



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:21 PM JST

PDB ID : 6M0P / pdb_00006m0p
Title : Hydroxylamine oxidoreductase in complex with juglone
Authors : Fujiwara, T.; Fujimoto, Z.; Nishigaya, Y.; Yamazaki, T.
Deposited on : 2020-02-22
Resolution : 2.78 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 : 1.8.5 (274361), CSD as541be (2020)
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

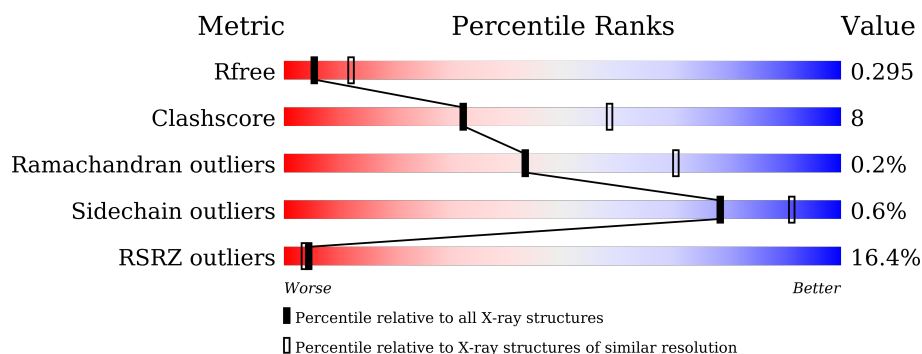
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	570	13% 70% 18% 12%
1	C	570	16% 71% 17% 12%
1	E	570	15% 72% 16% 12%
2	B	91	9% 58% 38%
2	D	91	8% 56% 5% 38%
2	F	91	12% 56% 5% 38%

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	601	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	E	601	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	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

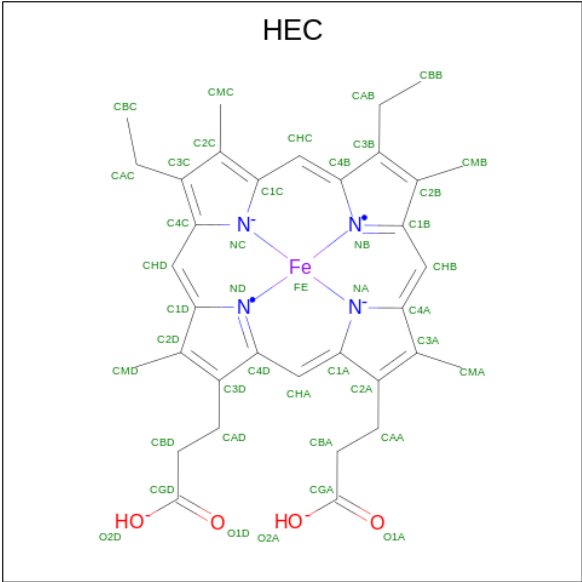
- Molecule 1 is a protein called Aerobic hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			
1	C	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			
1	E	503	Total	C	N	O	S	0	0	0
			4009	2493	711	773	32			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			423	263	75	82	3			
2	D	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			
2	F	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			

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



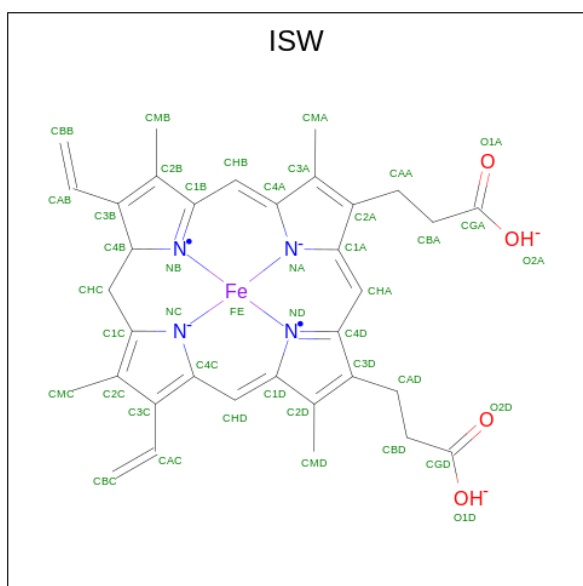
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0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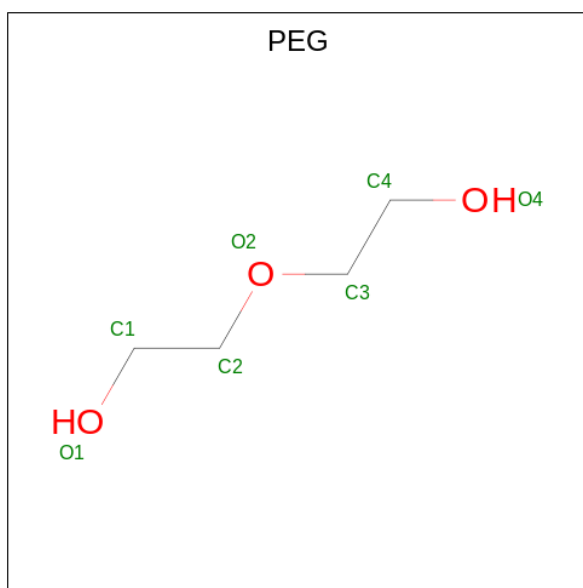
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is {3,3'-[(9S)-8,13-diethenyl-3,7,12,17-tetramethyl-9,10-dihydroporphyrin-2,18-diyl-kappa 4 N 21 ,N 22 ,N 23 ,N 24]dipropanoato(2-)}iron (CCD ID: ISW) (formula: C₃₄H₃₄FeN₄O₄).



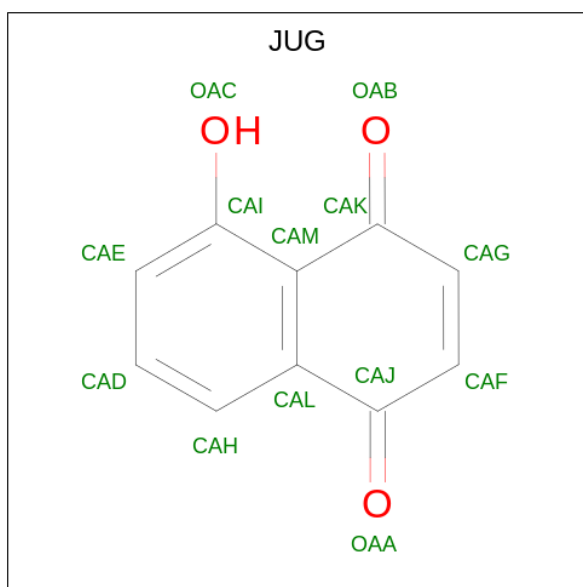
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



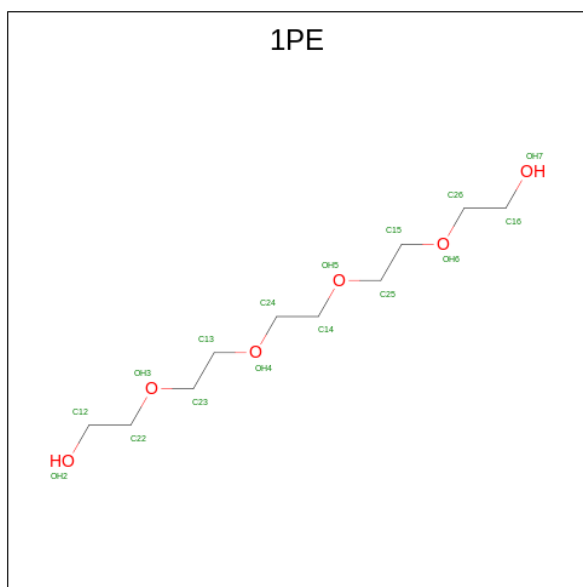
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 5-hydroxynaphthalene-1,4-dione (CCD ID: JUG) (formula: $C_{10}H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	10	3		
6	E	1	Total	C	O	0	0
			13	10	3		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			12	8	4		
7	C	1	Total	C	O	0	0
			16	10	6		

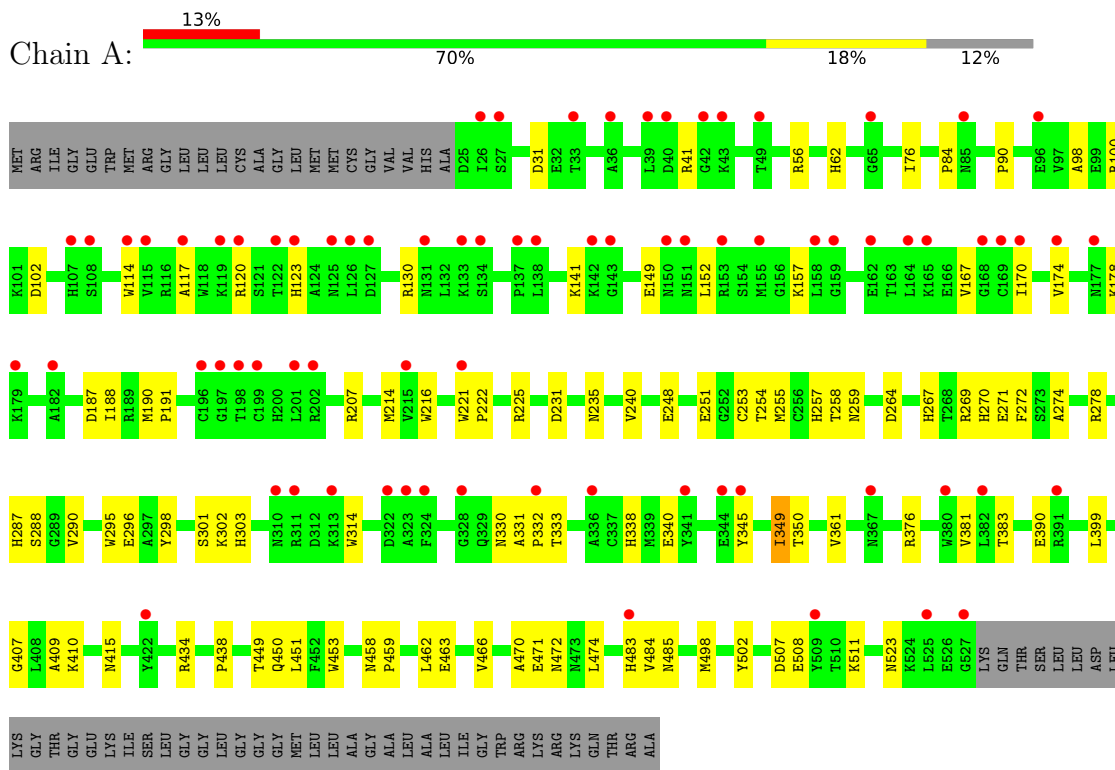
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	5	Total	O	0	0
			5	5		
8	C	31	Total	O	0	0
			31	31		
8	D	7	Total	O	0	0
			7	7		
8	E	26	Total	O	0	0
			26	26		
8	F	1	Total	O	0	0
			1	1		

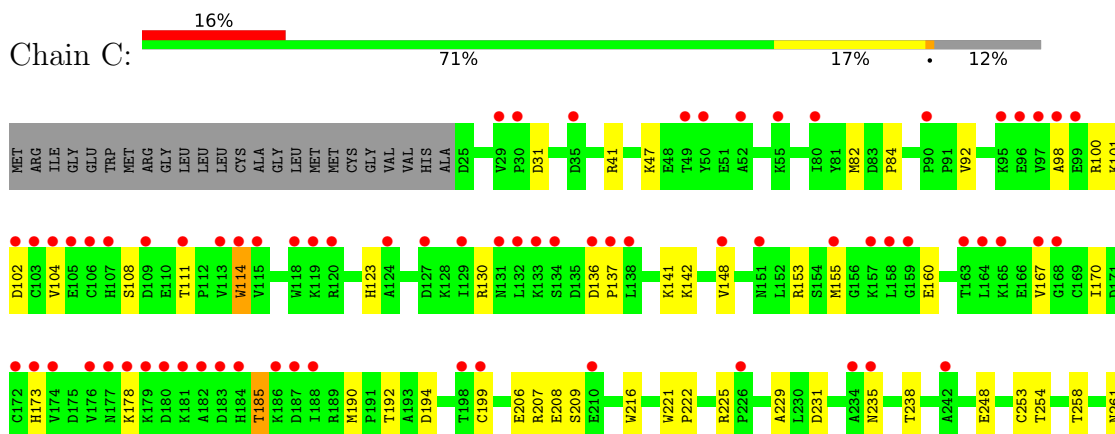
3 Residue-property plots [i](#)

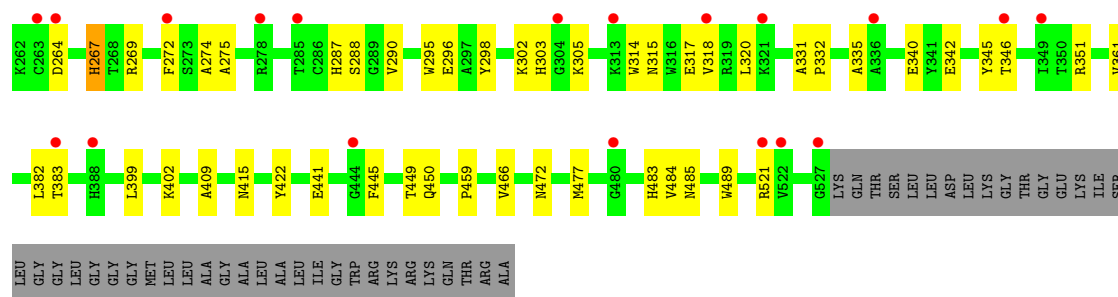
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Aerobic hydroxylamine oxidoreductase

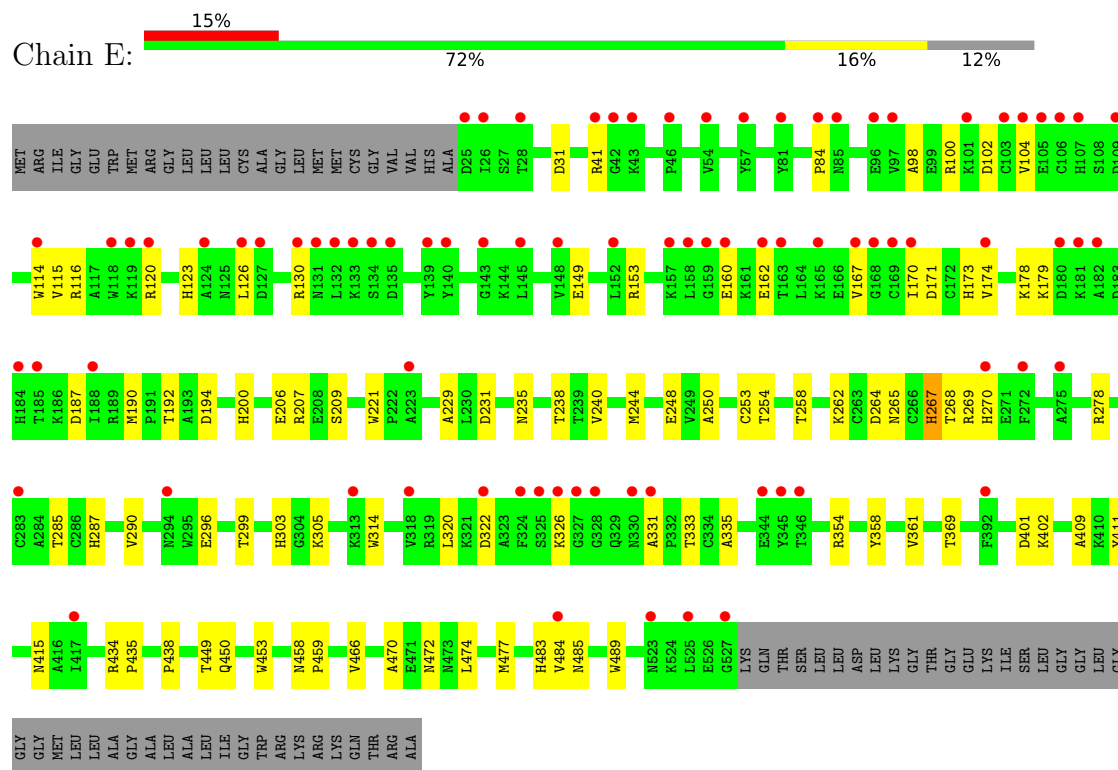


- Molecule 1: Aerobic hydroxylamine oxidoreductase

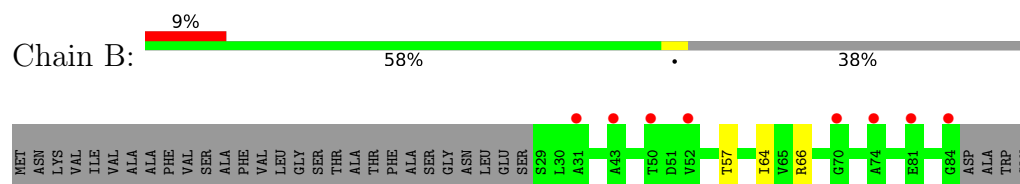




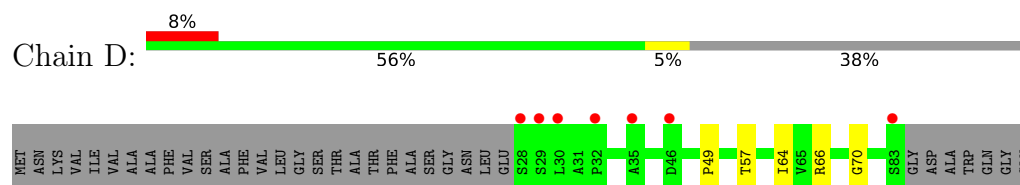
• Molecule 1: Aerobic hydroxylamine oxidoreductase



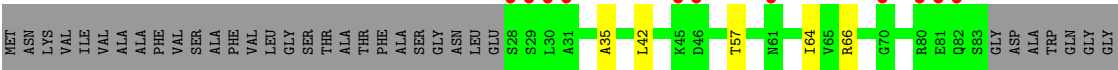
• Molecule 2: Uncharacterized protein



• Molecule 2: Uncharacterized protein



• Molecule 2: Uncharacterized protein



TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.34Å 141.07Å 106.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.77 – 2.78 46.77 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.77-2.78) 99.9 (46.77-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.256 , 0.292 0.258 , 0.295	Depositor DCC
R_{free} test set	2661 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14521	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 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ISW, 1PE, JUG, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/4112	0.26	0/5572
1	C	0.10	0/4112	0.27	0/5572
1	E	0.10	0/4112	0.27	0/5572
2	B	0.08	0/426	0.23	0/571
2	D	0.09	0/428	0.24	0/574
2	F	0.07	0/428	0.25	0/574
All	All	0.10	0/13618	0.26	0/18435

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4009	0	3808	79	0
1	C	4009	0	3808	69	0
1	E	4009	0	3808	71	0
2	B	423	0	444	2	0
2	D	425	0	446	3	0
2	F	425	0	446	4	0
3	A	301	0	210	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	301	0	209	16	0
3	E	301	0	210	14	0
4	A	86	0	56	8	0
4	C	43	0	28	4	0
5	A	14	0	20	1	0
5	E	7	0	10	0	0
6	C	13	0	6	1	0
6	E	13	0	6	2	0
7	C	28	0	37	1	0
8	A	44	0	0	2	0
8	B	5	0	0	0	0
8	C	31	0	0	1	0
8	D	7	0	0	0	0
8	E	26	0	0	1	0
8	F	1	0	0	0	0
All	All	14521	0	13552	223	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 8.

All (223) 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:123:HIS:HB3	1:C:167:VAL:HB	1.69	0.75
1:A:100:ARG:HG2	1:A:170:ILE:HG21	1.70	0.72
1:C:264:ASP:OD2	1:C:269:ARG:NH1	2.23	0.71
1:A:123:HIS:CD2	3:A:602:HEC:ND	2.60	0.69
1:A:123:HIS:HB3	1:A:167:VAL:HB	1.75	0.68
1:E:238:THR:HG23	6:E:608:JUG:HAD	1.75	0.66
1:A:120:ARG:NH2	8:A:701:HOH:O	2.28	0.66
4:A:608:ISW:HHB	1:E:235:ASN:HA	1.78	0.65
1:C:100:ARG:HG2	1:C:170:ILE:HG21	1.77	0.65
1:A:130:ARG:NH2	8:A:702:HOH:O	2.28	0.65
1:A:130:ARG:NH1	1:A:149:GLU:OE2	2.30	0.65
1:C:235:ASN:HA	4:C:611:ISW:HHB	1.79	0.63
1:A:330:ASN:HB3	1:E:120:ARG:HH12	1.64	0.62
1:C:153:ARG:HD3	1:C:160:GLU:HA	1.81	0.61
1:A:303:HIS:CD2	3:A:607:HEC:ND	2.68	0.61
1:A:235:ASN:HA	4:A:611:ISW:HHB	1.83	0.61
1:C:82:MET:O	1:C:261:ASN:ND2	2.30	0.60
1:E:130:ARG:NH2	1:E:149:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:VAL:HG13	1:E:187:ASP:HB3	1.84	0.60
1:E:173:HIS:HE1	3:E:604:HEC:ND	1.99	0.60
1:E:126:LEU:HD11	1:E:167:VAL:HG23	1.82	0.60
1:E:167:VAL:HG13	3:E:602:HEC:HBC2	1.85	0.59
1:C:207:ARG:HH21	1:C:229:ALA:HA	1.68	0.58
1:C:483:HIS:O	1:C:485:ASN:N	2.37	0.58
1:A:120:ARG:NH1	1:A:271:GLU:OE1	2.36	0.58
1:E:287:HIS:HE1	3:E:606:HEC:NA	2.02	0.58
2:F:64:ILE:HB	2:F:66:ARG:HH12	1.67	0.58
1:E:483:HIS:O	1:E:485:ASN:N	2.37	0.58
1:C:114:TRP:NE1	3:C:604:HEC:O1A	2.36	0.57
2:D:64:ILE:O	2:D:66:ARG:NH1	2.37	0.57
1:A:221:TRP:CZ3	4:A:611:ISW:HBA	2.39	0.56
1:A:483:HIS:O	1:A:485:ASN:N	2.37	0.56
1:A:152:LEU:HB3	1:A:157:LYS:HB2	1.88	0.56
1:A:31:ASP:OD1	1:A:41:ARG:NH1	2.39	0.56
1:A:207:ARG:NH1	1:A:259:ASN:O	2.29	0.56
1:C:253:CYS:SG	4:C:611:ISW:HHC	2.44	0.56
3:C:605:HEC:HMA3	3:C:606:HEC:HBA2	1.88	0.56
5:A:610:PEG:H32	4:A:611:ISW:HAA	1.88	0.55
1:C:302:LYS:NZ	8:C:703:HOH:O	2.38	0.55
1:C:238:THR:HG23	6:C:608:JUG:HAD	1.88	0.55
1:C:346:THR:OG1	1:C:351:ARG:NH2	2.40	0.55
2:B:64:ILE:O	2:B:66:ARG:NH2	2.40	0.55
1:A:84:PRO:HB3	1:A:190:MET:HB2	1.89	0.55
1:A:338:HIS:HE1	3:A:605:HEC:ND	2.05	0.54
4:A:608:ISW:HHC	1:E:253:CYS:SG	2.47	0.54
1:E:123:HIS:HD2	1:E:167:VAL:HG11	1.73	0.54
1:C:141:LYS:NZ	3:C:601:HEC:O2A	2.38	0.54
1:E:264:ASP:OD2	1:E:269:ARG:NH1	2.39	0.54
3:E:605:HEC:HMA3	3:E:606:HEC:HBA2	1.90	0.53
1:C:221:TRP:CZ2	1:C:361:VAL:HG21	2.43	0.53
1:A:450:GLN:HB3	1:A:459:PRO:HG3	1.90	0.53
1:C:207:ARG:NH2	1:C:208:GLU:OE2	2.42	0.53
1:C:98:ALA:HB2	3:C:603:HEC:HMC2	1.89	0.53
1:C:231:ASP:HB2	3:C:606:HEC:HMD2	1.91	0.53
1:E:450:GLN:HB3	1:E:459:PRO:HG3	1.90	0.53
1:C:148:VAL:HG13	1:C:199:CYS:HB3	1.91	0.53
1:C:415:ASN:HA	1:C:466:VAL:HG21	1.91	0.52
3:A:605:HEC:HMA3	3:A:606:HEC:HBA2	1.92	0.52
1:C:287:HIS:CD2	3:C:606:HEC:NC	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:VAL:HG22	3:C:602:HEC:HBC2	1.92	0.51
1:C:192:THR:OG1	1:C:194:ASP:OD1	2.28	0.51
1:A:253:CYS:SG	4:A:611:ISW:HHC	2.50	0.51
1:E:170:ILE:HD11	1:E:178:LYS:HD3	1.93	0.51
1:E:262:LYS:NZ	1:E:265:ASN:OD1	2.43	0.51
1:A:287:HIS:HE1	3:A:606:HEC:NA	2.05	0.51
1:A:330:ASN:HB3	1:E:120:ARG:NH1	2.25	0.50
1:E:162:GLU:OE2	1:E:179:LYS:NZ	2.31	0.50
1:C:31:ASP:HA	1:C:41:ARG:HH12	1.76	0.49
1:E:290:VAL:HG22	1:E:472:ASN:HB3	1.94	0.49
1:E:415:ASN:HA	1:E:466:VAL:HG21	1.94	0.49
1:C:221:TRP:CZ3	4:C:611:ISW:HBA	2.47	0.49
1:C:84:PRO:HB3	1:C:190:MET:HB2	1.93	0.49
1:C:47:LYS:HD2	1:C:155:MET:HA	1.95	0.49
1:E:231:ASP:HB2	3:E:606:HEC:HMD2	1.94	0.49
1:A:507:ASP:OD1	1:A:511:LYS:NZ	2.33	0.49
1:C:290:VAL:HG22	1:C:472:ASN:HB3	1.94	0.49
1:C:441:GLU:OE2	1:C:449:THR:OG1	2.25	0.49
1:C:173:HIS:HE1	3:C:604:HEC:ND	2.07	0.48
1:A:287:HIS:CD2	3:A:606:HEC:NC	2.78	0.48
1:A:170:ILE:HD11	1:A:178:LYS:HD3	1.94	0.48
1:A:314:TRP:HH2	1:A:331:ALA:HB3	1.79	0.48
1:A:98:ALA:HB1	1:A:102:ASP:HB2	1.94	0.48
1:C:173:HIS:HE1	3:C:604:HEC:C4D	2.27	0.48
1:C:450:GLN:HB3	1:C:459:PRO:HG3	1.94	0.48
1:E:84:PRO:HB3	1:E:190:MET:HB2	1.96	0.48
1:E:221:TRP:CZ2	1:E:361:VAL:HG21	2.49	0.48
1:A:167:VAL:HG22	3:A:602:HEC:HBC2	1.96	0.48
1:E:477:MET:HG3	1:E:489:TRP:HB2	1.96	0.48
1:A:231:ASP:HB3	3:A:606:HEC:HBD2	1.95	0.47
1:A:381:VAL:HG11	1:A:390:GLU:HG3	1.96	0.47
1:A:415:ASN:HA	1:A:466:VAL:HG21	1.95	0.47
1:E:314:TRP:HH2	1:E:331:ALA:HB3	1.79	0.47
1:E:470:ALA:HA	1:E:474:LEU:HB3	1.96	0.47
1:C:248:GLU:HG2	1:E:402:LYS:HB2	1.96	0.47
1:A:221:TRP:CZ2	1:A:361:VAL:HG21	2.49	0.47
1:E:153:ARG:HD3	1:E:160:GLU:HA	1.96	0.47
1:E:287:HIS:CD2	3:E:606:HEC:NC	2.76	0.47
1:A:332:PRO:N	3:A:607:HEC:HBC2	2.30	0.47
1:A:231:ASP:HB2	3:A:606:HEC:HMD2	1.97	0.47
1:A:269:ARG:HA	1:A:270:HIS:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:TYR:CZ	6:E:608:JUG:HAF	2.50	0.46
1:A:407:GLY:O	1:A:498:MET:HE1	2.16	0.46
1:C:477:MET:HG3	1:C:489:TRP:HB2	1.96	0.46
1:C:298:TYR:CE1	3:C:605:HEC:HMC2	2.51	0.46
1:E:100:ARG:NH2	1:E:171:ASP:OD1	2.45	0.46
1:A:191:PRO:HG2	3:A:604:HEC:CHD	2.46	0.46
1:E:153:ARG:HB3	1:E:160:GLU:OE2	2.16	0.46
1:C:303:HIS:CD2	3:C:607:HEC:ND	2.84	0.46
7:C:609:1PE:H252	7:C:609:1PE:H242	1.76	0.46
1:E:435:PRO:O	1:E:458:ASN:ND2	2.44	0.46
1:A:298:TYR:O	1:A:301:SER:OG	2.28	0.45
1:A:409:ALA:HB3	2:B:57:THR:HG21	1.98	0.45
1:A:222:PRO:HB2	1:A:225:ARG:HD3	1.98	0.45
1:A:434:ARG:HH22	1:A:463:GLU:CD	2.23	0.45
1:E:98:ALA:HB2	3:E:603:HEC:HMC2	1.98	0.45
1:C:254:THR:O	1:C:258:THR:HG23	2.17	0.45
1:C:315:ASN:O	1:C:318:VAL:HG22	2.16	0.45
1:E:303:HIS:CD2	3:E:607:HEC:ND	2.81	0.45
1:E:320:LEU:HD11	1:E:335:ALA:HB1	1.99	0.45
1:C:287:HIS:HE1	3:C:606:HEC:NA	2.11	0.45
1:E:322:ASP:HB3	1:E:326:LYS:HB2	1.99	0.45
1:A:90:PRO:HG3	1:A:188:ILE:O	2.17	0.45
1:C:272:PHE:CE2	3:C:604:HEC:HBC2	2.51	0.45
1:E:369:THR:HG21	2:F:42:LEU:HD11	1.99	0.45
1:E:409:ALA:HB3	2:F:57:THR:HG21	1.99	0.45
1:E:267:HIS:HE1	3:E:601:HEC:NB	2.07	0.44
1:C:320:LEU:HD11	1:C:335:ALA:HB1	1.98	0.44
1:A:272:PHE:CE2	3:A:604:HEC:HBC2	2.52	0.44
4:A:608:ISW:HBA	1:E:221:TRP:CZ3	2.52	0.44
1:C:288:SER:HB3	1:C:295:TRP:HB3	1.99	0.44
1:E:207:ARG:HH11	1:E:229:ALA:HA	1.81	0.44
1:A:270:HIS:HD2	3:A:604:HEC:NC	2.15	0.44
1:C:98:ALA:HB1	1:C:102:ASP:HB2	2.00	0.44
1:E:98:ALA:HB1	1:E:102:ASP:HB2	1.99	0.44
1:A:76:ILE:HD11	1:A:251:GLU:HG2	1.99	0.44
1:A:340:GLU:OE1	1:A:383:THR:OG1	2.29	0.44
1:C:111:THR:HB	1:C:114:TRP:HB2	2.00	0.44
1:A:56:ARG:HG3	1:A:62:HIS:CG	2.53	0.44
1:C:104:VAL:O	1:C:108:SER:OG	2.22	0.44
1:C:136:ASP:OD1	1:C:137:PRO:HD2	2.18	0.44
1:C:314:TRP:HH2	1:C:331:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:HIS:CE1	3:E:602:HEC:ND	2.86	0.44
1:E:269:ARG:HA	1:E:270:HIS:HA	1.67	0.44
2:D:49:PRO:O	2:D:70:GLY:N	2.51	0.43
1:A:350:THR:O	1:A:376:ARG:NH1	2.40	0.43
1:A:399:LEU:HG	1:E:248:GLU:HG3	1.99	0.43
1:A:470:ALA:HA	1:A:474:LEU:HB3	2.00	0.43
1:E:244:MET:SD	1:E:250:ALA:HB2	2.58	0.43
1:A:240:VAL:HB	1:A:449:THR:HA	2.01	0.43
1:A:298:TYR:CE1	3:A:605:HEC:HMC2	2.53	0.43
1:C:409:ALA:HB3	2:D:57:THR:HG21	2.01	0.43
1:A:451:LEU:HD11	1:A:471:GLU:HG2	2.01	0.43
1:E:434:ARG:HG3	1:E:458:ASN:HB2	2.00	0.43
1:A:141:LYS:NZ	3:A:601:HEC:O2A	2.50	0.43
1:A:167:VAL:HG13	3:A:602:HEC:HBC2	2.01	0.43
1:A:248:GLU:HG3	1:C:399:LEU:HG	2.01	0.43
1:E:206:GLU:O	1:E:209:SER:OG	2.24	0.43
1:E:296:GLU:OE1	1:E:296:GLU:N	2.44	0.43
1:C:275:ALA:HB2	1:C:317:GLU:HA	2.01	0.43
1:E:240:VAL:HB	1:E:449:THR:HA	2.00	0.43
1:A:349:ILE:HD13	3:A:606:HEC:C3A	2.49	0.42
1:C:101:LYS:HD3	1:C:101:LYS:HA	1.86	0.42
1:A:255:MET:HE2	1:A:255:MET:HB3	1.89	0.42
1:C:267:HIS:HE1	3:C:601:HEC:NB	2.15	0.42
1:E:192:THR:OG1	1:E:194:ASP:OD1	2.36	0.42
1:A:174:VAL:HG13	1:A:187:ASP:HB3	2.00	0.42
1:A:248:GLU:HG2	1:C:402:LYS:HB2	2.00	0.42
1:A:296:GLU:OE1	1:A:296:GLU:N	2.43	0.42
1:E:173:HIS:HE1	3:E:604:HEC:C4D	2.32	0.42
4:A:608:ISW:HHA	4:A:608:ISW:HAAA	2.00	0.42
1:A:274:ALA:O	1:A:278:ARG:HG3	2.20	0.42
1:A:290:VAL:HG22	1:A:472:ASN:HB3	2.00	0.42
1:C:206:GLU:O	1:C:209:SER:OG	2.24	0.42
1:C:340:GLU:HB2	1:C:345:TYR:CE2	2.54	0.42
4:C:611:ISW:HHA	4:C:611:ISW:HAAA	1.99	0.42
1:E:104:VAL:HG13	1:E:115:VAL:HG13	2.01	0.42
1:A:462:LEU:HG	1:A:508:GLU:CD	2.45	0.42
1:C:222:PRO:HB2	1:C:225:ARG:HD3	2.02	0.42
1:C:296:GLU:OE1	1:C:296:GLU:N	2.43	0.42
1:E:116:ARG:O	1:E:120:ARG:HG3	2.19	0.42
1:E:305:LYS:HD3	1:E:305:LYS:HA	1.89	0.42
1:A:214:MET:HE2	1:A:216:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:O	3:A:605:HEC:HMC3	2.20	0.42
1:C:216:TRP:NE1	1:C:221:TRP:HB2	2.35	0.41
1:C:92:VAL:HA	1:C:185:THR:HG23	2.03	0.41
1:A:257:HIS:CE1	3:A:606:HEC:HMD1	2.56	0.41
1:A:450:GLN:NE2	1:A:463:GLU:OE2	2.46	0.41
3:A:607:HEC:HBA2	1:E:269:ARG:HH22	1.85	0.41
1:C:207:ARG:NH2	1:C:229:ALA:HA	2.33	0.41
1:C:274:ALA:H	3:C:602:HEC:HBA1	1.86	0.41
1:E:254:THR:O	1:E:258:THR:HG23	2.20	0.41
1:A:117:ALA:HB1	1:A:271:GLU:HG3	2.02	0.41
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.94	0.41
1:A:434:ARG:HG3	1:A:458:ASN:HB2	2.01	0.41
1:A:523:ASN:OD1	1:C:521:ARG:NH1	2.51	0.41
1:E:354:ARG:NH2	1:E:401:ASP:OD1	2.53	0.41
1:E:31:ASP:OD1	1:E:41:ARG:NH2	2.54	0.41
1:E:278:ARG:NE	3:E:601:HEC:O2D	2.34	0.41
1:A:216:TRP:CD1	1:A:221:TRP:HB2	2.55	0.41
1:C:130:ARG:HA	1:C:142:LYS:HE2	2.02	0.41
1:C:332:PRO:N	3:C:607:HEC:HBC2	2.36	0.41
1:E:411:TYR:CE1	1:E:470:ALA:HB2	2.56	0.41
1:E:438:PRO:HD3	1:E:453:TRP:CE2	2.56	0.41
1:A:254:THR:O	1:A:258:THR:HG23	2.21	0.41
1:C:340:GLU:OE1	1:C:383:THR:OG1	2.31	0.41
1:E:333:THR:O	3:E:605:HEC:HMC3	2.21	0.41
1:A:288:SER:HB3	1:A:295:TRP:HB3	2.03	0.41
1:A:410:LYS:HE3	1:A:502:TYR:CG	2.55	0.41
1:E:31:ASP:HA	1:E:41:ARG:HH22	1.86	0.41
1:E:409:ALA:HB2	2:F:35:ALA:HB3	2.02	0.41
1:E:411:TYR:CE1	1:E:415:ASN:HB2	2.56	0.41
1:C:170:ILE:HD11	1:C:178:LYS:HD3	2.03	0.41
1:E:299:THR:O	1:E:305:LYS:HG2	2.20	0.41
1:A:31:ASP:HA	1:A:41:ARG:HH22	1.87	0.40
3:A:607:HEC:HBD1	1:E:268:THR:HB	2.03	0.40
1:C:305:LYS:HA	1:C:305:LYS:HD3	1.90	0.40
1:E:265:ASN:HB3	3:E:606:HEC:HBC3	2.03	0.40
1:A:264:ASP:OD2	1:A:269:ARG:NH1	2.49	0.40
1:C:422:TYR:CE1	1:C:445:PHE:HB2	2.56	0.40
1:A:340:GLU:HB2	1:A:345:TYR:CE2	2.56	0.40
1:E:285:THR:HB	8:E:720:HOH:O	2.21	0.40
1:A:438:PRO:HD3	1:A:453:TRP:CE2	2.56	0.40
1:C:342:GLU:HA	1:C:382:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	43	70
1	C	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	43	70
1	E	501/570 (88%)	479 (96%)	21 (4%)	1 (0%)	43	70
2	B	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
2	D	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
2	F	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
All	All	1665/1983 (84%)	1596 (96%)	66 (4%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	C	484	VAL
1	E	484	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/477 (90%)	426 (99%)	3 (1%)	76	90
1	C	429/477 (90%)	426 (99%)	3 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	429/477 (90%)	427 (100%)	2 (0%)	81	92
2	B	48/73 (66%)	48 (100%)	0	100	100
2	D	49/73 (67%)	49 (100%)	0	100	100
2	F	49/73 (67%)	49 (100%)	0	100	100
All	All	1433/1650 (87%)	1425 (99%)	8 (1%)	78	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TRP
1	A	267	HIS
1	A	349	ILE
1	C	114	TRP
1	C	185	THR
1	C	267	HIS
1	E	114	TRP
1	E	267	HIS

