



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:08 PM EDT

PDB ID : 4RWM / pdb_00004rwm
Title : Kuenenia stuttgartiensis hydroxylamine oxidoreductase cryoprotected with ethylene glycol
Authors : Dietl, A.; Maalcke, W.; Barends, T.R.M.
Deposited on : 2014-12-05
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

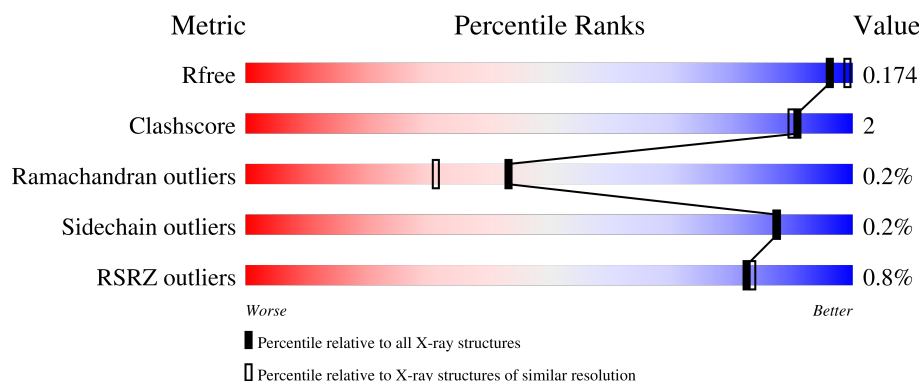
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

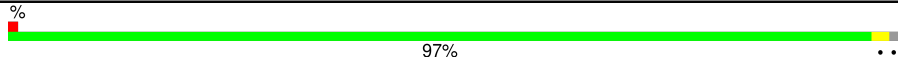
The reported resolution of this entry is 1.80 Å.

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	500	

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	HEC	A	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEC	A	611	X	-	-	-
5	HEC	A	612	X	-	-	-
5	HEC	A	613	X	-	-	-
5	HEC	A	614	X	-	-	-
5	HEC	A	615	X	-	-	-
5	HEC	A	616	X	-	-	-
5	HEC	A	617	X	-	-	-

2 Entry composition [i](#)

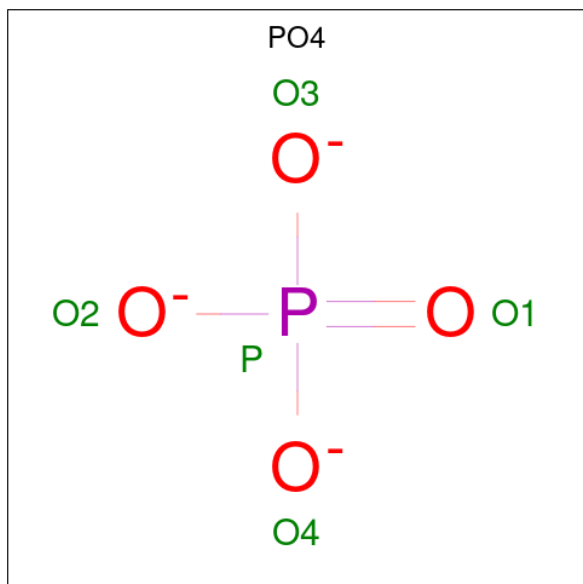
There are 6 unique types of molecules in this entry. The entry contains 4845 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Similar to hydroxylamine oxidoreductase hao.

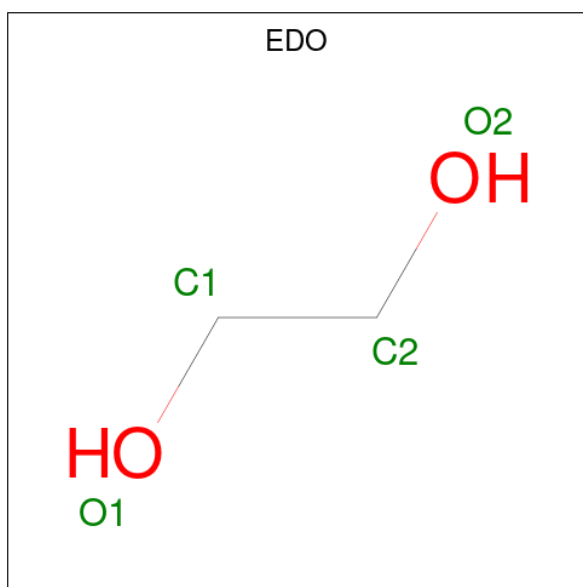
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			3945	2482	702	730	31			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



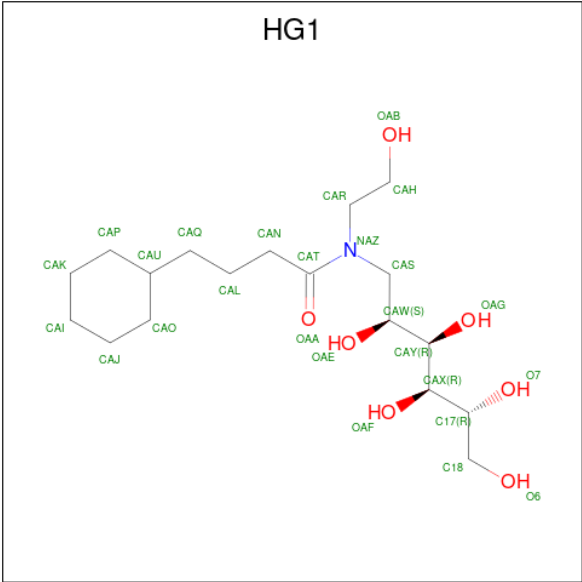
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



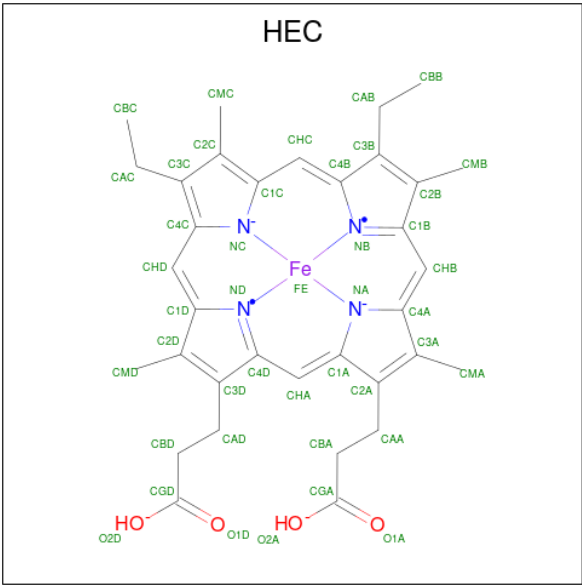
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1-[(4-cyclohexylbutanoyl)(2-hydroxyethyl)amino]-1-deoxy-D-glucitol (CCD ID: HG1) (formula: C₁₈H₃₅NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	10	1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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

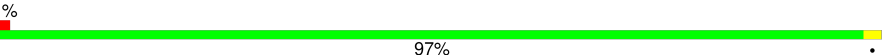
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	509	Total	O		
			509	509	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Similar to hydroxylamine oxidoreductase hao

Chain A:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	130.29Å 130.29Å 130.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.80) 99.7 (20.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.147 , 0.164 0.154 , 0.174	Depositor DCC
R_{free} test set	3361 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4845	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 2.35% 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: PO4, HG1, HEC, EDO

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	0.44	0/4063	0.66	0/5499

There are no bond length outliers.

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	3945	0	3738	7	0
2	A	15	0	0	0	0
3	A	20	0	29	1	0
4	A	12	0	17	0	0
5	A	344	0	240	10	0
6	A	509	0	0	0	0
All	All	4845	0	4024	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (14) 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)
5:A:613:HEC:HMC1	5:A:613:HEC:HBC3	1.72	0.70
5:A:613:HEC:HMB1	5:A:613:HEC:HBB3	1.73	0.68
1:A:323:MET:HE1	3:A:604:EDO:H21	1.80	0.64
1:A:53:VAL:HG11	1:A:69:LYS:HE3	1.90	0.54
5:A:617:HEC:HMB3	5:A:617:HEC:HBB3	1.93	0.51
1:A:345:LEU:C	1:A:345:LEU:HD13	2.39	0.47
1:A:234:CYS:HB2	5:A:612:HEC:HMB1	1.96	0.47
5:A:610:HEC:HMC3	5:A:610:HEC:HBC3	1.98	0.44
5:A:613:HEC:HMC1	5:A:613:HEC:CBC	2.45	0.44
1:A:427:LEU:C	1:A:427:LEU:HD13	2.44	0.42
5:A:610:HEC:HMC3	5:A:610:HEC:CBC	2.50	0.42
1:A:198:HIS:CD2	5:A:615:HEC:ND	2.87	0.42
1:A:205:ASN:O	5:A:613:HEC:HBB	2.20	0.42
5:A:613:HEC:HAD2	5:A:615:HEC:HBD2	2.02	0.41

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	496/500 (99%)	485 (98%)	10 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	HIS

