Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 06:23 PM JST

PDB ID	:	6M0Q
Title	:	Hydroxylamine oxidoreductase from Nitrosomonas europaea
Authors	:	Fujiwara, T.; Fujimoto, Z.; Nishigaya, Y.; Yamazaki, T.
Deposited on	:	2020-02-22
Resolution	:	1.99 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:

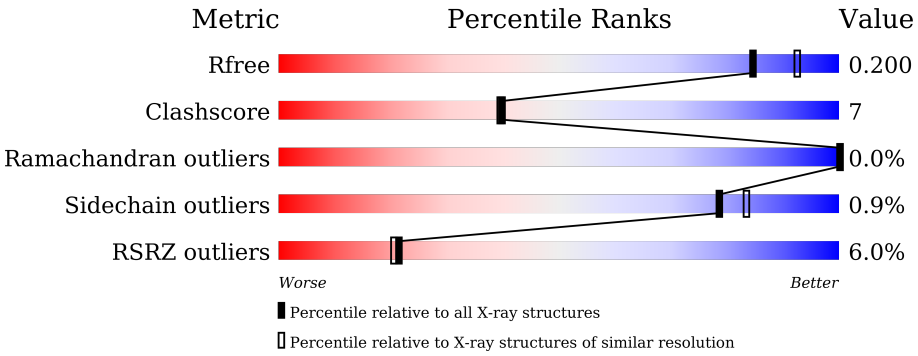
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	570	3% 79% 9% 12%
1	C	570	3% 80% 9% 12%
1	E	570	2% 79% 9% 12%
1	G	570	3% 81% 7% 12%
1	I	570	4% 78% 11% 12%
1	K	570	2% 77% 11% 12%

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Mol	Chain	Length	Quality of chain
2	B	91	15% 67% 30%
2	D	91	14% 67% 30%
2	F	91	23% 67% 30%
2	H	91	23% 66% 30%
2	J	91	10% 67% 30%
2	L	91	34% 64% 5% 30%

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
6	PGE	G	611	-	-	X	-
6	PGE	I	609	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31763 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.

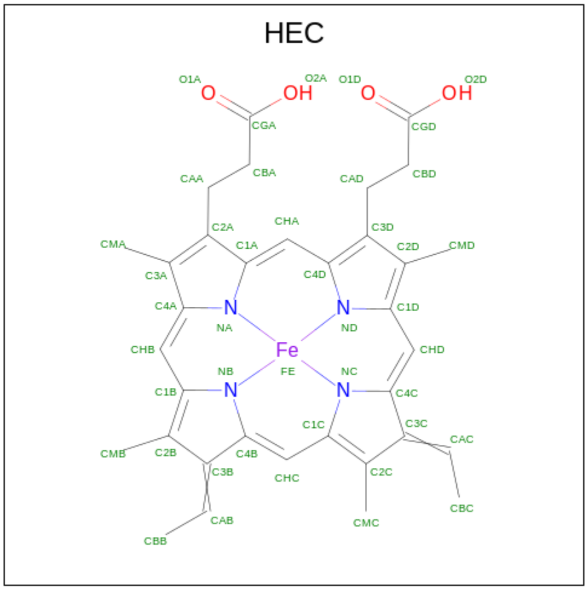
- Molecule 1 is a protein called Aerobic hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	E	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	G	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	I	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	K	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	D	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	F	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	H	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	J	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			
2	L	64	Total	C	N	O	S	0	0	0
			486	302	85	96	3			

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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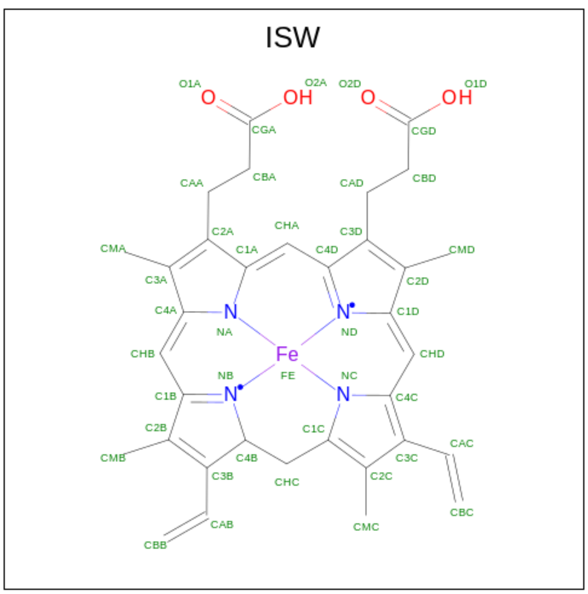
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0
3	K	1	43	34	1	4	4	0	0

- Molecule 4 is {3,3'-[(9S)-8,13-diethenyl-3,7,12,17-tetramethyl-9,10-dihydroporphyrin-2,18-diyl-kappa 4 N 21 ,N 22 ,N 23 ,N 24]dipropanoato(2-)}iron (three-letter code: ISW) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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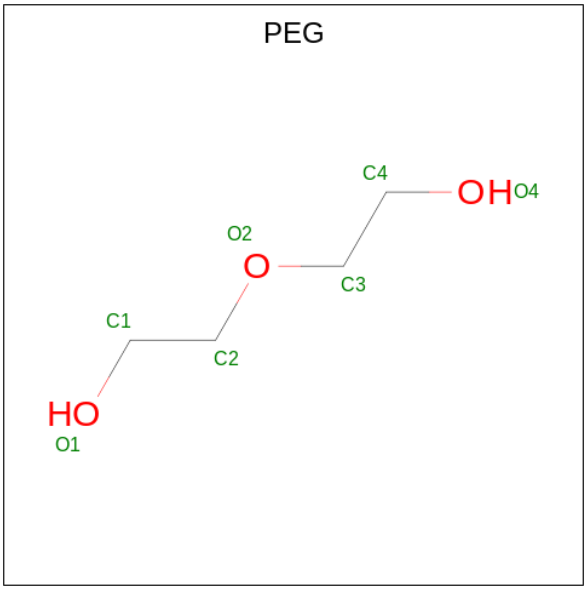
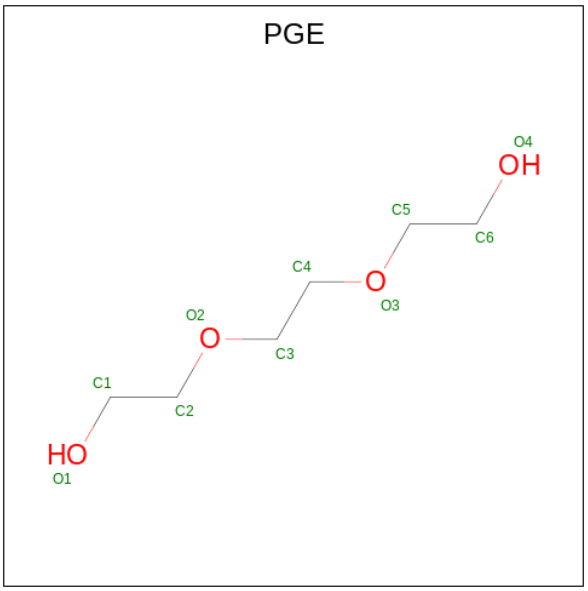
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



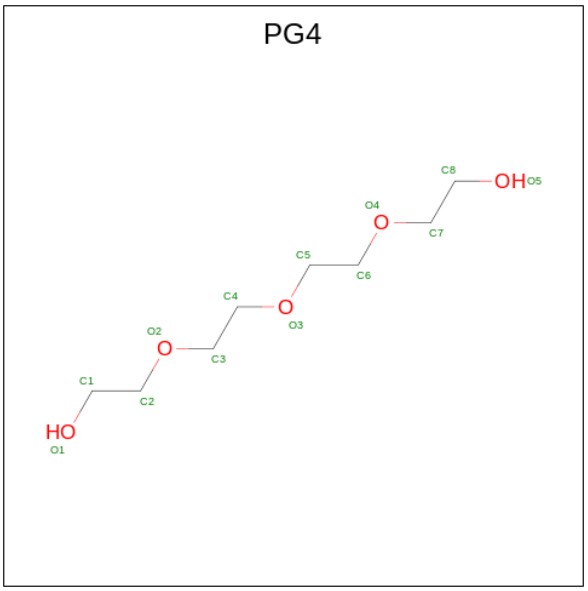
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	J	1	Total	C	O	0	0
			7	4	3		
5	K	1	Total	C	O	0	0
			7	4	3		
5	K	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	E	1	Total C O 10 6 4	0	0
6	E	1	Total C O 10 6 4	0	0
6	G	1	Total C O 10 6 4	0	0
6	G	1	Total C O 10 6 4	0	0
6	I	1	Total C O 10 6 4	0	0
6	I	1	Total C O 10 6 4	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	C	1	Total C O 13 8 5	0	0
7	E	1	Total C O 13 8 5	0	0
7	K	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	422	Total O 422 422	0	0
8	B	49	Total O 49 49	0	0
8	C	383	Total O 383 383	0	0
8	D	66	Total O 66 66	0	0
8	E	393	Total O 393 393	0	0
8	F	42	Total O 42 42	0	0
8	G	351	Total O 351 351	0	0
8	H	40	Total O 40 40	0	0

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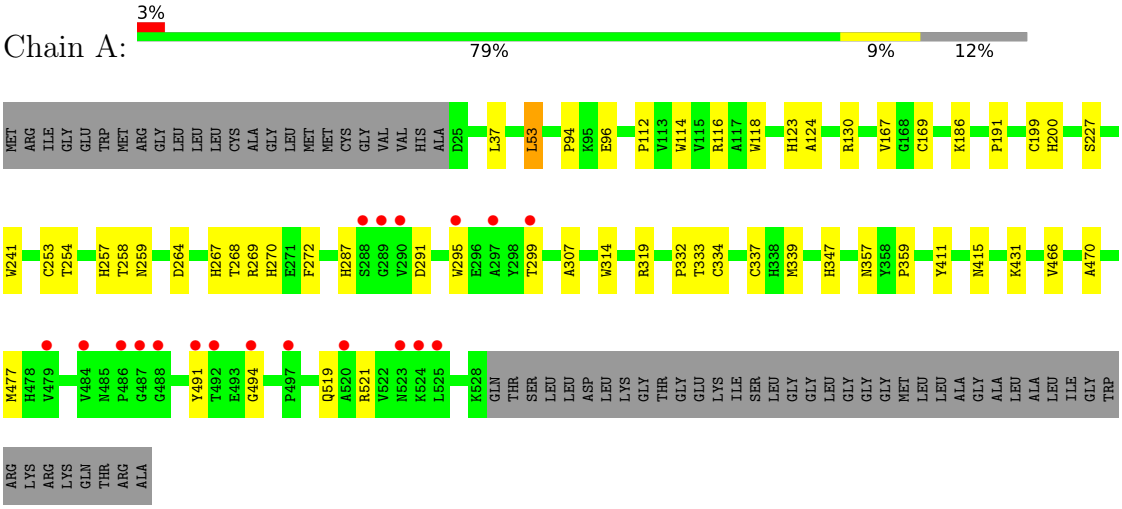
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	313	Total O 313 313	0	0
8	J	58	Total O 58 58	0	0
8	K	351	Total O 351 351	0	0
8	L	33	Total O 33 33	0	0

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.

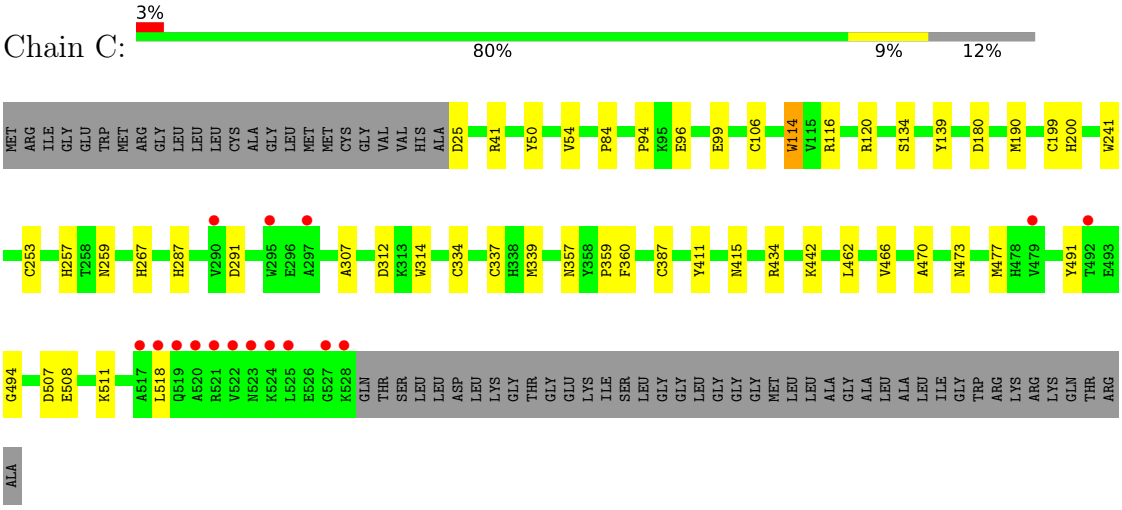
• Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain A:



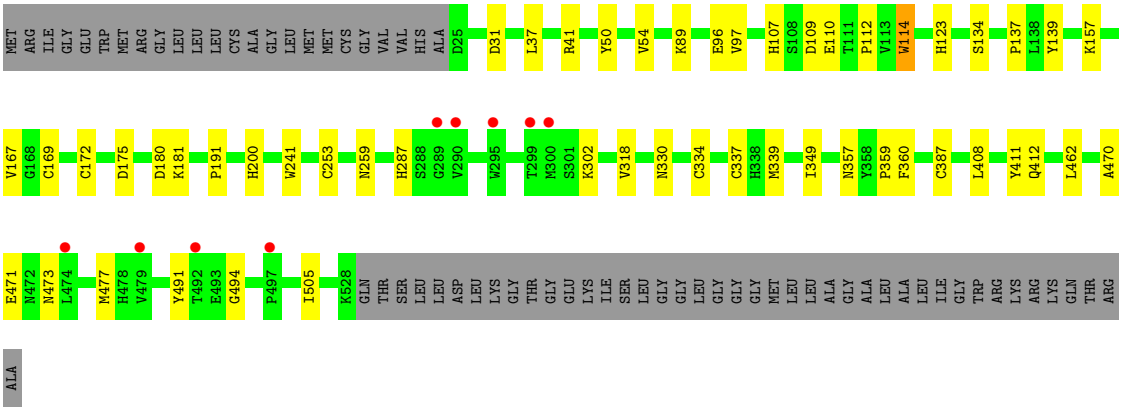
• Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain C:

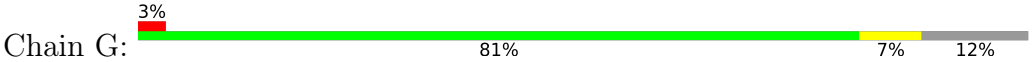


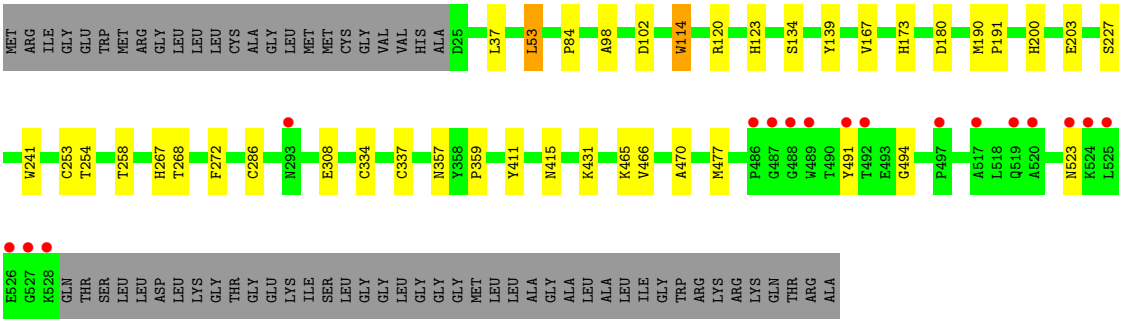
• Molecule 1: Aerobic hydroxylamine oxidoreductase

Chain E:

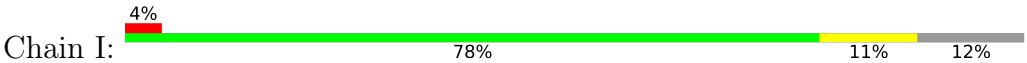


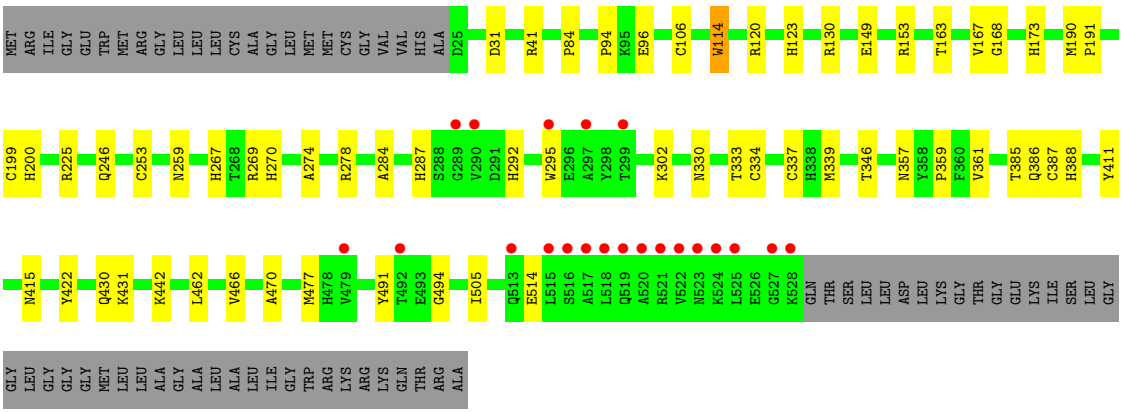
• Molecule 1: Aerobic hydroxylamine oxidoreductase



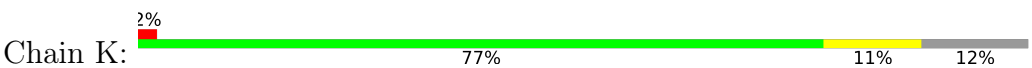


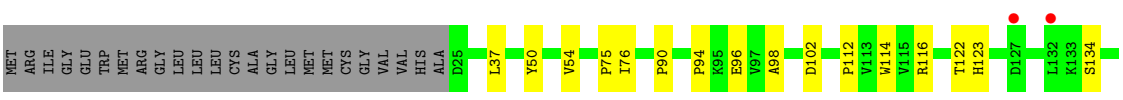
• Molecule 1: Aerobic hydroxylamine oxidoreductase

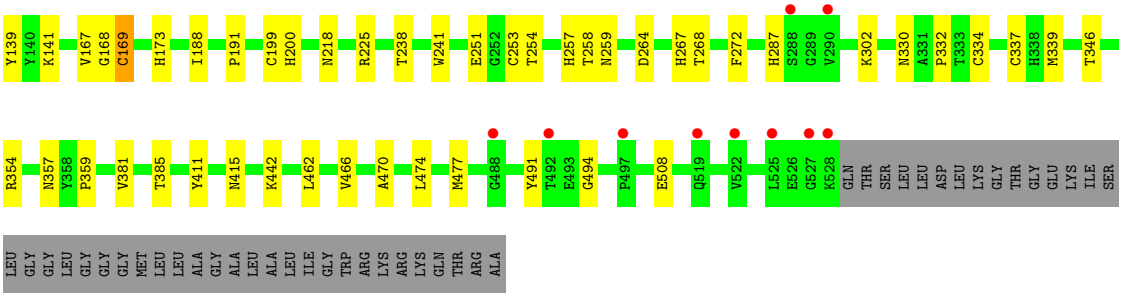




• Molecule 1: Aerobic hydroxylamine oxidoreductase

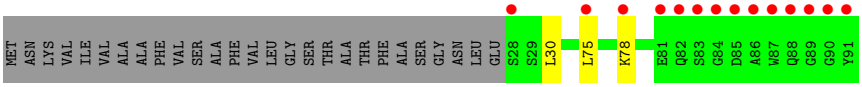






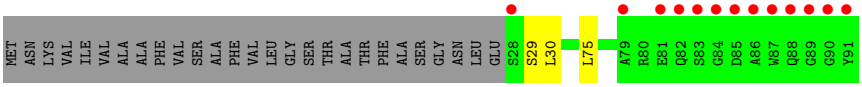
• Molecule 2: Uncharacterized protein

Chain B:



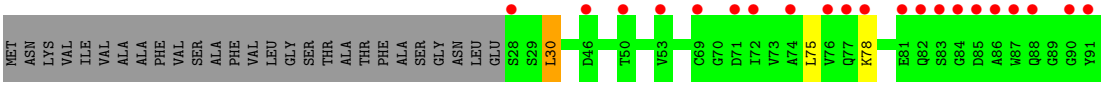
• Molecule 2: Uncharacterized protein

Chain D:



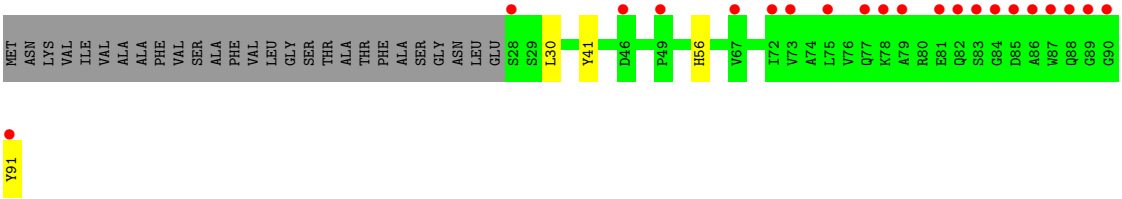
• Molecule 2: Uncharacterized protein

Chain F:



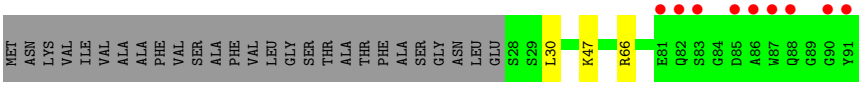
• Molecule 2: Uncharacterized protein

Chain H:



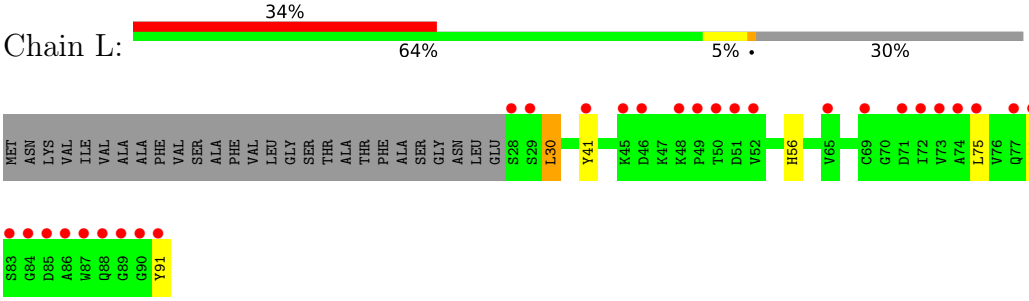
• Molecule 2: Uncharacterized protein

Chain J:



• Molecule 2: Uncharacterized protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.23Å 141.91Å 213.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 1.99 48.73 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.18-1.99) 99.9 (48.73-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.163 , 0.200 0.163 , 0.200	Depositor DCC
R_{free} test set	14603 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	31763	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ISW, PGE, PEG, PG4, 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	0.49	0/4121	0.62	0/5583
1	C	0.48	0/4121	0.62	0/5583
1	E	0.50	0/4121	0.62	0/5583
1	G	0.48	0/4121	0.59	0/5583
1	I	0.46	0/4121	0.59	0/5583
1	K	0.48	0/4121	0.61	1/5583 (0.0%)
2	B	0.45	0/492	0.62	0/660
2	D	0.42	0/492	0.64	1/660 (0.2%)
2	F	0.38	0/492	0.56	0/660
2	H	0.41	0/492	0.56	0/660
2	J	0.41	0/492	0.65	1/660 (0.2%)
2	L	0.34	0/492	0.55	0/660
All	All	0.47	0/27678	0.61	3/37458 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	354	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	J	66	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	D	75	LEU	CA-CB-CG	5.07	126.96	115.30

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	4018	0	3822	46	0
1	C	4018	0	3823	52	0
1	E	4018	0	3822	47	0
1	G	4018	0	3822	40	0
1	I	4018	0	3824	64	0
1	K	4018	0	3822	51	0
2	B	486	0	491	1	0
2	D	486	0	491	0	0
2	F	486	0	491	2	0
2	H	486	0	491	2	0
2	J	486	0	491	1	0
2	L	486	0	491	4	0
3	A	301	0	212	26	0
3	C	301	0	212	28	0
3	E	301	0	211	27	0
3	G	301	0	211	24	0
3	I	301	0	214	33	0
3	K	301	0	211	29	0
4	A	86	0	56	22	0
4	C	43	0	28	11	0
4	G	86	0	56	21	0
4	I	43	0	28	7	0
5	A	7	0	10	0	0
5	C	7	0	10	1	0
5	G	7	0	10	0	0
5	J	7	0	10	2	0
5	K	14	0	20	2	0
6	A	10	0	14	1	0
6	C	10	0	14	2	0
6	E	20	0	28	3	0
6	G	20	0	28	8	0
6	I	20	0	28	11	0
7	A	13	0	18	2	0
7	C	13	0	18	3	0
7	E	13	0	18	1	0
7	K	13	0	18	0	0
8	A	422	0	0	5	0
8	B	49	0	0	0	0
8	C	383	0	0	5	0
8	D	66	0	0	0	0
8	E	393	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	42	0	0	0	0
8	G	351	0	0	4	0
8	H	40	0	0	0	0
8	I	313	0	0	6	0
8	J	58	0	0	1	0
8	K	351	0	0	2	0
8	L	33	0	0	0	0
All	All	31763	0	27564	393	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 7.

All (393) 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:G:608:ISW:C4B	1:I:491:TYR:OH	1.74	1.21
1:I:337:CYS:SG	3:I:605:HEC:HAC	1.81	1.18
4:A:608:ISW:C4B	1:C:491:TYR:OH	1.75	1.15
1:C:337:CYS:SG	3:C:605:HEC:HAC	1.87	1.09
1:G:337:CYS:SG	3:G:605:HEC:HAC	1.82	1.09
1:I:387:CYS:SG	3:I:607:HEC:HAC	1.92	1.09
1:A:337:CYS:SG	3:A:605:HEC:HAC	1.91	1.05
1:K:337:CYS:SG	3:K:605:HEC:HAC	1.96	1.05
1:A:199:CYS:SG	3:A:602:HEC:HAC	1.95	1.05
1:E:337:CYS:SG	3:E:605:HEC:HAC	1.96	1.04
1:I:199:CYS:SG	3:I:602:HEC:HAC	1.93	1.04
1:I:106:CYS:SG	3:I:603:HEC:HAC	2.03	0.96
1:G:337:CYS:HG	3:G:605:HEC:HAC	1.31	0.93
4:G:608:ISW:HMAA	6:G:612:PGE:H22	1.51	0.89
1:I:106:CYS:SG	3:I:603:HEC:C3C	2.61	0.88
1:C:106:CYS:SG	3:C:603:HEC:C3C	2.62	0.87
1:C:106:CYS:SG	3:C:603:HEC:HAC	2.15	0.86
1:K:199:CYS:SG	3:K:602:HEC:C3C	2.64	0.85
1:A:37:LEU:HD11	1:A:53:LEU:HD13	1.57	0.84
1:C:199:CYS:SG	3:C:602:HEC:C3C	2.66	0.84
1:I:386:GLN:OE1	8:I:701:HOH:O	1.95	0.84
1:E:387:CYS:SG	3:E:607:HEC:C3C	2.66	0.83
1:G:337:CYS:SG	3:G:605:HEC:C3C	2.67	0.83
1:I:337:CYS:SG	3:I:605:HEC:C3C	2.68	0.82
1:E:337:CYS:SG	3:E:605:HEC:C3C	2.68	0.81
1:C:337:CYS:HG	3:C:605:HEC:HAC	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:CYS:SG	3:I:602:HEC:C3C	2.69	0.81
1:A:199:CYS:SG	3:A:602:HEC:C3C	2.68	0.80
1:C:106:CYS:SG	3:C:603:HEC:CBC	2.69	0.80
1:K:337:CYS:SG	3:K:605:HEC:C3C	2.70	0.80
1:A:337:CYS:SG	3:A:605:HEC:C3C	2.70	0.79
1:C:387:CYS:SG	3:C:607:HEC:C3C	2.70	0.79
1:I:387:CYS:SG	3:I:607:HEC:C3C	2.72	0.78
1:C:337:CYS:SG	3:C:605:HEC:C3C	2.72	0.77
1:A:186:LYS:NZ	8:A:701:HOH:O	2.16	0.77
1:G:286:CYS:SG	3:G:606:HEC:C3C	2.75	0.74
1:E:172:CYS:SG	3:E:604:HEC:C3C	2.76	0.74
1:I:106:CYS:SG	3:I:603:HEC:CBC	2.79	0.71
4:C:608:ISW:C3B	1:E:491:TYR:OH	2.38	0.70
4:G:609:ISW:HHC	1:K:253:CYS:SG	2.32	0.69
1:A:253:CYS:SG	4:A:608:ISW:HHC	2.33	0.69
1:G:253:CYS:SG	4:G:608:ISW:HHC	2.33	0.69
1:G:37:LEU:HD11	1:G:53:LEU:HD13	1.76	0.68
1:C:473:ASN:ND2	8:C:701:HOH:O	2.15	0.67
1:A:491:TYR:HD2	4:A:609:ISW:HMCA	1.60	0.67
1:G:120:ARG:HH22	1:I:330:ASN:HB3	1.61	0.65
1:I:153:ARG:NH2	8:I:706:HOH:O	2.29	0.65
1:G:491:TYR:OH	4:G:609:ISW:C3B	2.45	0.64
3:A:605:HEC:HBB3	3:A:605:HEC:HMB1	1.80	0.64
1:I:199:CYS:SG	3:I:602:HEC:CBC	2.87	0.63
4:C:608:ISW:NB	1:E:491:TYR:OH	2.30	0.63
1:G:491:TYR:HD2	4:G:609:ISW:HMCA	1.63	0.62
4:A:609:ISW:HHC	1:E:253:CYS:SG	2.39	0.62
3:C:607:HEC:HMB1	3:C:607:HEC:HBB3	1.82	0.62
5:J:101:PEG:H21	8:J:211:HOH:O	1.98	0.61
4:G:608:ISW:HMCA	1:I:491:TYR:HD2	1.66	0.61
4:A:608:ISW:HMCA	1:C:491:TYR:HD2	1.64	0.61
1:E:172:CYS:SG	3:E:604:HEC:CBC	2.87	0.61
1:A:199:CYS:SG	3:A:602:HEC:CBC	2.88	0.61
1:G:491:TYR:OH	4:G:609:ISW:NB	2.33	0.61
1:I:430:GLN:HE21	6:I:609:PGE:H4	1.66	0.60
3:G:605:HEC:HMB1	3:G:605:HEC:HBB3	1.83	0.60
1:K:359:PRO:HG2	1:K:474:LEU:HG	1.82	0.60
1:C:312:ASP:OD1	8:C:702:HOH:O	2.16	0.59
3:C:605:HEC:HBB3	3:C:605:HEC:HMB1	1.84	0.59
1:A:491:TYR:OH	4:A:609:ISW:C3B	2.49	0.59
1:C:116:ARG:NH1	8:C:711:HOH:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TYR:CE1	1:A:470:ALA:HB2	2.38	0.58
4:I:608:ISW:HMCA	1:K:491:TYR:HD2	1.68	0.58
1:C:253:CYS:SG	4:C:608:ISW:HHC	2.44	0.58
6:I:610:PGE:H1	8:I:978:HOH:O	2.05	0.57
4:C:608:ISW:HMCA	1:E:491:TYR:HD2	1.69	0.57
1:I:253:CYS:SG	4:I:608:ISW:HHC	2.44	0.57
3:I:606:HEC:HMB1	3:I:606:HEC:HBB3	1.87	0.57
1:C:99:GLU:OE1	8:C:703:HOH:O	2.17	0.56
4:A:609:ISW:HMAA	6:E:609:PGE:H2	1.87	0.56
3:E:603:HEC:CAA	3:E:604:HEC:HMA3	2.36	0.56
1:G:431:LYS:HZ3	6:G:611:PGE:H42	1.70	0.56
1:I:422:TYR:CZ	6:I:609:PGE:H42	2.40	0.56
1:I:31:ASP:OD1	1:I:41:ARG:HD2	2.06	0.56
1:G:286:CYS:SG	3:G:606:HEC:CBC	2.90	0.56
4:A:609:ISW:C2B	1:E:253:CYS:HB3	2.36	0.56
1:E:89:LYS:HZ2	7:E:610:PG4:H81	1.70	0.55
1:G:431:LYS:HZ3	6:G:611:PGE:C4	2.19	0.55
1:K:477:MET:HB2	1:K:494:GLY:HA2	1.88	0.55
4:A:608:ISW:C3B	1:C:491:TYR:OH	2.51	0.55
1:E:387:CYS:SG	3:E:607:HEC:CBC	2.92	0.55
2:B:75:LEU:HD12	2:B:78:LYS:HE2	1.88	0.54
3:I:605:HEC:HMB1	3:I:605:HEC:HBB3	1.88	0.54
6:G:611:PGE:H12	8:G:869:HOH:O	2.08	0.54
1:G:123:HIS:HB3	1:G:167:VAL:HB	1.90	0.54
1:E:109:ASP:HA	1:E:112:PRO:HG3	1.90	0.54
1:E:477:MET:HB2	1:E:494:GLY:HA2	1.88	0.53
3:G:607:HEC:HMB1	3:G:607:HEC:HBB3	1.90	0.53
1:I:387:CYS:SG	3:I:607:HEC:CBC	2.91	0.53
1:C:199:CYS:SG	3:C:602:HEC:CBC	2.91	0.53
1:A:337:CYS:HG	3:A:605:HEC:HAC	1.70	0.53
1:I:130:ARG:NH2	1:I:163:THR:HB	2.23	0.53
3:C:602:HEC:HMB1	3:C:602:HEC:HBB3	1.90	0.53
3:I:607:HEC:HMB1	3:I:607:HEC:HBB3	1.90	0.53
2:L:75:LEU:HD22	2:L:78:LYS:HE2	1.90	0.53
3:G:605:HEC:HMA3	3:G:606:HEC:HBA2	1.92	0.52
3:K:605:HEC:HBB3	3:K:605:HEC:HMB1	1.90	0.52
4:G:609:ISW:HBB	4:G:609:ISW:HMB	1.92	0.52
3:I:602:HEC:HBC3	3:I:602:HEC:HMC1	1.90	0.52
3:K:603:HEC:CAA	3:K:604:HEC:HMA3	2.40	0.52
1:I:477:MET:HB2	1:I:494:GLY:HA2	1.91	0.52
2:J:47:LYS:HZ2	5:J:101:PEG:H31	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ARG:HD3	6:C:610:PGE:H22	1.91	0.52
4:G:608:ISW:HMB	4:G:608:ISW:HBB	1.91	0.52
1:I:149:GLU:O	1:I:153:ARG:HG3	2.09	0.52
1:I:431:LYS:NZ	6:I:609:PGE:H1	2.24	0.52
3:A:604:HEC:HMC1	3:A:604:HEC:HBC3	1.91	0.52
1:C:387:CYS:SG	3:C:607:HEC:CBC	2.94	0.52
1:G:477:MET:HB2	1:G:494:GLY:HA2	1.91	0.52
1:C:287:HIS:CE1	4:C:608:ISW:HMD	2.45	0.52
3:E:607:HEC:HMB1	3:E:607:HEC:HBB3	1.92	0.52
1:G:357:ASN:O	1:G:359:PRO:HD3	2.10	0.52
6:I:610:PGE:H5	8:I:978:HOH:O	2.09	0.52
1:C:25:ASP:OD1	1:C:41:ARG:HG3	2.11	0.51
1:E:411:TYR:CE1	1:E:470:ALA:HB2	2.45	0.51
4:G:608:ISW:C3B	1:I:491:TYR:OH	2.54	0.51
4:A:609:ISW:HMD	1:E:287:HIS:CE1	2.45	0.51
3:C:605:HEC:HMA3	3:C:606:HEC:HBA2	1.92	0.51
1:E:357:ASN:O	1:E:359:PRO:HD3	2.10	0.51
4:G:609:ISW:HMD	1:K:287:HIS:CE1	2.45	0.51
3:I:604:HEC:HMC1	3:I:604:HEC:HBC3	1.92	0.51
1:C:411:TYR:CE1	1:C:470:ALA:HB2	2.45	0.51
1:A:339:MET:HE3	1:A:347:HIS:HA	1.93	0.51
1:A:123:HIS:HB3	1:A:167:VAL:HB	1.93	0.51
6:I:610:PGE:O1	8:I:702:HOH:O	2.19	0.51
1:C:106:CYS:SG	3:C:603:HEC:HBC3	2.51	0.51
1:G:191:PRO:HG2	3:G:604:HEC:CHD	2.40	0.51
1:K:415:ASN:HA	1:K:466:VAL:HG21	1.92	0.51
1:G:431:LYS:NZ	6:G:611:PGE:H1	2.25	0.51
4:G:609:ISW:O1D	3:K:605:HEC:HMA2	2.11	0.51
3:G:606:HEC:HBB3	3:G:606:HEC:HMB1	1.93	0.51
1:I:246:GLN:HG3	2:L:56:HIS:O	2.10	0.51
1:K:134:SER:HA	1:K:139:TYR:CG	2.46	0.50
1:A:431:LYS:NZ	6:A:611:PGE:H22	2.26	0.50
1:K:254:THR:O	1:K:258:THR:HG23	2.11	0.50
3:C:606:HEC:HMB1	3:C:606:HEC:HBB3	1.94	0.50
1:I:431:LYS:NZ	6:I:609:PGE:H62	2.26	0.50
1:K:123:HIS:HB3	1:K:167:VAL:HB	1.93	0.50
1:K:272:PHE:O	3:K:602:HEC:HBA1	2.11	0.50
1:E:473:ASN:ND2	8:E:705:HOH:O	2.35	0.50
3:K:607:HEC:HBB3	3:K:607:HEC:HMB1	1.93	0.50
1:E:97:VAL:HG12	1:E:181:LYS:HB3	1.94	0.50
1:I:94:PRO:HB2	1:I:96:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HA	1:C:466:VAL:HG21	1.94	0.49
4:G:609:ISW:O1A	1:K:225:ARG:NE	2.35	0.49
1:C:200:HIS:CD2	3:C:602:HEC:NB	2.79	0.49
1:G:415:ASN:HA	1:G:466:VAL:HG21	1.94	0.49
3:I:604:HEC:HBA1	3:I:604:HEC:HHA	1.94	0.49
1:G:334:CYS:HA	3:G:605:HEC:CHC	2.43	0.49
1:C:339:MET:SD	3:C:601:HEC:HMD2	2.53	0.49
1:G:431:LYS:HZ1	6:G:611:PGE:H6	1.77	0.49
1:A:295:TRP:CZ2	1:A:299:THR:HG21	2.48	0.49
1:C:120:ARG:HH22	1:E:330:ASN:HB3	1.78	0.49
7:C:611:PG4:H51	8:C:707:HOH:O	2.12	0.49
4:G:609:ISW:C2B	1:K:253:CYS:HB3	2.42	0.49
1:G:84:PRO:HB3	1:G:190:MET:HB2	1.95	0.49
1:G:411:TYR:CE1	1:G:470:ALA:HB2	2.47	0.48
3:I:603:HEC:CAA	3:I:604:HEC:HMA3	2.43	0.48
1:A:94:PRO:HB2	1:A:96:GLU:HG2	1.94	0.48
1:A:200:HIS:CD2	3:A:602:HEC:NB	2.81	0.48
1:C:462:LEU:HG	1:C:508:GLU:CD	2.34	0.48
1:K:357:ASN:O	1:K:359:PRO:HD3	2.14	0.48
4:A:609:ISW:HMB	4:A:609:ISW:HBB	1.95	0.48
1:E:137:PRO:HB2	1:E:318:VAL:HG12	1.94	0.48
3:K:604:HEC:HMC1	3:K:604:HEC:HBC3	1.95	0.48
2:H:56:HIS:HE1	8:K:714:HOH:O	1.97	0.48
1:I:84:PRO:HB3	1:I:190:MET:HB2	1.95	0.48
1:K:411:TYR:CE1	1:K:470:ALA:HB2	2.49	0.48
1:I:120:ARG:NH2	1:K:330:ASN:HB3	2.29	0.48
1:I:361:VAL:HG22	6:I:610:PGE:H6	1.95	0.48
1:A:241:TRP:HB2	4:A:608:ISW:HMB	1.95	0.47
2:H:41:TYR:OH	2:H:91:TYR:O	2.24	0.47
1:K:94:PRO:HB2	1:K:96:GLU:HG2	1.95	0.47
1:K:334:CYS:HA	3:K:605:HEC:CHC	2.44	0.47
1:G:200:HIS:CG	3:G:601:HEC:HMA1	2.49	0.47
1:A:254:THR:O	1:A:258:THR:HG23	2.15	0.47
1:E:408:LEU:O	1:E:412:GLN:HG3	2.15	0.47
3:E:606:HEC:HBB3	3:E:606:HEC:HMB1	1.96	0.47
1:I:411:TYR:CE1	1:I:470:ALA:HB2	2.50	0.47
1:C:357:ASN:O	1:C:359:PRO:HD3	2.14	0.47
1:E:471:GLU:OE2	6:E:609:PGE:H42	2.14	0.47
1:K:98:ALA:HB1	1:K:102:ASP:HB2	1.97	0.47
1:G:268:THR:HG21	1:I:302:LYS:HD2	1.96	0.47
1:I:334:CYS:HA	3:I:605:HEC:CHC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:OD1	1:C:291:ASP:N	2.47	0.47
1:C:334:CYS:HA	3:C:605:HEC:CHC	2.45	0.47
3:E:604:HEC:HBC3	3:E:604:HEC:HMC1	1.96	0.47
1:K:76:ILE:HD11	1:K:251:GLU:HG2	1.97	0.47
1:K:477:MET:HB2	1:K:494:GLY:CA	2.45	0.47
4:A:608:ISW:HMB	4:A:608:ISW:HBB	1.97	0.47
1:G:98:ALA:HB1	1:G:102:ASP:HB2	1.97	0.47
1:K:218:ASN:ND2	2:L:30:LEU:HD13	2.30	0.47
1:A:272:PHE:O	3:A:602:HEC:HBA1	2.15	0.46
3:A:603:HEC:HBB3	3:A:603:HEC:HMB1	1.98	0.46
1:K:168:GLY:O	3:K:604:HEC:HMC3	2.15	0.46
1:C:507:ASP:OD1	1:C:511:LYS:NZ	2.42	0.46
3:G:604:HEC:HBC3	3:G:604:HEC:HMC1	1.96	0.46
1:I:114:TRP:HA	1:I:114:TRP:CE3	2.51	0.46
4:G:609:ISW:HBAA	3:K:606:HEC:O1D	2.16	0.46
3:A:607:HEC:HBB3	3:A:607:HEC:HMB1	1.97	0.46
1:C:241:TRP:HB2	4:C:608:ISW:HMB	1.98	0.46
3:C:601:HEC:HBA1	3:C:602:HEC:CAA	2.46	0.46
3:E:602:HEC:HMC1	3:E:602:HEC:HBC3	1.96	0.46
2:F:75:LEU:HD22	2:F:78:LYS:HE2	1.96	0.46
6:C:610:PGE:H52	6:C:610:PGE:H32	1.55	0.46
3:G:601:HEC:HAA2	8:G:702:HOH:O	2.16	0.46
1:K:75:PRO:HG2	5:K:609:PEG:H32	1.98	0.46
1:K:339:MET:HE3	1:K:346:THR:O	2.15	0.46
1:E:123:HIS:HB3	1:E:167:VAL:HB	1.97	0.46
1:I:477:MET:HB2	1:I:494:GLY:CA	2.45	0.46
3:K:606:HEC:HMB1	3:K:606:HEC:HBB3	1.97	0.46
3:C:605:HEC:HMA2	4:C:608:ISW:O1D	2.15	0.46
1:E:302:LYS:HA	1:E:302:LYS:HD3	1.75	0.46
1:C:114:TRP:CE3	1:C:114:TRP:HA	2.51	0.46
1:C:259:ASN:HD21	3:C:606:HEC:C3C	2.28	0.46
1:K:259:ASN:HD21	3:K:606:HEC:C3C	2.29	0.46
1:I:430:GLN:NE2	6:I:609:PGE:H4	2.31	0.45
3:I:605:HEC:HMA2	4:I:608:ISW:O1D	2.15	0.45
1:K:50:TYR:CZ	1:K:54:VAL:HG21	2.50	0.45
1:G:114:TRP:HA	1:G:114:TRP:CE3	2.51	0.45
1:I:191:PRO:HG2	3:I:604:HEC:CHD	2.46	0.45
1:A:287:HIS:CE1	4:A:608:ISW:HMD	2.52	0.45
6:E:608:PGE:H32	6:E:608:PGE:H1	1.68	0.45
1:I:333:THR:C	3:I:605:HEC:HMC3	2.37	0.45
1:K:442:LYS:HE2	8:K:816:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:609:ISW:HMB	1:E:241:TRP:HB2	1.97	0.45
4:C:608:ISW:HMAA	7:C:611:PG4:H31	1.99	0.45
1:E:337:CYS:SG	3:E:605:HEC:CBC	2.98	0.45
1:I:287:HIS:CE1	4:I:608:ISW:HMD	2.52	0.45
1:I:431:LYS:HZ3	6:I:609:PGE:H62	1.80	0.45
1:I:462:LEU:HD21	1:I:505:ILE:HA	1.97	0.45
3:I:607:HEC:HBC3	3:I:607:HEC:HMC1	1.99	0.45
1:A:334:CYS:HA	3:A:605:HEC:CHC	2.47	0.45
1:A:477:MET:HB2	1:A:494:GLY:HA2	1.99	0.45
4:G:609:ISW:HMB	1:K:241:TRP:HB2	1.98	0.45
1:A:319:ARG:HG2	8:A:719:HOH:O	2.17	0.45
1:E:334:CYS:HA	3:E:605:HEC:CHC	2.46	0.45
3:A:603:HEC:CAA	3:A:604:HEC:HMA3	2.47	0.45
3:E:601:HEC:HBA1	3:E:602:HEC:CAA	2.47	0.45
1:C:477:MET:HB2	1:C:494:GLY:HA2	1.99	0.45
1:A:415:ASN:HA	1:A:466:VAL:HG21	2.00	0.44
1:C:200:HIS:CG	3:C:601:HEC:HMA1	2.52	0.44
1:E:134:SER:HA	1:E:139:TYR:CG	2.52	0.44
7:C:611:PG4:H51	7:C:611:PG4:H32	1.68	0.44
1:E:107:HIS:HA	1:E:110:GLU:HB3	1.98	0.44
6:G:612:PGE:H12	8:G:1027:HOH:O	2.17	0.44
3:A:604:HEC:HMB1	3:A:604:HEC:HBB3	2.00	0.44
1:C:180:ASP:N	1:C:180:ASP:OD1	2.49	0.44
1:C:253:CYS:HB3	4:C:608:ISW:C2B	2.47	0.44
1:E:31:ASP:OD1	1:E:41:ARG:HD2	2.17	0.44
1:K:122:THR:HB	3:K:602:HEC:HBA2	1.99	0.44
1:E:96:GLU:HG3	3:E:603:HEC:HBC2	2.00	0.44
1:E:339:MET:SD	3:E:601:HEC:HMD2	2.56	0.44
1:K:200:HIS:CG	3:K:601:HEC:HMA1	2.53	0.44
1:G:134:SER:HA	1:G:139:TYR:CG	2.52	0.44
1:E:157:LYS:NZ	1:E:175:ASP:OD1	2.47	0.44
1:I:200:HIS:CG	3:I:601:HEC:HMA1	2.53	0.44
1:K:332:PRO:HB2	3:K:605:HEC:HMC1	2.00	0.44
3:K:603:HEC:HBC3	3:K:603:HEC:HMC1	1.98	0.44
1:A:333:THR:C	3:A:605:HEC:HMC3	2.38	0.44
7:A:612:PG4:H72	8:A:1072:HOH:O	2.17	0.44
1:E:462:LEU:HD21	1:E:505:ILE:HA	1.99	0.44
1:G:254:THR:O	1:G:258:THR:HG23	2.17	0.44
1:K:169:CYS:HA	3:K:604:HEC:CHC	2.48	0.44
1:K:264:ASP:O	1:K:268:THR:HA	2.18	0.44
3:E:606:HEC:HBC3	3:E:606:HEC:HMC1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:603:HEC:CAA	3:G:604:HEC:HMA3	2.47	0.44
1:K:339:MET:SD	3:K:601:HEC:HMD2	2.57	0.44
1:I:274:ALA:O	1:I:278:ARG:HG3	2.17	0.43
1:I:514:GLU:OE2	8:I:703:HOH:O	2.21	0.43
2:L:41:TYR:OH	2:L:91:TYR:OXT	2.31	0.43
1:A:191:PRO:HG2	3:A:604:HEC:CHD	2.48	0.43
1:A:227:SER:O	3:A:606:HEC:HBD1	2.18	0.43
3:C:601:HEC:HBC3	3:C:601:HEC:HMC1	2.00	0.43
1:I:415:ASN:HA	1:I:466:VAL:HG21	2.01	0.43
3:K:605:HEC:HBA2	3:K:606:HEC:CGA	2.48	0.43
1:A:307:ALA:HA	1:A:314:TRP:CH2	2.53	0.43
1:E:169:CYS:HA	3:E:604:HEC:CHC	2.49	0.43
3:A:602:HEC:HMC1	3:A:602:HEC:HBC3	1.99	0.43
1:I:253:CYS:HB3	4:I:608:ISW:C2B	2.49	0.43
1:A:257:HIS:CE1	3:A:606:HEC:HMD1	2.54	0.43
1:A:287:HIS:ND1	4:A:608:ISW:HMD	2.33	0.43
3:E:605:HEC:HMB1	3:E:605:HEC:HBB3	2.00	0.43
4:G:609:ISW:HMA	1:K:238:THR:OG1	2.18	0.43
1:K:90:PRO:HB3	1:K:188:ILE:HB	2.00	0.43
1:K:337:CYS:SG	3:K:605:HEC:C2C	3.07	0.43
1:G:465:LYS:HE3	1:G:465:LYS:HB2	1.83	0.43
1:A:332:PRO:HB2	3:A:605:HEC:HMC1	2.01	0.43
1:A:357:ASN:O	1:A:359:PRO:HD3	2.19	0.43
1:I:123:HIS:HB3	1:I:167:VAL:HB	2.01	0.43
3:I:602:HEC:HBB3	3:I:602:HEC:HMB1	2.01	0.43
1:K:75:PRO:CG	5:K:609:PEG:H32	2.49	0.43
3:K:601:HEC:HMC1	3:K:601:HEC:HBC3	2.00	0.43
1:A:259:ASN:HD21	3:A:606:HEC:C3C	2.32	0.43
1:C:120:ARG:NH2	1:E:330:ASN:HB3	2.34	0.43
1:C:307:ALA:HA	1:C:314:TRP:CH2	2.53	0.43
1:E:191:PRO:HG2	3:E:604:HEC:CHD	2.49	0.43
1:I:337:CYS:HG	3:I:605:HEC:HAC	1.73	0.43
3:G:601:HEC:HMC1	3:G:601:HEC:HBC3	2.01	0.43
1:I:284:ALA:HB2	1:I:295:TRP:CE3	2.53	0.43
3:I:605:HEC:HMC1	3:I:605:HEC:HBC3	2.01	0.43
1:A:130:ARG:HG2	8:A:964:HOH:O	2.18	0.42
3:K:601:HEC:HBA1	3:K:602:HEC:CAA	2.49	0.42
1:A:167:VAL:HG21	3:A:602:HEC:CHD	2.49	0.42
4:A:608:ISW:C3A	7:A:612:PG4:H51	2.49	0.42
1:C:94:PRO:HB2	1:C:96:GLU:HG2	2.00	0.42
1:C:257:HIS:CE1	3:C:606:HEC:HMD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:HIS:CE1	1:G:191:PRO:HD3	2.53	0.42
3:I:605:HEC:HMA3	3:I:606:HEC:HBA2	2.00	0.42
1:K:462:LEU:HG	1:K:508:GLU:CD	2.39	0.42
4:A:609:ISW:O1D	3:E:605:HEC:HMA2	2.19	0.42
3:C:602:HEC:HMC1	3:C:602:HEC:HBC3	2.00	0.42
1:K:141:LYS:NZ	3:K:601:HEC:O1A	2.51	0.42
3:G:602:HEC:HBC3	3:G:602:HEC:HMC1	2.00	0.42
4:G:608:ISW:NB	1:I:491:TYR:OH	2.47	0.42
1:K:257:HIS:CE1	3:K:606:HEC:HMD1	2.54	0.42
1:C:84:PRO:HB3	1:C:190:MET:HB2	2.01	0.42
1:I:269:ARG:HA	1:I:270:HIS:HA	1.75	0.42
1:K:302:LYS:HD3	1:K:302:LYS:HA	1.75	0.42
1:C:50:TYR:CZ	1:C:54:VAL:HG21	2.55	0.42
3:E:604:HEC:HHA	3:E:604:HEC:HBA1	2.02	0.42
1:I:168:GLY:O	3:I:604:HEC:HMC3	2.19	0.42
1:I:259:ASN:HD21	3:I:606:HEC:C3C	2.32	0.42
1:K:442:LYS:HD3	1:K:442:LYS:HA	1.84	0.42
1:C:360:PHE:CD2	1:C:470:ALA:HB1	2.54	0.42
1:E:360:PHE:CD2	1:E:470:ALA:HB1	2.54	0.42
1:G:167:VAL:HG21	3:G:602:HEC:CHD	2.49	0.42
1:G:227:SER:O	3:G:606:HEC:HBD1	2.20	0.42
1:G:241:TRP:HB2	4:G:608:ISW:HMB	2.02	0.42
1:A:521:ARG:HG3	8:A:720:HOH:O	2.19	0.42
1:C:253:CYS:CB	4:C:608:ISW:HHC	2.50	0.42
1:E:50:TYR:CZ	1:E:54:VAL:HG21	2.54	0.42
1:K:381:VAL:O	1:K:385:THR:HG23	2.19	0.42
3:E:601:HEC:HHA	3:E:601:HEC:HAA2	1.85	0.42
1:G:431:LYS:HZ3	6:G:611:PGE:H1	1.85	0.42
3:A:605:HEC:HMA2	4:A:608:ISW:O1D	2.20	0.42
3:A:606:HEC:HMB1	3:A:606:HEC:HBB3	2.02	0.42
1:E:349:ILE:HD13	3:E:606:HEC:C2A	2.50	0.42
1:A:200:HIS:CG	3:A:601:HEC:HMA1	2.54	0.41
3:C:603:HEC:CAA	3:C:604:HEC:HMA3	2.50	0.41
1:I:173:HIS:CE1	1:I:191:PRO:HD3	2.55	0.41
1:I:225:ARG:NE	4:I:608:ISW:O1A	2.48	0.41
1:K:169:CYS:O	1:K:173:HIS:HB2	2.20	0.41
1:C:114:TRP:HA	1:C:114:TRP:HE3	1.85	0.41
1:I:114:TRP:HA	1:I:114:TRP:HE3	1.86	0.41
1:I:385:THR:HA	1:I:388:HIS:O	2.20	0.41
4:I:608:ISW:HBB	4:I:608:ISW:HMB	2.02	0.41
4:A:608:ISW:HHB	4:A:608:ISW:HMA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:ISW:NB	1:C:491:TYR:OH	2.48	0.41
1:E:200:HIS:CG	3:E:601:HEC:HMA1	2.56	0.41
1:G:167:VAL:HG13	3:G:602:HEC:HBC2	2.02	0.41
1:G:180:ASP:OD1	1:G:180:ASP:N	2.49	0.41
3:G:605:HEC:HMA2	4:G:608:ISW:O1D	2.20	0.41
1:E:41:ARG:HG3	8:E:882:HOH:O	2.20	0.41
3:C:605:HEC:HMC1	3:C:605:HEC:HBC3	2.02	0.41
1:E:259:ASN:HD21	3:E:606:HEC:C3C	2.33	0.41
1:I:339:MET:HE3	1:I:346:THR:O	2.21	0.41
1:K:112:PRO:O	1:K:116:ARG:HG3	2.21	0.41
1:A:112:PRO:O	1:A:116:ARG:HG3	2.20	0.41
1:A:264:ASP:O	1:A:268:THR:HA	2.21	0.41
1:E:114:TRP:HA	1:E:114:TRP:CE3	2.56	0.41
2:F:30:LEU:HD12	2:F:30:LEU:HA	1.90	0.41
1:G:272:PHE:O	3:G:602:HEC:HBA1	2.21	0.41
1:I:357:ASN:O	1:I:359:PRO:HD3	2.20	0.41
3:I:604:HEC:HBB3	3:I:604:HEC:HMB1	2.02	0.41
1:A:291:ASP:OD1	1:A:291:ASP:N	2.53	0.41
1:I:431:LYS:HZ3	6:I:609:PGE:H1	1.85	0.41
3:K:607:HEC:HMC1	3:K:607:HEC:HBC3	2.02	0.41
1:I:120:ARG:HH21	1:K:330:ASN:HB3	1.84	0.41
1:C:134:SER:HA	1:C:139:TYR:CG	2.56	0.40
5:C:609:PEG:H42	5:C:609:PEG:H21	1.93	0.40
1:G:203:GLU:HG2	3:G:601:HEC:C4A	2.51	0.40
3:G:605:HEC:HMC1	3:G:605:HEC:HBC3	2.03	0.40
3:I:603:HEC:CBC	3:I:603:HEC:HMC1	2.51	0.40
1:A:118:TRP:CE2	1:A:124:ALA:HB2	2.56	0.40
4:C:608:ISW:HMB	4:C:608:ISW:HBB	2.03	0.40
1:G:308:GLU:HG3	8:G:778:HOH:O	2.20	0.40
1:A:491:TYR:OH	4:A:609:ISW:NB	2.45	0.40
1:A:519:GLN:HG2	1:C:518:LEU:HD13	2.02	0.40
1:E:337:CYS:SG	3:E:605:HEC:C2C	3.09	0.40
1:C:442:LYS:HD3	1:C:442:LYS:HA	1.81	0.40
1:E:180:ASP:OD1	1:E:180:ASP:N	2.47	0.40
1:I:339:MET:SD	3:I:601:HEC:HMD2	2.61	0.40
1:I:442:LYS:HA	1:I:442:LYS:HD3	1.84	0.40
1:K:191:PRO:HG2	3:K:604:HEC:CHD	2.51	0.40
1:A:269:ARG:HA	1:A:270:HIS:HA	1.82	0.40
3:K:604:HEC:HBB3	3:K:604:HEC:HMB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/570 (88%)	487 (97%)	15 (3%)	0	100	100
1	C	502/570 (88%)	489 (97%)	13 (3%)	0	100	100
1	E	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
1	G	502/570 (88%)	486 (97%)	16 (3%)	0	100	100
1	I	502/570 (88%)	489 (97%)	12 (2%)	1 (0%)	47	44
1	K	502/570 (88%)	488 (97%)	14 (3%)	0	100	100
2	B	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	D	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	F	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	H	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	J	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
2	L	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
All	All	3384/3966 (85%)	3293 (97%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	292	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	430/477 (90%)	426 (99%)	4 (1%)	78	83
1	C	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	E	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	G	430/477 (90%)	426 (99%)	4 (1%)	78	83
1	I	430/477 (90%)	428 (100%)	2 (0%)	88	92
1	K	430/477 (90%)	426 (99%)	4 (1%)	78	83
2	B	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	D	53/73 (73%)	51 (96%)	2 (4%)	33	31
2	F	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	H	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	J	53/73 (73%)	52 (98%)	1 (2%)	57	61
2	L	53/73 (73%)	52 (98%)	1 (2%)	57	61
All	All	2898/3300 (88%)	2873 (99%)	25 (1%)	78	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	114	TRP
1	A	169	CYS
1	A	267	HIS
2	B	30	LEU
1	C	114	TRP
1	C	267	HIS
2	D	29	SER
2	D	30	LEU
1	E	37	LEU
1	E	114	TRP
2	F	30	LEU
1	G	53	LEU
1	G	114	TRP
1	G	267	HIS
1	G	523	ASN
2	H	30	LEU
1	I	114	TRP
1	I	267	HIS
2	J	30	LEU
1	K	37	LEU
1	K	114	TRP

