



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:19 AM UTC

PDB ID : 7QTH / pdb_00007qth
Title : Crystal structure of the Shewanella oneidensis MR1 MtrC mutant C453A
Authors : Edwards, M.J.; Clarke, T.A.
Deposited on : 2022-01-14
Resolution : 1.90 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

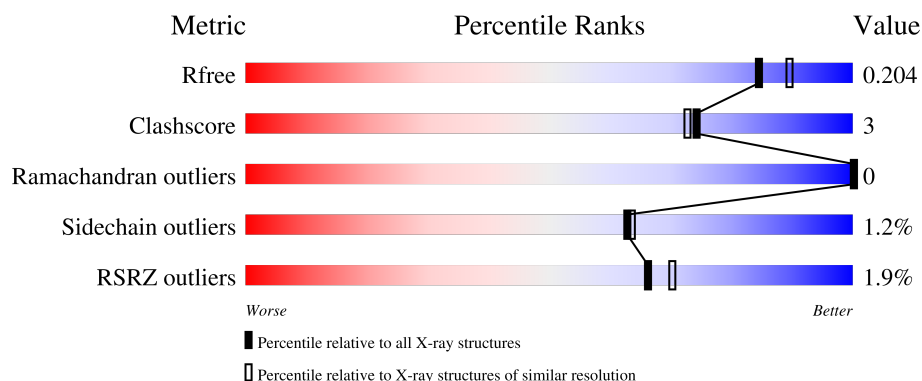
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

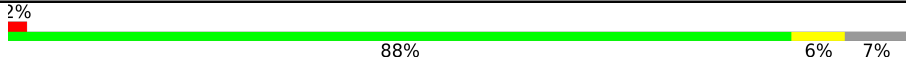
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	671	

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
5	ACT	A	823	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	827	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6167 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.

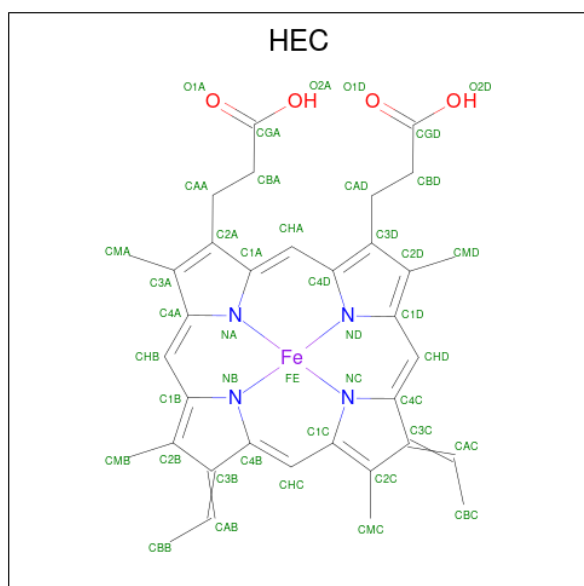
- Molecule 1 is a protein called Extracellular iron oxide respiratory system surface decaheme cytochrome c component MtrC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	627	Total	C	N	O	S	0	13	0
			4787	2961	825	968	33			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	ALA	CYS	engineered mutation	UNP Q8EG34

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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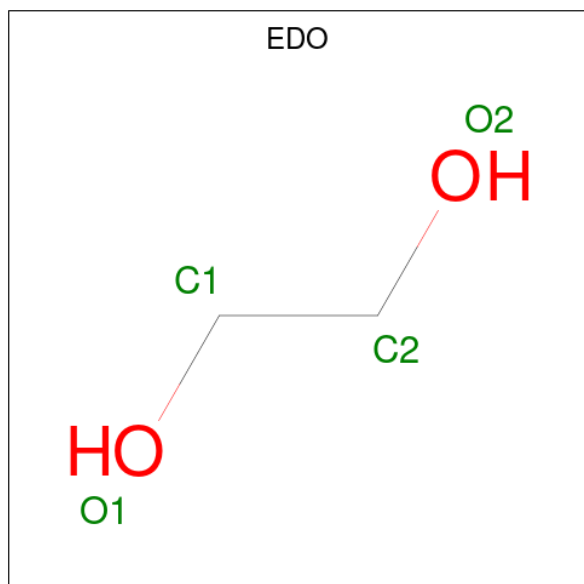
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1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

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

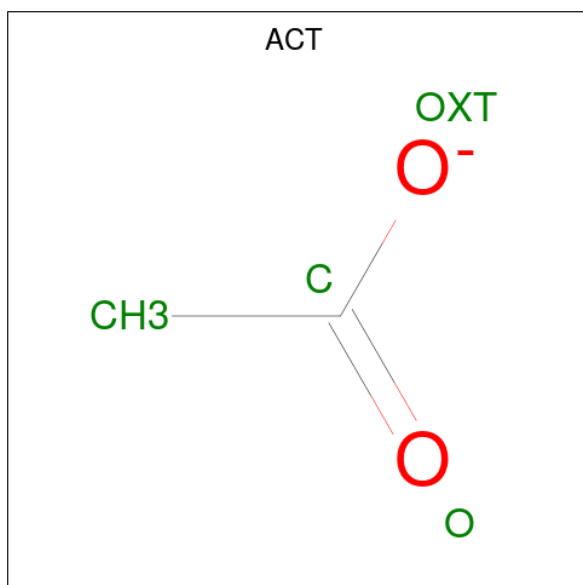
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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

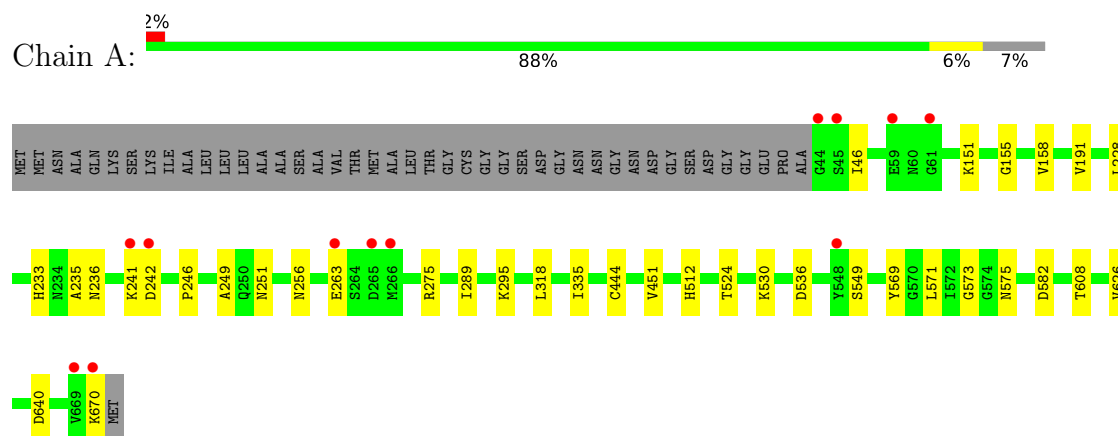
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	838	Total	O	0	0
			838	838		

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: Extracellular iron oxide respiratory system surface decaheme cytochrome c component MtrC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.06Å 89.80Å 154.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.73 – 1.90 77.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (77.73-1.90) 99.4 (77.61-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.151 , 0.196 0.162 , 0.204	Depositor DCC
R_{free} test set	2892 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6167	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 4.83% 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: ACT, HEC, EDO, CA

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	1.12	2/4876 (0.0%)	1.24	3/6623 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	C-O	6.25	1.30	1.24
1	A	575	ASN	C-O	5.48	1.30	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	608	THR	CB-CA-C	5.57	118.59	109.46
1	A	640	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4787	0	4587	26	0
2	A	473	0	330	9	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	48	0	72	2	0
5	A	16	0	12	5	0
6	A	838	0	0	10	0
All	All	6167	0	5001	32	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 3.

All (32) 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:289:ILE:HD11	2:A:805:HEC:HBA1	1.69	0.73
1:A:512:HIS:CE1	2:A:807:HEC:HBC2	2.30	0.67
1:A:530:LYS:HE3	6:A:1429:HOH:O	1.95	0.66
1:A:571:LEU:HD11	2:A:801[B]:HEC:HMD2	1.80	0.62
1:A:582[A]:ASP:OD1	4:A:826:EDO:H12	2.01	0.60
1:A:256:ASN:HB2	6:A:1509:HOH:O	2.01	0.59
1:A:626[A]:VAL:HG11	6:A:958:HOH:O	2.04	0.58
2:A:804:HEC:CHD	5:A:827:ACT:H2	2.34	0.58
1:A:251[B]:ASN:OD1	6:A:901:HOH:O	2.17	0.56
2:A:804:HEC:C1D	5:A:827:ACT:H2	2.36	0.55
1:A:46:ILE:HD11	5:A:823:ACT:H2	1.88	0.55
1:A:569:TYR:CD2	1:A:573:GLY:HA2	2.42	0.55
1:A:275:ARG:HD3	6:A:1633:HOH:O	2.07	0.55
1:A:191:VAL:HG23	1:A:571:LEU:O	2.08	0.54
5:A:823:ACT:H1	6:A:1263:HOH:O	2.08	0.53
2:A:801[B]:HEC:CHA	2:A:801[B]:HEC:HBA1	2.40	0.52
1:A:251[B]:ASN:ND2	6:A:927:HOH:O	2.43	0.51
1:A:569:TYR:CE2	1:A:573:GLY:HA2	2.49	0.48
2:A:801[B]:HEC:HBA1	2:A:801[B]:HEC:HHA	1.96	0.47
2:A:807:HEC:HBA1	6:A:1636:HOH:O	2.14	0.46
1:A:626[A]:VAL:HG22	2:A:810:HEC:HBA2	1.96	0.46
1:A:235:ALA:HA	1:A:246:PRO:HD2	1.98	0.44
1:A:582[A]:ASP:OD1	4:A:826:EDO:H21	2.17	0.44
1:A:251[B]:ASN:CG	6:A:903:HOH:O	2.60	0.44
1:A:524:THR:OG1	6:A:902:HOH:O	2.21	0.44
1:A:318:LEU:C	1:A:318:LEU:HD12	2.43	0.43
1:A:228:LEU:C	1:A:228:LEU:HD23	2.45	0.42
1:A:444:CYS:HB2	1:A:451:VAL:O	2.19	0.42
1:A:151:LYS:HD2	1:A:155:GLY:O	2.20	0.41
1:A:233:HIS:HA	1:A:249:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HD12	1:A:158[B]:VAL:HG12	2.02	0.40
1:A:236:ASN:HD21	5:A:827:ACT:C	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	638/671 (95%)	620 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/541 (97%)	519 (99%)	6 (1%)	65	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LYS
1	A	242	ASP
1	A	263	GLU
1	A	295	LYS

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Mol	Chain	Res	Type
1	A	549	SER
1	A	670	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 5 are monoatomic - leaving 27 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	A	806	1	46,50,50	2.32	21 (45%)	58,82,82	2.44	20 (34%)
2	HEC	A	805	1	46,50,50	2.53	21 (45%)	58,82,82	2.34	21 (36%)
5	ACT	A	825	3	3,3,3	0.79	0	3,3,3	1.02	0
4	EDO	A	830	-	3,3,3	0.32	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	824	-	3,3,3	1.33	0	3,3,3	0.66	0
2	HEC	A	808	1	46,50,50	2.43	23 (50%)	58,82,82	2.39	26 (44%)
4	EDO	A	819	-	3,3,3	0.39	0	2,2,2	0.18	0
4	EDO	A	829[B]	-	3,3,3	0.17	0	2,2,2	0.16	0
4	EDO	A	826	-	3,3,3	0.41	0	2,2,2	0.62	0
2	HEC	A	801[B]	1	46,50,50	2.32	21 (45%)	58,82,82	2.34	21 (36%)
2	HEC	A	803	1	46,50,50	2.45	22 (47%)	58,82,82	2.36	20 (34%)
4	EDO	A	818	-	3,3,3	0.19	0	2,2,2	0.27	0
2	HEC	A	804	1	46,50,50	2.32	19 (41%)	58,82,82	2.62	25 (43%)
2	HEC	A	802	1	46,50,50	2.14	17 (36%)	58,82,82	2.41	24 (41%)
4	EDO	A	829[A]	-	3,3,3	0.09	0	2,2,2	0.15	0
5	ACT	A	823	-	3,3,3	0.98	0	3,3,3	1.00	0
4	EDO	A	816	-	3,3,3	0.04	0	2,2,2	0.28	0
2	HEC	A	809	1	46,50,50	2.37	18 (39%)	58,82,82	2.54	20 (34%)
4	EDO	A	821	-	3,3,3	0.20	0	2,2,2	0.18	0
2	HEC	A	801[A]	1	46,50,50	2.38	22 (47%)	58,82,82	2.24	19 (32%)
2	HEC	A	807	1	46,50,50	2.20	17 (36%)	58,82,82	2.53	17 (29%)
4	EDO	A	817	-	3,3,3	0.10	0	2,2,2	0.01	0
4	EDO	A	820	-	3,3,3	0.23	0	2,2,2	0.12	0
4	EDO	A	828	-	3,3,3	0.21	0	2,2,2	0.42	0
5	ACT	A	827	-	3,3,3	0.69	0	3,3,3	1.03	0
4	EDO	A	822	-	3,3,3	0.22	0	2,2,2	0.19	0
2	HEC	A	810	1	46,50,50	2.44	21 (45%)	58,82,82	2.38	26 (44%)

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	A	806	1	-	6/14/54/54	-
2	HEC	A	805	1	-	5/14/54/54	-
4	EDO	A	830	-	-	1/1/1/1	-
2	HEC	A	808	1	-	8/14/54/54	-
4	EDO	A	819	-	-	1/1/1/1	-
4	EDO	A	829[B]	-	-	1/1/1/1	-
4	EDO	A	826	-	-	1/1/1/1	-
2	HEC	A	801[B]	1	-	8/14/54/54	-
2	HEC	A	803	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	818	-	-	0/1/1/1	-
2	HEC	A	804	1	-	6/14/54/54	-
2	HEC	A	802	1	-	6/14/54/54	-
4	EDO	A	829[A]	-	-	1/1/1/1	-
4	EDO	A	816	-	-	0/1/1/1	-
2	HEC	A	809	1	-	6/14/54/54	-
4	EDO	A	821	-	-	0/1/1/1	-
2	HEC	A	801[A]	1	-	6/14/54/54	-
2	HEC	A	807	1	-	8/14/54/54	-
4	EDO	A	817	-	-	0/1/1/1	-
4	EDO	A	820	-	-	0/1/1/1	-
4	EDO	A	828	-	-	1/1/1/1	-
4	EDO	A	822	-	-	1/1/1/1	-
2	HEC	A	810	1	-	4/14/54/54	-