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	414/416 (100%)	413 (100%)	1 (0%)	87 87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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	PO4	A	603	-	4,4,4	0.98	0	6,6,6	0.46	0
3	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.26	0
4	HG1	A	609	-	12,12,26	0.25	0	14,14,33	0.69	0
5	HEC	A	612	1	50,50,50	1.83	8 (16%)	68,82,82	1.35	7 (10%)
3	EDO	A	605	-	3,3,3	0.44	0	2,2,2	0.25	0
5	HEC	A	616	1	50,50,50	1.78	8 (16%)	68,82,82	1.36	6 (8%)
2	PO4	A	601	-	4,4,4	1.02	0	6,6,6	0.57	0
5	HEC	A	614	1	50,50,50	1.78	9 (18%)	68,82,82	1.23	5 (7%)
5	HEC	A	617	1	50,50,50	1.81	7 (14%)	68,82,82	1.19	3 (4%)
5	HEC	A	615	1	50,50,50	1.82	9 (18%)	68,82,82	1.35	10 (14%)
3	EDO	A	604	5	3,3,3	0.56	0	2,2,2	0.23	0
3	EDO	A	606	-	3,3,3	0.41	0	2,2,2	0.24	0
5	HEC	A	613	1,6,3	50,50,50	2.69	15 (30%)	68,82,82	2.35	25 (36%)
5	HEC	A	611	1	50,50,50	1.87	10 (20%)	68,82,82	1.33	7 (10%)
5	HEC	A	610	1	50,50,50	1.80	9 (18%)	68,82,82	1.35	7 (10%)
2	PO4	A	602	-	4,4,4	1.14	0	6,6,6	0.74	0
3	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.08	0

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
3	EDO	A	608	-	-	0/1/1/1	-
5	HEC	A	612	1	1/1/3/7	8/14/54/54	-
4	HG1	A	609	-	-	0/6/14/39	0/1/1/1
3	EDO	A	605	-	-	0/1/1/1	-
5	HEC	A	616	1	1/1/3/7	5/14/54/54	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	A	607	-	-	0/1/1/1	-
5	HEC	A	617	1	1/1/3/7	7/14/54/54	-
5	HEC	A	615	1	1/1/3/7	7/14/54/54	-
3	EDO	A	604	5	-	1/1/1/1	-
5	HEC	A	613	1,6,3	1/1/3/7	6/14/54/54	-
5	HEC	A	611	1	1/1/3/7	6/14/54/54	-
5	HEC	A	610	1	1/1/3/7	6/14/54/54	-
5	HEC	A	614	1	1/1/3/7	4/14/54/54	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	613	HEC	CHC-C4B	9.48	1.57	1.38
5	A	615	HEC	C3D-C2D	7.53	1.53	1.36
5	A	617	HEC	C3D-C2D	7.50	1.52	1.36
5	A	611	HEC	C3D-C2D	7.41	1.52	1.36
5	A	614	HEC	C3D-C2D	7.36	1.52	1.36
5	A	612	HEC	C3D-C2D	7.32	1.52	1.36
5	A	616	HEC	C3D-C2D	7.23	1.52	1.36
5	A	610	HEC	C3D-C2D	7.19	1.52	1.36
5	A	613	HEC	C4B-C3B	5.62	1.54	1.45
5	A	613	HEC	C1A-C2A	5.57	1.55	1.45
5	A	613	HEC	C4C-NC	5.30	1.49	1.39
5	A	613	HEC	C1A-NA	5.00	1.49	1.39
5	A	613	HEC	CHA-C1A	4.88	1.47	1.38
5	A	611	HEC	FE-ND	4.31	2.08	1.94
5	A	616	HEC	FE-ND	4.10	2.07	1.94
5	A	610	HEC	CBC-CAC	-4.02	1.34	1.51
5	A	611	HEC	CBC-CAC	-4.00	1.34	1.51
5	A	613	HEC	CHC-C1C	4.00	1.48	1.39
5	A	610	HEC	CBB-CAB	-3.94	1.34	1.51
5	A	613	HEC	C1C-NC	-3.91	1.32	1.39
5	A	612	HEC	CBC-CAC	-3.91	1.34	1.51
5	A	614	HEC	CBB-CAB	-3.91	1.34	1.51
5	A	617	HEC	CBC-CAC	-3.86	1.35	1.51
5	A	613	HEC	C4C-C3C	3.86	1.52	1.44
5	A	611	HEC	CBB-CAB	-3.85	1.35	1.51
5	A	617	HEC	CBB-CAB	-3.84	1.35	1.51
5	A	615	HEC	CBC-CAC	-3.84	1.35	1.51
5	A	612	HEC	CBB-CAB	-3.83	1.35	1.51
5	A	616	HEC	CBC-CAC	-3.80	1.35	1.51
5	A	615	HEC	CBB-CAB	-3.78	1.35	1.51
5	A	616	HEC	CBB-CAB	-3.73	1.35	1.51
5	A	614	HEC	CBC-CAC	-3.68	1.35	1.51
5	A	612	HEC	FE-ND	3.66	2.06	1.94
5	A	611	HEC	FE-NC	3.54	2.06	1.95
5	A	616	HEC	FE-NC	3.52	2.06	1.95
5	A	613	HEC	C4B-NB	3.49	1.46	1.40
5	A	610	HEC	FE-ND	3.49	2.05	1.94
5	A	614	HEC	FE-ND	3.37	2.05	1.94
5	A	613	HEC	CBD-CGD	3.27	1.58	1.50
5	A	615	HEC	FE-NA	3.25	2.05	1.95
5	A	610	HEC	FE-NA	3.25	2.05	1.95
5	A	613	HEC	CHD-C4C	3.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	617	HEC	FE-ND	3.22	2.04	1.94
5	A	615	HEC	FE-ND	3.20	2.04	1.94
5	A	612	HEC	FE-NC	3.07	2.05	1.95
5	A	617	HEC	FE-NB	3.06	2.04	1.94
5	A	612	HEC	FE-NB	3.04	2.04	1.94
5	A	612	HEC	FE-NA	3.01	2.05	1.95
5	A	615	HEC	FE-NC	2.98	2.05	1.95
5	A	617	HEC	FE-NA	2.97	2.05	1.95
5	A	614	HEC	FE-NC	2.85	2.04	1.95
5	A	613	HEC	C1C-C2C	2.81	1.49	1.43
5	A	610	HEC	FE-NB	2.72	2.03	1.94
5	A	614	HEC	FE-NA	2.57	2.03	1.95
5	A	615	HEC	FE-NB	2.51	2.02	1.94
5	A	611	HEC	FE-NA	2.50	2.03	1.95
5	A	610	HEC	FE-NC	2.47	2.03	1.95
5	A	617	HEC	FE-NC	2.45	2.03	1.95
5	A	611	HEC	FE-NB	2.44	2.02	1.94
5	A	613	HEC	C4A-NA	-2.34	1.35	1.39
5	A	614	HEC	FE-NB	2.31	2.02	1.94
5	A	611	HEC	CMA-C3A	2.26	1.55	1.50
5	A	611	HEC	CMB-C2B	2.23	1.55	1.50
5	A	616	HEC	CMB-C2B	2.23	1.55	1.50
5	A	616	HEC	CMC-C2C	2.19	1.55	1.50
5	A	614	HEC	CMA-C3A	2.18	1.55	1.50
5	A	614	HEC	CMB-C2B	2.11	1.55	1.50
5	A	615	HEC	CMA-C3A	2.11	1.55	1.50
5	A	616	HEC	CMA-C3A	2.06	1.55	1.50
5	A	611	HEC	CMC-C2C	2.04	1.54	1.50
5	A	612	HEC	CMA-C3A	2.03	1.54	1.50
5	A	615	HEC	CMC-C2C	2.03	1.54	1.50
5	A	610	HEC	CMA-C3A	2.03	1.54	1.50
5	A	610	HEC	CMB-C2B	2.03	1.54	1.50
5	A	613	HEC	C4D-ND	2.01	1.42	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	613	HEC	CHC-C4B-NB	-7.62	114.94	124.37
5	A	613	HEC	CHD-C4C-NC	-5.61	113.69	123.86
5	A	616	HEC	C1D-ND-C4D	5.46	111.67	105.21
5	A	613	HEC	C3C-C4C-NC	-5.20	104.39	110.15
5	A	612	HEC	C1D-ND-C4D	5.11	111.25	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	611	HEC	C1D-ND-C4D	5.04	111.17	105.21
5	A	615	HEC	C1D-ND-C4D	4.98	111.10	105.21
5	A	613	HEC	C3B-C4B-NB	-4.88	104.82	110.17
5	A	610	HEC	C1D-ND-C4D	4.70	110.78	105.21
5	A	613	HEC	C1C-CHC-C4B	-4.47	115.74	126.25
5	A	617	HEC	C1D-ND-C4D	4.41	110.43	105.21
5	A	614	HEC	C1D-ND-C4D	4.38	110.40	105.21
5	A	613	HEC	CAC-C3C-C4C	-4.01	119.39	124.91
5	A	613	HEC	CHD-C4C-C3C	-3.81	116.97	125.30
5	A	613	HEC	C4A-CHB-C1B	-3.68	118.20	126.02
5	A	613	HEC	CHC-C4B-C3B	-3.60	118.60	125.23
5	A	613	HEC	CAA-CBA-CGA	-3.36	104.76	113.67
5	A	614	HEC	CBD-CAD-C3D	-3.34	103.29	112.53
5	A	613	HEC	CHA-C1A-NA	-3.30	120.86	124.45
5	A	617	HEC	CBC-CAC-C3C	3.22	121.15	112.42
5	A	613	HEC	O2A-CGA-CBA	3.20	124.12	114.00
5	A	610	HEC	CBC-CAC-C3C	3.12	120.89	112.42
5	A	613	HEC	C3D-C4D-ND	-3.08	107.37	110.35
5	A	613	HEC	CAC-C3C-C2C	3.01	131.65	126.89
5	A	613	HEC	C2A-C1A-NA	-2.99	107.44	110.32
5	A	613	HEC	CHB-C4A-NA	-2.98	121.21	124.45
5	A	616	HEC	C4B-NB-C1B	2.84	108.57	105.21
5	A	612	HEC	CBC-CAC-C3C	2.83	120.08	112.42
5	A	613	HEC	C1A-C2A-C3A	-2.78	103.44	107.11
5	A	611	HEC	C2A-C1A-NA	-2.78	107.64	110.32
5	A	613	HEC	O2A-CGA-O1A	-2.75	116.27	123.33
5	A	615	HEC	CBB-CAB-C3B	2.73	119.81	112.42
5	A	616	HEC	CBC-CAC-C3C	2.73	119.81	112.42
5	A	616	HEC	C2A-C1A-NA	-2.72	107.70	110.32
5	A	610	HEC	C2A-C1A-NA	-2.66	107.76	110.32
5	A	616	HEC	C3B-C4B-NB	-2.65	107.26	110.17
5	A	615	HEC	CBC-CAC-C3C	2.64	119.57	112.42
5	A	611	HEC	CBC-CAC-C3C	2.59	119.44	112.42
5	A	615	HEC	C2A-C1A-NA	-2.54	107.87	110.32
5	A	611	HEC	CHD-C1D-ND	2.53	127.49	124.37
5	A	612	HEC	CBA-CAA-C2A	-2.52	105.57	112.53
5	A	613	HEC	CBA-CAA-C2A	-2.50	105.61	112.53
5	A	611	HEC	C4B-NB-C1B	2.45	108.11	105.21
5	A	615	HEC	C4B-NB-C1B	2.44	108.09	105.21
5	A	612	HEC	O2A-CGA-CBA	2.43	121.69	114.00
5	A	610	HEC	CBA-CAA-C2A	-2.38	105.95	112.53
5	A	610	HEC	C4B-NB-C1B	2.36	108.00	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	613	HEC	CHA-C4D-ND	2.32	126.92	124.42
5	A	615	HEC	C3D-C4D-ND	-2.30	108.13	110.35
5	A	611	HEC	CAD-C3D-C4D	2.29	128.70	124.70
5	A	616	HEC	CBA-CAA-C2A	-2.29	106.21	112.53
5	A	613	HEC	CAB-C3B-C4B	-2.25	121.87	124.79
5	A	612	HEC	C2A-C1A-NA	-2.24	108.16	110.32
5	A	615	HEC	CHD-C1D-ND	2.22	127.12	124.37
5	A	612	HEC	C4B-NB-C1B	2.21	107.82	105.21
5	A	614	HEC	C2A-C1A-NA	-2.19	108.21	110.32
5	A	611	HEC	C3B-C4B-NB	-2.18	107.78	110.17
5	A	614	HEC	CHD-C1D-ND	2.17	127.05	124.37
5	A	610	HEC	C3B-C4B-NB	-2.16	107.80	110.17
5	A	613	HEC	C4C-CHD-C1D	-2.15	121.20	126.25
5	A	615	HEC	CAD-C3D-C4D	2.14	128.43	124.70
5	A	613	HEC	C2D-C1D-ND	-2.06	107.47	109.84
5	A	612	HEC	O1A-CGA-CBA	-2.05	116.60	123.09
5	A	617	HEC	C2A-C1A-NA	-2.04	108.35	110.32
5	A	610	HEC	CMD-C2D-C1D	2.04	128.22	125.03
5	A	614	HEC	CAD-C3D-C4D	2.02	128.23	124.70
5	A	615	HEC	CAD-CBD-CGD	-2.01	108.33	113.67
5	A	613	HEC	CMA-C3A-C4A	-2.01	121.20	124.73
5	A	613	HEC	CMC-C2C-C3C	2.00	129.87	125.62
5	A	615	HEC	C3B-C4B-NB	-2.00	107.98	110.17

