



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 AM UTC

PDB ID : 6HIF / pdb_00006hif
Title : Kuenenia stuttgartiensis hydrazine dehydrogenase complex
Authors : Akram, M.; Dietl, A.; Mersdorf, U.; Prinz, S.; Maalcke, W.; Keltjens, J.; Ferousi, C.; de Almeida, N.M.; Reimann, J.; Kartal, B.; Jetten, M.S.M.; Parey, K.; Barends, T.R.M.
Deposited on : 2018-08-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

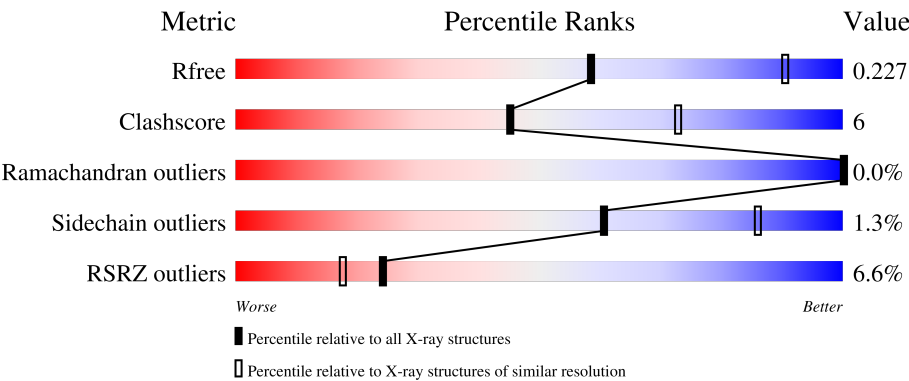
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	3% 79% 12% 9%
1	B	582	2% 80% 11% 9%
1	C	582	% 81% 11% 9%
1	D	582	4% 73% 18% 9%

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Mol	Chain	Length	Quality of chain
1	E	582	5% 81% 10% 9%
1	F	582	14% 80% 11% 9%
1	G	582	% 78% 13% 9%
1	H	582	% 78% 13% 9%
1	I	582	% 70% 19% 9%
1	J	582	% 79% 12% 9%
1	K	582	% 79% 13% 9%
1	L	582	% 80% 11% 9%
1	M	582	2% 82% 9% 9%
1	N	582	2% 80% 11% 9%
1	O	582	% 80% 11% 9%
1	P	582	2% 80% 11% 9%
1	Q	582	2% 79% 13% 9%
1	R	582	2% 78% 13% 9%
1	S	582	12% 80% 11% 9%
1	T	582	8% 80% 11% 9%
1	U	582	12% 82% 9% 9%
1	V	582	14% 81% 10% 9%
1	W	582	17% 79% 12% 9%
1	X	582	19% 80% 12% 9%
2	Y	114	5% 68% 8% 25%
2	Z	114	16% 69% 5% 25%
2	a	114	9% 68% 5% 25%
2	b	114	10% 67% 7% 25%
2	c	114	7% 68% 5% 25%

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Mol	Chain	Length	Quality of chain
2	d	114	
2	e	114	
2	f	114	
2	g	114	
2	h	114	
2	i	114	
2	j	114	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	G	610	-	-	X	-
4	SO4	J	611	-	-	X	-
5	GOL	H	614	-	-	X	-
5	GOL	H	615	-	-	X	-
5	GOL	I	614	-	-	X	-
5	GOL	K	614	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 118753 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 Hydrazine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	A	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	B	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	C	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	D	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	E	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	F	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	H	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	I	527	Total	C	N	O	S	0	0	0
			4201	2633	739	793	36			
1	J	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	K	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	L	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	M	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	N	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	O	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	P	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	R	531	Total	C	N	O	S	0	1	0
			4237	2653	749	799	36			
1	S	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	T	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	U	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	V	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	W	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	X	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

- Molecule 2 is a protein called hdh assembly factor Kustc1130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	Z	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	a	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	b	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	c	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	d	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	e	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	f	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	g	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	h	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	i	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	j	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

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



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

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

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

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

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

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

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

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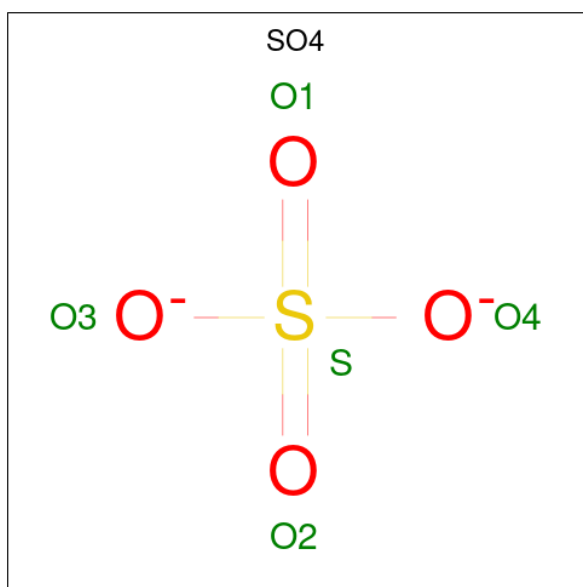
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

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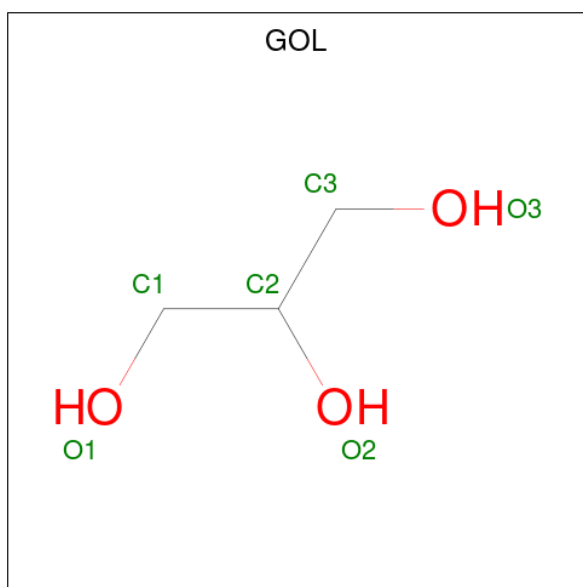
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	R	1	Total	O	S	0	0
			5	4	1		
4	R	1	Total	O	S	0	0
			5	4	1		
4	R	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	W	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	Y	1	Total	O	S	0	0
			5	4	1		
4	Y	1	Total	O	S	0	0
			5	4	1		
4	a	1	Total	O	S	0	0
			5	4	1		
4	c	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	K	0	0
			1	1		
6	K	1	Total	K	0	0
			1	1		
6	Q	1	Total	K	0	0
			1	1		
6	X	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	78	Total	O	0	0
			78	78		
7	A	33	Total	O	0	0
			33	33		
7	B	40	Total	O	0	0
			40	40		
7	C	36	Total	O	0	0
			36	36		
7	D	21	Total	O	0	0
			21	21		
7	E	21	Total	O	0	0
			21	21		
7	F	24	Total	O	0	0
			24	24		
7	H	70	Total	O	0	0
			70	70		
7	I	62	Total	O	0	0
			62	62		

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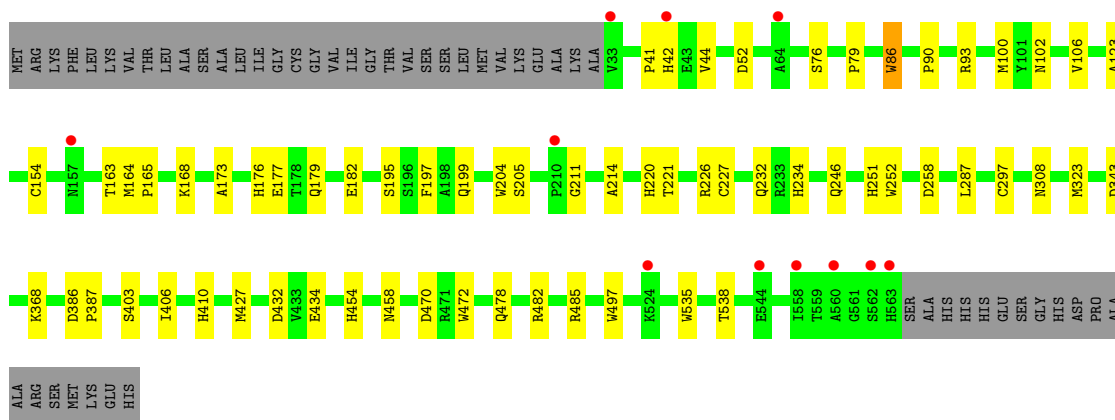
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	78	Total O 78 78	0	0
7	K	57	Total O 57 57	0	0
7	L	69	Total O 69 69	0	0
7	M	27	Total O 27 27	0	0
7	N	37	Total O 37 37	0	0
7	O	40	Total O 40 40	0	0
7	P	50	Total O 50 50	0	0
7	Q	48	Total O 48 48	0	0
7	R	49	Total O 49 49	0	0
7	S	4	Total O 4 4	0	0
7	T	15	Total O 15 15	0	0
7	U	15	Total O 15 15	0	0
7	V	17	Total O 17 17	0	0
7	W	12	Total O 12 12	0	0
7	X	13	Total O 13 13	0	0
7	Y	2	Total O 2 2	0	0
7	Z	1	Total O 1 1	0	0
7	a	2	Total O 2 2	0	0
7	b	2	Total O 2 2	0	0
7	c	2	Total O 2 2	0	0
7	d	2	Total O 2 2	0	0

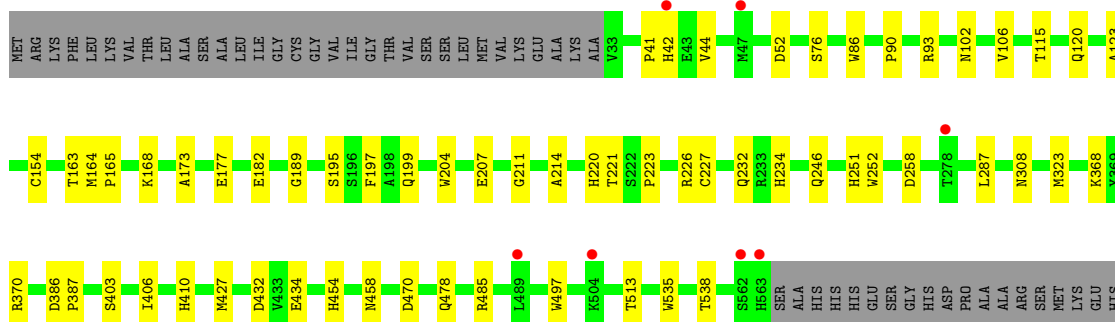
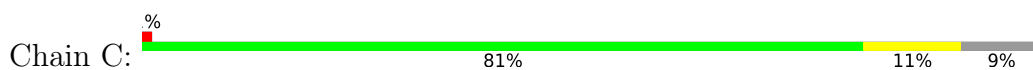
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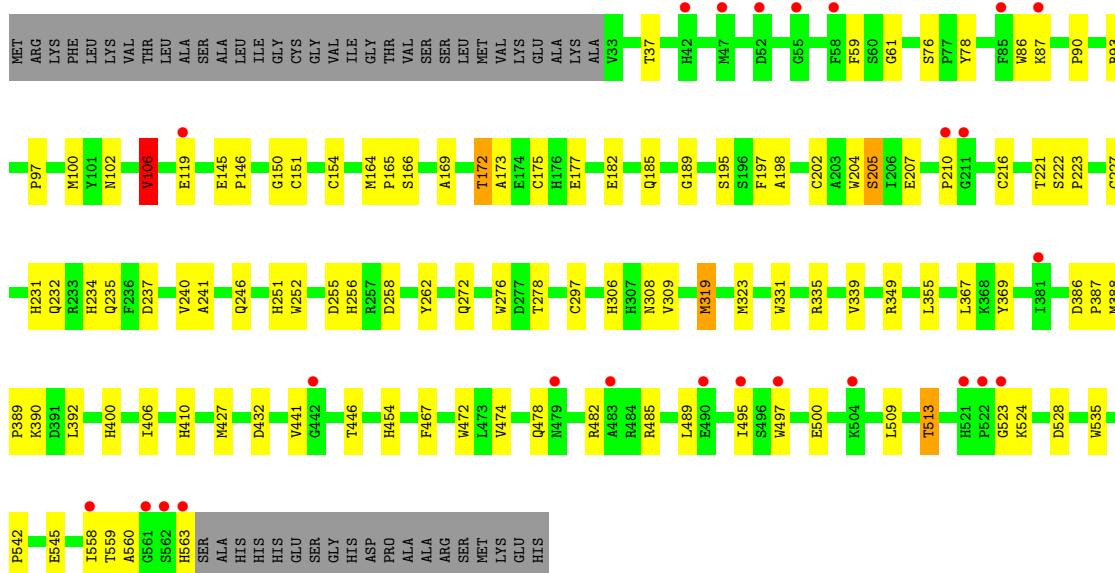
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	e	2	Total 2	O 2	0	0
7	f	2	Total 2	O 2	0	0
7	g	1	Total 1	O 1	0	0
7	i	2	Total 2	O 2	0	0
7	j	1	Total 1	O 1	0	0



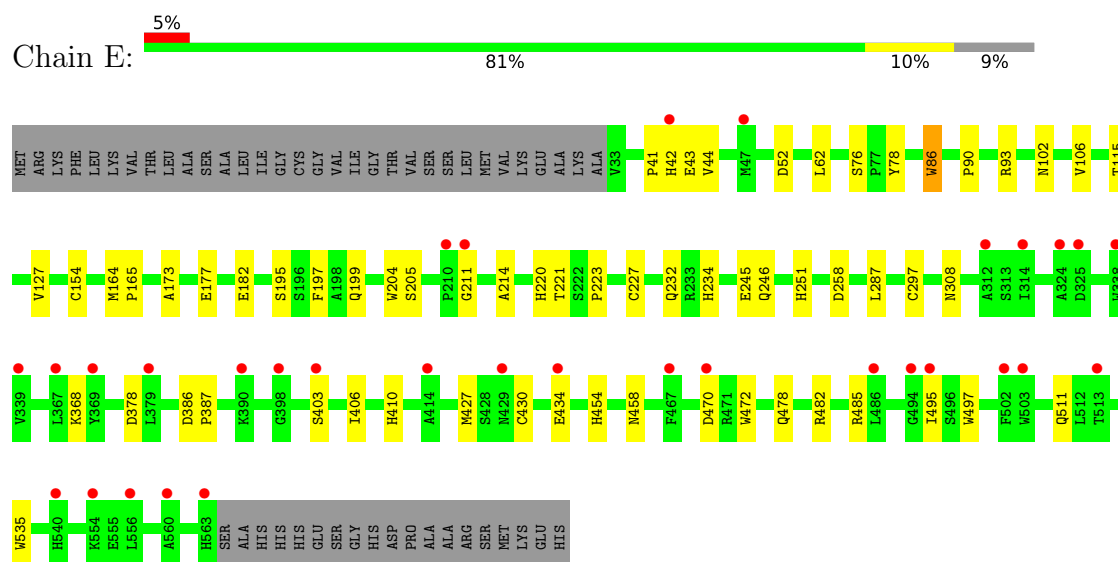
- Molecule 1: Hydrazine dehydrogenase



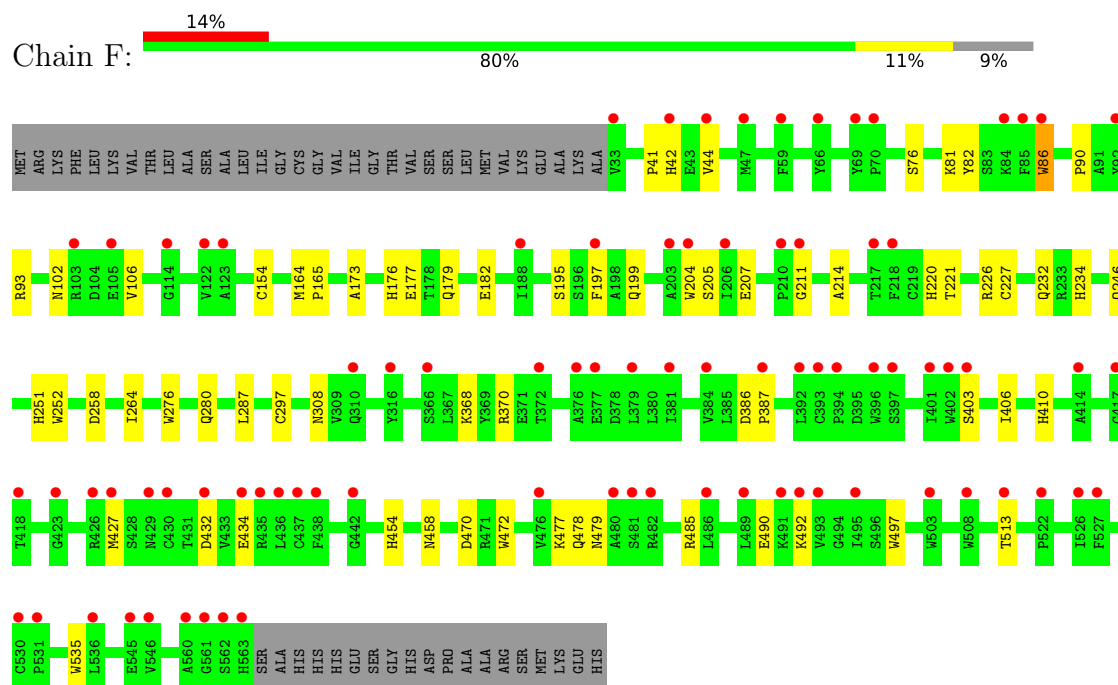
- Molecule 1: Hydrazine dehydrogenase



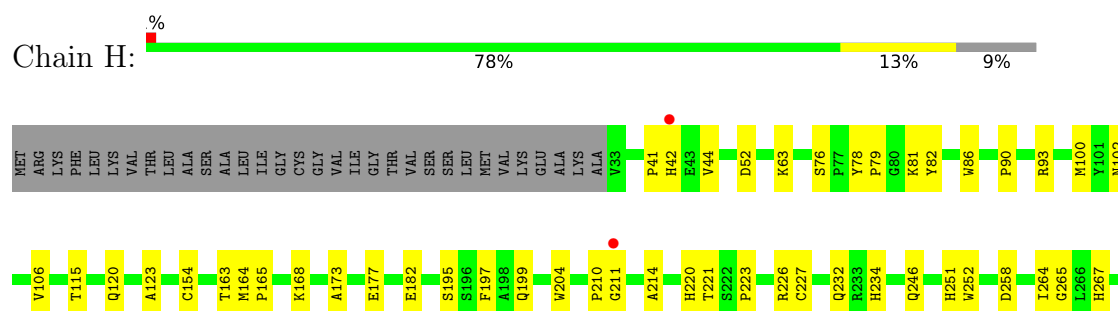
- Molecule 1: Hydrazine dehydrogenase

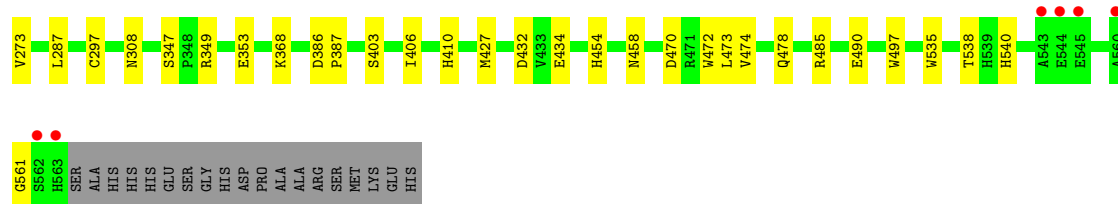


- Molecule 1: Hydrazine dehydrogenase



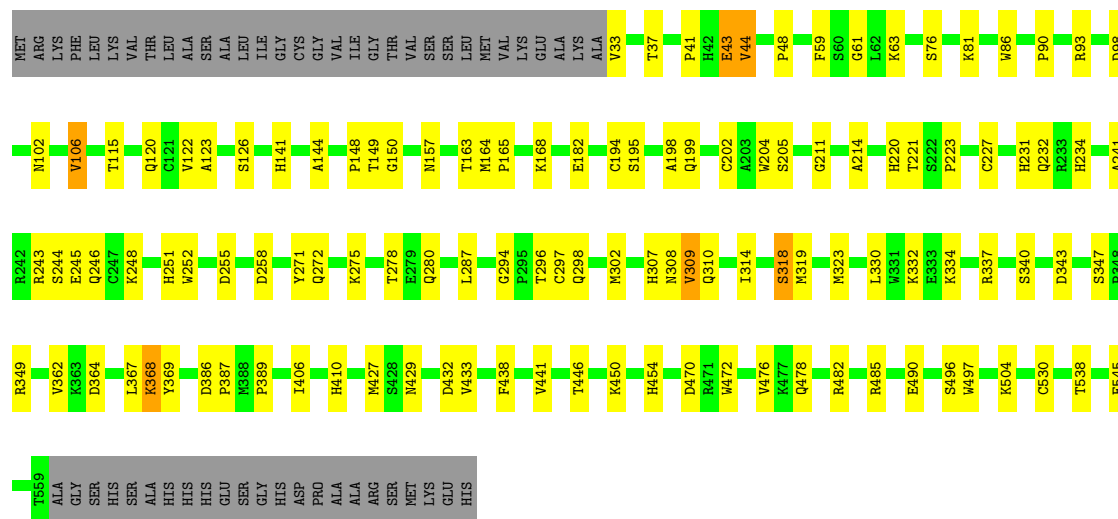
- Molecule 1: Hydrazine dehydrogenase





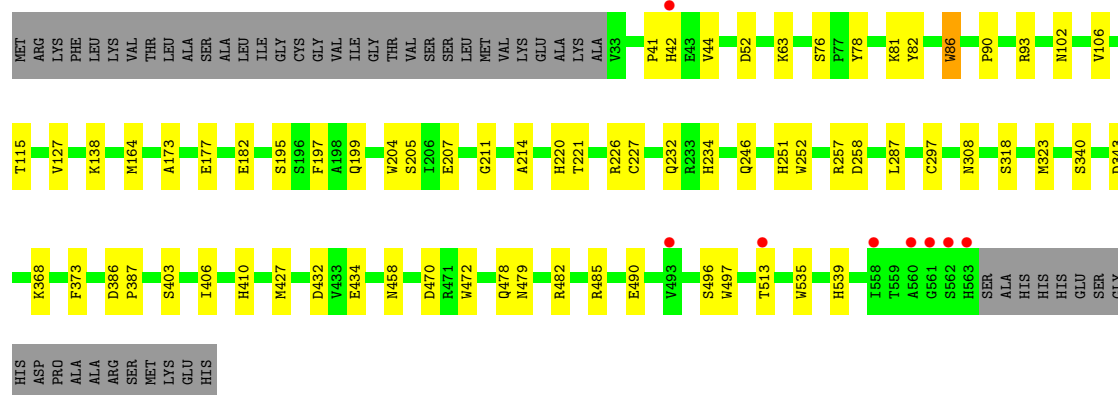
• Molecule 1: Hydrazine dehydrogenase

Chain I: 70% 19% 9%



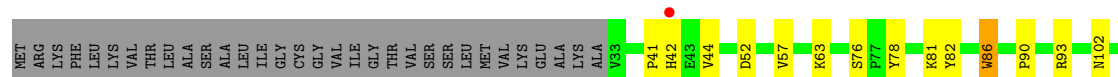
• Molecule 1: Hydrazine dehydrogenase

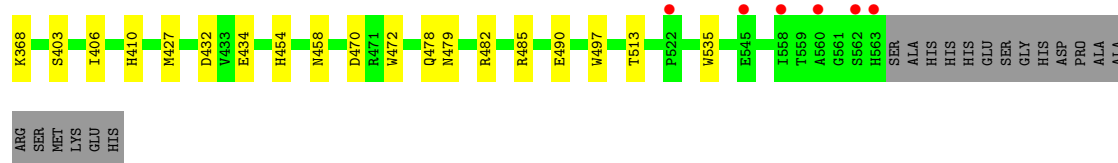
Chain J: 79% 12% 9%



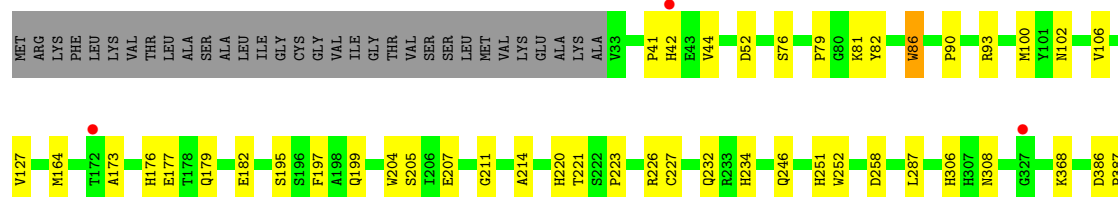
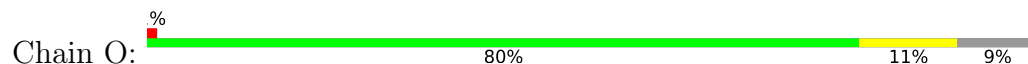
• Molecule 1: Hydrazine dehydrogenase

Chain K: 79% 13% 9%

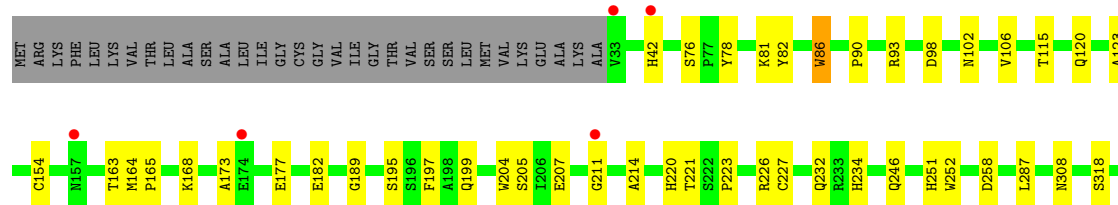
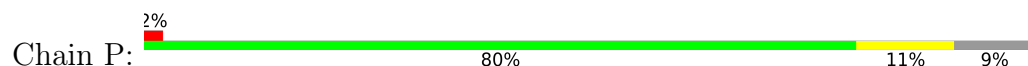




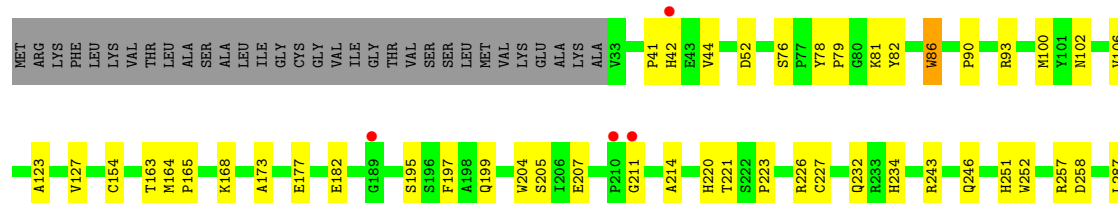
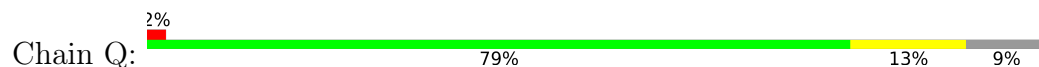
● Molecule 1: Hydrazine dehydrogenase

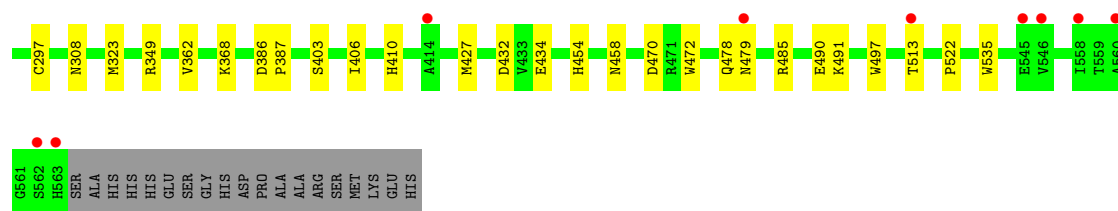


● Molecule 1: Hydrazine dehydrogenase

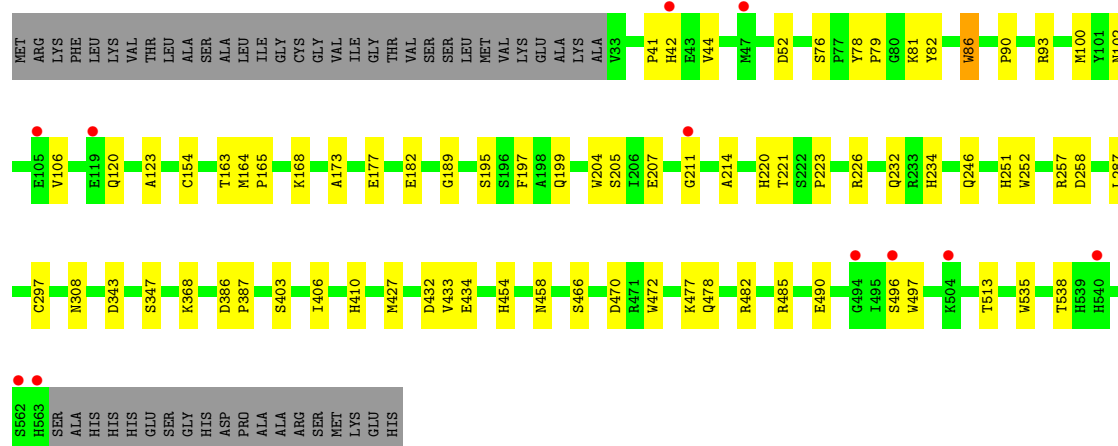
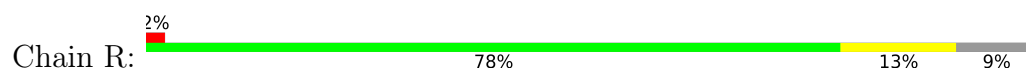


● Molecule 1: Hydrazine dehydrogenase

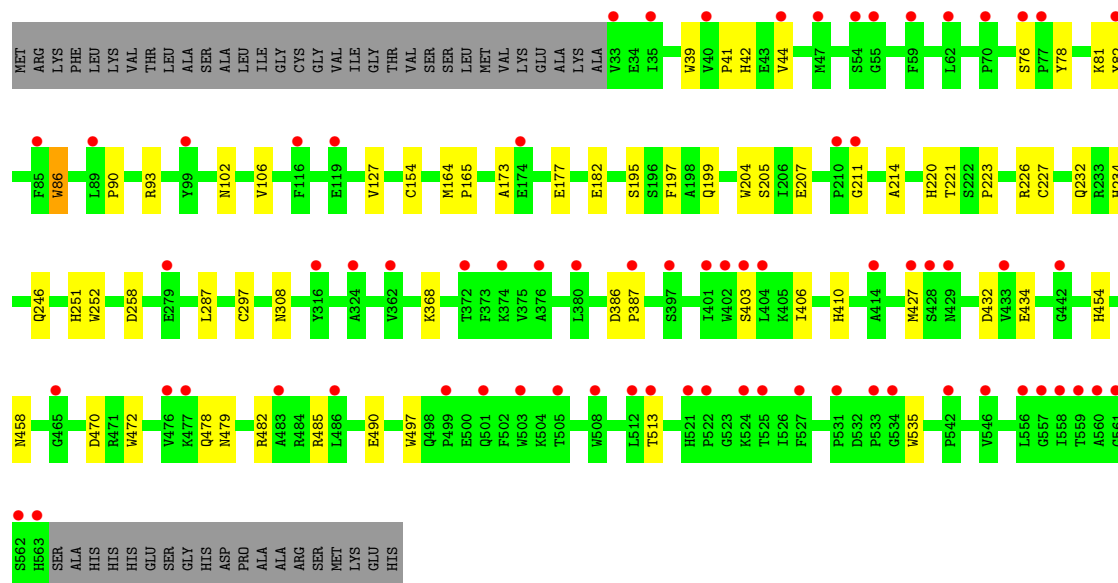
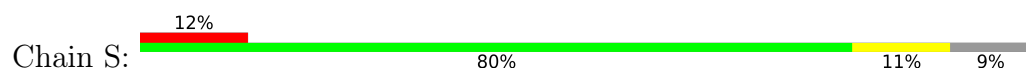




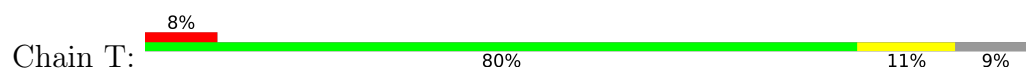
• Molecule 1: Hydrazine dehydrogenase

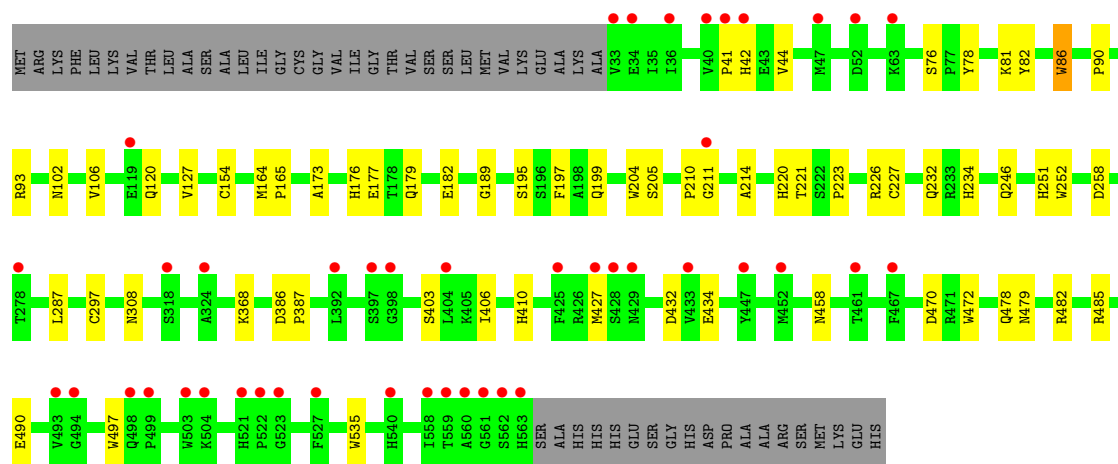


• Molecule 1: Hydrazine dehydrogenase

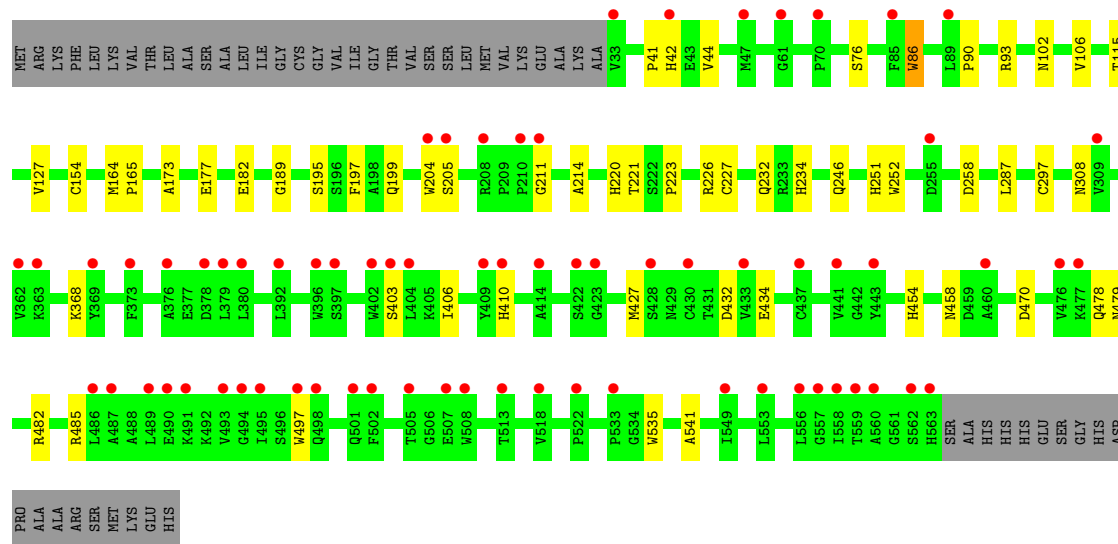
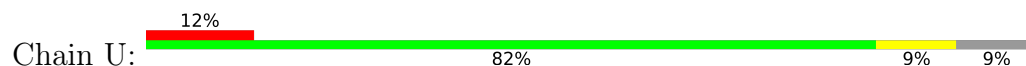


• Molecule 1: Hydrazine dehydrogenase

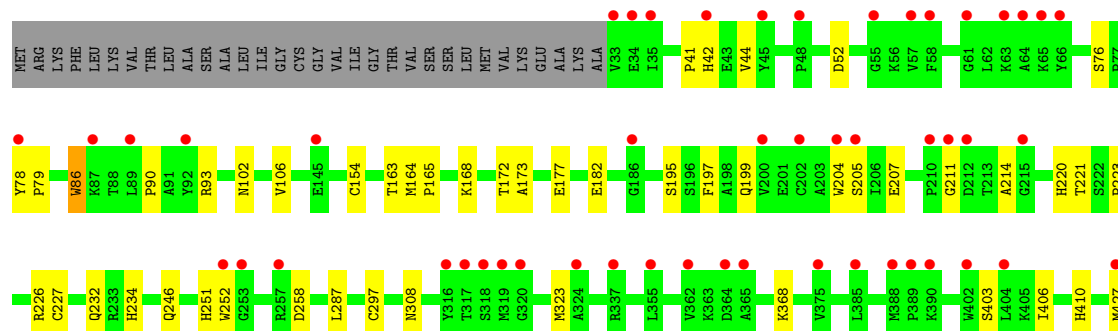
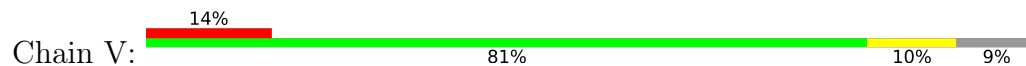


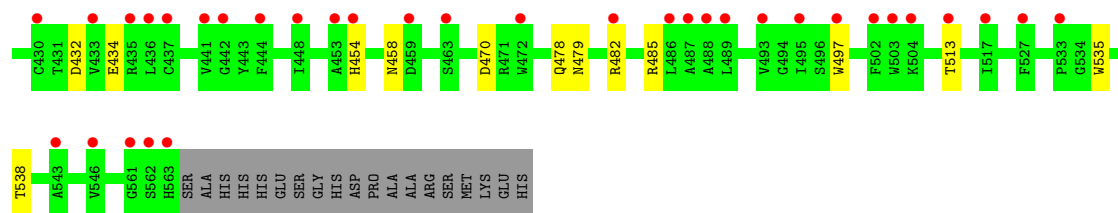


• Molecule 1: Hydrazine dehydrogenase

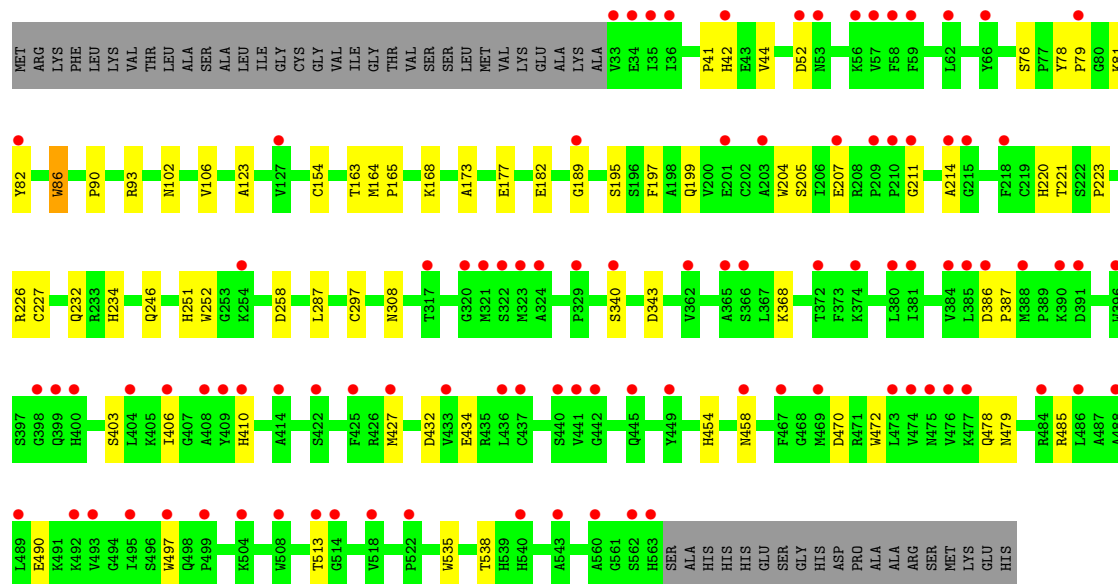
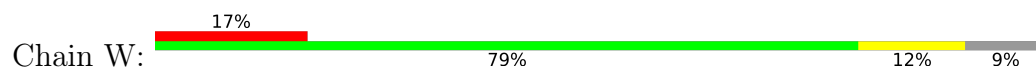


• Molecule 1: Hydrazine dehydrogenase

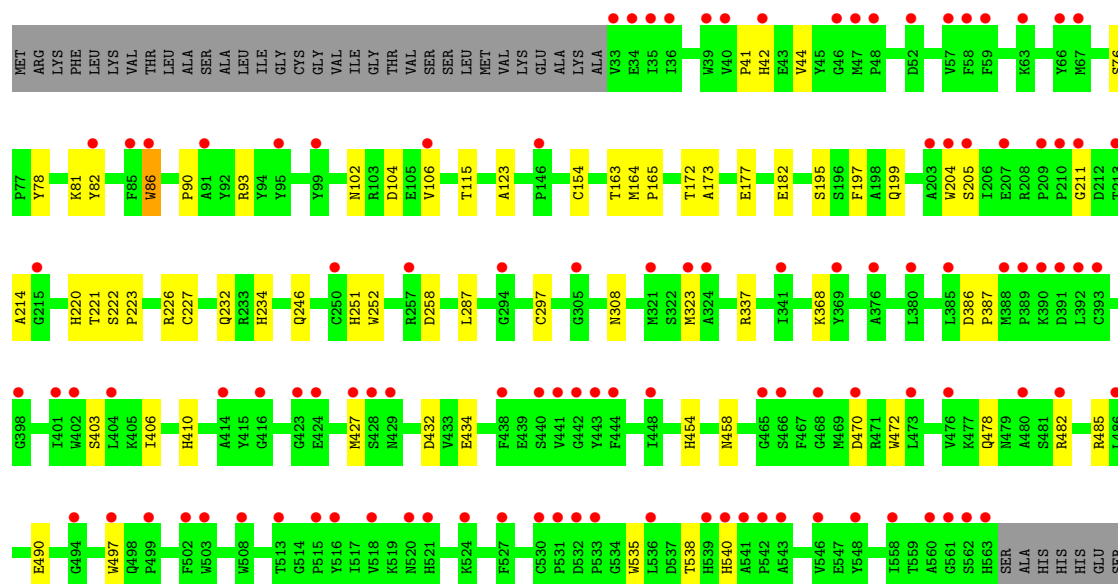
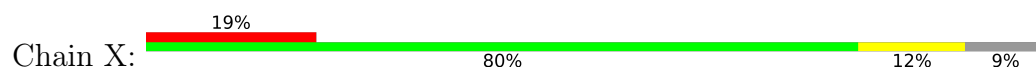




● Molecule 1: Hydrazine dehydrogenase



● Molecule 1: Hydrazine dehydrogenase



GLY
HIS
ASP
PRO
ALA
ALA
ARG
SER
MET
LYS
GLU
HIS

- Molecule 2: hdh assembly factor Kustc1130



MET LEU LYS LYS VAL VAL GLY MET MET PHE GLY ALA ALA LEU ILE ILE GLY GLY ILE ILE MET THR THR ALA ALA GLN ALA Y26 I38 L33 G41 E54 N61 E79 H80 F98 V99 S100 H109 P110 S111 GLY SER HIS

- Molecule 2: hdh assembly factor Kustc1130



MET LEU LYS LYS VAL VAL GLY MET MET PHE GLY ALA ALA LEU ILE ILE ILE ILE MET THR THR ALA ALA GLN ALA Y26 K32 L33 W34 A37 I38 A39 I40 G41 A47 E54 T57 N61 H78 E79 V69 I96 L97 F98 V99 S100 L101 D102 L103 A107 R108 H109 P110 S111 GLY SER HIS

- Molecule 2: hdh assembly factor Kustc1130



MET LEU LYS LYS VAL VAL GLY MET MET PHE GLY ALA ALA LEU ILE ILE ILE ILE MET THR THR ALA ALA GLN ALA Y26 I38 G41 A47 E54 T57 N61 E79 H80 F98 V99 S100 A107 R108 H109 P110 S111 GLY SER HIS

- Molecule 2: hdh assembly factor Kustc1130



MET LEU LYS LYS VAL VAL GLY MET MET PHE GLY ALA ALA LEU ILE ILE ILE ILE MET THR THR ALA ALA GLN ALA Y26 I38 G41 V51 G52 D53 E54 N61 F66 I75 E79 H78 H80 G81 G82 F98 V99 S100 R108 H109 P110 S111 GLY SER HIS

- Molecule 2: hdh assembly factor Kustc1130



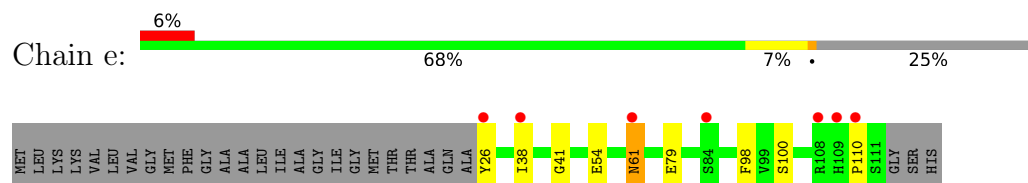
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- Molecule 2: hdh assembly factor Kustc1130

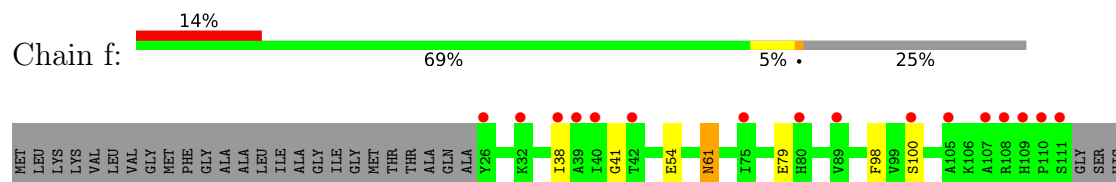


MET LEU LYS LYS VAL VAL GLY MET MET PHE GLY ALA ALA LEU ILE ILE ILE ILE MET THR THR ALA ALA GLN ALA Y26 I38 G41 E54 N61 E79 H80 F98 V99 S100 R108 H109 P110 S111 GLY SER HIS

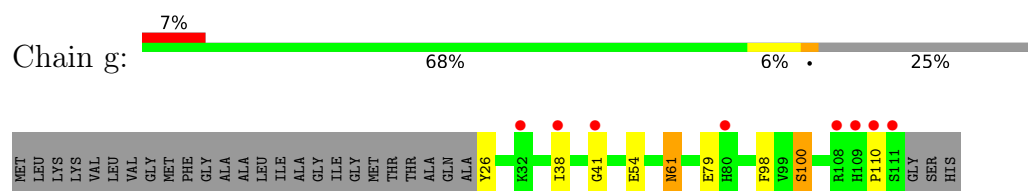
- Molecule 2: hdh assembly factor Kustc1130



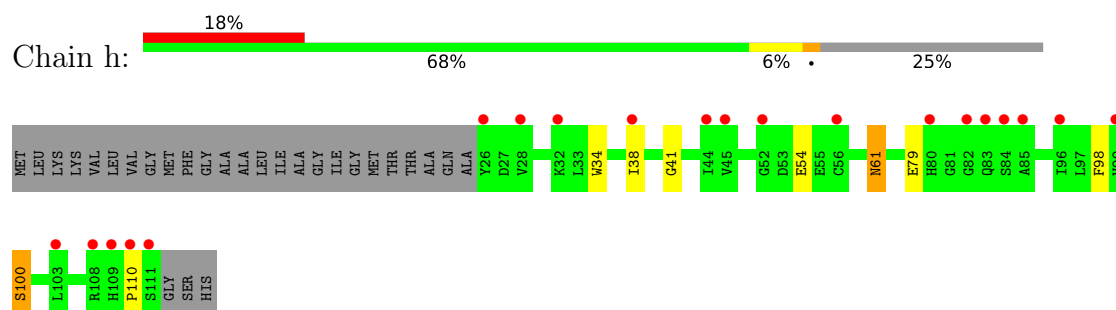
- Molecule 2: hdh assembly factor Kustc1130



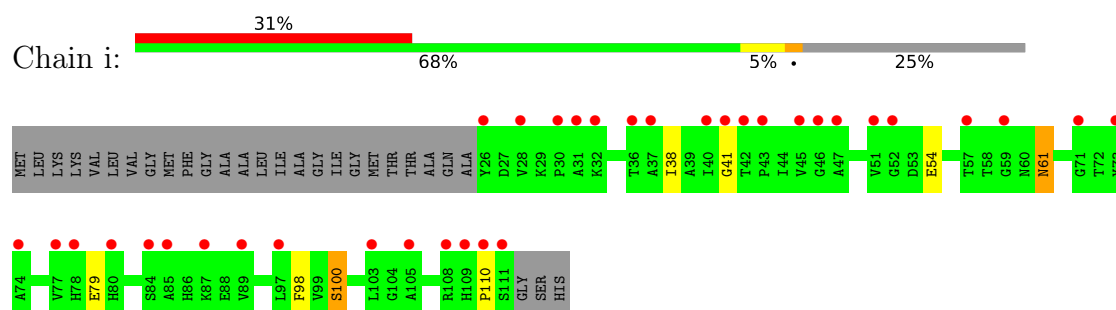
- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130

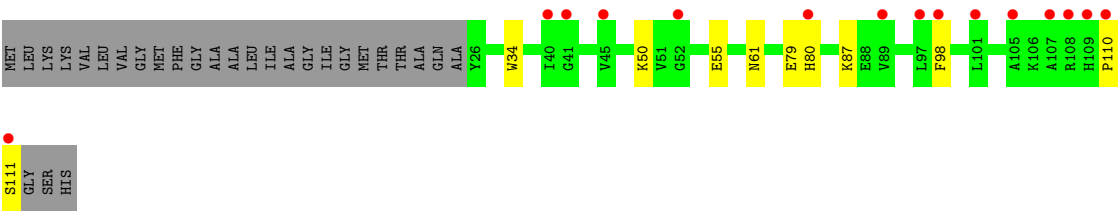


- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	211.86Å 211.86Å 398.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.71 – 2.80 93.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (93.71-2.80) 96.6 (93.71-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.221 , 0.238 (Not available) , 0.227	Depositor DCC
R_{free} test set	30022 reflections (6.09%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	118753	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, GOL, K, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/4355	0.91	0/5901
1	B	0.45	0/4355	0.90	0/5901
1	C	0.45	0/4355	0.92	0/5901
1	D	0.44	0/4355	0.95	0/5901
1	E	0.44	0/4355	0.91	0/5901
1	F	0.44	0/4355	0.91	0/5901
1	G	0.45	0/4355	0.91	0/5901
1	H	0.45	0/4355	0.91	0/5901
1	I	0.46	0/4329	0.95	0/5866
1	J	0.45	0/4355	0.90	0/5901
1	K	0.45	0/4355	0.90	0/5901
1	L	0.45	0/4355	0.91	0/5901
1	M	0.44	0/4355	0.91	0/5901
1	N	0.44	0/4355	0.91	0/5901
1	O	0.45	0/4355	0.90	0/5901
1	P	0.45	0/4355	0.91	0/5901
1	Q	0.45	0/4355	0.91	0/5901
1	R	0.45	0/4366	0.90	0/5915
1	S	0.44	0/4355	0.91	0/5901
1	T	0.44	0/4355	0.91	0/5901
1	U	0.44	0/4355	0.91	0/5901
1	V	0.44	0/4355	0.91	0/5901
1	W	0.44	0/4355	0.91	0/5901
1	X	0.44	0/4355	0.91	0/5901
2	Y	0.47	0/653	0.77	1/887 (0.1%)
2	Z	0.47	0/653	0.78	0/887
2	a	0.47	0/653	0.78	1/887 (0.1%)
2	b	0.47	0/653	0.77	1/887 (0.1%)
2	c	0.47	0/653	0.78	1/887 (0.1%)
2	d	0.48	0/653	0.78	1/887 (0.1%)
2	e	0.48	0/653	0.78	1/887 (0.1%)
2	f	0.47	0/653	0.78	1/887 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	g	0.47	0/653	0.78	1/887 (0.1%)
2	h	0.47	0/653	0.77	1/887 (0.1%)
2	i	0.48	0/653	0.77	1/887 (0.1%)
2	j	0.47	0/653	0.77	0/887
All	All	0.45	0/112341	0.90	10/152247 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	61	ASN	CB-CA-C	-5.58	101.53	110.79
2	e	61	ASN	CB-CA-C	-5.47	101.70	110.79
2	Y	61	ASN	CB-CA-C	-5.40	101.82	110.79
2	h	61	ASN	CB-CA-C	-5.36	101.89	110.79
2	d	61	ASN	CB-CA-C	-5.34	101.93	110.79
2	a	61	ASN	CB-CA-C	-5.25	102.07	110.79
2	g	61	ASN	CB-CA-C	-5.20	102.16	110.79
2	f	61	ASN	CB-CA-C	-5.17	102.22	110.79
2	i	61	ASN	CB-CA-C	-5.09	102.34	110.79
2	b	61	ASN	CB-CA-C	-5.05	102.40	110.79

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	4226	0	3941	52	1
1	B	4226	0	3941	51	0
1	C	4226	0	3941	52	0
1	D	4226	0	3941	75	0
1	E	4226	0	3941	49	0
1	F	4226	0	3941	46	0
1	G	4226	0	3941	71	2
1	H	4226	0	3941	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	4201	0	3921	101	0
1	J	4226	0	3941	62	1
1	K	4226	0	3941	70	0
1	L	4226	0	3941	53	0
1	M	4226	0	3941	44	0
1	N	4226	0	3941	51	0
1	O	4226	0	3941	51	0
1	P	4226	0	3941	55	0
1	Q	4226	0	3941	58	1
1	R	4237	0	3953	59	1
1	S	4226	0	3941	44	0
1	T	4226	0	3941	45	0
1	U	4226	0	3941	41	0
1	V	4226	0	3941	47	0
1	W	4226	0	3941	52	0
1	X	4226	0	3941	52	0
2	Y	640	0	627	5	0
2	Z	640	0	627	4	0
2	a	640	0	627	5	0
2	b	640	0	627	7	0
2	c	640	0	627	6	0
2	d	640	0	627	6	0
2	e	640	0	627	6	0
2	f	640	0	627	4	0
2	g	640	0	627	6	0
2	h	640	0	627	7	0
2	i	640	0	627	6	0
2	j	640	0	627	10	0
3	A	344	0	236	11	0
3	B	344	0	236	12	0
3	C	344	0	236	12	0
3	D	344	0	237	14	0
3	E	344	0	236	13	0
3	F	344	0	236	12	0
3	G	344	0	236	15	0
3	H	344	0	236	11	0
3	I	344	0	237	24	0
3	J	344	0	236	12	0
3	K	344	0	236	15	0
3	L	344	0	236	14	0
3	M	344	0	236	11	0
3	N	344	0	236	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	344	0	236	11	0
3	P	344	0	236	13	0
3	Q	344	0	236	17	0
3	R	344	0	236	14	0
3	S	344	0	236	14	0
3	T	344	0	236	11	0
3	U	344	0	236	14	0
3	V	344	0	236	14	0
3	W	344	0	236	17	0
3	X	344	0	236	14	0
4	A	15	0	0	0	0
4	B	10	0	0	1	0
4	C	15	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	30	0	0	3	0
4	H	25	0	0	1	0
4	I	20	0	0	0	0
4	J	15	0	0	2	0
4	K	15	0	0	0	0
4	L	20	0	0	1	0
4	M	20	0	0	0	0
4	N	15	0	0	1	0
4	O	15	0	0	0	0
4	P	5	0	0	0	0
4	Q	15	0	0	1	0
4	R	15	0	0	0	0
4	S	10	0	0	0	0
4	T	5	0	0	0	0
4	U	15	0	0	0	0
4	V	15	0	0	0	0
4	W	5	0	0	0	0
4	X	15	0	0	1	0
4	Y	10	0	0	0	0
4	a	5	0	0	0	0
4	c	5	0	0	0	0
5	A	18	0	24	2	0
5	D	6	0	8	0	0
5	G	12	0	16	2	0
5	H	12	0	16	20	0
5	I	18	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	12	0	16	3	0
5	K	24	0	32	14	0
5	L	6	0	8	1	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	Q	1	0	0	0	0
6	X	1	0	0	0	0
7	A	33	0	0	3	0
7	B	40	0	0	2	0
7	C	36	0	0	0	0
7	D	21	0	0	0	0
7	E	21	0	0	2	0
7	F	24	0	0	0	0
7	G	78	0	0	8	0
7	H	70	0	0	4	0
7	I	62	0	0	1	0
7	J	78	0	0	4	0
7	K	57	0	0	5	0
7	L	69	0	0	1	0
7	M	27	0	0	1	0
7	N	37	0	0	0	0
7	O	40	0	0	0	0
7	P	50	0	0	3	0
7	Q	48	0	0	4	0
7	R	49	0	0	5	0
7	S	4	0	0	0	0
7	T	15	0	0	1	0
7	U	15	0	0	0	0
7	V	17	0	0	0	0
7	W	12	0	0	0	0
7	X	13	0	0	0	0
7	Y	2	0	0	0	0
7	Z	1	0	0	0	0
7	a	2	0	0	0	0
7	b	2	0	0	0	0
7	c	2	0	0	1	0
7	d	2	0	0	0	0
7	e	2	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	i	2	0	0	0	0
7	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	118753	0	107910	1326	3

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 6.

All (1326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:HIS:HD1	5:H:614:GOL:H11	1.06	1.14
1:H:267:HIS:ND1	5:H:614:GOL:H11	1.65	1.12
1:H:267:HIS:HD1	5:H:614:GOL:C1	1.74	1.01
1:H:267:HIS:CE1	5:H:614:GOL:H31	2.01	0.96
1:I:406:ILE:H	1:I:410:HIS:HD2	1.14	0.95
1:B:406:ILE:H	1:B:410:HIS:HD2	1.16	0.93
5:H:615:GOL:H12	1:I:429:ASN:H	1.32	0.93
1:R:406:ILE:H	1:R:410:HIS:HD2	1.17	0.93
1:H:267:HIS:HE1	5:H:614:GOL:H31	1.32	0.92
1:N:406:ILE:H	1:N:410:HIS:HD2	1.17	0.92
1:G:406:ILE:H	1:G:410:HIS:HD2	1.16	0.92
1:Q:406:ILE:H	1:Q:410:HIS:HD2	1.17	0.92
1:A:406:ILE:H	1:A:410:HIS:HD2	1.16	0.91
1:H:474:VAL:HG22	5:H:615:GOL:H32	1.49	0.91
1:J:406:ILE:H	1:J:410:HIS:HD2	1.18	0.91
1:M:406:ILE:H	1:M:410:HIS:HD2	1.18	0.91
1:D:232:GLN:HE22	1:D:246:GLN:HE22	1.13	0.90
1:H:406:ILE:H	1:H:410:HIS:HD2	1.17	0.90
1:G:410:HIS:HA	5:G:616:GOL:H31	1.54	0.89
1:T:406:ILE:H	1:T:410:HIS:HD2	1.19	0.89
1:L:406:ILE:H	1:L:410:HIS:HD2	1.17	0.89
1:J:138:LYS:HE3	7:L:724:HOH:O	1.72	0.88
1:K:406:ILE:H	1:K:410:HIS:HD2	1.18	0.88
1:U:406:ILE:H	1:U:410:HIS:HD2	1.19	0.88
1:S:406:ILE:H	1:S:410:HIS:HD2	1.19	0.88
1:C:406:ILE:H	1:C:410:HIS:HD2	1.19	0.88
1:X:406:ILE:H	1:X:410:HIS:HD2	1.19	0.87
1:E:406:ILE:H	1:E:410:HIS:HD2	1.20	0.87
1:W:406:ILE:H	1:W:410:HIS:HD2	1.20	0.86
1:V:406:ILE:H	1:V:410:HIS:HD2	1.18	0.86
1:K:232:GLN:HE22	1:K:246:GLN:HE22	1.24	0.86
1:P:406:ILE:H	1:P:410:HIS:HD2	1.19	0.85
1:F:406:ILE:H	1:F:410:HIS:HD2	1.19	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:GLY:HA2	1:I:214:ALA:HB2	1.56	0.85
1:I:438:PHE:HZ	5:I:614:GOL:H31	1.41	0.84
1:O:406:ILE:H	1:O:410:HIS:HD2	1.18	0.84
1:L:232:GLN:HE22	1:L:246:GLN:HE22	1.26	0.84
1:W:232:GLN:HE22	1:W:246:GLN:HE22	1.27	0.82
1:R:232:GLN:HE22	1:R:246:GLN:HE22	1.27	0.81
1:E:232:GLN:HE22	1:E:246:GLN:HE22	1.27	0.81
1:J:232:GLN:HE22	1:J:246:GLN:HE22	1.27	0.81
1:X:232:GLN:HE22	1:X:246:GLN:HE22	1.29	0.81
1:D:207:GLU:HA	1:D:513:THR:OG1	1.79	0.81
1:J:76:SER:HB2	1:J:106:VAL:HG11	1.62	0.81
1:P:232:GLN:HE22	1:P:246:GLN:HE22	1.29	0.81
1:G:232:GLN:HE22	1:G:246:GLN:HE22	1.29	0.80
1:U:232:GLN:HE22	1:U:246:GLN:HE22	1.29	0.80
1:D:497:TRP:CD1	1:F:485:ARG:HD3	2.15	0.80
1:F:232:GLN:HE22	1:F:246:GLN:HE22	1.29	0.80
1:T:232:GLN:HE22	1:T:246:GLN:HE22	1.29	0.80
1:S:232:GLN:HE22	1:S:246:GLN:HE22	1.27	0.80
1:V:232:GLN:HE22	1:V:246:GLN:HE22	1.28	0.80
1:G:76:SER:HB2	1:G:106:VAL:HG11	1.64	0.80
1:Q:232:GLN:HE22	1:Q:246:GLN:HE22	1.30	0.80
1:B:76:SER:HB2	1:B:106:VAL:HG11	1.63	0.79
1:D:102:ASN:HD21	1:D:164:MET:H	1.27	0.79
1:N:232:GLN:HE22	1:N:246:GLN:HE22	1.30	0.79
1:C:163:THR:HG21	2:b:98:PHE:HB2	1.64	0.79
1:E:76:SER:HB2	1:E:106:VAL:HG11	1.64	0.79
1:H:454:HIS:HA	5:H:614:GOL:H2	1.61	0.79
1:C:232:GLN:HE22	1:C:246:GLN:HE22	1.31	0.79
1:C:76:SER:HB2	1:C:106:VAL:HG11	1.65	0.79
7:K:721:HOH:O	1:L:138:LYS:HE3	1.82	0.78
1:K:76:SER:HB2	1:K:106:VAL:HG11	1.65	0.78
1:O:232:GLN:HE22	1:O:246:GLN:HE22	1.32	0.78
1:N:76:SER:HB2	1:N:106:VAL:HG11	1.65	0.78
1:D:323:MET:HE1	1:E:52:ASP:HB2	1.66	0.78
1:H:76:SER:HB2	1:H:106:VAL:HG11	1.65	0.78
1:B:232:GLN:HE22	1:B:246:GLN:HE22	1.30	0.78
1:X:76:SER:HB2	1:X:106:VAL:HG11	1.66	0.77
1:F:76:SER:HB2	1:F:106:VAL:HG11	1.65	0.77
1:L:76:SER:HB2	1:L:106:VAL:HG11	1.63	0.77
1:S:76:SER:HB2	1:S:106:VAL:HG11	1.64	0.77
1:H:474:VAL:HG23	5:H:615:GOL:H11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:232:GLN:HE22	1:M:246:GLN:HE22	1.29	0.77
1:G:235:GLN:HE22	1:I:280:GLN:HE22	1.31	0.77
1:O:76:SER:HB2	1:O:106:VAL:HG11	1.65	0.77
1:W:163:THR:HG21	2:i:98:PHE:HB2	1.66	0.77
1:D:232:GLN:NE2	1:D:246:GLN:HE22	1.83	0.77
1:U:76:SER:HB2	1:U:106:VAL:HG11	1.67	0.77
1:M:76:SER:HB2	1:M:106:VAL:HG11	1.65	0.77
1:H:232:GLN:HE22	1:H:246:GLN:HE22	1.31	0.76
1:G:432:ASP:H	1:I:478:GLN:HE21	1.32	0.76
2:c:110:PRO:HG3	7:c:302:HOH:O	1.86	0.76
1:P:76:SER:HB2	1:P:106:VAL:HG11	1.67	0.76
1:H:267:HIS:CE1	5:H:614:GOL:H11	2.21	0.75
1:T:76:SER:HB2	1:T:106:VAL:HG11	1.65	0.75
1:I:102:ASN:HD21	1:I:164:MET:H	1.32	0.75
1:G:235:GLN:HE22	1:I:280:GLN:NE2	1.85	0.75
1:W:76:SER:HB2	1:W:106:VAL:HG11	1.68	0.75
1:I:232:GLN:HE22	1:I:246:GLN:HE22	1.33	0.75
1:A:76:SER:HB2	1:A:106:VAL:HG11	1.68	0.74
1:C:123:ALA:HB2	1:L:127:VAL:HG21	1.69	0.74
1:Q:76:SER:HB2	1:Q:106:VAL:HG11	1.67	0.74
1:R:76:SER:HB2	1:R:106:VAL:HG11	1.68	0.74
1:V:102:ASN:HD21	1:V:164:MET:H	1.36	0.74
1:A:232:GLN:HE22	1:A:246:GLN:HE22	1.33	0.74
1:H:540:HIS:HB2	7:H:770:HOH:O	1.87	0.74
1:G:163:THR:HG21	2:c:98:PHE:HB2	1.70	0.74
1:V:76:SER:HB2	1:V:106:VAL:HG11	1.67	0.74
1:A:400:HIS:H	5:A:613:GOL:H2	1.53	0.73
1:J:102:ASN:HD21	1:J:164:MET:H	1.34	0.73
1:P:102:ASN:HD21	1:P:164:MET:H	1.36	0.73
1:R:102:ASN:HD21	1:R:164:MET:H	1.36	0.73
1:O:102:ASN:HD21	1:O:164:MET:H	1.36	0.73
1:D:232:GLN:HE22	1:D:246:GLN:NE2	1.87	0.73
1:K:102:ASN:HD21	1:K:164:MET:H	1.35	0.73
1:K:132:ILE:HG12	5:K:614:GOL:H31	1.70	0.73
1:Q:102:ASN:HD21	1:Q:164:MET:H	1.36	0.73
1:G:343:ASP:HB2	7:G:701:HOH:O	1.89	0.72
1:R:163:THR:HG21	2:g:98:PHE:HB2	1.71	0.72
1:H:123:ALA:HB2	1:K:127:VAL:HG21	1.71	0.72
1:C:102:ASN:HD21	1:C:164:MET:H	1.36	0.72
1:M:102:ASN:HD21	1:M:164:MET:H	1.37	0.71
1:H:102:ASN:HD21	1:H:164:MET:H	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:318:SER:HB2	7:P:717:HOH:O	1.91	0.71
1:S:102:ASN:HD21	1:S:164:MET:H	1.38	0.71
1:N:127:VAL:HG21	1:R:123:ALA:HB2	1.71	0.71
1:I:163:THR:HG21	2:Y:98:PHE:HB2	1.73	0.70
1:G:102:ASN:HD21	1:G:164:MET:H	1.39	0.70
1:T:102:ASN:HD21	1:T:164:MET:H	1.37	0.70
1:I:406:ILE:H	1:I:410:HIS:CD2	2.04	0.70
1:I:438:PHE:CZ	5:I:614:GOL:H31	2.26	0.70
1:F:102:ASN:HD21	1:F:164:MET:H	1.37	0.70
1:J:127:VAL:HG21	1:P:123:ALA:HB2	1.73	0.70
1:G:343:ASP:CB	7:G:701:HOH:O	2.40	0.70
1:B:163:THR:HG21	2:a:98:PHE:HB2	1.74	0.70
1:A:102:ASN:HD21	1:A:164:MET:H	1.39	0.70
1:P:163:THR:HG21	2:e:98:PHE:HB2	1.74	0.70
1:L:102:ASN:HD21	1:L:164:MET:H	1.40	0.70
1:G:340:SER:O	7:G:701:HOH:O	2.10	0.69
1:E:102:ASN:HD21	1:E:164:MET:H	1.40	0.69
1:B:102:ASN:HD21	1:B:164:MET:H	1.39	0.69
1:X:163:THR:HG21	2:j:98:PHE:HB2	1.73	0.69
1:U:102:ASN:HD21	1:U:164:MET:H	1.39	0.69
3:O:600:HEC:HBC3	3:O:600:HEC:HHD	1.75	0.68
1:J:76:SER:HB2	1:J:106:VAL:CG1	2.23	0.68
1:X:102:ASN:HD21	1:X:164:MET:H	1.39	0.68
1:H:474:VAL:CG2	5:H:615:GOL:H32	2.22	0.68
3:I:600:HEC:HBC3	3:I:600:HEC:HHD	1.75	0.68
1:H:163:THR:HG21	2:d:98:PHE:HB2	1.76	0.68
1:G:76:SER:HB2	1:G:106:VAL:CG1	2.24	0.68
3:I:604:HEC:HBC1	3:I:605:HEC:HBB2	1.76	0.67
1:D:272:GLN:OE1	1:E:245:GLU:HG2	1.93	0.67
1:W:102:ASN:HD21	1:W:164:MET:H	1.40	0.67
1:B:76:SER:HB2	1:B:106:VAL:CG1	2.25	0.67
5:H:615:GOL:H12	1:I:429:ASN:N	2.08	0.67
1:W:168:LYS:HD3	2:i:61:ASN:O	1.93	0.67
3:F:600:HEC:HBC3	3:F:600:HEC:HHD	1.77	0.67
1:L:76:SER:HB2	1:L:106:VAL:CG1	2.24	0.67
3:G:600:HEC:HBC3	3:G:600:HEC:HHD	1.76	0.66
1:N:102:ASN:HD21	1:N:164:MET:H	1.41	0.66
3:D:604:HEC:HBC1	3:D:605:HEC:HBB2	1.76	0.66
1:D:172:THR:HG23	1:D:175:CYS:HB2	1.77	0.66
1:C:76:SER:HB2	1:C:106:VAL:CG1	2.26	0.66
1:K:234:HIS:HD1	5:K:614:GOL:H11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:604:HEC:HBC1	3:J:605:HEC:HBB2	1.78	0.66
1:T:76:SER:HB2	1:T:106:VAL:CG1	2.26	0.66
1:V:76:SER:HB2	1:V:106:VAL:CG1	2.26	0.66
3:L:600:HEC:HBC3	3:L:600:HEC:HHD	1.78	0.66
3:V:604:HEC:HBC1	3:V:605:HEC:HBB2	1.78	0.66
1:D:234:HIS:HD2	3:D:601:HEC:NC	1.93	0.65
1:D:182:GLU:O	1:D:308:ASN:HB2	1.97	0.65
1:G:235:GLN:NE2	1:I:280:GLN:HE22	1.94	0.65
1:M:76:SER:HB2	1:M:106:VAL:CG1	2.26	0.65
1:N:76:SER:HB2	1:N:106:VAL:CG1	2.27	0.65
2:Y:38:ILE:HD11	2:Y:100:SER:OG	1.97	0.65
2:d:38:ILE:HD11	2:d:100:SER:OG	1.97	0.65
1:F:76:SER:HB2	1:F:106:VAL:CG1	2.26	0.65
1:J:539:HIS:HE1	7:J:774:HOH:O	1.80	0.65
1:S:76:SER:HB2	1:S:106:VAL:CG1	2.26	0.65
3:W:604:HEC:HBC1	3:W:605:HEC:HBB2	1.79	0.65
1:G:226:ARG:NH2	3:I:607:HEC:O2A	2.30	0.65
1:H:76:SER:HB2	1:H:106:VAL:CG1	2.26	0.65
3:H:600:HEC:HBC3	3:H:600:HEC:HHD	1.79	0.65
3:K:600:HEC:HBC3	3:K:600:HEC:HHD	1.77	0.65
1:I:271:TYR:O	1:I:275:LYS:HB3	1.97	0.65
3:M:600:HEC:HBC3	3:M:600:HEC:HHD	1.80	0.64
1:O:76:SER:HB2	1:O:106:VAL:CG1	2.26	0.64
3:J:600:HEC:HBC3	3:J:600:HEC:HHD	1.79	0.64
1:R:76:SER:HB2	1:R:106:VAL:CG1	2.27	0.64
3:U:604:HEC:HBC1	3:U:605:HEC:HBB2	1.79	0.64
1:Q:76:SER:HB2	1:Q:106:VAL:CG1	2.27	0.64
1:G:123:ALA:HB2	1:E:127:VAL:HG21	1.80	0.64
1:E:76:SER:HB2	1:E:106:VAL:CG1	2.26	0.64
3:R:604:HEC:HBC1	3:R:605:HEC:HBB2	1.80	0.64
1:K:76:SER:HB2	1:K:106:VAL:CG1	2.26	0.64
1:K:411:ASP:H	5:K:613:GOL:H31	1.62	0.64
1:P:76:SER:HB2	1:P:106:VAL:CG1	2.27	0.64
3:B:604:HEC:HBC1	3:B:605:HEC:HBB2	1.79	0.64
1:V:163:THR:HG21	2:h:98:PHE:HB2	1.80	0.64
1:W:76:SER:HB2	1:W:106:VAL:CG1	2.28	0.64
3:X:600:HEC:HHD	3:X:600:HEC:HBC3	1.78	0.64
1:D:454:HIS:CD2	3:D:606:HEC:NC	2.66	0.64
1:A:76:SER:HB2	1:A:106:VAL:CG1	2.28	0.64
2:f:38:ILE:HD11	2:f:100:SER:OG	1.97	0.63
3:F:604:HEC:HBC1	3:F:605:HEC:HBB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:600:HEC:HBC3	3:T:600:HEC:HHD	1.81	0.63
3:W:600:HEC:HBC3	3:W:600:HEC:HHD	1.81	0.63
1:X:76:SER:HB2	1:X:106:VAL:CG1	2.27	0.63
1:G:432:ASP:H	1:I:478:GLN:NE2	1.96	0.63
1:U:76:SER:HB2	1:U:106:VAL:CG1	2.28	0.63
2:i:38:ILE:HD11	2:i:100:SER:OG	1.99	0.63
3:A:600:HEC:HBC3	3:A:600:HEC:HHD	1.81	0.63
1:J:226:ARG:HD3	7:J:708:HOH:O	1.99	0.63
3:V:600:HEC:HBC3	3:V:600:HEC:HHD	1.81	0.63
3:L:604:HEC:HBC1	3:L:605:HEC:HBB2	1.81	0.63
1:G:226:ARG:HH22	3:I:607:HEC:CGA	2.11	0.63
3:B:600:HEC:HBC3	3:B:600:HEC:HHD	1.80	0.63
1:I:340:SER:O	1:I:343:ASP:HB2	1.99	0.63
1:G:497:TRP:CD1	1:I:485:ARG:HD3	2.34	0.63
3:X:604:HEC:HBC1	3:X:605:HEC:HBB2	1.79	0.63
3:Q:600:HEC:HBC3	3:Q:600:HEC:HHD	1.81	0.63
3:S:600:HEC:HHD	3:S:600:HEC:HBC3	1.80	0.62
2:a:38:ILE:HD11	2:a:100:SER:OG	1.99	0.62
1:H:406:ILE:H	1:H:410:HIS:CD2	2.09	0.62
3:T:604:HEC:HBC1	3:T:605:HEC:HBB2	1.81	0.62
1:V:406:ILE:H	1:V:410:HIS:CD2	2.10	0.62
2:Z:38:ILE:HD11	2:Z:100:SER:OG	1.98	0.62
3:C:600:HEC:HBC3	3:C:600:HEC:HHD	1.80	0.62
1:I:182:GLU:O	1:I:308:ASN:HB2	1.99	0.62
3:R:600:HEC:HBC3	3:R:600:HEC:HHD	1.81	0.62
3:U:600:HEC:HBC3	3:U:600:HEC:HHD	1.81	0.62
1:B:406:ILE:H	1:B:410:HIS:CD2	2.09	0.62
1:Q:163:THR:HG21	2:f:98:PHE:HB2	1.80	0.62
1:R:168:LYS:HD3	2:g:61:ASN:O	2.00	0.62
3:D:600:HEC:HBC3	3:D:600:HEC:HHD	1.82	0.62
3:E:604:HEC:HBC1	3:E:605:HEC:HBB2	1.81	0.62
2:c:38:ILE:HD11	2:c:100:SER:OG	1.99	0.62
3:C:604:HEC:HBC1	3:C:605:HEC:HBB2	1.80	0.62
3:N:600:HEC:HHD	3:N:600:HEC:HBC3	1.82	0.61
1:H:474:VAL:HG22	5:H:615:GOL:C3	2.24	0.61
3:E:600:HEC:HBC3	3:E:600:HEC:HHD	1.81	0.61
1:H:454:HIS:CA	5:H:614:GOL:H2	2.29	0.61
1:I:98:ASP:OD2	1:I:168:LYS:HD2	2.00	0.61
1:L:84:LYS:HE2	4:L:610:SO4:S	2.41	0.61
2:e:38:ILE:HD11	2:e:100:SER:OG	2.00	0.61
2:h:38:ILE:HD11	2:h:100:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:406:ILE:H	1:L:410:HIS:CD2	2.09	0.61
1:R:406:ILE:H	1:R:410:HIS:CD2	2.09	0.61
3:P:604:HEC:HBC1	3:P:605:HEC:HBB2	1.82	0.60
3:S:604:HEC:HBC1	3:S:605:HEC:HBB2	1.81	0.60
1:I:251:HIS:HB3	1:I:258:ASP:HB2	1.81	0.60
1:X:234:HIS:HD2	3:X:601:HEC:NC	1.99	0.60
3:A:604:HEC:HBC1	3:A:605:HEC:HBB2	1.83	0.60
3:P:600:HEC:HBC3	3:P:600:HEC:HH2	1.81	0.60
3:Q:604:HEC:HBC1	3:Q:605:HEC:HBB2	1.81	0.60
1:T:210:PRO:HA	7:T:707:HOH:O	2.01	0.60
1:V:168:LYS:HD3	2:h:61:ASN:O	2.01	0.60
1:U:234:HIS:HD2	3:U:601:HEC:NC	2.00	0.60
1:W:234:HIS:HD2	3:W:601:HEC:NC	1.99	0.60
1:G:479:ASN:HD22	1:I:482:ARG:HH12	1.50	0.60
1:G:485:ARG:HD3	1:H:497:TRP:CD1	2.37	0.60
1:D:251:HIS:HB3	1:D:258:ASP:HB2	1.83	0.60
1:D:478:GLN:O	1:D:482:ARG:HG2	2.02	0.60
2:b:38:ILE:HD11	2:b:100:SER:OG	2.02	0.60
1:C:120:GLN:HA	1:L:127:VAL:HG11	1.82	0.59
1:N:211:GLY:HA2	1:N:214:ALA:HB2	1.84	0.59
1:N:234:HIS:HD2	3:N:601:HEC:NC	2.00	0.59
1:A:211:GLY:HA2	1:A:214:ALA:HB2	1.84	0.59
3:K:604:HEC:HBC1	3:K:605:HEC:HBB2	1.82	0.59
1:P:234:HIS:HD2	3:P:601:HEC:NC	2.00	0.59
1:G:182:GLU:O	1:G:308:ASN:HB2	2.03	0.59
1:I:165:PRO:HG2	3:I:601:HEC:HMD2	1.84	0.59
3:N:604:HEC:HBC1	3:N:605:HEC:HBB2	1.84	0.59
1:E:234:HIS:HD2	3:E:601:HEC:NC	2.00	0.59
1:H:168:LYS:HD3	2:d:61:ASN:O	2.03	0.59
1:G:234:HIS:HD2	3:G:601:HEC:NC	2.00	0.59
1:D:102:ASN:ND2	1:D:164:MET:H	1.99	0.59
1:P:211:GLY:HA2	1:P:214:ALA:HB2	1.84	0.59
1:X:406:ILE:H	1:X:410:HIS:CD2	2.11	0.59
1:F:406:ILE:H	1:F:410:HIS:CD2	2.11	0.59
1:J:482:ARG:NH1	4:J:611:SO4:O3	2.36	0.59
1:J:234:HIS:HD2	3:J:601:HEC:NC	2.00	0.59
1:T:234:HIS:HD2	3:T:601:HEC:NC	1.99	0.59
2:g:38:ILE:HD11	2:g:100:SER:OG	2.03	0.59
1:H:234:HIS:HD2	3:H:601:HEC:NC	2.01	0.59
1:K:406:ILE:H	1:K:410:HIS:CD2	2.10	0.59
1:L:234:HIS:HD2	3:L:601:HEC:NC	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:H	1:A:410:HIS:CD2	2.09	0.58
1:X:211:GLY:HA2	1:X:214:ALA:HB2	1.84	0.58
1:Q:234:HIS:HD2	3:Q:601:HEC:NC	2.00	0.58
1:V:234:HIS:HD2	3:V:601:HEC:NC	1.98	0.58
1:M:234:HIS:HD2	3:M:601:HEC:NC	1.99	0.58
1:B:538:THR:HA	2:a:110:PRO:HA	1.85	0.58
1:C:406:ILE:H	1:C:410:HIS:CD2	2.11	0.58
1:Q:406:ILE:H	1:Q:410:HIS:CD2	2.09	0.58
1:W:211:GLY:HA2	1:W:214:ALA:HB2	1.86	0.58
1:I:211:GLY:HA2	1:I:214:ALA:CB	2.30	0.58
1:A:343:ASP:HB3	7:A:715:HOH:O	2.02	0.58
1:B:211:GLY:HA2	1:B:214:ALA:HB2	1.86	0.58
1:S:211:GLY:HA2	1:S:214:ALA:HB2	1.85	0.58
1:F:234:HIS:HD2	3:F:601:HEC:NC	2.01	0.58
1:C:168:LYS:HD3	2:b:61:ASN:O	2.04	0.58
1:J:211:GLY:HA2	1:J:214:ALA:HB2	1.86	0.58
1:U:182:GLU:O	1:U:308:ASN:HB2	2.03	0.58
1:D:297:CYS:HB3	3:D:605:HEC:HMB1	1.85	0.58
3:H:604:HEC:HBC1	3:H:605:HEC:HBB2	1.84	0.58
1:K:234:HIS:HD2	3:K:601:HEC:NC	2.02	0.58
1:W:406:ILE:H	1:W:410:HIS:CD2	2.12	0.58
1:R:211:GLY:HA2	1:R:214:ALA:HB2	1.86	0.57
1:C:538:THR:HA	2:b:110:PRO:HA	1.86	0.57
1:K:211:GLY:HA2	1:K:214:ALA:HB2	1.85	0.57
1:U:211:GLY:HA2	1:U:214:ALA:HB2	1.85	0.57
1:C:211:GLY:HA2	1:C:214:ALA:HB2	1.87	0.57
1:E:211:GLY:HA2	1:E:214:ALA:HB2	1.86	0.57
1:H:182:GLU:O	1:H:308:ASN:HB2	2.03	0.57
1:S:234:HIS:HD2	3:S:601:HEC:NC	2.01	0.57
1:A:182:GLU:O	1:A:308:ASN:HB2	2.04	0.57
1:B:123:ALA:HB2	1:U:127:VAL:HG21	1.86	0.57
1:H:273:VAL:HG13	1:I:243:ARG:HG3	1.87	0.57
1:R:538:THR:HA	2:g:110:PRO:HA	1.87	0.57
1:B:234:HIS:HD2	3:B:601:HEC:NC	2.02	0.57
1:O:211:GLY:HA2	1:O:214:ALA:HB2	1.86	0.57
1:A:234:HIS:HD2	3:A:601:HEC:NC	2.01	0.57
1:D:237:ASP:HB3	1:D:240:VAL:HG22	1.85	0.57
1:F:211:GLY:HA2	1:F:214:ALA:HB2	1.86	0.57
1:A:226:ARG:HD3	7:A:702:HOH:O	2.04	0.57
1:R:234:HIS:HD2	3:R:601:HEC:NC	2.02	0.57
1:E:182:GLU:O	1:E:308:ASN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:182:GLU:O	1:W:308:ASN:HB2	2.04	0.57
1:C:234:HIS:HD2	3:C:601:HEC:NC	2.00	0.56
1:I:245:GLU:O	1:I:248:LYS:HG2	2.05	0.56
1:S:182:GLU:O	1:S:308:ASN:HB2	2.05	0.56
1:G:406:ILE:H	1:G:410:HIS:CD2	2.09	0.56
1:N:406:ILE:H	1:N:410:HIS:CD2	2.09	0.56
1:O:234:HIS:HD2	3:O:601:HEC:NC	2.02	0.56
1:P:406:ILE:H	1:P:410:HIS:CD2	2.11	0.56
1:Q:182:GLU:O	1:Q:308:ASN:HB2	2.05	0.56
1:G:251:HIS:HB3	1:G:258:ASP:HB2	1.88	0.56
1:H:195:SER:HB2	1:H:221:THR:HA	1.87	0.56
1:J:251:HIS:HB3	1:J:258:ASP:HB2	1.87	0.56
1:K:182:GLU:O	1:K:308:ASN:HB2	2.05	0.56
1:M:211:GLY:HA2	1:M:214:ALA:HB2	1.87	0.56
1:Q:211:GLY:HA2	1:Q:214:ALA:HB2	1.87	0.56
1:V:211:GLY:HA2	1:V:214:ALA:HB2	1.86	0.56
1:B:168:LYS:HD3	2:a:61:ASN:O	2.06	0.56
1:U:251:HIS:HB3	1:U:258:ASP:HB2	1.88	0.56
1:H:211:GLY:HA2	1:H:214:ALA:HB2	1.86	0.56
1:J:127:VAL:HG11	1:P:120:GLN:HA	1.87	0.56
1:L:182:GLU:OE1	2:e:26:TYR:HB3	2.05	0.56
1:R:195:SER:HB2	1:R:221:THR:HA	1.88	0.56
3:G:604:HEC:HBC1	3:G:605:HEC:HBB2	1.88	0.56
1:I:81:LYS:NZ	1:I:530:CYS:O	2.36	0.56
1:J:182:GLU:O	1:J:308:ASN:HB2	2.05	0.56
1:L:182:GLU:O	1:L:308:ASN:HB2	2.05	0.56
1:V:182:GLU:O	1:V:308:ASN:HB2	2.05	0.56
1:X:251:HIS:HB3	1:X:258:ASP:HB2	1.88	0.56
1:N:182:GLU:O	1:N:308:ASN:HB2	2.06	0.56
1:J:368:LYS:HE2	1:J:470:ASP:OD1	2.06	0.56
3:O:604:HEC:HBC1	3:O:605:HEC:HBB2	1.86	0.56
1:S:251:HIS:HB3	1:S:258:ASP:HB2	1.88	0.56
1:G:211:GLY:HA2	1:G:214:ALA:HB2	1.86	0.56
1:G:226:ARG:HD3	7:G:724:HOH:O	2.05	0.55
1:L:251:HIS:HB3	1:L:258:ASP:HB2	1.89	0.55
1:O:406:ILE:H	1:O:410:HIS:CD2	2.10	0.55
1:T:182:GLU:O	1:T:308:ASN:HB2	2.06	0.55
1:E:368:LYS:HE2	1:E:470:ASP:OD1	2.07	0.55
1:W:251:HIS:HB3	1:W:258:ASP:HB2	1.87	0.55
1:K:485:ARG:HD3	1:L:497:TRP:CD1	2.42	0.55
1:O:251:HIS:HB3	1:O:258:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:306:HIS:HD2	2:Y:26:TYR:CD2	2.25	0.55
1:W:538:THR:HA	2:i:110:PRO:HA	1.87	0.55
1:X:182:GLU:O	1:X:308:ASN:HB2	2.07	0.55
1:K:251:HIS:HB3	1:K:258:ASP:HB2	1.88	0.55
1:G:479:ASN:ND2	1:I:482:ARG:HH12	2.04	0.55
1:C:182:GLU:O	1:C:308:ASN:HB2	2.07	0.55
1:F:182:GLU:O	1:F:308:ASN:HB2	2.06	0.55
3:K:601:HEC:O1A	5:K:614:GOL:H32	2.06	0.55
1:L:211:GLY:HA2	1:L:214:ALA:HB2	1.87	0.55
1:M:182:GLU:O	1:M:308:ASN:HB2	2.07	0.55
1:P:168:LYS:HD3	2:e:61:ASN:O	2.06	0.55
1:R:182:GLU:O	1:R:308:ASN:HB2	2.07	0.55
1:B:485:ARG:HD3	1:C:497:TRP:CD1	2.42	0.55
1:K:132:ILE:HG12	5:K:614:GOL:H11	1.88	0.55
1:Q:251:HIS:HB3	1:Q:258:ASP:HB2	1.89	0.55
1:X:540:HIS:HD2	2:j:111:SER:HB3	1.71	0.55
1:I:195:SER:HB2	1:I:221:THR:HA	1.89	0.55
1:T:251:HIS:HB3	1:T:258:ASP:HB2	1.88	0.55
1:V:251:HIS:HB3	1:V:258:ASP:HB2	1.89	0.55
1:I:232:GLN:HE22	1:I:246:GLN:NE2	2.02	0.55
1:Q:123:ALA:HB2	1:T:127:VAL:HG21	1.89	0.55
1:T:406:ILE:H	1:T:410:HIS:CD2	2.11	0.55
1:I:504:LYS:HG3	7:I:734:HOH:O	2.05	0.54
1:P:182:GLU:O	1:P:308:ASN:HB2	2.07	0.54
1:P:251:HIS:HB3	1:P:258:ASP:HB2	1.89	0.54
1:B:251:HIS:HB3	1:B:258:ASP:HB2	1.90	0.54
1:M:251:HIS:HB3	1:M:258:ASP:HB2	1.88	0.54
1:N:251:HIS:HB3	1:N:258:ASP:HB2	1.90	0.54
1:A:163:THR:HG21	2:Z:98:PHE:HB2	1.89	0.54
1:H:251:HIS:HB3	1:H:258:ASP:HB2	1.90	0.54
1:I:337:ARG:O	1:I:340:SER:HB2	2.07	0.54
1:P:195:SER:HB2	1:P:221:THR:HA	1.90	0.54
1:W:195:SER:HB2	1:W:221:THR:HA	1.90	0.54
1:F:251:HIS:HB3	1:F:258:ASP:HB2	1.89	0.54
3:K:607:HEC:CGA	1:L:226:ARG:HH22	2.21	0.54
1:X:540:HIS:CD2	2:j:111:SER:HB3	2.43	0.54
3:I:601:HEC:HBA1	3:I:601:HEC:HHA	1.90	0.54
1:O:182:GLU:O	1:O:308:ASN:HB2	2.08	0.54
1:R:251:HIS:HB3	1:R:258:ASP:HB2	1.89	0.54
3:V:607:HEC:CGA	1:W:226:ARG:HH22	2.21	0.54
1:X:538:THR:HA	2:j:110:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:HIS:HB3	1:E:258:ASP:HB2	1.90	0.53
1:A:368:LYS:HE2	1:A:470:ASP:OD1	2.07	0.53
1:K:132:ILE:CG1	5:K:614:GOL:H31	2.38	0.53
1:R:368:LYS:HE2	1:R:470:ASP:OD1	2.08	0.53
1:D:255:ASP:HB2	1:D:319:MET:HE3	1.90	0.53
1:J:485:ARG:HD3	1:K:497:TRP:CD1	2.43	0.53
3:M:604:HEC:HBC1	3:M:605:HEC:HBB2	1.89	0.53
1:T:211:GLY:HA2	1:T:214:ALA:HB2	1.89	0.53
1:B:195:SER:HB2	1:B:221:THR:HA	1.91	0.53
1:J:497:TRP:CD1	1:L:485:ARG:HD3	2.43	0.53
3:I:600:HEC:HHD	3:I:600:HEC:CBC	2.39	0.53
1:U:406:ILE:H	1:U:410:HIS:CD2	2.11	0.53
1:P:485:ARG:HD3	1:Q:497:TRP:CD1	2.44	0.53
1:S:406:ILE:H	1:S:410:HIS:CD2	2.11	0.53
1:V:195:SER:HB2	1:V:221:THR:HA	1.91	0.53
1:G:195:SER:HB2	1:G:221:THR:HA	1.91	0.53
1:K:146:PRO:HD2	7:K:735:HOH:O	2.09	0.53
1:M:485:ARG:HD3	1:N:497:TRP:CD1	2.44	0.53
1:T:368:LYS:HE2	1:T:470:ASP:OD1	2.09	0.53
1:T:478:GLN:HE21	1:U:432:ASP:HB2	1.74	0.53
1:G:168:LYS:HD3	2:c:61:ASN:O	2.09	0.53
1:C:251:HIS:HB3	1:C:258:ASP:HB2	1.91	0.53
1:J:226:ARG:HH22	3:L:607:HEC:CGA	2.22	0.53
1:Q:485:ARG:HD3	1:R:497:TRP:CD1	2.44	0.53
1:R:343:ASP:CB	7:R:701:HOH:O	2.57	0.53
1:A:497:TRP:CD1	1:C:485:ARG:HD3	2.44	0.52
1:I:255:ASP:HB3	5:I:614:GOL:H2	1.91	0.52
1:K:234:HIS:HE1	5:K:614:GOL:O3	1.92	0.52
1:M:406:ILE:H	1:M:410:HIS:CD2	2.10	0.52
1:T:195:SER:HB2	1:T:221:THR:HA	1.91	0.52
1:V:368:LYS:HE2	1:V:470:ASP:OD1	2.09	0.52
1:A:251:HIS:HB3	1:A:258:ASP:HB2	1.90	0.52
1:D:173:ALA:HA	1:D:177:GLU:HB2	1.90	0.52
1:D:406:ILE:H	1:D:410:HIS:HD2	1.57	0.52
1:H:368:LYS:HE2	1:H:470:ASP:OD1	2.08	0.52
1:X:368:LYS:HE2	1:X:470:ASP:OD1	2.09	0.52
1:D:90:PRO:O	1:D:93:ARG:HG2	2.09	0.52
1:N:485:ARG:HD3	1:O:497:TRP:CD1	2.44	0.52
1:J:406:ILE:H	1:J:410:HIS:CD2	2.10	0.52
1:W:368:LYS:HE2	1:W:470:ASP:OD1	2.09	0.52
1:B:182:GLU:O	1:B:308:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:607:HEC:CGA	1:K:226:ARG:HH22	2.22	0.52
1:G:204:TRP:CZ3	1:G:427:MET:HE1	2.45	0.52
1:M:497:TRP:CD1	1:O:485:ARG:HD3	2.45	0.52
1:I:368:LYS:HE2	1:I:470:ASP:OD1	2.10	0.52
1:J:90:PRO:O	1:J:93:ARG:HG2	2.10	0.52
1:P:368:LYS:HE2	1:P:470:ASP:OD1	2.09	0.52
1:V:485:ARG:HD3	1:W:497:TRP:CD1	2.45	0.52
1:G:485:ARG:HD3	1:H:497:TRP:CG	2.45	0.52
1:M:195:SER:HB2	1:M:221:THR:HA	1.92	0.52
1:D:406:ILE:HD12	1:E:62:LEU:HD12	1.91	0.52
3:I:605:HEC:HMD1	3:I:605:HEC:HBD1	1.92	0.52
1:N:368:LYS:HE2	1:N:470:ASP:OD1	2.09	0.52
1:D:154:CYS:HB3	1:D:165:PRO:HG3	1.91	0.51
1:I:318:SER:O	1:I:319:MET:HB2	2.09	0.51
1:V:432:ASP:HB2	1:X:478:GLN:HE21	1.76	0.51
1:G:497:TRP:CG	1:I:485:ARG:HD3	2.46	0.51
1:Q:368:LYS:HE2	1:Q:470:ASP:OD1	2.10	0.51
1:V:538:THR:HA	2:h:110:PRO:HA	1.92	0.51
3:D:604:HEC:CBC	3:D:605:HEC:HBB2	2.40	0.51
1:M:287:LEU:HD12	3:M:604:HEC:HBD2	1.92	0.51
1:Q:287:LEU:HD12	3:Q:604:HEC:HBD2	1.92	0.51
3:D:601:HEC:HBA1	3:D:601:HEC:HHA	1.91	0.51
1:I:199:GLN:HB2	1:I:220:HIS:HB3	1.93	0.51
1:K:195:SER:HB2	1:K:221:THR:HA	1.93	0.51
1:F:287:LEU:HD12	3:F:604:HEC:HBD2	1.91	0.51
3:N:607:HEC:CGA	1:O:226:ARG:HH22	2.23	0.51
1:P:497:TRP:CD1	1:R:485:ARG:HD3	2.46	0.51
1:Q:257:ARG:HD3	7:Q:729:HOH:O	2.08	0.51
3:A:607:HEC:CGA	1:B:226:ARG:HH22	2.24	0.51
1:K:135:ASP:OD2	5:K:614:GOL:O1	2.28	0.51
1:K:374:LYS:NZ	7:K:701:HOH:O	2.25	0.51
1:V:287:LEU:HD12	3:V:604:HEC:HBD2	1.93	0.51
3:G:607:HEC:CGA	1:H:226:ARG:HH22	2.24	0.51
1:A:485:ARG:HD3	1:B:497:TRP:CD1	2.45	0.51
1:F:195:SER:HB2	1:F:221:THR:HA	1.92	0.51
1:J:182:GLU:OE1	2:d:26:TYR:HB3	2.11	0.51
1:O:368:LYS:HE2	1:O:470:ASP:OD1	2.10	0.51
1:C:368:LYS:HE2	1:C:470:ASP:OD1	2.11	0.51
1:D:195:SER:HB2	1:D:221:THR:HA	1.93	0.51
1:L:195:SER:HB2	1:L:221:THR:HA	1.93	0.51
1:L:368:LYS:HE2	1:L:470:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:SER:HB2	1:E:221:THR:HA	1.92	0.51
1:I:433:VAL:HG13	1:I:476:VAL:HG13	1.92	0.51
1:S:485:ARG:HD3	1:T:497:TRP:CD1	2.46	0.50
1:H:63:LYS:NZ	7:H:703:HOH:O	2.43	0.50
1:D:388:MET:HB3	1:D:389:PRO:HD2	1.93	0.50
1:S:368:LYS:HE2	1:S:470:ASP:OD1	2.11	0.50
1:W:79:PRO:HB2	2:i:41:GLY:HA3	1.93	0.50
1:D:331:TRP:CZ2	1:E:44:VAL:HG21	2.46	0.50
1:I:234:HIS:HD2	3:I:601:HEC:NC	2.06	0.50
3:M:607:HEC:CGA	1:N:226:ARG:HH22	2.23	0.50
1:A:195:SER:HB2	1:A:221:THR:HA	1.93	0.50
1:I:302:MET:HE3	1:I:307:HIS:HA	1.93	0.50
3:Q:607:HEC:CGA	1:R:226:ARG:HH22	2.24	0.50
1:W:287:LEU:HD12	3:W:604:HEC:HBD2	1.94	0.50
1:C:123:ALA:HB2	1:L:127:VAL:CG2	2.41	0.50
1:O:127:VAL:HG21	1:W:123:ALA:HB2	1.93	0.50
1:P:226:ARG:HD3	7:P:718:HOH:O	2.09	0.50
1:X:287:LEU:HD12	3:X:604:HEC:HBD2	1.92	0.50
1:I:48:PRO:HG3	1:I:63:LYS:HD2	1.92	0.50
1:V:226:ARG:HH22	3:X:607:HEC:CGA	2.24	0.50
1:C:195:SER:HB2	1:C:221:THR:HA	1.93	0.50
1:D:197:PHE:HB2	1:D:535:TRP:CD2	2.46	0.50
1:E:406:ILE:H	1:E:410:HIS:CD2	2.12	0.50
1:H:210:PRO:HA	7:H:709:HOH:O	2.12	0.50
1:P:287:LEU:HD12	3:P:604:HEC:HBD2	1.94	0.50
1:G:287:LEU:HD12	3:G:604:HEC:HBD2	1.93	0.50
1:S:432:ASP:HB2	1:U:478:GLN:HE21	1.77	0.50
1:I:194:CYS:HA	3:I:605:HEC:O1D	2.12	0.49
1:J:63:LYS:HD3	5:L:613:GOL:H12	1.94	0.49
1:K:234:HIS:CE1	5:K:614:GOL:O3	2.65	0.49
1:U:287:LEU:HD12	3:U:604:HEC:HBD2	1.93	0.49
1:D:495:ILE:HG12	1:F:492:LYS:HD3	1.93	0.49
1:I:144:ALA:HB3	1:I:148:PRO:HA	1.95	0.49
1:D:182:GLU:O	1:D:185:GLN:HB2	2.12	0.49
1:Q:195:SER:HB2	1:Q:221:THR:HA	1.95	0.49
1:Q:204:TRP:CZ3	1:Q:427:MET:HE1	2.47	0.49
1:G:429:ASN:ND2	7:G:706:HOH:O	2.46	0.49
1:K:204:TRP:CZ3	1:K:427:MET:HE1	2.48	0.49
1:K:368:LYS:HE2	1:K:470:ASP:OD1	2.12	0.49
1:O:195:SER:HB2	1:O:221:THR:HA	1.94	0.49
1:G:343:ASP:HB3	7:G:701:HOH:O	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:GLN:O	1:I:310:GLN:HG2	2.12	0.49
2:Y:38:ILE:HG22	2:Y:41:GLY:H	1.77	0.49
1:G:368:LYS:HE2	1:G:470:ASP:OD1	2.13	0.49
1:B:343:ASP:HB3	7:B:709:HOH:O	2.12	0.49
3:I:603:HEC:HMC1	3:I:603:HEC:HBC3	1.95	0.49
1:B:368:LYS:HE2	1:B:470:ASP:OD1	2.13	0.49
1:K:232:GLN:HE22	1:K:246:GLN:NE2	2.03	0.49
1:U:195:SER:HB2	1:U:221:THR:HA	1.94	0.49
3:W:607:HEC:CGA	1:X:226:ARG:HH22	2.25	0.49
1:L:204:TRP:CZ3	1:L:427:MET:HE1	2.47	0.49
1:A:497:TRP:CG	1:C:485:ARG:HD3	2.48	0.49
1:I:227:CYS:HB3	3:I:602:HEC:HMB2	1.95	0.49
1:I:538:THR:HA	2:Y:110:PRO:HA	1.94	0.49
1:N:287:LEU:HD12	3:N:604:HEC:HBD2	1.94	0.49
1:Q:522:PRO:HD2	7:Q:728:HOH:O	2.12	0.49
1:S:195:SER:HB2	1:S:221:THR:HA	1.94	0.49
2:a:38:ILE:HG22	2:a:41:GLY:H	1.78	0.49
1:I:59:PHE:C	1:I:61:GLY:H	2.20	0.48
1:S:90:PRO:O	1:S:93:ARG:HG2	2.13	0.48
1:H:349:ARG:NH2	4:H:609:SO4:O2	2.46	0.48
1:H:485:ARG:NH1	1:I:490:GLU:OE1	2.46	0.48
1:J:287:LEU:HD12	3:J:604:HEC:HBD2	1.95	0.48
1:K:233:ARG:NE	5:K:614:GOL:O3	2.43	0.48
1:P:226:ARG:HH22	3:R:607:HEC:CGA	2.26	0.48
2:d:38:ILE:HG22	2:d:41:GLY:H	1.78	0.48
1:D:560:ALA:HB1	1:E:43:GLU:HA	1.93	0.48
1:I:389:PRO:HB2	5:I:615:GOL:H32	1.95	0.48
1:P:432:ASP:HB2	1:R:478:GLN:HE21	1.78	0.48
1:V:479:ASN:HD22	1:X:482:ARG:HH22	1.60	0.48
1:C:287:LEU:HD12	3:C:604:HEC:HBD2	1.95	0.48
1:D:216:CYS:HA	3:D:603:HEC:HMC3	1.94	0.48
1:I:76:SER:HB2	1:I:106:VAL:CG1	2.43	0.48
1:J:497:TRP:CG	1:L:485:ARG:HD3	2.48	0.48
1:K:485:ARG:HD3	1:L:497:TRP:CG	2.48	0.48
1:N:127:VAL:HG11	1:R:120:GLN:HA	1.95	0.48
1:A:226:ARG:HH22	3:C:607:HEC:CGA	2.27	0.48
1:A:287:LEU:HD12	3:A:604:HEC:HBD2	1.93	0.48
1:B:485:ARG:HD3	1:C:497:TRP:CG	2.48	0.48
1:E:478:GLN:HE21	1:F:432:ASP:HB2	1.79	0.48
1:L:199:GLN:HB2	1:L:220:HIS:HB3	1.96	0.48
1:M:368:LYS:HE2	1:M:470:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:485:ARG:HD3	1:X:497:TRP:CD1	2.48	0.48
1:B:227:CYS:HB3	3:B:602:HEC:HMB2	1.95	0.48
1:H:123:ALA:HB2	1:K:127:VAL:CG2	2.40	0.48
1:H:454:HIS:C	5:H:614:GOL:H2	2.39	0.48
1:I:76:SER:HB2	1:I:106:VAL:HG13	1.96	0.48
1:V:90:PRO:O	1:V:93:ARG:HG2	2.14	0.48
3:B:607:HEC:CGA	1:C:226:ARG:HH22	2.27	0.48
1:D:37:THR:HA	1:D:59:PHE:CE1	2.49	0.48
1:N:195:SER:HB2	1:N:221:THR:HA	1.96	0.48
1:X:195:SER:HB2	1:X:221:THR:HA	1.96	0.48
1:E:199:GLN:HB2	1:E:220:HIS:HB3	1.95	0.48
1:I:120:GLN:HA	1:M:127:VAL:HG11	1.96	0.48
1:C:90:PRO:O	1:C:93:ARG:HG2	2.13	0.48
1:K:478:GLN:HE21	1:L:432:ASP:HB2	1.79	0.48
1:J:204:TRP:CZ3	1:J:427:MET:HE1	2.48	0.48
1:S:479:ASN:HD22	1:U:482:ARG:HH22	1.62	0.48
1:T:485:ARG:HD3	1:U:497:TRP:CD1	2.49	0.48
1:I:90:PRO:O	1:I:93:ARG:HG2	2.14	0.47
1:J:195:SER:HB2	1:J:221:THR:HA	1.95	0.47
2:e:38:ILE:HG22	2:e:41:GLY:H	1.79	0.47
1:G:204:TRP:CH2	1:G:427:MET:HE1	2.49	0.47
1:G:454:HIS:HD2	3:G:606:HEC:NC	2.12	0.47
1:A:478:GLN:HE21	1:B:432:ASP:HB2	1.79	0.47
1:D:231:HIS:HB3	1:D:241:ALA:HB2	1.96	0.47
1:F:227:CYS:HB3	3:F:602:HEC:HMB2	1.95	0.47
1:S:458:ASN:HB3	1:T:252:TRP:CZ2	2.49	0.47
1:U:368:LYS:HE2	1:U:470:ASP:OD1	2.13	0.47
1:X:90:PRO:O	1:X:93:ARG:HG2	2.14	0.47
1:A:227:CYS:HB3	3:A:602:HEC:HMB2	1.96	0.47
1:D:524:LYS:HG2	1:D:528:ASP:HB3	1.96	0.47
1:N:478:GLN:HE21	1:O:432:ASP:HB2	1.79	0.47
1:P:509:LEU:HD11	1:R:477:LYS:HZ3	1.79	0.47
1:G:44:VAL:HG23	1:I:330:LEU:HD21	1.96	0.47
1:G:120:GLN:HA	1:E:127:VAL:HG11	1.96	0.47
4:G:610:SO4:O4	1:I:482:ARG:HG3	2.15	0.47
1:D:390:LYS:HA	1:D:400:HIS:HB3	1.96	0.47
1:J:199:GLN:HB2	1:J:220:HIS:HB3	1.96	0.47
1:M:226:ARG:HH22	3:O:607:HEC:CGA	2.27	0.47
2:g:38:ILE:HG22	2:g:41:GLY:H	1.79	0.47
1:D:145:GLU:HA	1:D:146:PRO:C	2.39	0.47
1:D:198:ALA:O	3:D:603:HEC:HHB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:538:THR:HA	2:e:110:PRO:HA	1.95	0.47
1:S:287:LEU:HD12	3:S:604:HEC:HBD2	1.96	0.47
1:U:90:PRO:O	1:U:93:ARG:HG2	2.14	0.47
1:D:500:GLU:N	1:D:500:GLU:OE1	2.46	0.47
3:E:607:HEC:CGA	1:F:226:ARG:HH22	2.27	0.47
1:P:223:PRO:HG3	3:P:605:HEC:HBC2	1.97	0.47
1:R:287:LEU:HD12	3:R:604:HEC:HBD2	1.97	0.47
1:R:343:ASP:HB2	7:R:701:HOH:O	2.15	0.47
1:G:199:GLN:HB2	1:G:220:HIS:HB3	1.97	0.47
1:A:172:THR:HG21	2:Z:34:TRP:CH2	2.50	0.47
1:B:287:LEU:HD12	3:B:604:HEC:HBD2	1.96	0.47
1:D:97:PRO:HG2	1:D:166:SER:HB3	1.96	0.47
1:D:542:PRO:HG2	1:D:545:GLU:HB2	1.96	0.47
1:E:287:LEU:HD12	3:E:604:HEC:HBD2	1.95	0.47
1:F:204:TRP:CZ3	1:F:427:MET:HE1	2.50	0.47
1:J:485:ARG:HD3	1:K:497:TRP:CG	2.49	0.47
4:J:611:SO4:O2	1:K:482:ARG:NH1	2.48	0.47
1:K:204:TRP:CH2	1:K:427:MET:HE1	2.50	0.47
1:M:432:ASP:HB2	1:O:478:GLN:HE21	1.80	0.47
1:P:227:CYS:HB3	3:P:602:HEC:HMB2	1.96	0.47
1:R:199:GLN:HB2	1:R:220:HIS:HB3	1.97	0.47
3:X:604:HEC:CBC	3:X:605:HEC:HBB2	2.45	0.47
1:G:227:CYS:HB3	3:G:602:HEC:HMB2	1.97	0.47
1:C:207:GLU:HA	1:C:513:THR:OG1	2.15	0.47
1:D:523:GLY:O	1:D:524:LYS:HG3	2.14	0.47
1:Q:168:LYS:HD3	2:f:61:ASN:O	2.15	0.47
1:S:485:ARG:HD2	1:T:490:GLU:OE2	2.13	0.47
1:V:204:TRP:CZ3	1:V:427:MET:HE1	2.50	0.47
1:G:109:SER:HA	7:G:745:HOH:O	2.15	0.47
1:H:90:PRO:O	1:H:93:ARG:HG2	2.15	0.47
1:W:204:TRP:CZ3	1:W:427:MET:HE1	2.49	0.47
1:X:386:ASP:HA	1:X:387:PRO:HA	1.73	0.47
1:A:204:TRP:CZ3	1:A:427:MET:HE1	2.49	0.47
1:C:232:GLN:HE22	1:C:246:GLN:NE2	2.07	0.47
1:D:61:GLY:O	1:F:370:ARG:NH1	2.46	0.47
1:H:485:ARG:HD2	1:I:490:GLU:OE2	2.14	0.47
1:M:252:TRP:CZ2	1:O:458:ASN:HB3	2.50	0.47
1:O:287:LEU:HD12	3:O:604:HEC:HBD2	1.96	0.47
1:U:199:GLN:HB2	1:U:220:HIS:HB3	1.97	0.47
1:D:87:LYS:HB2	1:D:210:PRO:HD3	1.97	0.46
1:J:403:SER:HB3	1:J:434:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:343:ASP:HB3	7:R:701:HOH:O	2.15	0.46
1:F:173:ALA:HA	1:F:177:GLU:HB2	1.97	0.46
1:P:165:PRO:HG2	3:P:601:HEC:HMD2	1.97	0.46
1:Q:386:ASP:HA	1:Q:387:PRO:HA	1.73	0.46
1:R:204:TRP:CZ3	1:R:427:MET:HE1	2.50	0.46
1:S:199:GLN:HB2	1:S:220:HIS:HB3	1.98	0.46
1:S:252:TRP:CZ2	1:U:458:ASN:HB3	2.50	0.46
1:T:90:PRO:O	1:T:93:ARG:HG2	2.15	0.46
1:T:287:LEU:HD12	3:T:604:HEC:HBD2	1.96	0.46
1:T:482:ARG:HH22	1:U:479:ASN:HD22	1.62	0.46
1:W:199:GLN:HB2	1:W:220:HIS:HB3	1.97	0.46
1:X:204:TRP:CZ3	1:X:427:MET:HE1	2.51	0.46
2:h:38:ILE:HG22	2:h:41:GLY:H	1.81	0.46
1:G:323:MET:HE1	1:H:52:ASP:HB2	1.98	0.46
1:A:485:ARG:HD3	1:B:497:TRP:CG	2.50	0.46
1:K:403:SER:HB3	1:K:434:GLU:OE2	2.15	0.46
1:Q:173:ALA:HA	1:Q:177:GLU:HB2	1.97	0.46
2:f:38:ILE:HG22	2:f:41:GLY:H	1.81	0.46
1:G:349:ARG:NH2	4:G:609:SO4:O3	2.48	0.46
1:G:511:GLN:HG3	1:I:367:LEU:HD21	1.98	0.46
1:D:306:HIS:CE1	1:D:308:ASN:HB3	2.50	0.46
1:H:199:GLN:HB2	1:H:220:HIS:HB3	1.98	0.46
1:H:473:LEU:HG	5:H:615:GOL:H2	1.97	0.46
1:N:199:GLN:HB2	1:N:220:HIS:HB3	1.96	0.46
1:P:478:GLN:HE21	1:Q:432:ASP:HB2	1.80	0.46
1:Q:485:ARG:HD3	1:R:497:TRP:CG	2.50	0.46
1:S:204:TRP:CZ3	1:S:427:MET:HE1	2.49	0.46
1:A:432:ASP:H	1:C:478:GLN:NE2	2.14	0.46
1:B:482:ARG:HG3	4:B:609:SO4:O1	2.16	0.46
1:D:432:ASP:HB2	1:F:478:GLN:HE21	1.81	0.46
3:D:600:HEC:HAA2	3:D:601:HEC:HMA3	1.98	0.46
1:F:368:LYS:HE2	1:F:470:ASP:OD1	2.15	0.46
1:S:226:ARG:HH22	3:U:607:HEC:CGA	2.28	0.46
1:V:199:GLN:HB2	1:V:220:HIS:HB3	1.98	0.46
1:A:199:GLN:HB2	1:A:220:HIS:HB3	1.97	0.46
1:C:227:CYS:HB3	3:C:602:HEC:HMB2	1.97	0.46
1:J:318:SER:HB2	5:K:615:GOL:O3	2.15	0.46
1:P:252:TRP:CZ2	1:R:458:ASN:HB3	2.51	0.46
3:U:604:HEC:CBC	3:U:605:HEC:HBB2	2.45	0.46
1:V:252:TRP:CZ2	1:X:458:ASN:HB3	2.51	0.46
1:X:227:CYS:HB3	3:X:602:HEC:HMB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:38:ILE:HG22	2:b:41:GLY:H	1.79	0.46
1:B:204:TRP:CZ3	1:B:427:MET:HE1	2.51	0.46
1:C:199:GLN:HB2	1:C:220:HIS:HB3	1.97	0.46
1:F:199:GLN:HB2	1:F:220:HIS:HB3	1.98	0.46
1:I:123:ALA:HB2	1:M:127:VAL:HG21	1.98	0.46
1:I:255:ASP:HB2	1:I:319:MET:CE	2.46	0.46
3:P:607:HEC:CGA	1:Q:226:ARG:HH22	2.27	0.46
1:S:127:VAL:HG21	1:X:123:ALA:HB2	1.97	0.46
1:H:123:ALA:CB	1:K:127:VAL:HB	2.46	0.46
1:H:458:ASN:HB3	1:I:252:TRP:CZ2	2.51	0.46
1:O:227:CYS:HB3	3:O:602:HEC:HMB2	1.97	0.46
1:T:204:TRP:CZ3	1:T:427:MET:HE1	2.51	0.46
2:Z:38:ILE:HG22	2:Z:41:GLY:H	1.81	0.46
2:i:38:ILE:HG22	2:i:41:GLY:H	1.80	0.46
1:H:173:ALA:HA	1:H:177:GLU:HB2	1.98	0.46
1:I:255:ASP:HB2	1:I:319:MET:HE1	1.98	0.46
3:I:604:HEC:CBC	3:I:605:HEC:HBB2	2.45	0.46
1:K:90:PRO:O	1:K:93:ARG:HG2	2.16	0.46
1:M:485:ARG:HD3	1:N:497:TRP:CG	2.51	0.46
1:N:227:CYS:HB3	3:N:602:HEC:HMB2	1.97	0.46
1:H:485:ARG:HD3	1:I:497:TRP:CG	2.51	0.46
1:K:223:PRO:HG3	3:K:605:HEC:HBC2	1.98	0.46
1:M:497:TRP:CG	1:O:485:ARG:HD3	2.51	0.46
1:N:485:ARG:HD3	1:O:497:TRP:CG	2.51	0.46
1:O:207:GLU:HA	1:O:513:THR:OG1	2.16	0.46
1:O:386:ASP:HA	1:O:387:PRO:HA	1.73	0.46
1:O:403:SER:HB3	1:O:434:GLU:OE2	2.16	0.46
1:S:497:TRP:CD1	1:U:485:ARG:HD3	2.50	0.46
1:T:458:ASN:HB3	1:U:252:TRP:CZ2	2.51	0.46
1:G:63:LYS:NZ	5:G:615:GOL:O3	2.49	0.45
1:A:432:ASP:HB2	1:C:478:GLN:HE21	1.81	0.45
1:D:367:LEU:HD21	1:E:511:GLN:HG3	1.97	0.45
1:H:386:ASP:HA	1:H:387:PRO:HA	1.74	0.45
1:O:199:GLN:HB2	1:O:220:HIS:HB3	1.97	0.45
1:R:257:ARG:HD3	7:R:720:HOH:O	2.16	0.45
1:T:199:GLN:HB2	1:T:220:HIS:HB3	1.98	0.45
1:W:485:ARG:HD2	1:X:490:GLU:OE2	2.16	0.45
1:G:403:SER:HB3	1:G:434:GLU:OE2	2.16	0.45
1:D:252:TRP:CZ2	1:F:458:ASN:HB3	2.51	0.45
1:E:90:PRO:O	1:E:93:ARG:HG2	2.15	0.45
1:H:454:HIS:HA	5:H:614:GOL:C2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:VAL:CG2	1:P:123:ALA:HB2	2.45	0.45
1:K:173:ALA:HA	1:K:177:GLU:HB2	1.98	0.45
1:V:173:ALA:HA	1:V:177:GLU:HB2	1.98	0.45
1:E:482:ARG:HH22	1:F:479:ASN:HD22	1.65	0.45
3:J:604:HEC:CBC	3:J:605:HEC:HBB2	2.46	0.45
1:K:227:CYS:HB3	3:K:602:HEC:HMB2	1.98	0.45
1:K:478:GLN:NE2	1:L:432:ASP:H	2.13	0.45
1:M:199:GLN:HB2	1:M:220:HIS:HB3	1.97	0.45
1:M:204:TRP:CZ3	1:M:427:MET:HE1	2.51	0.45
1:P:90:PRO:O	1:P:93:ARG:HG2	2.17	0.45
1:P:199:GLN:HB2	1:P:220:HIS:HB3	1.97	0.45
1:Q:227:CYS:HB3	3:Q:602:HEC:HMB2	1.99	0.45
1:S:227:CYS:HB3	3:S:602:HEC:HMB2	1.99	0.45
3:T:607:HEC:CGA	1:U:226:ARG:HH22	2.30	0.45
1:G:478:GLN:NE2	1:H:432:ASP:H	2.13	0.45
1:G:482:ARG:HG3	4:G:610:SO4:O1	2.15	0.45
1:E:227:CYS:HB3	3:E:602:HEC:HMB2	1.98	0.45
1:Q:204:TRP:CH2	1:Q:427:MET:HE1	2.52	0.45
1:W:90:PRO:O	1:W:93:ARG:HG2	2.17	0.45
1:C:204:TRP:CZ3	1:C:427:MET:HE1	2.51	0.45
3:K:606:HEC:HBC1	3:K:607:HEC:HHC	1.99	0.45
1:L:287:LEU:HD12	3:L:604:HEC:HBD2	1.98	0.45
1:P:204:TRP:CZ3	1:P:427:MET:HE1	2.51	0.45
1:P:458:ASN:HB3	1:Q:252:TRP:CZ2	2.51	0.45
1:G:245:GLU:HG2	1:I:272:GLN:OE1	2.17	0.45
1:A:403:SER:HB3	1:A:434:GLU:OE2	2.16	0.45
1:J:432:ASP:HB2	1:L:478:GLN:HE21	1.81	0.45
1:L:227:CYS:HB3	3:L:602:HEC:HMB2	1.99	0.45
3:T:606:HEC:HBC1	3:T:607:HEC:HHC	1.99	0.45
1:V:454:HIS:HD2	3:V:606:HEC:NC	2.13	0.45
1:X:173:ALA:HA	1:X:177:GLU:HB2	1.98	0.45
1:G:90:PRO:O	1:G:93:ARG:HG2	2.16	0.45
1:A:490:GLU:OE2	1:C:485:ARG:HD2	2.17	0.45
1:E:204:TRP:CZ3	1:E:427:MET:HE1	2.52	0.45
5:J:613:GOL:O1	1:K:63:LYS:NZ	2.49	0.45
1:N:90:PRO:O	1:N:93:ARG:HG2	2.16	0.45
3:R:604:HEC:CBC	3:R:605:HEC:HBB2	2.47	0.45
3:S:607:HEC:CGA	1:T:226:ARG:HH22	2.29	0.45
1:U:173:ALA:HA	1:U:177:GLU:HB2	1.99	0.45
1:U:204:TRP:CZ3	1:U:427:MET:HE1	2.51	0.45
1:V:478:GLN:HE21	1:W:432:ASP:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PRO:O	1:A:93:ARG:HG2	2.17	0.45
1:A:252:TRP:CZ2	1:C:458:ASN:HB3	2.52	0.45
1:B:199:GLN:HB2	1:B:220:HIS:HB3	1.98	0.45
1:D:489:LEU:HD23	1:E:495:ILE:HD12	1.99	0.45
1:E:485:ARG:HD3	1:F:497:TRP:CD1	2.52	0.45
3:F:604:HEC:CBC	3:F:605:HEC:HBB2	2.46	0.45
1:I:369:TYR:CE1	1:I:441:VAL:HB	2.52	0.45
1:J:386:ASP:HA	1:J:387:PRO:HA	1.73	0.45
1:N:154:CYS:HB3	1:N:165:PRO:HG3	1.98	0.45
1:O:204:TRP:CZ3	1:O:427:MET:HE1	2.51	0.45
1:Q:199:GLN:HB2	1:Q:220:HIS:HB3	1.98	0.45
1:Q:478:GLN:HE21	1:R:432:ASP:HB2	1.82	0.45
3:R:606:HEC:HBC1	3:R:607:HEC:HHC	1.99	0.45
1:V:227:CYS:HB3	3:V:602:HEC:HMB2	1.99	0.45
1:V:497:TRP:CD1	1:X:485:ARG:HD3	2.52	0.45
3:V:604:HEC:CBC	3:V:605:HEC:HBB2	2.46	0.45
1:G:41:PRO:O	1:G:44:VAL:HG12	2.17	0.45
1:B:458:ASN:HB3	1:C:252:TRP:CZ2	2.52	0.45
1:E:458:ASN:HB3	1:F:252:TRP:CZ2	2.52	0.45
1:F:90:PRO:O	1:F:93:ARG:HG2	2.16	0.45
1:H:204:TRP:CZ3	1:H:427:MET:HE1	2.52	0.45
1:J:323:MET:HE1	1:K:52:ASP:HB2	1.99	0.45
1:K:199:GLN:HB2	1:K:220:HIS:HB3	1.98	0.45
1:M:403:SER:HB3	1:M:434:GLU:OE2	2.17	0.45
1:P:432:ASP:H	1:R:478:GLN:NE2	2.15	0.45
3:W:604:HEC:CBC	3:W:605:HEC:HBB2	2.46	0.45
1:X:104:ASP:CG	2:j:87:LYS:NZ	2.75	0.45
1:X:199:GLN:HB2	1:X:220:HIS:HB3	1.98	0.45
1:B:343:ASP:CB	7:B:709:HOH:O	2.64	0.45
1:M:478:GLN:HE21	1:N:432:ASP:HB2	1.82	0.45
1:M:490:GLU:OE2	1:O:485:ARG:HD2	2.17	0.45
1:N:403:SER:HB3	1:N:434:GLU:OE2	2.16	0.45
1:P:403:SER:HB3	1:P:434:GLU:OE2	2.17	0.45
1:Q:90:PRO:O	1:Q:93:ARG:HG2	2.16	0.45
1:A:458:ASN:HB3	1:B:252:TRP:CZ2	2.52	0.44
3:F:606:HEC:HBC1	3:F:607:HEC:HHC	2.00	0.44
1:I:241:ALA:O	1:I:298:GLN:NE2	2.50	0.44
1:J:227:CYS:HB3	3:J:602:HEC:HMB2	1.97	0.44
1:L:90:PRO:O	1:L:93:ARG:HG2	2.17	0.44
1:M:432:ASP:H	1:O:478:GLN:NE2	2.16	0.44
1:N:204:TRP:CZ3	1:N:427:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:41:PRO:O	1:S:44:VAL:HG12	2.17	0.44
1:C:403:SER:HB3	1:C:434:GLU:OE2	2.17	0.44
1:E:173:ALA:HA	1:E:177:GLU:HB2	2.00	0.44
1:J:340:SER:O	1:J:343:ASP:HB2	2.17	0.44
1:N:454:HIS:HD2	3:N:606:HEC:NC	2.15	0.44
1:T:227:CYS:HB3	3:T:602:HEC:HMB2	1.98	0.44
3:V:606:HEC:HBC1	3:V:607:HEC:HHC	1.99	0.44
1:A:154:CYS:HB3	1:A:165:PRO:HG3	2.00	0.44
1:E:154:CYS:HB3	1:E:165:PRO:HG3	1.98	0.44
1:H:287:LEU:HD12	3:H:604:HEC:HBD2	1.98	0.44
1:J:318:SER:HB2	5:K:615:GOL:C3	2.48	0.44
1:J:485:ARG:HD2	1:K:490:GLU:OE2	2.17	0.44
1:K:287:LEU:HD12	3:K:604:HEC:HBD2	1.98	0.44
1:M:323:MET:HE1	1:N:52:ASP:HB2	1.99	0.44
1:P:485:ARG:HD3	1:Q:497:TRP:CG	2.51	0.44
1:T:173:ALA:HA	1:T:177:GLU:HB2	1.97	0.44
2:j:50:LYS:HG3	2:j:55:GLU:HG2	1.99	0.44
1:B:154:CYS:HB3	1:B:165:PRO:HG3	1.99	0.44
3:B:606:HEC:HBC1	3:B:607:HEC:HHC	2.00	0.44
3:E:605:HEC:CBD	3:E:605:HEC:HMD1	2.48	0.44
1:H:223:PRO:HG3	3:H:605:HEC:HBC2	1.99	0.44
1:L:204:TRP:CH2	1:L:427:MET:HE1	2.52	0.44
1:G:478:GLN:HE21	1:H:432:ASP:HB2	1.81	0.44
1:D:222:SER:HB2	1:D:223:PRO:HD3	1.99	0.44
1:F:154:CYS:HB3	1:F:165:PRO:HG3	2.00	0.44
1:H:120:GLN:HA	1:K:127:VAL:HG11	1.99	0.44
1:J:197:PHE:HB2	1:J:535:TRP:CD2	2.53	0.44
1:J:490:GLU:OE2	1:L:485:ARG:HD2	2.17	0.44
1:S:403:SER:HB3	1:S:434:GLU:OE2	2.18	0.44
1:U:403:SER:HB3	1:U:434:GLU:OE2	2.17	0.44
1:B:173:ALA:HA	1:B:177:GLU:HB2	2.00	0.44
1:D:119:GLU:CD	1:D:119:GLU:H	2.26	0.44
1:D:204:TRP:CZ3	1:D:427:MET:HE1	2.52	0.44
1:K:323:MET:HE1	1:L:52:ASP:HB2	2.00	0.44
3:K:607:HEC:O2A	1:L:226:ARG:NH2	2.51	0.44
1:L:403:SER:HB3	1:L:434:GLU:OE2	2.18	0.44
1:M:227:CYS:HB3	3:M:602:HEC:HMB2	1.98	0.44
1:Q:458:ASN:HB3	1:R:252:TRP:CZ2	2.53	0.44
3:R:605:HEC:HMD1	3:R:605:HEC:HBD1	2.00	0.44
1:V:165:PRO:HG2	3:V:601:HEC:HMD2	1.99	0.44
1:V:223:PRO:HG3	3:V:605:HEC:HBC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:403:SER:HB3	1:W:434:GLU:OE2	2.17	0.44
1:G:197:PHE:HB2	1:G:535:TRP:CD2	2.53	0.44
1:D:331:TRP:HZ2	1:E:44:VAL:HG21	1.83	0.44
1:E:386:ASP:HA	1:E:387:PRO:HA	1.73	0.44
1:H:474:VAL:CG2	5:H:615:GOL:C3	2.93	0.44
1:J:478:GLN:HE21	1:K:432:ASP:HB2	1.83	0.44
1:T:197:PHE:HB2	1:T:535:TRP:CD2	2.53	0.44
1:W:223:PRO:HG3	3:W:605:HEC:HBC2	1.99	0.44
1:W:386:ASP:HA	1:W:387:PRO:HA	1.73	0.44
2:c:38:ILE:HG22	2:c:41:GLY:H	1.82	0.44
1:B:86:TRP:CH2	1:B:205:SER:HB3	2.53	0.44
1:B:90:PRO:O	1:B:93:ARG:HG2	2.17	0.44
1:B:403:SER:HB3	1:B:434:GLU:OE2	2.17	0.44
1:I:204:TRP:CH2	1:I:427:MET:HE1	2.53	0.44
1:I:241:ALA:HA	1:I:246:GLN:HG3	1.99	0.44
1:J:204:TRP:CH2	1:J:427:MET:HE1	2.52	0.44
1:J:373:PHE:CD1	5:J:613:GOL:H11	2.52	0.44
3:V:607:HEC:O2A	1:W:226:ARG:NH2	2.51	0.44
1:W:207:GLU:HA	1:W:513:THR:OG1	2.18	0.44
1:A:173:ALA:HA	1:A:177:GLU:HB2	1.98	0.44
1:D:389:PRO:HA	1:D:392:LEU:HD12	1.99	0.44
1:E:223:PRO:HG3	3:E:605:HEC:HBC2	2.00	0.44
1:H:154:CYS:HB3	1:H:165:PRO:HG3	2.00	0.44
1:H:227:CYS:HB3	3:H:602:HEC:HMB2	2.00	0.44
1:H:403:SER:HB3	1:H:434:GLU:OE2	2.17	0.44
1:J:173:ALA:HA	1:J:177:GLU:HB2	1.99	0.44
1:J:297:CYS:HB3	3:J:605:HEC:HMB1	2.00	0.44
1:L:81:LYS:HD3	1:L:82:TYR:CZ	2.53	0.44
1:O:90:PRO:O	1:O:93:ARG:HG2	2.17	0.44
1:Q:485:ARG:HD2	1:R:490:GLU:OE2	2.18	0.44
3:Q:604:HEC:CBC	3:Q:605:HEC:HBB2	2.48	0.44
1:R:403:SER:HB3	1:R:434:GLU:OE2	2.18	0.44
1:W:227:CYS:HB3	3:W:602:HEC:HMB2	1.99	0.44
1:W:478:GLN:HE21	1:X:432:ASP:HB2	1.83	0.44
1:G:538:THR:HA	2:c:110:PRO:HA	1.99	0.43
1:A:204:TRP:CH2	1:A:427:MET:HE1	2.53	0.43
1:H:265:GLY:HA3	7:H:732:HOH:O	2.18	0.43
1:P:497:TRP:CG	1:R:485:ARG:HD3	2.52	0.43
1:Q:41:PRO:O	1:Q:44:VAL:HG12	2.18	0.43
1:W:165:PRO:HG2	3:W:601:HEC:HMD2	1.99	0.43
1:B:41:PRO:O	1:B:44:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLU:HA	1:D:513:THR:HG1	1.81	0.43
1:L:173:ALA:HA	1:L:177:GLU:HB2	2.00	0.43
3:M:606:HEC:HBC1	3:M:607:HEC:HHC	2.00	0.43
1:N:173:ALA:HA	1:N:177:GLU:HB2	2.00	0.43
1:U:86:TRP:CH2	1:U:205:SER:HB3	2.54	0.43
3:U:606:HEC:HBC1	3:U:607:HEC:HHC	2.00	0.43
1:V:458:ASN:HB3	1:W:252:TRP:CZ2	2.53	0.43
1:X:232:GLN:HE22	1:X:246:GLN:NE2	2.07	0.43
1:G:458:ASN:HB3	1:H:252:TRP:CZ2	2.53	0.43
1:D:76:SER:HB2	1:D:106:VAL:HG13	2.00	0.43
1:F:41:PRO:O	1:F:44:VAL:HG12	2.18	0.43
1:I:150:GLY:C	3:I:601:HEC:HMC3	2.42	0.43
1:I:309:VAL:HG13	3:I:605:HEC:C3A	2.48	0.43
1:J:478:GLN:NE2	1:K:432:ASP:H	2.16	0.43
3:L:604:HEC:CBC	3:L:605:HEC:HBB2	2.47	0.43
1:P:485:ARG:HD2	1:Q:490:GLU:OE2	2.18	0.43
1:Q:362:VAL:HG13	7:Q:736:HOH:O	2.17	0.43
1:T:478:GLN:NE2	1:U:432:ASP:H	2.15	0.43
1:V:485:ARG:HD2	1:W:490:GLU:OE2	2.17	0.43
1:G:297:CYS:HB3	3:G:605:HEC:HMB1	2.00	0.43
1:E:86:TRP:CH2	1:E:205:SER:HB3	2.54	0.43
3:E:605:HEC:HMD1	3:E:605:HEC:HBD1	2.00	0.43
1:I:244:SER:OG	1:I:296:THR:HB	2.18	0.43
1:Q:127:VAL:HG13	1:T:120:GLN:NE2	2.33	0.43
1:R:204:TRP:CH2	1:R:427:MET:HE1	2.53	0.43
1:U:165:PRO:HG2	3:U:601:HEC:HMD2	2.00	0.43
1:W:297:CYS:HB3	3:W:605:HEC:HMB1	2.00	0.43
1:X:86:TRP:CH2	1:X:205:SER:HB3	2.53	0.43
1:X:223:PRO:HG3	3:X:605:HEC:HBC2	2.01	0.43
1:G:173:ALA:HA	1:G:177:GLU:HB2	2.00	0.43
1:E:197:PHE:HB2	1:E:535:TRP:CD2	2.53	0.43
3:H:606:HEC:HBC1	3:H:607:HEC:HHC	1.99	0.43
1:J:432:ASP:H	1:L:478:GLN:NE2	2.16	0.43
1:N:485:ARG:HD2	1:O:490:GLU:OE2	2.19	0.43
1:G:318:SER:HB2	7:G:703:HOH:O	2.18	0.43
1:D:204:TRP:CH2	1:D:427:MET:HE1	2.54	0.43
1:D:467:PHE:N	1:D:467:PHE:CD1	2.86	0.43
3:J:606:HEC:HBC1	3:J:607:HEC:HHC	2.00	0.43
1:K:76:SER:CB	1:K:106:VAL:HG11	2.44	0.43
1:M:173:ALA:HA	1:M:177:GLU:HB2	1.99	0.43
1:T:403:SER:HB3	1:T:434:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:173:ALA:HA	1:W:177:GLU:HB2	1.99	0.43
1:X:197:PHE:HB2	1:X:535:TRP:CD2	2.54	0.43
1:G:165:PRO:HG2	3:G:601:HEC:HMD2	2.00	0.43
1:B:478:GLN:HE21	1:C:432:ASP:HB2	1.83	0.43
1:E:454:HIS:HD2	3:E:606:HEC:NC	2.16	0.43
1:J:41:PRO:O	1:J:44:VAL:HG12	2.19	0.43
3:J:607:HEC:O2A	1:K:226:ARG:NH2	2.52	0.43
3:L:606:HEC:HBC1	3:L:607:HEC:HHC	2.01	0.43
3:P:604:HEC:CBC	3:P:605:HEC:HBB2	2.49	0.43
1:Q:165:PRO:HG2	3:Q:601:HEC:HMD2	2.00	0.43
1:Q:297:CYS:HB3	3:Q:605:HEC:HMB1	2.00	0.43
1:S:207:GLU:HA	1:S:513:THR:OG1	2.19	0.43
1:V:323:MET:HE1	1:W:52:ASP:HB2	2.01	0.43
1:W:204:TRP:CH2	1:W:427:MET:HE1	2.54	0.43
3:W:606:HEC:HBC1	3:W:607:HEC:HHC	2.00	0.43
2:j:79:GLU:HG2	2:j:80:HIS:N	2.34	0.43
1:E:403:SER:HB3	1:E:434:GLU:OE2	2.17	0.43
1:H:538:THR:HA	2:d:110:PRO:HA	2.01	0.43
1:I:204:TRP:HH2	5:I:614:GOL:H31	1.84	0.43
1:J:226:ARG:NH2	3:L:607:HEC:O2A	2.52	0.43
1:K:197:PHE:HB2	1:K:535:TRP:CD2	2.54	0.43
3:Q:605:HEC:HMD1	3:Q:605:HEC:HBD1	2.00	0.43
3:Q:606:HEC:HBC1	3:Q:607:HEC:HHC	1.99	0.43
1:S:86:TRP:CH2	1:S:205:SER:HB3	2.53	0.43
1:S:173:ALA:HA	1:S:177:GLU:HB2	2.00	0.43
1:W:454:HIS:HD2	3:W:606:HEC:NC	2.14	0.43
1:C:223:PRO:HG3	3:C:605:HEC:HBC2	2.00	0.43
1:C:454:HIS:HD2	3:C:606:HEC:NC	2.16	0.43
1:D:509:LEU:HD11	1:F:477:LYS:NZ	2.34	0.43
1:E:41:PRO:O	1:E:44:VAL:HG12	2.19	0.43
1:F:86:TRP:CH2	1:F:205:SER:HB3	2.54	0.43
1:H:232:GLN:HE22	1:H:246:GLN:NE2	2.08	0.43
1:K:458:ASN:HB3	1:L:252:TRP:CZ2	2.54	0.43
1:L:41:PRO:O	1:L:44:VAL:HG12	2.19	0.43
1:L:197:PHE:HB2	1:L:535:TRP:CD2	2.54	0.43
1:M:223:PRO:HG3	3:M:605:HEC:HBC2	2.00	0.43
1:Q:79:PRO:HD3	1:Q:100:MET:HE2	2.01	0.43
1:R:41:PRO:O	1:R:44:VAL:HG12	2.18	0.43
3:G:601:HEC:HMA3	1:I:347:SER:HB3	2.00	0.43
1:A:297:CYS:HB3	3:A:605:HEC:HMB1	2.01	0.43
1:C:41:PRO:O	1:C:44:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:CYS:HB3	3:D:602:HEC:HMB1	1.99	0.43
3:Q:607:HEC:O2A	1:R:226:ARG:NH2	2.51	0.43
1:R:297:CYS:HB3	3:R:605:HEC:HMB1	2.01	0.43
1:S:478:GLN:HE21	1:T:432:ASP:HB2	1.83	0.43
1:T:297:CYS:HB3	3:T:605:HEC:HMB1	2.01	0.43
1:U:197:PHE:HB2	1:U:535:TRP:CD2	2.54	0.43
1:V:79:PRO:HB2	2:h:41:GLY:HA3	2.01	0.43
1:G:81:LYS:HD3	1:G:82:TYR:CZ	2.54	0.42
1:A:197:PHE:HB2	1:A:535:TRP:CD2	2.54	0.42
1:B:232:GLN:HE22	1:B:246:GLN:NE2	2.09	0.42
3:B:605:HEC:HMD1	3:B:605:HEC:CBD	2.49	0.42
3:B:605:HEC:HMD1	3:B:605:HEC:HBD1	2.00	0.42
1:C:538:THR:HG21	2:b:108:ARG:HG2	2.00	0.42
1:D:276:TRP:CE2	1:F:276:TRP:HB2	2.54	0.42
1:F:197:PHE:HB2	1:F:535:TRP:CD2	2.54	0.42
1:I:454:HIS:HD2	3:I:606:HEC:C1C	2.32	0.42
1:J:81:LYS:HD3	1:J:82:TYR:CZ	2.53	0.42
1:K:454:HIS:HD2	3:K:606:HEC:NC	2.14	0.42
1:O:173:ALA:HA	1:O:177:GLU:HB2	2.00	0.42
3:T:604:HEC:CBC	3:T:605:HEC:HBB2	2.47	0.42
1:U:227:CYS:HB3	3:U:602:HEC:HMB2	2.01	0.42
1:V:297:CYS:HB3	3:V:605:HEC:HMB1	2.01	0.42
1:B:197:PHE:HB2	1:B:535:TRP:CD2	2.54	0.42
1:B:297:CYS:HB3	3:B:605:HEC:HMB1	2.00	0.42
1:C:173:ALA:HA	1:C:177:GLU:HB2	2.00	0.42
1:F:297:CYS:HB3	3:F:605:HEC:HMB1	2.01	0.42
1:I:122:VAL:O	1:I:126:SER:HB3	2.19	0.42
1:I:287:LEU:HD12	3:I:604:HEC:HBD2	2.01	0.42
1:I:386:ASP:HA	1:I:387:PRO:HA	1.68	0.42
3:I:603:HEC:HHA	3:I:603:HEC:HAD2	1.89	0.42
1:M:90:PRO:O	1:M:93:ARG:HG2	2.19	0.42
1:M:182:GLU:OE1	2:g:26:TYR:HB3	2.18	0.42
1:M:458:ASN:HB3	1:N:252:TRP:CZ2	2.53	0.42
1:Q:223:PRO:HG3	3:Q:605:HEC:HBC2	2.01	0.42
1:R:86:TRP:CH2	1:R:205:SER:HB3	2.54	0.42
1:R:173:ALA:HA	1:R:177:GLU:HB2	1.99	0.42
3:G:607:HEC:O2A	1:H:226:ARG:NH2	2.52	0.42
1:A:41:PRO:O	1:A:44:VAL:HG12	2.20	0.42
3:E:604:HEC:CBC	3:E:605:HEC:HBB2	2.47	0.42
1:K:41:PRO:O	1:K:44:VAL:HG12	2.19	0.42
1:O:79:PRO:HD3	1:O:100:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:173:ALA:HA	1:P:177:GLU:HB2	2.00	0.42
3:C:606:HEC:HBC1	3:C:607:HEC:HHC	2.01	0.42
1:F:81:LYS:HD3	1:F:82:TYR:CZ	2.55	0.42
1:K:207:GLU:HA	1:K:513:THR:OG1	2.20	0.42
1:M:204:TRP:CH2	1:M:427:MET:HE1	2.54	0.42
1:R:386:ASP:HA	1:R:387:PRO:HA	1.73	0.42
1:S:197:PHE:HB2	1:S:535:TRP:CD2	2.54	0.42
1:S:297:CYS:HB3	3:S:605:HEC:HMB1	2.01	0.42
1:U:297:CYS:HB3	3:U:605:HEC:HMB1	2.01	0.42
3:U:601:HEC:HBA1	3:U:601:HEC:HHA	2.02	0.42
1:V:482:ARG:HH22	1:W:479:ASN:HD22	1.67	0.42
1:X:297:CYS:HB3	3:X:605:HEC:HMB1	2.00	0.42
3:X:605:HEC:HBD1	3:X:605:HEC:HMD1	2.02	0.42
1:G:232:GLN:HE22	1:G:246:GLN:NE2	2.07	0.42
1:F:386:ASP:HA	1:F:387:PRO:HA	1.73	0.42
1:F:403:SER:HB3	1:F:434:GLU:OE2	2.18	0.42
1:H:264:ILE:HG12	1:I:252:TRP:CE2	2.54	0.42
1:T:86:TRP:CH2	1:T:205:SER:HB3	2.54	0.42
1:T:204:TRP:CH2	1:T:427:MET:HE1	2.55	0.42
1:V:172:THR:HG21	2:h:34:TRP:CH2	2.54	0.42
1:V:403:SER:HB3	1:V:434:GLU:OE2	2.20	0.42
3:X:606:HEC:HBC1	3:X:607:HEC:HHC	2.02	0.42
3:A:607:HEC:O2A	1:B:226:ARG:NH2	2.53	0.42
1:B:478:GLN:NE2	1:C:432:ASP:H	2.18	0.42
1:C:189:GLY:HA2	3:C:605:HEC:CGD	2.50	0.42
1:D:485:ARG:HD3	1:E:497:TRP:CD2	2.55	0.42
1:F:454:HIS:HD2	3:F:606:HEC:NC	2.14	0.42
1:H:353:GLU:OE2	1:I:93:ARG:NH1	2.53	0.42
1:I:37:THR:HA	1:I:59:PHE:CE1	2.55	0.42
1:I:364:ASP:O	1:I:367:LEU:HB3	2.20	0.42
1:K:429:ASN:ND2	7:K:706:HOH:O	2.50	0.42
1:P:454:HIS:HD2	3:P:606:HEC:NC	2.14	0.42
1:R:189:GLY:HA2	3:R:605:HEC:CGD	2.50	0.42
1:S:165:PRO:HG2	3:S:601:HEC:HMD2	2.00	0.42
1:X:222:SER:HB2	1:X:223:PRO:HD3	2.02	0.42
3:A:606:HEC:HBC1	3:A:607:HEC:HHC	2.01	0.42
3:C:604:HEC:CBC	3:C:605:HEC:HBB2	2.48	0.42
1:E:297:CYS:HB3	3:E:605:HEC:HMB1	2.02	0.42
1:I:227:CYS:CB	3:I:602:HEC:HMB2	2.48	0.42
1:J:52:ASP:HB2	1:L:323:MET:HE1	2.02	0.42
1:L:86:TRP:CH2	1:L:205:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:PRO:O	1:M:44:VAL:HG12	2.19	0.42
1:M:482:ARG:HH22	1:N:479:ASN:HD22	1.67	0.42
1:M:485:ARG:HD2	1:N:490:GLU:OE2	2.19	0.42
1:N:127:VAL:CG2	1:R:123:ALA:HB2	2.43	0.42
1:N:197:PHE:HB2	1:N:535:TRP:CD2	2.55	0.42
3:O:606:HEC:HBC1	3:O:607:HEC:HHC	2.01	0.42
3:S:605:HEC:HMD1	3:S:605:HEC:HBD1	2.02	0.42
1:W:197:PHE:HB2	1:W:535:TRP:CD2	2.55	0.42
1:H:478:GLN:NE2	1:I:432:ASP:H	2.18	0.42
3:H:604:HEC:CBC	3:H:605:HEC:HBB2	2.49	0.42
1:N:458:ASN:HB3	1:O:252:TRP:CZ2	2.55	0.42
3:N:607:HEC:O2A	1:O:226:ARG:NH2	2.52	0.42
1:O:454:HIS:HD2	3:O:606:HEC:NC	2.17	0.42
1:Q:403:SER:HB3	1:Q:434:GLU:OE2	2.19	0.42
1:R:197:PHE:HB2	1:R:535:TRP:CD2	2.55	0.42
1:W:86:TRP:CH2	1:W:205:SER:HB3	2.55	0.42
1:W:189:GLY:HA2	3:W:605:HEC:CGD	2.50	0.42
1:X:41:PRO:O	1:X:44:VAL:HG12	2.19	0.42
1:B:204:TRP:CH2	1:B:427:MET:HE1	2.55	0.42
1:E:76:SER:CB	1:E:106:VAL:HG11	2.43	0.42
3:F:605:HEC:HBD1	3:F:605:HEC:HMD1	2.02	0.42
1:H:561:GLY:H	1:I:43:GLU:HA	1.85	0.42
1:I:204:TRP:CZ3	1:I:427:MET:HE1	2.55	0.42
1:K:505:THR:HG22	7:K:707:HOH:O	2.18	0.42
1:N:79:PRO:HD3	1:N:100:MET:HE2	2.01	0.42
1:P:86:TRP:CH2	1:P:205:SER:HB3	2.55	0.42
1:Q:81:LYS:HD3	1:Q:82:TYR:CZ	2.55	0.42
1:S:454:HIS:HD2	3:S:606:HEC:NC	2.15	0.42
1:S:482:ARG:HH22	1:T:479:ASN:HD22	1.68	0.42
1:U:454:HIS:HD2	3:U:606:HEC:NC	2.14	0.42
3:G:606:HEC:HBC1	3:G:607:HEC:HHC	2.01	0.42
1:A:235:GLN:HG2	7:A:723:HOH:O	2.19	0.42
1:C:386:ASP:HA	1:C:387:PRO:HA	1.73	0.42
1:J:482:ARG:HH22	1:K:479:ASN:HD22	1.68	0.42
1:N:207:GLU:HA	1:N:513:THR:OG1	2.20	0.42
1:O:86:TRP:CH2	1:O:205:SER:HB3	2.55	0.42
1:O:223:PRO:HG3	3:O:605:HEC:HBC2	2.01	0.42
1:P:197:PHE:HB2	1:P:535:TRP:CD2	2.55	0.42
1:Q:154:CYS:HB3	1:Q:165:PRO:HG3	2.02	0.42
1:S:204:TRP:CH2	1:S:427:MET:HE1	2.54	0.42
1:S:223:PRO:HG3	3:S:605:HEC:HBC2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:490:GLU:OE2	1:U:485:ARG:HD2	2.20	0.42
1:V:204:TRP:CH2	1:V:427:MET:HE1	2.55	0.42
2:j:34:TRP:HB2	2:j:98:PHE:HA	2.01	0.42
1:G:485:ARG:HD2	1:H:490:GLU:OE2	2.20	0.41
1:D:235:GLN:HE22	1:F:280:GLN:NE2	2.18	0.41
1:D:262:TYR:CB	3:D:606:HEC:HBB2	2.50	0.41
1:H:41:PRO:O	1:H:44:VAL:HG12	2.19	0.41
1:I:450:LYS:HE2	3:I:606:HEC:HAA1	2.01	0.41
1:J:458:ASN:HB3	1:K:252:TRP:CZ2	2.54	0.41
1:N:41:PRO:O	1:N:44:VAL:HG12	2.20	0.41
1:N:86:TRP:CH2	1:N:205:SER:HB3	2.55	0.41
1:O:41:PRO:O	1:O:44:VAL:HG12	2.20	0.41
1:O:176:HIS:HB3	1:O:179:GLN:HE21	1.85	0.41
1:O:197:PHE:HB2	1:O:535:TRP:CD2	2.55	0.41
1:Q:86:TRP:CH2	1:Q:205:SER:HB3	2.54	0.41
3:Q:605:HEC:HMD1	3:Q:605:HEC:CBD	2.50	0.41
1:R:90:PRO:O	1:R:93:ARG:HG2	2.19	0.41
1:R:223:PRO:HG3	3:R:605:HEC:HBC2	2.02	0.41
3:S:605:HEC:HMD1	3:S:605:HEC:CBD	2.50	0.41
1:T:189:GLY:HA2	3:T:605:HEC:CGD	2.50	0.41
3:G:605:HEC:HBD1	3:G:605:HEC:HMD1	2.02	0.41
1:B:79:PRO:HD3	1:B:100:MET:HE2	2.01	0.41
1:E:378:ASP:HB2	7:E:711:HOH:O	2.20	0.41
1:F:232:GLN:HE22	1:F:246:GLN:NE2	2.08	0.41
1:H:197:PHE:HB2	1:H:535:TRP:CD2	2.55	0.41
3:K:604:HEC:CBC	3:K:605:HEC:HBB2	2.48	0.41
1:O:204:TRP:CH2	1:O:427:MET:HE1	2.55	0.41
1:R:81:LYS:HD3	1:R:82:TYR:CZ	2.55	0.41
3:R:605:HEC:HMD1	3:R:605:HEC:CBD	2.50	0.41
1:T:386:ASP:HA	1:T:387:PRO:HA	1.73	0.41
1:V:52:ASP:HB2	1:X:323:MET:HE1	2.02	0.41
3:W:605:HEC:HBD1	3:W:605:HEC:HMD1	2.02	0.41
1:G:52:ASP:HB2	1:I:323:MET:HE1	2.02	0.41
1:G:223:PRO:HG3	3:G:605:HEC:HBC2	2.02	0.41
1:A:323:MET:HE1	1:B:52:ASP:HB2	2.01	0.41
1:A:478:GLN:NE2	1:B:432:ASP:H	2.18	0.41
3:E:601:HEC:HBA1	3:E:601:HEC:HHA	2.02	0.41
1:H:81:LYS:HD3	1:H:82:TYR:CZ	2.55	0.41
1:H:485:ARG:HD3	1:I:497:TRP:CD1	2.55	0.41
1:K:57:VAL:HG11	5:K:615:GOL:O2	2.21	0.41
1:K:81:LYS:HD3	1:K:82:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:601:HEC:HBC1	3:K:602:HEC:CHC	2.50	0.41
1:L:154:CYS:HB3	1:L:165:PRO:HG3	2.02	0.41
1:N:323:MET:HE1	1:O:52:ASP:HB2	2.02	0.41
1:P:204:TRP:CH2	1:P:427:MET:HE1	2.55	0.41
3:P:601:HEC:HMA3	1:R:347:SER:HB3	2.03	0.41
1:R:433:VAL:HG23	7:R:709:HOH:O	2.19	0.41
1:R:454:HIS:HD2	3:R:606:HEC:NC	2.15	0.41
1:S:154:CYS:HB3	1:S:165:PRO:HG3	2.02	0.41
1:V:86:TRP:CH2	1:V:205:SER:HB3	2.55	0.41
1:V:197:PHE:HB2	1:V:535:TRP:CD2	2.55	0.41
1:A:81:LYS:HD3	1:A:82:TYR:CZ	2.56	0.41
1:B:323:MET:HE1	1:C:52:ASP:HB2	2.01	0.41
1:D:355:LEU:HD23	1:D:355:LEU:HA	1.92	0.41
1:H:79:PRO:HD3	1:H:100:MET:HE2	2.02	0.41
1:H:204:TRP:CH2	1:H:427:MET:HE1	2.55	0.41
1:I:141:HIS:CD2	1:I:149:THR:HB	2.56	0.41
1:L:165:PRO:HG2	3:L:601:HEC:HMD2	2.02	0.41
1:M:86:TRP:CH2	1:M:205:SER:HB3	2.55	0.41
1:O:232:GLN:HE22	1:O:246:GLN:NE2	2.10	0.41
1:Q:197:PHE:HB2	1:Q:535:TRP:CD2	2.55	0.41
1:T:154:CYS:HB3	1:T:165:PRO:HG3	2.01	0.41
1:X:154:CYS:HB3	1:X:165:PRO:HG3	2.02	0.41
3:G:605:HEC:HMD1	3:G:605:HEC:CBD	2.50	0.41
1:A:86:TRP:CH2	1:A:205:SER:HB3	2.54	0.41
1:A:226:ARG:NH2	3:C:607:HEC:O2A	2.53	0.41
1:A:386:ASP:HA	1:A:387:PRO:HA	1.74	0.41
1:B:454:HIS:HD2	3:B:606:HEC:NC	2.13	0.41
1:C:154:CYS:HB3	1:C:165:PRO:HG3	2.03	0.41
1:C:197:PHE:HB2	1:C:535:TRP:CD2	2.55	0.41
1:D:335:ARG:O	1:D:339:VAL:HG23	2.21	0.41
1:J:479:ASN:HD22	1:L:482:ARG:HH22	1.69	0.41
1:K:132:ILE:HG12	5:K:614:GOL:C1	2.50	0.41
1:M:479:ASN:HD22	1:O:482:ARG:HH22	1.69	0.41
1:T:81:LYS:HD3	1:T:82:TYR:CZ	2.55	0.41
1:U:223:PRO:HG3	3:U:605:HEC:HBC2	2.01	0.41
1:V:41:PRO:O	1:V:44:VAL:HG12	2.20	0.41
1:V:485:ARG:HD3	1:W:497:TRP:CG	2.55	0.41
3:W:607:HEC:O2A	1:X:226:ARG:NH2	2.54	0.41
1:G:154:CYS:HB3	1:G:165:PRO:HG3	2.02	0.41
1:A:454:HIS:HD2	3:A:606:HEC:NC	2.14	0.41
1:D:474:VAL:HG13	1:E:430:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:ASP:CB	7:E:711:HOH:O	2.69	0.41
1:I:41:PRO:O	1:I:44:VAL:HG12	2.20	0.41
1:I:198:ALA:O	1:I:202:CYS:HB2	2.20	0.41
1:J:76:SER:CB	1:J:106:VAL:HG11	2.43	0.41
1:L:454:HIS:HD2	3:L:606:HEC:NC	2.15	0.41
3:M:607:HEC:O2A	1:N:226:ARG:NH2	2.53	0.41
1:N:349:ARG:NH2	4:N:610:SO4:S	2.94	0.41
1:P:207:GLU:HA	1:P:513:THR:OG1	2.20	0.41
1:Q:207:GLU:HA	1:Q:513:THR:OG1	2.20	0.41
1:R:207:GLU:HA	1:R:513:THR:OG1	2.21	0.41
3:S:601:HEC:HBA1	3:S:601:HEC:HHA	2.02	0.41
3:V:605:HEC:HBD1	3:V:605:HEC:HMD1	2.01	0.41
1:W:41:PRO:O	1:W:44:VAL:HG12	2.20	0.41
1:W:340:SER:O	1:W:343:ASP:HB2	2.20	0.41
1:X:454:HIS:HD2	3:X:606:HEC:NC	2.15	0.41
1:C:204:TRP:CH2	1:C:427:MET:HE1	2.56	0.41
1:I:48:PRO:HA	1:I:63:LYS:HB3	2.02	0.41
3:K:601:HEC:HHA	3:K:601:HEC:HBA1	2.03	0.41
3:M:605:HEC:HBD1	3:M:605:HEC:HMD1	2.03	0.41
3:O:601:HEC:HBA1	3:O:601:HEC:HHA	2.02	0.41
1:P:154:CYS:HB3	1:P:165:PRO:HG3	2.03	0.41
1:P:479:ASN:HD22	1:R:482:ARG:HH22	1.68	0.41
1:W:458:ASN:HB3	1:X:252:TRP:CZ2	2.56	0.41
1:X:104:ASP:CG	2:j:87:LYS:HZ3	2.29	0.41
1:X:204:TRP:CH2	1:X:427:MET:HE1	2.56	0.41
1:D:485:ARG:HD3	1:E:497:TRP:CE2	2.56	0.41
1:J:207:GLU:HA	1:J:513:THR:OG1	2.21	0.41
3:J:605:HEC:HMD1	3:J:605:HEC:HBD1	2.03	0.41
1:K:86:TRP:CH2	1:K:205:SER:HB3	2.55	0.41
1:K:182:GLU:OE1	2:b:26:TYR:HB3	2.21	0.41
1:L:79:PRO:HD3	1:L:100:MET:HE2	2.02	0.41
3:L:605:HEC:CBD	3:L:605:HEC:HMD1	2.51	0.41
1:M:108:PRO:HD3	7:M:712:HOH:O	2.19	0.41
1:P:98:ASP:HB2	7:P:701:HOH:O	2.20	0.41
1:P:323:MET:HE1	1:Q:52:ASP:HB2	2.03	0.41
1:U:41:PRO:O	1:U:44:VAL:HG12	2.20	0.41
1:U:154:CYS:HB3	1:U:165:PRO:HG3	2.02	0.41
1:G:86:TRP:CH2	1:G:205:SER:HB3	2.56	0.41
1:D:169:ALA:O	1:D:172:THR:HG22	2.21	0.41
1:D:202:CYS:HB3	1:D:205:SER:HB2	2.01	0.41
1:D:223:PRO:HG3	3:D:605:HEC:HBC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:TRP:CH2	1:E:427:MET:HE1	2.56	0.41
1:E:485:ARG:HD2	1:F:490:GLU:OE2	2.20	0.41
3:F:600:HEC:HHH	3:F:600:HEC:CBC	2.49	0.41
3:F:605:HEC:HMD1	3:F:605:HEC:CBD	2.50	0.41
1:I:59:PHE:C	1:I:61:GLY:N	2.76	0.41
1:I:232:GLN:NE2	1:I:246:GLN:HE22	2.10	0.41
1:I:319:MET:SD	3:I:603:HEC:HBA1	2.61	0.41
1:J:252:TRP:CZ2	1:L:458:ASN:HB3	2.56	0.41
1:J:410:HIS:HE1	5:J:613:GOL:O1	2.04	0.41
1:K:386:ASP:HA	1:K:387:PRO:HA	1.72	0.41
1:L:232:GLN:HE22	1:L:246:GLN:NE2	2.04	0.41
1:M:478:GLN:NE2	1:N:432:ASP:H	2.18	0.41
3:M:605:HEC:HMD1	3:M:605:HEC:CBD	2.51	0.41
1:N:204:TRP:CH2	1:N:427:MET:HE1	2.55	0.41
1:N:482:ARG:HH22	1:O:479:ASN:HD22	1.68	0.41
3:O:600:HEC:HHH	3:O:600:HEC:CBC	2.48	0.41
1:Q:127:VAL:HG13	1:T:120:GLN:HE21	1.85	0.41
1:Q:323:MET:HE1	1:R:52:ASP:HB2	2.03	0.41
1:Q:349:ARG:NH2	4:Q:609:SO4:O1	2.53	0.41
1:S:81:LYS:HD3	1:S:82:TYR:CZ	2.56	0.41
1:S:386:ASP:HA	1:S:387:PRO:HA	1.73	0.41
1:T:176:HIS:HB3	1:T:179:GLN:HE21	1.86	0.41
1:T:223:PRO:HG3	3:T:605:HEC:HBC2	2.02	0.41
3:X:601:HEC:HBA1	3:X:601:HEC:HHA	2.03	0.41
1:D:386:ASP:HA	1:D:387:PRO:HA	1.76	0.41
1:F:204:TRP:CH2	1:F:427:MET:HE1	2.56	0.41
1:H:297:CYS:HB3	3:H:605:HEC:HMB1	2.03	0.41
1:H:347:SER:HB3	3:I:601:HEC:HMA3	2.03	0.41
3:H:606:HEC:CBC	5:H:614:GOL:H12	2.51	0.41
1:I:296:THR:O	1:I:297:CYS:C	2.64	0.41
1:N:478:GLN:NE2	1:O:432:ASP:H	2.19	0.41
1:O:76:SER:CB	1:O:106:VAL:HG11	2.44	0.41
1:Q:243:ARG:NH1	7:Q:702:HOH:O	2.47	0.41
3:Q:600:HEC:HAA2	3:Q:601:HEC:HMA3	2.03	0.41
3:Q:601:HEC:HBA1	3:Q:601:HEC:HHA	2.02	0.41
1:R:154:CYS:HB3	1:R:165:PRO:HG3	2.03	0.41
1:S:39:TRP:CZ2	1:U:541:ALA:HA	2.56	0.41
3:S:604:HEC:CBC	3:S:605:HEC:HBB2	2.48	0.41
1:V:154:CYS:HB3	1:V:165:PRO:HG3	2.02	0.41
1:X:172:THR:HG21	2:j:34:TRP:CH2	2.56	0.41
1:G:222:SER:HB2	1:G:223:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:HD3	1:A:100:MET:HE2	2.03	0.40
1:A:176:HIS:HB3	1:A:179:GLN:HE21	1.86	0.40
3:B:604:HEC:CBC	3:B:605:HEC:HBB2	2.46	0.40
1:D:150:GLY:O	1:D:151:CYS:C	2.64	0.40
1:H:454:HIS:HD2	3:H:606:HEC:NC	2.15	0.40
1:I:314:ILE:HA	1:I:334:LYS:HD3	2.03	0.40
1:M:207:GLU:HA	1:M:513:THR:OG1	2.21	0.40
1:O:81:LYS:HD3	1:O:82:TYR:CZ	2.56	0.40
1:P:189:GLY:HA2	3:P:605:HEC:CGD	2.51	0.40
1:P:478:GLN:NE2	1:Q:432:ASP:H	2.18	0.40
1:P:482:ARG:HH22	1:Q:479:ASN:HD22	1.69	0.40
1:R:368:LYS:NZ	1:R:466:SER:OG	2.54	0.40
1:V:207:GLU:HA	1:V:513:THR:OG1	2.21	0.40
1:W:154:CYS:HB3	1:W:165:PRO:HG3	2.02	0.40
1:W:485:ARG:HD3	1:X:497:TRP:CG	2.56	0.40
3:W:601:HEC:HHA	3:W:601:HEC:HBA1	2.02	0.40
1:X:81:LYS:HD3	1:X:82:TYR:CZ	2.56	0.40
1:X:337:ARG:NH2	4:X:610:SO4:S	2.91	0.40
1:X:403:SER:HB3	1:X:434:GLU:OE2	2.20	0.40
1:B:386:ASP:HA	1:B:387:PRO:HA	1.72	0.40
1:D:369:TYR:CE1	1:D:441:VAL:HB	2.56	0.40
1:F:176:HIS:HB3	1:F:179:GLN:HE21	1.86	0.40
1:H:353:GLU:CD	1:I:93:ARG:HH11	2.29	0.40
3:J:605:HEC:HMD1	3:J:605:HEC:CBD	2.51	0.40
1:K:485:ARG:HD2	1:L:490:GLU:OE2	2.21	0.40
3:N:604:HEC:CBC	3:N:605:HEC:HBB2	2.50	0.40
3:N:605:HEC:HBD1	3:N:605:HEC:HMD1	2.03	0.40
1:Q:79:PRO:CD	1:Q:100:MET:HE2	2.51	0.40
1:R:79:PRO:HD3	1:R:100:MET:HE2	2.03	0.40
1:U:189:GLY:HA2	3:U:605:HEC:CGD	2.50	0.40
1:D:189:GLY:HA2	3:D:605:HEC:O2D	2.22	0.40
1:F:207:GLU:HA	1:F:513:THR:OG1	2.21	0.40
1:H:473:LEU:HD23	5:H:615:GOL:O1	2.21	0.40
1:I:220:HIS:O	1:I:223:PRO:HD2	2.21	0.40
1:I:314:ILE:HD12	3:I:606:HEC:O2D	2.21	0.40
1:J:86:TRP:CH2	1:J:205:SER:HB3	2.56	0.40
1:J:257:ARG:HD3	7:J:763:HOH:O	2.20	0.40
1:K:154:CYS:HB3	1:K:165:PRO:HG3	2.03	0.40
1:L:207:GLU:HA	1:L:513:THR:OG1	2.22	0.40
3:L:605:HEC:HMD1	3:L:605:HEC:HBD1	2.02	0.40
1:N:297:CYS:HB3	3:N:605:HEC:HMB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:81:LYS:HD3	1:P:82:TYR:CZ	2.56	0.40
1:P:226:ARG:NH2	3:R:607:HEC:O2A	2.55	0.40
3:P:606:HEC:HBC1	3:P:607:HEC:HHC	2.02	0.40
1:T:41:PRO:O	1:T:44:VAL:HG12	2.21	0.40
3:W:605:HEC:HMD1	3:W:605:HEC:CBD	2.51	0.40
3:X:605:HEC:HMD1	3:X:605:HEC:CBD	2.51	0.40
1:G:235:GLN:NE2	1:I:280:GLN:NE2	2.60	0.40
5:A:612:GOL:H11	1:C:370:ARG:HG2	2.03	0.40
1:D:252:TRP:CE2	1:F:264:ILE:HG12	2.57	0.40
1:J:427:MET:CE	7:J:747:HOH:O	2.70	0.40
3:K:600:HEC:HAA2	3:K:601:HEC:HMA3	2.03	0.40
1:N:189:GLY:HA2	3:N:605:HEC:CGD	2.51	0.40
1:A:52:ASP:HB2	1:C:323:MET:HE1	2.03	0.40
1:A:189:GLY:HA2	3:A:605:HEC:CGD	2.51	0.40
1:B:176:HIS:HB3	1:B:179:GLN:HE21	1.85	0.40
1:C:76:SER:CB	1:C:106:VAL:HG11	2.44	0.40
1:I:294:GLY:C	3:I:607:HEC:HBC2	2.47	0.40
3:L:600:HEC:HAA2	3:L:601:HEC:HMA3	2.04	0.40
3:N:605:HEC:HMD1	3:N:605:HEC:CBD	2.52	0.40
3:N:606:HEC:HBC1	3:N:607:HEC:HHC	2.03	0.40
1:Q:454:HIS:HD2	3:Q:606:HEC:NC	2.14	0.40
1:W:81:LYS:HD3	1:W:82:TYR:CZ	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:O	1:R:496:SER:OG[1_545]	1.83	0.37
1:G:42:HIS:NE2	1:J:496:SER:CB[2_555]	2.03	0.17
1:G:496:SER:OG	1:Q:491:LYS:O[1_655]	2.18	0.02

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	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	B	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	C	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	D	529/582 (91%)	491 (93%)	36 (7%)	2 (0%)	30	60
1	E	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	F	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	G	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	H	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	I	525/582 (90%)	502 (96%)	23 (4%)	0	100	100
1	J	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	K	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	L	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	M	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	N	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	O	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	P	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	Q	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	R	530/582 (91%)	515 (97%)	15 (3%)	0	100	100
1	S	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	T	529/582 (91%)	511 (97%)	18 (3%)	0	100	100
1	U	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	V	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	W	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	X	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
2	Y	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	Z	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
2	a	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	b	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	c	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	d	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	e	84/114 (74%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	g	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	h	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	i	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	j	84/114 (74%)	79 (94%)	5 (6%)	0	100	100
All	All	13701/15336 (89%)	13279 (97%)	420 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	HIS
1	D	106	VAL

5.3.2 Protein sidechains ⓘ

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	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	B	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	C	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	D	451/491 (92%)	435 (96%)	16 (4%)	32	67
1	E	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	F	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	G	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	H	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	I	449/491 (91%)	429 (96%)	20 (4%)	24	58
1	J	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	K	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	L	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	M	451/491 (92%)	448 (99%)	3 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	O	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	P	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	Q	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	R	452/491 (92%)	448 (99%)	4 (1%)	70	89
1	S	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	T	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	U	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	V	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	W	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	X	451/491 (92%)	446 (99%)	5 (1%)	65	87
2	Y	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	Z	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	a	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	b	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	c	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	d	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	e	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	f	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	g	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	h	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	i	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	j	68/86 (79%)	67 (98%)	1 (2%)	57	84
All	All	11639/12816 (91%)	11485 (99%)	154 (1%)	61	86

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	42	HIS
1	G	78	TYR
1	G	86	TRP
1	G	115	THR
1	G	472	TRP
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	78	TYR
1	A	86	TRP
1	A	115	THR
1	A	472	TRP
1	B	42	HIS
1	B	86	TRP
1	B	472	TRP
1	C	42	HIS
1	C	86	TRP
1	C	115	THR
1	D	78	TYR
1	D	86	TRP
1	D	100	MET
1	D	106	VAL
1	D	172	THR
1	D	205	SER
1	D	278	THR
1	D	309	VAL
1	D	319	MET
1	D	349	ARG
1	D	446	THR
1	D	472	TRP
1	D	513	THR
1	D	558	ILE
1	D	559	THR
1	D	563	HIS
1	E	42	HIS
1	E	78	TYR
1	E	86	TRP
1	E	115	THR
1	E	472	TRP
1	F	42	HIS
1	F	86	TRP
1	F	472	TRP
1	H	42	HIS
1	H	78	TYR
1	H	86	TRP
1	H	115	THR
1	H	472	TRP
1	I	33	VAL
1	I	43	GLU
1	I	44	VAL

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Mol	Chain	Res	Type
1	I	86	TRP
1	I	106	VAL
1	I	115	THR
1	I	157	ASN
1	I	205	SER
1	I	231	HIS
1	I	278	THR
1	I	309	VAL
1	I	318	SER
1	I	332	LYS
1	I	349	ARG
1	I	362	VAL
1	I	368	LYS
1	I	446	THR
1	I	472	TRP
1	I	496	SER
1	I	545	GLU
1	J	42	HIS
1	J	78	TYR
1	J	86	TRP
1	J	115	THR
1	J	472	TRP
1	K	42	HIS
1	K	78	TYR
1	K	86	TRP
1	K	115	THR
1	K	472	TRP
1	L	42	HIS
1	L	86	TRP
1	L	115	THR
1	L	472	TRP
1	M	42	HIS
1	M	86	TRP
1	M	472	TRP
1	N	42	HIS
1	N	86	TRP
1	N	115	THR
1	N	472	TRP
1	O	42	HIS
1	O	86	TRP
1	O	472	TRP
1	P	42	HIS

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Mol	Chain	Res	Type
1	P	78	TYR
1	P	86	TRP
1	P	115	THR
1	Q	42	HIS
1	Q	78	TYR
1	Q	86	TRP
1	Q	472	TRP
1	R	42	HIS
1	R	78	TYR
1	R	86	TRP
1	R	472	TRP
1	S	42	HIS
1	S	78	TYR
1	S	86	TRP
1	S	472	TRP
1	T	42	HIS
1	T	78	TYR
1	T	86	TRP
1	T	472	TRP
1	U	42	HIS
1	U	86	TRP
1	U	115	THR
1	V	42	HIS
1	V	78	TYR
1	V	86	TRP
1	W	42	HIS
1	W	78	TYR
1	W	86	TRP
1	W	472	TRP
1	X	42	HIS
1	X	78	TYR
1	X	86	TRP
1	X	115	THR
1	X	472	TRP
2	Y	54	GLU
2	Y	79	GLU
2	Z	54	GLU
2	Z	79	GLU
2	Z	100	SER
2	a	54	GLU
2	a	79	GLU
2	a	100	SER

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Mol	Chain	Res	Type
2	b	54	GLU
2	b	79	GLU
2	b	100	SER
2	c	54	GLU
2	c	79	GLU
2	c	100	SER
2	d	54	GLU
2	d	79	GLU
2	e	54	GLU
2	e	79	GLU
2	f	54	GLU
2	f	79	GLU
2	g	54	GLU
2	g	79	GLU
2	g	100	SER
2	h	54	GLU
2	h	79	GLU
2	h	100	SER
2	i	54	GLU
2	i	79	GLU
2	i	100	SER
2	j	61	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (233) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	102	ASN
1	G	179	GLN
1	G	235	GLN
1	G	246	GLN
1	G	410	HIS
1	G	429	ASN
1	G	478	GLN
1	G	479	ASN
1	G	520	ASN
1	G	563	HIS
1	A	102	ASN
1	A	179	GLN
1	A	235	GLN
1	A	246	GLN
1	A	354	ASN
1	A	410	HIS

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Mol	Chain	Res	Type
1	A	478	GLN
1	A	479	ASN
1	A	520	ASN
1	B	102	ASN
1	B	179	GLN
1	B	235	GLN
1	B	246	GLN
1	B	410	HIS
1	B	478	GLN
1	B	479	ASN
1	B	520	ASN
1	B	563	HIS
1	C	102	ASN
1	C	179	GLN
1	C	235	GLN
1	C	246	GLN
1	C	354	ASN
1	C	410	HIS
1	C	478	GLN
1	C	479	ASN
1	C	520	ASN
1	D	102	ASN
1	D	157	ASN
1	D	179	GLN
1	D	185	GLN
1	D	235	GLN
1	D	246	GLN
1	D	410	HIS
1	D	429	ASN
1	D	478	GLN
1	D	498	GLN
1	E	102	ASN
1	E	179	GLN
1	E	235	GLN
1	E	246	GLN
1	E	410	HIS
1	E	478	GLN
1	E	520	ASN
1	F	102	ASN
1	F	179	GLN
1	F	235	GLN
1	F	246	GLN

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Mol	Chain	Res	Type
1	F	280	GLN
1	F	354	ASN
1	F	410	HIS
1	F	478	GLN
1	F	479	ASN
1	F	520	ASN
1	H	102	ASN
1	H	179	GLN
1	H	183	GLN
1	H	235	GLN
1	H	246	GLN
1	H	354	ASN
1	H	410	HIS
1	H	429	ASN
1	H	478	GLN
1	H	479	ASN
1	H	520	ASN
1	I	102	ASN
1	I	179	GLN
1	I	185	GLN
1	I	199	GLN
1	I	235	GLN
1	I	246	GLN
1	I	354	ASN
1	I	399	GLN
1	I	410	HIS
1	I	429	ASN
1	I	478	GLN
1	I	479	ASN
1	J	102	ASN
1	J	179	GLN
1	J	235	GLN
1	J	246	GLN
1	J	354	ASN
1	J	399	GLN
1	J	410	HIS
1	J	478	GLN
1	J	479	ASN
1	J	520	ASN
1	J	539	HIS
1	K	102	ASN
1	K	179	GLN

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Mol	Chain	Res	Type
1	K	235	GLN
1	K	246	GLN
1	K	410	HIS
1	K	429	ASN
1	K	478	GLN
1	K	479	ASN
1	K	520	ASN
1	L	42	HIS
1	L	102	ASN
1	L	179	GLN
1	L	235	GLN
1	L	246	GLN
1	L	354	ASN
1	L	410	HIS
1	L	429	ASN
1	L	478	GLN
1	L	479	ASN
1	L	520	ASN
1	M	102	ASN
1	M	179	GLN
1	M	235	GLN
1	M	246	GLN
1	M	410	HIS
1	M	478	GLN
1	M	479	ASN
1	M	520	ASN
1	N	102	ASN
1	N	179	GLN
1	N	235	GLN
1	N	246	GLN
1	N	410	HIS
1	N	429	ASN
1	N	478	GLN
1	N	479	ASN
1	N	520	ASN
1	O	102	ASN
1	O	179	GLN
1	O	235	GLN
1	O	246	GLN
1	O	410	HIS
1	O	478	GLN
1	O	479	ASN

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Mol	Chain	Res	Type
1	O	520	ASN
1	P	102	ASN
1	P	179	GLN
1	P	235	GLN
1	P	246	GLN
1	P	354	ASN
1	P	410	HIS
1	P	429	ASN
1	P	478	GLN
1	P	479	ASN
1	P	520	ASN
1	Q	102	ASN
1	Q	179	GLN
1	Q	235	GLN
1	Q	246	GLN
1	Q	354	ASN
1	Q	410	HIS
1	Q	478	GLN
1	Q	479	ASN
1	Q	520	ASN
1	R	102	ASN
1	R	179	GLN
1	R	235	GLN
1	R	246	GLN
1	R	410	HIS
1	R	429	ASN
1	R	478	GLN
1	R	479	ASN
1	R	520	ASN
1	R	563	HIS
1	S	102	ASN
1	S	179	GLN
1	S	235	GLN
1	S	246	GLN
1	S	354	ASN
1	S	410	HIS
1	S	429	ASN
1	S	478	GLN
1	S	479	ASN
1	S	520	ASN
1	T	102	ASN
1	T	179	GLN

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Mol	Chain	Res	Type
1	T	235	GLN
1	T	246	GLN
1	T	410	HIS
1	T	478	GLN
1	T	479	ASN
1	T	520	ASN
1	U	42	HIS
1	U	102	ASN
1	U	179	GLN
1	U	235	GLN
1	U	246	GLN
1	U	354	ASN
1	U	410	HIS
1	U	478	GLN
1	U	479	ASN
1	U	520	ASN
1	V	102	ASN
1	V	179	GLN
1	V	235	GLN
1	V	246	GLN
1	V	354	ASN
1	V	410	HIS
1	V	478	GLN
1	V	479	ASN
1	V	520	ASN
1	W	102	ASN
1	W	179	GLN
1	W	235	GLN
1	W	246	GLN
1	W	354	ASN
1	W	410	HIS
1	W	478	GLN
1	W	479	ASN
1	W	520	ASN
1	X	102	ASN
1	X	179	GLN
1	X	235	GLN
1	X	246	GLN
1	X	410	HIS
1	X	478	GLN
1	X	479	ASN
1	X	520	ASN

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Mol	Chain	Res	Type
1	X	540	HIS
1	X	563	HIS
2	Y	95	ASN
2	a	95	ASN
2	d	95	ASN
2	e	95	ASN
2	g	95	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 286 ligands modelled in this entry, 4 are monoatomic - leaving 282 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	K	610	-	4,4,4	0.44	0	6,6,6	0.12	0
4	SO4	J	611	-	4,4,4	0.39	0	6,6,6	0.08	0
3	HEC	N	603	7,1	46,50,50	2.92	16 (34%)	58,82,82	3.20	14 (24%)
4	SO4	M	609	-	4,4,4	0.45	0	6,6,6	0.11	0
3	HEC	W	600	1	46,50,50	1.71	8 (17%)	58,82,82	1.41	9 (15%)
3	HEC	E	602	1	46,50,50	1.74	9 (19%)	58,82,82	1.44	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	N	606	1	46,50,50	1.72	10 (21%)	58,82,82	1.46	8 (13%)
3	HEC	E	600	1	46,50,50	1.73	8 (17%)	58,82,82	1.43	8 (13%)
3	HEC	X	603	7,1	46,50,50	2.92	16 (34%)	58,82,82	3.26	14 (24%)
4	SO4	F	610	-	4,4,4	0.43	0	6,6,6	0.04	0
4	SO4	I	609	-	4,4,4	0.42	0	6,6,6	0.32	0
3	HEC	P	606	1	46,50,50	1.73	9 (19%)	58,82,82	1.41	8 (13%)
3	HEC	Q	607	1	46,50,50	1.73	10 (21%)	58,82,82	1.37	10 (17%)
3	HEC	U	601	1	46,50,50	1.70	9 (19%)	58,82,82	1.53	10 (17%)
5	GOL	J	613	-	5,5,5	0.27	0	5,5,5	0.53	0
3	HEC	U	600	1	46,50,50	1.70	8 (17%)	58,82,82	1.44	8 (13%)
3	HEC	C	602	1	46,50,50	1.74	8 (17%)	58,82,82	1.44	10 (17%)
4	SO4	H	611	-	4,4,4	0.42	0	6,6,6	0.22	0
4	SO4	N	610	-	4,4,4	0.45	0	6,6,6	0.11	0
5	GOL	A	614	-	5,5,5	0.36	0	5,5,5	0.21	0
5	GOL	I	614	-	5,5,5	0.23	0	5,5,5	0.21	0
3	HEC	S	602	1	46,50,50	1.72	9 (19%)	58,82,82	1.44	8 (13%)
3	HEC	L	605	1	46,50,50	1.73	10 (21%)	58,82,82	1.53	12 (20%)
3	HEC	G	600	1	46,50,50	1.69	8 (17%)	58,82,82	1.46	9 (15%)
3	HEC	J	600	1	46,50,50	1.70	9 (19%)	58,82,82	1.45	9 (15%)
5	GOL	L	613	-	5,5,5	0.26	0	5,5,5	0.39	0
3	HEC	R	600	1	46,50,50	1.71	8 (17%)	58,82,82	1.39	9 (15%)
5	GOL	I	615	-	5,5,5	0.34	0	5,5,5	0.38	0
3	HEC	F	604	1	46,50,50	1.73	9 (19%)	58,82,82	1.54	13 (22%)
3	HEC	Q	601	1	46,50,50	1.69	8 (17%)	58,82,82	1.51	11 (18%)
4	SO4	A	609	-	4,4,4	0.40	0	6,6,6	0.14	0
3	HEC	V	600	1	46,50,50	1.72	9 (19%)	58,82,82	1.42	10 (17%)
4	SO4	C	611	-	4,4,4	0.44	0	6,6,6	0.15	0
3	HEC	H	606	1	46,50,50	1.74	10 (21%)	58,82,82	1.42	8 (13%)
4	SO4	H	612	-	4,4,4	0.45	0	6,6,6	0.07	0
3	HEC	X	607	1	46,50,50	1.73	10 (21%)	58,82,82	1.35	7 (12%)
4	SO4	L	612	-	4,4,4	0.46	0	6,6,6	0.08	0
4	SO4	C	609	-	4,4,4	0.42	0	6,6,6	0.15	0
4	SO4	G	612	-	4,4,4	0.44	0	6,6,6	0.15	0
3	HEC	E	605	1	46,50,50	1.74	10 (21%)	58,82,82	1.46	11 (18%)
3	HEC	V	604	1	46,50,50	1.73	8 (17%)	58,82,82	1.57	13 (22%)
5	GOL	K	613	-	5,5,5	0.23	0	5,5,5	0.38	0
3	HEC	L	607	1	46,50,50	1.73	9 (19%)	58,82,82	1.32	9 (15%)
3	HEC	B	603	1	46,50,50	2.90	16 (34%)	58,82,82	3.21	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	O	611	-	4,4,4	0.42	0	6,6,6	0.08	0
3	HEC	D	607	1	46,50,50	1.75	10 (21%)	58,82,82	1.41	11 (18%)
3	HEC	C	605	1	46,50,50	1.71	9 (19%)	58,82,82	1.51	14 (24%)
4	SO4	O	609	-	4,4,4	0.45	0	6,6,6	0.09	0
3	HEC	J	602	1	46,50,50	1.77	10 (21%)	58,82,82	1.38	7 (12%)
3	HEC	S	605	1	46,50,50	1.73	9 (19%)	58,82,82	1.46	9 (15%)
3	HEC	V	602	1	46,50,50	1.75	11 (23%)	58,82,82	1.41	9 (15%)
3	HEC	E	606	1	46,50,50	1.71	11 (23%)	58,82,82	1.44	8 (13%)
3	HEC	B	601	1	46,50,50	1.76	10 (21%)	58,82,82	1.50	11 (18%)
3	HEC	F	601	1	46,50,50	1.74	10 (21%)	58,82,82	1.52	11 (18%)
4	SO4	M	610	-	4,4,4	0.42	0	6,6,6	0.11	0
3	HEC	Q	605	1	46,50,50	1.75	10 (21%)	58,82,82	1.45	10 (17%)
3	HEC	L	602	1	46,50,50	1.75	11 (23%)	58,82,82	1.37	8 (13%)
3	HEC	U	607	1	46,50,50	1.73	9 (19%)	58,82,82	1.33	7 (12%)
4	SO4	c	201	-	4,4,4	0.45	0	6,6,6	0.10	0
4	SO4	J	610	-	4,4,4	0.42	0	6,6,6	0.14	0
3	HEC	V	601	1	46,50,50	1.71	9 (19%)	58,82,82	1.53	12 (20%)
3	HEC	B	604	1	46,50,50	1.73	10 (21%)	58,82,82	1.55	14 (24%)
3	HEC	I	602	1	46,50,50	1.73	8 (17%)	58,82,82	1.45	11 (18%)
3	HEC	S	606	1	46,50,50	1.72	8 (17%)	58,82,82	1.45	8 (13%)
3	HEC	I	600	1	46,50,50	1.66	9 (19%)	58,82,82	1.47	11 (18%)
4	SO4	M	612	-	4,4,4	0.44	0	6,6,6	0.17	0
3	HEC	F	600	1	46,50,50	1.73	10 (21%)	58,82,82	1.46	9 (15%)
4	SO4	L	611	-	4,4,4	0.43	0	6,6,6	0.13	0
4	SO4	U	611	-	4,4,4	0.42	0	6,6,6	0.11	0
3	HEC	N	600	1	46,50,50	1.71	8 (17%)	58,82,82	1.45	9 (15%)
4	SO4	R	611	-	4,4,4	0.41	0	6,6,6	0.10	0
5	GOL	A	612	-	5,5,5	0.28	0	5,5,5	0.32	0
3	HEC	D	602	1	46,50,50	1.75	10 (21%)	58,82,82	1.38	9 (15%)
3	HEC	V	607	1	46,50,50	1.76	10 (21%)	58,82,82	1.32	10 (17%)
3	HEC	W	606	1	46,50,50	1.75	10 (21%)	58,82,82	1.44	8 (13%)
5	GOL	K	615	-	5,5,5	0.33	0	5,5,5	0.22	0
3	HEC	A	606	1	46,50,50	1.72	9 (19%)	58,82,82	1.43	9 (15%)
3	HEC	D	600	1	46,50,50	1.73	10 (21%)	58,82,82	1.43	10 (17%)
3	HEC	I	604	1	46,50,50	1.75	9 (19%)	58,82,82	1.58	10 (17%)
3	HEC	I	606	1	46,50,50	1.75	11 (23%)	58,82,82	1.46	8 (13%)
4	SO4	B	610	-	4,4,4	0.47	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	R	610	-	4,4,4	0.45	0	6,6,6	0.10	0
4	SO4	K	611	-	4,4,4	0.46	0	6,6,6	0.08	0
3	HEC	T	603	1	46,50,50	3.00	16 (34%)	58,82,82	3.19	13 (22%)
3	HEC	W	601	1	46,50,50	1.73	9 (19%)	58,82,82	1.47	10 (17%)
3	HEC	X	600	1	46,50,50	1.71	9 (19%)	58,82,82	1.48	9 (15%)
3	HEC	R	601	1	46,50,50	1.69	9 (19%)	58,82,82	1.48	11 (18%)
3	HEC	W	602	1	46,50,50	1.74	9 (19%)	58,82,82	1.43	9 (15%)
3	HEC	C	603	1	46,50,50	2.85	17 (36%)	58,82,82	3.26	13 (22%)
4	SO4	C	610	-	4,4,4	0.44	0	6,6,6	0.14	0
4	SO4	Q	610	-	4,4,4	0.43	0	6,6,6	0.08	0
3	HEC	A	602	1	46,50,50	1.77	9 (19%)	58,82,82	1.43	9 (15%)
4	SO4	I	610	-	4,4,4	0.45	0	6,6,6	0.06	0
4	SO4	V	610	-	4,4,4	0.45	0	6,6,6	0.15	0
3	HEC	F	602	1	46,50,50	1.74	9 (19%)	58,82,82	1.42	9 (15%)
4	SO4	N	609	-	4,4,4	0.46	0	6,6,6	0.14	0
3	HEC	M	600	1	46,50,50	1.71	8 (17%)	58,82,82	1.45	9 (15%)
3	HEC	A	604	1	46,50,50	1.74	11 (23%)	58,82,82	1.54	12 (20%)
4	SO4	Y	201	-	4,4,4	0.42	0	6,6,6	0.14	0
3	HEC	B	607	1	46,50,50	1.75	9 (19%)	58,82,82	1.38	10 (17%)
3	HEC	J	601	1	46,50,50	1.71	9 (19%)	58,82,82	1.51	11 (18%)
3	HEC	O	603	7,1	46,50,50	2.91	17 (36%)	58,82,82	3.24	15 (25%)
3	HEC	U	605	1	46,50,50	1.74	9 (19%)	58,82,82	1.47	11 (18%)
4	SO4	O	610	-	4,4,4	0.45	0	6,6,6	0.09	0
3	HEC	S	603	7,1	46,50,50	2.95	16 (34%)	58,82,82	3.21	16 (27%)
4	SO4	W	609	-	4,4,4	0.45	0	6,6,6	0.09	0
3	HEC	D	605	1	46,50,50	1.75	9 (19%)	58,82,82	1.50	13 (22%)
3	HEC	I	601	1	46,50,50	1.75	11 (23%)	58,82,82	1.59	12 (20%)
3	HEC	M	604	1	46,50,50	1.76	11 (23%)	58,82,82	1.56	12 (20%)
5	GOL	K	612	-	5,5,5	0.40	0	5,5,5	0.34	0
4	SO4	X	610	-	4,4,4	0.43	0	6,6,6	0.07	0
3	HEC	P	600	1	46,50,50	1.72	9 (19%)	58,82,82	1.46	10 (17%)
3	HEC	J	604	1	46,50,50	1.72	10 (21%)	58,82,82	1.59	13 (22%)
3	HEC	Q	602	1	46,50,50	1.74	9 (19%)	58,82,82	1.43	9 (15%)
3	HEC	A	603	7,1	46,50,50	2.92	16 (34%)	58,82,82	3.26	14 (24%)
4	SO4	H	613	-	4,4,4	0.43	0	6,6,6	0.22	0
3	HEC	V	605	1	46,50,50	1.75	10 (21%)	58,82,82	1.48	13 (22%)
3	HEC	H	601	1	46,50,50	1.71	10 (21%)	58,82,82	1.56	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	S	609	-	4,4,4	0.44	0	6,6,6	0.06	0
3	HEC	H	600	1	46,50,50	1.70	9 (19%)	58,82,82	1.49	10 (17%)
3	HEC	F	605	1	46,50,50	1.75	10 (21%)	58,82,82	1.46	12 (20%)
4	SO4	X	611	-	4,4,4	0.44	0	6,6,6	0.10	0
5	GOL	G	615	-	5,5,5	0.46	0	5,5,5	0.35	0
3	HEC	H	603	7,1	46,50,50	2.86	16 (34%)	58,82,82	3.20	14 (24%)
3	HEC	S	607	1	46,50,50	1.76	10 (21%)	58,82,82	1.36	9 (15%)
4	SO4	A	611	-	4,4,4	0.43	0	6,6,6	0.11	0
3	HEC	G	605	1	46,50,50	1.73	9 (19%)	58,82,82	1.49	14 (24%)
3	HEC	C	601	1	46,50,50	1.72	9 (19%)	58,82,82	1.49	11 (18%)
3	HEC	L	603	7,1	46,50,50	2.81	16 (34%)	58,82,82	3.26	12 (20%)
3	HEC	G	603	7,1	46,50,50	2.90	17 (36%)	58,82,82	3.22	13 (22%)
4	SO4	L	610	-	4,4,4	0.40	0	6,6,6	0.15	0
3	HEC	C	600	1	46,50,50	1.70	8 (17%)	58,82,82	1.46	8 (13%)
3	HEC	R	603	1	46,50,50	2.90	17 (36%)	58,82,82	3.19	13 (22%)
4	SO4	U	610	-	4,4,4	0.43	0	6,6,6	0.11	0
3	HEC	W	607	1	46,50,50	1.75	10 (21%)	58,82,82	1.35	8 (13%)
3	HEC	B	600	1	46,50,50	1.71	9 (19%)	58,82,82	1.42	9 (15%)
4	SO4	U	609	-	4,4,4	0.42	0	6,6,6	0.25	0
4	SO4	H	609	-	4,4,4	0.46	0	6,6,6	0.12	0
4	SO4	J	609	-	4,4,4	0.46	0	6,6,6	0.12	0
3	HEC	C	604	1	46,50,50	1.73	10 (21%)	58,82,82	1.58	12 (20%)
3	HEC	C	606	1	46,50,50	1.74	9 (19%)	58,82,82	1.46	8 (13%)
3	HEC	F	606	1	46,50,50	1.72	8 (17%)	58,82,82	1.50	8 (13%)
3	HEC	O	601	1	46,50,50	1.73	9 (19%)	58,82,82	1.51	11 (18%)
3	HEC	O	600	1	46,50,50	1.71	8 (17%)	58,82,82	1.47	10 (17%)
3	HEC	O	602	1	46,50,50	1.72	9 (19%)	58,82,82	1.42	9 (15%)
4	SO4	M	611	-	4,4,4	0.45	0	6,6,6	0.10	0
3	HEC	H	605	1	46,50,50	1.74	8 (17%)	58,82,82	1.47	13 (22%)
3	HEC	D	606	1	46,50,50	1.74	10 (21%)	58,82,82	1.45	8 (13%)
3	HEC	I	603	7,1	46,50,50	2.87	16 (34%)	58,82,82	3.68	22 (37%)
4	SO4	G	613	-	4,4,4	0.40	0	6,6,6	0.38	0
3	HEC	J	607	1	46,50,50	1.79	10 (21%)	58,82,82	1.34	9 (15%)
3	HEC	O	604	1	46,50,50	1.74	9 (19%)	58,82,82	1.55	12 (20%)
3	HEC	N	602	1	46,50,50	1.74	9 (19%)	58,82,82	1.42	8 (13%)
3	HEC	T	601	1	46,50,50	1.72	10 (21%)	58,82,82	1.48	10 (17%)
3	HEC	B	605	1	46,50,50	1.74	9 (19%)	58,82,82	1.47	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	T	600	1	46,50,50	1.70	8 (17%)	58,82,82	1.46	10 (17%)
3	HEC	H	607	1	46,50,50	1.71	9 (19%)	58,82,82	1.39	9 (15%)
4	SO4	Q	609	-	4,4,4	0.44	0	6,6,6	0.16	0
4	SO4	T	609	-	4,4,4	0.45	0	6,6,6	0.10	0
3	HEC	N	604	1	46,50,50	1.70	10 (21%)	58,82,82	1.55	13 (22%)
3	HEC	Q	603	7,1	46,50,50	2.94	16 (34%)	58,82,82	3.27	13 (22%)
3	HEC	R	602	1	46,50,50	1.73	9 (19%)	58,82,82	1.43	8 (13%)
3	HEC	D	604	1	46,50,50	1.75	9 (19%)	58,82,82	1.56	12 (20%)
3	HEC	I	605	1	46,50,50	1.74	9 (19%)	58,82,82	1.54	14 (24%)
3	HEC	J	606	1	46,50,50	1.74	10 (21%)	58,82,82	1.45	8 (13%)
3	HEC	W	604	1	46,50,50	1.73	11 (23%)	58,82,82	1.60	13 (22%)
4	SO4	G	611	-	4,4,4	0.44	0	6,6,6	0.10	0
4	SO4	V	611	-	4,4,4	0.44	0	6,6,6	0.08	0
3	HEC	C	607	1	46,50,50	1.71	8 (17%)	58,82,82	1.33	7 (12%)
3	HEC	F	603	7,1	46,50,50	2.90	16 (34%)	58,82,82	3.28	14 (24%)
4	SO4	E	610	-	4,4,4	0.45	0	6,6,6	0.10	0
3	HEC	K	603	7,1	46,50,50	2.87	16 (34%)	58,82,82	3.18	13 (22%)
3	HEC	K	602	1	46,50,50	1.73	9 (19%)	58,82,82	1.41	8 (13%)
3	HEC	L	606	1	46,50,50	1.71	9 (19%)	58,82,82	1.51	9 (15%)
3	HEC	E	603	7,1	46,50,50	2.91	16 (34%)	58,82,82	3.23	15 (25%)
3	HEC	K	600	1	46,50,50	1.68	8 (17%)	58,82,82	1.49	10 (17%)
3	HEC	N	605	1	46,50,50	1.75	9 (19%)	58,82,82	1.48	12 (20%)
3	HEC	Q	606	1	46,50,50	1.72	10 (21%)	58,82,82	1.45	8 (13%)
3	HEC	F	607	1	46,50,50	1.75	10 (21%)	58,82,82	1.33	8 (13%)
3	HEC	R	604	1	46,50,50	1.74	9 (19%)	58,82,82	1.55	13 (22%)
3	HEC	R	606	1	46,50,50	1.73	11 (23%)	58,82,82	1.50	10 (17%)
4	SO4	A	610	-	4,4,4	0.42	0	6,6,6	0.15	0
3	HEC	O	607	1	46,50,50	1.74	9 (19%)	58,82,82	1.37	8 (13%)
4	SO4	X	609	-	4,4,4	0.43	0	6,6,6	0.16	0
3	HEC	J	605	1	46,50,50	1.76	8 (17%)	58,82,82	1.40	11 (18%)
5	GOL	D	610	-	5,5,5	0.30	0	5,5,5	0.26	0
3	HEC	P	603	7,1	46,50,50	2.86	16 (34%)	58,82,82	3.27	15 (25%)
3	HEC	P	602	1	46,50,50	1.72	8 (17%)	58,82,82	1.40	8 (13%)
3	HEC	K	606	1	46,50,50	1.74	9 (19%)	58,82,82	1.45	10 (17%)
3	HEC	U	602	1	46,50,50	1.75	9 (19%)	58,82,82	1.46	8 (13%)
3	HEC	L	601	1	46,50,50	1.69	9 (19%)	58,82,82	1.52	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	B	602	1	46,50,50	1.71	9 (19%)	58,82,82	1.44	9 (15%)
4	SO4	a	201	-	4,4,4	0.44	0	6,6,6	0.12	0
4	SO4	D	609	-	4,4,4	0.45	0	6,6,6	0.10	0
3	HEC	M	603	7,1	46,50,50	2.92	17 (36%)	58,82,82	3.22	14 (24%)
3	HEC	A	601	1	46,50,50	1.68	9 (19%)	58,82,82	1.52	10 (17%)
3	HEC	U	604	1	46,50,50	1.73	8 (17%)	58,82,82	1.57	12 (20%)
3	HEC	K	607	1	46,50,50	1.77	9 (19%)	58,82,82	1.36	8 (13%)
3	HEC	A	600	1	46,50,50	1.70	8 (17%)	58,82,82	1.45	11 (18%)
3	HEC	S	600	1	46,50,50	1.73	8 (17%)	58,82,82	1.44	8 (13%)
3	HEC	G	601	1	46,50,50	1.68	9 (19%)	58,82,82	1.54	12 (20%)
3	HEC	M	605	1	46,50,50	1.77	9 (19%)	58,82,82	1.50	12 (20%)
3	HEC	T	607	1	46,50,50	1.73	9 (19%)	58,82,82	1.35	8 (13%)
4	SO4	R	609	-	4,4,4	0.42	0	6,6,6	0.23	0
3	HEC	H	604	1	46,50,50	1.72	10 (21%)	58,82,82	1.56	12 (20%)
3	HEC	T	605	1	46,50,50	1.73	9 (19%)	58,82,82	1.49	12 (20%)
3	HEC	M	601	1	46,50,50	1.70	8 (17%)	58,82,82	1.52	10 (17%)
5	GOL	I	613	-	5,5,5	0.26	0	5,5,5	0.27	0
3	HEC	G	604	1	46,50,50	1.71	8 (17%)	58,82,82	1.56	12 (20%)
3	HEC	R	607	1	46,50,50	1.77	9 (19%)	58,82,82	1.34	10 (17%)
3	HEC	X	602	1	46,50,50	1.72	9 (19%)	58,82,82	1.44	9 (15%)
3	HEC	P	605	1	46,50,50	1.75	10 (21%)	58,82,82	1.50	12 (20%)
3	HEC	E	601	1	46,50,50	1.73	10 (21%)	58,82,82	1.51	10 (17%)
3	HEC	M	607	1	46,50,50	1.75	9 (19%)	58,82,82	1.36	10 (17%)
3	HEC	N	607	1	46,50,50	1.74	9 (19%)	58,82,82	1.36	8 (13%)
3	HEC	W	603	7,1	46,50,50	2.89	16 (34%)	58,82,82	3.25	14 (24%)
3	HEC	T	602	1	46,50,50	1.75	10 (21%)	58,82,82	1.40	8 (13%)
4	SO4	G	609	-	4,4,4	0.45	0	6,6,6	0.10	0
4	SO4	Q	611	-	4,4,4	0.45	0	6,6,6	0.17	0
4	SO4	G	610	-	4,4,4	0.40	0	6,6,6	0.09	0
3	HEC	T	604	1	46,50,50	1.72	10 (21%)	58,82,82	1.56	13 (22%)
3	HEC	T	606	1	46,50,50	1.73	9 (19%)	58,82,82	1.45	8 (13%)
3	HEC	P	601	1	46,50,50	1.71	9 (19%)	58,82,82	1.46	9 (15%)
3	HEC	X	606	1	46,50,50	1.73	9 (19%)	58,82,82	1.46	9 (15%)
3	HEC	R	605	1	46,50,50	1.72	9 (19%)	58,82,82	1.51	12 (20%)
3	HEC	I	607	1	46,50,50	1.76	10 (21%)	58,82,82	1.47	10 (17%)
3	HEC	S	601	1	46,50,50	1.71	9 (19%)	58,82,82	1.50	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	Y	202	-	4,4,4	0.43	0	6,6,6	0.14	0
3	HEC	J	603	7,1	46,50,50	2.87	16 (34%)	58,82,82	3.26	14 (24%)
3	HEC	B	606	1	46,50,50	1.73	11 (23%)	58,82,82	1.50	10 (17%)
3	HEC	M	602	1	46,50,50	1.77	10 (21%)	58,82,82	1.43	9 (15%)
3	HEC	O	605	1	46,50,50	1.75	8 (17%)	58,82,82	1.46	13 (22%)
3	HEC	A	607	1	46,50,50	1.77	9 (19%)	58,82,82	1.31	8 (13%)
3	HEC	E	604	1	46,50,50	1.72	11 (23%)	58,82,82	1.58	12 (20%)
3	HEC	X	605	1	46,50,50	1.74	9 (19%)	58,82,82	1.46	11 (18%)
5	GOL	G	616	-	5,5,5	0.19	0	5,5,5	0.47	0
3	HEC	G	607	1	46,50,50	1.76	8 (17%)	58,82,82	1.35	9 (15%)
3	HEC	D	603	7,1	46,50,50	2.92	16 (34%)	58,82,82	3.34	18 (31%)
3	HEC	G	602	1	46,50,50	1.75	9 (19%)	58,82,82	1.41	9 (15%)
3	HEC	U	603	7,1	46,50,50	2.89	16 (34%)	58,82,82	3.21	12 (20%)
3	HEC	X	604	1	46,50,50	1.72	10 (21%)	58,82,82	1.54	12 (20%)
4	SO4	B	609	-	4,4,4	0.41	0	6,6,6	0.11	0
4	SO4	F	609	-	4,4,4	0.44	0	6,6,6	0.10	0
3	HEC	K	601	1	46,50,50	1.73	9 (19%)	58,82,82	1.48	11 (18%)
4	SO4	H	610	-	4,4,4	0.46	0	6,6,6	0.07	0
4	SO4	N	611	-	4,4,4	0.44	0	6,6,6	0.10	0
5	GOL	H	615	-	5,5,5	0.48	0	5,5,5	0.58	0
3	HEC	Q	600	1	46,50,50	1.71	9 (19%)	58,82,82	1.44	7 (12%)
4	SO4	V	609	-	4,4,4	0.50	0	6,6,6	0.19	0
3	HEC	S	604	1	46,50,50	1.75	10 (21%)	58,82,82	1.55	13 (22%)
4	SO4	I	611	-	4,4,4	0.44	0	6,6,6	0.06	0
3	HEC	L	604	1	46,50,50	1.73	10 (21%)	58,82,82	1.58	14 (24%)
3	HEC	O	606	1	46,50,50	1.70	9 (19%)	58,82,82	1.49	10 (17%)
3	HEC	U	606	1	46,50,50	1.73	8 (17%)	58,82,82	1.46	8 (13%)
5	GOL	H	614	-	5,5,5	0.43	0	5,5,5	0.79	0
3	HEC	E	607	1	46,50,50	1.75	10 (21%)	58,82,82	1.38	11 (18%)
3	HEC	Q	604	1	46,50,50	1.75	10 (21%)	58,82,82	1.56	12 (20%)
4	SO4	K	609	-	4,4,4	0.32	0	6,6,6	0.33	0
4	SO4	E	609	-	4,4,4	0.48	0	6,6,6	0.38	0
4	SO4	S	610	-	4,4,4	0.45	0	6,6,6	0.12	0
3	HEC	H	602	1	46,50,50	1.73	9 (19%)	58,82,82	1.39	9 (15%)
4	SO4	I	612	-	4,4,4	0.46	0	6,6,6	0.06	0
5	GOL	A	613	-	5,5,5	0.42	0	5,5,5	0.37	0
5	GOL	J	612	-	5,5,5	0.52	0	5,5,5	0.60	0
3	HEC	P	604	1	46,50,50	1.72	9 (19%)	58,82,82	1.56	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	P	607	1	46,50,50	1.73	8 (17%)	58,82,82	1.36	8 (13%)
3	HEC	X	601	1	46,50,50	1.70	9 (19%)	58,82,82	1.53	10 (17%)
3	HEC	G	606	1	46,50,50	1.76	10 (21%)	58,82,82	1.48	10 (17%)
3	HEC	K	604	1	46,50,50	1.73	10 (21%)	58,82,82	1.59	13 (22%)
3	HEC	V	606	1	46,50,50	1.74	9 (19%)	58,82,82	1.51	9 (15%)
3	HEC	V	603	7,1	46,50,50	2.88	16 (34%)	58,82,82	3.18	12 (20%)
4	SO4	P	609	-	4,4,4	0.43	0	6,6,6	0.15	0
5	GOL	K	614	-	5,5,5	0.18	0	5,5,5	0.40	0
4	SO4	G	614	-	4,4,4	0.46	0	6,6,6	0.17	0
3	HEC	K	605	1	46,50,50	1.74	9 (19%)	58,82,82	1.49	12 (20%)
3	HEC	M	606	1	46,50,50	1.74	11 (23%)	58,82,82	1.47	8 (13%)
3	HEC	W	605	1	46,50,50	1.76	11 (23%)	58,82,82	1.45	10 (17%)
3	HEC	N	601	1	46,50,50	1.74	9 (19%)	58,82,82	1.47	9 (15%)
3	HEC	L	600	1	46,50,50	1.68	8 (17%)	58,82,82	1.46	9 (15%)
3	HEC	A	605	1	46,50,50	1.73	8 (17%)	58,82,82	1.46	11 (18%)
4	SO4	L	609	-	4,4,4	0.44	0	6,6,6	0.08	0
3	HEC	D	601	1	46,50,50	1.71	10 (21%)	58,82,82	1.53	8 (13%)

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	N	603	7,1	-	6/14/54/54	-
3	HEC	W	600	1	-	8/14/54/54	-
3	HEC	E	602	1	-	8/14/54/54	-
3	HEC	N	606	1	-	7/14/54/54	-
3	HEC	E	600	1	-	8/14/54/54	-
3	HEC	X	603	7,1	-	6/14/54/54	-
3	HEC	P	606	1	-	6/14/54/54	-
3	HEC	Q	607	1	-	7/14/54/54	-
3	HEC	U	601	1	-	8/14/54/54	-
5	GOL	J	613	-	-	2/4/4/4	-
3	HEC	U	600	1	-	8/14/54/54	-
3	HEC	C	602	1	-	8/14/54/54	-
5	GOL	A	614	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	614	-	-	2/4/4/4	-
3	HEC	S	602	1	-	8/14/54/54	-
3	HEC	L	605	1	-	8/14/54/54	-
3	HEC	G	600	1	-	8/14/54/54	-
3	HEC	J	600	1	-	8/14/54/54	-
5	GOL	L	613	-	-	2/4/4/4	-
3	HEC	R	600	1	-	8/14/54/54	-
5	GOL	I	615	-	-	2/4/4/4	-
3	HEC	F	604	1	-	8/14/54/54	-
3	HEC	Q	601	1	-	8/14/54/54	-
3	HEC	V	600	1	-	8/14/54/54	-
3	HEC	H	606	1	-	6/14/54/54	-
3	HEC	X	607	1	-	7/14/54/54	-
3	HEC	E	605	1	-	8/14/54/54	-
3	HEC	V	604	1	-	8/14/54/54	-
5	GOL	K	613	-	-	2/4/4/4	-
3	HEC	L	607	1	-	7/14/54/54	-
3	HEC	B	603	1	-	4/14/54/54	-
3	HEC	D	607	1	-	9/14/54/54	-
3	HEC	C	605	1	-	8/14/54/54	-
3	HEC	J	602	1	-	8/14/54/54	-
3	HEC	S	605	1	-	8/14/54/54	-
3	HEC	V	602	1	-	8/14/54/54	-
3	HEC	E	606	1	-	6/14/54/54	-
3	HEC	B	601	1	-	8/14/54/54	-
3	HEC	F	601	1	-	8/14/54/54	-
3	HEC	Q	605	1	-	8/14/54/54	-
3	HEC	L	602	1	-	8/14/54/54	-
3	HEC	U	607	1	-	7/14/54/54	-
3	HEC	V	601	1	-	8/14/54/54	-
3	HEC	B	604	1	-	8/14/54/54	-
3	HEC	I	602	1	-	9/14/54/54	-
3	HEC	S	606	1	-	6/14/54/54	-
3	HEC	I	600	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	F	600	1	-	8/14/54/54	-
3	HEC	N	600	1	-	8/14/54/54	-
5	GOL	A	612	-	-	0/4/4/4	-
3	HEC	D	602	1	-	6/14/54/54	-
3	HEC	V	607	1	-	7/14/54/54	-
3	HEC	W	606	1	-	6/14/54/54	-
5	GOL	K	615	-	-	4/4/4/4	-
3	HEC	A	606	1	-	6/14/54/54	-
3	HEC	D	600	1	-	6/14/54/54	-
3	HEC	I	604	1	-	9/14/54/54	-
3	HEC	I	606	1	-	6/14/54/54	-
3	HEC	T	603	1	-	4/14/54/54	-
3	HEC	W	601	1	-	8/14/54/54	-
3	HEC	X	600	1	-	8/14/54/54	-
3	HEC	R	601	1	-	8/14/54/54	-
3	HEC	W	602	1	-	8/14/54/54	-
3	HEC	C	603	1	-	4/14/54/54	-
3	HEC	A	602	1	-	8/14/54/54	-
3	HEC	F	602	1	-	8/14/54/54	-
3	HEC	M	600	1	-	8/14/54/54	-
3	HEC	A	604	1	-	8/14/54/54	-
3	HEC	B	607	1	-	7/14/54/54	-
3	HEC	J	601	1	-	9/14/54/54	-
3	HEC	O	603	7,1	-	5/14/54/54	-
3	HEC	U	605	1	-	8/14/54/54	-
3	HEC	S	603	7,1	-	6/14/54/54	-
3	HEC	D	605	1	-	8/14/54/54	-
3	HEC	I	601	1	-	10/14/54/54	-
3	HEC	M	604	1	-	8/14/54/54	-
5	GOL	K	612	-	-	2/4/4/4	-
3	HEC	P	600	1	-	8/14/54/54	-
3	HEC	J	604	1	-	8/14/54/54	-
3	HEC	Q	602	1	-	8/14/54/54	-
3	HEC	A	603	7,1	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	V	605	1	-	8/14/54/54	-
3	HEC	H	601	1	-	10/14/54/54	-
3	HEC	H	600	1	-	8/14/54/54	-
3	HEC	F	605	1	-	8/14/54/54	-
5	GOL	G	615	-	-	2/4/4/4	-
3	HEC	H	603	7,1	-	6/14/54/54	-
3	HEC	S	607	1	-	7/14/54/54	-
3	HEC	G	605	1	-	8/14/54/54	-
3	HEC	C	601	1	-	8/14/54/54	-
3	HEC	L	603	7,1	-	4/14/54/54	-
3	HEC	G	603	7,1	-	6/14/54/54	-
3	HEC	C	600	1	-	8/14/54/54	-
3	HEC	R	603	1	-	4/14/54/54	-
3	HEC	W	607	1	-	7/14/54/54	-
3	HEC	B	600	1	-	8/14/54/54	-
3	HEC	C	604	1	-	8/14/54/54	-
3	HEC	C	606	1	-	6/14/54/54	-
3	HEC	F	606	1	-	6/14/54/54	-
3	HEC	O	601	1	-	8/14/54/54	-
3	HEC	O	600	1	-	8/14/54/54	-
3	HEC	O	602	1	-	8/14/54/54	-
3	HEC	H	605	1	-	8/14/54/54	-
3	HEC	D	606	1	-	6/14/54/54	-
3	HEC	I	603	7,1	-	6/14/54/54	-
3	HEC	J	607	1	-	7/14/54/54	-
3	HEC	O	604	1	-	8/14/54/54	-
3	HEC	N	602	1	-	8/14/54/54	-
3	HEC	T	601	1	-	8/14/54/54	-
3	HEC	B	605	1	-	8/14/54/54	-
3	HEC	T	600	1	-	8/14/54/54	-
3	HEC	H	607	1	-	7/14/54/54	-
3	HEC	N	604	1	-	8/14/54/54	-
3	HEC	Q	603	7,1	-	5/14/54/54	-
3	HEC	R	602	1	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	D	604	1	-	6/14/54/54	-
3	HEC	I	605	1	-	9/14/54/54	-
3	HEC	J	606	1	-	6/14/54/54	-
3	HEC	W	604	1	-	8/14/54/54	-
3	HEC	C	607	1	-	7/14/54/54	-
3	HEC	F	603	7,1	-	4/14/54/54	-
3	HEC	K	603	7,1	-	5/14/54/54	-
3	HEC	K	602	1	-	8/14/54/54	-
3	HEC	L	606	1	-	6/14/54/54	-
3	HEC	E	603	7,1	-	6/14/54/54	-
3	HEC	K	600	1	-	8/14/54/54	-
3	HEC	N	605	1	-	8/14/54/54	-
3	HEC	Q	606	1	-	6/14/54/54	-
3	HEC	F	607	1	-	7/14/54/54	-
3	HEC	R	604	1	-	8/14/54/54	-
3	HEC	R	606	1	-	6/14/54/54	-
3	HEC	O	607	1	-	7/14/54/54	-
3	HEC	J	605	1	-	8/14/54/54	-
5	GOL	D	610	-	-	2/4/4/4	-
3	HEC	P	603	7,1	-	4/14/54/54	-
3	HEC	P	602	1	-	8/14/54/54	-
3	HEC	K	606	1	-	7/14/54/54	-
3	HEC	U	602	1	-	8/14/54/54	-
3	HEC	L	601	1	-	8/14/54/54	-
3	HEC	B	602	1	-	8/14/54/54	-
3	HEC	M	603	7,1	-	6/14/54/54	-
3	HEC	A	601	1	-	8/14/54/54	-
3	HEC	U	604	1	-	8/14/54/54	-
3	HEC	K	607	1	-	7/14/54/54	-
3	HEC	A	600	1	-	8/14/54/54	-
3	HEC	S	600	1	-	8/14/54/54	-
3	HEC	G	601	1	-	8/14/54/54	-
3	HEC	M	605	1	-	8/14/54/54	-
3	HEC	T	607	1	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	H	604	1	-	8/14/54/54	-
3	HEC	T	605	1	-	8/14/54/54	-
3	HEC	M	601	1	-	8/14/54/54	-
5	GOL	I	613	-	-	4/4/4/4	-
3	HEC	G	604	1	-	8/14/54/54	-
3	HEC	R	607	1	-	7/14/54/54	-
3	HEC	X	602	1	-	8/14/54/54	-
3	HEC	P	605	1	-	8/14/54/54	-
3	HEC	E	601	1	-	8/14/54/54	-
3	HEC	M	607	1	-	7/14/54/54	-
3	HEC	N	607	1	-	7/14/54/54	-
3	HEC	W	603	7,1	-	6/14/54/54	-
3	HEC	T	602	1	-	8/14/54/54	-
3	HEC	T	604	1	-	8/14/54/54	-
3	HEC	T	606	1	-	6/14/54/54	-
3	HEC	P	601	1	-	9/14/54/54	-
3	HEC	X	606	1	-	6/14/54/54	-
3	HEC	R	605	1	-	8/14/54/54	-
3	HEC	I	607	1	-	8/14/54/54	-
3	HEC	S	601	1	-	8/14/54/54	-
3	HEC	J	603	7,1	-	5/14/54/54	-
3	HEC	B	606	1	-	7/14/54/54	-
3	HEC	M	602	1	-	8/14/54/54	-
3	HEC	O	605	1	-	8/14/54/54	-
3	HEC	A	607	1	-	7/14/54/54	-
3	HEC	E	604	1	-	8/14/54/54	-
3	HEC	X	605	1	-	8/14/54/54	-
5	GOL	G	616	-	-	2/4/4/4	-
3	HEC	G	607	1	-	7/14/54/54	-
3	HEC	D	603	7,1	-	6/14/54/54	-
3	HEC	G	602	1	-	8/14/54/54	-
3	HEC	U	603	7,1	-	4/14/54/54	-
3	HEC	X	604	1	-	8/14/54/54	-
5	GOL	H	615	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	K	601	1	-	8/14/54/54	-
3	HEC	Q	600	1	-	8/14/54/54	-
3	HEC	S	604	1	-	8/14/54/54	-
3	HEC	L	604	1	-	8/14/54/54	-
3	HEC	O	606	1	-	6/14/54/54	-
3	HEC	U	606	1	-	6/14/54/54	-
5	GOL	H	614	-	-	4/4/4/4	-
3	HEC	E	607	1	-	7/14/54/54	-
3	HEC	Q	604	1	-	8/14/54/54	-
3	HEC	H	602	1	-	8/14/54/54	-
5	GOL	A	613	-	-	2/4/4/4	-
5	GOL	J	612	-	-	4/4/4/4	-
3	HEC	P	604	1	-	8/14/54/54	-
3	HEC	P	607	1	-	7/14/54/54	-
3	HEC	X	601	1	-	8/14/54/54	-
3	HEC	G	606	1	-	6/14/54/54	-
3	HEC	K	604	1	-	8/14/54/54	-
3	HEC	V	606	1	-	6/14/54/54	-
3	HEC	V	603	7,1	-	4/14/54/54	-
5	GOL	K	614	-	-	3/4/4/4	-
3	HEC	K	605	1	-	8/14/54/54	-
3	HEC	M	606	1	-	6/14/54/54	-
3	HEC	W	605	1	-	8/14/54/54	-
3	HEC	N	601	1	-	8/14/54/54	-
3	HEC	L	600	1	-	8/14/54/54	-
3	HEC	A	605	1	-	8/14/54/54	-
3	HEC	D	601	1	-	8/14/54/54	-

