



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:41 AM EDT

PDB ID : 4N4O / pdb_00004n4o
Title : Nitrosomonas europea HAO soaked in NH₂OH
Authors : Maalcke, W.J.; Dietl, A.; Marritt, S.J.; Butt, J.N.; Jetten, M.S.M.; Keltjens, J.T.; Barends, T.R.M.B.; Kartal, B.
Deposited on : 2013-10-08
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

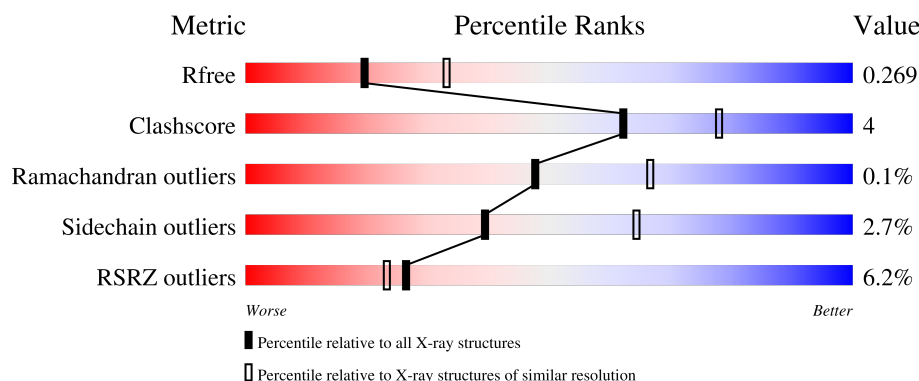
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	546	5% 82% 10% 8%
1	C	546	5% 82% 10% 8%
1	E	546	3% 81% 10% 8%
2	B	57	21% 86% 7% 7%
2	D	57	14% 95%

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Mol	Chain	Length	Quality of chain
2	F	57	26% 88% 7%

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
3	HEC	A	601	X	-	-	-
3	HEC	A	602	X	-	-	-
3	HEC	A	603	X	-	-	-
3	HEC	A	604	X	-	-	-
3	HEC	A	605	X	-	-	-
3	HEC	A	606	X	-	-	-
3	HEC	A	607	X	-	-	-
3	HEC	C	602	X	-	-	-
3	HEC	C	603	X	-	-	-
3	HEC	C	604	X	-	-	-
3	HEC	C	605	X	-	-	-
3	HEC	C	606	X	-	-	-
3	HEC	C	607	X	-	-	-
3	HEC	C	608	X	-	-	-
3	HEC	E	602	X	-	-	-
3	HEC	E	603	X	-	-	-
3	HEC	E	604	X	-	-	-
3	HEC	E	605	X	-	-	-
3	HEC	E	606	X	-	-	-
3	HEC	E	607	X	-	-	-
3	HEC	E	608	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15367 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

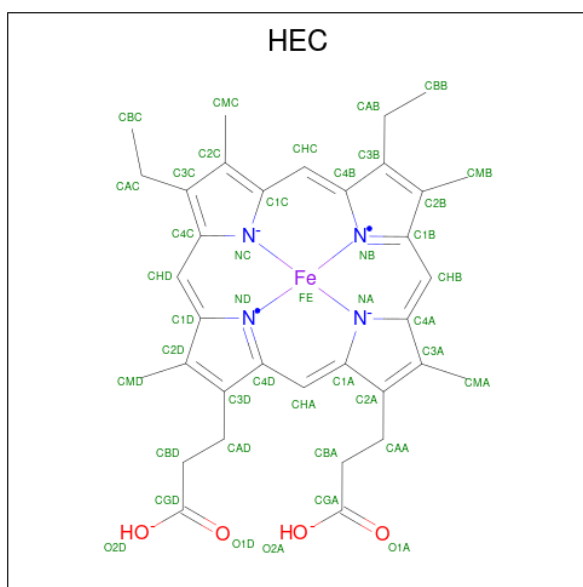
- Molecule 1 is a protein called Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			
1	E	503	Total	C	N	O	S	0	1	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	53	Total	C	N	O	S	0	0	0
			404	253	71	77	3			
2	D	57	Total	C	N	O	S	0	0	0
			429	266	76	84	3			
2	F	55	Total	C	N	O	S	0	0	0
			419	261	74	81	3			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).

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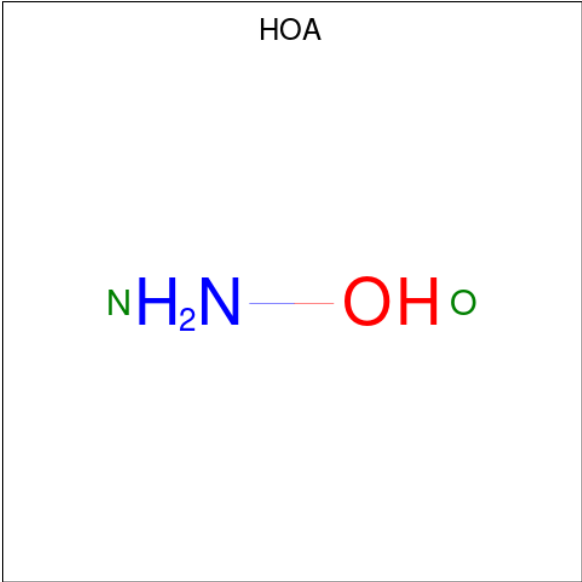
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
3	E	1	Total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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

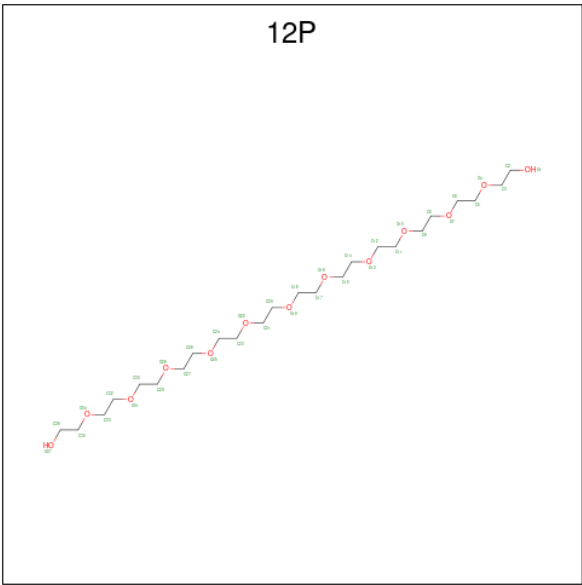
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K		
			1	1	0	0

- Molecule 5 is HYDROXYAMINE (CCD ID: HOA) (formula: H₃NO).



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

- Molecule 6 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



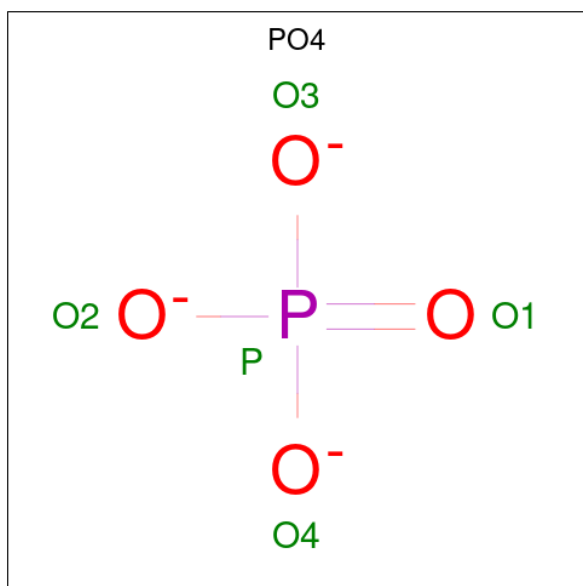
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	8	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			25	16	9		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

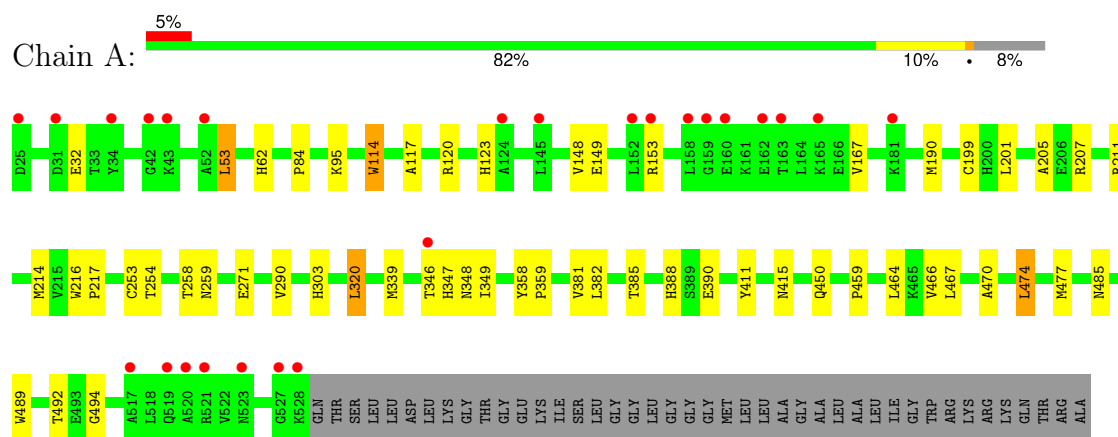
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	295	Total	O	0	0
			295	295		
8	B	37	Total	O	0	0
			37	37		
8	C	284	Total	O	0	0
			284	284		
8	D	41	Total	O	0	0
			41	41		
8	E	301	Total	O	0	0
			301	301		
8	F	35	Total	O	0	0
			35	35		

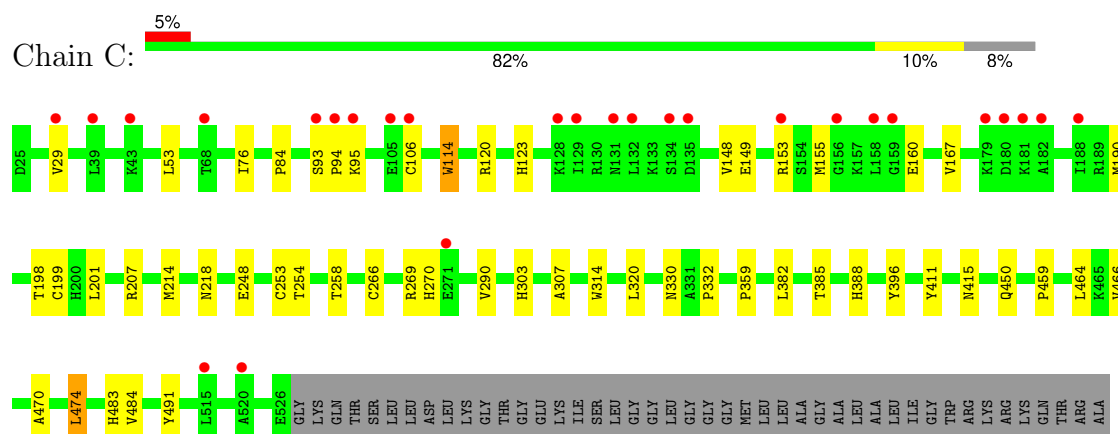
3 Residue-property plots [i](#)

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

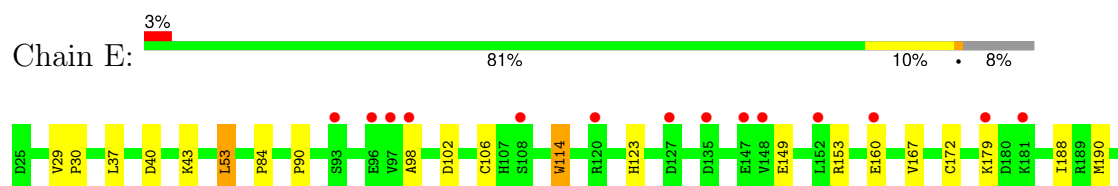
• Molecule 1: Hydroxylamine oxidoreductase

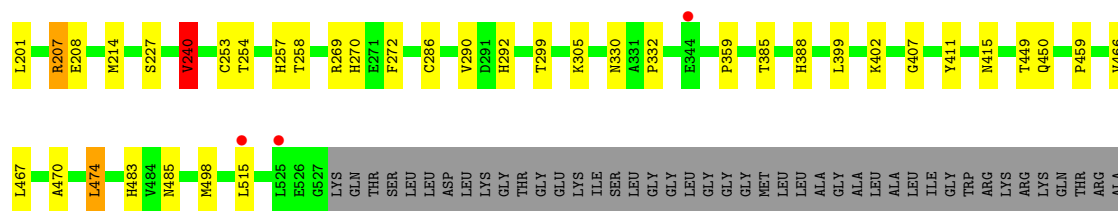


• Molecule 1: Hydroxylamine oxidoreductase

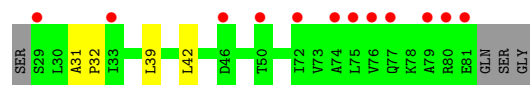
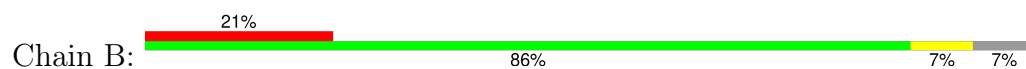


• Molecule 1: Hydroxylamine oxidoreductase

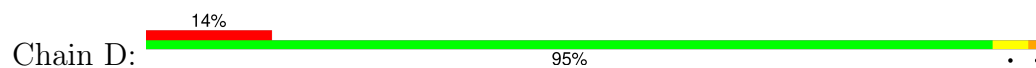




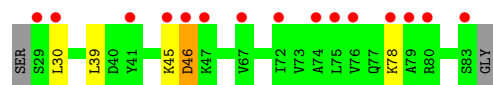
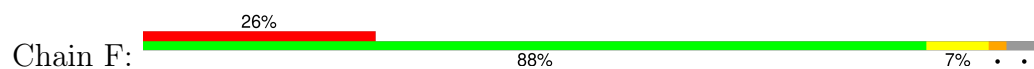
● Molecule 2: hydroxylamine oxidoreductase



● Molecule 2: hydroxylamine oxidoreductase



● Molecule 2: hydroxylamine oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.09Å 141.96Å 106.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.47 49.95 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.95-2.47) 98.1 (49.95-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.010	Depositor
R, R_{free}	0.224 , 0.273 0.221 , 0.269	Depositor DCC
R_{free} test set	7133 reflections (9.32%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15367	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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, PO4, HOA, 12P, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4121	0.81	2/5583 (0.0%)
1	C	0.41	0/4108	0.80	2/5567 (0.0%)
1	E	0.40	0/4121	0.79	3/5583 (0.1%)
2	B	0.43	0/407	0.75	0/546
2	D	0.43	0/432	0.77	0/579
2	F	0.44	0/422	0.77	0/566
All	All	0.41	0/13611	0.80	7/18424 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-C-N	5.88	125.35	119.24
1	A	485	ASN	C-N-CA	5.88	125.35	119.24
1	C	29	VAL	CA-C-N	5.85	125.86	119.89
1	C	29	VAL	C-N-CA	5.85	125.86	119.89
1	E	485	ASN	CA-C-N	5.25	124.71	119.24
1	E	485	ASN	C-N-CA	5.25	124.71	119.24
1	E	240	VAL	CB-CA-C	-5.02	105.45	111.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4018	0	3821	31	0
1	C	4005	0	3806	32	0
1	E	4018	0	3823	41	0
2	B	404	0	428	1	0
2	D	429	0	449	1	0
2	F	419	0	441	1	0
3	A	344	0	240	9	0
3	C	344	0	240	13	0
3	E	344	0	241	14	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
6	A	12	0	15	1	0
6	C	25	0	33	0	0
7	E	5	0	0	0	0
8	A	295	0	0	0	0
8	B	37	0	0	0	0
8	C	284	0	0	0	0
8	D	41	0	0	0	0
8	E	301	0	0	0	0
8	F	35	0	0	0	0
All	All	15367	0	13537	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (113) 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:C:253:CYS:HA	3:E:601:HEC:HMC3	1.64	0.78
1:E:37:LEU:HD21	1:E:53:LEU:HD13	1.68	0.76
1:A:346:THR:HG22	1:A:348:ASN:H	1.50	0.75
3:E:603:HEC:HBB2	3:E:605:HEC:HAC	1.69	0.72
1:A:253:CYS:HA	3:C:601:HEC:HMC3	1.71	0.72
1:E:179[B]:LYS:H	1:E:179[B]:LYS:HD3	1.54	0.72
3:A:608:HEC:HMC3	1:E:253:CYS:HA	1.75	0.69
1:C:167:VAL:HG22	3:C:603:HEC:HBC2	1.76	0.66
1:E:106:CYS:SG	3:E:604:HEC:HBC3	2.38	0.64
1:E:240:VAL:HG13	1:E:449:THR:HG23	1.80	0.63
3:C:606:HEC:HMA3	3:C:607:HEC:HBA2	1.79	0.63
1:C:149:GLU:O	1:C:153:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:HD3	1:C:160:GLU:HA	1.82	0.61
1:C:120:ARG:HH21	1:E:330:ASN:HB3	1.66	0.59
3:C:604:HEC:HBC2	3:C:604:HEC:HMC1	1.85	0.58
1:A:320:LEU:HD22	3:A:601:HEC:HBD2	1.85	0.58
1:C:214:MET:HE3	1:C:214:MET:HA	1.86	0.57
1:C:93:SER:HB3	1:C:94:PRO:HD3	1.86	0.57
3:E:606:HEC:HMA3	3:E:607:HEC:HBA2	1.85	0.57
3:C:601:HEC:HBB3	3:C:601:HEC:HMB1	1.85	0.57
6:A:611:12P:H82	3:C:601:HEC:HMA2	1.86	0.57
3:E:604:HEC:HMC1	3:E:604:HEC:HBC2	1.88	0.56
1:E:172:CYS:SG	3:E:605:HEC:CAC	2.94	0.56
1:C:120:ARG:NH2	1:E:330:ASN:HB3	2.22	0.54
3:A:604:HEC:HBA1	3:A:604:HEC:HHA	1.90	0.54
1:A:84:PRO:HB3	1:A:190:MET:HB2	1.89	0.53
1:A:381:VAL:HG11	1:A:390:GLU:HG3	1.90	0.53
1:E:149:GLU:O	1:E:153:ARG:HG3	2.09	0.53
1:A:167:VAL:HG22	3:A:602:HEC:HBC2	1.91	0.51
1:C:84:PRO:HB3	1:C:190:MET:HB2	1.91	0.51
1:C:123:HIS:HB3	1:C:167:VAL:HB	1.92	0.51
1:C:254:THR:O	1:C:258:THR:HG23	2.09	0.51
1:C:106:CYS:SG	3:C:604:HEC:HBC3	2.51	0.51
3:E:601:HEC:HBB3	3:E:601:HEC:HMB1	1.91	0.51
1:E:167:VAL:HG22	3:E:603:HEC:HBC2	1.93	0.51
1:C:359:PRO:HG2	1:C:474:LEU:HD22	1.92	0.50
1:A:114:TRP:HA	1:A:114:TRP:CE3	2.44	0.50
1:E:179[B]:LYS:H	1:E:179[B]:LYS:CD	2.23	0.50
1:E:407:GLY:HA2	1:E:498:MET:HE1	1.93	0.50
1:A:114:TRP:HA	1:A:114:TRP:HE3	1.77	0.50
1:A:359:PRO:HG2	1:A:474:LEU:HD22	1.92	0.50
1:C:385:THR:HA	1:C:388:HIS:O	2.11	0.50
1:A:492:THR:HG23	1:E:290:VAL:HG13	1.94	0.49
1:E:123:HIS:HB3	1:E:167:VAL:HB	1.93	0.49
1:A:303:HIS:CD2	3:A:607:HEC:ND	2.80	0.49
1:A:120:ARG:HH21	1:C:330:ASN:HB3	1.77	0.49
1:E:214:MET:HE3	1:E:214:MET:HA	1.95	0.49
1:E:411:TYR:CE1	1:E:470:ALA:HB2	2.48	0.49
3:C:603:HEC:CHC	3:C:605:HEC:HBC1	2.43	0.48
1:A:148:VAL:HG13	1:A:199:CYS:HB3	1.95	0.48
1:C:248:GLU:HG2	1:E:402:LYS:HB2	1.96	0.48
1:E:114:TRP:HA	1:E:114:TRP:CE3	2.48	0.48
1:A:117:ALA:HB1	1:A:271:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:605:HEC:HMA3	3:A:606:HEC:HBA2	1.96	0.47
1:E:450:GLN:HB3	1:E:459:PRO:HG3	1.96	0.47
3:A:608:HEC:HMB1	3:A:608:HEC:HBB3	1.95	0.47
1:C:76:ILE:HD11	1:E:399:LEU:HD12	1.96	0.47
1:A:259:ASN:HD21	3:A:606:HEC:C4C	2.28	0.47
1:E:359:PRO:HG2	1:E:474:LEU:HD22	1.96	0.47
1:A:214:MET:HE3	1:A:214:MET:HA	1.97	0.47
1:C:155:MET:HE1	1:C:198:THR:HG23	1.96	0.47
1:E:254:THR:O	1:E:258:THR:HG23	2.15	0.47
1:A:62:HIS:HB3	1:A:211:ARG:HH12	1.80	0.46
1:E:90:PRO:HG3	1:E:188:ILE:O	2.15	0.46
1:E:40:ASP:HB3	1:E:43:LYS:HB2	1.96	0.46
1:C:218:ASN:ND2	2:D:30:LEU:HD13	2.31	0.46
1:E:269:ARG:HA	1:E:270:HIS:HA	1.78	0.46
1:A:415:ASN:HA	1:A:466:VAL:HG21	1.98	0.46
1:E:114:TRP:HA	1:E:114:TRP:HE3	1.81	0.46
1:A:254:THR:O	1:A:258:THR:HG23	2.16	0.45
1:E:299:THR:O	1:E:305:LYS:HG2	2.17	0.45
1:E:272:PHE:O	3:E:603:HEC:HBA1	2.17	0.45
1:C:303:HIS:CD2	3:C:608:HEC:ND	2.86	0.44
1:E:179[B]:LYS:HD3	1:E:179[B]:LYS:N	2.22	0.44
1:E:207:ARG:NH1	1:E:208:GLU:OE2	2.49	0.44
1:A:477:MET:HG3	1:A:489:TRP:HB2	2.00	0.44
1:C:114:TRP:HA	1:C:114:TRP:CE3	2.52	0.44
1:A:53:LEU:HD21	1:A:205:ALA:HB2	2.00	0.44
3:A:608:HEC:HAC	1:E:286:CYS:O	2.17	0.44
1:C:415:ASN:HA	1:C:466:VAL:HG21	2.00	0.44
1:A:123:HIS:HB3	1:A:167:VAL:HB	2.00	0.44
1:E:84:PRO:HB3	1:E:190:MET:HB2	1.99	0.43
1:A:385:THR:HA	1:A:388:HIS:O	2.18	0.43
1:E:153:ARG:HD3	1:E:160:GLU:HA	2.00	0.43
1:C:332:PRO:HB2	3:C:606:HEC:HMC1	1.99	0.43
1:C:396:TYR:OH	1:C:484:VAL:HA	2.19	0.43
1:C:269:ARG:HA	1:C:270:HIS:HA	1.78	0.43
1:C:483:HIS:HD2	3:C:606:HEC:C1C	2.32	0.43
1:C:450:GLN:HB3	1:C:459:PRO:HG3	2.00	0.42
1:E:98:ALA:HB1	1:E:102:ASP:HB2	2.01	0.42
3:E:606:HEC:HBC1	3:E:608:HEC:HHC	2.01	0.42
1:A:450:GLN:HB3	1:A:459:PRO:HG3	2.02	0.42
1:E:483:HIS:HD2	3:E:606:HEC:C1C	2.33	0.42
2:F:45:LYS:O	2:F:46:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TRP:HA	1:A:217:PRO:HD3	1.92	0.42
1:C:266:CYS:SG	3:C:607:HEC:HHC	2.60	0.42
1:A:339:MET:HE3	1:A:347:HIS:HA	2.02	0.41
3:C:602:HEC:HBC1	3:C:607:HEC:C4B	2.50	0.41
1:A:290:VAL:HG12	1:C:491:TYR:HB3	2.01	0.41
2:B:31:ALA:HA	2:B:32:PRO:HD3	1.89	0.41
1:E:227:SER:O	3:E:607:HEC:HBD1	2.20	0.41
1:E:29:VAL:HA	1:E:30:PRO:HD3	1.93	0.41
1:E:257:HIS:CE1	3:E:607:HEC:HMD1	2.56	0.41
1:C:411:TYR:CE1	1:C:470:ALA:HB2	2.56	0.41
1:A:358:TYR:HA	1:A:359:PRO:HD3	1.93	0.41
1:C:148:VAL:HG13	1:C:199:CYS:HB3	2.02	0.41
1:E:415:ASN:HA	1:E:466:VAL:HG21	2.02	0.41
1:C:307:ALA:HA	1:C:314:TRP:CH2	2.56	0.41
1:A:149:GLU:O	1:A:153:ARG:HG3	2.21	0.40
1:E:332:PRO:HD3	3:E:608:HEC:C4C	2.52	0.40
1:E:385:THR:HA	1:E:388:HIS:O	2.22	0.40
1:A:411:TYR:CE1	1:A:470:ALA:HB2	2.55	0.40
1:A:477:MET:HB2	1:A:494:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/546 (92%)	484 (96%)	18 (4%)	0	100	100
1	C	500/546 (92%)	482 (96%)	18 (4%)	0	100	100
1	E	502/546 (92%)	484 (96%)	17 (3%)	1 (0%)	43	61
2	B	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
2	D	55/57 (96%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	53/57 (93%)	49 (92%)	3 (6%)	1 (2%)	6	10
All	All	1663/1809 (92%)	1602 (96%)	59 (4%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	46	ASP
1	E	292	HIS

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	430/459 (94%)	418 (97%)	12 (3%)	38	63
1	C	429/459 (94%)	419 (98%)	10 (2%)	44	69
1	E	430/459 (94%)	422 (98%)	8 (2%)	50	73
2	B	46/49 (94%)	44 (96%)	2 (4%)	26	48
2	D	49/49 (100%)	46 (94%)	3 (6%)	17	33
2	F	48/49 (98%)	45 (94%)	3 (6%)	16	31
All	All	1432/1524 (94%)	1394 (97%)	38 (3%)	39	64

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	53	LEU
1	A	95	LYS
1	A	114	TRP
1	A	201	LEU
1	A	207	ARG
1	A	320	LEU
1	A	349	ILE
1	A	382	LEU

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Mol	Chain	Res	Type
1	A	464	LEU
1	A	467	LEU
1	A	474	LEU
2	B	39	LEU
2	B	42	LEU
1	C	53	LEU
1	C	95	LYS
1	C	114	TRP
1	C	201	LEU
1	C	207	ARG
1	C	290	VAL
1	C	320	LEU
1	C	382	LEU
1	C	464	LEU
1	C	474	LEU
2	D	30	LEU
2	D	39	LEU
2	D	77	GLN
1	E	53	LEU
1	E	114	TRP
1	E	201	LEU
1	E	207	ARG
1	E	240	VAL
1	E	467	LEU
1	E	474	LEU
1	E	515	LEU
2	F	30	LEU
2	F	39	LEU
2	F	78	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	315	ASN
1	A	415	ASN
1	A	450	GLN
1	A	513	GLN
1	C	218	ASN
1	C	315	ASN
1	C	386	GLN
1	C	513	GLN