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

Mol	Chain	Res	Type
1	A	419	HIS
1	E	235	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

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	HEC	E	605	1	50,50,50	1.87	5 (10%)	68,82,82	1.38	6 (8%)
3	HEC	E	603	1	50,50,50	1.84	6 (12%)	68,82,82	1.40	7 (10%)
5	PEG	E	609	-	6,6,6	0.49	0	5,5,5	0.28	0
3	HEC	A	607	1	50,50,50	1.82	6 (12%)	68,82,82	1.41	6 (8%)
3	HEC	C	605	1	50,50,50	1.84	5 (10%)	68,82,82	1.34	5 (7%)
3	HEC	C	607	1	50,50,50	1.86	5 (10%)	68,82,82	1.54	8 (11%)
3	HEC	A	605	1	50,50,50	1.81	5 (10%)	68,82,82	1.32	6 (8%)
3	HEC	E	606	1	50,50,50	1.75	5 (10%)	68,82,82	1.37	6 (8%)
3	HEC	A	603	1	50,50,50	1.81	5 (10%)	68,82,82	1.37	6 (8%)
3	HEC	A	604	1	50,50,50	1.78	6 (12%)	68,82,82	1.36	7 (10%)
3	HEC	A	602	1	50,50,50	1.83	5 (10%)	68,82,82	1.47	7 (10%)
4	ISW	C	611	8,1	47,50,50	6.10	20 (42%)	56,82,82	4.43	27 (48%)
3	HEC	E	601	1	50,50,50	1.77	5 (10%)	68,82,82	1.37	6 (8%)
5	PEG	A	610	-	6,6,6	0.49	0	5,5,5	0.24	0
5	PEG	A	609	-	6,6,6	0.49	0	5,5,5	0.28	0
3	HEC	C	602	1	50,50,50	1.84	7 (14%)	68,82,82	1.35	5 (7%)
4	ISW	A	611	8,1	47,50,50	6.13	23 (48%)	56,82,82	4.37	27 (48%)
3	HEC	A	601	1	50,50,50	1.78	5 (10%)	68,82,82	1.40	7 (10%)
3	HEC	E	604	1	50,50,50	1.82	5 (10%)	68,82,82	1.41	6 (8%)
4	ISW	A	608	8,1	47,50,50	6.11	20 (42%)	56,82,82	4.38	27 (48%)
6	JUG	E	608	-	14,14,14	2.78	8 (57%)	20,20,20	1.05	0
3	HEC	C	603	1	50,50,50	1.77	6 (12%)	68,82,82	1.47	8 (11%)
3	HEC	C	604	1	50,50,50	1.84	5 (10%)	68,82,82	1.35	8 (11%)
3	HEC	A	606	1	50,50,50	1.75	5 (10%)	68,82,82	1.39	7 (10%)
6	JUG	C	608	-	14,14,14	2.79	7 (50%)	20,20,20	1.02	1 (5%)
7	1PE	C	609	-	11,11,15	0.55	0	10,10,14	0.25	0
3	HEC	E	602	1	50,50,50	1.80	6 (12%)	68,82,82	1.38	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1PE	C	610	-	15,15,15	0.53	0	14,14,14	0.23	0
3	HEC	E	607	1	50,50,50	1.79	6 (12%)	68,82,82	1.39	6 (8%)
3	HEC	C	601	1	50,50,50	1.75	5 (10%)	68,82,82	1.39	7 (10%)
3	HEC	C	606	1	50,50,50	1.76	6 (12%)	68,82,82	1.37	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	E	605	1	1/1/3/7	7/14/54/54	-
3	HEC	E	603	1	1/1/3/7	2/14/54/54	-
5	PEG	E	609	-	-	2/4/4/4	-
3	HEC	A	607	1	1/1/3/7	11/14/54/54	-
3	HEC	C	605	1	1/1/3/7	10/14/54/54	-
3	HEC	C	607	1	1/1/3/7	6/14/54/54	-
3	HEC	A	605	1	1/1/3/7	9/14/54/54	-
3	HEC	E	606	1	1/1/3/7	4/14/54/54	-
3	HEC	A	603	1	1/1/3/7	3/14/54/54	-
3	HEC	A	604	1	1/1/3/7	7/14/54/54	-
3	HEC	A	602	1	1/1/3/7	3/14/54/54	-
4	ISW	C	611	8,1	-	6/14/74/74	-
3	HEC	E	601	1	1/1/3/7	3/14/54/54	-
5	PEG	A	610	-	-	2/4/4/4	-
5	PEG	A	609	-	-	0/4/4/4	-
3	HEC	C	602	1	1/1/3/7	4/14/54/54	-
4	ISW	A	611	8,1	-	10/14/74/74	-
3	HEC	A	601	1	1/1/3/7	1/14/54/54	-
3	HEC	E	604	1	1/1/3/7	5/14/54/54	-
4	ISW	A	608	8,1	-	7/14/74/74	-
6	JUG	E	608	-	-	-	0/2/2/2
3	HEC	C	603	1	1/1/3/7	1/14/54/54	-
3	HEC	C	604	1	1/1/3/7	8/14/54/54	-
3	HEC	A	606	1	1/1/3/7	1/14/54/54	-
6	JUG	C	608	-	-	-	0/2/2/2
7	1PE	C	609	-	-	4/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	E	602	1	1/1/3/7	3/14/54/54	-
7	1PE	C	610	-	-	4/13/13/13	-
3	HEC	E	607	1	1/1/3/7	5/14/54/54	-
3	HEC	C	601	1	1/1/3/7	0/14/54/54	-
3	HEC	C	606	1	1/1/3/7	4/14/54/54	-

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	611	ISW	CHA-C1A	16.58	1.70	1.38
4	A	611	ISW	CHA-C1A	16.58	1.70	1.38
4	A	608	ISW	CHA-C1A	16.56	1.70	1.38
4	A	608	ISW	CHD-C4C	14.95	1.73	1.39
4	A	611	ISW	CHB-C4A	14.88	1.67	1.38
4	A	611	ISW	CHD-C4C	14.85	1.72	1.39
4	C	611	ISW	CHD-C4C	14.84	1.72	1.39
4	A	608	ISW	CHB-C4A	14.74	1.67	1.38
4	C	611	ISW	CHB-C4A	14.73	1.67	1.38
4	C	611	ISW	CHD-C1D	14.10	1.67	1.38
4	A	611	ISW	CHD-C1D	14.08	1.67	1.38
4	A	608	ISW	CHD-C1D	14.01	1.67	1.38
4	A	611	ISW	CHA-C4D	13.10	1.69	1.39
4	C	611	ISW	CHA-C4D	13.01	1.69	1.39
4	A	608	ISW	CHA-C4D	13.00	1.69	1.39
4	A	611	ISW	CHB-C1B	12.53	1.67	1.39
4	C	611	ISW	CHB-C1B	12.49	1.67	1.39
4	A	608	ISW	CHB-C1B	12.47	1.67	1.39
4	A	611	ISW	CHC-C1C	12.28	1.65	1.49
4	A	608	ISW	CHC-C1C	12.14	1.65	1.49
4	C	611	ISW	CHC-C1C	11.96	1.64	1.49
4	C	611	ISW	C1D-ND	9.11	1.56	1.40
4	A	608	ISW	C1D-ND	9.10	1.56	1.40
4	A	611	ISW	C1D-ND	9.01	1.55	1.40
4	C	611	ISW	CHC-C4B	-8.50	1.30	1.54
3	E	603	HEC	C3D-C2D	8.44	1.54	1.36
4	A	608	ISW	CHC-C4B	-8.42	1.30	1.54
4	A	611	ISW	CHC-C4B	-8.36	1.30	1.54
3	E	605	HEC	C3D-C2D	8.32	1.54	1.36
3	C	605	HEC	C3D-C2D	8.27	1.54	1.36
3	C	604	HEC	C3D-C2D	8.25	1.54	1.36
3	A	605	HEC	C3D-C2D	8.22	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEC	C3D-C2D	8.19	1.54	1.36
3	A	607	HEC	C3D-C2D	8.17	1.54	1.36
3	A	603	HEC	C3D-C2D	8.15	1.54	1.36
3	C	603	HEC	C3D-C2D	8.13	1.54	1.36
3	E	607	HEC	C3D-C2D	8.12	1.54	1.36
3	C	602	HEC	C3D-C2D	8.10	1.54	1.36
3	C	607	HEC	C3D-C2D	8.08	1.53	1.36
3	E	602	HEC	C3D-C2D	8.06	1.53	1.36
3	A	601	HEC	C3D-C2D	8.03	1.53	1.36
3	E	601	HEC	C3D-C2D	8.00	1.53	1.36
3	A	604	HEC	C3D-C2D	8.00	1.53	1.36
3	E	604	HEC	C3D-C2D	7.99	1.53	1.36
3	C	601	HEC	C3D-C2D	7.99	1.53	1.36
3	E	606	HEC	C3D-C2D	7.93	1.53	1.36
3	C	606	HEC	C3D-C2D	7.88	1.53	1.36
3	A	606	HEC	C3D-C2D	7.85	1.53	1.36
6	C	608	JUG	CAG-CAF	5.96	1.48	1.35
6	E	608	JUG	CAG-CAF	5.95	1.48	1.35
4	A	608	ISW	C1D-C2D	5.63	1.55	1.44
4	A	611	ISW	C1D-C2D	5.56	1.55	1.44
4	C	611	ISW	C1D-C2D	5.55	1.55	1.44
3	A	603	HEC	FE-ND	5.49	2.11	1.94
6	C	608	JUG	CAL-CAJ	5.40	1.57	1.48
6	E	608	JUG	CAL-CAJ	5.38	1.57	1.48
3	C	607	HEC	FE-NB	5.27	2.11	1.94
3	E	604	HEC	FE-ND	5.12	2.10	1.94
3	C	602	HEC	FE-ND	4.94	2.10	1.94
4	A	608	ISW	C4D-C3D	4.72	1.53	1.45
4	A	611	ISW	C4D-C3D	4.69	1.53	1.45
3	A	607	HEC	FE-ND	4.67	2.09	1.94
4	C	611	ISW	C4D-C3D	4.65	1.53	1.45
3	E	605	HEC	FE-NB	4.63	2.09	1.94
4	A	611	ISW	C4C-NC	-4.61	1.30	1.39
3	C	607	HEC	FE-ND	4.54	2.08	1.94
3	A	605	HEC	FE-ND	4.52	2.08	1.94
4	A	608	ISW	C4C-NC	-4.49	1.31	1.39
4	C	611	ISW	C4C-NC	-4.48	1.31	1.39
3	E	603	HEC	FE-ND	4.48	2.08	1.94
3	C	601	HEC	FE-ND	4.48	2.08	1.94
3	A	601	HEC	FE-ND	4.47	2.08	1.94
3	A	604	HEC	FE-ND	4.46	2.08	1.94
3	A	602	HEC	FE-ND	4.41	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	HEC	FE-NB	4.40	2.08	1.94
4	A	611	ISW	C3D-C2D	4.38	1.46	1.36
3	C	604	HEC	FE-ND	4.36	2.08	1.94
3	A	602	HEC	FE-NB	4.32	2.08	1.94
3	E	601	HEC	FE-ND	4.32	2.08	1.94
3	C	603	HEC	FE-ND	4.32	2.08	1.94
3	C	605	HEC	FE-NB	4.29	2.08	1.94
4	A	608	ISW	C1B-C2B	4.26	1.52	1.44
4	C	611	ISW	C1B-C2B	4.25	1.52	1.44
3	E	605	HEC	FE-ND	4.24	2.08	1.94
4	A	608	ISW	C4D-ND	4.21	1.47	1.38
4	A	611	ISW	C1B-C2B	4.20	1.52	1.44
3	E	606	HEC	FE-NB	4.20	2.07	1.94
6	C	608	JUG	CAM-CAK	4.18	1.57	1.46
4	C	611	ISW	C3D-C2D	4.18	1.45	1.36
3	C	605	HEC	FE-NA	4.17	2.09	1.95
3	E	607	HEC	FE-ND	4.14	2.07	1.94
3	E	607	HEC	FE-NB	4.13	2.07	1.94
4	A	608	ISW	C3D-C2D	4.13	1.45	1.36
3	E	601	HEC	FE-NB	4.13	2.07	1.94
4	C	611	ISW	C4D-ND	4.11	1.47	1.38
3	A	601	HEC	FE-NB	4.11	2.07	1.94
3	C	606	HEC	FE-NB	4.10	2.07	1.94
3	C	604	HEC	FE-NB	4.07	2.07	1.94
6	E	608	JUG	CAM-CAK	4.06	1.57	1.46
3	E	602	HEC	FE-NB	4.06	2.07	1.94
3	C	603	HEC	FE-NB	4.05	2.07	1.94
4	A	611	ISW	C4D-ND	4.04	1.47	1.38
3	C	605	HEC	FE-ND	3.99	2.07	1.94
3	A	607	HEC	FE-NA	3.95	2.08	1.95
3	E	602	HEC	FE-ND	3.94	2.07	1.94
3	A	606	HEC	FE-NB	3.94	2.07	1.94
3	E	605	HEC	FE-NA	3.87	2.08	1.95
3	C	602	HEC	FE-NA	3.77	2.07	1.95
3	E	604	HEC	FE-NC	3.77	2.07	1.95
3	C	606	HEC	FE-ND	3.70	2.06	1.94
3	E	602	HEC	FE-NA	3.69	2.07	1.95
3	A	605	HEC	FE-NB	3.67	2.06	1.94
4	C	611	ISW	C3C-C4C	3.63	1.51	1.42
3	C	601	HEC	FE-NB	3.61	2.06	1.94
3	A	606	HEC	FE-NA	3.60	2.07	1.95
3	A	604	HEC	FE-NB	3.60	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	ISW	C3C-C4C	3.58	1.51	1.42
3	C	602	HEC	FE-NB	3.57	2.05	1.94
3	A	602	HEC	FE-NA	3.55	2.07	1.95
3	A	606	HEC	FE-ND	3.53	2.05	1.94
3	A	607	HEC	FE-NB	3.53	2.05	1.94
4	A	611	ISW	C3C-C4C	3.49	1.50	1.42
3	C	606	HEC	FE-NA	3.47	2.06	1.95
3	E	606	HEC	FE-ND	3.47	2.05	1.94
3	C	604	HEC	FE-NA	3.36	2.06	1.95
3	E	604	HEC	FE-NB	3.35	2.05	1.94
3	A	605	HEC	FE-NA	3.31	2.06	1.95
3	C	604	HEC	FE-NC	3.30	2.06	1.95
3	E	606	HEC	FE-NC	3.29	2.06	1.95
3	E	607	HEC	FE-NC	3.29	2.06	1.95
3	A	604	HEC	FE-NC	3.20	2.06	1.95
3	C	607	HEC	FE-NA	3.17	2.05	1.95
3	A	603	HEC	FE-NB	3.17	2.04	1.94
3	E	603	HEC	FE-NC	3.15	2.05	1.95
4	A	608	ISW	C4B-NB	3.15	1.53	1.48
4	A	611	ISW	C4B-NB	3.13	1.53	1.48
4	C	611	ISW	C4B-NB	3.09	1.53	1.48
3	C	602	HEC	FE-NC	3.08	2.05	1.95
3	A	601	HEC	FE-NA	3.05	2.05	1.95
3	C	603	HEC	FE-NA	2.98	2.05	1.95
3	E	605	HEC	FE-NC	2.96	2.05	1.95
3	A	606	HEC	FE-NC	2.96	2.05	1.95
3	E	606	HEC	FE-NA	2.95	2.05	1.95
3	E	602	HEC	FE-NC	2.94	2.05	1.95
3	C	601	HEC	FE-NA	2.93	2.05	1.95
3	A	605	HEC	FE-NC	2.92	2.05	1.95
3	A	604	HEC	FE-NA	2.92	2.05	1.95
3	E	601	HEC	FE-NA	2.83	2.04	1.95
3	A	603	HEC	FE-NA	2.81	2.04	1.95
3	C	606	HEC	FE-NC	2.79	2.04	1.95
3	A	603	HEC	FE-NC	2.75	2.04	1.95
3	E	601	HEC	FE-NC	2.74	2.04	1.95
3	E	604	HEC	FE-NA	2.73	2.04	1.95
3	C	607	HEC	FE-NC	2.73	2.04	1.95
3	A	607	HEC	FE-NC	2.69	2.04	1.95
3	A	601	HEC	FE-NC	2.68	2.04	1.95
3	A	602	HEC	FE-NC	2.67	2.04	1.95
4	C	611	ISW	CAC-C3C	2.61	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	611	ISW	C1A-NA	-2.61	1.34	1.39
3	C	601	HEC	FE-NC	2.57	2.03	1.95
4	A	611	ISW	CAC-C3C	2.56	1.54	1.47
4	C	611	ISW	C1A-NA	-2.55	1.34	1.39
4	A	608	ISW	CAC-C3C	2.52	1.54	1.47
3	E	607	HEC	FE-NA	2.50	2.03	1.95
3	C	603	HEC	FE-NC	2.49	2.03	1.95
6	E	608	JUG	OAB-CAK	-2.48	1.18	1.24
6	C	608	JUG	OAA-CAJ	-2.45	1.19	1.24
6	E	608	JUG	OAA-CAJ	-2.44	1.19	1.24
6	C	608	JUG	OAB-CAK	-2.44	1.19	1.24
4	A	608	ISW	C1A-NA	-2.42	1.35	1.39
3	E	603	HEC	FE-NA	2.34	2.03	1.95
3	C	605	HEC	FE-NC	2.32	2.03	1.95
6	C	608	JUG	CAF-CAJ	2.16	1.51	1.46
6	E	608	JUG	CAF-CAJ	2.12	1.50	1.46
6	C	608	JUG	CAG-CAK	2.11	1.50	1.46
6	E	608	JUG	CAG-CAK	2.10	1.50	1.46
4	A	611	ISW	CMD-C2D	2.10	1.55	1.50
4	A	611	ISW	CMC-C2C	2.06	1.55	1.50
4	C	611	ISW	CMC-C2C	2.05	1.55	1.50
3	E	603	HEC	CMC-C2C	2.04	1.55	1.50
3	A	604	HEC	CMA-C3A	2.03	1.55	1.50
4	A	608	ISW	CMC-C2C	2.03	1.55	1.50
3	C	602	HEC	CMA-C3A	2.03	1.55	1.50
3	E	607	HEC	CMC-C2C	2.02	1.55	1.50
3	E	602	HEC	CMC-C2C	2.02	1.55	1.50
3	A	607	HEC	CMC-C2C	2.02	1.55	1.50
3	C	603	HEC	CMB-C2B	2.02	1.55	1.50
4	A	611	ISW	FE-ND	-2.02	1.88	1.94
3	C	602	HEC	CMC-C2C	2.01	1.55	1.50
3	C	606	HEC	CMB-C2B	2.01	1.55	1.50
4	A	611	ISW	FE-NA	-2.01	1.88	1.95
6	E	608	JUG	OAC-CAI	2.00	1.40	1.36