All (222) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	HEC	CAB-C3B	5.87	1.54	1.35
2	A	805	HEC	CAC-C3C	5.78	1.53	1.35
2	A	809	HEC	CAC-C3C	5.59	1.53	1.35
2	A	803	HEC	CAC-C3C	5.45	1.52	1.35
2	A	808	HEC	CAB-C3B	5.39	1.52	1.35
2	A	804	HEC	C1A-NA	-5.11	1.30	1.39
2	A	809	HEC	CAB-C3B	5.11	1.51	1.35
2	A	806	HEC	CAC-C3C	5.06	1.51	1.35
2	A	802	HEC	CAC-C3C	5.05	1.51	1.35
2	A	807	HEC	CAC-C3C	4.99	1.51	1.35
2	A	810	HEC	C2A-C3A	4.97	1.47	1.36
2	A	810	HEC	C4A-NA	-4.97	1.30	1.39
2	A	808	HEC	C1D-ND	-4.93	1.30	1.39
2	A	801[A]	HEC	CAB-C3B	4.91	1.50	1.35
2	A	808	HEC	CAC-C3C	4.88	1.50	1.35
2	A	801[A]	HEC	CAC-C3C	4.86	1.50	1.35
2	A	810	HEC	CAC-C3C	4.85	1.50	1.35
2	A	807	HEC	CAB-C3B	4.83	1.50	1.35
2	A	810	HEC	CAB-C3B	4.74	1.50	1.35
2	A	805	HEC	CHD-C4C	4.73	1.47	1.38
2	A	810	HEC	C1C-NC	-4.61	1.30	1.39
2	A	801[B]	HEC	CAB-C3B	4.59	1.49	1.35
2	A	803	HEC	CHA-C4D	4.52	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	HEC	C4B-NB	-4.50	1.31	1.39
2	A	801[B]	HEC	CHD-C4C	4.49	1.47	1.38
2	A	801[B]	HEC	CAC-C3C	4.46	1.49	1.35
2	A	805	HEC	CHA-C1A	4.40	1.47	1.38
2	A	810	HEC	CHA-C1A	4.28	1.46	1.38
2	A	802	HEC	CAB-C3B	4.26	1.48	1.35
2	A	808	HEC	C4A-NA	-4.26	1.31	1.39
2	A	806	HEC	CAB-C3B	4.24	1.48	1.35
2	A	807	HEC	C1D-ND	-4.22	1.31	1.39
2	A	805	HEC	C1B-NB	-4.21	1.31	1.39
2	A	804	HEC	CAB-C3B	4.15	1.48	1.35
2	A	808	HEC	C1C-NC	-4.14	1.31	1.39
2	A	803	HEC	C1D-ND	-4.14	1.31	1.39
2	A	809	HEC	C4A-NA	-4.11	1.31	1.39
2	A	804	HEC	C1C-NC	-4.11	1.31	1.39
2	A	804	HEC	CAC-C3C	4.09	1.48	1.35
2	A	803	HEC	C1B-NB	-4.05	1.32	1.39
2	A	806	HEC	CHA-C1A	4.05	1.46	1.38
2	A	805	HEC	CAB-C3B	4.05	1.48	1.35
2	A	804	HEC	C1B-NB	-4.02	1.32	1.39
2	A	809	HEC	C1C-NC	-3.99	1.32	1.39
2	A	806	HEC	C4B-NB	-3.98	1.32	1.39
2	A	801[A]	HEC	CHA-C1A	3.97	1.46	1.38
2	A	801[A]	HEC	CHC-C4B	3.97	1.46	1.38
2	A	803	HEC	C2A-C3A	3.96	1.45	1.36
2	A	803	HEC	CHA-C1A	3.95	1.46	1.38
2	A	805	HEC	C1D-ND	-3.94	1.32	1.39
2	A	801[A]	HEC	C2A-C3A	3.91	1.45	1.36
2	A	801[A]	HEC	CHD-C4C	3.89	1.46	1.38
2	A	805	HEC	C1A-NA	-3.89	1.32	1.39
2	A	801[B]	HEC	CHA-C1A	3.87	1.46	1.38
2	A	806	HEC	C1A-NA	-3.85	1.32	1.39
2	A	802	HEC	C1D-ND	-3.80	1.32	1.39
2	A	809	HEC	CHD-C4C	3.78	1.45	1.38
2	A	804	HEC	C4D-ND	-3.75	1.32	1.39
2	A	806	HEC	C4D-ND	-3.73	1.32	1.39
2	A	801[B]	HEC	CHC-C4B	3.72	1.45	1.38
2	A	801[B]	HEC	C1C-NC	-3.68	1.32	1.39
2	A	801[B]	HEC	C2A-C3A	3.68	1.44	1.36
2	A	809	HEC	CHA-C1A	3.67	1.45	1.38
2	A	804	HEC	C4C-NC	-3.65	1.32	1.39
2	A	809	HEC	CHC-C4B	3.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801[A]	HEC	C1C-NC	-3.62	1.32	1.39
2	A	804	HEC	C2A-C3A	3.62	1.44	1.36
2	A	806	HEC	CHC-C4B	3.62	1.45	1.38
2	A	804	HEC	CHA-C1A	3.61	1.45	1.38
2	A	806	HEC	CHB-C4A	3.60	1.45	1.38
2	A	808	HEC	C1A-NA	-3.58	1.32	1.39
2	A	805	HEC	C4B-NB	-3.58	1.32	1.39
2	A	801[A]	HEC	CHB-C4A	3.56	1.45	1.38
2	A	801[B]	HEC	C4B-NB	-3.55	1.32	1.39
2	A	805	HEC	CHA-C4D	3.54	1.47	1.39
2	A	808	HEC	C4D-ND	-3.54	1.32	1.39
2	A	809	HEC	C1D-ND	-3.53	1.33	1.39
2	A	805	HEC	C2A-C3A	3.51	1.44	1.36
2	A	808	HEC	CHD-C1D	3.51	1.47	1.39
2	A	807	HEC	C4A-NA	-3.50	1.33	1.39
2	A	805	HEC	CHB-C4A	3.48	1.45	1.38
2	A	810	HEC	C4C-NC	-3.47	1.33	1.39
2	A	810	HEC	C4B-NB	-3.40	1.33	1.39
2	A	802	HEC	CHA-C1A	3.39	1.45	1.38
2	A	808	HEC	CHB-C4A	3.39	1.45	1.38
2	A	801[A]	HEC	C4D-ND	-3.38	1.33	1.39
2	A	805	HEC	C3D-C2D	3.38	1.47	1.38
2	A	807	HEC	C1A-NA	-3.33	1.33	1.39
2	A	801[B]	HEC	CHA-C4D	3.28	1.46	1.39
2	A	807	HEC	CHA-C4D	3.25	1.46	1.39
2	A	810	HEC	CHD-C4C	3.24	1.44	1.38
2	A	808	HEC	C4C-NC	-3.24	1.33	1.39
2	A	803	HEC	C1A-C2A	3.22	1.50	1.45
2	A	804	HEC	C1D-ND	-3.21	1.33	1.39
2	A	807	HEC	C4D-ND	-3.21	1.33	1.39
2	A	801[A]	HEC	CHA-C4D	3.20	1.46	1.39
2	A	805	HEC	C1C-NC	-3.20	1.33	1.39
2	A	809	HEC	C4D-ND	-3.18	1.33	1.39
2	A	806	HEC	CHD-C1D	3.17	1.46	1.39
2	A	808	HEC	C2A-C3A	3.16	1.43	1.36
2	A	808	HEC	C1B-NB	-3.15	1.33	1.39
2	A	802	HEC	C1C-NC	-3.15	1.33	1.39
2	A	809	HEC	C4B-NB	-3.14	1.33	1.39
2	A	810	HEC	CHB-C4A	3.14	1.44	1.38
2	A	802	HEC	CHC-C4B	3.13	1.44	1.38
2	A	802	HEC	C1B-NB	-3.12	1.33	1.39
2	A	810	HEC	C1D-ND	-3.11	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	809	HEC	C1B-NB	-3.10	1.33	1.39
2	A	801[B]	HEC	C3D-C2D	3.10	1.47	1.38
2	A	801[A]	HEC	C4B-NB	-3.05	1.33	1.39
2	A	802	HEC	C2A-C3A	3.04	1.43	1.36
2	A	803	HEC	C1C-NC	-3.04	1.33	1.39
2	A	803	HEC	CHC-C4B	3.04	1.44	1.38
2	A	806	HEC	C1B-NB	-3.02	1.33	1.39
2	A	801[A]	HEC	CHB-C1B	3.00	1.46	1.39
2	A	804	HEC	CHB-C4A	2.98	1.44	1.38
2	A	802	HEC	CHA-C4D	2.97	1.46	1.39
2	A	809	HEC	C1A-NA	-2.96	1.34	1.39
2	A	805	HEC	C1D-C2D	2.95	1.50	1.43
2	A	803	HEC	C4A-NA	-2.94	1.34	1.39
2	A	803	HEC	CHB-C4A	2.92	1.44	1.38
2	A	807	HEC	C2A-C3A	2.92	1.43	1.36
2	A	806	HEC	C3D-C2D	2.91	1.46	1.38
2	A	807	HEC	C4C-NC	-2.87	1.34	1.39
2	A	804	HEC	C4A-NA	-2.84	1.34	1.39
2	A	801[B]	HEC	C4D-ND	-2.83	1.34	1.39
2	A	809	HEC	C4C-NC	-2.82	1.34	1.39
2	A	809	HEC	CHB-C1B	2.82	1.45	1.39
2	A	807	HEC	CHD-C4C	2.82	1.43	1.38
2	A	801[A]	HEC	C1B-NB	-2.81	1.34	1.39
2	A	807	HEC	CHB-C1B	2.80	1.45	1.39
2	A	802	HEC	CHB-C4A	2.80	1.43	1.38
2	A	808	HEC	C3B-C4B	2.80	1.50	1.46
2	A	803	HEC	C4D-ND	-2.76	1.34	1.39
2	A	801[B]	HEC	C1B-NB	-2.76	1.34	1.39
2	A	809	HEC	C1D-C2D	2.75	1.49	1.43
2	A	806	HEC	CHA-C4D	2.75	1.45	1.39
2	A	801[B]	HEC	C4A-NA	-2.74	1.34	1.39
2	A	802	HEC	CHB-C1B	2.74	1.45	1.39
2	A	805	HEC	CHC-C1C	2.74	1.45	1.39
2	A	801[B]	HEC	CHB-C4A	2.74	1.43	1.38
2	A	809	HEC	C2A-C3A	2.73	1.42	1.36
2	A	802	HEC	C4D-ND	-2.72	1.34	1.39
2	A	808	HEC	C4B-NB	-2.71	1.34	1.39
2	A	803	HEC	C3D-C2D	2.67	1.45	1.38
2	A	807	HEC	C1B-NB	-2.66	1.34	1.39
2	A	810	HEC	C1A-NA	-2.65	1.34	1.39
2	A	805	HEC	CHC-C4B	2.65	1.43	1.38
2	A	809	HEC	CHB-C4A	2.64	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	806	HEC	C2A-C3A	2.63	1.42	1.36
2	A	803	HEC	C4A-C3A	2.62	1.50	1.45
2	A	806	HEC	C1D-ND	-2.61	1.34	1.39
2	A	805	HEC	CHB-C1B	2.60	1.45	1.39
2	A	801[B]	HEC	C1D-ND	-2.59	1.34	1.39
2	A	810	HEC	O2D-CGD	-2.57	1.22	1.30
2	A	807	HEC	CHC-C4B	2.56	1.43	1.38
2	A	803	HEC	CHD-C4C	2.56	1.43	1.38
2	A	801[A]	HEC	C3D-C2D	2.55	1.45	1.38
2	A	806	HEC	C1B-C2B	2.55	1.49	1.43
2	A	801[A]	HEC	C4A-NA	-2.55	1.34	1.39
2	A	807	HEC	CHB-C4A	2.54	1.43	1.38
2	A	808	HEC	CHD-C4C	2.53	1.43	1.38
2	A	810	HEC	CHC-C4B	2.53	1.43	1.38
2	A	810	HEC	CHC-C1C	2.53	1.45	1.39
2	A	801[B]	HEC	CHD-C1D	2.52	1.45	1.39
2	A	805	HEC	CBD-CGD	2.51	1.56	1.50
2	A	804	HEC	C1A-C2A	2.51	1.49	1.45
2	A	801[A]	HEC	C1A-NA	-2.51	1.34	1.39
2	A	804	HEC	CHC-C4B	2.50	1.43	1.38
2	A	806	HEC	C1C-NC	-2.50	1.34	1.39
2	A	801[A]	HEC	C1D-ND	-2.48	1.34	1.39
2	A	808	HEC	C1C-C2C	2.46	1.48	1.43
2	A	810	HEC	C4D-ND	-2.45	1.35	1.39
2	A	801[B]	HEC	CHB-C1B	2.45	1.44	1.39
2	A	801[A]	HEC	C4C-NC	-2.45	1.35	1.39
2	A	805	HEC	C4A-NA	-2.44	1.35	1.39
2	A	804	HEC	C4B-NB	-2.39	1.35	1.39
2	A	810	HEC	C3D-C2D	2.39	1.45	1.38
2	A	806	HEC	O2D-CGD	-2.37	1.23	1.30
2	A	804	HEC	CHD-C4C	2.37	1.43	1.38
2	A	801[B]	HEC	C1A-NA	-2.37	1.35	1.39
2	A	810	HEC	CHA-C4D	2.36	1.44	1.39
2	A	802	HEC	C1A-NA	-2.35	1.35	1.39
2	A	803	HEC	C1A-NA	-2.34	1.35	1.39
2	A	806	HEC	C4C-NC	-2.33	1.35	1.39
2	A	808	HEC	CHA-C1A	2.33	1.42	1.38
2	A	801[B]	HEC	C4C-NC	-2.33	1.35	1.39
2	A	810	HEC	C1B-NB	-2.32	1.35	1.39
2	A	806	HEC	C4A-NA	-2.31	1.35	1.39
2	A	801[A]	HEC	C1C-C2C	2.30	1.48	1.43
2	A	804	HEC	CHC-C1C	2.27	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	806	HEC	C4A-C3A	2.27	1.49	1.45
2	A	806	HEC	C1D-C2D	2.26	1.48	1.43
2	A	802	HEC	O2D-CGD	-2.22	1.23	1.30
2	A	801[A]	HEC	CHC-C1C	2.22	1.44	1.39
2	A	808	HEC	CHC-C1C	2.22	1.44	1.39
2	A	808	HEC	C1B-C2B	2.20	1.48	1.43
2	A	802	HEC	CHD-C4C	2.20	1.42	1.38
2	A	807	HEC	CHA-C1A	2.20	1.42	1.38
2	A	808	HEC	CMC-C2C	-2.20	1.46	1.50
2	A	808	HEC	CHC-C4B	2.20	1.42	1.38
2	A	807	HEC	C1C-NC	-2.19	1.35	1.39
2	A	809	HEC	O2A-CGA	-2.16	1.23	1.30
2	A	801[A]	HEC	C1B-C2B	2.16	1.48	1.43
2	A	807	HEC	C3D-C2D	2.13	1.44	1.38
2	A	808	HEC	CHA-C4D	2.12	1.44	1.39
2	A	805	HEC	O2A-CGA	-2.12	1.23	1.30
2	A	805	HEC	C4D-ND	-2.12	1.35	1.39
2	A	810	HEC	CMD-C2D	2.12	1.55	1.50
2	A	808	HEC	O2A-CGA	-2.11	1.23	1.30
2	A	803	HEC	C4B-NB	-2.10	1.35	1.39
2	A	803	HEC	CHD-C1D	2.09	1.44	1.39
2	A	802	HEC	C3D-C2D	2.07	1.44	1.38
2	A	801[B]	HEC	O2D-CGD	-2.05	1.24	1.30
2	A	803	HEC	C1C-C2C	2.05	1.47	1.43
2	A	803	HEC	C4C-NC	-2.04	1.35	1.39
2	A	804	HEC	C3D-C2D	2.04	1.44	1.38
2	A	804	HEC	CHB-C1B	2.03	1.44	1.39
2	A	801[B]	HEC	C1D-C2D	2.02	1.47	1.43
2	A	810	HEC	CBD-CGD	2.01	1.55	1.50
2	A	801[A]	HEC	O2A-CGA	-2.01	1.24	1.30
2	A	803	HEC	C1B-C2B	2.01	1.47	1.43