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	610	HEC	NA
5	A	611	HEC	NA
5	A	612	HEC	NA
5	A	613	HEC	NA
5	A	614	HEC	NA
5	A	615	HEC	NA
5	A	616	HEC	NA
5	A	617	HEC	NA

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	613	HEC	C2C-C3C-CAC-CBC
5	A	610	HEC	C2C-C3C-CAC-CBC
5	A	613	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	A	613	HEC	C2B-C3B-CAB-CBB
5	A	613	HEC	C4C-C3C-CAC-CBC
5	A	610	HEC	C4C-C3C-CAC-CBC
5	A	615	HEC	C2B-C3B-CAB-CBB
5	A	614	HEC	C2C-C3C-CAC-CBC
5	A	617	HEC	C2C-C3C-CAC-CBC
5	A	615	HEC	C2C-C3C-CAC-CBC
5	A	616	HEC	C2B-C3B-CAB-CBB
5	A	617	HEC	C4C-C3C-CAC-CBC
5	A	615	HEC	C4B-C3B-CAB-CBB
5	A	610	HEC	C2B-C3B-CAB-CBB
5	A	612	HEC	C2C-C3C-CAC-CBC
5	A	615	HEC	C4C-C3C-CAC-CBC
5	A	612	HEC	C4C-C3C-CAC-CBC
5	A	617	HEC	C2B-C3B-CAB-CBB
5	A	614	HEC	C4C-C3C-CAC-CBC
5	A	614	HEC	C2B-C3B-CAB-CBB
5	A	611	HEC	C2C-C3C-CAC-CBC
5	A	616	HEC	C2C-C3C-CAC-CBC
5	A	611	HEC	C2B-C3B-CAB-CBB
5	A	611	HEC	C4C-C3C-CAC-CBC
5	A	616	HEC	C4C-C3C-CAC-CBC
5	A	616	HEC	C4B-C3B-CAB-CBB
5	A	610	HEC	C4B-C3B-CAB-CBB
5	A	617	HEC	C4B-C3B-CAB-CBB
5	A	614	HEC	C4B-C3B-CAB-CBB
5	A	617	HEC	C3D-CAD-CBD-CGD
5	A	612	HEC	C2B-C3B-CAB-CBB
5	A	611	HEC	C4B-C3B-CAB-CBB
5	A	616	HEC	C3D-CAD-CBD-CGD
5	A	610	HEC	CAD-CBD-CGD-O1D
5	A	610	HEC	CAD-CBD-CGD-O2D
5	A	612	HEC	CAD-CBD-CGD-O2D
5	A	617	HEC	CAD-CBD-CGD-O2D
5	A	613	HEC	CAA-CBA-CGA-O2A
5	A	613	HEC	CAA-CBA-CGA-O1A
5	A	617	HEC	CAD-CBD-CGD-O1D
5	A	612	HEC	CAD-CBD-CGD-O1D
5	A	612	HEC	CAA-CBA-CGA-O2A
5	A	615	HEC	CAA-CBA-CGA-O2A
3	A	604	EDO	O1-C1-C2-O2
5	A	615	HEC	CAA-CBA-CGA-O1A

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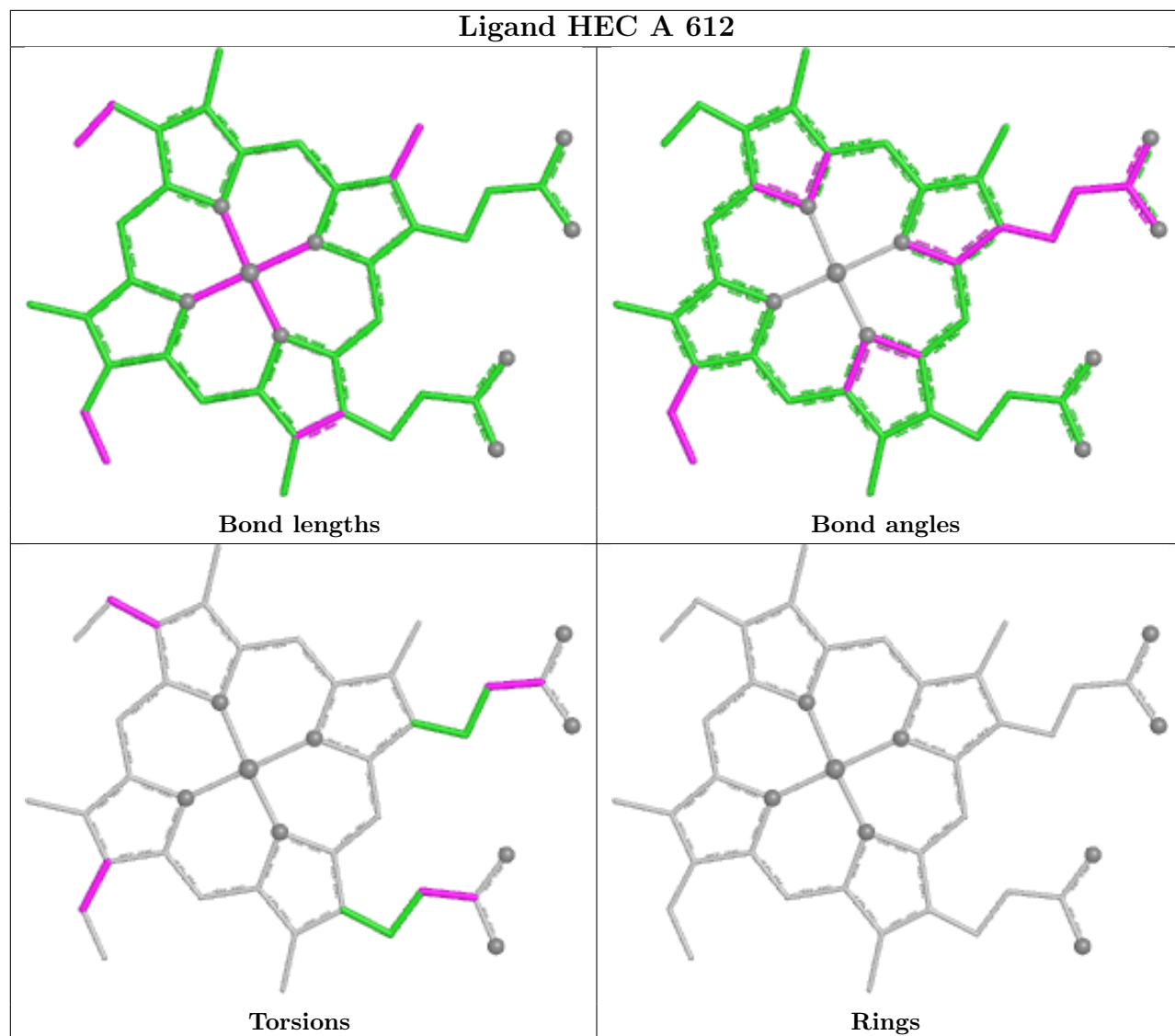
Mol	Chain	Res	Type	Atoms
5	A	612	HEC	C4B-C3B-CAB-CBB
5	A	611	HEC	CAA-CBA-CGA-O1A
5	A	612	HEC	CAA-CBA-CGA-O1A
5	A	615	HEC	CAD-CBD-CGD-O2D
5	A	611	HEC	CAA-CBA-CGA-O2A