All (1941) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	603	HEC	CHC-C4B	9.46	1.57	1.38
3	S	603	HEC	CHC-C4B	9.16	1.56	1.38
3	Q	603	HEC	CHC-C4B	9.13	1.56	1.38
3	O	603	HEC	CHC-C4B	9.10	1.56	1.38
3	M	603	HEC	CHC-C4B	9.08	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	603	HEC	CHC-C4B	9.08	1.56	1.38
3	N	603	HEC	CHC-C4B	9.08	1.56	1.38
3	B	603	HEC	CHC-C4B	9.04	1.56	1.38
3	E	603	HEC	CHC-C4B	9.03	1.56	1.38
3	F	603	HEC	CHC-C4B	9.02	1.56	1.38
3	G	603	HEC	CHC-C4B	8.98	1.56	1.38
3	R	603	HEC	CHC-C4B	8.98	1.56	1.38
3	W	603	HEC	CHC-C4B	8.95	1.56	1.38
3	A	603	HEC	CHC-C4B	8.95	1.55	1.38
3	D	603	HEC	CHC-C4B	8.94	1.55	1.38
3	J	603	HEC	CHC-C4B	8.83	1.55	1.38
3	V	603	HEC	CHC-C4B	8.80	1.55	1.38
3	P	603	HEC	CHC-C4B	8.76	1.55	1.38
3	K	603	HEC	CHC-C4B	8.66	1.55	1.38
3	U	603	HEC	CHC-C4B	8.66	1.55	1.38
3	C	603	HEC	CHC-C4B	8.64	1.55	1.38
3	L	603	HEC	CHC-C4B	8.60	1.55	1.38
3	H	603	HEC	CHC-C4B	8.55	1.55	1.38
3	I	603	HEC	CHC-C4B	8.33	1.54	1.38
3	A	603	HEC	C4C-NC	5.61	1.50	1.39
3	V	603	HEC	C4C-NC	5.61	1.50	1.39
3	P	603	HEC	C4C-NC	5.58	1.50	1.39
3	U	603	HEC	C4C-NC	5.57	1.50	1.39
3	D	603	HEC	C1A-C2A	5.50	1.54	1.45
3	D	603	HEC	C4C-NC	5.48	1.49	1.39
3	W	603	HEC	C4C-NC	5.47	1.49	1.39
3	I	603	HEC	C1A-NA	5.46	1.49	1.39
3	F	603	HEC	C4C-NC	5.45	1.49	1.39
3	H	603	HEC	C4C-NC	5.44	1.49	1.39
3	R	603	HEC	C4C-NC	5.43	1.49	1.39
3	S	603	HEC	C4C-NC	5.42	1.49	1.39
3	Q	603	HEC	C1A-C2A	5.42	1.54	1.45
3	H	603	HEC	C1A-C2A	5.42	1.54	1.45
3	X	603	HEC	C4C-NC	5.41	1.49	1.39
3	M	603	HEC	C4C-NC	5.40	1.49	1.39
3	S	603	HEC	C1A-C2A	5.39	1.54	1.45
3	B	603	HEC	C4C-NC	5.36	1.49	1.39
3	E	603	HEC	C1A-C2A	5.35	1.54	1.45
3	T	603	HEC	C4C-NC	5.34	1.49	1.39
3	N	603	HEC	C4C-NC	5.33	1.49	1.39
3	K	603	HEC	C4C-NC	5.33	1.49	1.39
3	Q	603	HEC	C4C-NC	5.33	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	603	HEC	C1A-C2A	5.32	1.54	1.45
3	I	603	HEC	C4C-NC	5.32	1.49	1.39
3	G	603	HEC	C4C-NC	5.31	1.49	1.39
3	B	603	HEC	C1A-C2A	5.30	1.54	1.45
3	N	603	HEC	C1A-C2A	5.30	1.54	1.45
3	U	603	HEC	C1A-C2A	5.30	1.54	1.45
3	A	603	HEC	C1A-C2A	5.28	1.54	1.45
3	C	603	HEC	C4C-NC	5.27	1.49	1.39
3	F	603	HEC	C1A-C2A	5.25	1.54	1.45
3	M	603	HEC	C1A-C2A	5.25	1.54	1.45
3	E	603	HEC	C4C-NC	5.25	1.49	1.39
3	K	603	HEC	C1A-C2A	5.23	1.54	1.45
3	W	603	HEC	C1A-C2A	5.23	1.54	1.45
3	R	603	HEC	C1A-C2A	5.23	1.54	1.45
3	P	603	HEC	C1A-C2A	5.22	1.54	1.45
3	O	603	HEC	C4C-NC	5.22	1.49	1.39
3	C	603	HEC	C1A-C2A	5.21	1.54	1.45
3	L	603	HEC	C4C-NC	5.21	1.49	1.39
3	N	603	HEC	C1A-NA	5.21	1.49	1.39
3	Q	603	HEC	C1A-NA	5.21	1.49	1.39
3	J	603	HEC	C1A-NA	5.20	1.49	1.39
3	T	603	HEC	C1A-NA	5.20	1.49	1.39
3	J	603	HEC	C4C-NC	5.17	1.49	1.39
3	J	603	HEC	C1A-C2A	5.16	1.54	1.45
3	T	603	HEC	C3B-C4B	5.16	1.55	1.46
3	X	603	HEC	C1A-C2A	5.14	1.54	1.45
3	I	603	HEC	C1A-C2A	5.13	1.54	1.45
3	U	603	HEC	C1A-NA	5.12	1.49	1.39
3	V	603	HEC	C1A-C2A	5.11	1.54	1.45
3	M	603	HEC	CHA-C1A	5.09	1.48	1.38
3	O	603	HEC	C1A-C2A	5.09	1.54	1.45
3	A	603	HEC	C1A-NA	5.09	1.49	1.39
3	E	603	HEC	C1A-NA	5.06	1.49	1.39
3	S	603	HEC	C1A-NA	5.06	1.49	1.39
3	G	603	HEC	C1A-C2A	5.05	1.54	1.45
3	L	603	HEC	C1A-C2A	5.04	1.54	1.45
3	G	603	HEC	C1A-NA	5.03	1.49	1.39
3	T	603	HEC	CHA-C1A	5.03	1.48	1.38
3	C	603	HEC	C1A-NA	5.02	1.49	1.39
3	N	603	HEC	CHA-C1A	5.01	1.48	1.38
3	B	603	HEC	C1A-NA	5.01	1.49	1.39
3	V	603	HEC	C1A-NA	5.01	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	603	HEC	CHA-C1A	5.00	1.48	1.38
3	D	603	HEC	CHA-C1A	4.99	1.48	1.38
3	S	603	HEC	CHA-C1A	4.97	1.48	1.38
3	M	603	HEC	C1A-NA	4.96	1.49	1.39
3	R	603	HEC	C1A-NA	4.96	1.49	1.39
3	P	603	HEC	C1A-NA	4.95	1.48	1.39
3	B	603	HEC	CHA-C1A	4.95	1.48	1.38
3	F	603	HEC	CHA-C1A	4.95	1.48	1.38
3	O	603	HEC	C1A-NA	4.94	1.48	1.39
3	X	603	HEC	C3B-C4B	4.94	1.54	1.46
3	C	603	HEC	CHA-C1A	4.93	1.48	1.38
3	H	603	HEC	C1A-NA	4.92	1.48	1.39
3	F	603	HEC	C1A-NA	4.92	1.48	1.39
3	U	603	HEC	CHA-C1A	4.91	1.48	1.38
3	O	603	HEC	C3B-C4B	4.91	1.54	1.46
3	Q	603	HEC	CHA-C1A	4.90	1.48	1.38
3	A	603	HEC	C3B-C4B	4.89	1.54	1.46
3	E	603	HEC	CHA-C1A	4.89	1.48	1.38
3	J	603	HEC	CHA-C1A	4.89	1.48	1.38
3	W	603	HEC	C1A-NA	4.89	1.48	1.39
3	K	603	HEC	CHA-C1A	4.88	1.48	1.38
3	E	603	HEC	C3B-C4B	4.88	1.54	1.46
3	P	603	HEC	CHA-C1A	4.87	1.47	1.38
3	A	603	HEC	CHA-C1A	4.86	1.47	1.38
3	K	603	HEC	C1A-NA	4.86	1.48	1.39
3	I	603	HEC	CHA-C1A	4.86	1.47	1.38
3	D	603	HEC	C1A-NA	4.85	1.48	1.39
3	X	603	HEC	CHA-C1A	4.84	1.47	1.38
3	V	603	HEC	CHA-C1A	4.84	1.47	1.38
3	Q	603	HEC	C3B-C4B	4.83	1.54	1.46
3	N	603	HEC	C3B-C4B	4.83	1.54	1.46
3	H	603	HEC	CHA-C1A	4.82	1.47	1.38
3	S	603	HEC	C3B-C4B	4.82	1.54	1.46
3	R	603	HEC	CHA-C1A	4.80	1.47	1.38
3	G	603	HEC	C3B-C4B	4.79	1.54	1.46
3	X	603	HEC	C1A-NA	4.79	1.48	1.39
3	L	603	HEC	C1A-NA	4.78	1.48	1.39
3	W	603	HEC	CHA-C1A	4.76	1.47	1.38
3	M	603	HEC	C3B-C4B	4.75	1.54	1.46
3	G	603	HEC	CHA-C1A	4.75	1.47	1.38
3	T	603	HEC	CHC-C1C	4.71	1.50	1.39
3	C	603	HEC	C3B-C4B	4.70	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	HEC	C3B-C4B	4.69	1.54	1.46
3	F	603	HEC	C3B-C4B	4.66	1.54	1.46
3	D	603	HEC	CHD-C4C	4.66	1.47	1.38
3	L	603	HEC	CHA-C1A	4.62	1.47	1.38
3	D	603	HEC	C3B-C4B	4.62	1.54	1.46
3	R	603	HEC	C3B-C4B	4.56	1.54	1.46
3	Q	603	HEC	CHD-C4C	4.56	1.47	1.38
3	H	606	HEC	CBC-CAC	-4.56	1.32	1.49
3	T	603	HEC	CHD-C4C	4.56	1.47	1.38
3	U	603	HEC	CHD-C4C	4.55	1.47	1.38
3	W	603	HEC	CAC-C3C	4.54	1.49	1.35
3	S	603	HEC	CHD-C4C	4.53	1.47	1.38
3	H	603	HEC	CAC-C3C	4.52	1.49	1.35
3	J	607	HEC	CBB-CAB	-4.52	1.32	1.49
3	V	603	HEC	C3B-C4B	4.51	1.53	1.46
3	H	603	HEC	C3B-C4B	4.51	1.53	1.46
3	K	603	HEC	CHD-C4C	4.51	1.47	1.38
3	E	605	HEC	CBC-CAC	-4.51	1.32	1.49
3	K	603	HEC	CAC-C3C	4.50	1.49	1.35
3	N	606	HEC	CBC-CAC	-4.50	1.32	1.49
3	E	603	HEC	CHD-C4C	4.50	1.47	1.38
3	K	605	HEC	CBB-CAB	-4.49	1.32	1.49
3	G	603	HEC	CHC-C1C	4.49	1.49	1.39
3	X	603	HEC	CAC-C3C	4.48	1.49	1.35
3	L	607	HEC	CBB-CAB	-4.48	1.32	1.49
3	K	607	HEC	CBB-CAB	-4.48	1.32	1.49
3	A	606	HEC	CBC-CAC	-4.48	1.32	1.49
3	W	604	HEC	CBB-CAB	-4.47	1.32	1.49
3	H	602	HEC	CBB-CAB	-4.47	1.32	1.49
3	N	603	HEC	CHD-C4C	4.47	1.47	1.38
3	T	603	HEC	CAC-C3C	4.47	1.49	1.35
3	K	602	HEC	CBB-CAB	-4.47	1.33	1.49
3	N	602	HEC	CBC-CAC	-4.46	1.33	1.49
3	I	607	HEC	CBC-CAC	-4.46	1.33	1.49
3	H	603	HEC	CHD-C4C	4.46	1.47	1.38
3	J	600	HEC	CBC-CAC	-4.46	1.33	1.49
3	H	606	HEC	CBB-CAB	-4.45	1.33	1.49
3	U	603	HEC	C3B-C4B	4.45	1.53	1.46
3	F	606	HEC	CBC-CAC	-4.45	1.33	1.49
3	W	603	HEC	C3B-C4B	4.45	1.53	1.46
3	D	605	HEC	CBB-CAB	-4.45	1.33	1.49
3	I	601	HEC	CBB-CAB	-4.45	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	603	HEC	CHD-C4C	4.45	1.47	1.38
3	E	606	HEC	CBC-CAC	-4.45	1.33	1.49
3	G	600	HEC	CBC-CAC	-4.44	1.33	1.49
3	A	603	HEC	CHD-C4C	4.44	1.47	1.38
3	W	606	HEC	CBC-CAC	-4.44	1.33	1.49
3	J	607	HEC	CBC-CAC	-4.44	1.33	1.49
3	K	601	HEC	CBC-CAC	-4.44	1.33	1.49
3	B	606	HEC	CBC-CAC	-4.44	1.33	1.49
3	L	604	HEC	CBB-CAB	-4.44	1.33	1.49
3	W	602	HEC	CBC-CAC	-4.44	1.33	1.49
3	S	606	HEC	CBC-CAC	-4.44	1.33	1.49
3	I	605	HEC	CBC-CAC	-4.43	1.33	1.49
3	L	603	HEC	C3B-C4B	4.43	1.53	1.46
3	E	602	HEC	CBB-CAB	-4.43	1.33	1.49
3	T	602	HEC	CBC-CAC	-4.43	1.33	1.49
3	R	606	HEC	CBC-CAC	-4.43	1.33	1.49
3	A	603	HEC	CAC-C3C	4.43	1.49	1.35
3	H	607	HEC	CBC-CAC	-4.43	1.33	1.49
3	V	604	HEC	CBC-CAC	-4.42	1.33	1.49
3	T	602	HEC	CBB-CAB	-4.42	1.33	1.49
3	G	603	HEC	CHD-C4C	4.42	1.47	1.38
3	K	604	HEC	CBC-CAC	-4.42	1.33	1.49
3	I	603	HEC	C3B-C4B	4.42	1.53	1.46
3	P	603	HEC	C3B-C4B	4.42	1.53	1.46
3	J	604	HEC	CBC-CAC	-4.42	1.33	1.49
3	H	602	HEC	CBC-CAC	-4.42	1.33	1.49
3	D	603	HEC	CAC-C3C	4.42	1.49	1.35
3	A	602	HEC	CBB-CAB	-4.42	1.33	1.49
3	P	602	HEC	CBC-CAC	-4.42	1.33	1.49
3	R	602	HEC	CBB-CAB	-4.42	1.33	1.49
3	A	602	HEC	CBC-CAC	-4.42	1.33	1.49
3	P	607	HEC	CBC-CAC	-4.42	1.33	1.49
3	L	602	HEC	CBB-CAB	-4.41	1.33	1.49
3	O	602	HEC	CBB-CAB	-4.41	1.33	1.49
3	P	605	HEC	CBC-CAC	-4.41	1.33	1.49
3	E	604	HEC	CBC-CAC	-4.41	1.33	1.49
3	V	606	HEC	CBC-CAC	-4.41	1.33	1.49
3	B	602	HEC	CBC-CAC	-4.41	1.33	1.49
3	P	603	HEC	CHD-C4C	4.41	1.47	1.38
3	D	603	HEC	CHC-C1C	4.41	1.49	1.39
3	M	601	HEC	CBB-CAB	-4.41	1.33	1.49
3	O	607	HEC	CBC-CAC	-4.41	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	603	HEC	CAC-C3C	4.41	1.49	1.35
3	C	605	HEC	CBC-CAC	-4.41	1.33	1.49
3	I	607	HEC	CBB-CAB	-4.41	1.33	1.49
3	O	604	HEC	CBB-CAB	-4.40	1.33	1.49
3	E	603	HEC	CAC-C3C	4.40	1.49	1.35
3	G	604	HEC	CBB-CAB	-4.40	1.33	1.49
3	L	603	HEC	CAC-C3C	4.40	1.49	1.35
3	V	603	HEC	CAC-C3C	4.40	1.49	1.35
3	P	607	HEC	CBB-CAB	-4.40	1.33	1.49
3	C	602	HEC	CBC-CAC	-4.40	1.33	1.49
3	S	601	HEC	CBC-CAC	-4.40	1.33	1.49
3	P	604	HEC	CBC-CAC	-4.40	1.33	1.49
3	O	604	HEC	CBC-CAC	-4.40	1.33	1.49
3	U	606	HEC	CBC-CAC	-4.40	1.33	1.49
3	N	604	HEC	CBB-CAB	-4.40	1.33	1.49
3	E	602	HEC	CBC-CAC	-4.40	1.33	1.49
3	N	600	HEC	CBC-CAC	-4.39	1.33	1.49
3	H	605	HEC	CBC-CAC	-4.39	1.33	1.49
3	G	607	HEC	CBB-CAB	-4.39	1.33	1.49
3	J	603	HEC	C3B-C4B	4.39	1.53	1.46
3	W	603	HEC	CHD-C4C	4.39	1.47	1.38
3	G	602	HEC	CBC-CAC	-4.39	1.33	1.49
3	Q	603	HEC	CAC-C3C	4.39	1.49	1.35
3	F	604	HEC	CBB-CAB	-4.39	1.33	1.49
3	M	606	HEC	CBC-CAC	-4.39	1.33	1.49
3	R	607	HEC	CBB-CAB	-4.39	1.33	1.49
3	S	600	HEC	CBC-CAC	-4.39	1.33	1.49
3	D	607	HEC	CBC-CAC	-4.39	1.33	1.49
3	M	607	HEC	CBC-CAC	-4.39	1.33	1.49
3	L	601	HEC	CBB-CAB	-4.39	1.33	1.49
3	U	600	HEC	CBC-CAC	-4.39	1.33	1.49
3	D	601	HEC	CBC-CAC	-4.38	1.33	1.49
3	F	603	HEC	CHC-C1C	4.38	1.49	1.39
3	R	602	HEC	CAC-C3C	4.38	1.49	1.35
3	J	603	HEC	CHC-C1C	4.38	1.49	1.39
3	X	602	HEC	CBC-CAC	-4.38	1.33	1.49
3	C	604	HEC	CBC-CAC	-4.38	1.33	1.49
3	K	603	HEC	C3B-C4B	4.38	1.53	1.46
3	B	601	HEC	CAC-C3C	4.38	1.49	1.35
3	D	606	HEC	CAC-C3C	4.38	1.49	1.35
3	T	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	P	602	HEC	CBB-CAB	-4.38	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	601	HEC	CBC-CAC	-4.38	1.33	1.49
3	K	607	HEC	CBC-CAC	-4.38	1.33	1.49
3	X	606	HEC	CBC-CAC	-4.38	1.33	1.49
3	U	603	HEC	CAC-C3C	4.38	1.49	1.35
3	E	607	HEC	CBC-CAC	-4.38	1.33	1.49
3	V	602	HEC	CBB-CAB	-4.38	1.33	1.49
3	I	603	HEC	CAB-C3B	4.38	1.49	1.35
3	I	603	HEC	CHD-C4C	4.38	1.47	1.38
3	I	602	HEC	CBB-CAB	-4.38	1.33	1.49
3	M	600	HEC	CBB-CAB	-4.38	1.33	1.49
3	I	606	HEC	CAC-C3C	4.38	1.49	1.35
3	I	602	HEC	CBC-CAC	-4.38	1.33	1.49
3	Q	607	HEC	CBB-CAB	-4.38	1.33	1.49
3	K	602	HEC	CBC-CAC	-4.37	1.33	1.49
3	G	604	HEC	CBC-CAC	-4.37	1.33	1.49
3	I	603	HEC	CAC-C3C	4.37	1.49	1.35
3	O	607	HEC	CBB-CAB	-4.37	1.33	1.49
3	V	602	HEC	CBC-CAC	-4.37	1.33	1.49
3	C	607	HEC	CBB-CAB	-4.37	1.33	1.49
3	B	602	HEC	CBB-CAB	-4.37	1.33	1.49
3	J	603	HEC	CAC-C3C	4.37	1.49	1.35
3	I	601	HEC	CBC-CAC	-4.37	1.33	1.49
3	Q	601	HEC	CBC-CAC	-4.37	1.33	1.49
3	F	600	HEC	CBB-CAB	-4.37	1.33	1.49
3	C	603	HEC	CAC-C3C	4.37	1.49	1.35
3	L	607	HEC	CAC-C3C	4.37	1.49	1.35
3	D	605	HEC	CBC-CAC	-4.37	1.33	1.49
3	S	605	HEC	CBB-CAB	-4.37	1.33	1.49
3	K	605	HEC	CBC-CAC	-4.37	1.33	1.49
3	Q	607	HEC	CBC-CAC	-4.37	1.33	1.49
3	S	602	HEC	CBB-CAB	-4.37	1.33	1.49
3	A	601	HEC	CBC-CAC	-4.37	1.33	1.49
3	S	604	HEC	CBC-CAC	-4.37	1.33	1.49
3	F	601	HEC	CBC-CAC	-4.37	1.33	1.49
3	P	600	HEC	CBC-CAC	-4.37	1.33	1.49
3	H	600	HEC	CBC-CAC	-4.37	1.33	1.49
3	V	601	HEC	CBC-CAC	-4.37	1.33	1.49
3	J	602	HEC	CBC-CAC	-4.36	1.33	1.49
3	O	605	HEC	CBB-CAB	-4.36	1.33	1.49
3	X	607	HEC	CBB-CAB	-4.36	1.33	1.49
3	B	600	HEC	CBC-CAC	-4.36	1.33	1.49
3	C	606	HEC	CBC-CAC	-4.36	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	605	HEC	CBB-CAB	-4.36	1.33	1.49
3	F	603	HEC	CHD-C4C	4.36	1.46	1.38
3	O	600	HEC	CBC-CAC	-4.36	1.33	1.49
3	U	607	HEC	CBC-CAC	-4.36	1.33	1.49
3	W	604	HEC	CBC-CAC	-4.36	1.33	1.49
3	H	601	HEC	CAC-C3C	4.36	1.49	1.35
3	E	600	HEC	CBC-CAC	-4.36	1.33	1.49
3	U	605	HEC	CBC-CAC	-4.36	1.33	1.49
3	Q	606	HEC	CBC-CAC	-4.36	1.33	1.49
3	R	601	HEC	CBC-CAC	-4.36	1.33	1.49
3	P	606	HEC	CBC-CAC	-4.36	1.33	1.49
3	H	607	HEC	CBB-CAB	-4.36	1.33	1.49
3	S	607	HEC	CBC-CAC	-4.36	1.33	1.49
3	F	602	HEC	CBB-CAB	-4.36	1.33	1.49
3	F	604	HEC	CBC-CAC	-4.36	1.33	1.49
3	V	600	HEC	CBC-CAC	-4.36	1.33	1.49
3	N	607	HEC	CBB-CAB	-4.36	1.33	1.49
3	P	606	HEC	CBB-CAB	-4.36	1.33	1.49
3	T	605	HEC	CBC-CAC	-4.36	1.33	1.49
3	P	601	HEC	CBB-CAB	-4.35	1.33	1.49
3	R	603	HEC	CHD-C4C	4.35	1.46	1.38
3	R	603	HEC	CHC-C1C	4.35	1.49	1.39
3	S	607	HEC	CBB-CAB	-4.35	1.33	1.49
3	M	600	HEC	CBC-CAC	-4.35	1.33	1.49
3	R	607	HEC	CBC-CAC	-4.35	1.33	1.49
3	X	607	HEC	CBC-CAC	-4.35	1.33	1.49
3	Q	602	HEC	CBC-CAC	-4.35	1.33	1.49
3	O	606	HEC	CBC-CAC	-4.35	1.33	1.49
3	O	607	HEC	CAC-C3C	4.35	1.49	1.35
3	S	603	HEC	CAC-C3C	4.35	1.49	1.35
3	B	605	HEC	CBC-CAC	-4.35	1.33	1.49
3	L	601	HEC	CAC-C3C	4.35	1.49	1.35
3	G	601	HEC	CBC-CAC	-4.35	1.33	1.49
3	F	606	HEC	CBB-CAB	-4.35	1.33	1.49
3	S	601	HEC	CBB-CAB	-4.35	1.33	1.49
3	N	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	R	600	HEC	CBC-CAC	-4.35	1.33	1.49
3	R	601	HEC	CBB-CAB	-4.35	1.33	1.49
3	T	600	HEC	CBC-CAC	-4.35	1.33	1.49
3	Q	604	HEC	CBC-CAC	-4.35	1.33	1.49
3	R	603	HEC	CAC-C3C	4.35	1.49	1.35
3	F	602	HEC	CBC-CAC	-4.35	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	602	HEC	CBB-CAB	-4.35	1.33	1.49
3	N	607	HEC	CBC-CAC	-4.35	1.33	1.49
3	W	600	HEC	CBB-CAB	-4.35	1.33	1.49
3	L	600	HEC	CBC-CAC	-4.34	1.33	1.49
3	L	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	T	601	HEC	CBC-CAC	-4.34	1.33	1.49
3	X	600	HEC	CBC-CAC	-4.34	1.33	1.49
3	X	606	HEC	CBB-CAB	-4.34	1.33	1.49
3	A	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	I	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	V	606	HEC	CBB-CAB	-4.34	1.33	1.49
3	S	603	HEC	CHC-C1C	4.34	1.49	1.39
3	C	602	HEC	CBB-CAB	-4.34	1.33	1.49
3	J	602	HEC	CBB-CAB	-4.34	1.33	1.49
3	T	604	HEC	CBC-CAC	-4.34	1.33	1.49
3	D	601	HEC	CBB-CAB	-4.34	1.33	1.49
3	E	601	HEC	CBC-CAC	-4.34	1.33	1.49
3	J	603	HEC	CHD-C4C	4.34	1.46	1.38
3	V	607	HEC	CAC-C3C	4.34	1.49	1.35
3	O	602	HEC	CAC-C3C	4.34	1.49	1.35
3	R	607	HEC	CAC-C3C	4.34	1.49	1.35
3	N	601	HEC	CBC-CAC	-4.34	1.33	1.49
3	N	605	HEC	CBC-CAC	-4.34	1.33	1.49
3	Q	605	HEC	CBB-CAB	-4.34	1.33	1.49
3	P	600	HEC	CAC-C3C	4.34	1.49	1.35
3	L	606	HEC	CBC-CAC	-4.34	1.33	1.49
3	L	606	HEC	CBB-CAB	-4.34	1.33	1.49
3	B	607	HEC	CBB-CAB	-4.34	1.33	1.49
3	M	607	HEC	CBB-CAB	-4.33	1.33	1.49
3	R	606	HEC	CBB-CAB	-4.33	1.33	1.49
3	M	604	HEC	CBC-CAC	-4.33	1.33	1.49
3	E	604	HEC	CBB-CAB	-4.33	1.33	1.49
3	X	601	HEC	CBB-CAB	-4.33	1.33	1.49
3	U	600	HEC	CAC-C3C	4.33	1.49	1.35
3	Q	600	HEC	CBB-CAB	-4.33	1.33	1.49
3	Q	603	HEC	CHC-C1C	4.33	1.49	1.39
3	B	600	HEC	CBB-CAB	-4.33	1.33	1.49
3	K	601	HEC	CAC-C3C	4.33	1.49	1.35
3	G	601	HEC	CBB-CAB	-4.33	1.33	1.49
3	I	600	HEC	CBC-CAC	-4.33	1.33	1.49
3	P	601	HEC	CBC-CAC	-4.33	1.33	1.49
3	F	607	HEC	CAC-C3C	4.33	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	604	HEC	CBC-CAC	-4.33	1.33	1.49
3	W	605	HEC	CBC-CAC	-4.33	1.33	1.49
3	X	604	HEC	CBC-CAC	-4.33	1.33	1.49
3	P	603	HEC	CAC-C3C	4.33	1.49	1.35
3	V	607	HEC	CBC-CAC	-4.33	1.33	1.49
3	M	604	HEC	CBB-CAB	-4.33	1.33	1.49
3	J	605	HEC	CBB-CAB	-4.33	1.33	1.49
3	X	602	HEC	CBB-CAB	-4.33	1.33	1.49
3	G	605	HEC	CBB-CAB	-4.33	1.33	1.49
3	G	606	HEC	CBB-CAB	-4.33	1.33	1.49
3	J	601	HEC	CBC-CAC	-4.33	1.33	1.49
3	M	602	HEC	CBB-CAB	-4.33	1.33	1.49
3	W	601	HEC	CBB-CAB	-4.33	1.33	1.49
3	P	600	HEC	CBB-CAB	-4.33	1.33	1.49
3	L	605	HEC	CBB-CAB	-4.33	1.33	1.49
3	X	603	HEC	CHC-C1C	4.33	1.49	1.39
3	I	606	HEC	CBC-CAC	-4.33	1.33	1.49
3	W	607	HEC	CBC-CAC	-4.33	1.33	1.49
3	B	601	HEC	CBC-CAC	-4.33	1.33	1.49
3	D	606	HEC	CBB-CAB	-4.33	1.33	1.49
3	J	602	HEC	CAC-C3C	4.33	1.49	1.35
3	S	604	HEC	CBB-CAB	-4.32	1.33	1.49
3	F	605	HEC	CBB-CAB	-4.32	1.33	1.49
3	B	601	HEC	CBB-CAB	-4.32	1.33	1.49
3	U	604	HEC	CBB-CAB	-4.32	1.33	1.49
3	G	606	HEC	CBC-CAC	-4.32	1.33	1.49
3	J	606	HEC	CBC-CAC	-4.32	1.33	1.49
3	R	602	HEC	CBC-CAC	-4.32	1.33	1.49
3	V	601	HEC	CAC-C3C	4.32	1.49	1.35
3	U	601	HEC	CBC-CAC	-4.32	1.33	1.49
3	D	600	HEC	CBC-CAC	-4.32	1.33	1.49
3	C	600	HEC	CBC-CAC	-4.32	1.33	1.49
3	W	602	HEC	CBB-CAB	-4.32	1.33	1.49
3	V	603	HEC	CHD-C4C	4.32	1.46	1.38
3	W	607	HEC	CBB-CAB	-4.32	1.33	1.49
3	S	600	HEC	CBB-CAB	-4.32	1.33	1.49
3	T	600	HEC	CBB-CAB	-4.32	1.33	1.49
3	C	605	HEC	CBB-CAB	-4.32	1.33	1.49
3	C	601	HEC	CBC-CAC	-4.32	1.33	1.49
3	K	600	HEC	CBC-CAC	-4.32	1.33	1.49
3	D	602	HEC	CBC-CAC	-4.32	1.33	1.49
3	N	605	HEC	CAB-C3B	4.32	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEC	CBB-CAB	-4.32	1.33	1.49
3	M	601	HEC	CBC-CAC	-4.32	1.33	1.49
3	W	601	HEC	CAC-C3C	4.32	1.49	1.35
3	F	600	HEC	CBC-CAC	-4.32	1.33	1.49
3	U	606	HEC	CBB-CAB	-4.32	1.33	1.49
3	D	606	HEC	CBC-CAC	-4.31	1.33	1.49
3	H	600	HEC	CAC-C3C	4.31	1.49	1.35
3	M	605	HEC	CAC-C3C	4.31	1.49	1.35
3	F	607	HEC	CBC-CAC	-4.31	1.33	1.49
3	C	604	HEC	CBB-CAB	-4.31	1.33	1.49
3	W	600	HEC	CAC-C3C	4.31	1.49	1.35
3	L	607	HEC	CBC-CAC	-4.31	1.33	1.49
3	M	605	HEC	CBB-CAB	-4.31	1.33	1.49
3	U	607	HEC	CBB-CAB	-4.31	1.33	1.49
3	X	601	HEC	CBC-CAC	-4.31	1.33	1.49
3	J	601	HEC	CAC-C3C	4.31	1.49	1.35
3	W	600	HEC	CBC-CAC	-4.31	1.33	1.49
3	O	603	HEC	CAC-C3C	4.31	1.49	1.35
3	D	604	HEC	CBB-CAB	-4.31	1.33	1.49
3	V	604	HEC	CBB-CAB	-4.31	1.33	1.49
3	J	606	HEC	CBB-CAB	-4.31	1.33	1.49
3	U	602	HEC	CBC-CAC	-4.31	1.33	1.49
3	F	600	HEC	CAC-C3C	4.31	1.49	1.35
3	O	601	HEC	CAC-C3C	4.31	1.49	1.35
3	P	601	HEC	CAC-C3C	4.31	1.49	1.35
3	Q	602	HEC	CBB-CAB	-4.31	1.33	1.49
3	Q	604	HEC	CBB-CAB	-4.31	1.33	1.49
3	A	601	HEC	CBB-CAB	-4.31	1.33	1.49
3	A	607	HEC	CBC-CAC	-4.31	1.33	1.49
3	E	601	HEC	CAC-C3C	4.31	1.49	1.35
3	A	605	HEC	CBB-CAB	-4.31	1.33	1.49
3	G	602	HEC	CAC-C3C	4.31	1.49	1.35
3	K	606	HEC	CBC-CAC	-4.30	1.33	1.49
3	T	607	HEC	CBB-CAB	-4.30	1.33	1.49
3	A	600	HEC	CBB-CAB	-4.30	1.33	1.49
3	R	605	HEC	CBC-CAC	-4.30	1.33	1.49
3	V	607	HEC	CBB-CAB	-4.30	1.33	1.49
3	R	604	HEC	CBC-CAC	-4.30	1.33	1.49
3	B	603	HEC	CAC-C3C	4.30	1.49	1.35
3	T	606	HEC	CBB-CAB	-4.30	1.33	1.49
3	E	605	HEC	CBB-CAB	-4.30	1.33	1.49
3	G	607	HEC	CBC-CAC	-4.30	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	600	HEC	CBB-CAB	-4.30	1.33	1.49
3	M	602	HEC	CBC-CAC	-4.30	1.33	1.49
3	L	602	HEC	CAC-C3C	4.30	1.49	1.35
3	T	607	HEC	CBC-CAC	-4.30	1.33	1.49
3	M	603	HEC	CHC-C1C	4.30	1.49	1.39
3	B	604	HEC	CBB-CAB	-4.30	1.33	1.49
3	T	604	HEC	CBB-CAB	-4.30	1.33	1.49
3	D	602	HEC	CAC-C3C	4.30	1.48	1.35
3	J	601	HEC	CBB-CAB	-4.30	1.33	1.49
3	O	601	HEC	CBC-CAC	-4.30	1.33	1.49
3	F	603	HEC	CAC-C3C	4.30	1.48	1.35
3	C	600	HEC	CBB-CAB	-4.30	1.33	1.49
3	V	601	HEC	CBB-CAB	-4.30	1.33	1.49
3	W	606	HEC	CBB-CAB	-4.29	1.33	1.49
3	T	605	HEC	CBB-CAB	-4.29	1.33	1.49
3	C	600	HEC	CAC-C3C	4.29	1.48	1.35
3	O	602	HEC	CBC-CAC	-4.29	1.33	1.49
3	M	605	HEC	CAB-C3B	4.29	1.48	1.35
3	Q	601	HEC	CBB-CAB	-4.29	1.33	1.49
3	F	605	HEC	CBC-CAC	-4.29	1.33	1.49
3	O	600	HEC	CBB-CAB	-4.29	1.33	1.49
3	P	604	HEC	CBB-CAB	-4.29	1.33	1.49
3	D	604	HEC	CBC-CAC	-4.29	1.33	1.49
3	G	603	HEC	CAC-C3C	4.29	1.48	1.35
3	C	601	HEC	CBB-CAB	-4.28	1.33	1.49
3	U	600	HEC	CBB-CAB	-4.28	1.33	1.49
3	E	606	HEC	CBB-CAB	-4.28	1.33	1.49
3	V	605	HEC	CBC-CAC	-4.28	1.33	1.49
3	Q	600	HEC	CBC-CAC	-4.28	1.33	1.49
3	U	602	HEC	CAC-C3C	4.28	1.48	1.35
3	R	605	HEC	CBB-CAB	-4.28	1.33	1.49
3	H	600	HEC	CBB-CAB	-4.28	1.33	1.49
3	X	601	HEC	CAC-C3C	4.28	1.48	1.35
3	E	601	HEC	CBB-CAB	-4.28	1.33	1.49
3	U	605	HEC	CAB-C3B	4.28	1.48	1.35
3	B	603	HEC	CHD-C4C	4.28	1.46	1.38
3	W	605	HEC	CBB-CAB	-4.28	1.33	1.49
3	T	606	HEC	CAC-C3C	4.28	1.48	1.35
3	V	605	HEC	CBB-CAB	-4.28	1.33	1.49
3	A	605	HEC	CAB-C3B	4.28	1.48	1.35
3	A	605	HEC	CBC-CAC	-4.28	1.33	1.49
3	S	602	HEC	CAC-C3C	4.28	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	602	HEC	CAC-C3C	4.28	1.48	1.35
3	I	604	HEC	CBB-CAB	-4.28	1.33	1.49
3	B	607	HEC	CBC-CAC	-4.27	1.33	1.49
3	U	601	HEC	CBB-CAB	-4.27	1.33	1.49
3	M	600	HEC	CAC-C3C	4.27	1.48	1.35
3	X	605	HEC	CBC-CAC	-4.27	1.33	1.49
3	V	602	HEC	CAC-C3C	4.27	1.48	1.35
3	L	603	HEC	CHD-C4C	4.27	1.46	1.38
3	Q	600	HEC	CAC-C3C	4.27	1.48	1.35
3	H	604	HEC	CBC-CAC	-4.27	1.33	1.49
3	A	604	HEC	CBB-CAB	-4.27	1.33	1.49
3	C	603	HEC	CHD-C4C	4.27	1.46	1.38
3	S	607	HEC	CAC-C3C	4.27	1.48	1.35
3	X	604	HEC	CBB-CAB	-4.27	1.33	1.49
3	M	603	HEC	CAC-C3C	4.27	1.48	1.35
3	X	600	HEC	CBB-CAB	-4.27	1.33	1.49
3	J	604	HEC	CBB-CAB	-4.27	1.33	1.49
3	N	601	HEC	CBB-CAB	-4.27	1.33	1.49
3	I	600	HEC	CBB-CAB	-4.27	1.33	1.49
3	G	605	HEC	CBC-CAC	-4.27	1.33	1.49
3	A	600	HEC	CAC-C3C	4.27	1.48	1.35
3	U	604	HEC	CBC-CAC	-4.27	1.33	1.49
3	B	606	HEC	CBB-CAB	-4.27	1.33	1.49
3	V	606	HEC	CAC-C3C	4.26	1.48	1.35
3	W	603	HEC	CHC-C1C	4.26	1.49	1.39
3	I	605	HEC	CAB-C3B	4.26	1.48	1.35
3	Q	606	HEC	CBB-CAB	-4.26	1.33	1.49
3	O	601	HEC	CBB-CAB	-4.26	1.33	1.49
3	C	601	HEC	CAC-C3C	4.26	1.48	1.35
3	M	606	HEC	CBB-CAB	-4.26	1.33	1.49
3	R	600	HEC	CAC-C3C	4.26	1.48	1.35
3	H	601	HEC	CBC-CAC	-4.26	1.33	1.49
3	K	604	HEC	CBB-CAB	-4.26	1.33	1.49
3	D	607	HEC	CBB-CAB	-4.26	1.33	1.49
3	B	604	HEC	CBC-CAC	-4.26	1.33	1.49
3	R	604	HEC	CBB-CAB	-4.26	1.33	1.49
3	T	601	HEC	CBB-CAB	-4.26	1.33	1.49
3	L	605	HEC	CBC-CAC	-4.26	1.33	1.49
3	S	605	HEC	CBC-CAC	-4.26	1.33	1.49
3	C	607	HEC	CBC-CAC	-4.26	1.33	1.49
3	F	601	HEC	CBB-CAB	-4.26	1.33	1.49
3	D	602	HEC	CBB-CAB	-4.26	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	605	HEC	CAB-C3B	4.26	1.48	1.35
3	K	600	HEC	CBB-CAB	-4.26	1.33	1.49
3	T	603	HEC	C4B-NB	4.26	1.47	1.39
3	J	605	HEC	CBC-CAC	-4.25	1.33	1.49
3	A	600	HEC	CBC-CAC	-4.25	1.33	1.49
3	I	605	HEC	CBB-CAB	-4.25	1.33	1.49
3	G	606	HEC	CAC-C3C	4.25	1.48	1.35
3	U	601	HEC	CAC-C3C	4.25	1.48	1.35
3	D	600	HEC	CBB-CAB	-4.25	1.33	1.49
3	S	606	HEC	CBB-CAB	-4.25	1.33	1.49
3	E	607	HEC	CBB-CAB	-4.25	1.33	1.49
3	A	601	HEC	CAC-C3C	4.25	1.48	1.35
3	O	603	HEC	CHD-C4C	4.25	1.46	1.38
3	T	607	HEC	CAC-C3C	4.25	1.48	1.35
3	W	607	HEC	CAC-C3C	4.25	1.48	1.35
3	V	600	HEC	CBB-CAB	-4.24	1.33	1.49
3	T	600	HEC	CAC-C3C	4.24	1.48	1.35
3	O	606	HEC	CBB-CAB	-4.24	1.33	1.49
3	H	602	HEC	CAC-C3C	4.24	1.48	1.35
3	N	605	HEC	CBB-CAB	-4.24	1.33	1.49
3	G	602	HEC	CBB-CAB	-4.24	1.33	1.49
3	S	602	HEC	CBC-CAC	-4.24	1.33	1.49
3	F	607	HEC	CBB-CAB	-4.24	1.33	1.49
3	Q	605	HEC	CBC-CAC	-4.24	1.33	1.49
3	P	605	HEC	CBB-CAB	-4.24	1.33	1.49
3	K	602	HEC	CAC-C3C	4.24	1.48	1.35
3	N	601	HEC	CAC-C3C	4.23	1.48	1.35
3	O	605	HEC	CAB-C3B	4.23	1.48	1.35
3	T	601	HEC	CAC-C3C	4.23	1.48	1.35
3	K	606	HEC	CBB-CAB	-4.23	1.33	1.49
3	M	605	HEC	CBC-CAC	-4.23	1.33	1.49
3	H	604	HEC	CBB-CAB	-4.23	1.33	1.49
3	L	601	HEC	CBC-CAC	-4.23	1.33	1.49
3	Q	606	HEC	CAC-C3C	4.23	1.48	1.35
3	N	606	HEC	CBB-CAB	-4.23	1.33	1.49
3	M	601	HEC	CAC-C3C	4.23	1.48	1.35
3	G	601	HEC	CAC-C3C	4.23	1.48	1.35
3	C	606	HEC	CAC-C3C	4.23	1.48	1.35
3	X	607	HEC	CAC-C3C	4.23	1.48	1.35
3	E	600	HEC	CBB-CAB	-4.22	1.33	1.49
3	J	603	HEC	C4B-NB	4.22	1.47	1.39
3	I	607	HEC	CAC-C3C	4.22	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	607	HEC	CAC-C3C	4.22	1.48	1.35
3	S	601	HEC	CAC-C3C	4.22	1.48	1.35
3	O	605	HEC	CBC-CAC	-4.22	1.33	1.49
3	L	602	HEC	CBC-CAC	-4.22	1.33	1.49
3	B	607	HEC	CAC-C3C	4.22	1.48	1.35
3	G	607	HEC	CAC-C3C	4.22	1.48	1.35
3	G	600	HEC	CBB-CAB	-4.22	1.33	1.49
3	S	603	HEC	CAB-C3B	4.22	1.48	1.35
3	J	600	HEC	CBB-CAB	-4.22	1.33	1.49
3	H	605	HEC	CBB-CAB	-4.22	1.33	1.49
3	F	607	HEC	CAB-C3B	4.22	1.48	1.35
3	M	606	HEC	CAC-C3C	4.22	1.48	1.35
3	J	606	HEC	CAC-C3C	4.21	1.48	1.35
3	F	605	HEC	CAB-C3B	4.21	1.48	1.35
3	S	600	HEC	CAC-C3C	4.21	1.48	1.35
3	P	605	HEC	CAB-C3B	4.21	1.48	1.35
3	W	605	HEC	CAB-C3B	4.21	1.48	1.35
3	U	604	HEC	CAC-C3C	4.21	1.48	1.35
3	U	605	HEC	CBB-CAB	-4.21	1.33	1.49
3	A	602	HEC	CAC-C3C	4.21	1.48	1.35
3	Q	607	HEC	CAC-C3C	4.21	1.48	1.35
3	N	600	HEC	CAC-C3C	4.21	1.48	1.35
3	M	603	HEC	CHD-C4C	4.20	1.46	1.38
3	Q	603	HEC	C4B-NB	4.20	1.47	1.39
3	I	606	HEC	CBB-CAB	-4.20	1.33	1.49
3	C	606	HEC	CBB-CAB	-4.20	1.33	1.49
3	R	601	HEC	CAC-C3C	4.20	1.48	1.35
3	C	602	HEC	CAC-C3C	4.20	1.48	1.35
3	O	603	HEC	C4B-NB	4.20	1.47	1.39
3	X	603	HEC	C4B-NB	4.20	1.47	1.39
3	K	601	HEC	CBB-CAB	-4.19	1.34	1.49
3	D	605	HEC	CAC-C3C	4.19	1.48	1.35
3	Q	605	HEC	CAC-C3C	4.19	1.48	1.35
3	V	605	HEC	CAC-C3C	4.19	1.48	1.35
3	F	601	HEC	CAC-C3C	4.19	1.48	1.35
3	Q	602	HEC	CAC-C3C	4.19	1.48	1.35
3	F	603	HEC	C4B-NB	4.19	1.47	1.39
3	A	607	HEC	CBB-CAB	-4.19	1.34	1.49
3	M	603	HEC	CAB-C3B	4.19	1.48	1.35
3	J	600	HEC	CAC-C3C	4.19	1.48	1.35
3	M	602	HEC	CAC-C3C	4.19	1.48	1.35
3	U	603	HEC	CAB-C3B	4.18	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	HEC	CBB-CAB	-4.18	1.34	1.49
3	H	601	HEC	CBB-CAB	-4.18	1.34	1.49
3	D	600	HEC	CAC-C3C	4.18	1.48	1.35
3	B	602	HEC	CAC-C3C	4.18	1.48	1.35
3	C	605	HEC	CAB-C3B	4.18	1.48	1.35
3	J	605	HEC	CAC-C3C	4.18	1.48	1.35
3	B	603	HEC	C4B-NB	4.18	1.47	1.39
3	J	605	HEC	CAB-C3B	4.18	1.48	1.35
3	E	603	HEC	CHC-C1C	4.18	1.48	1.39
3	B	600	HEC	CAC-C3C	4.18	1.48	1.35
3	L	600	HEC	CAC-C3C	4.18	1.48	1.35
3	T	603	HEC	CAB-C3B	4.18	1.48	1.35
3	X	600	HEC	CAC-C3C	4.17	1.48	1.35
3	T	605	HEC	CAC-C3C	4.17	1.48	1.35
3	R	606	HEC	CAC-C3C	4.17	1.48	1.35
3	B	603	HEC	CHC-C1C	4.17	1.48	1.39
3	G	605	HEC	CAC-C3C	4.17	1.48	1.35
3	G	605	HEC	CAB-C3B	4.17	1.48	1.35
3	W	602	HEC	CAC-C3C	4.17	1.48	1.35
3	P	606	HEC	CAC-C3C	4.16	1.48	1.35
3	Q	603	HEC	CAB-C3B	4.16	1.48	1.35
3	V	600	HEC	CAC-C3C	4.16	1.48	1.35
3	L	606	HEC	CAC-C3C	4.16	1.48	1.35
3	U	600	HEC	CAB-C3B	4.16	1.48	1.35
3	D	603	HEC	CAB-C3B	4.16	1.48	1.35
3	I	605	HEC	CAC-C3C	4.16	1.48	1.35
3	B	603	HEC	CAB-C3B	4.16	1.48	1.35
3	N	600	HEC	CBB-CAB	-4.16	1.34	1.49
3	X	603	HEC	CAB-C3B	4.16	1.48	1.35
3	U	606	HEC	CAC-C3C	4.15	1.48	1.35
3	R	604	HEC	CAC-C3C	4.15	1.48	1.35
3	O	603	HEC	CAB-C3B	4.15	1.48	1.35
3	R	605	HEC	CAC-C3C	4.15	1.48	1.35
3	J	607	HEC	CAC-C3C	4.15	1.48	1.35
3	E	600	HEC	CAC-C3C	4.15	1.48	1.35
3	A	606	HEC	CBB-CAB	-4.15	1.34	1.49
3	E	602	HEC	CAC-C3C	4.15	1.48	1.35
3	M	604	HEC	CAC-C3C	4.15	1.48	1.35
3	C	607	HEC	CAC-C3C	4.15	1.48	1.35
3	A	603	HEC	CAB-C3B	4.15	1.48	1.35
3	O	606	HEC	CAC-C3C	4.15	1.48	1.35
3	D	601	HEC	CAC-C3C	4.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	603	HEC	C3C-C4C	4.15	1.53	1.46
3	H	604	HEC	CAC-C3C	4.14	1.48	1.35
3	A	605	HEC	CAC-C3C	4.14	1.48	1.35
3	K	603	HEC	CHC-C1C	4.14	1.48	1.39
3	K	600	HEC	CAC-C3C	4.14	1.48	1.35
3	P	602	HEC	CAC-C3C	4.14	1.48	1.35
3	F	602	HEC	CAC-C3C	4.14	1.48	1.35
3	O	605	HEC	CAC-C3C	4.14	1.48	1.35
3	S	604	HEC	CAB-C3B	4.14	1.48	1.35
3	S	605	HEC	CAC-C3C	4.13	1.48	1.35
3	A	606	HEC	CAC-C3C	4.13	1.48	1.35
3	W	605	HEC	CAC-C3C	4.13	1.48	1.35
3	X	606	HEC	CAC-C3C	4.13	1.48	1.35
3	W	603	HEC	CAB-C3B	4.13	1.48	1.35
3	X	604	HEC	CAC-C3C	4.13	1.48	1.35
3	K	606	HEC	CAC-C3C	4.13	1.48	1.35
3	W	603	HEC	C4B-NB	4.13	1.47	1.39
3	I	600	HEC	CAC-C3C	4.13	1.48	1.35
3	U	607	HEC	CAC-C3C	4.12	1.48	1.35
3	I	603	HEC	CHC-C1C	4.12	1.48	1.39
3	N	605	HEC	CAC-C3C	4.12	1.48	1.35
3	V	603	HEC	CHC-C1C	4.12	1.48	1.39
3	B	604	HEC	CAC-C3C	4.12	1.48	1.35
3	X	602	HEC	CAC-C3C	4.12	1.48	1.35
3	N	603	HEC	CHC-C1C	4.12	1.48	1.39
3	H	606	HEC	CAC-C3C	4.12	1.48	1.35
3	V	603	HEC	C4B-NB	4.12	1.47	1.39
3	L	605	HEC	CAC-C3C	4.12	1.48	1.35
3	R	605	HEC	CAB-C3B	4.12	1.48	1.35
3	D	607	HEC	CAC-C3C	4.11	1.48	1.35
3	F	605	HEC	CAC-C3C	4.11	1.48	1.35
3	Q	604	HEC	CAC-C3C	4.11	1.48	1.35
3	X	605	HEC	CAC-C3C	4.11	1.48	1.35
3	U	607	HEC	CAB-C3B	4.11	1.48	1.35
3	V	605	HEC	CAB-C3B	4.10	1.48	1.35
3	N	607	HEC	CAC-C3C	4.10	1.48	1.35
3	O	603	HEC	CHC-C1C	4.10	1.48	1.39
3	D	604	HEC	CAB-C3B	4.10	1.48	1.35
3	F	604	HEC	CAC-C3C	4.10	1.48	1.35
3	M	607	HEC	CAB-C3B	4.10	1.48	1.35
3	Q	601	HEC	CAC-C3C	4.09	1.48	1.35
3	J	607	HEC	CAB-C3B	4.09	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	606	HEC	CAC-C3C	4.09	1.48	1.35
3	A	607	HEC	CAB-C3B	4.09	1.48	1.35
3	M	607	HEC	CAC-C3C	4.09	1.48	1.35
3	O	600	HEC	CAC-C3C	4.09	1.48	1.35
3	W	604	HEC	CAC-C3C	4.08	1.48	1.35
3	S	603	HEC	C4B-NB	4.08	1.47	1.39
3	I	607	HEC	CAB-C3B	4.08	1.48	1.35
3	T	602	HEC	CAC-C3C	4.08	1.48	1.35
3	K	601	HEC	CAB-C3B	4.07	1.48	1.35
3	D	600	HEC	CAB-C3B	4.07	1.48	1.35
3	U	602	HEC	CAB-C3B	4.07	1.48	1.35
3	S	606	HEC	CAC-C3C	4.07	1.48	1.35
3	E	607	HEC	CAC-C3C	4.07	1.48	1.35
3	V	607	HEC	CAB-C3B	4.07	1.48	1.35
3	L	603	HEC	CHC-C1C	4.07	1.48	1.39
3	B	606	HEC	CAC-C3C	4.07	1.48	1.35
3	F	603	HEC	CAB-C3B	4.07	1.48	1.35
3	B	605	HEC	CAC-C3C	4.07	1.48	1.35
3	W	607	HEC	CAB-C3B	4.07	1.48	1.35
3	N	602	HEC	CAC-C3C	4.07	1.48	1.35
3	U	603	HEC	CHC-C1C	4.07	1.48	1.39
3	G	607	HEC	CAB-C3B	4.06	1.48	1.35
3	J	603	HEC	CAB-C3B	4.06	1.48	1.35
3	V	604	HEC	CAB-C3B	4.06	1.48	1.35
3	I	601	HEC	CAC-C3C	4.06	1.48	1.35
3	F	606	HEC	CAC-C3C	4.06	1.48	1.35
3	C	603	HEC	CAB-C3B	4.06	1.48	1.35
3	D	607	HEC	CAB-C3B	4.06	1.48	1.35
3	K	604	HEC	CAB-C3B	4.06	1.48	1.35
3	A	607	HEC	CAC-C3C	4.05	1.48	1.35
3	T	605	HEC	CAB-C3B	4.05	1.48	1.35
3	R	607	HEC	CAB-C3B	4.05	1.48	1.35
3	X	605	HEC	CAB-C3B	4.05	1.48	1.35
3	D	602	HEC	CAB-C3B	4.05	1.48	1.35
3	M	602	HEC	CAB-C3B	4.05	1.48	1.35
3	P	607	HEC	CAC-C3C	4.04	1.48	1.35
3	T	604	HEC	CAC-C3C	4.04	1.48	1.35
3	E	603	HEC	CAB-C3B	4.04	1.48	1.35
3	D	603	HEC	C4B-NB	4.04	1.47	1.39
3	R	603	HEC	C4B-NB	4.04	1.47	1.39
3	A	603	HEC	CHC-C1C	4.04	1.48	1.39
3	Q	604	HEC	CAB-C3B	4.04	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	604	HEC	CAB-C3B	4.03	1.48	1.35
3	J	604	HEC	CAC-C3C	4.03	1.48	1.35
3	G	600	HEC	CAB-C3B	4.03	1.48	1.35
3	H	605	HEC	CAB-C3B	4.02	1.48	1.35
3	N	606	HEC	CAC-C3C	4.02	1.48	1.35
3	S	605	HEC	CAB-C3B	4.02	1.48	1.35
3	X	607	HEC	CAB-C3B	4.02	1.48	1.35
3	R	603	HEC	CAB-C3B	4.02	1.48	1.35
3	T	604	HEC	CAB-C3B	4.02	1.48	1.35
3	Q	602	HEC	CAB-C3B	4.02	1.48	1.35
3	S	604	HEC	CAC-C3C	4.02	1.48	1.35
3	P	603	HEC	CAB-C3B	4.02	1.48	1.35
3	I	600	HEC	CAB-C3B	4.02	1.48	1.35
3	L	603	HEC	C4B-NB	4.02	1.47	1.39
3	E	606	HEC	CAC-C3C	4.01	1.48	1.35
3	S	607	HEC	CAB-C3B	4.01	1.48	1.35
3	G	603	HEC	C4B-NB	4.01	1.47	1.39
3	O	604	HEC	CAC-C3C	4.01	1.48	1.35
3	P	605	HEC	CAC-C3C	4.01	1.48	1.35
3	X	600	HEC	CAB-C3B	4.01	1.48	1.35
3	U	605	HEC	CAC-C3C	4.01	1.48	1.35
3	L	605	HEC	CAB-C3B	4.01	1.48	1.35
3	Q	606	HEC	CAB-C3B	4.01	1.48	1.35
3	B	605	HEC	CAB-C3B	4.01	1.48	1.35
3	H	603	HEC	CHC-C1C	4.00	1.48	1.39
3	G	600	HEC	CAC-C3C	4.00	1.48	1.35
3	K	603	HEC	CAB-C3B	4.00	1.48	1.35
3	X	602	HEC	CAB-C3B	4.00	1.48	1.35
3	J	600	HEC	CAB-C3B	4.00	1.48	1.35
3	P	607	HEC	CAB-C3B	4.00	1.48	1.35
3	V	602	HEC	CAB-C3B	4.00	1.48	1.35
3	O	600	HEC	CAB-C3B	4.00	1.48	1.35
3	P	603	HEC	CHC-C1C	3.99	1.48	1.39
3	F	604	HEC	CAB-C3B	3.99	1.48	1.35
3	E	605	HEC	CAC-C3C	3.99	1.47	1.35
3	O	607	HEC	CAB-C3B	3.99	1.47	1.35
3	T	607	HEC	CAB-C3B	3.99	1.47	1.35
3	C	603	HEC	CHC-C1C	3.99	1.48	1.39
3	I	603	HEC	C3C-C4C	3.99	1.53	1.46
3	E	605	HEC	CAB-C3B	3.98	1.47	1.35
3	V	600	HEC	CAB-C3B	3.98	1.47	1.35
3	G	602	HEC	CAB-C3B	3.98	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	603	HEC	C1C-NC	-3.98	1.32	1.39
3	G	603	HEC	CAB-C3B	3.98	1.47	1.35
3	N	607	HEC	CAB-C3B	3.98	1.47	1.35
3	H	603	HEC	CAB-C3B	3.98	1.47	1.35
3	N	603	HEC	CAB-C3B	3.98	1.47	1.35
3	R	600	HEC	CAB-C3B	3.98	1.47	1.35
3	N	600	HEC	CAB-C3B	3.98	1.47	1.35
3	N	603	HEC	C4B-NB	3.98	1.47	1.39
3	E	600	HEC	CAB-C3B	3.98	1.47	1.35
3	T	606	HEC	CAB-C3B	3.98	1.47	1.35
3	M	603	HEC	C4B-NB	3.97	1.47	1.39
3	C	605	HEC	CAC-C3C	3.97	1.47	1.35
3	U	604	HEC	CAB-C3B	3.97	1.47	1.35
3	V	604	HEC	CAC-C3C	3.97	1.47	1.35
3	P	604	HEC	CAC-C3C	3.97	1.47	1.35
3	P	603	HEC	C3C-C4C	3.97	1.52	1.46
3	Q	607	HEC	CAB-C3B	3.96	1.47	1.35
3	L	604	HEC	CAC-C3C	3.96	1.47	1.35
3	I	604	HEC	CAC-C3C	3.96	1.47	1.35
3	E	607	HEC	CAB-C3B	3.96	1.47	1.35
3	I	601	HEC	CAB-C3B	3.96	1.47	1.35
3	O	604	HEC	CAB-C3B	3.96	1.47	1.35
3	A	603	HEC	C4B-NB	3.96	1.47	1.39
3	U	603	HEC	C3C-C4C	3.96	1.52	1.46
3	J	604	HEC	CAB-C3B	3.95	1.47	1.35
3	H	605	HEC	CAC-C3C	3.95	1.47	1.35
3	K	604	HEC	CAC-C3C	3.95	1.47	1.35
3	A	604	HEC	CAB-C3B	3.95	1.47	1.35
3	B	601	HEC	CAB-C3B	3.95	1.47	1.35
3	S	602	HEC	CAB-C3B	3.95	1.47	1.35
3	A	602	HEC	CAB-C3B	3.95	1.47	1.35
3	S	600	HEC	CAB-C3B	3.95	1.47	1.35
3	H	607	HEC	CAB-C3B	3.95	1.47	1.35
3	C	604	HEC	CAC-C3C	3.95	1.47	1.35
3	B	604	HEC	CAB-C3B	3.94	1.47	1.35
3	H	601	HEC	CAB-C3B	3.94	1.47	1.35
3	B	600	HEC	CAB-C3B	3.93	1.47	1.35
3	W	602	HEC	CAB-C3B	3.93	1.47	1.35
3	W	606	HEC	CAB-C3B	3.93	1.47	1.35
3	V	601	HEC	CAB-C3B	3.93	1.47	1.35
3	A	604	HEC	CAC-C3C	3.93	1.47	1.35
3	T	602	HEC	CAB-C3B	3.93	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	604	HEC	CAB-C3B	3.93	1.47	1.35
3	H	604	HEC	CAB-C3B	3.93	1.47	1.35
3	B	607	HEC	CAB-C3B	3.93	1.47	1.35
3	W	600	HEC	CAB-C3B	3.93	1.47	1.35
3	G	604	HEC	CAC-C3C	3.93	1.47	1.35
3	F	602	HEC	CAB-C3B	3.93	1.47	1.35
3	P	600	HEC	CAB-C3B	3.93	1.47	1.35
3	D	604	HEC	CAC-C3C	3.92	1.47	1.35
3	N	606	HEC	CAB-C3B	3.92	1.47	1.35
3	V	603	HEC	CAB-C3B	3.92	1.47	1.35
3	L	600	HEC	CAB-C3B	3.92	1.47	1.35
3	I	602	HEC	CAB-C3B	3.92	1.47	1.35
3	K	603	HEC	C4B-NB	3.91	1.47	1.39
3	U	603	HEC	C4B-NB	3.91	1.47	1.39
3	S	606	HEC	CAB-C3B	3.91	1.47	1.35
3	S	603	HEC	C3C-C4C	3.91	1.52	1.46
3	T	600	HEC	CAB-C3B	3.91	1.47	1.35
3	O	603	HEC	C1C-NC	-3.90	1.32	1.39
3	A	606	HEC	CAB-C3B	3.90	1.47	1.35
3	U	601	HEC	CAB-C3B	3.90	1.47	1.35
3	K	605	HEC	CAB-C3B	3.90	1.47	1.35
3	L	603	HEC	C3C-C4C	3.90	1.52	1.46
3	N	604	HEC	CAC-C3C	3.90	1.47	1.35
3	E	604	HEC	CAB-C3B	3.90	1.47	1.35
3	D	605	HEC	CAB-C3B	3.90	1.47	1.35
3	W	603	HEC	C3C-C4C	3.89	1.52	1.46
3	N	602	HEC	CAB-C3B	3.89	1.47	1.35
3	U	606	HEC	CAB-C3B	3.89	1.47	1.35
3	C	607	HEC	CAB-C3B	3.89	1.47	1.35
3	K	605	HEC	CAC-C3C	3.89	1.47	1.35
3	P	604	HEC	CAB-C3B	3.88	1.47	1.35
3	K	607	HEC	CAB-C3B	3.88	1.47	1.35
3	D	601	HEC	CAB-C3B	3.88	1.47	1.35
3	E	601	HEC	CAB-C3B	3.88	1.47	1.35
3	C	603	HEC	C1C-NC	-3.87	1.32	1.39
3	C	601	HEC	CAB-C3B	3.87	1.47	1.35
3	E	603	HEC	C4B-NB	3.87	1.46	1.39
3	P	602	HEC	CAB-C3B	3.87	1.47	1.35
3	L	604	HEC	CAB-C3B	3.87	1.47	1.35
3	I	603	HEC	C4B-NB	3.87	1.46	1.39
3	W	601	HEC	CAB-C3B	3.86	1.47	1.35
3	X	601	HEC	CAB-C3B	3.86	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	606	HEC	CAB-C3B	3.86	1.47	1.35
3	K	606	HEC	CAB-C3B	3.86	1.47	1.35
3	Q	600	HEC	CAB-C3B	3.86	1.47	1.35
3	M	604	HEC	CAB-C3B	3.86	1.47	1.35
3	P	601	HEC	CAB-C3B	3.85	1.47	1.35
3	H	607	HEC	CAC-C3C	3.85	1.47	1.35
3	L	607	HEC	CAB-C3B	3.84	1.47	1.35
3	C	600	HEC	CAB-C3B	3.84	1.47	1.35
3	W	604	HEC	CAB-C3B	3.84	1.47	1.35
3	J	601	HEC	CAB-C3B	3.84	1.47	1.35
3	N	604	HEC	CAB-C3B	3.84	1.47	1.35
3	E	604	HEC	CAC-C3C	3.83	1.47	1.35
3	N	601	HEC	CAB-C3B	3.83	1.47	1.35
3	A	600	HEC	CAB-C3B	3.83	1.47	1.35
3	C	602	HEC	CAB-C3B	3.83	1.47	1.35
3	A	603	HEC	C3C-C4C	3.83	1.52	1.46
3	P	606	HEC	CAB-C3B	3.83	1.47	1.35
3	X	603	HEC	C3C-C4C	3.83	1.52	1.46
3	X	606	HEC	CAB-C3B	3.83	1.47	1.35
3	L	601	HEC	CAB-C3B	3.82	1.47	1.35
3	L	603	HEC	CAB-C3B	3.82	1.47	1.35
3	I	606	HEC	CAB-C3B	3.82	1.47	1.35
3	F	601	HEC	CAB-C3B	3.81	1.47	1.35
3	M	600	HEC	CAB-C3B	3.81	1.47	1.35
3	C	606	HEC	CAB-C3B	3.81	1.47	1.35
3	H	600	HEC	CAB-C3B	3.80	1.47	1.35
3	O	601	HEC	CAB-C3B	3.80	1.47	1.35
3	H	603	HEC	C3C-C4C	3.80	1.52	1.46
3	G	604	HEC	CAB-C3B	3.80	1.47	1.35
3	M	606	HEC	CAB-C3B	3.80	1.47	1.35
3	V	606	HEC	CAB-C3B	3.80	1.47	1.35
3	K	602	HEC	CAB-C3B	3.80	1.47	1.35
3	C	603	HEC	C3C-C4C	3.80	1.52	1.46
3	E	602	HEC	CAB-C3B	3.80	1.47	1.35
3	R	602	HEC	CAB-C3B	3.79	1.47	1.35
3	G	601	HEC	CAB-C3B	3.79	1.47	1.35
3	F	600	HEC	CAB-C3B	3.79	1.47	1.35
3	K	600	HEC	CAB-C3B	3.79	1.47	1.35
3	B	602	HEC	CAB-C3B	3.78	1.47	1.35
3	I	604	HEC	CAB-C3B	3.78	1.47	1.35
3	N	603	HEC	C3C-C4C	3.78	1.52	1.46
3	Q	601	HEC	CAB-C3B	3.78	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	602	HEC	CAB-C3B	3.77	1.47	1.35
3	N	603	HEC	C1C-NC	-3.77	1.32	1.39
3	H	603	HEC	C4B-NB	3.76	1.46	1.39
3	E	603	HEC	C1C-NC	-3.75	1.32	1.39
3	E	603	HEC	C3C-C4C	3.75	1.52	1.46
3	O	602	HEC	CAB-C3B	3.75	1.47	1.35
3	C	604	HEC	CAB-C3B	3.74	1.47	1.35
3	T	601	HEC	CAB-C3B	3.73	1.47	1.35
3	O	606	HEC	CAB-C3B	3.72	1.47	1.35
3	S	601	HEC	CAB-C3B	3.72	1.47	1.35
3	R	601	HEC	CAB-C3B	3.72	1.47	1.35
3	J	602	HEC	CAB-C3B	3.71	1.47	1.35
3	Q	603	HEC	C3C-C4C	3.70	1.52	1.46
3	H	602	HEC	CAB-C3B	3.70	1.47	1.35
3	A	603	HEC	C1C-NC	-3.69	1.32	1.39
3	B	606	HEC	CAB-C3B	3.69	1.47	1.35
3	J	606	HEC	CAB-C3B	3.69	1.47	1.35
3	R	606	HEC	CAB-C3B	3.68	1.47	1.35
3	E	606	HEC	CAB-C3B	3.68	1.46	1.35
3	B	603	HEC	C1C-NC	-3.67	1.32	1.39
3	D	606	HEC	CAB-C3B	3.67	1.46	1.35
3	T	603	HEC	C1C-NC	-3.66	1.32	1.39
3	R	603	HEC	C3C-C4C	3.66	1.52	1.46
3	B	603	HEC	C3C-C4C	3.66	1.52	1.46
3	M	601	HEC	CAB-C3B	3.66	1.46	1.35
3	U	603	HEC	C1C-NC	-3.65	1.32	1.39
3	V	603	HEC	C3C-C4C	3.65	1.52	1.46
3	M	603	HEC	C3C-C4C	3.64	1.52	1.46
3	T	603	HEC	C3C-C4C	3.64	1.52	1.46
3	A	601	HEC	CAB-C3B	3.64	1.46	1.35
3	L	606	HEC	CAB-C3B	3.64	1.46	1.35
3	P	603	HEC	C4B-NB	3.63	1.46	1.39
3	G	603	HEC	C3C-C4C	3.63	1.52	1.46
3	D	603	HEC	C3C-C4C	3.62	1.52	1.46
3	C	603	HEC	C4B-NB	3.62	1.46	1.39
3	G	603	HEC	C1C-NC	-3.62	1.32	1.39
3	R	603	HEC	C1C-NC	-3.61	1.32	1.39
3	V	603	HEC	C1C-NC	-3.60	1.32	1.39
3	J	603	HEC	C3C-C4C	3.60	1.52	1.46
3	L	603	HEC	C1C-NC	-3.60	1.32	1.39
3	Q	603	HEC	C1C-NC	-3.59	1.32	1.39
3	F	606	HEC	CAB-C3B	3.59	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	603	HEC	C1C-NC	-3.58	1.32	1.39
3	S	603	HEC	C1C-NC	-3.58	1.32	1.39
3	S	603	HEC	CBD-CGD	3.58	1.58	1.50
3	P	603	HEC	C1C-NC	-3.57	1.32	1.39
3	K	603	HEC	C1C-NC	-3.57	1.32	1.39
3	F	603	HEC	C1C-NC	-3.56	1.32	1.39
3	D	603	HEC	C1C-NC	-3.54	1.32	1.39
3	G	603	HEC	CBD-CGD	3.54	1.58	1.50
3	A	603	HEC	CBD-CGD	3.53	1.58	1.50
3	O	603	HEC	C3C-C4C	3.52	1.52	1.46
3	R	603	HEC	CBD-CGD	3.51	1.58	1.50
3	H	606	HEC	CAB-C3B	3.51	1.46	1.35
3	W	603	HEC	C1C-NC	-3.49	1.33	1.39
3	X	603	HEC	C1C-NC	-3.49	1.33	1.39
3	X	603	HEC	CBD-CGD	3.46	1.58	1.50
3	J	603	HEC	C1C-NC	-3.45	1.33	1.39
3	U	603	HEC	CBD-CGD	3.44	1.58	1.50
3	I	603	HEC	C1C-NC	-3.44	1.33	1.39
3	F	603	HEC	C3C-C4C	3.42	1.52	1.46
3	V	603	HEC	CBD-CGD	3.41	1.58	1.50
3	O	603	HEC	CBD-CGD	3.39	1.58	1.50
3	P	603	HEC	CBD-CGD	3.39	1.58	1.50
3	C	603	HEC	CBD-CGD	3.38	1.58	1.50
3	M	603	HEC	CBD-CGD	3.38	1.58	1.50
3	H	603	HEC	CBD-CGD	3.37	1.58	1.50
3	K	603	HEC	CBD-CGD	3.37	1.58	1.50
3	F	603	HEC	CBD-CGD	3.37	1.58	1.50
3	D	603	HEC	CBD-CGD	3.35	1.58	1.50
3	T	603	HEC	CBD-CGD	3.34	1.58	1.50
3	N	603	HEC	CBD-CGD	3.29	1.58	1.50
3	W	603	HEC	CBD-CGD	3.27	1.58	1.50
3	I	603	HEC	CBD-CGD	3.25	1.58	1.50
3	E	603	HEC	CBD-CGD	3.25	1.58	1.50
3	E	602	HEC	C1B-NB	-3.23	1.33	1.39
3	Q	603	HEC	CBD-CGD	3.23	1.58	1.50
3	B	603	HEC	CBD-CGD	3.19	1.58	1.50
3	G	602	HEC	C1B-NB	-3.17	1.33	1.39
3	J	603	HEC	CBD-CGD	3.17	1.57	1.50
3	L	605	HEC	C1B-NB	-3.15	1.33	1.39
3	J	607	HEC	C4B-NB	-3.14	1.33	1.39
3	J	606	HEC	C4B-NB	-3.13	1.33	1.39
3	N	605	HEC	C1B-NB	-3.13	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	605	HEC	C1B-NB	-3.13	1.33	1.39
3	B	601	HEC	C1B-NB	-3.12	1.33	1.39
3	T	601	HEC	C1B-NB	-3.10	1.33	1.39
3	D	606	HEC	C4B-NB	-3.10	1.33	1.39
3	O	605	HEC	C1D-ND	-3.09	1.33	1.39
3	G	606	HEC	C4B-NB	-3.09	1.33	1.39
3	G	606	HEC	C1B-NB	-3.09	1.33	1.39
3	N	602	HEC	C4D-ND	-3.08	1.33	1.39
3	F	601	HEC	C1B-NB	-3.07	1.33	1.39
3	L	603	HEC	CBD-CGD	3.07	1.57	1.50
3	Q	602	HEC	C1B-NB	-3.06	1.33	1.39
3	K	606	HEC	C4B-NB	-3.06	1.33	1.39
3	J	602	HEC	C4D-ND	-3.06	1.33	1.39
3	J	604	HEC	C1B-NB	-3.05	1.33	1.39
3	C	601	HEC	C4B-NB	-3.05	1.33	1.39
3	J	606	HEC	C1B-NB	-3.05	1.33	1.39
3	C	601	HEC	C1B-NB	-3.04	1.33	1.39
3	I	606	HEC	C1B-NB	-3.04	1.33	1.39
3	I	604	HEC	C4B-NB	-3.03	1.33	1.39
3	D	602	HEC	C1B-NB	-3.03	1.33	1.39
3	N	602	HEC	C1B-NB	-3.03	1.33	1.39
3	C	606	HEC	C4B-NB	-3.03	1.33	1.39
3	G	604	HEC	C1B-NB	-3.02	1.33	1.39
3	P	606	HEC	C4B-NB	-3.02	1.33	1.39
3	F	602	HEC	C1B-NB	-3.02	1.33	1.39
3	F	606	HEC	C1B-NB	-3.01	1.33	1.39
3	D	605	HEC	C4B-NB	-3.01	1.34	1.39
3	M	604	HEC	C4B-NB	-3.00	1.34	1.39
3	X	606	HEC	C1B-NB	-3.00	1.34	1.39
3	G	603	HEC	C1C-C2C	2.99	1.50	1.43
3	B	601	HEC	C4B-NB	-2.99	1.34	1.39
3	I	603	HEC	C1C-C2C	2.99	1.50	1.43
3	F	601	HEC	C4B-NB	-2.99	1.34	1.39
3	L	604	HEC	C4B-NB	-2.98	1.34	1.39
3	C	602	HEC	C4B-NB	-2.98	1.34	1.39
3	O	602	HEC	C1B-NB	-2.98	1.34	1.39
3	F	605	HEC	C1B-NB	-2.98	1.34	1.39
3	F	602	HEC	C4B-NB	-2.97	1.34	1.39
3	J	605	HEC	C1B-NB	-2.97	1.34	1.39
3	A	602	HEC	C1B-NB	-2.97	1.34	1.39
3	R	601	HEC	C1B-NB	-2.97	1.34	1.39
3	K	606	HEC	C1B-NB	-2.96	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	606	HEC	C4B-NB	-2.96	1.34	1.39
3	B	604	HEC	C4B-NB	-2.96	1.34	1.39
3	B	606	HEC	C4B-NB	-2.96	1.34	1.39
3	W	603	HEC	C1C-C2C	2.96	1.50	1.43
3	A	602	HEC	C4D-ND	-2.96	1.34	1.39
3	X	606	HEC	C4B-NB	-2.95	1.34	1.39
3	O	601	HEC	C1B-NB	-2.95	1.34	1.39
3	K	602	HEC	C1B-NB	-2.95	1.34	1.39
3	T	601	HEC	C4B-NB	-2.95	1.34	1.39
3	F	606	HEC	C4B-NB	-2.94	1.34	1.39
3	I	601	HEC	C4B-NB	-2.94	1.34	1.39
3	L	606	HEC	C4B-NB	-2.94	1.34	1.39
3	U	602	HEC	C1B-NB	-2.94	1.34	1.39
3	K	607	HEC	C1D-ND	-2.94	1.34	1.39
3	K	606	HEC	C4D-ND	-2.93	1.34	1.39
3	W	606	HEC	C4B-NB	-2.93	1.34	1.39
3	D	601	HEC	C1B-NB	-2.93	1.34	1.39
3	V	602	HEC	C1B-NB	-2.93	1.34	1.39
3	D	601	HEC	C4B-NB	-2.93	1.34	1.39
3	P	604	HEC	C1B-NB	-2.92	1.34	1.39
3	X	602	HEC	C1B-NB	-2.92	1.34	1.39
3	E	600	HEC	C1B-NB	-2.92	1.34	1.39
3	F	606	HEC	C4D-ND	-2.92	1.34	1.39
3	V	606	HEC	C1B-NB	-2.92	1.34	1.39
3	R	604	HEC	C1B-NB	-2.92	1.34	1.39
3	T	602	HEC	C1B-NB	-2.92	1.34	1.39
3	O	601	HEC	C4B-NB	-2.92	1.34	1.39
3	C	602	HEC	C1B-NB	-2.91	1.34	1.39
3	H	602	HEC	C1B-NB	-2.91	1.34	1.39
3	P	605	HEC	C1B-NB	-2.91	1.34	1.39
3	H	600	HEC	C1B-NB	-2.91	1.34	1.39
3	X	600	HEC	C4B-NB	-2.91	1.34	1.39
3	K	607	HEC	C4B-NB	-2.91	1.34	1.39
3	S	605	HEC	C1B-NB	-2.91	1.34	1.39
3	D	604	HEC	C4D-ND	-2.90	1.34	1.39
3	Q	602	HEC	C4B-NB	-2.90	1.34	1.39
3	S	601	HEC	C1B-NB	-2.90	1.34	1.39
3	B	606	HEC	C1B-NB	-2.90	1.34	1.39
3	E	600	HEC	C4B-NB	-2.90	1.34	1.39
3	M	603	HEC	C4A-NA	-2.90	1.34	1.39
3	R	606	HEC	C1B-NB	-2.90	1.34	1.39
3	O	601	HEC	C4D-ND	-2.90	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	607	HEC	C1B-NB	-2.89	1.34	1.39
3	E	601	HEC	C1B-NB	-2.89	1.34	1.39
3	D	604	HEC	C1B-NB	-2.89	1.34	1.39
3	G	600	HEC	C1D-ND	-2.89	1.34	1.39
3	L	605	HEC	C4B-NB	-2.89	1.34	1.39
3	L	602	HEC	C1B-NB	-2.88	1.34	1.39
3	I	605	HEC	C1D-ND	-2.88	1.34	1.39
3	C	606	HEC	C1B-NB	-2.88	1.34	1.39
3	M	602	HEC	C4D-ND	-2.88	1.34	1.39
3	G	605	HEC	C4B-NB	-2.88	1.34	1.39
3	H	606	HEC	C1B-NB	-2.88	1.34	1.39
3	G	607	HEC	C4B-NB	-2.88	1.34	1.39
3	P	603	HEC	C1C-C2C	2.87	1.49	1.43
3	L	605	HEC	C1D-ND	-2.87	1.34	1.39
3	R	607	HEC	C1B-NB	-2.87	1.34	1.39
3	J	601	HEC	C4B-NB	-2.87	1.34	1.39
3	W	602	HEC	C4B-NB	-2.87	1.34	1.39
3	D	605	HEC	C1B-NB	-2.87	1.34	1.39
3	M	600	HEC	C1B-NB	-2.87	1.34	1.39
3	A	603	HEC	C1C-C2C	2.87	1.49	1.43
3	N	600	HEC	C1B-NB	-2.87	1.34	1.39
3	W	604	HEC	C1B-NB	-2.86	1.34	1.39
3	C	603	HEC	C1C-C2C	2.86	1.49	1.43
3	M	601	HEC	C4D-ND	-2.86	1.34	1.39
3	R	607	HEC	C4B-NB	-2.86	1.34	1.39
3	R	606	HEC	C4B-NB	-2.86	1.34	1.39
3	I	602	HEC	C1B-NB	-2.86	1.34	1.39
3	J	605	HEC	C4B-NB	-2.86	1.34	1.39
3	A	602	HEC	C4B-NB	-2.86	1.34	1.39
3	V	606	HEC	C4D-ND	-2.85	1.34	1.39
3	A	606	HEC	C1B-NB	-2.85	1.34	1.39
3	L	606	HEC	C1B-NB	-2.85	1.34	1.39
3	O	607	HEC	C1B-NB	-2.85	1.34	1.39
3	A	606	HEC	C4B-NB	-2.85	1.34	1.39
3	D	602	HEC	C4B-NB	-2.85	1.34	1.39
3	S	602	HEC	C1B-NB	-2.85	1.34	1.39
3	R	604	HEC	C4B-NB	-2.85	1.34	1.39
3	K	604	HEC	C1B-NB	-2.85	1.34	1.39
3	X	603	HEC	C1C-C2C	2.85	1.49	1.43
3	M	606	HEC	C4B-NB	-2.85	1.34	1.39
3	U	604	HEC	C1D-ND	-2.85	1.34	1.39
3	A	601	HEC	C4B-NB	-2.85	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	604	HEC	C1B-NB	-2.85	1.34	1.39
3	C	604	HEC	C4B-NB	-2.85	1.34	1.39
3	E	602	HEC	C4B-NB	-2.84	1.34	1.39
3	S	600	HEC	C1B-NB	-2.84	1.34	1.39
3	C	605	HEC	C1B-NB	-2.84	1.34	1.39
3	C	607	HEC	C4D-ND	-2.84	1.34	1.39
3	H	605	HEC	C1B-NB	-2.84	1.34	1.39
3	K	604	HEC	C4B-NB	-2.84	1.34	1.39
3	X	600	HEC	C1B-NB	-2.84	1.34	1.39
3	H	606	HEC	C4B-NB	-2.84	1.34	1.39
3	M	602	HEC	C4B-NB	-2.84	1.34	1.39
3	S	606	HEC	C1D-ND	-2.84	1.34	1.39
3	A	604	HEC	C4D-ND	-2.84	1.34	1.39
3	I	605	HEC	C1B-NB	-2.84	1.34	1.39
3	M	605	HEC	C1B-NB	-2.83	1.34	1.39
3	N	601	HEC	C4D-ND	-2.83	1.34	1.39
3	L	600	HEC	C1B-NB	-2.83	1.34	1.39
3	U	605	HEC	C1D-ND	-2.83	1.34	1.39
3	U	605	HEC	C1B-NB	-2.83	1.34	1.39
3	U	603	HEC	C1C-C2C	2.83	1.49	1.43
3	S	604	HEC	C1D-ND	-2.83	1.34	1.39
3	G	604	HEC	C4B-NB	-2.83	1.34	1.39
3	Q	604	HEC	C1B-NB	-2.83	1.34	1.39
3	K	600	HEC	C1B-NB	-2.83	1.34	1.39
3	J	603	HEC	C1C-C2C	2.83	1.49	1.43
3	G	602	HEC	C4B-NB	-2.82	1.34	1.39
3	O	602	HEC	C4B-NB	-2.82	1.34	1.39
3	T	606	HEC	C1B-NB	-2.82	1.34	1.39
3	B	607	HEC	C1D-ND	-2.82	1.34	1.39
3	Q	601	HEC	C1D-ND	-2.82	1.34	1.39
3	O	604	HEC	C4B-NB	-2.82	1.34	1.39
3	F	600	HEC	C1B-NB	-2.82	1.34	1.39
3	M	604	HEC	C1B-NB	-2.82	1.34	1.39
3	J	602	HEC	C4B-NB	-2.82	1.34	1.39
3	K	601	HEC	C1D-ND	-2.82	1.34	1.39
3	J	604	HEC	C4B-NB	-2.82	1.34	1.39
3	G	607	HEC	C1B-NB	-2.81	1.34	1.39
3	C	604	HEC	C4D-ND	-2.81	1.34	1.39
3	M	602	HEC	C1B-NB	-2.81	1.34	1.39
3	V	604	HEC	C1B-NB	-2.81	1.34	1.39
3	G	607	HEC	C4D-ND	-2.81	1.34	1.39
3	P	602	HEC	C4B-NB	-2.81	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	605	HEC	C1B-NB	-2.81	1.34	1.39
3	J	601	HEC	C1B-NB	-2.81	1.34	1.39
3	H	605	HEC	C1D-ND	-2.81	1.34	1.39
3	O	604	HEC	C1B-NB	-2.81	1.34	1.39
3	V	601	HEC	C1B-NB	-2.81	1.34	1.39
3	Q	606	HEC	C4B-NB	-2.80	1.34	1.39
3	A	605	HEC	C1D-ND	-2.80	1.34	1.39
3	M	606	HEC	C1B-NB	-2.80	1.34	1.39
3	R	603	HEC	C1C-C2C	2.80	1.49	1.43
3	S	606	HEC	C1B-NB	-2.80	1.34	1.39
3	F	604	HEC	C1B-NB	-2.80	1.34	1.39
3	E	604	HEC	C4B-NB	-2.80	1.34	1.39
3	J	602	HEC	C1D-ND	-2.80	1.34	1.39
3	Q	605	HEC	C1B-NB	-2.80	1.34	1.39
3	M	605	HEC	C4B-NB	-2.80	1.34	1.39
3	Q	603	HEC	C1C-C2C	2.80	1.49	1.43
3	R	601	HEC	C4B-NB	-2.80	1.34	1.39
3	C	600	HEC	C4B-NB	-2.79	1.34	1.39
3	S	604	HEC	C1B-NB	-2.79	1.34	1.39
3	S	600	HEC	C1D-ND	-2.79	1.34	1.39
3	F	603	HEC	C1C-C2C	2.79	1.49	1.43
3	E	607	HEC	C4B-NB	-2.79	1.34	1.39
3	H	602	HEC	C4B-NB	-2.79	1.34	1.39
3	S	602	HEC	C1D-ND	-2.79	1.34	1.39
3	J	605	HEC	C1D-ND	-2.79	1.34	1.39
3	U	601	HEC	C1B-NB	-2.79	1.34	1.39
3	K	605	HEC	C4B-NB	-2.79	1.34	1.39
3	P	604	HEC	C4B-NB	-2.79	1.34	1.39
3	M	603	HEC	C1C-C2C	2.78	1.49	1.43
3	N	602	HEC	C4B-NB	-2.78	1.34	1.39
3	I	602	HEC	C4D-ND	-2.78	1.34	1.39
3	V	606	HEC	C4B-NB	-2.78	1.34	1.39
3	U	606	HEC	C4B-NB	-2.78	1.34	1.39
3	K	601	HEC	C4B-NB	-2.78	1.34	1.39
3	V	605	HEC	C1B-NB	-2.78	1.34	1.39
3	O	607	HEC	C4B-NB	-2.78	1.34	1.39
3	W	602	HEC	C1B-NB	-2.78	1.34	1.39
3	A	607	HEC	C1D-ND	-2.78	1.34	1.39
3	D	600	HEC	C1D-ND	-2.78	1.34	1.39
3	L	601	HEC	C4B-NB	-2.78	1.34	1.39
3	M	607	HEC	C4B-NB	-2.77	1.34	1.39
3	O	606	HEC	C4D-ND	-2.77	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	605	HEC	C1B-NB	-2.77	1.34	1.39
3	I	602	HEC	C1D-ND	-2.77	1.34	1.39
3	S	603	HEC	C1C-C2C	2.77	1.49	1.43
3	E	605	HEC	C1D-ND	-2.77	1.34	1.39
3	N	607	HEC	C1D-ND	-2.77	1.34	1.39
3	U	606	HEC	C1B-NB	-2.77	1.34	1.39
3	W	606	HEC	C1D-ND	-2.77	1.34	1.39
3	J	602	HEC	C1B-NB	-2.77	1.34	1.39
3	E	600	HEC	C1D-ND	-2.77	1.34	1.39
3	N	605	HEC	C4D-ND	-2.77	1.34	1.39
3	J	600	HEC	C4B-NB	-2.77	1.34	1.39
3	C	600	HEC	C1B-NB	-2.76	1.34	1.39
3	I	606	HEC	C4B-NB	-2.76	1.34	1.39
3	T	602	HEC	C4D-ND	-2.76	1.34	1.39
3	S	607	HEC	C4B-NB	-2.76	1.34	1.39
3	B	604	HEC	C1B-NB	-2.76	1.34	1.39
3	B	602	HEC	C1B-NB	-2.76	1.34	1.39
3	D	604	HEC	C4B-NB	-2.76	1.34	1.39
3	X	604	HEC	C1B-NB	-2.76	1.34	1.39
3	L	603	HEC	C1C-C2C	2.76	1.49	1.43
3	K	603	HEC	C1C-C2C	2.76	1.49	1.43
3	W	605	HEC	C1D-ND	-2.76	1.34	1.39
3	Q	604	HEC	C4B-NB	-2.76	1.34	1.39
3	U	604	HEC	C4B-NB	-2.76	1.34	1.39
3	H	603	HEC	C1C-C2C	2.75	1.49	1.43
3	R	600	HEC	C1B-NB	-2.75	1.34	1.39
3	E	605	HEC	C4B-NB	-2.75	1.34	1.39
3	T	602	HEC	C4B-NB	-2.75	1.34	1.39
3	V	600	HEC	C1B-NB	-2.75	1.34	1.39
3	D	606	HEC	C4D-ND	-2.75	1.34	1.39
3	K	602	HEC	C4D-ND	-2.75	1.34	1.39
3	K	605	HEC	C1B-NB	-2.75	1.34	1.39
3	P	600	HEC	C1B-NB	-2.75	1.34	1.39
3	E	603	HEC	C1C-C2C	2.75	1.49	1.43
3	P	606	HEC	C1B-NB	-2.75	1.34	1.39
3	L	607	HEC	C1D-ND	-2.75	1.34	1.39
3	B	600	HEC	C4B-NB	-2.75	1.34	1.39
3	R	600	HEC	C4B-NB	-2.75	1.34	1.39
3	D	607	HEC	C4B-NB	-2.75	1.34	1.39
3	L	602	HEC	C4B-NB	-2.75	1.34	1.39
3	O	605	HEC	C1B-NB	-2.75	1.34	1.39
3	N	601	HEC	C4B-NB	-2.74	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	606	HEC	C1B-NB	-2.74	1.34	1.39
3	U	606	HEC	C4D-ND	-2.74	1.34	1.39
3	M	607	HEC	C1B-NB	-2.74	1.34	1.39
3	B	605	HEC	C1B-NB	-2.74	1.34	1.39
3	H	601	HEC	C1B-NB	-2.74	1.34	1.39
3	W	606	HEC	C1B-NB	-2.74	1.34	1.39
3	L	607	HEC	C4B-NB	-2.74	1.34	1.39
3	T	606	HEC	C4D-ND	-2.74	1.34	1.39
3	J	607	HEC	C1B-NB	-2.74	1.34	1.39
3	U	604	HEC	C1B-NB	-2.73	1.34	1.39
3	T	603	HEC	C1C-C2C	2.73	1.49	1.43
3	Q	600	HEC	C1D-ND	-2.73	1.34	1.39
3	W	607	HEC	C4D-ND	-2.73	1.34	1.39
3	V	603	HEC	C1C-C2C	2.73	1.49	1.43
3	U	607	HEC	C4D-ND	-2.73	1.34	1.39
3	W	601	HEC	C4D-ND	-2.73	1.34	1.39
3	N	600	HEC	C1D-ND	-2.73	1.34	1.39
3	P	607	HEC	C4D-ND	-2.72	1.34	1.39
3	V	601	HEC	C4B-NB	-2.72	1.34	1.39
3	A	604	HEC	C1B-NB	-2.72	1.34	1.39
3	V	602	HEC	C4B-NB	-2.72	1.34	1.39
3	H	607	HEC	C1B-NB	-2.72	1.34	1.39
3	U	602	HEC	C4D-ND	-2.72	1.34	1.39
3	V	604	HEC	C1D-ND	-2.72	1.34	1.39
3	A	605	HEC	C1B-NB	-2.72	1.34	1.39
3	E	605	HEC	C1B-NB	-2.72	1.34	1.39
3	O	603	HEC	C4A-NA	-2.72	1.34	1.39
3	S	600	HEC	C4D-ND	-2.72	1.34	1.39
3	A	600	HEC	C1B-NB	-2.72	1.34	1.39
3	W	604	HEC	C1D-ND	-2.72	1.34	1.39
3	I	606	HEC	C1D-ND	-2.72	1.34	1.39
3	M	604	HEC	C1D-ND	-2.72	1.34	1.39
3	R	602	HEC	C1B-NB	-2.71	1.34	1.39
3	L	604	HEC	C1B-NB	-2.71	1.34	1.39
3	T	605	HEC	C1B-NB	-2.71	1.34	1.39
3	M	602	HEC	C1D-ND	-2.71	1.34	1.39
3	Q	605	HEC	C1D-ND	-2.71	1.34	1.39
3	T	600	HEC	C1D-ND	-2.71	1.34	1.39
3	F	600	HEC	C4B-NB	-2.71	1.34	1.39
3	N	606	HEC	C1B-NB	-2.71	1.34	1.39
3	O	600	HEC	C4B-NB	-2.71	1.34	1.39
3	X	606	HEC	C4D-ND	-2.71	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	HEC	C4A-NA	-2.71	1.34	1.39
3	J	605	HEC	C4D-ND	-2.71	1.34	1.39
3	B	606	HEC	C4D-ND	-2.71	1.34	1.39
3	I	605	HEC	C4D-ND	-2.71	1.34	1.39
3	M	605	HEC	C4D-ND	-2.71	1.34	1.39
3	R	606	HEC	C4D-ND	-2.71	1.34	1.39
3	H	604	HEC	C1B-NB	-2.71	1.34	1.39
3	P	601	HEC	C4D-ND	-2.71	1.34	1.39
3	V	603	HEC	C4A-NA	-2.70	1.34	1.39
3	M	601	HEC	C1B-NB	-2.70	1.34	1.39
3	V	607	HEC	C1D-ND	-2.70	1.34	1.39
3	I	602	HEC	C4B-NB	-2.70	1.34	1.39
3	I	601	HEC	C1B-NB	-2.70	1.34	1.39
3	N	601	HEC	C1B-NB	-2.70	1.34	1.39
3	A	600	HEC	C4B-NB	-2.70	1.34	1.39
3	Q	601	HEC	C4D-ND	-2.70	1.34	1.39
3	V	607	HEC	C4B-NB	-2.70	1.34	1.39
3	W	600	HEC	C1B-NB	-2.70	1.34	1.39
3	G	600	HEC	C1B-NB	-2.70	1.34	1.39
3	F	606	HEC	C1D-ND	-2.70	1.34	1.39
3	V	600	HEC	C4B-NB	-2.70	1.34	1.39
3	R	607	HEC	C1D-ND	-2.70	1.34	1.39
3	H	602	HEC	C4D-ND	-2.69	1.34	1.39
3	K	602	HEC	C4B-NB	-2.69	1.34	1.39
3	E	604	HEC	C1B-NB	-2.69	1.34	1.39
3	F	604	HEC	C4B-NB	-2.69	1.34	1.39
3	E	607	HEC	C1B-NB	-2.69	1.34	1.39
3	Q	607	HEC	C4B-NB	-2.69	1.34	1.39
3	T	607	HEC	C4D-ND	-2.69	1.34	1.39
3	O	605	HEC	C4B-NB	-2.69	1.34	1.39
3	X	605	HEC	C1D-ND	-2.69	1.34	1.39
3	W	601	HEC	C1B-NB	-2.69	1.34	1.39
3	O	602	HEC	C4D-ND	-2.68	1.34	1.39
3	T	604	HEC	C1B-NB	-2.68	1.34	1.39
3	B	600	HEC	C1B-NB	-2.68	1.34	1.39
3	R	605	HEC	C1D-ND	-2.68	1.34	1.39
3	P	601	HEC	C1B-NB	-2.68	1.34	1.39
3	T	606	HEC	C4B-NB	-2.68	1.34	1.39
3	N	606	HEC	C4B-NB	-2.68	1.34	1.39
3	I	607	HEC	C4B-NB	-2.68	1.34	1.39
3	U	602	HEC	C4B-NB	-2.68	1.34	1.39
3	P	607	HEC	C1B-NB	-2.68	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	601	HEC	C4B-NB	-2.68	1.34	1.39
3	I	601	HEC	C4D-ND	-2.68	1.34	1.39
3	W	605	HEC	C4D-ND	-2.68	1.34	1.39
3	D	603	HEC	C1C-C2C	2.67	1.49	1.43
3	R	602	HEC	C4B-NB	-2.67	1.34	1.39
3	N	603	HEC	C1C-C2C	2.67	1.49	1.43
3	G	600	HEC	C4B-NB	-2.67	1.34	1.39
3	C	604	HEC	C1B-NB	-2.67	1.34	1.39
3	S	606	HEC	C4D-ND	-2.67	1.34	1.39
3	H	607	HEC	C4B-NB	-2.67	1.34	1.39
3	N	606	HEC	C4D-ND	-2.67	1.34	1.39
3	B	600	HEC	C1D-ND	-2.67	1.34	1.39
3	W	601	HEC	C1D-ND	-2.67	1.34	1.39
3	B	603	HEC	C1C-C2C	2.67	1.49	1.43
3	W	607	HEC	C4B-NB	-2.66	1.34	1.39
3	X	602	HEC	C4B-NB	-2.66	1.34	1.39
3	J	600	HEC	C1B-NB	-2.66	1.34	1.39
3	Q	607	HEC	C1B-NB	-2.66	1.34	1.39
3	M	601	HEC	C4B-NB	-2.66	1.34	1.39
3	C	602	HEC	C4D-ND	-2.66	1.34	1.39
3	S	601	HEC	C4D-ND	-2.66	1.34	1.39
3	D	607	HEC	C4D-ND	-2.66	1.34	1.39
3	V	605	HEC	C1D-ND	-2.66	1.34	1.39
3	I	607	HEC	C1B-NB	-2.66	1.34	1.39
3	J	601	HEC	C4D-ND	-2.66	1.34	1.39
3	K	603	HEC	C4A-NA	-2.66	1.34	1.39
3	T	604	HEC	C4B-NB	-2.66	1.34	1.39
3	V	600	HEC	C1D-ND	-2.66	1.34	1.39
3	R	602	HEC	C4D-ND	-2.65	1.34	1.39
3	V	607	HEC	C1B-NB	-2.65	1.34	1.39
3	F	602	HEC	C4D-ND	-2.65	1.34	1.39
3	H	601	HEC	C4D-ND	-2.65	1.34	1.39
3	D	607	HEC	C1D-ND	-2.65	1.34	1.39
3	B	607	HEC	C4D-ND	-2.65	1.34	1.39
3	L	606	HEC	C4D-ND	-2.65	1.34	1.39
3	Q	600	HEC	C1B-NB	-2.65	1.34	1.39
3	E	607	HEC	C4D-ND	-2.65	1.34	1.39
3	A	607	HEC	C4B-NB	-2.65	1.34	1.39
3	D	606	HEC	C1D-ND	-2.65	1.34	1.39
3	W	600	HEC	C1D-ND	-2.65	1.34	1.39
3	I	607	HEC	C1D-ND	-2.65	1.34	1.39
3	Q	606	HEC	C1B-NB	-2.65	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	HEC	C4D-ND	-2.65	1.34	1.39
3	U	600	HEC	C1D-ND	-2.65	1.34	1.39
3	U	605	HEC	C4B-NB	-2.65	1.34	1.39
3	P	601	HEC	C1D-ND	-2.65	1.34	1.39
3	P	601	HEC	C4B-NB	-2.64	1.34	1.39
3	W	607	HEC	C1B-NB	-2.64	1.34	1.39
3	S	602	HEC	C4D-ND	-2.64	1.34	1.39
3	K	601	HEC	C1B-NB	-2.64	1.34	1.39
3	S	601	HEC	C4B-NB	-2.64	1.34	1.39
3	K	600	HEC	C4B-NB	-2.64	1.34	1.39
3	X	602	HEC	C4D-ND	-2.64	1.34	1.39
3	Q	600	HEC	C4B-NB	-2.64	1.34	1.39
3	I	601	HEC	C1D-ND	-2.64	1.34	1.39
3	T	600	HEC	C4B-NB	-2.64	1.34	1.39
3	X	606	HEC	C1D-ND	-2.64	1.34	1.39
3	O	600	HEC	C1B-NB	-2.63	1.34	1.39
3	M	605	HEC	C1D-ND	-2.63	1.34	1.39
3	A	600	HEC	C1D-ND	-2.63	1.34	1.39
3	K	607	HEC	C4D-ND	-2.63	1.34	1.39
3	M	600	HEC	C1D-ND	-2.63	1.34	1.39
3	O	606	HEC	C1B-NB	-2.63	1.34	1.39
3	X	605	HEC	C1B-NB	-2.63	1.34	1.39
3	M	607	HEC	C1D-ND	-2.63	1.34	1.39
3	B	602	HEC	C4D-ND	-2.63	1.34	1.39
3	B	605	HEC	C4B-NB	-2.63	1.34	1.39
3	T	605	HEC	C1D-ND	-2.63	1.34	1.39
3	M	606	HEC	C4D-ND	-2.63	1.34	1.39
3	B	602	HEC	C4B-NB	-2.63	1.34	1.39
3	D	604	HEC	C1D-ND	-2.63	1.34	1.39
3	U	604	HEC	C4D-ND	-2.62	1.34	1.39
3	K	601	HEC	C4D-ND	-2.62	1.34	1.39
3	Q	607	HEC	C1D-ND	-2.62	1.34	1.39
3	N	605	HEC	C1D-ND	-2.62	1.34	1.39
3	P	605	HEC	C1D-ND	-2.62	1.34	1.39
3	X	603	HEC	C4A-NA	-2.62	1.34	1.39
3	H	607	HEC	C4D-ND	-2.62	1.34	1.39
3	T	607	HEC	C1B-NB	-2.62	1.34	1.39
3	L	603	HEC	C4A-NA	-2.62	1.34	1.39
3	X	601	HEC	C1B-NB	-2.62	1.34	1.39
3	G	604	HEC	C1D-ND	-2.62	1.34	1.39
3	P	600	HEC	C1D-ND	-2.62	1.34	1.39
3	J	607	HEC	C4D-ND	-2.62	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	606	HEC	C1D-ND	-2.62	1.34	1.39
3	W	604	HEC	C4B-NB	-2.62	1.34	1.39
3	N	600	HEC	C4B-NB	-2.62	1.34	1.39
3	D	606	HEC	C1B-NB	-2.62	1.34	1.39
3	E	600	HEC	C4D-ND	-2.62	1.34	1.39
3	X	607	HEC	C4D-ND	-2.62	1.34	1.39
3	T	600	HEC	C1B-NB	-2.61	1.34	1.39
3	O	600	HEC	C1D-ND	-2.61	1.34	1.39
3	L	602	HEC	C4D-ND	-2.61	1.34	1.39
3	E	603	HEC	C4A-NA	-2.61	1.34	1.39
3	G	607	HEC	C1D-ND	-2.61	1.34	1.39
3	W	601	HEC	C4B-NB	-2.61	1.34	1.39
3	K	607	HEC	C1B-NB	-2.61	1.34	1.39
3	P	605	HEC	C4B-NB	-2.61	1.34	1.39
3	W	606	HEC	C4D-ND	-2.61	1.34	1.39
3	V	604	HEC	C4D-ND	-2.61	1.34	1.39
3	K	605	HEC	C4D-ND	-2.61	1.34	1.39
3	U	607	HEC	C1B-NB	-2.61	1.34	1.39
3	S	605	HEC	C4D-ND	-2.61	1.34	1.39
3	T	607	HEC	C4B-NB	-2.60	1.34	1.39
3	A	607	HEC	C4D-ND	-2.60	1.34	1.39
3	E	607	HEC	C1D-ND	-2.60	1.34	1.39
3	V	605	HEC	C4B-NB	-2.60	1.34	1.39
3	S	606	HEC	C4B-NB	-2.60	1.34	1.39
3	U	600	HEC	C1B-NB	-2.60	1.34	1.39
3	X	605	HEC	C4D-ND	-2.60	1.34	1.39
3	R	600	HEC	C1D-ND	-2.60	1.34	1.39
3	C	600	HEC	C1D-ND	-2.60	1.34	1.39
3	H	605	HEC	C4B-NB	-2.60	1.34	1.39
3	V	606	HEC	C1D-ND	-2.59	1.34	1.39
3	G	603	HEC	C4A-NA	-2.59	1.34	1.39
3	B	605	HEC	C1D-ND	-2.59	1.34	1.39
3	Q	604	HEC	C1D-ND	-2.59	1.34	1.39
3	V	604	HEC	C4B-NB	-2.59	1.34	1.39
3	W	604	HEC	C4D-ND	-2.59	1.34	1.39
3	G	601	HEC	C4B-NB	-2.59	1.34	1.39
3	W	603	HEC	C4A-NA	-2.59	1.34	1.39
3	C	605	HEC	C4B-NB	-2.59	1.34	1.39
3	P	605	HEC	C4D-ND	-2.59	1.34	1.39
3	X	601	HEC	C4B-NB	-2.59	1.34	1.39
3	J	600	HEC	C1D-ND	-2.59	1.34	1.39
3	K	600	HEC	C1D-ND	-2.59	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	HEC	C1D-ND	-2.58	1.34	1.39
3	I	603	HEC	C4A-NA	-2.58	1.34	1.39
3	N	601	HEC	C1D-ND	-2.58	1.34	1.39
3	K	605	HEC	C1D-ND	-2.58	1.34	1.39
3	Q	605	HEC	C4B-NB	-2.58	1.34	1.39
3	H	607	HEC	C1D-ND	-2.58	1.34	1.39
3	B	601	HEC	C1D-ND	-2.58	1.34	1.39
3	C	605	HEC	C1D-ND	-2.58	1.34	1.39
3	F	605	HEC	C4B-NB	-2.58	1.34	1.39
3	U	601	HEC	C4D-ND	-2.57	1.34	1.39
3	S	607	HEC	C1B-NB	-2.57	1.34	1.39
3	A	602	HEC	C1D-ND	-2.57	1.34	1.39
3	B	601	HEC	C4D-ND	-2.57	1.34	1.39
3	C	607	HEC	C1D-ND	-2.57	1.34	1.39
3	W	607	HEC	C1D-ND	-2.57	1.34	1.39
3	W	602	HEC	C4D-ND	-2.57	1.34	1.39
3	A	605	HEC	C4D-ND	-2.57	1.34	1.39
3	H	605	HEC	C4D-ND	-2.57	1.34	1.39
3	X	604	HEC	C4D-ND	-2.57	1.34	1.39
3	F	607	HEC	C1B-NB	-2.57	1.34	1.39
3	H	606	HEC	C4D-ND	-2.57	1.34	1.39
3	H	604	HEC	C4B-NB	-2.56	1.34	1.39
3	P	606	HEC	C1D-ND	-2.56	1.34	1.39
3	W	600	HEC	C4B-NB	-2.56	1.34	1.39
3	X	601	HEC	C4D-ND	-2.56	1.34	1.39
3	G	601	HEC	C1D-ND	-2.56	1.34	1.39
3	Q	606	HEC	C1D-ND	-2.56	1.34	1.39
3	Q	602	HEC	C4D-ND	-2.56	1.34	1.39
3	D	600	HEC	C4D-ND	-2.56	1.34	1.39
3	C	607	HEC	C1B-NB	-2.56	1.34	1.39
3	V	602	HEC	C4D-ND	-2.55	1.34	1.39
3	V	601	HEC	C4D-ND	-2.55	1.34	1.39
3	X	605	HEC	C4B-NB	-2.55	1.34	1.39
3	N	600	HEC	C4D-ND	-2.55	1.34	1.39
3	P	602	HEC	C4D-ND	-2.55	1.34	1.39
3	S	604	HEC	C4B-NB	-2.55	1.34	1.39
3	N	604	HEC	C1B-NB	-2.55	1.34	1.39
3	T	607	HEC	C1D-ND	-2.55	1.34	1.39
3	C	607	HEC	C4B-NB	-2.55	1.34	1.39
3	H	604	HEC	C1D-ND	-2.55	1.34	1.39
3	I	600	HEC	C1B-NB	-2.55	1.34	1.39
3	F	604	HEC	C1D-ND	-2.54	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	604	HEC	C4B-NB	-2.54	1.34	1.39
3	L	604	HEC	C1D-ND	-2.54	1.34	1.39
3	P	602	HEC	C1B-NB	-2.54	1.34	1.39
3	E	606	HEC	C4B-NB	-2.54	1.34	1.39
3	W	600	HEC	C4D-ND	-2.54	1.34	1.39
3	U	602	HEC	C1D-ND	-2.54	1.34	1.39
3	C	602	HEC	C1D-ND	-2.54	1.34	1.39
3	Q	601	HEC	C1B-NB	-2.54	1.34	1.39
3	S	600	HEC	C4B-NB	-2.54	1.34	1.39
3	T	601	HEC	C1D-ND	-2.54	1.34	1.39
3	A	601	HEC	C1B-NB	-2.54	1.34	1.39
3	N	605	HEC	C4B-NB	-2.54	1.34	1.39
3	T	605	HEC	C4B-NB	-2.54	1.34	1.39
3	O	605	HEC	C4D-ND	-2.54	1.34	1.39
3	X	600	HEC	C1D-ND	-2.54	1.34	1.39
3	L	607	HEC	C1B-NB	-2.54	1.34	1.39
3	N	607	HEC	C4B-NB	-2.54	1.34	1.39
3	F	600	HEC	C1D-ND	-2.53	1.34	1.39
3	R	607	HEC	C4D-ND	-2.53	1.34	1.39
3	E	606	HEC	C4D-ND	-2.53	1.34	1.39
3	Q	604	HEC	C4D-ND	-2.53	1.34	1.39
3	L	606	HEC	C1D-ND	-2.53	1.34	1.39
3	W	602	HEC	C1D-ND	-2.53	1.34	1.39
3	X	607	HEC	C1D-ND	-2.53	1.34	1.39
3	N	607	HEC	C1B-NB	-2.53	1.34	1.39
3	P	602	HEC	C1D-ND	-2.53	1.34	1.39
3	B	604	HEC	C4D-ND	-2.53	1.34	1.39
3	G	601	HEC	C1B-NB	-2.53	1.34	1.39
3	A	604	HEC	C4B-NB	-2.53	1.34	1.39
3	B	605	HEC	C4D-ND	-2.53	1.34	1.39
3	F	607	HEC	C4B-NB	-2.53	1.34	1.39
3	T	604	HEC	C1D-ND	-2.52	1.34	1.39
3	A	606	HEC	C1D-ND	-2.52	1.34	1.39
3	L	600	HEC	C4B-NB	-2.52	1.34	1.39
3	H	601	HEC	C4B-NB	-2.52	1.34	1.39
3	R	604	HEC	C1D-ND	-2.52	1.34	1.39
3	E	601	HEC	C4D-ND	-2.52	1.34	1.39
3	T	604	HEC	C4D-ND	-2.52	1.34	1.39
3	U	605	HEC	C4D-ND	-2.52	1.34	1.39
3	P	604	HEC	C4D-ND	-2.52	1.34	1.39
3	J	603	HEC	C4A-NA	-2.52	1.34	1.39
3	O	604	HEC	C1D-ND	-2.52	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	605	HEC	C1D-ND	-2.52	1.34	1.39
3	I	604	HEC	C1D-ND	-2.52	1.34	1.39
3	E	606	HEC	C1D-ND	-2.51	1.34	1.39
3	F	602	HEC	C1D-ND	-2.51	1.34	1.39
3	J	607	HEC	C1D-ND	-2.51	1.34	1.39
3	F	604	HEC	C4D-ND	-2.51	1.34	1.39
3	X	602	HEC	C1D-ND	-2.51	1.34	1.39
3	O	604	HEC	C4D-ND	-2.51	1.34	1.39
3	S	604	HEC	C4D-ND	-2.51	1.34	1.39
3	Q	605	HEC	C4D-ND	-2.51	1.34	1.39
3	V	601	HEC	C1D-ND	-2.51	1.34	1.39
3	D	602	HEC	C4D-ND	-2.50	1.34	1.39
3	L	601	HEC	C1B-NB	-2.50	1.34	1.39
3	P	607	HEC	C4B-NB	-2.50	1.34	1.39
3	U	606	HEC	C1D-ND	-2.50	1.34	1.39
3	F	605	HEC	C1D-ND	-2.50	1.34	1.39
3	O	603	HEC	C1C-C2C	2.49	1.49	1.43
3	T	605	HEC	C4D-ND	-2.49	1.34	1.39
3	H	606	HEC	C1D-ND	-2.49	1.34	1.39
3	C	604	HEC	C1D-ND	-2.49	1.34	1.39
3	U	607	HEC	C4B-NB	-2.49	1.34	1.39
3	U	600	HEC	C4D-ND	-2.49	1.34	1.39
3	N	604	HEC	C4D-ND	-2.49	1.34	1.39
3	H	600	HEC	C4B-NB	-2.49	1.34	1.39
3	N	602	HEC	C1D-ND	-2.49	1.34	1.39
3	A	601	HEC	C1D-ND	-2.49	1.34	1.39
3	T	601	HEC	C4D-ND	-2.48	1.34	1.39
3	X	604	HEC	C1D-ND	-2.48	1.34	1.39
3	L	601	HEC	C4D-ND	-2.48	1.34	1.39
3	V	607	HEC	C4D-ND	-2.48	1.34	1.39
3	X	607	HEC	C1B-NB	-2.48	1.34	1.39
3	E	601	HEC	C4B-NB	-2.48	1.34	1.39
3	R	605	HEC	C4B-NB	-2.48	1.34	1.39
3	F	601	HEC	C4D-ND	-2.48	1.34	1.39
3	H	604	HEC	C4D-ND	-2.47	1.35	1.39
3	R	606	HEC	C1D-ND	-2.47	1.35	1.39
3	A	605	HEC	C4B-NB	-2.47	1.35	1.39
3	D	602	HEC	C1D-ND	-2.47	1.35	1.39
3	U	600	HEC	C4B-NB	-2.47	1.35	1.39
3	O	607	HEC	C4D-ND	-2.46	1.35	1.39
3	G	606	HEC	C4D-ND	-2.46	1.35	1.39
3	C	606	HEC	C4D-ND	-2.46	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	607	HEC	C4D-ND	-2.46	1.35	1.39
3	F	605	HEC	C4D-ND	-2.46	1.35	1.39
3	B	602	HEC	C1D-ND	-2.46	1.35	1.39
3	A	606	HEC	C4D-ND	-2.46	1.35	1.39
3	S	605	HEC	C4B-NB	-2.45	1.35	1.39
3	B	603	HEC	C4A-NA	-2.45	1.35	1.39
3	E	604	HEC	C4D-ND	-2.45	1.35	1.39
3	F	603	HEC	C4A-NA	-2.45	1.35	1.39
3	S	603	HEC	C4A-NA	-2.45	1.35	1.39
3	S	602	HEC	C4B-NB	-2.45	1.35	1.39
3	A	600	HEC	C4D-ND	-2.45	1.35	1.39
3	D	600	HEC	C4B-NB	-2.45	1.35	1.39
3	S	601	HEC	C1D-ND	-2.45	1.35	1.39
3	Q	606	HEC	C4D-ND	-2.44	1.35	1.39
3	F	600	HEC	C4D-ND	-2.44	1.35	1.39
3	O	601	HEC	C1D-ND	-2.44	1.35	1.39
3	I	604	HEC	C4D-ND	-2.44	1.35	1.39
3	D	605	HEC	C4D-ND	-2.44	1.35	1.39
3	S	607	HEC	C4D-ND	-2.44	1.35	1.39
3	J	600	HEC	C4D-ND	-2.44	1.35	1.39
3	X	601	HEC	C1D-ND	-2.44	1.35	1.39
3	B	607	HEC	C4B-NB	-2.44	1.35	1.39
3	H	602	HEC	C1D-ND	-2.43	1.35	1.39
3	U	601	HEC	C1D-ND	-2.43	1.35	1.39
3	J	606	HEC	C1D-ND	-2.43	1.35	1.39
3	A	607	HEC	C1B-NB	-2.43	1.35	1.39
3	U	607	HEC	C1D-ND	-2.42	1.35	1.39
3	I	600	HEC	C4B-NB	-2.42	1.35	1.39
3	P	604	HEC	C1D-ND	-2.42	1.35	1.39
3	K	606	HEC	C1D-ND	-2.42	1.35	1.39
3	F	607	HEC	C1D-ND	-2.42	1.35	1.39
3	T	602	HEC	C1D-ND	-2.42	1.35	1.39
3	X	607	HEC	C4B-NB	-2.42	1.35	1.39
3	P	600	HEC	C4B-NB	-2.42	1.35	1.39
3	H	600	HEC	C1D-ND	-2.42	1.35	1.39
3	W	605	HEC	C4B-NB	-2.42	1.35	1.39
3	J	606	HEC	C4D-ND	-2.42	1.35	1.39
3	R	605	HEC	C4D-ND	-2.41	1.35	1.39
3	V	602	HEC	C1D-ND	-2.41	1.35	1.39
3	D	605	HEC	C1D-ND	-2.41	1.35	1.39
3	M	604	HEC	C4D-ND	-2.41	1.35	1.39
3	Q	602	HEC	C1D-ND	-2.41	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	604	HEC	C4B-NB	-2.40	1.35	1.39
3	M	600	HEC	C4B-NB	-2.40	1.35	1.39
3	L	600	HEC	C1D-ND	-2.40	1.35	1.39
3	F	607	HEC	C4D-ND	-2.40	1.35	1.39
3	I	605	HEC	C4B-NB	-2.39	1.35	1.39
3	G	602	HEC	C4D-ND	-2.39	1.35	1.39
3	F	601	HEC	C1D-ND	-2.39	1.35	1.39
3	E	604	HEC	C1D-ND	-2.39	1.35	1.39
3	U	601	HEC	C4B-NB	-2.39	1.35	1.39
3	O	602	HEC	C1D-ND	-2.39	1.35	1.39
3	A	604	HEC	C1D-ND	-2.38	1.35	1.39
3	A	603	HEC	C4A-NA	-2.38	1.35	1.39
3	V	605	HEC	C4D-ND	-2.38	1.35	1.39
3	N	606	HEC	C1D-ND	-2.38	1.35	1.39
3	R	600	HEC	C4D-ND	-2.38	1.35	1.39
3	O	607	HEC	C1D-ND	-2.38	1.35	1.39
3	K	604	HEC	C1D-ND	-2.37	1.35	1.39
3	P	603	HEC	C4A-NA	-2.37	1.35	1.39
3	R	601	HEC	C4D-ND	-2.37	1.35	1.39
3	G	601	HEC	C4D-ND	-2.37	1.35	1.39
3	Q	603	HEC	C4A-NA	-2.36	1.35	1.39
3	D	601	HEC	C1D-ND	-2.36	1.35	1.39
3	T	603	HEC	C4A-NA	-2.36	1.35	1.39
3	R	604	HEC	C4D-ND	-2.35	1.35	1.39
3	K	600	HEC	C4D-ND	-2.35	1.35	1.39
3	L	607	HEC	C4D-ND	-2.35	1.35	1.39
3	R	603	HEC	C4A-NA	-2.35	1.35	1.39
3	B	600	HEC	C4D-ND	-2.35	1.35	1.39
3	C	605	HEC	C4D-ND	-2.34	1.35	1.39
3	A	601	HEC	C4D-ND	-2.34	1.35	1.39
3	J	601	HEC	C1D-ND	-2.34	1.35	1.39
3	V	600	HEC	C4D-ND	-2.34	1.35	1.39
3	H	603	HEC	C4A-NA	-2.34	1.35	1.39
3	I	607	HEC	C4D-ND	-2.34	1.35	1.39
3	I	600	HEC	C1D-ND	-2.34	1.35	1.39
3	I	601	HEC	C4A-C3A	-2.33	1.40	1.45
3	E	602	HEC	C1D-ND	-2.33	1.35	1.39
3	D	607	HEC	C1B-NB	-2.33	1.35	1.39
3	T	600	HEC	C4D-ND	-2.33	1.35	1.39
3	C	600	HEC	C4D-ND	-2.33	1.35	1.39
3	K	602	HEC	C1D-ND	-2.33	1.35	1.39
3	G	604	HEC	C4D-ND	-2.32	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	HEC	C1D-C2D	2.32	1.48	1.43
3	D	601	HEC	C4D-ND	-2.32	1.35	1.39
3	S	607	HEC	C1D-ND	-2.32	1.35	1.39
3	A	607	HEC	C1D-C2D	2.32	1.48	1.43
3	L	601	HEC	C1D-ND	-2.32	1.35	1.39
3	P	607	HEC	C1D-ND	-2.32	1.35	1.39
3	X	600	HEC	C4D-ND	-2.32	1.35	1.39
3	C	601	HEC	C1D-ND	-2.32	1.35	1.39
3	M	606	HEC	C4A-C3A	-2.32	1.40	1.45
3	O	606	HEC	C1D-ND	-2.31	1.35	1.39
3	L	605	HEC	C4D-ND	-2.31	1.35	1.39
3	P	605	HEC	C1A-C2A	-2.31	1.41	1.45
3	I	607	HEC	C1A-C2A	-2.31	1.41	1.45
3	C	606	HEC	C1D-ND	-2.31	1.35	1.39
3	U	603	HEC	C4A-NA	-2.30	1.35	1.39
3	D	600	HEC	C1B-NB	-2.30	1.35	1.39
3	G	605	HEC	C4D-ND	-2.30	1.35	1.39
3	B	605	HEC	C1D-C2D	2.30	1.48	1.43
3	O	600	HEC	C4D-ND	-2.30	1.35	1.39
3	P	606	HEC	C4D-ND	-2.30	1.35	1.39
3	Q	600	HEC	C4D-ND	-2.30	1.35	1.39
3	F	607	HEC	C1A-C2A	-2.29	1.41	1.45
3	L	604	HEC	C1A-C2A	-2.29	1.41	1.45
3	N	603	HEC	C4A-NA	-2.29	1.35	1.39
3	M	600	HEC	C4D-ND	-2.29	1.35	1.39
3	N	604	HEC	C1D-ND	-2.29	1.35	1.39
3	C	601	HEC	C4D-ND	-2.28	1.35	1.39
3	G	600	HEC	C4D-ND	-2.28	1.35	1.39
3	H	600	HEC	C4D-ND	-2.28	1.35	1.39
3	E	605	HEC	C4D-ND	-2.28	1.35	1.39
3	M	607	HEC	C4D-ND	-2.27	1.35	1.39
3	K	604	HEC	C4D-ND	-2.27	1.35	1.39
3	L	601	HEC	C1D-C2D	2.27	1.48	1.43
3	G	606	HEC	C1D-C2D	2.27	1.48	1.43
3	E	601	HEC	C4A-C3A	-2.27	1.40	1.45
3	R	604	HEC	C4A-C3A	-2.27	1.40	1.45
3	S	607	HEC	C1D-C2D	2.27	1.48	1.43
3	E	601	HEC	C1D-ND	-2.26	1.35	1.39
3	P	600	HEC	C4D-ND	-2.26	1.35	1.39
3	M	606	HEC	C1D-ND	-2.26	1.35	1.39
3	C	604	HEC	C4A-C3A	-2.25	1.40	1.45
3	E	605	HEC	C1D-C2D	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	604	HEC	C4A-C3A	-2.24	1.40	1.45
3	J	604	HEC	C1D-ND	-2.24	1.35	1.39
3	B	606	HEC	C1D-ND	-2.24	1.35	1.39
3	J	604	HEC	C4D-ND	-2.24	1.35	1.39
3	V	605	HEC	C1D-C2D	2.24	1.48	1.43
3	Q	607	HEC	C4D-ND	-2.24	1.35	1.39
3	H	601	HEC	C1D-ND	-2.23	1.35	1.39
3	G	601	HEC	C1D-C2D	2.23	1.48	1.43
3	C	603	HEC	C4A-NA	-2.23	1.35	1.39
3	E	602	HEC	C1D-C2D	2.22	1.48	1.43
3	P	606	HEC	C1D-C2D	2.22	1.48	1.43
3	I	604	HEC	C4A-C3A	-2.22	1.40	1.45
3	B	601	HEC	C1D-C2D	2.22	1.48	1.43
3	I	606	HEC	C1A-C2A	-2.22	1.41	1.45
3	L	602	HEC	C1A-C2A	-2.22	1.41	1.45
3	L	604	HEC	C4D-ND	-2.22	1.35	1.39
3	L	602	HEC	C1D-C2D	2.22	1.48	1.43
3	R	601	HEC	C1D-ND	-2.22	1.35	1.39
3	O	602	HEC	C1D-C2D	2.21	1.48	1.43
3	R	605	HEC	C1D-C2D	2.21	1.48	1.43
3	L	606	HEC	C1D-C2D	2.21	1.48	1.43
3	R	602	HEC	C1D-ND	-2.21	1.35	1.39
3	A	604	HEC	C3C-C4C	-2.20	1.42	1.46
3	Q	606	HEC	C1D-C2D	2.20	1.48	1.43
3	G	605	HEC	C1D-ND	-2.20	1.35	1.39
3	J	607	HEC	C1D-C2D	2.20	1.48	1.43
3	M	602	HEC	C1D-C2D	2.20	1.48	1.43
3	G	602	HEC	C1D-ND	-2.20	1.35	1.39
3	I	600	HEC	C4D-ND	-2.20	1.35	1.39
3	J	604	HEC	C4A-C3A	-2.19	1.41	1.45
3	H	604	HEC	C4A-C3A	-2.19	1.41	1.45
3	J	606	HEC	C1D-C2D	2.19	1.48	1.43
3	S	604	HEC	C4A-C3A	-2.19	1.41	1.45
3	Q	602	HEC	C1D-C2D	2.19	1.48	1.43
3	M	602	HEC	C4A-C3A	-2.19	1.41	1.45
3	U	602	HEC	C1D-C2D	2.19	1.48	1.43
3	F	605	HEC	C1D-C2D	2.19	1.48	1.43
3	K	606	HEC	C1D-C2D	2.19	1.48	1.43
3	I	607	HEC	C1D-C2D	2.19	1.48	1.43
3	V	602	HEC	C1D-C2D	2.19	1.48	1.43
3	B	606	HEC	C3C-C4C	-2.18	1.42	1.46
3	I	606	HEC	C4D-ND	-2.18	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	606	HEC	C1D-C2D	2.18	1.48	1.43
3	W	602	HEC	C1D-C2D	2.18	1.48	1.43
3	I	601	HEC	C1A-C2A	-2.17	1.41	1.45
3	K	604	HEC	C4A-C3A	-2.17	1.41	1.45
3	W	605	HEC	C1D-C2D	2.17	1.48	1.43
3	D	607	HEC	C1D-C2D	2.17	1.48	1.43
3	N	602	HEC	C1D-C2D	2.17	1.48	1.43
3	D	606	HEC	C1D-C2D	2.16	1.48	1.43
3	A	604	HEC	C4A-C3A	-2.16	1.41	1.45
3	D	602	HEC	C1D-C2D	2.16	1.48	1.43
3	E	606	HEC	C1D-C2D	2.16	1.48	1.43
3	E	604	HEC	C3C-C4C	-2.16	1.42	1.46
3	R	601	HEC	C1D-C2D	2.16	1.48	1.43
3	R	606	HEC	C1A-C2A	-2.16	1.41	1.45
3	X	604	HEC	C4A-C3A	-2.15	1.41	1.45
3	D	600	HEC	C1D-C2D	2.15	1.48	1.43
3	J	607	HEC	C1A-C2A	-2.15	1.41	1.45
3	C	606	HEC	C1D-C2D	2.15	1.48	1.43
3	A	602	HEC	C1D-C2D	2.15	1.48	1.43
3	D	601	HEC	C4A-C3A	-2.14	1.41	1.45
3	H	602	HEC	C1D-C2D	2.14	1.48	1.43
3	I	606	HEC	C1D-C2D	2.14	1.48	1.43
3	L	602	HEC	C1D-ND	-2.14	1.35	1.39
3	R	607	HEC	C1D-C2D	2.14	1.48	1.43
3	N	605	HEC	C1A-C2A	-2.14	1.41	1.45
3	X	604	HEC	C1A-C2A	-2.14	1.41	1.45
3	F	607	HEC	C1D-C2D	2.14	1.48	1.43
3	J	601	HEC	C1D-C2D	2.14	1.48	1.43
3	B	604	HEC	C1D-ND	-2.13	1.35	1.39
3	A	606	HEC	C1D-C2D	2.13	1.48	1.43
3	M	606	HEC	C1D-C2D	2.13	1.48	1.43
3	T	602	HEC	C1D-C2D	2.13	1.48	1.43
3	R	602	HEC	C1D-C2D	2.13	1.48	1.43
3	M	604	HEC	C1D-C2D	2.13	1.48	1.43
3	G	606	HEC	C1D-ND	-2.12	1.35	1.39
3	F	600	HEC	C1A-C2A	-2.12	1.41	1.45
3	F	605	HEC	C1A-C2A	-2.12	1.41	1.45
3	D	602	HEC	C4A-C3A	-2.12	1.41	1.45
3	W	605	HEC	C1A-C2A	-2.12	1.41	1.45
3	K	605	HEC	C3C-C4C	-2.12	1.42	1.46
3	G	605	HEC	C1D-C2D	2.12	1.48	1.43
3	O	607	HEC	C1D-C2D	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	601	HEC	C1D-C2D	2.12	1.48	1.43
3	G	606	HEC	C4A-C3A	-2.12	1.41	1.45
3	R	603	HEC	O1D-CGD	2.11	1.29	1.22
3	C	603	HEC	O1D-CGD	2.11	1.29	1.22
3	C	601	HEC	C1D-C2D	2.11	1.48	1.43
3	U	605	HEC	C1D-C2D	2.11	1.48	1.43
3	M	605	HEC	C1D-C2D	2.11	1.48	1.43
3	Q	604	HEC	C4A-C3A	-2.10	1.41	1.45
3	M	606	HEC	C1A-C2A	-2.10	1.41	1.45
3	R	606	HEC	C4A-C3A	-2.10	1.41	1.45
3	D	601	HEC	C1D-C2D	2.10	1.48	1.43
3	H	601	HEC	C1D-C2D	2.10	1.48	1.43
3	H	604	HEC	C1D-C2D	2.10	1.48	1.43
3	F	601	HEC	C1D-C2D	2.10	1.48	1.43
3	W	605	HEC	C4A-C3A	-2.10	1.41	1.45
3	I	601	HEC	C1D-C2D	2.10	1.48	1.43
3	T	604	HEC	C4A-C3A	-2.10	1.41	1.45
3	L	604	HEC	C4A-C3A	-2.09	1.41	1.45
3	T	602	HEC	C4A-C3A	-2.09	1.41	1.45
3	E	607	HEC	C1A-C2A	-2.09	1.41	1.45
3	D	600	HEC	C1A-C2A	-2.09	1.41	1.45
3	J	602	HEC	C1D-C2D	2.09	1.48	1.43
3	L	600	HEC	C4D-ND	-2.09	1.35	1.39
3	X	605	HEC	C1D-C2D	2.09	1.48	1.43
3	B	606	HEC	C4A-C3A	-2.09	1.41	1.45
3	W	607	HEC	C1D-C2D	2.09	1.48	1.43
3	R	606	HEC	C1D-C2D	2.09	1.48	1.43
3	P	600	HEC	C1D-C2D	2.08	1.48	1.43
3	N	604	HEC	C1A-C2A	-2.08	1.41	1.45
3	W	604	HEC	C1A-C2A	-2.08	1.41	1.45
3	H	607	HEC	C1A-C2A	-2.08	1.41	1.45
3	B	604	HEC	C4A-C3A	-2.08	1.41	1.45
3	Q	605	HEC	C1A-C2A	-2.08	1.41	1.45
3	N	606	HEC	C1D-C2D	2.08	1.48	1.43
3	J	602	HEC	C4A-C3A	-2.08	1.41	1.45
3	V	607	HEC	C1D-C2D	2.08	1.48	1.43
3	M	603	HEC	O1D-CGD	2.08	1.28	1.22
3	T	604	HEC	C1A-C2A	-2.08	1.41	1.45
3	O	606	HEC	C1D-C2D	2.08	1.48	1.43
3	X	602	HEC	C1D-C2D	2.08	1.48	1.43
3	N	601	HEC	C1D-C2D	2.07	1.48	1.43
3	S	607	HEC	C1A-C2A	-2.07	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	607	HEC	C1A-C2A	-2.07	1.41	1.45
3	E	604	HEC	C1A-C2A	-2.07	1.41	1.45
3	B	602	HEC	C1D-C2D	2.07	1.48	1.43
3	A	604	HEC	C1A-C2A	-2.07	1.41	1.45
3	I	606	HEC	C3C-C4C	-2.07	1.42	1.46
3	M	604	HEC	C1A-C2A	-2.07	1.41	1.45
3	S	605	HEC	C1D-C2D	2.07	1.48	1.43
3	O	601	HEC	C4A-C3A	-2.07	1.41	1.45
3	K	602	HEC	C1D-C2D	2.07	1.48	1.43
3	T	605	HEC	C1D-C2D	2.07	1.48	1.43
3	H	600	HEC	C4A-C3A	-2.06	1.41	1.45
3	T	601	HEC	C4A-C3A	-2.06	1.41	1.45
3	X	606	HEC	C1D-C2D	2.06	1.48	1.43
3	O	604	HEC	C3C-C4C	-2.06	1.42	1.46
3	S	602	HEC	C1D-C2D	2.06	1.48	1.43
3	V	600	HEC	C1D-C2D	2.06	1.48	1.43
3	D	605	HEC	C1A-C2A	-2.06	1.41	1.45
3	J	604	HEC	C1A-C2A	-2.06	1.41	1.45
3	X	601	HEC	C4A-C3A	-2.05	1.41	1.45
3	L	602	HEC	C4A-C3A	-2.05	1.41	1.45
3	C	605	HEC	C1D-C2D	2.05	1.47	1.43
3	P	601	HEC	C1D-C2D	2.05	1.47	1.43
3	B	600	HEC	C1A-C2A	-2.05	1.41	1.45
3	L	607	HEC	C1A-C2A	-2.05	1.41	1.45
3	T	606	HEC	C1D-C2D	2.05	1.47	1.43
3	Q	604	HEC	C1A-C2A	-2.05	1.41	1.45
3	Q	605	HEC	C1D-C2D	2.04	1.47	1.43
3	V	602	HEC	C4A-C3A	-2.04	1.41	1.45
3	F	600	HEC	C1D-C2D	2.04	1.47	1.43
3	F	602	HEC	C1D-C2D	2.04	1.47	1.43
3	D	604	HEC	C4A-C3A	-2.04	1.41	1.45
3	E	607	HEC	C4A-C3A	-2.04	1.41	1.45
3	V	606	HEC	C1A-C2A	-2.04	1.41	1.45
3	M	607	HEC	C1D-C2D	2.04	1.47	1.43
3	G	603	HEC	O1D-CGD	2.04	1.28	1.22
3	Q	600	HEC	C1D-C2D	2.04	1.47	1.43
3	B	601	HEC	C4A-C3A	-2.04	1.41	1.45
3	D	606	HEC	C1A-C2A	-2.04	1.41	1.45
3	W	604	HEC	C1D-C2D	2.04	1.47	1.43
3	W	607	HEC	C1A-C2A	-2.04	1.41	1.45
3	B	604	HEC	C1D-C2D	2.04	1.47	1.43
3	K	601	HEC	C1D-C2D	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	606	HEC	C1D-C2D	2.04	1.47	1.43
3	S	604	HEC	C1A-C2A	-2.03	1.41	1.45
3	V	607	HEC	C1A-C2A	-2.03	1.41	1.45
3	N	607	HEC	C3C-C4C	-2.03	1.42	1.46
3	J	600	HEC	C1D-C2D	2.03	1.47	1.43
3	W	604	HEC	C4A-C3A	-2.03	1.41	1.45
3	Q	607	HEC	C1D-C2D	2.03	1.47	1.43
3	N	604	HEC	C3C-C4C	-2.03	1.42	1.46
3	E	601	HEC	C1D-C2D	2.03	1.47	1.43
3	N	606	HEC	C4A-C3A	-2.03	1.41	1.45
3	Q	606	HEC	C1A-C2A	-2.03	1.41	1.45
3	W	606	HEC	C4A-C3A	-2.03	1.41	1.45
3	I	600	HEC	C1D-C2D	2.02	1.47	1.43
3	V	605	HEC	C1A-C2A	-2.02	1.41	1.45
3	O	603	HEC	O1D-CGD	2.02	1.28	1.22
3	T	601	HEC	C1D-C2D	2.02	1.47	1.43
3	E	606	HEC	C4A-C3A	-2.02	1.41	1.45
3	K	604	HEC	C1D-C2D	2.02	1.47	1.43
3	F	604	HEC	C4A-C3A	-2.02	1.41	1.45
3	H	606	HEC	C1A-C2A	-2.02	1.41	1.45
3	L	605	HEC	C1A-C2A	-2.02	1.41	1.45
3	F	601	HEC	C4A-C3A	-2.02	1.41	1.45
3	Q	607	HEC	C1A-C2A	-2.02	1.41	1.45
3	H	601	HEC	C4A-C3A	-2.02	1.41	1.45
3	E	604	HEC	C4A-C3A	-2.02	1.41	1.45
3	P	604	HEC	C4A-C3A	-2.02	1.41	1.45
3	C	604	HEC	C3C-C4C	-2.02	1.42	1.46
3	V	601	HEC	C1D-C2D	2.02	1.47	1.43
3	T	607	HEC	C1D-C2D	2.01	1.47	1.43
3	X	607	HEC	C1D-C2D	2.01	1.47	1.43
3	A	601	HEC	C1D-C2D	2.01	1.47	1.43
3	X	607	HEC	C1A-C2A	-2.01	1.41	1.45
3	J	606	HEC	C1A-C2A	-2.01	1.41	1.45
3	S	601	HEC	C1D-C2D	2.01	1.47	1.43
3	B	607	HEC	C1A-C2A	-2.01	1.41	1.45
3	W	601	HEC	C1D-C2D	2.01	1.47	1.43
3	I	605	HEC	C3B-C4B	2.01	1.49	1.46
3	U	607	HEC	C1D-C2D	2.01	1.47	1.43
3	L	605	HEC	C1D-C2D	2.01	1.47	1.43
3	X	600	HEC	C1D-C2D	2.00	1.47	1.43
3	P	605	HEC	C1D-C2D	2.00	1.47	1.43
3	E	605	HEC	C1A-C2A	-2.00	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	607	HEC	C4A-C3A	-2.00	1.41	1.45
3	B	606	HEC	C1D-C2D	2.00	1.47	1.43
3	E	606	HEC	C1A-C2A	-2.00	1.41	1.45
3	V	602	HEC	C1A-C2A	-2.00	1.41	1.45

All (2028) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	603	HEC	CHD-C4C-NC	-12.60	110.73	124.45
3	C	603	HEC	CHD-C4C-NC	-12.26	111.10	124.45
3	G	603	HEC	CHD-C4C-NC	-12.20	111.17	124.45
3	J	603	HEC	CHD-C4C-NC	-11.99	111.40	124.45
3	P	603	HEC	CHD-C4C-NC	-11.87	111.52	124.45
3	K	603	HEC	CHD-C4C-NC	-11.86	111.54	124.45
3	A	603	HEC	CHD-C4C-NC	-11.81	111.59	124.45
3	O	603	HEC	CHD-C4C-NC	-11.76	111.65	124.45
3	X	603	HEC	CHD-C4C-NC	-11.74	111.67	124.45
3	W	603	HEC	CHD-C4C-NC	-11.73	111.68	124.45
3	E	603	HEC	CHD-C4C-NC	-11.72	111.69	124.45
3	M	603	HEC	CHD-C4C-NC	-11.67	111.75	124.45
3	I	603	HEC	CHD-C4C-NC	-11.65	111.77	124.45
3	F	603	HEC	CHD-C4C-NC	-11.56	111.86	124.45
3	Q	603	HEC	CHD-C4C-NC	-11.56	111.87	124.45
3	S	603	HEC	CHD-C4C-NC	-11.54	111.89	124.45
3	U	603	HEC	CHD-C4C-NC	-11.47	111.97	124.45
3	V	603	HEC	CHD-C4C-NC	-11.46	111.97	124.45
3	N	603	HEC	CHD-C4C-NC	-11.46	111.98	124.45
3	B	603	HEC	CHD-C4C-NC	-11.35	112.09	124.45
3	R	603	HEC	CHD-C4C-NC	-11.27	112.18	124.45
3	T	603	HEC	CHD-C4C-NC	-11.25	112.20	124.45
3	H	603	HEC	CHD-C4C-NC	-11.09	112.38	124.45
3	D	603	HEC	CHD-C4C-NC	-10.84	112.65	124.45
3	I	603	HEC	CBA-CAA-C2A	10.79	142.36	112.53
3	G	603	HEC	CHA-C1A-NA	-10.31	113.23	124.45
3	L	603	HEC	CHA-C1A-NA	-10.24	113.30	124.45
3	F	603	HEC	CHA-C1A-NA	-10.24	113.31	124.45
3	X	603	HEC	CHA-C1A-NA	-10.24	113.31	124.45
3	D	603	HEC	CHA-C1A-NA	-10.23	113.31	124.45
3	P	603	HEC	CHA-C1A-NA	-10.22	113.32	124.45
3	C	603	HEC	CHA-C1A-NA	-10.19	113.35	124.45
3	A	603	HEC	CHA-C1A-NA	-10.16	113.39	124.45
3	B	603	HEC	CHA-C1A-NA	-10.06	113.49	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	603	HEC	CHA-C1A-NA	-10.05	113.51	124.45
3	E	603	HEC	CHA-C1A-NA	-10.02	113.54	124.45
3	V	603	HEC	CHA-C1A-NA	-10.02	113.54	124.45
3	Q	603	HEC	CHA-C1A-NA	-10.02	113.55	124.45
3	J	603	HEC	CHA-C1A-NA	-10.01	113.56	124.45
3	U	603	HEC	CHA-C1A-NA	-9.97	113.59	124.45
3	S	603	HEC	CHA-C1A-NA	-9.97	113.60	124.45
3	T	603	HEC	CHA-C1A-NA	-9.92	113.65	124.45
3	N	603	HEC	CHA-C1A-NA	-9.92	113.65	124.45
3	H	603	HEC	CHA-C1A-NA	-9.90	113.67	124.45
3	R	603	HEC	CHA-C1A-NA	-9.85	113.72	124.45
3	O	603	HEC	CHA-C1A-NA	-9.78	113.81	124.45
3	M	603	HEC	CHA-C1A-NA	-9.74	113.84	124.45
3	K	603	HEC	CHA-C1A-NA	-9.56	114.04	124.45
3	I	603	HEC	CAA-C2A-C1A	-9.07	106.40	124.85
3	I	603	HEC	CHA-C1A-NA	-7.90	115.85	124.45
3	I	603	HEC	C2A-C1A-NA	-7.34	103.25	110.32
3	I	603	HEC	CHC-C4B-NB	-7.13	116.68	124.45
3	D	603	HEC	C2A-C1A-NA	-7.08	103.49	110.32
3	K	603	HEC	C2A-C1A-NA	-7.02	103.55	110.32
3	K	603	HEC	CHC-C4B-C3B	-6.96	113.47	125.21
3	W	603	HEC	C2A-C1A-NA	-6.87	103.69	110.32
3	O	603	HEC	CHC-C4B-NB	-6.87	116.97	124.45
3	O	603	HEC	CBB-CAB-C3B	-6.83	113.78	127.43
3	R	603	HEC	CHC-C4B-C3B	-6.83	113.70	125.21
3	I	603	HEC	CHC-C4B-C3B	-6.82	113.71	125.21
3	C	603	HEC	CHC-C4B-NB	-6.82	117.03	124.45
3	P	603	HEC	CBB-CAB-C3B	-6.81	113.83	127.43
3	J	603	HEC	CHC-C4B-C3B	-6.80	113.75	125.21
3	D	603	HEC	CBB-CAB-C3B	-6.79	113.87	127.43
3	E	603	HEC	CHA-C1A-C2A	-6.78	114.15	124.86
3	M	603	HEC	CHC-C4B-C3B	-6.78	113.78	125.21
3	Q	603	HEC	CHC-C4B-C3B	-6.77	113.79	125.21
3	X	603	HEC	C2A-C1A-NA	-6.76	103.80	110.32
3	F	603	HEC	C2A-C1A-NA	-6.76	103.80	110.32
3	M	603	HEC	C2A-C1A-NA	-6.75	103.81	110.32
3	S	603	HEC	CBB-CAB-C3B	-6.75	113.95	127.43
3	T	603	HEC	CBB-CAB-C3B	-6.72	114.00	127.43
3	U	603	HEC	C2A-C1A-NA	-6.72	103.84	110.32
3	R	603	HEC	C2A-C1A-NA	-6.71	103.85	110.32
3	P	603	HEC	C2A-C1A-NA	-6.70	103.86	110.32
3	Q	603	HEC	C2A-C1A-NA	-6.70	103.86	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	HEC	CHC-C4B-NB	-6.67	117.19	124.45
3	H	603	HEC	CHC-C4B-C3B	-6.67	113.97	125.21
3	Q	603	HEC	CHA-C1A-C2A	-6.66	114.35	124.86
3	X	603	HEC	CHA-C1A-C2A	-6.66	114.36	124.86
3	B	603	HEC	CHC-C4B-NB	-6.65	117.21	124.45
3	L	603	HEC	CHC-C4B-C3B	-6.65	114.00	125.21
3	U	603	HEC	CBB-CAB-C3B	-6.64	114.15	127.43
3	R	603	HEC	CBB-CAB-C3B	-6.64	114.16	127.43
3	Q	603	HEC	CBB-CAB-C3B	-6.64	114.17	127.43
3	N	603	HEC	CHC-C4B-NB	-6.63	117.24	124.45
3	A	603	HEC	C2A-C1A-NA	-6.63	103.93	110.32
3	S	603	HEC	C2A-C1A-NA	-6.62	103.94	110.32
3	B	603	HEC	CHC-C4B-C3B	-6.61	114.06	125.21
3	T	603	HEC	CHC-C4B-C3B	-6.60	114.09	125.21
3	B	603	HEC	CBB-CAB-C3B	-6.57	114.30	127.43
3	C	603	HEC	CHC-C4B-C3B	-6.56	114.14	125.21
3	X	603	HEC	CHC-C4B-C3B	-6.54	114.17	125.21
3	U	603	HEC	CHC-C4B-C3B	-6.54	114.18	125.21
3	P	603	HEC	CHC-C4B-C3B	-6.54	114.18	125.21
3	K	603	HEC	CHA-C1A-C2A	-6.54	114.54	124.86
3	F	603	HEC	CHC-C4B-NB	-6.53	117.35	124.45
3	B	603	HEC	C2A-C1A-NA	-6.53	104.03	110.32
3	N	603	HEC	C2A-C1A-NA	-6.52	104.03	110.32
3	F	603	HEC	CBB-CAB-C3B	-6.52	114.41	127.43
3	G	603	HEC	CHA-C1A-C2A	-6.52	114.58	124.86
3	O	603	HEC	CHC-C4B-C3B	-6.51	114.23	125.21
3	S	603	HEC	CHA-C1A-C2A	-6.50	114.60	124.86
3	U	603	HEC	CHA-C1A-C2A	-6.50	114.61	124.86
3	A	603	HEC	CHA-C1A-C2A	-6.50	114.61	124.86
3	G	603	HEC	CHC-C4B-C3B	-6.50	114.26	125.21
3	H	603	HEC	C2A-C1A-NA	-6.49	104.06	110.32
3	J	603	HEC	C2A-C1A-NA	-6.49	104.06	110.32
3	W	603	HEC	CHC-C4B-C3B	-6.48	114.28	125.21
3	H	603	HEC	CHC-C4B-NB	-6.47	117.41	124.45
3	V	603	HEC	CBB-CAB-C3B	-6.47	114.51	127.43
3	V	603	HEC	CHA-C1A-C2A	-6.46	114.66	124.86
3	H	603	HEC	CHA-C1A-C2A	-6.46	114.67	124.86
3	V	603	HEC	CHC-C4B-C3B	-6.45	114.33	125.21
3	T	603	HEC	CHA-C1A-C2A	-6.44	114.69	124.86
3	W	603	HEC	CHA-C1A-C2A	-6.44	114.69	124.86
3	N	603	HEC	CHC-C4B-C3B	-6.44	114.36	125.21
3	F	603	HEC	CHC-C4B-C3B	-6.42	114.38	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	HEC	CHC-C4B-C3B	-6.42	114.39	125.21
3	V	603	HEC	C2A-C1A-NA	-6.42	104.13	110.32
3	A	603	HEC	CHC-C4B-NB	-6.42	117.47	124.45
3	R	603	HEC	CHC-C4B-NB	-6.41	117.47	124.45
3	A	603	HEC	CBB-CAB-C3B	-6.41	114.62	127.43
3	W	603	HEC	CBC-CAC-C3C	-6.40	114.64	127.43
3	W	603	HEC	CBB-CAB-C3B	-6.40	114.64	127.43
3	W	603	HEC	CHC-C4B-NB	-6.39	117.49	124.45
3	C	603	HEC	CHA-C1A-C2A	-6.38	114.79	124.86
3	E	603	HEC	CBB-CAB-C3B	-6.37	114.69	127.43
3	O	603	HEC	CHA-C1A-C2A	-6.37	114.80	124.86
3	L	603	HEC	C2A-C1A-NA	-6.37	104.18	110.32
3	H	603	HEC	CBB-CAB-C3B	-6.36	114.72	127.43
3	I	603	HEC	CHA-C1A-C2A	-6.35	114.83	124.86
3	H	603	HEC	CBC-CAC-C3C	-6.33	114.78	127.43
3	A	603	HEC	CHC-C4B-C3B	-6.33	114.53	125.21
3	J	603	HEC	CHC-C4B-NB	-6.33	117.56	124.45
3	F	603	HEC	CHA-C1A-C2A	-6.32	114.89	124.86
3	P	603	HEC	CHC-C4B-NB	-6.32	117.57	124.45
3	P	603	HEC	CHA-C1A-C2A	-6.31	114.90	124.86
3	S	603	HEC	CHC-C4B-C3B	-6.31	114.57	125.21
3	M	603	HEC	CHA-C1A-C2A	-6.31	114.91	124.86
3	X	603	HEC	CBB-CAB-C3B	-6.30	114.83	127.43
3	J	603	HEC	CBB-CAB-C3B	-6.30	114.84	127.43
3	L	603	HEC	CHC-C4B-NB	-6.30	117.59	124.45
3	C	603	HEC	C2A-C1A-NA	-6.28	104.26	110.32
3	M	603	HEC	CHC-C4B-NB	-6.28	117.61	124.45
3	R	603	HEC	CHA-C1A-C2A	-6.28	114.95	124.86
3	N	603	HEC	CBC-CAC-C3C	-6.27	114.90	127.43
3	M	603	HEC	CBB-CAB-C3B	-6.26	114.92	127.43
3	J	603	HEC	CBC-CAC-C3C	-6.26	114.92	127.43
3	X	603	HEC	CHC-C4B-NB	-6.26	117.64	124.45
3	C	603	HEC	CBB-CAB-C3B	-6.26	114.93	127.43
3	A	603	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
3	J	603	HEC	CHA-C1A-C2A	-6.25	115.00	124.86
3	L	603	HEC	CBB-CAB-C3B	-6.25	114.95	127.43
3	N	603	HEC	CBB-CAB-C3B	-6.24	114.97	127.43
3	N	603	HEC	CHA-C1A-C2A	-6.23	115.03	124.86
3	F	603	HEC	CBC-CAC-C3C	-6.23	114.99	127.43
3	G	603	HEC	C2A-C1A-NA	-6.21	104.33	110.32
3	S	603	HEC	CHC-C4B-NB	-6.20	117.70	124.45
3	B	603	HEC	CHA-C1A-C2A	-6.20	115.07	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	603	HEC	CHC-C4B-NB	-6.20	117.70	124.45
3	T	603	HEC	CHC-C4B-NB	-6.19	117.71	124.45
3	E	603	HEC	C2A-C1A-NA	-6.19	104.35	110.32
3	P	603	HEC	CBC-CAC-C3C	-6.19	115.07	127.43
3	G	603	HEC	CHC-C4B-NB	-6.17	117.73	124.45
3	R	603	HEC	CHD-C4C-C3C	-6.16	114.81	125.21
3	X	603	HEC	CBC-CAC-C3C	-6.16	115.12	127.43
3	L	603	HEC	CHA-C1A-C2A	-6.16	115.14	124.86
3	Q	603	HEC	CBC-CAC-C3C	-6.14	115.15	127.43
3	T	603	HEC	C2A-C1A-NA	-6.14	104.40	110.32
3	D	603	HEC	CHA-C1A-C2A	-6.13	115.18	124.86
3	C	603	HEC	CBC-CAC-C3C	-6.12	115.19	127.43
3	O	603	HEC	C2A-C1A-NA	-6.09	104.44	110.32
3	D	603	HEC	CHC-C4B-C3B	-6.07	114.97	125.21
3	M	603	HEC	CHD-C4C-C3C	-6.05	115.01	125.21
3	U	603	HEC	CBC-CAC-C3C	-6.02	115.41	127.43
3	E	603	HEC	CBC-CAC-C3C	-5.98	115.49	127.43
3	J	603	HEC	CHD-C4C-C3C	-5.97	115.15	125.21
3	F	603	HEC	CHD-C4C-C3C	-5.96	115.15	125.21
3	E	603	HEC	CHC-C4B-NB	-5.96	117.96	124.45
3	T	603	HEC	CHD-C4C-C3C	-5.96	115.16	125.21
3	I	603	HEC	CHD-C4C-C3C	-5.95	115.18	125.21
3	B	603	HEC	CBC-CAC-C3C	-5.94	115.55	127.43
3	B	603	HEC	CHD-C4C-C3C	-5.94	115.19	125.21
3	U	603	HEC	CHC-C4B-NB	-5.93	117.99	124.45
3	K	603	HEC	CBB-CAB-C3B	-5.91	115.61	127.43
3	G	603	HEC	CBB-CAB-C3B	-5.91	115.62	127.43
3	S	603	HEC	CBC-CAC-C3C	-5.91	115.62	127.43
3	V	603	HEC	CHD-C4C-C3C	-5.89	115.28	125.21
3	D	603	HEC	CHD-C4C-C3C	-5.85	115.35	125.21
3	O	603	HEC	CBC-CAC-C3C	-5.85	115.75	127.43
3	H	603	HEC	CHD-C4C-C3C	-5.84	115.36	125.21
3	K	603	HEC	CHC-C4B-NB	-5.83	118.10	124.45
3	O	603	HEC	CHD-C4C-C3C	-5.82	115.39	125.21
3	W	603	HEC	CHD-C4C-C3C	-5.81	115.42	125.21
3	K	603	HEC	CHD-C4C-C3C	-5.80	115.43	125.21
3	C	603	HEC	CHD-C4C-C3C	-5.80	115.44	125.21
3	E	603	HEC	CHD-C4C-C3C	-5.79	115.44	125.21
3	Q	603	HEC	CHD-C4C-C3C	-5.75	115.52	125.21
3	V	603	HEC	CHC-C4B-NB	-5.74	118.20	124.45
3	V	603	HEC	CBC-CAC-C3C	-5.74	115.96	127.43
3	R	603	HEC	CBC-CAC-C3C	-5.73	115.98	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	HEC	CHD-C4C-C3C	-5.73	115.55	125.21
3	P	603	HEC	CHD-C4C-C3C	-5.72	115.56	125.21
3	G	603	HEC	CBC-CAC-C3C	-5.69	116.06	127.43
3	D	603	HEC	CBC-CAC-C3C	-5.69	116.06	127.43
3	S	603	HEC	CHD-C4C-C3C	-5.66	115.67	125.21
3	L	603	HEC	CHD-C4C-C3C	-5.66	115.67	125.21
3	G	603	HEC	CHD-C4C-C3C	-5.65	115.68	125.21
3	M	603	HEC	CBC-CAC-C3C	-5.63	116.19	127.43
3	N	603	HEC	CHD-C4C-C3C	-5.61	115.74	125.21
3	X	603	HEC	CHD-C4C-C3C	-5.59	115.79	125.21
3	T	603	HEC	CBC-CAC-C3C	-5.57	116.31	127.43
3	D	603	HEC	CAA-C2A-C1A	5.54	136.12	124.85
3	U	603	HEC	CHD-C4C-C3C	-5.52	115.90	125.21
3	L	603	HEC	CBC-CAC-C3C	-5.51	116.42	127.43
3	I	603	HEC	CBC-CAC-C3C	-5.48	116.48	127.43
3	I	603	HEC	CBB-CAB-C3B	-5.29	116.86	127.43
3	K	603	HEC	CBC-CAC-C3C	-5.22	117.01	127.43
3	F	603	HEC	CAA-CBA-CGA	5.09	127.17	113.67
3	A	603	HEC	CAA-CBA-CGA	5.06	127.09	113.67
3	W	604	HEC	CHC-C4B-NB	5.04	129.94	124.45
3	E	603	HEC	CAA-CBA-CGA	5.04	127.03	113.67
3	D	604	HEC	CHC-C4B-NB	4.97	129.86	124.45
3	L	603	HEC	CAA-CBA-CGA	4.96	126.82	113.67
3	M	603	HEC	CAA-CBA-CGA	4.93	126.75	113.67
3	P	601	HEC	CHC-C4B-NB	4.93	129.82	124.45
3	I	601	HEC	CHC-C4B-NB	4.92	129.81	124.45
3	B	604	HEC	CHC-C4B-NB	4.90	129.79	124.45
3	E	601	HEC	CHC-C4B-NB	4.90	129.79	124.45
3	U	604	HEC	CHC-C4B-NB	4.90	129.79	124.45
3	K	600	HEC	CHC-C4B-NB	4.89	129.78	124.45
3	M	600	HEC	CHC-C4B-NB	4.88	129.77	124.45
3	H	601	HEC	CHC-C4B-NB	4.88	129.77	124.45
3	O	601	HEC	CHC-C4B-NB	4.82	129.71	124.45
3	Q	603	HEC	CAA-CBA-CGA	4.82	126.45	113.67
3	P	604	HEC	CHC-C4B-NB	4.80	129.68	124.45
3	V	604	HEC	CHC-C4B-NB	4.80	129.68	124.45
3	B	601	HEC	CHC-C4B-NB	4.80	129.68	124.45
3	I	600	HEC	CHC-C4B-NB	4.79	129.67	124.45
3	X	603	HEC	CAA-CBA-CGA	4.79	126.36	113.67
3	P	603	HEC	CAA-CBA-CGA	4.78	126.33	113.67
3	N	604	HEC	CHC-C4B-NB	4.77	129.65	124.45
3	J	604	HEC	CHC-C4B-NB	4.76	129.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	604	HEC	CHC-C4B-NB	4.75	129.63	124.45
3	R	604	HEC	CHC-C4B-NB	4.75	129.63	124.45
3	L	600	HEC	CHC-C4B-NB	4.75	129.62	124.45
3	F	604	HEC	CHC-C4B-NB	4.75	129.62	124.45
3	N	600	HEC	CHC-C4B-NB	4.75	129.62	124.45
3	X	604	HEC	CHC-C4B-NB	4.74	129.61	124.45
3	M	601	HEC	CHC-C4B-NB	4.74	129.61	124.45
3	T	604	HEC	CHC-C4B-NB	4.73	129.60	124.45
3	L	606	HEC	CHC-C4B-NB	4.73	129.60	124.45
3	M	604	HEC	CHC-C4B-NB	4.72	129.59	124.45
3	K	604	HEC	CHC-C4B-NB	4.71	129.58	124.45
3	U	600	HEC	CHC-C4B-NB	4.71	129.58	124.45
3	R	601	HEC	CHC-C4B-NB	4.70	129.57	124.45
3	U	603	HEC	CAA-CBA-CGA	4.70	126.13	113.67
3	V	601	HEC	CHC-C4B-NB	4.70	129.57	124.45
3	X	601	HEC	CHC-C4B-NB	4.70	129.57	124.45
3	C	601	HEC	CHC-C4B-NB	4.70	129.57	124.45
3	T	601	HEC	CHC-C4B-NB	4.69	129.56	124.45
3	F	601	HEC	CHC-C4B-NB	4.69	129.56	124.45
3	S	601	HEC	CHC-C4B-NB	4.68	129.55	124.45
3	J	600	HEC	CHC-C4B-NB	4.67	129.54	124.45
3	Q	604	HEC	CHC-C4B-NB	4.67	129.54	124.45
3	F	600	HEC	CHC-C4B-NB	4.67	129.54	124.45
3	I	604	HEC	CBB-CAB-C3B	-4.67	118.11	127.43
3	L	604	HEC	CHC-C4B-NB	4.66	129.53	124.45
3	I	601	HEC	CBC-CAC-C3C	-4.66	118.12	127.43
3	J	603	HEC	CAA-CBA-CGA	4.66	126.02	113.67
3	S	604	HEC	CHC-C4B-NB	4.66	129.52	124.45
3	G	601	HEC	CHC-C4B-NB	4.65	129.52	124.45
3	H	600	HEC	CHC-C4B-NB	4.65	129.52	124.45
3	A	600	HEC	CHC-C4B-NB	4.65	129.51	124.45
3	U	601	HEC	CHC-C4B-NB	4.65	129.51	124.45
3	A	601	HEC	CHC-C4B-NB	4.64	129.50	124.45
3	J	601	HEC	CHC-C4B-NB	4.64	129.50	124.45
3	E	604	HEC	CHC-C4B-NB	4.63	129.49	124.45
3	E	600	HEC	CHC-C4B-NB	4.62	129.49	124.45
3	F	606	HEC	CHC-C4B-NB	4.62	129.48	124.45
3	T	603	HEC	CAA-CBA-CGA	4.61	125.90	113.67
3	C	600	HEC	CHC-C4B-NB	4.61	129.47	124.45
3	X	600	HEC	CHC-C4B-NB	4.61	129.47	124.45
3	D	606	HEC	CBB-CAB-C3B	-4.61	118.23	127.43
3	D	606	HEC	CHC-C4B-NB	4.60	129.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	603	HEC	CAA-CBA-CGA	4.60	125.87	113.67
3	I	604	HEC	CHC-C4B-NB	4.58	129.44	124.45
3	V	606	HEC	CHC-C4B-NB	4.58	129.44	124.45
3	A	604	HEC	CHC-C4B-NB	4.58	129.44	124.45
3	L	601	HEC	CHC-C4B-NB	4.57	129.42	124.45
3	P	600	HEC	CHC-C4B-NB	4.56	129.42	124.45
3	E	602	HEC	CHC-C4B-NB	4.55	129.41	124.45
3	I	607	HEC	CHC-C4B-NB	4.54	129.40	124.45
3	O	604	HEC	CHC-C4B-NB	4.53	129.39	124.45
3	N	605	HEC	CHC-C4B-NB	4.53	129.39	124.45
3	K	601	HEC	CHC-C4B-NB	4.53	129.38	124.45
3	W	600	HEC	CHC-C4B-NB	4.52	129.38	124.45
3	O	603	HEC	CAA-CBA-CGA	4.52	125.66	113.67
3	I	606	HEC	CHC-C4B-NB	4.52	129.38	124.45
3	G	600	HEC	CHC-C4B-NB	4.52	129.37	124.45
3	R	606	HEC	CHC-C4B-NB	4.52	129.37	124.45
3	S	600	HEC	CHC-C4B-NB	4.52	129.37	124.45
3	O	600	HEC	CHC-C4B-NB	4.51	129.37	124.45
3	V	600	HEC	CHC-C4B-NB	4.51	129.36	124.45
3	X	602	HEC	CHC-C4B-NB	4.50	129.36	124.45
3	D	603	HEC	CAA-C2A-C3A	-4.50	119.43	127.87
3	H	604	HEC	CHC-C4B-NB	4.49	129.35	124.45
3	W	601	HEC	CHC-C4B-NB	4.49	129.34	124.45
3	M	606	HEC	CHC-C4B-NB	4.49	129.34	124.45
3	D	603	HEC	CAA-CBA-CGA	4.49	125.57	113.67
3	K	606	HEC	CHC-C4B-NB	4.49	129.34	124.45
3	Q	601	HEC	CHC-C4B-NB	4.49	129.34	124.45
3	B	606	HEC	CHC-C4B-NB	4.48	129.34	124.45
3	Q	600	HEC	CHC-C4B-NB	4.48	129.33	124.45
3	N	603	HEC	CAA-CBA-CGA	4.48	125.54	113.67
3	V	603	HEC	CAA-CBA-CGA	4.48	125.53	113.67
3	T	600	HEC	CHC-C4B-NB	4.47	129.32	124.45
3	O	602	HEC	CHC-C4B-NB	4.47	129.32	124.45
3	H	604	HEC	CBB-CAB-C3B	-4.47	118.51	127.43
3	D	600	HEC	CHC-C4B-NB	4.46	129.31	124.45
3	U	602	HEC	CHC-C4B-NB	4.46	129.31	124.45
3	W	603	HEC	CAA-CBA-CGA	4.45	125.47	113.67
3	B	600	HEC	CHC-C4B-NB	4.45	129.30	124.45
3	C	604	HEC	CHC-C4B-NB	4.44	129.29	124.45
3	S	602	HEC	CHC-C4B-NB	4.43	129.28	124.45
3	B	602	HEC	CHC-C4B-NB	4.43	129.28	124.45
3	I	603	HEC	C1A-C2A-C3A	-4.42	101.29	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	HEC	CAA-CBA-CGA	4.41	125.37	113.67
3	F	606	HEC	CBB-CAB-C3B	-4.41	118.62	127.43
3	U	606	HEC	CHC-C4B-NB	4.39	129.23	124.45
3	N	601	HEC	CHC-C4B-NB	4.38	129.23	124.45
3	G	606	HEC	CHC-C4B-NB	4.35	129.19	124.45
3	K	602	HEC	CHC-C4B-NB	4.35	129.19	124.45
3	D	601	HEC	CHC-C4B-NB	4.34	129.18	124.45
3	A	602	HEC	CHC-C4B-NB	4.32	129.16	124.45
3	N	606	HEC	CBB-CAB-C3B	-4.32	118.80	127.43
3	C	604	HEC	CBB-CAB-C3B	-4.32	118.80	127.43
3	Q	604	HEC	CBB-CAB-C3B	-4.32	118.81	127.43
3	S	604	HEC	CBB-CAB-C3B	-4.30	118.83	127.43
3	N	602	HEC	CHC-C4B-NB	4.30	129.14	124.45
3	V	606	HEC	CBB-CAB-C3B	-4.30	118.83	127.43
3	C	606	HEC	CBB-CAB-C3B	-4.30	118.84	127.43
3	C	603	HEC	CAA-CBA-CGA	4.30	125.07	113.67
3	O	606	HEC	CBB-CAB-C3B	-4.30	118.84	127.43
3	L	605	HEC	CHC-C4B-NB	4.29	129.12	124.45
3	C	605	HEC	CHC-C4B-NB	4.29	129.12	124.45
3	R	602	HEC	CHC-C4B-NB	4.29	129.12	124.45
3	V	602	HEC	CHC-C4B-NB	4.29	129.12	124.45
3	J	602	HEC	CHC-C4B-NB	4.28	129.11	124.45
3	X	606	HEC	CHC-C4B-NB	4.28	129.11	124.45
3	Q	602	HEC	CHC-C4B-NB	4.27	129.10	124.45
3	H	603	HEC	CAA-CBA-CGA	4.27	124.98	113.67
3	W	602	HEC	CHC-C4B-NB	4.26	129.09	124.45
3	O	606	HEC	CHC-C4B-NB	4.25	129.09	124.45
3	G	601	HEC	CBB-CAB-C3B	-4.25	118.93	127.43
3	E	606	HEC	CHC-C4B-NB	4.25	129.08	124.45
3	S	602	HEC	CBB-CAB-C3B	-4.25	118.94	127.43
3	H	606	HEC	CBB-CAB-C3B	-4.24	118.95	127.43
3	G	602	HEC	CHC-C4B-NB	4.24	129.07	124.45
3	M	602	HEC	CBB-CAB-C3B	-4.23	118.98	127.43
3	M	605	HEC	CHC-C4B-NB	4.23	129.06	124.45
3	N	606	HEC	CHC-C4B-NB	4.22	129.05	124.45
3	S	606	HEC	CHC-C4B-NB	4.22	129.05	124.45
3	P	604	HEC	CBB-CAB-C3B	-4.22	119.00	127.43
3	M	602	HEC	CHC-C4B-NB	4.22	129.05	124.45
3	Q	606	HEC	CHC-C4B-NB	4.22	129.04	124.45
3	E	604	HEC	CBB-CAB-C3B	-4.21	119.02	127.43
3	I	607	HEC	CBB-CAB-C3B	-4.20	119.04	127.43
3	T	602	HEC	CHC-C4B-NB	4.20	129.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	606	HEC	CHC-C4B-NB	4.20	129.02	124.45
3	U	601	HEC	CBB-CAB-C3B	-4.20	119.05	127.43
3	H	606	HEC	CHC-C4B-NB	4.19	129.02	124.45
3	R	600	HEC	CHC-C4B-NB	4.19	129.02	124.45
3	F	602	HEC	CHC-C4B-NB	4.17	129.00	124.45
3	A	606	HEC	CHC-C4B-NB	4.17	129.00	124.45
3	P	602	HEC	CHC-C4B-NB	4.16	128.99	124.45
3	C	602	HEC	CHC-C4B-NB	4.16	128.98	124.45
3	D	604	HEC	CBB-CAB-C3B	-4.16	119.13	127.43
3	T	606	HEC	CHC-C4B-NB	4.16	128.98	124.45
3	C	606	HEC	CHC-C4B-NB	4.15	128.98	124.45
3	G	603	HEC	CAA-CBA-CGA	4.15	124.68	113.67
3	I	602	HEC	CBB-CAB-C3B	-4.14	119.17	127.43
3	J	604	HEC	CBB-CAB-C3B	-4.13	119.18	127.43
3	H	607	HEC	CHC-C4B-NB	4.13	128.95	124.45
3	J	606	HEC	CHC-C4B-NB	4.12	128.94	124.45
3	T	606	HEC	CBB-CAB-C3B	-4.12	119.21	127.43
3	D	601	HEC	CBC-CAC-C3C	-4.11	119.21	127.43
3	U	602	HEC	CBB-CAB-C3B	-4.11	119.22	127.43
3	H	602	HEC	CHC-C4B-NB	4.10	128.92	124.45
3	W	606	HEC	CHC-C4B-NB	4.08	128.89	124.45
3	R	605	HEC	CHC-C4B-NB	4.07	128.89	124.45
3	K	603	HEC	CAA-CBA-CGA	4.07	124.46	113.67
3	S	606	HEC	CBB-CAB-C3B	-4.07	119.30	127.43
3	R	604	HEC	CBB-CAB-C3B	-4.07	119.30	127.43
3	U	605	HEC	CHC-C4B-NB	4.07	128.88	124.45
3	T	605	HEC	CHC-C4B-NB	4.06	128.88	124.45
3	L	604	HEC	CBB-CAB-C3B	-4.06	119.31	127.43
3	H	602	HEC	CBB-CAB-C3B	-4.05	119.34	127.43
3	D	605	HEC	CHC-C4B-NB	4.05	128.86	124.45
3	M	604	HEC	CBB-CAB-C3B	-4.04	119.36	127.43
3	X	604	HEC	CBB-CAB-C3B	-4.03	119.39	127.43
3	E	606	HEC	CBB-CAB-C3B	-4.02	119.39	127.43
3	P	605	HEC	CHC-C4B-NB	4.02	128.83	124.45
3	D	602	HEC	CHC-C4B-NB	4.02	128.83	124.45
3	K	604	HEC	CBB-CAB-C3B	-4.02	119.41	127.43
3	M	606	HEC	CBB-CAB-C3B	-4.02	119.41	127.43
3	D	607	HEC	CBB-CAB-C3B	-4.00	119.45	127.43
3	E	605	HEC	CHC-C4B-NB	3.99	128.80	124.45
3	L	605	HEC	CBB-CAB-C3B	-3.99	119.46	127.43
3	S	605	HEC	CHC-C4B-NB	3.99	128.79	124.45
3	L	602	HEC	CHC-C4B-NB	3.98	128.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	606	HEC	CBB-CAB-C3B	-3.98	119.48	127.43
3	U	606	HEC	CBB-CAB-C3B	-3.98	119.48	127.43
3	X	606	HEC	CBB-CAB-C3B	-3.97	119.49	127.43
3	B	607	HEC	CHC-C4B-NB	3.97	128.77	124.45
3	E	607	HEC	CHC-C4B-NB	3.97	128.77	124.45
3	V	605	HEC	CHC-C4B-NB	3.96	128.77	124.45
3	H	600	HEC	CBB-CAB-C3B	-3.96	119.52	127.43
3	V	602	HEC	CBB-CAB-C3B	-3.96	119.52	127.43
3	L	600	HEC	CBB-CAB-C3B	-3.95	119.54	127.43
3	G	605	HEC	CHC-C4B-NB	3.95	128.75	124.45
3	Q	605	HEC	CHC-C4B-NB	3.95	128.75	124.45
3	O	604	HEC	CBB-CAB-C3B	-3.95	119.55	127.43
3	B	604	HEC	CBB-CAB-C3B	-3.94	119.55	127.43
3	F	600	HEC	CBB-CAB-C3B	-3.94	119.56	127.43
3	W	606	HEC	CBB-CAB-C3B	-3.94	119.56	127.43
3	A	605	HEC	CHC-C4B-NB	3.94	128.74	124.45
3	R	602	HEC	CBB-CAB-C3B	-3.93	119.57	127.43
3	A	604	HEC	CBB-CAB-C3B	-3.93	119.58	127.43
3	V	604	HEC	CBB-CAB-C3B	-3.93	119.58	127.43
3	U	607	HEC	CHC-C4B-NB	3.93	128.73	124.45
3	B	605	HEC	CHC-C4B-NB	3.92	128.72	124.45
3	O	607	HEC	CHC-C4B-NB	3.92	128.72	124.45
3	Q	607	HEC	CHC-C4B-NB	3.92	128.72	124.45
3	I	606	HEC	CBB-CAB-C3B	-3.92	119.61	127.43
3	R	603	HEC	CAA-CBA-CGA	3.91	124.05	113.67
3	F	605	HEC	CHC-C4B-NB	3.91	128.71	124.45
3	V	601	HEC	CBB-CAB-C3B	-3.91	119.62	127.43
3	T	604	HEC	CBB-CAB-C3B	-3.91	119.63	127.43
3	W	604	HEC	CBB-CAB-C3B	-3.90	119.64	127.43
3	T	607	HEC	CHC-C4B-NB	3.89	128.69	124.45
3	W	607	HEC	CHC-C4B-NB	3.89	128.69	124.45
3	K	605	HEC	CHC-C4B-NB	3.89	128.69	124.45
3	P	602	HEC	CBB-CAB-C3B	-3.89	119.66	127.43
3	U	604	HEC	CBB-CAB-C3B	-3.88	119.67	127.43
3	N	602	HEC	CBB-CAB-C3B	-3.88	119.68	127.43
3	I	605	HEC	CHC-C4B-NB	3.88	128.67	124.45
3	L	601	HEC	CBB-CAB-C3B	-3.88	119.69	127.43
3	I	602	HEC	CHC-C4B-NB	3.87	128.66	124.45
3	P	600	HEC	CBB-CAB-C3B	-3.86	119.71	127.43
3	B	606	HEC	CBB-CAB-C3B	-3.86	119.71	127.43
3	F	602	HEC	CBB-CAB-C3B	-3.86	119.72	127.43
3	O	604	HEC	CBC-CAC-C3C	-3.86	119.72	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	607	HEC	CHC-C4B-NB	3.86	128.65	124.45
3	C	602	HEC	CBB-CAB-C3B	-3.86	119.73	127.43
3	W	602	HEC	CBB-CAB-C3B	-3.85	119.74	127.43
3	G	602	HEC	CBB-CAB-C3B	-3.84	119.76	127.43
3	X	607	HEC	CHC-C4B-NB	3.84	128.63	124.45
3	A	602	HEC	CBB-CAB-C3B	-3.84	119.77	127.43
3	L	606	HEC	CBB-CAB-C3B	-3.83	119.77	127.43
3	N	607	HEC	CBB-CAB-C3B	-3.82	119.79	127.43
3	X	606	HEC	CBC-CAC-C3C	-3.82	119.80	127.43
3	W	605	HEC	CHC-C4B-NB	3.82	128.61	124.45
3	X	601	HEC	CBB-CAB-C3B	-3.82	119.81	127.43
3	J	606	HEC	CBB-CAB-C3B	-3.81	119.81	127.43
3	C	600	HEC	CBB-CAB-C3B	-3.81	119.81	127.43
3	Q	600	HEC	CBB-CAB-C3B	-3.81	119.81	127.43
3	G	604	HEC	CBB-CAB-C3B	-3.81	119.82	127.43
3	N	600	HEC	CBB-CAB-C3B	-3.81	119.83	127.43
3	K	600	HEC	CBB-CAB-C3B	-3.81	119.83	127.43
3	Q	602	HEC	CBB-CAB-C3B	-3.80	119.85	127.43
3	H	607	HEC	CBB-CAB-C3B	-3.79	119.86	127.43
3	R	606	HEC	CBB-CAB-C3B	-3.79	119.86	127.43
3	X	600	HEC	CBB-CAB-C3B	-3.79	119.86	127.43
3	X	605	HEC	CHC-C4B-NB	3.78	128.57	124.45
3	H	605	HEC	CHC-C4B-NB	3.78	128.57	124.45
3	J	602	HEC	CBB-CAB-C3B	-3.76	119.91	127.43
3	S	606	HEC	CBC-CAC-C3C	-3.76	119.92	127.43
3	N	604	HEC	CBB-CAB-C3B	-3.76	119.92	127.43
3	O	605	HEC	CHC-C4B-NB	3.76	128.54	124.45
3	G	600	HEC	CBB-CAB-C3B	-3.75	119.94	127.43
3	B	602	HEC	CBB-CAB-C3B	-3.75	119.94	127.43
3	T	600	HEC	CBB-CAB-C3B	-3.75	119.95	127.43
3	P	606	HEC	CBB-CAB-C3B	-3.74	119.95	127.43
3	C	607	HEC	CHC-C4B-NB	3.74	128.52	124.45
3	U	600	HEC	CBB-CAB-C3B	-3.74	119.96	127.43
3	D	601	HEC	CBB-CAB-C3B	-3.74	119.96	127.43
3	V	607	HEC	CHC-C4B-NB	3.73	128.52	124.45
3	L	602	HEC	CBB-CAB-C3B	-3.73	119.98	127.43
3	C	607	HEC	CBB-CAB-C3B	-3.73	119.98	127.43
3	H	601	HEC	CBB-CAB-C3B	-3.72	120.00	127.43
3	O	602	HEC	CBB-CAB-C3B	-3.71	120.02	127.43
3	L	606	HEC	CBC-CAC-C3C	-3.71	120.02	127.43
3	M	600	HEC	CBB-CAB-C3B	-3.70	120.04	127.43
3	F	604	HEC	CBB-CAB-C3B	-3.69	120.05	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	HEC	CBB-CAB-C3B	-3.69	120.06	127.43
3	A	601	HEC	CBB-CAB-C3B	-3.69	120.07	127.43
3	K	607	HEC	CBB-CAB-C3B	-3.68	120.07	127.43
3	W	601	HEC	CBB-CAB-C3B	-3.68	120.07	127.43
3	G	607	HEC	CHC-C4B-NB	3.68	128.46	124.45
3	S	607	HEC	CHC-C4B-NB	3.68	128.46	124.45
3	Q	606	HEC	CBC-CAC-C3C	-3.67	120.09	127.43
3	X	602	HEC	CBB-CAB-C3B	-3.67	120.10	127.43
3	G	606	HEC	CBB-CAB-C3B	-3.67	120.11	127.43
3	A	604	HEC	CBC-CAC-C3C	-3.67	120.11	127.43
3	R	607	HEC	CHC-C4B-NB	3.66	128.44	124.45
3	K	604	HEC	CBC-CAC-C3C	-3.66	120.11	127.43
3	B	606	HEC	CBC-CAC-C3C	-3.66	120.11	127.43
3	F	601	HEC	CBB-CAB-C3B	-3.66	120.11	127.43
3	M	601	HEC	CBB-CAB-C3B	-3.66	120.12	127.43
3	M	607	HEC	CHC-C4B-NB	3.65	128.43	124.45
3	B	605	HEC	CBB-CAB-C3B	-3.65	120.13	127.43
3	K	602	HEC	CBB-CAB-C3B	-3.65	120.14	127.43
3	L	607	HEC	CHC-C4B-NB	3.65	128.43	124.45
3	T	602	HEC	CBB-CAB-C3B	-3.65	120.14	127.43
3	J	606	HEC	CBC-CAC-C3C	-3.65	120.15	127.43
3	I	600	HEC	CBB-CAB-C3B	-3.64	120.16	127.43
3	F	607	HEC	CHC-C4B-NB	3.64	128.41	124.45
3	A	606	HEC	CBB-CAB-C3B	-3.64	120.17	127.43
3	S	600	HEC	CBB-CAB-C3B	-3.63	120.18	127.43
3	X	607	HEC	CBB-CAB-C3B	-3.63	120.19	127.43
3	O	600	HEC	CBB-CAB-C3B	-3.60	120.23	127.43
3	K	606	HEC	CBC-CAC-C3C	-3.60	120.23	127.43
3	N	607	HEC	CHC-C4B-NB	3.60	128.37	124.45
3	D	607	HEC	CHC-C4B-NB	3.59	128.37	124.45
3	K	607	HEC	CHC-C4B-NB	3.59	128.37	124.45
3	E	600	HEC	CBB-CAB-C3B	-3.59	120.26	127.43
3	B	607	HEC	CBB-CAB-C3B	-3.59	120.26	127.43
3	D	604	HEC	CBD-CAD-C3D	-3.59	102.61	112.53
3	E	607	HEC	CBB-CAB-C3B	-3.58	120.28	127.43
3	E	601	HEC	CBB-CAB-C3B	-3.58	120.28	127.43
3	I	604	HEC	CBC-CAC-C3C	-3.58	120.28	127.43
3	U	606	HEC	CBC-CAC-C3C	-3.58	120.28	127.43
3	O	601	HEC	CBB-CAB-C3B	-3.57	120.30	127.43
3	J	607	HEC	CHC-C4B-NB	3.57	128.34	124.45
3	I	605	HEC	CBB-CAB-C3B	-3.56	120.32	127.43
3	M	607	HEC	CBB-CAB-C3B	-3.56	120.32	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	606	HEC	CBC-CAC-C3C	-3.55	120.33	127.43
3	A	607	HEC	CBB-CAB-C3B	-3.54	120.35	127.43
3	S	605	HEC	CBB-CAB-C3B	-3.54	120.36	127.43
3	T	605	HEC	CBB-CAB-C3B	-3.53	120.37	127.43
3	F	606	HEC	CBC-CAC-C3C	-3.53	120.38	127.43
3	L	604	HEC	CBC-CAC-C3C	-3.53	120.38	127.43
3	N	601	HEC	CBB-CAB-C3B	-3.53	120.38	127.43
3	A	600	HEC	CBB-CAB-C3B	-3.52	120.39	127.43
3	Q	601	HEC	CBB-CAB-C3B	-3.52	120.39	127.43
3	K	606	HEC	CBB-CAB-C3B	-3.52	120.41	127.43
3	J	601	HEC	CBC-CAC-C3C	-3.51	120.41	127.43
3	E	602	HEC	CBB-CAB-C3B	-3.51	120.42	127.43
3	R	600	HEC	CBB-CAB-C3B	-3.51	120.42	127.43
3	E	605	HEC	CBB-CAB-C3B	-3.51	120.43	127.43
3	J	600	HEC	CBB-CAB-C3B	-3.49	120.45	127.43
3	X	605	HEC	CBB-CAB-C3B	-3.49	120.45	127.43
3	W	606	HEC	CBC-CAC-C3C	-3.49	120.46	127.43
3	S	607	HEC	CBB-CAB-C3B	-3.49	120.46	127.43
3	O	607	HEC	CBB-CAB-C3B	-3.48	120.47	127.43
3	D	600	HEC	CBB-CAB-C3B	-3.48	120.47	127.43
3	H	604	HEC	CBC-CAC-C3C	-3.48	120.48	127.43
3	A	607	HEC	CHC-C4B-NB	3.48	128.24	124.45
3	V	605	HEC	CBB-CAB-C3B	-3.47	120.49	127.43
3	R	601	HEC	CBB-CAB-C3B	-3.47	120.50	127.43
3	D	605	HEC	CBB-CAB-C3B	-3.47	120.50	127.43
3	M	601	HEC	CBC-CAC-C3C	-3.46	120.51	127.43
3	S	601	HEC	CBB-CAB-C3B	-3.46	120.51	127.43
3	F	602	HEC	CBC-CAC-C3C	-3.46	120.52	127.43
3	T	601	HEC	CBB-CAB-C3B	-3.46	120.52	127.43
3	C	604	HEC	CBC-CAC-C3C	-3.45	120.54	127.43
3	J	605	HEC	CHC-C4B-NB	3.44	128.19	124.45
3	B	600	HEC	CBB-CAB-C3B	-3.44	120.57	127.43
3	F	604	HEC	CBC-CAC-C3C	-3.43	120.57	127.43
3	J	601	HEC	CBB-CAB-C3B	-3.43	120.58	127.43
3	K	605	HEC	CBB-CAB-C3B	-3.42	120.59	127.43
3	I	604	HEC	CBD-CAD-C3D	-3.42	103.08	112.53
3	A	606	HEC	CBC-CAC-C3C	-3.41	120.61	127.43
3	B	601	HEC	CBB-CAB-C3B	-3.41	120.61	127.43
3	L	601	HEC	CBC-CAC-C3C	-3.40	120.64	127.43
3	W	600	HEC	CBB-CAB-C3B	-3.40	120.65	127.43
3	Q	607	HEC	CBB-CAB-C3B	-3.39	120.67	127.43
3	G	601	HEC	CBC-CAC-C3C	-3.38	120.68	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	607	HEC	CBB-CAB-C3B	-3.38	120.68	127.43
3	C	602	HEC	CBC-CAC-C3C	-3.38	120.69	127.43
3	W	605	HEC	CBB-CAB-C3B	-3.38	120.69	127.43
3	K	605	HEC	CBC-CAC-C3C	-3.37	120.69	127.43
3	Q	604	HEC	CBC-CAC-C3C	-3.36	120.72	127.43
3	E	606	HEC	CBC-CAC-C3C	-3.36	120.72	127.43
3	I	601	HEC	CBB-CAB-C3B	-3.36	120.73	127.43
3	T	604	HEC	CBC-CAC-C3C	-3.35	120.73	127.43
3	P	607	HEC	CBB-CAB-C3B	-3.35	120.74	127.43
3	F	605	HEC	CBB-CAB-C3B	-3.35	120.74	127.43
3	T	607	HEC	CBB-CAB-C3B	-3.34	120.77	127.43
3	C	605	HEC	CBB-CAB-C3B	-3.33	120.77	127.43
3	O	606	HEC	CBC-CAC-C3C	-3.32	120.80	127.43
3	J	607	HEC	CBB-CAB-C3B	-3.32	120.80	127.43
3	V	604	HEC	CBC-CAC-C3C	-3.32	120.80	127.43
3	G	607	HEC	CBB-CAB-C3B	-3.32	120.80	127.43
3	H	601	HEC	CBC-CAC-C3C	-3.31	120.82	127.43
3	H	604	HEC	CBD-CAD-C3D	-3.31	103.39	112.53
3	K	604	HEC	CBD-CAD-C3D	-3.31	103.39	112.53
3	Q	601	HEC	CBC-CAC-C3C	-3.30	120.83	127.43
3	V	600	HEC	CBB-CAB-C3B	-3.30	120.83	127.43
3	U	607	HEC	CBB-CAB-C3B	-3.30	120.84	127.43
3	N	606	HEC	CBC-CAC-C3C	-3.30	120.84	127.43
3	R	605	HEC	CBB-CAB-C3B	-3.29	120.85	127.43
3	R	606	HEC	CBC-CAC-C3C	-3.29	120.87	127.43
3	A	601	HEC	CBC-CAC-C3C	-3.28	120.89	127.43
3	E	604	HEC	CBC-CAC-C3C	-3.27	120.89	127.43
3	U	604	HEC	CBC-CAC-C3C	-3.26	120.91	127.43
3	W	604	HEC	CBD-CAD-C3D	-3.26	103.51	112.53
3	A	605	HEC	CBB-CAB-C3B	-3.26	120.92	127.43
3	G	606	HEC	CBC-CAC-C3C	-3.25	120.93	127.43
3	S	601	HEC	CBC-CAC-C3C	-3.25	120.93	127.43
3	F	601	HEC	CBC-CAC-C3C	-3.25	120.93	127.43
3	Q	605	HEC	CBB-CAB-C3B	-3.25	120.94	127.43
3	D	605	HEC	CBC-CAC-C3C	-3.24	120.96	127.43
3	N	604	HEC	CBD-CAD-C3D	-3.23	103.60	112.53
3	F	607	HEC	CBB-CAB-C3B	-3.23	120.98	127.43
3	L	607	HEC	CBB-CAB-C3B	-3.23	120.98	127.43
3	V	604	HEC	CBD-CAD-C3D	-3.23	103.61	112.53
3	P	605	HEC	CBB-CAB-C3B	-3.22	120.99	127.43
3	T	604	HEC	CBD-CAD-C3D	-3.22	103.63	112.53
3	W	604	HEC	CBC-CAC-C3C	-3.22	121.00	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	601	HEC	CBC-CAC-C3C	-3.22	121.01	127.43
3	O	604	HEC	CBD-CAD-C3D	-3.21	103.65	112.53
3	X	601	HEC	CBC-CAC-C3C	-3.20	121.03	127.43
3	A	604	HEC	CBD-CAD-C3D	-3.20	103.68	112.53
3	G	604	HEC	CBC-CAC-C3C	-3.20	121.04	127.43
3	B	604	HEC	CBD-CAD-C3D	-3.20	103.69	112.53
3	T	606	HEC	CBC-CAC-C3C	-3.20	121.04	127.43
3	L	604	HEC	CBD-CAD-C3D	-3.20	103.69	112.53
3	R	607	HEC	CBB-CAB-C3B	-3.20	121.05	127.43
3	W	607	HEC	CBB-CAB-C3B	-3.19	121.05	127.43
3	H	605	HEC	CBB-CAB-C3B	-3.19	121.06	127.43
3	T	603	HEC	C1C-CHC-C4B	-3.19	114.82	124.66
3	M	604	HEC	CBD-CAD-C3D	-3.19	103.72	112.53
3	P	606	HEC	CBC-CAC-C3C	-3.19	121.06	127.43
3	E	604	HEC	CBD-CAD-C3D	-3.18	103.73	112.53
3	S	604	HEC	CBD-CAD-C3D	-3.18	103.74	112.53
3	X	605	HEC	CBC-CAC-C3C	-3.18	121.08	127.43
3	P	601	HEC	CBB-CAB-C3B	-3.17	121.10	127.43
3	M	604	HEC	CBC-CAC-C3C	-3.17	121.10	127.43
3	Q	605	HEC	CBC-CAC-C3C	-3.17	121.10	127.43
3	P	605	HEC	CBC-CAC-C3C	-3.17	121.10	127.43
3	P	604	HEC	CBD-CAD-C3D	-3.17	103.78	112.53
3	T	601	HEC	CBC-CAC-C3C	-3.17	121.11	127.43
3	F	604	HEC	CBD-CAD-C3D	-3.15	103.81	112.53
3	N	604	HEC	CBC-CAC-C3C	-3.15	121.14	127.43
3	U	602	HEC	CBC-CAC-C3C	-3.14	121.16	127.43
3	U	601	HEC	CBC-CAC-C3C	-3.14	121.16	127.43
3	J	604	HEC	CBD-CAD-C3D	-3.13	103.87	112.53
3	M	605	HEC	CBC-CAC-C3C	-3.13	121.17	127.43
3	U	604	HEC	CBD-CAD-C3D	-3.13	103.87	112.53
3	J	605	HEC	CBB-CAB-C3B	-3.13	121.18	127.43
3	R	601	HEC	CBC-CAC-C3C	-3.13	121.18	127.43
3	E	601	HEC	CBC-CAC-C3C	-3.13	121.18	127.43
3	S	604	HEC	CBC-CAC-C3C	-3.12	121.19	127.43
3	T	602	HEC	CBC-CAC-C3C	-3.12	121.20	127.43
3	D	606	HEC	CBC-CAC-C3C	-3.12	121.20	127.43
3	X	604	HEC	CBC-CAC-C3C	-3.12	121.20	127.43
3	I	605	HEC	CBC-CAC-C3C	-3.11	121.22	127.43
3	D	602	HEC	CBB-CAB-C3B	-3.10	121.23	127.43
3	S	602	HEC	CBC-CAC-C3C	-3.10	121.23	127.43
3	C	606	HEC	CBC-CAC-C3C	-3.09	121.25	127.43
3	M	605	HEC	CBB-CAB-C3B	-3.09	121.25	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	602	HEC	CBC-CAC-C3C	-3.09	121.26	127.43
3	K	601	HEC	CBB-CAB-C3B	-3.09	121.26	127.43
3	R	602	HEC	CBC-CAC-C3C	-3.08	121.27	127.43
3	G	605	HEC	CBB-CAB-C3B	-3.08	121.28	127.43
3	K	602	HEC	CBC-CAC-C3C	-3.08	121.28	127.43
3	V	601	HEC	CBC-CAC-C3C	-3.08	121.28	127.43
3	B	601	HEC	CBC-CAC-C3C	-3.08	121.29	127.43
3	J	607	HEC	CBC-CAC-C3C	-3.08	121.29	127.43
3	G	605	HEC	CBC-CAC-C3C	-3.07	121.29	127.43
3	Q	604	HEC	CBD-CAD-C3D	-3.07	104.05	112.53
3	W	605	HEC	CBC-CAC-C3C	-3.07	121.30	127.43
3	N	605	HEC	CBB-CAB-C3B	-3.06	121.32	127.43
3	G	604	HEC	CBD-CAD-C3D	-3.06	104.08	112.53
3	C	604	HEC	CBD-CAD-C3D	-3.06	104.08	112.53
3	V	605	HEC	CBC-CAC-C3C	-3.05	121.33	127.43
3	X	604	HEC	CBD-CAD-C3D	-3.05	104.10	112.53
3	D	604	HEC	CBC-CAC-C3C	-3.05	121.34	127.43
3	C	601	HEC	CBC-CAC-C3C	-3.05	121.35	127.43
3	B	605	HEC	CBC-CAC-C3C	-3.03	121.37	127.43
3	O	601	HEC	CBC-CAC-C3C	-3.03	121.38	127.43
3	P	601	HEC	CBC-CAC-C3C	-3.03	121.38	127.43
3	C	605	HEC	CBC-CAC-C3C	-3.03	121.38	127.43
3	I	602	HEC	CBC-CAC-C3C	-3.02	121.39	127.43
3	U	605	HEC	CBB-CAB-C3B	-3.02	121.40	127.43
3	N	607	HEC	CBC-CAC-C3C	-3.02	121.40	127.43
3	P	602	HEC	CBC-CAC-C3C	-3.02	121.40	127.43
3	Q	602	HEC	CBC-CAC-C3C	-3.02	121.40	127.43
3	R	604	HEC	CBD-CAD-C3D	-3.01	104.20	112.53
3	O	605	HEC	CBC-CAC-C3C	-3.00	121.43	127.43
3	N	601	HEC	CBC-CAC-C3C	-3.00	121.44	127.43
3	L	602	HEC	CBC-CAC-C3C	-2.99	121.45	127.43
3	J	604	HEC	CBC-CAC-C3C	-2.99	121.45	127.43
3	O	602	HEC	CBC-CAC-C3C	-2.99	121.45	127.43
3	E	605	HEC	CBC-CAC-C3C	-2.99	121.46	127.43
3	P	604	HEC	CBC-CAC-C3C	-2.97	121.50	127.43
3	R	605	HEC	CBC-CAC-C3C	-2.97	121.51	127.43
3	M	606	HEC	CBC-CAC-C3C	-2.96	121.52	127.43
3	H	602	HEC	CBC-CAC-C3C	-2.96	121.52	127.43
3	M	602	HEC	CBC-CAC-C3C	-2.96	121.52	127.43
3	I	607	HEC	CBC-CAC-C3C	-2.96	121.52	127.43
3	H	606	HEC	CBC-CAC-C3C	-2.95	121.53	127.43
3	G	600	HEC	CBC-CAC-C3C	-2.95	121.53	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	605	HEC	CBC-CAC-C3C	-2.95	121.55	127.43
3	E	602	HEC	CBC-CAC-C3C	-2.94	121.55	127.43
3	P	607	HEC	CBC-CAC-C3C	-2.94	121.55	127.43
3	V	603	HEC	C1C-CHC-C4B	-2.94	115.58	124.66
3	K	600	HEC	CBC-CAC-C3C	-2.93	121.57	127.43
3	U	603	HEC	C1C-CHC-C4B	-2.93	115.61	124.66
3	A	602	HEC	CBC-CAC-C3C	-2.93	121.58	127.43
3	K	601	HEC	CHA-C4D-ND	2.92	129.16	123.86
3	K	607	HEC	CBC-CAC-C3C	-2.92	121.61	127.43
3	R	604	HEC	CBC-CAC-C3C	-2.92	121.61	127.43
3	P	604	HEC	CHD-C4C-NC	2.91	127.63	124.45
3	B	602	HEC	CBC-CAC-C3C	-2.91	121.61	127.43
3	T	607	HEC	CBC-CAC-C3C	-2.90	121.64	127.43
3	X	603	HEC	C1C-CHC-C4B	-2.90	115.71	124.66
3	O	600	HEC	CBC-CAC-C3C	-2.90	121.64	127.43
3	W	602	HEC	CBC-CAC-C3C	-2.89	121.65	127.43
3	C	607	HEC	CBC-CAC-C3C	-2.89	121.65	127.43
3	I	601	HEC	CHB-C1B-NB	2.89	129.10	123.86
3	U	605	HEC	CBC-CAC-C3C	-2.88	121.67	127.43
3	K	601	HEC	CBC-CAC-C3C	-2.88	121.67	127.43
3	J	603	HEC	C1C-CHC-C4B	-2.88	115.78	124.66
3	E	604	HEC	CHD-C4C-NC	2.87	127.58	124.45
3	A	605	HEC	CBC-CAC-C3C	-2.87	121.70	127.43
3	S	605	HEC	CBC-CAC-C3C	-2.86	121.71	127.43
3	W	607	HEC	CBC-CAC-C3C	-2.86	121.72	127.43
3	E	603	HEC	C1C-CHC-C4B	-2.85	115.86	124.66
3	R	603	HEC	C1C-CHC-C4B	-2.85	115.86	124.66
3	T	605	HEC	CBC-CAC-C3C	-2.85	121.74	127.43
3	U	604	HEC	CHA-C4D-ND	2.84	129.02	123.86
3	X	602	HEC	CBC-CAC-C3C	-2.84	121.76	127.43
3	S	607	HEC	CBC-CAC-C3C	-2.84	121.76	127.43
3	D	600	HEC	CBC-CAC-C3C	-2.84	121.77	127.43
3	J	600	HEC	CBC-CAC-C3C	-2.83	121.78	127.43
3	V	601	HEC	CHA-C4D-ND	2.83	128.99	123.86
3	D	602	HEC	CBC-CAC-C3C	-2.83	121.79	127.43
3	H	603	HEC	C1C-CHC-C4B	-2.83	115.94	124.66
3	G	602	HEC	CBC-CAC-C3C	-2.82	121.79	127.43
3	X	607	HEC	CBC-CAC-C3C	-2.82	121.79	127.43
3	L	605	HEC	CBC-CAC-C3C	-2.82	121.79	127.43
3	M	604	HEC	CHD-C4C-NC	2.82	127.52	124.45
3	M	603	HEC	C1C-CHC-C4B	-2.82	115.97	124.66
3	Q	601	HEC	CHA-C4D-ND	2.81	128.95	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	607	HEC	CHD-C4C-NC	2.80	127.51	124.45
3	K	603	HEC	C1C-CHC-C4B	-2.80	116.02	124.66
3	F	603	HEC	C1C-CHC-C4B	-2.80	116.03	124.66
3	D	607	HEC	CHD-C4C-NC	2.80	127.50	124.45
3	Q	603	HEC	C1C-CHC-C4B	-2.79	116.04	124.66
3	G	606	HEC	C4B-NB-C1B	2.79	110.37	105.82
3	D	604	HEC	CHA-C4D-ND	2.79	128.91	123.86
3	S	603	HEC	C1C-CHC-C4B	-2.78	116.07	124.66
3	F	607	HEC	CBC-CAC-C3C	-2.78	121.88	127.43
3	V	602	HEC	CBC-CAC-C3C	-2.78	121.88	127.43
3	D	601	HEC	O2D-CGD-CBD	2.77	122.77	114.00
3	G	604	HEC	CHA-C4D-ND	2.77	128.89	123.86
3	J	604	HEC	CHA-C1A-NA	2.77	127.47	124.45
3	A	607	HEC	CBC-CAC-C3C	-2.76	121.91	127.43
3	L	603	HEC	C1C-CHC-C4B	-2.76	116.13	124.66
3	B	603	HEC	C1C-CHC-C4B	-2.76	116.16	124.66
3	V	607	HEC	CBC-CAC-C3C	-2.75	121.93	127.43
3	J	602	HEC	CBC-CAC-C3C	-2.75	121.94	127.43
3	I	601	HEC	CHA-C4D-ND	2.75	128.85	123.86
3	H	607	HEC	CBC-CAC-C3C	-2.75	121.94	127.43
3	E	607	HEC	CBC-CAC-C3C	-2.74	121.95	127.43
3	W	604	HEC	CHA-C4D-ND	2.74	128.84	123.86
3	C	604	HEC	CHD-C4C-NC	2.74	127.44	124.45
3	G	603	HEC	C1C-CHC-C4B	-2.74	116.21	124.66
3	F	605	HEC	CBC-CAC-C3C	-2.74	121.96	127.43
3	D	603	HEC	C1A-C2A-C3A	-2.73	103.51	107.11
3	O	605	HEC	CBB-CAB-C3B	-2.73	121.98	127.43
3	P	603	HEC	C1C-CHC-C4B	-2.73	116.25	124.66
3	S	601	HEC	CHA-C4D-ND	2.72	128.80	123.86
3	C	601	HEC	CHA-C4D-ND	2.72	128.79	123.86
3	D	607	HEC	CBC-CAC-C3C	-2.72	122.01	127.43
3	I	603	HEC	C1C-CHC-C4B	-2.72	116.28	124.66
3	N	603	HEC	C1C-CHC-C4B	-2.71	116.31	124.66
3	J	601	HEC	CHA-C4D-ND	2.70	128.76	123.86
3	L	606	HEC	C4B-NB-C1B	2.70	110.22	105.82
3	G	600	HEC	CHA-C4D-ND	2.70	128.75	123.86
3	I	604	HEC	CHD-C1D-ND	2.69	128.74	123.86
3	I	607	HEC	CHD-C4C-NC	2.69	127.38	124.45
3	P	606	HEC	C4B-NB-C1B	2.69	110.21	105.82
3	E	607	HEC	CHD-C4C-NC	2.68	127.37	124.45
3	V	604	HEC	CHA-C4D-ND	2.68	128.72	123.86
3	G	601	HEC	CHA-C4D-ND	2.67	128.71	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	601	HEC	CHA-C4D-ND	2.67	128.71	123.86
3	A	601	HEC	CHA-C4D-ND	2.67	128.70	123.86
3	B	604	HEC	CHD-C4C-NC	2.67	127.36	124.45
3	X	601	HEC	CHA-C4D-ND	2.66	128.69	123.86
3	M	601	HEC	CHA-C4D-ND	2.66	128.69	123.86
3	U	604	HEC	CHD-C4C-NC	2.66	127.35	124.45
3	T	601	HEC	CHA-C4D-ND	2.66	128.68	123.86
3	B	606	HEC	C4B-NB-C1B	2.66	110.15	105.82
3	R	604	HEC	CHA-C4D-ND	2.65	128.67	123.86
3	I	606	HEC	CHA-C4D-ND	2.65	128.67	123.86
3	E	600	HEC	CBC-CAC-C3C	-2.65	122.14	127.43
3	N	605	HEC	CBC-CAC-C3C	-2.65	122.14	127.43
3	L	607	HEC	CHD-C4C-NC	2.64	127.33	124.45
3	H	601	HEC	CHA-C4D-ND	2.64	128.66	123.86
3	E	602	HEC	C4B-NB-C1B	2.64	110.13	105.82
3	G	607	HEC	CBC-CAC-C3C	-2.64	122.15	127.43
3	B	604	HEC	CBC-CAC-C3C	-2.64	122.15	127.43
3	C	606	HEC	C4B-NB-C1B	2.64	110.13	105.82
3	M	606	HEC	C4B-NB-C1B	2.64	110.13	105.82
3	S	604	HEC	CHA-C4D-ND	2.64	128.65	123.86
3	N	604	HEC	CHD-C4C-NC	2.64	127.33	124.45
3	M	601	HEC	O2D-CGD-CBD	2.64	122.34	114.00
3	N	604	HEC	CHA-C4D-ND	2.64	128.64	123.86
3	U	606	HEC	C4B-NB-C1B	2.63	110.11	105.82
3	V	600	HEC	CBC-CAC-C3C	-2.63	122.17	127.43
3	W	603	HEC	C1C-CHC-C4B	-2.63	116.54	124.66
3	M	600	HEC	CBC-CAC-C3C	-2.63	122.19	127.43
3	M	607	HEC	CHD-C4C-NC	2.62	127.31	124.45
3	G	602	HEC	C4B-NB-C1B	2.62	110.09	105.82
3	C	603	HEC	C1C-CHC-C4B	-2.61	116.60	124.66
3	S	600	HEC	CBC-CAC-C3C	-2.61	122.21	127.43
3	Q	604	HEC	CHD-C4C-NC	2.61	127.29	124.45
3	L	600	HEC	CBC-CAC-C3C	-2.61	122.22	127.43
3	T	600	HEC	CBC-CAC-C3C	-2.61	122.22	127.43
3	O	607	HEC	CHD-C4C-NC	2.60	127.29	124.45
3	D	606	HEC	C4B-NB-C1B	2.60	110.07	105.82
3	Q	600	HEC	CHA-C4D-ND	2.60	128.58	123.86
3	R	606	HEC	C4B-NB-C1B	2.60	110.06	105.82
3	N	600	HEC	CBC-CAC-C3C	-2.60	122.25	127.43
3	P	601	HEC	O2D-CGD-CBD	2.59	122.20	114.00
3	Q	604	HEC	CHA-C4D-ND	2.59	128.56	123.86
3	I	601	HEC	O2D-CGD-CBD	2.59	122.19	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	604	HEC	CHA-C4D-ND	2.59	128.56	123.86
3	V	601	HEC	O2D-CGD-CBD	2.59	122.18	114.00
3	I	600	HEC	CHD-C1D-ND	2.59	128.55	123.86
3	Q	607	HEC	CHD-C4C-NC	2.59	127.27	124.45
3	T	604	HEC	CHA-C4D-ND	2.59	128.55	123.86
3	G	601	HEC	O2D-CGD-CBD	2.58	122.17	114.00
3	I	605	HEC	CAD-C3D-C2D	2.58	132.87	127.07
3	D	603	HEC	CMC-C2C-C1C	-2.58	121.49	125.42
3	G	604	HEC	CBA-CAA-C2A	-2.58	105.39	112.53
3	N	601	HEC	O2D-CGD-CBD	2.58	122.16	114.00
3	K	602	HEC	C4B-NB-C1B	2.58	110.03	105.82
3	A	603	HEC	C1C-CHC-C4B	-2.58	116.71	124.66
3	I	605	HEC	CHA-C4D-ND	2.58	128.53	123.86
3	I	600	HEC	CHA-C4D-ND	2.58	128.53	123.86
3	W	601	HEC	CHA-C4D-ND	2.58	128.53	123.86
3	R	607	HEC	CBC-CAC-C3C	-2.58	122.29	127.43
3	X	604	HEC	CHA-C4D-ND	2.58	128.53	123.86
3	L	601	HEC	CHB-C1B-NB	2.57	128.52	123.86
3	G	605	HEC	CHD-C4C-NC	2.57	127.25	124.45
3	R	602	HEC	C4B-NB-C1B	2.57	110.00	105.82
3	H	604	HEC	CHA-C4D-ND	2.56	128.51	123.86
3	R	601	HEC	CHA-C4D-ND	2.56	128.51	123.86
3	J	604	HEC	CHD-C1D-ND	2.56	128.51	123.86
3	I	607	HEC	CHA-C1A-NA	2.56	127.24	124.45
3	J	604	HEC	CHA-C4D-ND	2.56	128.51	123.86
3	F	601	HEC	CHA-C4D-ND	2.56	128.51	123.86
3	P	600	HEC	CBC-CAC-C3C	-2.56	122.32	127.43
3	W	602	HEC	C4B-NB-C1B	2.56	109.99	105.82
3	F	604	HEC	CHA-C4D-ND	2.56	128.50	123.86
3	Q	601	HEC	O2D-CGD-CBD	2.56	122.08	114.00
3	F	606	HEC	C4B-NB-C1B	2.56	109.99	105.82
3	M	605	HEC	CHB-C1B-NB	2.56	128.50	123.86
3	B	601	HEC	CHA-C4D-ND	2.56	128.50	123.86
3	X	601	HEC	O2D-CGD-CBD	2.56	122.07	114.00
3	E	604	HEC	CHA-C4D-ND	2.56	128.49	123.86
3	P	604	HEC	CHA-C4D-ND	2.55	128.49	123.86
3	P	607	HEC	CHD-C4C-NC	2.55	127.23	124.45
3	H	601	HEC	CHD-C1D-ND	2.55	128.49	123.86
3	G	601	HEC	CHB-C1B-NB	2.55	128.49	123.86
3	N	606	HEC	C4B-NB-C1B	2.55	109.97	105.82
3	D	605	HEC	CBD-CAD-C3D	2.55	119.57	112.53
3	I	602	HEC	CAD-CBD-CGD	-2.55	106.91	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	HEC	CHA-C4D-ND	2.55	128.48	123.86
3	D	602	HEC	CHB-C1B-NB	2.54	128.47	123.86
3	L	604	HEC	CHA-C4D-ND	2.54	128.47	123.86
3	M	607	HEC	CBC-CAC-C3C	-2.54	122.35	127.43
3	G	604	HEC	CHA-C1A-NA	2.54	127.22	124.45
3	H	600	HEC	CHA-C4D-ND	2.54	128.46	123.86
3	O	605	HEC	CHA-C4D-ND	2.54	128.46	123.86
3	K	604	HEC	CBA-CAA-C2A	-2.54	105.52	112.53
3	I	606	HEC	CHA-C1A-NA	2.53	127.21	124.45
3	I	601	HEC	CHB-C1B-C2B	-2.53	120.07	127.43
3	M	604	HEC	CHA-C4D-ND	2.53	128.46	123.86
3	E	604	HEC	CBA-CAA-C2A	-2.53	105.53	112.53
3	B	607	HEC	CBC-CAC-C3C	-2.53	122.38	127.43
3	A	600	HEC	CBC-CAC-C3C	-2.53	122.38	127.43
3	J	600	HEC	CHA-C4D-ND	2.53	128.44	123.86
3	W	604	HEC	CHD-C4C-NC	2.53	127.20	124.45
3	J	604	HEC	CBA-CAA-C2A	-2.53	105.55	112.53
3	U	607	HEC	CBC-CAC-C3C	-2.53	122.39	127.43
3	W	606	HEC	C4B-NB-C1B	2.53	109.94	105.82
3	L	605	HEC	CHD-C4C-NC	2.53	127.20	124.45
3	J	604	HEC	CHD-C4C-NC	2.52	127.20	124.45
3	F	601	HEC	O2D-CGD-CBD	2.52	121.97	114.00
3	O	603	HEC	C1C-CHC-C4B	-2.52	116.87	124.66
3	C	600	HEC	CBC-CAC-C3C	-2.52	122.39	127.43
3	O	604	HEC	CHA-C4D-ND	2.52	128.43	123.86
3	K	601	HEC	O2D-CGD-CBD	2.52	121.97	114.00
3	E	606	HEC	C4B-NB-C1B	2.52	109.93	105.82
3	H	607	HEC	CHD-C4C-NC	2.52	127.20	124.45
3	O	604	HEC	CBA-CAA-C2A	-2.52	105.56	112.53
3	B	604	HEC	CHB-C1B-NB	2.52	128.43	123.86
3	B	602	HEC	CAD-CBD-CGD	-2.52	106.99	113.67
3	B	600	HEC	CBC-CAC-C3C	-2.52	122.40	127.43
3	K	601	HEC	CHD-C1D-ND	2.52	128.42	123.86
3	X	600	HEC	CHA-C4D-ND	2.52	128.42	123.86
3	K	607	HEC	CHD-C4C-NC	2.52	127.19	124.45
3	W	602	HEC	CHB-C1B-NB	2.52	128.42	123.86
3	Q	606	HEC	C4B-NB-C1B	2.51	109.92	105.82
3	Q	607	HEC	CBC-CAC-C3C	-2.51	122.41	127.43
3	K	604	HEC	CHD-C4C-NC	2.51	127.19	124.45
3	O	601	HEC	CHB-C1B-NB	2.51	128.41	123.86
3	B	604	HEC	CHA-C4D-ND	2.51	128.41	123.86
3	N	607	HEC	CHD-C4C-NC	2.51	127.19	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	604	HEC	CHB-C1B-NB	2.51	128.41	123.86
3	Q	602	HEC	C4B-NB-C1B	2.51	109.91	105.82
3	I	606	HEC	C4B-NB-C1B	2.50	109.90	105.82
3	I	600	HEC	CHB-C1B-NB	2.50	128.40	123.86
3	X	602	HEC	C4B-NB-C1B	2.50	109.90	105.82
3	U	602	HEC	C4B-NB-C1B	2.50	109.90	105.82
3	B	600	HEC	CHA-C4D-ND	2.50	128.39	123.86
3	O	602	HEC	C4B-NB-C1B	2.50	109.89	105.82
3	G	602	HEC	CHB-C1B-NB	2.50	128.39	123.86
3	A	604	HEC	CHA-C4D-ND	2.50	128.39	123.86
3	J	607	HEC	CHD-C4C-NC	2.50	127.17	124.45
3	L	601	HEC	CHA-C4D-ND	2.50	128.39	123.86
3	N	601	HEC	CHA-C4D-ND	2.50	128.39	123.86
3	P	602	HEC	C4B-NB-C1B	2.49	109.89	105.82
3	U	600	HEC	CBC-CAC-C3C	-2.49	122.45	127.43
3	L	602	HEC	C4B-NB-C1B	2.49	109.89	105.82
3	X	600	HEC	CBC-CAC-C3C	-2.49	122.45	127.43
3	I	602	HEC	CHB-C1B-NB	2.49	128.38	123.86
3	L	604	HEC	CHA-C1A-NA	2.49	127.17	124.45
3	D	604	HEC	CHD-C1D-ND	2.49	128.38	123.86
3	R	604	HEC	CHD-C4C-NC	2.49	127.16	124.45
3	T	600	HEC	CHA-C4D-ND	2.49	128.37	123.86
3	S	601	HEC	O2D-CGD-CBD	2.48	121.85	114.00
3	R	605	HEC	CAD-C3D-C2D	2.48	132.64	127.07
3	B	601	HEC	O2D-CGD-CBD	2.48	121.85	114.00
3	M	607	HEC	CHA-C4D-ND	2.48	128.36	123.86
3	C	604	HEC	CHB-C1B-NB	2.48	128.36	123.86
3	M	603	HEC	CHB-C4A-NA	-2.48	121.75	124.45
3	Q	601	HEC	CHB-C1B-NB	2.48	128.36	123.86
3	T	606	HEC	C4B-NB-C1B	2.48	109.86	105.82
3	C	602	HEC	C4B-NB-C1B	2.48	109.86	105.82
3	B	607	HEC	CHD-C4C-NC	2.48	127.15	124.45
3	E	600	HEC	CHA-C4D-ND	2.48	128.35	123.86
3	C	600	HEC	CHA-C4D-ND	2.47	128.35	123.86
3	F	600	HEC	CHA-C4D-ND	2.47	128.35	123.86
3	J	601	HEC	CHD-C1D-ND	2.47	128.35	123.86
3	W	606	HEC	O2A-CGA-CBA	2.47	121.81	114.00
3	V	606	HEC	C4B-NB-C1B	2.47	109.85	105.82
3	C	601	HEC	CHB-C1B-NB	2.47	128.34	123.86
3	M	605	HEC	CHD-C4C-NC	2.47	127.14	124.45
3	A	602	HEC	C4B-NB-C1B	2.47	109.85	105.82
3	L	606	HEC	CHB-C1B-NB	2.47	128.34	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	607	HEC	CHD-C4C-NC	2.47	127.14	124.45
3	I	600	HEC	CBC-CAC-C3C	-2.47	122.50	127.43
3	N	602	HEC	CAD-CBD-CGD	-2.46	107.13	113.67
3	D	603	HEC	CHB-C4A-NA	-2.46	121.77	124.45
3	I	604	HEC	CHD-C4C-NC	2.46	127.14	124.45
3	K	606	HEC	C4B-NB-C1B	2.46	109.84	105.82
3	X	606	HEC	C4B-NB-C1B	2.46	109.83	105.82
3	H	600	HEC	CHD-C1D-ND	2.46	128.32	123.86
3	S	600	HEC	CHD-C1D-ND	2.46	128.32	123.86
3	Q	607	HEC	C4B-NB-C1B	2.46	109.83	105.82
3	A	606	HEC	C4B-NB-C1B	2.46	109.83	105.82
3	F	602	HEC	C4B-NB-C1B	2.46	109.83	105.82
3	U	604	HEC	CBA-CAA-C2A	-2.46	105.73	112.53
3	D	605	HEC	CHD-C4C-NC	2.46	127.13	124.45
3	H	601	HEC	O2D-CGD-CBD	2.46	121.76	114.00
3	A	604	HEC	CHD-C4C-NC	2.46	127.13	124.45
3	S	602	HEC	C4B-NB-C1B	2.46	109.83	105.82
3	P	600	HEC	CHD-C1D-ND	2.46	128.31	123.86
3	V	600	HEC	CHA-C4D-ND	2.46	128.31	123.86
3	J	606	HEC	C4B-NB-C1B	2.45	109.82	105.82
3	I	604	HEC	CHB-C1B-NB	2.45	128.31	123.86
3	B	602	HEC	C4B-NB-C1B	2.45	109.82	105.82
3	G	607	HEC	CHD-C4C-NC	2.45	127.12	124.45
3	R	605	HEC	O2A-CGA-CBA	2.45	121.75	114.00
3	P	605	HEC	CAD-C3D-C2D	2.45	132.56	127.07
3	N	604	HEC	CHD-C1D-ND	2.45	128.30	123.86
3	F	604	HEC	CBA-CAA-C2A	-2.45	105.77	112.53
3	X	601	HEC	CHB-C1B-NB	2.45	128.30	123.86
3	L	600	HEC	CHB-C1B-NB	2.45	128.30	123.86
3	O	602	HEC	CHB-C1B-NB	2.44	128.29	123.86
3	O	606	HEC	C4B-NB-C1B	2.44	109.80	105.82
3	N	600	HEC	CHA-C4D-ND	2.44	128.29	123.86
3	A	602	HEC	CAD-CBD-CGD	-2.44	107.19	113.67
3	V	604	HEC	CBA-CAA-C2A	-2.44	105.78	112.53
3	A	604	HEC	CHD-C1D-ND	2.44	128.28	123.86
3	L	607	HEC	CBC-CAC-C3C	-2.44	122.56	127.43
3	R	600	HEC	CHD-C1D-ND	2.44	128.28	123.86
3	F	604	HEC	CHD-C4C-NC	2.44	127.11	124.45
3	T	604	HEC	CHD-C4C-NC	2.44	127.11	124.45
3	O	607	HEC	CBC-CAC-C3C	-2.44	122.56	127.43
3	M	601	HEC	CHB-C1B-NB	2.44	128.28	123.86
3	A	600	HEC	CHA-C4D-ND	2.44	128.28	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	602	HEC	CHB-C1B-NB	2.44	128.28	123.86
3	U	601	HEC	O2D-CGD-CBD	2.44	121.70	114.00
3	H	606	HEC	C4B-NB-C1B	2.44	109.79	105.82
3	P	602	HEC	CHB-C1B-NB	2.43	128.27	123.86
3	U	602	HEC	CAD-CBD-CGD	-2.43	107.21	113.67
3	P	600	HEC	CHA-C4D-ND	2.43	128.27	123.86
3	T	602	HEC	C4B-NB-C1B	2.43	109.78	105.82
3	G	600	HEC	CHD-C1D-ND	2.43	128.27	123.86
3	L	604	HEC	CHB-C1B-NB	2.43	128.27	123.86
3	A	601	HEC	O2D-CGD-CBD	2.43	121.68	114.00
3	C	602	HEC	CHB-C1B-NB	2.43	128.27	123.86
3	L	604	HEC	CBA-CAA-C2A	-2.43	105.81	112.53
3	V	604	HEC	CHD-C4C-NC	2.43	127.10	124.45
3	K	607	HEC	CHA-C4D-ND	2.43	128.26	123.86
3	D	601	HEC	CHA-C4D-ND	2.43	128.26	123.86
3	B	600	HEC	CHD-C1D-ND	2.43	128.26	123.86
3	X	602	HEC	CHB-C1B-NB	2.43	128.26	123.86
3	C	600	HEC	CHD-C1D-ND	2.43	128.26	123.86
3	S	600	HEC	CHA-C4D-ND	2.43	128.26	123.86
3	C	601	HEC	O2D-CGD-CBD	2.42	121.66	114.00
3	F	600	HEC	CHD-C1D-ND	2.42	128.26	123.86
3	R	606	HEC	O2A-CGA-CBA	2.42	121.66	114.00
3	Q	604	HEC	CBA-CAA-C2A	-2.42	105.83	112.53
3	T	600	HEC	CHB-C1B-NB	2.42	128.25	123.86
3	S	606	HEC	CHA-C4D-ND	2.42	128.25	123.86
3	T	605	HEC	CHD-C4C-NC	2.42	127.09	124.45
3	E	601	HEC	CHB-C1B-NB	2.42	128.25	123.86
3	M	606	HEC	CHB-C1B-NB	2.42	128.25	123.86
3	R	606	HEC	CHA-C4D-ND	2.42	128.25	123.86
3	A	606	HEC	CHA-C4D-ND	2.42	128.25	123.86
3	U	600	HEC	CHD-C1D-ND	2.42	128.25	123.86
3	V	601	HEC	CHB-C1B-NB	2.42	128.25	123.86
3	T	604	HEC	CHD-C1D-ND	2.42	128.25	123.86
3	P	605	HEC	O2A-CGA-CBA	2.42	121.64	114.00
3	P	604	HEC	CHB-C1B-NB	2.42	128.25	123.86
3	N	604	HEC	CBA-CAA-C2A	-2.42	105.85	112.53
3	V	602	HEC	C4B-NB-C1B	2.42	109.76	105.82
3	D	601	HEC	O2A-CGA-CBA	2.42	121.63	114.00
3	B	605	HEC	CHD-C4C-NC	2.42	127.08	124.45
3	H	600	HEC	CBC-CAC-C3C	-2.42	122.61	127.43
3	R	605	HEC	CHD-C4C-NC	2.41	127.08	124.45
3	F	607	HEC	CHD-C4C-NC	2.41	127.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	604	HEC	CHD-C4C-NC	2.41	127.08	124.45
3	B	606	HEC	CHB-C1B-NB	2.41	128.24	123.86
3	Q	600	HEC	CBC-CAC-C3C	-2.41	122.61	127.43
3	M	601	HEC	CHD-C1D-ND	2.41	128.23	123.86
3	U	605	HEC	O2A-CGA-CBA	2.41	121.62	114.00
3	K	604	HEC	CHA-C1A-NA	2.41	127.08	124.45
3	R	607	HEC	CHD-C4C-NC	2.41	127.08	124.45
3	B	605	HEC	CAD-C3D-C2D	2.41	132.47	127.07
3	N	600	HEC	CHD-C1D-ND	2.41	128.22	123.86
3	R	604	HEC	CHB-C1B-NB	2.41	128.22	123.86
3	R	601	HEC	CHB-C1B-NB	2.40	128.22	123.86
3	D	603	HEC	CHC-C1C-C2C	-2.40	120.45	127.43
3	E	602	HEC	CHB-C1B-NB	2.40	128.22	123.86
3	L	607	HEC	CHA-C4D-ND	2.40	128.22	123.86
3	A	601	HEC	CHB-C1B-NB	2.40	128.21	123.86
3	B	601	HEC	CHB-C1B-NB	2.40	128.21	123.86
3	U	604	HEC	CHB-C1B-NB	2.40	128.21	123.86
3	J	602	HEC	C4B-NB-C1B	2.40	109.73	105.82
3	R	600	HEC	CHA-C4D-ND	2.40	128.21	123.86
3	J	602	HEC	CAD-CBD-CGD	-2.40	107.31	113.67
3	J	600	HEC	CHB-C1B-NB	2.40	128.21	123.86
3	X	600	HEC	CHB-C1B-NB	2.40	128.21	123.86
3	D	605	HEC	CAD-CBD-CGD	-2.40	107.31	113.67
3	L	605	HEC	CAD-C3D-C2D	2.40	132.44	127.07
3	L	601	HEC	O2D-CGD-CBD	2.40	121.57	114.00
3	O	601	HEC	CHA-C4D-ND	2.39	128.20	123.86
3	D	600	HEC	CHB-C1B-NB	2.39	128.20	123.86
3	V	606	HEC	CHA-C4D-ND	2.39	128.20	123.86
3	O	605	HEC	O2D-CGD-CBD	2.39	121.56	114.00
3	S	602	HEC	CHB-C1B-NB	2.39	128.20	123.86
3	E	604	HEC	CHD-C1D-ND	2.39	128.20	123.86
3	O	600	HEC	CHA-C4D-ND	2.39	128.20	123.86
3	W	600	HEC	CHD-C1D-ND	2.39	128.20	123.86
3	U	607	HEC	CHD-C4C-NC	2.39	127.06	124.45
3	O	601	HEC	O2D-CGD-CBD	2.39	121.56	114.00
3	P	601	HEC	CHB-C1B-NB	2.39	128.20	123.86
3	N	600	HEC	CHB-C1B-NB	2.39	128.19	123.86
3	G	605	HEC	CHB-C1B-NB	2.39	128.19	123.86
3	K	601	HEC	CBD-CAD-C3D	-2.39	105.93	112.53
3	O	600	HEC	O2A-CGA-CBA	2.39	121.55	114.00
3	B	604	HEC	CHD-C1D-ND	2.39	128.19	123.86
3	P	601	HEC	CHA-C4D-ND	2.39	128.19	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	604	HEC	CBA-CAA-C2A	-2.39	105.93	112.53
3	F	600	HEC	CBC-CAC-C3C	-2.39	122.66	127.43
3	K	600	HEC	CHB-C1B-NB	2.39	128.19	123.86
3	O	602	HEC	CAD-CBD-CGD	-2.39	107.34	113.67
3	G	605	HEC	O2A-CGA-CBA	2.39	121.54	114.00
3	W	604	HEC	CHD-C1D-ND	2.38	128.19	123.86
3	A	607	HEC	CHD-C4C-NC	2.38	127.05	124.45
3	S	604	HEC	CBA-CAA-C2A	-2.38	105.94	112.53
3	D	604	HEC	CHB-C1B-NB	2.38	128.18	123.86
3	X	604	HEC	CHD-C1D-ND	2.38	128.18	123.86
3	H	604	HEC	CHD-C1D-ND	2.38	128.18	123.86
3	M	604	HEC	CBA-CAA-C2A	-2.38	105.95	112.53
3	F	601	HEC	CHD-C1D-ND	2.38	128.18	123.86
3	U	606	HEC	CHB-C1B-NB	2.38	128.18	123.86
3	D	604	HEC	CHD-C4C-NC	2.38	127.05	124.45
3	M	606	HEC	O2A-CGA-CBA	2.38	121.52	114.00
3	A	602	HEC	CHB-C1B-NB	2.38	128.18	123.86
3	I	603	HEC	C3D-C4D-ND	-2.38	107.51	110.15
3	O	605	HEC	CAD-C3D-C2D	2.38	132.40	127.07
3	I	606	HEC	CHB-C1B-NB	2.38	128.17	123.86
3	W	600	HEC	CHA-C4D-ND	2.38	128.17	123.86
3	E	600	HEC	CHD-C1D-ND	2.38	128.17	123.86
3	Q	606	HEC	O2A-CGA-CBA	2.38	121.50	114.00
3	H	604	HEC	CBA-CAA-C2A	-2.37	105.97	112.53
3	V	601	HEC	CHD-C1D-ND	2.37	128.16	123.86
3	U	602	HEC	CHB-C1B-NB	2.37	128.16	123.86
3	A	605	HEC	CAD-C3D-C2D	2.37	132.39	127.07
3	C	604	HEC	CHD-C1D-ND	2.37	128.16	123.86
3	E	600	HEC	CHB-C1B-NB	2.37	128.16	123.86
3	Q	604	HEC	CHB-C1B-NB	2.37	128.16	123.86
3	U	600	HEC	CHA-C4D-ND	2.37	128.16	123.86
3	Q	605	HEC	O2A-CGA-CBA	2.37	121.50	114.00
3	C	605	HEC	CHA-C4D-ND	2.37	128.16	123.86
3	V	604	HEC	CHB-C1B-NB	2.37	128.16	123.86
3	F	603	HEC	CAA-C2A-C1A	2.37	129.67	124.85
3	H	601	HEC	CHB-C1B-NB	2.37	128.16	123.86
3	E	606	HEC	O2A-CGA-CBA	2.37	121.49	114.00
3	X	600	HEC	CHA-C1A-NA	2.37	127.03	124.45
3	C	605	HEC	CAD-C3D-C2D	2.37	132.38	127.07
3	M	602	HEC	C4B-NB-C1B	2.37	109.68	105.82
3	M	602	HEC	CHB-C1B-NB	2.37	128.15	123.86
3	K	604	HEC	CHD-C1D-ND	2.37	128.15	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	604	HEC	CHB-C1B-NB	2.37	128.15	123.86
3	J	602	HEC	CHB-C1B-NB	2.37	128.15	123.86
3	V	606	HEC	CHB-C1B-NB	2.37	128.15	123.86
3	N	605	HEC	CAD-C3D-C2D	2.37	132.38	127.07
3	I	605	HEC	CHB-C1B-NB	2.36	128.15	123.86
3	U	601	HEC	CBD-CAD-C3D	-2.36	106.00	112.53
3	R	602	HEC	CHB-C1B-NB	2.36	128.14	123.86
3	U	604	HEC	CHD-C1D-ND	2.36	128.14	123.86
3	V	604	HEC	CHD-C1D-ND	2.36	128.14	123.86
3	G	604	HEC	CHD-C1D-ND	2.36	128.14	123.86
3	K	601	HEC	CHB-C1B-NB	2.36	128.14	123.86
3	A	601	HEC	CBD-CAD-C3D	-2.36	106.01	112.53
3	R	605	HEC	O2D-CGD-CBD	2.36	121.45	114.00
3	H	605	HEC	CAD-C3D-C2D	2.36	132.36	127.07
3	T	601	HEC	O2D-CGD-CBD	2.36	121.45	114.00
3	F	602	HEC	CHB-C1B-NB	2.36	128.14	123.86
3	F	604	HEC	CHD-C1D-ND	2.36	128.13	123.86
3	B	602	HEC	CHB-C1B-NB	2.36	128.13	123.86
3	F	605	HEC	O2A-CGA-CBA	2.36	121.44	114.00
3	M	602	HEC	CAD-CBD-CGD	-2.35	107.42	113.67
3	S	601	HEC	CHD-C1D-ND	2.35	128.13	123.86
3	E	605	HEC	CHD-C4C-NC	2.35	127.02	124.45
3	P	605	HEC	CHD-C4C-NC	2.35	127.02	124.45
3	J	605	HEC	CBD-CAD-C3D	2.35	119.04	112.53
3	J	601	HEC	CHB-C1B-NB	2.35	128.12	123.86
3	L	602	HEC	CAD-CBD-CGD	-2.35	107.43	113.67
3	C	604	HEC	CBA-CAA-C2A	-2.35	106.04	112.53
3	L	600	HEC	CHA-C4D-ND	2.35	128.11	123.86
3	B	601	HEC	CBD-CAD-C3D	-2.35	106.05	112.53
3	O	603	HEC	CAA-C2A-C1A	2.34	129.62	124.85
3	O	604	HEC	CHD-C4C-NC	2.34	127.00	124.45
3	U	605	HEC	CAD-C3D-C2D	2.34	132.33	127.07
3	G	606	HEC	CHB-C1B-NB	2.34	128.11	123.86
3	V	605	HEC	CAD-C3D-C2D	2.34	132.32	127.07
3	Q	601	HEC	CHD-C1D-ND	2.34	128.11	123.86
3	D	605	HEC	CHD-C1D-ND	2.34	128.11	123.86
3	O	601	HEC	CHD-C1D-ND	2.34	128.11	123.86
3	H	600	HEC	CHA-C1A-NA	2.34	127.00	124.45
3	F	606	HEC	CHB-C1B-NB	2.34	128.10	123.86
3	L	605	HEC	CHB-C1B-NB	2.34	128.10	123.86
3	H	607	HEC	C4B-NB-C1B	2.34	109.63	105.82
3	N	602	HEC	CHB-C1B-NB	2.34	128.10	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	604	HEC	CHA-C1A-NA	2.34	127.00	124.45
3	P	601	HEC	CBD-CAD-C3D	-2.34	106.07	112.53
3	W	601	HEC	O2D-CGD-CBD	2.34	121.39	114.00
3	A	600	HEC	CHD-C1D-ND	2.34	128.10	123.86
3	I	605	HEC	O2A-CGA-CBA	2.34	121.38	114.00
3	T	605	HEC	CAD-C3D-C2D	2.34	132.31	127.07
3	U	605	HEC	CHD-C4C-NC	2.34	127.00	124.45
3	B	600	HEC	CHB-C1B-NB	2.33	128.09	123.86
3	M	600	HEC	CHA-C4D-ND	2.33	128.09	123.86
3	O	601	HEC	CBD-CAD-C3D	-2.33	106.08	112.53
3	T	602	HEC	CHB-C1B-NB	2.33	128.09	123.86
3	B	605	HEC	O2A-CGA-CBA	2.33	121.37	114.00
3	K	604	HEC	CHB-C1B-NB	2.33	128.09	123.86
3	O	606	HEC	O2A-CGA-CBA	2.33	121.36	114.00
3	M	605	HEC	CAD-C3D-C2D	2.33	132.30	127.07
3	C	605	HEC	CHD-C4C-NC	2.33	126.99	124.45
3	S	601	HEC	CHB-C1B-NB	2.33	128.09	123.86
3	W	606	HEC	CHB-C1B-NB	2.33	128.09	123.86
3	D	607	HEC	CHB-C1B-NB	2.33	128.08	123.86
3	W	601	HEC	CHD-C1D-ND	2.33	128.08	123.86
3	T	606	HEC	O2A-CGA-CBA	2.33	121.36	114.00
3	V	602	HEC	O2A-CGA-CBA	2.33	121.36	114.00
3	O	607	HEC	C4B-NB-C1B	2.33	109.61	105.82
3	S	604	HEC	CHD-C1D-ND	2.33	128.08	123.86
3	O	600	HEC	CHB-C1B-NB	2.32	128.08	123.86
3	H	605	HEC	CHD-C4C-NC	2.32	126.98	124.45
3	O	604	HEC	CHB-C1B-NB	2.32	128.07	123.86
3	F	601	HEC	CHB-C1B-NB	2.32	128.07	123.86
3	S	605	HEC	CHD-C4C-NC	2.32	126.98	124.45
3	I	604	HEC	CHD-C1D-C2D	-2.32	120.68	127.43
3	Q	602	HEC	CHB-C1B-NB	2.32	128.07	123.86
3	T	606	HEC	CHB-C1B-NB	2.32	128.07	123.86
3	R	601	HEC	CBD-CAD-C3D	-2.32	106.11	112.53
3	A	600	HEC	CHB-C1B-NB	2.32	128.07	123.86
3	K	601	HEC	O2A-CGA-CBA	2.32	121.33	114.00
3	V	601	HEC	O2A-CGA-CBA	2.32	121.33	114.00
3	W	602	HEC	O2A-CGA-CBA	2.32	121.33	114.00
3	C	601	HEC	CBD-CAD-C3D	-2.32	106.12	112.53
3	O	603	HEC	CHB-C4A-NA	-2.32	121.93	124.45
3	G	605	HEC	C4B-NB-C1B	2.32	109.60	105.82
3	L	600	HEC	C4B-NB-C1B	2.32	109.60	105.82
3	I	601	HEC	CHA-C4D-C3D	-2.32	120.23	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	600	HEC	CHA-C4D-ND	2.31	128.06	123.86
3	S	607	HEC	C4B-NB-C1B	2.31	109.59	105.82
3	S	601	HEC	CBD-CAD-C3D	-2.31	106.13	112.53
3	E	601	HEC	CHA-C4D-ND	2.31	128.06	123.86
3	L	605	HEC	CHA-C4D-ND	2.31	128.06	123.86
3	U	601	HEC	CHD-C1D-ND	2.31	128.06	123.86
3	U	606	HEC	O2A-CGA-CBA	2.31	121.31	114.00
3	X	600	HEC	CHD-C1D-ND	2.31	128.05	123.86
3	H	602	HEC	C4B-NB-C1B	2.31	109.59	105.82
3	G	600	HEC	CHB-C1B-NB	2.31	128.05	123.86
3	D	603	HEC	C1C-CHC-C4B	-2.31	117.53	124.66
3	E	601	HEC	O2D-CGD-CBD	2.31	121.30	114.00
3	E	604	HEC	CHA-C1A-NA	2.31	126.97	124.45
3	G	604	HEC	CHD-C4C-NC	2.31	126.97	124.45
3	N	601	HEC	CHB-C1B-NB	2.31	128.04	123.86
3	O	606	HEC	CHA-C4D-ND	2.31	128.04	123.86
3	U	601	HEC	CHB-C1B-NB	2.31	128.04	123.86
3	T	601	HEC	CBD-CAD-C3D	-2.30	106.16	112.53
3	W	601	HEC	CBD-CAD-C3D	-2.30	106.16	112.53
3	M	605	HEC	C4B-NB-C1B	2.30	109.58	105.82
3	E	607	HEC	C4B-NB-C1B	2.30	109.58	105.82
3	Q	603	HEC	CAA-C2A-C1A	2.30	129.53	124.85
3	T	600	HEC	CHD-C1D-ND	2.30	128.03	123.86
3	E	602	HEC	CAD-CBD-CGD	-2.30	107.56	113.67
3	O	606	HEC	CHB-C1B-NB	2.30	128.03	123.86
3	C	606	HEC	CHB-C1B-NB	2.30	128.03	123.86
3	P	602	HEC	CAD-CBD-CGD	-2.30	107.57	113.67
3	T	601	HEC	CHB-C1B-NB	2.30	128.03	123.86
3	H	601	HEC	CBD-CAD-C3D	-2.30	106.18	112.53
3	O	600	HEC	CHD-C1D-ND	2.30	128.03	123.86
3	S	604	HEC	CHB-C1B-NB	2.30	128.03	123.86
3	A	606	HEC	CHB-C1B-NB	2.30	128.03	123.86
3	Q	600	HEC	CHD-C1D-ND	2.30	128.03	123.86
3	F	606	HEC	O2A-CGA-CBA	2.30	121.25	114.00
3	R	604	HEC	CHD-C1D-ND	2.30	128.02	123.86
3	F	602	HEC	CAD-CBD-CGD	-2.29	107.58	113.67
3	K	605	HEC	CHD-C4C-NC	2.29	126.95	124.45
3	I	604	HEC	CHA-C4D-ND	2.29	128.02	123.86
3	T	601	HEC	CHD-C1D-ND	2.29	128.02	123.86
3	D	602	HEC	CHD-C1D-ND	2.29	128.02	123.86
3	P	603	HEC	O1A-CGA-CBA	-2.29	115.82	123.09
3	I	605	HEC	CHD-C4C-NC	2.29	126.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	604	HEC	CBA-CAA-C2A	-2.29	106.19	112.53
3	W	607	HEC	CHD-C4C-NC	2.29	126.95	124.45
3	W	600	HEC	CBC-CAC-C3C	-2.29	122.86	127.43
3	X	605	HEC	O2A-CGA-CBA	2.29	121.23	114.00
3	I	601	HEC	CHD-C1D-ND	2.29	128.01	123.86
3	P	600	HEC	CHB-C1B-NB	2.29	128.01	123.86
3	A	600	HEC	CAD-CBD-CGD	-2.29	107.59	113.67
3	R	604	HEC	CBA-CAA-C2A	-2.29	106.20	112.53
3	A	605	HEC	CHA-C4D-ND	2.29	128.01	123.86
3	L	601	HEC	CBD-CAD-C3D	-2.29	106.21	112.53
3	W	604	HEC	CHB-C1B-NB	2.29	128.00	123.86
3	X	604	HEC	CBA-CAA-C2A	-2.28	106.22	112.53
3	X	606	HEC	CHB-C1B-NB	2.28	128.00	123.86
3	H	600	HEC	CHB-C1B-NB	2.28	128.00	123.86
3	X	602	HEC	CAD-CBD-CGD	-2.28	107.61	113.67
3	C	601	HEC	CHD-C1D-ND	2.28	128.00	123.86
3	R	601	HEC	O2D-CGD-CBD	2.28	121.21	114.00
3	P	607	HEC	C4B-NB-C1B	2.28	109.54	105.82
3	T	604	HEC	CHB-C1B-NB	2.28	127.99	123.86
3	I	603	HEC	C2D-C1D-ND	-2.28	106.49	110.14
3	O	604	HEC	CHA-C1A-NA	2.28	126.94	124.45
3	X	605	HEC	CAD-C3D-C2D	2.28	132.18	127.07
3	W	605	HEC	O2A-CGA-CBA	2.28	121.20	114.00
3	M	602	HEC	O2A-CGA-CBA	2.28	121.20	114.00
3	U	602	HEC	O2A-CGA-CBA	2.28	121.20	114.00
3	H	605	HEC	O2A-CGA-CBA	2.28	121.20	114.00
3	J	604	HEC	CHB-C1B-NB	2.28	127.99	123.86
3	B	606	HEC	CHA-C4D-ND	2.28	127.99	123.86
3	K	602	HEC	CAD-CBD-CGD	-2.28	107.63	113.67
3	H	605	HEC	O2D-CGD-CBD	2.28	121.19	114.00
3	C	600	HEC	CHB-C1B-NB	2.28	127.99	123.86
3	K	600	HEC	CHD-C1D-ND	2.28	127.99	123.86
3	B	606	HEC	O2A-CGA-CBA	2.28	121.19	114.00
3	I	607	HEC	CHA-C4D-ND	2.27	127.98	123.86
3	J	601	HEC	O2D-CGD-CBD	2.27	121.19	114.00
3	B	604	HEC	CHA-C1A-NA	2.27	126.93	124.45
3	V	605	HEC	CHD-C4C-NC	2.27	126.93	124.45
3	Q	606	HEC	CHA-C4D-ND	2.27	127.98	123.86
3	T	605	HEC	CHB-C1B-NB	2.27	127.98	123.86
3	S	606	HEC	C4B-NB-C1B	2.27	109.52	105.82
3	G	606	HEC	CHA-C1A-NA	2.27	126.93	124.45
3	J	600	HEC	O2A-CGA-CBA	2.27	121.17	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	606	HEC	CHA-C4D-ND	2.27	127.98	123.86
3	C	602	HEC	CAD-CBD-CGD	-2.27	107.64	113.67
3	Q	606	HEC	CHB-C1B-NB	2.27	127.98	123.86
3	Q	605	HEC	CAD-C3D-C2D	2.27	132.16	127.07
3	H	603	HEC	CHB-C4A-NA	-2.27	121.98	124.45
3	A	601	HEC	CHD-C1D-ND	2.27	127.97	123.86
3	K	605	HEC	O2D-CGD-CBD	2.27	121.17	114.00
3	R	606	HEC	CHB-C1B-NB	2.27	127.97	123.86
3	E	603	HEC	CHB-C4A-NA	-2.27	121.98	124.45
3	I	602	HEC	CAA-CBA-CGA	-2.27	107.65	113.67
3	B	606	HEC	CHD-C1D-ND	2.27	127.97	123.86
3	X	601	HEC	CHD-C1D-ND	2.27	127.97	123.86
3	K	605	HEC	O2A-CGA-CBA	2.27	121.16	114.00
3	G	601	HEC	CBD-CAD-C3D	-2.27	106.27	112.53
3	G	606	HEC	C2A-C1A-NA	-2.26	108.14	110.32
3	V	600	HEC	CHD-C1D-ND	2.26	127.97	123.86
3	O	606	HEC	CHD-C1D-ND	2.26	127.96	123.86
3	B	605	HEC	CHB-C1B-NB	2.26	127.96	123.86
3	S	605	HEC	O2A-CGA-CBA	2.26	121.14	114.00
3	M	600	HEC	CHB-C1B-NB	2.26	127.96	123.86
3	P	604	HEC	CHD-C1D-ND	2.26	127.96	123.86
3	H	607	HEC	CHA-C4D-ND	2.26	127.95	123.86
3	N	602	HEC	CHD-C1D-ND	2.26	127.95	123.86
3	M	600	HEC	CHD-C1D-ND	2.26	127.95	123.86
3	S	606	HEC	O2A-CGA-CBA	2.26	121.13	114.00
3	K	607	HEC	CHD-C1D-ND	2.26	127.95	123.86
3	L	606	HEC	O2A-CGA-CBA	2.26	121.13	114.00
3	D	600	HEC	C4B-NB-C1B	2.26	109.50	105.82
3	D	604	HEC	CHA-C4D-C3D	-2.25	120.36	125.30
3	N	602	HEC	C4B-NB-C1B	2.25	109.50	105.82
3	W	604	HEC	CHA-C4D-C3D	-2.25	120.37	125.30
3	J	605	HEC	CBC-CAC-C3C	-2.25	122.93	127.43
3	B	602	HEC	CHD-C1D-ND	2.25	127.94	123.86
3	H	602	HEC	CHB-C1B-NB	2.25	127.94	123.86
3	B	604	HEC	CBA-CAA-C2A	-2.25	106.31	112.53
3	W	606	HEC	CHA-C4D-ND	2.25	127.94	123.86
3	W	605	HEC	CAD-C3D-C2D	2.25	132.12	127.07
3	J	606	HEC	O2A-CGA-CBA	2.25	121.11	114.00
3	I	600	HEC	CHB-C1B-C2B	-2.25	120.89	127.43
3	D	605	HEC	CAD-C3D-C2D	2.25	132.12	127.07
3	S	603	HEC	O1A-CGA-CBA	-2.25	115.96	123.09
3	E	604	HEC	CHB-C1B-NB	2.25	127.94	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	607	HEC	CHD-C4C-NC	2.25	126.90	124.45
3	Q	602	HEC	O2A-CGA-CBA	2.25	121.10	114.00
3	Q	602	HEC	CAD-CBD-CGD	-2.25	107.71	113.67
3	D	607	HEC	CHA-C4D-ND	2.25	127.93	123.86
3	Q	600	HEC	CHA-C1A-NA	2.25	126.90	124.45
3	F	605	HEC	C4B-NB-C1B	2.25	109.48	105.82
3	J	600	HEC	CHD-C1D-ND	2.25	127.93	123.86
3	E	601	HEC	C4B-NB-C1B	2.24	109.48	105.82
3	N	604	HEC	CHB-C1B-NB	2.24	127.93	123.86
3	F	607	HEC	C4B-NB-C1B	2.24	109.48	105.82
3	G	602	HEC	CAD-CBD-CGD	-2.24	107.71	113.67
3	F	604	HEC	CHB-C1B-NB	2.24	127.93	123.86
3	V	600	HEC	CHB-C1B-NB	2.24	127.93	123.86
3	T	602	HEC	CAD-CBD-CGD	-2.24	107.72	113.67
3	L	604	HEC	CHD-C1D-ND	2.24	127.92	123.86
3	C	606	HEC	O2A-CGA-CBA	2.24	121.08	114.00
3	A	604	HEC	CBA-CAA-C2A	-2.24	106.34	112.53
3	S	604	HEC	CHD-C4C-NC	2.24	126.89	124.45
3	T	603	HEC	CHB-C4A-NA	-2.24	122.02	124.45
3	I	605	HEC	CHD-C1D-ND	2.24	127.92	123.86
3	M	605	HEC	CHA-C4D-ND	2.24	127.92	123.86
3	V	607	HEC	C4B-NB-C1B	2.24	109.47	105.82
3	U	605	HEC	CHA-C4D-ND	2.24	127.91	123.86
3	L	607	HEC	C4B-NB-C1B	2.23	109.46	105.82
3	H	604	HEC	CHB-C1B-NB	2.23	127.91	123.86
3	V	605	HEC	CHA-C4D-ND	2.23	127.91	123.86
3	E	605	HEC	CAD-C3D-C2D	2.23	132.08	127.07
3	V	602	HEC	CHB-C1B-NB	2.23	127.91	123.86
3	X	602	HEC	O2A-CGA-CBA	2.23	121.06	114.00
3	G	606	HEC	O2D-CGD-CBD	2.23	121.06	114.00
3	J	605	HEC	O2A-CGA-CBA	2.23	121.05	114.00
3	E	601	HEC	CBD-CAD-C3D	-2.23	106.36	112.53
3	G	606	HEC	O2A-CGA-CBA	2.23	121.05	114.00
3	U	600	HEC	O2A-CGA-CBA	2.23	121.05	114.00
3	N	606	HEC	CHB-C1B-NB	2.23	127.91	123.86
3	R	601	HEC	CHD-C1D-ND	2.23	127.91	123.86
3	E	605	HEC	CHA-C4D-ND	2.23	127.90	123.86
3	J	601	HEC	CBD-CAD-C3D	-2.23	106.37	112.53
3	P	606	HEC	CHB-C1B-NB	2.23	127.90	123.86
3	B	602	HEC	O2A-CGA-CBA	2.23	121.04	114.00
3	L	602	HEC	CHB-C1B-NB	2.23	127.90	123.86
3	K	606	HEC	CHA-C4D-ND	2.23	127.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	605	HEC	CAD-C3D-C2D	2.23	132.06	127.07
3	V	602	HEC	CAD-CBD-CGD	-2.23	107.76	113.67
3	V	605	HEC	O2A-CGA-CBA	2.23	121.03	114.00
3	N	603	HEC	O1A-CGA-CBA	-2.23	116.03	123.09
3	O	607	HEC	O2D-CGD-O1D	-2.23	117.61	123.33
3	D	602	HEC	C4B-NB-C1B	2.23	109.45	105.82
3	R	602	HEC	CAD-CBD-CGD	-2.23	107.76	113.67
3	G	601	HEC	CHA-C4D-C3D	-2.22	120.43	125.30
3	C	605	HEC	CHB-C1B-NB	2.22	127.89	123.86
3	X	604	HEC	CHB-C1B-NB	2.22	127.89	123.86
3	W	604	HEC	CHA-C1A-NA	2.22	126.87	124.45
3	H	602	HEC	CHD-C1D-ND	2.22	127.89	123.86
3	E	606	HEC	CHB-C1B-NB	2.22	127.89	123.86
3	W	602	HEC	CHA-C4D-ND	2.22	127.89	123.86
3	K	606	HEC	CHB-C1B-NB	2.22	127.88	123.86
3	R	600	HEC	CHB-C1B-NB	2.22	127.88	123.86
3	U	605	HEC	CHB-C1B-NB	2.22	127.88	123.86
3	I	605	HEC	CHA-C4D-C3D	-2.22	120.44	125.30
3	N	606	HEC	CHA-C4D-ND	2.22	127.88	123.86
3	N	605	HEC	CHA-C4D-ND	2.22	127.88	123.86
3	U	600	HEC	CHB-C1B-NB	2.22	127.88	123.86
3	U	604	HEC	CHA-C4D-C3D	-2.22	120.45	125.30
3	I	603	HEC	O1D-CGD-CBD	-2.21	116.07	123.09
3	W	600	HEC	CHB-C1B-NB	2.21	127.88	123.86
3	O	607	HEC	CHB-C1B-NB	2.21	127.87	123.86
3	W	603	HEC	O1A-CGA-CBA	-2.21	116.08	123.09
3	F	605	HEC	CHD-C4C-NC	2.21	126.86	124.45
3	W	601	HEC	CHB-C1B-NB	2.21	127.87	123.86
3	K	606	HEC	O2A-CGA-CBA	2.21	120.99	114.00
3	V	604	HEC	CHA-C4D-C3D	-2.21	120.46	125.30
3	K	605	HEC	CHA-C4D-ND	2.21	127.87	123.86
3	F	600	HEC	CHB-C1B-NB	2.21	127.87	123.86
3	X	607	HEC	C4B-NB-C1B	2.21	109.42	105.82
3	P	604	HEC	CBA-CAA-C2A	-2.21	106.43	112.53
3	E	601	HEC	CHD-C1D-ND	2.21	127.86	123.86
3	R	606	HEC	CHD-C1D-ND	2.21	127.86	123.86
3	I	606	HEC	O2A-CGA-CBA	2.21	120.98	114.00
3	N	606	HEC	O2A-CGA-CBA	2.21	120.97	114.00
3	F	603	HEC	C3D-C4D-ND	-2.21	107.70	110.15
3	N	600	HEC	O2A-CGA-CBA	2.21	120.97	114.00
3	H	607	HEC	CHD-C1D-ND	2.21	127.86	123.86
3	O	604	HEC	CHD-C1D-ND	2.21	127.86	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	604	HEC	CHB-C1B-C2B	-2.21	121.02	127.43
3	L	605	HEC	C4B-NB-C1B	2.21	109.42	105.82
3	K	600	HEC	C4B-NB-C1B	2.21	109.42	105.82
3	X	602	HEC	CHD-C1D-ND	2.20	127.86	123.86
3	G	604	HEC	CHA-C4D-C3D	-2.20	120.48	125.30
3	X	605	HEC	CHD-C4C-NC	2.20	126.85	124.45
3	E	603	HEC	C1A-C2A-C3A	-2.20	104.21	107.11
3	M	600	HEC	CHA-C1A-NA	2.20	126.85	124.45
3	Q	605	HEC	CHD-C4C-NC	2.20	126.85	124.45
3	A	606	HEC	CBA-CAA-C2A	-2.20	106.45	112.53
3	G	603	HEC	CAA-C2A-C1A	2.20	129.32	124.85
3	R	600	HEC	CBC-CAC-C3C	-2.20	123.04	127.43
3	S	602	HEC	CAD-CBD-CGD	-2.20	107.83	113.67
3	V	604	HEC	CHB-C1B-C2B	-2.20	121.05	127.43
3	F	602	HEC	O2A-CGA-CBA	2.20	120.94	114.00
3	W	603	HEC	CHB-C4A-NA	-2.20	122.06	124.45
3	J	601	HEC	CHA-C4D-C3D	-2.20	120.49	125.30
3	A	602	HEC	CHD-C1D-ND	2.20	127.84	123.86
3	I	602	HEC	C4B-NB-C1B	2.20	109.40	105.82
3	T	607	HEC	CHB-C1B-NB	2.19	127.84	123.86
3	Q	601	HEC	CBD-CAD-C3D	-2.19	106.47	112.53
3	F	606	HEC	CHA-C4D-ND	2.19	127.84	123.86
3	N	602	HEC	CHA-C4D-ND	2.19	127.84	123.86
3	B	607	HEC	C4B-NB-C1B	2.19	109.40	105.82
3	Q	601	HEC	O2A-CGA-CBA	2.19	120.93	114.00
3	K	603	HEC	O1A-CGA-CBA	-2.19	116.14	123.09
3	C	607	HEC	CHA-C4D-ND	2.19	127.84	123.86
3	E	607	HEC	CHB-C1B-NB	2.19	127.84	123.86
3	L	606	HEC	CHA-C4D-ND	2.19	127.84	123.86
3	N	607	HEC	CHA-C4D-ND	2.19	127.84	123.86
3	G	607	HEC	C4B-NB-C1B	2.19	109.39	105.82
3	I	605	HEC	CHB-C1B-C2B	-2.19	121.07	127.43
3	D	600	HEC	CHA-C1A-NA	2.19	126.84	124.45
3	H	605	HEC	CHD-C1D-ND	2.19	127.83	123.86
3	N	603	HEC	CHB-C4A-NA	-2.19	122.07	124.45
3	B	604	HEC	CHB-C1B-C2B	-2.19	121.07	127.43
3	J	607	HEC	O2D-CGD-O1D	-2.19	117.70	123.33
3	Q	607	HEC	C4C-NC-C1C	2.19	109.39	105.82
3	K	605	HEC	CHD-C1D-ND	2.19	127.82	123.86
3	P	603	HEC	O2A-CGA-CBA	2.19	120.91	114.00
3	J	605	HEC	CHB-C1B-NB	2.18	127.82	123.86
3	A	605	HEC	CBD-CAD-C3D	2.18	118.57	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	605	HEC	CAD-C3D-C2D	2.18	131.97	127.07
3	X	606	HEC	CHA-C4D-ND	2.18	127.82	123.86
3	C	602	HEC	CHD-C1D-ND	2.18	127.82	123.86
3	T	605	HEC	CBD-CAD-C3D	2.18	118.56	112.53
3	F	601	HEC	CBD-CAD-C3D	-2.18	106.50	112.53
3	P	605	HEC	CHA-C4D-ND	2.18	127.81	123.86
3	S	606	HEC	CHB-C1B-NB	2.18	127.81	123.86
3	W	607	HEC	CHD-C1D-ND	2.18	127.81	123.86
3	D	600	HEC	CHA-C4D-ND	2.18	127.81	123.86
3	O	605	HEC	CHD-C1D-ND	2.18	127.81	123.86
3	N	601	HEC	CBD-CAD-C3D	-2.18	106.51	112.53
3	X	602	HEC	CHA-C4D-ND	2.18	127.81	123.86
3	X	605	HEC	CHA-C4D-ND	2.18	127.81	123.86
3	M	600	HEC	C4B-NB-C1B	2.18	109.37	105.82
3	X	603	HEC	CHB-C4A-NA	-2.18	122.08	124.45
3	T	607	HEC	C4B-NB-C1B	2.18	109.37	105.82
3	F	605	HEC	CHA-C1A-NA	2.17	126.82	124.45
3	P	600	HEC	CHA-C1A-NA	2.17	126.82	124.45
3	K	601	HEC	CHA-C4D-C3D	-2.17	120.54	125.30
3	E	605	HEC	O2A-CGA-CBA	2.17	120.87	114.00
3	R	606	HEC	O2D-CGD-CBD	2.17	120.87	114.00
3	R	605	HEC	CHA-C4D-ND	2.17	127.80	123.86
3	K	605	HEC	CBD-CAD-C3D	2.17	118.55	112.53
3	V	601	HEC	CBD-CAD-C3D	-2.17	106.52	112.53
3	M	604	HEC	CHB-C1B-C2B	-2.17	121.12	127.43
3	I	601	HEC	O2A-CGA-CBA	2.17	120.87	114.00
3	C	603	HEC	CHB-C4A-NA	-2.17	122.09	124.45
3	X	604	HEC	CHD-C4C-NC	2.17	126.82	124.45
3	T	601	HEC	O2A-CGA-CBA	2.17	120.86	114.00
3	C	603	HEC	O1A-CGA-CBA	-2.17	116.20	123.09
3	D	601	HEC	CHB-C1B-NB	2.17	127.80	123.86
3	H	602	HEC	O2A-CGA-CBA	2.17	120.86	114.00
3	H	600	HEC	C2A-C1A-NA	-2.17	108.23	110.32
3	H	604	HEC	CHD-C4C-NC	2.17	126.82	124.45
3	X	601	HEC	CBD-CAD-C3D	-2.17	106.53	112.53
3	K	600	HEC	O2A-CGA-CBA	2.17	120.86	114.00
3	C	605	HEC	C4B-NB-C1B	2.17	109.36	105.82
3	W	607	HEC	C4B-NB-C1B	2.17	109.36	105.82
3	X	600	HEC	C4B-NB-C1B	2.17	109.36	105.82
3	T	605	HEC	CHA-C4D-ND	2.17	127.79	123.86
3	R	603	HEC	O1A-CGA-CBA	-2.17	116.22	123.09
3	H	605	HEC	O2D-CGD-O1D	-2.17	117.76	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEC	O2D-CGD-CBD	2.17	120.84	114.00
3	T	607	HEC	CHD-C4C-NC	2.17	126.81	124.45
3	H	606	HEC	CHA-C4D-ND	2.17	127.79	123.86
3	P	606	HEC	CHA-C4D-ND	2.17	127.79	123.86
3	H	601	HEC	O2A-CGA-CBA	2.17	120.84	114.00
3	K	607	HEC	C4C-NC-C1C	2.16	109.35	105.82
3	A	603	HEC	O2A-CGA-CBA	2.16	120.84	114.00
3	N	605	HEC	O2A-CGA-CBA	2.16	120.83	114.00
3	G	605	HEC	CBD-CAD-C3D	2.16	118.51	112.53
3	T	600	HEC	O2A-CGA-CBA	2.16	120.83	114.00
3	F	605	HEC	CHB-C1B-NB	2.16	127.78	123.86
3	H	606	HEC	CHB-C1B-NB	2.16	127.78	123.86
3	I	604	HEC	CHB-C1B-C2B	-2.16	121.15	127.43
3	C	601	HEC	O2A-CGA-CBA	2.16	120.83	114.00
3	W	601	HEC	O2A-CGA-CBA	2.16	120.83	114.00
3	V	601	HEC	CHA-C4D-C3D	-2.16	120.57	125.30
3	A	602	HEC	CHA-C4D-ND	2.16	127.78	123.86
3	L	600	HEC	CHD-C1D-ND	2.16	127.78	123.86
3	S	605	HEC	CAD-C3D-C2D	2.16	131.91	127.07
3	E	601	HEC	O2A-CGA-CBA	2.16	120.82	114.00
3	D	606	HEC	CHB-C1B-NB	2.16	127.78	123.86
3	U	607	HEC	C4B-NB-C1B	2.16	109.34	105.82
3	D	605	HEC	CHD-C1D-C2D	-2.16	121.16	127.43
3	B	603	HEC	C3D-C4D-ND	-2.16	107.76	110.15
3	K	604	HEC	CHB-C1B-C2B	-2.16	121.16	127.43
3	F	605	HEC	CBD-CAD-C3D	2.16	118.50	112.53
3	D	606	HEC	O2A-CGA-CBA	2.16	120.82	114.00
3	G	605	HEC	CAD-C3D-C2D	2.16	131.91	127.07
3	W	605	HEC	CHA-C4D-ND	2.16	127.77	123.86
3	T	605	HEC	C4B-NB-C1B	2.16	109.34	105.82
3	W	604	HEC	CHB-C1B-C2B	-2.16	121.17	127.43
3	K	606	HEC	CBA-CAA-C2A	-2.15	106.58	112.53
3	V	604	HEC	CHA-C1A-NA	2.15	126.80	124.45
3	I	600	HEC	O2A-CGA-CBA	2.15	120.81	114.00
3	G	604	HEC	CHB-C1B-C2B	-2.15	121.17	127.43
3	F	606	HEC	CHD-C1D-ND	2.15	127.77	123.86
3	U	607	HEC	CHD-C1D-ND	2.15	127.77	123.86
3	M	604	HEC	CHA-C4D-C3D	-2.15	120.59	125.30
3	W	605	HEC	CHB-C1B-NB	2.15	127.76	123.86
3	A	605	HEC	O2A-CGA-CBA	2.15	120.80	114.00
3	I	605	HEC	O2D-CGD-CBD	2.15	120.80	114.00
3	R	607	HEC	C4B-NB-C1B	2.15	109.33	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	607	HEC	CHB-C1B-NB	2.15	127.76	123.86
3	S	605	HEC	CBD-CAD-C3D	2.15	118.48	112.53
3	S	603	HEC	CHB-C4A-NA	-2.15	122.11	124.45
3	S	600	HEC	O2A-CGA-CBA	2.15	120.80	114.00
3	W	607	HEC	CHB-C1B-NB	2.15	127.76	123.86
3	X	607	HEC	CHD-C1D-ND	2.15	127.76	123.86
3	D	605	HEC	CHB-C1B-NB	2.15	127.76	123.86
3	F	607	HEC	CHA-C4D-ND	2.15	127.76	123.86
3	Q	604	HEC	CHD-C1D-ND	2.15	127.76	123.86
3	R	607	HEC	CHB-C1B-NB	2.15	127.76	123.86
3	M	607	HEC	CHD-C1D-ND	2.15	127.76	123.86
3	B	607	HEC	CHD-C1D-ND	2.15	127.76	123.86
3	D	607	HEC	CHD-C1D-ND	2.15	127.76	123.86
3	K	606	HEC	CHD-C1D-ND	2.15	127.75	123.86
3	V	602	HEC	CHD-C1D-ND	2.15	127.75	123.86
3	S	600	HEC	CHB-C1B-NB	2.15	127.75	123.86
3	H	602	HEC	CAD-CBD-CGD	-2.15	107.97	113.67
3	G	605	HEC	O2D-CGD-CBD	2.14	120.78	114.00
3	C	602	HEC	O2A-CGA-CBA	2.14	120.78	114.00
3	H	605	HEC	CHB-C1B-NB	2.14	127.75	123.86
3	V	606	HEC	CHD-C1D-ND	2.14	127.75	123.86
3	L	600	HEC	CHA-C1A-NA	2.14	126.79	124.45
3	L	605	HEC	C4C-NC-C1C	2.14	109.32	105.82
3	J	605	HEC	CHA-C4D-ND	2.14	127.75	123.86
3	L	607	HEC	CHB-C1B-NB	2.14	127.75	123.86
3	W	607	HEC	CHA-C4D-ND	2.14	127.75	123.86
3	X	606	HEC	O2A-CGA-CBA	2.14	120.77	114.00
3	I	602	HEC	C2A-C1A-NA	-2.14	108.25	110.32
3	T	604	HEC	CHB-C1B-C2B	-2.14	121.20	127.43
3	S	602	HEC	CHA-C4D-ND	2.14	127.75	123.86
3	J	604	HEC	CHD-C1D-C2D	-2.14	121.21	127.43
3	C	605	HEC	O2D-CGD-CBD	2.14	120.77	114.00
3	D	607	HEC	C4C-NC-C1C	2.14	109.31	105.82
3	N	607	HEC	CHD-C1D-ND	2.14	127.74	123.86
3	B	604	HEC	CHD-C1D-C2D	-2.14	121.21	127.43
3	R	604	HEC	CHB-C1B-C2B	-2.14	121.21	127.43
3	T	602	HEC	O2A-CGA-CBA	2.14	120.76	114.00
3	Q	605	HEC	C4B-NB-C1B	2.14	109.31	105.82
3	M	604	HEC	CHA-C1A-NA	2.14	126.78	124.45
3	N	605	HEC	CHB-C1B-NB	2.14	127.74	123.86
3	I	607	HEC	C4B-NB-C1B	2.14	109.31	105.82
3	Q	607	HEC	CHA-C4D-ND	2.14	127.74	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	604	HEC	CHA-C4D-C3D	-2.14	120.62	125.30
3	F	601	HEC	O2A-CGA-CBA	2.14	120.76	114.00
3	R	602	HEC	O2A-CGA-CBA	2.14	120.75	114.00
3	P	604	HEC	CHA-C1A-NA	2.14	126.78	124.45
3	X	605	HEC	CHB-C1B-NB	2.14	127.73	123.86
3	D	604	HEC	CHB-C1B-C2B	-2.14	121.22	127.43
3	B	600	HEC	O2A-CGA-CBA	2.14	120.75	114.00
3	F	605	HEC	O2D-CGD-CBD	2.14	120.75	114.00
3	C	601	HEC	C4B-NB-C1B	2.14	109.30	105.82
3	W	600	HEC	O2A-CGA-CBA	2.14	120.75	114.00
3	P	606	HEC	O2A-CGA-CBA	2.13	120.75	114.00
3	L	601	HEC	CHA-C4D-C3D	-2.13	120.63	125.30
3	M	602	HEC	CHD-C1D-ND	2.13	127.73	123.86
3	T	607	HEC	CHD-C1D-ND	2.13	127.73	123.86
3	Q	602	HEC	CHA-C4D-ND	2.13	127.73	123.86
3	B	606	HEC	C2A-C1A-NA	-2.13	108.27	110.32
3	T	604	HEC	CHA-C1A-NA	2.13	126.78	124.45
3	M	606	HEC	CHA-C4D-ND	2.13	127.73	123.86
3	R	605	HEC	CHB-C1B-NB	2.13	127.73	123.86
3	D	605	HEC	CHA-C4D-ND	2.13	127.72	123.86
3	R	607	HEC	CHA-C4D-ND	2.13	127.72	123.86
3	W	605	HEC	CBD-CAD-C3D	2.13	118.42	112.53
3	B	605	HEC	C4B-NB-C1B	2.13	109.29	105.82
3	H	607	HEC	C4C-NC-C1C	2.13	109.29	105.82
3	C	607	HEC	CHD-C1D-ND	2.13	127.72	123.86
3	I	607	HEC	CHA-C4D-C3D	-2.13	120.64	125.30
3	J	603	HEC	CHB-C4A-NA	-2.13	122.14	124.45
3	O	603	HEC	O1A-CGA-CBA	-2.13	116.34	123.09
3	B	601	HEC	CHD-C1D-ND	2.13	127.72	123.86
3	R	607	HEC	CHD-C1D-ND	2.13	127.72	123.86
3	L	601	HEC	O2A-CGA-CBA	2.13	120.72	114.00
3	U	606	HEC	CHA-C4D-ND	2.13	127.72	123.86
3	S	604	HEC	CHB-C1B-C2B	-2.13	121.25	127.43
3	N	601	HEC	CHD-C1D-ND	2.13	127.72	123.86
3	V	605	HEC	CHB-C1B-NB	2.13	127.72	123.86
3	O	602	HEC	CHA-C4D-ND	2.13	127.72	123.86
3	I	605	HEC	CAD-CBD-CGD	-2.13	108.03	113.67
3	B	605	HEC	CHA-C4D-ND	2.13	127.71	123.86
3	A	605	HEC	CHD-C1D-ND	2.12	127.71	123.86
3	E	606	HEC	CHA-C4D-ND	2.12	127.71	123.86
3	C	600	HEC	O2A-CGA-CBA	2.12	120.71	114.00
3	R	604	HEC	CHA-C4D-C3D	-2.12	120.65	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	607	HEC	CHA-C4D-ND	2.12	127.71	123.86
3	D	602	HEC	O2A-CGA-CBA	2.12	120.71	114.00
3	F	604	HEC	CHA-C1A-NA	2.12	126.76	124.45
3	I	603	HEC	O1A-CGA-CBA	-2.12	116.36	123.09
3	I	602	HEC	CHD-C1D-ND	2.12	127.71	123.86
3	V	606	HEC	O2A-CGA-CBA	2.12	120.70	114.00
3	G	605	HEC	CHA-C1A-NA	2.12	126.76	124.45
3	Q	604	HEC	CHA-C4D-C3D	-2.12	120.66	125.30
3	C	606	HEC	CHA-C4D-ND	2.12	127.71	123.86
3	D	606	HEC	CHA-C4D-ND	2.12	127.71	123.86
3	O	605	HEC	O2A-CGA-CBA	2.12	120.70	114.00
3	I	600	HEC	O2A-CGA-O1A	-2.12	117.88	123.33
3	D	607	HEC	O2D-CGD-CBD	2.12	120.70	114.00
3	M	607	HEC	C4B-NB-C1B	2.12	109.28	105.82
3	R	601	HEC	CHA-C4D-C3D	-2.12	120.66	125.30
3	Q	604	HEC	CHB-C1B-C2B	-2.12	121.27	127.43
3	S	605	HEC	CHA-C4D-ND	2.12	127.70	123.86
3	G	606	HEC	CHA-C4D-ND	2.12	127.70	123.86
3	N	605	HEC	CBD-CAD-C3D	2.12	118.39	112.53
3	L	607	HEC	CHD-C1D-ND	2.12	127.70	123.86
3	H	606	HEC	CHD-C1D-ND	2.12	127.70	123.86
3	C	605	HEC	O2A-CGA-CBA	2.12	120.69	114.00
3	F	602	HEC	CHA-C4D-ND	2.12	127.70	123.86
3	N	605	HEC	CHD-C1D-ND	2.12	127.70	123.86
3	E	607	HEC	CHD-C1D-ND	2.11	127.69	123.86
3	P	602	HEC	CHA-C4D-ND	2.11	127.69	123.86
3	U	607	HEC	CHA-C4D-ND	2.11	127.69	123.86
3	R	602	HEC	CHD-C1D-ND	2.11	127.69	123.86
3	L	601	HEC	C4B-NB-C1B	2.11	109.26	105.82
3	I	605	HEC	CHD-C1D-C2D	-2.11	121.30	127.43
3	S	602	HEC	O2A-CGA-CBA	2.11	120.67	114.00
3	C	604	HEC	CHB-C1B-C2B	-2.11	121.30	127.43
3	J	607	HEC	C4B-NB-C1B	2.11	109.26	105.82
3	P	605	HEC	O2D-CGD-CBD	2.11	120.67	114.00
3	A	600	HEC	O2A-CGA-CBA	2.11	120.67	114.00
3	E	604	HEC	CHB-C1B-C2B	-2.11	121.30	127.43
3	E	605	HEC	O2D-CGD-CBD	2.11	120.67	114.00
3	S	601	HEC	O2A-CGA-CBA	2.11	120.67	114.00
3	C	602	HEC	CHA-C4D-ND	2.11	127.69	123.86
3	C	605	HEC	CHD-C1D-ND	2.11	127.69	123.86
3	T	606	HEC	CHA-C4D-ND	2.11	127.69	123.86
3	P	604	HEC	CHB-C1B-C2B	-2.11	121.31	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	605	HEC	CHA-C4D-C3D	-2.11	120.68	125.30
3	L	605	HEC	O2D-CGD-CBD	2.11	120.66	114.00
3	V	600	HEC	O2A-CGA-CBA	2.11	120.66	114.00
3	O	605	HEC	CHA-C4D-C3D	-2.11	120.69	125.30
3	G	601	HEC	CHD-C1D-ND	2.11	127.68	123.86
3	I	607	HEC	CHB-C1B-NB	2.11	127.68	123.86
3	R	607	HEC	C4C-NC-C1C	2.11	109.25	105.82
3	A	604	HEC	CHB-C1B-NB	2.11	127.68	123.86
3	L	601	HEC	CHD-C1D-ND	2.11	127.68	123.86
3	S	605	HEC	CHD-C1D-ND	2.11	127.68	123.86
3	K	604	HEC	CHA-C4D-C3D	-2.10	120.69	125.30
3	P	603	HEC	CHB-C4A-NA	-2.10	122.16	124.45
3	D	602	HEC	C2A-C1A-NA	-2.10	108.29	110.32
3	R	600	HEC	O2D-CGD-CBD	2.10	120.65	114.00
3	C	602	HEC	CHD-C4C-NC	2.10	126.74	124.45
3	M	604	HEC	CHD-C1D-ND	2.10	127.67	123.86
3	C	604	HEC	CHA-C4D-C3D	-2.10	120.70	125.30
3	B	607	HEC	CHA-C4D-ND	2.10	127.67	123.86
3	H	604	HEC	CHB-C1B-C2B	-2.10	121.32	127.43
3	F	602	HEC	CHD-C1D-ND	2.10	127.67	123.86
3	E	605	HEC	C4C-NC-C1C	2.10	109.25	105.82
3	O	604	HEC	CHB-C1B-C2B	-2.10	121.33	127.43
3	C	604	HEC	CHD-C1D-C2D	-2.10	121.33	127.43
3	D	600	HEC	O2A-CGA-CBA	2.10	120.63	114.00
3	L	606	HEC	CBA-CAA-C2A	-2.10	106.73	112.53
3	Q	602	HEC	CHD-C1D-ND	2.10	127.67	123.86
3	L	605	HEC	O2A-CGA-CBA	2.10	120.63	114.00
3	O	605	HEC	CHB-C1B-NB	2.10	127.67	123.86
3	X	606	HEC	CHD-C1D-ND	2.10	127.67	123.86
3	B	601	HEC	CHA-C4D-C3D	-2.10	120.70	125.30
3	M	607	HEC	C4C-NC-C1C	2.10	109.24	105.82
3	I	603	HEC	CHC-C1C-C2C	-2.10	121.34	127.43
3	E	602	HEC	CHD-C1D-ND	2.10	127.66	123.86
3	F	607	HEC	CHD-C1D-ND	2.10	127.66	123.86
3	M	601	HEC	CBD-CAD-C3D	-2.10	106.73	112.53
3	T	605	HEC	CHD-C1D-ND	2.10	127.66	123.86
3	G	607	HEC	CHB-C1B-NB	2.10	127.66	123.86
3	M	602	HEC	CHA-C4D-ND	2.10	127.66	123.86
3	S	606	HEC	CHD-C1D-ND	2.10	127.66	123.86
3	M	607	HEC	CHA-C1A-NA	2.10	126.73	124.45
3	X	601	HEC	O2A-CGA-CBA	2.10	120.62	114.00
3	Q	600	HEC	CHB-C1B-NB	2.10	127.66	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	607	HEC	O2D-CGD-O1D	-2.10	117.94	123.33
3	M	605	HEC	CHA-C4D-C3D	-2.09	120.71	125.30
3	N	606	HEC	CHD-C1D-ND	2.09	127.66	123.86
3	B	600	HEC	CHA-C1A-NA	2.09	126.73	124.45
3	H	605	HEC	CHA-C4D-ND	2.09	127.66	123.86
3	R	605	HEC	C4B-NB-C1B	2.09	109.23	105.82
3	N	607	HEC	C4C-NC-C1C	2.09	109.23	105.82
3	T	605	HEC	O2A-CGA-CBA	2.09	120.61	114.00
3	U	602	HEC	CHA-C4D-ND	2.09	127.66	123.86
3	X	605	HEC	CHD-C1D-ND	2.09	127.66	123.86
3	J	605	HEC	CHA-C1A-NA	2.09	126.73	124.45
3	D	600	HEC	CHD-C1D-ND	2.09	127.66	123.86
3	P	600	HEC	O2D-CGD-CBD	2.09	120.61	114.00
3	N	607	HEC	C4B-NB-C1B	2.09	109.23	105.82
3	B	604	HEC	CHA-C4D-C3D	-2.09	120.72	125.30
3	F	607	HEC	CHB-C1B-NB	2.09	127.65	123.86
3	J	602	HEC	O2A-CGA-CBA	2.09	120.61	114.00
3	Q	605	HEC	CHB-C1B-NB	2.09	127.65	123.86
3	P	605	HEC	C4B-NB-C1B	2.09	109.23	105.82
3	J	601	HEC	CAA-C2A-C1A	2.09	129.10	124.85
3	J	604	HEC	CHB-C1B-C2B	-2.09	121.36	127.43
3	F	601	HEC	C4B-NB-C1B	2.09	109.23	105.82
3	J	605	HEC	O2D-CGD-CBD	2.09	120.60	114.00
3	R	605	HEC	O2A-CGA-O1A	-2.09	117.96	123.33
3	T	601	HEC	CHA-C4D-C3D	-2.09	120.73	125.30
3	Q	601	HEC	CHB-C1B-C2B	-2.09	121.36	127.43
3	R	604	HEC	CHD-C1D-C2D	-2.09	121.36	127.43
3	L	600	HEC	O2A-CGA-CBA	2.09	120.60	114.00
3	C	605	HEC	CBD-CAD-C3D	2.09	118.31	112.53
3	B	601	HEC	C4B-NB-C1B	2.09	109.22	105.82
3	L	603	HEC	O1A-CGA-CBA	-2.09	116.47	123.09
3	I	602	HEC	O2A-CGA-CBA	2.09	120.59	114.00
3	L	606	HEC	C2A-C1A-NA	-2.09	108.31	110.32
3	D	605	HEC	O2A-CGA-CBA	2.09	120.59	114.00
3	V	604	HEC	CHD-C1D-C2D	-2.09	121.37	127.43
3	J	603	HEC	O1A-CGA-CBA	-2.09	116.48	123.09
3	C	607	HEC	CHD-C4C-NC	2.08	126.72	124.45
3	B	602	HEC	CHA-C4D-ND	2.08	127.64	123.86
3	G	601	HEC	C4B-NB-C1B	2.08	109.22	105.82
3	X	604	HEC	CHB-C1B-C2B	-2.08	121.38	127.43
3	P	605	HEC	CHD-C1D-ND	2.08	127.64	123.86
3	E	607	HEC	C4C-NC-C1C	2.08	109.22	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	605	HEC	CHD-C4C-NC	2.08	126.72	124.45
3	R	601	HEC	O2A-CGA-CBA	2.08	120.58	114.00
3	X	603	HEC	O1A-CGA-CBA	-2.08	116.49	123.09
3	E	602	HEC	CHA-C4D-ND	2.08	127.63	123.86
3	U	603	HEC	O1A-CGA-CBA	-2.08	116.49	123.09
3	W	605	HEC	CHD-C1D-ND	2.08	127.63	123.86
3	O	601	HEC	C4B-NB-C1B	2.08	109.21	105.82
3	A	601	HEC	O2A-CGA-CBA	2.08	120.57	114.00
3	E	605	HEC	CHB-C1B-NB	2.08	127.63	123.86
3	I	603	HEC	C1B-CHB-C4A	-2.08	118.24	124.66
3	D	603	HEC	C3D-C4D-ND	-2.08	107.84	110.15
3	L	602	HEC	O2A-CGA-CBA	2.08	120.57	114.00
3	B	607	HEC	CHB-C1B-NB	2.08	127.63	123.86
3	F	604	HEC	CHD-C1D-C2D	-2.08	121.39	127.43
3	L	604	HEC	CHB-C1B-C2B	-2.08	121.39	127.43
3	S	604	HEC	CHD-C1D-C2D	-2.08	121.39	127.43
3	G	607	HEC	O2D-CGD-O1D	-2.08	117.99	123.33
3	K	601	HEC	CHB-C1B-C2B	-2.08	121.40	127.43
3	S	600	HEC	O2D-CGD-CBD	2.08	120.56	114.00
3	A	605	HEC	CHB-C1B-NB	2.08	127.62	123.86
3	J	605	HEC	CAD-C3D-C2D	2.08	131.73	127.07
3	T	602	HEC	CHD-C1D-ND	2.08	127.62	123.86
3	A	603	HEC	O1A-CGA-CBA	-2.08	116.51	123.09
3	D	601	HEC	CHD-C1D-ND	2.08	127.62	123.86
3	F	604	HEC	CHB-C1B-C2B	-2.07	121.40	127.43
3	G	602	HEC	O2D-CGD-CBD	2.07	120.56	114.00
3	E	607	HEC	CHA-C4D-ND	2.07	127.62	123.86
3	M	606	HEC	CHD-C1D-ND	2.07	127.62	123.86
3	X	600	HEC	O2A-CGA-CBA	2.07	120.55	114.00
3	E	603	HEC	O1A-CGA-CBA	-2.07	116.52	123.09
3	O	600	HEC	C4B-NB-C1B	2.07	109.20	105.82
3	Q	603	HEC	C3D-C4D-ND	-2.07	107.85	110.15
3	H	605	HEC	C4B-NB-C1B	2.07	109.20	105.82
3	J	600	HEC	C4B-NB-C1B	2.07	109.19	105.82
3	F	600	HEC	CHA-C1A-NA	2.07	126.71	124.45
3	M	605	HEC	O2D-CGD-CBD	2.07	120.54	114.00
3	T	606	HEC	CHD-C1D-ND	2.07	127.61	123.86
3	D	600	HEC	O2D-CGD-CBD	2.07	120.53	114.00
3	L	607	HEC	C4C-NC-C1C	2.07	109.19	105.82
3	U	604	HEC	CHD-C1D-C2D	-2.07	121.42	127.43
3	S	607	HEC	C4C-NC-C1C	2.07	109.19	105.82
3	J	607	HEC	CHA-C4D-ND	2.07	127.61	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	606	HEC	O2D-CGD-CBD	2.07	120.53	114.00
3	M	601	HEC	CHA-C4D-C3D	-2.07	120.78	125.30
3	M	600	HEC	O2A-CGA-CBA	2.07	120.53	114.00
3	H	604	HEC	CHD-C1D-C2D	-2.07	121.43	127.43
3	C	605	HEC	C4C-NC-C1C	2.07	109.19	105.82
3	P	601	HEC	CHD-C1D-ND	2.07	127.61	123.86
3	A	602	HEC	O2A-CGA-CBA	2.07	120.53	114.00
3	N	604	HEC	CHA-C1A-NA	2.07	126.70	124.45
3	C	601	HEC	CHA-C4D-C3D	-2.07	120.78	125.30
3	P	607	HEC	CHD-C1D-ND	2.07	127.61	123.86
3	U	601	HEC	O2A-CGA-CBA	2.06	120.52	114.00
3	K	605	HEC	CHB-C1B-NB	2.06	127.60	123.86
3	W	606	HEC	CHD-C1D-ND	2.06	127.60	123.86
3	F	601	HEC	CHA-C4D-C3D	-2.06	120.78	125.30
3	N	601	HEC	CHA-C4D-C3D	-2.06	120.78	125.30
3	A	606	HEC	O2A-CGA-CBA	2.06	120.52	114.00
3	Q	605	HEC	CHA-C4D-ND	2.06	127.60	123.86
3	V	607	HEC	CHD-C1D-ND	2.06	127.60	123.86
3	U	605	HEC	CBD-CAD-C3D	2.06	118.23	112.53
3	K	606	HEC	O2D-CGD-CBD	2.06	120.52	114.00
3	E	600	HEC	CHB-C1B-C2B	-2.06	121.44	127.43
3	Q	607	HEC	CHB-C1B-NB	2.06	127.60	123.86
3	K	600	HEC	CHA-C1A-NA	2.06	126.70	124.45
3	B	605	HEC	O2D-CGD-CBD	2.06	120.51	114.00
3	O	601	HEC	CHB-C1B-C2B	-2.06	121.44	127.43
3	O	605	HEC	CBD-CAD-C3D	2.06	118.23	112.53
3	T	607	HEC	CHA-C4D-ND	2.06	127.60	123.86
3	P	603	HEC	O1D-CGD-CBD	-2.06	116.56	123.09
3	O	605	HEC	C4C-NC-C1C	2.06	109.18	105.82
3	C	600	HEC	CHA-C1A-NA	2.06	126.70	124.45
3	H	604	HEC	CHA-C1A-NA	2.06	126.70	124.45
3	V	605	HEC	C4B-NB-C1B	2.06	109.18	105.82
3	S	604	HEC	CHA-C1A-NA	2.06	126.70	124.45
3	V	602	HEC	CHA-C4D-ND	2.06	127.59	123.86
3	B	606	HEC	CBA-CAA-C2A	-2.06	106.84	112.53
3	V	605	HEC	CHD-C1D-ND	2.06	127.59	123.86
3	V	601	HEC	C4B-NB-C1B	2.06	109.18	105.82
3	M	607	HEC	CHB-C1B-NB	2.06	127.59	123.86
3	G	603	HEC	O1A-CGA-CBA	-2.06	116.57	123.09
3	N	604	HEC	CHA-C4D-C3D	-2.06	120.80	125.30
3	Q	601	HEC	CHA-C4D-C3D	-2.06	120.80	125.30
3	O	602	HEC	CHD-C1D-ND	2.06	127.59	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	607	HEC	CHA-C4D-ND	2.06	127.59	123.86
3	O	604	HEC	CHA-C4D-C3D	-2.06	120.80	125.30
3	H	603	HEC	O2A-CGA-CBA	2.06	120.50	114.00
3	Q	607	HEC	CHA-C1A-NA	2.06	126.69	124.45
3	J	606	HEC	CHB-C1B-NB	2.06	127.59	123.86
3	A	601	HEC	CHA-C4D-C3D	-2.06	120.80	125.30
3	B	601	HEC	CHB-C1B-C2B	-2.06	121.46	127.43
3	G	600	HEC	O2D-CGD-CBD	2.06	120.49	114.00
3	K	604	HEC	CHD-C1D-C2D	-2.05	121.46	127.43
3	S	603	HEC	O2D-CGD-CBD	2.05	120.49	114.00
3	A	604	HEC	CHB-C1B-C2B	-2.05	121.46	127.43
3	J	604	HEC	CHA-C4D-C3D	-2.05	120.80	125.30
3	D	606	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	S	603	HEC	O2A-CGA-CBA	2.05	120.49	114.00
3	U	600	HEC	O2D-CGD-CBD	2.05	120.49	114.00
3	P	604	HEC	CHD-C1D-C2D	-2.05	121.47	127.43
3	A	607	HEC	C4B-NB-C1B	2.05	109.17	105.82
3	N	600	HEC	C4B-NB-C1B	2.05	109.17	105.82
3	U	605	HEC	C4C-NC-C1C	2.05	109.17	105.82
3	A	607	HEC	CHB-C1B-NB	2.05	127.58	123.86
3	P	605	HEC	CHB-C1B-NB	2.05	127.58	123.86
3	Q	606	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	W	602	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	E	603	HEC	CAA-C2A-C1A	2.05	129.02	124.85
3	V	607	HEC	CHB-C1B-NB	2.05	127.58	123.86
3	H	601	HEC	CHD-C1D-C2D	-2.05	121.47	127.43
3	N	605	HEC	O2D-CGD-CBD	2.05	120.48	114.00
3	C	606	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	A	604	HEC	CHA-C1A-NA	2.05	126.69	124.45
3	R	603	HEC	O2A-CGA-CBA	2.05	120.48	114.00
3	B	600	HEC	C4B-NB-C1B	2.05	109.16	105.82
3	N	605	HEC	C4B-NB-C1B	2.05	109.16	105.82
3	T	604	HEC	CHD-C1D-C2D	-2.05	121.48	127.43
3	H	605	HEC	CBD-CAD-C3D	2.05	118.20	112.53
3	F	605	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	R	607	HEC	CHA-C1A-NA	2.05	126.68	124.45
3	E	606	HEC	CHD-C1D-ND	2.05	127.57	123.86
3	C	605	HEC	CHA-C4D-C3D	-2.05	120.82	125.30
3	V	601	HEC	CHB-C1B-C2B	-2.05	121.48	127.43
3	U	606	HEC	CHD-C1D-ND	2.05	127.57	123.86
3	R	601	HEC	C4B-NB-C1B	2.05	109.16	105.82
3	F	603	HEC	CHB-C4A-NA	-2.05	122.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	606	HEC	C2A-C1A-NA	-2.04	108.35	110.32
3	B	604	HEC	C4B-NB-C1B	2.04	109.15	105.82
3	P	600	HEC	O2A-CGA-CBA	2.04	120.46	114.00
3	G	601	HEC	CAA-C2A-C1A	2.04	129.01	124.85
3	C	607	HEC	C4B-NB-C1B	2.04	109.15	105.82
3	J	603	HEC	O1D-CGD-CBD	-2.04	116.61	123.09
3	H	602	HEC	CHA-C4D-ND	2.04	127.56	123.86
3	H	600	HEC	O2A-CGA-CBA	2.04	120.45	114.00
3	D	607	HEC	C4B-NB-C1B	2.04	109.15	105.82
3	O	602	HEC	O2A-CGA-CBA	2.04	120.45	114.00
3	G	607	HEC	CHA-C4D-ND	2.04	127.56	123.86
3	D	605	HEC	C4B-NB-C1B	2.04	109.15	105.82
3	E	604	HEC	CHD-C1D-C2D	-2.04	121.50	127.43
3	O	601	HEC	CHA-C4D-C3D	-2.04	120.83	125.30
3	Q	604	HEC	CHA-C1A-NA	2.04	126.67	124.45
3	F	600	HEC	O2D-CGD-CBD	2.04	120.44	114.00
3	N	604	HEC	CHB-C1B-C2B	-2.04	121.51	127.43
3	S	601	HEC	CHA-C4D-C3D	-2.04	120.84	125.30
3	O	607	HEC	CHD-C1D-ND	2.04	127.56	123.86
3	W	604	HEC	CHD-C1D-C2D	-2.04	121.51	127.43
3	G	605	HEC	CAD-CBD-CGD	-2.04	108.26	113.67
3	O	603	HEC	C3D-C4D-ND	-2.04	107.89	110.15
3	J	605	HEC	CHD-C1D-ND	2.04	127.56	123.86
3	G	600	HEC	CHB-C1B-C2B	-2.04	121.51	127.43
3	A	607	HEC	C4C-NC-C1C	2.04	109.14	105.82
3	K	602	HEC	CHD-C1D-ND	2.04	127.55	123.86
3	Q	605	HEC	CHD-C1D-ND	2.04	127.55	123.86
3	D	602	HEC	CHB-C1B-C2B	-2.04	121.52	127.43
3	B	605	HEC	CHA-C4D-C3D	-2.04	120.84	125.30
3	R	606	HEC	CBA-CAA-C2A	-2.04	106.91	112.53
3	S	607	HEC	CHB-C1B-NB	2.04	127.55	123.86
3	P	604	HEC	CHA-C4D-C3D	-2.04	120.84	125.30
3	X	607	HEC	CHA-C4D-ND	2.03	127.55	123.86
3	R	605	HEC	CHA-C4D-C3D	-2.03	120.84	125.30
3	S	607	HEC	O2D-CGD-O1D	-2.03	118.10	123.33
3	W	600	HEC	O2D-CGD-CBD	2.03	120.43	114.00
3	X	605	HEC	C4B-NB-C1B	2.03	109.14	105.82
3	T	603	HEC	O1A-CGA-CBA	-2.03	116.64	123.09
3	S	607	HEC	CHD-C1D-ND	2.03	127.55	123.86
3	T	604	HEC	CHA-C4D-C3D	-2.03	120.85	125.30
3	I	601	HEC	C4B-NB-C1B	2.03	109.14	105.82
3	X	603	HEC	C3D-C4D-ND	-2.03	107.90	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	604	HEC	CHA-C1A-NA	2.03	126.67	124.45
3	K	602	HEC	CHA-C4D-ND	2.03	127.55	123.86
3	H	606	HEC	CBA-CAA-C2A	-2.03	106.92	112.53
3	X	604	HEC	CHD-C1D-C2D	-2.03	121.53	127.43
3	V	603	HEC	O1A-CGA-CBA	-2.03	116.65	123.09
3	B	607	HEC	O2D-CGD-O1D	-2.03	118.11	123.33
3	N	603	HEC	O2A-CGA-CBA	2.03	120.42	114.00
3	A	604	HEC	CHD-C1D-C2D	-2.03	121.53	127.43
3	V	600	HEC	O2D-CGD-CBD	2.03	120.42	114.00
3	K	603	HEC	CAA-C2A-C1A	2.03	128.98	124.85
3	S	603	HEC	CAA-C2A-C1A	2.03	128.98	124.85
3	E	602	HEC	CHD-C4C-NC	2.03	126.66	124.45
3	P	606	HEC	CBA-CAA-C2A	-2.03	106.92	112.53
3	U	605	HEC	C4B-NB-C1B	2.03	109.13	105.82
3	B	603	HEC	CAA-C2A-C1A	2.03	128.97	124.85
3	D	604	HEC	CHD-C1D-C2D	-2.03	121.54	127.43
3	P	601	HEC	CHB-C1B-C2B	-2.03	121.54	127.43
3	R	600	HEC	CHD-C1D-C2D	-2.03	121.54	127.43
3	E	605	HEC	C4B-NB-C1B	2.03	109.13	105.82
3	J	607	HEC	CHB-C1B-NB	2.03	127.53	123.86
3	I	607	HEC	CHD-C1D-ND	2.03	127.53	123.86
3	S	601	HEC	CHB-C1B-C2B	-2.02	121.55	127.43
3	J	601	HEC	C4B-NB-C1B	2.02	109.12	105.82
3	X	605	HEC	C4C-NC-C1C	2.02	109.12	105.82
3	D	607	HEC	CHB-C1B-C2B	-2.02	121.55	127.43
3	F	604	HEC	CHA-C4D-C3D	-2.02	120.87	125.30
3	B	603	HEC	CHB-C4A-NA	-2.02	122.25	124.45
3	G	601	HEC	CHB-C1B-C2B	-2.02	121.55	127.43
3	T	600	HEC	CHA-C1A-NA	2.02	126.66	124.45
3	N	600	HEC	CHB-C1B-C2B	-2.02	121.56	127.43
3	E	602	HEC	O2A-CGA-CBA	2.02	120.39	114.00
3	G	607	HEC	CHD-C1D-ND	2.02	127.53	123.86
3	A	607	HEC	CHA-C4D-ND	2.02	127.53	123.86
3	P	602	HEC	CHD-C1D-ND	2.02	127.53	123.86
3	N	604	HEC	CHD-C1D-C2D	-2.02	121.56	127.43
3	I	603	HEC	O2D-CGD-CBD	2.02	120.38	114.00
3	P	600	HEC	CHB-C1B-C2B	-2.02	121.56	127.43
3	A	600	HEC	C4B-NB-C1B	2.02	109.11	105.82
3	E	607	HEC	O2D-CGD-O1D	-2.02	118.14	123.33
3	G	602	HEC	O2A-CGA-CBA	2.02	120.38	114.00
3	G	602	HEC	CHD-C4C-NC	2.02	126.65	124.45
3	V	600	HEC	CHA-C1A-NA	2.02	126.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	600	HEC	CHD-C1D-C2D	-2.02	121.56	127.43
3	T	605	HEC	C4C-NC-C1C	2.02	109.11	105.82
3	M	603	HEC	O1A-CGA-CBA	-2.02	116.69	123.09
3	M	605	HEC	O2A-CGA-CBA	2.02	120.38	114.00
3	V	605	HEC	O2D-CGD-CBD	2.02	120.38	114.00
3	E	602	HEC	O2D-CGD-CBD	2.02	120.37	114.00
3	M	605	HEC	CHB-C1B-C2B	-2.02	121.57	127.43
3	N	605	HEC	CHD-C4C-NC	2.02	126.65	124.45
3	M	601	HEC	CHB-C1B-C2B	-2.02	121.57	127.43
3	E	607	HEC	O2D-CGD-CBD	2.02	120.37	114.00
3	X	601	HEC	C4B-NB-C1B	2.02	109.11	105.82
3	U	601	HEC	CHA-C4D-C3D	-2.02	120.89	125.30
3	X	606	HEC	CBA-CAA-C2A	-2.02	106.96	112.53
3	D	604	HEC	CHC-C4B-C3B	-2.02	121.81	125.21
3	P	605	HEC	CBD-CAD-C3D	2.02	118.11	112.53
3	I	600	HEC	O2D-CGD-CBD	2.01	120.36	114.00
3	V	605	HEC	CHA-C1A-NA	2.01	126.65	124.45
3	W	600	HEC	CHD-C1D-C2D	-2.01	121.58	127.43
3	Q	607	HEC	CHD-C1D-ND	2.01	127.51	123.86
3	H	600	HEC	C4B-NB-C1B	2.01	109.10	105.82
3	I	606	HEC	C4C-NC-C1C	2.01	109.10	105.82
3	T	600	HEC	C4B-NB-C1B	2.01	109.10	105.82
3	O	606	HEC	C4C-NC-C1C	2.01	109.10	105.82
3	I	603	HEC	O2A-CGA-CBA	2.01	120.36	114.00
3	L	604	HEC	CHD-C1D-C2D	-2.01	121.59	127.43
3	J	606	HEC	O2D-CGD-CBD	2.01	120.36	114.00
3	T	600	HEC	CHB-C1B-C2B	-2.01	121.59	127.43
3	I	602	HEC	CAA-C2A-C3A	-2.01	124.10	127.87
3	G	600	HEC	CHD-C1D-C2D	-2.01	121.59	127.43
3	A	603	HEC	O2D-CGD-CBD	2.01	120.35	114.00
3	V	605	HEC	CHA-C4D-C3D	-2.01	120.90	125.30
3	G	605	HEC	CHA-C4D-ND	2.01	127.50	123.86
3	F	600	HEC	O2A-CGA-CBA	2.01	120.35	114.00
3	A	605	HEC	CHD-C4C-NC	2.01	126.64	124.45
3	G	605	HEC	C4C-NC-C1C	2.01	109.09	105.82
3	V	607	HEC	C4C-NC-C1C	2.01	109.09	105.82
3	E	600	HEC	CHD-C1D-C2D	-2.01	121.60	127.43
3	A	600	HEC	CHB-C1B-C2B	-2.01	121.60	127.43
3	W	603	HEC	O2A-CGA-CBA	2.01	120.34	114.00
3	O	600	HEC	O2D-CGD-CBD	2.01	120.34	114.00
3	P	607	HEC	CHB-C1B-NB	2.01	127.50	123.86
3	M	603	HEC	C1A-C2A-C3A	-2.00	104.47	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	601	HEC	CHA-C4D-C3D	-2.00	120.91	125.30
3	L	604	HEC	C4B-NB-C1B	2.00	109.09	105.82
3	W	605	HEC	C4B-NB-C1B	2.00	109.09	105.82
3	B	607	HEC	O2D-CGD-CBD	2.00	120.33	114.00
3	R	600	HEC	O2A-CGA-CBA	2.00	120.33	114.00
3	K	600	HEC	CHD-C1D-C2D	-2.00	121.61	127.43
3	I	603	HEC	CAD-C3D-C4D	-2.00	121.03	124.94
3	H	603	HEC	O1A-CGA-CBA	-2.00	116.74	123.09
3	J	607	HEC	C4C-NC-C1C	2.00	109.09	105.82
3	A	600	HEC	CHD-C1D-C2D	-2.00	121.61	127.43
3	I	601	HEC	CBD-CAD-C3D	-2.00	107.00	112.53
3	O	600	HEC	CHA-C1A-NA	2.00	126.63	124.45
3	W	602	HEC	CAD-CBD-CGD	-2.00	108.36	113.67
3	S	604	HEC	CHA-C4D-C3D	-2.00	120.92	125.30
3	V	607	HEC	O2D-CGD-O1D	-2.00	118.18	123.33
3	K	605	HEC	C4B-NB-C1B	2.00	109.08	105.82
3	J	600	HEC	CHB-C1B-C2B	-2.00	121.62	127.43
3	A	606	HEC	CHD-C1D-ND	2.00	127.49	123.86
3	V	600	HEC	C4B-NB-C1B	2.00	109.08	105.82
3	L	602	HEC	CHD-C1D-ND	2.00	127.49	123.86