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	HEC	CBB-CAB-C3B	-9.72	108.00	127.43
2	A	805	HEC	CBB-CAB-C3B	-9.41	108.63	127.43
2	A	804	HEC	CBB-CAB-C3B	-8.95	109.54	127.43
2	A	809	HEC	CBB-CAB-C3B	-8.86	109.72	127.43
2	A	807	HEC	CBB-CAB-C3B	-8.24	110.97	127.43
2	A	803	HEC	CBB-CAB-C3B	-7.90	111.65	127.43
2	A	801[A]	HEC	CBB-CAB-C3B	-7.86	111.73	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[B]	HEC	CBB-CAB-C3B	-7.71	112.03	127.43
2	A	809	HEC	C2A-C1A-NA	6.89	116.97	110.32
2	A	807	HEC	CBC-CAC-C3C	-6.86	113.73	127.43
2	A	802	HEC	CBB-CAB-C3B	-6.74	113.96	127.43
2	A	802	HEC	C2A-C1A-NA	6.43	116.52	110.32
2	A	810	HEC	CBC-CAC-C3C	-6.33	114.79	127.43
2	A	807	HEC	C2A-C1A-NA	6.29	116.39	110.32
2	A	808	HEC	CBB-CAB-C3B	-6.13	115.17	127.43
2	A	807	HEC	C3D-C4D-ND	6.13	116.96	110.15
2	A	810	HEC	CBB-CAB-C3B	-6.10	115.25	127.43
2	A	804	HEC	C2A-C1A-NA	5.97	116.09	110.32
2	A	808	HEC	CBC-CAC-C3C	-5.94	115.56	127.43
2	A	804	HEC	CBC-CAC-C3C	-5.72	116.01	127.43
2	A	806	HEC	CBC-CAC-C3C	-5.69	116.06	127.43
2	A	808	HEC	C2A-C1A-NA	5.66	115.79	110.32
2	A	810	HEC	C3D-C4D-ND	5.65	116.42	110.15
2	A	803	HEC	C3D-C4D-ND	5.60	116.37	110.15
2	A	803	HEC	CBC-CAC-C3C	-5.59	116.26	127.43
2	A	809	HEC	CBC-CAC-C3C	-5.39	116.65	127.43
2	A	801[B]	HEC	CBC-CAC-C3C	-5.27	116.90	127.43
2	A	801[B]	HEC	C2A-C1A-NA	5.23	115.37	110.32
2	A	801[A]	HEC	C1D-C2D-C3D	-5.09	100.99	106.82
2	A	804	HEC	C3D-C4D-ND	5.03	115.73	110.15
2	A	801[A]	HEC	C2A-C1A-NA	5.00	115.15	110.32
2	A	806	HEC	CMA-C3A-C4A	5.00	133.53	124.73
2	A	805	HEC	C3D-C4D-ND	4.94	115.63	110.15
2	A	804	HEC	CBD-CAD-C3D	-4.71	99.51	112.53
2	A	802	HEC	CBC-CAC-C3C	-4.54	118.37	127.43
2	A	806	HEC	C3D-C4D-ND	4.51	115.16	110.15
2	A	801[A]	HEC	CBC-CAC-C3C	-4.40	118.64	127.43
2	A	808	HEC	C1A-C2A-C3A	-4.39	101.33	107.11
2	A	809	HEC	C1D-C2D-C3D	-4.38	101.80	106.82
2	A	805	HEC	C2A-C1A-NA	4.34	114.52	110.32
2	A	805	HEC	CBC-CAC-C3C	-4.25	118.94	127.43
2	A	803	HEC	C2A-C1A-NA	4.21	114.39	110.32
2	A	807	HEC	C1A-C2A-C3A	-4.17	101.62	107.11
2	A	810	HEC	C1D-C2D-C3D	-4.16	102.05	106.82
2	A	809	HEC	C2C-C1C-NC	4.14	116.78	110.14
2	A	809	HEC	C1A-C2A-C3A	-4.14	101.66	107.11
2	A	801[B]	HEC	C2B-C1B-NB	4.09	116.70	110.14
2	A	804	HEC	C2C-C1C-NC	4.07	116.67	110.14
2	A	806	HEC	C4A-C3A-C2A	-3.96	101.09	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	HEC	C2A-C1A-NA	3.96	114.14	110.32
2	A	803	HEC	CMD-C2D-C1D	3.94	131.41	125.42
2	A	801[B]	HEC	C2C-C1C-NC	3.93	116.44	110.14
2	A	801[A]	HEC	C2C-C1C-NC	3.92	116.43	110.14
2	A	802	HEC	C3D-C4D-ND	3.89	114.47	110.15
2	A	810	HEC	C2B-C1B-NB	3.88	116.37	110.14
2	A	805	HEC	CMA-C3A-C4A	3.88	131.56	124.73
2	A	802	HEC	C2D-C1D-ND	3.86	116.32	110.14
2	A	810	HEC	C2A-C1A-NA	3.82	114.01	110.32
2	A	810	HEC	C2D-C1D-ND	3.80	116.23	110.14
2	A	801[B]	HEC	C3D-C4D-ND	3.74	114.30	110.15
2	A	802	HEC	C2C-C1C-NC	3.72	116.10	110.14
2	A	807	HEC	C2D-C1D-ND	3.72	116.10	110.14
2	A	802	HEC	C2B-C1B-NB	3.70	116.07	110.14
2	A	801[B]	HEC	C1D-C2D-C3D	-3.66	102.63	106.82
2	A	804	HEC	C3A-C4A-NA	3.65	116.38	109.64
2	A	805	HEC	C4D-C3D-C2D	-3.64	101.23	106.87
2	A	807	HEC	C4D-C3D-C2D	-3.63	101.25	106.87
2	A	809	HEC	C3D-C4D-ND	3.58	114.13	110.15
2	A	804	HEC	C1A-C2A-C3A	-3.56	102.42	107.11
2	A	808	HEC	CAD-CBD-CGD	-3.56	104.22	113.67
2	A	801[A]	HEC	C2D-C1D-ND	3.56	115.85	110.14
2	A	805	HEC	C2B-C1B-NB	3.56	115.84	110.14
2	A	808	HEC	C2D-C1D-ND	3.54	115.81	110.14
2	A	802	HEC	CBA-CAA-C2A	-3.53	102.77	112.53
2	A	802	HEC	C1D-C2D-C3D	-3.52	102.78	106.82
2	A	801[A]	HEC	C1A-C2A-C3A	-3.52	102.47	107.11
2	A	809	HEC	C2B-C1B-NB	3.50	115.75	110.14
2	A	808	HEC	C2B-C1B-NB	3.49	115.74	110.14
2	A	804	HEC	C4A-C3A-C2A	-3.43	101.89	106.97
2	A	801[A]	HEC	C2B-C1B-NB	3.42	115.63	110.14
2	A	803	HEC	C2B-C1B-NB	3.42	115.63	110.14
2	A	807	HEC	C2C-C1C-NC	3.42	115.62	110.14
2	A	801[B]	HEC	C1A-C2A-C3A	-3.41	102.62	107.11
2	A	808	HEC	C3D-C4D-ND	3.41	113.93	110.15
2	A	803	HEC	C1D-C2D-C3D	-3.37	102.96	106.82
2	A	802	HEC	CMB-C2B-C1B	3.37	130.54	125.42
2	A	806	HEC	C2C-C1C-NC	3.35	115.52	110.14
2	A	808	HEC	CAD-C3D-C4D	3.35	131.48	124.94
2	A	804	HEC	C2B-C1B-NB	3.29	115.42	110.14
2	A	809	HEC	CHC-C1C-C2C	-3.28	117.89	127.43
2	A	808	HEC	C1D-C2D-C3D	-3.23	103.11	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	HEC	C3A-C4A-NA	3.22	115.60	109.64
2	A	802	HEC	C1A-C2A-C3A	-3.22	102.87	107.11
2	A	804	HEC	C4D-C3D-C2D	-3.20	101.91	106.87
2	A	809	HEC	CMD-C2D-C3D	3.19	132.40	125.62
2	A	807	HEC	C1D-C2D-C3D	-3.17	103.18	106.82
2	A	803	HEC	C2D-C1D-ND	3.17	115.22	110.14
2	A	807	HEC	CAD-C3D-C4D	3.16	131.10	124.94
2	A	805	HEC	C2C-C1C-NC	3.15	115.20	110.14
2	A	808	HEC	CMD-C2D-C1D	3.15	130.22	125.42
2	A	808	HEC	C3A-C4A-NA	3.14	115.44	109.64
2	A	809	HEC	C2D-C1D-ND	3.14	115.17	110.14
2	A	801[B]	HEC	CHC-C1C-C2C	-3.14	118.32	127.43
2	A	803	HEC	C4D-C3D-C2D	-3.13	102.02	106.87
2	A	803	HEC	CAD-C3D-C4D	3.11	131.02	124.94
2	A	805	HEC	C1A-C2A-C3A	-3.11	103.01	107.11
2	A	803	HEC	C4A-C3A-C2A	-3.10	102.37	106.97
2	A	802	HEC	CMD-C2D-C3D	3.08	132.15	125.62
2	A	810	HEC	C4A-C3A-C2A	-3.07	102.41	106.97
2	A	809	HEC	CAD-CBD-CGD	-3.01	105.67	113.67
2	A	810	HEC	CMD-C2D-C1D	3.00	129.99	125.42
2	A	806	HEC	C1D-C2D-C3D	-2.99	103.40	106.82
2	A	802	HEC	CMC-C2C-C3C	2.97	133.53	126.55
2	A	801[A]	HEC	CMD-C2D-C1D	2.95	129.91	125.42
2	A	801[B]	HEC	O1A-CGA-CBA	-2.94	113.78	123.09
2	A	804	HEC	CHB-C4A-C3A	-2.94	119.38	125.49
2	A	807	HEC	CHC-C1C-C2C	-2.93	118.91	127.43
2	A	810	HEC	C1A-C2A-C3A	-2.90	103.28	107.11
2	A	801[B]	HEC	CMB-C2B-C1B	2.90	129.83	125.42
2	A	808	HEC	CMC-C2C-C1C	2.89	129.82	125.42
2	A	801[B]	HEC	C3A-C4A-NA	2.88	114.97	109.64
2	A	806	HEC	C4D-C3D-C2D	-2.88	102.41	106.87
2	A	804	HEC	CHA-C1A-C2A	-2.85	120.37	124.86
2	A	801[A]	HEC	C3D-C4D-ND	2.84	113.31	110.15
2	A	807	HEC	CHA-C1A-C2A	-2.84	120.38	124.86
2	A	803	HEC	C1A-C2A-C3A	-2.84	103.37	107.11
2	A	801[B]	HEC	C2D-C1D-ND	2.83	114.68	110.14
2	A	810	HEC	C2C-C1C-NC	2.83	114.67	110.14
2	A	808	HEC	C4D-C3D-C2D	-2.81	102.52	106.87
2	A	802	HEC	C3A-C4A-NA	2.79	114.80	109.64
2	A	804	HEC	CHC-C1C-C2C	-2.77	119.39	127.43
2	A	805	HEC	CMD-C2D-C1D	2.75	129.61	125.42
2	A	810	HEC	CBA-CAA-C2A	-2.75	104.92	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[A]	HEC	CHC-C1C-C2C	-2.75	119.44	127.43
2	A	804	HEC	CMD-C2D-C1D	2.74	129.59	125.42
2	A	809	HEC	CHA-C1A-C2A	-2.74	120.55	124.86
2	A	809	HEC	C3A-C4A-NA	2.73	114.69	109.64
2	A	801[A]	HEC	CHD-C1D-C2D	-2.73	119.52	127.43
2	A	805	HEC	CHC-C4B-C3B	-2.72	120.61	125.21
2	A	803	HEC	CMA-C3A-C4A	2.71	129.51	124.73
2	A	804	HEC	O2A-CGA-CBA	2.71	122.56	114.00
2	A	806	HEC	CAD-C3D-C2D	2.70	133.13	127.07
2	A	810	HEC	CHC-C4B-C3B	-2.70	120.65	125.21
2	A	804	HEC	CMC-C2C-C3C	2.69	132.87	126.55
2	A	808	HEC	O1D-CGD-CBD	-2.68	114.61	123.09
2	A	806	HEC	CMC-C2C-C3C	2.67	132.83	126.55
2	A	802	HEC	CBD-CAD-C3D	-2.67	105.15	112.53
2	A	810	HEC	C4B-NB-C1B	-2.67	101.47	105.82
2	A	805	HEC	CBD-CAD-C3D	-2.66	105.19	112.53
2	A	804	HEC	O1A-CGA-CBA	-2.64	114.72	123.09
2	A	810	HEC	CHA-C1A-C2A	-2.64	120.70	124.86
2	A	810	HEC	O1A-CGA-CBA	-2.62	114.79	123.09
2	A	804	HEC	CAD-C3D-C4D	2.61	130.04	124.94
2	A	802	HEC	CHA-C1A-NA	-2.61	121.61	124.45
2	A	806	HEC	CHD-C4C-C3C	-2.60	120.82	125.21
2	A	803	HEC	C2C-C1C-NC	2.60	114.31	110.14
2	A	807	HEC	C2B-C1B-NB	2.60	114.31	110.14
2	A	809	HEC	CHD-C1D-C2D	-2.59	119.91	127.43
2	A	801[B]	HEC	CHA-C1A-C2A	-2.59	120.78	124.86
2	A	805	HEC	CAD-C3D-C4D	2.58	129.98	124.94
2	A	808	HEC	CHB-C1B-C2B	-2.58	119.93	127.43
2	A	802	HEC	CHC-C4B-C3B	-2.58	120.86	125.21
2	A	801[A]	HEC	CHD-C4C-C3C	-2.58	120.87	125.21
2	A	804	HEC	CHC-C4B-C3B	-2.57	120.88	125.21
2	A	801[B]	HEC	CHB-C1B-C2B	-2.55	120.02	127.43
2	A	802	HEC	C4D-C3D-C2D	-2.54	102.94	106.87
2	A	807	HEC	CHD-C1D-C2D	-2.54	120.06	127.43
2	A	806	HEC	C2B-C1B-NB	2.53	114.20	110.14
2	A	805	HEC	CHB-C1B-C2B	-2.53	120.08	127.43
2	A	806	HEC	CBA-CAA-C2A	-2.50	105.63	112.53
2	A	801[A]	HEC	CHA-C1A-C2A	-2.49	120.93	124.86
2	A	804	HEC	CMA-C3A-C4A	2.48	129.09	124.73
2	A	806	HEC	CHA-C4D-C3D	-2.48	119.88	125.30
2	A	801[A]	HEC	CMB-C2B-C1B	2.46	129.16	125.42
2	A	805	HEC	C1D-C2D-C3D	-2.45	104.01	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	808	HEC	C2C-C1C-NC	2.45	114.07	110.14
2	A	802	HEC	CHD-C1D-C2D	-2.43	120.36	127.43
2	A	806	HEC	O1D-CGD-CBD	-2.43	115.39	123.09
2	A	807	HEC	CHC-C4B-C3B	-2.42	121.13	125.21
2	A	803	HEC	CHB-C1B-C2B	-2.42	120.41	127.43
2	A	808	HEC	CHC-C1C-C2C	-2.41	120.43	127.43
2	A	808	HEC	CHD-C1D-C2D	-2.37	120.53	127.43
2	A	810	HEC	C4D-C3D-C2D	-2.36	103.22	106.87
2	A	810	HEC	CBD-CAD-C3D	-2.35	106.03	112.53
2	A	802	HEC	C4A-NA-C1A	-2.35	101.98	105.82
2	A	801[A]	HEC	C3A-C4A-NA	2.35	113.98	109.64
2	A	806	HEC	C3A-C4A-NA	2.34	113.97	109.64
2	A	801[B]	HEC	C4A-C3A-C2A	-2.33	103.52	106.97
2	A	810	HEC	CHA-C4D-C3D	-2.32	120.23	125.30
2	A	809	HEC	CHD-C4C-NC	-2.32	121.93	124.45
2	A	804	HEC	CHB-C1B-C2B	-2.31	120.72	127.43
2	A	808	HEC	CHB-C4A-C3A	-2.30	120.69	125.49
2	A	810	HEC	C4D-ND-C1D	-2.30	102.07	105.82
2	A	801[B]	HEC	C4D-C3D-C2D	-2.29	103.33	106.87
2	A	801[B]	HEC	CHD-C1D-C2D	-2.29	120.79	127.43
2	A	801[B]	HEC	CHB-C4A-C3A	-2.28	120.74	125.49
2	A	803	HEC	CAA-CBA-CGA	-2.28	107.61	113.67
2	A	801[A]	HEC	CHB-C1B-C2B	-2.27	120.83	127.43
2	A	802	HEC	C4A-C3A-C2A	-2.24	103.64	106.97
2	A	810	HEC	CHC-C1C-C2C	-2.23	120.96	127.43
2	A	804	HEC	C1D-C2D-C3D	-2.22	104.27	106.82
2	A	809	HEC	CMC-C2C-C3C	2.22	131.77	126.55
2	A	805	HEC	C4A-C3A-C2A	-2.22	103.68	106.97
2	A	806	HEC	CHC-C4B-C3B	-2.21	121.49	125.21
2	A	810	HEC	C3A-C4A-NA	2.20	113.71	109.64
2	A	808	HEC	O2D-CGD-CBD	2.20	120.94	114.00
2	A	808	HEC	CHA-C1A-C2A	-2.19	121.41	124.86
2	A	802	HEC	O2A-CGA-CBA	2.19	120.91	114.00
2	A	810	HEC	CHD-C1D-C2D	-2.18	121.09	127.43
2	A	805	HEC	C2D-C1D-ND	2.17	113.62	110.14
2	A	804	HEC	CAA-C2A-C1A	2.15	129.23	124.85
2	A	802	HEC	CHB-C1B-C2B	-2.15	121.19	127.43
2	A	805	HEC	CMC-C2C-C1C	2.14	128.68	125.42
2	A	808	HEC	CHC-C4B-NB	-2.13	122.13	124.45
2	A	809	HEC	CMB-C2B-C1B	2.12	128.65	125.42
2	A	805	HEC	C3A-C4A-NA	2.11	113.55	109.64
2	A	803	HEC	CHD-C1D-C2D	-2.11	121.29	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	810	HEC	CHC-C4B-NB	-2.10	122.16	124.45
2	A	808	HEC	CAA-C2A-C1A	2.10	129.12	124.85
2	A	801[B]	HEC	CBA-CAA-C2A	-2.10	106.73	112.53
2	A	802	HEC	CHB-C4A-C3A	-2.10	121.12	125.49
2	A	806	HEC	O2D-CGD-CBD	2.09	120.60	114.00
2	A	804	HEC	CMB-C2B-C1B	2.09	128.60	125.42
2	A	805	HEC	CHC-C1C-C2C	-2.08	121.40	127.43
2	A	805	HEC	CHC-C4B-NB	2.07	126.71	124.45
2	A	810	HEC	CAD-CBD-CGD	-2.07	108.19	113.67
2	A	808	HEC	CHA-C4D-C3D	-2.06	120.79	125.30
2	A	806	HEC	C2D-C1D-ND	2.05	113.44	110.14
2	A	809	HEC	C4A-C3A-C2A	-2.05	103.93	106.97
2	A	808	HEC	CMA-C3A-C4A	2.05	128.33	124.73
2	A	809	HEC	CAA-C2A-C1A	2.04	129.01	124.85
2	A	801[B]	HEC	CBD-CAD-C3D	-2.04	106.89	112.53
2	A	803	HEC	CHA-C4D-C3D	-2.04	120.84	125.30
2	A	807	HEC	C4D-ND-C1D	-2.04	102.50	105.82
2	A	810	HEC	CHB-C1B-C2B	-2.04	121.52	127.43
2	A	803	HEC	CMC-C2C-C3C	2.03	131.32	126.55
2	A	807	HEC	C3A-C4A-NA	2.02	113.37	109.64
2	A	801[A]	HEC	C4A-C3A-C2A	-2.01	104.00	106.97
2	A	801[A]	HEC	CMA-C3A-C4A	2.00	128.25	124.73