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Mol	Chain	Res	Type
1	K	169	CYS
1	K	267	HIS
2	L	30	LEU

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

Mol	Chain	Res	Type
2	H	56	HIS
2	L	61	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

66 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	$\#\|Z\| > 2$
3	HEC	G	604	1	32,50,50	2.23	4 (12%)	24,82,82	1.77	6 (25%)
6	PGE	A	611	-	9,9,9	0.35	0	8,8,8	0.35	0
3	HEC	E	607	1	32,50,50	2.06	4 (12%)	24,82,82	2.35	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	K	602	1	32,50,50	2.08	4 (12%)	24,82,82	1.79	5 (20%)
3	HEC	K	605	1	32,50,50	2.09	4 (12%)	24,82,82	2.16	8 (33%)
3	HEC	A	602	1	32,50,50	2.10	5 (15%)	24,82,82	2.11	6 (25%)
6	PGE	G	611	-	9,9,9	0.34	0	8,8,8	0.40	0
5	PEG	J	101	-	6,6,6	0.48	0	5,5,5	0.52	0
4	ISW	A	609	1,8	40,50,50	4.38	17 (42%)	38,82,82	5.18	17 (44%)
3	HEC	C	605	1	32,50,50	2.27	4 (12%)	24,82,82	2.05	5 (20%)
6	PGE	E	608	-	9,9,9	0.36	0	8,8,8	0.31	0
3	HEC	E	602	1	32,50,50	2.14	4 (12%)	24,82,82	1.98	9 (37%)
3	HEC	G	607	1	32,50,50	2.14	5 (15%)	24,82,82	2.16	7 (29%)
4	ISW	C	608	1,8	40,50,50	4.54	16 (40%)	38,82,82	5.25	21 (55%)
3	HEC	C	602	1	32,50,50	2.11	3 (9%)	24,82,82	2.18	7 (29%)
3	HEC	E	601	1	32,50,50	2.05	4 (12%)	24,82,82	2.35	7 (29%)
3	HEC	K	601	1	32,50,50	1.88	3 (9%)	24,82,82	2.33	9 (37%)
3	HEC	I	605	1	32,50,50	2.17	3 (9%)	24,82,82	2.23	7 (29%)
5	PEG	C	609	-	6,6,6	0.48	0	5,5,5	0.38	0
6	PGE	I	610	-	9,9,9	0.29	0	8,8,8	0.24	0
3	HEC	K	603	1	32,50,50	2.00	4 (12%)	24,82,82	2.09	6 (25%)
3	HEC	K	604	1	32,50,50	2.19	3 (9%)	24,82,82	1.72	7 (29%)
5	PEG	K	609	-	6,6,6	0.47	0	5,5,5	0.41	0
3	HEC	I	607	1	32,50,50	2.19	3 (9%)	24,82,82	2.34	9 (37%)
4	ISW	G	609	1,8	40,50,50	4.45	18 (45%)	38,82,82	5.02	17 (44%)
4	ISW	A	608	1,8	40,50,50	4.46	16 (40%)	38,82,82	5.36	22 (57%)
5	PEG	G	610	-	6,6,6	0.50	0	5,5,5	0.25	0
3	HEC	C	601	1	32,50,50	2.10	3 (9%)	24,82,82	2.15	7 (29%)
3	HEC	G	605	1	32,50,50	2.11	3 (9%)	24,82,82	2.23	7 (29%)
3	HEC	A	606	1	32,50,50	2.16	6 (18%)	24,82,82	2.24	7 (29%)
3	HEC	I	601	1	32,50,50	2.14	3 (9%)	24,82,82	1.76	4 (16%)
3	HEC	C	603	1	32,50,50	1.91	3 (9%)	24,82,82	2.09	7 (29%)
3	HEC	K	607	1	32,50,50	2.10	3 (9%)	24,82,82	2.31	9 (37%)
3	HEC	C	604	1	32,50,50	2.31	5 (15%)	24,82,82	1.92	8 (33%)
4	ISW	G	608	1	40,50,50	4.49	16 (40%)	38,82,82	5.50	21 (55%)
3	HEC	I	602	1	32,50,50	2.16	3 (9%)	24,82,82	2.10	7 (29%)
5	PEG	A	610	-	6,6,6	0.50	0	5,5,5	0.41	0
6	PGE	C	610	-	9,9,9	0.36	0	8,8,8	0.31	0
6	PGE	G	612	-	9,9,9	0.39	0	8,8,8	0.41	0
3	HEC	E	603	1	32,50,50	2.09	5 (15%)	24,82,82	2.21	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	E	606	1	32,50,50	2.12	3 (9%)	24,82,82	2.00	7 (29%)
3	HEC	A	601	1	32,50,50	1.80	3 (9%)	24,82,82	2.45	5 (20%)
6	PGE	E	609	-	9,9,9	0.31	0	8,8,8	0.50	0
3	HEC	A	603	1	32,50,50	2.07	5 (15%)	24,82,82	2.34	9 (37%)
3	HEC	C	606	1	32,50,50	2.13	4 (12%)	24,82,82	2.26	6 (25%)
3	HEC	C	607	1	32,50,50	2.25	7 (21%)	24,82,82	2.34	9 (37%)
3	HEC	A	604	1	32,50,50	2.01	3 (9%)	24,82,82	2.17	5 (20%)
3	HEC	K	606	1	32,50,50	2.20	4 (12%)	24,82,82	2.17	9 (37%)
5	PEG	K	608	-	6,6,6	0.42	0	5,5,5	0.33	0
4	ISW	I	608	1,8	40,50,50	4.57	16 (40%)	38,82,82	4.98	20 (52%)
7	PG4	A	612	-	12,12,12	0.53	0	11,11,11	0.31	0
3	HEC	E	604	1	32,50,50	2.06	5 (15%)	24,82,82	1.80	6 (25%)
7	PG4	C	611	-	12,12,12	0.52	0	11,11,11	0.29	0
3	HEC	G	602	1	32,50,50	2.11	4 (12%)	24,82,82	1.90	6 (25%)
3	HEC	A	607	1	32,50,50	2.23	3 (9%)	24,82,82	2.06	10 (41%)
3	HEC	A	605	1	32,50,50	2.08	3 (9%)	24,82,82	2.15	6 (25%)
3	HEC	G	606	1	32,50,50	2.10	3 (9%)	24,82,82	2.50	7 (29%)
3	HEC	I	603	1	32,50,50	2.18	5 (15%)	24,82,82	2.03	7 (29%)
3	HEC	I	606	1	32,50,50	2.10	3 (9%)	24,82,82	2.23	5 (20%)
6	PGE	I	609	-	9,9,9	0.32	0	8,8,8	0.25	0
7	PG4	E	610	-	12,12,12	0.52	0	11,11,11	0.32	0
3	HEC	E	605	1	32,50,50	2.08	3 (9%)	24,82,82	2.09	6 (25%)
3	HEC	G	601	1	32,50,50	1.99	4 (12%)	24,82,82	2.16	7 (29%)
7	PG4	K	610	-	12,12,12	0.56	0	11,11,11	0.34	0
3	HEC	G	603	1	32,50,50	1.86	3 (9%)	24,82,82	2.50	7 (29%)
3	HEC	I	604	1	32,50,50	2.21	4 (12%)	24,82,82	1.52	4 (16%)

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	HEC	G	604	1	-	3/10/54/54	-
6	PGE	A	611	-	-	3/7/7/7	-
3	HEC	E	607	1	-	3/10/54/54	-
3	HEC	K	602	1	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	K	605	1	-	5/10/54/54	-
3	HEC	A	602	1	-	4/10/54/54	-
6	PGE	G	611	-	-	6/7/7/7	-
5	PEG	J	101	-	-	2/4/4/4	-
4	ISW	A	609	1,8	-	3/12/74/74	-
3	HEC	C	605	1	-	5/10/54/54	-
6	PGE	E	608	-	-	4/7/7/7	-
3	HEC	E	602	1	-	4/10/54/54	-
3	HEC	G	607	1	-	3/10/54/54	-
4	ISW	C	608	1,8	-	3/12/74/74	-
3	HEC	C	602	1	-	4/10/54/54	-
3	HEC	E	601	1	-	4/10/54/54	-
3	HEC	K	601	1	-	3/10/54/54	-
3	HEC	I	605	1	-	5/10/54/54	-
5	PEG	C	609	-	-	2/4/4/4	-
6	PGE	I	610	-	-	6/7/7/7	-
3	HEC	K	603	1	-	1/10/54/54	-
3	HEC	K	604	1	-	2/10/54/54	-
5	PEG	K	609	-	-	2/4/4/4	-
3	HEC	I	607	1	-	4/10/54/54	-
4	ISW	G	609	1,8	-	5/12/74/74	-
4	ISW	A	608	1,8	-	3/12/74/74	-
5	PEG	G	610	-	-	3/4/4/4	-
3	HEC	C	601	1	-	4/10/54/54	-
3	HEC	G	605	1	-	5/10/54/54	-
3	HEC	A	606	1	-	2/10/54/54	-
3	HEC	I	601	1	-	2/10/54/54	-
3	HEC	C	603	1	-	2/10/54/54	-
3	HEC	K	607	1	-	4/10/54/54	-
3	HEC	C	604	1	-	3/10/54/54	-
4	ISW	G	608	1	-	2/12/74/74	-
3	HEC	I	602	1	-	4/10/54/54	-
5	PEG	A	610	-	-	3/4/4/4	-
6	PGE	C	610	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	G	612	-	-	5/7/7/7	-
3	HEC	E	603	1	-	1/10/54/54	-
3	HEC	E	606	1	-	2/10/54/54	-
3	HEC	A	601	1	-	2/10/54/54	-
6	PGE	E	609	-	-	2/7/7/7	-
3	HEC	A	603	1	-	0/10/54/54	-
3	HEC	C	606	1	-	4/10/54/54	-
3	HEC	C	607	1	-	5/10/54/54	-
3	HEC	A	604	1	-	2/10/54/54	-
3	HEC	K	606	1	-	2/10/54/54	-
5	PEG	K	608	-	-	2/4/4/4	-
4	ISW	I	608	1,8	-	5/12/74/74	-
7	PG4	A	612	-	-	7/10/10/10	-
3	HEC	E	604	1	-	2/10/54/54	-
7	PG4	C	611	-	-	6/10/10/10	-
3	HEC	G	602	1	-	4/10/54/54	-
3	HEC	A	607	1	-	2/10/54/54	-
3	HEC	A	605	1	-	5/10/54/54	-
3	HEC	G	606	1	-	4/10/54/54	-
3	HEC	I	603	1	-	0/10/54/54	-
3	HEC	I	606	1	-	2/10/54/54	-
6	PGE	I	609	-	-	5/7/7/7	-
7	PG4	E	610	-	-	3/10/10/10	-
3	HEC	E	605	1	-	5/10/54/54	-
3	HEC	G	601	1	-	4/10/54/54	-
7	PG4	K	610	-	-	5/10/10/10	-
3	HEC	G	603	1	-	2/10/54/54	-
3	HEC	I	604	1	-	4/10/54/54	-

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	608	ISW	CHC-C4B	-14.98	1.30	1.53
4	I	608	ISW	CHC-C4B	-14.90	1.30	1.53
4	A	608	ISW	CHC-C4B	-14.51	1.30	1.53
4	G	608	ISW	CHC-C4B	-14.50	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	609	ISW	CHC-C4B	-13.77	1.32	1.53
4	G	609	ISW	CHC-C4B	-13.48	1.32	1.53
4	G	608	ISW	CHD-C1D	11.36	1.64	1.35
4	A	609	ISW	CHD-C1D	11.32	1.64	1.35
4	G	609	ISW	CHD-C1D	11.21	1.63	1.35
4	C	608	ISW	CHD-C1D	11.20	1.63	1.35
4	I	608	ISW	CHD-C1D	11.02	1.63	1.35
4	A	608	ISW	CHD-C1D	10.76	1.62	1.35
4	I	608	ISW	C4C-CHD	10.17	1.69	1.41
4	C	608	ISW	C4C-CHD	10.08	1.69	1.41
4	A	608	ISW	C4C-CHD	10.00	1.68	1.41
4	G	609	ISW	C4C-CHD	9.88	1.68	1.41
4	A	609	ISW	C4C-CHD	9.85	1.68	1.41
4	G	608	ISW	C4C-CHD	9.78	1.68	1.41
4	G	608	ISW	CHA-C4D	9.53	1.68	1.41
4	A	608	ISW	CHA-C4D	9.42	1.68	1.41
4	I	608	ISW	CHA-C4D	9.39	1.68	1.41
4	C	608	ISW	CHA-C4D	9.36	1.68	1.41
4	A	609	ISW	CHA-C4D	9.14	1.67	1.41
4	G	609	ISW	CHA-C4D	9.10	1.67	1.41
4	I	608	ISW	CHB-C1B	8.93	1.66	1.41
4	A	609	ISW	CHB-C1B	8.83	1.66	1.41
4	C	608	ISW	CHB-C1B	8.81	1.66	1.41
4	A	608	ISW	CHB-C1B	8.77	1.66	1.41
4	G	609	ISW	CHB-C1B	8.64	1.66	1.41
4	G	608	ISW	CHB-C1B	8.40	1.65	1.41
4	I	608	ISW	C1D-ND	8.23	1.54	1.40
4	G	608	ISW	C1D-ND	8.13	1.54	1.40
4	C	608	ISW	C1D-ND	7.76	1.53	1.40
3	A	607	HEC	C2B-C3B	-7.75	1.32	1.40
4	G	609	ISW	C1D-ND	7.72	1.53	1.40
3	I	602	HEC	C2B-C3B	-7.67	1.32	1.40
4	A	608	ISW	C1D-ND	7.55	1.53	1.40
3	C	605	HEC	C2B-C3B	-7.48	1.32	1.40
3	I	607	HEC	C2B-C3B	-7.46	1.33	1.40
3	C	604	HEC	C2B-C3B	-7.33	1.33	1.40
3	I	605	HEC	C2B-C3B	-7.26	1.33	1.40
3	C	607	HEC	C3C-C2C	-7.25	1.33	1.40
3	G	604	HEC	C3C-C2C	-7.22	1.33	1.40
3	E	603	HEC	C2B-C3B	-7.09	1.33	1.40
3	K	606	HEC	C2B-C3B	-7.08	1.33	1.40
3	G	607	HEC	C2B-C3B	-7.01	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	604	HEC	C2B-C3B	-6.95	1.33	1.40
3	A	605	HEC	C2B-C3B	-6.94	1.33	1.40
3	K	604	HEC	C2B-C3B	-6.87	1.33	1.40
3	G	604	HEC	C2B-C3B	-6.87	1.33	1.40
3	I	601	HEC	C3C-C2C	-6.86	1.33	1.40
3	K	606	HEC	C3C-C2C	-6.85	1.33	1.40
3	G	606	HEC	C2B-C3B	-6.80	1.33	1.40
3	K	605	HEC	C2B-C3B	-6.78	1.33	1.40
3	G	605	HEC	C2B-C3B	-6.76	1.33	1.40
4	A	609	ISW	C1D-ND	6.75	1.51	1.40
3	A	606	HEC	C3C-C2C	-6.75	1.33	1.40
3	E	605	HEC	C2B-C3B	-6.73	1.33	1.40
3	G	602	HEC	C2B-C3B	-6.59	1.33	1.40
3	C	602	HEC	C2B-C3B	-6.52	1.33	1.40
3	C	604	HEC	C3C-C2C	-6.51	1.34	1.40
3	C	605	HEC	C3C-C2C	-6.48	1.34	1.40
3	E	602	HEC	C2B-C3B	-6.47	1.34	1.40
3	C	601	HEC	C2B-C3B	-6.45	1.34	1.40
3	C	602	HEC	C3C-C2C	-6.41	1.34	1.40
3	A	603	HEC	C2B-C3B	-6.36	1.34	1.40
3	K	604	HEC	C3C-C2C	-6.36	1.34	1.40
3	K	602	HEC	C2B-C3B	-6.29	1.34	1.40
3	E	607	HEC	C3C-C2C	-6.28	1.34	1.40
3	A	602	HEC	C2B-C3B	-6.28	1.34	1.40
3	G	606	HEC	C3C-C2C	-6.25	1.34	1.40
3	I	605	HEC	C3C-C2C	-6.24	1.34	1.40
3	I	603	HEC	C2B-C3B	-6.23	1.34	1.40
3	K	607	HEC	C2B-C3B	-6.23	1.34	1.40
3	I	604	HEC	C3C-C2C	-6.22	1.34	1.40
3	E	606	HEC	C3C-C2C	-6.20	1.34	1.40
3	G	601	HEC	C2B-C3B	-6.18	1.34	1.40
3	I	606	HEC	C2B-C3B	-6.14	1.34	1.40
3	E	606	HEC	C2B-C3B	-6.13	1.34	1.40
3	C	607	HEC	C2B-C3B	-6.12	1.34	1.40
3	C	606	HEC	C2B-C3B	-6.11	1.34	1.40
3	K	607	HEC	C3C-C2C	-6.09	1.34	1.40
3	A	607	HEC	C3C-C2C	-6.03	1.34	1.40
3	K	605	HEC	C3C-C2C	-6.03	1.34	1.40
3	E	601	HEC	C2B-C3B	-6.01	1.34	1.40
3	A	604	HEC	C3C-C2C	-6.00	1.34	1.40
3	C	606	HEC	C3C-C2C	-5.97	1.34	1.40
3	I	607	HEC	C3C-C2C	-5.97	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	606	HEC	C3C-C2C	-5.93	1.34	1.40
3	I	601	HEC	C2B-C3B	-5.92	1.34	1.40
3	A	606	HEC	C2B-C3B	-5.90	1.34	1.40
3	I	602	HEC	C3C-C2C	-5.90	1.34	1.40
3	C	601	HEC	C3C-C2C	-5.89	1.34	1.40
3	C	603	HEC	C2B-C3B	-5.84	1.34	1.40
3	E	607	HEC	C2B-C3B	-5.80	1.34	1.40
3	E	602	HEC	C3C-C2C	-5.78	1.34	1.40
3	E	604	HEC	C3C-C2C	-5.73	1.34	1.40
3	G	605	HEC	C3C-C2C	-5.71	1.34	1.40
3	E	604	HEC	C2B-C3B	-5.70	1.34	1.40
3	A	604	HEC	C2B-C3B	-5.70	1.34	1.40
3	I	603	HEC	C3D-C2D	5.70	1.54	1.37
3	G	603	HEC	C2B-C3B	-5.68	1.34	1.40
3	G	607	HEC	C3C-C2C	-5.62	1.34	1.40
3	A	601	HEC	C3C-C2C	-5.60	1.34	1.40
3	A	605	HEC	C3C-C2C	-5.58	1.34	1.40
4	G	609	ISW	CHC-C1C	5.49	1.64	1.51
4	A	608	ISW	CHC-C1C	5.49	1.64	1.51
3	A	602	HEC	C3C-C2C	-5.44	1.35	1.40
3	E	605	HEC	C3C-C2C	-5.44	1.35	1.40
3	G	601	HEC	C3C-C2C	-5.44	1.35	1.40
3	G	602	HEC	C3C-C2C	-5.43	1.35	1.40
3	K	603	HEC	C2B-C3B	-5.41	1.35	1.40
4	C	608	ISW	CHC-C1C	5.30	1.64	1.51
3	K	601	HEC	C3C-C2C	-5.28	1.35	1.40
3	K	602	HEC	C3D-C2D	5.22	1.53	1.37
3	E	601	HEC	C3C-C2C	-5.21	1.35	1.40
3	I	603	HEC	C3C-C2C	-5.18	1.35	1.40
4	G	608	ISW	CHC-C1C	5.15	1.64	1.51
4	I	608	ISW	CHC-C1C	5.13	1.64	1.51
3	A	603	HEC	C3D-C2D	5.13	1.52	1.37
3	K	603	HEC	C3D-C2D	5.11	1.52	1.37
3	G	602	HEC	C3D-C2D	5.10	1.52	1.37
3	K	601	HEC	C2B-C3B	-5.06	1.35	1.40
4	A	609	ISW	CHC-C1C	5.03	1.63	1.51
3	E	602	HEC	C3D-C2D	5.01	1.52	1.37
3	G	605	HEC	C3D-C2D	4.99	1.52	1.37
3	K	602	HEC	C3C-C2C	-4.99	1.35	1.40
3	E	603	HEC	C3D-C2D	4.94	1.52	1.37
3	K	603	HEC	C3C-C2C	-4.94	1.35	1.40
3	E	601	HEC	C3D-C2D	4.93	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	606	HEC	C3D-C2D	4.89	1.52	1.37
3	C	604	HEC	C3D-C2D	4.88	1.52	1.37
3	C	603	HEC	C3C-C2C	-4.87	1.35	1.40
3	I	601	HEC	C3D-C2D	4.86	1.52	1.37
3	E	605	HEC	C3D-C2D	4.83	1.52	1.37
3	A	602	HEC	C3D-C2D	4.82	1.51	1.37
3	E	603	HEC	C3C-C2C	-4.80	1.35	1.40
3	C	606	HEC	C3D-C2D	4.79	1.51	1.37
3	E	606	HEC	C3D-C2D	4.77	1.51	1.37
3	G	607	HEC	C3D-C2D	4.76	1.51	1.37
3	K	601	HEC	C3D-C2D	4.72	1.51	1.37
3	G	603	HEC	C3D-C2D	4.70	1.51	1.37
3	C	603	HEC	C3D-C2D	4.68	1.51	1.37
3	E	607	HEC	C3D-C2D	4.67	1.51	1.37
3	I	607	HEC	C3D-C2D	4.66	1.51	1.37
3	I	604	HEC	C3D-C2D	4.66	1.51	1.37
3	K	607	HEC	C3D-C2D	4.61	1.51	1.37
3	C	605	HEC	C3D-C2D	4.61	1.51	1.37
3	A	605	HEC	C3D-C2D	4.59	1.51	1.37
3	C	607	HEC	C3D-C2D	4.59	1.51	1.37
3	K	604	HEC	C3D-C2D	4.59	1.51	1.37
3	C	601	HEC	C3D-C2D	4.58	1.51	1.37
3	G	601	HEC	C3D-C2D	4.54	1.51	1.37
3	A	606	HEC	C3D-C2D	4.51	1.51	1.37
3	I	602	HEC	C3D-C2D	4.47	1.50	1.37
3	C	602	HEC	C3D-C2D	4.46	1.50	1.37
3	K	606	HEC	C3D-C2D	4.46	1.50	1.37
3	A	604	HEC	C3D-C2D	4.45	1.50	1.37
3	A	603	HEC	C3C-C2C	-4.45	1.36	1.40
3	I	605	HEC	C3D-C2D	4.40	1.50	1.37
3	E	604	HEC	C3D-C2D	4.37	1.50	1.37
3	A	607	HEC	C3D-C2D	4.28	1.50	1.37
3	A	601	HEC	C3D-C2D	4.27	1.50	1.37
3	G	606	HEC	C3D-C2D	4.25	1.50	1.37
3	A	601	HEC	C2B-C3B	-4.23	1.36	1.40
3	K	605	HEC	C3D-C2D	4.22	1.50	1.37
4	G	609	ISW	C1D-C2D	4.15	1.52	1.44
3	G	604	HEC	C3D-C2D	4.10	1.49	1.37
3	G	603	HEC	C3C-C2C	-4.03	1.36	1.40
4	C	608	ISW	C1B-C2B	4.03	1.52	1.44
4	I	608	ISW	C4D-ND	3.99	1.47	1.38
4	I	608	ISW	C4D-C3D	3.92	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	608	ISW	C1D-C2D	3.81	1.51	1.44
4	C	608	ISW	C3C-CAC	3.81	1.55	1.47
4	G	609	ISW	C4D-ND	3.80	1.46	1.38
4	G	609	ISW	C4D-C3D	3.78	1.51	1.45
4	I	608	ISW	C1B-C2B	3.71	1.51	1.44
4	A	609	ISW	C1D-C2D	3.67	1.51	1.44
4	G	608	ISW	C4D-C3D	3.65	1.51	1.45
4	A	608	ISW	C3C-CAC	3.64	1.55	1.47
4	A	609	ISW	C1B-C2B	3.63	1.51	1.44
4	A	609	ISW	C4C-NC	-3.49	1.29	1.36
4	A	608	ISW	C4C-NC	-3.44	1.29	1.36
4	A	608	ISW	C1B-C2B	3.43	1.51	1.44
4	C	608	ISW	C4D-C3D	3.37	1.50	1.45
4	G	609	ISW	C3D-C2D	3.36	1.43	1.36
4	G	609	ISW	C1B-C2B	3.35	1.51	1.44
4	C	608	ISW	C4D-ND	3.34	1.45	1.38
4	C	608	ISW	C1D-C2D	3.33	1.51	1.44
4	G	608	ISW	C3D-C2D	3.33	1.43	1.36
4	G	608	ISW	C4C-NC	-3.26	1.29	1.36
4	G	608	ISW	C1B-C2B	3.22	1.50	1.44
4	I	608	ISW	C1D-C2D	3.21	1.50	1.44
4	G	609	ISW	C3C-CAC	3.20	1.54	1.47
4	A	609	ISW	C4D-C3D	3.20	1.50	1.45
4	I	608	ISW	C3C-CAC	3.17	1.54	1.47
4	I	608	ISW	C3D-C2D	3.16	1.43	1.36
4	A	609	ISW	C4D-ND	3.15	1.45	1.38
4	A	608	ISW	C1D-C2D	3.14	1.50	1.44
4	G	608	ISW	C4D-ND	3.12	1.45	1.38
4	G	609	ISW	C4C-NC	-3.03	1.29	1.36
4	A	608	ISW	C3D-C2D	3.00	1.43	1.36
4	C	608	ISW	C3D-C2D	2.95	1.43	1.36
4	A	608	ISW	C4D-C3D	2.93	1.50	1.45
4	G	608	ISW	C3C-CAC	2.92	1.53	1.47
4	C	608	ISW	C4C-NC	-2.92	1.30	1.36
4	A	609	ISW	C3C-C2C	2.82	1.44	1.40
4	A	609	ISW	C3C-CAC	2.74	1.53	1.47
4	A	608	ISW	C4D-ND	2.72	1.44	1.38
3	I	603	HEC	CAD-C3D	2.71	1.56	1.52
4	A	609	ISW	C3D-C2D	2.64	1.42	1.36
3	A	603	HEC	CAA-C2A	2.59	1.56	1.52
4	G	609	ISW	CBA-CGA	2.52	1.56	1.50
4	I	608	ISW	C4C-NC	-2.52	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	603	HEC	CMD-C2D	2.49	1.56	1.51
4	G	609	ISW	C4B-NB	2.47	1.52	1.48
3	A	606	HEC	O2D-CGD	-2.45	1.22	1.30
4	C	608	ISW	C3C-C2C	2.42	1.43	1.40
4	A	608	ISW	CBA-CGA	2.40	1.56	1.50
4	G	609	ISW	C3C-C2C	2.36	1.43	1.40
4	I	608	ISW	CBA-CGA	2.33	1.56	1.50
3	C	605	HEC	CAA-C2A	2.32	1.56	1.52
3	I	604	HEC	CAA-C2A	2.29	1.56	1.52
3	K	605	HEC	CMD-C2D	2.26	1.56	1.51
4	G	608	ISW	CBA-CGA	2.26	1.55	1.50
3	E	604	HEC	CMA-C3A	2.24	1.56	1.51
4	A	609	ISW	CBA-CGA	2.24	1.55	1.50
3	A	606	HEC	C1D-CHD	-2.23	1.34	1.41
3	G	607	HEC	CMC-C2C	2.21	1.56	1.51
3	C	607	HEC	CMD-C2D	2.21	1.56	1.51
3	K	602	HEC	C4D-ND	2.19	1.40	1.36
3	K	603	HEC	C1D-ND	2.17	1.40	1.36
3	G	602	HEC	CAD-C3D	2.15	1.55	1.52
4	I	608	ISW	C3C-C2C	2.14	1.43	1.40
3	C	607	HEC	C1D-CHD	-2.12	1.35	1.41
3	E	602	HEC	C4D-ND	2.12	1.40	1.36
3	E	607	HEC	CAA-C2A	2.11	1.55	1.52
3	C	604	HEC	C1D-ND	2.11	1.40	1.36
3	E	604	HEC	CAA-C2A	2.10	1.55	1.52
4	G	608	ISW	C4B-NB	2.10	1.52	1.48
4	G	609	ISW	CMB-C2B	2.09	1.55	1.50
4	C	608	ISW	CBA-CGA	2.09	1.55	1.50
4	A	609	ISW	C4B-NB	2.08	1.51	1.48
3	E	603	HEC	CMD-C2D	2.08	1.56	1.51
3	C	604	HEC	CMA-C3A	2.08	1.56	1.51
3	K	606	HEC	CMB-C2B	2.06	1.56	1.51
3	A	602	HEC	C1D-ND	2.06	1.40	1.36
3	A	606	HEC	C1B-NB	2.06	1.40	1.36
3	E	603	HEC	C1D-ND	2.05	1.40	1.36
3	G	607	HEC	CAA-C2A	2.04	1.55	1.52
3	E	601	HEC	CMD-C2D	2.04	1.55	1.51
3	G	604	HEC	C1D-ND	2.04	1.40	1.36
3	C	607	HEC	C1C-NC	2.04	1.40	1.36
3	A	602	HEC	C4D-ND	2.03	1.40	1.36
3	C	606	HEC	C4B-C3B	2.02	1.46	1.43
4	A	608	ISW	C4B-NB	2.02	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	HEC	CAA-C2A	2.01	1.55	1.52
3	C	607	HEC	C1D-ND	2.01	1.40	1.36
3	A	603	HEC	CMD-C2D	2.01	1.55	1.51

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	608	ISW	C4D-CHA-C1A	-19.55	96.76	122.56
4	C	608	ISW	C4D-CHA-C1A	-19.29	97.11	122.56
4	G	608	ISW	C4D-CHA-C1A	-19.12	97.32	122.56
4	A	609	ISW	C4D-CHA-C1A	-18.05	98.73	122.56
4	I	608	ISW	C4D-CHA-C1A	-18.04	98.75	122.56
4	G	609	ISW	C4D-CHA-C1A	-17.53	99.42	122.56
4	G	608	ISW	CHB-C1B-C2B	-14.57	102.22	124.98
4	A	609	ISW	CHB-C1B-C2B	-9.89	109.53	124.98
4	G	609	ISW	CHB-C1B-C2B	-9.59	110.00	124.98
4	A	608	ISW	CHA-C4D-C3D	-9.48	110.91	124.84
4	A	609	ISW	CBA-CAA-C2A	9.22	128.15	112.60
4	C	608	ISW	CHB-C1B-C2B	-9.18	110.64	124.98
4	G	608	ISW	CHA-C4D-C3D	-8.88	111.78	124.84
4	A	608	ISW	CBA-CAA-C2A	8.86	127.53	112.60
4	C	608	ISW	CHA-C4D-C3D	-8.79	111.92	124.84
4	G	609	ISW	CHA-C4D-C3D	-8.74	112.00	124.84
4	A	608	ISW	CHA-C4D-ND	8.62	133.80	124.43
4	A	608	ISW	CMA-C3A-C2A	8.57	141.11	124.94
4	A	609	ISW	C4A-CHB-C1B	-8.55	111.28	122.56
4	G	608	ISW	CMA-C3A-C2A	8.46	140.89	124.94
4	G	608	ISW	CBA-CAA-C2A	8.43	126.81	112.60
4	I	608	ISW	CHB-C1B-C2B	-8.29	112.03	124.98
4	G	609	ISW	C4A-CHB-C1B	-8.20	111.74	122.56
4	G	608	ISW	CHA-C4D-ND	8.14	133.28	124.43
4	C	608	ISW	C3C-C4C-NC	8.13	119.72	109.21
4	C	608	ISW	CAD-CBD-CGD	-8.13	96.12	113.60
4	A	608	ISW	CHB-C1B-C2B	-8.11	112.31	124.98
4	A	608	ISW	C4A-CHB-C1B	-8.07	111.91	122.56
4	I	608	ISW	CHA-C4D-C3D	-8.00	113.07	124.84
4	I	608	ISW	CBA-CAA-C2A	7.96	126.01	112.60
4	C	608	ISW	CMA-C3A-C2A	7.95	139.94	124.94
4	C	608	ISW	CHA-C4D-ND	7.95	133.06	124.43
4	A	608	ISW	C3C-C4C-NC	7.94	119.48	109.21
4	A	609	ISW	CAD-CBD-CGD	-7.89	96.62	113.60
4	A	609	ISW	CHA-C4D-C3D	-7.80	113.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	608	ISW	CBA-CAA-C2A	7.80	125.75	112.60
4	G	608	ISW	C3C-C4C-NC	7.78	119.26	109.21
4	I	608	ISW	CMA-C3A-C2A	7.74	139.54	124.94
4	I	608	ISW	C3C-C4C-NC	7.73	119.21	109.21
4	A	609	ISW	C3C-C4C-NC	7.63	119.07	109.21
4	G	609	ISW	C3C-C4C-NC	7.62	119.06	109.21
4	G	609	ISW	CMA-C3A-C2A	7.61	139.29	124.94
4	I	608	ISW	C4A-CHB-C1B	-7.49	112.67	122.56
4	G	609	ISW	CAD-CBD-CGD	-7.45	97.58	113.60
4	C	608	ISW	C4A-CHB-C1B	-7.35	112.85	122.56
4	G	608	ISW	CAD-CBD-CGD	-7.29	97.91	113.60
4	I	608	ISW	CHA-C4D-ND	7.20	132.26	124.43
4	A	609	ISW	CMA-C3A-C2A	7.18	138.48	124.94
4	I	608	ISW	CAD-CBD-CGD	-7.11	98.31	113.60
4	G	608	ISW	C4A-CHB-C1B	-6.96	113.37	122.56
3	C	601	HEC	CBD-CAD-C3D	-6.89	100.87	112.62
3	K	601	HEC	CBD-CAD-C3D	-6.83	100.96	112.62
4	A	608	ISW	CAD-CBD-CGD	-6.81	98.94	113.60
3	G	601	HEC	CBD-CAD-C3D	-6.80	101.02	112.62
4	A	609	ISW	CHA-C4D-ND	6.69	131.69	124.43
3	A	601	HEC	CBD-CAD-C3D	-6.68	101.23	112.62
4	G	609	ISW	CHA-C4D-ND	6.60	131.60	124.43
3	G	606	HEC	CBA-CAA-C2A	-6.31	101.97	112.60
4	A	609	ISW	CMB-C2B-C1B	-6.30	115.44	125.04
4	G	609	ISW	C1D-ND-C4D	-6.29	98.58	105.07
3	G	605	HEC	CBD-CAD-C3D	-6.24	101.97	112.62
4	G	609	ISW	C3D-C4D-ND	6.22	116.38	110.36
4	G	609	ISW	CBA-CAA-C2A	6.19	123.03	112.60
3	G	607	HEC	CBD-CAD-C3D	-5.87	102.60	112.62
3	G	603	HEC	CMC-C2C-C1C	-5.86	119.46	128.46
3	I	605	HEC	CMB-C2B-C1B	-5.85	119.47	128.46
3	C	605	HEC	CMB-C2B-C1B	-5.84	119.48	128.46
3	A	603	HEC	CBA-CAA-C2A	-5.84	102.76	112.60
3	I	606	HEC	CBA-CAA-C2A	-5.64	103.10	112.60
3	E	601	HEC	CBD-CAD-C3D	-5.64	103.00	112.62
3	G	603	HEC	CMC-C2C-C3C	5.63	132.44	125.82
3	G	606	HEC	CBD-CAD-C3D	-5.62	103.03	112.62
3	I	602	HEC	CMC-C2C-C1C	-5.61	119.84	128.46
3	K	607	HEC	CBD-CAD-C3D	-5.61	103.05	112.62
3	A	601	HEC	CMB-C2B-C1B	-5.48	120.04	128.46
3	I	607	HEC	CBD-CAD-C3D	-5.46	103.30	112.62
3	E	607	HEC	CBD-CAD-C3D	-5.45	103.31	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	608	ISW	C1D-ND-C4D	-5.35	99.55	105.07
3	E	603	HEC	CMC-C2C-C1C	-5.32	120.29	128.46
3	K	605	HEC	CBD-CAD-C3D	-5.21	103.73	112.62
3	C	606	HEC	CBA-CAA-C2A	-5.19	103.86	112.60
3	E	601	HEC	CMC-C2C-C1C	-5.18	120.51	128.46
3	A	604	HEC	CBD-CAD-C3D	-5.16	103.82	112.62
4	I	608	ISW	C1D-ND-C4D	-5.15	99.75	105.07
3	E	605	HEC	CBD-CAD-C3D	-5.15	103.83	112.62
3	C	607	HEC	C1D-C2D-C3D	-5.14	103.42	107.00
3	G	603	HEC	CBA-CAA-C2A	-5.12	103.97	112.60
3	A	605	HEC	CMB-C2B-C1B	-5.11	120.61	128.46
3	K	603	HEC	CMC-C2C-C1C	-5.10	120.62	128.46
4	A	608	ISW	C3D-C4D-ND	5.10	115.29	110.36
3	I	601	HEC	CBD-CAD-C3D	-5.04	104.02	112.62
3	A	602	HEC	CMC-C2C-C1C	-5.03	120.73	128.46
4	C	608	ISW	C1D-ND-C4D	-5.03	99.88	105.07
3	K	606	HEC	CBD-CAD-C3D	-5.00	104.08	112.62
3	C	603	HEC	CMC-C2C-C1C	-4.97	120.82	128.46
3	A	602	HEC	CMC-C2C-C3C	4.94	131.62	125.82
3	A	606	HEC	CBA-CAA-C2A	-4.90	104.34	112.60
3	C	606	HEC	CBD-CAD-C3D	-4.85	104.34	112.62
4	A	609	ISW	C1D-ND-C4D	-4.82	100.09	105.07
3	E	607	HEC	CMB-C2B-C1B	-4.82	121.05	128.46
3	I	607	HEC	CMC-C2C-C1C	-4.82	121.06	128.46
4	C	608	ISW	C3D-C4D-ND	4.79	115.00	110.36
4	G	608	ISW	C3D-C4D-ND	4.73	114.94	110.36
4	A	609	ISW	C3D-C4D-ND	4.73	114.94	110.36
4	G	608	ISW	C1D-ND-C4D	-4.72	100.20	105.07
3	C	605	HEC	CBD-CAD-C3D	-4.72	104.57	112.62
3	I	606	HEC	CMB-C2B-C1B	-4.69	121.25	128.46
3	C	607	HEC	CMB-C2B-C1B	-4.67	121.28	128.46
3	E	602	HEC	CBD-CAD-C3D	-4.67	104.66	112.62
3	C	604	HEC	CMC-C2C-C1C	-4.66	121.30	128.46
3	E	605	HEC	CMB-C2B-C1B	-4.63	121.35	128.46
3	A	601	HEC	CMB-C2B-C3B	4.61	131.25	125.82
3	A	606	HEC	CBD-CAD-C3D	-4.60	104.76	112.62
3	G	605	HEC	CMB-C2B-C1B	-4.60	121.40	128.46
3	A	603	HEC	CMC-C2C-C1C	-4.57	121.44	128.46
4	G	609	ISW	CMB-C2B-C1B	-4.57	118.08	125.04
3	I	605	HEC	CMB-C2B-C3B	4.54	131.16	125.82
3	A	602	HEC	CBD-CAD-C3D	-4.53	104.89	112.62
3	K	603	HEC	CBA-CAA-C2A	-4.52	104.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	605	HEC	CBD-CAD-C3D	-4.48	104.97	112.62
3	C	606	HEC	CMC-C2C-C1C	-4.48	121.58	128.46
4	I	608	ISW	C3D-C4D-ND	4.42	114.64	110.36
3	E	601	HEC	C1D-C2D-C3D	-4.41	103.92	107.00
3	I	606	HEC	CBD-CAD-C3D	-4.40	105.12	112.62
3	A	604	HEC	CMC-C2C-C1C	-4.38	121.73	128.46
3	G	602	HEC	CMC-C2C-C1C	-4.38	121.73	128.46
3	C	602	HEC	CMC-C2C-C1C	-4.38	121.74	128.46
3	K	607	HEC	CMB-C2B-C1B	-4.34	121.80	128.46
3	I	603	HEC	CBA-CAA-C2A	-4.32	105.32	112.60
3	A	606	HEC	CMC-C2C-C1C	-4.31	121.84	128.46
3	A	604	HEC	CMC-C2C-C3C	4.31	130.88	125.82
3	I	603	HEC	CMC-C2C-C1C	-4.31	121.85	128.46
3	K	602	HEC	CBD-CAD-C3D	-4.29	105.30	112.62
4	C	608	ISW	CMB-C2B-C1B	-4.28	118.52	125.04
3	I	607	HEC	CMC-C2C-C3C	4.26	130.83	125.82
3	E	606	HEC	CBA-CAA-C2A	-4.26	105.43	112.60
3	C	602	HEC	CMB-C2B-C1B	-4.21	122.00	128.46
3	A	607	HEC	CBD-CAD-C3D	-4.19	105.47	112.62
3	C	607	HEC	CMB-C2B-C3B	4.18	130.74	125.82
4	I	608	ISW	CMB-C2B-C1B	-4.14	118.74	125.04
3	G	604	HEC	CMB-C2B-C1B	-4.13	122.11	128.46
3	A	605	HEC	CMC-C2C-C1C	-4.13	122.11	128.46
3	C	605	HEC	CMB-C2B-C3B	4.10	130.64	125.82
3	I	606	HEC	CMC-C2C-C1C	-4.09	122.17	128.46
3	G	604	HEC	CBD-CAD-C3D	-4.09	105.64	112.62
3	K	606	HEC	CBA-CAA-C2A	-4.08	105.73	112.60
3	C	607	HEC	CBD-CAD-C3D	-4.07	105.67	112.62
3	K	606	HEC	CMB-C2B-C1B	-4.03	122.27	128.46
3	C	602	HEC	CMC-C2C-C3C	4.00	130.53	125.82
3	G	603	HEC	CAD-CBD-CGD	-4.00	102.56	113.76
3	G	601	HEC	C1D-C2D-C3D	-3.99	104.22	107.00
3	C	602	HEC	CBA-CAA-C2A	-3.98	105.90	112.60
3	A	606	HEC	CMC-C2C-C3C	3.95	130.47	125.82
3	G	602	HEC	CBD-CAD-C3D	-3.95	105.88	112.62
3	A	607	HEC	CMC-C2C-C1C	-3.92	122.44	128.46
3	K	603	HEC	CMC-C2C-C3C	3.91	130.42	125.82
3	E	604	HEC	CBD-CAD-C3D	-3.90	105.97	112.62
3	K	605	HEC	CMC-C2C-C1C	-3.88	122.50	128.46
3	K	601	HEC	C1D-C2D-C3D	-3.85	104.31	107.00
3	K	605	HEC	CMB-C2B-C1B	-3.85	122.55	128.46
3	G	607	HEC	C1D-C2D-C3D	-3.82	104.34	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	HEC	CMC-C2C-C3C	3.82	130.31	125.82
3	E	603	HEC	CBA-CAA-C2A	-3.78	106.22	112.60
3	C	606	HEC	CMC-C2C-C3C	3.78	130.27	125.82
3	K	607	HEC	CMB-C2B-C3B	3.78	130.27	125.82
3	A	605	HEC	CBD-CAD-C3D	-3.77	106.18	112.62
3	K	607	HEC	C1D-C2D-C3D	-3.74	104.39	107.00
3	G	606	HEC	CMC-C2C-C1C	-3.74	122.72	128.46
3	E	602	HEC	CMC-C2C-C1C	-3.70	122.77	128.46
3	E	603	HEC	CAD-CBD-CGD	-3.68	103.43	113.76
3	I	602	HEC	CBD-CAD-C3D	-3.68	106.33	112.62
3	E	603	HEC	C1D-C2D-C3D	-3.68	104.44	107.00
3	C	603	HEC	CBA-CAA-C2A	-3.67	106.42	112.60
3	A	607	HEC	CMB-C2B-C1B	-3.66	122.83	128.46
3	I	604	HEC	CMC-C2C-C1C	-3.66	122.83	128.46
3	G	602	HEC	CMC-C2C-C3C	3.66	130.12	125.82
3	G	607	HEC	CMC-C2C-C1C	-3.66	122.84	128.46
3	K	602	HEC	CMC-C2C-C1C	-3.65	122.85	128.46
3	E	603	HEC	CMC-C2C-C3C	3.65	130.11	125.82
3	C	606	HEC	CMB-C2B-C1B	-3.64	122.86	128.46
3	K	604	HEC	CMB-C2B-C1B	-3.64	122.86	128.46
3	G	606	HEC	C1D-C2D-C3D	-3.61	104.49	107.00
3	I	603	HEC	CMC-C2C-C3C	3.60	130.06	125.82
4	A	609	ISW	C1B-C2B-C3B	-3.60	102.50	106.80
3	E	605	HEC	CBA-CAA-C2A	-3.56	106.60	112.60
3	I	606	HEC	CMB-C2B-C3B	3.54	129.99	125.82
3	E	607	HEC	CMC-C2C-C1C	-3.53	123.03	128.46
4	I	608	ISW	CHD-C1D-ND	3.51	128.72	124.38
3	K	605	HEC	C1D-C2D-C3D	-3.51	104.56	107.00
3	I	602	HEC	CMB-C2B-C1B	-3.50	123.08	128.46
3	G	606	HEC	CAD-CBD-CGD	-3.50	103.95	113.76
3	E	605	HEC	CMB-C2B-C3B	3.49	129.93	125.82
3	K	602	HEC	CAA-CBA-CGA	-3.47	104.02	113.76
3	E	606	HEC	CBD-CAD-C3D	-3.43	106.76	112.62
3	E	604	HEC	CMC-C2C-C1C	-3.42	123.21	128.46
3	K	607	HEC	CMC-C2C-C1C	-3.39	123.25	128.46
3	A	606	HEC	CMB-C2B-C1B	-3.37	123.29	128.46
3	A	605	HEC	CMB-C2B-C3B	3.35	129.76	125.82
3	G	607	HEC	CMC-C2C-C3C	3.35	129.76	125.82
3	G	605	HEC	C1D-C2D-C3D	-3.34	104.67	107.00
3	I	607	HEC	C1D-C2D-C3D	-3.33	104.68	107.00
3	C	602	HEC	CAA-CBA-CGA	-3.33	104.43	113.76
3	A	604	HEC	CMB-C2B-C1B	-3.32	123.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	606	HEC	C1D-C2D-C3D	-3.31	104.70	107.00
3	E	606	HEC	CMB-C2B-C1B	-3.30	123.39	128.46
3	C	607	HEC	CMC-C2C-C1C	-3.29	123.40	128.46
3	K	601	HEC	CBA-CAA-C2A	3.29	118.14	112.60
3	C	603	HEC	CMB-C2B-C1B	-3.28	123.43	128.46
3	G	606	HEC	CMC-C2C-C3C	3.25	129.65	125.82
3	E	607	HEC	C1D-C2D-C3D	-3.25	104.73	107.00
3	K	601	HEC	CMC-C2C-C1C	-3.23	123.51	128.46
3	C	603	HEC	CAD-CBD-CGD	-3.21	104.76	113.76
3	A	603	HEC	C1D-C2D-C3D	-3.20	104.77	107.00
3	E	604	HEC	CMB-C2B-C1B	-3.20	123.54	128.46
3	K	606	HEC	C1D-C2D-C3D	-3.20	104.77	107.00
3	C	604	HEC	CBA-CAA-C2A	3.17	117.94	112.60
3	I	607	HEC	CMB-C2B-C1B	-3.16	123.60	128.46
3	G	606	HEC	CMB-C2B-C1B	-3.16	123.61	128.46
3	I	603	HEC	C1D-C2D-C3D	-3.14	104.81	107.00
3	K	606	HEC	CMC-C2C-C1C	-3.14	123.64	128.46
3	E	602	HEC	CBA-CAA-C2A	-3.14	107.32	112.60
3	A	606	HEC	C1D-C2D-C3D	-3.14	104.81	107.00
3	G	603	HEC	CMB-C2B-C1B	-3.14	123.64	128.46
3	C	603	HEC	CMB-C2B-C3B	3.13	129.50	125.82
3	C	602	HEC	CBD-CAD-C3D	-3.13	107.29	112.62
3	E	607	HEC	CMB-C2B-C3B	3.12	129.49	125.82
3	I	605	HEC	CBA-CAA-C2A	-3.12	107.35	112.60
3	E	603	HEC	CMB-C2B-C1B	-3.09	123.72	128.46
3	K	603	HEC	CMB-C2B-C1B	-3.07	123.75	128.46
3	I	601	HEC	CMC-C2C-C1C	-3.06	123.76	128.46
3	E	601	HEC	CMB-C2B-C1B	-3.00	123.86	128.46
4	A	608	ISW	CMB-C2B-C1B	-2.99	120.49	125.04
3	C	604	HEC	CMB-C2B-C1B	-2.98	123.88	128.46
3	C	604	HEC	CMC-C2C-C3C	2.98	129.33	125.82
3	G	605	HEC	CMB-C2B-C3B	2.98	129.32	125.82
3	A	607	HEC	C1D-C2D-C3D	-2.97	104.93	107.00
3	K	601	HEC	CMB-C2B-C1B	-2.97	123.90	128.46
4	A	608	ISW	C2B-C1B-NB	2.96	113.42	109.88
3	G	604	HEC	CMB-C2B-C3B	2.96	129.30	125.82
3	K	605	HEC	CBA-CAA-C2A	-2.95	107.62	112.60
4	G	609	ISW	C4B-NB-C1B	2.95	110.61	107.63
3	E	607	HEC	CMC-C2C-C3C	2.94	129.27	125.82
3	E	606	HEC	CMC-C2C-C1C	-2.92	123.97	128.46
3	E	602	HEC	CAA-CBA-CGA	-2.92	105.58	113.76
3	A	605	HEC	CBA-CAA-C2A	-2.92	107.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	604	HEC	CBD-CAD-C3D	-2.91	107.65	112.62
3	A	601	HEC	CMC-C2C-C1C	-2.91	123.99	128.46
4	I	608	ISW	C1B-C2B-C3B	-2.88	103.35	106.80
3	K	602	HEC	CMB-C2B-C1B	-2.86	124.06	128.46
3	C	602	HEC	CMB-C2B-C3B	2.86	129.19	125.82
3	E	605	HEC	C1D-C2D-C3D	-2.85	105.02	107.00
3	G	602	HEC	CMB-C2B-C1B	-2.85	124.09	128.46
3	G	605	HEC	CBA-CAA-C2A	-2.84	107.83	112.60
3	G	605	HEC	CMC-C2C-C1C	-2.83	124.11	128.46
3	I	602	HEC	CMB-C2B-C3B	2.83	129.15	125.82
3	A	602	HEC	CAA-CBA-CGA	-2.82	105.86	113.76
3	G	602	HEC	CAA-CBA-CGA	-2.81	105.87	113.76
3	E	602	HEC	CMC-C2C-C3C	2.81	129.12	125.82
3	I	601	HEC	CMB-C2B-C1B	-2.80	124.16	128.46
3	E	607	HEC	CAD-CBD-CGD	-2.80	105.91	113.76
3	K	603	HEC	CAD-CBD-CGD	-2.80	105.92	113.76
3	K	604	HEC	CMC-C2C-C1C	-2.78	124.19	128.46
3	K	601	HEC	CAA-CBA-CGA	-2.78	105.96	113.76
3	A	605	HEC	CMC-C2C-C3C	2.78	129.09	125.82
3	A	603	HEC	CAD-CBD-CGD	-2.78	105.97	113.76
3	I	604	HEC	CAA-CBA-CGA	-2.77	105.99	113.76
3	A	601	HEC	C1D-C2D-C3D	-2.76	105.08	107.00
4	G	608	ISW	CMB-C2B-C1B	-2.75	120.84	125.04
3	I	607	HEC	CMB-C2B-C3B	2.75	129.06	125.82
3	A	604	HEC	CMB-C2B-C3B	2.74	129.04	125.82
3	I	602	HEC	CMC-C2C-C3C	2.73	129.03	125.82
4	I	608	ISW	CHD-C1D-C2D	-2.73	119.17	126.72
3	K	607	HEC	CMC-C2C-C3C	2.71	129.01	125.82
3	K	607	HEC	CAD-CBD-CGD	-2.71	106.16	113.76
3	A	603	HEC	CMB-C2B-C1B	-2.71	124.30	128.46
4	A	609	ISW	C2B-C1B-NB	2.70	113.12	109.88
4	G	609	ISW	C2D-C1D-ND	2.70	113.04	109.84
3	C	607	HEC	O1A-CGA-CBA	-2.69	114.43	123.08
3	C	601	HEC	C4C-C3C-C2C	2.69	109.26	106.35
4	A	608	ISW	C1B-C2B-C3B	-2.68	103.59	106.80
3	I	601	HEC	C1D-C2D-C3D	-2.67	105.14	107.00
3	G	601	HEC	CMC-C2C-C1C	-2.67	124.36	128.46
3	K	606	HEC	CMB-C2B-C3B	2.67	128.96	125.82
3	K	607	HEC	O1A-CGA-CBA	-2.66	114.53	123.08
4	A	608	ISW	CMD-C2D-C1D	-2.64	121.01	125.04
3	K	604	HEC	CAA-CBA-CGA	-2.62	106.40	113.76
3	C	601	HEC	CMB-C2B-C1B	-2.61	124.45	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	607	HEC	CMC-C2C-C3C	2.61	128.89	125.82
3	E	601	HEC	CBA-CAA-C2A	2.61	117.00	112.60
4	A	608	ISW	CBD-CAD-C3D	-2.59	105.42	112.63
3	I	605	HEC	CAD-CBD-CGD	-2.59	106.49	113.76
3	G	601	HEC	CMB-C2B-C1B	-2.59	124.48	128.46
3	A	607	HEC	CAD-CBD-CGD	-2.58	106.51	113.76
4	A	609	ISW	C4B-NB-C1B	2.58	110.25	107.63
3	E	601	HEC	CMC-C2C-C3C	2.57	128.84	125.82
3	C	601	HEC	CMC-C2C-C1C	-2.56	124.53	128.46
4	A	608	ISW	CMD-C2D-C3D	2.56	133.06	126.12
4	C	608	ISW	O1D-CGD-CBD	2.55	122.21	114.03
3	G	603	HEC	C1D-C2D-C3D	-2.54	105.23	107.00
3	K	604	HEC	CBD-CAD-C3D	-2.54	108.28	112.62
3	K	605	HEC	CMB-C2B-C3B	2.53	128.79	125.82
4	A	608	ISW	CBB-CAB-C3B	-2.52	118.43	127.20
3	I	604	HEC	CBD-CAD-C3D	-2.52	108.32	112.62
3	E	607	HEC	O1A-CGA-CBA	-2.52	115.00	123.08
3	G	607	HEC	CMB-C2B-C1B	-2.51	124.60	128.46
3	C	606	HEC	CMB-C2B-C3B	2.51	128.77	125.82
3	K	604	HEC	CMB-C2B-C3B	2.50	128.76	125.82
3	G	607	HEC	O2A-CGA-CBA	2.50	122.07	114.03
3	K	601	HEC	CMB-C2B-C3B	2.50	128.75	125.82
3	I	603	HEC	CMB-C2B-C1B	-2.49	124.63	128.46
4	C	608	ISW	C1B-C2B-C3B	-2.48	103.84	106.80
4	G	608	ISW	CHD-C1D-ND	2.48	127.44	124.38
3	I	604	HEC	CAD-CBD-CGD	-2.47	106.83	113.76
4	C	608	ISW	C2B-C1B-NB	2.47	112.84	109.88
4	C	608	ISW	O2D-CGD-CBD	-2.47	115.16	123.08
4	A	608	ISW	CHD-C1D-ND	2.46	127.43	124.38
3	E	602	HEC	CAD-CBD-CGD	-2.46	106.86	113.76
3	K	603	HEC	C1D-C2D-C3D	-2.46	105.28	107.00
3	A	603	HEC	CMA-C3A-C2A	2.46	129.58	124.94
4	G	609	ISW	C1B-C2B-C3B	-2.45	103.88	106.80
3	C	601	HEC	C1D-C2D-C3D	-2.44	105.30	107.00
4	A	608	ISW	CHD-C1D-C2D	-2.43	119.99	126.72
3	E	604	HEC	CAD-CBD-CGD	-2.42	106.97	113.76
3	C	603	HEC	C2B-C3B-C4B	2.40	108.94	106.35
3	E	606	HEC	CMC-C2C-C3C	2.39	128.63	125.82
3	E	604	HEC	CMC-C2C-C3C	2.38	128.62	125.82
3	I	605	HEC	C1D-C2D-C3D	-2.38	105.34	107.00
4	I	608	ISW	C4B-NB-C1B	2.37	110.03	107.63
3	A	607	HEC	O1A-CGA-CBA	-2.37	115.47	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	602	HEC	CMB-C2B-C1B	-2.36	124.83	128.46
4	G	609	ISW	CBB-CAB-C3B	-2.36	119.00	127.20
4	C	608	ISW	CHD-C1D-ND	2.35	127.28	124.38
3	C	607	HEC	CBA-CAA-C2A	-2.35	108.64	112.60
3	G	604	HEC	C1D-C2D-C3D	-2.35	105.36	107.00
3	C	601	HEC	CAA-CBA-CGA	-2.34	107.19	113.76
3	I	602	HEC	C1D-C2D-C3D	-2.34	105.37	107.00
3	I	607	HEC	O1A-CGA-CBA	-2.34	115.58	123.08
3	E	607	HEC	O2A-CGA-CBA	2.33	121.52	114.03
4	G	608	ISW	O2D-CGD-CBD	-2.33	115.60	123.08
3	G	607	HEC	O1A-CGA-CBA	-2.33	115.61	123.08
3	K	607	HEC	O2A-CGA-CBA	2.32	121.48	114.03
3	E	606	HEC	CAD-CBD-CGD	-2.32	107.26	113.76
3	K	606	HEC	CMC-C2C-C3C	2.32	128.54	125.82
3	C	604	HEC	CAA-CBA-CGA	-2.30	107.30	113.76
3	I	602	HEC	CAA-CBA-CGA	-2.30	107.32	113.76
4	A	608	ISW	C2D-C1D-ND	2.30	112.56	109.84
3	G	603	HEC	CMB-C2B-C3B	2.29	128.52	125.82
3	G	601	HEC	CMB-C2B-C3B	2.29	128.51	125.82
4	I	608	ISW	C2B-C1B-NB	2.29	112.62	109.88
3	K	604	HEC	C1D-C2D-C3D	-2.29	105.40	107.00
3	E	602	HEC	C1D-C2D-C3D	-2.28	105.41	107.00
4	G	608	ISW	O2A-CGA-CBA	2.28	121.35	114.03
3	C	605	HEC	CMC-C2C-C1C	-2.28	124.97	128.46
4	I	608	ISW	CMD-C2D-C1D	-2.27	121.59	125.04
3	K	602	HEC	CMA-C3A-C2A	2.26	129.21	124.94
3	K	601	HEC	O1D-CGD-CBD	-2.25	115.84	123.08
3	C	604	HEC	C1D-C2D-C3D	-2.25	105.43	107.00
3	E	601	HEC	CAA-CBA-CGA	-2.25	107.45	113.76
3	A	607	HEC	CMB-C2B-C3B	2.25	128.46	125.82
3	C	607	HEC	O2A-CGA-CBA	2.24	121.23	114.03
4	A	608	ISW	O2A-CGA-CBA	2.24	121.22	114.03
4	G	608	ISW	C1B-C2B-C3B	-2.24	104.13	106.80
4	G	609	ISW	C2B-C1B-NB	2.23	112.55	109.88
3	E	602	HEC	O2A-CGA-CBA	2.22	121.17	114.03
3	G	602	HEC	CBA-CAA-C2A	-2.22	108.86	112.60
4	A	609	ISW	CBB-CAB-C3B	-2.22	119.50	127.20
3	K	604	HEC	CMC-C2C-C3C	2.20	128.41	125.82
3	G	601	HEC	C2B-C3B-C4B	2.19	108.72	106.35
3	A	607	HEC	CBA-CAA-C2A	-2.19	108.91	112.60
3	K	605	HEC	CAD-CBD-CGD	-2.18	107.64	113.76
3	C	604	HEC	CAD-CBD-CGD	-2.18	107.64	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	608	ISW	CHD-C1D-C2D	-2.18	120.70	126.72
3	A	602	HEC	CMB-C2B-C1B	-2.18	125.12	128.46
3	E	607	HEC	CBA-CAA-C2A	-2.17	108.94	112.60
3	A	607	HEC	O2A-CGA-CBA	2.16	120.98	114.03
4	G	608	ISW	O1D-CGD-CBD	2.16	120.98	114.03
3	A	602	HEC	O1D-CGD-CBD	-2.16	116.14	123.08
4	G	608	ISW	CBB-CAB-C3B	-2.15	119.72	127.20
3	C	605	HEC	CBA-CAA-C2A	-2.15	108.98	112.60
3	A	603	HEC	O1A-CGA-CBA	-2.15	116.17	123.08
4	C	608	ISW	CHD-C1D-C2D	-2.15	120.78	126.72
3	E	605	HEC	CMC-C2C-C1C	-2.15	125.16	128.46
4	C	608	ISW	CBB-CAB-C3B	-2.15	119.75	127.20
3	G	604	HEC	O1A-CGA-CBA	-2.14	116.20	123.08
3	I	605	HEC	CMC-C2C-C1C	-2.14	125.18	128.46
3	A	603	HEC	CAA-CBA-CGA	-2.13	107.79	113.76
3	C	607	HEC	CMC-C2C-C3C	2.12	128.31	125.82
4	C	608	ISW	CHB-C1B-NB	-2.11	122.14	124.43
4	I	608	ISW	O1D-CGD-CBD	2.11	120.81	114.03
3	K	606	HEC	CAD-CBD-CGD	-2.10	107.86	113.76
3	K	601	HEC	O2D-CGD-CBD	2.10	120.78	114.03
3	I	607	HEC	O2A-CGA-CBA	2.08	120.72	114.03
3	E	604	HEC	CBA-CAA-C2A	2.08	116.11	112.60
4	G	608	ISW	C4B-NB-C1B	2.08	109.73	107.63
3	K	606	HEC	CAA-CBA-CGA	-2.07	107.95	113.76
3	G	601	HEC	O1A-CGA-CBA	-2.07	116.43	123.08
3	K	605	HEC	O2A-CGA-CBA	2.06	120.65	114.03
4	I	608	ISW	O2A-CGA-CBA	2.05	120.62	114.03
3	I	603	HEC	CMB-C2B-C3B	2.04	128.22	125.82
4	A	609	ISW	CHB-C1B-NB	-2.04	122.22	124.43
3	C	601	HEC	CBA-CAA-C2A	2.03	116.03	112.60
3	C	603	HEC	CBD-CAD-C3D	-2.02	109.17	112.62
3	I	607	HEC	CAD-CBD-CGD	-2.01	108.12	113.76
3	A	606	HEC	CMB-C2B-C3B	2.01	128.18	125.82
4	C	608	ISW	C4B-NB-C1B	2.01	109.66	107.63
3	G	605	HEC	CAD-CBD-CGD	-2.01	108.13	113.76
4	G	608	ISW	CHB-C1B-NB	-2.01	122.25	124.43
3	G	604	HEC	O2A-CGA-CBA	2.00	120.47	114.03
3	E	603	HEC	O1A-CGA-CBA	-2.00	116.65	123.08
3	I	603	HEC	CAD-CBD-CGD	-2.00	108.14	113.76

There are no chirality outliers.