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	ISW	C1A-CHA-C4D	-13.32	97.33	126.06
4	A	608	ISW	C1A-CHA-C4D	-13.30	97.37	126.06
4	A	611	ISW	C1A-CHA-C4D	-13.27	97.42	126.06
4	A	611	ISW	C4C-CHD-C1D	-10.67	101.03	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	ISW	C4C-CHD-C1D	-10.58	101.25	126.34
4	A	608	ISW	C4C-CHD-C1D	-10.51	101.41	126.34
4	A	611	ISW	C4A-CHB-C1B	-9.62	105.31	126.06
4	C	611	ISW	C4A-CHB-C1B	-9.33	105.94	126.06
4	A	608	ISW	C4A-CHB-C1B	-9.26	106.09	126.06
4	C	611	ISW	C3C-C4C-NC	8.89	115.72	110.25
4	A	611	ISW	C3C-C4C-NC	8.50	115.48	110.25
4	A	608	ISW	C3C-C4C-NC	8.24	115.32	110.25
4	C	611	ISW	C4C-NC-C1C	-7.77	101.97	106.96
4	A	611	ISW	CMA-C3A-C4A	-7.59	111.34	124.71
4	A	608	ISW	CMA-C3A-C4A	-7.41	111.65	124.71
4	C	611	ISW	CMA-C3A-C4A	-7.36	111.73	124.71
4	A	608	ISW	CHA-C1A-C2A	-7.22	113.23	124.94
4	C	611	ISW	CHA-C1A-C2A	-7.20	113.27	124.94
4	A	608	ISW	C4C-NC-C1C	-7.17	102.36	106.96
4	C	611	ISW	CHA-C4D-C3D	-7.11	114.39	124.84
4	A	608	ISW	CHA-C4D-C3D	-7.06	114.46	124.84
4	A	611	ISW	C4C-NC-C1C	-7.01	102.46	106.96
4	A	611	ISW	CHA-C1A-C2A	-6.84	113.85	124.94
3	A	602	HEC	C1D-ND-C4D	6.81	112.11	105.07
4	A	611	ISW	CHA-C4D-C3D	-6.79	114.86	124.84
3	C	603	HEC	C1D-ND-C4D	6.72	112.01	105.07
4	C	611	ISW	CHA-C1A-NA	6.65	131.64	124.44
3	E	605	HEC	C1D-ND-C4D	6.62	111.91	105.07
3	E	602	HEC	C1D-ND-C4D	6.53	111.82	105.07
4	A	608	ISW	CHA-C1A-NA	6.49	131.46	124.44
3	E	607	HEC	C1D-ND-C4D	6.47	111.76	105.07
3	A	604	HEC	C1D-ND-C4D	6.46	111.75	105.07
3	C	604	HEC	C1D-ND-C4D	6.45	111.74	105.07
3	E	603	HEC	C1D-ND-C4D	6.45	111.74	105.07
3	C	605	HEC	C1D-ND-C4D	6.45	111.73	105.07
3	C	602	HEC	C1D-ND-C4D	6.40	111.69	105.07
3	E	604	HEC	C1D-ND-C4D	6.38	111.66	105.07
3	A	601	HEC	C1D-ND-C4D	6.36	111.64	105.07
3	C	607	HEC	C1D-ND-C4D	6.36	111.64	105.07
3	E	601	HEC	C1D-ND-C4D	6.33	111.61	105.07
3	C	606	HEC	C1D-ND-C4D	6.33	111.61	105.07
4	C	611	ISW	C4B-CHC-C1C	6.32	120.40	109.08
3	A	607	HEC	C1D-ND-C4D	6.30	111.58	105.07
3	A	606	HEC	C1D-ND-C4D	6.27	111.55	105.07
4	A	611	ISW	C4B-CHC-C1C	6.25	120.28	109.08
3	A	605	HEC	C1D-ND-C4D	6.22	111.50	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	606	HEC	C1D-ND-C4D	6.21	111.49	105.07
4	A	611	ISW	CHA-C1A-NA	6.21	131.16	124.44
4	A	608	ISW	C4B-CHC-C1C	6.21	120.21	109.08
3	C	601	HEC	C1D-ND-C4D	6.19	111.47	105.07
3	A	603	HEC	C1D-ND-C4D	6.09	111.37	105.07
4	A	611	ISW	CMA-C3A-C2A	6.05	142.53	126.12
4	A	611	ISW	CBA-CAA-C2A	5.98	129.24	112.63
4	C	611	ISW	CMA-C3A-C2A	5.97	142.33	126.12
4	A	608	ISW	CMA-C3A-C2A	5.86	142.03	126.12
4	A	608	ISW	C3D-C4D-ND	5.75	115.93	110.36
4	C	611	ISW	C3D-C4D-ND	5.67	115.85	110.36
4	C	611	ISW	CBA-CAA-C2A	5.58	128.14	112.63
4	A	608	ISW	CBA-CAA-C2A	5.57	128.10	112.63
4	A	611	ISW	C3D-C4D-ND	5.43	115.62	110.36
4	A	608	ISW	C2A-C1A-NA	5.09	115.28	110.32
4	A	608	ISW	C4A-NA-C1A	-4.96	100.49	105.35
4	C	611	ISW	C4A-NA-C1A	-4.93	100.52	105.35
4	C	611	ISW	CHA-C4D-ND	4.89	129.73	124.42
4	C	611	ISW	C2A-C1A-NA	4.88	115.07	110.32
4	A	608	ISW	CHA-C4D-ND	4.76	129.59	124.42
4	A	611	ISW	C2A-C1A-NA	4.75	114.95	110.32
4	A	611	ISW	CHB-C4A-NA	-4.68	119.38	124.44
4	A	611	ISW	CHA-C4D-ND	4.67	129.50	124.42
4	A	608	ISW	CHD-C4C-NC	4.61	132.33	123.85
4	A	611	ISW	CHD-C4C-NC	4.61	132.32	123.85
4	A	608	ISW	CHB-C4A-NA	-4.59	119.47	124.44
4	A	608	ISW	C1D-ND-C4D	-4.56	100.36	105.07
4	A	611	ISW	C4A-NA-C1A	-4.55	100.89	105.35
4	C	611	ISW	CHD-C4C-NC	4.54	132.21	123.85
4	C	611	ISW	C1D-ND-C4D	-4.42	100.51	105.07
4	C	611	ISW	CHB-C4A-NA	-4.39	119.69	124.44
4	A	611	ISW	C1D-ND-C4D	-4.14	100.79	105.07
4	A	608	ISW	CHB-C1B-C2B	-4.06	118.64	124.98
4	C	611	ISW	CHB-C1B-C2B	-4.02	118.70	124.98
4	A	611	ISW	CHB-C1B-C2B	-3.67	119.25	124.98
3	C	607	HEC	CAB-C3B-C4B	3.58	129.46	124.81
4	C	611	ISW	CHD-C4C-C3C	-3.52	112.06	127.71
4	A	611	ISW	CHD-C4C-C3C	-3.49	112.19	127.71
4	A	608	ISW	CHD-C4C-C3C	-3.46	112.33	127.71
4	A	611	ISW	CAD-CBD-CGD	-3.33	106.43	113.60
4	A	608	ISW	C2B-C1B-NB	3.20	113.72	109.88
4	C	611	ISW	C2B-C1B-NB	3.14	113.64	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	611	ISW	CAA-C2A-C3A	3.12	133.70	127.88
4	A	611	ISW	CAA-C2A-C3A	3.12	133.69	127.88
3	A	602	HEC	CAD-C3D-C4D	3.06	130.00	124.66
3	E	603	HEC	C4A-NA-C1A	3.01	108.30	105.35
4	C	611	ISW	CAD-CBD-CGD	-3.01	107.13	113.60
4	A	611	ISW	C2B-C1B-NB	3.00	113.48	109.88
4	A	608	ISW	CAA-C2A-C3A	2.97	133.42	127.88
3	A	603	HEC	C4B-NB-C1B	2.97	108.14	105.07
3	C	602	HEC	C4B-NB-C1B	2.92	108.08	105.07
3	C	603	HEC	C4A-NA-C1A	2.91	108.20	105.35
4	C	611	ISW	CHB-C1B-NB	2.90	127.58	124.43
3	E	604	HEC	C4A-NA-C1A	2.89	108.18	105.35
3	A	601	HEC	C4B-NB-C1B	2.88	108.04	105.07
4	A	608	ISW	CHB-C1B-NB	2.87	127.55	124.43
3	C	603	HEC	C4C-NC-C1C	2.86	108.15	105.35
3	C	603	HEC	C4B-NB-C1B	2.85	108.02	105.07
3	C	607	HEC	C4B-NB-C1B	2.79	107.95	105.07
3	C	607	HEC	C4A-NA-C1A	2.78	108.07	105.35
3	C	601	HEC	C4B-NB-C1B	2.76	107.93	105.07
3	A	607	HEC	C4B-NB-C1B	2.76	107.92	105.07
3	E	601	HEC	C4B-NB-C1B	2.76	107.92	105.07
3	A	602	HEC	C4A-NA-C1A	2.74	108.03	105.35
3	A	603	HEC	C4C-NC-C1C	2.72	108.01	105.35
3	A	607	HEC	C4A-NA-C1A	2.71	108.00	105.35
3	E	603	HEC	C2A-C1A-NA	-2.71	107.69	110.32
3	E	604	HEC	C4B-NB-C1B	2.69	107.86	105.07
3	A	607	HEC	C4C-NC-C1C	2.69	107.98	105.35
3	A	603	HEC	C4A-NA-C1A	2.68	107.97	105.35
3	E	607	HEC	C4A-NA-C1A	2.68	107.97	105.35
4	A	608	ISW	CAD-CBD-CGD	-2.67	107.85	113.60
3	A	601	HEC	C4A-NA-C1A	2.67	107.97	105.35
3	E	606	HEC	C4A-NA-C1A	2.67	107.96	105.35
3	E	604	HEC	C2A-C1A-NA	-2.66	107.74	110.32
3	C	603	HEC	C2A-C1A-NA	-2.65	107.74	110.32
3	C	607	HEC	C4C-NC-C1C	2.65	107.94	105.35
3	C	601	HEC	C4A-NA-C1A	2.65	107.94	105.35
3	E	602	HEC	C4B-NB-C1B	2.65	107.81	105.07
3	E	602	HEC	C4A-NA-C1A	2.64	107.94	105.35
3	C	604	HEC	C4C-NC-C1C	2.64	107.94	105.35
3	C	602	HEC	C4C-NC-C1C	2.64	107.93	105.35
3	C	607	HEC	CAB-C3B-C2B	-2.64	123.02	127.53
3	E	601	HEC	C4A-NA-C1A	2.62	107.92	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEC	C4C-NC-C1C	2.61	107.91	105.35
3	C	604	HEC	C4B-NB-C1B	2.61	107.77	105.07
3	A	602	HEC	C4B-NB-C1B	2.60	107.75	105.07
3	A	602	HEC	C4C-NC-C1C	2.59	107.89	105.35
3	A	604	HEC	C4A-NA-C1A	2.58	107.88	105.35
3	C	606	HEC	C4B-NB-C1B	2.57	107.73	105.07
3	E	601	HEC	C4C-NC-C1C	2.57	107.86	105.35
3	E	603	HEC	C4B-NB-C1B	2.56	107.71	105.07
3	C	604	HEC	C4A-NA-C1A	2.55	107.84	105.35
3	C	601	HEC	C4C-NC-C1C	2.54	107.83	105.35
4	A	611	ISW	CHB-C1B-NB	2.54	127.19	124.43
3	E	606	HEC	C4B-NB-C1B	2.54	107.69	105.07
3	A	606	HEC	C4B-NB-C1B	2.54	107.69	105.07
3	A	606	HEC	C4A-NA-C1A	2.53	107.82	105.35
3	A	602	HEC	C2A-C1A-NA	-2.52	107.88	110.32
3	E	605	HEC	C3C-C4C-NC	-2.51	107.34	110.15
3	E	607	HEC	C4B-NB-C1B	2.51	107.67	105.07
3	C	605	HEC	C4C-NC-C1C	2.51	107.81	105.35
3	C	606	HEC	C4A-NA-C1A	2.51	107.80	105.35
3	E	603	HEC	C4C-NC-C1C	2.50	107.80	105.35
3	C	604	HEC	CAD-CBD-CGD	-2.50	108.22	113.60
3	E	607	HEC	C4C-NC-C1C	2.50	107.79	105.35
3	E	602	HEC	C4C-NC-C1C	2.48	107.78	105.35
3	E	606	HEC	C2A-C1A-NA	-2.48	107.91	110.32
3	E	605	HEC	C4C-NC-C1C	2.47	107.77	105.35
4	A	608	ISW	C1B-C2B-C3B	-2.47	103.84	106.80
4	C	611	ISW	C1B-C2B-C3B	-2.47	103.85	106.80
3	C	602	HEC	C4A-NA-C1A	2.47	107.76	105.35
3	C	607	HEC	C2A-C1A-NA	-2.45	107.94	110.32
3	A	603	HEC	C2A-C1A-NA	-2.44	107.95	110.32
3	A	604	HEC	C2A-C1A-NA	-2.43	107.96	110.32
3	A	604	HEC	C4B-NB-C1B	2.43	107.58	105.07
3	A	605	HEC	C4B-NB-C1B	2.43	107.58	105.07
3	E	607	HEC	C2A-C1A-NA	-2.43	107.96	110.32
3	A	607	HEC	C2A-C1A-NA	-2.42	107.97	110.32
3	A	606	HEC	C2A-C1A-NA	-2.41	107.98	110.32
3	E	605	HEC	C4B-NB-C1B	2.40	107.55	105.07
3	E	605	HEC	C4A-NA-C1A	2.38	107.67	105.35
3	C	601	HEC	C2A-C1A-NA	-2.37	108.02	110.32
3	C	603	HEC	C3C-C4C-NC	-2.36	107.51	110.15
3	C	605	HEC	C3C-C4C-NC	-2.36	107.51	110.15
3	A	606	HEC	CHD-C1D-ND	2.35	127.28	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	604	HEC	C4C-NC-C1C	2.34	107.64	105.35
3	C	603	HEC	CAD-CBD-CGD	-2.32	108.60	113.60
3	A	605	HEC	C3C-C4C-NC	-2.32	107.55	110.15
3	C	606	HEC	C2A-C1A-NA	-2.32	108.07	110.32
3	E	602	HEC	C2A-C1A-NA	-2.31	108.08	110.32
4	A	611	ISW	C1B-C2B-C3B	-2.30	104.05	106.80
3	A	605	HEC	C4C-NC-C1C	2.29	107.59	105.35
3	C	606	HEC	C4C-NC-C1C	2.29	107.59	105.35
3	A	605	HEC	C4A-NA-C1A	2.26	107.56	105.35
3	E	606	HEC	CHD-C1D-ND	2.26	127.16	124.37
3	C	605	HEC	C4B-NB-C1B	2.24	107.38	105.07
3	A	606	HEC	C4C-NC-C1C	2.23	107.53	105.35
3	A	601	HEC	C2A-C1A-NA	-2.23	108.15	110.32
3	E	605	HEC	C2A-C1A-NA	-2.23	108.16	110.32
3	E	603	HEC	C3C-C4C-NC	-2.23	107.66	110.15
3	A	601	HEC	C3C-C4C-NC	-2.22	107.67	110.15
3	A	603	HEC	C3C-C4C-NC	-2.21	107.67	110.15
3	A	604	HEC	C4C-NC-C1C	2.21	107.51	105.35
3	E	607	HEC	CAA-CBA-CGA	-2.21	108.85	113.60
3	C	601	HEC	C3C-C4C-NC	-2.20	107.69	110.15
3	C	604	HEC	C2A-C1A-NA	-2.19	108.19	110.32
3	E	601	HEC	C3C-C4C-NC	-2.19	107.70	110.15
3	A	601	HEC	CAA-CBA-CGA	-2.17	108.93	113.60
3	E	601	HEC	C2A-C1A-NA	-2.17	108.22	110.32
3	C	604	HEC	C3C-C4C-NC	-2.16	107.73	110.15
3	C	606	HEC	CHD-C1D-ND	2.13	127.00	124.37
4	C	611	ISW	CAA-C2A-C1A	-2.12	120.90	124.89
3	C	602	HEC	C3C-C4C-NC	-2.12	107.78	110.15
3	E	603	HEC	CAD-CBD-CGD	-2.11	109.07	113.60
3	C	604	HEC	CHA-C4D-ND	2.10	126.70	124.42
3	A	606	HEC	CAD-C3D-C4D	2.09	128.31	124.66
3	A	607	HEC	CAD-CBD-CGD	-2.08	109.13	113.60
3	A	602	HEC	C3C-C4C-NC	-2.08	107.82	110.15
3	E	604	HEC	C3C-C4C-NC	-2.07	107.83	110.15
3	E	606	HEC	C4C-NC-C1C	2.07	107.38	105.35
3	A	604	HEC	CHB-C4A-NA	2.07	126.68	124.44
3	C	607	HEC	CAA-CBA-CGA	-2.07	109.16	113.60
3	C	605	HEC	C2A-C1A-NA	-2.05	108.33	110.32
3	A	605	HEC	C2A-C1A-NA	-2.05	108.33	110.32
3	C	601	HEC	CAA-CBA-CGA	-2.02	109.25	113.60
3	A	604	HEC	C3D-C4D-ND	-2.02	108.40	110.36
3	C	603	HEC	CAA-CBA-CGA	-2.02	109.26	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	ISW	O2A-CGA-CBA	2.01	120.49	114.03
4	A	611	ISW	CAA-C2A-C1A	-2.01	121.11	124.89
6	C	608	JUG	CAL-CAJ-CAF	2.00	120.04	116.99

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
3	A	604	HEC	NA
3	A	605	HEC	NA
3	A	606	HEC	NA
3	A	607	HEC	NA
3	C	601	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	E	601	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

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	603	HEC	C2D-C3D-CAD-CBD
3	E	603	HEC	C4D-C3D-CAD-CBD
3	A	602	HEC	C4D-C3D-CAD-CBD
7	C	609	1PE	OH5-C14-C24-OH4
7	C	609	1PE	OH6-C15-C25-OH5
3	C	604	HEC	C2A-CAA-CBA-CGA
3	C	605	HEC	C2A-CAA-CBA-CGA
3	A	602	HEC	C2D-C3D-CAD-CBD
3	C	607	HEC	C2B-C3B-CAB-CBB
7	C	610	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
4	A	608	ISW	C4B-C3B-CAB-CBB
4	A	611	ISW	C4B-C3B-CAB-CBB
4	C	611	ISW	C4B-C3B-CAB-CBB
3	A	605	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	C2A-CAA-CBA-CGA
3	A	604	HEC	C1A-C2A-CAA-CBA
3	A	607	HEC	C2C-C3C-CAC-CBC
3	C	605	HEC	C2B-C3B-CAB-CBB
3	E	607	HEC	C2C-C3C-CAC-CBC
3	A	607	HEC	C1A-C2A-CAA-CBA
3	A	607	HEC	C4C-C3C-CAC-CBC
7	C	609	1PE	C24-C14-OH5-C25
3	E	604	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	C4D-C3D-CAD-CBD
3	C	604	HEC	C4D-C3D-CAD-CBD
3	C	605	HEC	C4D-C3D-CAD-CBD
3	E	605	HEC	C4D-C3D-CAD-CBD
4	A	611	ISW	C4D-C3D-CAD-CBD
4	A	608	ISW	C4C-C3C-CAC-CBC
4	A	611	ISW	C4C-C3C-CAC-CBC
3	E	605	HEC	C2A-CAA-CBA-CGA
7	C	610	1PE	OH6-C15-C25-OH5
3	E	602	HEC	C2C-C3C-CAC-CBC
4	A	611	ISW	C2C-C3C-CAC-CBC
4	A	611	ISW	C2B-C3B-CAB-CBB
3	A	604	HEC	C3A-C2A-CAA-CBA
3	C	605	HEC	C2D-C3D-CAD-CBD
3	E	605	HEC	C2D-C3D-CAD-CBD
3	C	604	HEC	C2D-C3D-CAD-CBD
3	A	605	HEC	C2D-C3D-CAD-CBD
4	A	611	ISW	C2D-C3D-CAD-CBD
3	E	604	HEC	C1A-C2A-CAA-CBA
3	E	605	HEC	C2B-C3B-CAB-CBB
3	E	607	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	C4B-C3B-CAB-CBB
3	C	605	HEC	C4B-C3B-CAB-CBB
5	E	609	PEG	C1-C2-O2-C3
3	A	607	HEC	C3A-C2A-CAA-CBA
3	A	607	HEC	C2B-C3B-CAB-CBB
3	C	607	HEC	C2C-C3C-CAC-CBC
4	A	608	ISW	C2C-C3C-CAC-CBC
4	C	611	ISW	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	E	604	HEC	C4B-C3B-CAB-CBB
3	A	603	HEC	C2D-C3D-CAD-CBD
3	E	607	HEC	C4C-C3C-CAC-CBC
3	C	604	HEC	C2B-C3B-CAB-CBB
7	C	610	1PE	C25-C15-OH6-C26
3	C	602	HEC	C2C-C3C-CAC-CBC
3	C	607	HEC	C4B-C3B-CAB-CBB
3	A	604	HEC	C2A-CAA-CBA-CGA
3	C	606	HEC	C2B-C3B-CAB-CBB
4	C	611	ISW	C4C-C3C-CAC-CBC
3	C	605	HEC	CAA-CBA-CGA-O1A
3	A	607	HEC	CAA-CBA-CGA-O1A
3	E	607	HEC	C4B-C3B-CAB-CBB
4	A	611	ISW	CAA-CBA-CGA-O1A
3	A	607	HEC	C3D-CAD-CBD-CGD
3	C	603	HEC	C3D-CAD-CBD-CGD
3	E	605	HEC	C4B-C3B-CAB-CBB
3	A	604	HEC	C2B-C3B-CAB-CBB
3	A	604	HEC	CAA-CBA-CGA-O1A
3	A	607	HEC	CAA-CBA-CGA-O2A
3	C	604	HEC	C2C-C3C-CAC-CBC
3	A	603	HEC	C4D-C3D-CAD-CBD
3	A	605	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O1D
3	C	602	HEC	CAD-CBD-CGD-O2D
4	A	611	ISW	CAA-CBA-CGA-O2A
7	C	609	1PE	C15-C25-OH5-C14
3	A	602	HEC	C2C-C3C-CAC-CBC
4	C	611	ISW	C3D-CAD-CBD-CGD
3	A	604	HEC	CAA-CBA-CGA-O2A
4	C	611	ISW	C2B-C3B-CAB-CBB
5	A	610	PEG	O2-C3-C4-O4
3	E	604	HEC	C3A-C2A-CAA-CBA
3	E	602	HEC	CAD-CBD-CGD-O1D
3	A	605	HEC	CAD-CBD-CGD-O2D
5	E	609	PEG	C4-C3-O2-C2
3	A	607	HEC	C4B-C3B-CAB-CBB
3	C	605	HEC	C3D-CAD-CBD-CGD
3	E	604	HEC	C2A-CAA-CBA-CGA
4	A	611	ISW	C3D-CAD-CBD-CGD
3	E	602	HEC	CAD-CBD-CGD-O2D
3	C	605	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	E	601	HEC	CAD-CBD-CGD-O2D
3	C	604	HEC	CAA-CBA-CGA-O2A
3	E	607	HEC	C1A-C2A-CAA-CBA
3	C	604	HEC	CAA-CBA-CGA-O1A
4	A	608	ISW	C3D-CAD-CBD-CGD
4	A	608	ISW	CAA-CBA-CGA-O2A
3	C	604	HEC	C4B-C3B-CAB-CBB
3	C	605	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	CAD-CBD-CGD-O2D
3	C	606	HEC	C4B-C3B-CAB-CBB
3	A	605	HEC	CAA-CBA-CGA-O1A
3	C	606	HEC	CAD-CBD-CGD-O1D
3	E	606	HEC	CAD-CBD-CGD-O1D
5	A	610	PEG	C1-C2-O2-C3
3	E	606	HEC	C2B-C3B-CAB-CBB
3	A	605	HEC	CAA-CBA-CGA-O2A
3	C	605	HEC	CAD-CBD-CGD-O1D
3	E	601	HEC	CAD-CBD-CGD-O1D
3	E	605	HEC	CAD-CBD-CGD-O2D
4	A	608	ISW	CAA-CBA-CGA-O1A
3	A	606	HEC	C2B-C3B-CAB-CBB
4	A	608	ISW	C2B-C3B-CAB-CBB
4	A	611	ISW	C2A-CAA-CBA-CGA
3	A	604	HEC	C4B-C3B-CAB-CBB
3	C	607	HEC	CAA-CBA-CGA-O2A
3	A	607	HEC	CAD-CBD-CGD-O2D
3	E	601	HEC	CAA-CBA-CGA-O2A
3	E	606	HEC	CAD-CBD-CGD-O2D
3	C	607	HEC	CAD-CBD-CGD-O1D
3	C	607	HEC	CAD-CBD-CGD-O2D
3	E	605	HEC	CAD-CBD-CGD-O1D
3	A	607	HEC	CAD-CBD-CGD-O1D
7	C	610	1PE	OH4-C13-C23-OH3
4	C	611	ISW	CAA-CBA-CGA-O2A
3	A	601	HEC	C2A-CAA-CBA-CGA
3	C	602	HEC	CAA-CBA-CGA-O1A
3	A	603	HEC	C2B-C3B-CAB-CBB
3	E	606	HEC	C4B-C3B-CAB-CBB

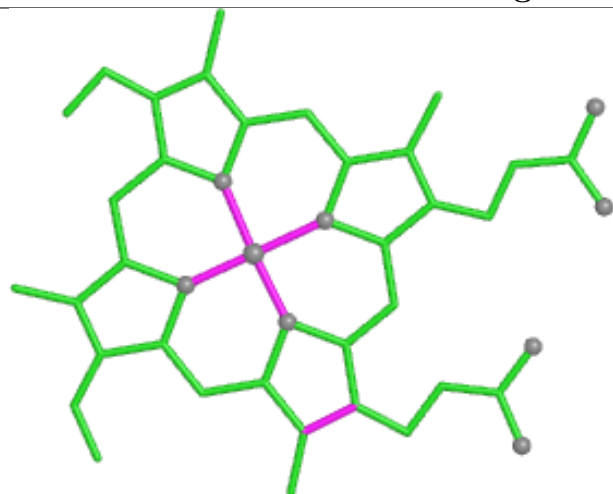
There are no ring outliers.

27 monomers are involved in 67 short contacts:

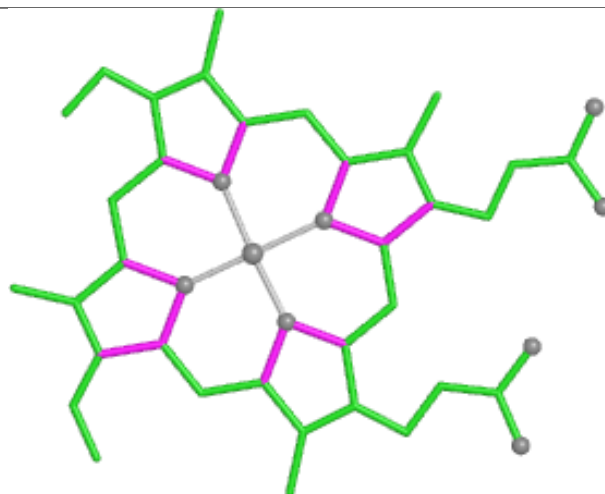
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	605	HEC	2	0
3	E	603	HEC	1	0
3	A	607	HEC	4	0
3	C	605	HEC	2	0
3	C	607	HEC	2	0
3	A	605	HEC	4	0
3	E	606	HEC	5	0
3	A	604	HEC	3	0
3	A	602	HEC	3	0
4	C	611	ISW	4	0
3	E	601	HEC	2	0
5	A	610	PEG	1	0
3	C	602	HEC	2	0
4	A	611	ISW	4	0
3	A	601	HEC	1	0
3	E	604	HEC	2	0
4	A	608	ISW	4	0
6	E	608	JUG	2	0
3	C	603	HEC	1	0
3	C	604	HEC	4	0
3	A	606	HEC	7	0
6	C	608	JUG	1	0
7	C	609	1PE	1	0
3	E	602	HEC	2	0
3	E	607	HEC	1	0
3	C	601	HEC	2	0
3	C	606	HEC	4	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.

