Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 09:03 pm BST

PDB ID	:	1GWS
Title	:	hexadecaheme high molecular weight cytochrome Hmc from Desulfovibrio vulgaris Hildenborough
Authors	:	Czjzek, M.; Haser, R.; Bruschi, M.
Deposited on	:	2002-03-25
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

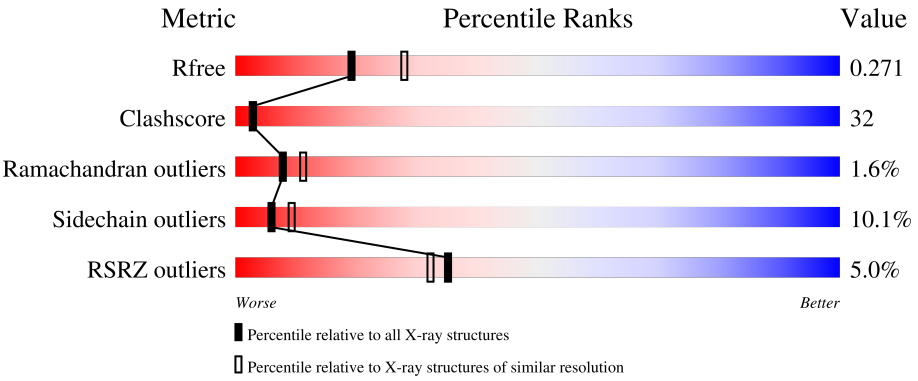
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	545	5% 57% 28% 6% • 8%

2 Entry composition (i)

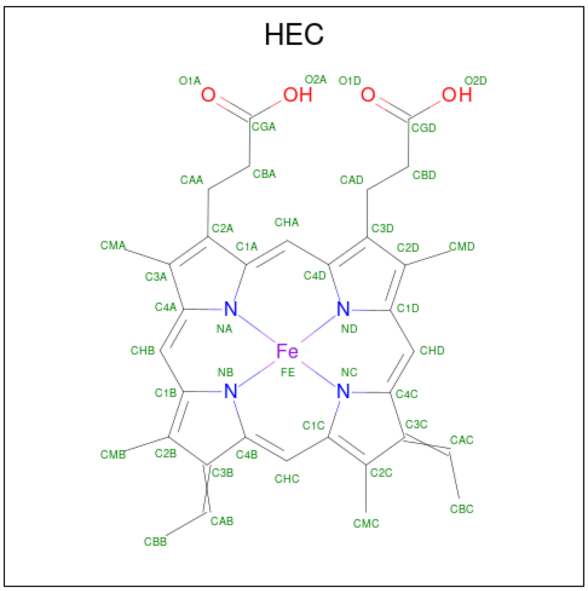
There are 3 unique types of molecules in this entry. The entry contains 4631 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIGH-MOLECULAR-WEIGHT CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	503	3792	2331	715	702	44	0	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
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.

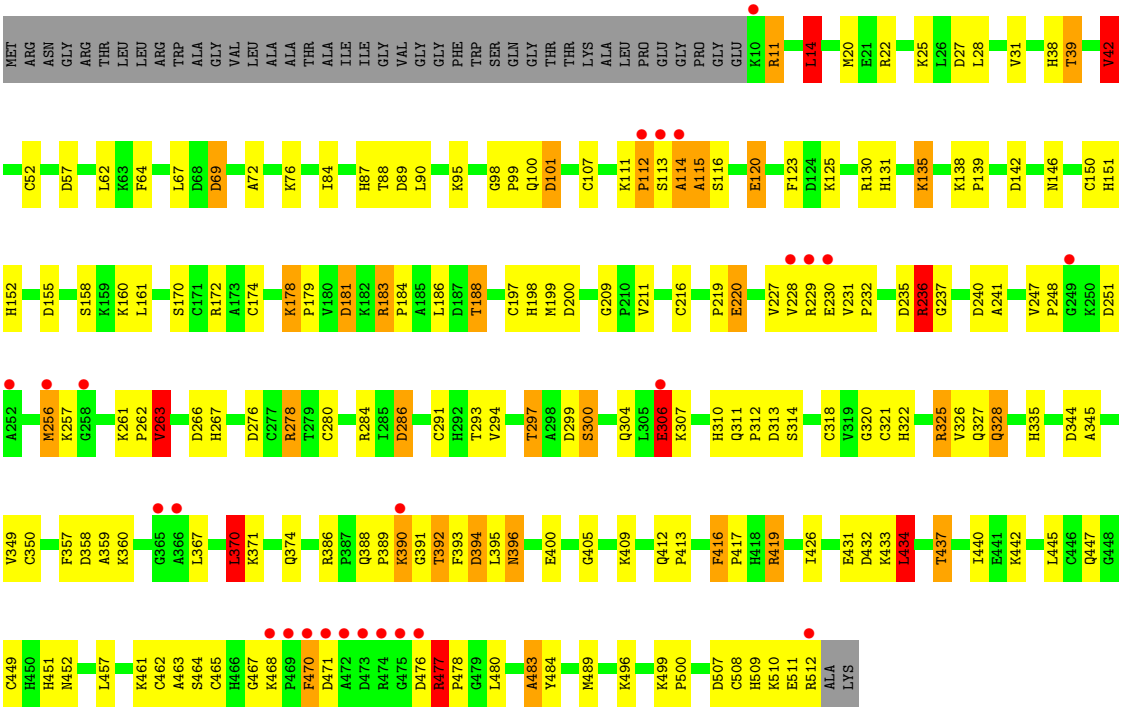
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0

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: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain A: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	108.39Å 108.39Å 102.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.52 – 2.40 33.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.52-2.40) 99.0 (33.52-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.201 , 0.276 0.199 , 0.271	Depositor DCC
R_{free} test set	1281 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4631	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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	1.16	12/3875 (0.3%)	1.29	34/5221 (0.7%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	VAL	CB-CG1	6.94	1.67	1.52
1	A	489	MET	SD-CE	-5.97	1.44	1.77
1	A	14	LEU	CG-CD2	5.66	1.72	1.51
1	A	483	ALA	CA-CB	-5.58	1.40	1.52
1	A	306	GLU	CD-OE1	5.56	1.31	1.25
1	A	120	GLU	CG-CD	5.33	1.59	1.51
1	A	328	GLN	CG-CD	5.28	1.63	1.51
1	A	57	ASP	CB-CG	5.24	1.62	1.51
1	A	345	ALA	CA-CB	-5.20	1.41	1.52
1	A	42	VAL	CA-CB	5.12	1.65	1.54
1	A	328	GLN	CB-CG	5.06	1.66	1.52
1	A	241	ALA	CA-CB	5.03	1.63	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	ASP	CB-CG-OD2	9.55	126.89	118.30
1	A	240	ASP	CB-CG-OD2	9.47	126.83	118.30
1	A	394	ASP	CB-CG-OD2	9.06	126.45	118.30
1	A	236	ARG	C-N-CA	-8.73	103.97	122.30
1	A	69	ASP	CB-CG-OD2	8.61	126.05	118.30
1	A	266	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	358	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	278	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	181	ASP	CB-CG-OD2	7.61	125.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	313	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	507	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	386	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	300	SER	C-N-CA	-6.39	105.72	121.70
1	A	370	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	101	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	286	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	89	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	300	SER	N-CA-C	-5.82	95.29	111.00
1	A	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	199	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	57	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	276	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	263	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	A	236	ARG	N-CA-C	-5.40	96.42	111.00
1	A	419	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	130	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	A	251	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	470	PHE	N-CA-C	5.29	125.29	111.00
1	A	434	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	11	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	39	THR	N-CA-CB	-5.03	100.75	110.30
1	A	278	ARG	CA-CB-CG	5.03	124.46	113.40
1	A	344	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3792	0	3721	220	0
2	A	688	0	491	131	0
3	A	151	0	0	9	1
All	All	4631	0	4212	273	1

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 32.