All (223) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	604	HEC	C1A-C2A-CAA-CBA
3	I	604	HEC	C3A-C2A-CAA-CBA
3	K	604	HEC	C1A-C2A-CAA-CBA
3	K	604	HEC	C3A-C2A-CAA-CBA
6	I	609	PGE	O3-C5-C6-O4
7	A	612	PG4	O4-C7-C8-O5
7	E	610	PG4	O2-C3-C4-O3
6	E	609	PGE	O2-C3-C4-O3
6	G	611	PGE	O1-C1-C2-O2
3	A	605	HEC	C2A-CAA-CBA-CGA
3	C	605	HEC	C2A-CAA-CBA-CGA
3	K	605	HEC	C2A-CAA-CBA-CGA
7	A	612	PG4	O2-C3-C4-O3
6	I	610	PGE	C1-C2-O2-C3
6	C	610	PGE	C3-C4-O3-C5
5	C	609	PEG	O1-C1-C2-O2
5	K	608	PEG	O1-C1-C2-O2
6	A	611	PGE	O1-C1-C2-O2
6	I	609	PGE	O1-C1-C2-O2
6	G	611	PGE	O2-C3-C4-O3
5	A	610	PEG	O2-C3-C4-O4
5	K	608	PEG	O2-C3-C4-O4
7	A	612	PG4	O1-C1-C2-O2
7	K	610	PG4	O3-C5-C6-O4
6	C	610	PGE	O1-C1-C2-O2
7	E	610	PG4	O3-C5-C6-O4
3	E	605	HEC	C2A-CAA-CBA-CGA
4	C	608	ISW	C2B-C3B-CAB-CBB
4	I	608	ISW	C2B-C3B-CAB-CBB
6	E	609	PGE	O3-C5-C6-O4
6	I	610	PGE	O1-C1-C2-O2
7	C	611	PG4	O3-C5-C6-O4
7	A	612	PG4	C6-C5-O3-C4
5	A	610	PEG	O1-C1-C2-O2
5	K	609	PEG	O1-C1-C2-O2
6	G	612	PGE	O3-C5-C6-O4
3	I	605	HEC	C2A-CAA-CBA-CGA
6	E	608	PGE	O1-C1-C2-O2
6	E	608	PGE	C1-C2-O2-C3
6	I	609	PGE	O2-C3-C4-O3
5	G	610	PEG	O2-C3-C4-O4
5	J	101	PEG	O2-C3-C4-O4
5	C	609	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
7	A	612	PG4	O3-C5-C6-O4
3	G	605	HEC	C2A-CAA-CBA-CGA
4	A	608	ISW	C2B-C3B-CAB-CBB
4	A	609	ISW	C2B-C3B-CAB-CBB
4	G	609	ISW	C2B-C3B-CAB-CBB
6	E	608	PGE	C6-C5-O3-C4
6	G	612	PGE	C1-C2-O2-C3
7	K	610	PG4	O4-C7-C8-O5
7	C	611	PG4	C3-C4-O3-C5
7	C	611	PG4	C1-C2-O2-C3
5	A	610	PEG	C1-C2-O2-C3
6	G	611	PGE	C6-C5-O3-C4
6	G	612	PGE	C3-C4-O3-C5
6	I	609	PGE	C6-C5-O3-C4
7	A	612	PG4	C3-C4-O3-C5
7	K	610	PG4	C1-C2-O2-C3
6	G	612	PGE	O2-C3-C4-O3
3	K	607	HEC	C3D-CAD-CBD-CGD
3	A	604	HEC	C1A-C2A-CAA-CBA
3	A	604	HEC	C3A-C2A-CAA-CBA
3	C	604	HEC	C1A-C2A-CAA-CBA
3	C	604	HEC	C3A-C2A-CAA-CBA
3	E	601	HEC	C1A-C2A-CAA-CBA
3	E	604	HEC	C1A-C2A-CAA-CBA
3	E	604	HEC	C3A-C2A-CAA-CBA
3	G	604	HEC	C1A-C2A-CAA-CBA
3	G	604	HEC	C3A-C2A-CAA-CBA
6	E	608	PGE	O2-C3-C4-O3
6	I	610	PGE	C3-C4-O3-C5
6	I	610	PGE	O2-C3-C4-O3
7	K	610	PG4	C3-C4-O3-C5
5	G	610	PEG	C1-C2-O2-C3
7	K	610	PG4	O2-C3-C4-O3
6	G	611	PGE	C4-C3-O2-C2
3	C	607	HEC	C3D-CAD-CBD-CGD
7	C	611	PG4	C6-C5-O3-C4
6	G	611	PGE	C1-C2-O2-C3
6	A	611	PGE	O2-C3-C4-O3
5	K	609	PEG	C1-C2-O2-C3
7	A	612	PG4	C1-C2-O2-C3
6	I	610	PGE	C4-C3-O2-C2
3	C	605	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	605	HEC	CAA-CBA-CGA-O1A
3	G	605	HEC	CAD-CBD-CGD-O2D
3	G	605	HEC	CAA-CBA-CGA-O1A
3	I	605	HEC	CAA-CBA-CGA-O1A
3	K	605	HEC	CAA-CBA-CGA-O1A
3	I	607	HEC	CAD-CBD-CGD-O1D
7	E	610	PG4	C3-C4-O3-C5
3	G	602	HEC	CAA-CBA-CGA-O1A
3	C	601	HEC	C2A-CAA-CBA-CGA
3	G	602	HEC	CAD-CBD-CGD-O1D
3	E	602	HEC	CAD-CBD-CGD-O2D
3	K	602	HEC	CAD-CBD-CGD-O1D
3	C	605	HEC	CAA-CBA-CGA-O2A
3	I	606	HEC	CAD-CBD-CGD-O1D
4	I	608	ISW	CAD-CBD-CGD-O2D
3	I	606	HEC	CAD-CBD-CGD-O2D
6	G	612	PGE	O1-C1-C2-O2
3	E	602	HEC	CAA-CBA-CGA-O1A
3	E	602	HEC	CAA-CBA-CGA-O2A
3	A	606	HEC	CAD-CBD-CGD-O1D
3	A	606	HEC	CAD-CBD-CGD-O2D
3	E	602	HEC	CAD-CBD-CGD-O1D
3	G	602	HEC	CAA-CBA-CGA-O2A
3	K	602	HEC	CAD-CBD-CGD-O2D
3	K	606	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	CAA-CBA-CGA-O2A
3	G	602	HEC	CAD-CBD-CGD-O2D
3	I	602	HEC	CAA-CBA-CGA-O1A
4	C	608	ISW	CAD-CBD-CGD-O1D
3	G	606	HEC	CAD-CBD-CGD-O1D
6	I	609	PGE	C1-C2-O2-C3
3	E	601	HEC	CAD-CBD-CGD-O2D
3	I	605	HEC	CAA-CBA-CGA-O2A
3	I	607	HEC	CAA-CBA-CGA-O2A
5	J	101	PEG	C1-C2-O2-C3
6	C	610	PGE	O2-C3-C4-O3
3	G	605	HEC	CAA-CBA-CGA-O2A
3	I	602	HEC	CAA-CBA-CGA-O2A
4	A	609	ISW	CAD-CBD-CGD-O1D
3	G	605	HEC	CAD-CBD-CGD-O1D
3	K	605	HEC	CAA-CBA-CGA-O2A
3	I	605	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	K	601	HEC	CAD-CBD-CGD-O2D
4	I	608	ISW	CAD-CBD-CGD-O1D
3	G	606	HEC	CAD-CBD-CGD-O2D
3	K	606	HEC	CAD-CBD-CGD-O2D
6	G	611	PGE	O3-C5-C6-O4
6	I	610	PGE	O3-C5-C6-O4
3	C	603	HEC	CAD-CBD-CGD-O2D
3	I	607	HEC	CAD-CBD-CGD-O2D
3	A	602	HEC	CAD-CBD-CGD-O2D
3	K	601	HEC	CAD-CBD-CGD-O1D
3	K	602	HEC	CAA-CBA-CGA-O2A
3	A	602	HEC	CAA-CBA-CGA-O2A
3	I	602	HEC	CAD-CBD-CGD-O2D
4	G	608	ISW	CAD-CBD-CGD-O1D
4	G	609	ISW	CAD-CBD-CGD-O1D
6	A	611	PGE	C4-C3-O2-C2
3	A	605	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAA-CBA-CGA-O2A
3	E	601	HEC	CAD-CBD-CGD-O1D
4	A	609	ISW	CAD-CBD-CGD-O2D
3	C	607	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	CAD-CBD-CGD-O2D
4	C	608	ISW	CAD-CBD-CGD-O2D
3	C	602	HEC	CAA-CBA-CGA-O2A
3	E	606	HEC	CAD-CBD-CGD-O2D
3	A	602	HEC	CAA-CBA-CGA-O1A
3	E	606	HEC	CAD-CBD-CGD-O1D
3	G	603	HEC	CAD-CBD-CGD-O1D
3	A	607	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAD-CBD-CGD-O2D
3	G	607	HEC	CAD-CBD-CGD-O2D
3	K	602	HEC	CAA-CBA-CGA-O1A
3	E	607	HEC	CAD-CBD-CGD-O2D
3	K	607	HEC	CAD-CBD-CGD-O2D
3	I	602	HEC	CAD-CBD-CGD-O1D
3	K	605	HEC	CAD-CBD-CGD-O2D
3	A	602	HEC	CAD-CBD-CGD-O1D
3	C	603	HEC	CAD-CBD-CGD-O1D
3	C	605	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAD-CBD-CGD-O1D
3	C	605	HEC	CAD-CBD-CGD-O2D
3	E	605	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	E	605	HEC	CAD-CBD-CGD-O2D
3	G	601	HEC	CAA-CBA-CGA-O1A
3	G	607	HEC	CAD-CBD-CGD-O1D
3	K	605	HEC	CAD-CBD-CGD-O1D
4	A	608	ISW	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O2D
3	E	607	HEC	CAD-CBD-CGD-O1D
3	I	605	HEC	CAD-CBD-CGD-O1D
4	G	609	ISW	CAD-CBD-CGD-O2D
3	A	607	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAA-CBA-CGA-O1A
3	C	607	HEC	CAD-CBD-CGD-O2D
4	A	608	ISW	CAD-CBD-CGD-O2D
4	G	608	ISW	CAD-CBD-CGD-O2D
3	A	601	HEC	CAD-CBD-CGD-O2D
3	C	607	HEC	CAA-CBA-CGA-O2A
3	G	601	HEC	CAA-CBA-CGA-O2A
3	I	607	HEC	CAA-CBA-CGA-O1A
3	G	603	HEC	CAD-CBD-CGD-O2D
3	G	606	HEC	CAA-CBA-CGA-O2A
3	I	601	HEC	CAA-CBA-CGA-O1A
3	G	601	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAA-CBA-CGA-O1A
3	K	607	HEC	CAA-CBA-CGA-O2A
6	C	610	PGE	C1-C2-O2-C3
3	K	607	HEC	CAD-CBD-CGD-O1D
3	E	605	HEC	CAA-CBA-CGA-O2A
3	G	604	HEC	CAA-CBA-CGA-O2A
4	I	608	ISW	CAA-CBA-CGA-O1A
3	C	604	HEC	CAA-CBA-CGA-O2A
3	G	601	HEC	CAD-CBD-CGD-O1D
7	C	611	PG4	O4-C7-C8-O5
3	I	601	HEC	CAA-CBA-CGA-O2A
3	E	605	HEC	CAA-CBA-CGA-O1A
3	A	601	HEC	CAD-CBD-CGD-O1D
3	E	603	HEC	CAA-CBA-CGA-O2A
3	G	607	HEC	CAA-CBA-CGA-O2A
4	I	608	ISW	CAA-CBA-CGA-O2A
3	C	607	HEC	CAA-CBA-CGA-O1A
3	I	604	HEC	CAA-CBA-CGA-O1A
4	G	609	ISW	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	601	HEC	CAD-CBD-CGD-O1D
3	I	604	HEC	CAA-CBA-CGA-O2A
7	C	611	PG4	O2-C3-C4-O3
3	C	601	HEC	CAA-CBA-CGA-O2A
3	C	601	HEC	CAA-CBA-CGA-O1A
3	E	601	HEC	CAA-CBA-CGA-O2A
4	G	609	ISW	CAA-CBA-CGA-O1A
3	E	607	HEC	CAA-CBA-CGA-O2A
3	K	601	HEC	CAA-CBA-CGA-O2A
5	G	610	PEG	O1-C1-C2-O2
3	G	606	HEC	CAA-CBA-CGA-O1A
3	K	603	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

62 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	604	HEC	3	0
6	A	611	PGE	1	0
3	E	607	HEC	3	0
3	K	602	HEC	4	0
3	K	605	HEC	8	0
3	A	602	HEC	7	0
6	G	611	PGE	6	0
5	J	101	PEG	2	0
4	A	609	ISW	10	0
3	C	605	HEC	8	0
6	E	608	PGE	1	0
3	E	602	HEC	2	0
3	G	607	HEC	1	0
4	C	608	ISW	11	0
3	C	602	HEC	6	0
3	E	601	HEC	4	0
3	K	601	HEC	5	0
3	I	605	HEC	9	0
5	C	609	PEG	1	0
6	I	610	PGE	4	0
3	K	603	HEC	2	0
3	K	604	HEC	6	0
5	K	609	PEG	2	0
3	I	607	HEC	5	0
4	G	609	ISW	12	0

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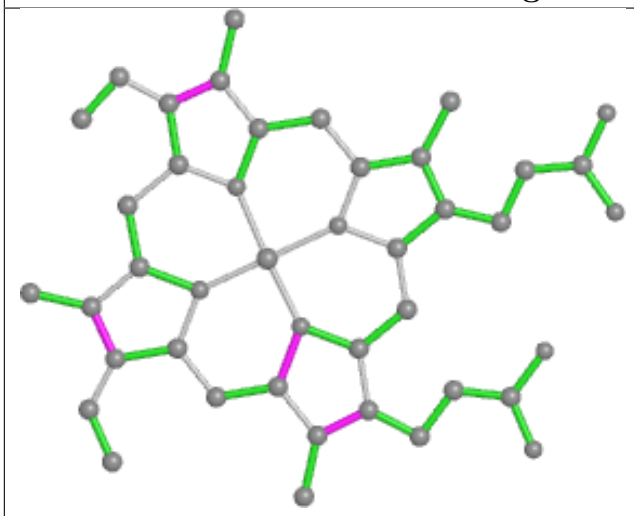
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	ISW	12	0
3	C	601	HEC	4	0
3	G	605	HEC	8	0
3	A	606	HEC	4	0
3	I	601	HEC	2	0
3	C	603	HEC	5	0
3	K	607	HEC	2	0
3	C	604	HEC	1	0
4	G	608	ISW	9	0
3	I	602	HEC	5	0
6	C	610	PGE	2	0
6	G	612	PGE	2	0
3	E	603	HEC	2	0
3	E	606	HEC	4	0
3	A	601	HEC	1	0
6	E	609	PGE	2	0
3	A	603	HEC	2	0
3	C	606	HEC	4	0
3	C	607	HEC	3	0
3	A	604	HEC	4	0
3	K	606	HEC	5	0
4	I	608	ISW	7	0
7	A	612	PG4	2	0
3	E	604	HEC	7	0
7	C	611	PG4	3	0
3	G	602	HEC	4	0
3	A	607	HEC	1	0
3	A	605	HEC	8	0
3	G	606	HEC	5	0
3	I	603	HEC	5	0
3	I	606	HEC	3	0
6	I	609	PGE	7	0
7	E	610	PG4	1	0
3	E	605	HEC	7	0
3	G	601	HEC	4	0
3	G	603	HEC	1	0
3	I	604	HEC	6	0

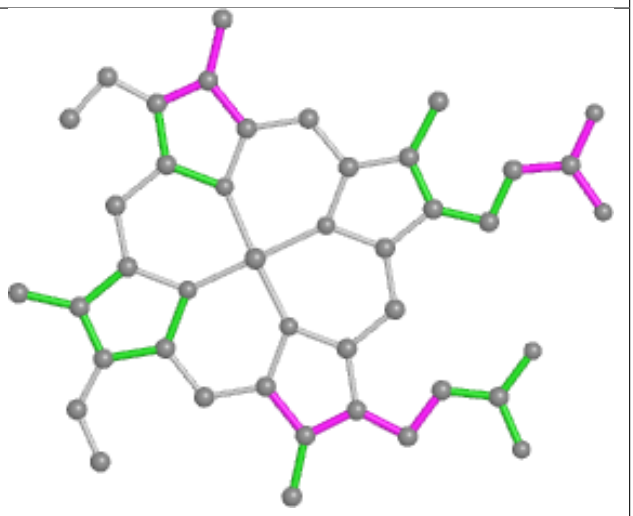
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

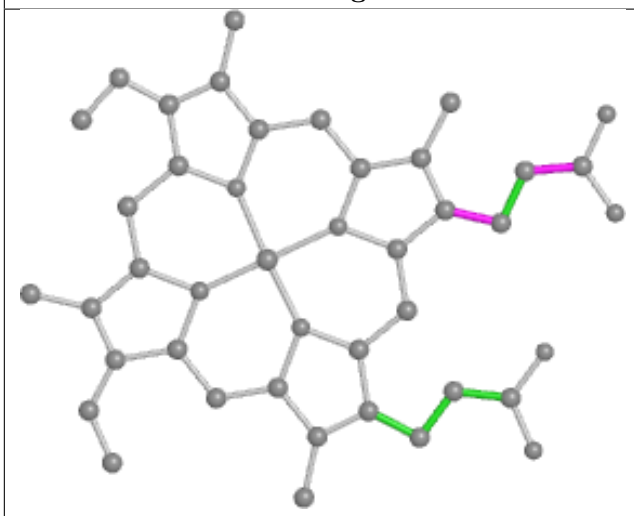
Ligand HEC G 604



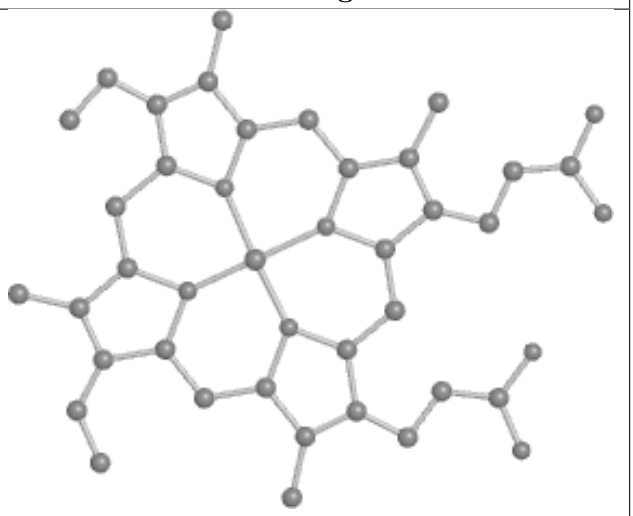
Bond lengths



Bond angles

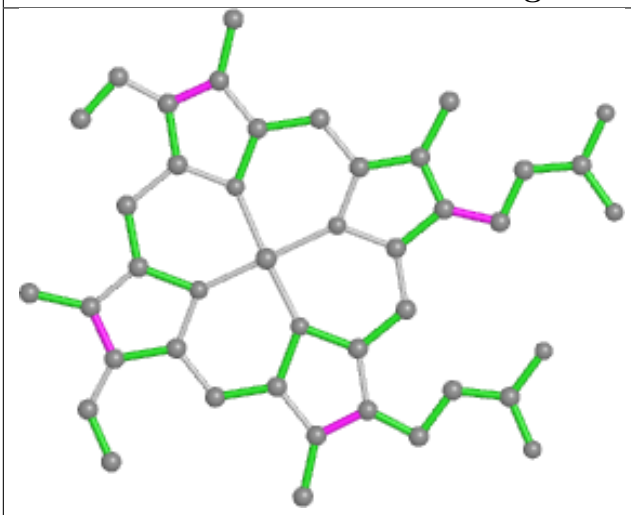


Torsions

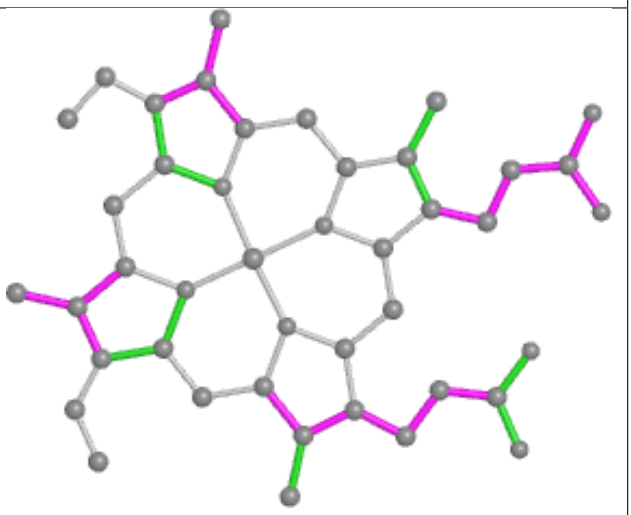


Rings

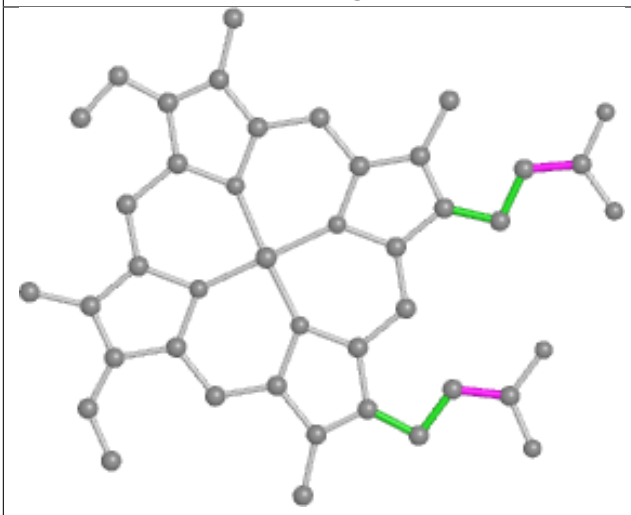
Ligand HEC E 607



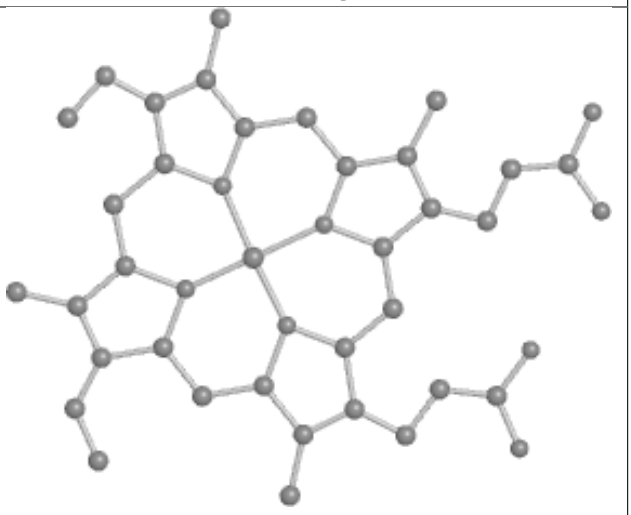
Bond lengths



Bond angles

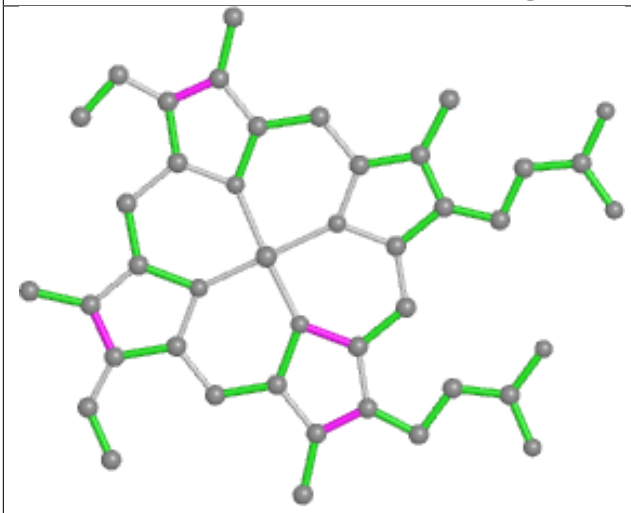


Torsions

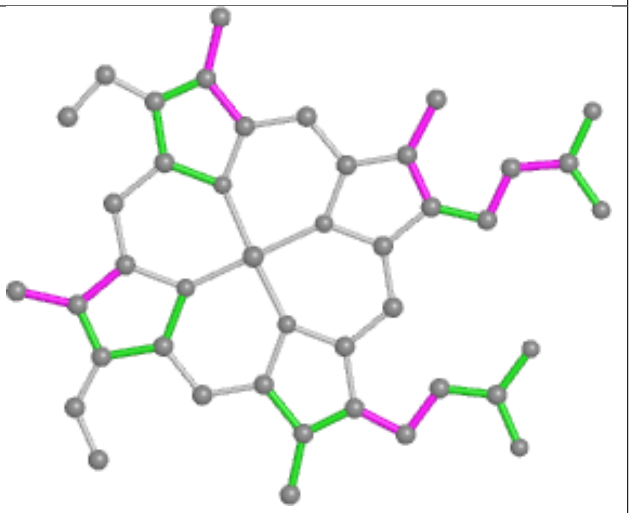


Rings

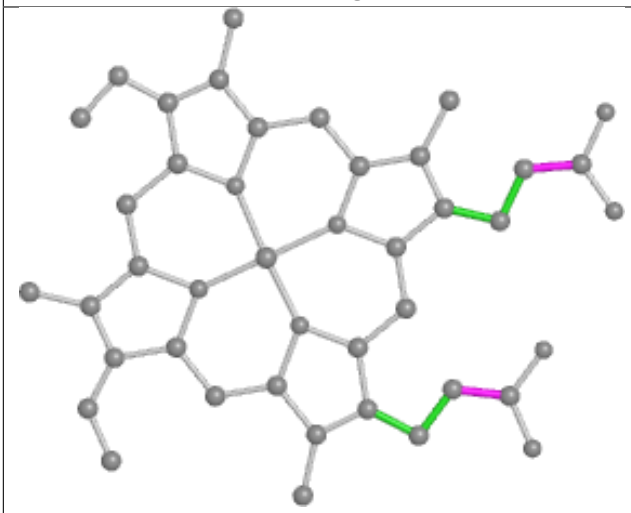
Ligand HEC K 602



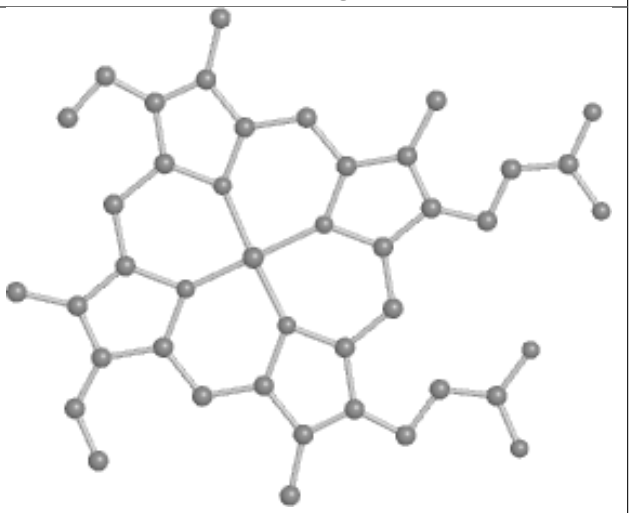
Bond lengths



Bond angles

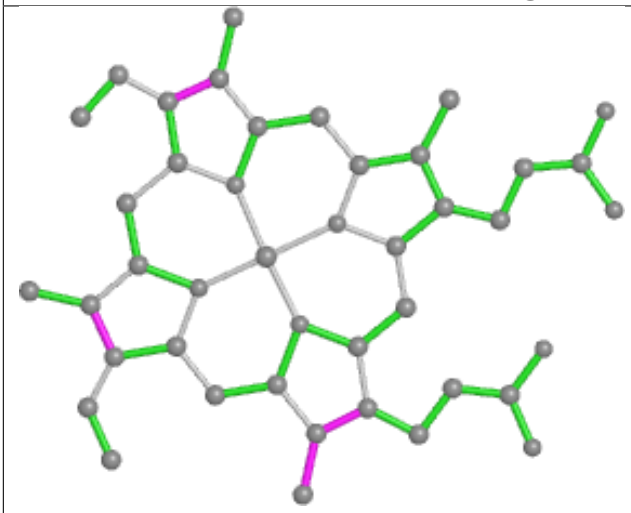


Torsions

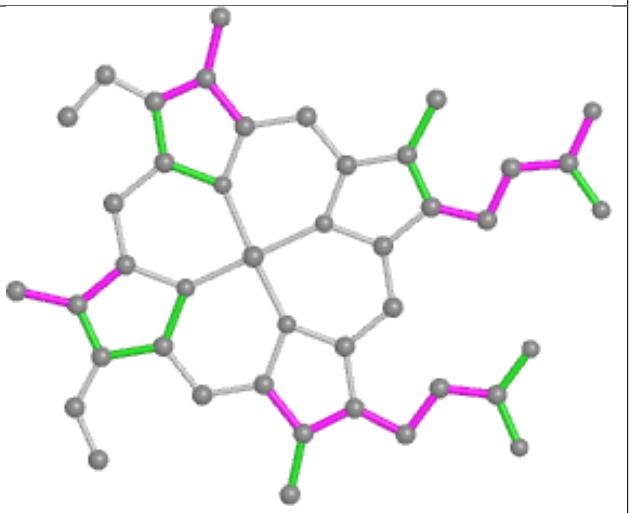


Rings

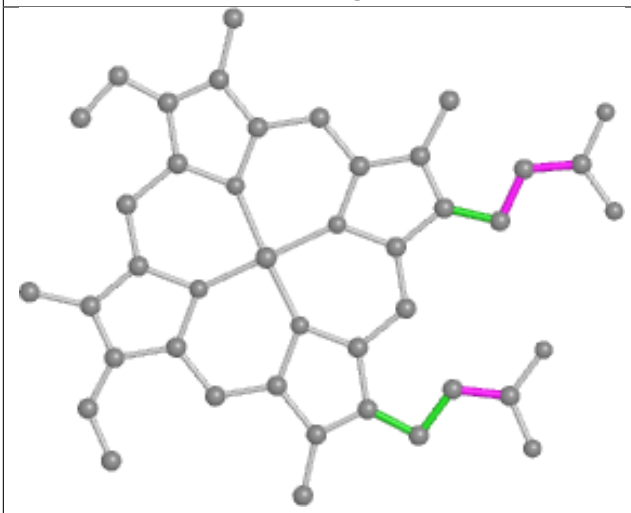
Ligand HEC K 605



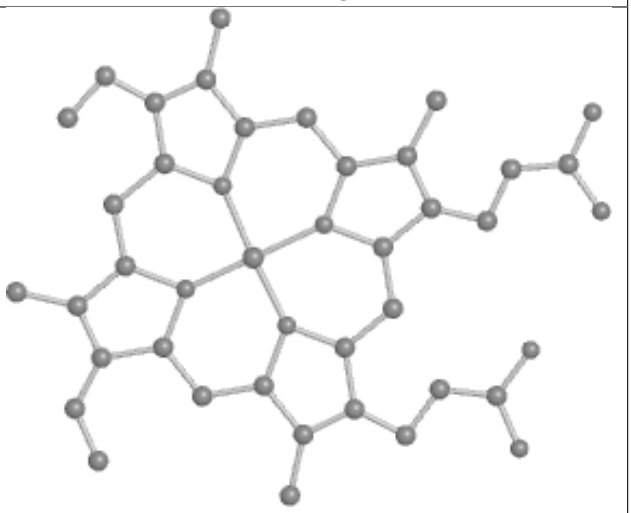
Bond lengths



Bond angles

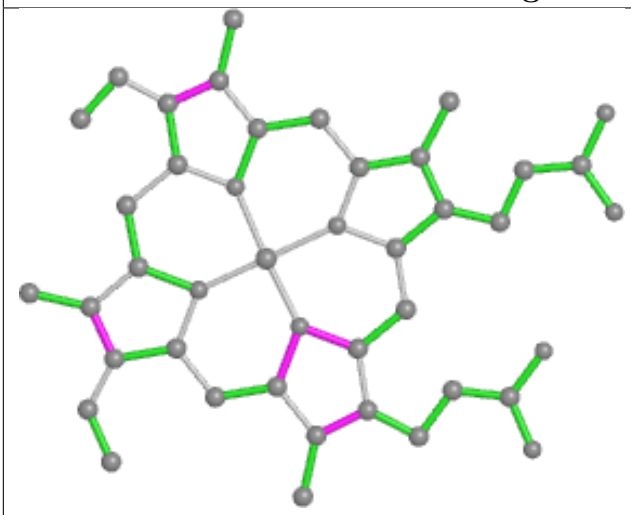


Torsions

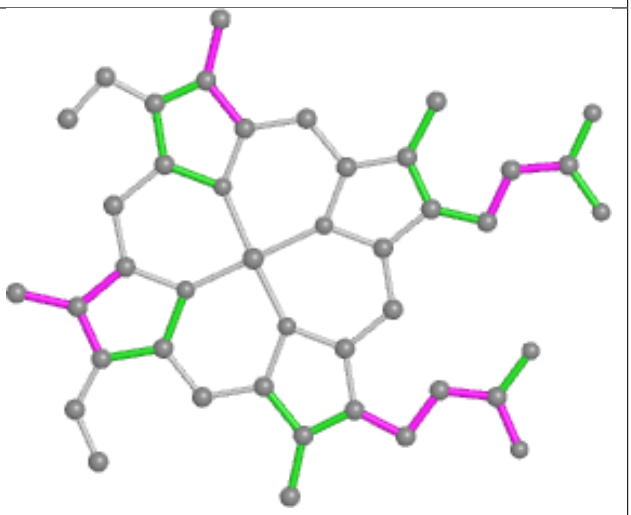


Rings

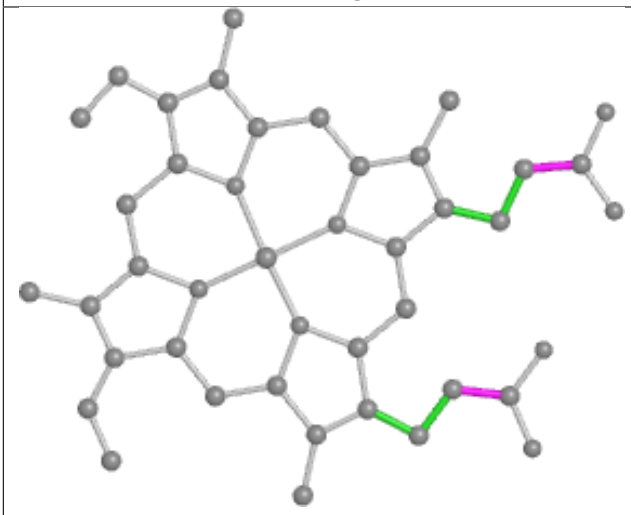
Ligand HEC A 602



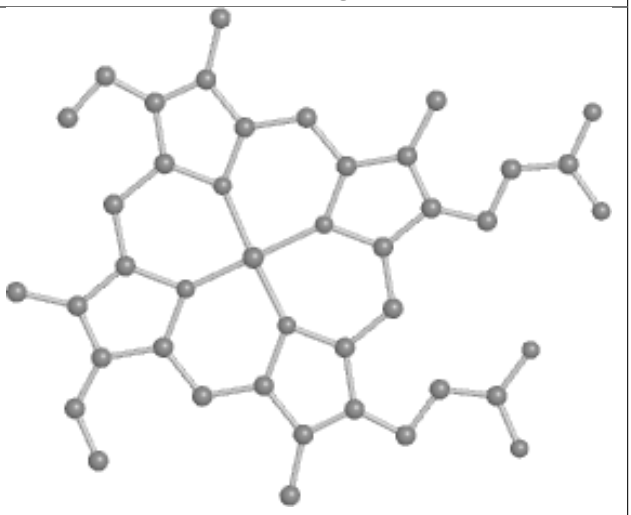
Bond lengths



Bond angles

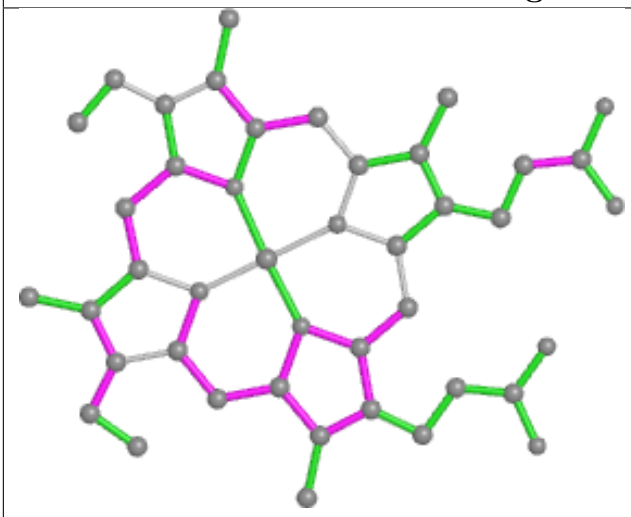


Torsions



Rings

Ligand ISW A 609



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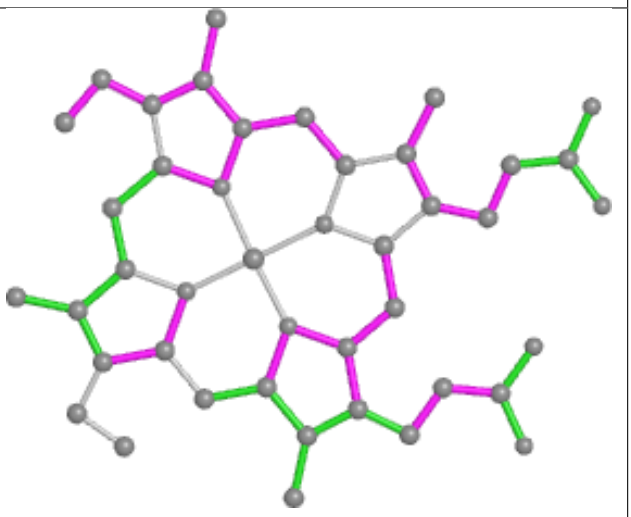

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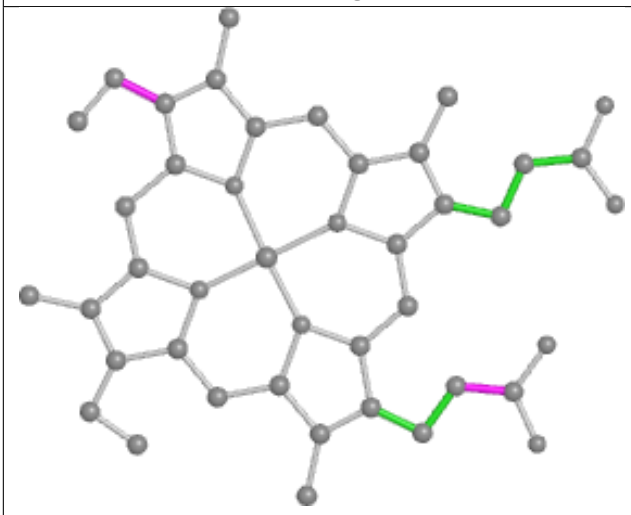

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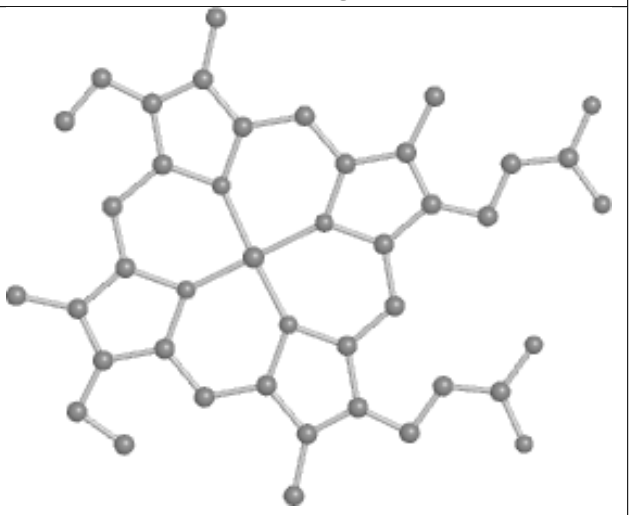
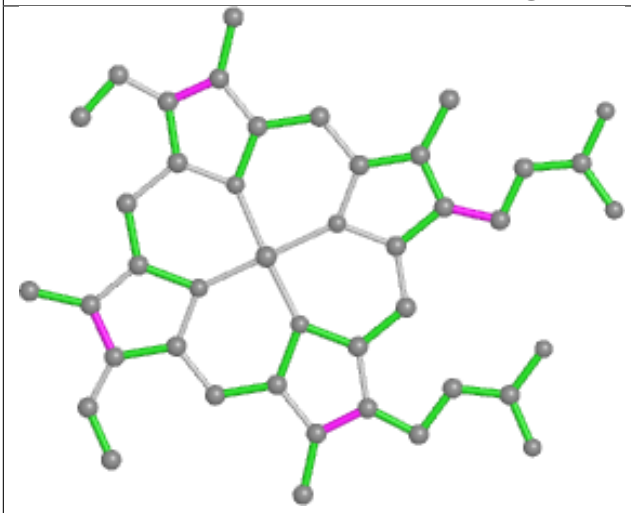


Rings

Ligand HEC C 605



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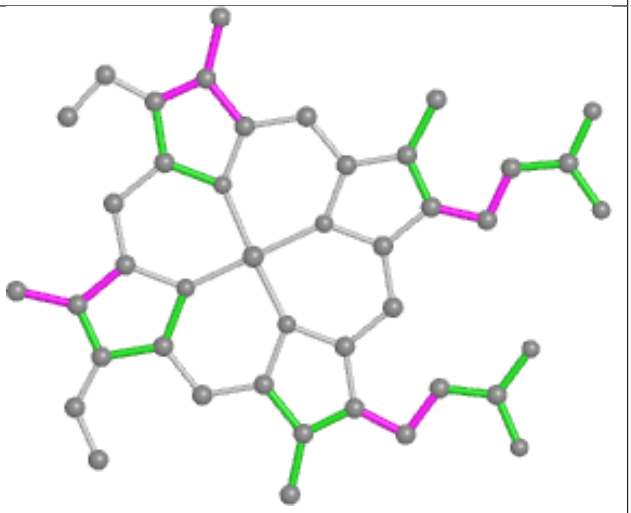

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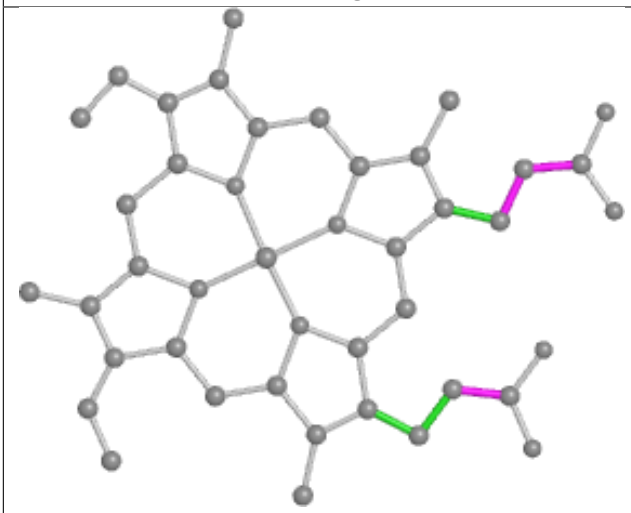

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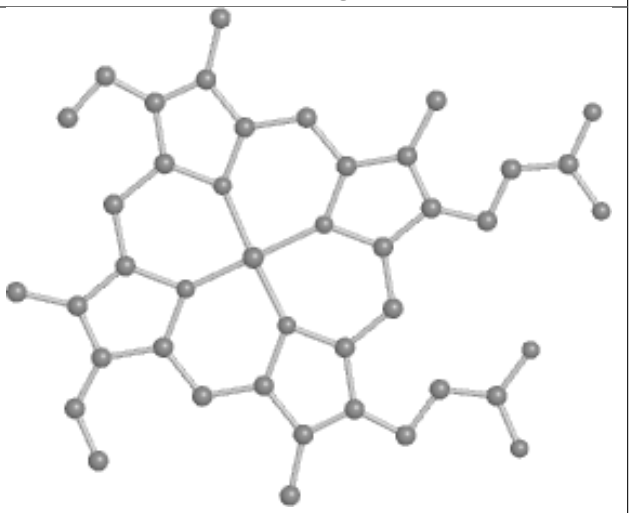
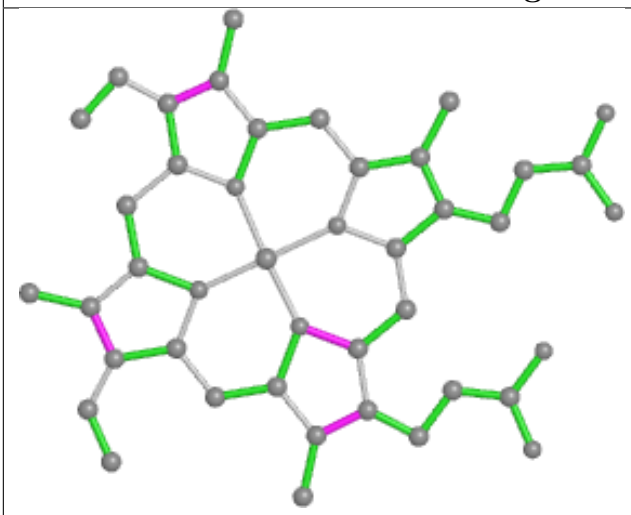


Rings

Ligand HEC E 602



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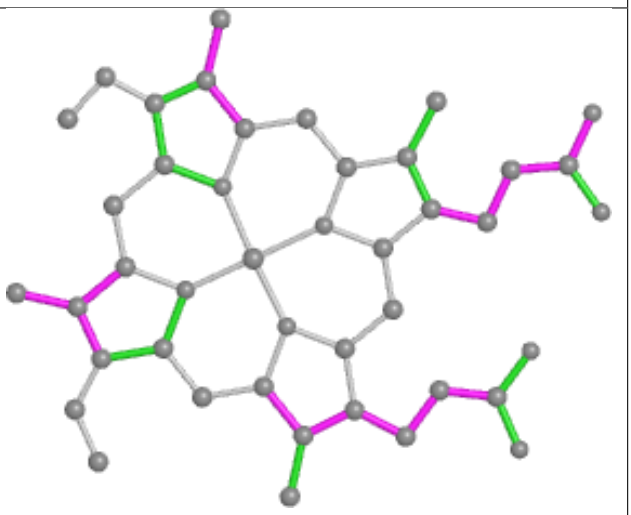

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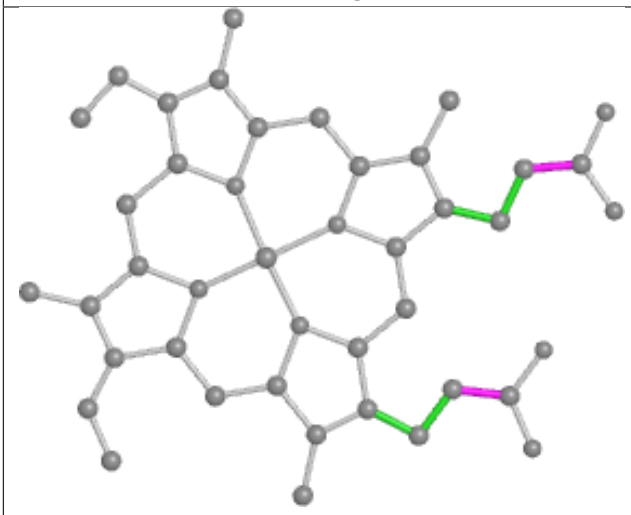
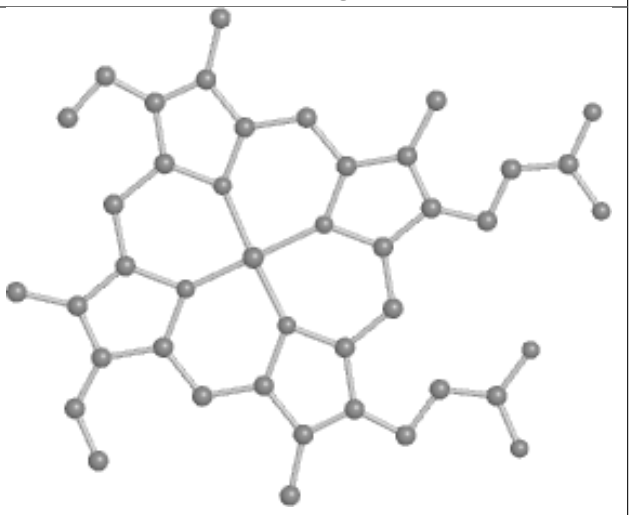
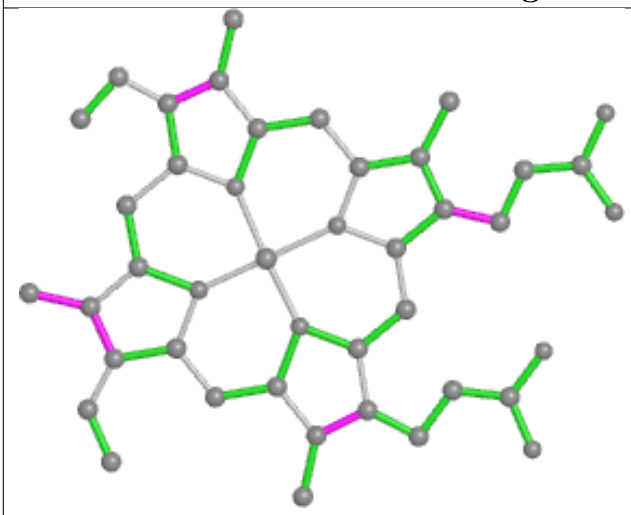


Torsions



Rings

Ligand HEC G 607



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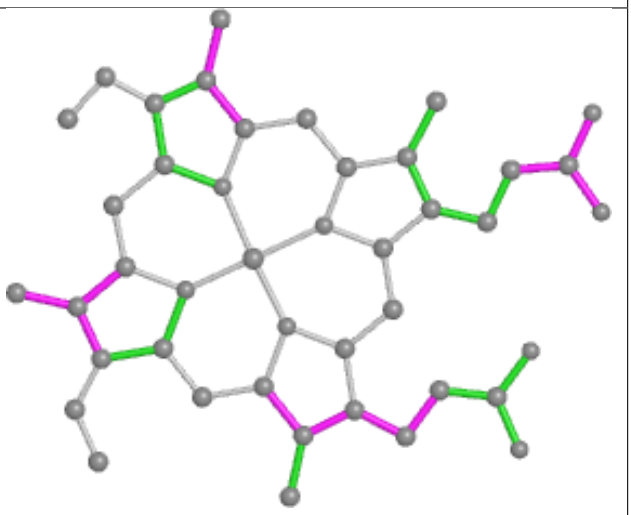

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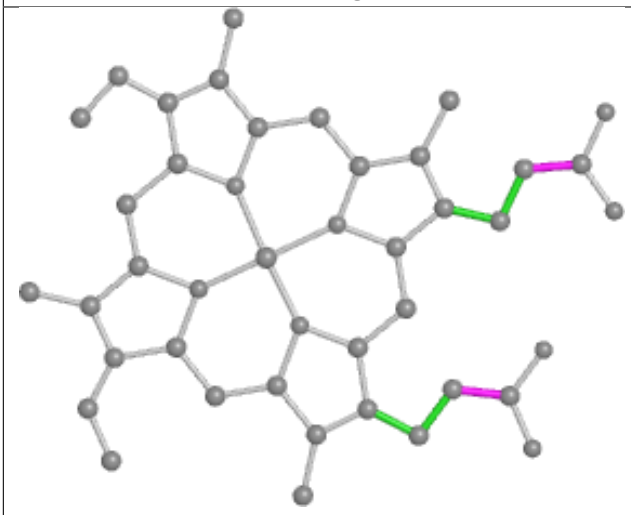

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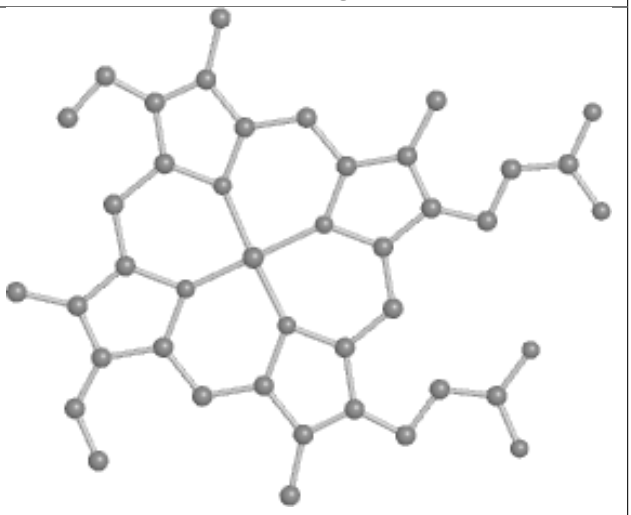
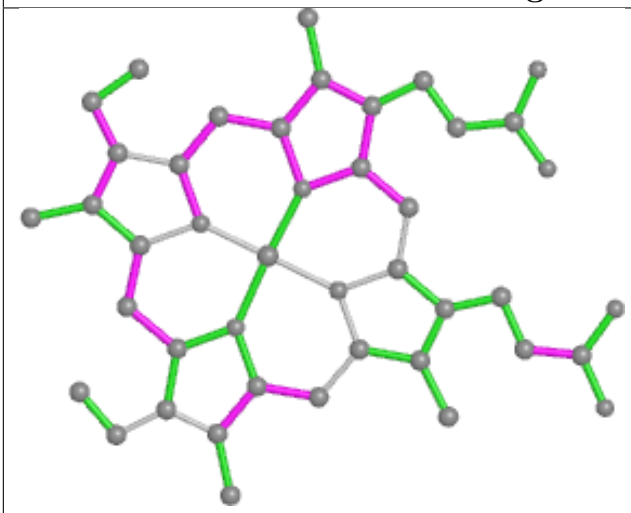


Rings

Ligand ISW C 608



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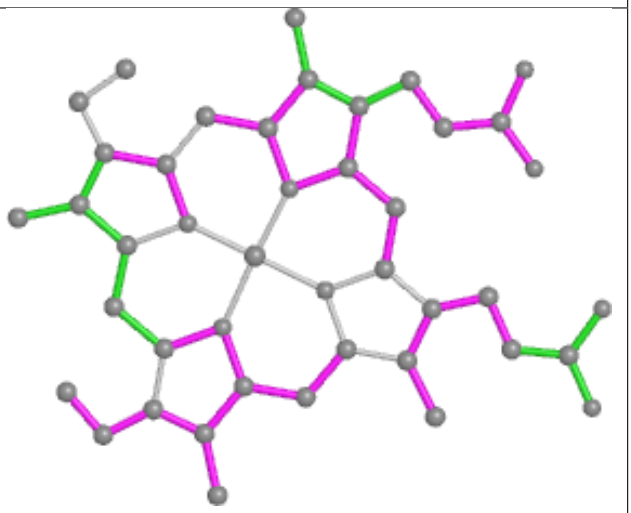

