



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 AM UTC

PDB ID : 4N4J / pdb_00004n4j
Title : Kuenenia stuttgartiensis hydroxylamine oxidoreductase
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 : 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 : 9.0.010 (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

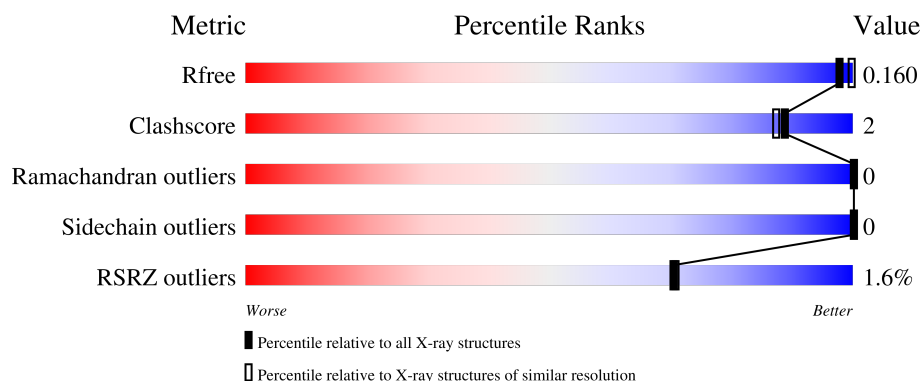
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	 2% 97%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4872 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.

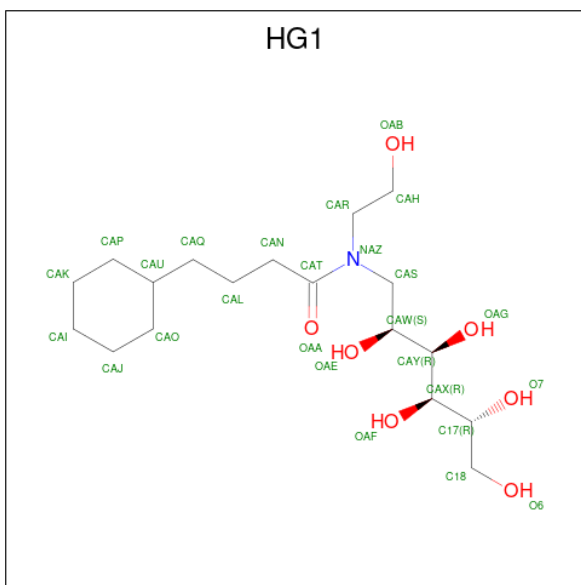
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	6	0
			3979	2499	708	741	31			

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



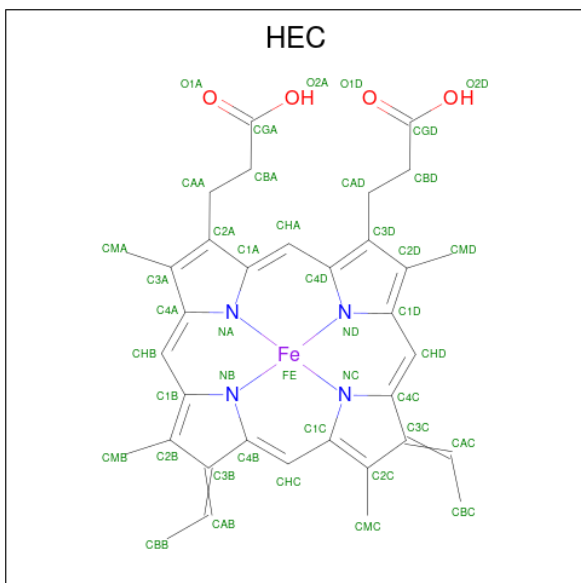
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1-[(4-cyclohexylbutanoyl)(2-hydroxyethyl)amino]-1-deoxy-D-glucitol (CCD ID: HG1) (formula: C₁₈H₃₅NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 10	N 1	O 1	0	0
3	A	1	Total 21	C 16	N 1	O 4	0	0
3	A	1	Total 15	C 12	N 1	O 2	0	0
3	A	1	Total 9	C 9			0	0

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



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

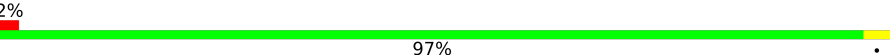
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	472	Total	O	0	0
			472	472		

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	130.00Å 130.00Å 130.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.96 – 1.80 45.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.96-1.80) 100.0 (45.96-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.010	Depositor
R, R_{free}	0.143 , 0.157 0.150 , 0.160	Depositor DCC
R_{free} test set	3340 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4872	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: HG1, PO4, 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	0.41	0/4097	0.66	0/5545

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 [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	3979	0	3758	10	2
2	A	20	0	0	0	0
3	A	57	0	81	1	0
4	A	344	0	240	10	2
5	A	472	0	0	0	0
All	All	4872	0	4079	16	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 2.

All (16) 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:612:HEC:HMC1	4:A:612:HEC:HBC3	1.69	0.75
1:A:98:GLU:OE1	1:A:177:LYS:HD2	1.98	0.62
4:A:612:HEC:HMC1	4:A:612:HEC:CBC	2.38	0.54
4:A:609:HEC:HBC3	4:A:609:HEC:HMC3	1.93	0.49
4:A:616:HEC:HMB3	4:A:616:HEC:HBB3	1.96	0.48
4:A:612:HEC:HAD2	4:A:614:HEC:HBD2	1.96	0.47
1:A:180:ASN:HB2	1:A:187:THR:HG21	1.98	0.46
4:A:609:HEC:HMC3	4:A:609:HEC:CBC	2.47	0.45
1:A:205:ASN:O	4:A:612:HEC:HHB	2.19	0.43
1:A:345:LEU:C	1:A:345:LEU:HD13	2.43	0.42
1:A:273:ILE:HD12	4:A:616:HEC:HAA2	2.01	0.42
1:A:62:TYR:CG	1:A:68:ALA:HB2	2.54	0.42
1:A:414:PRO:HB2	3:A:606:HG1:H4	2.01	0.42
1:A:427:LEU:C	1:A:427:LEU:HD13	2.45	0.42
1:A:234:CYS:HB3	4:A:611:HEC:HMB2	2.01	0.41
1:A:198:HIS:CD2	4:A:614:HEC:ND	2.88	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)
1:A:451:TYR:OH	4:A:612:HEC:C4B[12_455]	1.49	0.71
1:A:451:TYR:CE2	4:A:612:HEC:CHC[12_455]	1.51	0.69

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/500 (100%)	491 (98%)	10 (2%)	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	419/416 (101%)	419 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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](#)

16 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	604	-	4,4,4	0.86	0	6,6,6	0.51	0
4	HEC	A	616	1	46,50,50	1.95	7 (15%)	58,82,82	1.35	3 (5%)
3	HG1	A	607	-	15,15,26	0.57	0	17,17,33	0.47	0
4	HEC	A	612	1,5	46,50,50	2.89	18 (39%)	58,82,82	3.28	16 (27%)
4	HEC	A	613	1	46,50,50	1.94	7 (15%)	58,82,82	1.54	5 (8%)
3	HG1	A	605	-	12,12,26	0.24	0	14,14,33	0.76	0
2	PO4	A	601	-	4,4,4	0.97	0	6,6,6	0.66	0
4	HEC	A	614	1	46,50,50	1.96	8 (17%)	58,82,82	1.36	6 (10%)
4	HEC	A	615	1	46,50,50	1.90	7 (15%)	58,82,82	1.48	6 (10%)
3	HG1	A	608	-	9,9,26	0.47	0	10,10,33	0.58	0
4	HEC	A	611	1	46,50,50	1.93	6 (13%)	58,82,82	1.44	8 (13%)
2	PO4	A	602	-	4,4,4	0.99	0	6,6,6	0.68	0
4	HEC	A	610	1	46,50,50	1.92	8 (17%)	58,82,82	1.37	5 (8%)
3	HG1	A	606	-	21,21,26	0.61	0	23,25,33	0.88	1 (4%)
4	HEC	A	609	1	46,50,50	1.96	9 (19%)	58,82,82	1.35	5 (8%)
2	PO4	A	603	-	4,4,4	1.15	0	6,6,6	0.33	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	616	1	-	7/14/54/54	-
3	HG1	A	607	-	-	3/10/18/39	0/1/1/1
4	HEC	A	612	1,5	-	6/14/54/54	-
4	HEC	A	613	1	-	4/14/54/54	-
3	HG1	A	605	-	-	0/6/14/39	0/1/1/1
4	HEC	A	614	1	-	8/14/54/54	-
4	HEC	A	615	1	-	5/14/54/54	-
4	HEC	A	611	1	-	7/14/54/54	-
4	HEC	A	610	1	-	4/14/54/54	-
3	HG1	A	606	-	-	6/20/28/39	0/1/1/1
4	HEC	A	609	1	-	6/14/54/54	-
3	HG1	A	608	-	-	1/3/11/39	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	612	HEC	CHC-C4B	9.57	1.57	1.38
4	A	609	HEC	CAC-C3C	6.22	1.55	1.35
4	A	615	HEC	CAC-C3C	6.17	1.55	1.35
4	A	611	HEC	CAC-C3C	6.16	1.55	1.35
4	A	611	HEC	CAB-C3B	6.10	1.54	1.35
4	A	614	HEC	CAC-C3C	6.08	1.54	1.35
4	A	614	HEC	CAB-C3B	6.06	1.54	1.35
4	A	610	HEC	CAC-C3C	6.03	1.54	1.35
4	A	616	HEC	CAC-C3C	6.00	1.54	1.35
4	A	613	HEC	CAC-C3C	5.91	1.54	1.35
4	A	613	HEC	CAB-C3B	5.86	1.54	1.35
4	A	609	HEC	CAB-C3B	5.84	1.54	1.35
4	A	610	HEC	CAB-C3B	5.72	1.53	1.35
4	A	616	HEC	CAB-C3B	5.71	1.53	1.35
4	A	615	HEC	CAB-C3B	5.48	1.52	1.35
4	A	613	HEC	C3D-C2D	5.28	1.52	1.38
4	A	612	HEC	C1A-C2A	5.27	1.54	1.45
4	A	609	HEC	C3D-C2D	5.25	1.52	1.38
4	A	612	HEC	C3B-C4B	5.18	1.55	1.46
4	A	614	HEC	C3D-C2D	5.17	1.52	1.38
4	A	612	HEC	C4C-NC	5.08	1.49	1.39
4	A	616	HEC	C3D-C2D	5.08	1.52	1.38
4	A	615	HEC	C3D-C2D	5.06	1.52	1.38
4	A	611	HEC	C3D-C2D	5.01	1.52	1.38
4	A	610	HEC	C3D-C2D	4.95	1.51	1.38
4	A	612	HEC	C1A-NA	4.59	1.48	1.39
4	A	612	HEC	CHA-C1A	4.57	1.47	1.38
4	A	612	HEC	CAC-C3C	4.31	1.49	1.35
4	A	612	HEC	CAB-C3B	4.29	1.48	1.35
4	A	612	HEC	CHD-C4C	4.09	1.46	1.38
4	A	609	HEC	CBC-CAC	-4.07	1.34	1.49
4	A	609	HEC	CBB-CAB	-4.07	1.34	1.49
4	A	616	HEC	CBB-CAB	-4.02	1.34	1.49
4	A	614	HEC	CBC-CAC	-4.01	1.34	1.49
4	A	612	HEC	CHC-C1C	4.00	1.48	1.39
4	A	616	HEC	CBC-CAC	-4.00	1.34	1.49
4	A	613	HEC	CBB-CAB	-4.00	1.34	1.49
4	A	610	HEC	CBB-CAB	-3.97	1.34	1.49
4	A	613	HEC	CBC-CAC	-3.95	1.34	1.49
4	A	610	HEC	CBC-CAC	-3.95	1.34	1.49
4	A	611	HEC	CBC-CAC	-3.94	1.34	1.49
4	A	614	HEC	CBB-CAB	-3.93	1.34	1.49
4	A	615	HEC	CBC-CAC	-3.91	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	615	HEC	CBB-CAB	-3.88	1.35	1.49
4	A	611	HEC	CBB-CAB	-3.82	1.35	1.49
4	A	612	HEC	C4B-NB	3.73	1.46	1.39
4	A	612	HEC	C1C-NC	-3.60	1.32	1.39
4	A	612	HEC	C3C-C4C	3.11	1.51	1.46
4	A	612	HEC	CBD-CGD	2.96	1.57	1.50
4	A	612	HEC	O1A-CGA	2.78	1.31	1.22
4	A	612	HEC	C1C-C2C	2.59	1.49	1.43
4	A	612	HEC	O2A-CGA	-2.54	1.22	1.30
4	A	612	HEC	C4A-NA	-2.30	1.35	1.39
4	A	616	HEC	C3C-C2C	-2.21	1.33	1.41
4	A	613	HEC	C3B-C2B	-2.19	1.33	1.41
4	A	610	HEC	C3B-C2B	-2.19	1.33	1.41
4	A	613	HEC	C3C-C2C	-2.16	1.33	1.41
4	A	610	HEC	C3C-C2C	-2.14	1.33	1.41
4	A	610	HEC	CMA-C3A	2.11	1.55	1.50
4	A	615	HEC	C3B-C2B	-2.10	1.34	1.41
4	A	611	HEC	C3C-C2C	-2.10	1.34	1.41
4	A	609	HEC	C3B-C2B	-2.09	1.34	1.41
4	A	614	HEC	C3B-C2B	-2.09	1.34	1.41
4	A	609	HEC	CMC-C2C	2.08	1.55	1.50
4	A	609	HEC	CMA-C3A	2.05	1.55	1.50
4	A	614	HEC	C3C-C2C	-2.05	1.34	1.41
4	A	614	HEC	CMA-C3A	2.04	1.55	1.50
4	A	616	HEC	C3B-C2B	-2.04	1.34	1.41
4	A	609	HEC	CMB-C2B	2.01	1.54	1.50
4	A	615	HEC	CMA-C3A	2.00	1.54	1.50