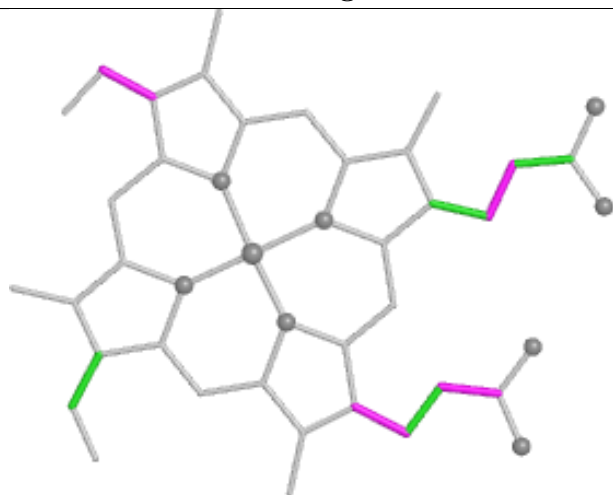
Ligand HEC E 605



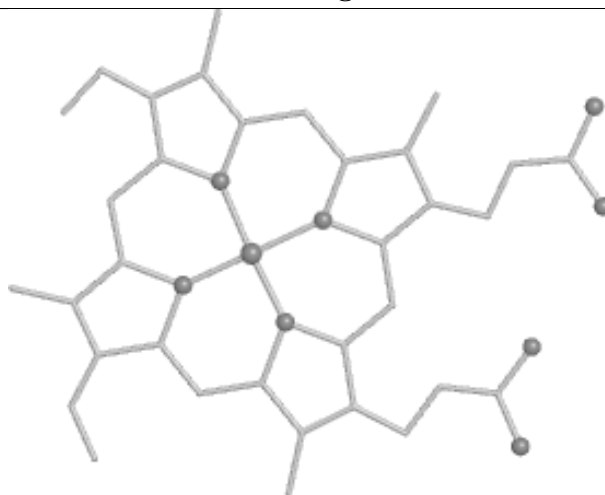
Bond lengths



Bond angles

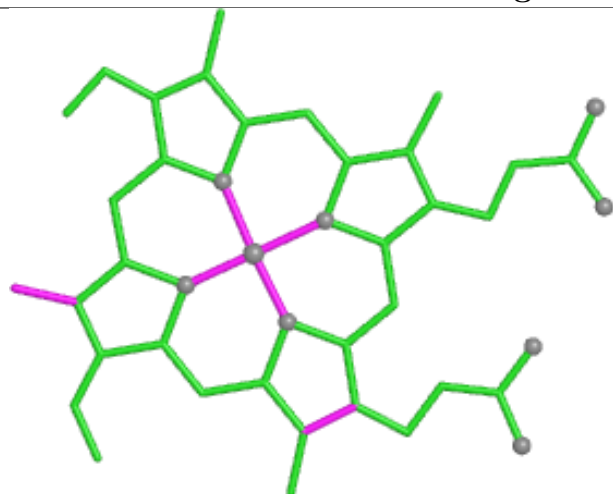


Torsions

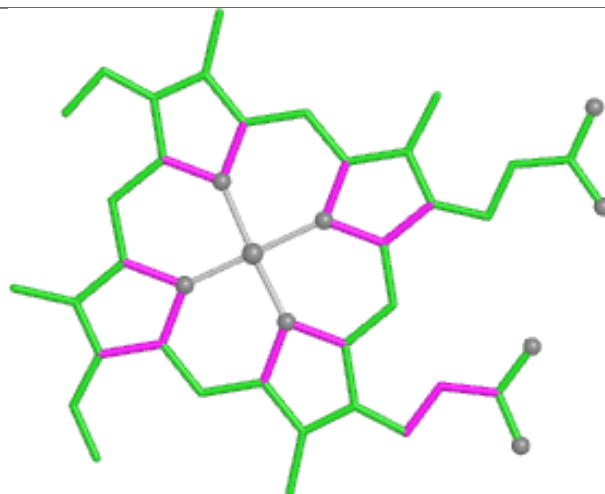


Rings

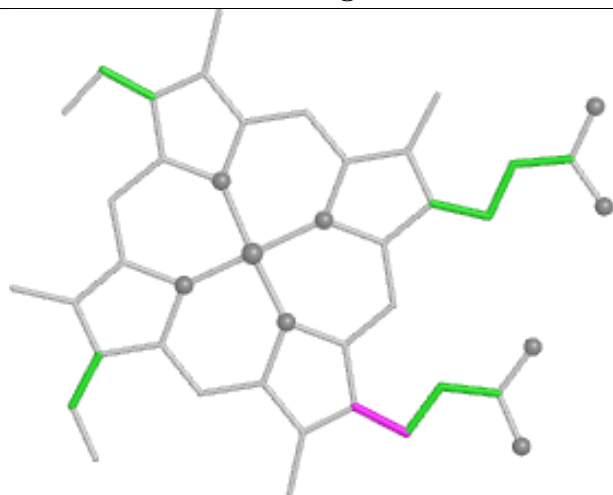
Ligand HEC E 603



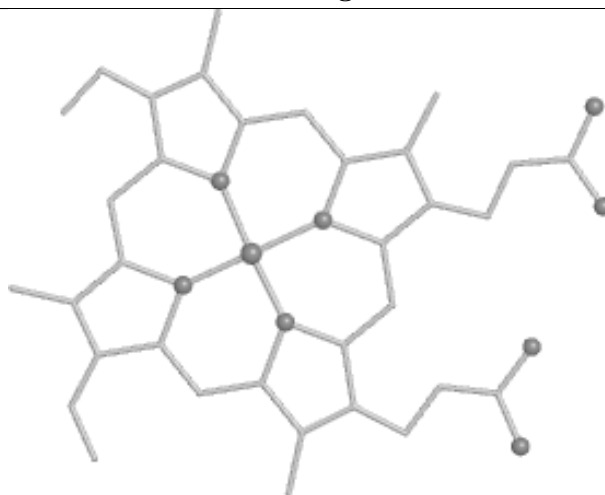
Bond lengths



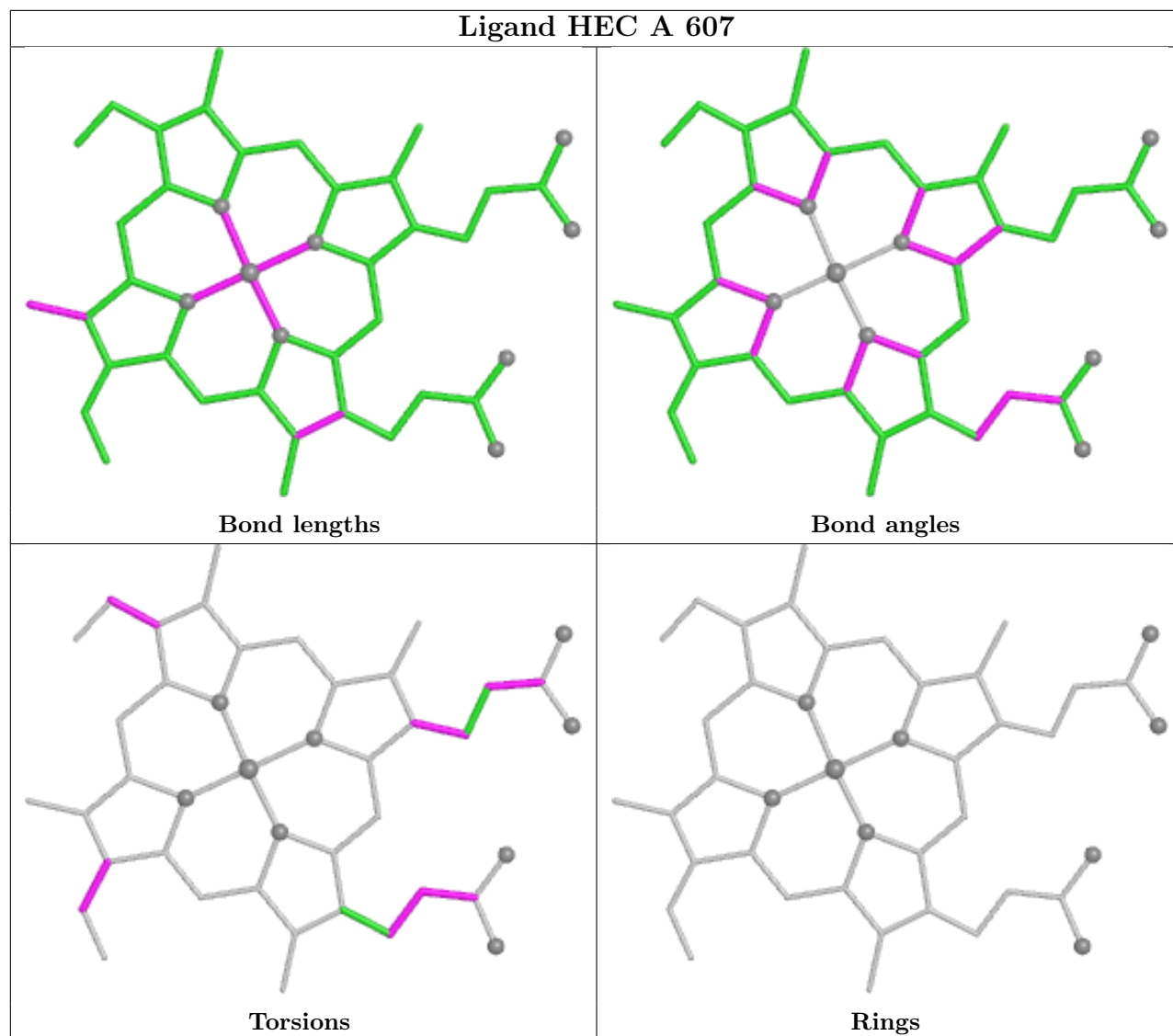
Bond angles



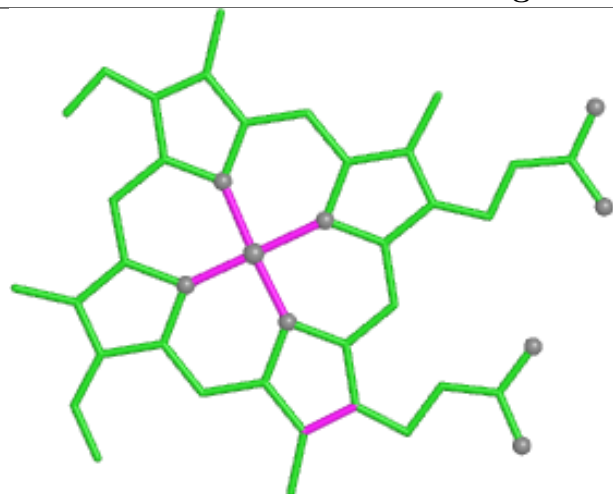
Torsions



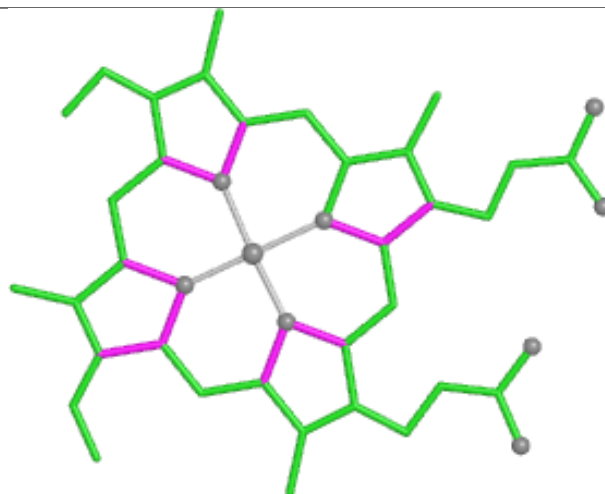
Rings



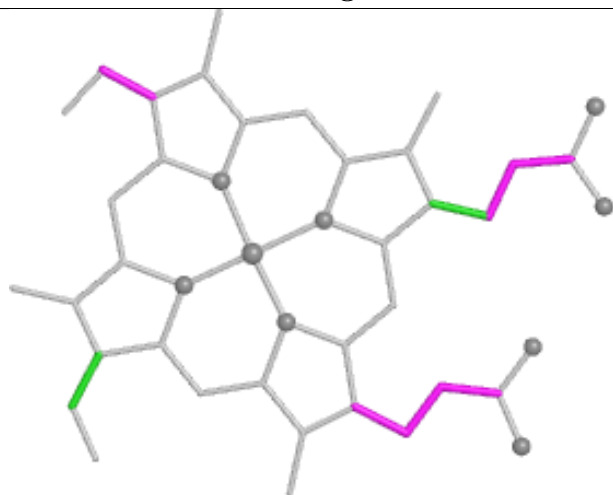
Ligand HEC C 605



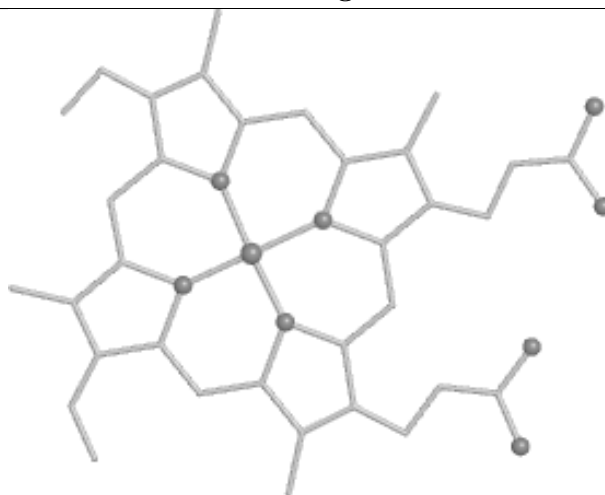
Bond lengths



Bond angles

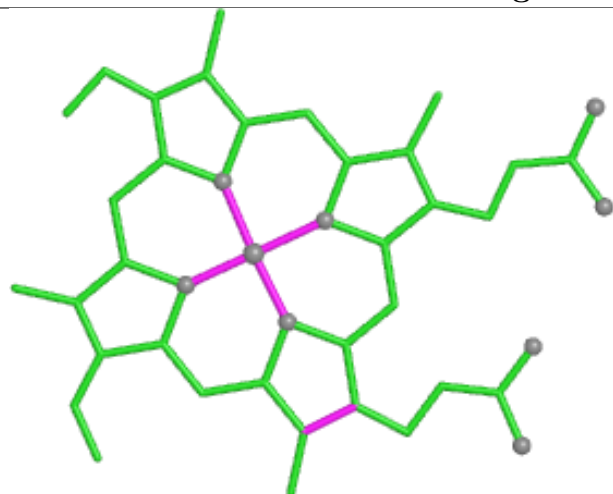


Torsions

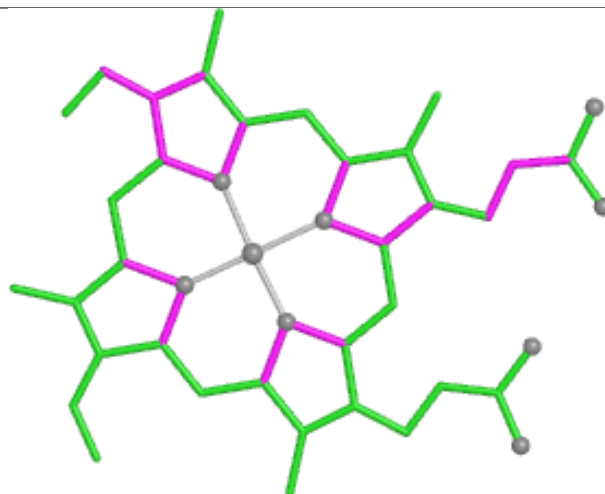


Rings

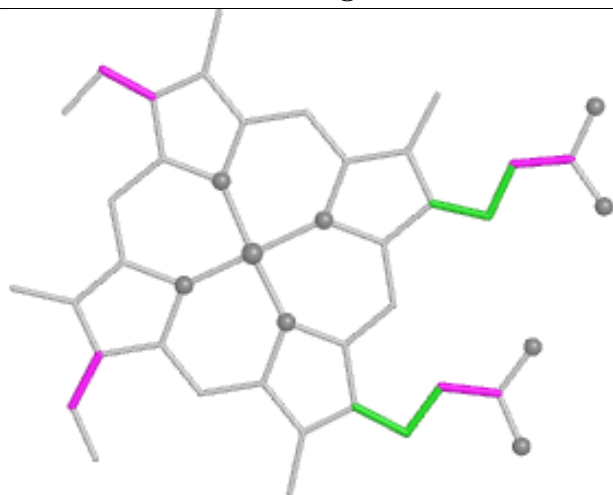
Ligand HEC C 607



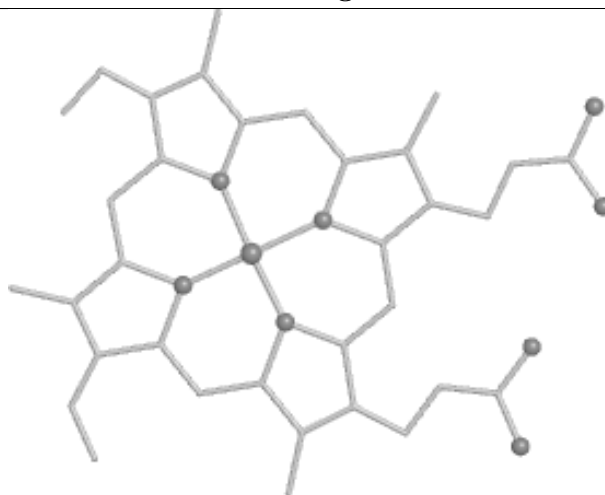
Bond lengths



Bond angles

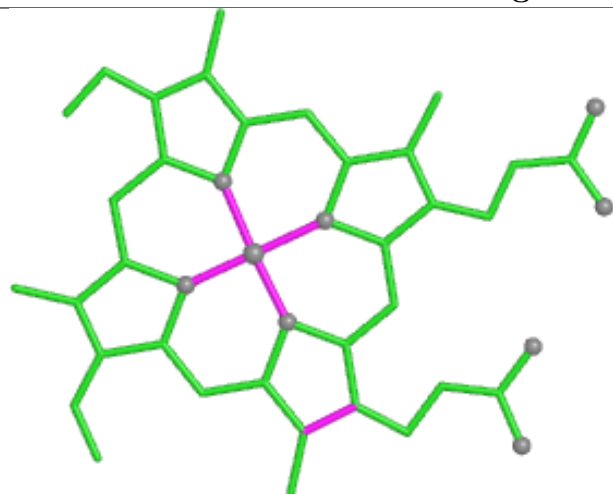


Torsions

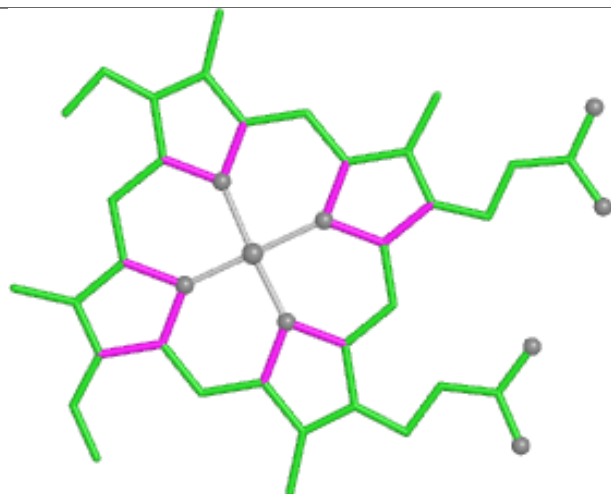


Rings

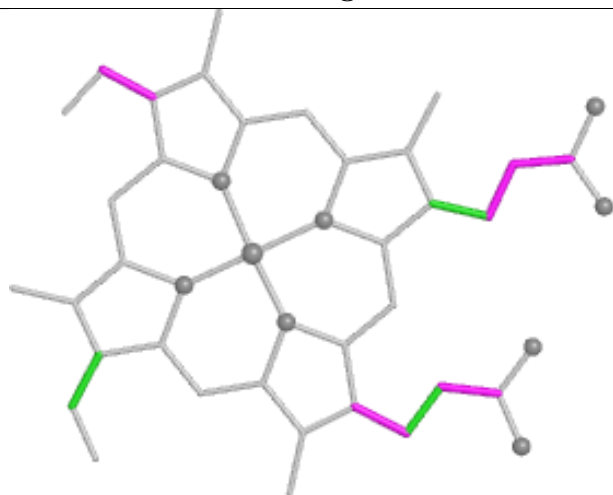
Ligand HEC A 605



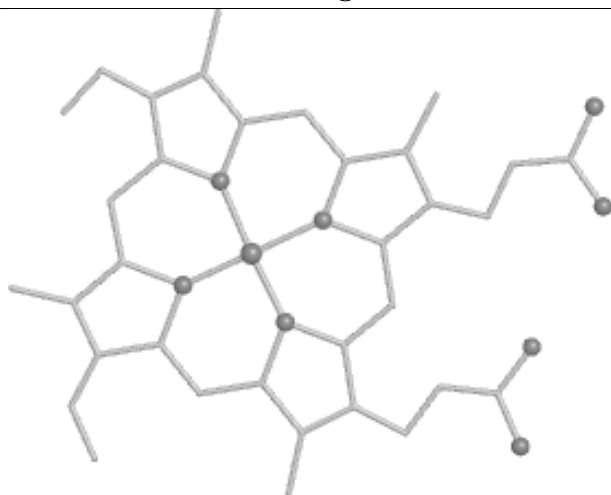
Bond lengths



Bond angles

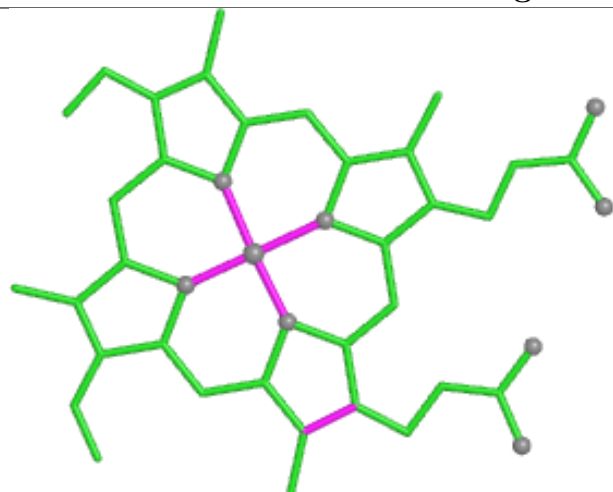


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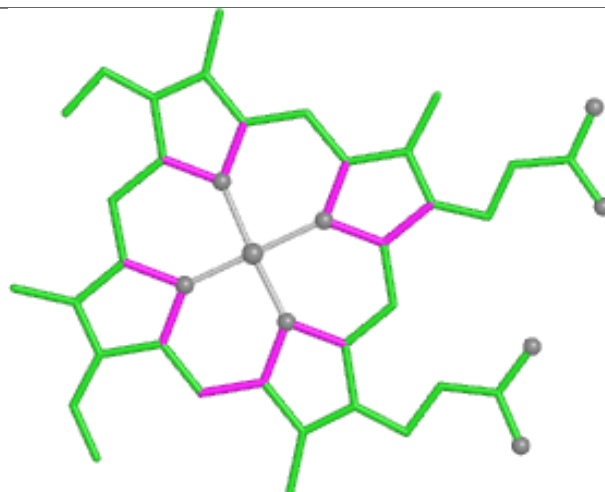


Rings

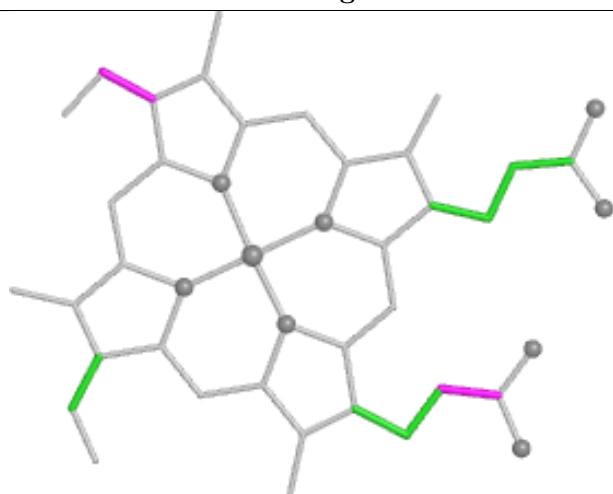
Ligand HEC E 606



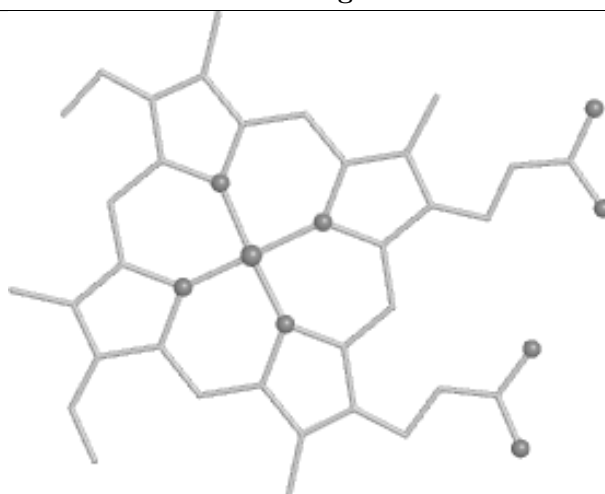
Bond lengths



Bond angles

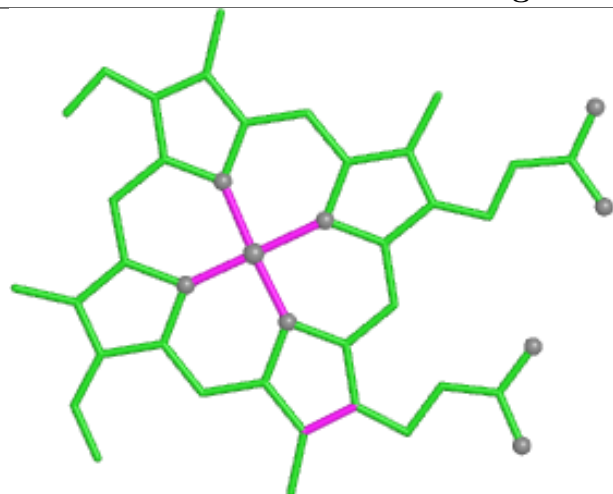


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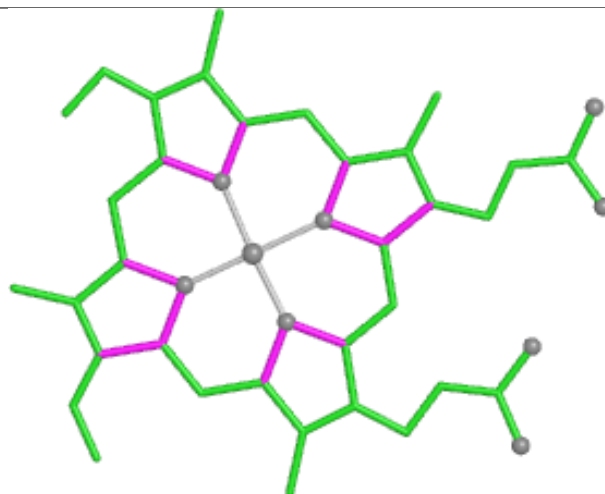


Rings

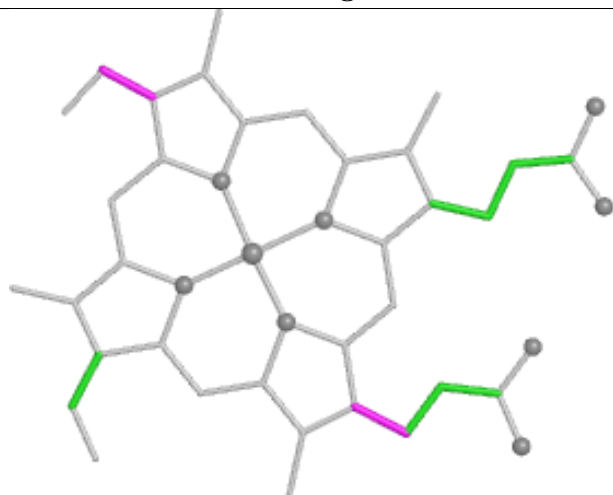
Ligand HEC A 603



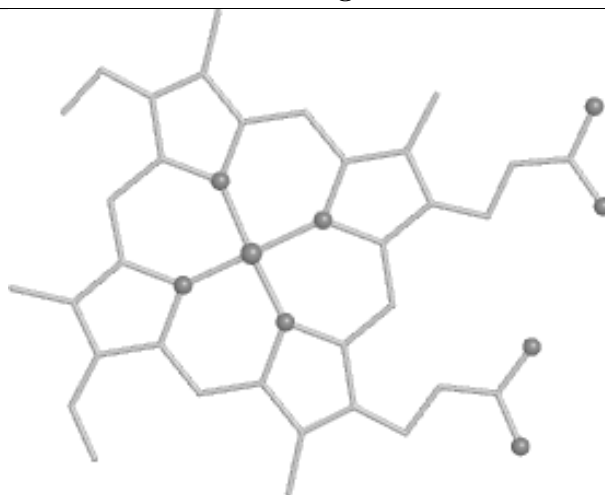
Bond lengths



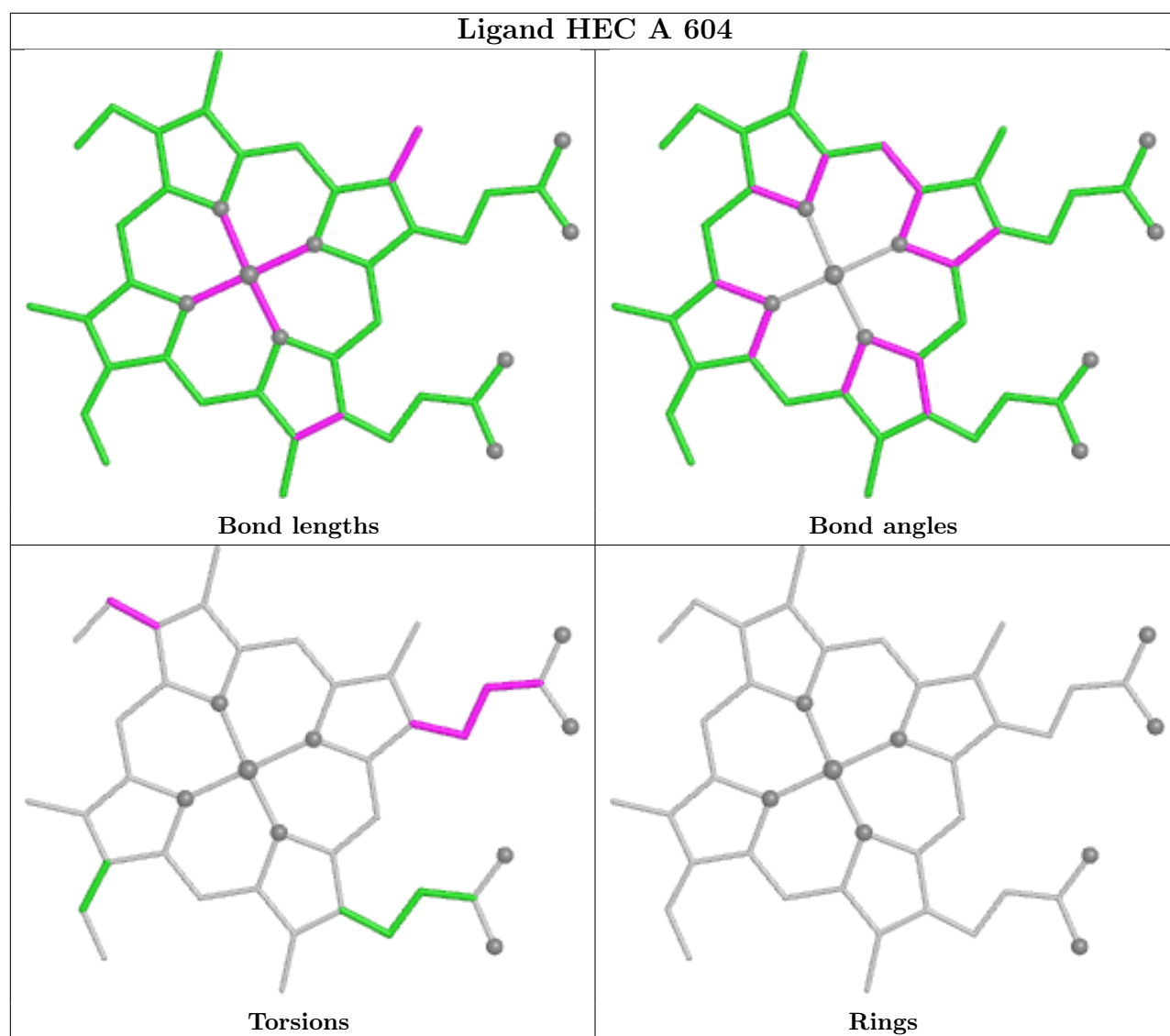
Bond angles

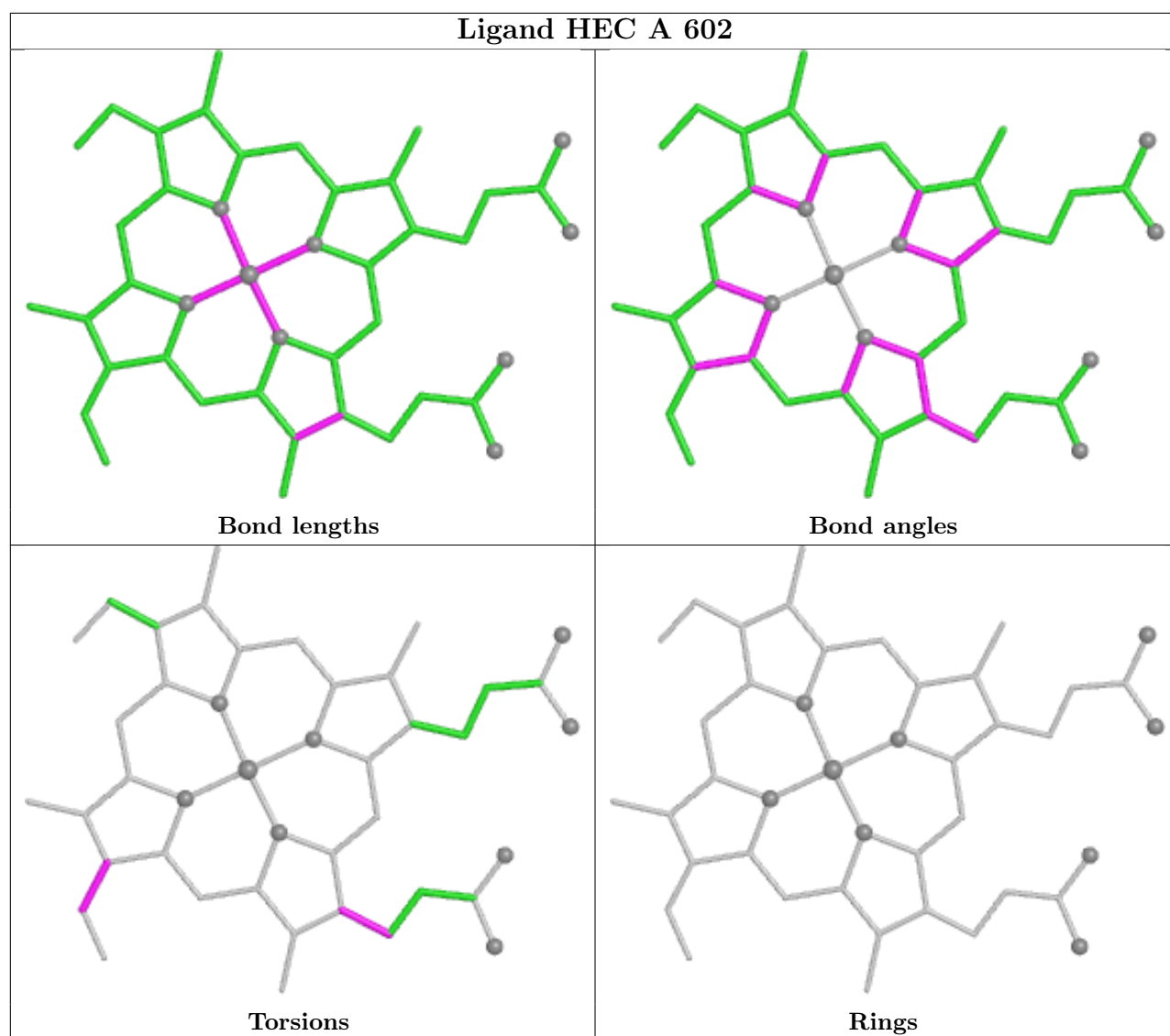


Torsions

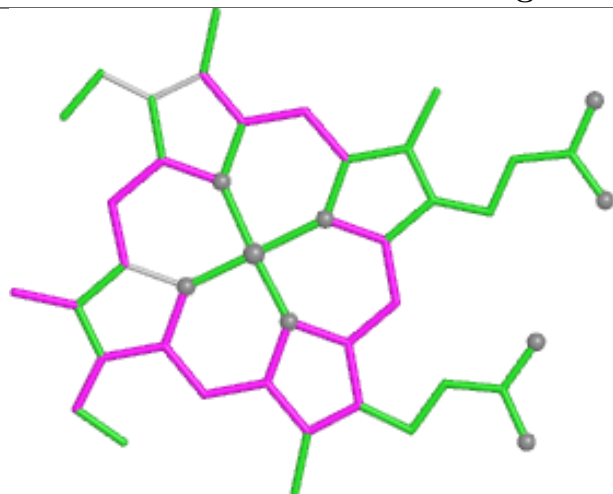


Rings

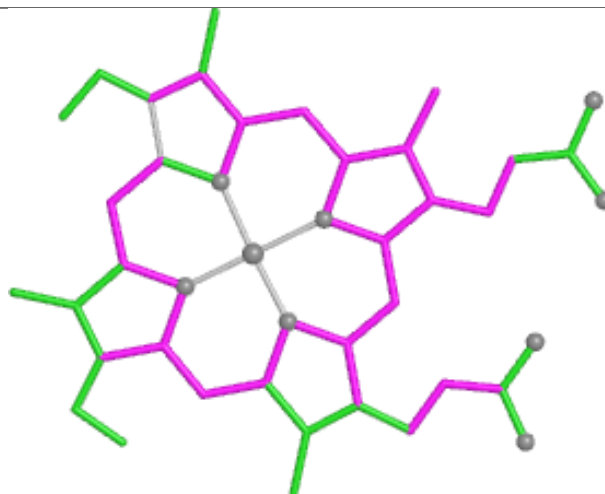




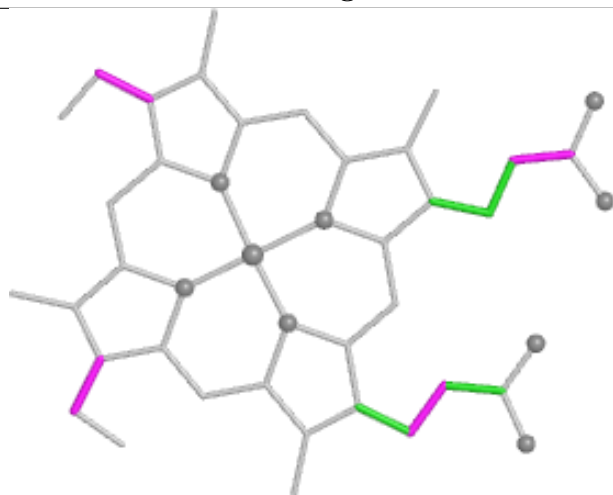
Ligand ISW C 611



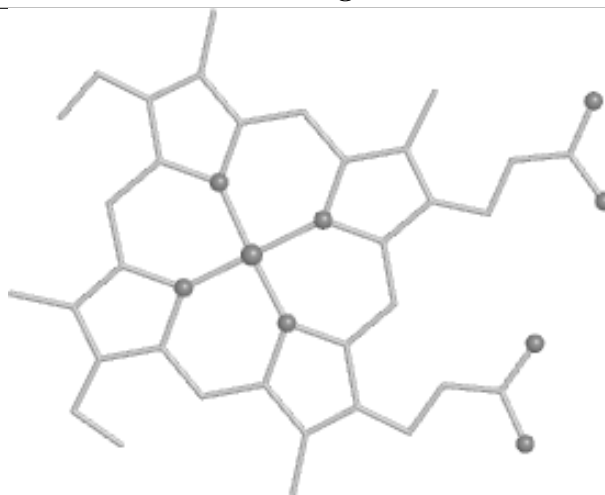
Bond lengths



Bond angles

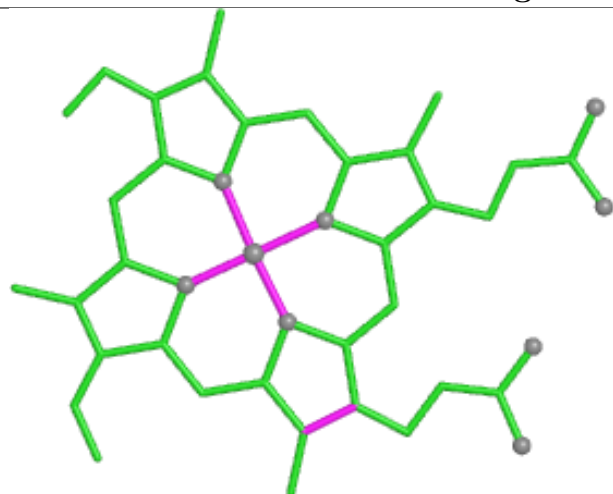


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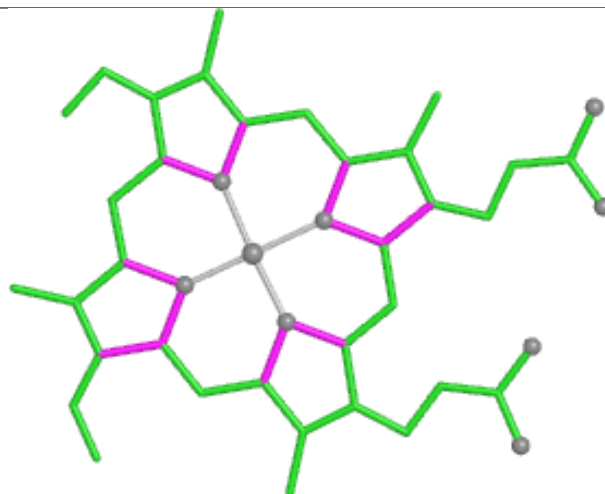