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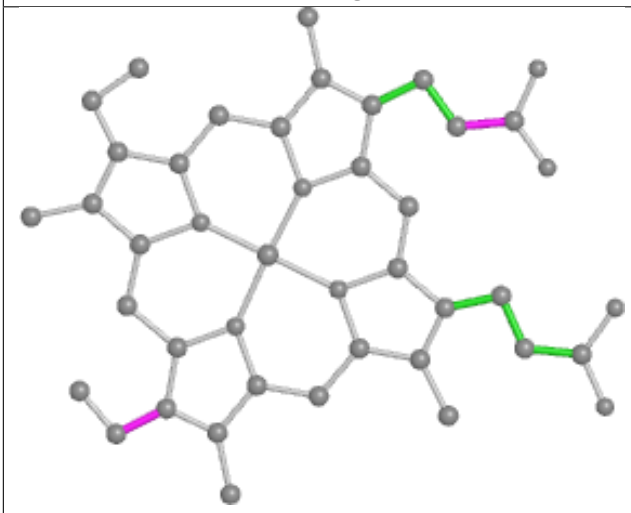

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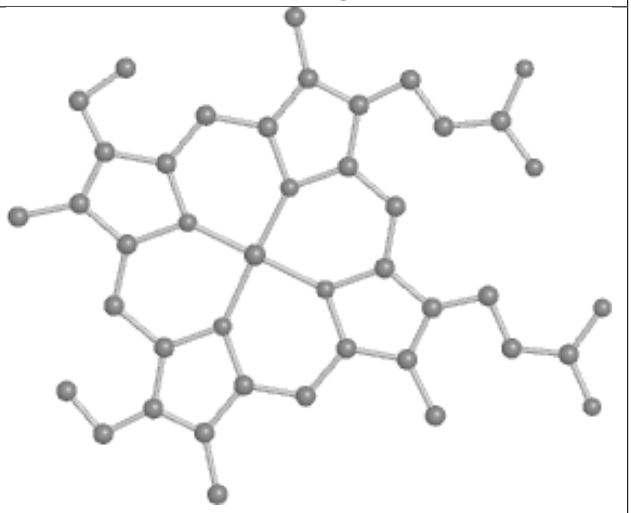
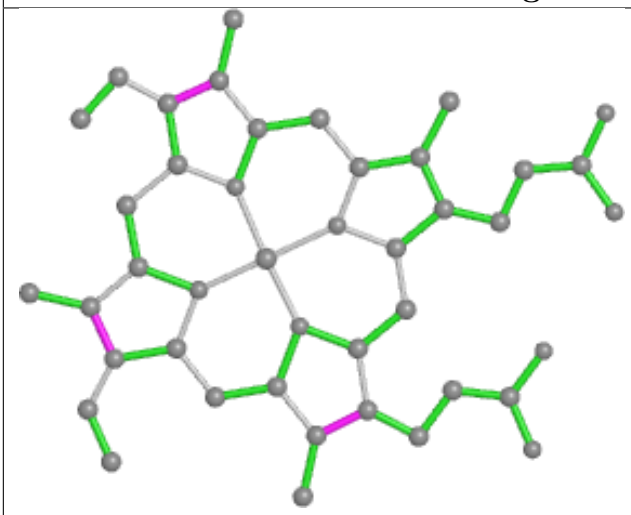


Rings

Ligand HEC C 602



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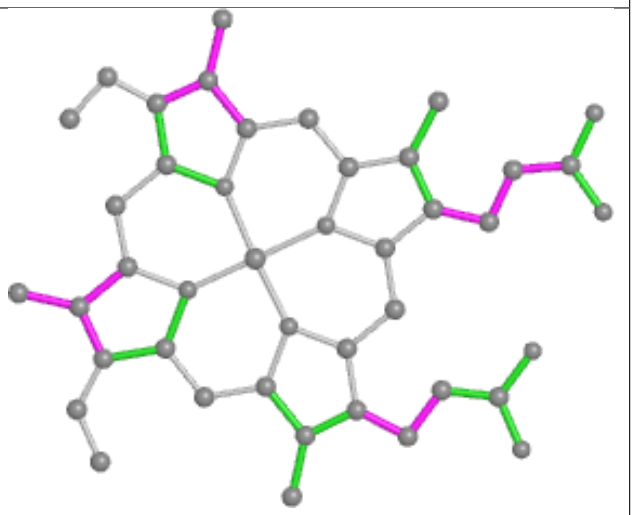
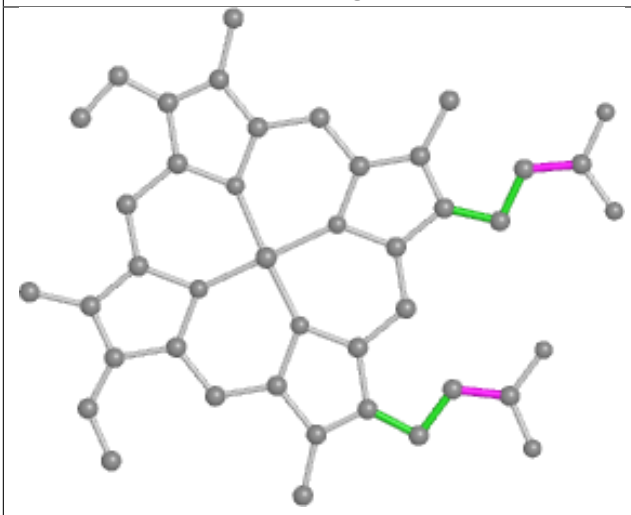
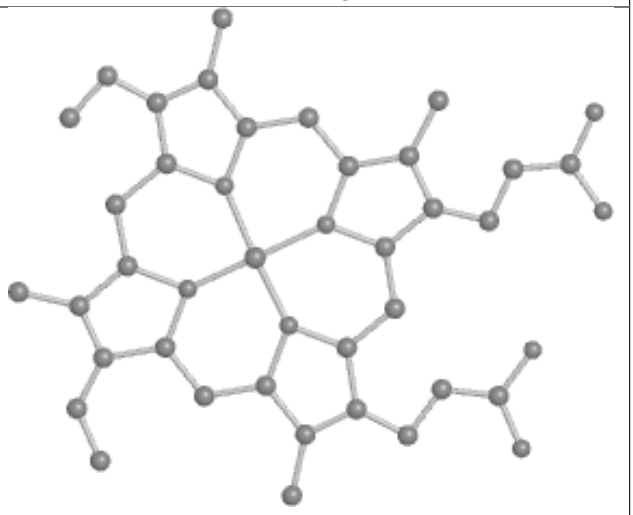


Bond angles

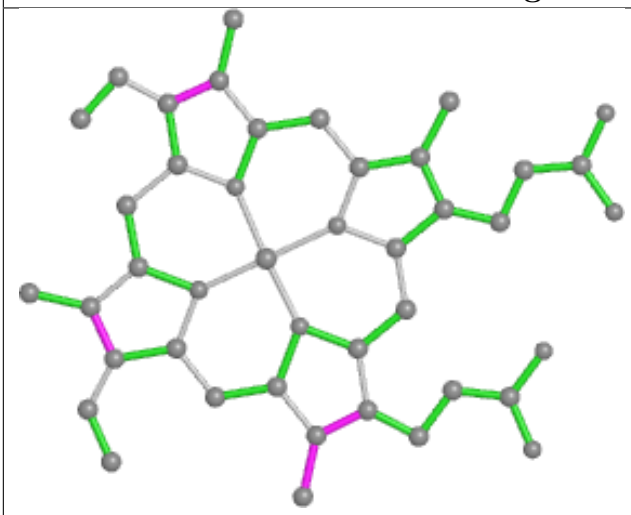


Torsions



Rings

Ligand HEC E 601



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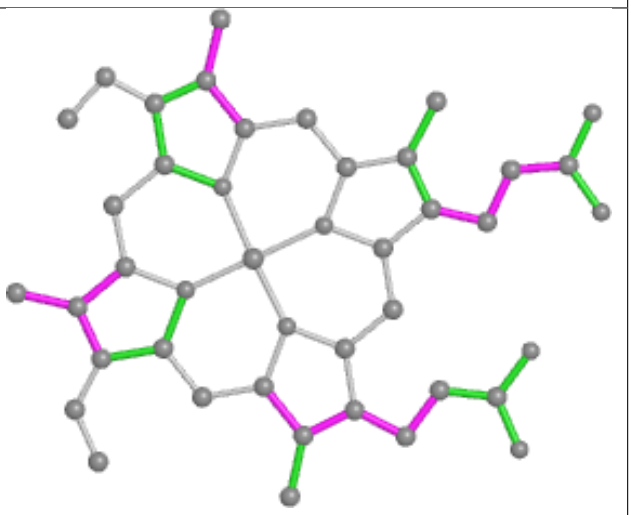
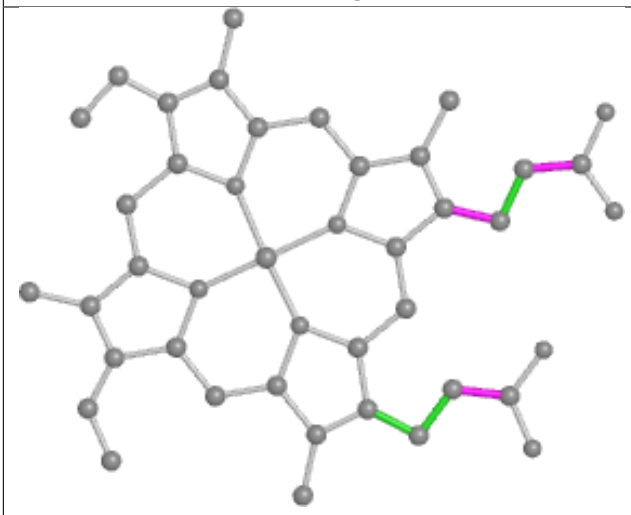


Bond angles



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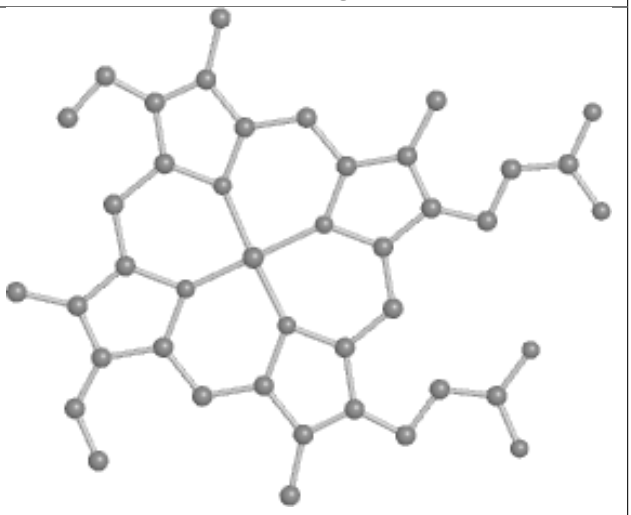
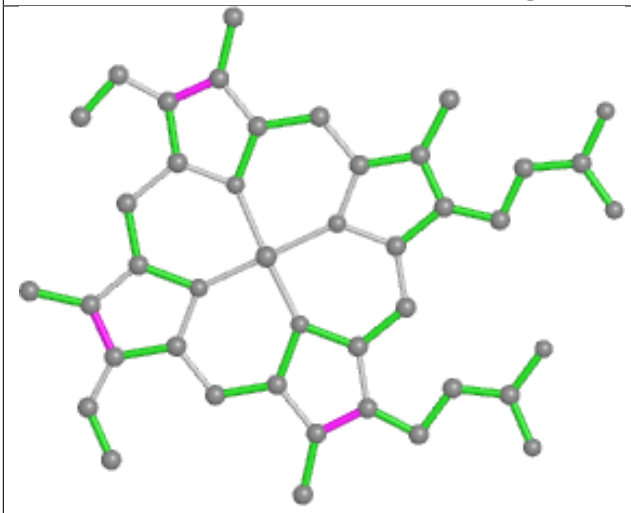


Rings

Ligand HEC K 601



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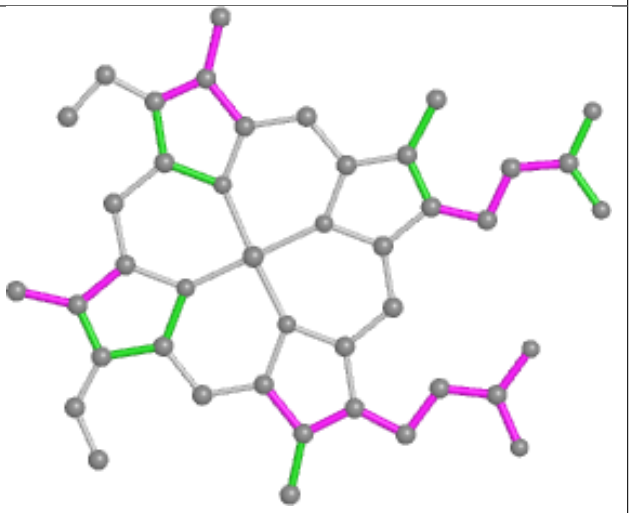
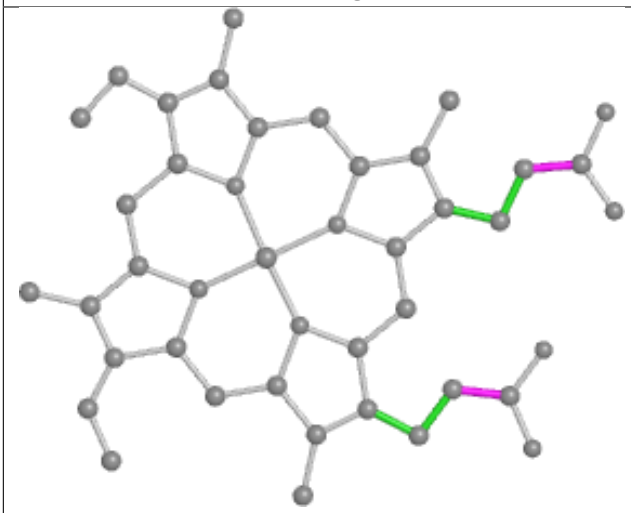
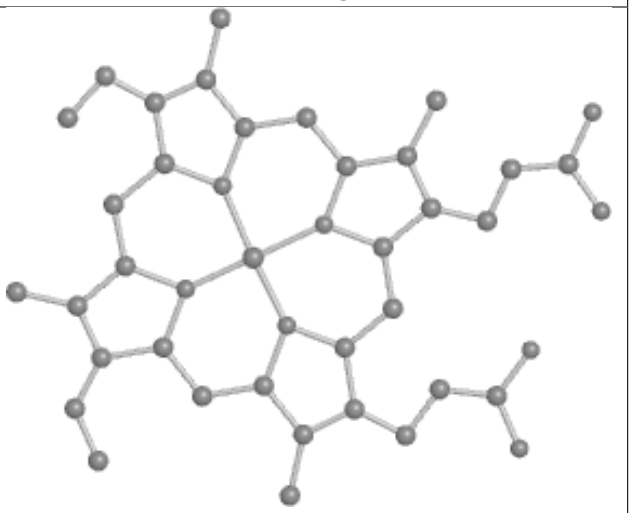


Bond angles

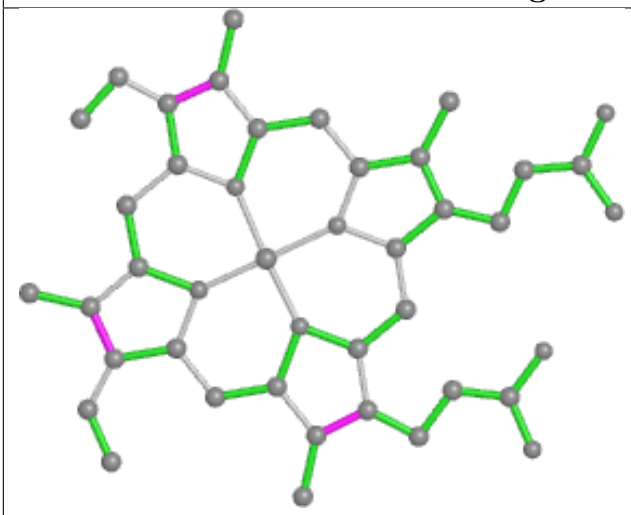


Torsions



Rings

Ligand HEC I 605



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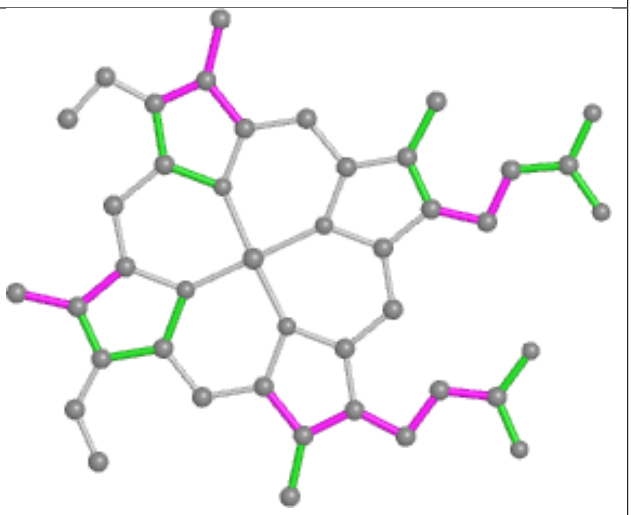
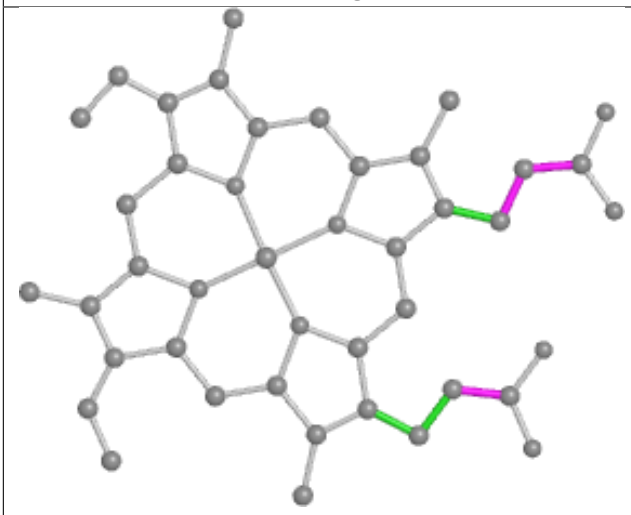
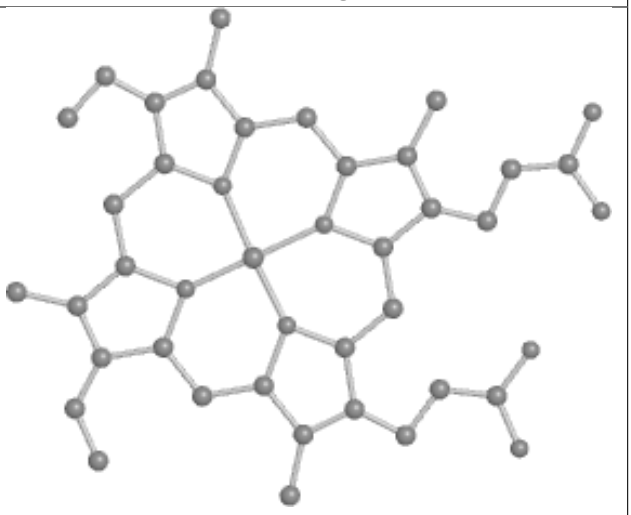


Bond angles

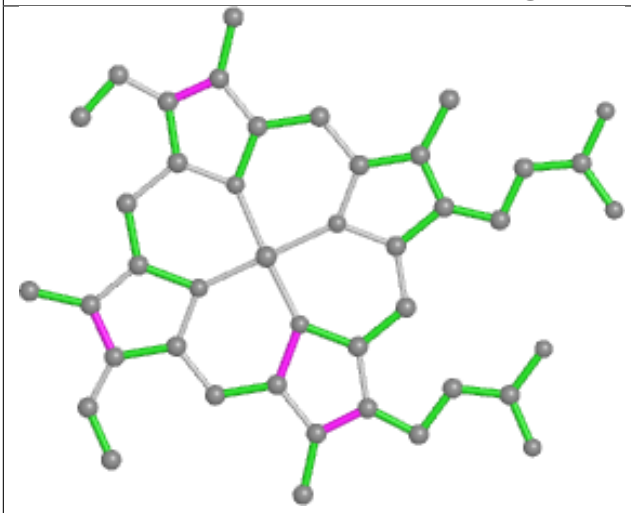


Torsions

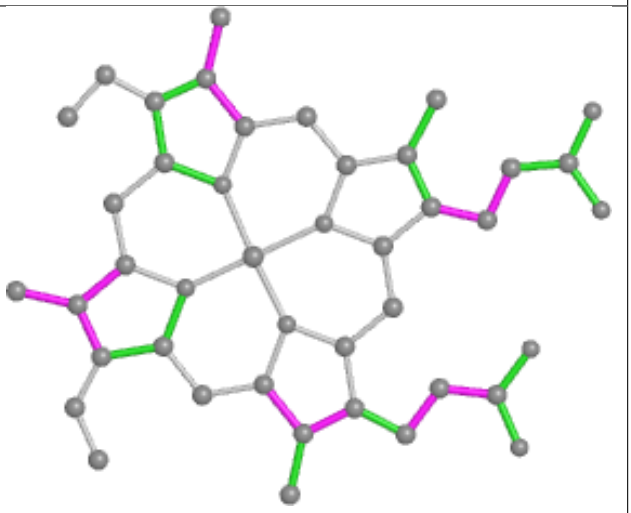


Rings

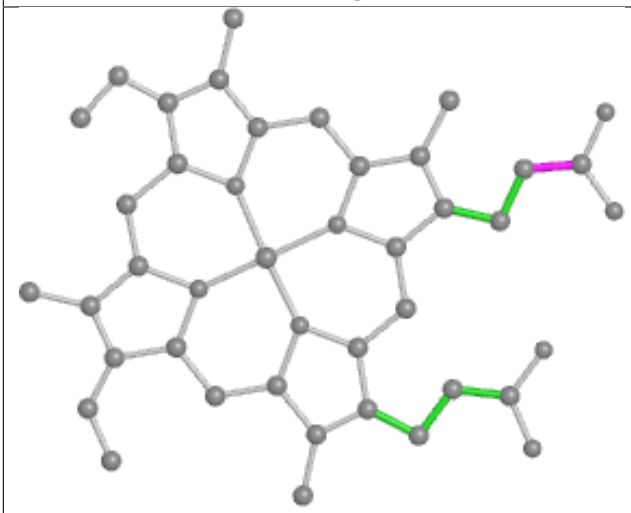
Ligand HEC K 603



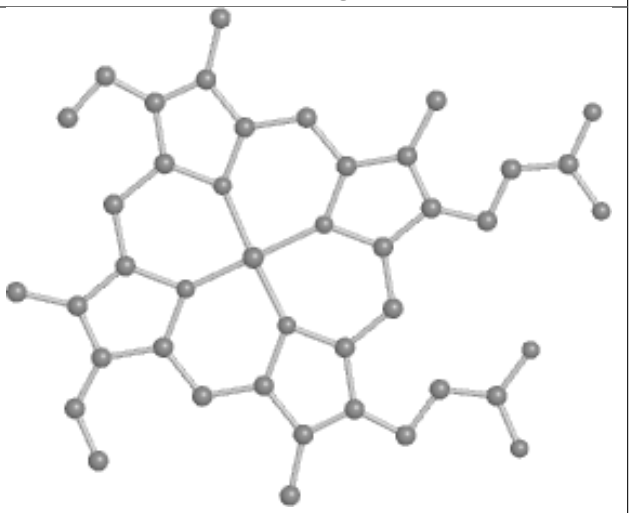
Bond lengths



Bond angles

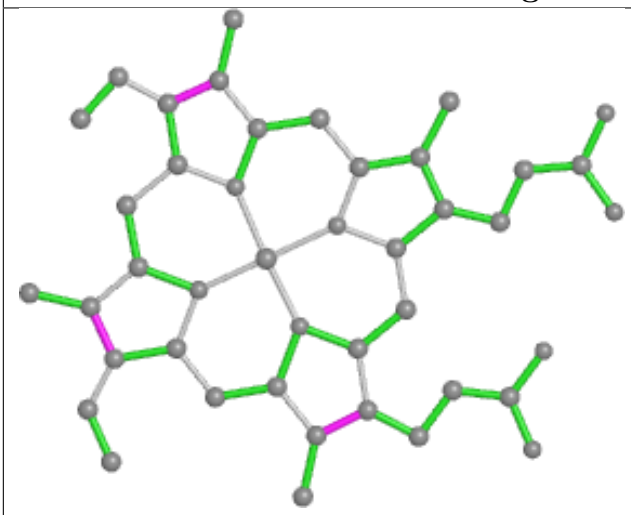


Torsions



Rings

Ligand HEC K 604



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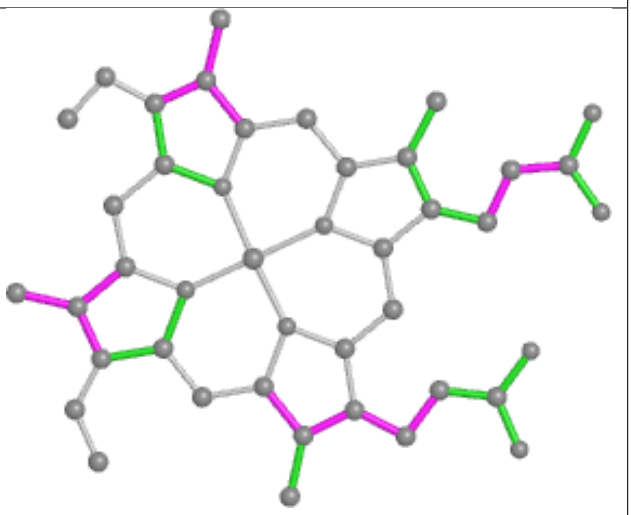
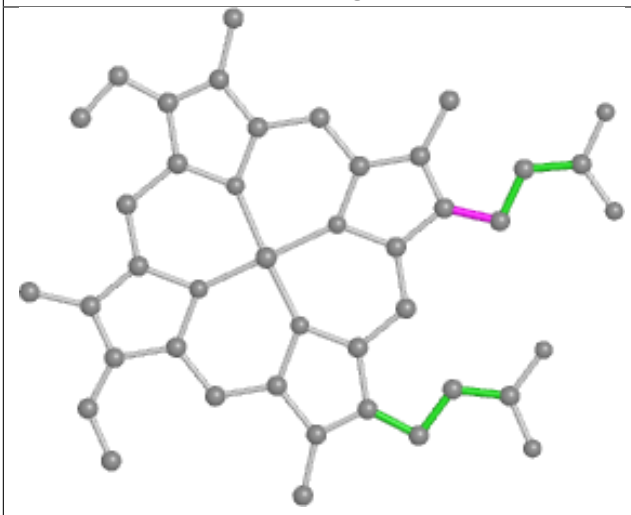


Bond angles



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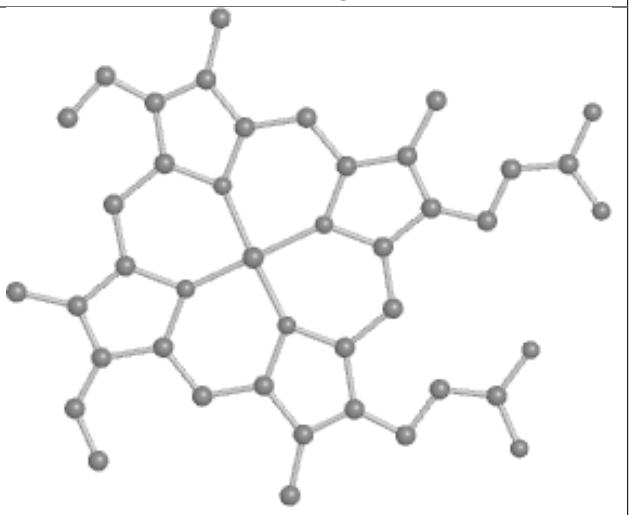
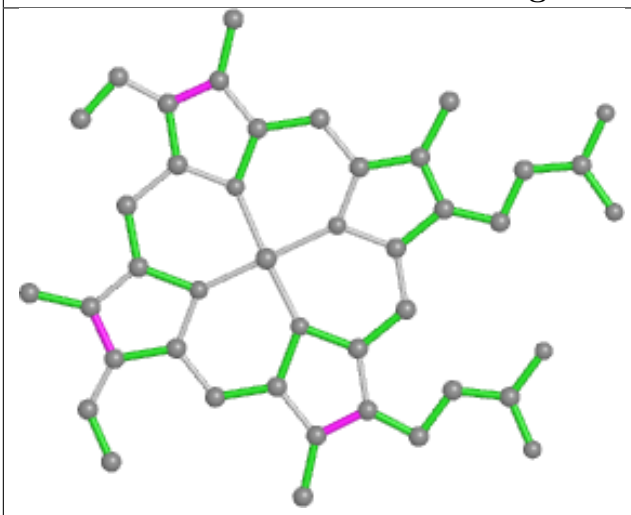


Rings

Ligand HEC I 607



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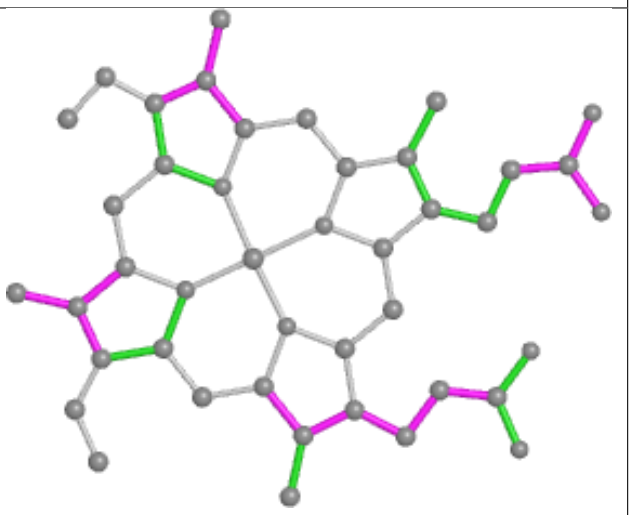

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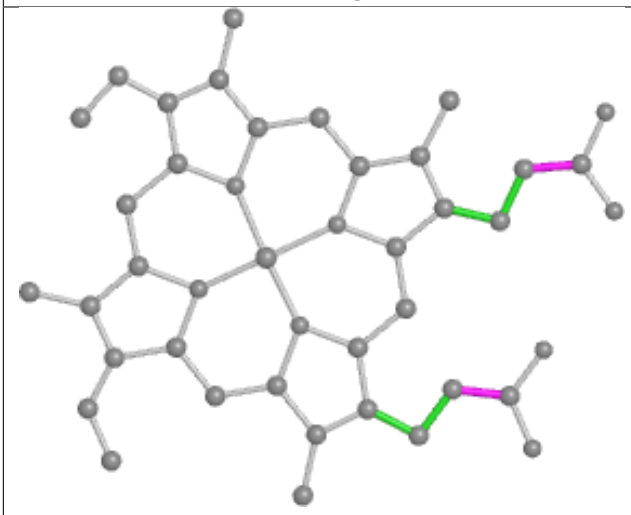

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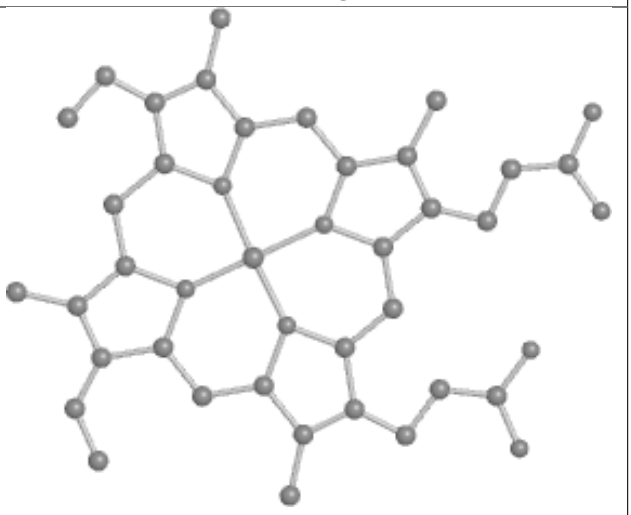
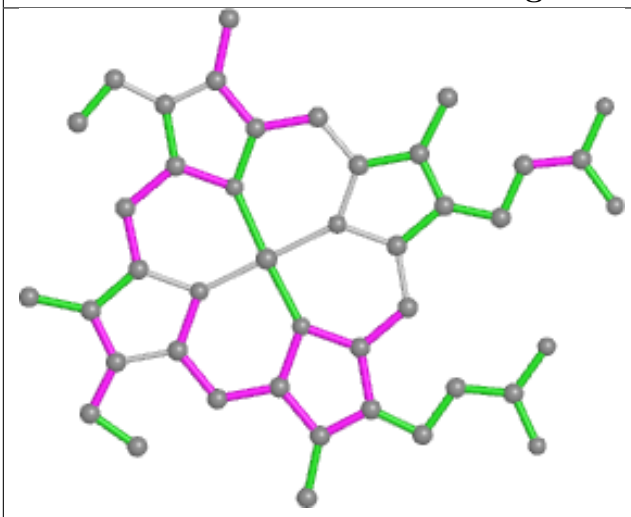


Rings

Ligand ISW G 609



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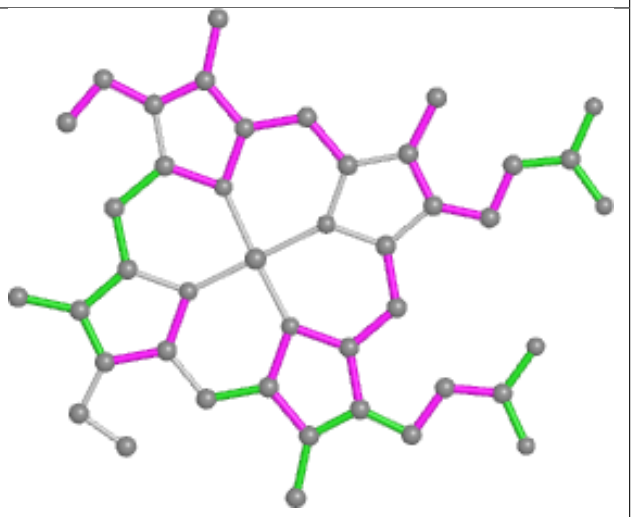
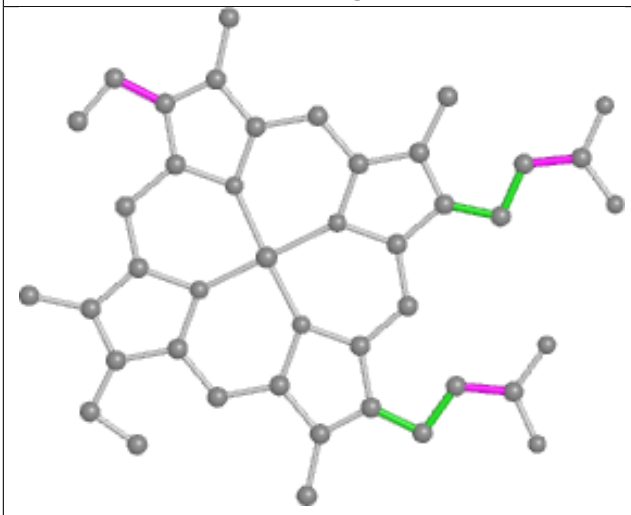


Bond angles



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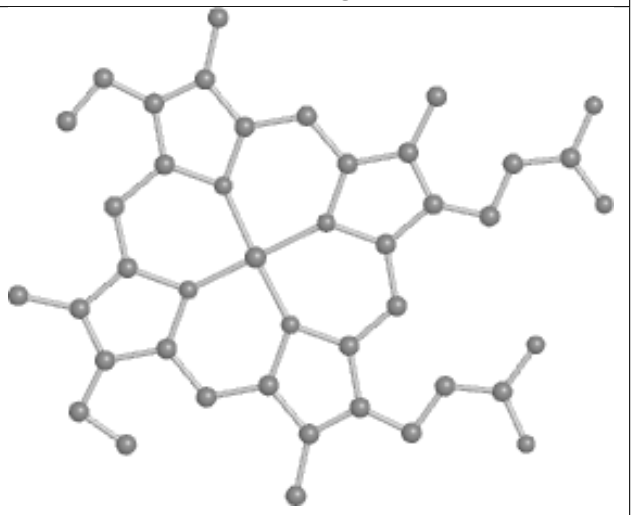
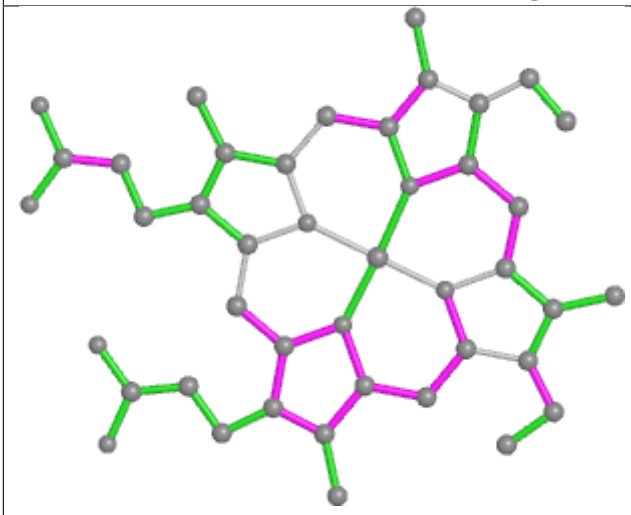


Rings

Ligand ISW A 608



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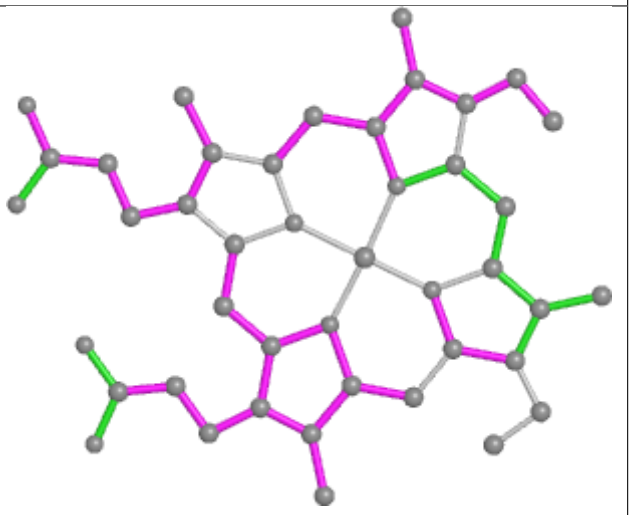
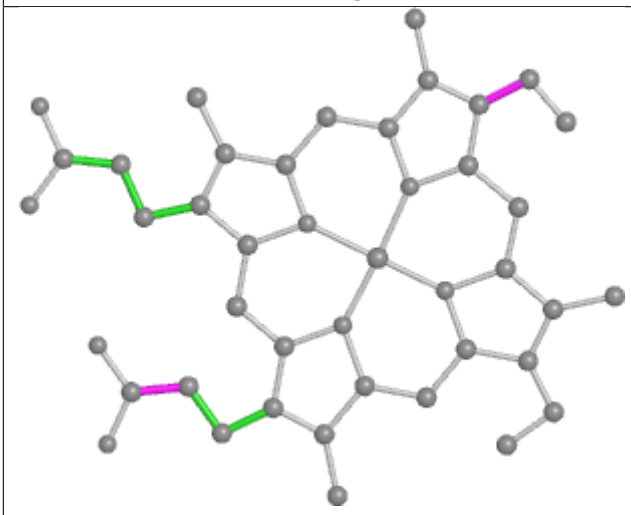


Bond angles



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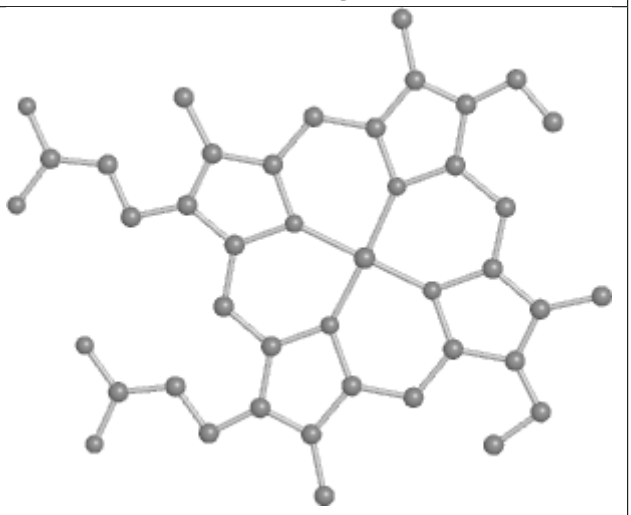
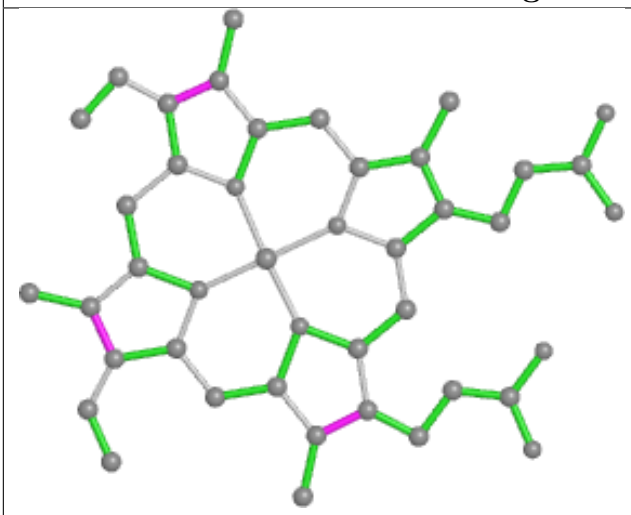


Rings

Ligand HEC C 601



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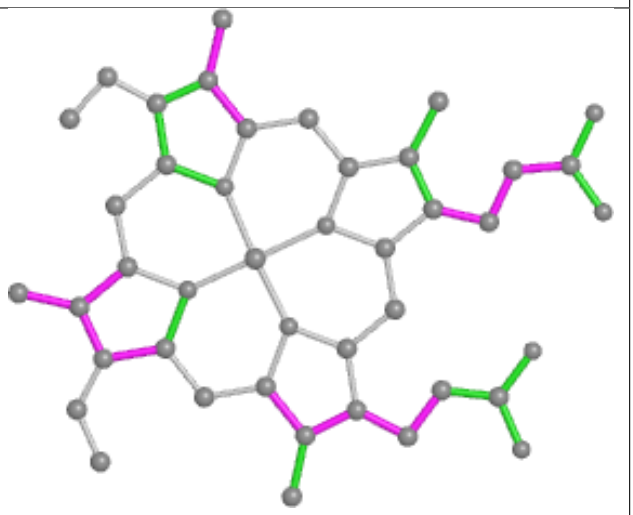
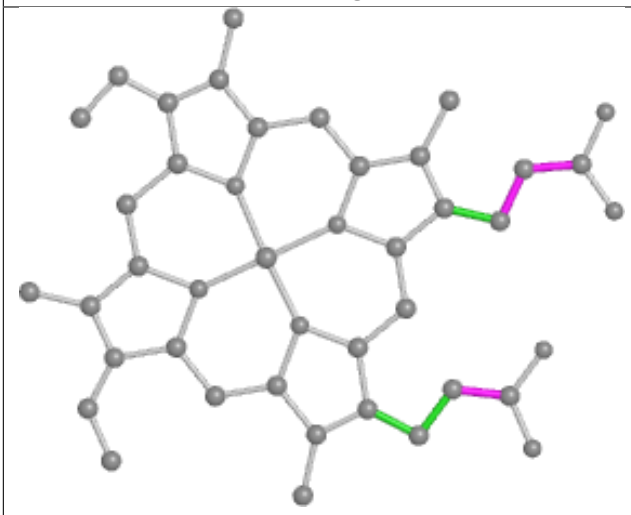


Bond angles



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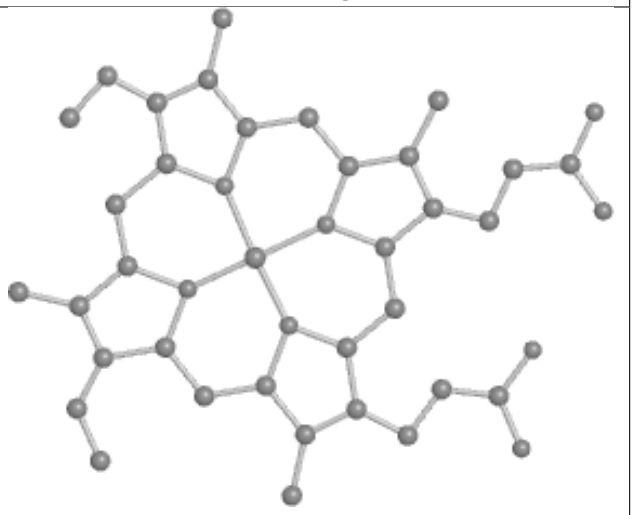
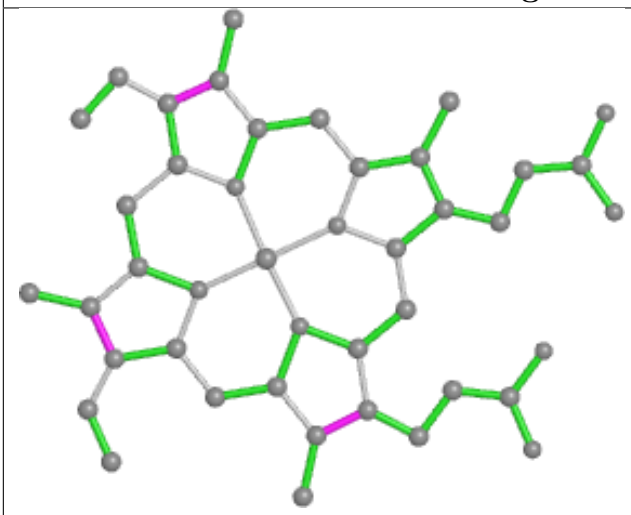


Rings

Ligand HEC G 605



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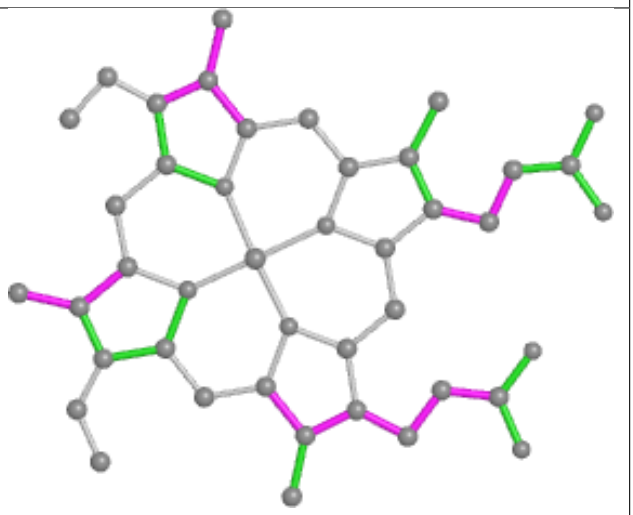
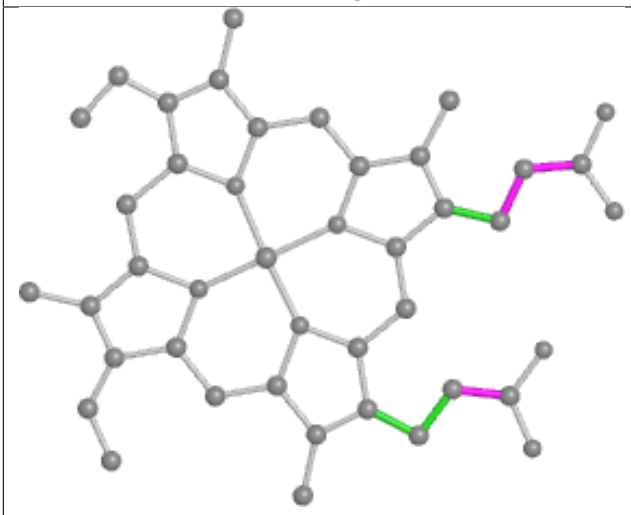


Bond angles



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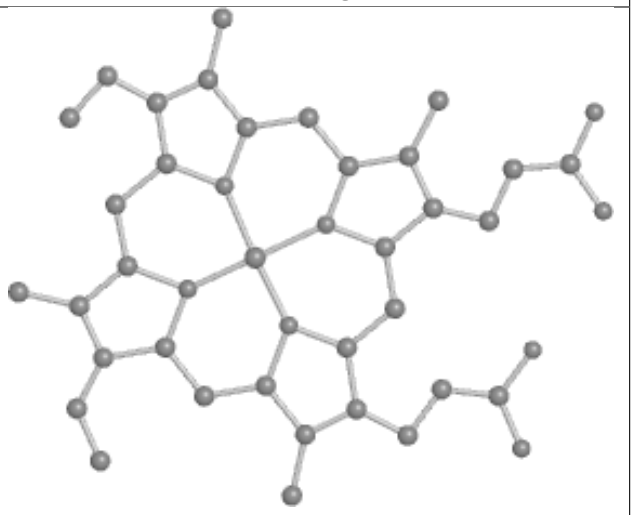
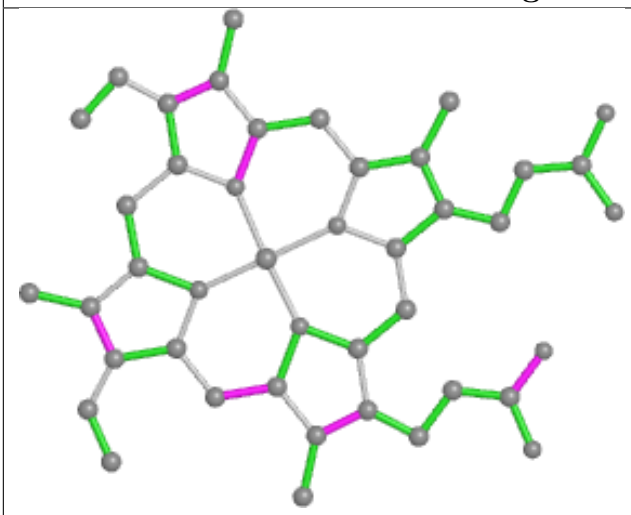


Rings

Ligand HEC A 606



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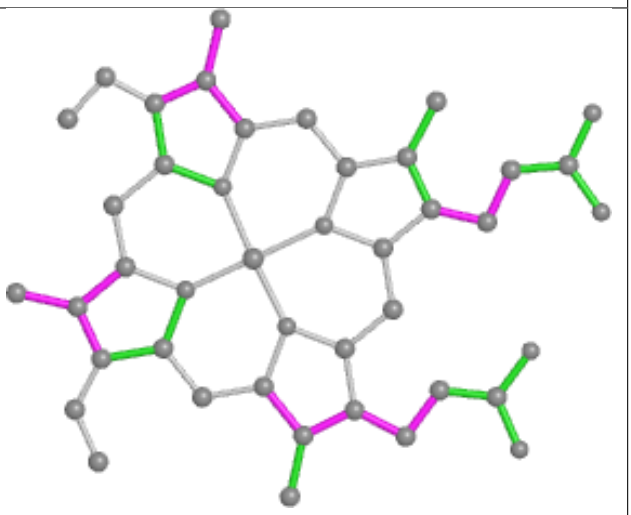
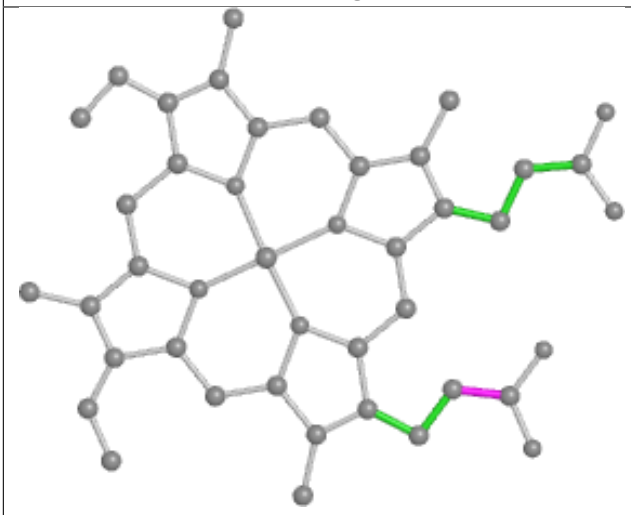


Bond angles



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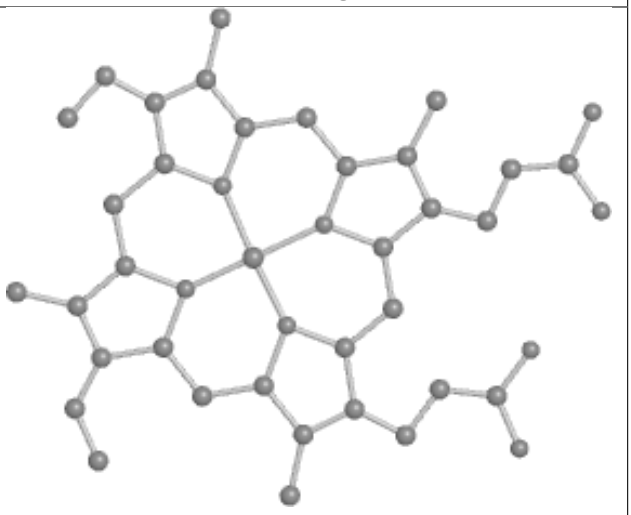
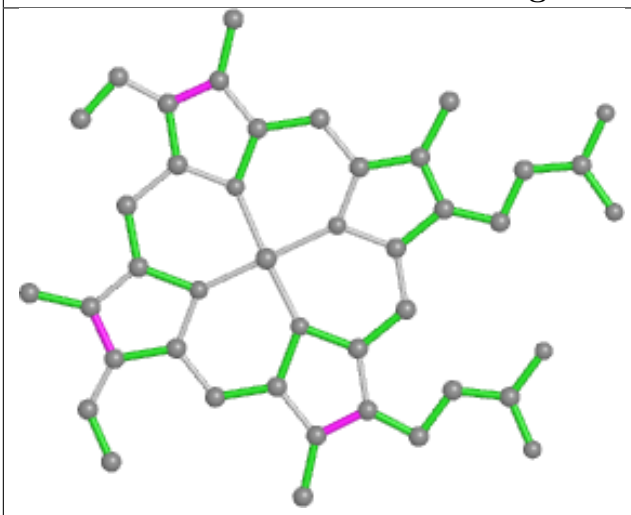


Rings

Ligand HEC I 601



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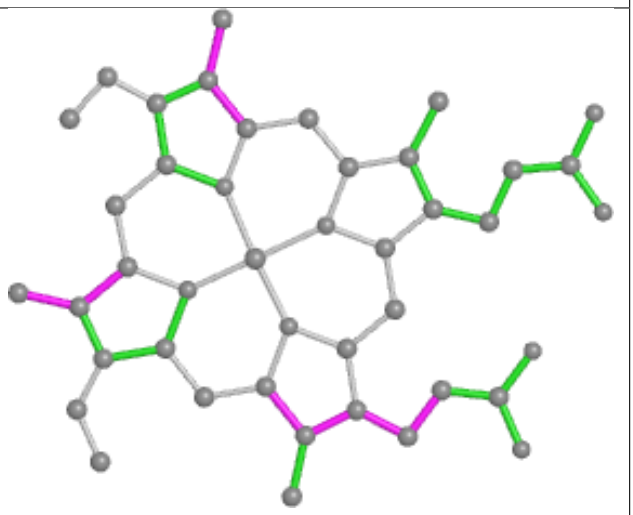
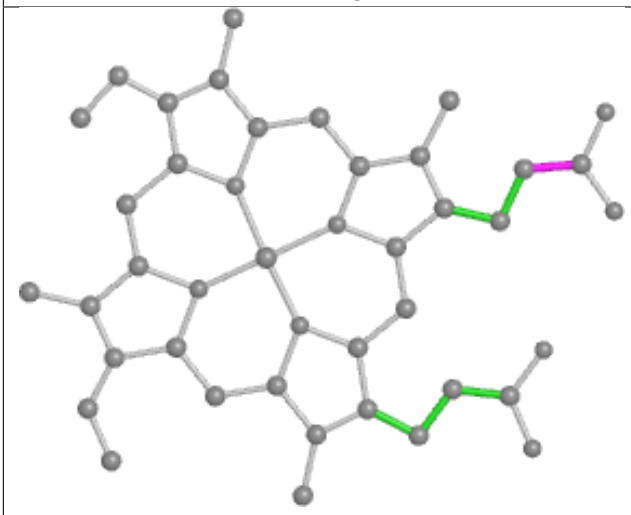


Bond angles



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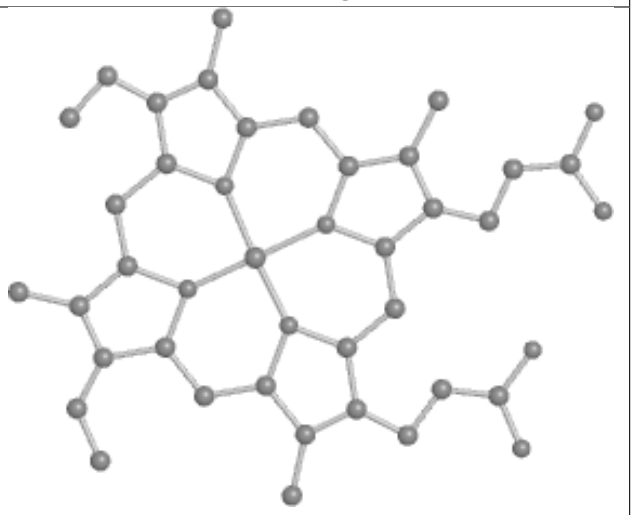
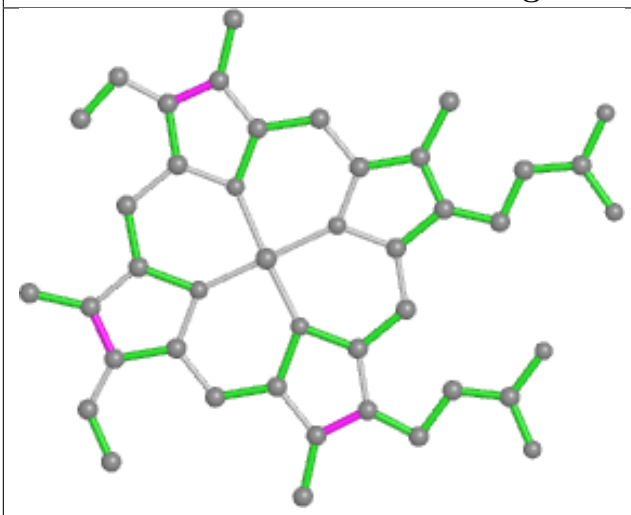