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	612	HEC	CHD-C4C-NC	-10.83	112.66	124.45
4	A	612	HEC	CHC-C4B-NB	-9.25	114.38	124.45
4	A	612	HEC	CHA-C1A-NA	-8.71	114.97	124.45
4	A	612	HEC	C2A-C1A-NA	-7.17	103.40	110.32
4	A	612	HEC	CBC-CAC-C3C	-6.63	114.18	127.43
4	A	612	HEC	CHA-C1A-C2A	-6.37	114.80	124.86
4	A	616	HEC	CBB-CAB-C3B	-6.17	115.11	127.43
4	A	612	HEC	O2A-CGA-CBA	6.16	133.46	114.00
4	A	613	HEC	CBB-CAB-C3B	-5.91	115.62	127.43
4	A	615	HEC	CBB-CAB-C3B	-5.80	115.84	127.43
4	A	612	HEC	CBB-CAB-C3B	-5.21	117.03	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	HEC	CBB-CAB-C3B	-5.18	117.08	127.43
4	A	612	HEC	CHD-C4C-C3C	-4.96	116.85	125.21
4	A	610	HEC	CBB-CAB-C3B	-4.87	117.70	127.43
4	A	613	HEC	CBC-CAC-C3C	-4.78	117.88	127.43
4	A	609	HEC	CBB-CAB-C3B	-4.74	117.97	127.43
4	A	614	HEC	CBC-CAC-C3C	-4.36	118.71	127.43
4	A	615	HEC	CBC-CAC-C3C	-4.29	118.86	127.43
4	A	612	HEC	CHC-C4B-C3B	-4.18	118.16	125.21
4	A	610	HEC	CBC-CAC-C3C	-4.17	119.09	127.43
4	A	612	HEC	CAA-CBA-CGA	-4.10	102.79	113.67
4	A	614	HEC	CBB-CAB-C3B	-4.02	119.39	127.43
4	A	612	HEC	O2A-CGA-O1A	-3.60	114.06	123.33
4	A	613	HEC	CBD-CAD-C3D	-3.55	102.72	112.53
4	A	616	HEC	CBC-CAC-C3C	-3.52	120.41	127.43
4	A	611	HEC	CBC-CAC-C3C	-3.48	120.47	127.43
4	A	609	HEC	CBC-CAC-C3C	-3.45	120.55	127.43
4	A	612	HEC	O1A-CGA-CBA	-3.41	112.27	123.09
4	A	612	HEC	CAA-C2A-C3A	-3.39	121.51	127.87
4	A	614	HEC	C4D-ND-C1D	3.33	111.25	105.82
4	A	615	HEC	C4D-ND-C1D	3.31	111.21	105.82
4	A	609	HEC	C4D-ND-C1D	3.30	111.20	105.82
4	A	611	HEC	C4D-ND-C1D	3.28	111.18	105.82
4	A	613	HEC	C4D-ND-C1D	3.12	110.91	105.82
4	A	612	HEC	C1C-CHC-C4B	-3.01	115.36	124.66
4	A	616	HEC	C4D-ND-C1D	2.86	110.48	105.82
4	A	610	HEC	C4D-ND-C1D	2.83	110.44	105.82
4	A	612	HEC	C3D-C4D-ND	-2.78	107.07	110.15
4	A	614	HEC	CAD-CBD-CGD	-2.78	106.30	113.67
4	A	615	HEC	C2A-C1A-NA	-2.71	107.71	110.32
4	A	611	HEC	CBA-CAA-C2A	-2.66	105.19	112.53
4	A	611	HEC	CBD-CAD-C3D	-2.52	105.56	112.53
4	A	610	HEC	C2A-C1A-NA	-2.52	107.89	110.32
4	A	609	HEC	C2A-C1A-NA	-2.44	107.97	110.32
4	A	615	HEC	CBD-CAD-C3D	-2.42	105.83	112.53
4	A	609	HEC	CBA-CAA-C2A	-2.35	106.04	112.53
4	A	615	HEC	CBA-CAA-C2A	-2.34	106.07	112.53
4	A	611	HEC	CMD-C2D-C1D	2.33	128.97	125.42
4	A	613	HEC	C2A-C1A-NA	-2.30	108.10	110.32
3	A	606	HG1	CAN-CAT-NAZ	-2.24	114.70	118.09
4	A	614	HEC	C3D-C4D-ND	-2.19	107.73	110.15
4	A	611	HEC	O2A-CGA-CBA	2.18	120.90	114.00
4	A	611	HEC	O1A-CGA-CBA	-2.18	116.18	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	HEC	CHC-C4B-NB	2.16	126.80	124.45
4	A	614	HEC	C1D-C2D-C3D	-2.14	104.37	106.82

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	HEC	C2B-C3B-CAB-CBB
4	A	609	HEC	C4B-C3B-CAB-CBB
4	A	609	HEC	C2C-C3C-CAC-CBC
4	A	609	HEC	C4C-C3C-CAC-CBC
4	A	610	HEC	C2B-C3B-CAB-CBB
4	A	610	HEC	C4B-C3B-CAB-CBB
4	A	610	HEC	C2C-C3C-CAC-CBC
4	A	610	HEC	C4C-C3C-CAC-CBC
4	A	611	HEC	C2B-C3B-CAB-CBB
4	A	611	HEC	C4B-C3B-CAB-CBB
4	A	611	HEC	C2C-C3C-CAC-CBC
4	A	611	HEC	C4C-C3C-CAC-CBC
4	A	612	HEC	C2B-C3B-CAB-CBB
4	A	612	HEC	C4B-C3B-CAB-CBB
4	A	612	HEC	C2C-C3C-CAC-CBC
4	A	613	HEC	C2B-C3B-CAB-CBB
4	A	613	HEC	C4B-C3B-CAB-CBB
4	A	613	HEC	C2C-C3C-CAC-CBC
4	A	613	HEC	C4C-C3C-CAC-CBC
4	A	614	HEC	C2B-C3B-CAB-CBB
4	A	614	HEC	C4B-C3B-CAB-CBB
4	A	614	HEC	C2C-C3C-CAC-CBC
4	A	614	HEC	C4C-C3C-CAC-CBC
4	A	615	HEC	C2B-C3B-CAB-CBB
4	A	615	HEC	C4B-C3B-CAB-CBB
4	A	615	HEC	C2C-C3C-CAC-CBC
4	A	615	HEC	C4C-C3C-CAC-CBC
4	A	616	HEC	C2B-C3B-CAB-CBB
4	A	616	HEC	C4B-C3B-CAB-CBB
4	A	616	HEC	C2C-C3C-CAC-CBC
4	A	616	HEC	C4C-C3C-CAC-CBC
3	A	607	HG1	CAQ-CAL-CAN-CAT
3	A	606	HG1	CAW-CAS-NAZ-CAR
3	A	606	HG1	CAW-CAS-NAZ-CAT
3	A	608	HG1	CAN-CAL-CAQ-CAU

