



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:38 PM EDT

PDB ID : 4N4K / pdb_00004n4k
Title : Kuenenia stuttgartiensis hydroxylamine oxidoreductase soaked in hydroxylamine
Authors : Maalcke, W.J.; Dietl, A.; Marritt, S.J.; Butt, J.N.; Jetten, M.S.M.; Keltjens, J.T.; Barends, T.R.M.B.; Kartal, B.
Deposited on : 2013-10-08
Resolution : 2.20 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

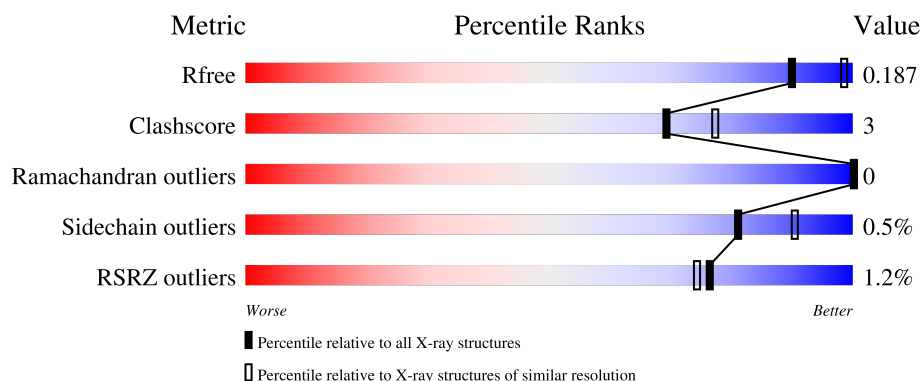
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

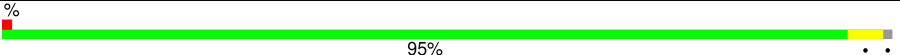
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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
4	HEC	A	607	X	-	-	-
4	HEC	A	608	X	-	-	-
4	HEC	A	609	X	-	-	-
4	HEC	A	610	X	-	-	-
4	HEC	A	611	X	-	-	-
4	HEC	A	612	X	-	-	-
4	HEC	A	613	X	-	-	-
4	HEC	A	614	X	-	-	-

2 Entry composition [i](#)

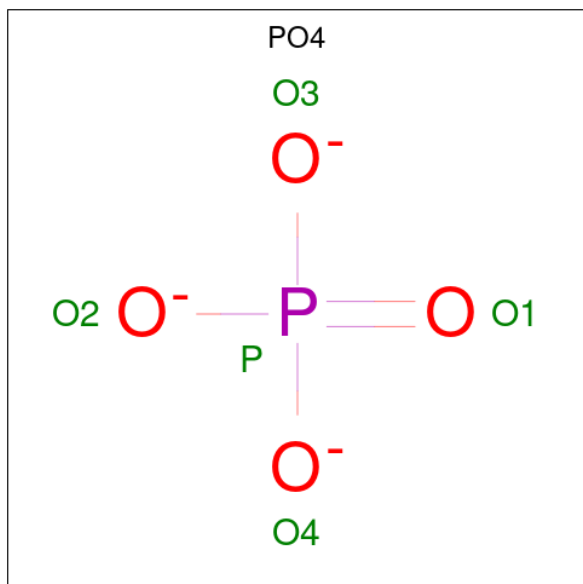
There are 6 unique types of molecules in this entry. The entry contains 4647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 hydroxylamine oxidoreductase.

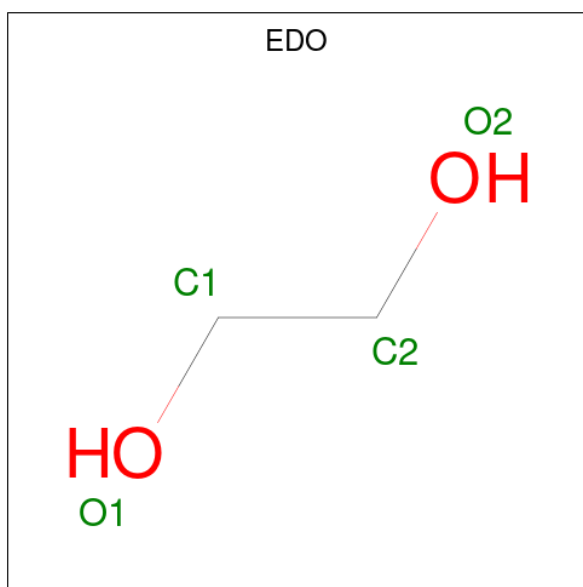
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	3	0
			3968	2494	708	735	31			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



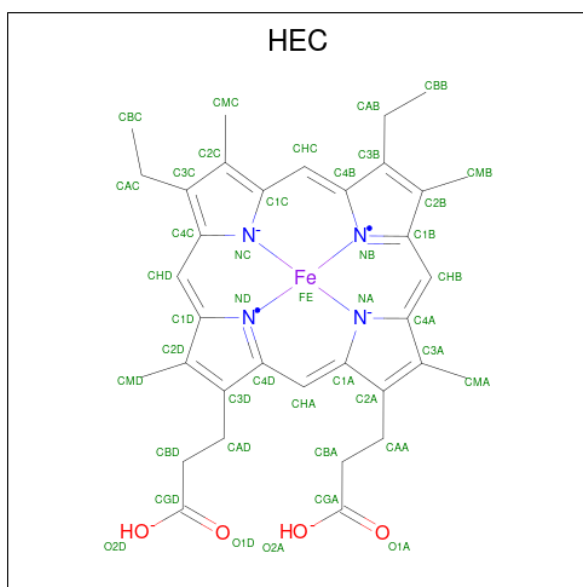
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



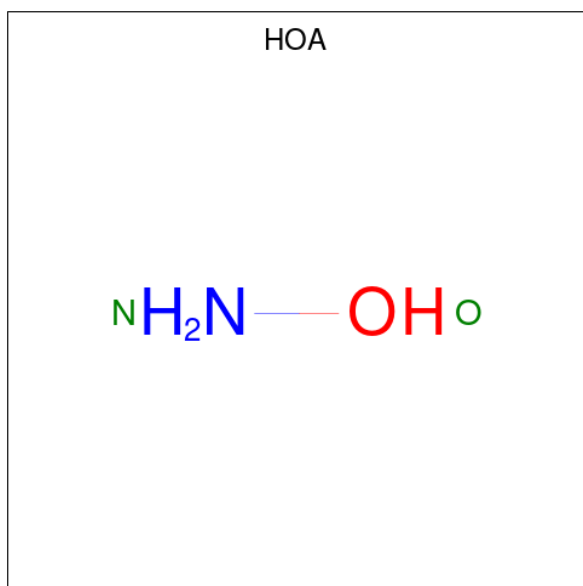
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 5 is HYDROXYAMINE (CCD ID: HOA) (formula: H_3NO).



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

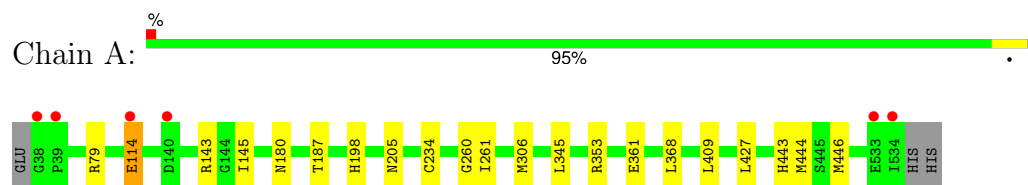
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total	O		
			306	306	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: hydroxylamine oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	130.07 Å 130.07 Å 130.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.99 – 2.20 45.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.99-2.20) 99.9 (45.99-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.010	Depositor
R, R_{free}	0.167 , 0.187 0.166 , 0.187	Depositor DCC
R_{free} test set	1786 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4647	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: HOA, PO4, EDO, HEC

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	0.43	0/4083	0.65	0/5525

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	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLY	Mainchain
1	A	443	HIS	Sidechain
1	A	79	ARG	Sidechain

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	3968	0	3754	19	1
2	A	15	0	0	0	0
3	A	12	0	18	0	0
4	A	344	0	239	17	0
5	A	2	0	0	0	0
6	A	306	0	0	2	2
All	All	4647	0	4011	29	2

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 (29) 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)
4:A:610:HEC:HBB3	4:A:610:HEC:HMB1	1.46	0.94
1:A:353[B]:ARG:HH21	1:A:353[B]:ARG:HG3	1.31	0.91
1:A:353[B]:ARG:HH21	1:A:353[B]:ARG:CG	1.88	0.86
4:A:610:HEC:HMC1	4:A:610:HEC:HBC3	1.63	0.79
1:A:446:MET:HE2	6:A:741:HOH:O	1.88	0.71
4:A:610:HEC:HMB1	4:A:610:HEC:CBB	2.22	0.63
4:A:607:HEC:HMC1	4:A:607:HEC:HBC3	1.81	0.62
4:A:614:HEC:HMB3	4:A:614:HEC:HBB3	1.81	0.60
4:A:607:HEC:HMB1	4:A:607:HEC:HBB3	1.86	0.58
4:A:613:HEC:HBC3	4:A:613:HEC:HMC3	1.85	0.57
1:A:353[B]:ARG:HG3	1:A:353[B]:ARG:NH2	2.09	0.56
1:A:444:MET:HE3	4:A:614:HEC:CMB	2.37	0.55
1:A:444:MET:HE3	4:A:614:HEC:HMB1	1.89	0.54
1:A:345:LEU:C	1:A:345:LEU:HD13	2.33	0.54
1:A:427:LEU:C	1:A:427:LEU:HD13	2.35	0.52
1:A:114[A]:GLU:H	1:A:114[A]:GLU:CD	2.19	0.49
1:A:353[B]:ARG:CG	1:A:353[B]:ARG:NH2	2.60	0.49
1:A:261:ILE:HG22	6:A:798:HOH:O	2.14	0.47
1:A:234:CYS:HB2	4:A:609:HEC:HMB1	1.96	0.46
1:A:143:ARG:NH2	1:A:145:ILE:HD11	2.31	0.46
1:A:306:MET:HE1	4:A:611:HEC:CHD	2.47	0.45
1:A:368:LEU:HD13	1:A:368:LEU:C	2.41	0.45
1:A:180:ASN:HB2	1:A:187:THR:HG21	2.00	0.44
1:A:444:MET:CE	4:A:614:HEC:HMB1	2.48	0.43
4:A:610:HEC:HMC1	4:A:610:HEC:CBC	2.44	0.43
1:A:198:HIS:CD2	4:A:612:HEC:ND	2.88	0.42
4:A:611:HEC:HMB3	4:A:611:HEC:CBB	2.50	0.42
1:A:205:ASN:HD22	4:A:612:HEC:CGD	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:610:HEC:CBB	4:A:610:HEC:CMB	2.94	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:739:HOH:O	6:A:810:HOH:O[5_555]	2.13	0.07
1:A:361:GLU:OE1	6:A:739:HOH:O[9_555]	2.16	0.04