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Mol	Chain	Res	Type
1	E	450	GLN
1	E	513	GLN
1	E	523	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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\# Z > 2$
3	HEC	C	603	1	50,50,50	1.97	10 (20%)	68,82,82	1.40	7 (10%)
3	HEC	C	608	1	50,50,50	1.98	11 (22%)	68,82,82	1.37	7 (10%)
3	HEC	A	602	1	50,50,50	1.97	10 (20%)	68,82,82	1.42	8 (11%)
3	HEC	E	608	1	50,50,50	1.96	11 (22%)	68,82,82	1.40	6 (8%)
6	12P	C	610	-	24,24,36	0.51	0	23,23,35	0.22	0
3	HEC	A	601	1	50,50,50	2.05	9 (18%)	68,82,82	1.42	8 (11%)
3	HEC	C	604	1	50,50,50	2.09	10 (20%)	68,82,82	1.41	6 (8%)
3	HEC	E	605	1	50,50,50	2.05	10 (20%)	68,82,82	1.40	6 (8%)
5	HOA	A	610	3	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	C	602	1	50,50,50	2.02	9 (18%)	68,82,82	1.36	8 (11%)
3	HEC	A	604	1	50,50,50	2.01	10 (20%)	68,82,82	1.34	7 (10%)
3	HEC	A	606	1	50,50,50	1.93	10 (20%)	68,82,82	1.37	6 (8%)
3	HEC	C	607	1	50,50,50	1.94	9 (18%)	68,82,82	1.36	7 (10%)
3	HEC	E	607	1	50,50,50	1.92	10 (20%)	68,82,82	1.38	7 (10%)
3	HEC	A	605	1	50,50,50	1.95	9 (18%)	68,82,82	1.41	7 (10%)
3	HEC	C	605	1	50,50,50	2.05	10 (20%)	68,82,82	1.40	8 (11%)
3	HEC	E	603	1	50,50,50	1.93	10 (20%)	68,82,82	1.41	7 (10%)
3	HEC	A	607	1	50,50,50	1.98	11 (22%)	68,82,82	1.42	8 (11%)
7	PO4	E	609	-	4,4,4	0.99	0	6,6,6	0.46	0
3	HEC	E	601	1,5	50,50,50	2.70	17 (34%)	68,82,82	3.09	20 (29%)
3	HEC	C	601	1,5	50,50,50	2.68	16 (32%)	68,82,82	3.07	22 (32%)
3	HEC	E	602	1	50,50,50	2.03	9 (18%)	68,82,82	1.33	8 (11%)
5	HOA	C	609	3	0,1,1	-	-	-	-	-
3	HEC	A	608	1,5	50,50,50	2.71	17 (34%)	68,82,82	3.53	21 (30%)
3	HEC	A	603	1	50,50,50	1.98	10 (20%)	68,82,82	1.42	7 (10%)
3	HEC	C	606	1	50,50,50	1.98	9 (18%)	68,82,82	1.42	7 (10%)
3	HEC	E	606	1	50,50,50	2.01	9 (18%)	68,82,82	1.46	8 (11%)
6	12P	A	611	-	11,11,36	0.52	0	10,10,35	0.17	0
5	HOA	E	610	3	0,1,1	-	-	-	-	-
3	HEC	E	604	1	50,50,50	2.07	10 (20%)	68,82,82	1.39	6 (8%)

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	C	603	1	1/1/3/7	4/14/54/54	-
3	HEC	C	608	1	1/1/3/7	3/14/54/54	-
3	HEC	A	602	1	1/1/3/7	4/14/54/54	-
3	HEC	E	608	1	1/1/3/7	2/14/54/54	-
6	12P	C	610	-	-	16/22/22/34	-
3	HEC	A	601	1	1/1/3/7	2/14/54/54	-
3	HEC	C	604	1	1/1/3/7	2/14/54/54	-
3	HEC	E	605	1	1/1/3/7	3/14/54/54	-
3	HEC	C	602	1	1/1/3/7	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	604	1	1/1/3/7	2/14/54/54	-
3	HEC	A	606	1	1/1/3/7	5/14/54/54	-
3	HEC	C	607	1	1/1/3/7	3/14/54/54	-
3	HEC	E	607	1	1/1/3/7	2/14/54/54	-
3	HEC	A	605	1	1/1/3/7	7/14/54/54	-
3	HEC	C	605	1	1/1/3/7	2/14/54/54	-
3	HEC	E	603	1	1/1/3/7	4/14/54/54	-
3	HEC	A	607	1	1/1/3/7	4/14/54/54	-
3	HEC	C	601	1,5	-	6/14/54/54	-
3	HEC	E	601	1,5	-	6/14/54/54	-
3	HEC	E	602	1	1/1/3/7	3/14/54/54	-
3	HEC	A	608	1,5	-	7/14/54/54	-
3	HEC	A	603	1	1/1/3/7	6/14/54/54	-
3	HEC	C	606	1	1/1/3/7	7/14/54/54	-
3	HEC	E	606	1	1/1/3/7	7/14/54/54	-
6	12P	A	611	-	-	7/9/9/34	-
3	HEC	E	604	1	1/1/3/7	3/14/54/54	-

All (256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	608	HEC	CHC-C4B	9.03	1.56	1.38
3	C	601	HEC	CHC-C4B	8.94	1.56	1.38
3	E	601	HEC	CHC-C4B	8.83	1.56	1.38
3	E	606	HEC	C3D-C2D	8.23	1.54	1.36
3	A	605	HEC	C3D-C2D	8.16	1.54	1.36
3	E	608	HEC	C3D-C2D	8.08	1.54	1.36
3	C	608	HEC	C3D-C2D	8.08	1.54	1.36
3	A	607	HEC	C3D-C2D	8.05	1.54	1.36
3	C	606	HEC	C3D-C2D	8.04	1.54	1.36
3	C	604	HEC	C3D-C2D	8.02	1.54	1.36
3	E	604	HEC	C3D-C2D	7.98	1.54	1.36
3	A	602	HEC	C3D-C2D	7.98	1.54	1.36
3	C	603	HEC	C3D-C2D	7.97	1.54	1.36
3	E	603	HEC	C3D-C2D	7.97	1.54	1.36
3	C	605	HEC	C3D-C2D	7.94	1.53	1.36
3	A	604	HEC	C3D-C2D	7.94	1.53	1.36
3	E	605	HEC	C3D-C2D	7.93	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HEC	C3D-C2D	7.93	1.53	1.36
3	A	606	HEC	C3D-C2D	7.92	1.53	1.36
3	E	602	HEC	C3D-C2D	7.91	1.53	1.36
3	C	607	HEC	C3D-C2D	7.91	1.53	1.36
3	A	603	HEC	C3D-C2D	7.89	1.53	1.36
3	A	601	HEC	C3D-C2D	7.88	1.53	1.36
3	E	607	HEC	C3D-C2D	7.81	1.53	1.36
3	C	601	HEC	C4B-C3B	5.65	1.54	1.45
3	A	608	HEC	C4B-C3B	5.61	1.54	1.45
3	E	604	HEC	FE-ND	5.60	2.12	1.94
3	E	601	HEC	C4B-C3B	5.49	1.54	1.45
3	A	608	HEC	C4C-NC	5.49	1.50	1.39
3	E	601	HEC	C4C-NC	5.43	1.49	1.39
3	C	604	HEC	FE-ND	5.37	2.11	1.94
3	C	601	HEC	C4C-NC	5.30	1.49	1.39
3	C	605	HEC	FE-ND	5.27	2.11	1.94
3	E	605	HEC	FE-ND	5.25	2.11	1.94
3	E	601	HEC	C1A-C2A	5.22	1.54	1.45
3	A	601	HEC	FE-ND	5.20	2.10	1.94
3	E	606	HEC	FE-ND	5.18	2.10	1.94
3	E	602	HEC	FE-ND	5.17	2.10	1.94
3	C	601	HEC	C1A-C2A	5.17	1.54	1.45
3	E	601	HEC	C1A-NA	5.14	1.49	1.39
3	A	608	HEC	C1A-NA	5.10	1.49	1.39
3	A	608	HEC	C1A-C2A	5.06	1.54	1.45
3	C	601	HEC	C1A-NA	5.06	1.49	1.39
3	E	601	HEC	CHA-C1A	4.98	1.48	1.38
3	A	608	HEC	CHA-C1A	4.91	1.48	1.38
3	A	604	HEC	FE-ND	4.78	2.09	1.94
3	C	601	HEC	CHA-C1A	4.71	1.47	1.38
3	A	602	HEC	FE-ND	4.71	2.09	1.94
3	A	603	HEC	FE-ND	4.69	2.09	1.94
3	A	607	HEC	FE-ND	4.65	2.09	1.94
3	C	602	HEC	FE-ND	4.60	2.09	1.94
3	C	608	HEC	FE-ND	4.58	2.09	1.94
3	C	603	HEC	FE-ND	4.57	2.09	1.94
3	A	601	HEC	FE-NB	4.57	2.09	1.94
3	E	608	HEC	FE-ND	4.49	2.08	1.94
3	C	607	HEC	FE-ND	4.45	2.08	1.94
3	C	606	HEC	FE-ND	4.42	2.08	1.94
3	A	605	HEC	FE-ND	4.40	2.08	1.94
3	A	608	HEC	C4B-NB	4.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	608	HEC	CHC-C1C	4.34	1.49	1.39
3	E	601	HEC	CHC-C1C	4.28	1.49	1.39
3	E	604	HEC	FE-NC	4.28	2.09	1.95
3	C	604	HEC	FE-NC	4.26	2.09	1.95
3	C	602	HEC	FE-NB	4.24	2.08	1.94
3	C	601	HEC	CHC-C1C	4.21	1.48	1.39
3	C	601	HEC	C4B-NB	4.21	1.47	1.40
3	E	601	HEC	C4B-NB	4.17	1.47	1.40
3	C	606	HEC	CBC-CAC	-4.13	1.33	1.51
3	C	608	HEC	CBC-CAC	-4.12	1.34	1.51
3	A	603	HEC	FE-NB	4.12	2.07	1.94
3	E	606	HEC	CBC-CAC	-4.12	1.34	1.51
3	C	605	HEC	CBC-CAC	-4.11	1.34	1.51
3	A	601	HEC	CBB-CAB	-4.11	1.34	1.51
3	C	602	HEC	CBC-CAC	-4.11	1.34	1.51
3	A	602	HEC	CBC-CAC	-4.11	1.34	1.51
3	C	607	HEC	CBC-CAC	-4.10	1.34	1.51
3	C	608	HEC	CBB-CAB	-4.10	1.34	1.51
3	E	605	HEC	CBC-CAC	-4.10	1.34	1.51
3	C	603	HEC	CBB-CAB	-4.09	1.34	1.51
3	C	602	HEC	CBB-CAB	-4.09	1.34	1.51
3	E	608	HEC	FE-NB	4.09	2.07	1.94
3	E	602	HEC	CBC-CAC	-4.09	1.34	1.51
3	A	602	HEC	CBB-CAB	-4.09	1.34	1.51
3	A	607	HEC	CBC-CAC	-4.08	1.34	1.51
3	E	604	HEC	CBB-CAB	-4.08	1.34	1.51
3	A	603	HEC	CBB-CAB	-4.08	1.34	1.51
3	A	605	HEC	CBC-CAC	-4.08	1.34	1.51
3	C	603	HEC	CBC-CAC	-4.08	1.34	1.51
3	A	606	HEC	CBC-CAC	-4.08	1.34	1.51
3	E	602	HEC	CBB-CAB	-4.08	1.34	1.51
3	A	605	HEC	CBB-CAB	-4.07	1.34	1.51
3	E	607	HEC	CBB-CAB	-4.07	1.34	1.51
3	A	604	HEC	CBC-CAC	-4.07	1.34	1.51
3	A	601	HEC	CBC-CAC	-4.07	1.34	1.51
3	A	603	HEC	CBC-CAC	-4.07	1.34	1.51
3	A	606	HEC	FE-ND	4.07	2.07	1.94
3	C	604	HEC	CBB-CAB	-4.06	1.34	1.51
3	A	606	HEC	CBB-CAB	-4.06	1.34	1.51
3	E	608	HEC	CBB-CAB	-4.06	1.34	1.51
3	E	603	HEC	CBC-CAC	-4.06	1.34	1.51
3	A	607	HEC	CBB-CAB	-4.06	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	HEC	CBB-CAB	-4.06	1.34	1.51
3	C	605	HEC	CBB-CAB	-4.06	1.34	1.51
3	E	607	HEC	CBC-CAC	-4.06	1.34	1.51
3	E	603	HEC	FE-ND	4.05	2.07	1.94
3	E	606	HEC	CBB-CAB	-4.04	1.34	1.51
3	C	607	HEC	CBB-CAB	-4.04	1.34	1.51
3	E	608	HEC	CBC-CAC	-4.04	1.34	1.51
3	A	604	HEC	CBB-CAB	-4.04	1.34	1.51
3	C	606	HEC	CBB-CAB	-4.02	1.34	1.51
3	E	604	HEC	CBC-CAC	-4.01	1.34	1.51
3	E	601	HEC	C4C-C3C	4.01	1.52	1.44
3	E	605	HEC	CBB-CAB	-4.01	1.34	1.51
3	C	604	HEC	CBC-CAC	-4.01	1.34	1.51
3	C	604	HEC	FE-NB	4.00	2.07	1.94
3	C	605	HEC	FE-NC	3.99	2.08	1.95
3	C	603	HEC	FE-NB	3.97	2.07	1.94
3	A	607	HEC	FE-NB	3.94	2.07	1.94
3	E	602	HEC	FE-NB	3.92	2.07	1.94
3	C	601	HEC	C4C-C3C	3.84	1.52	1.44
3	E	607	HEC	FE-ND	3.84	2.06	1.94
3	E	605	HEC	FE-NA	3.83	2.07	1.95
3	A	604	HEC	FE-NC	3.76	2.07	1.95
3	A	608	HEC	C4C-C3C	3.72	1.52	1.44
3	C	604	HEC	FE-NA	3.71	2.07	1.95
3	C	602	HEC	FE-NA	3.71	2.07	1.95
3	C	608	HEC	FE-NB	3.68	2.06	1.94
3	E	605	HEC	FE-NB	3.67	2.06	1.94
3	A	601	HEC	FE-NC	3.67	2.07	1.95
3	E	607	HEC	FE-NB	3.64	2.06	1.94
3	C	605	HEC	FE-NA	3.63	2.07	1.95
3	E	602	HEC	FE-NA	3.62	2.07	1.95
3	A	604	HEC	FE-NA	3.61	2.07	1.95
3	E	603	HEC	FE-NB	3.61	2.06	1.94
3	C	606	HEC	FE-NB	3.60	2.06	1.94
3	A	605	HEC	FE-NC	3.58	2.07	1.95
3	E	604	HEC	FE-NB	3.57	2.05	1.94
3	E	601	HEC	C1C-NC	-3.57	1.32	1.39
3	C	605	HEC	FE-NB	3.54	2.05	1.94
3	C	601	HEC	C1C-NC	-3.51	1.33	1.39
3	A	606	HEC	FE-NA	3.50	2.06	1.95
3	E	605	HEC	FE-NC	3.49	2.06	1.95
3	E	606	HEC	FE-NC	3.44	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEC	FE-NB	3.40	2.05	1.94
3	A	608	HEC	CHD-C4C	3.40	1.47	1.39
3	E	607	HEC	FE-NA	3.39	2.06	1.95
3	C	606	HEC	FE-NA	3.38	2.06	1.95
3	C	607	HEC	FE-NB	3.35	2.05	1.94
3	E	602	HEC	FE-NC	3.31	2.06	1.95
3	C	602	HEC	FE-NC	3.31	2.06	1.95
3	A	603	HEC	FE-NC	3.29	2.06	1.95
3	E	604	HEC	FE-NA	3.28	2.06	1.95
3	A	602	HEC	FE-NA	3.28	2.06	1.95
3	E	601	HEC	CHD-C4C	3.27	1.46	1.39
3	C	608	HEC	FE-NA	3.25	2.05	1.95
3	A	606	HEC	FE-NB	3.24	2.04	1.94
3	A	601	HEC	FE-NA	3.23	2.05	1.95
3	C	606	HEC	FE-NC	3.23	2.05	1.95
3	A	608	HEC	C1C-NC	-3.22	1.33	1.39
3	E	603	HEC	FE-NC	3.22	2.05	1.95
3	A	604	HEC	FE-NB	3.22	2.04	1.94
3	E	606	HEC	FE-NB	3.19	2.04	1.94
3	C	601	HEC	CHD-C4C	3.19	1.46	1.39
3	E	606	HEC	FE-NA	3.16	2.05	1.95
3	C	607	HEC	FE-NC	3.05	2.05	1.95
3	C	607	HEC	FE-NA	3.02	2.05	1.95
3	E	601	HEC	O1A-CGA	3.00	1.31	1.22
3	C	603	HEC	FE-NA	3.00	2.05	1.95
3	C	601	HEC	CBD-CGD	2.97	1.57	1.50
3	A	608	HEC	O1A-CGA	2.97	1.31	1.22
3	C	601	HEC	O1A-CGA	2.95	1.31	1.22
3	A	607	HEC	FE-NA	2.94	2.04	1.95
3	A	608	HEC	CBD-CGD	2.92	1.57	1.50
3	C	603	HEC	FE-NC	2.91	2.04	1.95
3	A	607	HEC	FE-NC	2.87	2.04	1.95
3	A	602	HEC	FE-NC	2.82	2.04	1.95
3	E	601	HEC	CBD-CGD	2.81	1.57	1.50
3	A	608	HEC	C1C-C2C	2.80	1.49	1.43
3	A	606	HEC	FE-NC	2.74	2.04	1.95
3	C	608	HEC	FE-NC	2.73	2.04	1.95
3	E	601	HEC	C1C-C2C	2.66	1.49	1.43
3	A	605	HEC	FE-NA	2.66	2.03	1.95
3	E	607	HEC	FE-NC	2.64	2.03	1.95
3	C	601	HEC	C1C-C2C	2.64	1.49	1.43
3	E	608	HEC	FE-NC	2.62	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	HEC	C4A-NA	-2.61	1.34	1.39
3	A	608	HEC	C4A-NA	-2.60	1.34	1.39
3	E	601	HEC	C4A-NA	-2.58	1.34	1.39
3	E	608	HEC	FE-NA	2.57	2.03	1.95
3	A	603	HEC	FE-NA	2.56	2.03	1.95
3	A	605	HEC	FE-NB	2.51	2.02	1.94
3	C	601	HEC	O2A-CGA	-2.44	1.22	1.30
3	E	603	HEC	FE-NA	2.42	2.03	1.95
3	A	608	HEC	O2A-CGA	-2.41	1.22	1.30
3	E	601	HEC	O2A-CGA	-2.39	1.22	1.30
3	A	602	HEC	CMA-C3A	2.20	1.55	1.50
3	C	603	HEC	CMA-C3A	2.20	1.55	1.50
3	C	603	HEC	CMC-C2C	2.20	1.55	1.50
3	C	608	HEC	CMB-C2B	2.19	1.55	1.50
3	C	608	HEC	CMC-C2C	2.19	1.55	1.50
3	E	603	HEC	CMA-C3A	2.19	1.55	1.50
3	A	606	HEC	CMA-C3A	2.18	1.55	1.50
3	A	607	HEC	CMC-C2C	2.18	1.55	1.50
3	A	602	HEC	CMC-C2C	2.18	1.55	1.50
3	E	604	HEC	CMB-C2B	2.18	1.55	1.50
3	E	607	HEC	CMA-C3A	2.17	1.55	1.50
3	A	607	HEC	CMB-C2B	2.17	1.55	1.50
3	A	603	HEC	CMC-C2C	2.16	1.55	1.50
3	C	604	HEC	CMB-C2B	2.16	1.55	1.50
3	E	602	HEC	CMC-C2C	2.15	1.55	1.50
3	E	607	HEC	CMB-C2B	2.15	1.55	1.50
3	A	601	HEC	CMC-C2C	2.14	1.55	1.50
3	C	602	HEC	CMC-C2C	2.14	1.55	1.50
3	E	603	HEC	CMC-C2C	2.14	1.55	1.50
3	A	605	HEC	CMD-C2D	2.14	1.55	1.50
3	C	607	HEC	CMA-C3A	2.13	1.55	1.50
3	C	604	HEC	CMC-C2C	2.13	1.55	1.50
3	C	605	HEC	CMA-C3A	2.13	1.55	1.50
3	C	606	HEC	CMD-C2D	2.13	1.55	1.50
3	E	606	HEC	CMD-C2D	2.12	1.55	1.50
3	E	605	HEC	CMC-C2C	2.12	1.55	1.50
3	E	605	HEC	CMA-C3A	2.12	1.55	1.50
3	A	606	HEC	CMB-C2B	2.12	1.55	1.50
3	A	601	HEC	CMB-C2B	2.12	1.55	1.50
3	A	604	HEC	CMA-C3A	2.12	1.55	1.50
3	C	607	HEC	CMB-C2B	2.11	1.55	1.50
3	E	608	HEC	CMD-C2D	2.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	604	HEC	CMD-C2D	2.10	1.55	1.50
3	E	608	HEC	CMB-C2B	2.10	1.55	1.50
3	A	607	HEC	CMA-C3A	2.10	1.55	1.50
3	E	604	HEC	CMC-C2C	2.09	1.55	1.50
3	A	603	HEC	CMD-C2D	2.09	1.55	1.50
3	E	605	HEC	CMD-C2D	2.09	1.55	1.50
3	A	606	HEC	CMC-C2C	2.08	1.55	1.50
3	C	605	HEC	CMD-C2D	2.08	1.55	1.50
3	E	601	HEC	C4D-ND	2.08	1.42	1.38
3	A	607	HEC	CMD-C2D	2.07	1.55	1.50
3	C	608	HEC	CMA-C3A	2.07	1.55	1.50
3	A	603	HEC	CMB-C2B	2.07	1.55	1.50
3	C	604	HEC	CMA-C3A	2.07	1.55	1.50
3	E	608	HEC	CMA-C3A	2.07	1.55	1.50
3	C	608	HEC	CMD-C2D	2.06	1.55	1.50
3	E	602	HEC	CMB-C2B	2.06	1.55	1.50
3	A	602	HEC	CMB-C2B	2.06	1.55	1.50
3	C	603	HEC	CMB-C2B	2.06	1.55	1.50
3	C	602	HEC	CMB-C2B	2.05	1.55	1.50
3	A	604	HEC	CMD-C2D	2.05	1.55	1.50
3	C	606	HEC	CMA-C3A	2.05	1.55	1.50
3	C	605	HEC	CMC-C2C	2.05	1.55	1.50
3	E	603	HEC	CMB-C2B	2.03	1.54	1.50
3	A	605	HEC	CMA-C3A	2.03	1.54	1.50
3	E	608	HEC	CMC-C2C	2.03	1.54	1.50
3	A	604	HEC	CMC-C2C	2.02	1.54	1.50
3	E	607	HEC	CMC-C2C	2.02	1.54	1.50
3	A	608	HEC	C4D-ND	2.01	1.42	1.38
3	E	606	HEC	CMA-C3A	2.00	1.54	1.50