All (273) 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:321:CYS:SG	2:A:610:HEC:CAC	2.10	1.39
1:A:508:CYS:SG	2:A:616:HEC:CAC	2.10	1.39
1:A:449:CYS:SG	2:A:613:HEC:CAC	2.10	1.39
1:A:280:CYS:SG	2:A:608:HEC:CAC	2.12	1.37
1:A:107:CYS:SG	2:A:603:HEC:CAC	2.18	1.31
1:A:52:CYS:SG	2:A:601:HEC:CAC	2.23	1.26
1:A:216:CYS:SG	2:A:607:HEC:CAC	2.26	1.24
1:A:150:CYS:SG	2:A:604:HEC:CAC	2.33	1.17
1:A:465:CYS:SG	2:A:614:HEC:CAC	2.33	1.16
1:A:321:CYS:SG	2:A:610:HEC:HAC	1.86	1.15
1:A:14:LEU:HD22	1:A:14:LEU:H	1.07	1.14
1:A:11:ARG:HB2	1:A:14:LEU:HD11	1.17	1.13
1:A:508:CYS:SG	2:A:616:HEC:HAC	1.87	1.11
2:A:608:HEC:HMB1	2:A:608:HEC:HBB3	1.27	1.11
1:A:178:LYS:HE3	1:A:179:PRO:HD3	1.33	1.09
1:A:280:CYS:SG	2:A:608:HEC:HAC	1.93	1.04
1:A:174:CYS:SG	2:A:605:HEC:HAC	1.97	1.03
2:A:609:HEC:HMC1	2:A:609:HEC:HBC3	1.40	1.03
1:A:476:ASP:O	1:A:477:ARG:O	1.76	1.02
1:A:216:CYS:SG	2:A:607:HEC:CBC	2.50	0.98
1:A:135:LYS:HB2	1:A:135:LYS:NZ	1.80	0.95
1:A:449:CYS:SG	2:A:613:HEC:CBC	2.52	0.95
1:A:14:LEU:H	1:A:14:LEU:CD2	1.76	0.95
2:A:602:HEC:HMB1	2:A:602:HEC:HBB3	1.49	0.94
1:A:371:LYS:H	1:A:374:GLN:HE21	1.14	0.94
2:A:606:HEC:HMC1	2:A:606:HEC:HBC3	1.50	0.94
2:A:606:HEC:HMB1	2:A:606:HEC:HBB3	1.50	0.93
2:A:615:HEC:HBB3	2:A:615:HEC:HMB1	1.50	0.93
1:A:216:CYS:SG	2:A:607:HEC:HBC3	2.10	0.92
1:A:69:ASP:OD1	3:A:2016:HOH:O	1.88	0.91
1:A:476:ASP:HA	3:A:2126:HOH:O	1.70	0.90
1:A:174:CYS:SG	2:A:605:HEC:CBC	2.60	0.89
2:A:611:HEC:HBB3	2:A:611:HEC:HMB1	1.54	0.88
1:A:449:CYS:SG	2:A:613:HEC:HAC	2.12	0.87
1:A:107:CYS:SG	2:A:603:HEC:CBC	2.62	0.87
1:A:220:GLU:H	1:A:220:GLU:CD	1.76	0.87
1:A:465:CYS:SG	2:A:614:HEC:CBC	2.63	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:CB	1:A:14:LEU:HD11	2.05	0.86
1:A:371:LYS:H	1:A:374:GLN:NE2	1.74	0.85
1:A:20:MET:HE3	1:A:72:ALA:O	1.77	0.84
1:A:135:LYS:HB2	1:A:135:LYS:HZ3	1.41	0.84
1:A:174:CYS:O	1:A:183:ARG:HD3	1.78	0.84
1:A:350:CYS:SG	2:A:612:HEC:CBC	2.67	0.83
2:A:607:HEC:HBB3	2:A:607:HEC:HMB1	1.61	0.82
1:A:465:CYS:SG	2:A:614:HEC:HBC3	2.20	0.82
2:A:611:HEC:HBC3	2:A:611:HEC:HMC1	1.62	0.81
2:A:614:HEC:HBD2	2:A:614:HEC:HHA	1.61	0.81
1:A:14:LEU:HD22	1:A:14:LEU:N	1.91	0.81
1:A:111:LYS:O	1:A:113:SER:N	2.14	0.81
1:A:150:CYS:SG	2:A:604:HEC:HAC	2.22	0.80
1:A:114:ALA:O	1:A:115:ALA:HB3	1.80	0.80
1:A:107:CYS:SG	2:A:603:HEC:C3C	2.71	0.79
1:A:178:LYS:CE	1:A:179:PRO:HD3	2.14	0.78
1:A:256:MET:O	1:A:256:MET:HG2	1.82	0.78
1:A:263:VAL:HG13	2:A:612:HEC:HBD2	1.66	0.77
2:A:608:HEC:HMB1	2:A:608:HEC:CBB	2.10	0.77
2:A:603:HEC:HBC3	2:A:603:HEC:HMC1	1.65	0.77
2:A:605:HEC:HBC3	2:A:605:HEC:HMC1	1.66	0.77
1:A:307:LYS:HG3	1:A:311:GLN:NE2	2.00	0.76
1:A:297:THR:HG22	1:A:299:ASP:H	1.50	0.76
2:A:602:HEC:HMC1	2:A:602:HEC:HBC3	1.67	0.76
1:A:172:ARG:NH1	2:A:604:HEC:O1D	2.18	0.76
2:A:613:HEC:HBB3	2:A:613:HEC:HMB1	1.68	0.76
1:A:38:HIS:O	1:A:42:VAL:HG13	1.87	0.75
2:A:607:HEC:HBC3	2:A:607:HEC:HMC1	1.68	0.75
2:A:606:HEC:HMC1	2:A:606:HEC:CBC	2.17	0.74
1:A:131:HIS:HB3	2:A:604:HEC:HBC2	1.69	0.74
1:A:20:MET:CE	1:A:72:ALA:O	2.36	0.74
1:A:52:CYS:SG	2:A:601:HEC:HAC	2.24	0.74
1:A:20:MET:HG3	2:A:603:HEC:O1D	1.88	0.73
1:A:280:CYS:SG	2:A:608:HEC:CBC	2.73	0.73
1:A:52:CYS:SG	2:A:601:HEC:CBC	2.76	0.73
1:A:174:CYS:SG	2:A:605:HEC:C3C	2.76	0.73
1:A:27:ASP:C	1:A:28:LEU:HD12	2.09	0.73
2:A:609:HEC:HBB3	2:A:609:HEC:HMB1	1.71	0.72
1:A:508:CYS:SG	2:A:616:HEC:CBC	2.77	0.72
1:A:465:CYS:SG	2:A:614:HEC:C3C	2.77	0.72
2:A:609:HEC:HMC1	2:A:609:HEC:CBC	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:THR:HG21	1:A:426:ILE:HD11	1.72	0.72
1:A:172:ARG:HD2	1:A:278:ARG:HD3	1.71	0.71
1:A:197:CYS:SG	2:A:606:HEC:C3C	2.78	0.71
1:A:219:PRO:HD2	1:A:220:GLU:OE1	1.90	0.71
1:A:114:ALA:O	1:A:115:ALA:CB	2.39	0.70
1:A:297:THR:HG22	1:A:299:ASP:N	2.07	0.70
2:A:603:HEC:HBB3	2:A:603:HEC:HMB1	1.74	0.70
1:A:28:LEU:HD12	1:A:28:LEU:N	2.05	0.69
1:A:52:CYS:SG	2:A:601:HEC:C3C	2.81	0.69
2:A:610:HEC:HMA2	2:A:610:HEC:O1A	1.91	0.69
1:A:120:GLU:HG3	2:A:607:HEC:CGD	2.23	0.69
2:A:612:HEC:HMC1	2:A:612:HEC:HBC3	1.75	0.69
1:A:476:ASP:OD1	3:A:2126:HOH:O	2.10	0.68
1:A:461:LYS:HZ2	2:A:613:HEC:CGA	2.06	0.68
1:A:449:CYS:SG	2:A:613:HEC:HBC3	2.33	0.68
1:A:216:CYS:SG	2:A:607:HEC:C3C	2.82	0.68
2:A:607:HEC:CBC	2:A:607:HEC:HMC1	2.25	0.67
1:A:350:CYS:SG	2:A:612:HEC:C3C	2.81	0.67
1:A:321:CYS:SG	2:A:610:HEC:CBC	2.82	0.67
1:A:388:GLN:HG3	1:A:389:PRO:HD2	1.75	0.67
1:A:371:LYS:N	1:A:374:GLN:HE21	1.87	0.67
1:A:183:ARG:CG	1:A:183:ARG:O	2.44	0.66
1:A:107:CYS:SG	2:A:603:HEC:HBC3	2.34	0.65
1:A:508:CYS:SG	2:A:616:HEC:C3C	2.85	0.65
1:A:107:CYS:SG	2:A:603:HEC:HAC	2.30	0.65
2:A:611:HEC:HBB3	2:A:611:HEC:CMB	2.27	0.65
1:A:220:GLU:OE1	1:A:220:GLU:N	2.25	0.64
1:A:360:LYS:NZ	3:A:2094:HOH:O	2.29	0.64
1:A:230:GLU:O	1:A:230:GLU:HG2	1.96	0.64
1:A:321:CYS:SG	2:A:610:HEC:C3C	2.86	0.64
1:A:297:THR:CG2	1:A:299:ASP:H	2.11	0.63
1:A:449:CYS:SG	2:A:613:HEC:C3C	2.86	0.63
1:A:280:CYS:SG	2:A:608:HEC:C3C	2.86	0.62
2:A:615:HEC:HMC1	2:A:615:HEC:HBC3	1.81	0.62
1:A:14:LEU:N	1:A:14:LEU:HD13	2.16	0.61
1:A:90:LEU:HD13	2:A:602:HEC:HMD3	1.81	0.61
2:A:613:HEC:HBC3	2:A:613:HEC:HMC1	1.81	0.61
1:A:113:SER:OG	1:A:114:ALA:N	2.33	0.61
1:A:367:LEU:HA	1:A:370:LEU:HD22	1.82	0.61
1:A:412:GLN:HB2	1:A:413:PRO:CD	2.31	0.60
1:A:390:LYS:NZ	1:A:440:ILE:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:HA	1:A:100:GLN:HE22	1.65	0.59
1:A:111:LYS:O	1:A:112:PRO:C	2.41	0.59
1:A:437:THR:HG21	2:A:610:HEC:HAA2	1.84	0.59
1:A:400:GLU:HA	1:A:419:ARG:HB2	1.85	0.58
2:A:612:HEC:HMA3	2:A:612:HEC:O2A	2.03	0.58
1:A:135:LYS:NZ	1:A:135:LYS:CB	2.61	0.58
1:A:150:CYS:SG	2:A:604:HEC:C3C	2.92	0.58
1:A:412:GLN:HB2	1:A:413:PRO:HD2	1.84	0.58
1:A:178:LYS:HE3	1:A:178:LYS:HA	1.84	0.58
1:A:198:HIS:CE1	1:A:209:GLY:HA3	2.39	0.57
2:A:611:HEC:HBC3	2:A:611:HEC:CMC	2.34	0.57
1:A:52:CYS:HB3	1:A:64:PHE:CE1	2.40	0.57
1:A:465:CYS:HG	2:A:614:HEC:HBC3	1.69	0.57
1:A:14:LEU:CD2	1:A:14:LEU:N	2.57	0.56
1:A:183:ARG:O	1:A:183:ARG:HG3	2.04	0.56
1:A:325:ARG:HH11	1:A:325:ARG:CG	2.18	0.56
1:A:112:PRO:HA	3:A:2029:HOH:O	2.05	0.55
1:A:123:PHE:HB2	2:A:604:HEC:CBD	2.36	0.55
2:A:603:HEC:HBB3	2:A:603:HEC:CMB	2.35	0.55
1:A:318:CYS:HA	2:A:610:HEC:CHC	2.36	0.55
1:A:219:PRO:CD	1:A:220:GLU:OE1	2.53	0.55
2:A:606:HEC:HMB1	2:A:606:HEC:CBB	2.30	0.54
1:A:11:ARG:O	1:A:116:SER:HA	2.08	0.54
1:A:123:PHE:HB2	2:A:604:HEC:HBD2	1.89	0.54
1:A:230:GLU:O	1:A:232:PRO:HD3	2.08	0.54
1:A:220:GLU:CD	1:A:220:GLU:N	2.55	0.54
1:A:416:PHE:HB2	2:A:615:HEC:HMB2	1.89	0.53
1:A:461:LYS:NZ	2:A:613:HEC:O1A	2.39	0.53
2:A:602:HEC:HMC1	2:A:602:HEC:CBC	2.37	0.53
1:A:412:GLN:HG2	1:A:510:LYS:O	2.08	0.53
1:A:310:HIS:HE1	2:A:612:HEC:C1A	2.20	0.53
1:A:52:CYS:HB3	1:A:64:PHE:CD1	2.44	0.53
1:A:111:LYS:N	1:A:112:PRO:HD2	2.24	0.53
1:A:294:VAL:O	1:A:304:GLN:HB2	2.09	0.53
1:A:197:CYS:SG	2:A:606:HEC:CBC	2.88	0.52
2:A:602:HEC:HBB3	2:A:602:HEC:CMB	2.21	0.52
1:A:335:HIS:HE1	2:A:611:HEC:C1A	2.22	0.52
1:A:392:THR:OG1	1:A:393:PHE:N	2.42	0.52
2:A:605:HEC:CBC	2:A:605:HEC:HMC1	2.38	0.52
2:A:604:HEC:HMC1	2:A:604:HEC:HBC3	1.90	0.52
2:A:606:HEC:HBA2	2:A:606:HEC:HMA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:604:HEC:HMB1	2:A:604:HEC:HBB3	1.92	0.52
1:A:28:LEU:N	1:A:28:LEU:CD1	2.72	0.52
1:A:87:HIS:CE1	1:A:98:GLY:HA3	2.44	0.52
1:A:135:LYS:HE2	3:A:2036:HOH:O	2.10	0.52
1:A:20:MET:HG3	2:A:603:HEC:CGD	2.40	0.51
1:A:511:GLU:O	1:A:512:ARG:CB	2.58	0.51
2:A:613:HEC:HBB3	2:A:613:HEC:CMB	2.38	0.51
2:A:614:HEC:HBD2	2:A:614:HEC:CHA	2.33	0.51
1:A:123:PHE:O	1:A:278:ARG:NH2	2.42	0.51
1:A:357:PHE:O	3:A:2092:HOH:O	2.19	0.51
1:A:230:GLU:O	1:A:230:GLU:CG	2.59	0.51
1:A:509:HIS:HE1	2:A:616:HEC:NB	2.08	0.51
1:A:178:LYS:CE	1:A:178:LYS:HA	2.41	0.50
1:A:150:CYS:SG	2:A:604:HEC:CBC	2.95	0.50
1:A:433:LYS:O	1:A:437:THR:CG2	2.59	0.50
2:A:615:HEC:HHA	2:A:615:HEC:CBA	2.40	0.50
1:A:467:GLY:C	1:A:468:LYS:O	2.47	0.50
2:A:612:HEC:HMB1	2:A:612:HEC:HBB3	1.93	0.50
1:A:395:LEU:HD11	1:A:426:ILE:HD12	1.92	0.50
1:A:499:LYS:HA	1:A:500:PRO:C	2.31	0.49
1:A:314:SER:O	1:A:320:GLY:HA3	2.12	0.49
1:A:84:ILE:HG21	1:A:101:ASP:HB3	1.95	0.49
1:A:174:CYS:SG	2:A:605:HEC:HBC3	2.49	0.49
2:A:606:HEC:HBA2	2:A:606:HEC:CMA	2.43	0.49
1:A:480:LEU:HG	1:A:484:TYR:CE2	2.48	0.49
1:A:120:GLU:HG3	2:A:607:HEC:O2D	2.13	0.49
1:A:322:HIS:CG	1:A:434:LEU:HD11	2.47	0.48
1:A:325:ARG:HH11	1:A:325:ARG:HB3	1.77	0.48
2:A:609:HEC:HBD1	2:A:609:HEC:HMD1	1.94	0.48
1:A:27:ASP:HB3	1:A:28:LEU:HD12	1.96	0.48
1:A:27:ASP:CB	1:A:28:LEU:HD12	2.43	0.48
1:A:135:LYS:CB	3:A:2035:HOH:O	2.61	0.48
2:A:608:HEC:CBB	2:A:608:HEC:CMB	2.83	0.48
1:A:135:LYS:HB2	1:A:135:LYS:HZ2	1.76	0.48
1:A:235:ASP:OD2	1:A:235:ASP:C	2.53	0.48
1:A:11:ARG:O	1:A:14:LEU:HD21	2.14	0.47
1:A:371:LYS:HB2	1:A:374:GLN:HE21	1.79	0.47
2:A:608:HEC:HBB3	2:A:608:HEC:CMB	2.15	0.47
1:A:131:HIS:CB	2:A:604:HEC:HBC2	2.43	0.47
1:A:437:THR:CG2	2:A:610:HEC:HAA2	2.44	0.47
1:A:52:CYS:SG	2:A:601:HEC:HBC3	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:O	1:A:160:LYS:HG2	2.14	0.47
1:A:247:VAL:O	1:A:293:THR:HB	2.15	0.47
1:A:248:PRO:HB3	1:A:256:MET:CE	2.44	0.47
1:A:311:GLN:HA	1:A:312:PRO:HD3	1.64	0.47
1:A:388:GLN:HG3	1:A:389:PRO:CD	2.43	0.47
1:A:307:LYS:HG3	1:A:311:GLN:HE21	1.74	0.47
1:A:158:SER:HB2	1:A:160:LYS:HE3	1.98	0.46
1:A:235:ASP:OD2	1:A:236:ARG:O	2.34	0.46
1:A:388:GLN:CG	1:A:389:PRO:CD	2.93	0.46
1:A:463:ALA:O	1:A:464:SER:C	2.51	0.46
1:A:367:LEU:HD23	1:A:370:LEU:HD22	1.97	0.46
1:A:227:VAL:HG12	1:A:228:VAL:N	2.30	0.46
1:A:391:GLY:O	1:A:442:LYS:HA	2.15	0.46
1:A:452:ASN:HD22	2:A:614:HEC:CHD	2.30	0.45
2:A:608:HEC:HMC1	2:A:608:HEC:HBC3	1.98	0.45
2:A:609:HEC:HBD1	2:A:609:HEC:CMD	2.47	0.45
1:A:219:PRO:N	1:A:220:GLU:OE1	2.50	0.45
1:A:463:ALA:C	1:A:465:CYS:N	2.67	0.45
1:A:462:CYS:N	2:A:613:HEC:O2D	2.44	0.45
2:A:606:HEC:CBC	2:A:606:HEC:CMC	2.90	0.45
1:A:464:SER:O	1:A:465:CYS:HB3	2.17	0.44
1:A:405:GLY:HA2	2:A:616:HEC:O1D	2.17	0.44
1:A:138:LYS:HA	1:A:139:PRO:HD3	1.89	0.44
1:A:170:SER:OG	1:A:172:ARG:HG3	2.18	0.44
1:A:307:LYS:HD2	1:A:307:LYS:HA	1.65	0.44
1:A:262:PRO:HD3	1:A:359:ALA:HB3	1.99	0.44
2:A:609:HEC:HBB3	2:A:609:HEC:CMB	2.44	0.44
1:A:325:ARG:HH11	1:A:325:ARG:HG3	1.83	0.43
2:A:614:HEC:HBC3	2:A:614:HEC:HMC1	2.00	0.43
1:A:291:CYS:O	1:A:297:THR:HB	2.19	0.43
1:A:151:HIS:CD2	2:A:604:HEC:NB	2.87	0.43
1:A:349:VAL:O	1:A:349:VAL:HG12	2.18	0.43
1:A:477:ARG:HB2	1:A:478:PRO:HD3	1.98	0.43
1:A:483:ALA:HB1	2:A:614:HEC:CHB	2.48	0.43
1:A:62:LEU:HD12	1:A:188:THR:HB	2.01	0.43
1:A:198:HIS:NE2	1:A:209:GLY:HA3	2.34	0.43
1:A:125:LYS:HE3	1:A:229:ARG:NH1	2.35	0.42
1:A:299:ASP:C	1:A:300:SER:O	2.54	0.42
1:A:183:ARG:HA	1:A:184:PRO:HD3	1.87	0.42
1:A:227:VAL:CG1	1:A:228:VAL:N	2.82	0.42
1:A:304:GLN:HG3	1:A:306:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:CYS:HB3	2:A:610:HEC:C4B	2.46	0.42
1:A:477:ARG:CB	1:A:478:PRO:CD	2.97	0.42
1:A:87:HIS:CE1	1:A:99:PRO:HD2	2.55	0.42
1:A:447:GLN:NE2	3:A:2118:HOH:O	2.52	0.42
1:A:467:GLY:O	1:A:468:LYS:C	2.58	0.42
1:A:311:GLN:HE21	1:A:311:GLN:HB2	1.52	0.42
2:A:610:HEC:HMC1	2:A:610:HEC:HBC3	2.02	0.42
1:A:20:MET:HE1	1:A:72:ALA:O	2.20	0.42
1:A:135:LYS:O	1:A:135:LYS:HG3	2.19	0.42
1:A:183:ARG:O	1:A:183:ARG:HG2	2.17	0.42
2:A:615:HEC:HMB1	2:A:615:HEC:CBB	2.30	0.41
2:A:616:HEC:HBC3	2:A:616:HEC:HMC1	2.02	0.41
1:A:236:ARG:HB2	1:A:237:GLY:H	1.69	0.41
1:A:248:PRO:HB3	1:A:256:MET:HE2	2.02	0.41
1:A:477:ARG:HB2	1:A:478:PRO:CD	2.50	0.41
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.81	0.41
1:A:367:LEU:HD23	1:A:370:LEU:CD2	2.51	0.41
1:A:433:LYS:O	1:A:437:THR:HG22	2.21	0.41
1:A:228:VAL:O	1:A:231:VAL:CG2	2.69	0.41
1:A:416:PHE:HA	1:A:417:PRO:HD3	1.87	0.41
1:A:432:ASP:OD2	1:A:434:LEU:N	2.54	0.41
1:A:261:LYS:HB3	1:A:262:PRO:HD2	2.02	0.41
1:A:267:HIS:CE1	2:A:608:HEC:C4B	3.04	0.40
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.33	0.40
1:A:433:LYS:O	1:A:437:THR:HG23	2.22	0.40
1:A:452:ASN:HD22	2:A:614:HEC:C1D	2.33	0.40
2:A:613:HEC:HBC1	2:A:615:HEC:C2C	2.51	0.40
1:A:152:HIS:CD2	1:A:161:LEU:HD22	2.57	0.40
1:A:299:ASP:O	2:A:609:HEC:HMD3	2.22	0.40
1:A:335:HIS:CE1	2:A:611:HEC:C1A	3.04	0.40
1:A:394:ASP:OD2	1:A:396:ASN:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2028:HOH:O	3:A:2136:HOH:O[4_675]	0.64	1.56

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	501/545 (92%)	460 (92%)	33 (7%)	8 (2%)	8 11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	A	181	ASP
1	A	257	LYS
1	A	477	ARG
1	A	115	ALA
1	A	114	ALA
1	A	409	LYS
1	A	286	ASP

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	405/435 (93%)	364 (90%)	41 (10%)	6 9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	ARG
1	A	25	LYS

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Mol	Chain	Res	Type
1	A	39	THR
1	A	42	VAL
1	A	67	LEU
1	A	76	LYS
1	A	95	LYS
1	A	135	LYS
1	A	146	ASN
1	A	178	LYS
1	A	183	ARG
1	A	186	LEU
1	A	188	THR
1	A	211	VAL
1	A	220	GLU
1	A	236	ARG
1	A	256	MET
1	A	263	VAL
1	A	284	ARG
1	A	297	THR
1	A	306	GLU
1	A	325	ARG
1	A	326	VAL
1	A	327	GLN
1	A	328	GLN
1	A	370	LEU
1	A	390	LYS
1	A	392	THR
1	A	396	ASN
1	A	416	PHE
1	A	431	GLU
1	A	434	LEU
1	A	437	THR
1	A	445	LEU
1	A	451	HIS
1	A	457	LEU
1	A	470	PHE
1	A	471	ASP
1	A	477	ARG
1	A	496	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	100	GLN
1	A	146	ASN
1	A	222	GLN
1	A	282	HIS
1	A	311	GLN
1	A	323	ASN
1	A	346	GLN
1	A	374	GLN
1	A	447	GLN
1	A	452	ASN
1	A	486	GLN
1	A	487	GLN

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

16 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	605	1	32,50,50	2.50	9 (28%)	24,82,82	1.47	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEC	A	601	1	32,50,50	2.47	10 (31%)	24,82,82	1.93	5 (20%)
2	HEC	A	604	1	32,50,50	2.40	8 (25%)	24,82,82	2.13	2 (8%)
2	HEC	A	602	1	32,50,50	2.75	9 (28%)	24,82,82	2.59	7 (29%)
2	HEC	A	613	1	32,50,50	2.44	8 (25%)	24,82,82	2.36	9 (37%)
2	HEC	A	611	1	32,50,50	2.95	6 (18%)	24,82,82	2.33	10 (41%)
2	HEC	A	616	1	32,50,50	2.76	8 (25%)	24,82,82	2.45	8 (33%)
2	HEC	A	606	1	32,50,50	2.85	9 (28%)	24,82,82	1.92	7 (29%)
2	HEC	A	607	1	32,50,50	2.48	9 (28%)	24,82,82	2.35	12 (50%)
2	HEC	A	612	1	32,50,50	2.36	9 (28%)	24,82,82	2.39	8 (33%)
2	HEC	A	614	1	32,50,50	2.39	8 (25%)	24,82,82	1.69	6 (25%)
2	HEC	A	609	1	32,50,50	2.83	9 (28%)	24,82,82	2.07	5 (20%)
2	HEC	A	610	1	32,50,50	2.31	10 (31%)	24,82,82	2.63	9 (37%)
2	HEC	A	608	1	32,50,50	2.74	8 (25%)	24,82,82	1.89	7 (29%)
2	HEC	A	603	1	32,50,50	2.80	8 (25%)	24,82,82	2.03	9 (37%)
2	HEC	A	615	1	32,50,50	2.28	7 (21%)	24,82,82	2.50	9 (37%)

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	605	1	-	2/10/54/54	-
2	HEC	A	601	1	-	3/10/54/54	-
2	HEC	A	604	1	-	3/10/54/54	-
2	HEC	A	602	1	-	2/10/54/54	-
2	HEC	A	613	1	-	2/10/54/54	-
2	HEC	A	611	1	-	4/10/54/54	-
2	HEC	A	616	1	-	1/10/54/54	-
2	HEC	A	606	1	-	6/10/54/54	-
2	HEC	A	607	1	-	4/10/54/54	-
2	HEC	A	612	1	-	4/10/54/54	-
2	HEC	A	614	1	-	4/10/54/54	-
2	HEC	A	609	1	-	5/10/54/54	-
2	HEC	A	610	1	-	3/10/54/54	-
2	HEC	A	608	1	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	603	1	-	4/10/54/54	-
2	HEC	A	615	1	-	6/10/54/54	-