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	498/500 (100%)	482 (97%)	16 (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	416/416 (100%)	413 (99%)	3 (1%)	76 87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114[A]	GLU
1	A	114[B]	GLU
1	A	409	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	106	GLN
1	A	166	ASN
1	A	335	HIS
1	A	459	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 ⓘ

15 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	$\# Z > 2$
4	HEC	A	612	1	50,50,50	1.86	9 (18%)	68,82,82	1.26	4 (5%)
4	HEC	A	609	1	50,50,50	1.87	10 (20%)	68,82,82	1.36	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	605	-	3,3,3	0.54	0	2,2,2	0.07	0
4	HEC	A	614	1	50,50,50	1.88	9 (18%)	68,82,82	1.27	4 (5%)
3	EDO	A	604	-	3,3,3	0.52	0	2,2,2	0.09	0
4	HEC	A	611	1	50,50,50	1.87	10 (20%)	68,82,82	1.30	8 (11%)
5	HOA	A	615	4	0,1,1	-	-	-	-	-
2	PO4	A	601	-	4,4,4	0.99	0	6,6,6	0.50	0
4	HEC	A	608	1	50,50,50	1.95	8 (16%)	68,82,82	1.35	7 (10%)
3	EDO	A	606	-	3,3,3	0.41	0	2,2,2	0.25	0
4	HEC	A	613	1	50,50,50	1.86	9 (18%)	68,82,82	1.31	7 (10%)
4	HEC	A	607	1	50,50,50	1.88	9 (18%)	68,82,82	1.33	7 (10%)
2	PO4	A	602	-	4,4,4	1.08	0	6,6,6	0.35	0
4	HEC	A	610	5,1	50,50,50	1.50	3 (6%)	68,82,82	1.70	11 (16%)
2	PO4	A	603	-	4,4,4	1.48	1 (25%)	6,6,6	0.45	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
4	HEC	A	612	1	1/1/3/7	9/14/54/54	-
3	EDO	A	605	-	-	1/1/1/1	-
4	HEC	A	614	1	1/1/3/7	7/14/54/54	-
4	HEC	A	611	1	1/1/3/7	4/14/54/54	-
3	EDO	A	604	-	-	0/1/1/1	-
4	HEC	A	608	1	1/1/3/7	6/14/54/54	-
4	HEC	A	613	1	1/1/3/7	4/14/54/54	-
3	EDO	A	606	-	-	1/1/1/1	-
4	HEC	A	607	1	1/1/3/7	7/14/54/54	-
4	HEC	A	610	5,1	1/1/3/7	6/14/54/54	-
4	HEC	A	609	1	1/1/3/7	7/14/54/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	HEC	C3D-C2D	7.73	1.53	1.36
4	A	608	HEC	C3D-C2D	7.70	1.53	1.36
4	A	611	HEC	C3D-C2D	7.56	1.53	1.36
4	A	607	HEC	C3D-C2D	7.53	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	614	HEC	C3D-C2D	7.52	1.53	1.36
4	A	612	HEC	C3D-C2D	7.51	1.53	1.36
4	A	613	HEC	C3D-C2D	7.38	1.52	1.36
4	A	609	HEC	C3D-C2D	7.37	1.52	1.36
4	A	608	HEC	FE-ND	5.25	2.11	1.94
4	A	613	HEC	FE-ND	4.67	2.09	1.94
4	A	611	HEC	CBB-CAB	-4.42	1.32	1.51
4	A	607	HEC	FE-ND	4.11	2.07	1.94
4	A	607	HEC	CBB-CAB	-4.04	1.34	1.51
4	A	609	HEC	FE-ND	4.02	2.07	1.94
4	A	614	HEC	CBB-CAB	-4.02	1.34	1.51
4	A	608	HEC	CBC-CAC	-4.00	1.34	1.51
4	A	612	HEC	CBC-CAC	-4.00	1.34	1.51
4	A	608	HEC	CBB-CAB	-3.99	1.34	1.51
4	A	611	HEC	CBC-CAC	-3.98	1.34	1.51
4	A	609	HEC	CBB-CAB	-3.97	1.34	1.51
4	A	613	HEC	CBC-CAC	-3.94	1.34	1.51
4	A	607	HEC	CBC-CAC	-3.93	1.34	1.51
4	A	612	HEC	CBB-CAB	-3.89	1.35	1.51
4	A	613	HEC	CBB-CAB	-3.89	1.35	1.51
4	A	614	HEC	CBC-CAC	-3.88	1.35	1.51
4	A	609	HEC	CBC-CAC	-3.84	1.35	1.51
4	A	612	HEC	FE-ND	3.83	2.06	1.94
4	A	608	HEC	FE-NB	3.56	2.05	1.94
4	A	614	HEC	FE-ND	3.52	2.05	1.94
4	A	614	HEC	FE-NB	3.45	2.05	1.94
4	A	611	HEC	FE-ND	3.38	2.05	1.94
4	A	612	HEC	FE-NA	3.32	2.06	1.95
4	A	613	HEC	FE-NC	3.26	2.05	1.95
4	A	608	HEC	FE-NC	3.20	2.05	1.95
4	A	607	HEC	FE-NC	3.13	2.05	1.95
4	A	611	HEC	FE-NC	3.12	2.05	1.95
4	A	614	HEC	FE-NC	3.08	2.05	1.95
4	A	607	HEC	FE-NA	3.07	2.05	1.95
4	A	612	HEC	FE-NC	3.07	2.05	1.95
4	A	607	HEC	FE-NB	3.04	2.04	1.94
4	A	609	HEC	FE-NC	3.04	2.05	1.95
4	A	609	HEC	FE-NA	2.92	2.04	1.95
4	A	611	HEC	FE-NA	2.87	2.04	1.95
4	A	609	HEC	FE-NB	2.80	2.03	1.94
4	A	614	HEC	FE-NA	2.77	2.04	1.95
4	A	612	HEC	FE-NB	2.46	2.02	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	PO4	P-O3	-2.35	1.47	1.54
4	A	613	HEC	C3C-C2C	-2.21	1.33	1.38
4	A	611	HEC	CMB-C2B	2.21	1.55	1.50
4	A	613	HEC	CMC-C2C	2.19	1.55	1.50
4	A	613	HEC	CMA-C3A	2.18	1.55	1.50
4	A	607	HEC	CMA-C3A	2.18	1.55	1.50
4	A	609	HEC	CMC-C2C	2.17	1.55	1.50
4	A	609	HEC	CMD-C2D	2.16	1.55	1.50
4	A	612	HEC	CMB-C2B	2.15	1.55	1.50
4	A	611	HEC	CMC-C2C	2.15	1.55	1.50
4	A	611	HEC	CMD-C2D	2.13	1.55	1.50
4	A	607	HEC	CMD-C2D	2.10	1.55	1.50
4	A	610	HEC	CMA-C3A	2.09	1.55	1.50
4	A	610	HEC	CMC-C2C	2.08	1.55	1.50
4	A	614	HEC	CMA-C3A	2.07	1.55	1.50
4	A	608	HEC	CMD-C2D	2.05	1.55	1.50
4	A	611	HEC	CMA-C3A	2.05	1.55	1.50
4	A	608	HEC	C3C-C2C	-2.05	1.33	1.38
4	A	613	HEC	FE-NA	2.04	2.01	1.95
4	A	612	HEC	CMA-C3A	2.03	1.54	1.50
4	A	609	HEC	CMB-C2B	2.02	1.54	1.50
4	A	614	HEC	C3C-C2C	-2.01	1.33	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	HEC	C1D-ND-C4D	5.73	111.99	105.21
4	A	610	HEC	C3B-C4B-NB	-5.21	104.46	110.17
4	A	609	HEC	C1D-ND-C4D	5.15	111.31	105.21
4	A	608	HEC	C1D-ND-C4D	5.14	111.30	105.21
4	A	613	HEC	C1D-ND-C4D	5.04	111.18	105.21
4	A	612	HEC	C1D-ND-C4D	5.04	111.17	105.21
4	A	614	HEC	C1D-ND-C4D	4.85	110.94	105.21
4	A	607	HEC	C1D-ND-C4D	4.73	110.81	105.21
4	A	611	HEC	C1D-ND-C4D	4.46	110.49	105.21
4	A	610	HEC	C4B-NB-C1B	4.34	110.34	105.21
4	A	610	HEC	C2A-C1A-NA	-3.27	107.17	110.32
4	A	607	HEC	CBC-CAC-C3C	3.22	121.14	112.42
4	A	608	HEC	CBC-CAC-C3C	3.16	120.98	112.42
4	A	610	HEC	C2C-C1C-NC	-3.15	105.09	110.14
4	A	611	HEC	CBB-CAB-C3B	3.15	120.96	112.42
4	A	610	HEC	CHC-C4B-NB	-3.14	120.48	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	HEC	C3C-C4C-NC	-2.97	106.86	110.15
4	A	607	HEC	C2A-C1A-NA	-2.96	107.47	110.32
4	A	609	HEC	CBC-CAC-C3C	2.96	120.44	112.42
4	A	614	HEC	CBC-CAC-C3C	2.83	120.09	112.42
4	A	607	HEC	CBB-CAB-C3B	2.82	120.05	112.42
4	A	610	HEC	C2B-C1B-NB	-2.79	106.68	109.90
4	A	612	HEC	CBB-CAB-C3B	2.75	119.89	112.42
4	A	614	HEC	CBB-CAB-C3B	2.72	119.79	112.42
4	A	611	HEC	CAB-C3B-C4B	-2.70	121.27	124.79
4	A	608	HEC	C2A-C1A-NA	-2.69	107.73	110.32
4	A	613	HEC	CBC-CAC-C3C	2.60	119.46	112.42
4	A	611	HEC	CHC-C4B-NB	2.57	127.54	124.37
4	A	608	HEC	CBB-CAB-C3B	2.52	119.24	112.42
4	A	613	HEC	C4B-NB-C1B	2.48	108.14	105.21
4	A	611	HEC	CBC-CAC-C3C	2.47	119.12	112.42
4	A	611	HEC	C2A-C1A-NA	-2.47	107.94	110.32
4	A	613	HEC	C2A-C1A-NA	-2.43	107.97	110.32
4	A	612	HEC	C2A-C1A-NA	-2.43	107.98	110.32
4	A	613	HEC	C3B-C4B-NB	-2.43	107.50	110.17
4	A	609	HEC	CBB-CAB-C3B	2.30	118.65	112.42
4	A	610	HEC	CHA-C1A-C2A	2.29	128.47	124.86
4	A	609	HEC	C3D-C4D-ND	-2.27	108.16	110.35
4	A	612	HEC	CBC-CAC-C3C	2.25	118.52	112.42
4	A	607	HEC	C3B-C4B-NB	-2.23	107.73	110.17
4	A	614	HEC	C4B-NB-C1B	2.23	107.84	105.21
4	A	609	HEC	C2A-C1A-NA	-2.22	108.18	110.32
4	A	610	HEC	C3D-C4D-ND	-2.19	108.23	110.35
4	A	611	HEC	C3B-C4B-NB	-2.18	107.78	110.17
4	A	608	HEC	C4B-NB-C1B	2.16	107.76	105.21
4	A	608	HEC	C3B-C4B-NB	-2.16	107.80	110.17
4	A	607	HEC	CBA-CAA-C2A	-2.13	106.65	112.53
4	A	611	HEC	CHD-C1D-ND	2.12	126.99	124.37
4	A	613	HEC	CAC-C3C-C2C	-2.12	123.54	126.89
4	A	609	HEC	CAD-CBD-CGD	-2.11	108.07	113.67
4	A	608	HEC	CHB-C4A-NA	2.10	126.74	124.45
4	A	607	HEC	C1D-C2D-C3D	-2.08	104.79	106.98
4	A	610	HEC	CAD-C3D-C2D	-2.04	124.05	127.87
4	A	613	HEC	CBB-CAB-C3B	2.03	117.92	112.42
4	A	609	HEC	O1A-CGA-CBA	-2.01	116.72	123.09
4	A	609	HEC	CHD-C1D-ND	2.00	126.84	124.37