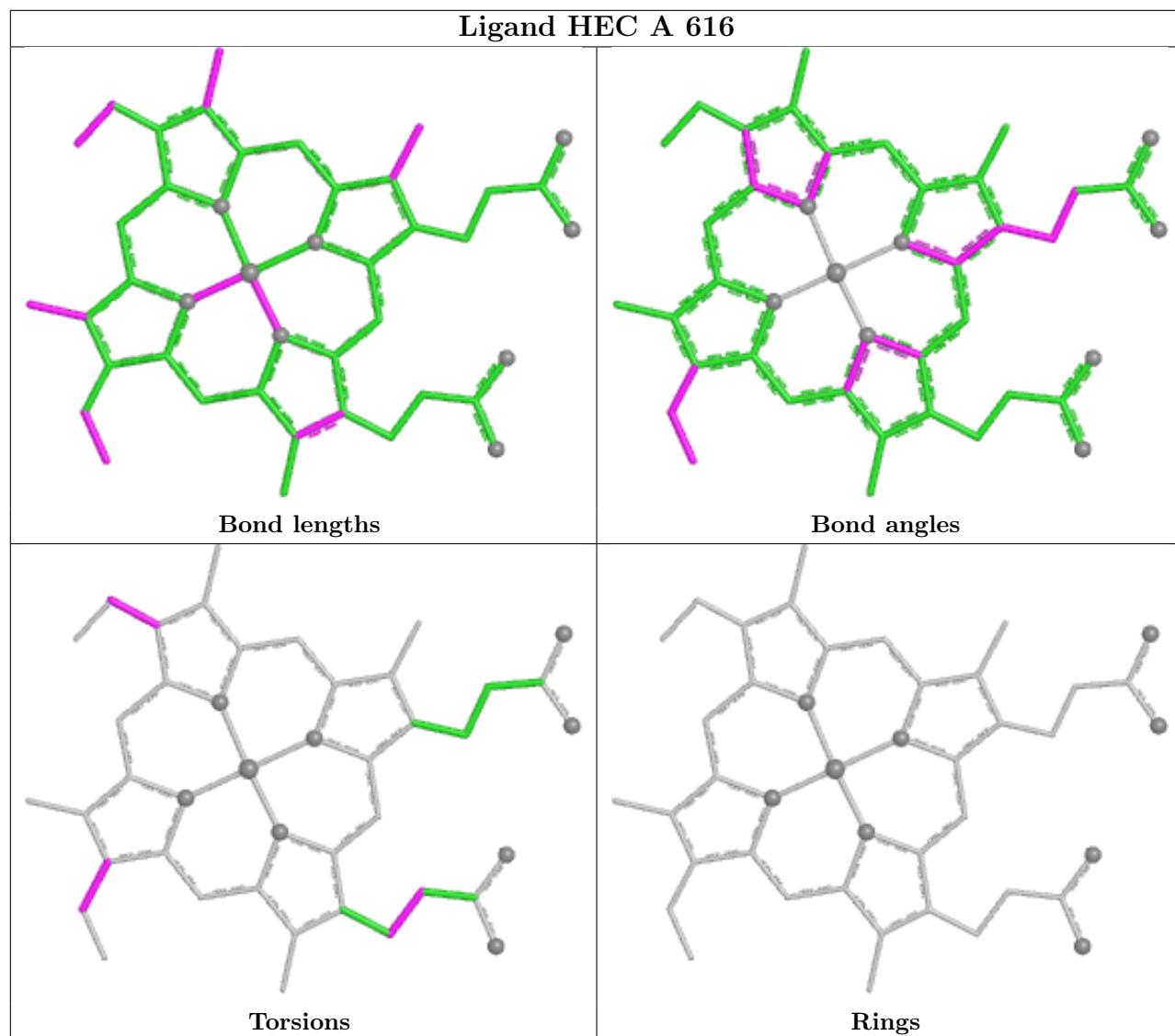
There are no ring outliers.

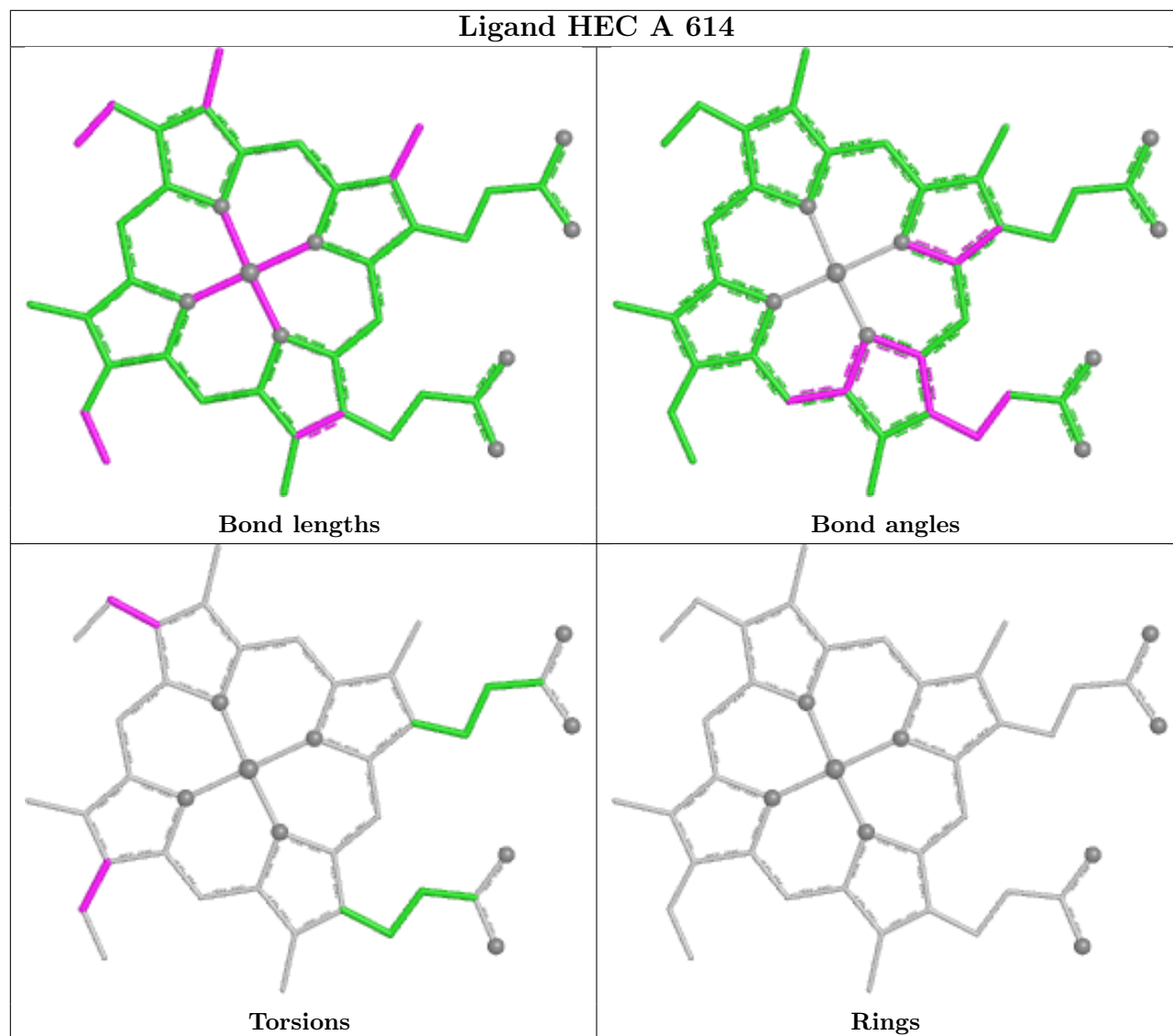
6 monomers are involved in 11 short contacts:

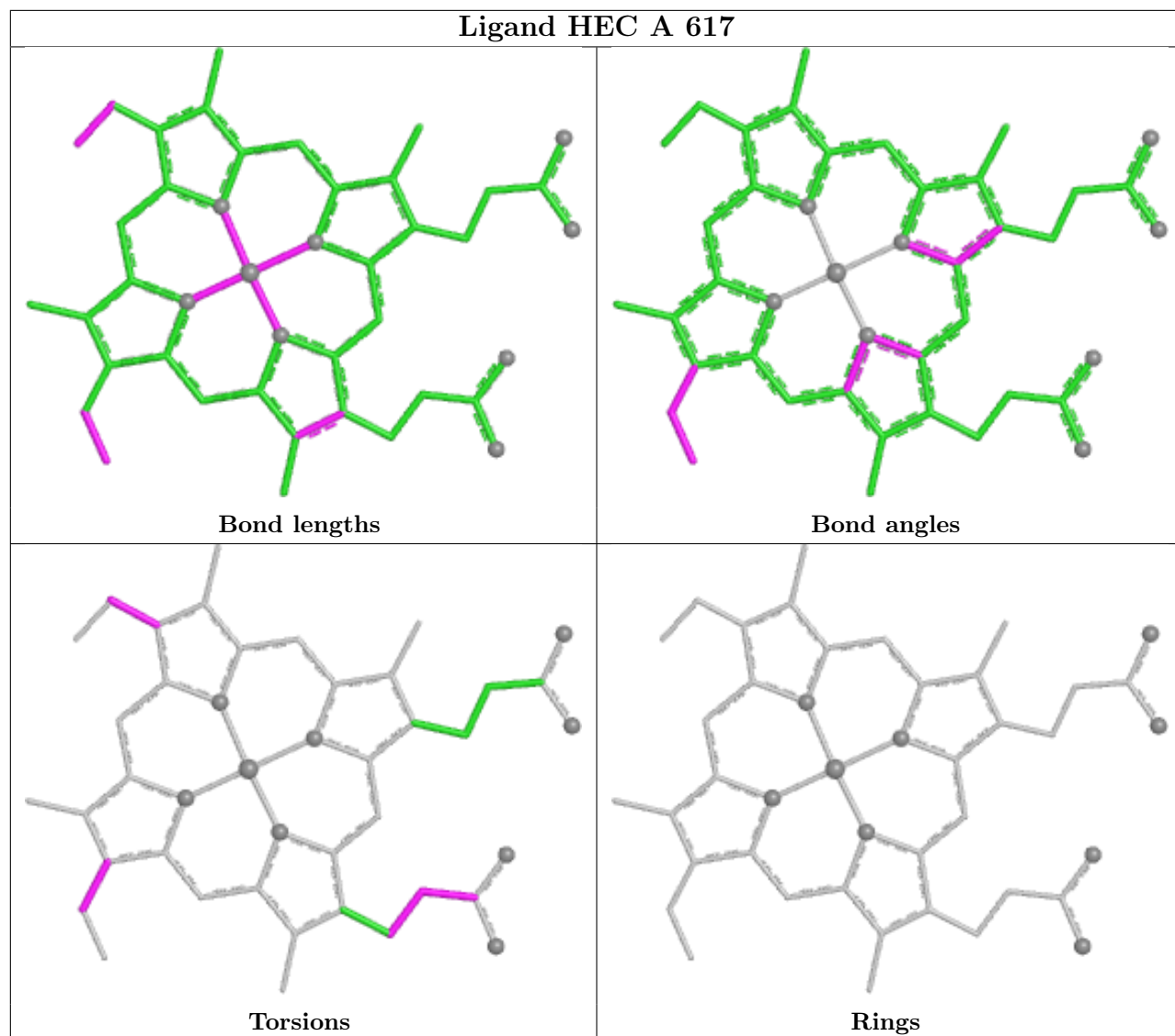
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	612	HEC	1	0
5	A	617	HEC	1	0
5	A	615	HEC	2	0
3	A	604	EDO	1	0
5	A	613	HEC	5	0
5	A	610	HEC	2	0

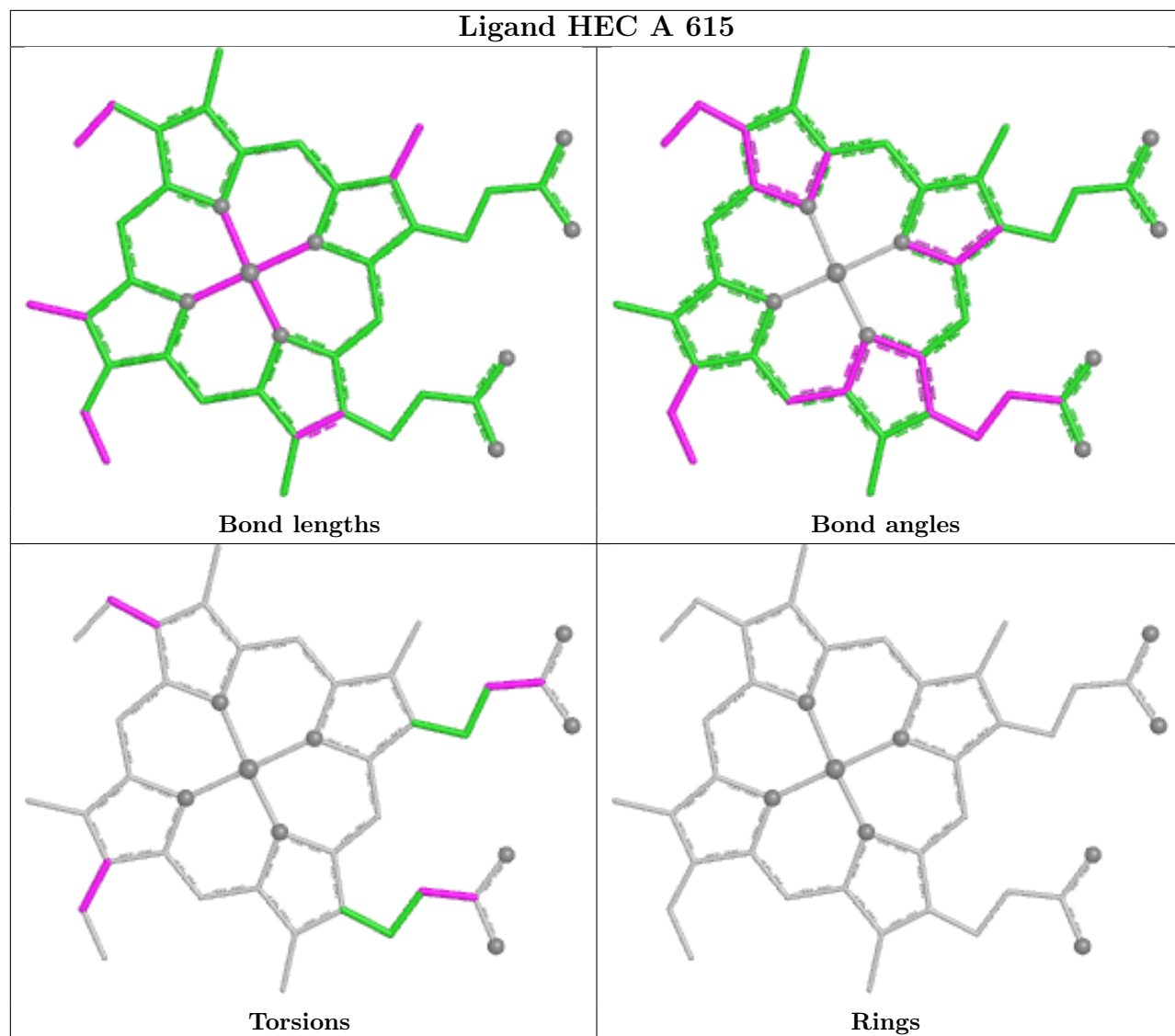
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