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	609	HEC	C3C-C2C	-11.68	1.28	1.40
2	A	611	HEC	C2B-C3B	-10.10	1.30	1.40
2	A	608	HEC	C2B-C3B	-9.85	1.30	1.40
2	A	606	HEC	C2B-C3B	-9.40	1.30	1.40
2	A	616	HEC	C3C-C2C	-9.30	1.31	1.40
2	A	602	HEC	C2B-C3B	-9.08	1.31	1.40
2	A	603	HEC	C3C-C2C	-8.92	1.31	1.40
2	A	611	HEC	C3C-C2C	-8.63	1.31	1.40
2	A	613	HEC	C2B-C3B	-8.62	1.31	1.40
2	A	604	HEC	C2B-C3B	-8.34	1.32	1.40
2	A	606	HEC	C3C-C2C	-8.12	1.32	1.40
2	A	605	HEC	C3C-C2C	-7.92	1.32	1.40
2	A	603	HEC	C2B-C3B	-7.88	1.32	1.40
2	A	601	HEC	C2B-C3B	-7.63	1.32	1.40
2	A	612	HEC	C3C-C2C	-7.55	1.32	1.40
2	A	615	HEC	C2B-C3B	-7.29	1.33	1.40
2	A	607	HEC	C3C-C2C	-7.25	1.33	1.40
2	A	610	HEC	C2B-C3B	-7.09	1.33	1.40
2	A	608	HEC	C3C-C2C	-7.08	1.33	1.40
2	A	602	HEC	C3C-C2C	-6.89	1.33	1.40
2	A	614	HEC	C2B-C3B	-6.89	1.33	1.40
2	A	615	HEC	C3C-C2C	-5.87	1.34	1.40
2	A	616	HEC	C3D-C2D	5.68	1.54	1.37
2	A	601	HEC	C3C-C2C	-5.66	1.34	1.40
2	A	616	HEC	C2B-C3B	-5.65	1.34	1.40
2	A	613	HEC	C3C-C2C	-5.57	1.34	1.40
2	A	604	HEC	C3C-C2C	-5.07	1.35	1.40
2	A	601	HEC	C3D-C2D	5.01	1.52	1.37
2	A	605	HEC	CBB-CAB	-5.00	1.30	1.49
2	A	605	HEC	C2B-C3B	-5.00	1.35	1.40
2	A	610	HEC	C3D-C2D	4.90	1.52	1.37
2	A	602	HEC	C3D-C2D	4.86	1.52	1.37
2	A	607	HEC	C2B-C3B	-4.83	1.35	1.40
2	A	614	HEC	C3C-C2C	-4.77	1.35	1.40
2	A	609	HEC	C3D-C2D	4.75	1.51	1.37
2	A	612	HEC	C2B-C3B	-4.67	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	614	HEC	C3D-C2D	4.62	1.51	1.37
2	A	603	HEC	CBC-CAC	-4.60	1.32	1.49
2	A	613	HEC	C3D-C2D	4.55	1.51	1.37
2	A	614	HEC	CBB-CAB	-4.53	1.32	1.49
2	A	605	HEC	C3D-C2D	4.42	1.50	1.37
2	A	607	HEC	CAA-C2A	4.40	1.59	1.52
2	A	612	HEC	C3D-C2D	4.39	1.50	1.37
2	A	608	HEC	CBC-CAC	-4.38	1.33	1.49
2	A	603	HEC	C3D-C2D	4.30	1.50	1.37
2	A	615	HEC	C3D-C2D	4.28	1.50	1.37
2	A	607	HEC	CBC-CAC	-4.24	1.33	1.49
2	A	607	HEC	C3D-C2D	4.23	1.50	1.37
2	A	606	HEC	C3D-C2D	4.21	1.50	1.37
2	A	608	HEC	C3D-C2D	4.19	1.50	1.37
2	A	616	HEC	CBC-CAC	-4.19	1.33	1.49
2	A	611	HEC	C3D-C2D	4.16	1.50	1.37
2	A	609	HEC	C2B-C3B	-4.15	1.36	1.40
2	A	609	HEC	CBC-CAC	-4.13	1.34	1.49
2	A	611	HEC	CBC-CAC	-4.09	1.34	1.49
2	A	612	HEC	CBB-CAB	-4.03	1.34	1.49
2	A	610	HEC	CBB-CAB	-3.94	1.34	1.49
2	A	613	HEC	CBC-CAC	-3.94	1.34	1.49
2	A	611	HEC	CBB-CAB	-3.92	1.34	1.49
2	A	603	HEC	CBB-CAB	-3.87	1.35	1.49
2	A	610	HEC	C3C-C4C	3.87	1.50	1.43
2	A	607	HEC	CBB-CAB	-3.87	1.35	1.49
2	A	606	HEC	CBB-CAB	-3.85	1.35	1.49
2	A	616	HEC	CBB-CAB	-3.79	1.35	1.49
2	A	604	HEC	C3D-C2D	3.78	1.48	1.37
2	A	602	HEC	CBB-CAB	-3.78	1.35	1.49
2	A	614	HEC	CBC-CAC	-3.76	1.35	1.49
2	A	610	HEC	C3C-C2C	-3.63	1.37	1.40
2	A	604	HEC	CBB-CAB	-3.58	1.36	1.49
2	A	614	HEC	O1D-CGD	3.58	1.34	1.22
2	A	605	HEC	CBC-CAC	-3.51	1.36	1.49
2	A	609	HEC	CAA-C2A	3.49	1.58	1.52
2	A	603	HEC	CAA-C2A	3.44	1.58	1.52
2	A	610	HEC	CBC-CAC	-3.44	1.36	1.49
2	A	607	HEC	C1D-ND	3.41	1.43	1.36
2	A	604	HEC	CBC-CAC	-3.39	1.36	1.49
2	A	602	HEC	CBC-CAC	-3.37	1.36	1.49
2	A	601	HEC	CBC-CAC	-3.36	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	612	HEC	CBC-CAC	-3.34	1.37	1.49
2	A	615	HEC	CBC-CAC	-3.32	1.37	1.49
2	A	606	HEC	CBC-CAC	-3.28	1.37	1.49
2	A	615	HEC	CBB-CAB	-3.20	1.37	1.49
2	A	605	HEC	O1D-CGD	3.18	1.32	1.22
2	A	605	HEC	C3C-C4C	3.10	1.48	1.43
2	A	608	HEC	CBB-CAB	-3.07	1.38	1.49
2	A	614	HEC	O1A-CGA	2.96	1.31	1.22
2	A	601	HEC	CMC-C2C	2.89	1.58	1.51
2	A	608	HEC	C1D-CHD	-2.89	1.32	1.41
2	A	601	HEC	CBB-CAB	-2.84	1.38	1.49
2	A	616	HEC	CMB-C2B	2.79	1.58	1.51
2	A	610	HEC	CAA-C2A	2.77	1.57	1.52
2	A	616	HEC	C1D-CHD	-2.75	1.33	1.41
2	A	613	HEC	CAD-C3D	2.70	1.56	1.52
2	A	601	HEC	CAA-C2A	2.68	1.56	1.52
2	A	602	HEC	CAA-C2A	2.62	1.56	1.52
2	A	614	HEC	CAA-C2A	2.58	1.56	1.52
2	A	611	HEC	CMD-C2D	2.58	1.57	1.51
2	A	616	HEC	C1B-NB	2.56	1.41	1.36
2	A	615	HEC	C4D-ND	2.55	1.41	1.36
2	A	608	HEC	C1C-CHC	-2.55	1.33	1.41
2	A	602	HEC	C3C-C4C	2.55	1.47	1.43
2	A	607	HEC	CMA-C3A	2.53	1.57	1.51
2	A	606	HEC	C2A-C3A	-2.51	1.30	1.37
2	A	608	HEC	C2A-C3A	-2.50	1.30	1.37
2	A	609	HEC	O1A-CGA	2.48	1.30	1.22
2	A	602	HEC	C1C-CHC	-2.46	1.34	1.41
2	A	612	HEC	C1C-CHC	-2.44	1.34	1.41
2	A	610	HEC	O1D-CGD	2.41	1.30	1.22
2	A	604	HEC	O1D-CGD	2.34	1.29	1.22
2	A	604	HEC	CAD-C3D	2.34	1.55	1.52
2	A	603	HEC	CMB-C2B	2.34	1.57	1.51
2	A	610	HEC	CAD-C3D	2.33	1.55	1.52
2	A	601	HEC	C1C-CHC	-2.32	1.34	1.41
2	A	613	HEC	CBB-CAB	-2.32	1.40	1.49
2	A	601	HEC	C4D-CHA	-2.31	1.34	1.41
2	A	612	HEC	C1D-ND	2.26	1.40	1.36
2	A	609	HEC	C1C-NC	2.23	1.40	1.36
2	A	612	HEC	CMB-C2B	2.22	1.56	1.51
2	A	606	HEC	O1D-CGD	2.20	1.29	1.22
2	A	606	HEC	C4D-CHA	-2.19	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	613	HEC	C4B-C3B	2.19	1.47	1.43
2	A	603	HEC	CAD-C3D	2.17	1.55	1.52
2	A	607	HEC	C4D-ND	2.16	1.40	1.36
2	A	601	HEC	CMB-C2B	2.15	1.56	1.51
2	A	606	HEC	CBD-CGD	2.14	1.55	1.50
2	A	605	HEC	C4D-CHA	-2.10	1.35	1.41
2	A	604	HEC	C1D-CHD	-2.08	1.35	1.41
2	A	609	HEC	CBB-CAB	-2.08	1.41	1.49
2	A	605	HEC	CAD-C3D	2.07	1.55	1.52
2	A	612	HEC	O2A-CGA	-2.04	1.23	1.30
2	A	602	HEC	O1D-CGD	2.03	1.28	1.22
2	A	615	HEC	CAD-C3D	2.03	1.55	1.52
2	A	613	HEC	CMA-C3A	2.02	1.56	1.51
2	A	610	HEC	CMC-C2C	2.01	1.56	1.51
2	A	609	HEC	CBA-CGA	2.00	1.55	1.50

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	604	HEC	CBA-CAA-C2A	-7.82	99.42	112.60
2	A	615	HEC	CMC-C2C-C1C	-6.58	118.35	128.46
2	A	602	HEC	C1D-C2D-C3D	-6.30	102.61	107.00
2	A	612	HEC	CBD-CAD-C3D	-6.14	102.13	112.62
2	A	613	HEC	CBA-CAA-C2A	-6.07	102.37	112.60
2	A	602	HEC	CMB-C2B-C1B	-5.90	119.39	128.46
2	A	611	HEC	CAA-CBA-CGA	-5.77	97.59	113.76
2	A	612	HEC	C1D-C2D-C3D	-5.70	103.03	107.00
2	A	609	HEC	CAD-CBD-CGD	-5.53	98.26	113.76
2	A	616	HEC	C1D-C2D-C3D	-5.46	103.19	107.00
2	A	610	HEC	CMC-C2C-C1C	-5.40	120.16	128.46
2	A	602	HEC	CMB-C2B-C3B	5.40	132.17	125.82
2	A	616	HEC	CBD-CAD-C3D	-5.37	103.46	112.62
2	A	607	HEC	CBD-CAD-C3D	-5.27	103.63	112.62
2	A	609	HEC	CBD-CAD-C3D	-5.18	103.78	112.62
2	A	616	HEC	CMB-C2B-C3B	5.10	131.81	125.82
2	A	604	HEC	CMC-C2C-C1C	-5.09	120.64	128.46
2	A	610	HEC	CBD-CAD-C3D	-5.08	103.95	112.62
2	A	610	HEC	CMC-C2C-C3C	4.89	131.57	125.82
2	A	614	HEC	CBD-CAD-C3D	-4.82	104.40	112.62
2	A	610	HEC	CBA-CAA-C2A	-4.78	104.55	112.60
2	A	605	HEC	CBD-CAD-C3D	-4.78	104.47	112.62
2	A	607	HEC	CMB-C2B-C1B	-4.74	121.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	615	HEC	O2D-CGD-CBD	4.65	128.99	114.03
2	A	601	HEC	CMC-C2C-C1C	-4.62	121.37	128.46
2	A	613	HEC	CMC-C2C-C3C	4.61	131.24	125.82
2	A	613	HEC	CMC-C2C-C1C	-4.52	121.52	128.46
2	A	609	HEC	CMC-C2C-C1C	-4.51	121.53	128.46
2	A	606	HEC	CBD-CAD-C3D	-4.49	104.95	112.62
2	A	615	HEC	CAD-CBD-CGD	4.44	126.21	113.76
2	A	611	HEC	CMC-C2C-C3C	-4.39	120.66	125.82
2	A	603	HEC	CBD-CAD-C3D	-4.39	105.13	112.62
2	A	610	HEC	CMB-C2B-C1B	-4.35	121.78	128.46
2	A	602	HEC	CBD-CAD-C3D	-4.33	105.24	112.62
2	A	606	HEC	CMB-C2B-C1B	-4.29	121.88	128.46
2	A	601	HEC	CMC-C2C-C3C	4.19	130.75	125.82
2	A	608	HEC	CMC-C2C-C1C	-3.97	122.36	128.46
2	A	616	HEC	CMB-C2B-C1B	-3.97	122.37	128.46
2	A	608	HEC	C1D-C2D-C3D	-3.94	104.26	107.00
2	A	612	HEC	CMC-C2C-C1C	-3.85	122.55	128.46
2	A	607	HEC	CMB-C2B-C3B	3.80	130.29	125.82
2	A	606	HEC	CMB-C2B-C3B	3.60	130.06	125.82
2	A	615	HEC	O1D-CGD-CBD	-3.59	111.55	123.08
2	A	611	HEC	C1D-C2D-C3D	-3.59	104.50	107.00
2	A	607	HEC	CAD-CBD-CGD	-3.55	103.80	113.76
2	A	611	HEC	CAA-C2A-C3A	-3.52	117.13	127.25
2	A	607	HEC	O1D-CGD-CBD	-3.49	111.85	123.08
2	A	609	HEC	CMB-C2B-C1B	-3.39	123.26	128.46
2	A	614	HEC	CMC-C2C-C1C	-3.37	123.28	128.46
2	A	608	HEC	CMB-C2B-C1B	-3.32	123.36	128.46
2	A	606	HEC	C1D-C2D-C3D	-3.30	104.70	107.00
2	A	611	HEC	O1A-CGA-CBA	-3.26	112.61	123.08
2	A	612	HEC	CAA-CBA-CGA	-3.25	104.64	113.76
2	A	615	HEC	CAA-CBA-CGA	-3.23	104.72	113.76
2	A	615	HEC	CBD-CAD-C3D	-3.12	107.29	112.62
2	A	616	HEC	CMD-C2D-C3D	3.11	130.80	124.94
2	A	611	HEC	C2B-C3B-C4B	3.09	109.69	106.35
2	A	601	HEC	C1D-C2D-C3D	-3.09	104.84	107.00
2	A	610	HEC	C1D-C2D-C3D	-3.05	104.88	107.00
2	A	603	HEC	CMD-C2D-C1D	2.97	133.02	128.46
2	A	601	HEC	CBD-CAD-C3D	-2.96	107.56	112.62
2	A	602	HEC	O2A-CGA-O1A	-2.92	116.02	123.30
2	A	614	HEC	CAD-CBD-CGD	-2.90	105.63	113.76
2	A	603	HEC	C2B-C3B-C4B	2.86	109.44	106.35
2	A	613	HEC	CMD-C2D-C1D	-2.85	124.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	603	HEC	CAA-CBA-CGA	-2.84	105.79	113.76
2	A	612	HEC	CMC-C2C-C3C	2.81	129.13	125.82
2	A	616	HEC	O2D-CGD-CBD	2.81	123.06	114.03
2	A	603	HEC	CMC-C2C-C1C	-2.81	124.15	128.46
2	A	610	HEC	O2A-CGA-O1A	-2.80	116.32	123.30
2	A	607	HEC	O2D-CGD-CBD	2.65	122.53	114.03
2	A	612	HEC	CMD-C2D-C1D	2.64	132.53	128.46
2	A	610	HEC	O1D-CGD-CBD	-2.64	114.59	123.08
2	A	606	HEC	CAA-CBA-CGA	-2.62	106.42	113.76
2	A	614	HEC	O2D-CGD-O1D	2.57	129.71	123.30
2	A	615	HEC	CAD-C3D-C2D	-2.56	119.89	127.25
2	A	613	HEC	O2D-CGD-CBD	2.51	122.08	114.03
2	A	612	HEC	CMB-C2B-C1B	-2.50	124.63	128.46
2	A	603	HEC	CMA-C3A-C2A	2.50	129.65	124.94
2	A	614	HEC	CMD-C2D-C1D	-2.48	124.65	128.46
2	A	607	HEC	CMC-C2C-C1C	-2.48	124.65	128.46
2	A	613	HEC	CMD-C2D-C3D	2.48	129.62	124.94
2	A	603	HEC	C1D-C2D-C3D	-2.46	105.29	107.00
2	A	607	HEC	O2A-CGA-CBA	2.43	121.84	114.03
2	A	608	HEC	CAA-CBA-CGA	-2.42	106.97	113.76
2	A	611	HEC	CAD-C3D-C2D	-2.39	120.36	127.25
2	A	613	HEC	CAA-CBA-CGA	-2.37	107.11	113.76
2	A	602	HEC	CMC-C2C-C1C	-2.35	124.85	128.46
2	A	610	HEC	O2A-CGA-CBA	2.34	121.55	114.03
2	A	616	HEC	O1D-CGD-CBD	-2.31	115.67	123.08
2	A	611	HEC	CMD-C2D-C1D	2.31	132.01	128.46
2	A	608	HEC	CAD-CBD-CGD	-2.30	107.31	113.76
2	A	606	HEC	C2B-C3B-C4B	2.28	108.81	106.35
2	A	616	HEC	CBA-CAA-C2A	-2.27	108.77	112.60
2	A	606	HEC	CMC-C2C-C1C	-2.26	124.99	128.46
2	A	607	HEC	CMC-C2C-C3C	-2.26	123.17	125.82
2	A	613	HEC	O1A-CGA-CBA	-2.25	115.85	123.08
2	A	608	HEC	CMD-C2D-C3D	2.24	129.17	124.94
2	A	608	HEC	C2B-C3B-C4B	-2.22	103.95	106.35
2	A	603	HEC	CMB-C2B-C1B	-2.19	125.09	128.46
2	A	615	HEC	CAA-C2A-C3A	-2.18	120.98	127.25
2	A	611	HEC	O2A-CGA-CBA	2.17	120.99	114.03
2	A	601	HEC	O2D-CGD-O1D	-2.14	117.95	123.30
2	A	615	HEC	CMB-C2B-C1B	-2.14	125.18	128.46
2	A	607	HEC	CMA-C3A-C2A	2.13	128.96	124.94
2	A	602	HEC	O2A-CGA-CBA	2.12	120.83	114.03
2	A	607	HEC	O1A-CGA-CBA	-2.10	116.34	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	605	HEC	O2A-CGA-CBA	2.10	120.77	114.03
2	A	609	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
2	A	613	HEC	CBD-CAD-C3D	-2.07	109.10	112.62
2	A	612	HEC	CMB-C2B-C3B	2.05	128.23	125.82
2	A	614	HEC	CMD-C2D-C3D	2.03	128.77	124.94
2	A	603	HEC	CMB-C2B-C3B	2.02	128.20	125.82
2	A	611	HEC	CBD-CAD-C3D	-2.02	109.17	112.62
2	A	607	HEC	C1D-C2D-C3D	-2.01	105.60	107.00

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	606	HEC	C1A-C2A-CAA-CBA
2	A	606	HEC	C3A-C2A-CAA-CBA
2	A	611	HEC	C1A-C2A-CAA-CBA
2	A	611	HEC	C3A-C2A-CAA-CBA
2	A	614	HEC	C2D-C3D-CAD-CBD
2	A	614	HEC	C4D-C3D-CAD-CBD
2	A	615	HEC	C1A-C2A-CAA-CBA
2	A	615	HEC	C3A-C2A-CAA-CBA
2	A	615	HEC	C2D-C3D-CAD-CBD
2	A	615	HEC	C4D-C3D-CAD-CBD
2	A	601	HEC	C3D-CAD-CBD-CGD
2	A	604	HEC	C2A-CAA-CBA-CGA
2	A	602	HEC	C2A-CAA-CBA-CGA
2	A	609	HEC	C2D-C3D-CAD-CBD
2	A	609	HEC	C4D-C3D-CAD-CBD
2	A	607	HEC	CAA-CBA-CGA-O1A
2	A	612	HEC	CAD-CBD-CGD-O1D
2	A	609	HEC	CAD-CBD-CGD-O1D
2	A	603	HEC	C3D-CAD-CBD-CGD
2	A	603	HEC	CAA-CBA-CGA-O1A
2	A	608	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAA-CBA-CGA-O1A
2	A	607	HEC	CAA-CBA-CGA-O2A
2	A	611	HEC	CAA-CBA-CGA-O1A
2	A	611	HEC	CAA-CBA-CGA-O2A
2	A	615	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O2A
2	A	603	HEC	CAA-CBA-CGA-O2A
2	A	607	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	A	608	HEC	CAD-CBD-CGD-O2D
2	A	606	HEC	CAD-CBD-CGD-O2D
2	A	609	HEC	CAD-CBD-CGD-O2D
2	A	612	HEC	CAD-CBD-CGD-O2D
2	A	606	HEC	CAD-CBD-CGD-O1D
2	A	602	HEC	CAA-CBA-CGA-O2A
2	A	612	HEC	CAA-CBA-CGA-O1A
2	A	613	HEC	CAA-CBA-CGA-O1A
2	A	604	HEC	CAA-CBA-CGA-O2A
2	A	615	HEC	CAA-CBA-CGA-O1A
2	A	610	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	CAA-CBA-CGA-O1A
2	A	605	HEC	CAD-CBD-CGD-O2D
2	A	606	HEC	CAA-CBA-CGA-O2A
2	A	607	HEC	CAD-CBD-CGD-O1D
2	A	614	HEC	CAD-CBD-CGD-O1D
2	A	610	HEC	CAA-CBA-CGA-O1A
2	A	605	HEC	CAD-CBD-CGD-O1D
2	A	606	HEC	CAA-CBA-CGA-O1A
2	A	612	HEC	CAA-CBA-CGA-O2A
2	A	613	HEC	CAA-CBA-CGA-O2A
2	A	614	HEC	CAD-CBD-CGD-O2D
2	A	610	HEC	C2A-CAA-CBA-CGA
2	A	616	HEC	CAA-CBA-CGA-O2A
2	A	609	HEC	CAA-CBA-CGA-O1A
2	A	603	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

16 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	HEC	6	0
2	A	601	HEC	5	0
2	A	604	HEC	12	0
2	A	602	HEC	5	0
2	A	613	HEC	12	0
2	A	611	HEC	6	0
2	A	616	HEC	7	0
2	A	606	HEC	9	0
2	A	607	HEC	9	0
2	A	612	HEC	7	0
2	A	614	HEC	11	0

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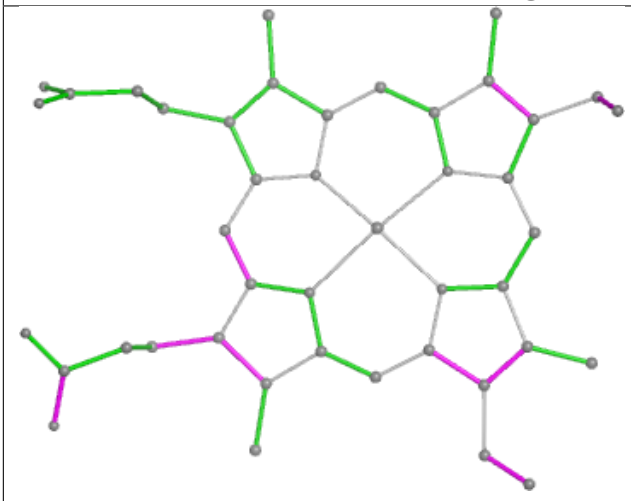
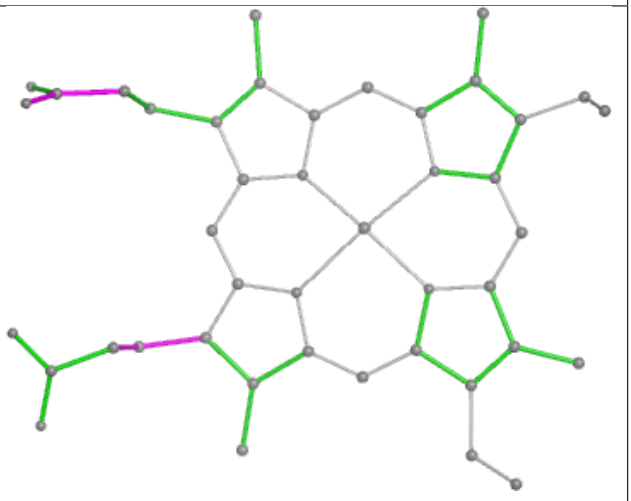
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	609	HEC	7	0
2	A	610	HEC	10	0
2	A	608	HEC	10	0
2	A	603	HEC	10	0
2	A	615	HEC	6	0

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.