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	607	HEC	NA
4	A	608	HEC	NA
4	A	609	HEC	NA
4	A	610	HEC	NA
4	A	611	HEC	NA
4	A	612	HEC	NA
4	A	613	HEC	NA
4	A	614	HEC	NA

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	607	HEC	C2C-C3C-CAC-CBC
4	A	611	HEC	C2B-C3B-CAB-CBB
4	A	610	HEC	C2B-C3B-CAB-CBB
4	A	610	HEC	C4C-C3C-CAC-CBC
4	A	610	HEC	C4B-C3B-CAB-CBB
4	A	611	HEC	C4B-C3B-CAB-CBB
4	A	607	HEC	C4C-C3C-CAC-CBC
4	A	612	HEC	C4B-C3B-CAB-CBB
4	A	612	HEC	C2B-C3B-CAB-CBB
4	A	607	HEC	C2B-C3B-CAB-CBB
4	A	608	HEC	C4C-C3C-CAC-CBC
4	A	609	HEC	C4C-C3C-CAC-CBC
4	A	614	HEC	C2B-C3B-CAB-CBB
4	A	611	HEC	C2C-C3C-CAC-CBC
4	A	610	HEC	C2C-C3C-CAC-CBC
4	A	614	HEC	C4B-C3B-CAB-CBB
4	A	609	HEC	C2B-C3B-CAB-CBB
4	A	613	HEC	C2B-C3B-CAB-CBB
3	A	606	EDO	O1-C1-C2-O2
4	A	613	HEC	C4C-C3C-CAC-CBC
4	A	614	HEC	C4C-C3C-CAC-CBC
4	A	611	HEC	C4C-C3C-CAC-CBC
4	A	612	HEC	C4C-C3C-CAC-CBC
4	A	612	HEC	C4D-C3D-CAD-CBD
4	A	612	HEC	C2C-C3C-CAC-CBC
4	A	607	HEC	C4B-C3B-CAB-CBB
4	A	608	HEC	C2B-C3B-CAB-CBB
4	A	608	HEC	C2C-C3C-CAC-CBC
4	A	608	HEC	C4B-C3B-CAB-CBB
4	A	614	HEC	C3D-CAD-CBD-CGD
4	A	614	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	A	610	HEC	CAA-CBA-CGA-O2A
4	A	607	HEC	CAD-CBD-CGD-O1D
4	A	609	HEC	C2C-C3C-CAC-CBC
4	A	612	HEC	CAA-CBA-CGA-O2A
4	A	607	HEC	CAD-CBD-CGD-O2D
3	A	605	EDO	O1-C1-C2-O2
4	A	614	HEC	CAD-CBD-CGD-O2D
4	A	609	HEC	CAD-CBD-CGD-O2D
4	A	607	HEC	C2D-C3D-CAD-CBD
4	A	609	HEC	CAD-CBD-CGD-O1D
4	A	610	HEC	CAA-CBA-CGA-O1A
4	A	612	HEC	CAD-CBD-CGD-O1D
4	A	612	HEC	CAD-CBD-CGD-O2D
4	A	609	HEC	C4B-C3B-CAB-CBB
4	A	614	HEC	CAD-CBD-CGD-O1D
4	A	612	HEC	CAA-CBA-CGA-O1A
4	A	609	HEC	CAA-CBA-CGA-O1A
4	A	608	HEC	CAA-CBA-CGA-O2A
4	A	613	HEC	CAD-CBD-CGD-O2D
4	A	608	HEC	CAD-CBD-CGD-O2D
4	A	613	HEC	CAD-CBD-CGD-O1D

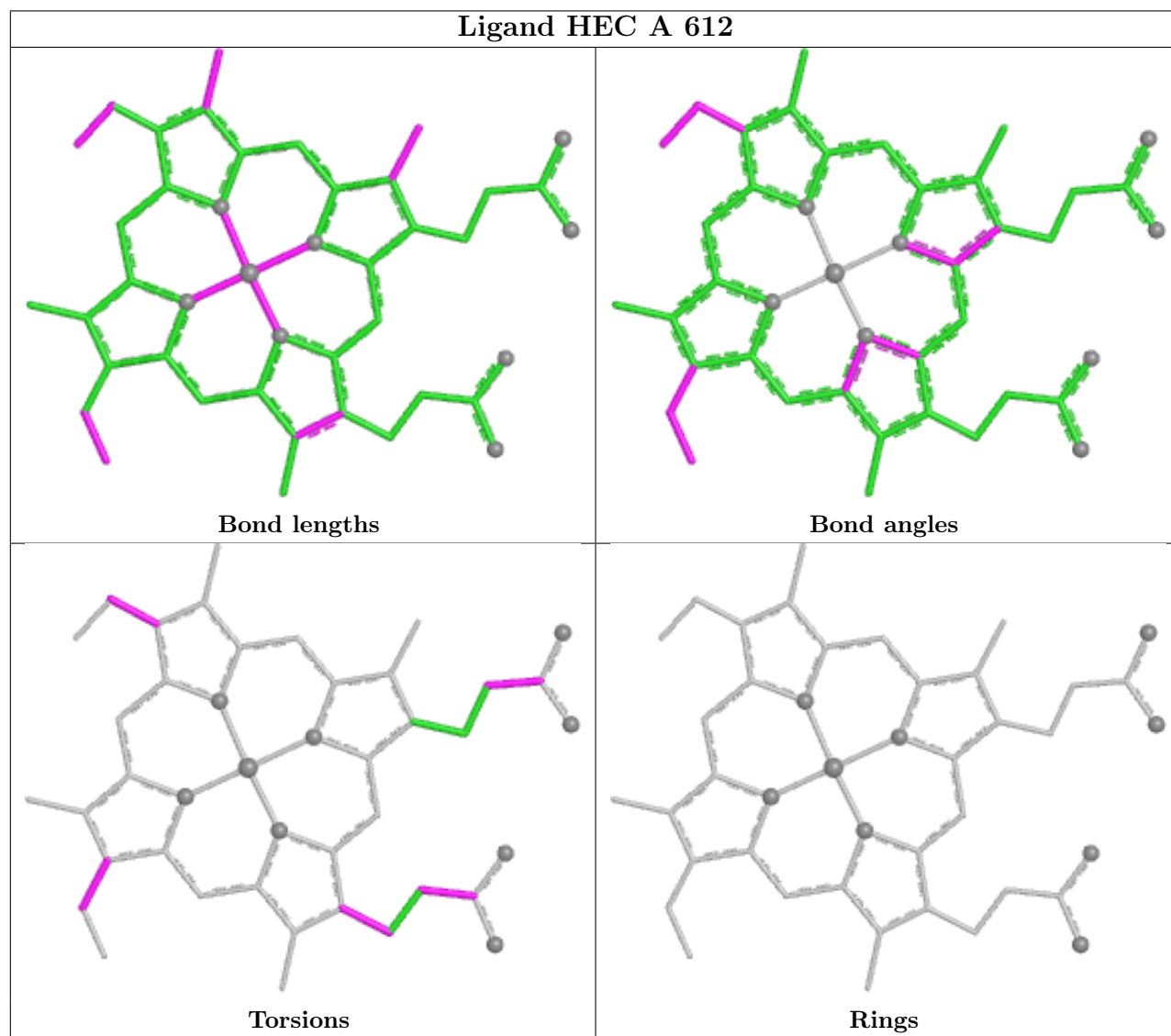
There are no ring outliers.