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	608	HEC	O2A-CGA-O1A	-14.66	85.63	123.33
3	C	601	HEC	CHA-C1A-NA	-11.96	111.43	124.45
3	A	608	HEC	CHA-C1A-NA	-10.75	112.75	124.45
3	E	601	HEC	CHA-C1A-NA	-10.56	112.95	124.45
3	E	601	HEC	O2A-CGA-O1A	-10.20	97.09	123.33
3	A	608	HEC	O2A-CGA-CBA	9.94	145.42	114.00
3	C	601	HEC	O2A-CGA-O1A	-8.82	100.65	123.33
3	A	608	HEC	C3C-C4C-NC	-7.08	102.29	110.15
3	C	601	HEC	CHC-C4B-NB	-7.02	115.68	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	HEC	C2A-C1A-NA	-6.90	103.67	110.32
3	E	601	HEC	CHC-C4B-NB	-6.86	115.89	124.37
3	A	608	HEC	C2A-C1A-NA	-6.71	103.85	110.32
3	A	608	HEC	C3B-C4B-NB	-6.49	103.06	110.17
3	E	601	HEC	O2A-CGA-CBA	6.34	134.03	114.00
3	C	601	HEC	C2A-C1A-NA	-6.32	104.22	110.32
3	A	608	HEC	CHC-C4B-NB	-6.25	116.64	124.37
3	C	601	HEC	CHD-C4C-NC	-6.24	112.55	123.86
3	A	608	HEC	CHA-C1A-C2A	-6.20	115.07	124.86
3	E	601	HEC	CHA-C1A-C2A	-6.14	115.16	124.86
3	C	601	HEC	CHA-C1A-C2A	-6.11	115.21	124.86
3	C	601	HEC	O2A-CGA-CBA	6.06	133.15	114.00
3	E	606	HEC	C1D-ND-C4D	6.05	112.38	105.21
3	E	601	HEC	C3B-C4B-NB	-6.04	103.54	110.17
3	C	601	HEC	C3B-C4B-NB	-5.94	103.65	110.17
3	E	603	HEC	C1D-ND-C4D	5.93	112.23	105.21
3	A	607	HEC	C1D-ND-C4D	5.93	112.22	105.21
3	E	608	HEC	C1D-ND-C4D	5.93	112.22	105.21
3	A	602	HEC	C1D-ND-C4D	5.88	112.17	105.21
3	C	606	HEC	C1D-ND-C4D	5.83	112.11	105.21
3	C	608	HEC	C1D-ND-C4D	5.78	112.06	105.21
3	A	605	HEC	C1D-ND-C4D	5.78	112.05	105.21
3	C	605	HEC	C1D-ND-C4D	5.75	112.02	105.21
3	C	603	HEC	C1D-ND-C4D	5.69	111.94	105.21
3	A	603	HEC	C1D-ND-C4D	5.66	111.91	105.21
3	E	607	HEC	C1D-ND-C4D	5.64	111.89	105.21
3	E	601	HEC	CHD-C4C-NC	-5.64	113.64	123.86
3	A	601	HEC	C1D-ND-C4D	5.63	111.88	105.21
3	A	606	HEC	C1D-ND-C4D	5.62	111.86	105.21
3	C	602	HEC	C1D-ND-C4D	5.59	111.83	105.21
3	A	604	HEC	C1D-ND-C4D	5.59	111.83	105.21
3	C	604	HEC	C1D-ND-C4D	5.59	111.83	105.21
3	E	605	HEC	C1D-ND-C4D	5.55	111.78	105.21
3	E	604	HEC	C1D-ND-C4D	5.51	111.73	105.21
3	C	607	HEC	C1D-ND-C4D	5.43	111.64	105.21
3	E	602	HEC	C1D-ND-C4D	5.35	111.55	105.21
3	E	601	HEC	CHD-C4C-C3C	-4.99	114.39	125.30
3	A	608	HEC	CHD-C4C-C3C	-4.97	114.43	125.30
3	C	601	HEC	CHD-C4C-C3C	-4.94	114.49	125.30
3	C	601	HEC	C3C-C4C-NC	-4.85	104.77	110.15
3	E	601	HEC	C3C-C4C-NC	-4.67	104.97	110.15
3	E	601	HEC	CHC-C4B-C3B	-4.62	116.71	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	HEC	CHC-C4B-C3B	-4.53	116.88	125.23
3	A	608	HEC	CHC-C4B-C3B	-4.39	117.13	125.23
3	A	608	HEC	CAC-C3C-C2C	4.18	133.50	126.89
3	A	608	HEC	C1C-CHC-C4B	-4.06	116.69	126.25
3	C	601	HEC	C1C-CHC-C4B	-3.95	116.95	126.25
3	E	605	HEC	CBC-CAC-C3C	3.94	123.10	112.42
3	C	604	HEC	CBC-CAC-C3C	3.93	123.08	112.42
3	E	601	HEC	C1C-CHC-C4B	-3.78	117.36	126.25
3	E	604	HEC	CBC-CAC-C3C	3.67	122.36	112.42
3	A	608	HEC	CHD-C4C-NC	-3.65	117.25	123.86
3	E	601	HEC	CHA-C4D-ND	3.54	128.23	124.42
3	A	608	HEC	CHA-C4D-ND	3.36	128.04	124.42
3	C	607	HEC	CBC-CAC-C3C	3.35	121.49	112.42
3	E	606	HEC	CBB-CAB-C3B	3.32	121.42	112.42
3	C	603	HEC	CBC-CAC-C3C	3.30	121.36	112.42
3	A	608	HEC	CAA-CBA-CGA	3.25	122.28	113.67
3	A	606	HEC	CBC-CAC-C3C	3.22	121.16	112.42
3	A	603	HEC	CBC-CAC-C3C	3.21	121.11	112.42
3	E	607	HEC	CBC-CAC-C3C	3.19	121.08	112.42
3	C	601	HEC	C4A-CHB-C1B	-3.18	119.26	126.02
3	E	608	HEC	CBC-CAC-C3C	3.16	120.98	112.42
3	C	606	HEC	CBB-CAB-C3B	3.15	120.95	112.42
3	A	603	HEC	CBB-CAB-C3B	3.13	120.91	112.42
3	A	607	HEC	CBB-CAB-C3B	3.13	120.90	112.42
3	A	606	HEC	CBB-CAB-C3B	3.12	120.86	112.42
3	E	605	HEC	CBB-CAB-C3B	3.09	120.81	112.42
3	E	601	HEC	C4A-CHB-C1B	-3.06	119.53	126.02
3	A	602	HEC	CBB-CAB-C3B	3.05	120.69	112.42
3	E	608	HEC	CBB-CAB-C3B	3.03	120.62	112.42
3	E	606	HEC	C2A-C1A-NA	-3.01	107.42	110.32
3	E	601	HEC	CAC-C3C-C4C	-3.00	120.79	124.91
3	A	607	HEC	CBC-CAC-C3C	2.99	120.51	112.42
3	C	608	HEC	CBC-CAC-C3C	2.98	120.50	112.42
3	A	601	HEC	CBB-CAB-C3B	2.95	120.41	112.42
3	A	602	HEC	CBC-CAC-C3C	2.94	120.39	112.42
3	C	604	HEC	CBB-CAB-C3B	2.94	120.38	112.42
3	E	603	HEC	CBC-CAC-C3C	2.93	120.36	112.42
3	C	607	HEC	CBB-CAB-C3B	2.90	120.28	112.42
3	A	605	HEC	CBB-CAB-C3B	2.90	120.28	112.42
3	A	608	HEC	C4A-CHB-C1B	-2.90	119.86	126.02
3	E	602	HEC	CBB-CAB-C3B	2.89	120.26	112.42
3	A	603	HEC	C2A-C1A-NA	-2.88	107.54	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	HEC	CBB-CAB-C3B	2.88	120.22	112.42
3	A	605	HEC	C2A-C1A-NA	-2.87	107.56	110.32
3	A	605	HEC	CBC-CAC-C3C	2.87	120.19	112.42
3	C	608	HEC	CBB-CAB-C3B	2.86	120.17	112.42
3	C	605	HEC	CBC-CAC-C3C	2.86	120.16	112.42
3	C	601	HEC	CAC-C3C-C4C	-2.84	121.01	124.91
3	C	603	HEC	CBB-CAB-C3B	2.83	120.10	112.42
3	C	606	HEC	CBC-CAC-C3C	2.78	119.96	112.42
3	A	602	HEC	C4B-NB-C1B	2.78	108.50	105.21
3	C	606	HEC	C2A-C1A-NA	-2.77	107.65	110.32
3	A	607	HEC	C2A-C1A-NA	-2.77	107.65	110.32
3	C	605	HEC	CBB-CAB-C3B	2.74	119.86	112.42
3	A	604	HEC	CBB-CAB-C3B	2.74	119.84	112.42
3	C	608	HEC	C4B-NB-C1B	2.73	108.44	105.21
3	E	603	HEC	C2A-C1A-NA	-2.72	107.69	110.32
3	A	604	HEC	CBC-CAC-C3C	2.72	119.80	112.42
3	E	606	HEC	CBC-CAC-C3C	2.72	119.78	112.42
3	E	607	HEC	CBB-CAB-C3B	2.71	119.77	112.42
3	E	604	HEC	C2A-C1A-NA	-2.70	107.71	110.32
3	E	606	HEC	C4B-NB-C1B	2.69	108.39	105.21
3	C	603	HEC	C4B-NB-C1B	2.68	108.38	105.21
3	A	601	HEC	C4B-NB-C1B	2.68	108.38	105.21
3	A	605	HEC	C4B-NB-C1B	2.67	108.37	105.21
3	E	604	HEC	C4B-NB-C1B	2.67	108.37	105.21
3	E	607	HEC	C2A-C1A-NA	-2.65	107.77	110.32
3	C	602	HEC	CBC-CAC-C3C	2.65	119.59	112.42
3	C	602	HEC	CBB-CAB-C3B	2.64	119.58	112.42
3	C	604	HEC	C4B-NB-C1B	2.64	108.33	105.21
3	C	606	HEC	C4B-NB-C1B	2.63	108.33	105.21
3	C	604	HEC	C2A-C1A-NA	-2.62	107.80	110.32
3	E	601	HEC	C3D-C4D-ND	-2.61	107.83	110.35
3	E	602	HEC	C4B-NB-C1B	2.59	108.27	105.21
3	A	602	HEC	C2A-C1A-NA	-2.56	107.85	110.32
3	E	605	HEC	C2A-C1A-NA	-2.56	107.85	110.32
3	E	603	HEC	C4B-NB-C1B	2.56	108.24	105.21
3	A	606	HEC	C4B-NB-C1B	2.55	108.23	105.21
3	E	601	HEC	CAA-CBA-CGA	2.55	120.42	113.67
3	E	604	HEC	CBB-CAB-C3B	2.55	119.33	112.42
3	E	605	HEC	C4B-NB-C1B	2.54	108.21	105.21
3	C	602	HEC	C4B-NB-C1B	2.53	108.20	105.21
3	E	608	HEC	C4B-NB-C1B	2.51	108.18	105.21
3	E	607	HEC	C4B-NB-C1B	2.50	108.17	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	HEC	CBC-CAC-C3C	2.50	119.20	112.42
3	C	605	HEC	C2A-C1A-NA	-2.50	107.91	110.32
3	C	607	HEC	C4B-NB-C1B	2.50	108.17	105.21
3	A	601	HEC	C2A-C1A-NA	-2.50	107.91	110.32
3	C	603	HEC	C2A-C1A-NA	-2.49	107.92	110.32
3	E	608	HEC	C2A-C1A-NA	-2.48	107.93	110.32
3	A	607	HEC	C4B-NB-C1B	2.47	108.13	105.21
3	C	605	HEC	C4B-NB-C1B	2.46	108.12	105.21
3	A	606	HEC	C2A-C1A-NA	-2.46	107.95	110.32
3	C	607	HEC	C2A-C1A-NA	-2.46	107.95	110.32
3	A	608	HEC	C3D-C4D-ND	-2.40	108.04	110.35
3	C	601	HEC	CAA-C2A-C3A	2.39	132.35	127.87
3	A	601	HEC	CBD-CAD-C3D	-2.39	105.93	112.53
3	A	608	HEC	C4B-NB-C1B	2.39	108.03	105.21
3	A	603	HEC	C4B-NB-C1B	2.38	108.02	105.21
3	C	601	HEC	C1A-CHA-C4D	-2.37	120.99	126.02
3	E	604	HEC	C3B-C4B-NB	-2.35	107.60	110.17
3	A	601	HEC	CBC-CAC-C3C	2.34	118.76	112.42
3	E	606	HEC	C3C-C4C-NC	-2.33	107.57	110.15
3	C	608	HEC	C3C-C4C-NC	-2.33	107.57	110.15
3	A	604	HEC	C2A-C1A-NA	-2.32	108.08	110.32
3	C	608	HEC	C2A-C1A-NA	-2.32	108.08	110.32
3	C	604	HEC	C3B-C4B-NB	-2.32	107.63	110.17
3	A	608	HEC	CHB-C4A-NA	-2.32	121.93	124.45
3	A	602	HEC	C3B-C4B-NB	-2.31	107.64	110.17
3	A	601	HEC	C3C-C4C-NC	-2.28	107.62	110.15
3	A	602	HEC	C3C-C4C-NC	-2.27	107.64	110.15
3	C	602	HEC	C3C-C4C-NC	-2.25	107.65	110.15
3	A	607	HEC	C3D-C4D-ND	-2.25	108.17	110.35
3	A	605	HEC	C3B-C4B-NB	-2.25	107.70	110.17
3	A	607	HEC	C3C-C4C-NC	-2.24	107.67	110.15
3	C	601	HEC	C4B-NB-C1B	2.24	107.85	105.21
3	C	606	HEC	C3C-C4C-NC	-2.23	107.68	110.15
3	E	602	HEC	C3C-C4C-NC	-2.23	107.68	110.15
3	C	601	HEC	CHB-C4A-NA	-2.22	122.03	124.45
3	A	601	HEC	C3B-C4B-NB	-2.22	107.74	110.17
3	E	601	HEC	CAA-C2A-C3A	2.21	132.01	127.87
3	E	608	HEC	C3C-C4C-NC	-2.21	107.70	110.15
3	C	602	HEC	C2A-C1A-NA	-2.21	108.19	110.32
3	C	603	HEC	C3B-C4B-NB	-2.20	107.75	110.17
3	C	601	HEC	C4C-CHD-C1D	-2.20	121.07	126.25
3	A	603	HEC	CAD-C3D-C4D	2.20	128.53	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	HEC	C4B-NB-C1B	2.20	107.81	105.21
3	C	601	HEC	CAA-C2A-C1A	-2.16	120.46	124.85
3	C	608	HEC	C3B-C4B-NB	-2.16	107.81	110.17
3	C	601	HEC	CAA-CBA-CGA	2.15	119.36	113.67
3	C	602	HEC	C3B-C4B-NB	-2.14	107.82	110.17
3	A	607	HEC	CBD-CAD-C3D	-2.14	106.61	112.53
3	E	602	HEC	C3B-C4B-NB	-2.14	107.82	110.17
3	C	605	HEC	C3B-C4B-NB	-2.14	107.82	110.17
3	E	603	HEC	C3D-C4D-ND	-2.13	108.30	110.35
3	C	601	HEC	CHA-C4D-ND	2.13	126.71	124.42
3	A	604	HEC	CHA-C4D-ND	2.12	126.70	124.42
3	E	603	HEC	C3B-C4B-NB	-2.11	107.85	110.17
3	C	605	HEC	C3C-C4C-NC	-2.11	107.81	110.15
3	E	607	HEC	C3B-C4B-NB	-2.11	107.86	110.17
3	E	601	HEC	C4B-NB-C1B	2.11	107.70	105.21
3	A	608	HEC	CAC-C3C-C4C	-2.11	122.02	124.91
3	C	602	HEC	CBD-CAD-C3D	-2.10	106.72	112.53
3	E	602	HEC	CBD-CAD-C3D	-2.09	106.77	112.53
3	C	606	HEC	C3B-C4B-NB	-2.08	107.89	110.17
3	E	605	HEC	C3B-C4B-NB	-2.08	107.89	110.17
3	A	603	HEC	C3C-C4C-NC	-2.07	107.86	110.15
3	E	606	HEC	C3B-C4B-NB	-2.07	107.90	110.17
3	C	607	HEC	C3B-C4B-NB	-2.07	107.90	110.17
3	A	606	HEC	C3B-C4B-NB	-2.06	107.91	110.17
3	E	602	HEC	C2A-C1A-NA	-2.06	108.34	110.32
3	E	601	HEC	CAA-C2A-C1A	-2.04	120.70	124.85
3	E	607	HEC	C3D-C4D-ND	-2.04	108.38	110.35
3	C	605	HEC	C3D-C4D-ND	-2.04	108.38	110.35
3	A	604	HEC	C3C-C4C-NC	-2.04	107.89	110.15
3	C	607	HEC	O2A-CGA-CBA	2.03	120.43	114.00
3	A	602	HEC	C2B-C1B-NB	-2.03	107.56	109.90
3	C	603	HEC	C3C-C4C-NC	-2.02	107.91	110.15
3	A	605	HEC	C3C-C4C-NC	-2.02	107.91	110.15
3	A	608	HEC	CBC-CAC-C3C	2.01	117.88	112.42
3	E	606	HEC	C2B-C1B-NB	-2.00	107.59	109.90

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	HEC	NA
3	A	602	HEC	NA
3	A	603	HEC	NA

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Mol	Chain	Res	Type	Atom
3	A	604	HEC	NA
3	A	605	HEC	NA
3	A	606	HEC	NA
3	A	607	HEC	NA
3	C	602	HEC	NA
3	C	603	HEC	NA
3	C	604	HEC	NA
3	C	605	HEC	NA
3	C	606	HEC	NA
3	C	607	HEC	NA
3	C	608	HEC	NA
3	E	602	HEC	NA
3	E	603	HEC	NA
3	E	604	HEC	NA
3	E	605	HEC	NA
3	E	606	HEC	NA
3	E	607	HEC	NA
3	E	608	HEC	NA

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	604	HEC	C2C-C3C-CAC-CBC
3	A	608	HEC	C4C-C3C-CAC-CBC
3	C	604	HEC	C4C-C3C-CAC-CBC
3	A	608	HEC	C2C-C3C-CAC-CBC
3	C	601	HEC	C4B-C3B-CAB-CBB
3	E	605	HEC	C2C-C3C-CAC-CBC
3	E	605	HEC	C4C-C3C-CAC-CBC
3	E	604	HEC	C2C-C3C-CAC-CBC
6	C	610	12P	O19-C20-C21-O22
6	C	610	12P	O31-C32-C33-O34
6	C	610	12P	O25-C26-C27-O28
6	C	610	12P	O16-C17-C18-O19
3	A	603	HEC	C2C-C3C-CAC-CBC
3	E	604	HEC	C4C-C3C-CAC-CBC
3	E	601	HEC	C4C-C3C-CAC-CBC
3	C	606	HEC	C2B-C3B-CAB-CBB
6	C	610	12P	O13-C14-C15-O16
6	C	610	12P	O22-C23-C24-O25
3	E	601	HEC	C4B-C3B-CAB-CBB
3	C	601	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	E	606	HEC	C2B-C3B-CAB-CBB
3	A	603	HEC	C4C-C3C-CAC-CBC
3	A	608	HEC	C4B-C3B-CAB-CBB
3	C	601	HEC	C2B-C3B-CAB-CBB
3	A	604	HEC	C1A-C2A-CAA-CBA
6	C	610	12P	O34-C35-C36-O37
3	C	606	HEC	C4B-C3B-CAB-CBB
3	E	606	HEC	C4B-C3B-CAB-CBB
6	A	611	12P	O7-C8-C9-O10
6	A	611	12P	O1-C2-C3-O4
3	A	605	HEC	C2B-C3B-CAB-CBB
3	A	604	HEC	C3A-C2A-CAA-CBA
6	A	611	12P	C12-C11-O10-C9
6	C	610	12P	C36-C35-O34-C33
3	C	606	HEC	C2A-CAA-CBA-CGA
6	C	610	12P	C32-C33-O34-C35
6	C	610	12P	C26-C27-O28-C29
6	C	610	12P	C21-C20-O19-C18
6	C	610	12P	C17-C18-O19-C20
6	A	611	12P	C9-C8-O7-C6
6	C	610	12P	O28-C29-C30-O31
3	E	601	HEC	C2A-CAA-CBA-CGA
6	C	610	12P	C18-C17-O16-C15
6	C	610	12P	C33-C32-O31-C30
6	C	610	12P	C27-C26-O25-C24
3	C	601	HEC	C2A-CAA-CBA-CGA
3	C	605	HEC	C1A-C2A-CAA-CBA
3	A	605	HEC	C4B-C3B-CAB-CBB
6	A	611	12P	C6-C5-O4-C3
3	A	605	HEC	CAD-CBD-CGD-O2D
3	E	602	HEC	C2A-CAA-CBA-CGA
3	A	602	HEC	CAD-CBD-CGD-O1D
3	E	601	HEC	C2B-C3B-CAB-CBB
3	C	607	HEC	CAD-CBD-CGD-O1D
3	A	602	HEC	CAD-CBD-CGD-O2D
3	A	606	HEC	CAD-CBD-CGD-O2D
3	C	607	HEC	CAD-CBD-CGD-O2D
3	E	607	HEC	CAD-CBD-CGD-O2D
6	A	611	12P	C2-C3-O4-C5
3	A	602	HEC	CAA-CBA-CGA-O1A
3	A	602	HEC	CAA-CBA-CGA-O2A
3	C	603	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	602	HEC	CAA-CBA-CGA-O2A
3	C	603	HEC	CAA-CBA-CGA-O1A
3	E	603	HEC	CAA-CBA-CGA-O2A
3	C	603	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAA-CBA-CGA-O1A
3	E	606	HEC	CAA-CBA-CGA-O1A
3	A	605	HEC	CAA-CBA-CGA-O1A
3	C	605	HEC	C3A-C2A-CAA-CBA
3	A	606	HEC	CAD-CBD-CGD-O1D
3	E	606	HEC	CAA-CBA-CGA-O2A
3	A	605	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAA-CBA-CGA-O1A
3	C	603	HEC	CAD-CBD-CGD-O2D
3	E	603	HEC	CAA-CBA-CGA-O1A
3	E	607	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	C2A-CAA-CBA-CGA
3	A	608	HEC	C2A-CAA-CBA-CGA
3	E	601	HEC	CAD-CBD-CGD-O2D
3	C	601	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAA-CBA-CGA-O2A
3	E	606	HEC	CAD-CBD-CGD-O1D
3	E	606	HEC	CAD-CBD-CGD-O2D
3	E	608	HEC	CAD-CBD-CGD-O2D
3	A	605	HEC	CAA-CBA-CGA-O2A
3	E	603	HEC	CAD-CBD-CGD-O2D
3	E	603	HEC	CAD-CBD-CGD-O1D
3	A	608	HEC	CAD-CBD-CGD-O2D
3	A	601	HEC	CAA-CBA-CGA-O1A
3	A	607	HEC	CAD-CBD-CGD-O2D
3	A	607	HEC	C2B-C3B-CAB-CBB
3	C	601	HEC	CAD-CBD-CGD-O1D
3	C	608	HEC	CAD-CBD-CGD-O2D
3	A	606	HEC	C2B-C3B-CAB-CBB
3	C	606	HEC	CAD-CBD-CGD-O2D
3	E	601	HEC	CAD-CBD-CGD-O1D
3	C	606	HEC	CAD-CBD-CGD-O1D
3	A	607	HEC	CAD-CBD-CGD-O1D
3	C	608	HEC	CAD-CBD-CGD-O1D
3	A	608	HEC	CAD-CBD-CGD-O1D
3	E	608	HEC	CAD-CBD-CGD-O1D
3	E	602	HEC	CAA-CBA-CGA-O1A
3	E	606	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	E	605	HEC	C1A-C2A-CAA-CBA
3	A	601	HEC	CAA-CBA-CGA-O2A
3	A	603	HEC	CAD-CBD-CGD-O1D
3	A	603	HEC	CAD-CBD-CGD-O2D
3	A	608	HEC	C2B-C3B-CAB-CBB
3	A	603	HEC	CAA-CBA-CGA-O2A
3	A	607	HEC	C4B-C3B-CAB-CBB
3	A	606	HEC	C4B-C3B-CAB-CBB
3	E	602	HEC	CAA-CBA-CGA-O2A
3	A	606	HEC	CAA-CBA-CGA-O2A
6	A	611	12P	C5-C6-O7-C8
3	C	607	HEC	C2B-C3B-CAB-CBB
3	A	603	HEC	CAA-CBA-CGA-O1A
3	E	604	HEC	CAD-CBD-CGD-O2D
3	C	608	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

23 monomers are involved in 36 short contacts:

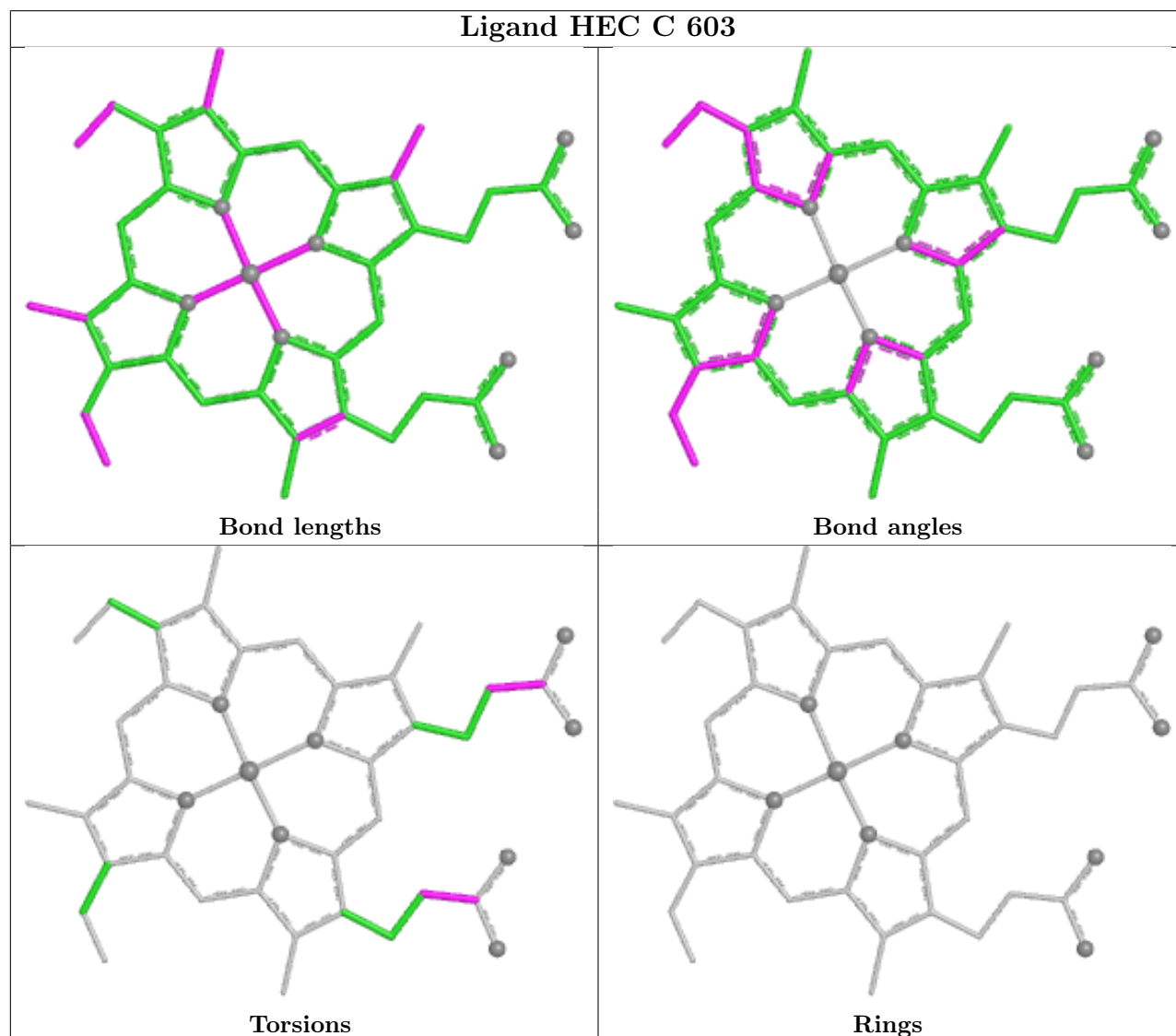
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	HEC	2	0
3	C	608	HEC	1	0
3	A	602	HEC	1	0
3	E	608	HEC	2	0
3	A	601	HEC	1	0
3	C	604	HEC	2	0
3	E	605	HEC	2	0
3	C	602	HEC	1	0
3	A	604	HEC	1	0
3	A	606	HEC	2	0
3	C	607	HEC	3	0
3	E	607	HEC	3	0
3	A	605	HEC	1	0
3	C	605	HEC	1	0
3	E	603	HEC	3	0
3	A	607	HEC	1	0
3	E	601	HEC	2	0
3	C	601	HEC	3	0
3	A	608	HEC	3	0
3	C	606	HEC	3	0
3	E	606	HEC	3	0
6	A	611	12P	1	0

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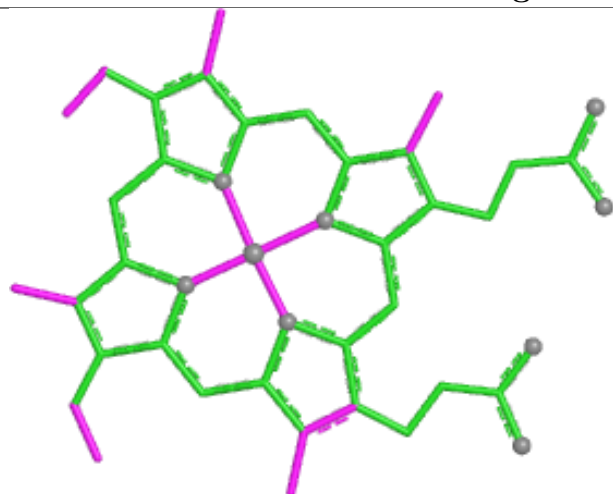
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	604	HEC	2	0

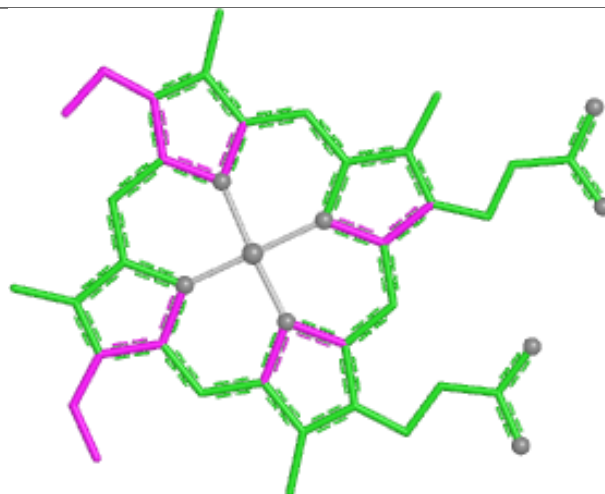
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