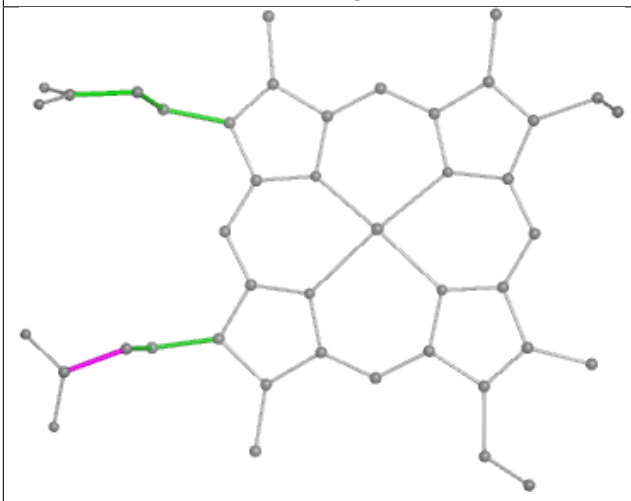
Ligand HEC A 605



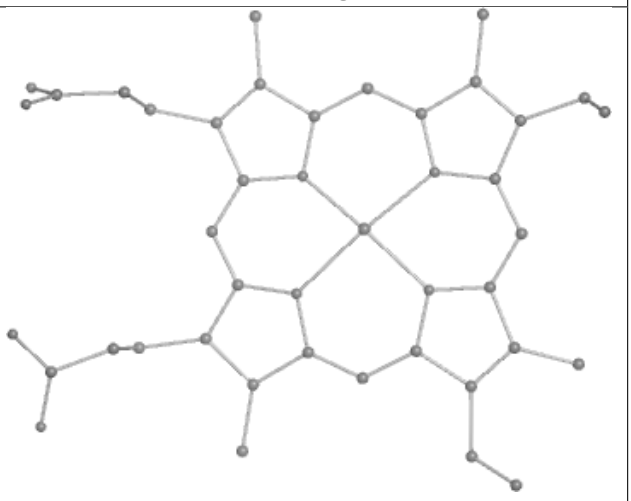
Bond lengths



Bond angles

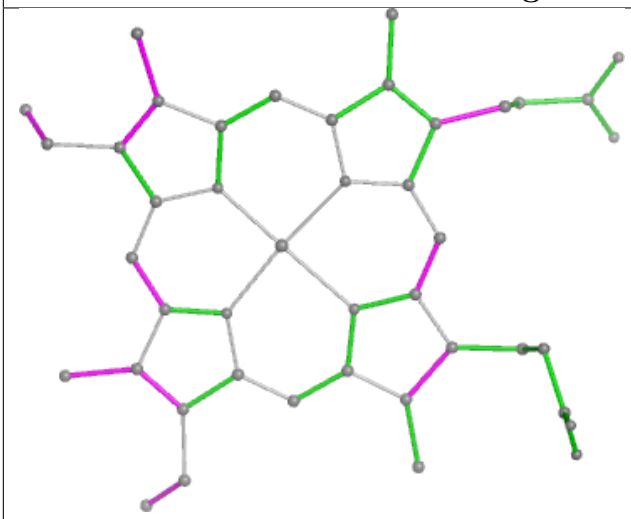


Torsions

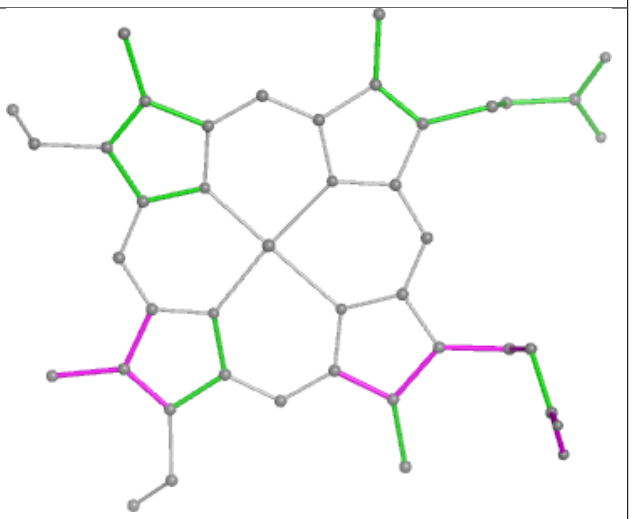


Rings

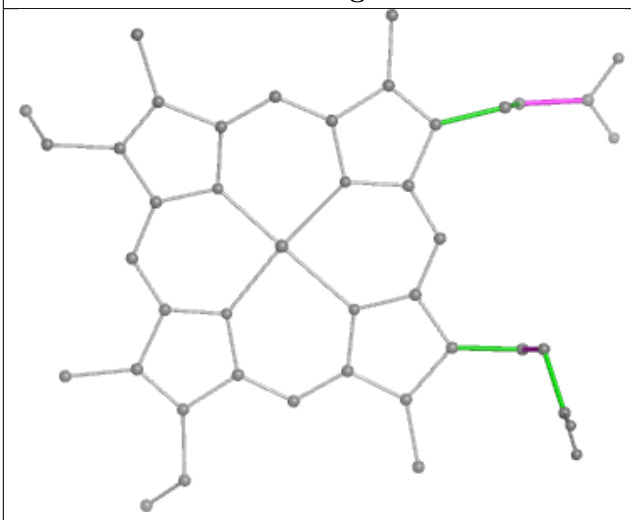
Ligand HEC A 601



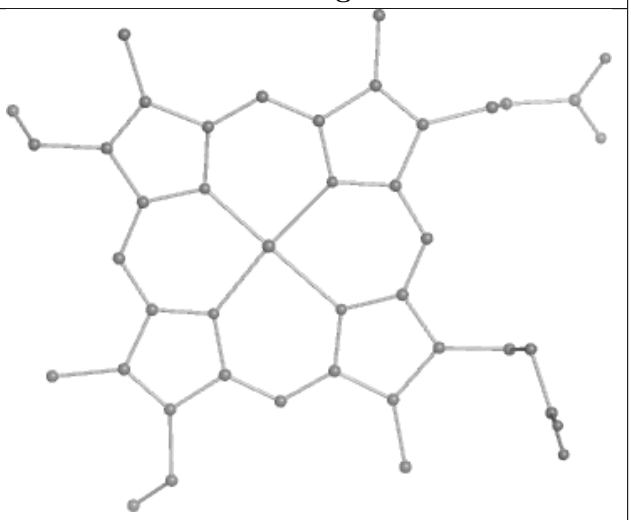
Bond lengths



Bond angles

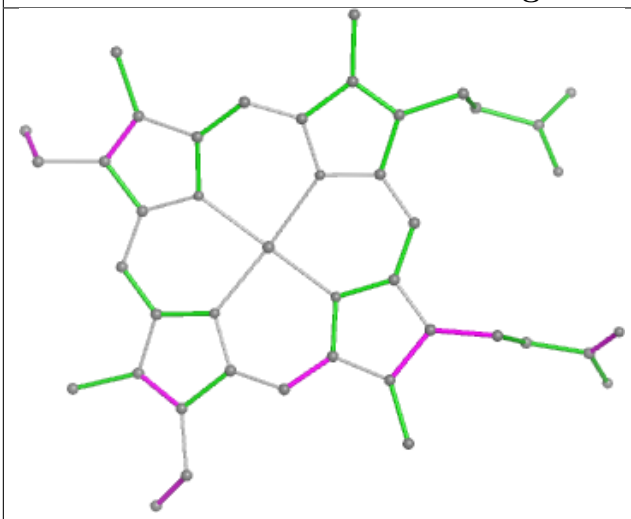


Torsions

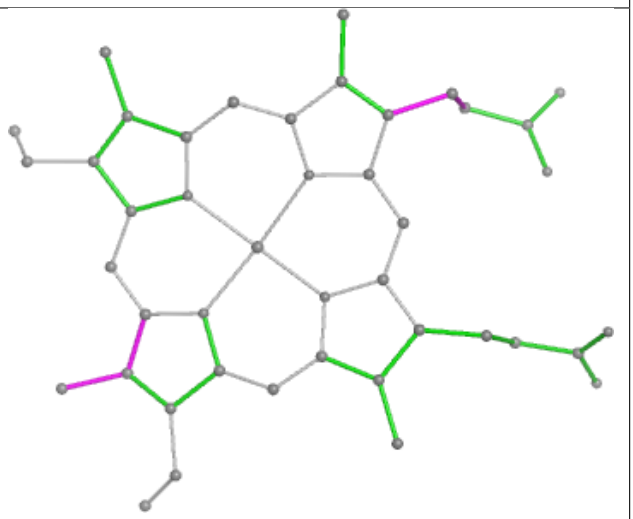


Rings

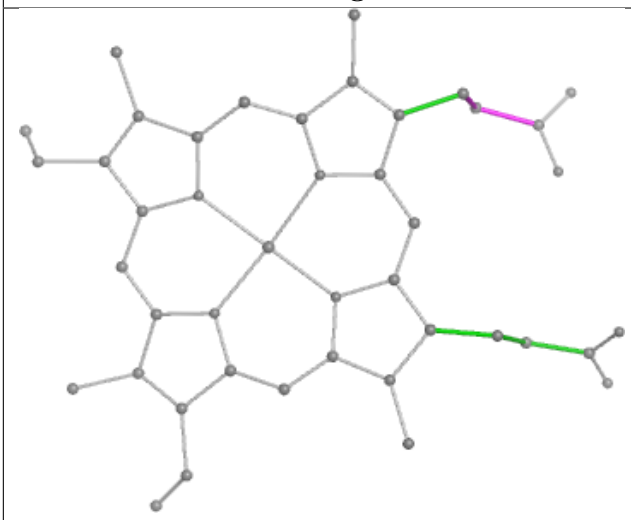
Ligand HEC A 604



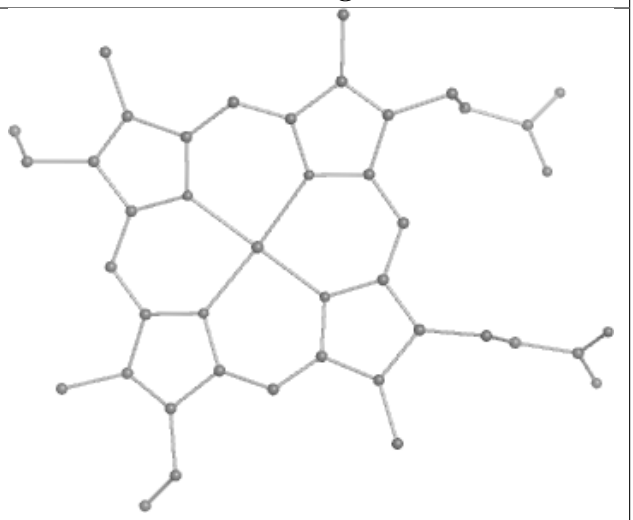
Bond lengths



Bond angles

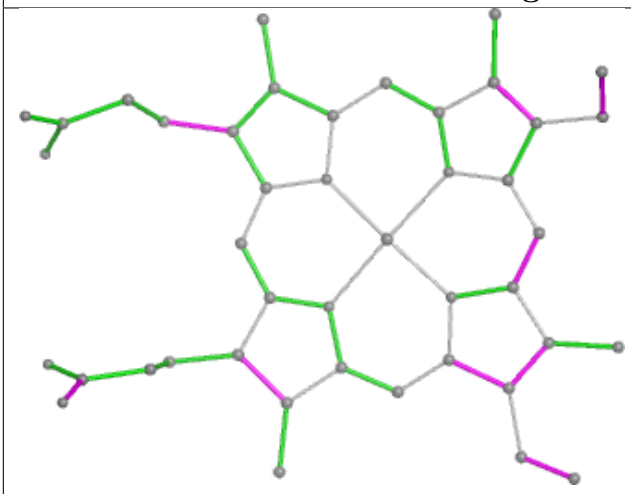


Torsions

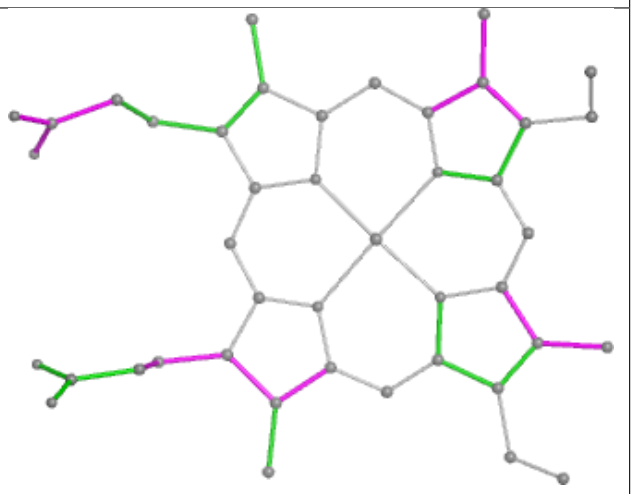


Rings

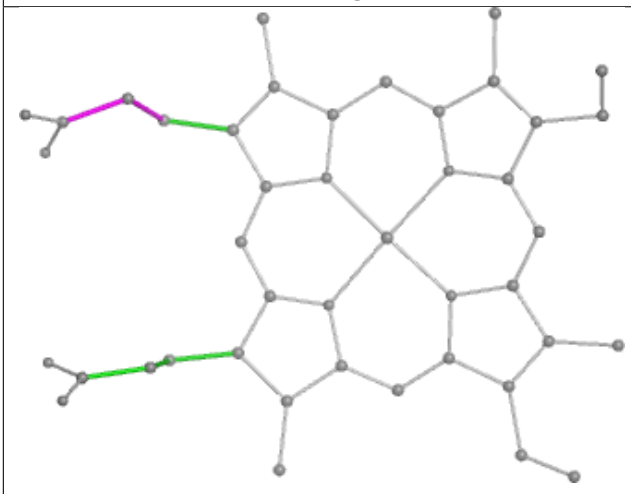
Ligand HEC A 602



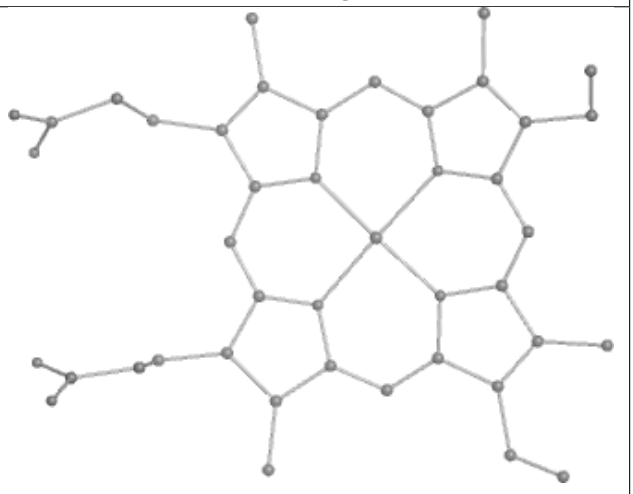
Bond lengths



Bond angles

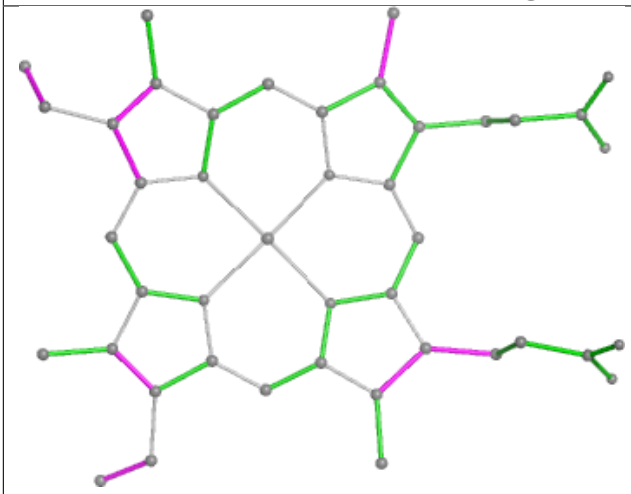


Torsions

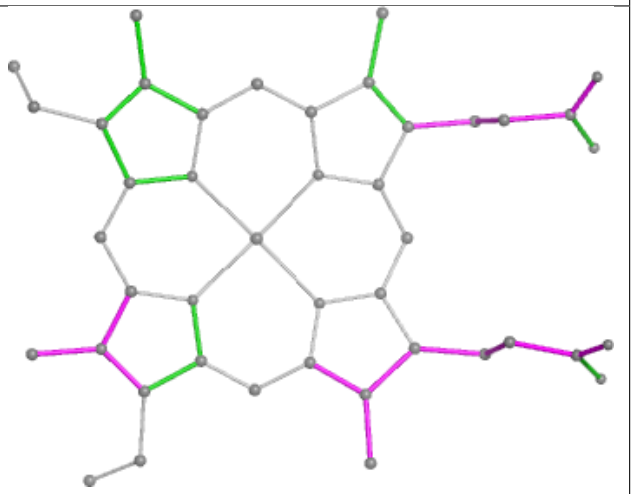


Rings

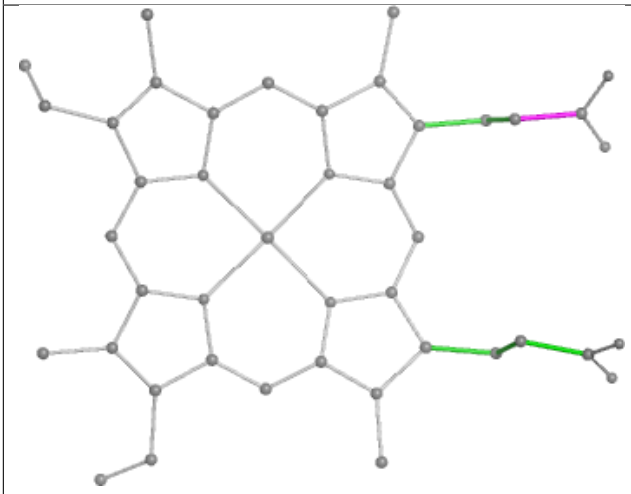
Ligand HEC A 613



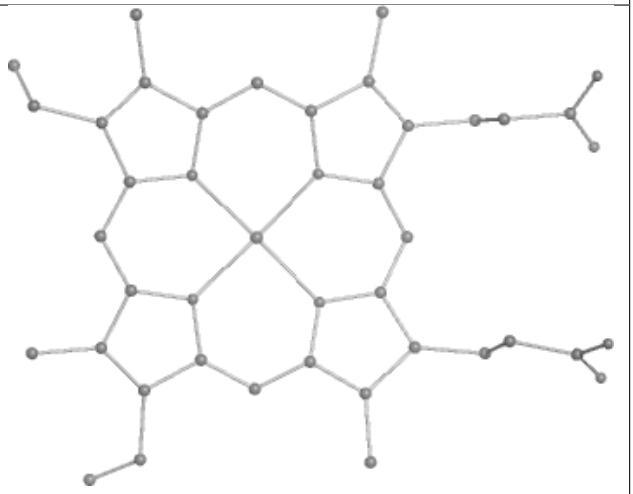
