Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 09:17 PM EST

PDB ID	:	3OV0
Title	:	Structure of dodecaheme cytochrome c GSU1996
Authors	:	Pokkuluri, P.R.; Schiffer, M.
Deposited on	:	2010-09-15
Resolution	:	3.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

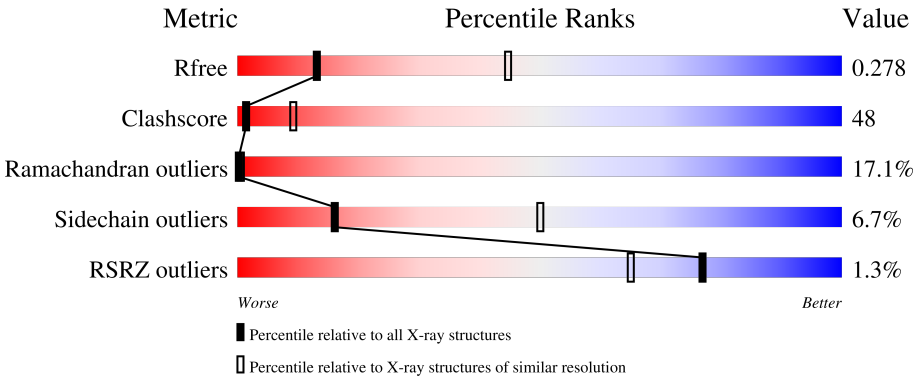
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	318	% 41% 44% 13%

2 Entry composition (i)

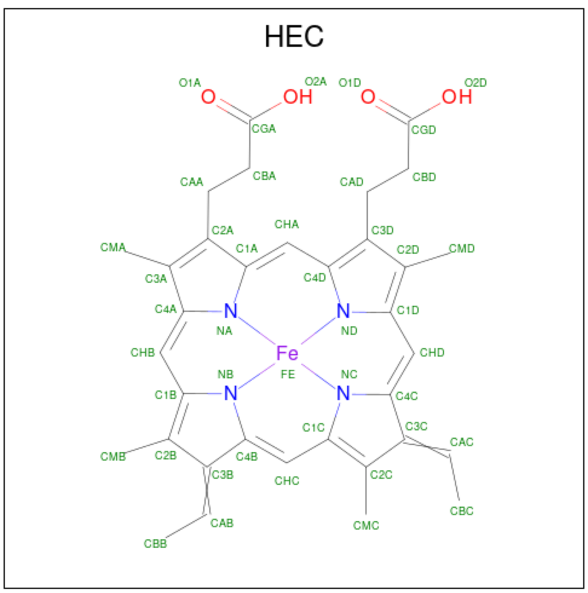
There are 3 unique types of molecules in this entry. The entry contains 2749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome c family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2224	1369	402	416	37	18	0	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

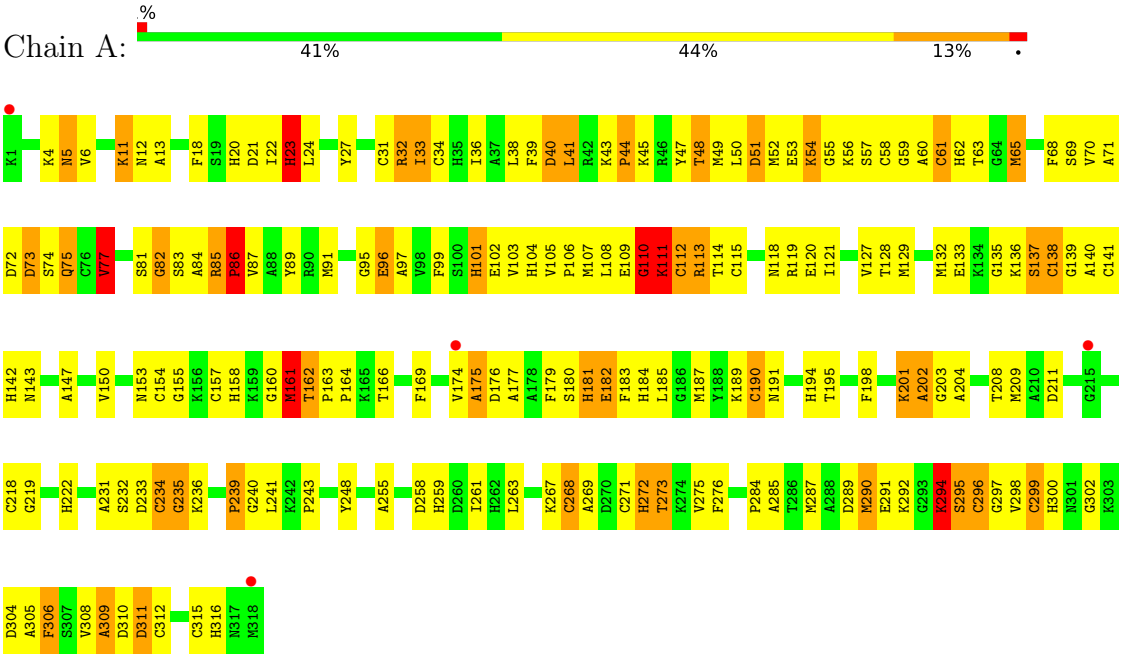
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0

3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c family protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	150.90Å 150.90Å 76.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 41.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-3.20) 96.6 (41.96-3.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.266 , 0.298 0.253 , 0.278	Depositor DCC
R_{free} test set	1751 reflections (6.53%)	wwPDB-VP
Wilson B-factor (Å^2)	94.4	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2749	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/2277	0.73	2/3083 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	GLY	N-CA-C	-5.77	98.67	113.10
1	A	111	LYS	N-CA-C	5.48	125.80	111.00

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	2224	0	1922	208	0
2	A	516	0	361	71	0
3	A	9	0	0	3	0
All	All	2749	0	2283	237	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 48.