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Mol	Chain	Res	Type	Atoms
3	A	606	HG1	OAF-CAX-CAY-CAW
3	A	607	HG1	CAN-CAL-CAQ-CAU
3	A	607	HG1	OAB-CAH-CAR-NAZ
4	A	616	HEC	C3D-CAD-CBD-CGD
3	A	606	HG1	OAF-CAX-CAY-OAG
4	A	612	HEC	CAA-CBA-CGA-O1A
4	A	612	HEC	CAA-CBA-CGA-O2A
4	A	609	HEC	CAD-CBD-CGD-O1D
3	A	606	HG1	CAQ-CAL-CAN-CAT
4	A	615	HEC	C3D-CAD-CBD-CGD
4	A	609	HEC	CAD-CBD-CGD-O2D
4	A	611	HEC	CAD-CBD-CGD-O2D
4	A	614	HEC	CAA-CBA-CGA-O2A
4	A	614	HEC	CAD-CBD-CGD-O2D
4	A	614	HEC	CAA-CBA-CGA-O1A
4	A	614	HEC	CAD-CBD-CGD-O1D
4	A	616	HEC	CAD-CBD-CGD-O2D
4	A	611	HEC	CAD-CBD-CGD-O1D
4	A	616	HEC	CAD-CBD-CGD-O1D
4	A	612	HEC	CAD-CBD-CGD-O2D
3	A	606	HG1	CAS-CAW-CAY-CAX
4	A	611	HEC	CAA-CBA-CGA-O2A

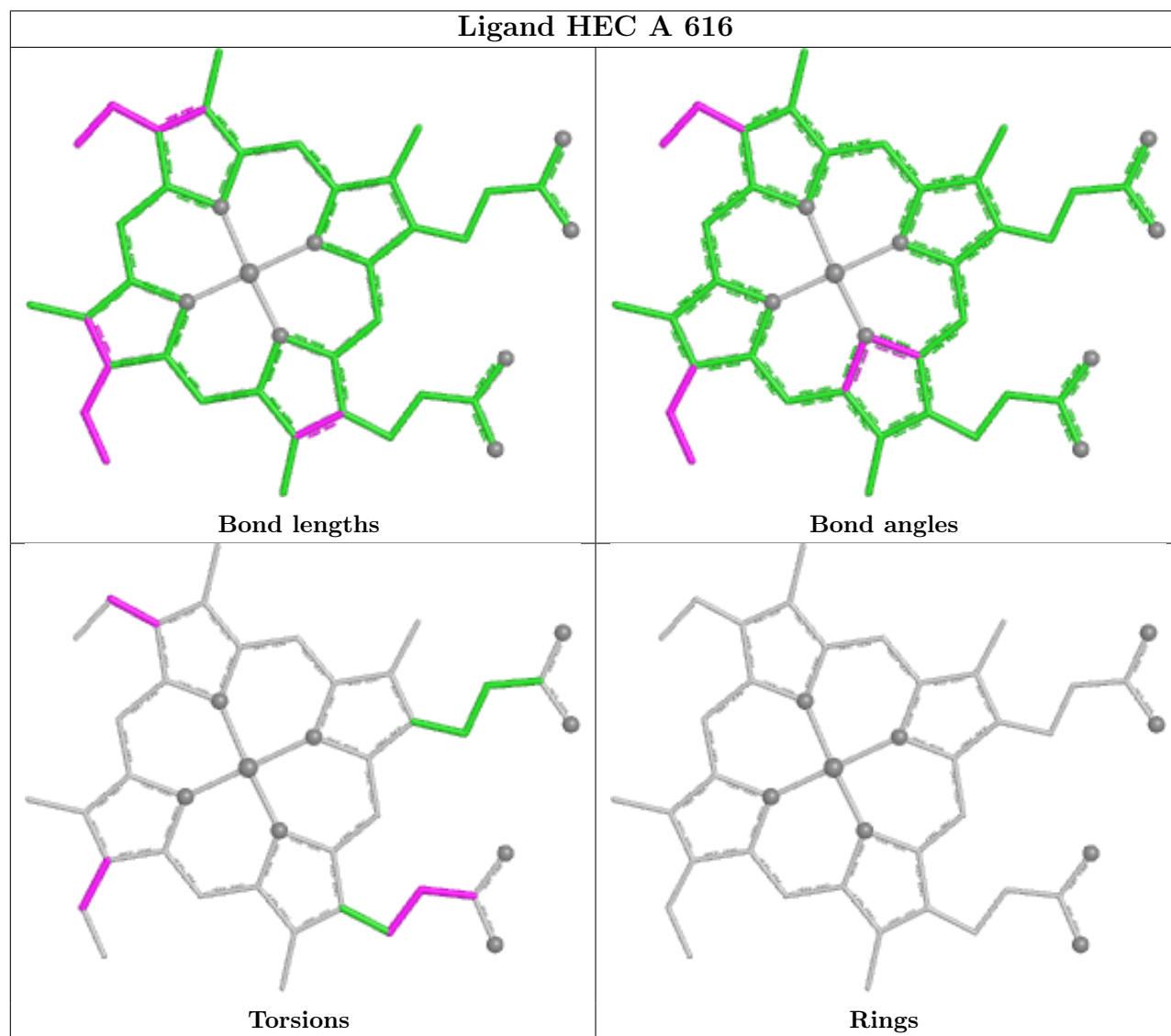
There are no ring outliers.

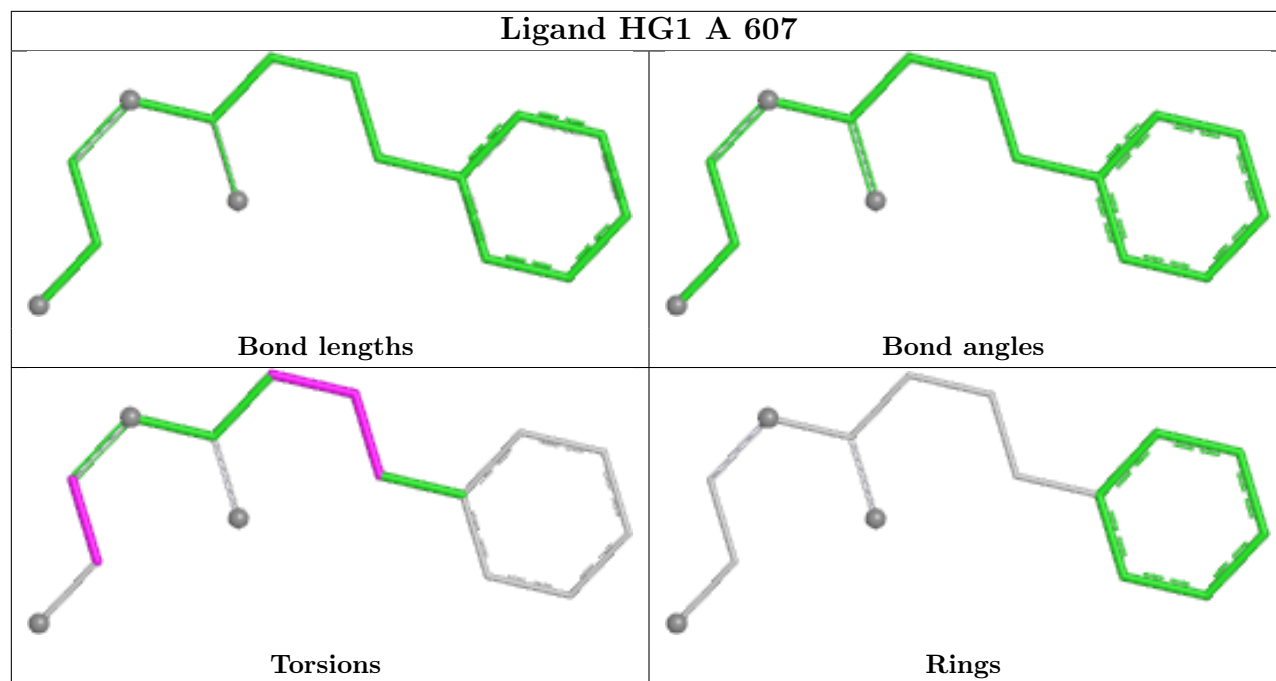
6 monomers are involved in 13 short contacts:

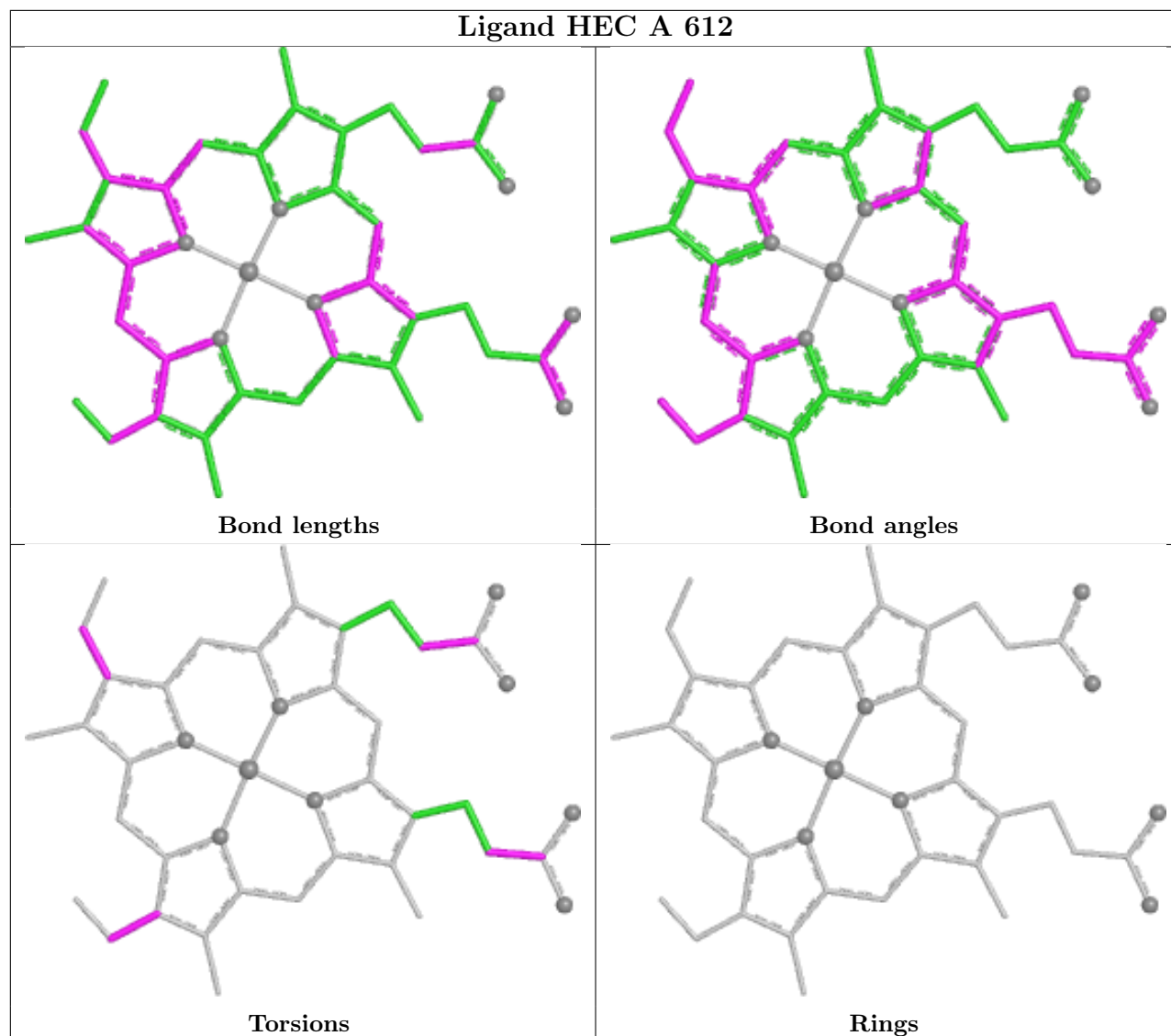
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	616	HEC	2	0
4	A	612	HEC	4	2
4	A	614	HEC	2	0
4	A	611	HEC	1	0
3	A	606	HG1	1	0
4	A	609	HEC	2	0