Bond lengths



Bond angles



Torsions



Rings

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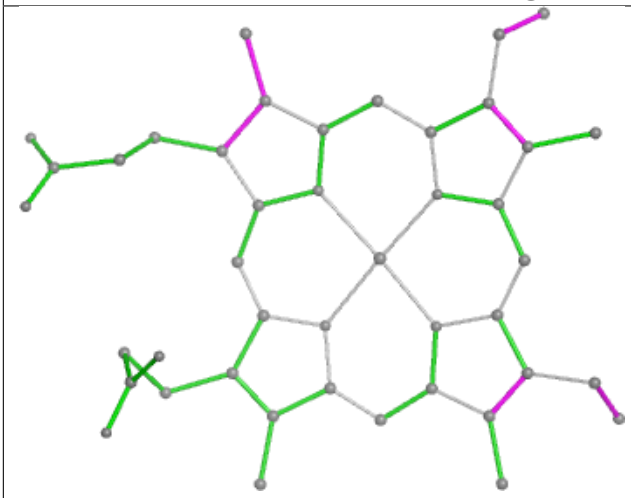

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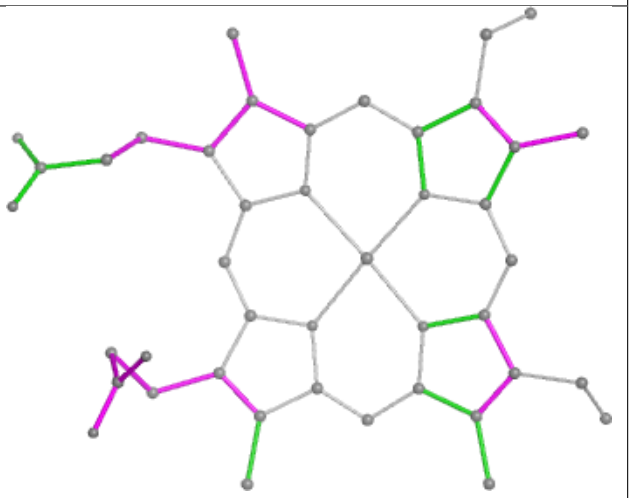
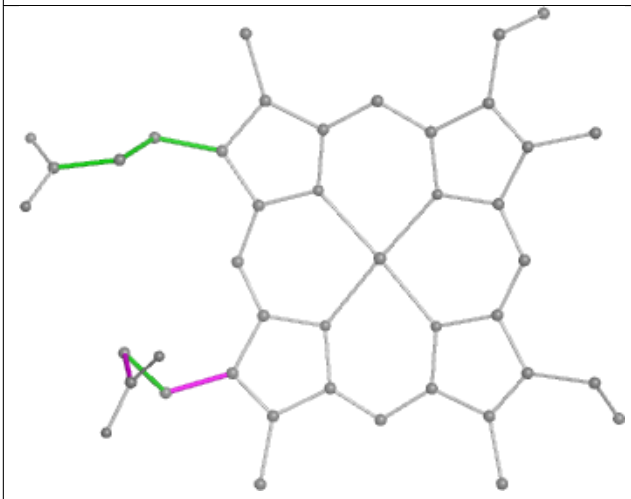
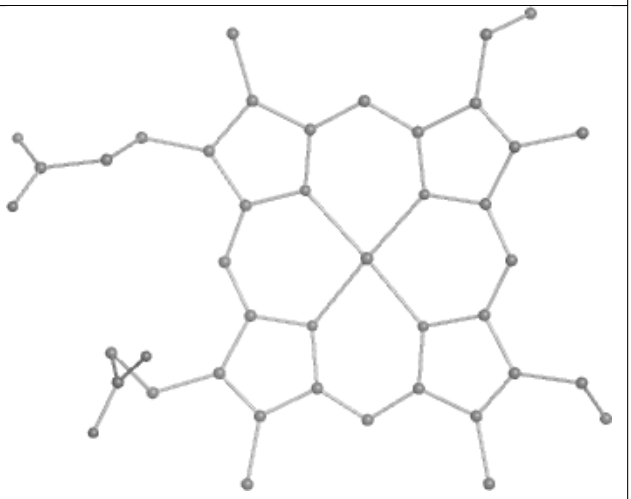


Bond angles

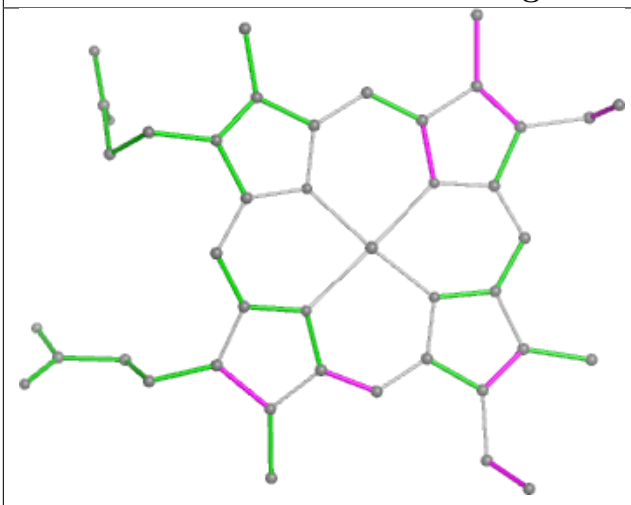


Torsions

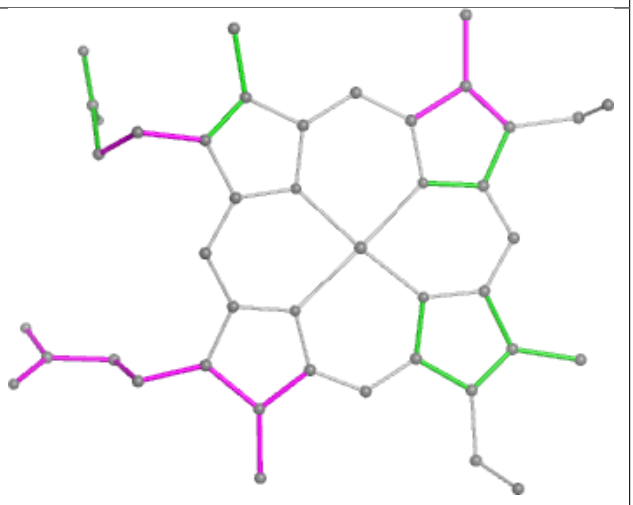


Rings

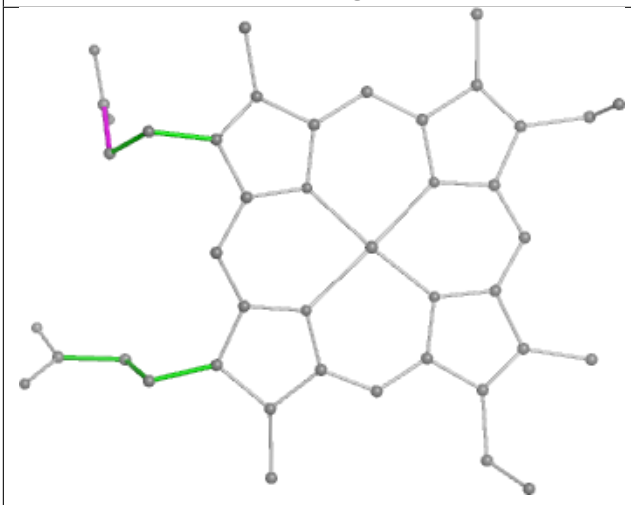
Ligand HEC A 616



Bond lengths



Bond angles



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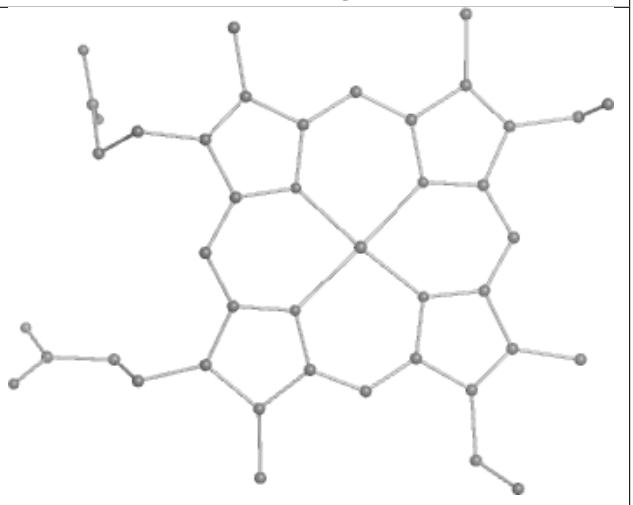
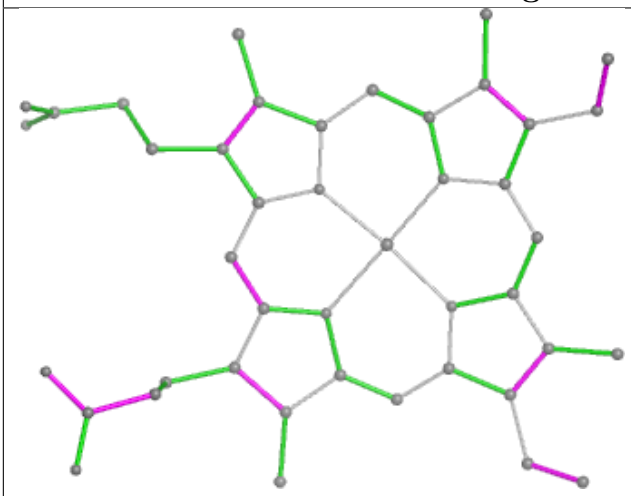
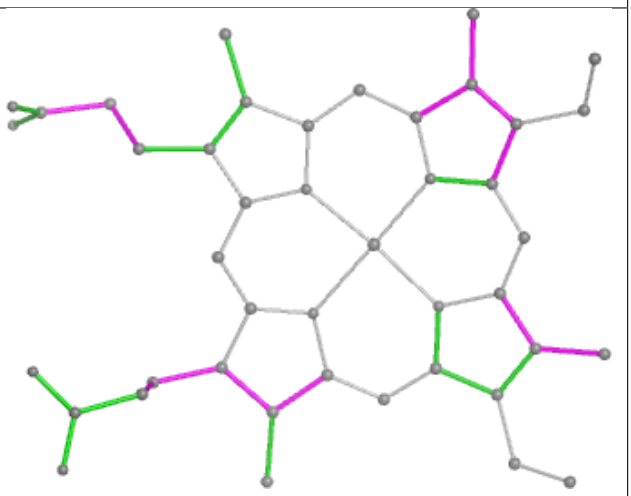


Rings

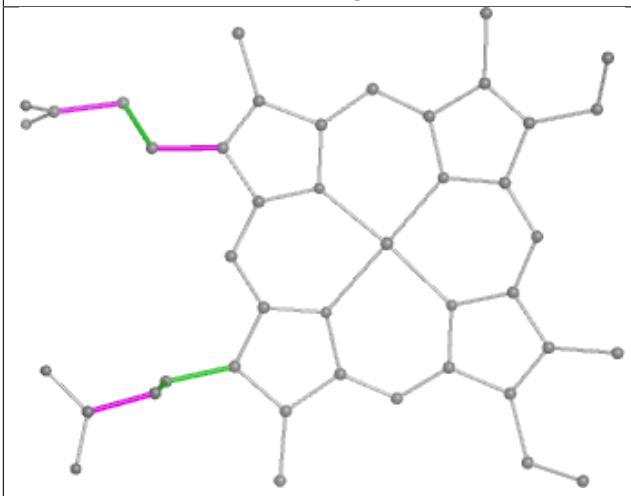
Ligand HEC A 606



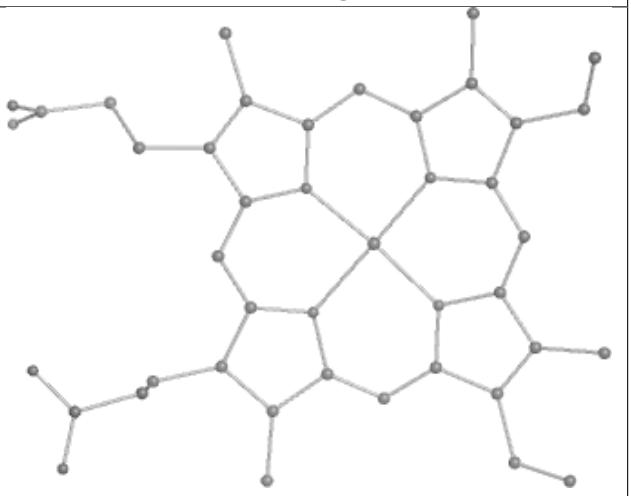
Bond lengths



Bond angles



Torsions



Rings

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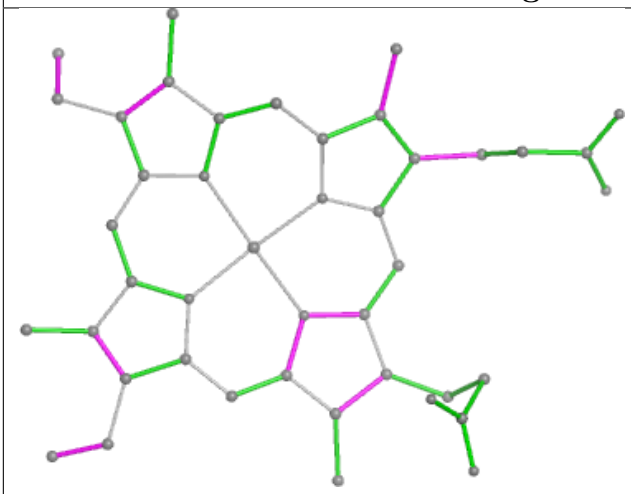
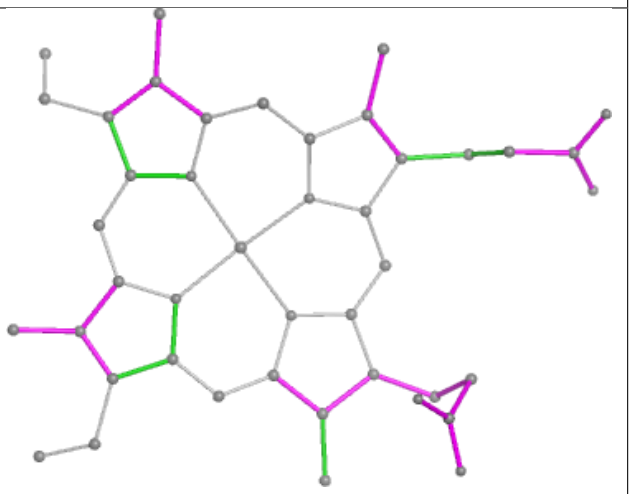
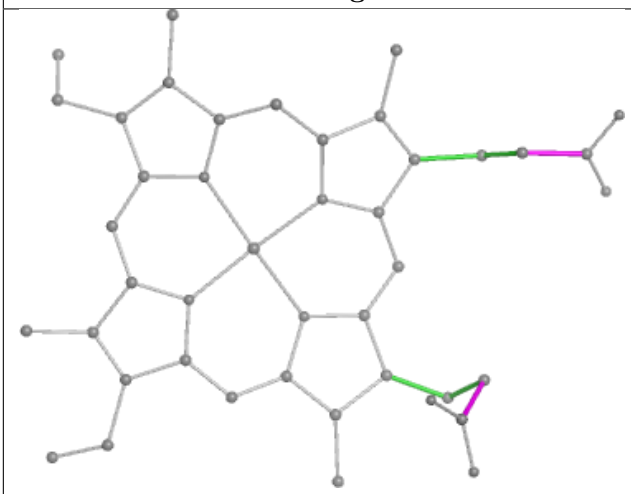