Rings

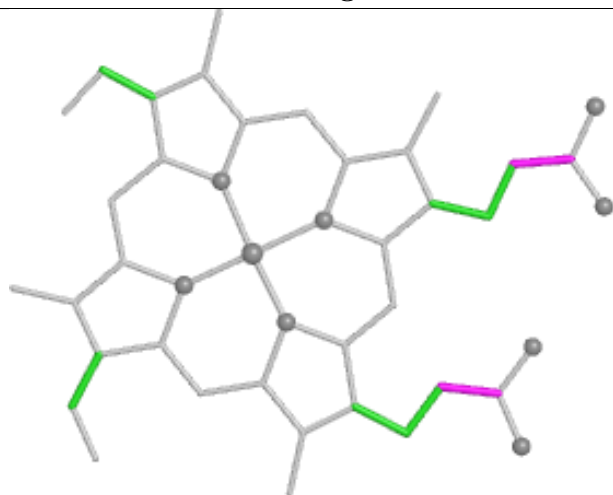
Ligand HEC E 601



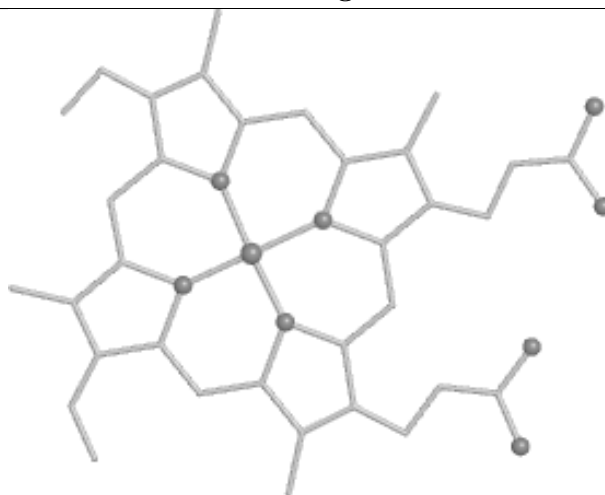
Bond lengths



Bond angles

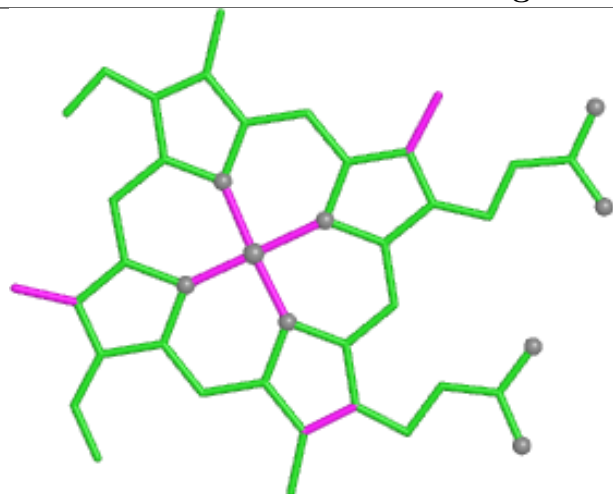


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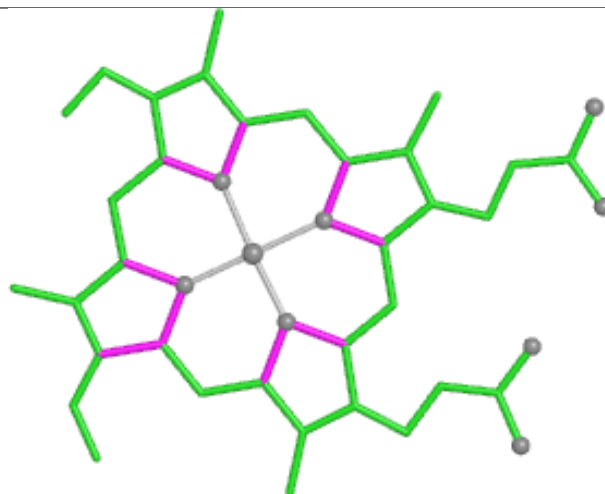


Rings

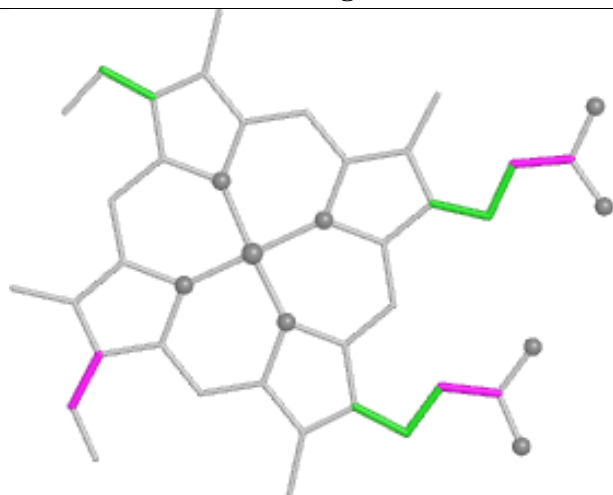
Ligand HEC C 602



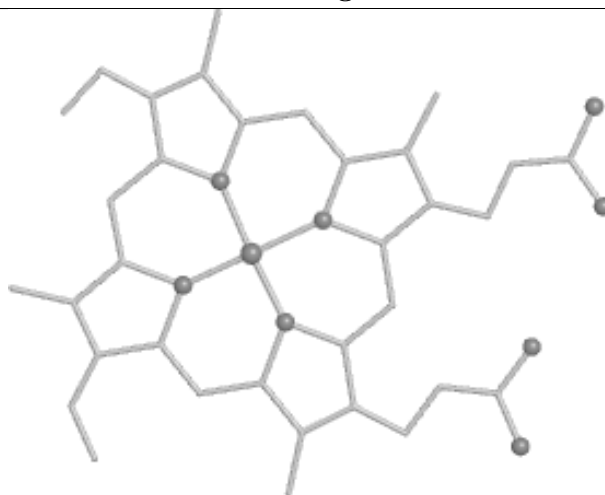
Bond lengths



Bond angles

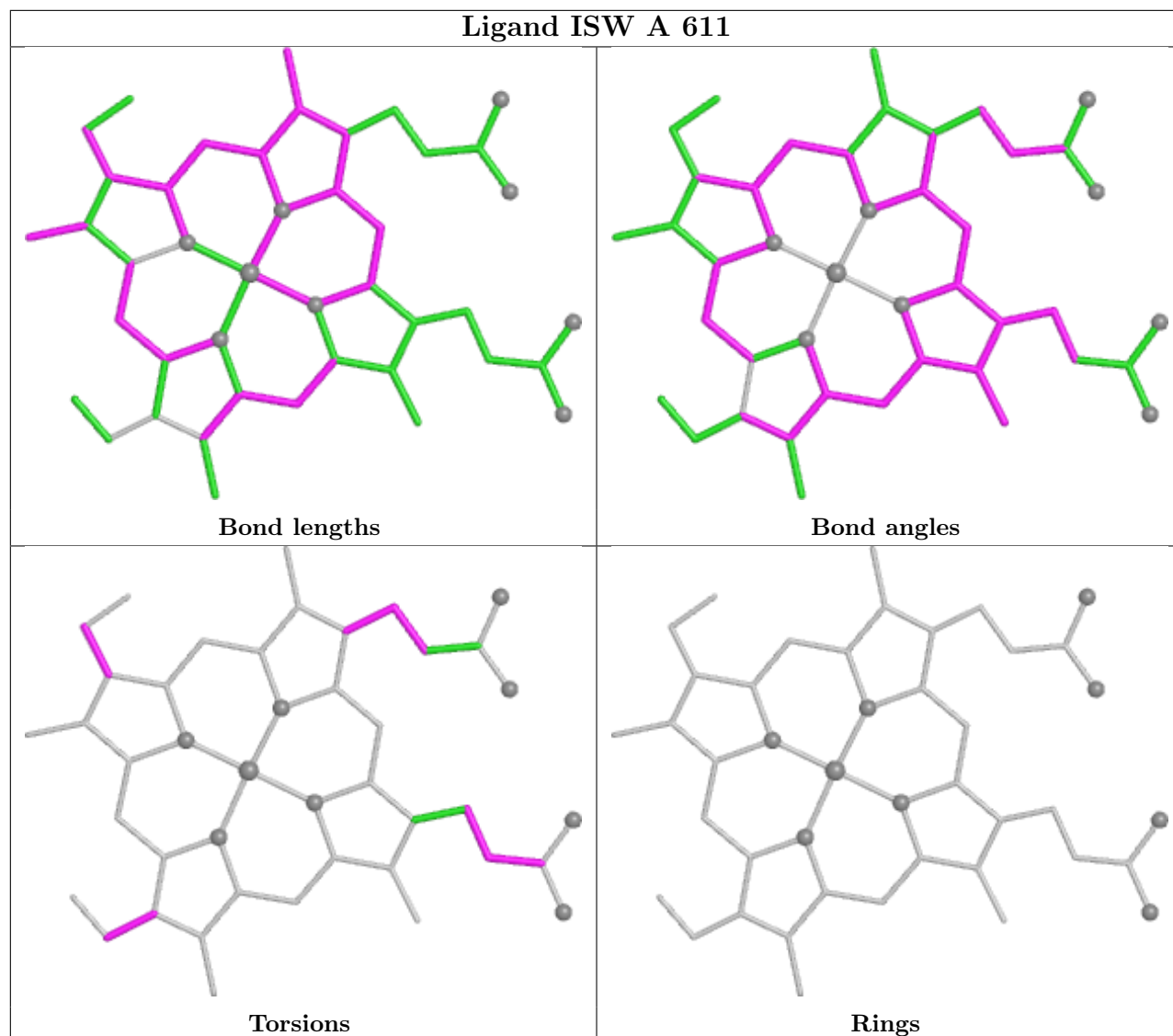


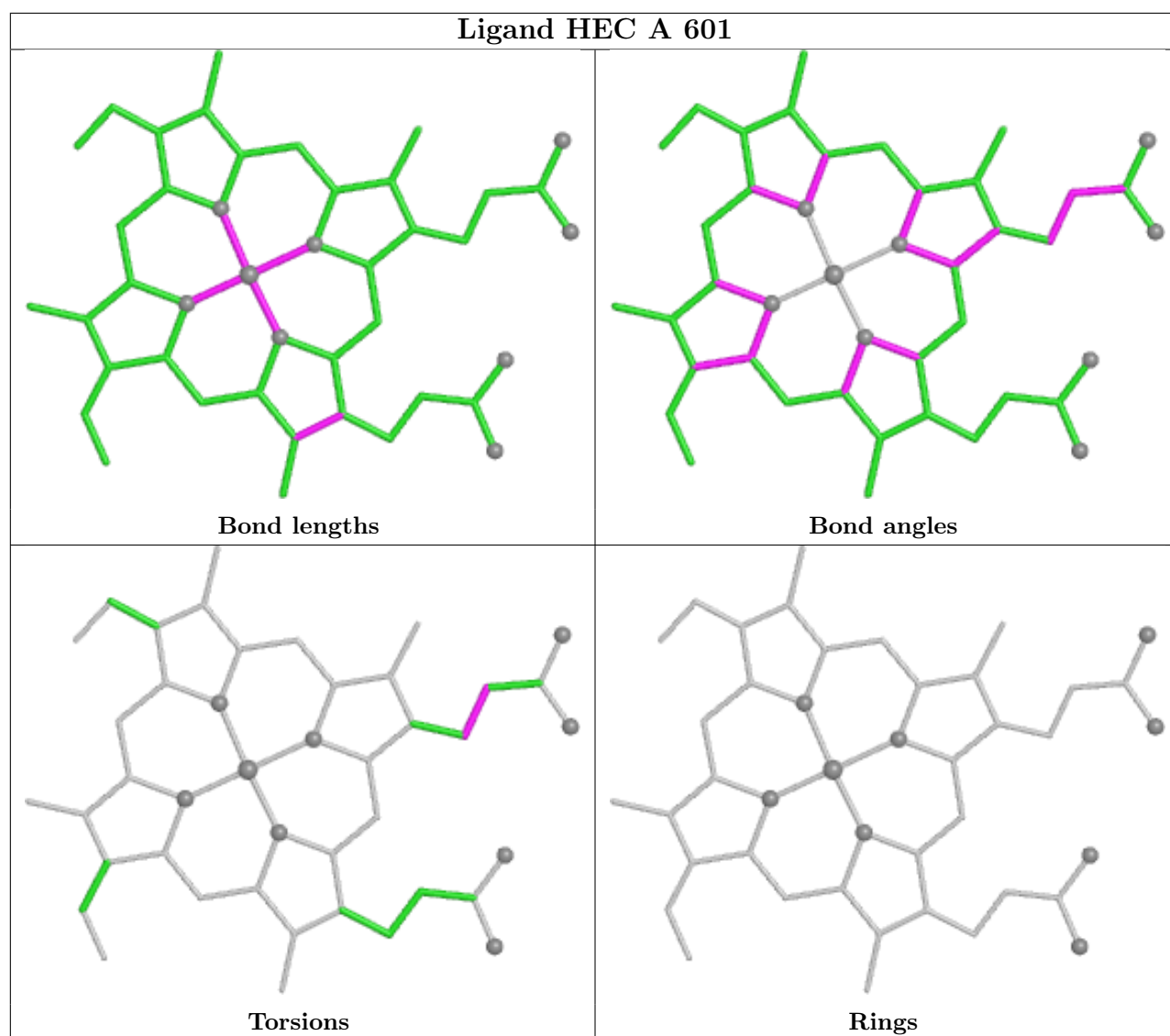
Torsions



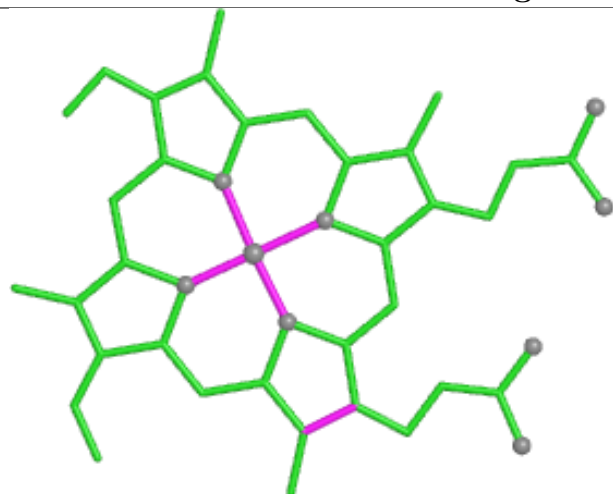
Rings

Ligand ISW A 611

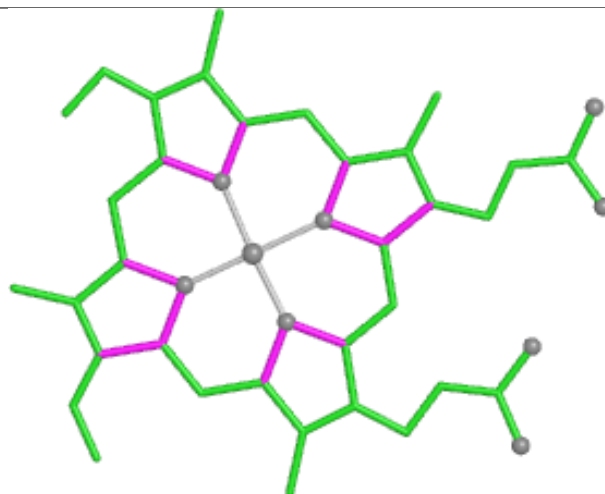




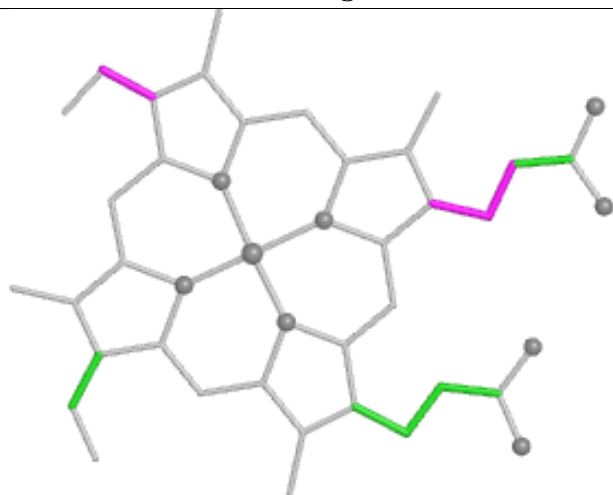
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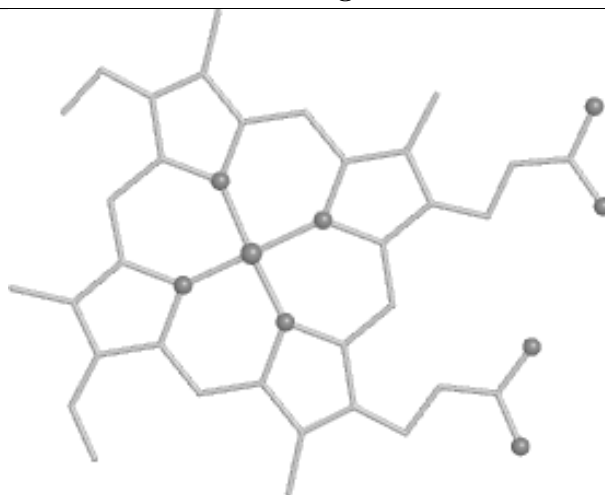
Bond lengths