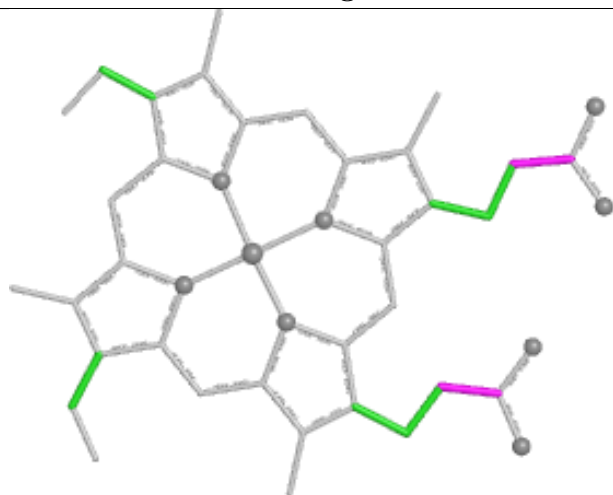
Ligand HEC C 608



Bond lengths



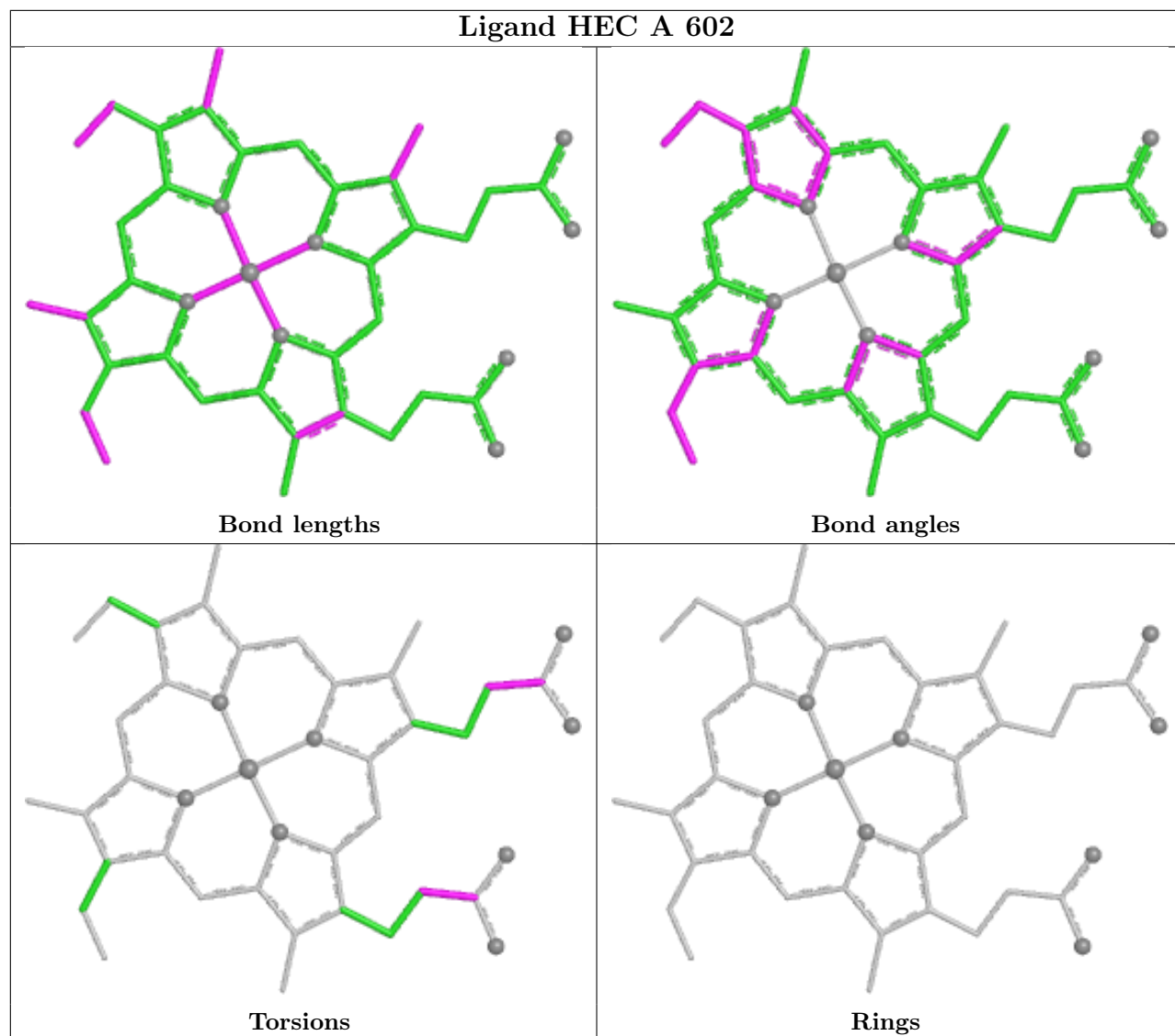
Bond angles



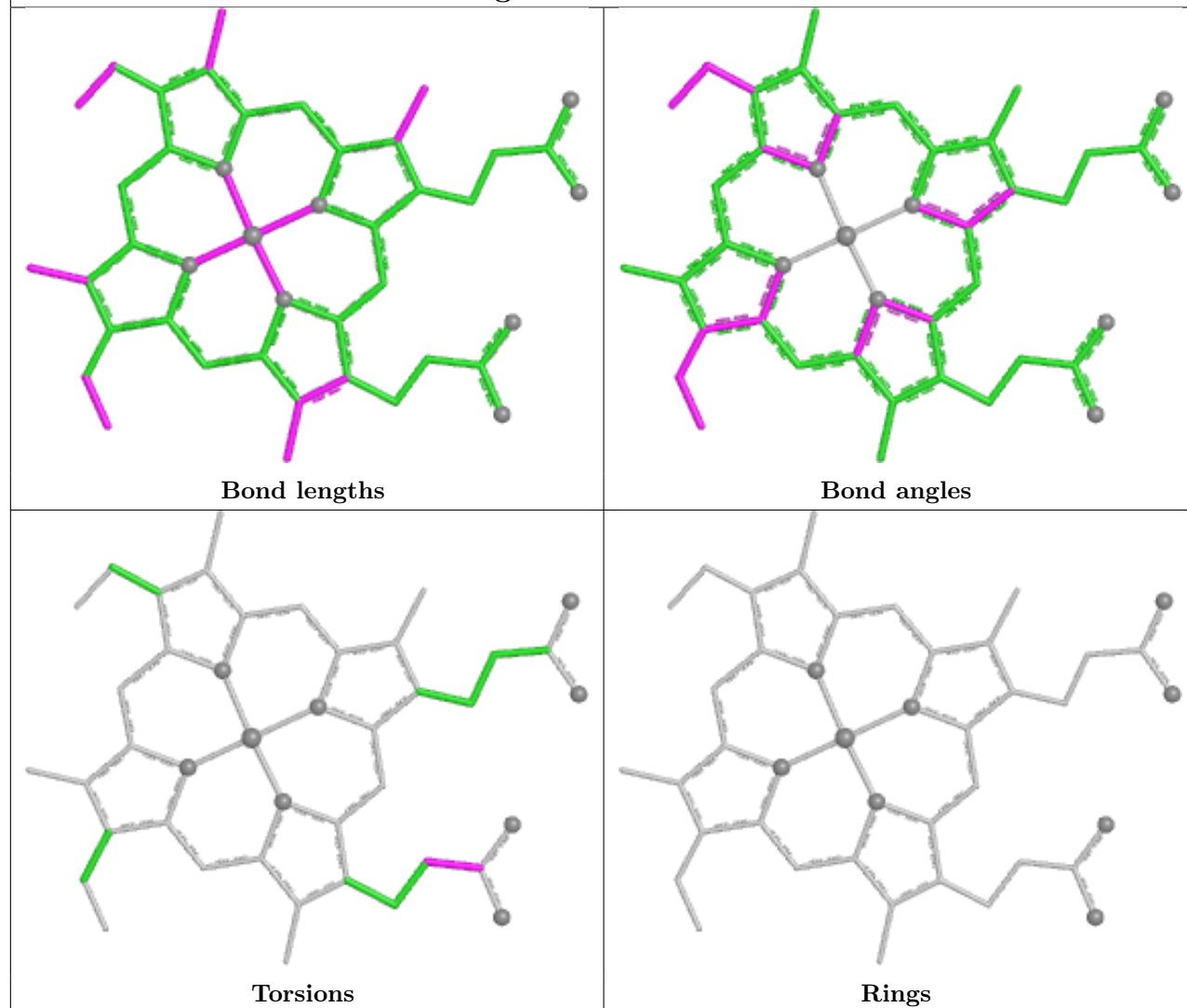
Torsions



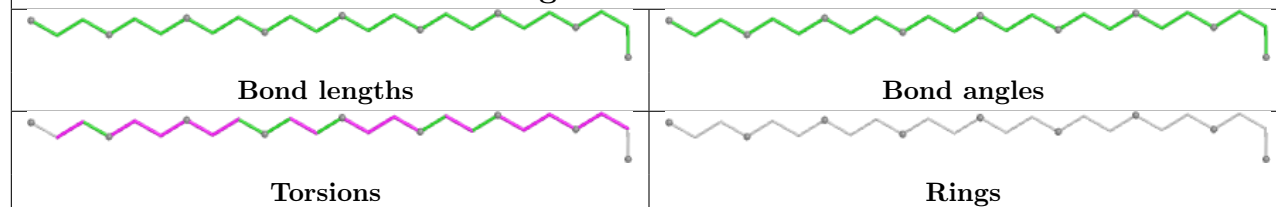
Rings

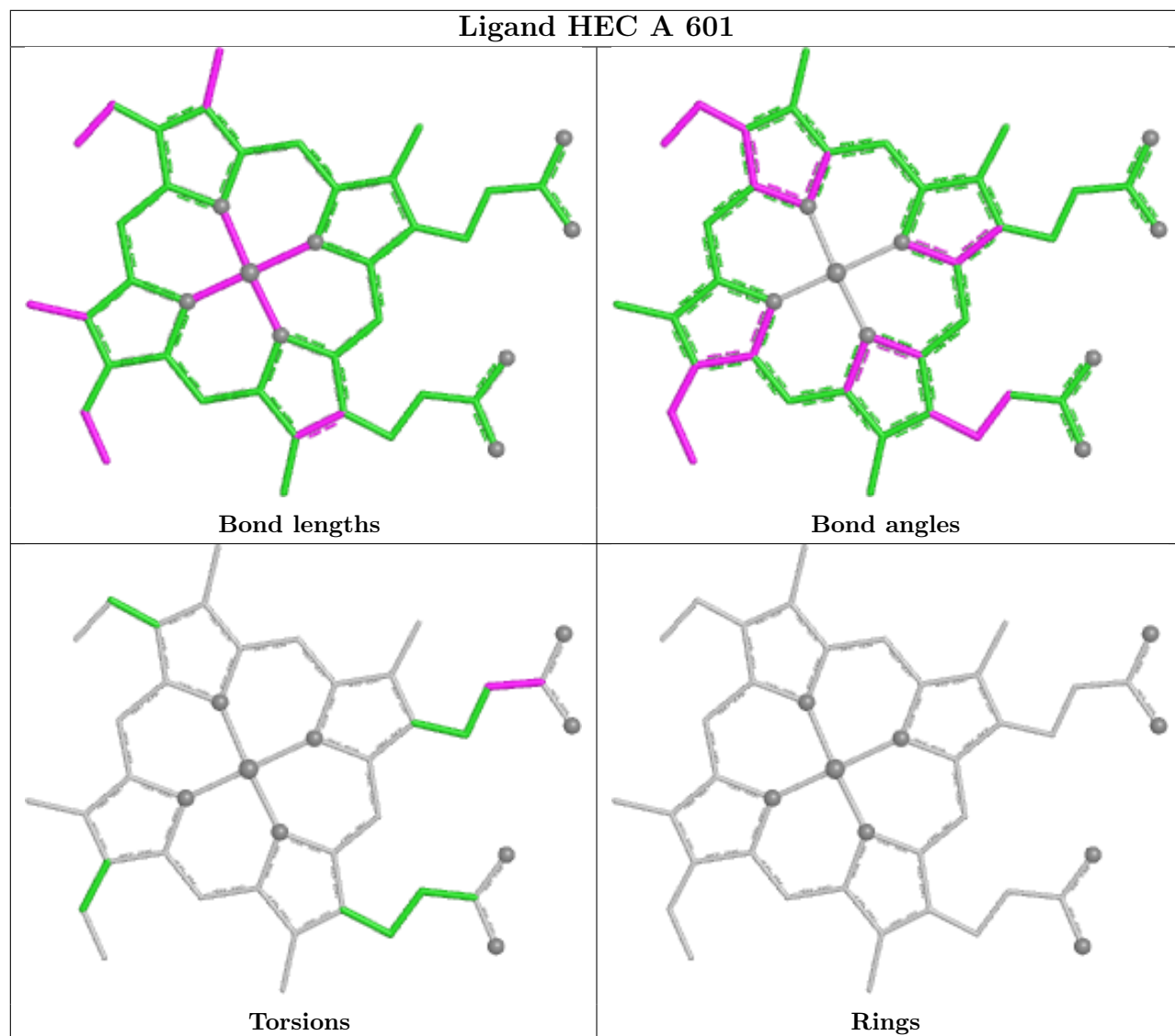


Ligand HEC E 608

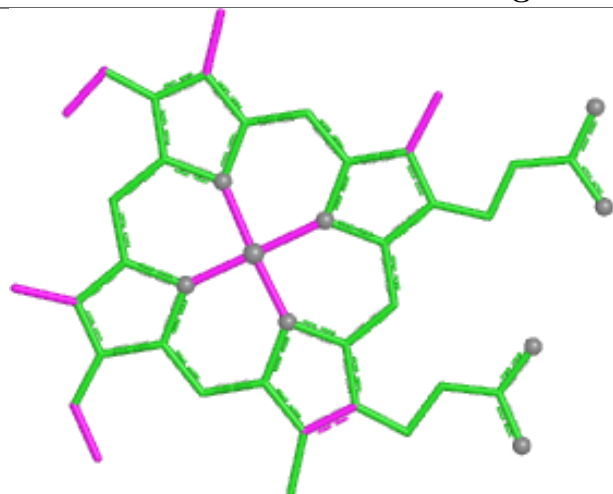


Ligand 12P C 610

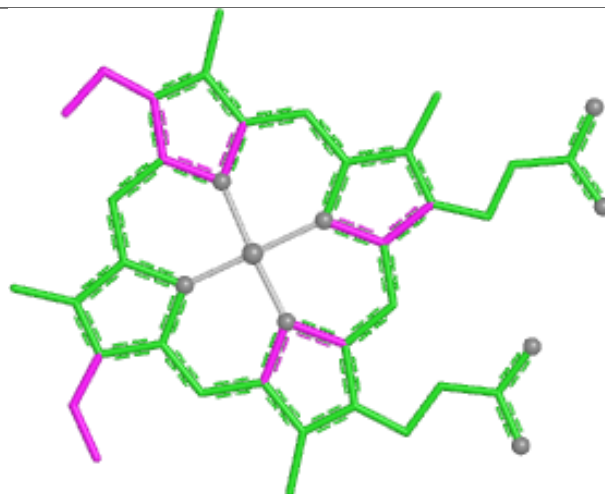




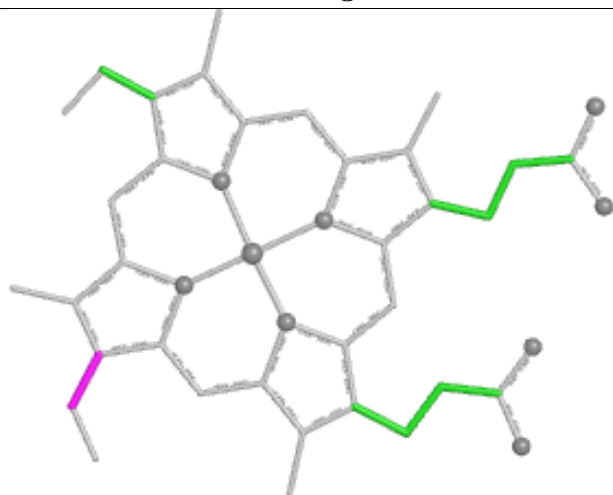
Ligand HEC C 604



Bond lengths



Bond angles

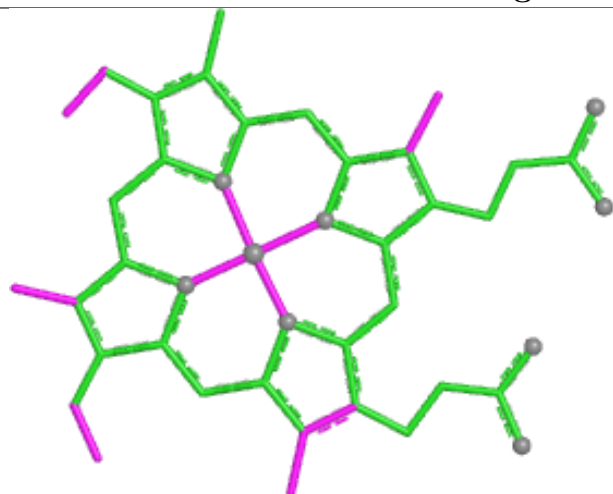


Torsions

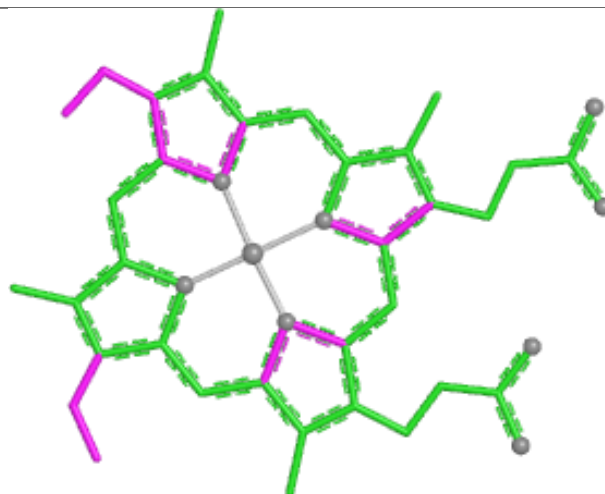


Rings

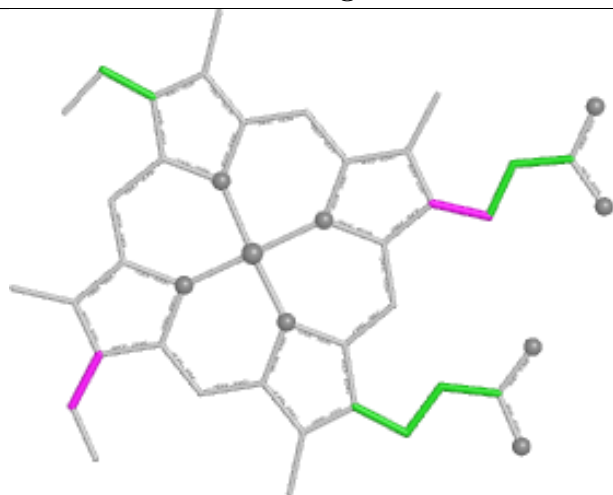
Ligand HEC E 605



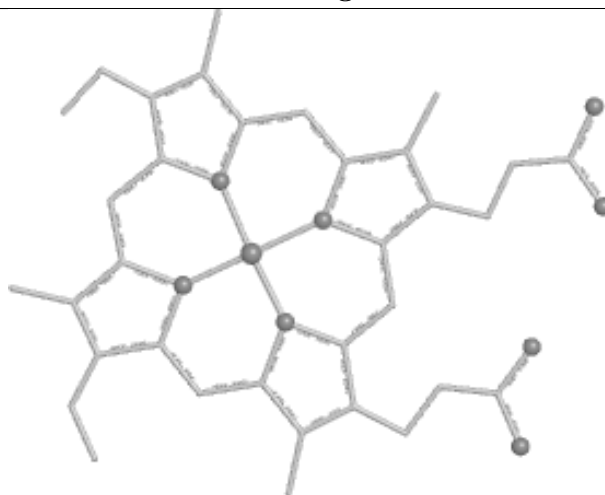
Bond lengths



Bond angles

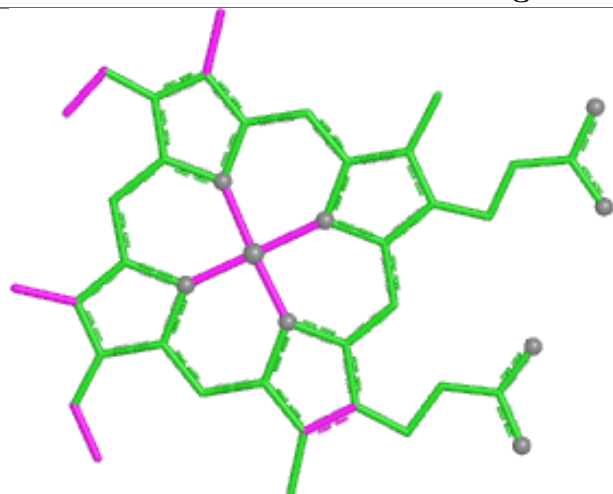


Torsions

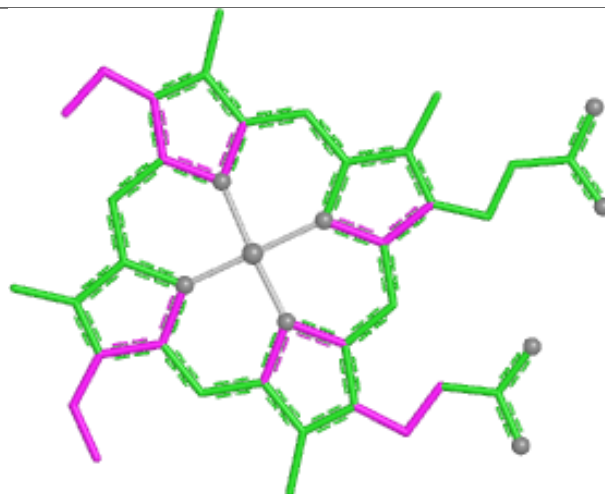


Rings

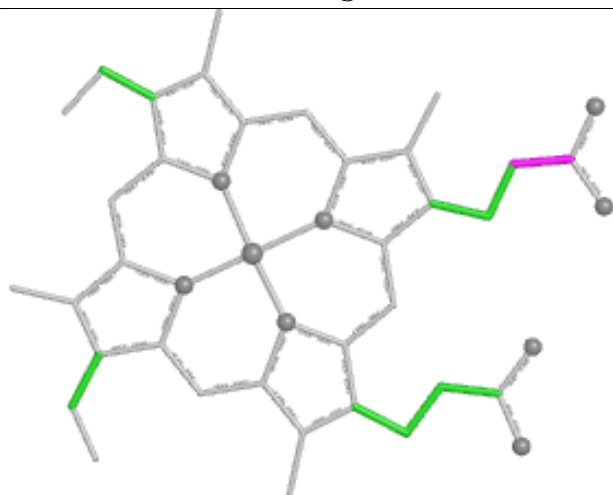
Ligand HEC C 602



Bond lengths



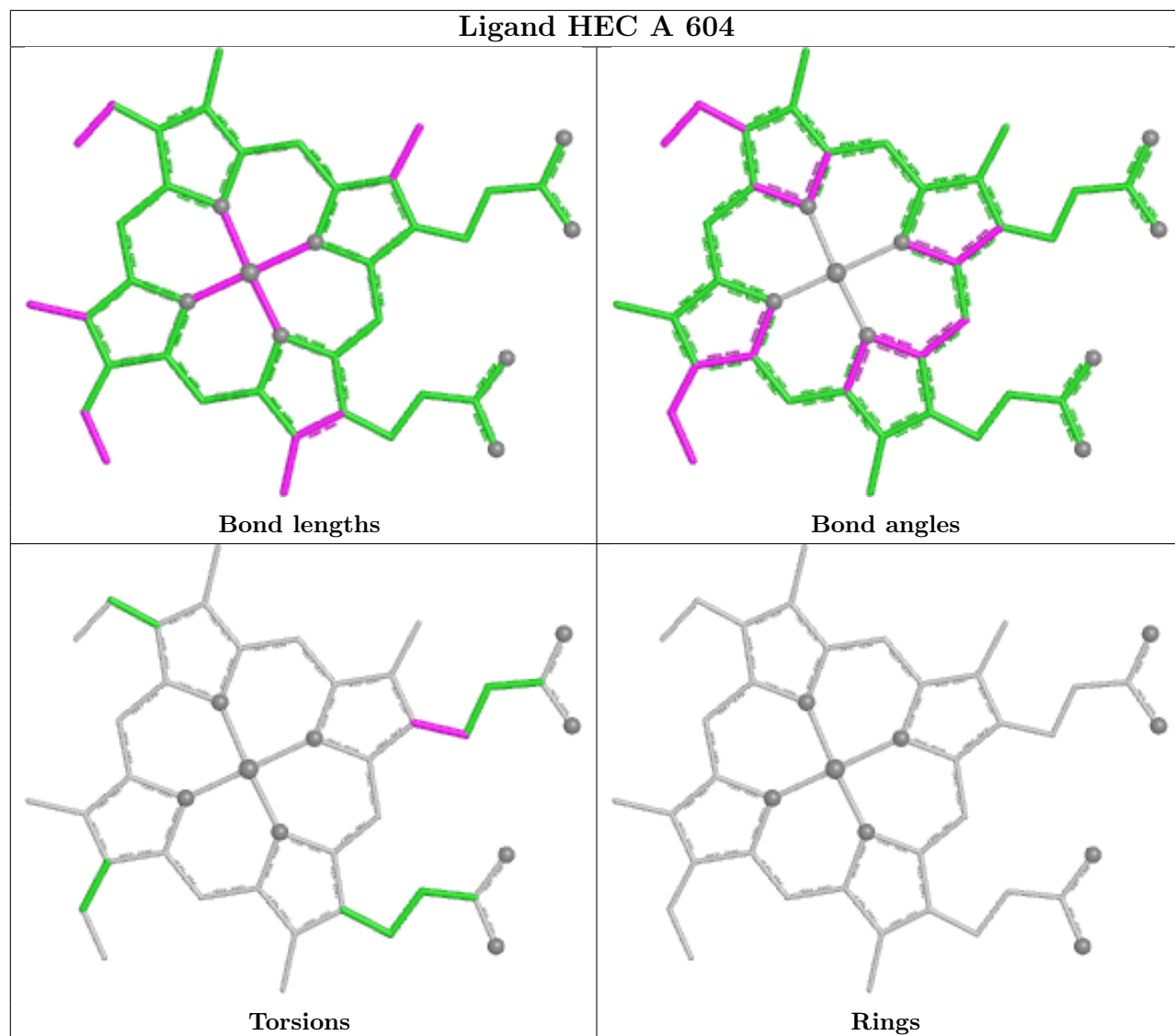
Bond angles

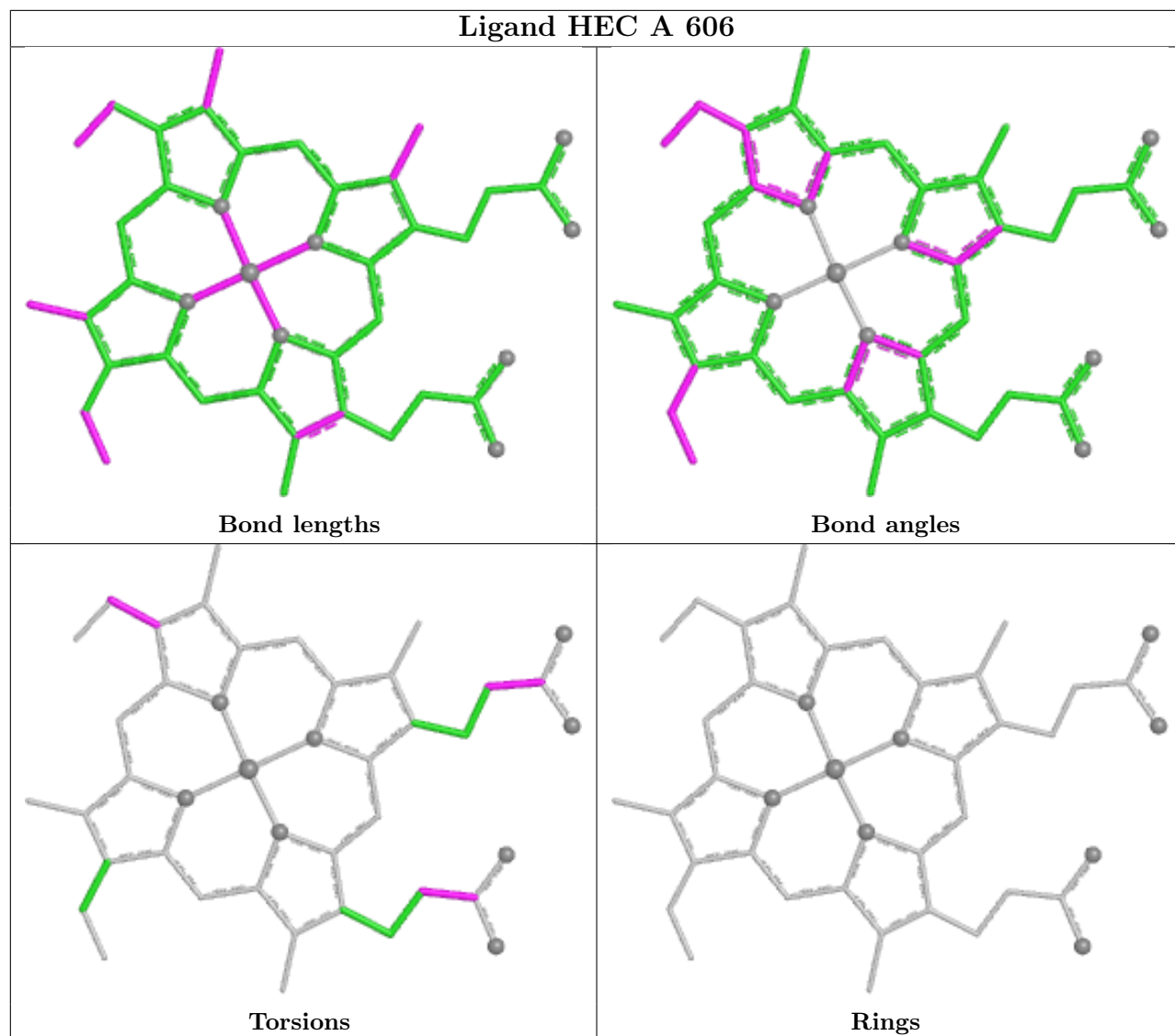


Torsions

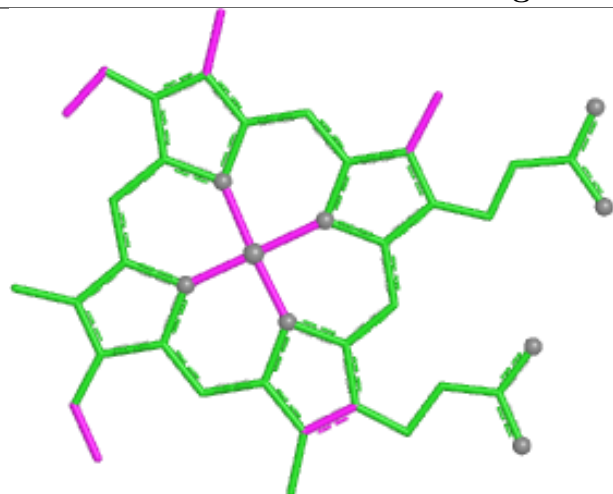


Rings

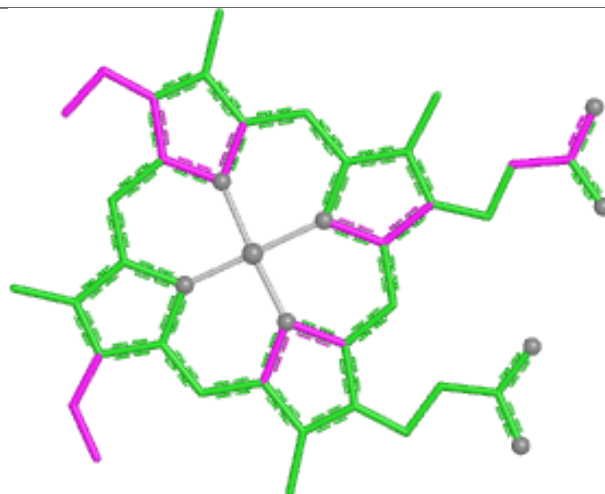




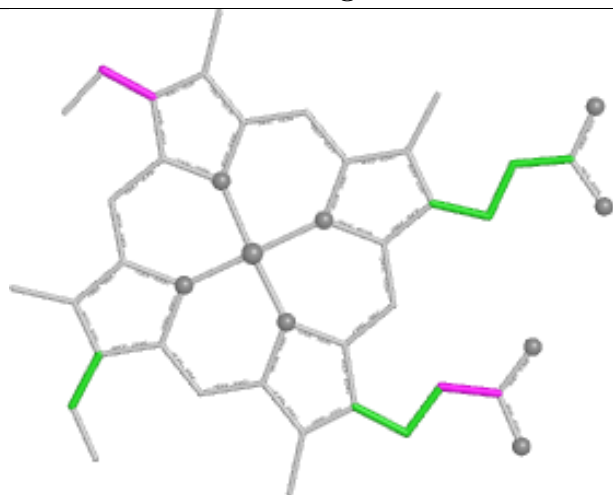
Ligand HEC C 607



Bond lengths



Bond angles

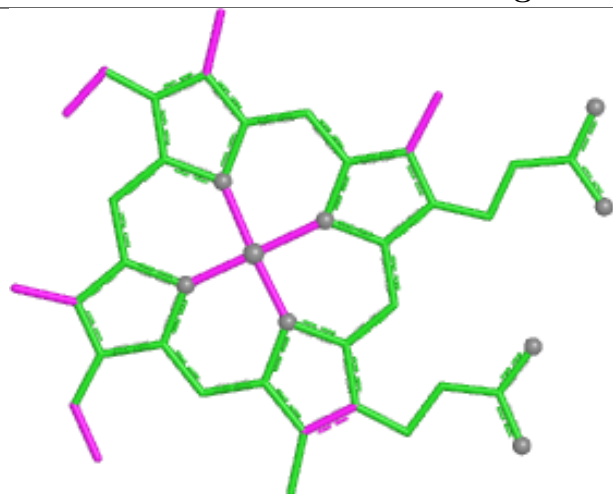


Torsions

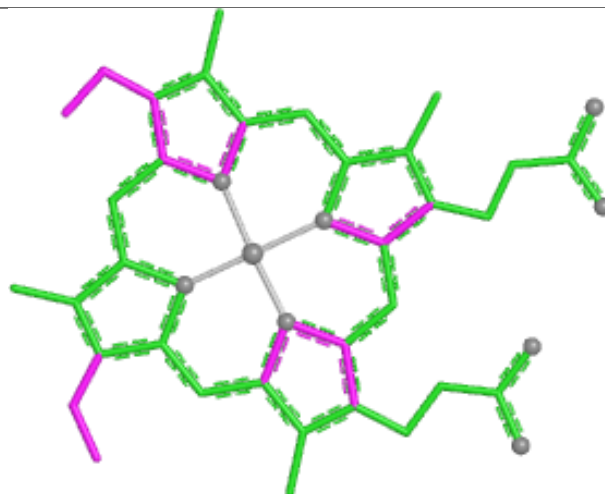


Rings

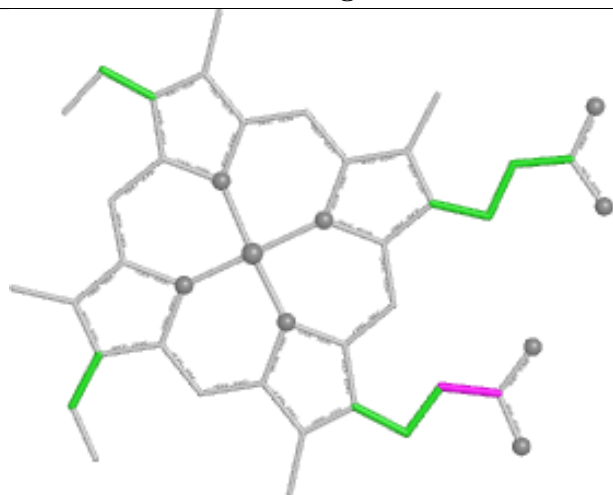
Ligand HEC E 607



Bond lengths



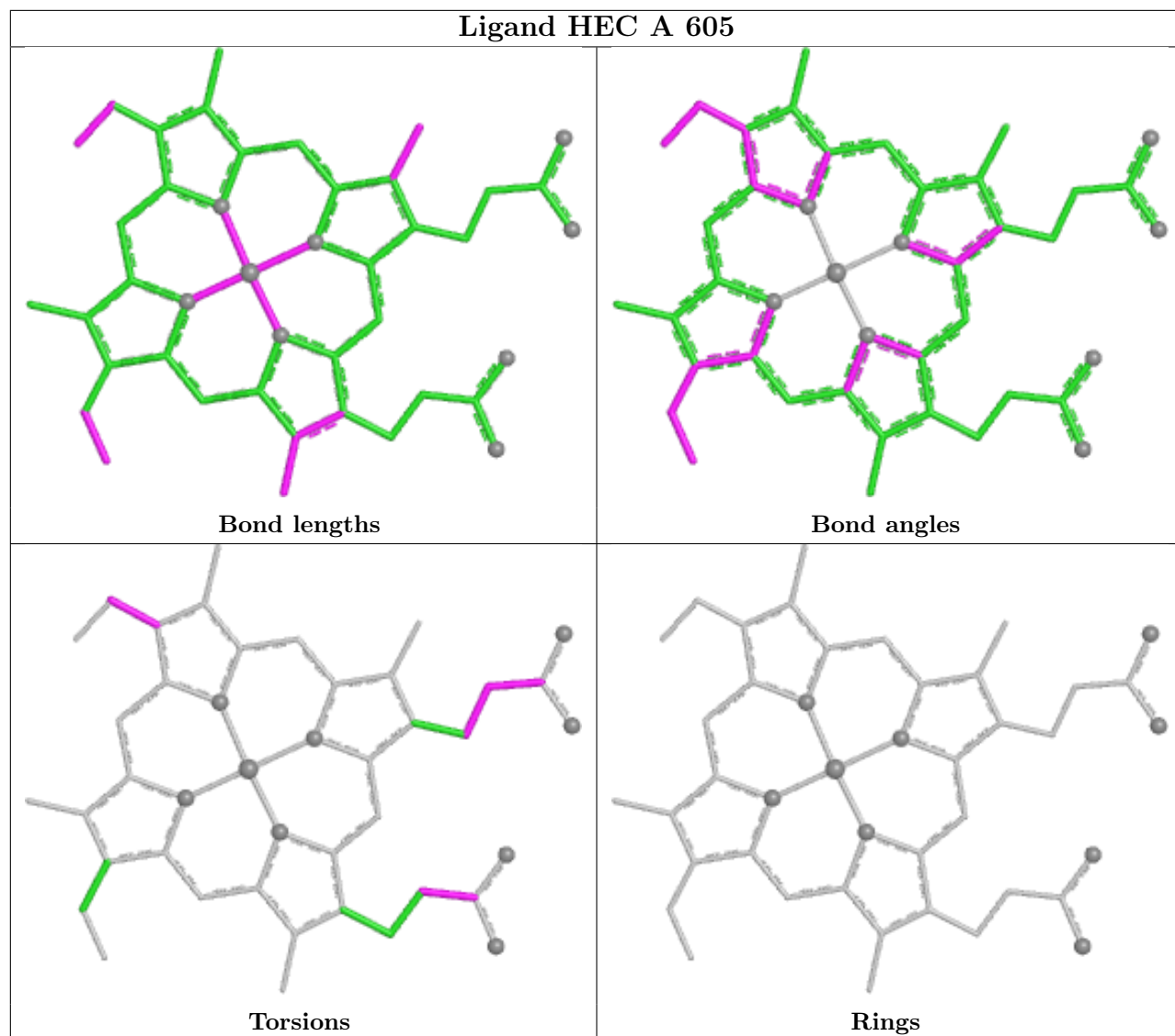
Bond angles



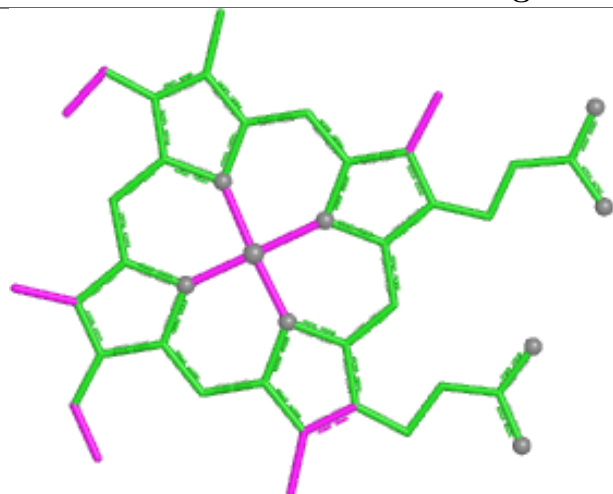
Torsions



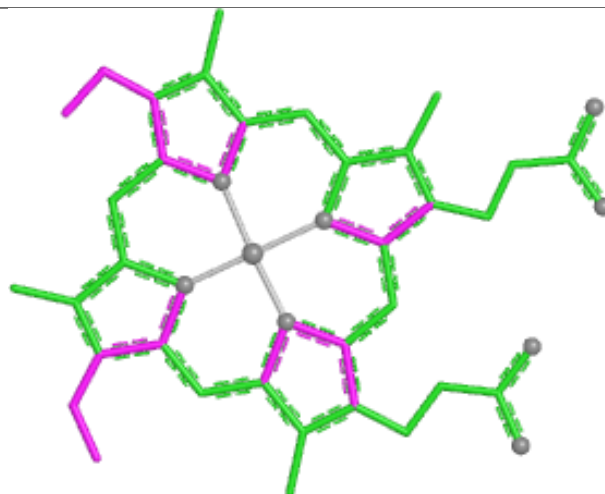
Rings



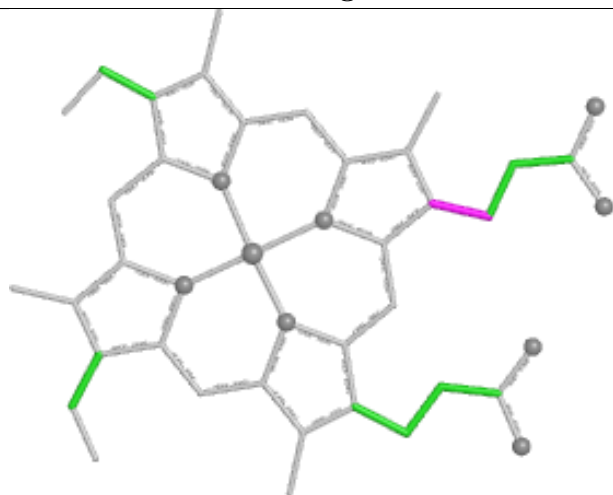
Ligand HEC C 605



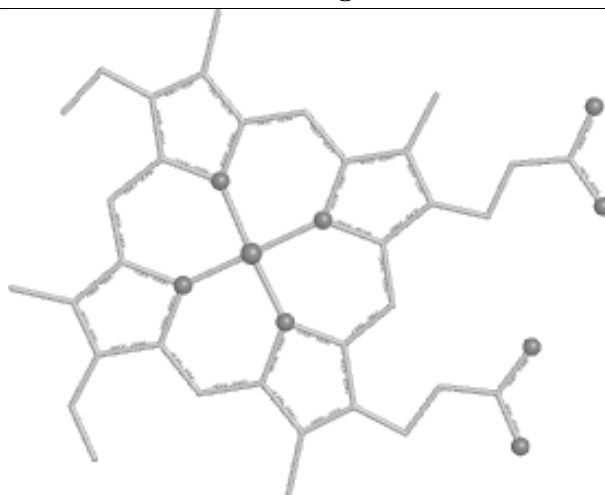
Bond lengths



Bond angles

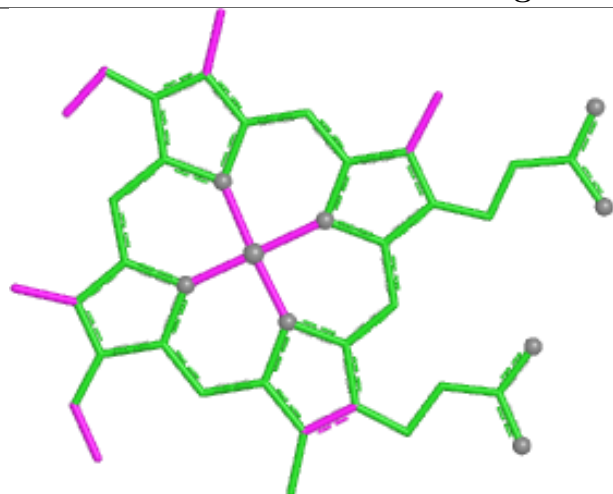


Torsions

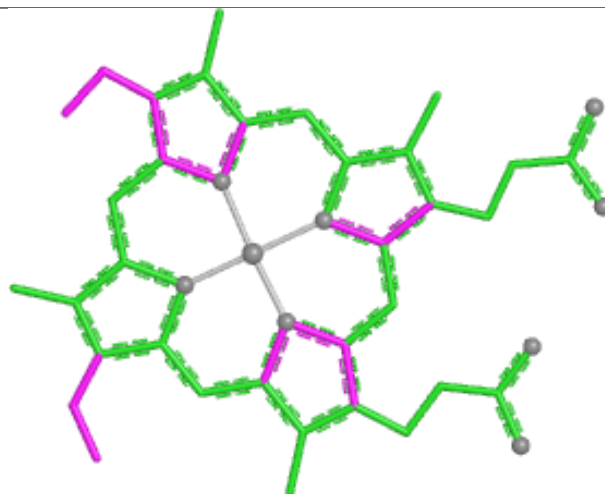


Rings

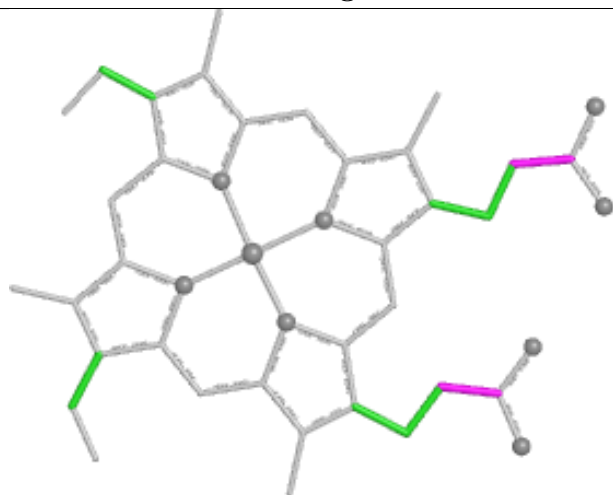
Ligand HEC E 603



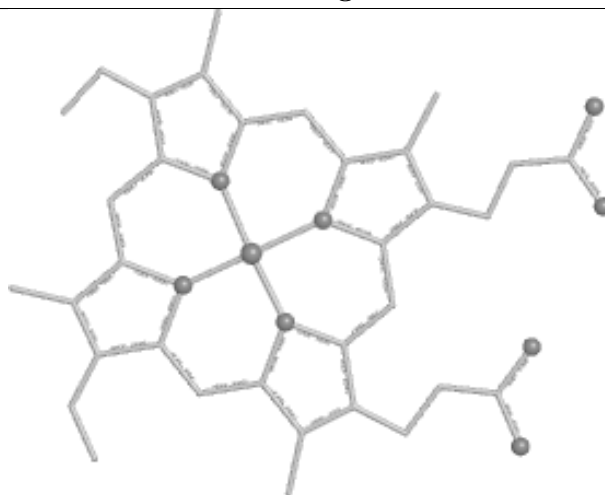
Bond lengths



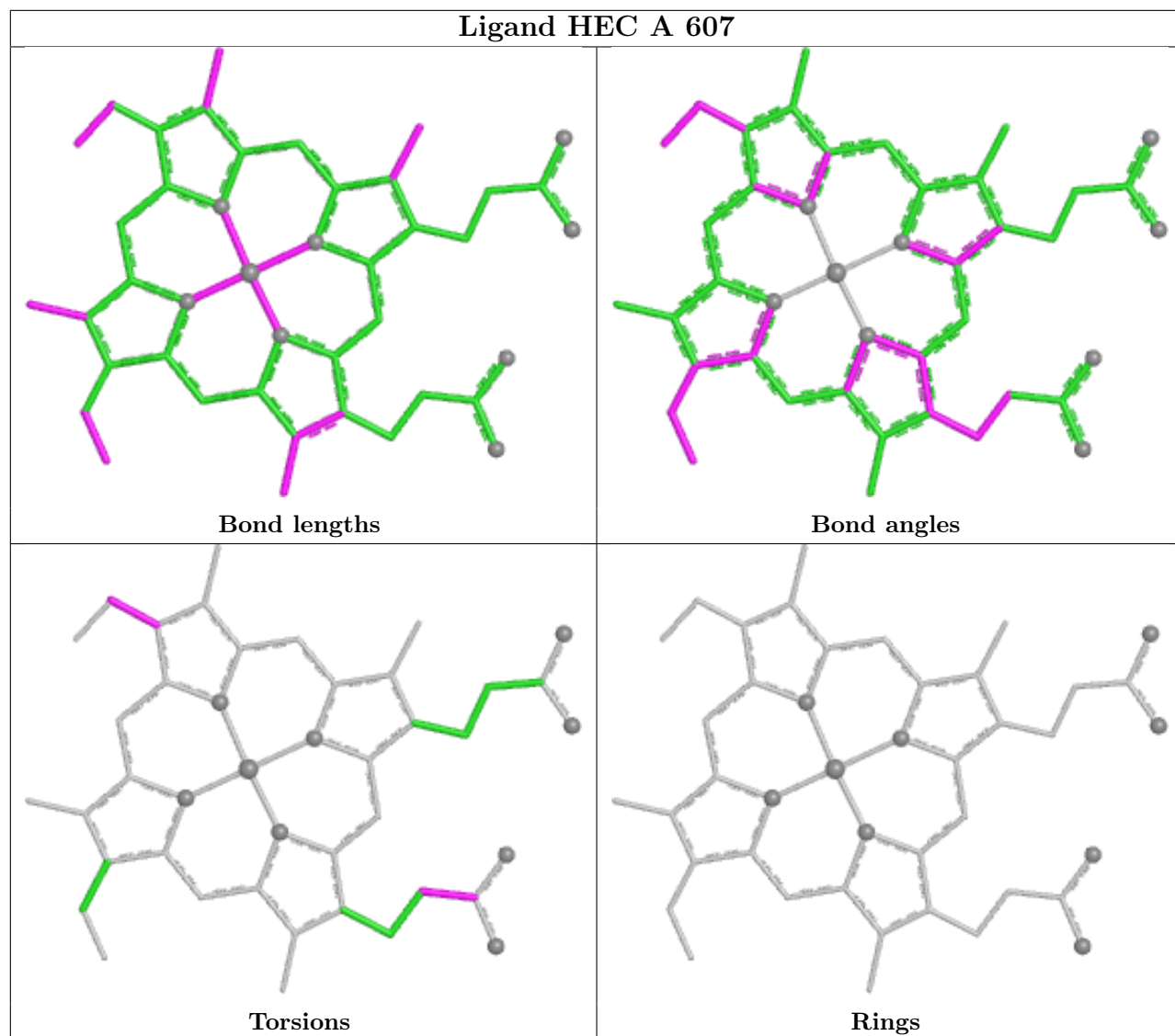
Bond angles



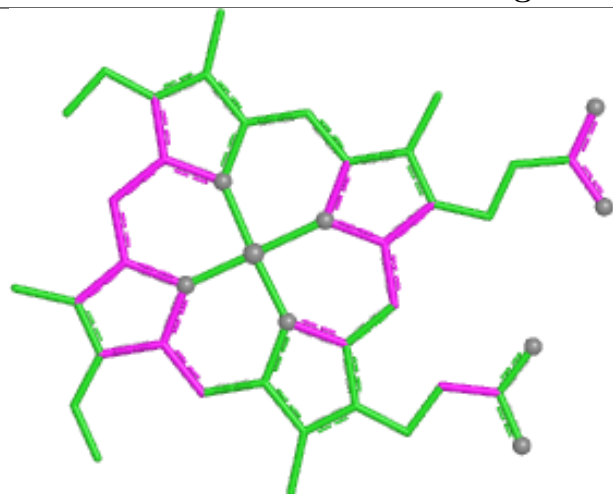
Torsions



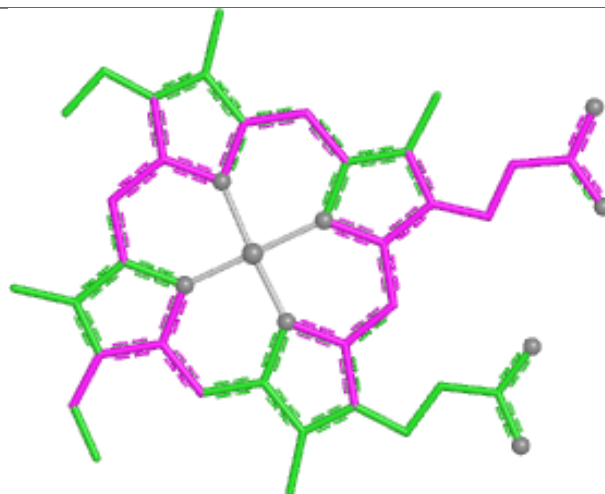
Rings



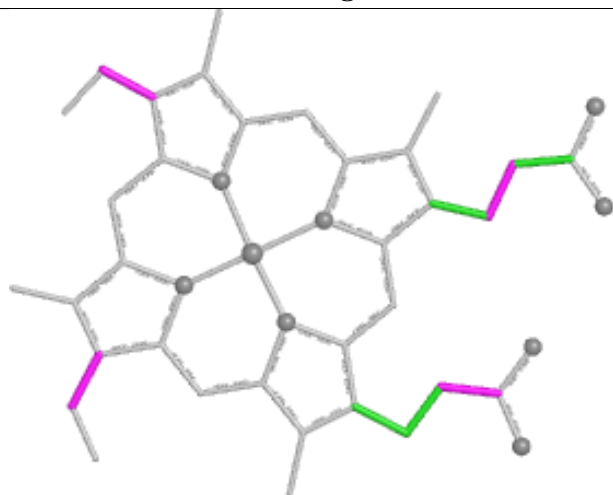
Ligand HEC E 601



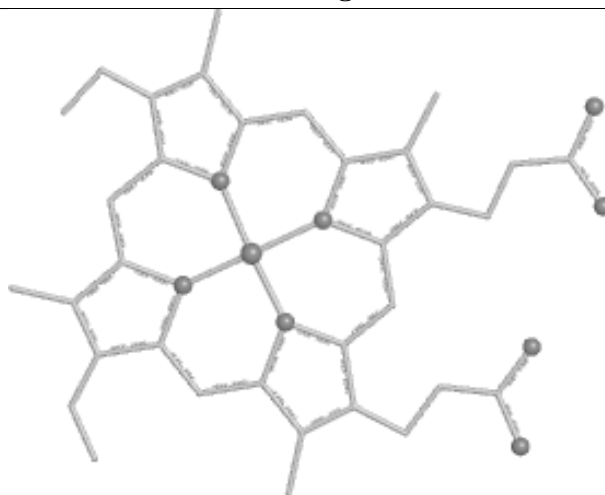
Bond lengths



Bond angles

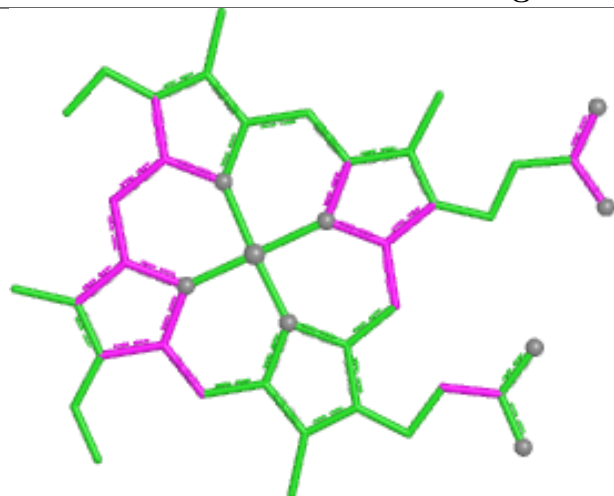


Torsions

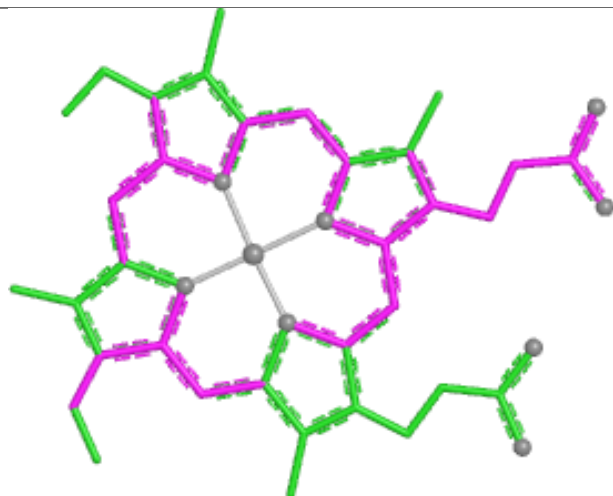


Rings

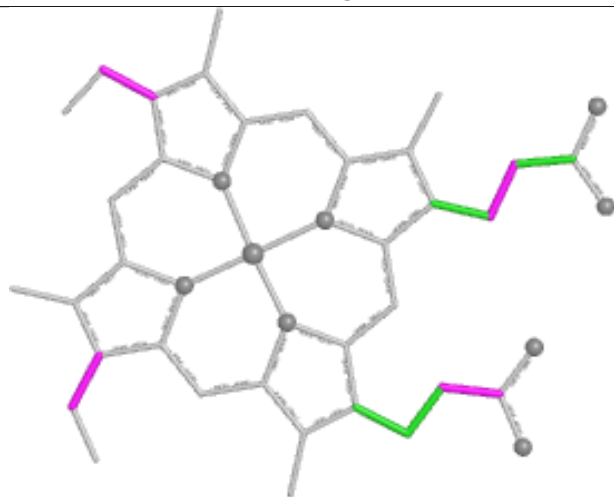