There are no chirality outliers.

All (1445) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	600	HEC	C2B-C3B-CAB-CBB
3	G	600	HEC	C4B-C3B-CAB-CBB
3	G	600	HEC	C2C-C3C-CAC-CBC
3	G	600	HEC	C4C-C3C-CAC-CBC
3	G	601	HEC	C2C-C3C-CAC-CBC
3	G	604	HEC	C2C-C3C-CAC-CBC
3	G	604	HEC	C4C-C3C-CAC-CBC
3	G	605	HEC	C2B-C3B-CAB-CBB
3	G	605	HEC	C4B-C3B-CAB-CBB
3	G	605	HEC	C2C-C3C-CAC-CBC
3	G	605	HEC	C4C-C3C-CAC-CBC
3	G	606	HEC	C2B-C3B-CAB-CBB
3	G	607	HEC	C2B-C3B-CAB-CBB
3	G	607	HEC	C4B-C3B-CAB-CBB
3	G	607	HEC	C2C-C3C-CAC-CBC
3	G	607	HEC	C4C-C3C-CAC-CBC
3	G	603	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	G	603	HEC	C4C-C3C-CAC-CBC
3	A	600	HEC	C2B-C3B-CAB-CBB
3	A	600	HEC	C4B-C3B-CAB-CBB
3	A	600	HEC	C2C-C3C-CAC-CBC
3	A	600	HEC	C4C-C3C-CAC-CBC
3	A	601	HEC	C2C-C3C-CAC-CBC
3	A	604	HEC	C2C-C3C-CAC-CBC
3	A	604	HEC	C4C-C3C-CAC-CBC
3	A	605	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	C4B-C3B-CAB-CBB
3	A	605	HEC	C2C-C3C-CAC-CBC
3	A	605	HEC	C4C-C3C-CAC-CBC
3	A	606	HEC	C2B-C3B-CAB-CBB
3	A	607	HEC	C2B-C3B-CAB-CBB
3	A	607	HEC	C4B-C3B-CAB-CBB
3	A	607	HEC	C2C-C3C-CAC-CBC
3	A	607	HEC	C4C-C3C-CAC-CBC
3	A	603	HEC	C2C-C3C-CAC-CBC
3	A	603	HEC	C4C-C3C-CAC-CBC
3	B	603	HEC	C4B-C3B-CAB-CBB
3	B	603	HEC	C2C-C3C-CAC-CBC
3	B	603	HEC	C4C-C3C-CAC-CBC
3	B	600	HEC	C2B-C3B-CAB-CBB
3	B	600	HEC	C4B-C3B-CAB-CBB
3	B	600	HEC	C2C-C3C-CAC-CBC
3	B	600	HEC	C4C-C3C-CAC-CBC
3	B	601	HEC	C2C-C3C-CAC-CBC
3	B	602	HEC	C4C-C3C-CAC-CBC
3	B	604	HEC	C2C-C3C-CAC-CBC
3	B	604	HEC	C4C-C3C-CAC-CBC
3	B	605	HEC	C2B-C3B-CAB-CBB
3	B	605	HEC	C4B-C3B-CAB-CBB
3	B	605	HEC	C2C-C3C-CAC-CBC
3	B	605	HEC	C4C-C3C-CAC-CBC
3	B	607	HEC	C2B-C3B-CAB-CBB
3	B	607	HEC	C4B-C3B-CAB-CBB
3	B	607	HEC	C2C-C3C-CAC-CBC
3	B	607	HEC	C4C-C3C-CAC-CBC
3	C	603	HEC	C4B-C3B-CAB-CBB
3	C	603	HEC	C2C-C3C-CAC-CBC
3	C	603	HEC	C4C-C3C-CAC-CBC
3	C	600	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	600	HEC	C4B-C3B-CAB-CBB
3	C	600	HEC	C2C-C3C-CAC-CBC
3	C	600	HEC	C4C-C3C-CAC-CBC
3	C	601	HEC	C2C-C3C-CAC-CBC
3	C	604	HEC	C2C-C3C-CAC-CBC
3	C	604	HEC	C4C-C3C-CAC-CBC
3	C	605	HEC	C2B-C3B-CAB-CBB
3	C	605	HEC	C4B-C3B-CAB-CBB
3	C	605	HEC	C2C-C3C-CAC-CBC
3	C	605	HEC	C4C-C3C-CAC-CBC
3	C	607	HEC	C2B-C3B-CAB-CBB
3	C	607	HEC	C4B-C3B-CAB-CBB
3	C	607	HEC	C2C-C3C-CAC-CBC
3	C	607	HEC	C4C-C3C-CAC-CBC
3	D	600	HEC	C2B-C3B-CAB-CBB
3	D	600	HEC	C4B-C3B-CAB-CBB
3	D	600	HEC	C2C-C3C-CAC-CBC
3	D	600	HEC	C4C-C3C-CAC-CBC
3	D	601	HEC	C2B-C3B-CAB-CBB
3	D	602	HEC	C2B-C3B-CAB-CBB
3	D	602	HEC	C4B-C3B-CAB-CBB
3	D	604	HEC	C2C-C3C-CAC-CBC
3	D	604	HEC	C4C-C3C-CAC-CBC
3	D	605	HEC	C2B-C3B-CAB-CBB
3	D	605	HEC	C4B-C3B-CAB-CBB
3	D	605	HEC	C2C-C3C-CAC-CBC
3	D	605	HEC	C4C-C3C-CAC-CBC
3	D	606	HEC	C2C-C3C-CAC-CBC
3	D	606	HEC	C4C-C3C-CAC-CBC
3	D	607	HEC	C2B-C3B-CAB-CBB
3	D	607	HEC	C2C-C3C-CAC-CBC
3	D	607	HEC	C4C-C3C-CAC-CBC
3	D	603	HEC	C2B-C3B-CAB-CBB
3	D	603	HEC	C4B-C3B-CAB-CBB
3	D	603	HEC	C2C-C3C-CAC-CBC
3	D	603	HEC	C4C-C3C-CAC-CBC
3	E	603	HEC	C4C-C3C-CAC-CBC
3	E	600	HEC	C2B-C3B-CAB-CBB
3	E	600	HEC	C4B-C3B-CAB-CBB
3	E	600	HEC	C2C-C3C-CAC-CBC
3	E	600	HEC	C4C-C3C-CAC-CBC
3	E	601	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	E	601	HEC	C4C-C3C-CAC-CBC
3	E	604	HEC	C2C-C3C-CAC-CBC
3	E	604	HEC	C4C-C3C-CAC-CBC
3	E	605	HEC	C2B-C3B-CAB-CBB
3	E	605	HEC	C4B-C3B-CAB-CBB
3	E	605	HEC	C2C-C3C-CAC-CBC
3	E	605	HEC	C4C-C3C-CAC-CBC
3	E	606	HEC	C2B-C3B-CAB-CBB
3	E	606	HEC	C2C-C3C-CAC-CBC
3	E	607	HEC	C2B-C3B-CAB-CBB
3	E	607	HEC	C4B-C3B-CAB-CBB
3	E	607	HEC	C2C-C3C-CAC-CBC
3	E	607	HEC	C4C-C3C-CAC-CBC
3	F	603	HEC	C2C-C3C-CAC-CBC
3	F	603	HEC	C4C-C3C-CAC-CBC
3	F	600	HEC	C2B-C3B-CAB-CBB
3	F	600	HEC	C4B-C3B-CAB-CBB
3	F	600	HEC	C2C-C3C-CAC-CBC
3	F	600	HEC	C4C-C3C-CAC-CBC
3	F	601	HEC	C2C-C3C-CAC-CBC
3	F	604	HEC	C2C-C3C-CAC-CBC
3	F	604	HEC	C4C-C3C-CAC-CBC
3	F	605	HEC	C2B-C3B-CAB-CBB
3	F	605	HEC	C4B-C3B-CAB-CBB
3	F	605	HEC	C2C-C3C-CAC-CBC
3	F	605	HEC	C4C-C3C-CAC-CBC
3	F	606	HEC	C2B-C3B-CAB-CBB
3	F	607	HEC	C2B-C3B-CAB-CBB
3	F	607	HEC	C4B-C3B-CAB-CBB
3	F	607	HEC	C2C-C3C-CAC-CBC
3	F	607	HEC	C4C-C3C-CAC-CBC
3	H	603	HEC	C2C-C3C-CAC-CBC
3	H	603	HEC	C4C-C3C-CAC-CBC
3	H	600	HEC	C2B-C3B-CAB-CBB
3	H	600	HEC	C4B-C3B-CAB-CBB
3	H	600	HEC	C2C-C3C-CAC-CBC
3	H	600	HEC	C4C-C3C-CAC-CBC
3	H	601	HEC	C2C-C3C-CAC-CBC
3	H	604	HEC	C2C-C3C-CAC-CBC
3	H	604	HEC	C4C-C3C-CAC-CBC
3	H	605	HEC	C2B-C3B-CAB-CBB
3	H	605	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	H	605	HEC	C2C-C3C-CAC-CBC
3	H	605	HEC	C4C-C3C-CAC-CBC
3	H	606	HEC	C2B-C3B-CAB-CBB
3	H	607	HEC	C2B-C3B-CAB-CBB
3	H	607	HEC	C4B-C3B-CAB-CBB
3	H	607	HEC	C2C-C3C-CAC-CBC
3	H	607	HEC	C4C-C3C-CAC-CBC
3	I	603	HEC	C2B-C3B-CAB-CBB
3	I	603	HEC	C4B-C3B-CAB-CBB
3	I	603	HEC	C2C-C3C-CAC-CBC
3	I	603	HEC	C4C-C3C-CAC-CBC
3	I	600	HEC	C2B-C3B-CAB-CBB
3	I	600	HEC	C2C-C3C-CAC-CBC
3	I	600	HEC	C4C-C3C-CAC-CBC
3	I	601	HEC	C2C-C3C-CAC-CBC
3	I	602	HEC	C2B-C3B-CAB-CBB
3	I	604	HEC	C2B-C3B-CAB-CBB
3	I	604	HEC	C2C-C3C-CAC-CBC
3	I	604	HEC	C4C-C3C-CAC-CBC
3	I	605	HEC	C2B-C3B-CAB-CBB
3	I	605	HEC	C4B-C3B-CAB-CBB
3	I	605	HEC	C2C-C3C-CAC-CBC
3	I	605	HEC	C4C-C3C-CAC-CBC
3	I	605	HEC	C2D-C3D-CAD-CBD
3	I	606	HEC	C2B-C3B-CAB-CBB
3	I	606	HEC	C4B-C3B-CAB-CBB
3	I	606	HEC	C2C-C3C-CAC-CBC
3	I	606	HEC	C4C-C3C-CAC-CBC
3	I	607	HEC	C2C-C3C-CAC-CBC
3	I	607	HEC	C4C-C3C-CAC-CBC
3	J	600	HEC	C2B-C3B-CAB-CBB
3	J	600	HEC	C4B-C3B-CAB-CBB
3	J	600	HEC	C2C-C3C-CAC-CBC
3	J	600	HEC	C4C-C3C-CAC-CBC
3	J	601	HEC	C2C-C3C-CAC-CBC
3	J	604	HEC	C2C-C3C-CAC-CBC
3	J	604	HEC	C4C-C3C-CAC-CBC
3	J	605	HEC	C2B-C3B-CAB-CBB
3	J	605	HEC	C4B-C3B-CAB-CBB
3	J	605	HEC	C2C-C3C-CAC-CBC
3	J	605	HEC	C4C-C3C-CAC-CBC
3	J	606	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	J	607	HEC	C2B-C3B-CAB-CBB
3	J	607	HEC	C4B-C3B-CAB-CBB
3	J	607	HEC	C2C-C3C-CAC-CBC
3	J	607	HEC	C4C-C3C-CAC-CBC
3	J	603	HEC	C2B-C3B-CAB-CBB
3	J	603	HEC	C4B-C3B-CAB-CBB
3	J	603	HEC	C2C-C3C-CAC-CBC
3	J	603	HEC	C4C-C3C-CAC-CBC
3	K	603	HEC	C2C-C3C-CAC-CBC
3	K	603	HEC	C4C-C3C-CAC-CBC
3	K	600	HEC	C2B-C3B-CAB-CBB
3	K	600	HEC	C4B-C3B-CAB-CBB
3	K	600	HEC	C2C-C3C-CAC-CBC
3	K	600	HEC	C4C-C3C-CAC-CBC
3	K	601	HEC	C2C-C3C-CAC-CBC
3	K	604	HEC	C2C-C3C-CAC-CBC
3	K	604	HEC	C4C-C3C-CAC-CBC
3	K	605	HEC	C2B-C3B-CAB-CBB
3	K	605	HEC	C4B-C3B-CAB-CBB
3	K	605	HEC	C2C-C3C-CAC-CBC
3	K	605	HEC	C4C-C3C-CAC-CBC
3	K	606	HEC	C2B-C3B-CAB-CBB
3	K	607	HEC	C2B-C3B-CAB-CBB
3	K	607	HEC	C4B-C3B-CAB-CBB
3	K	607	HEC	C2C-C3C-CAC-CBC
3	K	607	HEC	C4C-C3C-CAC-CBC
3	L	603	HEC	C2B-C3B-CAB-CBB
3	L	603	HEC	C4B-C3B-CAB-CBB
3	L	603	HEC	C2C-C3C-CAC-CBC
3	L	603	HEC	C4C-C3C-CAC-CBC
3	L	600	HEC	C2B-C3B-CAB-CBB
3	L	600	HEC	C4B-C3B-CAB-CBB
3	L	600	HEC	C2C-C3C-CAC-CBC
3	L	600	HEC	C4C-C3C-CAC-CBC
3	L	601	HEC	C2C-C3C-CAC-CBC
3	L	604	HEC	C2C-C3C-CAC-CBC
3	L	604	HEC	C4C-C3C-CAC-CBC
3	L	605	HEC	C2B-C3B-CAB-CBB
3	L	605	HEC	C4B-C3B-CAB-CBB
3	L	605	HEC	C2C-C3C-CAC-CBC
3	L	605	HEC	C4C-C3C-CAC-CBC
3	L	606	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	L	607	HEC	C2B-C3B-CAB-CBB
3	L	607	HEC	C4B-C3B-CAB-CBB
3	L	607	HEC	C2C-C3C-CAC-CBC
3	L	607	HEC	C4C-C3C-CAC-CBC
3	M	600	HEC	C2B-C3B-CAB-CBB
3	M	600	HEC	C4B-C3B-CAB-CBB
3	M	600	HEC	C2C-C3C-CAC-CBC
3	M	600	HEC	C4C-C3C-CAC-CBC
3	M	601	HEC	C2C-C3C-CAC-CBC
3	M	604	HEC	C2C-C3C-CAC-CBC
3	M	604	HEC	C4C-C3C-CAC-CBC
3	M	605	HEC	C2B-C3B-CAB-CBB
3	M	605	HEC	C4B-C3B-CAB-CBB
3	M	605	HEC	C2C-C3C-CAC-CBC
3	M	605	HEC	C4C-C3C-CAC-CBC
3	M	607	HEC	C2B-C3B-CAB-CBB
3	M	607	HEC	C4B-C3B-CAB-CBB
3	M	607	HEC	C2C-C3C-CAC-CBC
3	M	607	HEC	C4C-C3C-CAC-CBC
3	M	603	HEC	C4C-C3C-CAC-CBC
3	N	603	HEC	C4C-C3C-CAC-CBC
3	N	600	HEC	C2B-C3B-CAB-CBB
3	N	600	HEC	C4B-C3B-CAB-CBB
3	N	600	HEC	C2C-C3C-CAC-CBC
3	N	600	HEC	C4C-C3C-CAC-CBC
3	N	601	HEC	C2C-C3C-CAC-CBC
3	N	601	HEC	C4C-C3C-CAC-CBC
3	N	604	HEC	C2C-C3C-CAC-CBC
3	N	604	HEC	C4C-C3C-CAC-CBC
3	N	605	HEC	C2B-C3B-CAB-CBB
3	N	605	HEC	C4B-C3B-CAB-CBB
3	N	605	HEC	C2C-C3C-CAC-CBC
3	N	605	HEC	C4C-C3C-CAC-CBC
3	N	607	HEC	C2B-C3B-CAB-CBB
3	N	607	HEC	C4B-C3B-CAB-CBB
3	N	607	HEC	C2C-C3C-CAC-CBC
3	N	607	HEC	C4C-C3C-CAC-CBC
3	O	603	HEC	C4C-C3C-CAC-CBC
3	O	600	HEC	C2B-C3B-CAB-CBB
3	O	600	HEC	C4B-C3B-CAB-CBB
3	O	600	HEC	C2C-C3C-CAC-CBC
3	O	600	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	O	601	HEC	C2C-C3C-CAC-CBC
3	O	604	HEC	C2C-C3C-CAC-CBC
3	O	604	HEC	C4C-C3C-CAC-CBC
3	O	605	HEC	C2B-C3B-CAB-CBB
3	O	605	HEC	C4B-C3B-CAB-CBB
3	O	605	HEC	C2C-C3C-CAC-CBC
3	O	605	HEC	C4C-C3C-CAC-CBC
3	O	606	HEC	C2B-C3B-CAB-CBB
3	O	607	HEC	C2B-C3B-CAB-CBB
3	O	607	HEC	C4B-C3B-CAB-CBB
3	O	607	HEC	C2C-C3C-CAC-CBC
3	O	607	HEC	C4C-C3C-CAC-CBC
3	P	600	HEC	C2B-C3B-CAB-CBB
3	P	600	HEC	C4B-C3B-CAB-CBB
3	P	600	HEC	C2C-C3C-CAC-CBC
3	P	600	HEC	C4C-C3C-CAC-CBC
3	P	601	HEC	C2C-C3C-CAC-CBC
3	P	604	HEC	C2C-C3C-CAC-CBC
3	P	604	HEC	C4C-C3C-CAC-CBC
3	P	605	HEC	C2B-C3B-CAB-CBB
3	P	605	HEC	C4B-C3B-CAB-CBB
3	P	605	HEC	C2C-C3C-CAC-CBC
3	P	605	HEC	C4C-C3C-CAC-CBC
3	P	607	HEC	C2B-C3B-CAB-CBB
3	P	607	HEC	C4B-C3B-CAB-CBB
3	P	607	HEC	C2C-C3C-CAC-CBC
3	P	607	HEC	C4C-C3C-CAC-CBC
3	P	603	HEC	C4B-C3B-CAB-CBB
3	P	603	HEC	C2C-C3C-CAC-CBC
3	P	603	HEC	C4C-C3C-CAC-CBC
3	Q	603	HEC	C2C-C3C-CAC-CBC
3	Q	603	HEC	C4C-C3C-CAC-CBC
3	Q	600	HEC	C2B-C3B-CAB-CBB
3	Q	600	HEC	C4B-C3B-CAB-CBB
3	Q	600	HEC	C2C-C3C-CAC-CBC
3	Q	600	HEC	C4C-C3C-CAC-CBC
3	Q	601	HEC	C2C-C3C-CAC-CBC
3	Q	604	HEC	C2C-C3C-CAC-CBC
3	Q	604	HEC	C4C-C3C-CAC-CBC
3	Q	605	HEC	C2B-C3B-CAB-CBB
3	Q	605	HEC	C4B-C3B-CAB-CBB
3	Q	605	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	Q	605	HEC	C4C-C3C-CAC-CBC
3	Q	607	HEC	C2B-C3B-CAB-CBB
3	Q	607	HEC	C4B-C3B-CAB-CBB
3	Q	607	HEC	C2C-C3C-CAC-CBC
3	Q	607	HEC	C4C-C3C-CAC-CBC
3	R	603	HEC	C2C-C3C-CAC-CBC
3	R	603	HEC	C4C-C3C-CAC-CBC
3	R	600	HEC	C2B-C3B-CAB-CBB
3	R	600	HEC	C4B-C3B-CAB-CBB
3	R	600	HEC	C2C-C3C-CAC-CBC
3	R	600	HEC	C4C-C3C-CAC-CBC
3	R	601	HEC	C2C-C3C-CAC-CBC
3	R	604	HEC	C2C-C3C-CAC-CBC
3	R	604	HEC	C4C-C3C-CAC-CBC
3	R	605	HEC	C2B-C3B-CAB-CBB
3	R	605	HEC	C4B-C3B-CAB-CBB
3	R	605	HEC	C2C-C3C-CAC-CBC
3	R	605	HEC	C4C-C3C-CAC-CBC
3	R	606	HEC	C2B-C3B-CAB-CBB
3	R	607	HEC	C2B-C3B-CAB-CBB
3	R	607	HEC	C4B-C3B-CAB-CBB
3	R	607	HEC	C2C-C3C-CAC-CBC
3	R	607	HEC	C4C-C3C-CAC-CBC
3	S	600	HEC	C2B-C3B-CAB-CBB
3	S	600	HEC	C4B-C3B-CAB-CBB
3	S	600	HEC	C2C-C3C-CAC-CBC
3	S	600	HEC	C4C-C3C-CAC-CBC
3	S	601	HEC	C2C-C3C-CAC-CBC
3	S	604	HEC	C2C-C3C-CAC-CBC
3	S	604	HEC	C4C-C3C-CAC-CBC
3	S	605	HEC	C2B-C3B-CAB-CBB
3	S	605	HEC	C4B-C3B-CAB-CBB
3	S	605	HEC	C2C-C3C-CAC-CBC
3	S	605	HEC	C4C-C3C-CAC-CBC
3	S	607	HEC	C2B-C3B-CAB-CBB
3	S	607	HEC	C4B-C3B-CAB-CBB
3	S	607	HEC	C2C-C3C-CAC-CBC
3	S	607	HEC	C4C-C3C-CAC-CBC
3	S	603	HEC	C2C-C3C-CAC-CBC
3	S	603	HEC	C4C-C3C-CAC-CBC
3	T	603	HEC	C2C-C3C-CAC-CBC
3	T	603	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	T	600	HEC	C2B-C3B-CAB-CBB
3	T	600	HEC	C4B-C3B-CAB-CBB
3	T	600	HEC	C2C-C3C-CAC-CBC
3	T	600	HEC	C4C-C3C-CAC-CBC
3	T	601	HEC	C2C-C3C-CAC-CBC
3	T	604	HEC	C2C-C3C-CAC-CBC
3	T	604	HEC	C4C-C3C-CAC-CBC
3	T	605	HEC	C2B-C3B-CAB-CBB
3	T	605	HEC	C4B-C3B-CAB-CBB
3	T	605	HEC	C2C-C3C-CAC-CBC
3	T	605	HEC	C4C-C3C-CAC-CBC
3	T	607	HEC	C2B-C3B-CAB-CBB
3	T	607	HEC	C4B-C3B-CAB-CBB
3	T	607	HEC	C2C-C3C-CAC-CBC
3	T	607	HEC	C4C-C3C-CAC-CBC
3	U	603	HEC	C4B-C3B-CAB-CBB
3	U	603	HEC	C4C-C3C-CAC-CBC
3	U	600	HEC	C2B-C3B-CAB-CBB
3	U	600	HEC	C4B-C3B-CAB-CBB
3	U	600	HEC	C2C-C3C-CAC-CBC
3	U	600	HEC	C4C-C3C-CAC-CBC
3	U	601	HEC	C2C-C3C-CAC-CBC
3	U	604	HEC	C2C-C3C-CAC-CBC
3	U	604	HEC	C4C-C3C-CAC-CBC
3	U	605	HEC	C2B-C3B-CAB-CBB
3	U	605	HEC	C4B-C3B-CAB-CBB
3	U	605	HEC	C2C-C3C-CAC-CBC
3	U	605	HEC	C4C-C3C-CAC-CBC
3	U	607	HEC	C2B-C3B-CAB-CBB
3	U	607	HEC	C4B-C3B-CAB-CBB
3	U	607	HEC	C2C-C3C-CAC-CBC
3	U	607	HEC	C4C-C3C-CAC-CBC
3	V	600	HEC	C2B-C3B-CAB-CBB
3	V	600	HEC	C4B-C3B-CAB-CBB
3	V	600	HEC	C2C-C3C-CAC-CBC
3	V	600	HEC	C4C-C3C-CAC-CBC
3	V	601	HEC	C2C-C3C-CAC-CBC
3	V	601	HEC	C4C-C3C-CAC-CBC
3	V	604	HEC	C2C-C3C-CAC-CBC
3	V	604	HEC	C4C-C3C-CAC-CBC
3	V	605	HEC	C2B-C3B-CAB-CBB
3	V	605	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	V	605	HEC	C2C-C3C-CAC-CBC
3	V	605	HEC	C4C-C3C-CAC-CBC
3	V	607	HEC	C2B-C3B-CAB-CBB
3	V	607	HEC	C4B-C3B-CAB-CBB
3	V	607	HEC	C2C-C3C-CAC-CBC
3	V	607	HEC	C4C-C3C-CAC-CBC
3	V	603	HEC	C2C-C3C-CAC-CBC
3	V	603	HEC	C4C-C3C-CAC-CBC
3	W	603	HEC	C4B-C3B-CAB-CBB
3	W	603	HEC	C4C-C3C-CAC-CBC
3	W	600	HEC	C2B-C3B-CAB-CBB
3	W	600	HEC	C4B-C3B-CAB-CBB
3	W	600	HEC	C2C-C3C-CAC-CBC
3	W	600	HEC	C4C-C3C-CAC-CBC
3	W	601	HEC	C2C-C3C-CAC-CBC
3	W	604	HEC	C2C-C3C-CAC-CBC
3	W	604	HEC	C4C-C3C-CAC-CBC
3	W	605	HEC	C2B-C3B-CAB-CBB
3	W	605	HEC	C4B-C3B-CAB-CBB
3	W	605	HEC	C2C-C3C-CAC-CBC
3	W	605	HEC	C4C-C3C-CAC-CBC
3	W	607	HEC	C2B-C3B-CAB-CBB
3	W	607	HEC	C4B-C3B-CAB-CBB
3	W	607	HEC	C2C-C3C-CAC-CBC
3	W	607	HEC	C4C-C3C-CAC-CBC
3	X	603	HEC	C2C-C3C-CAC-CBC
3	X	603	HEC	C4C-C3C-CAC-CBC
3	X	600	HEC	C2B-C3B-CAB-CBB
3	X	600	HEC	C4B-C3B-CAB-CBB
3	X	600	HEC	C2C-C3C-CAC-CBC
3	X	600	HEC	C4C-C3C-CAC-CBC
3	X	601	HEC	C2C-C3C-CAC-CBC
3	X	604	HEC	C2C-C3C-CAC-CBC
3	X	604	HEC	C4C-C3C-CAC-CBC
3	X	605	HEC	C2B-C3B-CAB-CBB
3	X	605	HEC	C4B-C3B-CAB-CBB
3	X	605	HEC	C2C-C3C-CAC-CBC
3	X	605	HEC	C4C-C3C-CAC-CBC
3	X	607	HEC	C2B-C3B-CAB-CBB
3	X	607	HEC	C4B-C3B-CAB-CBB
3	X	607	HEC	C2C-C3C-CAC-CBC
3	X	607	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	G	615	GOL	C1-C2-C3-O3
5	G	616	GOL	O1-C1-C2-C3
5	A	613	GOL	C1-C2-C3-O3
5	A	614	GOL	O1-C1-C2-C3
5	A	614	GOL	C1-C2-C3-O3
5	A	614	GOL	O2-C2-C3-O3
5	D	610	GOL	O1-C1-C2-C3
5	H	614	GOL	O1-C1-C2-C3
5	H	615	GOL	C1-C2-C3-O3
5	I	613	GOL	O1-C1-C2-C3
5	I	613	GOL	C1-C2-C3-O3
5	I	614	GOL	C1-C2-C3-O3
5	I	615	GOL	C1-C2-C3-O3
5	J	612	GOL	O1-C1-C2-C3
5	J	613	GOL	C1-C2-C3-O3
5	J	613	GOL	O2-C2-C3-O3
5	K	615	GOL	O1-C1-C2-O2
5	K	615	GOL	O1-C1-C2-C3
5	L	613	GOL	C1-C2-C3-O3
3	G	605	HEC	C2D-C3D-CAD-CBD
3	A	605	HEC	C2D-C3D-CAD-CBD
3	B	605	HEC	C2D-C3D-CAD-CBD
3	C	605	HEC	C2D-C3D-CAD-CBD
3	D	605	HEC	C2D-C3D-CAD-CBD
3	E	605	HEC	C2D-C3D-CAD-CBD
3	F	605	HEC	C2D-C3D-CAD-CBD
3	H	605	HEC	C2D-C3D-CAD-CBD
3	J	605	HEC	C2D-C3D-CAD-CBD
3	K	605	HEC	C2D-C3D-CAD-CBD
3	L	605	HEC	C2D-C3D-CAD-CBD
3	M	605	HEC	C2D-C3D-CAD-CBD
3	N	605	HEC	C2D-C3D-CAD-CBD
3	O	605	HEC	C2D-C3D-CAD-CBD
3	P	605	HEC	C2D-C3D-CAD-CBD
3	Q	605	HEC	C2D-C3D-CAD-CBD
3	R	605	HEC	C2D-C3D-CAD-CBD
3	S	605	HEC	C2D-C3D-CAD-CBD
3	T	605	HEC	C2D-C3D-CAD-CBD
3	U	605	HEC	C2D-C3D-CAD-CBD
3	V	605	HEC	C2D-C3D-CAD-CBD
3	W	605	HEC	C2D-C3D-CAD-CBD
3	X	605	HEC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
3	D	604	HEC	C2A-CAA-CBA-CGA
5	G	615	GOL	O2-C2-C3-O3
5	A	614	GOL	O1-C1-C2-O2
5	J	612	GOL	O1-C1-C2-O2
5	K	614	GOL	O2-C2-C3-O3
5	L	613	GOL	O2-C2-C3-O3
3	G	605	HEC	C4D-C3D-CAD-CBD
3	A	605	HEC	C4D-C3D-CAD-CBD
3	B	605	HEC	C4D-C3D-CAD-CBD
3	C	605	HEC	C4D-C3D-CAD-CBD
3	D	605	HEC	C4D-C3D-CAD-CBD
3	E	605	HEC	C4D-C3D-CAD-CBD
3	F	605	HEC	C4D-C3D-CAD-CBD
3	H	605	HEC	C4D-C3D-CAD-CBD
3	I	605	HEC	C4D-C3D-CAD-CBD
3	J	605	HEC	C4D-C3D-CAD-CBD
3	K	605	HEC	C4D-C3D-CAD-CBD
3	L	605	HEC	C4D-C3D-CAD-CBD
3	M	605	HEC	C4D-C3D-CAD-CBD
3	N	605	HEC	C4D-C3D-CAD-CBD
3	O	605	HEC	C4D-C3D-CAD-CBD
3	P	605	HEC	C4D-C3D-CAD-CBD
3	Q	605	HEC	C4D-C3D-CAD-CBD
3	R	605	HEC	C4D-C3D-CAD-CBD
3	S	605	HEC	C4D-C3D-CAD-CBD
3	T	605	HEC	C4D-C3D-CAD-CBD
3	U	605	HEC	C4D-C3D-CAD-CBD
3	V	605	HEC	C4D-C3D-CAD-CBD
3	W	605	HEC	C4D-C3D-CAD-CBD
3	X	605	HEC	C4D-C3D-CAD-CBD
5	H	614	GOL	C1-C2-C3-O3
5	J	612	GOL	C1-C2-C3-O3
5	K	612	GOL	O1-C1-C2-C3
5	K	613	GOL	O1-C1-C2-C3
5	K	614	GOL	C1-C2-C3-O3
5	K	615	GOL	C1-C2-C3-O3
5	G	616	GOL	O1-C1-C2-O2
5	A	613	GOL	O2-C2-C3-O3
5	D	610	GOL	O1-C1-C2-O2
5	H	614	GOL	O1-C1-C2-O2
5	H	614	GOL	O2-C2-C3-O3
5	I	613	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	I	613	GOL	O2-C2-C3-O3
5	I	614	GOL	O2-C2-C3-O3
5	I	615	GOL	O2-C2-C3-O3
3	I	607	HEC	C2A-CAA-CBA-CGA
3	I	603	HEC	C1A-C2A-CAA-CBA
5	H	615	GOL	O2-C2-C3-O3
5	J	612	GOL	O2-C2-C3-O3
3	D	601	HEC	C1A-C2A-CAA-CBA
3	I	601	HEC	C1A-C2A-CAA-CBA
3	I	603	HEC	C4D-C3D-CAD-CBD
5	K	615	GOL	O2-C2-C3-O3
3	D	603	HEC	C2A-CAA-CBA-CGA
3	C	607	HEC	C2A-CAA-CBA-CGA
3	N	607	HEC	C2A-CAA-CBA-CGA
3	O	607	HEC	C2A-CAA-CBA-CGA
3	P	607	HEC	C2A-CAA-CBA-CGA
3	Q	607	HEC	C2A-CAA-CBA-CGA
3	D	601	HEC	C3A-C2A-CAA-CBA
3	G	607	HEC	C2A-CAA-CBA-CGA
3	A	602	HEC	C3D-CAD-CBD-CGD
3	A	607	HEC	C2A-CAA-CBA-CGA
3	B	602	HEC	C3D-CAD-CBD-CGD
3	D	607	HEC	C2A-CAA-CBA-CGA
3	E	607	HEC	C2A-CAA-CBA-CGA
3	F	602	HEC	C3D-CAD-CBD-CGD
3	F	607	HEC	C2A-CAA-CBA-CGA
3	H	607	HEC	C2A-CAA-CBA-CGA
3	I	602	HEC	C3D-CAD-CBD-CGD
3	J	602	HEC	C3D-CAD-CBD-CGD
3	J	607	HEC	C2A-CAA-CBA-CGA
3	K	607	HEC	C2A-CAA-CBA-CGA
3	L	607	HEC	C2A-CAA-CBA-CGA
3	M	602	HEC	C3D-CAD-CBD-CGD
3	M	607	HEC	C2A-CAA-CBA-CGA
3	N	602	HEC	C3D-CAD-CBD-CGD
3	O	602	HEC	C3D-CAD-CBD-CGD
3	Q	602	HEC	C3D-CAD-CBD-CGD
3	R	602	HEC	C3D-CAD-CBD-CGD
3	R	607	HEC	C2A-CAA-CBA-CGA
3	S	607	HEC	C2A-CAA-CBA-CGA
3	T	607	HEC	C2A-CAA-CBA-CGA
3	U	602	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
3	U	607	HEC	C2A-CAA-CBA-CGA
3	V	602	HEC	C3D-CAD-CBD-CGD
3	V	607	HEC	C2A-CAA-CBA-CGA
3	W	602	HEC	C3D-CAD-CBD-CGD
3	W	607	HEC	C2A-CAA-CBA-CGA
3	X	602	HEC	C3D-CAD-CBD-CGD
3	X	607	HEC	C2A-CAA-CBA-CGA
3	I	601	HEC	C3A-C2A-CAA-CBA
3	D	603	HEC	C1A-C2A-CAA-CBA
3	G	602	HEC	C3D-CAD-CBD-CGD
3	B	607	HEC	C2A-CAA-CBA-CGA
3	C	602	HEC	C3D-CAD-CBD-CGD
3	E	602	HEC	C3D-CAD-CBD-CGD
3	H	602	HEC	C3D-CAD-CBD-CGD
3	K	602	HEC	C3D-CAD-CBD-CGD
3	L	602	HEC	C3D-CAD-CBD-CGD
3	P	602	HEC	C3D-CAD-CBD-CGD
3	S	602	HEC	C3D-CAD-CBD-CGD
3	T	602	HEC	C3D-CAD-CBD-CGD
5	K	613	GOL	O1-C1-C2-O2
5	K	614	GOL	O1-C1-C2-O2
3	G	601	HEC	C4B-C3B-CAB-CBB
3	G	601	HEC	C4C-C3C-CAC-CBC
3	G	602	HEC	C4B-C3B-CAB-CBB
3	G	602	HEC	C4C-C3C-CAC-CBC
3	G	604	HEC	C4B-C3B-CAB-CBB
3	G	606	HEC	C4B-C3B-CAB-CBB
3	G	606	HEC	C4C-C3C-CAC-CBC
3	G	603	HEC	C4B-C3B-CAB-CBB
3	A	601	HEC	C4B-C3B-CAB-CBB
3	A	601	HEC	C4C-C3C-CAC-CBC
3	A	602	HEC	C4B-C3B-CAB-CBB
3	A	602	HEC	C4C-C3C-CAC-CBC
3	A	604	HEC	C4B-C3B-CAB-CBB
3	A	606	HEC	C4B-C3B-CAB-CBB
3	A	606	HEC	C4C-C3C-CAC-CBC
3	A	603	HEC	C4B-C3B-CAB-CBB
3	B	601	HEC	C4B-C3B-CAB-CBB
3	B	601	HEC	C4C-C3C-CAC-CBC
3	B	602	HEC	C4B-C3B-CAB-CBB
3	B	604	HEC	C4B-C3B-CAB-CBB
3	B	606	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	B	606	HEC	C4C-C3C-CAC-CBC
3	C	601	HEC	C4B-C3B-CAB-CBB
3	C	601	HEC	C4C-C3C-CAC-CBC
3	C	602	HEC	C4C-C3C-CAC-CBC
3	C	604	HEC	C4B-C3B-CAB-CBB
3	C	606	HEC	C4B-C3B-CAB-CBB
3	C	606	HEC	C4C-C3C-CAC-CBC
3	D	601	HEC	C4B-C3B-CAB-CBB
3	D	602	HEC	C4C-C3C-CAC-CBC
3	D	604	HEC	C4B-C3B-CAB-CBB
3	D	607	HEC	C4B-C3B-CAB-CBB
3	E	603	HEC	C4B-C3B-CAB-CBB
3	E	601	HEC	C4B-C3B-CAB-CBB
3	E	602	HEC	C4C-C3C-CAC-CBC
3	E	604	HEC	C4B-C3B-CAB-CBB
3	E	606	HEC	C4B-C3B-CAB-CBB
3	E	606	HEC	C4C-C3C-CAC-CBC
3	F	603	HEC	C4B-C3B-CAB-CBB
3	F	601	HEC	C4B-C3B-CAB-CBB
3	F	601	HEC	C4C-C3C-CAC-CBC
3	F	602	HEC	C4B-C3B-CAB-CBB
3	F	602	HEC	C4C-C3C-CAC-CBC
3	F	604	HEC	C4B-C3B-CAB-CBB
3	F	606	HEC	C4B-C3B-CAB-CBB
3	F	606	HEC	C4C-C3C-CAC-CBC
3	H	603	HEC	C4B-C3B-CAB-CBB
3	H	601	HEC	C4B-C3B-CAB-CBB
3	H	601	HEC	C4C-C3C-CAC-CBC
3	H	602	HEC	C4B-C3B-CAB-CBB
3	H	602	HEC	C4C-C3C-CAC-CBC
3	H	604	HEC	C4B-C3B-CAB-CBB
3	H	606	HEC	C4B-C3B-CAB-CBB
3	H	606	HEC	C4C-C3C-CAC-CBC
3	I	600	HEC	C4B-C3B-CAB-CBB
3	I	601	HEC	C4C-C3C-CAC-CBC
3	I	602	HEC	C4B-C3B-CAB-CBB
3	I	602	HEC	C4C-C3C-CAC-CBC
3	I	604	HEC	C4B-C3B-CAB-CBB
3	I	607	HEC	C4B-C3B-CAB-CBB
3	J	601	HEC	C4B-C3B-CAB-CBB
3	J	601	HEC	C4C-C3C-CAC-CBC
3	J	602	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	J	602	HEC	C4C-C3C-CAC-CBC
3	J	604	HEC	C4B-C3B-CAB-CBB
3	J	606	HEC	C4B-C3B-CAB-CBB
3	J	606	HEC	C4C-C3C-CAC-CBC
3	K	603	HEC	C4B-C3B-CAB-CBB
3	K	601	HEC	C4B-C3B-CAB-CBB
3	K	601	HEC	C4C-C3C-CAC-CBC
3	K	602	HEC	C4C-C3C-CAC-CBC
3	K	604	HEC	C4B-C3B-CAB-CBB
3	K	606	HEC	C4B-C3B-CAB-CBB
3	K	606	HEC	C4C-C3C-CAC-CBC
3	L	601	HEC	C4B-C3B-CAB-CBB
3	L	601	HEC	C4C-C3C-CAC-CBC
3	L	602	HEC	C4B-C3B-CAB-CBB
3	L	602	HEC	C4C-C3C-CAC-CBC
3	L	604	HEC	C4B-C3B-CAB-CBB
3	L	606	HEC	C4B-C3B-CAB-CBB
3	L	606	HEC	C4C-C3C-CAC-CBC
3	M	601	HEC	C4B-C3B-CAB-CBB
3	M	601	HEC	C4C-C3C-CAC-CBC
3	M	602	HEC	C4B-C3B-CAB-CBB
3	M	602	HEC	C4C-C3C-CAC-CBC
3	M	606	HEC	C4B-C3B-CAB-CBB
3	M	606	HEC	C4C-C3C-CAC-CBC
3	M	603	HEC	C4B-C3B-CAB-CBB
3	N	603	HEC	C4B-C3B-CAB-CBB
3	N	601	HEC	C4B-C3B-CAB-CBB
3	N	602	HEC	C4C-C3C-CAC-CBC
3	N	604	HEC	C4B-C3B-CAB-CBB
3	N	606	HEC	C4B-C3B-CAB-CBB
3	N	606	HEC	C4C-C3C-CAC-CBC
3	O	603	HEC	C4B-C3B-CAB-CBB
3	O	601	HEC	C4B-C3B-CAB-CBB
3	O	601	HEC	C4C-C3C-CAC-CBC
3	O	602	HEC	C4C-C3C-CAC-CBC
3	O	604	HEC	C4B-C3B-CAB-CBB
3	O	606	HEC	C4B-C3B-CAB-CBB
3	O	606	HEC	C4C-C3C-CAC-CBC
3	P	601	HEC	C4B-C3B-CAB-CBB
3	P	601	HEC	C4C-C3C-CAC-CBC
3	P	602	HEC	C4C-C3C-CAC-CBC
3	P	604	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	P	606	HEC	C4B-C3B-CAB-CBB
3	P	606	HEC	C4C-C3C-CAC-CBC
3	Q	603	HEC	C4B-C3B-CAB-CBB
3	Q	601	HEC	C4B-C3B-CAB-CBB
3	Q	601	HEC	C4C-C3C-CAC-CBC
3	Q	602	HEC	C4B-C3B-CAB-CBB
3	Q	602	HEC	C4C-C3C-CAC-CBC
3	Q	604	HEC	C4B-C3B-CAB-CBB
3	Q	606	HEC	C4B-C3B-CAB-CBB
3	Q	606	HEC	C4C-C3C-CAC-CBC
3	R	603	HEC	C4B-C3B-CAB-CBB
3	R	601	HEC	C4B-C3B-CAB-CBB
3	R	601	HEC	C4C-C3C-CAC-CBC
3	R	602	HEC	C4B-C3B-CAB-CBB
3	R	602	HEC	C4C-C3C-CAC-CBC
3	R	604	HEC	C4B-C3B-CAB-CBB
3	R	606	HEC	C4B-C3B-CAB-CBB
3	R	606	HEC	C4C-C3C-CAC-CBC
3	S	601	HEC	C4B-C3B-CAB-CBB
3	S	601	HEC	C4C-C3C-CAC-CBC
3	S	602	HEC	C4B-C3B-CAB-CBB
3	S	602	HEC	C4C-C3C-CAC-CBC
3	S	604	HEC	C4B-C3B-CAB-CBB
3	S	606	HEC	C4B-C3B-CAB-CBB
3	S	606	HEC	C4C-C3C-CAC-CBC
3	S	603	HEC	C4B-C3B-CAB-CBB
3	T	603	HEC	C4B-C3B-CAB-CBB
3	T	601	HEC	C4B-C3B-CAB-CBB
3	T	601	HEC	C4C-C3C-CAC-CBC
3	T	602	HEC	C4B-C3B-CAB-CBB
3	T	602	HEC	C4C-C3C-CAC-CBC
3	T	604	HEC	C4B-C3B-CAB-CBB
3	T	606	HEC	C4B-C3B-CAB-CBB
3	T	606	HEC	C4C-C3C-CAC-CBC
3	U	601	HEC	C4B-C3B-CAB-CBB
3	U	601	HEC	C4C-C3C-CAC-CBC
3	U	602	HEC	C4B-C3B-CAB-CBB
3	U	602	HEC	C4C-C3C-CAC-CBC
3	U	604	HEC	C4B-C3B-CAB-CBB
3	U	606	HEC	C4B-C3B-CAB-CBB
3	U	606	HEC	C4C-C3C-CAC-CBC
3	V	601	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	V	602	HEC	C4B-C3B-CAB-CBB
3	V	602	HEC	C4C-C3C-CAC-CBC
3	V	604	HEC	C4B-C3B-CAB-CBB
3	V	606	HEC	C4B-C3B-CAB-CBB
3	V	606	HEC	C4C-C3C-CAC-CBC
3	V	603	HEC	C4B-C3B-CAB-CBB
3	W	601	HEC	C4B-C3B-CAB-CBB
3	W	601	HEC	C4C-C3C-CAC-CBC
3	W	602	HEC	C4B-C3B-CAB-CBB
3	W	602	HEC	C4C-C3C-CAC-CBC
3	W	604	HEC	C4B-C3B-CAB-CBB
3	W	606	HEC	C4B-C3B-CAB-CBB
3	W	606	HEC	C4C-C3C-CAC-CBC
3	X	603	HEC	C4B-C3B-CAB-CBB
3	X	601	HEC	C4B-C3B-CAB-CBB
3	X	601	HEC	C4C-C3C-CAC-CBC
3	X	602	HEC	C4C-C3C-CAC-CBC
3	X	604	HEC	C4B-C3B-CAB-CBB
3	X	606	HEC	C4B-C3B-CAB-CBB
3	X	606	HEC	C4C-C3C-CAC-CBC
3	G	601	HEC	C1A-C2A-CAA-CBA
3	G	601	HEC	C2B-C3B-CAB-CBB
3	G	602	HEC	C2C-C3C-CAC-CBC
3	G	604	HEC	C2B-C3B-CAB-CBB
3	G	606	HEC	C2C-C3C-CAC-CBC
3	G	603	HEC	C2B-C3B-CAB-CBB
3	A	601	HEC	C2B-C3B-CAB-CBB
3	A	602	HEC	C2C-C3C-CAC-CBC
3	A	604	HEC	C2B-C3B-CAB-CBB
3	A	606	HEC	C2C-C3C-CAC-CBC
3	A	603	HEC	C2B-C3B-CAB-CBB
3	B	603	HEC	C2B-C3B-CAB-CBB
3	B	601	HEC	C2B-C3B-CAB-CBB
3	B	602	HEC	C2C-C3C-CAC-CBC
3	B	604	HEC	C2B-C3B-CAB-CBB
3	B	606	HEC	C2B-C3B-CAB-CBB
3	B	606	HEC	C2C-C3C-CAC-CBC
3	C	603	HEC	C2B-C3B-CAB-CBB
3	C	601	HEC	C2B-C3B-CAB-CBB
3	C	602	HEC	C2C-C3C-CAC-CBC
3	C	604	HEC	C2B-C3B-CAB-CBB
3	C	606	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	606	HEC	C2C-C3C-CAC-CBC
3	D	601	HEC	C2C-C3C-CAC-CBC
3	D	602	HEC	C2C-C3C-CAC-CBC
3	D	606	HEC	C2B-C3B-CAB-CBB
3	E	603	HEC	C2B-C3B-CAB-CBB
3	E	603	HEC	C2C-C3C-CAC-CBC
3	E	601	HEC	C2B-C3B-CAB-CBB
3	E	602	HEC	C2C-C3C-CAC-CBC
3	E	604	HEC	C2B-C3B-CAB-CBB
3	F	603	HEC	C2B-C3B-CAB-CBB
3	F	601	HEC	C2B-C3B-CAB-CBB
3	F	602	HEC	C2C-C3C-CAC-CBC
3	F	604	HEC	C2B-C3B-CAB-CBB
3	F	606	HEC	C2C-C3C-CAC-CBC
3	H	603	HEC	C2B-C3B-CAB-CBB
3	H	601	HEC	C2B-C3B-CAB-CBB
3	H	602	HEC	C2C-C3C-CAC-CBC
3	H	604	HEC	C2B-C3B-CAB-CBB
3	H	606	HEC	C2C-C3C-CAC-CBC
3	I	601	HEC	C2B-C3B-CAB-CBB
3	I	602	HEC	C2C-C3C-CAC-CBC
3	I	607	HEC	C2B-C3B-CAB-CBB
3	J	601	HEC	C2B-C3B-CAB-CBB
3	J	602	HEC	C2C-C3C-CAC-CBC
3	J	604	HEC	C2B-C3B-CAB-CBB
3	J	606	HEC	C2C-C3C-CAC-CBC
3	K	603	HEC	C2B-C3B-CAB-CBB
3	K	601	HEC	C2B-C3B-CAB-CBB
3	K	602	HEC	C2C-C3C-CAC-CBC
3	K	604	HEC	C2B-C3B-CAB-CBB
3	K	606	HEC	C2C-C3C-CAC-CBC
3	L	601	HEC	C2B-C3B-CAB-CBB
3	L	602	HEC	C2C-C3C-CAC-CBC
3	L	604	HEC	C2B-C3B-CAB-CBB
3	L	606	HEC	C2C-C3C-CAC-CBC
3	M	601	HEC	C2B-C3B-CAB-CBB
3	M	602	HEC	C2C-C3C-CAC-CBC
3	M	604	HEC	C2B-C3B-CAB-CBB
3	M	606	HEC	C2B-C3B-CAB-CBB
3	M	606	HEC	C2C-C3C-CAC-CBC
3	M	603	HEC	C2B-C3B-CAB-CBB
3	M	603	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	N	603	HEC	C2B-C3B-CAB-CBB
3	N	603	HEC	C2C-C3C-CAC-CBC
3	N	601	HEC	C2B-C3B-CAB-CBB
3	N	602	HEC	C2C-C3C-CAC-CBC
3	N	604	HEC	C2B-C3B-CAB-CBB
3	N	606	HEC	C2B-C3B-CAB-CBB
3	N	606	HEC	C2C-C3C-CAC-CBC
3	O	603	HEC	C2B-C3B-CAB-CBB
3	O	603	HEC	C2C-C3C-CAC-CBC
3	O	601	HEC	C2B-C3B-CAB-CBB
3	O	602	HEC	C2C-C3C-CAC-CBC
3	O	604	HEC	C2B-C3B-CAB-CBB
3	O	606	HEC	C2C-C3C-CAC-CBC
3	P	601	HEC	C2B-C3B-CAB-CBB
3	P	602	HEC	C2C-C3C-CAC-CBC
3	P	604	HEC	C2B-C3B-CAB-CBB
3	P	606	HEC	C2B-C3B-CAB-CBB
3	P	606	HEC	C2C-C3C-CAC-CBC
3	P	603	HEC	C2B-C3B-CAB-CBB
3	Q	603	HEC	C2B-C3B-CAB-CBB
3	Q	601	HEC	C2B-C3B-CAB-CBB
3	Q	602	HEC	C2C-C3C-CAC-CBC
3	Q	604	HEC	C2B-C3B-CAB-CBB
3	Q	606	HEC	C2B-C3B-CAB-CBB
3	Q	606	HEC	C2C-C3C-CAC-CBC
3	R	603	HEC	C2B-C3B-CAB-CBB
3	R	601	HEC	C2B-C3B-CAB-CBB
3	R	602	HEC	C2C-C3C-CAC-CBC
3	R	604	HEC	C2B-C3B-CAB-CBB
3	R	606	HEC	C2C-C3C-CAC-CBC
3	S	601	HEC	C2B-C3B-CAB-CBB
3	S	602	HEC	C2C-C3C-CAC-CBC
3	S	604	HEC	C2B-C3B-CAB-CBB
3	S	606	HEC	C2B-C3B-CAB-CBB
3	S	606	HEC	C2C-C3C-CAC-CBC
3	S	603	HEC	C2B-C3B-CAB-CBB
3	T	603	HEC	C2B-C3B-CAB-CBB
3	T	601	HEC	C2B-C3B-CAB-CBB
3	T	602	HEC	C2C-C3C-CAC-CBC
3	T	604	HEC	C2B-C3B-CAB-CBB
3	T	606	HEC	C2B-C3B-CAB-CBB
3	T	606	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	U	603	HEC	C2B-C3B-CAB-CBB
3	U	603	HEC	C2C-C3C-CAC-CBC
3	U	601	HEC	C2B-C3B-CAB-CBB
3	U	602	HEC	C2C-C3C-CAC-CBC
3	U	604	HEC	C2B-C3B-CAB-CBB
3	U	606	HEC	C2B-C3B-CAB-CBB
3	U	606	HEC	C2C-C3C-CAC-CBC
3	V	601	HEC	C2B-C3B-CAB-CBB
3	V	602	HEC	C2C-C3C-CAC-CBC
3	V	604	HEC	C2B-C3B-CAB-CBB
3	V	606	HEC	C2B-C3B-CAB-CBB
3	V	606	HEC	C2C-C3C-CAC-CBC
3	V	603	HEC	C2B-C3B-CAB-CBB
3	W	603	HEC	C2B-C3B-CAB-CBB
3	W	603	HEC	C2C-C3C-CAC-CBC
3	W	601	HEC	C2B-C3B-CAB-CBB
3	W	602	HEC	C2C-C3C-CAC-CBC
3	W	604	HEC	C2B-C3B-CAB-CBB
3	W	606	HEC	C2B-C3B-CAB-CBB
3	W	606	HEC	C2C-C3C-CAC-CBC
3	X	603	HEC	C2B-C3B-CAB-CBB
3	X	601	HEC	C2B-C3B-CAB-CBB
3	X	602	HEC	C2C-C3C-CAC-CBC
3	X	604	HEC	C2B-C3B-CAB-CBB
3	X	606	HEC	C2B-C3B-CAB-CBB
3	X	606	HEC	C2C-C3C-CAC-CBC
3	O	601	HEC	C3A-C2A-CAA-CBA
3	G	601	HEC	C3A-C2A-CAA-CBA
3	E	601	HEC	C1A-C2A-CAA-CBA
3	J	601	HEC	C1A-C2A-CAA-CBA
3	O	601	HEC	C1A-C2A-CAA-CBA
3	Q	601	HEC	C1A-C2A-CAA-CBA
3	U	601	HEC	C1A-C2A-CAA-CBA
3	E	601	HEC	C3A-C2A-CAA-CBA
3	X	601	HEC	C1A-C2A-CAA-CBA
3	M	602	HEC	CAD-CBD-CGD-O1D
3	X	602	HEC	CAD-CBD-CGD-O1D
3	O	602	HEC	CAD-CBD-CGD-O1D
3	G	602	HEC	CAD-CBD-CGD-O1D
3	B	601	HEC	C3A-C2A-CAA-CBA
3	S	601	HEC	C3A-C2A-CAA-CBA
3	U	601	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	A	601	HEC	C1A-C2A-CAA-CBA
3	W	601	HEC	C1A-C2A-CAA-CBA
3	A	600	HEC	CAD-CBD-CGD-O1D
3	E	600	HEC	CAD-CBD-CGD-O1D
3	I	600	HEC	CAD-CBD-CGD-O1D
3	K	602	HEC	CAD-CBD-CGD-O1D
3	M	600	HEC	CAD-CBD-CGD-O1D
3	B	602	HEC	CAD-CBD-CGD-O1D
3	D	604	HEC	CAA-CBA-CGA-O1A
3	E	602	HEC	CAD-CBD-CGD-O1D
3	F	602	HEC	CAD-CBD-CGD-O1D
3	J	602	HEC	CAD-CBD-CGD-O1D
3	L	602	HEC	CAD-CBD-CGD-O1D
3	P	600	HEC	CAD-CBD-CGD-O1D
3	P	602	HEC	CAD-CBD-CGD-O1D
3	V	602	HEC	CAD-CBD-CGD-O1D
3	F	606	HEC	CAD-CBD-CGD-O2D
3	I	606	HEC	CAD-CBD-CGD-O2D
3	L	600	HEC	CAD-CBD-CGD-O1D
3	M	606	HEC	CAD-CBD-CGD-O1D
3	T	606	HEC	CAD-CBD-CGD-O2D
3	W	606	HEC	CAD-CBD-CGD-O1D
3	B	601	HEC	C1A-C2A-CAA-CBA
3	K	601	HEC	C1A-C2A-CAA-CBA
3	R	601	HEC	C1A-C2A-CAA-CBA
3	S	601	HEC	C1A-C2A-CAA-CBA
3	A	602	HEC	CAD-CBD-CGD-O1D
3	B	600	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O1D
3	H	602	HEC	CAD-CBD-CGD-O1D
3	K	606	HEC	CAD-CBD-CGD-O2D
3	L	606	HEC	CAD-CBD-CGD-O2D
3	O	600	HEC	CAD-CBD-CGD-O1D
3	Q	602	HEC	CAD-CBD-CGD-O1D
3	S	602	HEC	CAD-CBD-CGD-O1D
3	U	602	HEC	CAD-CBD-CGD-O1D
3	V	600	HEC	CAD-CBD-CGD-O1D
3	G	606	HEC	CAD-CBD-CGD-O2D
3	B	606	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAD-CBD-CGD-O2D
3	E	606	HEC	CAD-CBD-CGD-O2D
3	H	606	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	I	600	HEC	CAD-CBD-CGD-O2D
3	N	600	HEC	CAD-CBD-CGD-O1D
3	P	606	HEC	CAD-CBD-CGD-O2D
3	R	606	HEC	CAD-CBD-CGD-O2D
3	S	600	HEC	CAD-CBD-CGD-O1D
3	T	602	HEC	CAD-CBD-CGD-O1D
3	U	600	HEC	CAD-CBD-CGD-O1D
3	W	602	HEC	CAD-CBD-CGD-O1D
3	A	606	HEC	CAD-CBD-CGD-O2D
3	J	606	HEC	CAD-CBD-CGD-O1D
3	K	600	HEC	CAD-CBD-CGD-O1D
3	N	600	HEC	CAD-CBD-CGD-O2D
3	N	602	HEC	CAD-CBD-CGD-O1D
3	N	606	HEC	CAD-CBD-CGD-O2D
3	Q	606	HEC	CAD-CBD-CGD-O2D
3	R	602	HEC	CAD-CBD-CGD-O1D
3	S	606	HEC	CAD-CBD-CGD-O2D
3	U	606	HEC	CAD-CBD-CGD-O2D
3	V	600	HEC	CAD-CBD-CGD-O2D
3	W	600	HEC	CAD-CBD-CGD-O1D
3	X	606	HEC	CAD-CBD-CGD-O2D
3	A	601	HEC	C3A-C2A-CAA-CBA
3	J	601	HEC	C3A-C2A-CAA-CBA
3	X	601	HEC	C3A-C2A-CAA-CBA
3	A	600	HEC	CAD-CBD-CGD-O2D
3	C	600	HEC	CAD-CBD-CGD-O2D
3	E	600	HEC	CAD-CBD-CGD-O2D
3	H	600	HEC	CAD-CBD-CGD-O1D
3	J	600	HEC	CAD-CBD-CGD-O1D
3	J	600	HEC	CAD-CBD-CGD-O2D
3	J	606	HEC	CAD-CBD-CGD-O2D
3	M	602	HEC	CAD-CBD-CGD-O2D
3	O	602	HEC	CAD-CBD-CGD-O2D
3	T	600	HEC	CAD-CBD-CGD-O2D
3	X	602	HEC	CAD-CBD-CGD-O2D
3	G	600	HEC	CAD-CBD-CGD-O1D
3	G	602	HEC	CAD-CBD-CGD-O2D
3	A	602	HEC	CAD-CBD-CGD-O2D
3	C	600	HEC	CAD-CBD-CGD-O1D
3	F	600	HEC	CAD-CBD-CGD-O2D
3	H	600	HEC	CAD-CBD-CGD-O2D
3	M	606	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	O	606	HEC	CAD-CBD-CGD-O2D
3	Q	600	HEC	CAD-CBD-CGD-O2D
3	R	600	HEC	CAD-CBD-CGD-O1D
3	R	600	HEC	CAD-CBD-CGD-O2D
3	S	600	HEC	CAD-CBD-CGD-O2D
3	U	600	HEC	CAD-CBD-CGD-O2D
3	V	606	HEC	CAD-CBD-CGD-O2D
3	W	600	HEC	CAD-CBD-CGD-O2D
3	X	600	HEC	CAD-CBD-CGD-O1D
3	X	600	HEC	CAD-CBD-CGD-O2D
3	V	601	HEC	C1A-C2A-CAA-CBA
3	G	600	HEC	CAD-CBD-CGD-O2D
3	B	600	HEC	CAD-CBD-CGD-O2D
3	D	604	HEC	CAA-CBA-CGA-O2A
3	F	600	HEC	CAD-CBD-CGD-O1D
3	I	601	HEC	CAD-CBD-CGD-O1D
3	I	602	HEC	CAD-CBD-CGD-O2D
3	O	600	HEC	CAD-CBD-CGD-O2D
3	P	600	HEC	CAD-CBD-CGD-O2D
3	T	600	HEC	CAD-CBD-CGD-O1D
3	V	602	HEC	CAD-CBD-CGD-O2D
3	V	606	HEC	CAD-CBD-CGD-O1D
3	D	600	HEC	CAD-CBD-CGD-O2D
3	D	606	HEC	CAD-CBD-CGD-O1D
3	E	602	HEC	CAD-CBD-CGD-O2D
3	F	602	HEC	CAD-CBD-CGD-O2D
3	H	602	HEC	CAD-CBD-CGD-O2D
3	I	602	HEC	CAD-CBD-CGD-O1D
3	J	602	HEC	CAD-CBD-CGD-O2D
3	K	600	HEC	CAD-CBD-CGD-O2D
3	K	602	HEC	CAD-CBD-CGD-O2D
3	M	600	HEC	CAD-CBD-CGD-O2D
3	Q	600	HEC	CAD-CBD-CGD-O1D
3	R	602	HEC	CAD-CBD-CGD-O2D
3	B	602	HEC	CAD-CBD-CGD-O2D
3	I	606	HEC	CAD-CBD-CGD-O1D
3	L	600	HEC	CAD-CBD-CGD-O2D
3	M	601	HEC	CAA-CBA-CGA-O1A
3	O	606	HEC	CAD-CBD-CGD-O1D
3	P	602	HEC	CAD-CBD-CGD-O2D
3	U	602	HEC	CAD-CBD-CGD-O2D
3	U	606	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	X	606	HEC	CAD-CBD-CGD-O1D
3	K	601	HEC	C3A-C2A-CAA-CBA
3	N	601	HEC	C3A-C2A-CAA-CBA
3	Q	601	HEC	C3A-C2A-CAA-CBA
3	R	601	HEC	C3A-C2A-CAA-CBA
3	W	601	HEC	C3A-C2A-CAA-CBA
3	G	606	HEC	CAD-CBD-CGD-O1D
3	A	606	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O2D
3	D	600	HEC	CAD-CBD-CGD-O1D
3	K	606	HEC	CAD-CBD-CGD-O1D
3	L	602	HEC	CAD-CBD-CGD-O2D
3	N	602	HEC	CAD-CBD-CGD-O2D
3	N	606	HEC	CAD-CBD-CGD-O1D
3	P	606	HEC	CAD-CBD-CGD-O1D
3	S	602	HEC	CAD-CBD-CGD-O2D
3	T	602	HEC	CAD-CBD-CGD-O2D
3	W	602	HEC	CAD-CBD-CGD-O2D
3	E	606	HEC	CAD-CBD-CGD-O1D
3	F	606	HEC	CAD-CBD-CGD-O1D
3	L	606	HEC	CAD-CBD-CGD-O1D
3	Q	602	HEC	CAD-CBD-CGD-O2D
3	Q	606	HEC	CAD-CBD-CGD-O1D
3	W	606	HEC	CAD-CBD-CGD-O2D
3	B	606	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAD-CBD-CGD-O1D
3	H	606	HEC	CAD-CBD-CGD-O1D
3	R	606	HEC	CAD-CBD-CGD-O1D
3	S	606	HEC	CAD-CBD-CGD-O1D
3	T	606	HEC	CAD-CBD-CGD-O1D
3	D	607	HEC	C1A-C2A-CAA-CBA
3	N	601	HEC	C1A-C2A-CAA-CBA
3	F	601	HEC	C3A-C2A-CAA-CBA
3	V	601	HEC	C3A-C2A-CAA-CBA
3	I	604	HEC	C2A-CAA-CBA-CGA
3	C	605	HEC	CAD-CBD-CGD-O2D
3	I	604	HEC	CAA-CBA-CGA-O2A
3	I	604	HEC	CAD-CBD-CGD-O2D
3	O	605	HEC	CAD-CBD-CGD-O2D
3	B	601	HEC	CAA-CBA-CGA-O1A
3	L	601	HEC	CAA-CBA-CGA-O1A
3	P	605	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	W	605	HEC	CAD-CBD-CGD-O2D
3	J	605	HEC	CAD-CBD-CGD-O2D
3	N	601	HEC	CAA-CBA-CGA-O1A
3	O	605	HEC	CAD-CBD-CGD-O1D
3	C	601	HEC	CAA-CBA-CGA-O1A
3	C	602	HEC	CAA-CBA-CGA-O2A
3	C	605	HEC	CAD-CBD-CGD-O1D
3	D	606	HEC	CAD-CBD-CGD-O2D
3	E	602	HEC	CAA-CBA-CGA-O2A
3	E	604	HEC	CAA-CBA-CGA-O2A
3	K	605	HEC	CAD-CBD-CGD-O2D
3	L	605	HEC	CAD-CBD-CGD-O2D
3	N	602	HEC	CAA-CBA-CGA-O2A
3	P	602	HEC	CAA-CBA-CGA-O2A
3	Q	602	HEC	CAA-CBA-CGA-O2A
3	R	605	HEC	CAD-CBD-CGD-O2D
3	V	602	HEC	CAA-CBA-CGA-O2A
3	T	601	HEC	C3A-C2A-CAA-CBA
3	F	601	HEC	C1A-C2A-CAA-CBA
3	H	601	HEC	C1A-C2A-CAA-CBA
3	L	601	HEC	C1A-C2A-CAA-CBA
3	T	601	HEC	C1A-C2A-CAA-CBA
3	B	604	HEC	CAA-CBA-CGA-O2A
3	B	605	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAA-CBA-CGA-O1A
3	F	605	HEC	CAD-CBD-CGD-O2D
3	I	601	HEC	CAD-CBD-CGD-O2D
3	J	604	HEC	CAA-CBA-CGA-O2A
3	J	605	HEC	CAD-CBD-CGD-O1D
3	K	604	HEC	CAA-CBA-CGA-O1A
3	L	604	HEC	CAA-CBA-CGA-O2A
3	M	605	HEC	CAD-CBD-CGD-O2D
3	N	604	HEC	CAA-CBA-CGA-O1A
3	N	604	HEC	CAA-CBA-CGA-O2A
3	P	604	HEC	CAA-CBA-CGA-O2A
3	U	605	HEC	CAD-CBD-CGD-O2D
3	X	604	HEC	CAA-CBA-CGA-O2A
3	G	604	HEC	CAA-CBA-CGA-O1A
3	G	605	HEC	CAD-CBD-CGD-O2D
3	A	602	HEC	CAA-CBA-CGA-O2A
3	B	602	HEC	CAA-CBA-CGA-O2A
3	B	604	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	E	601	HEC	CAA-CBA-CGA-O1A
3	I	605	HEC	CAD-CBD-CGD-O1D
3	J	601	HEC	CAA-CBA-CGA-O1A
3	M	604	HEC	CAA-CBA-CGA-O1A
3	M	604	HEC	CAD-CBD-CGD-O2D
3	P	601	HEC	CAA-CBA-CGA-O1A
3	P	605	HEC	CAD-CBD-CGD-O1D
3	U	604	HEC	CAA-CBA-CGA-O1A
3	U	604	HEC	CAA-CBA-CGA-O2A
3	U	604	HEC	CAD-CBD-CGD-O2D
3	V	604	HEC	CAA-CBA-CGA-O1A
3	W	604	HEC	CAA-CBA-CGA-O2A
3	W	605	HEC	CAD-CBD-CGD-O1D
3	X	602	HEC	CAA-CBA-CGA-O2A
3	G	604	HEC	CAA-CBA-CGA-O2A
3	A	604	HEC	CAA-CBA-CGA-O2A
3	H	604	HEC	CAA-CBA-CGA-O2A
3	H	607	HEC	CAA-CBA-CGA-O2A
3	K	607	HEC	CAA-CBA-CGA-O2A
3	M	604	HEC	CAA-CBA-CGA-O2A
3	M	607	HEC	CAA-CBA-CGA-O2A
3	N	607	HEC	CAA-CBA-CGA-O2A
3	R	604	HEC	CAA-CBA-CGA-O1A
3	S	604	HEC	CAA-CBA-CGA-O1A
3	T	604	HEC	CAA-CBA-CGA-O2A
3	T	607	HEC	CAA-CBA-CGA-O2A
3	V	604	HEC	CAA-CBA-CGA-O2A
3	V	607	HEC	CAA-CBA-CGA-O2A
3	W	607	HEC	CAA-CBA-CGA-O2A
3	E	604	HEC	CAA-CBA-CGA-O1A
3	F	602	HEC	CAA-CBA-CGA-O2A
3	F	604	HEC	CAA-CBA-CGA-O1A
3	F	604	HEC	CAA-CBA-CGA-O2A
3	H	604	HEC	CAA-CBA-CGA-O1A
3	I	605	HEC	CAD-CBD-CGD-O2D
3	O	604	HEC	CAA-CBA-CGA-O1A
3	Q	604	HEC	CAA-CBA-CGA-O1A
3	X	604	HEC	CAA-CBA-CGA-O1A
3	A	604	HEC	CAA-CBA-CGA-O1A
3	A	604	HEC	CAD-CBD-CGD-O2D
3	K	604	HEC	CAA-CBA-CGA-O2A
3	L	604	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	M	602	HEC	CAA-CBA-CGA-O2A
3	P	604	HEC	CAA-CBA-CGA-O1A
3	S	604	HEC	CAA-CBA-CGA-O2A
3	T	602	HEC	CAA-CBA-CGA-O2A
3	T	604	HEC	CAA-CBA-CGA-O1A
3	V	605	HEC	CAD-CBD-CGD-O2D
3	W	604	HEC	CAA-CBA-CGA-O1A
3	X	607	HEC	CAA-CBA-CGA-O2A
3	H	601	HEC	C3A-C2A-CAA-CBA
3	D	602	HEC	CAD-CBD-CGD-O2D
3	J	604	HEC	CAA-CBA-CGA-O1A
3	O	604	HEC	CAA-CBA-CGA-O2A
3	Q	604	HEC	CAA-CBA-CGA-O2A
3	R	604	HEC	CAA-CBA-CGA-O2A
3	U	607	HEC	CAA-CBA-CGA-O2A
3	X	604	HEC	CAD-CBD-CGD-O2D
3	M	601	HEC	C1A-C2A-CAA-CBA
3	P	601	HEC	C1A-C2A-CAA-CBA
3	A	601	HEC	CAA-CBA-CGA-O1A
3	A	607	HEC	CAA-CBA-CGA-O2A
3	B	607	HEC	CAA-CBA-CGA-O2A
3	C	604	HEC	CAA-CBA-CGA-O2A
3	E	607	HEC	CAA-CBA-CGA-O2A
3	F	604	HEC	CAD-CBD-CGD-O2D
3	I	607	HEC	CAD-CBD-CGD-O2D
3	J	607	HEC	CAA-CBA-CGA-O2A
3	L	604	HEC	CAD-CBD-CGD-O2D
3	O	604	HEC	CAD-CBD-CGD-O2D
3	P	604	HEC	CAD-CBD-CGD-O2D
3	Q	604	HEC	CAD-CBD-CGD-O2D
3	R	605	HEC	CAD-CBD-CGD-O1D
3	U	602	HEC	CAA-CBA-CGA-O2A
3	V	604	HEC	CAD-CBD-CGD-O2D
3	W	602	HEC	CAA-CBA-CGA-O2A
3	C	607	HEC	CAA-CBA-CGA-O2A
3	K	602	HEC	CAA-CBA-CGA-O2A
3	K	605	HEC	CAD-CBD-CGD-O1D
3	N	600	HEC	CAA-CBA-CGA-O2A
3	O	607	HEC	CAA-CBA-CGA-O2A
3	P	607	HEC	CAA-CBA-CGA-O2A
3	Q	600	HEC	CAA-CBA-CGA-O2A
3	R	600	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	R	604	HEC	CAD-CBD-CGD-O2D
3	S	605	HEC	CAD-CBD-CGD-O2D
3	S	607	HEC	CAA-CBA-CGA-O2A
3	W	600	HEC	CAA-CBA-CGA-O2A
3	G	600	HEC	CAA-CBA-CGA-O2A
3	G	602	HEC	CAA-CBA-CGA-O2A
3	G	607	HEC	CAA-CBA-CGA-O2A
3	B	600	HEC	CAA-CBA-CGA-O2A
3	B	605	HEC	CAD-CBD-CGD-O1D
3	C	600	HEC	CAA-CBA-CGA-O2A
3	E	600	HEC	CAA-CBA-CGA-O2A
3	E	602	HEC	CAA-CBA-CGA-O1A
3	F	600	HEC	CAA-CBA-CGA-O2A
3	F	604	HEC	CAD-CBD-CGD-O1D
3	F	607	HEC	CAA-CBA-CGA-O2A
3	H	604	HEC	CAD-CBD-CGD-O2D
3	K	604	HEC	CAD-CBD-CGD-O2D
3	M	605	HEC	CAD-CBD-CGD-O1D
3	N	607	HEC	CAA-CBA-CGA-O1A
3	O	600	HEC	CAA-CBA-CGA-O2A
3	P	602	HEC	CAA-CBA-CGA-O1A
3	R	607	HEC	CAA-CBA-CGA-O2A
3	S	600	HEC	CAA-CBA-CGA-O2A
3	W	604	HEC	CAD-CBD-CGD-O2D
3	X	600	HEC	CAA-CBA-CGA-O2A
3	L	601	HEC	C3A-C2A-CAA-CBA
3	P	601	HEC	C3A-C2A-CAA-CBA
3	A	600	HEC	CAA-CBA-CGA-O2A
3	A	607	HEC	CAA-CBA-CGA-O1A
3	B	604	HEC	CAD-CBD-CGD-O2D
3	F	605	HEC	CAD-CBD-CGD-O1D
3	H	600	HEC	CAA-CBA-CGA-O2A
3	I	604	HEC	CAA-CBA-CGA-O1A
3	I	604	HEC	CAD-CBD-CGD-O1D
3	L	604	HEC	CAD-CBD-CGD-O1D
3	L	605	HEC	CAD-CBD-CGD-O1D
3	M	601	HEC	CAA-CBA-CGA-O2A
3	M	607	HEC	CAA-CBA-CGA-O1A
3	N	604	HEC	CAD-CBD-CGD-O2D
3	P	604	HEC	CAD-CBD-CGD-O1D
3	Q	604	HEC	CAD-CBD-CGD-O1D
3	Q	607	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	S	604	HEC	CAD-CBD-CGD-O2D
3	U	600	HEC	CAA-CBA-CGA-O2A
3	V	600	HEC	CAA-CBA-CGA-O2A
3	V	602	HEC	CAA-CBA-CGA-O1A
3	V	604	HEC	CAD-CBD-CGD-O1D
3	V	607	HEC	CAA-CBA-CGA-O1A
3	X	604	HEC	CAD-CBD-CGD-O1D
3	X	607	HEC	CAA-CBA-CGA-O1A
3	G	604	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAD-CBD-CGD-O1D
3	E	604	HEC	CAD-CBD-CGD-O1D
3	E	604	HEC	CAD-CBD-CGD-O2D
3	H	601	HEC	CAA-CBA-CGA-O1A
3	J	600	HEC	CAA-CBA-CGA-O2A
3	J	604	HEC	CAD-CBD-CGD-O1D
3	J	604	HEC	CAD-CBD-CGD-O2D
3	K	607	HEC	CAA-CBA-CGA-O1A
3	L	607	HEC	CAA-CBA-CGA-O2A
3	M	600	HEC	CAA-CBA-CGA-O2A
3	N	602	HEC	CAA-CBA-CGA-O1A
3	O	602	HEC	CAA-CBA-CGA-O2A
3	P	607	HEC	CAA-CBA-CGA-O1A
3	S	604	HEC	CAD-CBD-CGD-O1D
3	T	600	HEC	CAA-CBA-CGA-O2A
3	T	607	HEC	CAA-CBA-CGA-O1A
3	U	605	HEC	CAD-CBD-CGD-O1D
3	U	607	HEC	CAA-CBA-CGA-O1A
3	A	604	HEC	CAD-CBD-CGD-O1D
3	C	604	HEC	CAD-CBD-CGD-O2D
3	H	607	HEC	CAA-CBA-CGA-O1A
3	M	604	HEC	CAD-CBD-CGD-O1D
3	O	604	HEC	CAD-CBD-CGD-O1D
3	T	604	HEC	CAD-CBD-CGD-O2D
3	W	607	HEC	CAA-CBA-CGA-O1A
3	E	605	HEC	CAD-CBD-CGD-O2D
3	F	600	HEC	CAA-CBA-CGA-O1A
3	L	600	HEC	CAA-CBA-CGA-O2A
3	O	601	HEC	CAA-CBA-CGA-O1A
3	T	605	HEC	CAD-CBD-CGD-O2D
3	U	604	HEC	CAD-CBD-CGD-O1D
5	K	612	GOL	O1-C1-C2-O2
3	M	601	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	C	602	HEC	CAA-CBA-CGA-O1A
3	F	601	HEC	CAA-CBA-CGA-O1A
3	J	602	HEC	CAA-CBA-CGA-O2A
3	K	600	HEC	CAA-CBA-CGA-O2A
3	Q	602	HEC	CAA-CBA-CGA-O1A
3	G	601	HEC	CAA-CBA-CGA-O1A
3	B	607	HEC	CAA-CBA-CGA-O1A
3	E	607	HEC	CAA-CBA-CGA-O1A
3	H	605	HEC	CAD-CBD-CGD-O2D
3	K	601	HEC	CAA-CBA-CGA-O1A
3	R	604	HEC	CAD-CBD-CGD-O1D
3	S	601	HEC	CAA-CBA-CGA-O1A
3	S	607	HEC	CAA-CBA-CGA-O1A
3	U	601	HEC	CAA-CBA-CGA-O1A
3	V	601	HEC	CAA-CBA-CGA-O1A
3	X	605	HEC	CAD-CBD-CGD-O1D
3	G	605	HEC	CAD-CBD-CGD-O1D
3	G	607	HEC	CAA-CBA-CGA-O1A
3	A	605	HEC	CAD-CBD-CGD-O2D
3	B	600	HEC	CAA-CBA-CGA-O1A
3	B	604	HEC	CAD-CBD-CGD-O1D
3	C	607	HEC	CAA-CBA-CGA-O1A
3	D	605	HEC	CAD-CBD-CGD-O1D
3	D	607	HEC	CAA-CBA-CGA-O2A
3	H	604	HEC	CAD-CBD-CGD-O1D
3	I	607	HEC	CAD-CBD-CGD-O1D
3	J	607	HEC	CAA-CBA-CGA-O1A
3	L	607	HEC	CAA-CBA-CGA-O1A
3	N	604	HEC	CAD-CBD-CGD-O1D
3	N	605	HEC	CAD-CBD-CGD-O1D
3	O	607	HEC	CAA-CBA-CGA-O1A
3	Q	601	HEC	CAA-CBA-CGA-O1A
3	Q	605	HEC	CAD-CBD-CGD-O2D
3	Q	607	HEC	CAA-CBA-CGA-O1A
3	R	607	HEC	CAA-CBA-CGA-O1A
3	S	602	HEC	CAA-CBA-CGA-O2A
3	T	601	HEC	CAA-CBA-CGA-O1A
3	T	604	HEC	CAD-CBD-CGD-O1D
3	T	605	HEC	CAD-CBD-CGD-O1D
3	U	600	HEC	CAA-CBA-CGA-O1A
3	W	604	HEC	CAD-CBD-CGD-O1D
3	X	600	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	G	604	HEC	CAD-CBD-CGD-O1D
3	E	605	HEC	CAD-CBD-CGD-O1D
3	F	607	HEC	CAA-CBA-CGA-O1A
3	H	605	HEC	CAD-CBD-CGD-O1D
3	Q	605	HEC	CAD-CBD-CGD-O1D
3	S	605	HEC	CAD-CBD-CGD-O1D
3	A	602	HEC	CAA-CBA-CGA-O1A
3	D	605	HEC	CAD-CBD-CGD-O2D
3	K	604	HEC	CAD-CBD-CGD-O1D
3	L	602	HEC	CAA-CBA-CGA-O2A
3	N	605	HEC	CAD-CBD-CGD-O2D
3	V	600	HEC	CAA-CBA-CGA-O1A
3	V	605	HEC	CAD-CBD-CGD-O1D
3	X	601	HEC	CAA-CBA-CGA-O1A
3	X	602	HEC	CAA-CBA-CGA-O1A
3	X	605	HEC	CAD-CBD-CGD-O2D
3	D	602	HEC	CAD-CBD-CGD-O1D
3	G	600	HEC	CAA-CBA-CGA-O1A
3	B	602	HEC	CAA-CBA-CGA-O1A
3	Q	600	HEC	CAA-CBA-CGA-O1A
3	R	601	HEC	CAA-CBA-CGA-O1A
3	A	605	HEC	CAD-CBD-CGD-O1D
3	O	600	HEC	CAA-CBA-CGA-O1A
3	P	600	HEC	CAA-CBA-CGA-O2A
3	W	601	HEC	CAA-CBA-CGA-O1A
3	D	601	HEC	C2A-CAA-CBA-CGA
3	D	607	HEC	CAA-CBA-CGA-O1A
3	I	601	HEC	CAA-CBA-CGA-O1A
3	N	600	HEC	CAA-CBA-CGA-O1A
3	N	601	HEC	CAA-CBA-CGA-O2A
3	R	600	HEC	CAA-CBA-CGA-O1A
3	E	600	HEC	CAA-CBA-CGA-O1A
3	H	600	HEC	CAA-CBA-CGA-O1A
3	M	602	HEC	CAA-CBA-CGA-O1A
3	R	602	HEC	CAA-CBA-CGA-O2A
3	S	600	HEC	CAA-CBA-CGA-O1A
3	C	601	HEC	CAA-CBA-CGA-O2A
3	T	602	HEC	CAA-CBA-CGA-O1A
3	W	600	HEC	CAA-CBA-CGA-O1A
3	A	600	HEC	CAA-CBA-CGA-O1A
3	B	601	HEC	CAA-CBA-CGA-O2A
3	C	600	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	F	602	HEC	CAA-CBA-CGA-O1A
3	J	600	HEC	CAA-CBA-CGA-O1A
3	K	600	HEC	CAA-CBA-CGA-O1A
3	L	600	HEC	CAA-CBA-CGA-O1A
3	T	600	HEC	CAA-CBA-CGA-O1A
3	M	600	HEC	CAA-CBA-CGA-O1A
3	E	603	HEC	CAA-CBA-CGA-O2A
3	H	603	HEC	CAA-CBA-CGA-O2A
3	E	601	HEC	CAA-CBA-CGA-O2A
3	H	602	HEC	CAA-CBA-CGA-O2A
3	J	601	HEC	CAA-CBA-CGA-O2A
3	L	601	HEC	CAA-CBA-CGA-O2A
3	P	601	HEC	CAA-CBA-CGA-O2A
3	W	602	HEC	CAA-CBA-CGA-O1A
3	G	602	HEC	CAA-CBA-CGA-O1A
3	I	602	HEC	CAA-CBA-CGA-O1A
3	X	603	HEC	CAA-CBA-CGA-O2A
3	A	601	HEC	CAA-CBA-CGA-O2A
3	H	601	HEC	CAA-CBA-CGA-O2A
3	K	601	HEC	CAA-CBA-CGA-O2A
3	K	602	HEC	CAA-CBA-CGA-O1A
3	M	603	HEC	CAA-CBA-CGA-O2A
3	U	602	HEC	CAA-CBA-CGA-O1A
3	C	601	HEC	C1A-C2A-CAA-CBA
3	S	603	HEC	CAA-CBA-CGA-O2A
3	W	603	HEC	CAA-CBA-CGA-O2A
3	G	601	HEC	CAA-CBA-CGA-O2A
3	J	602	HEC	CAA-CBA-CGA-O1A
3	N	603	HEC	CAA-CBA-CGA-O2A
3	G	603	HEC	CAA-CBA-CGA-O2A
3	F	601	HEC	CAA-CBA-CGA-O2A
3	H	601	HEC	CAD-CBD-CGD-O1D
3	P	600	HEC	CAA-CBA-CGA-O1A
3	L	602	HEC	CAA-CBA-CGA-O1A
3	O	601	HEC	CAA-CBA-CGA-O2A
3	O	602	HEC	CAA-CBA-CGA-O1A
3	S	601	HEC	CAA-CBA-CGA-O2A
3	T	601	HEC	CAA-CBA-CGA-O2A
3	V	601	HEC	CAA-CBA-CGA-O2A
3	C	602	HEC	C4B-C3B-CAB-CBB
3	D	601	HEC	C4C-C3C-CAC-CBC
3	D	606	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	E	602	HEC	C4B-C3B-CAB-CBB
3	I	601	HEC	C4B-C3B-CAB-CBB
3	K	602	HEC	C4B-C3B-CAB-CBB
3	M	604	HEC	C4B-C3B-CAB-CBB
3	N	602	HEC	C4B-C3B-CAB-CBB
3	O	602	HEC	C4B-C3B-CAB-CBB
3	P	602	HEC	C4B-C3B-CAB-CBB
3	X	602	HEC	C4B-C3B-CAB-CBB
3	S	602	HEC	CAA-CBA-CGA-O1A
3	U	601	HEC	CAA-CBA-CGA-O2A
3	W	601	HEC	CAA-CBA-CGA-O2A
3	X	601	HEC	CAA-CBA-CGA-O2A
3	R	601	HEC	CAA-CBA-CGA-O2A
3	R	602	HEC	CAA-CBA-CGA-O1A
3	H	603	HEC	CAA-CBA-CGA-O1A
3	Q	601	HEC	CAA-CBA-CGA-O2A
3	E	603	HEC	CAA-CBA-CGA-O1A
3	I	601	HEC	CAA-CBA-CGA-O2A
3	I	602	HEC	CAA-CBA-CGA-O2A
3	M	603	HEC	CAA-CBA-CGA-O1A
3	X	603	HEC	CAA-CBA-CGA-O1A
3	D	607	HEC	C3A-C2A-CAA-CBA
3	K	603	HEC	C1A-C2A-CAA-CBA
3	A	603	HEC	CAA-CBA-CGA-O2A
3	H	601	HEC	CAD-CBD-CGD-O2D
3	H	602	HEC	CAA-CBA-CGA-O1A
3	I	607	HEC	CAA-CBA-CGA-O2A
3	G	603	HEC	CAA-CBA-CGA-O1A
3	W	603	HEC	CAA-CBA-CGA-O1A
3	N	603	HEC	CAA-CBA-CGA-O1A
3	J	603	HEC	CAA-CBA-CGA-O2A
3	O	603	HEC	CAA-CBA-CGA-O2A
3	Q	603	HEC	CAA-CBA-CGA-O2A
3	I	605	HEC	CAA-CBA-CGA-O2A
3	S	603	HEC	CAA-CBA-CGA-O1A
3	B	606	HEC	CAA-CBA-CGA-O2A
3	D	601	HEC	CAD-CBD-CGD-O2D
3	N	606	HEC	CAA-CBA-CGA-O2A
3	C	601	HEC	CAD-CBD-CGD-O1D
3	J	601	HEC	CAD-CBD-CGD-O1D
3	K	606	HEC	CAA-CBA-CGA-O2A
3	P	601	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

190 monomers are involved in 385 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	611	SO4	2	0
3	W	600	HEC	1	0
3	E	602	HEC	1	0
3	N	606	HEC	2	0
3	E	600	HEC	1	0
3	P	606	HEC	2	0
3	Q	607	HEC	3	0
3	U	601	HEC	3	0
5	J	613	GOL	3	0
3	U	600	HEC	1	0
3	C	602	HEC	1	0
4	N	610	SO4	1	0
5	I	614	GOL	4	0
3	S	602	HEC	1	0
3	L	605	HEC	4	0
3	G	600	HEC	1	0
3	J	600	HEC	1	0
5	L	613	GOL	1	0
3	R	600	HEC	1	0
5	I	615	GOL	1	0
3	F	604	HEC	3	0
3	Q	601	HEC	4	0
3	V	600	HEC	1	0
3	H	606	HEC	3	0
3	X	607	HEC	2	0
3	E	605	HEC	6	0
3	V	604	HEC	3	0
5	K	613	GOL	1	0
3	L	607	HEC	3	0
3	C	605	HEC	4	0
3	J	602	HEC	1	0
3	S	605	HEC	6	0
3	V	602	HEC	1	0
3	E	606	HEC	1	0
3	B	601	HEC	1	0
3	F	601	HEC	1	0
3	Q	605	HEC	6	0
3	L	602	HEC	1	0
3	U	607	HEC	2	0
3	V	601	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	HEC	3	0
3	I	602	HEC	2	0
3	S	606	HEC	1	0
3	I	600	HEC	2	0
3	F	600	HEC	2	0
3	N	600	HEC	1	0
5	A	612	GOL	1	0
3	D	602	HEC	1	0
3	V	607	HEC	3	0
3	W	606	HEC	2	0
5	K	615	GOL	3	0
3	A	606	HEC	2	0
3	D	600	HEC	2	0
3	I	604	HEC	3	0
3	I	606	HEC	3	0
3	W	601	HEC	3	0
3	X	600	HEC	1	0
3	R	601	HEC	1	0
3	W	602	HEC	1	0
3	A	602	HEC	1	0
3	F	602	HEC	1	0
3	M	600	HEC	1	0
3	A	604	HEC	2	0
3	B	607	HEC	2	0
3	J	601	HEC	1	0
3	U	605	HEC	5	0
3	D	605	HEC	5	0
3	I	601	HEC	5	0
3	M	604	HEC	2	0
4	X	610	SO4	1	0
3	P	600	HEC	1	0
3	J	604	HEC	3	0
3	Q	602	HEC	1	0
3	V	605	HEC	5	0
3	H	601	HEC	1	0
3	H	600	HEC	1	0
3	F	605	HEC	5	0
5	G	615	GOL	1	0
3	S	607	HEC	1	0
3	G	605	HEC	5	0
3	C	601	HEC	1	0
4	L	610	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	600	HEC	1	0
3	W	607	HEC	3	0
3	B	600	HEC	1	0
4	H	609	SO4	1	0
3	C	604	HEC	3	0
3	C	606	HEC	2	0
3	F	606	HEC	2	0
3	O	601	HEC	2	0
3	O	600	HEC	2	0
3	O	602	HEC	1	0
3	H	605	HEC	4	0
3	D	606	HEC	2	0
3	I	603	HEC	3	0
3	J	607	HEC	3	0
3	O	604	HEC	2	0
3	N	602	HEC	1	0
3	T	601	HEC	1	0
3	B	605	HEC	5	0
3	T	600	HEC	1	0
3	H	607	HEC	1	0
4	Q	609	SO4	1	0
3	N	604	HEC	3	0
3	D	604	HEC	2	0
3	I	605	HEC	5	0
3	J	606	HEC	1	0
3	W	604	HEC	3	0
3	C	607	HEC	3	0
3	K	602	HEC	2	0
3	L	606	HEC	2	0
3	K	600	HEC	2	0
3	N	605	HEC	6	0
3	Q	606	HEC	2	0
3	F	607	HEC	1	0
3	R	604	HEC	3	0
3	R	606	HEC	2	0
3	O	607	HEC	2	0
3	J	605	HEC	5	0
3	P	602	HEC	1	0
3	K	606	HEC	2	0
3	U	602	HEC	1	0
3	L	601	HEC	3	0
3	B	602	HEC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEC	1	0
3	U	604	HEC	3	0
3	K	607	HEC	3	0
3	A	600	HEC	1	0
3	S	600	HEC	1	0
3	G	601	HEC	3	0
3	M	605	HEC	4	0
3	T	607	HEC	2	0
3	H	604	HEC	3	0
3	T	605	HEC	5	0
3	M	601	HEC	1	0
3	G	604	HEC	2	0
3	R	607	HEC	3	0
3	X	602	HEC	1	0
3	P	605	HEC	4	0
3	E	601	HEC	2	0
3	M	607	HEC	3	0
3	N	607	HEC	3	0
3	T	602	HEC	1	0
4	G	609	SO4	1	0
4	G	610	SO4	2	0
3	T	604	HEC	3	0
3	T	606	HEC	1	0
3	P	601	HEC	3	0
3	X	606	HEC	2	0
3	R	605	HEC	7	0
3	I	607	HEC	3	0
3	S	601	HEC	3	0
3	B	606	HEC	2	0
3	M	602	HEC	1	0
3	O	605	HEC	2	0
3	A	607	HEC	3	0
3	E	604	HEC	3	0
3	X	605	HEC	6	0
5	G	616	GOL	1	0
3	G	607	HEC	3	0
3	D	603	HEC	2	0
3	G	602	HEC	1	0
3	X	604	HEC	3	0
4	B	609	SO4	1	0
3	K	601	HEC	5	0
5	H	615	GOL	9	0

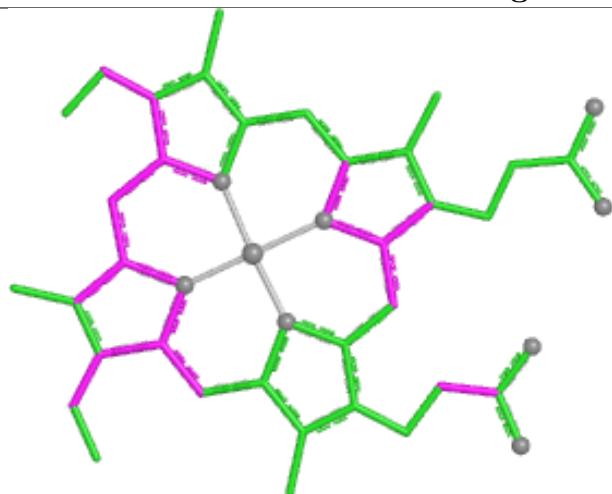
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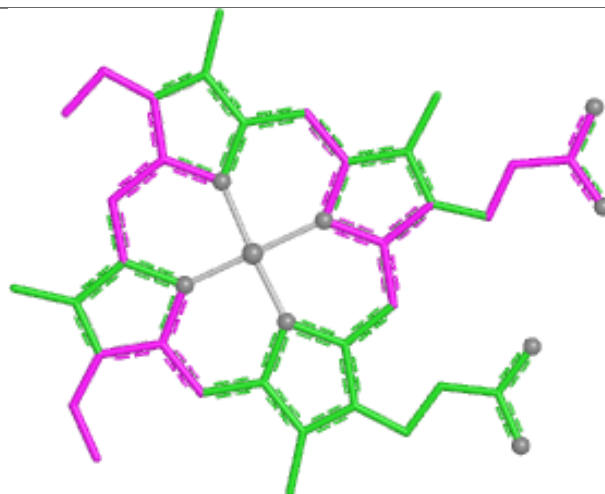
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	600	HEC	2	0
3	S	604	HEC	3	0
3	L	604	HEC	3	0
3	O	606	HEC	2	0
3	U	606	HEC	2	0
5	H	614	GOL	11	0
3	E	607	HEC	1	0
3	Q	604	HEC	3	0
3	H	602	HEC	1	0
5	A	613	GOL	1	0
3	P	604	HEC	3	0
3	P	607	HEC	2	0
3	X	601	HEC	2	0
3	G	606	HEC	2	0
3	K	604	HEC	3	0
3	V	606	HEC	2	0
5	K	614	GOL	10	0
3	K	605	HEC	3	0
3	M	606	HEC	1	0
3	W	605	HEC	7	0
3	N	601	HEC	1	0
3	L	600	HEC	2	0
3	A	605	HEC	3	0
3	D	601	HEC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

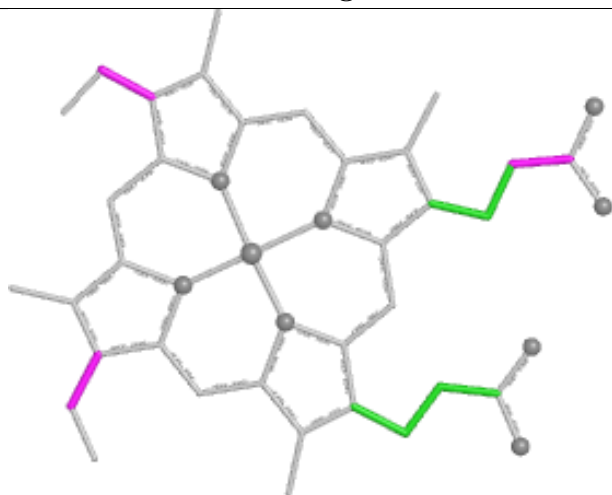
Ligand HEC N 603



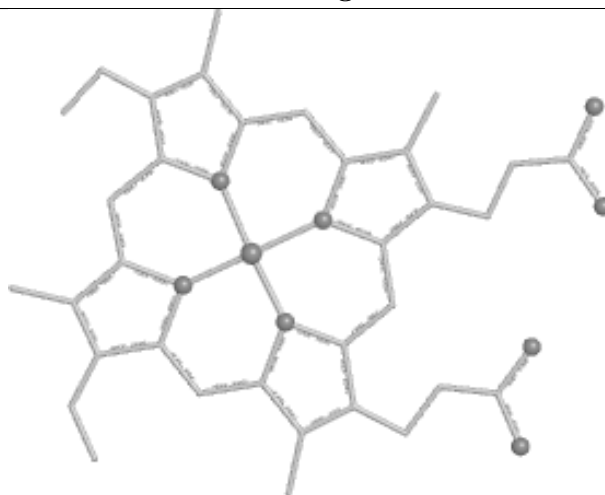
Bond lengths



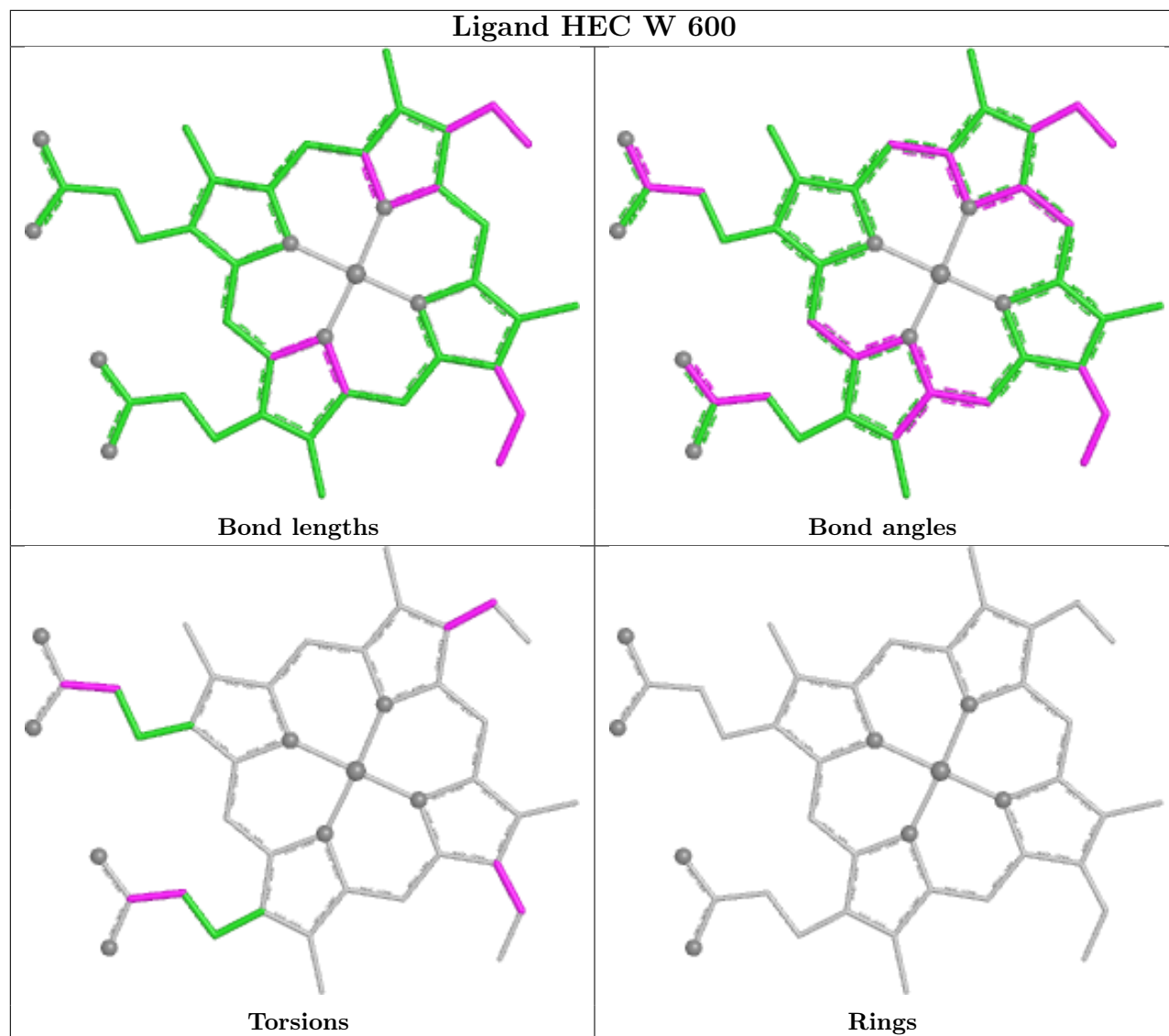
Bond angles



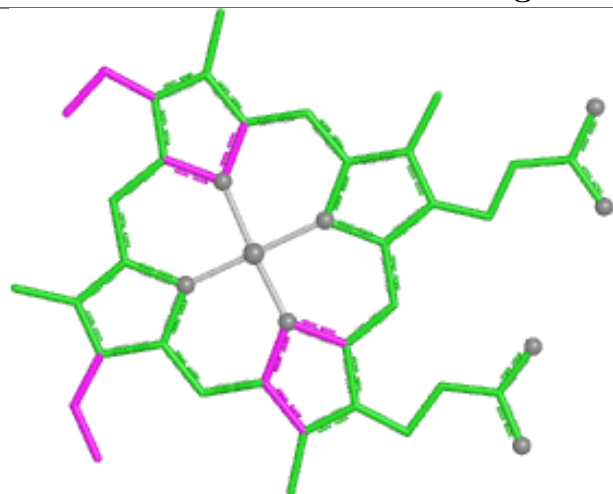
Torsions



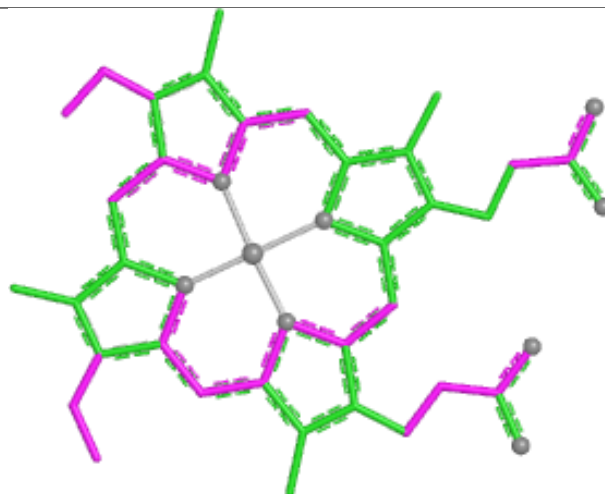
Rings



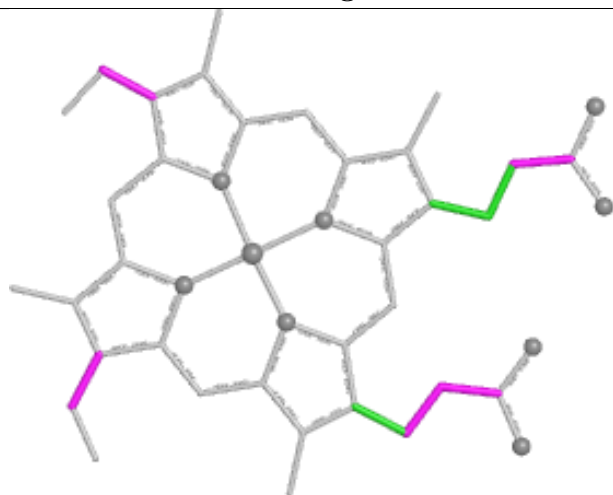
Ligand HEC E 602



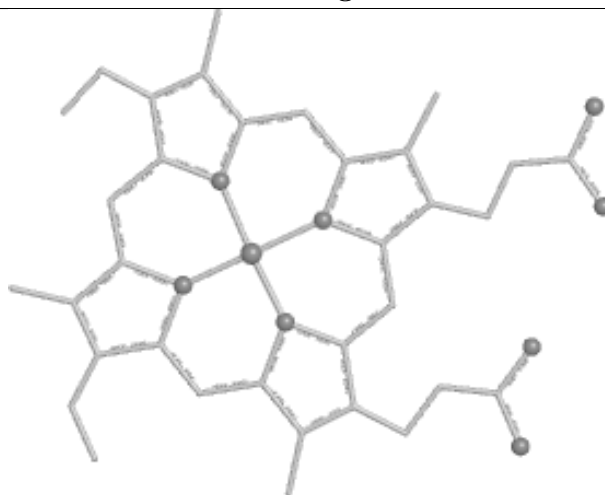
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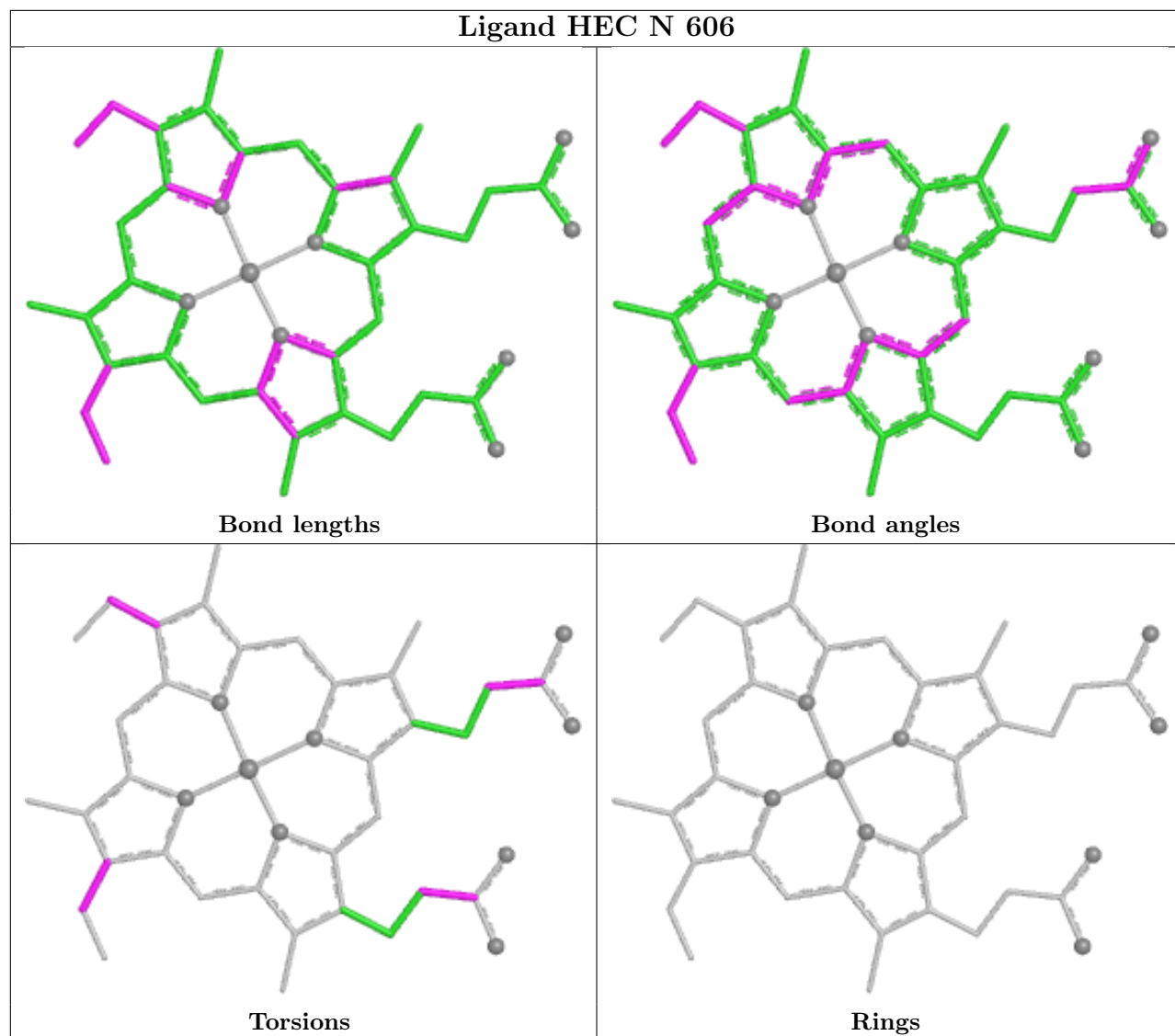
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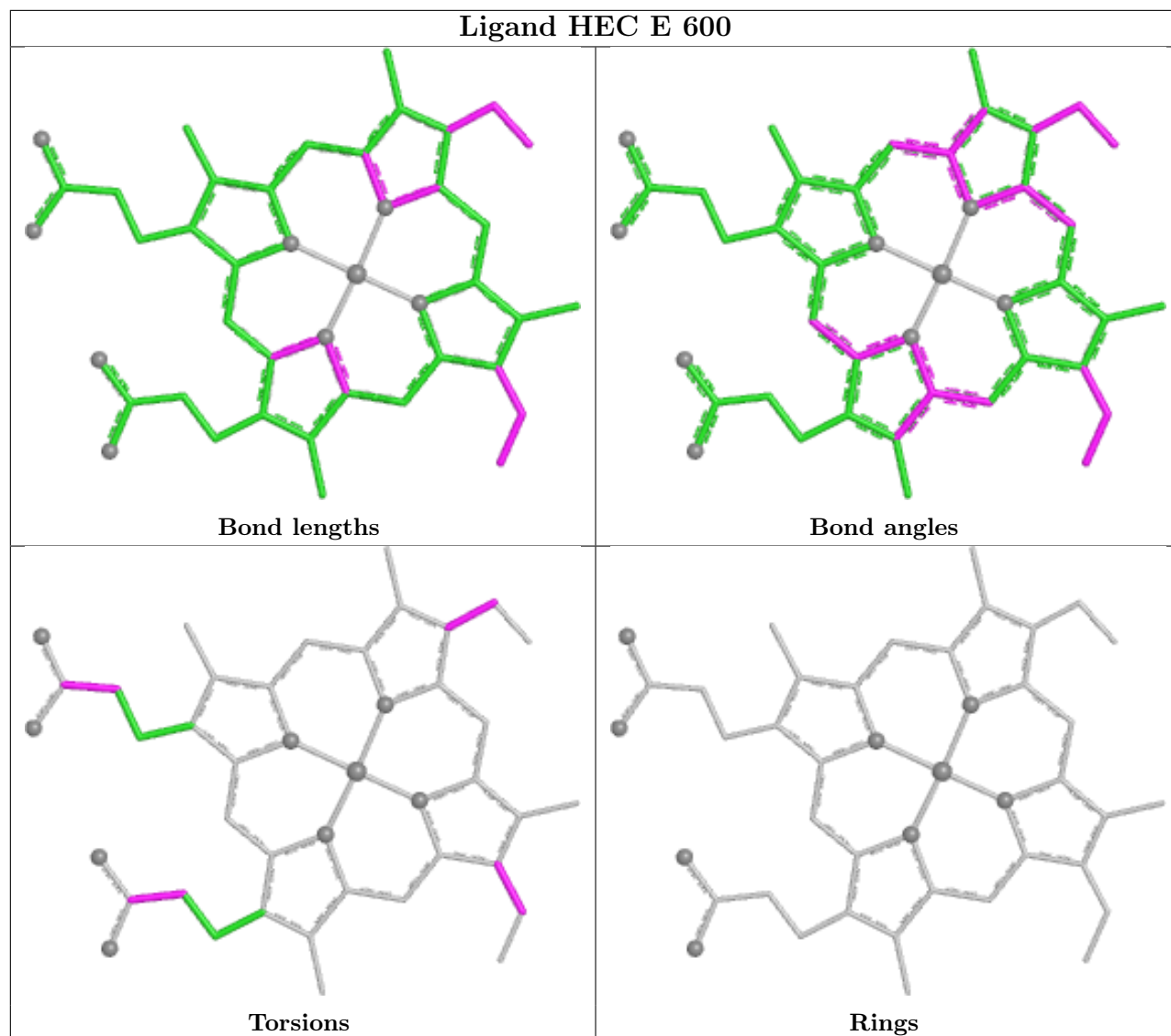


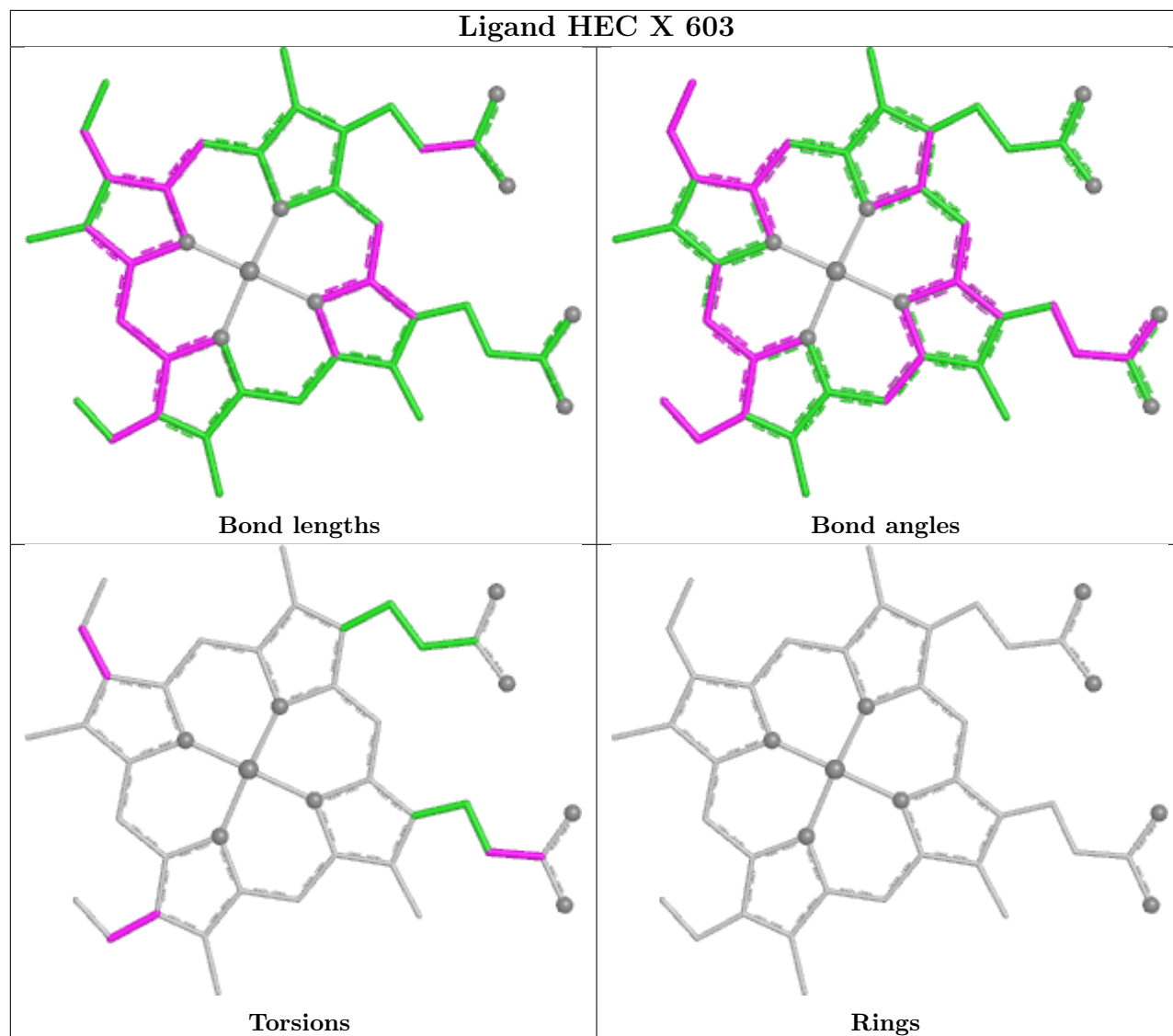
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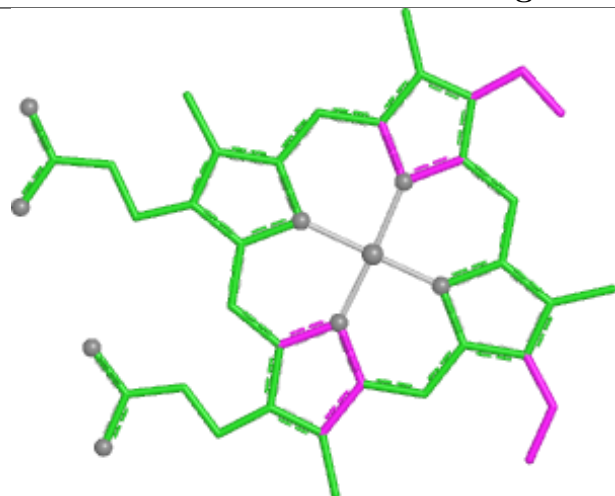
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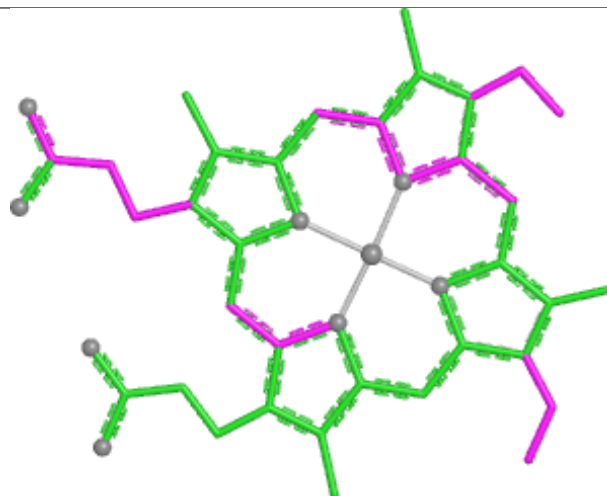




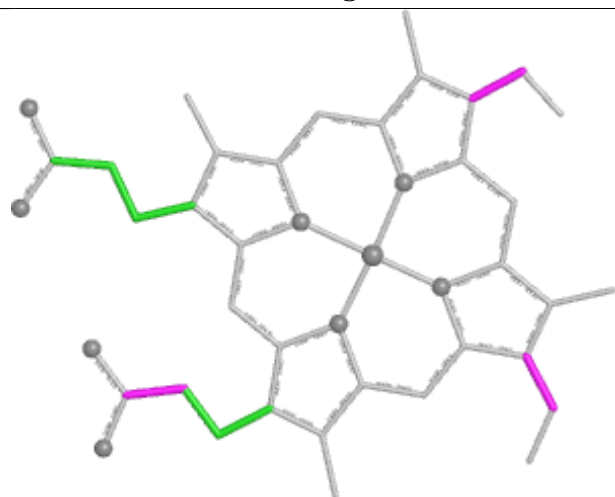
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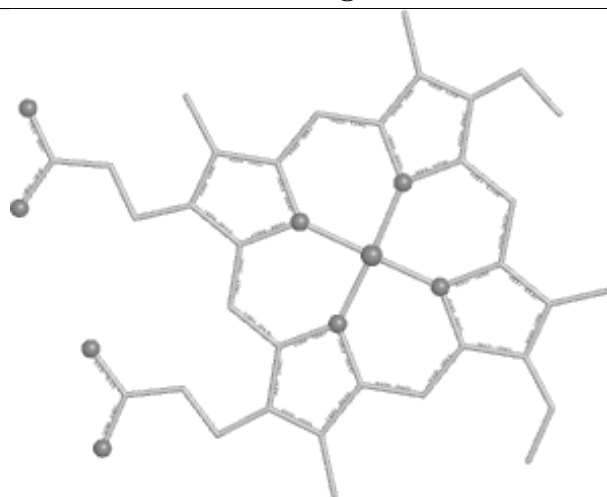
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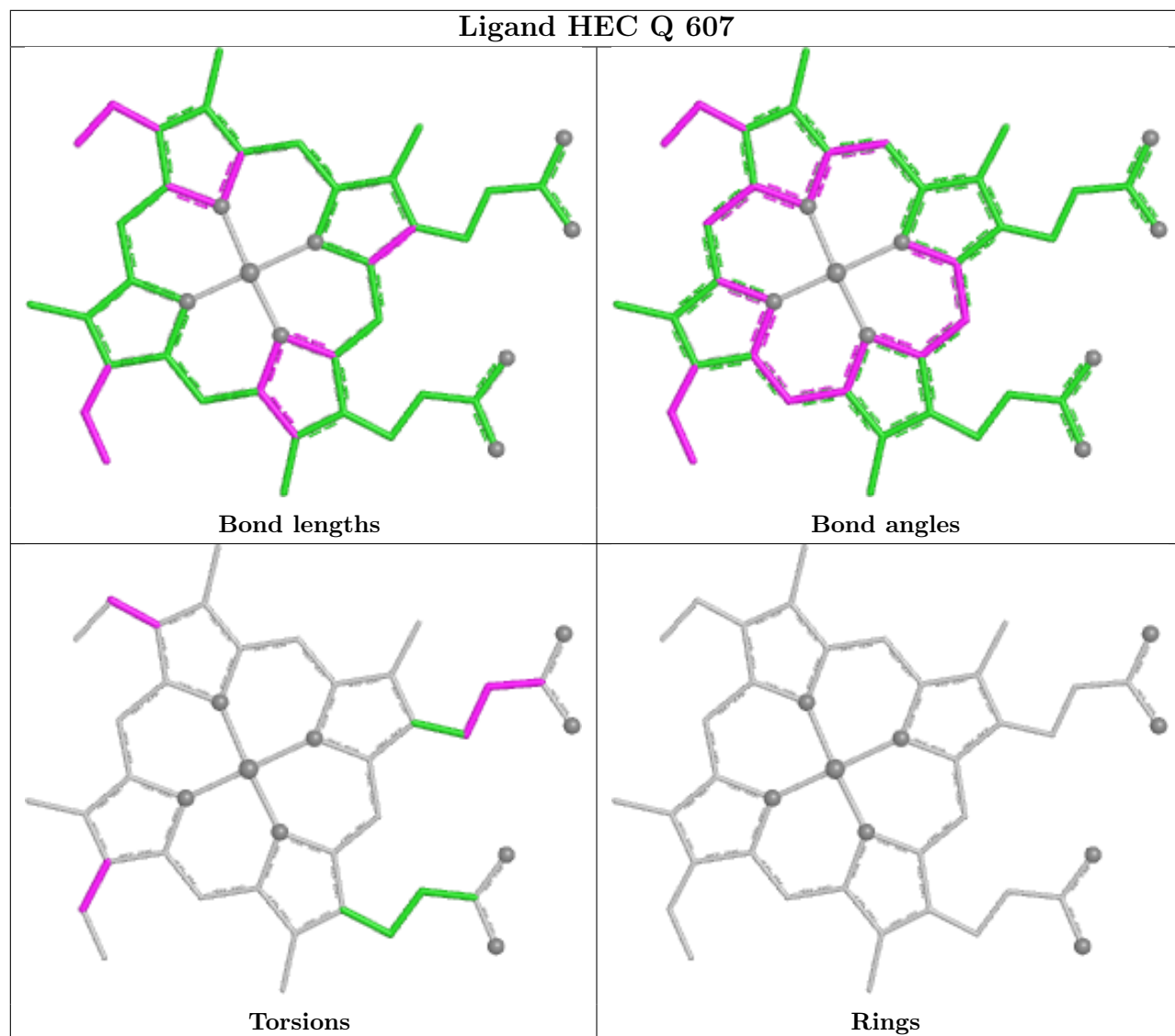
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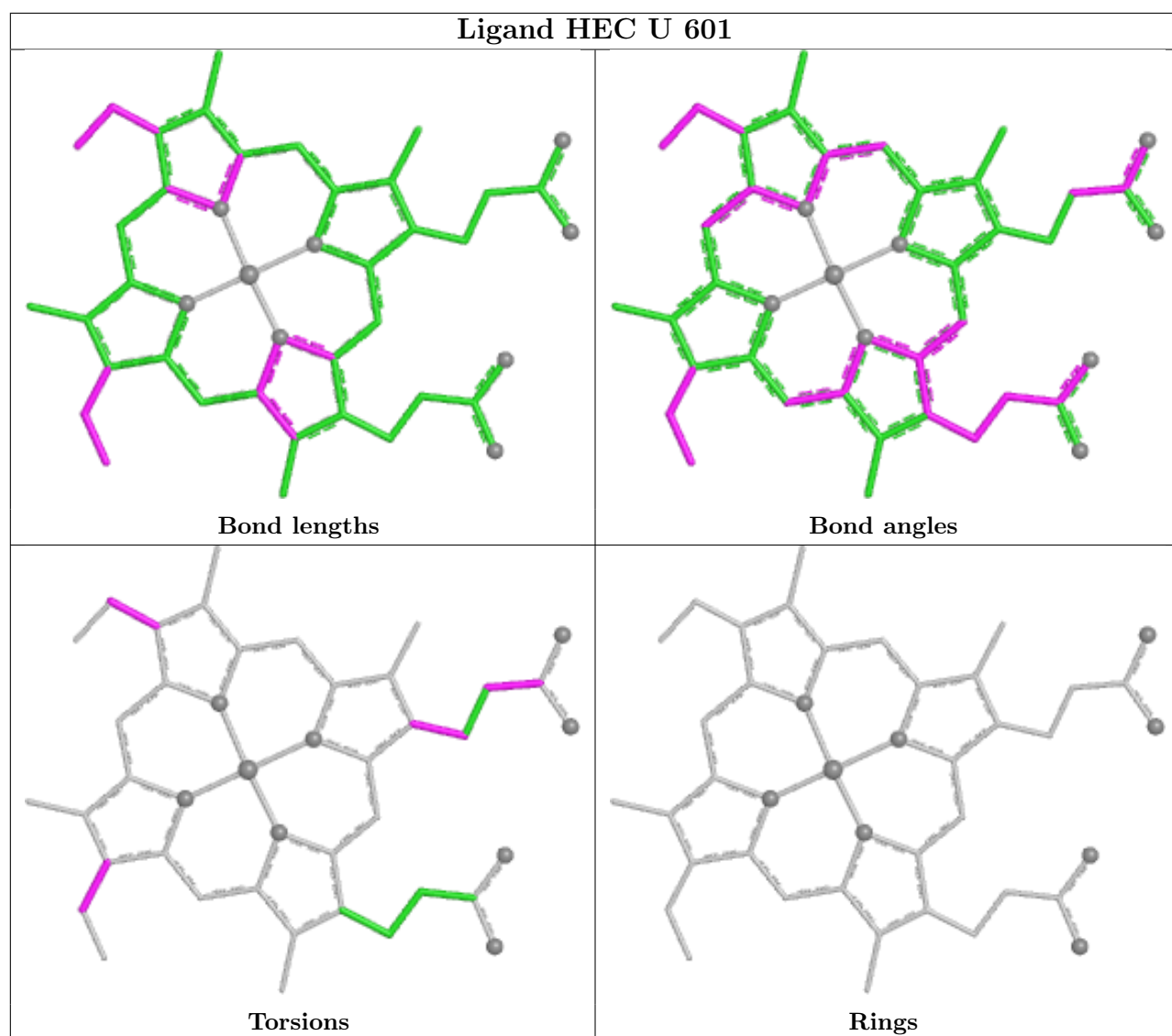


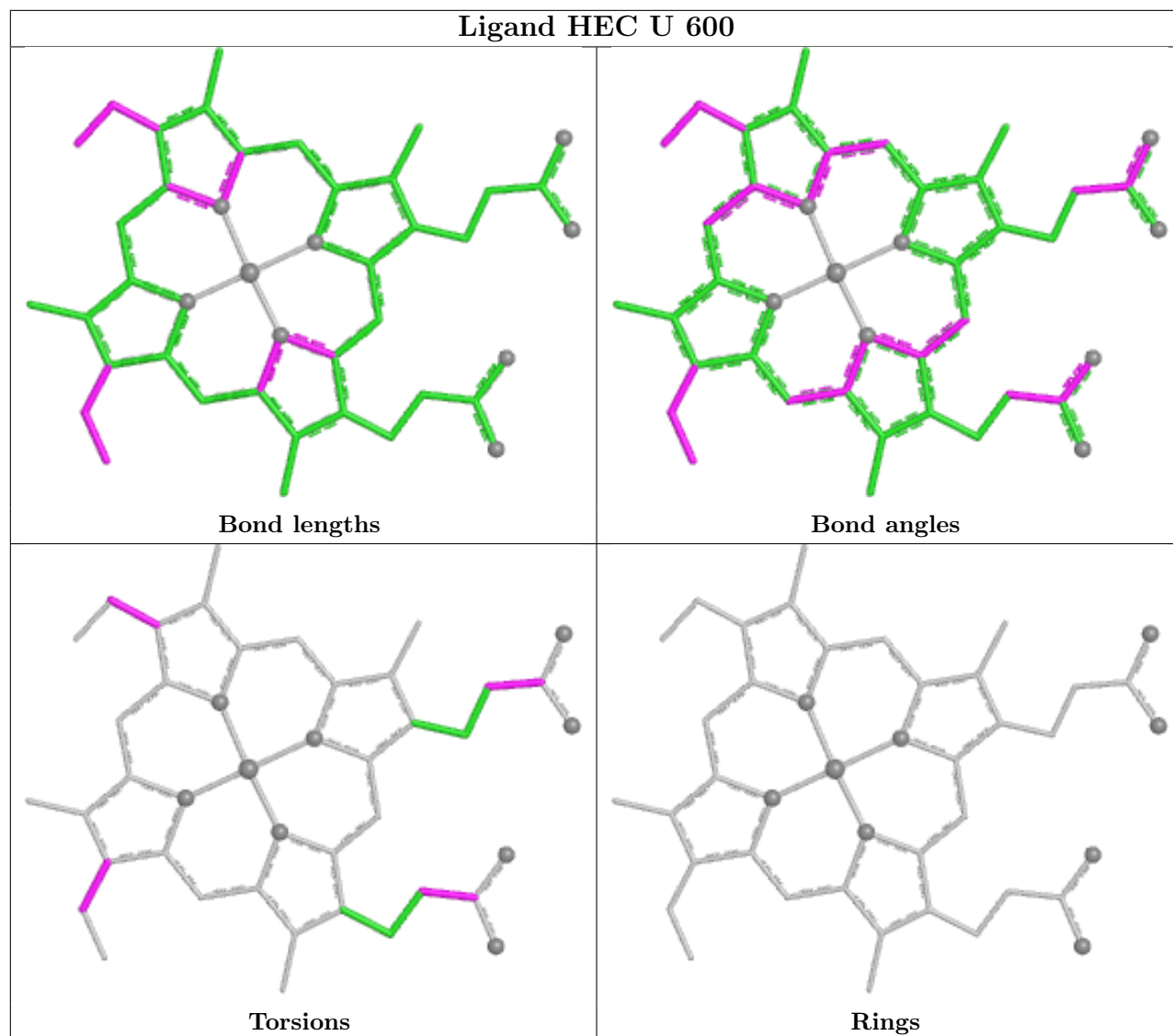
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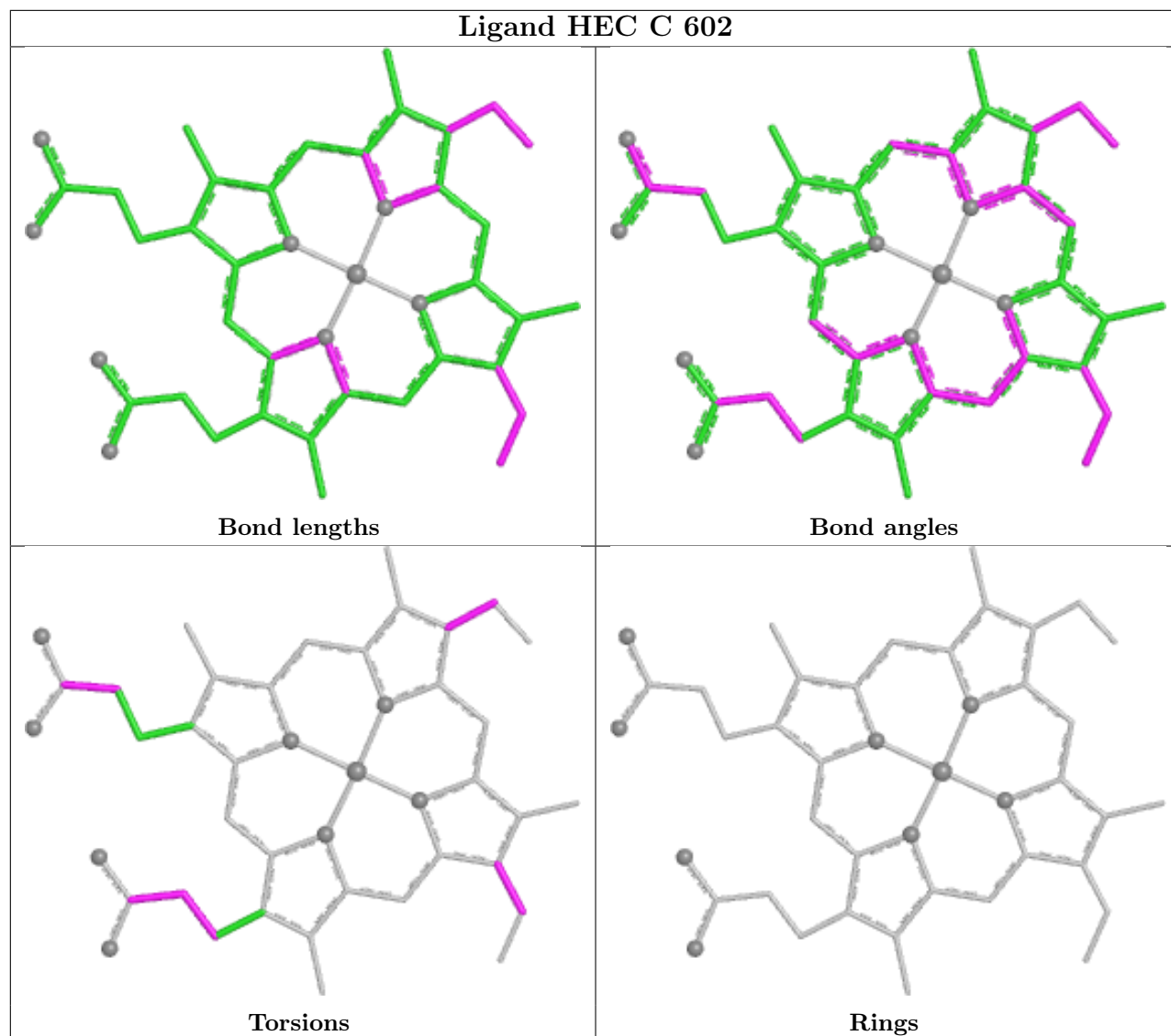


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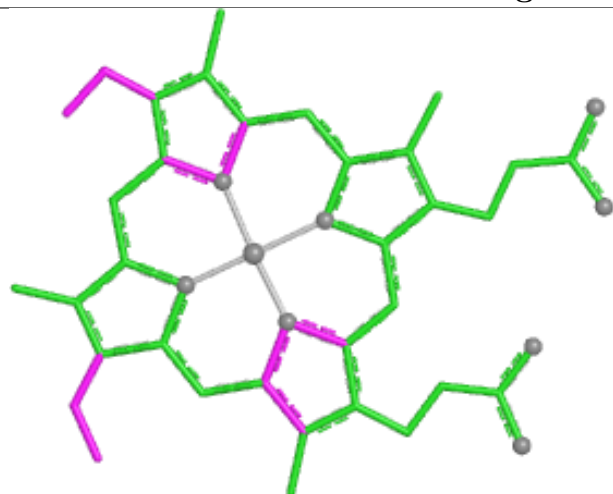




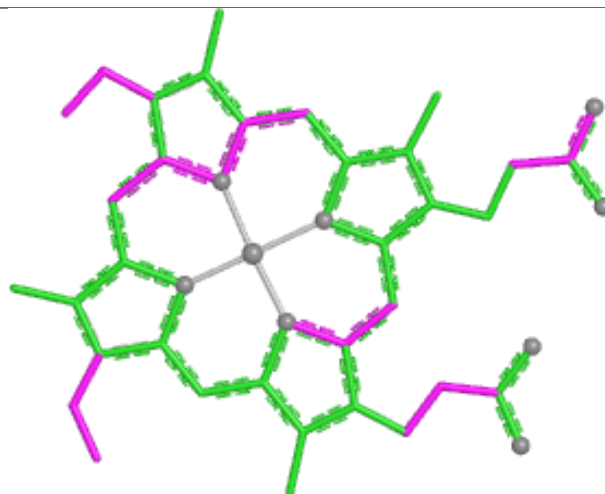




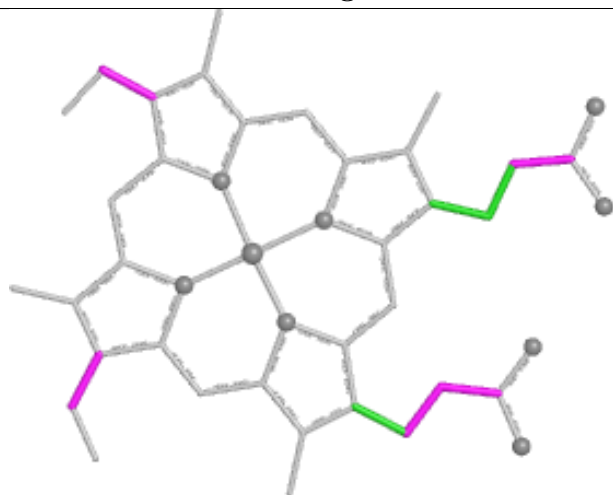
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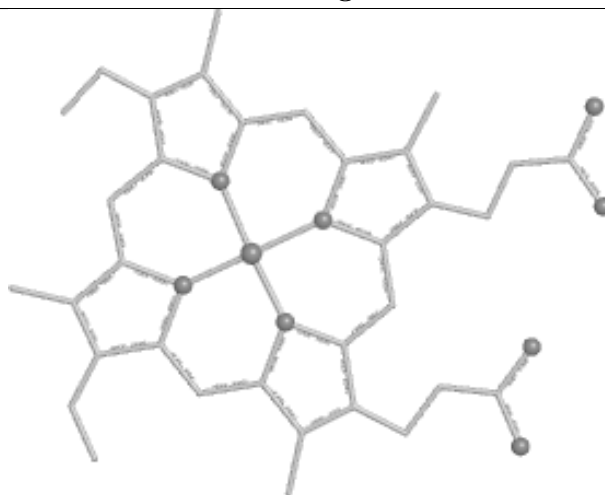
Bond lengths



