	908	43/43	0.99	0.05	15,21,34,39	0
2	HEC	A	909	43/43	0.99	0.05	13,21,27,41	0
2	HEC	A	903	43/43	0.99	0.05	11,17,23,24	0
2	HEC	A	904	43/43	0.99	0.04	8,15,21,24	0
2	HEC	A	905	43/43	0.99	0.04	4,11,18,27	0
3	MG	A	914	1/1	1.00	0.01	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.

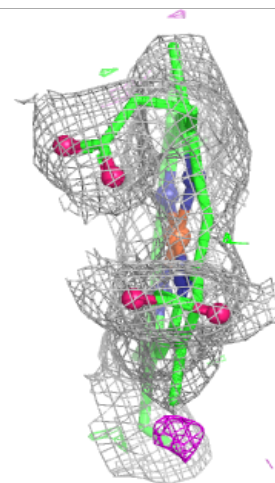
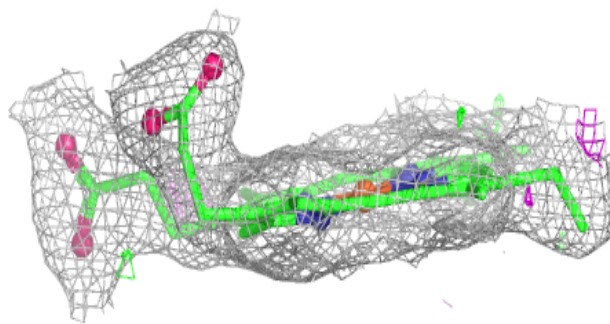
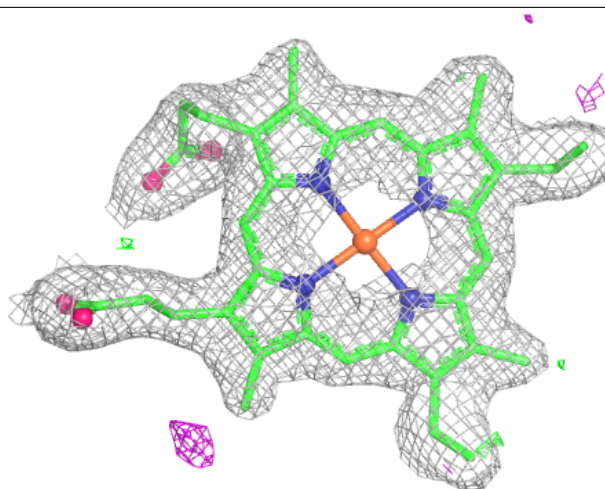
Electron density around HEC A 901:

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



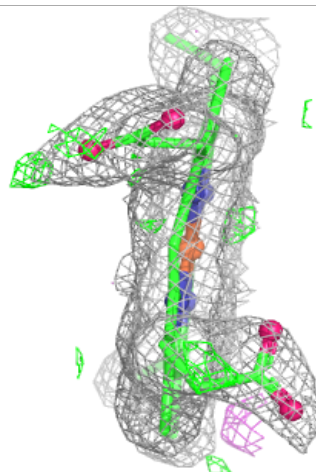
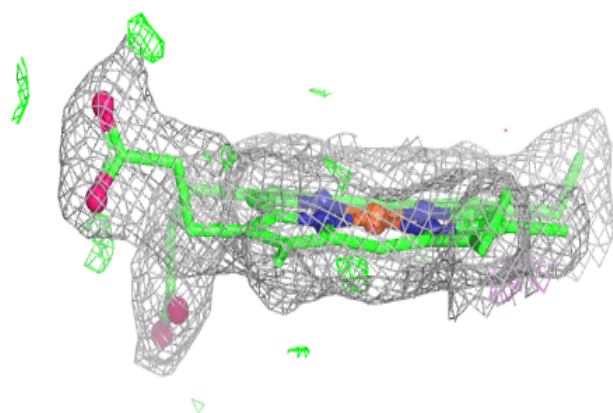
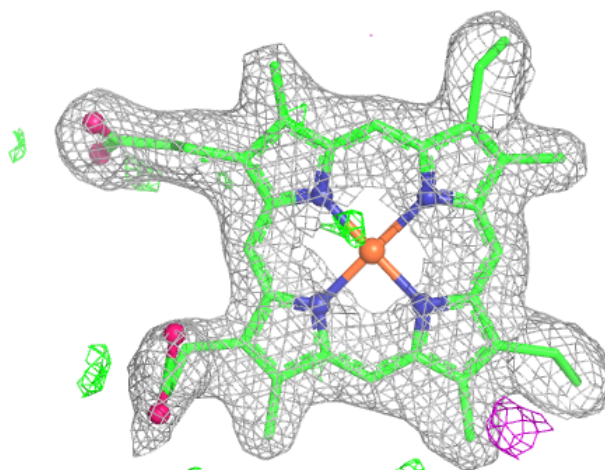
Electron density around HEC A 910:

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



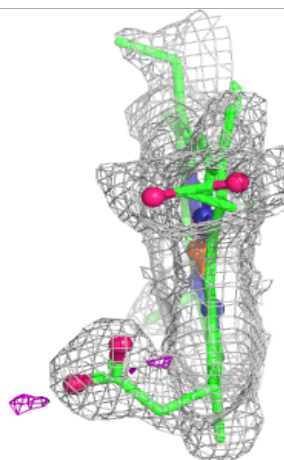
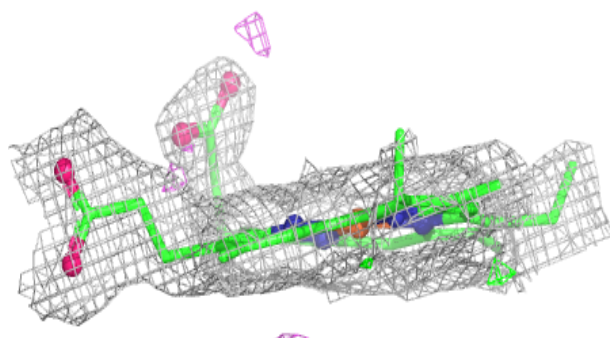
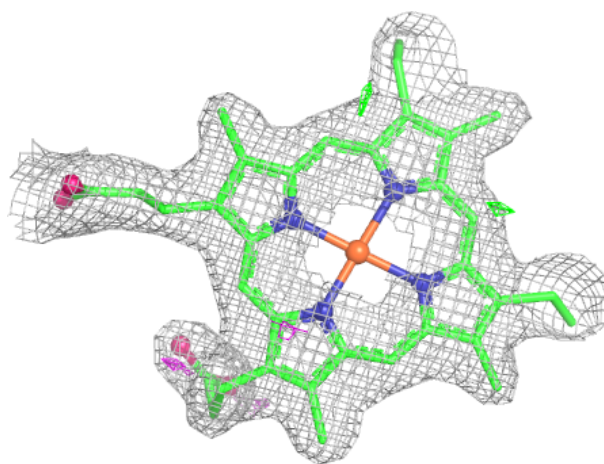
Electron density around HEC A 911:

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and green (positive)



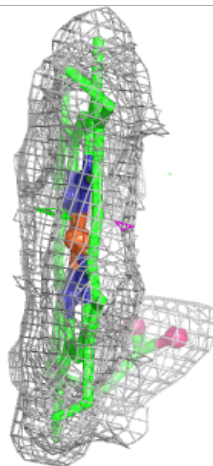
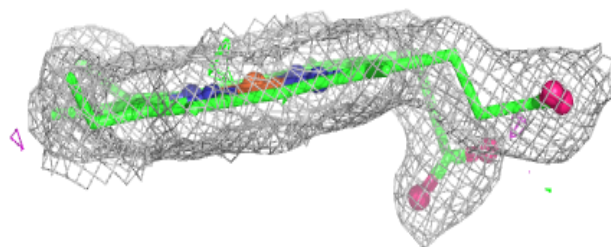
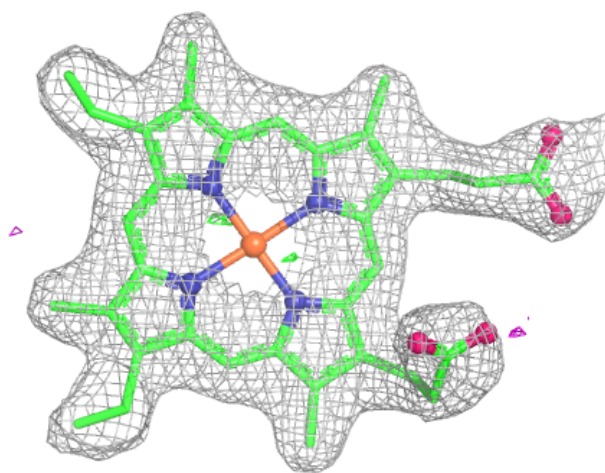
Electron density around HEC A 907:

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



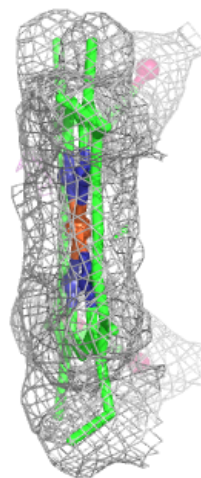
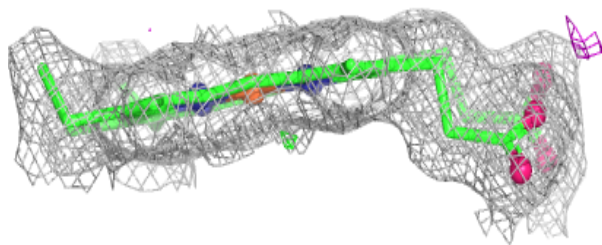
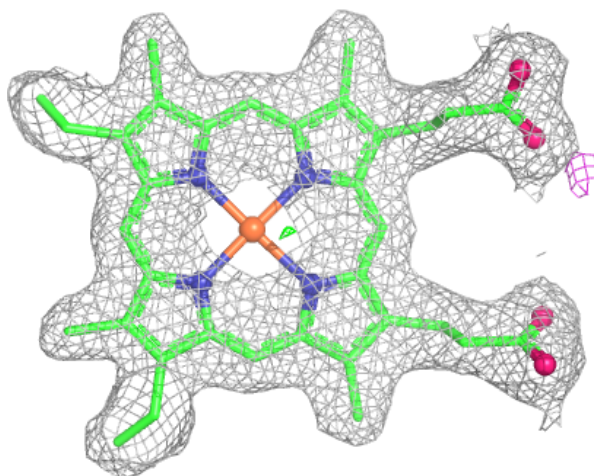
Electron density around HEC A 906:

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



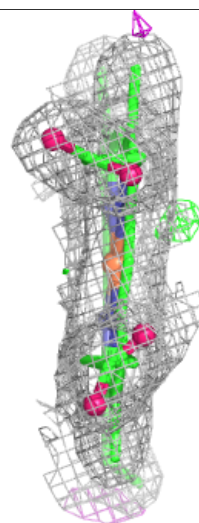
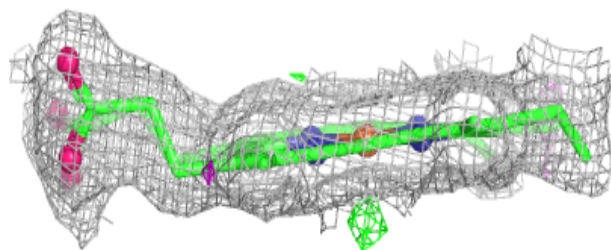
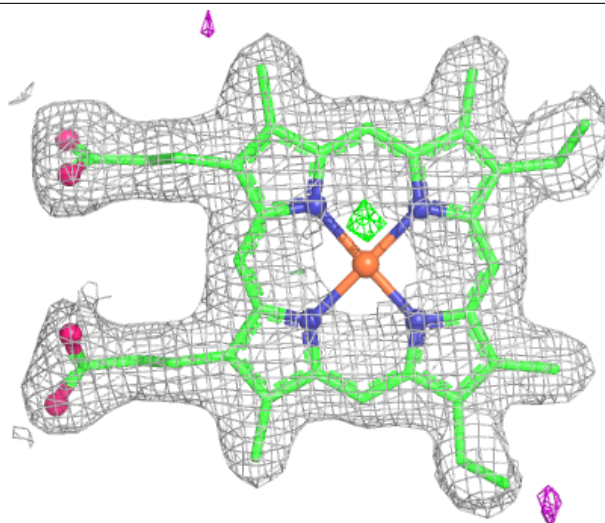
Electron density around HEC A 902:

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and green (positive)