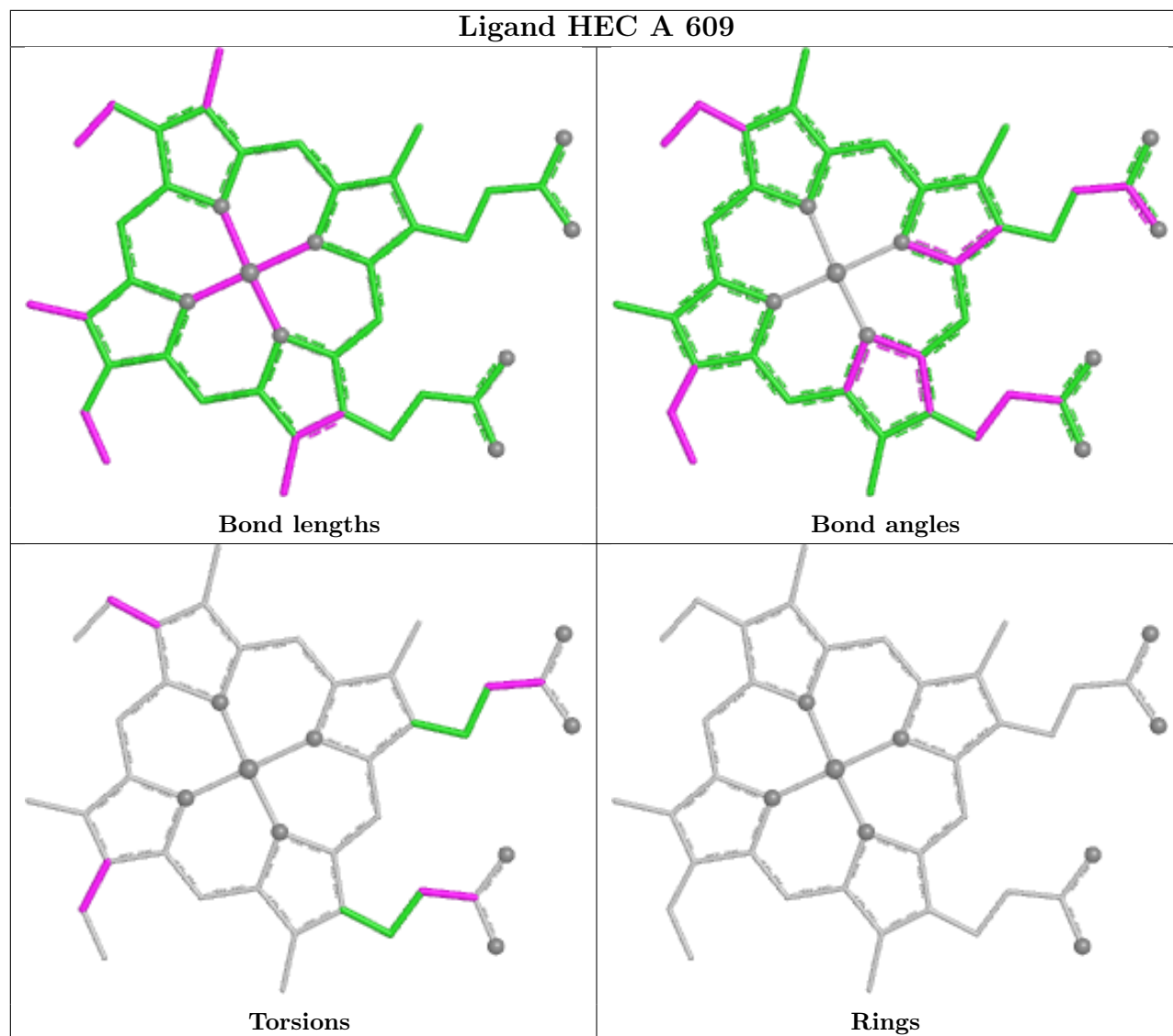
7 monomers are involved in 17 short contacts:

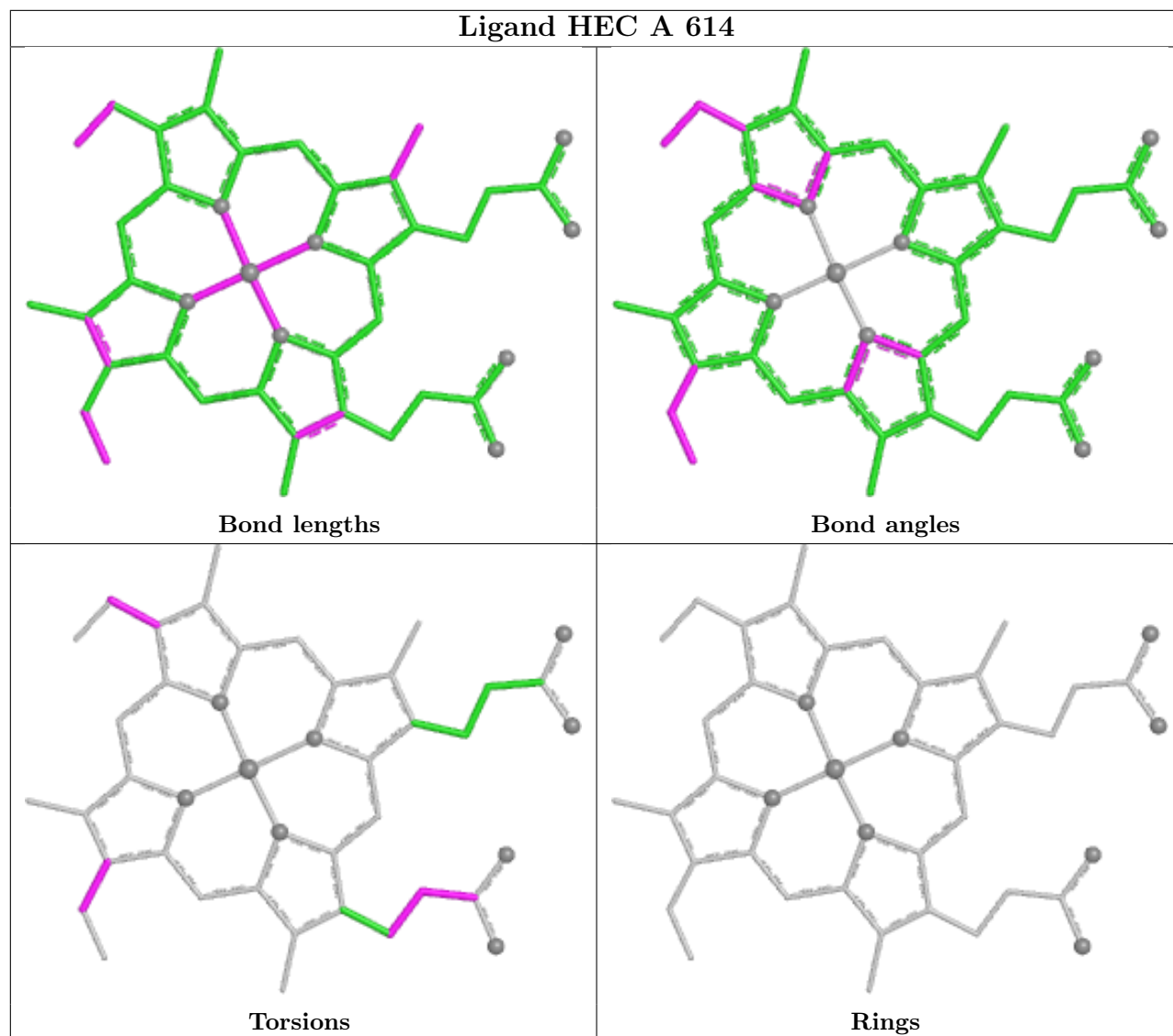
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	612	HEC	2	0
4	A	609	HEC	1	0
4	A	614	HEC	4	0
4	A	611	HEC	2	0
4	A	613	HEC	1	0
4	A	607	HEC	2	0
4	A	610	HEC	5	0