Rings

Ligand HEC C 603



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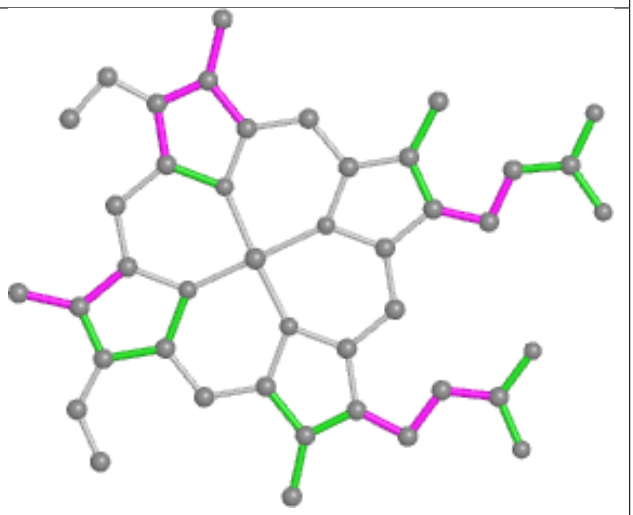
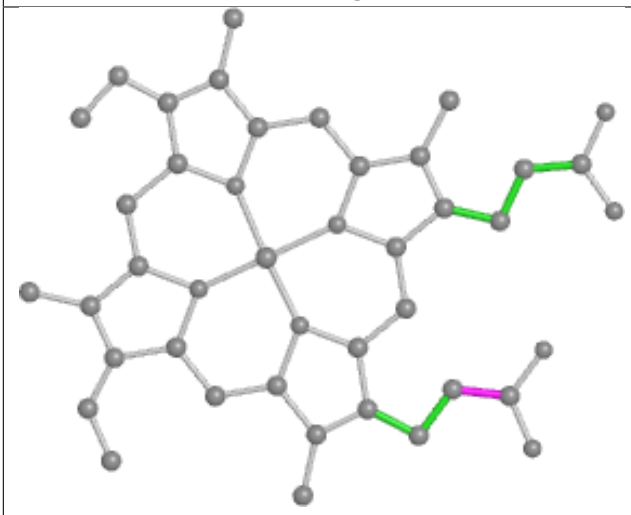
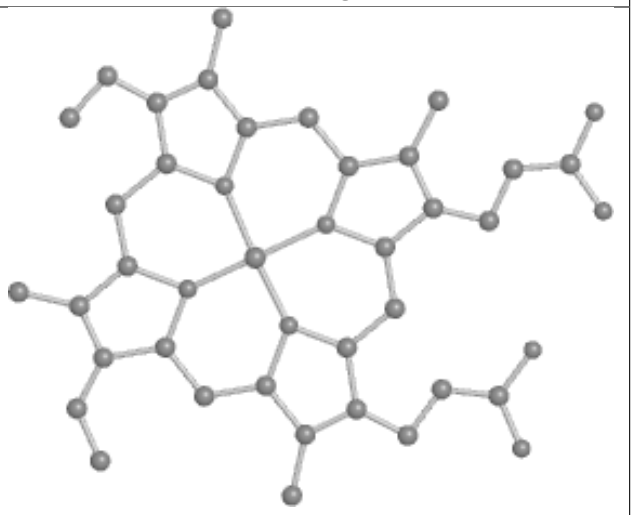


Bond angles

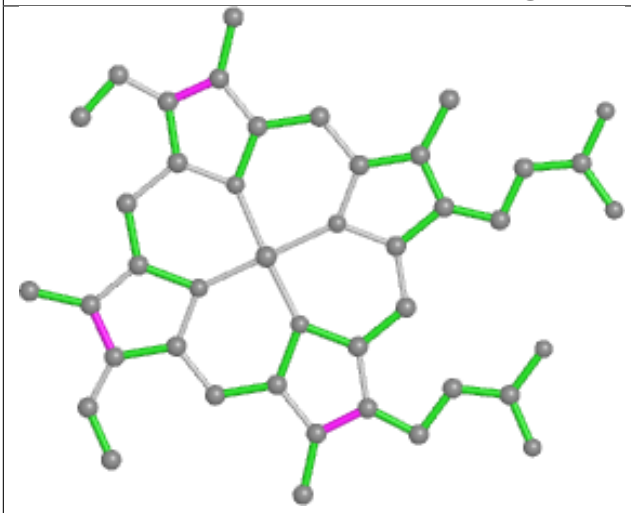


Torsions



Rings

Ligand HEC K 607



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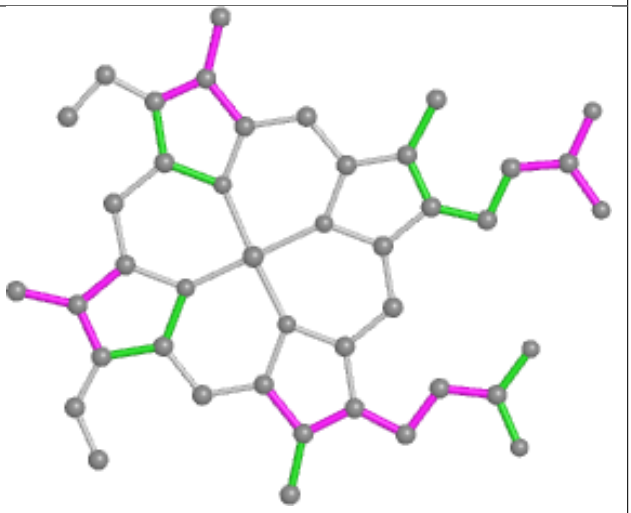

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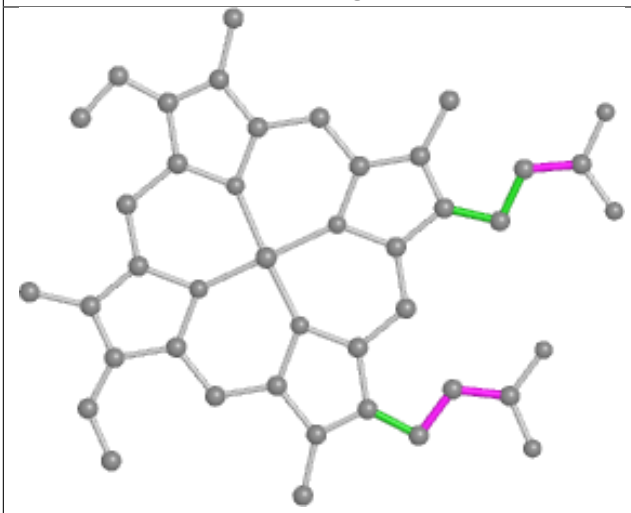

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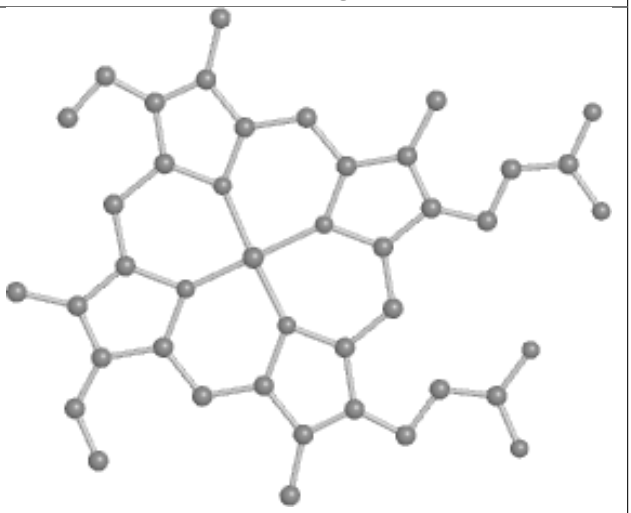
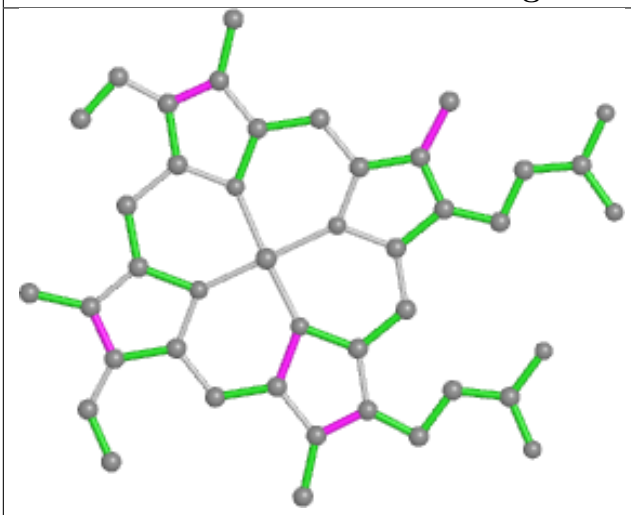


Rings

Ligand HEC C 604



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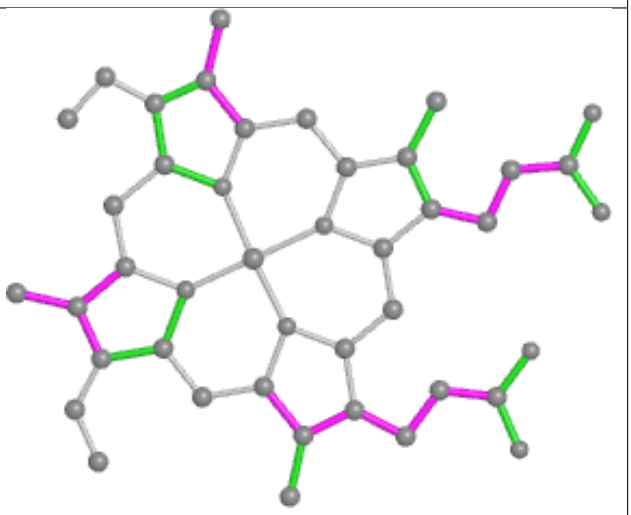

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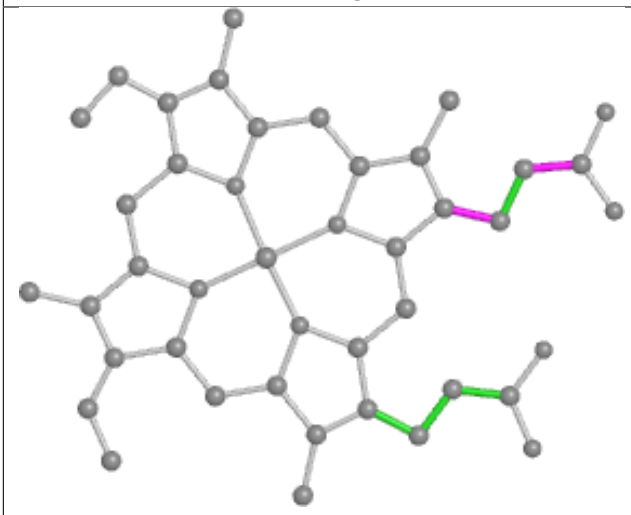

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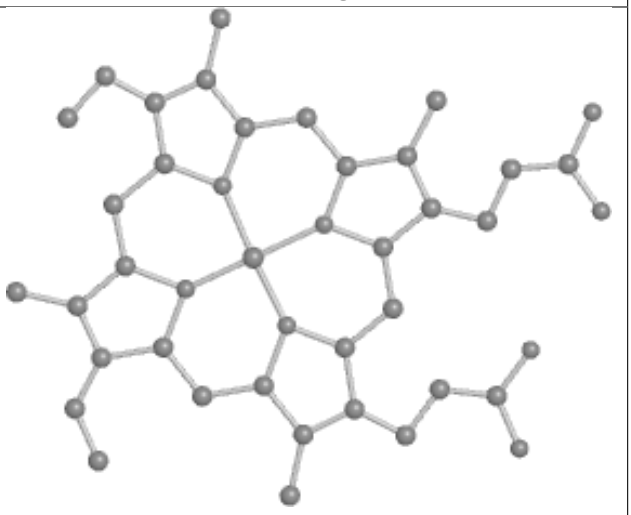
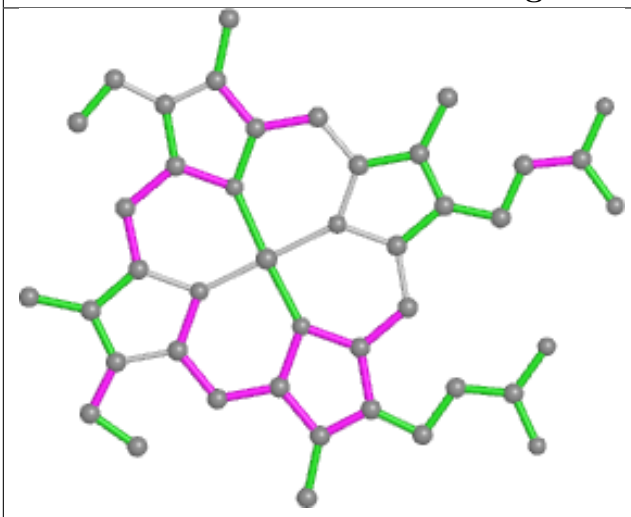


Rings

Ligand ISW G 608



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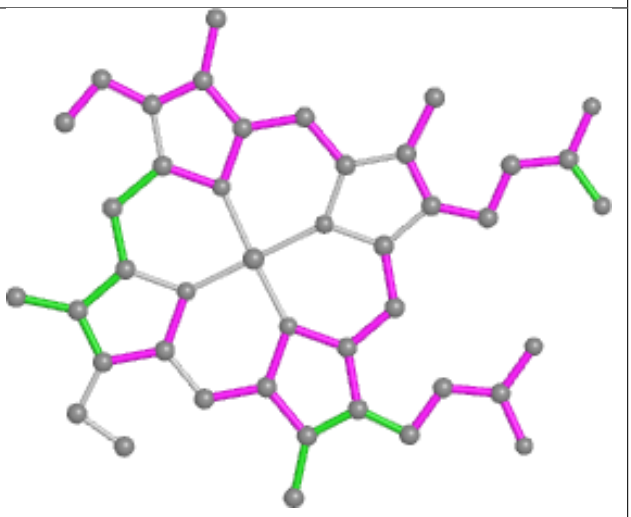
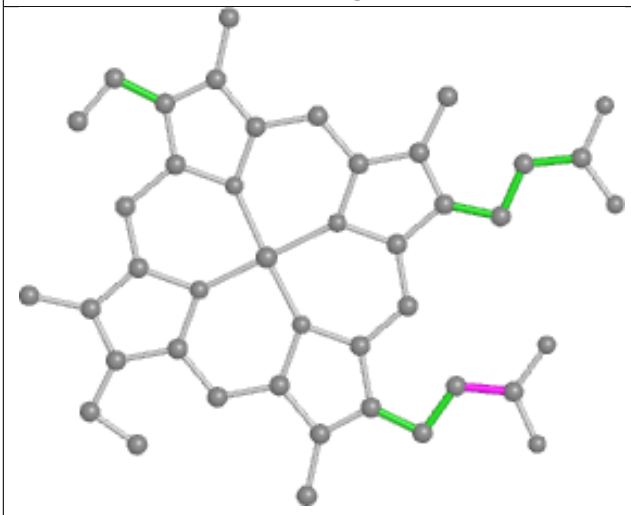
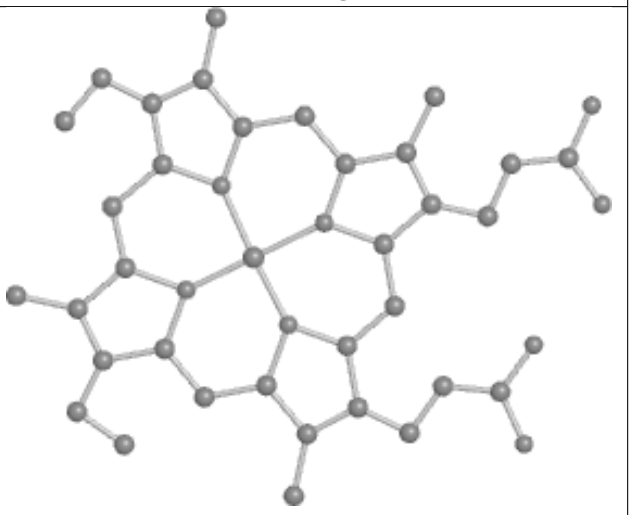


Bond angles

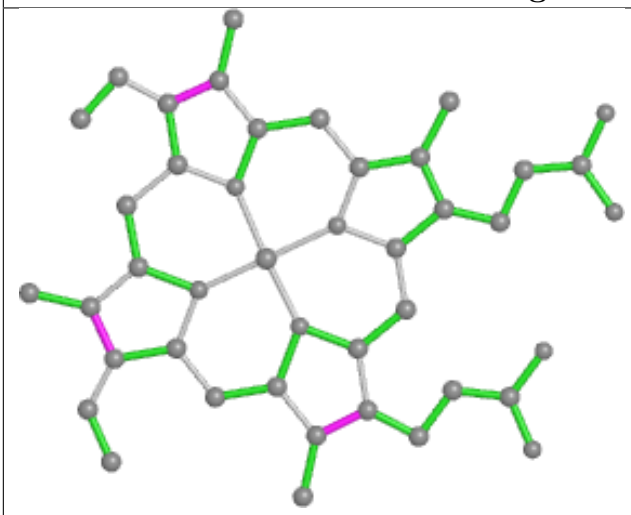


Torsions

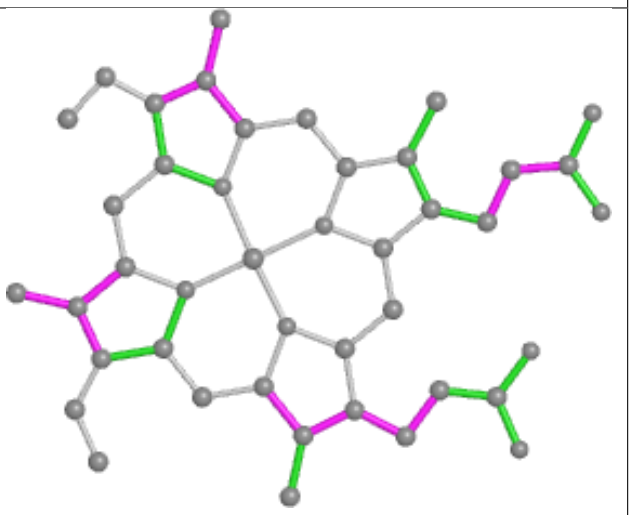


Rings

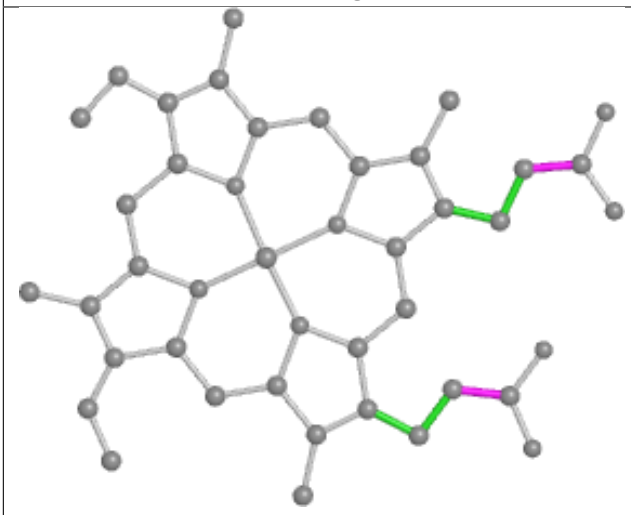
Ligand HEC I 602



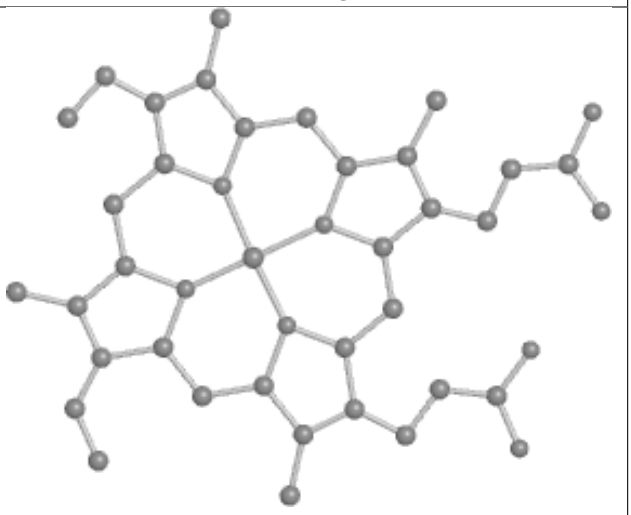
Bond lengths



Bond angles

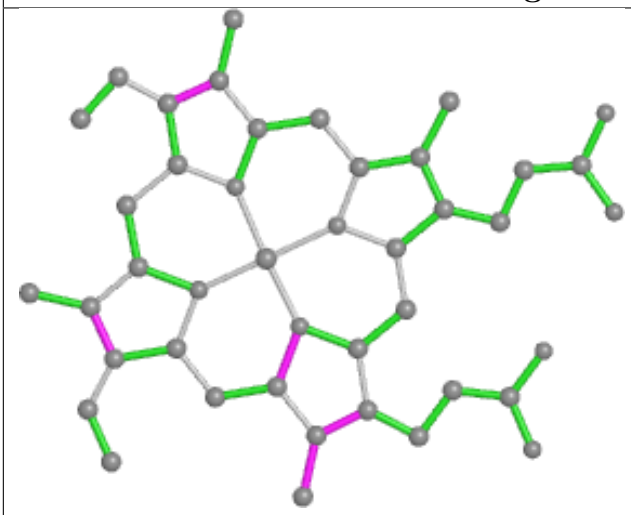


Torsions



Rings

Ligand HEC E 603



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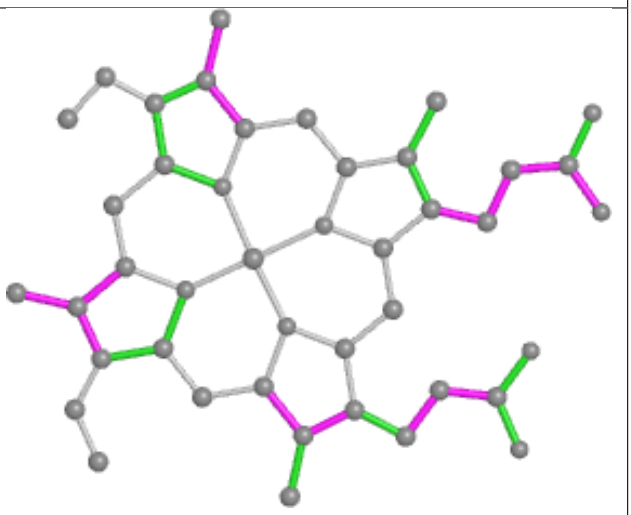
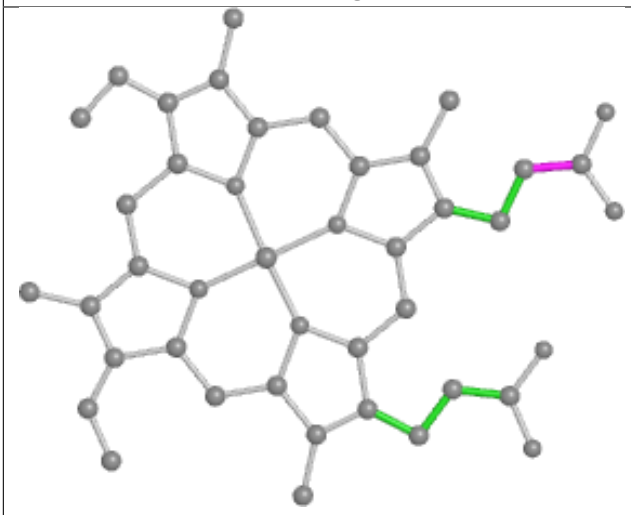
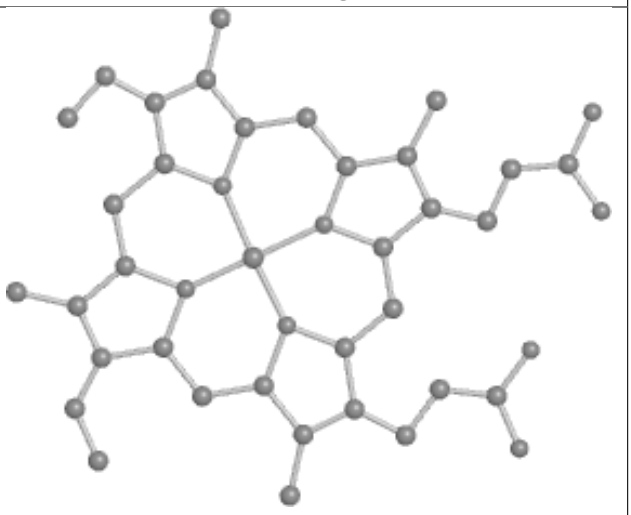


Bond angles

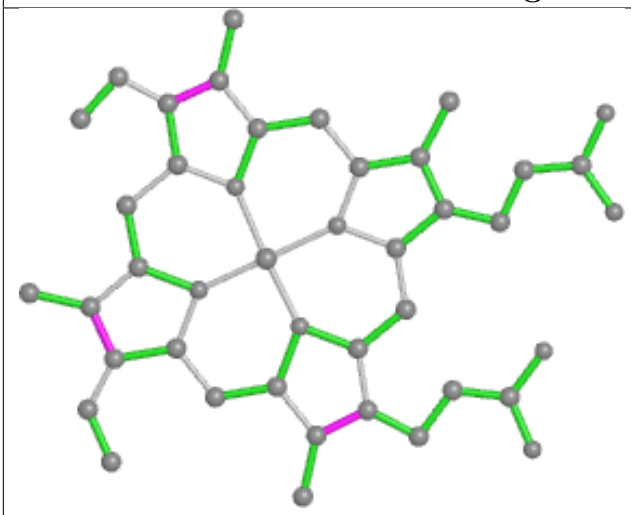


Torsions



Rings

Ligand HEC E 606



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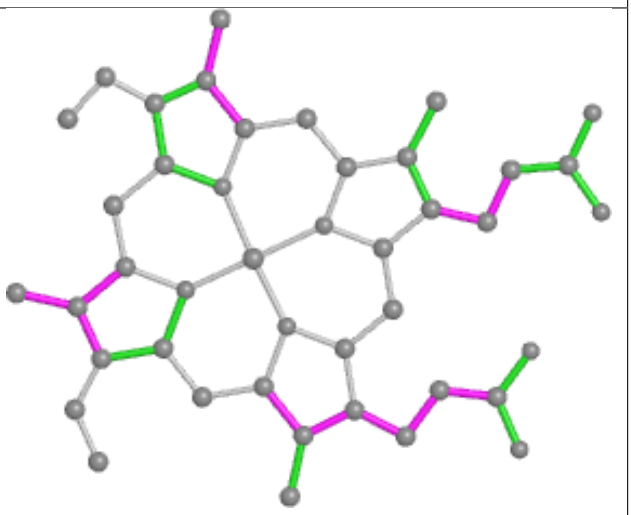
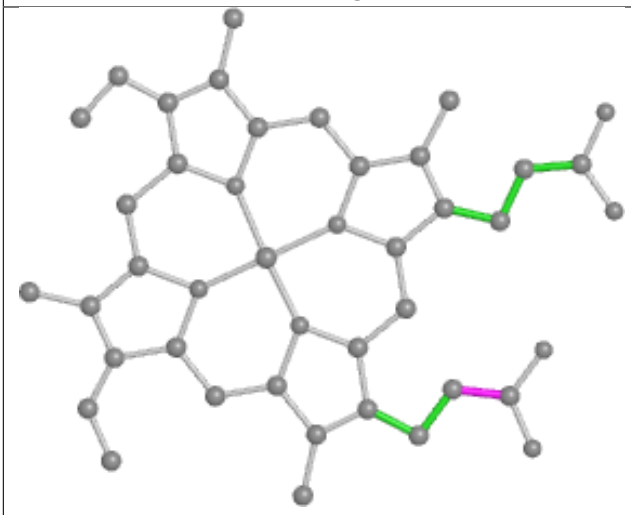
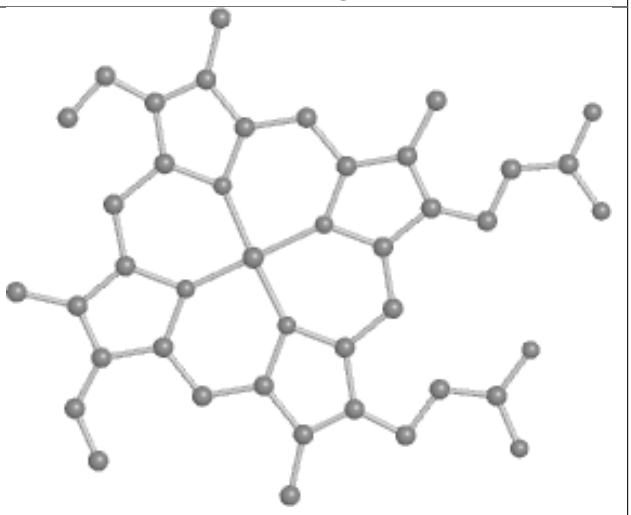


Bond angles

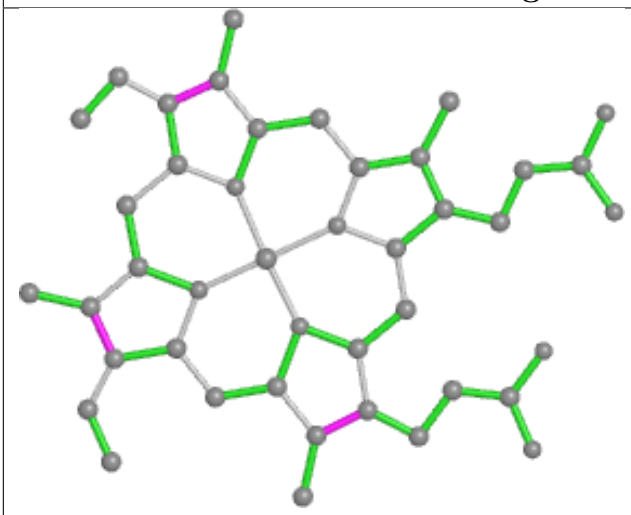


Torsions



Rings

Ligand HEC A 601



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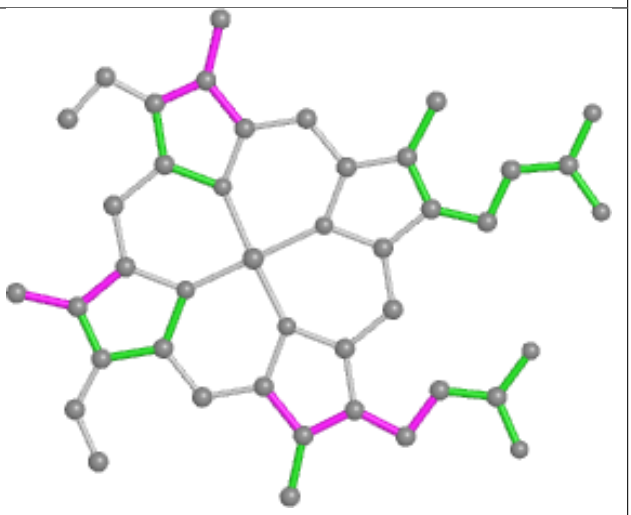
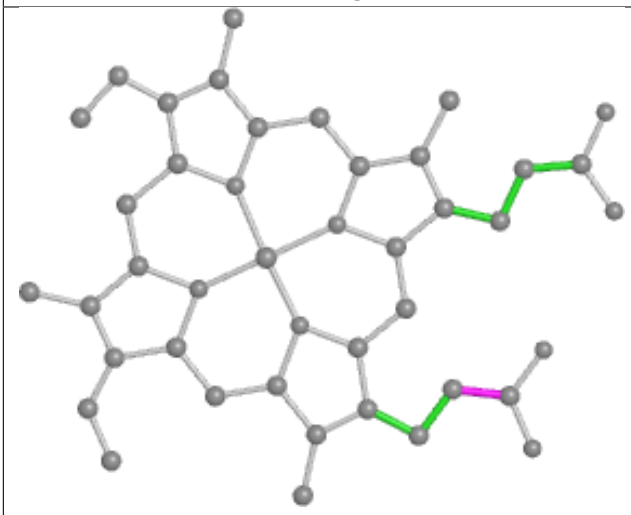
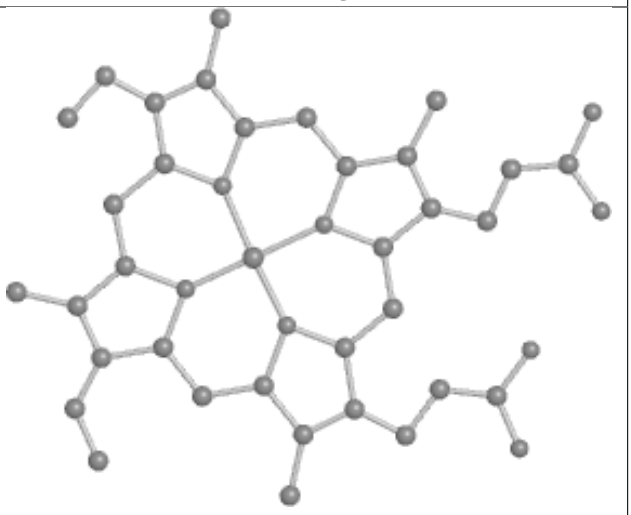


Bond angles

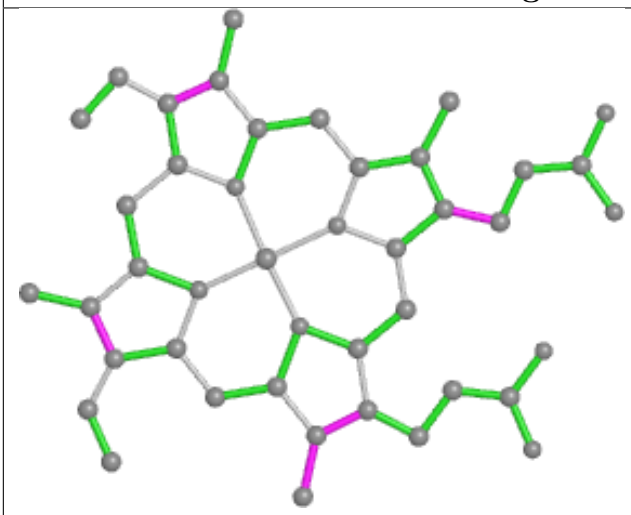


Torsions



Rings

Ligand HEC A 603



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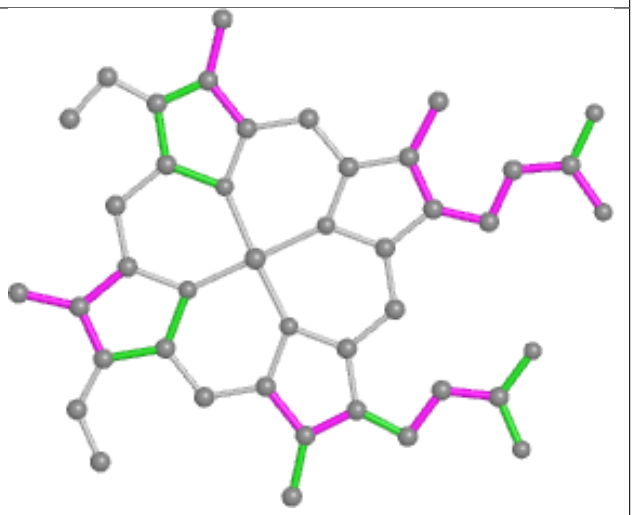
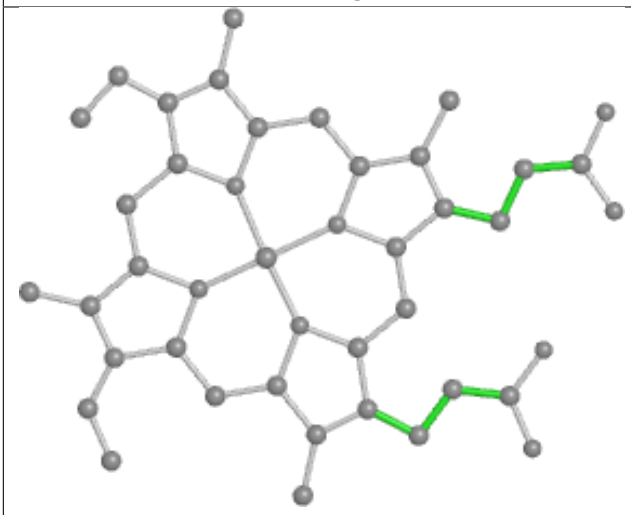
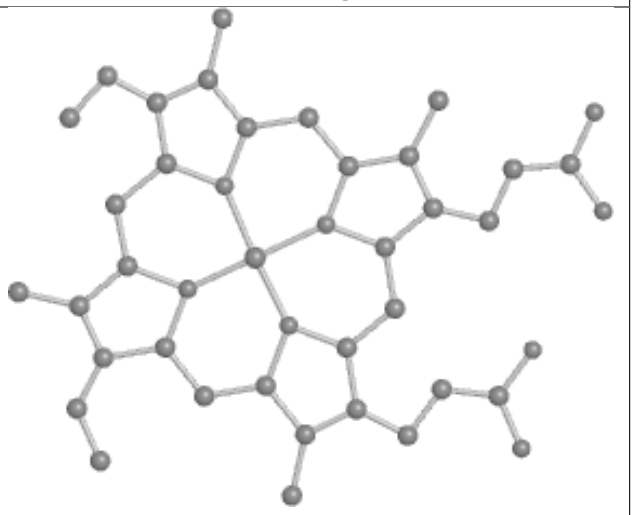


Bond angles

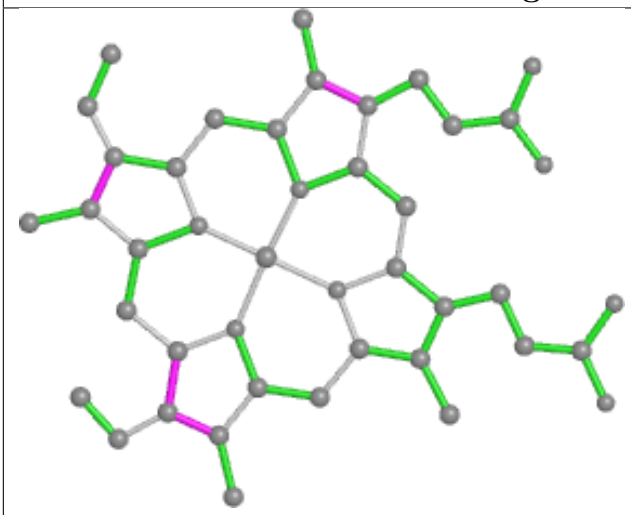


Torsions



Rings

Ligand HEC C 606



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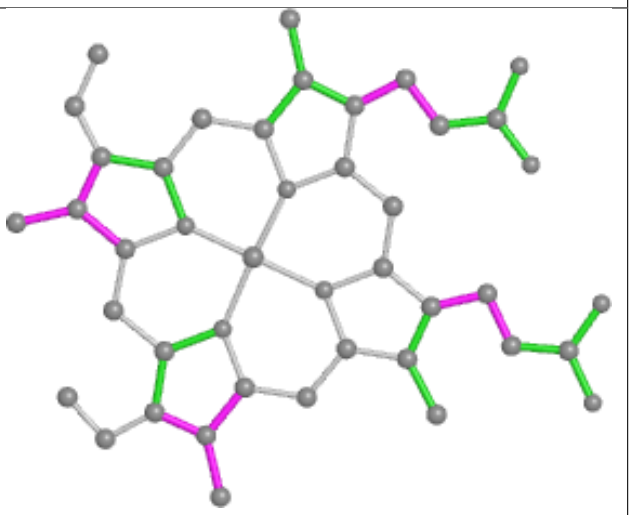
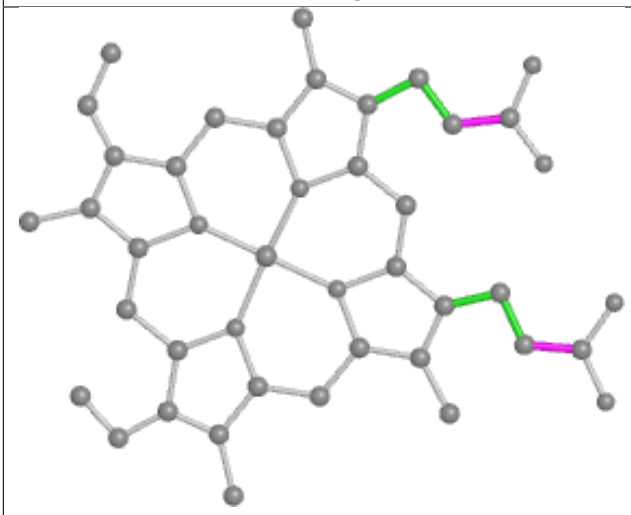
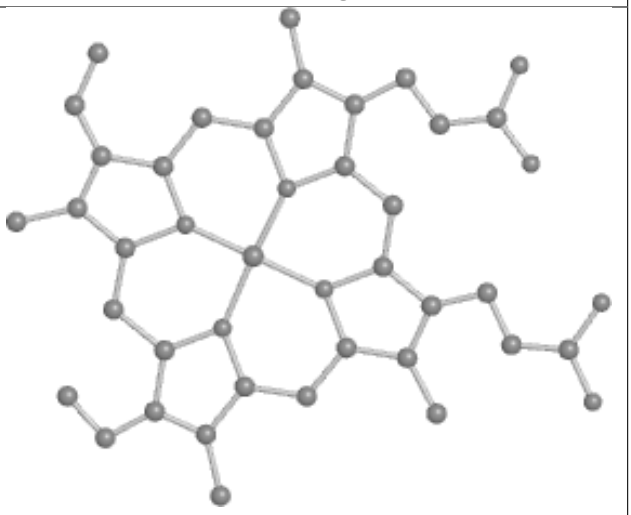


Bond angles

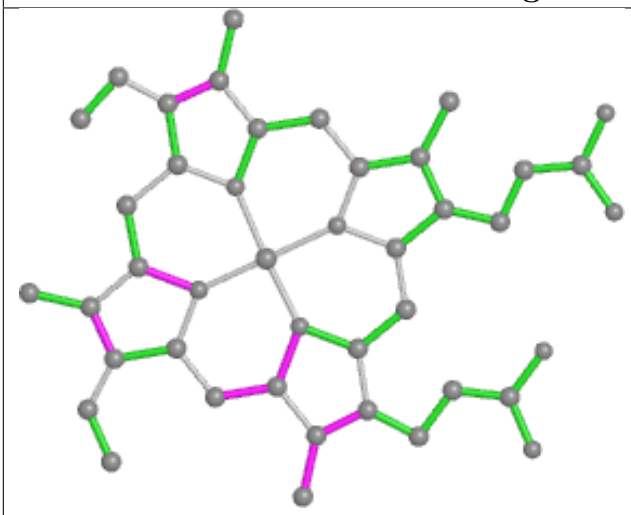


Torsions



Rings

Ligand HEC C 607



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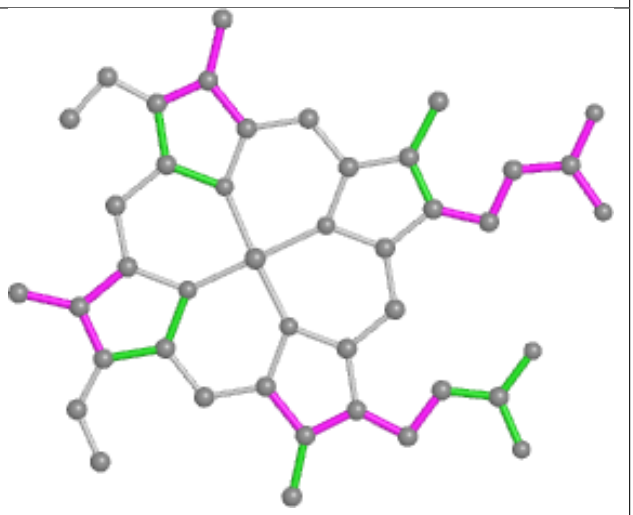

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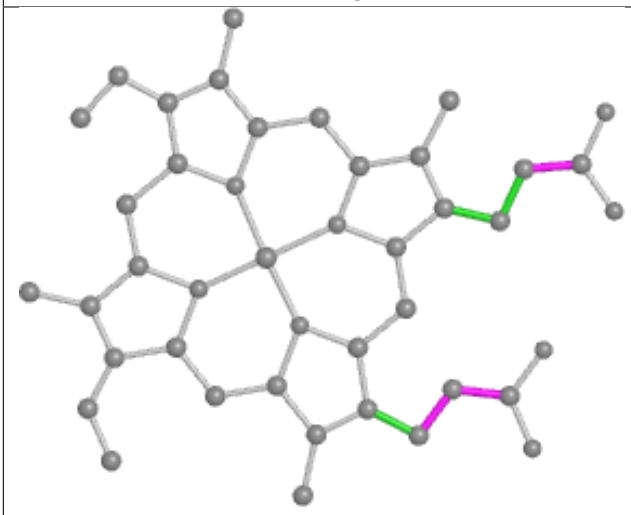

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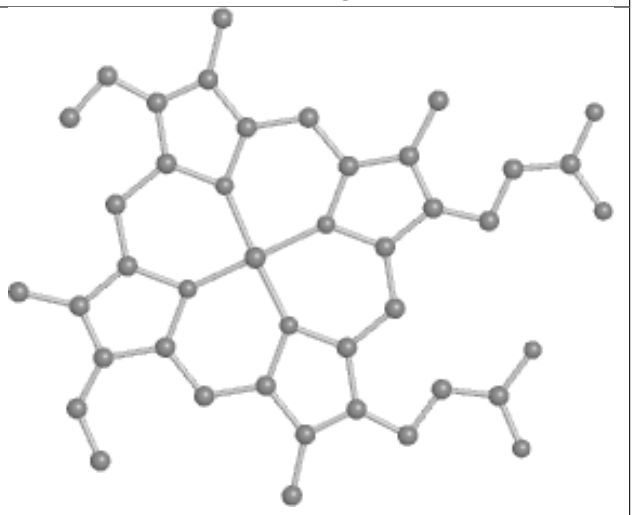
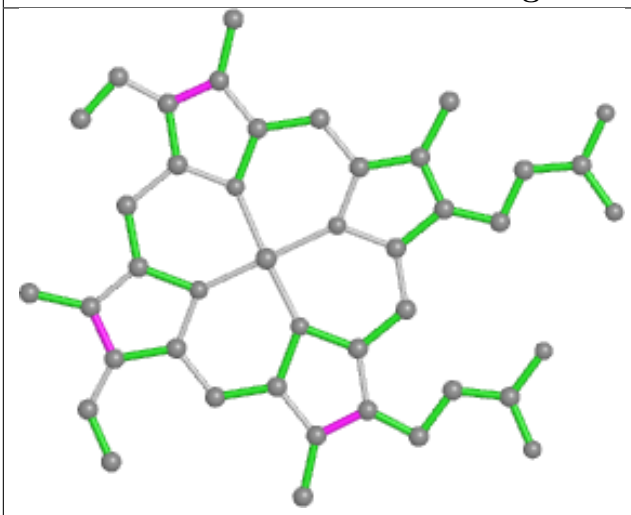


Rings

Ligand HEC A 604



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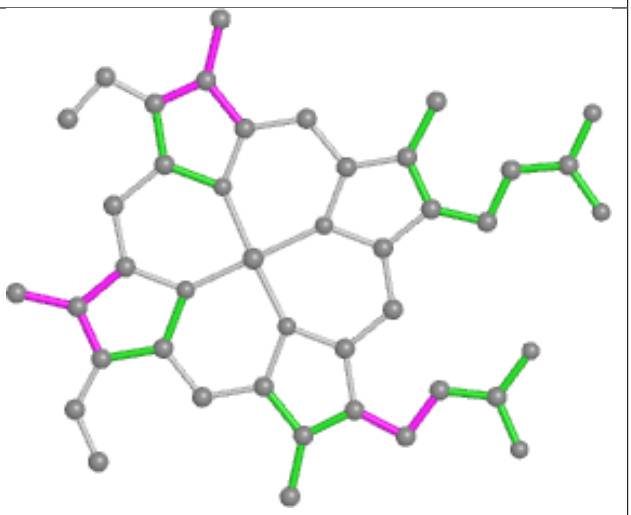
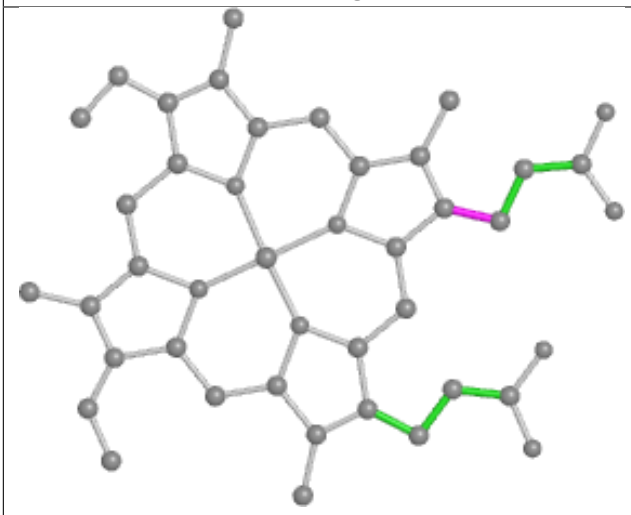


Bond angles



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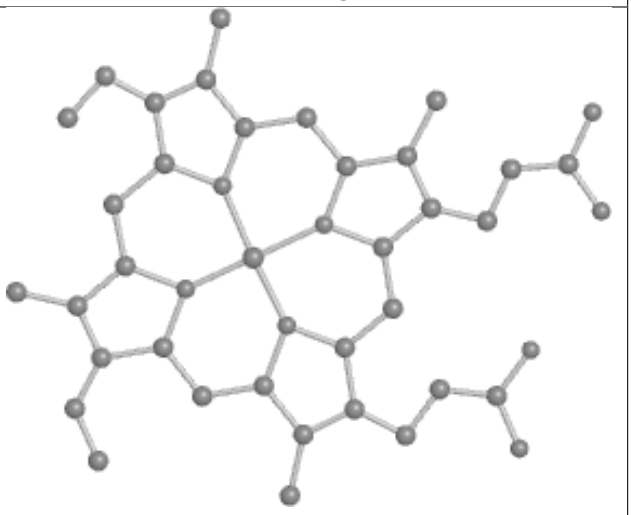
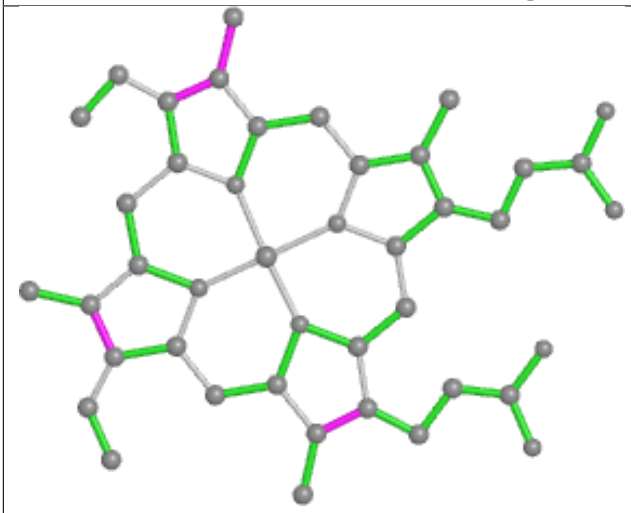


Rings

Ligand HEC K 606



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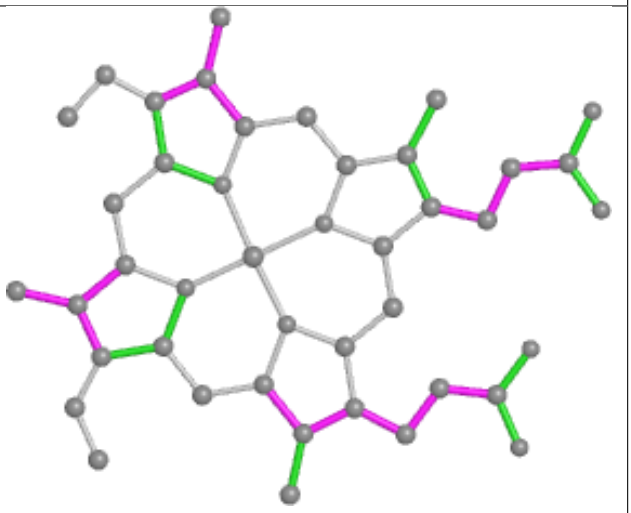
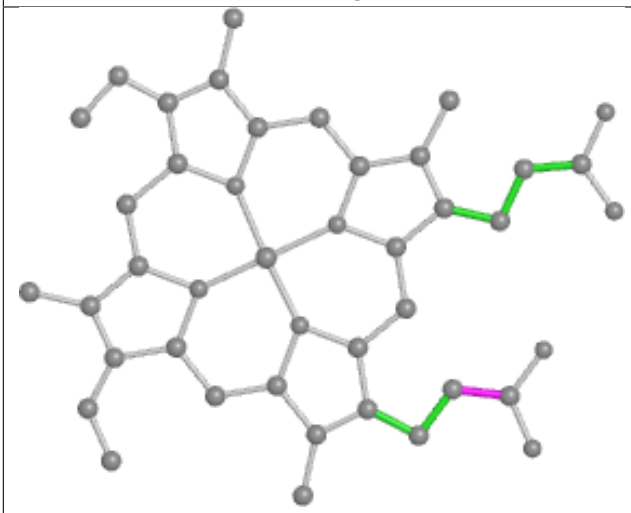
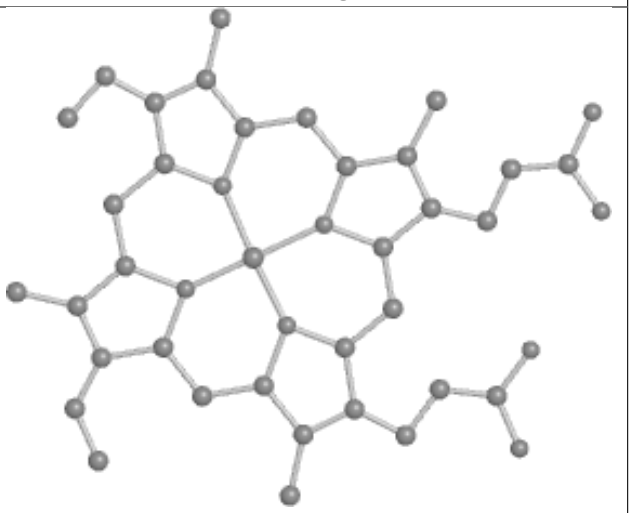


Bond angles

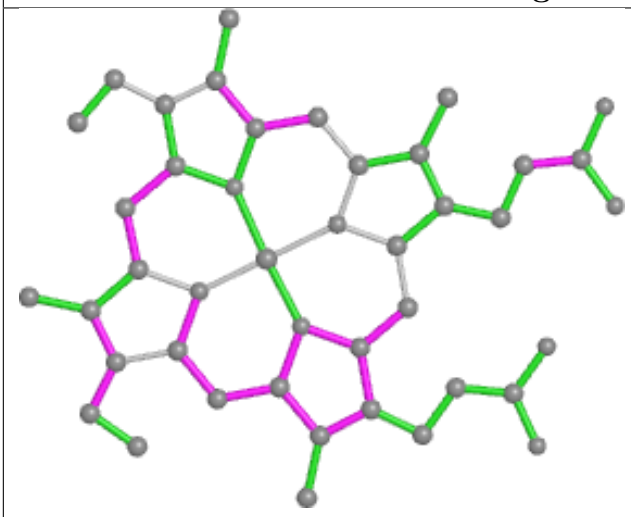


Torsions



Rings

Ligand ISW I 608



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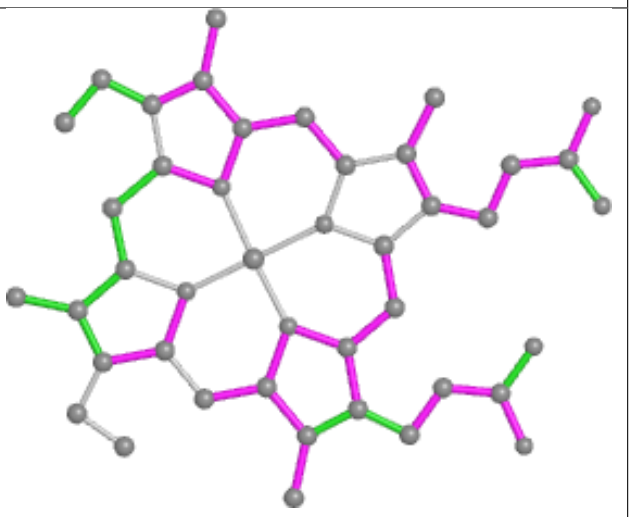
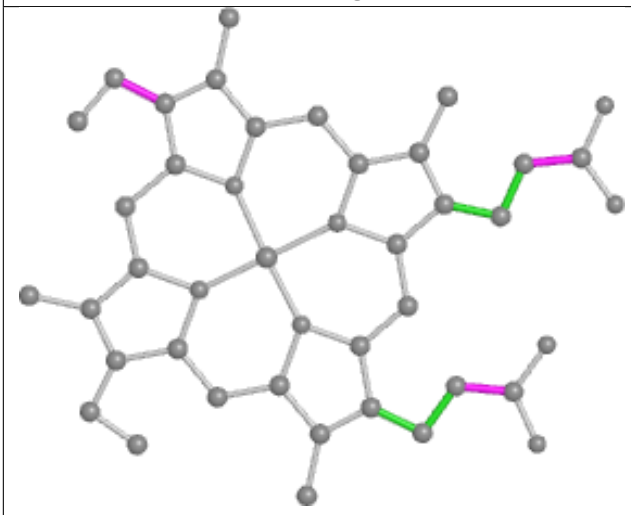
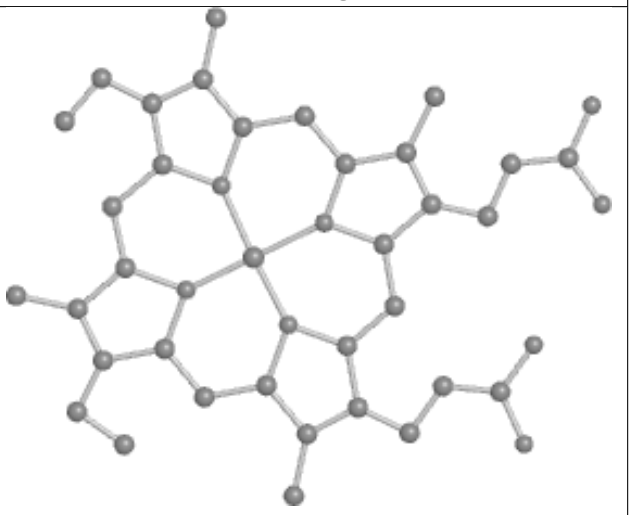