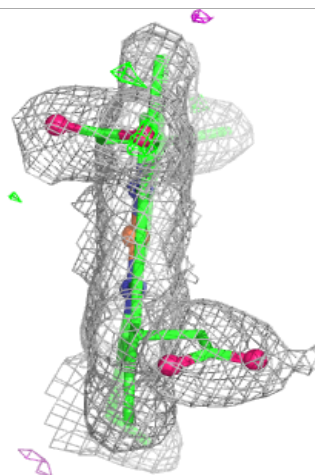
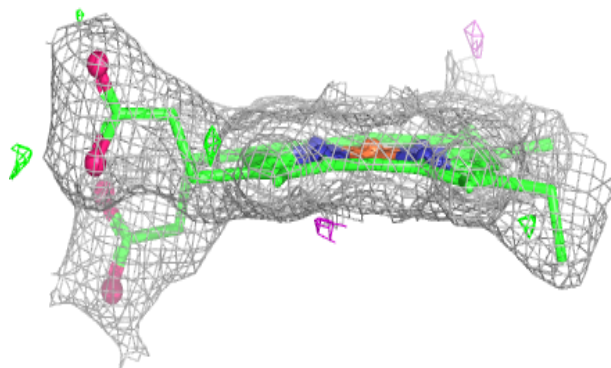
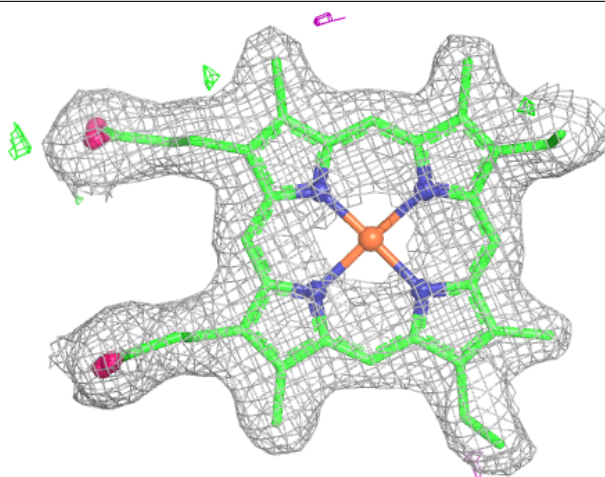
Electron density around HEC A 908:

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



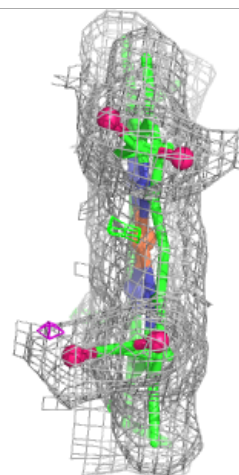
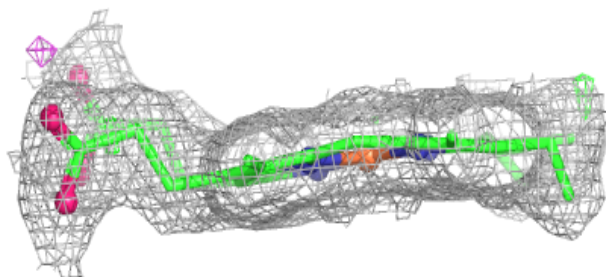
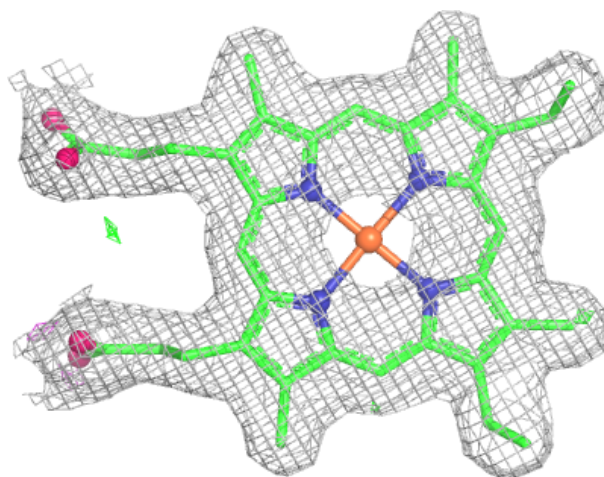
Electron density around HEC A 909:

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and green (positive)