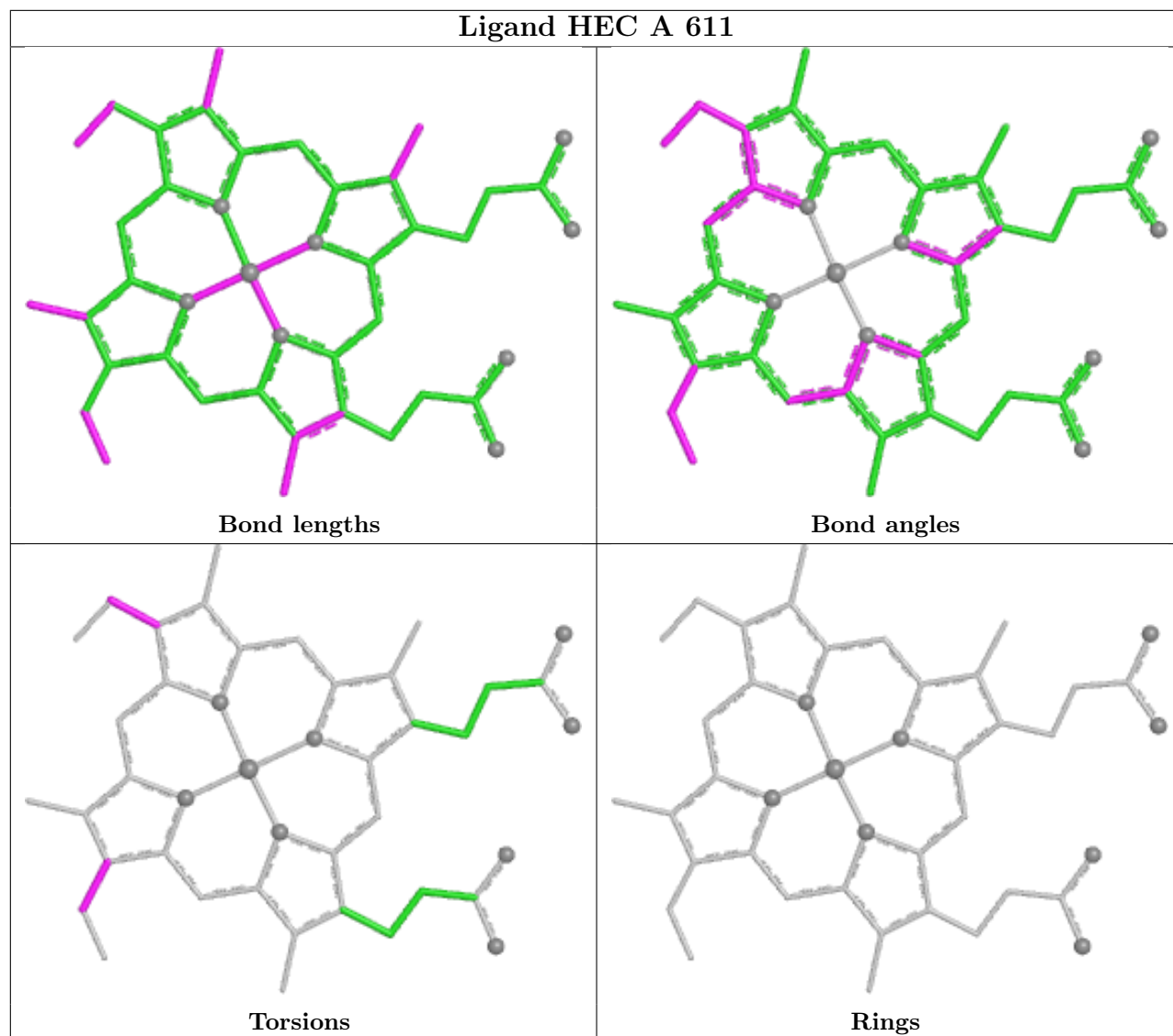
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

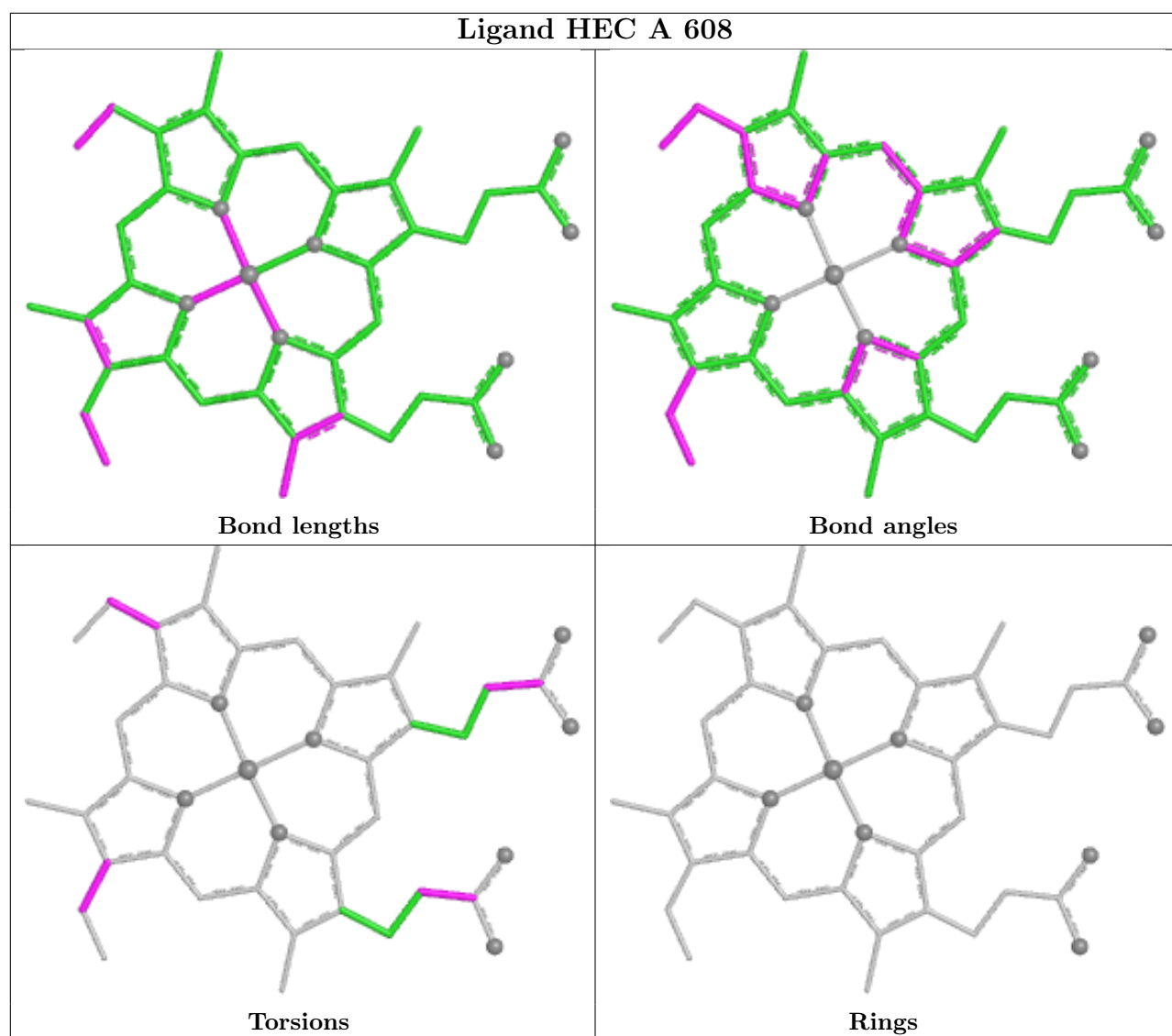
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