Ligand HEC C 601



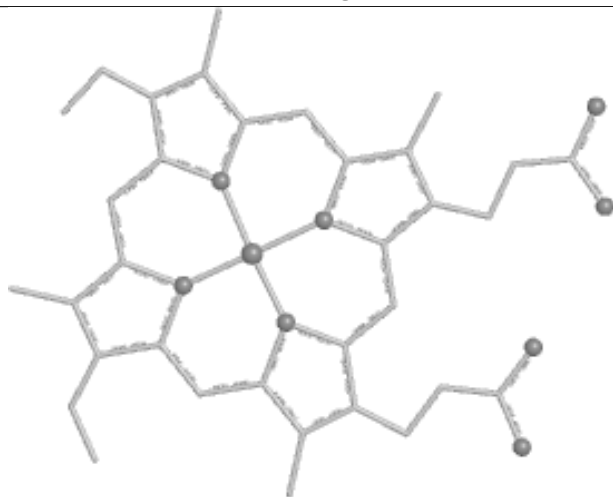
Bond lengths



Bond angles

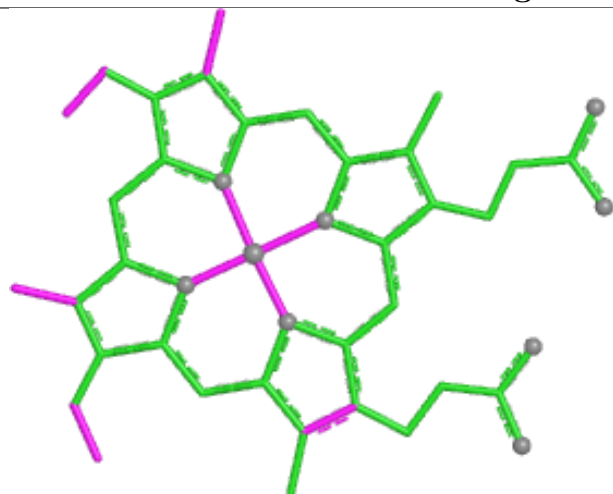


Torsions

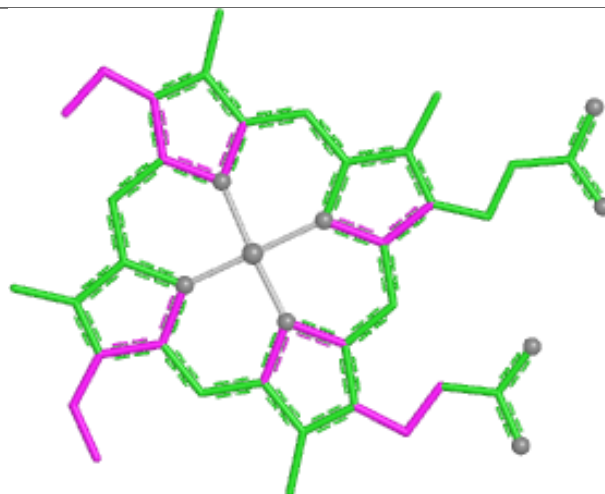


Rings

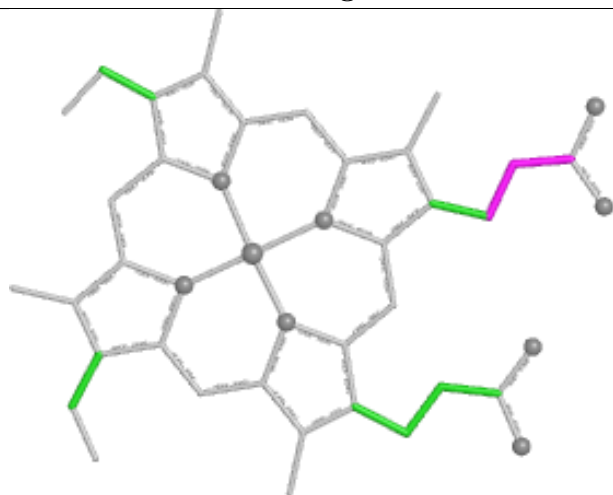
Ligand HEC E 602



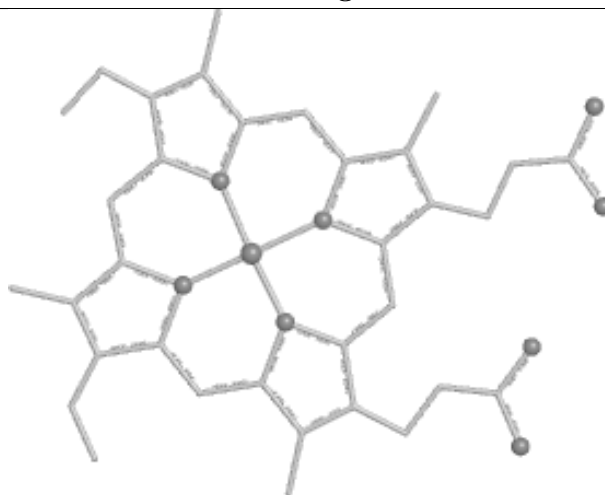
Bond lengths



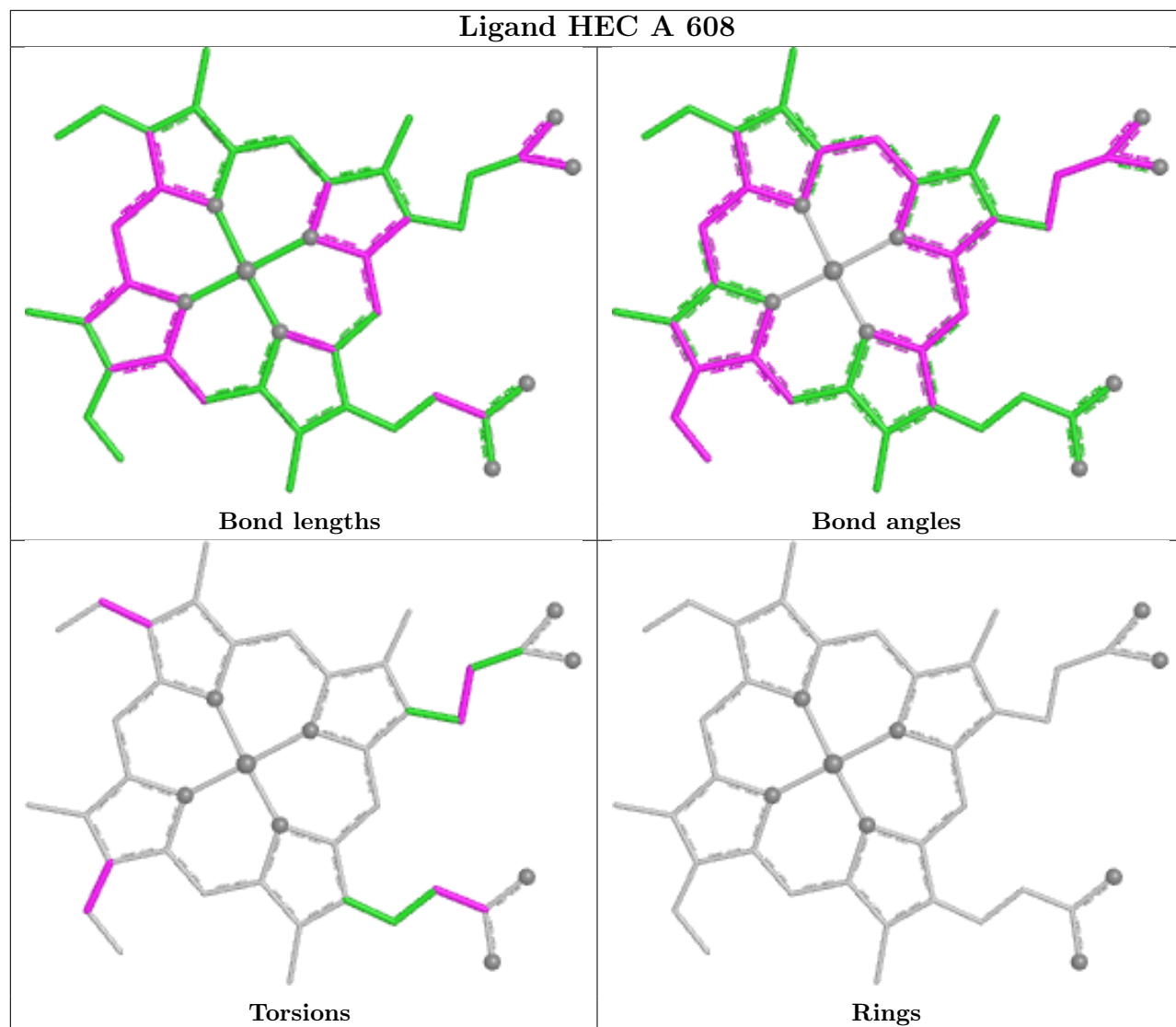
Bond angles

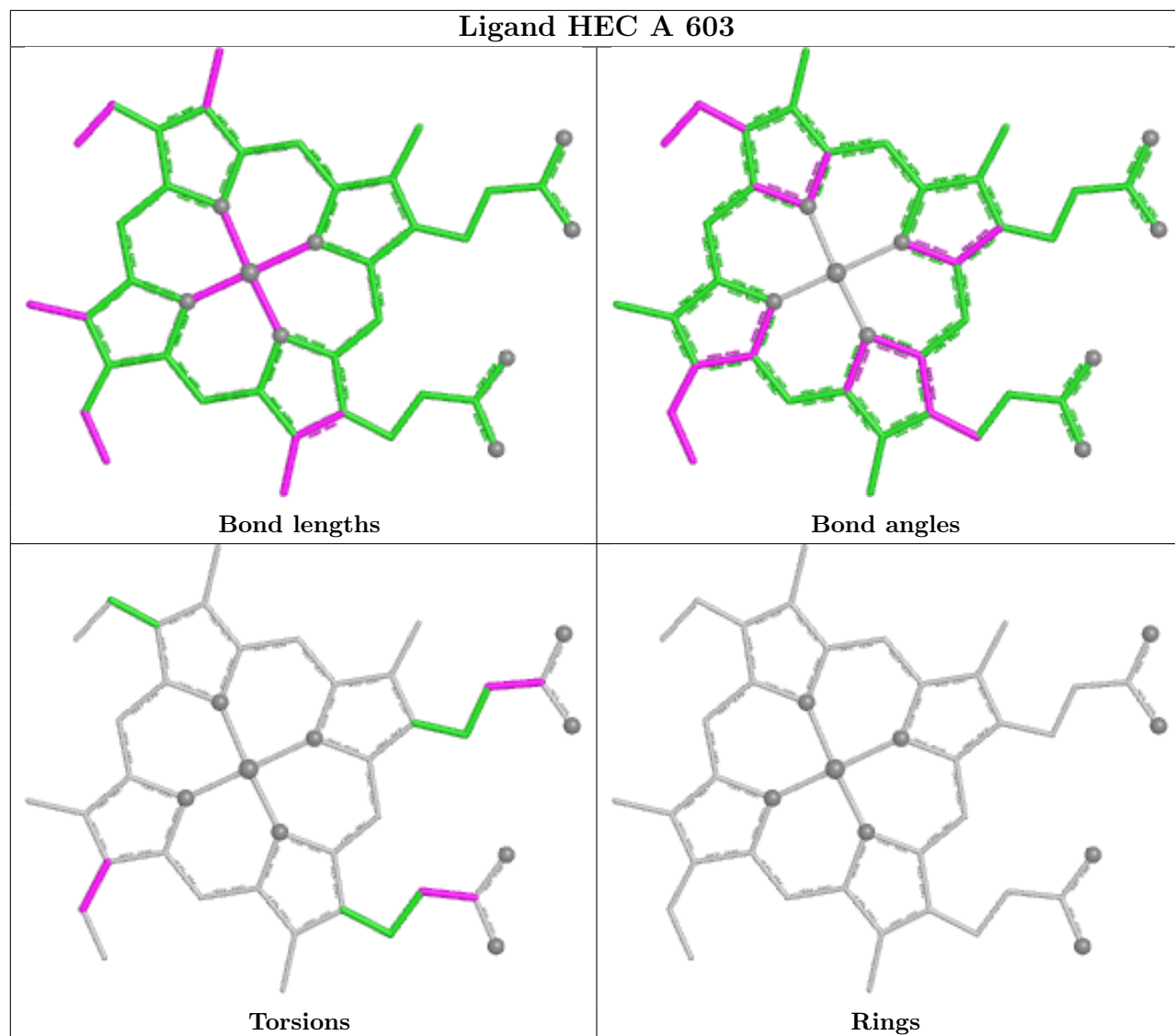


Torsions

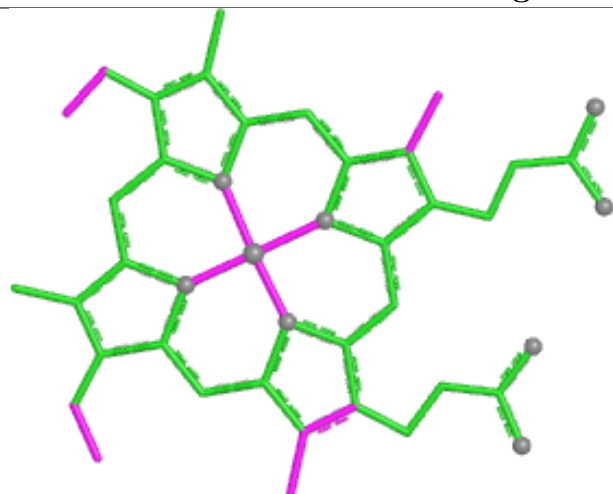


Rings

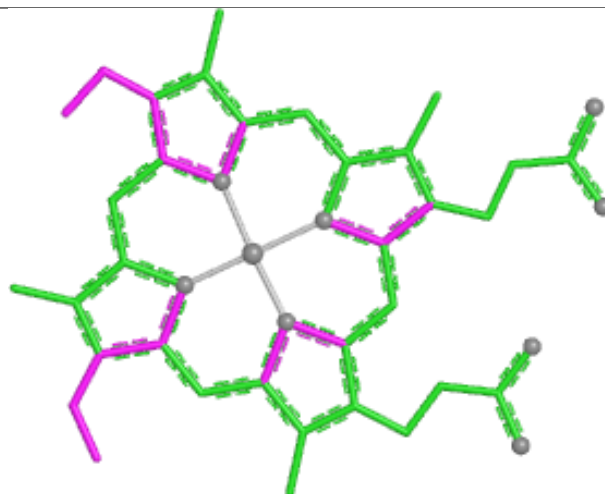




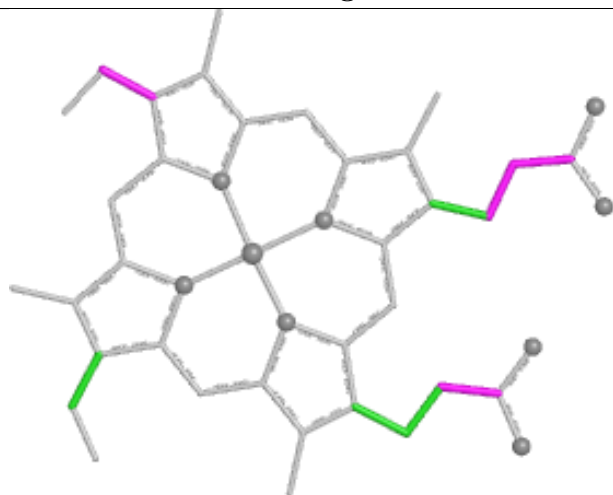
Ligand HEC C 606



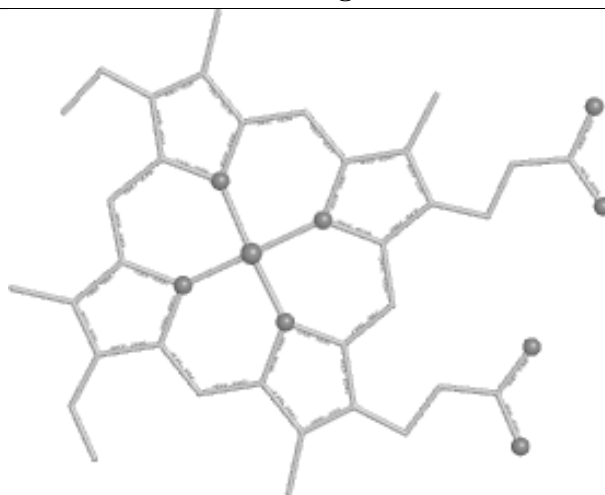
Bond lengths



Bond angles

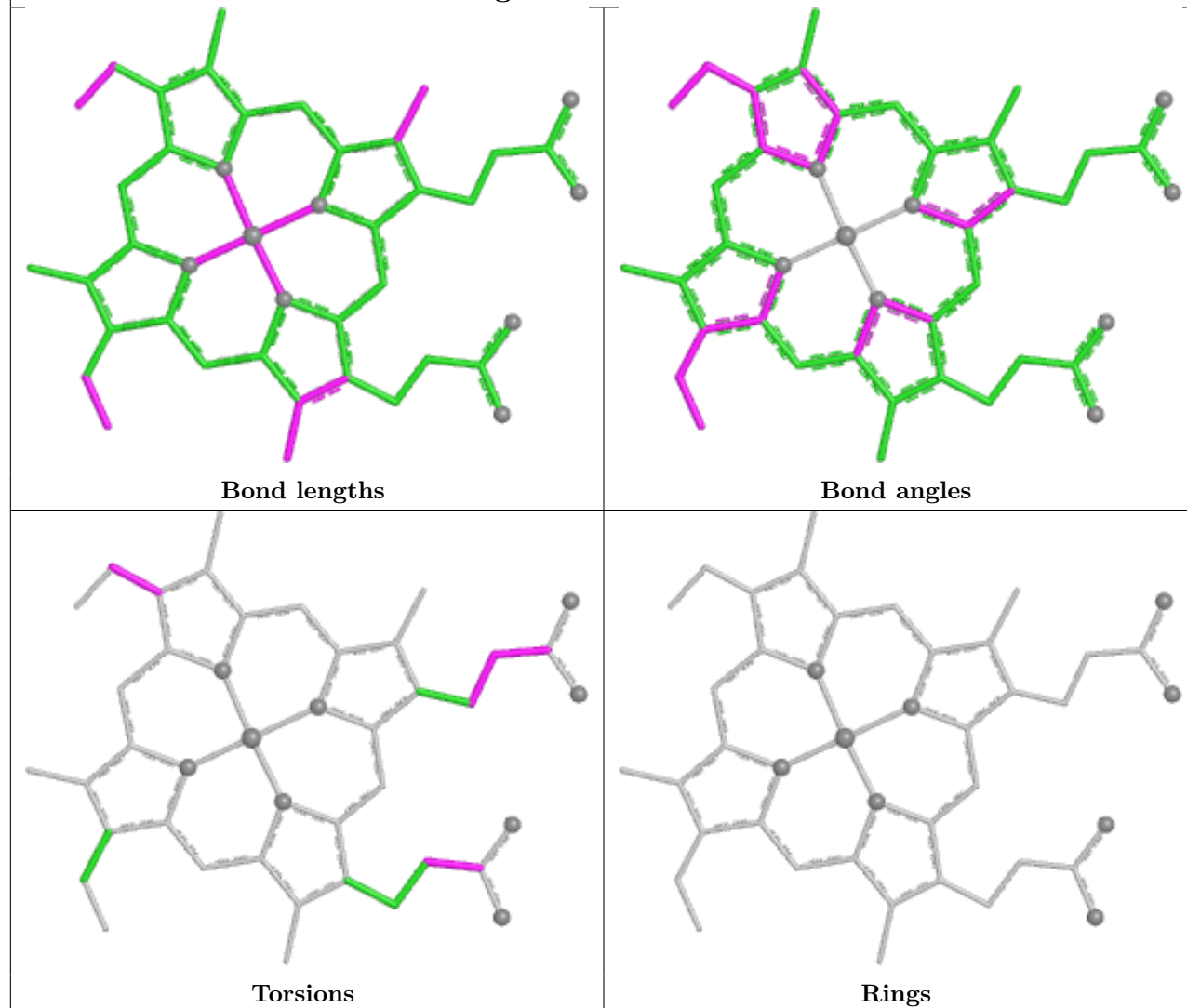


Torsions

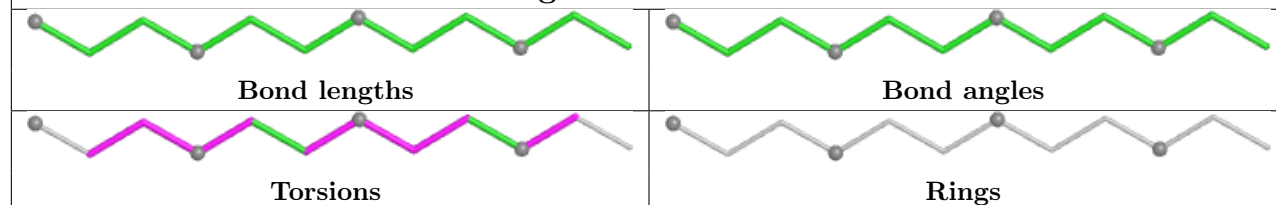


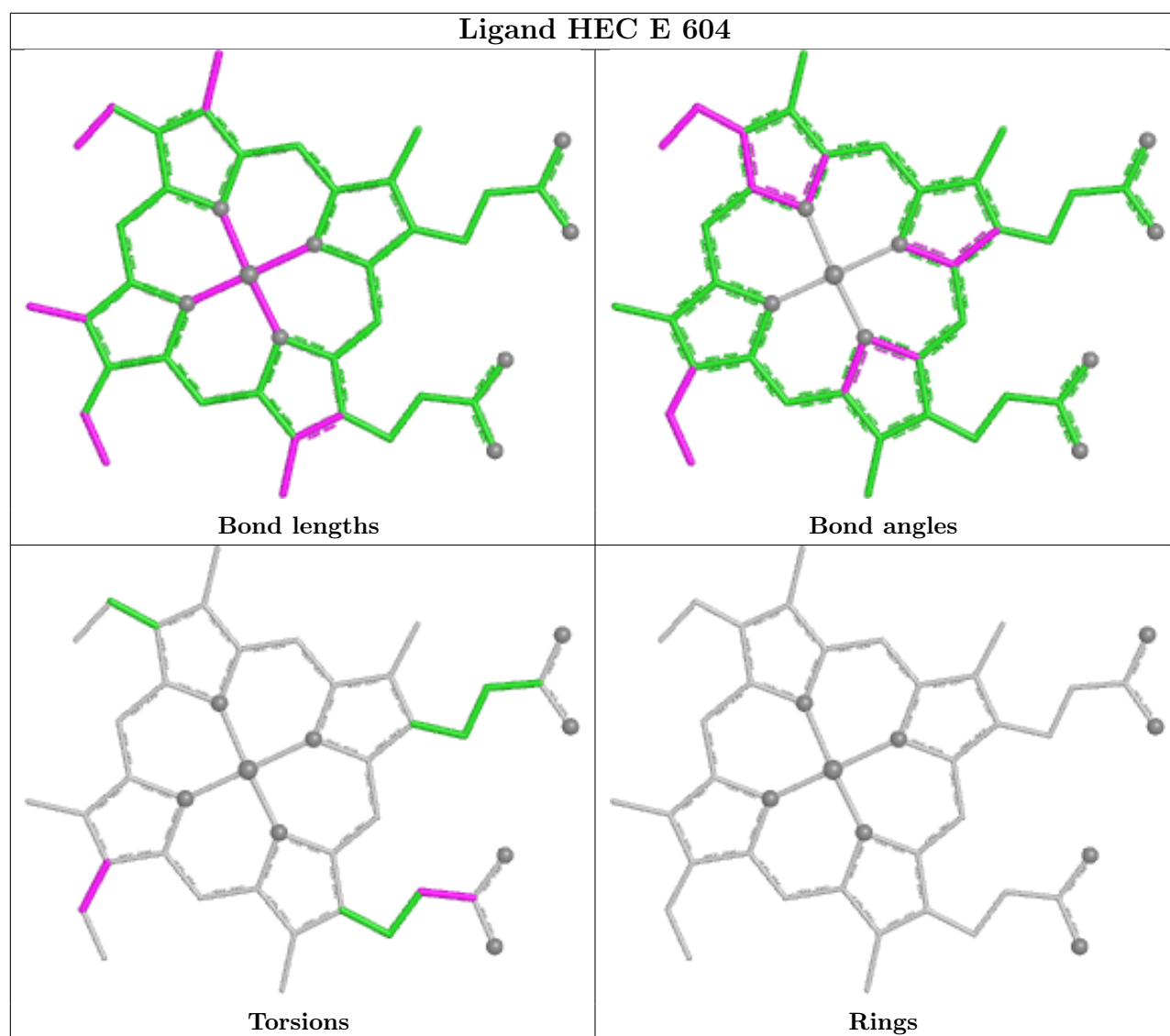
Rings

Ligand HEC E 606



Ligand 12P A 611





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	504/546 (92%)	0.57	25 (4%) 34 30	18, 31, 50, 60	0
1	C	502/546 (91%)	0.57	27 (5%) 31 28	18, 32, 48, 51	0
1	E	503/546 (92%)	0.42	17 (3%) 48 44	18, 29, 45, 56	1 (0%)
2	B	53/57 (92%)	1.20	12 (22%) 2 2	32, 43, 62, 64	0
2	D	57/57 (100%)	0.82	8 (14%) 6 5	25, 33, 58, 59	0
2	F	55/57 (96%)	1.53	15 (27%) 1 1	40, 46, 68, 68	0
All	All	1674/1809 (92%)	0.59	104 (6%) 26 23	18, 32, 50, 68	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	SER	5.6
1	A	527	GLY	4.8
1	E	179[A]	LYS	4.5
2	F	79	ALA	4.4
1	A	528	LYS	3.9
2	D	28	SER	3.8
2	D	84	GLY	3.8
2	F	83	SER	3.6
1	C	94	PRO	3.6
1	C	156	GLY	3.4
2	B	79	ALA	3.3
1	C	132	LEU	3.3
2	D	83	SER	3.3
1	A	163	THR	3.3
2	F	46	ASP	3.2
1	C	43	LYS	3.2
2	F	80	ARG	3.1
1	C	271	GLU	3.0
2	F	74	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	179	LYS	3.0
2	B	74	ALA	2.9
2	B	29	SER	2.9
2	B	77	GLN	2.8
1	E	147	GLU	2.8
1	A	520	ALA	2.8
2	B	81	GLU	2.8
1	C	520	ALA	2.8
1	A	159	GLY	2.7
1	A	34	TYR	2.7
1	A	160	GLU	2.7
2	F	72	ILE	2.7
1	A	31	ASP	2.6
1	C	129	ILE	2.6
2	B	75	LEU	2.6
1	C	134	SER	2.6
2	F	76	VAL	2.6
2	D	82	GLN	2.5
1	C	182	ALA	2.5
2	D	29	SER	2.5
1	E	97	VAL	2.5
1	A	25	ASP	2.5
1	A	152	LEU	2.5
2	F	47	LYS	2.5
2	D	76	VAL	2.5
1	C	68	THR	2.5
1	C	106	CYS	2.4
2	D	30	LEU	2.4
1	C	95	LYS	2.4
2	F	41	TYR	2.4
1	A	346	THR	2.4
1	A	162	GLU	2.4
2	F	75	LEU	2.4
2	F	29	SER	2.4
1	E	120	ARG	2.4
2	F	30	LEU	2.4
2	F	45	LYS	2.4
1	E	93	SER	2.3
1	A	153	ARG	2.3
1	E	525	LEU	2.3
1	C	29	VAL	2.3