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

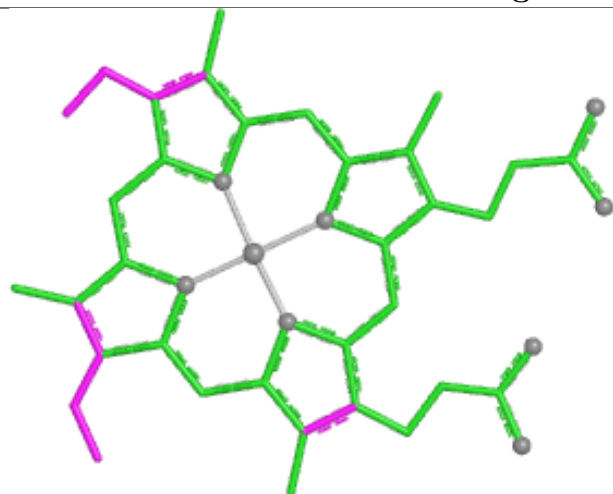
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



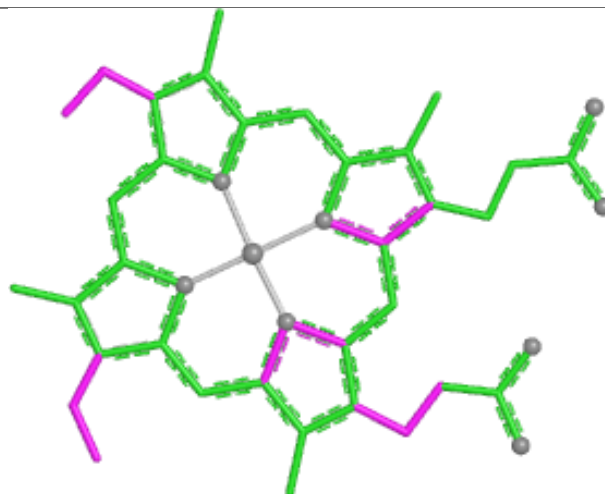




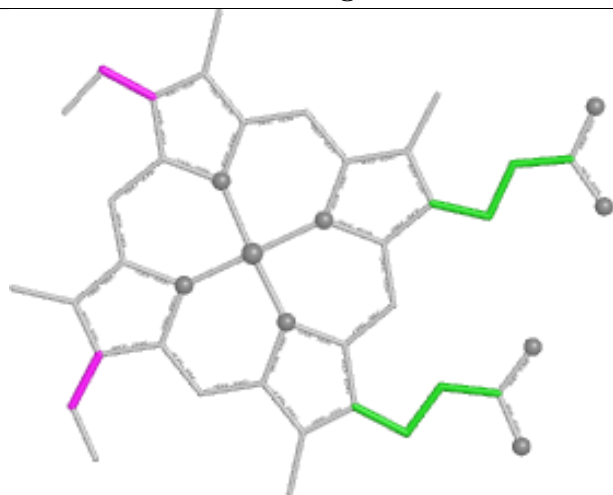
Ligand HEC A 613



Bond lengths



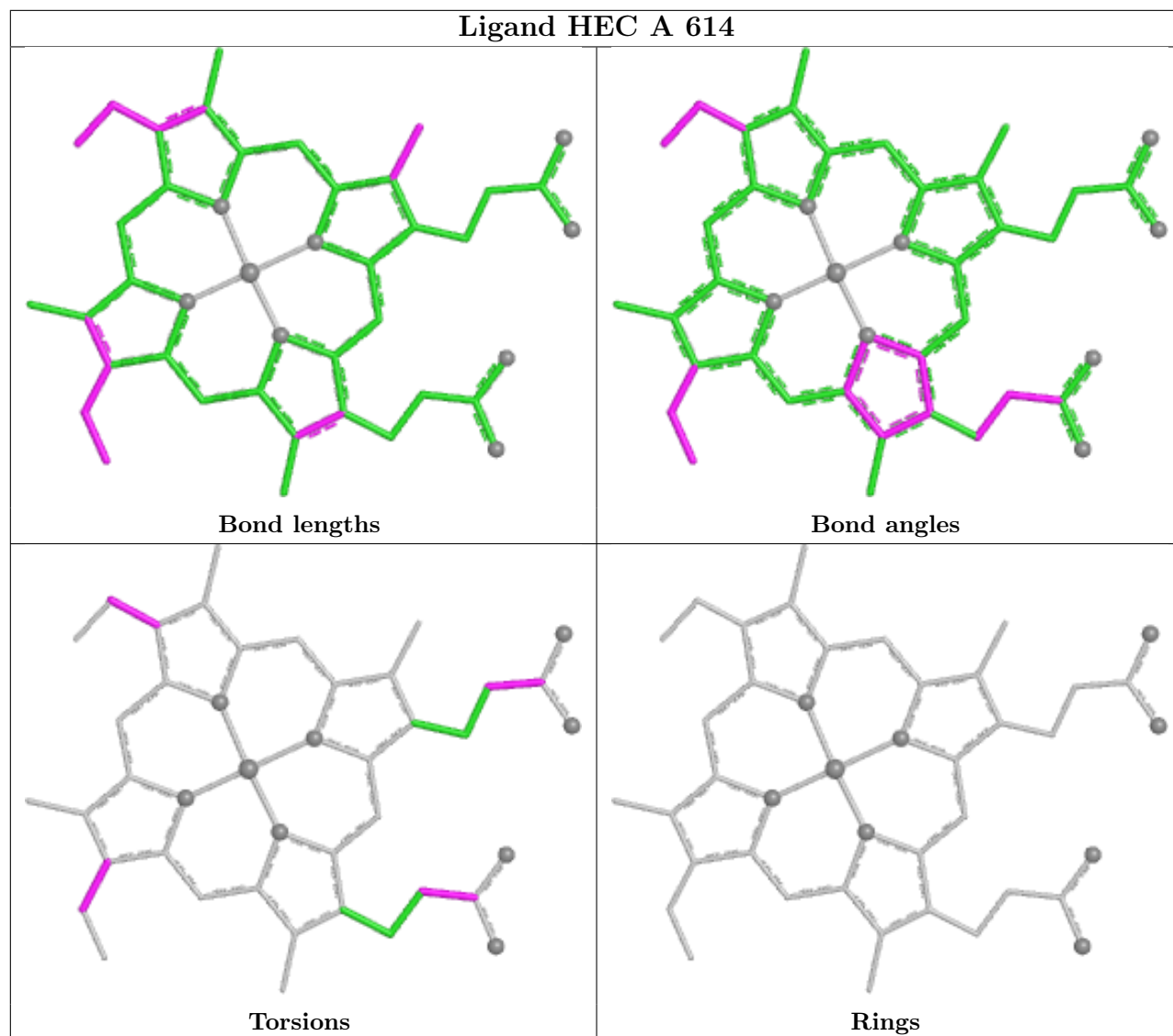
Bond angles



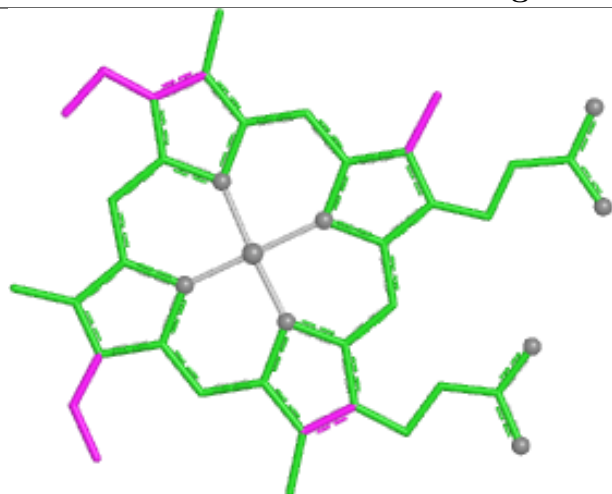
Torsions



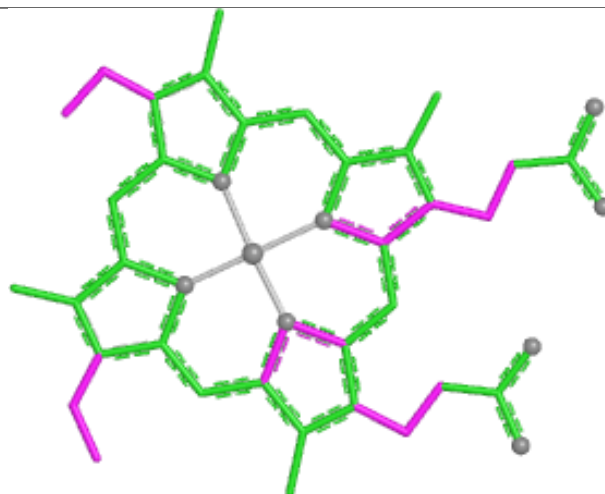
Rings



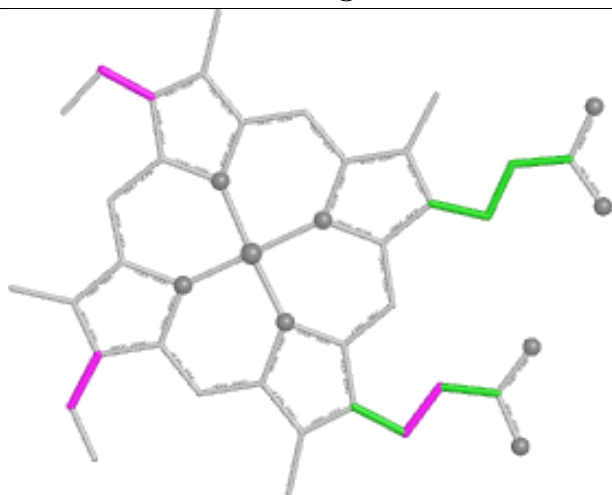
Ligand HEC A 615



Bond lengths



Bond angles

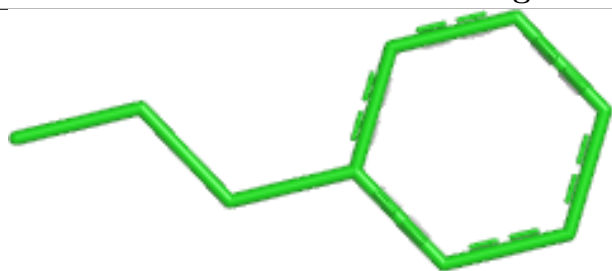


Torsions

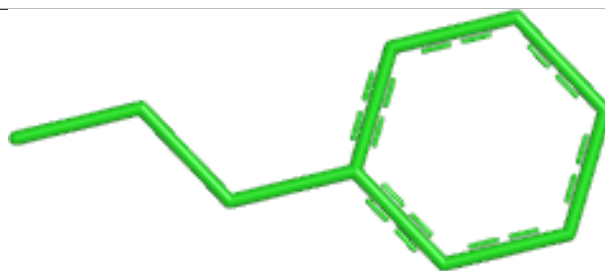


Rings

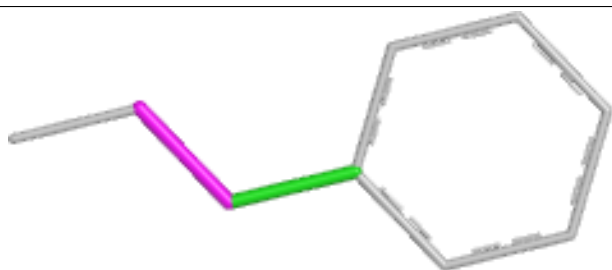
Ligand HG1 A 608



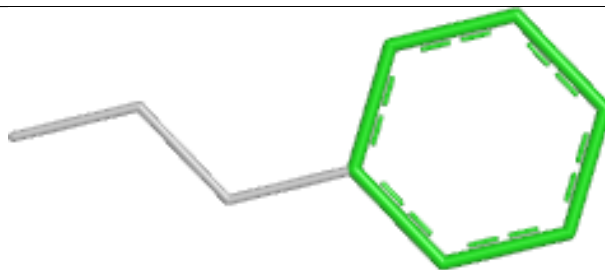