All (237) 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:A:32:ARG:HE	1:A:36:ILE:HD11	1.16	1.08
1:A:308:VAL:HA	2:A:612:HEC:HMC2	1.36	1.08
1:A:105:VAL:HB	1:A:106:PRO:HD3	1.42	1.02
1:A:248:TYR:HB2	1:A:255:ALA:HB3	1.42	1.00
1:A:169:PHE:HB2	1:A:177:ALA:HB3	1.43	1.00
1:A:49:MET:HA	1:A:52:MET:HE3	1.46	0.97
2:A:603:HEC:O1A	2:A:603:HEC:HMA2	1.69	0.92
2:A:604:HEC:HBA1	2:A:604:HEC:O1D	1.70	0.91
1:A:32:ARG:HB3	1:A:36:ILE:HD11	1.55	0.89
1:A:294:LYS:H	1:A:294:LYS:HD2	1.41	0.86
1:A:163:PRO:HD3	2:A:607:HEC:HMB2	1.58	0.85
1:A:32:ARG:NE	1:A:36:ILE:HD11	1.92	0.84
1:A:241:LEU:HD21	2:A:609:HEC:HMB3	1.58	0.84
1:A:294:LYS:HD2	1:A:294:LYS:N	1.91	0.84
2:A:611:HEC:HBB3	2:A:611:HEC:HMB1	1.61	0.82
1:A:32:ARG:HE	1:A:36:ILE:CD1	1.93	0.82
1:A:55:GLY:O	1:A:60:ALA:HB2	1.78	0.82
1:A:73:ASP:OD1	1:A:113:ARG:HB2	1.81	0.80
1:A:137:SER:O	1:A:139:GLY:N	2.13	0.80
2:A:601:HEC:HBC3	2:A:601:HEC:HMC1	1.64	0.80
1:A:296:CYS:O	1:A:300:HIS:HB2	1.83	0.79
1:A:32:ARG:O	1:A:36:ILE:HG13	1.82	0.79
1:A:299:CYS:SG	2:A:611:HEC:HMC1	2.22	0.78
1:A:258:ASP:OD2	1:A:261:ILE:HG13	1.85	0.77
1:A:49:MET:HA	1:A:52:MET:CE	2.15	0.77
1:A:18:PHE:CG	2:A:601:HEC:HMD2	2.20	0.76
1:A:101:HIS:O	1:A:103:VAL:N	2.19	0.75
1:A:23:HIS:HD1	1:A:23:HIS:H	1.33	0.75
2:A:610:HEC:HMC1	2:A:610:HEC:HBC2	1.69	0.74
1:A:50:LEU:HD21	1:A:54:LYS:HE3	1.68	0.74
1:A:32:ARG:HB3	1:A:36:ILE:CD1	2.18	0.73
2:A:608:HEC:HMC1	2:A:608:HEC:HBC3	1.71	0.73
1:A:263:LEU:HD21	2:A:610:HEC:HHC	1.72	0.72
1:A:147:ALA:HB2	2:A:605:HEC:HMD3	1.72	0.71
2:A:602:HEC:HMB3	2:A:603:HEC:CAC	2.20	0.71
1:A:52:MET:HA	1:A:56:LYS:O	1.90	0.71
1:A:34:CYS:HA	1:A:38:LEU:HD12	1.72	0.71
2:A:604:HEC:HMC1	2:A:604:HEC:HBC3	1.71	0.71
1:A:27:TYR:HD2	1:A:33:ILE:HD12	1.55	0.70
1:A:105:VAL:CB	1:A:106:PRO:HD3	2.19	0.70
1:A:62:HIS:O	1:A:69:SER:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:O	1:A:235:GLY:N	2.25	0.70
1:A:135:GLY:O	1:A:140:ALA:HA	1.92	0.69
1:A:312:CYS:O	1:A:316:HIS:HB2	1.93	0.69
1:A:20:HIS:HE1	2:A:601:HEC:ND	1.91	0.68
1:A:308:VAL:CA	2:A:612:HEC:HMC2	2.21	0.68
1:A:187:MET:SD	2:A:608:HEC:HMD2	2.35	0.67
1:A:104:HIS:HE1	2:A:605:HEC:NA	1.93	0.67
1:A:185:LEU:C	1:A:187:MET:H	1.99	0.66
1:A:48:THR:HG23	1:A:51:ASP:OD2	1.97	0.64
1:A:50:LEU:HD21	1:A:54:LYS:CE	2.28	0.64
1:A:47:TYR:CD2	1:A:57:SER:HB2	2.33	0.64
1:A:241:LEU:CD2	2:A:609:HEC:HMB3	2.27	0.64
1:A:57:SER:OG	1:A:58:CYS:N	2.30	0.63
1:A:52:MET:O	1:A:59:GLY:HA3	1.98	0.63
1:A:84:ALA:O	1:A:85:ARG:HB2	1.97	0.63
1:A:72:ASP:O	1:A:74:SER:N	2.32	0.63
1:A:89:TYR:HB2	1:A:97:ALA:HB3	1.81	0.63
1:A:89:TYR:CD2	2:A:606:HEC:HAD1	2.35	0.62
1:A:22:ILE:HB	1:A:23:HIS:HD1	1.62	0.62
1:A:99:PHE:HB2	2:A:605:HEC:HBB3	1.82	0.61
1:A:49:MET:SD	1:A:52:MET:HE1	2.39	0.61
2:A:606:HEC:HMB1	2:A:606:HEC:CBB	2.30	0.61
1:A:89:TYR:HB2	1:A:97:ALA:O	2.00	0.61
2:A:611:HEC:HHA	2:A:611:HEC:HBA1	1.82	0.61
1:A:241:LEU:HD11	2:A:610:HEC:CMA	2.31	0.60
2:A:610:HEC:HMB1	2:A:610:HEC:HBB3	1.82	0.60
1:A:295:SER:O	1:A:297:GLY:N	2.34	0.60
1:A:49:MET:O	1:A:52:MET:HB2	2.01	0.59
1:A:155:GLY:HA3	1:A:162:THR:OG1	2.02	0.59
2:A:612:HEC:CGA	2:A:612:HEC:HMA2	2.31	0.59
1:A:48:THR:HA	2:A:603:HEC:HBA2	1.85	0.59
1:A:22:ILE:C	1:A:24:LEU:H	2.06	0.59
2:A:608:HEC:HMB1	2:A:608:HEC:HBB3	1.84	0.59
1:A:23:HIS:HD1	1:A:23:HIS:N	2.01	0.59
1:A:50:LEU:HD23	1:A:50:LEU:C	2.23	0.59
1:A:49:MET:H	2:A:603:HEC:HBA1	1.67	0.58
1:A:161:MET:O	1:A:162:THR:C	2.42	0.58
1:A:72:ASP:C	1:A:74:SER:H	2.07	0.58
2:A:606:HEC:HMB1	2:A:606:HEC:HBB3	1.86	0.58
1:A:132:MET:SD	1:A:138:CYS:HB2	2.44	0.57
1:A:181:HIS:O	1:A:182:GLU:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:610:HEC:HMC1	2:A:610:HEC:CBC	2.34	0.57
1:A:295:SER:OG	1:A:296:CYS:N	2.38	0.57
2:A:604:HEC:O1D	2:A:604:HEC:CBA	2.49	0.57
1:A:185:LEU:O	1:A:187:MET:N	2.34	0.56
1:A:135:GLY:O	1:A:140:ALA:CA	2.54	0.56
1:A:63:THR:HG22	3:A:402:HOH:O	2.06	0.56
2:A:611:HEC:HMB1	2:A:611:HEC:CBB	2.35	0.55
1:A:89:TYR:CB	1:A:97:ALA:HB3	2.36	0.55
2:A:606:HEC:CBC	2:A:606:HEC:HMC1	2.37	0.55
1:A:24:LEU:HD21	2:A:601:HEC:HBB2	1.89	0.55
1:A:89:TYR:O	1:A:96:GLU:HA	2.06	0.55
1:A:129:MET:O	1:A:133:GLU:HB2	2.06	0.55
1:A:95:GLY:O	1:A:96:GLU:C	2.45	0.55
1:A:23:HIS:N	1:A:23:HIS:ND1	2.56	0.54
2:A:606:HEC:HMA2	2:A:606:HEC:O2A	2.07	0.54
1:A:295:SER:O	1:A:298:VAL:HG23	2.07	0.54
1:A:201:LYS:O	1:A:202:ALA:HB2	2.08	0.53
1:A:231:ALA:O	2:A:609:HEC:HBB1	2.08	0.53
1:A:111:LYS:O	1:A:112:CYS:C	2.44	0.53
1:A:128:THR:O	1:A:132:MET:HB2	2.08	0.53
1:A:71:ALA:HB1	1:A:113:ARG:HH21	1.74	0.52
1:A:305:ALA:HA	2:A:611:HEC:O2D	2.09	0.52
1:A:40:ASP:O	1:A:41:LEU:CB	2.58	0.52
1:A:87:VAL:HG23	1:A:99:PHE:O	2.10	0.52
1:A:195:THR:HA	1:A:198:PHE:O	2.09	0.52
1:A:60:ALA:O	1:A:61:CYS:SG	2.67	0.52
1:A:27:TYR:N	1:A:27:TYR:CD1	2.77	0.52
1:A:22:ILE:O	1:A:24:LEU:N	2.41	0.51
1:A:52:MET:HG2	1:A:57:SER:HB3	1.92	0.51
1:A:136:LYS:O	1:A:137:SER:O	2.27	0.51
1:A:47:TYR:HD2	1:A:57:SER:HB2	1.74	0.51
1:A:141:CYS:O	1:A:143:ASN:N	2.43	0.51
1:A:20:HIS:O	1:A:24:LEU:HG	2.11	0.51
1:A:285:ALA:N	2:A:612:HEC:O1D	2.43	0.51
1:A:299:CYS:SG	2:A:611:HEC:CMC	2.98	0.51
1:A:108:LEU:CB	1:A:111:LYS:HD2	2.40	0.51
1:A:218:CYS:HB3	2:A:609:HEC:HBC2	1.93	0.51
1:A:185:LEU:C	1:A:187:MET:N	2.63	0.50
1:A:174:VAL:O	1:A:175:ALA:HB2	2.11	0.50
1:A:176:ASP:O	1:A:239:PRO:HD2	2.11	0.50
1:A:72:ASP:HB3	1:A:75:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:O	1:A:13:ALA:HB2	2.12	0.50
2:A:604:HEC:O1D	2:A:604:HEC:HHA	2.12	0.50
1:A:53:GLU:OE2	1:A:113:ARG:NH2	2.45	0.49
1:A:191:ASN:HA	1:A:194:HIS:O	2.12	0.49
1:A:71:ALA:CB	1:A:113:ARG:HH21	2.26	0.49
1:A:27:TYR:N	1:A:27:TYR:HD1	2.11	0.49
1:A:51:ASP:O	1:A:56:LYS:HB2	2.13	0.49
1:A:110:GLY:O	1:A:112:CYS:SG	2.71	0.49
1:A:118:ASN:O	1:A:120:GLU:N	2.45	0.49
2:A:603:HEC:O1A	2:A:603:HEC:CMA	2.53	0.48
2:A:612:HEC:HMC1	2:A:612:HEC:HBC3	1.95	0.48
1:A:272:HIS:O	1:A:273:THR:OG1	2.25	0.48
1:A:49:MET:SD	1:A:52:MET:CE	3.01	0.48
1:A:294:LYS:O	1:A:295:SER:O	2.32	0.48
1:A:83:SER:O	1:A:84:ALA:HB3	2.14	0.48
1:A:302:GLY:H	1:A:306:PHE:C	2.16	0.48
1:A:27:TYR:CD2	1:A:33:ILE:HD12	2.43	0.48
1:A:132:MET:CE	1:A:138:CYS:HB2	2.43	0.48
1:A:6:VAL:HG11	2:A:601:HEC:HAD1	1.95	0.48
1:A:18:PHE:CD1	2:A:601:HEC:HMD2	2.47	0.48
1:A:157:CYS:SG	2:A:606:HEC:HMC1	2.54	0.48
1:A:275:VAL:HG12	1:A:276:PHE:CD1	2.49	0.48
1:A:294:LYS:H	1:A:294:LYS:CD	2.20	0.48
1:A:306:PHE:C	1:A:306:PHE:CD1	2.87	0.48
1:A:111:LYS:HB3	1:A:114:THR:OG1	2.13	0.47
1:A:287:MET:HE1	1:A:308:VAL:HB	1.96	0.47
1:A:41:LEU:HD21	2:A:601:HEC:CMA	2.45	0.47
1:A:306:PHE:C	1:A:306:PHE:HD1	2.17	0.47
1:A:127:VAL:HG12	1:A:128:THR:N	2.29	0.47
1:A:27:TYR:HE1	2:A:602:HEC:HMD2	1.80	0.47
1:A:154:CYS:O	1:A:158:HIS:HB2	2.14	0.47
1:A:39:PHE:HA	3:A:401:HOH:O	2.15	0.47
1:A:4:LYS:O	1:A:5:ASN:O	2.33	0.47
1:A:101:HIS:O	1:A:104:HIS:N	2.24	0.47
1:A:234:CYS:C	1:A:236:LYS:H	2.18	0.46
1:A:181:HIS:O	1:A:184:HIS:N	2.49	0.46
1:A:289:ASP:O	1:A:292:LYS:N	2.48	0.46
1:A:84:ALA:O	1:A:85:ARG:CB	2.62	0.46
1:A:232:SER:O	1:A:233:ASP:HB2	2.16	0.46
1:A:36:ILE:HG22	1:A:36:ILE:O	2.16	0.46
1:A:52:MET:C	1:A:59:GLY:HA3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HB2	2:A:605:HEC:HMB2	1.98	0.45
1:A:73:ASP:HB2	1:A:113:ARG:HD2	1.98	0.45
1:A:77:VAL:O	1:A:77:VAL:HG23	2.16	0.45
1:A:306:PHE:HD1	1:A:306:PHE:O	1.99	0.45
1:A:183:PHE:C	1:A:183:PHE:CD2	2.89	0.45
1:A:43:LYS:O	1:A:44:PRO:O	2.34	0.45
1:A:284:PRO:HA	2:A:612:HEC:O1D	2.17	0.45
1:A:43:LYS:N	1:A:44:PRO:CD	2.80	0.45
2:A:604:HEC:HAD2	2:A:604:HEC:HMD1	1.83	0.45
1:A:267:LYS:O	1:A:269:ALA:N	2.50	0.44
1:A:89:TYR:CE2	2:A:606:HEC:HMD1	2.52	0.44
1:A:208:THR:O	1:A:211:ASP:N	2.51	0.44
1:A:27:TYR:HD2	1:A:33:ILE:CD1	2.27	0.44
1:A:209:MET:N	2:A:609:HEC:O2A	2.51	0.44
1:A:11:LYS:O	1:A:12:ASN:ND2	2.51	0.44
1:A:49:MET:HE1	1:A:70:VAL:HB	2.00	0.44
1:A:85:ARG:O	1:A:86:PRO:C	2.56	0.44
1:A:72:ASP:C	1:A:74:SER:N	2.70	0.44
2:A:602:HEC:HMB3	2:A:603:HEC:CBC	2.47	0.44
1:A:89:TYR:CD2	2:A:606:HEC:HMD1	2.53	0.43
1:A:52:MET:O	1:A:55:GLY:N	2.47	0.43
1:A:65:MET:HB2	3:A:408:HOH:O	2.18	0.43
1:A:105:VAL:O	1:A:107:MET:N	2.49	0.43
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.62	0.43
1:A:295:SER:C	1:A:297:GLY:N	2.69	0.43
1:A:133:GLU:HG3	1:A:150:VAL:HG12	2.01	0.43
1:A:184:HIS:HE1	2:A:608:HEC:NA	2.17	0.43
1:A:243:PRO:HD3	2:A:610:HEC:HMB2	2.00	0.43
1:A:290:MET:HG2	1:A:308:VAL:HG11	2.00	0.43
2:A:606:HEC:HAD1	2:A:606:HEC:HMD1	1.72	0.43
1:A:105:VAL:CB	1:A:106:PRO:CD	2.93	0.43
1:A:240:GLY:O	1:A:241:LEU:C	2.57	0.43
1:A:22:ILE:C	1:A:24:LEU:N	2.72	0.43
1:A:45:LYS:HE2	1:A:45:LYS:HB3	1.91	0.43
1:A:219:GLY:HA2	1:A:222:HIS:O	2.18	0.43
1:A:234:CYS:O	1:A:236:LYS:N	2.51	0.43
1:A:50:LEU:O	1:A:52:MET:N	2.52	0.43
1:A:231:ALA:O	2:A:609:HEC:CBB	2.67	0.43
1:A:299:CYS:O	1:A:304:ASP:HB2	2.19	0.43
1:A:287:MET:HE2	1:A:287:MET:HB3	1.83	0.43
1:A:32:ARG:CB	1:A:36:ILE:HD11	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:CYS:O	1:A:33:ILE:N	2.51	0.43
1:A:115:CYS:SG	1:A:121:ILE:HD13	2.58	0.43
1:A:310:ASP:OD1	1:A:311:ASP:N	2.42	0.42
2:A:603:HEC:CBD	2:A:603:HEC:HMD1	2.49	0.42
1:A:181:HIS:HD2	1:A:185:LEU:HD21	1.84	0.42
1:A:99:PHE:HB2	2:A:605:HEC:CMB	2.49	0.42
1:A:295:SER:C	1:A:297:GLY:H	2.23	0.42
1:A:189:LYS:O	1:A:190:CYS:C	2.57	0.42
1:A:289:ASP:C	1:A:291:GLU:N	2.72	0.42
1:A:267:LYS:O	1:A:268:CYS:C	2.58	0.42
1:A:50:LEU:HD23	1:A:51:ASP:N	2.34	0.41
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.90	0.41
1:A:48:THR:HB	2:A:603:HEC:O2A	2.20	0.41
1:A:99:PHE:CB	2:A:605:HEC:HBB3	2.49	0.41
1:A:50:LEU:C	1:A:52:MET:N	2.73	0.41
1:A:308:VAL:HG23	1:A:309:ALA:N	2.35	0.41
1:A:127:VAL:N	2:A:606:HEC:O2D	2.53	0.41
2:A:608:HEC:HMB3	2:A:609:HEC:CAC	2.51	0.41
1:A:53:GLU:C	1:A:55:GLY:H	2.23	0.41
1:A:18:PHE:HE2	1:A:20:HIS:ND1	2.19	0.41
1:A:91:MET:HE1	1:A:97:ALA:H	1.86	0.41
1:A:132:MET:HA	1:A:136:LYS:O	2.20	0.41
1:A:181:HIS:O	1:A:185:LEU:HG	2.21	0.41
1:A:275:VAL:HG12	1:A:276:PHE:CE1	2.56	0.41
2:A:603:HEC:HMD1	2:A:603:HEC:HBD1	2.03	0.41
1:A:179:PHE:CE2	2:A:607:HEC:HMD2	2.56	0.41
1:A:272:HIS:HA	1:A:276:PHE:O	2.21	0.41
2:A:605:HEC:HMB3	2:A:606:HEC:HAC	2.02	0.41
1:A:81:SER:O	1:A:82:GLY:O	2.39	0.40
1:A:289:ASP:O	1:A:291:GLU:N	2.54	0.40
1:A:138:CYS:HA	2:A:605:HEC:HHC	2.02	0.40
1:A:160:GLY:O	1:A:161:MET:C	2.59	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	316/318 (99%)	187 (59%)	75 (24%)	54 (17%)	0 0

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	33	ILE
1	A	44	PRO
1	A	68	PHE
1	A	73	ASP
1	A	82	GLY
1	A	85	ARG
1	A	102	GLU
1	A	109	GLU
1	A	111	LYS
1	A	112	CYS
1	A	137	SER
1	A	138	CYS
1	A	142	HIS
1	A	161	MET
1	A	175	ALA
1	A	201	LYS
1	A	202	ALA
1	A	204	ALA
1	A	234	CYS
1	A	239	PRO
1	A	295	SER
1	A	11	LYS
1	A	23	HIS
1	A	32	ARG
1	A	61	CYS
1	A	113	ARG
1	A	119	ARG
1	A	153	ASN
1	A	235	GLY
1	A	272	HIS
1	A	273	THR
1	A	294	LYS
1	A	296	CYS

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Mol	Chain	Res	Type
1	A	309	ALA
1	A	86	PRO
1	A	96	GLU
1	A	21	ASP
1	A	41	LEU
1	A	51	ASP
1	A	65	MET
1	A	162	THR
1	A	182	GLU
1	A	40	ASP
1	A	54	LYS
1	A	190	CYS
1	A	268	CYS
1	A	271	CYS
1	A	290	MET
1	A	101	HIS
1	A	311	ASP
1	A	110	GLY
1	A	77	VAL
1	A	203	GLY

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	209/259 (81%)	195 (93%)	14 (7%)	16 50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	48	THR
1	A	75	GLN
1	A	77	VAL
1	A	86	PRO
1	A	161	MET

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Mol	Chain	Res	Type
1	A	166	THR
1	A	180	SER
1	A	181	HIS
1	A	259	HIS
1	A	294	LYS
1	A	299	CYS
1	A	306	PHE
1	A	315	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	GLN
1	A	131	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEC	A	603	1	26,50,50	1.86	4 (15%)	18,82,82	2.07	3 (16%)
2	HEC	A	608	1	26,50,50	2.06	4 (15%)	18,82,82	2.99	9 (50%)
2	HEC	A	602	1	26,50,50	2.44	3 (11%)	18,82,82	1.72	3 (16%)
2	HEC	A	611	1	26,50,50	2.14	4 (15%)	18,82,82	2.24	5 (27%)
2	HEC	A	601	1	26,50,50	1.87	7 (26%)	18,82,82	1.71	3 (16%)
2	HEC	A	606	1	26,50,50	1.75	3 (11%)	18,82,82	1.93	7 (38%)
2	HEC	A	607	1	26,50,50	2.05	7 (26%)	18,82,82	0.97	1 (5%)
2	HEC	A	609	1	26,50,50	1.85	4 (15%)	18,82,82	0.77	0
2	HEC	A	605	1	26,50,50	1.99	7 (26%)	18,82,82	1.49	3 (16%)
2	HEC	A	610	1	26,50,50	1.62	6 (23%)	18,82,82	1.63	4 (22%)
2	HEC	A	604	1	26,50,50	2.30	4 (15%)	18,82,82	2.30	4 (22%)
2	HEC	A	612	1	26,50,50	1.48	5 (19%)	18,82,82	1.11	2 (11%)