Bond angles

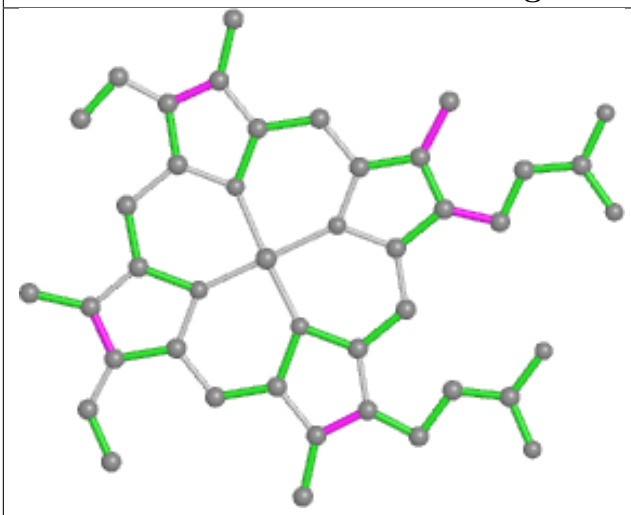


Torsions

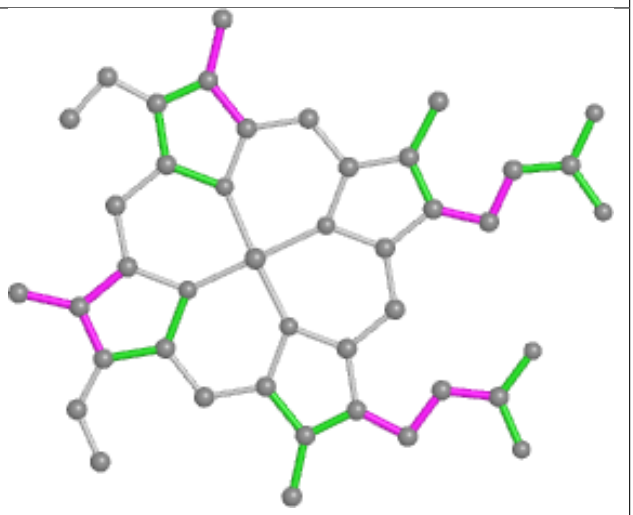


Rings

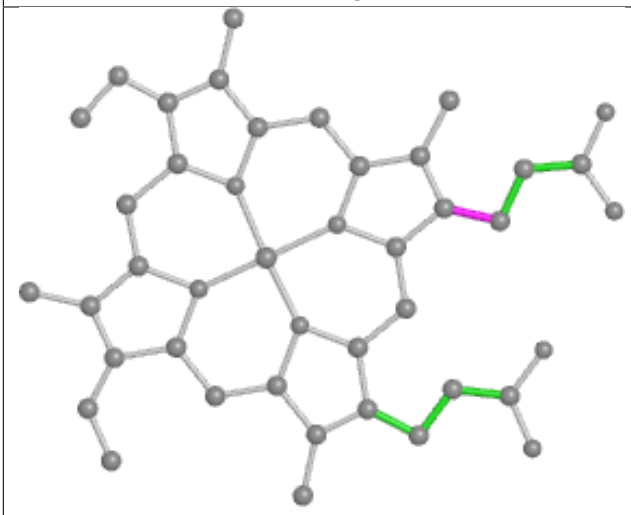
Ligand HEC E 604



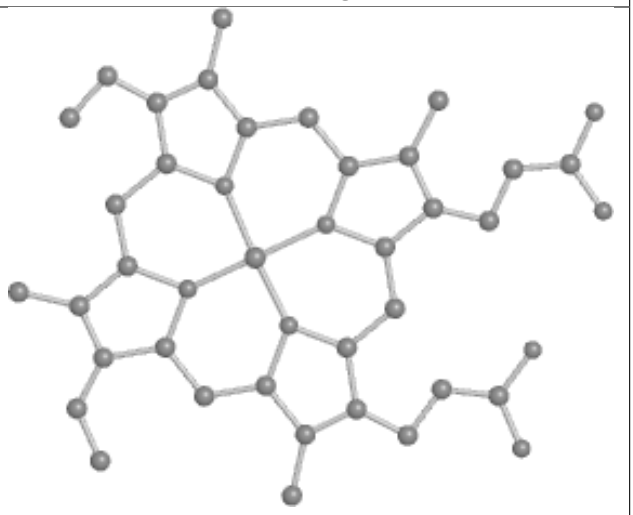
Bond lengths



Bond angles

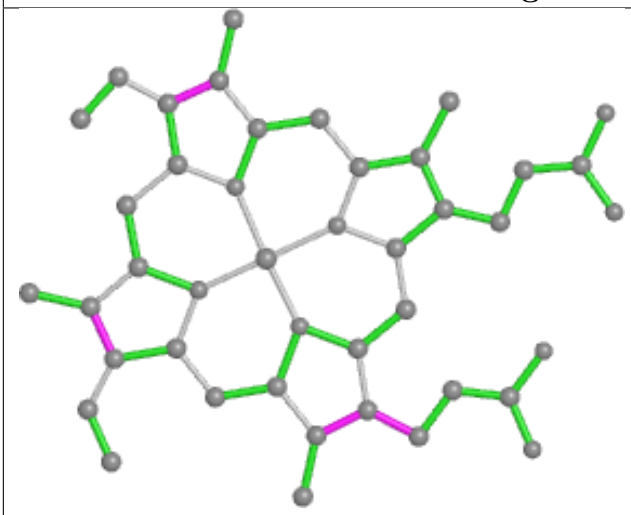


Torsions



Rings

Ligand HEC G 602



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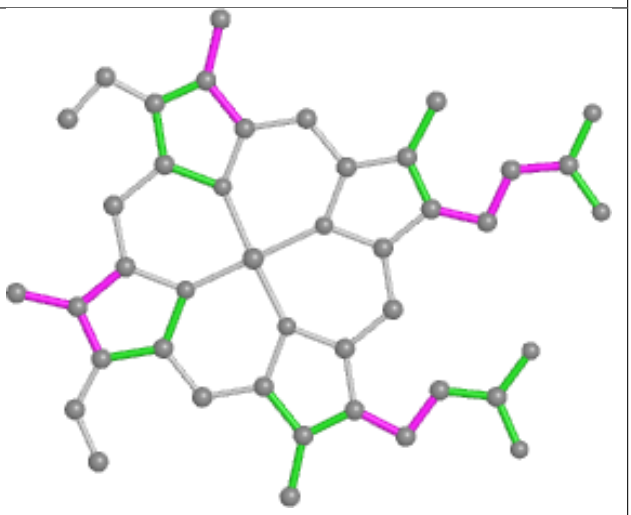
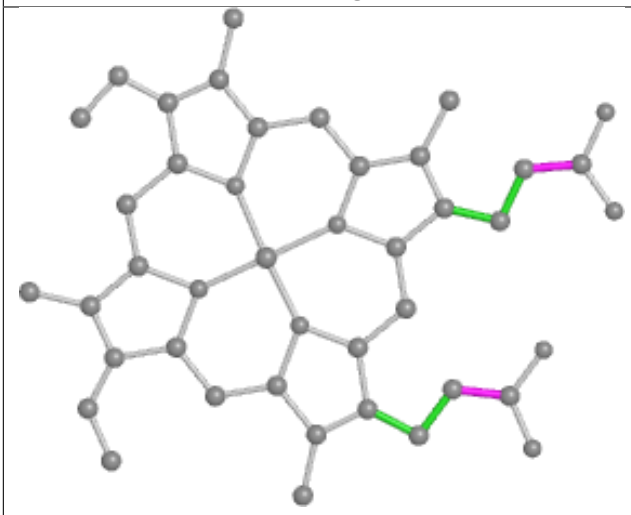
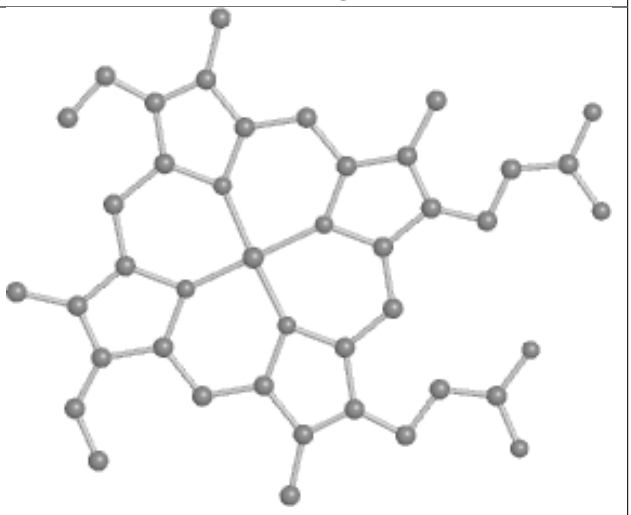


Bond angles

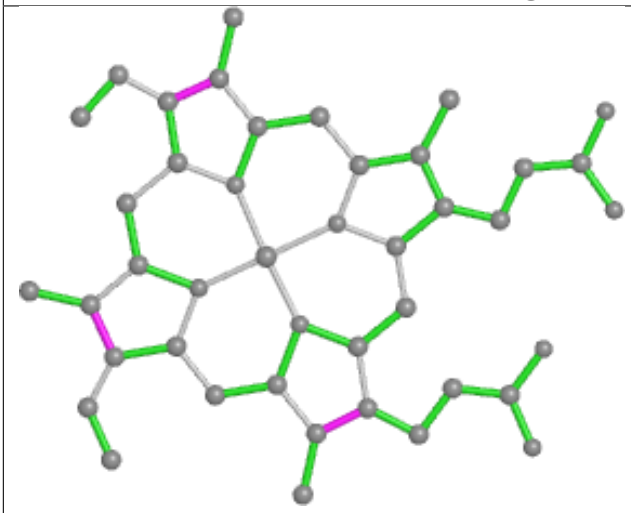


Torsions



Rings

Ligand HEC A 607



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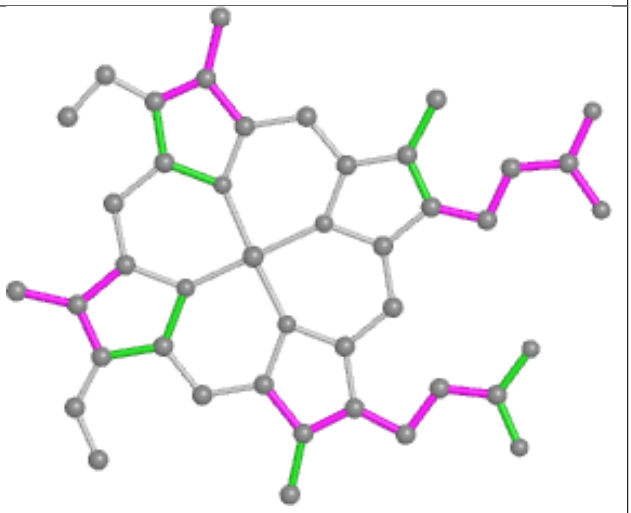
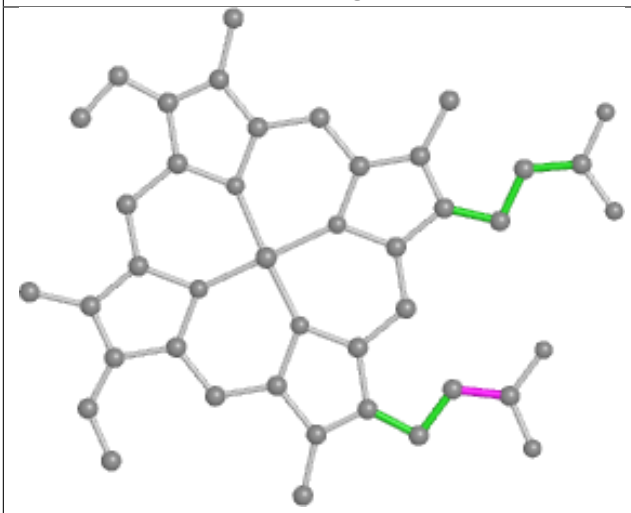
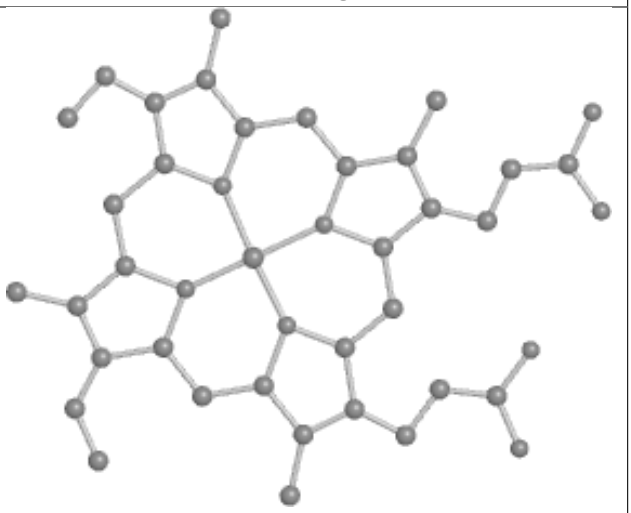


Bond angles

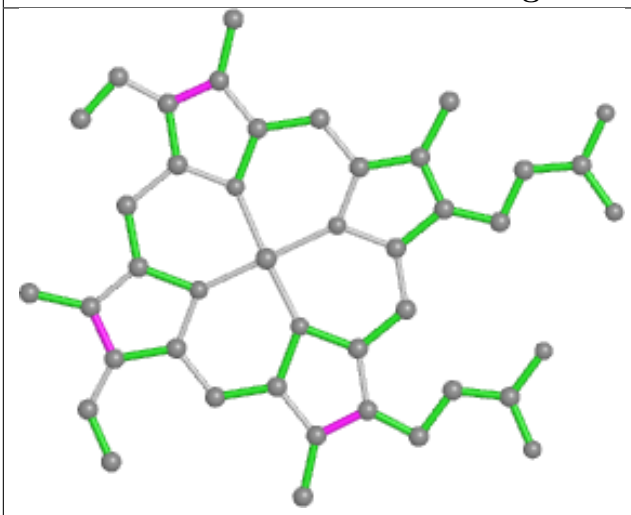


Torsions



Rings

Ligand HEC A 605



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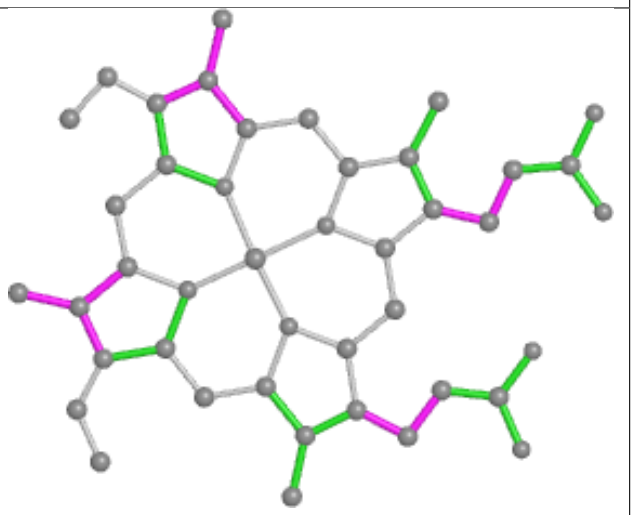
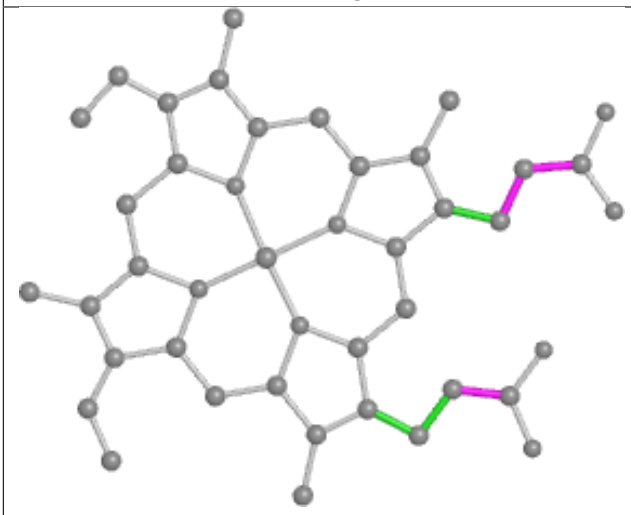
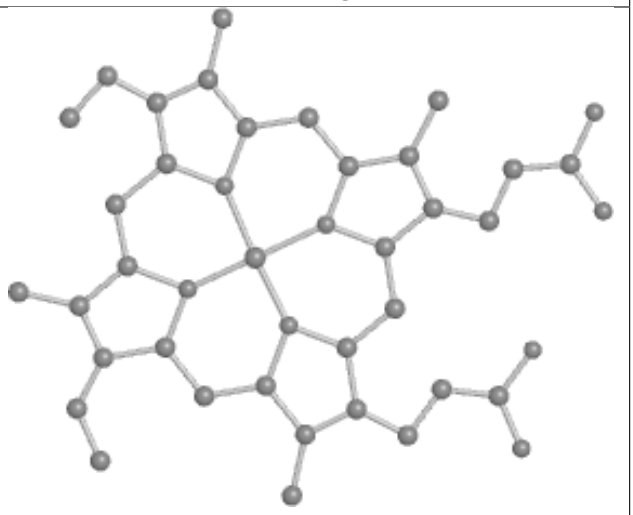


Bond angles

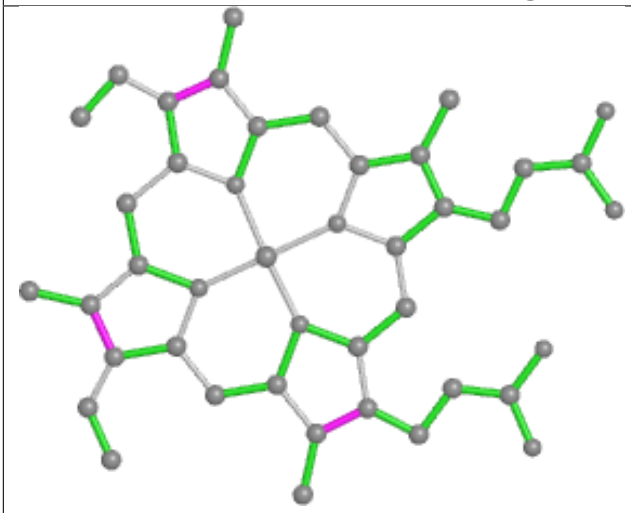


Torsions

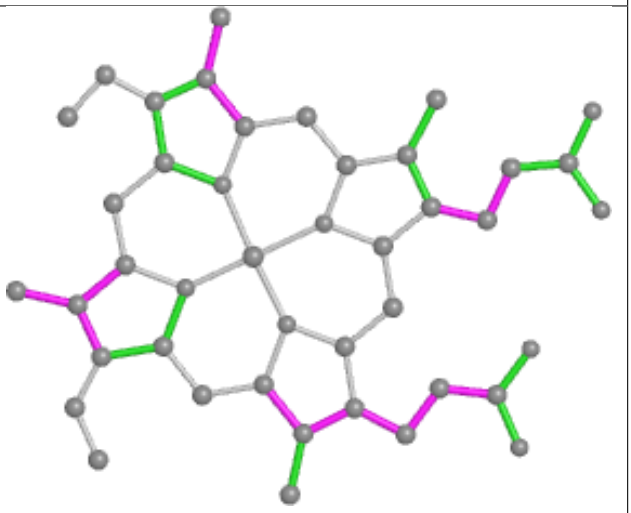


Rings

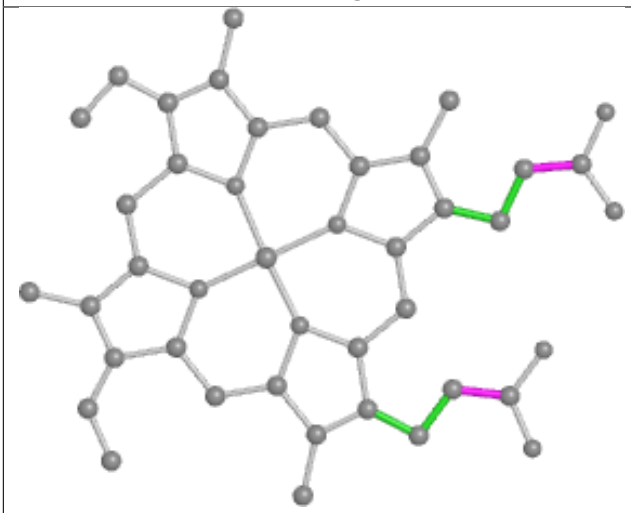
Ligand HEC G 606



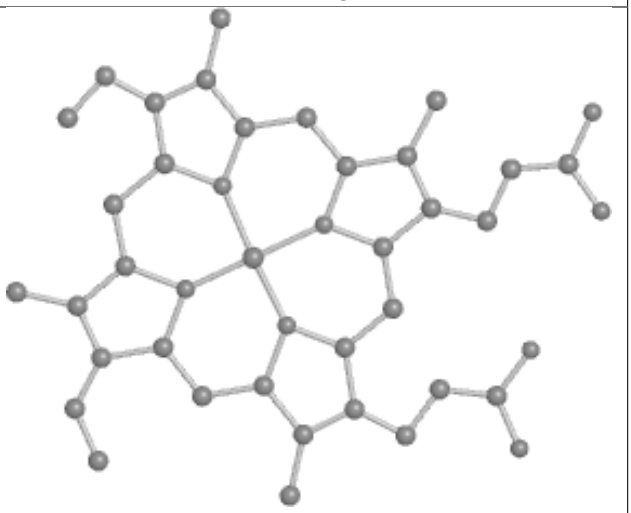
Bond lengths



Bond angles

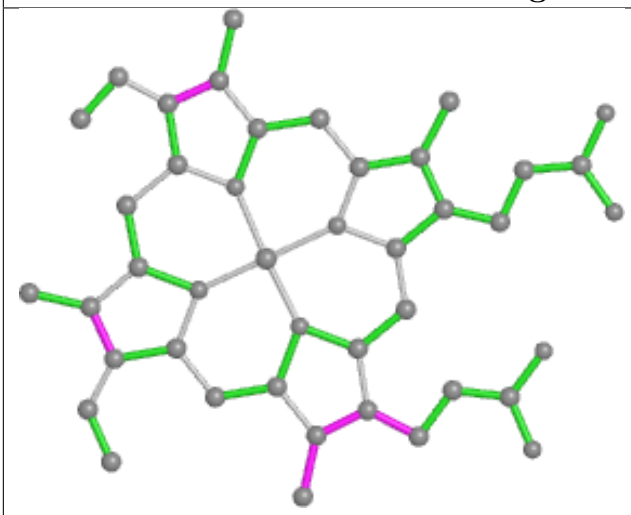


Torsions

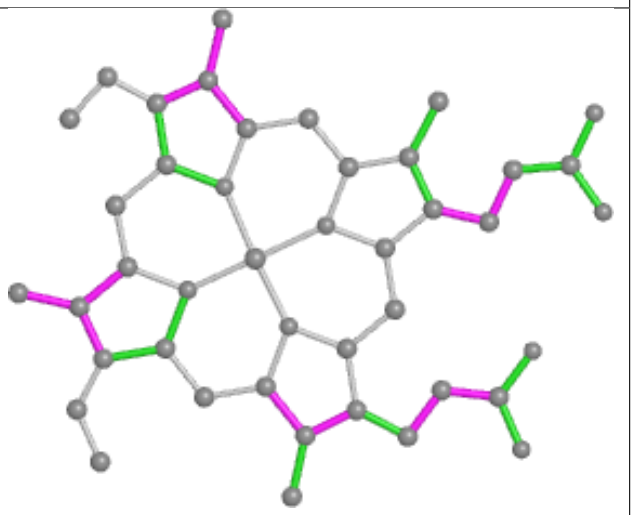


Rings

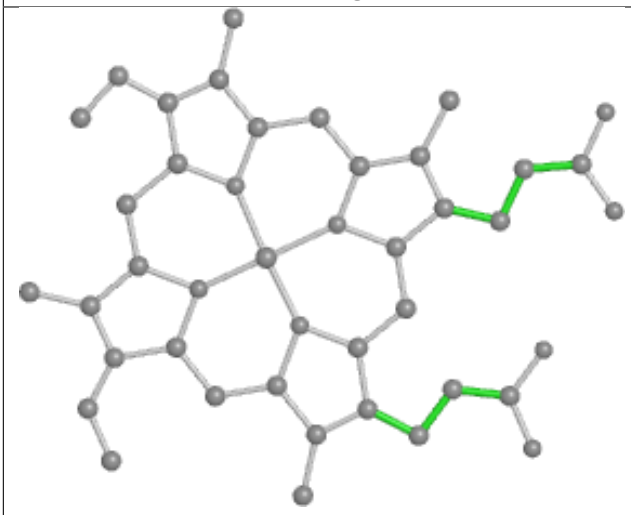
Ligand HEC I 603



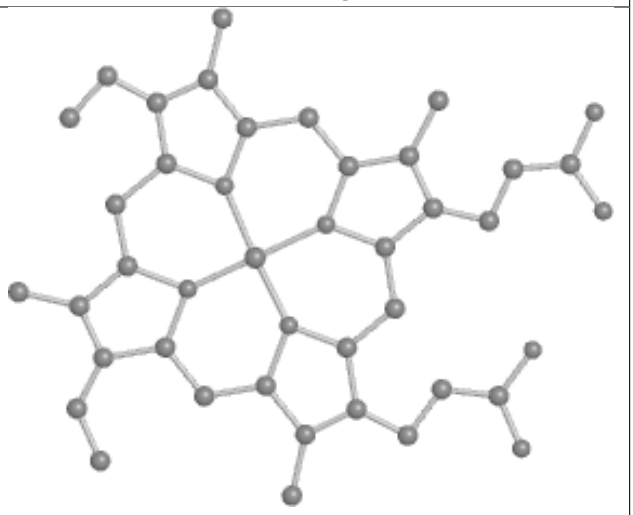
Bond lengths



Bond angles

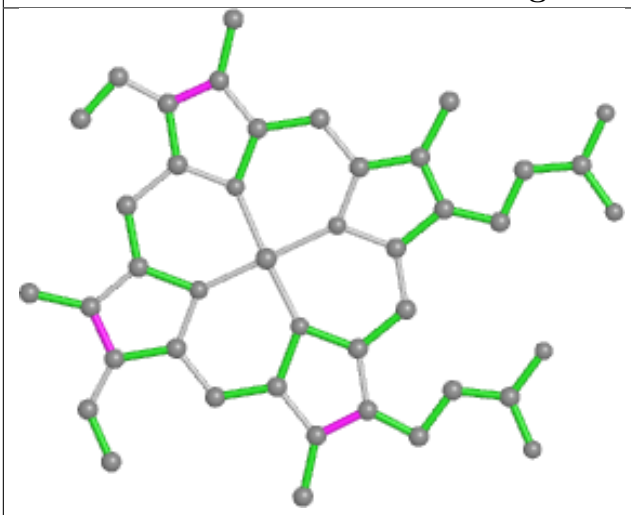


Torsions

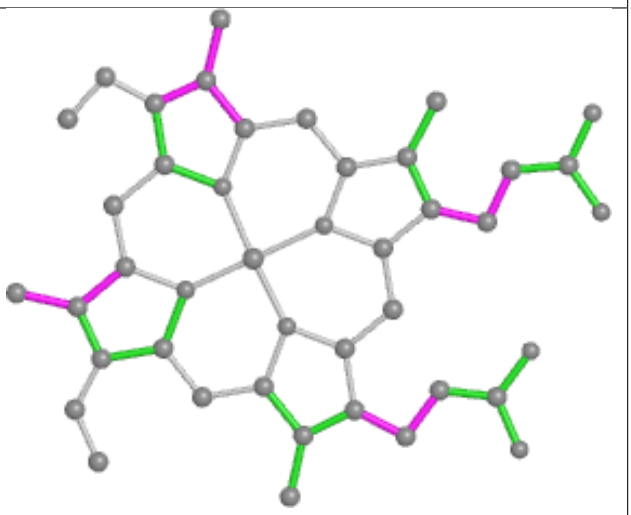


Rings

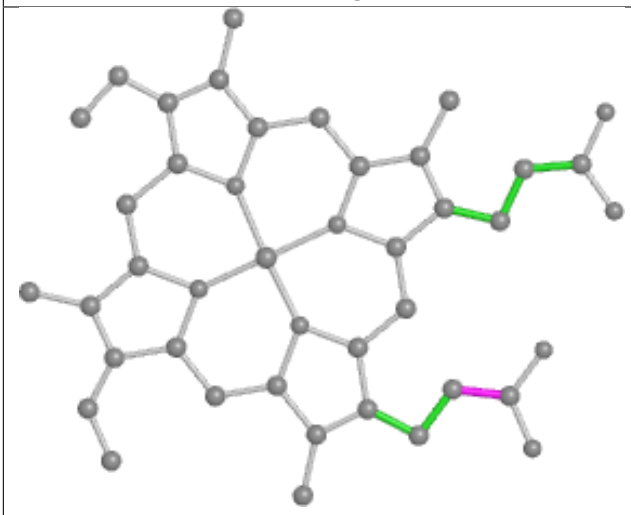
Ligand HEC I 606



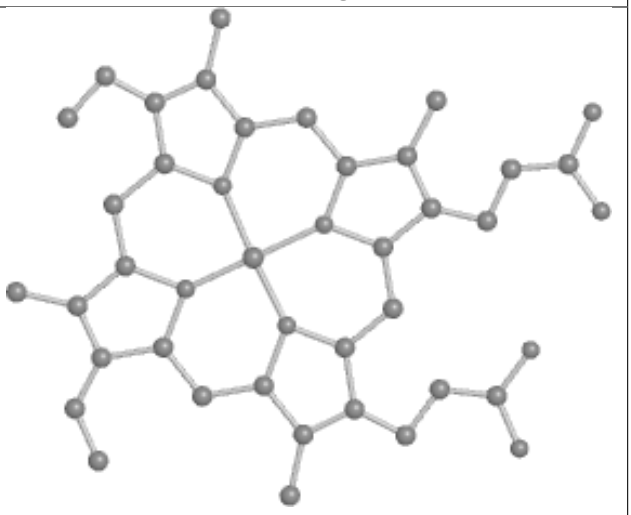
Bond lengths



Bond angles

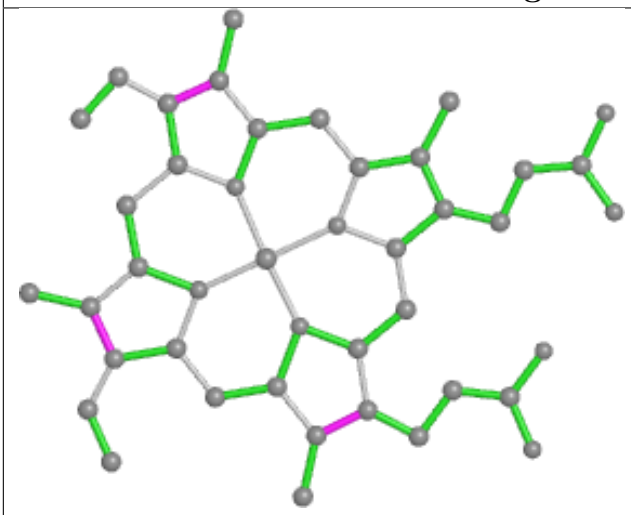


Torsions

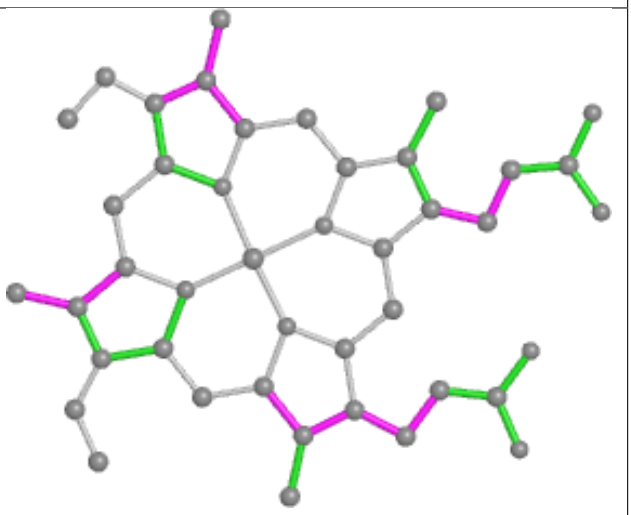


Rings

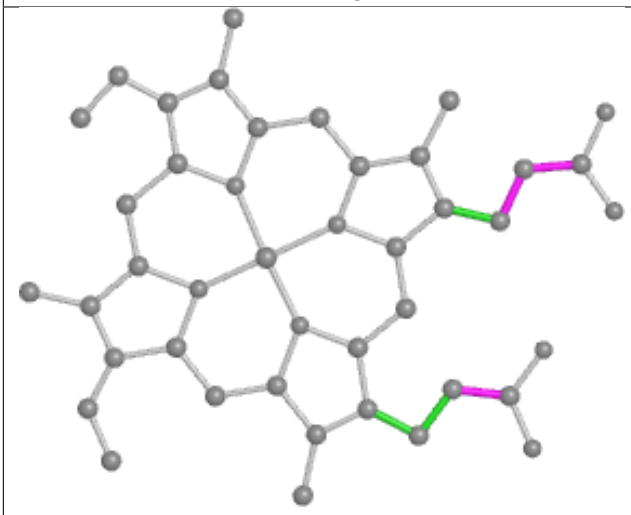
Ligand HEC E 605



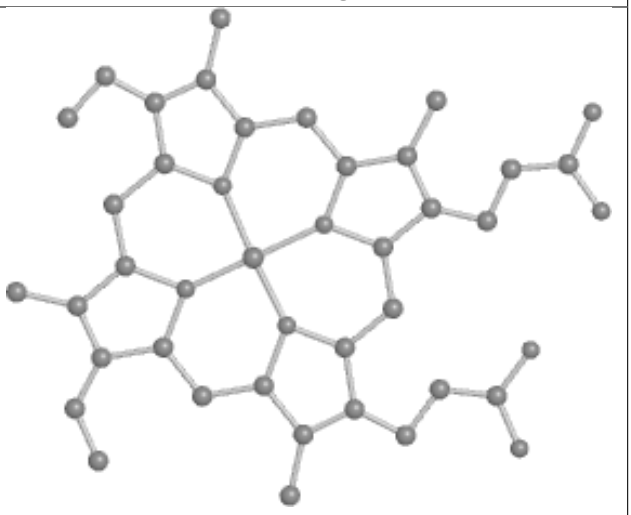
Bond lengths



Bond angles

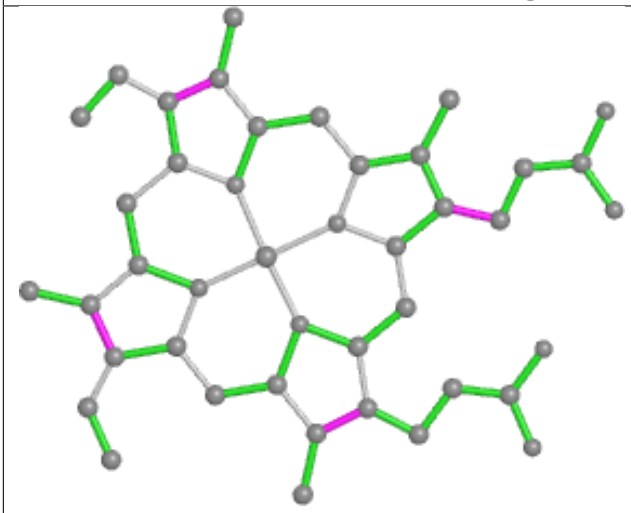


Torsions

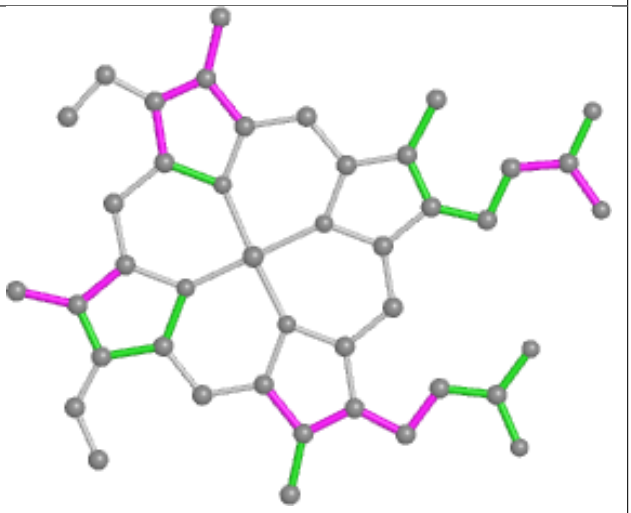


Rings

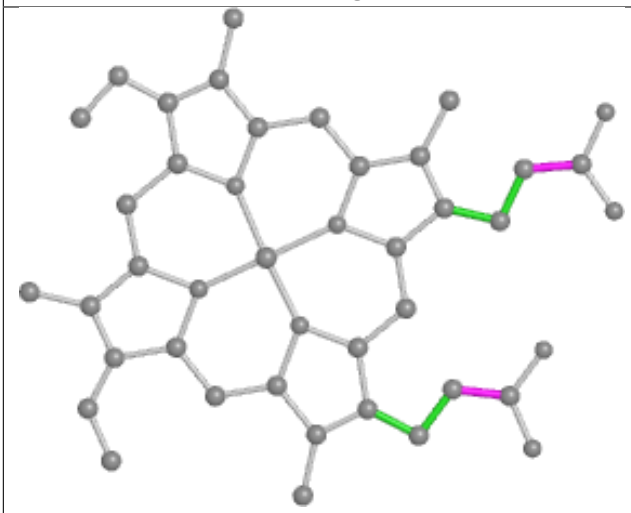
Ligand HEC G 601



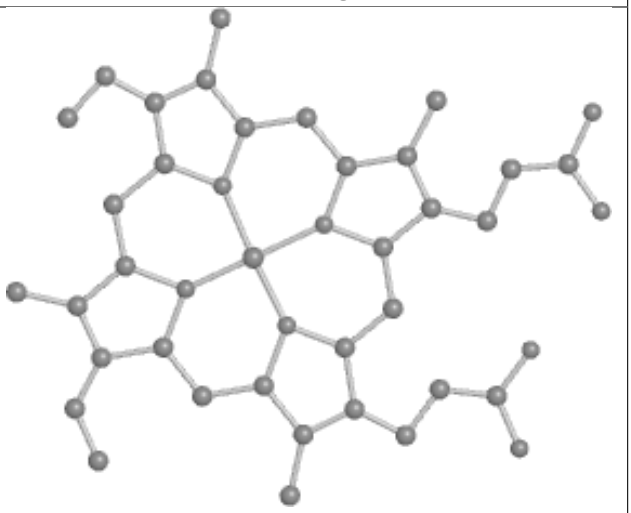
Bond lengths



Bond angles

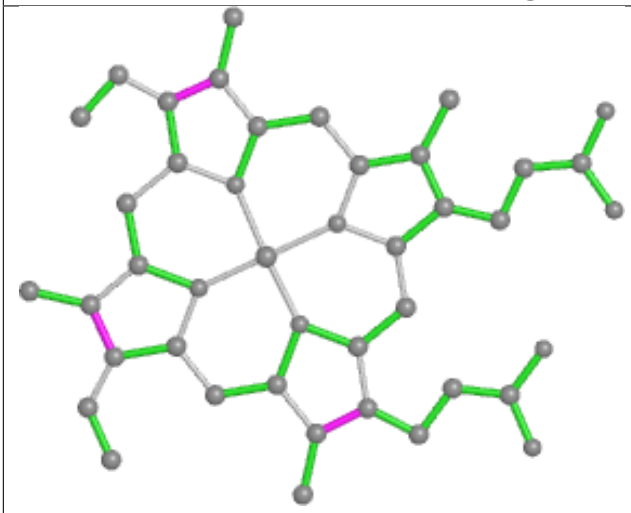


Torsions

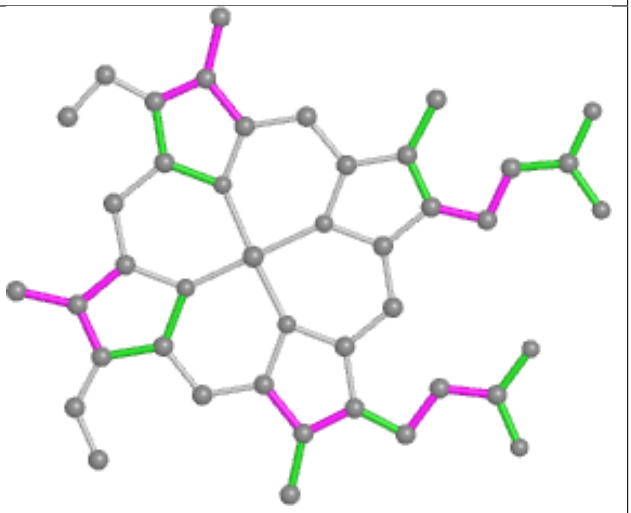


Rings

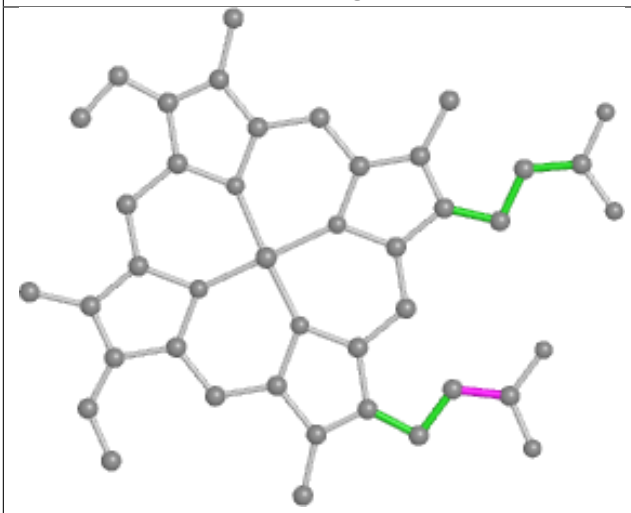
Ligand HEC G 603



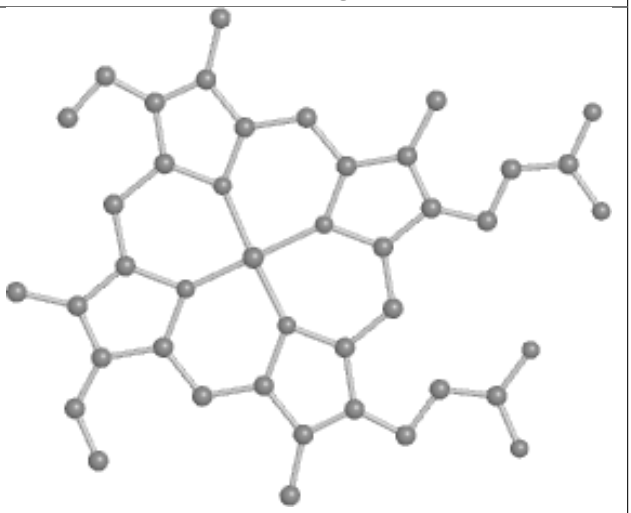
Bond lengths



Bond angles

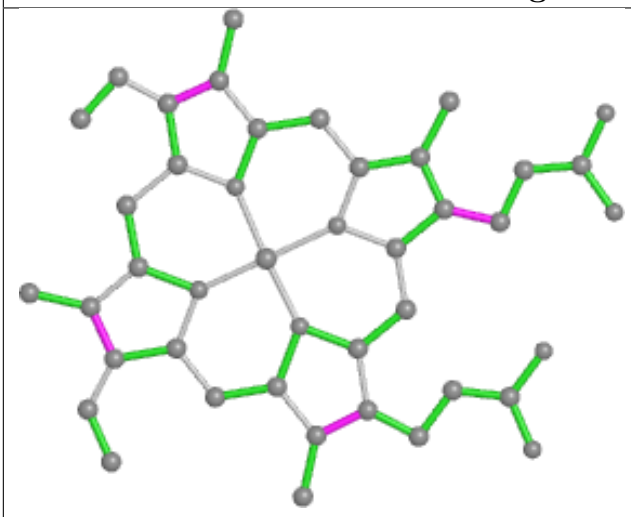


Torsions

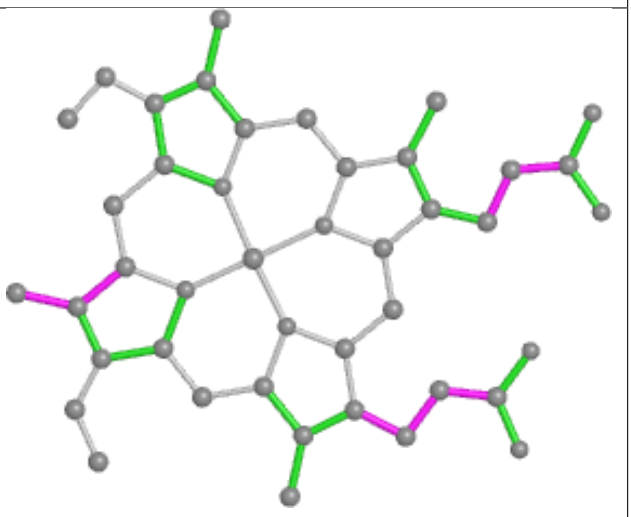


Rings

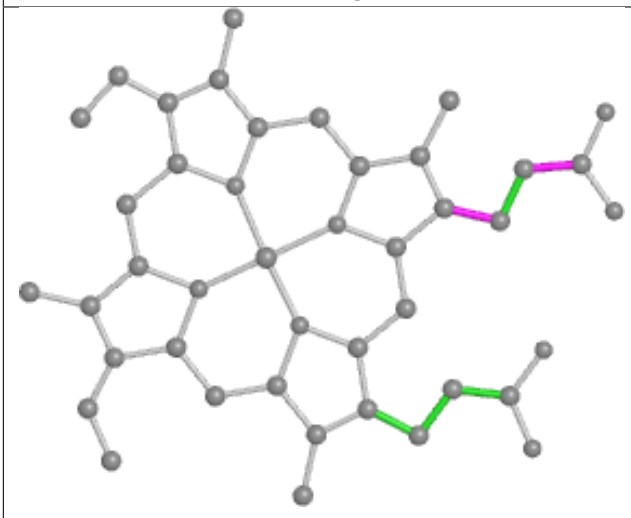
Ligand HEC I 604



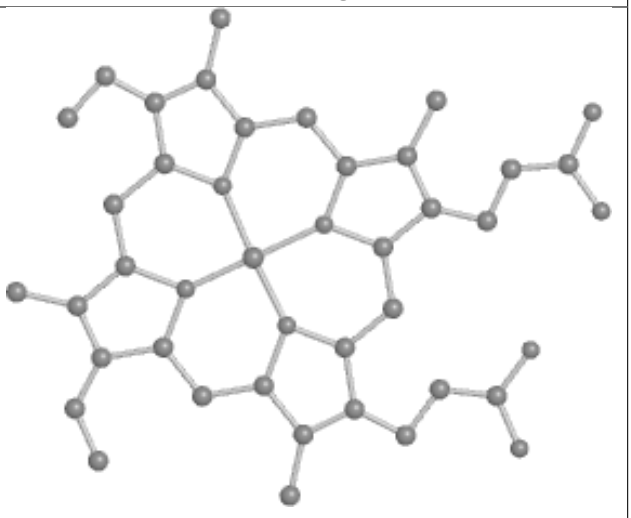
Bond lengths



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	504/570 (88%)	0.02	19 (3%)	40	39	19, 27, 46, 69	0
1	C	504/570 (88%)	-0.02	16 (3%)	47	46	18, 29, 46, 82	0
1	E	504/570 (88%)	-0.02	9 (1%)	68	66	19, 27, 46, 76	0
1	G	504/570 (88%)	0.02	17 (3%)	45	44	20, 30, 52, 81	0
1	I	504/570 (88%)	0.09	21 (4%)	36	35	19, 32, 53, 90	0
1	K	504/570 (88%)	0.01	12 (2%)	59	57	21, 30, 50, 87	0
2	B	64/91 (70%)	1.05	14 (21%)	0	0	23, 43, 77, 85	0
2	D	64/91 (70%)	0.54	13 (20%)	1	0	25, 34, 69, 85	0
2	F	64/91 (70%)	1.54	21 (32%)	0	0	26, 45, 70, 87	0
2	H	64/91 (70%)	1.23	21 (32%)	0	0	25, 44, 73, 80	0
2	J	64/91 (70%)	0.40	9 (14%)	2	2	26, 37, 69, 90	0
2	L	64/91 (70%)	1.80	31 (48%)	0	0	30, 50, 81, 91	0
All	All	3408/3966 (85%)	0.14	203 (5%)	21	20	18, 30, 56, 91	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	87	TRP	6.1
2	J	85	ASP	5.9
2	L	85	ASP	5.5
2	B	91	TYR	5.5
2	L	91	TYR	5.4
2	H	86	ALA	5.3
2	L	86	ALA	5.2
2	D	85	ASP	5.2
2	L	81	GLU	5.0
2	F	81	GLU	4.8
2	B	85	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	87	TRP	4.7
2	B	86	ALA	4.7
2	B	83	SER	4.7
2	F	91	TYR	4.6
2	H	91	TYR	4.6
2	L	88	GLN	4.5
1	I	524	LYS	4.5
2	L	90	GLY	4.5
2	H	84	GLY	4.5
2	H	85	ASP	4.5
2	F	84	GLY	4.4
1	I	525	LEU	4.4
2	D	87	TRP	4.4
2	F	83	SER	4.3
2	F	88	GLN	4.3
2	F	86	ALA	4.3
2	B	88	GLN	4.3
2	D	84	GLY	4.2
2	H	28	SER	4.2
1	I	528	LYS	4.1
1	I	519	GLN	4.0
1	C	527	GLY	4.0
1	I	290	VAL	4.0
2	L	83	SER	3.9
1	G	525	LEU	3.9
2	J	82	GLN	3.9
2	L	72	ILE	3.8
2	H	88	GLN	3.8
2	D	88	GLN	3.8
2	L	28	SER	3.7
2	B	28	SER	3.7
2	L	84	GLY	3.7
2	B	90	GLY	3.7
1	G	520	ALA	3.7
2	D	28	SER	3.7
2	D	86	ALA	3.6
1	I	520	ALA	3.6
1	I	522	VAL	3.6
2	D	91	TYR	3.6
2	F	46	ASP	3.6
1	I	517	ALA	3.5
2	F	78	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	527	GLY	3.5
1	C	522	VAL	3.5
2	F	74	ALA	3.5
1	G	526	GLU	3.5
1	C	518	LEU	3.4
2	F	87	TRP	3.4
2	F	28	SER	3.4
1	G	528	LYS	3.4
1	C	517	ALA	3.4
1	K	527	GLY	3.4
1	I	518	LEU	3.3
2	L	77	GLN	3.3
1	C	520	ALA	3.3
2	F	85	ASP	3.3
2	H	77	GLN	3.3
1	K	290	VAL	3.2
2	J	88	GLN	3.2
1	A	520	ALA	3.2
1	I	527	GLY	3.2
2	F	77	GLN	3.2
2	F	82	GLN	3.2
2	L	46	ASP	3.2
2	L	75	LEU	3.2
2	L	78	LYS	3.2
2	L	50	THR	3.2
2	L	52	VAL	3.2
1	C	519	GLN	3.1
2	J	91	TYR	3.1
2	F	69	CYS	3.1
1	C	528	LYS	3.1
1	G	524	LYS	3.1
2	H	90	GLY	3.1
2	H	83	SER	3.0
1	A	492	THR	3.0
2	H	82	GLN	3.0
2	J	87	TRP	3.0
2	B	81	GLU	3.0
2	D	82	GLN	2.9
2	L	82	GLN	2.9
2	L	87	TRP	2.9
1	A	290	VAL	2.9
2	B	82	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	525	LEU	2.9
2	B	84	GLY	2.9
1	G	491	TYR	2.9
1	I	523	ASN	2.9
1	K	492	THR	2.9
2	H	46	ASP	2.9
2	B	75	LEU	2.8
1	G	492	THR	2.8
2	J	81	GLU	2.8
1	I	516	SER	2.8
1	I	492	THR	2.8
1	E	290	VAL	2.8
2	D	81	GLU	2.7
1	A	491	TYR	2.7
1	E	492	THR	2.7
1	K	132	LEU	2.7
2	H	75	LEU	2.7
1	C	523	ASN	2.7
2	L	69	CYS	2.7
1	G	523	ASN	2.7
2	L	89	GLY	2.7
1	G	487	GLY	2.6
1	A	297	ALA	2.6
1	G	519	GLN	2.6
2	H	81	GLU	2.6
2	B	78	LYS	2.6
1	C	492	THR	2.6
1	I	521	ARG	2.6
2	F	76	VAL	2.6
2	B	89	GLY	2.5
1	C	525	LEU	2.5
1	C	524	LYS	2.5
1	I	297	ALA	2.5
1	G	489	TRP	2.5
2	J	83	SER	2.5
1	A	497	PRO	2.5
2	L	49	PRO	2.5
1	I	289	GLY	2.5
1	G	497	PRO	2.5
1	K	497	PRO	2.5
1	E	299	THR	2.5
1	K	127	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	79	ALA	2.4
2	F	53	VAL	2.4
2	H	89	GLY	2.4
1	E	289	GLY	2.4
2	J	90	GLY	2.4
1	A	295	TRP	2.4
1	A	525	LEU	2.4
1	A	288	SER	2.4
2	F	72	ILE	2.4
1	A	484	VAL	2.4
1	K	528	LYS	2.4
1	K	519	GLN	2.4
2	H	72	ILE	2.4
2	H	73	VAL	2.4
1	G	488	GLY	2.3
2	D	90	GLY	2.3
2	L	51	ASP	2.3
1	A	289	GLY	2.3
1	I	295	TRP	2.3
1	C	290	VAL	2.3
1	E	300	MET	2.3
2	J	86	ALA	2.3
2	L	73	VAL	2.3
2	F	50	THR	2.3
1	C	521	ARG	2.3
1	C	297	ALA	2.2
1	C	479	VAL	2.2
2	F	71	ASP	2.2
1	E	474	LEU	2.2
1	A	479	VAL	2.2
2	F	90	GLY	2.2
1	E	295	TRP	2.2
1	I	515	LEU	2.2
1	A	524	LYS	2.2
2	H	78	LYS	2.2
2	L	74	ALA	2.2
1	K	288	SER	2.1
1	A	523	ASN	2.1
2	H	79	ALA	2.1
1	E	497	PRO	2.1
2	L	48	LYS	2.1
1	A	486	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	65	VAL	2.1
2	D	89	GLY	2.1
1	A	299	THR	2.1
2	L	29	SER	2.1
1	A	487	GLY	2.1
1	A	494	GLY	2.1
1	K	488	GLY	2.1
1	I	479	VAL	2.1
2	H	67	VAL	2.1
1	G	517	ALA	2.1
1	A	488	GLY	2.1
1	C	295	TRP	2.1
1	G	293	ASN	2.1
2	D	79	ALA	2.1
2	L	45	LYS	2.1
2	L	71	ASP	2.0
1	K	522	VAL	2.0
1	G	486	PRO	2.0
1	I	299	THR	2.0
1	I	513	GLN	2.0
2	L	41	TYR	2.0
1	E	479	VAL	2.0
2	H	49	PRO	2.0
2	D	83	SER	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	J	101	7/7	0.80	0.19	58,59,61,61	0
6	PGE	E	608	10/10	0.80	0.16	60,62,65,66	0
7	PG4	C	611	13/13	0.80	0.21	60,64,67,67	0
6	PGE	G	612	10/10	0.81	0.21	49,52,56,58	0
5	PEG	K	608	7/7	0.82	0.29	49,51,54,55	0
7	PG4	A	612	13/13	0.84	0.21	50,56,60,60	0
7	PG4	K	610	13/13	0.85	0.18	48,55,61,63	0
6	PGE	A	611	10/10	0.86	0.17	46,50,61,63	0
5	PEG	K	609	7/7	0.86	0.14	49,51,55,56	0
7	PG4	E	610	13/13	0.87	0.16	61,63,64,65	0
6	PGE	I	610	10/10	0.87	0.20	49,53,55,55	0
6	PGE	E	609	10/10	0.90	0.22	52,52,55,56	0
5	PEG	G	610	7/7	0.90	0.12	50,51,52,53	0
6	PGE	I	609	10/10	0.90	0.21	56,58,60,60	0
5	PEG	C	609	7/7	0.90	0.14	42,44,52,54	0
6	PGE	C	610	10/10	0.93	0.19	53,55,57,57	0
5	PEG	A	610	7/7	0.93	0.10	43,46,50,51	0
6	PGE	G	611	10/10	0.94	0.17	52,53,55,55	0
4	ISW	A	608	43/43	0.95	0.14	16,25,36,39	0
4	ISW	A	609	43/43	0.95	0.15	16,25,34,37	0
4	ISW	G	608	43/43	0.95	0.12	21,27,36,38	0
4	ISW	C	608	43/43	0.96	0.12	14,27,37,38	0
4	ISW	G	609	43/43	0.96	0.14	19,28,35,37	0
4	ISW	I	608	43/43	0.96	0.13	20,28,40,41	0
3	HEC	K	605	43/43	0.98	0.12	14,21,25,27	0
3	HEC	K	606	43/43	0.98	0.10	17,22,34,37	0
3	HEC	K	607	43/43	0.98	0.10	16,21,35,36	0
3	HEC	A	602	43/43	0.98	0.09	18,22,28,35	0
3	HEC	A	603	43/43	0.98	0.09	19,27,31,33	0
3	HEC	A	605	43/43	0.98	0.15	15,19,22,24	0
3	HEC	A	606	43/43	0.98	0.12	14,20,28,32	0
3	HEC	C	603	43/43	0.98	0.09	22,26,29,36	0
3	HEC	C	605	43/43	0.98	0.12	16,21,23,25	0
3	HEC	C	607	43/43	0.98	0.12	14,17,28,33	0
3	HEC	E	602	43/43	0.98	0.09	17,23,28,30	0
3	HEC	E	605	43/43	0.98	0.12	15,20,22,23	0
3	HEC	E	607	43/43	0.98	0.10	16,21,32,37	0
3	HEC	G	603	43/43	0.98	0.08	22,28,34,38	0
3	HEC	G	604	43/43	0.98	0.09	19,24,28,30	0
3	HEC	G	605	43/43	0.98	0.12	16,20,25,27	0
3	HEC	G	606	43/43	0.98	0.11	17,23,33,36	0
3	HEC	G	607	43/43	0.98	0.12	16,22,31,36	0
3	HEC	I	601	43/43	0.98	0.10	19,25,31,33	0

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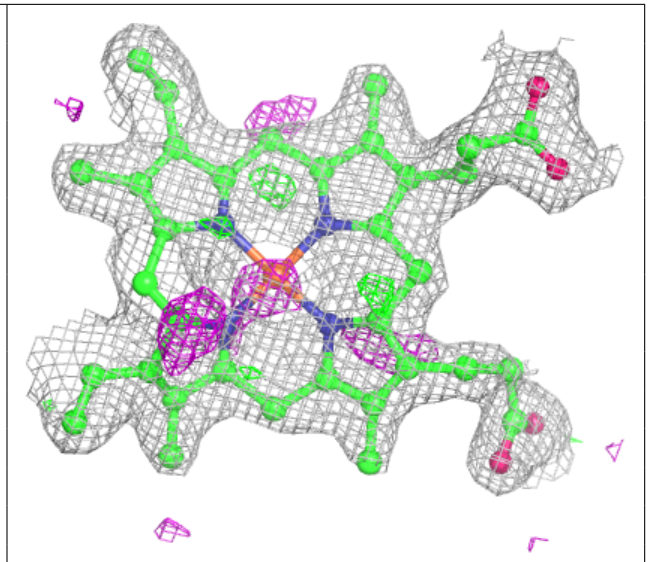
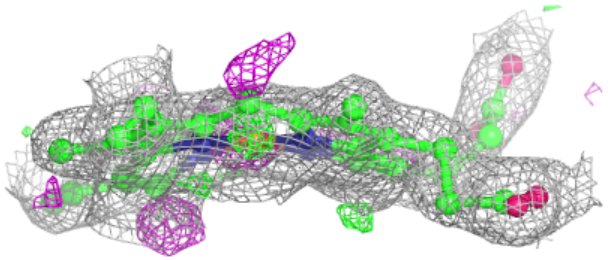
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	I	602	43/43	0.98	0.10	19,26,33,36	0
3	HEC	I	603	43/43	0.98	0.09	25,31,35,39	0
3	HEC	I	605	43/43	0.98	0.13	15,21,25,26	0
3	HEC	I	607	43/43	0.98	0.11	16,20,30,36	0
3	HEC	K	601	43/43	0.98	0.09	16,27,31,37	0
3	HEC	K	602	43/43	0.98	0.10	22,27,33,35	0
3	HEC	K	603	43/43	0.98	0.09	23,27,33,42	0
3	HEC	K	604	43/43	0.98	0.09	19,23,27,29	0
3	HEC	G	601	43/43	0.99	0.08	14,22,29,33	0
3	HEC	G	602	43/43	0.99	0.08	18,27,31,32	0
3	HEC	C	604	43/43	0.99	0.09	18,21,25,27	0
3	HEC	A	604	43/43	0.99	0.09	17,22,26,30	0
3	HEC	C	606	43/43	0.99	0.11	15,21,32,36	0
3	HEC	A	607	43/43	0.99	0.13	16,20,28,31	0
3	HEC	E	601	43/43	0.99	0.09	16,21,27,30	0
3	HEC	C	601	43/43	0.99	0.07	17,23,26,29	0
3	HEC	E	603	43/43	0.99	0.08	21,26,30,34	0
3	HEC	E	604	43/43	0.99	0.09	17,22,25,27	0
3	HEC	I	604	43/43	0.99	0.09	20,26,29,31	0
3	HEC	C	602	43/43	0.99	0.09	17,23,28,32	0
3	HEC	I	606	43/43	0.99	0.12	14,22,34,39	0
3	HEC	E	606	43/43	0.99	0.11	15,19,29,32	0
3	HEC	A	601	43/43	0.99	0.09	14,21,28,29	0