Bond angles

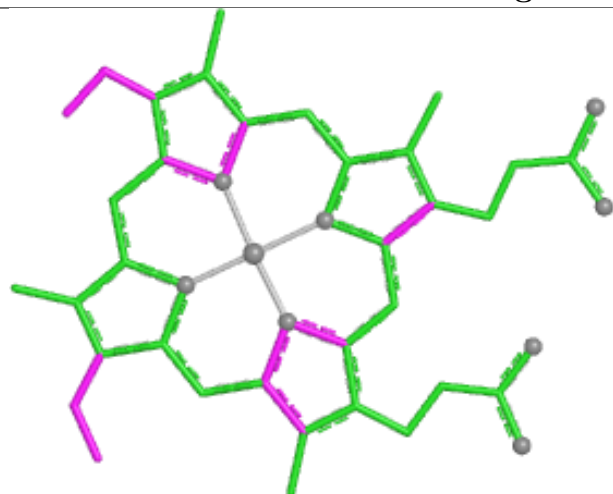


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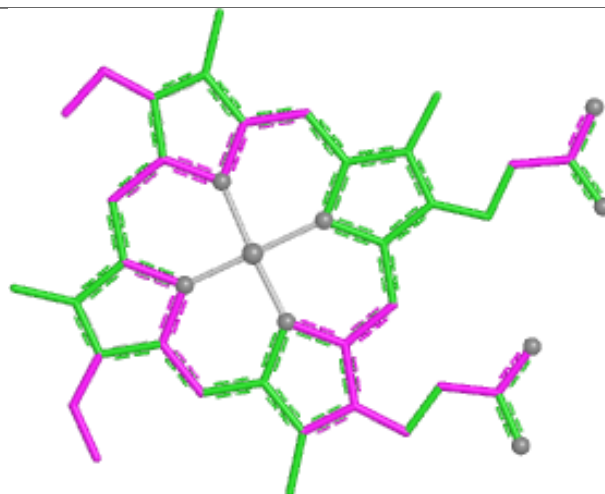


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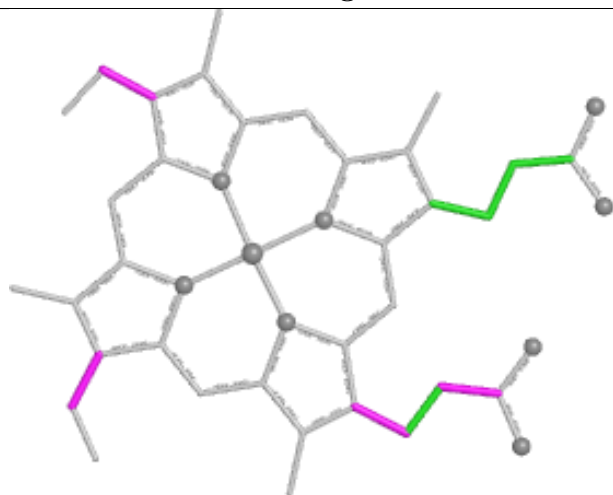
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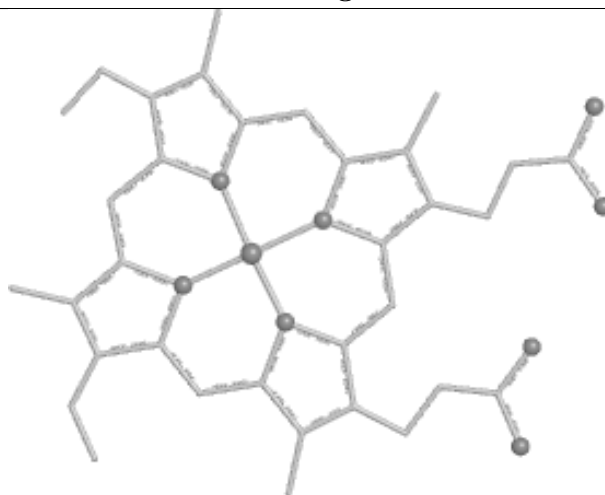
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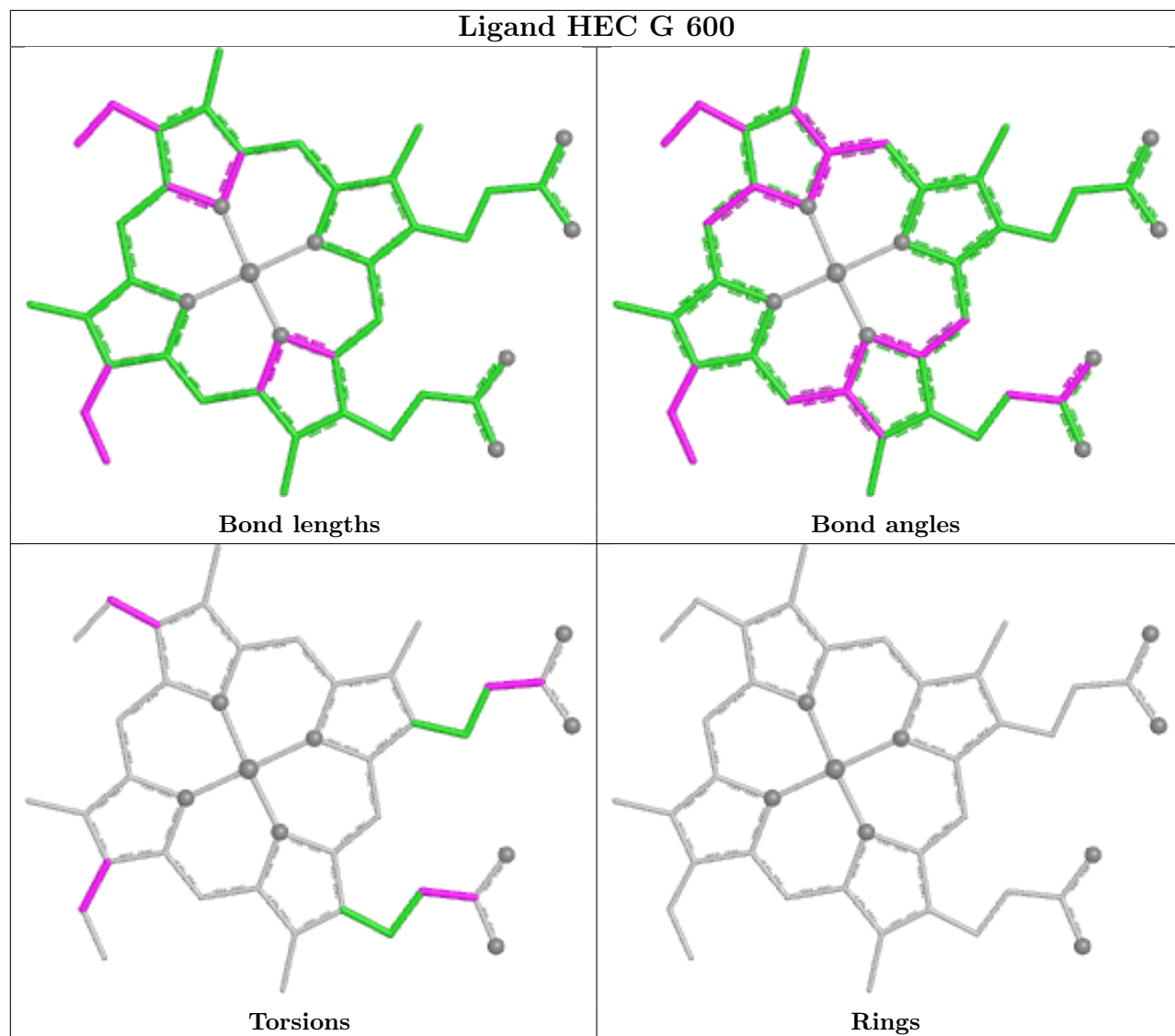
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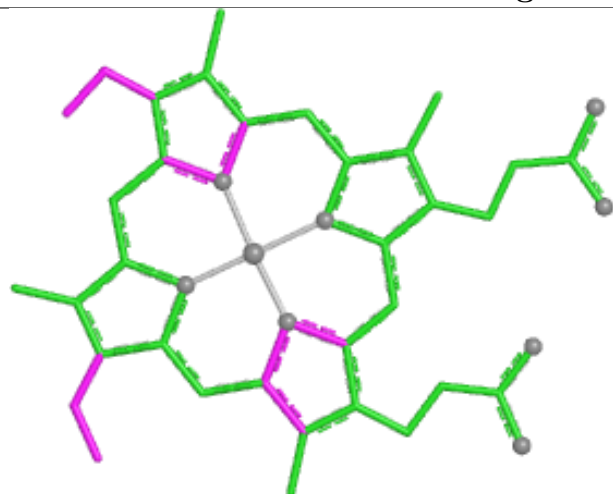
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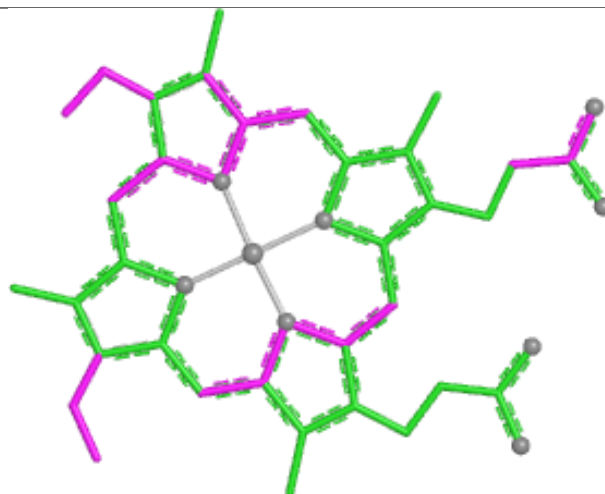
Rings



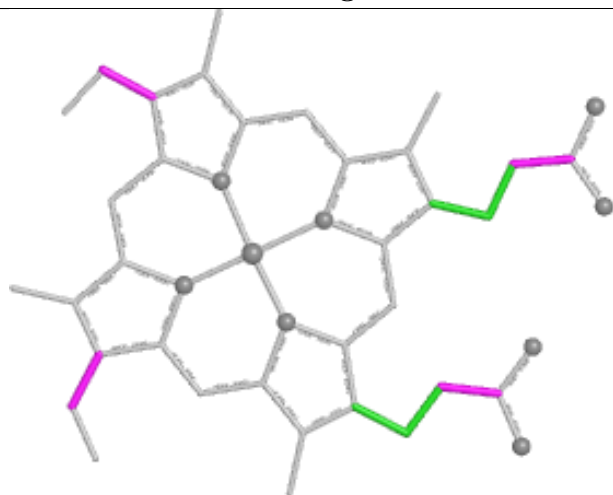
Ligand HEC J 600



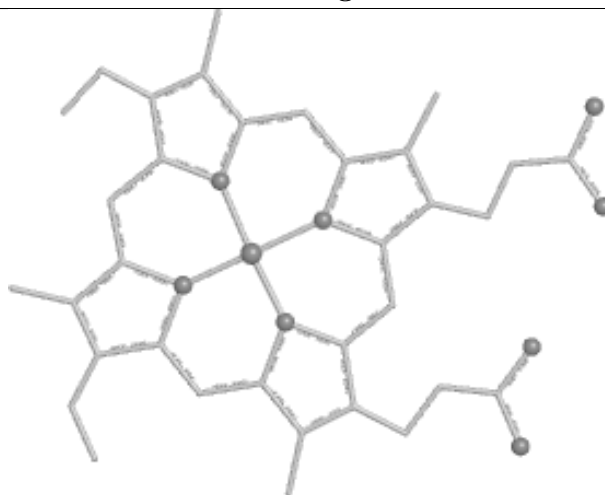
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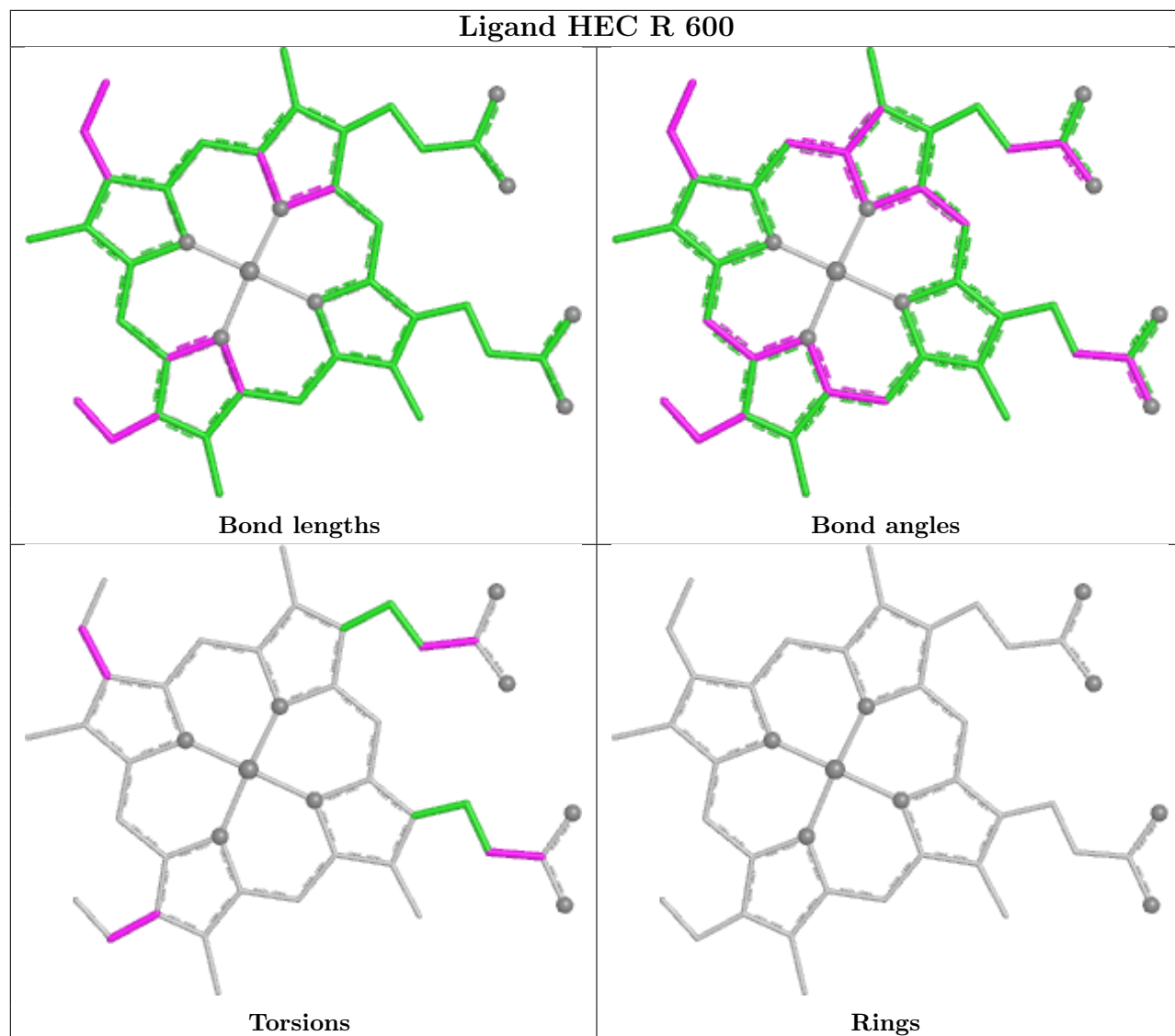
Bond angles



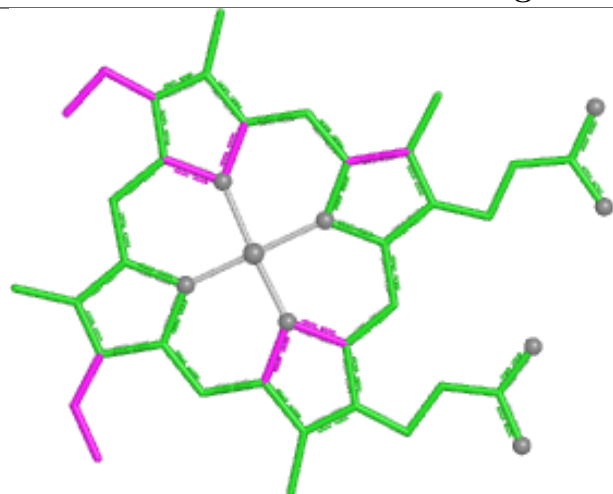
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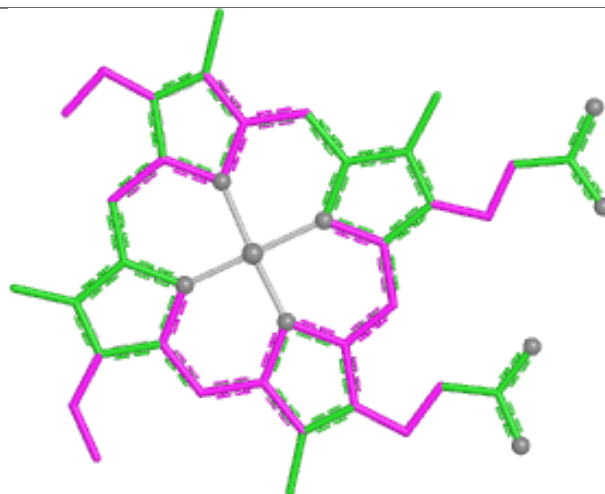
Rings



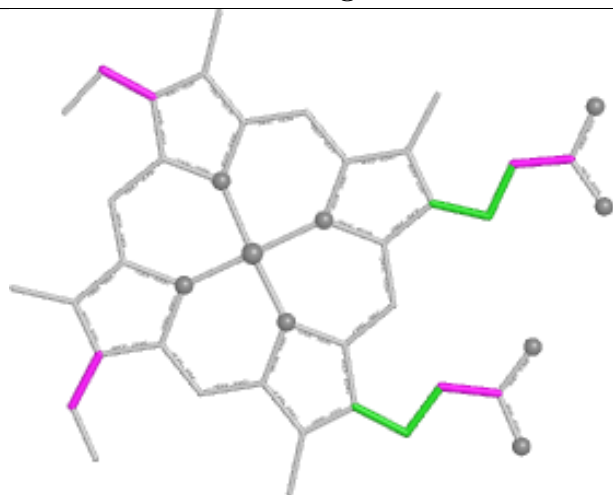
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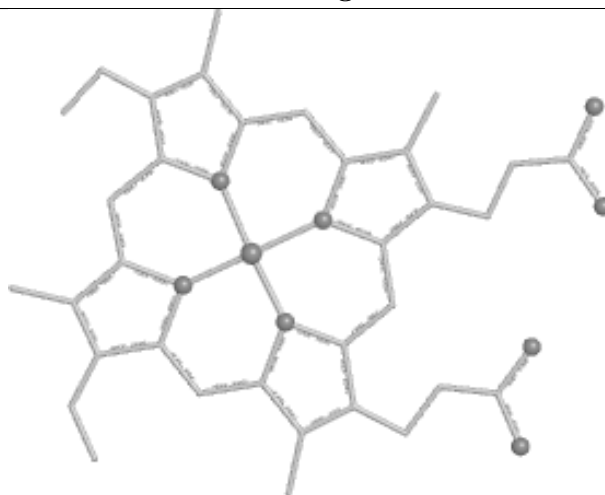
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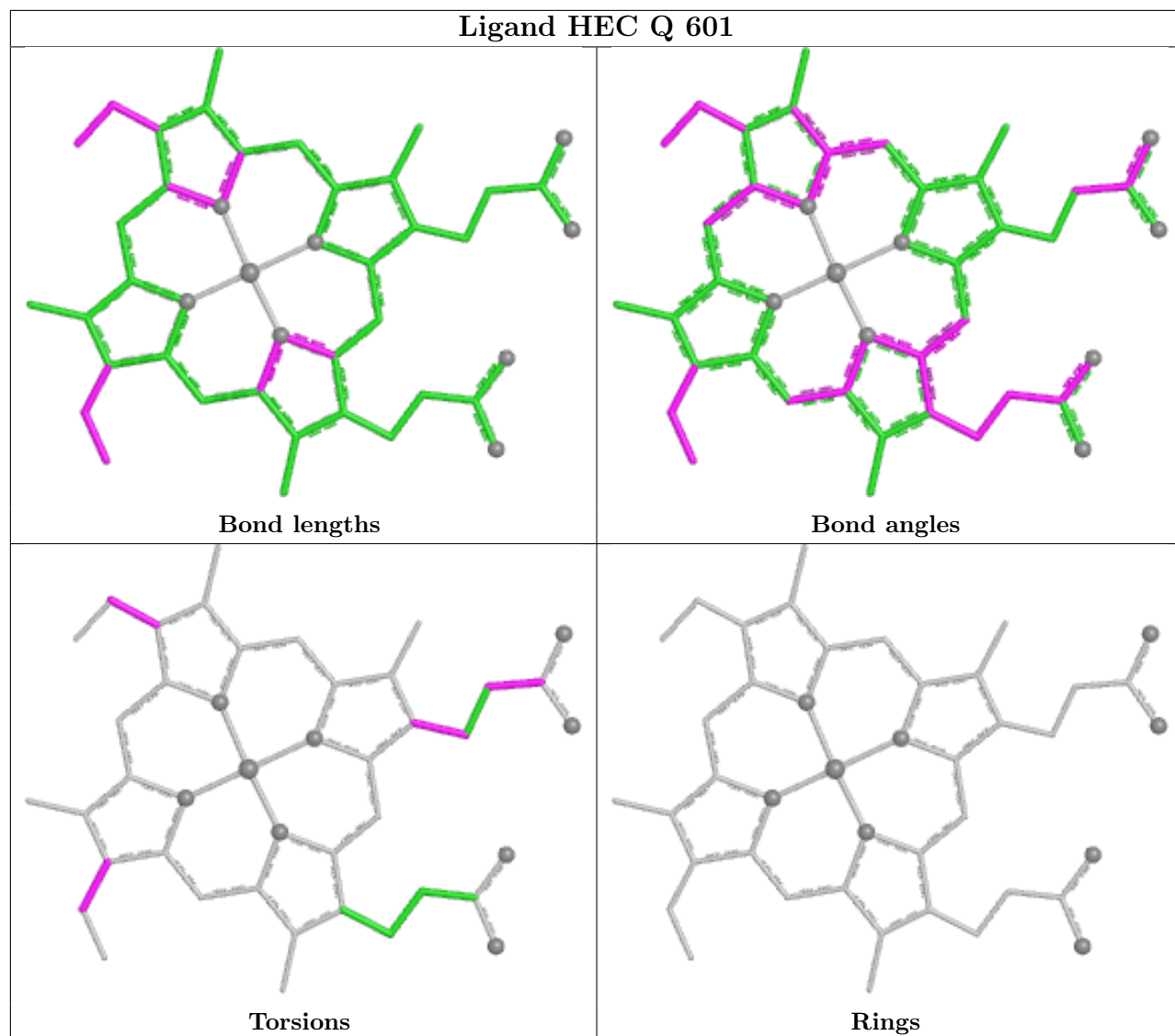
Bond angles

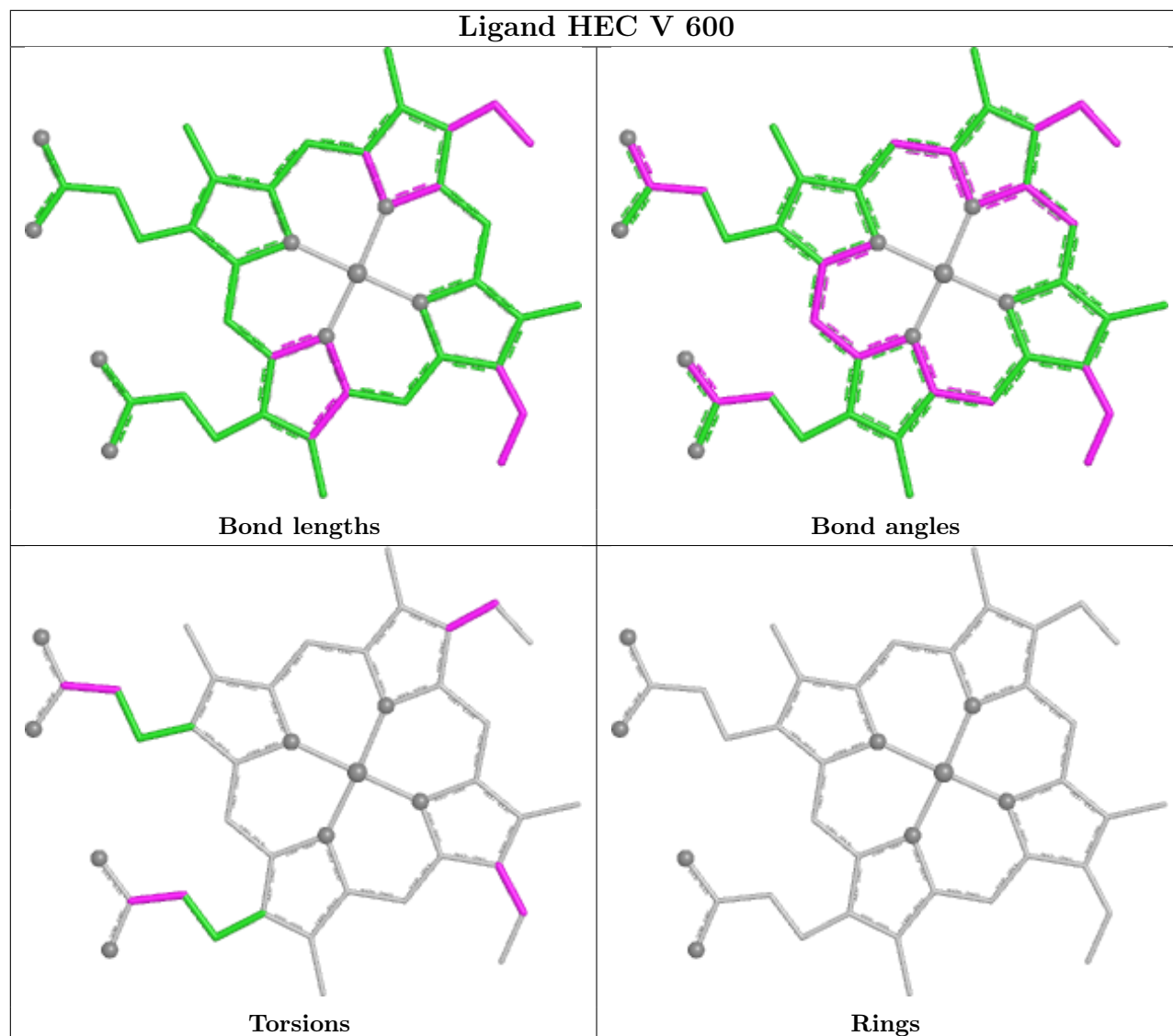


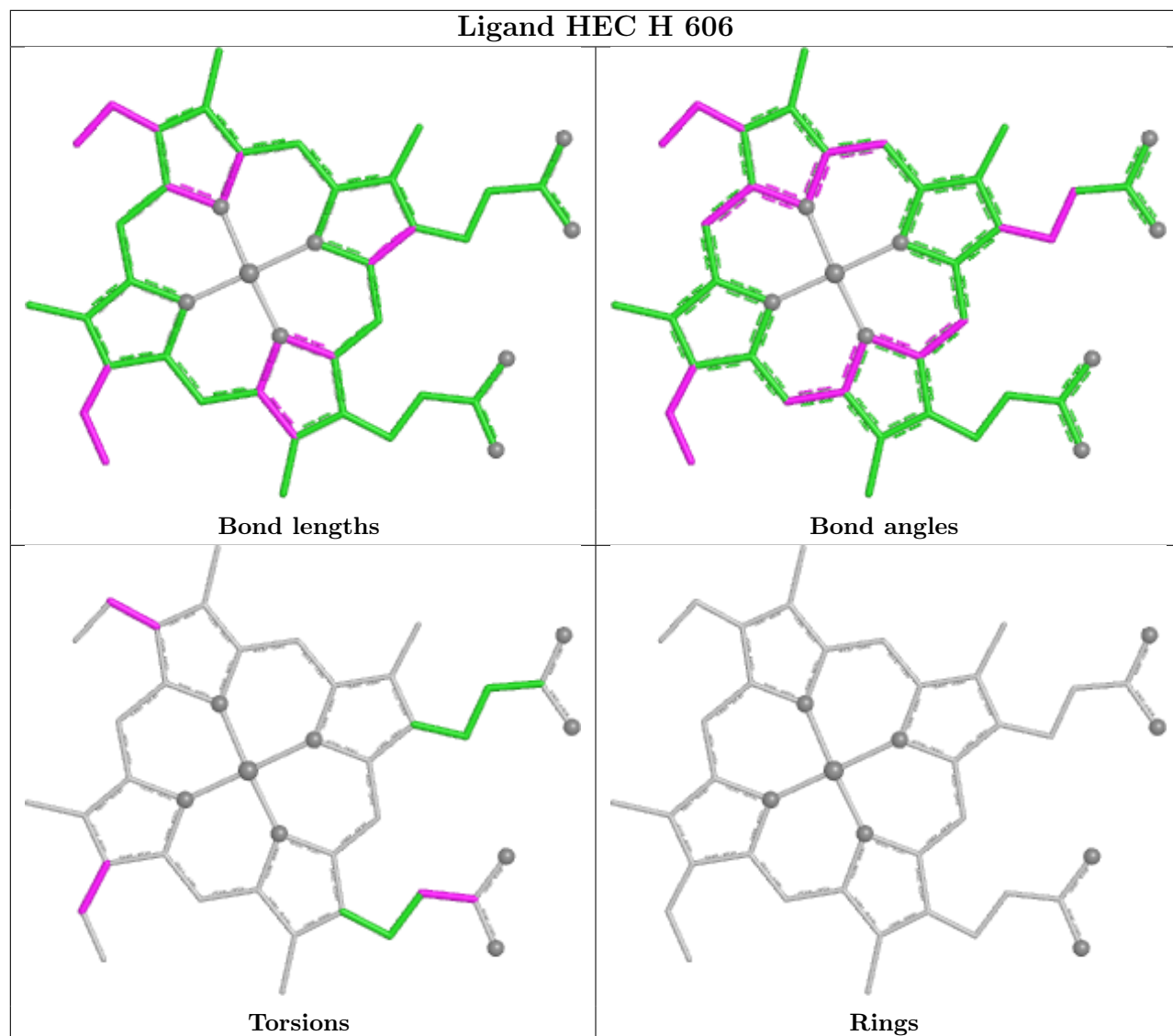
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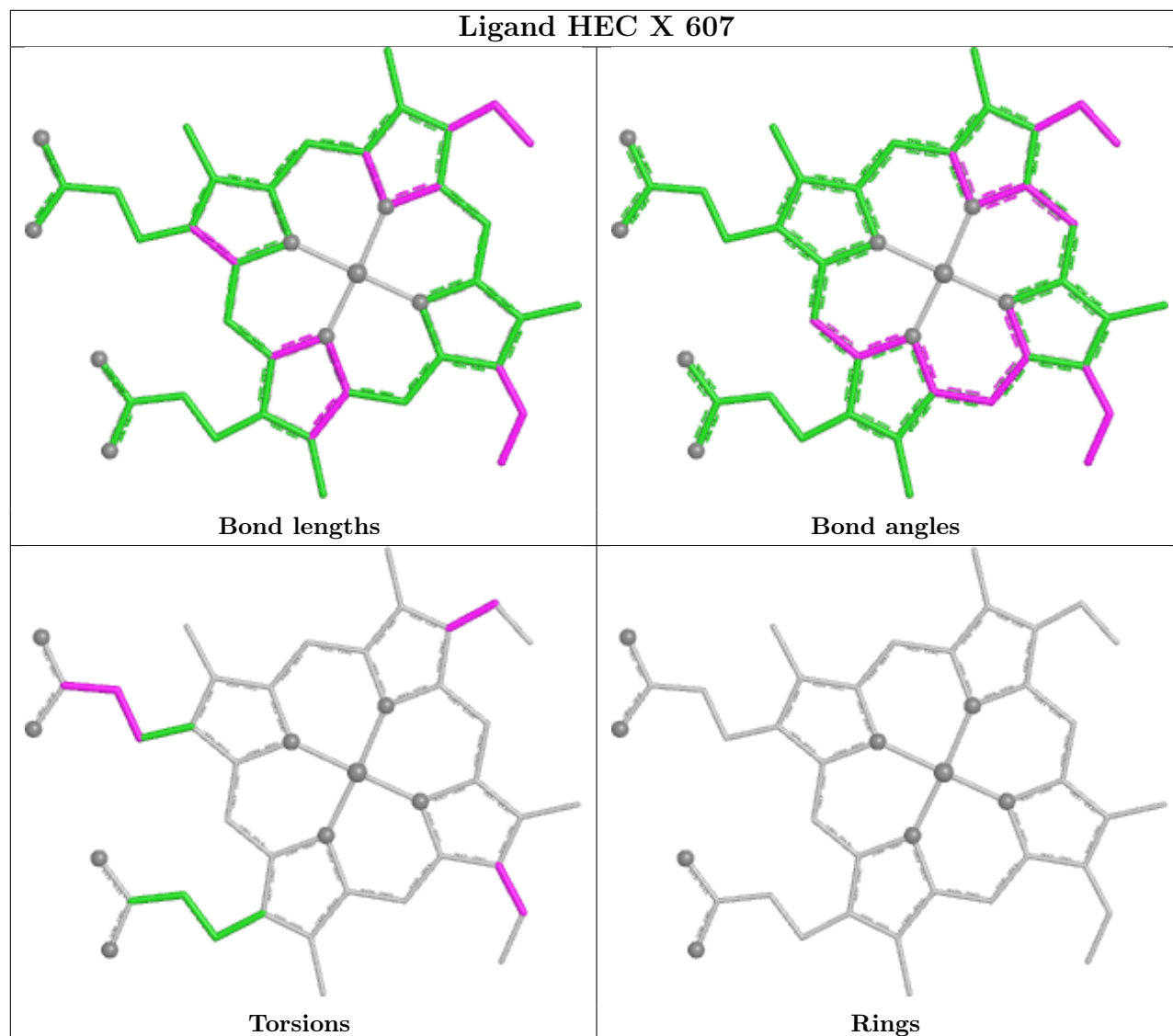


Rings

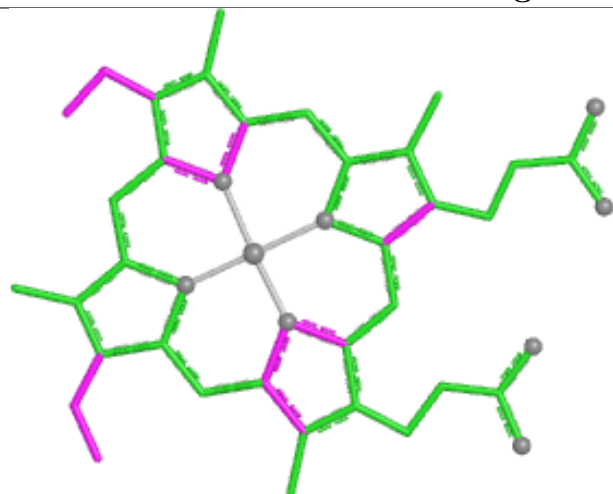




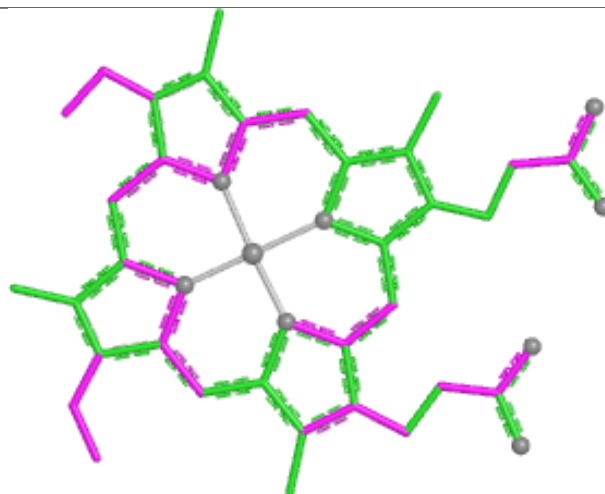




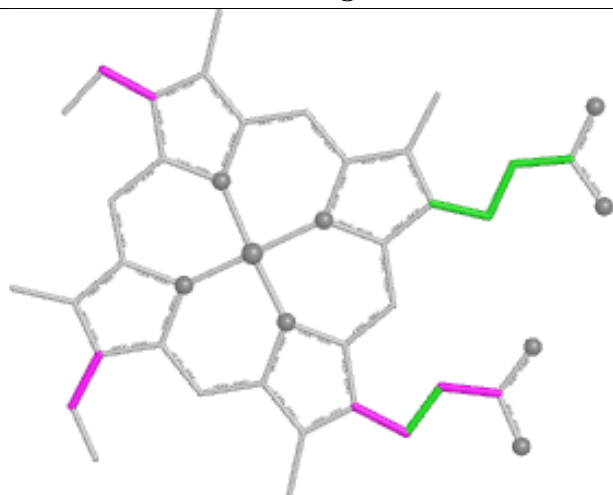
Ligand HEC E 605



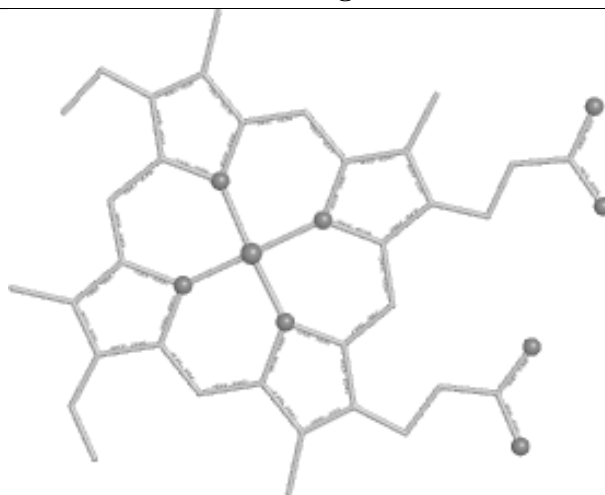
Bond lengths



Bond angles

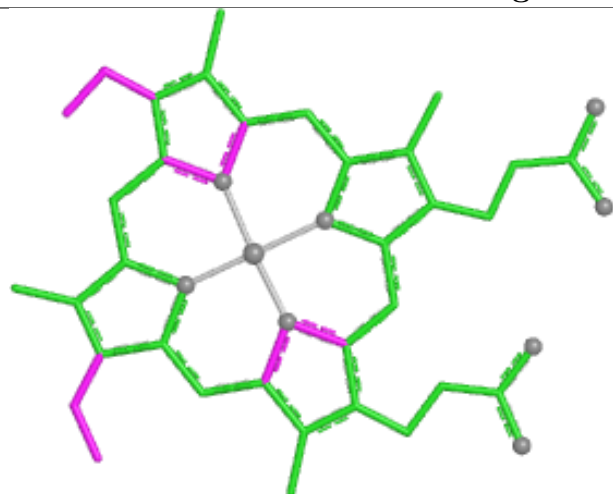


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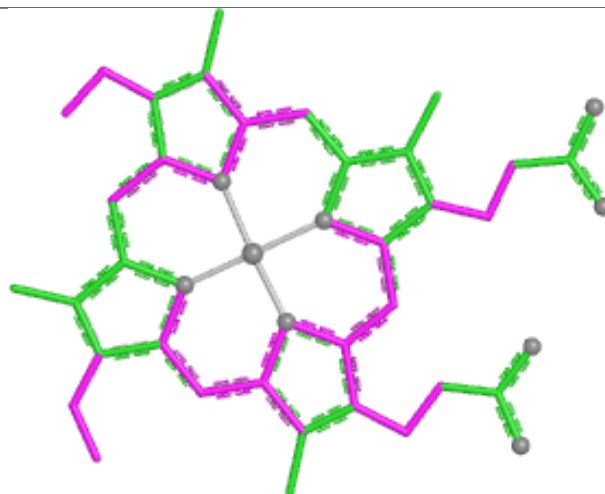


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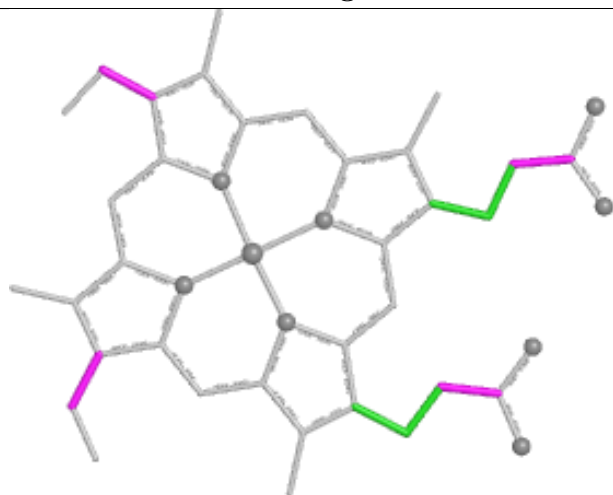
Ligand HEC V 604



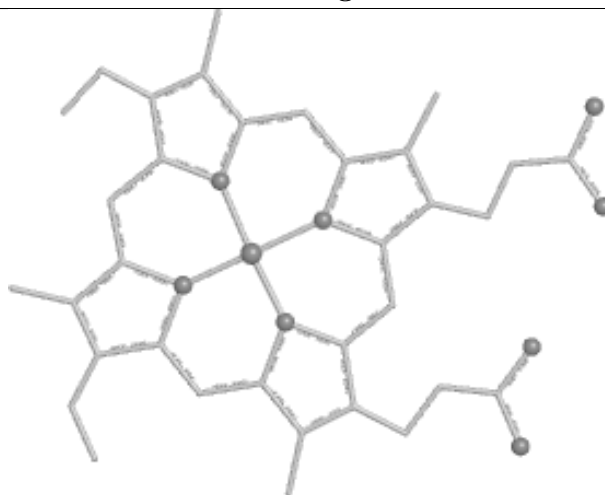
Bond lengths



Bond angles

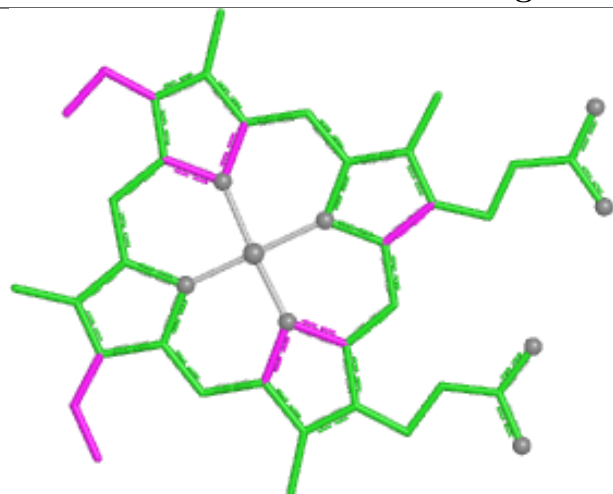


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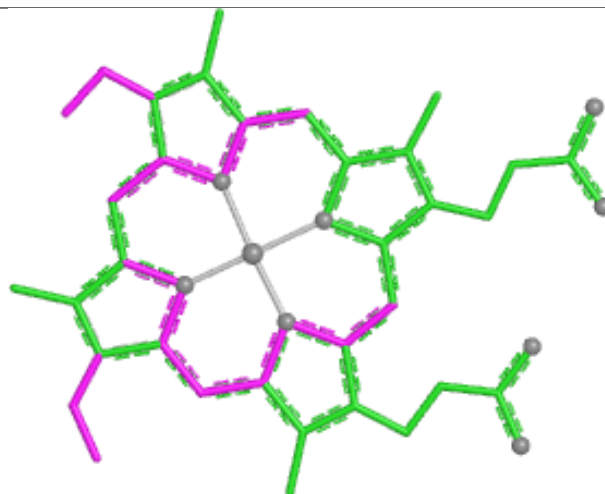


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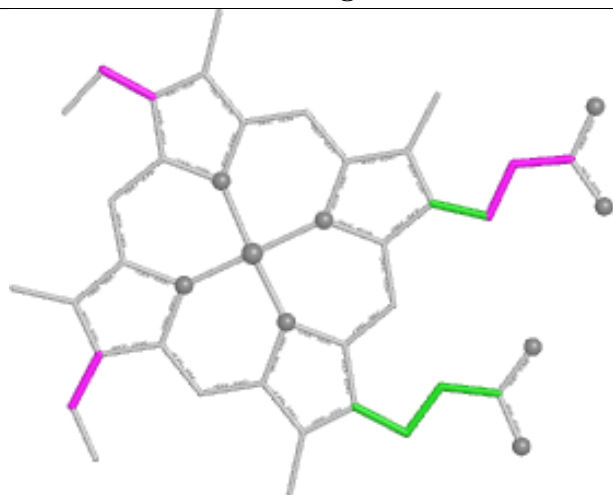
Ligand HEC L 607



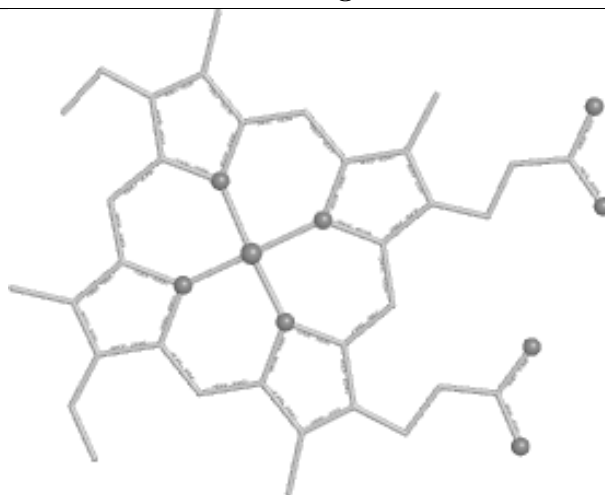
Bond lengths



Bond angles

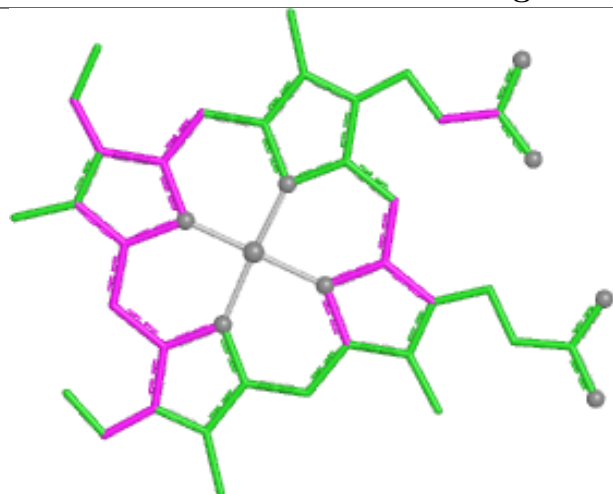


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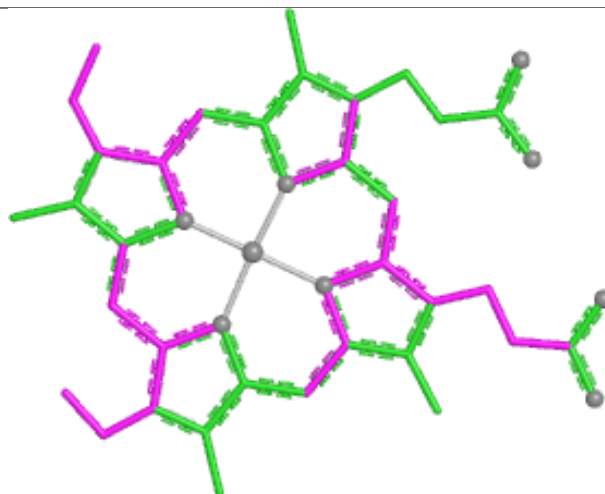


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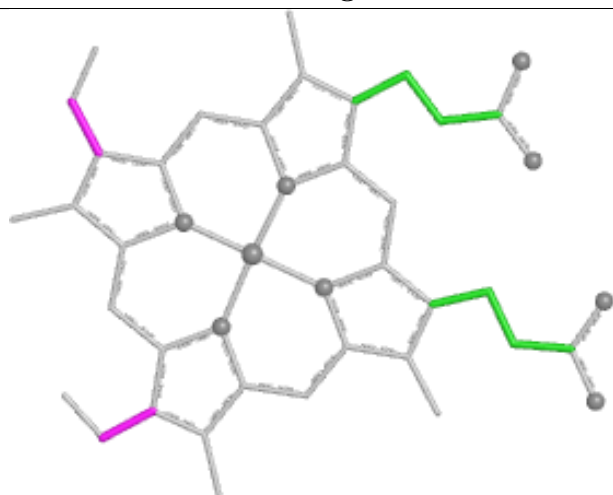
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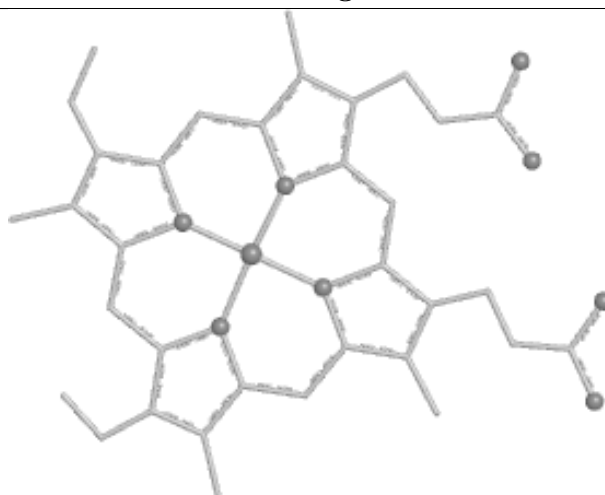
Bond lengths



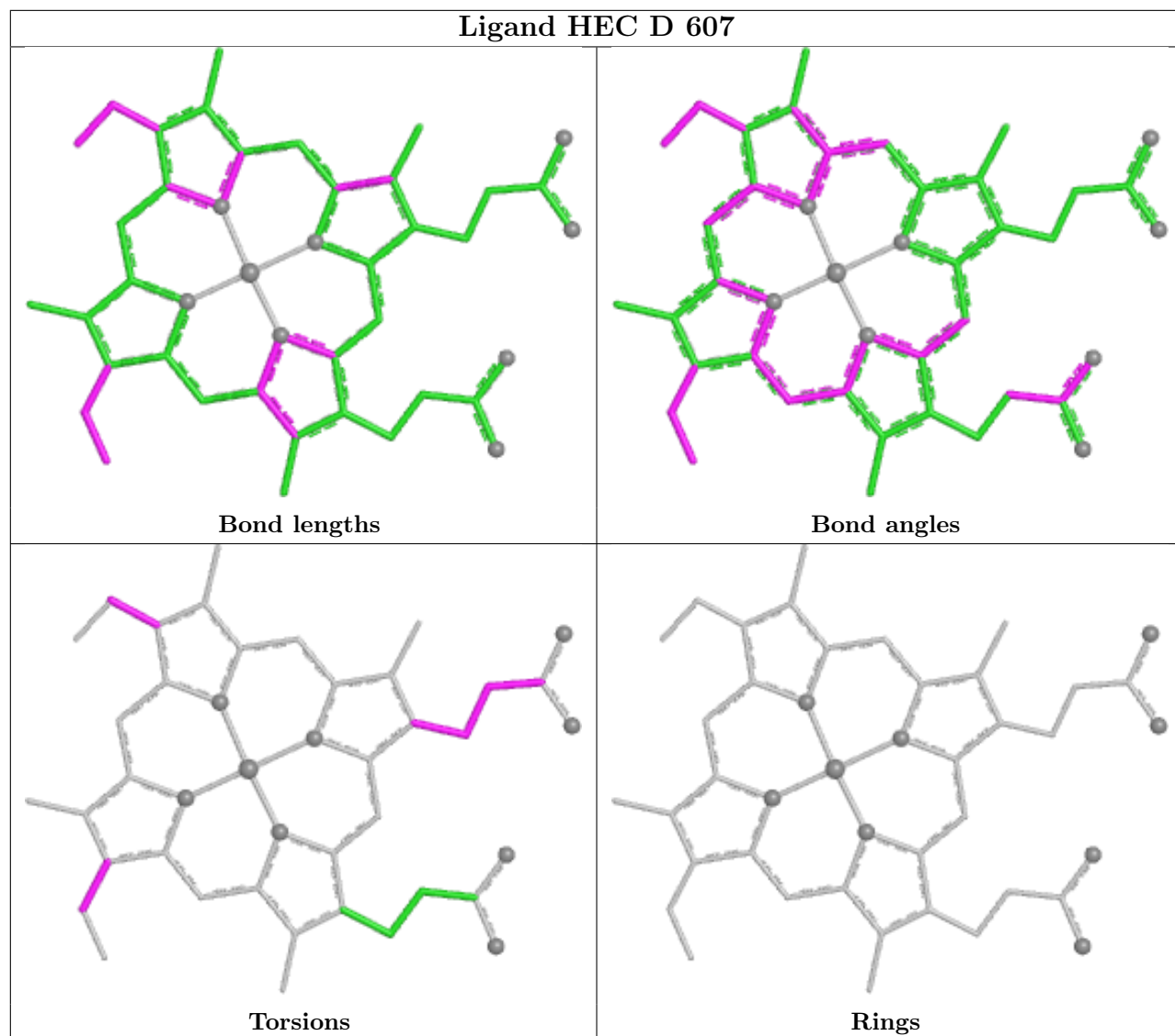
Bond angles



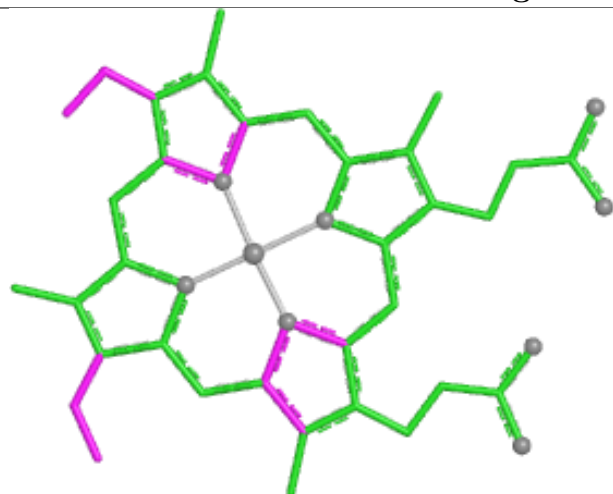
Torsions



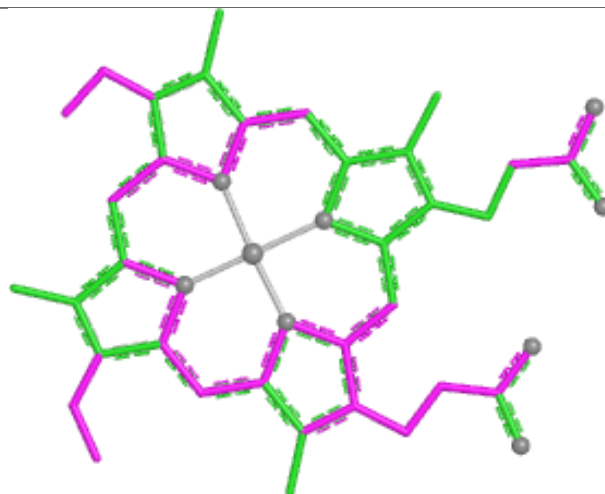
Rings



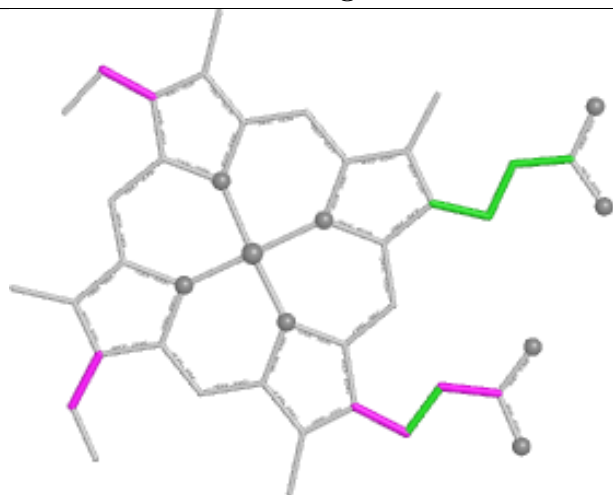
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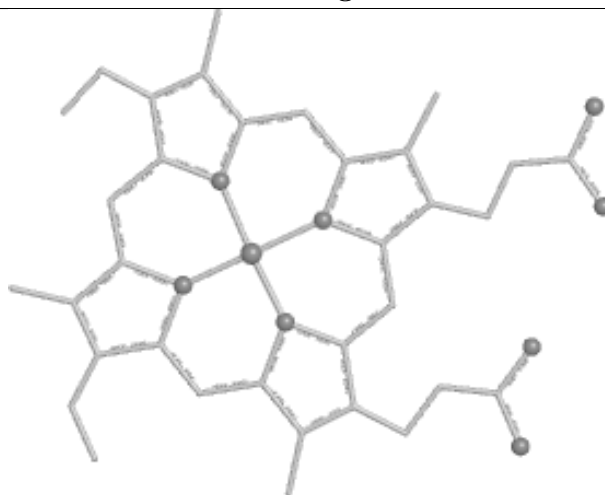
Bond lengths



Bond angles

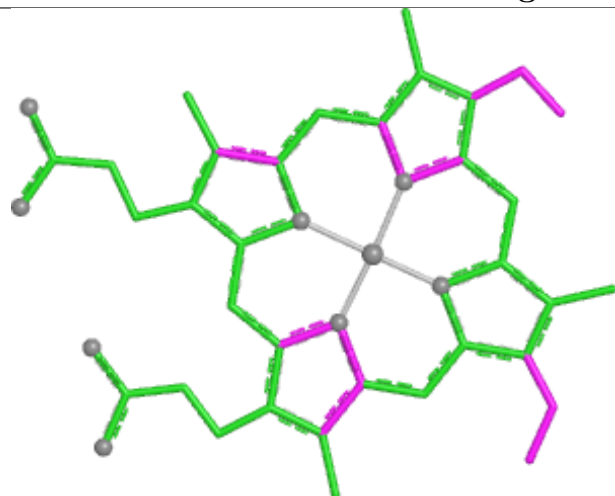


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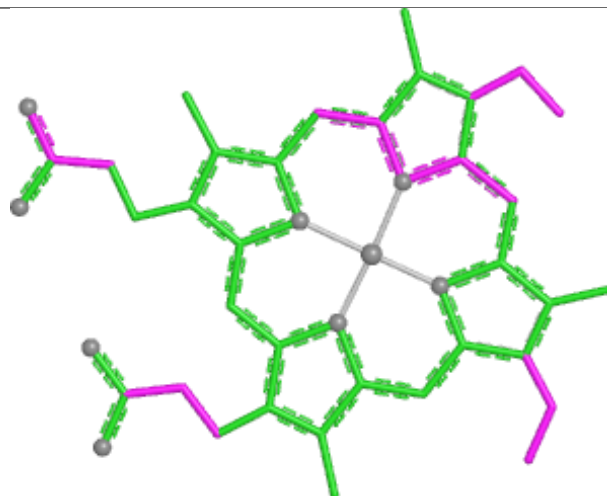


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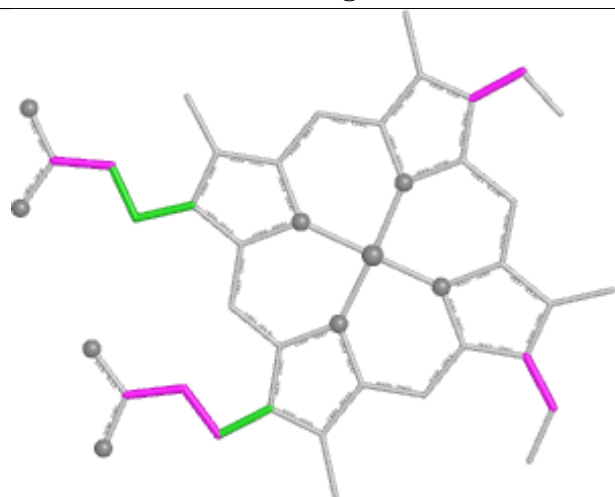
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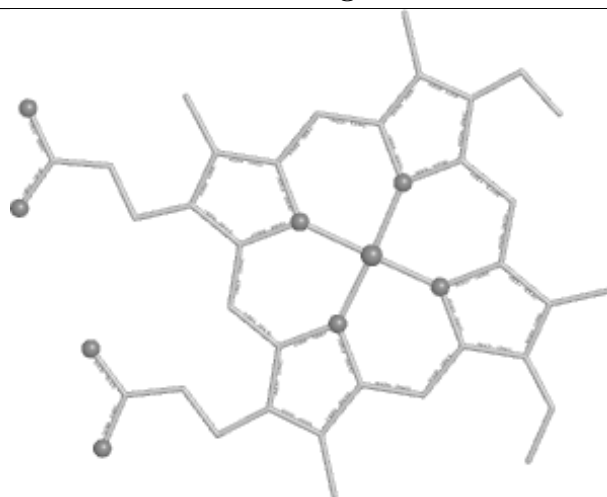
Bond lengths



Bond angles

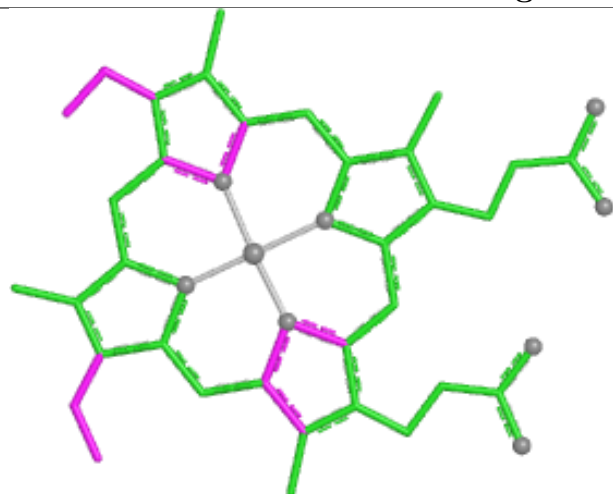


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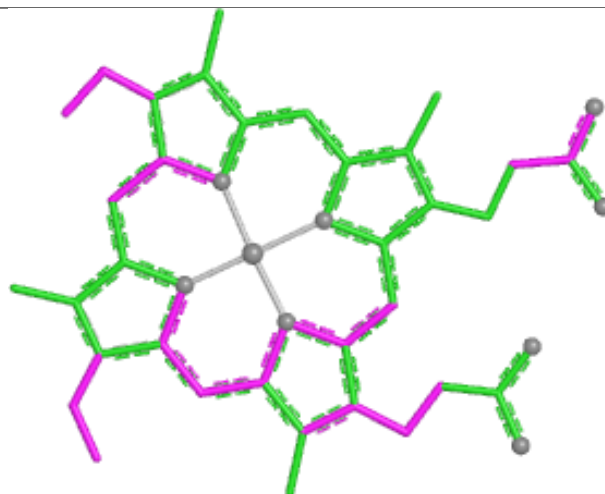


Rings

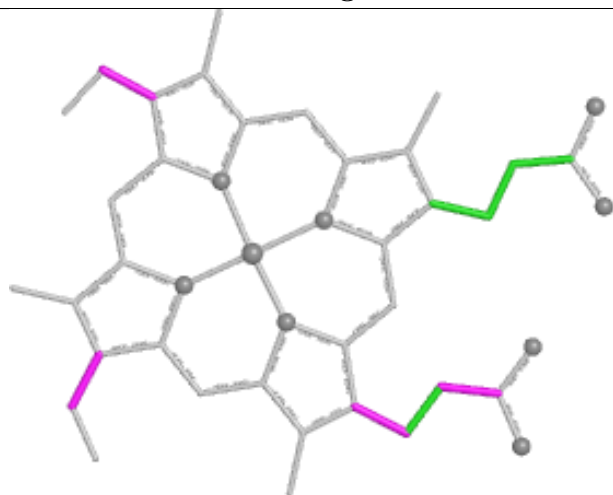
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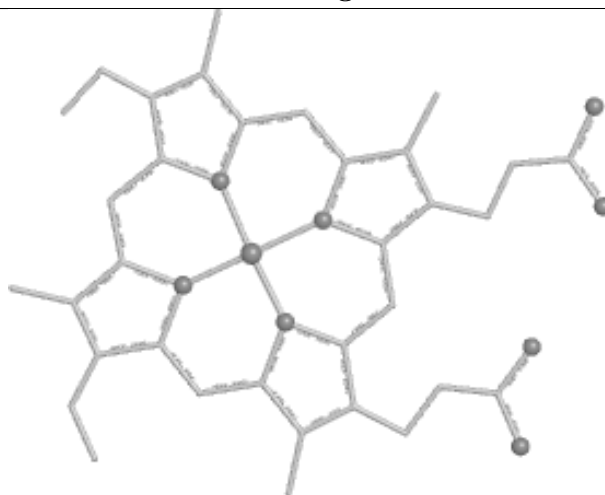
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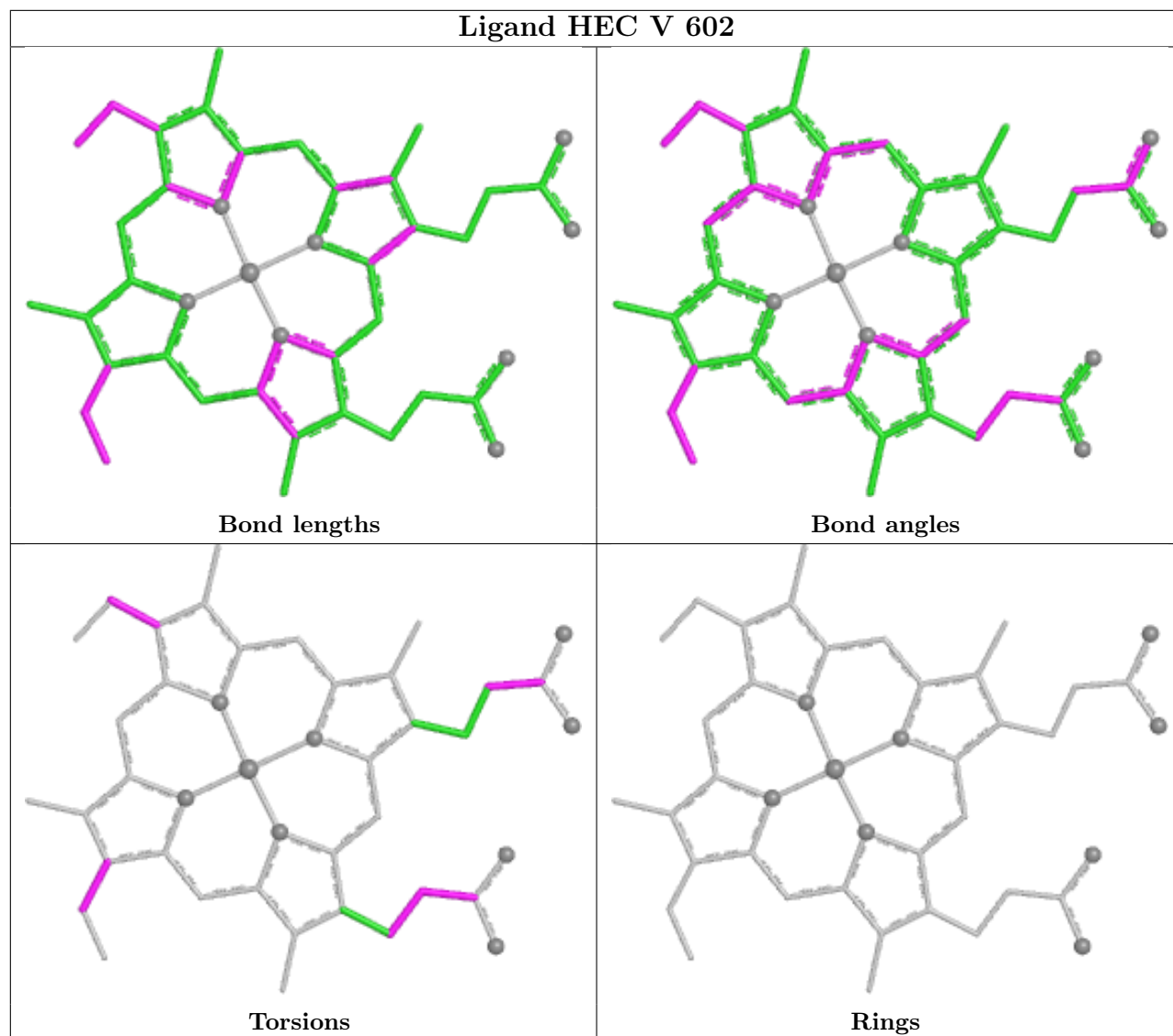
Bond angles



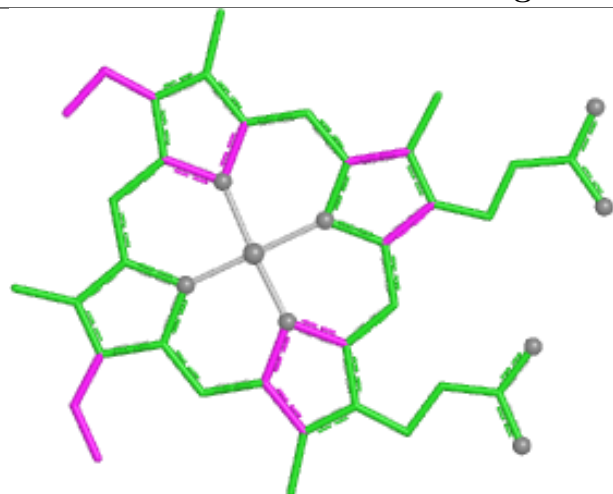
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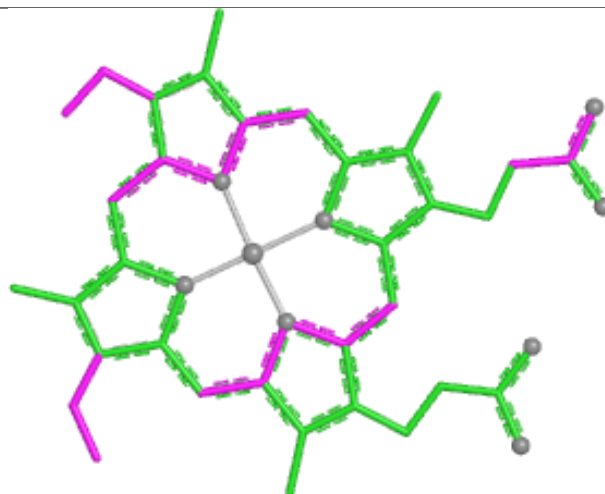
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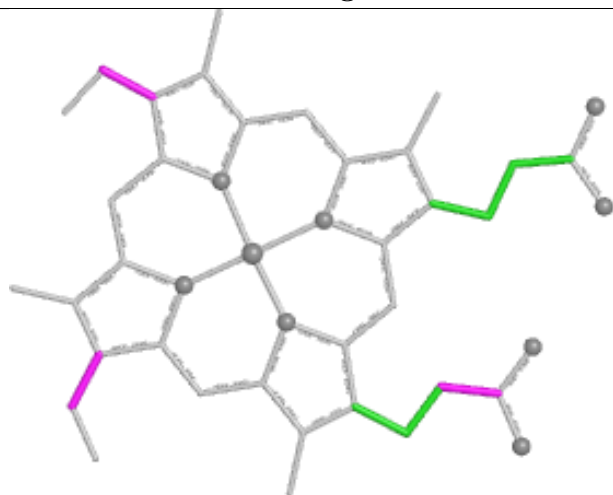
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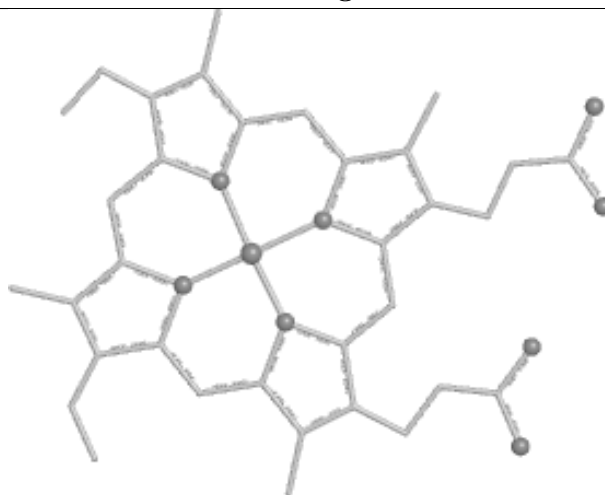
Bond lengths



Bond angles

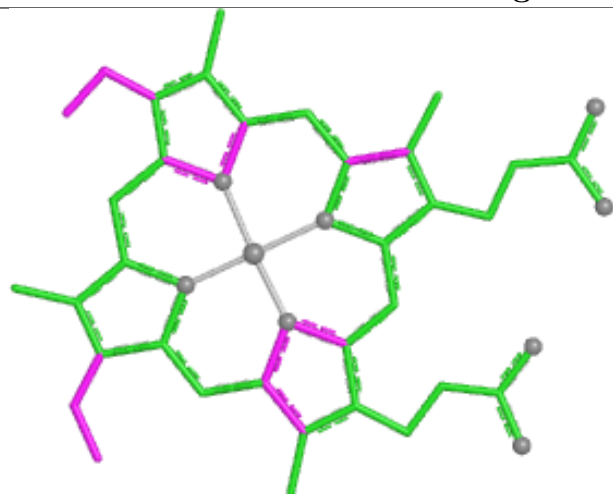


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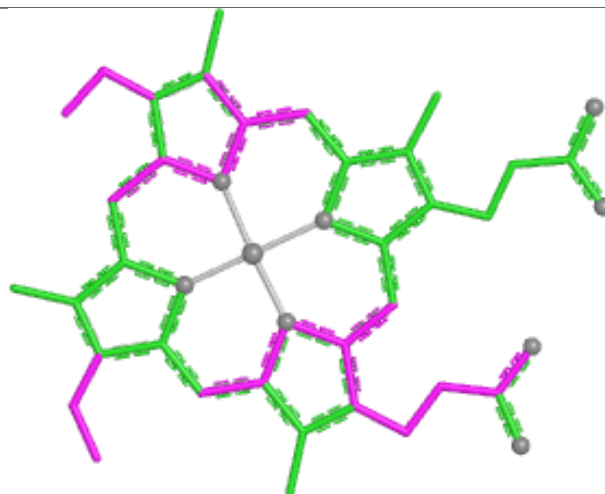


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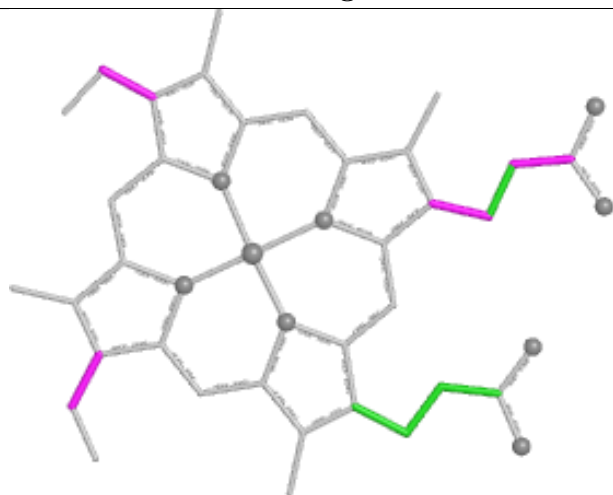
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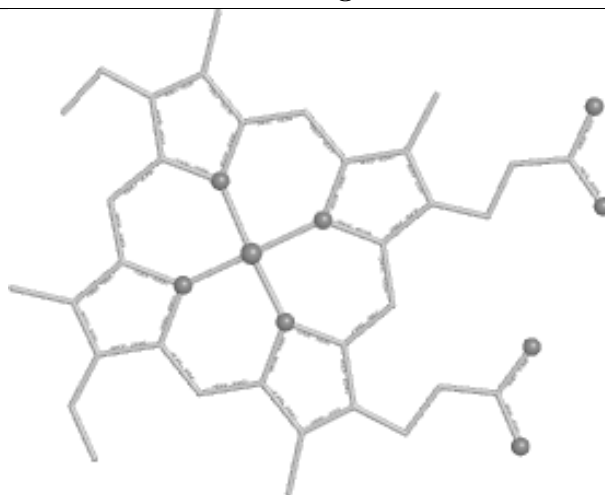
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Bond angles

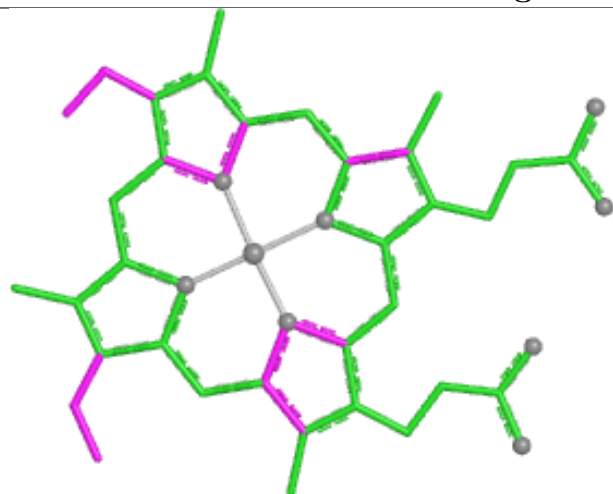


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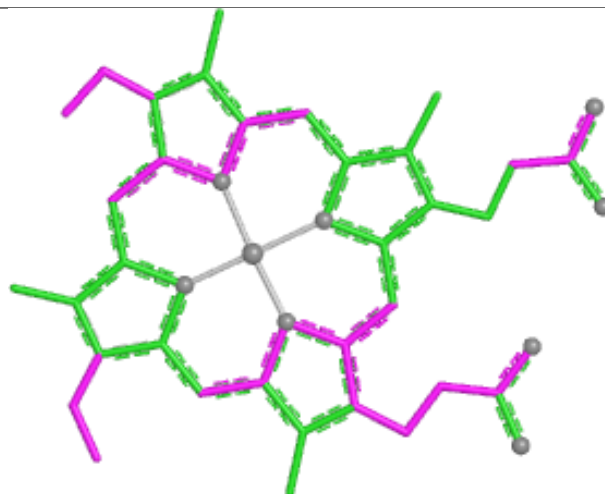


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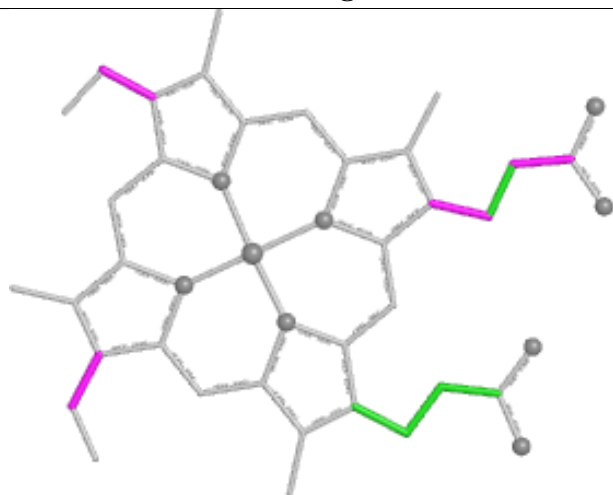
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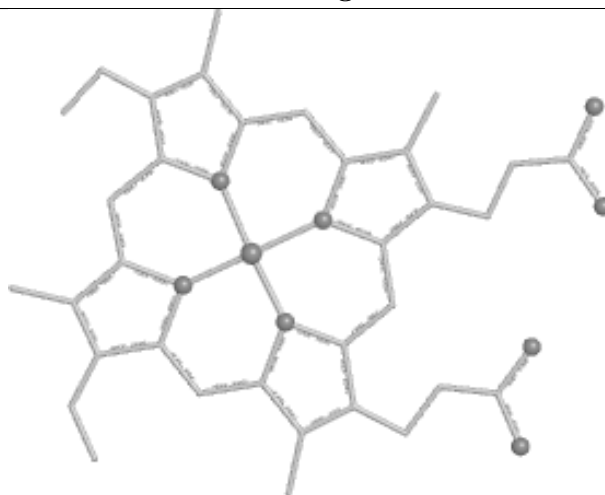
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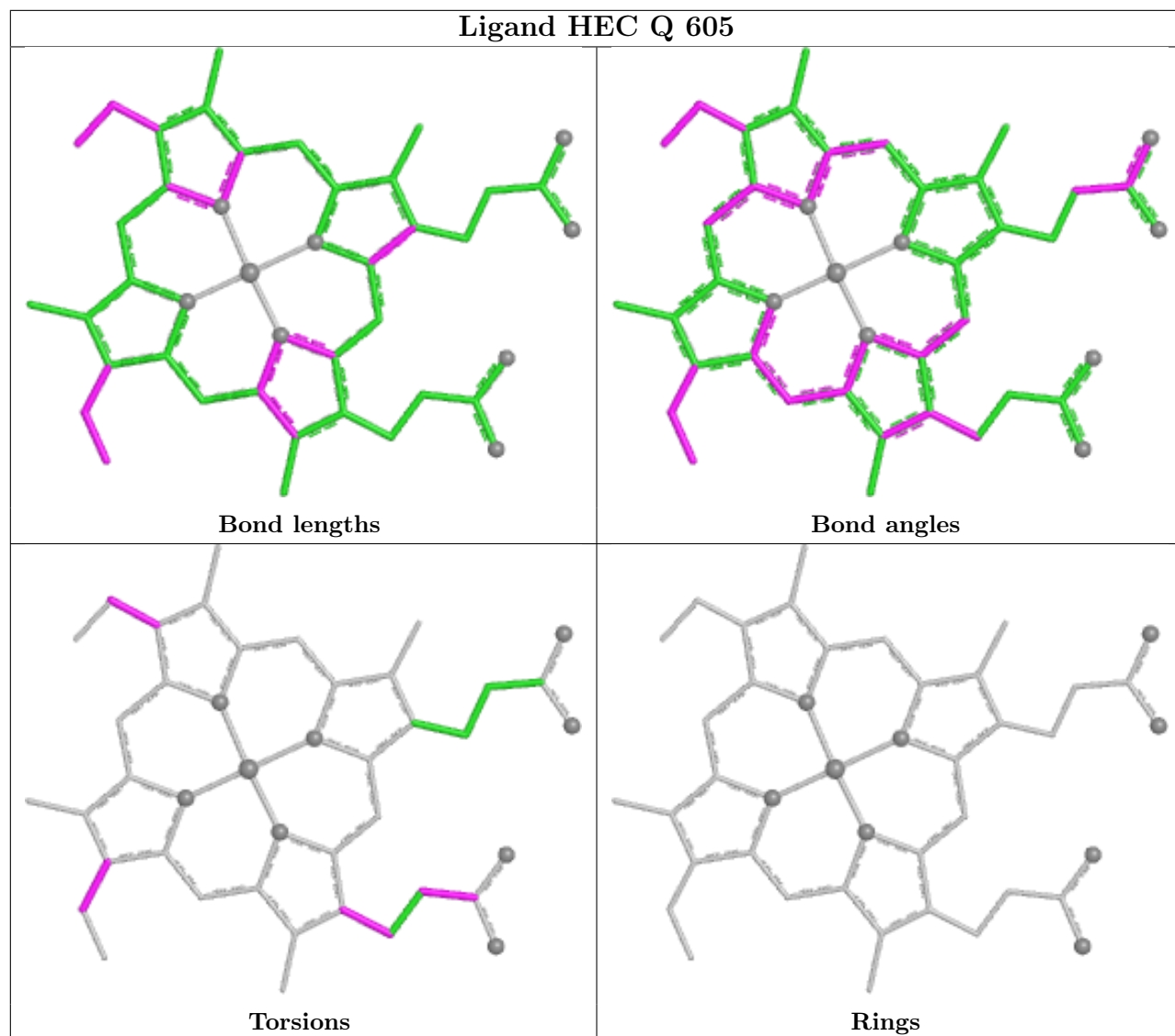
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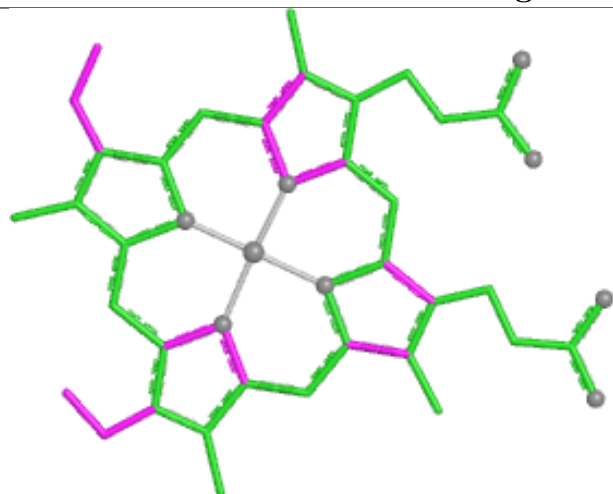
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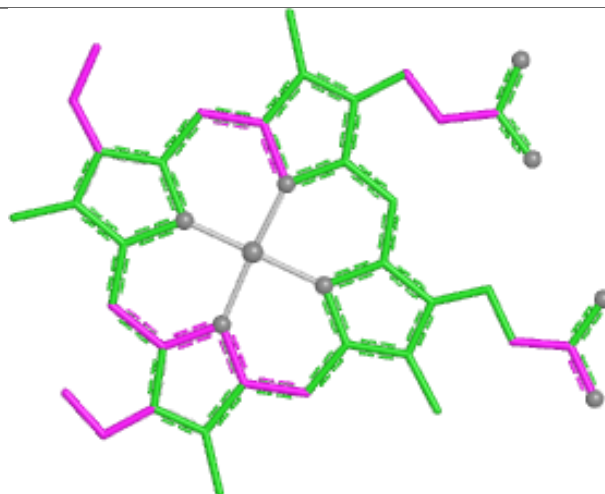
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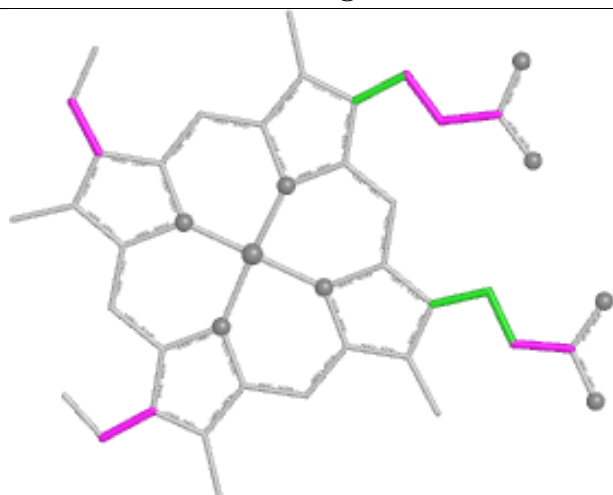
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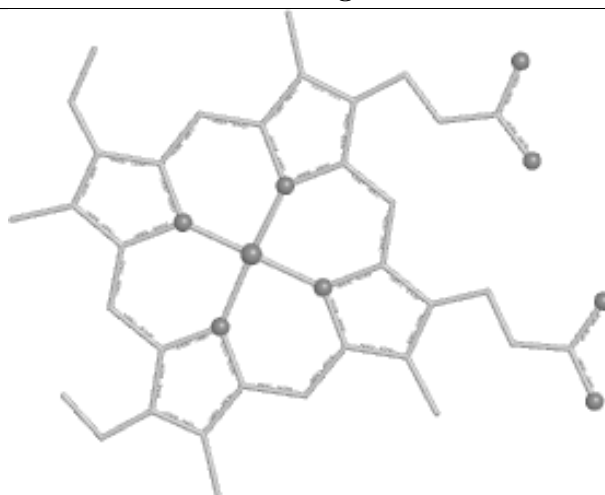
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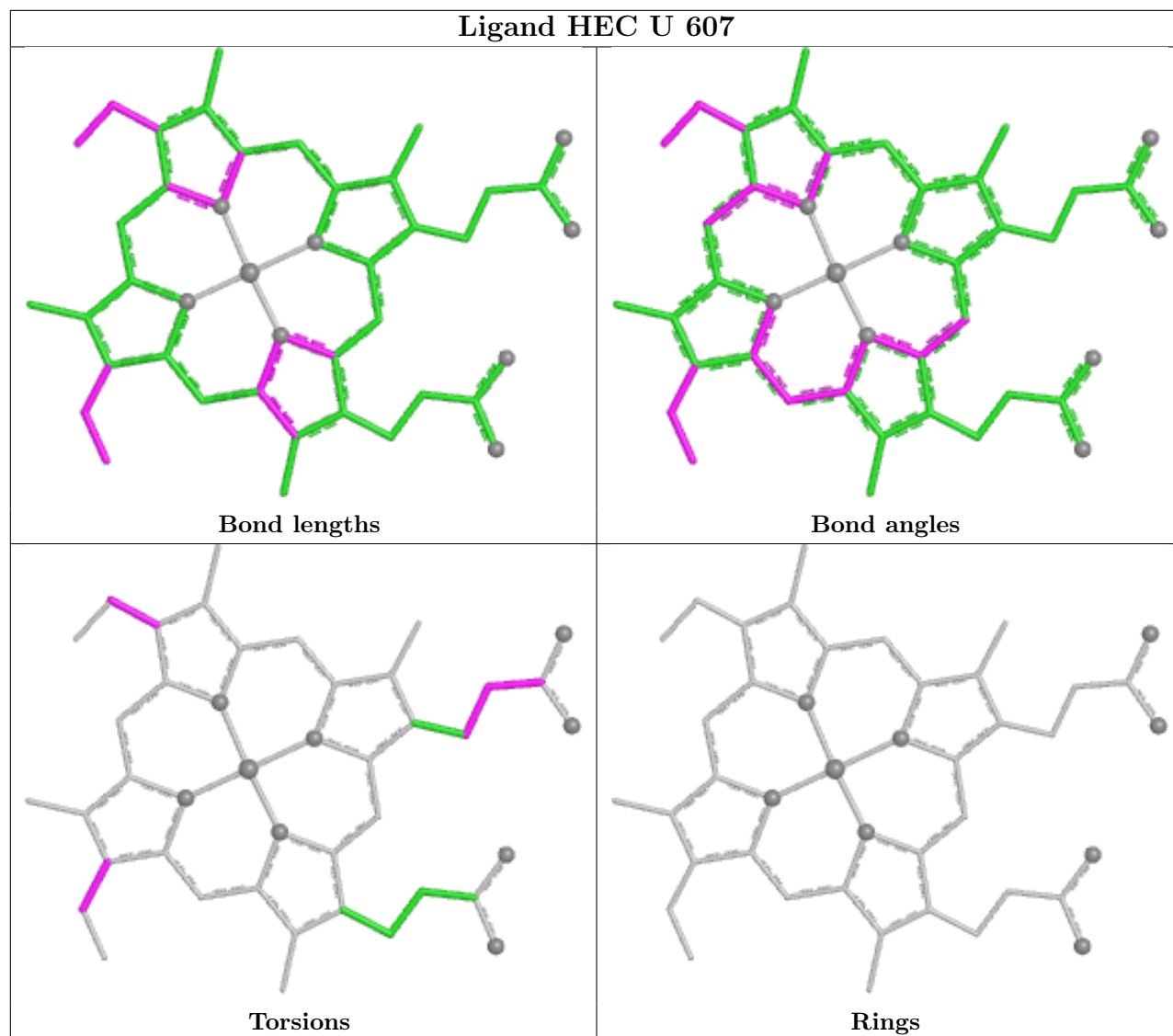
Bond angles



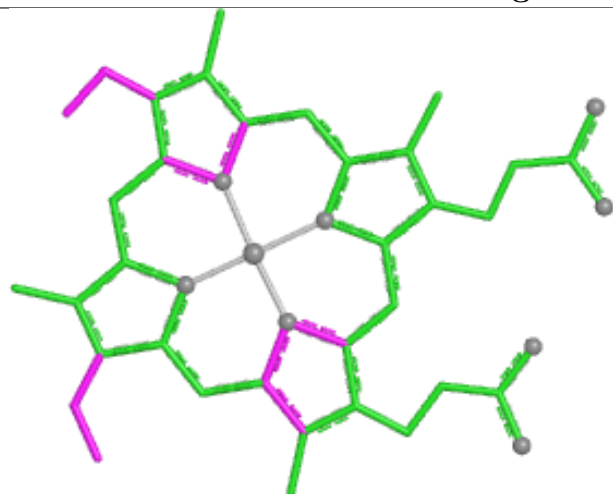
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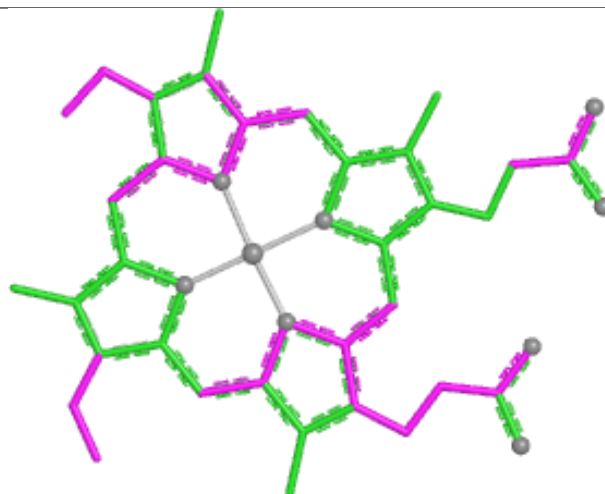
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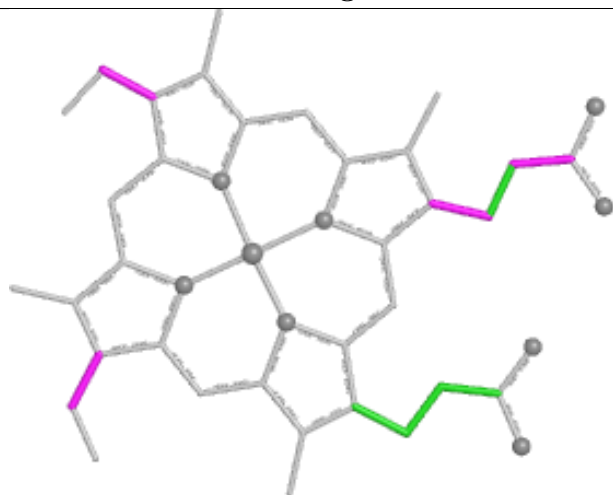
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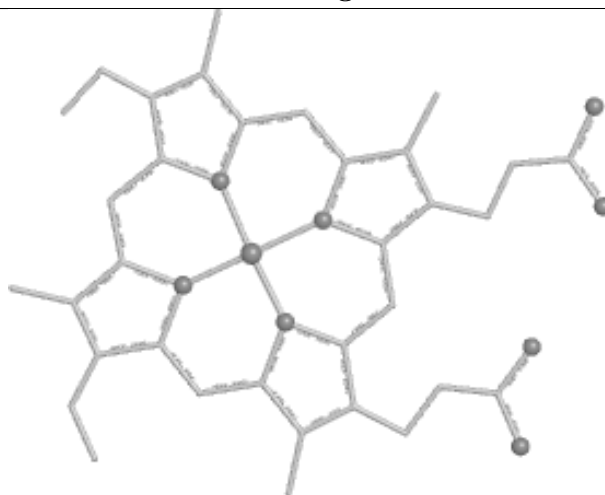
Bond lengths



Bond angles

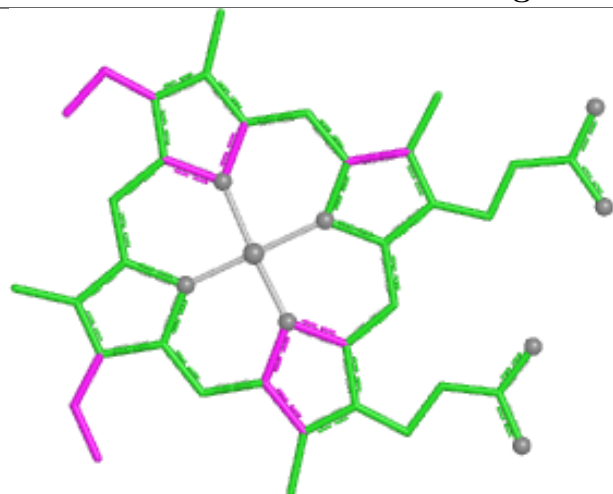


Torsions

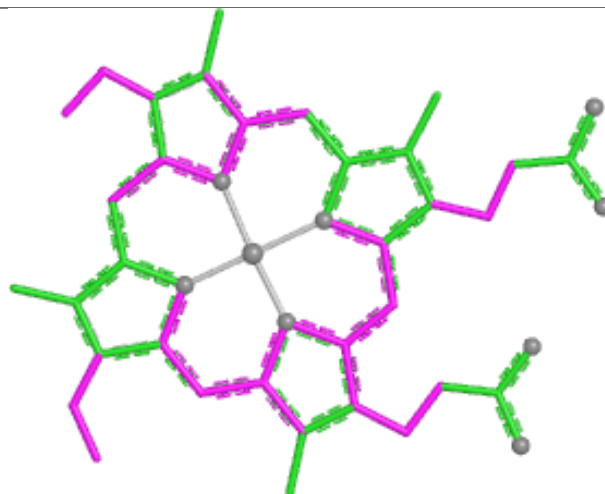


Rings

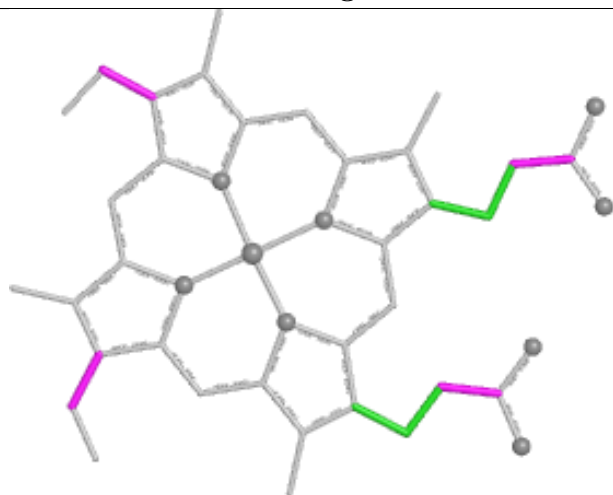
Ligand HEC B 604



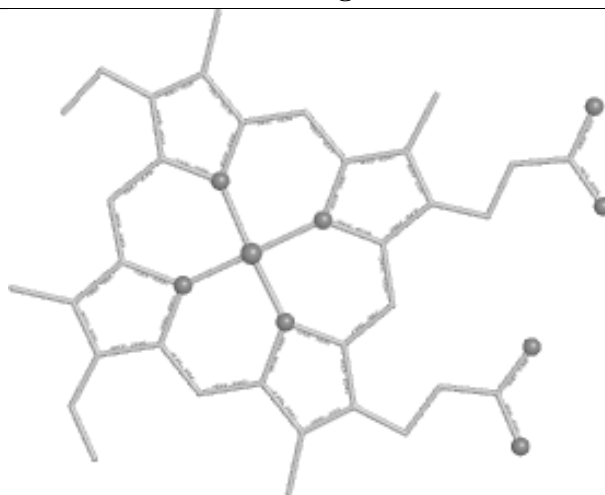
Bond lengths



Bond angles

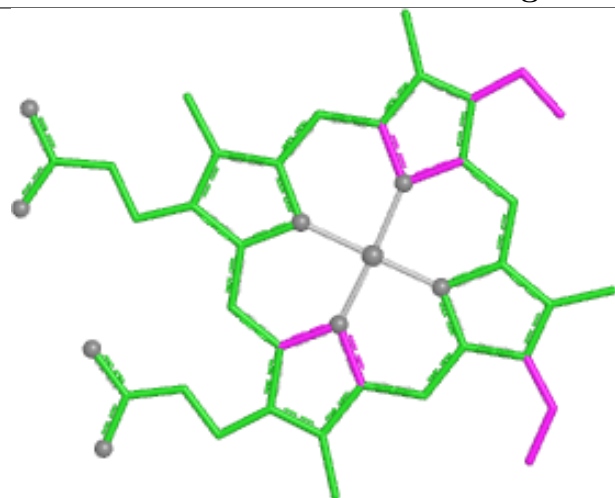


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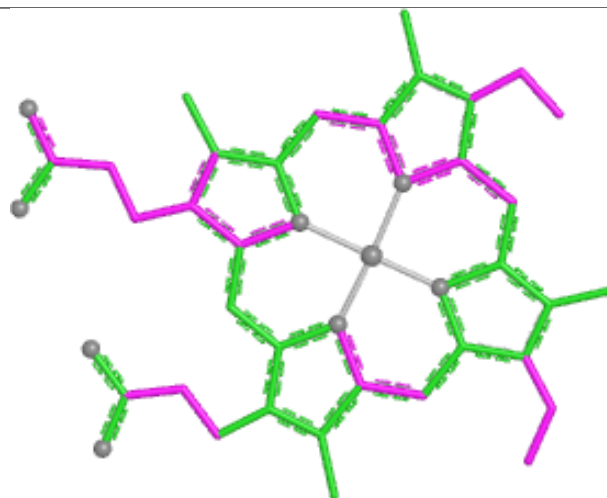


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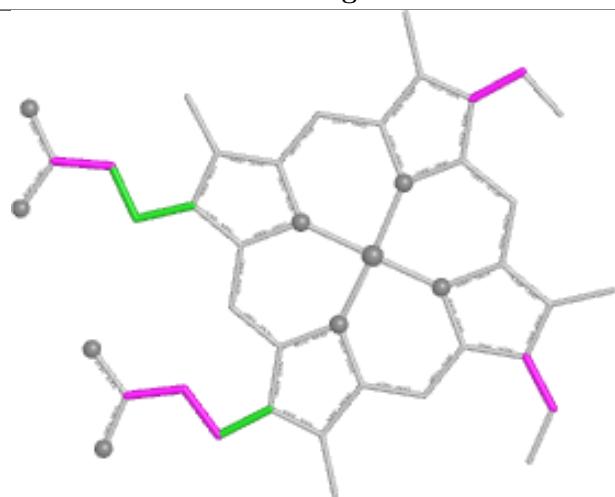
Ligand HEC I 602



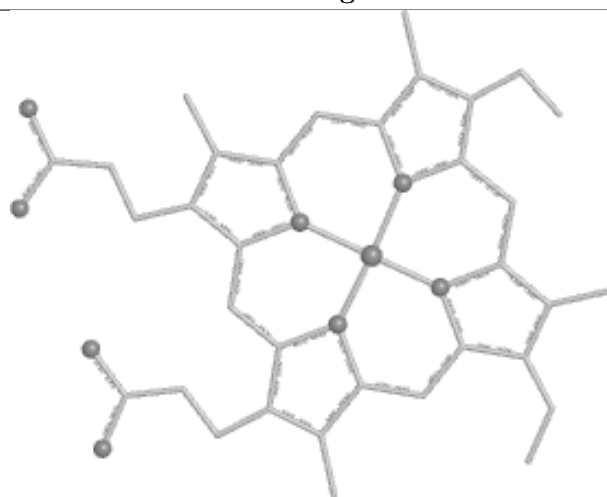
Bond lengths



Bond angles

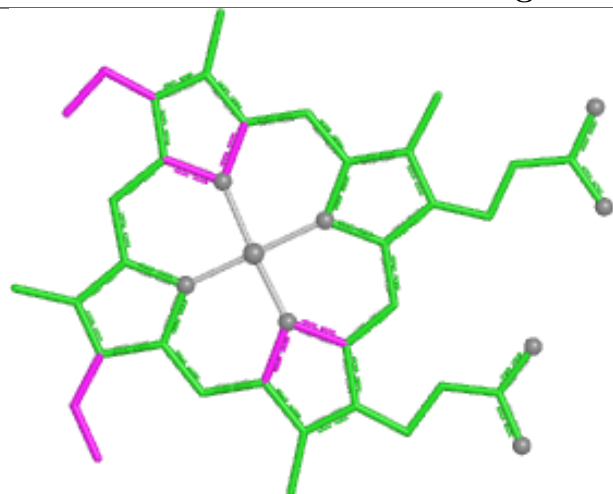


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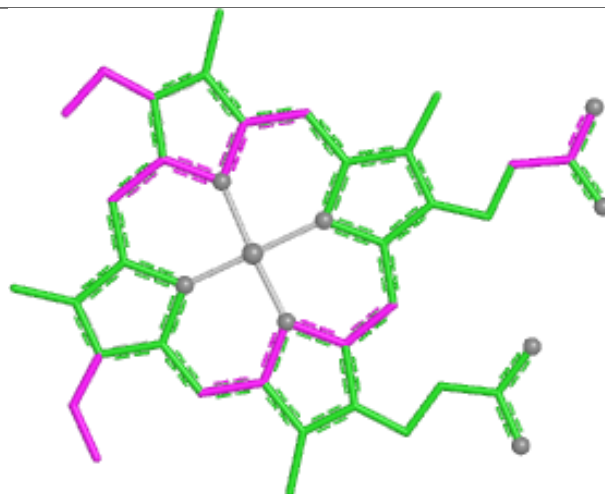


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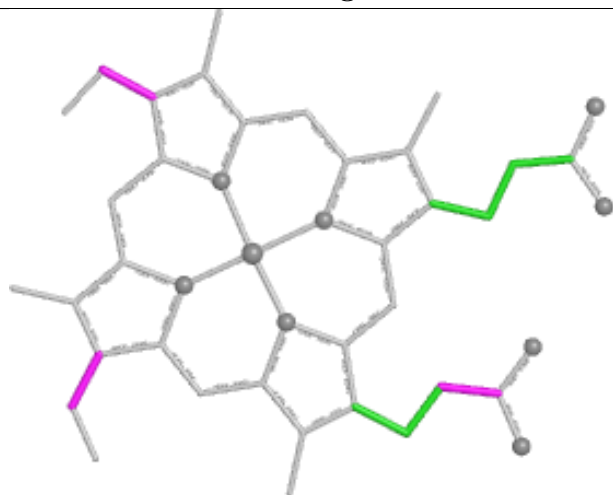
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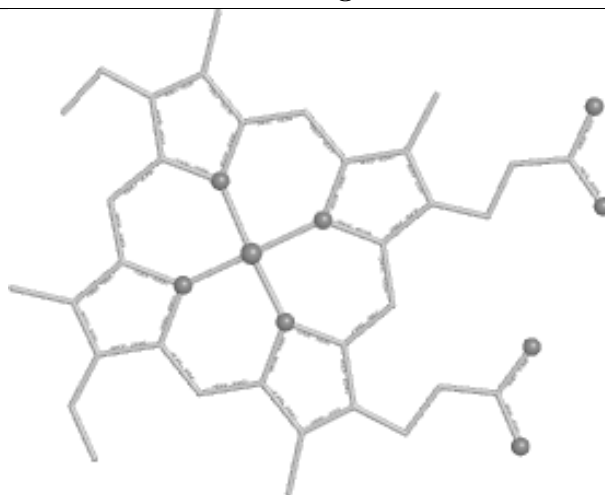
Bond lengths



Bond angles

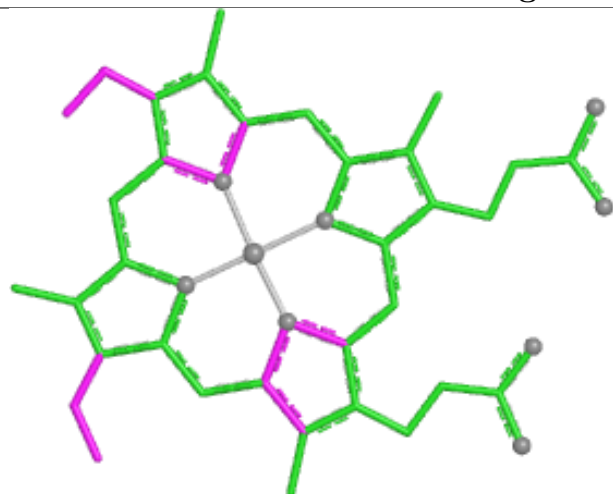


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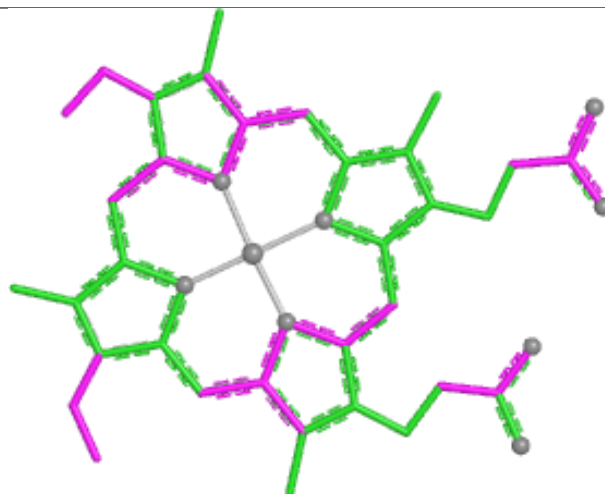


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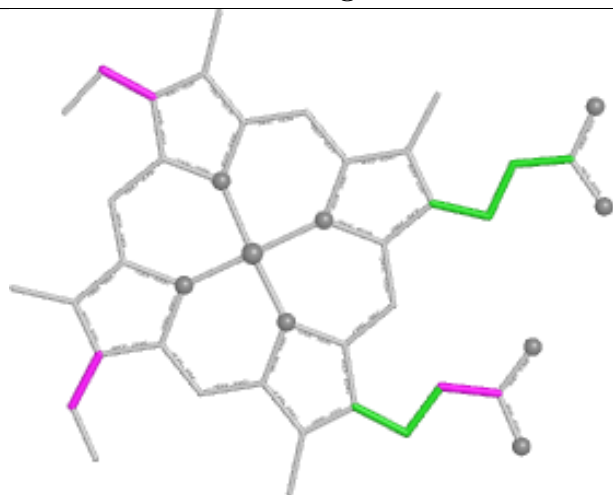
Ligand HEC I 600



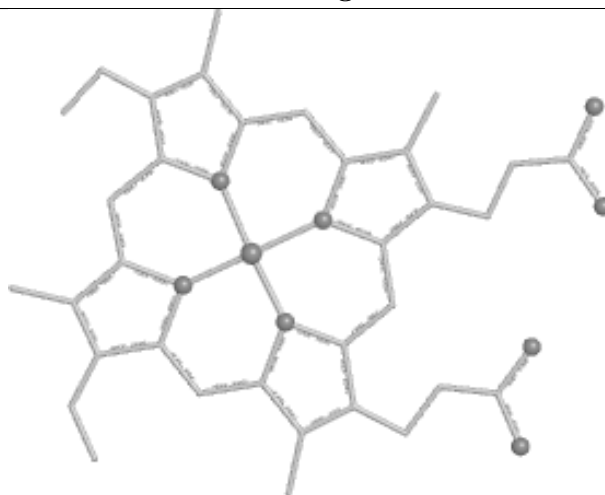
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Bond angles

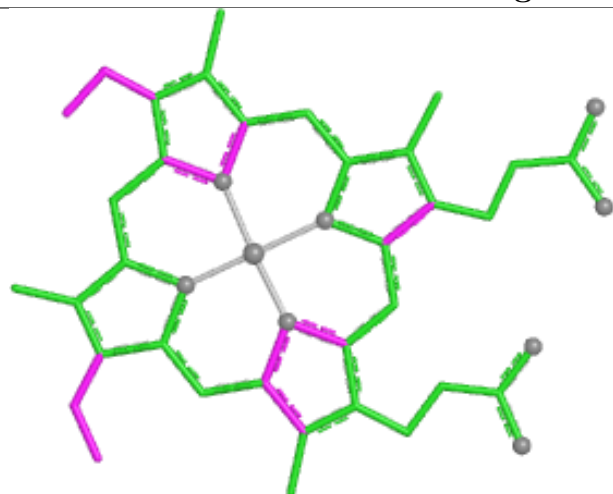


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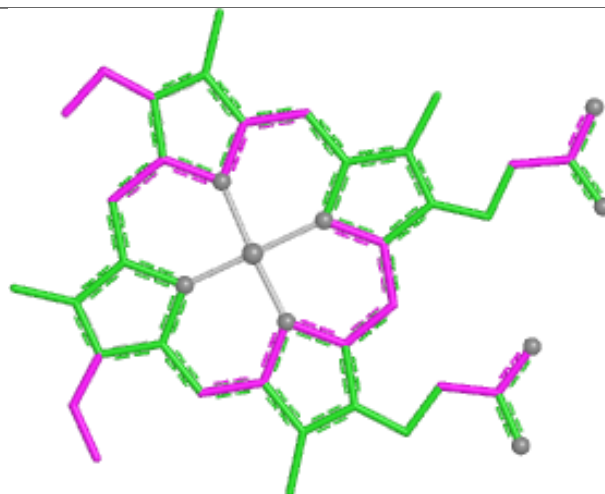


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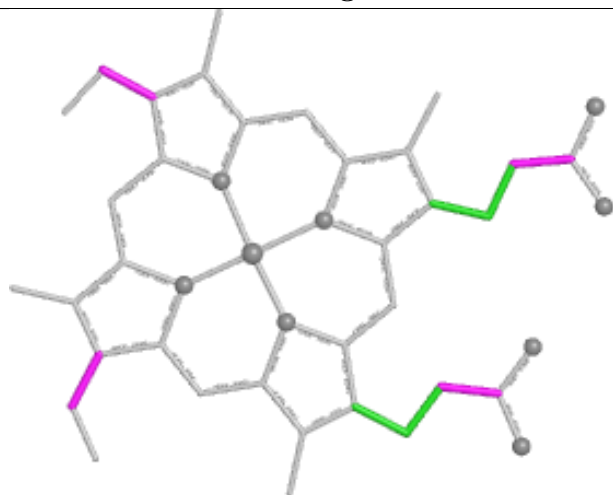
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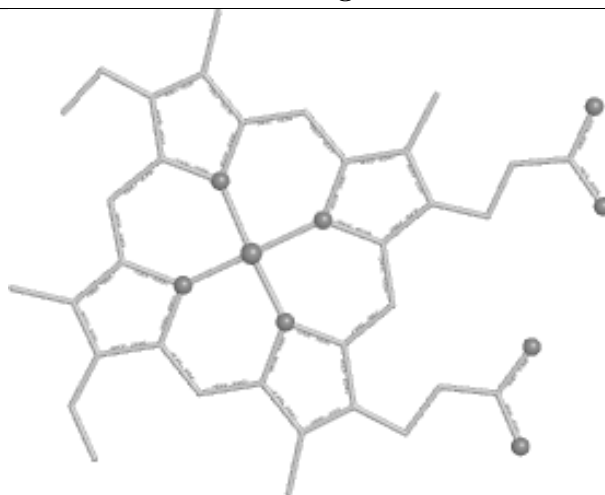
Bond lengths



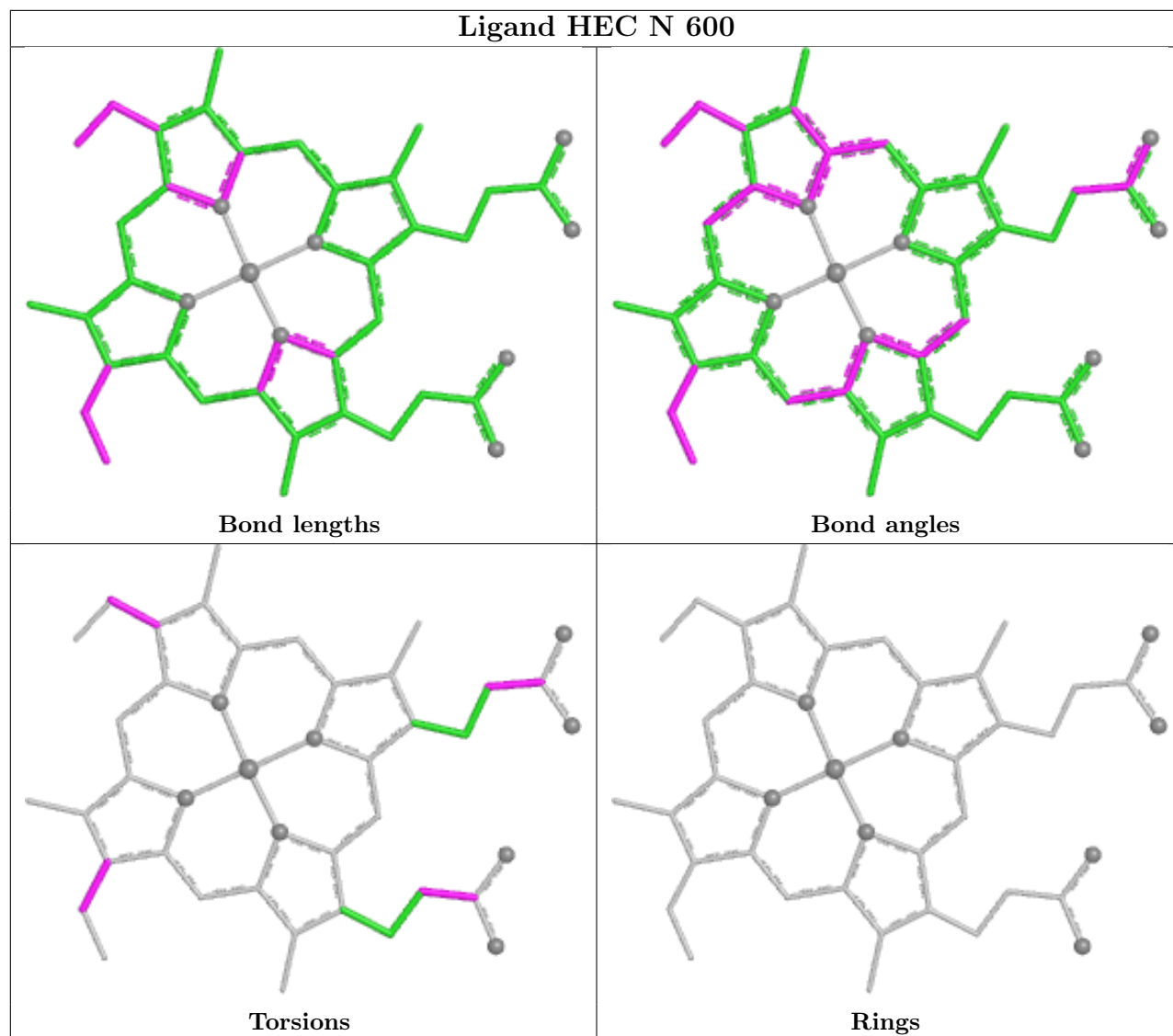
Bond angles

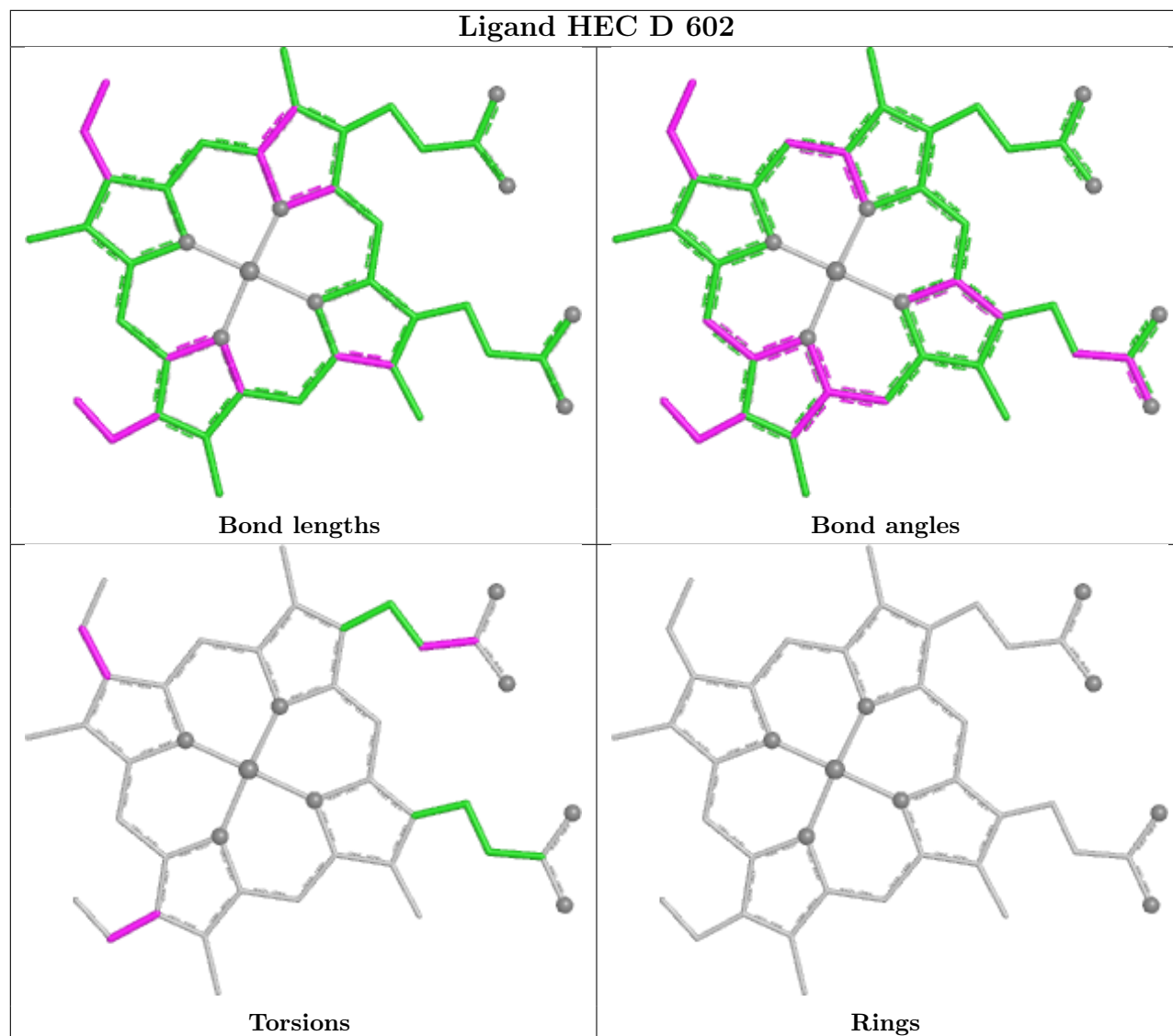


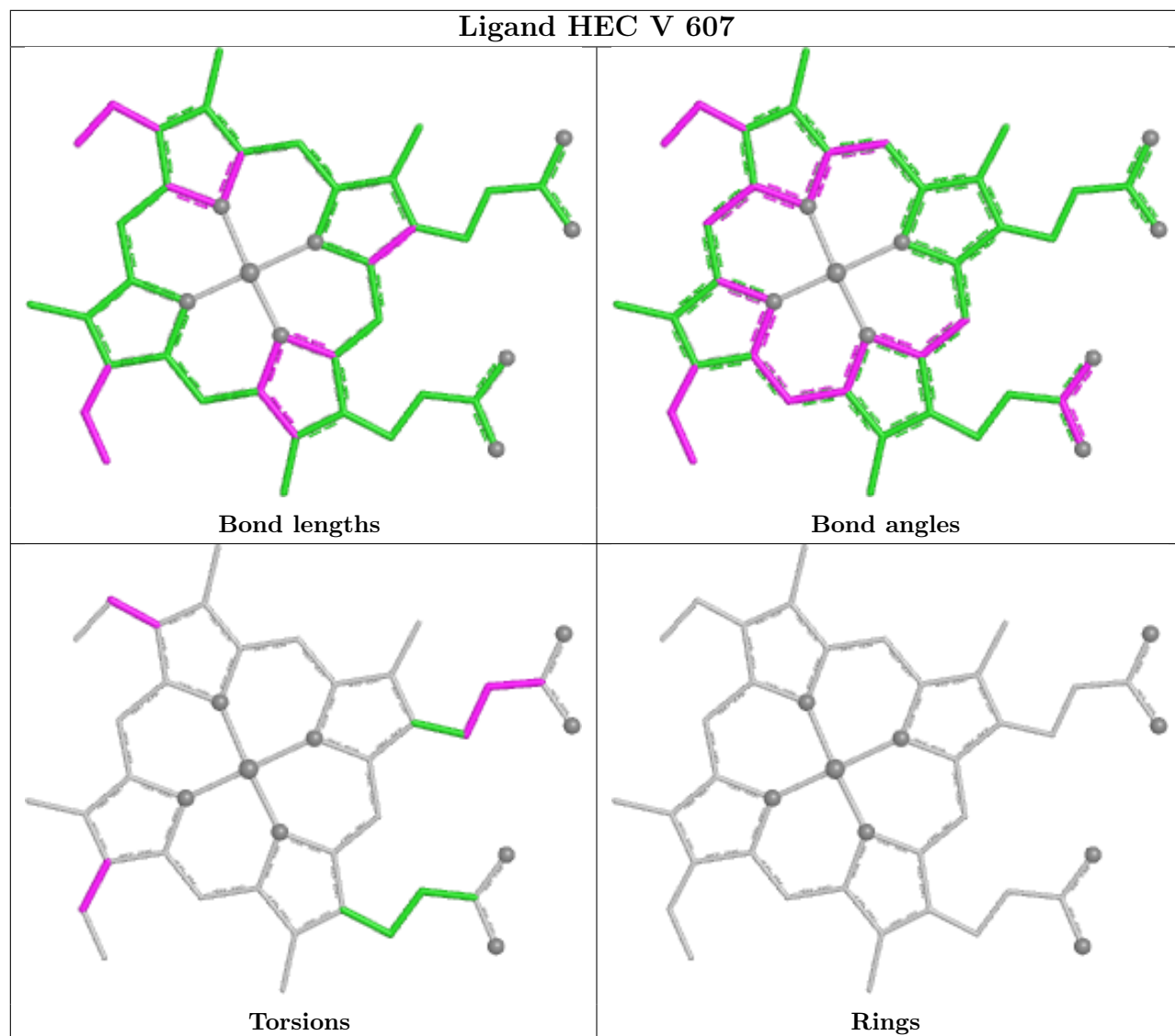
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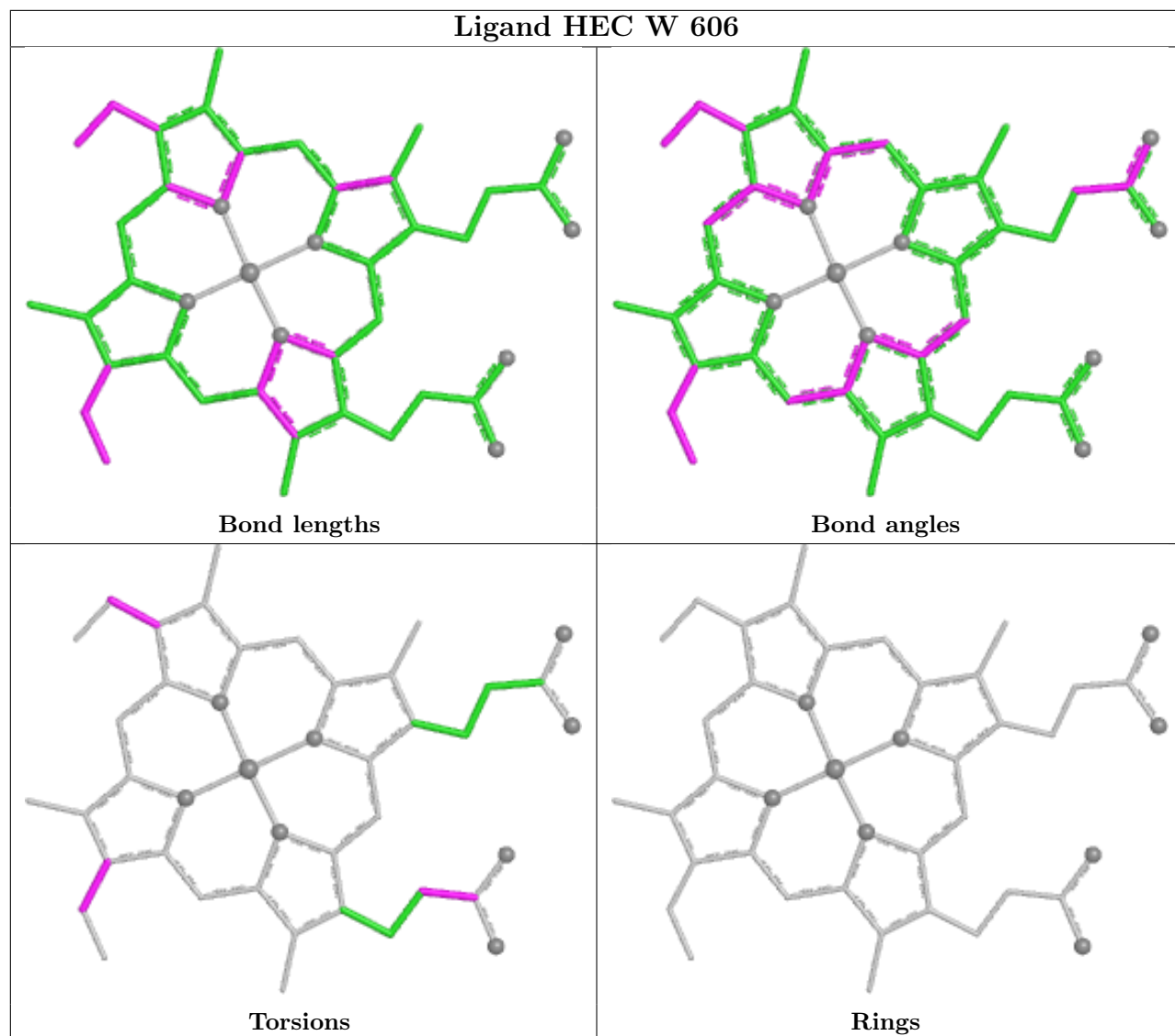


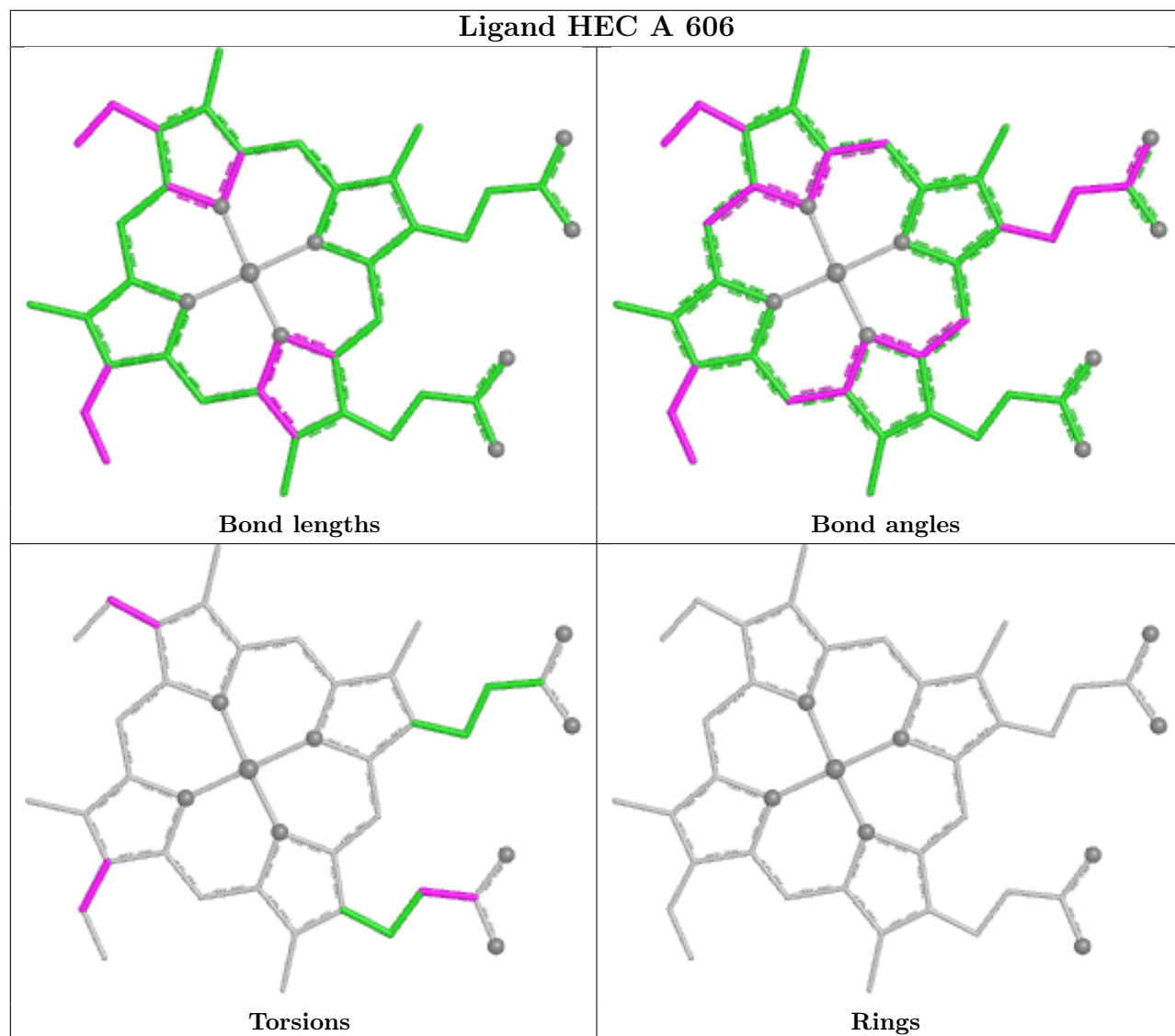
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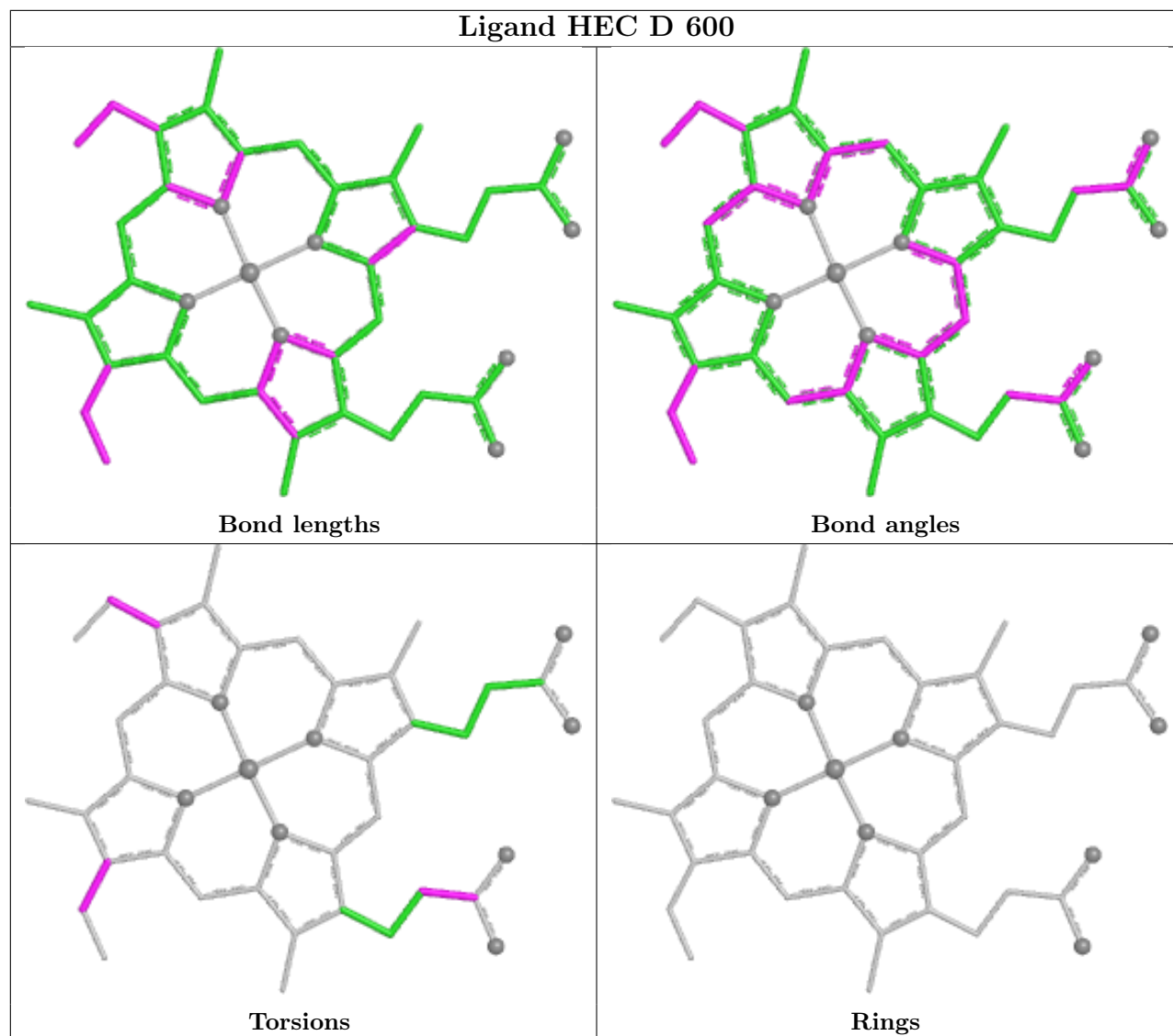




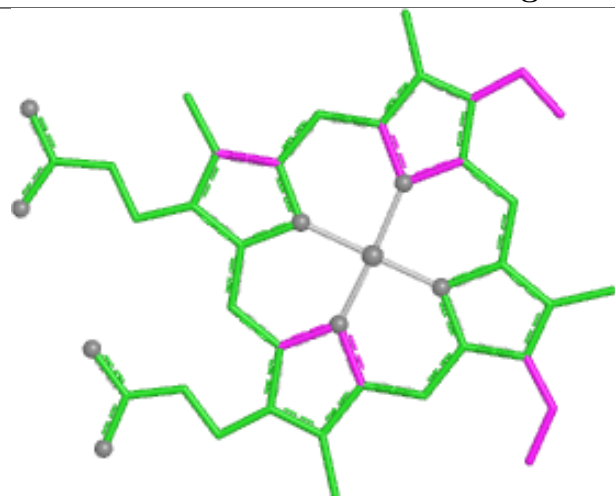




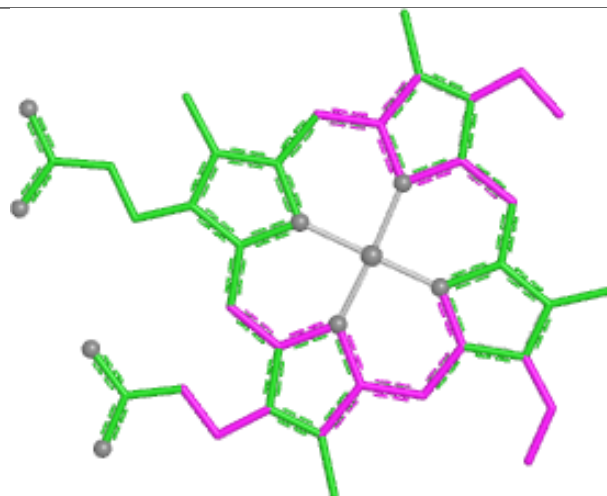




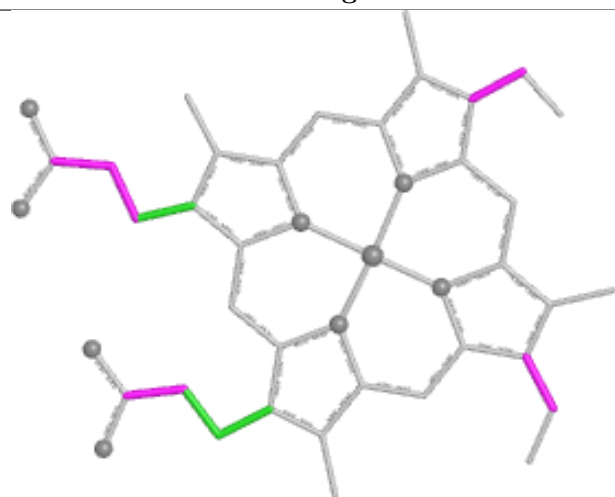
Ligand HEC I 604



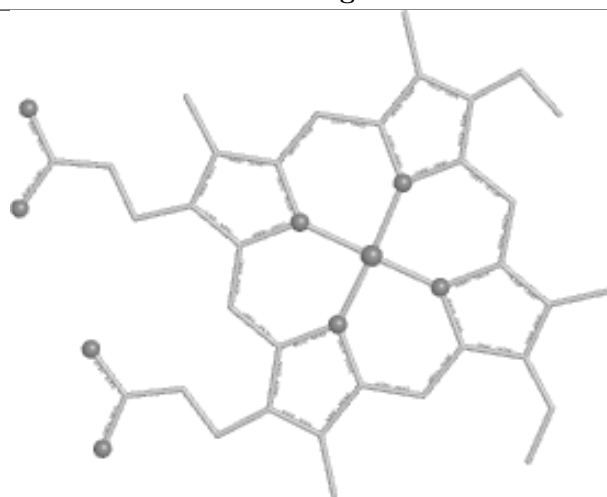
Bond lengths



Bond angles

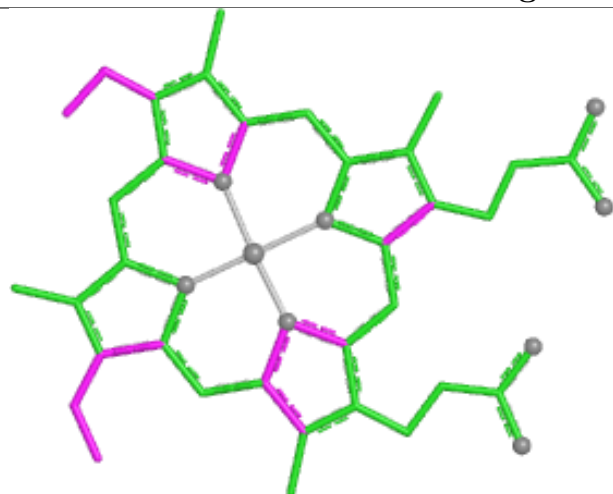


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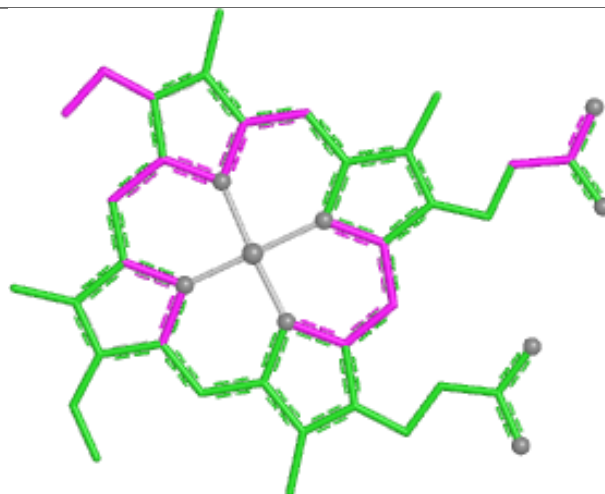


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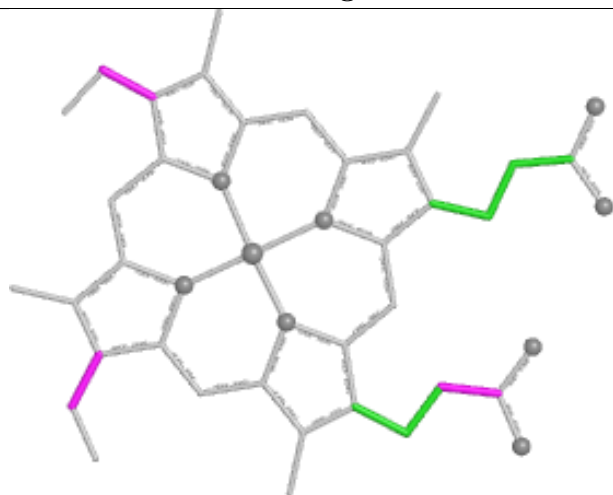
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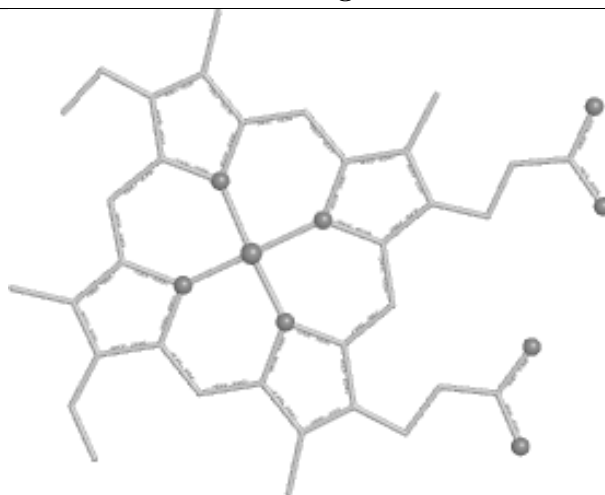
Bond lengths



Bond angles

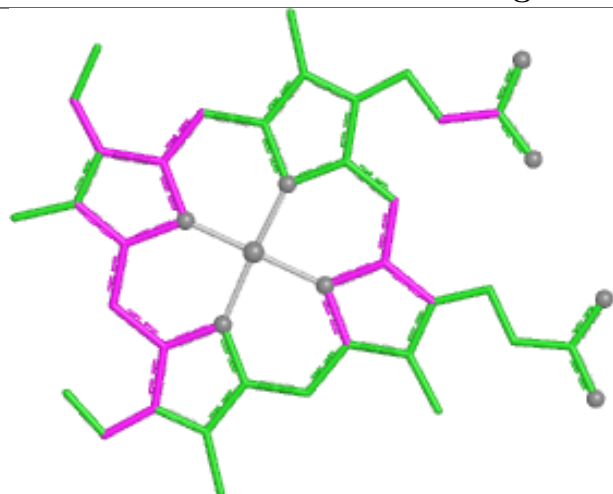


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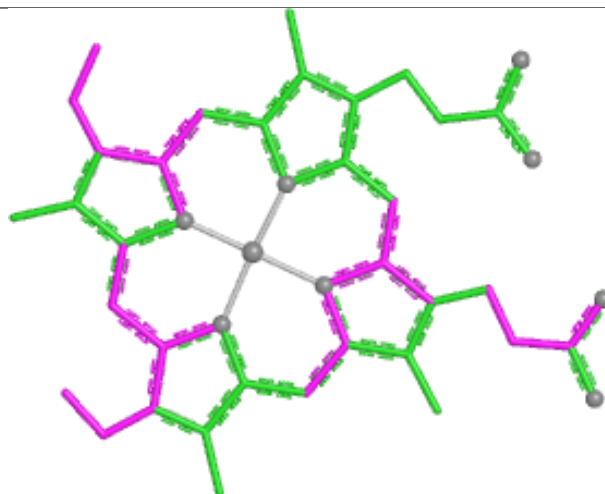


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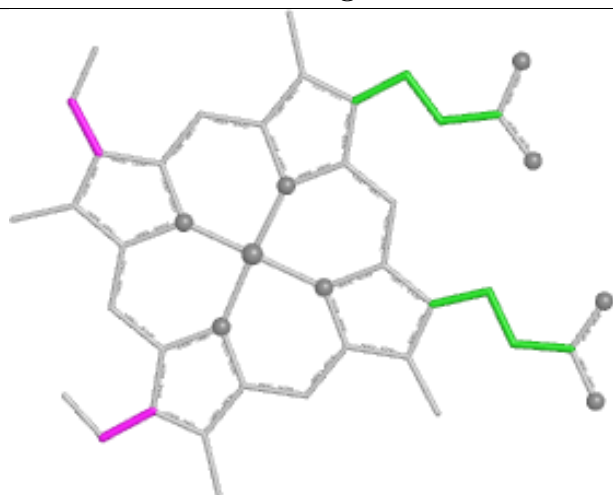
Ligand HEC T 603



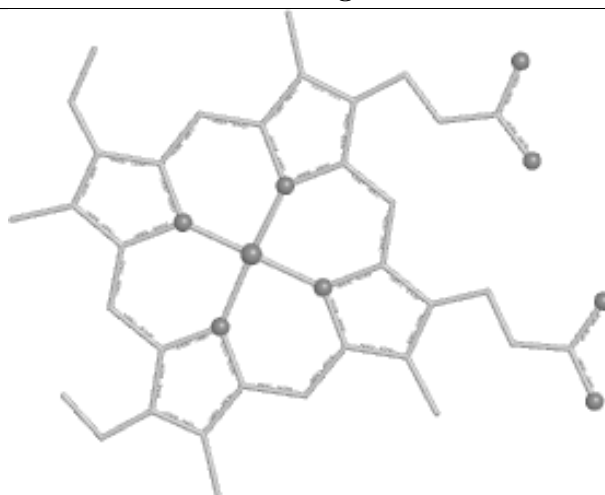
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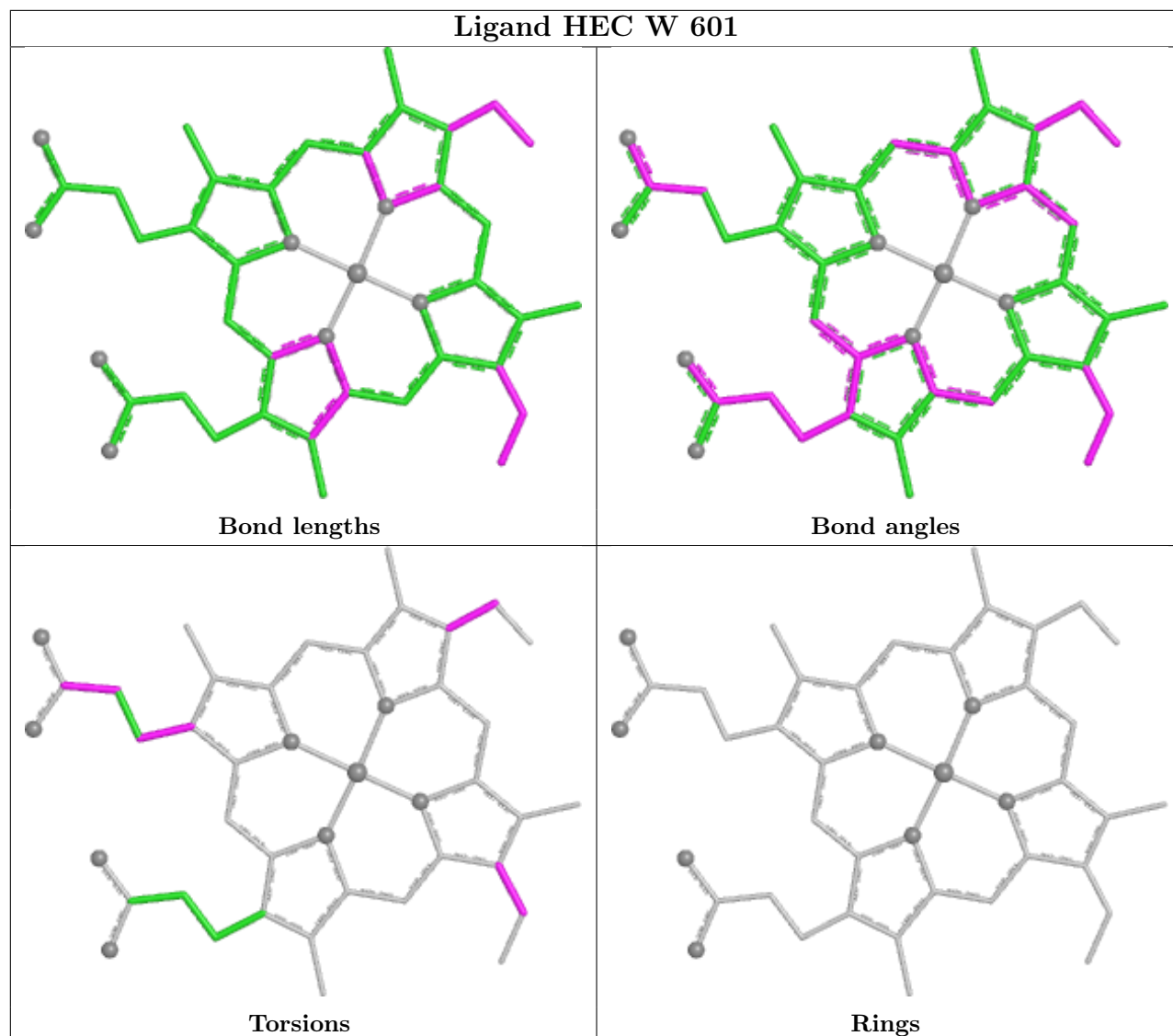
Bond angles

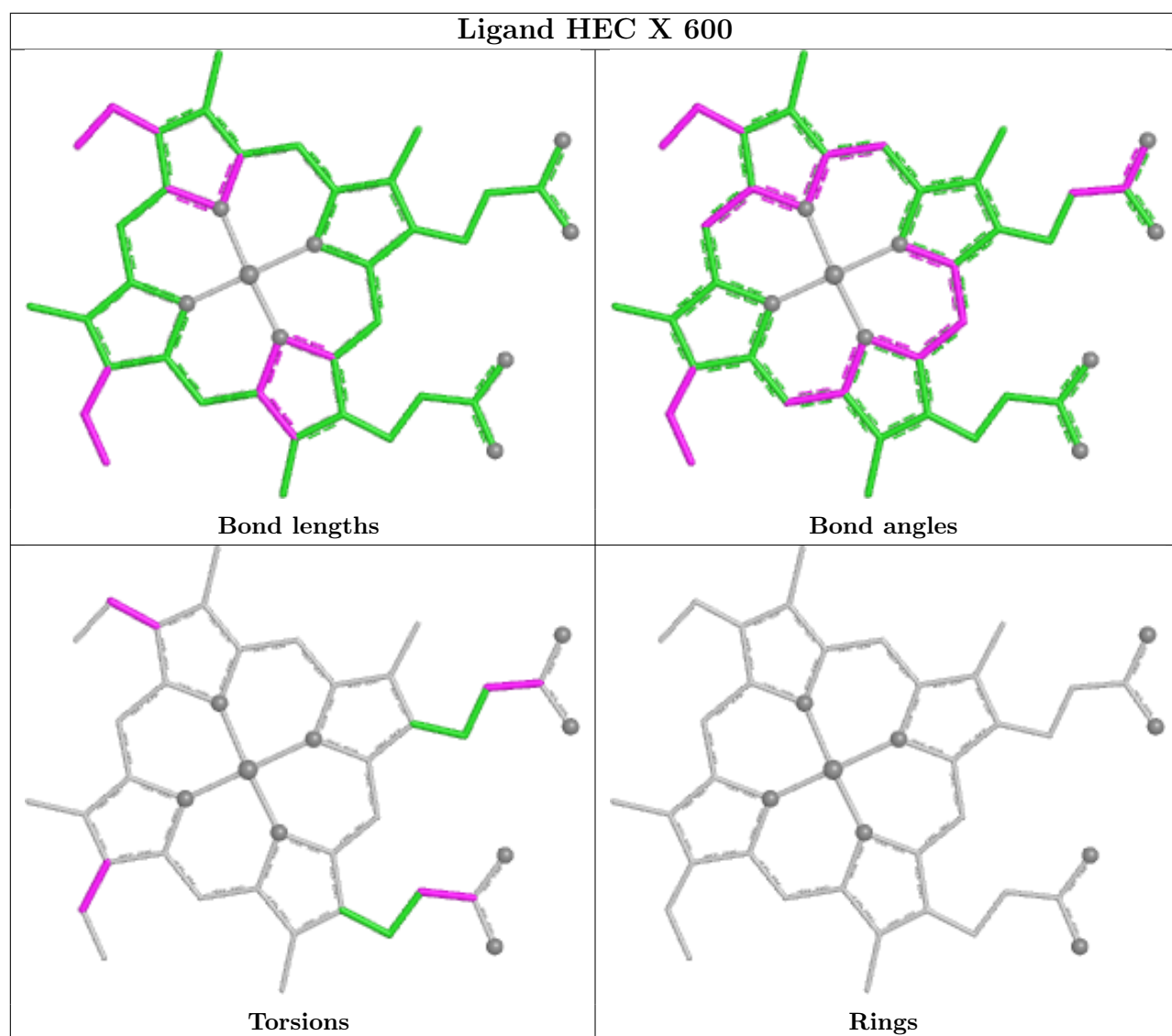


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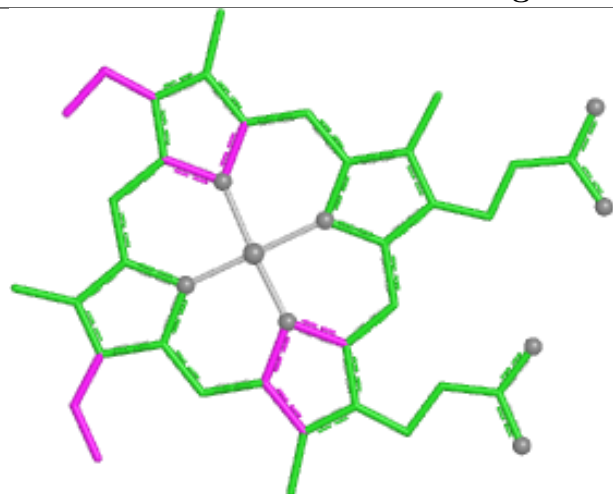


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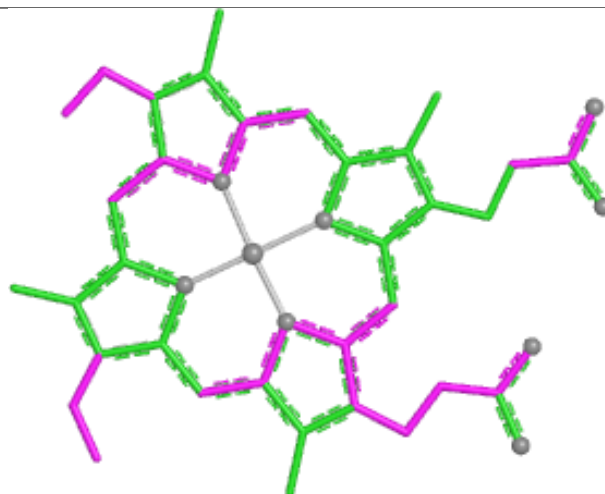




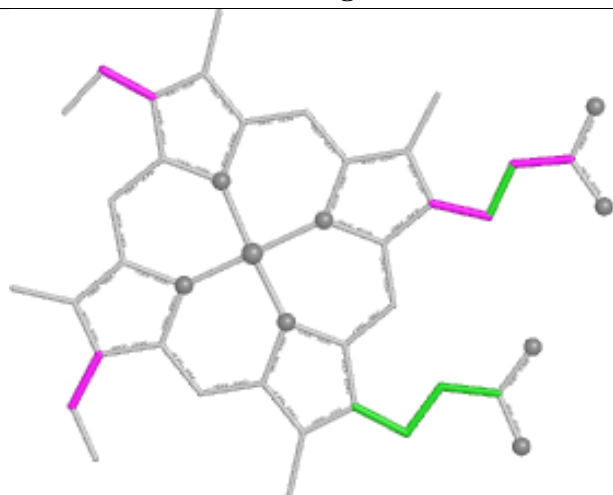
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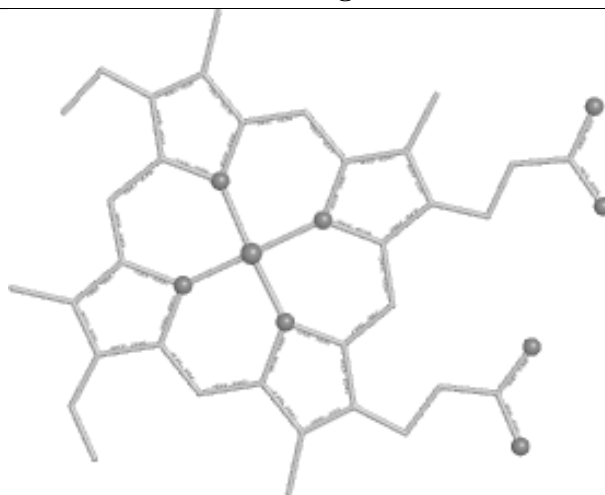
Bond lengths



Bond angles

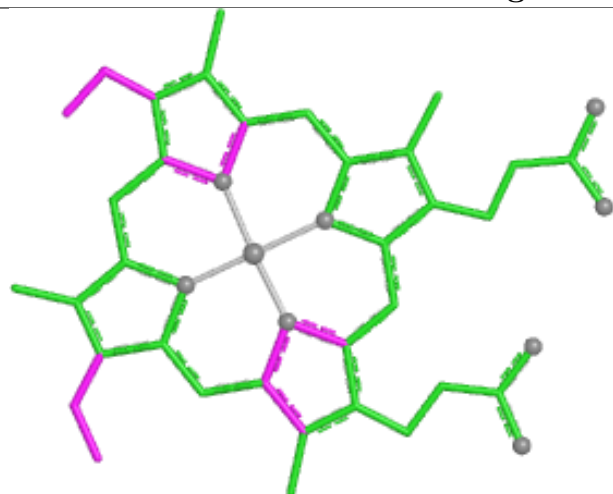


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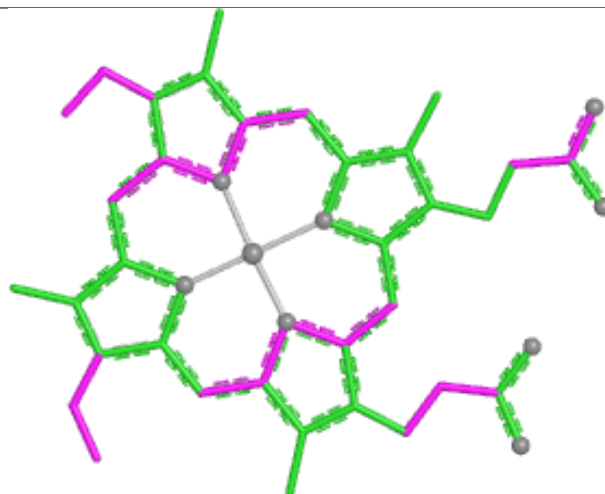


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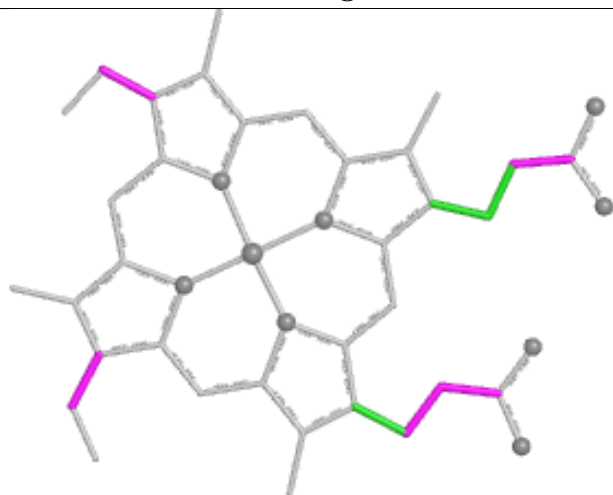
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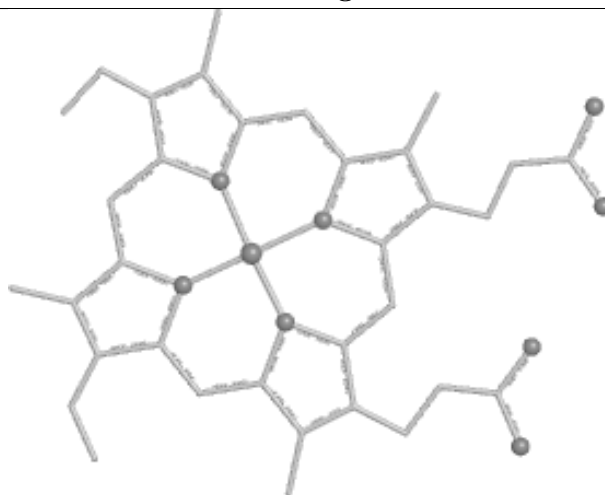
Bond lengths



Bond angles

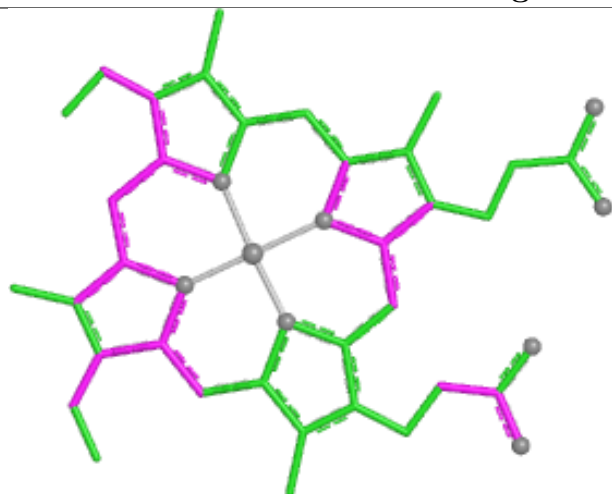


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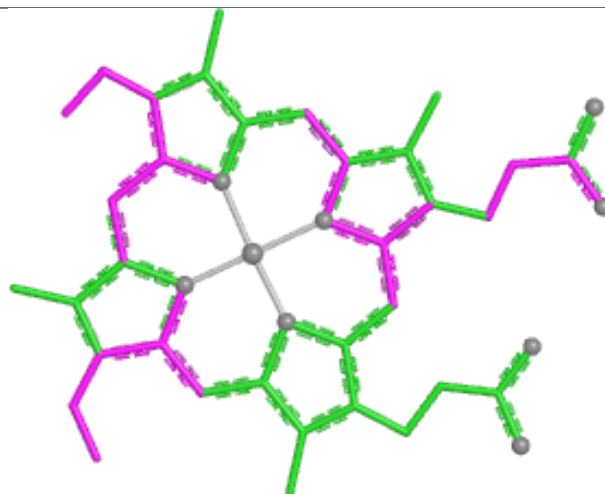


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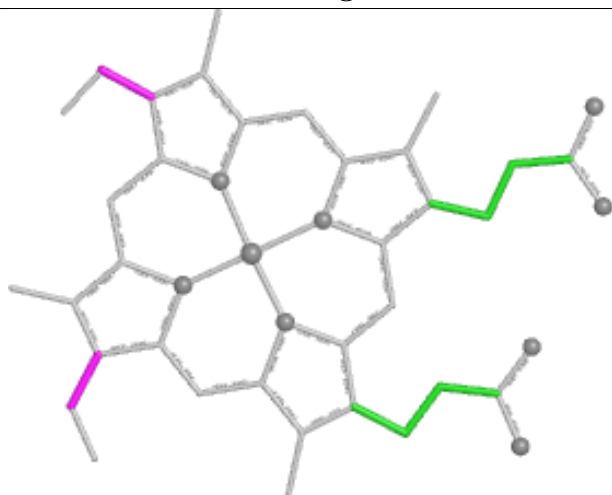
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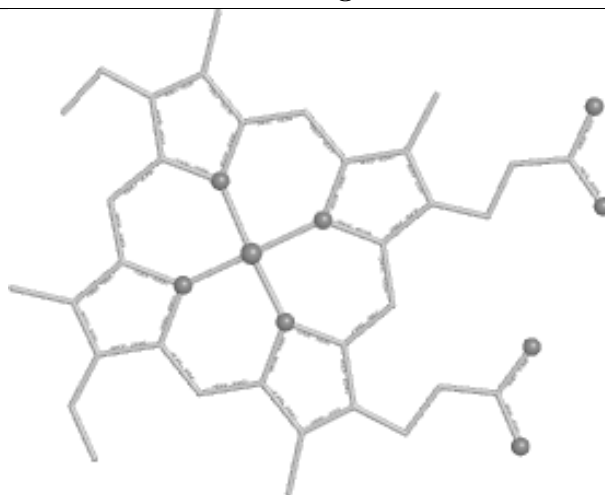
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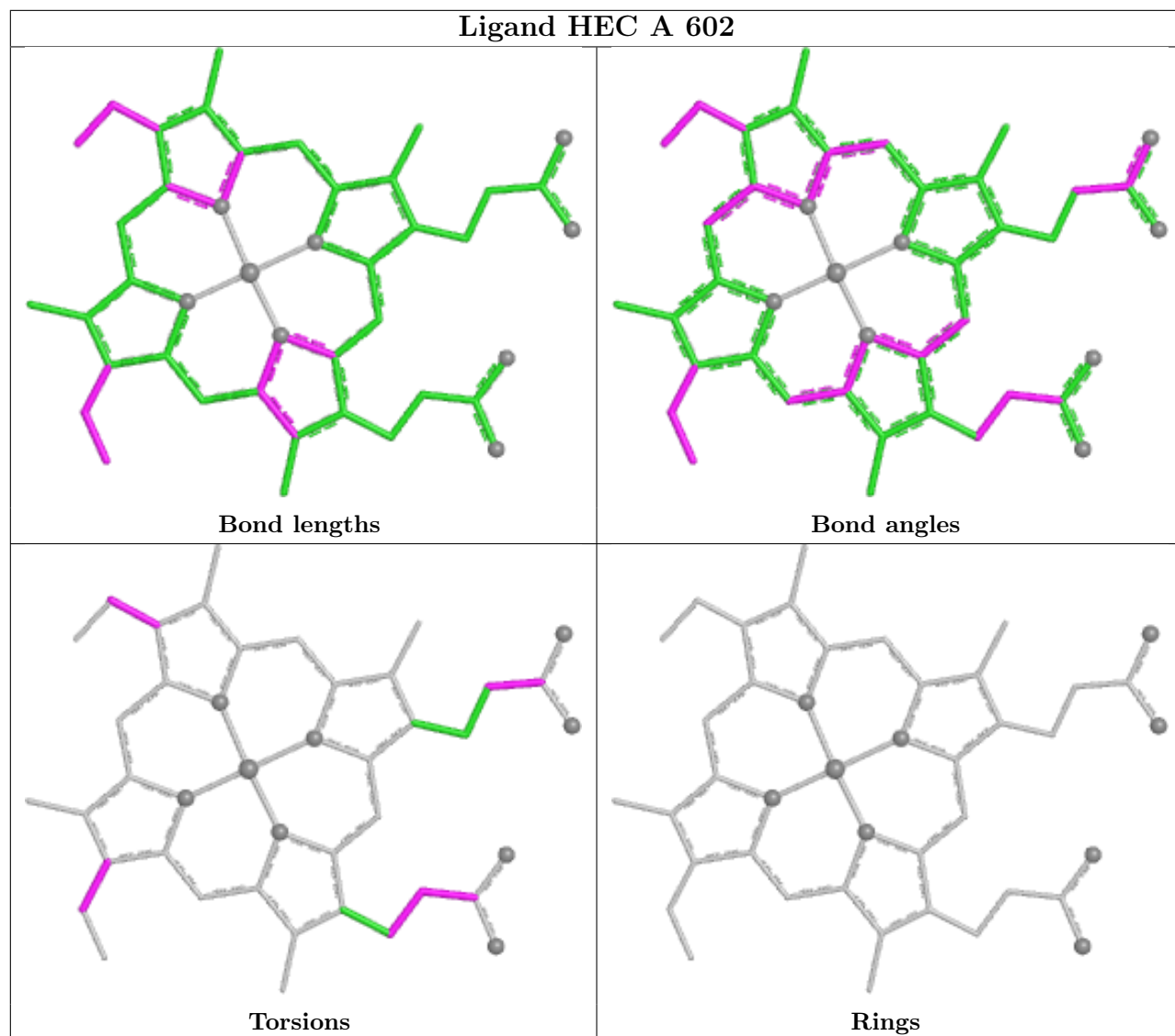
Bond angles



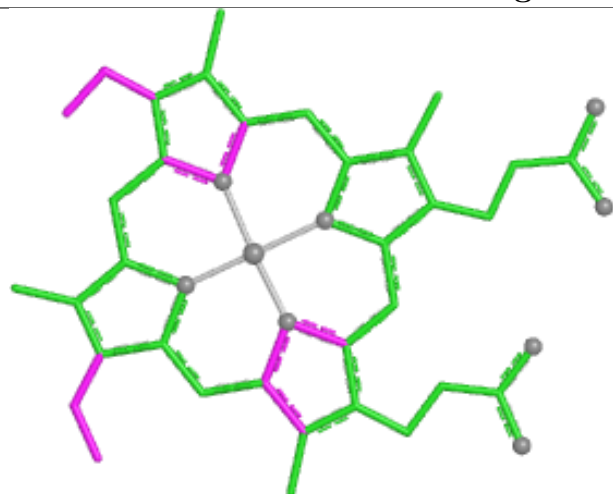
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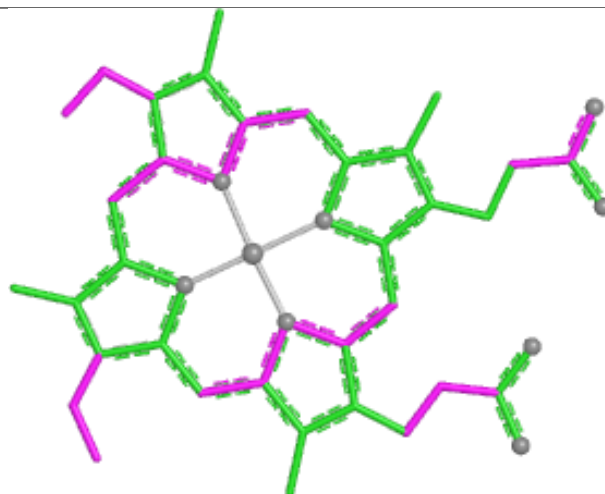
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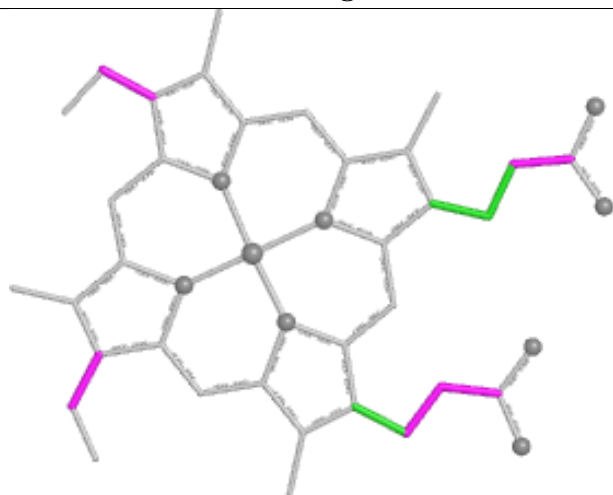
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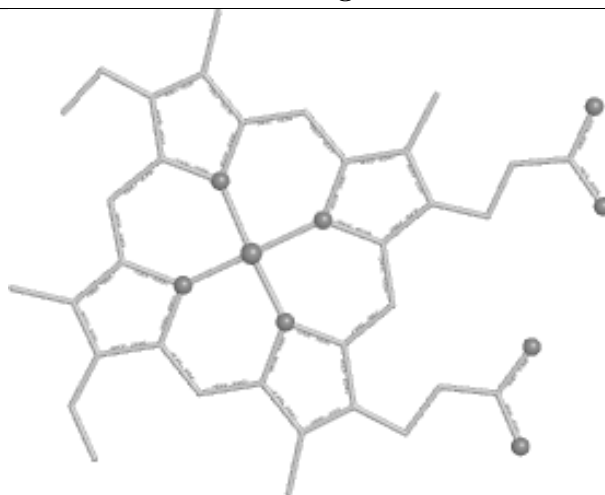
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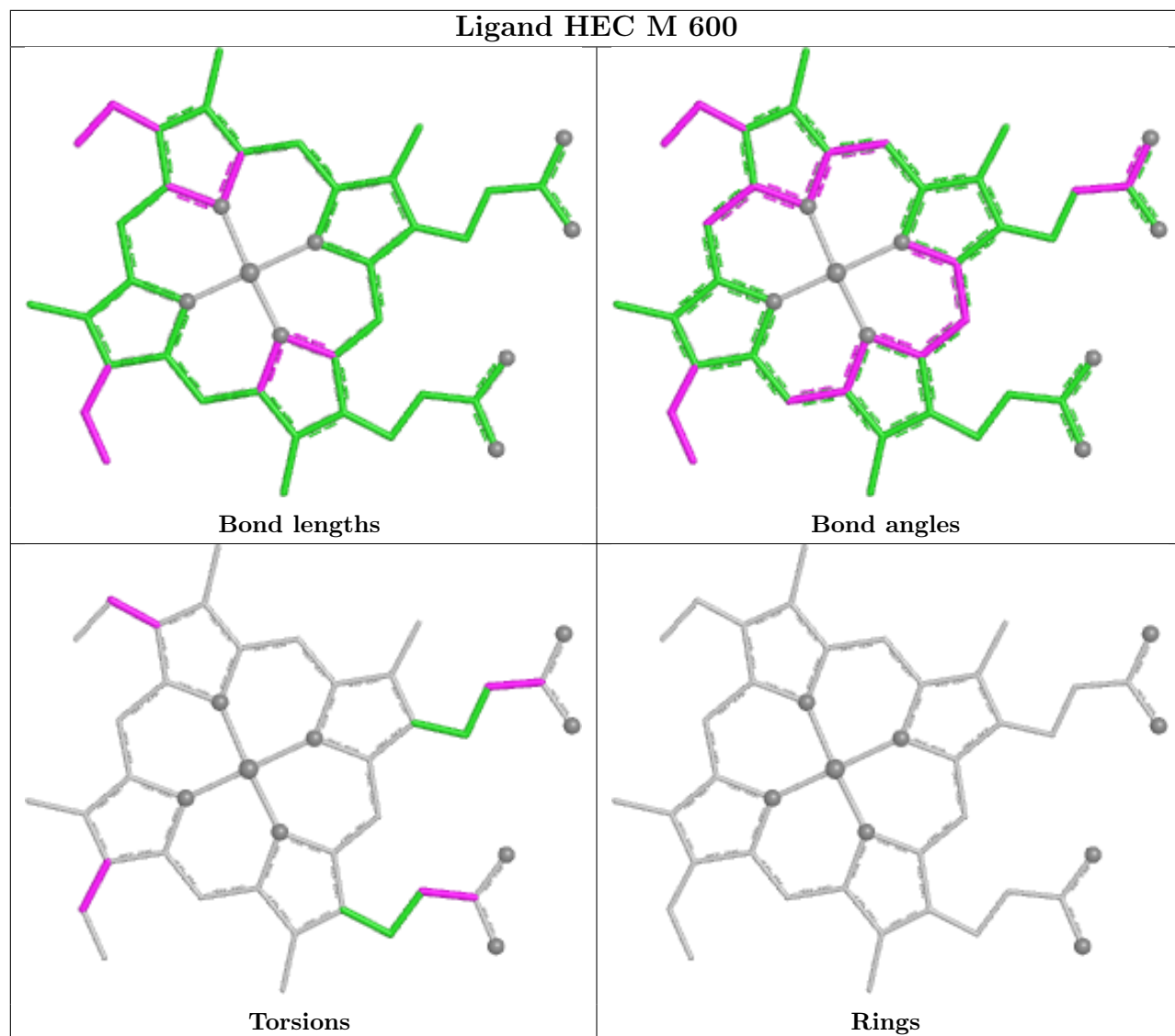
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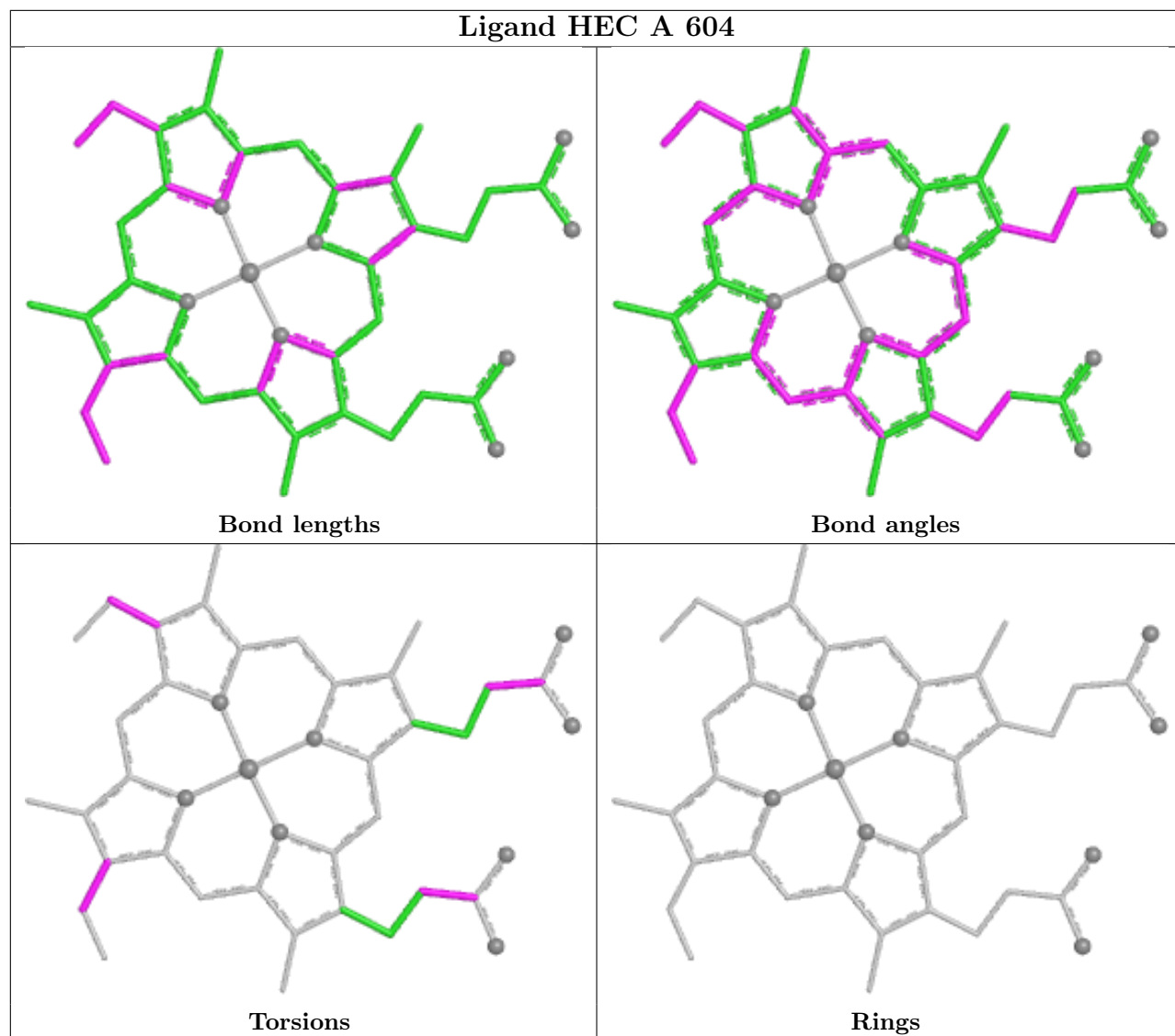


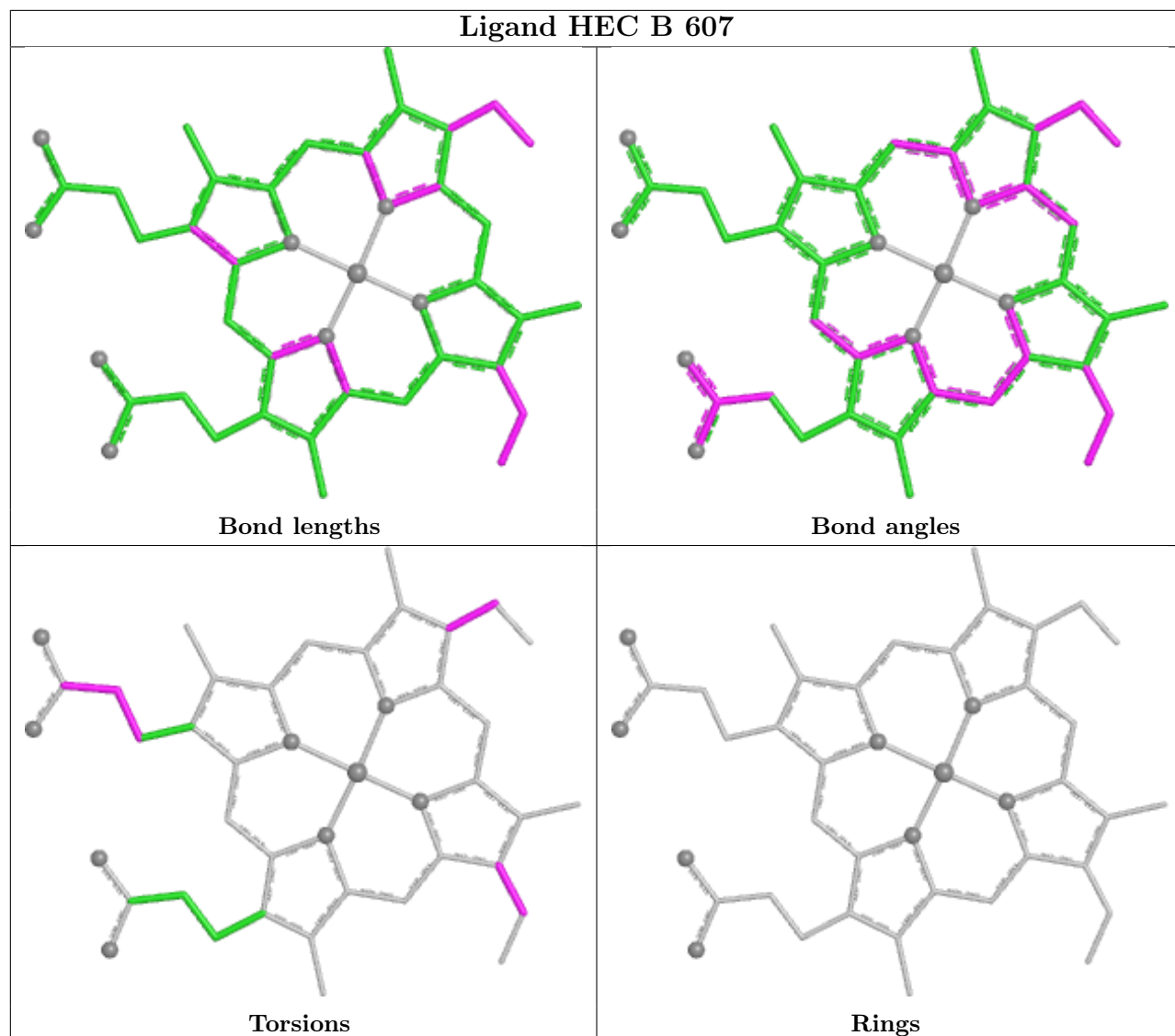
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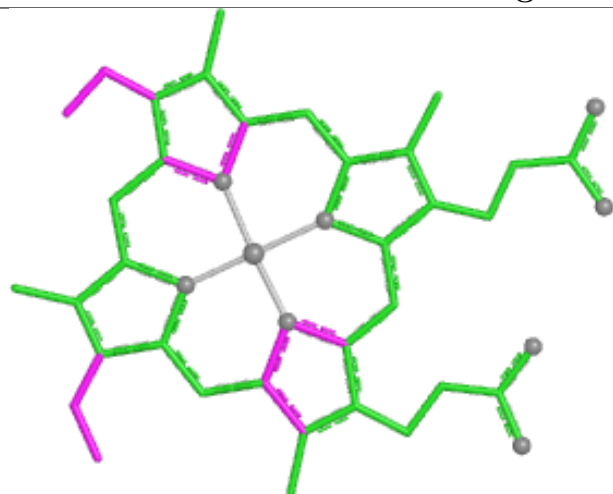
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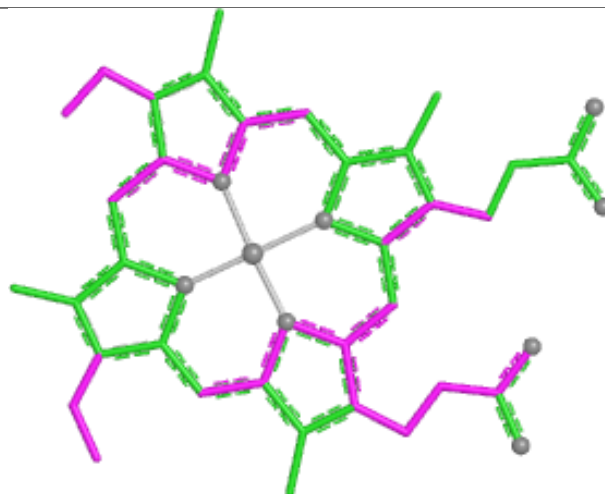




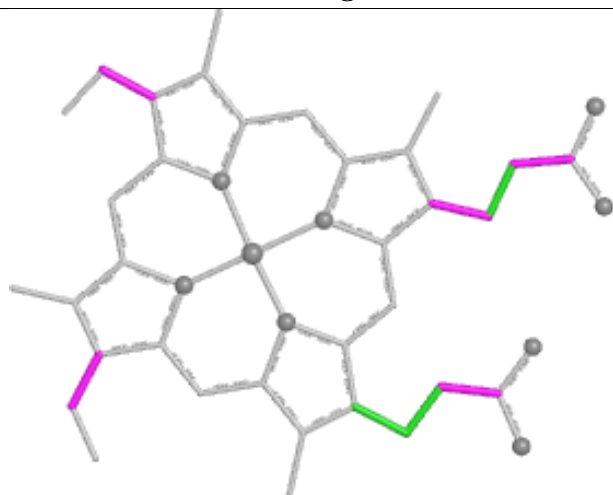
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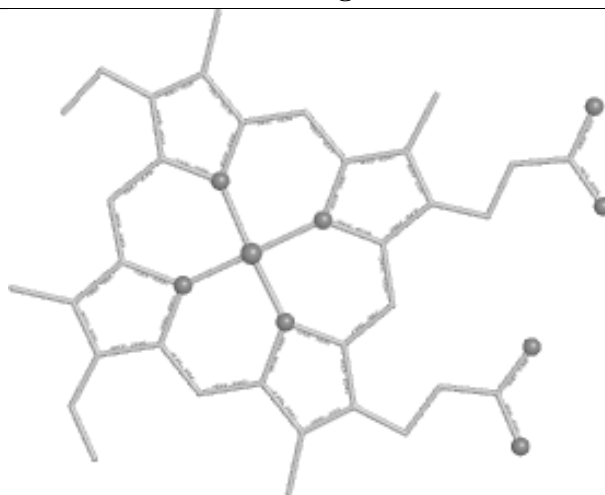
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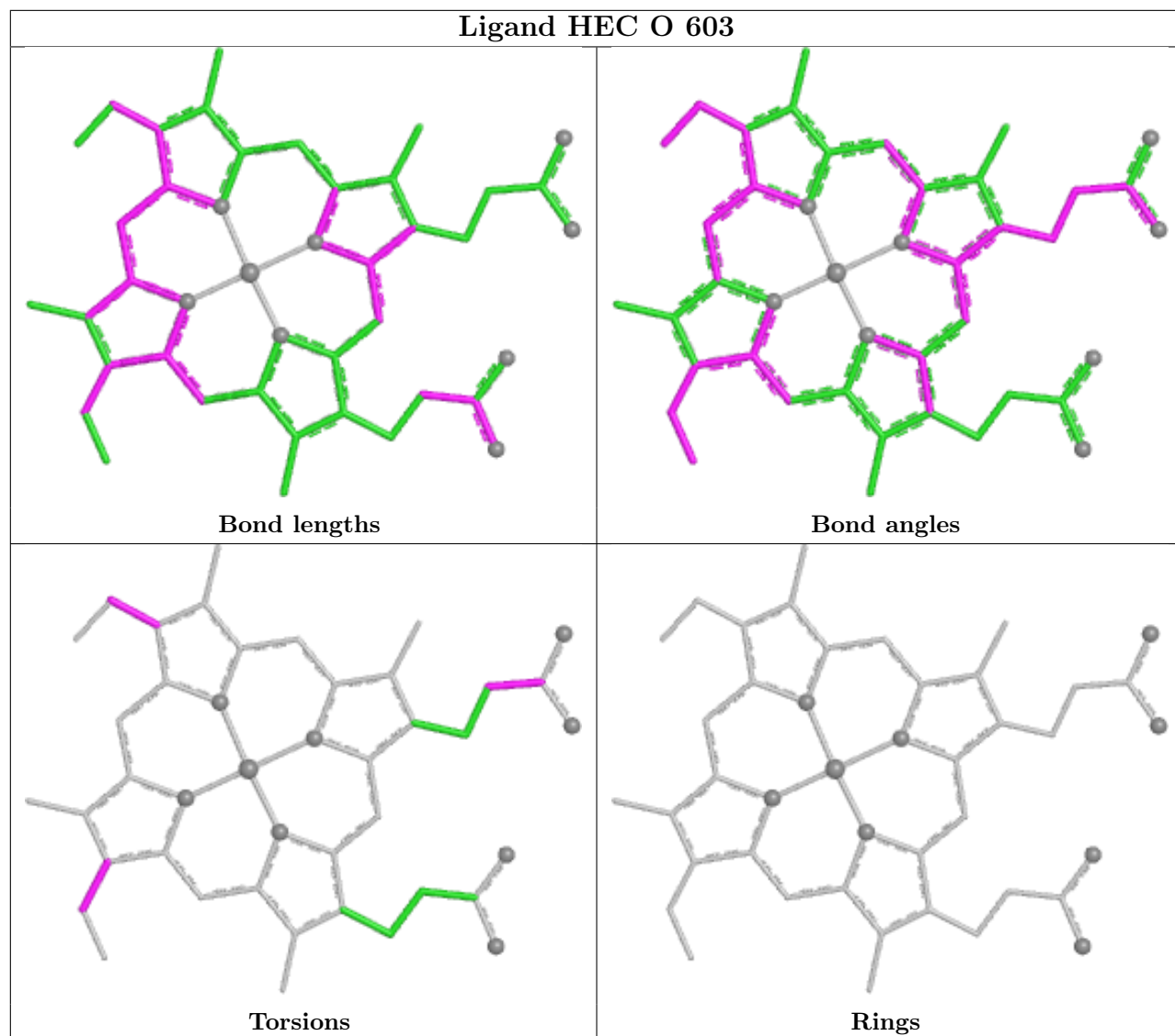
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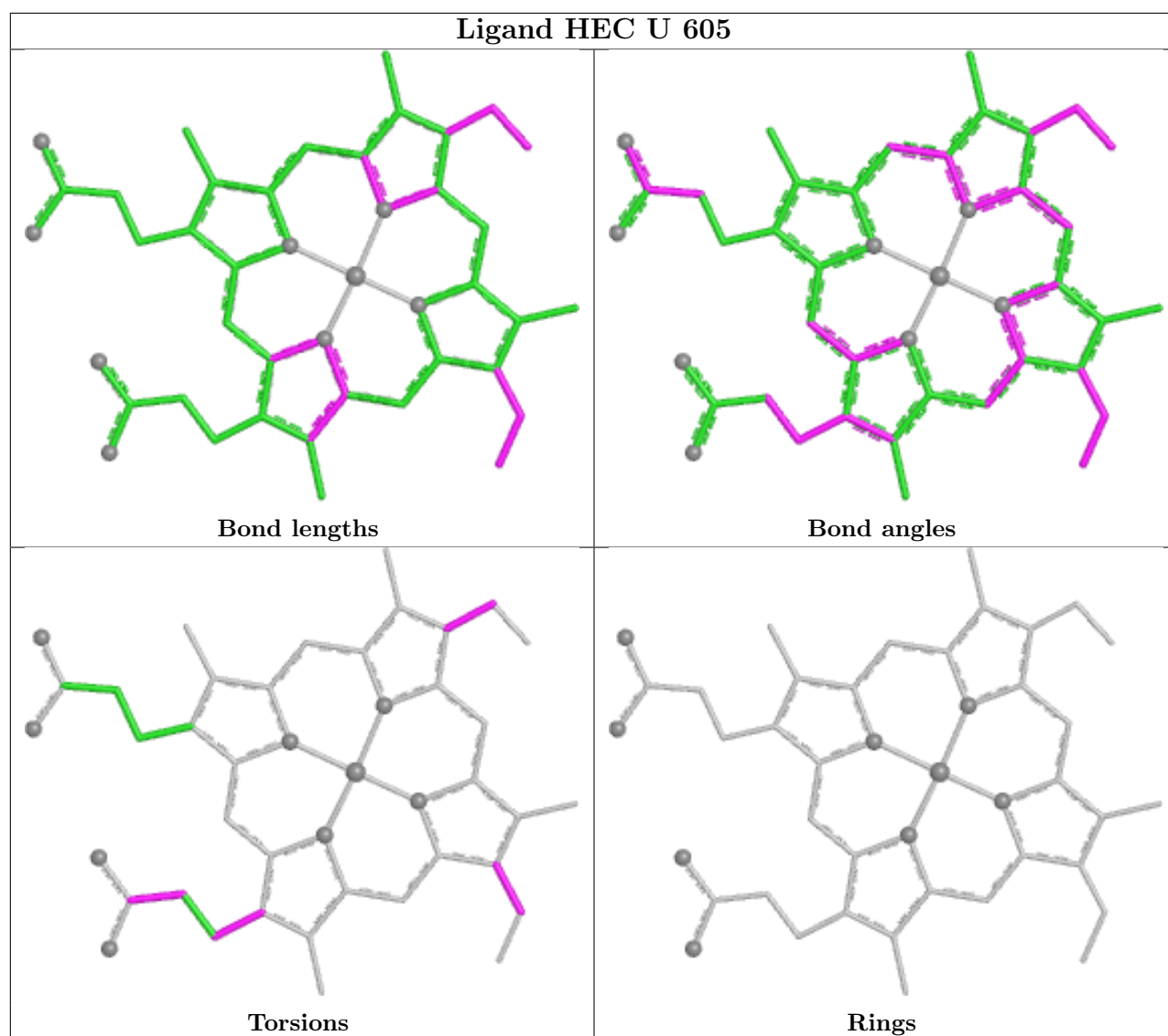


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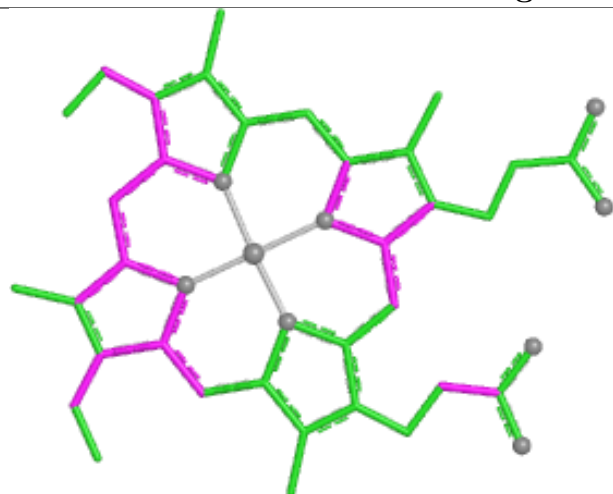


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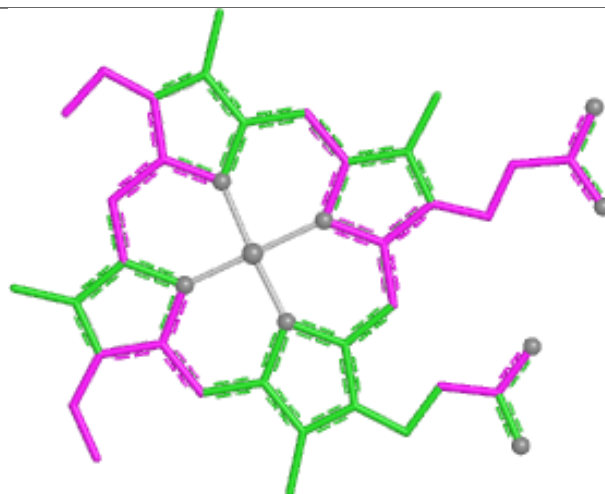




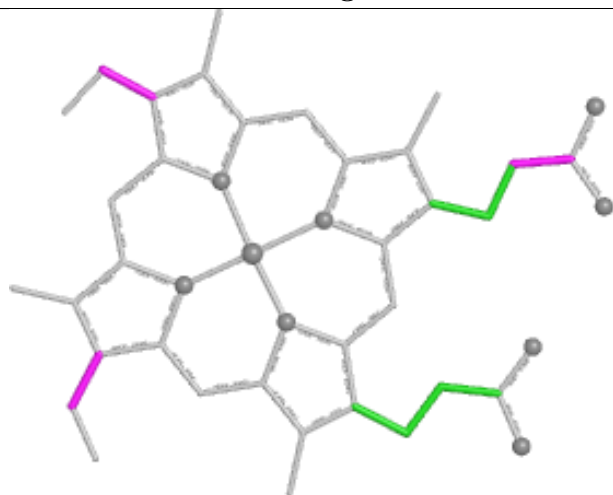
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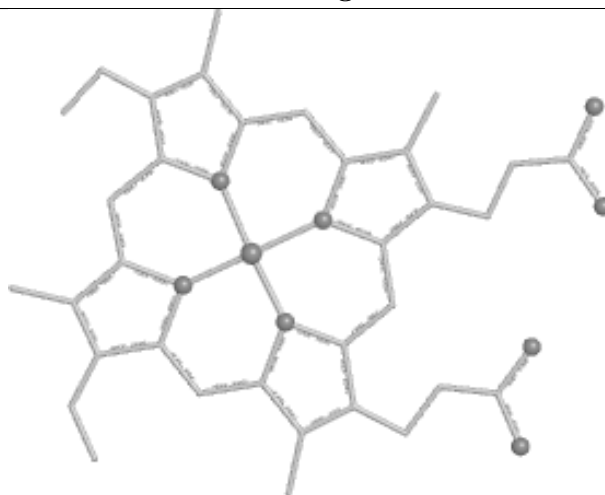
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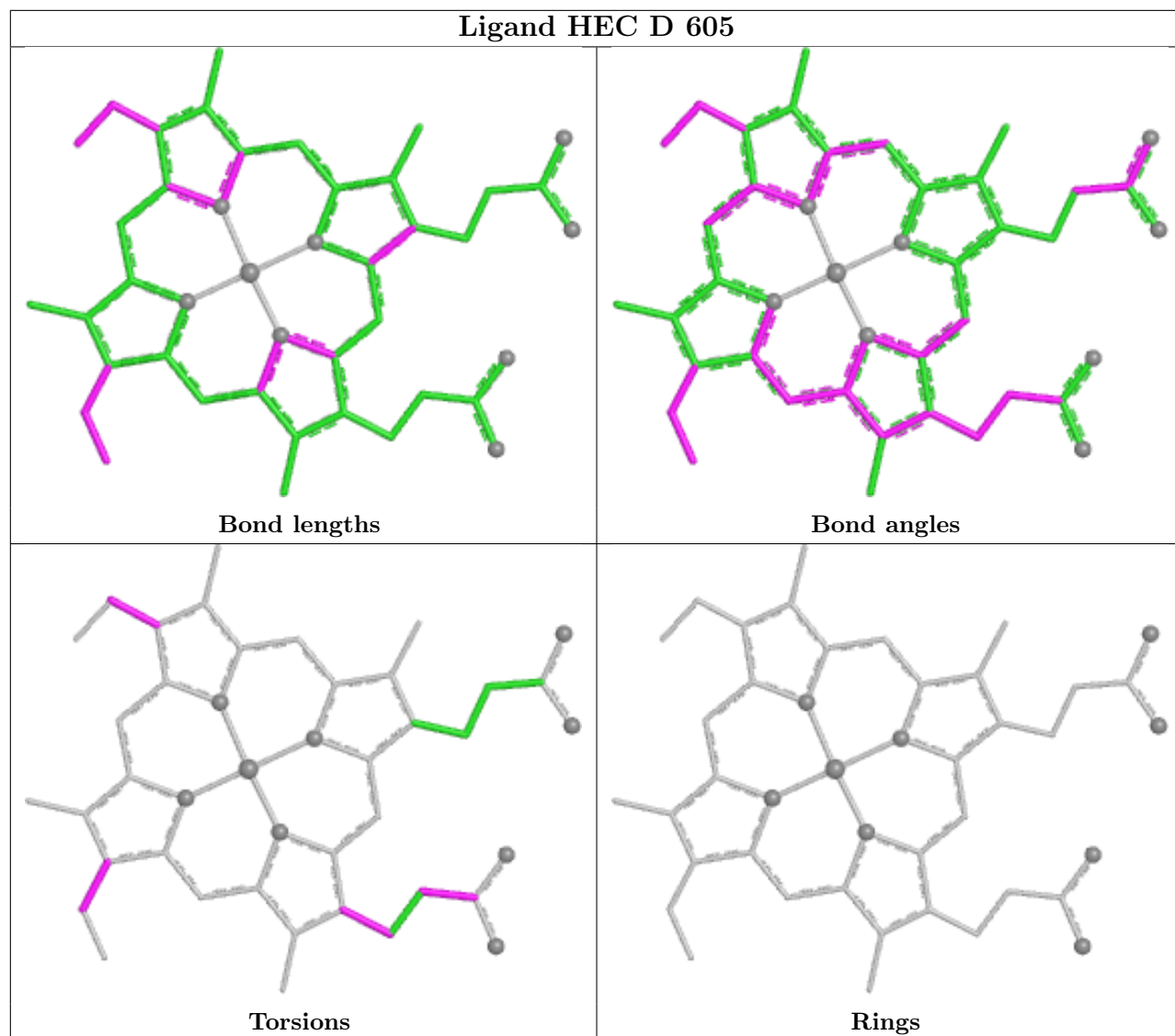
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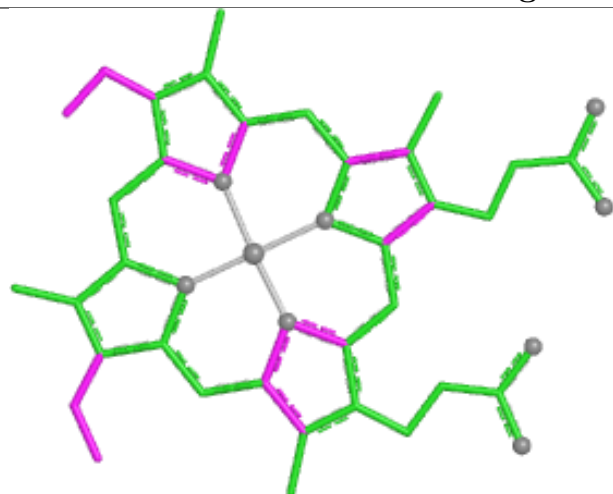
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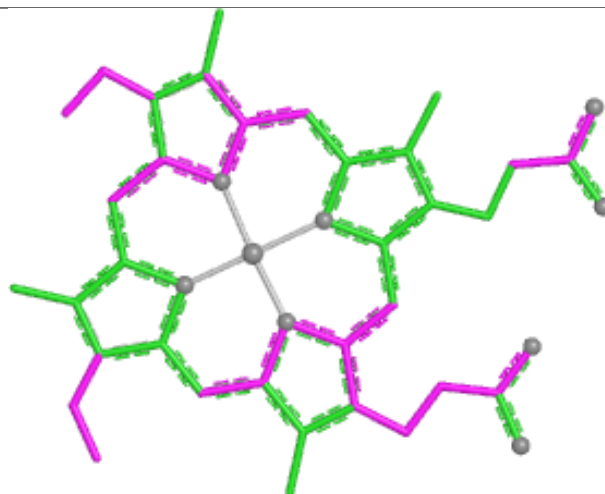
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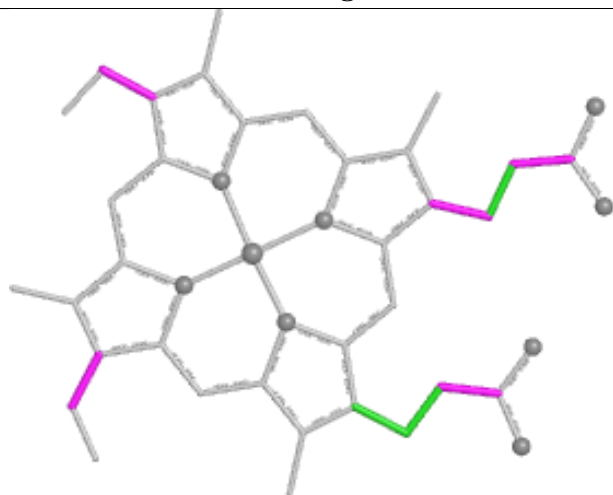
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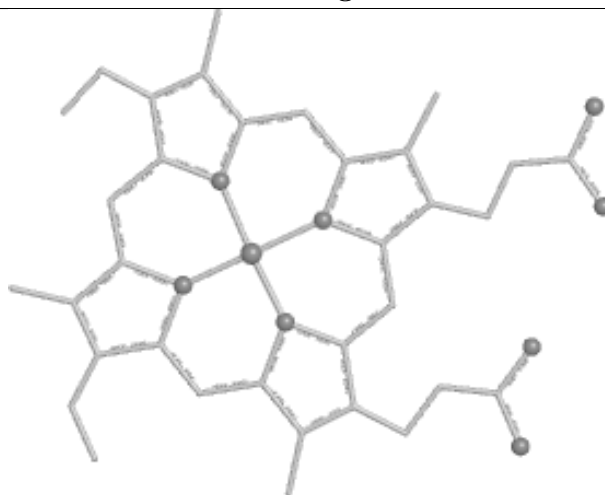
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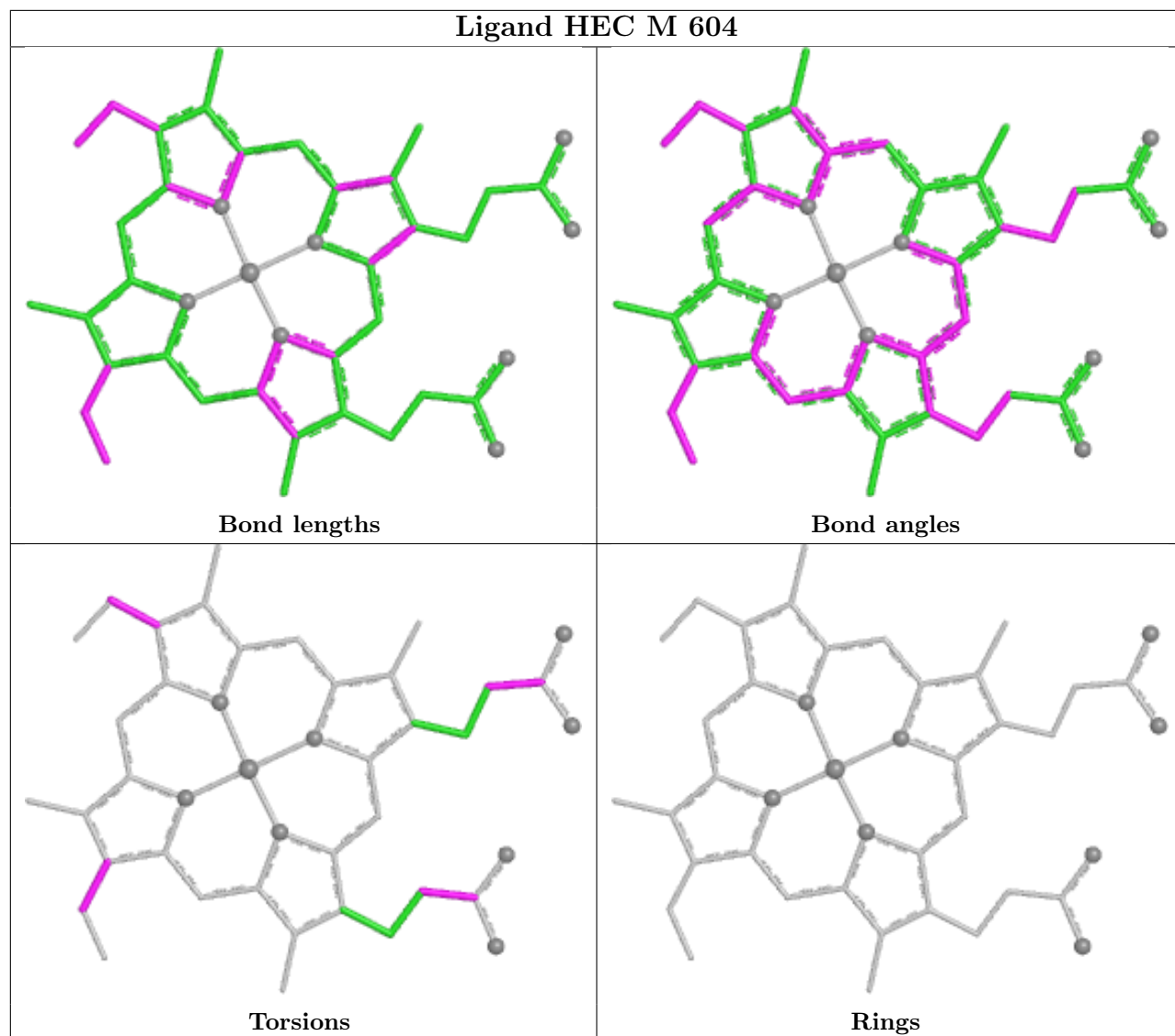
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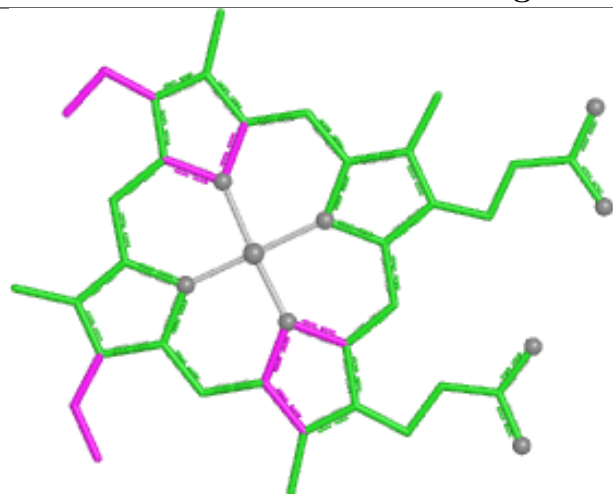
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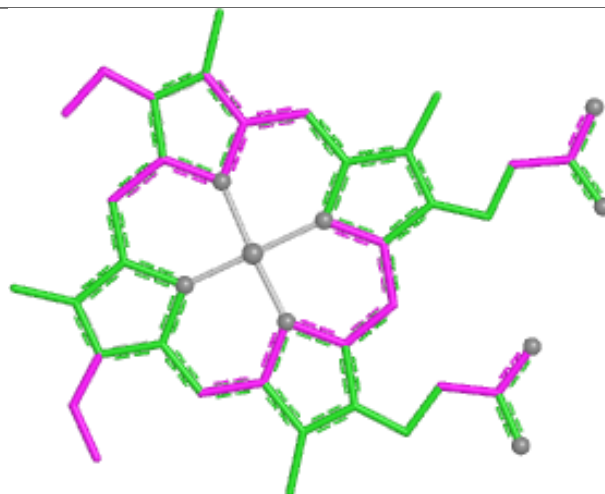
Rings



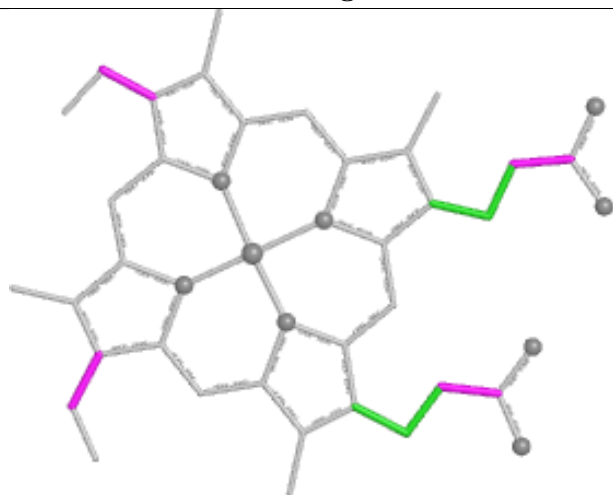
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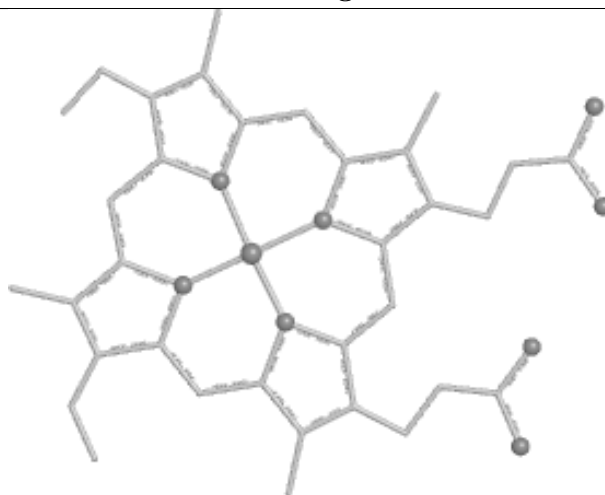
Bond lengths



Bond angles

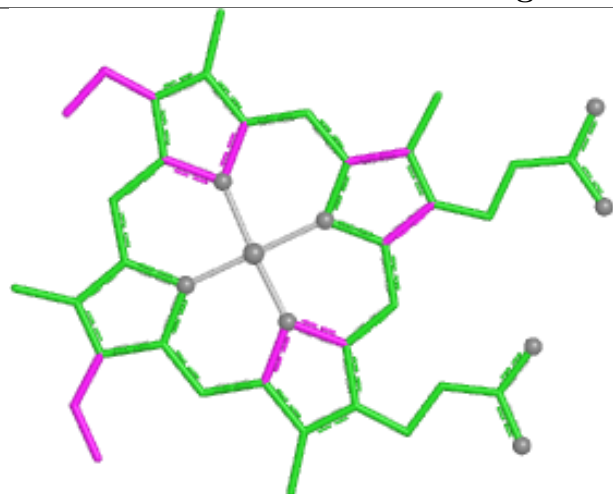


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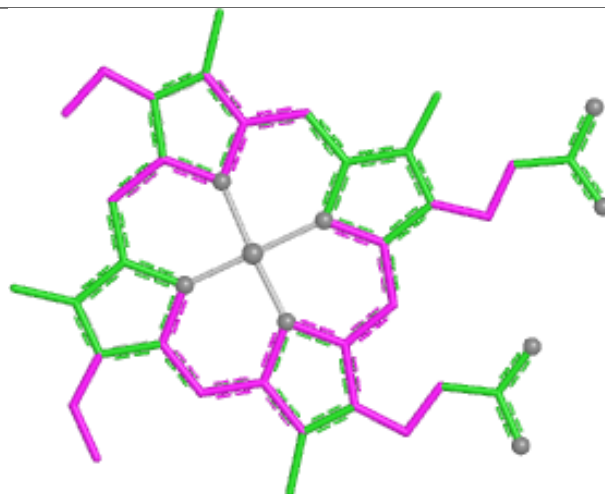


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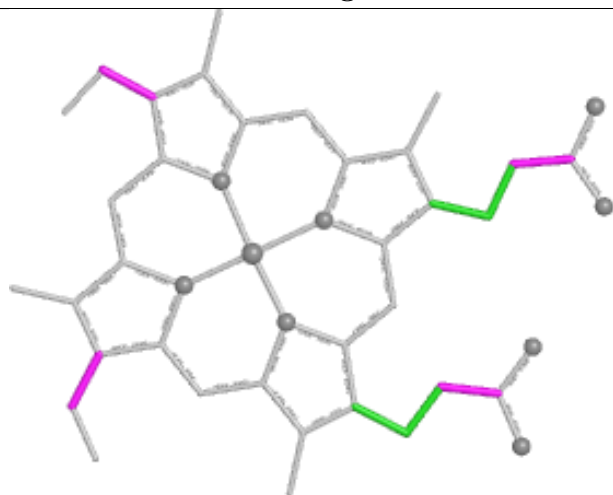
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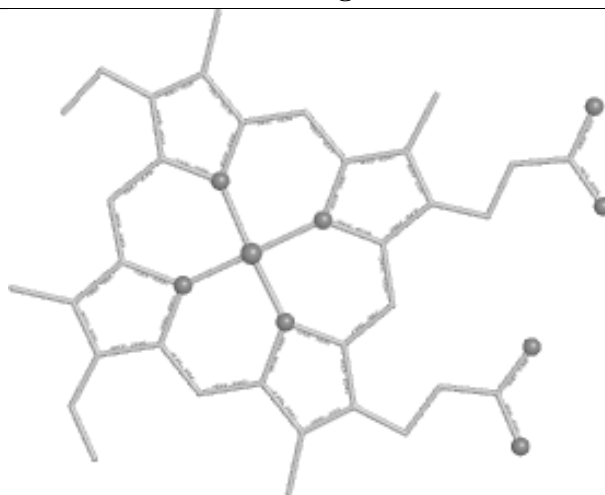
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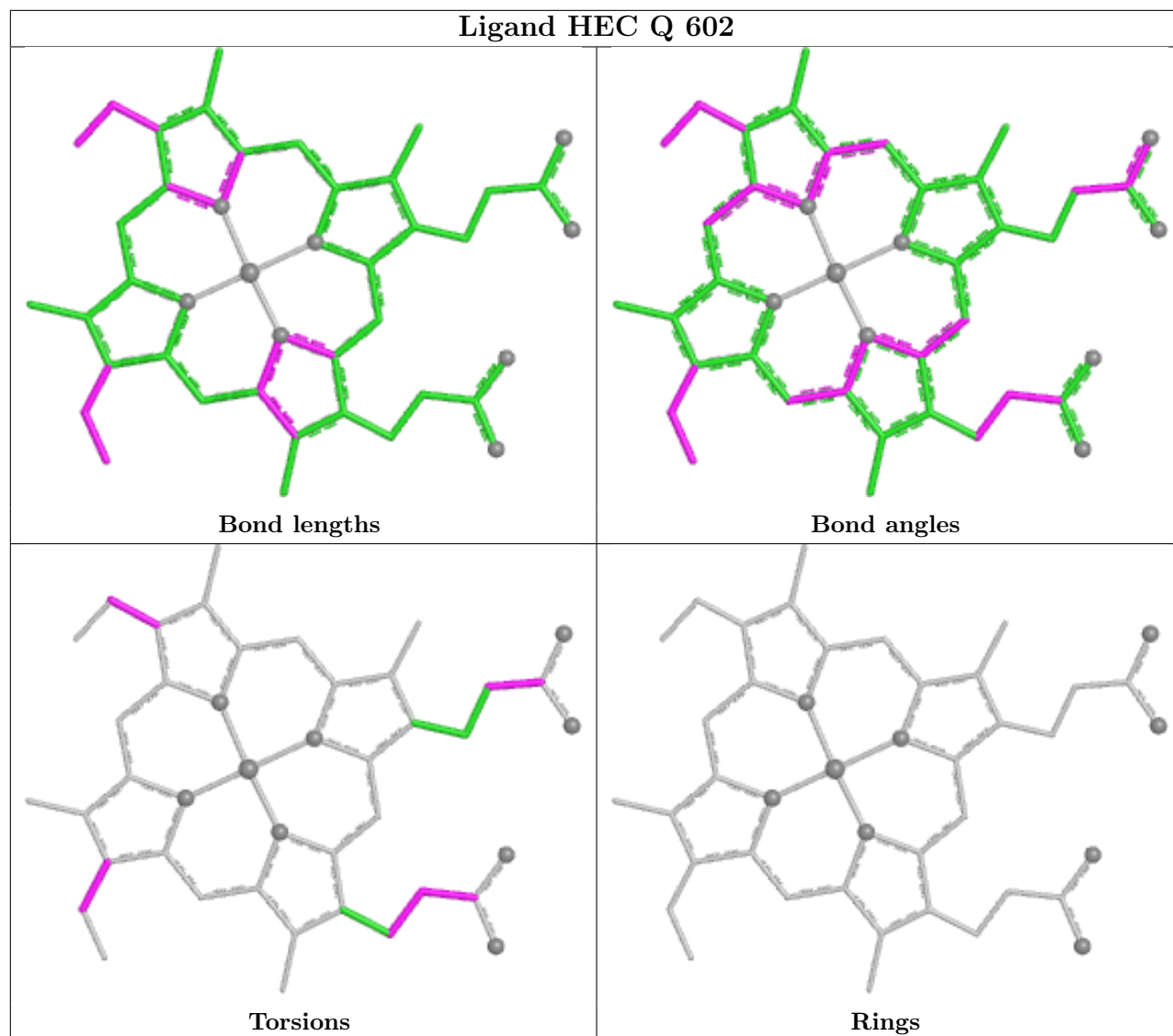
Bond angles