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
2	HEC	A	603	1	-	3/6/54/54	-
2	HEC	A	608	1	-	4/6/54/54	-
2	HEC	A	602	1	-	0/6/54/54	-
2	HEC	A	611	1	-	2/6/54/54	-
2	HEC	A	601	1	-	1/6/54/54	-
2	HEC	A	606	1	-	0/6/54/54	-
2	HEC	A	607	1	-	1/6/54/54	-
2	HEC	A	609	1	-	0/6/54/54	-
2	HEC	A	605	1	-	1/6/54/54	-
2	HEC	A	610	1	-	2/6/54/54	-
2	HEC	A	604	1	-	2/6/54/54	-
2	HEC	A	612	1	-	1/6/54/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	HEC	C3B-C2B	-9.87	1.30	1.40
2	A	604	HEC	C3C-C2C	-8.39	1.32	1.40
2	A	607	HEC	C3C-C2C	-7.45	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	C3B-C2B	-6.90	1.33	1.40
2	A	609	HEC	C3B-C2B	-6.65	1.33	1.40
2	A	611	HEC	C3B-C2B	-6.63	1.33	1.40
2	A	603	HEC	C3C-C2C	-6.55	1.33	1.40
2	A	608	HEC	C3C-C2C	-6.22	1.34	1.40
2	A	611	HEC	C3C-C2C	-6.18	1.34	1.40
2	A	608	HEC	C3B-C2B	-6.02	1.34	1.40
2	A	604	HEC	C3B-C2B	-5.76	1.34	1.40
2	A	606	HEC	C3B-C2B	-5.51	1.35	1.40
2	A	602	HEC	C3C-C2C	-5.16	1.35	1.40
2	A	606	HEC	C3C-C2C	-4.95	1.35	1.40
2	A	601	HEC	C3B-C2B	-4.90	1.35	1.40
2	A	605	HEC	C3C-C2C	-4.28	1.36	1.40
2	A	603	HEC	C3B-C2B	-4.25	1.36	1.40
2	A	610	HEC	C3B-C2B	-3.91	1.36	1.40
2	A	610	HEC	C3C-C2C	-3.91	1.36	1.40
2	A	601	HEC	C3C-C2C	-3.88	1.36	1.40
2	A	607	HEC	C4D-ND	3.73	1.43	1.36
2	A	601	HEC	C3C-C4C	3.63	1.49	1.43
2	A	609	HEC	C3C-C2C	-3.61	1.37	1.40
2	A	608	HEC	C1C-CHC	-3.31	1.31	1.41
2	A	602	HEC	CAD-C3D	3.27	1.56	1.52
2	A	612	HEC	C1B-NB	3.14	1.42	1.36
2	A	607	HEC	C3B-C2B	-3.09	1.37	1.40
2	A	601	HEC	C1C-NC	3.04	1.42	1.36
2	A	610	HEC	C3B-C4B	2.95	1.48	1.43
2	A	612	HEC	C3B-C4B	2.94	1.48	1.43
2	A	612	HEC	C3B-C2B	-2.92	1.37	1.40
2	A	601	HEC	C4D-ND	2.83	1.42	1.36
2	A	604	HEC	C4D-ND	2.77	1.41	1.36
2	A	612	HEC	C3C-C2C	-2.77	1.37	1.40
2	A	610	HEC	C1D-ND	2.76	1.41	1.36
2	A	611	HEC	C3C-C4C	-2.75	1.38	1.43
2	A	608	HEC	C4D-ND	2.74	1.41	1.36
2	A	603	HEC	C1C-NC	2.65	1.41	1.36
2	A	603	HEC	C3B-C4B	2.58	1.47	1.43
2	A	601	HEC	CAD-C3D	2.48	1.55	1.52
2	A	609	HEC	C3C-C4C	2.46	1.47	1.43
2	A	607	HEC	C4A-C3A	2.42	1.48	1.42
2	A	605	HEC	C3C-C4C	2.39	1.47	1.43
2	A	607	HEC	C1D-ND	2.25	1.40	1.36
2	A	606	HEC	C1D-CHD	-2.18	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	612	HEC	C1D-ND	2.14	1.40	1.36
2	A	607	HEC	CAD-C3D	2.13	1.55	1.52
2	A	611	HEC	C1D-CHD	-2.13	1.35	1.41
2	A	610	HEC	C3C-C4C	2.12	1.46	1.43
2	A	604	HEC	CAA-C2A	2.10	1.55	1.52
2	A	609	HEC	C1B-NB	2.08	1.40	1.36
2	A	601	HEC	C1A-C2A	2.07	1.47	1.42
2	A	610	HEC	C1B-NB	2.05	1.40	1.36
2	A	605	HEC	C4D-ND	2.04	1.40	1.36
2	A	605	HEC	C1D-ND	2.04	1.40	1.36
2	A	605	HEC	CAA-C2A	2.03	1.55	1.52
2	A	605	HEC	C4A-C3A	2.03	1.47	1.42
2	A	607	HEC	C1C-NC	2.01	1.40	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	608	HEC	CBA-CAA-C2A	8.35	127.86	112.48
2	A	604	HEC	CBD-CAD-C3D	7.71	126.70	112.49
2	A	611	HEC	CBD-CAD-C3D	7.36	126.06	112.49
2	A	603	HEC	CBD-CAD-C3D	6.23	123.97	112.49
2	A	601	HEC	CBA-CAA-C2A	-5.27	102.77	112.48
2	A	608	HEC	CBD-CAD-C3D	5.25	122.17	112.49
2	A	608	HEC	C1D-C2D-C3D	4.30	109.99	107.00
2	A	605	HEC	CBA-CAA-C2A	4.08	120.00	112.48
2	A	602	HEC	CBD-CAD-C3D	3.89	119.66	112.49
2	A	602	HEC	CMB-C2B-C3B	-3.87	121.27	125.82
2	A	603	HEC	C4C-C3C-C2C	3.59	110.22	106.35
2	A	610	HEC	CBD-CAD-C3D	3.47	118.89	112.49
2	A	606	HEC	CMD-C2D-C1D	3.32	133.56	128.46
2	A	606	HEC	C1D-C2D-C3D	-3.27	104.72	107.00
2	A	608	HEC	C4C-C3C-C2C	3.20	109.80	106.35
2	A	611	HEC	C4C-C3C-C2C	3.18	109.79	106.35
2	A	606	HEC	CMB-C2B-C3B	3.15	129.53	125.82
2	A	604	HEC	C1D-C2D-C3D	3.01	109.09	107.00
2	A	610	HEC	CMD-C2D-C1D	-2.99	123.87	128.46
2	A	605	HEC	C4C-C3C-C2C	-2.92	103.20	106.35
2	A	612	HEC	CMB-C2B-C1B	-2.92	123.98	128.46
2	A	606	HEC	CMC-C2C-C3C	2.80	129.11	125.82
2	A	610	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
2	A	604	HEC	CBA-CAA-C2A	2.72	117.49	112.48
2	A	606	HEC	CMA-C3A-C2A	2.72	130.07	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	608	HEC	C4B-C3B-C2B	-2.65	103.49	106.35
2	A	602	HEC	CMB-C2B-C1B	2.57	132.41	128.46
2	A	608	HEC	CMC-C2C-C3C	2.48	128.74	125.82
2	A	607	HEC	CBD-CAD-C3D	2.47	117.05	112.49
2	A	601	HEC	CMD-C2D-C3D	-2.46	120.31	124.94
2	A	608	HEC	CAD-C3D-C2D	-2.33	120.54	127.25
2	A	612	HEC	CMC-C2C-C3C	2.22	128.43	125.82
2	A	611	HEC	CAA-C2A-C3A	-2.21	120.89	127.25
2	A	608	HEC	CMB-C2B-C3B	-2.21	123.22	125.82
2	A	610	HEC	CBA-CAA-C2A	-2.20	108.43	112.48
2	A	604	HEC	CMD-C2D-C3D	-2.13	120.92	124.94
2	A	606	HEC	CMB-C2B-C1B	-2.10	125.23	128.46
2	A	603	HEC	CMC-C2C-C3C	-2.09	123.36	125.82
2	A	611	HEC	CMC-C2C-C3C	2.06	128.25	125.82
2	A	601	HEC	CBD-CAD-C3D	2.05	116.27	112.49
2	A	611	HEC	CBA-CAA-C2A	2.05	116.25	112.48
2	A	605	HEC	CAD-C3D-C2D	-2.04	121.39	127.25
2	A	608	HEC	CMD-C2D-C1D	-2.04	125.33	128.46
2	A	606	HEC	CMC-C2C-C1C	-2.02	125.36	128.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	HEC	C2D-C3D-CAD-CBD
2	A	603	HEC	C4D-C3D-CAD-CBD
2	A	604	HEC	C1A-C2A-CAA-CBA
2	A	604	HEC	C3A-C2A-CAA-CBA
2	A	605	HEC	C3A-C2A-CAA-CBA
2	A	607	HEC	C3D-CAD-CBD-CGD
2	A	608	HEC	C1A-C2A-CAA-CBA
2	A	608	HEC	C3A-C2A-CAA-CBA
2	A	608	HEC	C2D-C3D-CAD-CBD
2	A	608	HEC	C4D-C3D-CAD-CBD
2	A	610	HEC	C2D-C3D-CAD-CBD
2	A	610	HEC	C4D-C3D-CAD-CBD
2	A	611	HEC	C1A-C2A-CAA-CBA
2	A	611	HEC	C3A-C2A-CAA-CBA
2	A	601	HEC	C4D-C3D-CAD-CBD
2	A	612	HEC	C2A-CAA-CBA-CGA
2	A	603	HEC	C2A-CAA-CBA-CGA

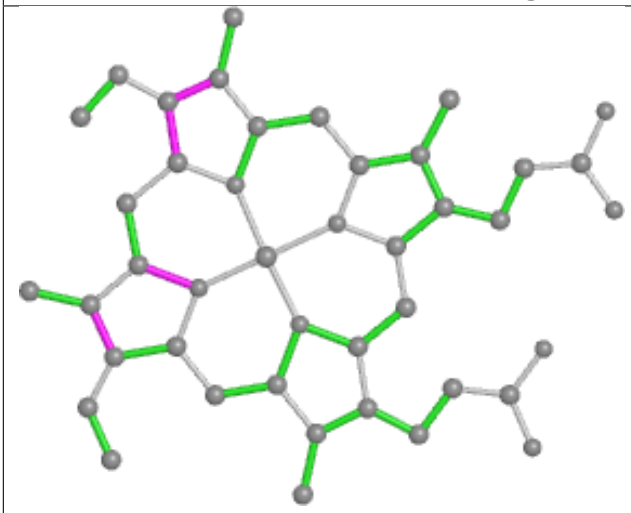
There are no ring outliers.

12 monomers are involved in 71 short contacts:

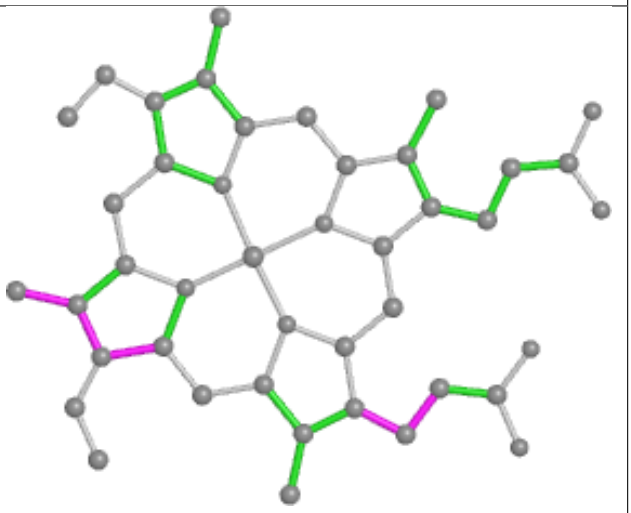
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	HEC	9	0
2	A	608	HEC	5	0
2	A	602	HEC	3	0
2	A	611	HEC	6	0
2	A	601	HEC	7	0
2	A	606	HEC	11	0
2	A	607	HEC	2	0
2	A	609	HEC	7	0
2	A	605	HEC	8	0
2	A	610	HEC	6	0
2	A	604	HEC	5	0
2	A	612	HEC	6	0