Bond lengths



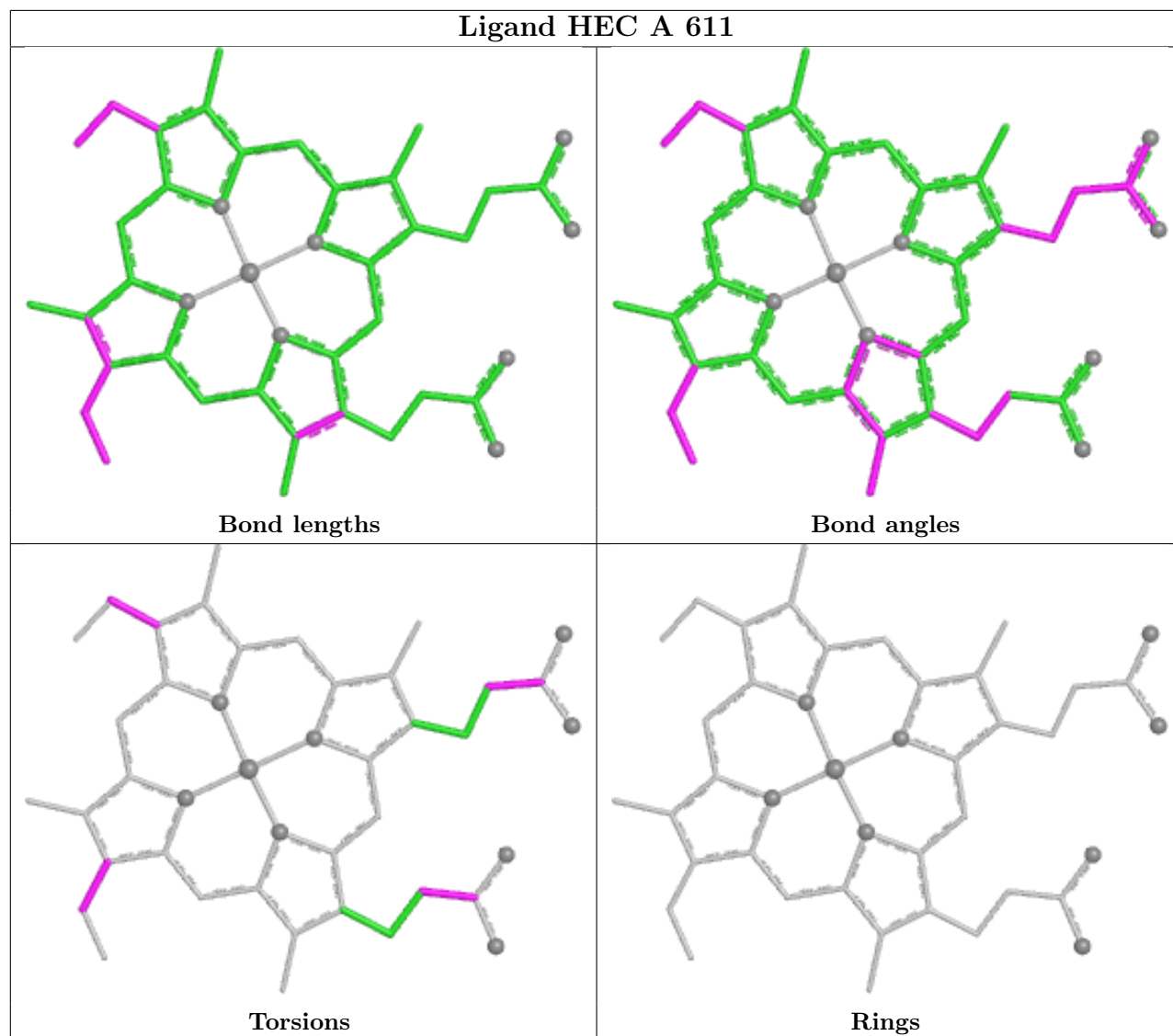
Bond angles



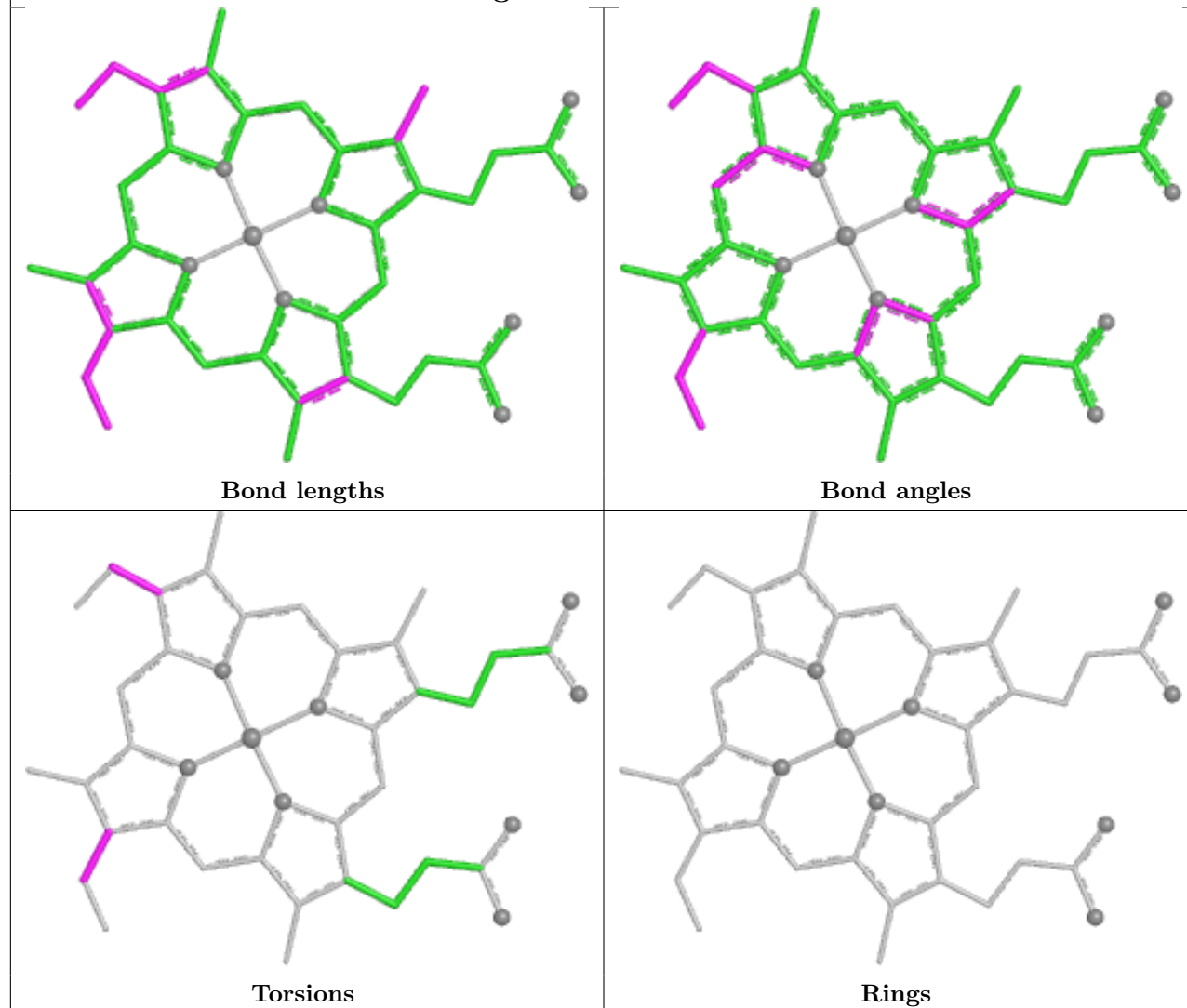
Torsions



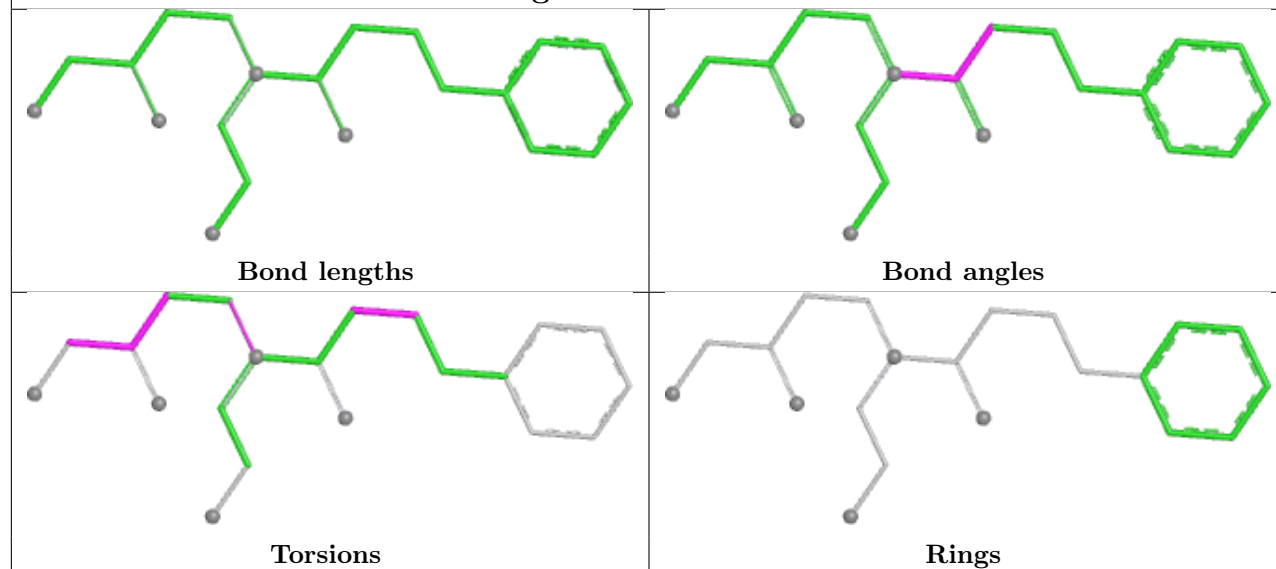
Rings

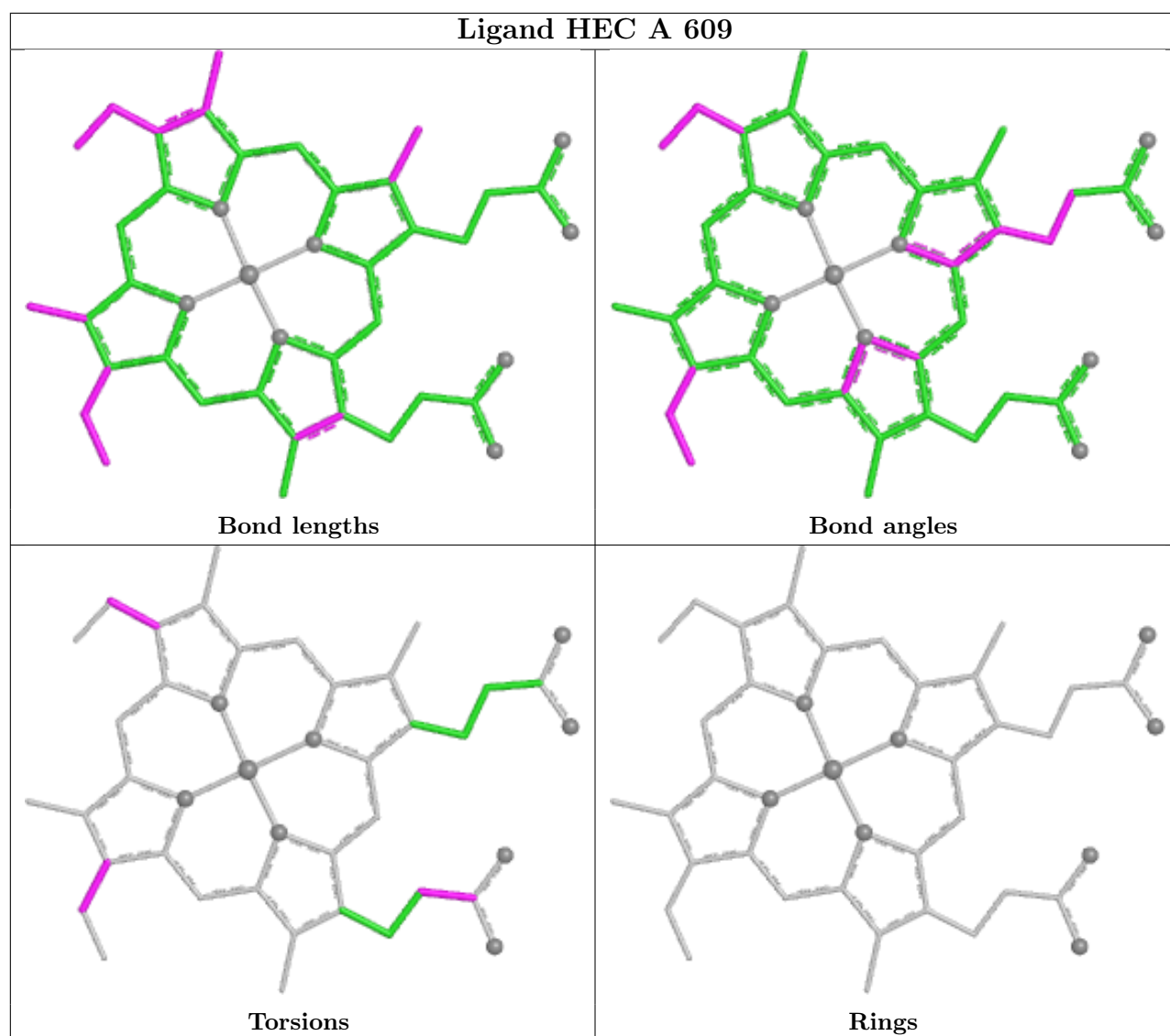


Ligand HEC A 610



Ligand HG1 A 606





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	8 (1%) 70 71	6, 14, 24, 33	6 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	5.0
1	A	534	ILE	4.8
1	A	486	GLU	2.8
1	A	114	GLU	2.4
1	A	394	GLU	2.4
1	A	140	ASP	2.3
1	A	48	VAL	2.2
1	A	488	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

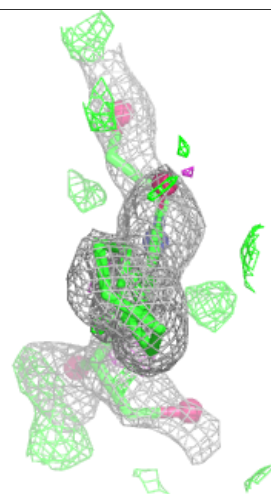
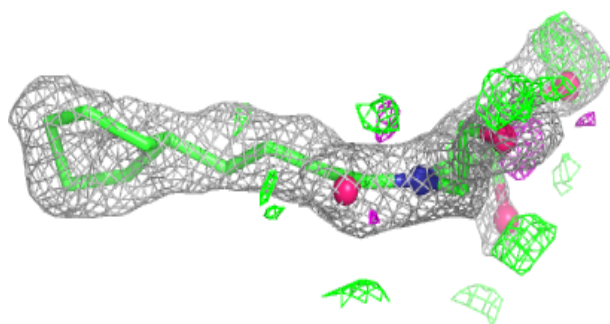
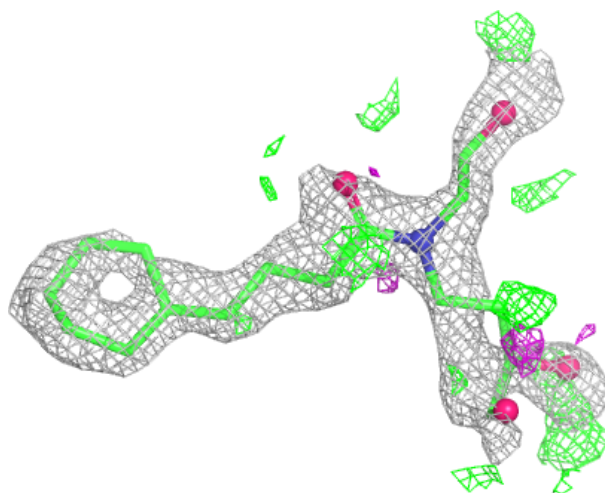
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG1	A	606	21/26	0.75	0.24	47,50,52,53	0
3	HG1	A	607	15/26	0.80	0.21	47,49,53,53	0
3	HG1	A	608	9/26	0.81	0.20	47,48,48,48	0
3	HG1	A	605	12/26	0.90	0.13	35,35,37,38	0
2	PO4	A	604	5/5	0.90	0.26	31,33,34,34	0
2	PO4	A	602	5/5	0.93	0.15	25,27,28,28	0
2	PO4	A	601	5/5	0.96	0.12	24,25,26,27	0
4	HEC	A	611	43/43	0.98	0.05	8,11,13,15	0
4	HEC	A	612	43/43	0.98	0.06	11,13,17,21	0
4	HEC	A	610	43/43	0.99	0.05	9,11,12,12	0
2	PO4	A	603	5/5	0.99	0.05	14,14,15,15	5
4	HEC	A	609	43/43	0.99	0.05	12,13,16,17	0
4	HEC	A	613	43/43	0.99	0.05	8,10,13,16	0
4	HEC	A	614	43/43	0.99	0.05	7,9,14,16	0
4	HEC	A	615	43/43	0.99	0.05	7,9,12,14	0
4	HEC	A	616	43/43	0.99	0.04	8,9,11,11	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.