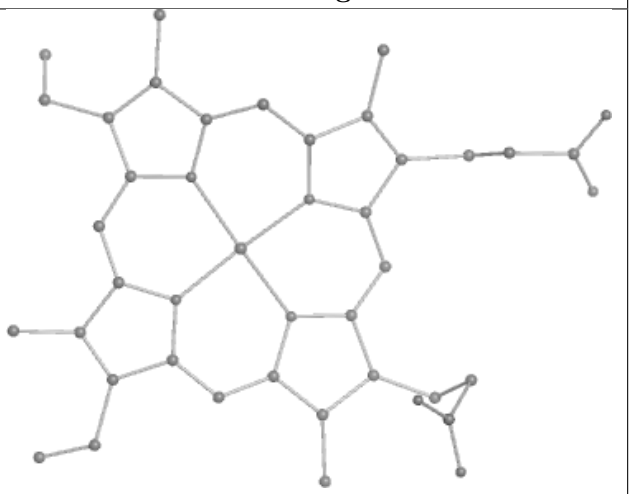
Bond lengths



Bond angles

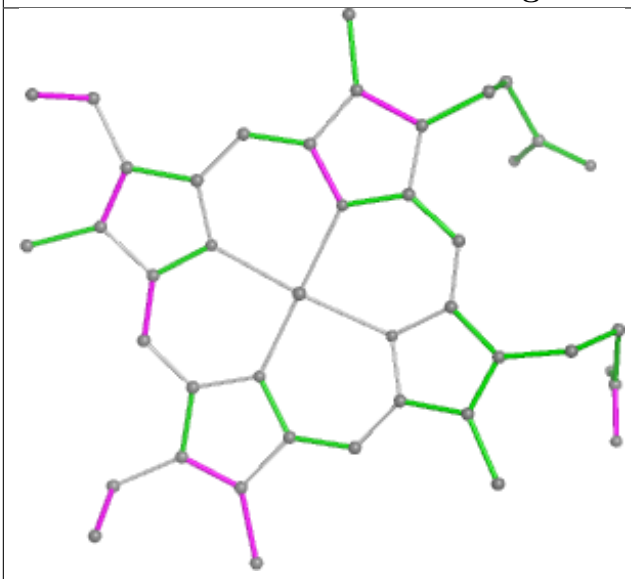


Torsions

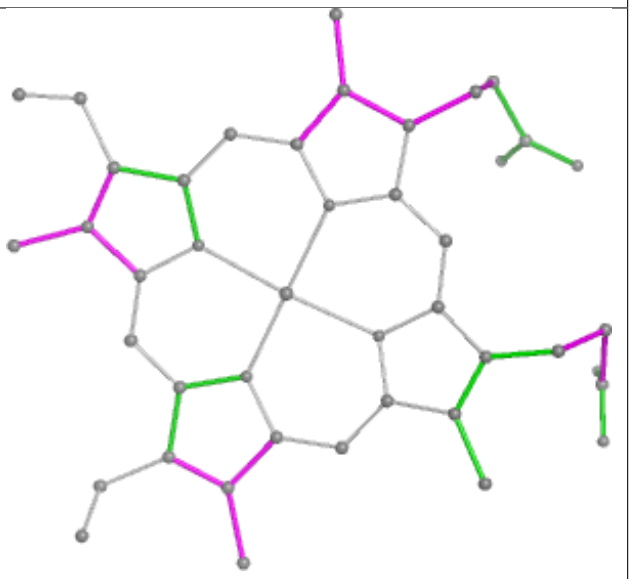


Rings

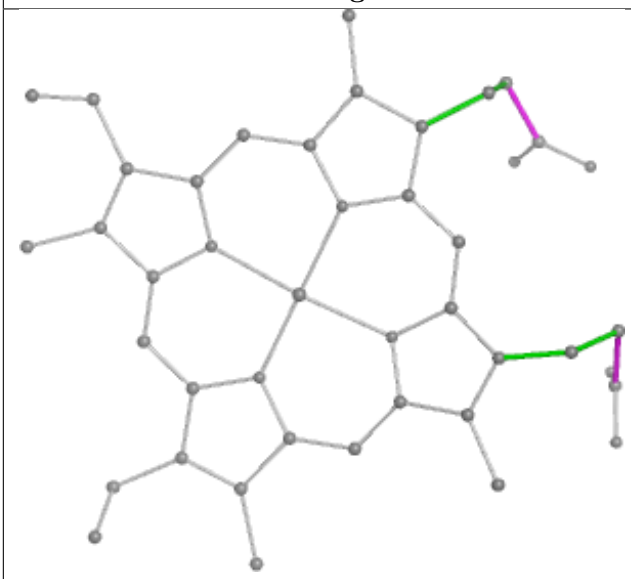
Ligand HEC A 612



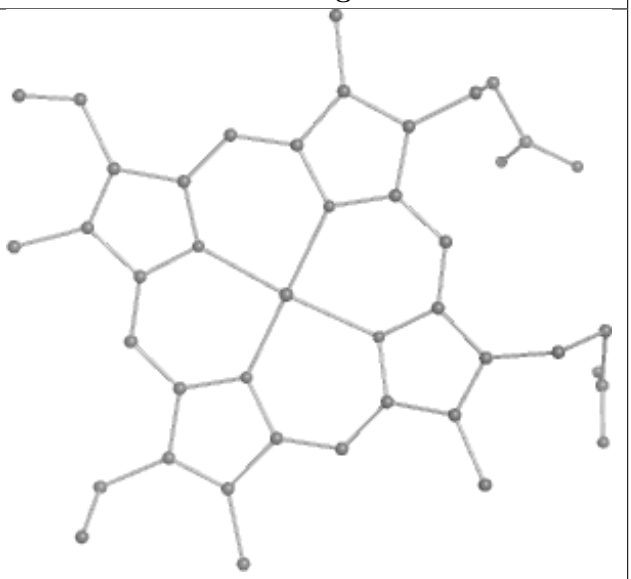
Bond lengths



Bond angles

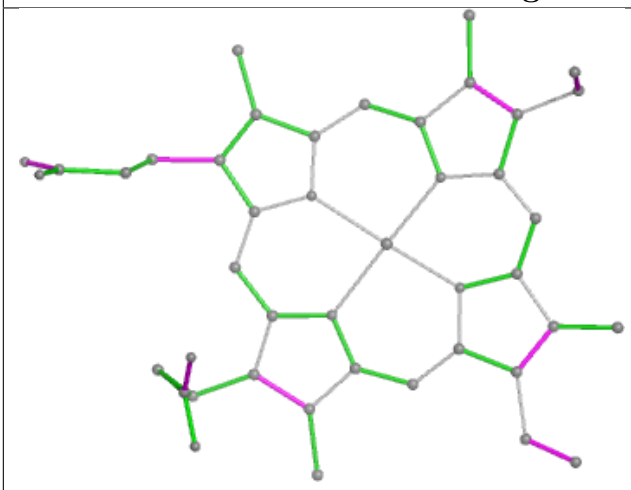


Torsions

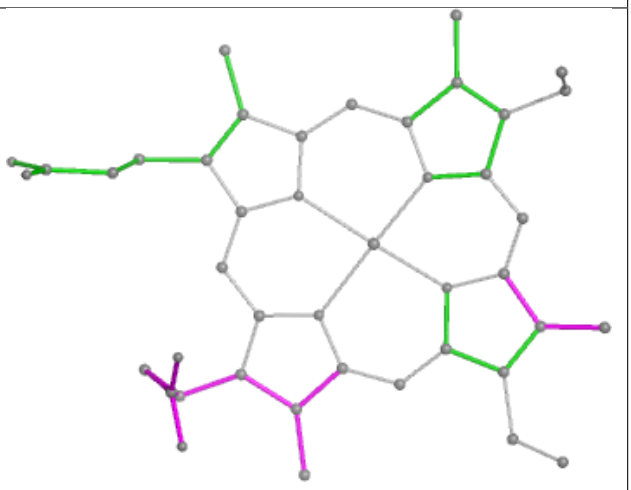


Rings

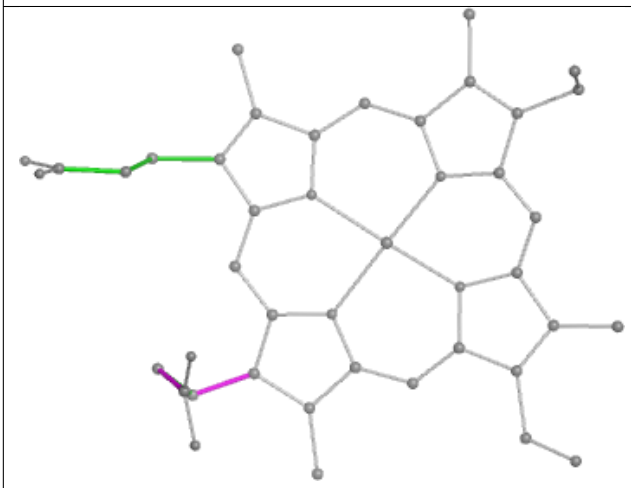
Ligand HEC A 614



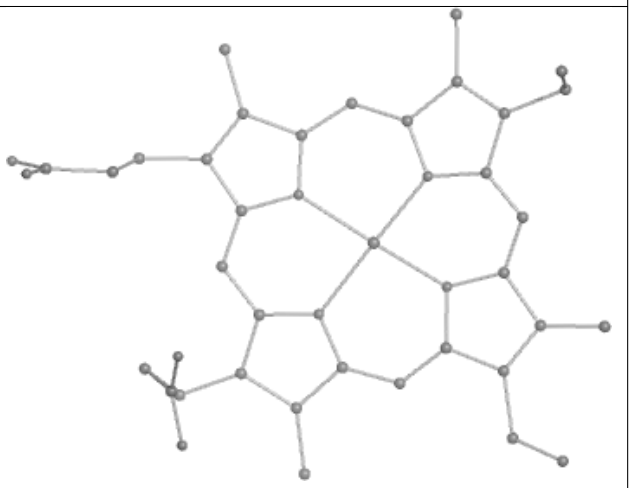
Bond lengths



Bond angles

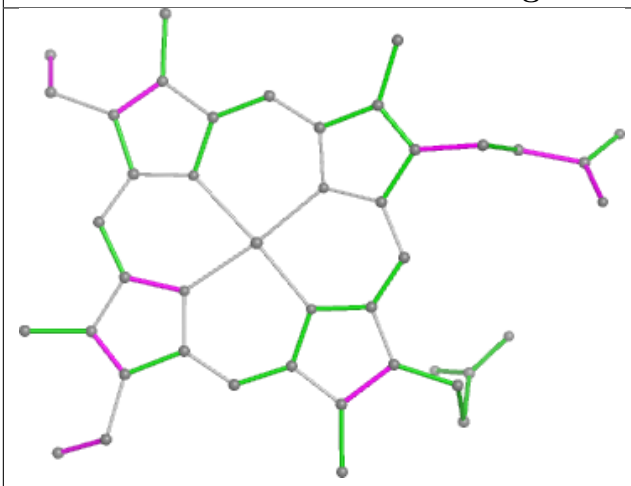


Torsions

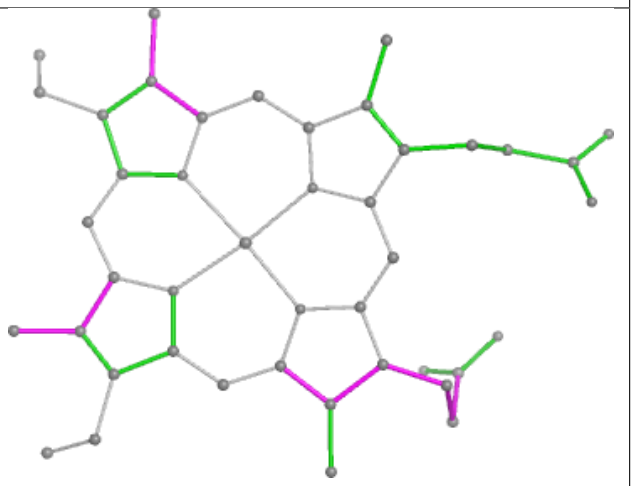


Rings

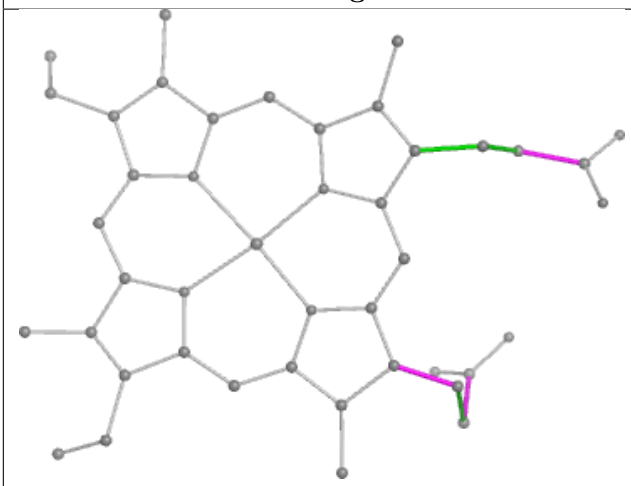
Ligand HEC A 609



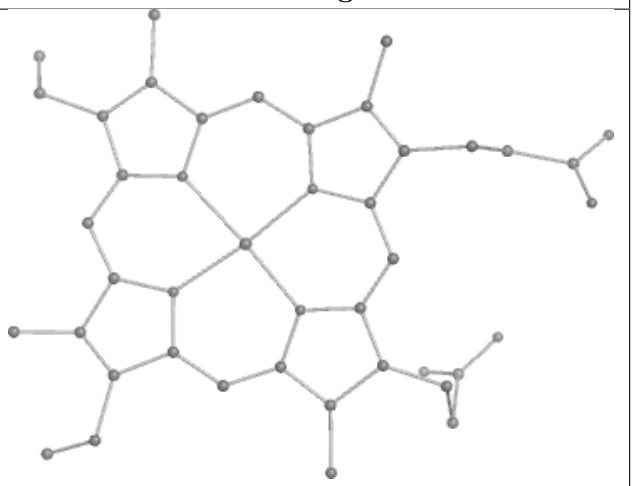
Bond lengths



Bond angles

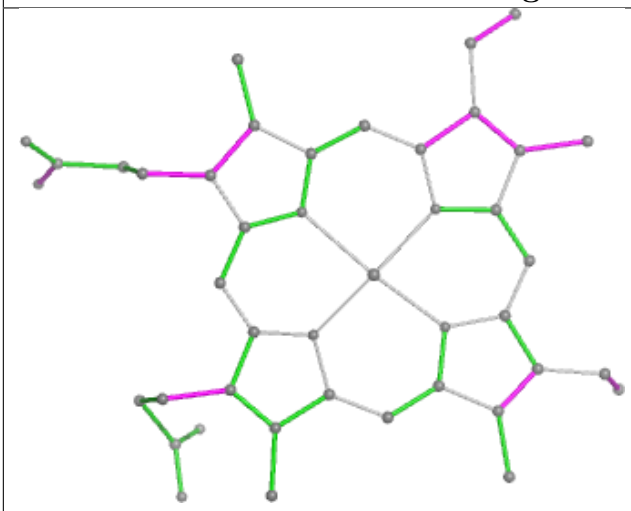


Torsions

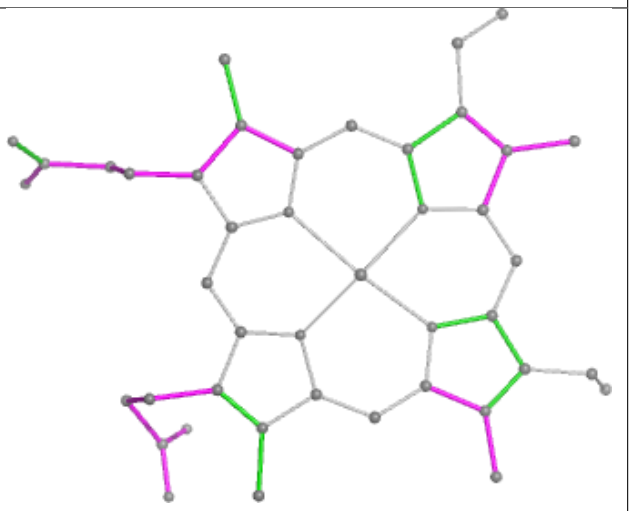


Rings

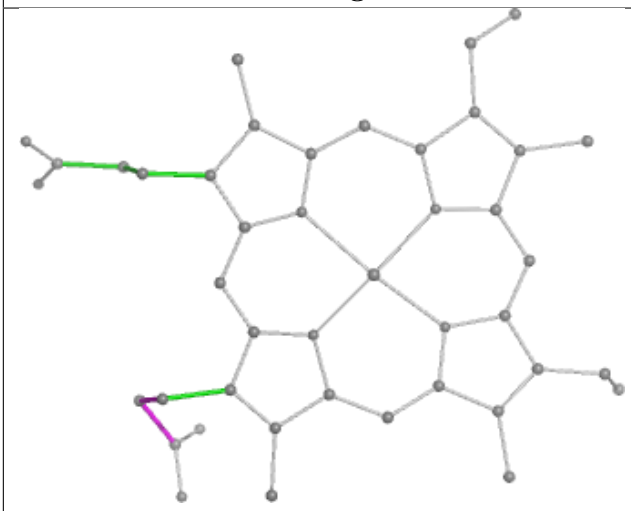
Ligand HEC A 610



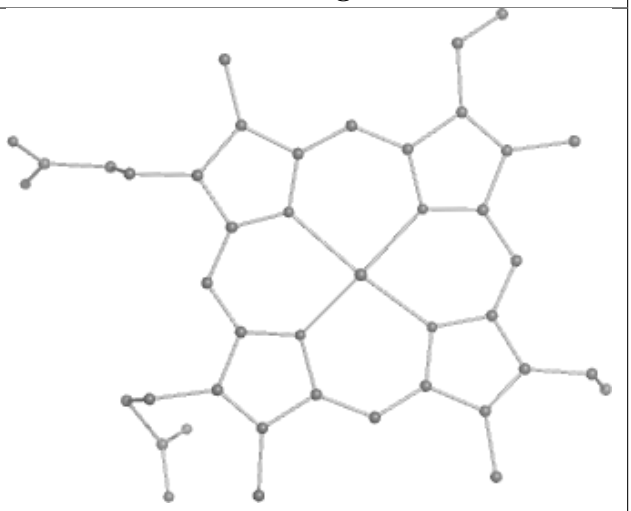
Bond lengths



Bond angles

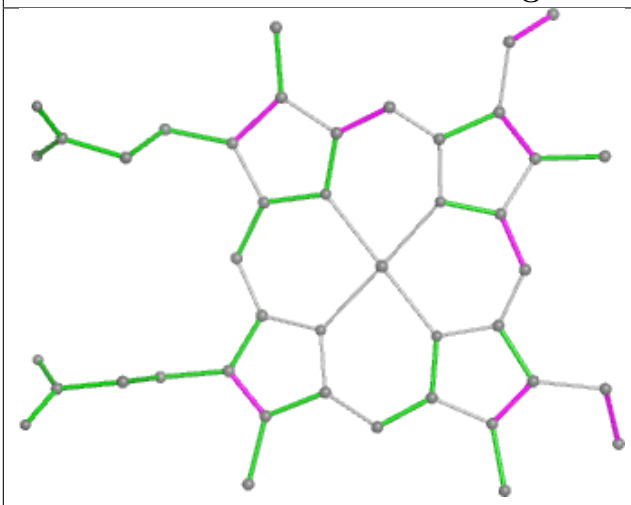


Torsions

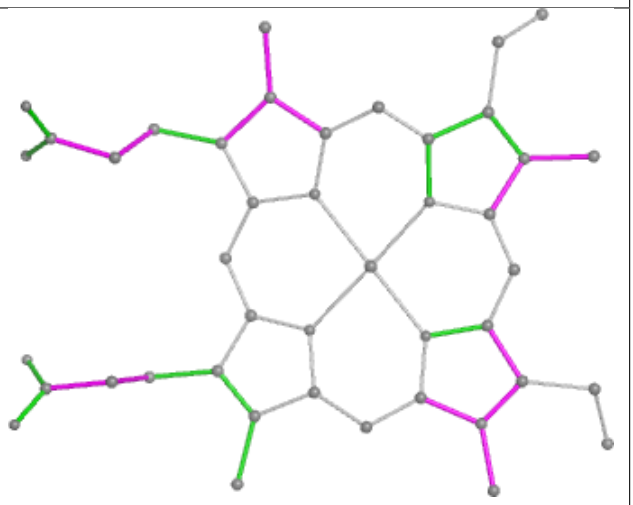


Rings

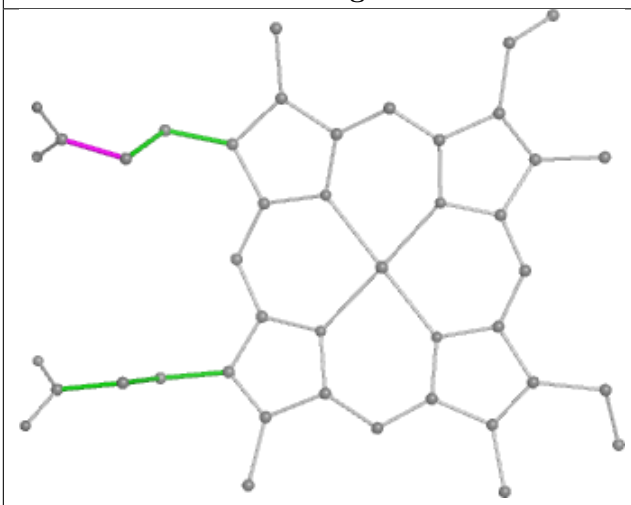
Ligand HEC A 608



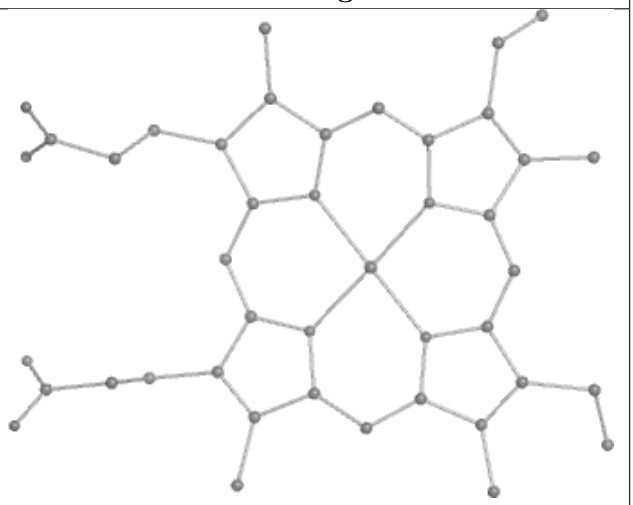
Bond lengths



Bond angles

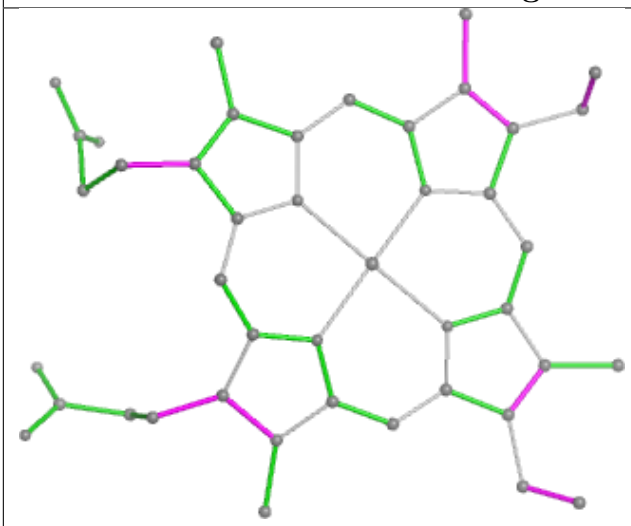


Torsions

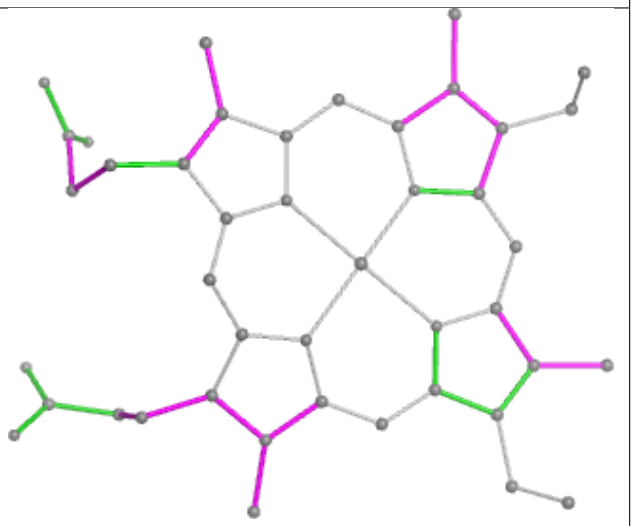


Rings

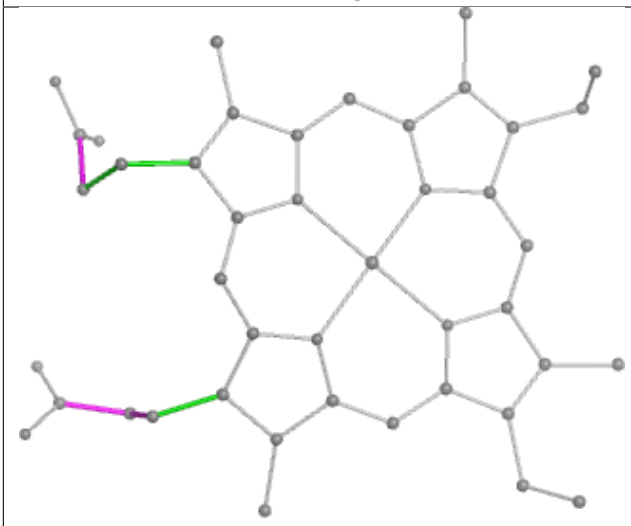
Ligand HEC A 603



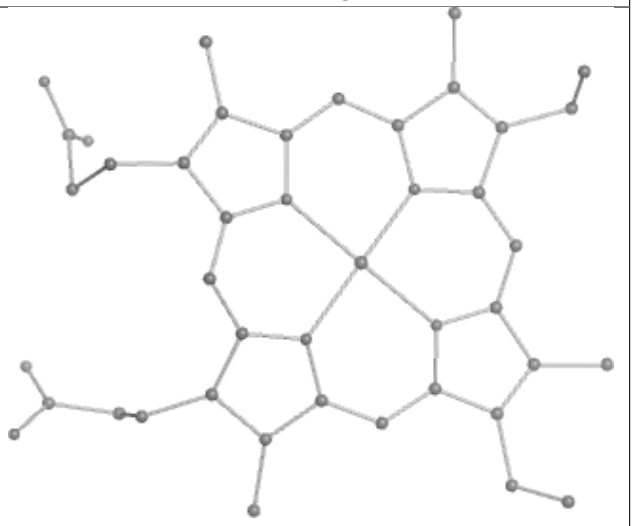
Bond lengths



Bond angles