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

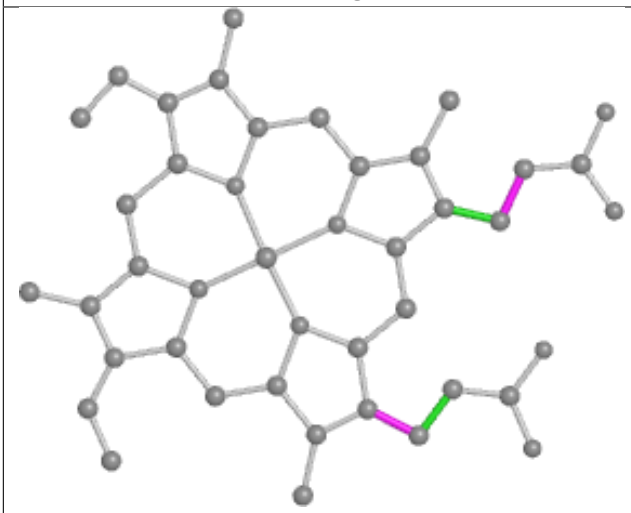
Ligand HEC A 603



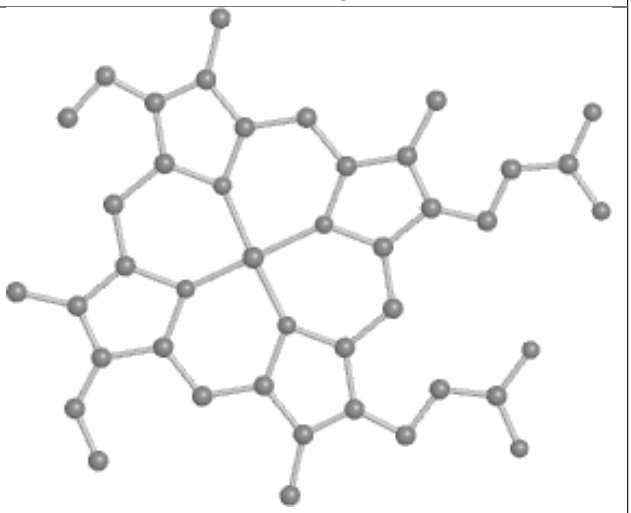
Bond lengths



Bond angles

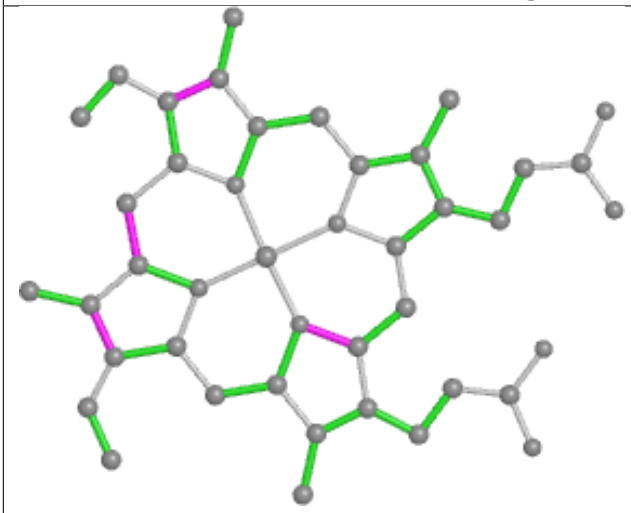


Torsions

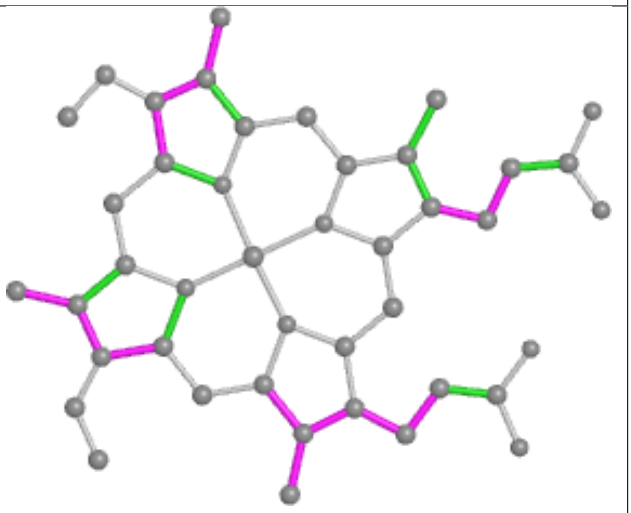


Rings

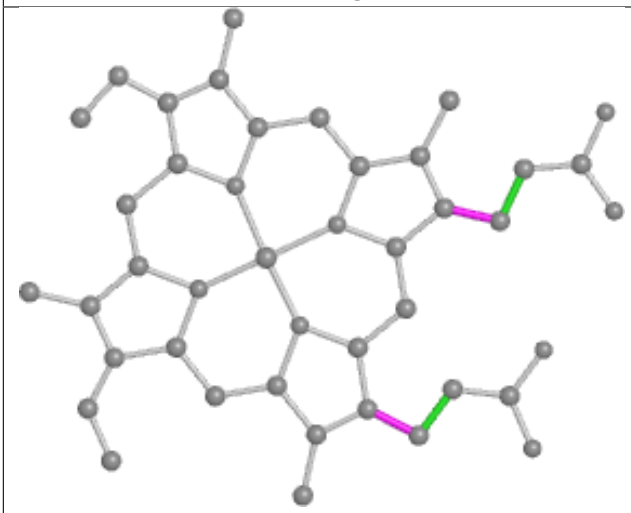
Ligand HEC A 608



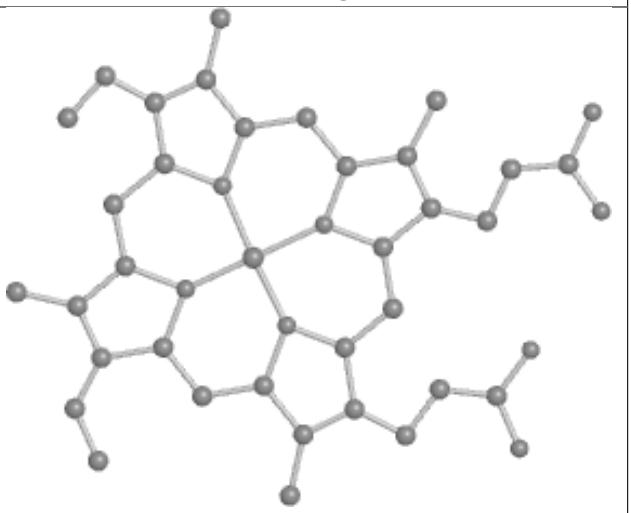
Bond lengths



Bond angles

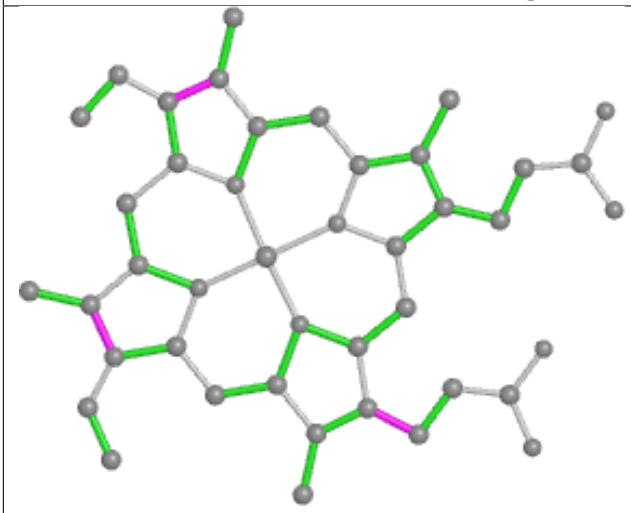


Torsions

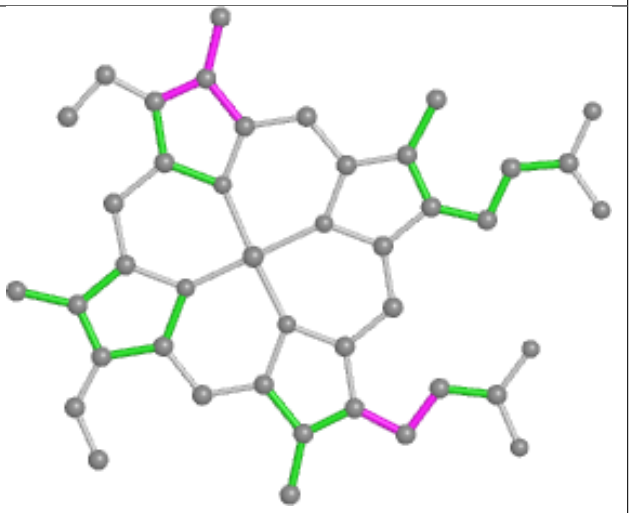


Rings

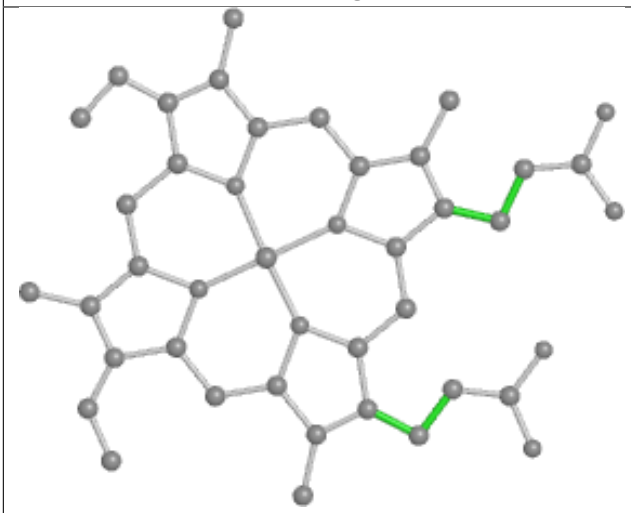
Ligand HEC A 602



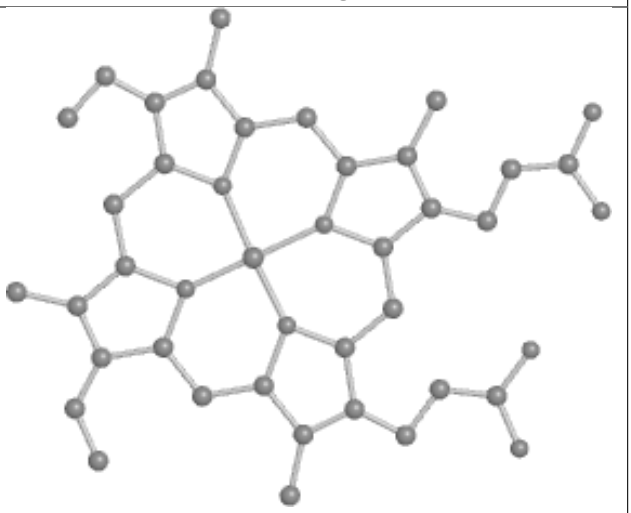
Bond lengths



Bond angles

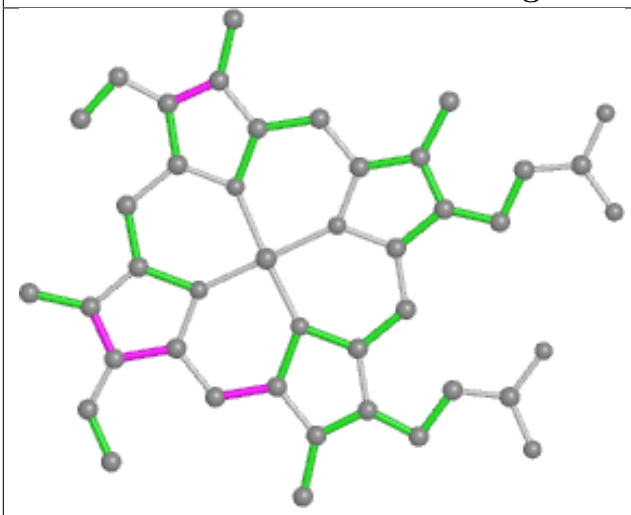


Torsions

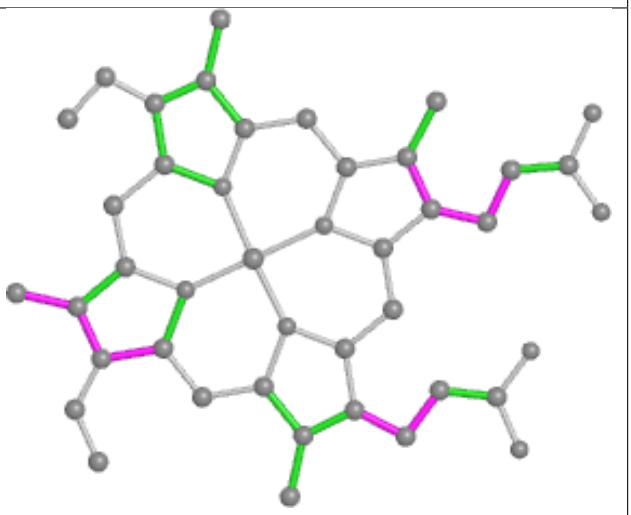


Rings

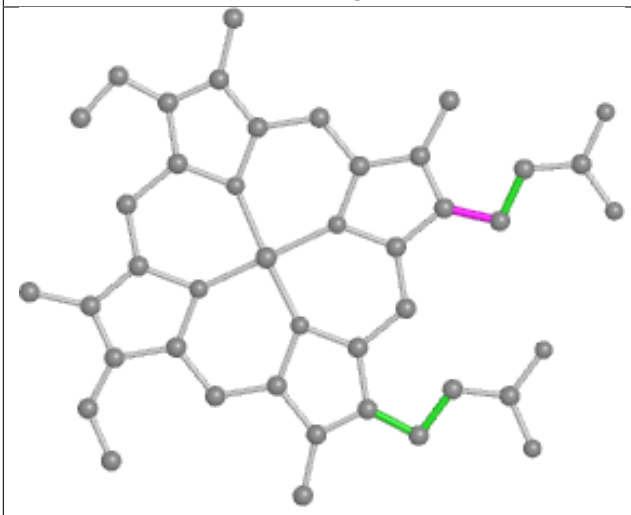
Ligand HEC A 611



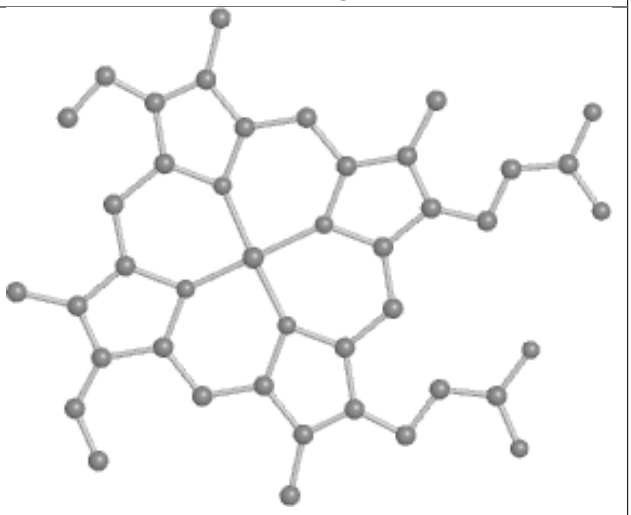
Bond lengths



Bond angles

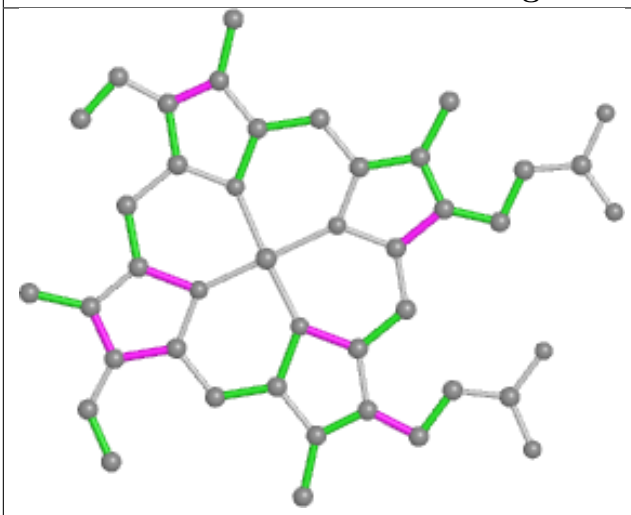


Torsions

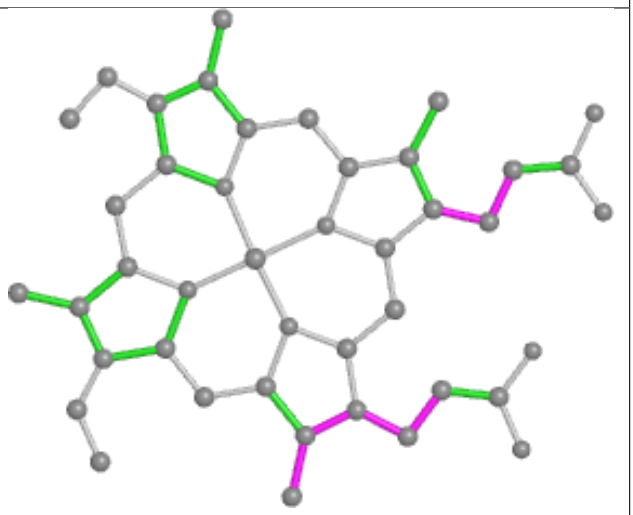


Rings

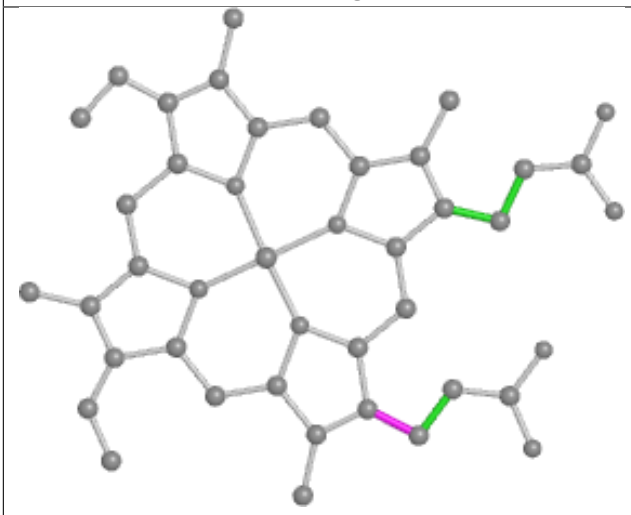
Ligand HEC A 601



Bond lengths



Bond angles



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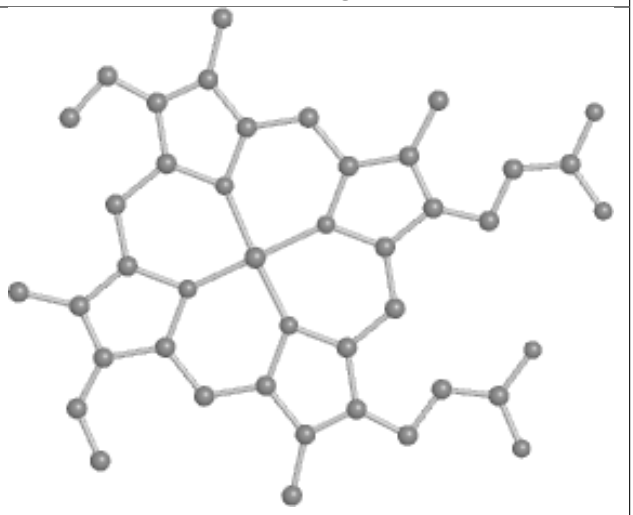
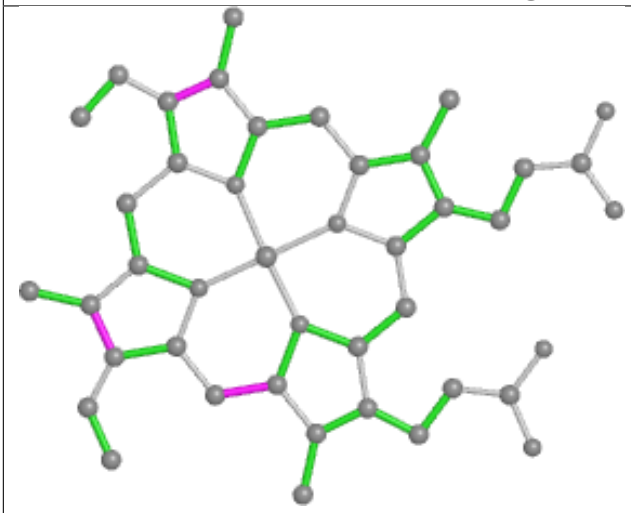