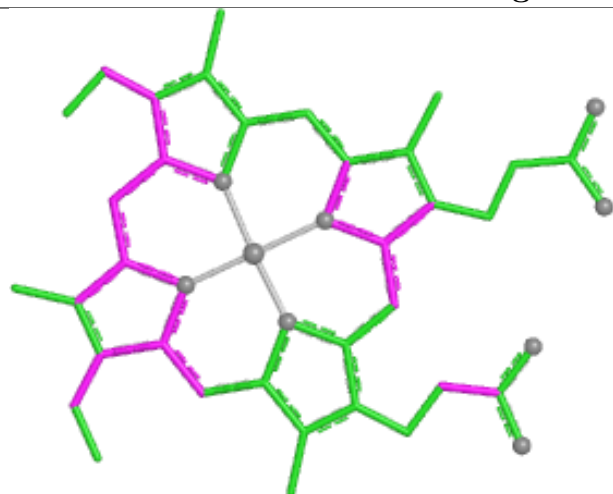
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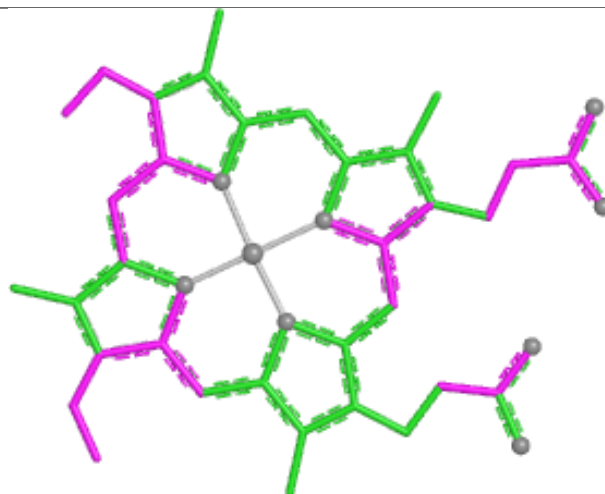
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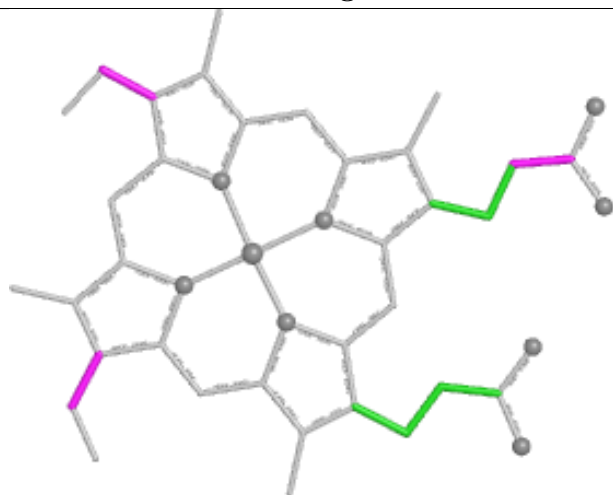
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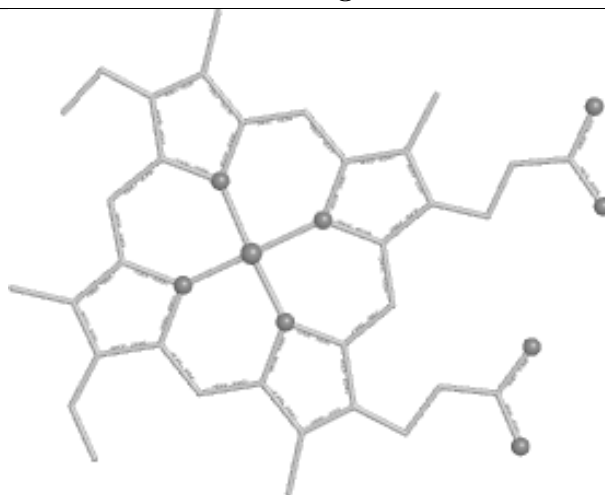
Bond lengths



Bond angles

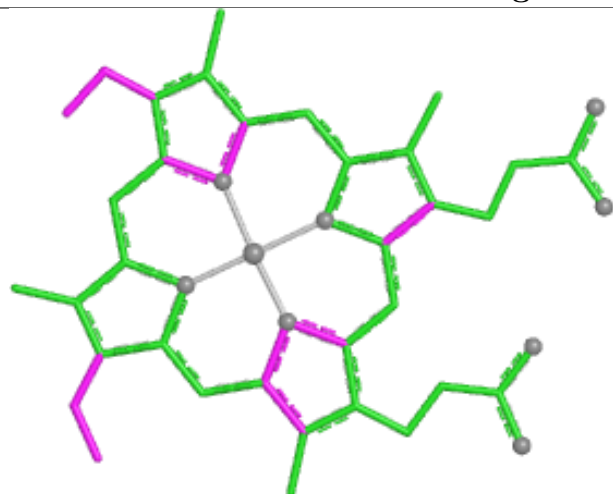


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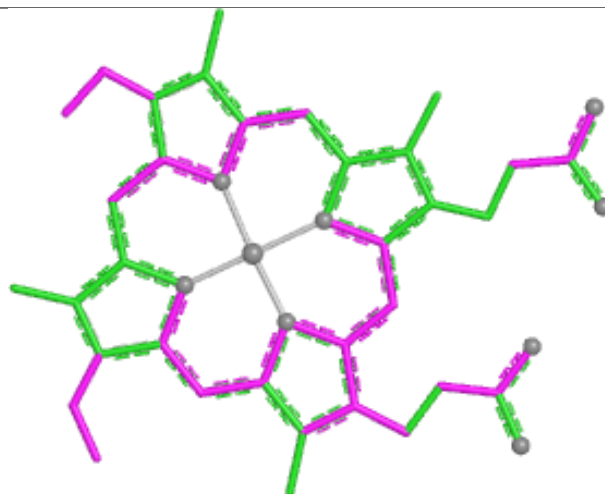


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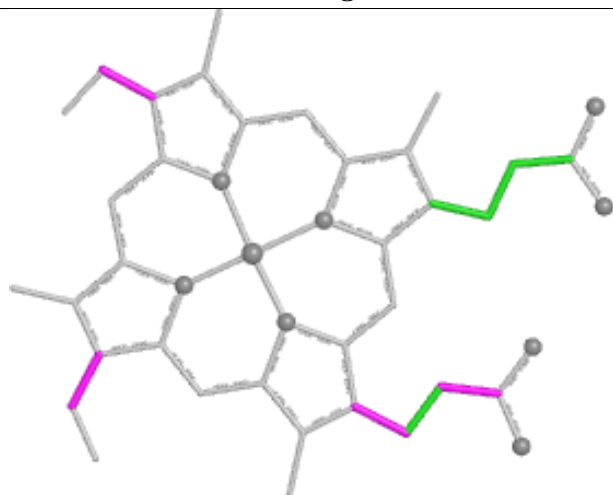
Ligand HEC V 605



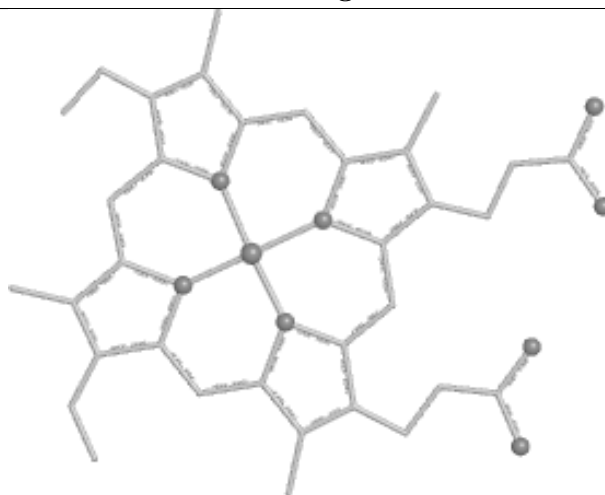
Bond lengths



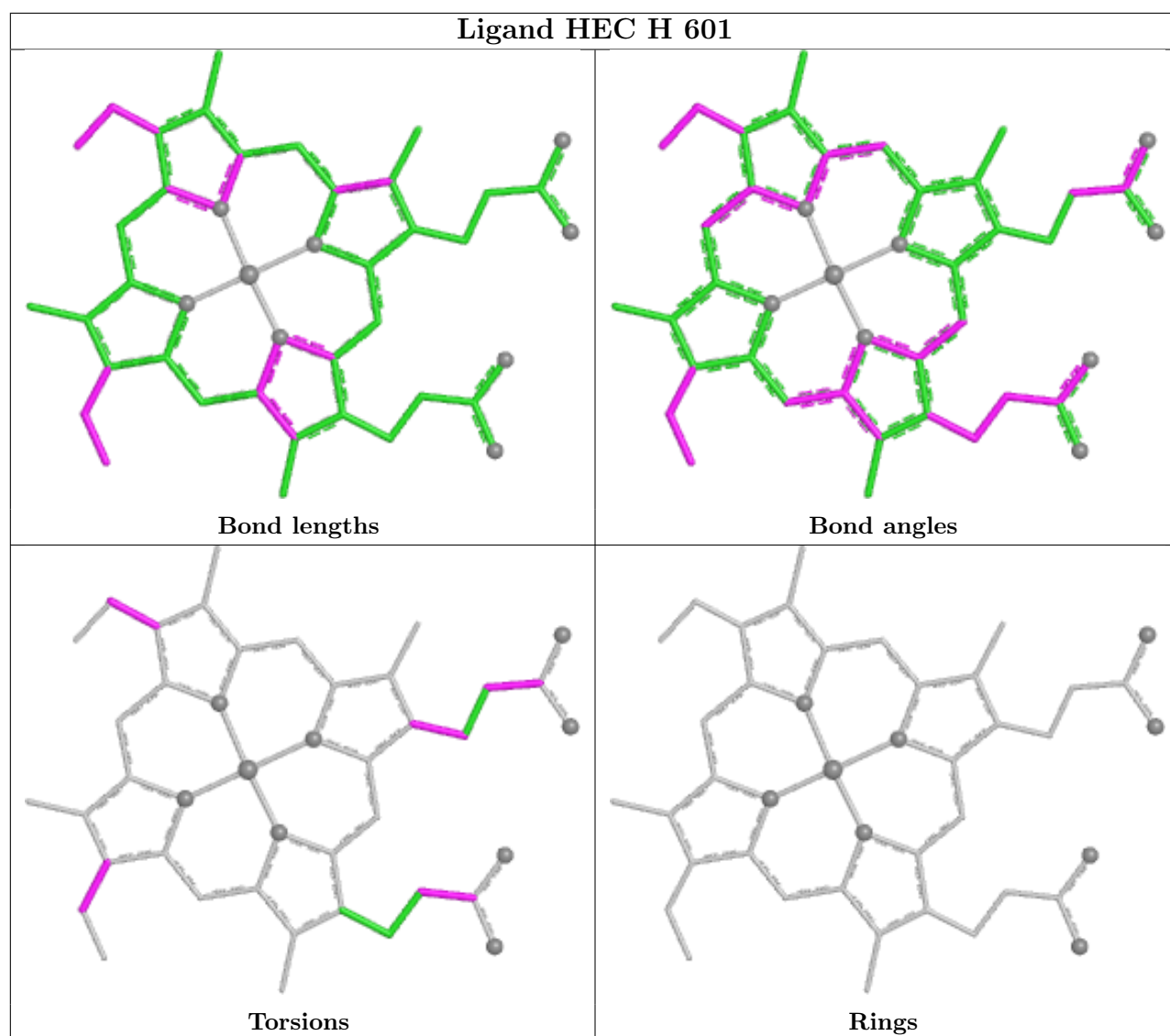
Bond angles

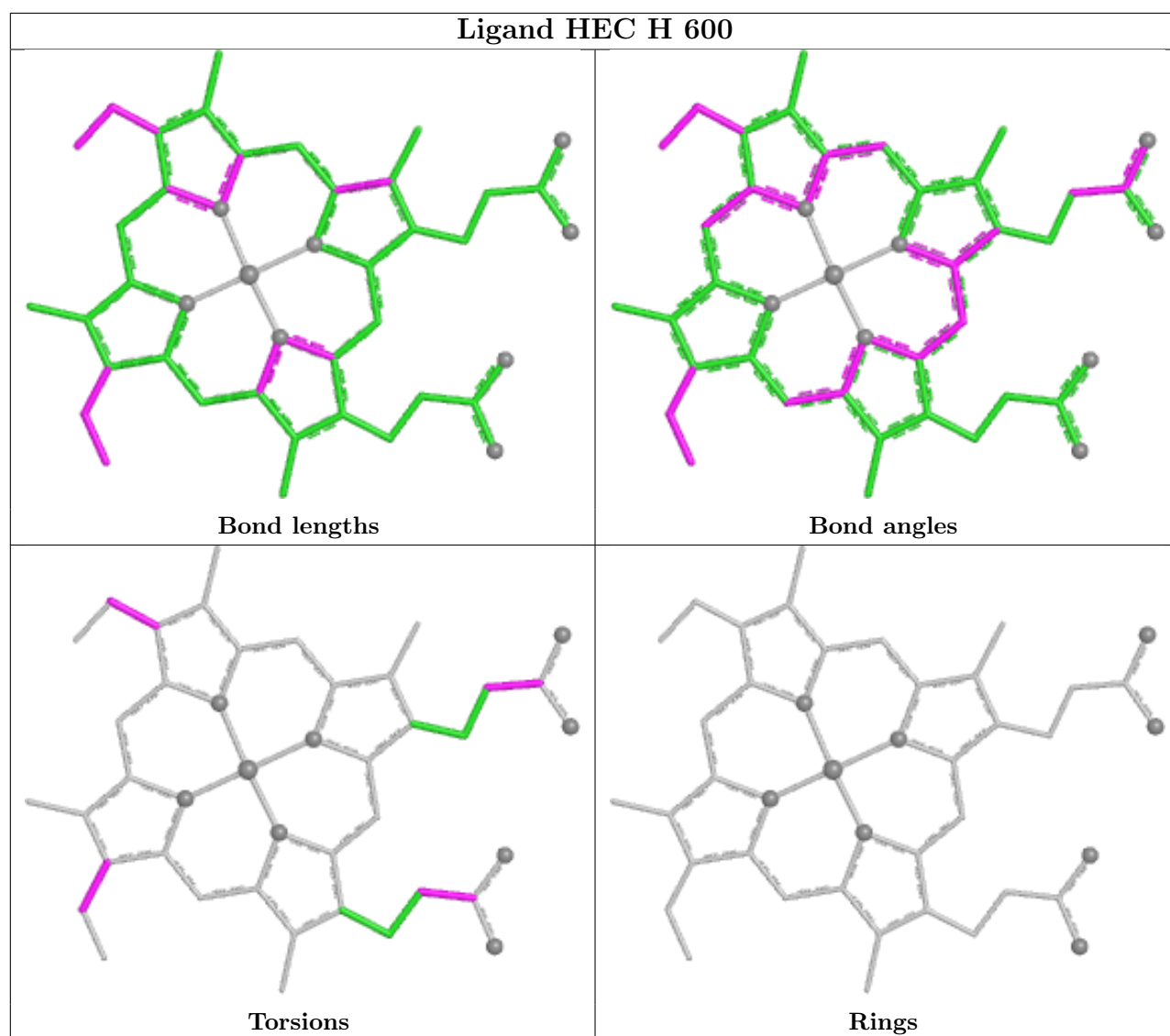


Torsions

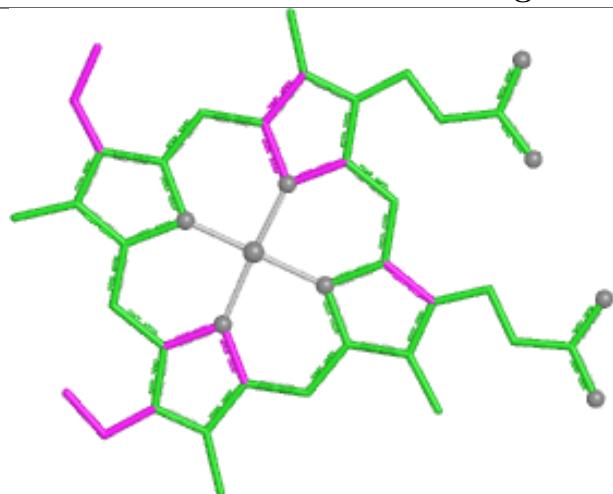


Rings

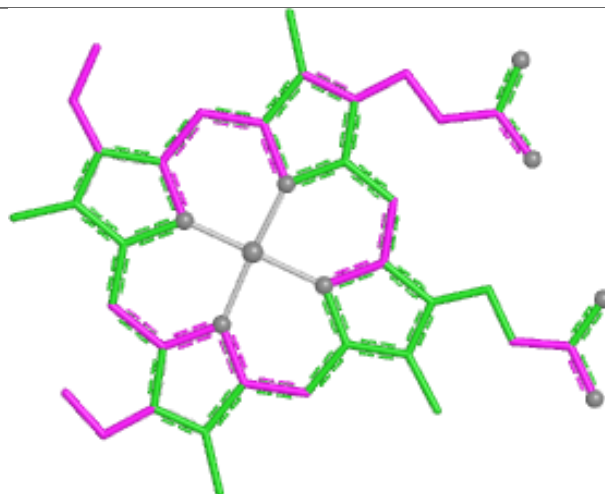




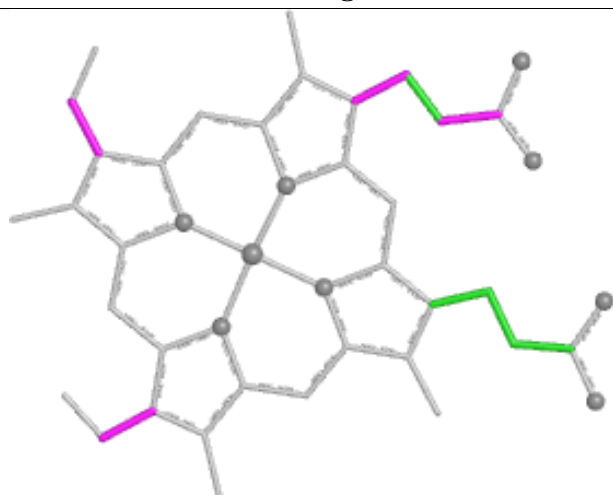
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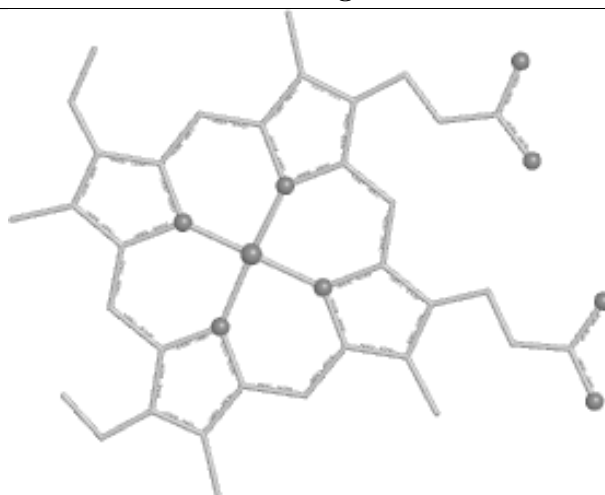
Bond lengths



Bond angles

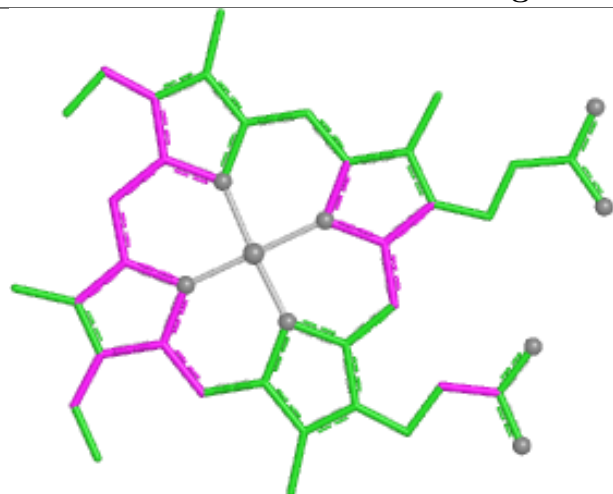


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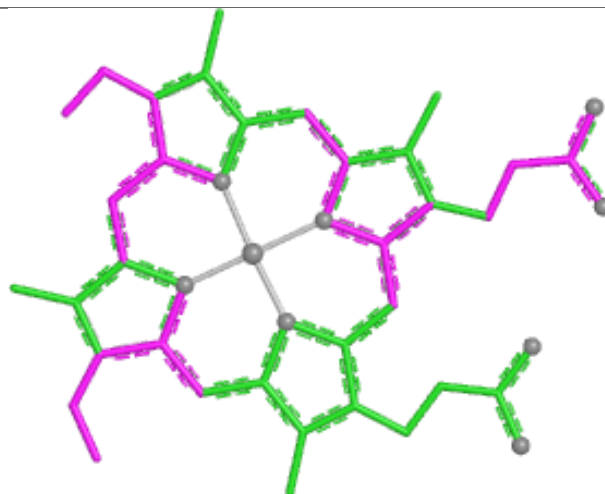


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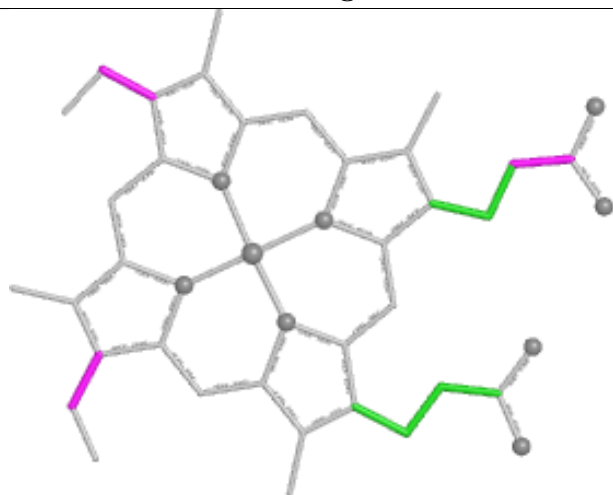
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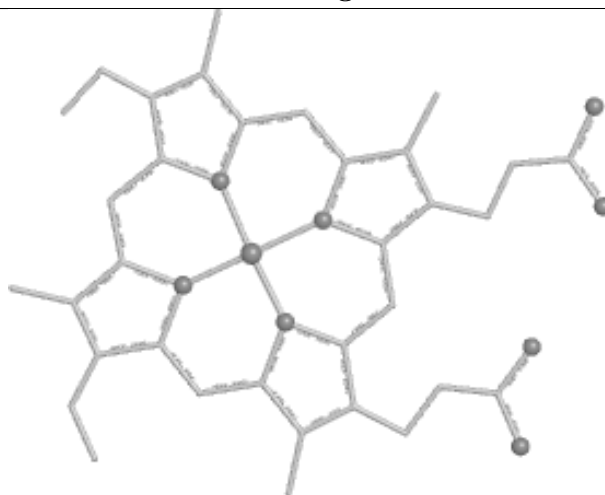
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Bond angles

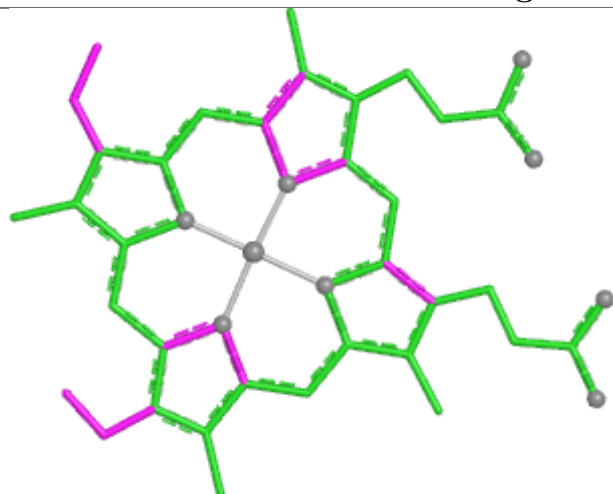


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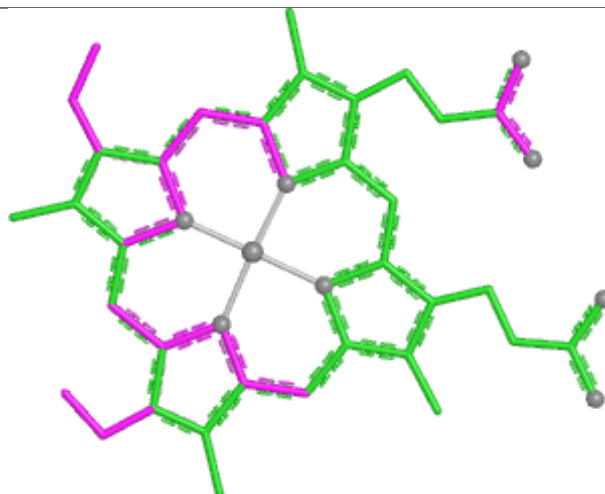


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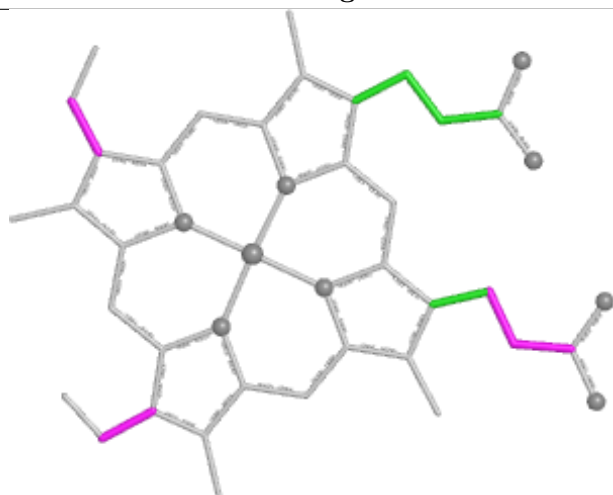
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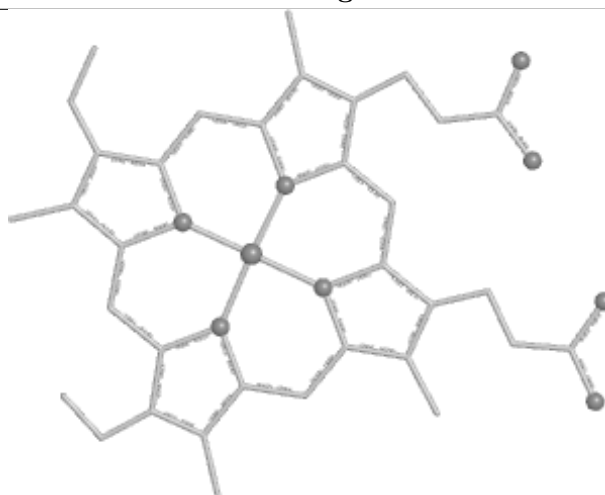
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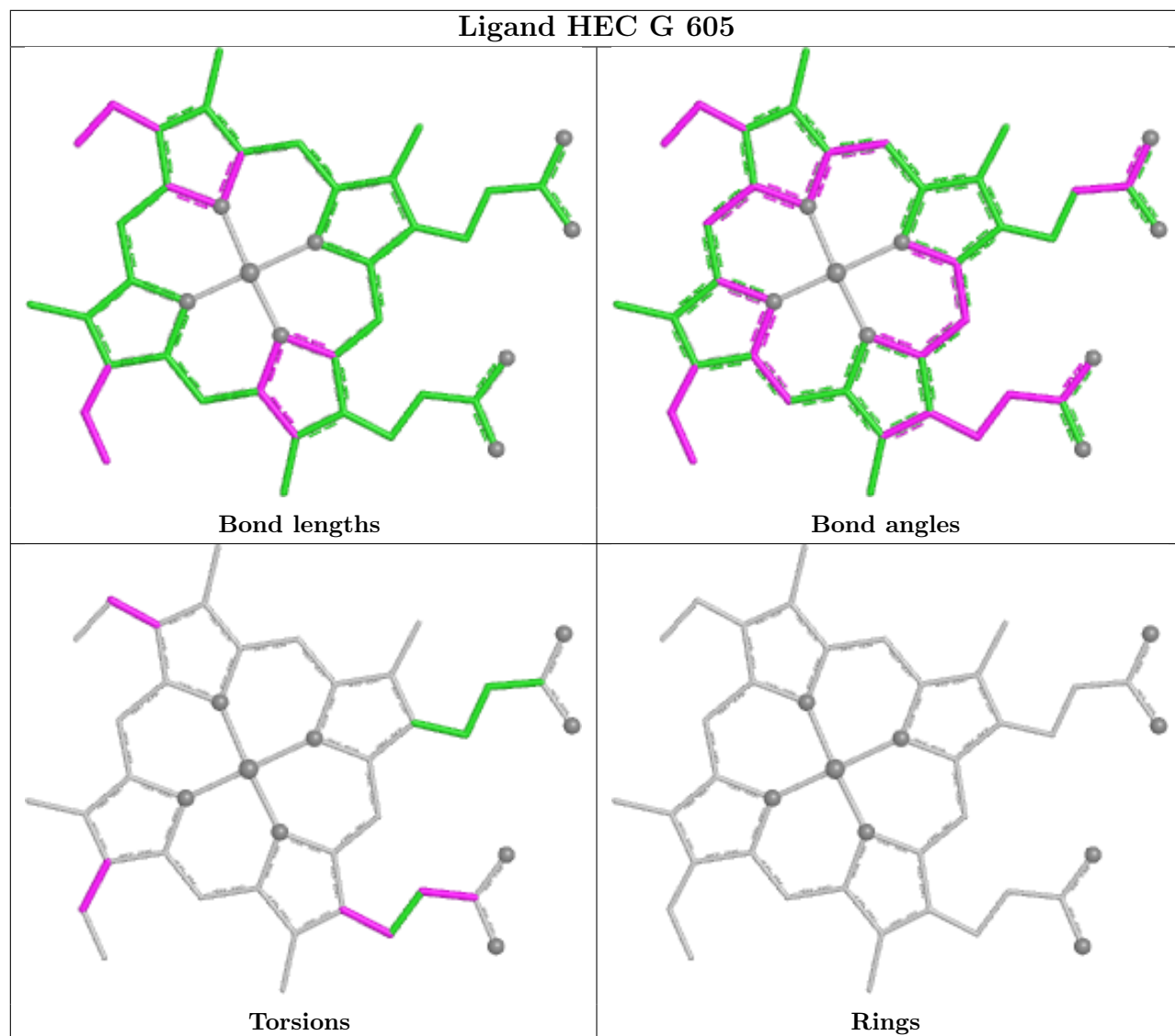
Bond angles



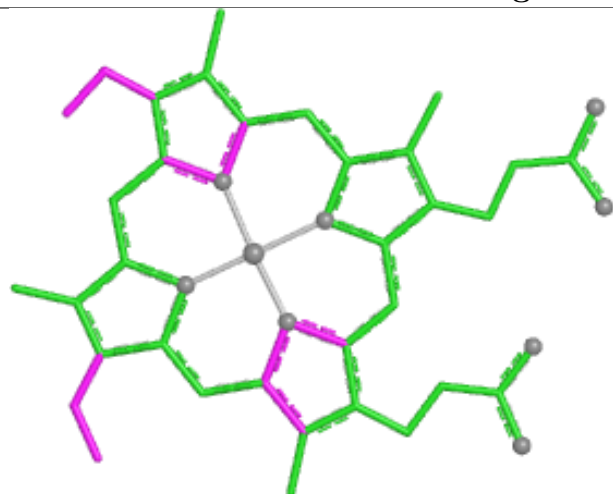
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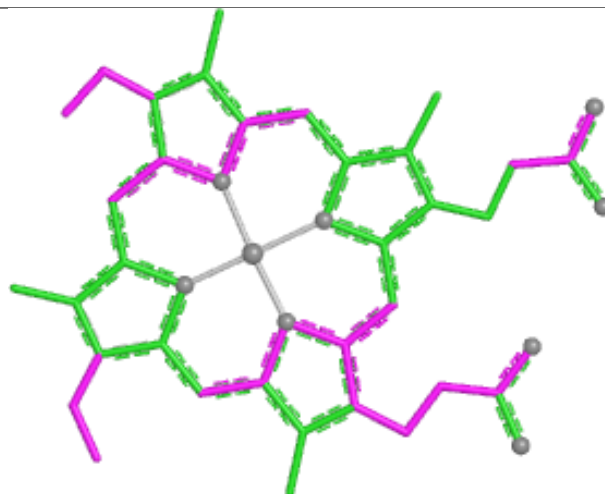
Rings



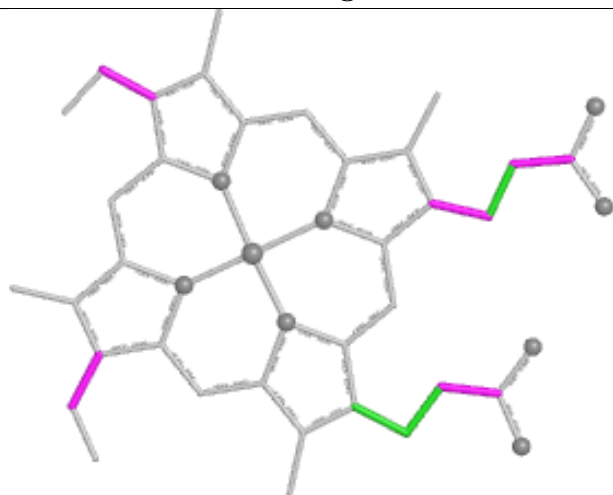
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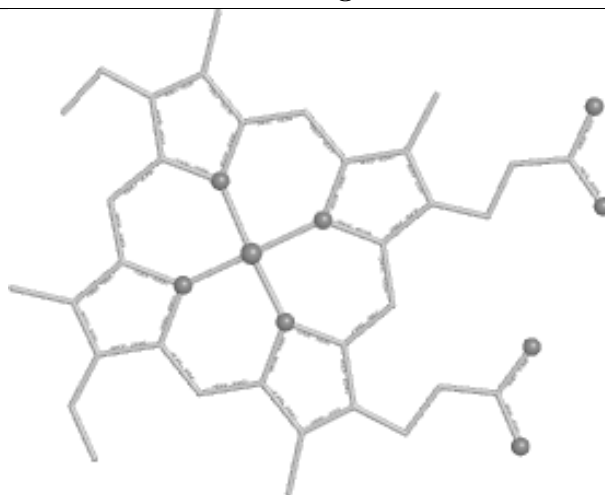
Bond lengths



Bond angles

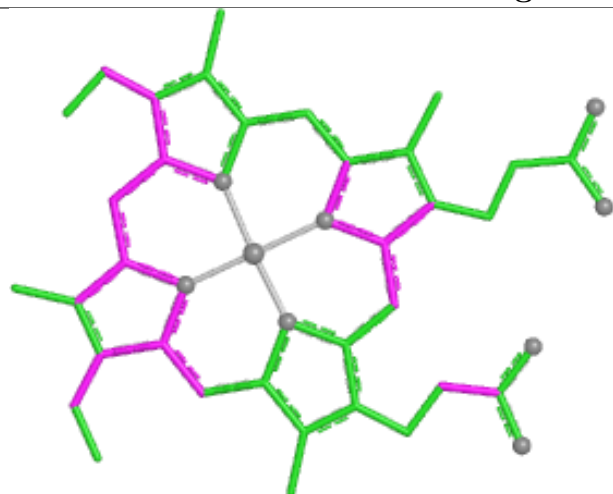


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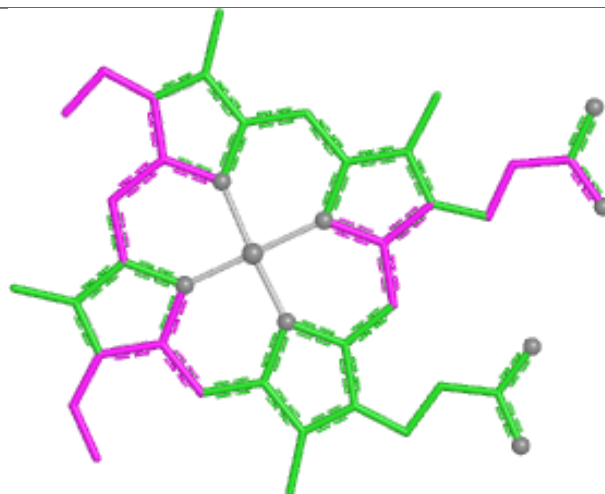


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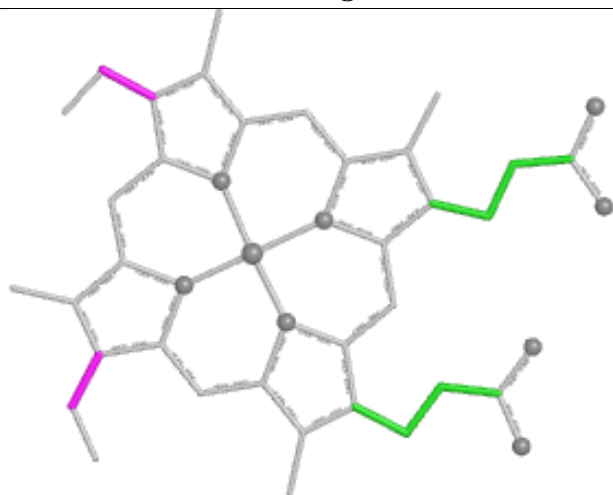
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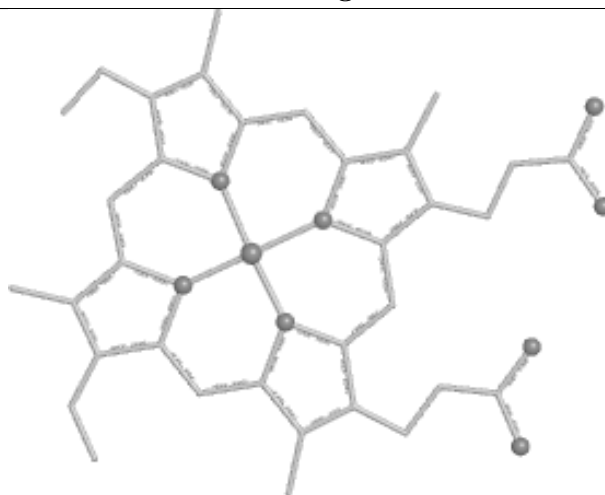
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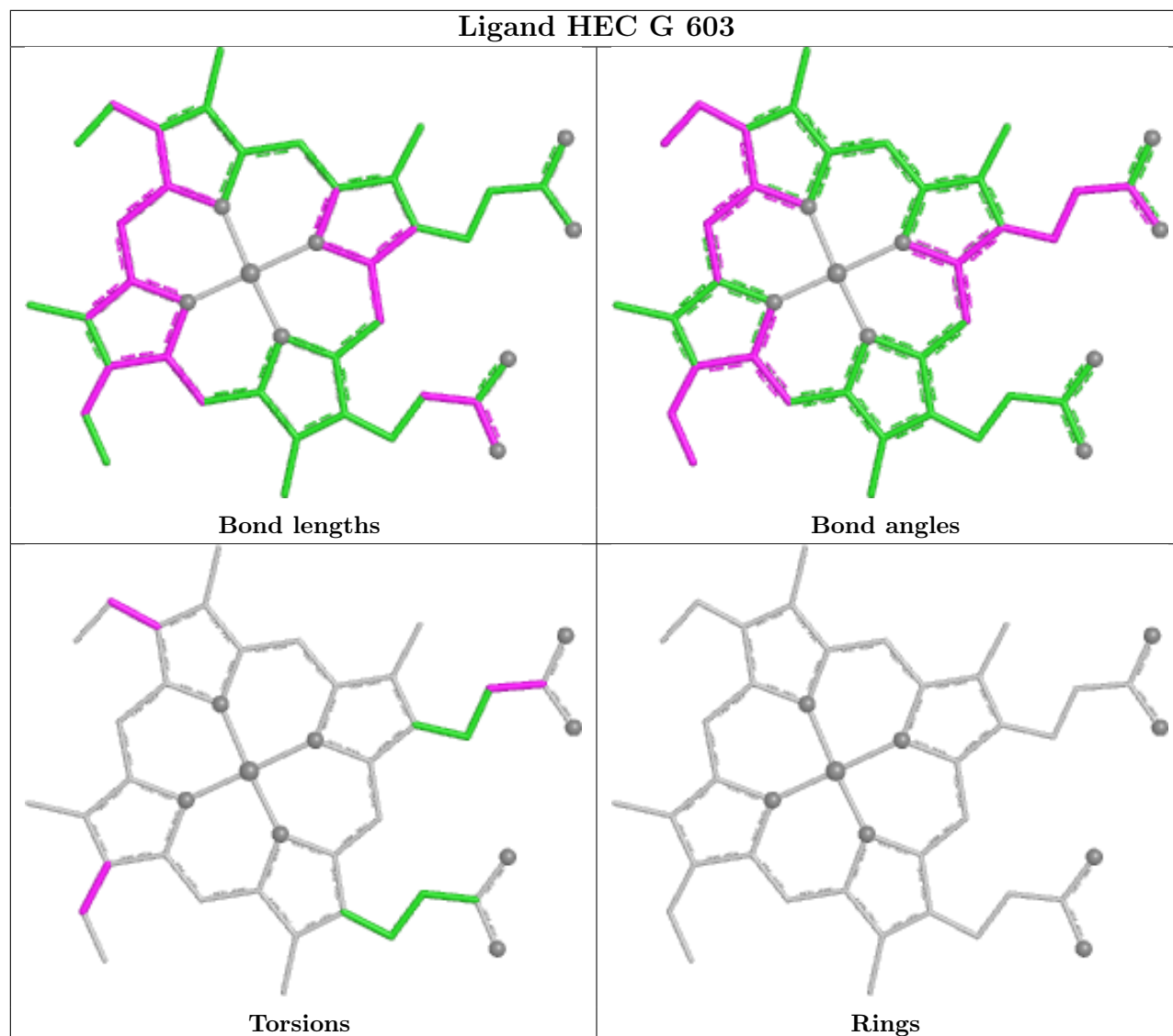
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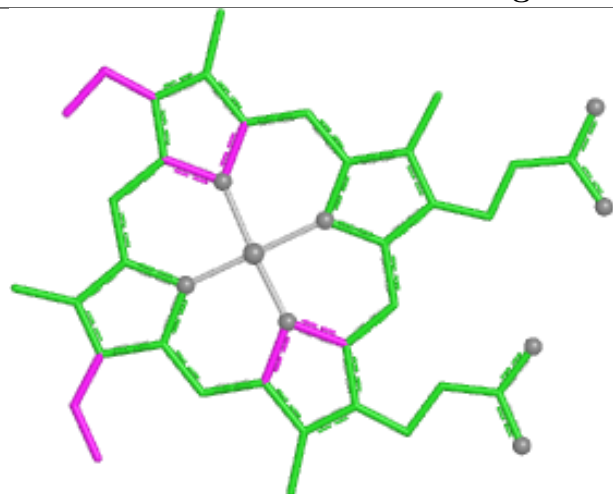
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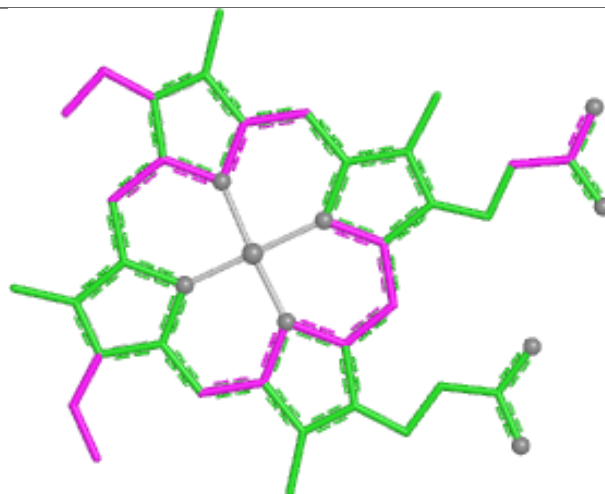
Rings



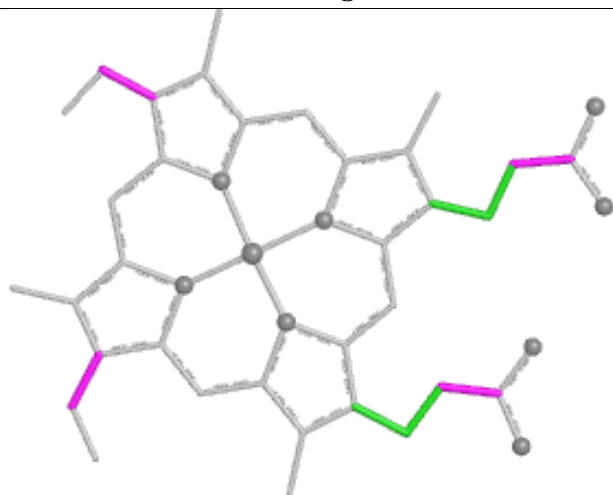
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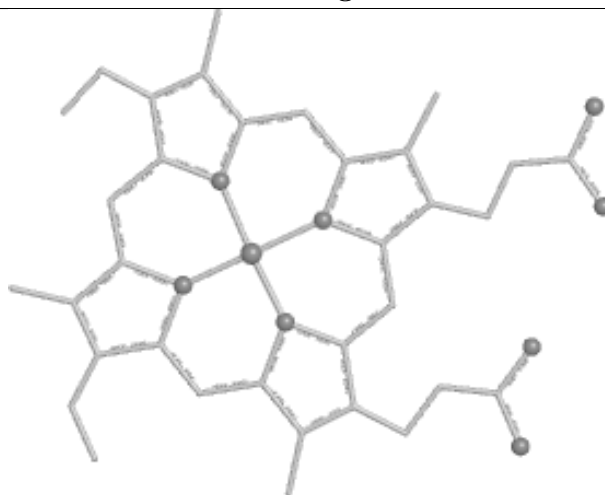
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Bond angles

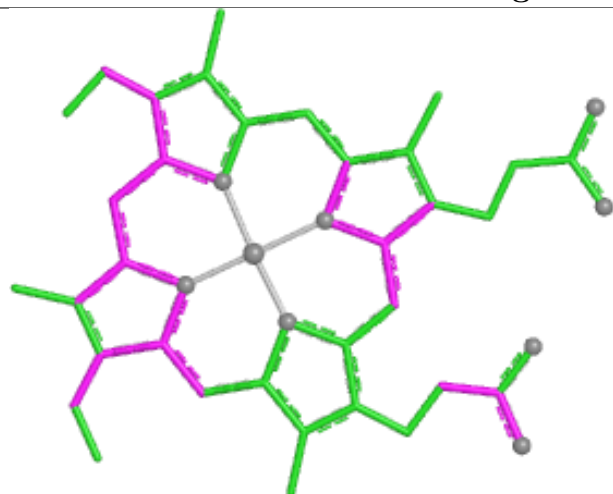


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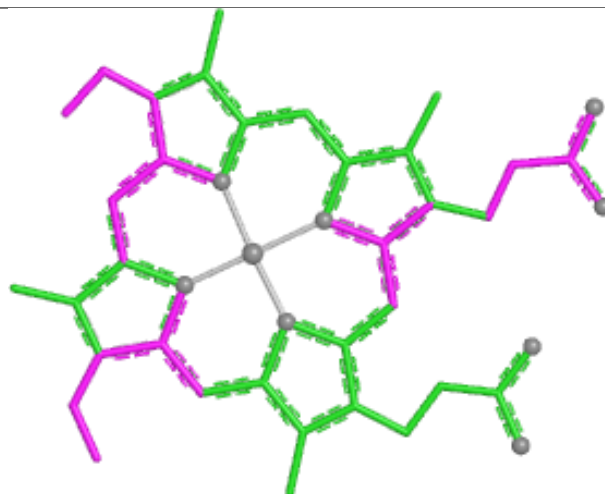


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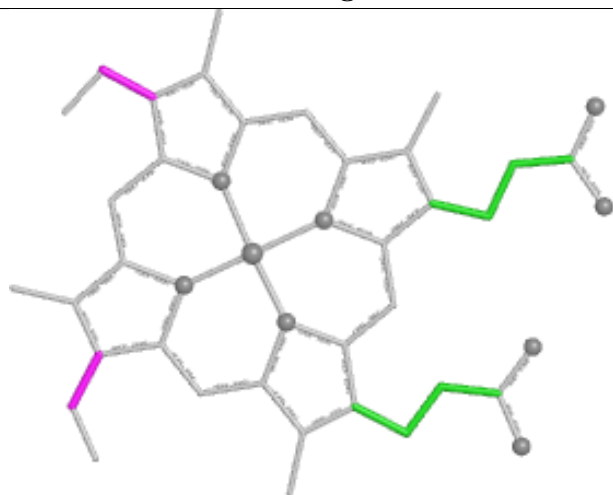
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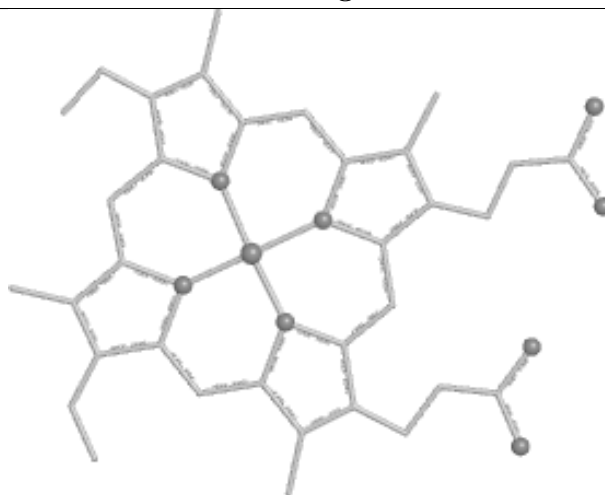
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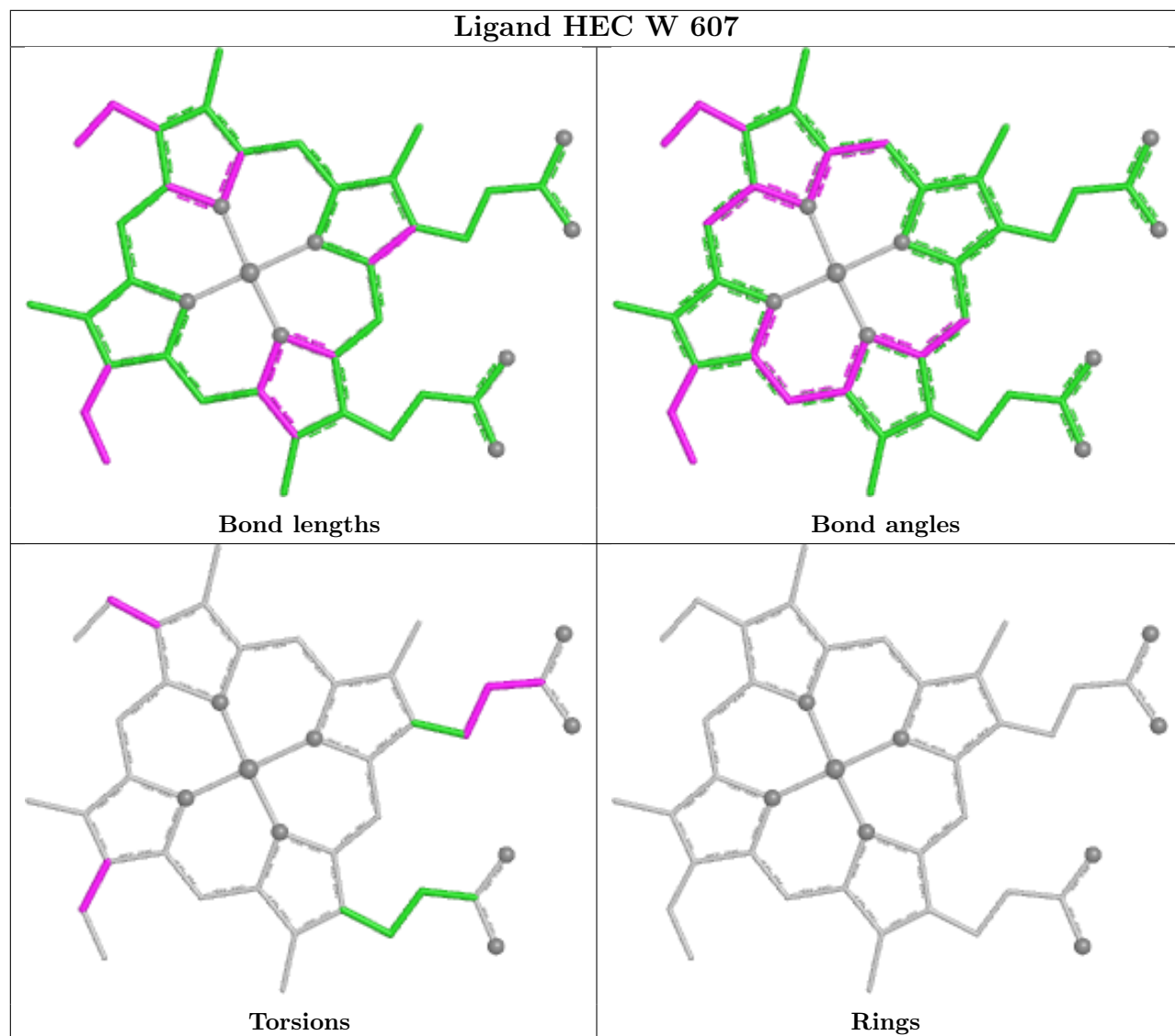
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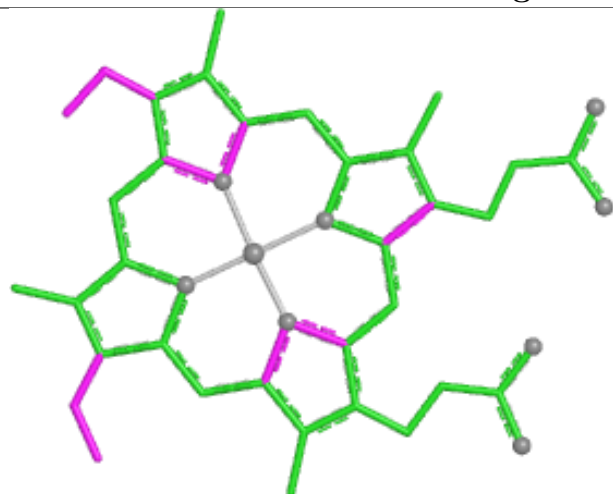
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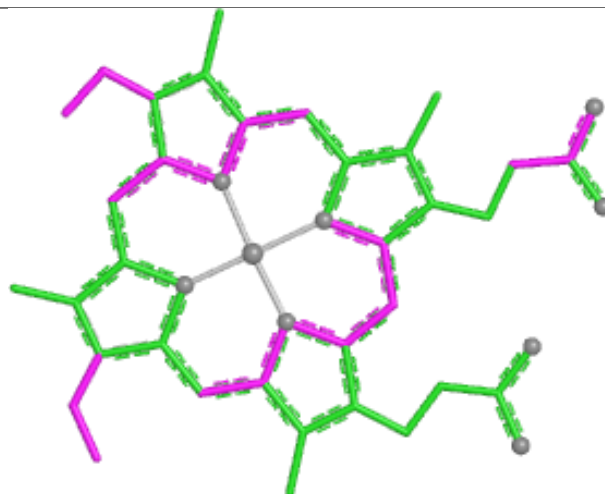
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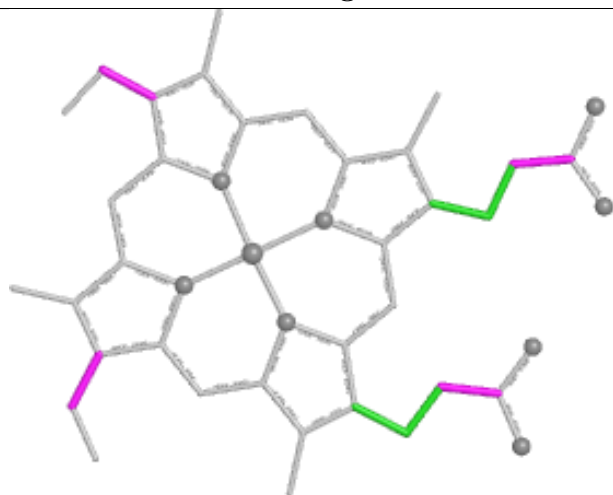
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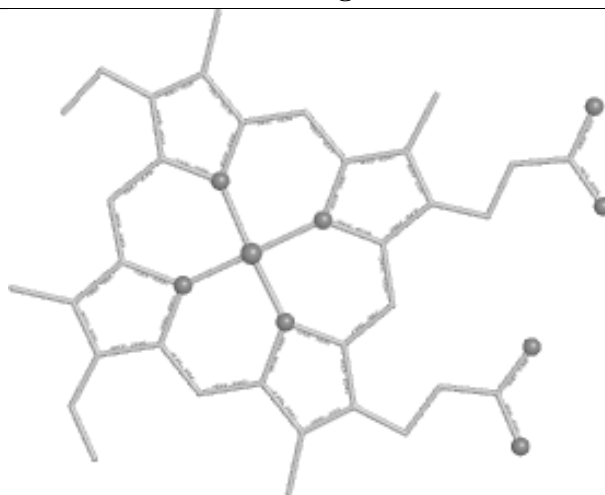
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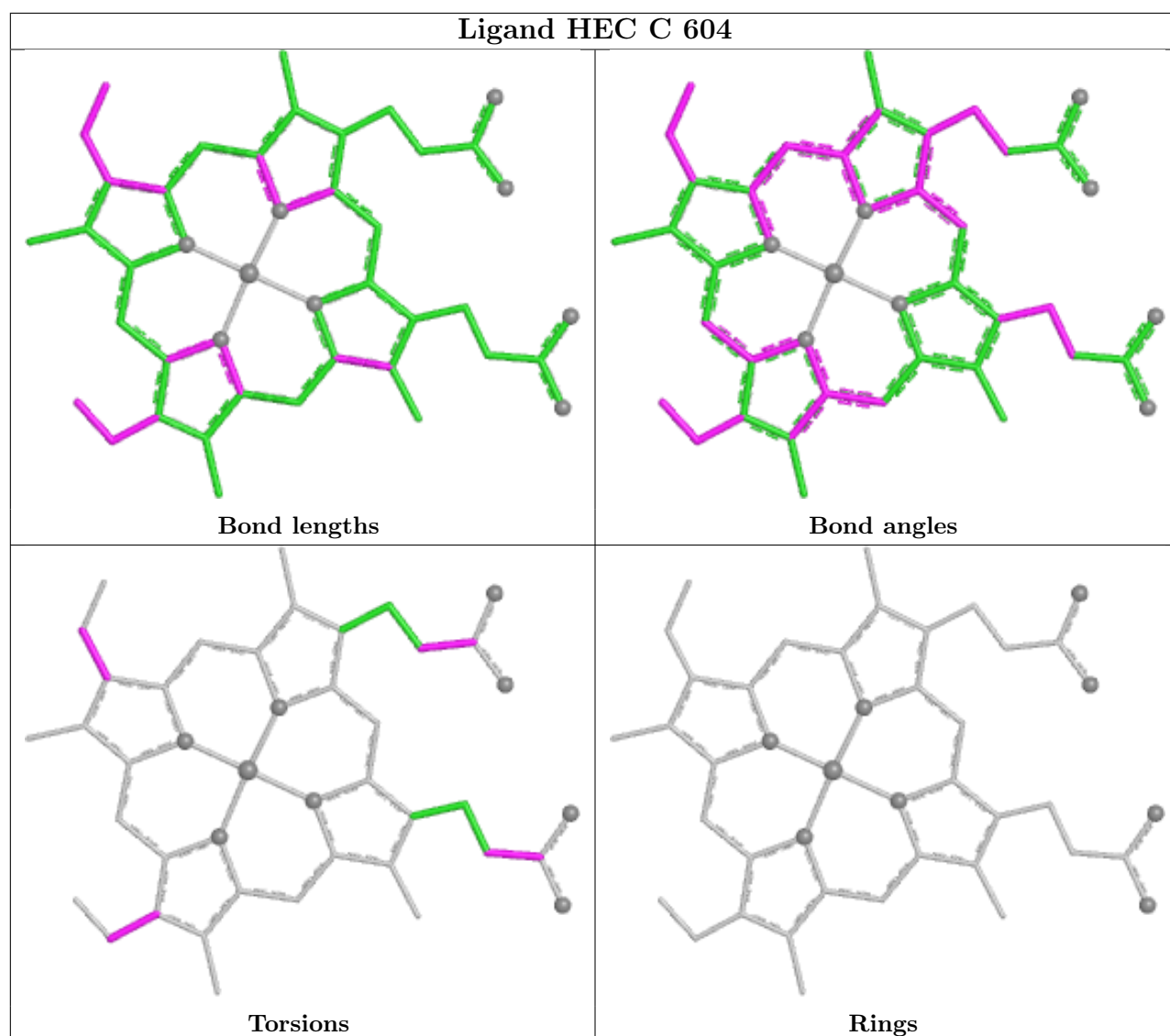
Bond angles



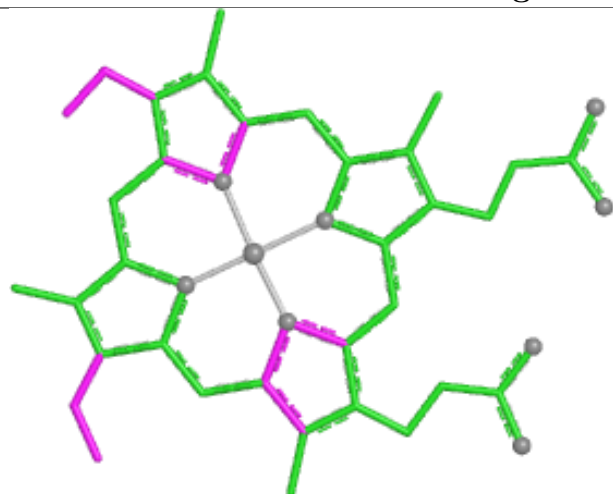
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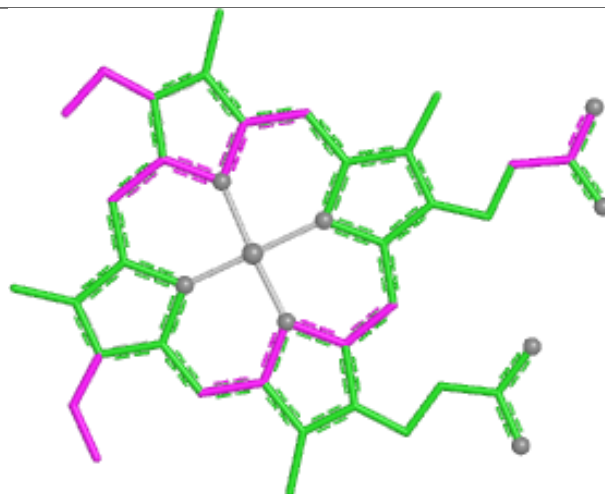
Rings



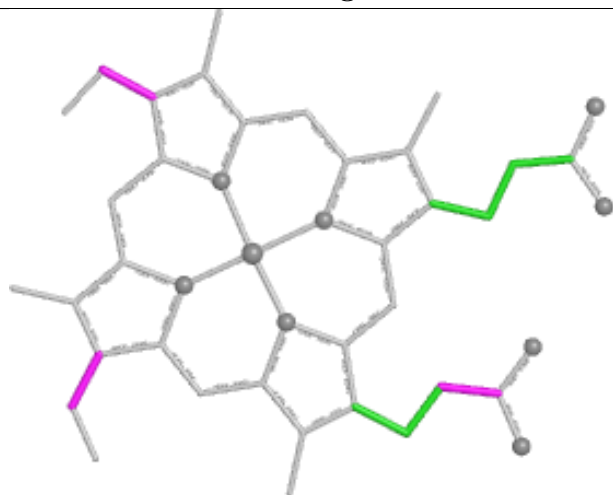
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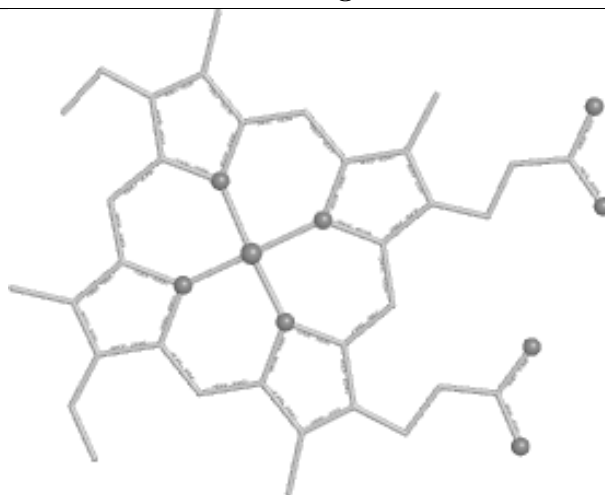
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Bond angles

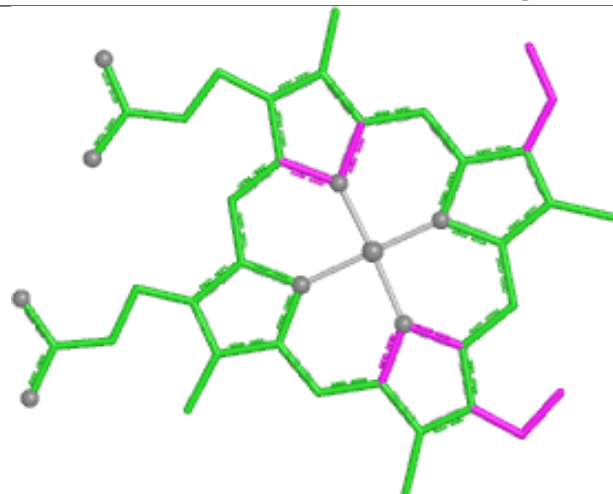


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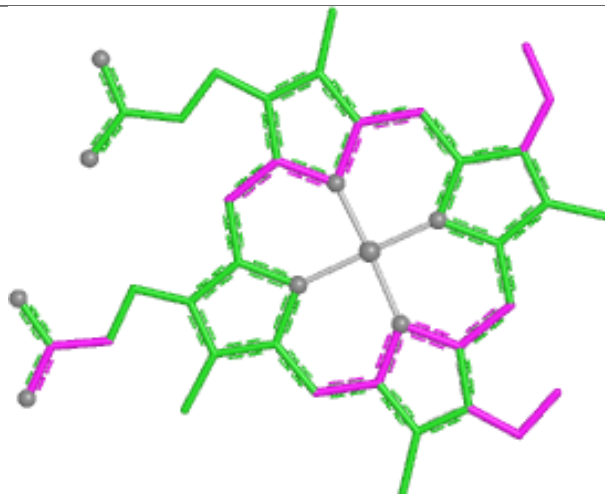


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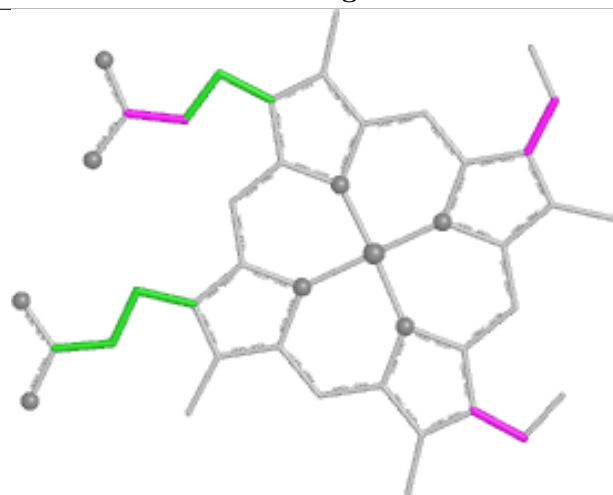
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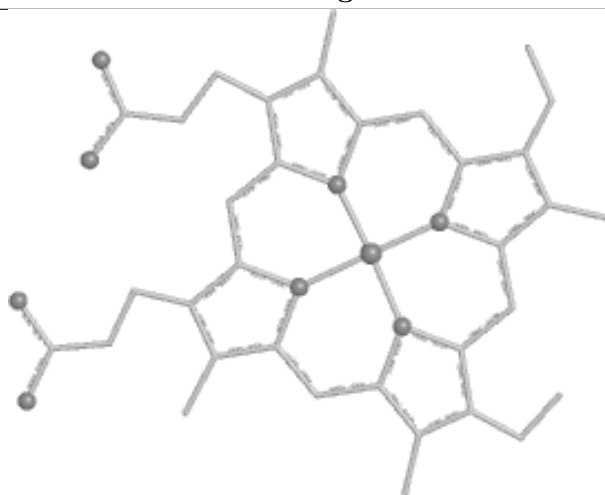
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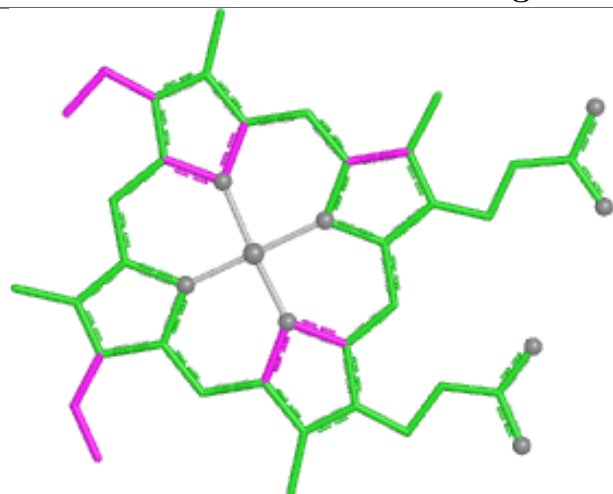


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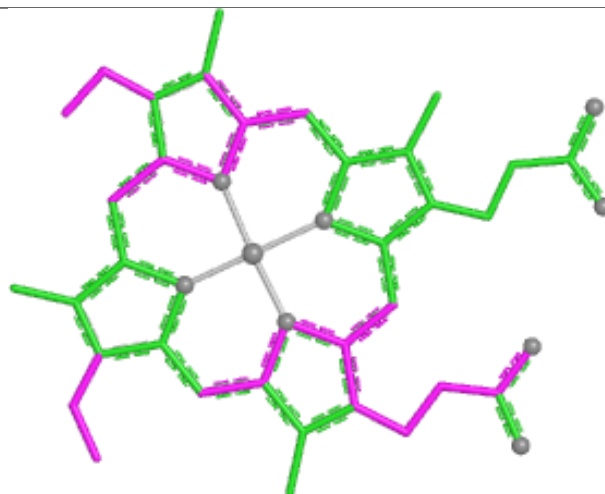


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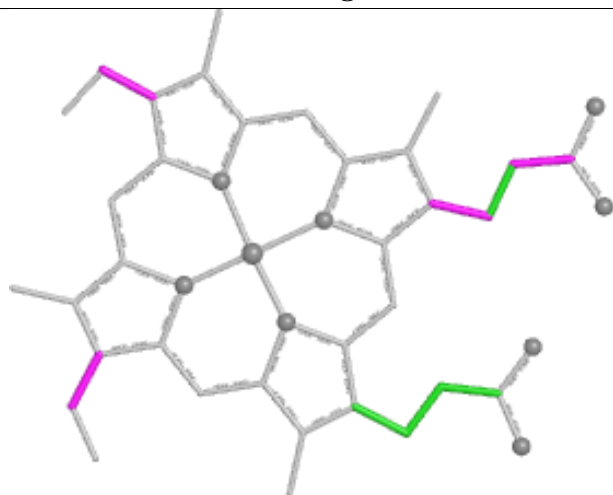
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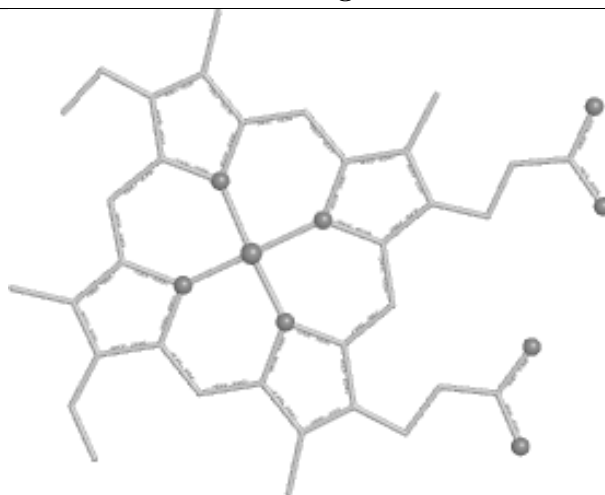
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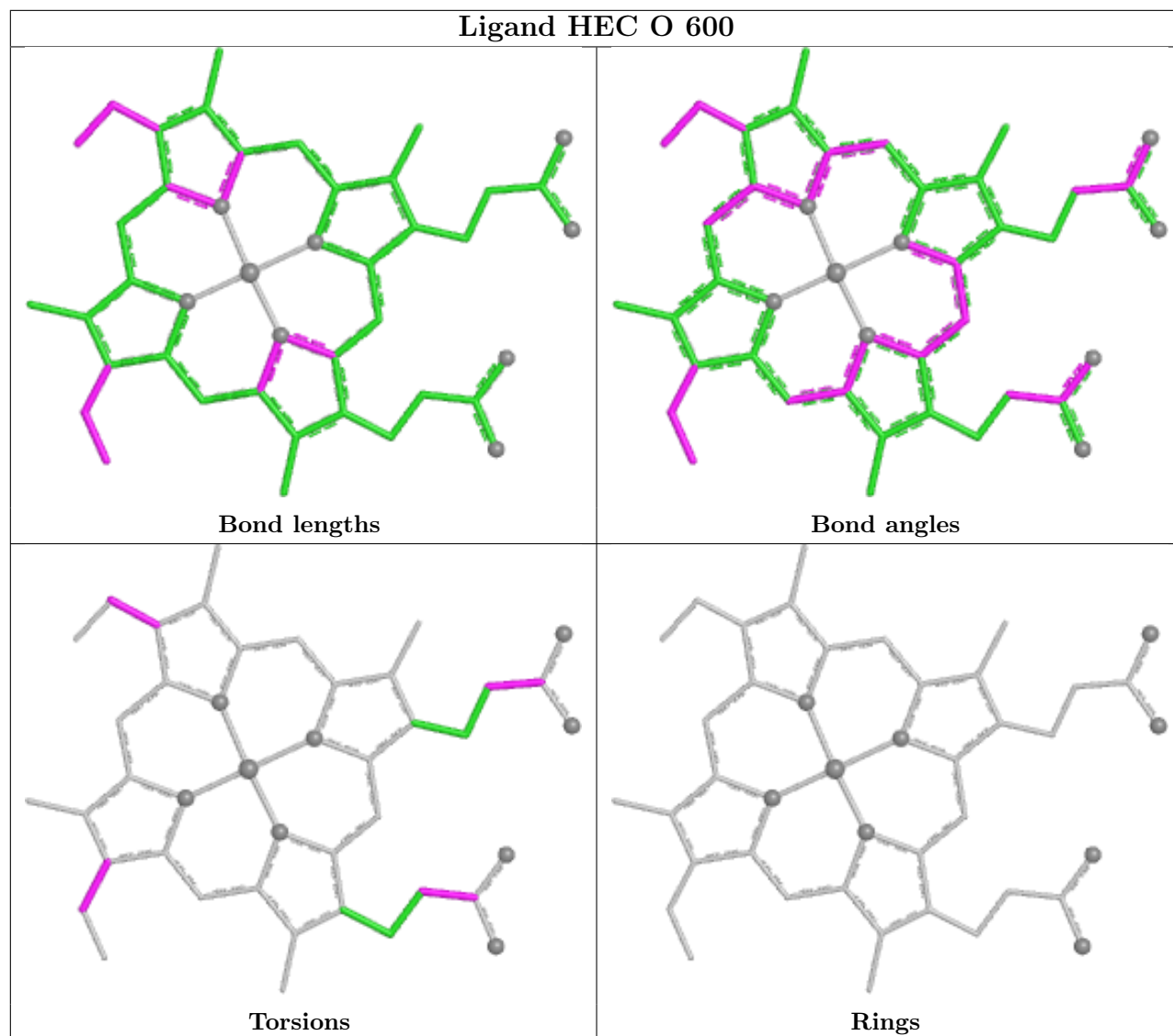
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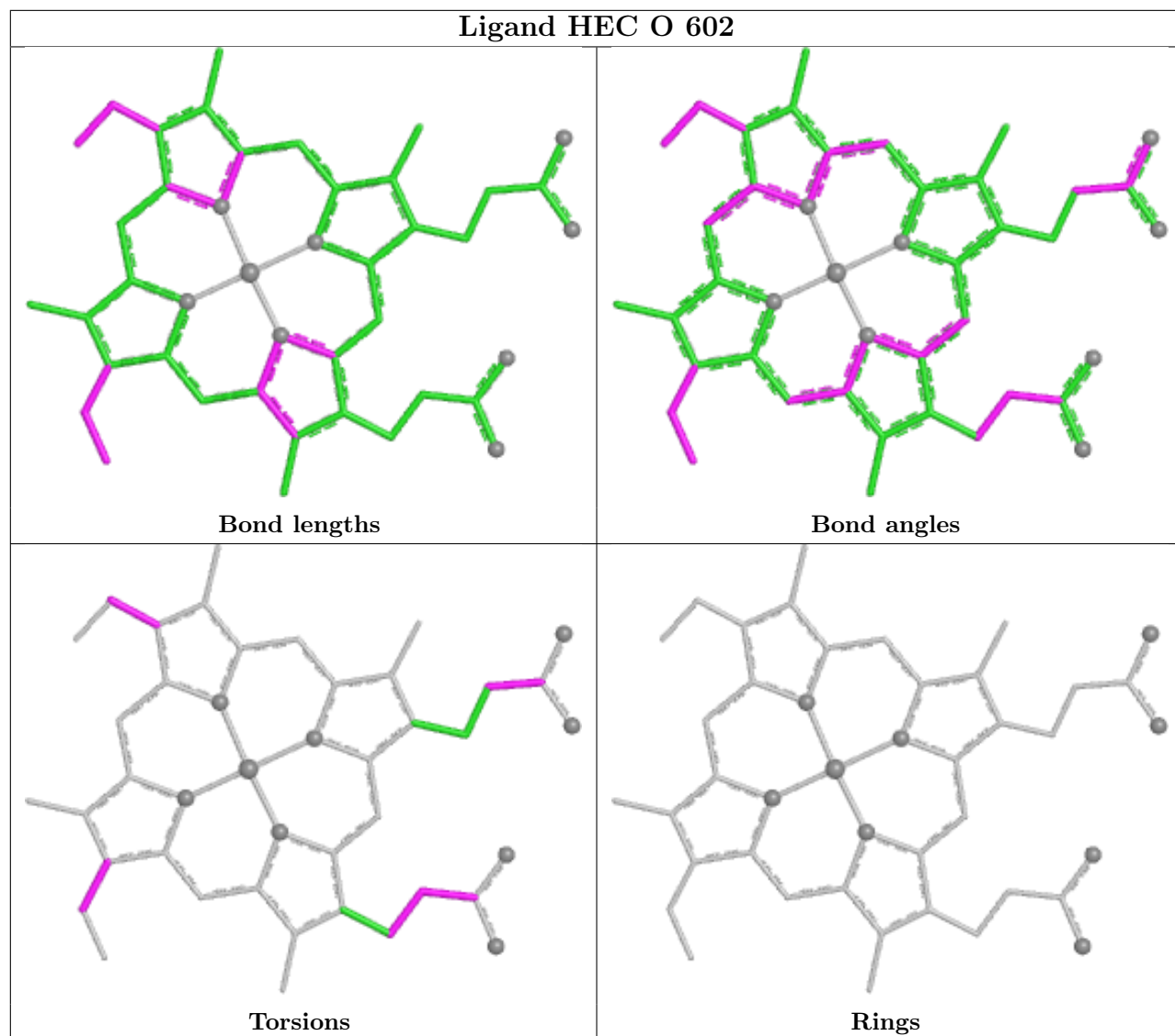


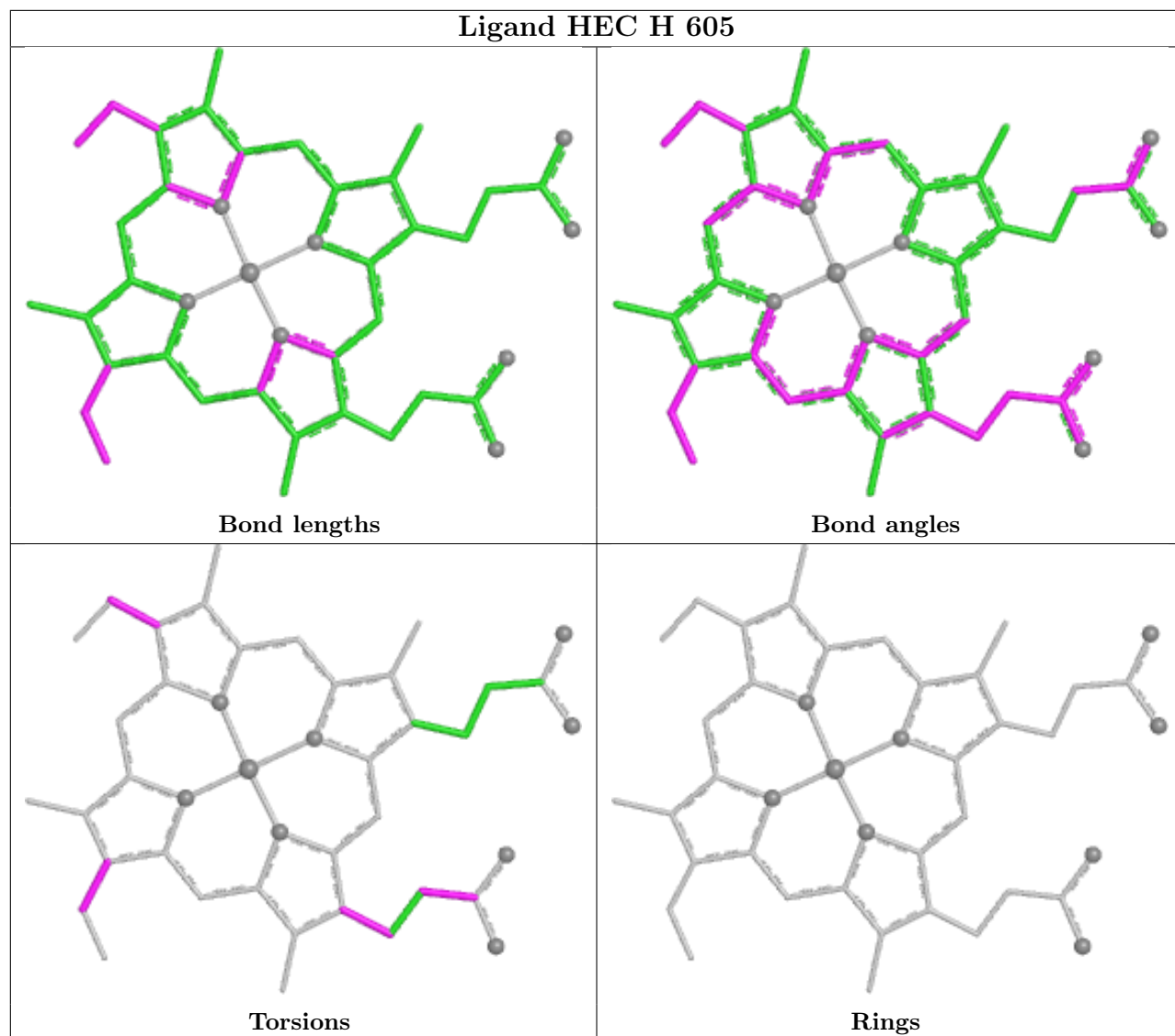
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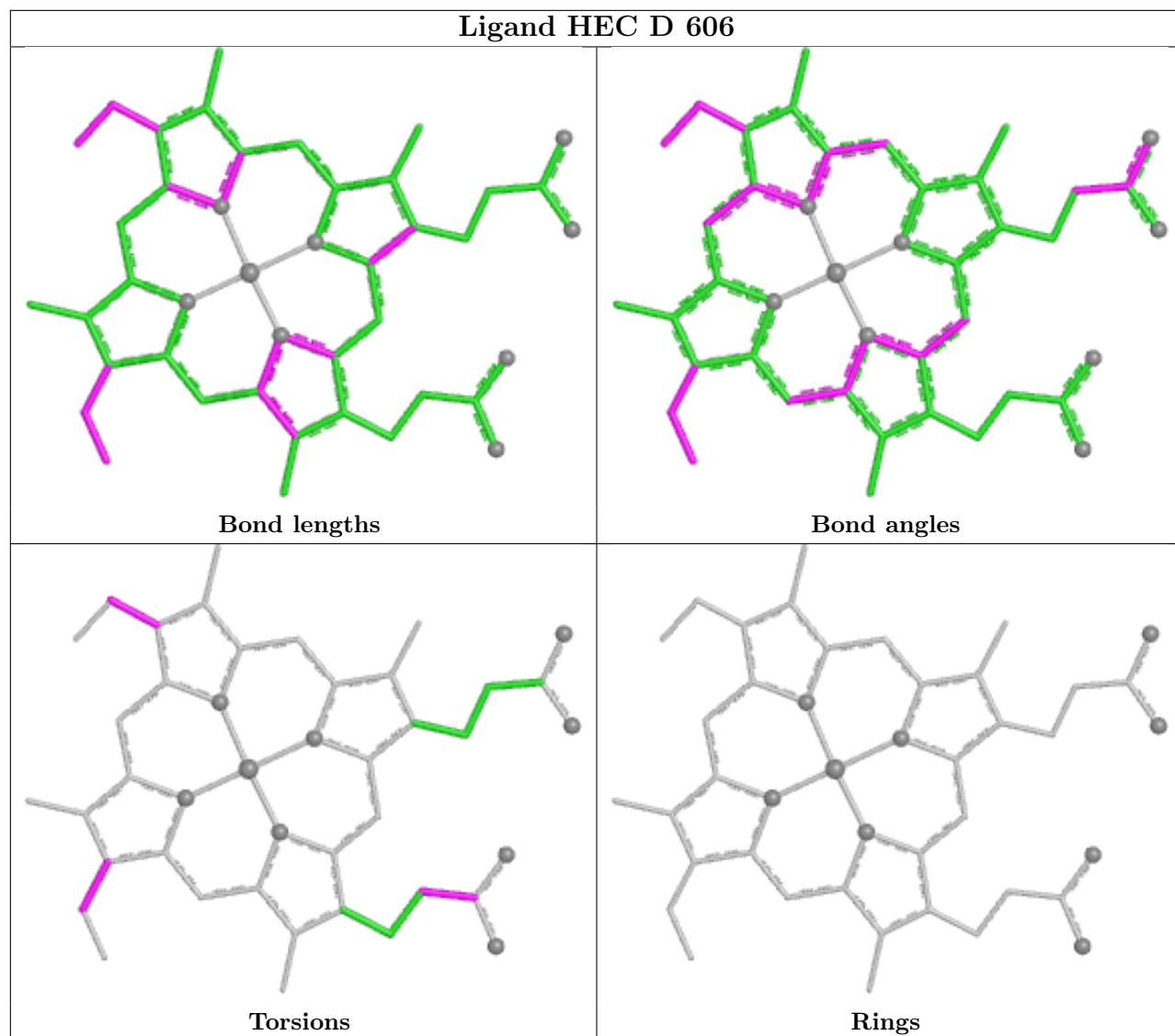


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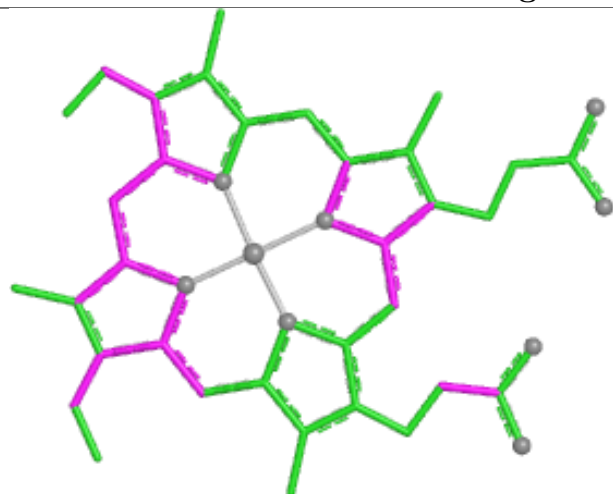




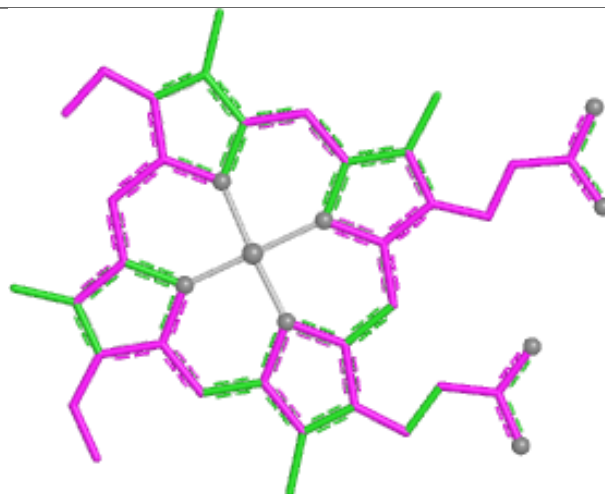




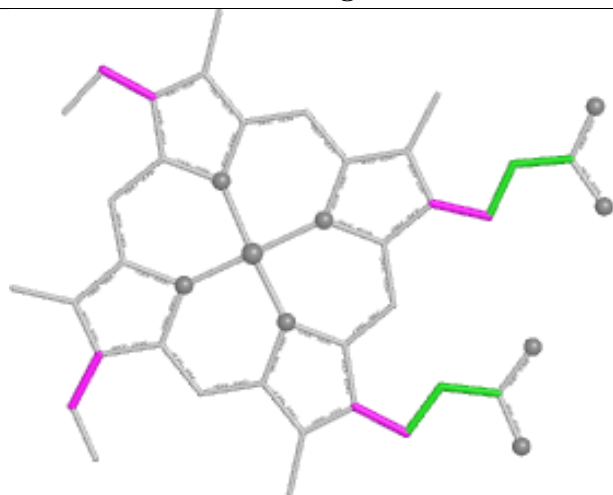
Ligand HEC I 603



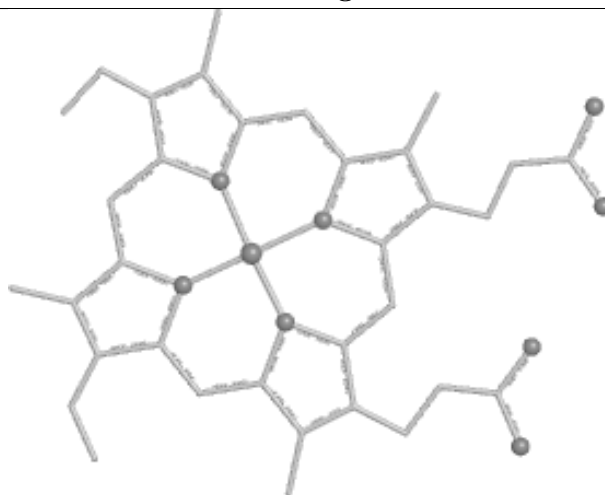
Bond lengths



Bond angles

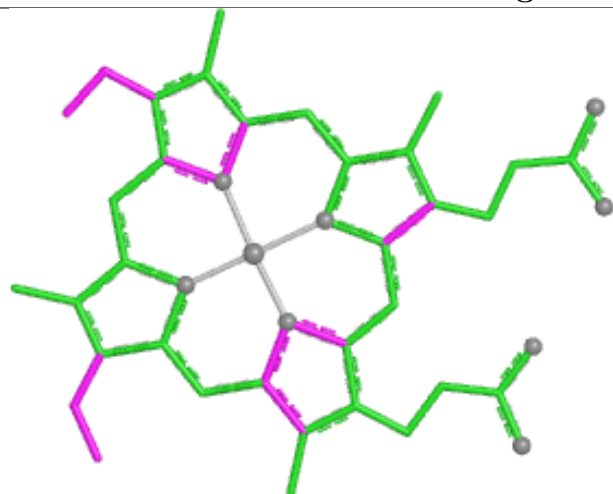


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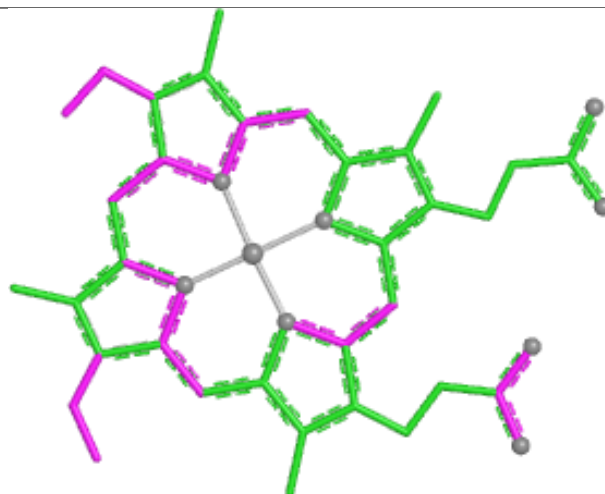


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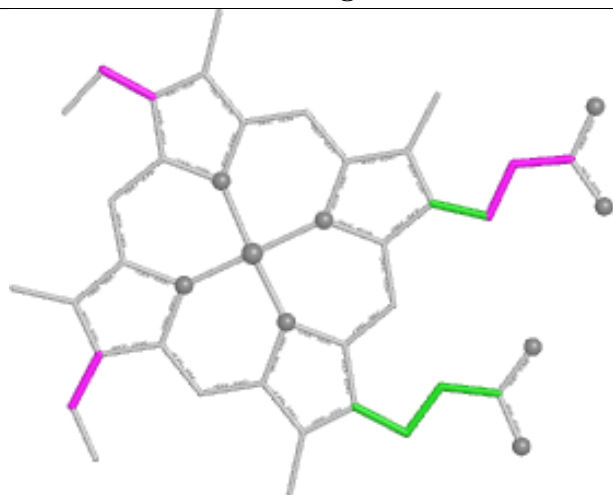
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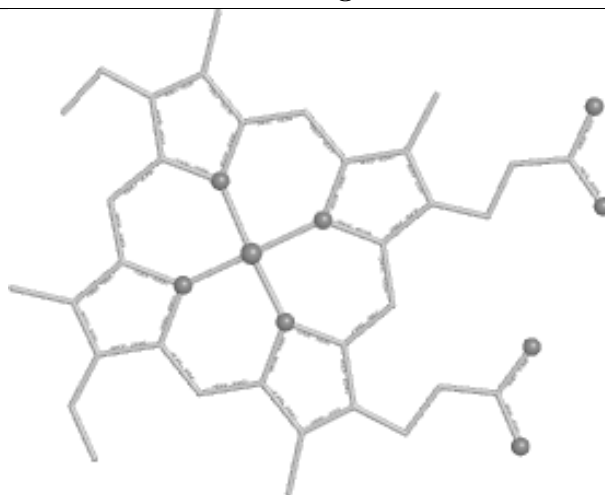
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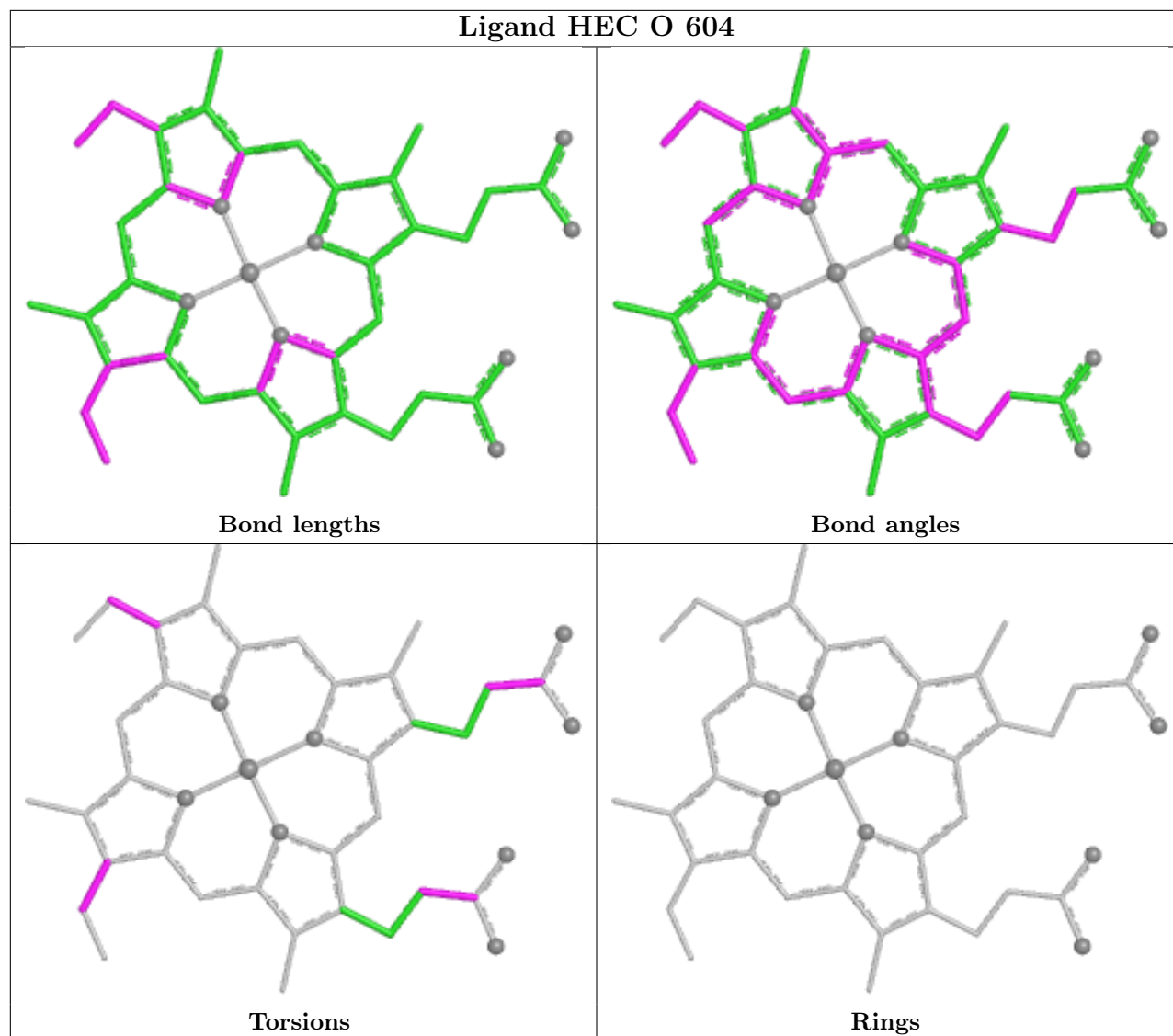
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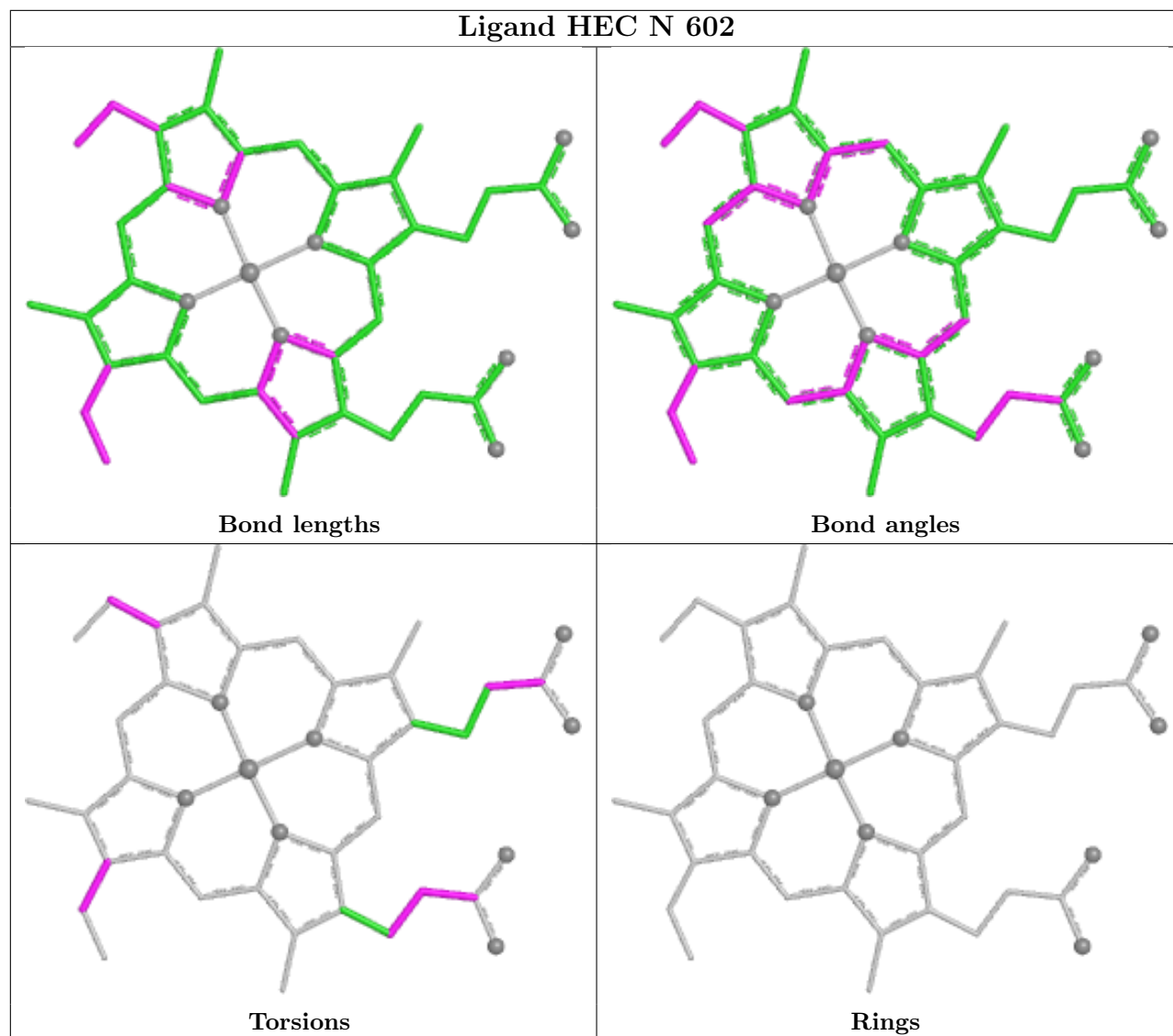


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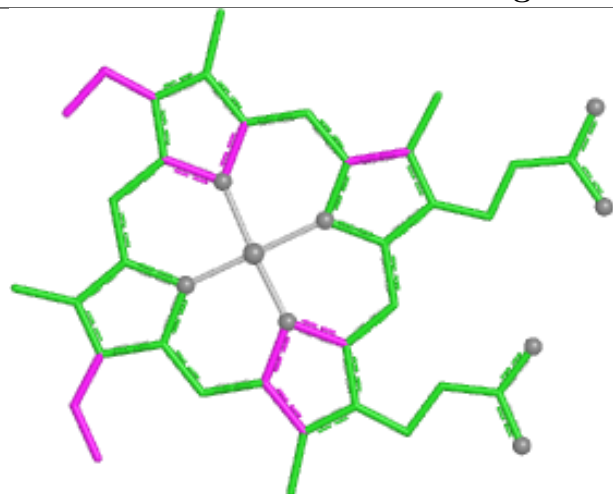


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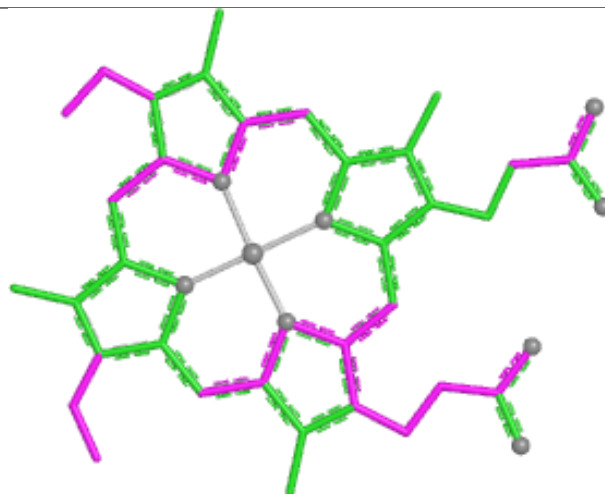




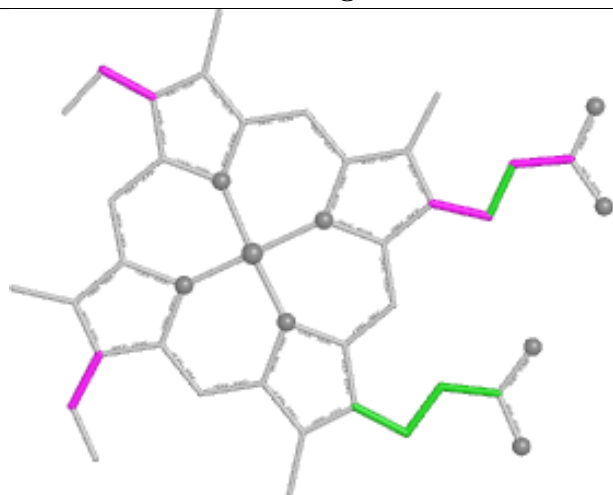
Ligand HEC T 601



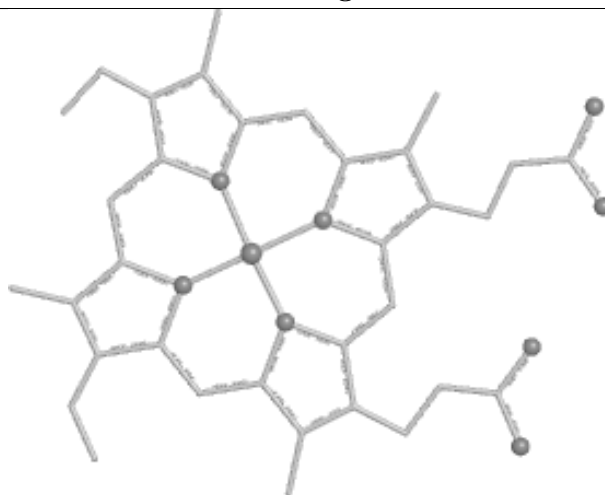
Bond lengths



Bond angles

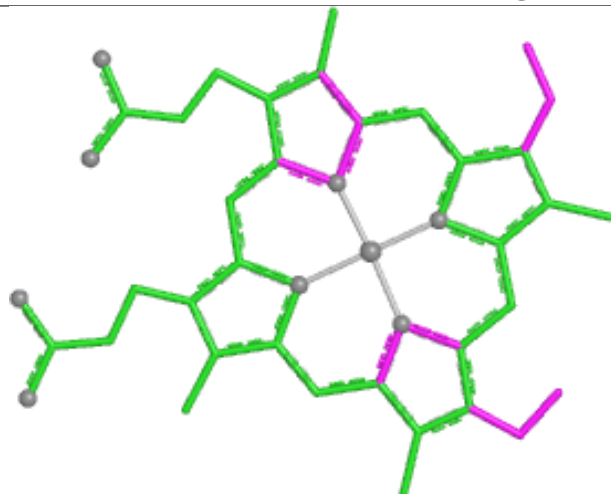


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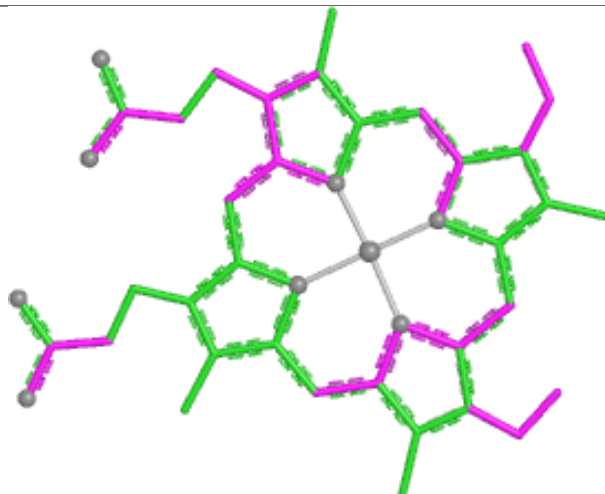


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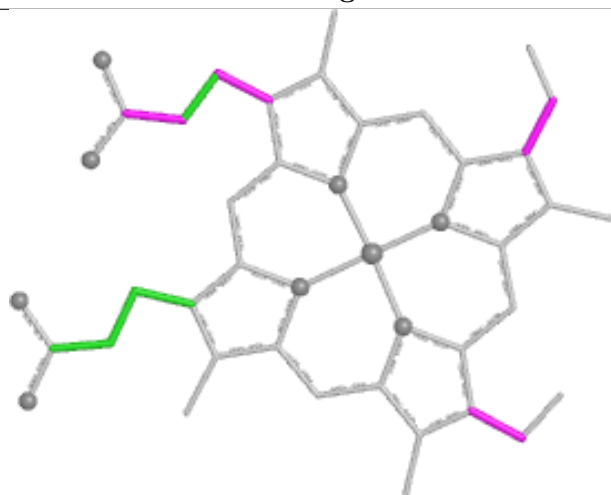
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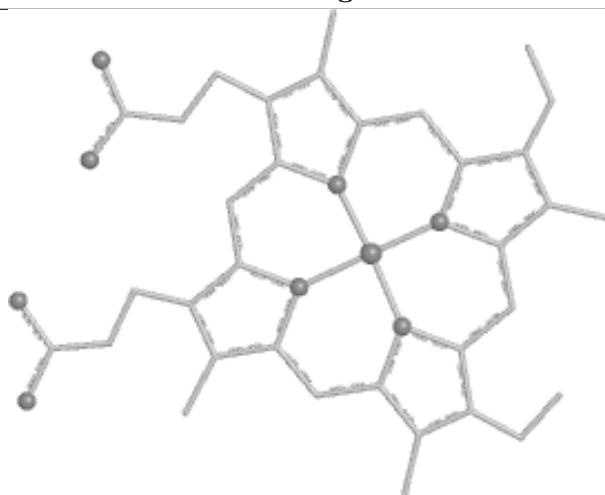
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Bond angles

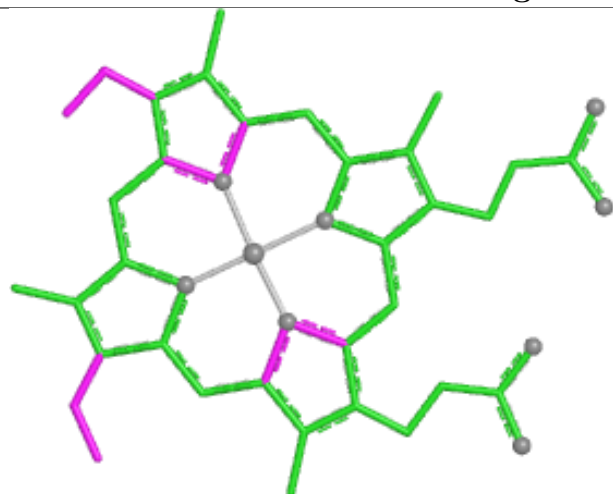


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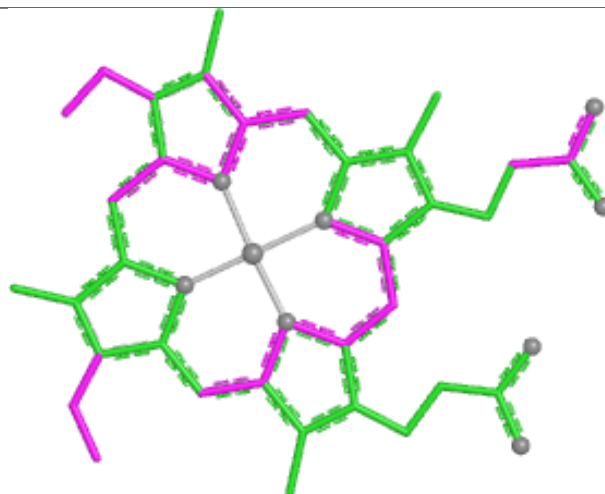


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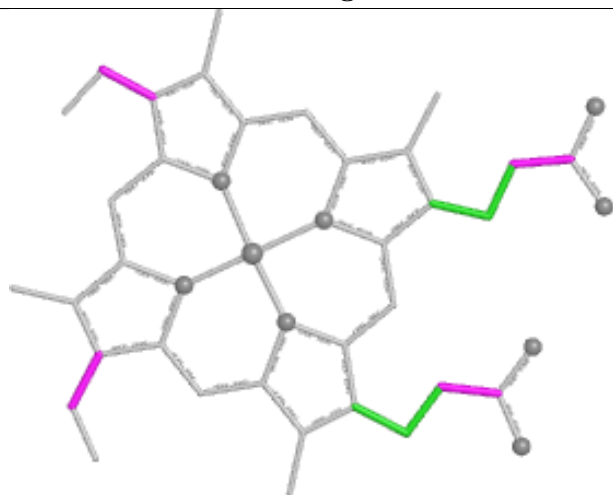
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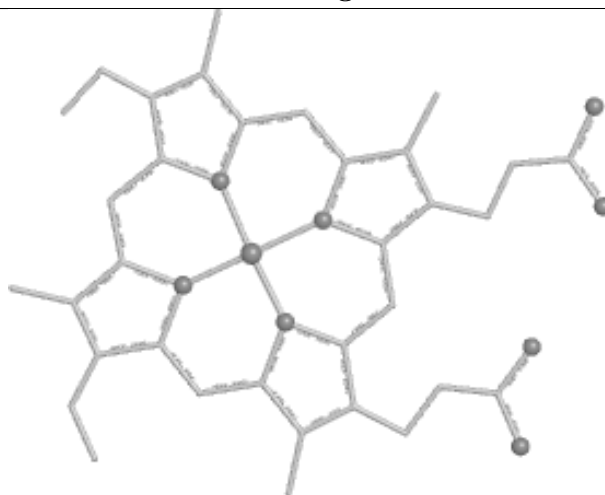
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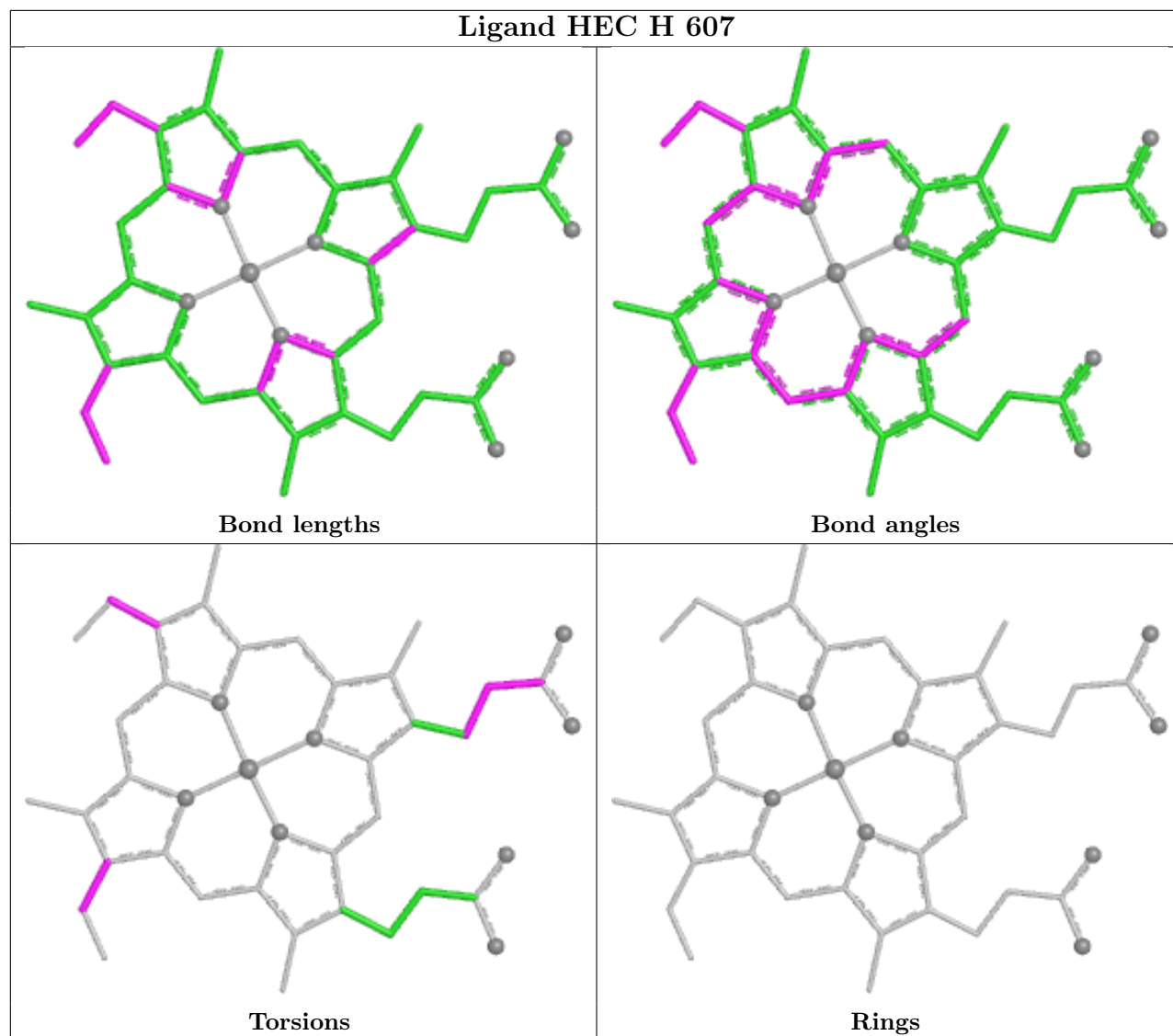
Bond angles

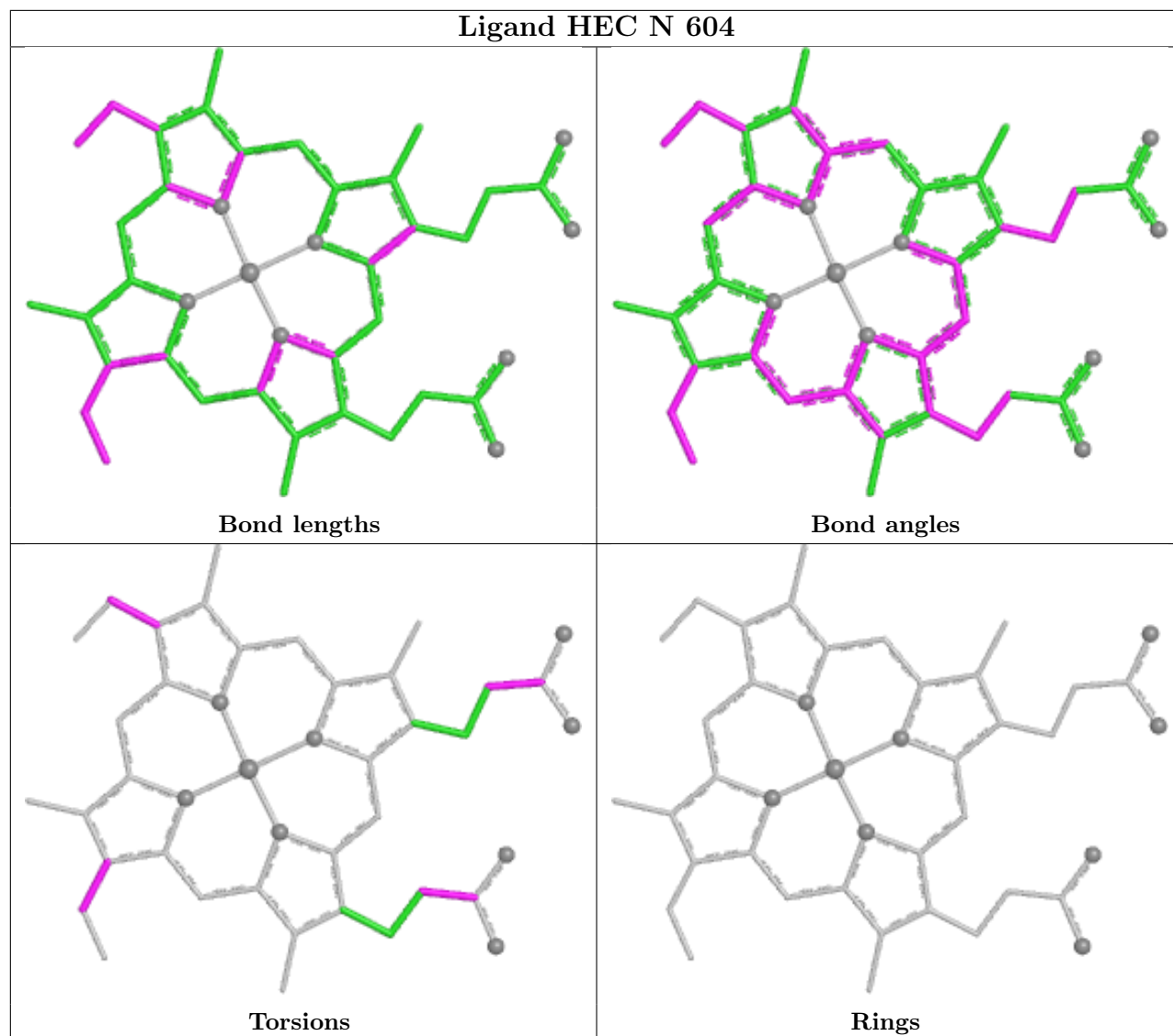


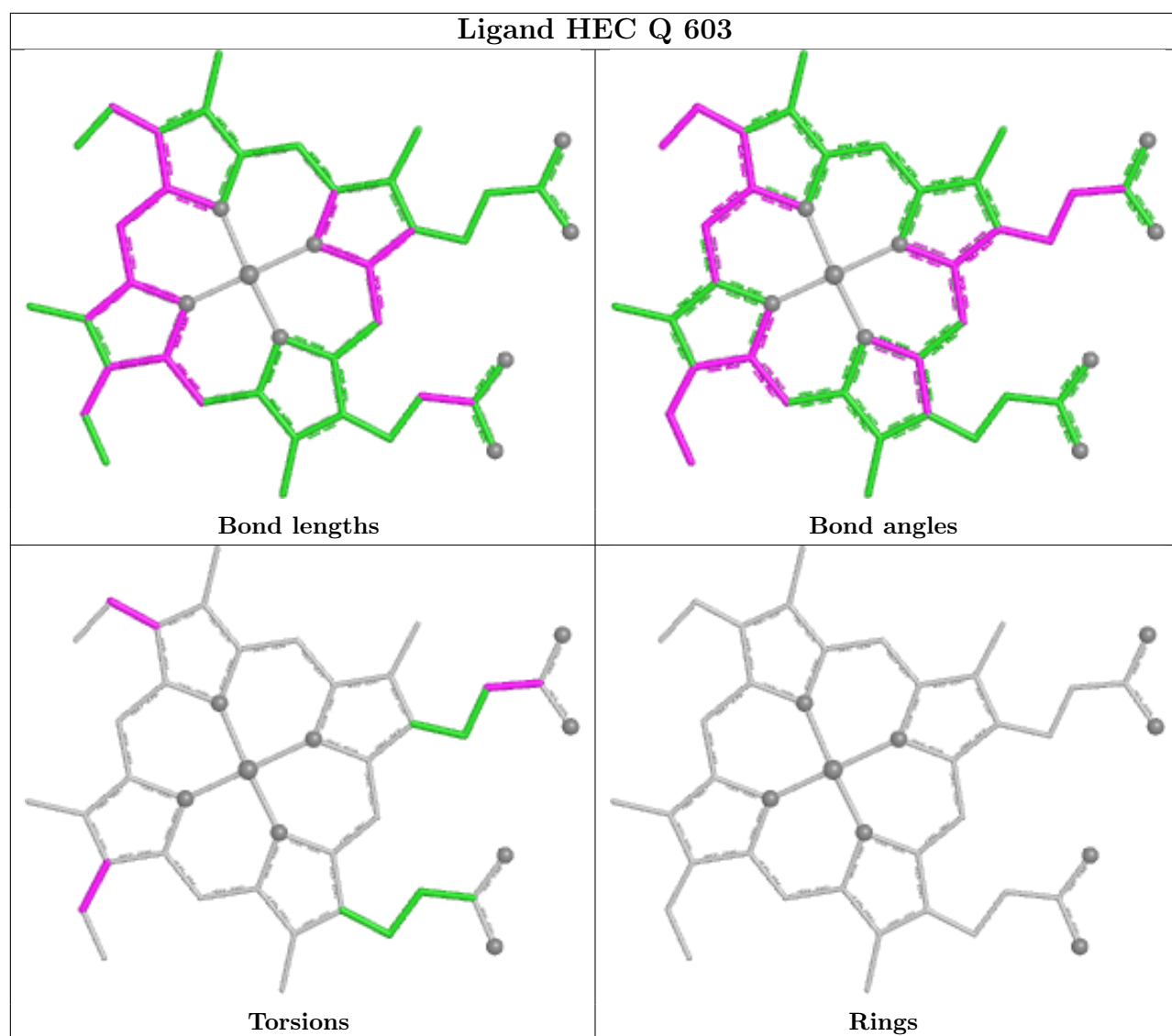
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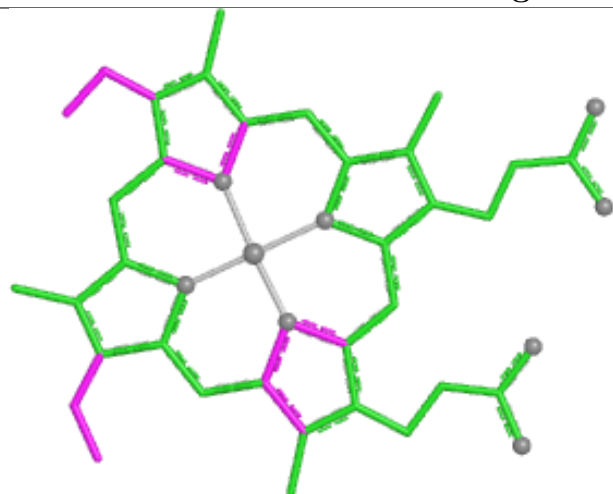
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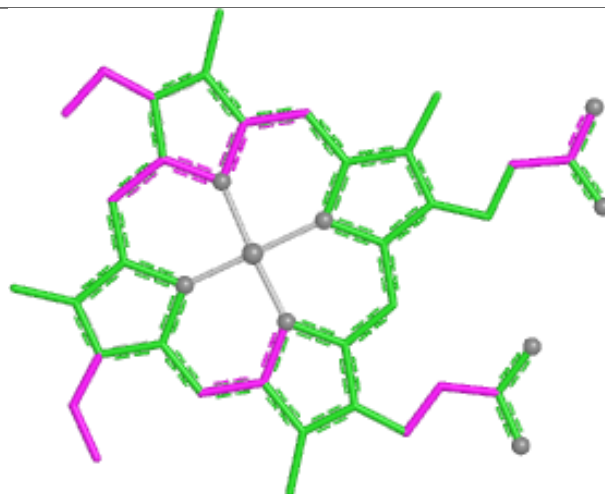




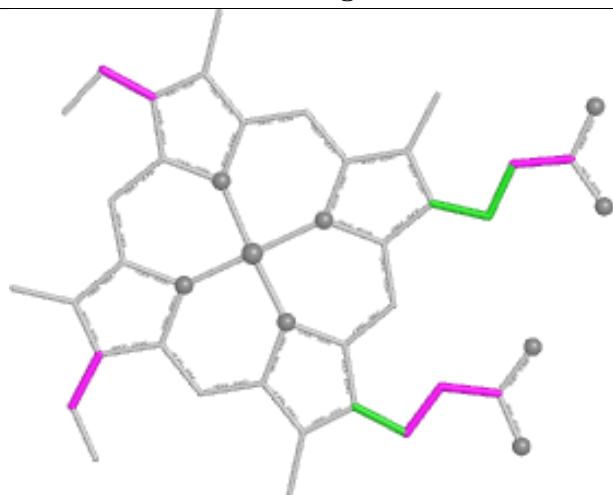
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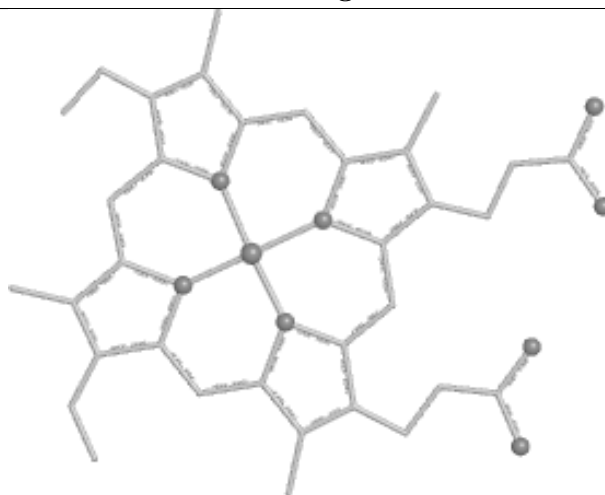
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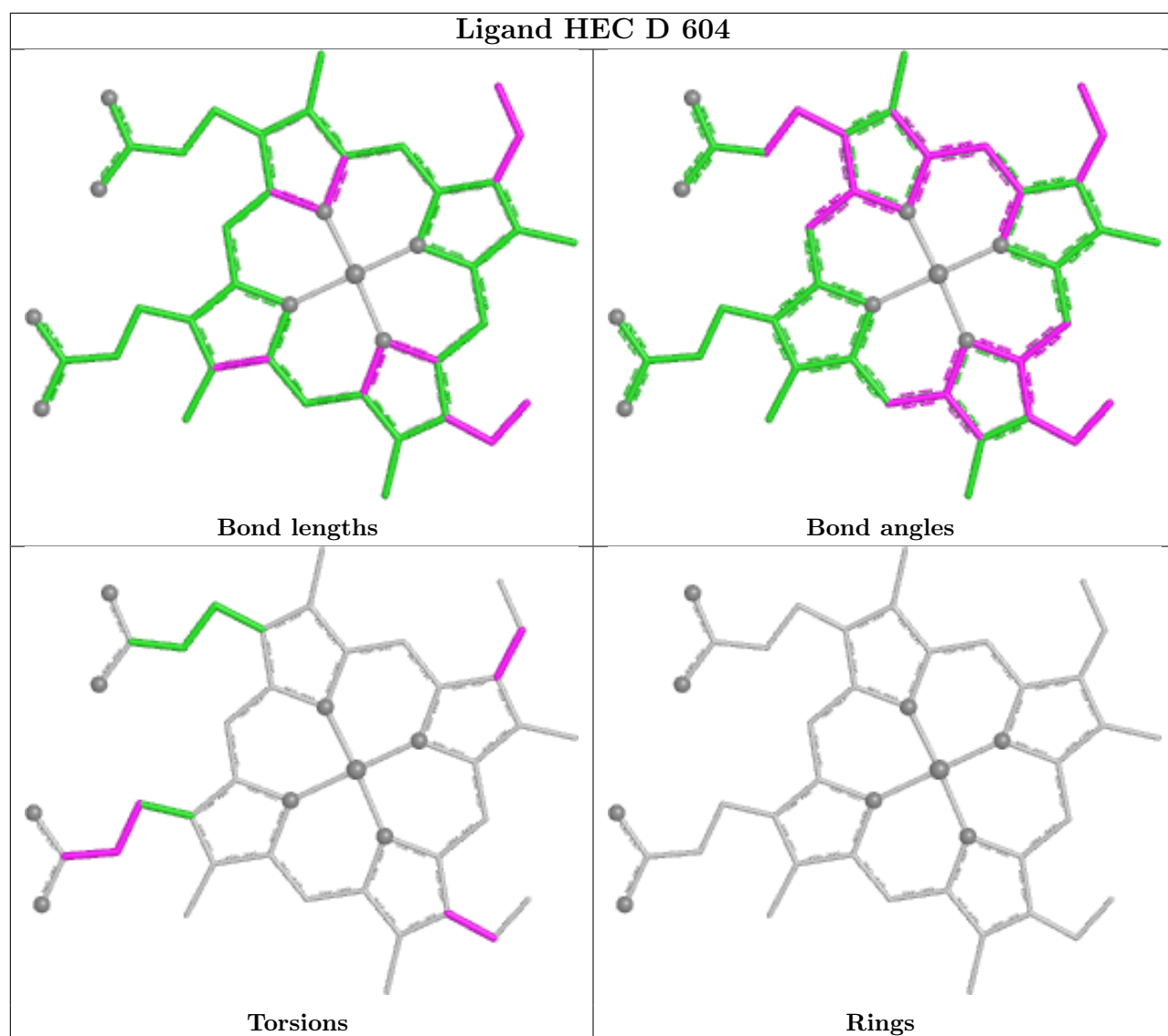
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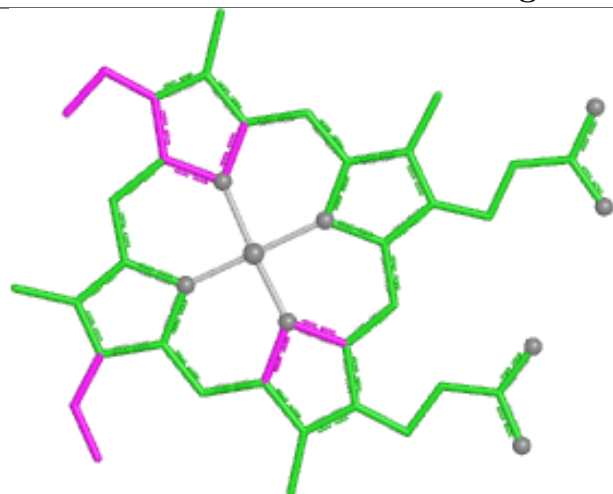
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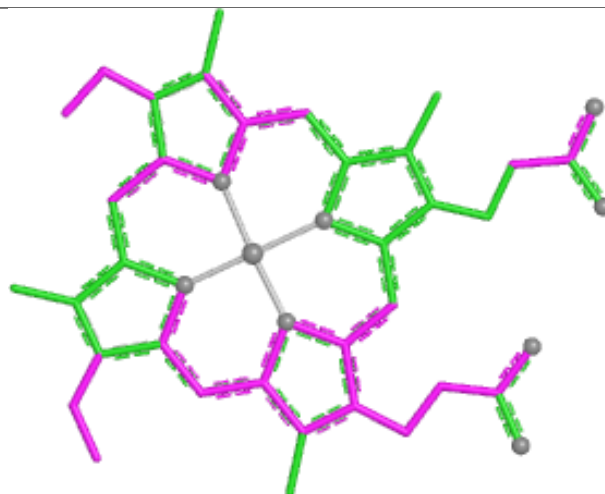
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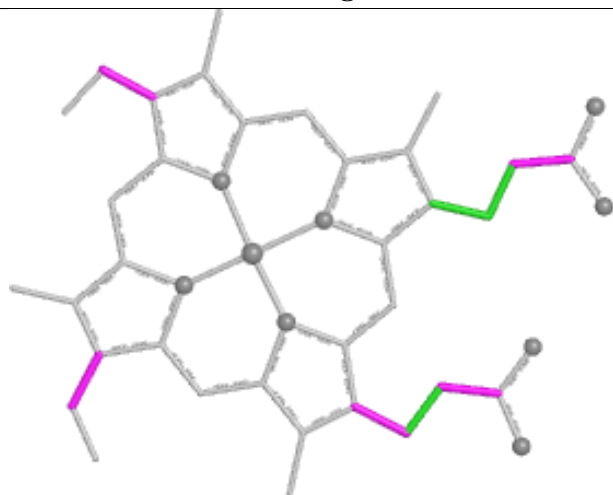
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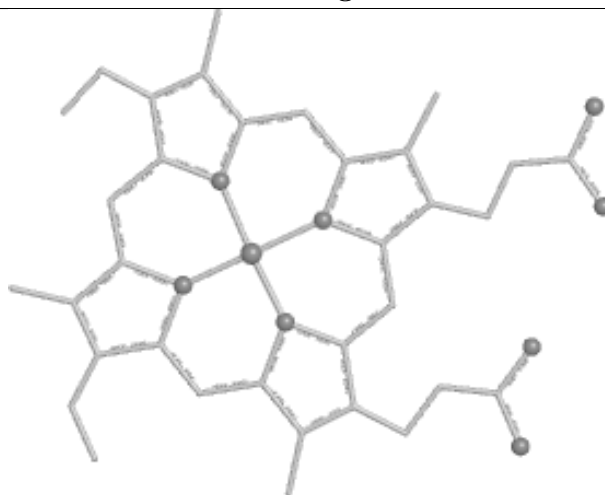
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Bond angles

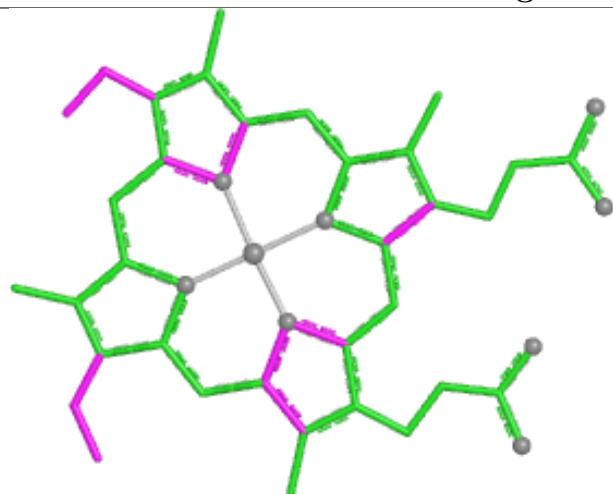


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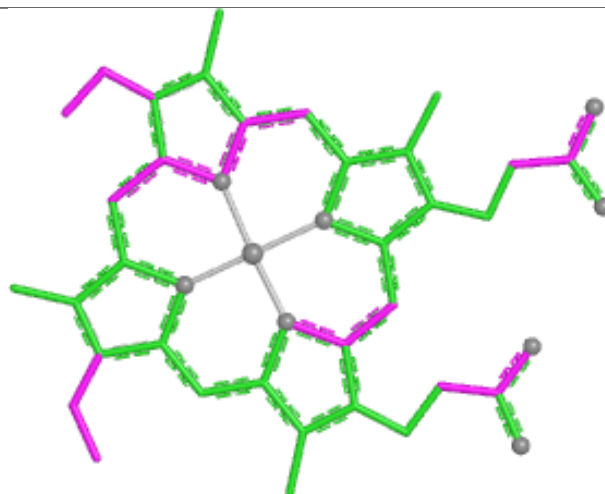


Rings

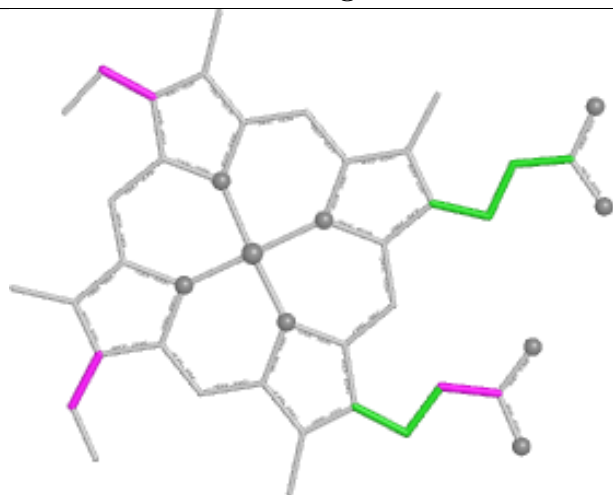
Ligand HEC J 606



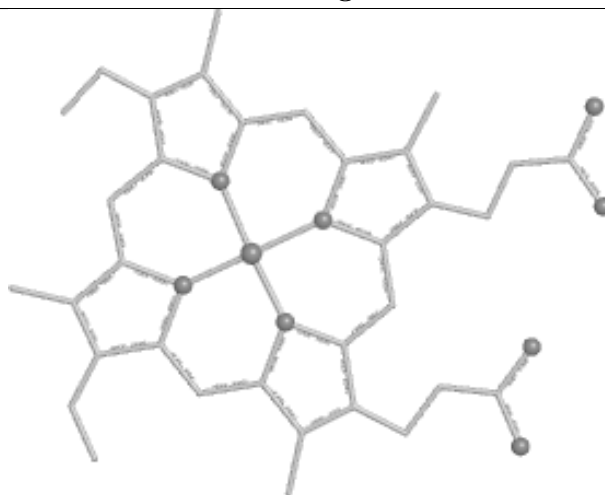
Bond lengths



Bond angles

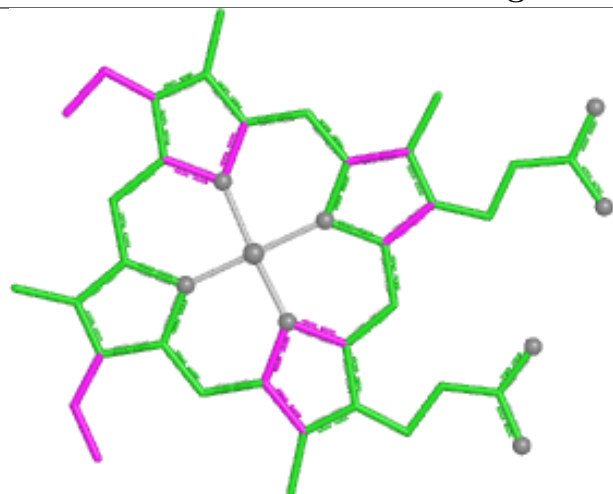


Torsions

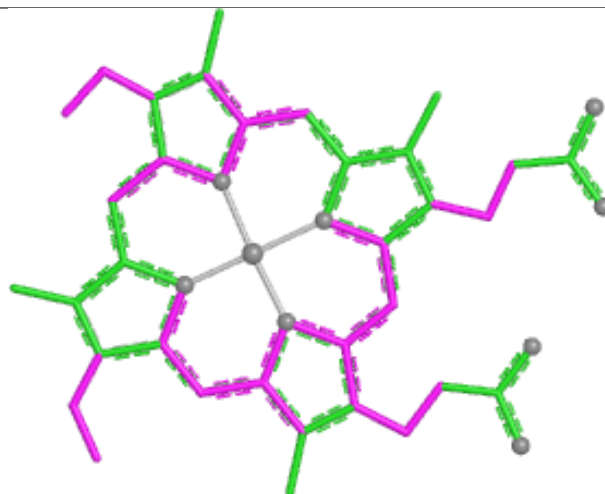


Rings

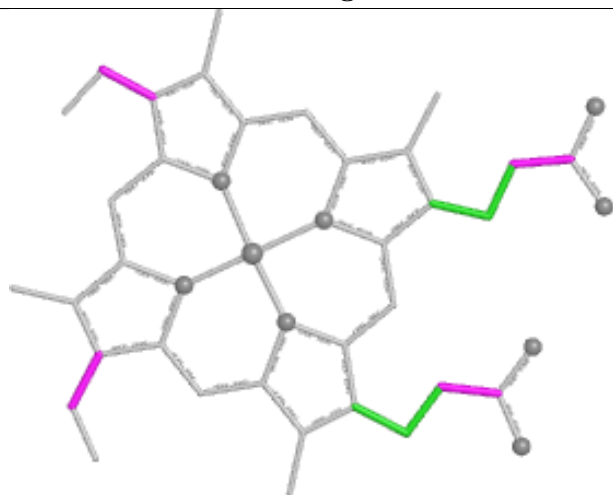
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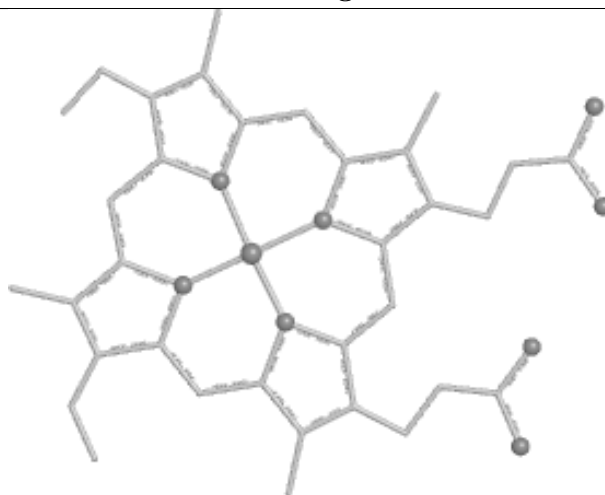
Bond lengths



Bond angles

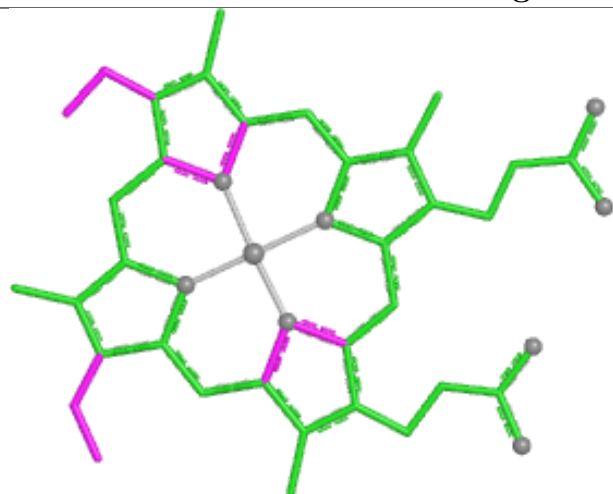


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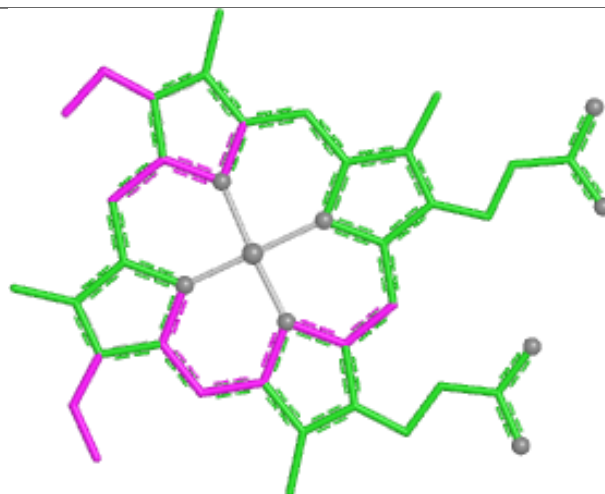


Rings

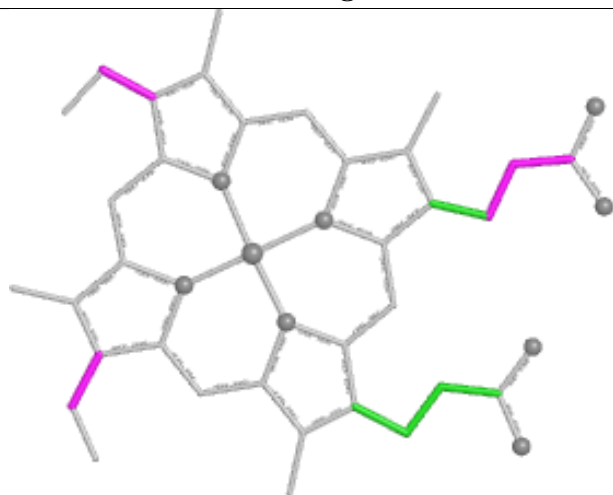
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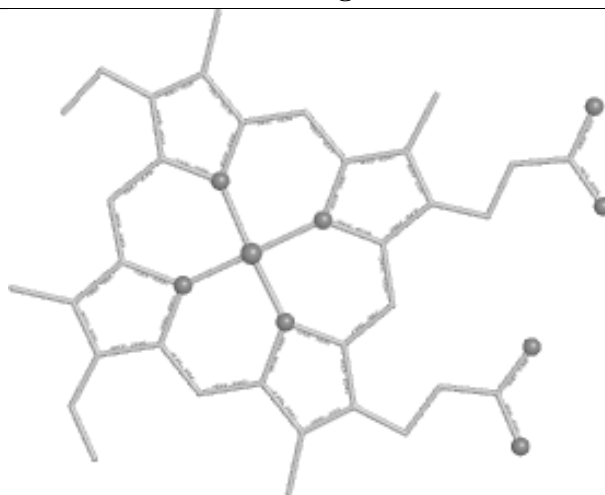
Bond lengths



Bond angles

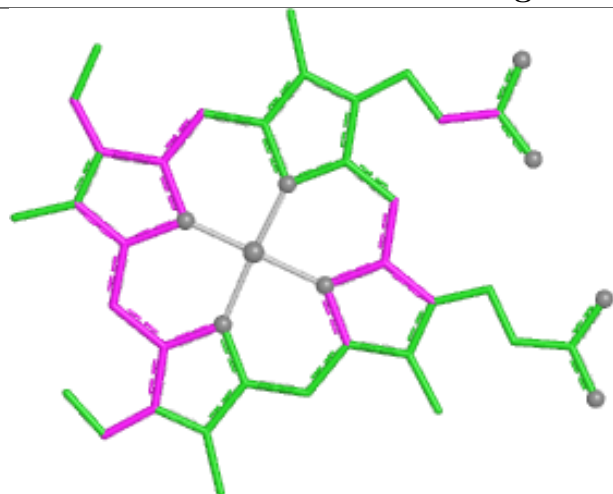


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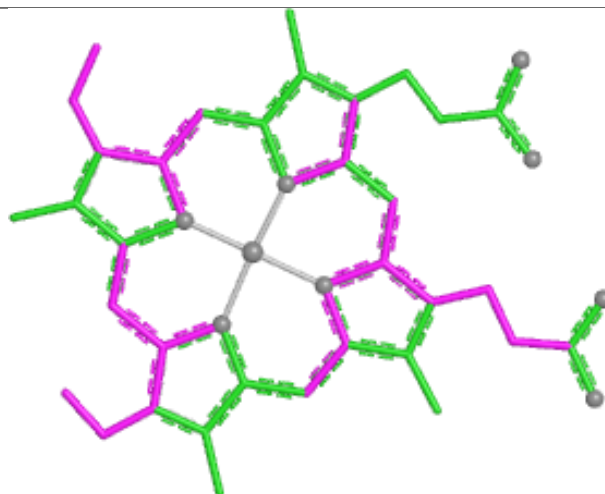


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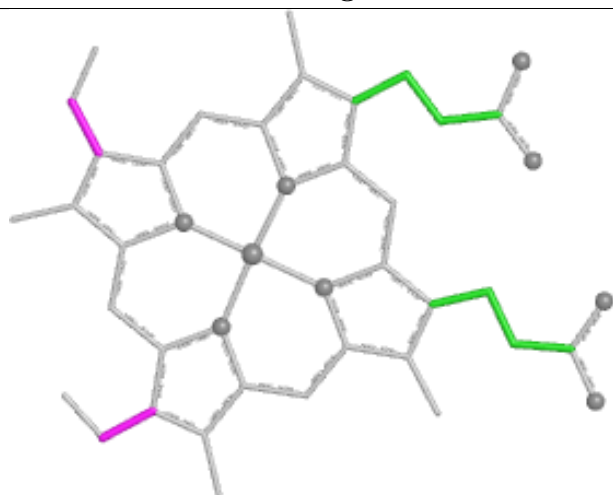
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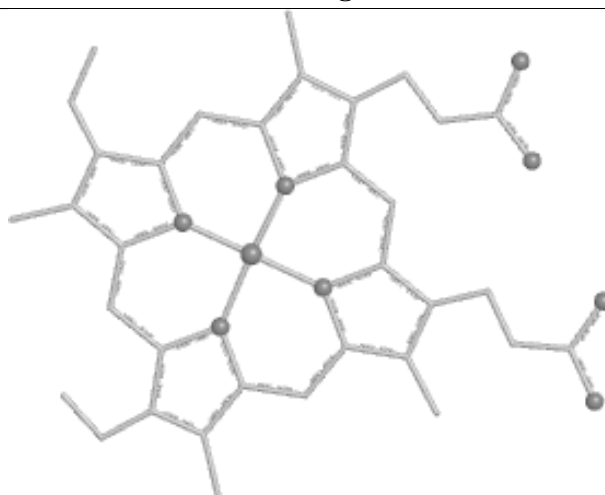
Bond lengths



Bond angles

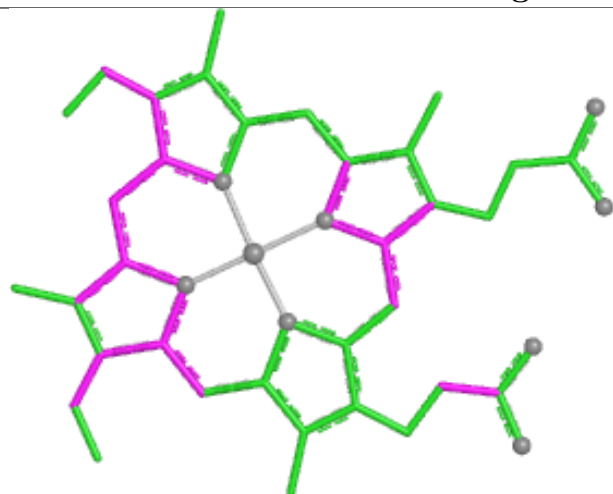


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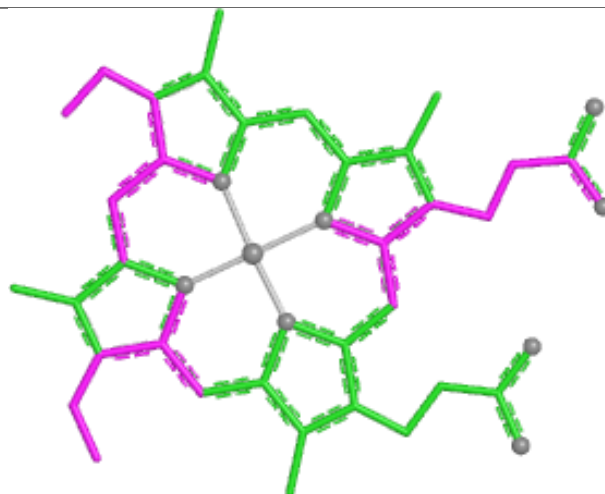


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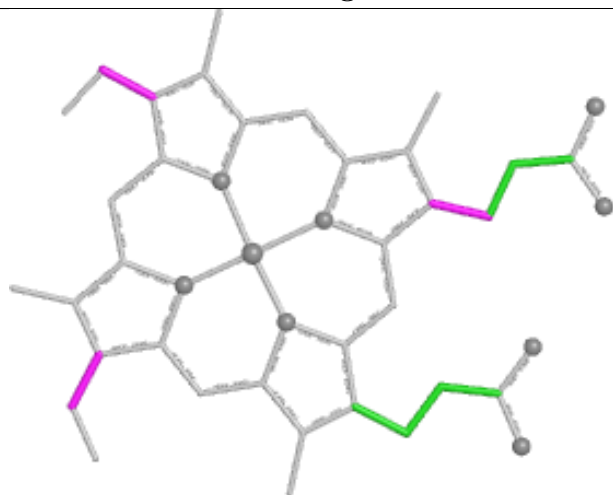
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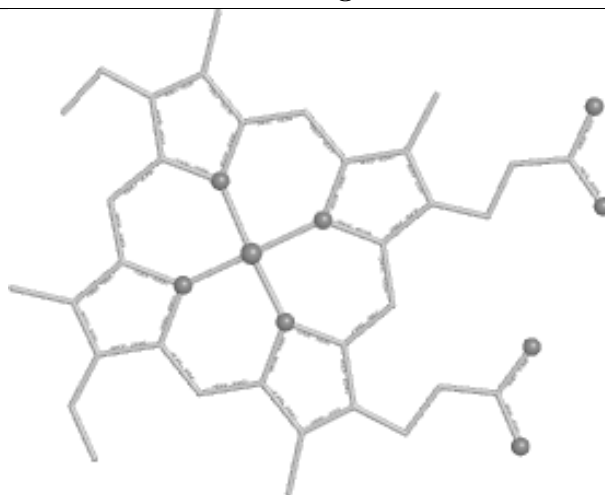
Bond lengths



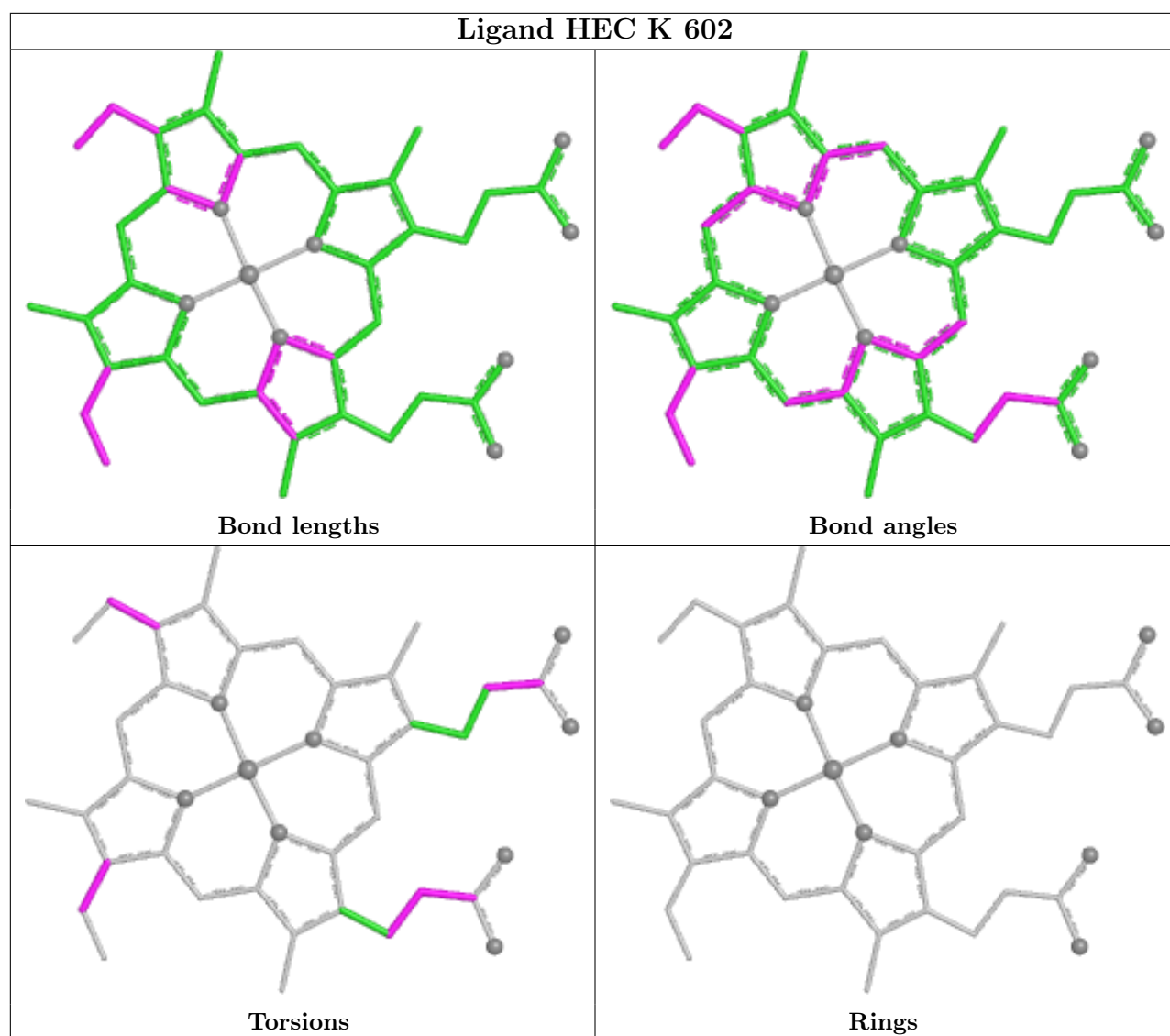
Bond angles



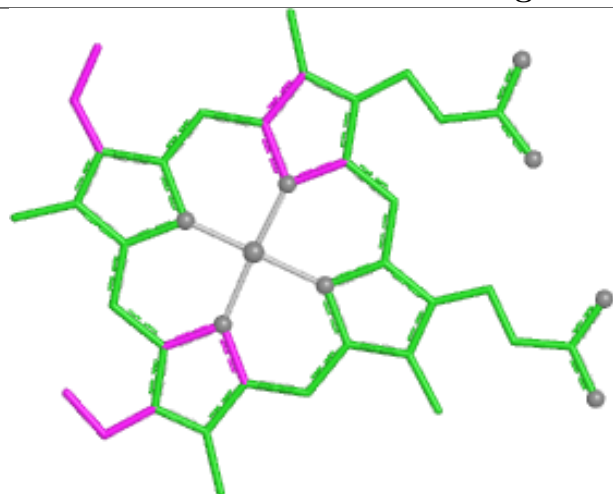
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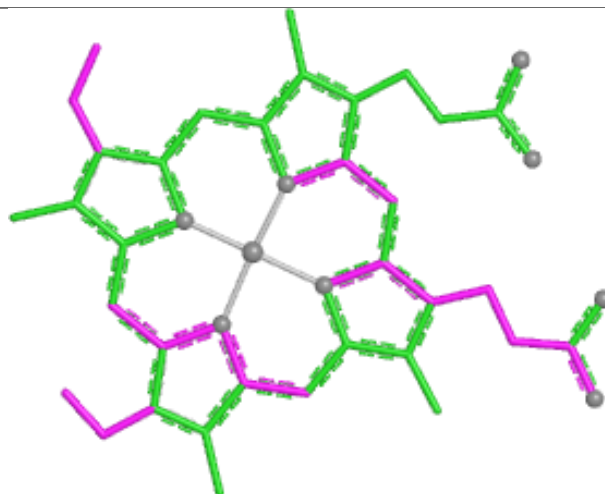
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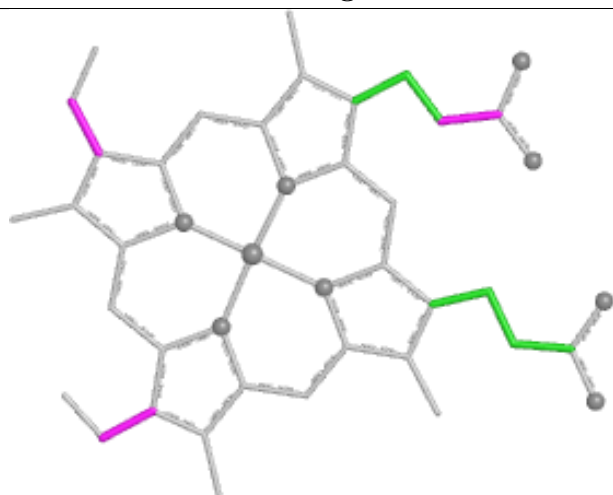
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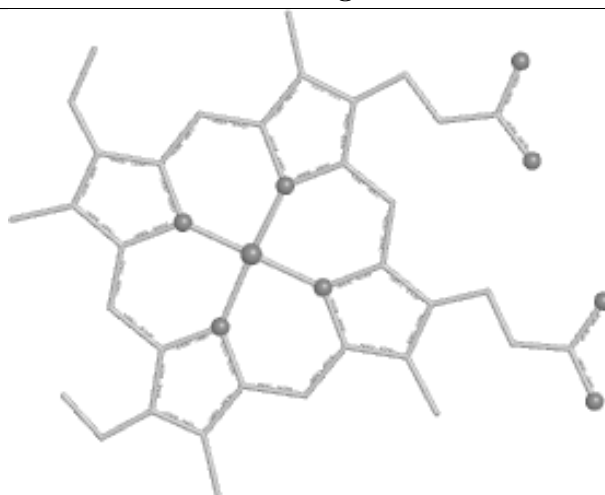
Bond lengths



Bond angles

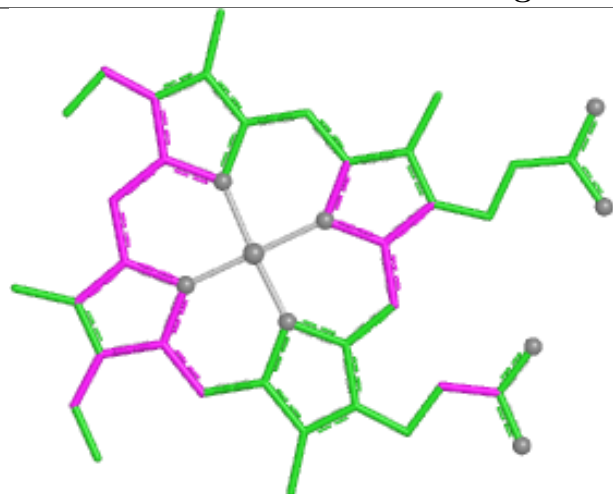


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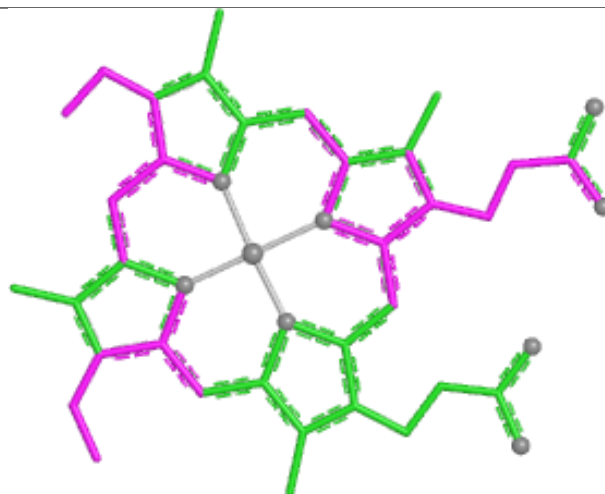


Rings

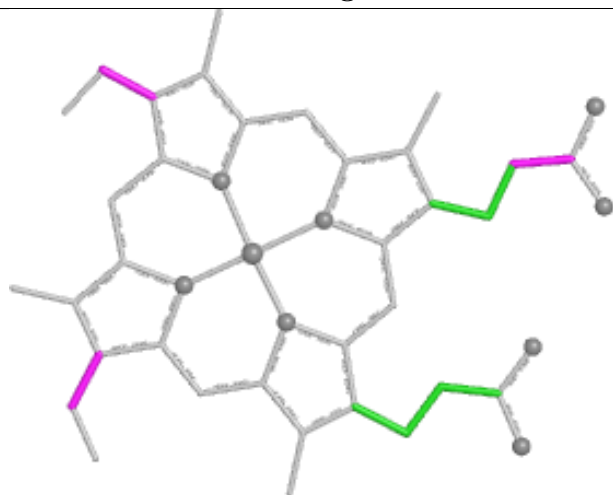
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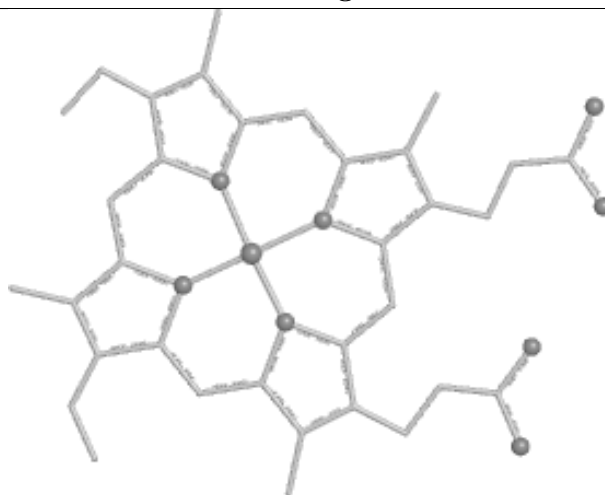
Bond lengths



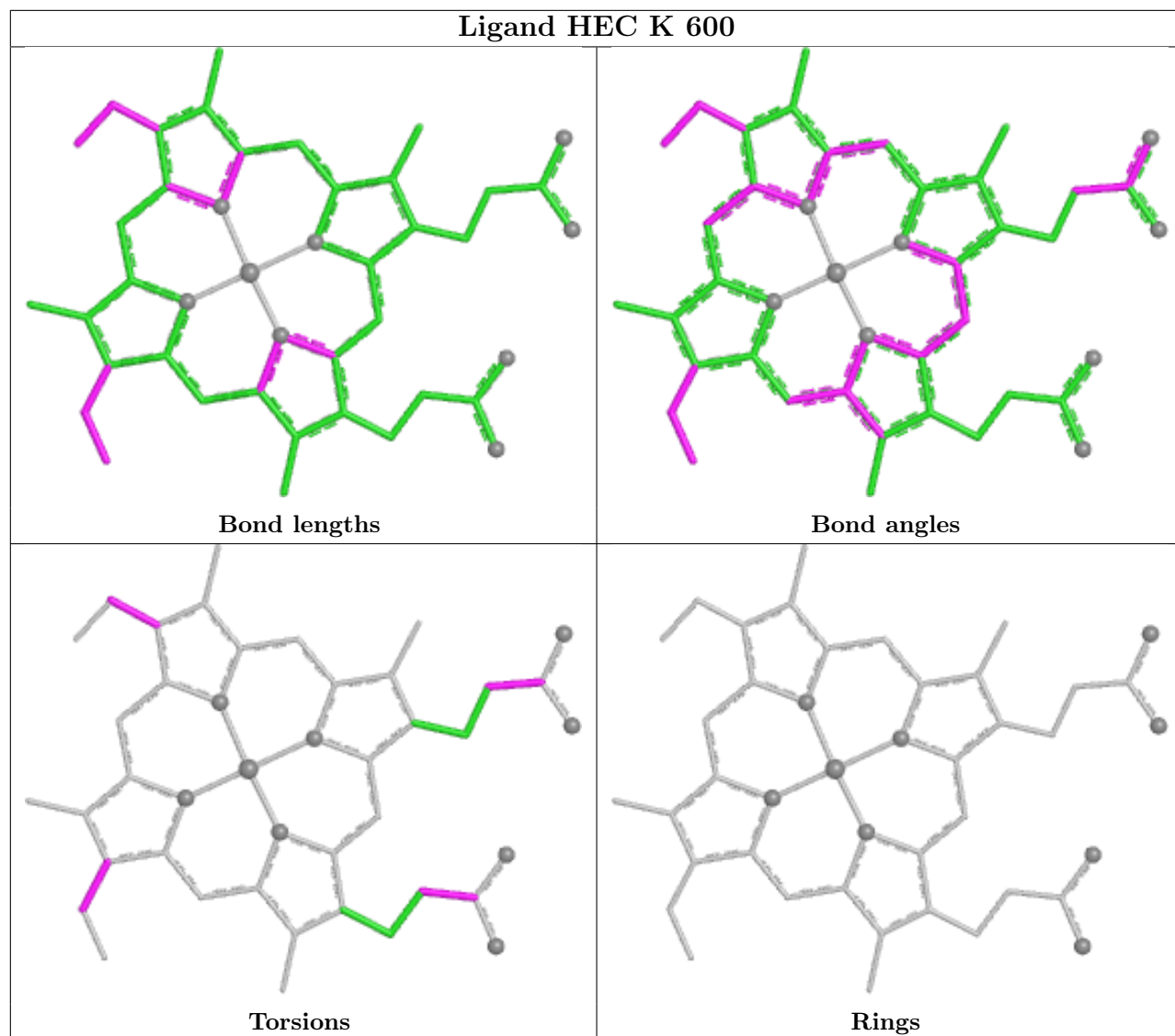
Bond angles

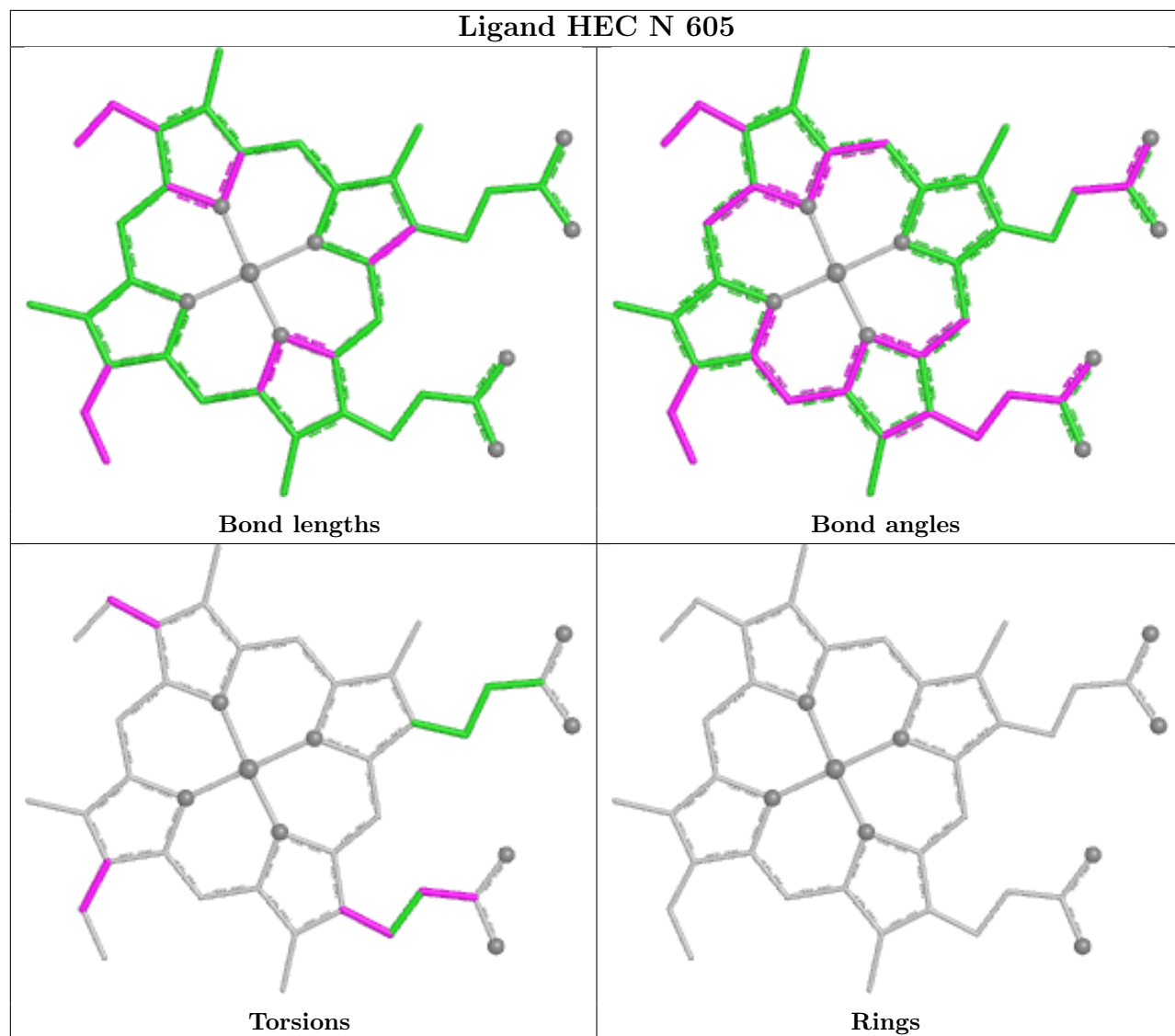


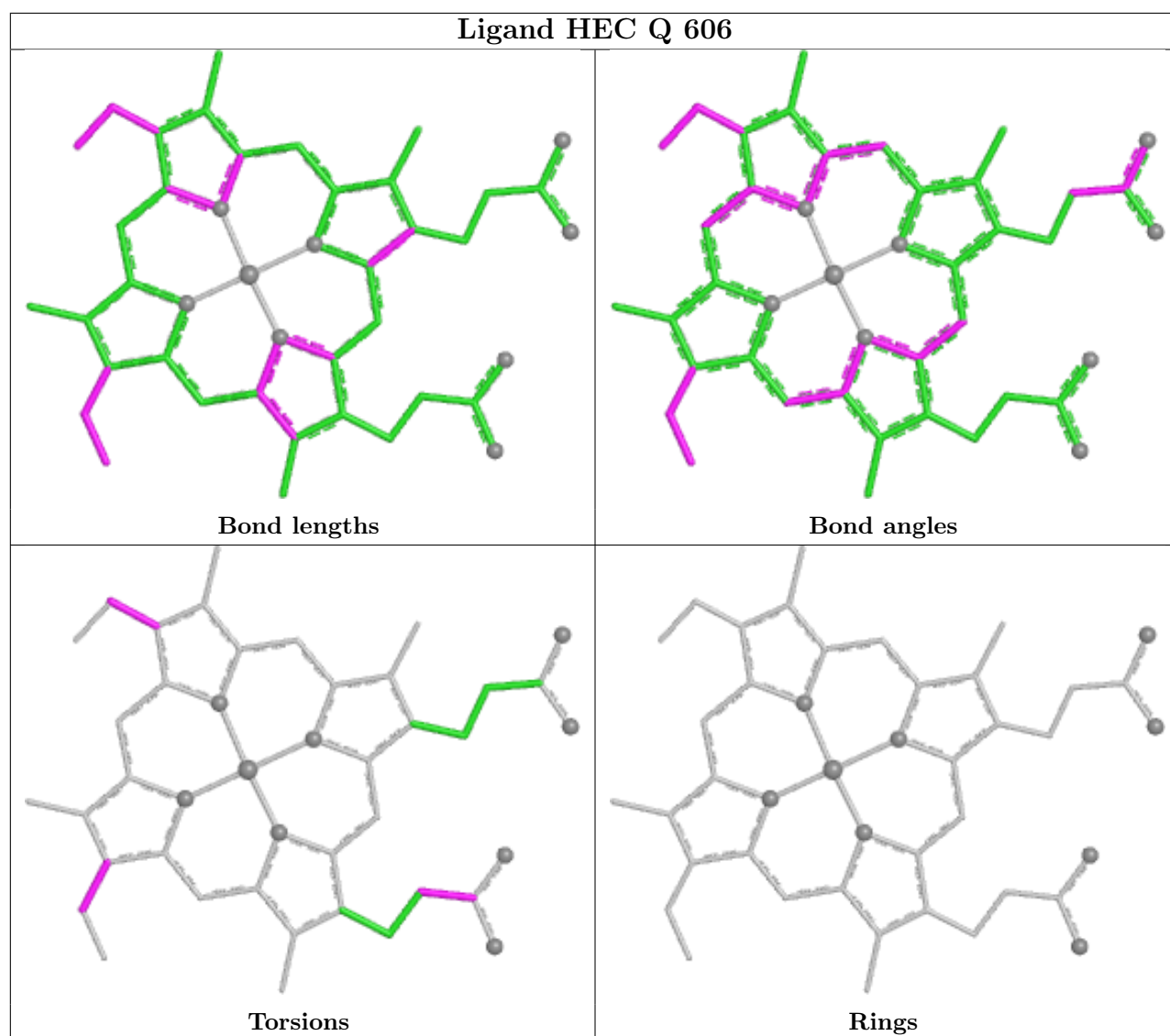
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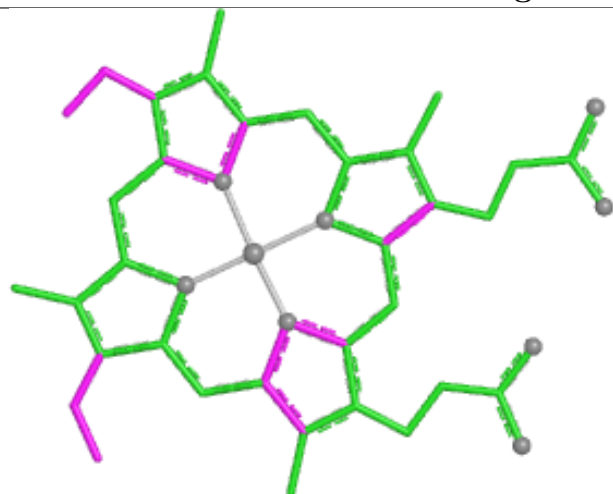
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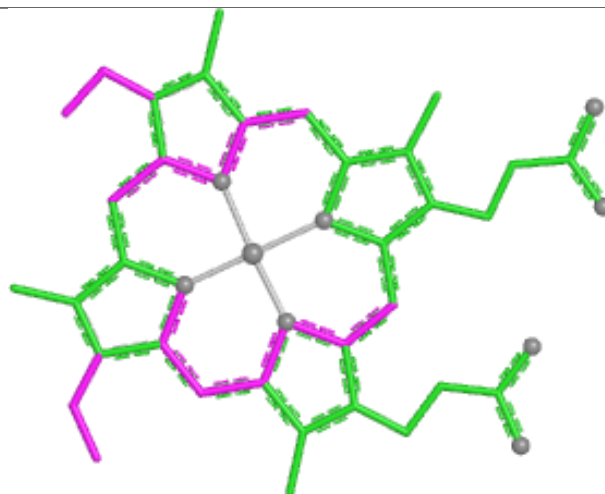




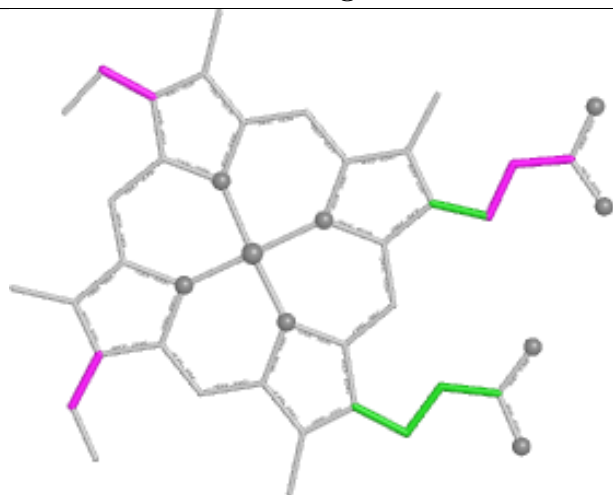
Ligand HEC F 607



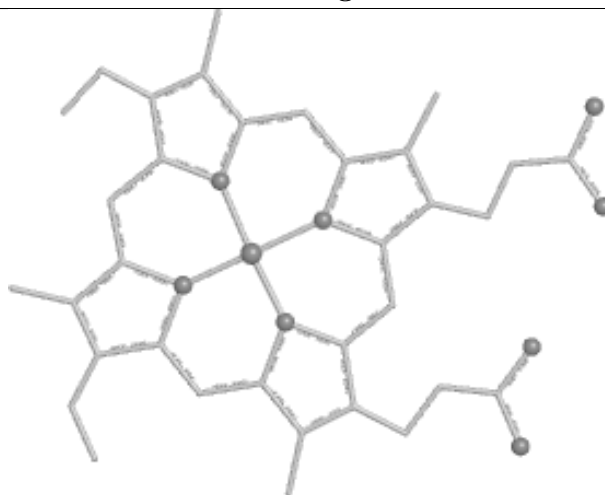
Bond lengths



Bond angles

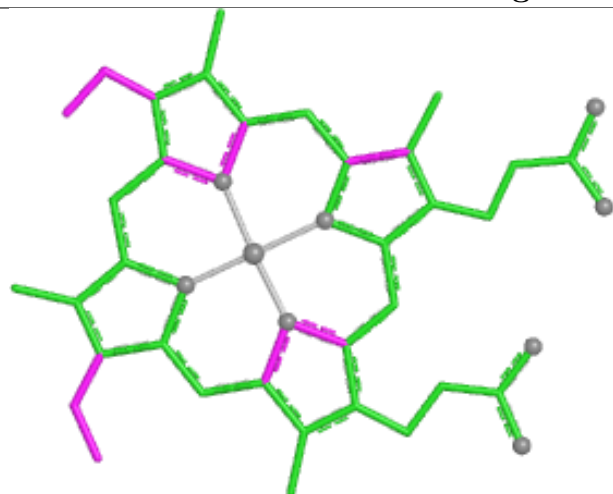


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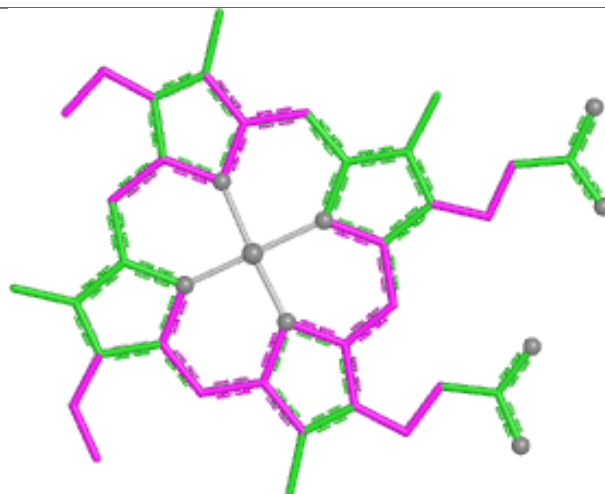


Rings

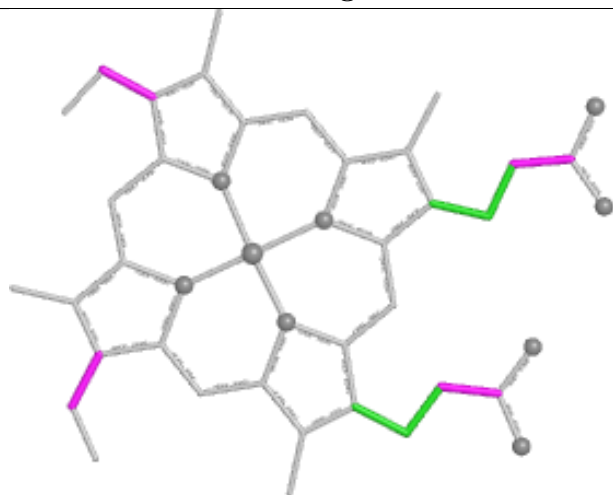
Ligand HEC R 604



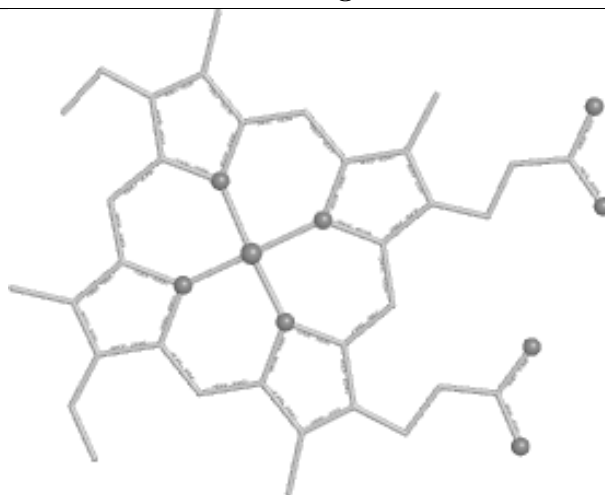
Bond lengths



Bond angles

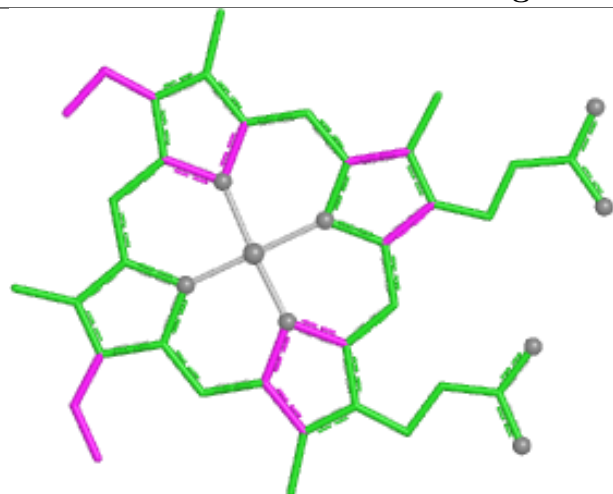


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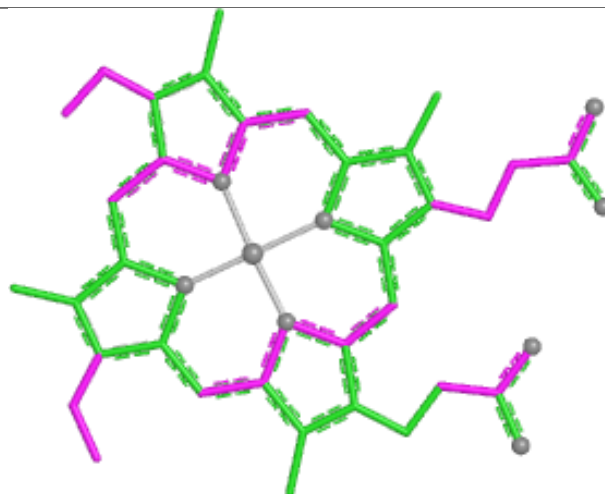


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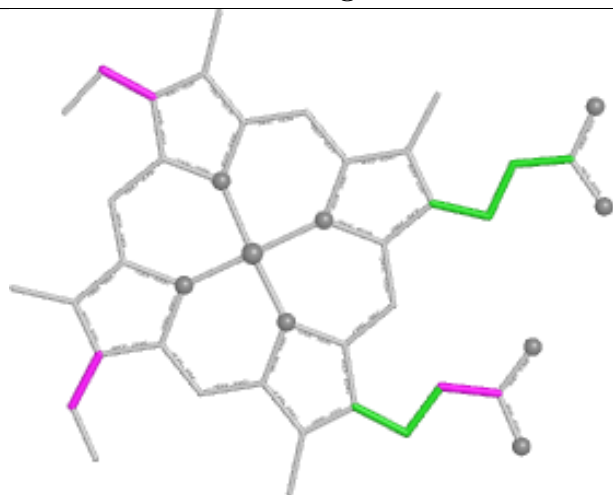
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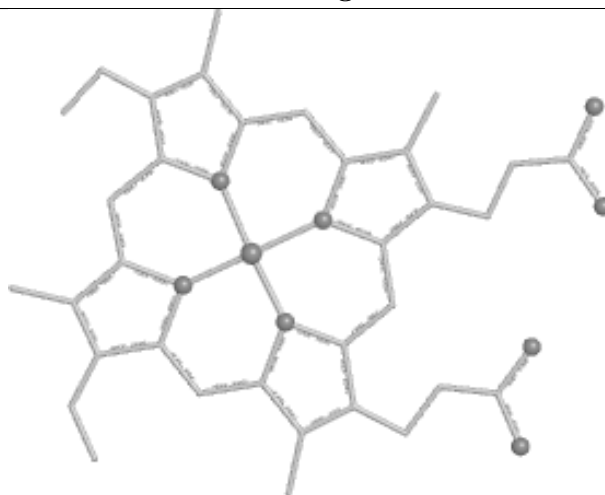
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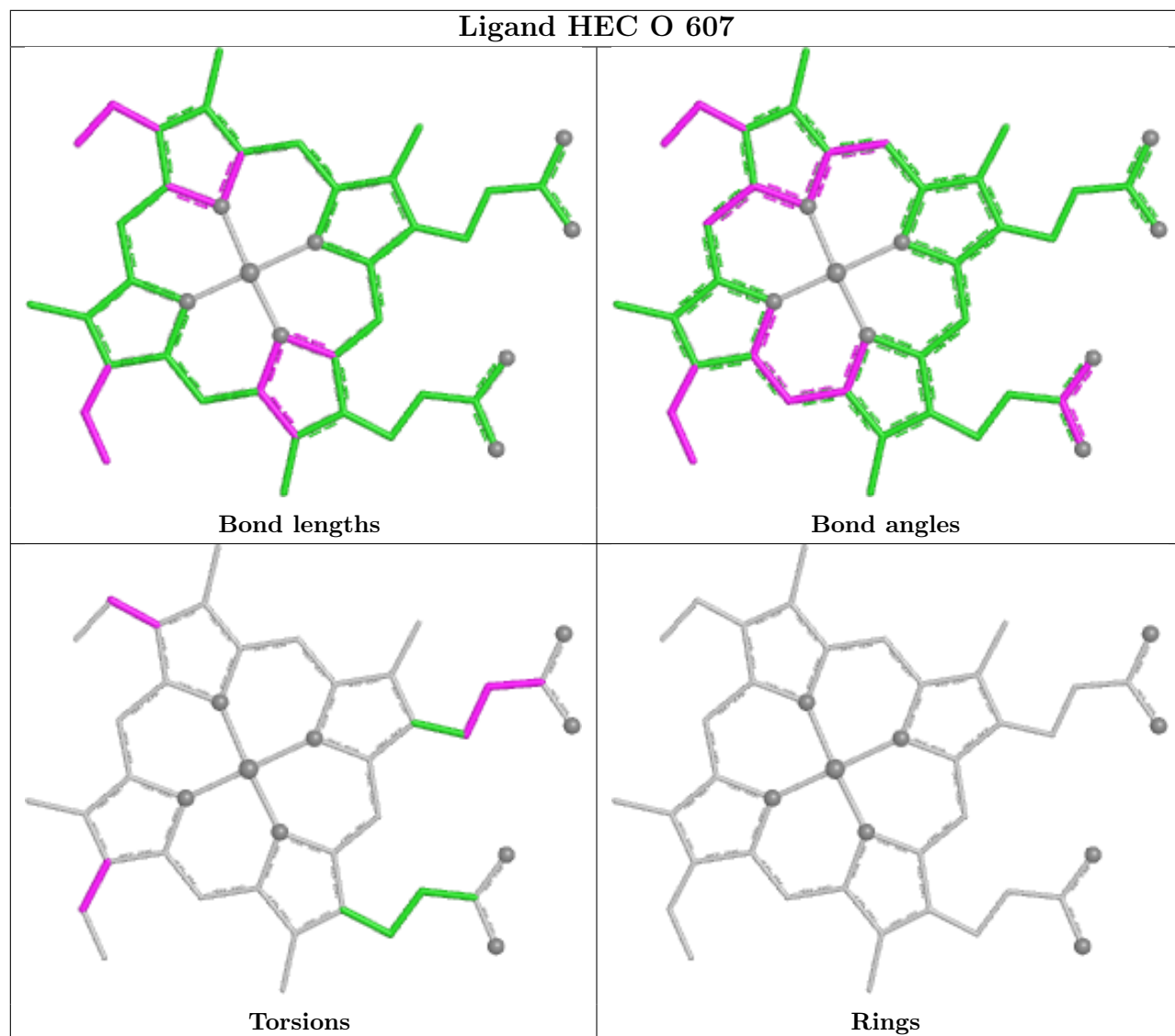
Bond angles



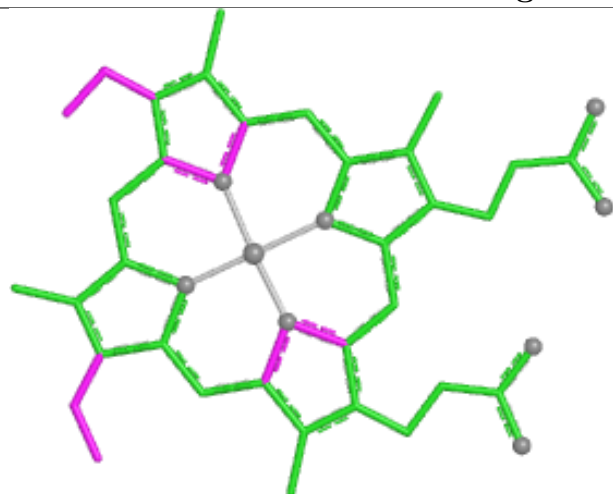
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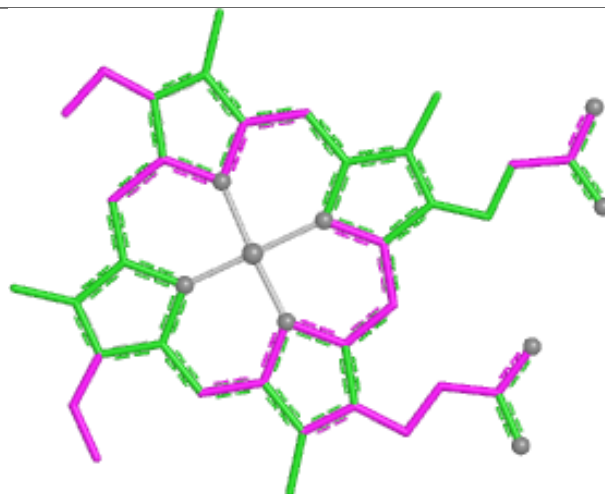
Rings



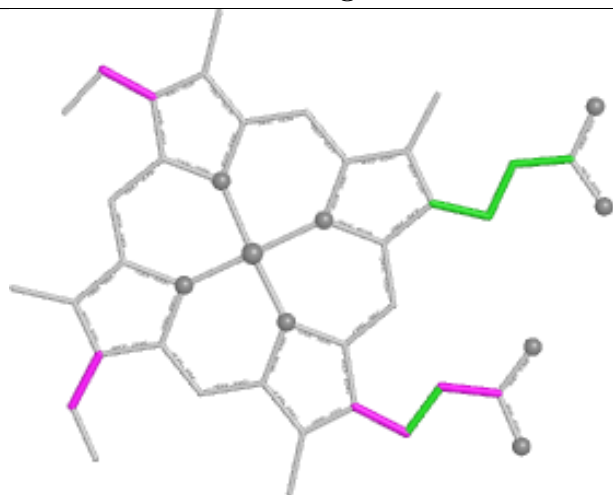
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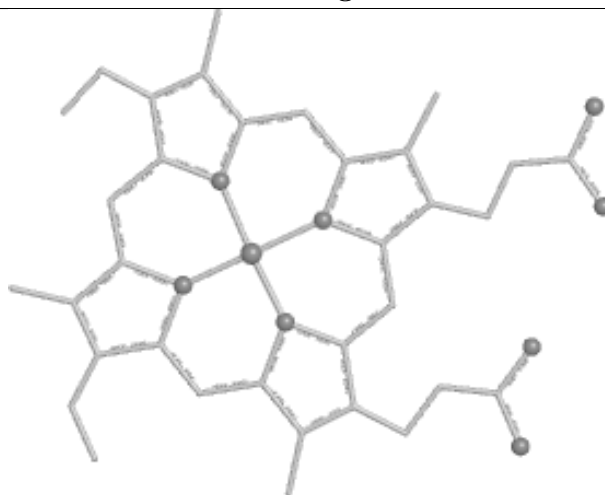
Bond lengths



Bond angles

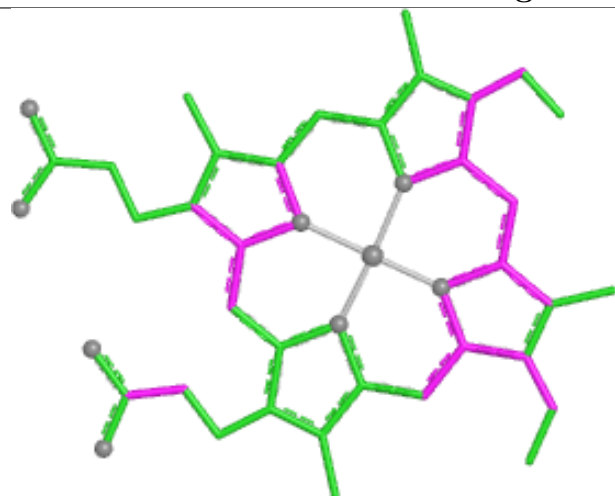


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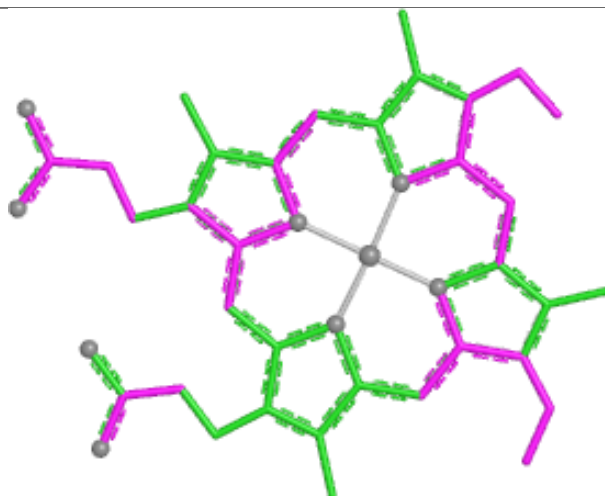


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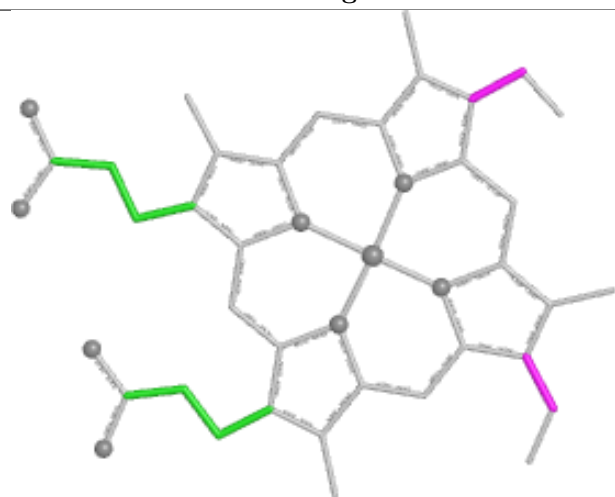
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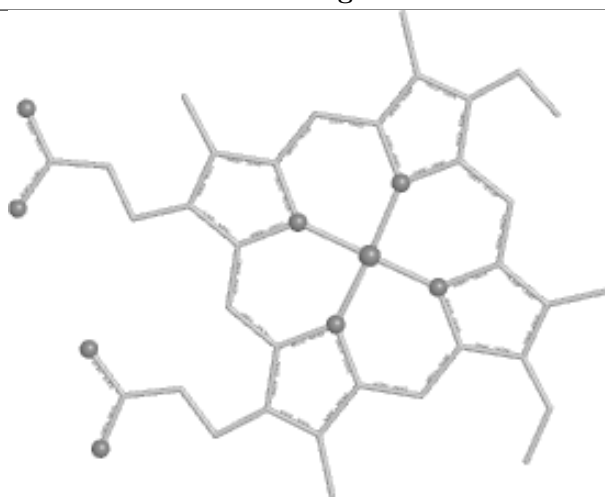
Bond lengths



Bond angles

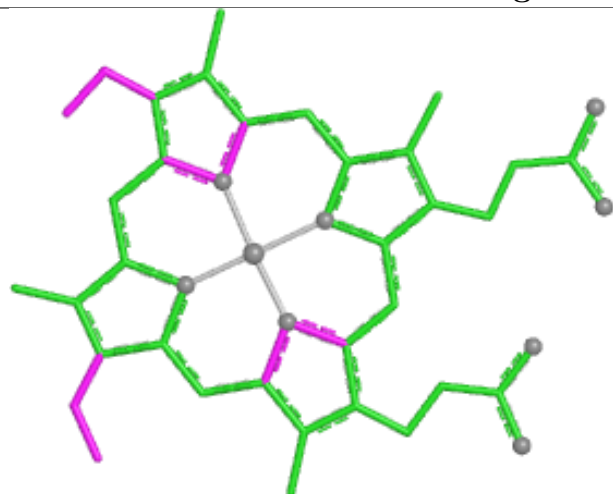


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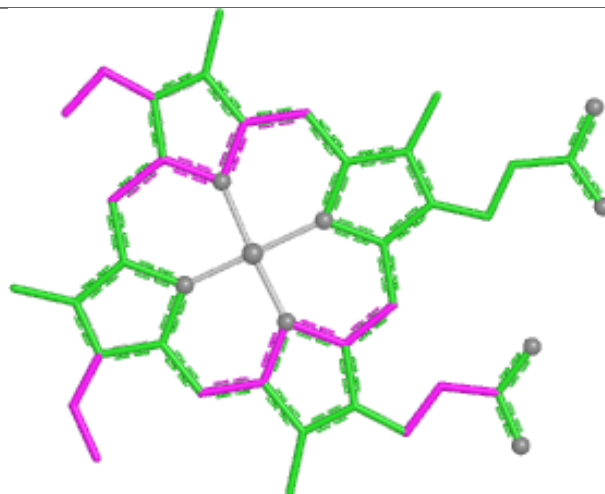


Rings

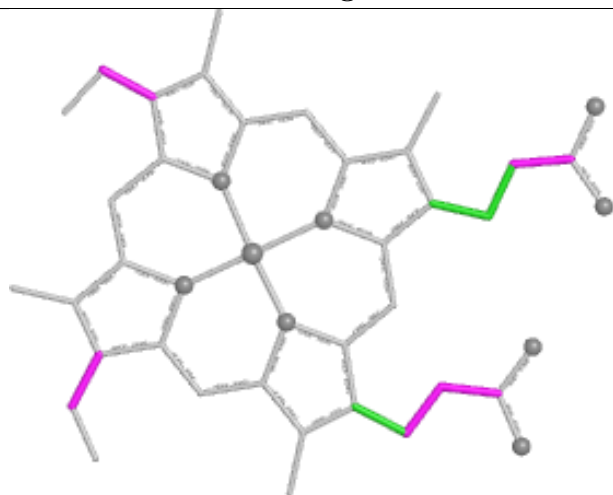
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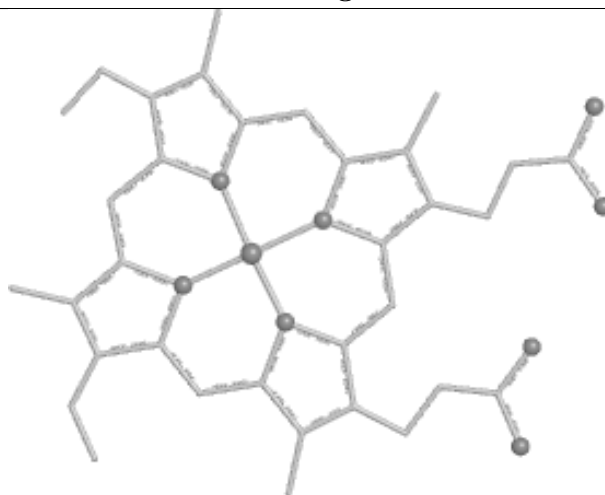
Bond lengths



Bond angles

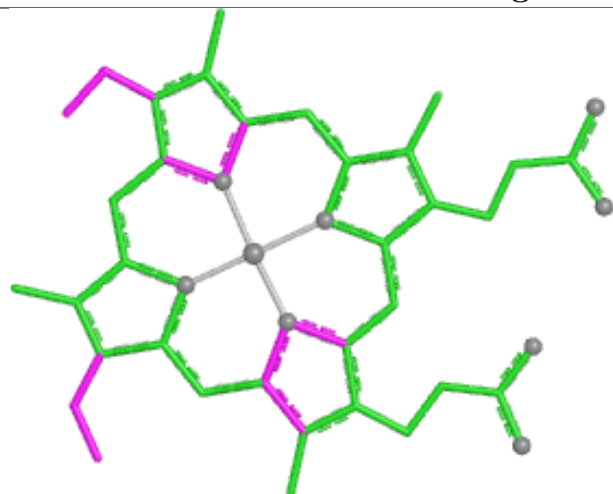


Torsions

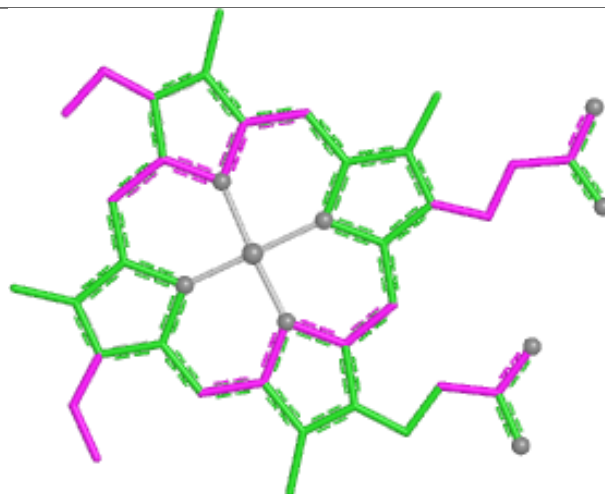


Rings

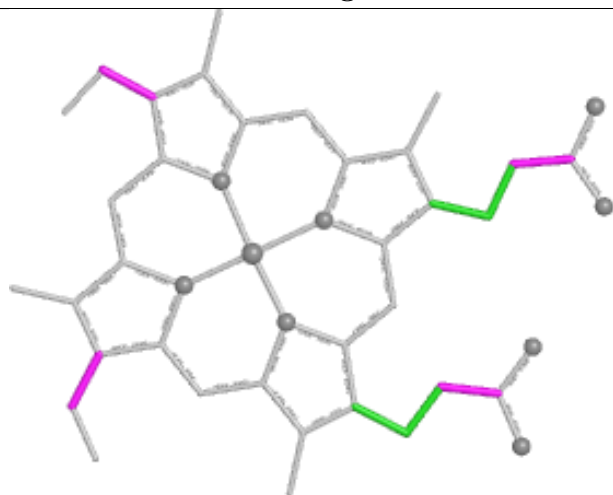
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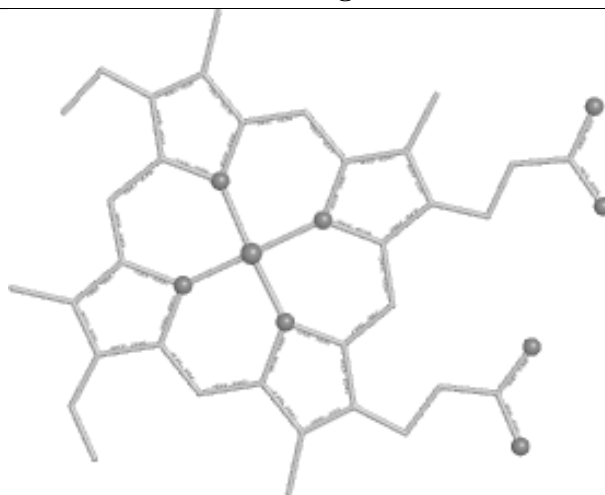
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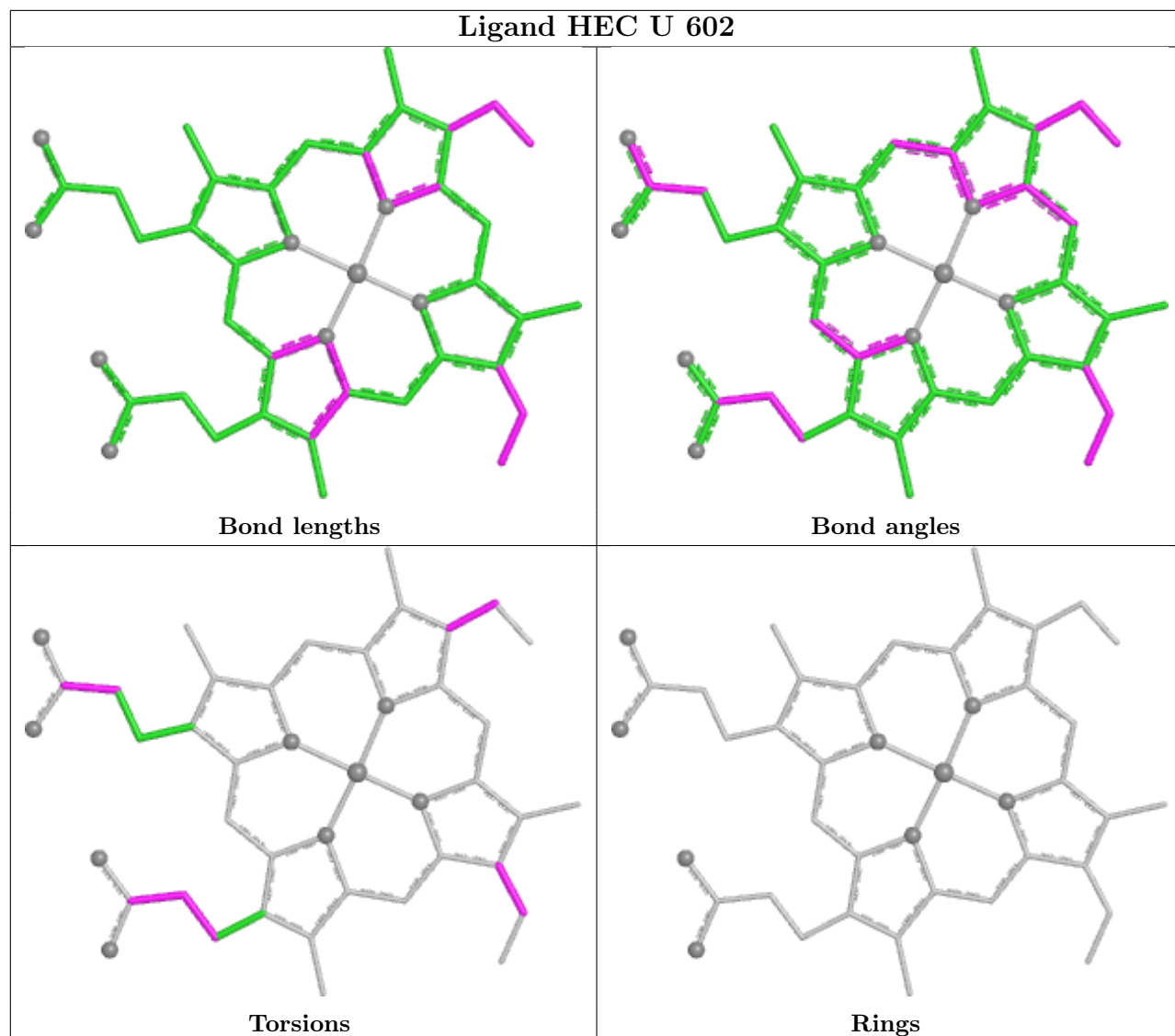
Bond angles



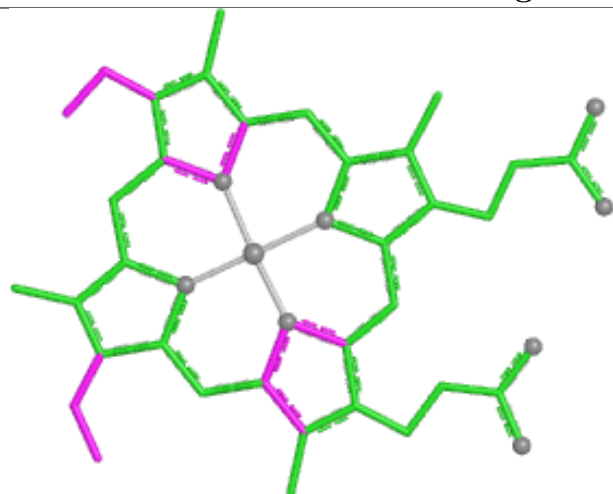
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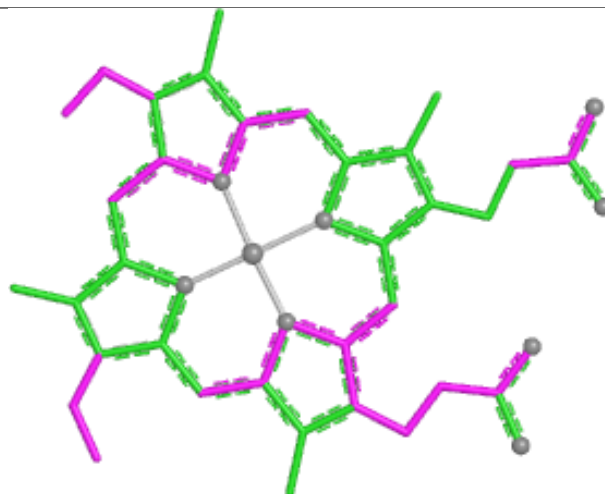
Rings



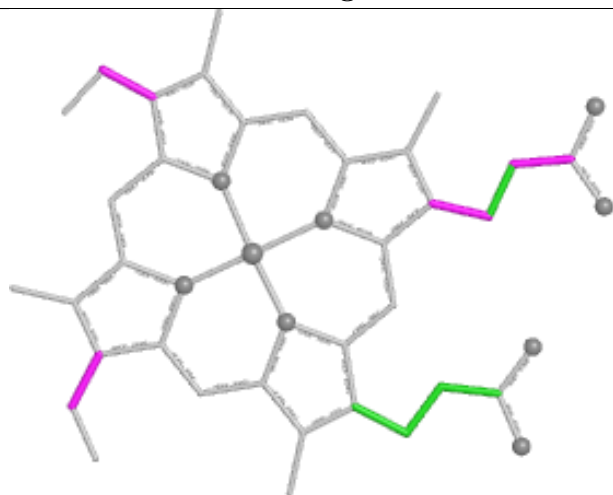
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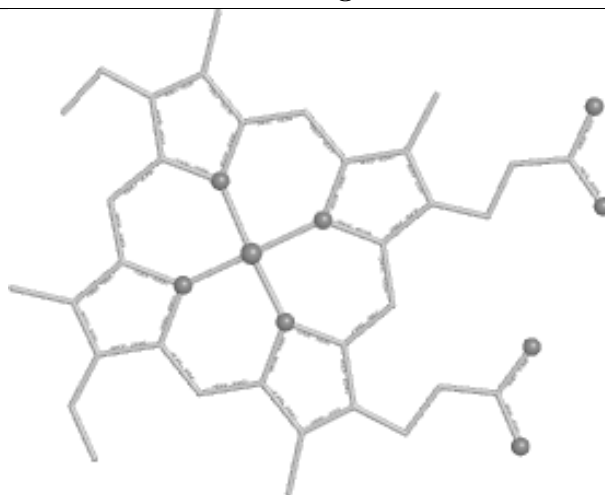
Bond lengths