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801[A]	HEC	C2B-C3B-CAB-CBB
2	A	801[A]	HEC	C4B-C3B-CAB-CBB
2	A	801[A]	HEC	C2C-C3C-CAC-CBC
2	A	801[A]	HEC	C4C-C3C-CAC-CBC
2	A	801[B]	HEC	C2B-C3B-CAB-CBB
2	A	801[B]	HEC	C4B-C3B-CAB-CBB
2	A	801[B]	HEC	C2C-C3C-CAC-CBC
2	A	801[B]	HEC	C4C-C3C-CAC-CBC
2	A	802	HEC	C2B-C3B-CAB-CBB
2	A	802	HEC	C4B-C3B-CAB-CBB
2	A	802	HEC	C2C-C3C-CAC-CBC
2	A	802	HEC	C4C-C3C-CAC-CBC
2	A	803	HEC	C2B-C3B-CAB-CBB
2	A	803	HEC	C4B-C3B-CAB-CBB
2	A	803	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	A	803	HEC	C4C-C3C-CAC-CBC
2	A	804	HEC	C2B-C3B-CAB-CBB
2	A	804	HEC	C4B-C3B-CAB-CBB
2	A	804	HEC	C2C-C3C-CAC-CBC
2	A	804	HEC	C4C-C3C-CAC-CBC
2	A	805	HEC	C2B-C3B-CAB-CBB
2	A	805	HEC	C4B-C3B-CAB-CBB
2	A	805	HEC	C2C-C3C-CAC-CBC
2	A	805	HEC	C4C-C3C-CAC-CBC
2	A	806	HEC	C2B-C3B-CAB-CBB
2	A	806	HEC	C2C-C3C-CAC-CBC
2	A	806	HEC	C4C-C3C-CAC-CBC
2	A	807	HEC	C2B-C3B-CAB-CBB
2	A	807	HEC	C4B-C3B-CAB-CBB
2	A	807	HEC	C2C-C3C-CAC-CBC
2	A	807	HEC	C4C-C3C-CAC-CBC
2	A	808	HEC	C2B-C3B-CAB-CBB
2	A	808	HEC	C4B-C3B-CAB-CBB
2	A	808	HEC	C2C-C3C-CAC-CBC
2	A	808	HEC	C4C-C3C-CAC-CBC
2	A	809	HEC	C2B-C3B-CAB-CBB
2	A	809	HEC	C4B-C3B-CAB-CBB
2	A	809	HEC	C2C-C3C-CAC-CBC
2	A	809	HEC	C4C-C3C-CAC-CBC
2	A	810	HEC	C2B-C3B-CAB-CBB
2	A	810	HEC	C4B-C3B-CAB-CBB
2	A	810	HEC	C2C-C3C-CAC-CBC
2	A	810	HEC	C4C-C3C-CAC-CBC
4	A	819	EDO	O1-C1-C2-O2
4	A	829[B]	EDO	O1-C1-C2-O2
4	A	829[A]	EDO	O1-C1-C2-O2
4	A	830	EDO	O1-C1-C2-O2
4	A	826	EDO	O1-C1-C2-O2
2	A	806	HEC	C4B-C3B-CAB-CBB
2	A	801[B]	HEC	C3A-C2A-CAA-CBA
4	A	828	EDO	O1-C1-C2-O2
2	A	802	HEC	CAD-CBD-CGD-O2D
2	A	801[B]	HEC	CAA-CBA-CGA-O1A
2	A	801[A]	HEC	CAA-CBA-CGA-O2A
2	A	807	HEC	CAA-CBA-CGA-O2A
2	A	801[A]	HEC	CAA-CBA-CGA-O1A
2	A	807	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	802	HEC	CAD-CBD-CGD-O1D
2	A	801[B]	HEC	CAA-CBA-CGA-O2A
2	A	801[B]	HEC	C1A-C2A-CAA-CBA
2	A	808	HEC	CAA-CBA-CGA-O2A
2	A	809	HEC	CAD-CBD-CGD-O2D
2	A	807	HEC	CAD-CBD-CGD-O2D
2	A	807	HEC	CAD-CBD-CGD-O1D
4	A	822	EDO	O1-C1-C2-O2
2	A	809	HEC	CAD-CBD-CGD-O1D
2	A	806	HEC	CAD-CBD-CGD-O1D
2	A	808	HEC	CAA-CBA-CGA-O1A
2	A	808	HEC	CAD-CBD-CGD-O2D
2	A	804	HEC	CAD-CBD-CGD-O1D
2	A	804	HEC	CAD-CBD-CGD-O2D
2	A	806	HEC	CAD-CBD-CGD-O2D
2	A	808	HEC	CAD-CBD-CGD-O1D
2	A	805	HEC	CAD-CBD-CGD-O2D

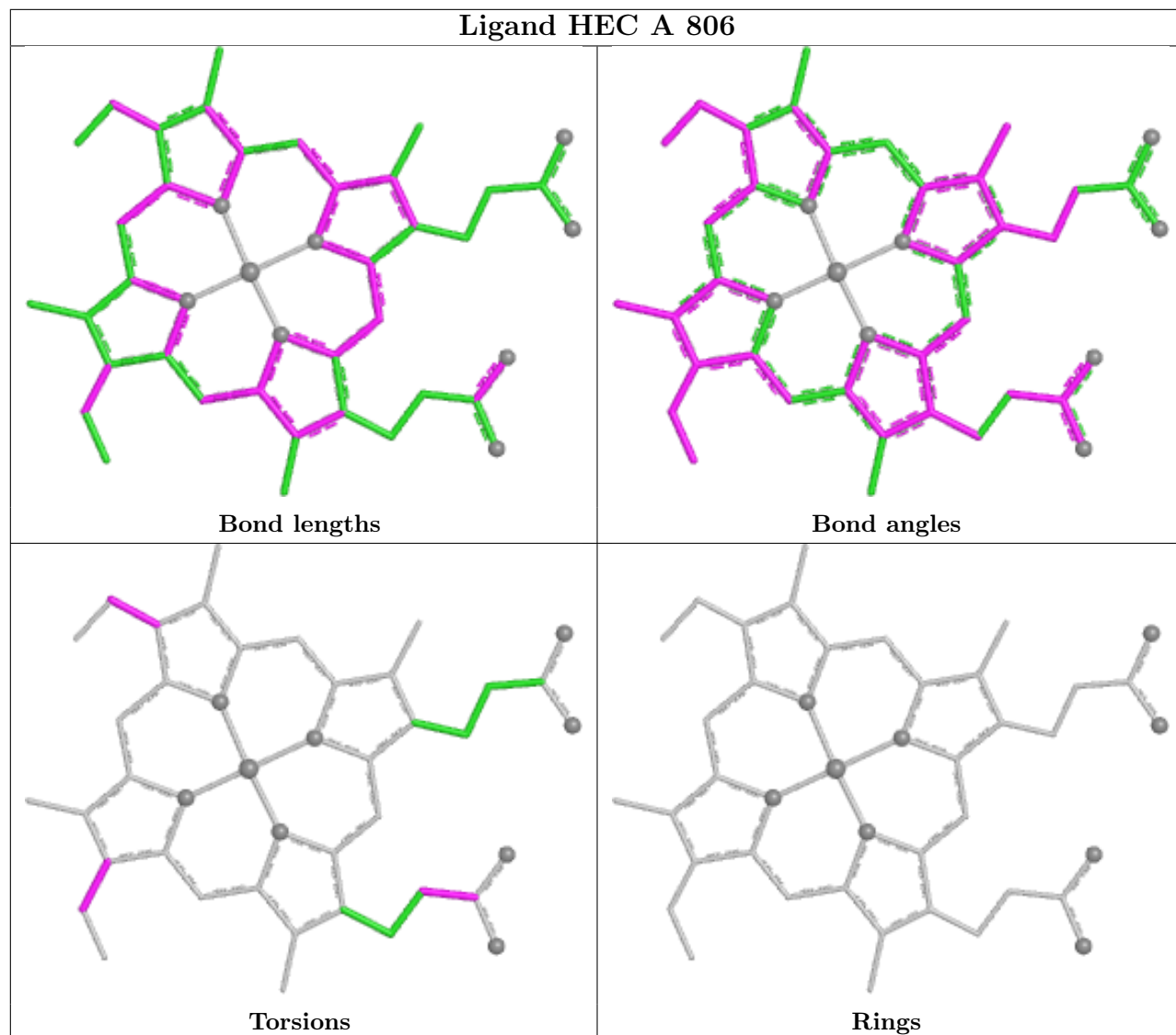
There are no ring outliers.