Rings

Ligand HEC A 606



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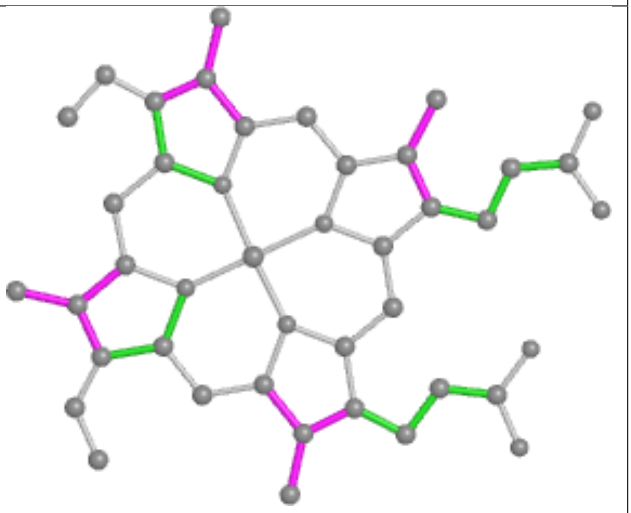
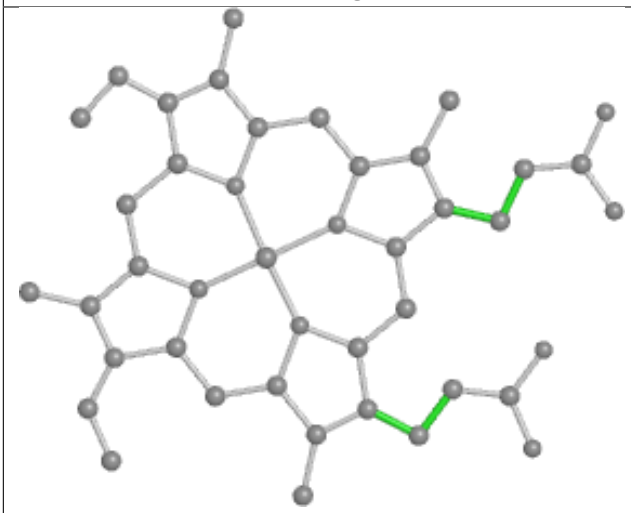
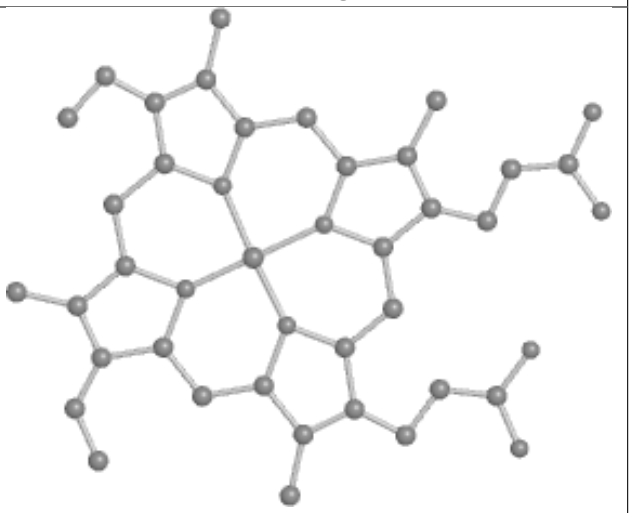