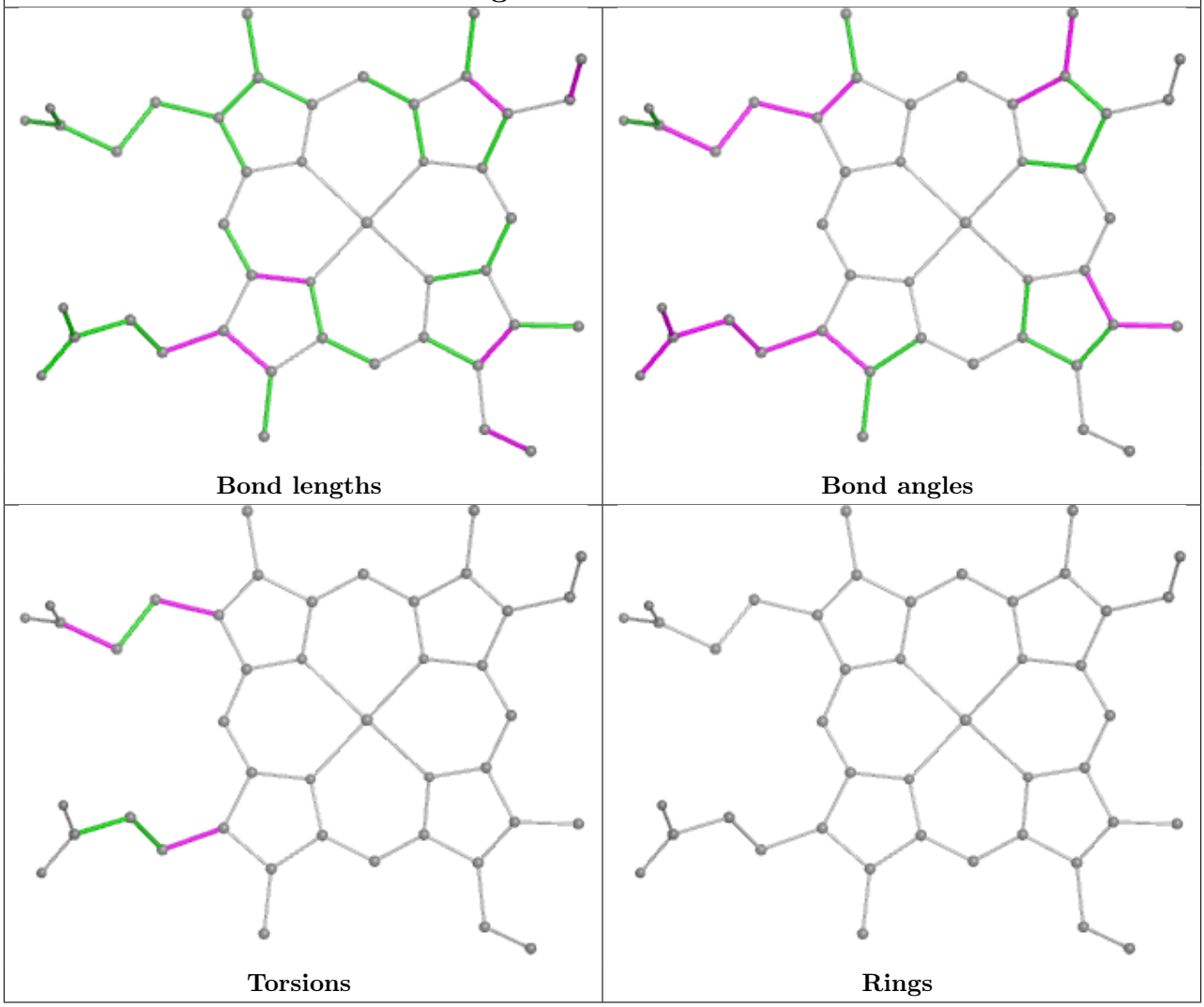


Torsions



Rings

Ligand HEC A 615



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	503/545 (92%)	0.00	25 (4%) 35 32	13, 33, 62, 91	11 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	PRO	26.4
1	A	468	LYS	17.5
1	A	474	ARG	10.1
1	A	512	ARG	8.3
1	A	473	ASP	5.9
1	A	470	PHE	5.2
1	A	476	ASP	3.8
1	A	472	ALA	3.7
1	A	475	GLY	3.5
1	A	10	LYS	3.5
1	A	114	ALA	3.3
1	A	258	GLY	3.3
1	A	471	ASP	3.0
1	A	365	GLY	2.9
1	A	256	MET	2.7
1	A	228	VAL	2.6
1	A	249	GLY	2.6
1	A	229	ARG	2.5
1	A	306	GLU	2.5
1	A	230	GLU	2.4
1	A	112	PRO	2.3
1	A	113	SER	2.3
1	A	390	LYS	2.2
1	A	252	ALA	2.1
1	A	366	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

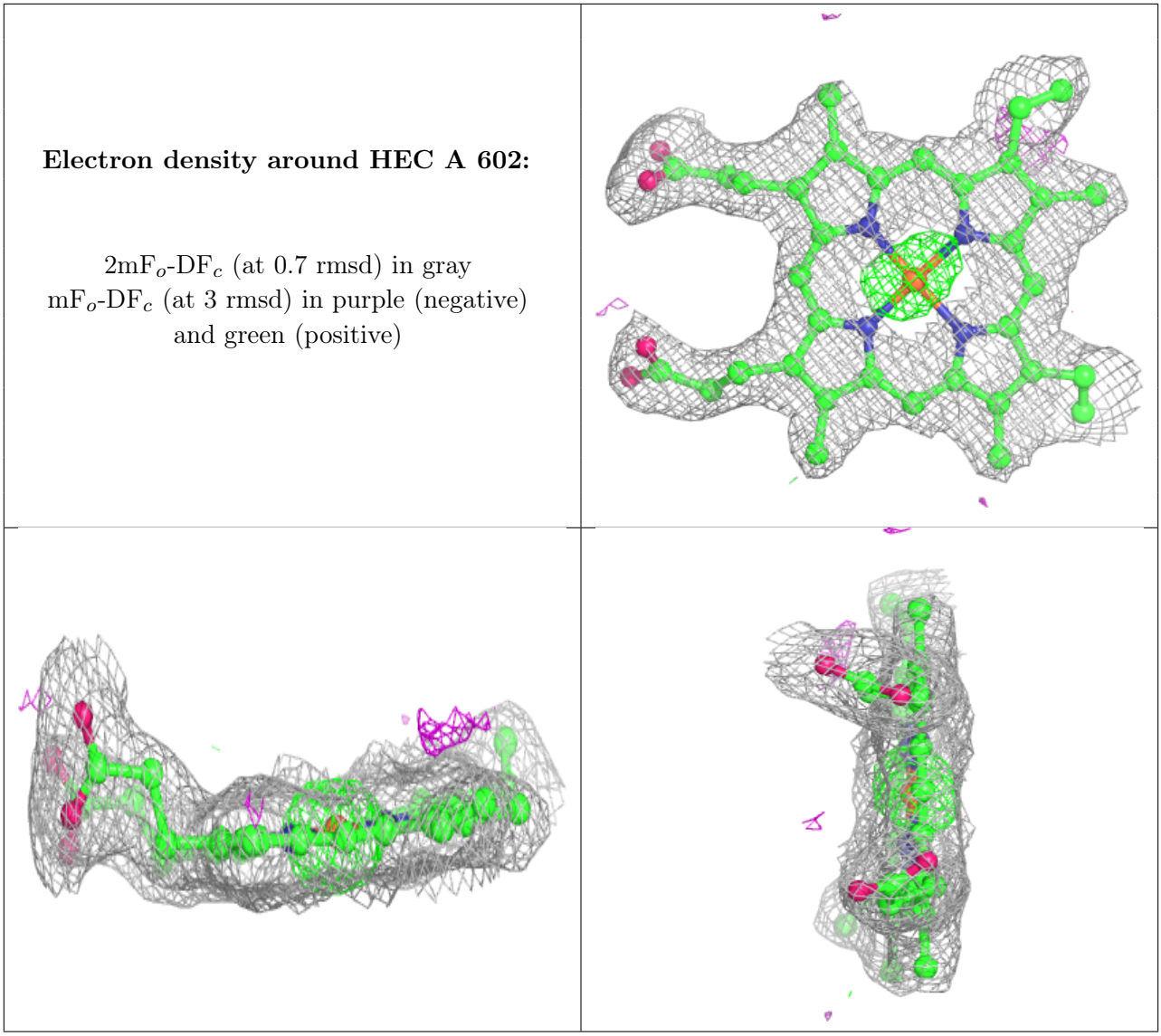
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	602	43/43	0.96	0.08	15,21,31,42	0
2	HEC	A	603	43/43	0.96	0.08	16,22,25,31	0
2	HEC	A	604	43/43	0.96	0.08	22,27,33,37	0
2	HEC	A	605	43/43	0.96	0.08	19,27,41,53	0
2	HEC	A	606	43/43	0.96	0.08	16,24,34,35	0
2	HEC	A	607	43/43	0.96	0.09	20,26,40,43	0
2	HEC	A	608	43/43	0.96	0.08	9,21,27,30	0
2	HEC	A	609	43/43	0.96	0.07	14,27,50,58	0
2	HEC	A	610	43/43	0.96	0.08	13,21,32,38	0
2	HEC	A	613	43/43	0.96	0.09	11,25,39,43	0
2	HEC	A	614	43/43	0.96	0.09	17,27,40,44	0
2	HEC	A	615	43/43	0.96	0.09	16,23,42,46	0
2	HEC	A	616	43/43	0.96	0.08	12,25,31,34	0
2	HEC	A	611	43/43	0.97	0.08	13,20,25,28	0
2	HEC	A	612	43/43	0.97	0.06	15,22,29,35	0
2	HEC	A	601	43/43	0.97	0.07	6,22,30,42	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.