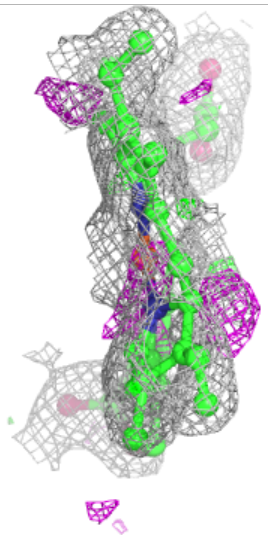
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ISW 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)

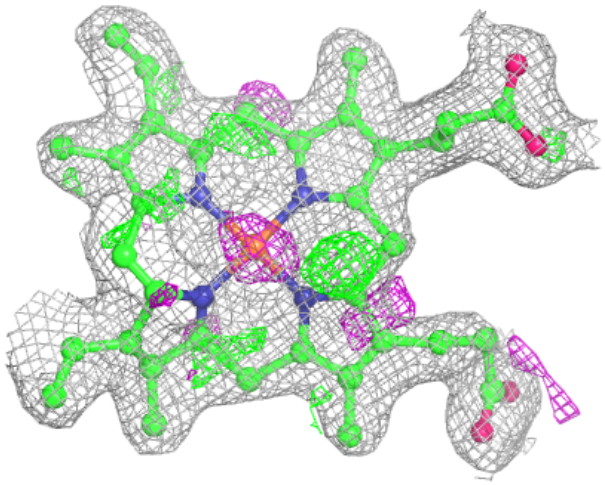


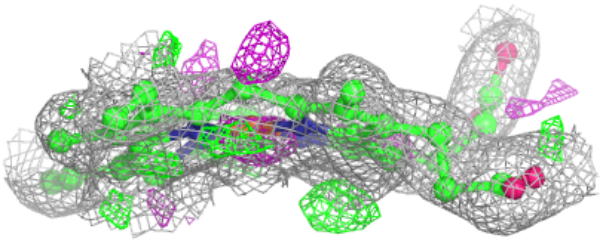


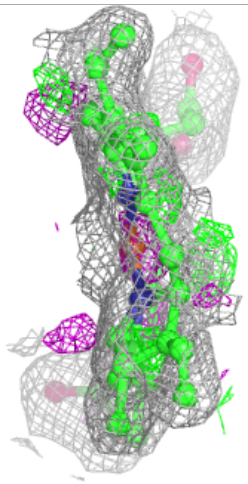


Electron density around ISW A 609:

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

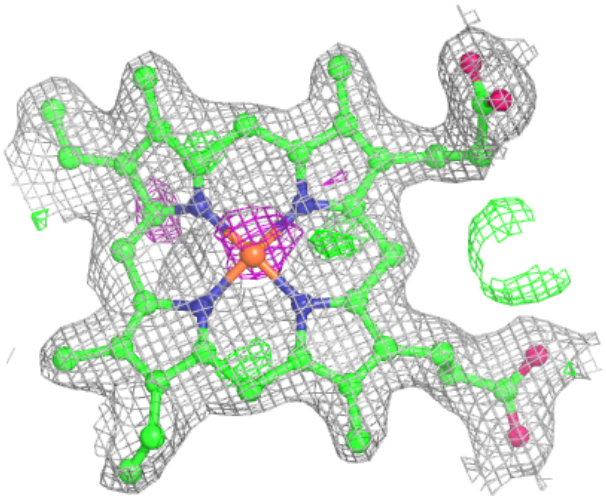


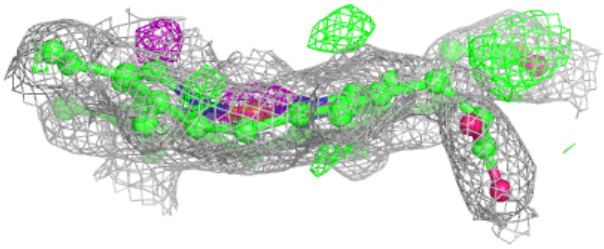


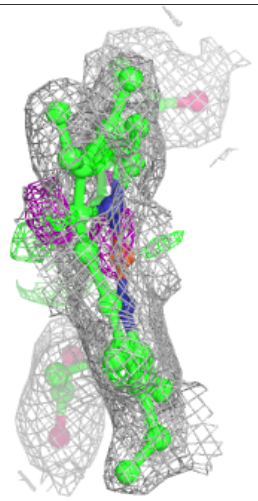


Electron density around ISW G 608:

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

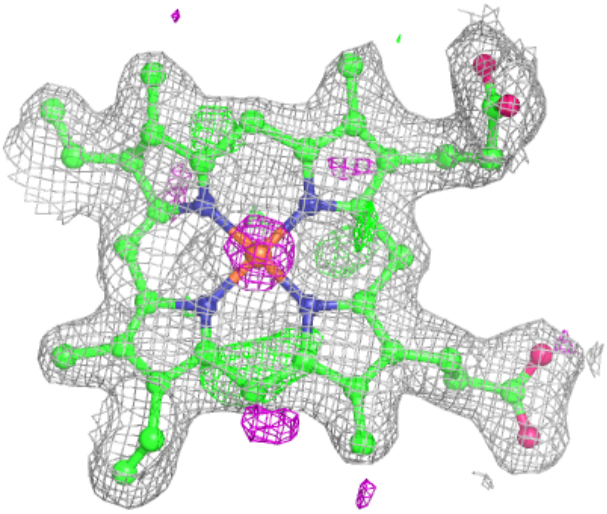


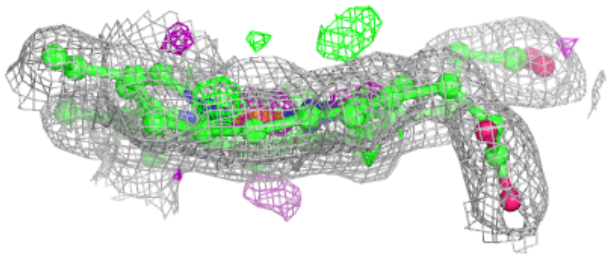


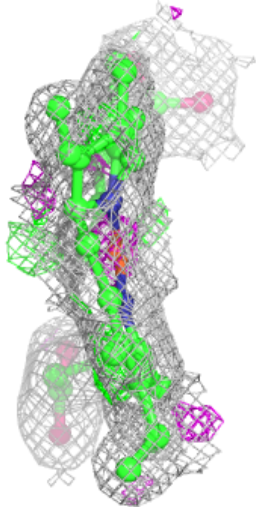


Electron density around ISW C 608:

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

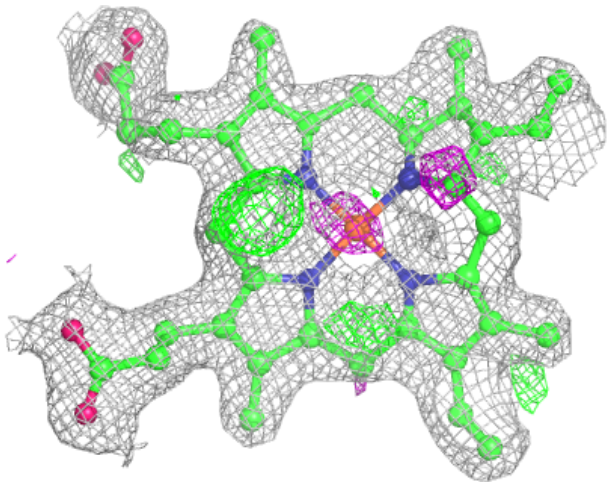


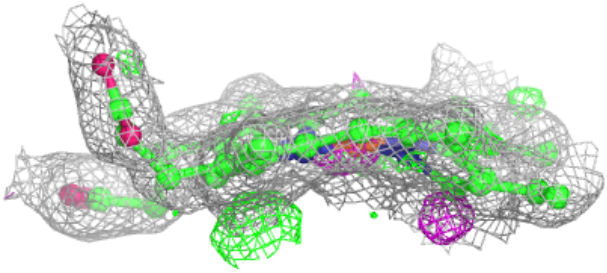


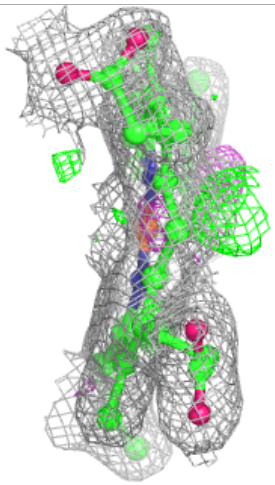


Electron density around ISW G 609:

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

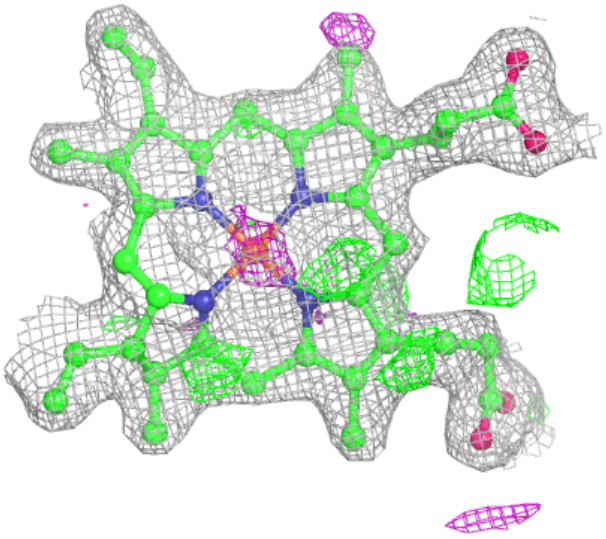


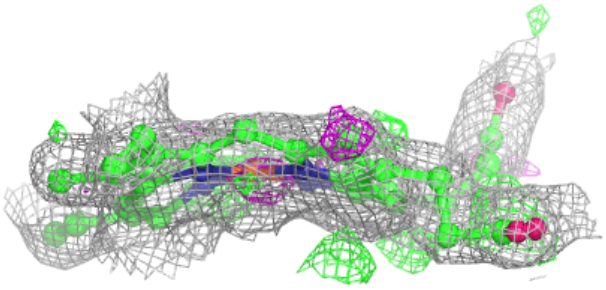


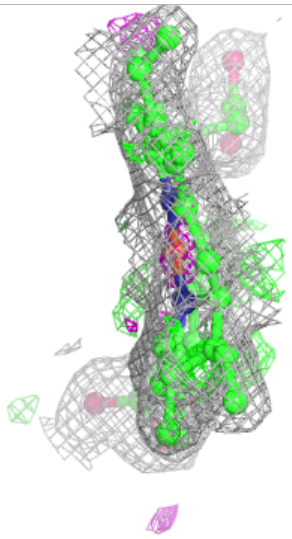


Electron density around ISW I 608:

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

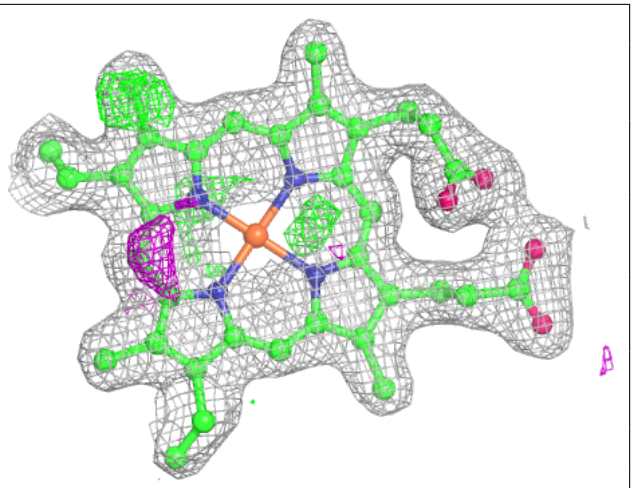


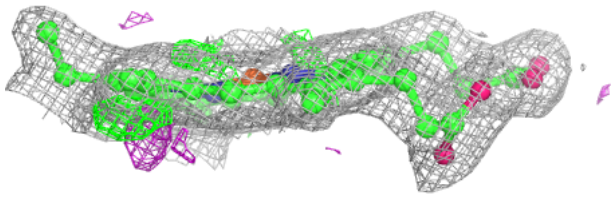


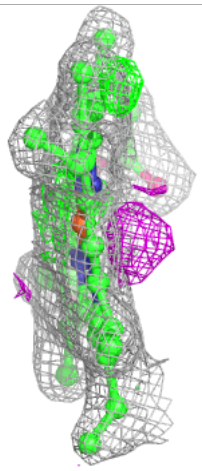


Electron density around HEC K 605:

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

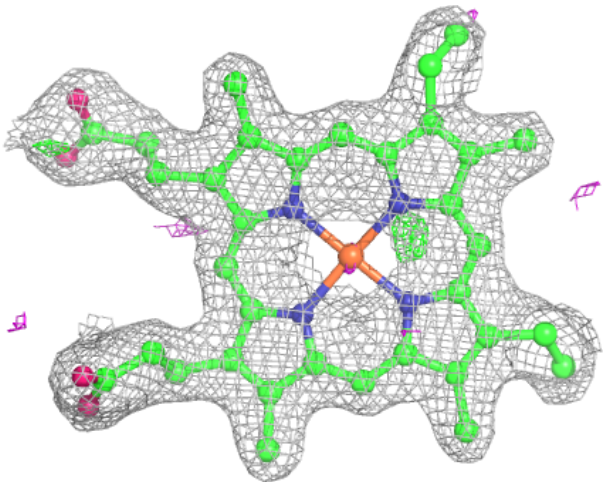


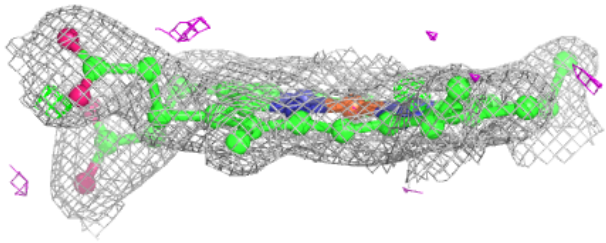


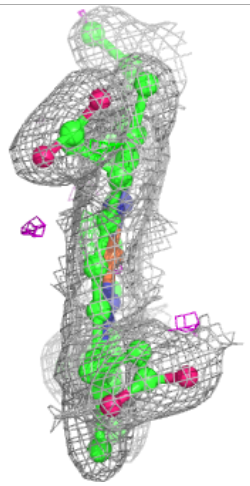


Electron density around HEC K 606:

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

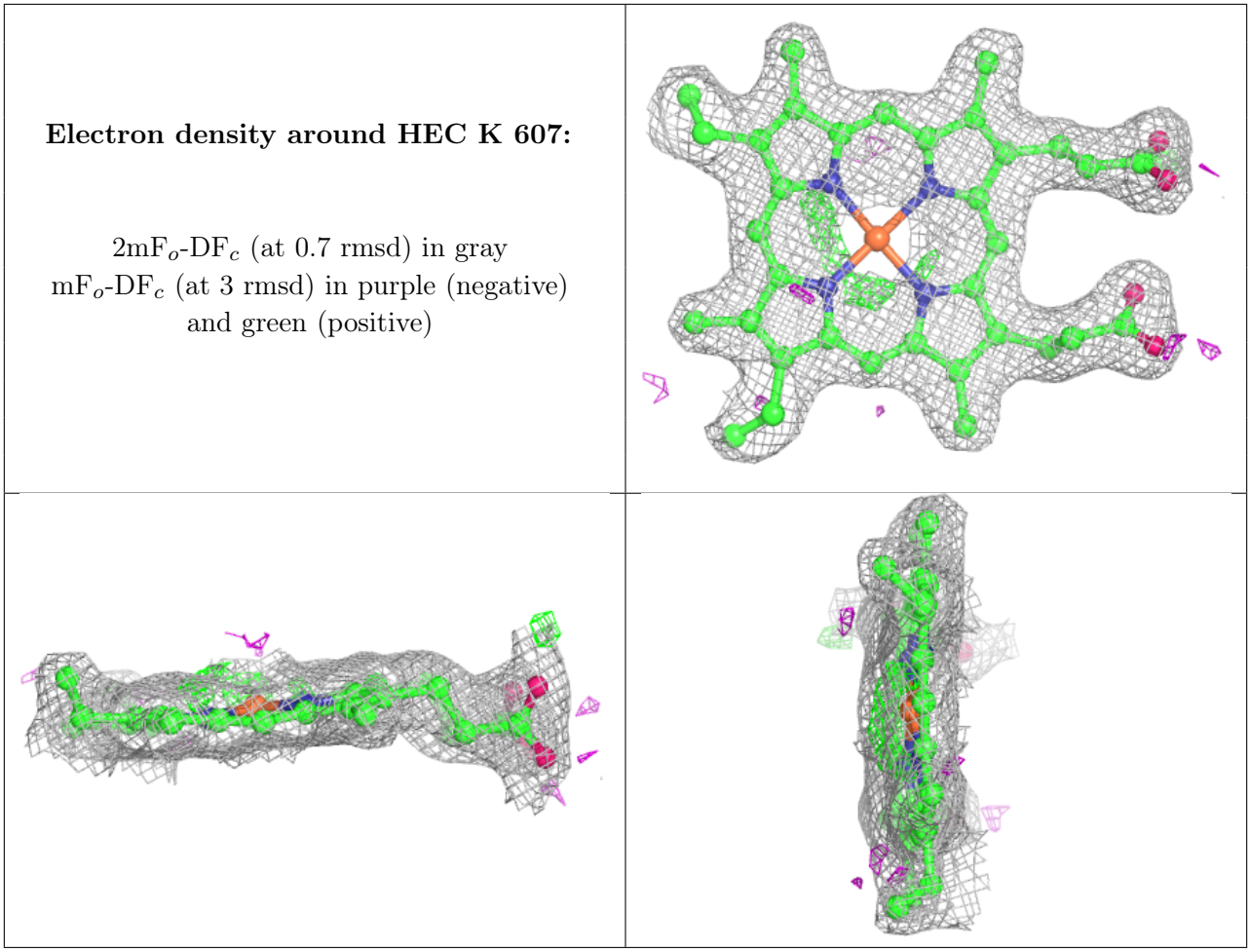






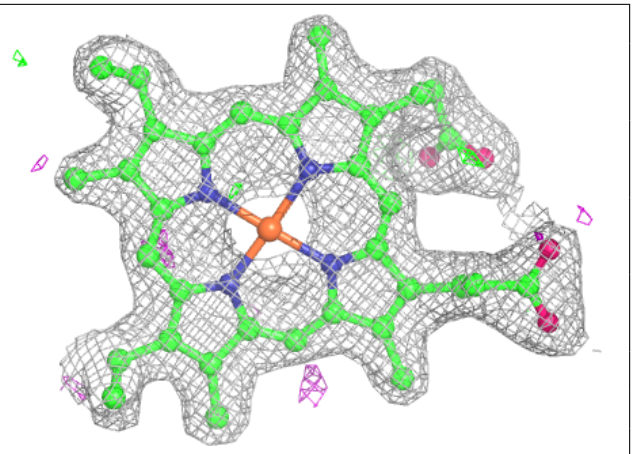
Electron density around HEC K 607:

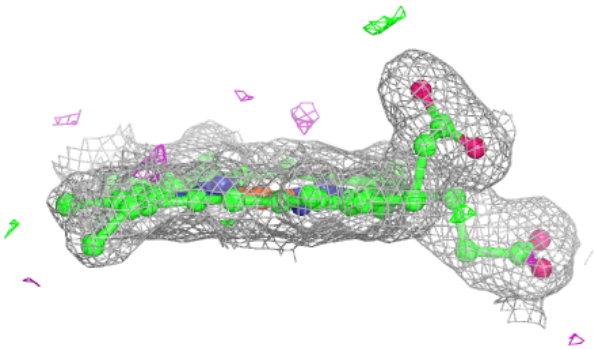
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

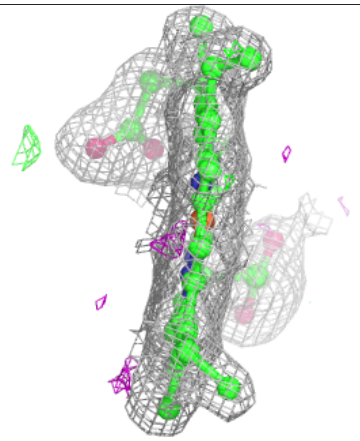


Electron density around HEC A 602:

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

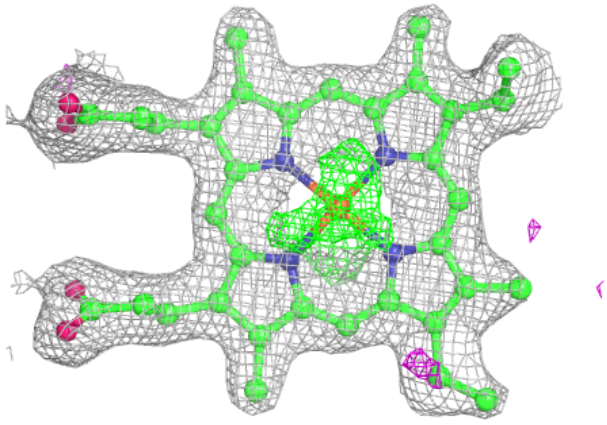


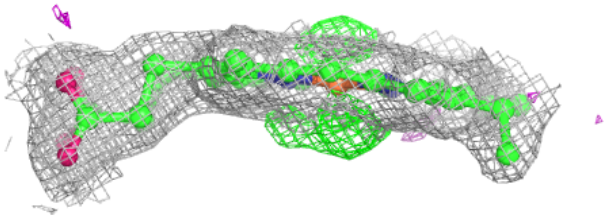


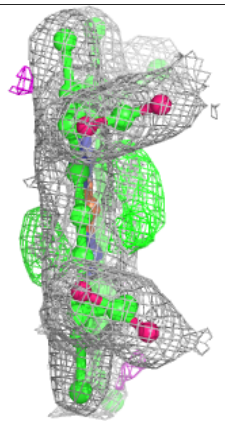


Electron density around HEC A 603:

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

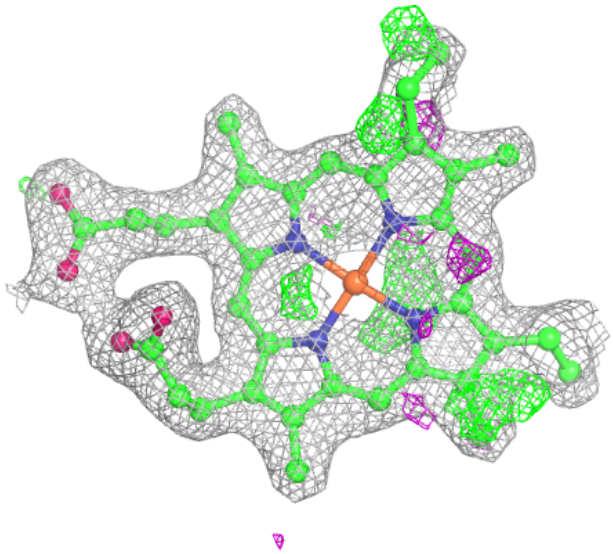


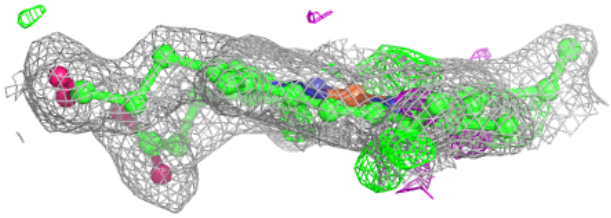


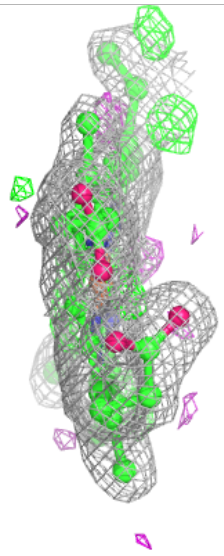


Electron density around HEC A 605:

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

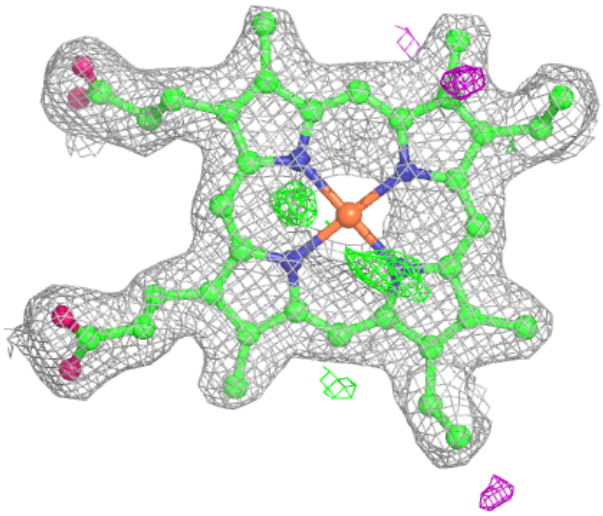


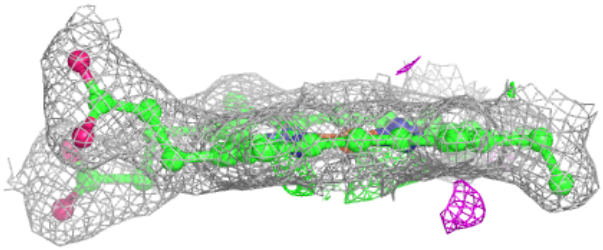


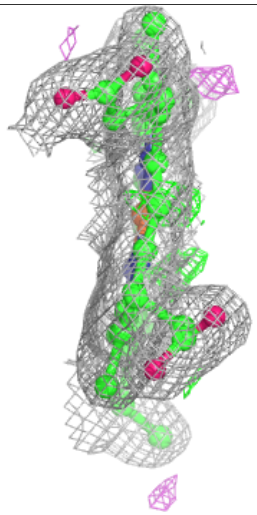


Electron density around HEC A 606:

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

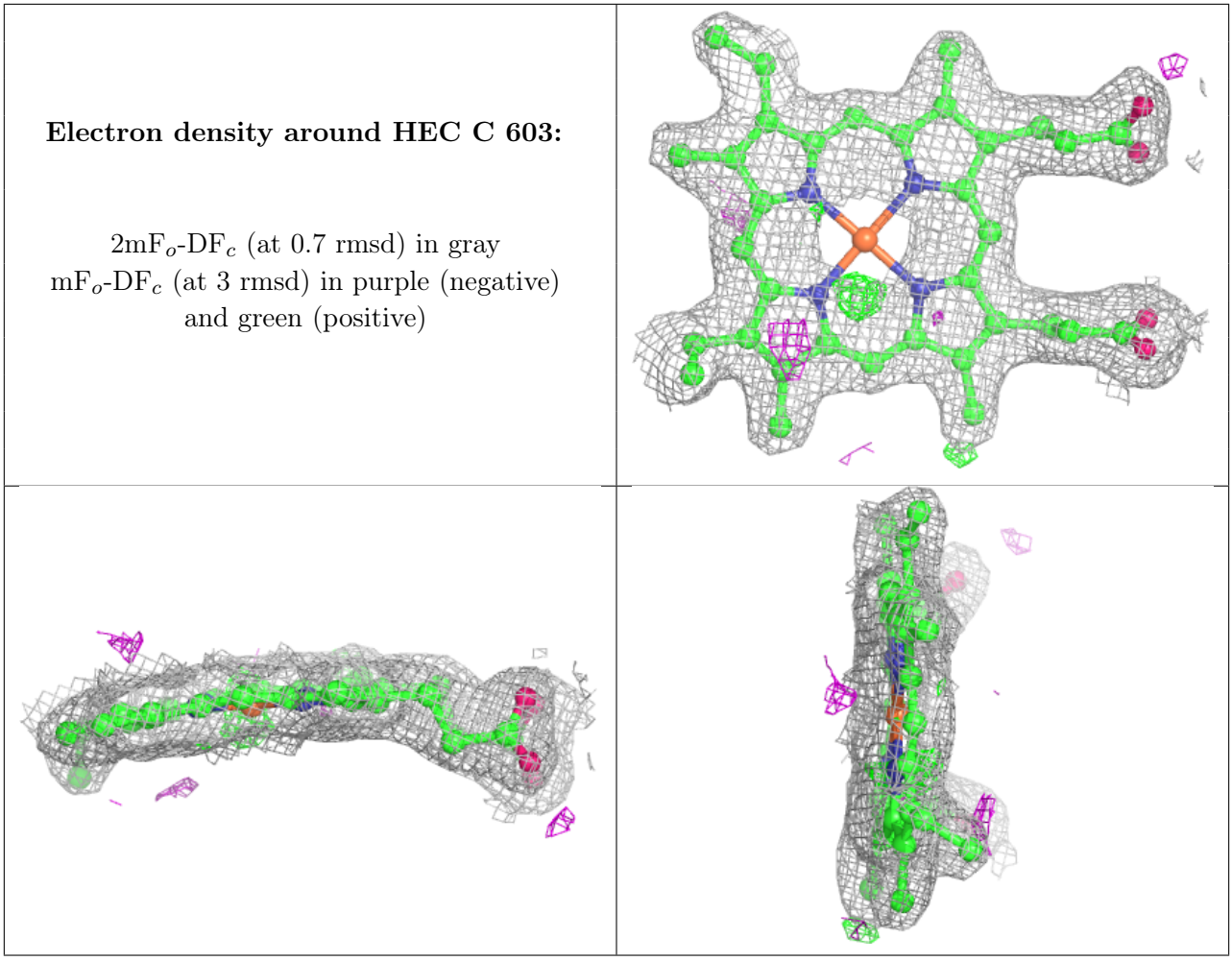






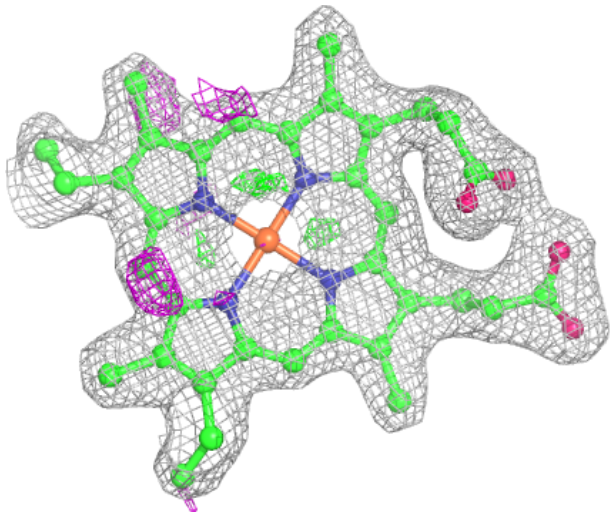
Electron density around HEC C 603:

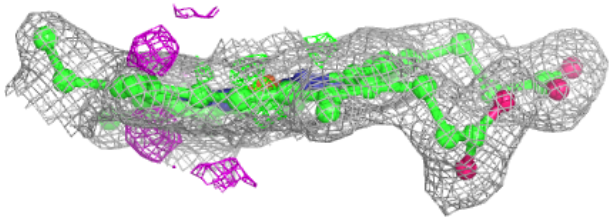
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

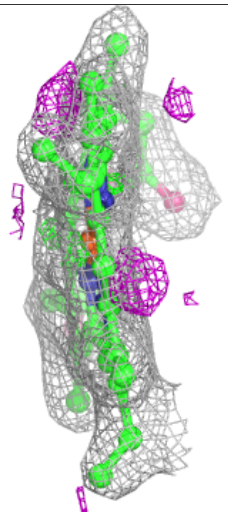


Electron density around HEC C 605:

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

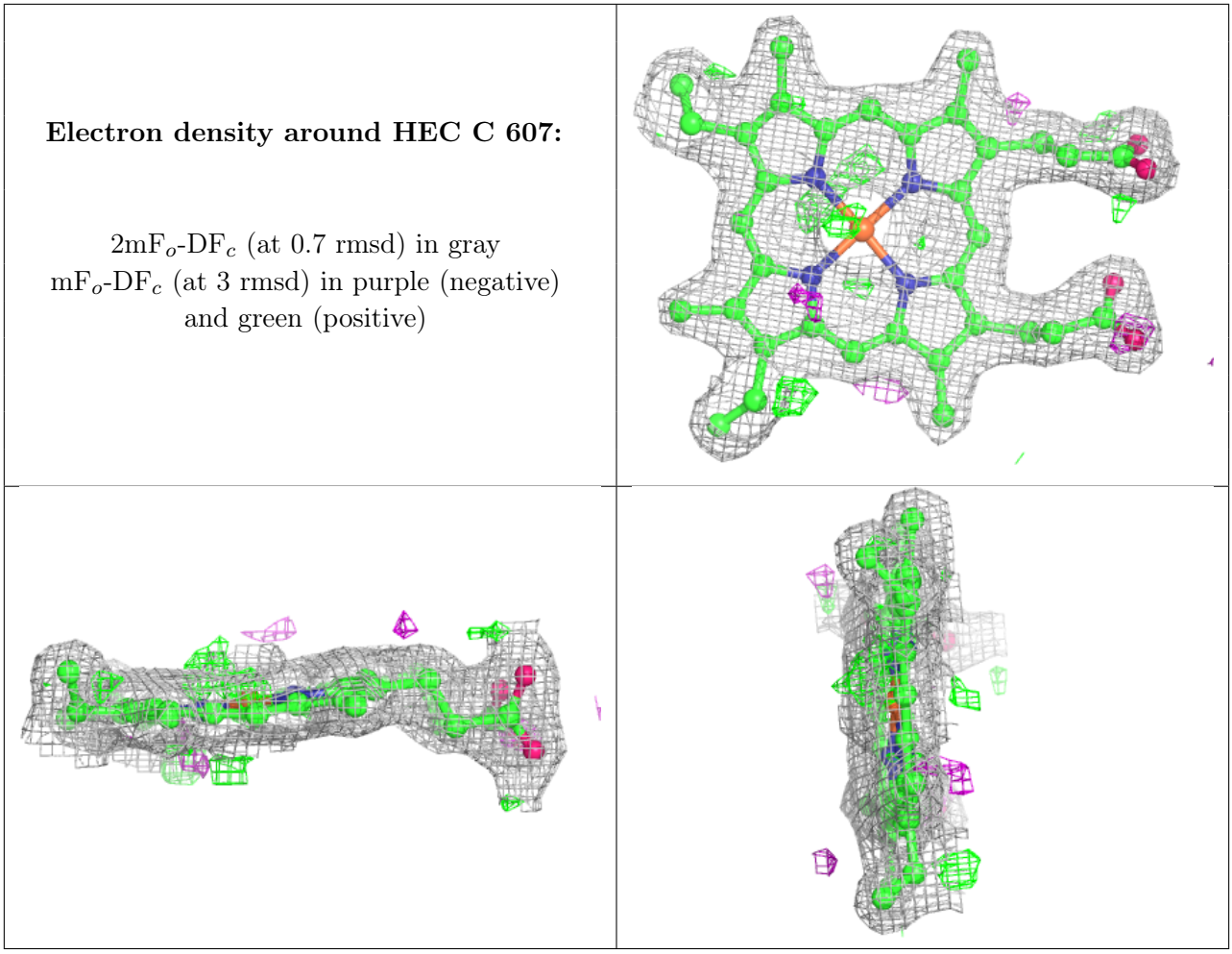






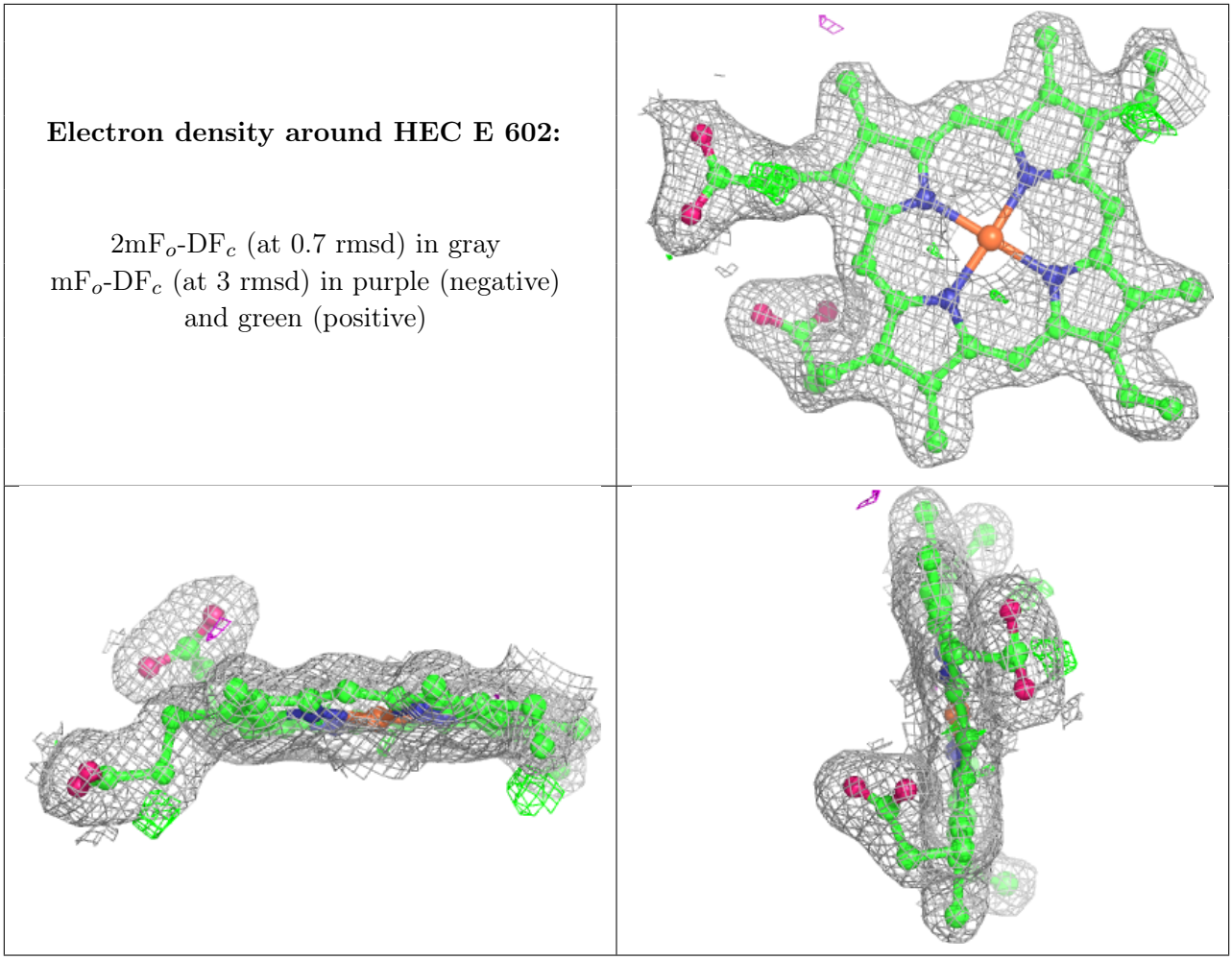
Electron density around HEC C 607:

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



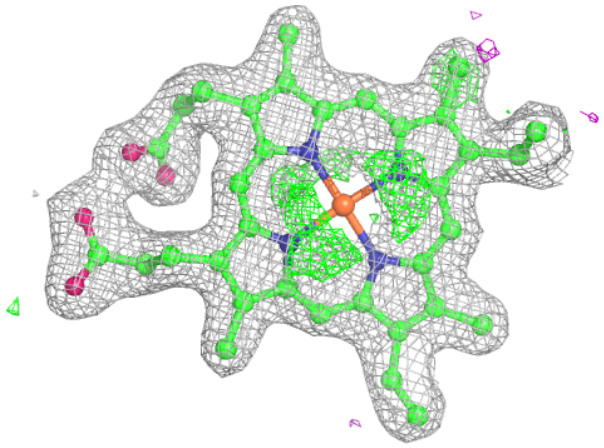
Electron density around HEC E 602:

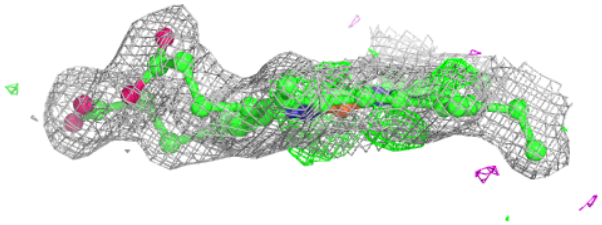
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

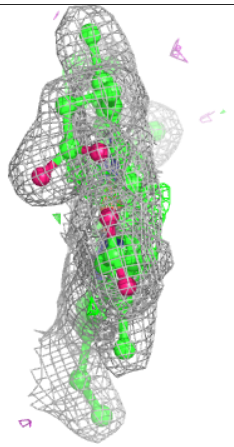


Electron density around HEC E 605:

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

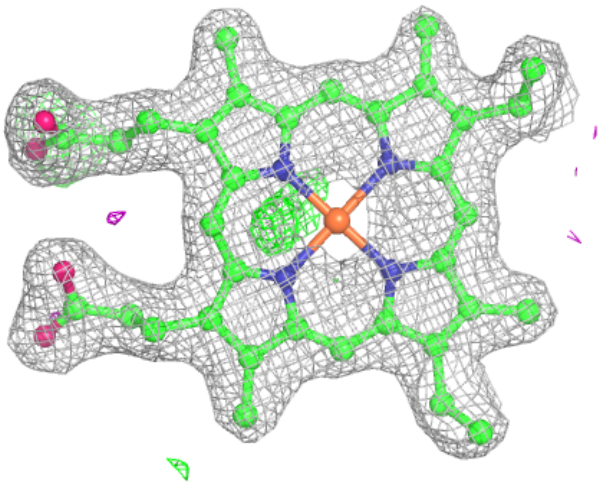


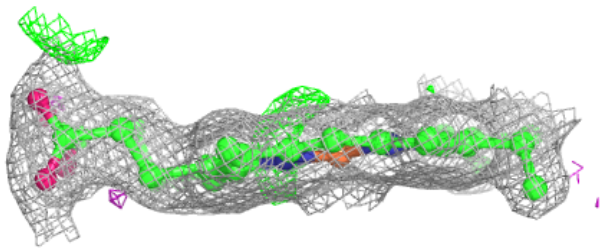


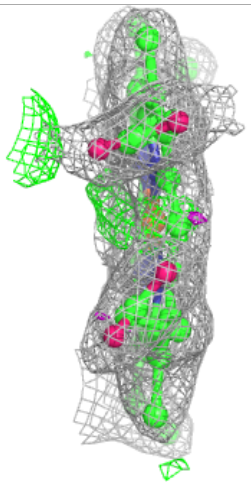


Electron density around HEC E 607:

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

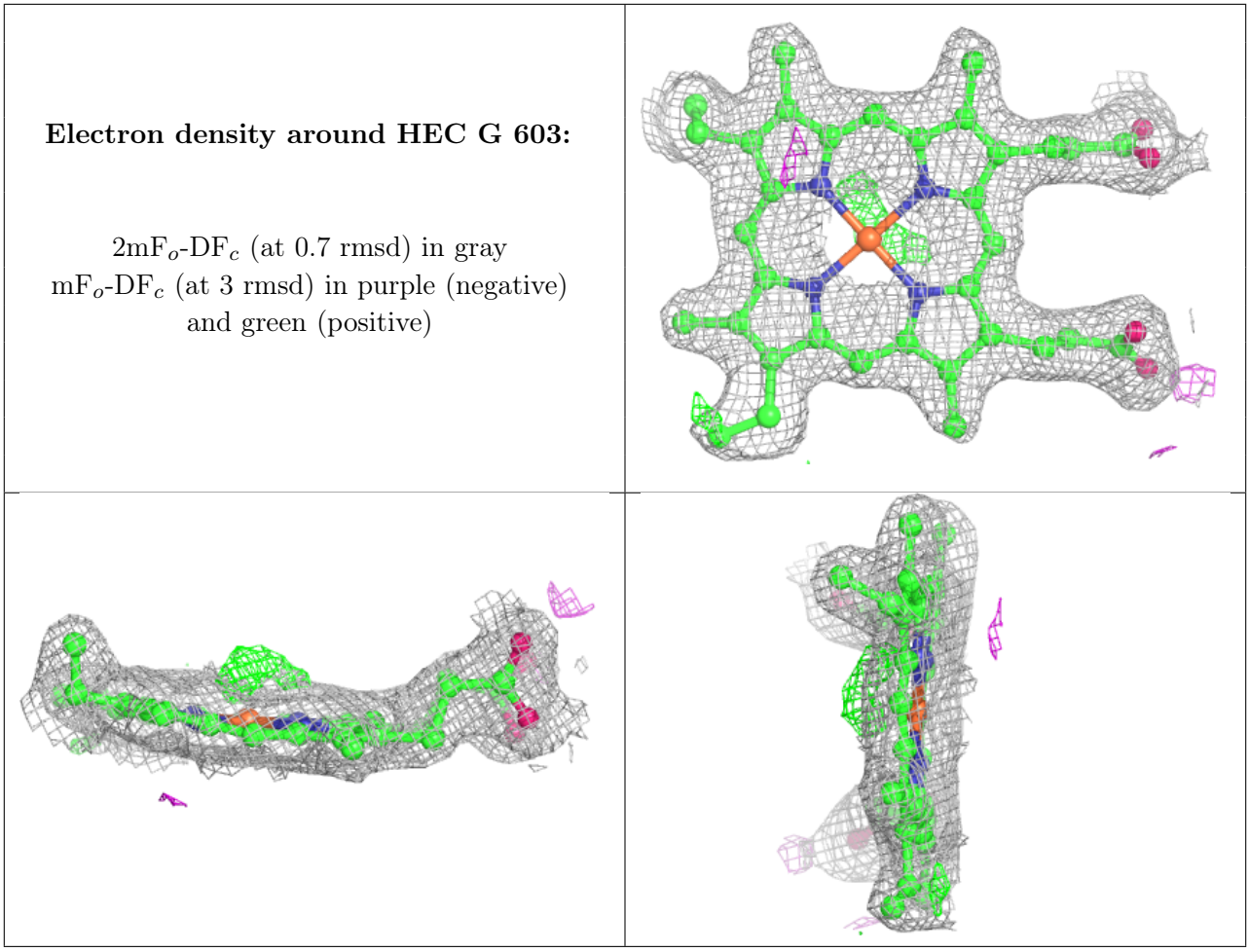






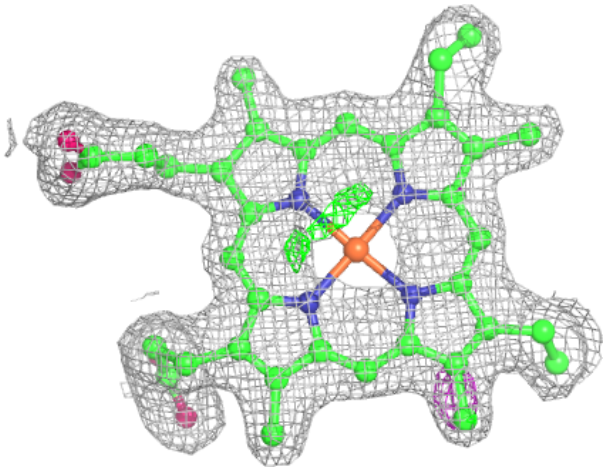
Electron density around HEC G 603:

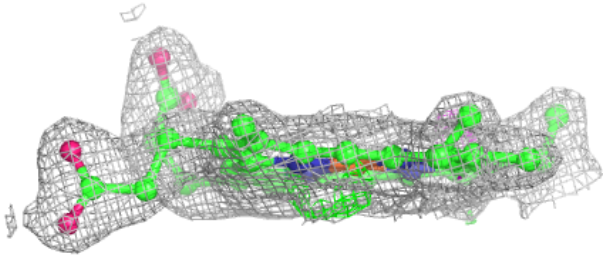
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

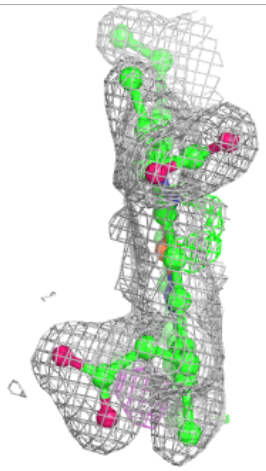


Electron density around HEC G 604:

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

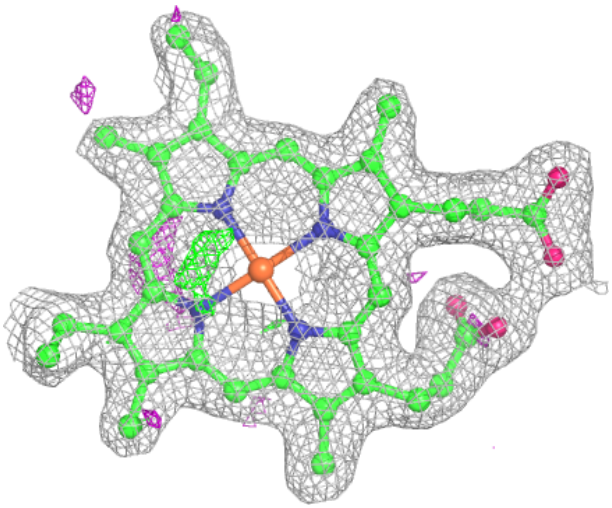


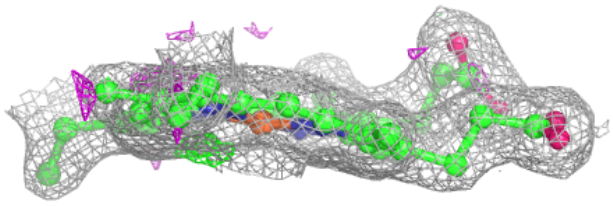


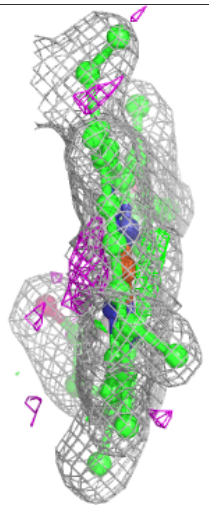


Electron density around HEC G 605:

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

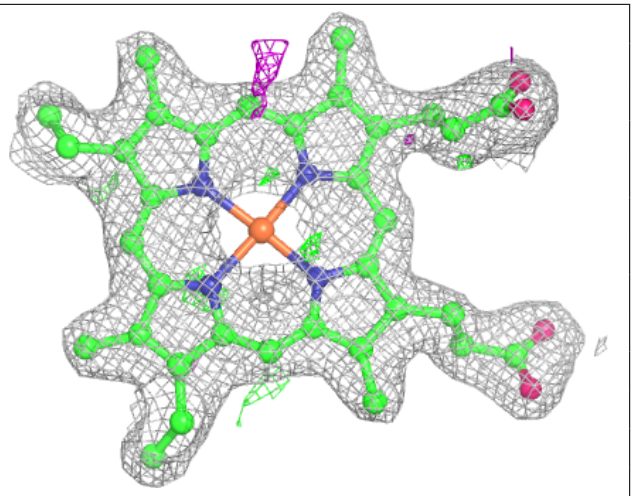


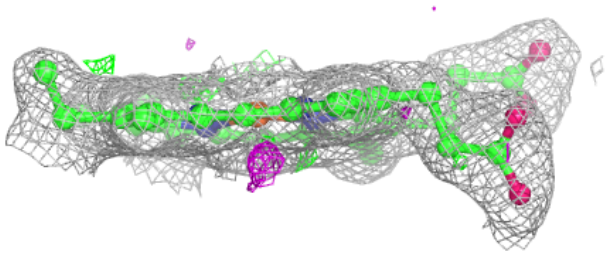


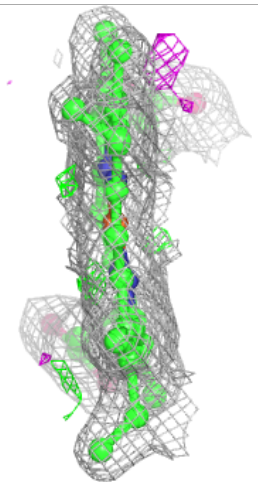


Electron density around HEC G 606:

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

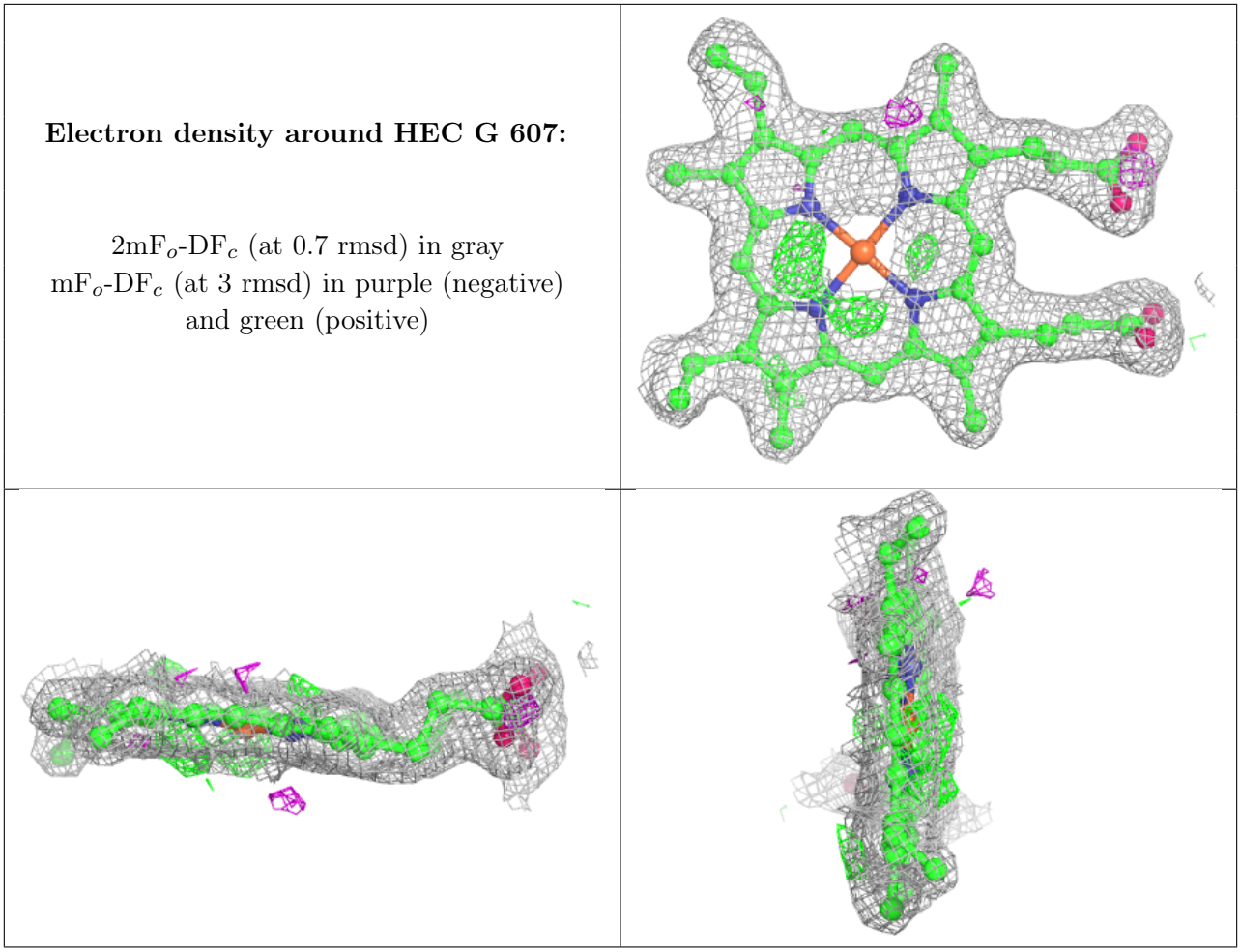






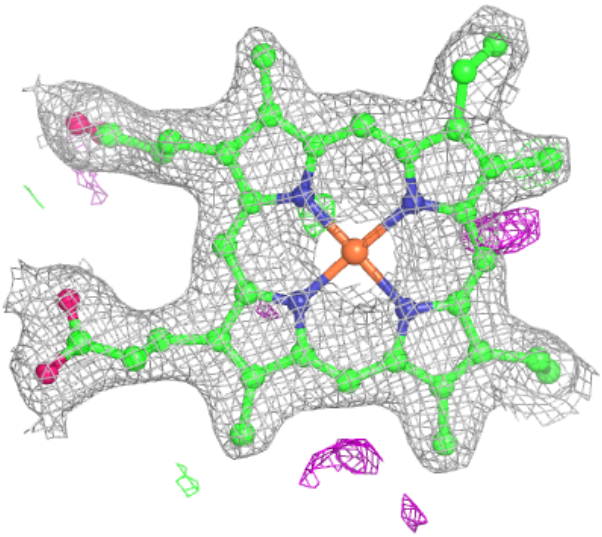
Electron density around HEC G 607:

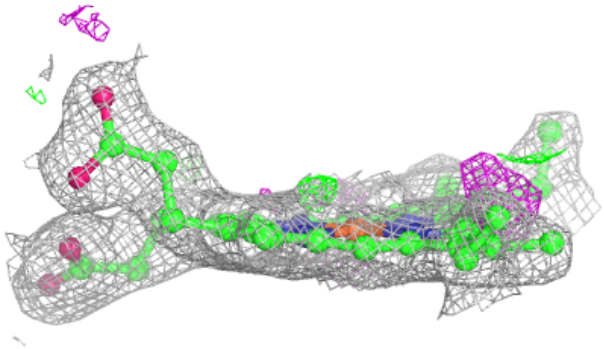
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

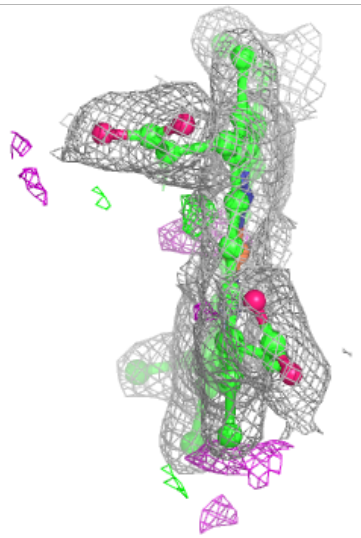


Electron density around HEC I 601:

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

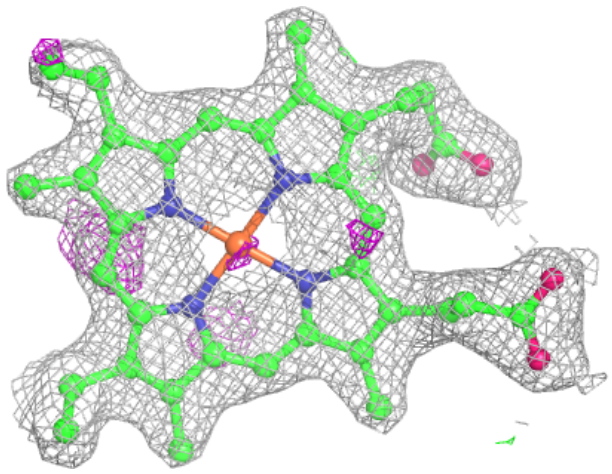


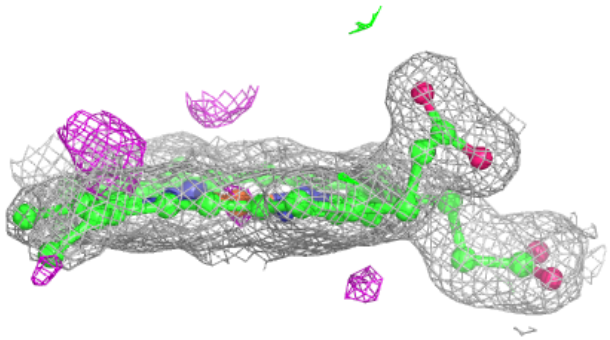


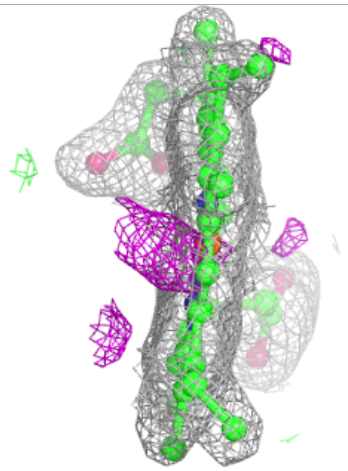


Electron density around HEC I 602:

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

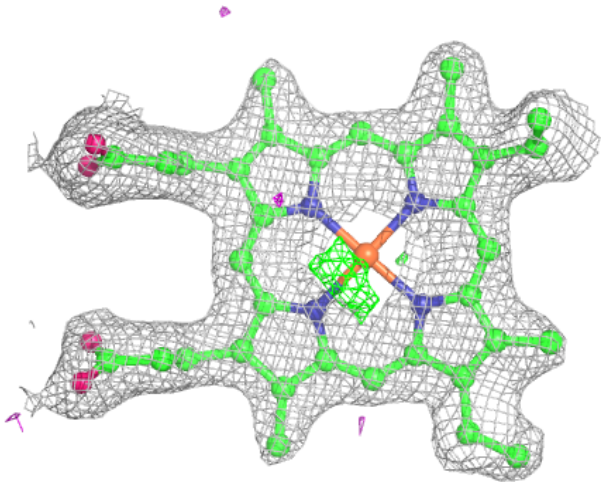


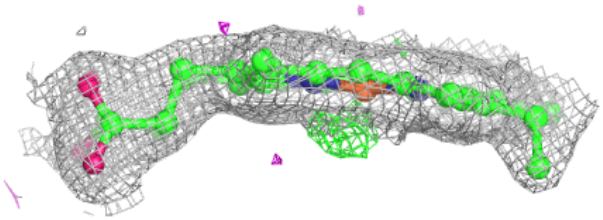


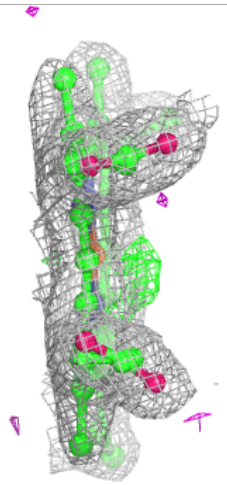


Electron density around HEC I 603:

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

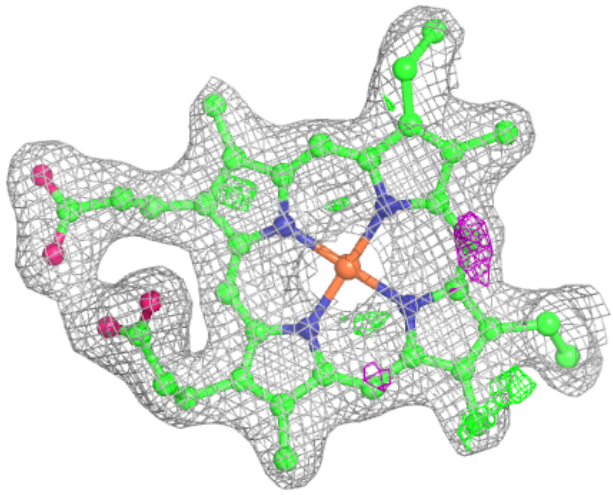


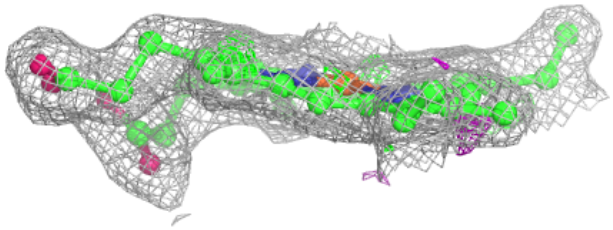


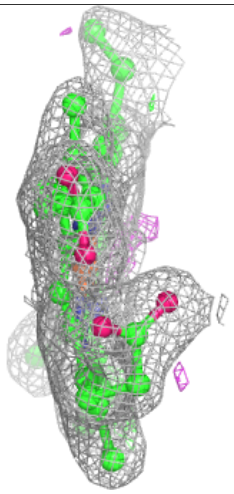


Electron density around HEC I 605:

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

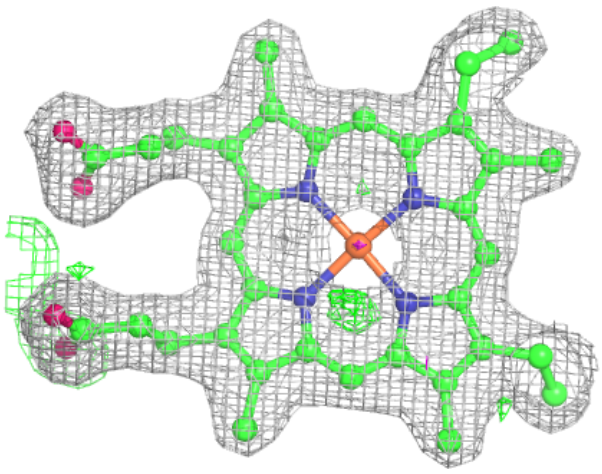


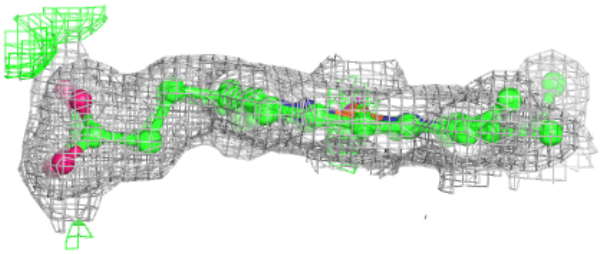


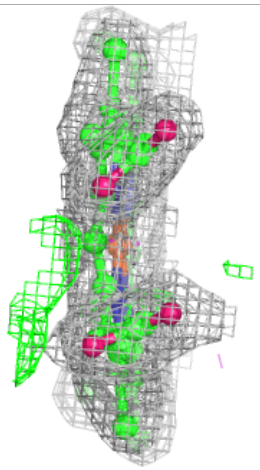


Electron density around HEC I 607:

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

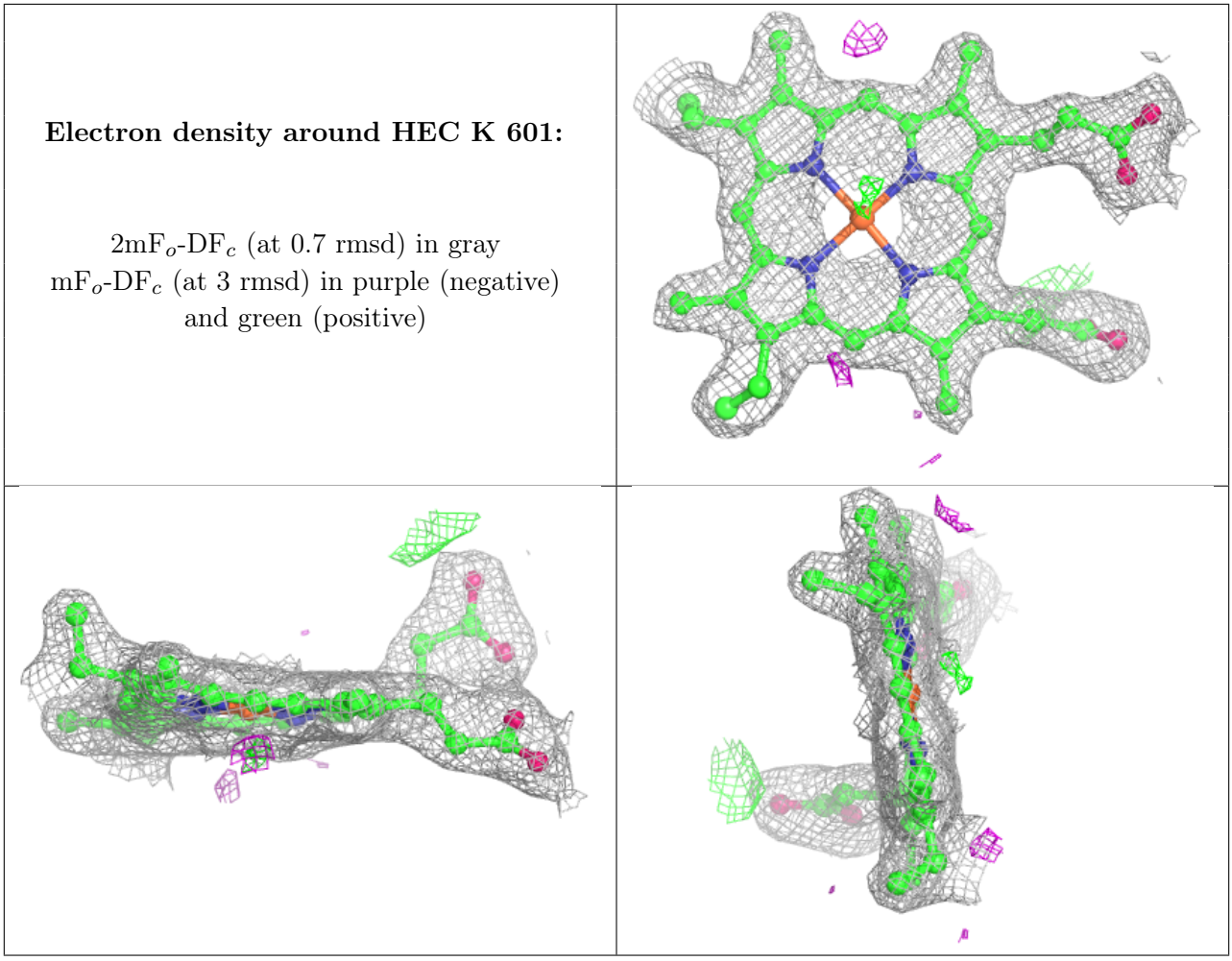






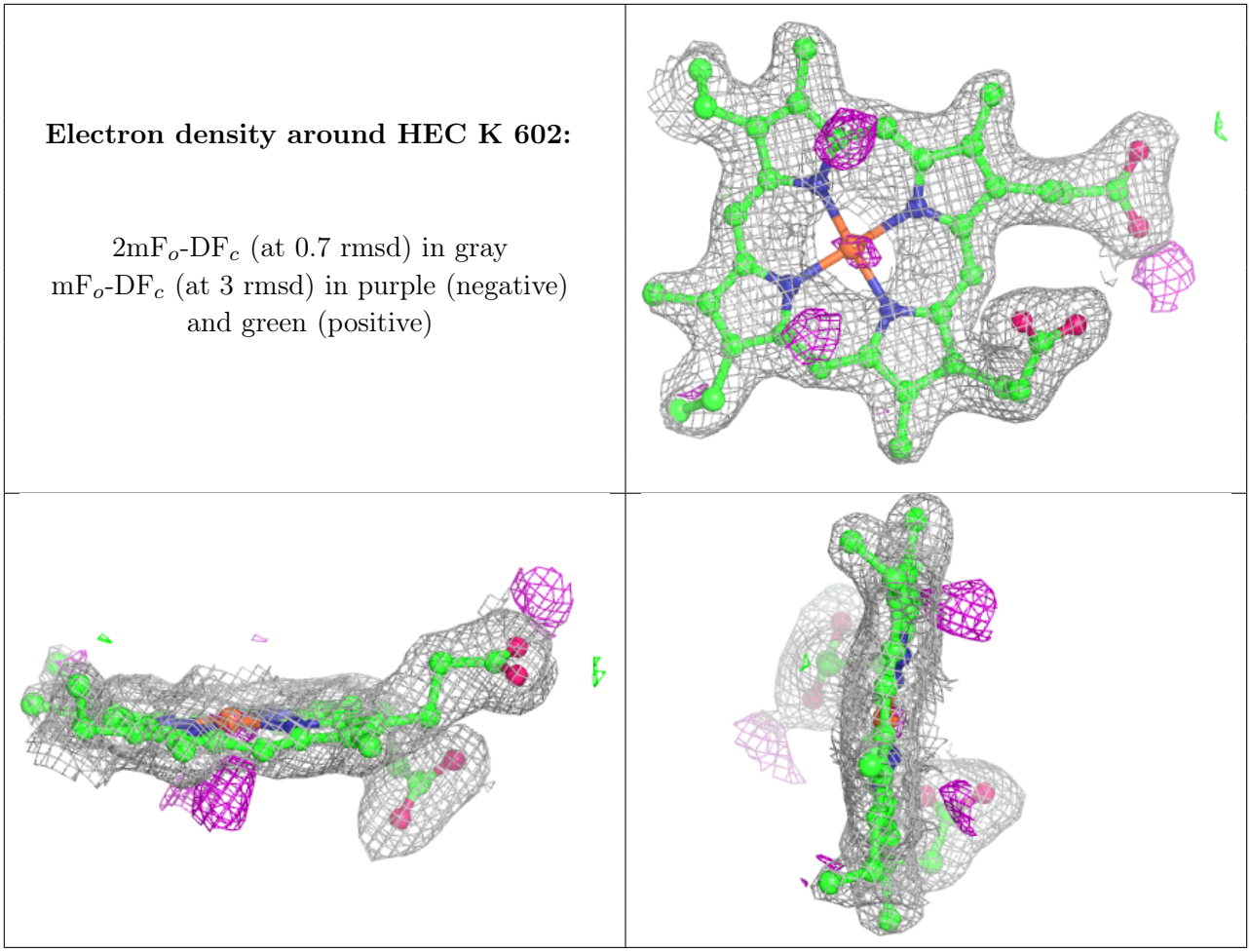
Electron density around HEC K 601:

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



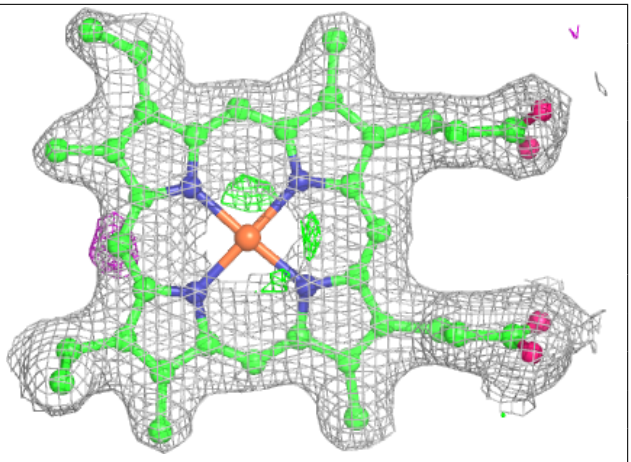
Electron density around HEC K 602:

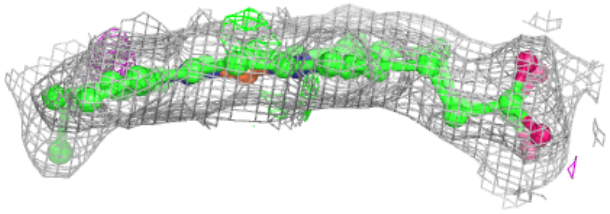
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

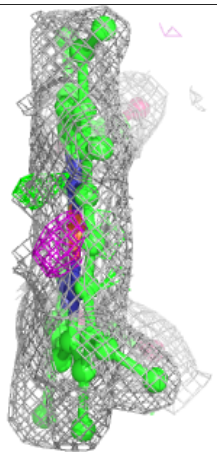


Electron density around HEC K 603:

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

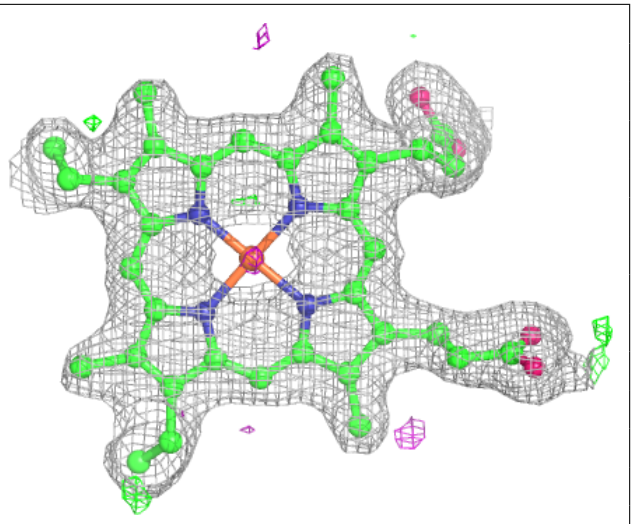


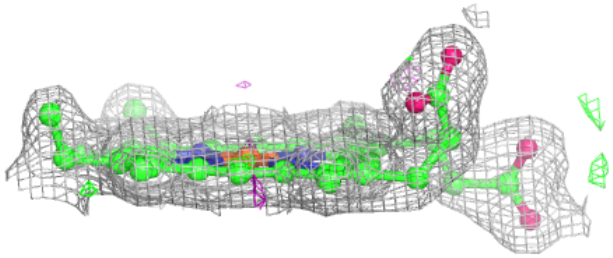


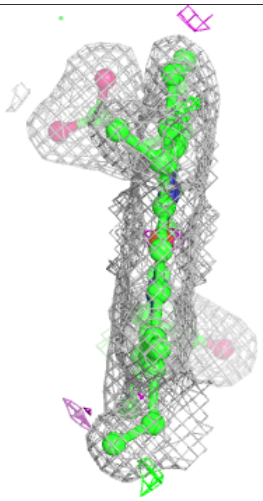


Electron density around HEC K 604:

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

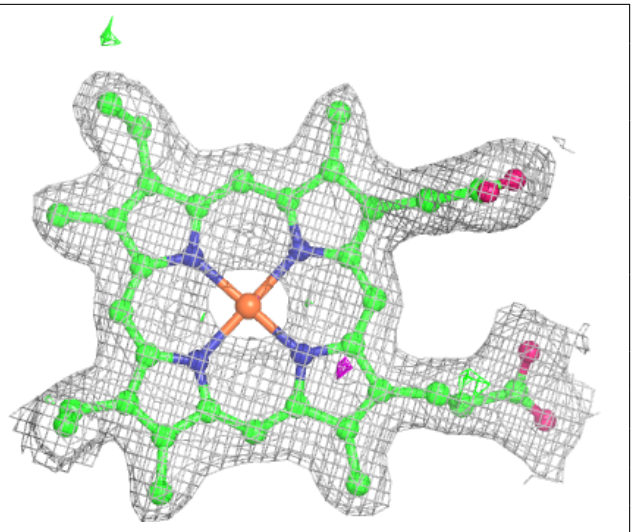


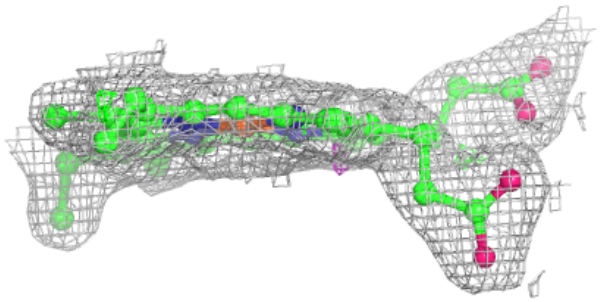


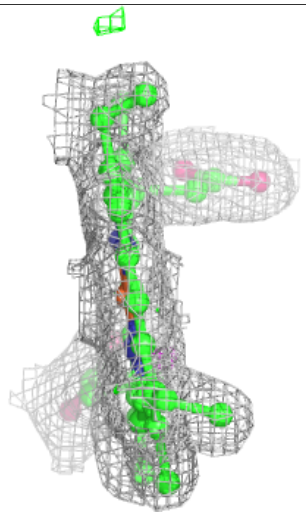


Electron density around HEC G 601:

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

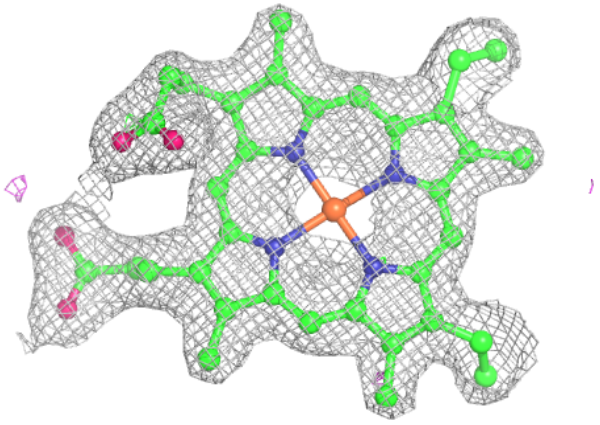


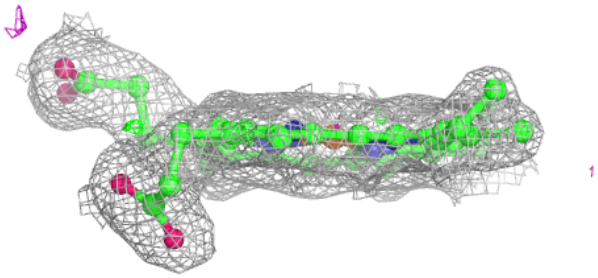


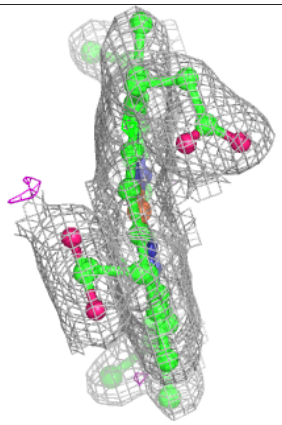


Electron density around HEC G 602:

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

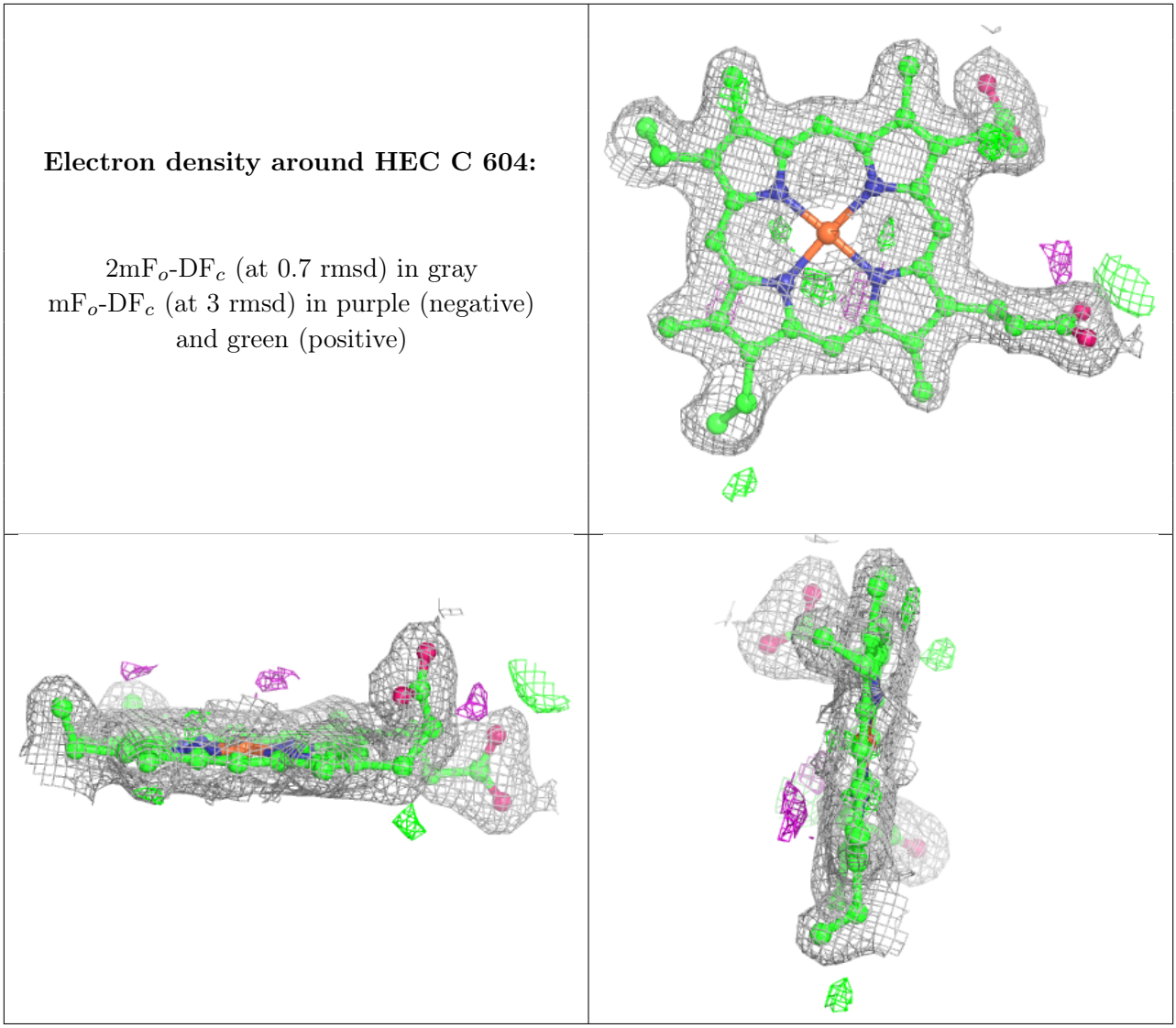






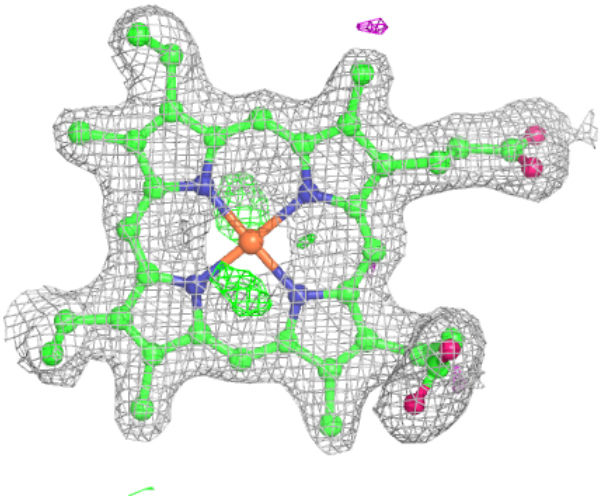
Electron density around HEC C 604:

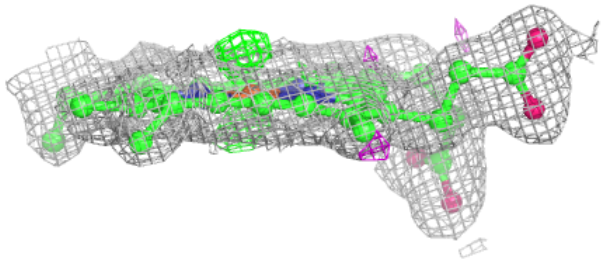
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

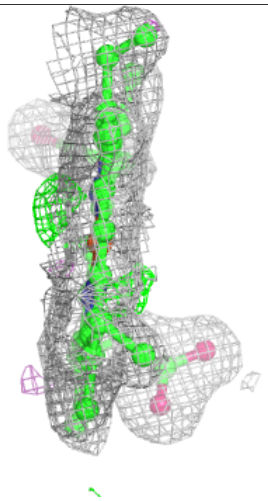


Electron density around HEC A 604:

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

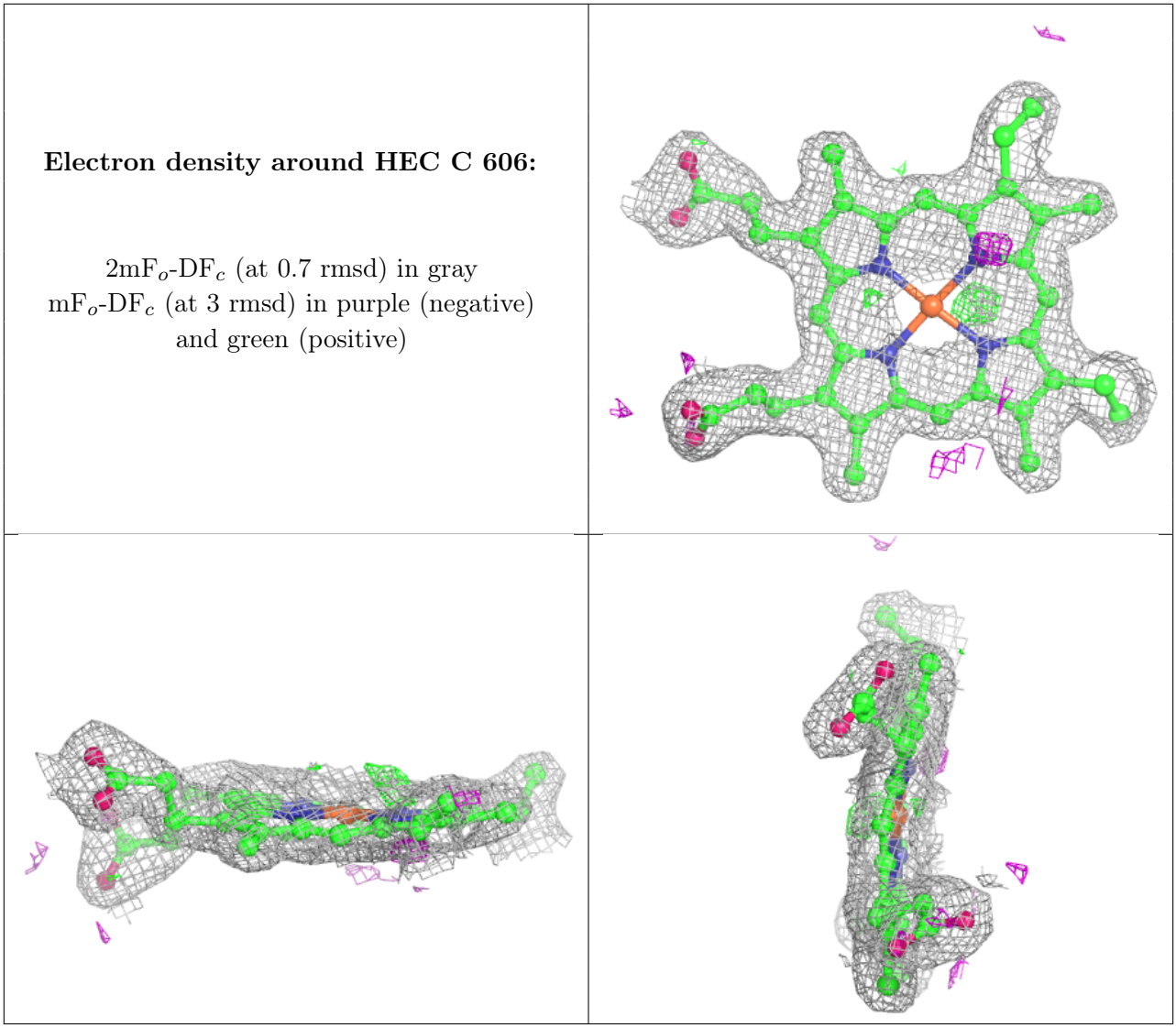






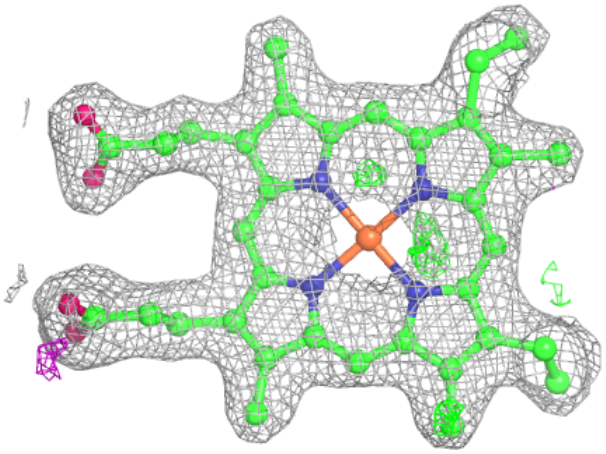
Electron density around HEC C 606:

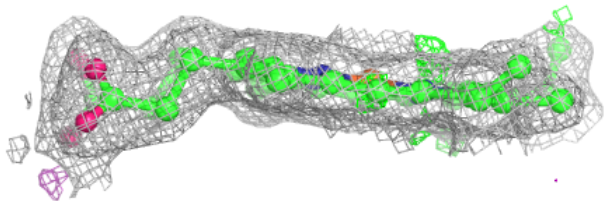
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

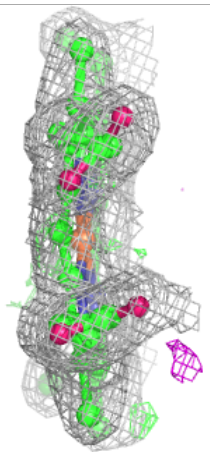


Electron density around HEC A 607:

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

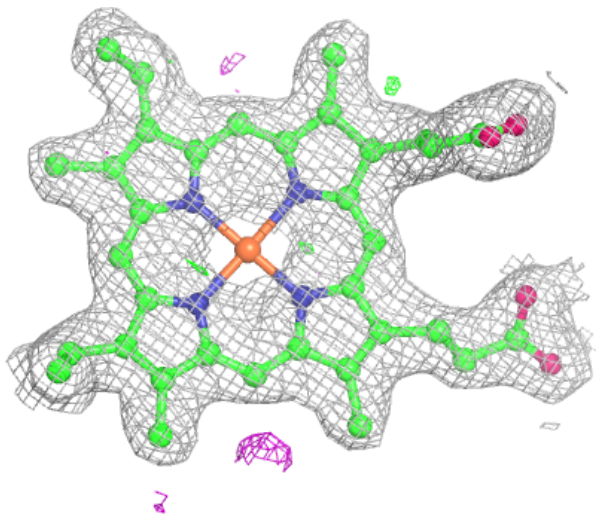


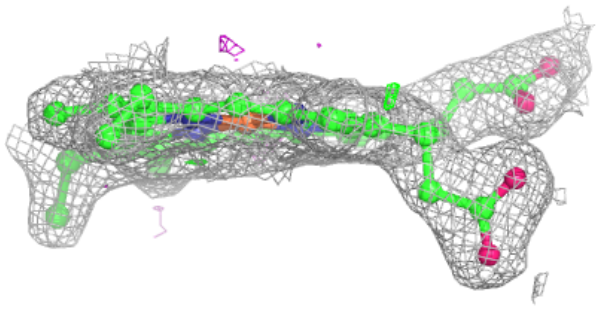


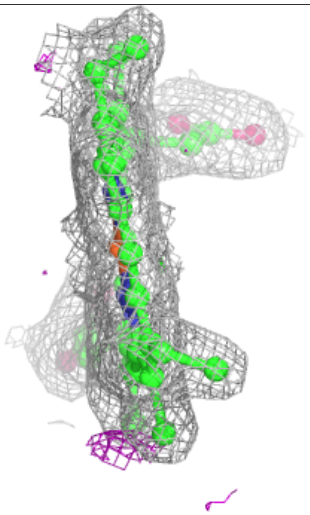


Electron density around HEC E 601:

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

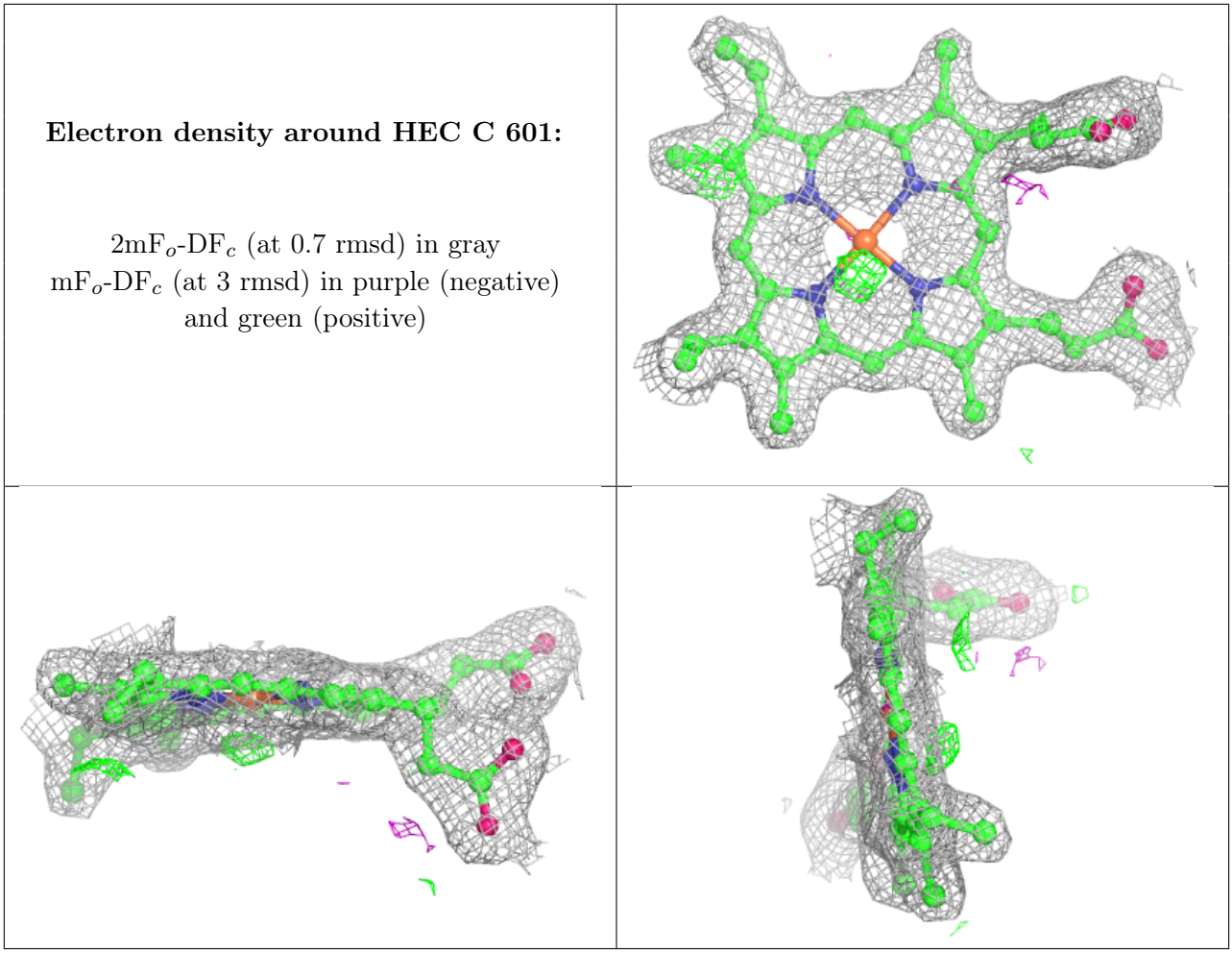






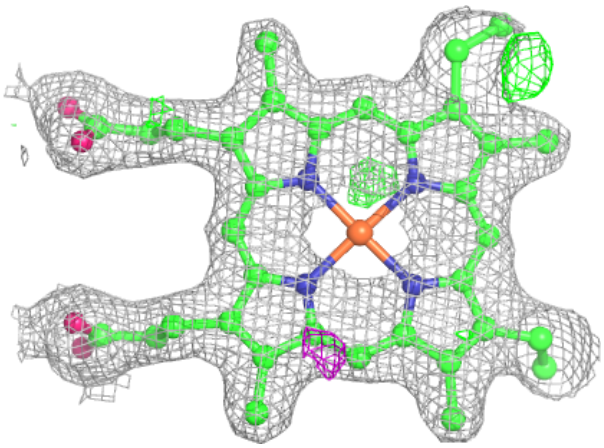
Electron density around HEC C 601:

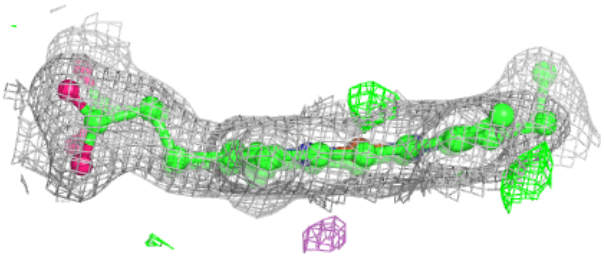
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

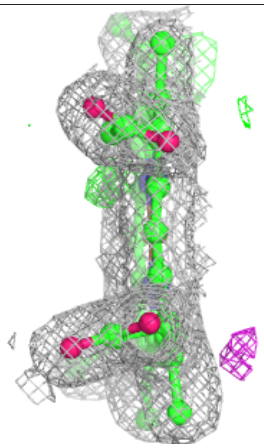


Electron density around HEC E 603:

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

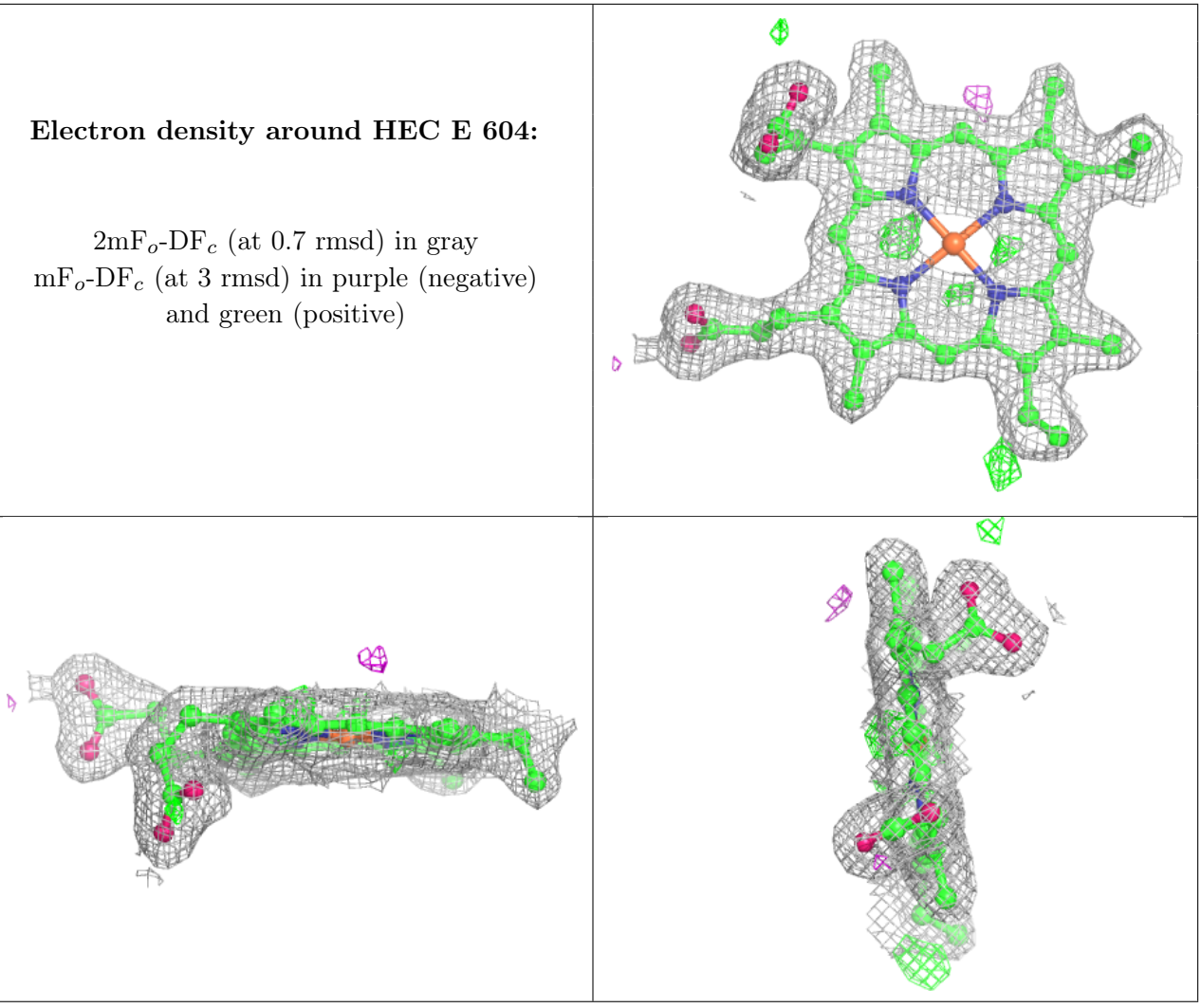






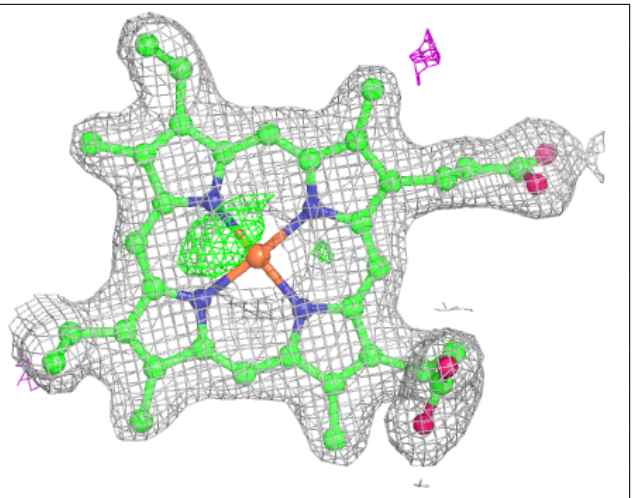
Electron density around HEC E 604:

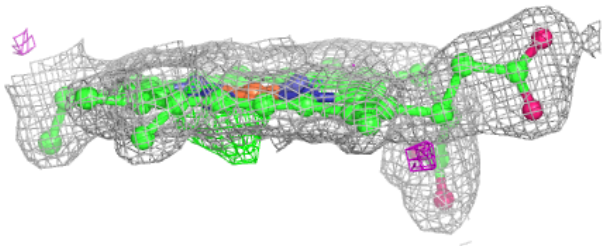
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

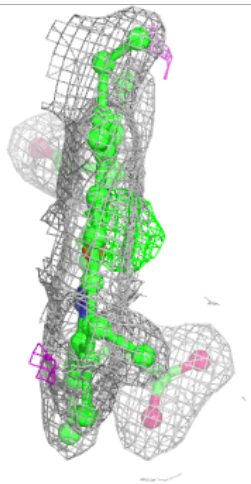


Electron density around HEC I 604:

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

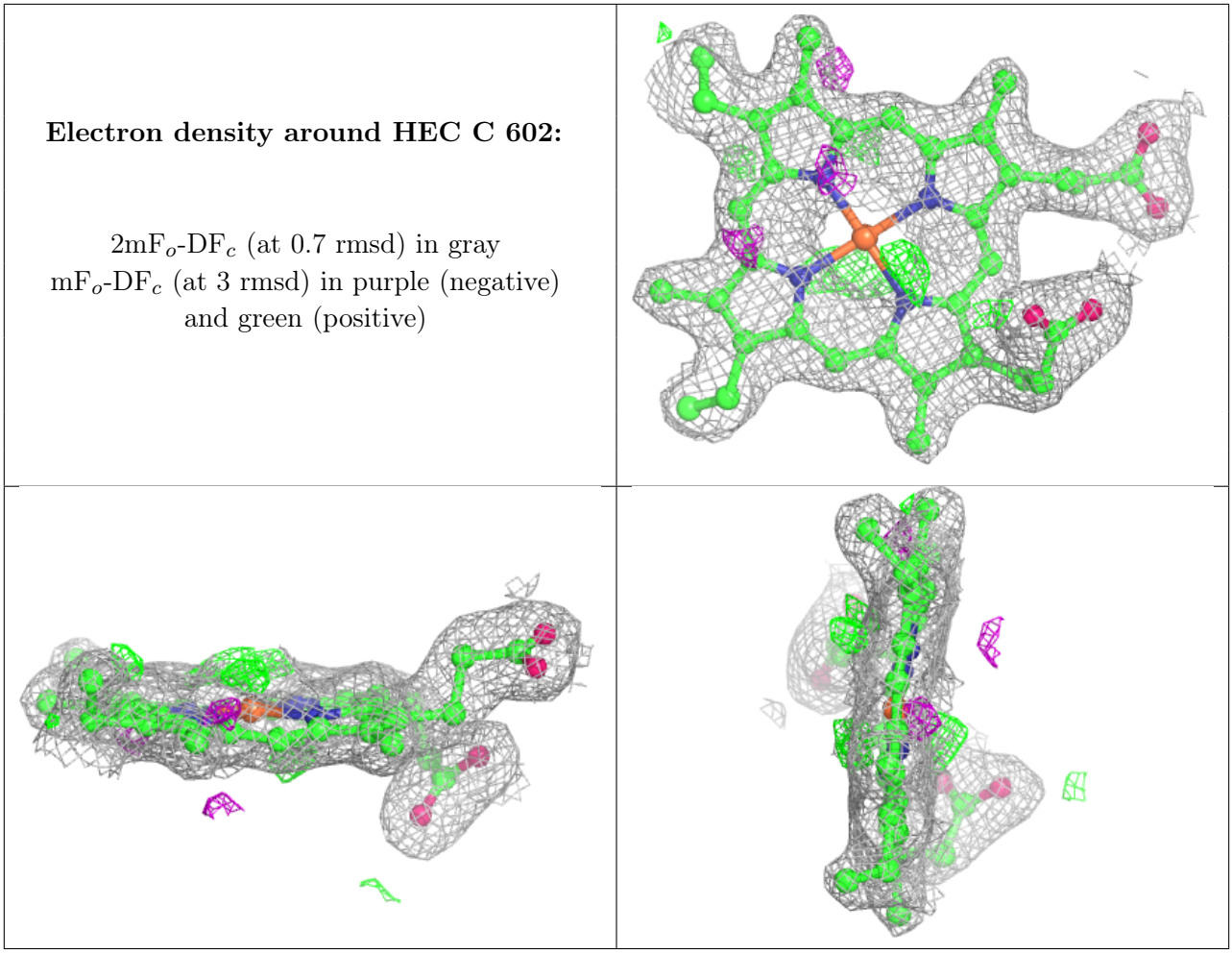






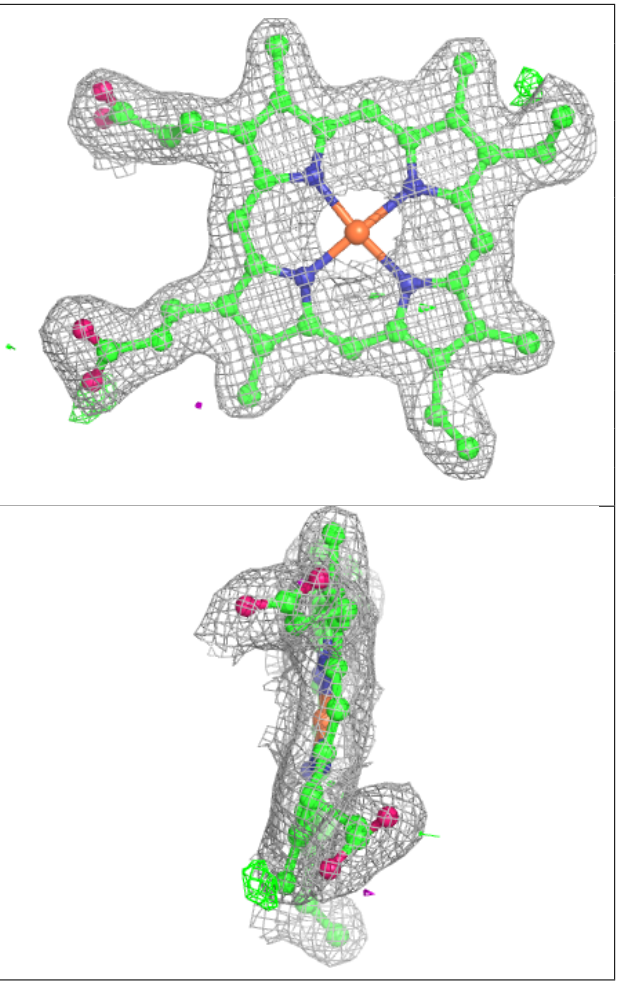
Electron density around HEC C 602:

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



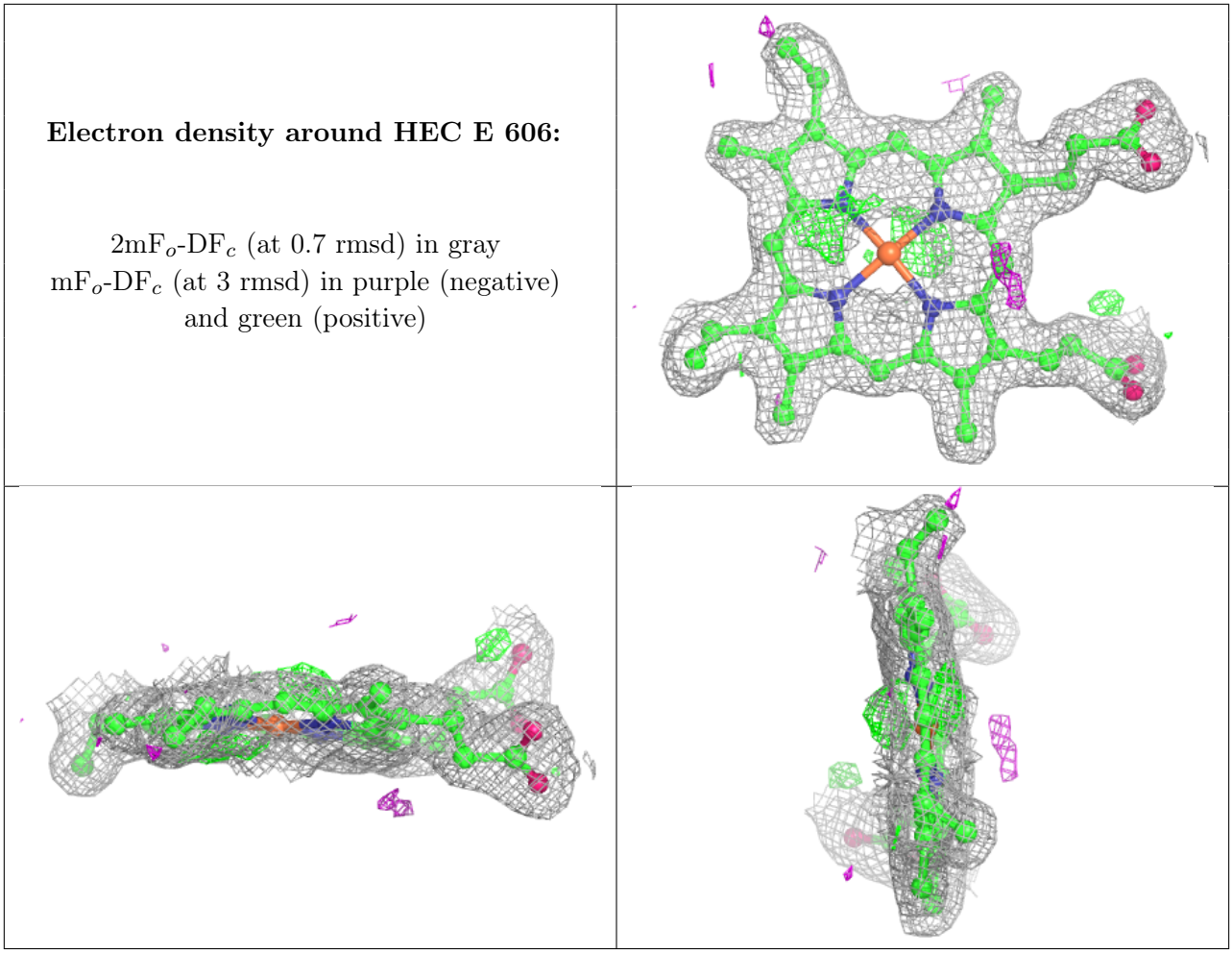
Electron density around HEC I 606:

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



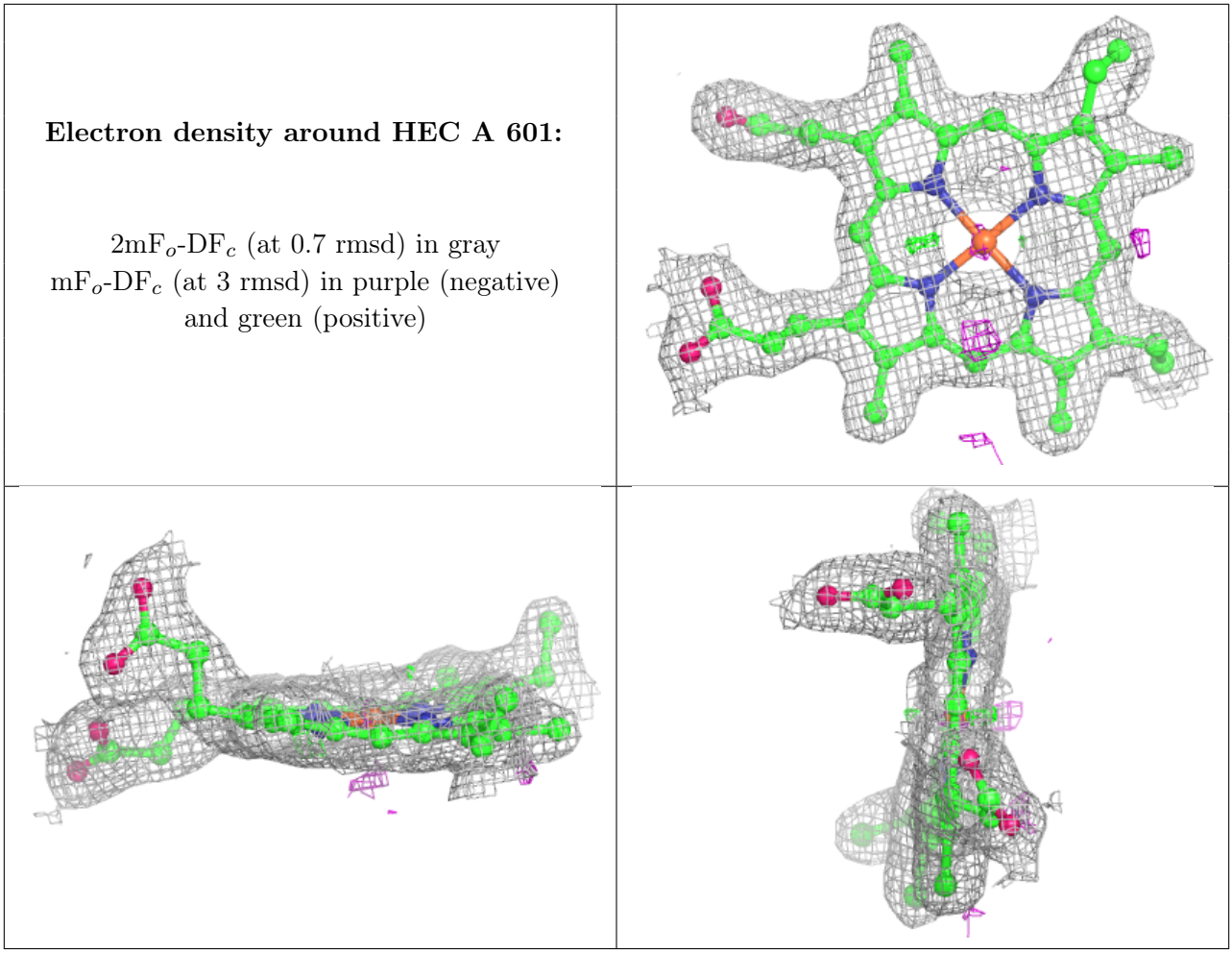
Electron density around HEC E 606:

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



Electron density around HEC A 601:

$2mF_o$-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.