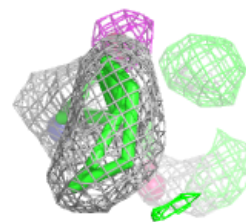
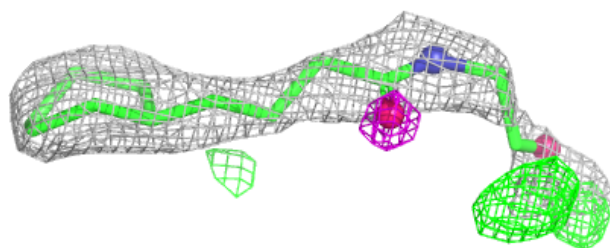
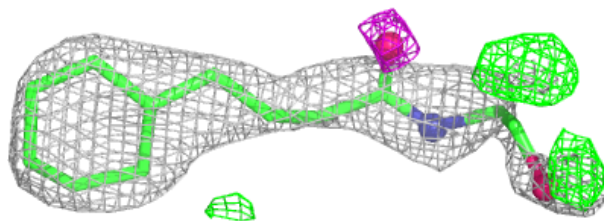
Electron density around HG1 A 606:

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

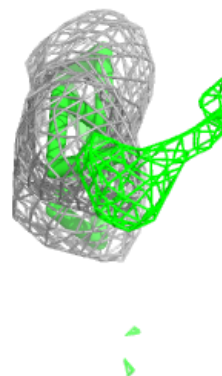
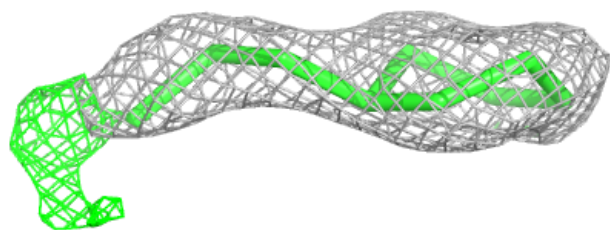
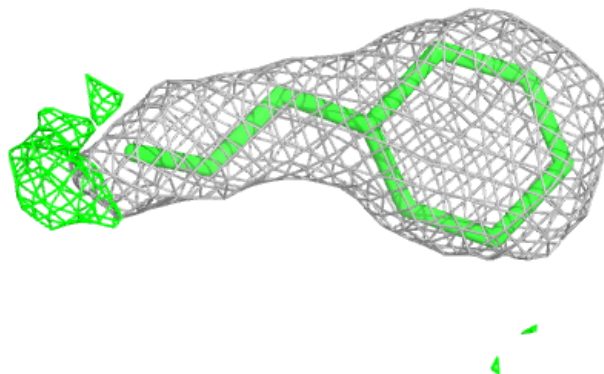


Electron density around HG1 A 607:

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

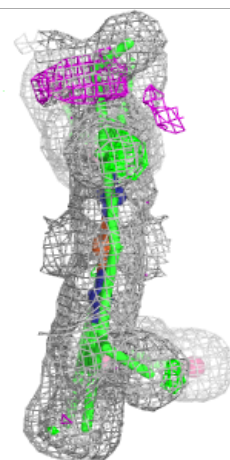
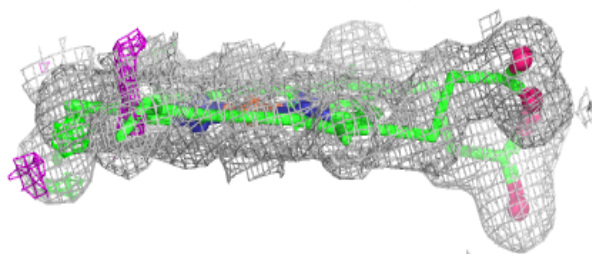
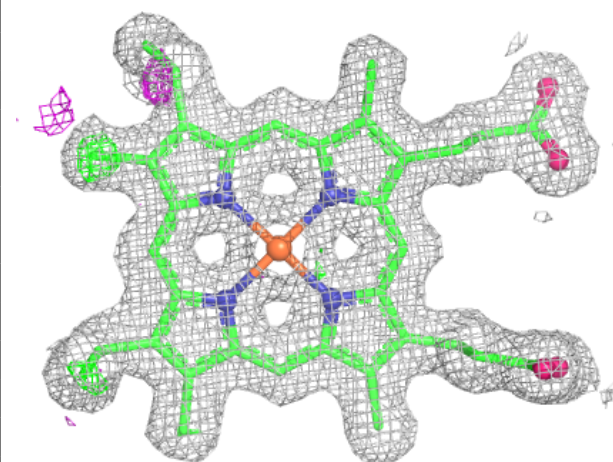
**Electron density around HG1 A 608:**

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



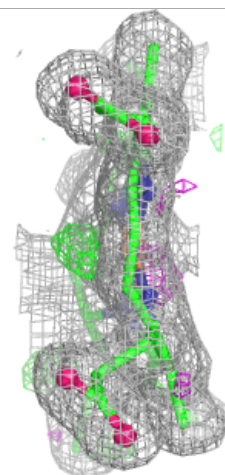
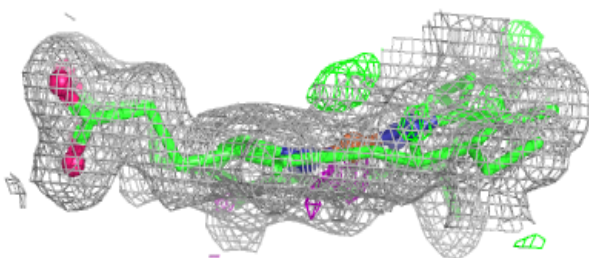
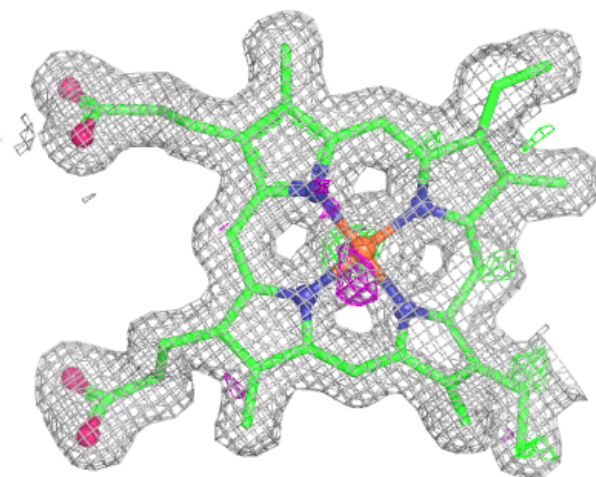
Electron density around HEC A 611:

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



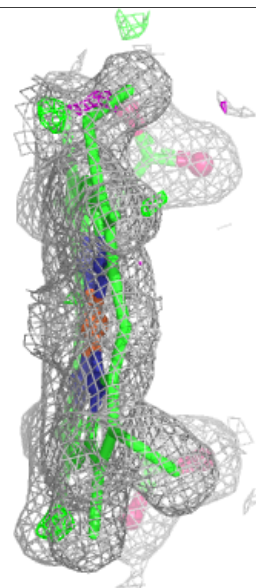
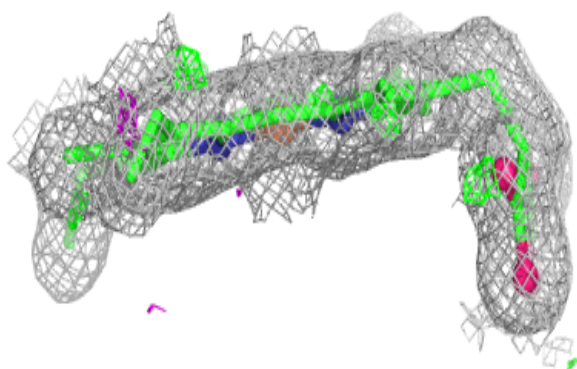
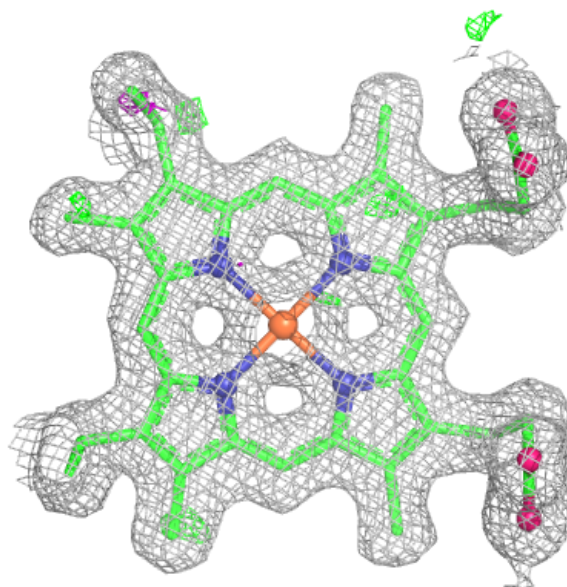
Electron density around HEC A 612:

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



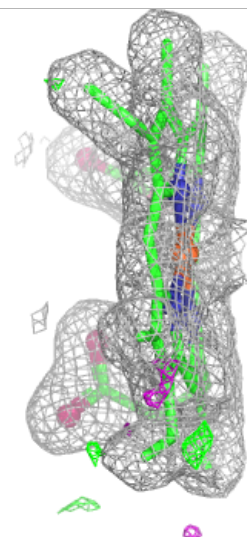
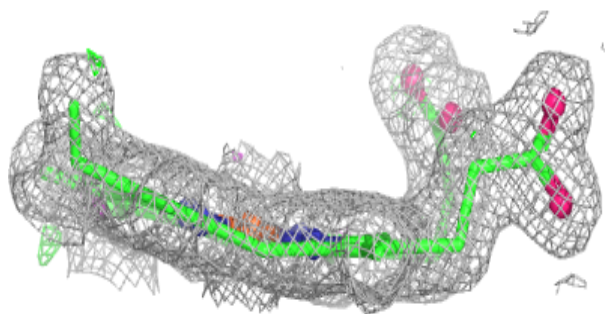
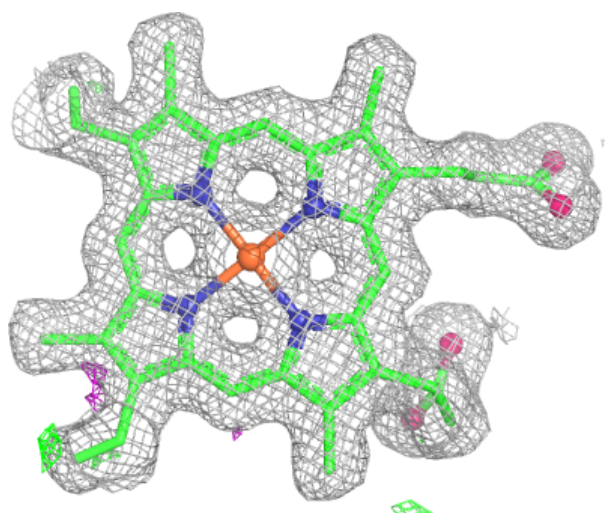
Electron density around HEC A 610:

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



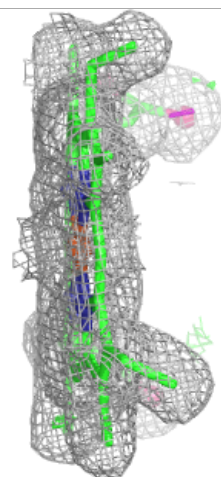
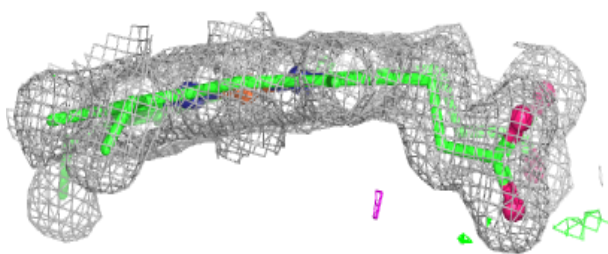
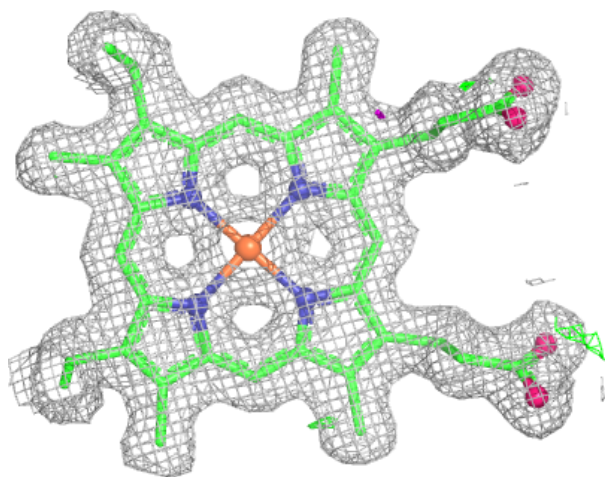
Electron density around HEC A 609:

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



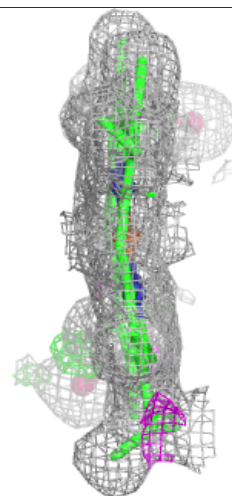
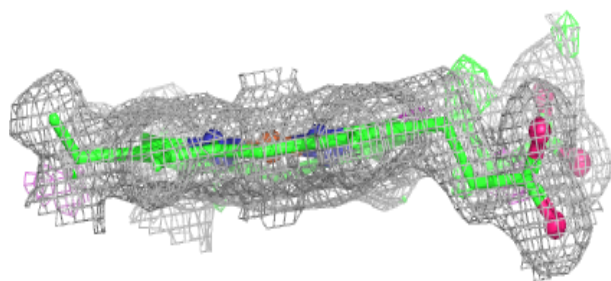
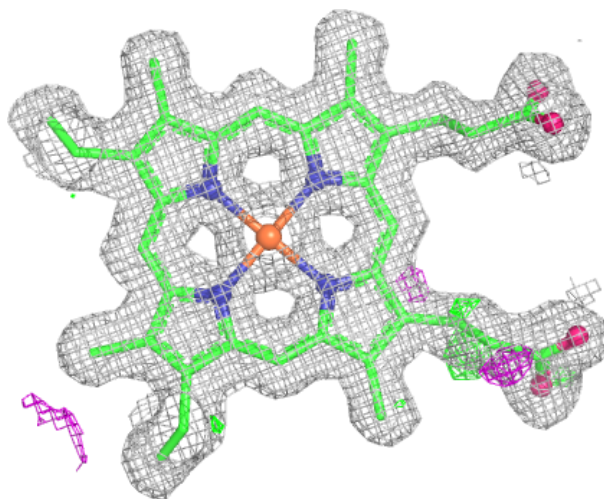
Electron density around HEC A 613:

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



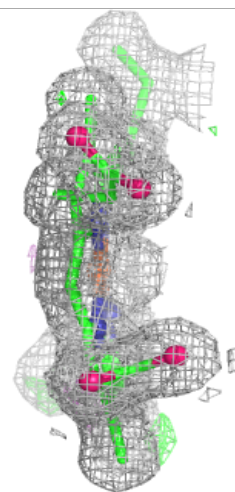
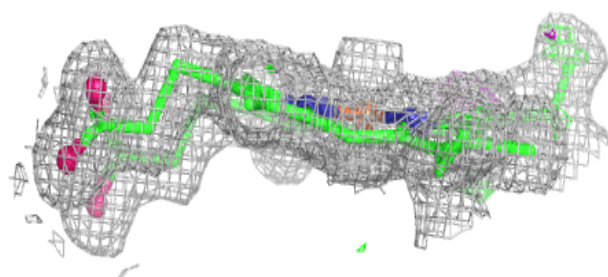
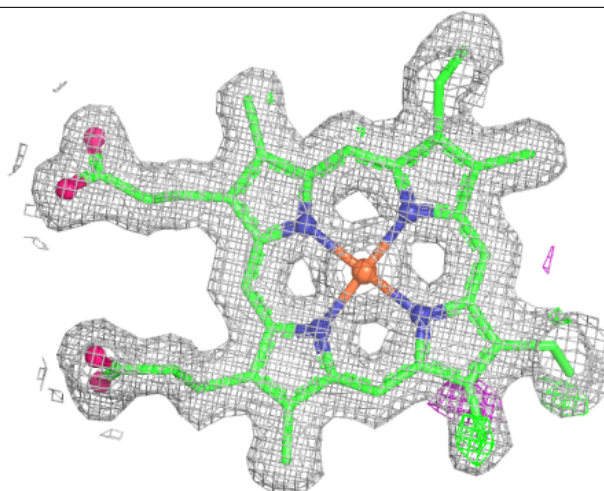
Electron density around HEC A 614:

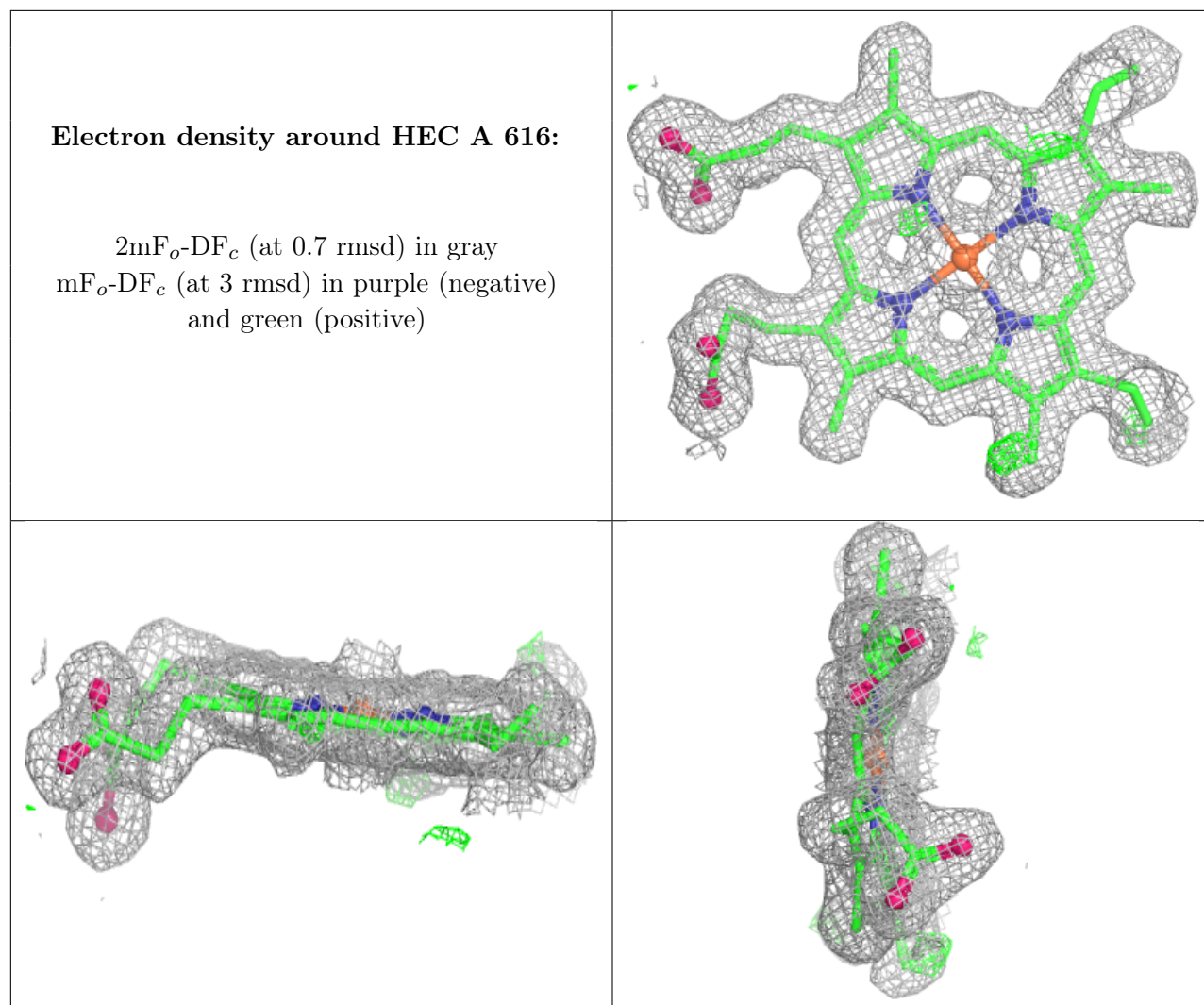
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.