2	B	76	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	80	ARG	2.3
1	C	181	LYS	2.3
1	A	181	LYS	2.3
1	C	128	LYS	2.3
2	F	67	VAL	2.3
1	E	152	LEU	2.3
2	B	46	ASP	2.3
1	E	344	GLU	2.3
1	C	131	ASN	2.2
1	A	158	LEU	2.2
1	C	180	ASP	2.2
1	E	148	VAL	2.2
1	A	523	ASN	2.2
2	B	50	THR	2.2
1	C	188	ILE	2.2
1	E	135	ASP	2.2
1	A	124	ALA	2.2
1	E	96	GLU	2.2
1	E	181	LYS	2.2
1	E	160	GLU	2.2
2	D	46	ASP	2.2
1	A	52	ALA	2.1
1	A	517	ALA	2.1
1	A	145	LEU	2.1
1	C	135	ASP	2.1
1	E	108	SER	2.1
1	C	39	LEU	2.1
1	C	158	LEU	2.1
1	E	515	LEU	2.1
1	A	43	LYS	2.1
1	E	98	ALA	2.1
1	C	159	GLY	2.1
1	A	165	LYS	2.1
1	E	127	ASP	2.1
2	F	78	LYS	2.1
1	A	519	GLN	2.1
1	C	153	ARG	2.0
1	C	515	LEU	2.0
1	A	42	GLY	2.0
1	C	105	GLU	2.0
1	A	521	ARG	2.0
2	B	33	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	72	ILE	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
6	12P	A	611	12/37	0.65	0.26	50,51,51,51	0
6	12P	C	610	25/37	0.73	0.23	57,58,59,59	0
4	K	A	609	1/1	0.80	0.22	31,31,31,31	0
3	HEC	C	604	43/43	0.90	0.16	39,42,43,43	0
3	HEC	E	604	43/43	0.91	0.14	38,40,41,42	0
5	HOA	E	610	2/2	0.91	0.12	23,23,23,24	0
7	PO4	E	609	5/5	0.91	0.11	51,51,52,52	0
5	HOA	A	610	2/2	0.93	0.13	21,21,21,22	0
5	HOA	C	609	2/2	0.93	0.09	26,26,26,26	0
3	HEC	A	608	43/43	0.94	0.10	22,24,27,28	0
3	HEC	E	605	43/43	0.94	0.11	29,30,32,34	0
3	HEC	A	602	43/43	0.94	0.11	34,36,37,37	0
3	HEC	C	605	43/43	0.95	0.10	34,36,37,37	0
3	HEC	E	601	43/43	0.95	0.09	23,25,27,28	0
3	HEC	E	603	43/43	0.95	0.11	31,32,33,35	0
3	HEC	A	601	43/43	0.95	0.10	27,28,29,29	0
3	HEC	C	601	43/43	0.95	0.10	20,21,23,23	0
3	HEC	A	605	43/43	0.95	0.10	22,23,24,25	0
3	HEC	E	606	43/43	0.96	0.08	19,20,21,22	0
3	HEC	A	603	43/43	0.96	0.10	27,30,31,32	0
3	HEC	C	607	43/43	0.96	0.09	18,19,21,22	0
3	HEC	A	606	43/43	0.96	0.09	21,23,25,26	0

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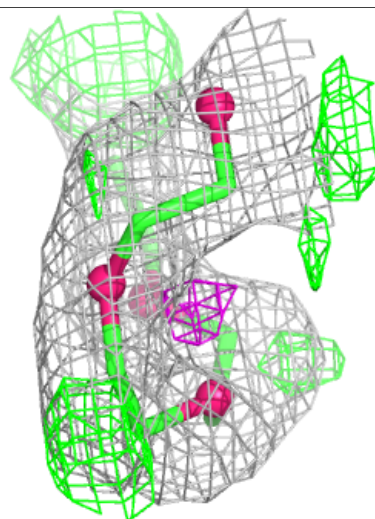
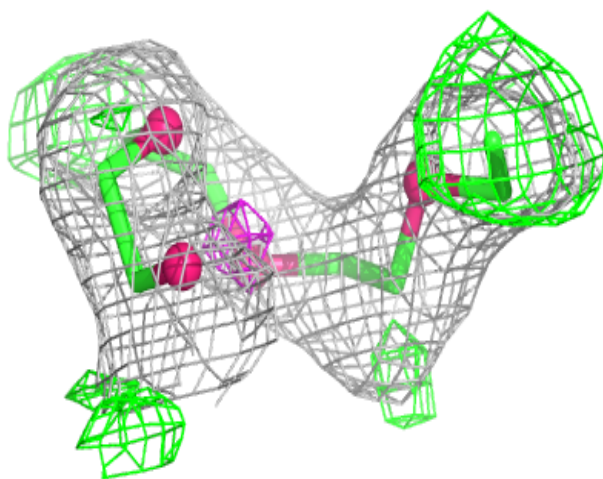
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	E	602	43/43	0.96	0.09	26,26,27,27	0
3	HEC	C	602	43/43	0.96	0.09	25,26,28,29	0
3	HEC	C	603	43/43	0.96	0.10	31,32,33,33	0
3	HEC	A	607	43/43	0.96	0.09	26,27,27,28	0
3	HEC	C	608	43/43	0.97	0.09	19,21,23,23	0
3	HEC	E	607	43/43	0.97	0.08	19,19,20,21	0
3	HEC	E	608	43/43	0.97	0.08	24,24,27,28	0
3	HEC	C	606	43/43	0.97	0.08	19,20,21,22	0
3	HEC	A	604	43/43	0.97	0.09	25,27,30,31	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.