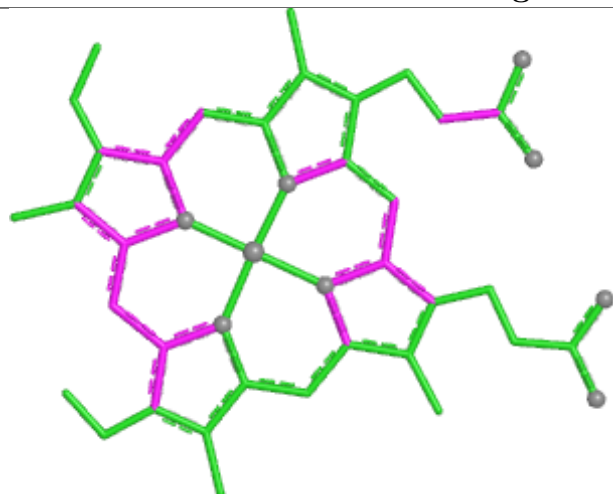




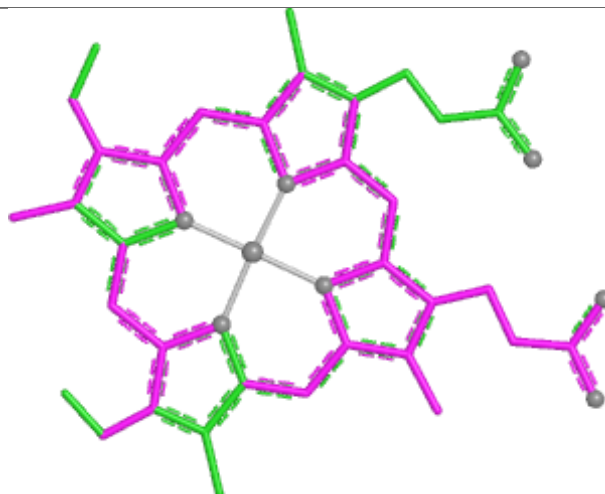




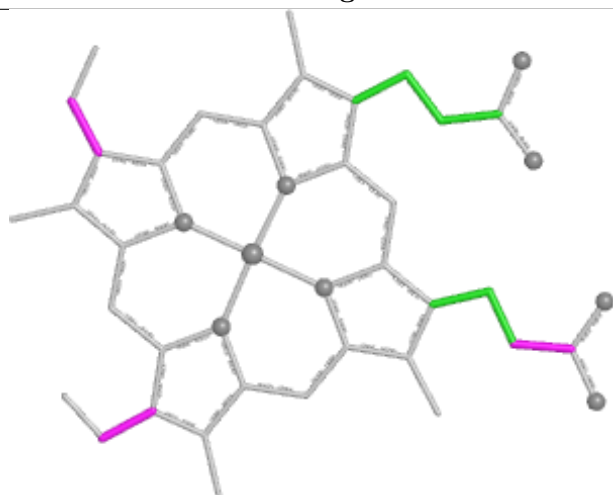
Ligand HEC A 613



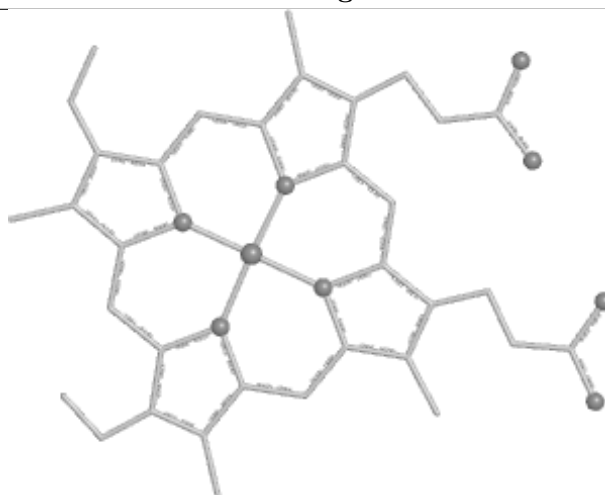
Bond lengths



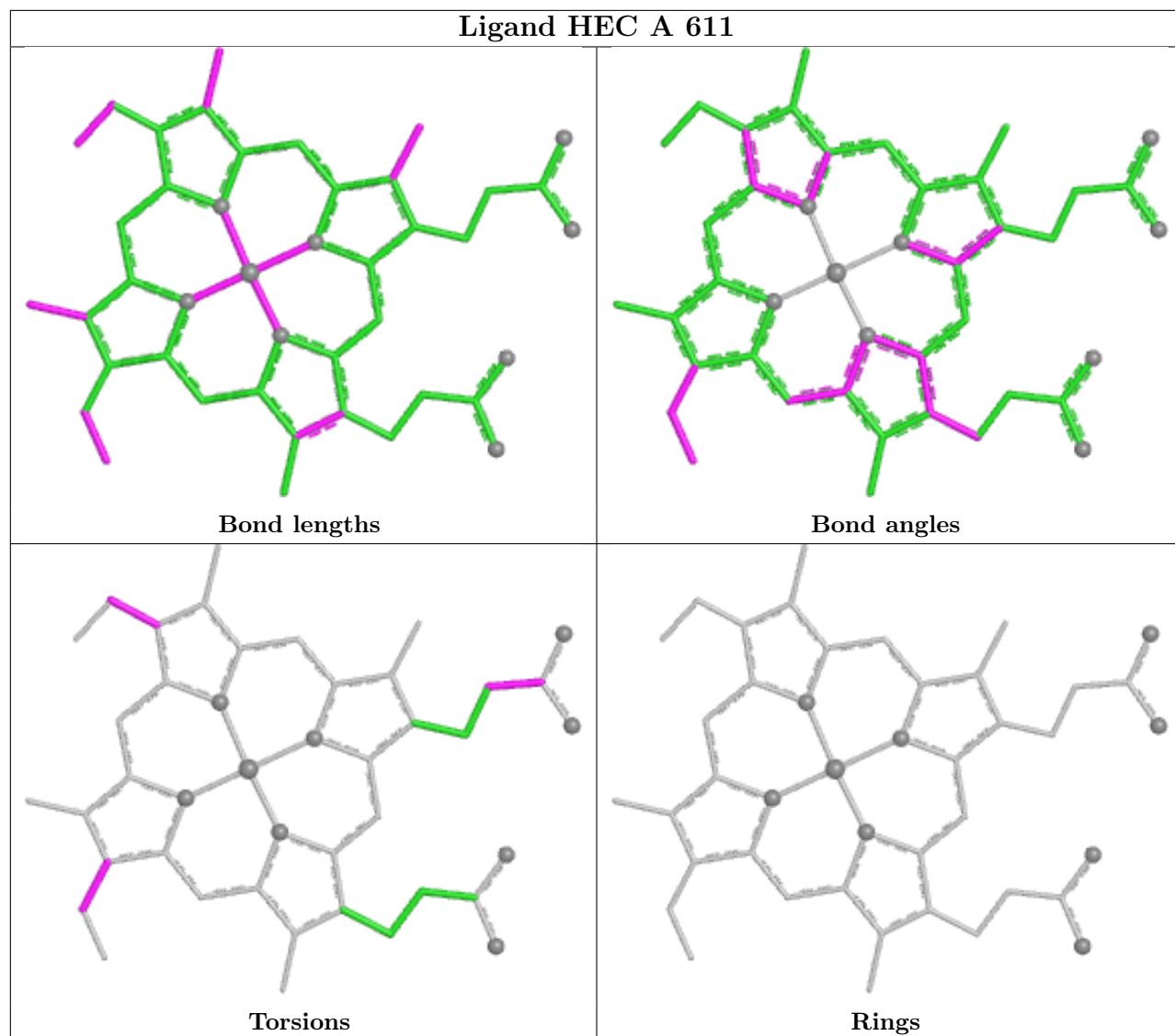
Bond angles

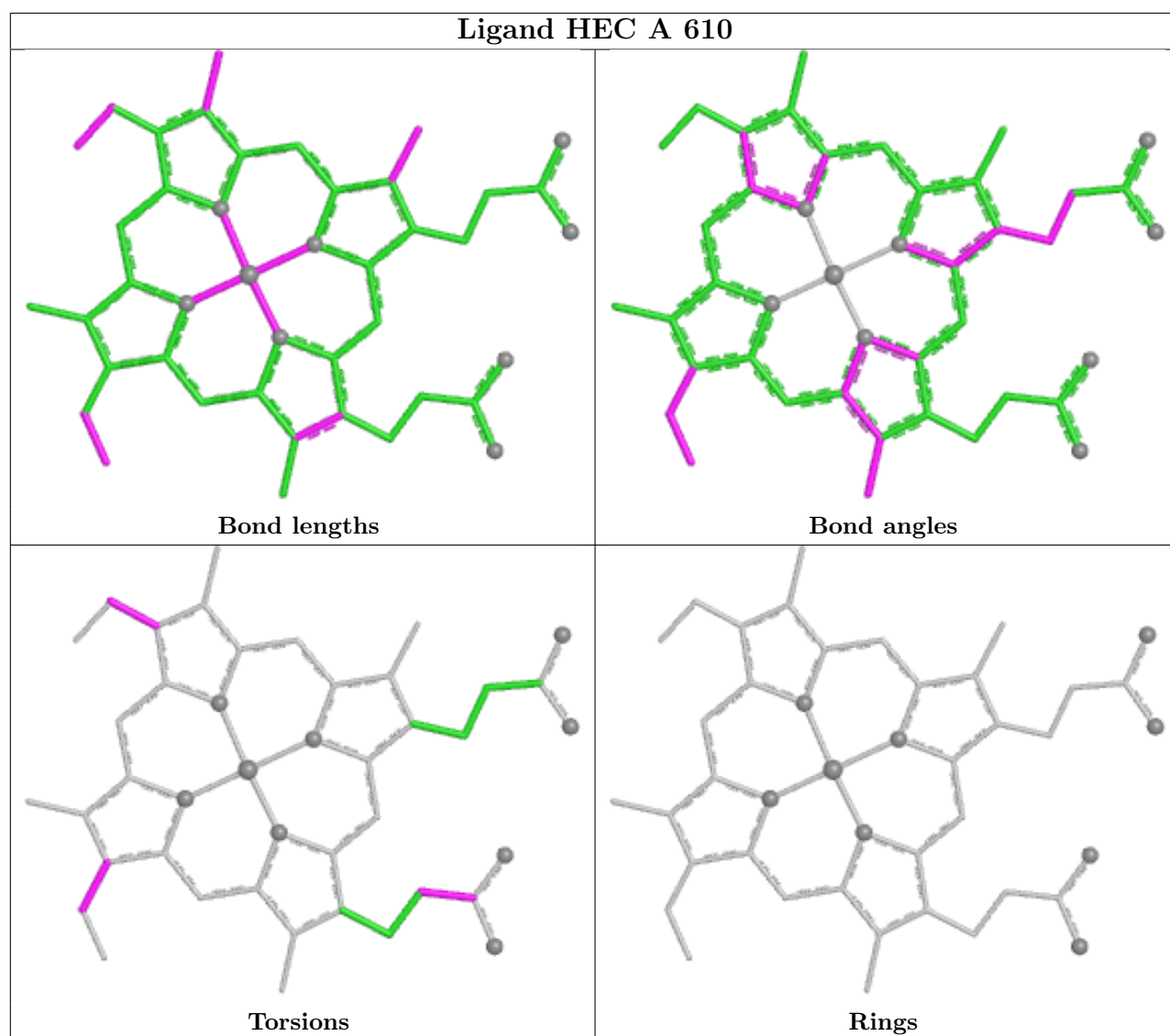


Torsions



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	497/500 (99%)	-0.49	4 (0%) 82 83	13, 18, 28, 38	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	ILE	3.6
1	A	38	GLY	3.3
1	A	39	PRO	2.1
1	A	533	GLU	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
4	HG1	A	609	12/26	0.90	0.09	39,40,43,43	0
3	EDO	A	604	4/4	0.91	0.12	23,24,25,25	0
3	EDO	A	605	4/4	0.92	0.10	19,21,22,24	0

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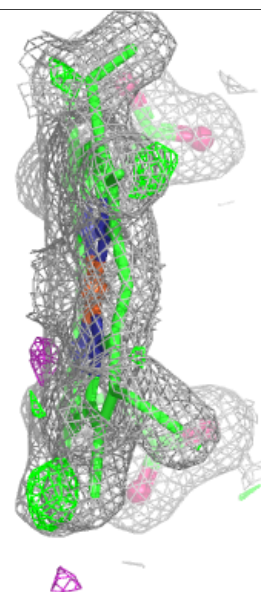
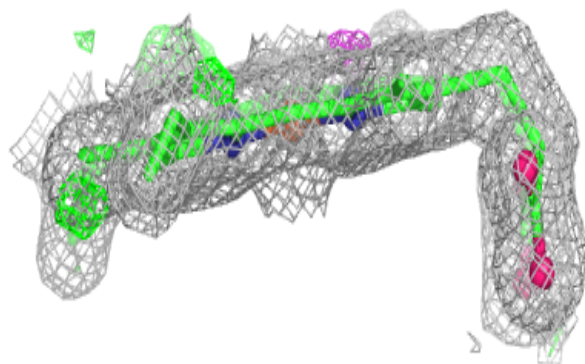
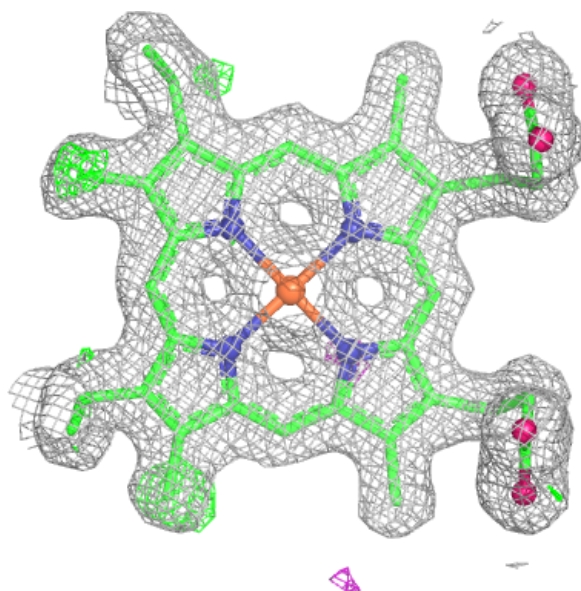
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	608	4/4	0.94	0.08	28,28,28,29	0