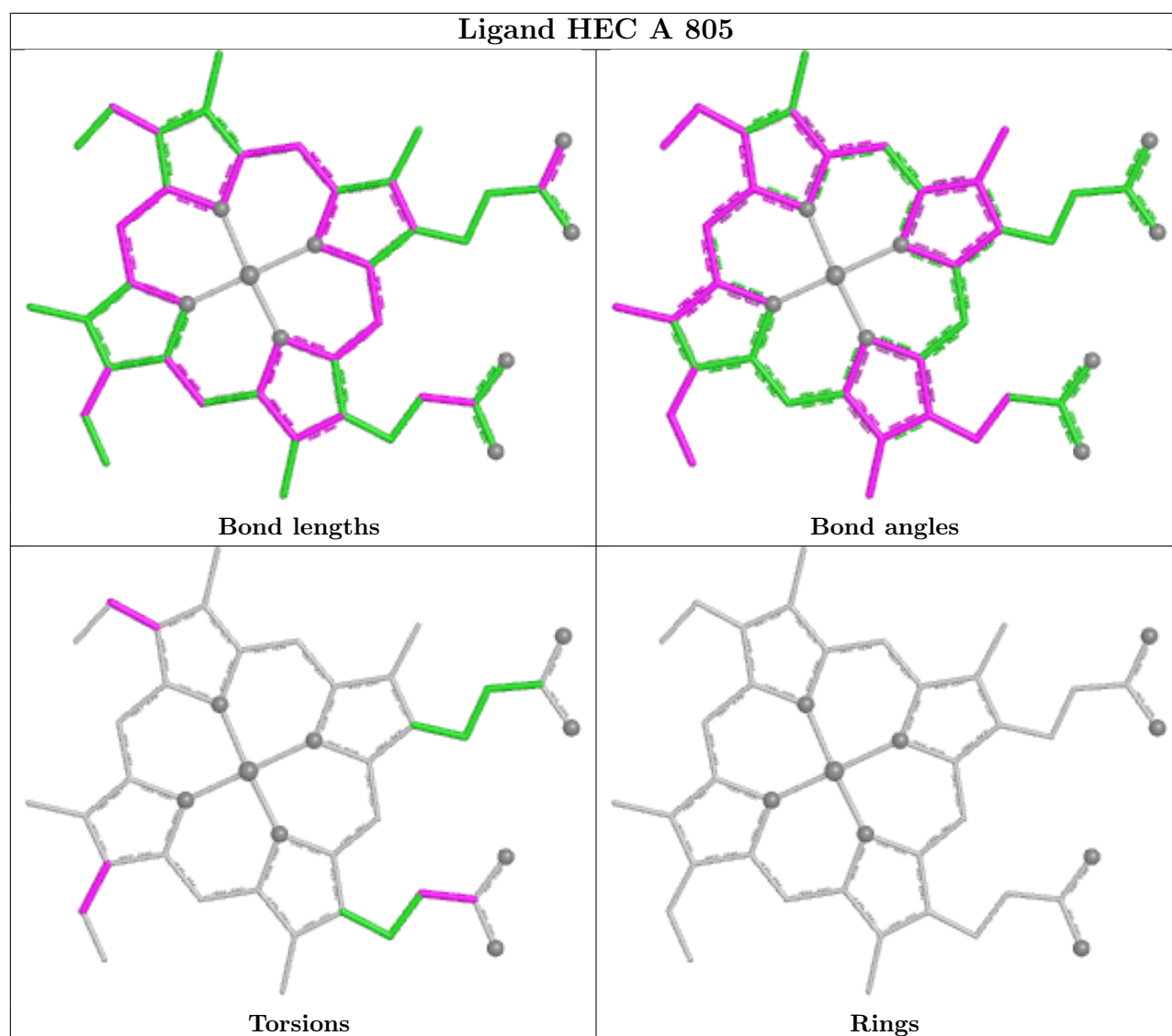
8 monomers are involved in 14 short contacts:

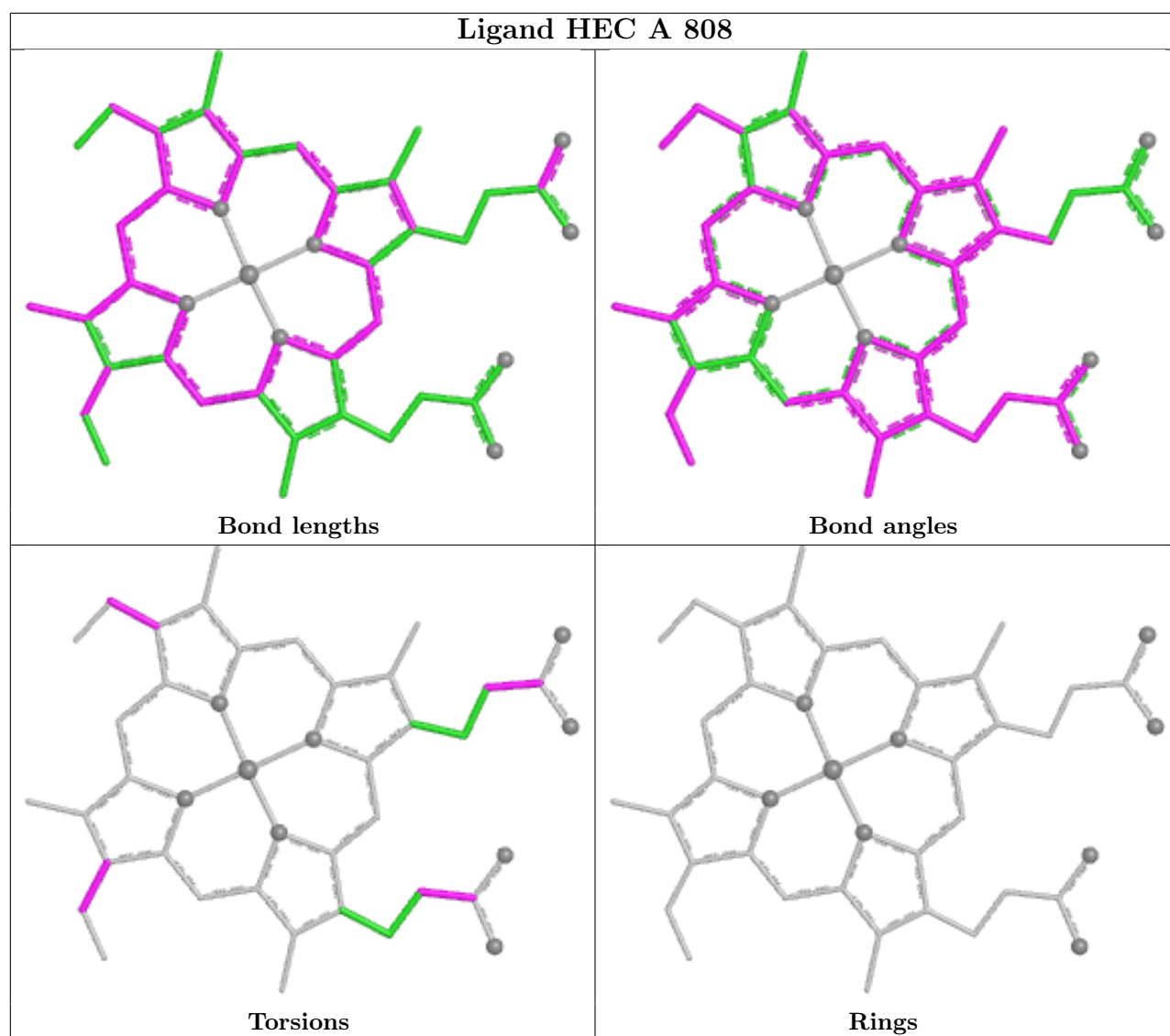
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	805	HEC	1	0
4	A	826	EDO	2	0
2	A	801[B]	HEC	3	0
2	A	804	HEC	2	0
5	A	823	ACT	2	0
2	A	807	HEC	2	0
5	A	827	ACT	3	0
2	A	810	HEC	1	0

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

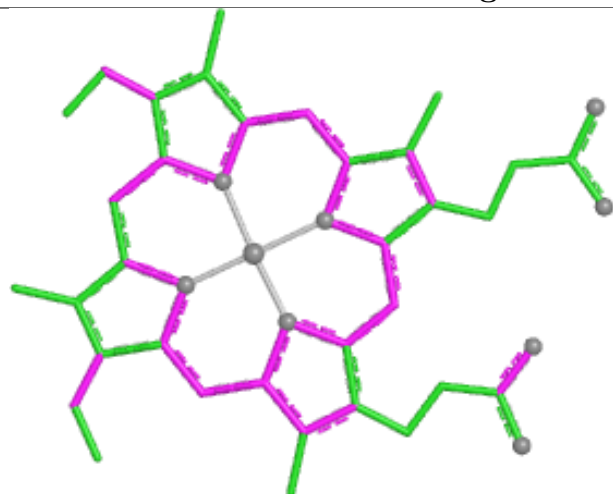
equivalents in the CSD to analyse the geometry.



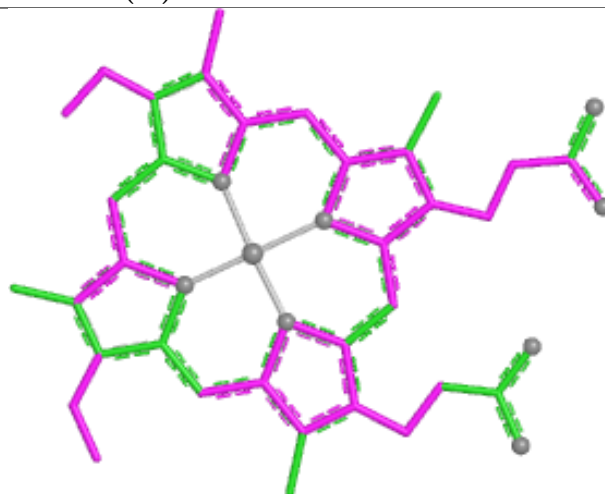




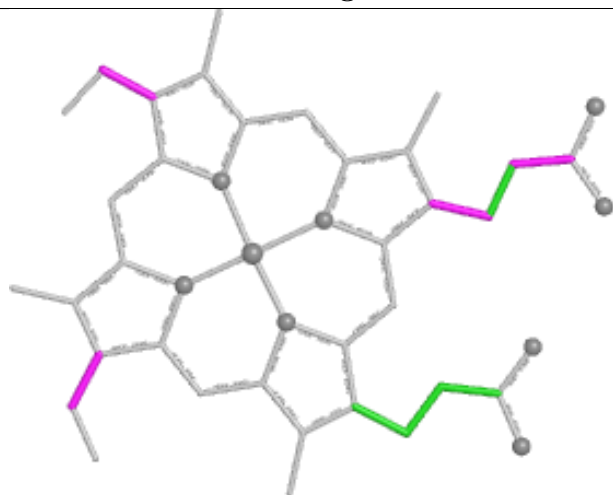
Ligand HEC A 801 (B)