Bond angles

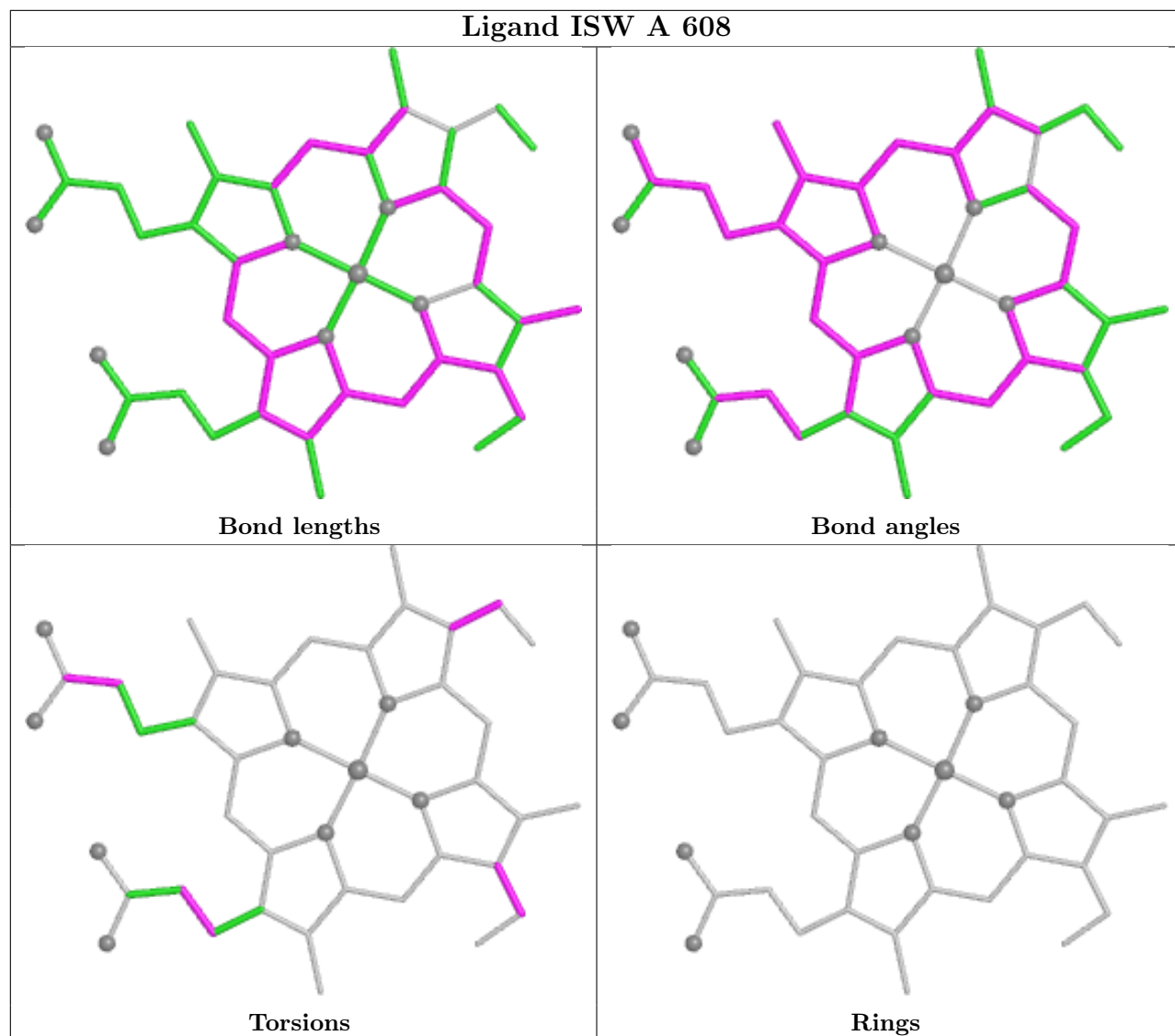


Torsions

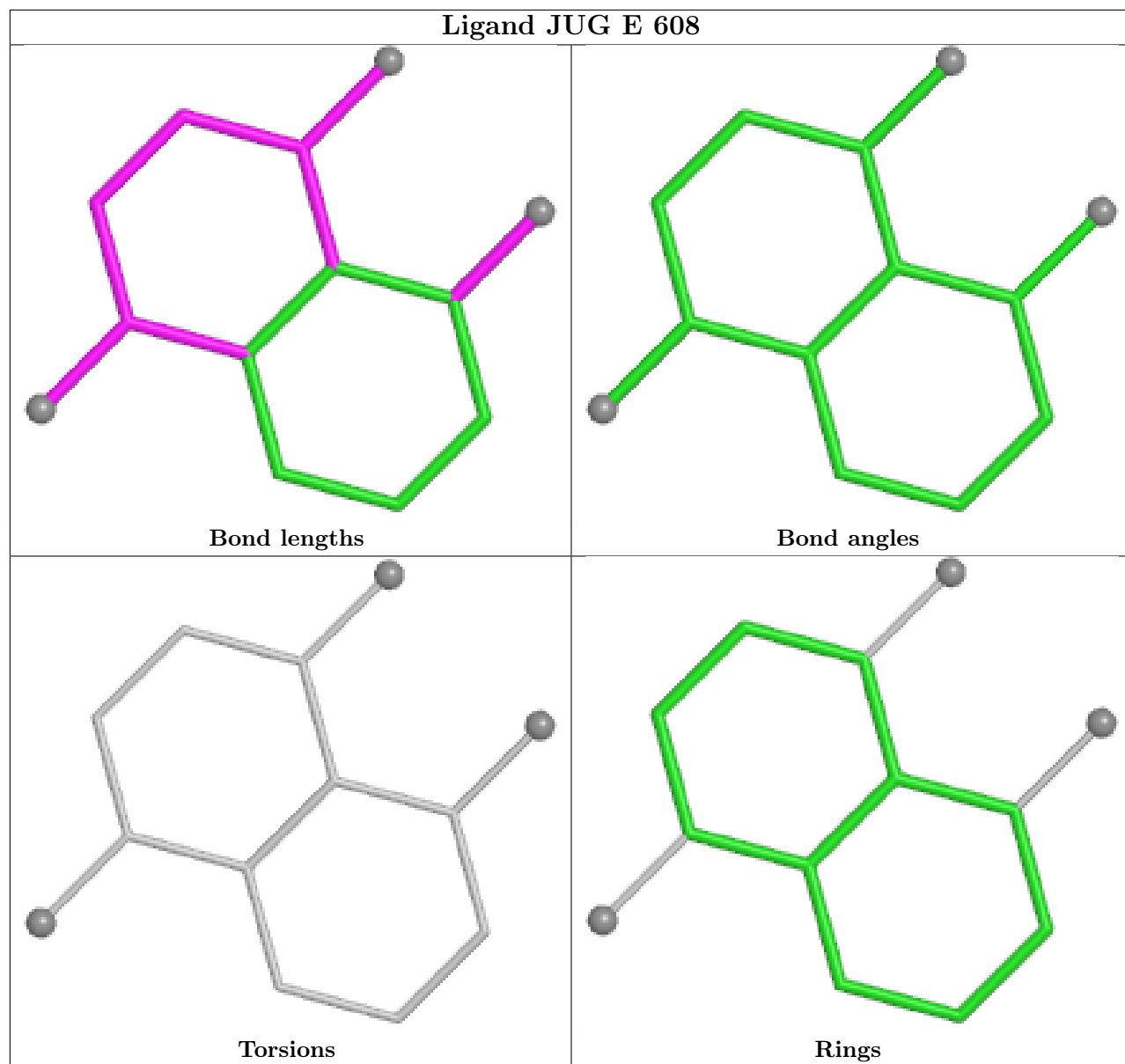


Rings

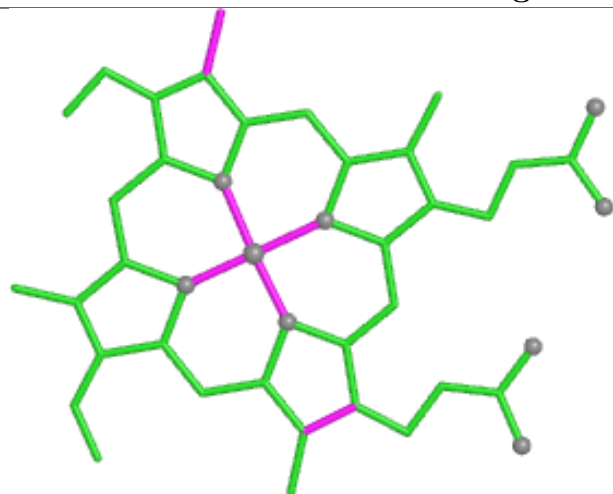
Ligand ISW A 608



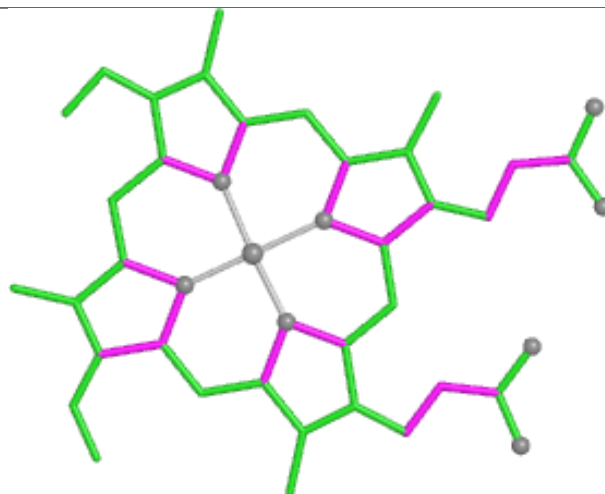
Ligand JUG E 608



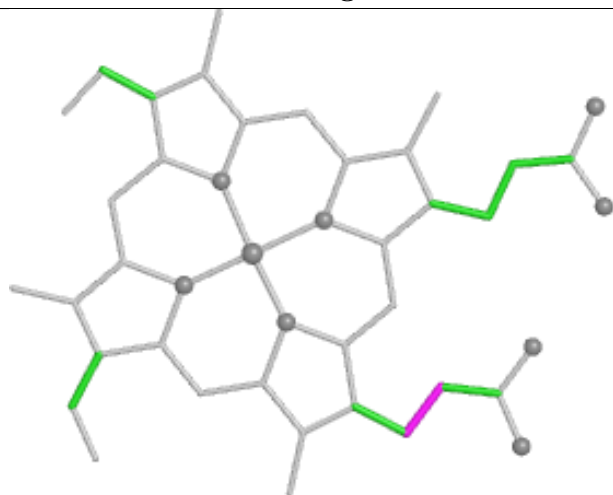
Ligand HEC C 603



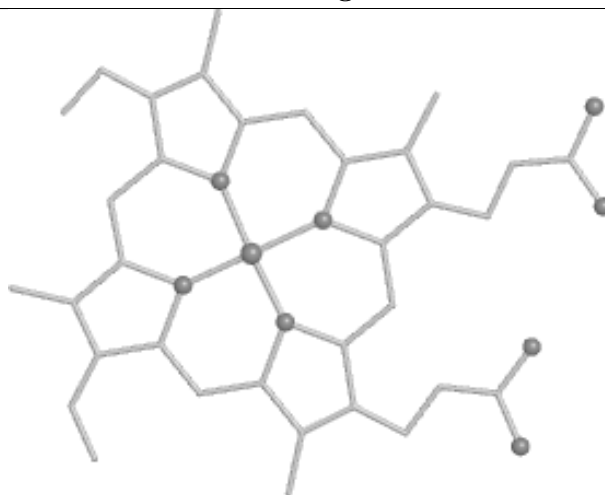
Bond lengths



Bond angles

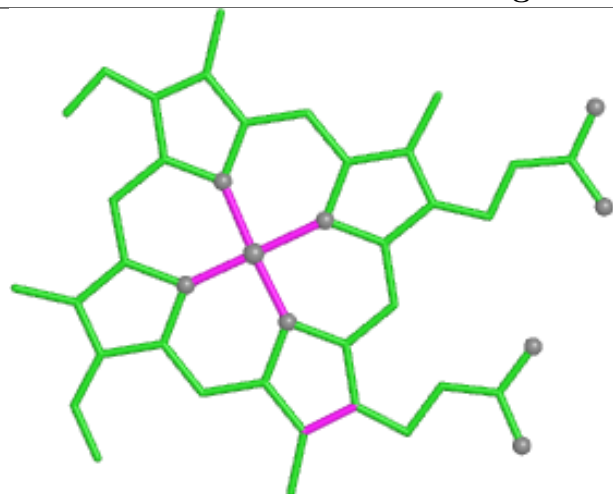


Torsions

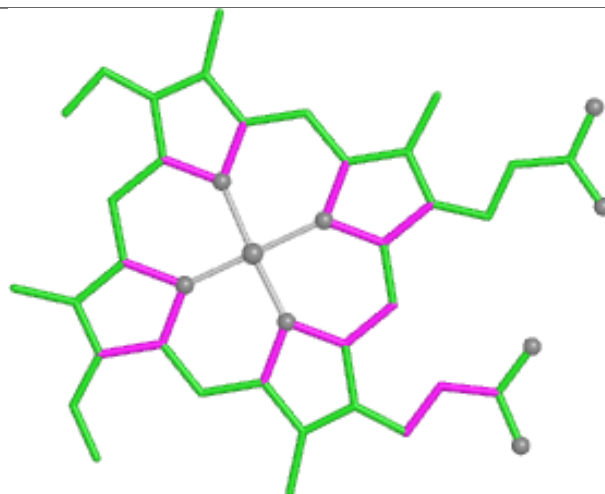


Rings

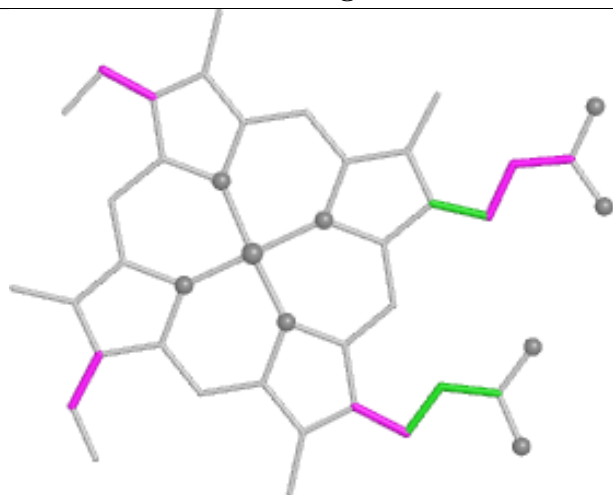
Ligand HEC C 604



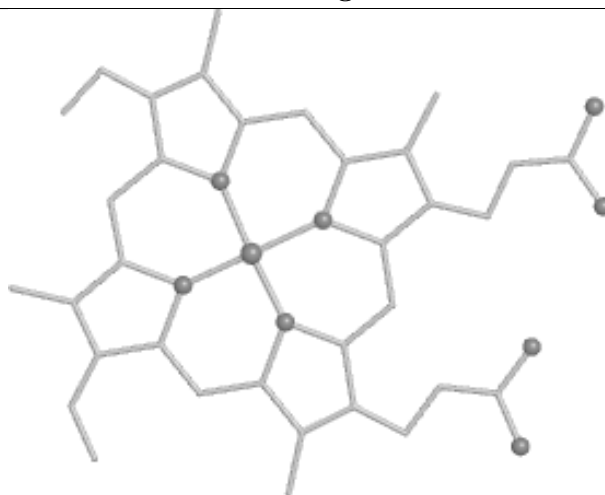
Bond lengths



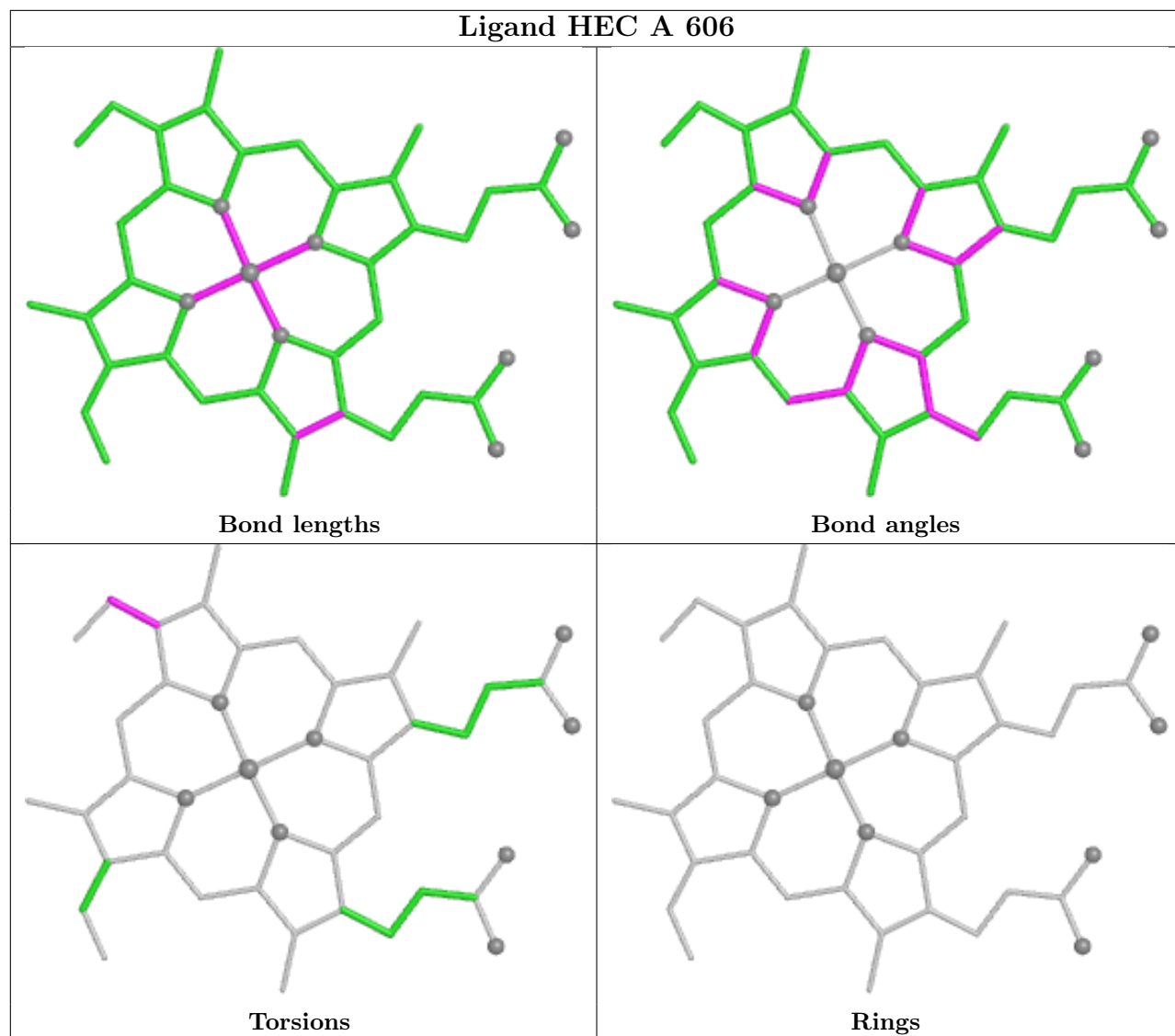
Bond angles



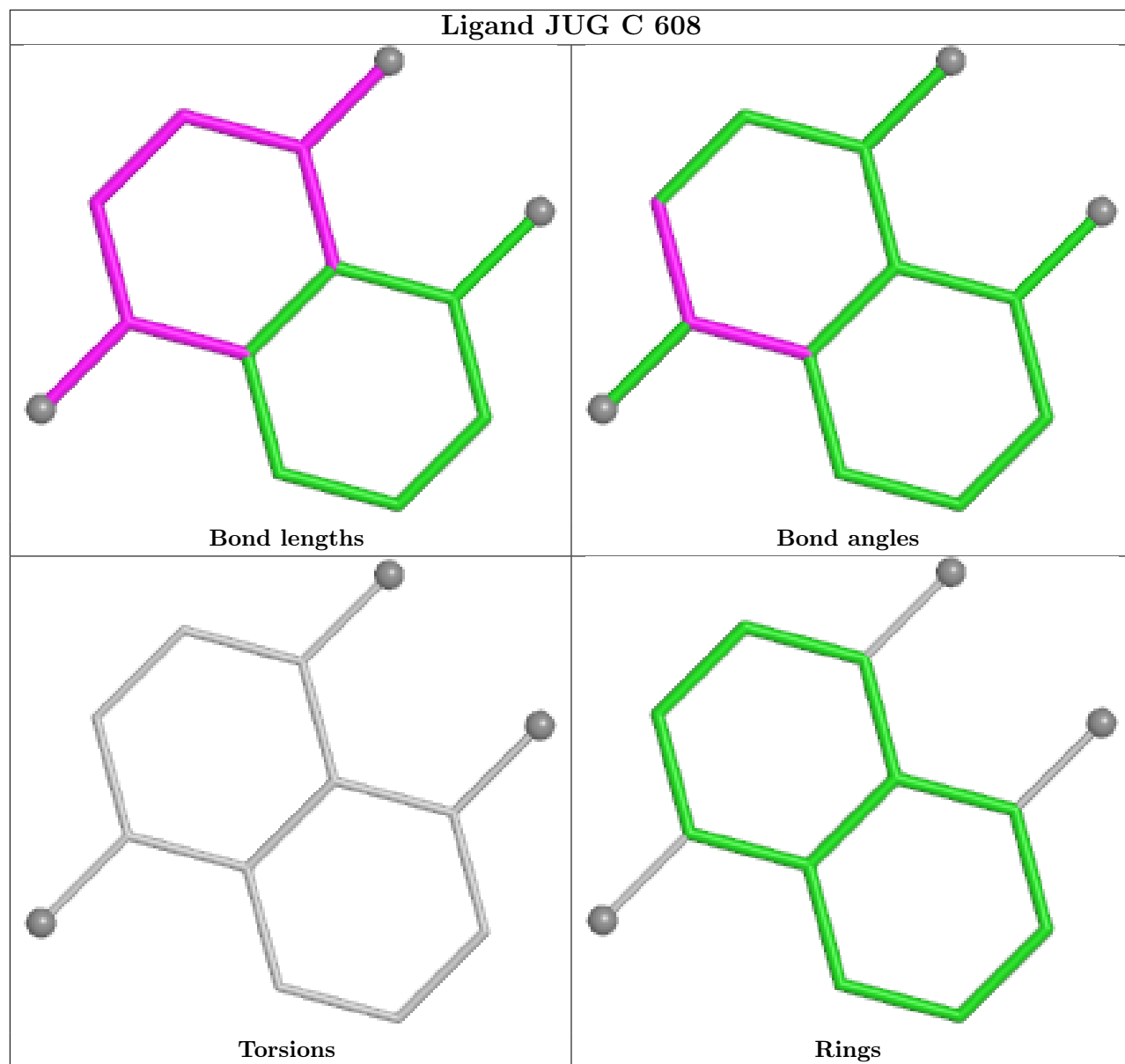
Torsions



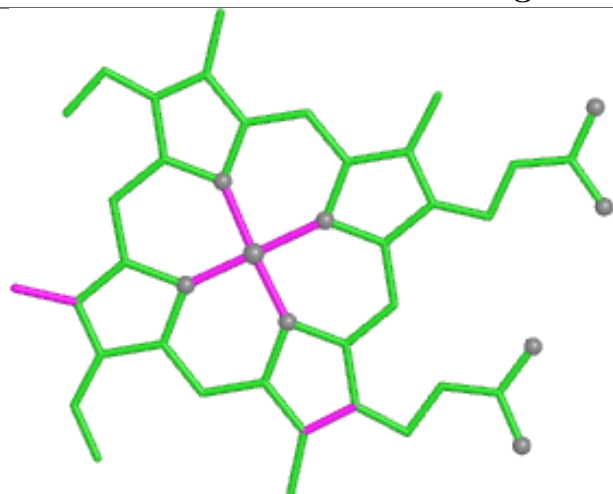
Rings



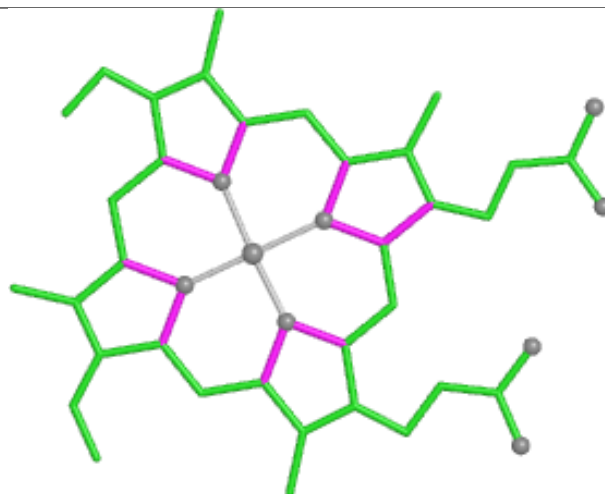
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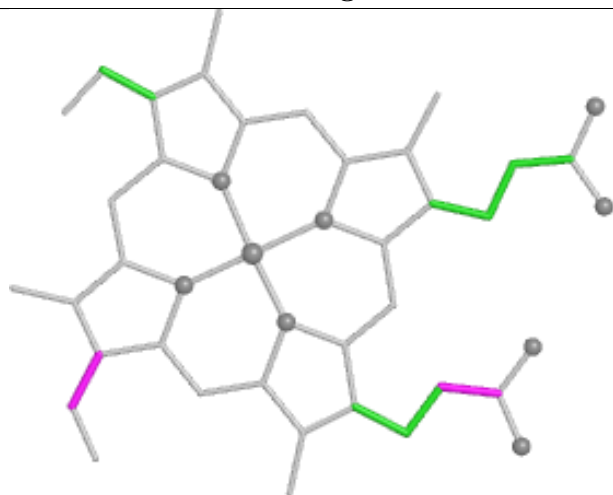
Ligand HEC E 602