3	EDO	A	607	4/4	0.96	0.07	17,18,18,19	0
2	PO4	A	602	5/5	0.96	0.09	23,23,25,26	0
3	EDO	A	606	4/4	0.96	0.07	21,23,24,25	0
2	PO4	A	601	5/5	0.98	0.07	24,24,26,26	0
5	HEC	A	611	43/43	0.98	0.05	13,14,16,17	0
5	HEC	A	612	43/43	0.98	0.05	14,15,18,19	0
5	HEC	A	613	43/43	0.98	0.06	13,15,21,27	0
5	HEC	A	616	43/43	0.98	0.05	11,12,16,17	0
5	HEC	A	614	43/43	0.99	0.05	11,13,16,18	0
5	HEC	A	615	43/43	0.99	0.05	11,13,17,19	0
5	HEC	A	610	43/43	0.99	0.05	15,17,19,21	0
5	HEC	A	617	43/43	0.99	0.04	11,13,15,16	0
2	PO4	A	603	5/5	1.00	0.03	18,18,19,19	5

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.

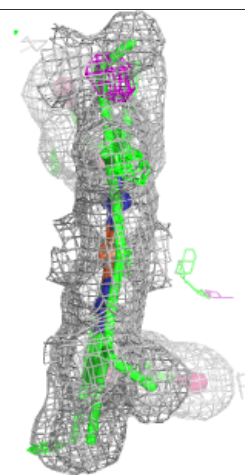
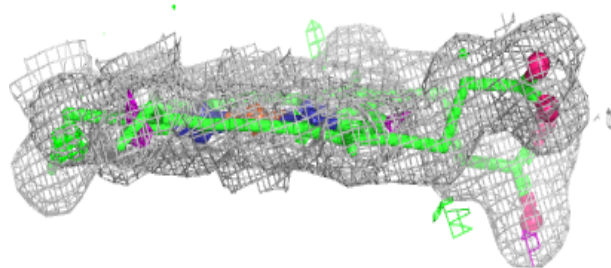
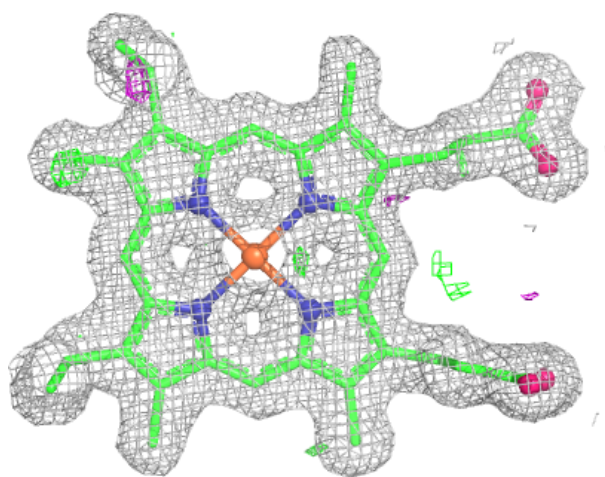
Electron density around HEC A 611:

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



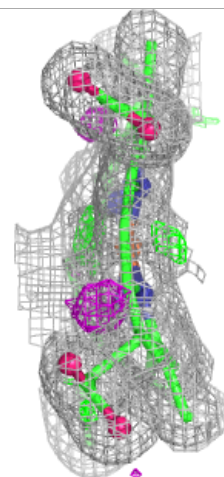
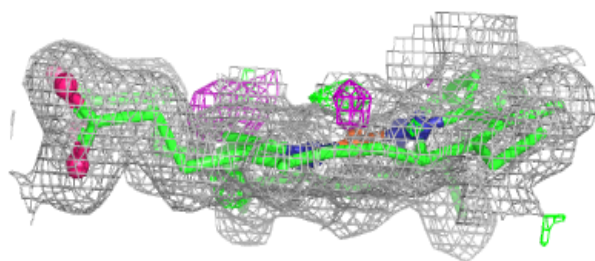
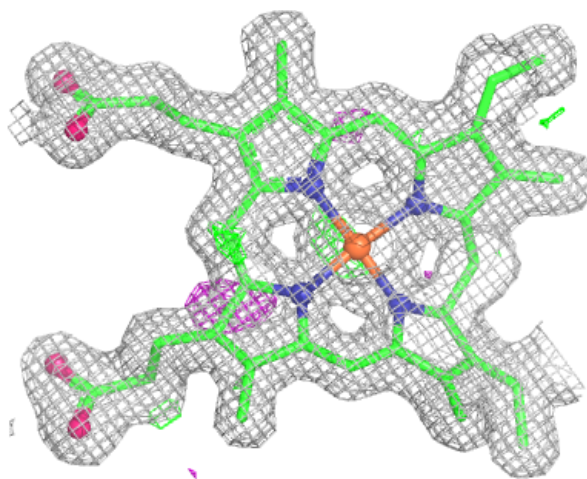
Electron density around HEC A 612:

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



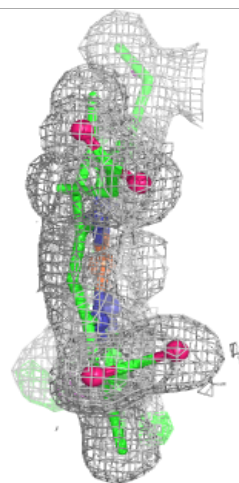
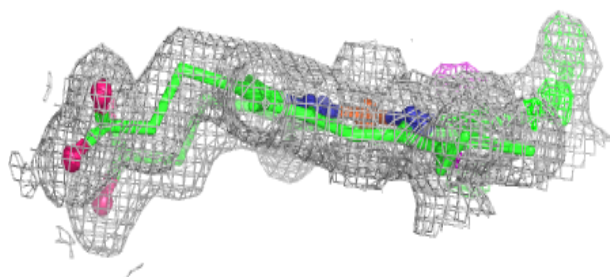
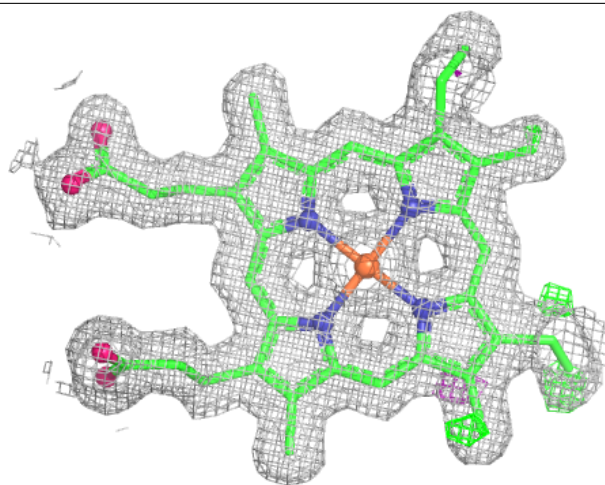
Electron density around HEC A 613:

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



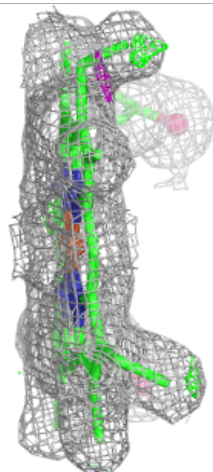
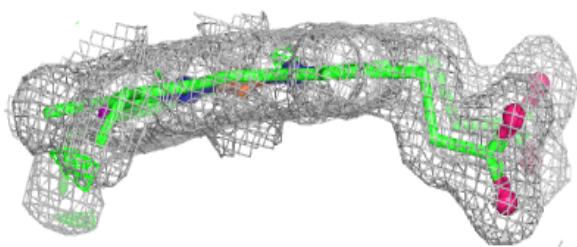
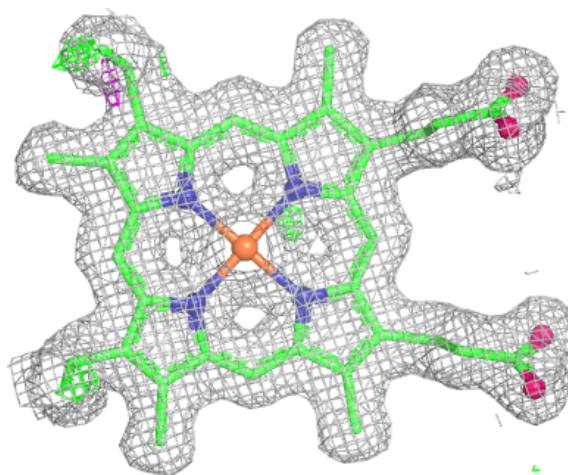
Electron density around HEC A 616:

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



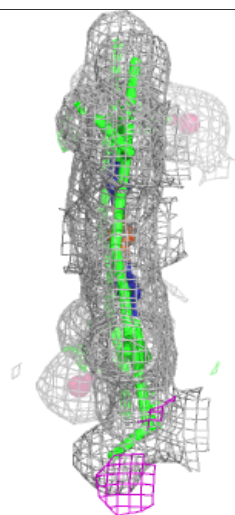
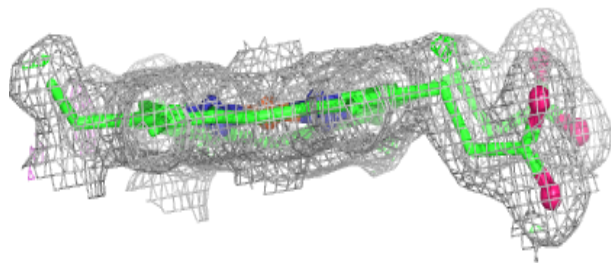
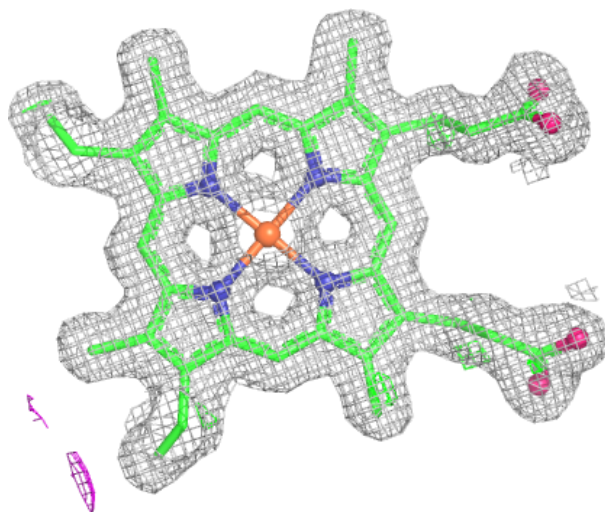
Electron density around HEC A 614:

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



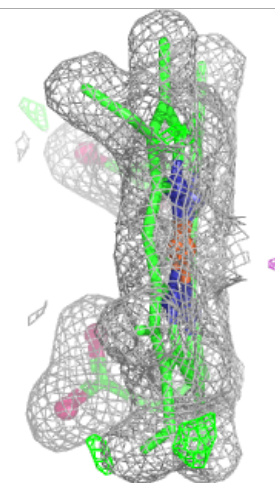
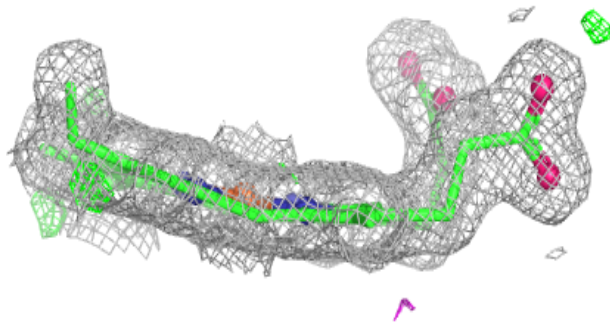
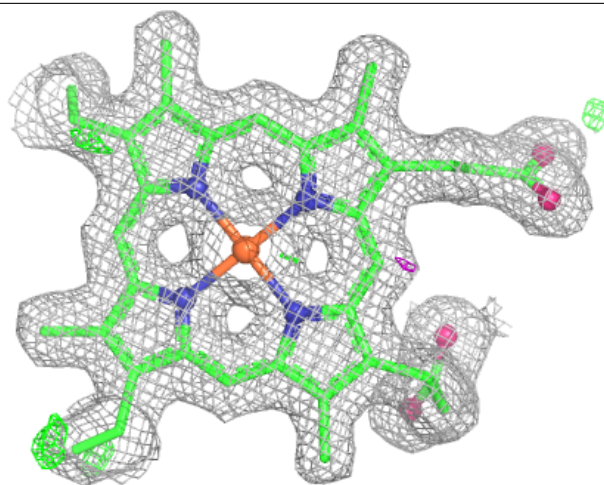
Electron density around HEC A 615:

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



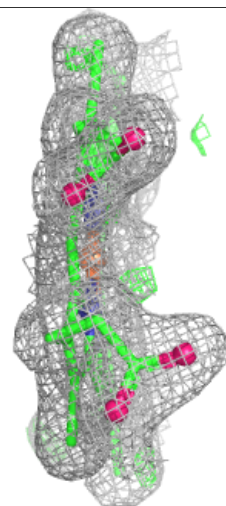
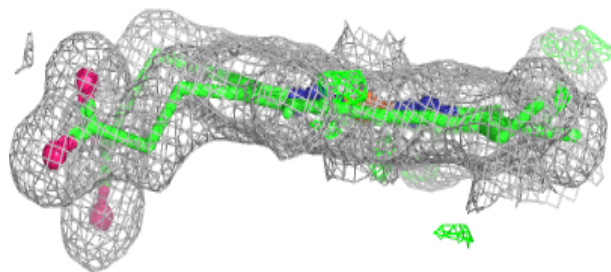
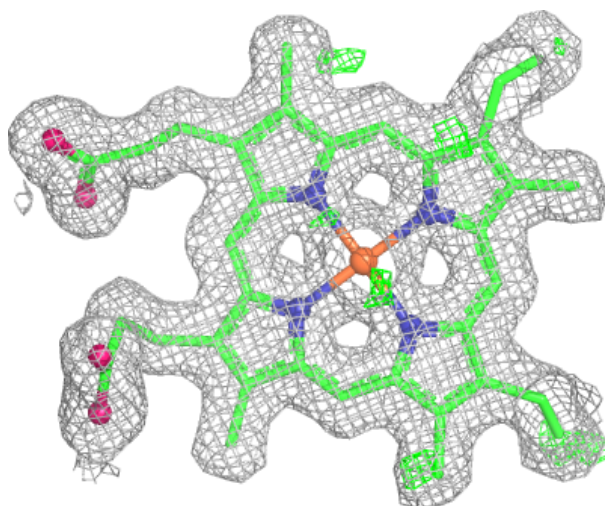
Electron density around HEC A 610:

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



Electron density around HEC A 617:

$2mF_o-DF_c$ (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.