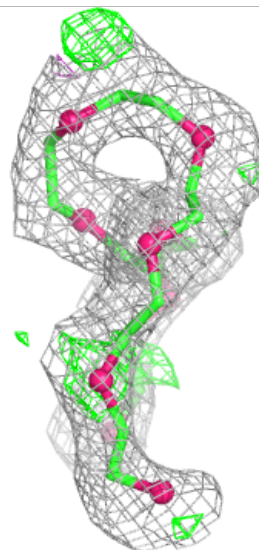
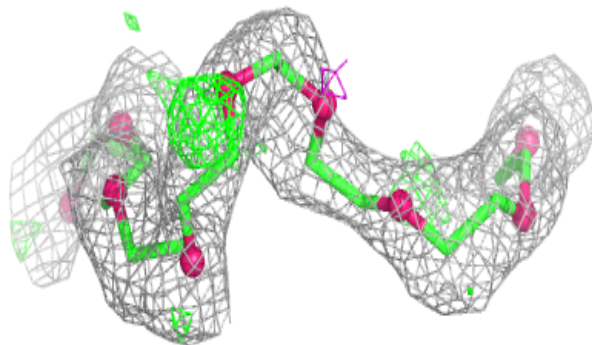
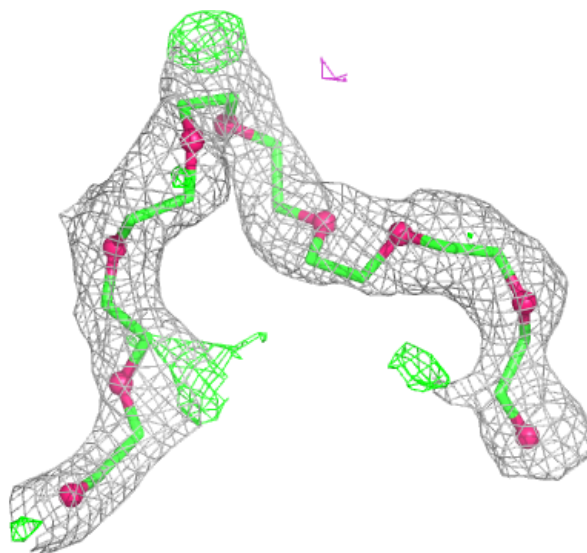
Electron density around 12P A 611:

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



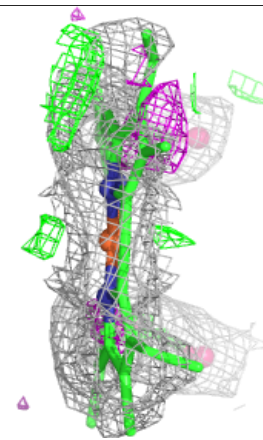
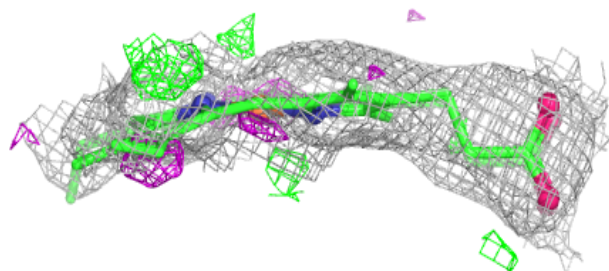
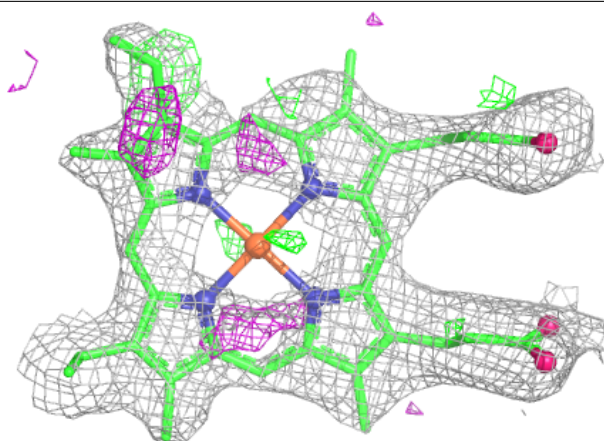
Electron density around 12P C 610:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



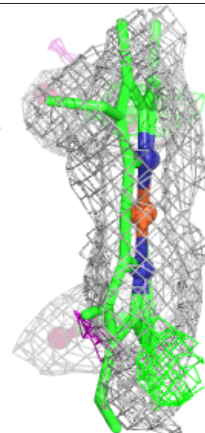
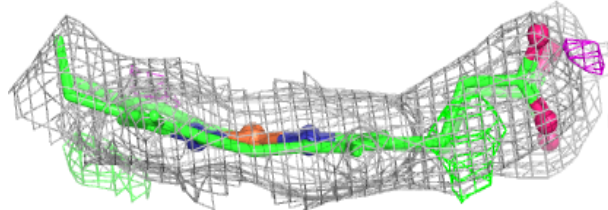
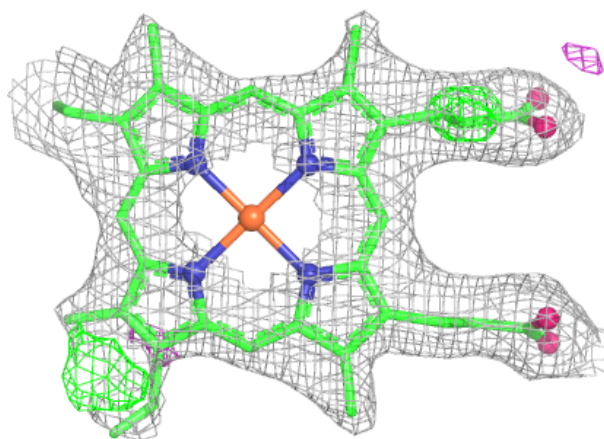
Electron density around HEC C 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



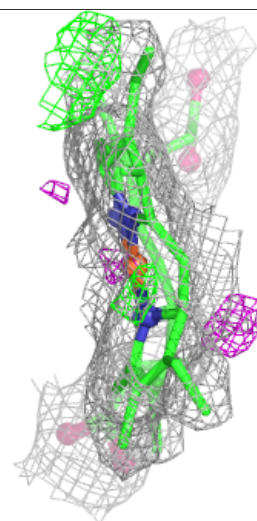
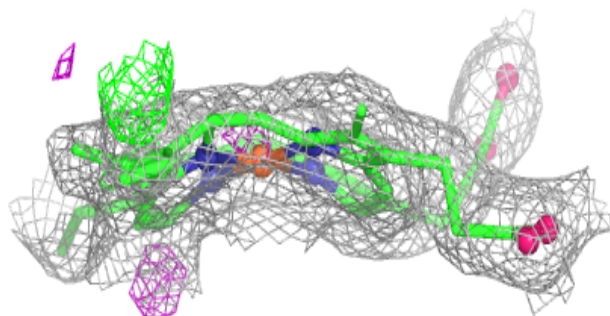
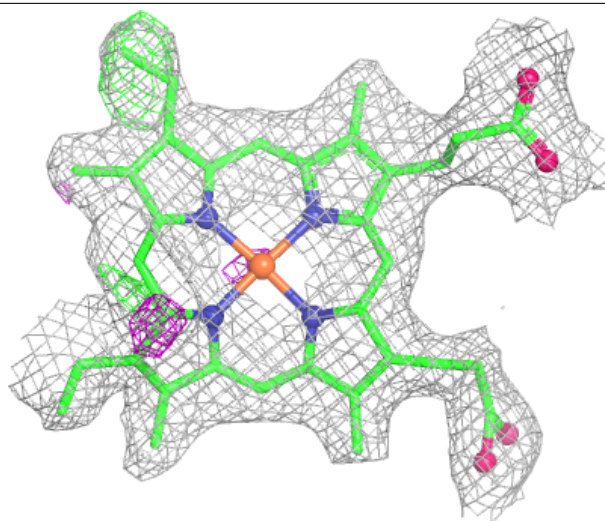
Electron density around HEC E 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



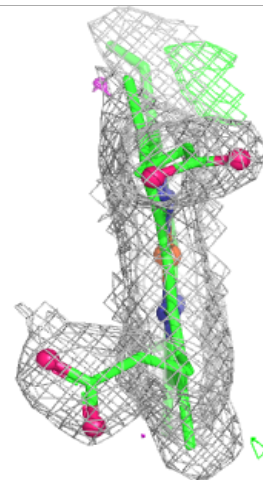
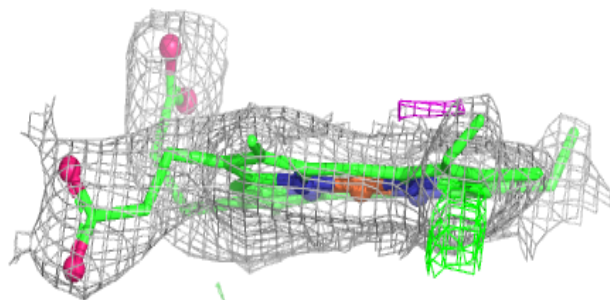
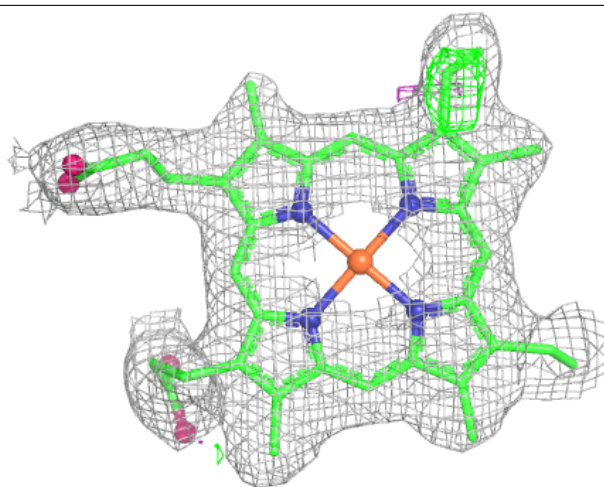
Electron density around HEC A 608:

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



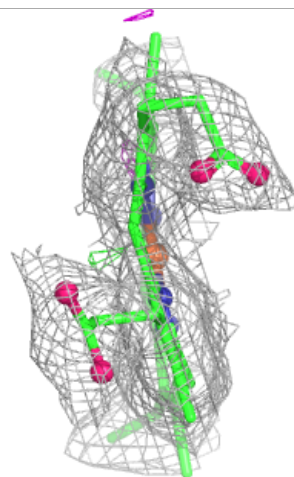
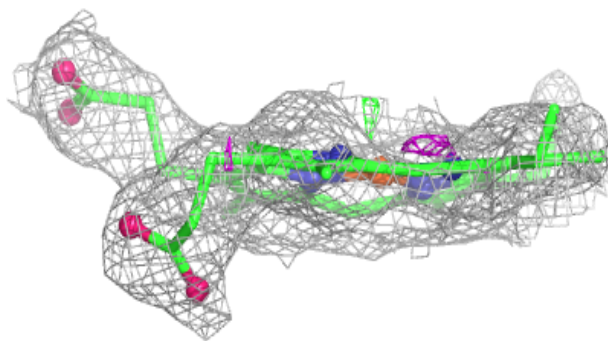
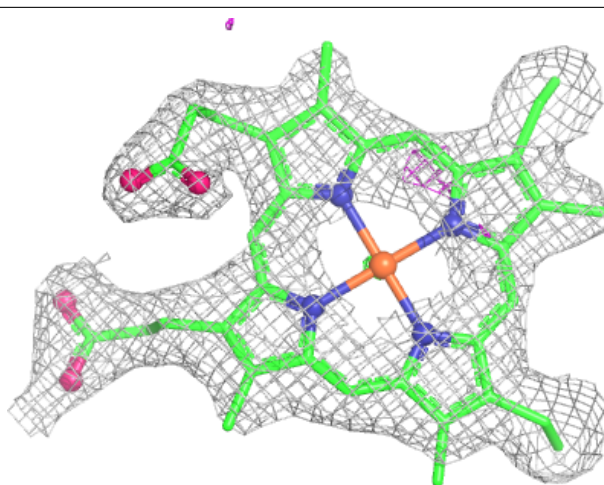
Electron density around HEC E 605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



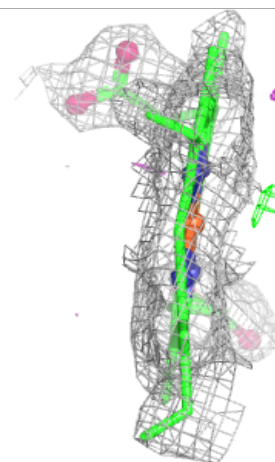
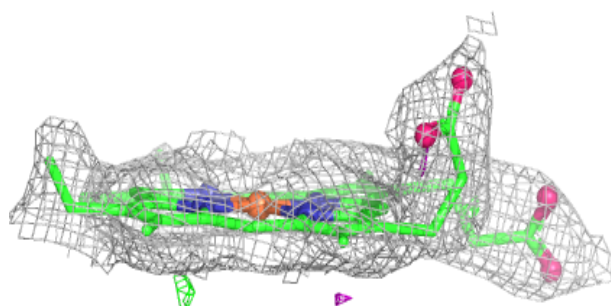
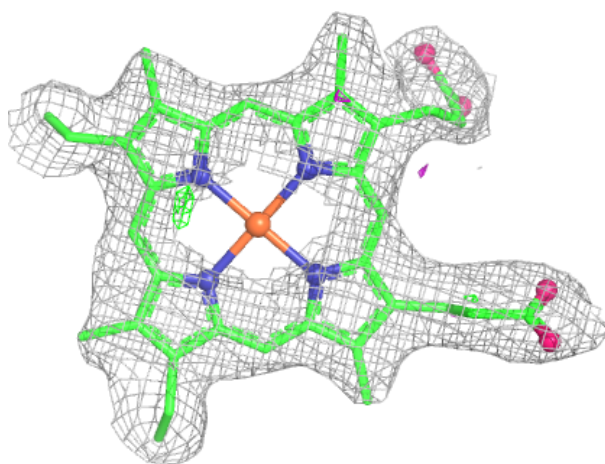
Electron density around HEC A 602:

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



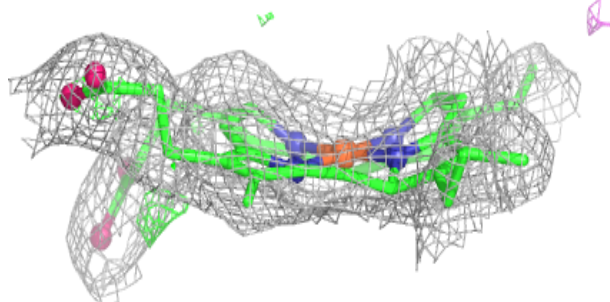
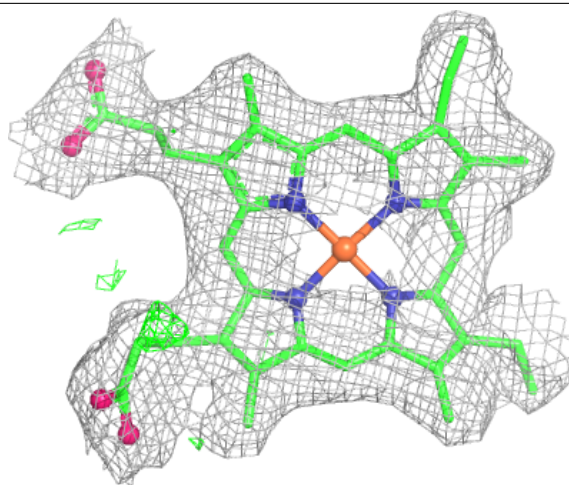
Electron density around HEC C 605:

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



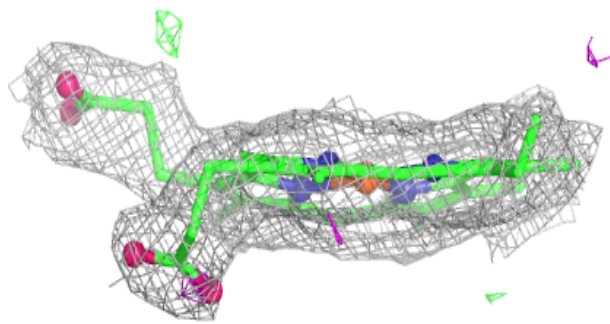
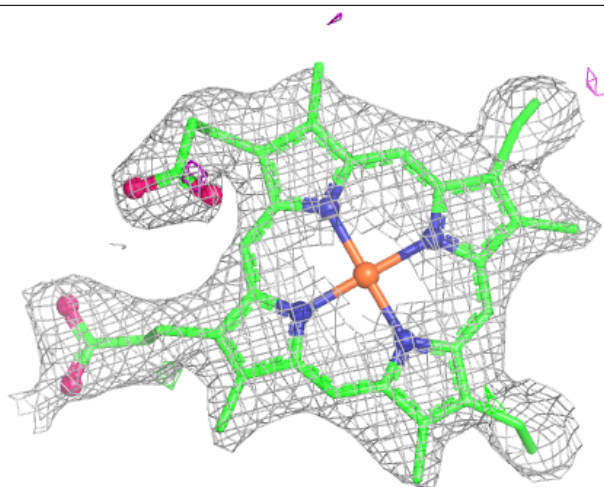
Electron density around HEC E 601:

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



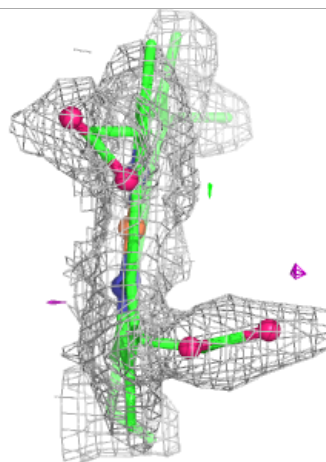
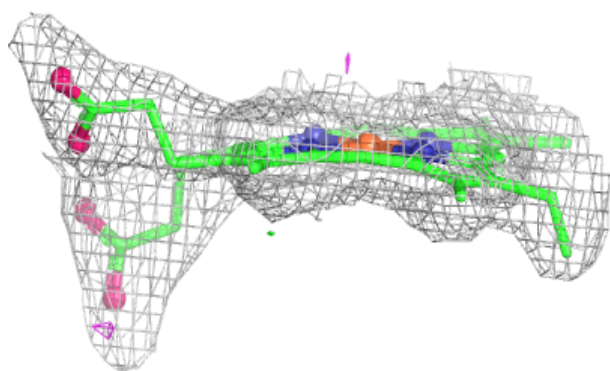
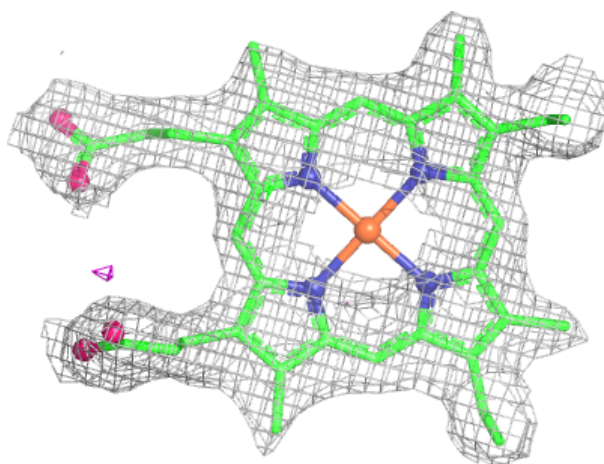
Electron density around HEC E 603:

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and green (positive)



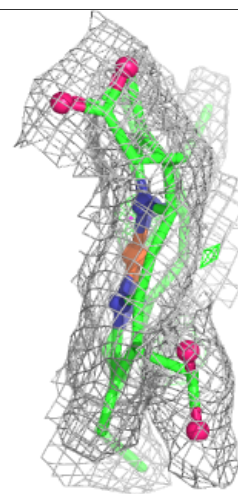
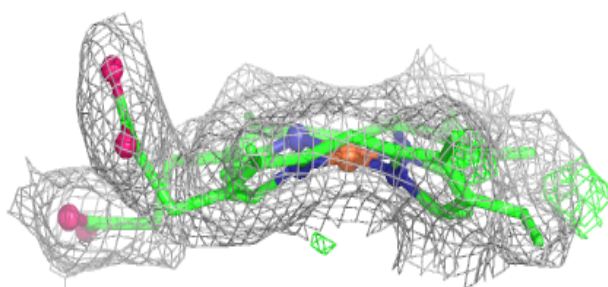
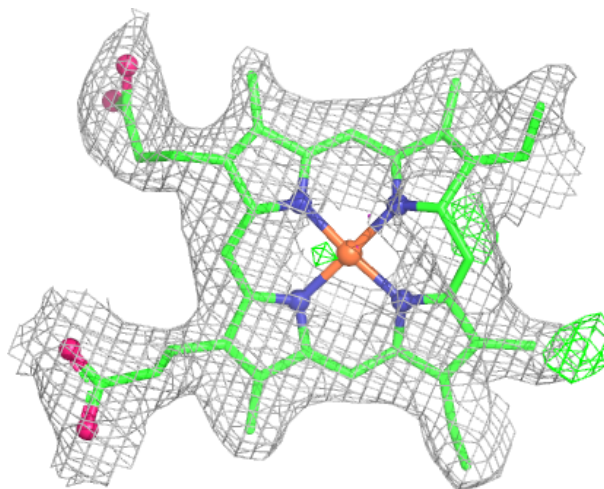
Electron density around HEC A 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