Bond lengths



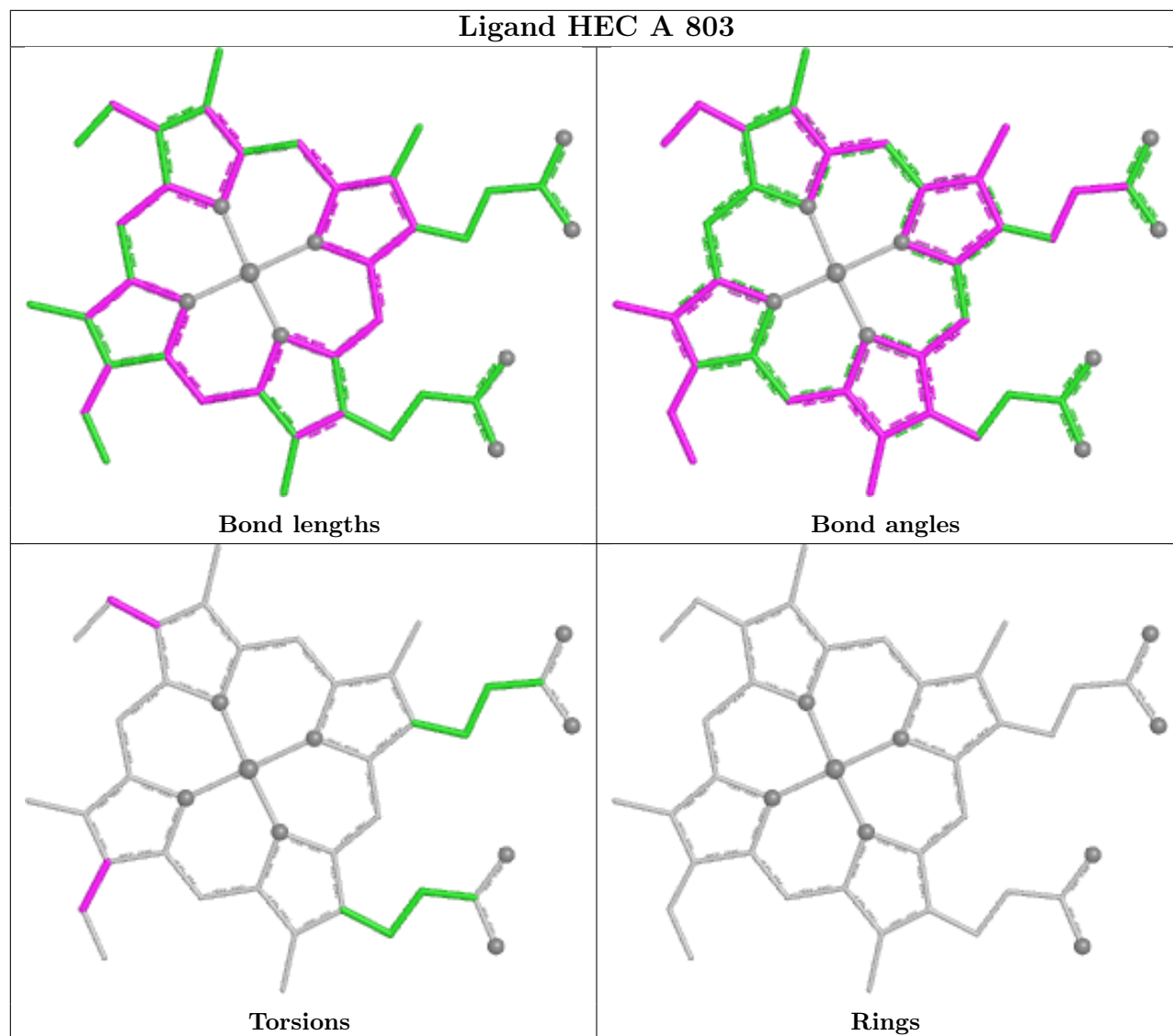
Bond angles

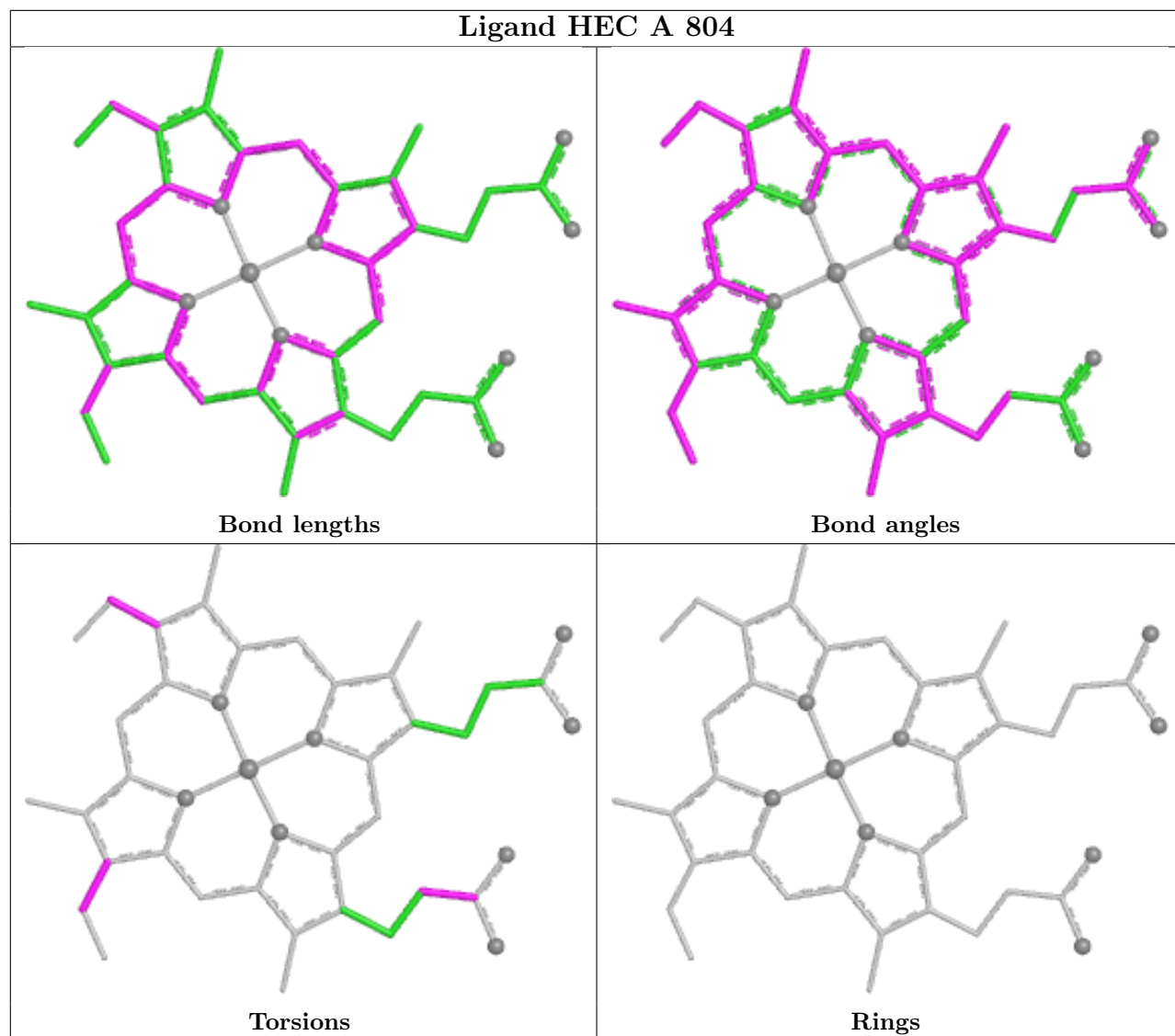


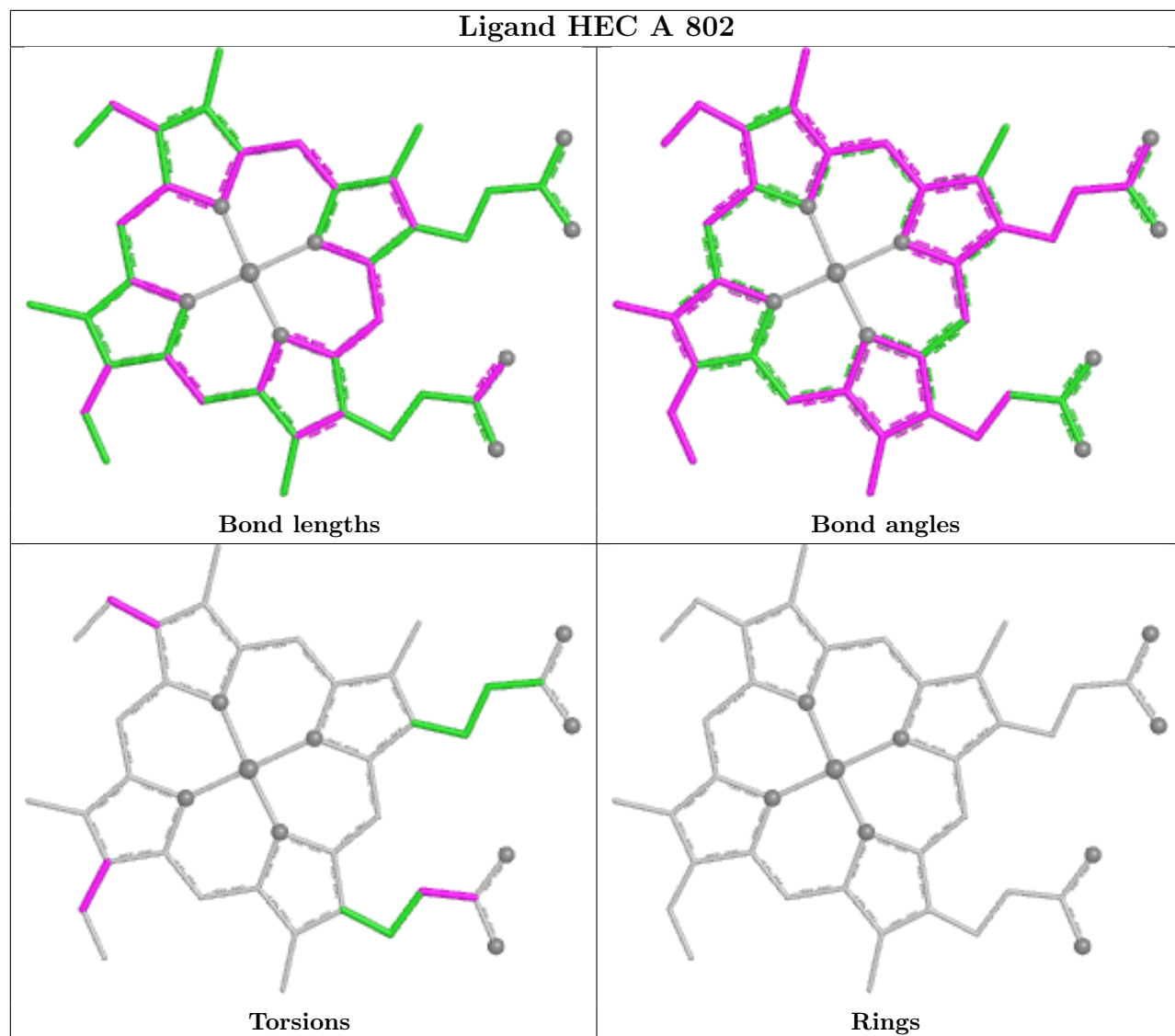
Torsions



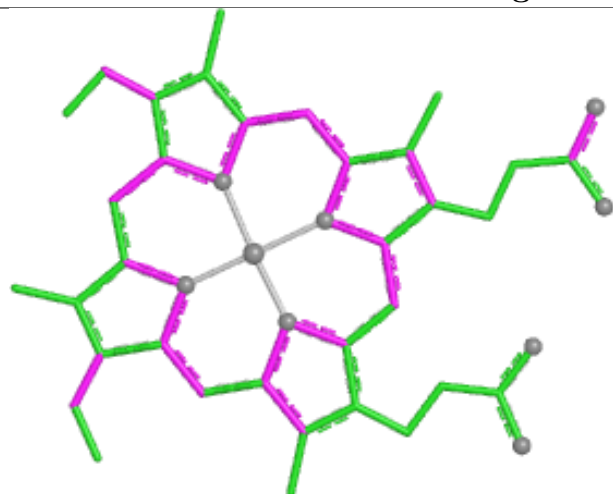
Rings



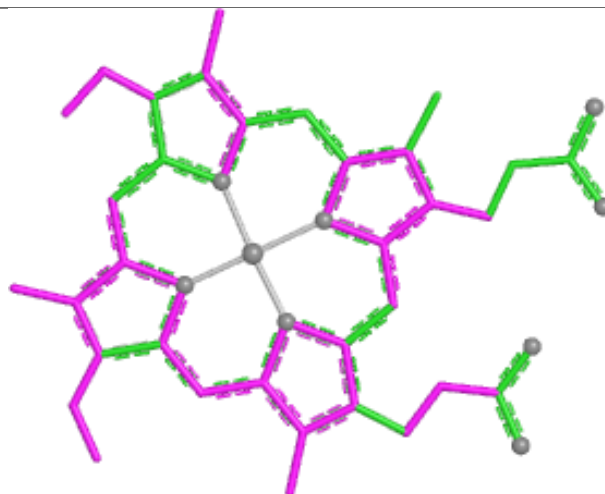




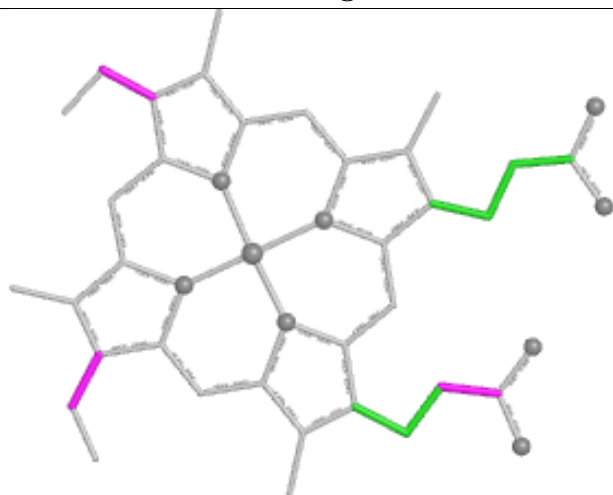
Ligand HEC A 809



Bond lengths



Bond angles

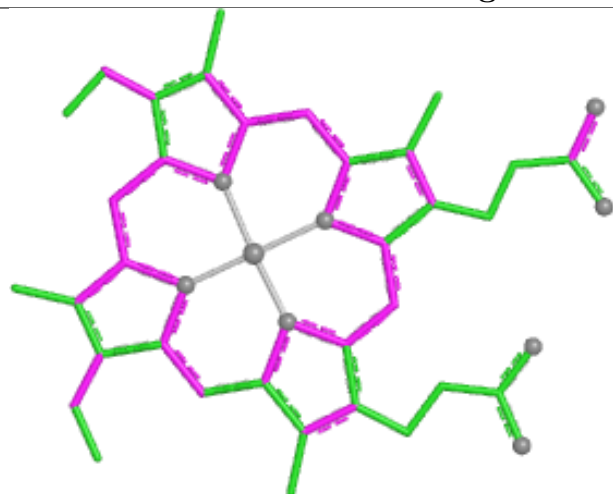


Torsions

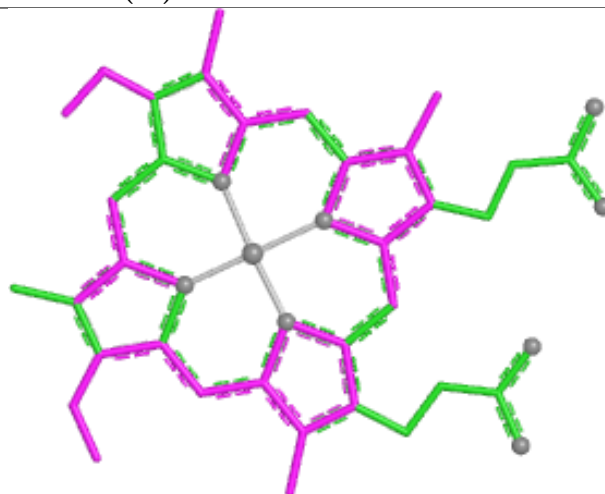


Rings

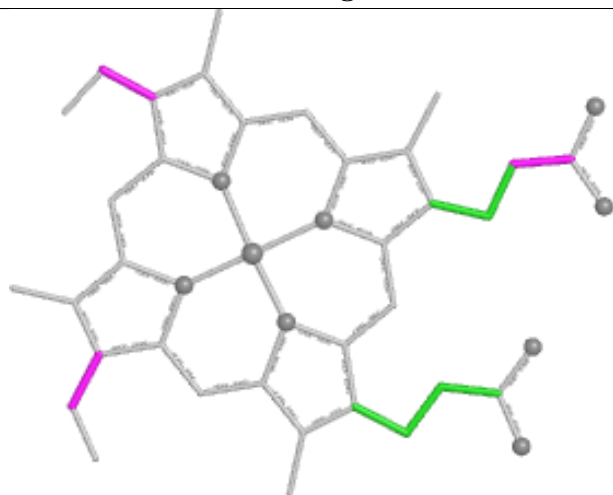
Ligand HEC A 801 (A)