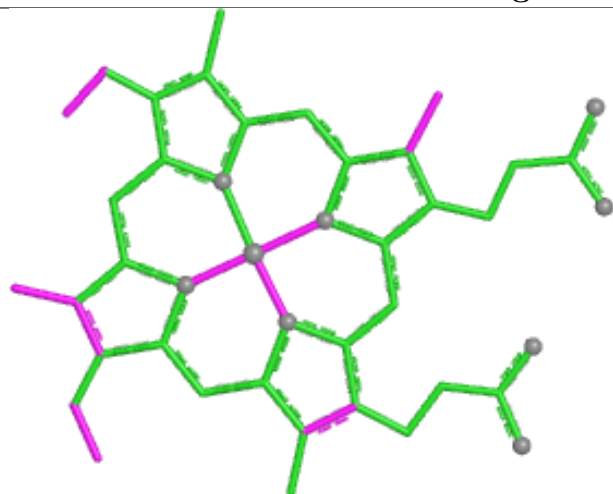




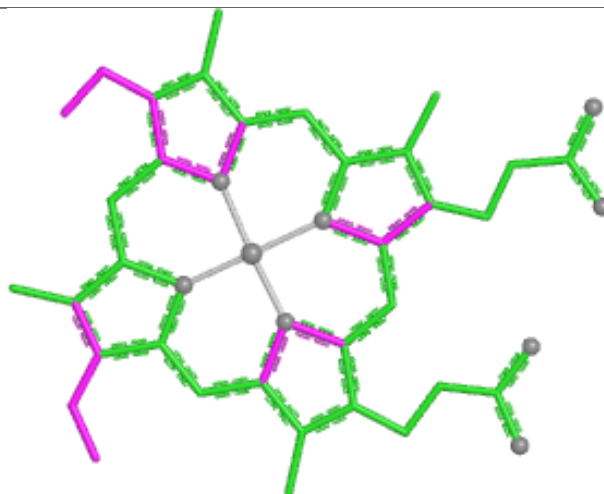




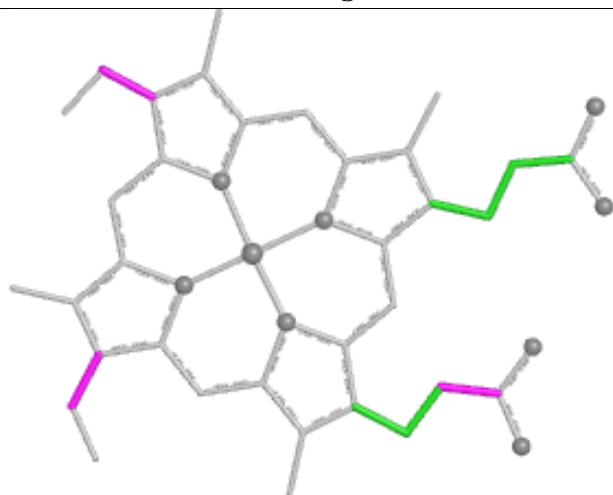
Ligand HEC A 613



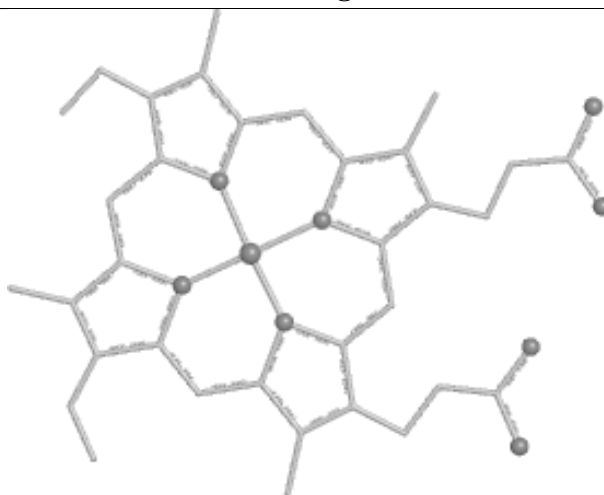
Bond lengths



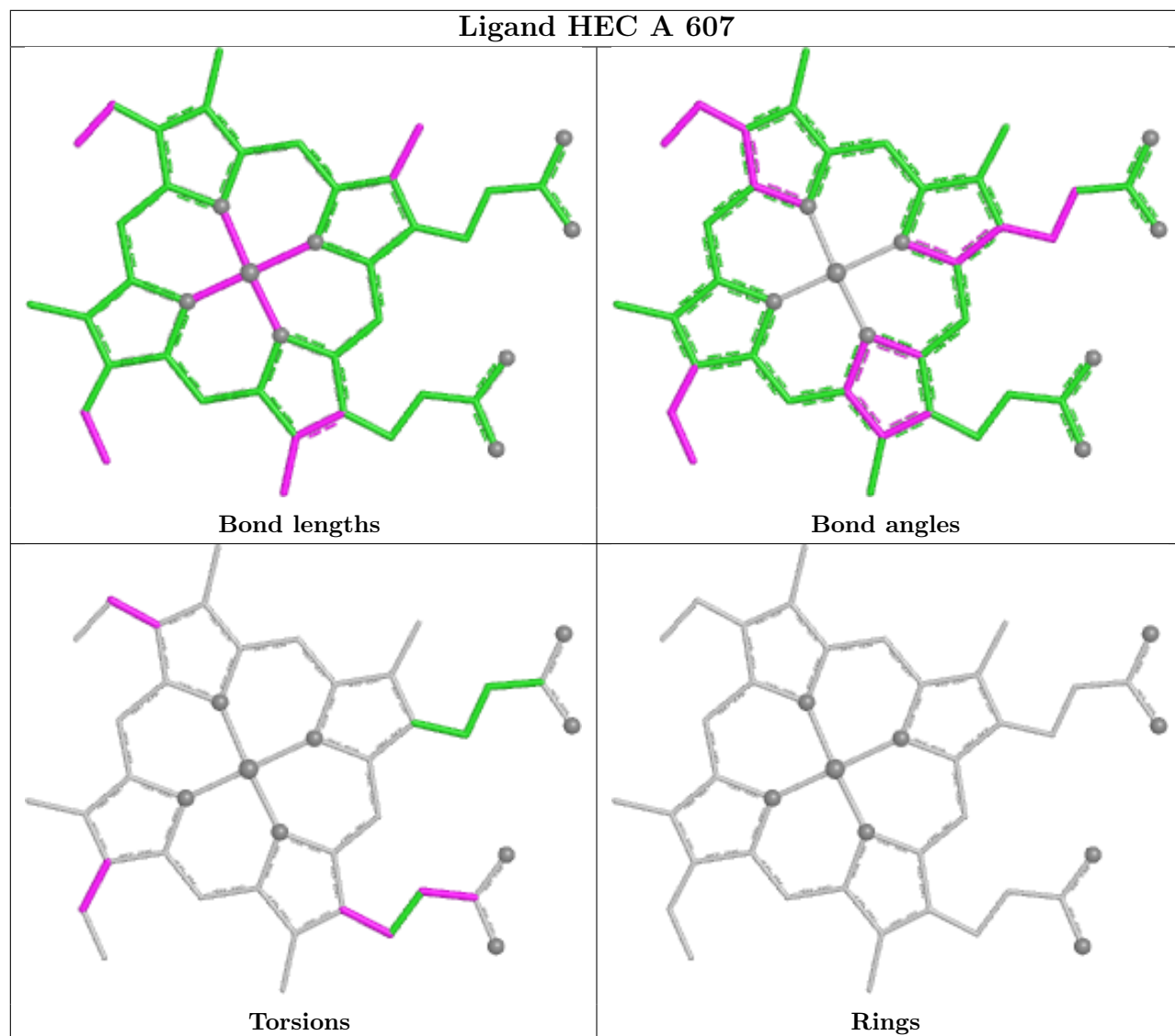
Bond angles

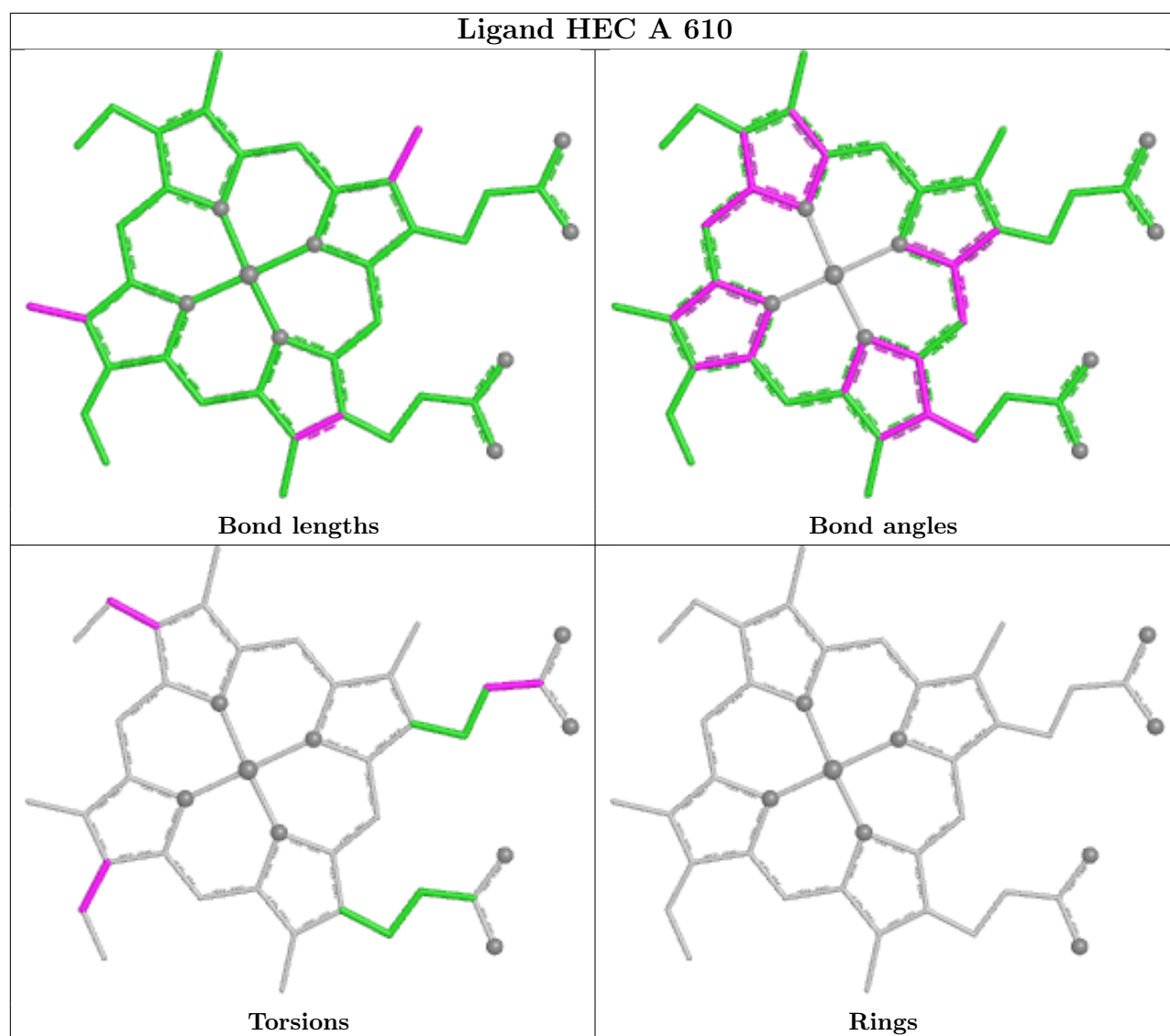


Torsions



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%)	-0.38	6 (1%) 76 74	11, 25, 39, 55	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	ILE	4.6
1	A	39	PRO	3.0
1	A	38	GLY	2.8
1	A	533	GLU	2.8
1	A	140	ASP	2.4
1	A	114[A]	GLU	2.2

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.