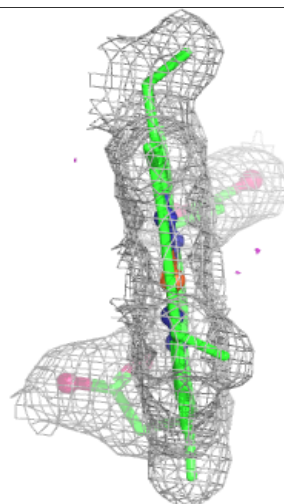
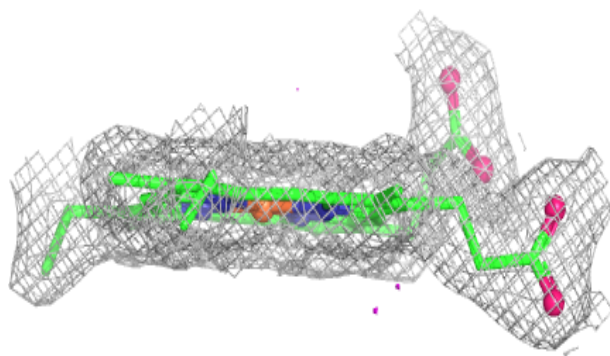
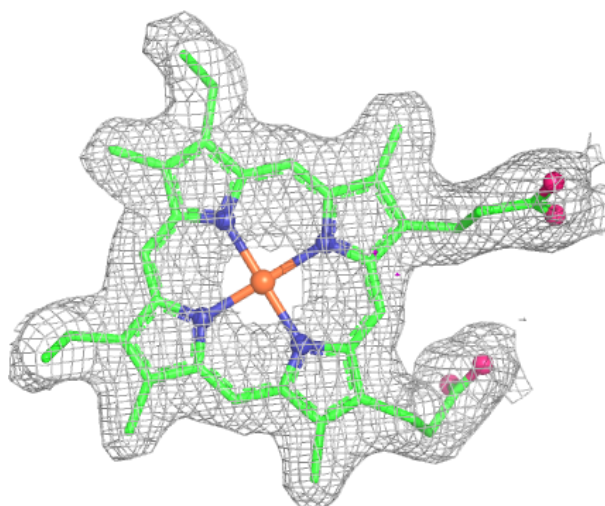
Electron density around HEC A 903:

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and green (positive)



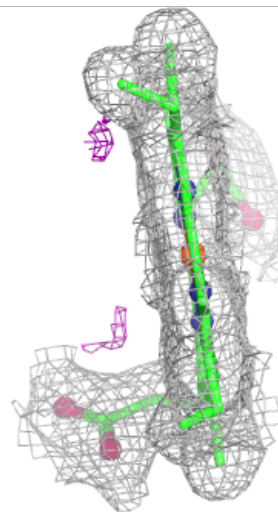
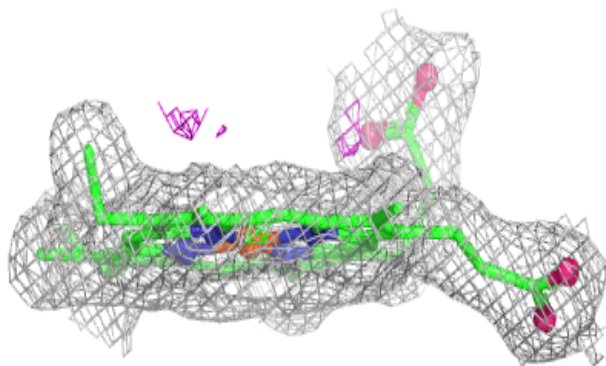
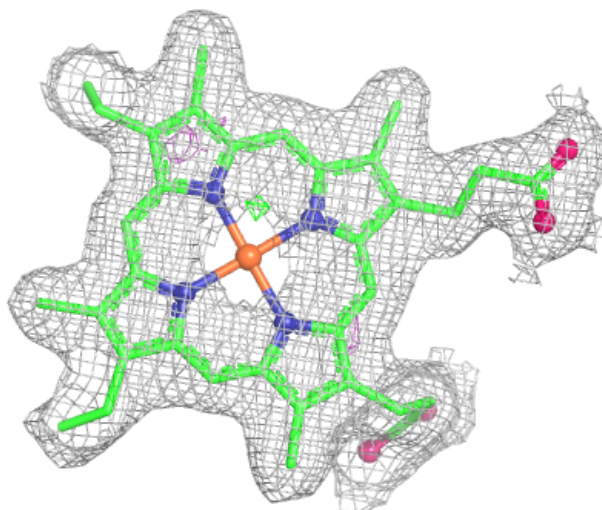
Electron density around HEC A 904:

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



Electron density around HEC A 905:

$2mF_o-DF_c$ (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.