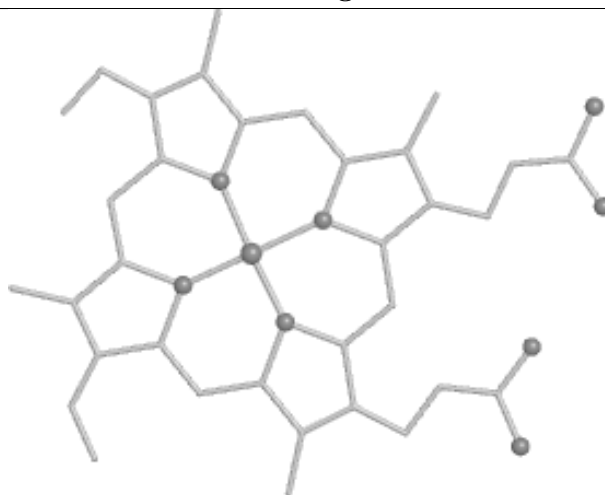
Bond lengths



Bond angles

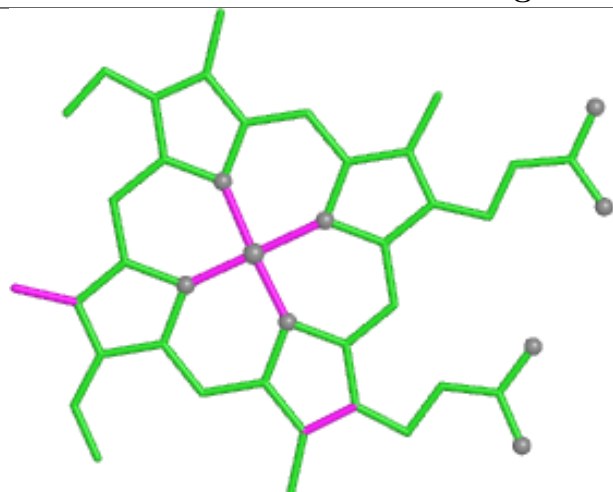


Torsions

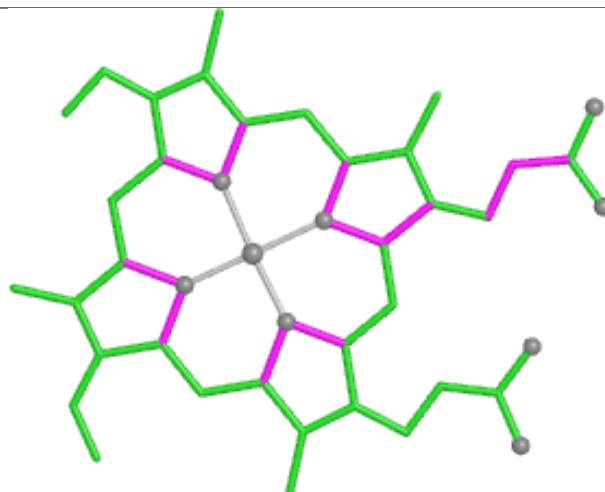


Rings

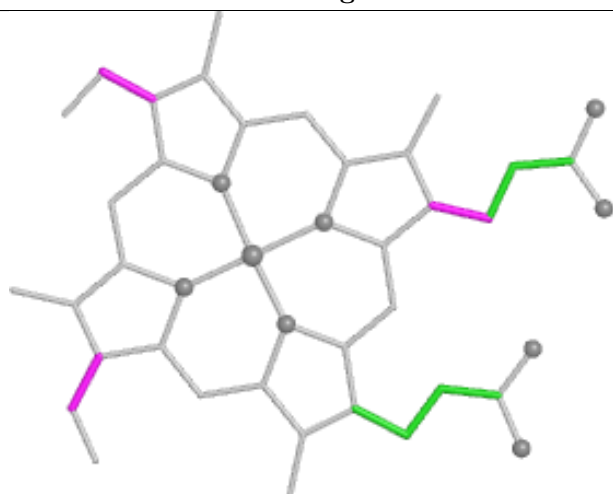
Ligand HEC E 607



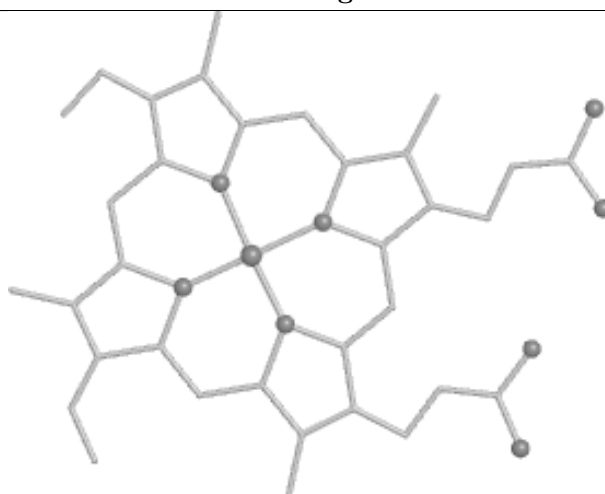
Bond lengths



Bond angles

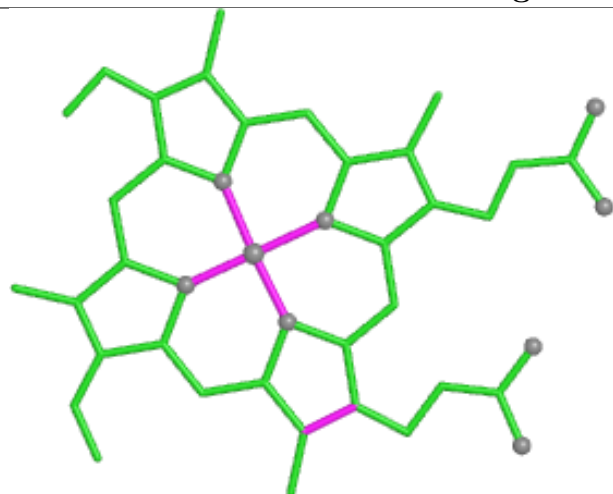


Torsions

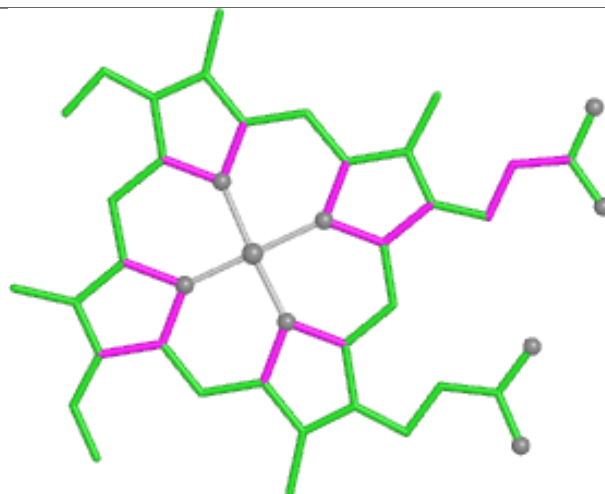


Rings

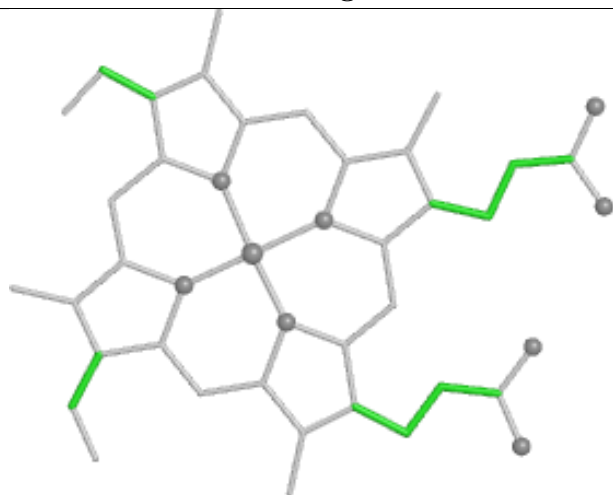
Ligand HEC C 601



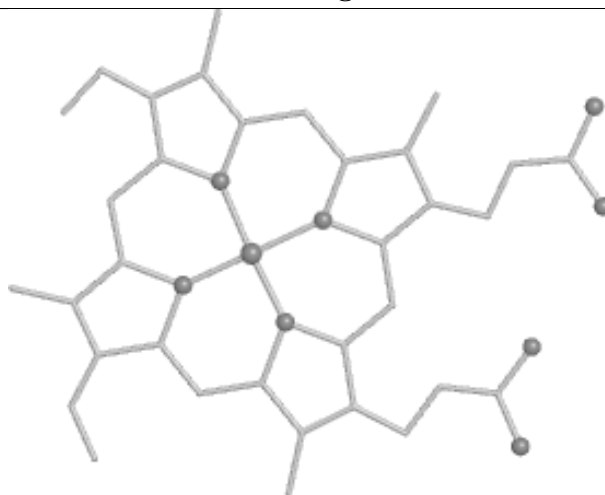
Bond lengths



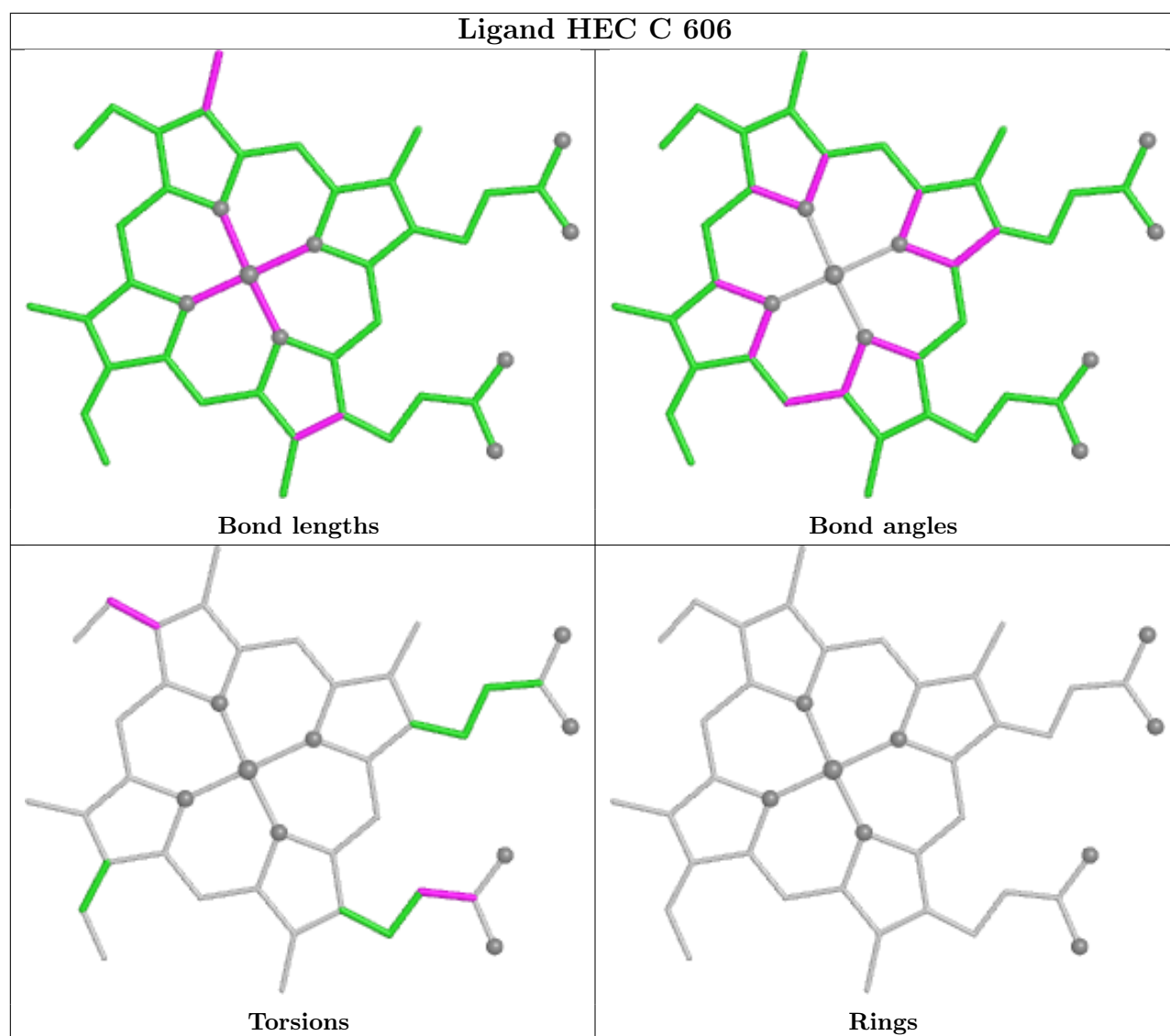
Bond angles



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	503/570 (88%)	1.19	76 (15%) 5 4	31, 60, 103, 142	0
1	C	503/570 (88%)	1.25	90 (17%) 3 3	22, 59, 103, 145	0
1	E	503/570 (88%)	1.15	83 (16%) 4 3	32, 61, 114, 171	0
2	B	56/91 (61%)	1.24	8 (14%) 6 5	48, 71, 121, 145	0
2	D	56/91 (61%)	0.87	7 (12%) 8 6	33, 48, 123, 156	0
2	F	56/91 (61%)	1.27	11 (19%) 3 2	53, 74, 133, 165	0
All	All	1677/1983 (84%)	1.19	275 (16%) 4 4	22, 61, 110, 171	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	5.7
1	C	159	GLY	5.0
1	C	158	LEU	4.9
1	A	36	ALA	4.6
1	E	170	ILE	4.5
1	C	182	ALA	4.4
2	F	70	GLY	4.3
1	A	158	LEU	4.2
1	C	304	GLY	4.0
1	E	159	GLY	4.0
1	E	181	LYS	4.0
1	E	25	ASP	3.9
1	E	109	ASP	3.9
1	E	143	GLY	3.9
2	B	84	GLY	3.9
1	C	172	CYS	3.9
1	C	187	ASP	3.9
1	A	198	THR	3.9
1	C	155	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	3.8
1	E	97	VAL	3.8
1	A	49	THR	3.8
1	C	174	VAL	3.8
1	E	324	PHE	3.7
1	C	176	VAL	3.7
1	C	179	LYS	3.7
1	C	113	VAL	3.7
1	A	125	ASN	3.7
2	D	30	LEU	3.6
1	E	120	ARG	3.6
1	E	139	TYR	3.6
1	C	263	CYS	3.6
1	A	197	GLY	3.6
1	E	118	TRP	3.6
1	C	52	ALA	3.5
2	B	43	ALA	3.5
1	C	115	VAL	3.5
1	E	318	VAL	3.5
1	C	138	LEU	3.4
1	A	310	ASN	3.4
1	E	346	THR	3.4
1	E	158	LEU	3.4
1	C	181	LYS	3.3
1	C	186	LYS	3.3
1	C	527	GLY	3.3
2	F	30	LEU	3.3
1	E	126	LEU	3.3
1	E	275	ALA	3.3
2	B	31	ALA	3.3
1	C	95	LYS	3.3
1	C	177	ASN	3.3
1	A	199	CYS	3.3
1	C	127	ASP	3.3
1	C	119	LYS	3.3
1	E	43	LYS	3.3
1	E	103	CYS	3.2
1	A	221	TRP	3.2
1	E	46	PRO	3.2
1	E	42	GLY	3.2
1	E	134	SER	3.2
1	C	234	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	TYR	3.2
1	A	177	ASN	3.2
1	A	126	LEU	3.2
1	E	344	GLU	3.2
1	E	527	GLY	3.2
1	C	167	VAL	3.2
1	C	96	GLU	3.1
1	E	484	VAL	3.1
1	A	196	CYS	3.1
1	A	108	SER	3.1
1	A	115	VAL	3.1
1	C	318	VAL	3.1
1	A	138	LEU	3.1
1	E	96	GLU	3.1
1	C	80	ILE	3.1
1	C	129	ILE	3.1
1	A	114	TRP	3.1
1	E	131	ASN	3.0
1	C	183	ASP	3.0
1	E	223	ALA	3.0
1	C	132	LEU	3.0
2	F	28	SER	3.0
1	A	345	TYR	3.0
1	E	322	ASP	3.0
1	E	331	ALA	3.0
1	C	97	VAL	3.0
1	A	323	ALA	2.9
1	C	165	LYS	2.9
1	E	325	SER	2.9
1	A	142	LYS	2.9
1	E	152	LEU	2.9
1	A	137	PRO	2.9
1	C	278	ARG	2.9
1	C	235	ASN	2.9
1	E	133	LYS	2.9
1	A	174	VAL	2.9
1	C	131	ASN	2.8
1	A	127	ASP	2.8
1	A	165	LYS	2.8
1	C	99	GLU	2.8
1	C	118	TRP	2.8
1	A	131	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	264	ASP	2.8
1	C	285	THR	2.8
1	E	41	ARG	2.8
2	F	29	SER	2.8
1	E	345	TYR	2.8
1	C	106	CYS	2.8
1	E	26	ILE	2.8
1	C	134	SER	2.8
1	E	130	ARG	2.8
1	A	27	SER	2.7
1	A	150	ASN	2.7
1	E	104	VAL	2.7
1	C	157	LYS	2.7
1	C	188	ILE	2.7
1	A	119	LYS	2.7
1	A	527	GLY	2.7
1	A	382	LEU	2.7
2	F	81	GLU	2.7
1	C	313	LYS	2.7
1	E	57	TYR	2.6
1	C	111	THR	2.6
1	E	163	THR	2.6
1	C	164	LEU	2.6
1	E	160	GLU	2.6
1	E	330	ASN	2.6
1	A	324	PHE	2.6
2	F	31	ALA	2.6
1	A	39	LEU	2.6
1	A	201	LEU	2.6
1	E	145	LEU	2.6
1	C	184	HIS	2.6
1	E	270	HIS	2.6
1	C	321	LYS	2.6
1	C	29	VAL	2.6
1	C	49	THR	2.6
1	C	336	ALA	2.6
1	A	42	GLY	2.5
1	A	215	VAL	2.5
1	C	137	PRO	2.5
1	C	124	ALA	2.5
1	A	322	ASP	2.5
1	C	180	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	178	LYS	2.5
1	E	107	HIS	2.5
1	A	341	TYR	2.5
1	A	33	THR	2.5
1	A	43	LYS	2.5
1	E	165	LYS	2.5
1	E	132	LEU	2.5
2	B	81	GLU	2.5
1	C	148	VAL	2.5
1	E	157	LYS	2.5
1	A	168	GLY	2.5
1	C	522	VAL	2.5
1	E	54	VAL	2.5
2	B	52	VAL	2.5
1	A	336	ALA	2.5
1	A	122	THR	2.4
2	F	80	ARG	2.4
2	D	28	SER	2.4
1	E	135	ASP	2.4
1	A	332	PRO	2.4
1	A	151	ASN	2.4
2	D	46	ASP	2.4
1	C	210	GLU	2.4
1	A	328	GLY	2.4
1	A	391	ARG	2.4
2	D	35	ALA	2.4
1	C	346	THR	2.4
1	E	294	ASN	2.4
1	A	162	GLU	2.4
1	C	114	TRP	2.4
1	E	101	LYS	2.4
1	E	328	GLY	2.4
1	C	104	VAL	2.4
1	C	272	PHE	2.4
1	E	140	TYR	2.4
1	E	182	ALA	2.4
1	E	392	PHE	2.4
1	A	107	HIS	2.4
2	F	61	ASN	2.4
1	C	133	LYS	2.4
1	E	283	CYS	2.4
1	A	344	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	155	MET	2.3
1	C	35	ASP	2.3
1	E	105	GLU	2.3
2	F	45	LYS	2.3
1	A	120	ARG	2.3
1	E	174	VAL	2.3
1	A	117	ALA	2.3
1	E	525	LEU	2.3
1	E	84	PRO	2.3
1	C	444	GLY	2.3
1	E	169	CYS	2.3
1	E	124	ALA	2.3
1	C	163	THR	2.3
1	C	105	GLU	2.3
1	C	151	ASN	2.3
1	C	90	PRO	2.3
1	C	109	ASP	2.3
1	A	170	ILE	2.2
1	C	199	CYS	2.2
1	A	422	TYR	2.2
1	C	102	ASP	2.2
1	E	180	ASP	2.2
2	D	83	SER	2.2
1	A	164	LEU	2.2
1	A	123	HIS	2.2
1	A	313	LYS	2.2
1	E	188	ILE	2.2
1	A	96	GLU	2.2
1	A	143	GLY	2.2
1	C	168	GLY	2.2
2	B	70	GLY	2.2
1	E	119	LYS	2.2
1	C	107	HIS	2.2
1	C	98	ALA	2.2
1	E	162	GLU	2.2
1	A	65	GLY	2.2
1	C	55	LYS	2.2
1	E	127	ASP	2.2
1	E	168	GLY	2.2
1	C	388	HIS	2.2
1	E	272	PHE	2.2
1	E	417	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	50	THR	2.2
1	E	106	CYS	2.2
1	E	313	LYS	2.2
1	E	326	LYS	2.2
1	A	525	LEU	2.2
1	C	349	ILE	2.2
1	A	169	CYS	2.1
1	C	226	PRO	2.1
1	A	133	LYS	2.1
1	E	523	ASN	2.1
1	C	136	ASP	2.1
2	D	29	SER	2.1
1	A	182	ALA	2.1
1	E	114	TRP	2.1
1	E	28	THR	2.1
1	C	30	PRO	2.1
1	A	85	ASN	2.1
1	A	40	ASP	2.1
1	E	167	VAL	2.1
1	A	202	ARG	2.1
1	C	198	THR	2.1
1	E	185	THR	2.1
2	F	82	GLN	2.1
1	E	148	VAL	2.1
2	F	46	ASP	2.1
1	A	483	HIS	2.1
1	C	242	ALA	2.0
1	A	179	LYS	2.0
2	D	32	PRO	2.0
1	E	85	ASN	2.0
1	E	184	HIS	2.0
1	E	327	GLY	2.0
1	A	509	TYR	2.0
1	C	103	CYS	2.0
1	E	81	TYR	2.0
1	C	521	ARG	2.0
2	B	74	ALA	2.0
1	A	134	SER	2.0
1	A	380	TRP	2.0
1	C	383	THR	2.0
1	C	173	HIS	2.0
1	A	367	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	480	GLY	2.0
1	A	153	ARG	2.0
1	A	311	ARG	2.0
1	C	120	ARG	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.

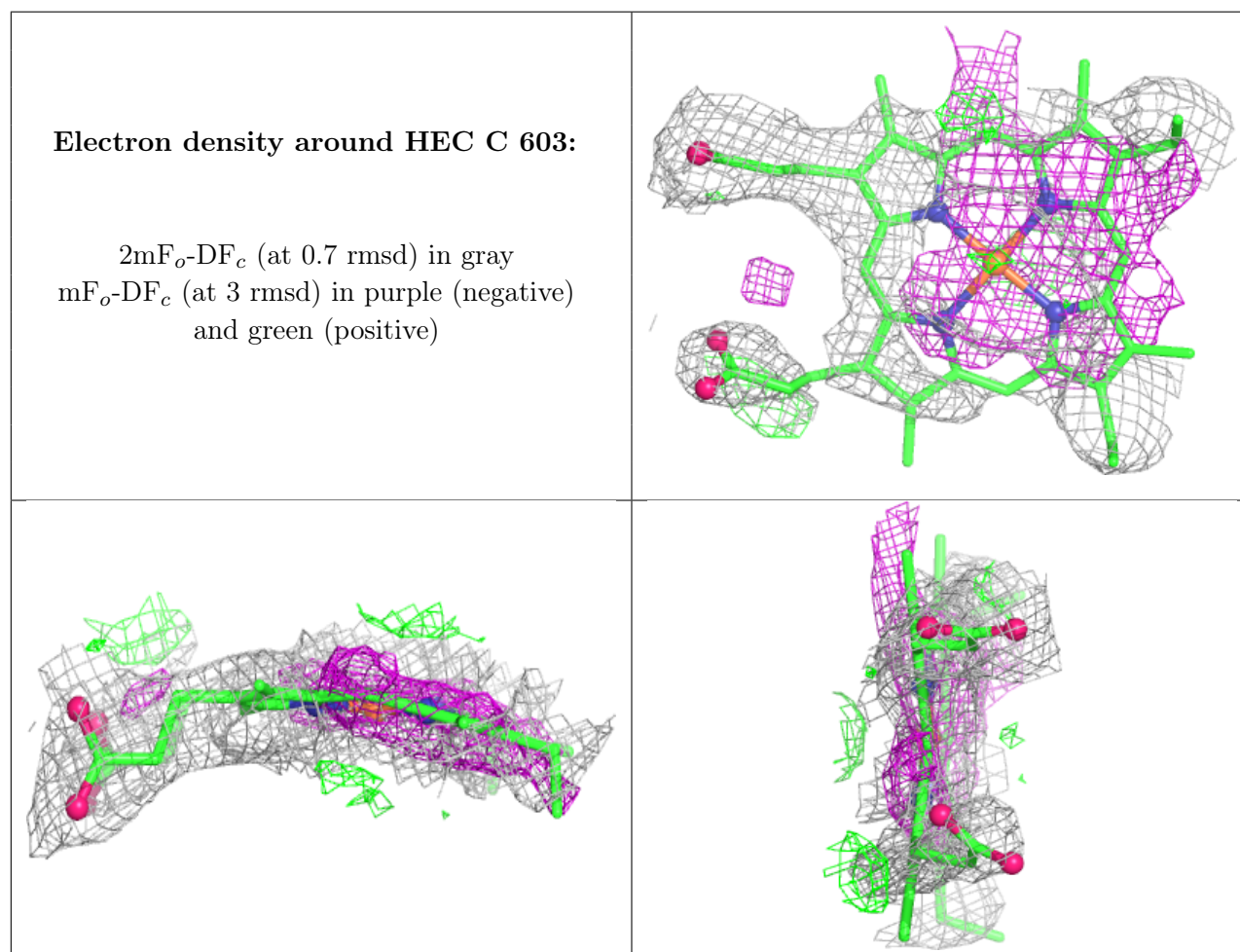
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	E	609	7/7	0.62	0.21	48,55,60,62	0
7	1PE	C	609	12/16	0.68	0.21	51,61,65,66	0
7	1PE	C	610	16/16	0.75	0.20	66,78,81,82	0
3	HEC	C	603	43/43	0.79	0.21	42,84,90,92	0
6	JUG	C	608	13/13	0.83	0.16	48,54,64,70	0
5	PEG	A	609	7/7	0.84	0.15	44,50,56,56	0
5	PEG	A	610	7/7	0.84	0.15	42,46,53,54	0
3	HEC	E	603	43/43	0.85	0.17	45,71,80,84	0
6	JUG	E	608	13/13	0.86	0.17	63,65,70,72	0
3	HEC	C	604	43/43	0.88	0.17	28,52,63,67	0
3	HEC	C	602	43/43	0.89	0.14	19,54,65,67	0
3	HEC	A	602	43/43	0.90	0.17	27,64,85,93	0
3	HEC	E	604	43/43	0.91	0.14	40,53,67,70	0
3	HEC	E	601	43/43	0.91	0.13	25,42,60,68	0
3	HEC	E	602	43/43	0.91	0.14	31,52,64,70	0
3	HEC	A	601	43/43	0.91	0.14	19,56,76,84	0
3	HEC	A	604	43/43	0.92	0.12	20,32,39,41	0
4	ISW	A	608	43/43	0.92	0.14	24,37,41,46	0
4	ISW	A	611	43/43	0.92	0.15	28,41,55,57	0

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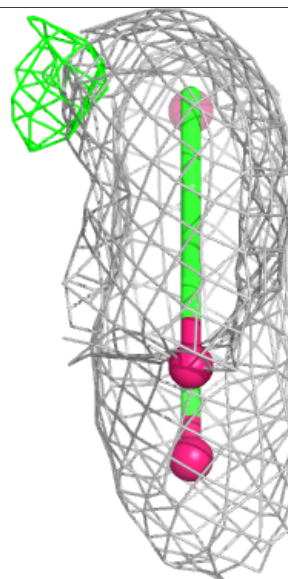
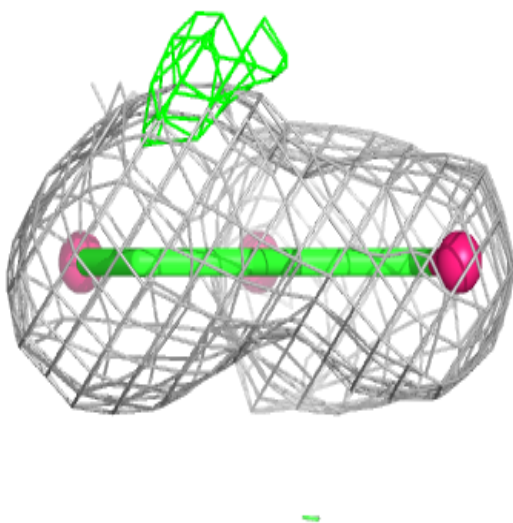
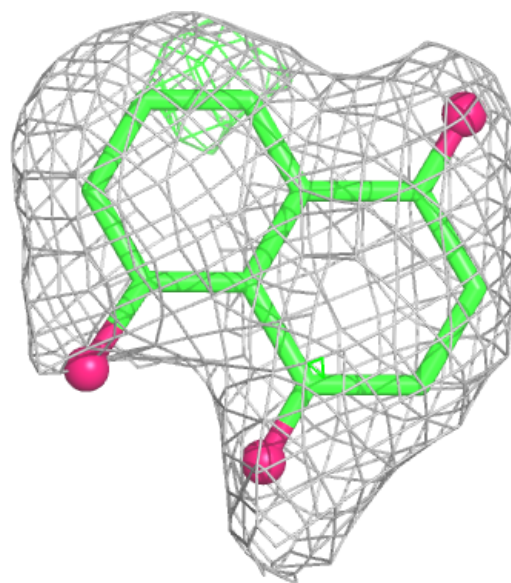
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEC	A	607	43/43	0.92	0.13	16,45,65,77	0
3	HEC	C	601	43/43	0.92	0.13	29,51,58,63	0
4	ISW	C	611	43/43	0.93	0.13	18,39,53,59	0
3	HEC	E	606	43/43	0.93	0.14	30,42,60,68	0
3	HEC	C	605	43/43	0.93	0.14	18,35,43,48	0
3	HEC	E	605	43/43	0.93	0.12	13,36,45,51	0
3	HEC	A	605	43/43	0.94	0.11	20,33,53,57	0
3	HEC	C	606	43/43	0.94	0.11	18,34,50,55	0
3	HEC	A	603	43/43	0.94	0.11	26,41,52,57	0
3	HEC	A	606	43/43	0.95	0.10	15,27,38,47	0
3	HEC	E	607	43/43	0.95	0.11	14,35,51,60	0
3	HEC	C	607	43/43	0.96	0.10	11,27,42,47	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.



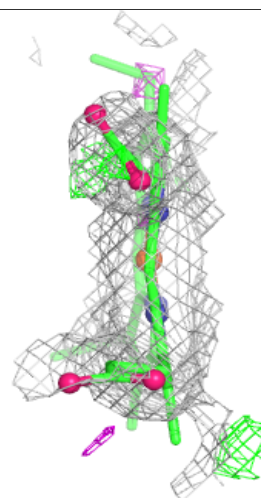
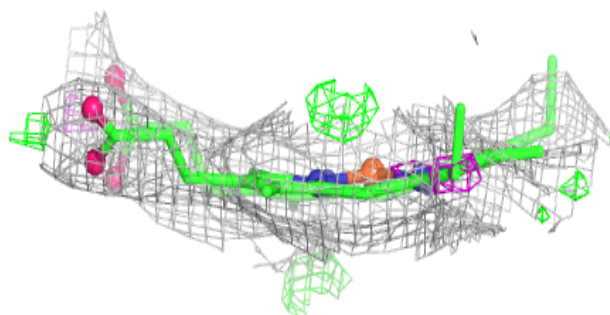
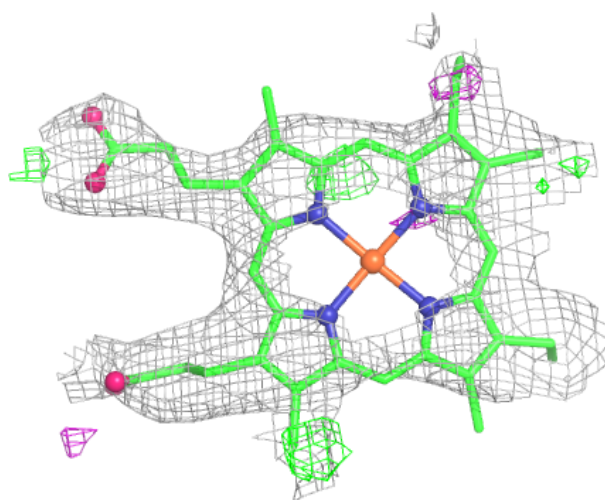
Electron density around JUG C 608:

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



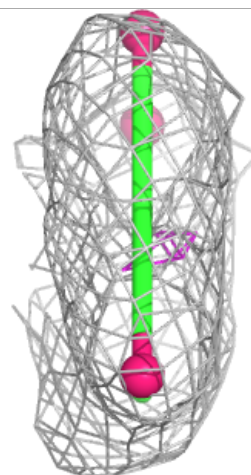
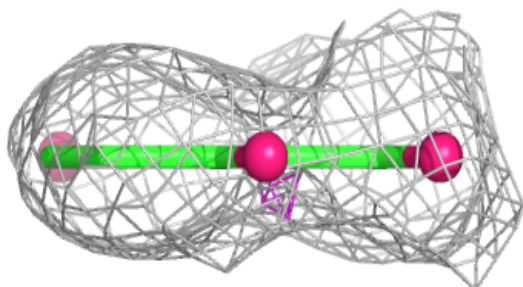
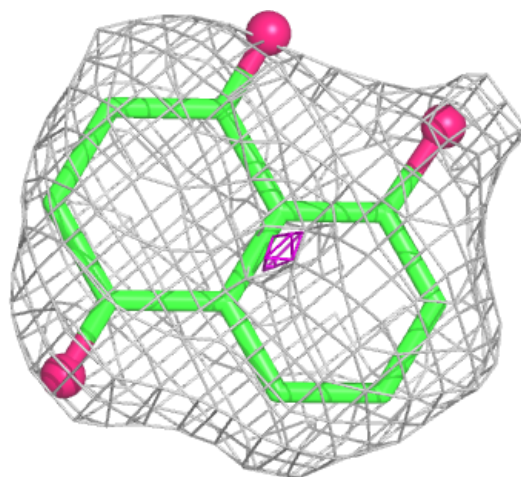
Electron density around HEC E 603:

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



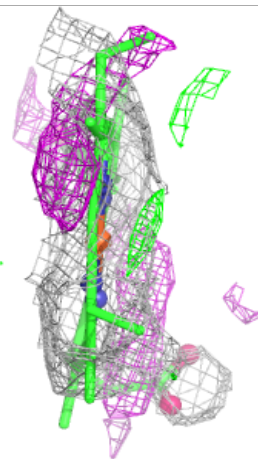
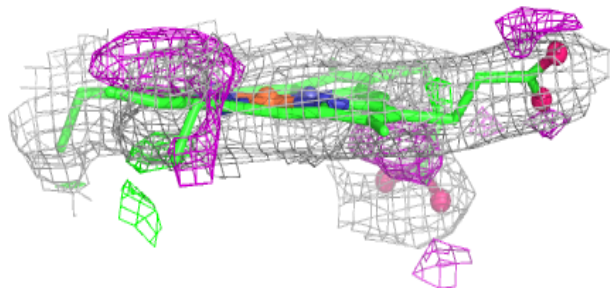
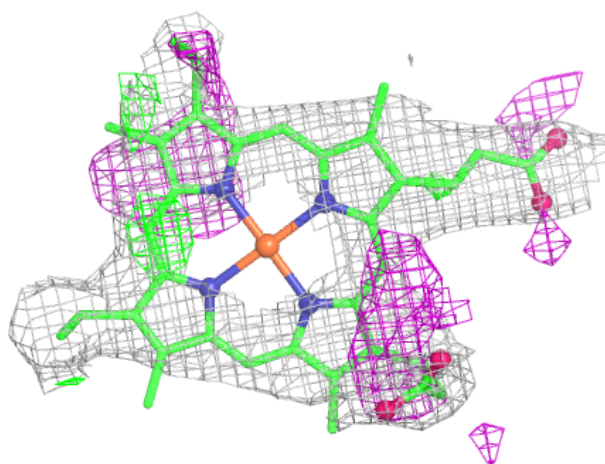
Electron density around JUG E 608:

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



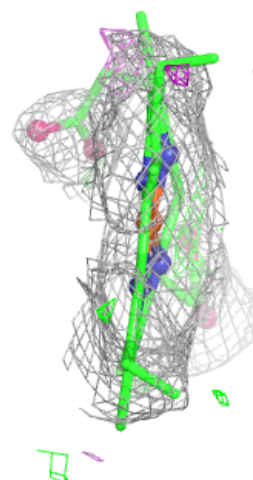
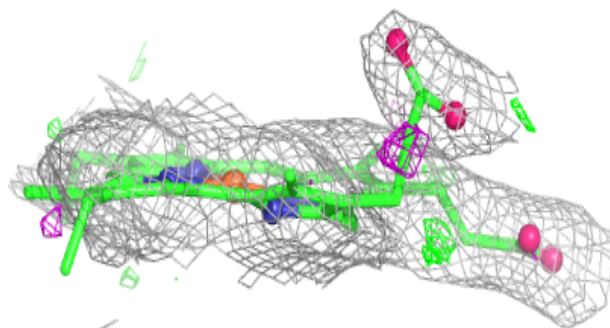
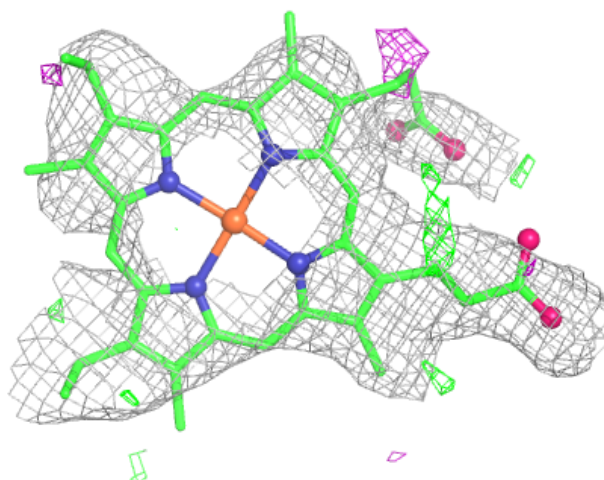
Electron density around HEC C 604:

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



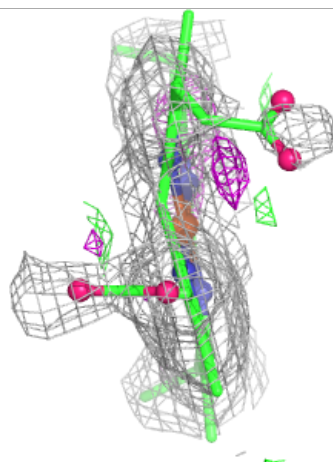
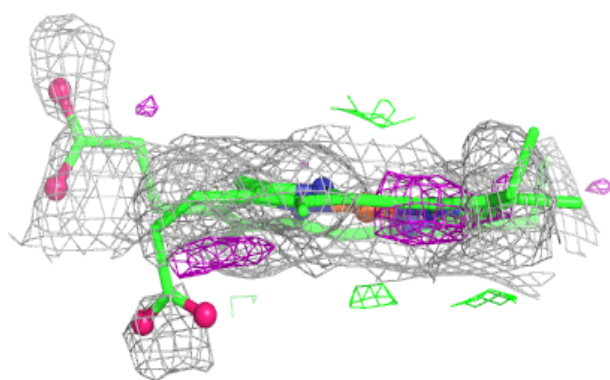
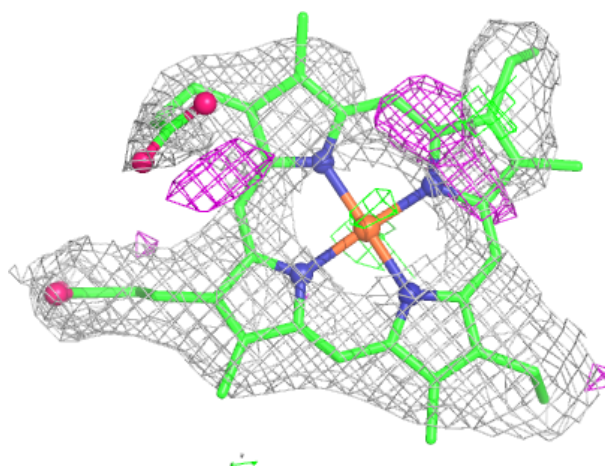
Electron density around HEC C 602:

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



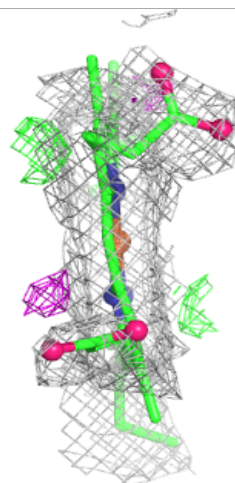
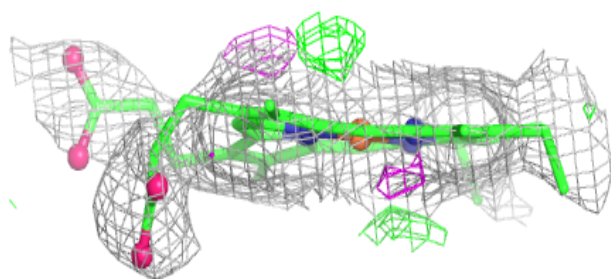
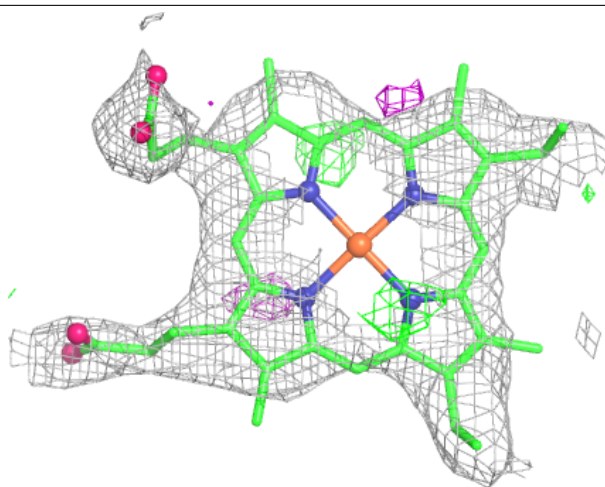
Electron density around HEC A 602:

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



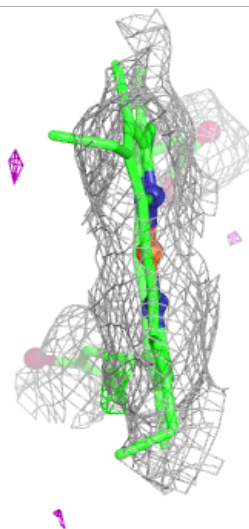
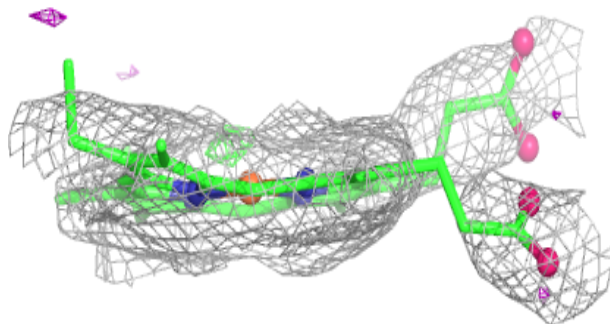
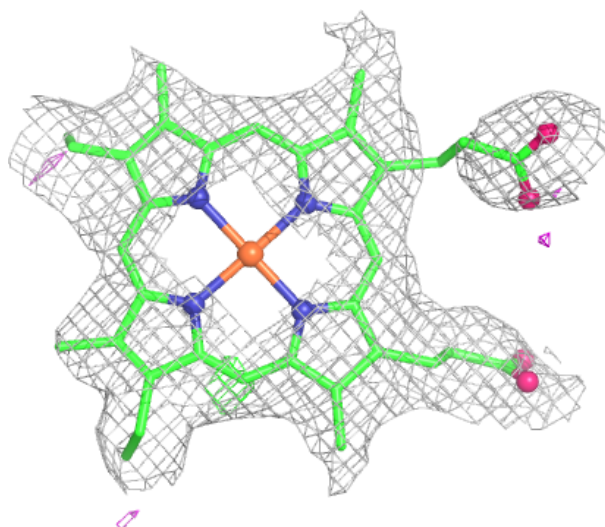
Electron density around HEC E 604:

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



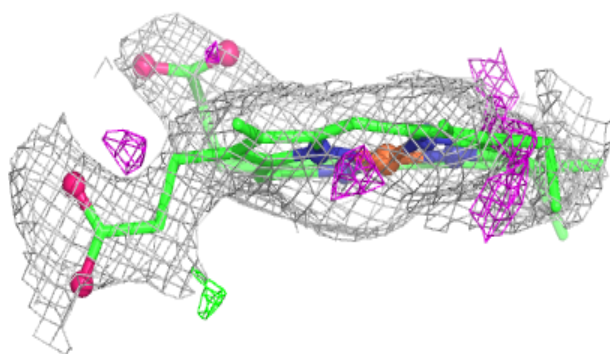
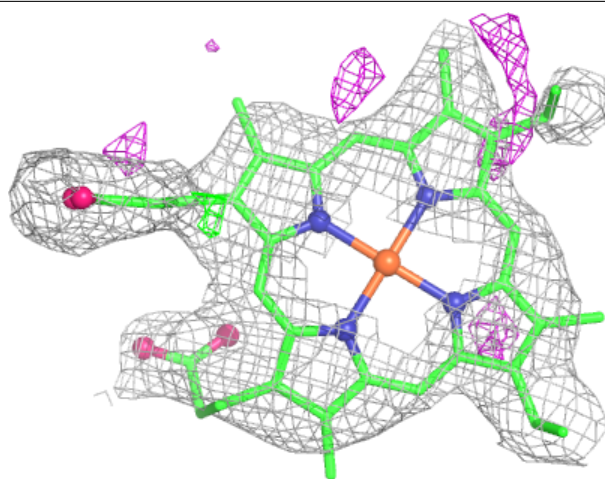
Electron density around HEC E 601:

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



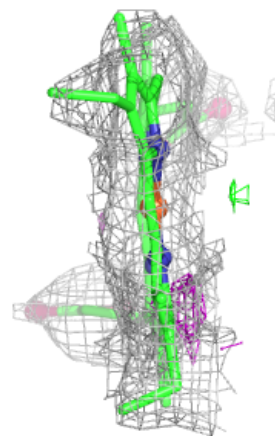
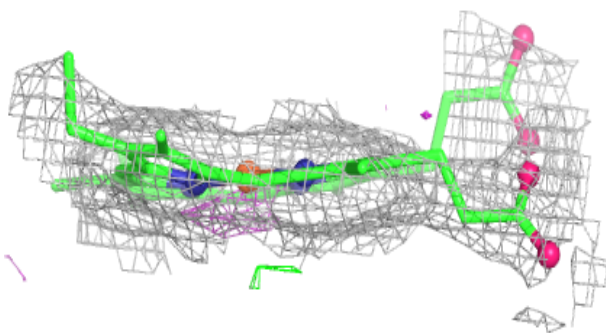
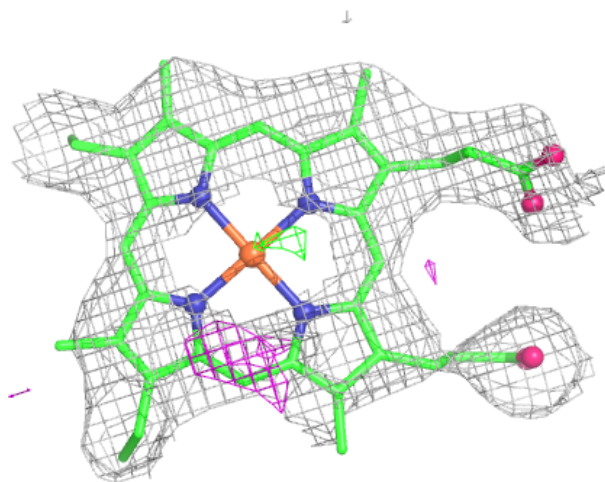
Electron density around HEC E 602:

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



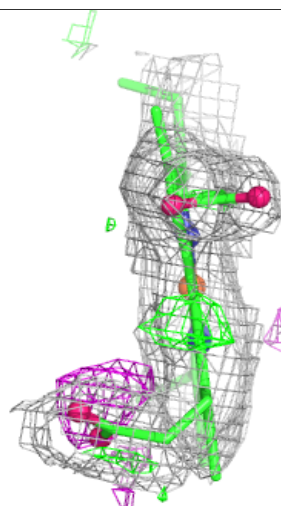
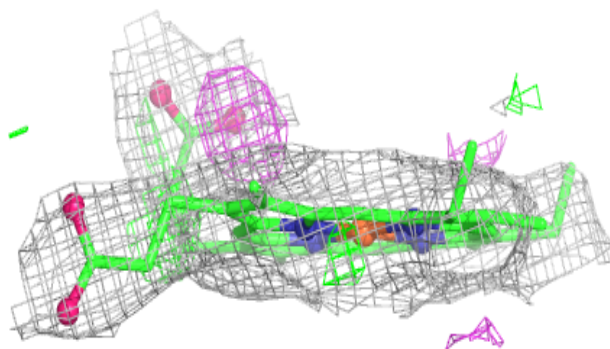
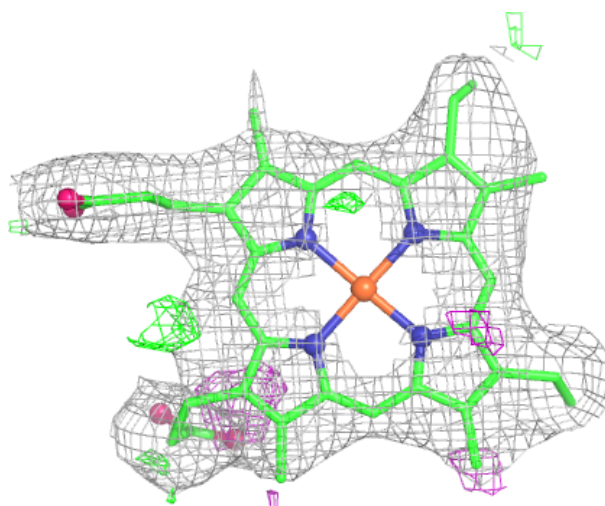
Electron density around HEC A 601:

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



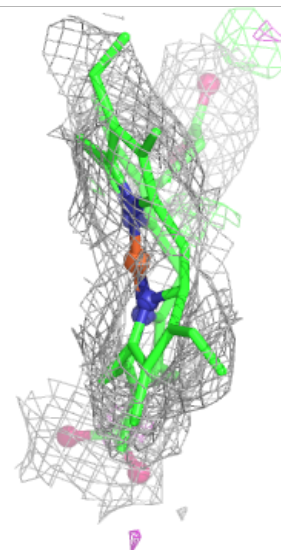
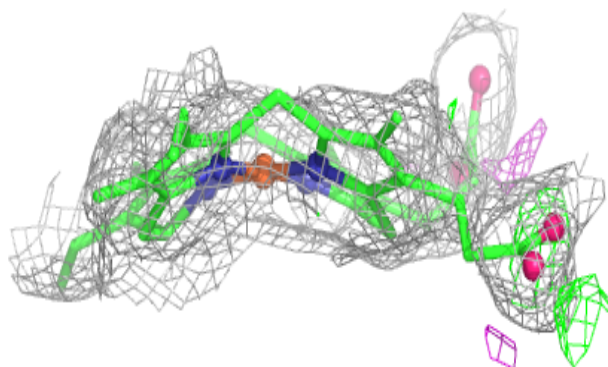
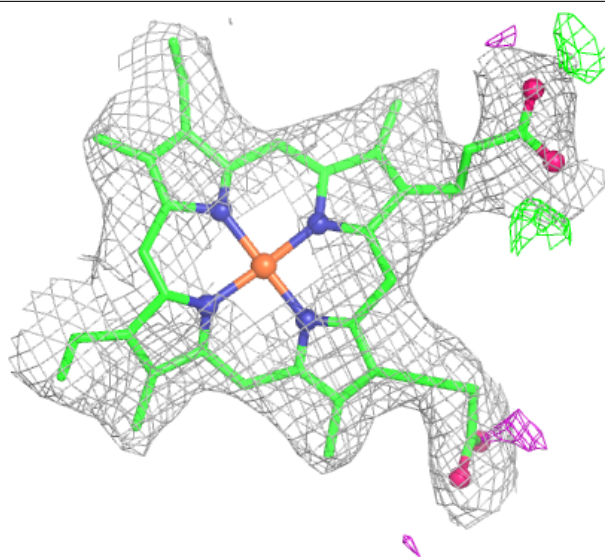
Electron density around HEC A 604:

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



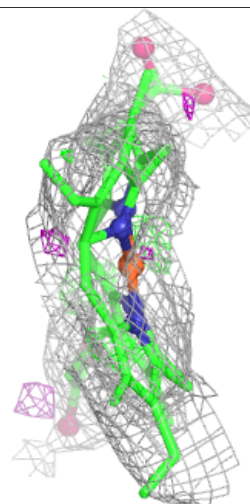
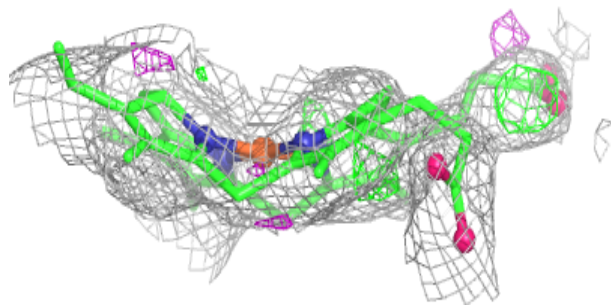
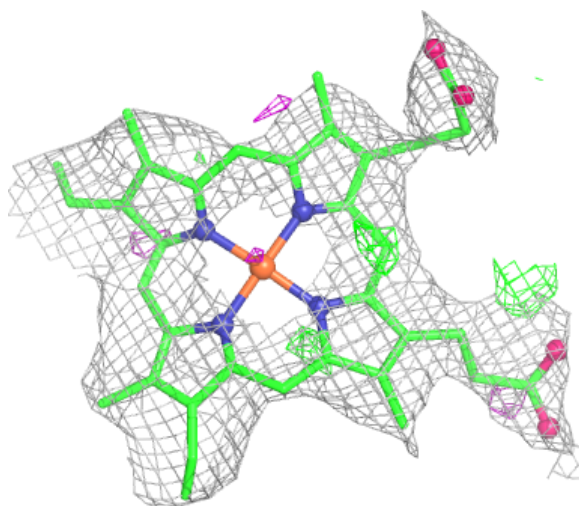
Electron density around ISW A 608:

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



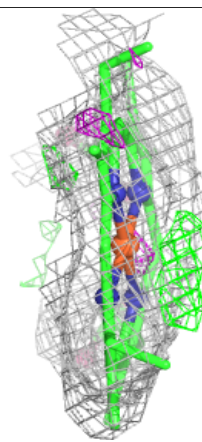
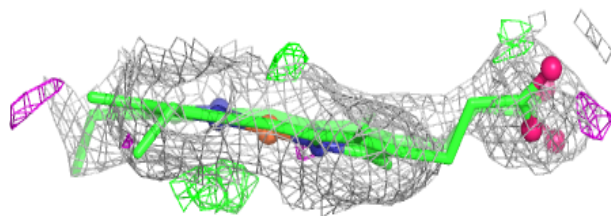
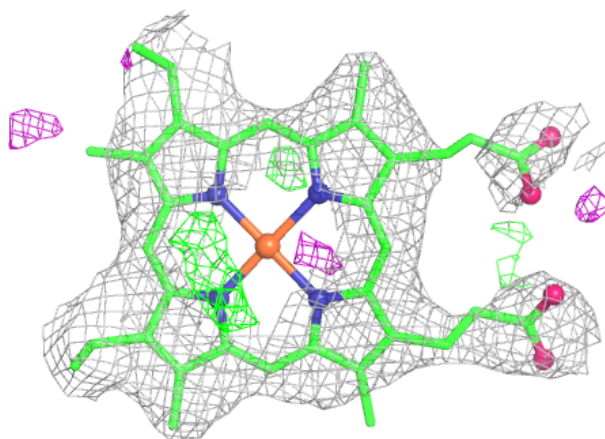
Electron density around ISW A 611:

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



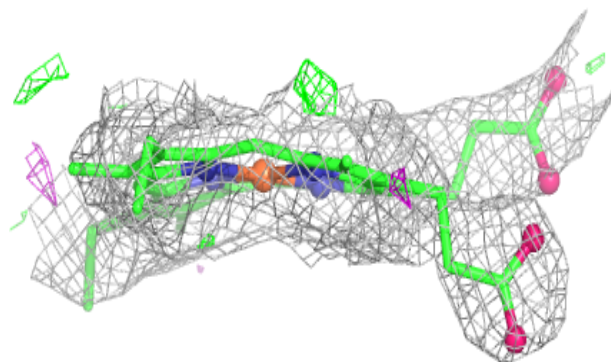
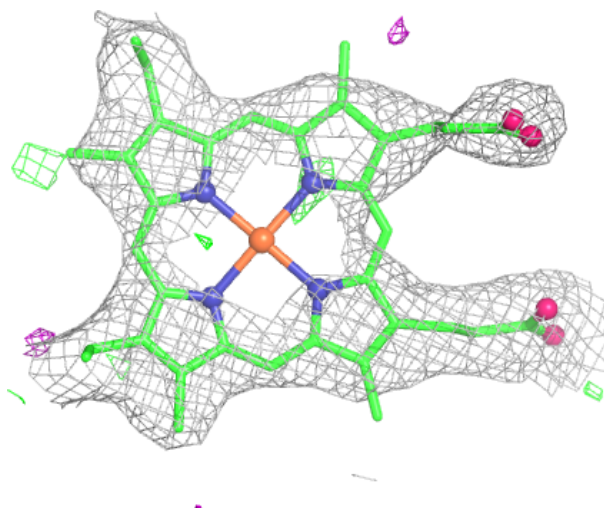
Electron density around HEC A 607:

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



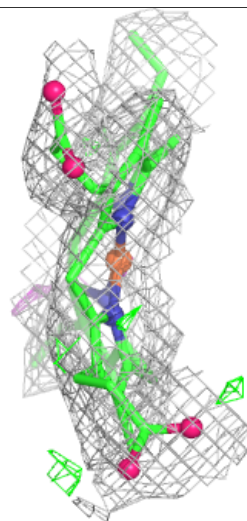
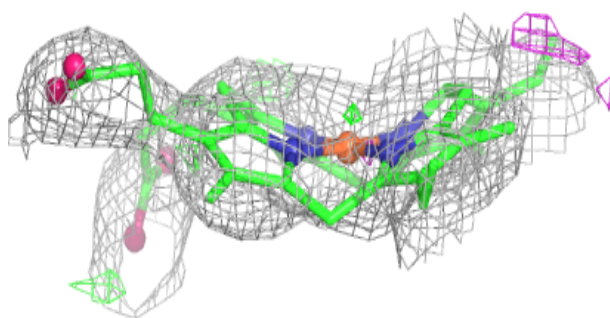
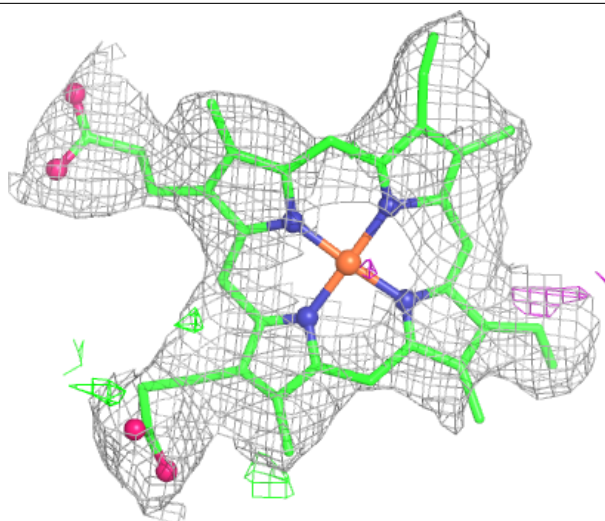
Electron density around HEC C 601:

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



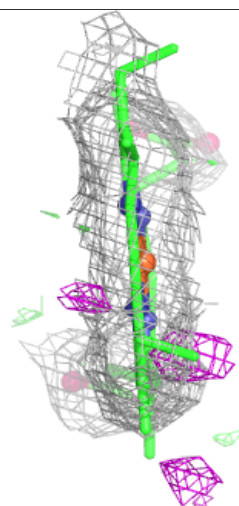
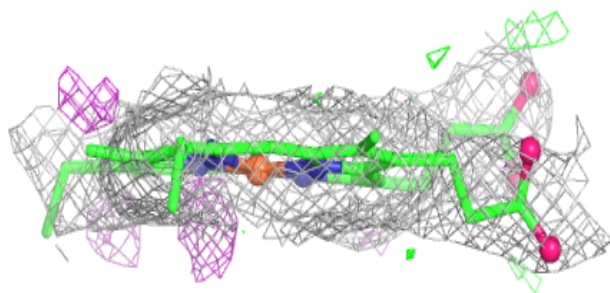
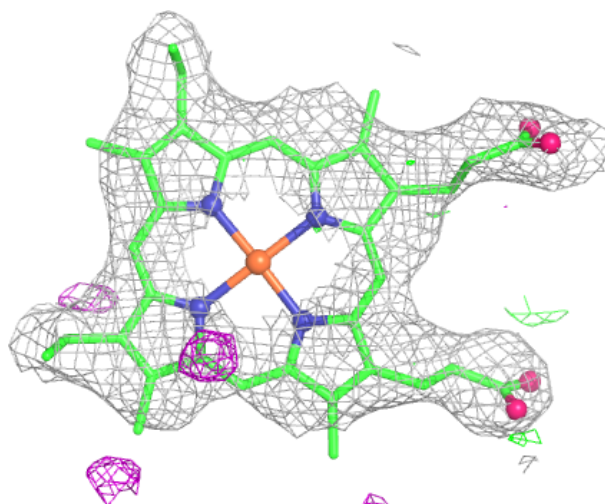
Electron density around ISW C 611:

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



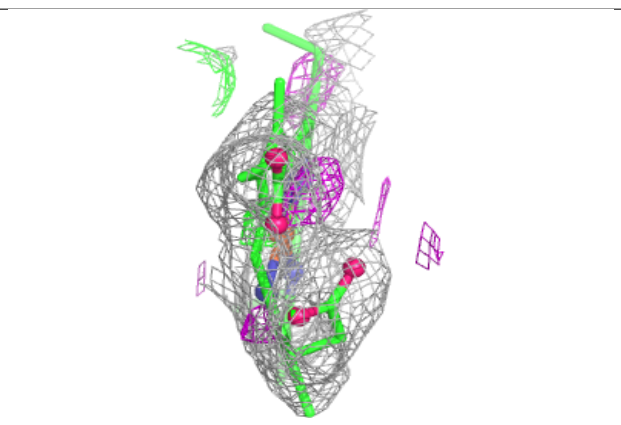
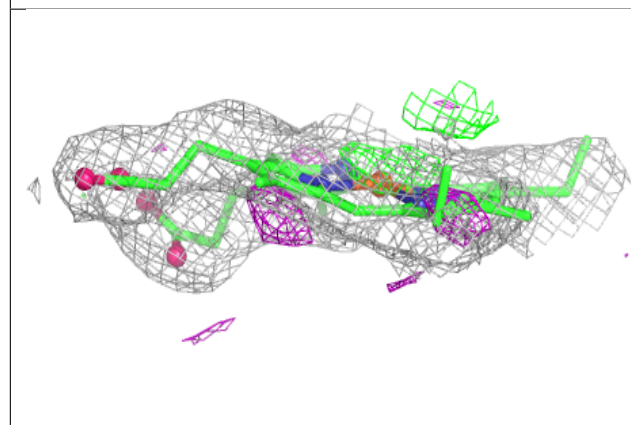
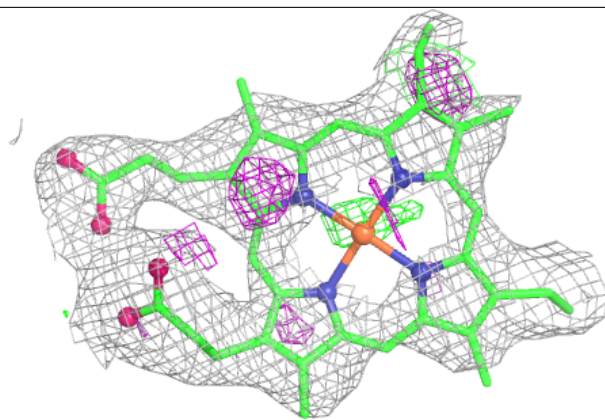
Electron density around HEC E 606:

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



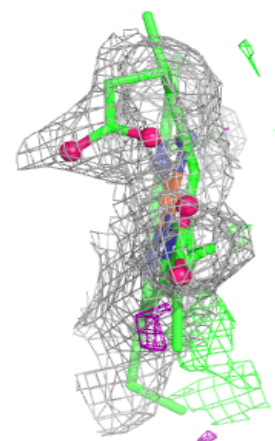
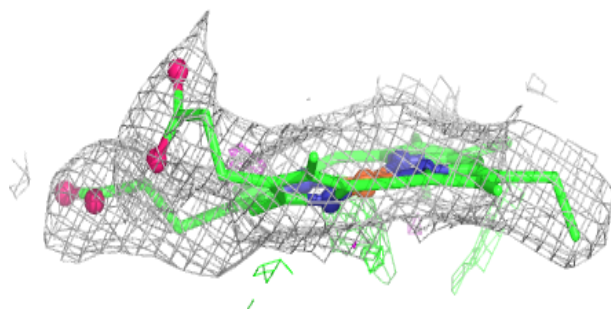
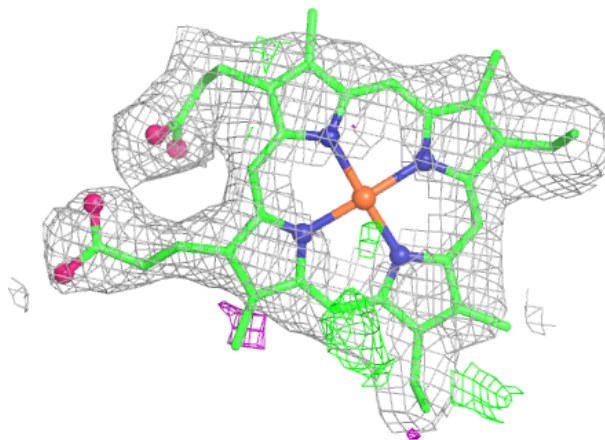
Electron density around HEC C 605:

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



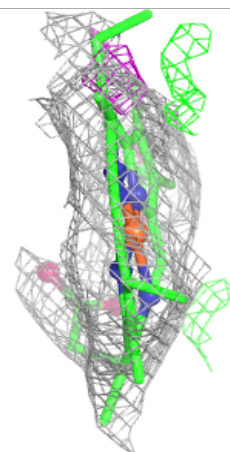
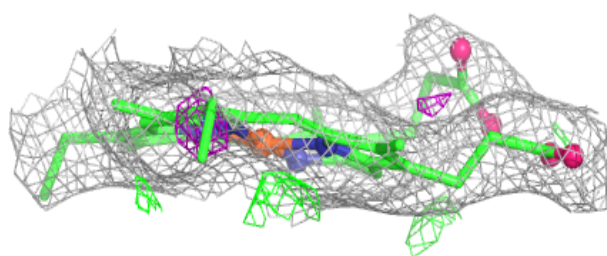
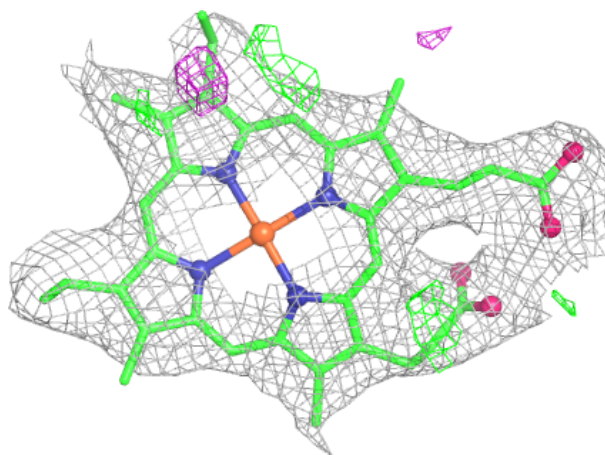
Electron density around HEC E 605:

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



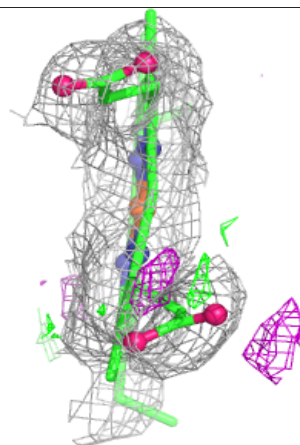
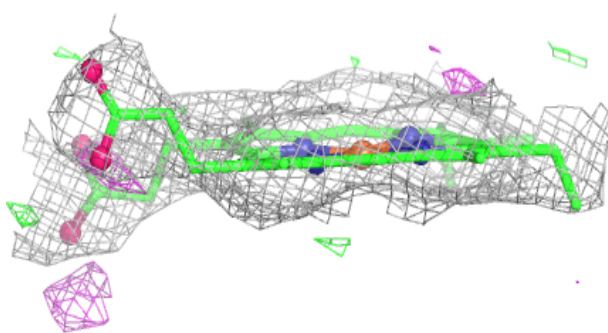
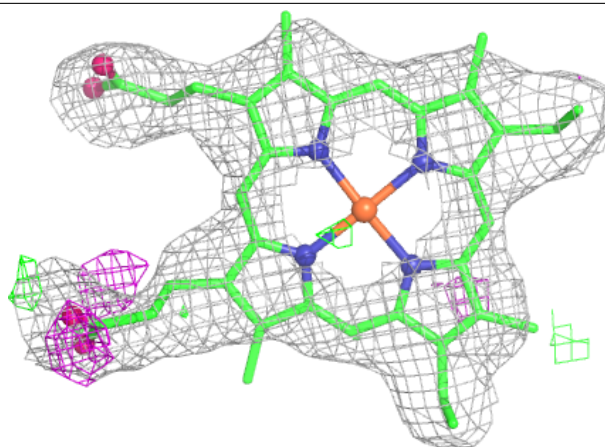
Electron density around HEC A 605:

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



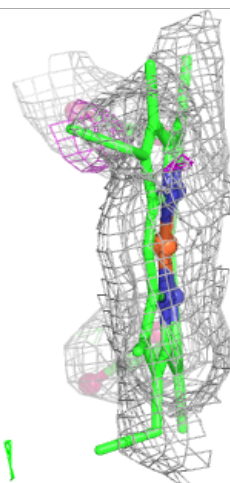
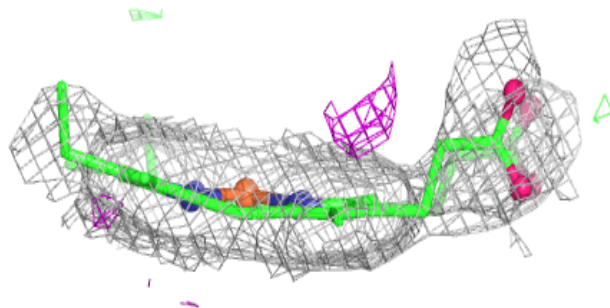
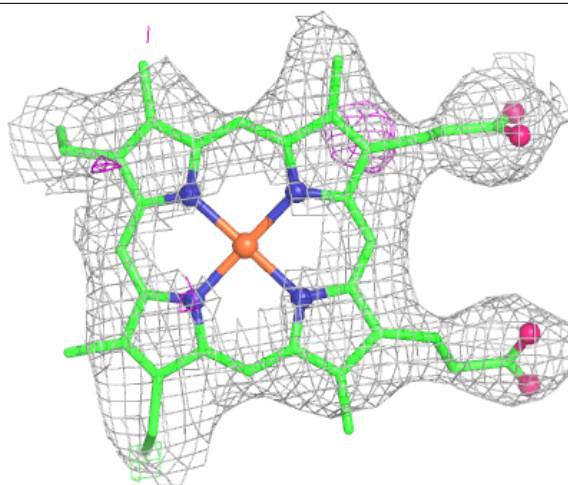
Electron density around HEC C 606:

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



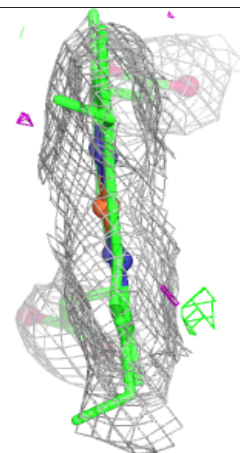
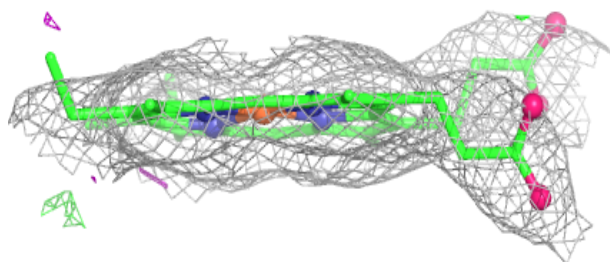
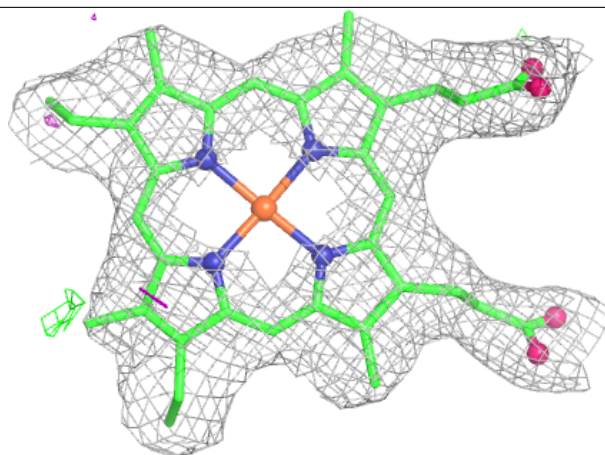
Electron density around HEC A 603:

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



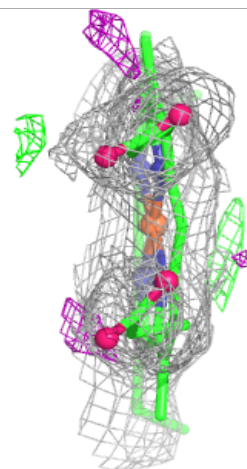
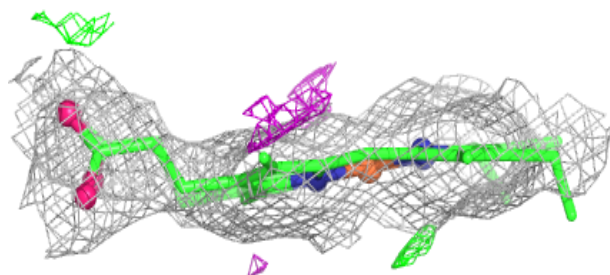
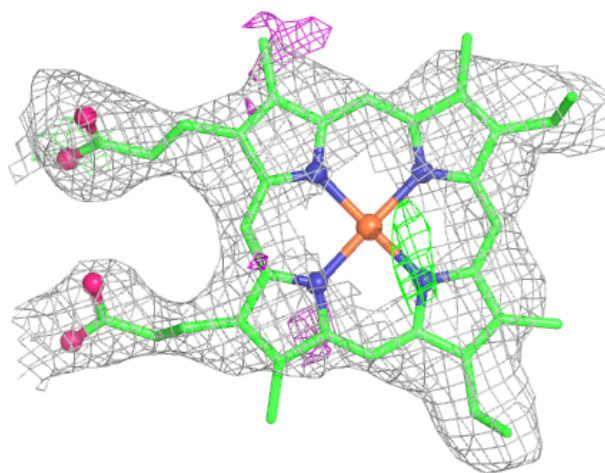
Electron density around HEC A 606:

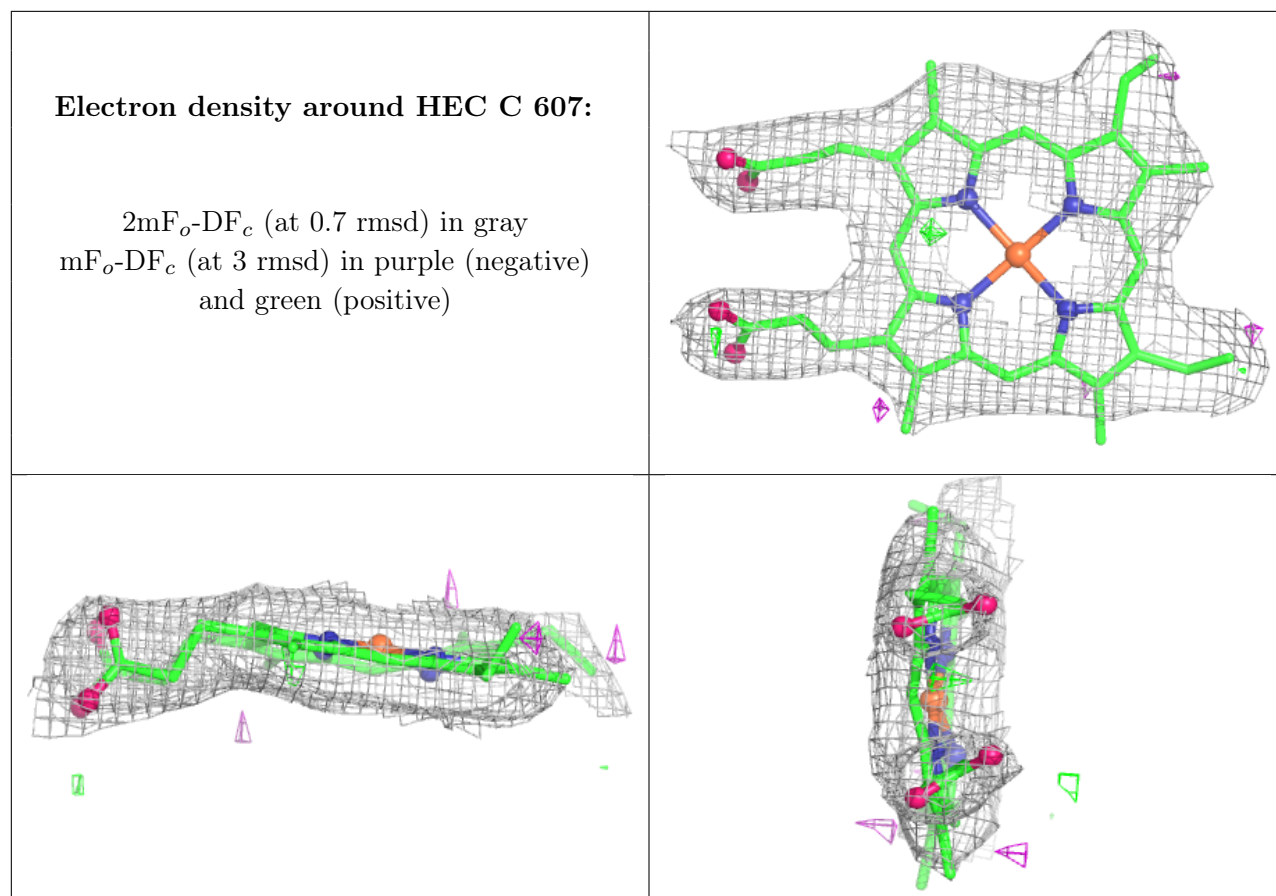
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC E 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 ⓘ

There are no such residues in this entry.