Bond lengths



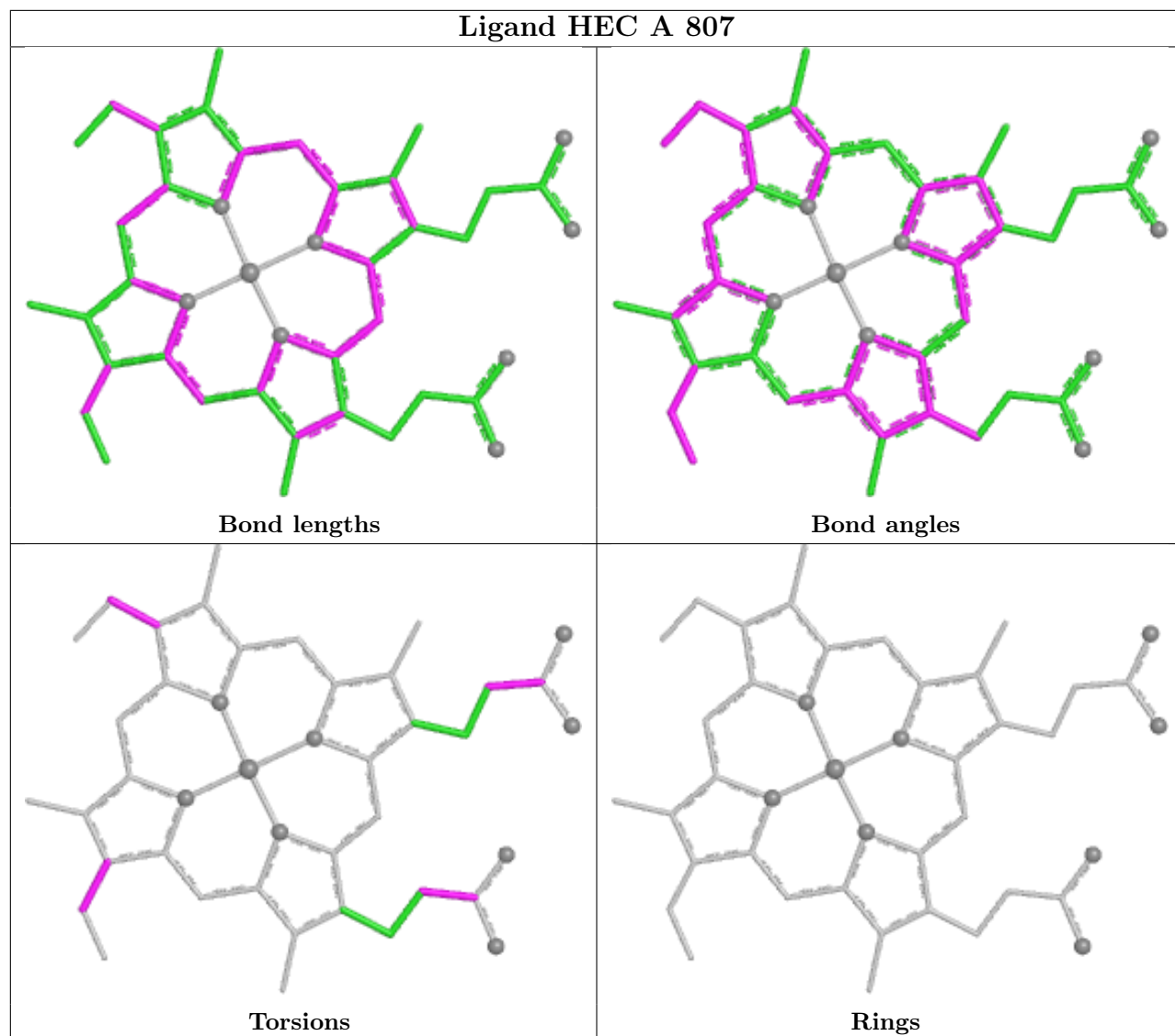
Bond angles

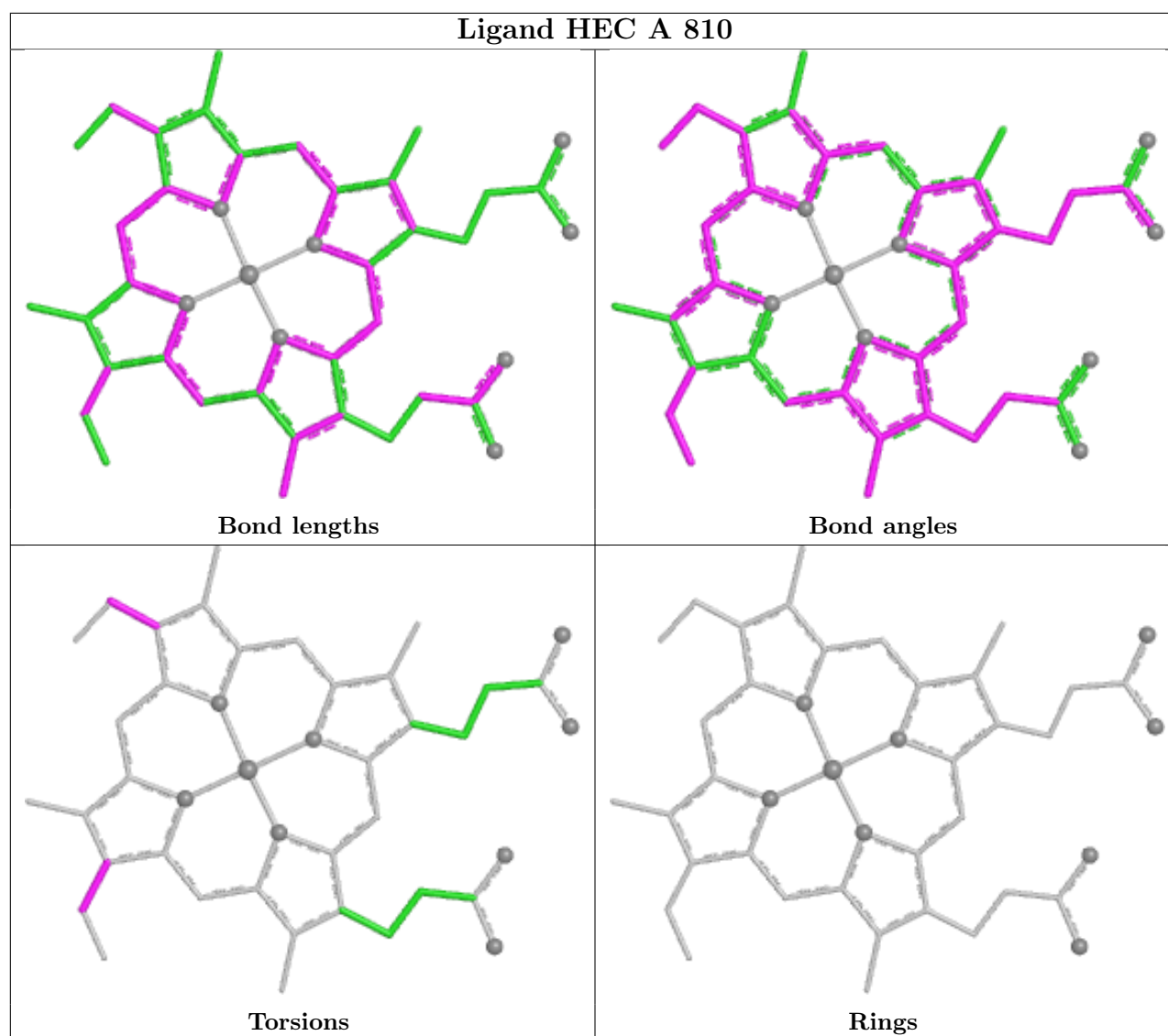


Torsions



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	627/671 (93%)	-0.29	12 (1%) 66 70	5, 16, 31, 57	13 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	4.5
1	A	242	ASP	3.2
1	A	670	LYS	3.1
1	A	61	GLY	2.6
1	A	265	ASP	2.6
1	A	263	GLU	2.5
1	A	266	MET	2.5
1	A	59	GLU	2.4
1	A	45	SER	2.4
1	A	669	VAL	2.1
1	A	241	LYS	2.1
1	A	548	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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,

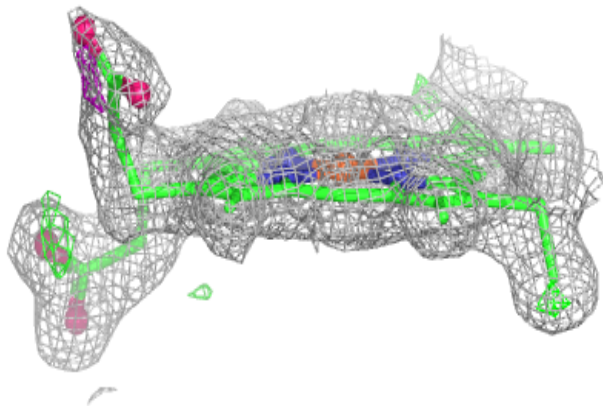
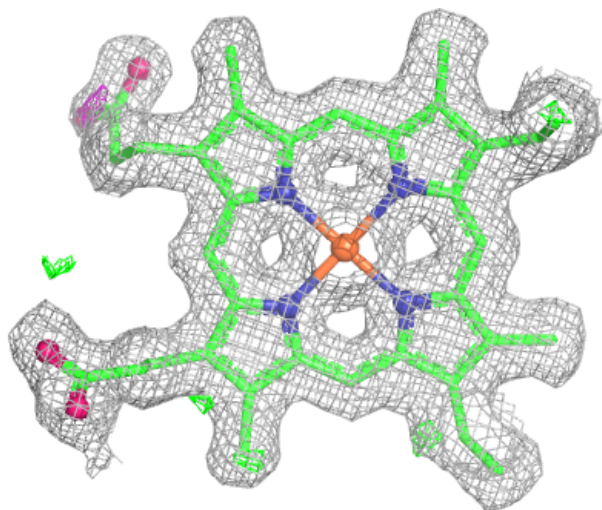
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	824	4/4	0.70	0.20	44,47,47,50	0
5	ACT	A	823	4/4	0.82	0.16	50,51,55,58	0
5	ACT	A	827	4/4	0.85	0.15	32,36,39,40	0
4	EDO	A	826	4/4	0.86	0.17	26,32,37,39	0
4	EDO	A	830	4/4	0.87	0.12	27,29,33,39	0
4	EDO	A	822	4/4	0.89	0.14	35,38,41,41	0
4	EDO	A	816	4/4	0.89	0.11	25,28,29,32	0
4	EDO	A	829[A]	4/4	0.89	0.19	44,49,50,51	4
4	EDO	A	829[B]	4/4	0.89	0.19	15,17,18,19	4
4	EDO	A	818	4/4	0.91	0.09	29,29,29,30	0
4	EDO	A	819	4/4	0.91	0.11	29,31,33,34	0
5	ACT	A	825	4/4	0.91	0.13	33,34,35,36	0
4	EDO	A	828	4/4	0.91	0.11	19,19,21,27	0
4	EDO	A	820	4/4	0.93	0.09	26,29,29,32	0
4	EDO	A	821	4/4	0.94	0.08	27,30,32,33	0
4	EDO	A	817	4/4	0.95	0.08	19,19,24,25	0
2	HEC	A	804	43/43	0.98	0.06	10,12,25,40	0
2	HEC	A	805	43/43	0.98	0.07	13,15,33,36	0
2	HEC	A	806	43/43	0.98	0.06	10,12,24,46	0
2	HEC	A	809	43/43	0.98	0.06	9,10,21,33	0
3	CA	A	815	1/1	0.98	0.10	31,31,31,31	0
2	HEC	A	801[A]	43/43	0.98	0.05	10,11,14,19	43
2	HEC	A	801[B]	43/43	0.98	0.05	9,10,11,12	43
2	HEC	A	803	43/43	0.99	0.04	8,9,10,11	0
2	HEC	A	810	43/43	0.99	0.05	10,11,16,20	0
3	CA	A	812	1/1	0.99	0.03	9,9,9,9	1
3	CA	A	814	1/1	0.99	0.05	10,10,10,10	1
2	HEC	A	802	43/43	0.99	0.05	9,11,15,19	0
2	HEC	A	807	43/43	0.99	0.05	11,12,22,36	0
2	HEC	A	808	43/43	0.99	0.04	8,10,12,12	0
3	CA	A	811	1/1	1.00	0.03	10,10,10,10	0
3	CA	A	813	1/1	1.00	0.03	15,15,15,15	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.

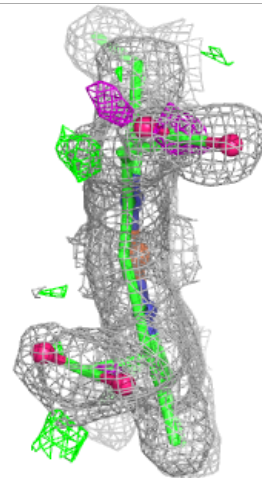
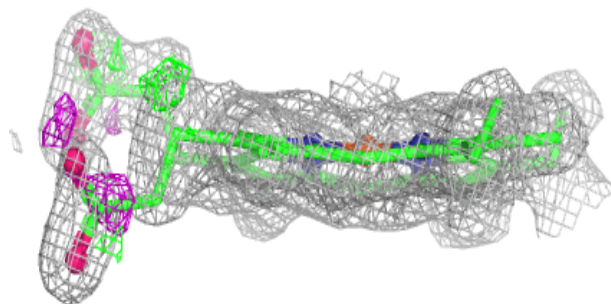
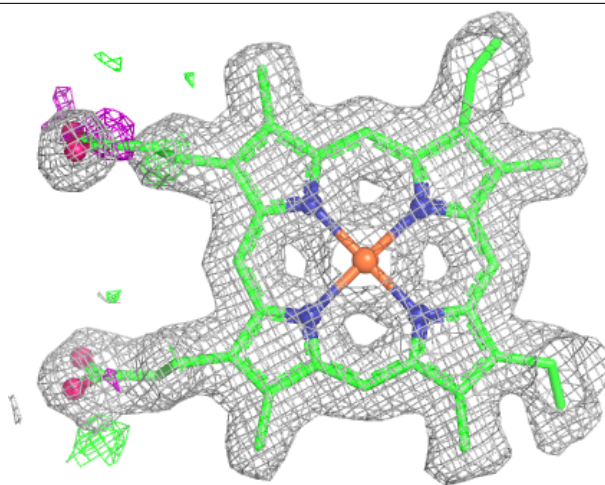
Electron density around HEC A 804:

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



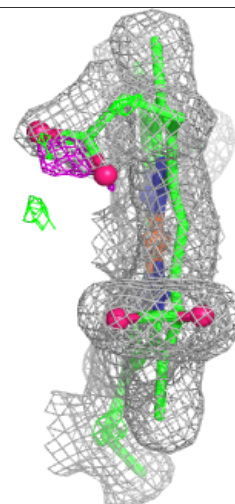
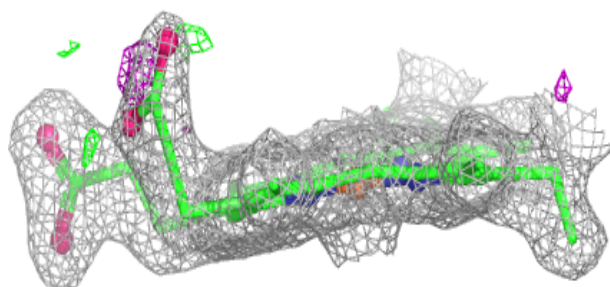
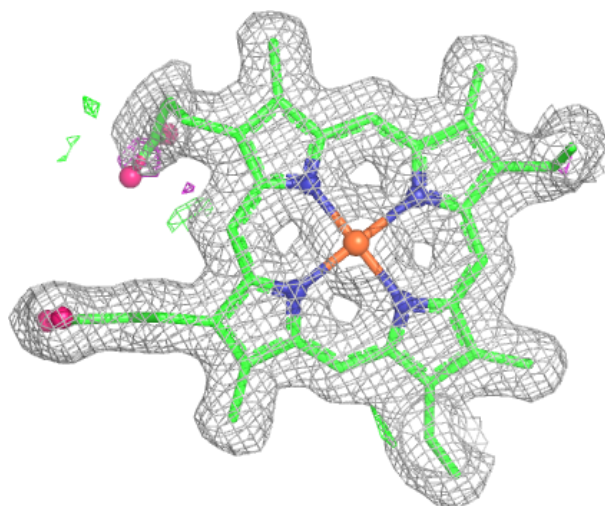
Electron density around HEC A 805:

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



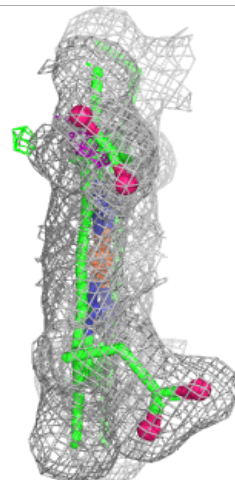
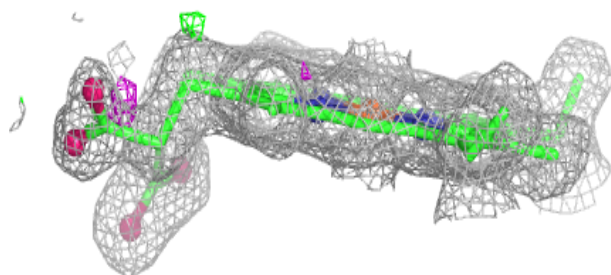
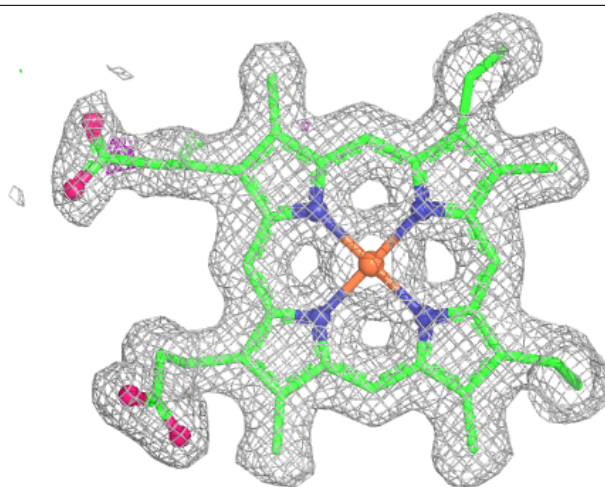
Electron density around HEC A 806:

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



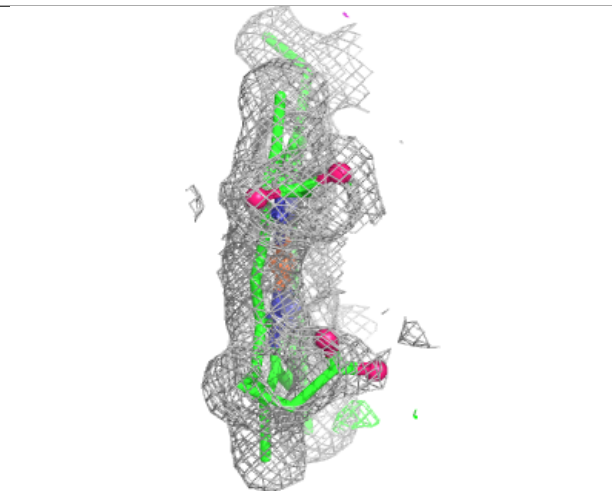
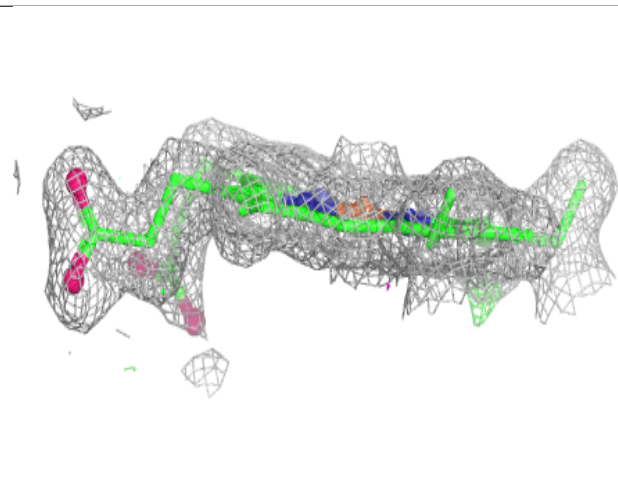
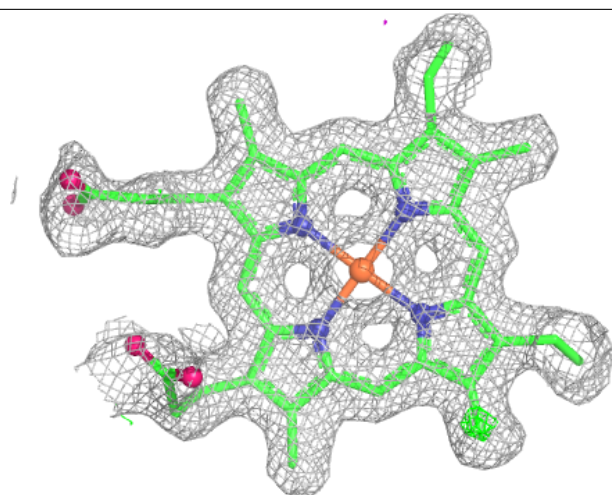
Electron density around HEC A 809:

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



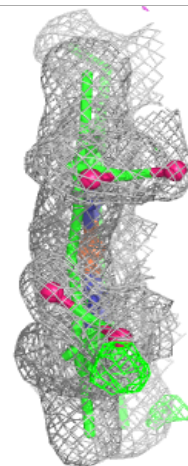
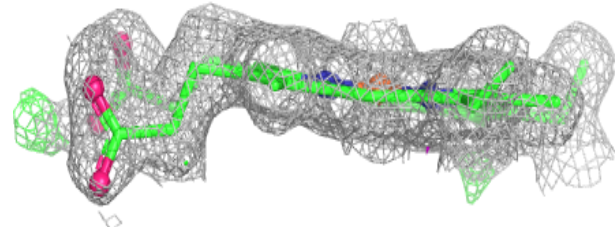
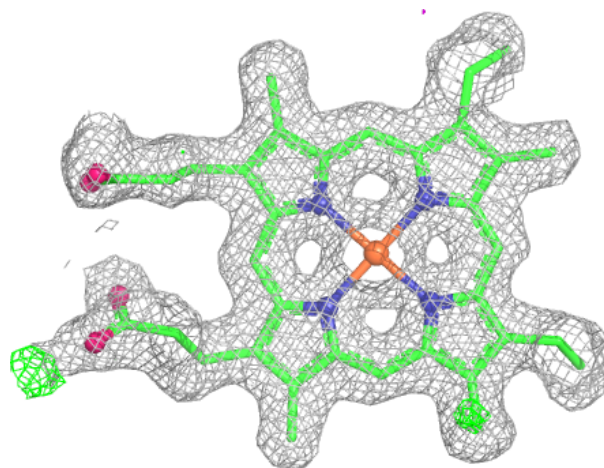
Electron density around HEC A 801 (A):

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and green (positive)



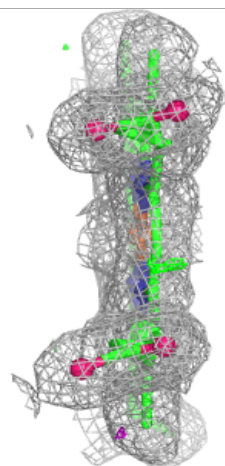
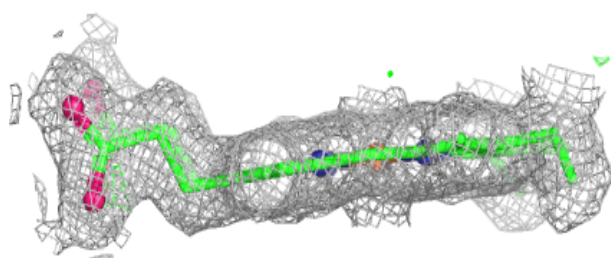
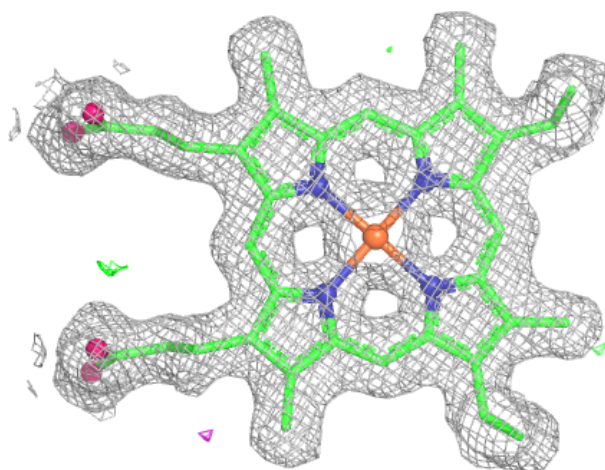
Electron density around HEC A 801 (B):

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and green (positive)



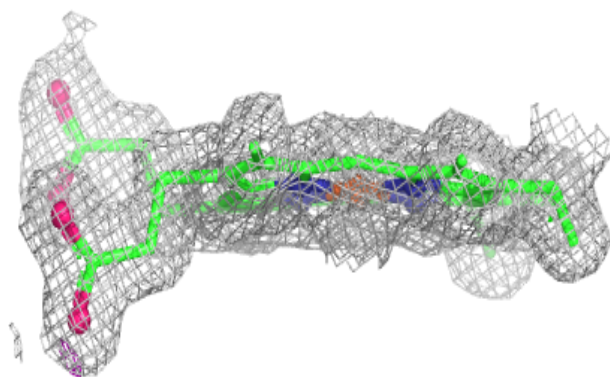
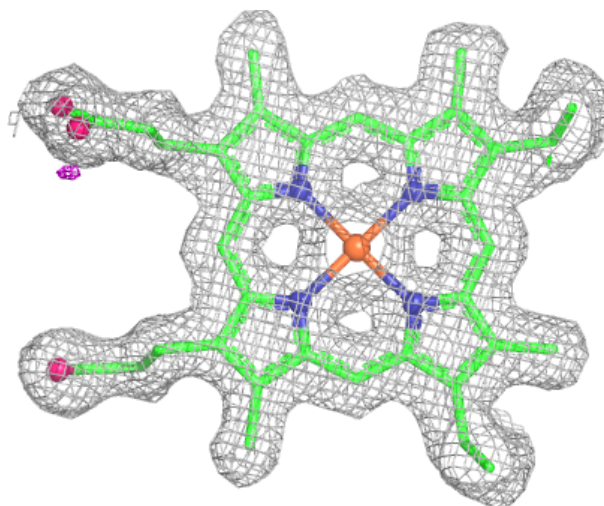
Electron density around HEC A 803:

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and green (positive)



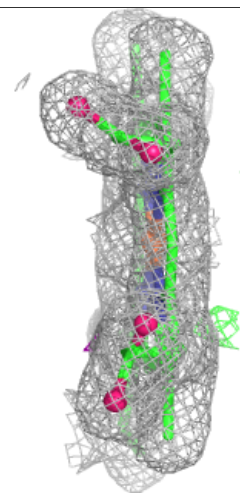
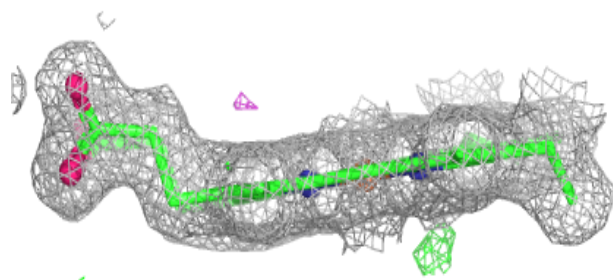
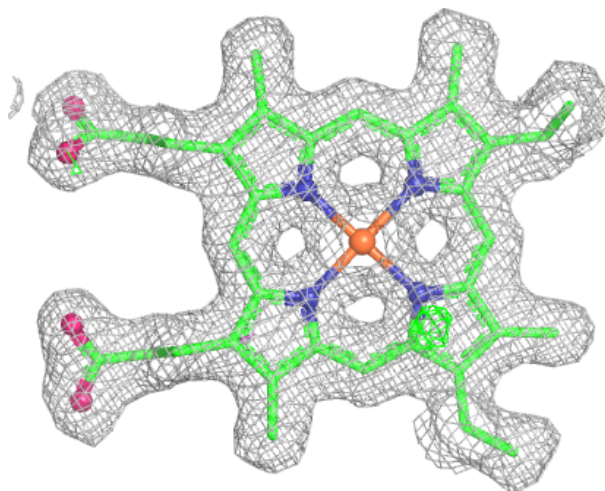
Electron density around HEC A 810:

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



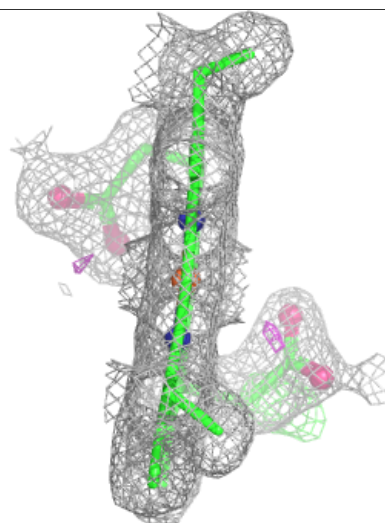
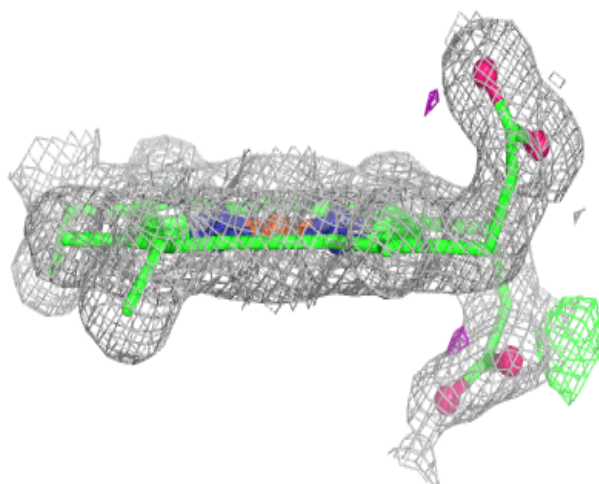
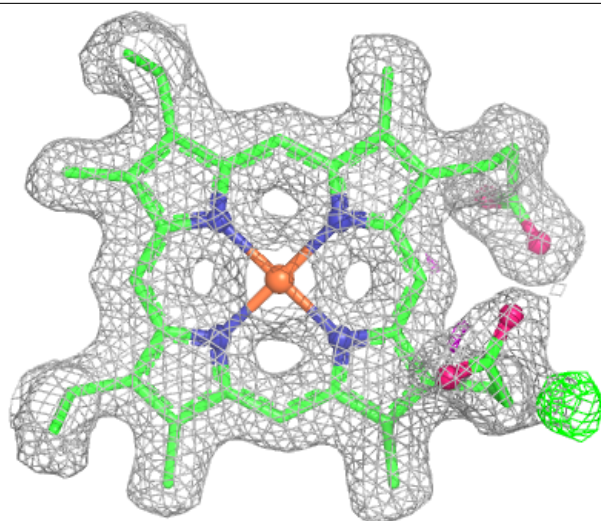
Electron density around HEC A 802:

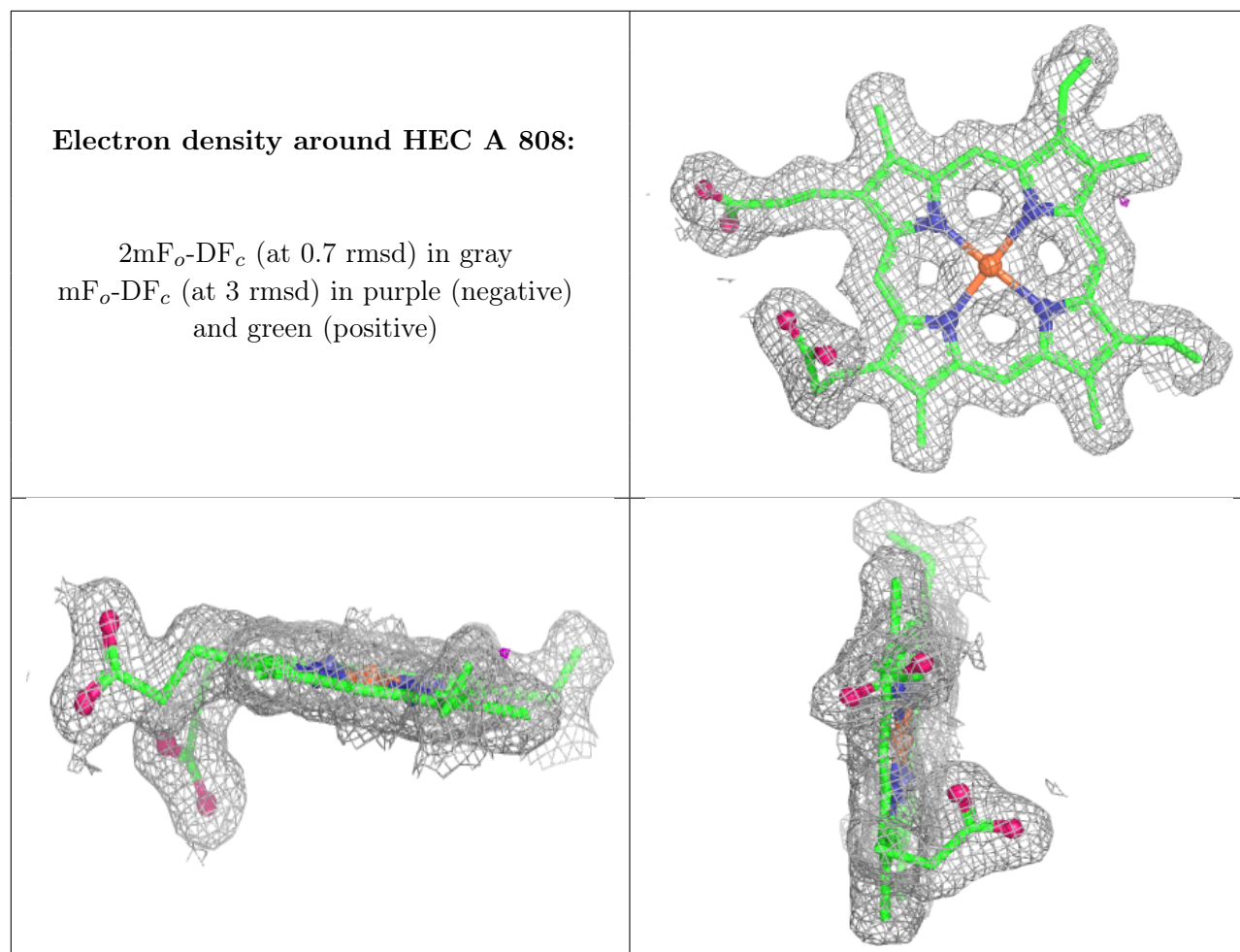
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 807:

$2mF_o-DF_c$ (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.