Bond angles

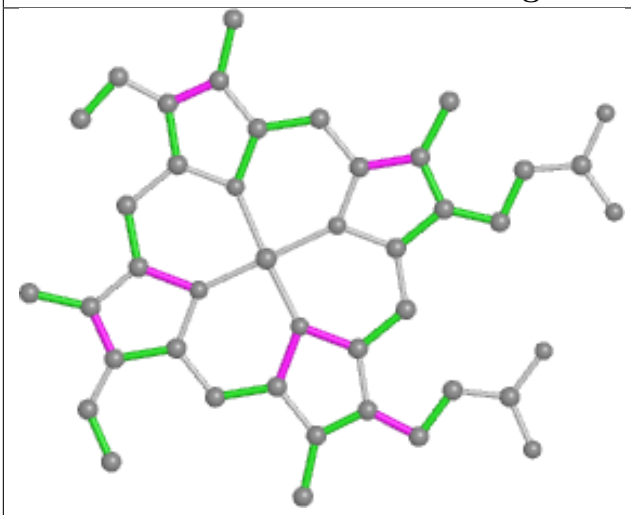


Torsions

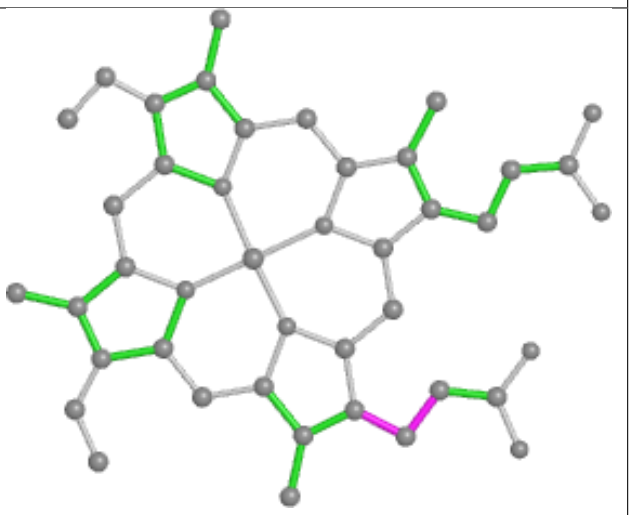


Rings

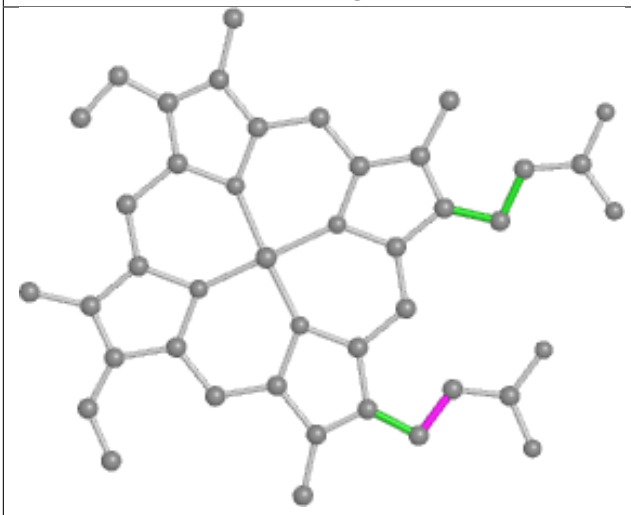
Ligand HEC A 607



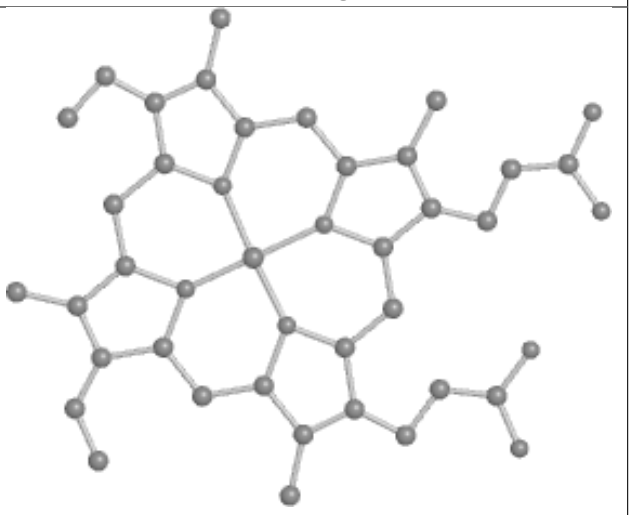
Bond lengths



Bond angles

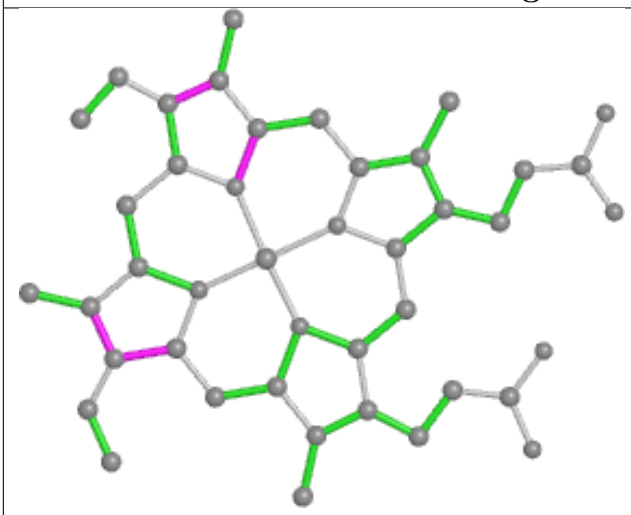


Torsions

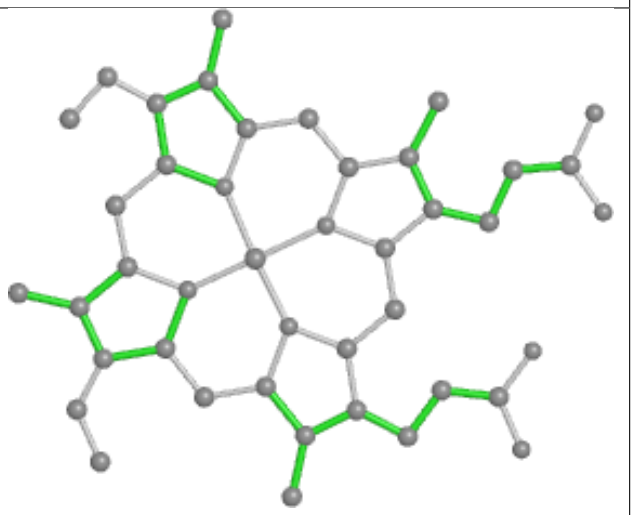


Rings

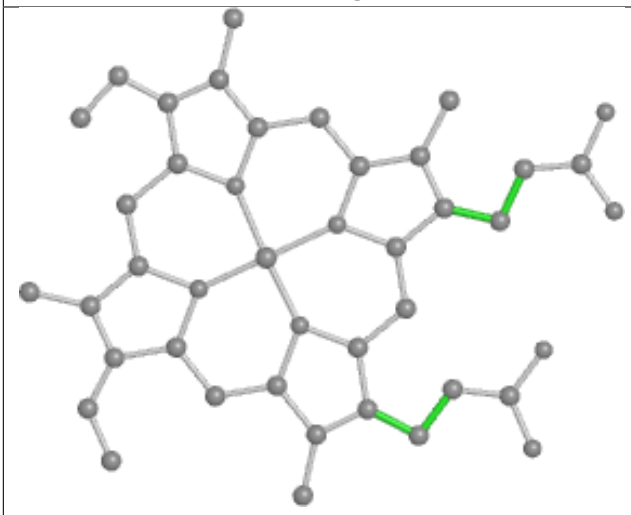
Ligand HEC A 609



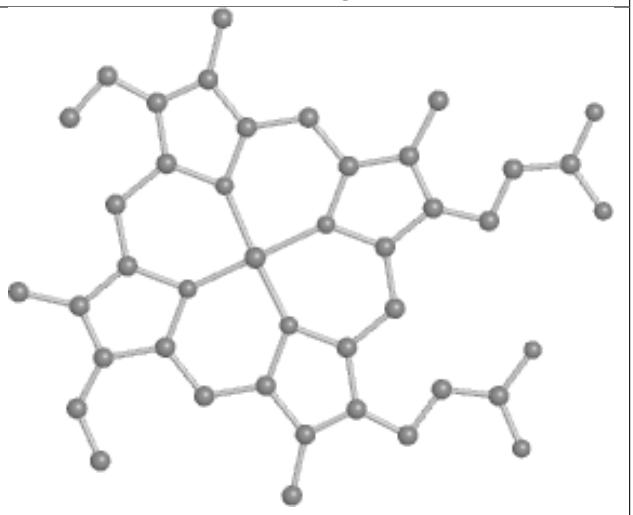
Bond lengths



Bond angles

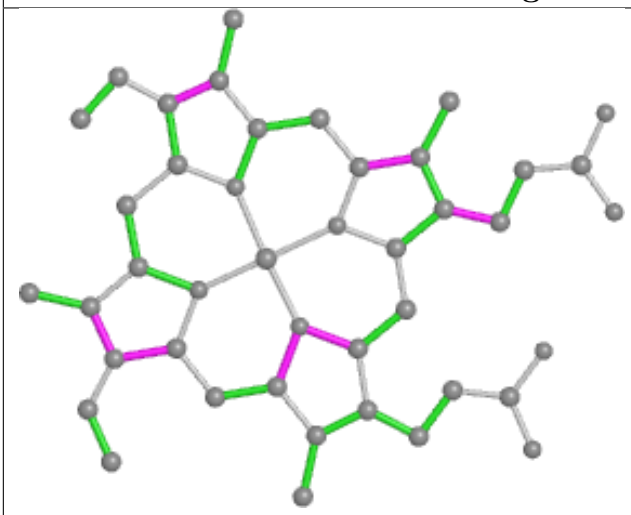


Torsions

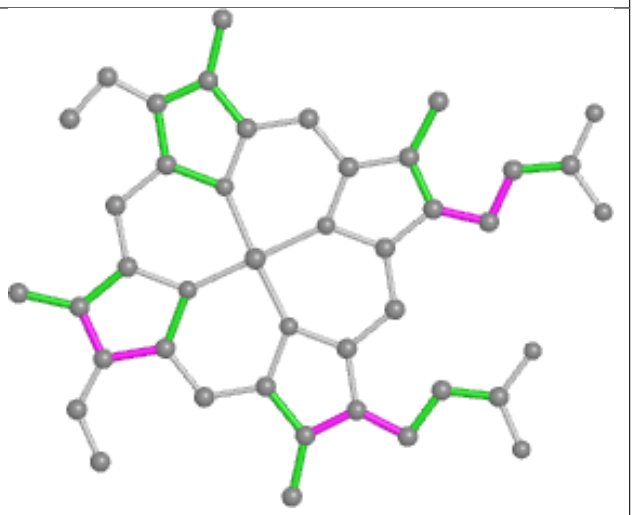


Rings

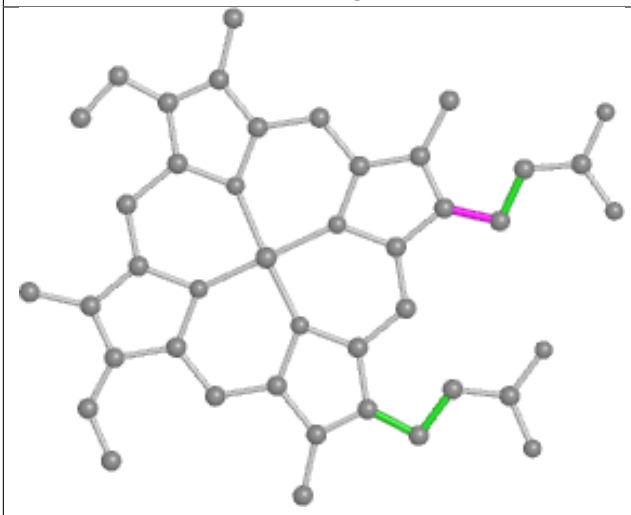
Ligand HEC A 605



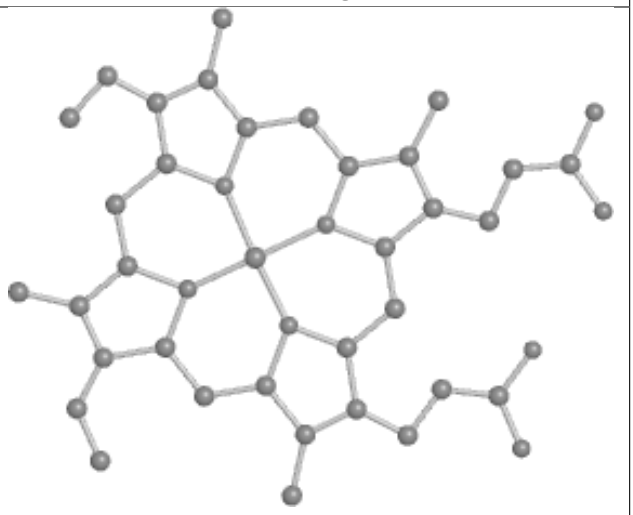
Bond lengths



Bond angles

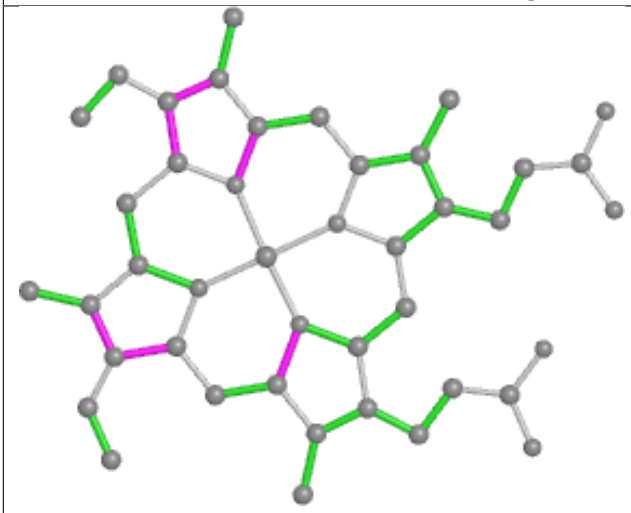


Torsions

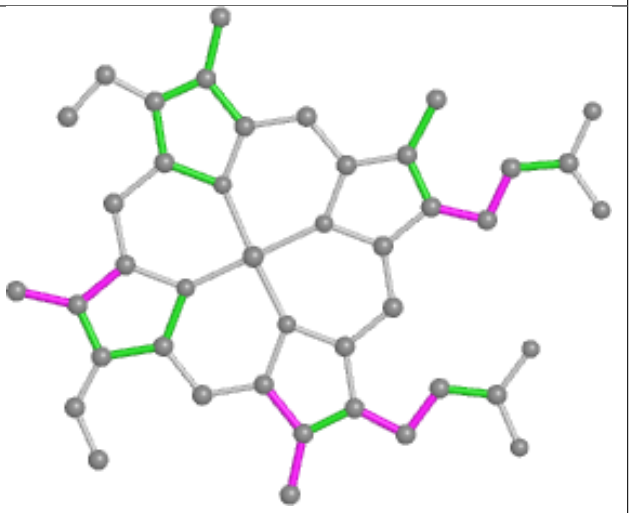


Rings

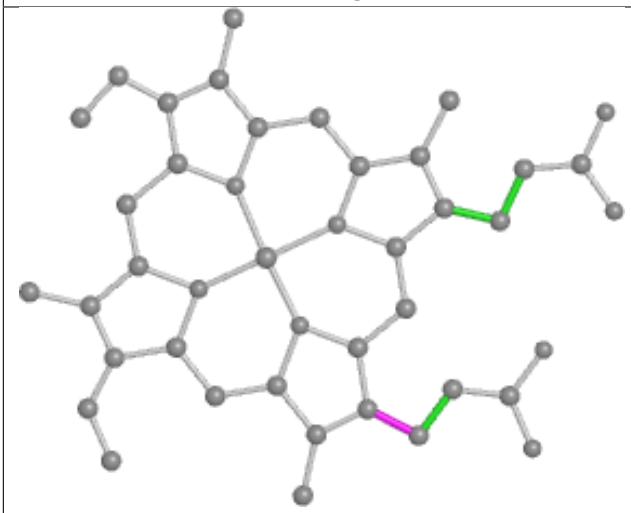
Ligand HEC A 610



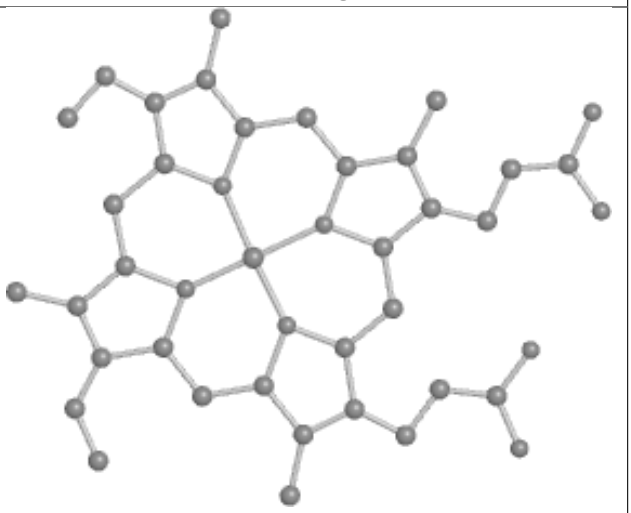
Bond lengths



Bond angles

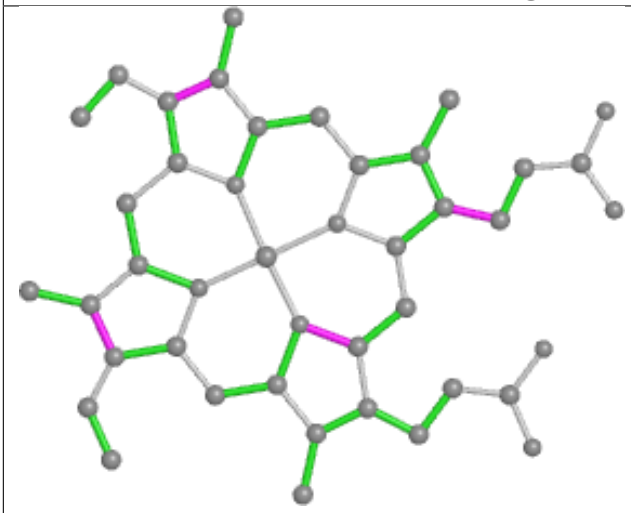


Torsions

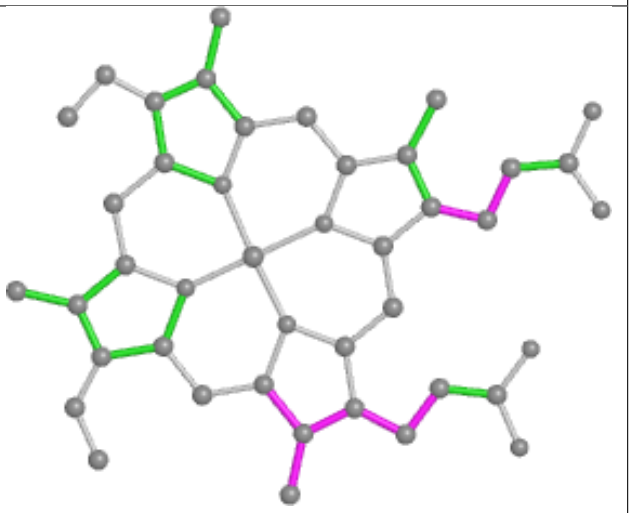


Rings

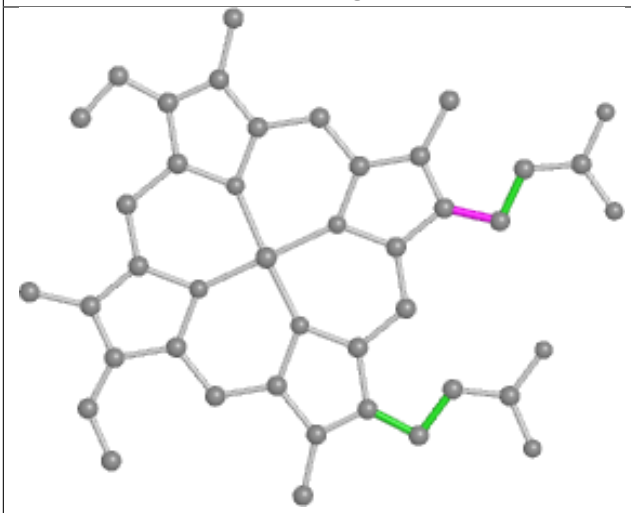
Ligand HEC A 604



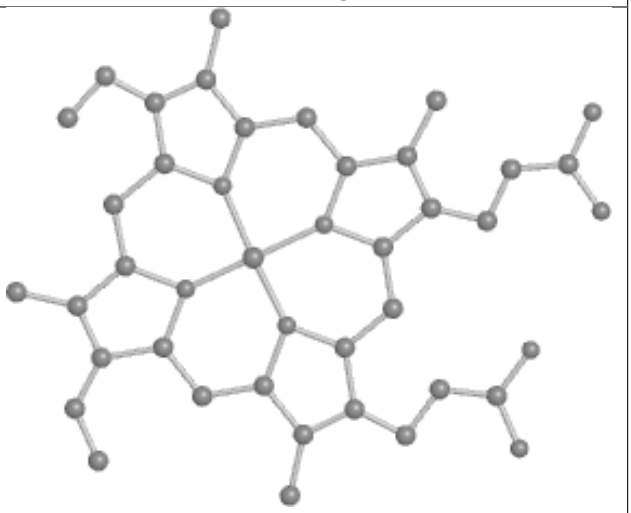
Bond lengths



Bond angles

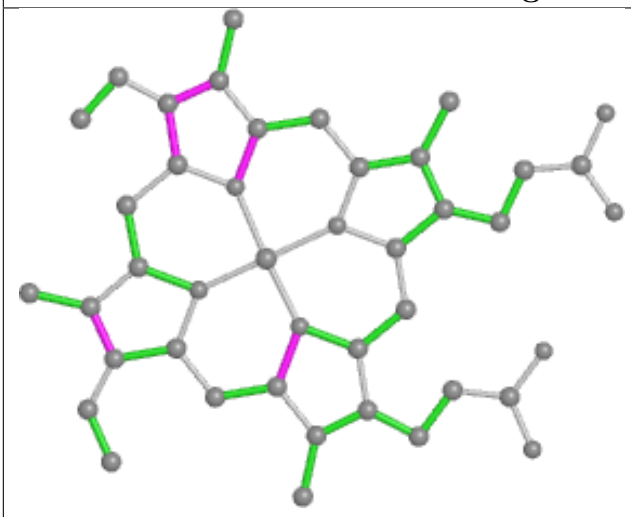


Torsions

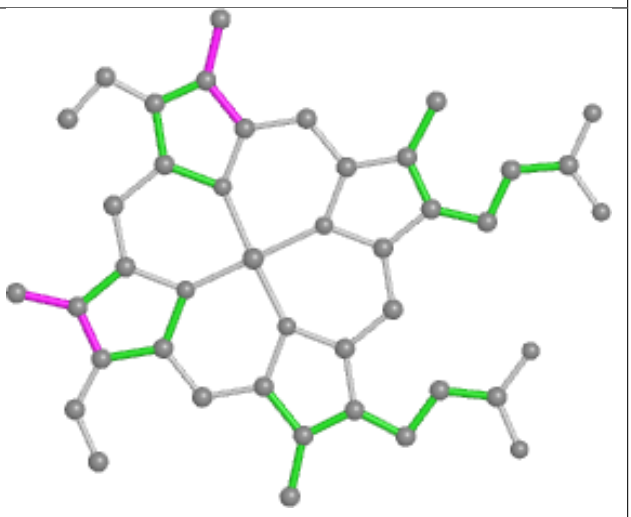


Rings

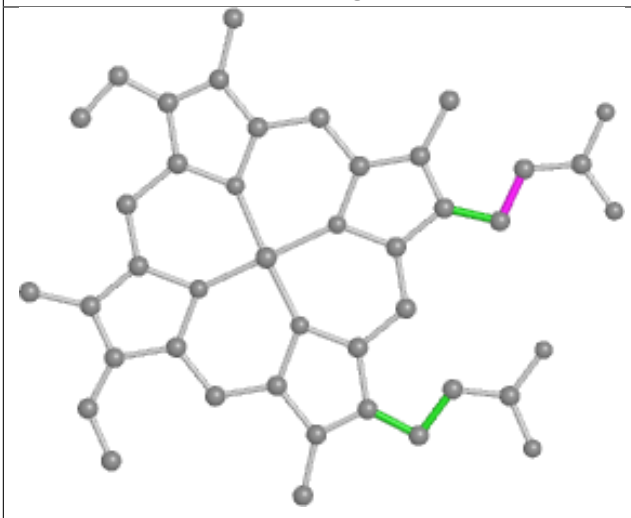
Ligand HEC A 612



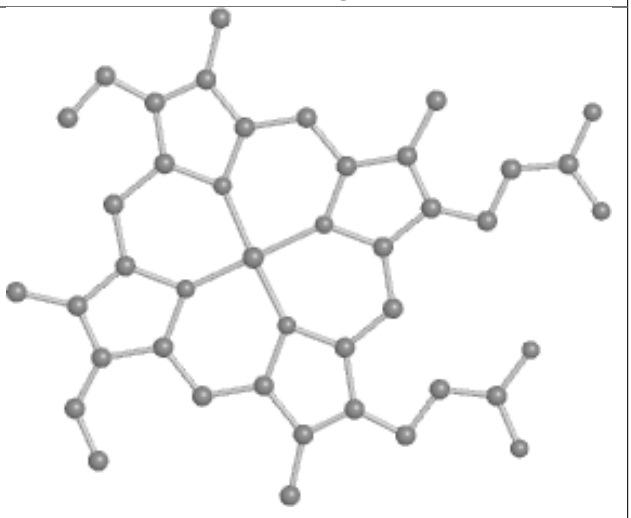
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/318 (100%)	-0.11	4 (1%)	77	65	23, 63, 98, 109	8 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	VAL	3.7
1	A	1	LYS	2.7
1	A	215	GLY	2.5
1	A	318	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	605	43/43	0.95	0.30	67,80,91,93	0
2	HEC	A	609	43/43	0.95	0.35	75,82,89,92	0
2	HEC	A	604	43/43	0.96	0.27	33,39,44,46	0