Bond angles

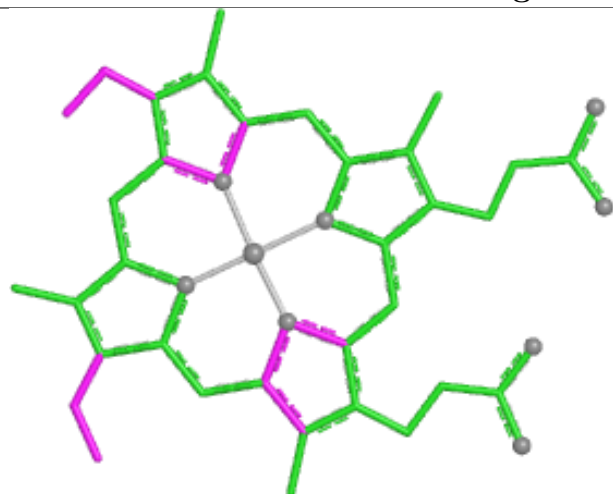


Torsions

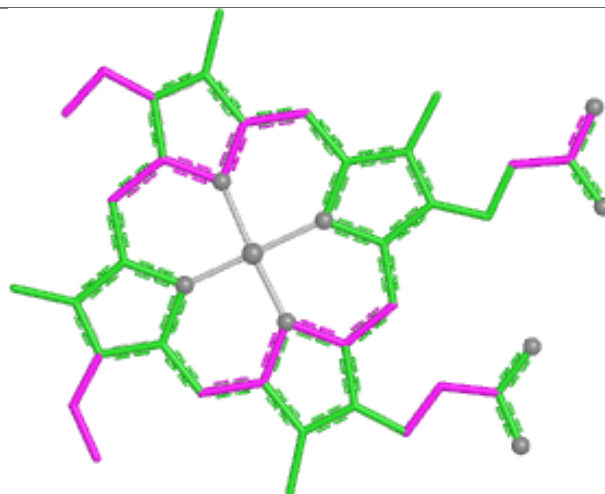


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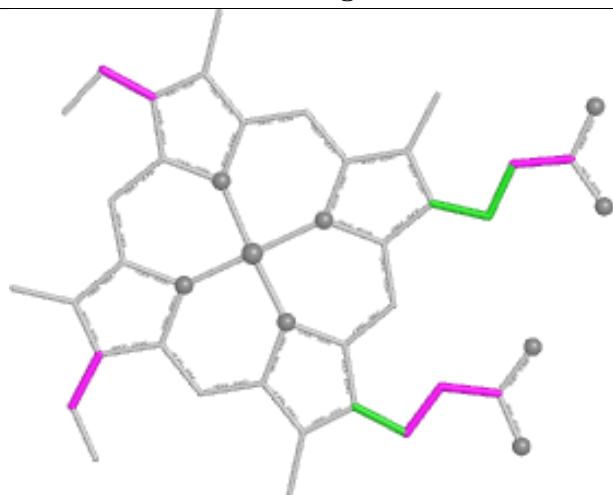
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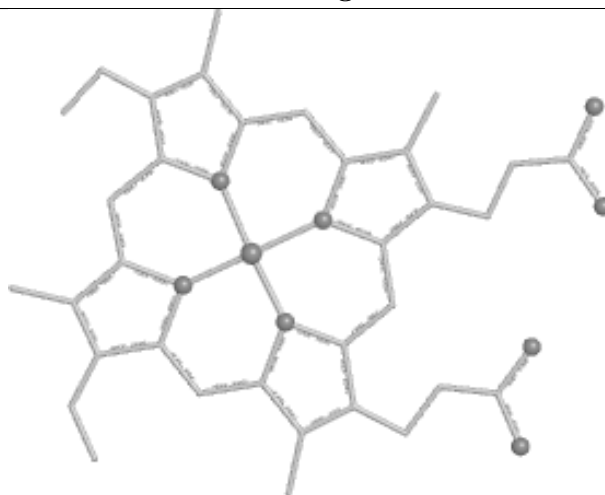
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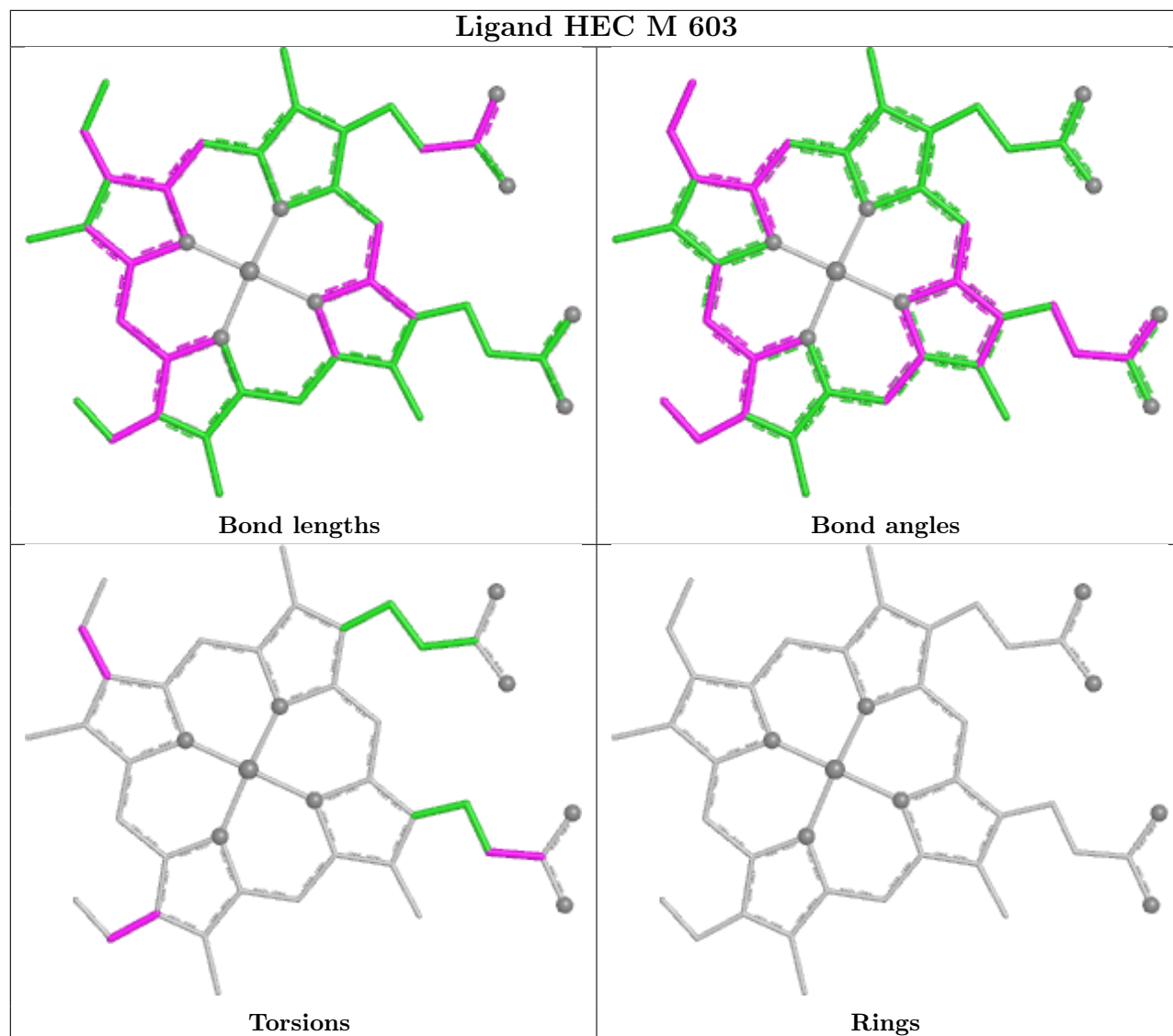
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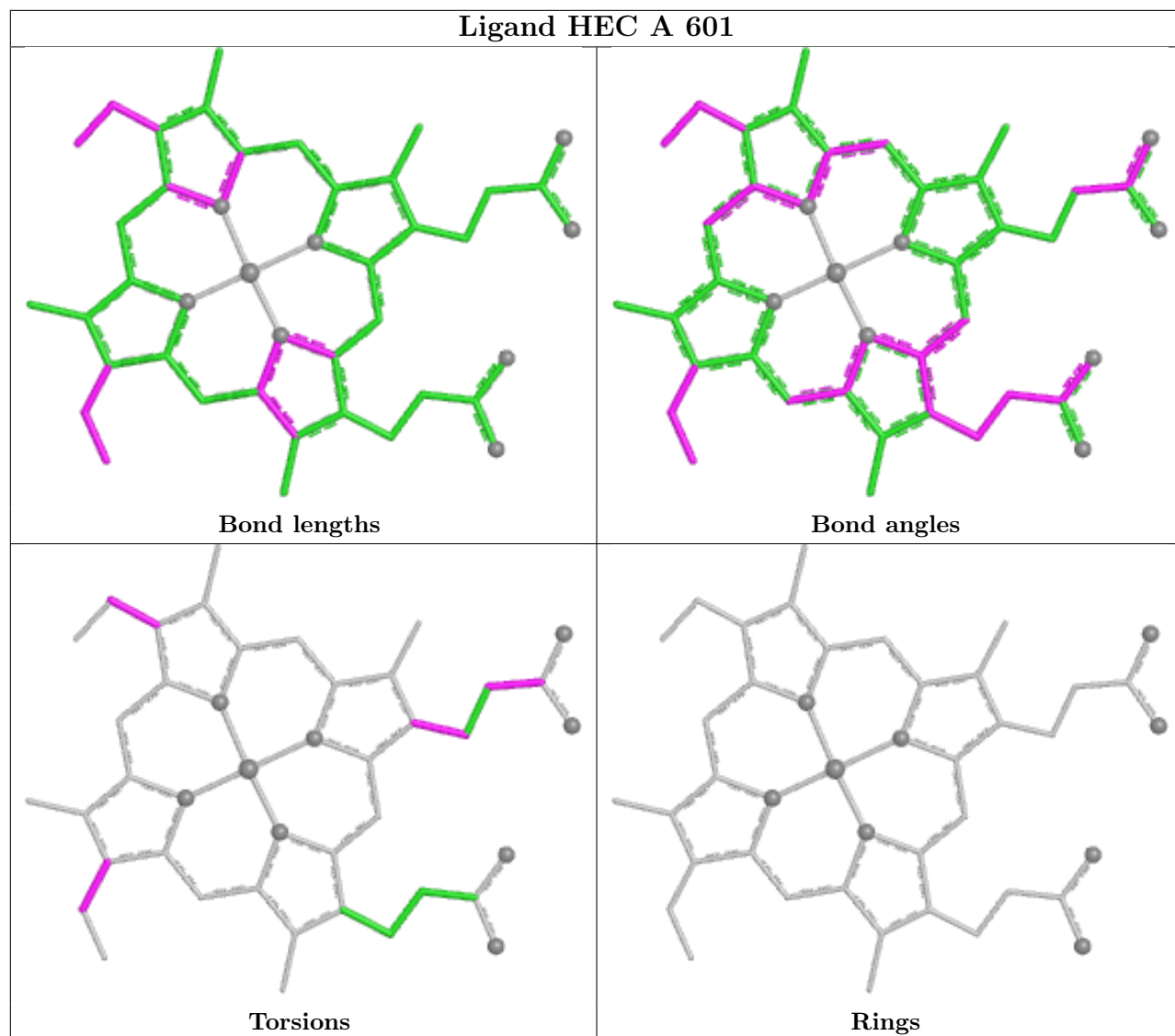


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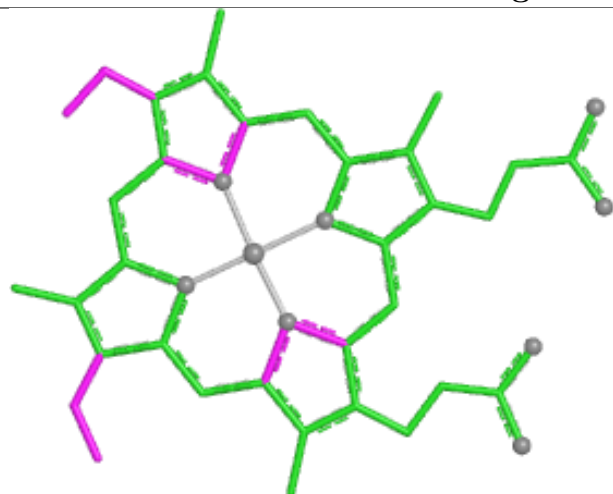


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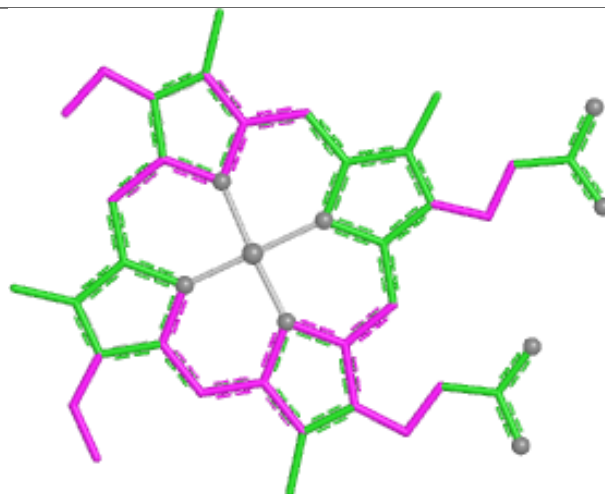




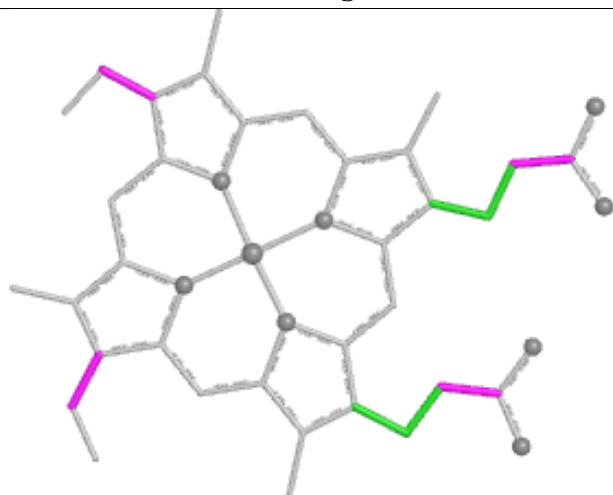
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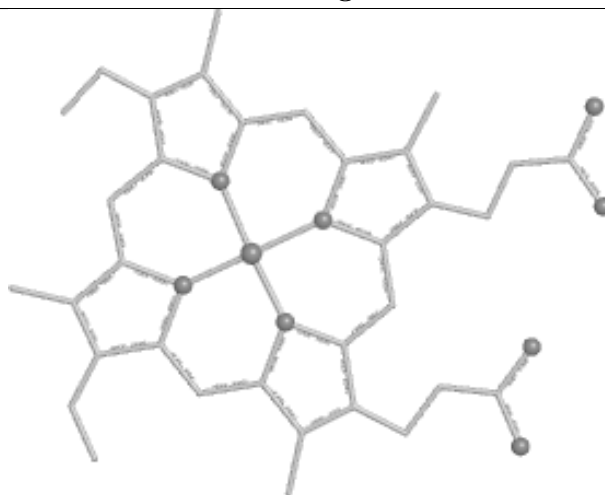
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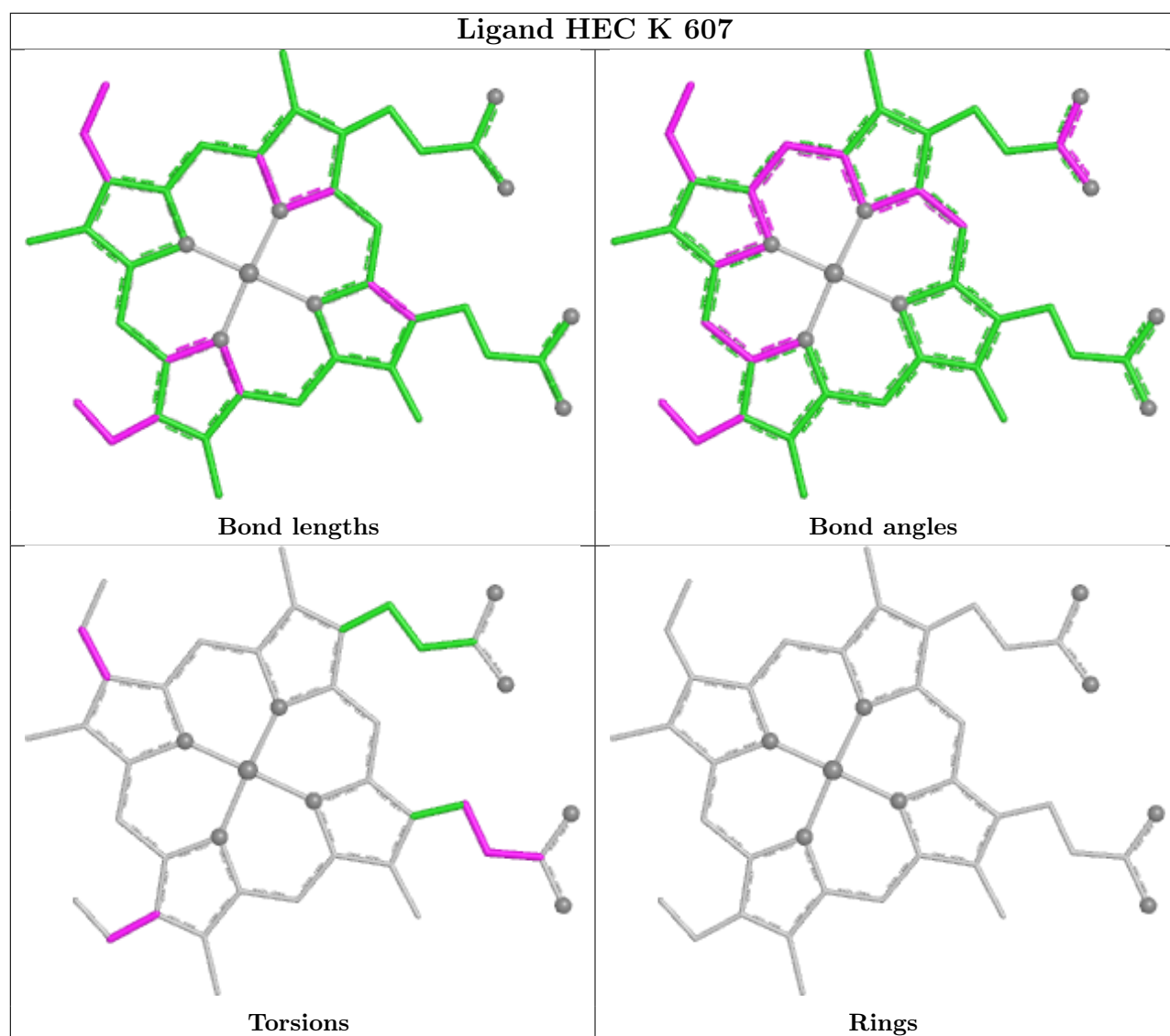
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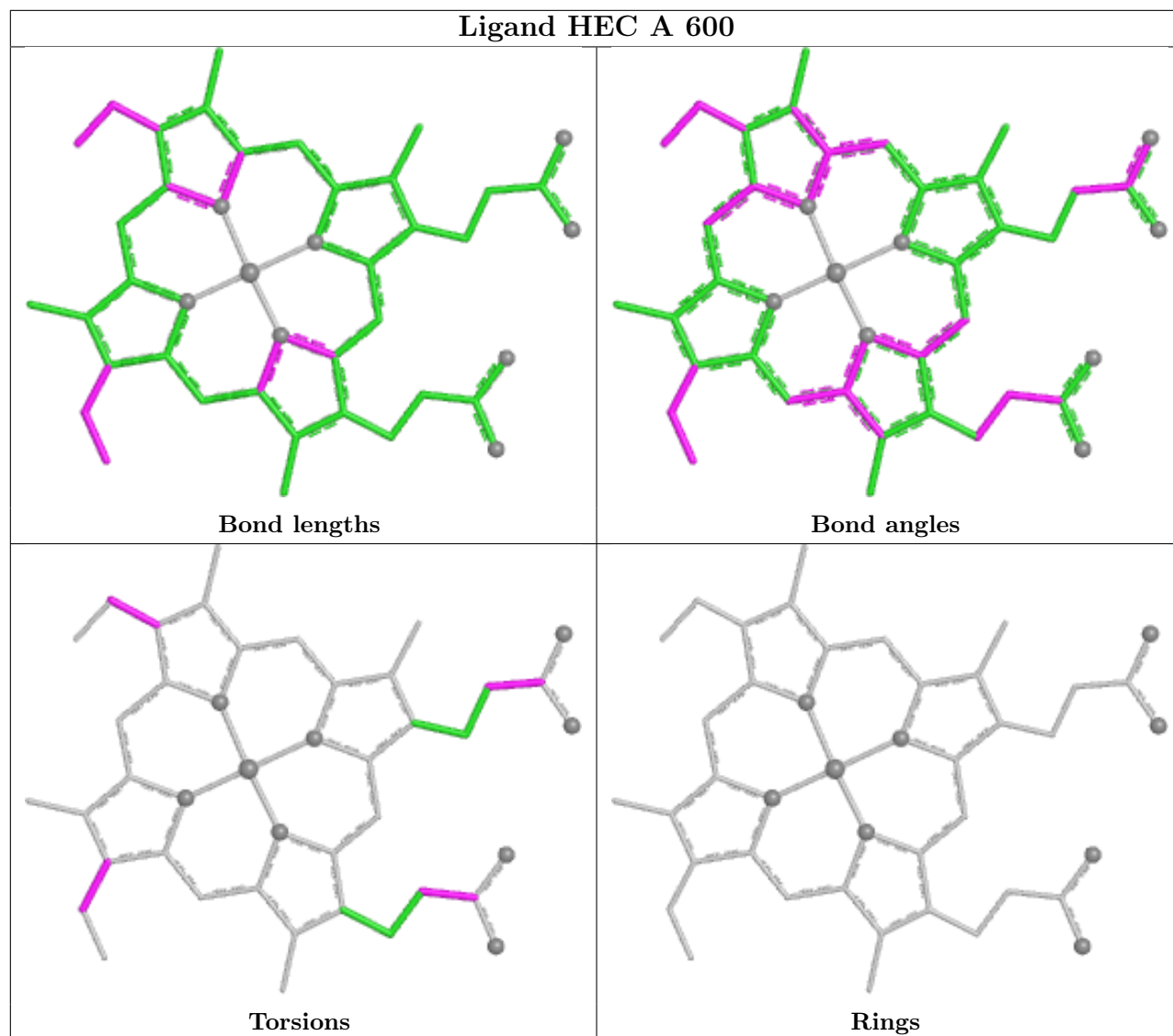


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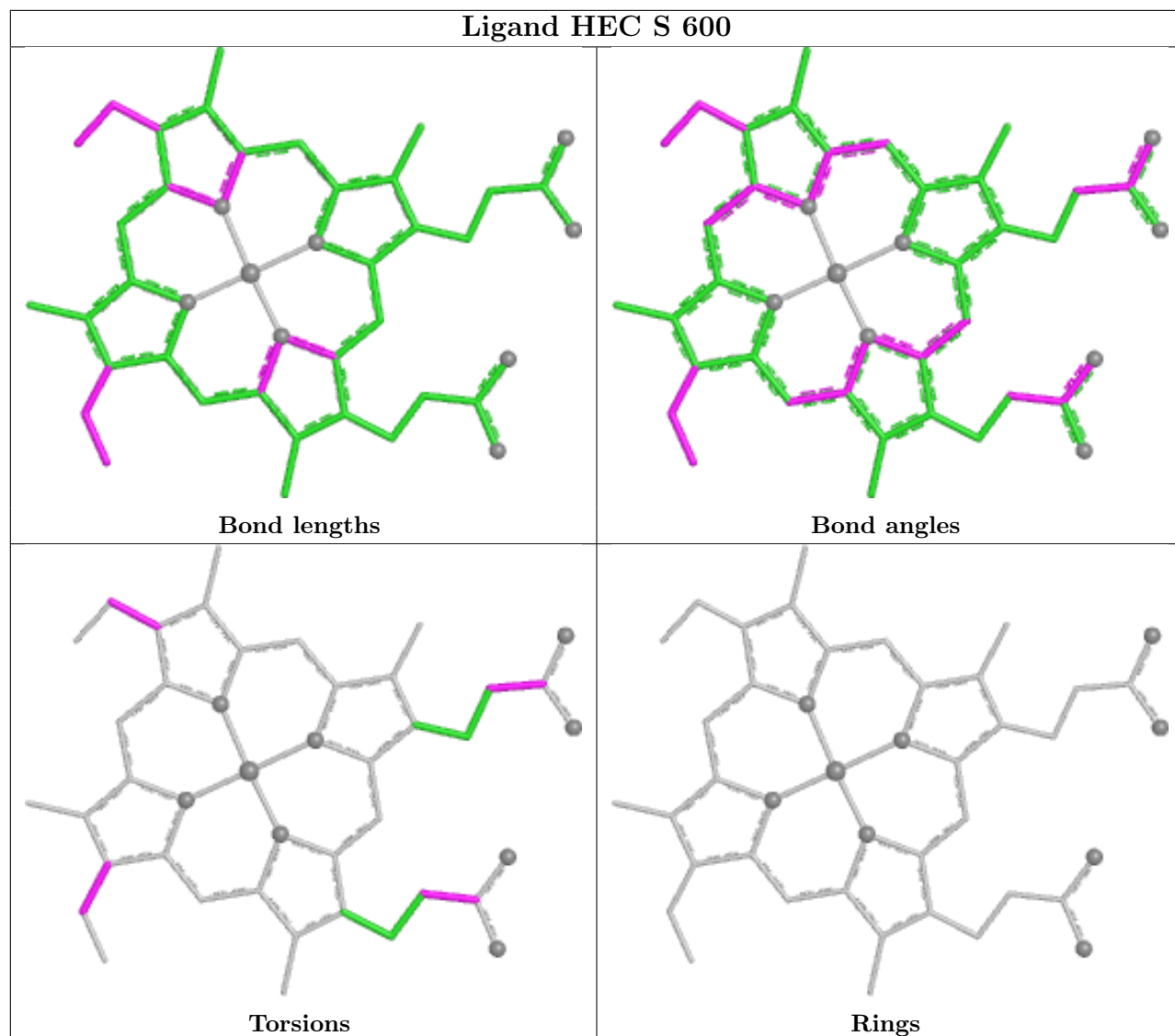


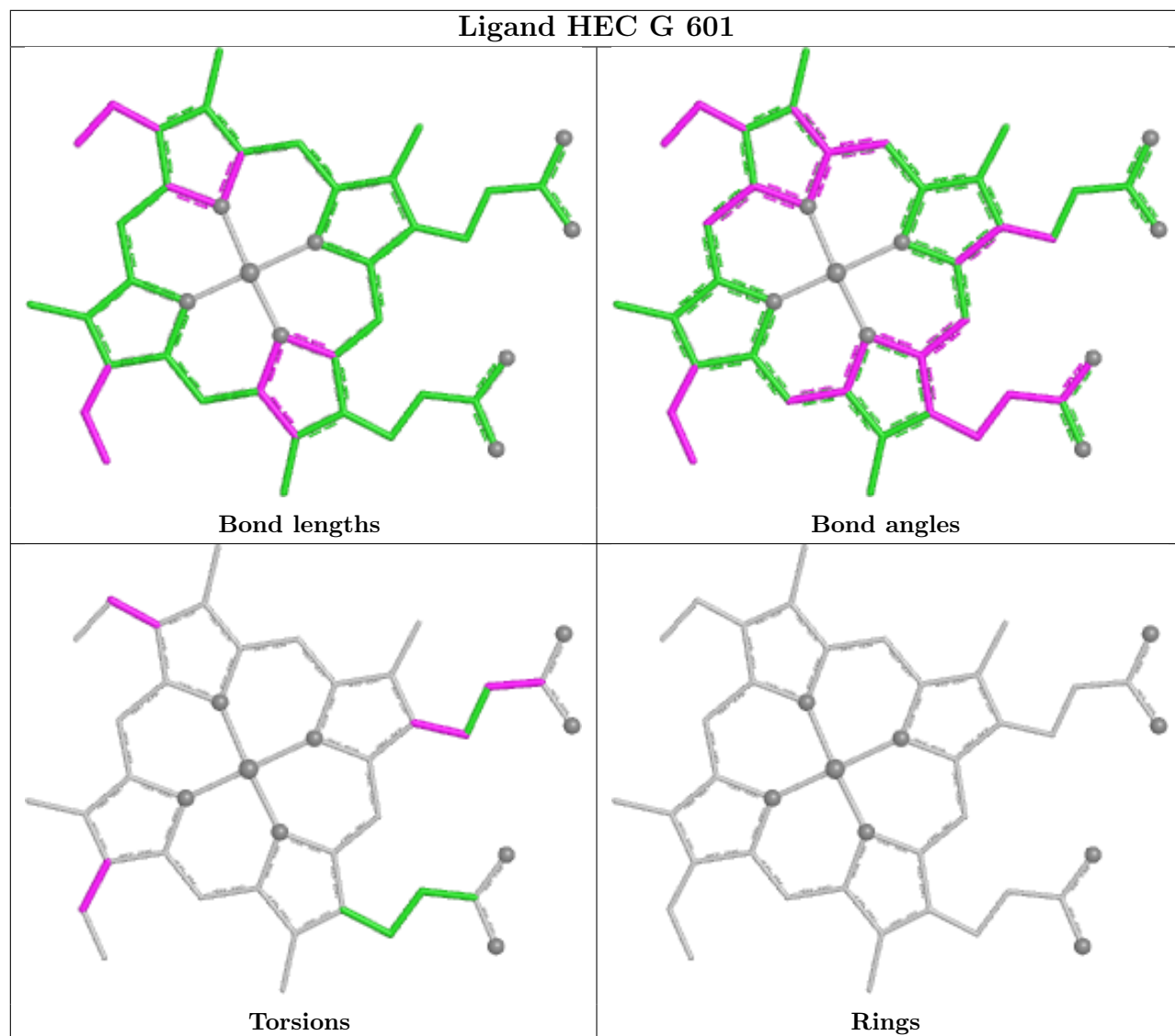
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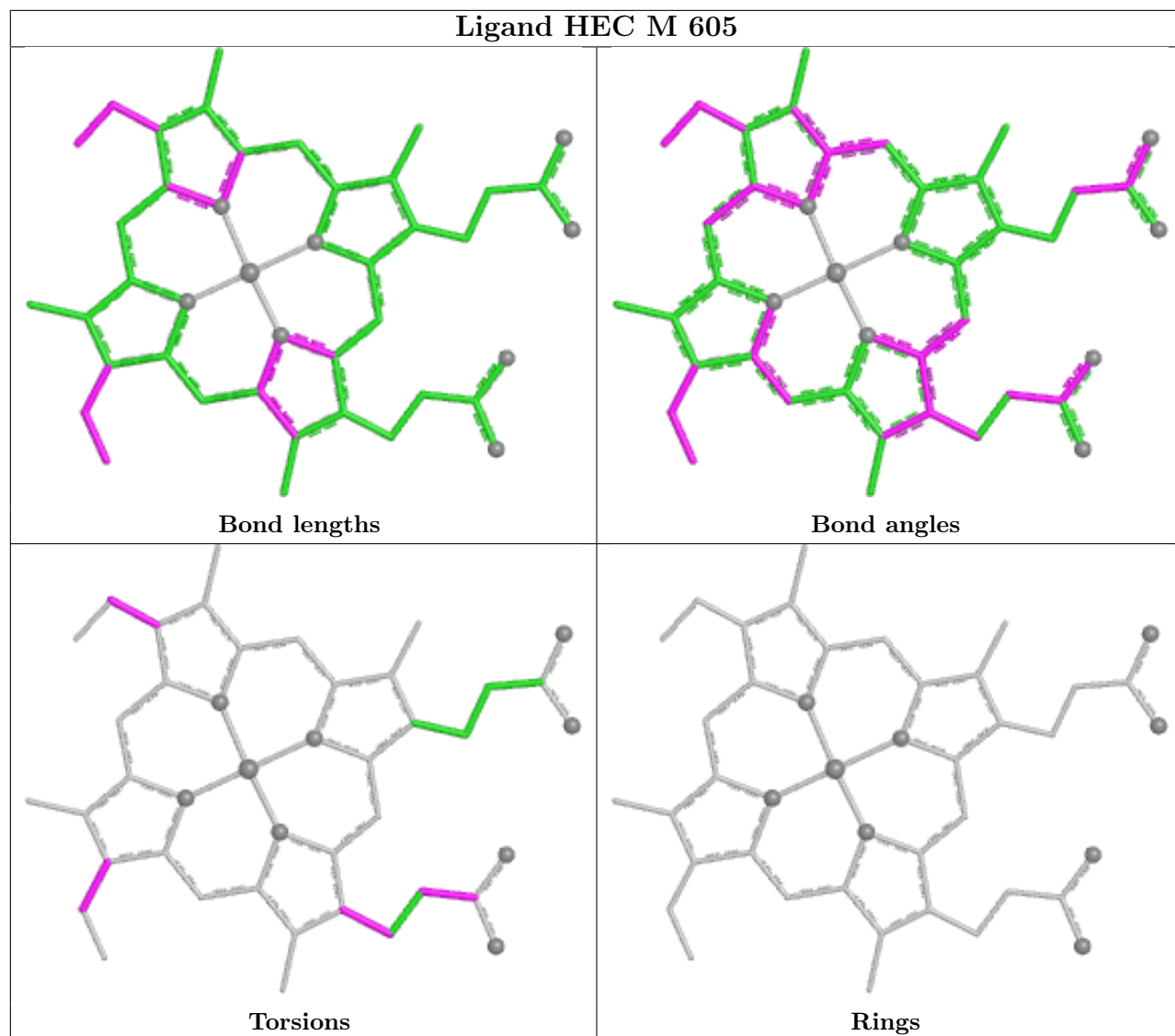




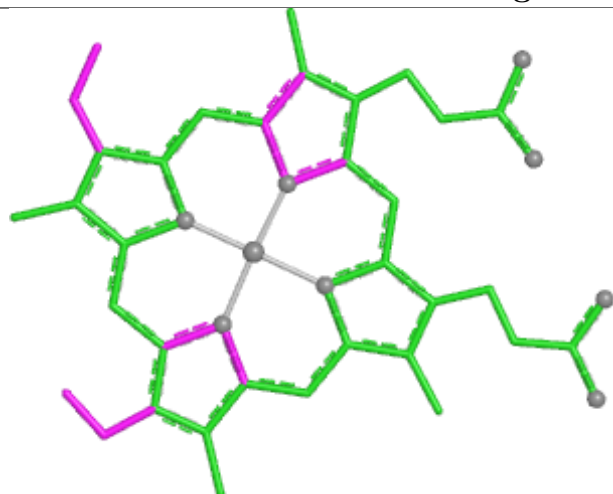
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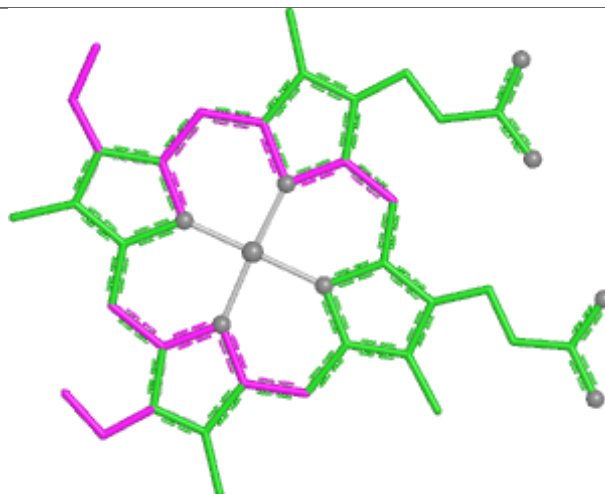




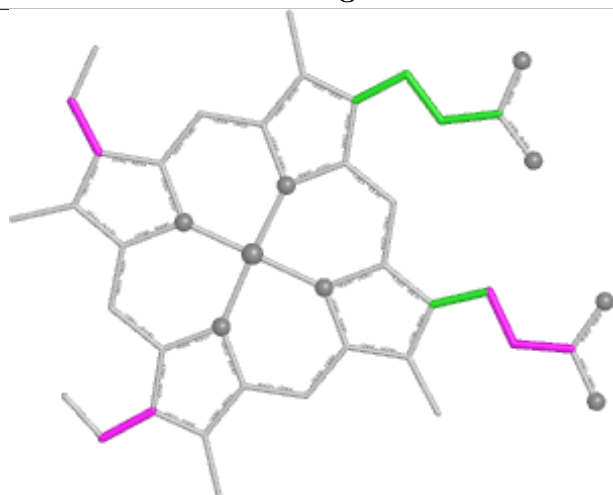
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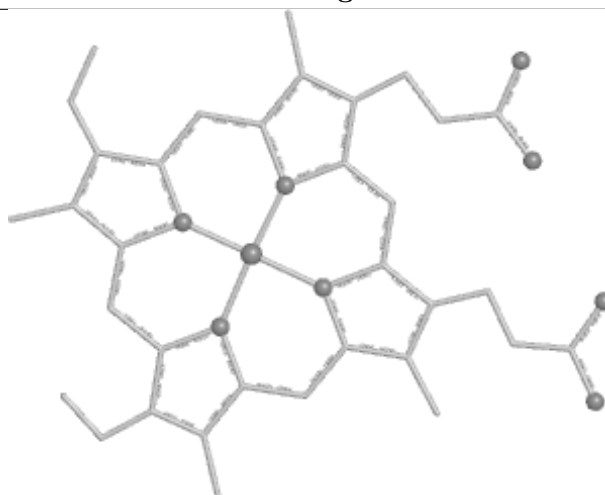
Bond lengths



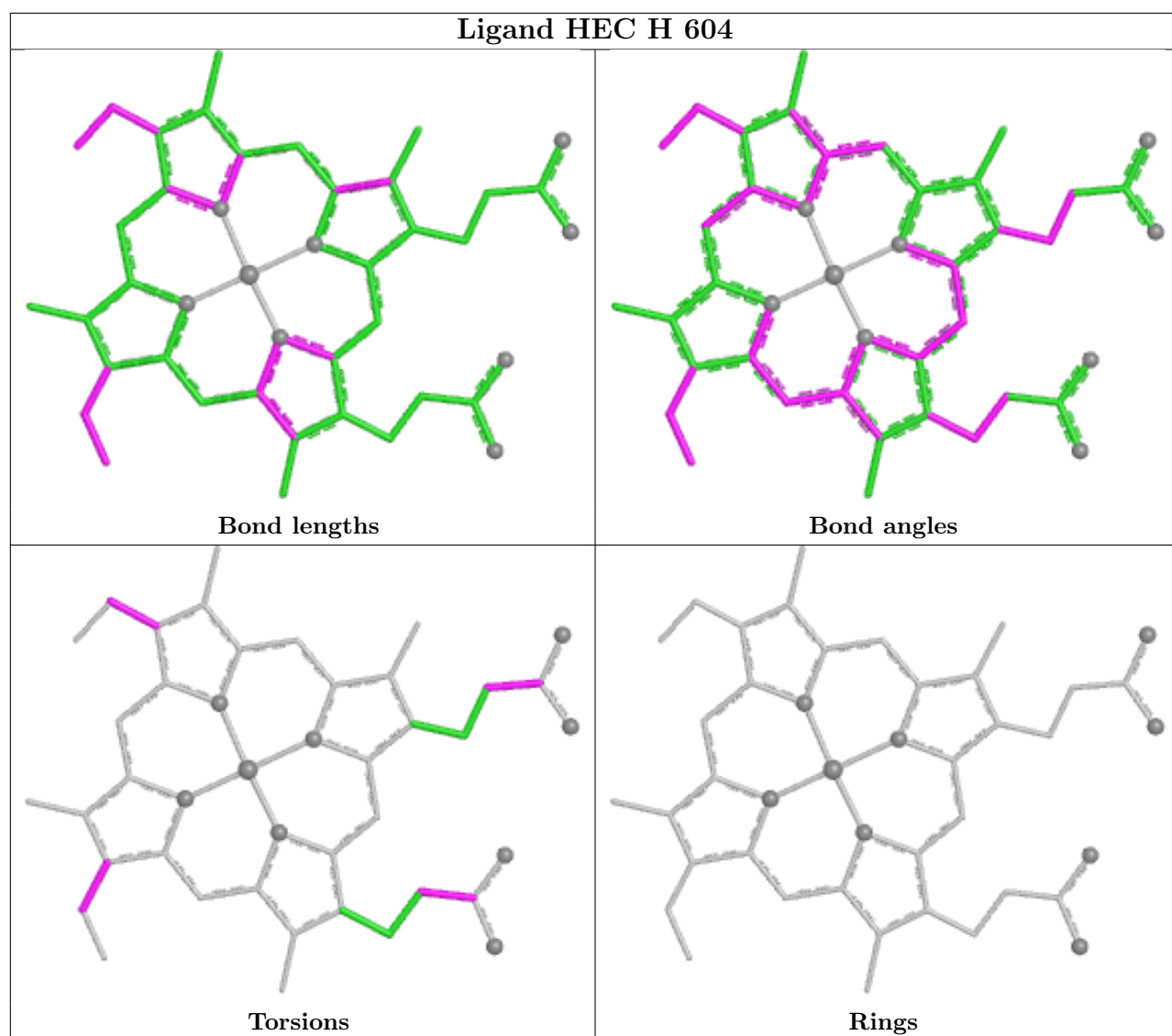
Bond angles



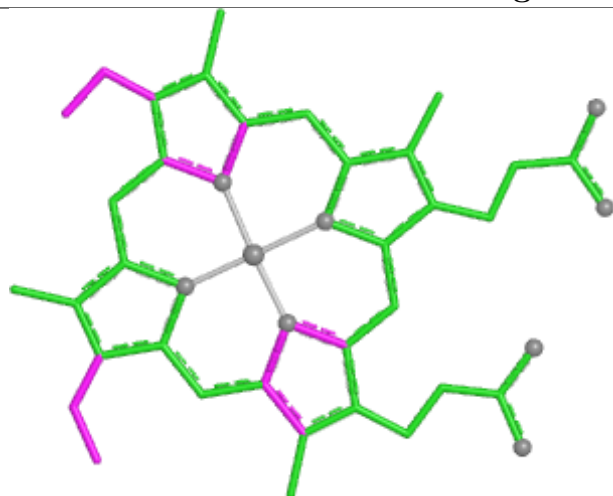
Torsions



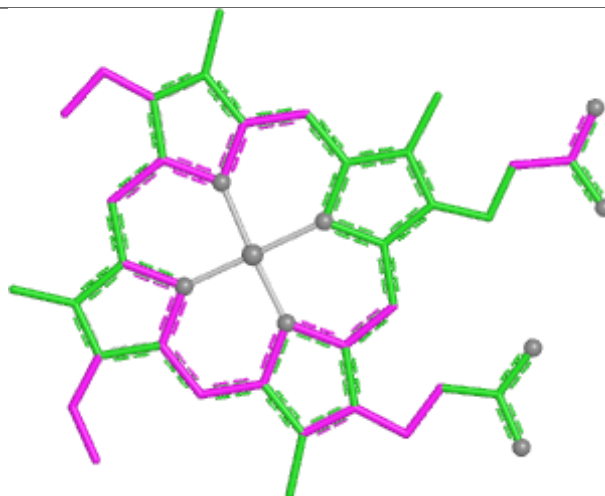
Rings



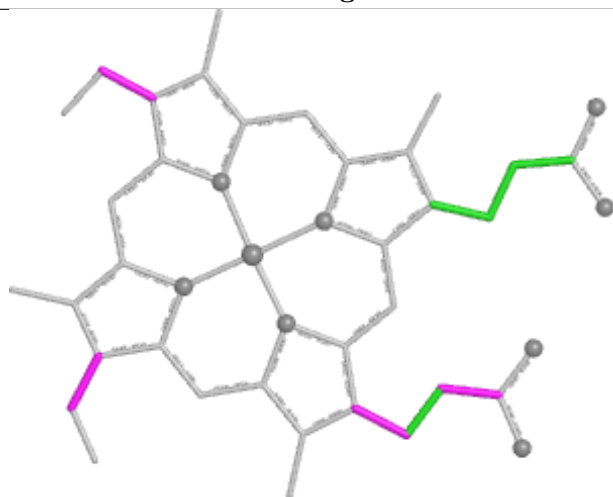
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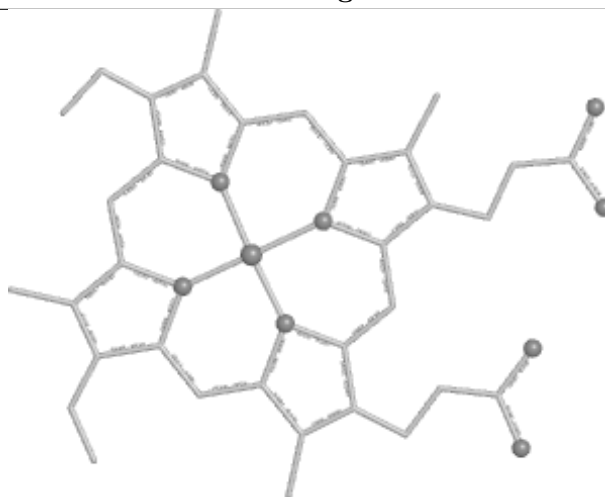
Bond lengths



Bond angles

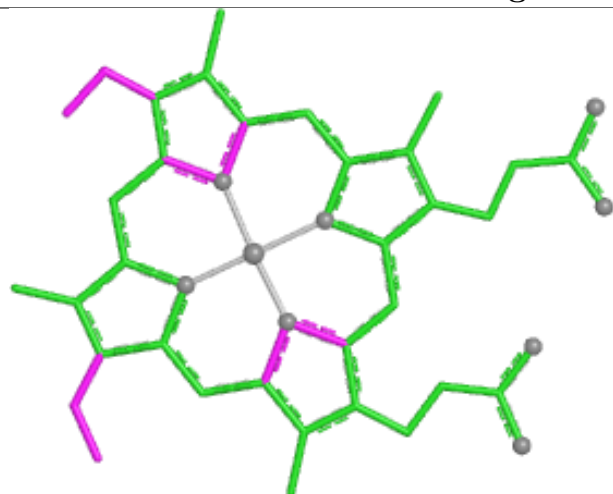


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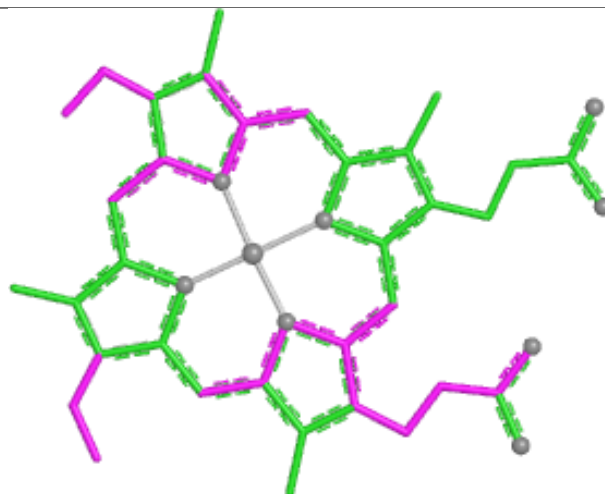


Rings

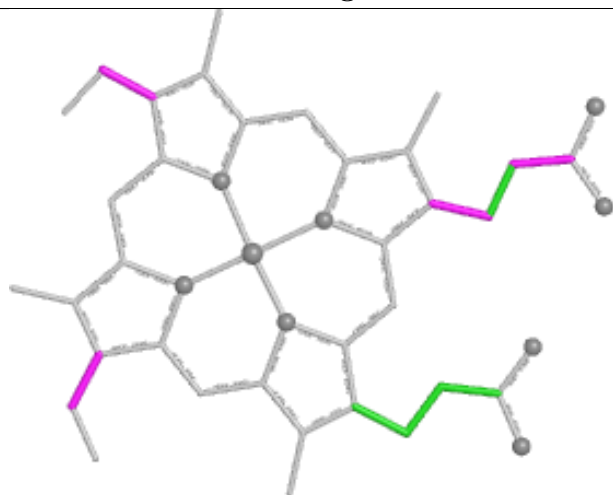
Ligand HEC M 601



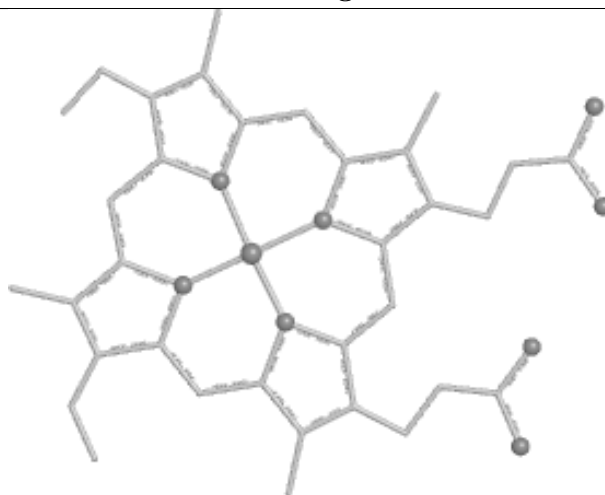
Bond lengths



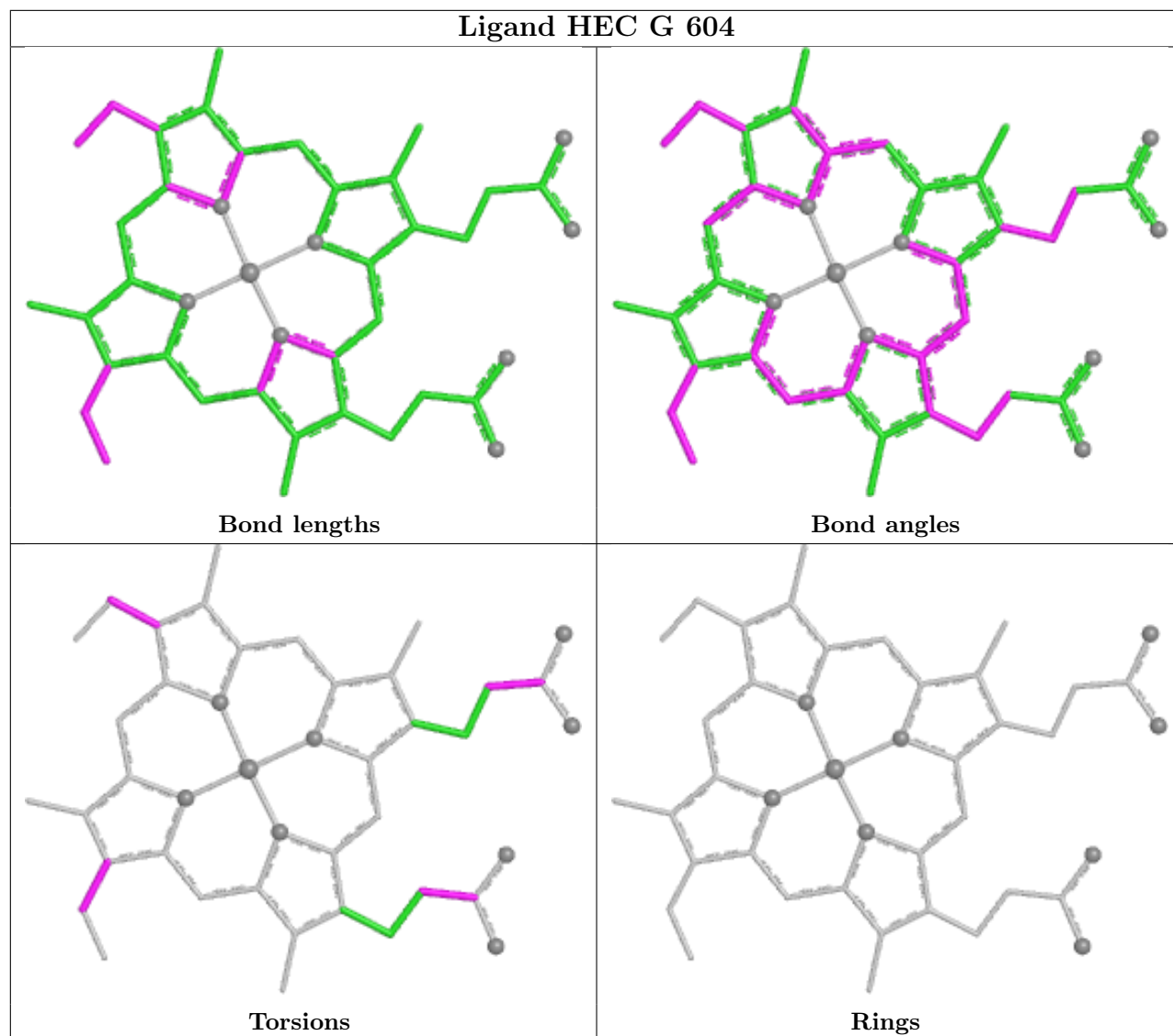
Bond angles



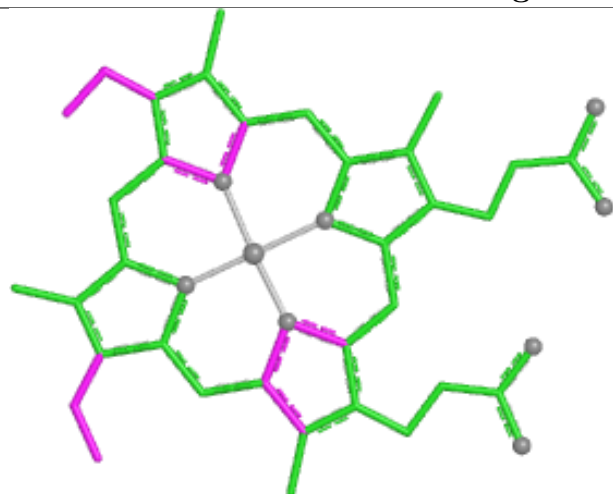
Torsions



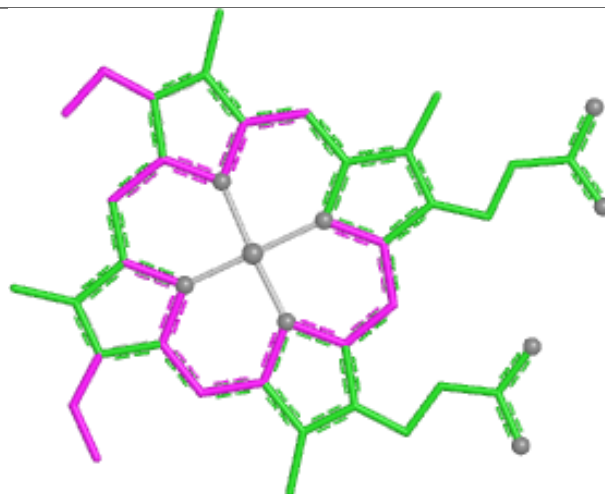
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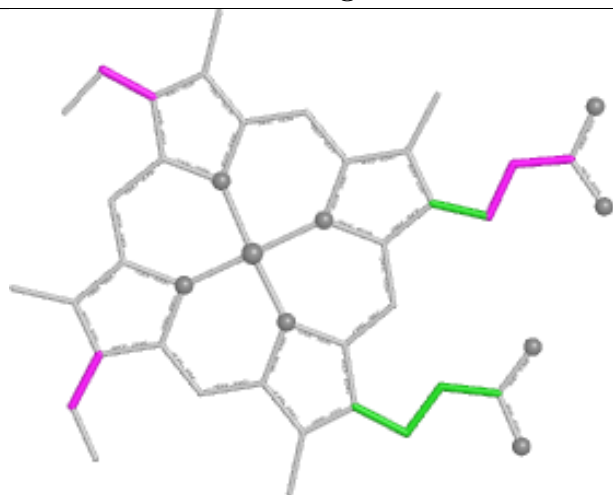
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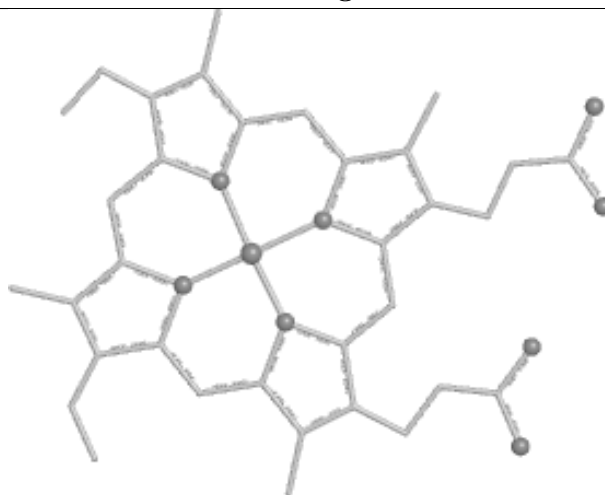
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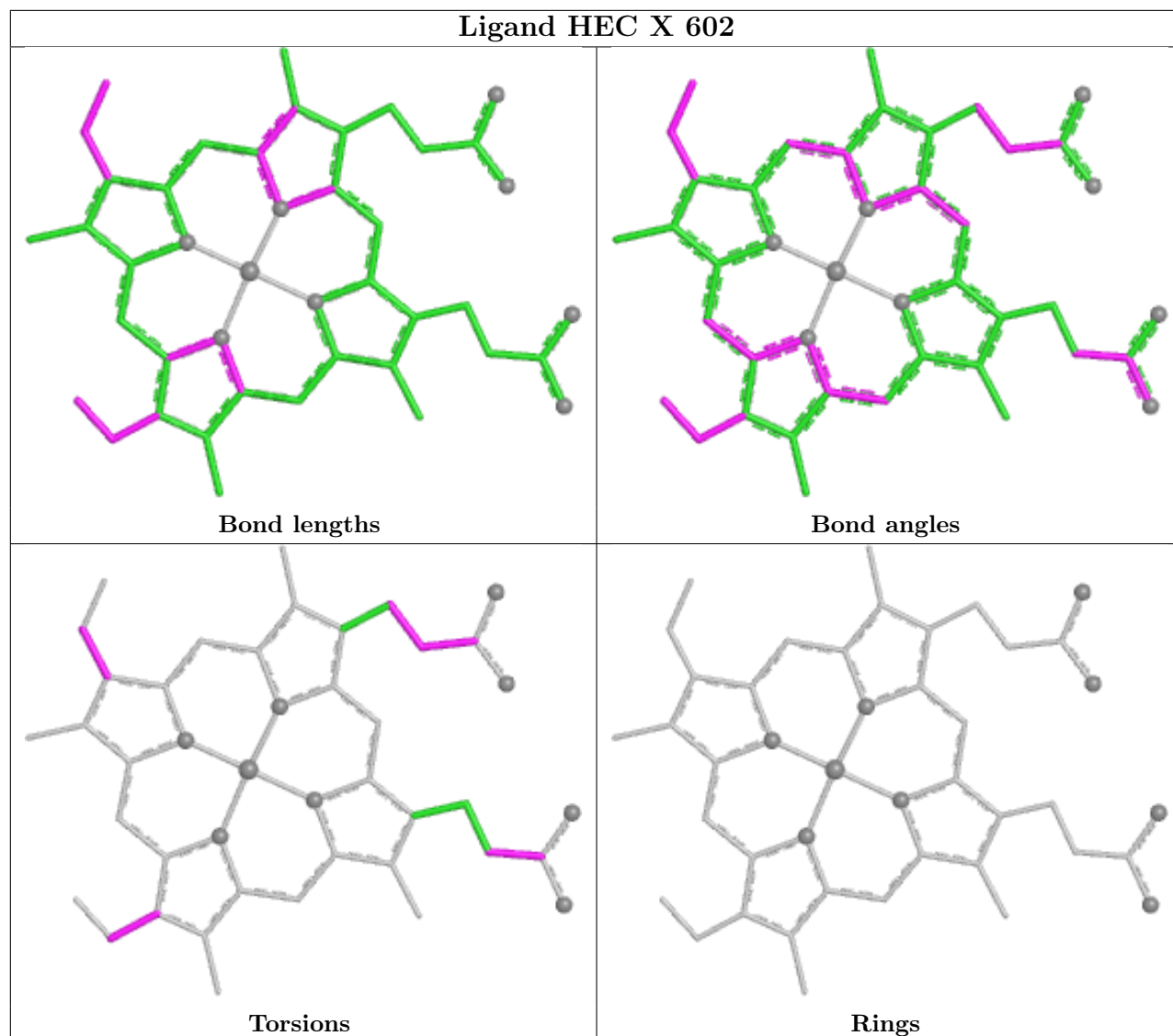
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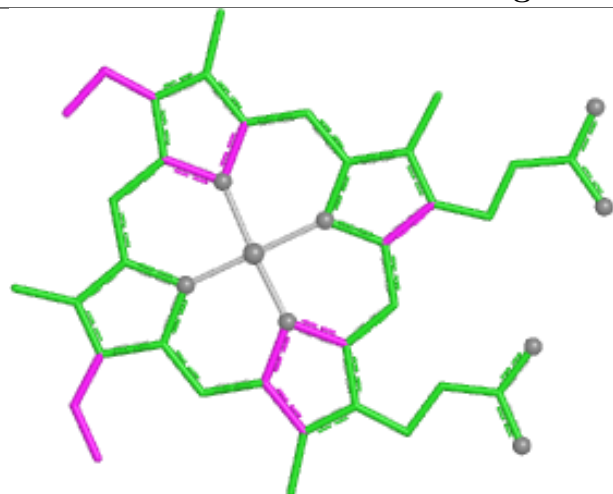
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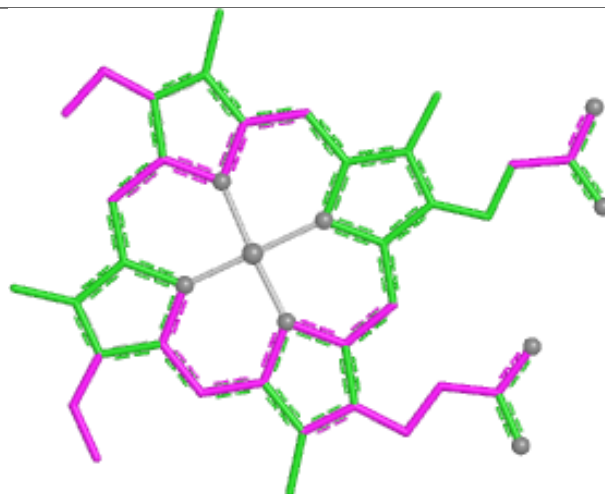
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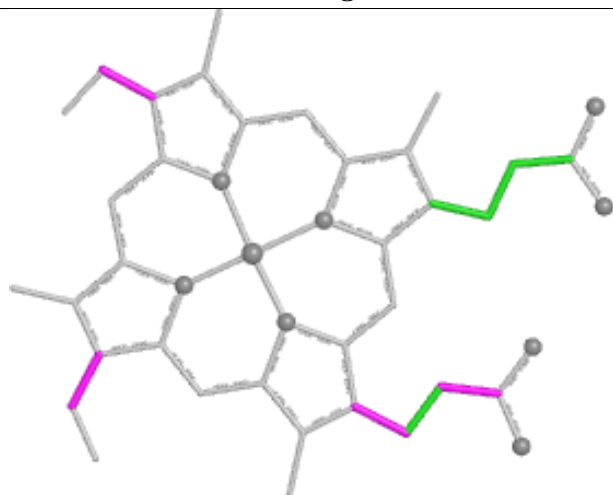
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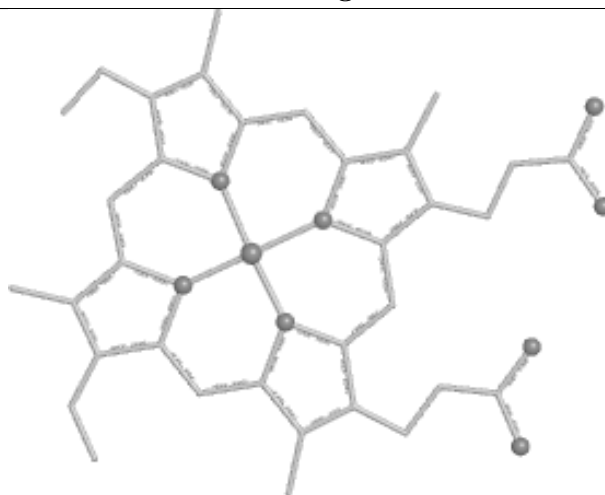
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Bond angles

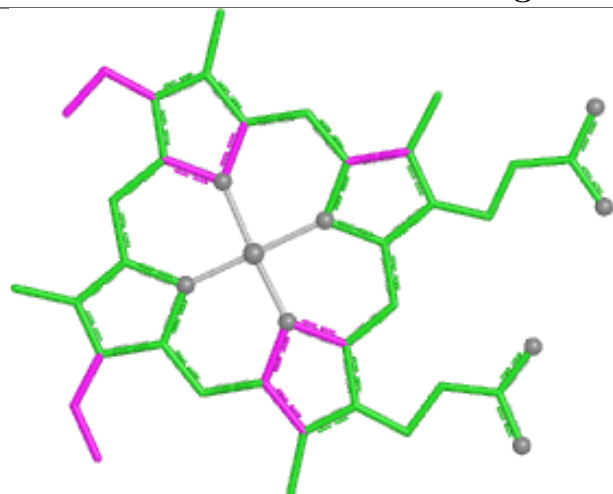


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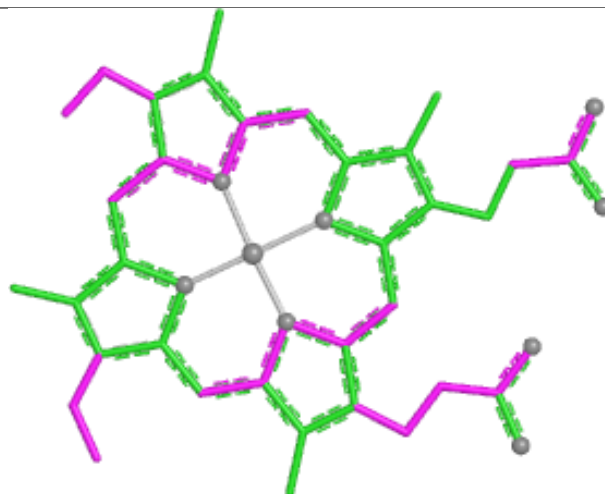


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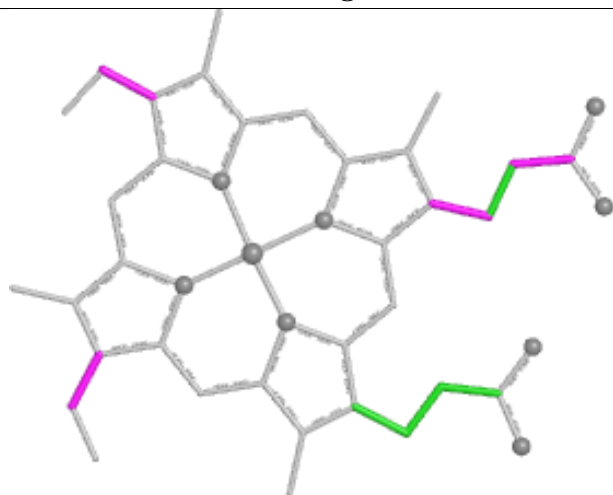
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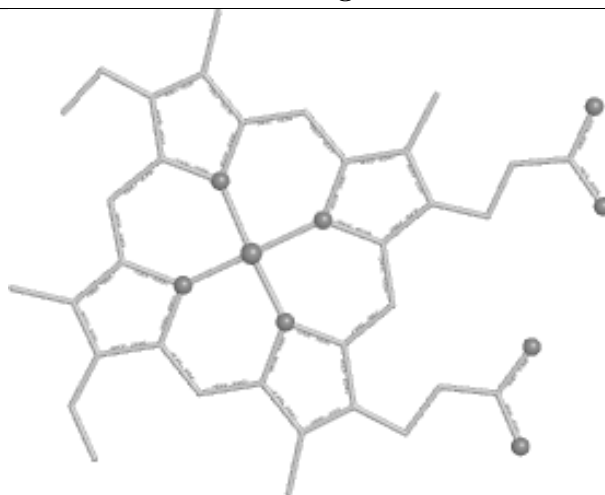
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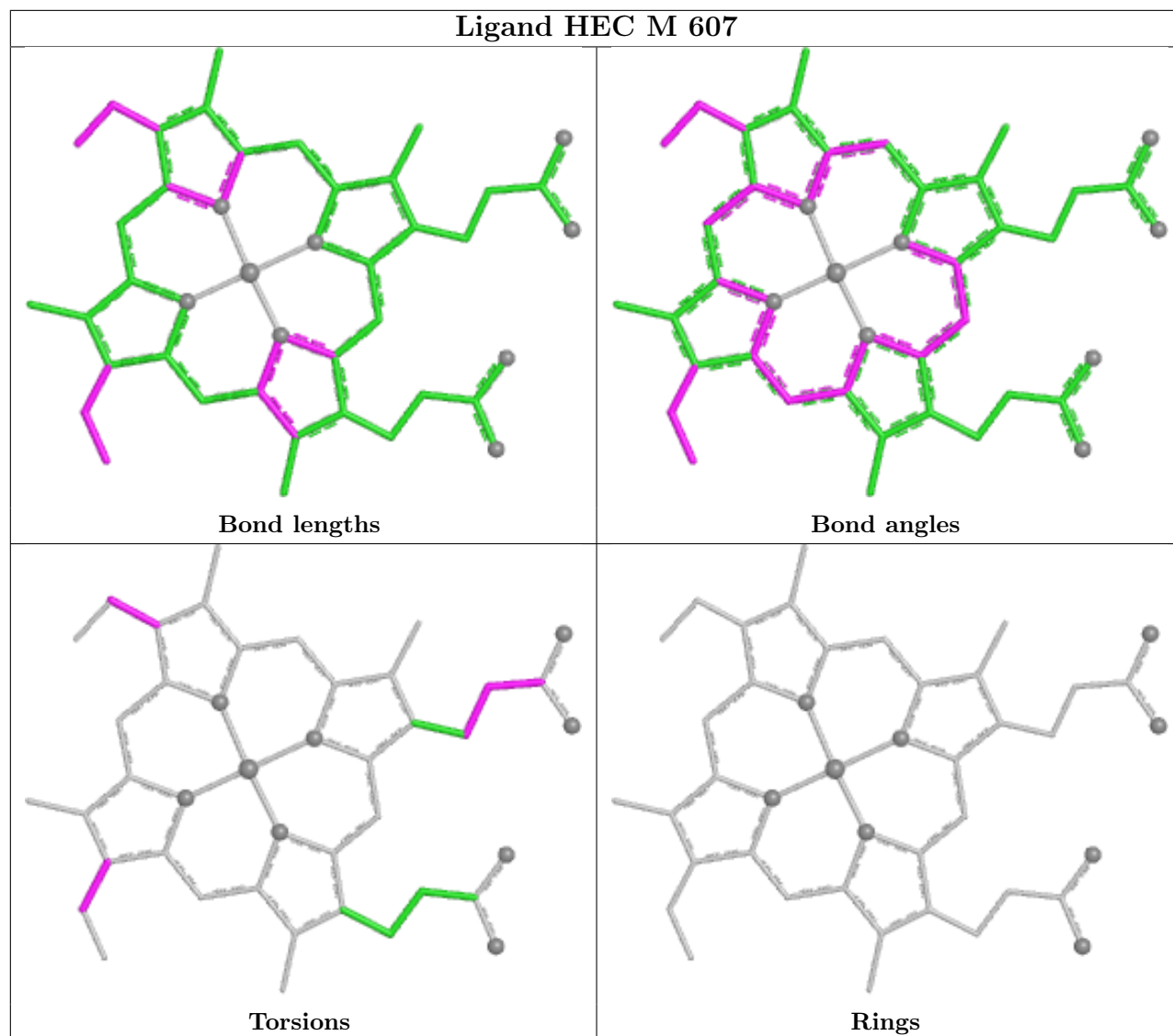
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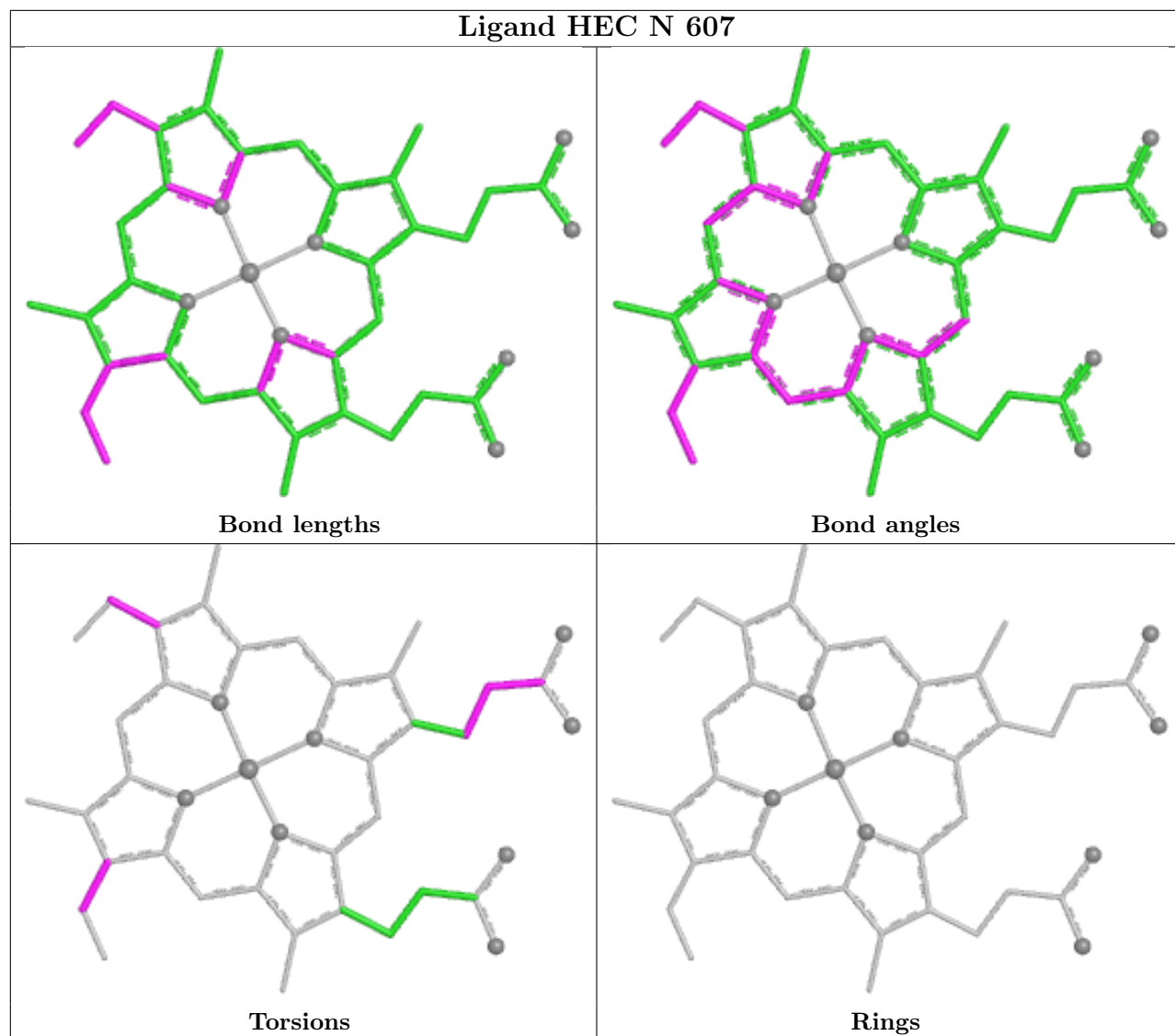


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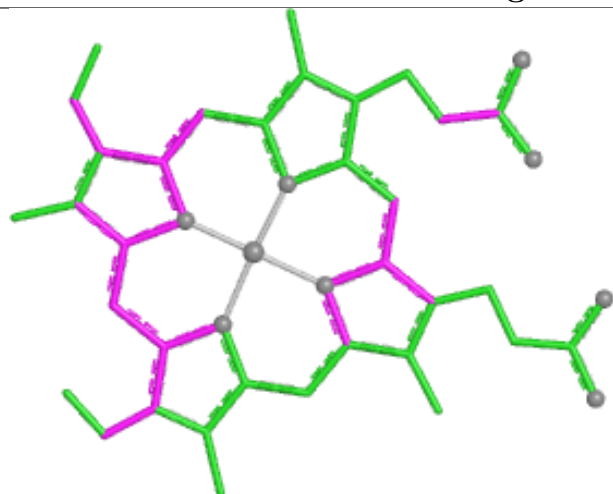


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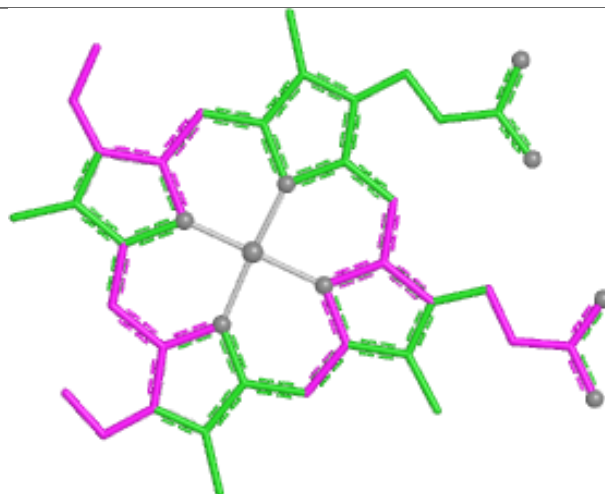




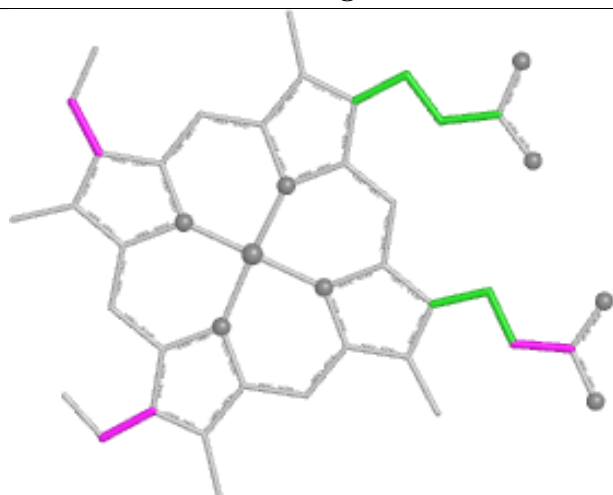
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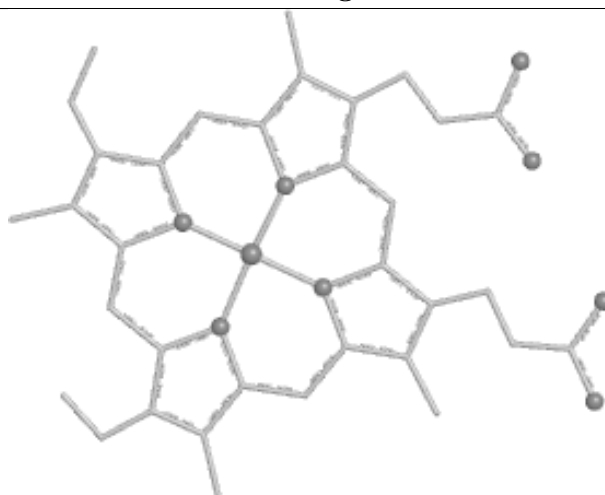
Bond lengths



Bond angles

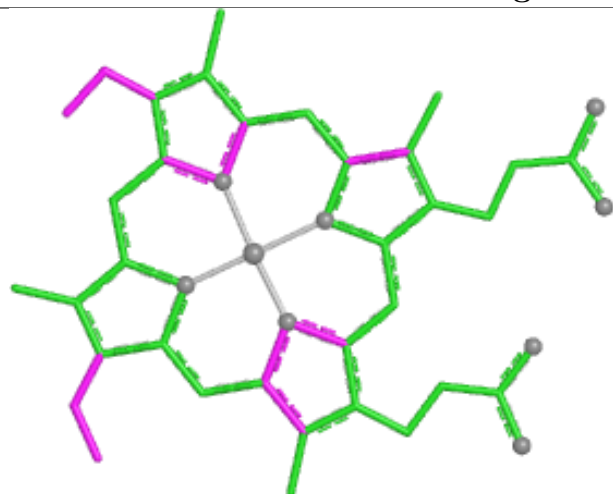


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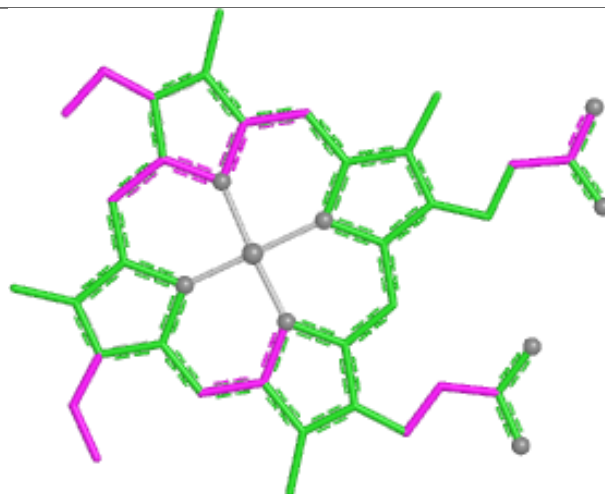


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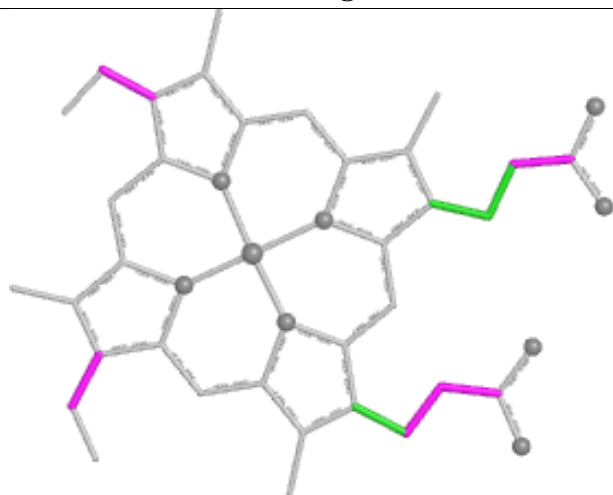
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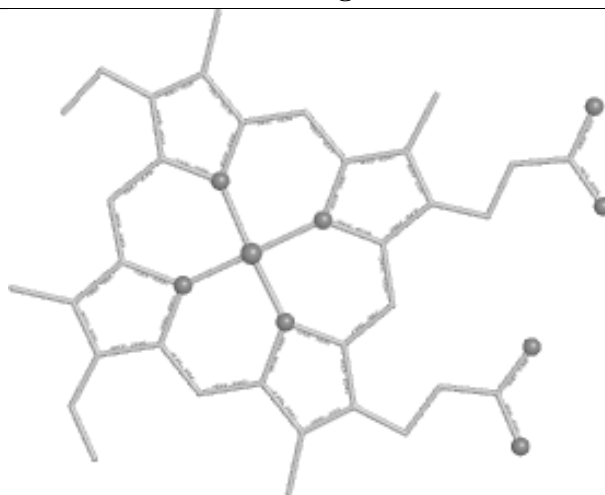
Bond lengths



Bond angles

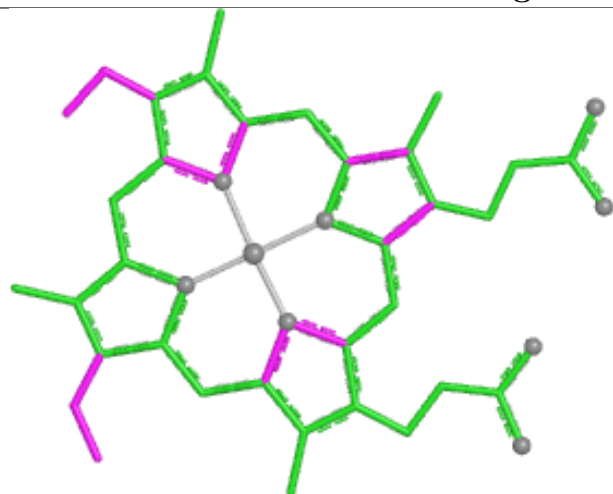


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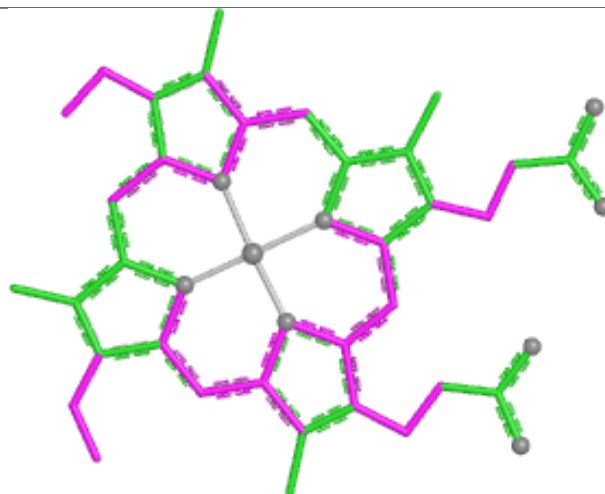


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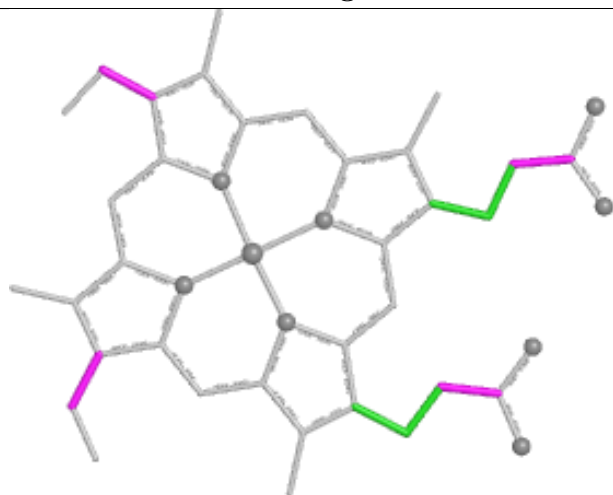
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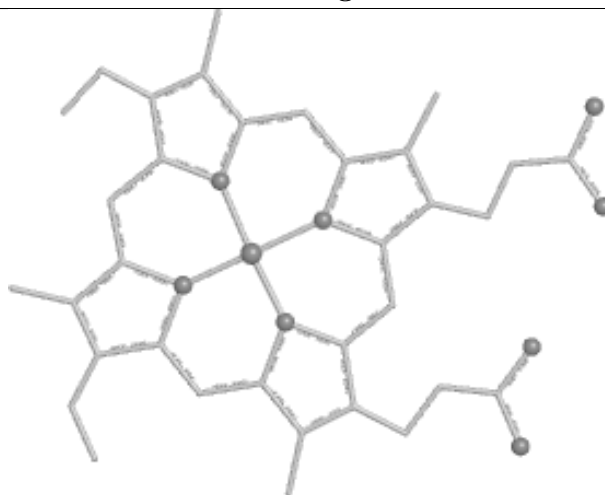
Bond lengths



Bond angles

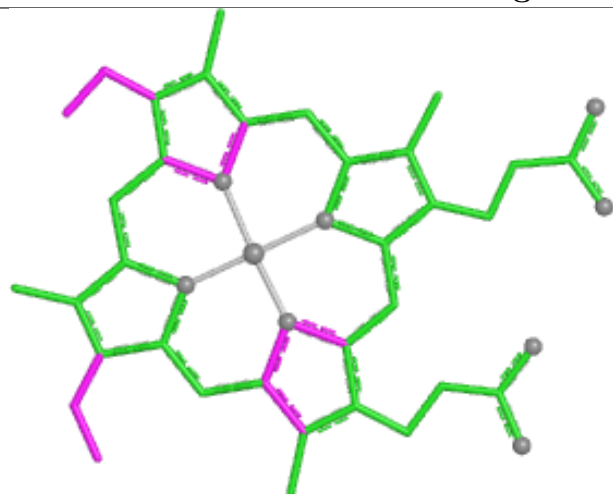


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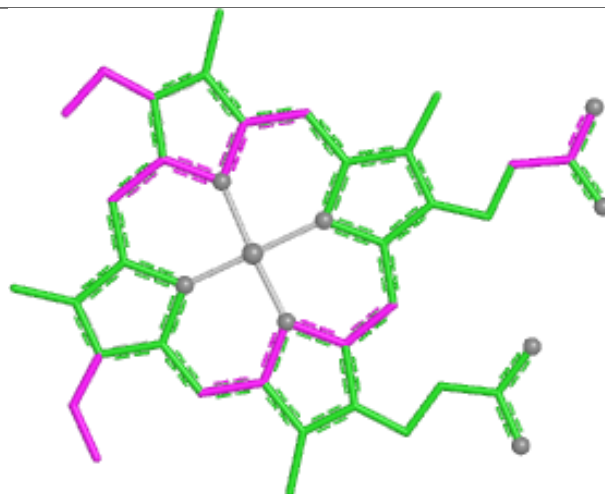


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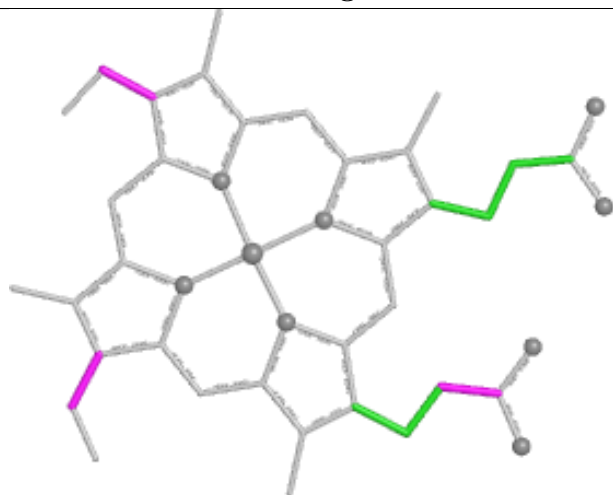
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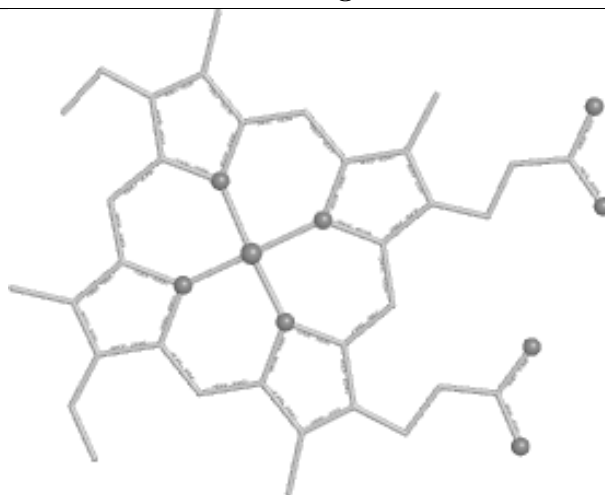
Bond lengths



Bond angles

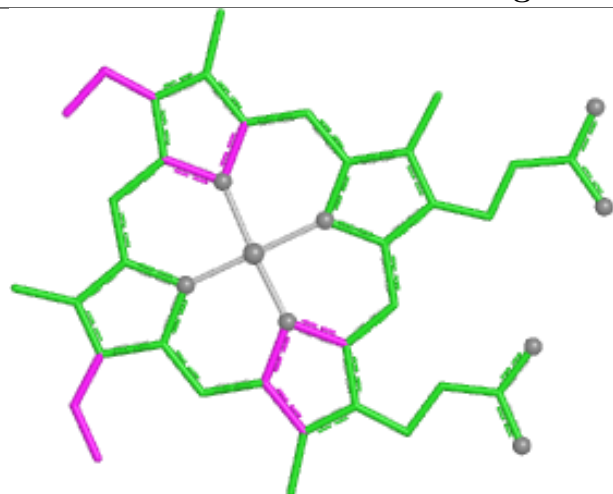


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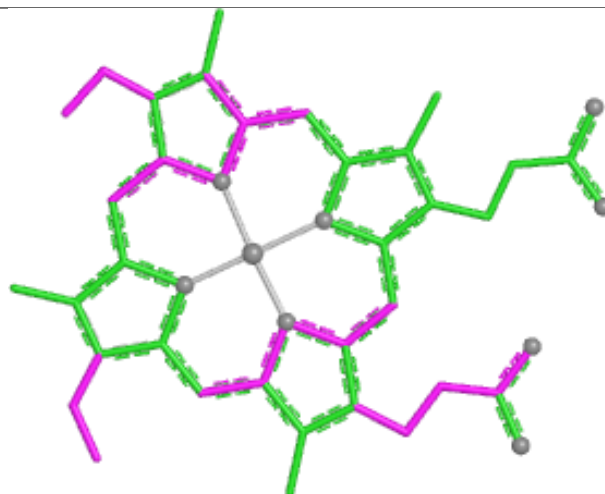


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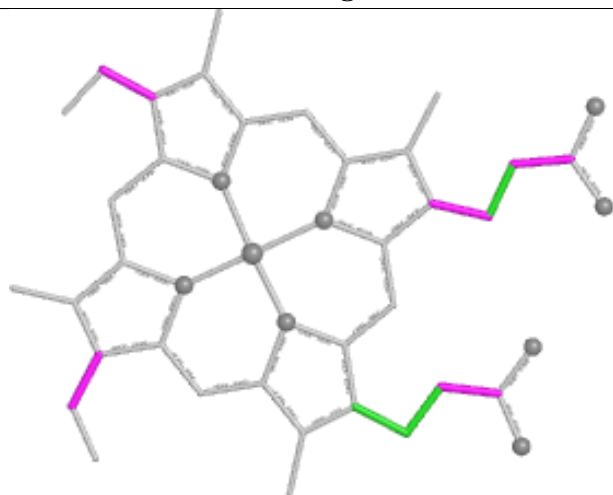
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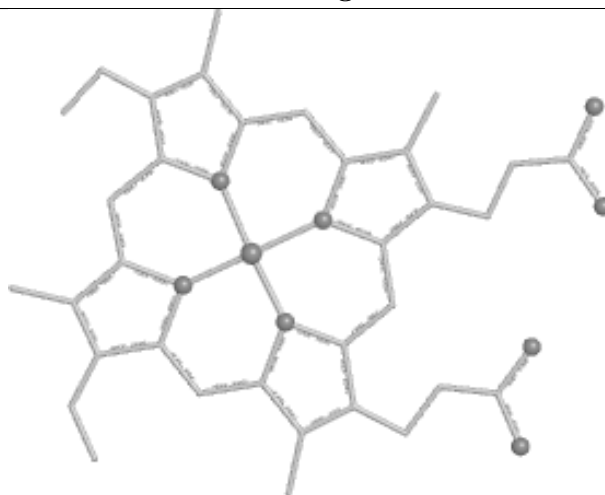
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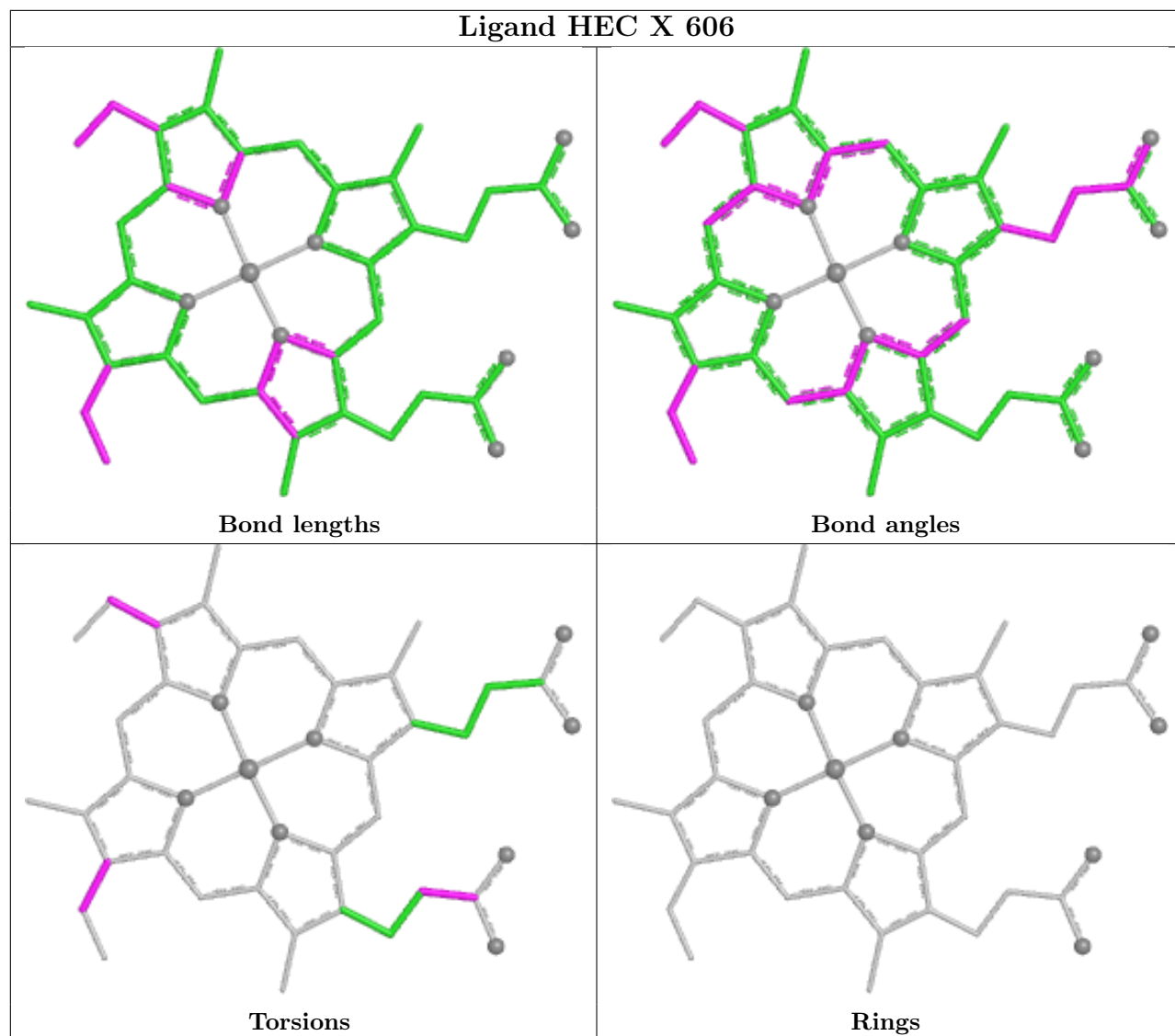
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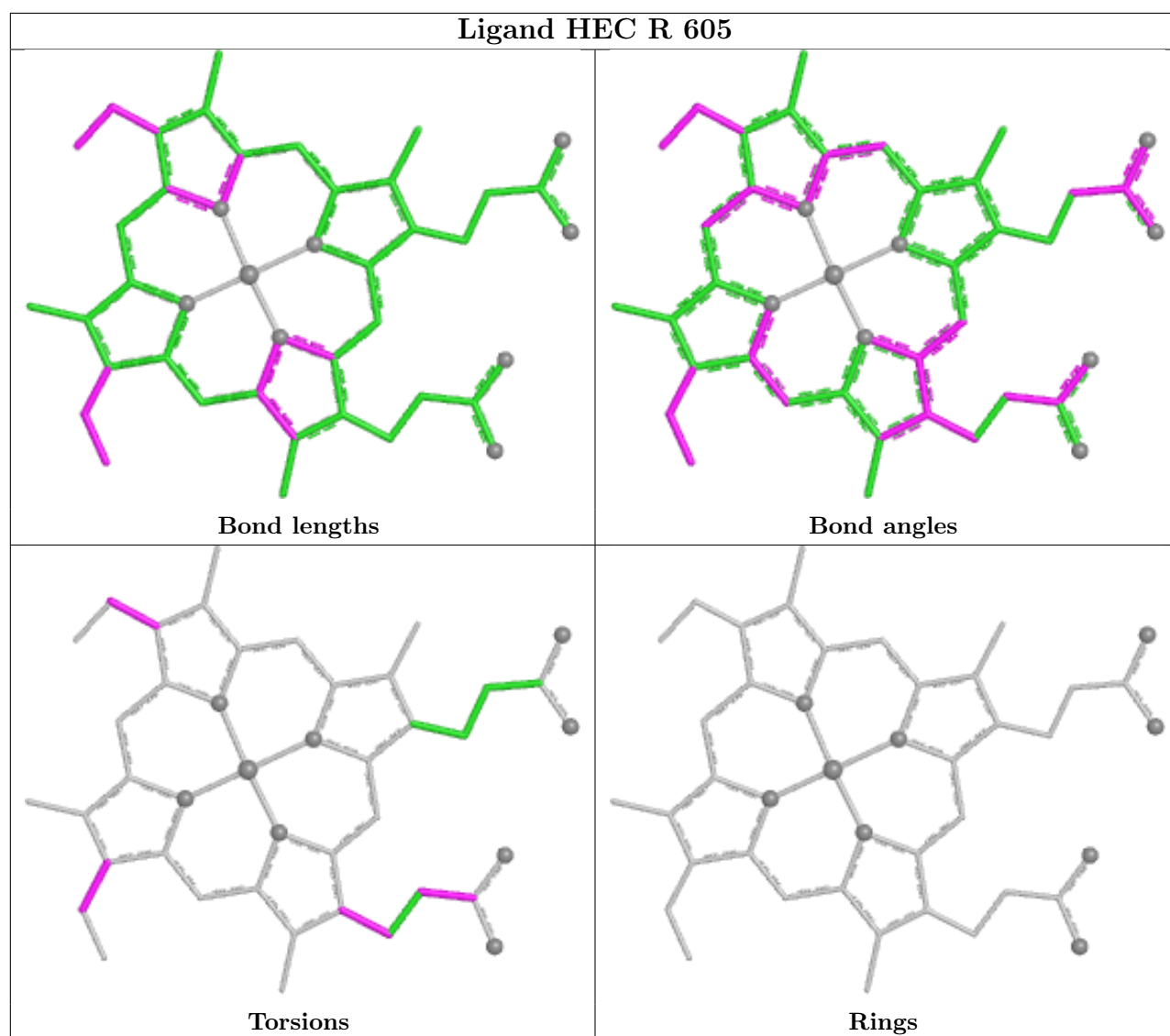


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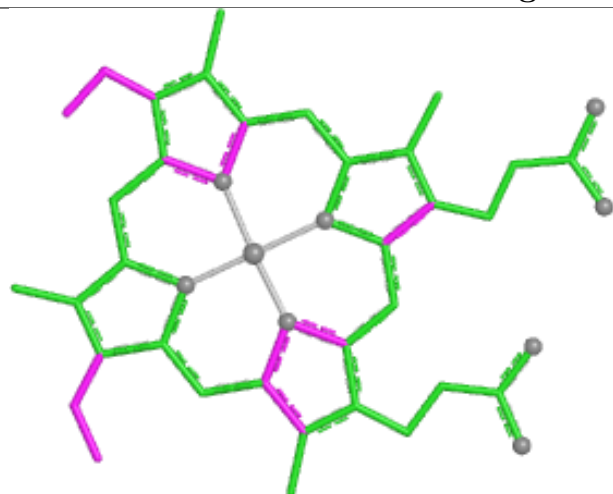


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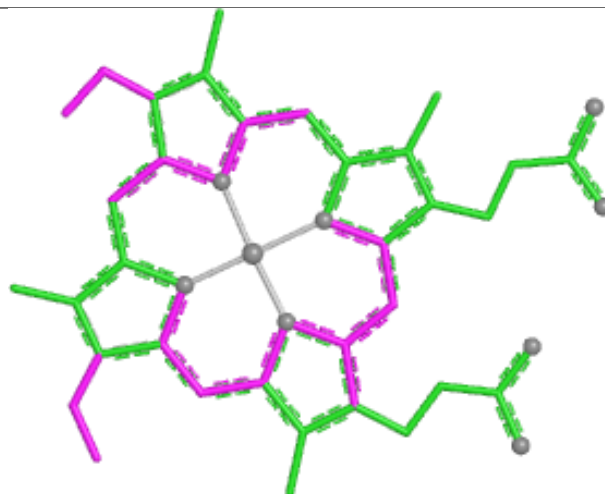




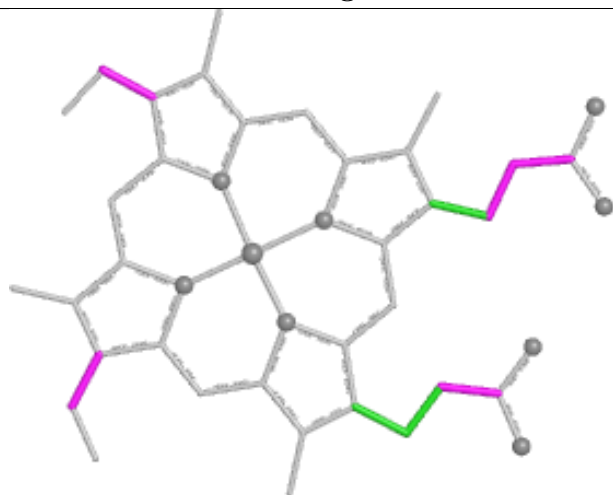
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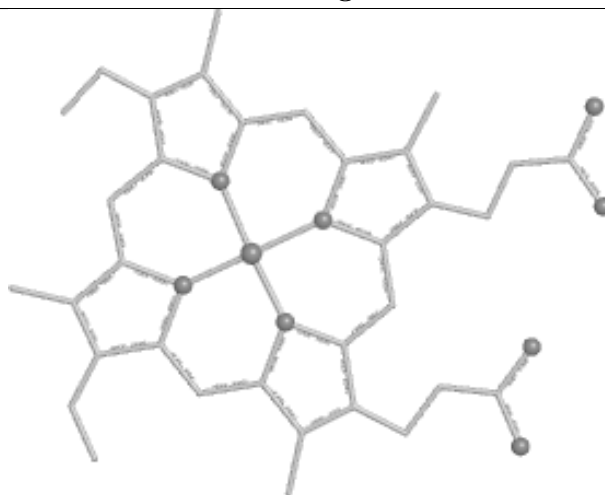
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Bond angles

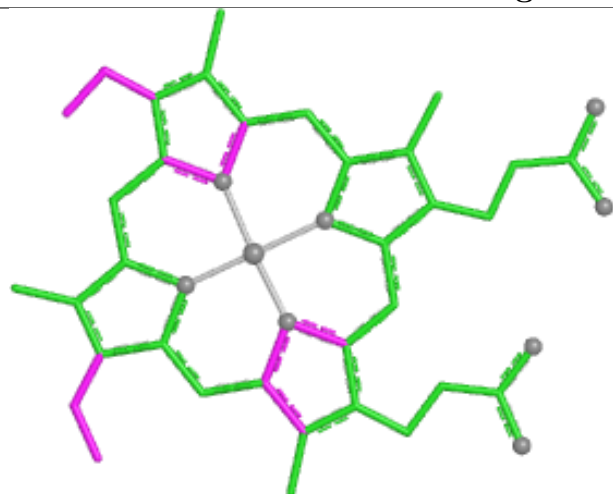


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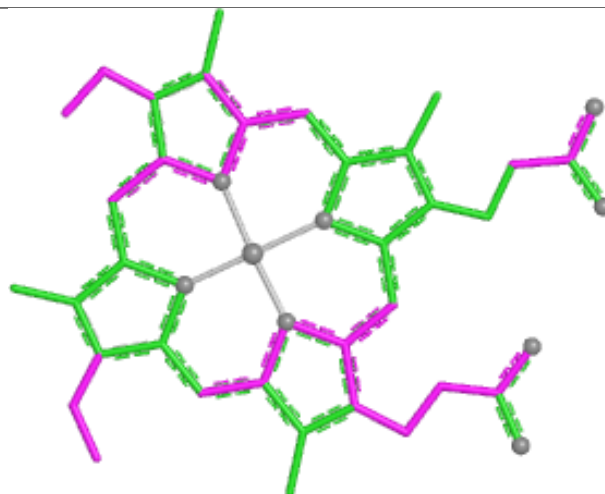


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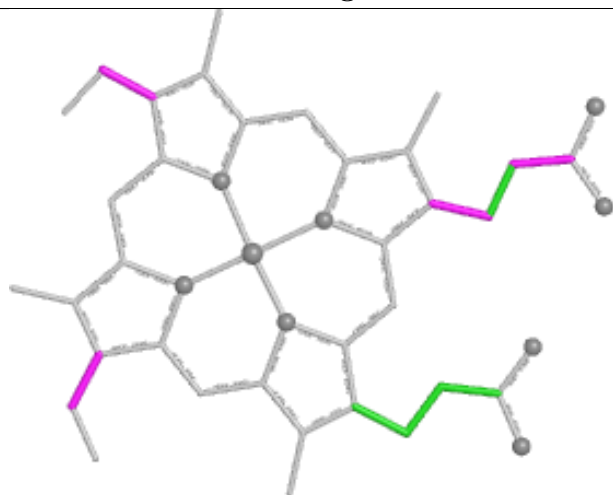
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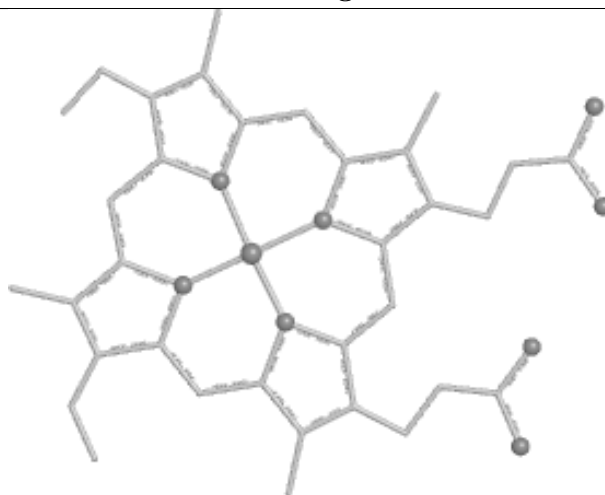
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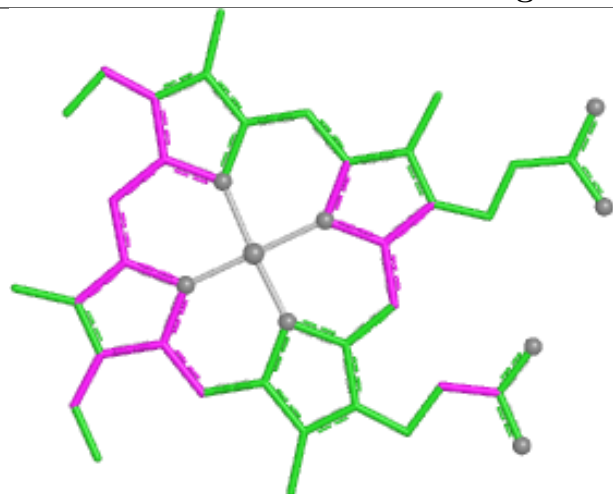


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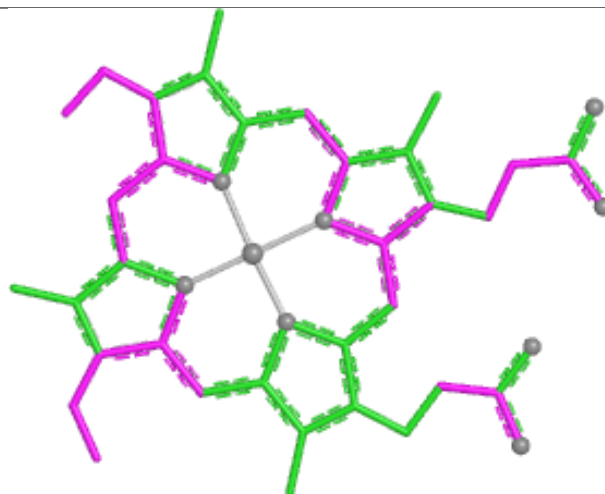


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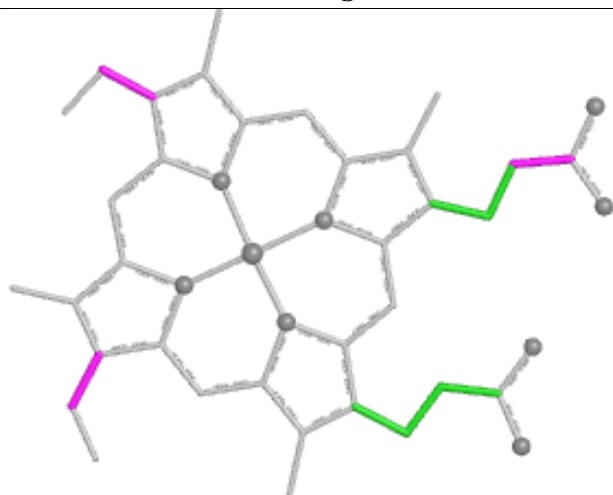
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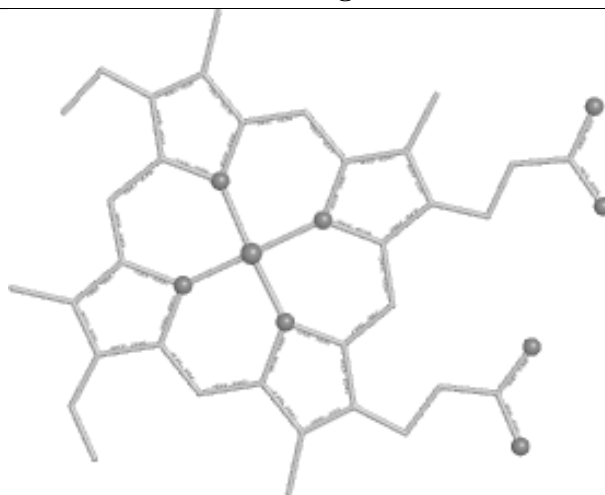
Bond lengths



Bond angles

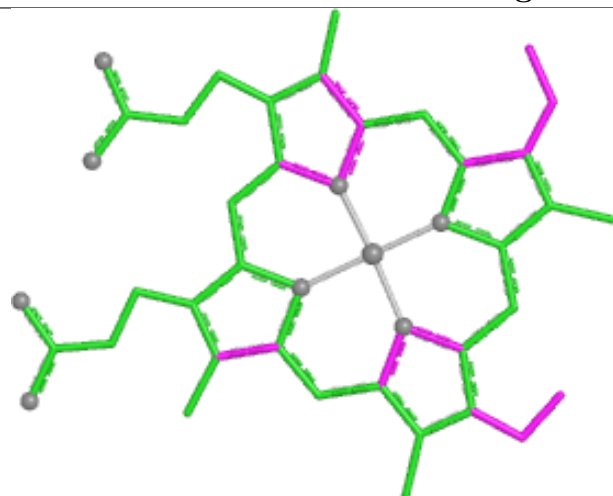


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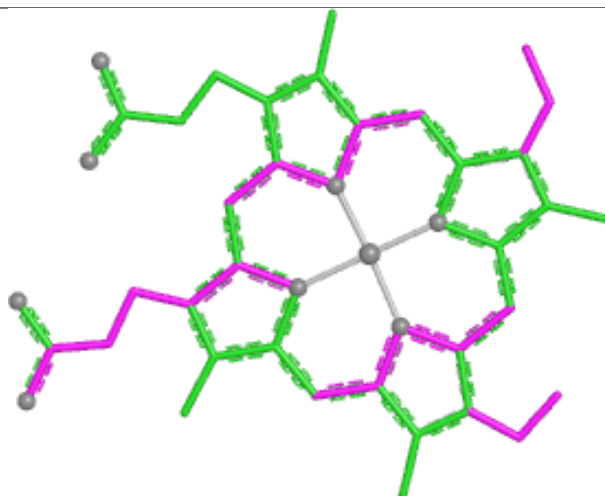


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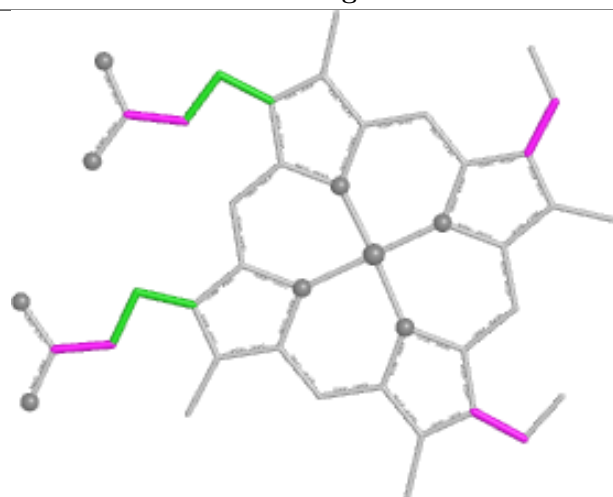
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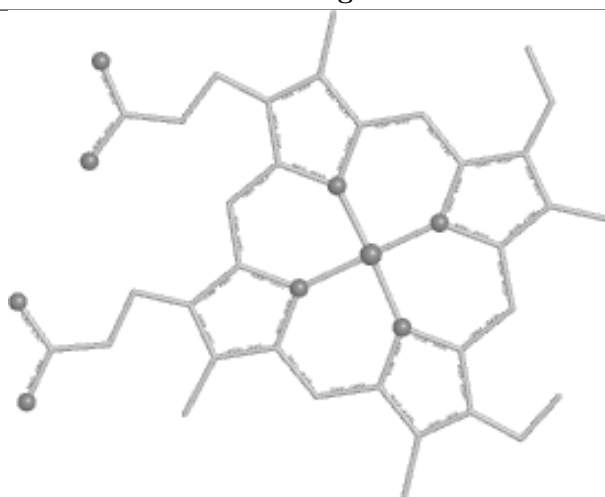
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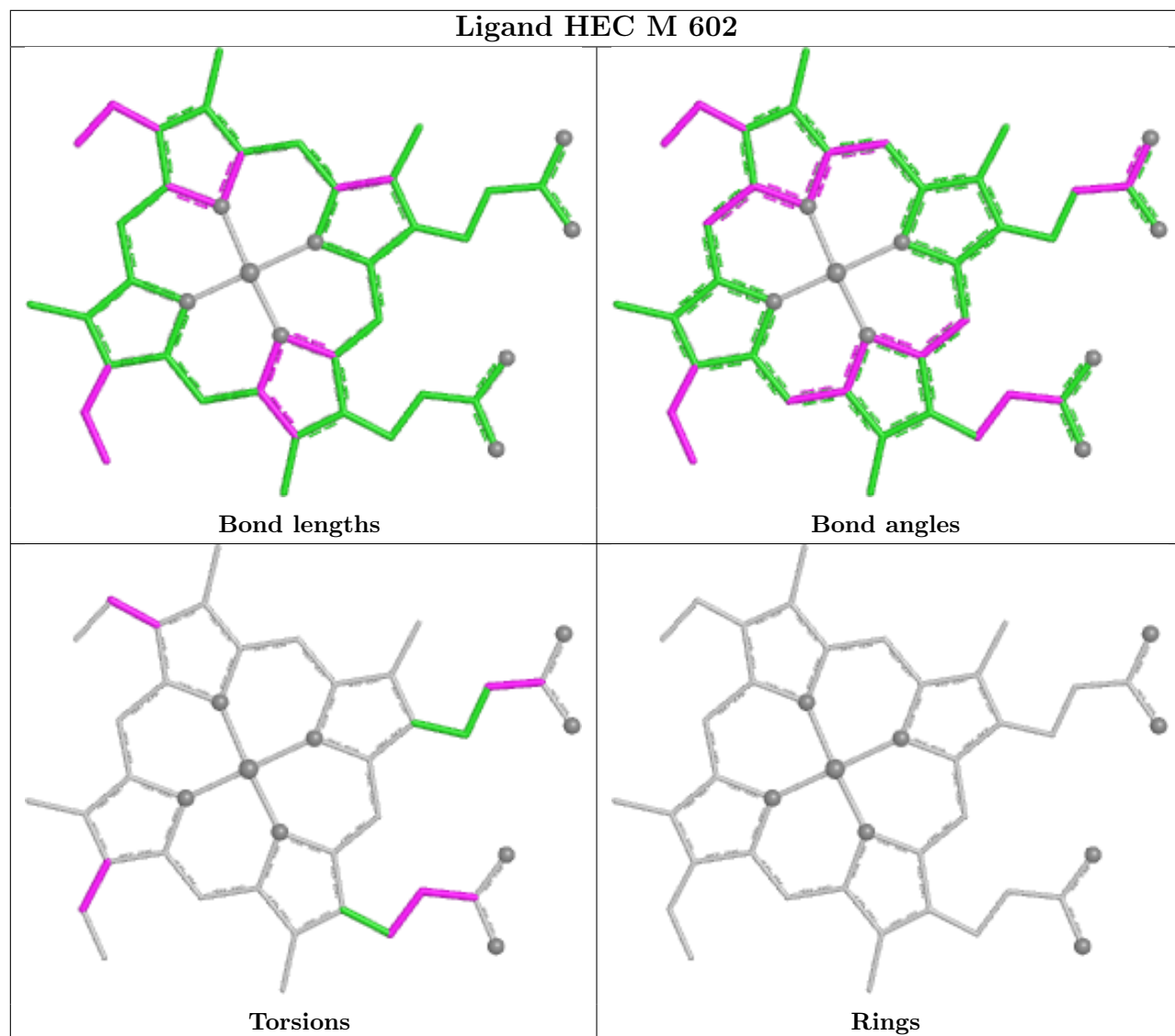
Bond angles



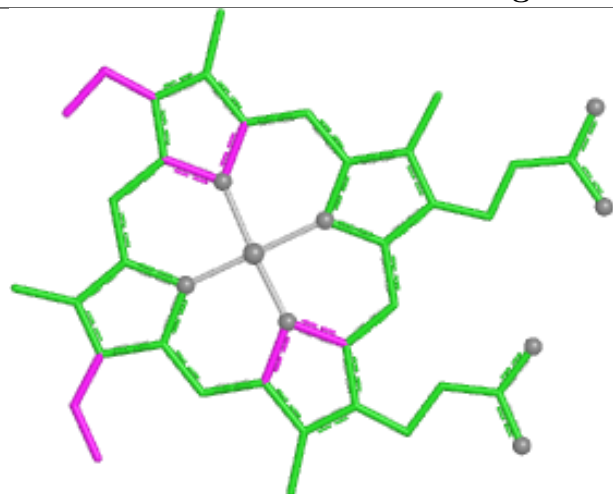
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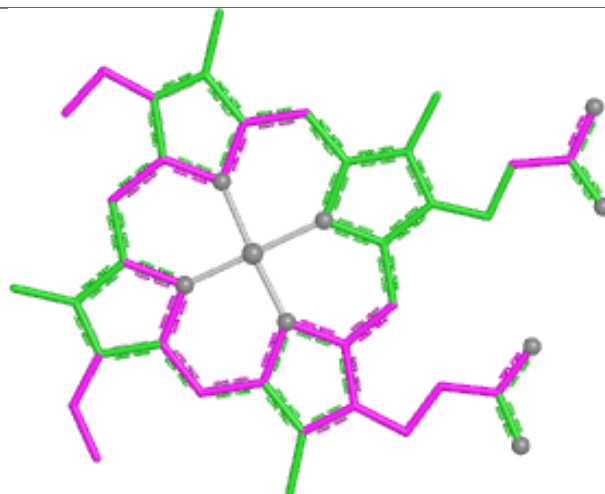
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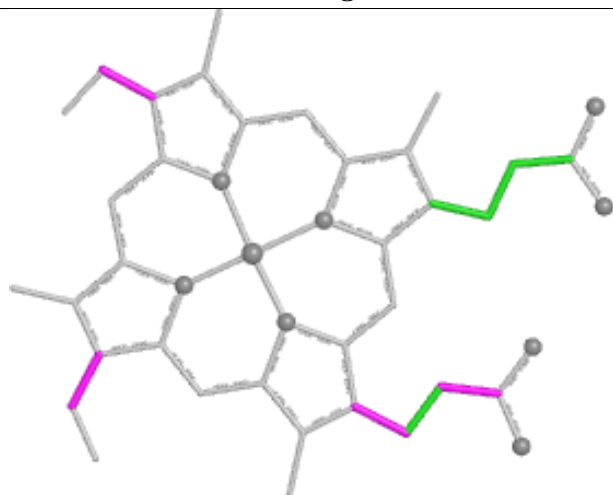
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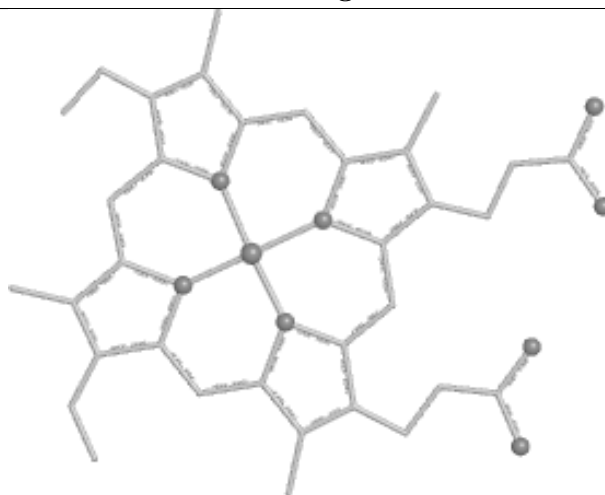
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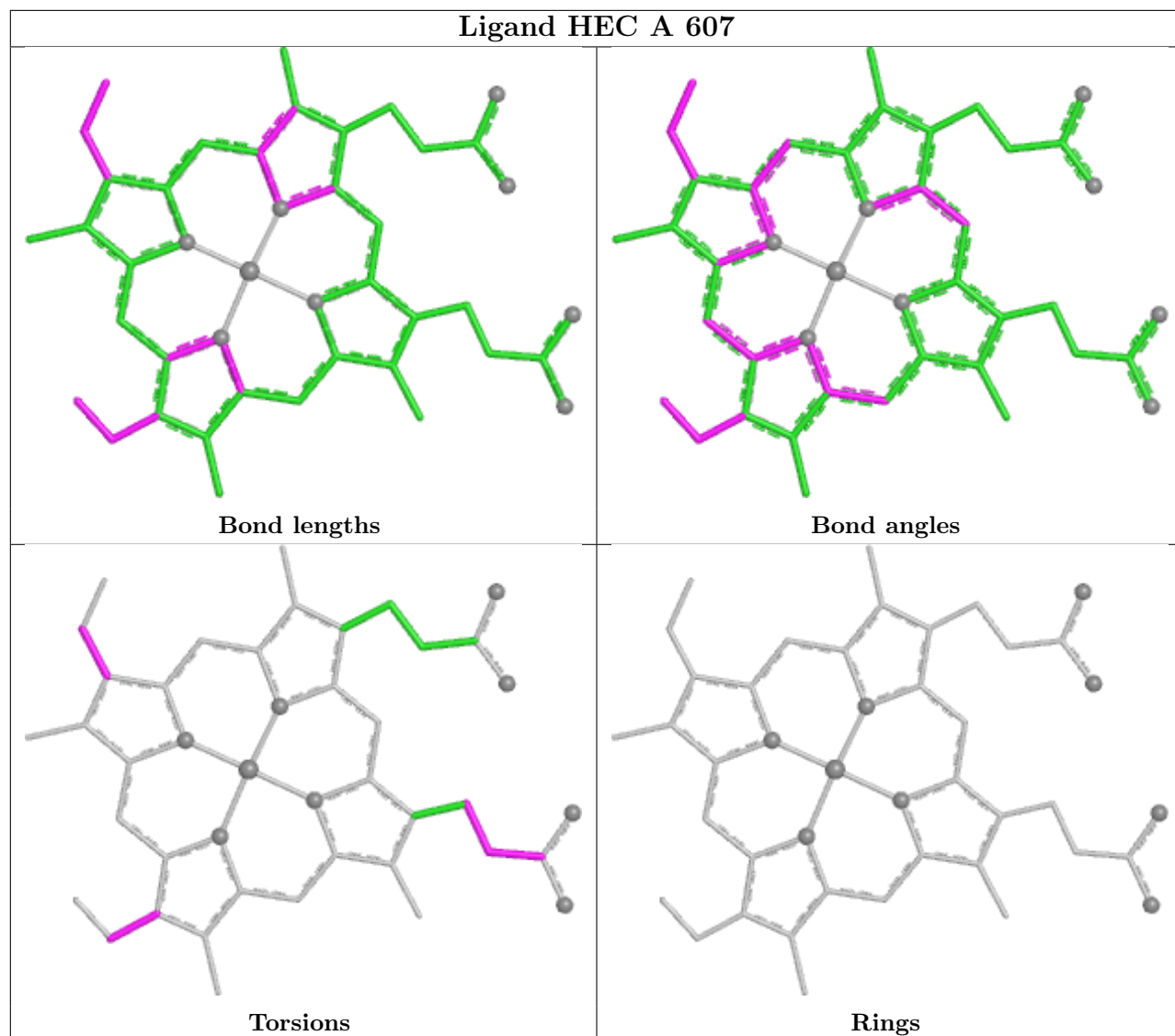
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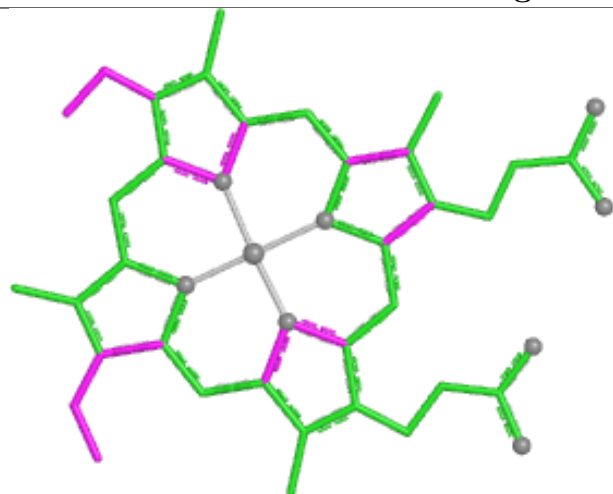
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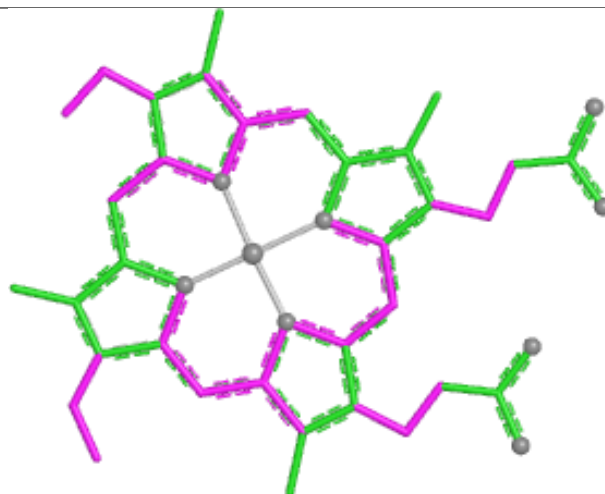
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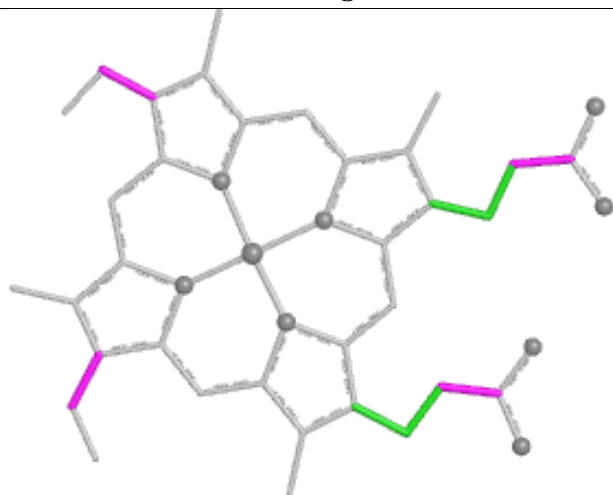
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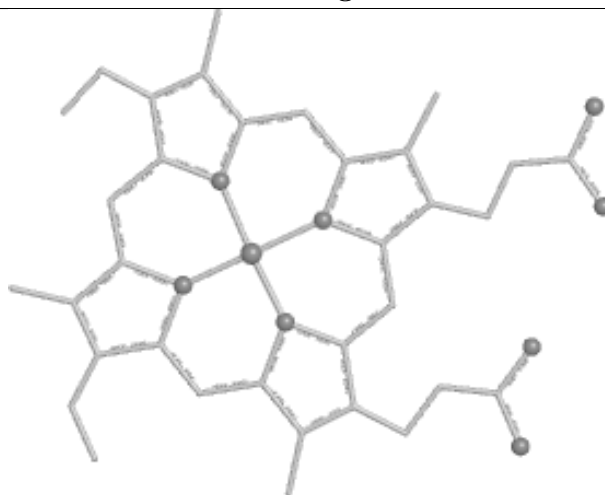
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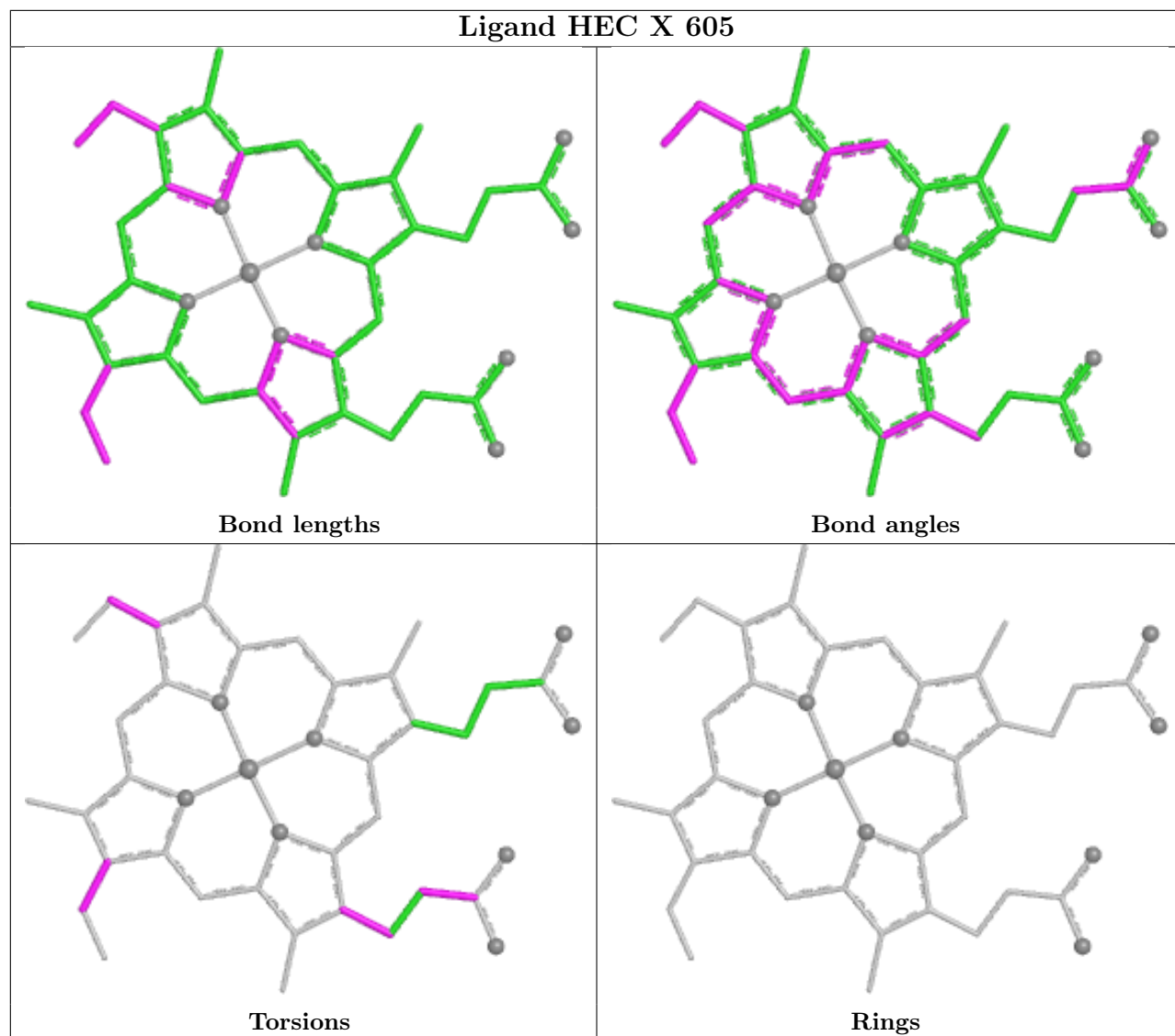
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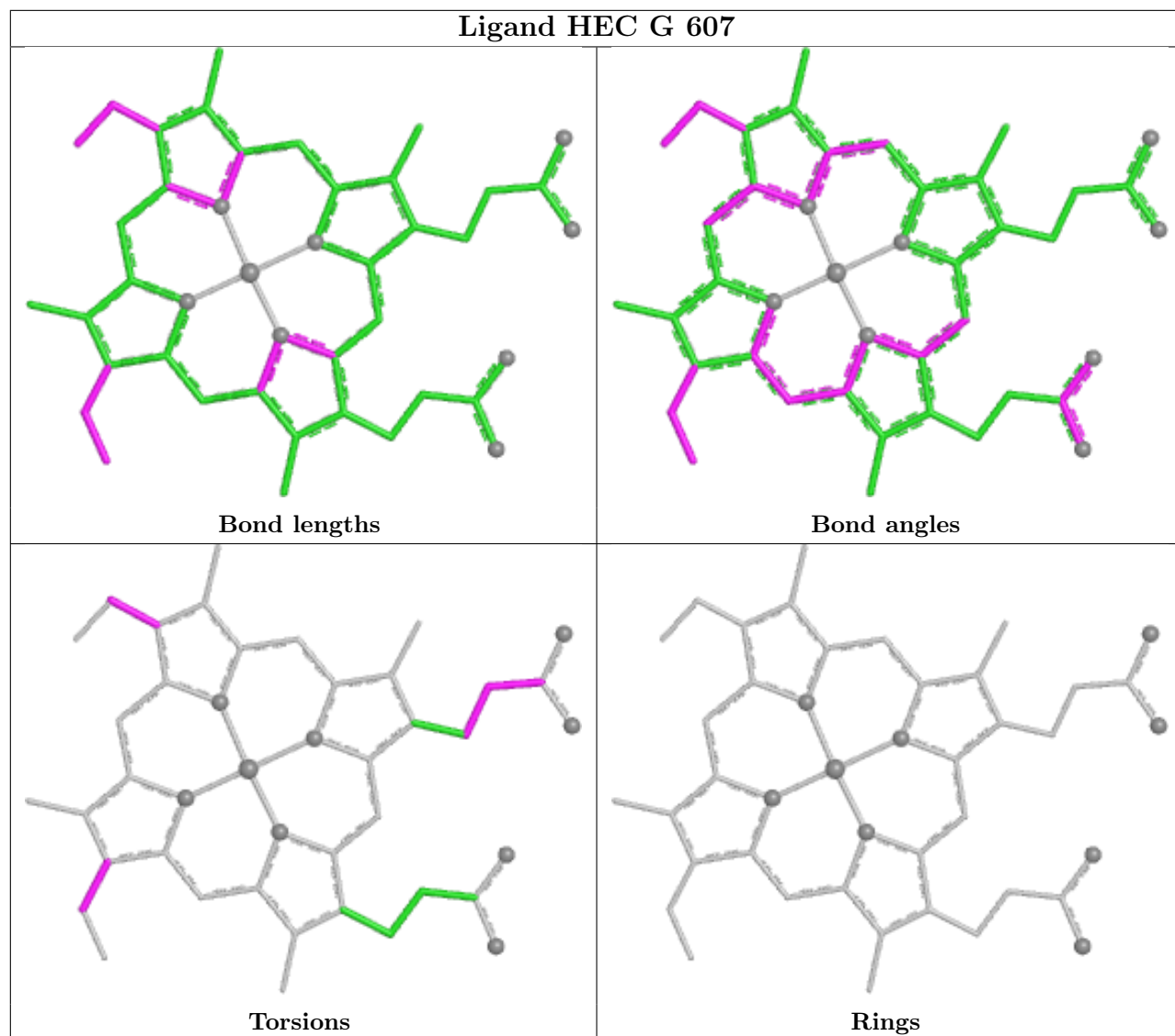


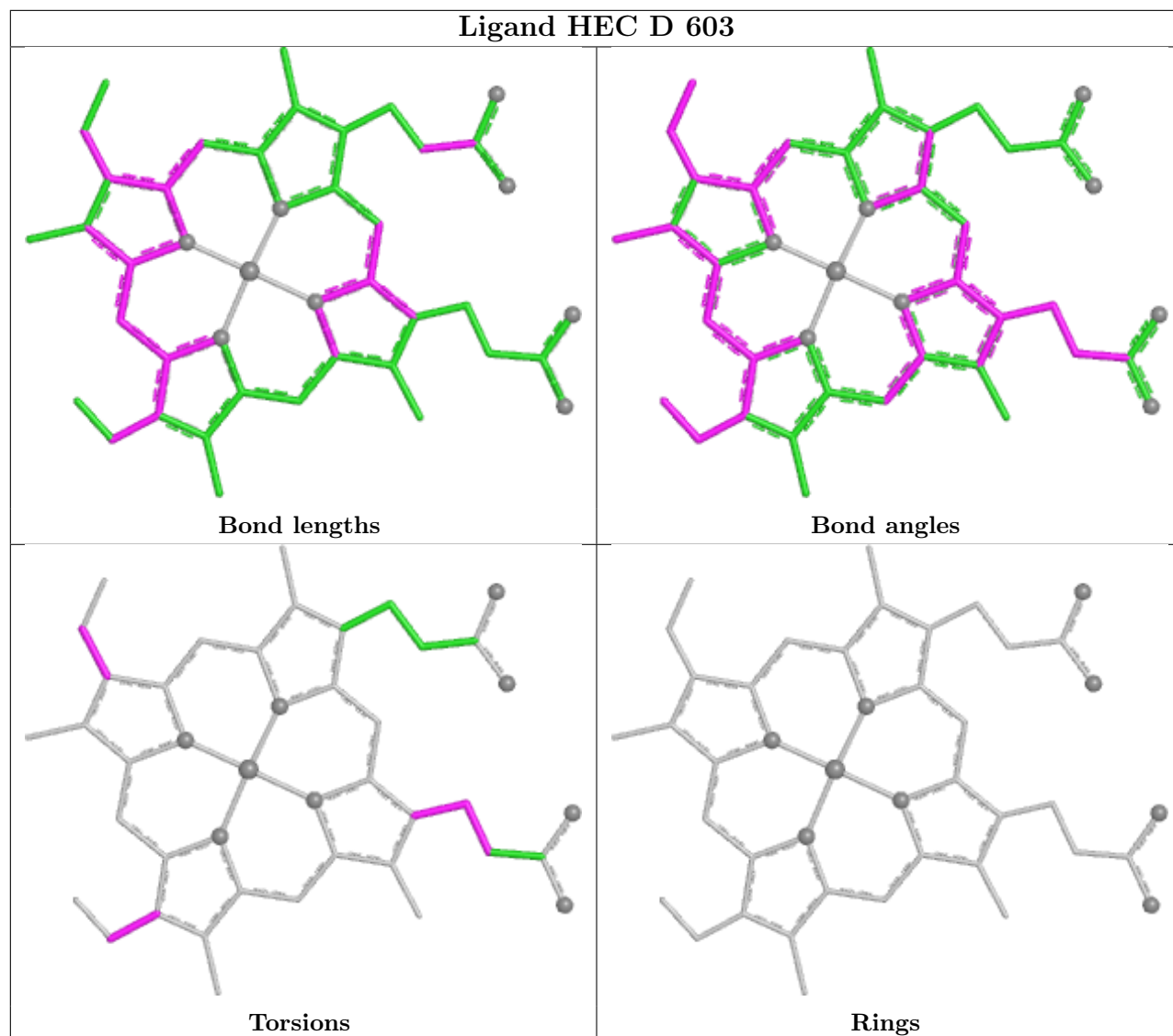
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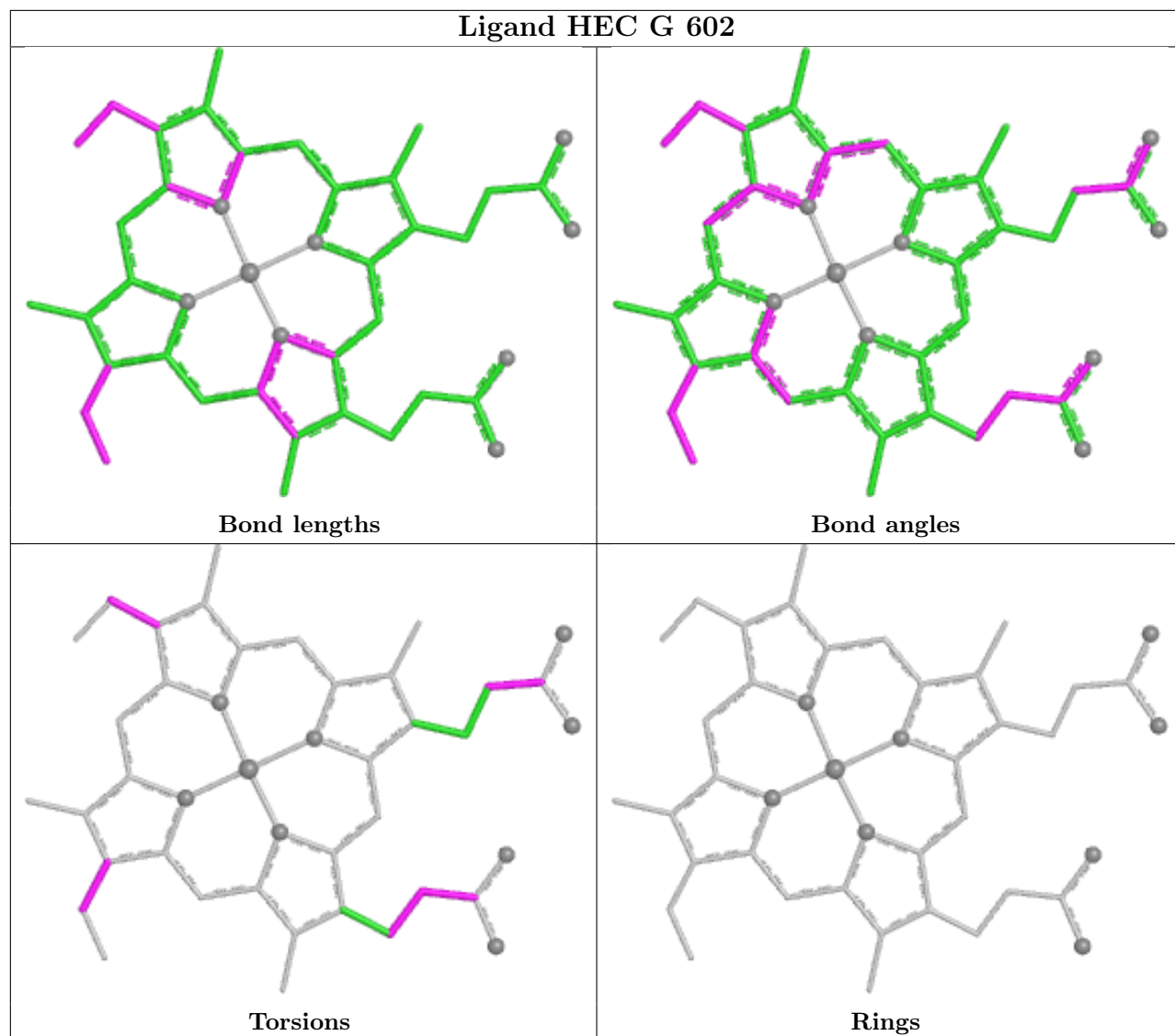


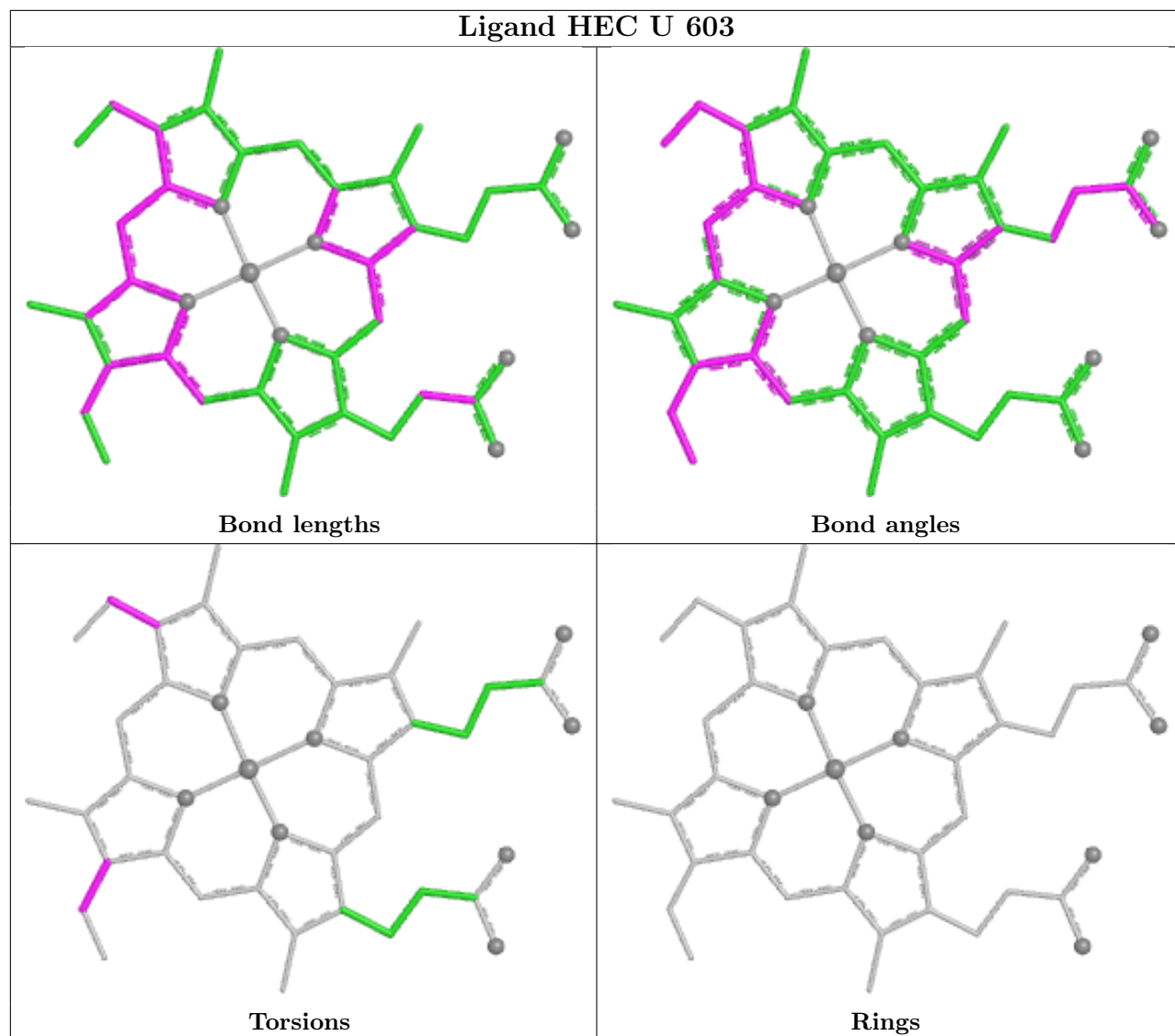
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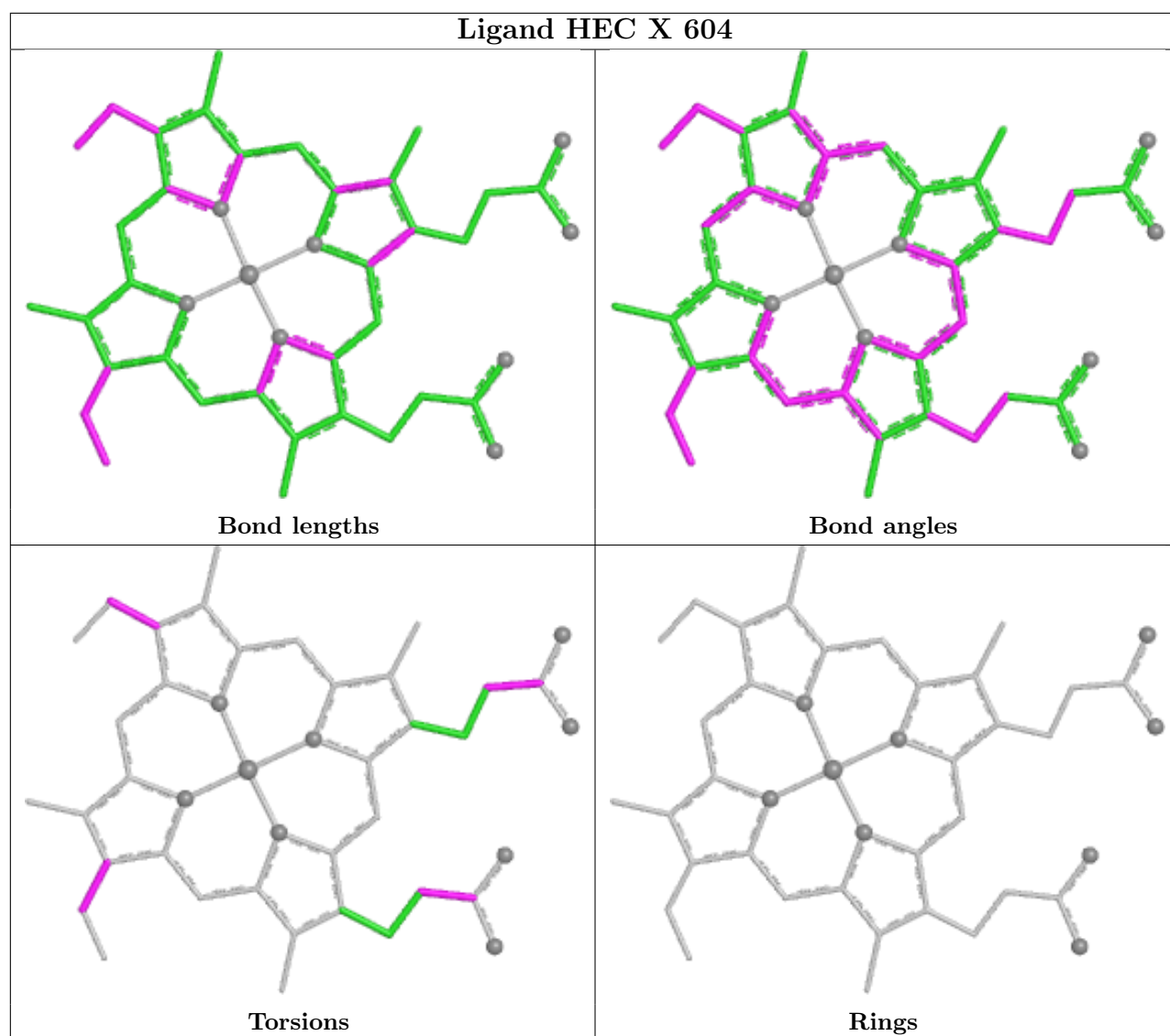


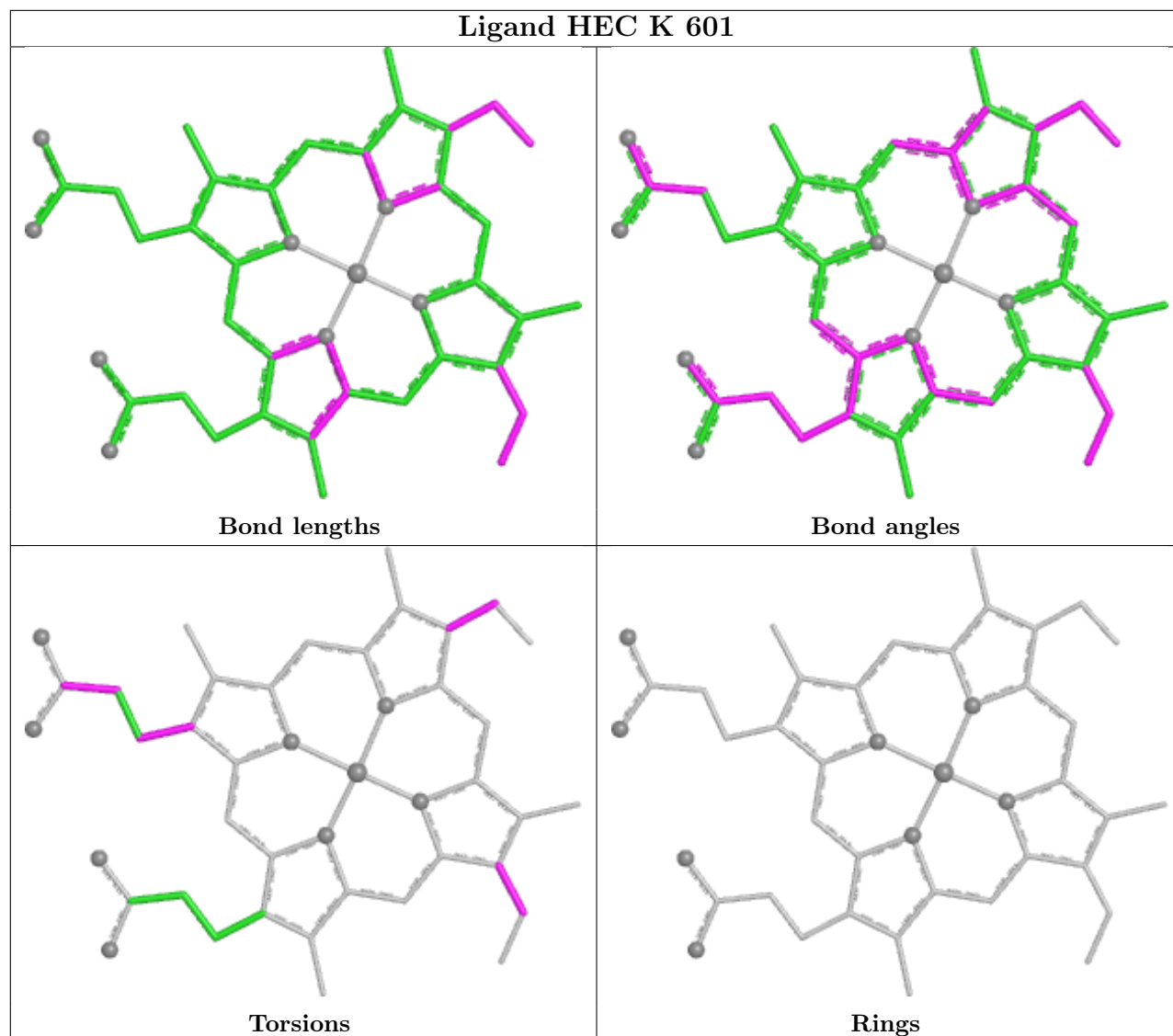


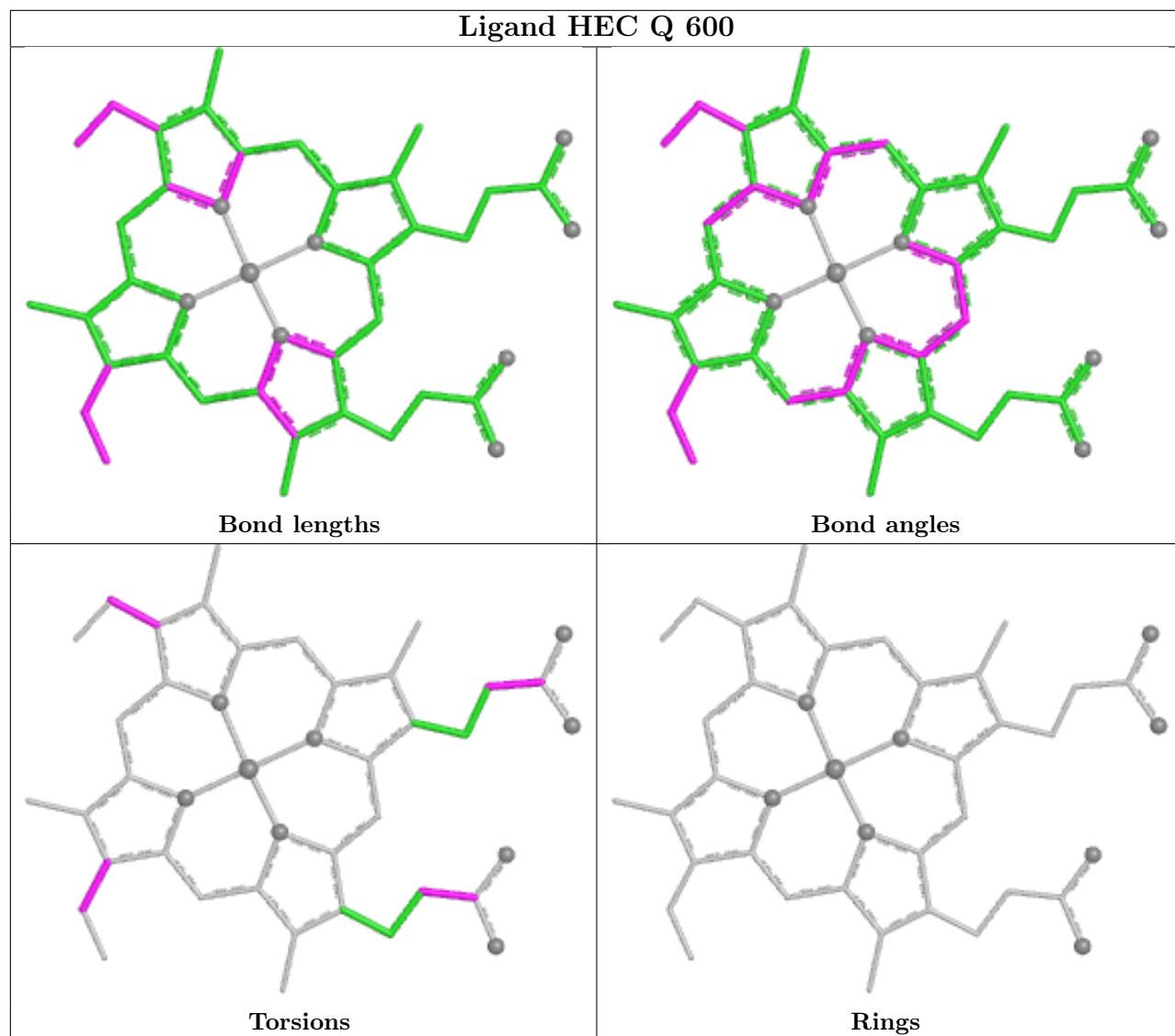




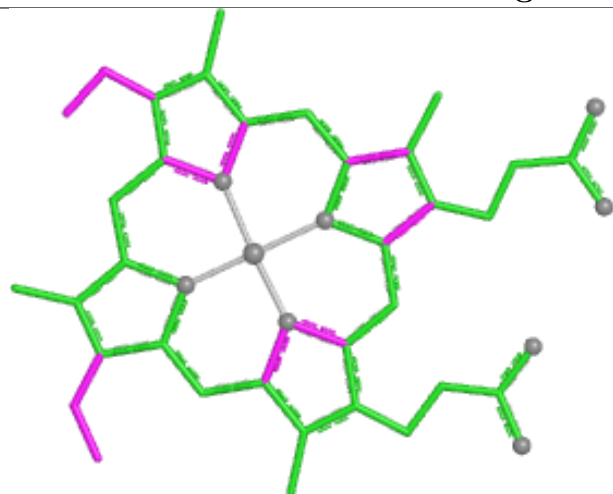




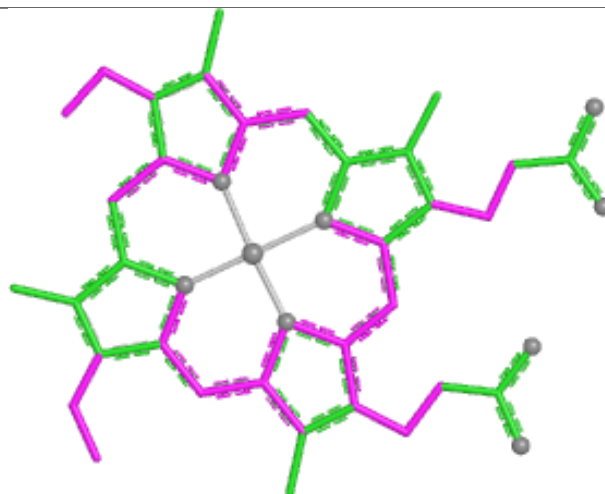




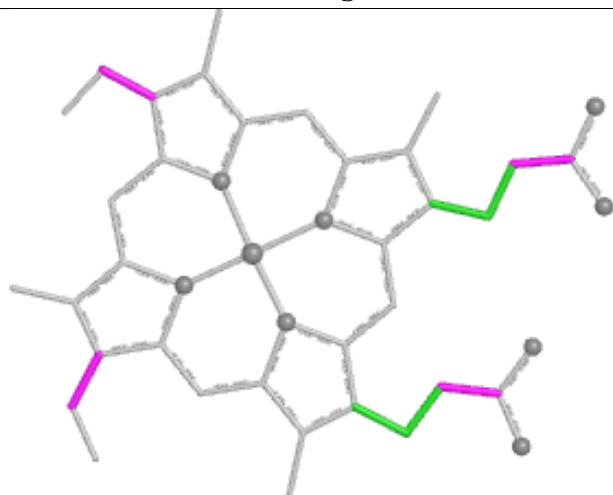
Ligand HEC S 604



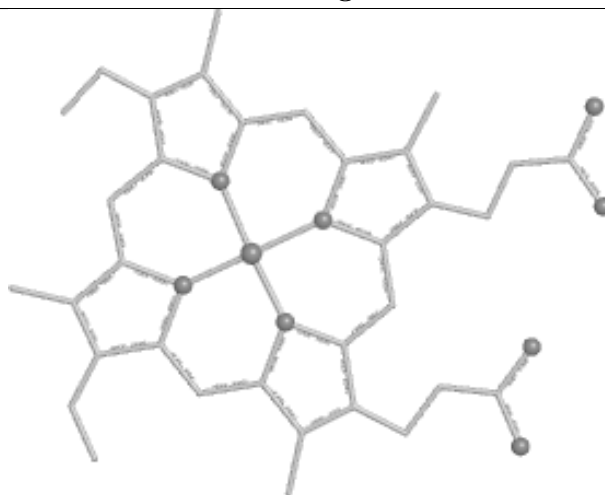
Bond lengths



Bond angles

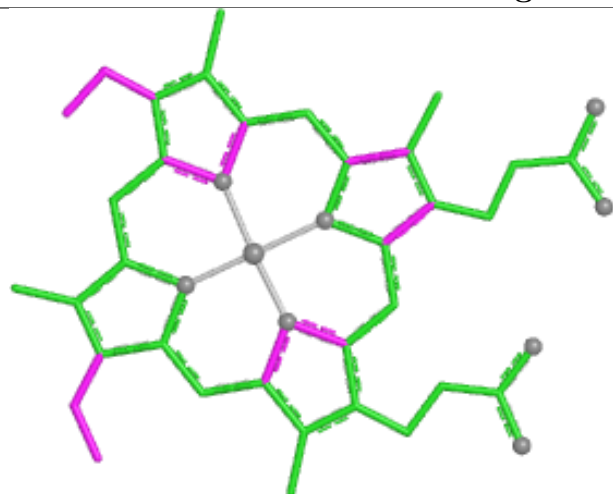


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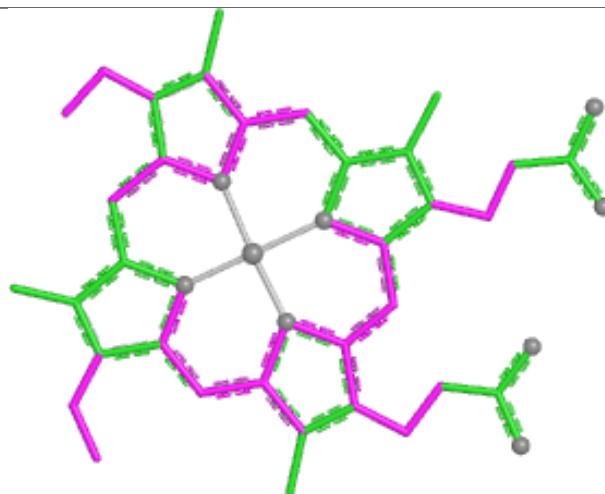


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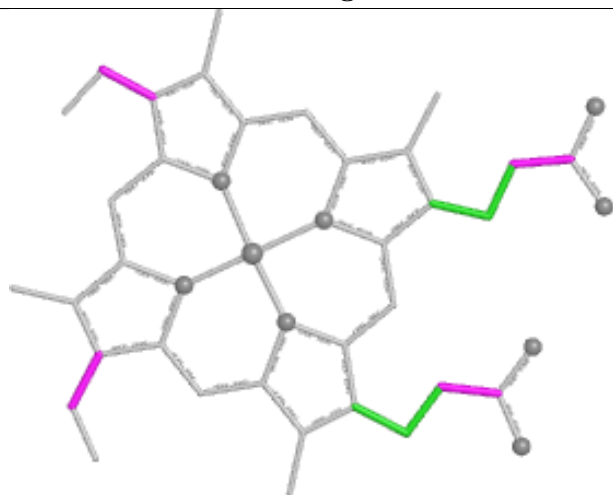
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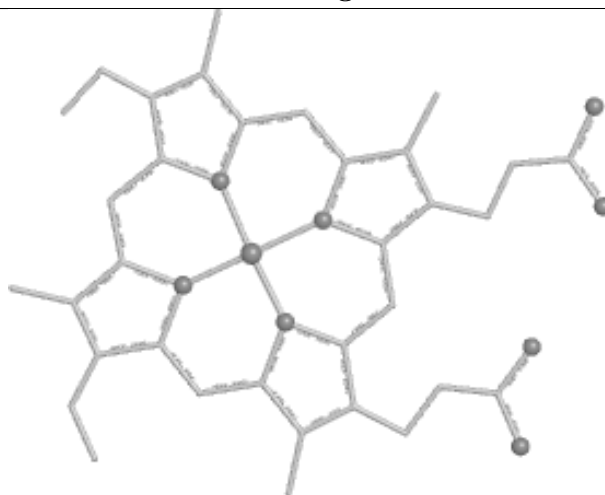
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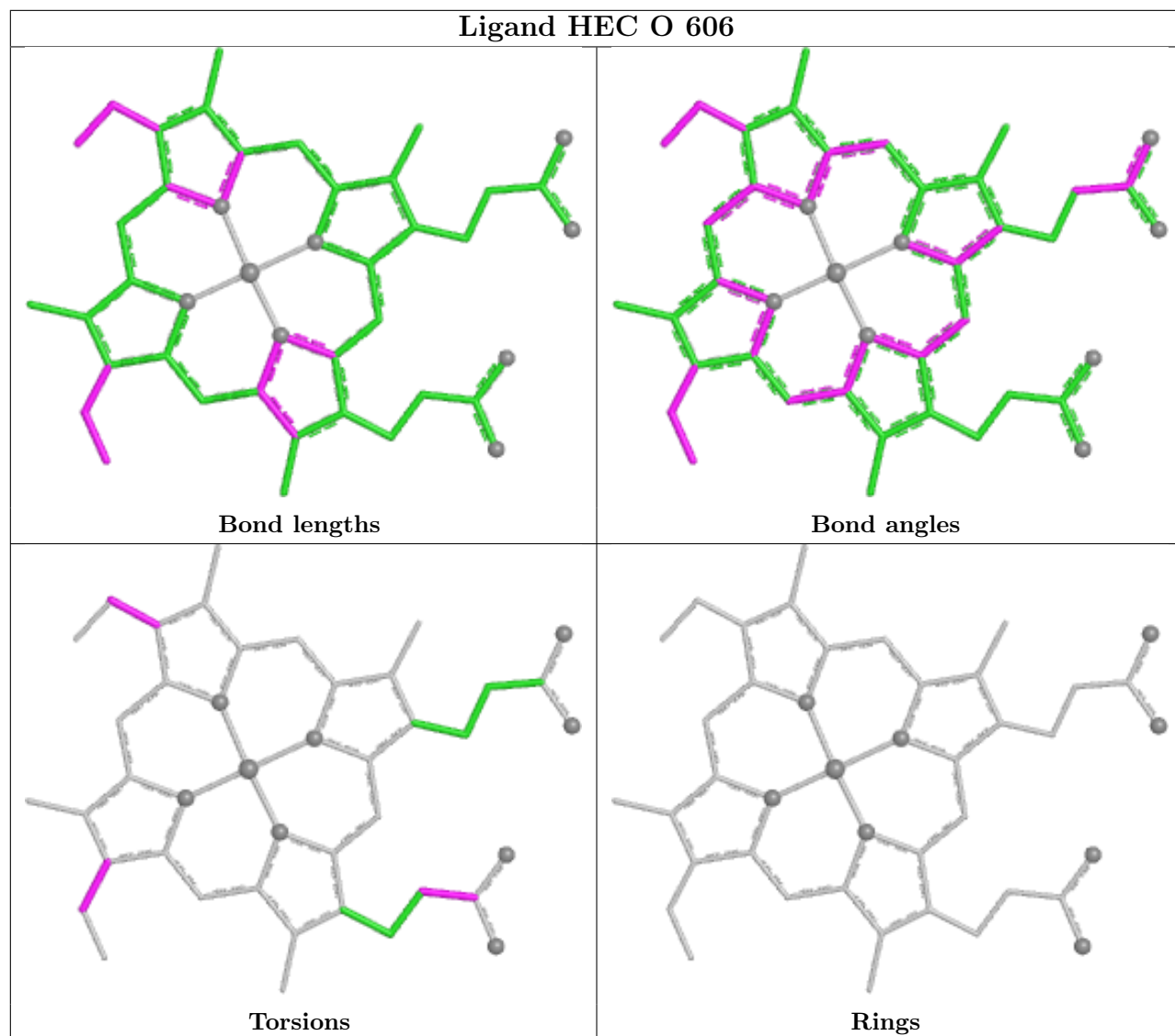
Bond angles

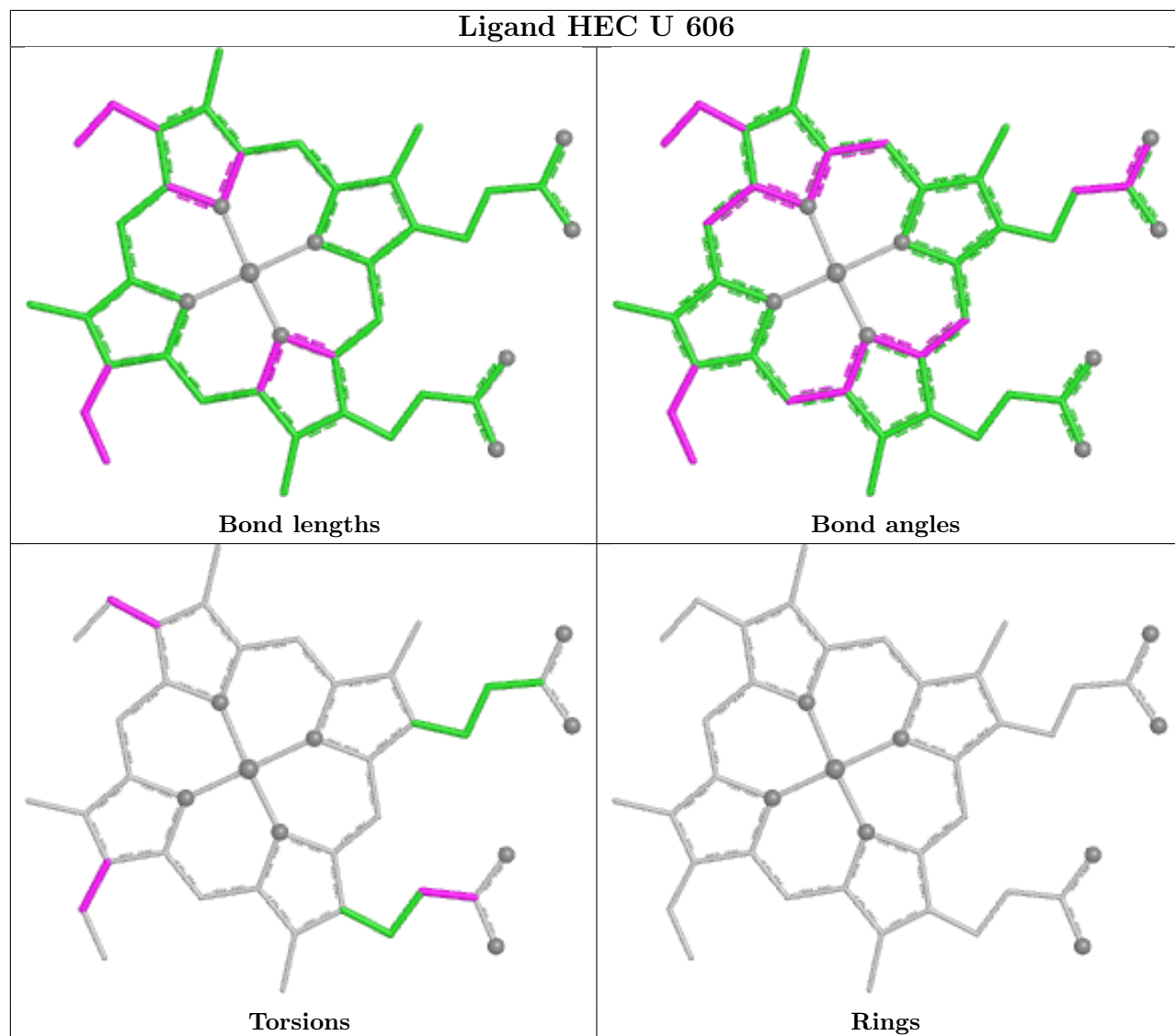


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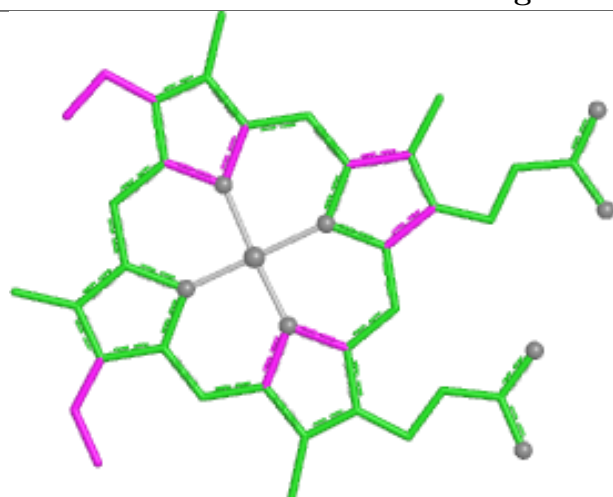


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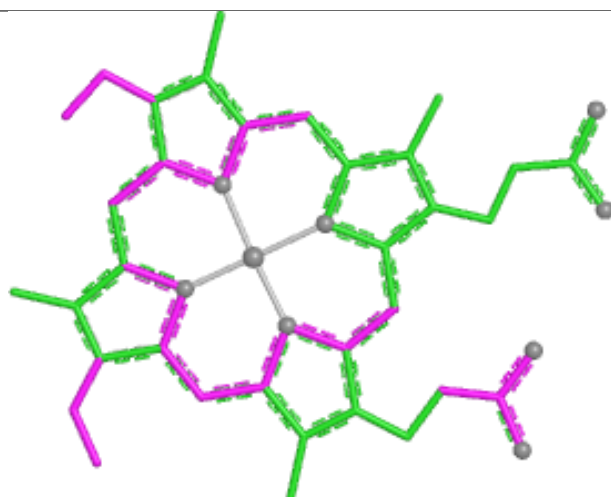




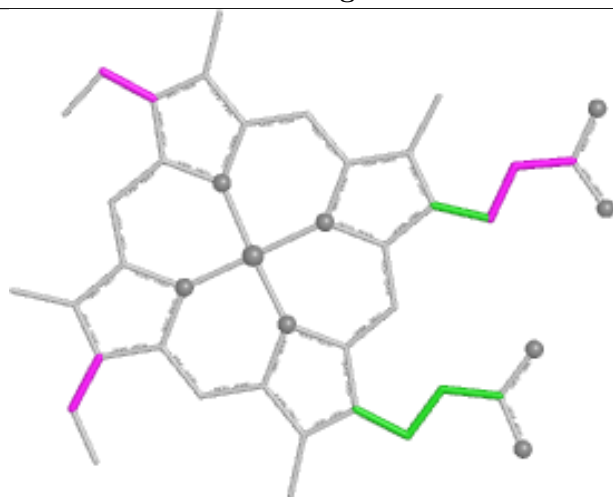
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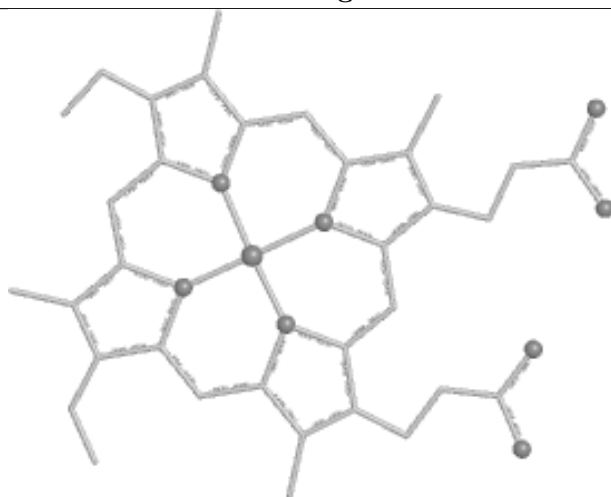
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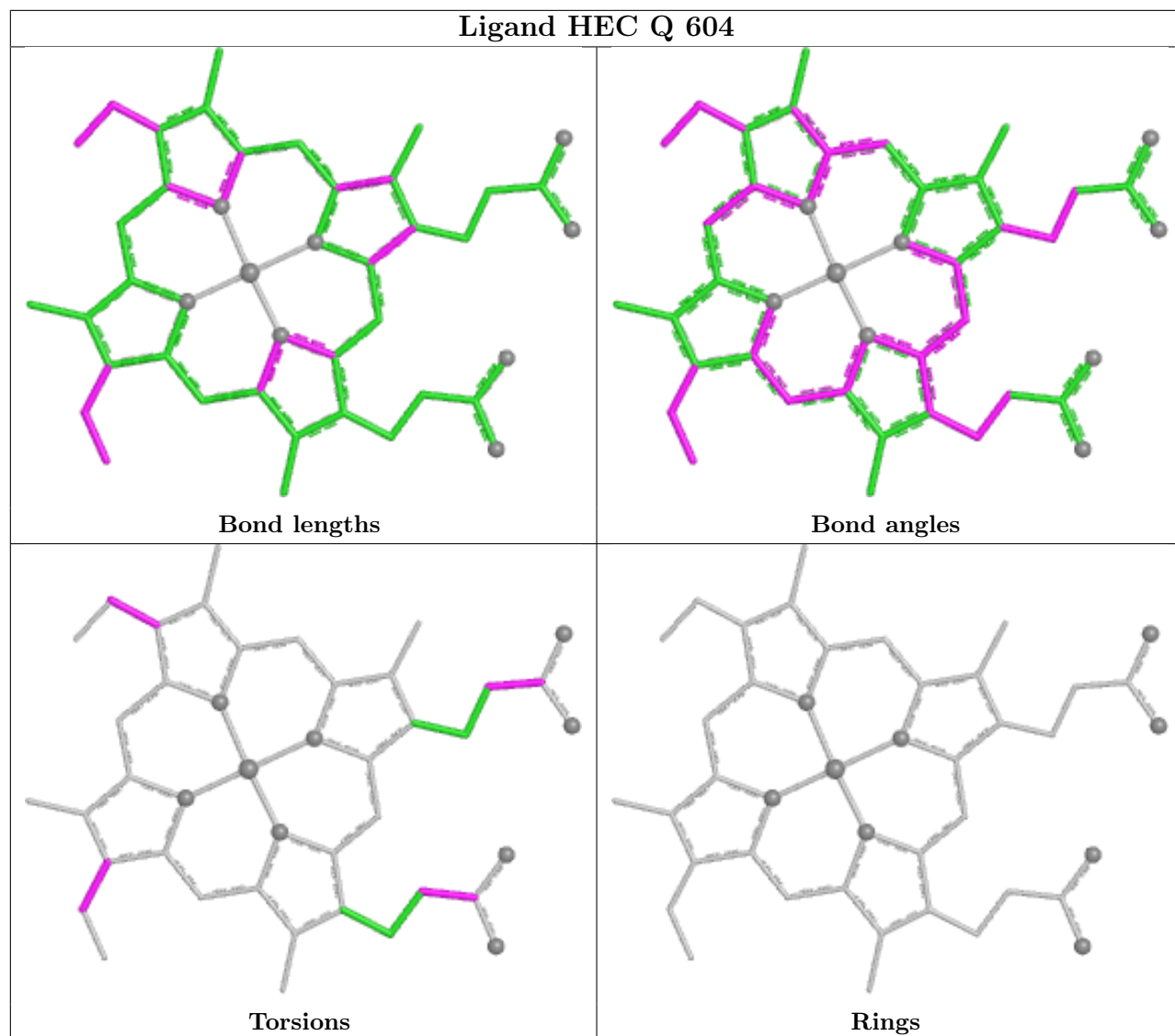
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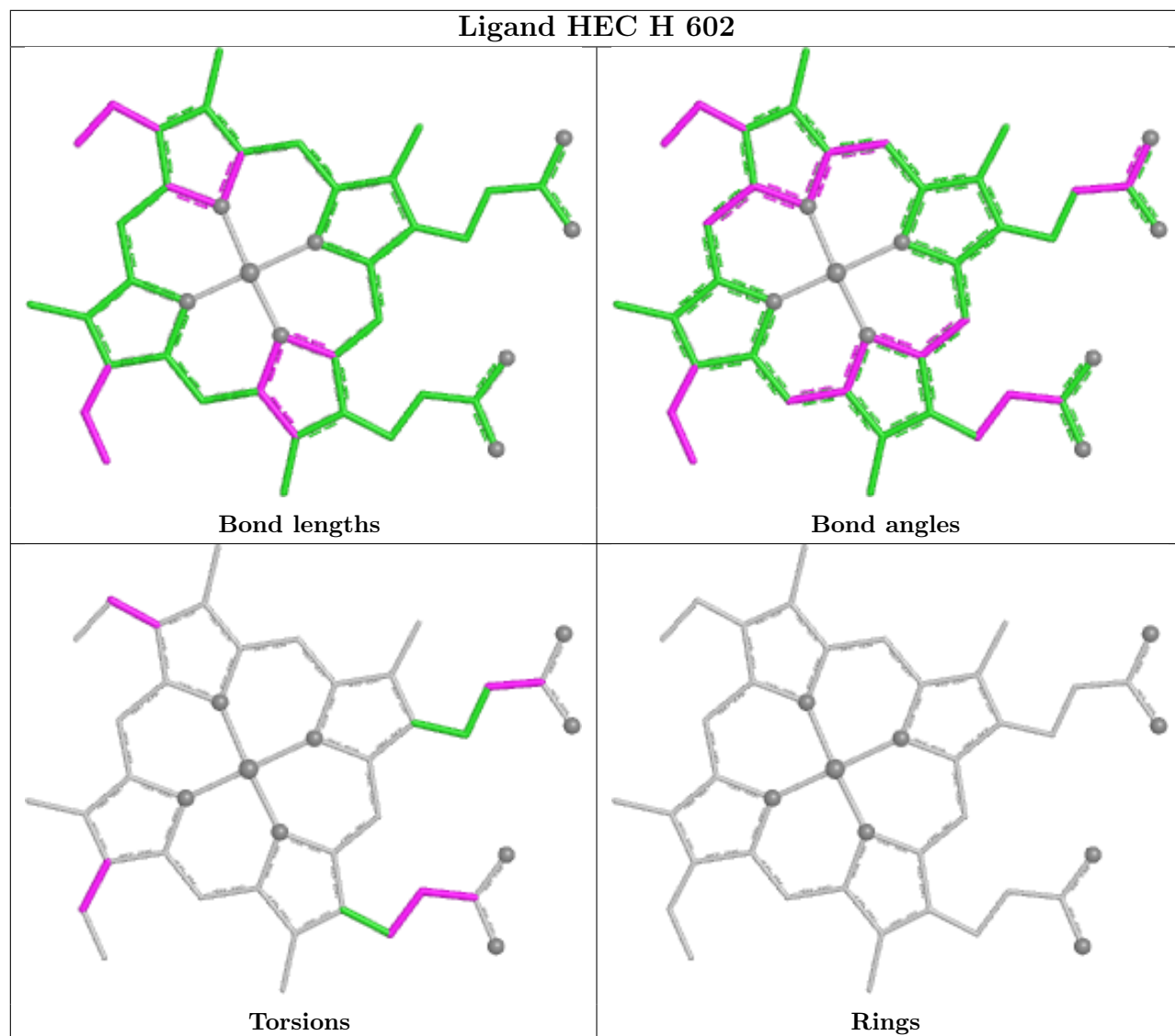


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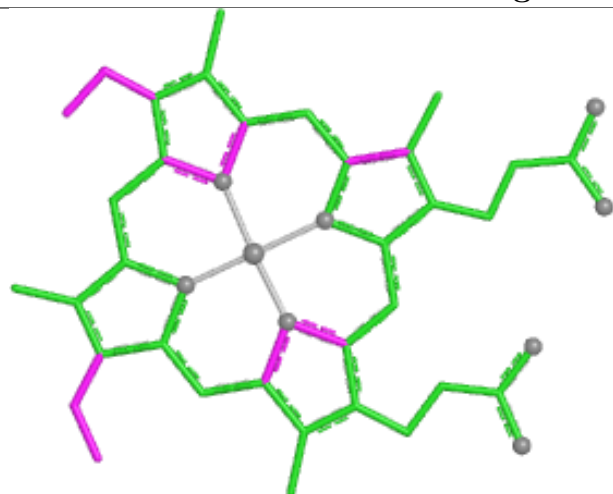


Rings

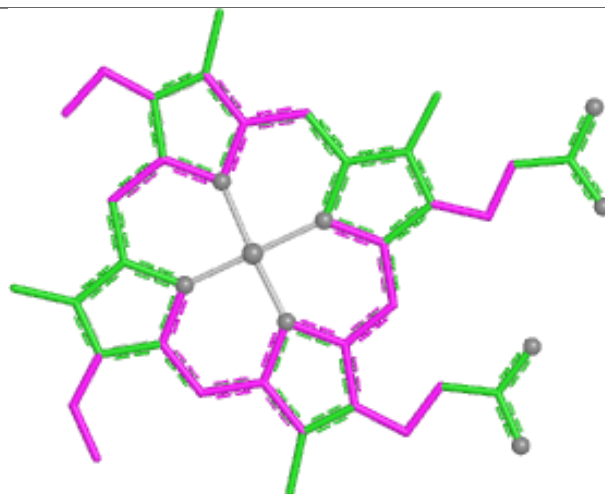




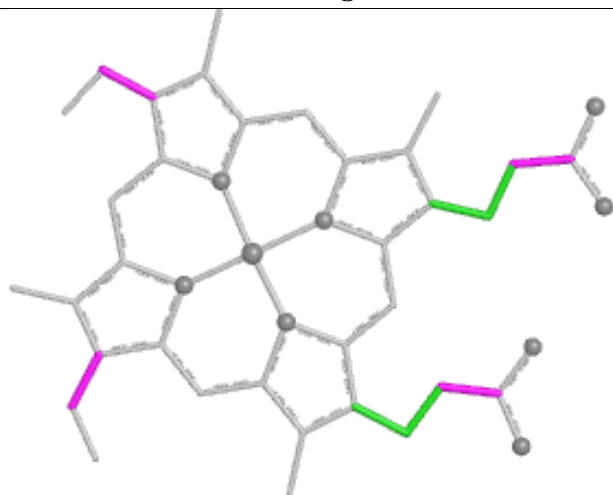
Ligand HEC P 604



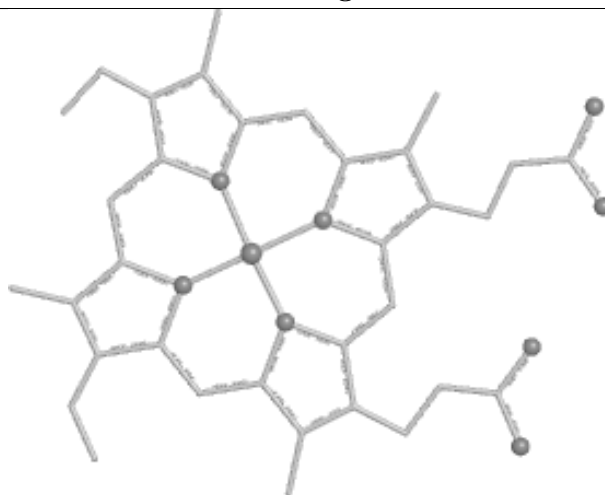
Bond lengths



Bond angles

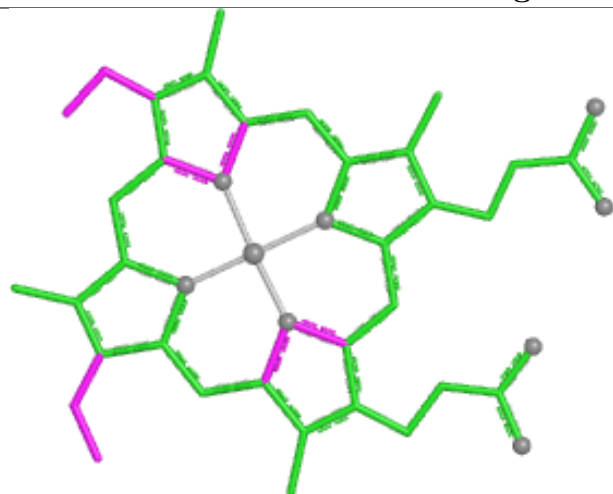


Torsions

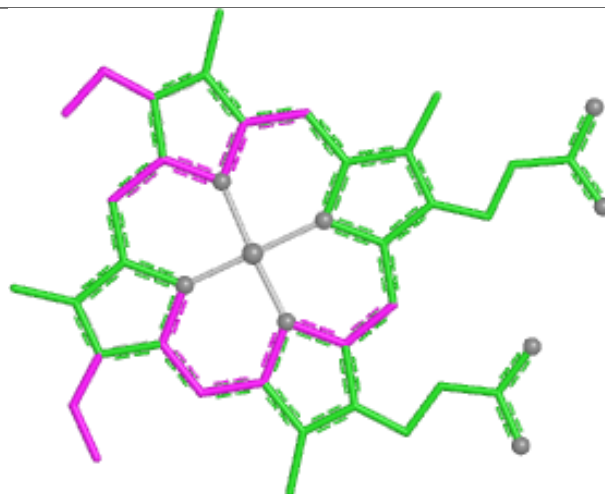


Rings

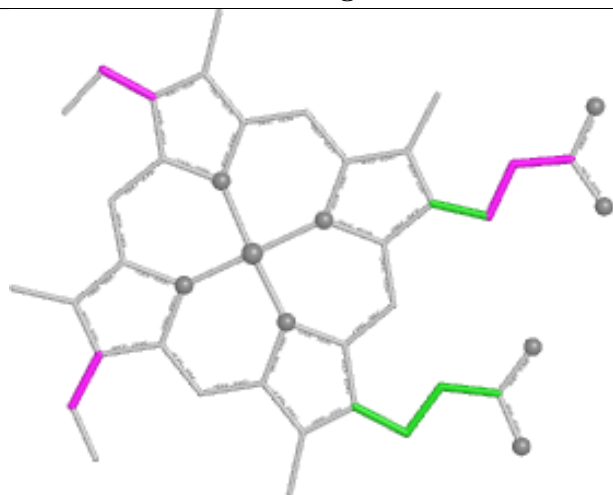
Ligand HEC P 607



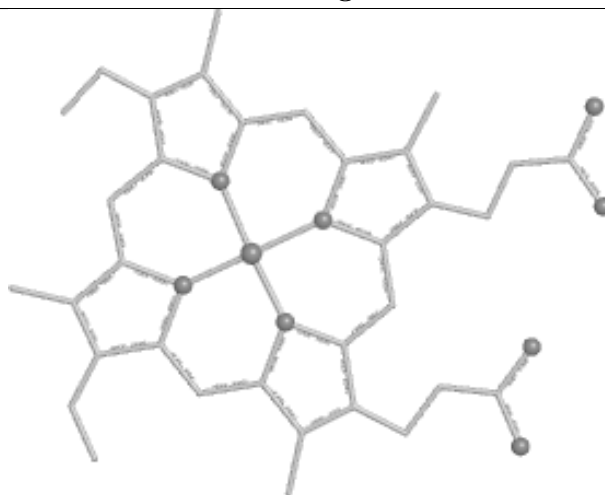
Bond lengths



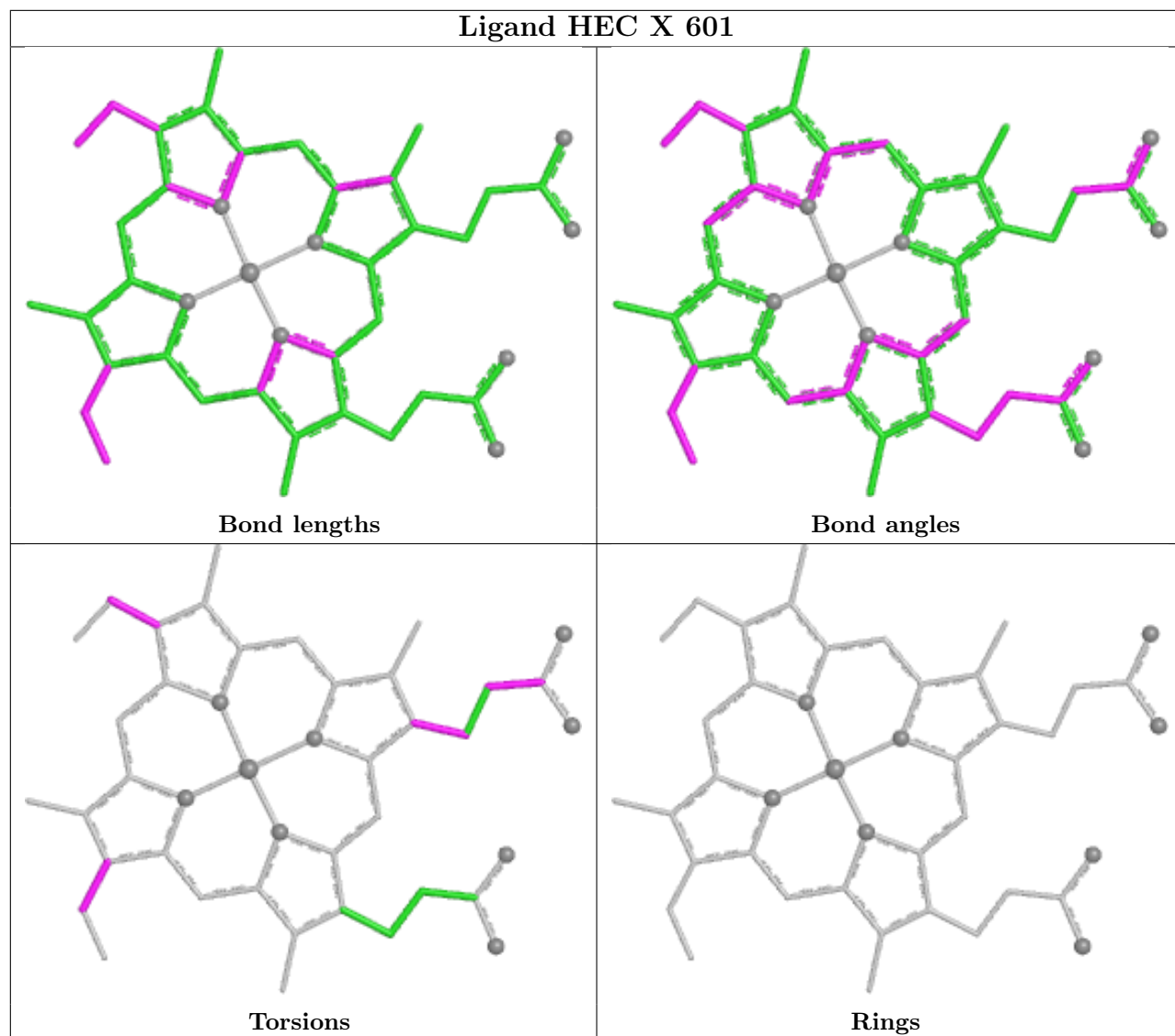
Bond angles

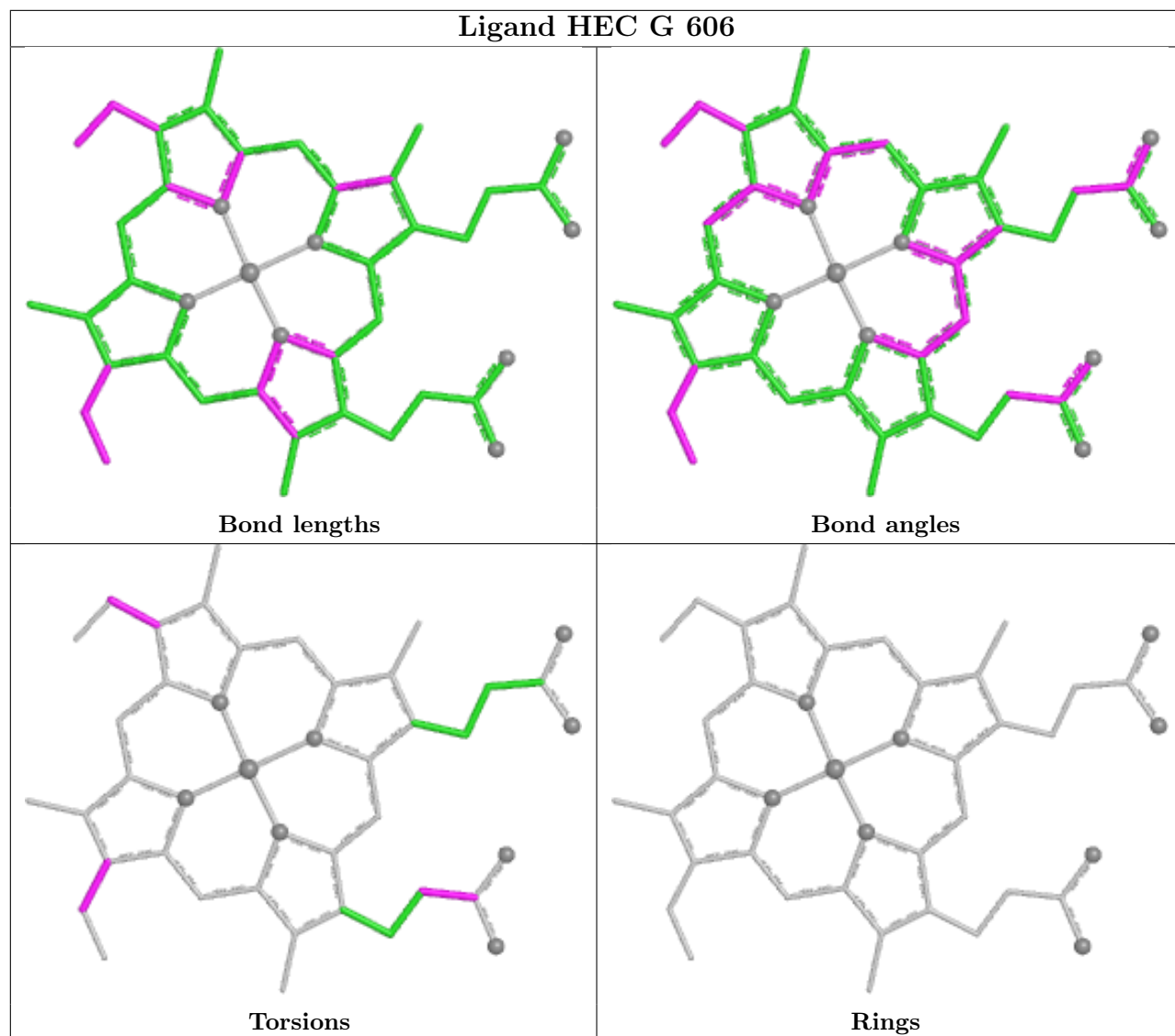


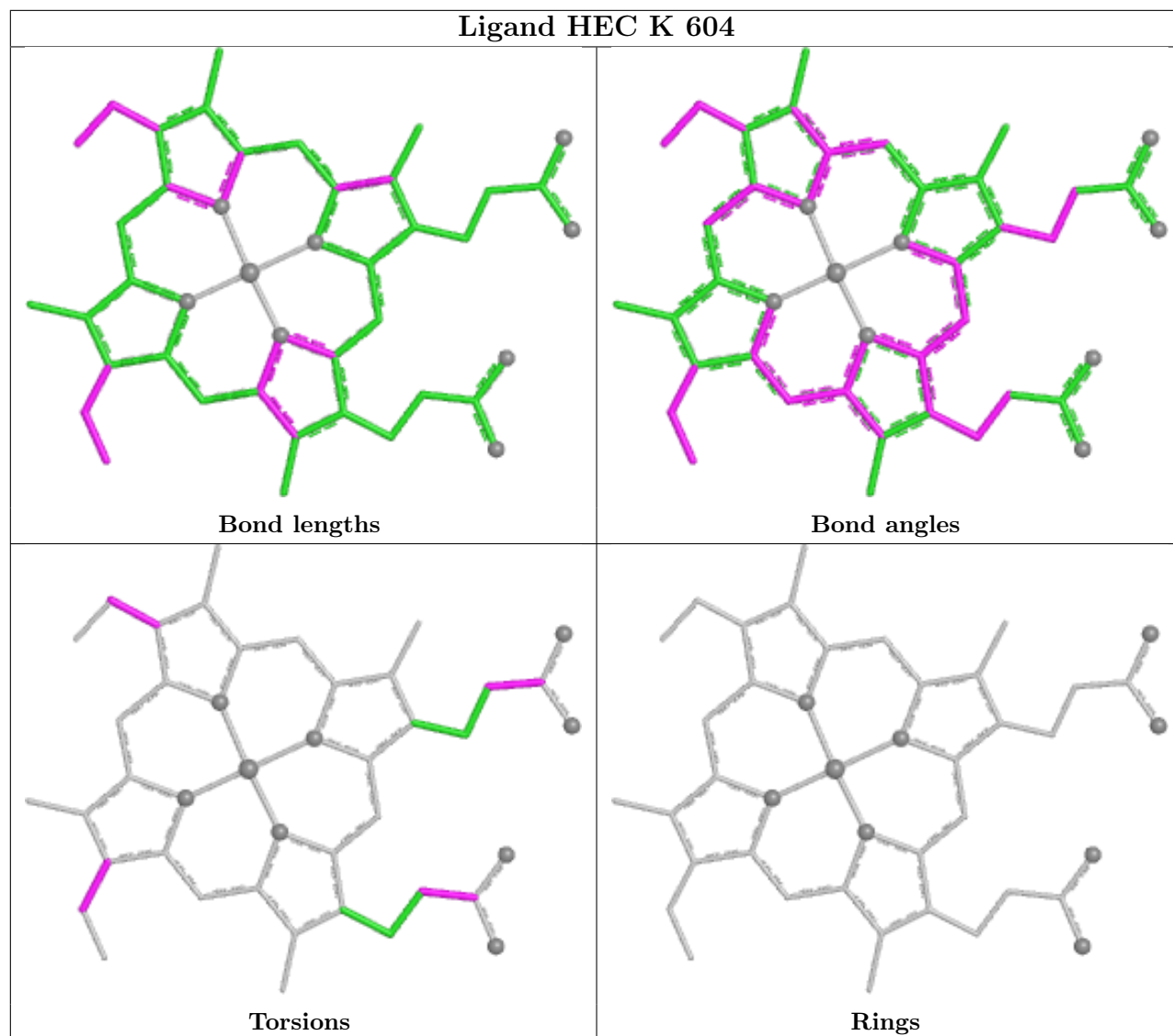
Torsions



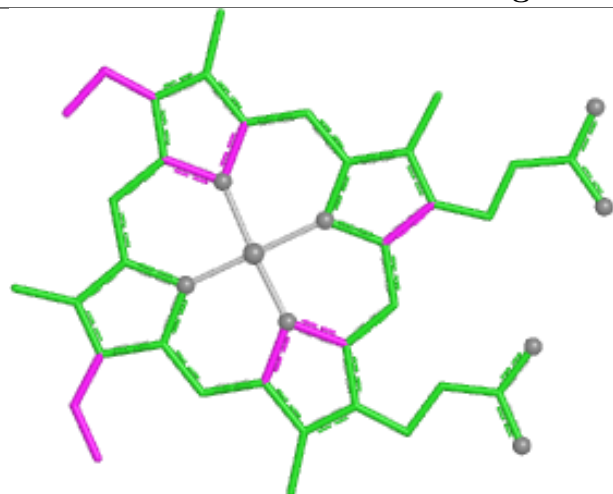
Rings



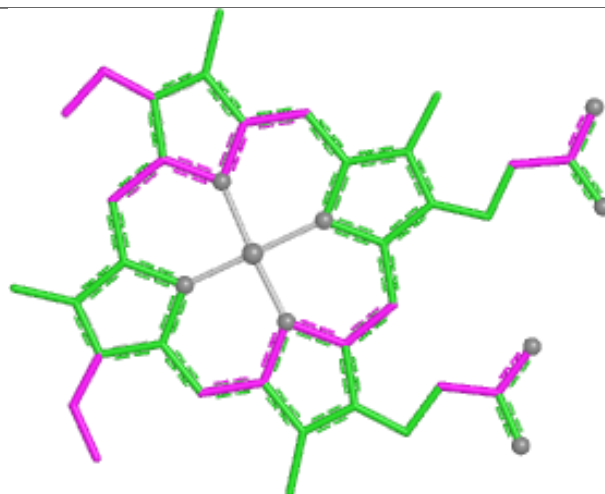




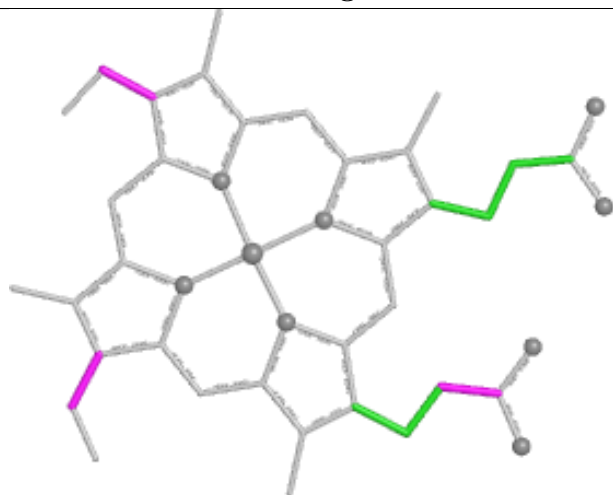
Ligand HEC V 606



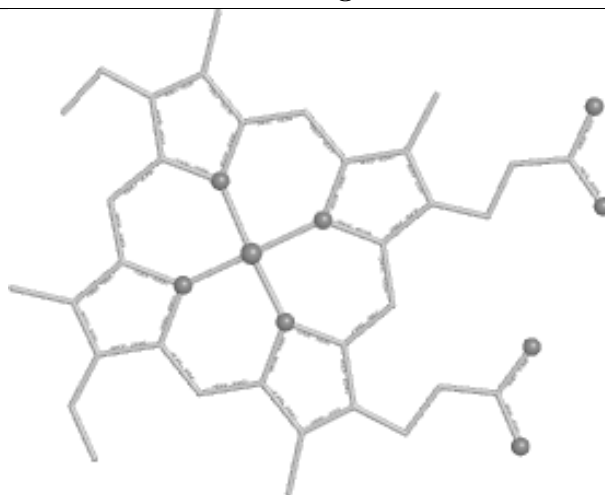
Bond lengths



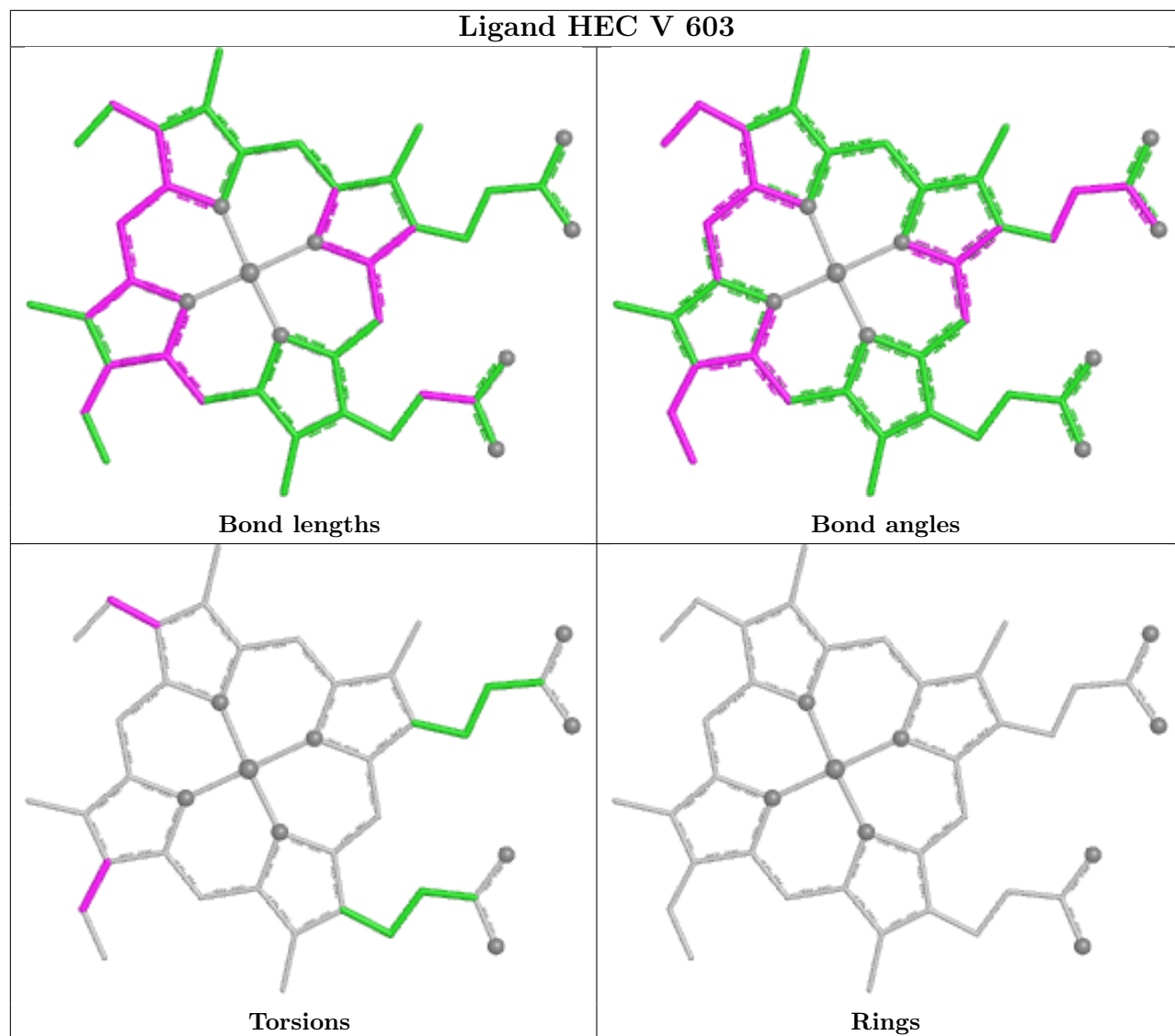
Bond angles



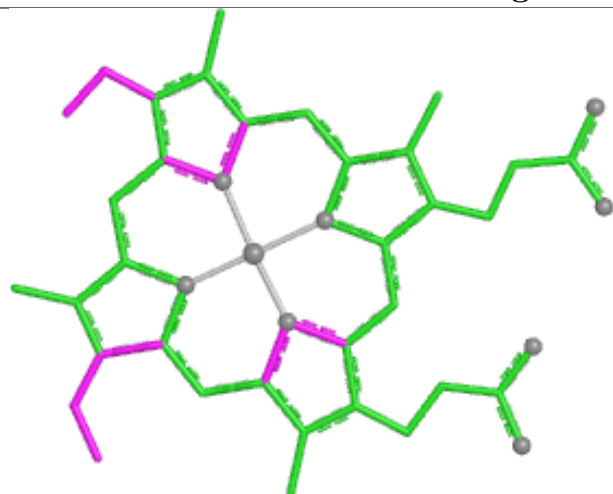
Torsions



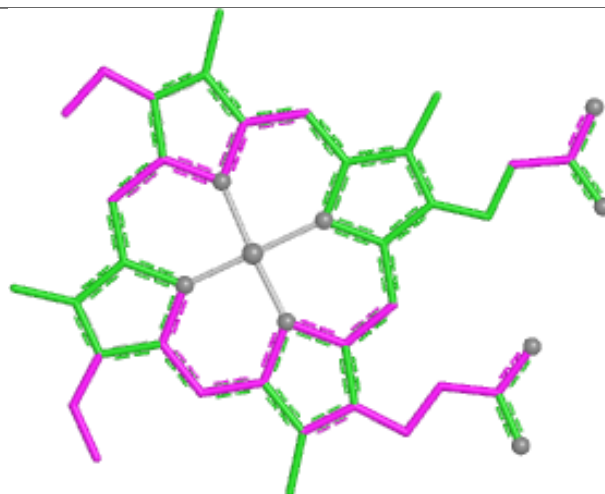
Rings



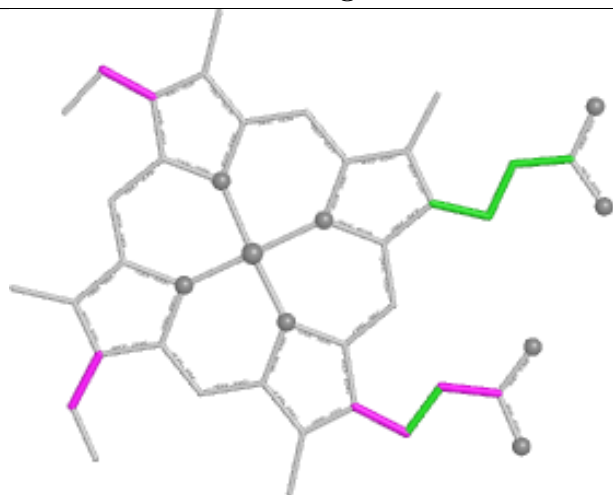
Ligand HEC K 605



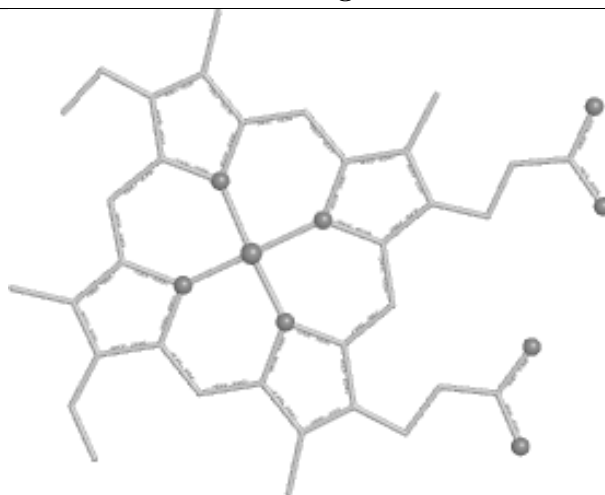
Bond lengths



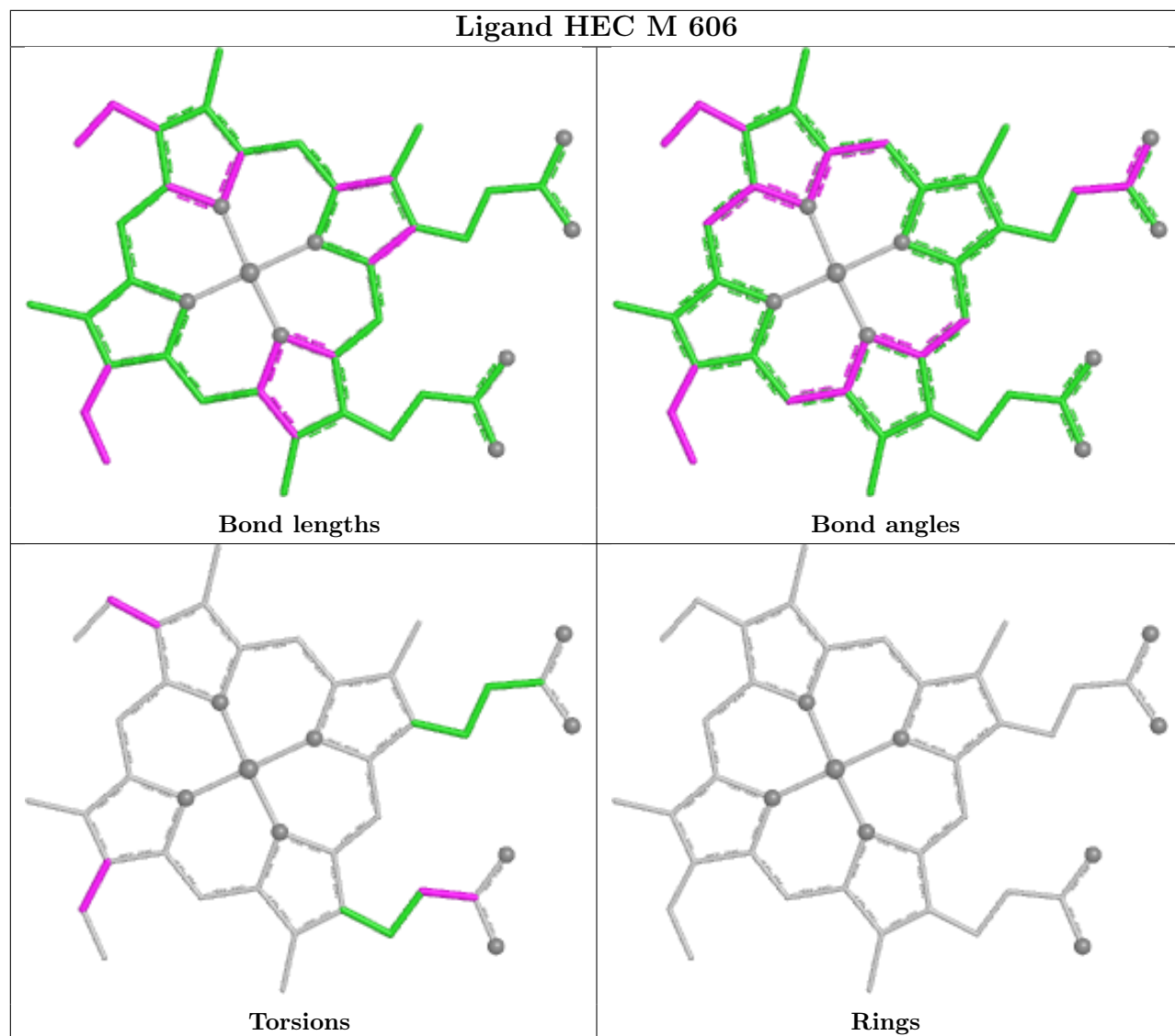
Bond angles



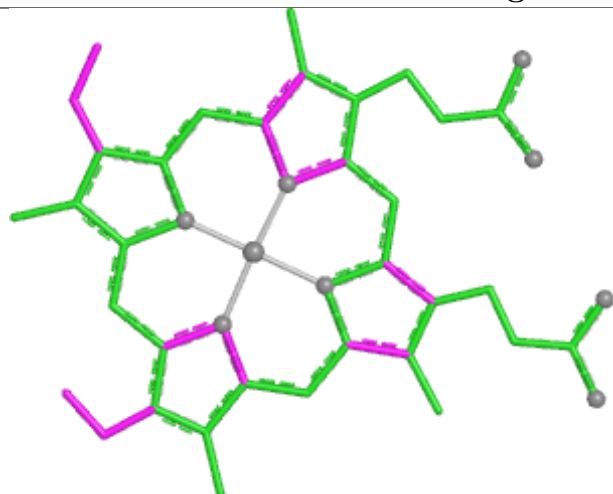
Torsions



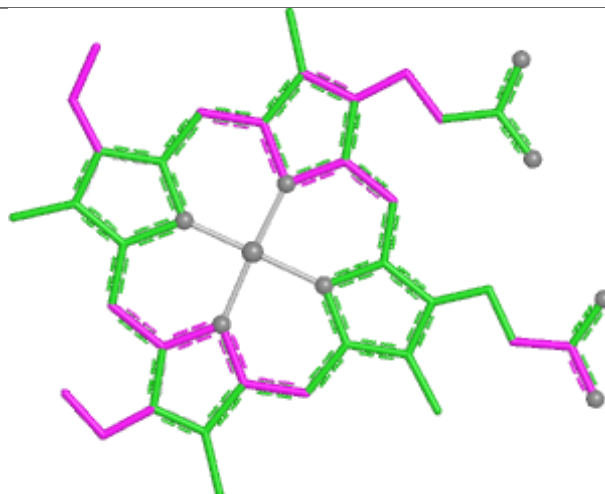
Rings



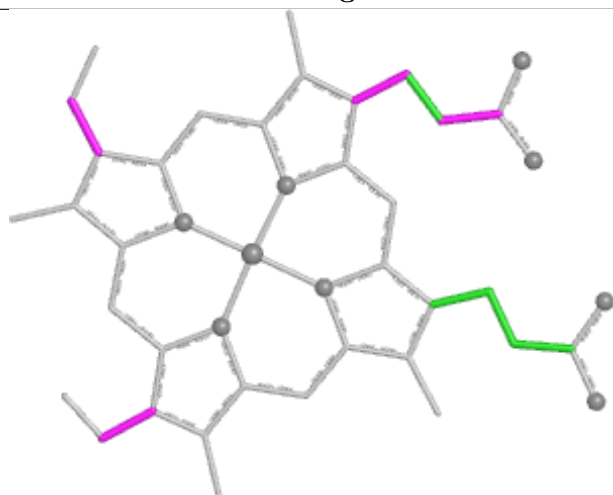
Ligand HEC W 605



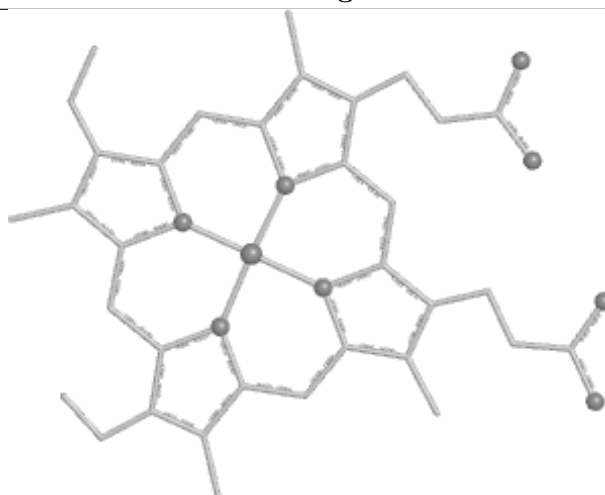
Bond lengths



Bond angles

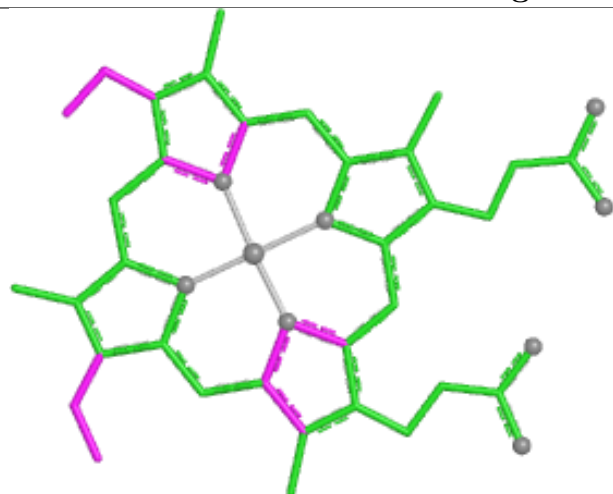


Torsions

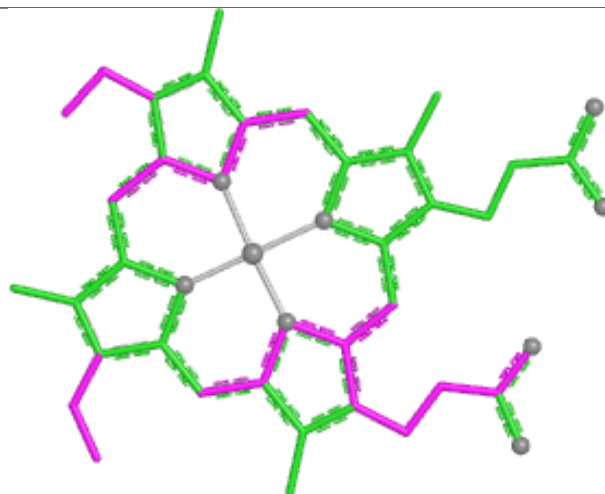


Rings

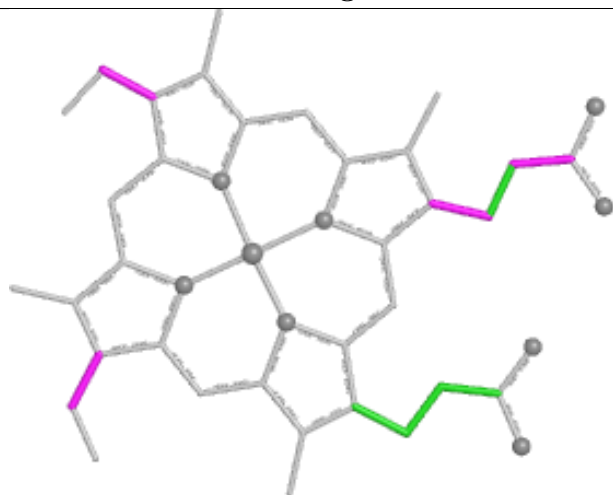
Ligand HEC N 601



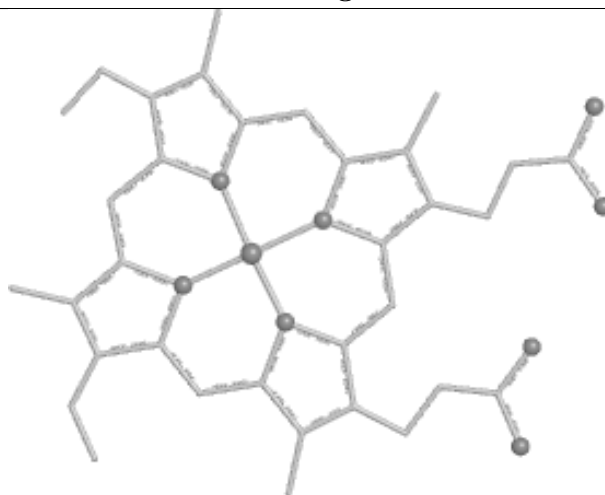
Bond lengths



Bond angles

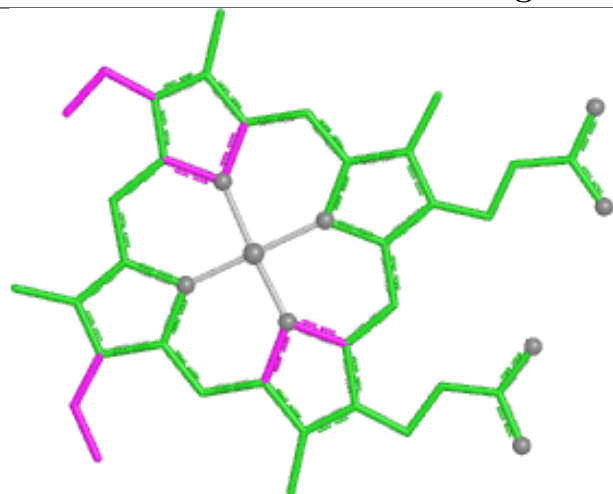


Torsions

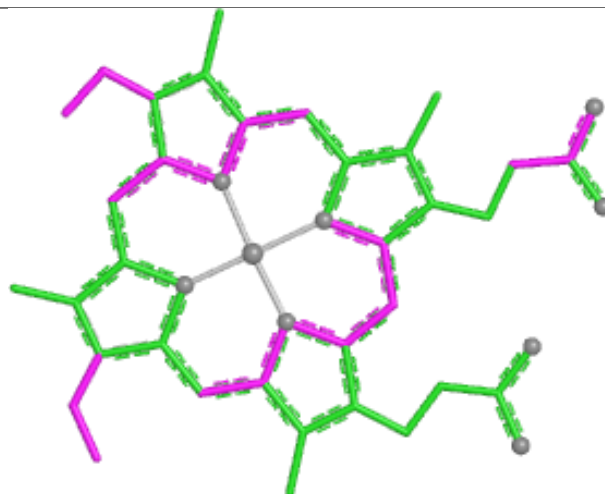


Rings

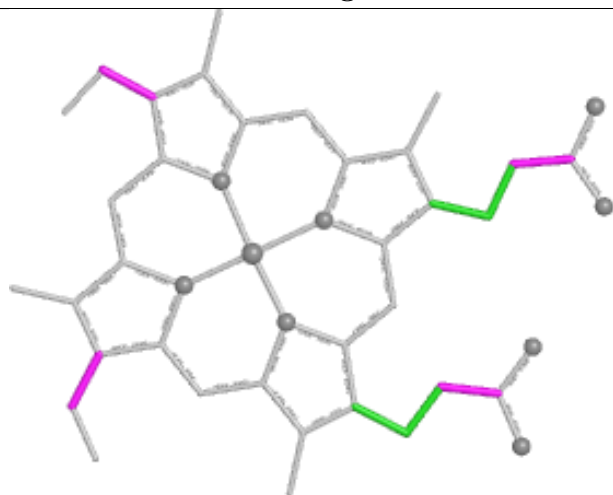
Ligand HEC L 600



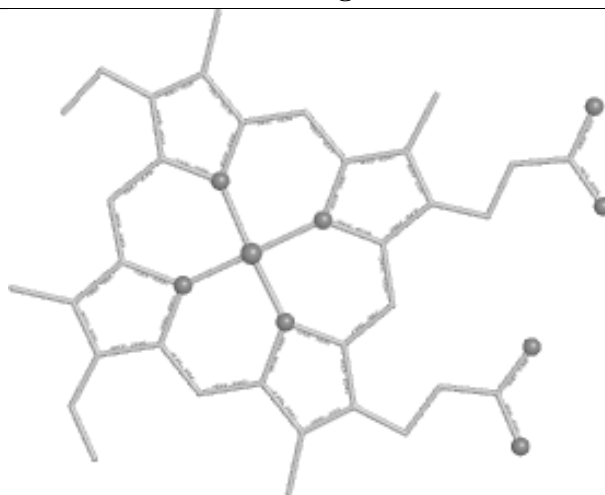
Bond lengths



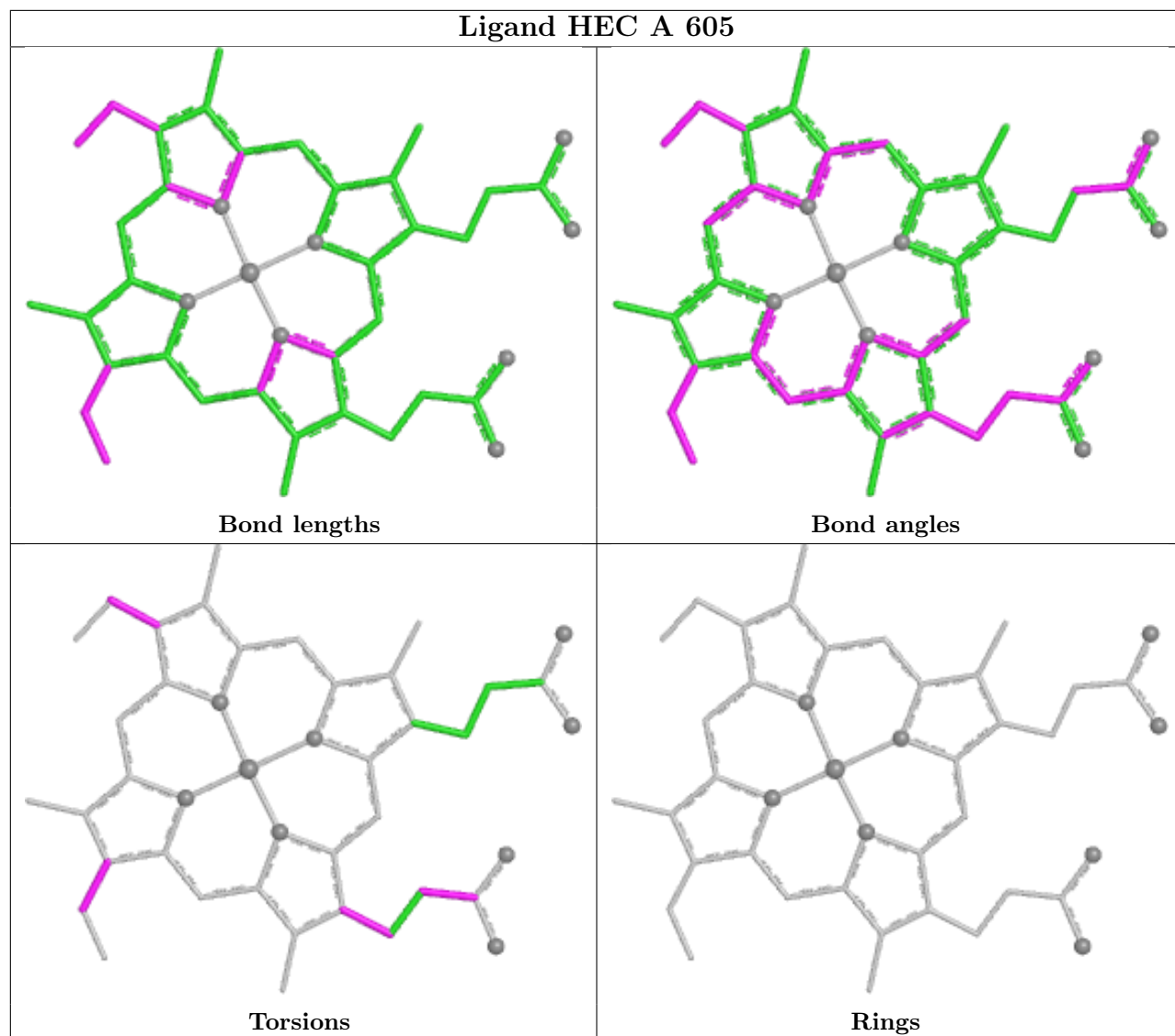
Bond angles

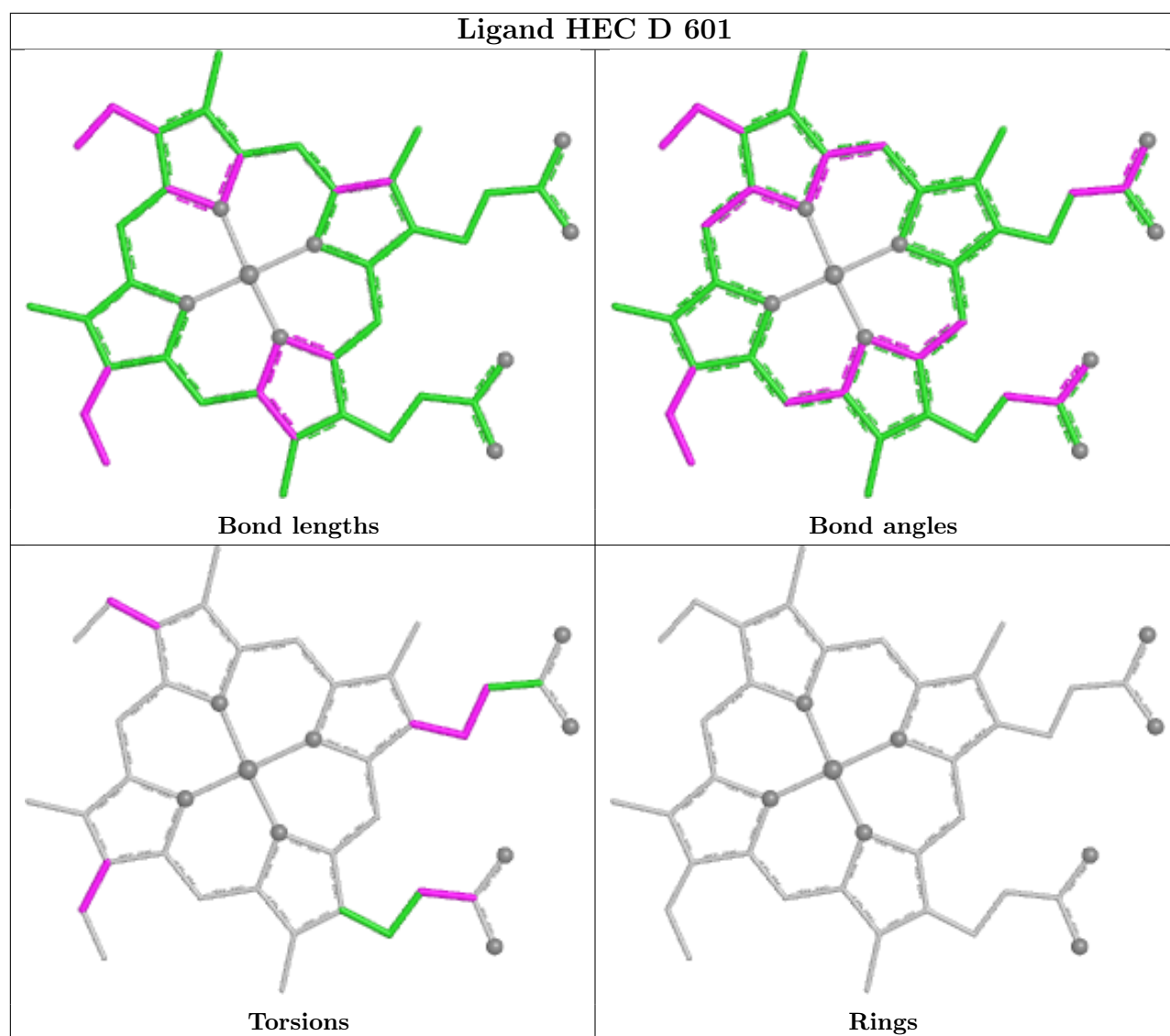


Torsions



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	531/582 (91%)	0.59	20 (3%) 44 35	39, 59, 87, 153	0
1	B	531/582 (91%)	0.43	11 (2%) 63 54	39, 57, 81, 173	0
1	C	531/582 (91%)	0.32	7 (1%) 75 66	40, 54, 84, 123	0
1	D	531/582 (91%)	0.52	25 (4%) 36 29	42, 68, 100, 140	0
1	E	531/582 (91%)	0.81	32 (6%) 27 21	39, 69, 104, 165	0
1	F	531/582 (91%)	1.18	84 (15%) 5 4	43, 76, 108, 158	0
1	G	531/582 (91%)	-0.08	6 (1%) 78 70	29, 41, 64, 139	0
1	H	531/582 (91%)	-0.08	8 (1%) 72 63	29, 39, 63, 156	0
1	I	527/582 (90%)	-0.34	0 100 100	27, 38, 57, 104	0
1	J	531/582 (91%)	-0.02	8 (1%) 72 63	29, 42, 66, 166	0
1	K	531/582 (91%)	0.04	8 (1%) 72 63	32, 44, 70, 159	0
1	L	531/582 (91%)	0.09	5 (0%) 81 74	32, 45, 73, 157	0
1	M	531/582 (91%)	0.31	11 (2%) 63 54	37, 54, 84, 150	0
1	N	531/582 (91%)	0.47	10 (1%) 66 57	37, 58, 85, 157	0
1	O	531/582 (91%)	0.21	6 (1%) 78 70	37, 51, 77, 133	0
1	P	531/582 (91%)	0.18	10 (1%) 66 57	37, 51, 72, 124	0
1	Q	531/582 (91%)	0.44	13 (2%) 59 49	34, 57, 82, 124	0
1	R	531/582 (91%)	0.28	11 (2%) 63 54	20, 52, 78, 142	1 (0%)
1	S	531/582 (91%)	1.07	71 (13%) 7 5	51, 80, 111, 158	0
1	T	531/582 (91%)	0.88	44 (8%) 17 12	50, 74, 107, 184	0
1	U	531/582 (91%)	1.06	70 (13%) 7 6	50, 80, 111, 150	0
1	V	531/582 (91%)	1.17	84 (15%) 5 4	52, 79, 108, 161	0
1	W	531/582 (91%)	1.18	97 (18%) 3 2	50, 80, 105, 163	0
1	X	531/582 (91%)	1.34	110 (20%) 2 2	56, 83, 111, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	86/114 (75%)	0.66	6 (6%) 22 16	38, 54, 76, 105	0
2	Z	86/114 (75%)	1.43	18 (20%) 2 2	76, 96, 128, 192	0
2	a	86/114 (75%)	1.10	10 (11%) 9 7	64, 87, 116, 166	0
2	b	86/114 (75%)	1.08	11 (12%) 7 6	61, 83, 118, 167	0
2	c	86/114 (75%)	0.94	8 (9%) 14 10	58, 76, 101, 166	0
2	d	86/114 (75%)	0.93	9 (10%) 11 8	54, 68, 107, 152	0
2	e	86/114 (75%)	0.91	7 (8%) 18 13	57, 76, 109, 155	0
2	f	86/114 (75%)	1.34	16 (18%) 3 2	71, 96, 131, 168	0
2	g	86/114 (75%)	1.11	8 (9%) 14 10	68, 82, 114, 179	0
2	h	86/114 (75%)	1.43	20 (23%) 2 1	82, 96, 130, 166	0
2	i	86/114 (75%)	1.78	35 (40%) 0 0	85, 107, 137, 185	0
2	j	86/114 (75%)	1.39	15 (17%) 4 3	96, 109, 147, 178	0
All	All	13772/15336 (89%)	0.55	914 (6%) 24 18	20, 60, 104, 192	1 (0%)