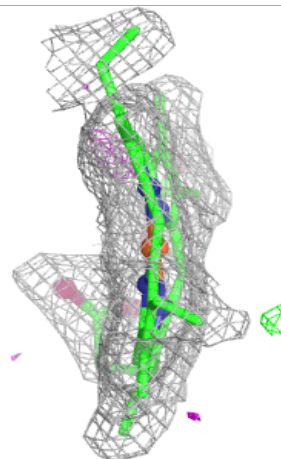
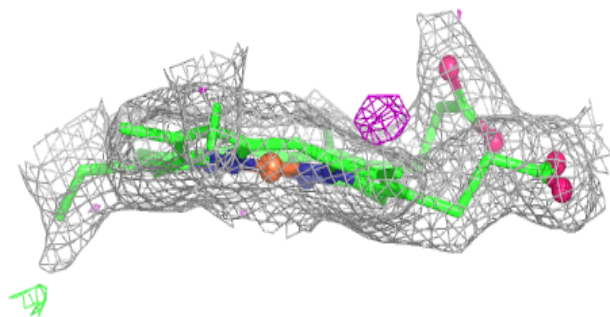
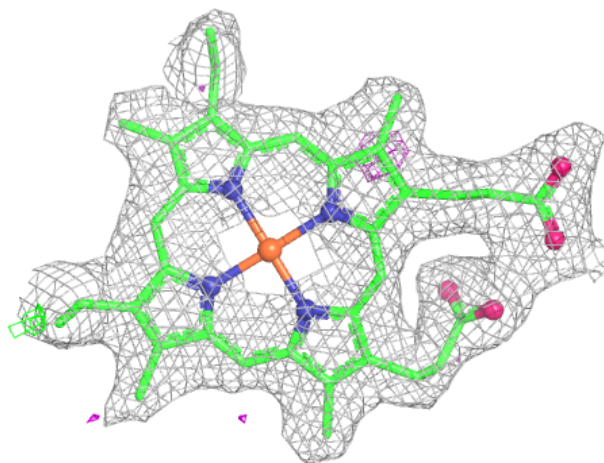
Electron density around HEC C 601:

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



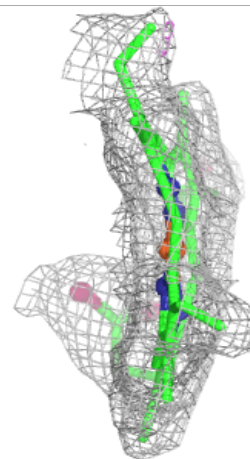
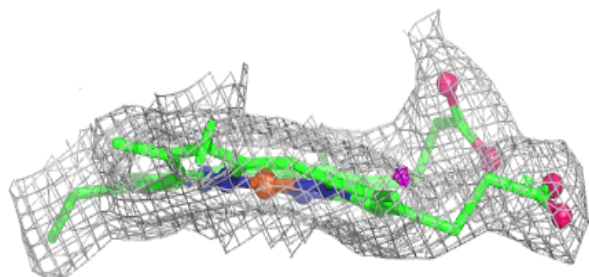
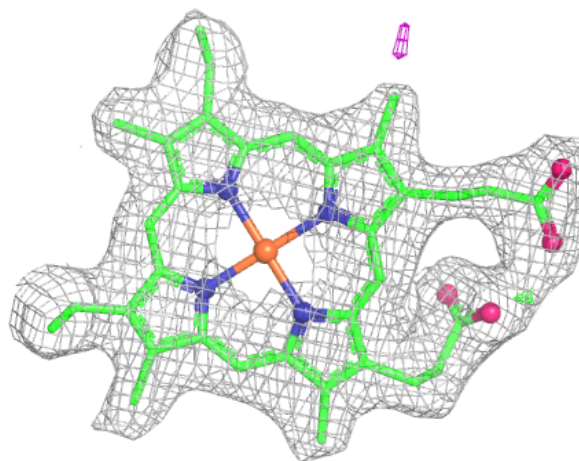
Electron density around HEC A 605:

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



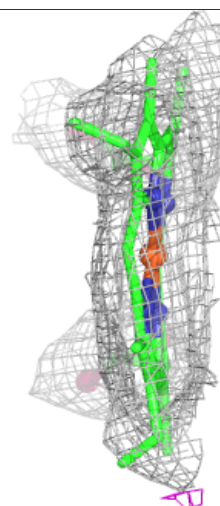
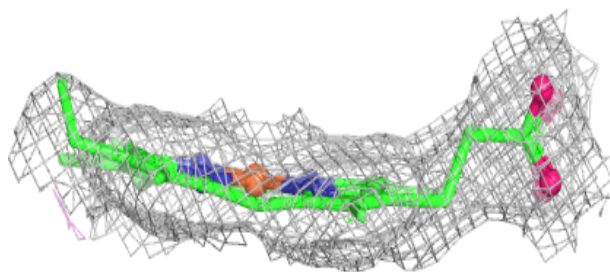
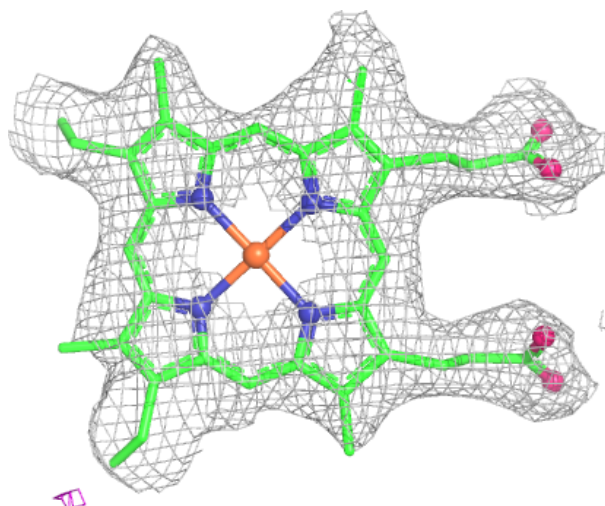
Electron density around HEC E 606:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



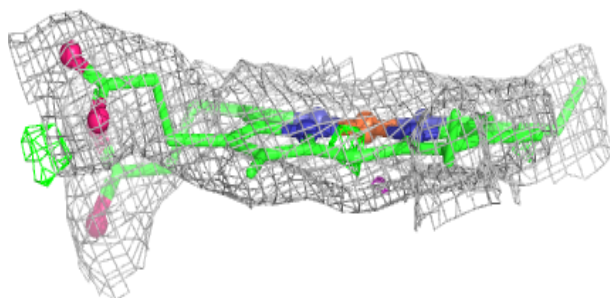
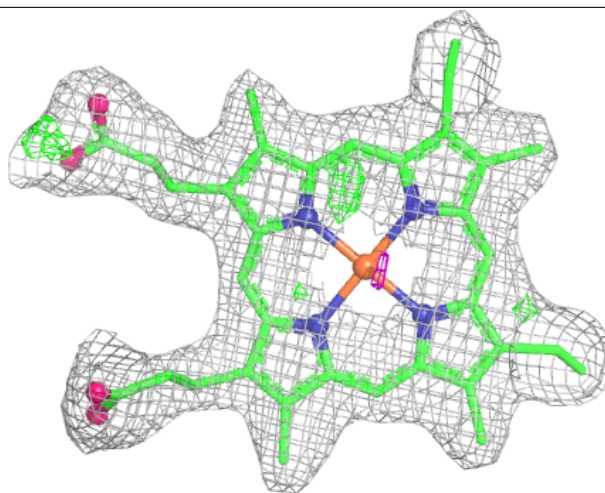
Electron density around HEC A 603:

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



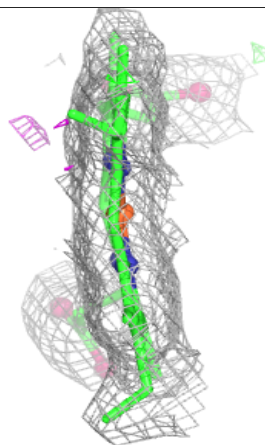
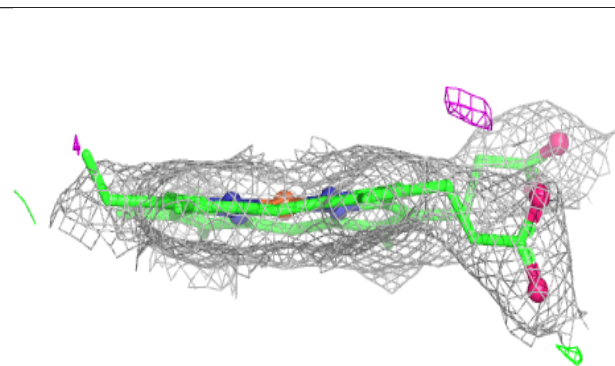
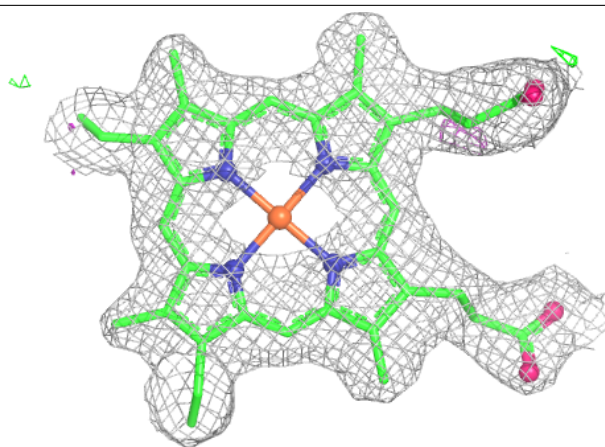
Electron density around HEC C 607:

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



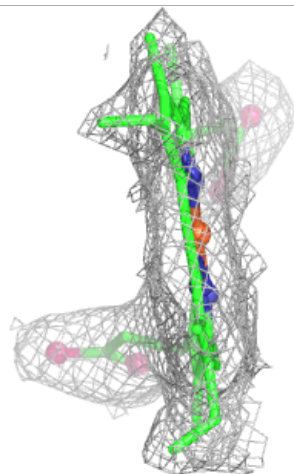
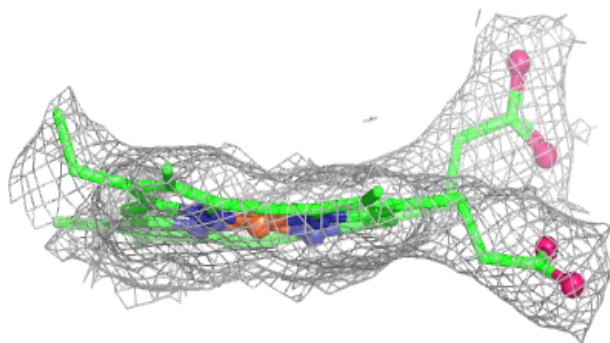
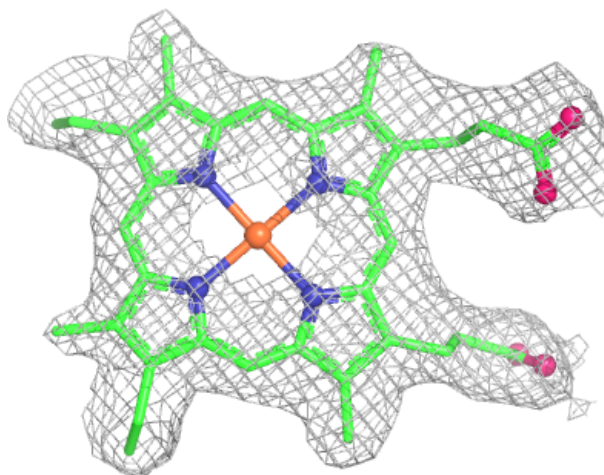
Electron density around HEC A 606:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



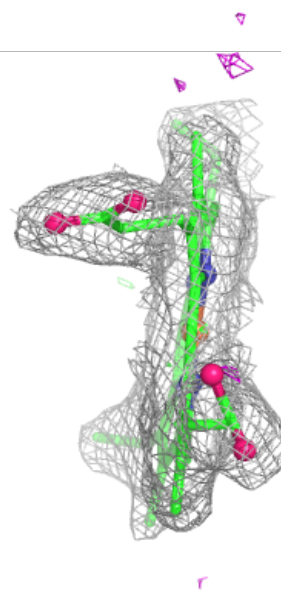
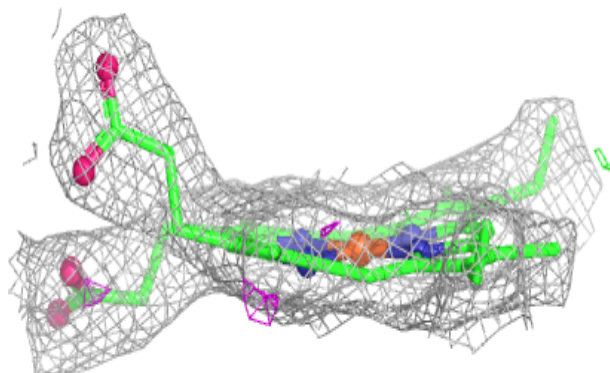
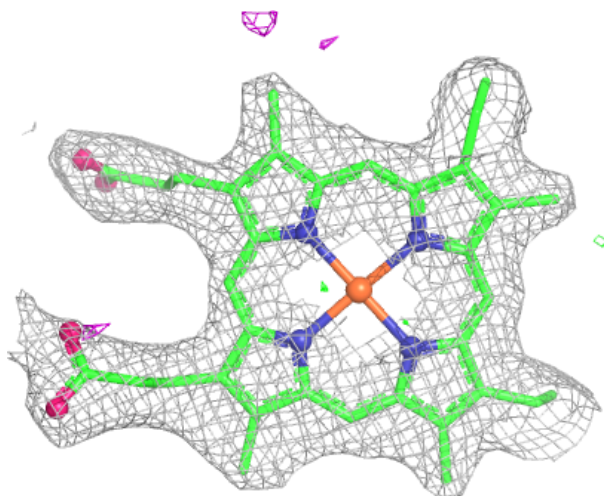
Electron density around HEC E 602:

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



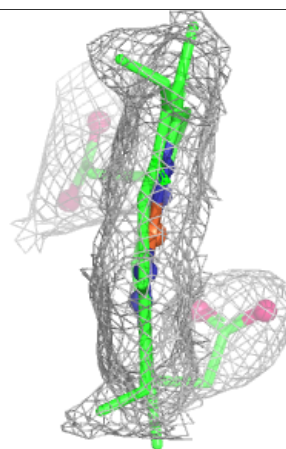
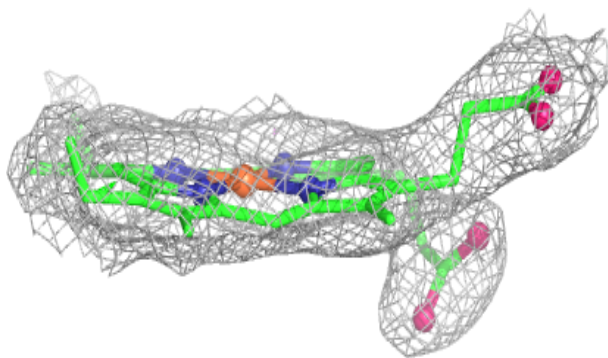
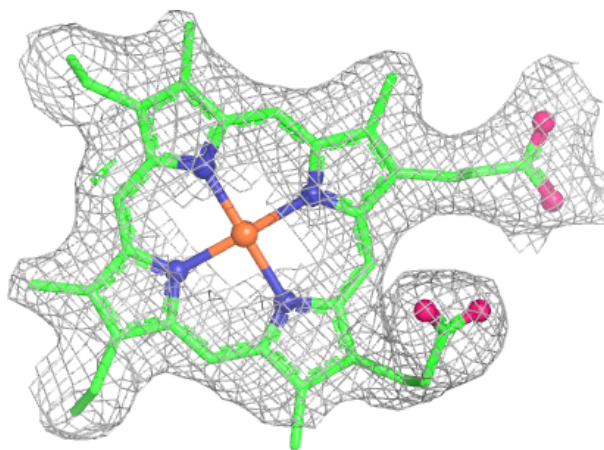
Electron density around HEC C 602:

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and green (positive)



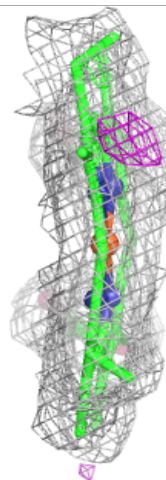
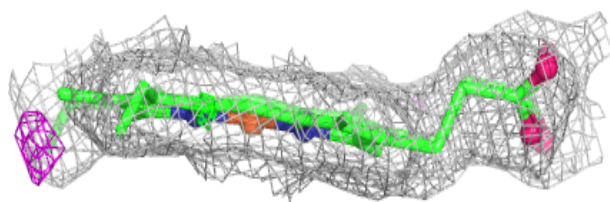
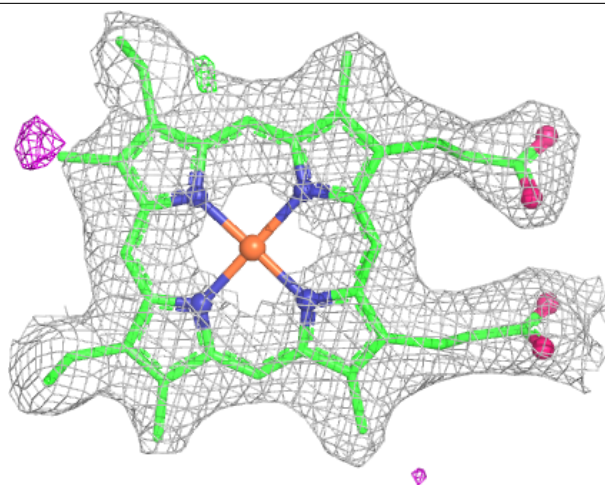
Electron density around HEC C 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



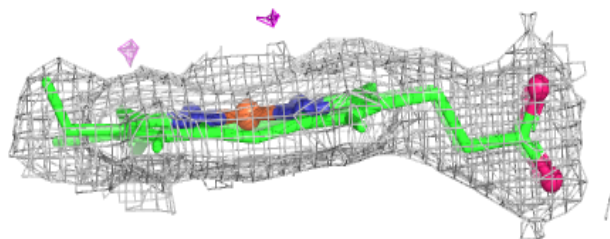
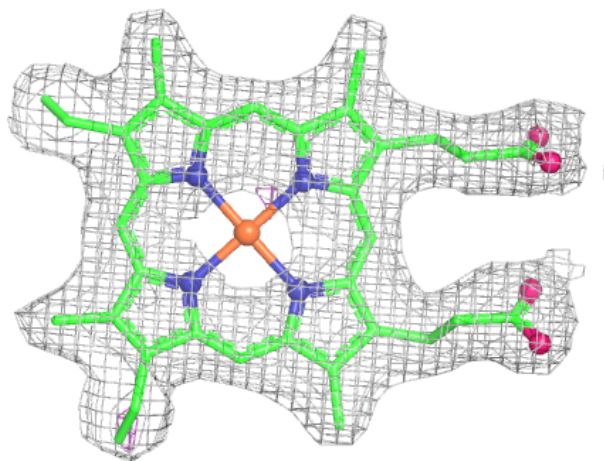
Electron density around HEC A 607:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



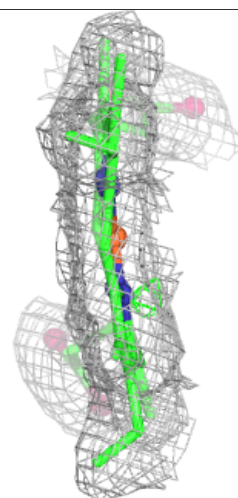
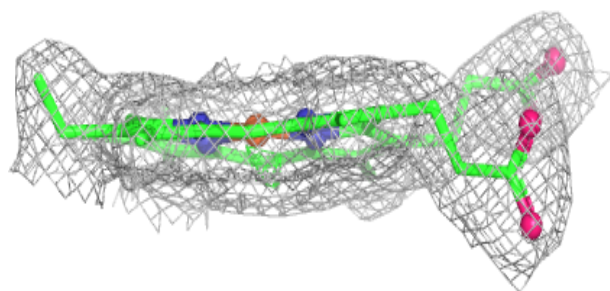
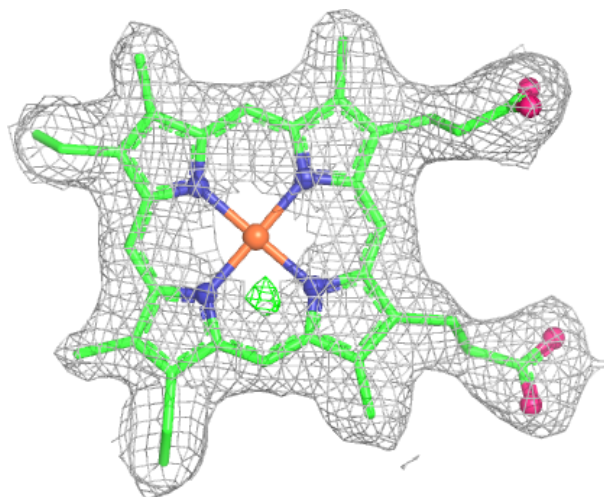
Electron density around HEC C 608:

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



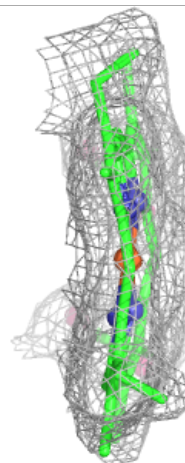
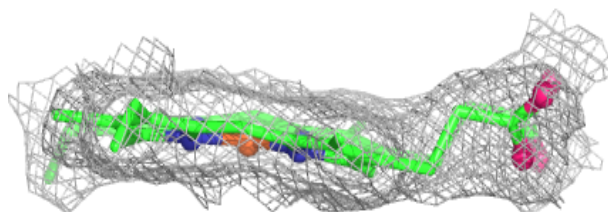
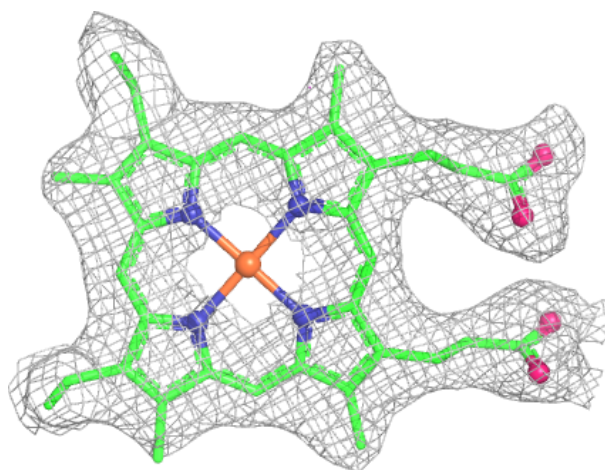
Electron density around HEC E 607:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



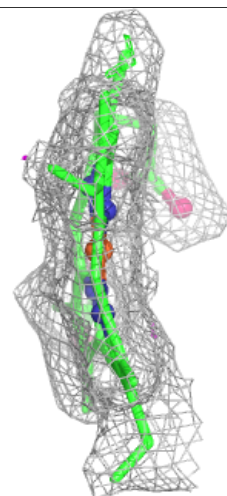
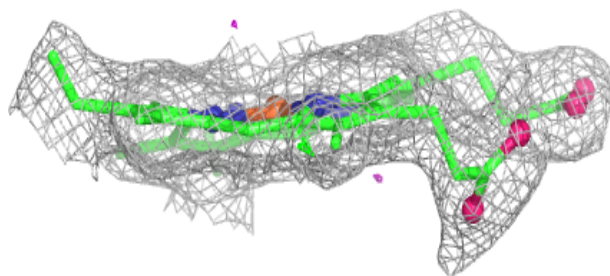
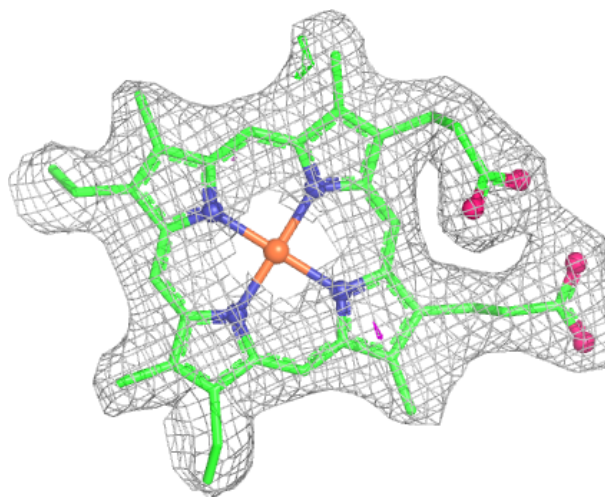
Electron density around HEC E 608:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



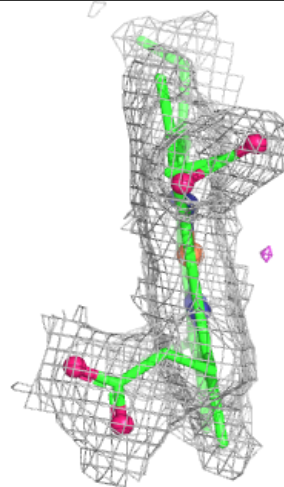
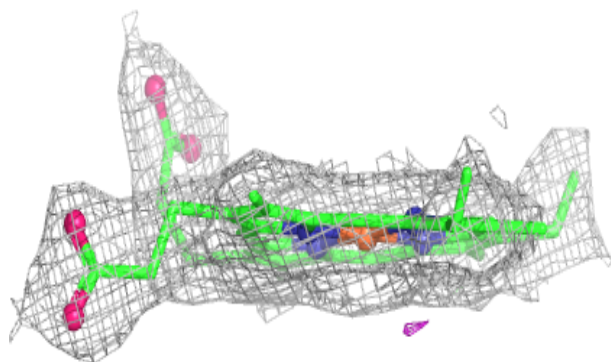
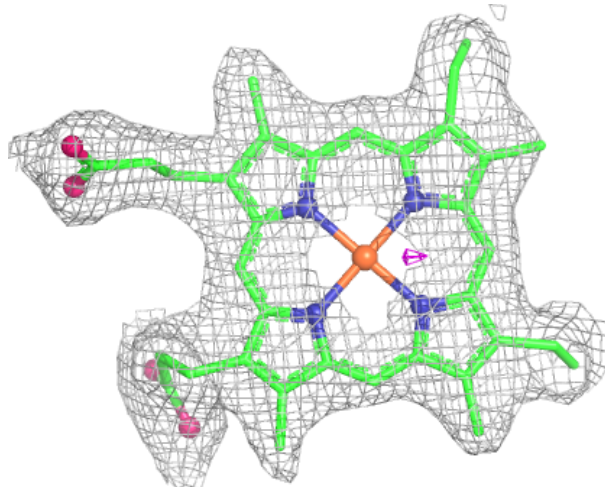
Electron density around HEC C 606:

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



Electron density around HEC A 604:

$2mF_o-DF_c$ (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.