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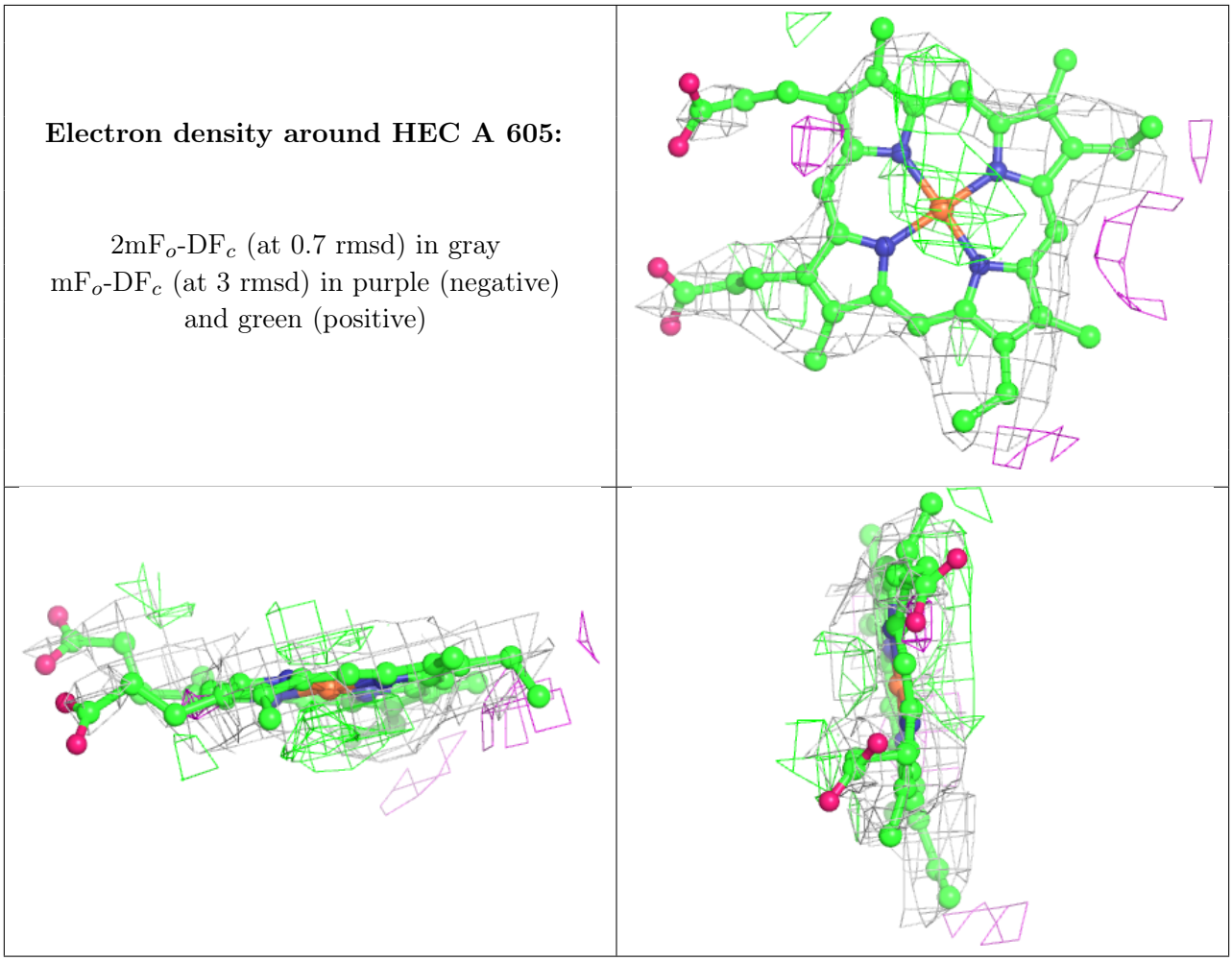
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	601	43/43	0.96	0.27	50,55,66,71	0
2	HEC	A	607	43/43	0.96	0.31	42,53,69,75	0
2	HEC	A	608	43/43	0.96	0.25	24,29,36,41	0
2	HEC	A	602	43/43	0.96	0.30	40,47,65,68	0
2	HEC	A	611	43/43	0.96	0.21	12,22,44,47	0
2	HEC	A	612	43/43	0.96	0.26	46,52,54,54	0
2	HEC	A	610	43/43	0.97	0.28	52,61,65,67	0
2	HEC	A	606	43/43	0.97	0.21	16,24,32,33	0
2	HEC	A	603	43/43	0.97	0.22	24,33,41,43	0

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

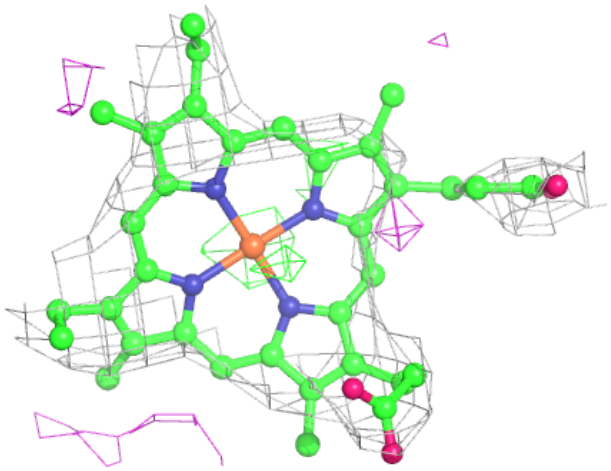
Electron density around HEC A 605:

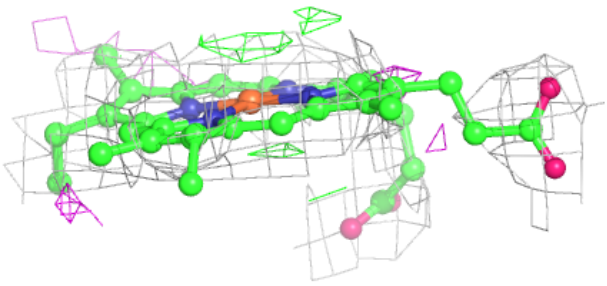
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

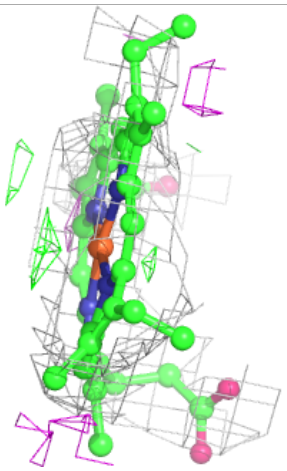


Electron density around HEC A 609:

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

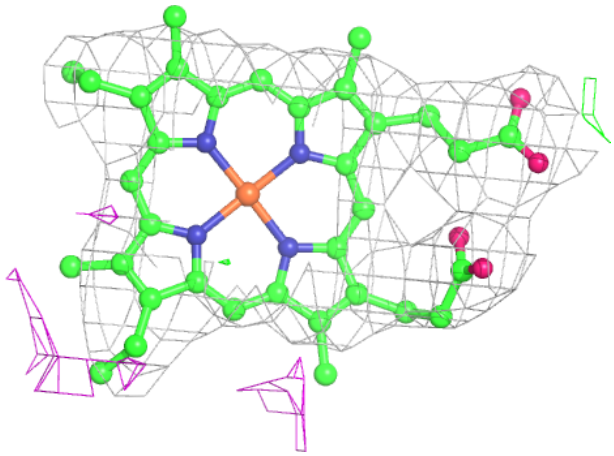


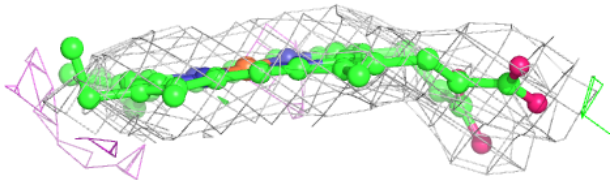


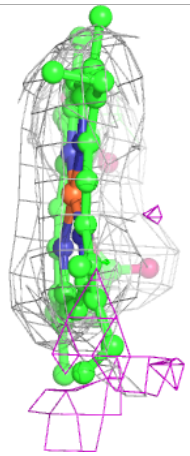


Electron density around HEC A 604:

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

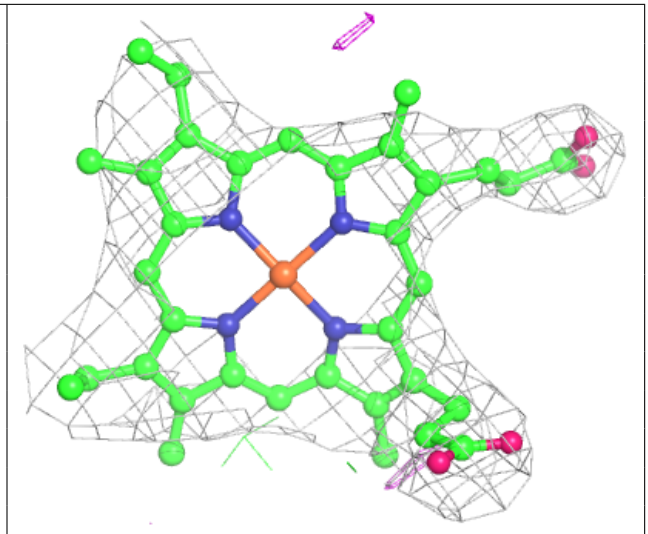


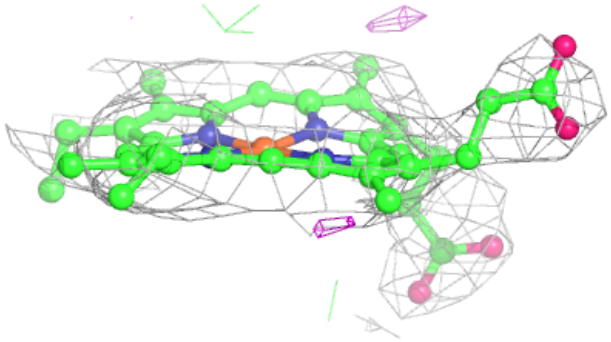


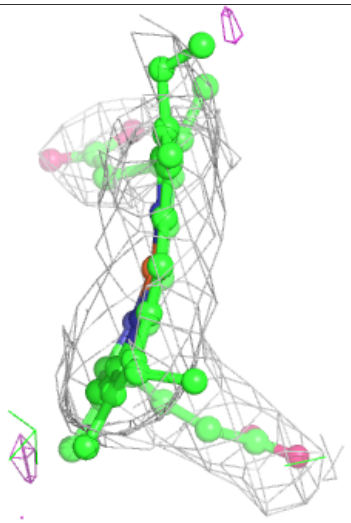


Electron density around HEC A 601:

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

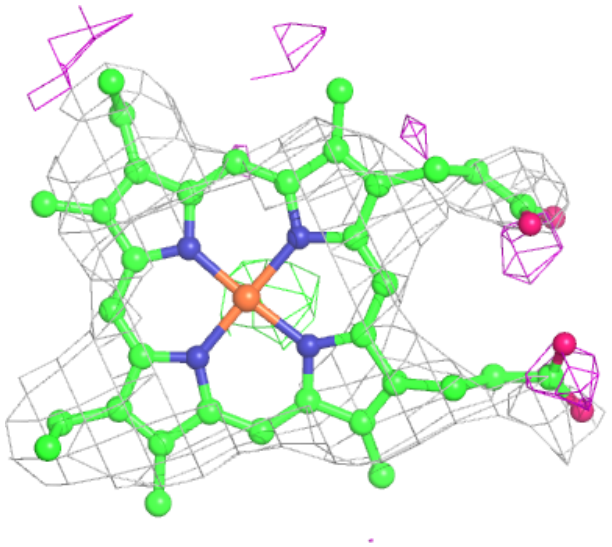


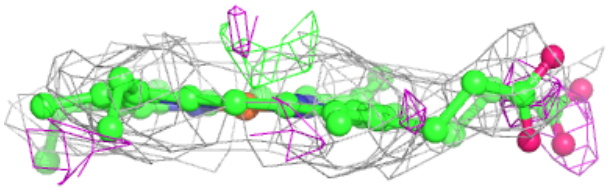


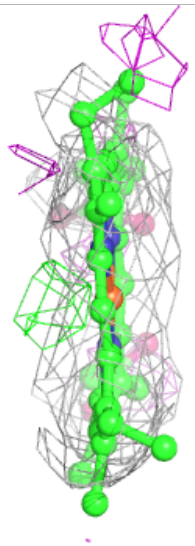


Electron density around HEC A 607:

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

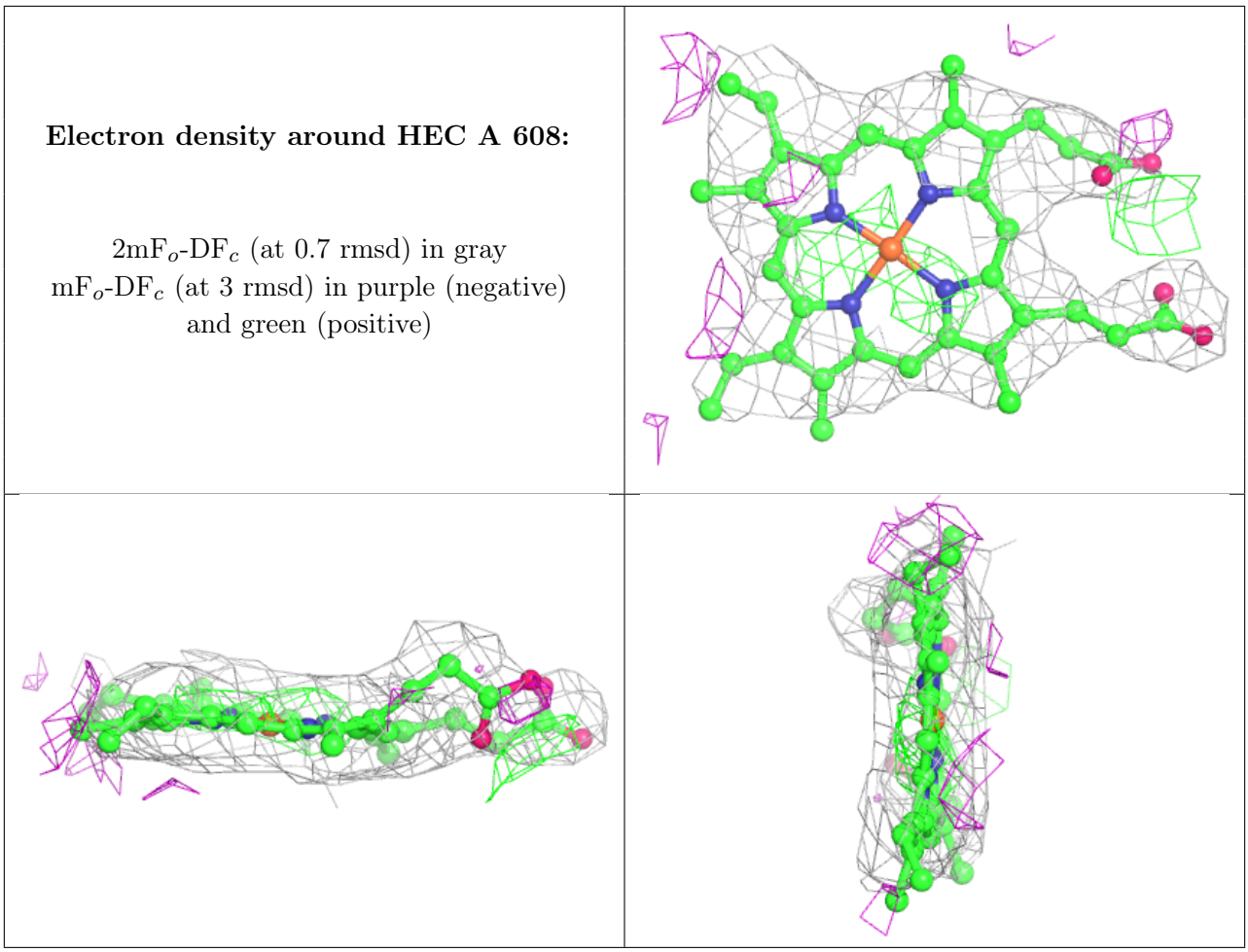






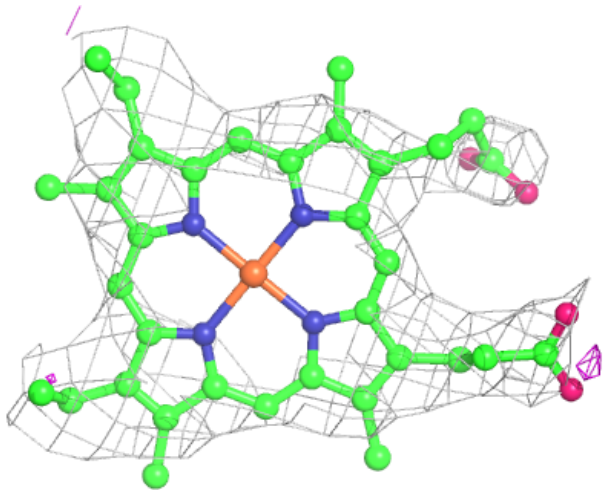
Electron density around HEC A 608:

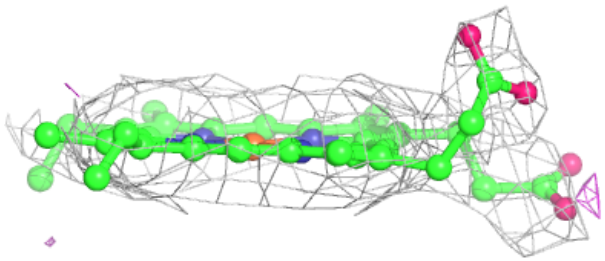
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

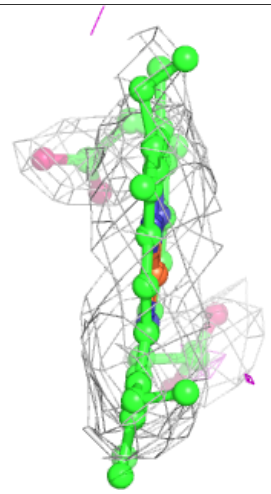


Electron density around HEC A 602:

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

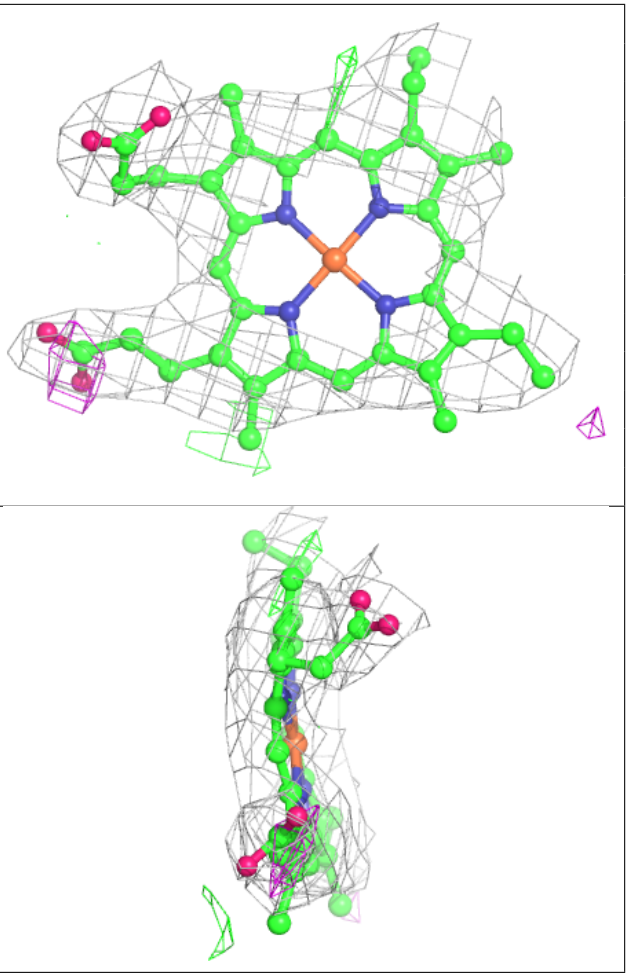






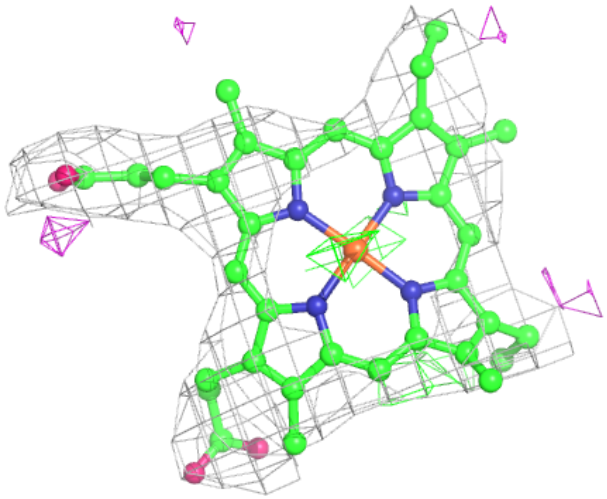
Electron density around HEC A 611:

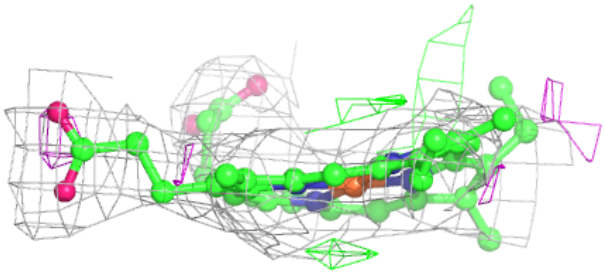
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

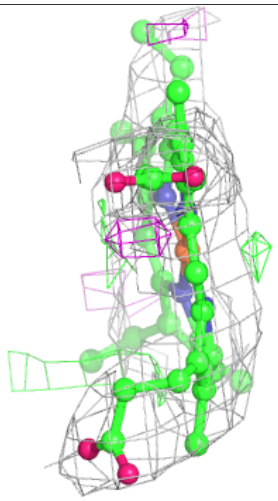


Electron density around HEC A 612:

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

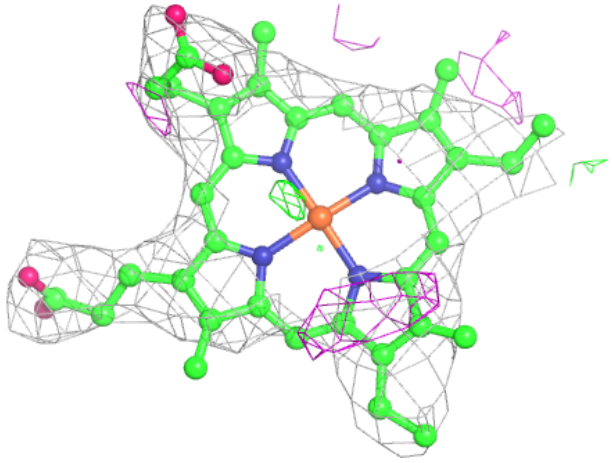


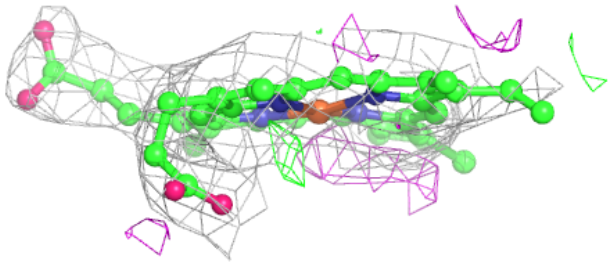




Electron density around HEC A 610:

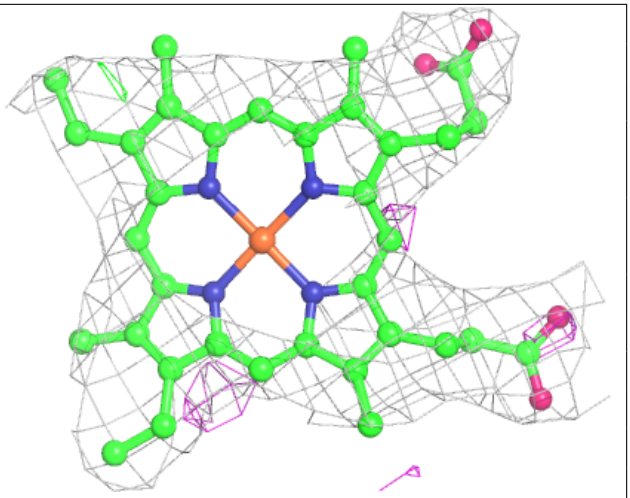
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

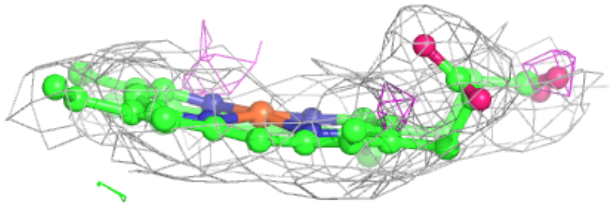


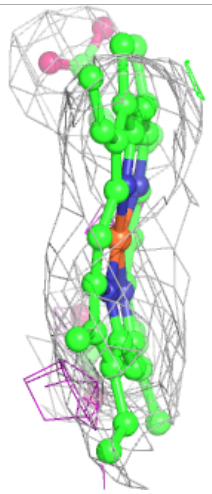


Electron density around HEC A 606:

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

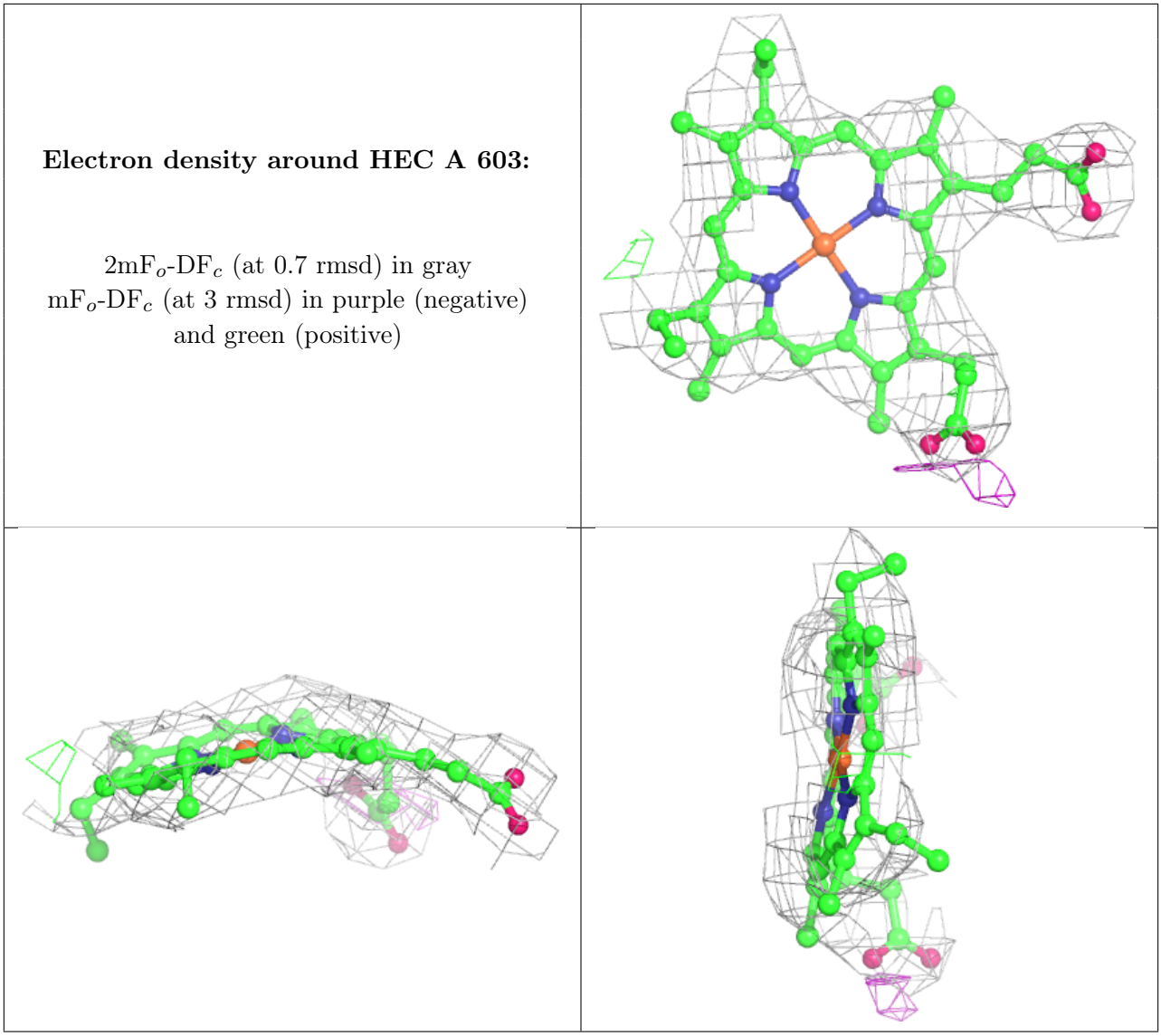






Electron density around HEC A 603:

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



6.5 Other polymers

There are no such residues in this entry.