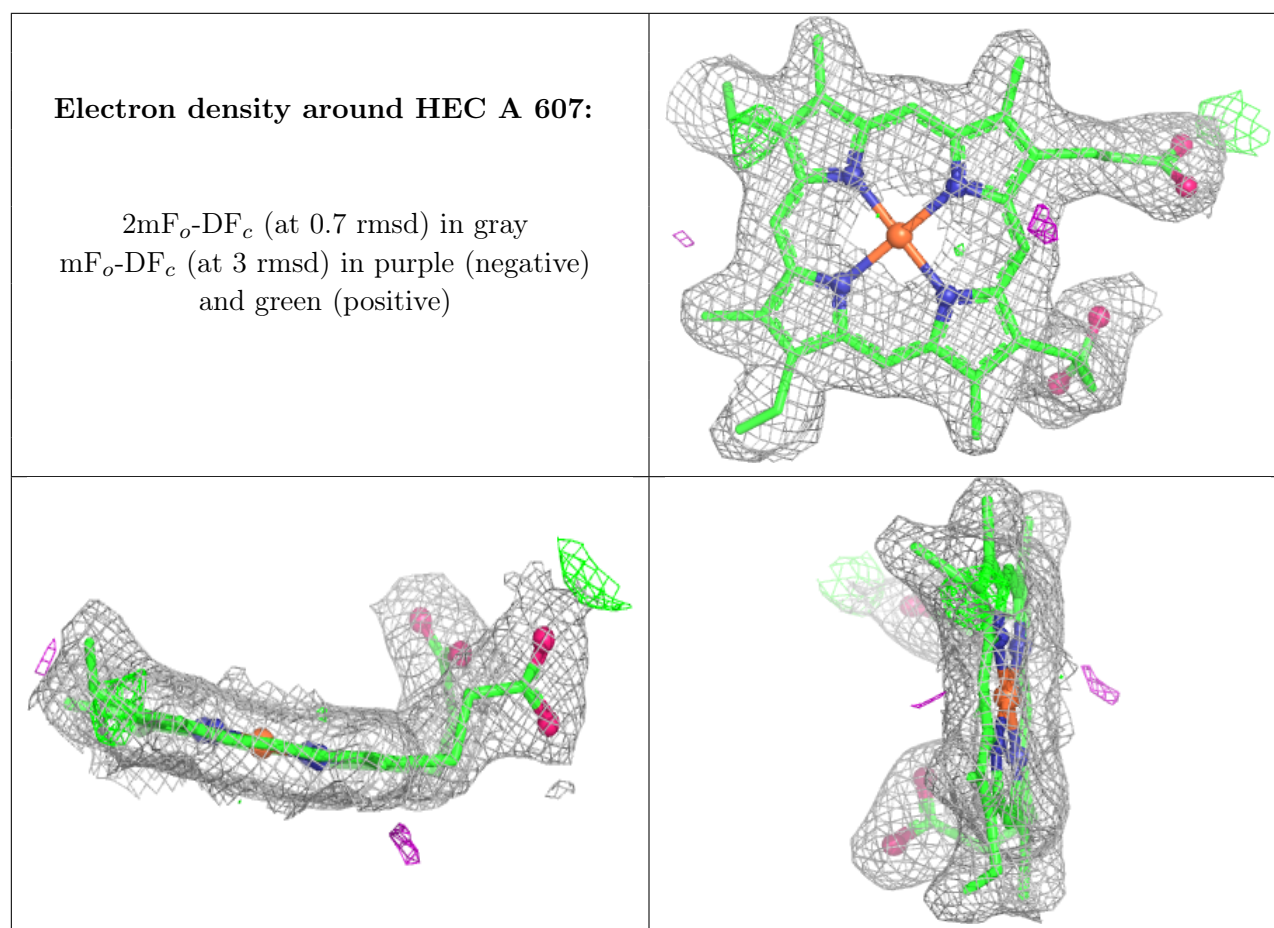
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	605	4/4	0.61	0.32	43,44,44,44	0

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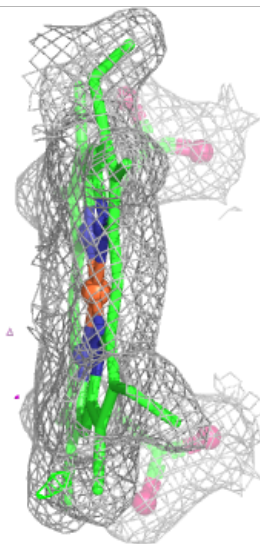
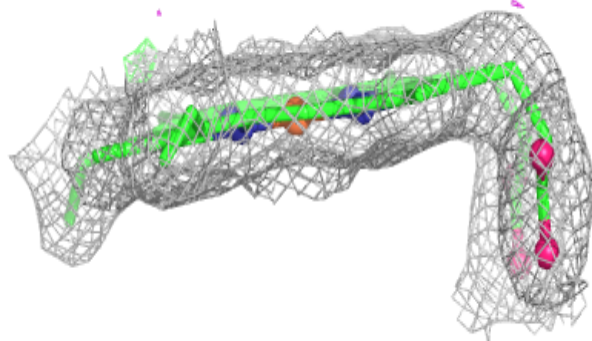
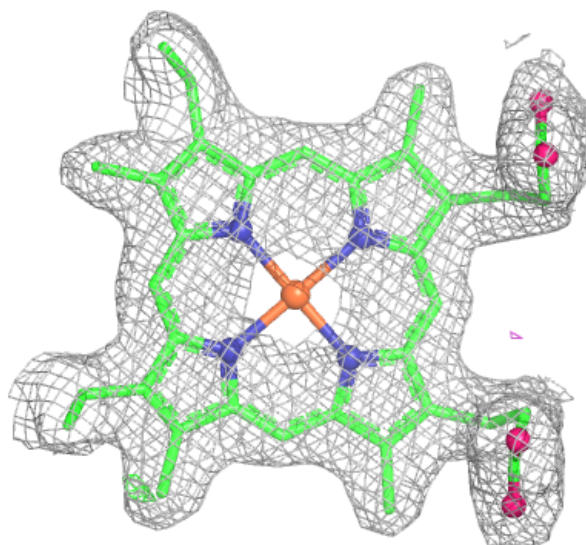
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	606	4/4	0.80	0.43	78,78,78,78	0
3	EDO	A	604	4/4	0.94	0.08	26,26,26,26	0
2	PO4	A	602	5/5	0.97	0.09	30,30,32,32	0
2	PO4	A	603	5/5	0.98	0.06	31,31,31,32	5
2	PO4	A	601	5/5	0.98	0.07	30,30,32,33	0
4	HEC	A	607	43/43	0.98	0.07	23,25,28,28	0
4	HEC	A	608	43/43	0.98	0.05	19,20,21,22	0
4	HEC	A	609	43/43	0.98	0.06	19,21,24,24	0
4	HEC	A	610	43/43	0.98	0.06	18,21,25,29	0
4	HEC	A	611	43/43	0.98	0.06	16,18,21,23	0
4	HEC	A	612	43/43	0.98	0.06	17,18,21,22	0
4	HEC	A	613	43/43	0.98	0.06	15,17,22,24	0
5	HOA	A	615	2/2	0.98	0.05	23,23,23,23	0
4	HEC	A	614	43/43	0.99	0.05	17,18,19,20	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.



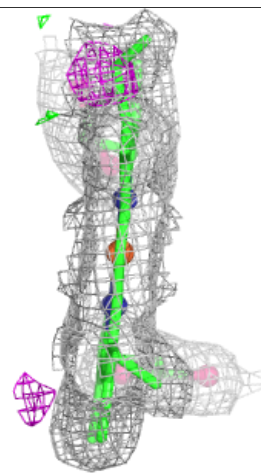
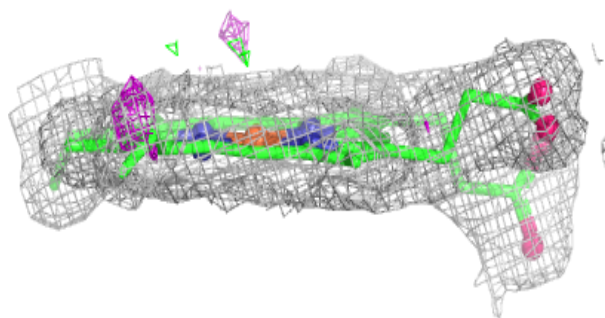
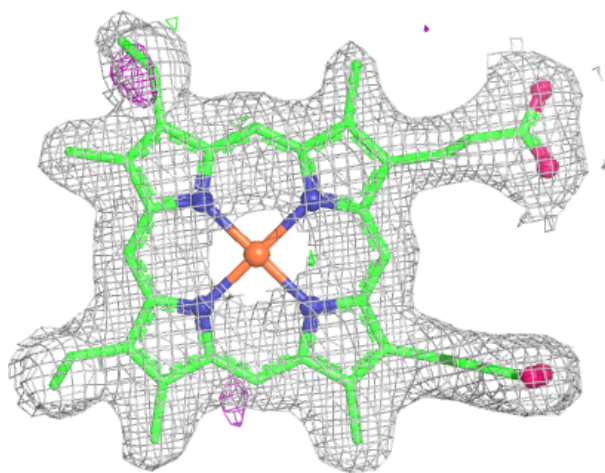
Electron density around HEC A 608:

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



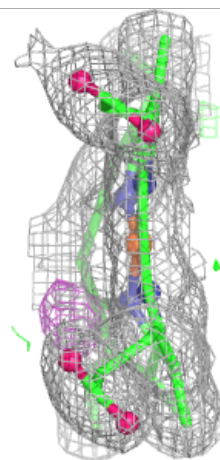
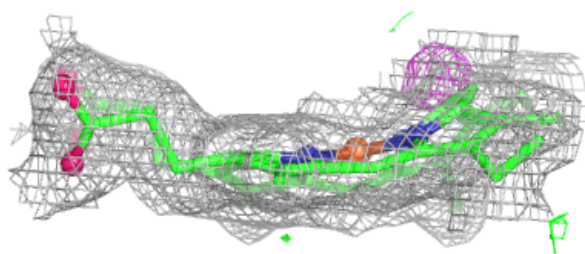
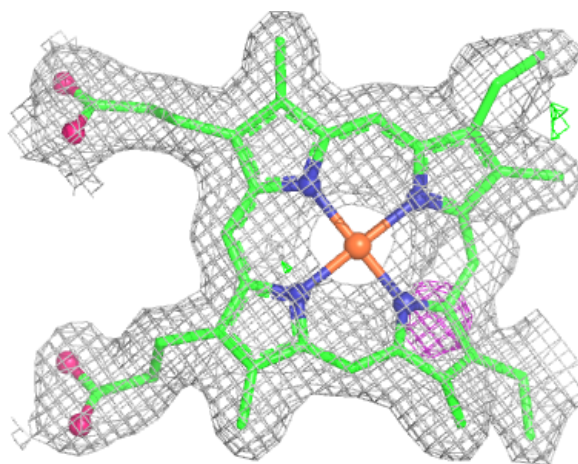
Electron density around HEC A 609:

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



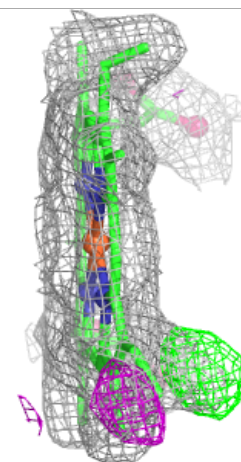
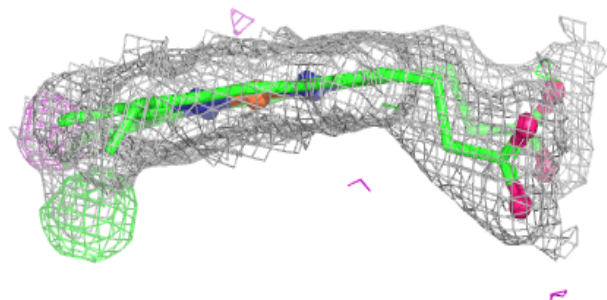
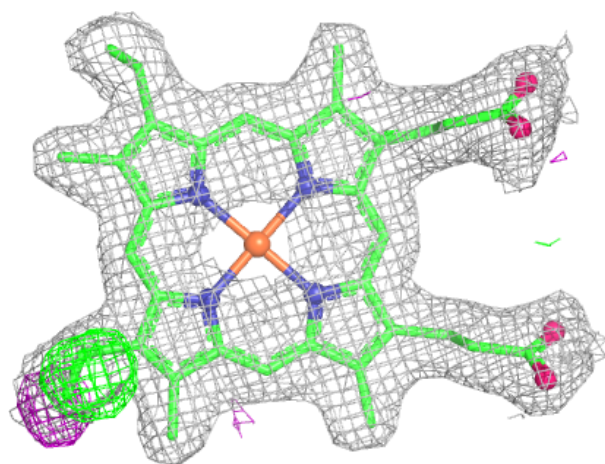
Electron density around HEC A 610:

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



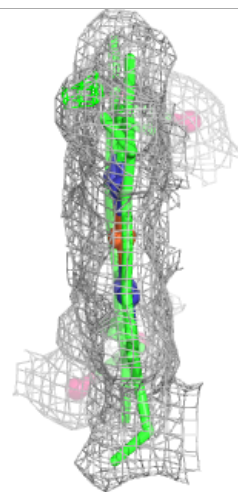
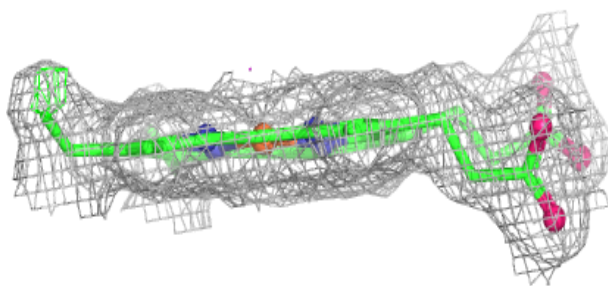
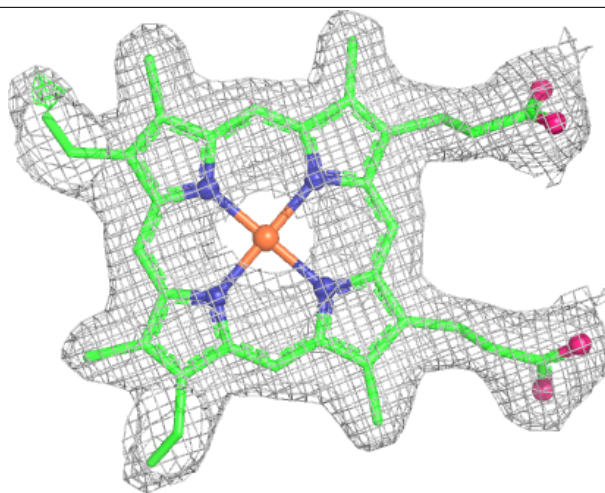
Electron density around HEC A 611:

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



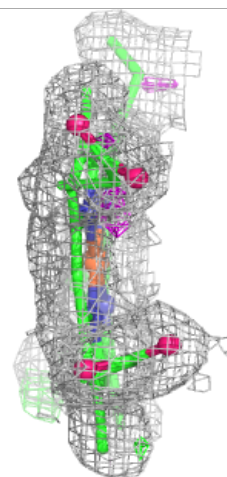
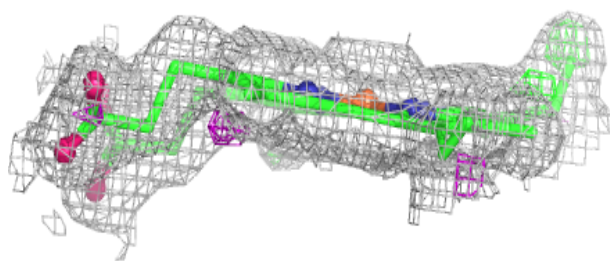
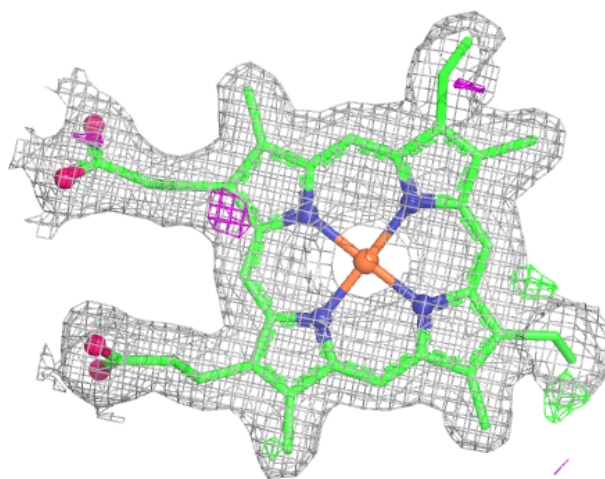
Electron density around HEC A 612:

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



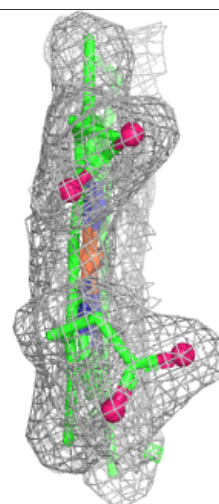
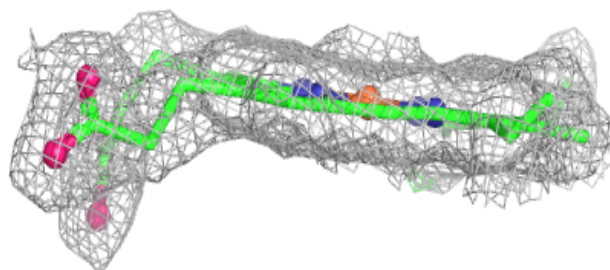
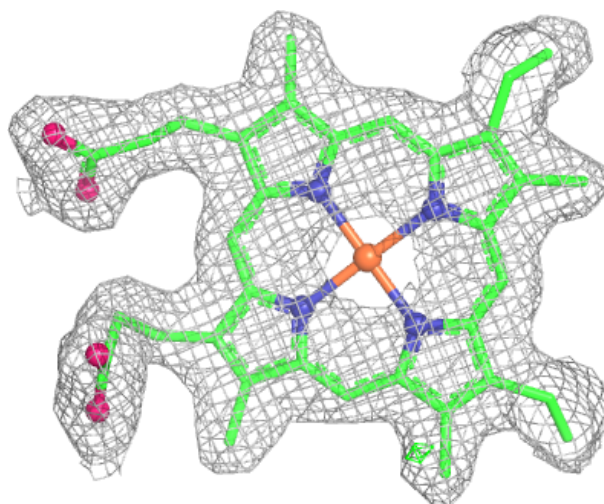
Electron density around HEC A 613:

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



Electron density around HEC A 614:

$2mF_o-DF_c$ (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.