All (914) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	h	110	PRO	7.0
2	Y	111	SER	6.5
2	c	110	PRO	6.2
2	d	110	PRO	6.1
2	a	110	PRO	5.4
2	e	110	PRO	5.3
2	g	110	PRO	4.8
2	d	111	SER	4.8
1	H	563	HIS	4.7
1	X	562	SER	4.6
2	Z	110	PRO	4.6
1	V	362	VAL	4.6
2	f	110	PRO	4.5
2	j	110	PRO	4.5
2	a	108	ARG	4.4
1	K	563	HIS	4.4
1	W	209	PRO	4.4
1	R	42	HIS	4.4
1	X	429	ASN	4.4
2	Y	110	PRO	4.4
1	O	563	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
2	b	110	PRO	4.2
1	X	323	MET	4.2
1	J	562	SER	4.2
1	W	441	VAL	4.1
1	X	210	PRO	4.1
1	V	513	THR	4.1
1	X	448	ILE	4.1
1	X	531	PRO	4.1
1	L	562	SER	4.1
1	S	508	TRP	4.0
1	W	445	GLN	4.0
2	i	110	PRO	4.0
1	W	211	GLY	4.0
1	X	442	GLY	4.0
1	D	562	SER	4.0
1	J	42	HIS	3.9
1	T	211	GLY	3.9
1	X	211	GLY	3.9
1	S	414	ALA	3.8
1	W	488	ALA	3.8
1	V	89	LEU	3.8
2	j	41	GLY	3.8
1	C	563	HIS	3.8
1	T	429	ASN	3.8
1	A	211	GLY	3.8
1	U	476	VAL	3.8
1	H	562	SER	3.7
1	G	563	HIS	3.7
1	F	392	LEU	3.7
1	Q	560	ALA	3.7
1	V	34	GLU	3.7
1	L	563	HIS	3.7
1	G	42	HIS	3.6
1	T	563	HIS	3.6
1	V	563	HIS	3.6
1	N	562	SER	3.6
1	V	253	GLY	3.6
2	g	41	GLY	3.6
1	L	560	ALA	3.6
2	f	107	ALA	3.6
2	i	111	SER	3.6
1	K	211	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	T	36	ILE	3.5
1	V	459	ASP	3.5
1	B	42	HIS	3.5
1	U	61	GLY	3.5
1	C	47	MET	3.5
1	X	57	VAL	3.5
1	F	394	PRO	3.5
2	Z	37	ALA	3.5
1	F	211	GLY	3.5
1	N	563	HIS	3.4
1	U	513	THR	3.4
1	W	433	VAL	3.4
1	A	42	HIS	3.4
1	F	562	SER	3.4
1	K	562	SER	3.4
2	Z	107	ALA	3.4
2	b	109	HIS	3.4
1	X	85	PHE	3.4
1	X	441	VAL	3.4
1	X	508	TRP	3.4
1	V	437	CYS	3.3
1	B	563	HIS	3.3
1	S	560	ALA	3.3
1	F	66	TYR	3.3
1	F	476	VAL	3.3
1	R	211	GLY	3.3
1	Q	545	GLU	3.3
1	D	563	HIS	3.3
1	V	318	SER	3.3
2	c	108	ARG	3.3
1	E	429	ASN	3.3
1	X	34	GLU	3.3
1	F	426	ARG	3.3
1	F	513	THR	3.3
1	W	320	GLY	3.3
1	T	34	GLU	3.3
1	S	376	ALA	3.3
1	X	543	ALA	3.3
2	Z	109	HIS	3.3
1	F	33	VAL	3.3
1	F	563	HIS	3.2
2	Y	80	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	80	HIS	3.2
1	B	562	SER	3.2
2	h	111	SER	3.2
1	F	427	MET	3.2
1	U	560	ALA	3.2
1	X	392	LEU	3.2
2	Z	108	ARG	3.2
1	W	518	VAL	3.2
2	f	38	ILE	3.2
1	N	42	HIS	3.2
2	f	108	ARG	3.2
2	j	108	ARG	3.2
1	X	497	TRP	3.2
1	W	324	ALA	3.2
1	U	373	PHE	3.2
1	X	33	VAL	3.2
1	S	210	PRO	3.2
1	U	489	LEU	3.1
1	A	560	ALA	3.1
1	F	429	ASN	3.1
2	e	61	ASN	3.1
2	e	108	ARG	3.1
1	G	560	ALA	3.1
1	W	366	SER	3.1
1	W	543	ALA	3.1
1	O	42	HIS	3.1
1	P	563	HIS	3.1
1	U	493	VAL	3.1
1	X	46	GLY	3.1
1	S	33	VAL	3.1
1	T	562	SER	3.1
2	e	84	SER	3.1
1	J	563	HIS	3.1
1	S	403	SER	3.1
1	S	55	GLY	3.1
1	X	561	GLY	3.1
1	T	558	ILE	3.1
2	i	40	ILE	3.1
1	W	34	GLU	3.1
1	H	42	HIS	3.0
1	W	493	VAL	3.0
2	b	108	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	h	108	ARG	3.0
2	Z	101	LEU	3.0
1	D	42	HIS	3.0
1	K	42	HIS	3.0
1	V	33	VAL	3.0
1	W	400	HIS	3.0
1	F	47	MET	3.0
1	X	47	MET	3.0
1	X	204	TRP	3.0
1	X	66	TYR	3.0
1	X	82	TYR	3.0
1	P	562	SER	3.0
1	X	486	LEU	3.0
1	N	210	PRO	3.0
1	T	560	ALA	3.0
1	V	324	ALA	3.0
2	i	37	ALA	3.0
1	W	540	HIS	3.0
2	c	80	HIS	3.0
1	F	69	TYR	3.0
1	V	442	GLY	3.0
2	f	111	SER	3.0
1	A	210	PRO	3.0
1	S	372	THR	3.0
1	W	365	ALA	3.0
2	j	105	ALA	3.0
1	D	523	GLY	2.9
1	S	380	LEU	2.9
1	V	186	GLY	2.9
1	V	320	GLY	2.9
1	Q	210	PRO	2.9
2	a	111	SER	2.9
1	F	560	ALA	2.9
1	F	493	VAL	2.9
1	X	518	VAL	2.9
2	Y	109	HIS	2.9
1	R	504	LYS	2.9
1	A	563	HIS	2.9
1	W	513	THR	2.9
1	X	563	HIS	2.9
1	V	436	LEU	2.9
1	S	533	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	h	84	SER	2.9
1	G	540	HIS	2.9
1	Q	563	HIS	2.9
1	X	540	HIS	2.9
1	V	430	CYS	2.9
1	Q	189	GLY	2.9
1	U	494	GLY	2.9
1	X	468	GLY	2.9
1	F	387	PRO	2.9
1	S	387	PRO	2.9
1	X	209	PRO	2.9
1	X	207	GLU	2.9
1	B	560	ALA	2.9
2	Z	89	VAL	2.9
1	V	502	PHE	2.9
1	X	440	SER	2.9
2	i	108	ARG	2.9
2	j	111	SER	2.9
2	a	80	HIS	2.9
2	e	109	HIS	2.9
1	F	489	LEU	2.9
1	U	369	TYR	2.8
1	W	409	TYR	2.8
1	X	63	LYS	2.8
2	h	26	TYR	2.8
1	X	91	ALA	2.8
2	i	77	VAL	2.8
2	i	85	ALA	2.8
1	X	428	SER	2.8
2	a	109	HIS	2.8
2	f	109	HIS	2.8
1	U	495	ILE	2.8
1	F	105	GLU	2.8
1	F	316	TYR	2.8
1	S	324	ALA	2.8
1	E	495	ILE	2.8
1	M	563	HIS	2.8
1	T	42	HIS	2.8
1	V	364	ASP	2.8
1	M	559	THR	2.8
2	c	111	SER	2.8
1	D	211	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	114	GLY	2.8
1	T	561	GLY	2.8
1	V	427	MET	2.8
2	i	41	GLY	2.8
2	i	30	PRO	2.8
1	T	433	VAL	2.8
1	V	200	VAL	2.8
1	X	443	TYR	2.8
2	g	108	ARG	2.8
1	F	414	ALA	2.8
1	H	560	ALA	2.8
1	C	42	HIS	2.8
1	W	62	LEU	2.8
2	d	109	HIS	2.8
1	T	559	THR	2.8
1	E	211	GLY	2.8
1	S	211	GLY	2.8
1	W	442	GLY	2.8
1	A	544	GLU	2.8
1	F	435	ARG	2.8
1	B	33	VAL	2.8
1	X	99	TYR	2.8
1	E	367	LEU	2.8
1	F	206	ILE	2.8
1	U	558	ILE	2.8
1	V	495	ILE	2.8
1	W	489	LEU	2.8
2	d	80	HIS	2.8
1	W	427	MET	2.8
1	V	61	GLY	2.8
1	X	203	ALA	2.7
1	F	495	ILE	2.7
1	U	380	LEU	2.7
1	D	52	ASP	2.7
1	K	561	GLY	2.7
1	V	463	SER	2.7
1	D	210	PRO	2.7
1	X	389	PRO	2.7
1	E	502	PHE	2.7
1	U	396	TRP	2.7
1	U	430	CYS	2.7
1	U	460	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	42	HIS	2.7
1	T	521	HIS	2.7
1	V	42	HIS	2.7
2	d	78	HIS	2.7
1	X	427	MET	2.7
2	d	61	ASN	2.7
1	T	398	GLY	2.7
1	S	522	PRO	2.7
1	W	422	SER	2.7
1	N	545	GLU	2.7
1	U	33	VAL	2.7
1	D	558	ILE	2.7
1	E	486	LEU	2.7
1	E	560	ALA	2.7
1	U	379	LEU	2.7
1	W	214	ALA	2.7
1	W	385	LEU	2.7
1	X	560	ALA	2.7
1	M	42	HIS	2.7
1	Q	211	GLY	2.7
1	H	545	GLU	2.7
1	S	76	SER	2.7
1	X	40	VAL	2.7
1	X	106	VAL	2.7
1	S	404	LEU	2.7
1	U	556	LEU	2.7
2	i	97	LEU	2.7
1	E	467	PHE	2.7
1	W	374	LYS	2.7
1	V	257	ARG	2.7
1	F	217	THR	2.7
1	F	522	PRO	2.7
1	S	534	GLY	2.7
1	U	559	THR	2.7
1	S	433	VAL	2.7
1	U	490	GLU	2.7
1	V	493	VAL	2.7
1	W	562	SER	2.7
1	W	469	MET	2.6
1	W	42	HIS	2.6
2	i	80	HIS	2.6
2	j	80	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	d	108	ARG	2.6
1	D	522	PRO	2.6
1	O	327	GLY	2.6
1	T	33	VAL	2.6
1	U	441	VAL	2.6
1	U	507	GLU	2.6
1	X	380	LEU	2.6
1	Q	562	SER	2.6
1	U	422	SER	2.6
1	E	42	HIS	2.6
1	X	516	TYR	2.6
1	X	398	GLY	2.6
1	T	392	LEU	2.6
1	U	85	PHE	2.6
1	U	410	HIS	2.6
1	X	42	HIS	2.6
1	F	92	TYR	2.6
1	D	55	GLY	2.6
1	U	210	PRO	2.6
1	X	416	GLY	2.6
2	i	43	PRO	2.6
1	F	491	LYS	2.6
1	W	492	LYS	2.6
1	X	250	CYS	2.6
2	Z	103	LEU	2.6
1	U	47	MET	2.6
2	i	31	ALA	2.6
1	F	403	SER	2.6
1	R	563	HIS	2.6
2	b	111	SER	2.6
2	h	80	HIS	2.6
1	X	482	ARG	2.6
1	W	254	LYS	2.6
2	Z	32	LYS	2.6
1	X	423	GLY	2.6
1	S	89	LEU	2.6
1	A	315	VAL	2.6
1	D	495	ILE	2.6
1	T	461	THR	2.6
1	W	52	ASP	2.6
1	X	257	ARG	2.5
1	S	556	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	V	489	LEU	2.5
1	W	404	LEU	2.5
1	L	174	GLU	2.5
1	T	324	ALA	2.5
2	a	47	ALA	2.5
1	F	84	LYS	2.5
1	U	397	SER	2.5
1	U	403	SER	2.5
1	D	497	TRP	2.5
1	F	417	GLY	2.5
1	U	89	LEU	2.5
1	V	211	GLY	2.5
2	h	52	GLY	2.5
1	T	452	MET	2.5
1	W	33	VAL	2.5
1	W	57	VAL	2.5
1	W	384	VAL	2.5
1	S	513	THR	2.5
2	j	98	PHE	2.5
1	D	483	ALA	2.5
1	H	543	ALA	2.5
2	f	39	ALA	2.5
2	h	85	ALA	2.5
1	D	479	ASN	2.5
1	P	157	ASN	2.5
1	Q	42	HIS	2.5
1	S	563	HIS	2.5
1	X	539	HIS	2.5
2	j	109	HIS	2.5
1	C	562	SER	2.5
1	R	47	MET	2.5
1	T	427	MET	2.5
1	W	436	LEU	2.5
1	U	211	GLY	2.5
2	d	41	GLY	2.5
1	U	518	VAL	2.5
1	W	396	TRP	2.5
1	W	476	VAL	2.5
1	X	402	TRP	2.5
1	M	548	TYR	2.5
1	U	409	TYR	2.5
1	H	544	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	W	425	PHE	2.5
1	P	560	ALA	2.5
2	Z	78	HIS	2.5
1	X	52	ASP	2.5
1	F	486	LEU	2.5
1	M	533	PRO	2.5
1	S	427	MET	2.5
1	D	381	ILE	2.5
1	S	558	ILE	2.5
2	e	38	ILE	2.5
2	i	51	VAL	2.5
1	W	508	TRP	2.5
1	S	59	PHE	2.5
1	T	467	PHE	2.5
1	E	554	LYS	2.5
1	W	477	LYS	2.5
2	h	32	LYS	2.5
2	g	109	HIS	2.5
2	Y	61	ASN	2.5
1	V	389	PRO	2.4
2	h	96	ILE	2.4
1	F	397	SER	2.4
1	W	340	SER	2.4
1	B	544	GLU	2.4
1	F	434	GLU	2.4
1	X	503	TRP	2.4
1	X	438	PHE	2.4
1	E	324	ALA	2.4
1	Q	414	ALA	2.4
1	S	501	GLN	2.4
1	W	504	LYS	2.4
1	X	390	LYS	2.4
1	D	47	MET	2.4
1	F	530	CYS	2.4
1	T	41	PRO	2.4
1	W	522	PRO	2.4
1	F	122	VAL	2.4
1	F	442	GLY	2.4
1	P	211	GLY	2.4
1	R	494	GLY	2.4
1	S	476	VAL	2.4
1	T	493	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	441	VAL	2.4
1	W	127	VAL	2.4
2	i	46	GLY	2.4
2	Z	111	SER	2.4
1	D	490	GLU	2.4
1	B	64	ALA	2.4
1	F	203	ALA	2.4
1	N	560	ALA	2.4
1	V	365	ALA	2.4
1	S	82	TYR	2.4
1	X	513	THR	2.4
2	a	57	THR	2.4
1	C	489	LEU	2.4
1	X	520	ASN	2.4
1	S	401	ILE	2.4
1	F	437	CYS	2.4
1	W	437	CYS	2.4
1	Q	546	VAL	2.4
1	U	255	ASP	2.4
1	X	494	GLY	2.4
1	C	504	LYS	2.4
1	D	85	PHE	2.4
1	F	218	PHE	2.4
1	A	365	ALA	2.4
1	F	204	TRP	2.4
1	K	560	ALA	2.4
1	U	414	ALA	2.4
1	V	497	TRP	2.4
2	a	107	ALA	2.4
1	F	310	GLN	2.4
1	C	278	THR	2.4
1	W	317	THR	2.4
2	i	57	THR	2.4
2	f	80	HIS	2.4
2	g	80	HIS	2.4
1	F	526	ILE	2.4
2	f	75	ILE	2.4
1	F	210	PRO	2.4
1	F	531	PRO	2.4
1	S	429	ASN	2.4
1	S	531	PRO	2.4
1	F	384	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	T	40	VAL	2.4
1	U	309	VAL	2.4
1	U	362	VAL	2.4
1	F	492	LYS	2.4
1	H	211	GLY	2.4
1	V	63	LYS	2.4
1	X	305	GLY	2.4
2	i	89	VAL	2.4
1	U	477	LYS	2.4
1	X	524	LYS	2.4
1	F	85	PHE	2.4
1	T	527	PHE	2.4
1	U	502	PHE	2.4
1	W	203	ALA	2.4
1	G	496	SER	2.4
1	S	562	SER	2.4
1	U	205	SER	2.4
1	U	204	TRP	2.4
1	N	172	THR	2.4
1	O	172	THR	2.4
1	W	321	MET	2.4
1	E	563	HIS	2.4
1	U	392	LEU	2.4
2	h	109	HIS	2.4
1	F	401	ILE	2.4
1	V	533	PRO	2.4
1	U	491	LYS	2.3
1	V	435	ARG	2.3
2	i	32	LYS	2.3
1	E	470	ASP	2.3
1	U	437	CYS	2.3
1	S	279	GLU	2.3
2	Z	79	GLU	2.3
2	j	107	ALA	2.3
2	h	83	GLN	2.3
1	S	54	SER	2.3
1	S	428	SER	2.3
1	T	503	TRP	2.3
1	U	508	TRP	2.3
1	V	562	SER	2.3
1	X	86	TRP	2.3
1	D	521	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	369	TYR	2.3
1	E	513	THR	2.3
1	L	42	HIS	2.3
1	R	540	HIS	2.3
1	S	505	THR	2.3
1	U	42	HIS	2.3
1	W	380	LEU	2.3
1	X	473	LEU	2.3
2	c	109	HIS	2.3
1	J	558	ILE	2.3
1	Q	558	ILE	2.3
1	S	35	ILE	2.3
2	d	38	ILE	2.3
1	V	55	GLY	2.3
2	c	61	ASN	2.3
1	S	527	PHE	2.3
1	V	444	PHE	2.3
1	E	325	ASP	2.3
1	E	312	ALA	2.3
1	V	202	CYS	2.3
1	X	376	ALA	2.3
1	W	388	MET	2.3
1	X	388	MET	2.3
1	F	366	SER	2.3
1	X	404	LEU	2.3
1	E	540	HIS	2.3
1	V	402	TRP	2.3
1	B	558	ILE	2.3
1	V	45	TYR	2.3
1	V	316	TYR	2.3
1	U	363	LYS	2.3
1	U	70	PRO	2.3
1	W	79	PRO	2.3
1	X	146	PRO	2.3
1	X	515	PRO	2.3
1	A	127	VAL	2.3
1	S	546	VAL	2.3
2	h	28	VAL	2.3
1	W	215	GLY	2.3
1	X	215	GLY	2.3
1	W	458	ASN	2.3
1	X	527	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	424	GLU	2.3
1	E	556	LEU	2.3
1	S	374	LYS	2.3
1	X	39	TRP	2.3
1	A	513	THR	2.3
1	S	525	THR	2.3
1	S	559	THR	2.3
2	e	26	TYR	2.3
2	i	26	TYR	2.3
1	T	499	PRO	2.3
1	U	433	VAL	2.3
2	j	45	VAL	2.3
1	V	215	GLY	2.3
2	j	52	GLY	2.3
1	W	207	GLU	2.3
1	F	436	LEU	2.3
1	T	504	LYS	2.3
1	E	314	ILE	2.3
1	F	188	ILE	2.3
1	F	393	CYS	2.3
1	N	558	ILE	2.3
1	U	549	ILE	2.3
2	j	40	ILE	2.3
1	F	86	TRP	2.3
1	F	482	ARG	2.3
1	R	562	SER	2.3
2	Z	57	THR	2.3
2	Z	100	SER	2.3
1	S	99	TYR	2.3
1	S	316	TYR	2.3
1	P	33	VAL	2.3
1	V	48	PRO	2.3
1	V	210	PRO	2.3
1	W	362	VAL	2.3
1	X	499	PRO	2.3
1	X	533	PRO	2.3
2	b	51	VAL	2.3
1	W	514	GLY	2.3
1	X	465	GLY	2.3
2	h	82	GLY	2.3
1	F	527	PHE	2.2
1	V	58	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	59	PHE	2.2
1	J	560	ALA	2.2
1	O	545	GLU	2.2
1	W	414	ALA	2.2
1	W	560	ALA	2.2
1	W	486	LEU	2.2
1	V	87	LYS	2.2
1	V	212	ASP	2.2
1	W	35	ILE	2.2
1	X	36	ILE	2.2
1	U	497	TRP	2.2
1	S	77	PRO	2.2
1	V	66	TYR	2.2
1	W	66	TYR	2.2
1	W	449	TYR	2.2
1	X	95	TYR	2.2
1	X	466	SER	2.2
2	g	111	SER	2.2
2	i	73	TYR	2.2
1	D	442	GLY	2.2
1	E	494	GLY	2.2
1	E	47	MET	2.2
1	X	58	PHE	2.2
1	R	105	GLU	2.2
1	W	408	ALA	2.2
2	f	105	ALA	2.2
1	S	477	LYS	2.2
1	T	404	LEU	2.2
1	W	473	LEU	2.2
1	W	475	ASN	2.2
2	i	103	LEU	2.2
1	K	540	HIS	2.2
1	T	52	ASP	2.2
1	U	563	HIS	2.2
1	W	386	ASP	2.2
1	W	391	ASP	2.2
1	W	410	HIS	2.2
1	W	484	ARG	2.2
2	b	78	HIS	2.2
1	F	418	THR	2.2
1	F	508	TRP	2.2
1	F	546	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	533	PRO	2.2
1	W	210	PRO	2.2
1	W	499	PRO	2.2
1	X	542	PRO	2.2
1	A	562	SER	2.2
1	T	428	SER	2.2
1	T	447	TYR	2.2
1	U	428	SER	2.2
1	V	78	TYR	2.2
2	f	26	TYR	2.2
1	M	523	GLY	2.2
1	D	119	GLU	2.2
1	E	379	LEU	2.2
1	F	123	ALA	2.2
1	N	365	ALA	2.2
1	V	355	LEU	2.2
1	X	414	ALA	2.2
1	W	53	ASN	2.2
2	Z	61	ASN	2.2
1	U	501	GLN	2.2
1	V	35	ILE	2.2
1	X	35	ILE	2.2
2	h	38	ILE	2.2
1	X	476	VAL	2.2
1	M	513	THR	2.2
1	S	503	TRP	2.2
1	T	278	THR	2.2
2	f	42	THR	2.2
1	S	557	GLY	2.2
1	X	369	TYR	2.2
1	X	548	TYR	2.2
1	V	65	LYS	2.2
1	W	59	PHE	2.2
1	F	376	ALA	2.2
1	F	377	GLU	2.2
1	F	480	ALA	2.2
1	S	174	GLU	2.2
1	V	453	ALA	2.2
1	W	399	GLN	2.2
1	S	521	HIS	2.2
1	V	454	HIS	2.2
1	A	546	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	339	VAL	2.2
1	W	474	VAL	2.2
1	W	372	THR	2.2
1	E	398	GLY	2.2
1	F	561	GLY	2.2
1	U	557	GLY	2.2
1	V	503	TRP	2.2
1	W	398	GLY	2.2
1	W	497	TRP	2.2
1	X	294	GLY	2.2
1	S	85	PHE	2.2
1	A	556	LEU	2.2
1	E	403	SER	2.2
1	U	562	SER	2.2
1	W	218	PHE	2.2
1	X	502	PHE	2.2
1	X	536	LEU	2.2
1	T	119	GLU	2.2
1	V	543	ALA	2.2
1	V	337	ARG	2.1
1	W	36	ILE	2.1
1	X	401	ILE	2.1
1	T	540	HIS	2.1
2	a	61	ASN	2.1
2	i	109	HIS	2.1
1	S	70	PRO	2.1
1	S	362	VAL	2.1
1	U	522	PRO	2.1
1	V	375	VAL	2.1
1	S	47	MET	2.1
1	K	559	THR	2.1
1	V	504	LYS	2.1
1	V	561	GLY	2.1
2	b	82	GLY	2.1
2	i	36	THR	2.1
1	S	402	TRP	2.1
1	F	379	LEU	2.1
1	F	438	PHE	2.1
1	T	425	PHE	2.1
1	V	204	TRP	2.1
1	U	404	LEU	2.1
1	U	553	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	66	PHE	2.1
1	V	92	TYR	2.1
1	A	403	SER	2.1
1	X	393	CYS	2.1
1	X	324	ALA	2.1
1	X	480	ALA	2.1
1	X	541	ALA	2.1
1	E	434	GLU	2.1
1	F	103	ARG	2.1
1	S	119	GLU	2.1
1	A	549	ILE	2.1
1	V	517	ILE	2.1
1	W	381	ILE	2.1
1	X	558	ILE	2.1
1	A	47	MET	2.1
1	S	499	PRO	2.1
1	X	67	MET	2.1
1	O	524	LYS	2.1
2	g	32	LYS	2.1
2	i	87	LYS	2.1
1	F	432	ASP	2.1
1	G	211	GLY	2.1
1	F	423	GLY	2.1
1	M	172	THR	2.1
1	P	561	GLY	2.1
1	S	465	GLY	2.1
1	U	505	THR	2.1
1	X	213	THR	2.1
1	F	59	PHE	2.1
1	V	404	LEU	2.1
1	W	467	PHE	2.1
1	X	385	LEU	2.1
2	j	97	LEU	2.1
2	i	47	ALA	2.1
1	F	545	GLU	2.1
1	S	397	SER	2.1
2	Z	40	ILE	2.1
2	f	40	ILE	2.1
2	f	100	SER	2.1
1	U	498	GLN	2.1
2	i	78	HIS	2.1
1	S	524	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	542	PRO	2.1
1	T	63	LYS	2.1
1	W	56	LYS	2.1
1	X	546	VAL	2.1
2	h	45	VAL	2.1
2	h	99	VAL	2.1
1	D	561	GLY	2.1
1	J	561	GLY	2.1
1	S	486	LEU	2.1
1	S	512	LEU	2.1
1	T	523	GLY	2.1
1	U	423	GLY	2.1
1	V	486	LEU	2.1
1	V	527	PHE	2.1
1	X	391	ASP	2.1
2	h	103	LEU	2.1
2	j	101	LEU	2.1
1	V	482	ARG	2.1
1	A	558	ILE	2.1
1	V	448	ILE	2.1
1	W	82	TYR	2.1
1	W	495	ILE	2.1
2	c	74	ALA	2.1
1	P	174	GLU	2.1
1	U	443	TYR	2.1
2	Y	79	GLU	2.1
2	h	44	ILE	2.1
1	F	481	SER	2.1
1	M	562	SER	2.1
1	R	496	SER	2.1
1	V	205	SER	2.1
1	W	322	SER	2.1
2	h	56	CYS	2.1
1	T	498	GLN	2.1
1	A	410	HIS	2.1
1	F	42	HIS	2.1
1	T	47	MET	2.1
1	B	210	PRO	2.1
1	F	70	PRO	2.1
1	N	522	PRO	2.1
1	T	522	PRO	2.1
1	W	329	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	48	PRO	2.1
1	V	385	LEU	2.1
1	S	116	PHE	2.1
1	S	442	GLY	2.1
1	S	561	GLY	2.1
1	T	494	GLY	2.1
1	W	189	GLY	2.1
1	M	343	ASP	2.1
1	U	378	ASP	2.1
1	X	470	ASP	2.1
1	X	532	ASP	2.1
2	b	53	ASP	2.1
2	i	42	THR	2.1
1	A	543	ALA	2.1
1	E	503	TRP	2.1
1	F	381	ILE	2.1
1	F	396	TRP	2.1
1	S	483	ALA	2.1
1	U	487	ALA	2.1
1	V	64	ALA	2.1
1	V	472	TRP	2.1
1	V	487	ALA	2.1
1	W	406	ILE	2.1
2	b	75	ILE	2.1
2	i	74	ALA	2.1
1	W	201	GLU	2.1
1	D	504	LYS	2.0
1	T	397	SER	2.0
1	V	390	LYS	2.0
1	W	390	LYS	2.0
1	W	440	SER	2.0
1	F	430	CYS	2.0
1	X	321	MET	2.0
2	f	32	LYS	2.0
1	X	521	HIS	2.0
1	F	44	VAL	2.0
1	S	44	VAL	2.0
2	f	89	VAL	2.0
2	j	89	VAL	2.0
1	B	157	ASN	2.0
1	F	536	LEU	2.0
1	P	392	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	479	ASN	2.0
1	U	486	LEU	2.0
1	F	197	PHE	2.0
1	U	208	ARG	2.0
2	i	59	GLY	2.0
1	F	372	THR	2.0
1	M	381	ILE	2.0
1	X	341	ILE	2.0
2	g	38	ILE	2.0
1	E	338	TRP	2.0
1	F	503	TRP	2.0
1	R	119	GLU	2.0
1	U	402	TRP	2.0
1	V	145	GLU	2.0
1	B	524	LYS	2.0
1	D	87	LYS	2.0
1	V	319	MET	2.0
1	V	388	MET	2.0
1	J	493	VAL	2.0
1	S	40	VAL	2.0
1	T	318	SER	2.0
1	V	433	VAL	2.0
1	W	563	HIS	2.0
1	X	205	SER	2.0
2	i	84	SER	2.0
1	A	533	PRO	2.0
1	E	210	PRO	2.0
1	X	530	CYS	2.0
1	S	62	LEU	2.0
1	D	58	PHE	2.0
1	W	58	PHE	2.0
1	X	444	PHE	2.0
2	i	52	GLY	2.0
2	i	71	GLY	2.0
2	Z	96	ILE	2.0
1	E	414	ALA	2.0
1	J	513	THR	2.0
1	Q	513	THR	2.0
1	U	376	ALA	2.0
1	V	317	THR	2.0
1	V	488	ALA	2.0
2	Z	47	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	c	85	ALA	2.0
2	i	105	ALA	2.0
1	E	390	LYS	2.0
1	F	402	TRP	2.0
1	V	252	TRP	2.0
1	W	323	MET	2.0
2	a	26	TYR	2.0
1	V	57	VAL	2.0
1	V	546	VAL	2.0
2	i	28	VAL	2.0
2	i	45	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	X	610	5/5	0.31	0.13	158,161,161,162	0
6	K	X	612	1/1	0.44	0.20	93,93,93,93	0
6	K	K	616	1/1	0.46	0.17	85,85,85,85	0
4	SO4	c	201	5/5	0.54	0.12	132,133,135,135	0
6	K	H	616	1/1	0.54	0.17	82,82,82,82	0
4	SO4	X	611	5/5	0.55	0.12	139,139,141,144	0
4	SO4	a	201	5/5	0.63	0.11	139,139,140,140	0
4	SO4	X	609	5/5	0.64	0.11	107,108,110,112	0
4	SO4	O	610	5/5	0.66	0.12	109,111,112,112	0
4	SO4	S	609	5/5	0.66	0.11	129,133,135,135	0
4	SO4	Q	611	5/5	0.67	0.12	112,118,119,119	0
4	SO4	A	611	5/5	0.68	0.14	117,118,119,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	H	610	5/5	0.69	0.14	106,111,113,114	0
4	SO4	H	613	5/5	0.70	0.17	116,120,125,127	0
4	SO4	U	611	5/5	0.70	0.12	127,130,131,133	0
4	SO4	L	612	5/5	0.71	0.14	110,112,115,115	0
4	SO4	V	611	5/5	0.71	0.11	131,133,134,135	0
4	SO4	C	609	5/5	0.72	0.14	96,102,106,108	0
5	GOL	A	614	6/6	0.73	0.21	82,89,90,91	0
6	K	Q	612	1/1	0.73	0.10	96,96,96,96	0
4	SO4	I	612	5/5	0.73	0.13	120,121,124,125	0
4	SO4	C	610	5/5	0.74	0.27	143,145,147,149	0
4	SO4	C	611	5/5	0.74	0.13	111,111,114,116	0
4	SO4	M	610	5/5	0.74	0.23	134,135,138,139	0
4	SO4	Y	202	5/5	0.75	0.09	130,130,132,136	0
4	SO4	M	612	5/5	0.75	0.14	121,122,123,125	0
4	SO4	G	611	5/5	0.77	0.12	139,139,143,149	0
4	SO4	N	610	5/5	0.77	0.16	101,105,107,109	0
4	SO4	H	612	5/5	0.78	0.14	110,113,116,118	0
5	GOL	J	612	6/6	0.78	0.18	58,64,67,67	0
4	SO4	K	611	5/5	0.79	0.15	102,104,105,105	0
4	SO4	I	611	5/5	0.79	0.11	115,115,116,117	0
4	SO4	J	611	5/5	0.79	0.21	118,118,120,123	0
4	SO4	Q	609	5/5	0.79	0.11	84,87,88,89	0
5	GOL	I	615	6/6	0.80	0.15	51,55,56,57	0
4	SO4	W	609	5/5	0.80	0.09	114,118,119,124	0
4	SO4	M	611	5/5	0.80	0.20	129,131,136,137	0
4	SO4	F	610	5/5	0.80	0.10	135,136,139,139	0
5	GOL	G	615	6/6	0.80	0.20	61,67,68,68	0
4	SO4	E	610	5/5	0.80	0.09	103,105,106,109	0
4	SO4	L	610	5/5	0.81	0.13	142,143,145,150	0
5	GOL	H	615	6/6	0.81	0.37	78,86,90,100	0
4	SO4	U	610	5/5	0.81	0.11	99,101,103,104	0
4	SO4	Y	201	5/5	0.81	0.11	136,136,137,141	0
4	SO4	L	611	5/5	0.81	0.10	116,119,121,122	0
4	SO4	G	612	5/5	0.81	0.16	120,124,126,126	0
4	SO4	H	609	5/5	0.81	0.17	78,81,82,83	0
4	SO4	B	609	5/5	0.81	0.18	116,117,119,124	0
5	GOL	A	612	6/6	0.82	0.17	76,78,79,81	0
4	SO4	O	611	5/5	0.82	0.10	114,114,119,120	0
5	GOL	D	610	6/6	0.82	0.15	86,88,88,89	0
5	GOL	K	612	6/6	0.82	0.24	76,80,86,90	0
4	SO4	Q	610	5/5	0.83	0.20	133,136,137,137	0
4	SO4	T	609	5/5	0.84	0.10	98,100,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	610	5/5	0.84	0.14	88,89,91,91	0
4	SO4	P	609	5/5	0.84	0.19	95,95,96,98	0
4	SO4	F	609	5/5	0.85	0.08	95,99,102,104	0
4	SO4	N	611	5/5	0.85	0.10	123,126,127,129	0
4	SO4	A	610	5/5	0.85	0.13	73,77,79,80	0
5	GOL	A	613	6/6	0.85	0.14	74,77,78,79	0
4	SO4	H	611	5/5	0.85	0.13	97,100,101,105	0
4	SO4	R	610	5/5	0.85	0.15	75,77,79,79	0
4	SO4	R	611	5/5	0.85	0.21	142,143,145,147	0
4	SO4	K	610	5/5	0.86	0.15	84,84,86,88	0
4	SO4	L	609	5/5	0.87	0.10	91,94,94,97	0
4	SO4	J	610	5/5	0.87	0.13	99,100,101,103	0
5	GOL	I	613	6/6	0.87	0.13	59,64,66,73	0
4	SO4	G	610	5/5	0.87	0.24	104,106,107,108	0
4	SO4	S	610	5/5	0.87	0.13	92,93,94,95	0
4	SO4	V	610	5/5	0.88	0.12	94,97,98,99	0
4	SO4	D	609	5/5	0.89	0.10	82,82,84,87	0
4	SO4	G	614	5/5	0.89	0.14	91,94,95,95	0
4	SO4	O	609	5/5	0.89	0.11	77,78,80,82	0
5	GOL	L	613	6/6	0.89	0.17	56,59,60,61	0
5	GOL	J	613	6/6	0.90	0.16	58,61,62,63	0
4	SO4	J	609	5/5	0.90	0.11	77,79,80,80	0
5	GOL	K	615	6/6	0.90	0.33	53,55,58,59	0
5	GOL	H	614	6/6	0.90	0.30	56,63,64,68	0
4	SO4	M	609	5/5	0.91	0.12	89,90,91,92	0
4	SO4	V	609	5/5	0.91	0.10	56,59,60,62	0
5	GOL	K	613	6/6	0.91	0.09	45,51,52,53	0
5	GOL	I	614	6/6	0.92	0.33	67,78,80,83	0
4	SO4	E	609	5/5	0.92	0.10	50,51,53,53	0
4	SO4	G	613	5/5	0.93	0.10	63,63,64,66	0
3	HEC	V	602	43/43	0.93	0.14	68,73,87,100	0
3	HEC	W	606	43/43	0.93	0.14	64,76,88,96	0
3	HEC	X	606	43/43	0.93	0.15	69,83,87,90	0
5	GOL	G	616	6/6	0.93	0.10	37,40,41,41	0
4	SO4	U	609	5/5	0.93	0.10	57,58,60,64	0
3	HEC	V	603	43/43	0.94	0.12	51,65,82,86	0
3	HEC	W	603	43/43	0.94	0.13	67,77,85,89	0
5	GOL	K	614	6/6	0.94	0.20	49,56,57,59	0
3	HEC	W	605	43/43	0.94	0.13	74,81,87,89	0
3	HEC	S	603	43/43	0.94	0.13	72,77,88,94	0
3	HEC	U	606	43/43	0.94	0.13	65,72,88,96	0
4	SO4	G	609	5/5	0.94	0.10	72,72,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	S	605	43/43	0.94	0.13	63,72,82,83	0
4	SO4	I	610	5/5	0.94	0.10	67,67,69,69	0
3	HEC	V	606	43/43	0.95	0.11	57,60,76,81	0
3	HEC	V	607	43/43	0.95	0.11	54,66,69,70	0
3	HEC	E	605	43/43	0.95	0.12	53,63,75,82	0
3	HEC	E	606	43/43	0.95	0.13	55,60,68,75	0
3	HEC	F	603	43/43	0.95	0.12	62,70,74,79	0
3	HEC	F	605	43/43	0.95	0.11	54,60,69,78	0
3	HEC	X	603	43/43	0.95	0.12	70,80,103,109	0
3	HEC	X	601	43/43	0.95	0.11	62,69,78,82	0
3	HEC	X	602	43/43	0.95	0.12	69,75,91,106	0
3	HEC	X	605	43/43	0.95	0.15	79,86,97,100	0
3	HEC	N	601	43/43	0.95	0.11	41,44,55,65	0
3	HEC	Q	602	43/43	0.95	0.13	64,68,88,97	0
3	HEC	S	602	43/43	0.95	0.13	63,71,86,104	0
3	HEC	S	604	43/43	0.95	0.12	59,66,75,86	0
3	HEC	A	604	43/43	0.95	0.11	47,50,61,73	0
3	HEC	S	606	43/43	0.95	0.11	61,69,74,79	0
3	HEC	A	606	43/43	0.95	0.12	45,60,73,78	0
3	HEC	T	602	43/43	0.95	0.12	59,68,83,97	0
3	HEC	T	607	43/43	0.95	0.11	49,57,60,62	0
3	HEC	U	603	43/43	0.95	0.11	61,72,83,85	0
3	HEC	U	600	43/43	0.95	0.11	58,64,71,72	0
3	HEC	U	605	43/43	0.95	0.12	62,68,80,87	0
3	HEC	D	600	43/43	0.95	0.10	54,60,68,74	0
3	HEC	E	603	43/43	0.95	0.11	56,66,92,96	0
3	HEC	V	605	43/43	0.95	0.12	56,65,73,76	0
4	SO4	I	609	5/5	0.96	0.08	28,28,29,30	0
3	HEC	S	607	43/43	0.96	0.11	51,57,59,60	0
3	HEC	E	602	43/43	0.96	0.11	48,53,73,94	0
3	HEC	T	603	43/43	0.96	0.10	60,66,71,73	0
3	HEC	T	600	43/43	0.96	0.10	53,60,68,69	0
3	HEC	T	601	43/43	0.96	0.10	55,58,61,63	0
3	HEC	E	604	43/43	0.96	0.10	40,45,53,63	0
3	HEC	T	604	43/43	0.96	0.10	59,65,70,80	0
3	HEC	T	605	43/43	0.96	0.11	54,60,74,76	0
3	HEC	T	606	43/43	0.96	0.10	52,56,65,74	0
3	HEC	A	605	43/43	0.96	0.11	50,59,63,64	0
3	HEC	A	600	43/43	0.96	0.10	47,49,56,59	0
3	HEC	E	607	43/43	0.96	0.10	47,54,60,62	0
3	HEC	U	601	43/43	0.96	0.11	54,57,67,73	0
3	HEC	U	602	43/43	0.96	0.11	60,69,94,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	U	604	43/43	0.96	0.11	52,60,72,81	0
3	HEC	A	607	43/43	0.96	0.10	41,45,50,53	0
3	HEC	F	600	43/43	0.96	0.10	46,52,62,68	0
3	HEC	U	607	43/43	0.96	0.11	53,70,73,74	0
3	HEC	V	600	43/43	0.96	0.11	67,70,84,91	0
3	HEC	V	601	43/43	0.96	0.10	52,63,65,67	0
3	HEC	F	601	43/43	0.96	0.12	51,55,68,70	0
3	HEC	V	604	43/43	0.96	0.11	59,71,81,85	0
3	HEC	F	602	43/43	0.96	0.12	64,75,85,96	0
3	HEC	F	604	43/43	0.96	0.10	58,65,74,84	0
3	HEC	A	603	43/43	0.96	0.11	54,66,71,73	0
4	SO4	R	609	5/5	0.96	0.08	36,39,40,40	0
3	HEC	F	606	43/43	0.96	0.11	50,56,67,76	0
3	HEC	F	607	43/43	0.96	0.11	49,56,57,60	0
3	HEC	W	600	43/43	0.96	0.10	61,68,74,77	0
3	HEC	W	601	43/43	0.96	0.11	61,70,77,80	0
3	HEC	W	602	43/43	0.96	0.11	54,58,83,99	0
3	HEC	W	604	43/43	0.96	0.10	50,57,67,74	0
3	HEC	H	602	43/43	0.96	0.10	35,44,64,77	0
3	HEC	I	602	43/43	0.96	0.10	37,42,59,70	0
3	HEC	W	607	43/43	0.96	0.11	63,68,71,71	0
3	HEC	J	600	43/43	0.96	0.10	37,41,52,60	0
3	HEC	X	600	43/43	0.96	0.10	57,63,75,81	0
3	HEC	J	602	43/43	0.96	0.11	38,41,67,86	0
3	HEC	K	600	43/43	0.96	0.10	38,40,46,55	0
3	HEC	X	604	43/43	0.96	0.10	63,73,78,80	0
3	HEC	L	600	43/43	0.96	0.10	41,44,50,51	0
3	HEC	M	600	43/43	0.96	0.10	44,48,56,62	0
3	HEC	X	607	43/43	0.96	0.11	57,61,65,67	0
3	HEC	N	600	43/43	0.96	0.10	46,49,57,63	0
3	HEC	B	602	43/43	0.96	0.10	49,56,80,99	0
3	HEC	N	602	43/43	0.96	0.11	48,52,75,92	0
3	HEC	N	605	43/43	0.96	0.10	48,52,66,73	0
3	HEC	N	606	43/43	0.96	0.11	47,51,60,64	0
3	HEC	O	600	43/43	0.96	0.09	44,48,58,60	0
4	SO4	A	609	5/5	0.96	0.07	47,49,49,52	0
3	HEC	O	602	43/43	0.96	0.10	47,51,72,91	0
3	HEC	P	601	43/43	0.96	0.10	39,44,46,47	0
3	HEC	P	602	43/43	0.96	0.09	41,45,63,76	0
3	HEC	Q	603	43/43	0.96	0.09	52,55,58,59	0
3	HEC	Q	600	43/43	0.96	0.10	47,52,59,65	0
3	HEC	Q	601	43/43	0.96	0.11	46,50,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	B	604	43/43	0.96	0.10	44,51,62,67	0
3	HEC	Q	604	43/43	0.96	0.11	54,60,68,76	0
3	HEC	Q	606	43/43	0.96	0.11	44,55,65,69	0
3	HEC	R	603	43/43	0.96	0.09	37,43,48,52	0
3	HEC	R	600	43/43	0.96	0.10	49,54,62,64	0
3	HEC	S	600	43/43	0.96	0.10	60,65,73,75	0
3	HEC	S	601	43/43	0.96	0.12	67,70,81,85	0
3	HEC	C	606	43/43	0.96	0.10	41,43,59,65	0
3	HEC	C	607	43/43	0.96	0.10	44,48,49,52	0
3	HEC	A	602	43/43	0.96	0.10	51,56,79,99	0
3	HEC	G	602	43/43	0.96	0.10	34,38,59,77	0
3	HEC	B	603	43/43	0.97	0.08	45,49,53,54	0
3	HEC	H	604	43/43	0.97	0.08	38,43,53,64	0
3	HEC	H	606	43/43	0.97	0.08	32,34,39,44	0
3	HEC	I	600	43/43	0.97	0.08	39,43,50,52	0
3	HEC	I	601	43/43	0.97	0.08	35,37,41,44	0
3	HEC	D	601	43/43	0.97	0.10	51,59,61,62	0
3	HEC	D	602	43/43	0.97	0.10	45,48,65,79	0
3	HEC	D	605	43/43	0.97	0.10	48,53,61,66	0
3	HEC	J	604	43/43	0.97	0.09	32,35,44,55	0
3	HEC	J	605	43/43	0.97	0.09	32,38,43,47	0
3	HEC	J	606	43/43	0.97	0.09	33,39,41,46	0
3	HEC	D	606	43/43	0.97	0.09	46,51,62,66	0
3	HEC	K	601	43/43	0.97	0.08	33,34,38,43	0
3	HEC	K	602	43/43	0.97	0.10	44,47,65,81	0
3	HEC	K	604	43/43	0.97	0.09	36,41,49,57	0
3	HEC	K	605	43/43	0.97	0.09	35,38,43,48	0
3	HEC	K	606	43/43	0.97	0.09	33,39,42,46	0
3	HEC	L	603	43/43	0.97	0.08	35,41,50,52	0
3	HEC	D	603	43/43	0.97	0.09	54,66,69,72	0
4	SO4	N	609	5/5	0.97	0.07	40,40,41,42	0
3	HEC	L	601	43/43	0.97	0.09	36,40,45,46	0
3	HEC	L	602	43/43	0.97	0.10	42,45,57,72	0
3	HEC	L	604	43/43	0.97	0.09	35,41,48,58	0
3	HEC	L	605	43/43	0.97	0.09	35,37,41,45	0
3	HEC	L	606	43/43	0.97	0.08	35,37,43,47	0
3	HEC	B	600	43/43	0.97	0.10	48,52,59,61	0
3	HEC	M	601	43/43	0.97	0.09	41,44,47,51	0
3	HEC	M	602	43/43	0.97	0.10	44,48,72,89	0
3	HEC	M	604	43/43	0.97	0.09	40,43,51,62	0
3	HEC	M	605	43/43	0.97	0.10	36,38,46,51	0
3	HEC	M	606	43/43	0.97	0.10	37,40,50,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	M	607	43/43	0.97	0.09	36,39,52,62	0
3	HEC	M	603	43/43	0.97	0.09	42,46,49,50	0
3	HEC	N	603	43/43	0.97	0.08	47,56,60,62	0
3	HEC	E	600	43/43	0.97	0.09	39,41,53,55	0
3	HEC	E	601	43/43	0.97	0.09	39,43,47,55	0
3	HEC	B	601	43/43	0.97	0.09	43,47,56,68	0
3	HEC	N	604	43/43	0.97	0.08	42,47,56,59	0
3	HEC	G	601	43/43	0.97	0.09	37,41,43,48	0
3	HEC	A	601	43/43	0.97	0.09	44,47,53,54	0
3	HEC	N	607	43/43	0.97	0.09	37,41,44,46	0
3	HEC	O	603	43/43	0.97	0.09	40,44,49,51	0
3	HEC	B	605	43/43	0.97	0.09	42,45,53,59	0
3	HEC	B	607	43/43	0.97	0.07	37,40,45,47	0
3	HEC	O	604	43/43	0.97	0.10	34,41,50,60	0
3	HEC	O	605	43/43	0.97	0.09	36,41,49,52	0
3	HEC	O	606	43/43	0.97	0.09	37,41,49,52	0
3	HEC	O	607	43/43	0.97	0.08	34,37,38,39	0
3	HEC	P	600	43/43	0.97	0.09	44,46,51,53	0
3	HEC	C	603	43/43	0.97	0.10	44,48,58,63	0
3	HEC	C	600	43/43	0.97	0.09	49,52,56,58	0
3	HEC	P	604	43/43	0.97	0.08	36,40,52,63	0
3	HEC	P	605	43/43	0.97	0.08	43,46,49,50	0
3	HEC	P	606	43/43	0.97	0.09	43,47,48,49	0
3	HEC	P	607	43/43	0.97	0.09	38,48,52,54	0
3	HEC	P	603	43/43	0.97	0.10	40,49,56,62	0
3	HEC	C	601	43/43	0.97	0.09	41,45,50,51	0
3	HEC	C	602	43/43	0.97	0.09	45,48,66,80	0
3	HEC	C	604	43/43	0.97	0.09	42,47,53,60	0
3	HEC	C	605	43/43	0.97	0.09	38,43,53,57	0
3	HEC	G	600	43/43	0.97	0.09	40,42,45,49	0
3	HEC	Q	605	43/43	0.97	0.09	45,51,57,60	0
3	HEC	G	604	43/43	0.97	0.08	31,34,49,57	0
3	HEC	Q	607	43/43	0.97	0.08	36,40,44,46	0
3	HEC	H	600	43/43	0.97	0.07	32,37,42,44	0
3	HEC	H	601	43/43	0.97	0.09	34,36,41,47	0
3	HEC	R	601	43/43	0.97	0.09	43,48,50,50	0
3	HEC	R	602	43/43	0.97	0.10	45,48,74,89	0
3	HEC	R	604	43/43	0.97	0.09	38,43,53,61	0
3	HEC	R	606	43/43	0.97	0.09	37,43,59,63	0
3	HEC	R	607	43/43	0.97	0.08	37,38,43,48	0
3	HEC	J	603	43/43	0.98	0.07	37,39,44,46	0
3	HEC	K	603	43/43	0.98	0.07	37,39,42,44	0

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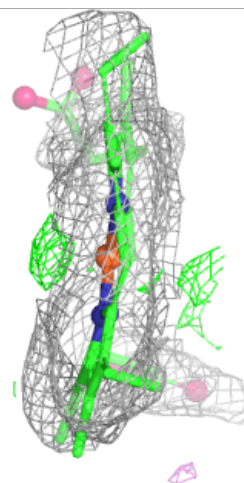
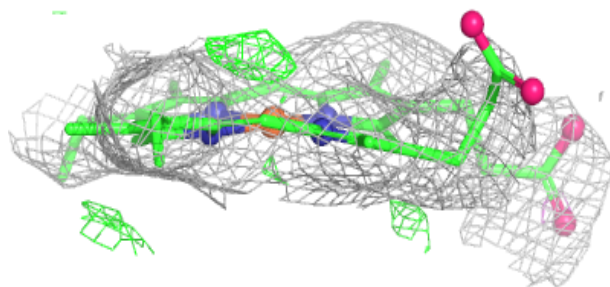
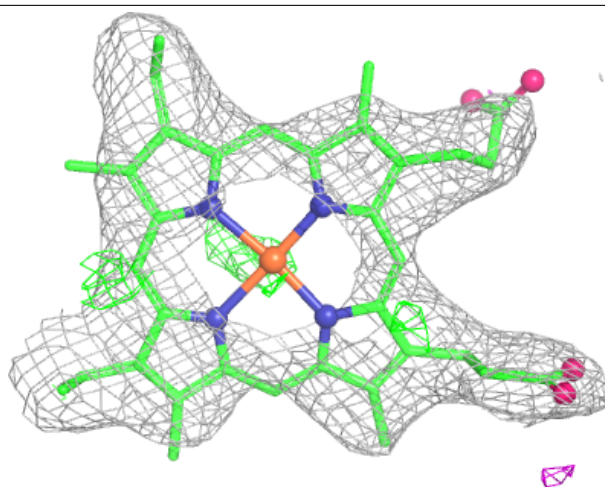
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	B	606	43/43	0.98	0.09	39,42,50,57	0
3	HEC	H	607	43/43	0.98	0.07	28,30,32,35	0
3	HEC	I	603	43/43	0.98	0.06	30,33,37,39	0
3	HEC	G	607	43/43	0.98	0.07	30,31,34,34	0
3	HEC	G	603	43/43	0.98	0.07	34,36,39,42	0
3	HEC	H	603	43/43	0.98	0.07	31,34,42,48	0
3	HEC	K	607	43/43	0.98	0.07	30,32,34,36	0
4	SO4	K	609	5/5	0.98	0.06	28,28,29,30	0
3	HEC	I	604	43/43	0.98	0.07	36,38,51,58	0
3	HEC	I	605	43/43	0.98	0.07	29,33,38,40	0
3	HEC	I	606	43/43	0.98	0.07	34,35,44,47	0
3	HEC	I	607	43/43	0.98	0.07	32,34,36,38	0
3	HEC	D	604	43/43	0.98	0.08	44,47,54,60	0
3	HEC	O	601	43/43	0.98	0.09	40,44,49,56	0
3	HEC	J	601	43/43	0.98	0.08	34,37,41,47	0
3	HEC	G	605	43/43	0.98	0.08	33,36,41,43	0
3	HEC	L	607	43/43	0.98	0.07	32,34,35,36	0
3	HEC	G	606	43/43	0.98	0.08	35,37,42,46	0
3	HEC	R	605	43/43	0.98	0.07	35,40,45,46	0
3	HEC	D	607	43/43	0.98	0.08	40,45,55,61	0
3	HEC	H	605	43/43	0.98	0.07	28,32,34,35	0
3	HEC	J	607	43/43	0.98	0.08	28,30,33,37	0

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

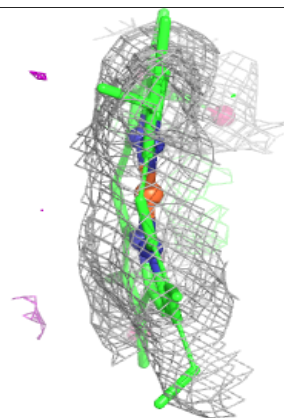
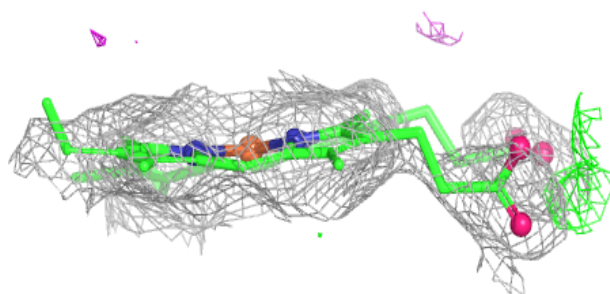
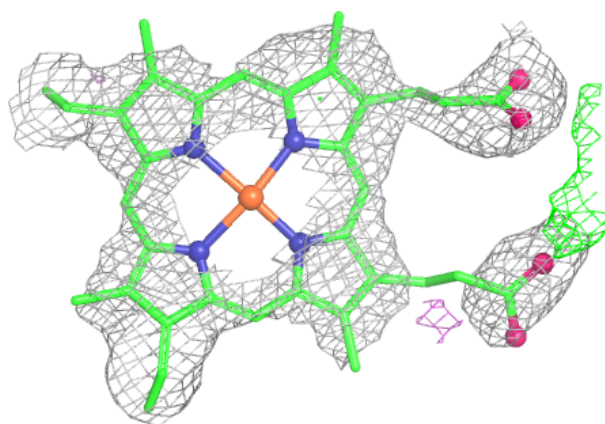
Electron density around HEC V 602:

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



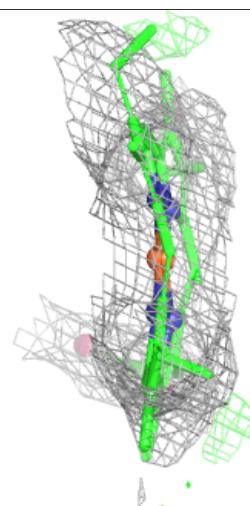
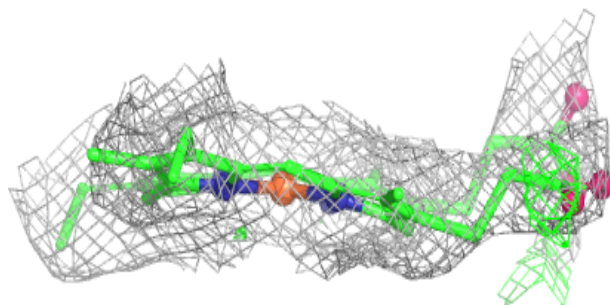
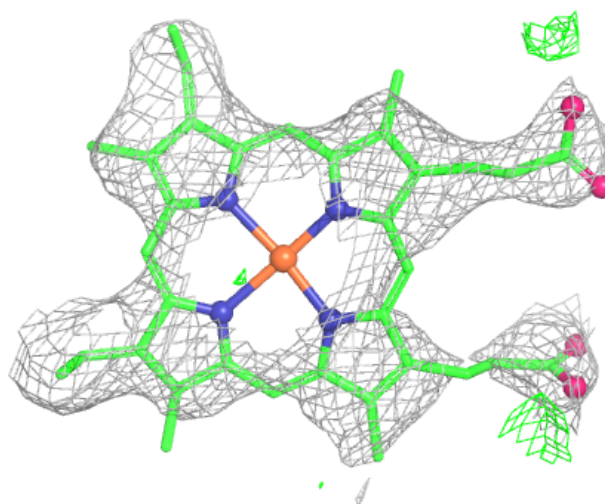
Electron density around HEC W 606:

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



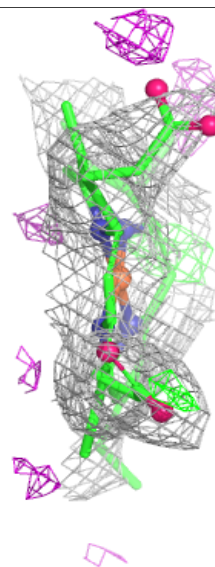
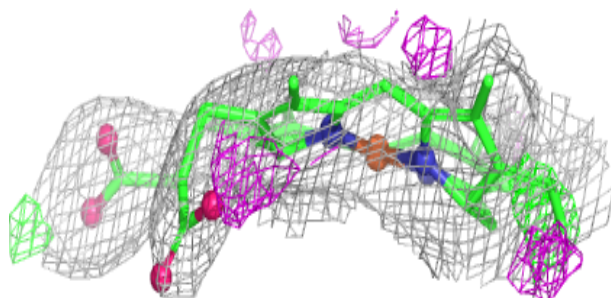
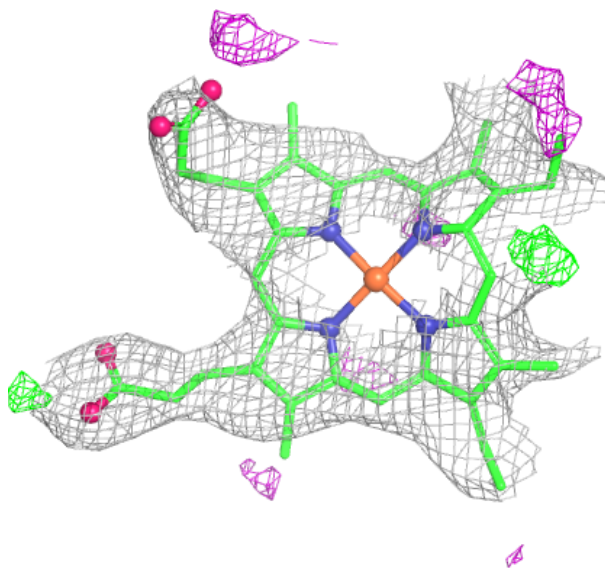
Electron density around HEC X 606:

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



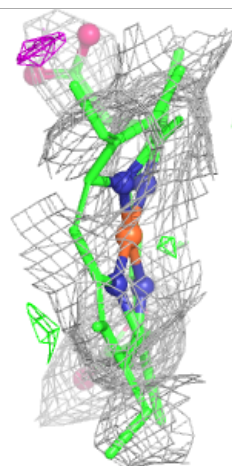
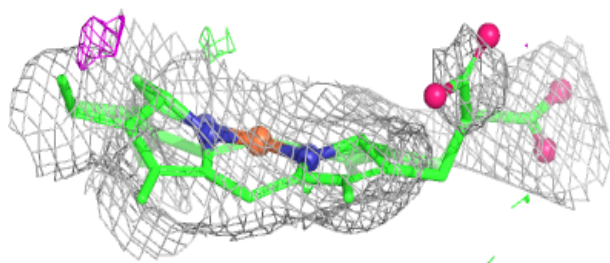
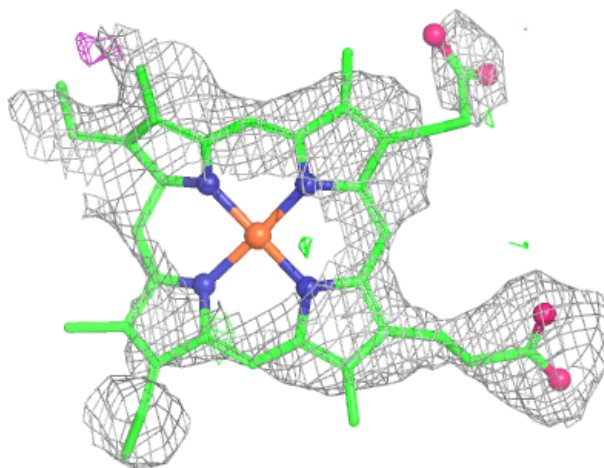
Electron density around HEC V 603:

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



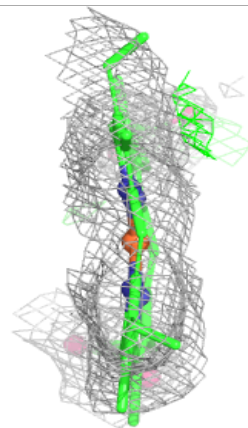
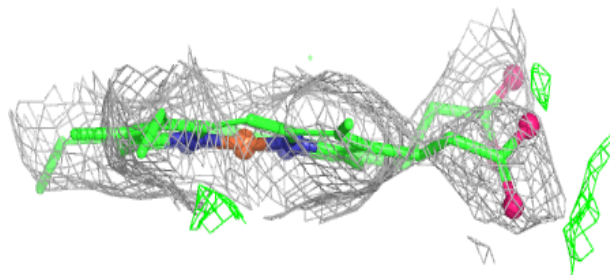
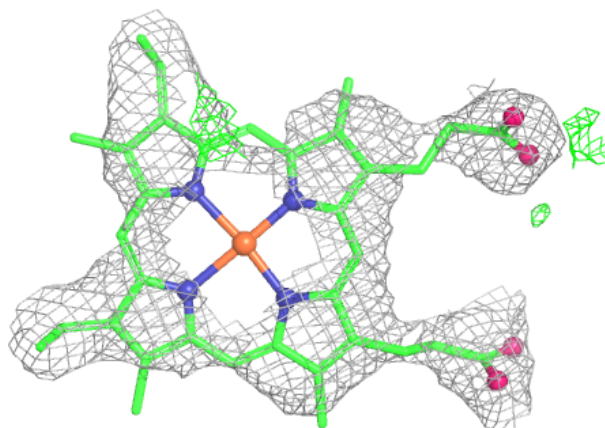
Electron density around HEC W 603:

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



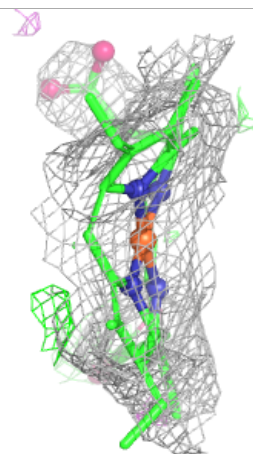
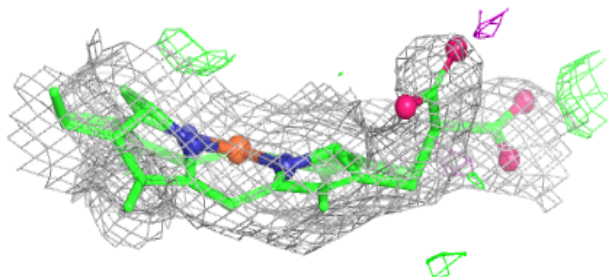
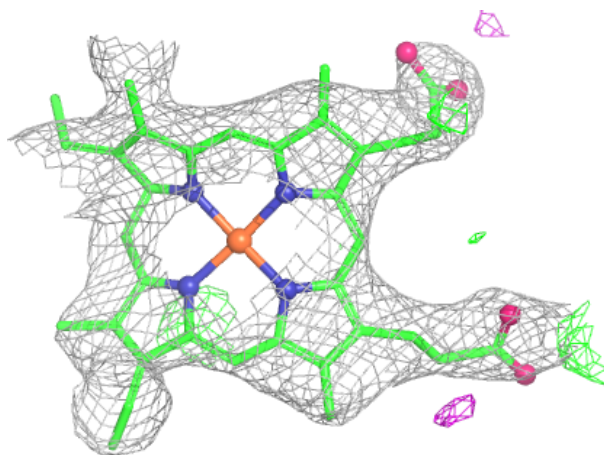
Electron density around HEC W 605:

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



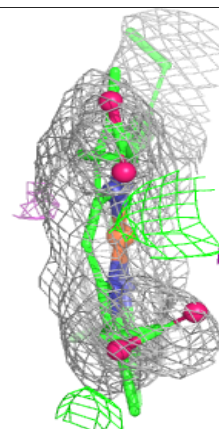
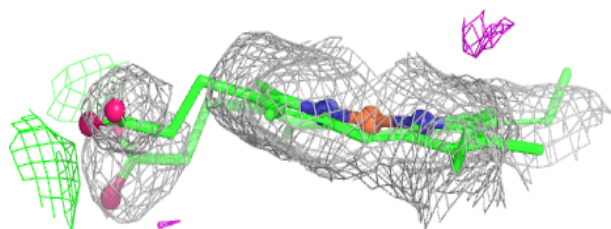
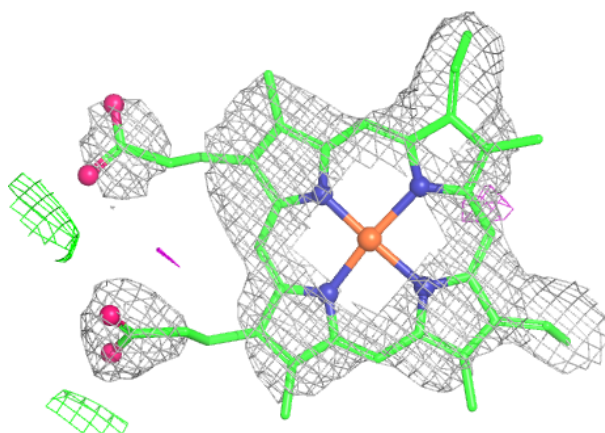
Electron density around HEC S 603:

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



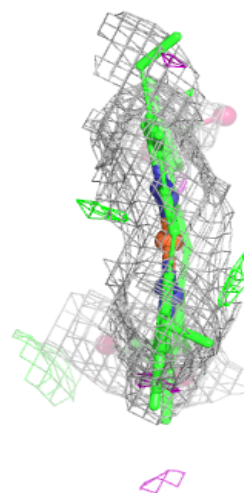
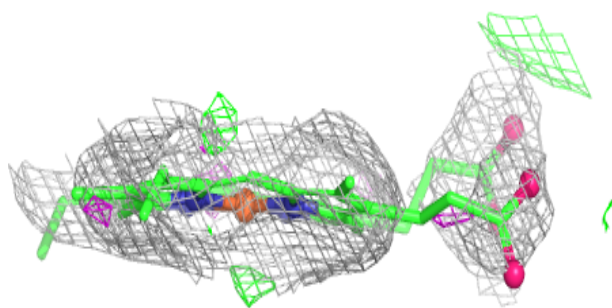
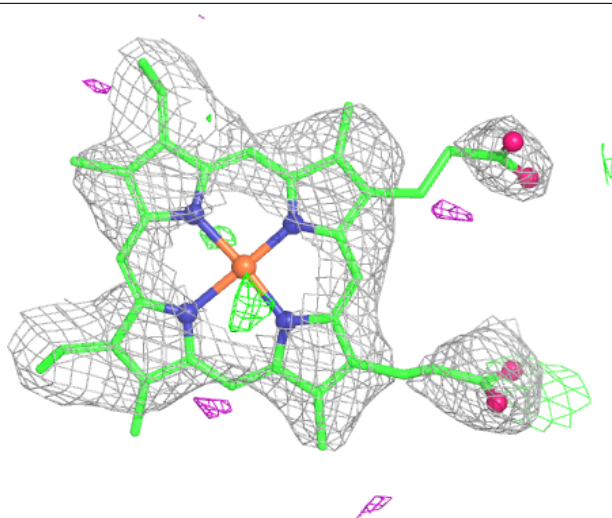
Electron density around HEC U 606:

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



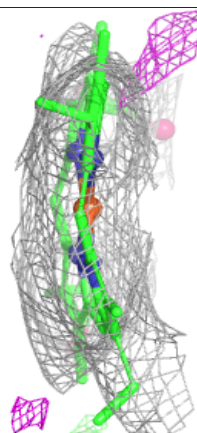
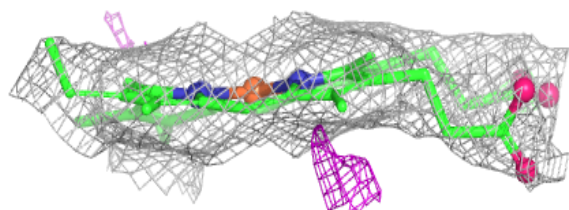
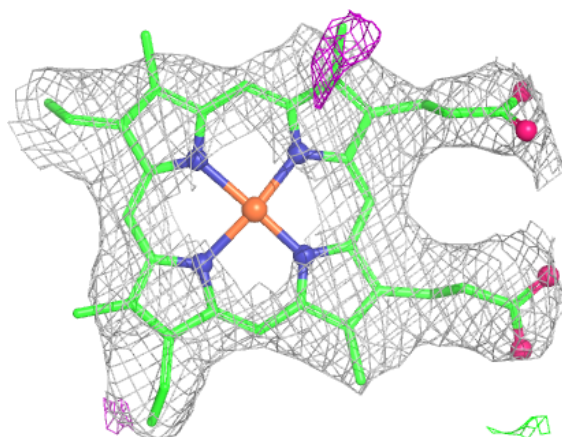
Electron density around HEC S 605:

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and green (positive)



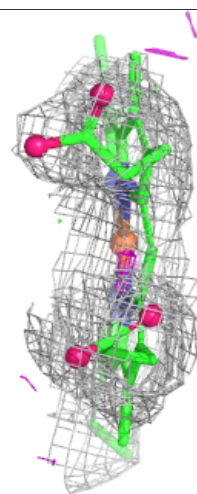
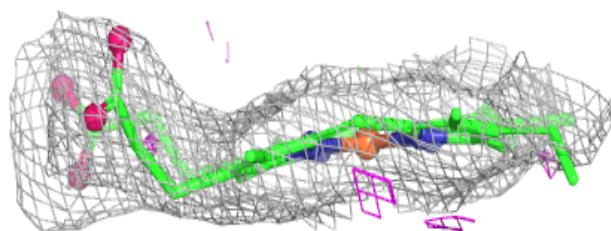
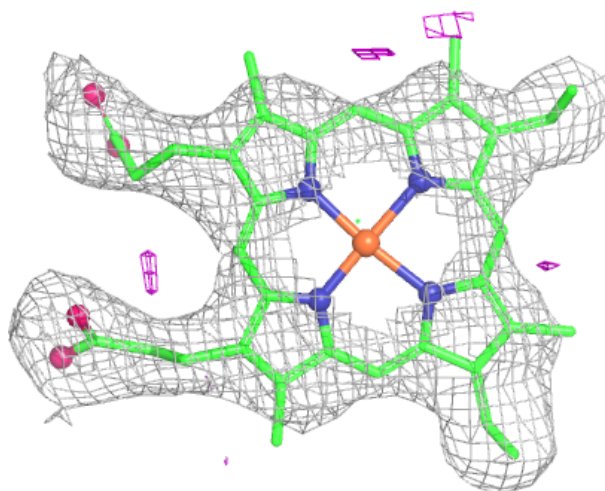
Electron density around HEC V 606:

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and green (positive)



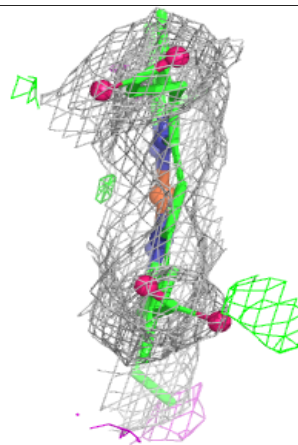
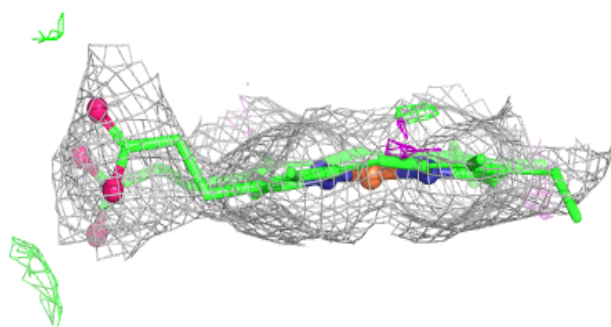
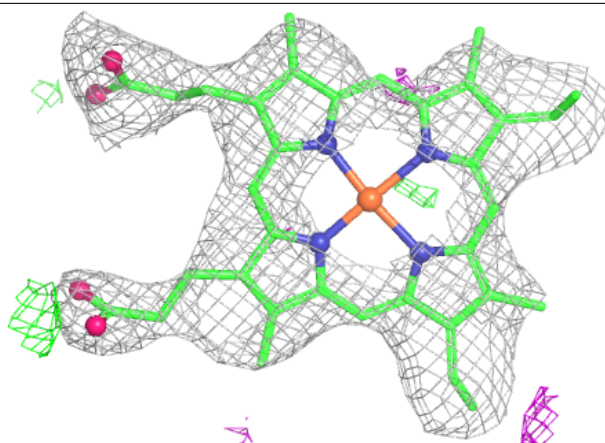
Electron density around HEC V 607:

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



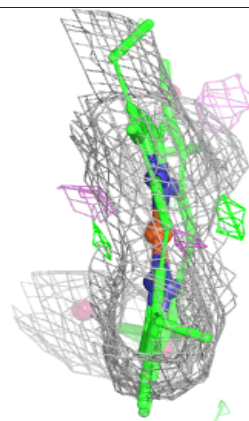
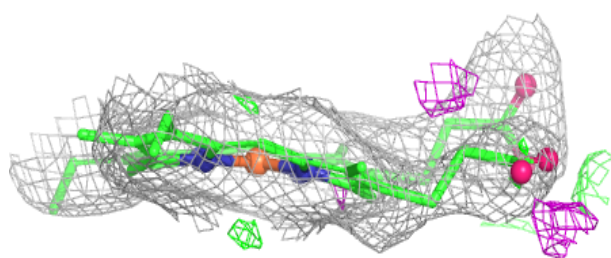
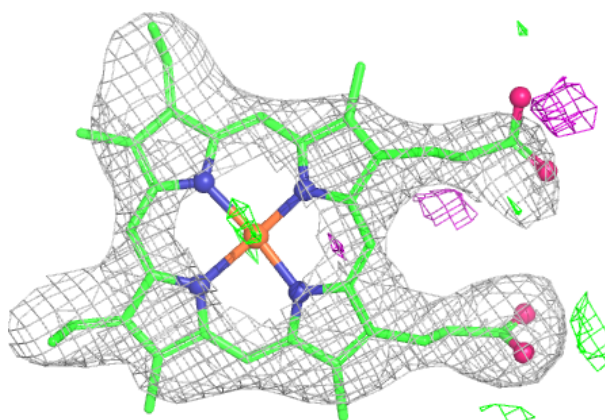
Electron density around HEC E 605:

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and green (positive)



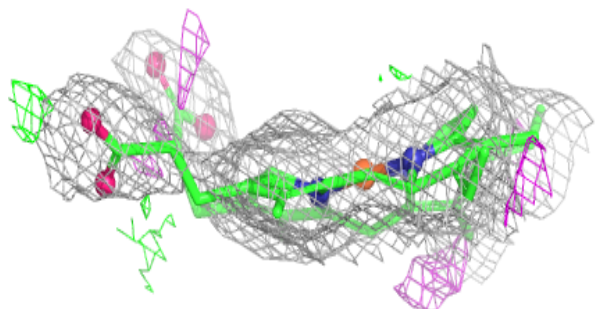
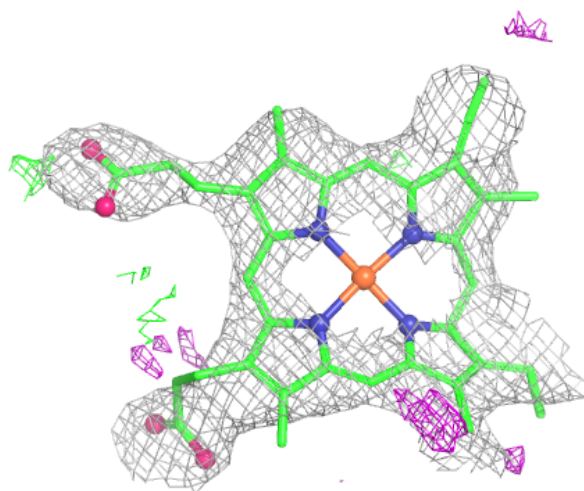
Electron density around HEC E 606:

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and green (positive)



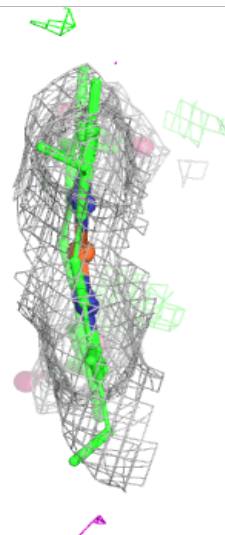
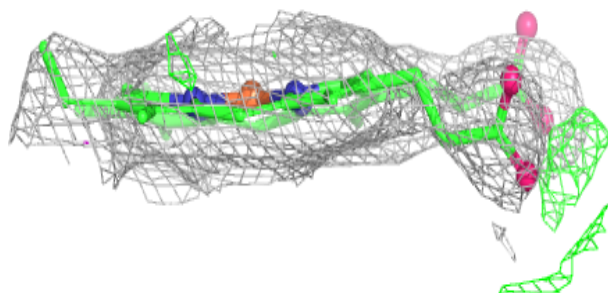
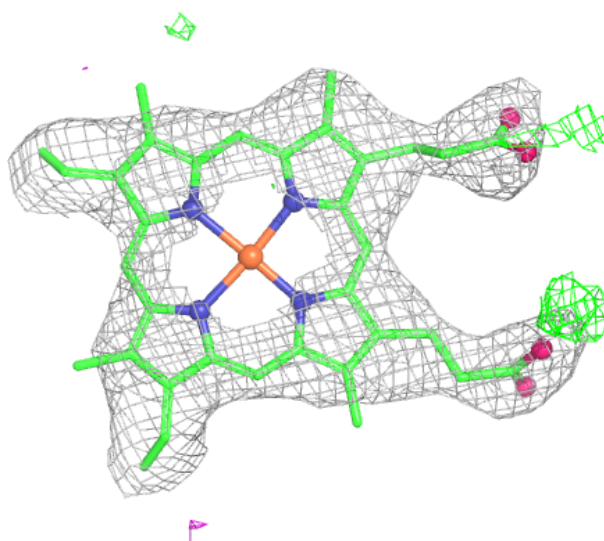
Electron density around HEC F 603:

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



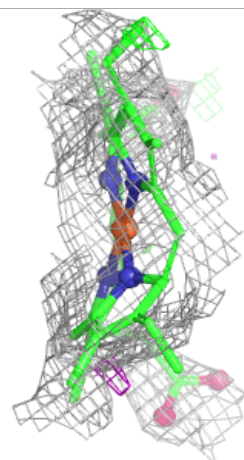
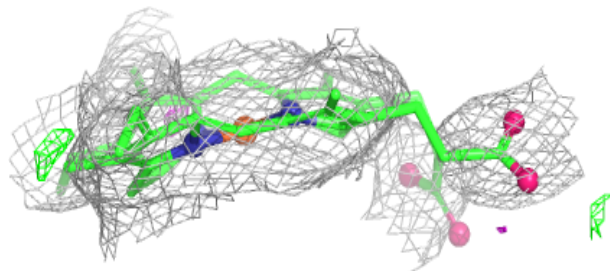
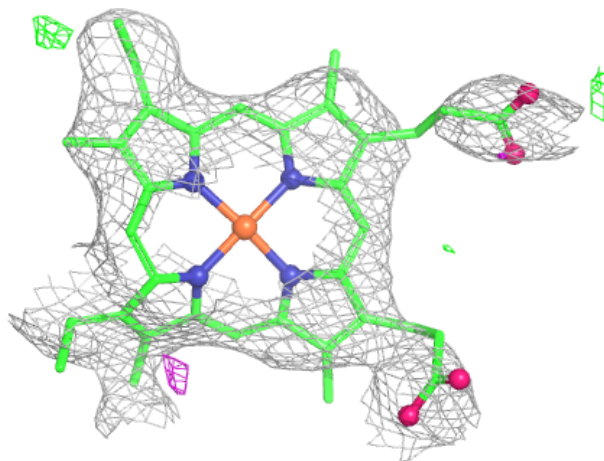
Electron density around HEC F 605:

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and green (positive)



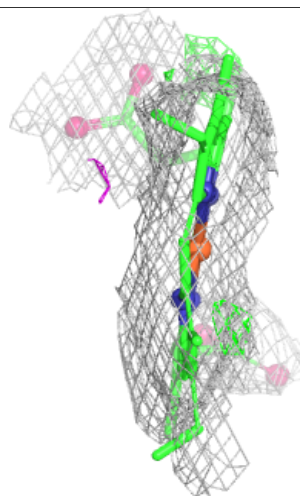
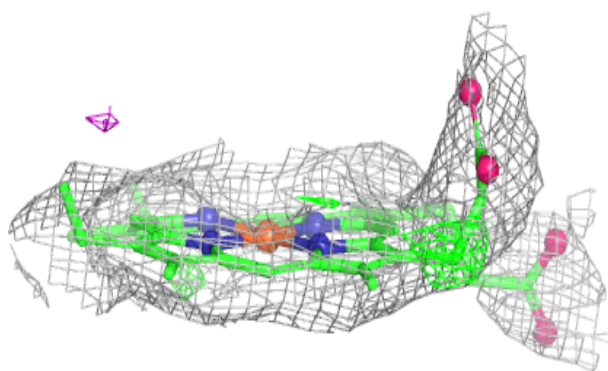
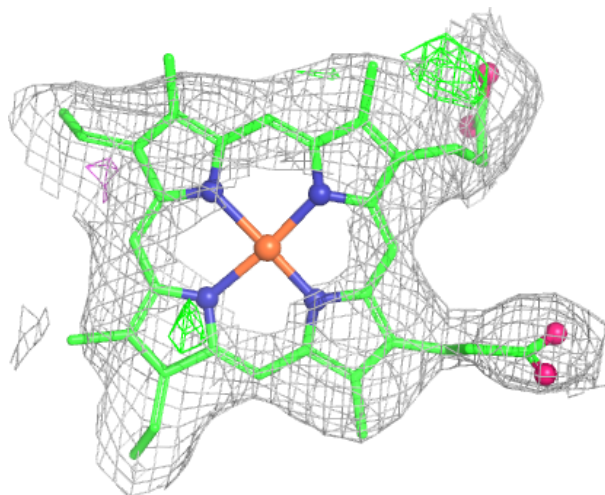
Electron density around HEC X 603:

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



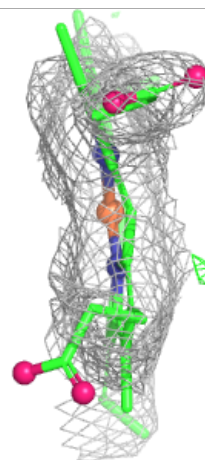
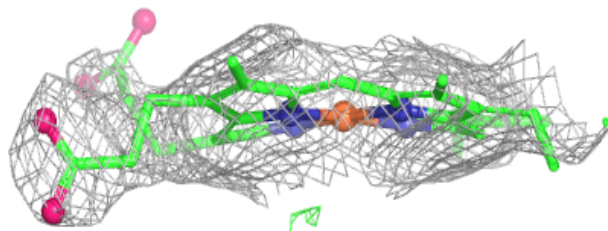
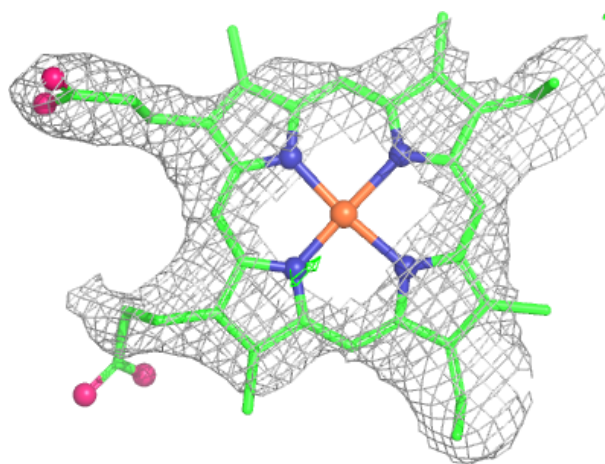
Electron density around HEC X 601:

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



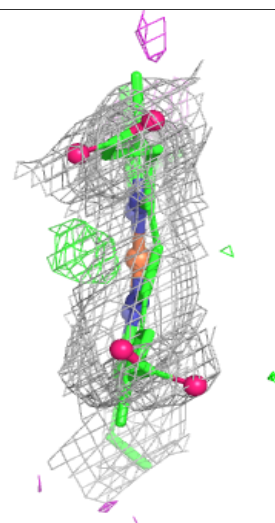
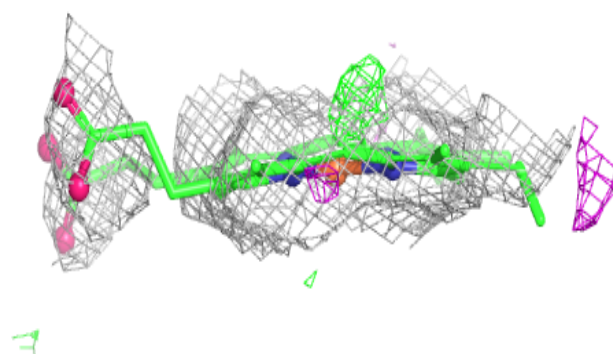
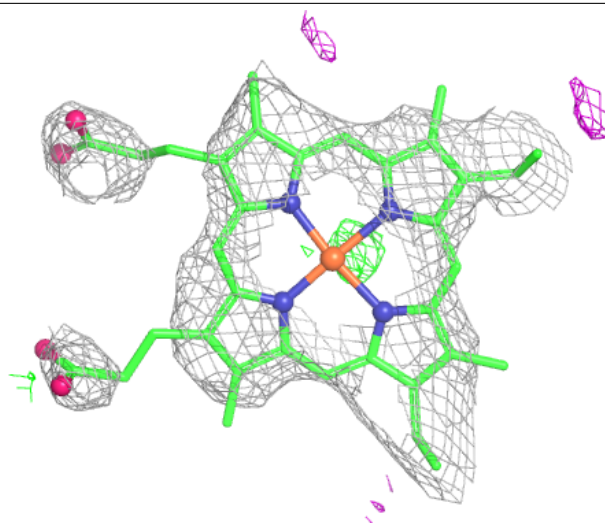
Electron density around HEC X 602:

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



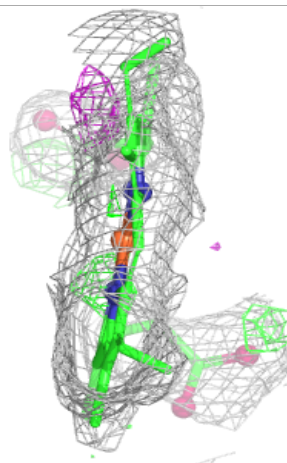
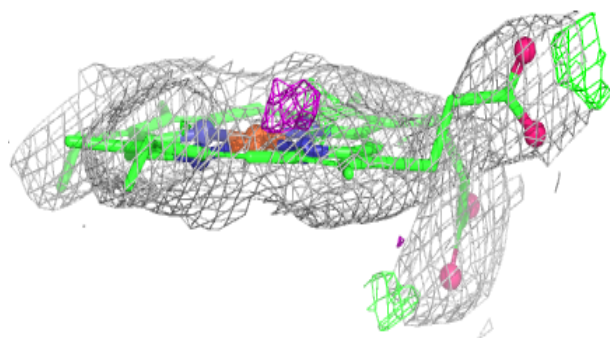
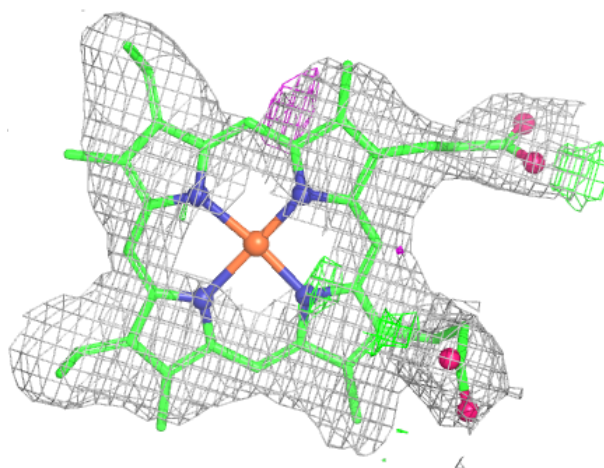
Electron density around HEC X 605:

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



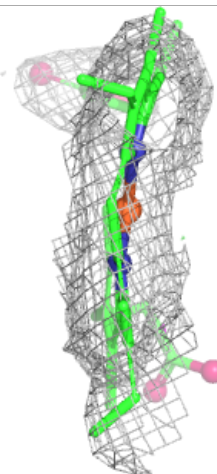
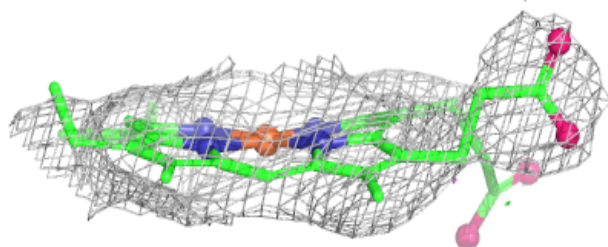
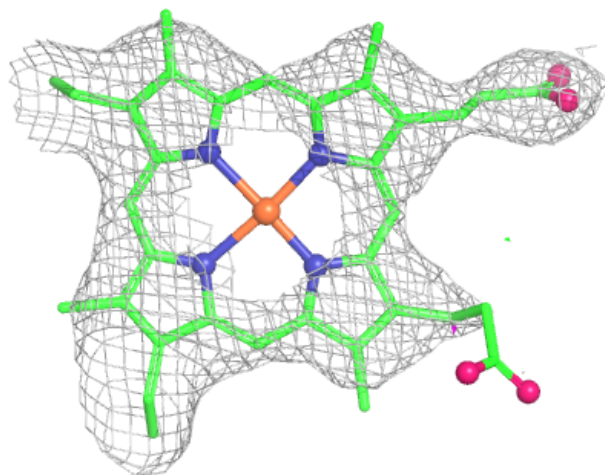
Electron density around HEC N 601:

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



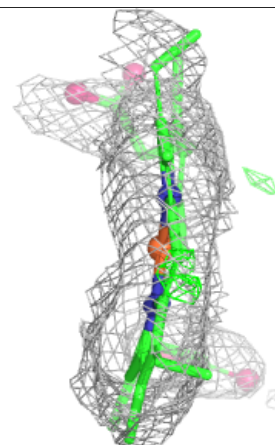
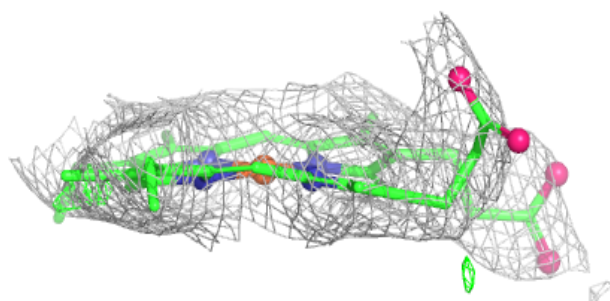
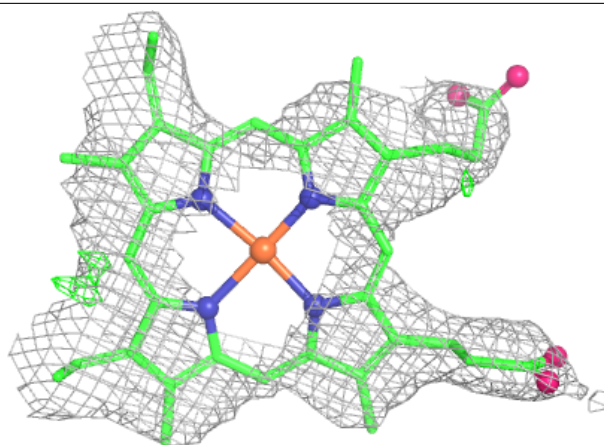
Electron density around HEC Q 602:

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



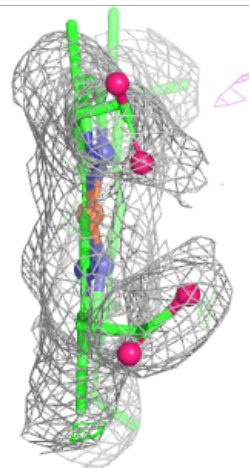
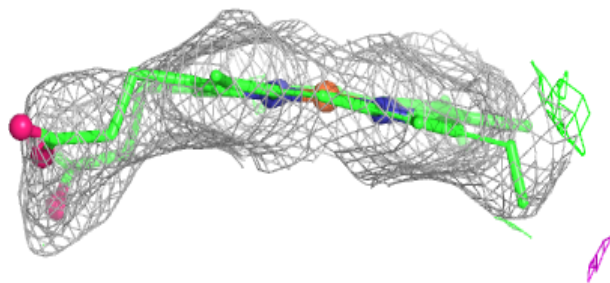
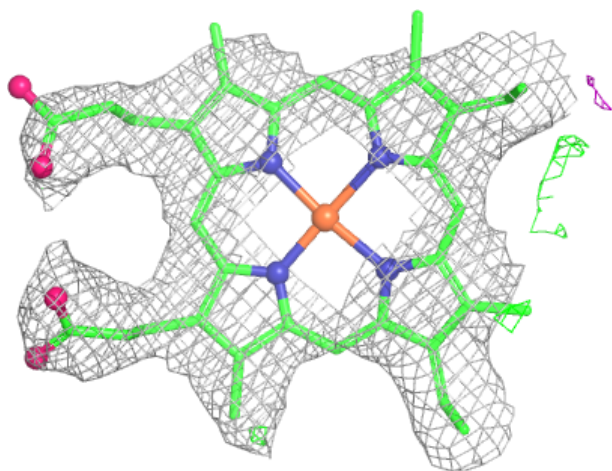
Electron density around HEC S 602:

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



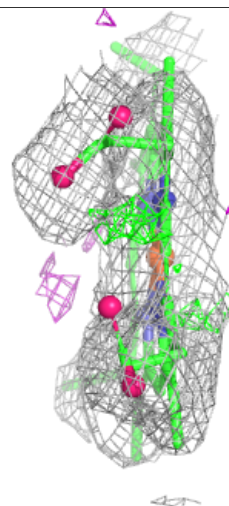
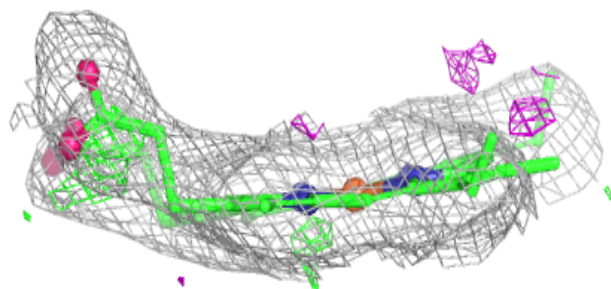
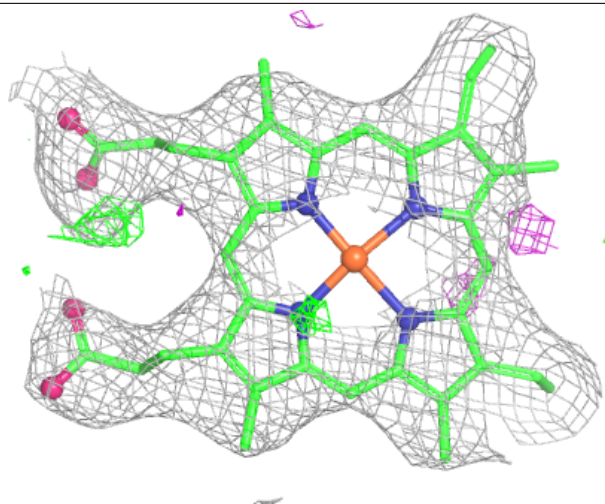
Electron density around HEC S 604:

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



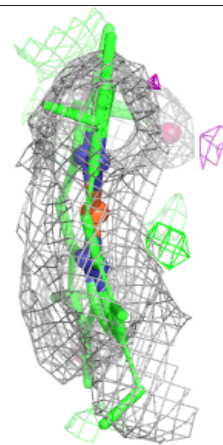
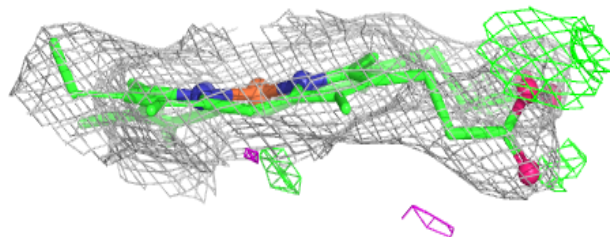
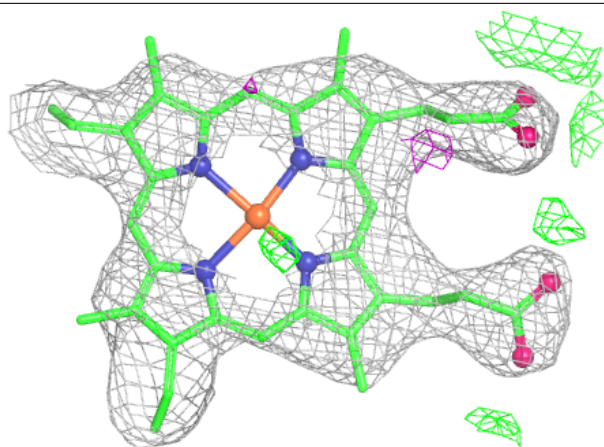
Electron density around HEC A 604:

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



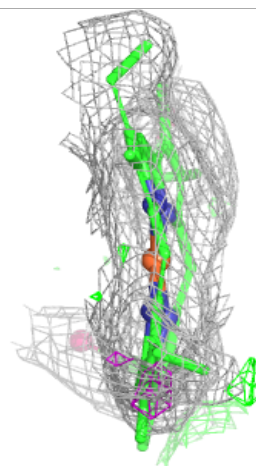
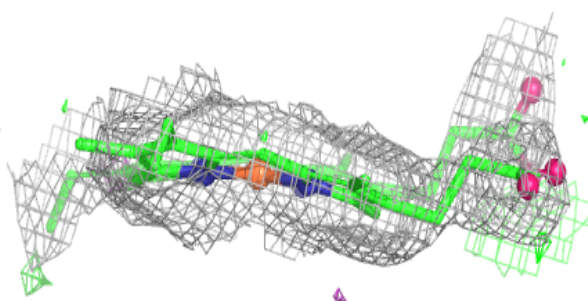
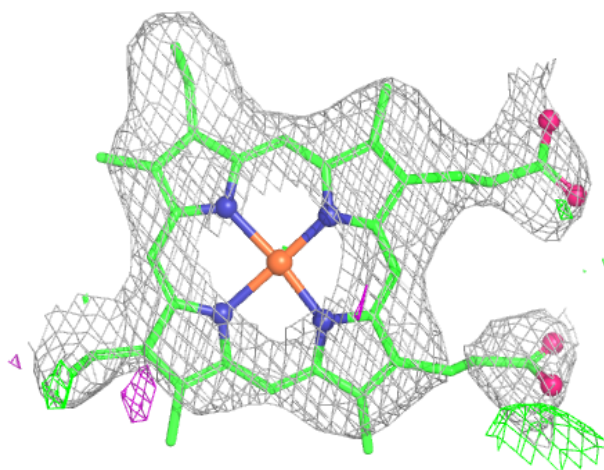
Electron density around HEC S 606:

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



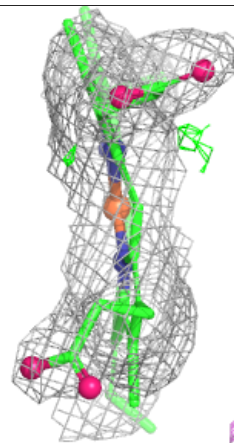
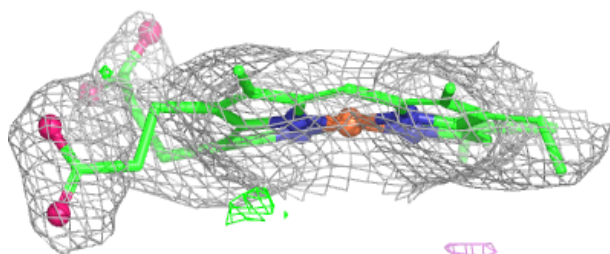
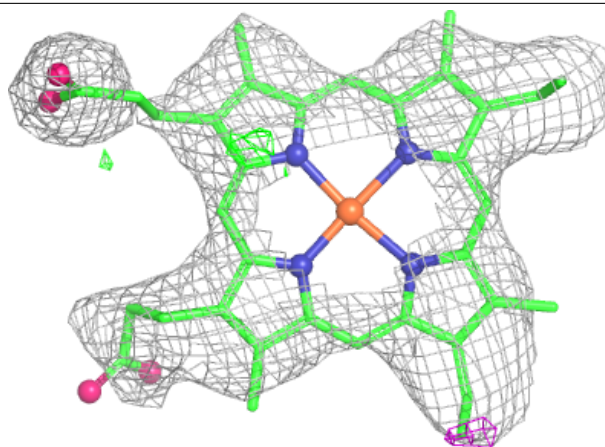
Electron density around HEC A 606:

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



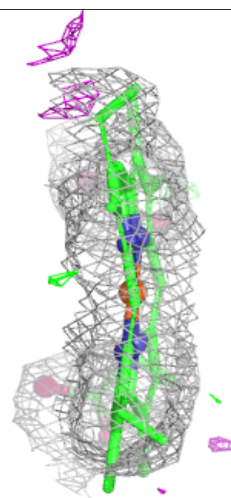
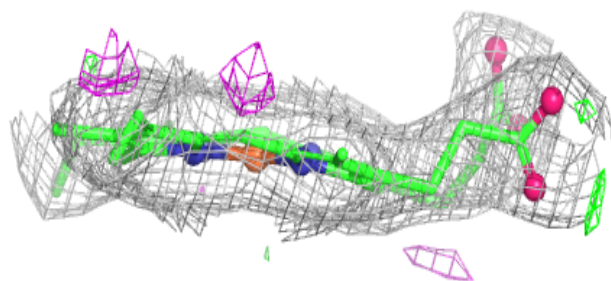
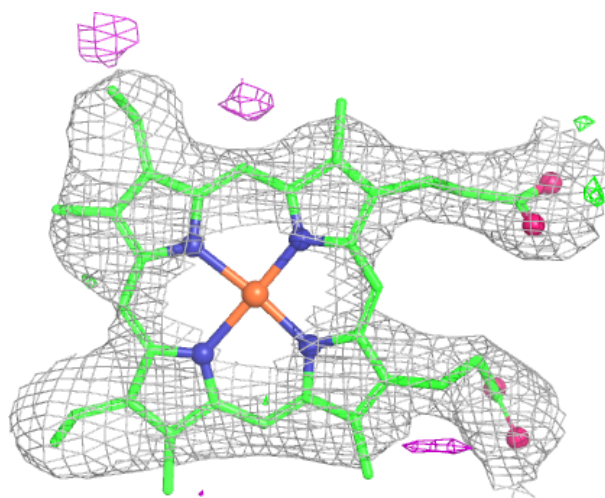
Electron density around HEC T 602:

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



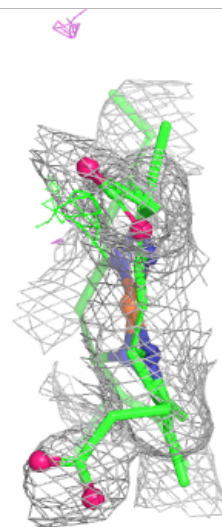
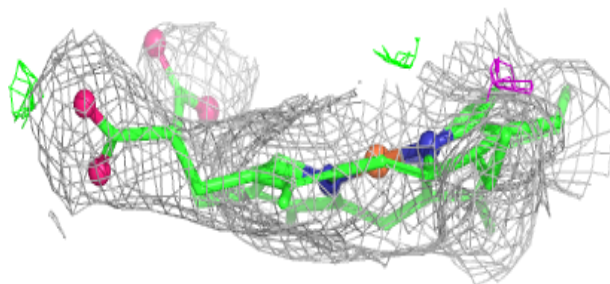
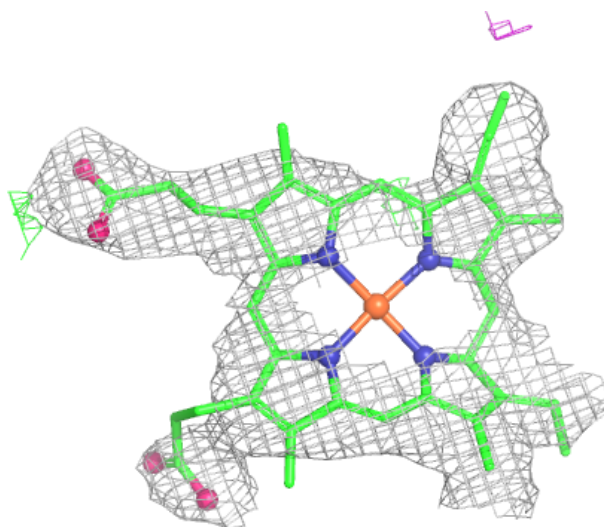
Electron density around HEC T 607:

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



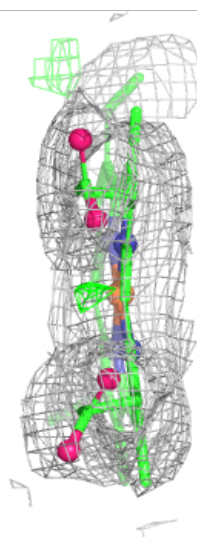
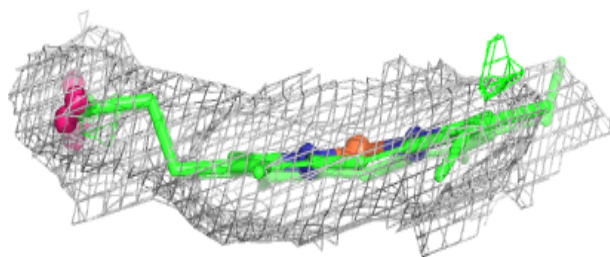
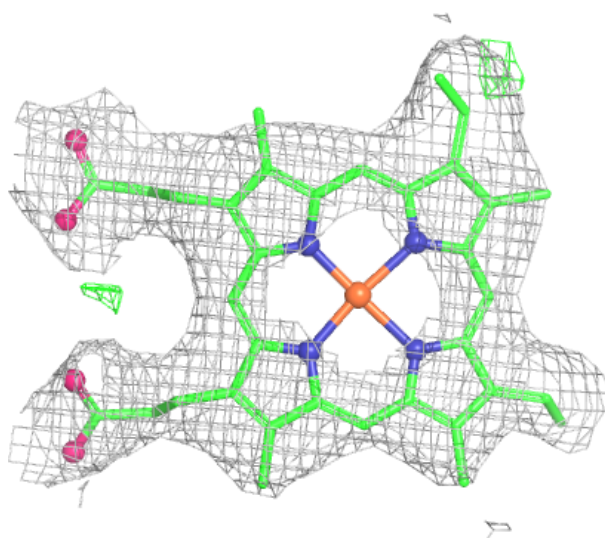
Electron density around HEC U 603:

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



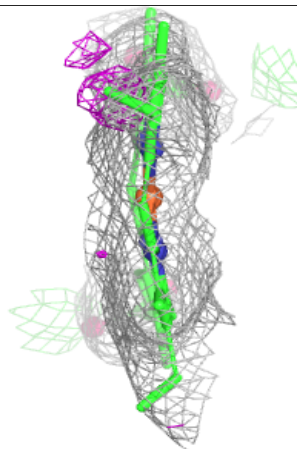
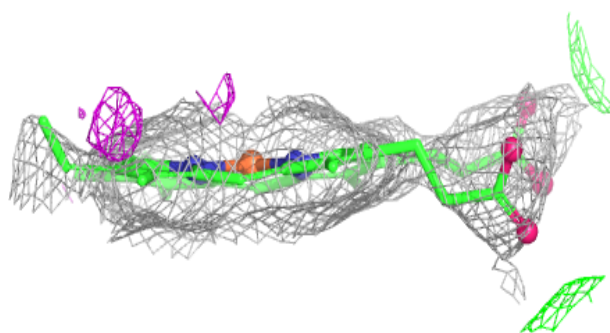
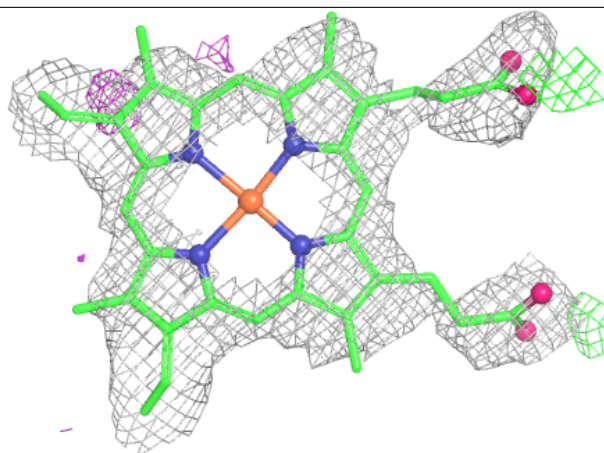
Electron density around HEC U 600:

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



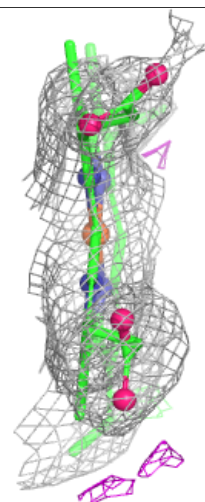
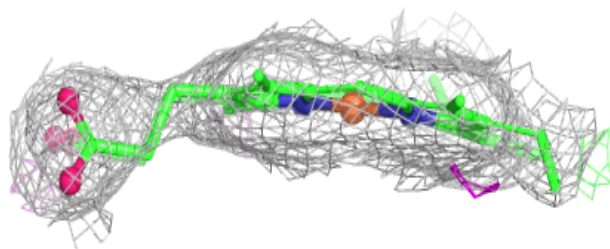
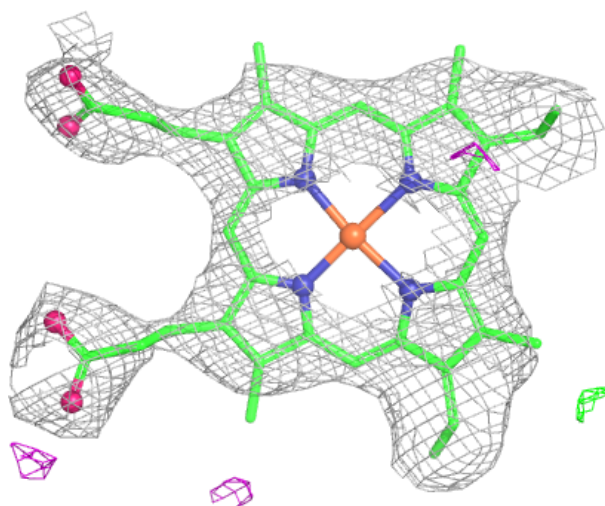
Electron density around HEC U 605:

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



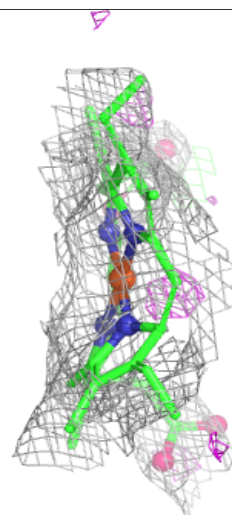
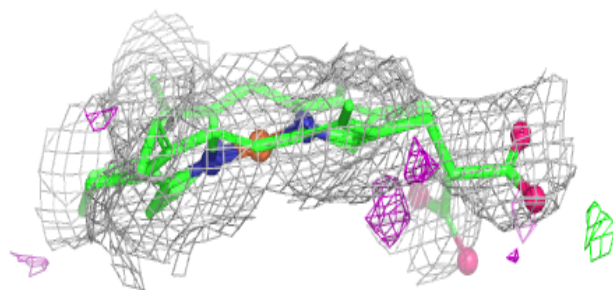
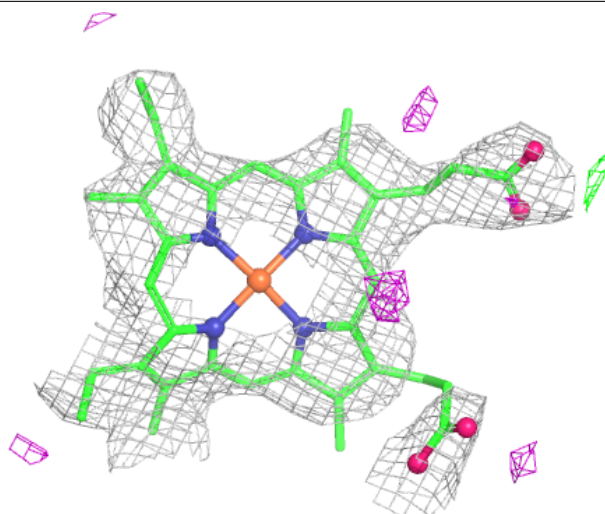
Electron density around HEC D 600:

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



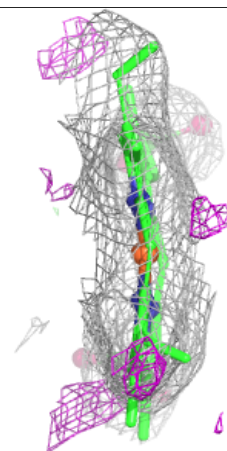
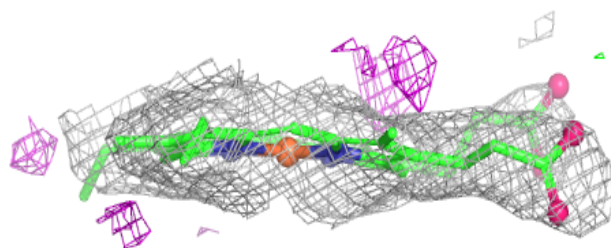
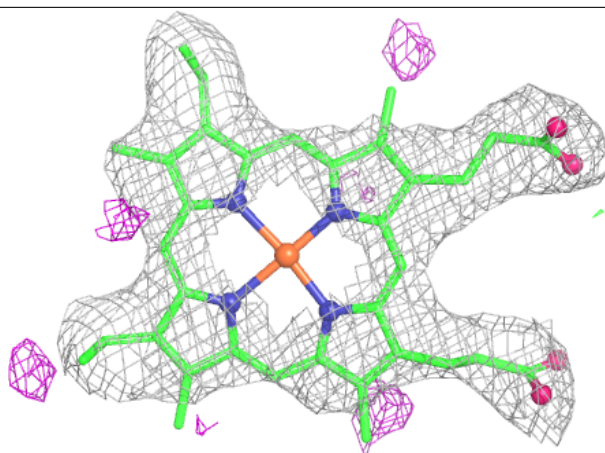
Electron density around HEC E 603:

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



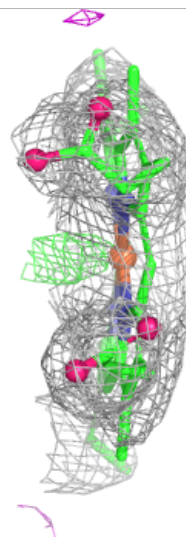
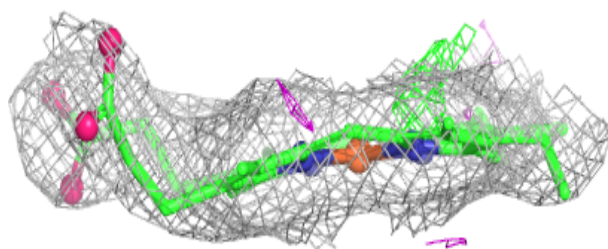
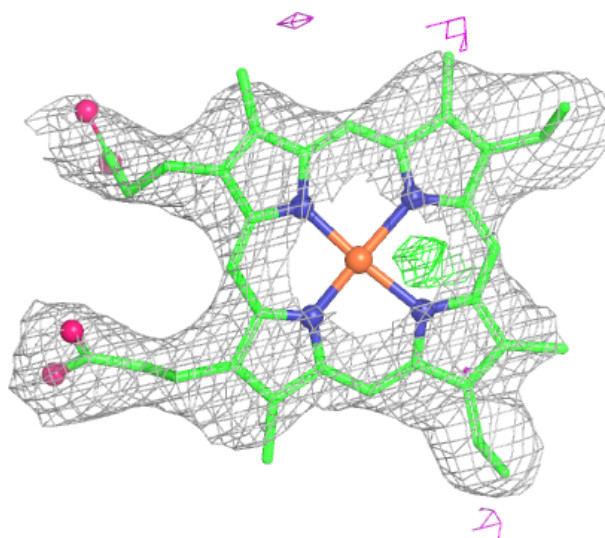
Electron density around HEC V 605:

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



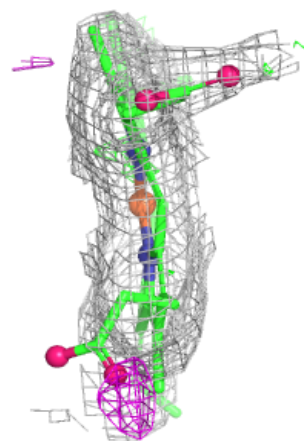
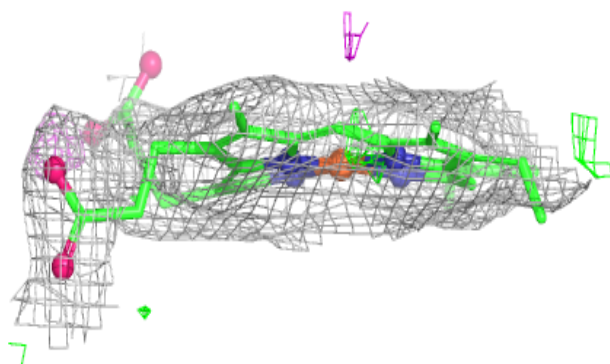
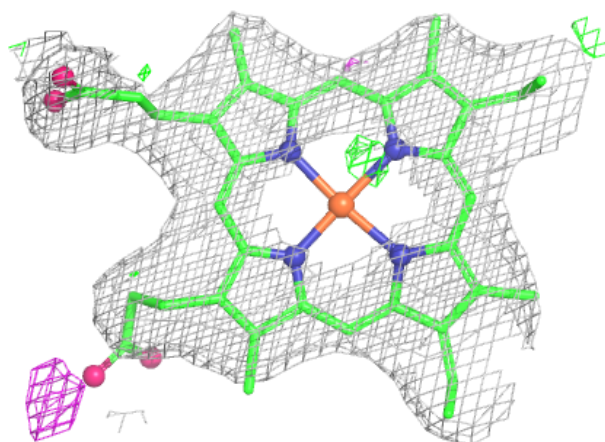
Electron density around HEC S 607:

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



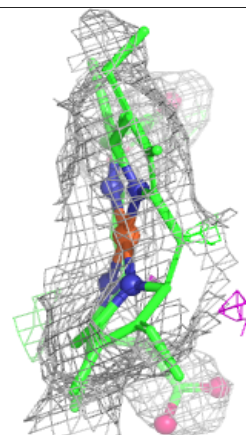
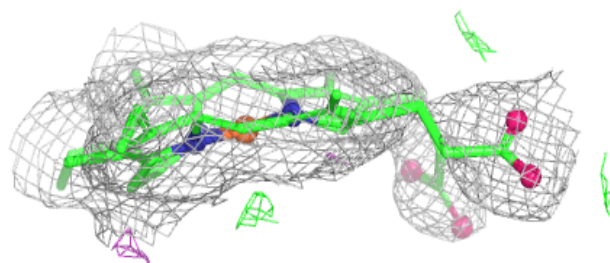
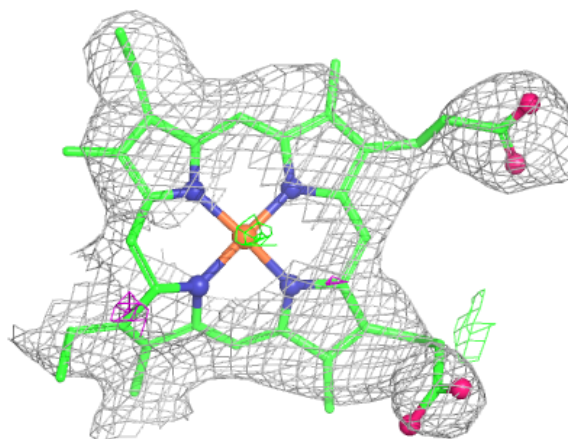
Electron density around HEC E 602:

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



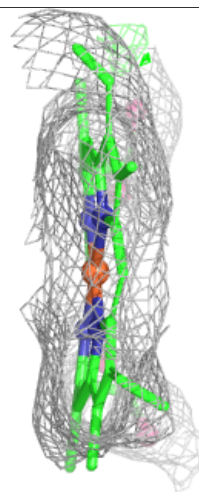
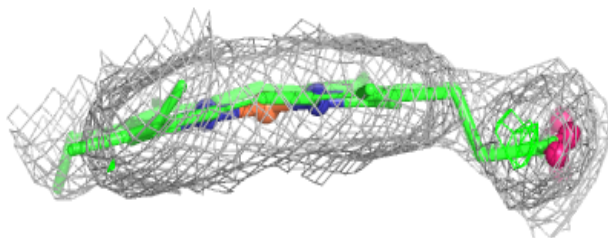
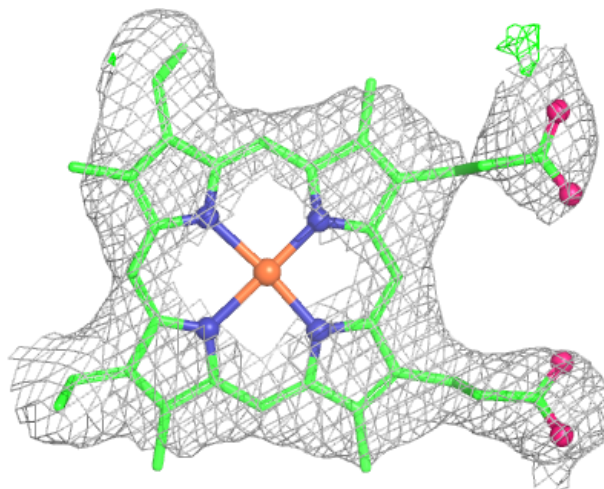
Electron density around HEC T 603:

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



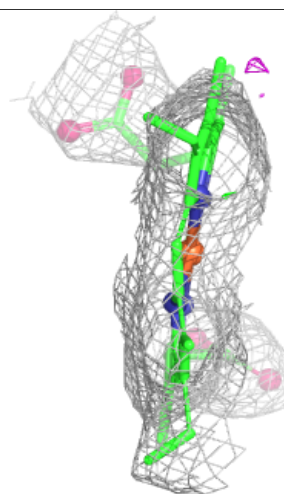
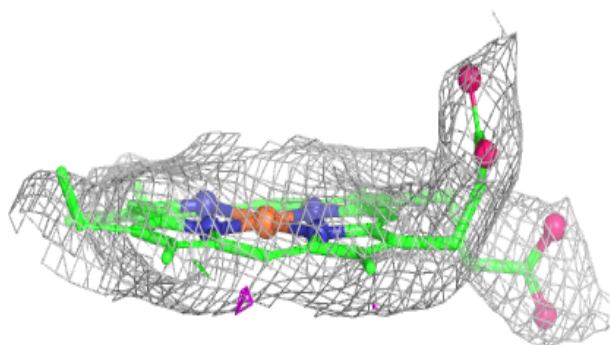
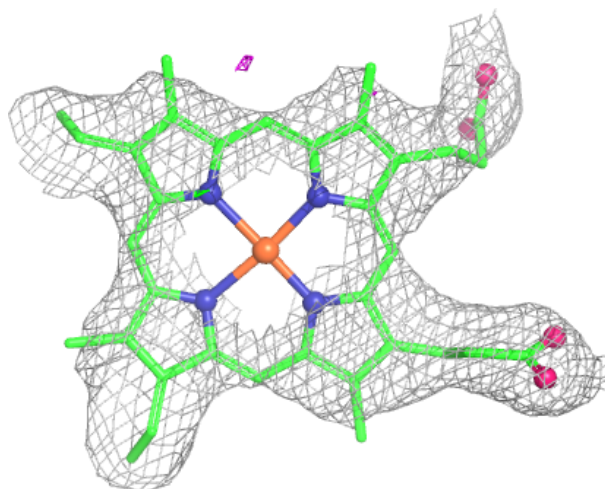
Electron density around HEC T 600:

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



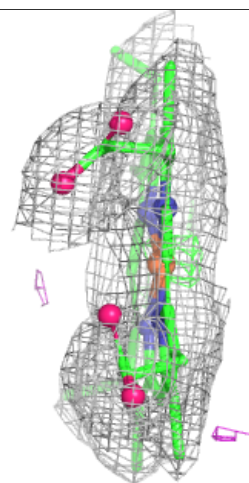
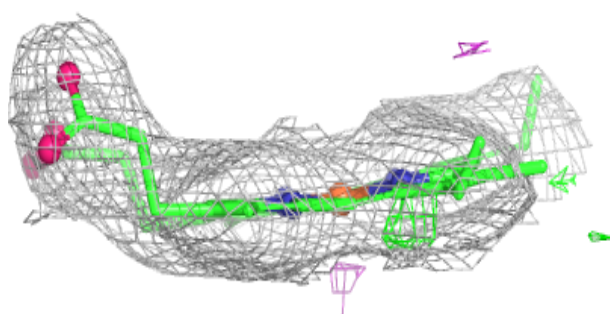
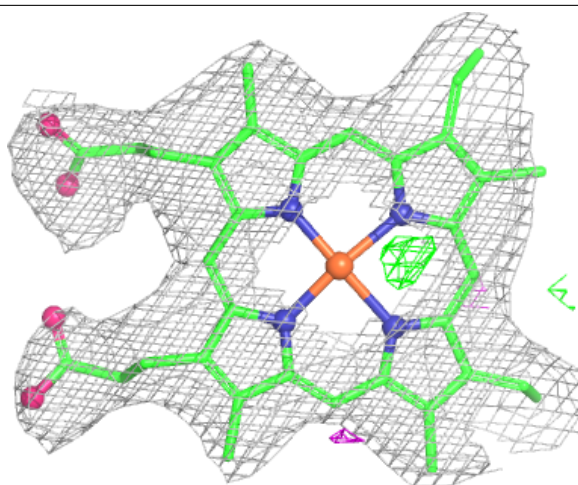
Electron density around HEC T 601:

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



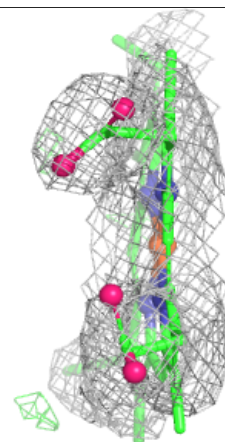
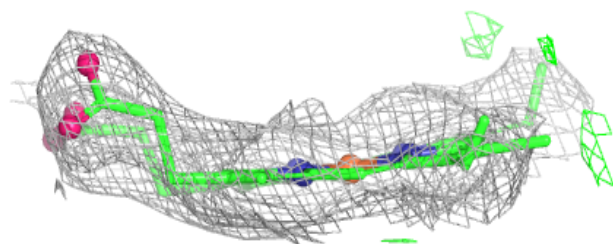
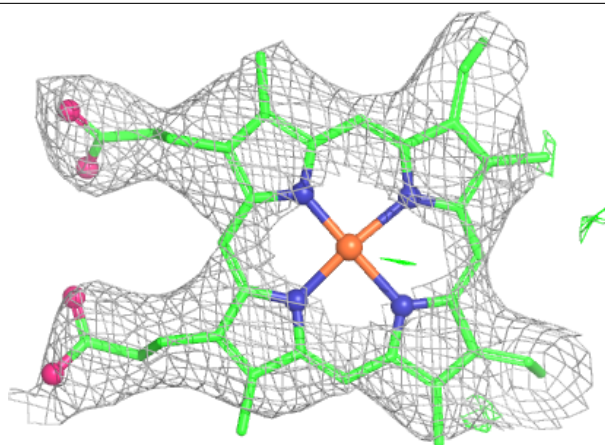
Electron density around HEC E 604:

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

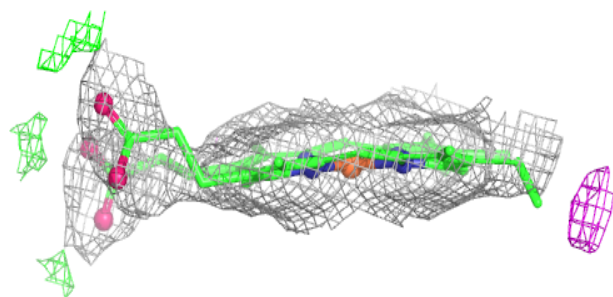
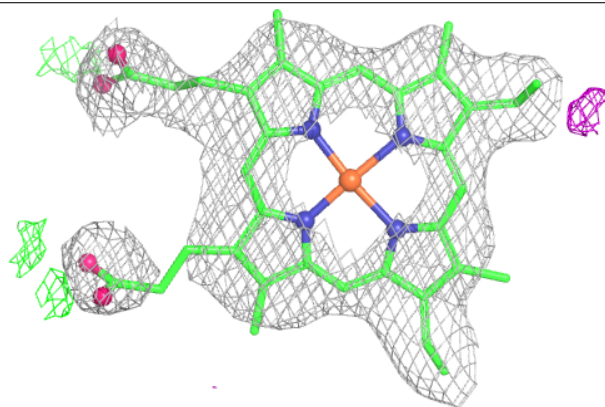


Electron density around HEC T 604:

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

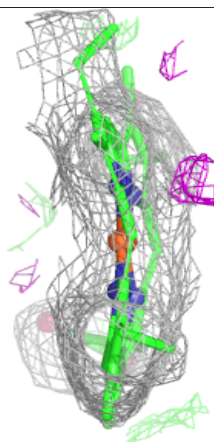
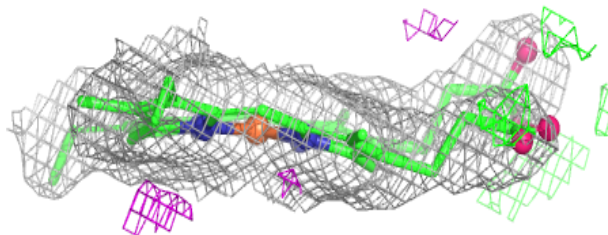
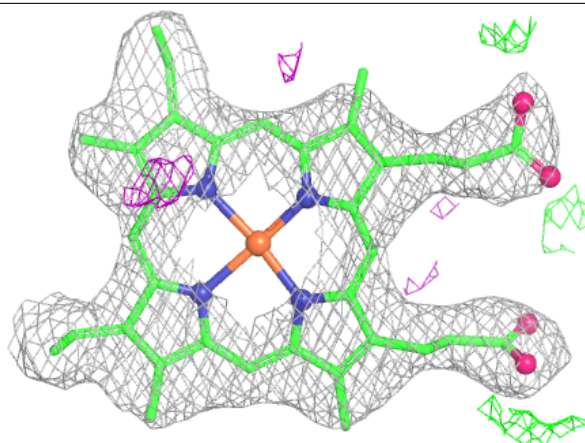
**Electron density around HEC T 605:**

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



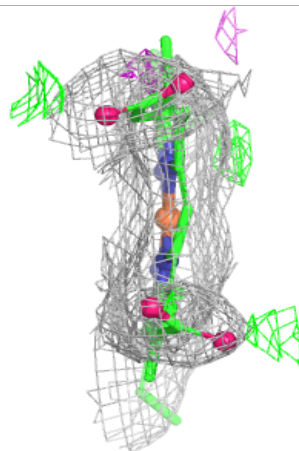
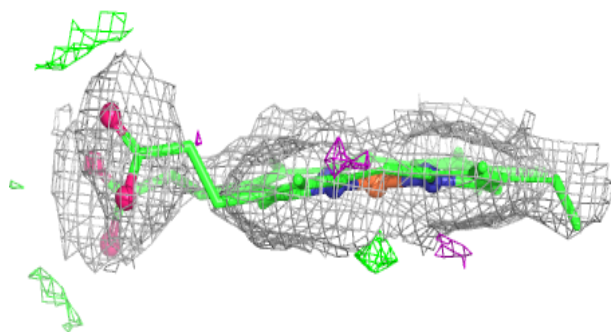
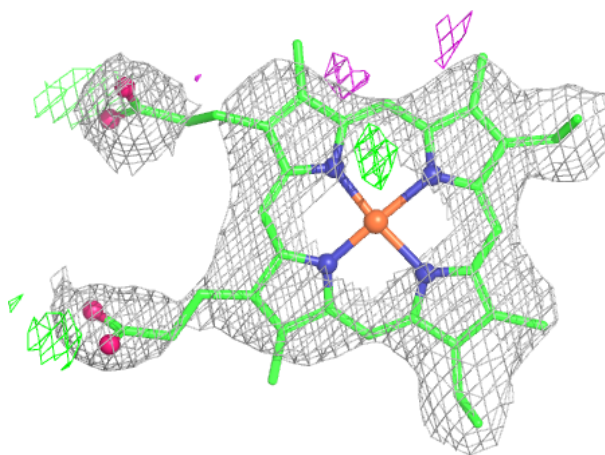
Electron density around HEC T 606:

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



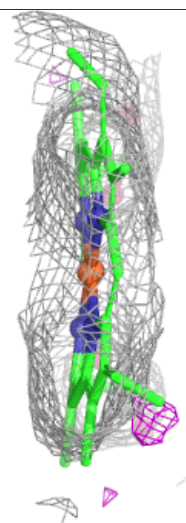
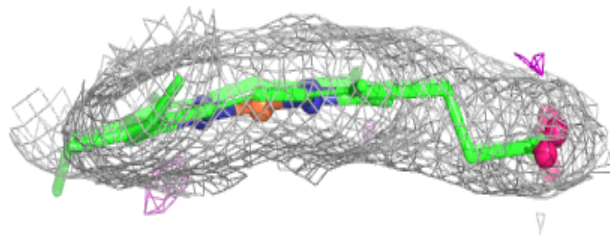
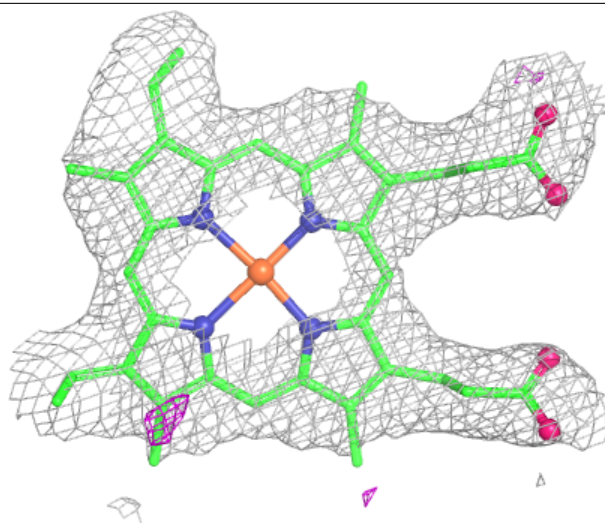
Electron density around HEC A 605:

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



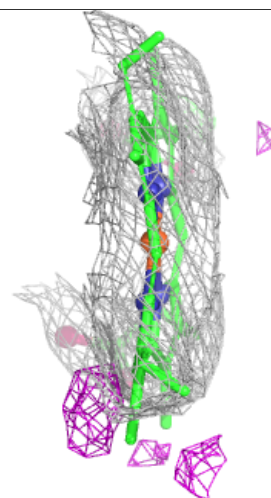
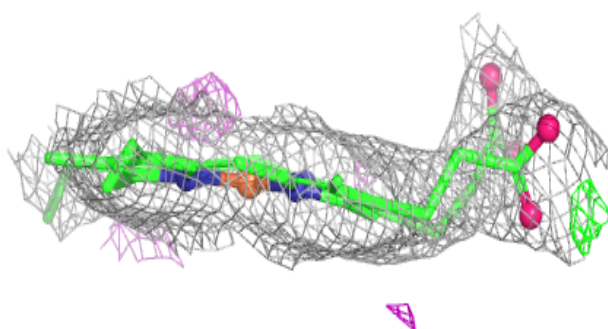
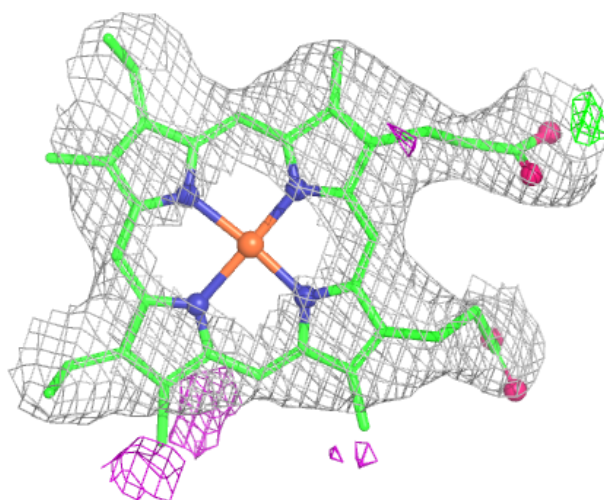
Electron density around HEC A 600:

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



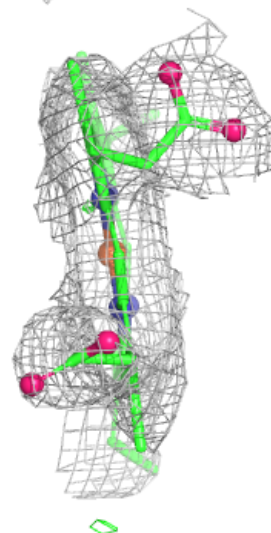
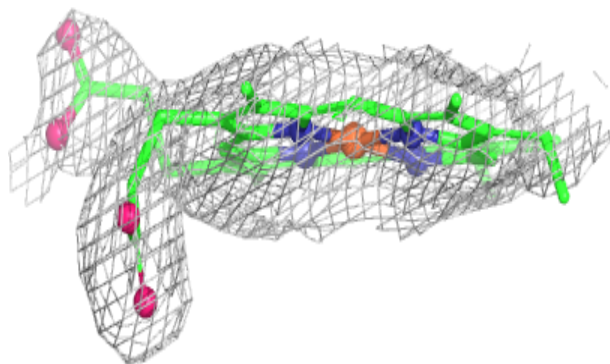
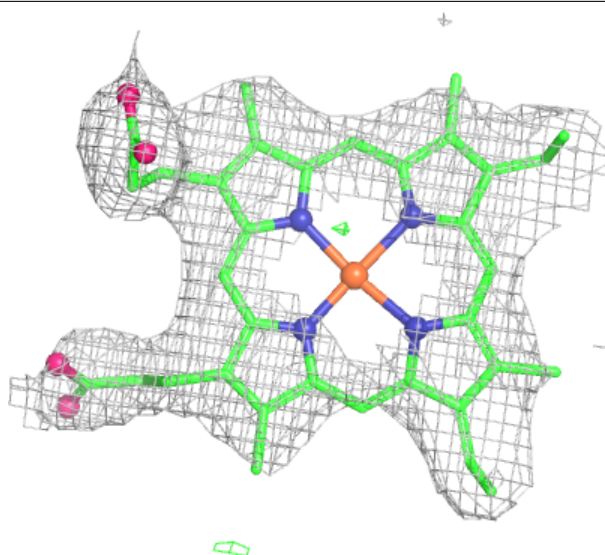
Electron density around HEC E 607:

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



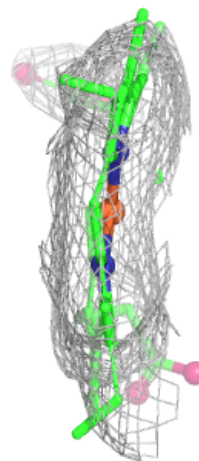
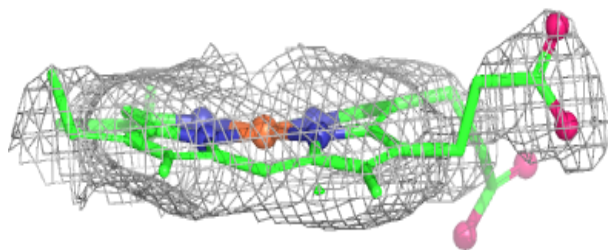
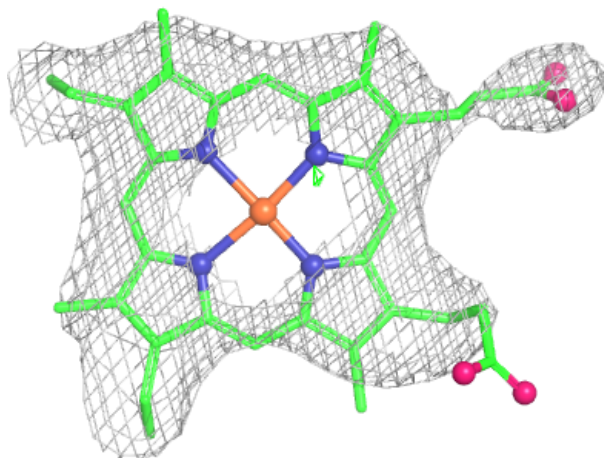
Electron density around HEC U 601:

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



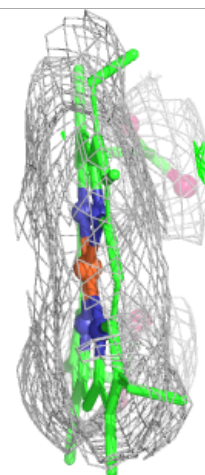
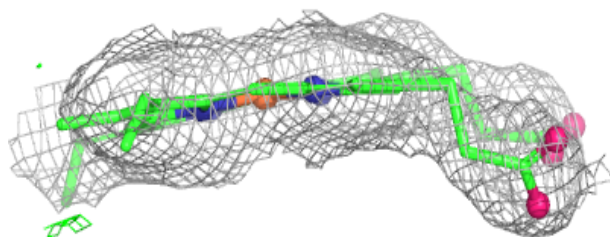
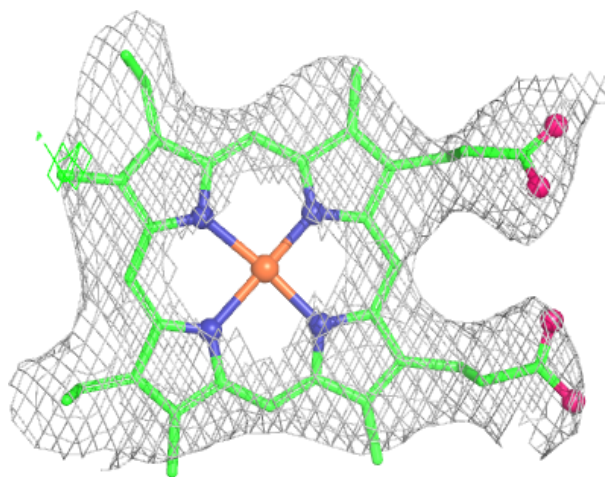
Electron density around HEC U 602:

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



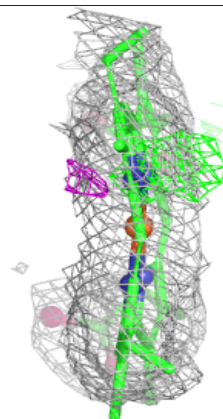
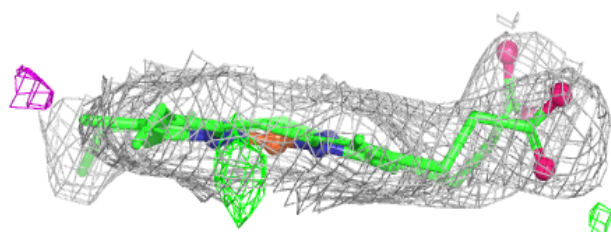
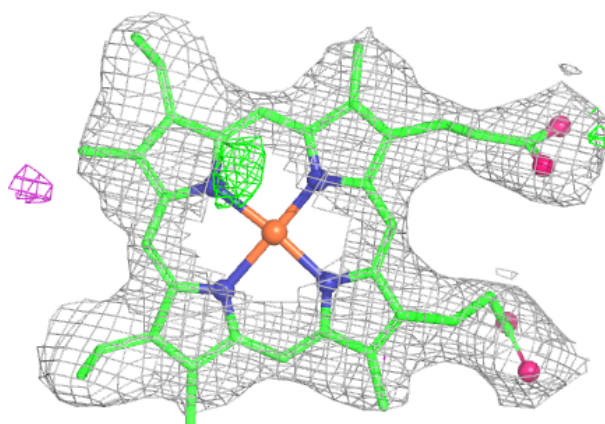
Electron density around HEC U 604:

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



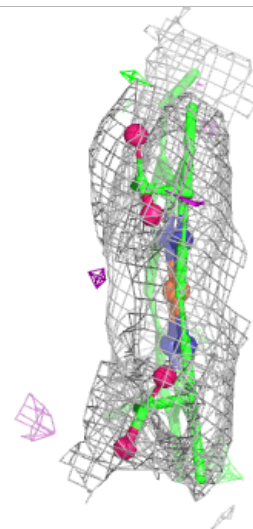
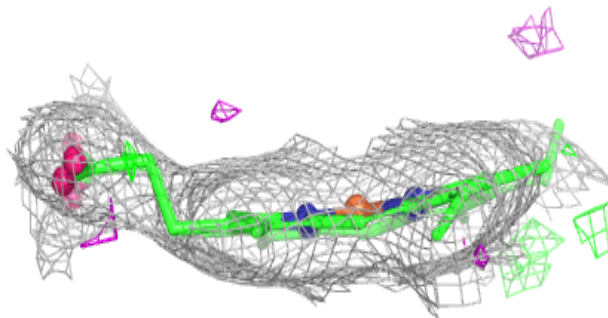
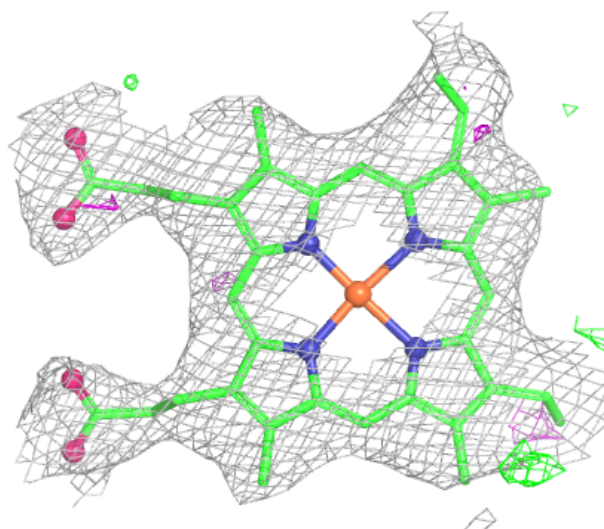
Electron density around HEC A 607:

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



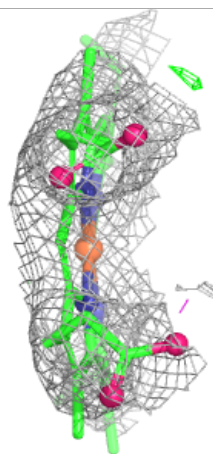
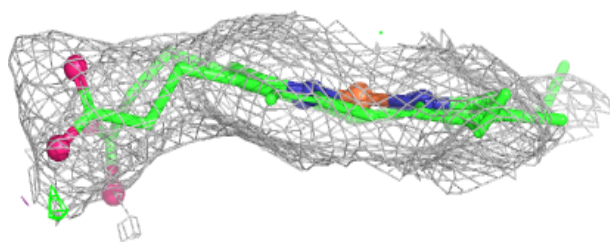
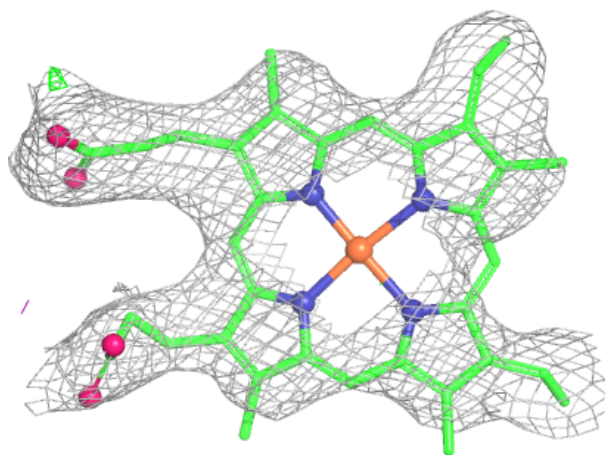
Electron density around HEC F 600:

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



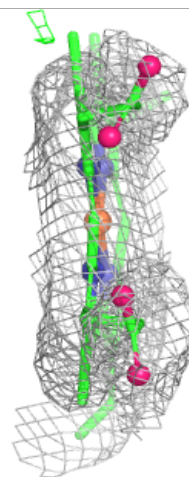
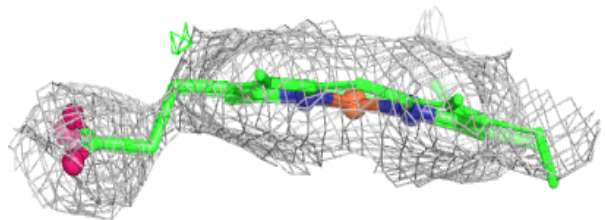
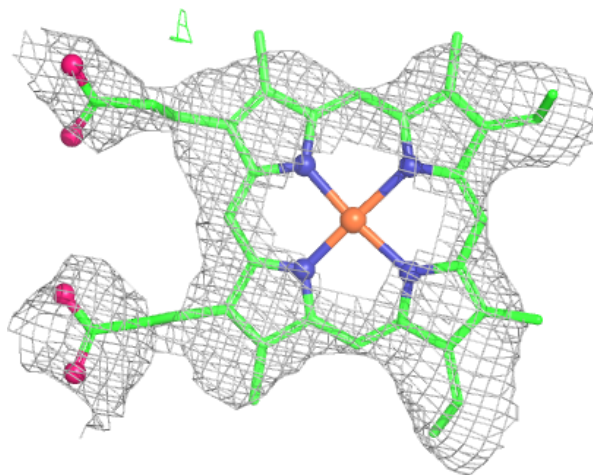
Electron density around HEC U 607:

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



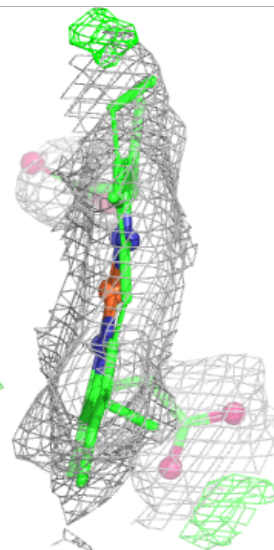
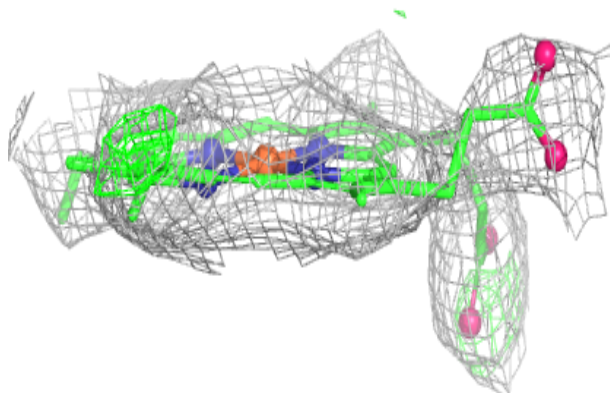
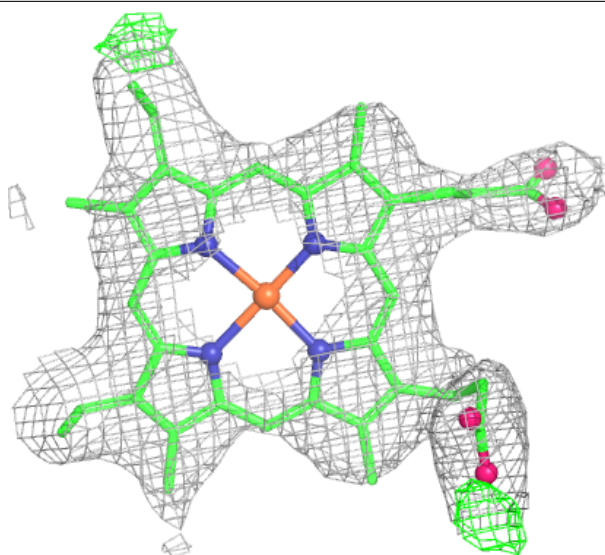
Electron density around HEC V 600:

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



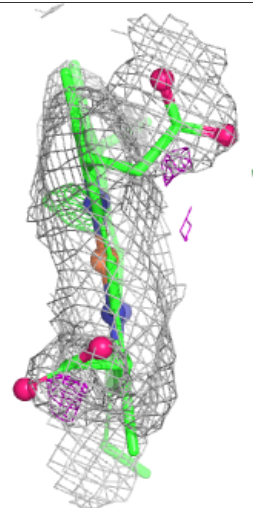
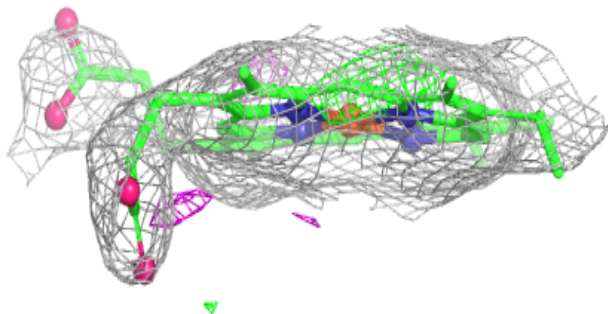
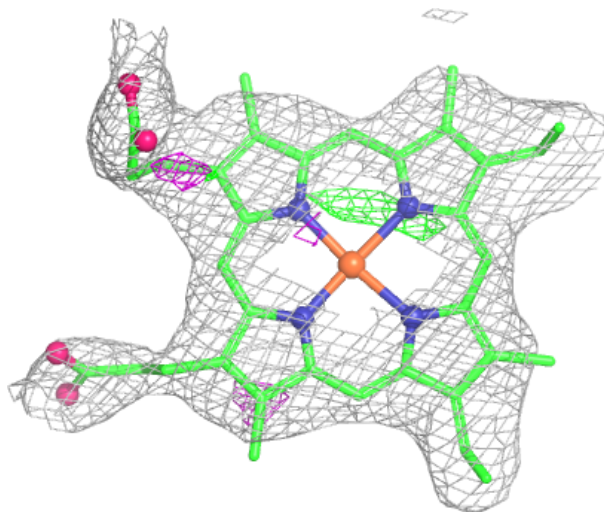
Electron density around HEC V 601:

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



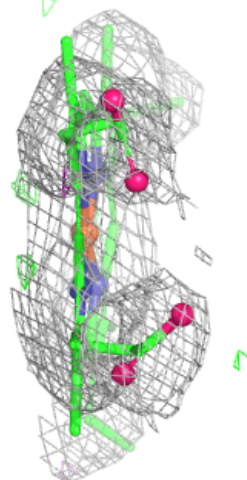
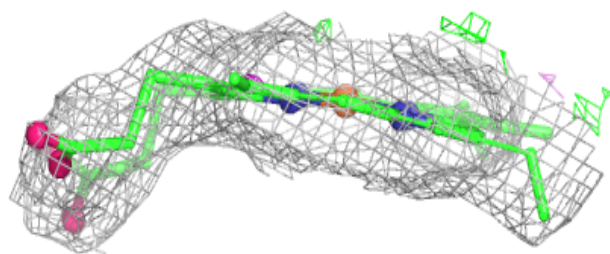
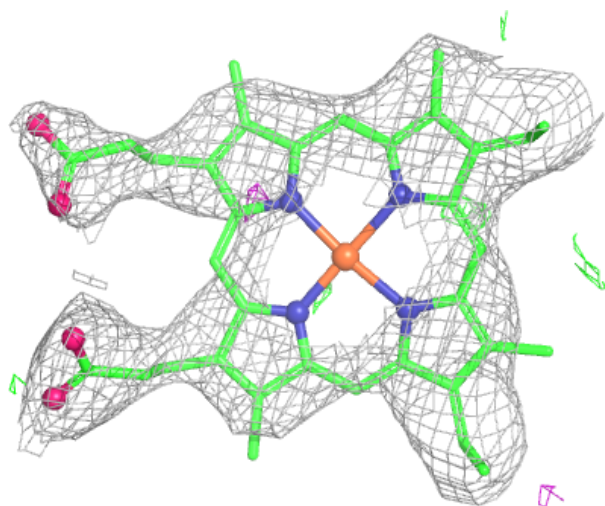
Electron density around HEC F 601:

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



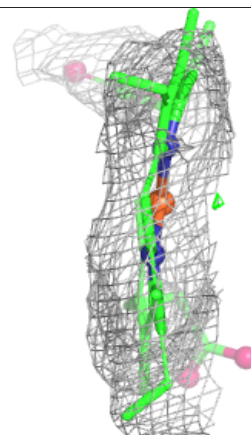
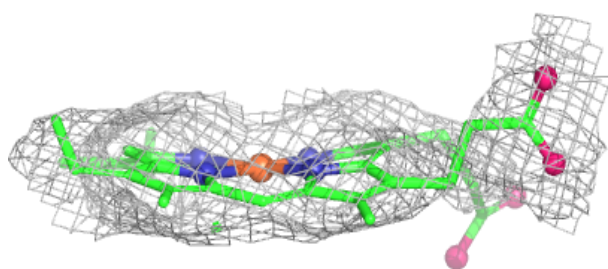
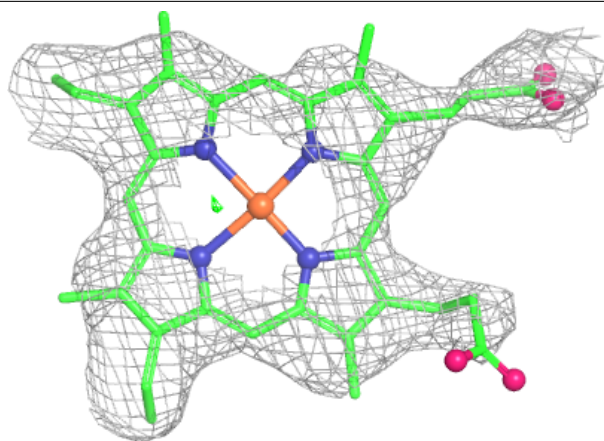
Electron density around HEC V 604:

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



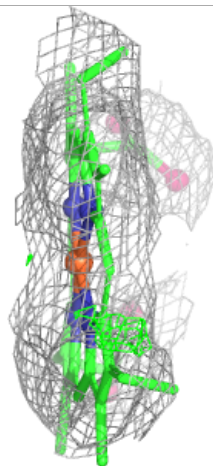
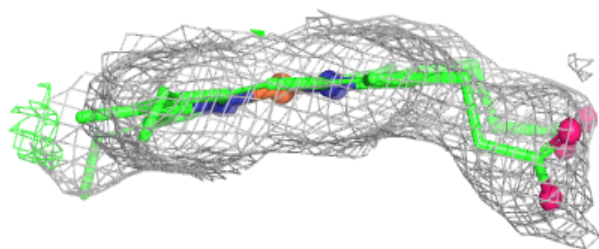
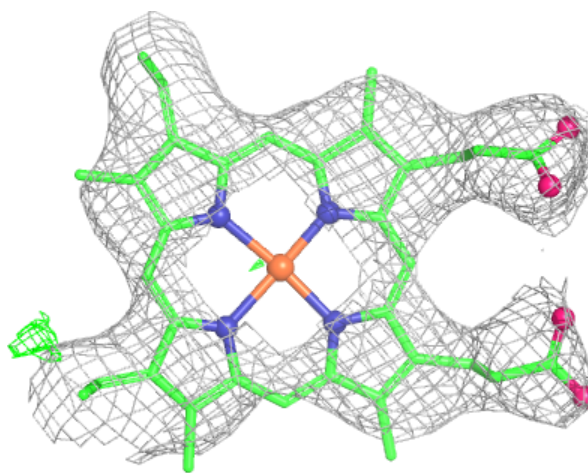
Electron density around HEC F 602:

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



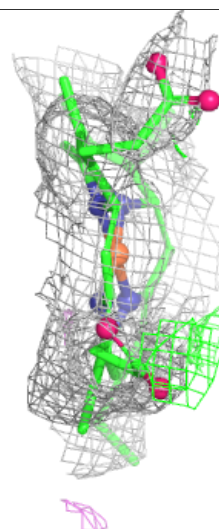
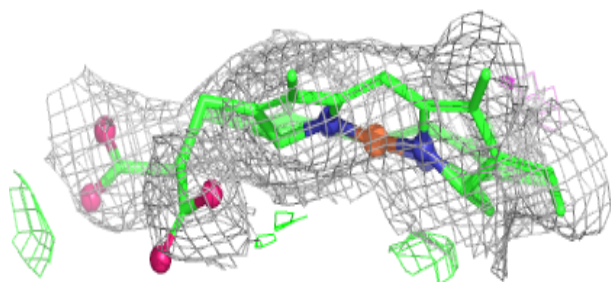
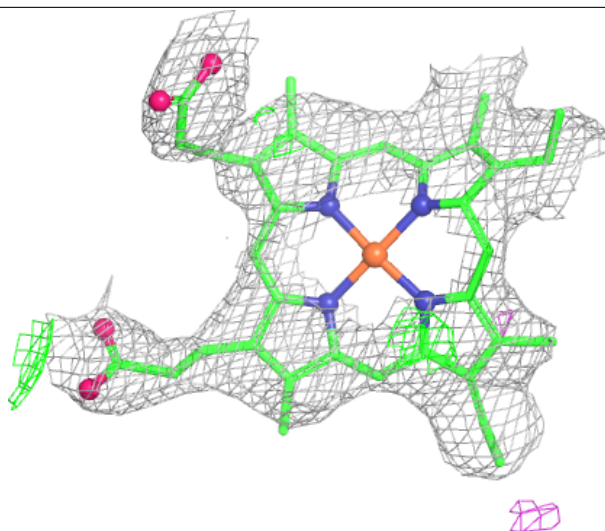
Electron density around HEC F 604:

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



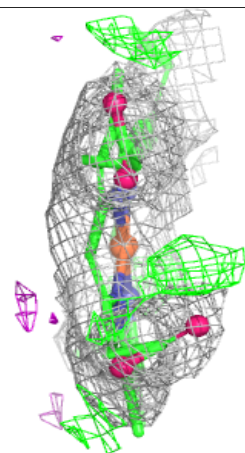
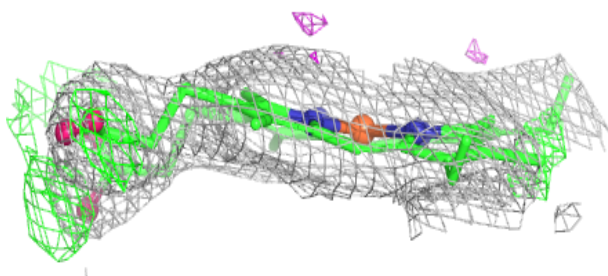
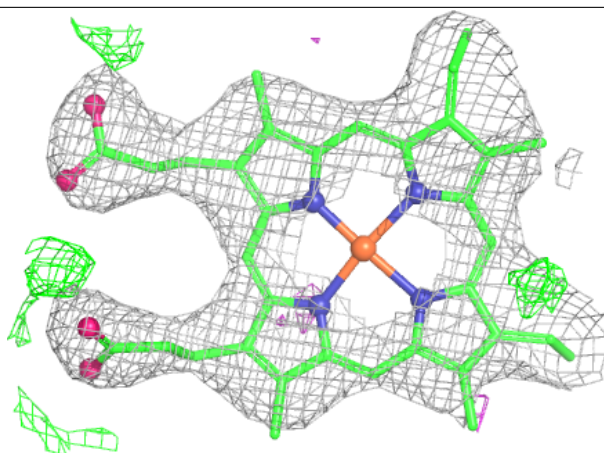
Electron density around HEC A 603:

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



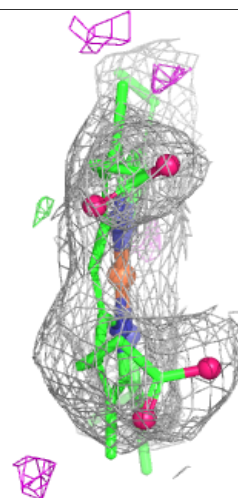
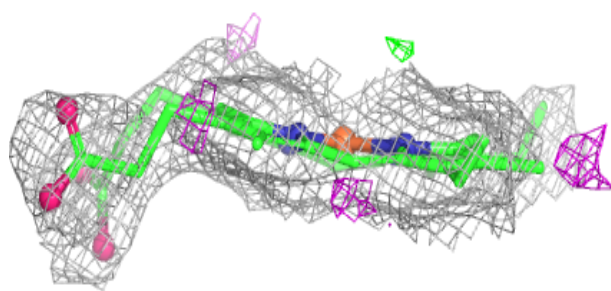
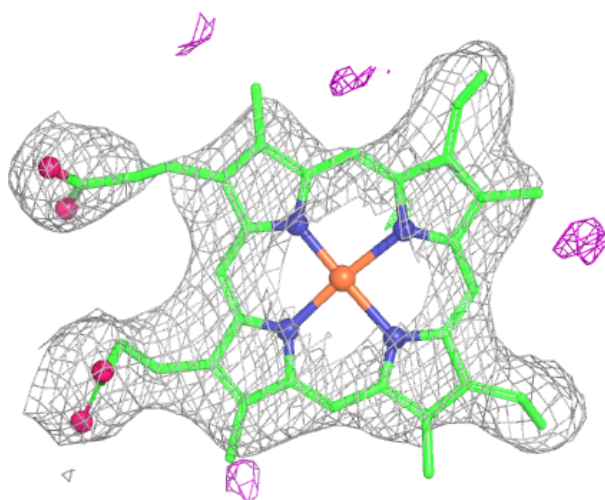
Electron density around HEC F 606:

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



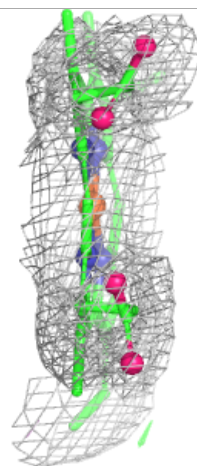
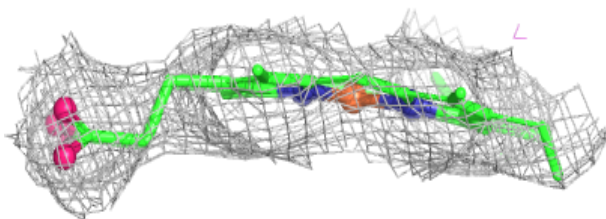
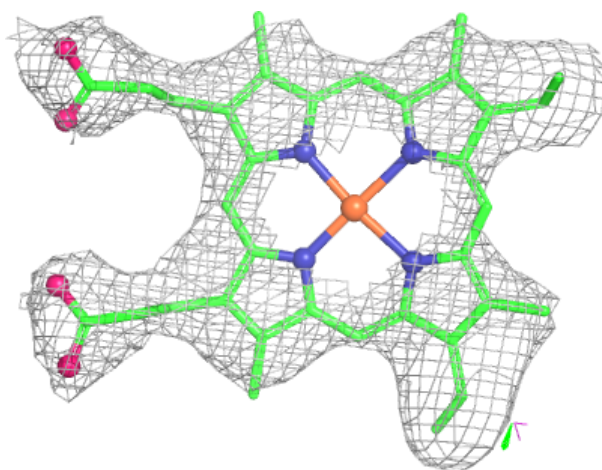
Electron density around HEC F 607:

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



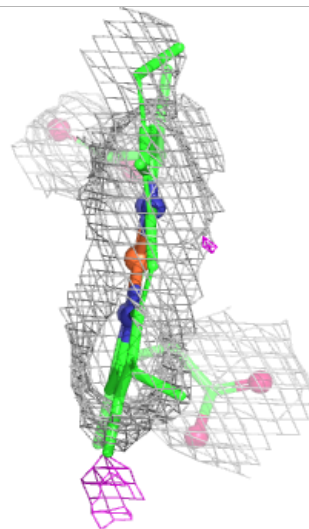
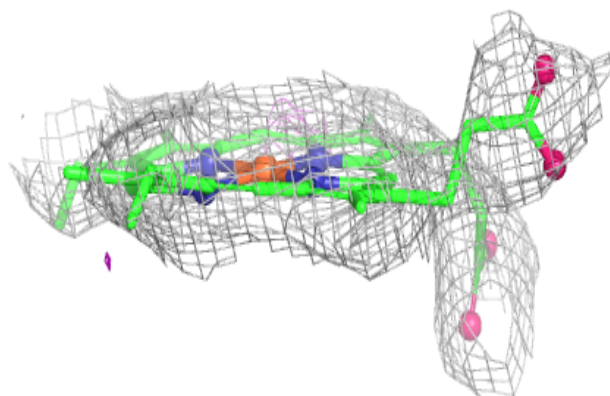
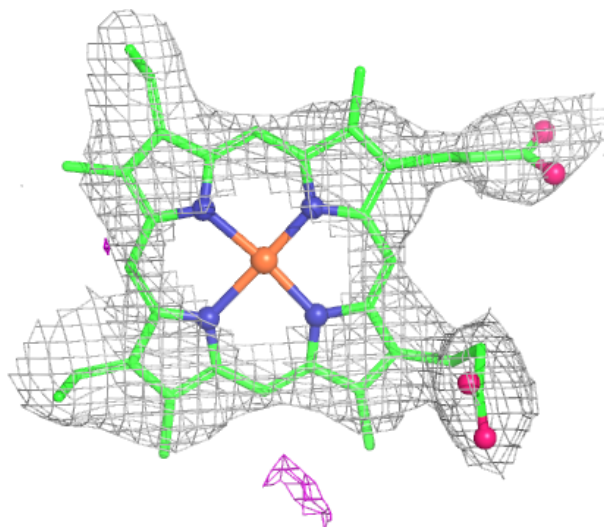
Electron density around HEC W 600:

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



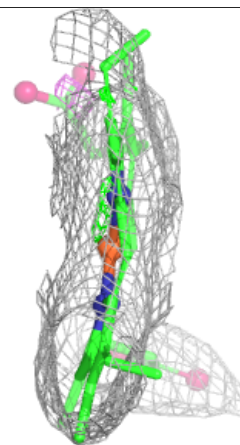
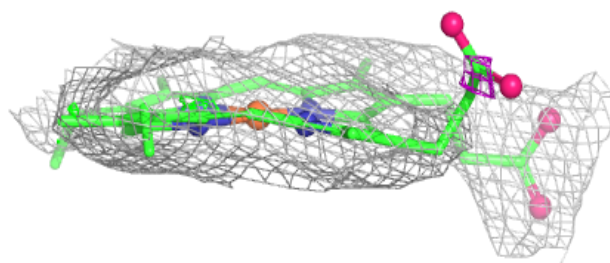
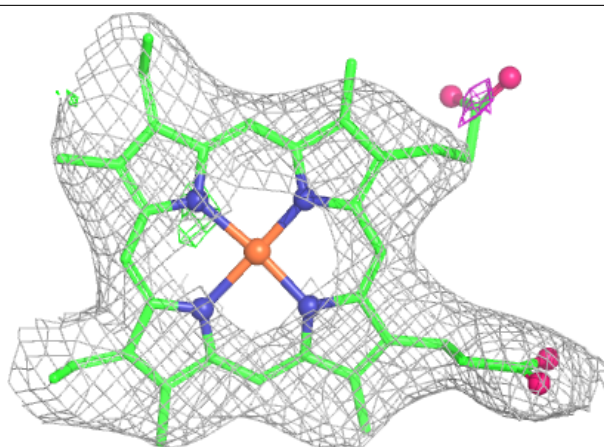
Electron density around HEC W 601:

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



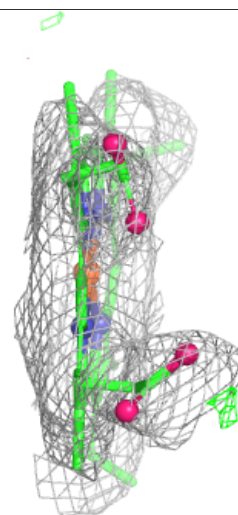
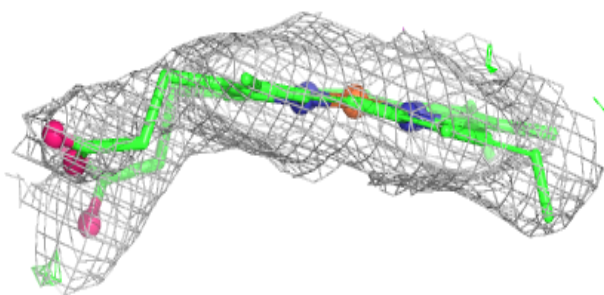
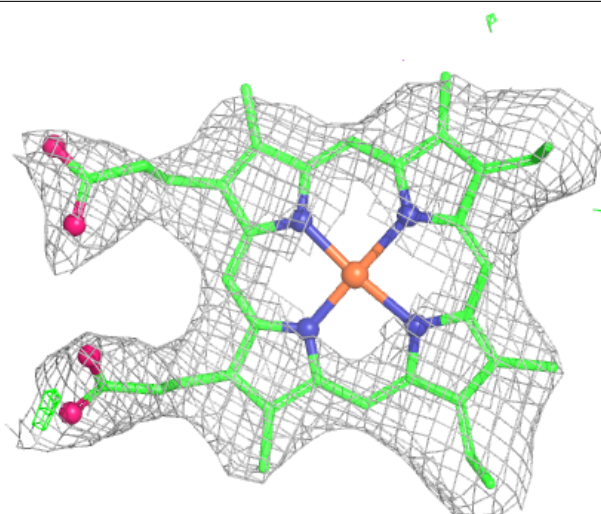
Electron density around HEC W 602:

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



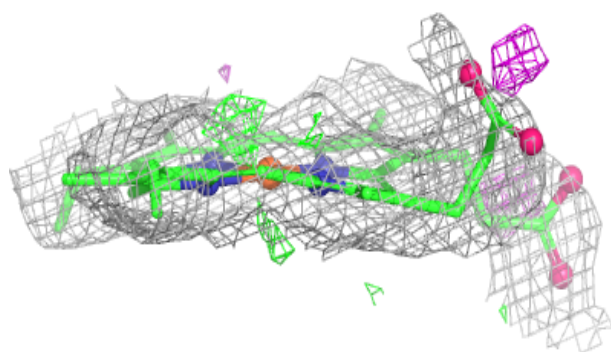
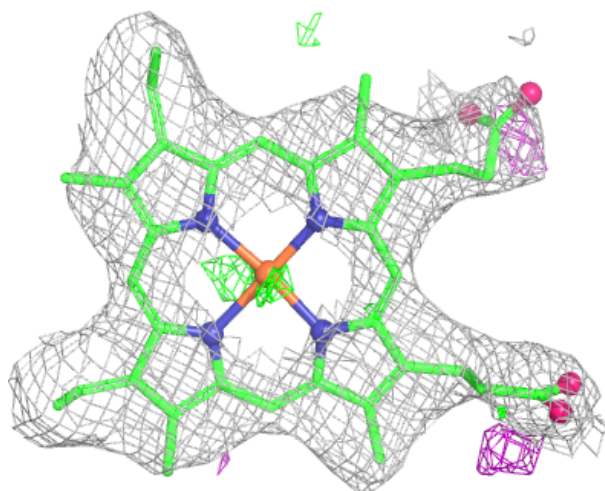
Electron density around HEC W 604:

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



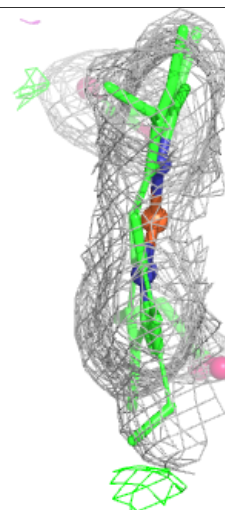
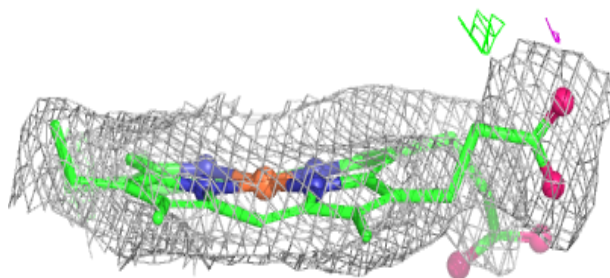
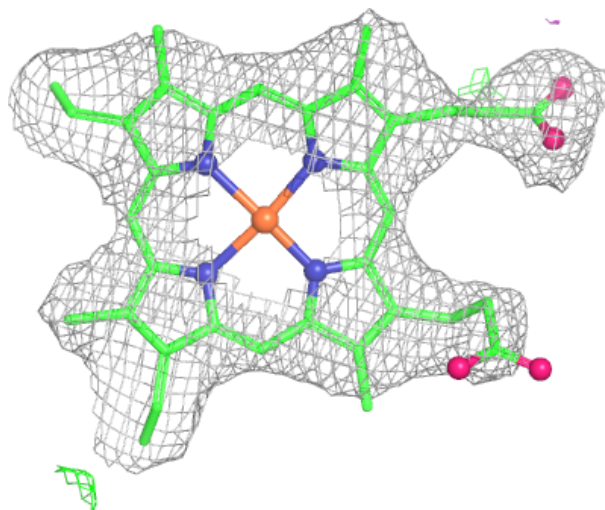
Electron density around HEC H 602:

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



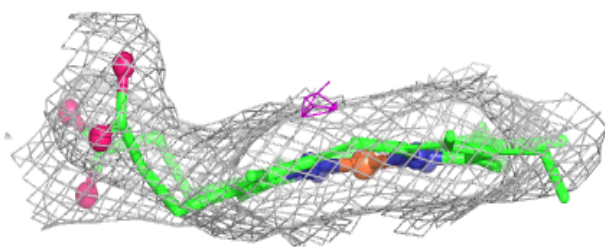
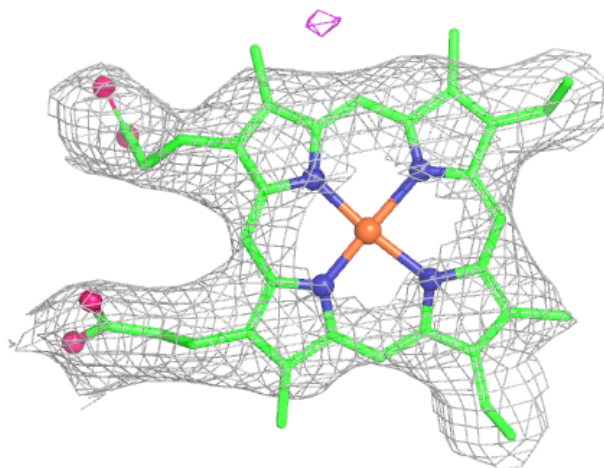
Electron density around HEC I 602:

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



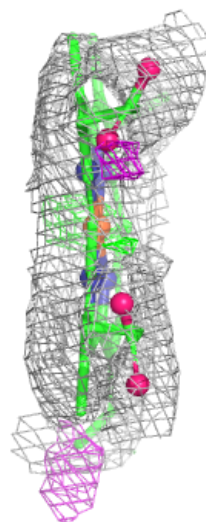
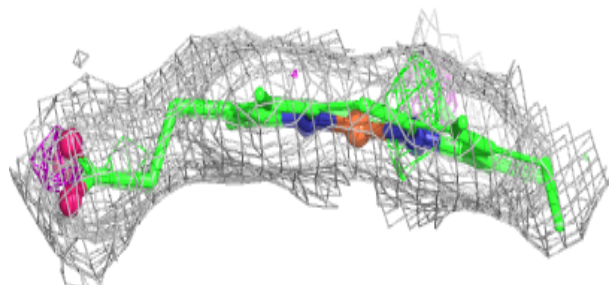
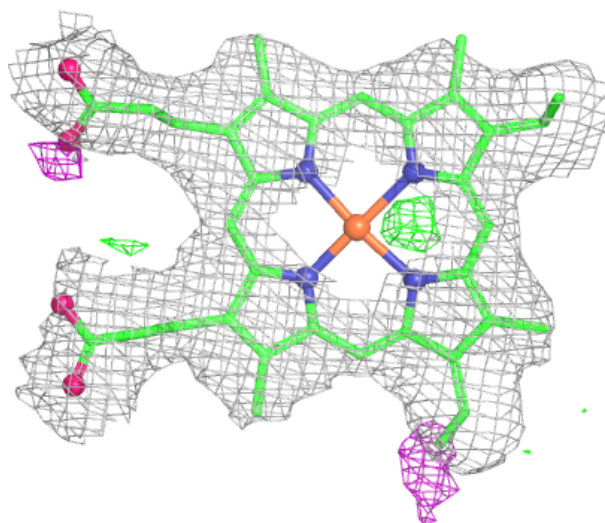
Electron density around HEC W 607:

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



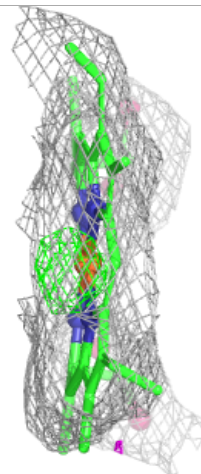
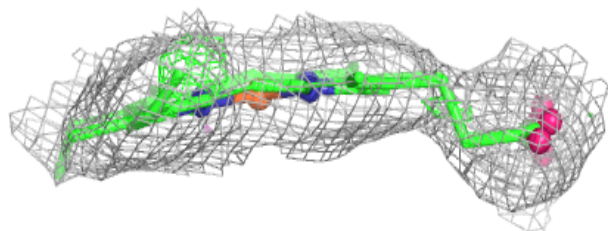
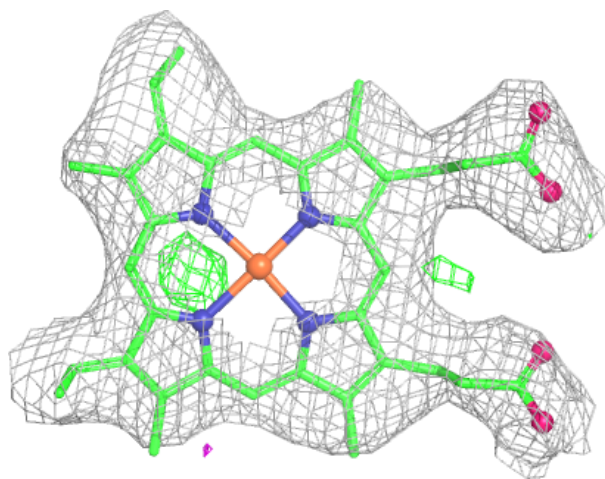
Electron density around HEC J 600:

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



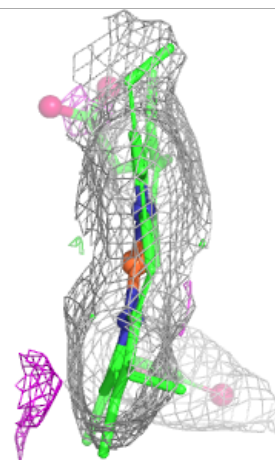
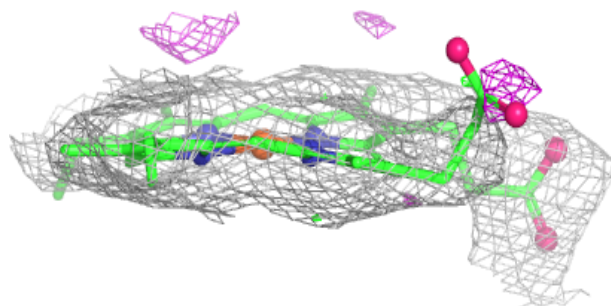
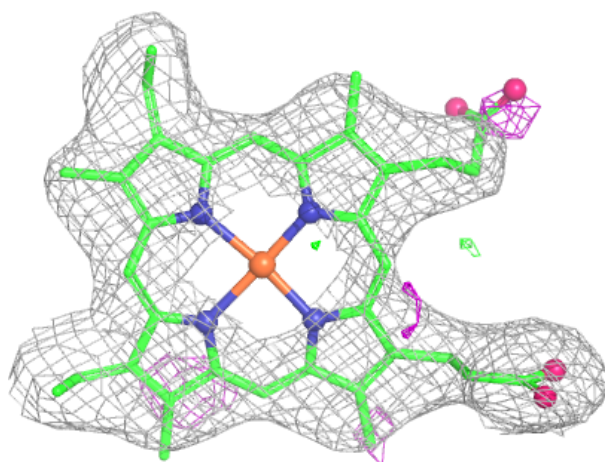
Electron density around HEC X 600:

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



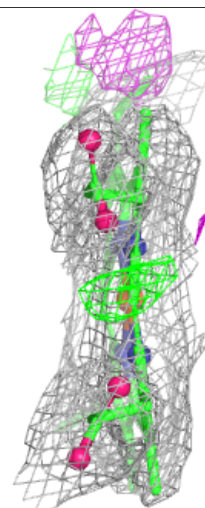
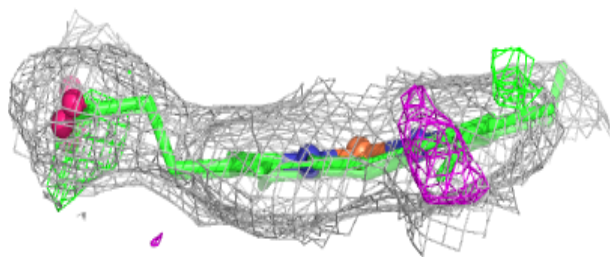
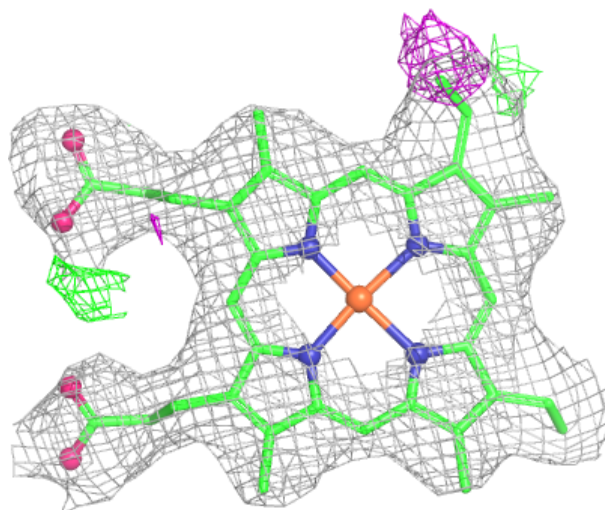
Electron density around HEC J 602:

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



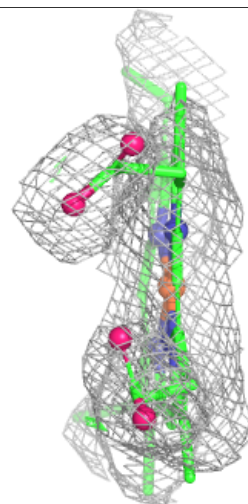
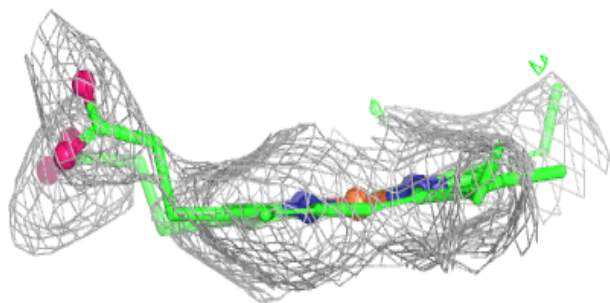
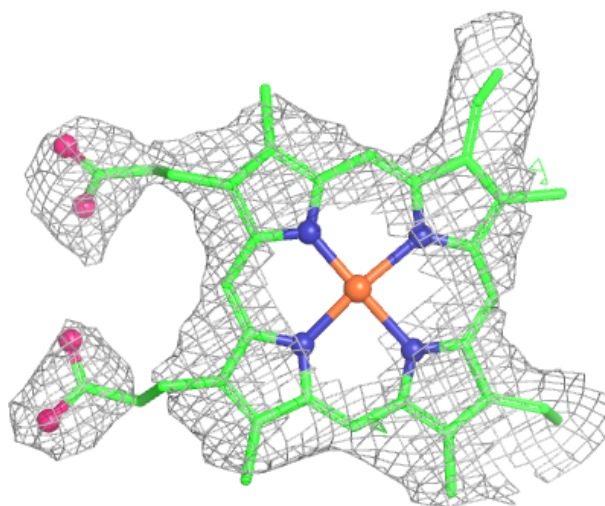
Electron density around HEC K 600:

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



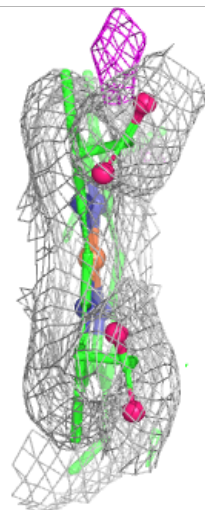
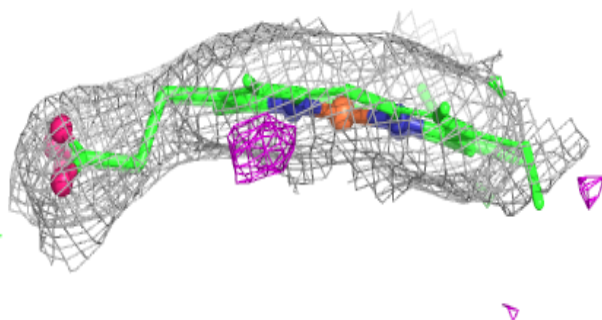
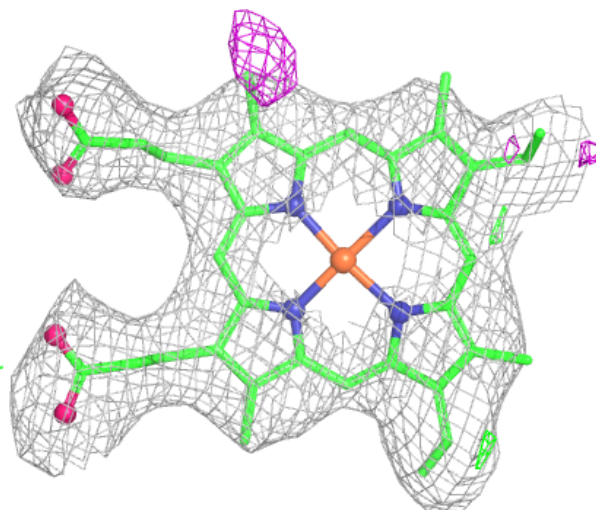
Electron density around HEC X 604:

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



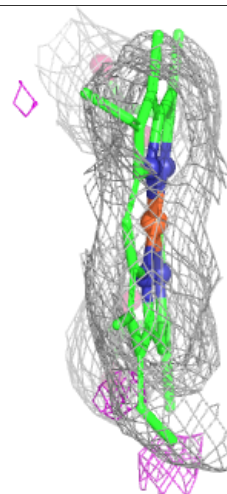
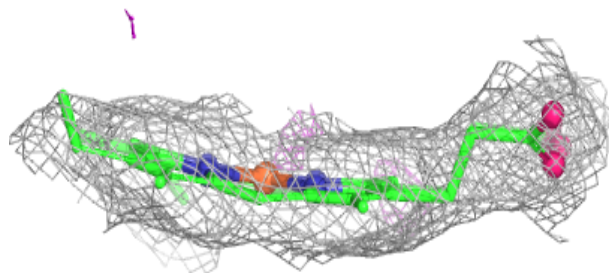
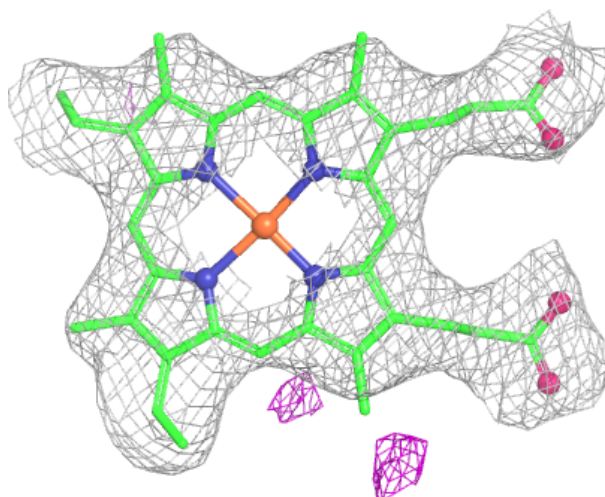
Electron density around HEC L 600:

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



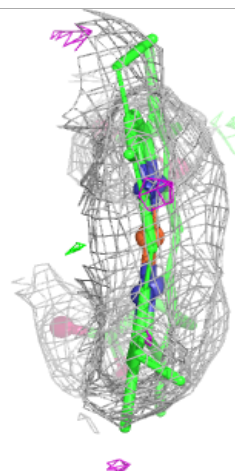
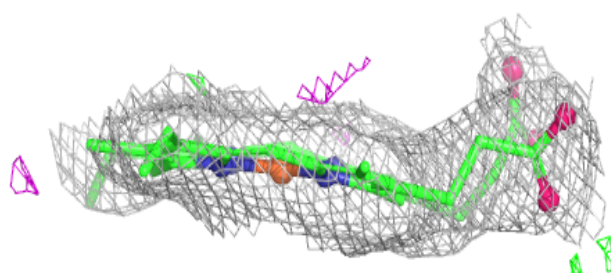
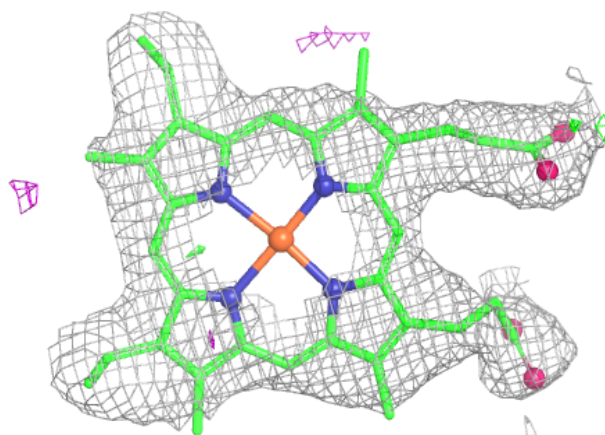
Electron density around HEC M 600:

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



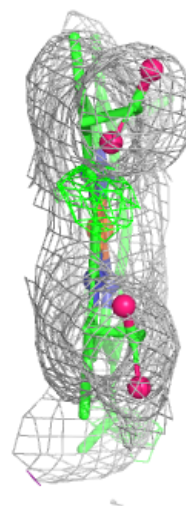
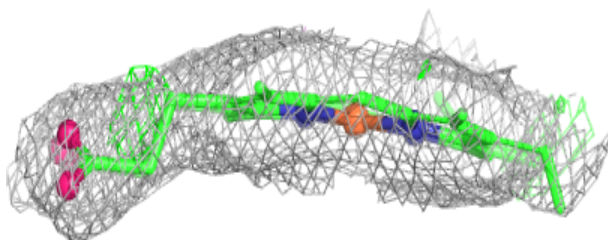
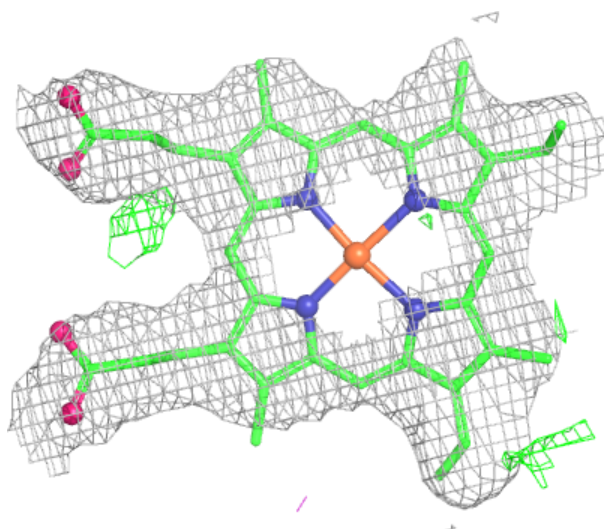
Electron density around HEC X 607:

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



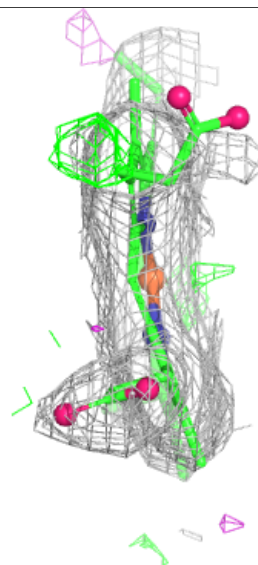
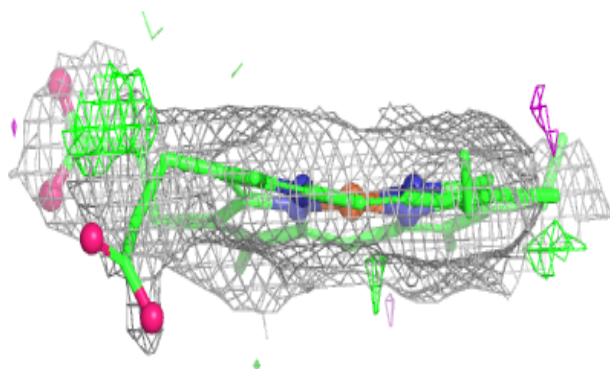
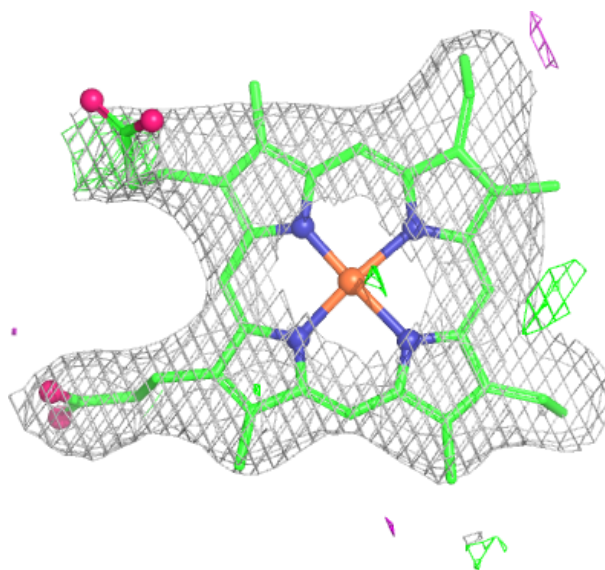
Electron density around HEC N 600:

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



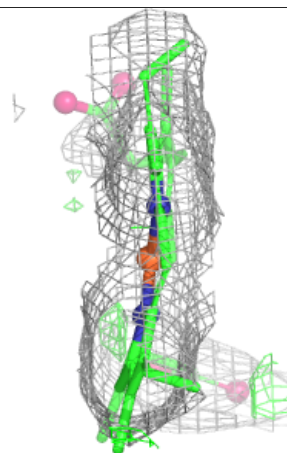
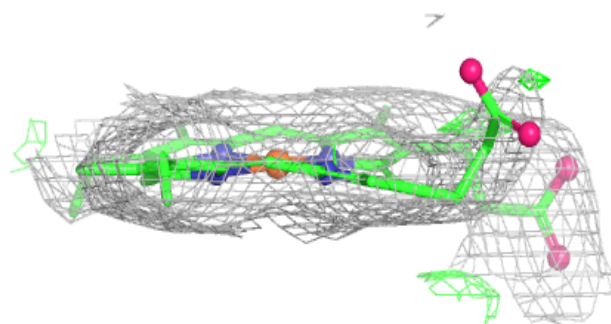
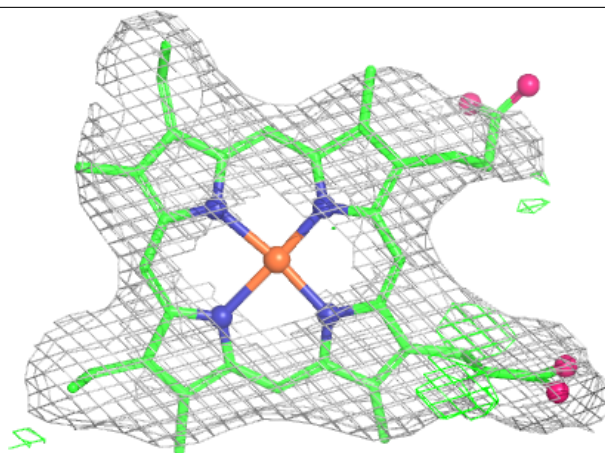
Electron density around HEC B 602:

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



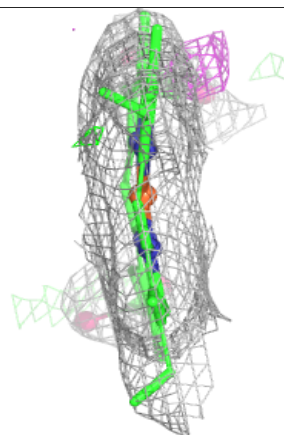
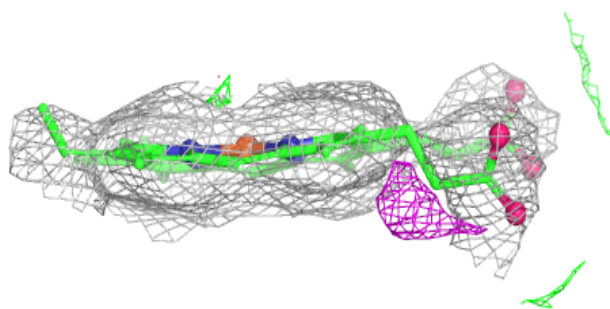
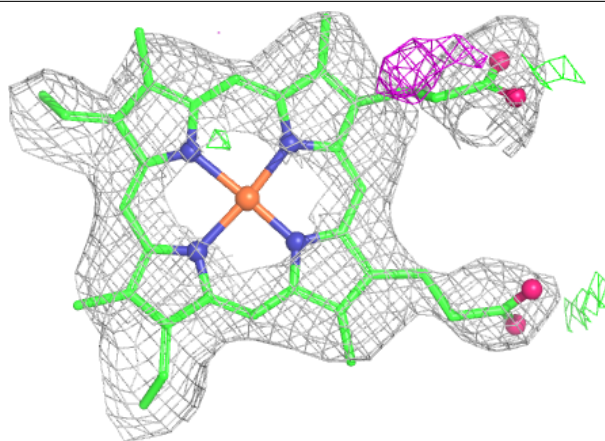
Electron density around HEC N 602:

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



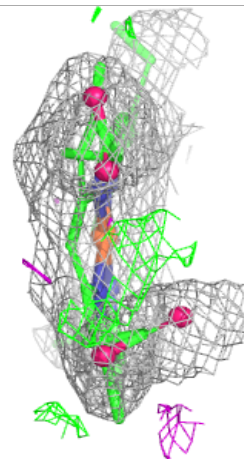
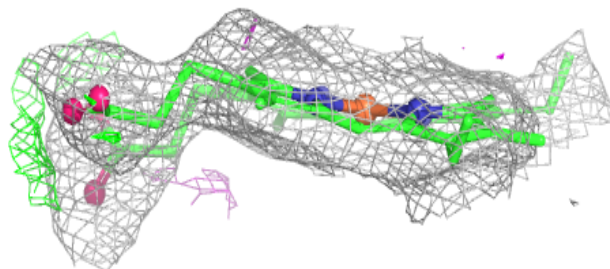
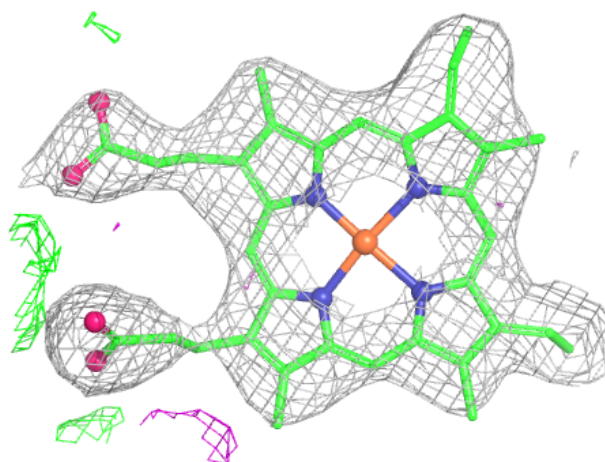
Electron density around HEC N 605:

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



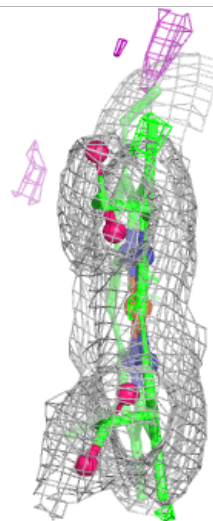
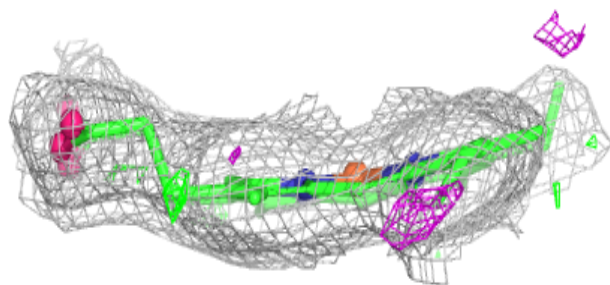
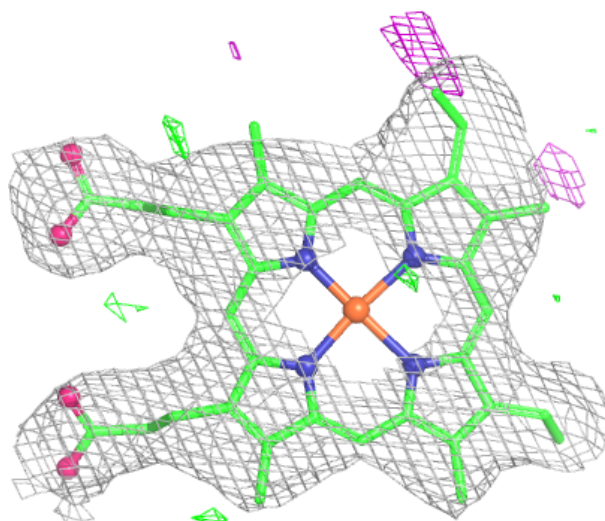
Electron density around HEC N 606:

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



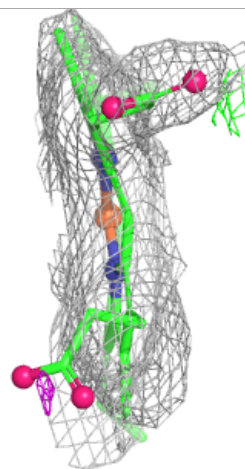
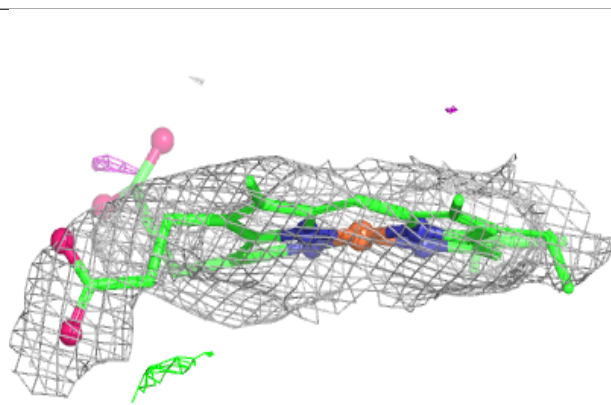
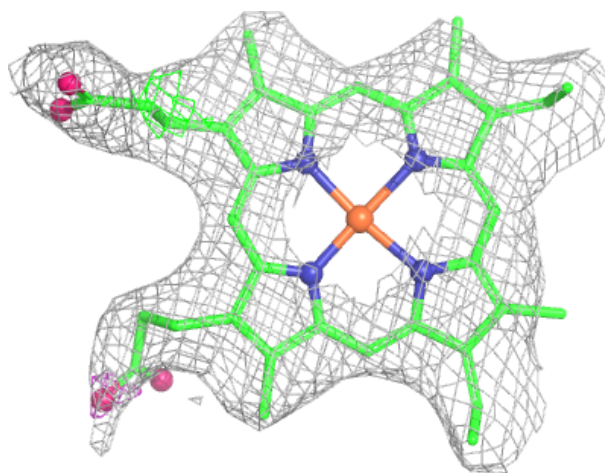
Electron density around HEC O 600:

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



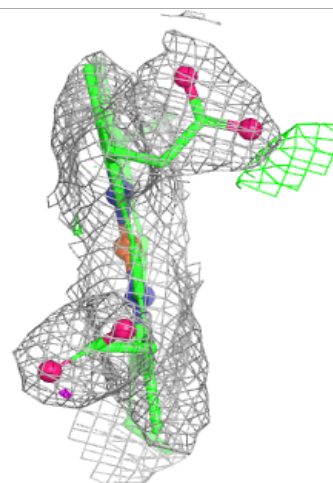
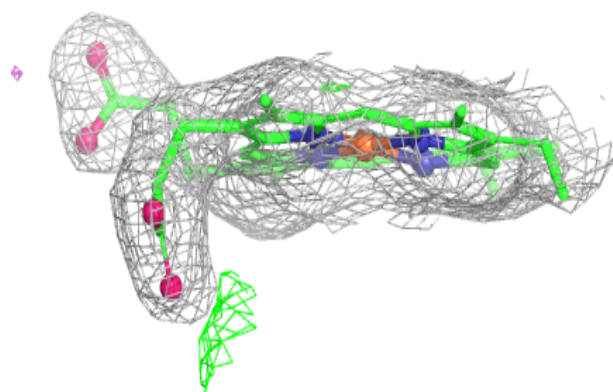
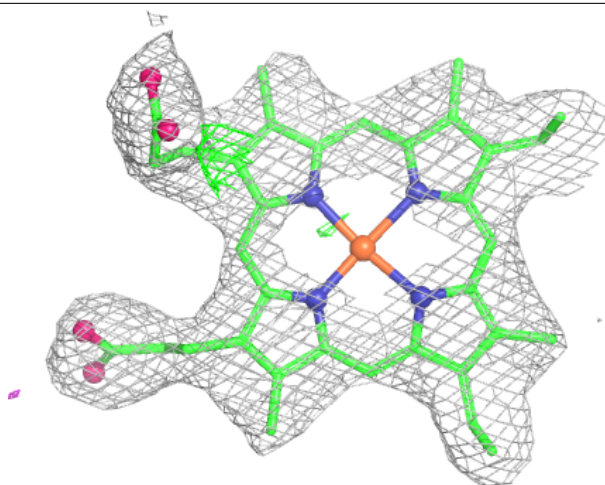
Electron density around HEC O 602:

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



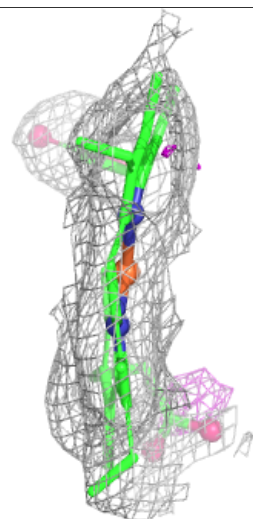
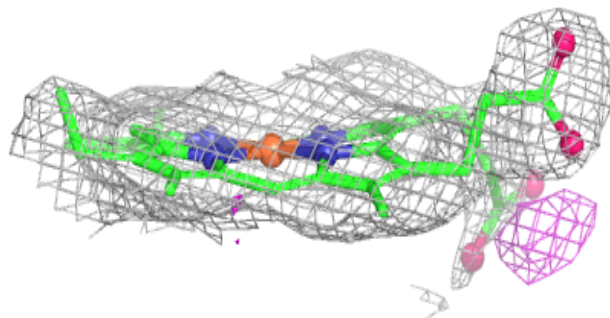
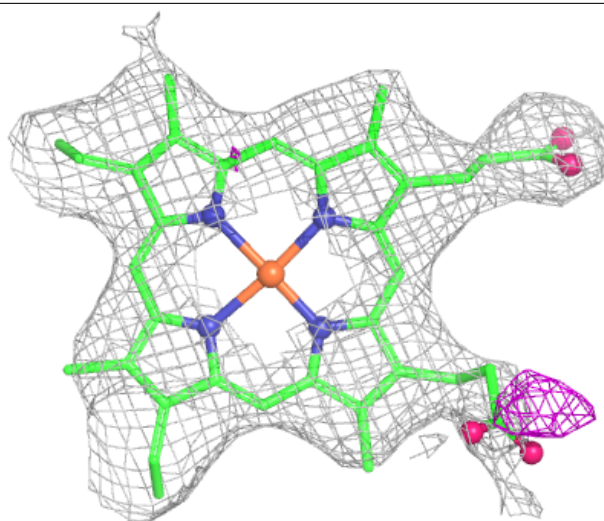
Electron density around HEC P 601:

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



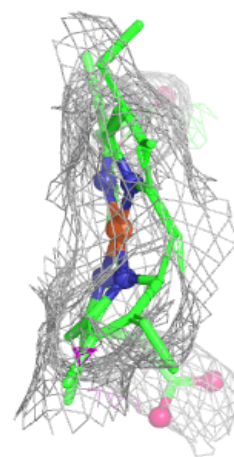
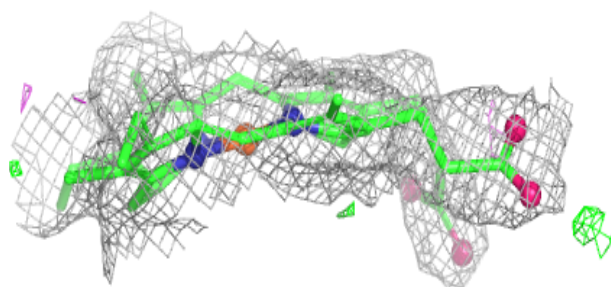
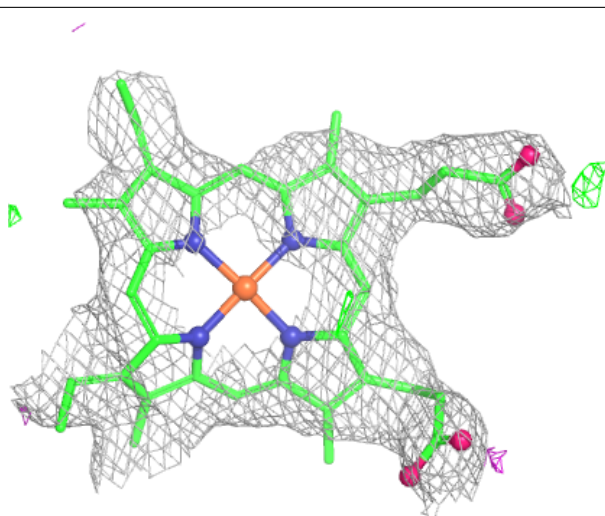
Electron density around HEC P 602:

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



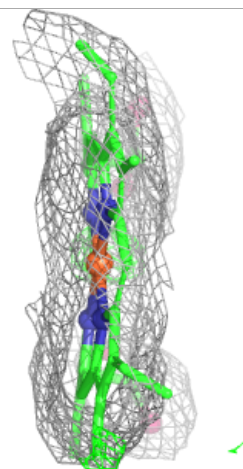
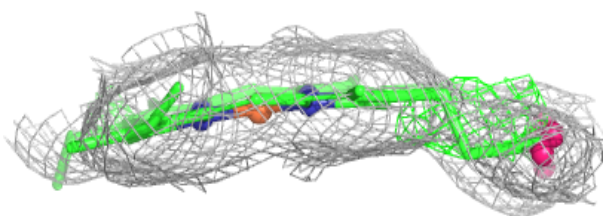
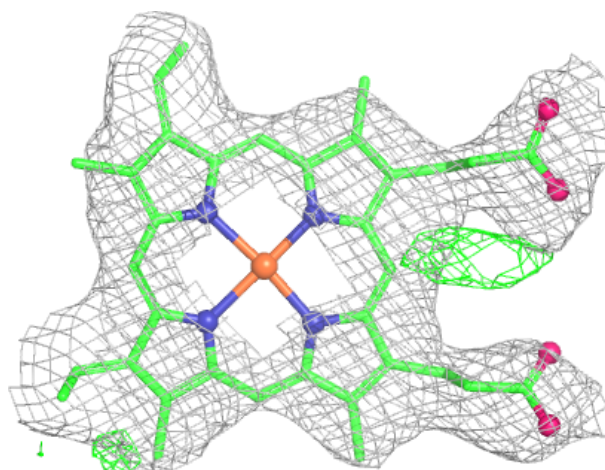
Electron density around HEC Q 603:

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



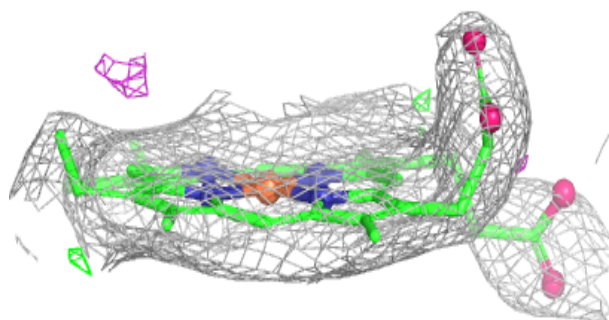
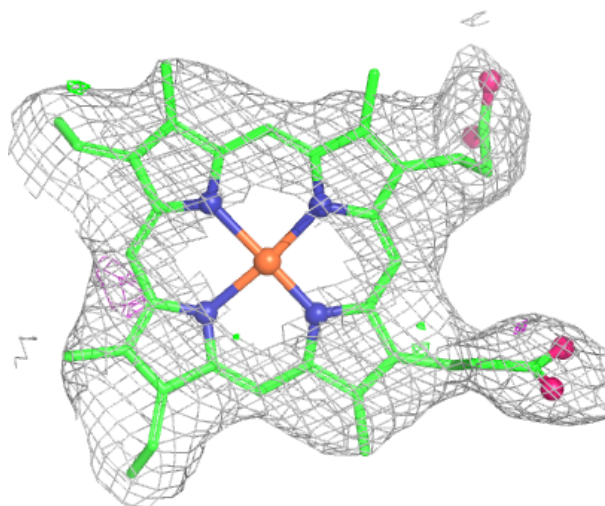
Electron density around HEC Q 600:

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



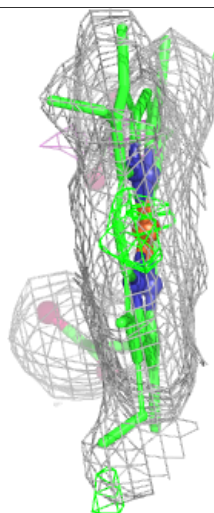
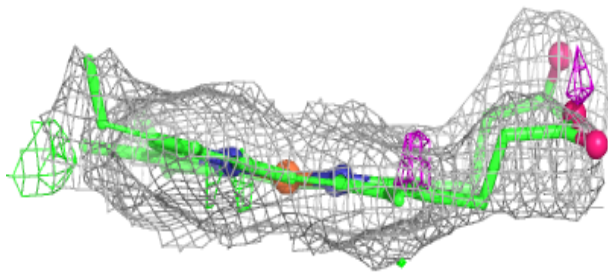
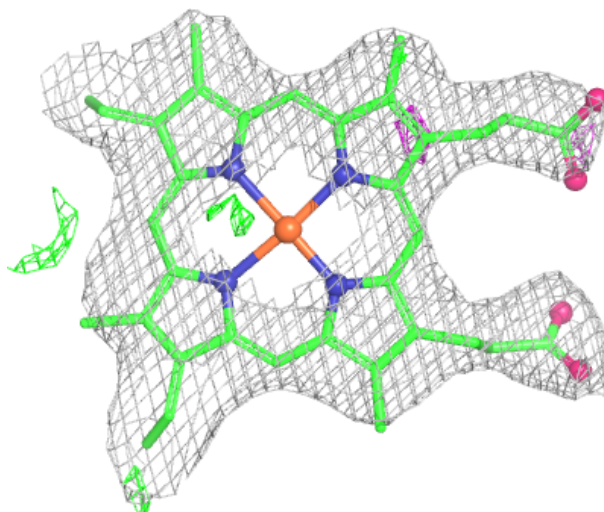
Electron density around HEC Q 601:

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



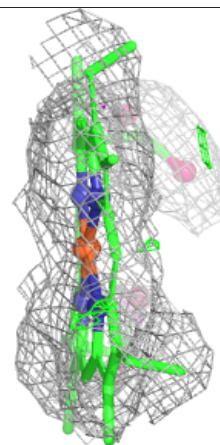
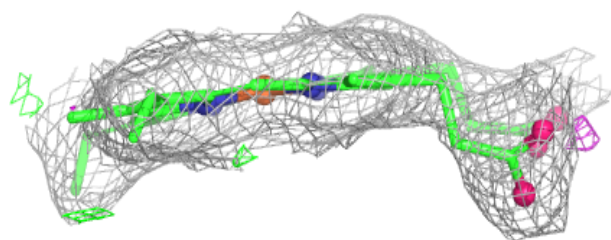
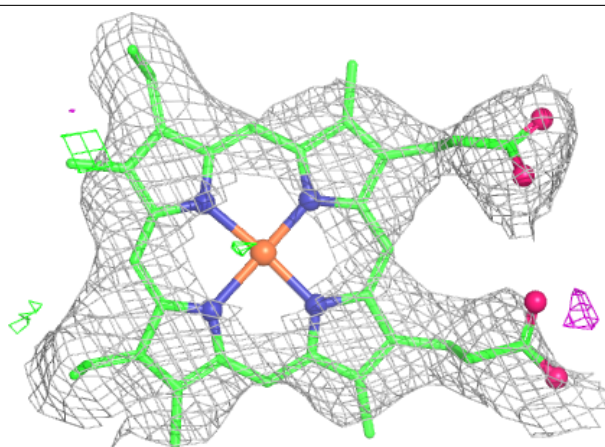
Electron density around HEC B 604:

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



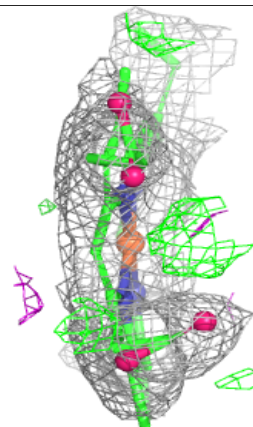
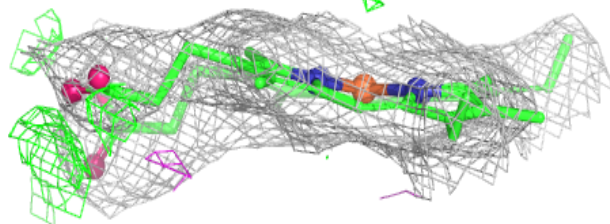
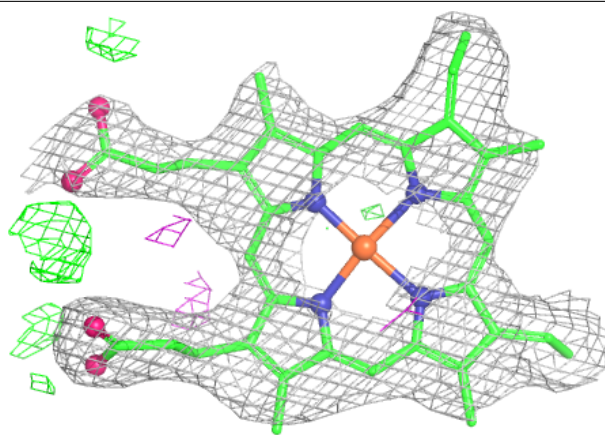
Electron density around HEC Q 604:

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



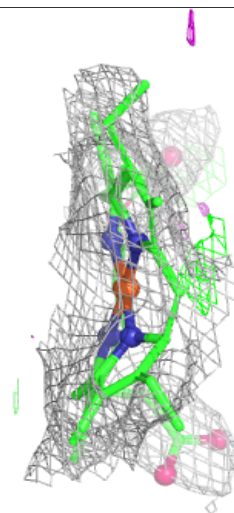
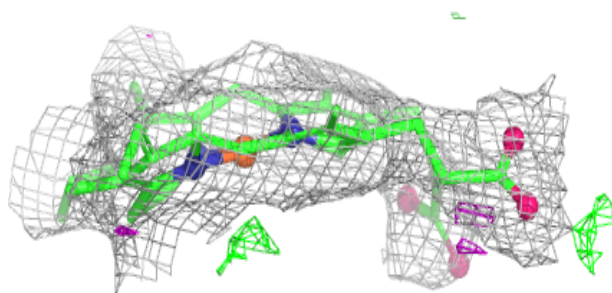
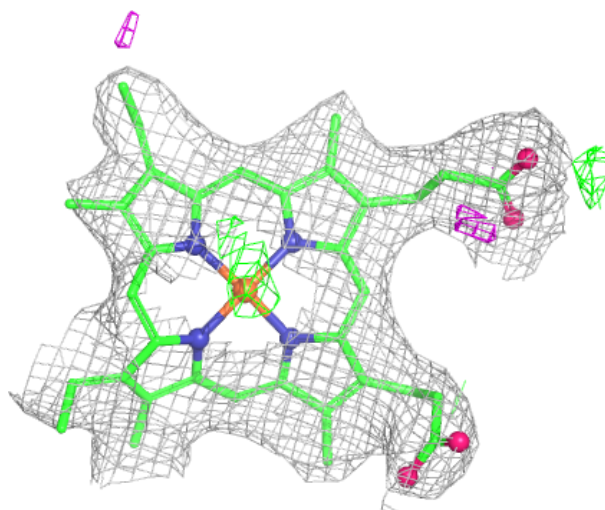
Electron density around HEC Q 606:

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



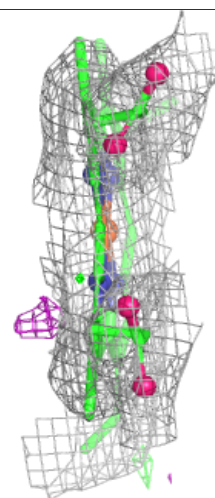
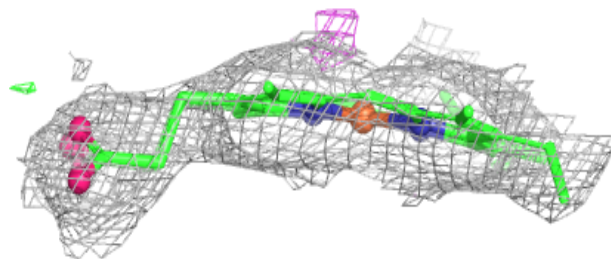
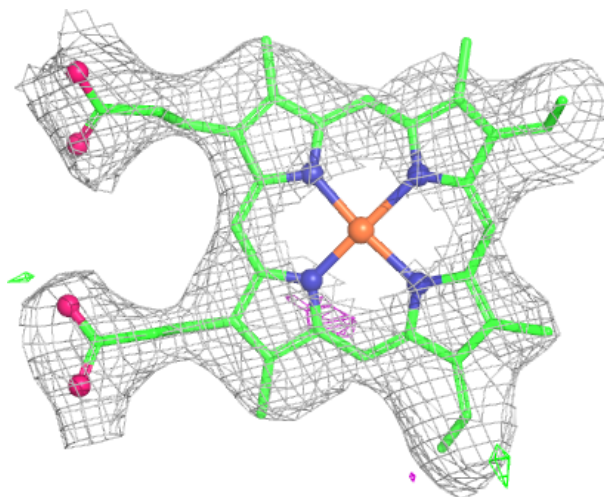
Electron density around HEC R 603:

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



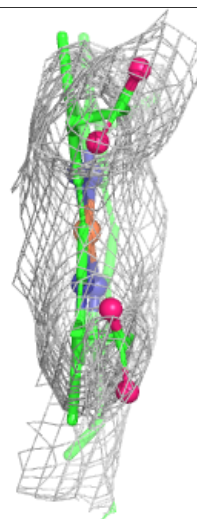
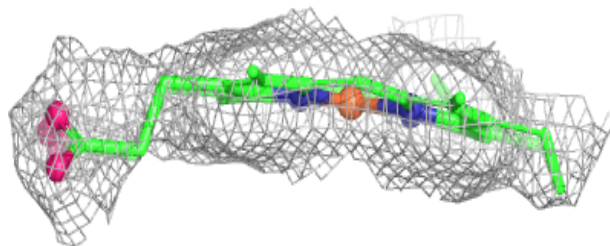
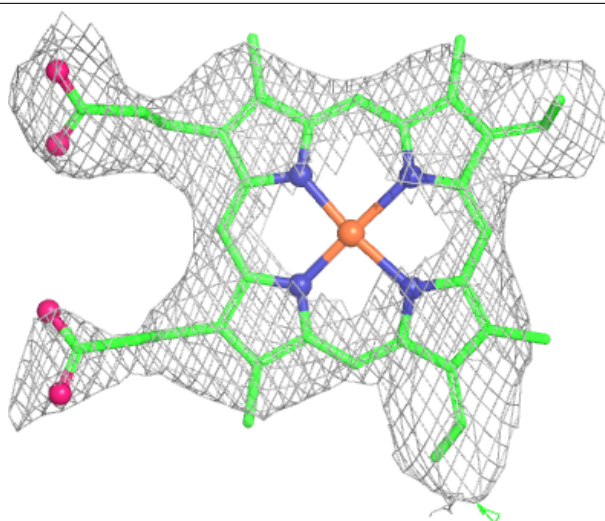
Electron density around HEC R 600:

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



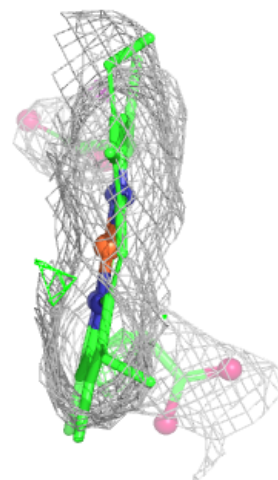
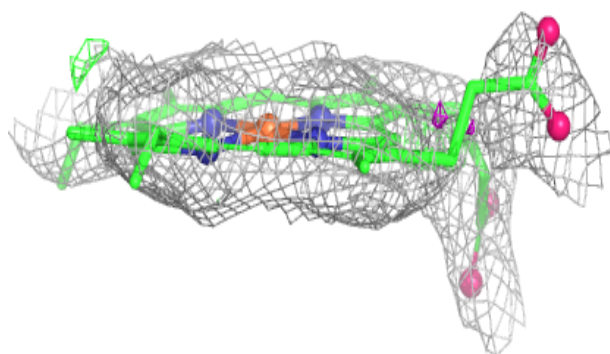
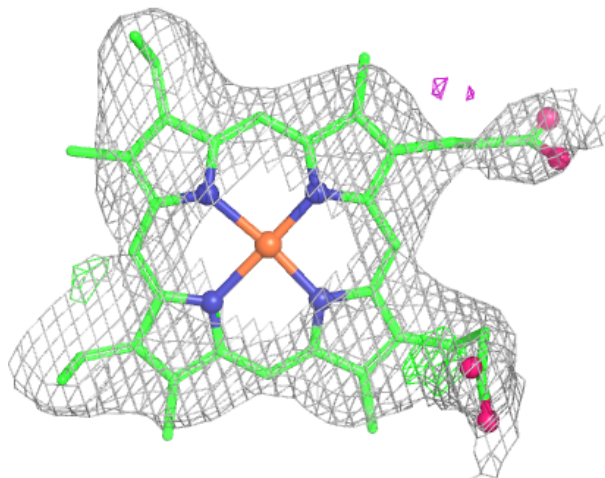
Electron density around HEC S 600:

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



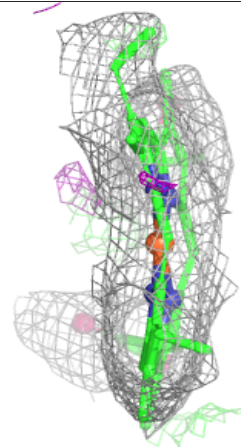
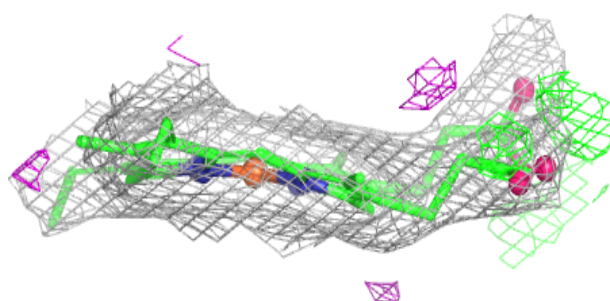
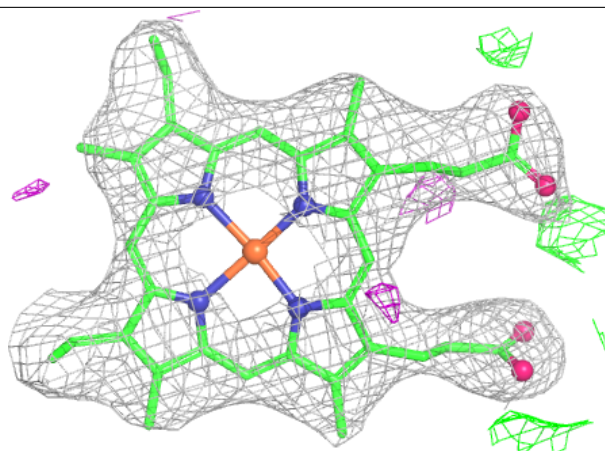
Electron density around HEC S 601:

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



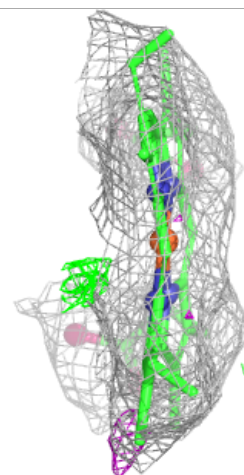
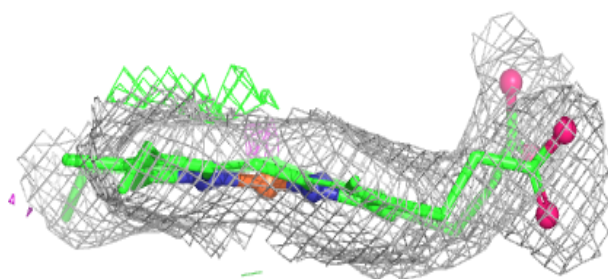
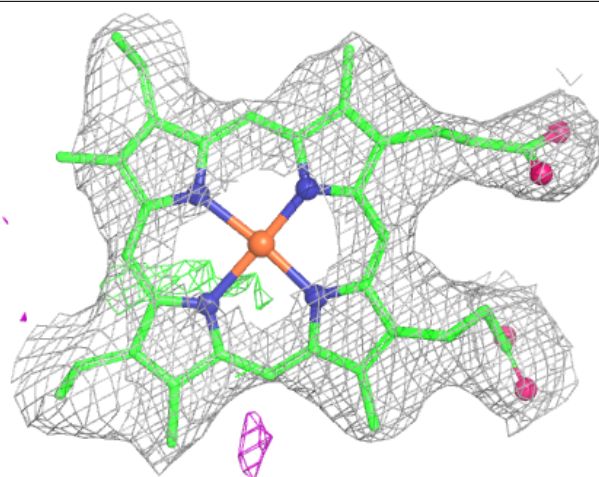
Electron density around HEC C 606:

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



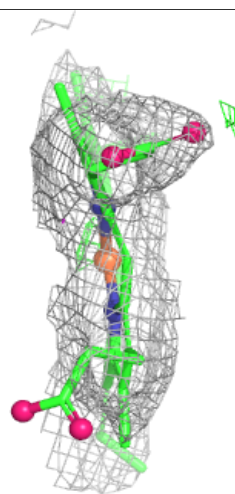
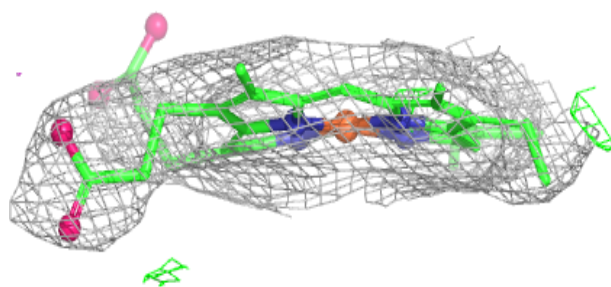
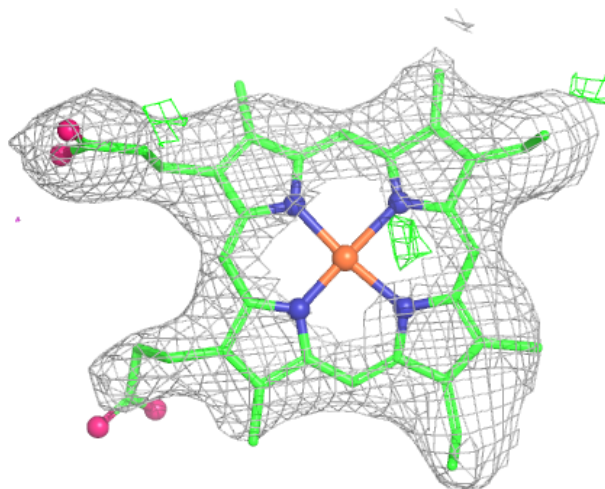
Electron density around HEC C 607:

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



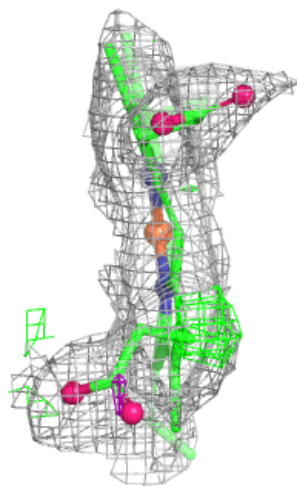
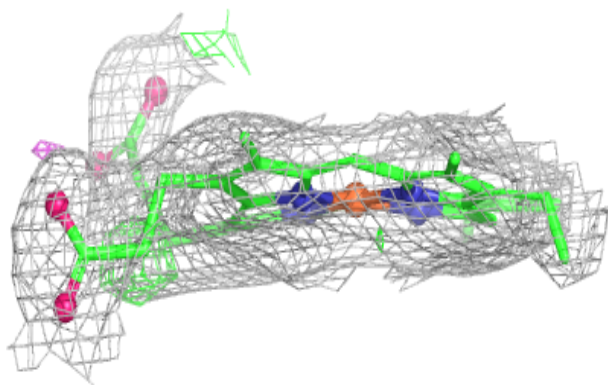
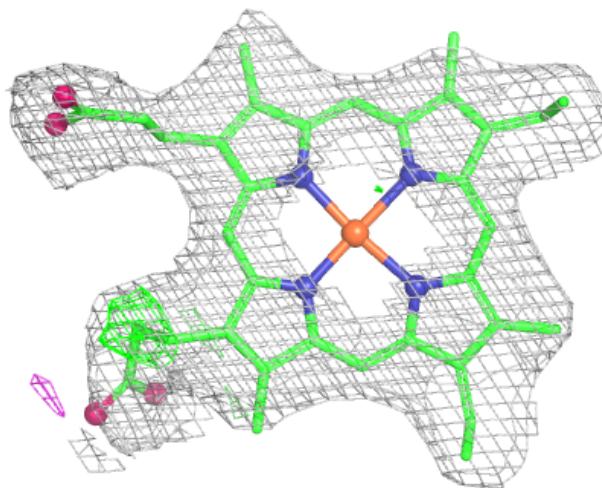
Electron density around HEC A 602:

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



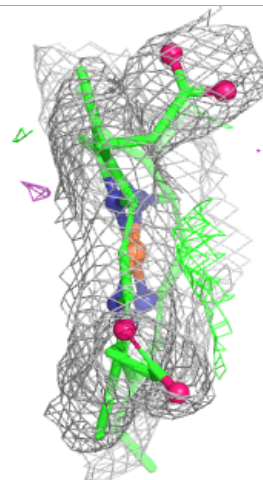
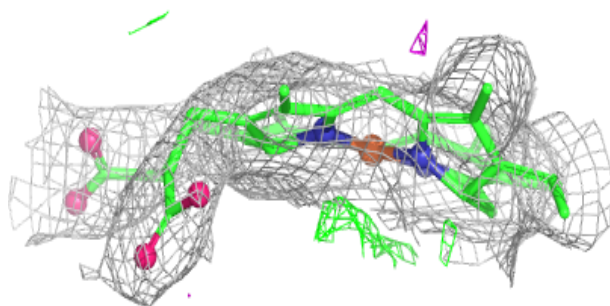
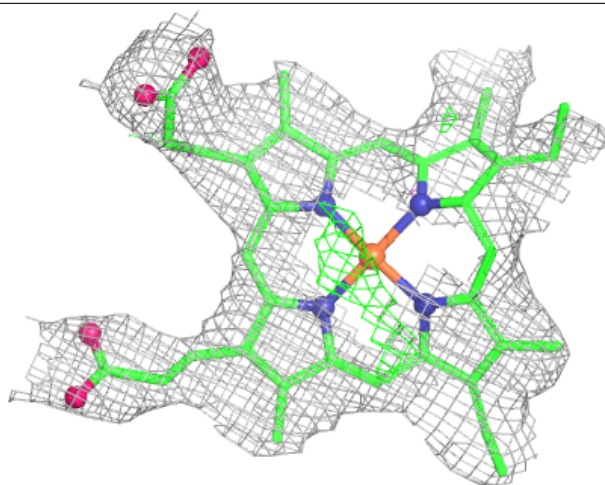
Electron density around HEC G 602:

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



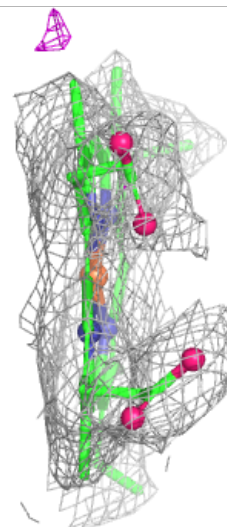
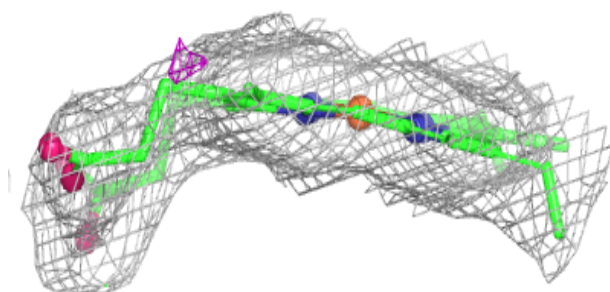
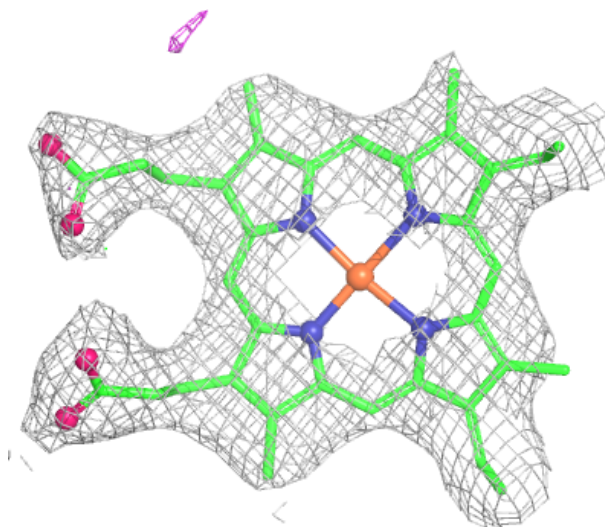
Electron density around HEC B 603:

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



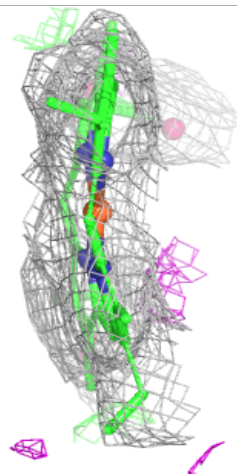
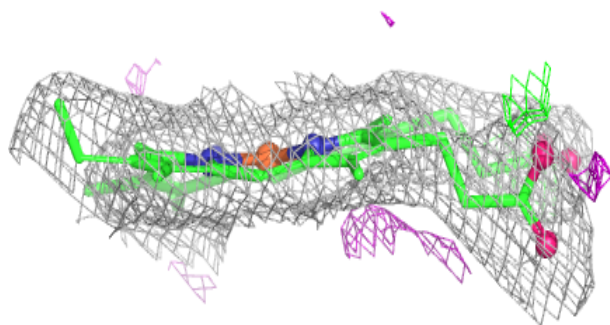
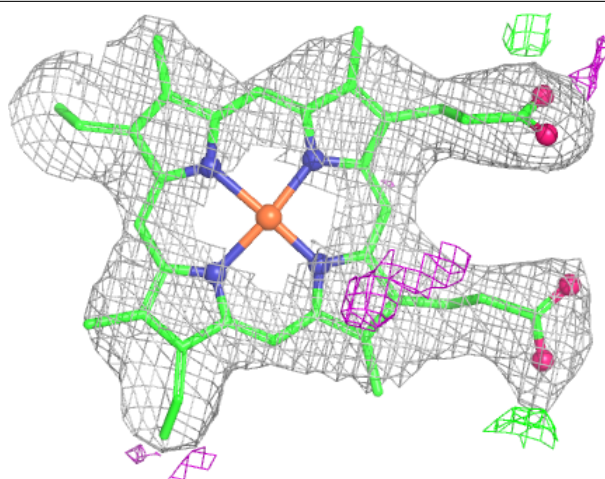
Electron density around HEC H 604:

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



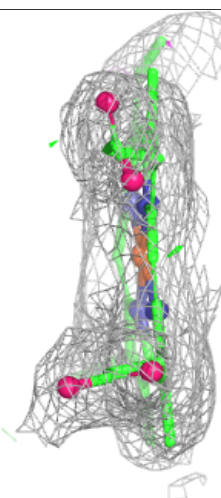
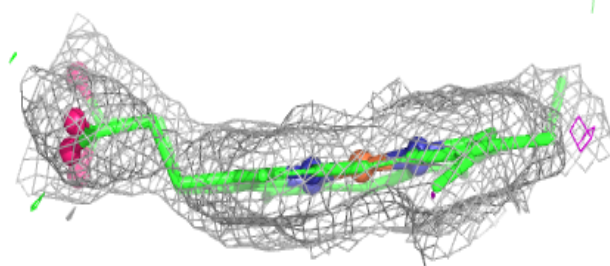
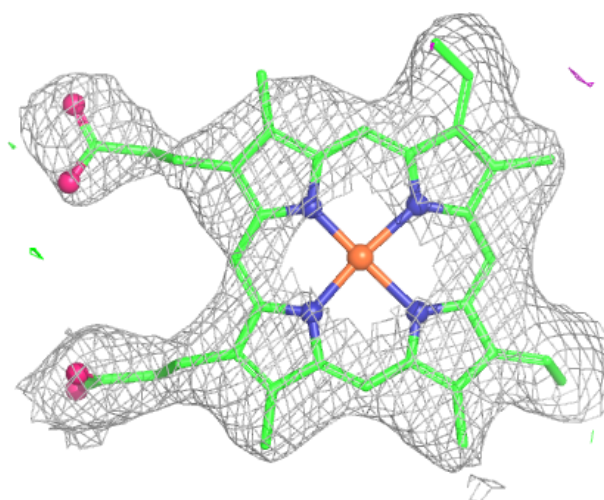
Electron density around HEC H 606:

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



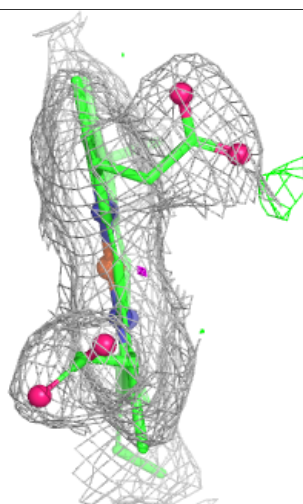
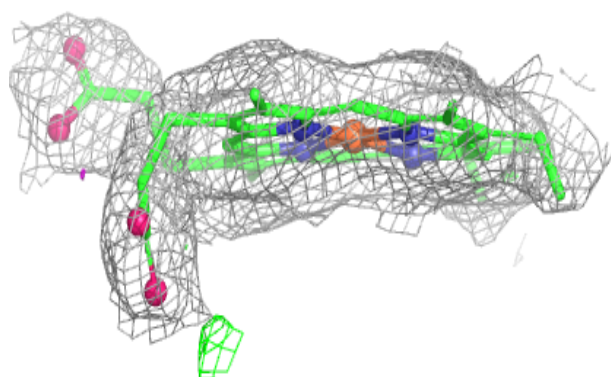
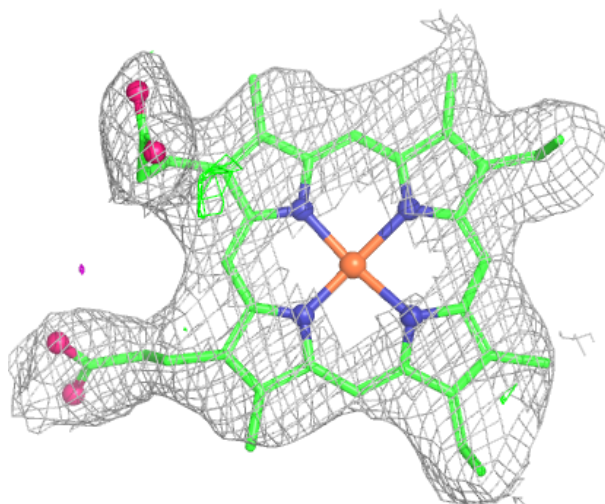
Electron density around HEC I 600:

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



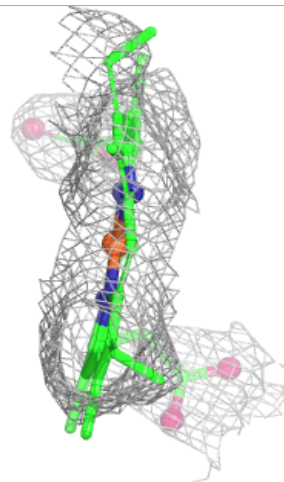
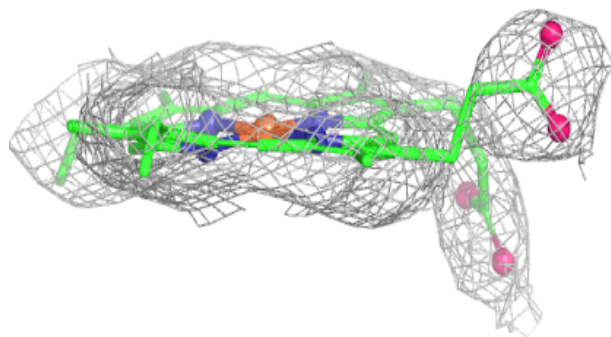
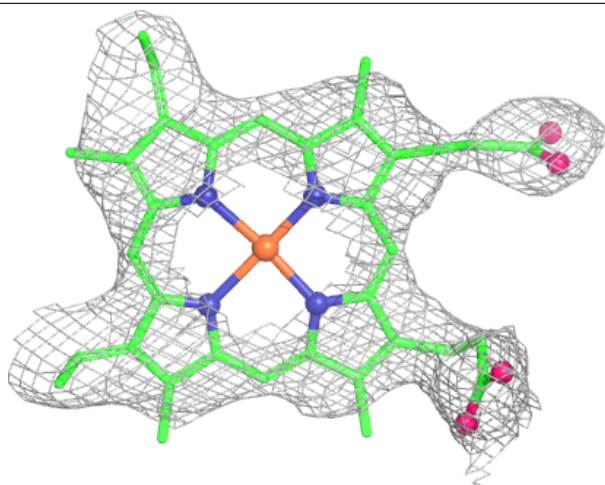
Electron density around HEC I 601:

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



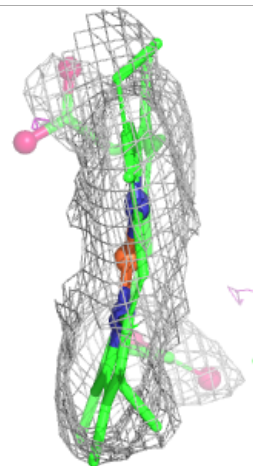
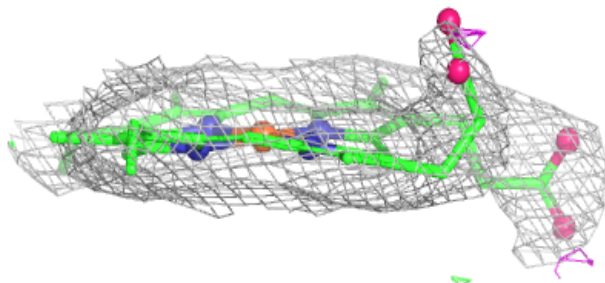
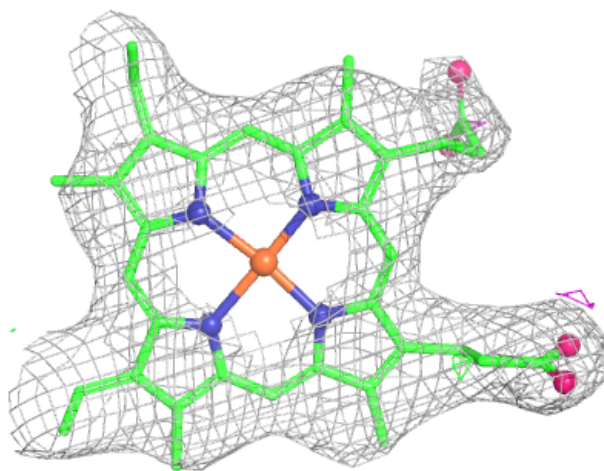
Electron density around HEC D 601:

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



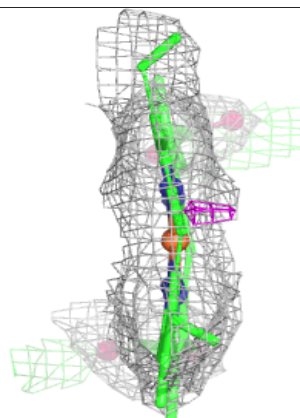
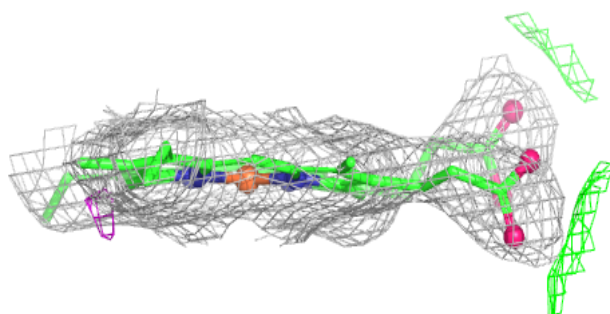
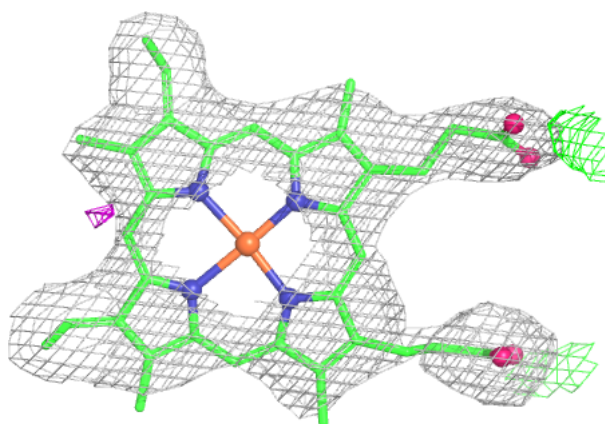
Electron density around HEC D 602:

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



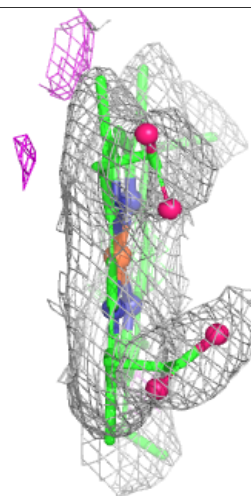
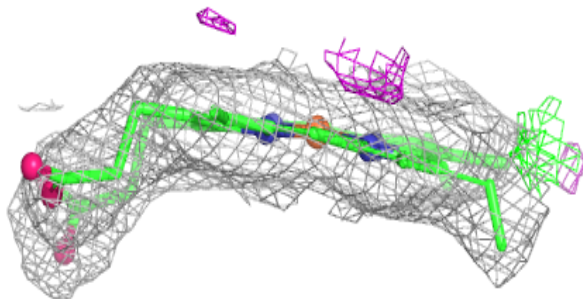
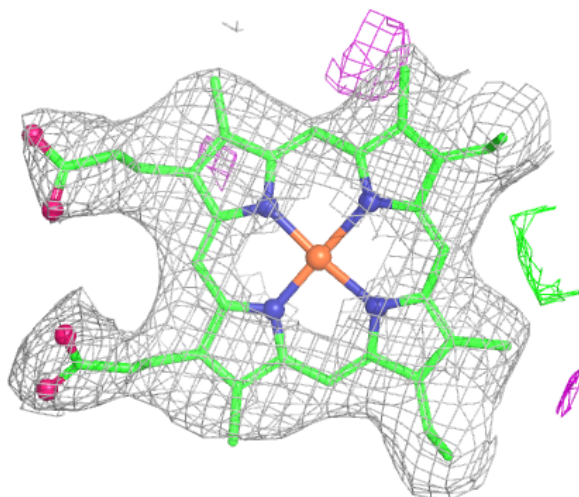
Electron density around HEC D 605:

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



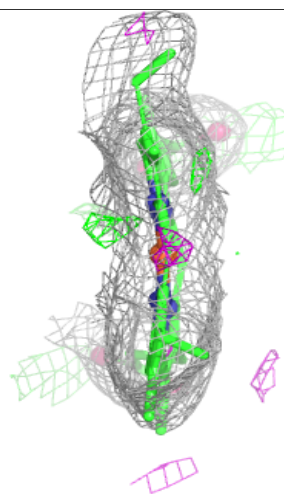
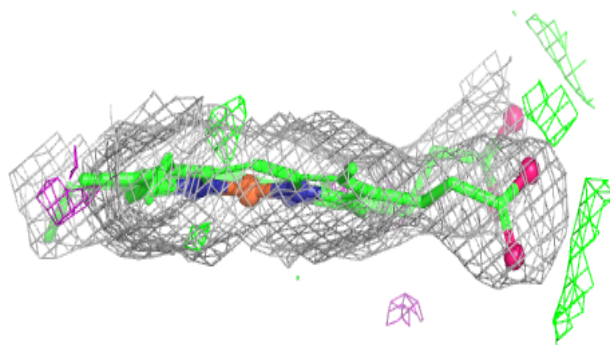
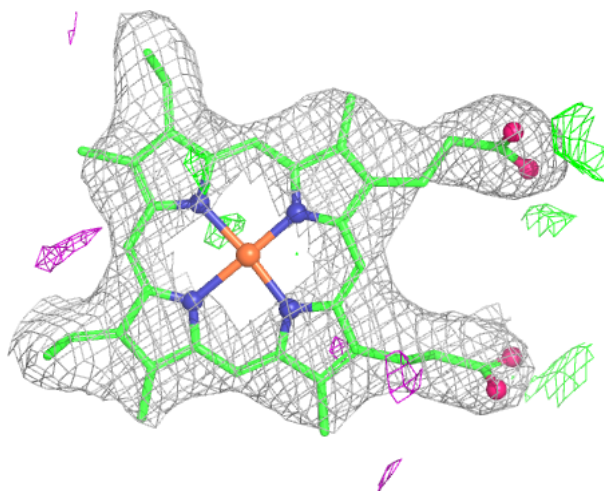
Electron density around HEC J 604:

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



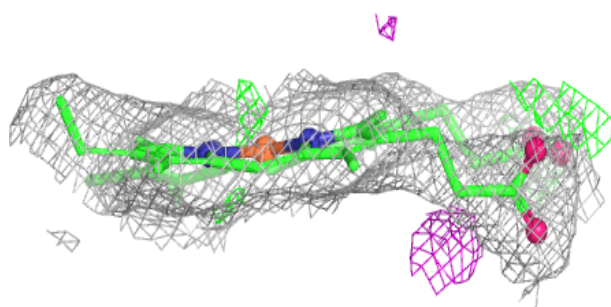
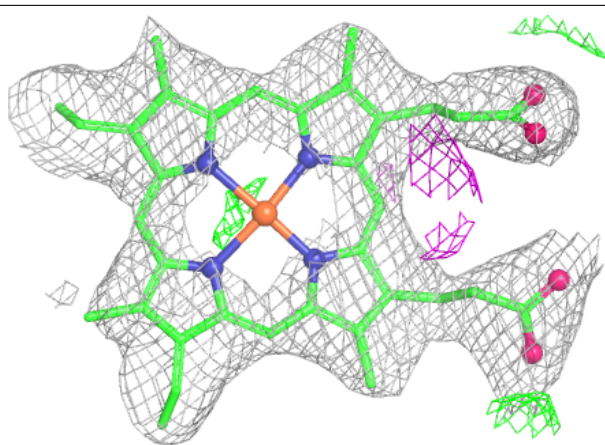
Electron density around HEC J 605:

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



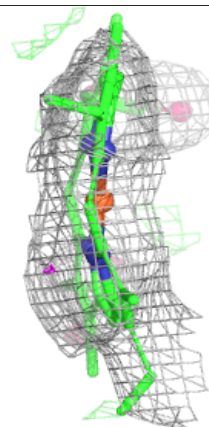
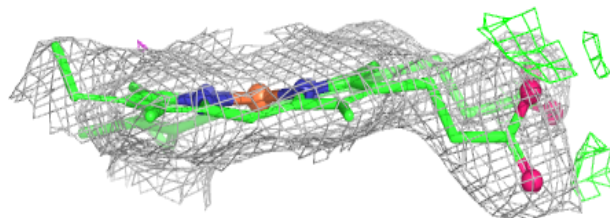
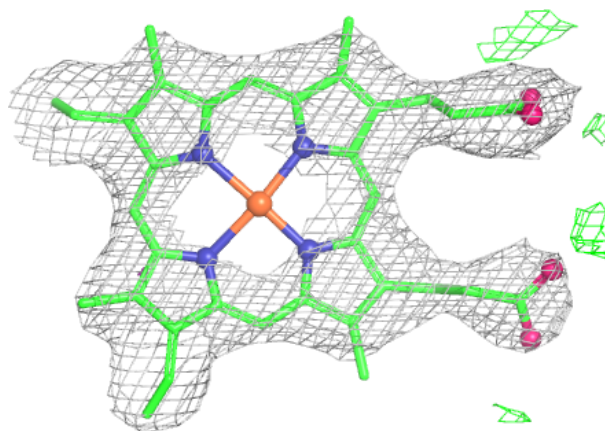
Electron density around HEC J 606:

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



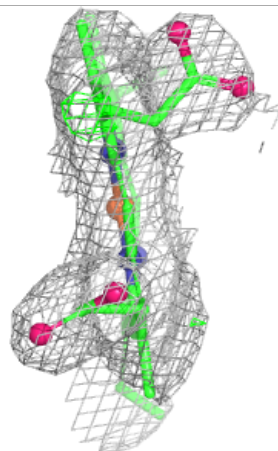
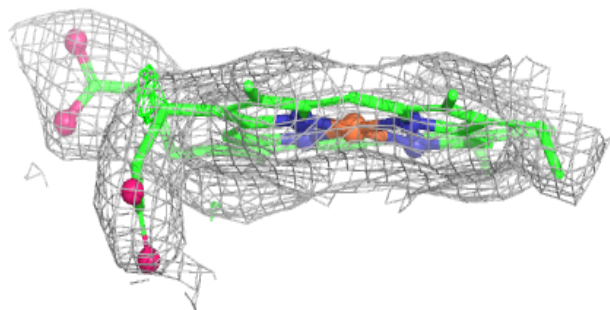
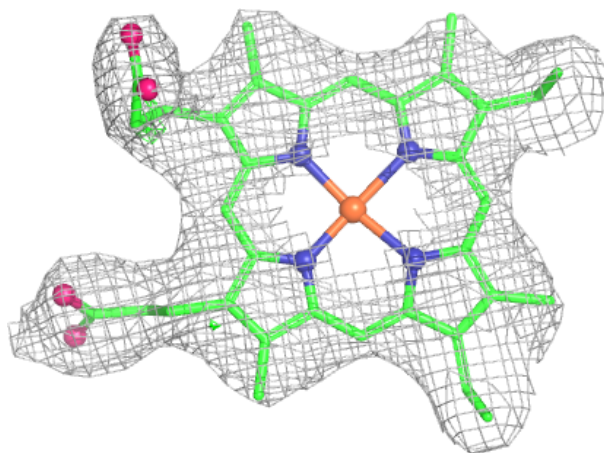
Electron density around HEC D 606:

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



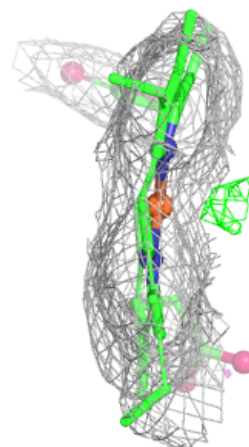
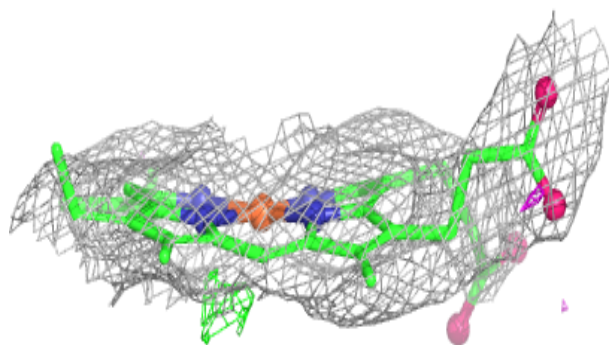
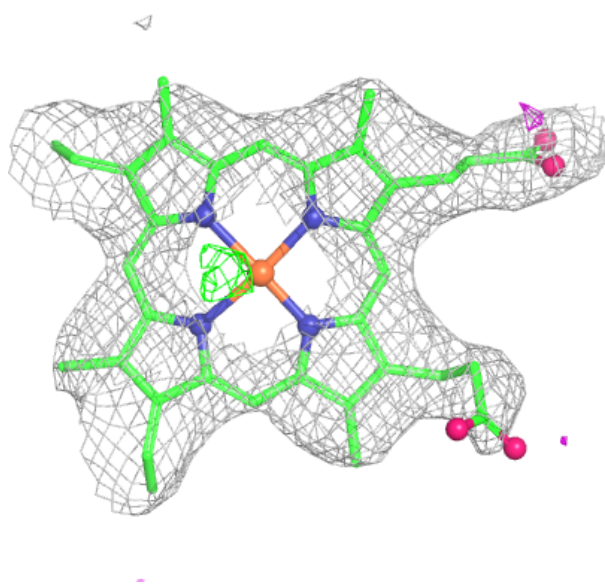
Electron density around HEC K 601:

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



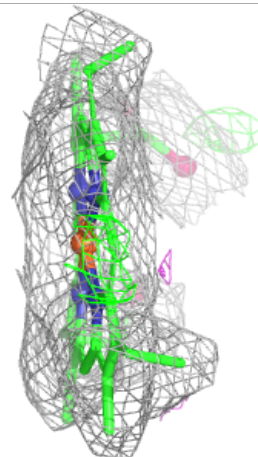
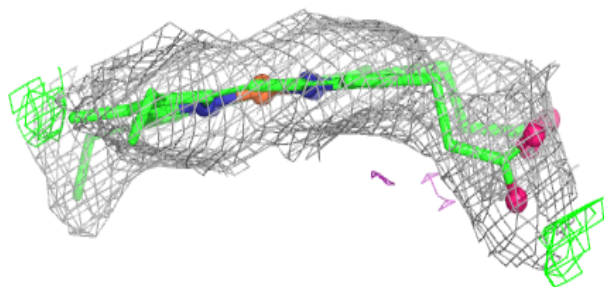
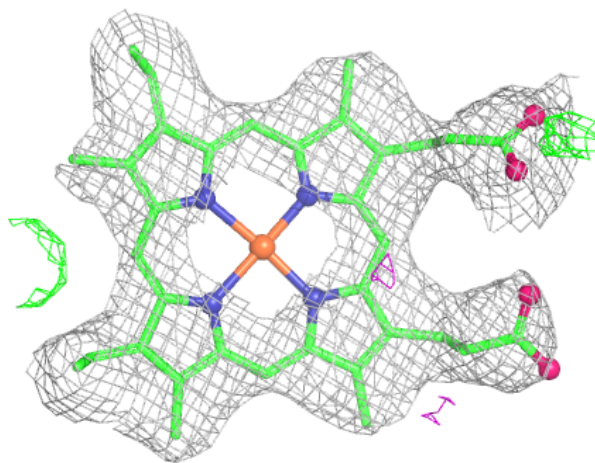
Electron density around HEC K 602:

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



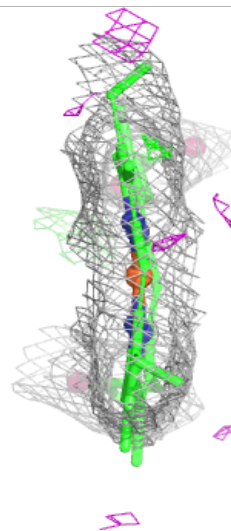
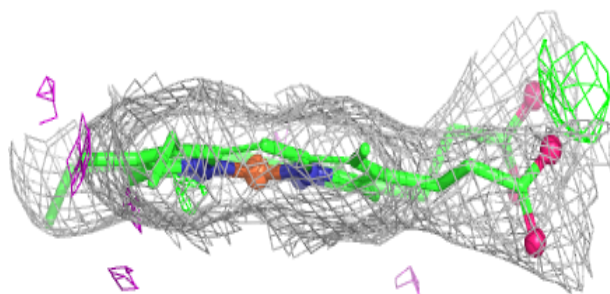
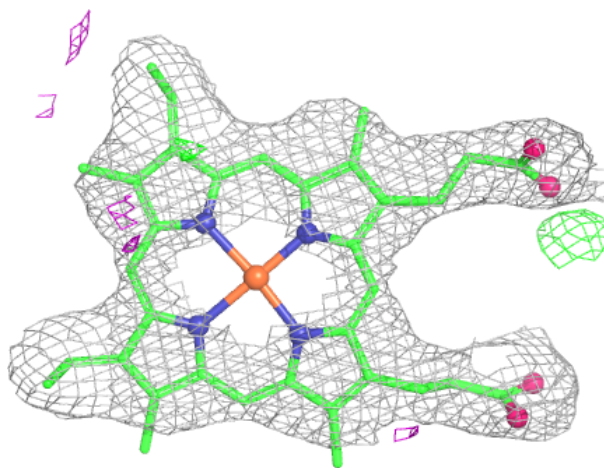
Electron density around HEC K 604:

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



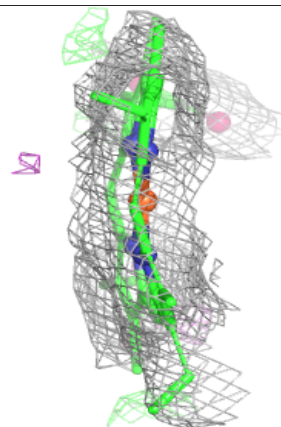
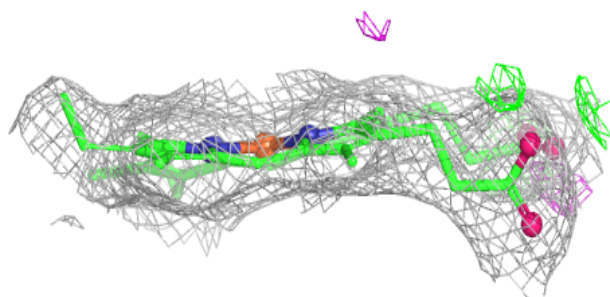
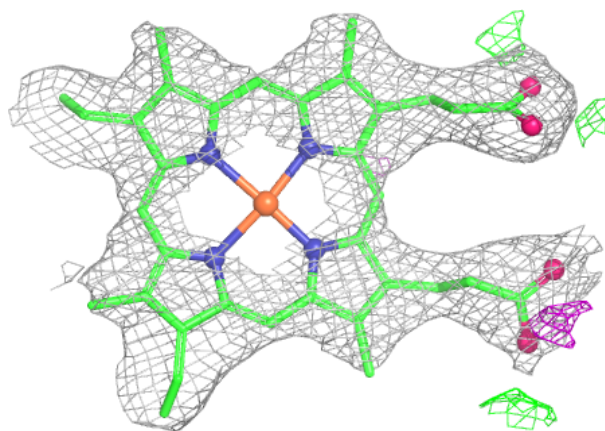
Electron density around HEC K 605:

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



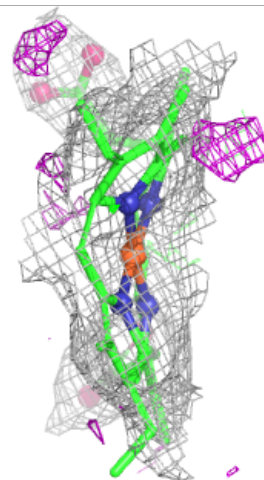
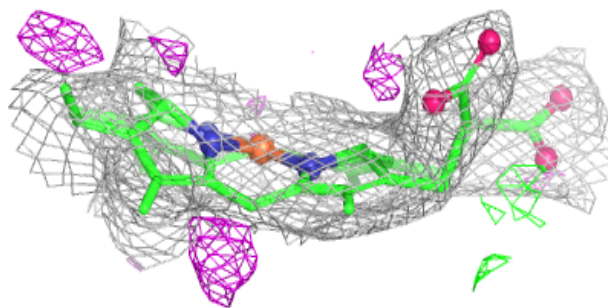
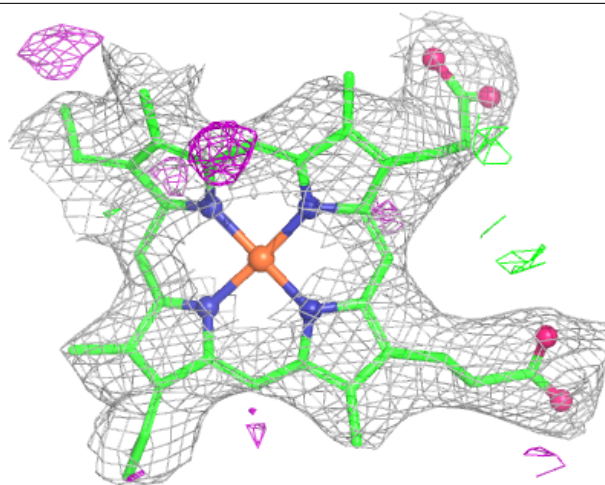
Electron density around HEC K 606:

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



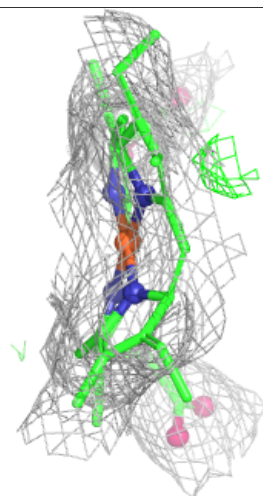
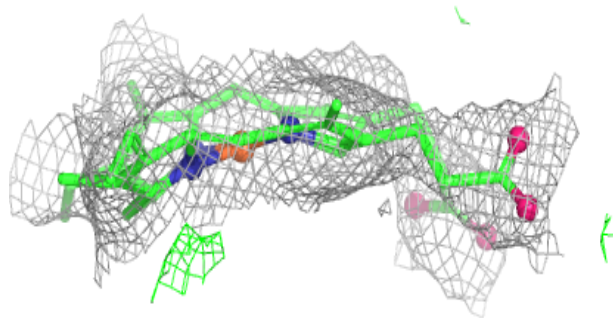
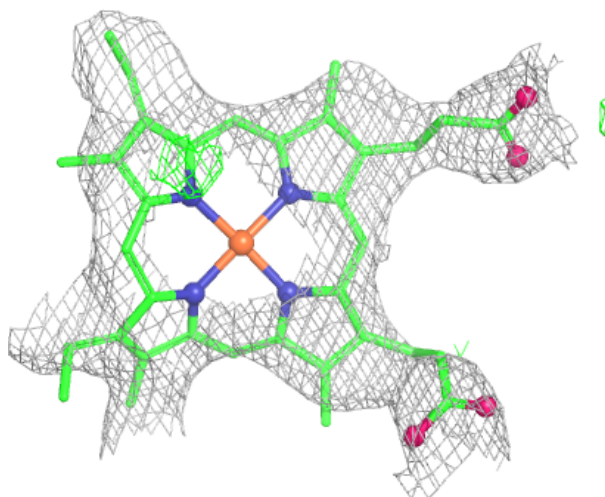
Electron density around HEC L 603:

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



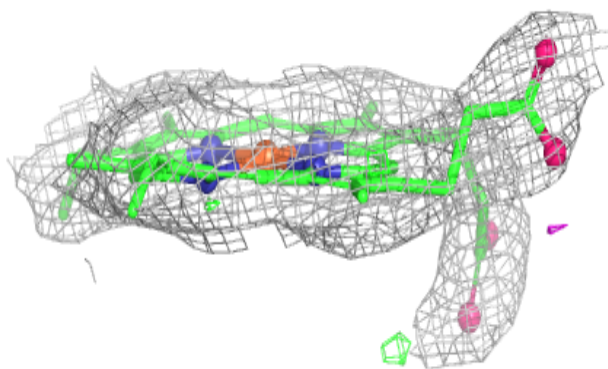
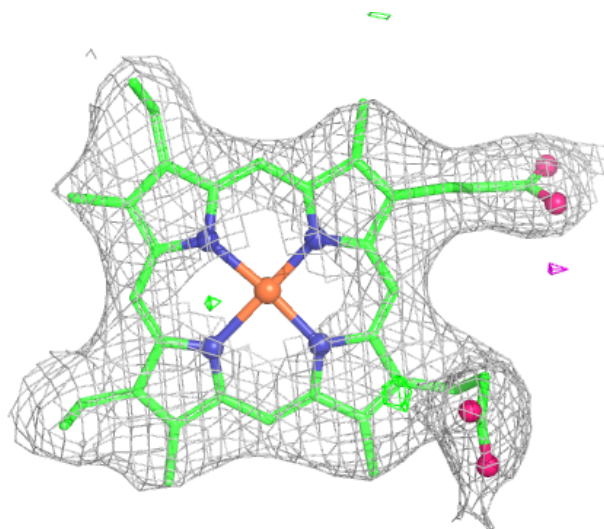
Electron density around HEC D 603:

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



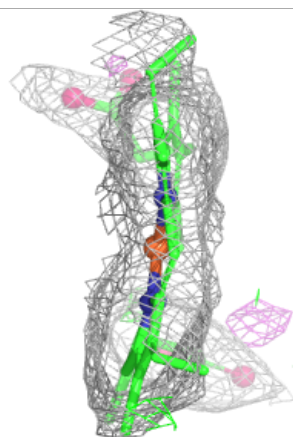
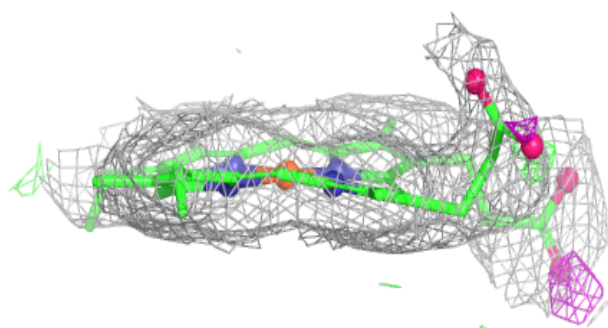
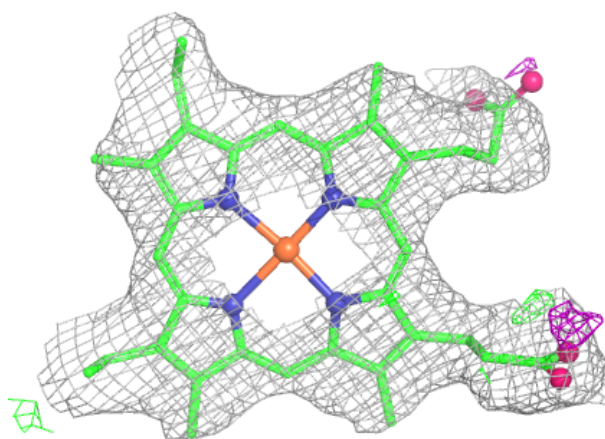
Electron density around HEC L 601:

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



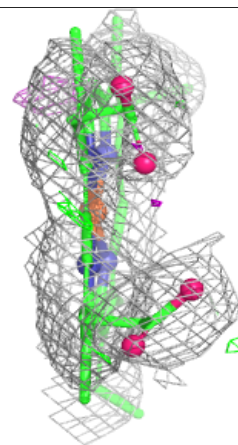
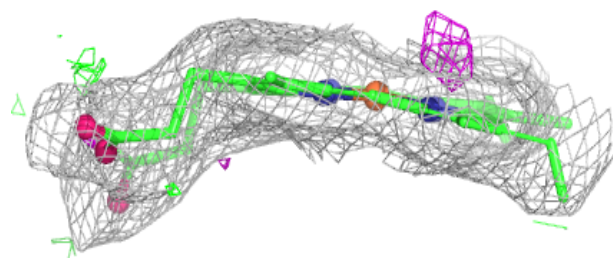
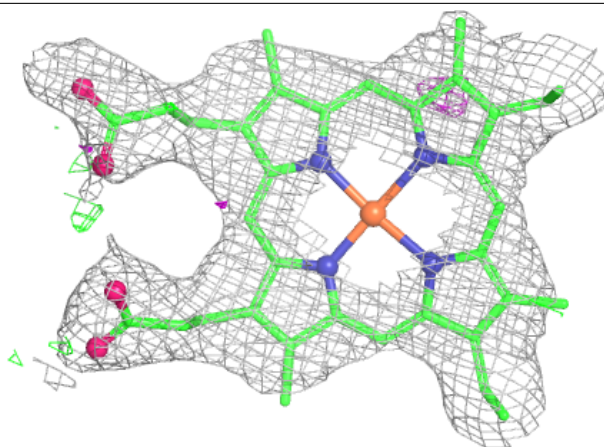
Electron density around HEC L 602:

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



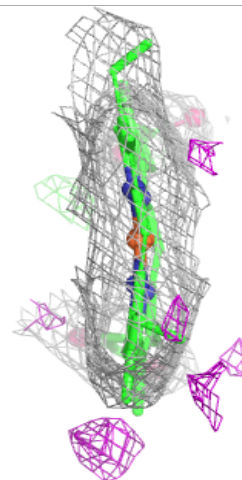
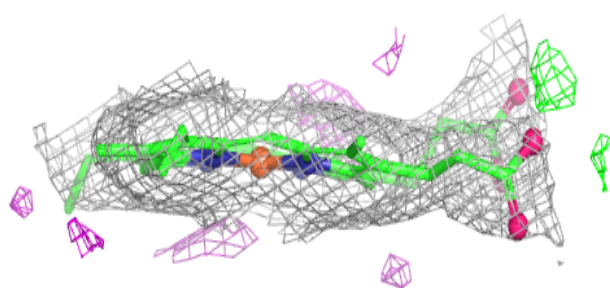
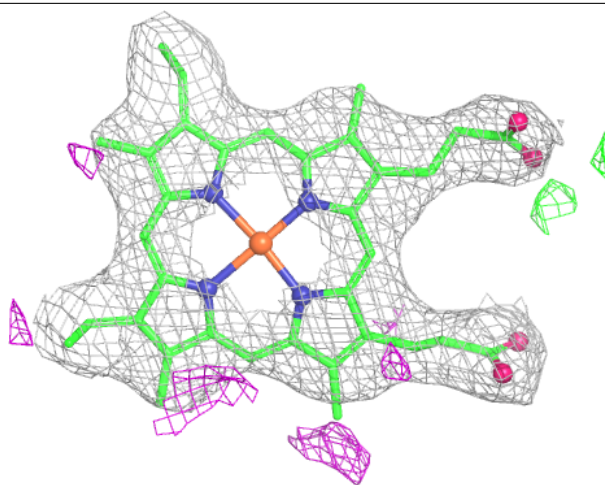
Electron density around HEC L 604:

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



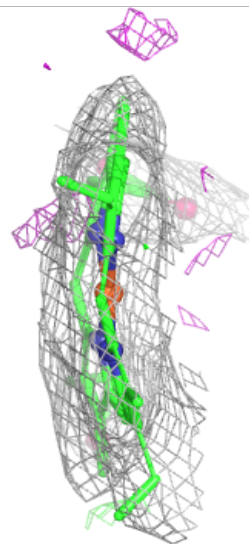
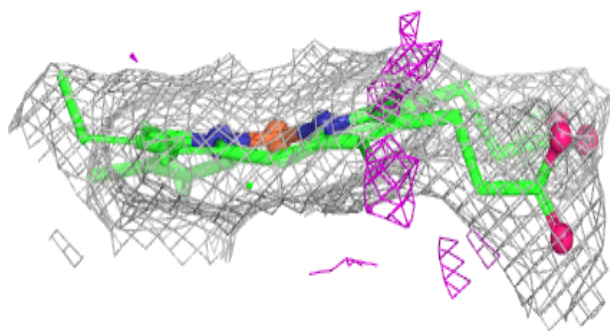
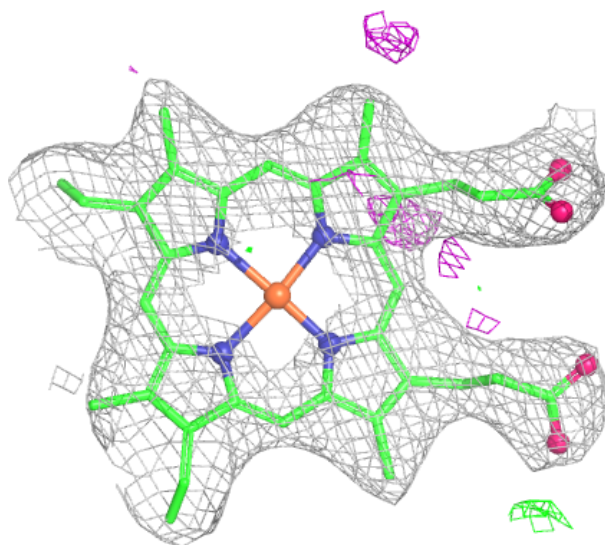
Electron density around HEC L 605:

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



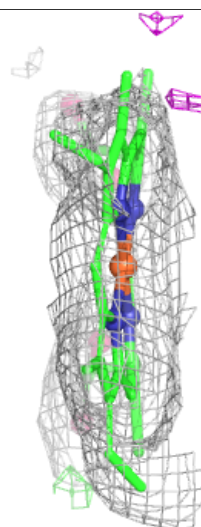
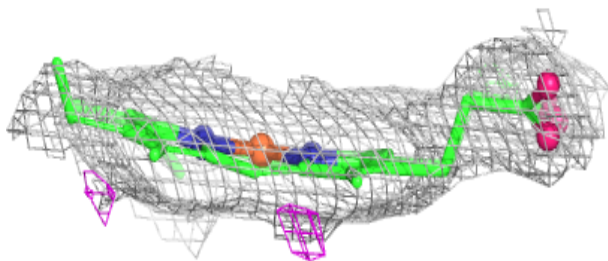
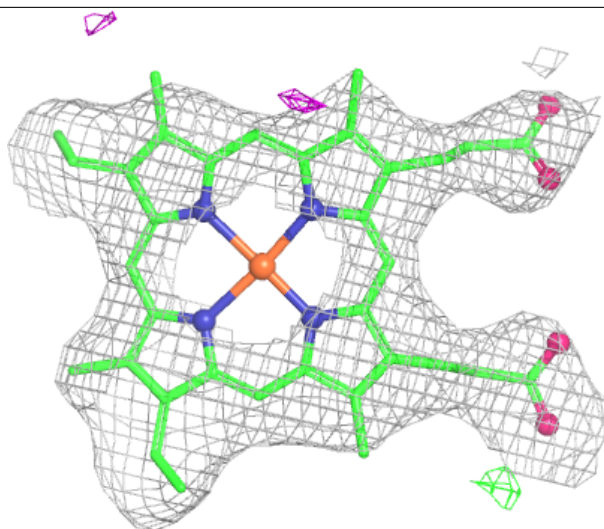
Electron density around HEC L 606:

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



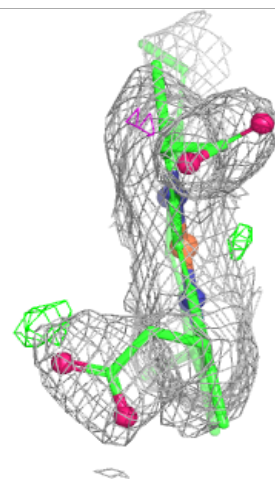
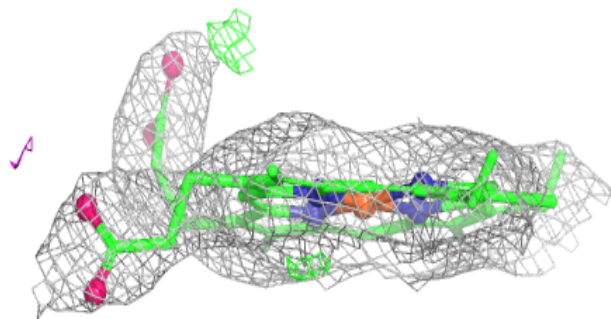
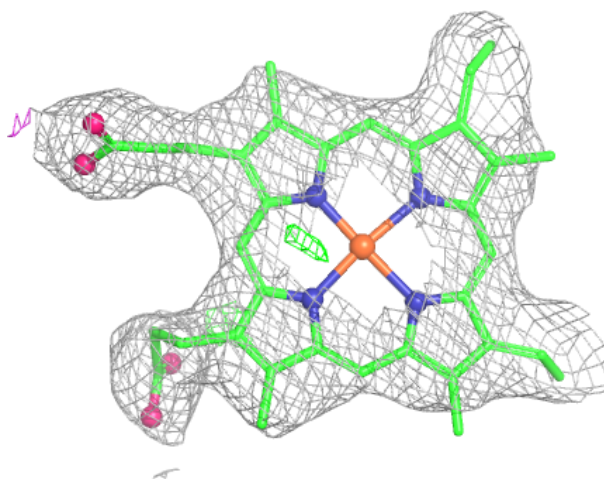
Electron density around HEC B 600:

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



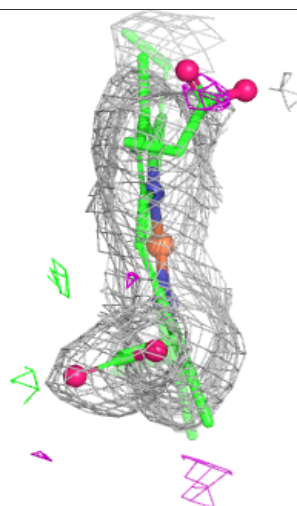
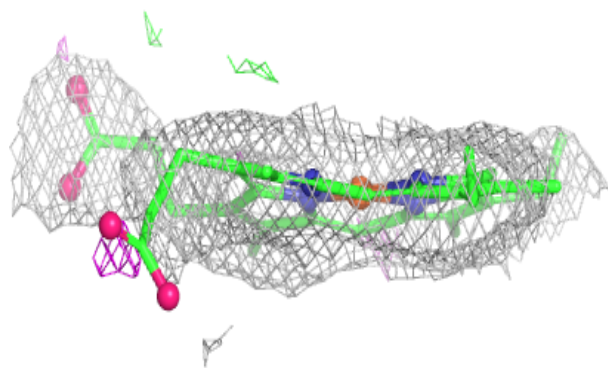
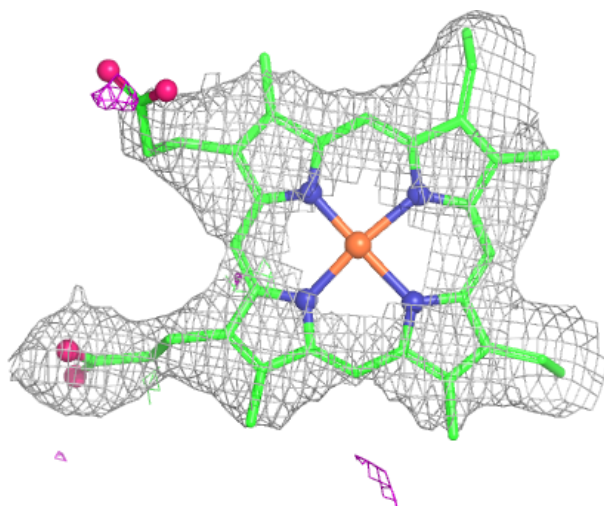
Electron density around HEC M 601:

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



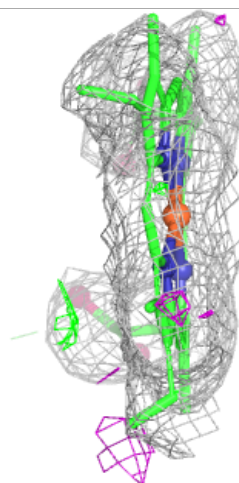
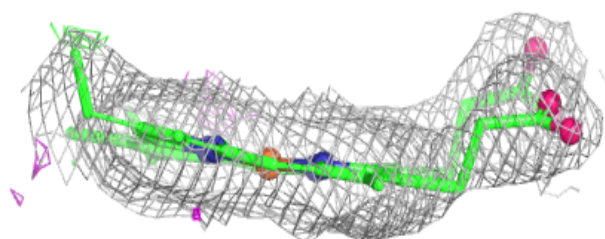
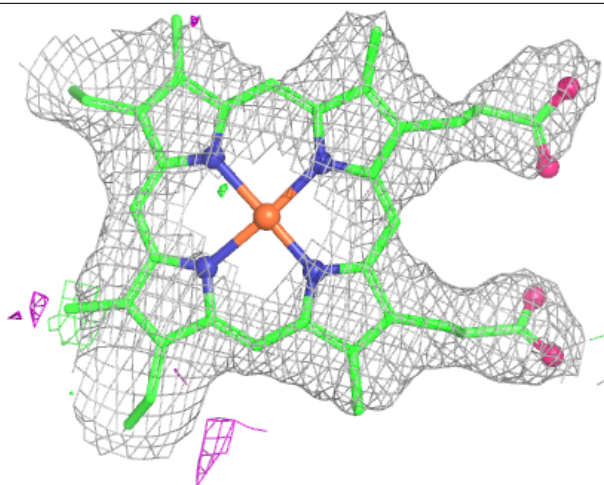
Electron density around HEC M 602:

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



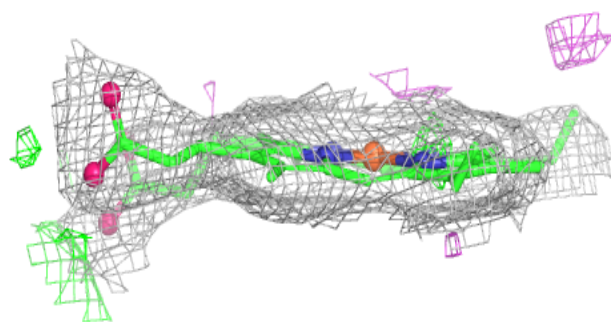
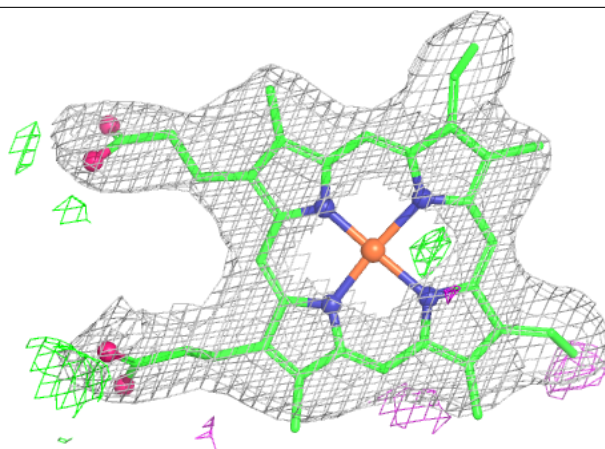
Electron density around HEC M 604:

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



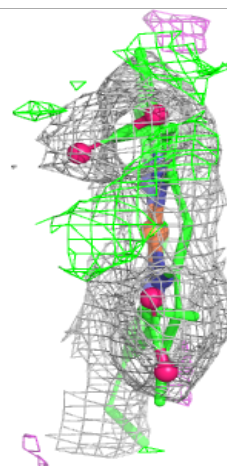
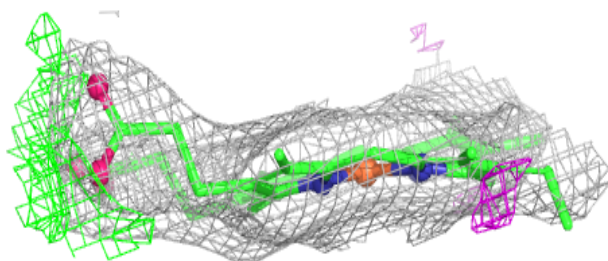
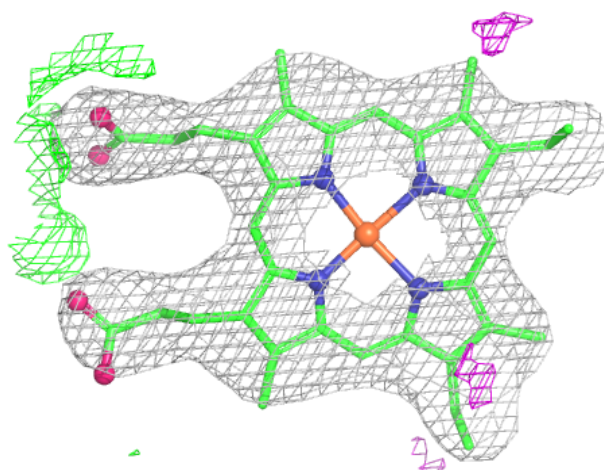
Electron density around HEC M 605:

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



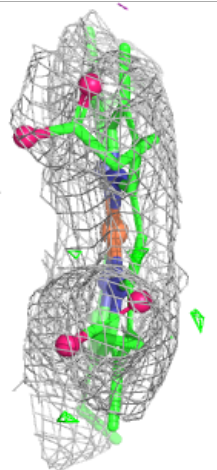
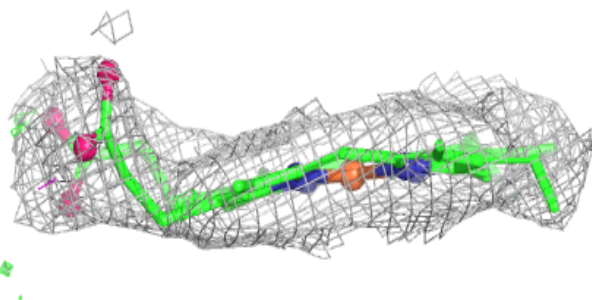
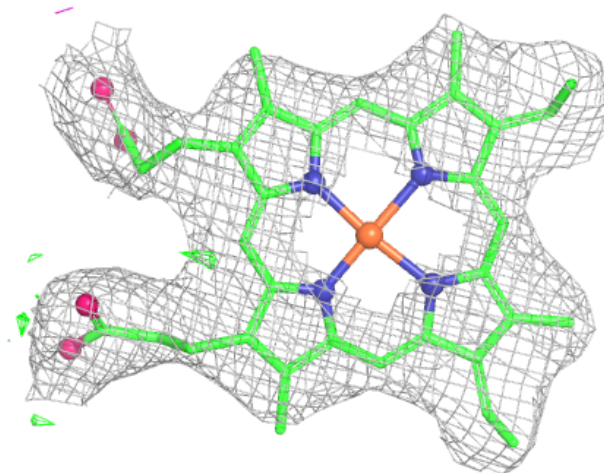
Electron density around HEC M 606:

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



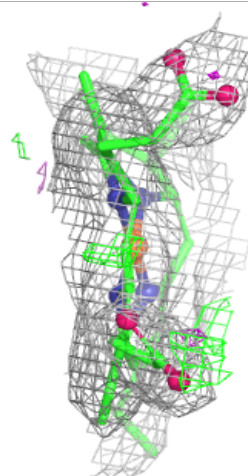
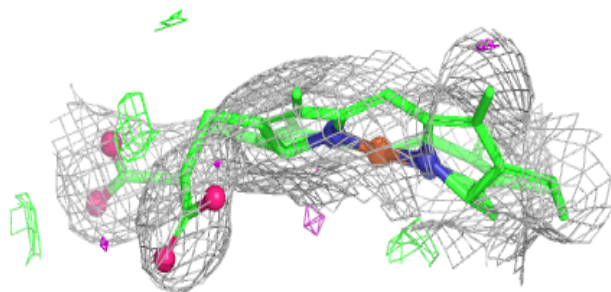
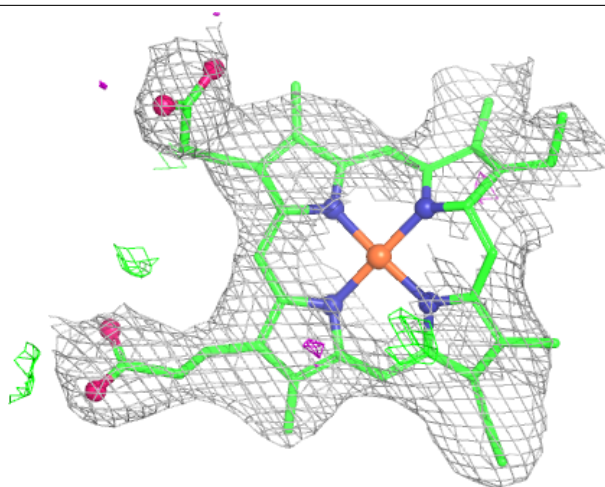
Electron density around HEC M 607:

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



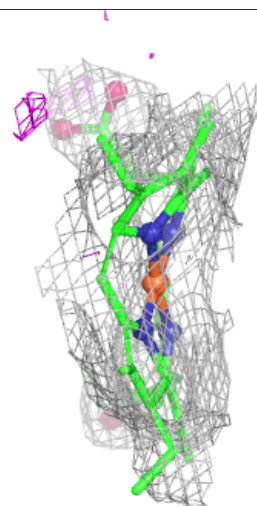
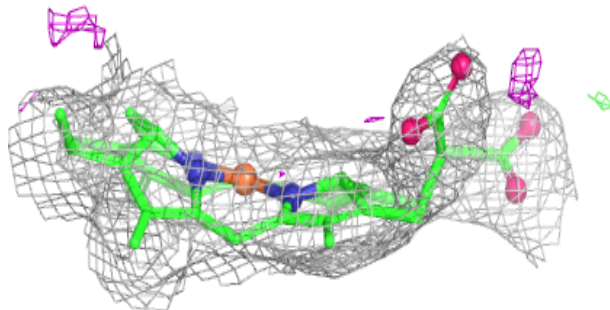
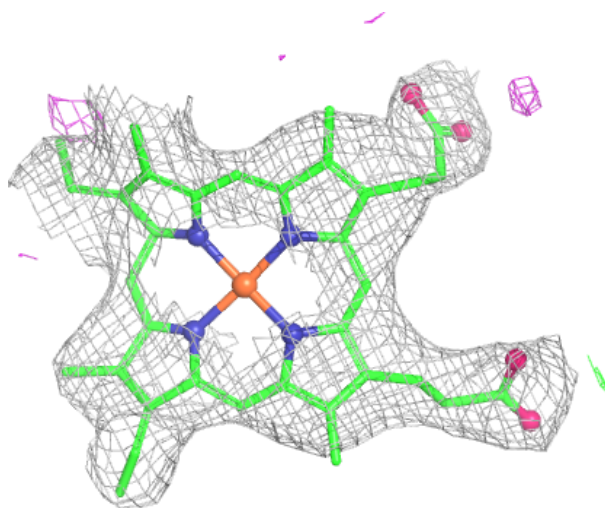
Electron density around HEC M 603:

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



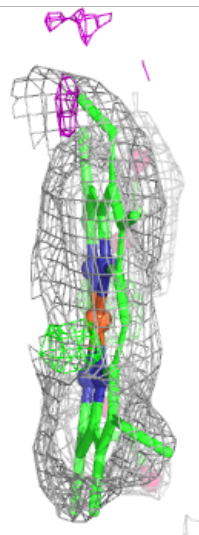
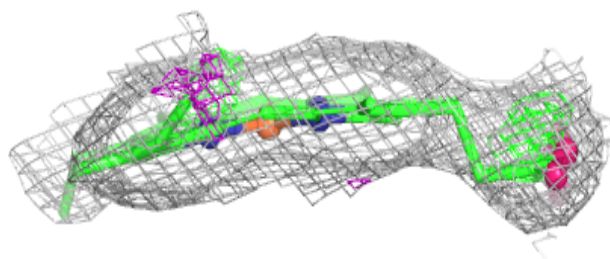
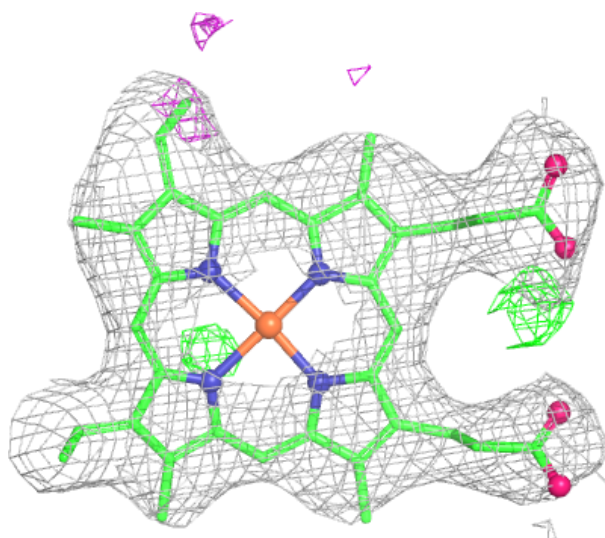
Electron density around HEC N 603:

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



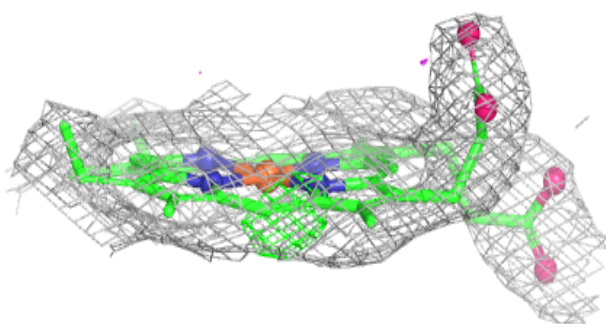
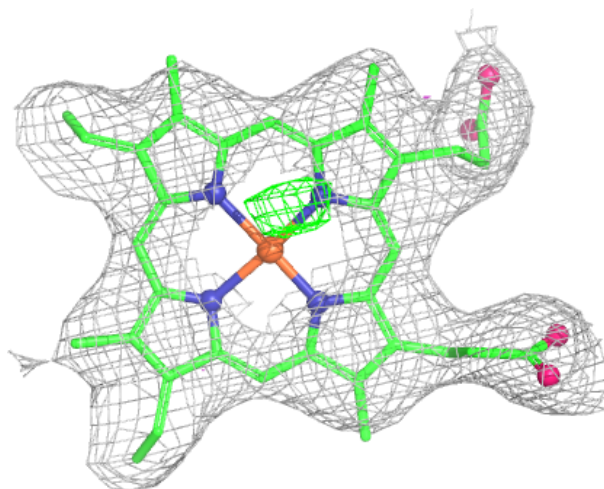
Electron density around HEC E 600:

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



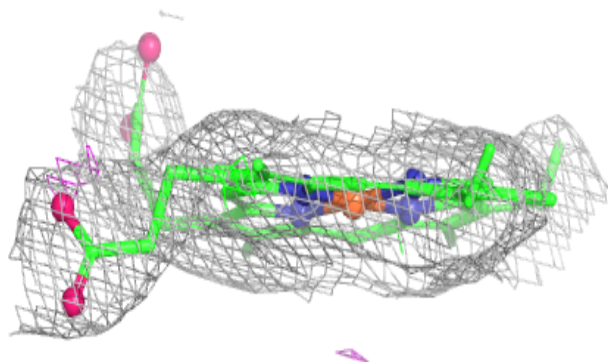
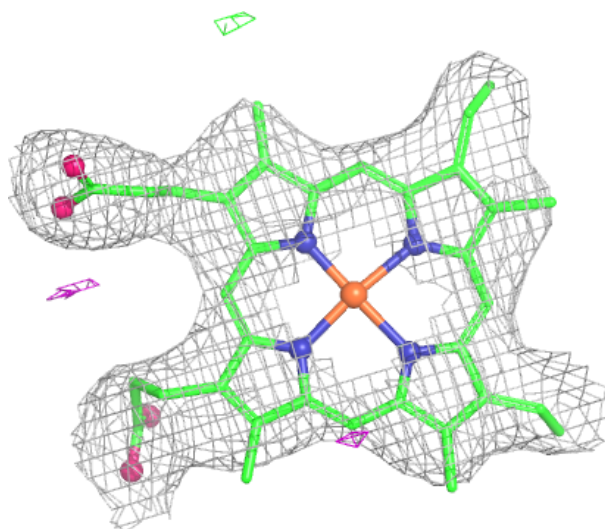
Electron density around HEC E 601:

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



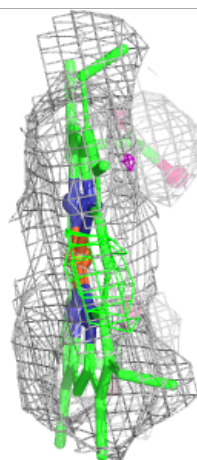
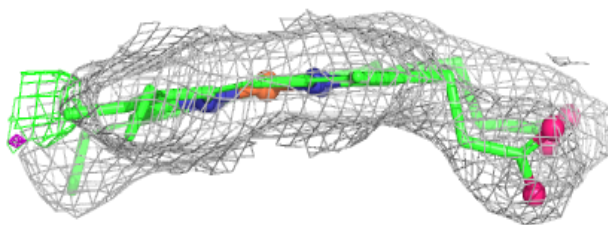
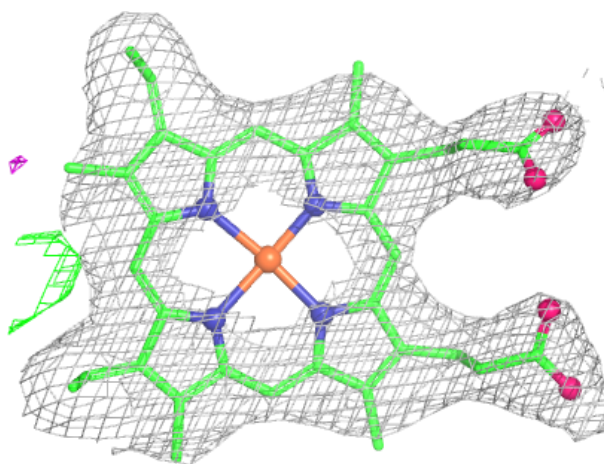
Electron density around HEC B 601:

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



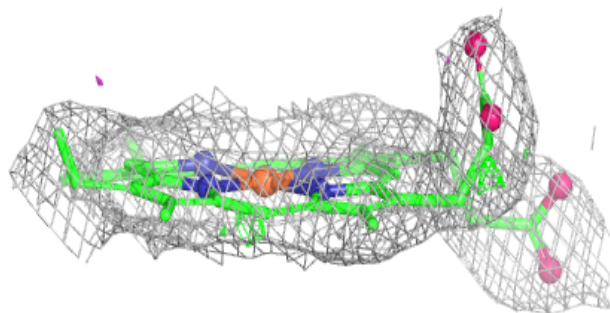
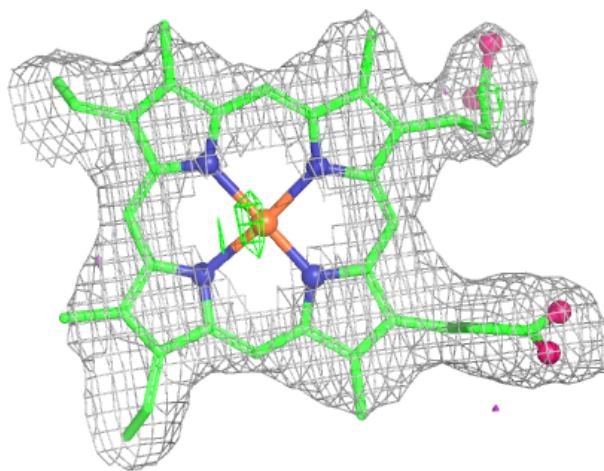
Electron density around HEC N 604:

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



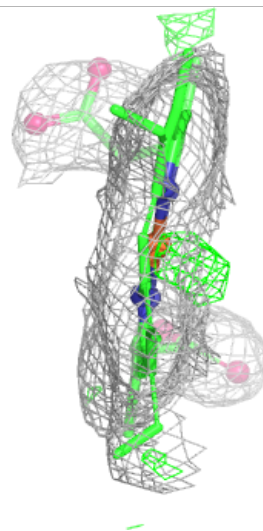
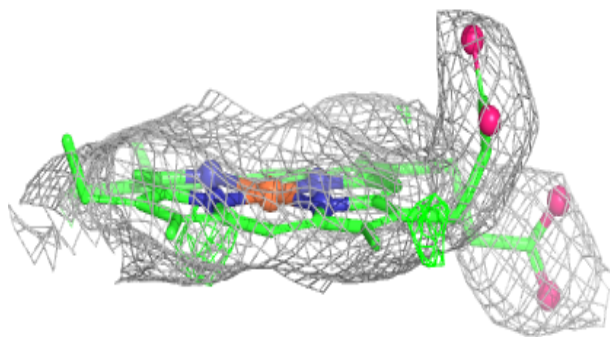
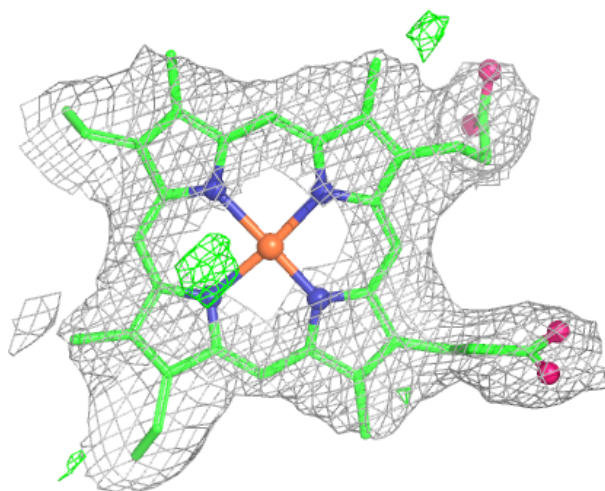
Electron density around HEC G 601:

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



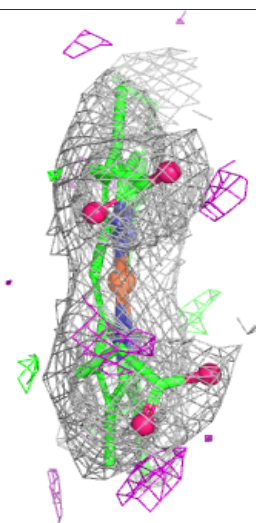
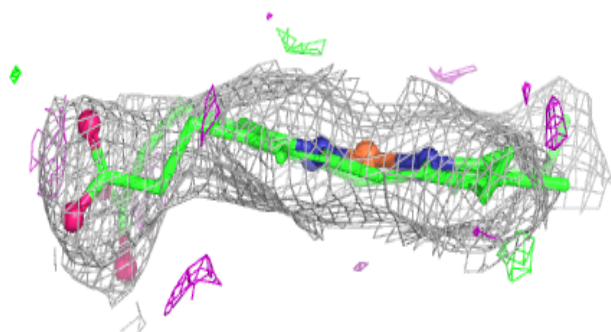
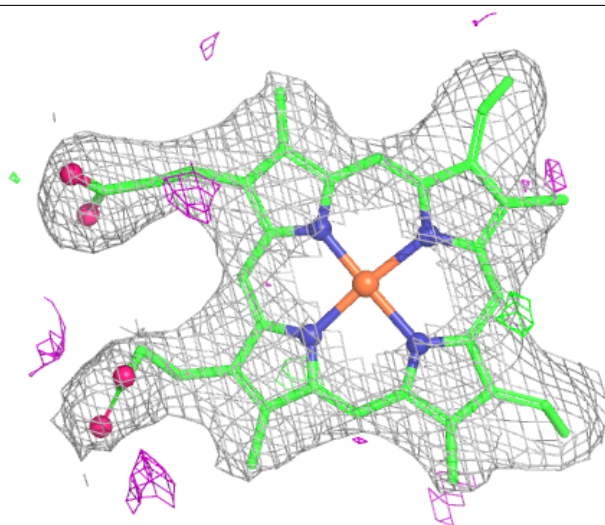
Electron density around HEC A 601:

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



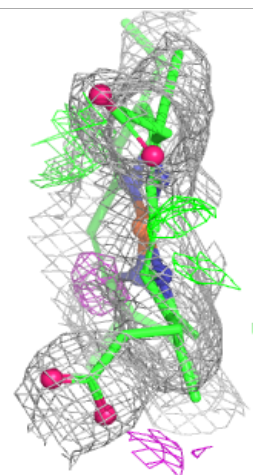
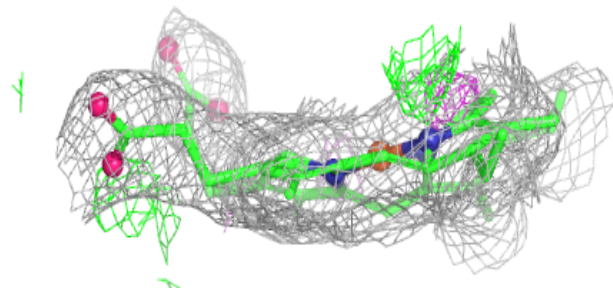
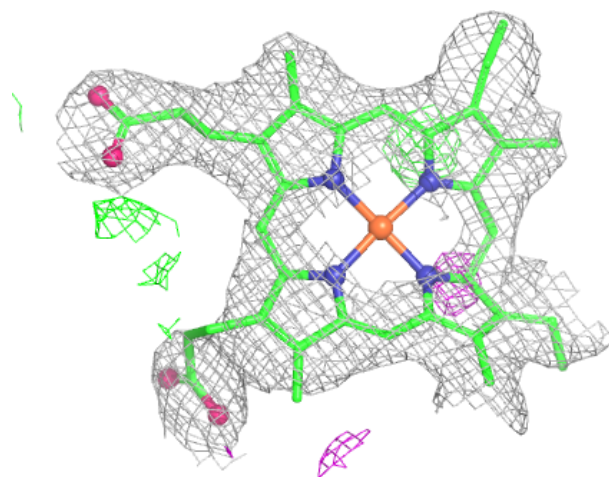
Electron density around HEC N 607:

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



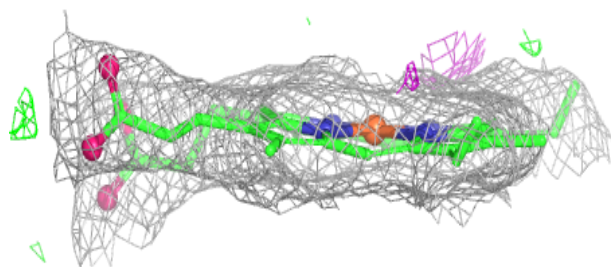
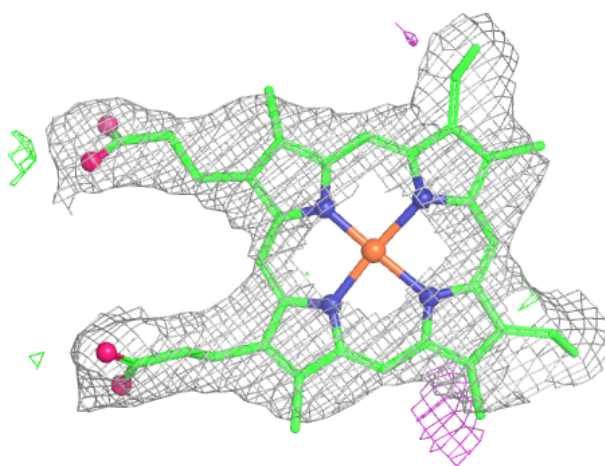
Electron density around HEC O 603:

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



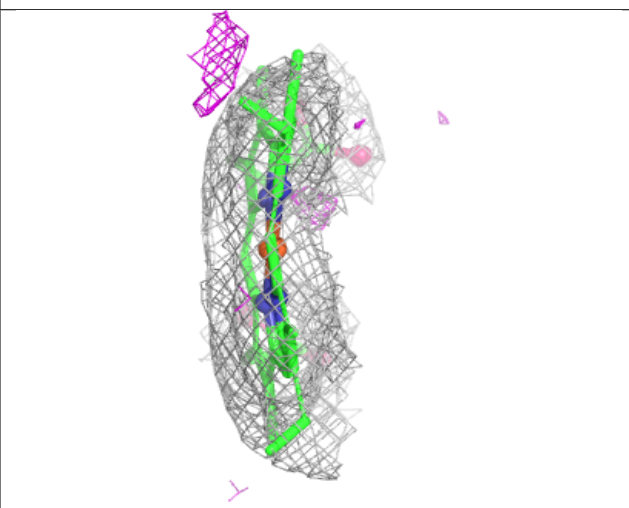
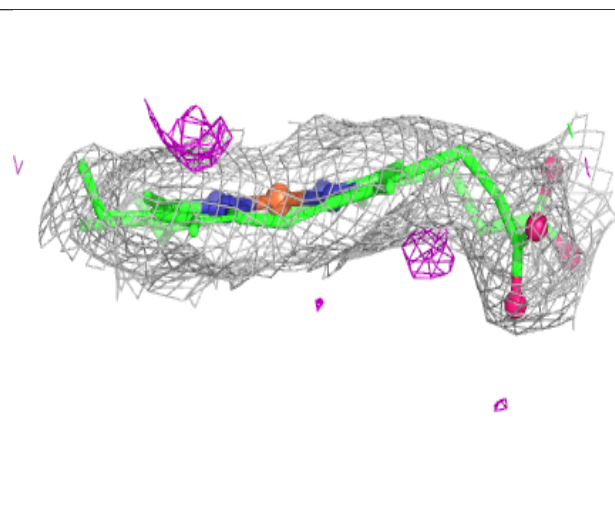
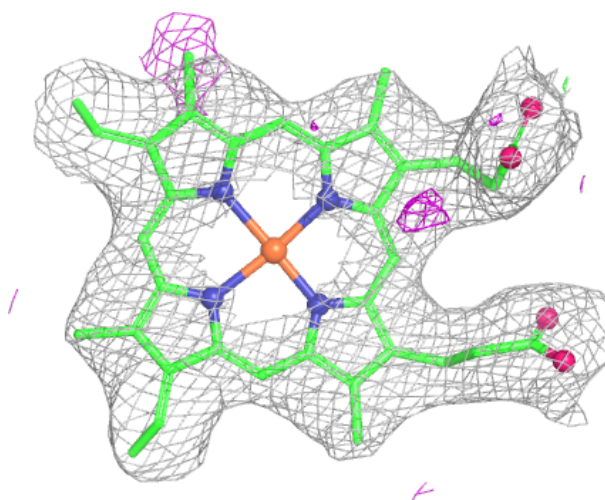
Electron density around HEC B 605:

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



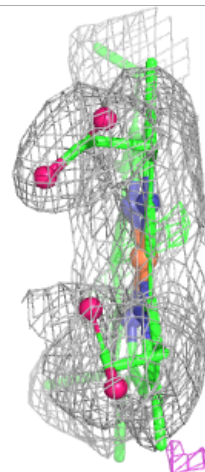
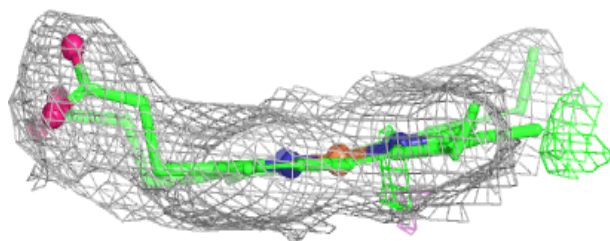
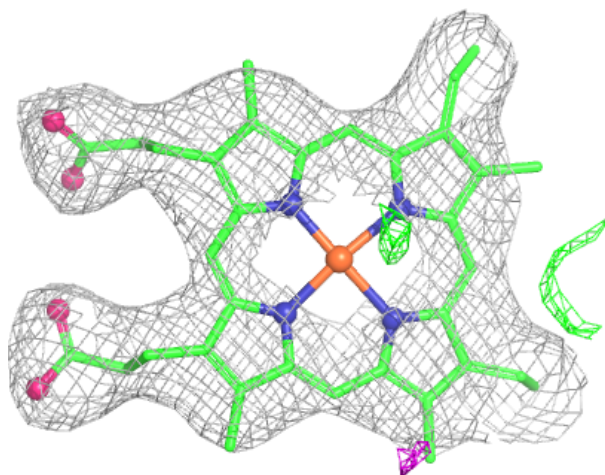
Electron density around HEC B 607:

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



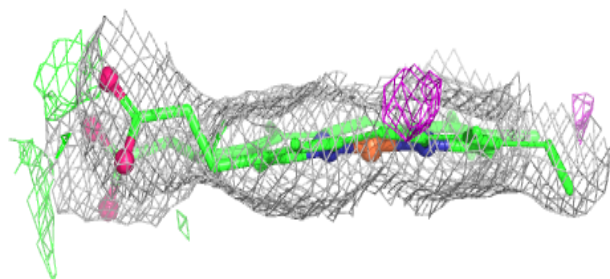
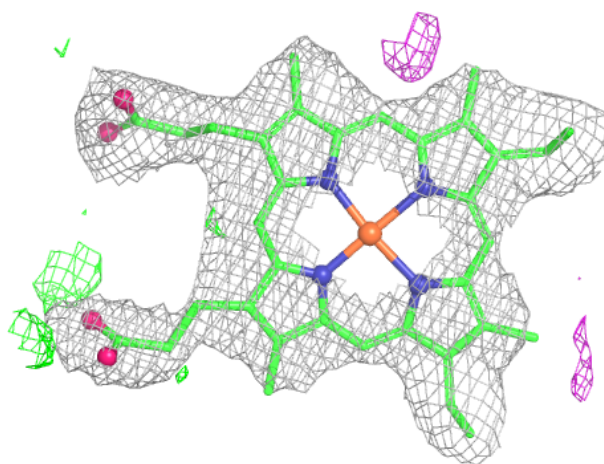
Electron density around HEC O 604:

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



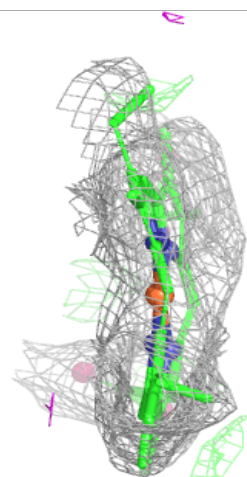
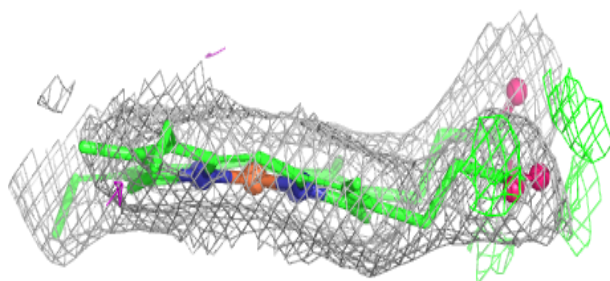
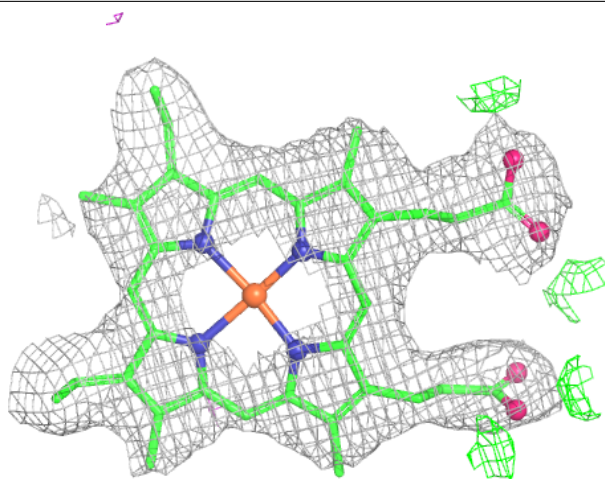
Electron density around HEC O 605:

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



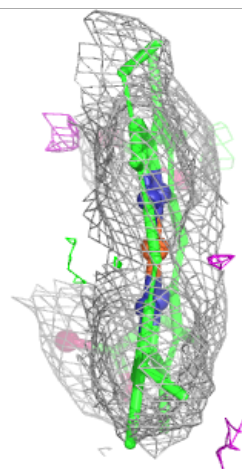
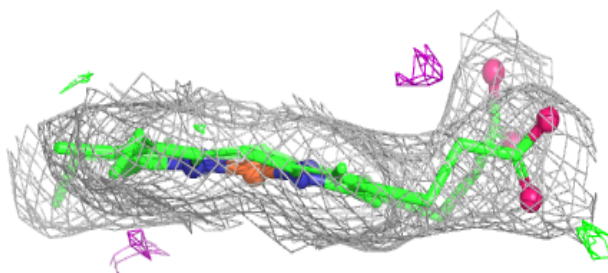
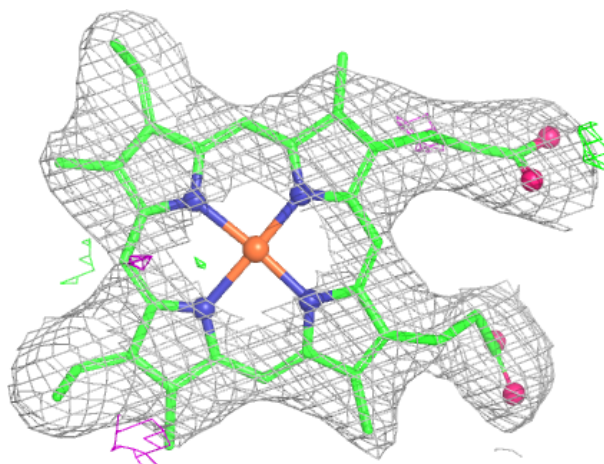
Electron density around HEC O 606:

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



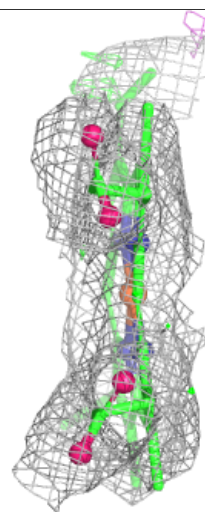
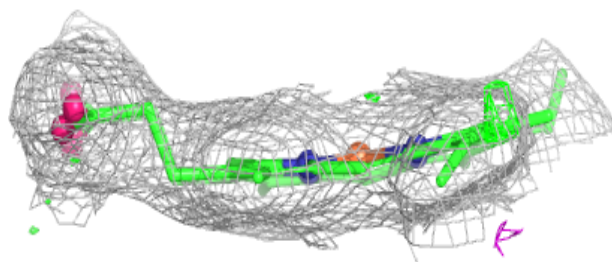
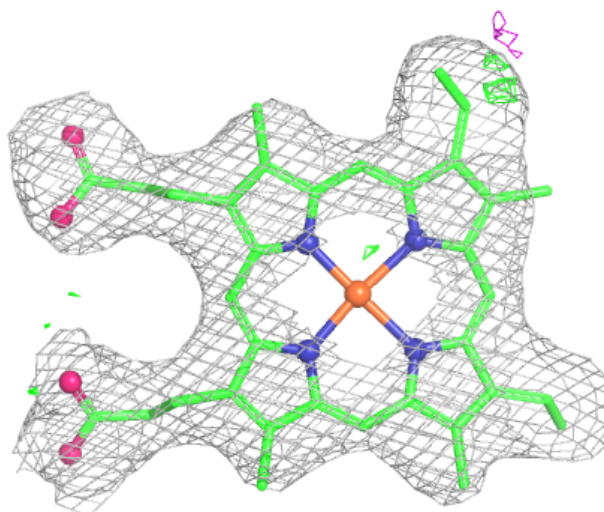
Electron density around HEC O 607:

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



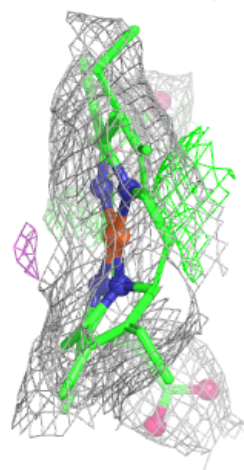
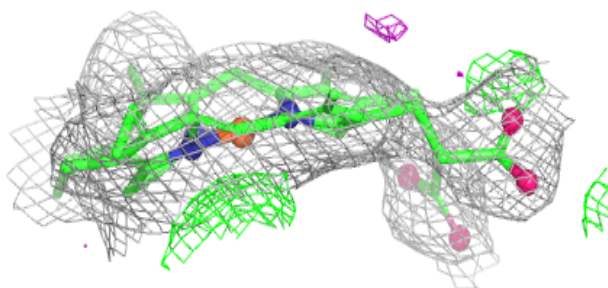
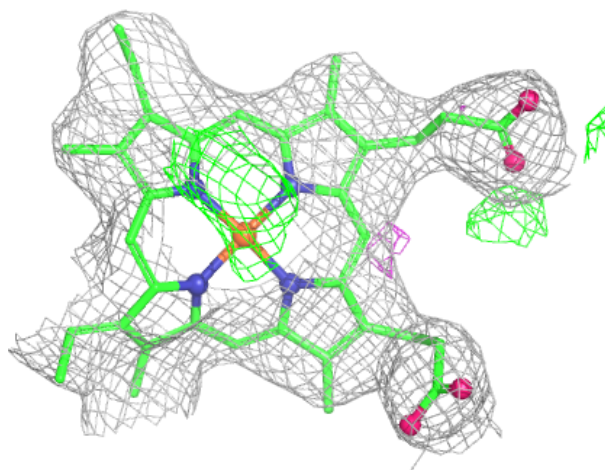
Electron density around HEC P 600:

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



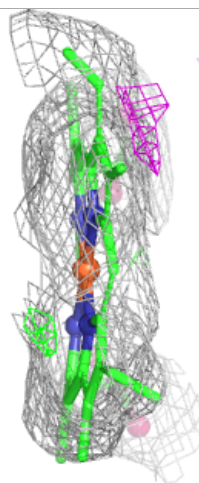
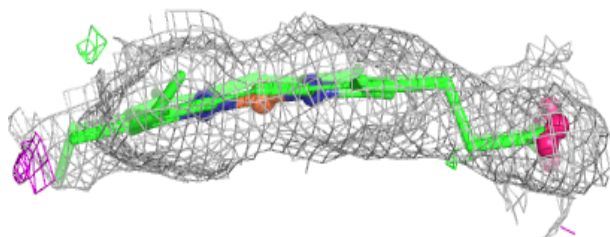
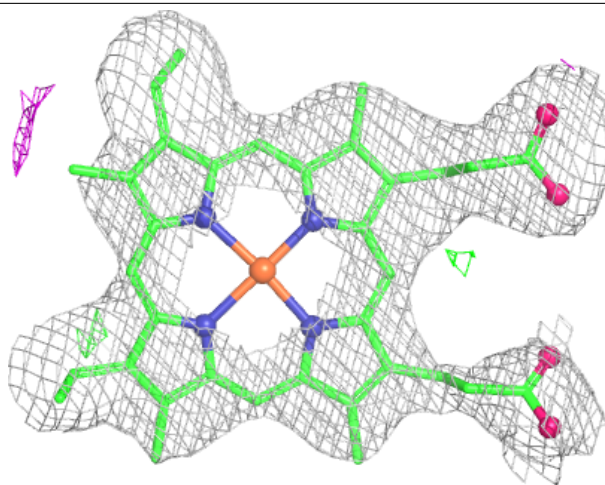
Electron density around HEC C 603:

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



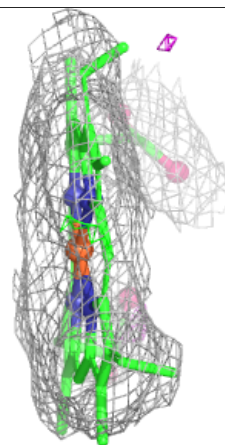
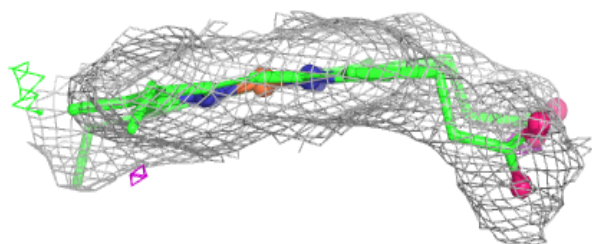
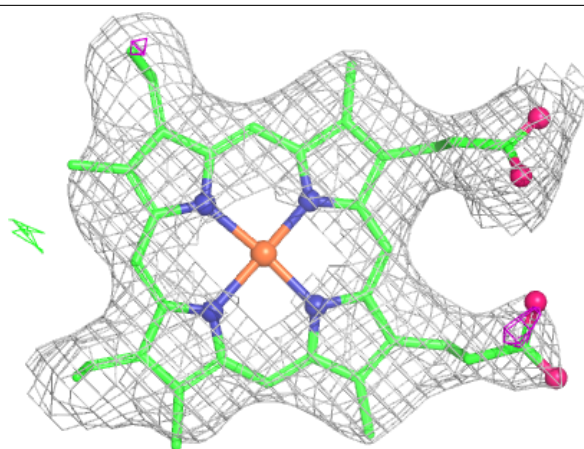
Electron density around HEC C 600:

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



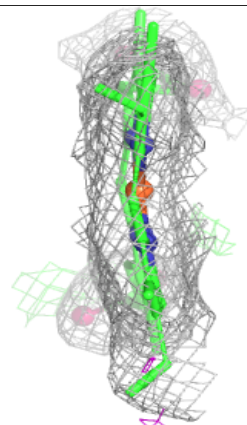
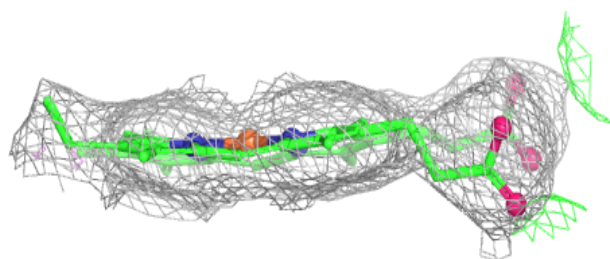
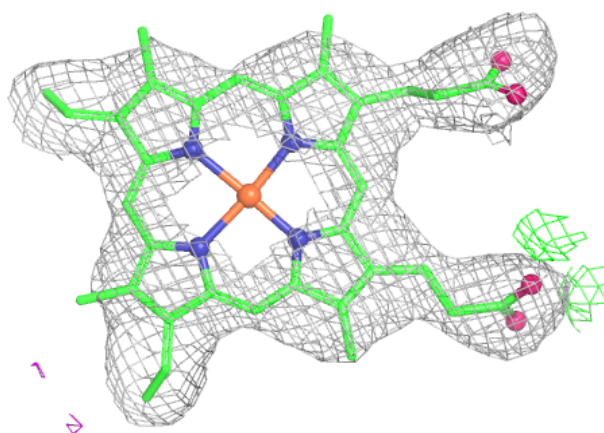
Electron density around HEC P 604:

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



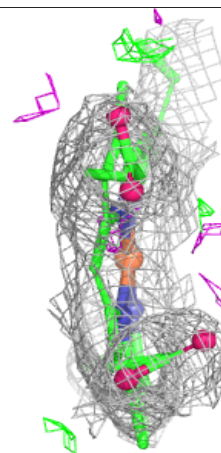
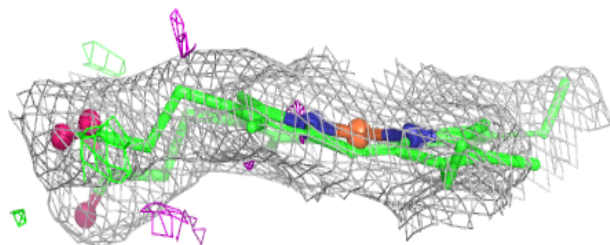
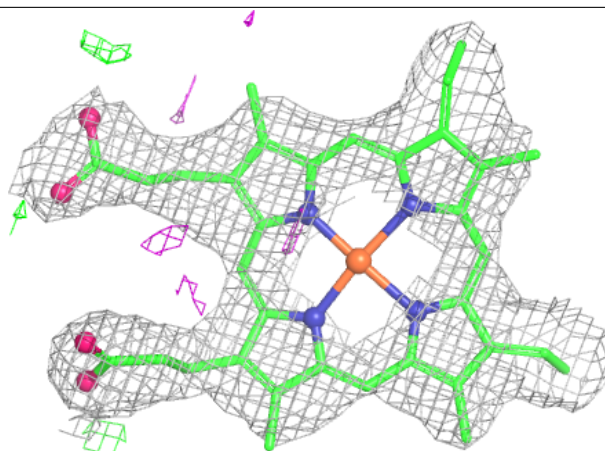
Electron density around HEC P 605:

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



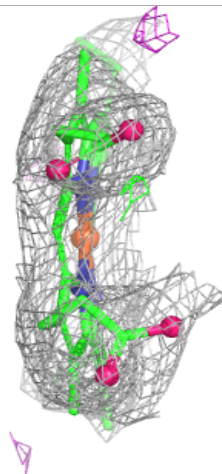
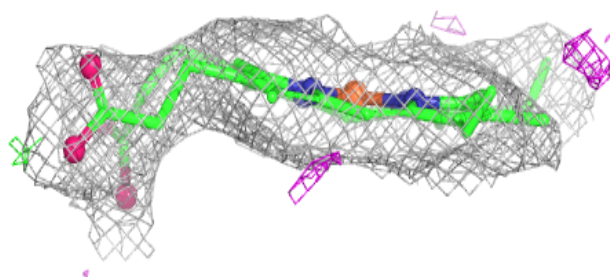
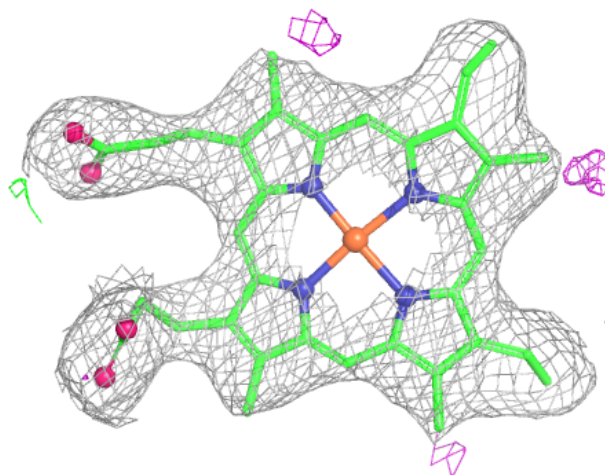
Electron density around HEC P 606:

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



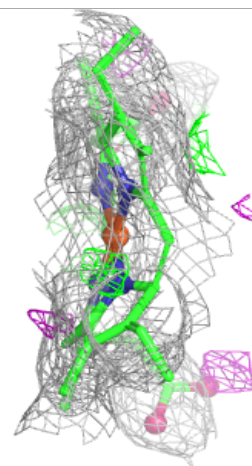
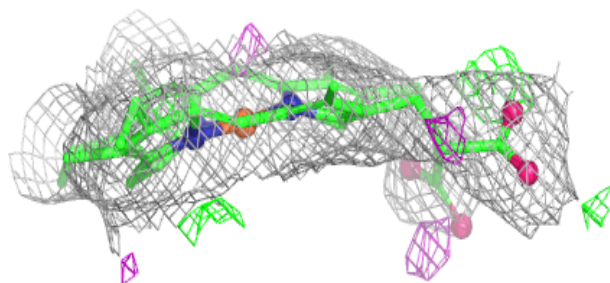
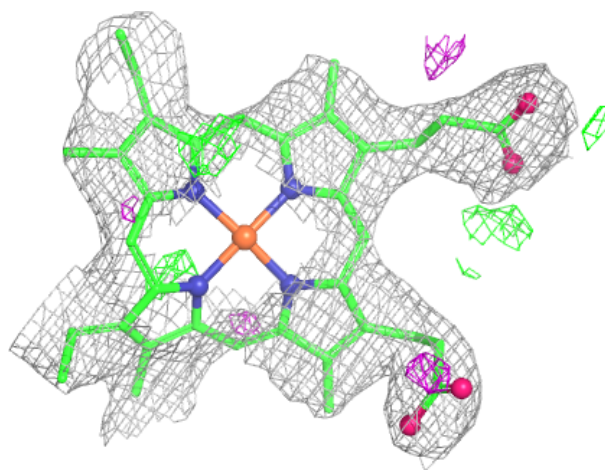
Electron density around HEC P 607:

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



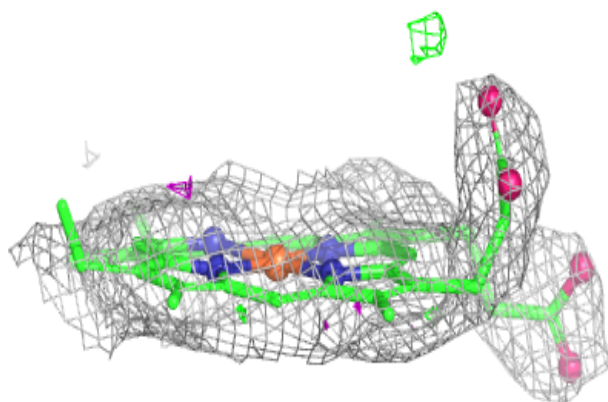
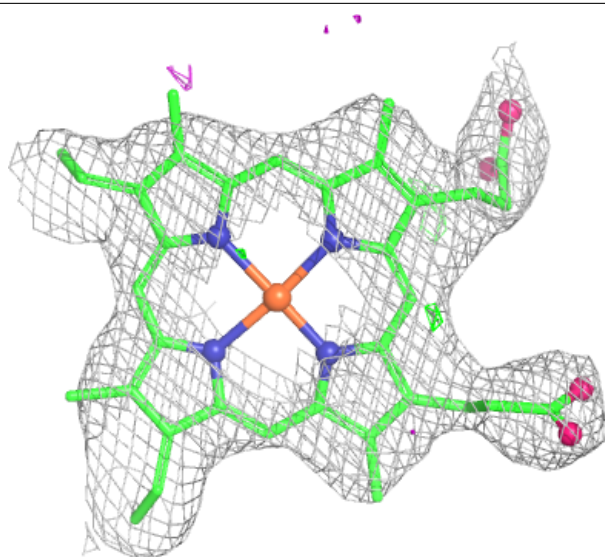
Electron density around HEC P 603:

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



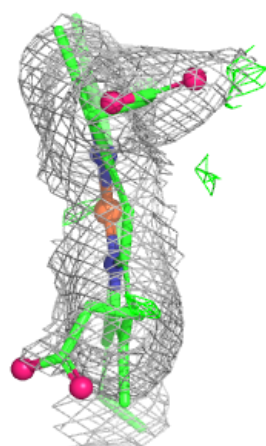
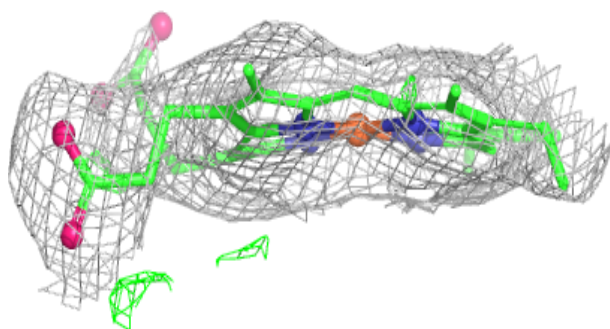
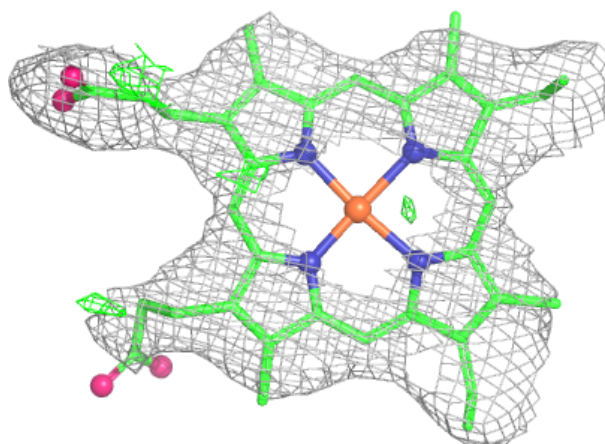
Electron density around HEC C 601:

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



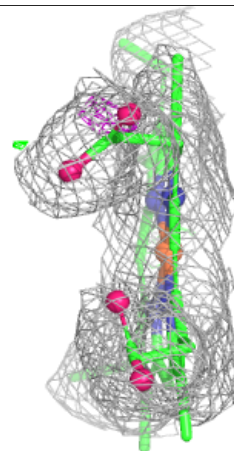
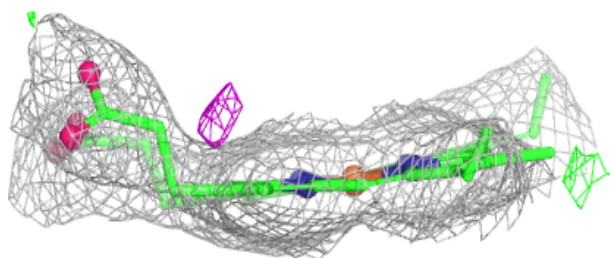
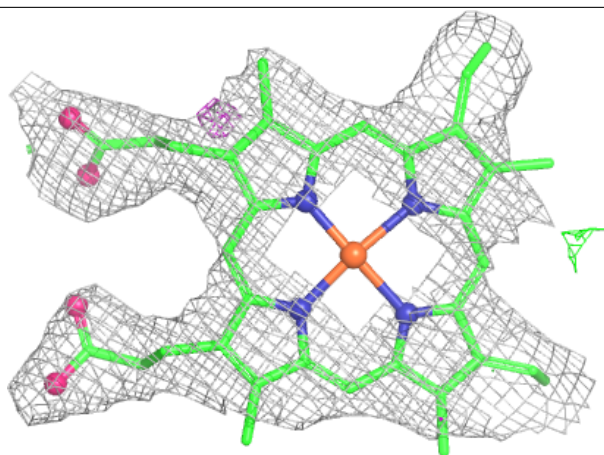
Electron density around HEC C 602:

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



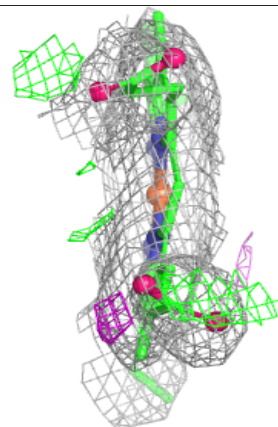
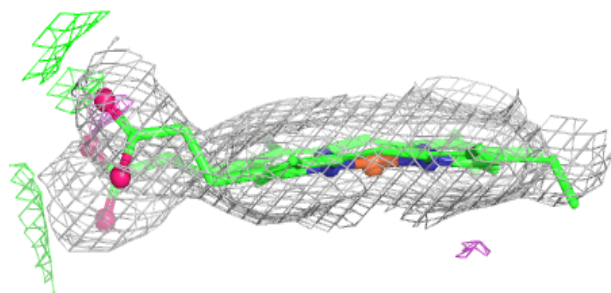
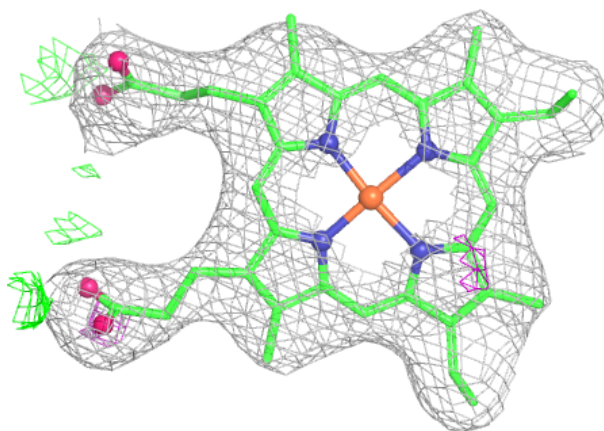
Electron density around HEC C 604:

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



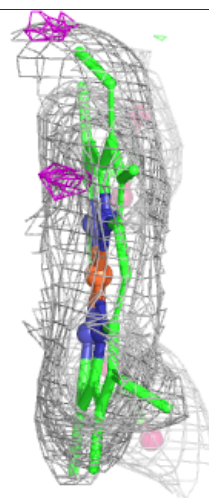
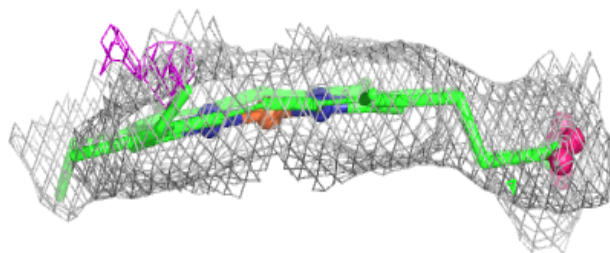
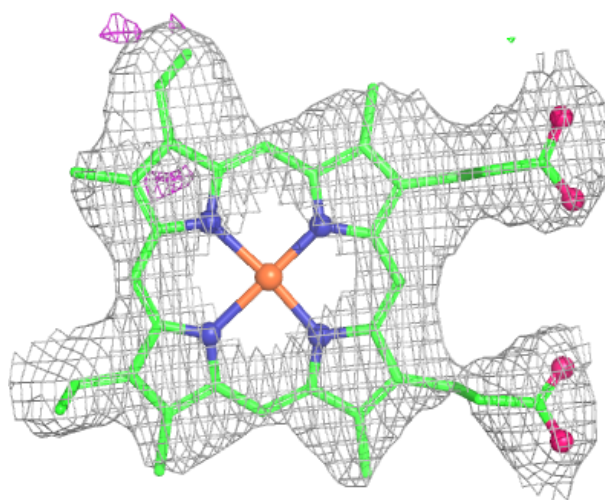
Electron density around HEC C 605:

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



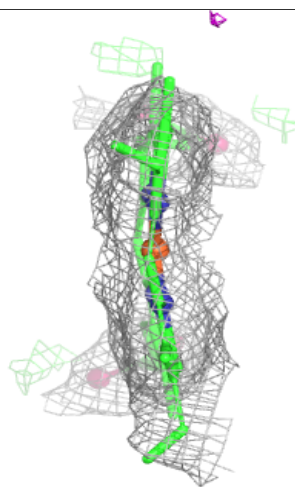
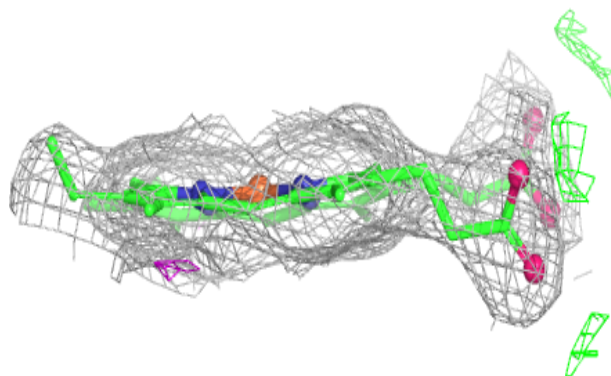
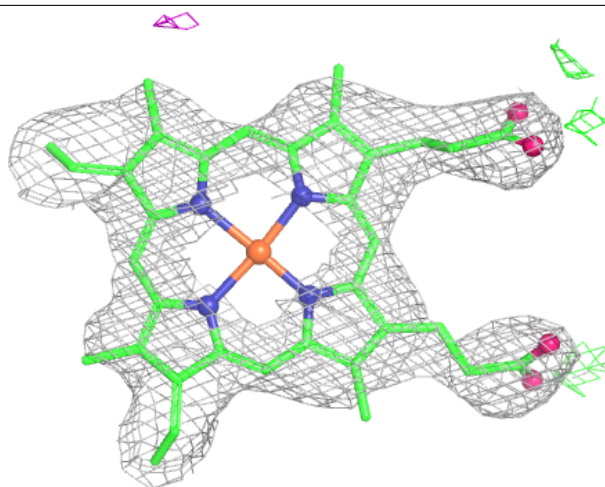
Electron density around HEC G 600:

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



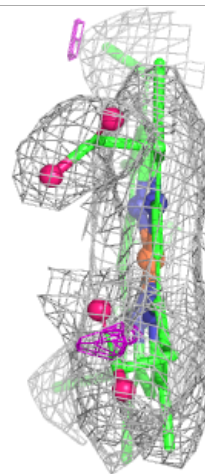
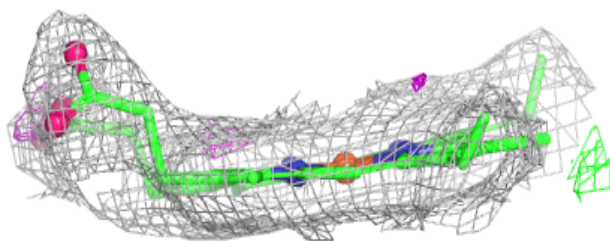
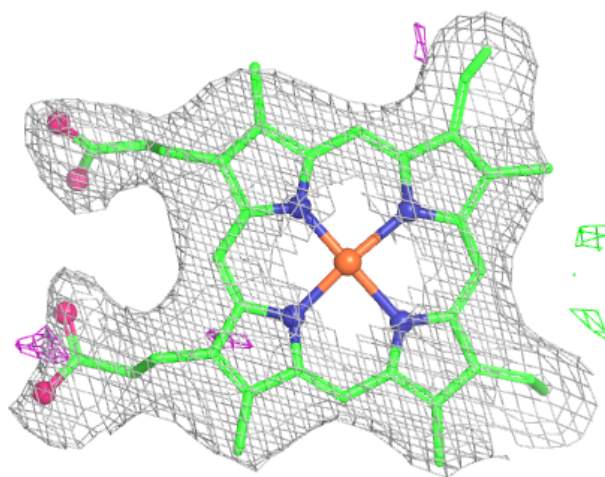
Electron density around HEC Q 605:

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



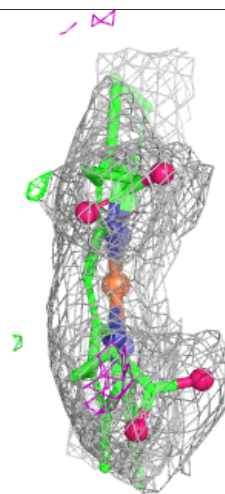
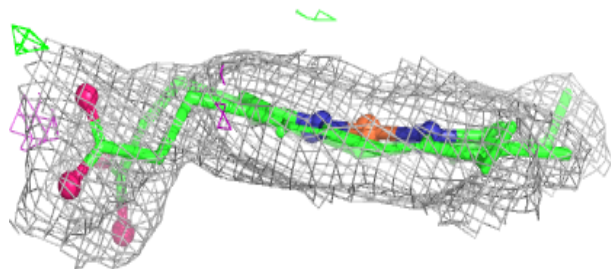
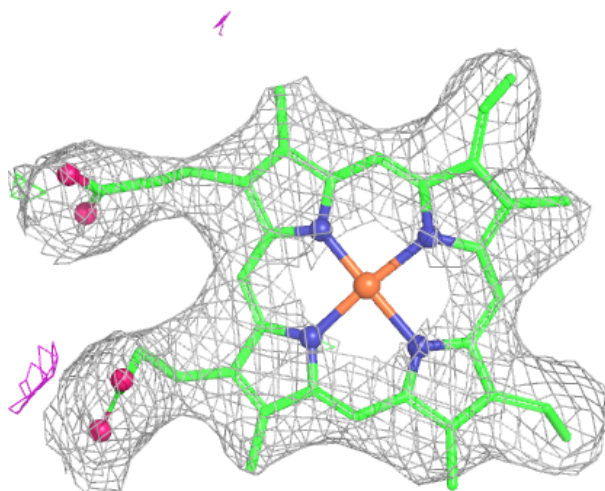
Electron density around HEC G 604:

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



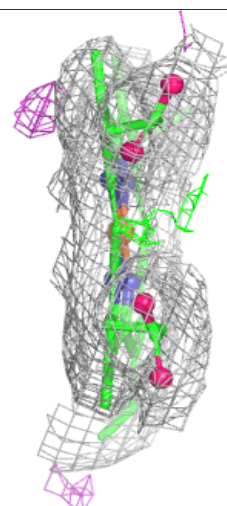
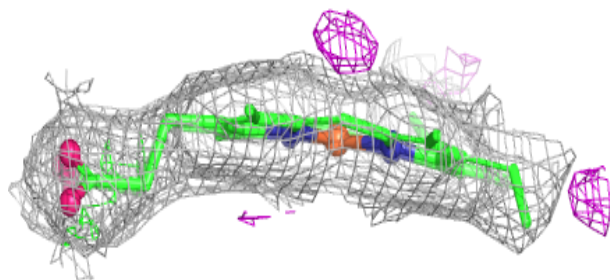
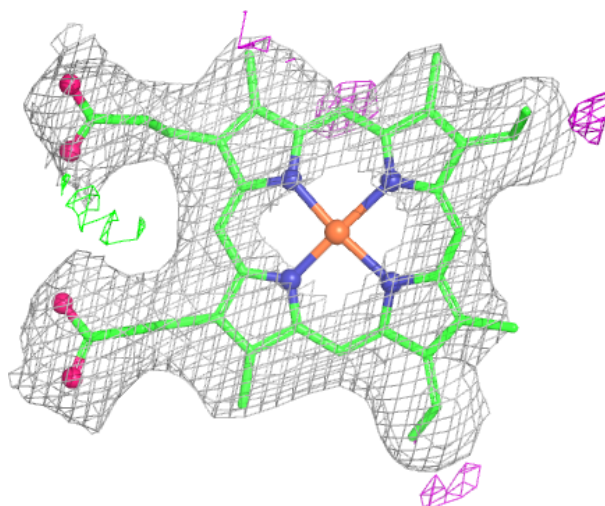
Electron density around HEC Q 607:

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



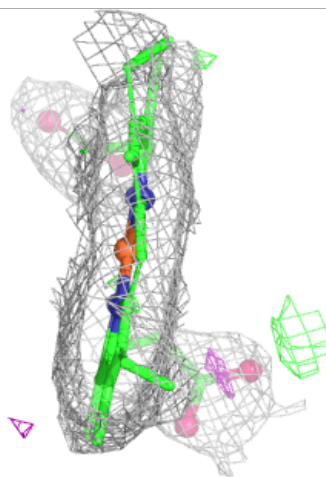
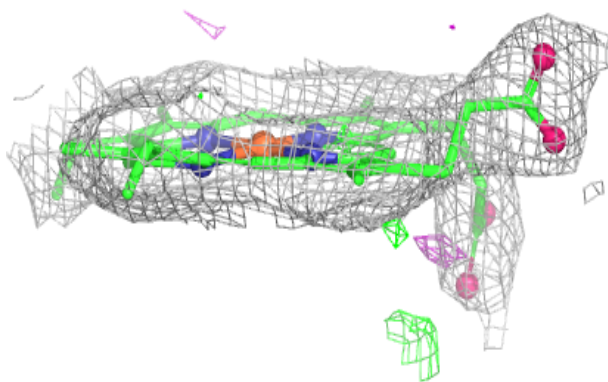
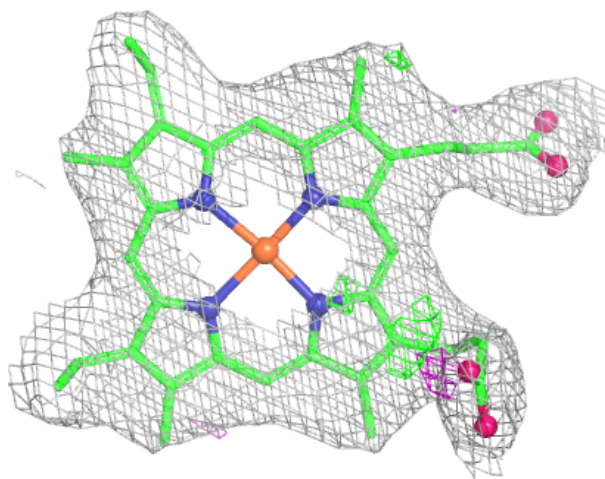
Electron density around HEC H 600:

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



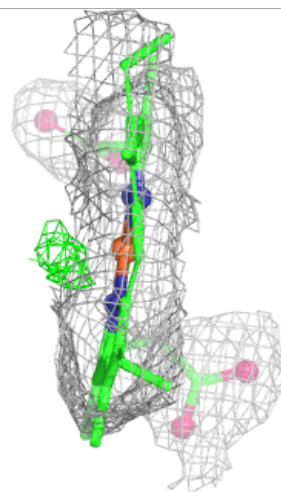
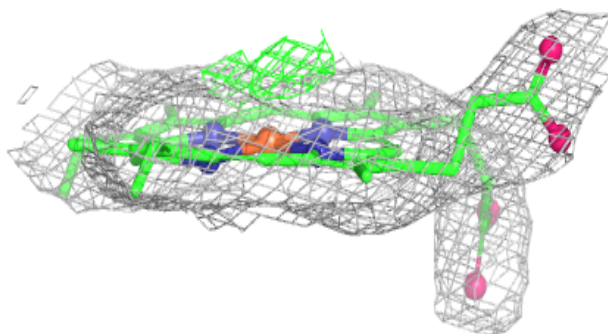
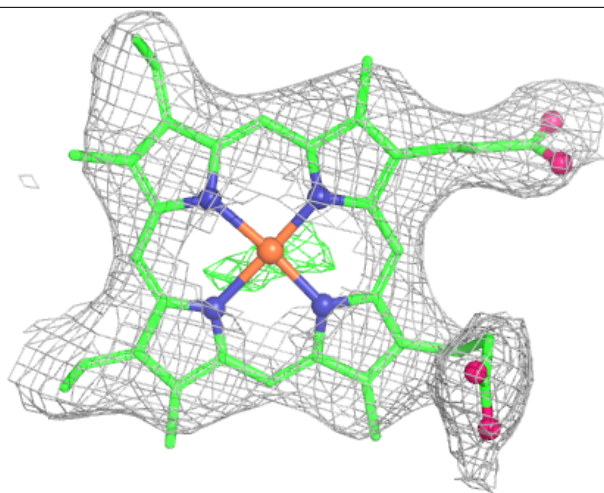
Electron density around HEC H 601:

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



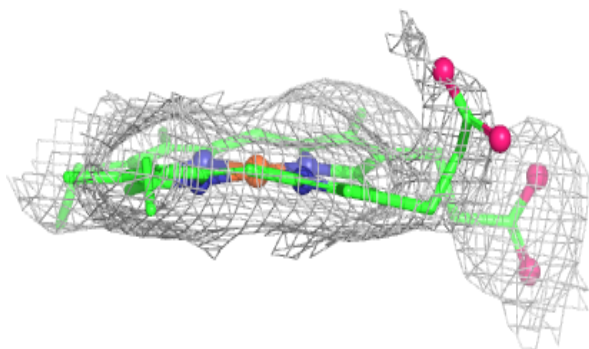
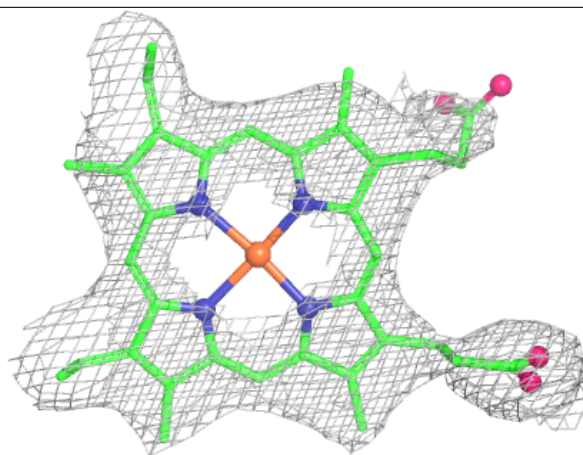
Electron density around HEC R 601:

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



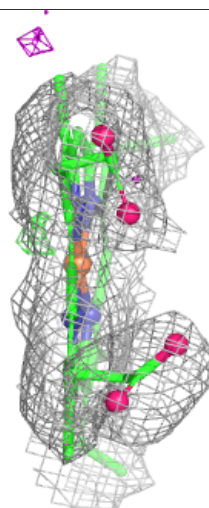
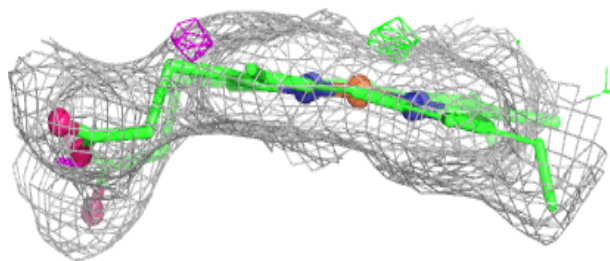
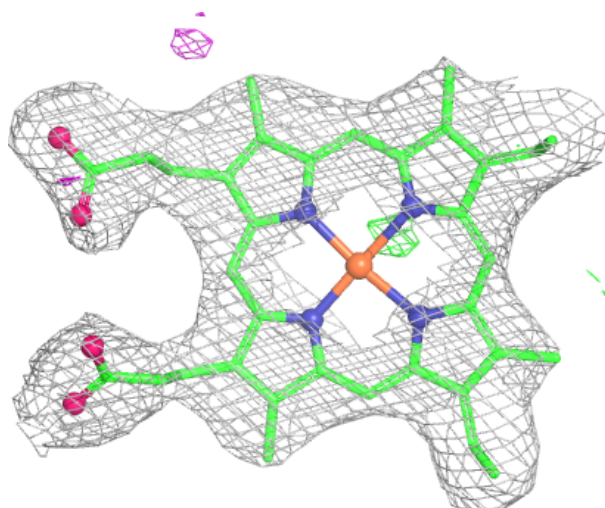
Electron density around HEC R 602:

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



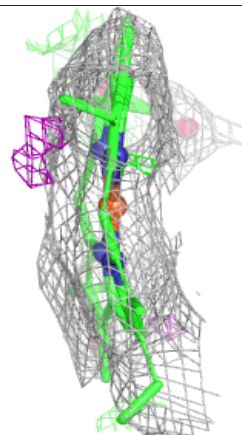
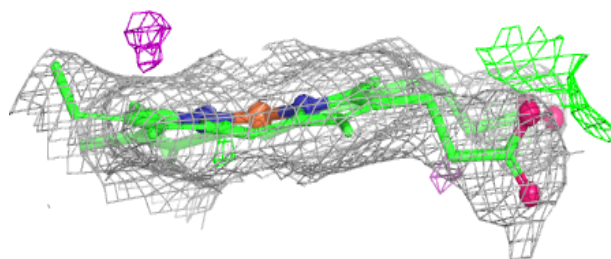
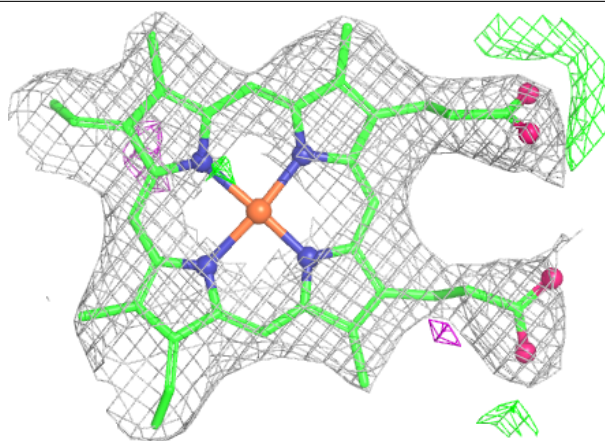
Electron density around HEC R 604:

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



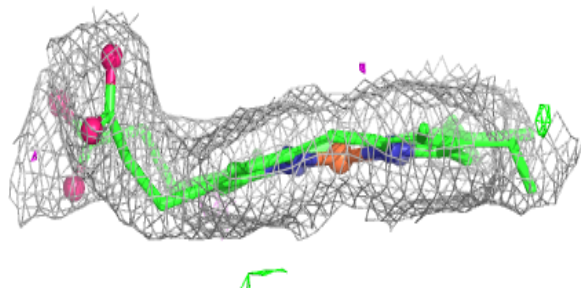
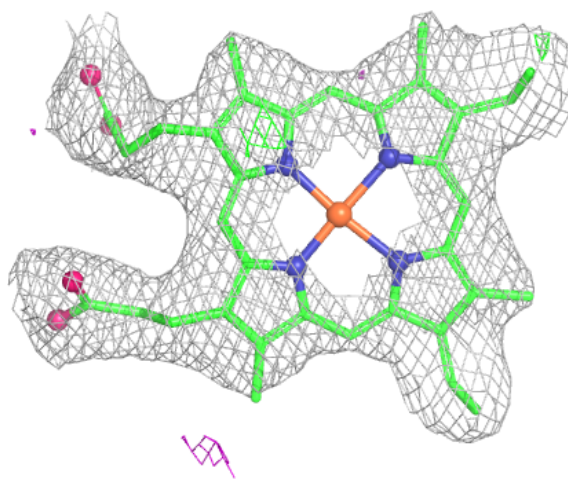
Electron density around HEC R 606:

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



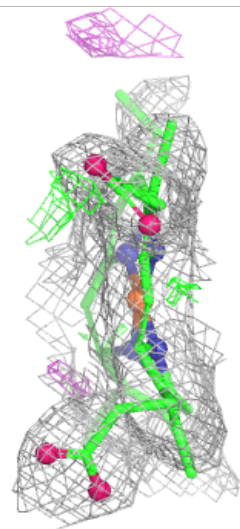
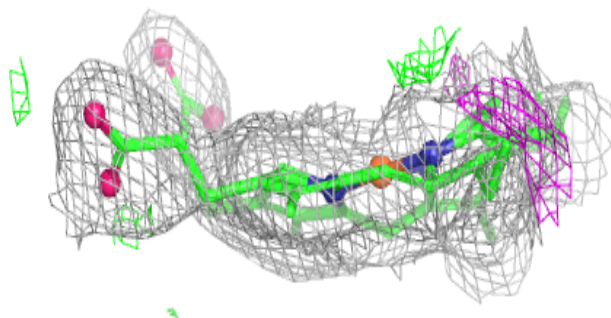
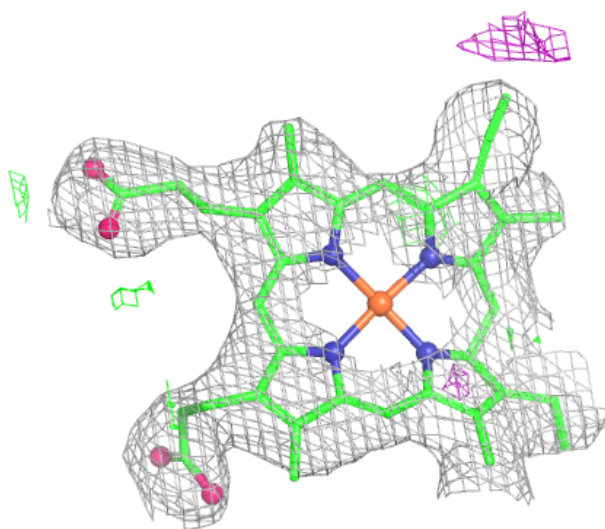
Electron density around HEC R 607:

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



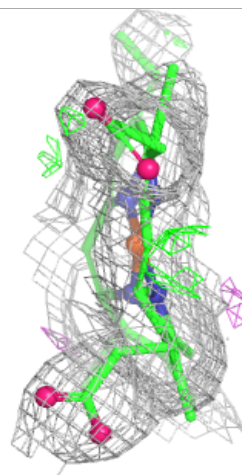
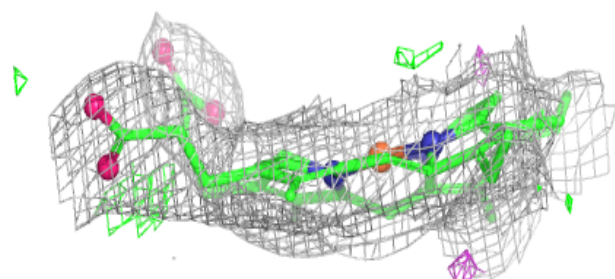
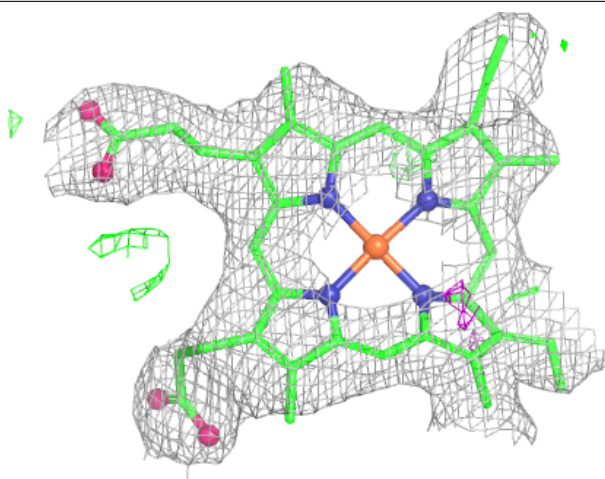
Electron density around HEC J 603:

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



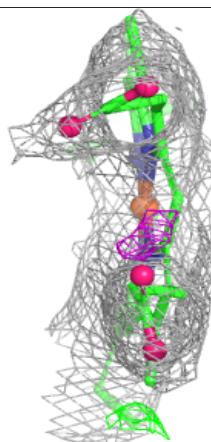
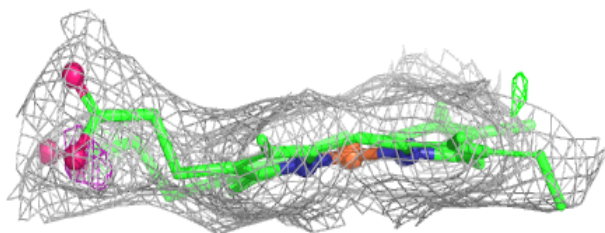
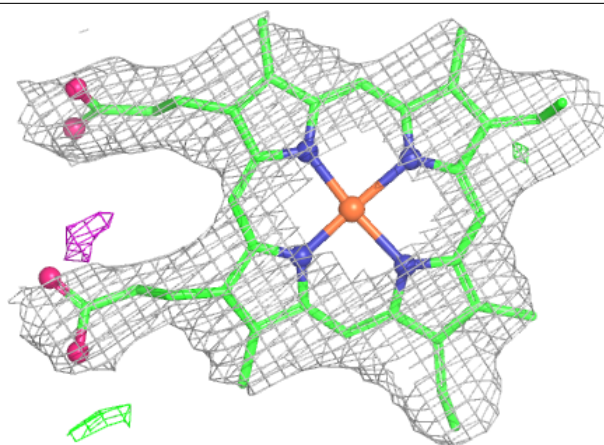
Electron density around HEC K 603:

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



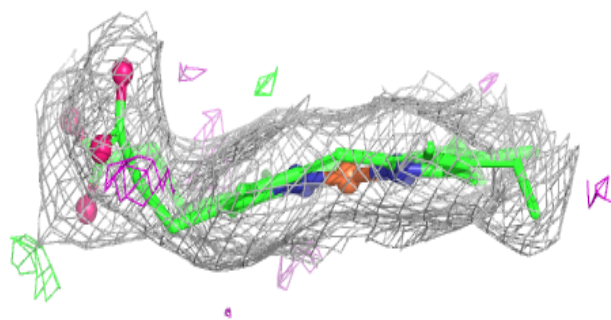
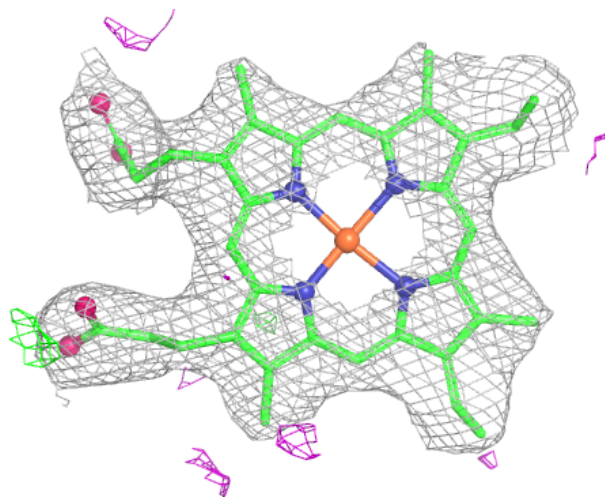
Electron density around HEC B 606:

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



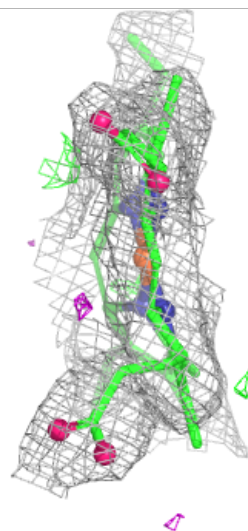
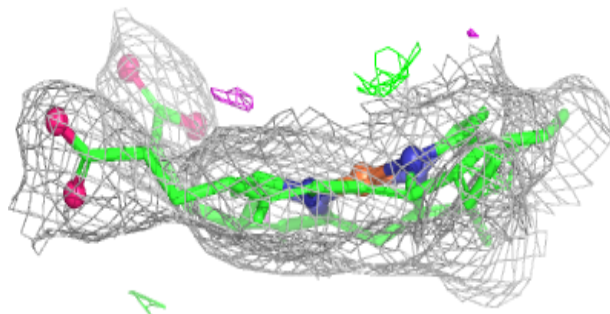
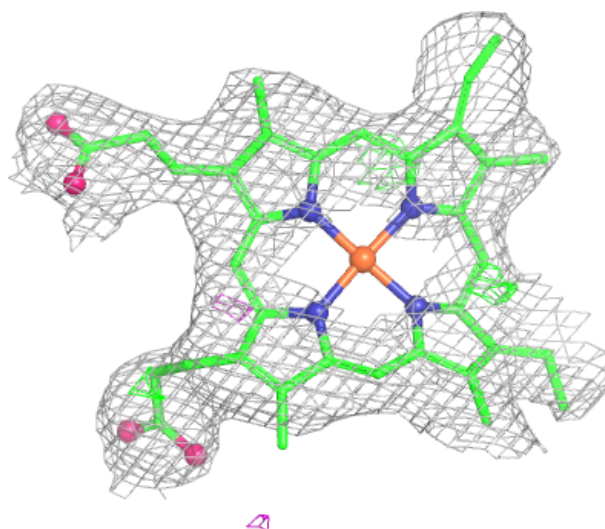
Electron density around HEC H 607:

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



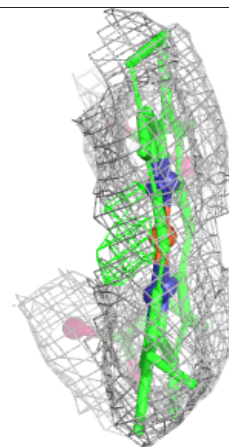
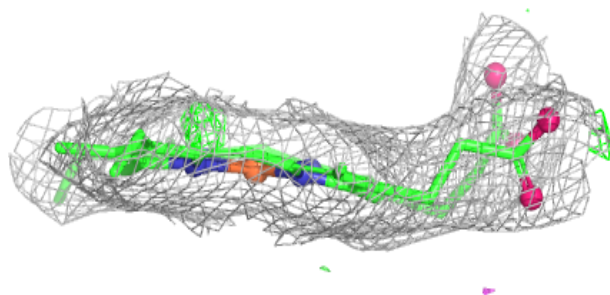
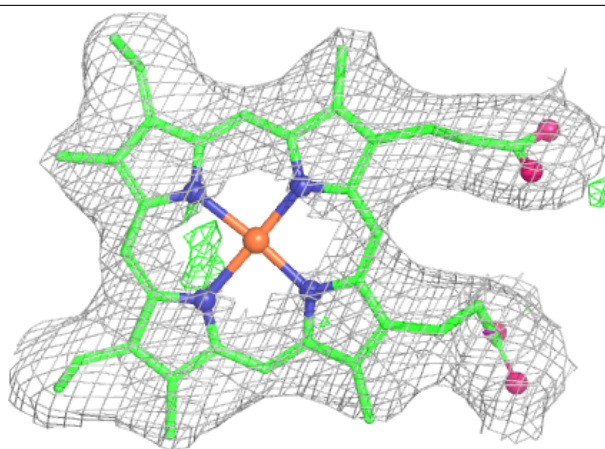
Electron density around HEC I 603:

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



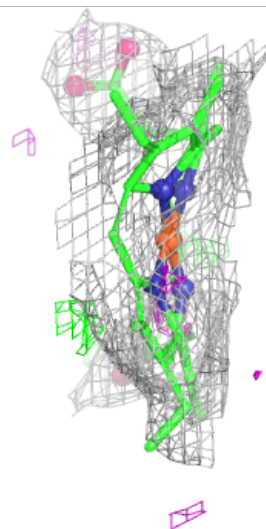
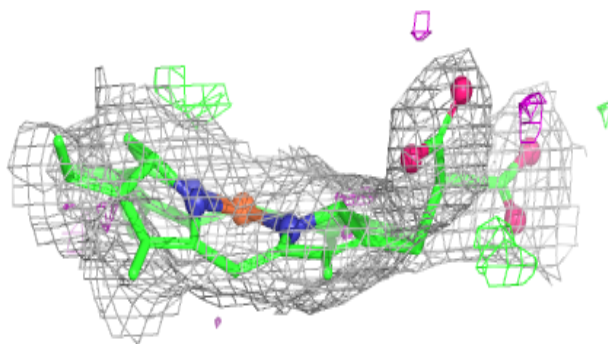
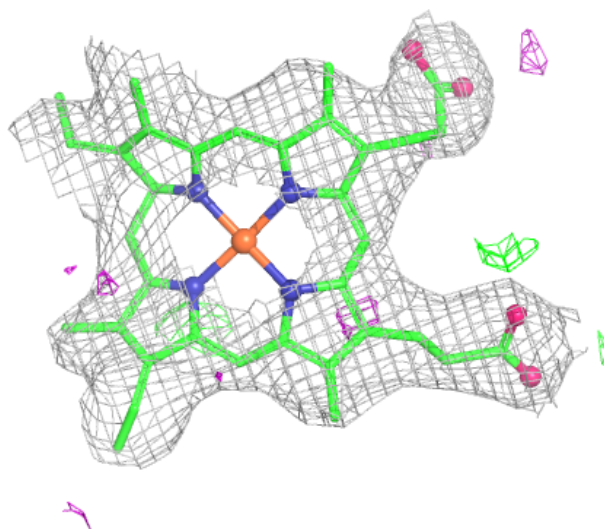
Electron density around HEC G 607:

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



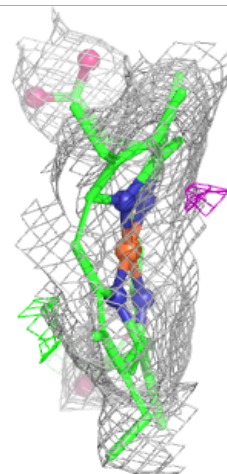
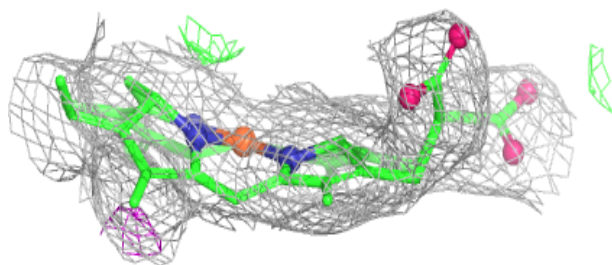
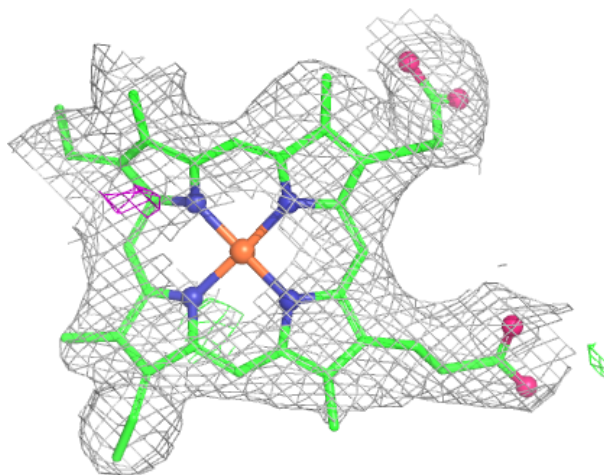
Electron density around HEC G 603:

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



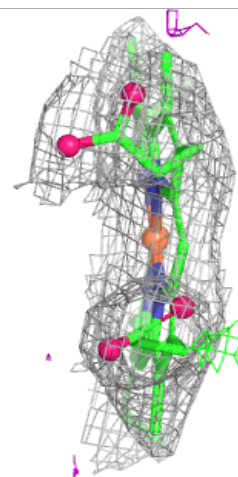
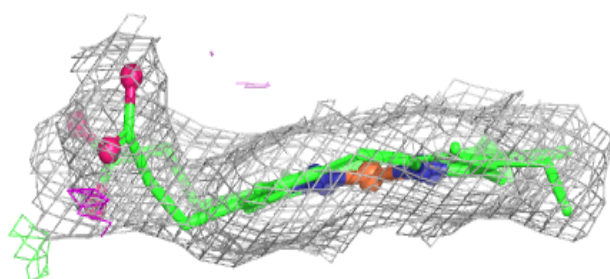
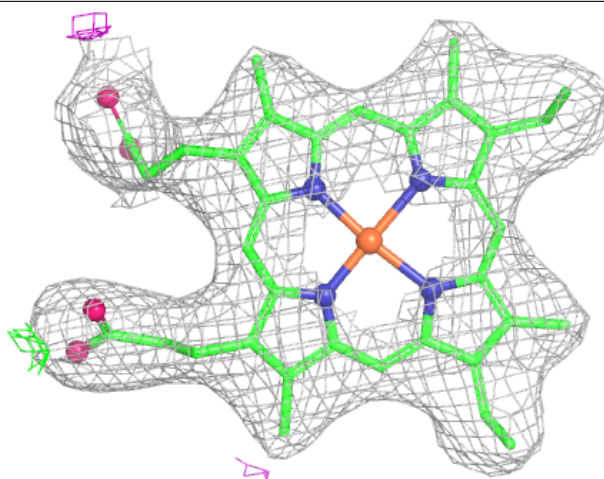
Electron density around HEC H 603:

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



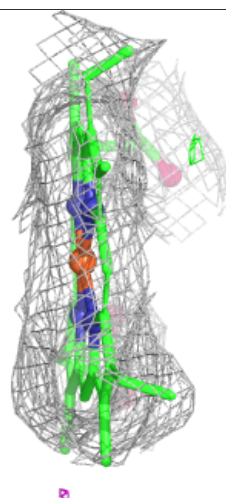
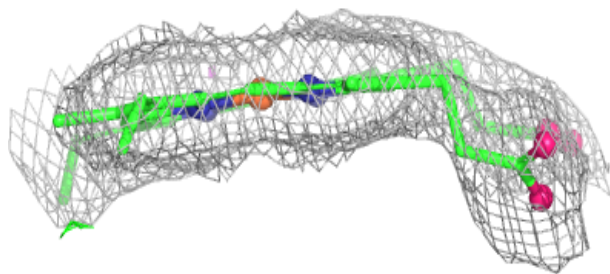
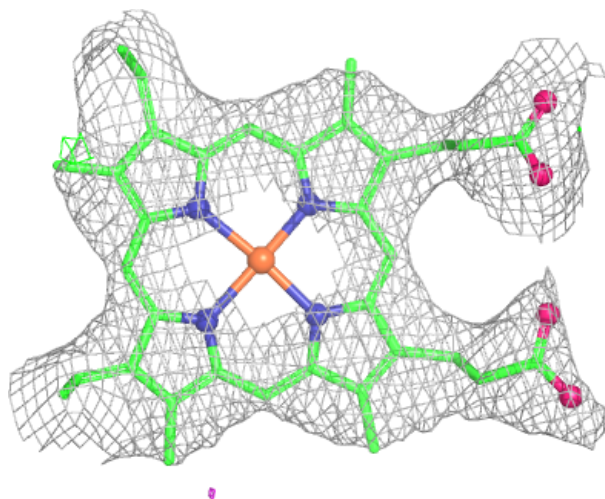
Electron density around HEC K 607:

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



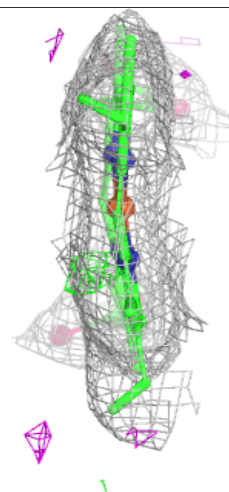
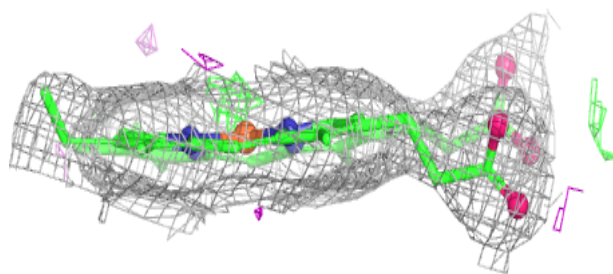
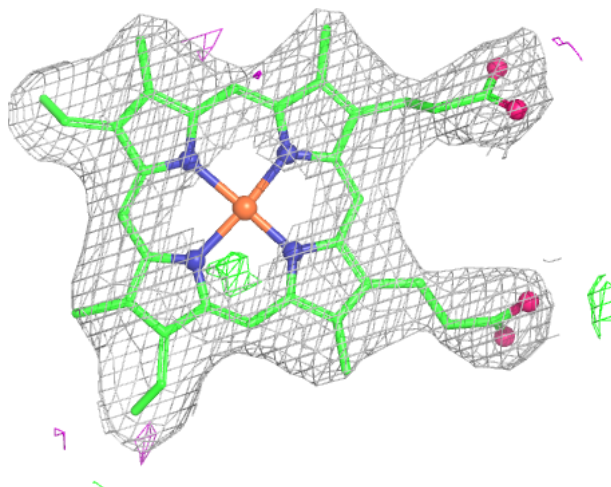
Electron density around HEC I 604:

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



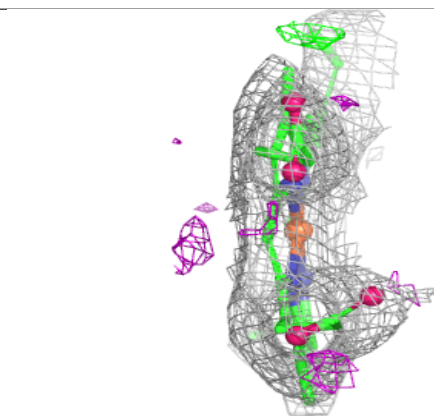
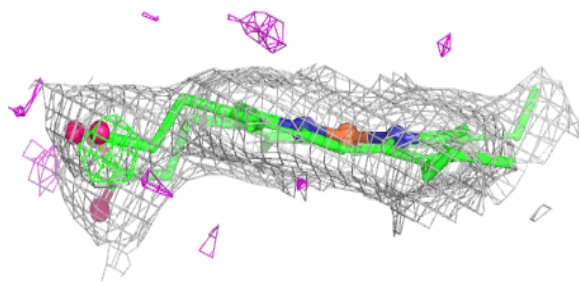
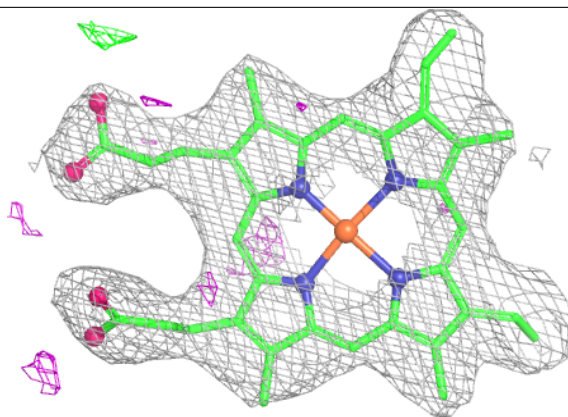
Electron density around HEC I 605:

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

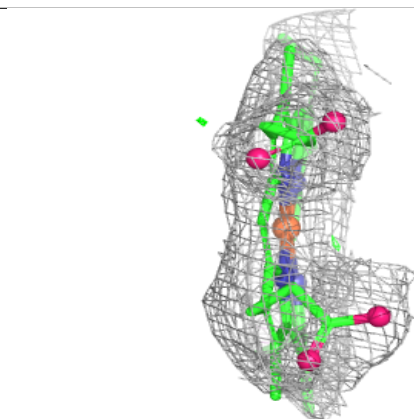
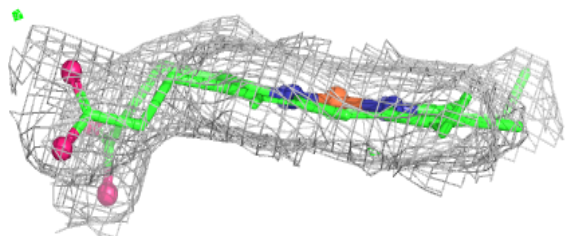
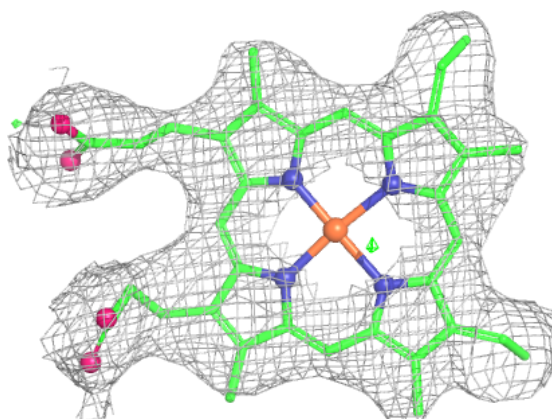


Electron density around HEC I 606:

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

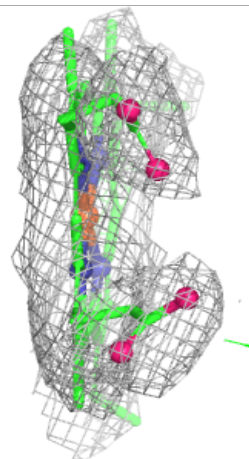
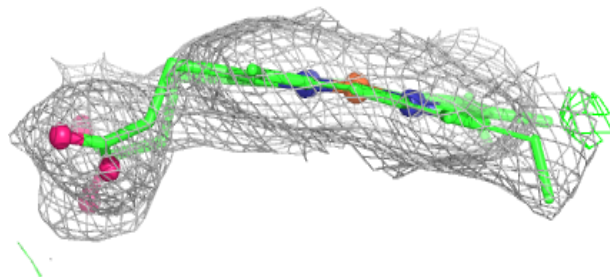
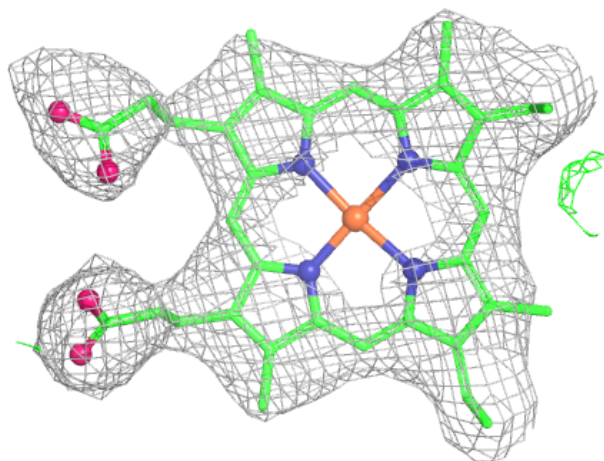
**Electron density around HEC I 607:**

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



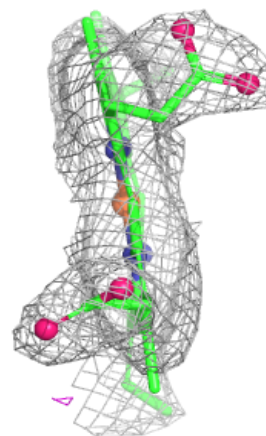
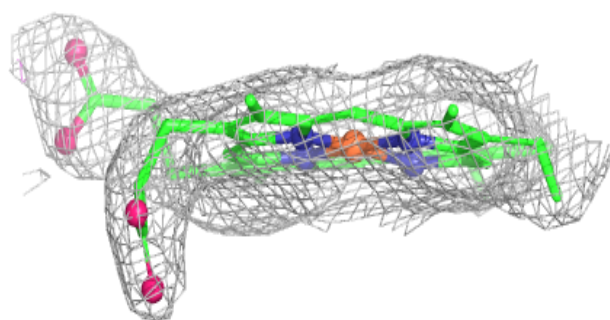
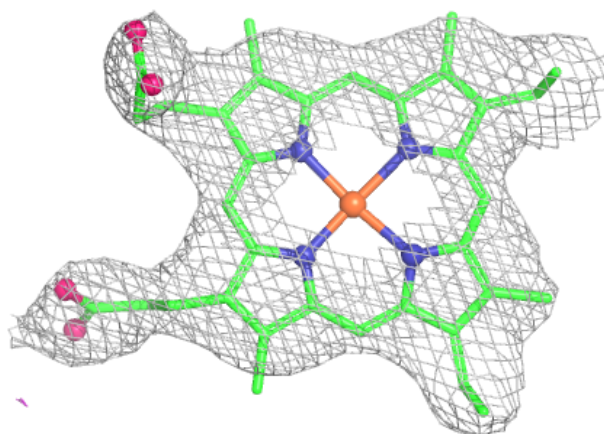
Electron density around HEC D 604:

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



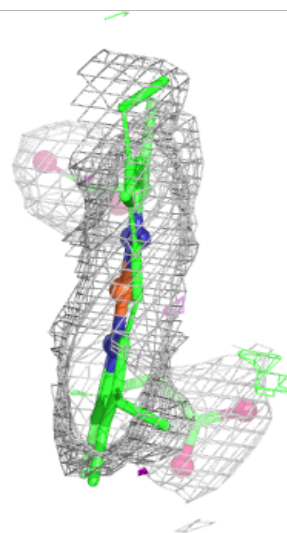
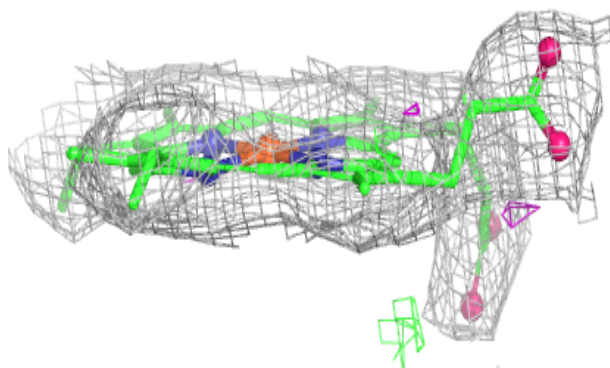
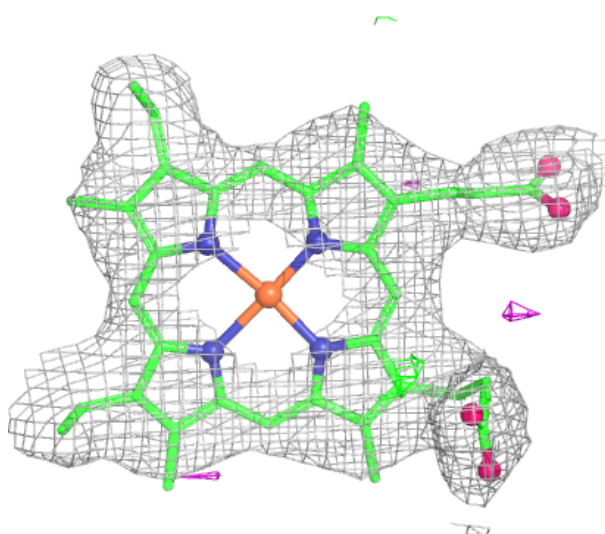
Electron density around HEC O 601:

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



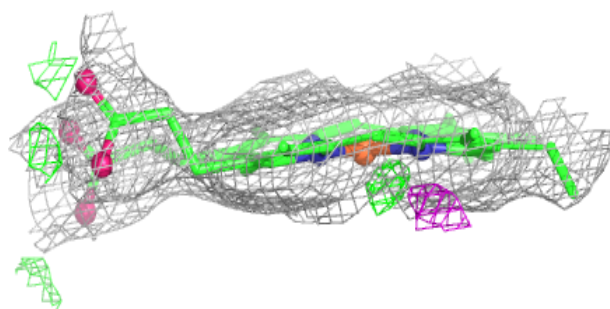
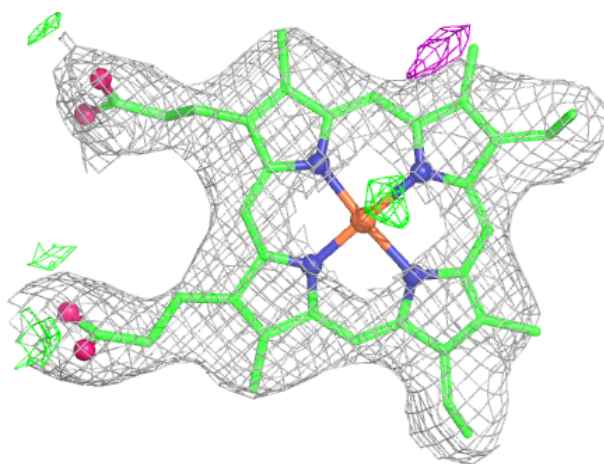
Electron density around HEC J 601:

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



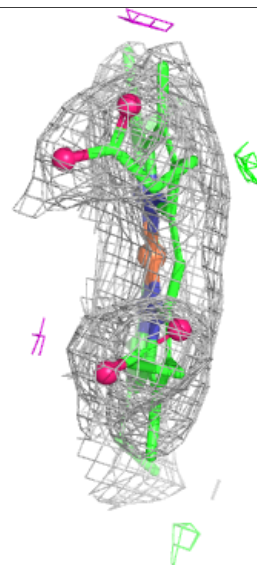
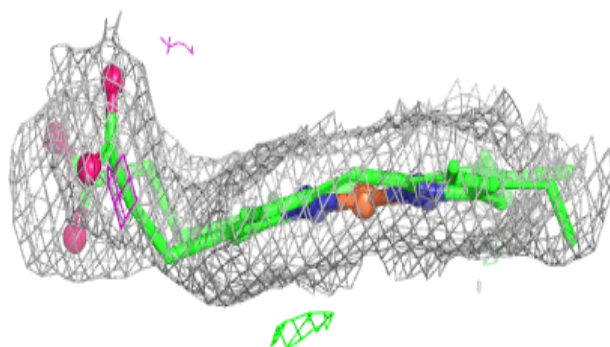
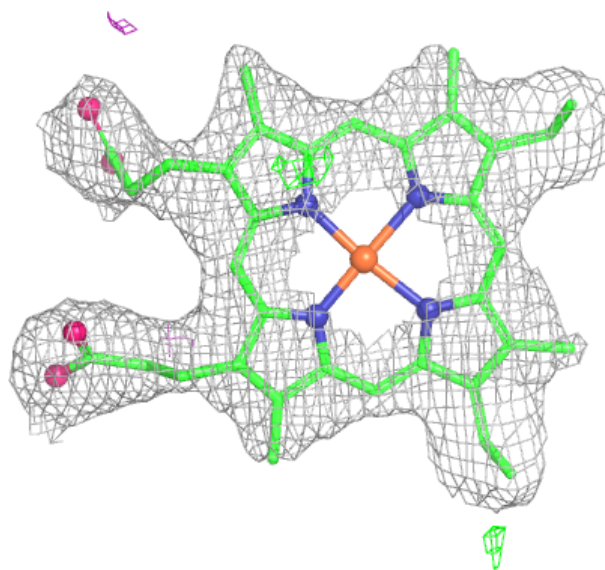
Electron density around HEC G 605:

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



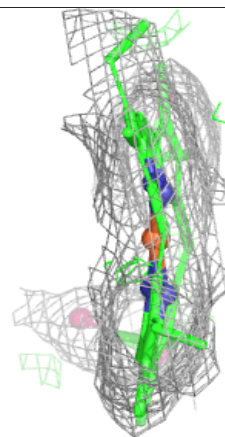
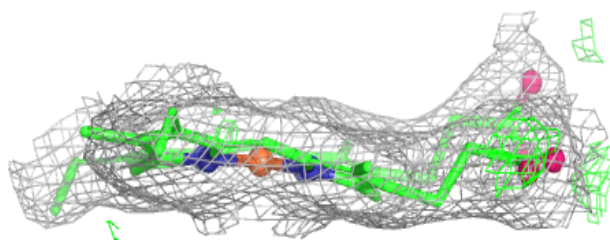
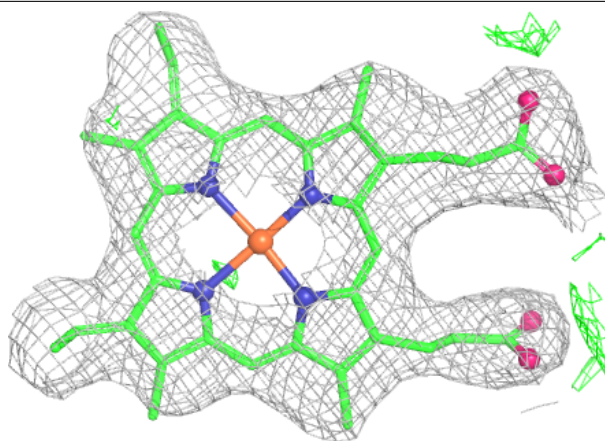
Electron density around HEC L 607:

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



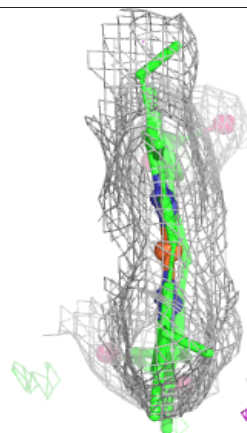
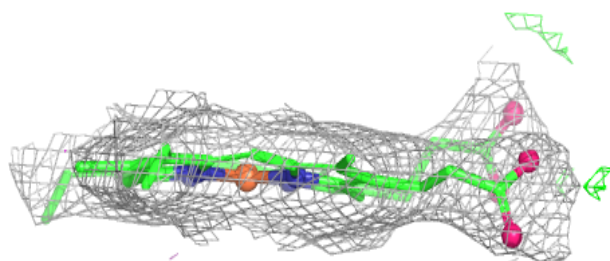
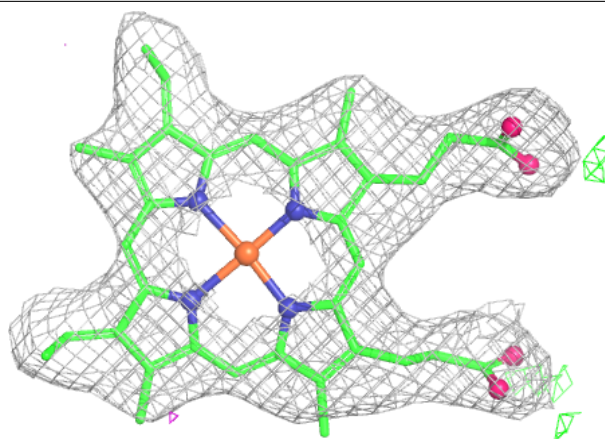
Electron density around HEC G 606:

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



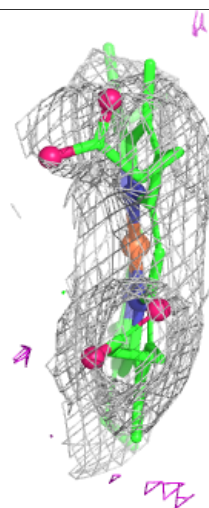
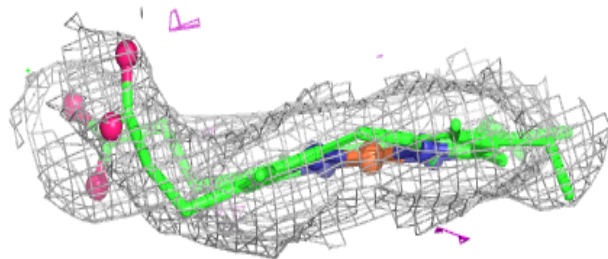
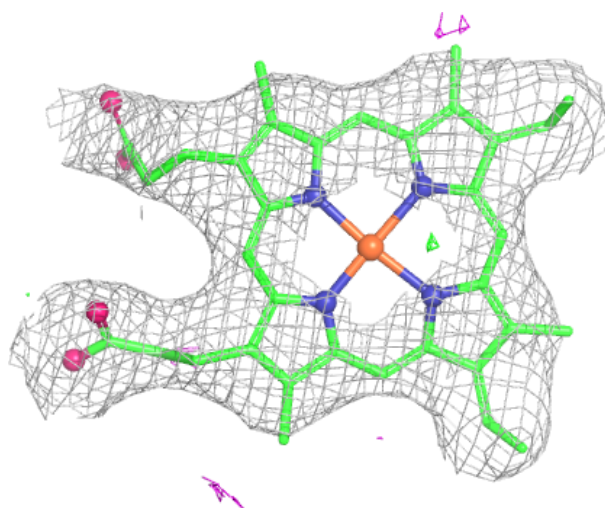
Electron density around HEC R 605:

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



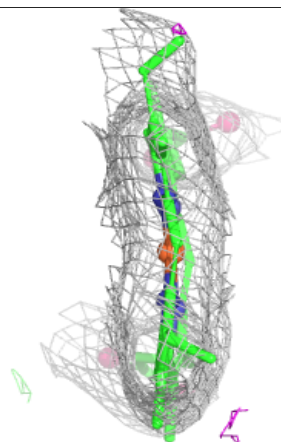
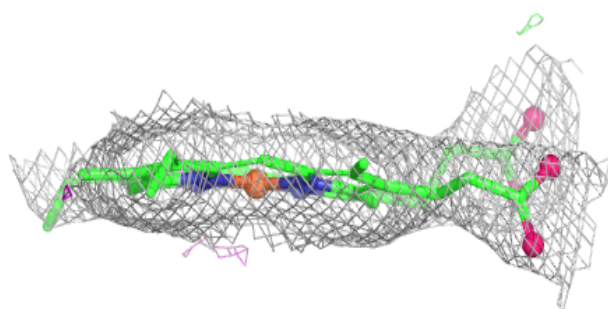
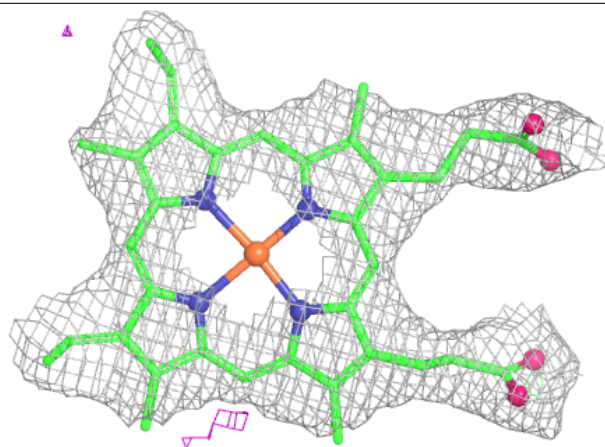
Electron density around HEC D 607:

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



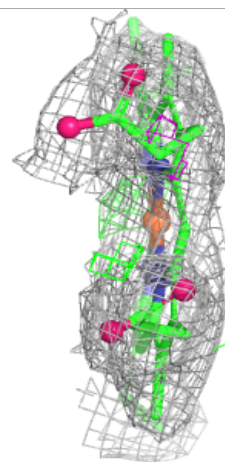
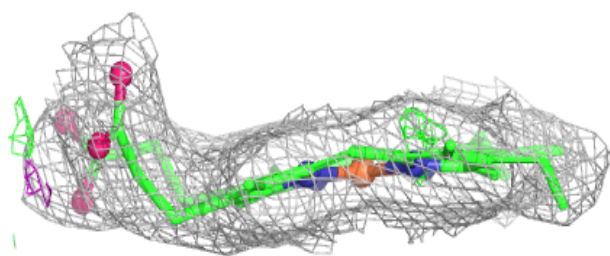
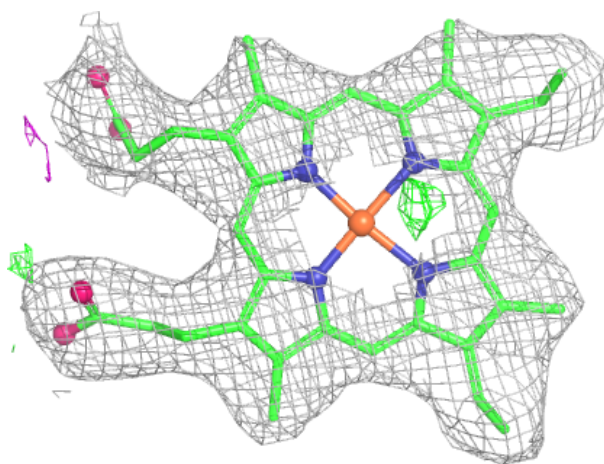
Electron density around HEC H 605:

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



Electron density around HEC J 607:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.