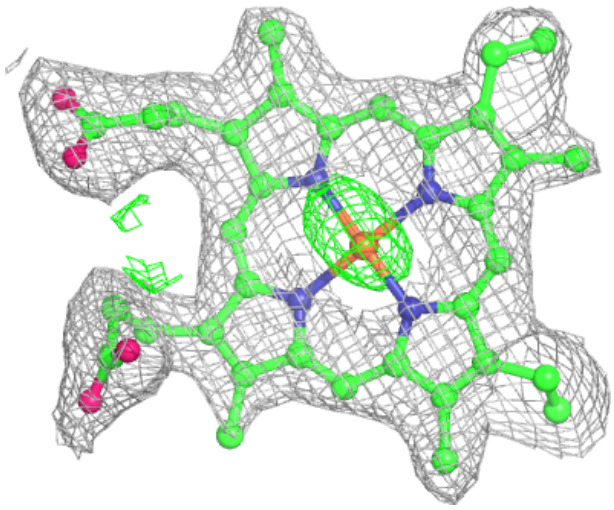
Electron density around HEC A 602:

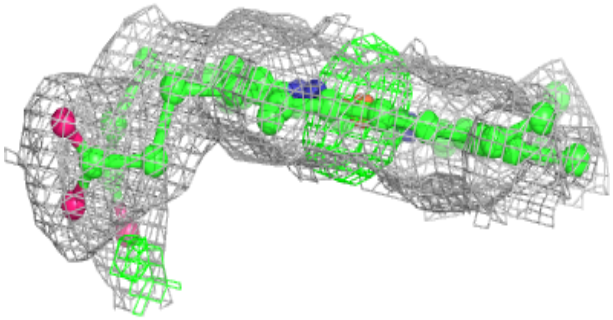
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

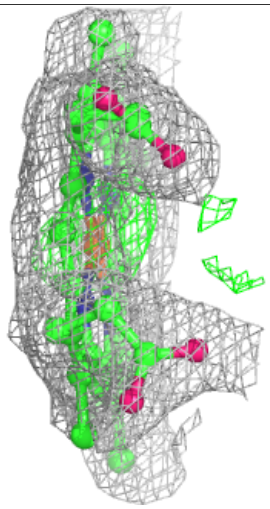


Electron density around HEC A 603:

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

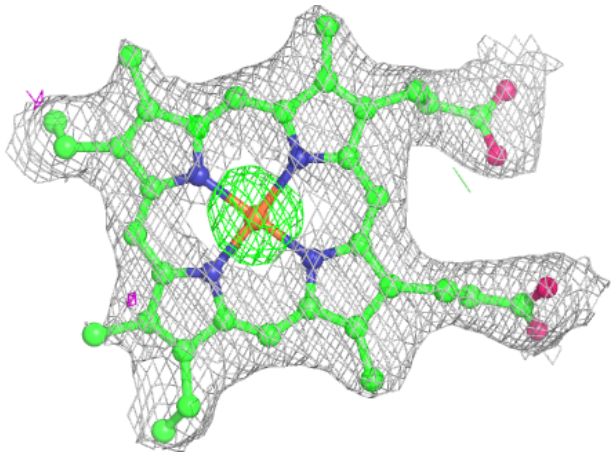


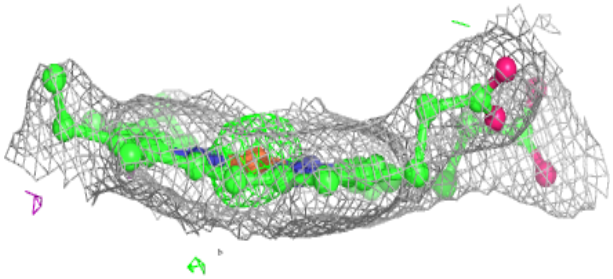


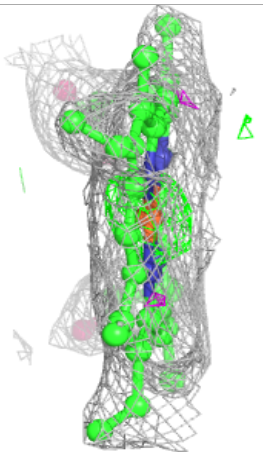


Electron density around HEC A 604:

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

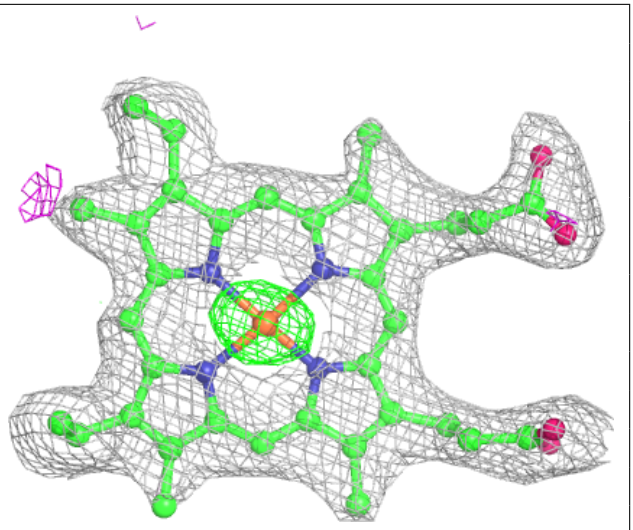


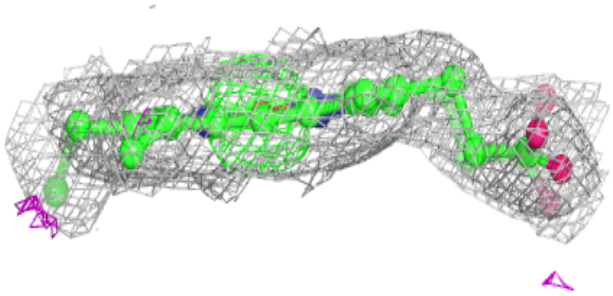


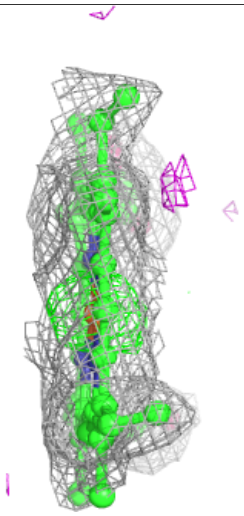


Electron density around HEC A 605:

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

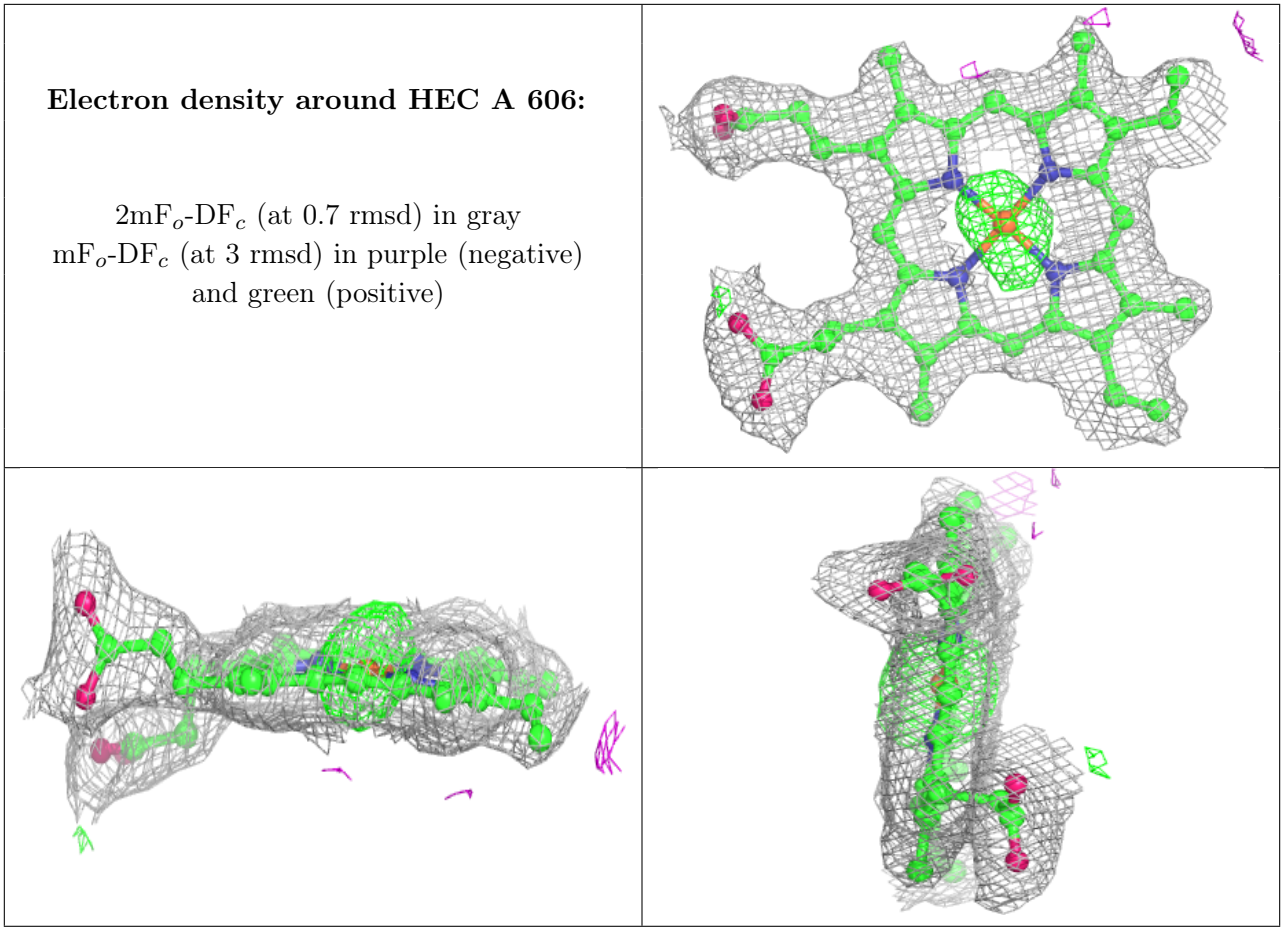






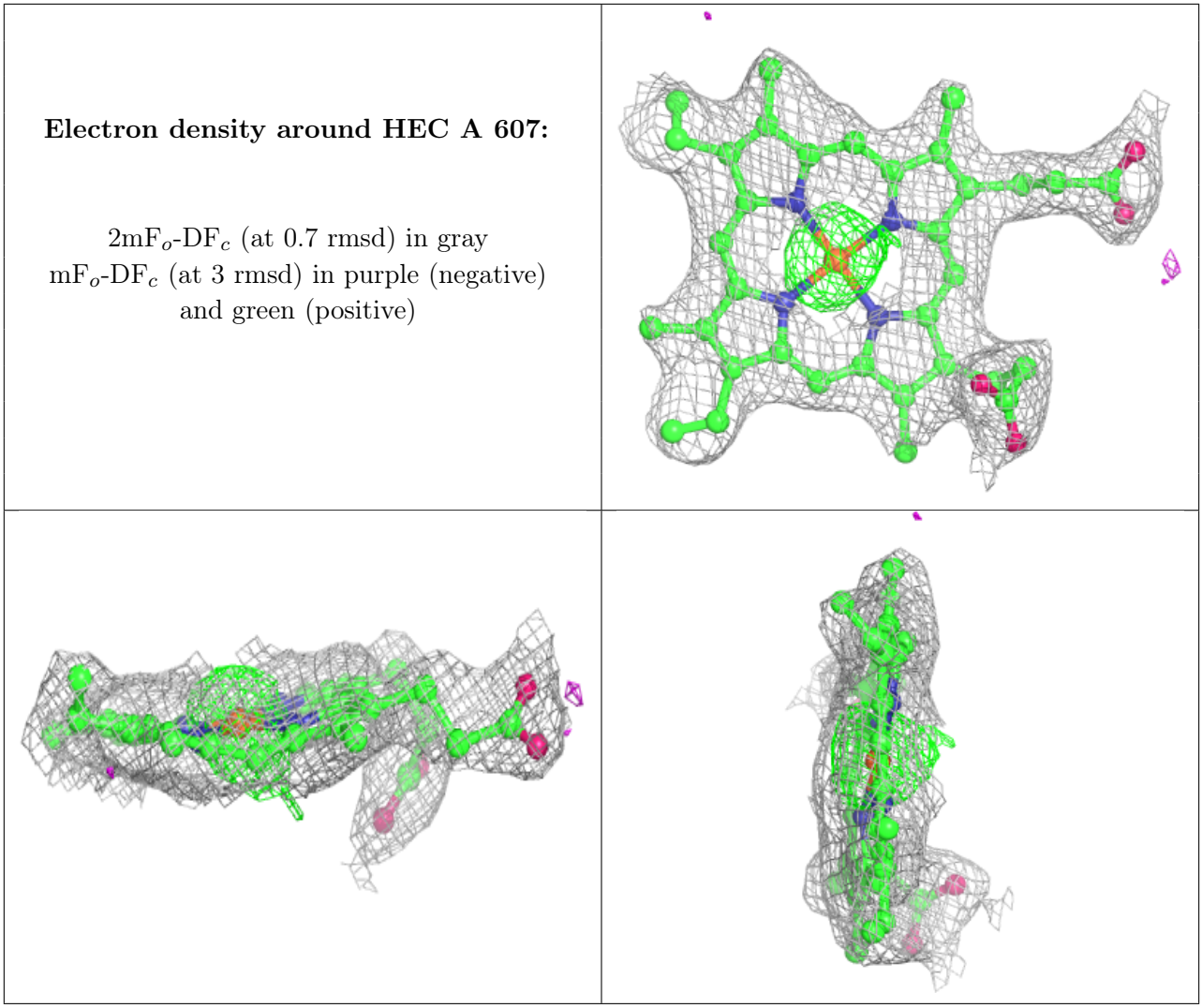
Electron density around HEC A 606:

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



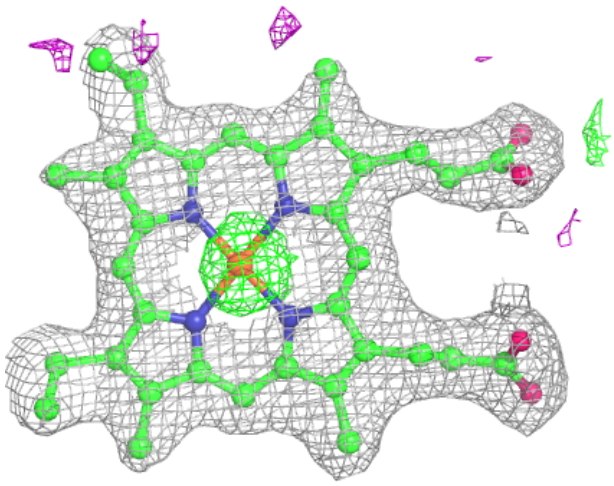
Electron density around HEC A 607:

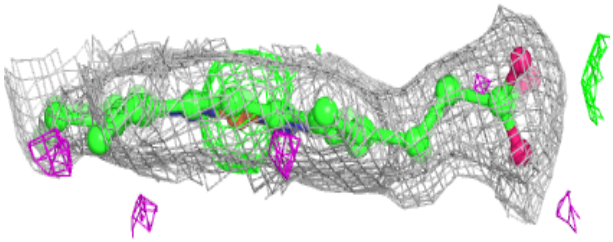
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

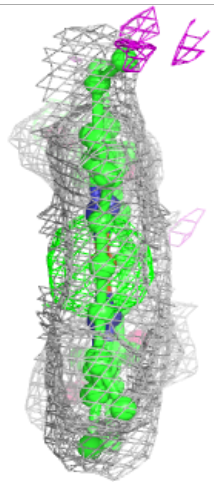


Electron density around HEC A 608:

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

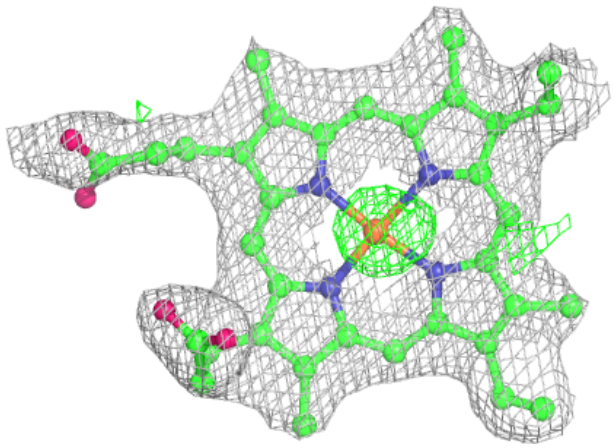


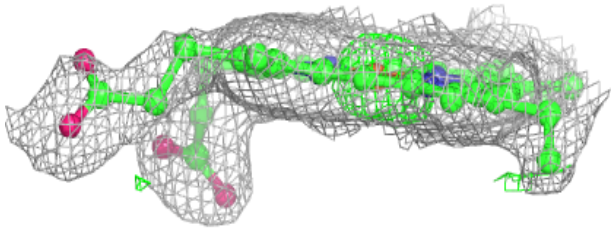


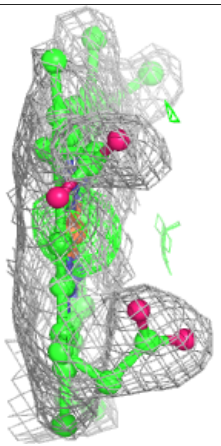


Electron density around HEC A 609:

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

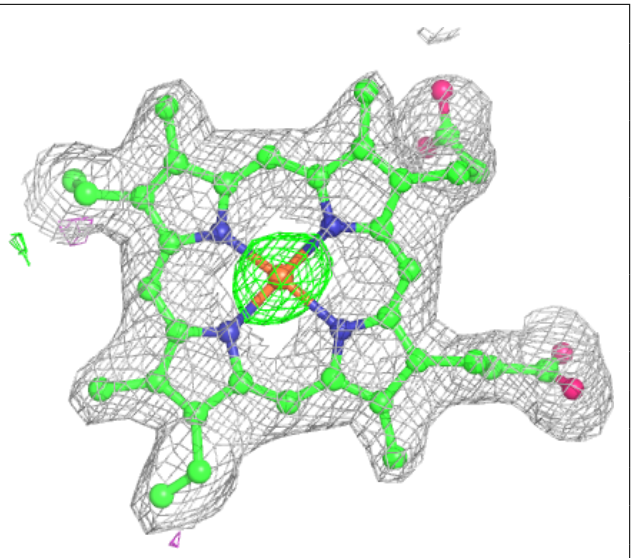


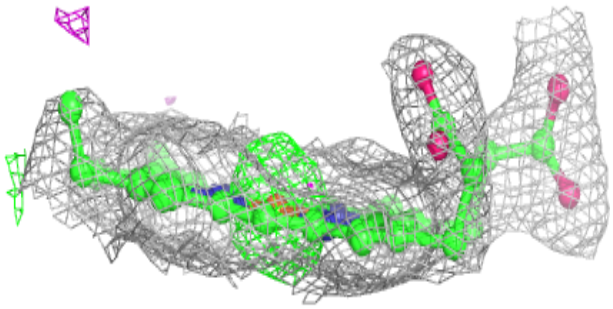


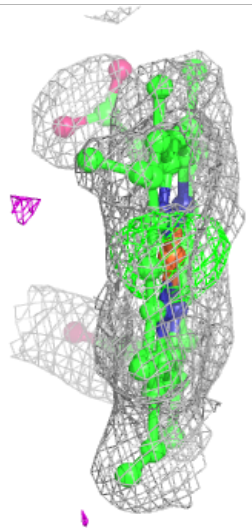


Electron density around HEC A 610:

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

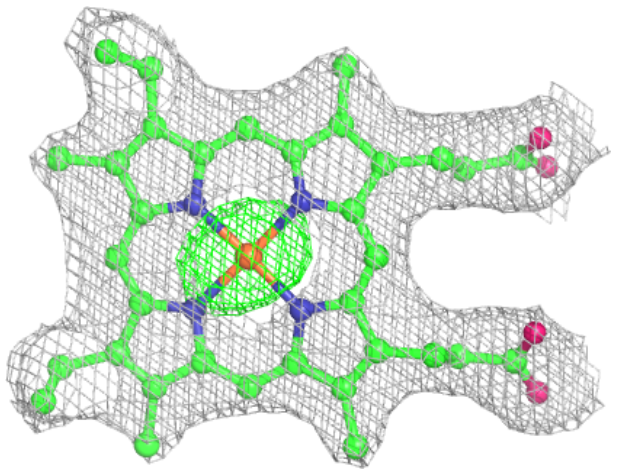


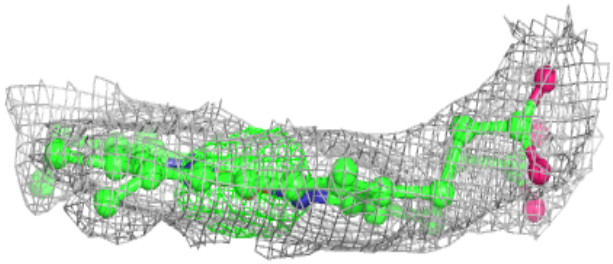


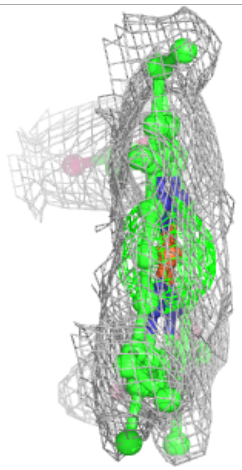


Electron density around HEC A 613:

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

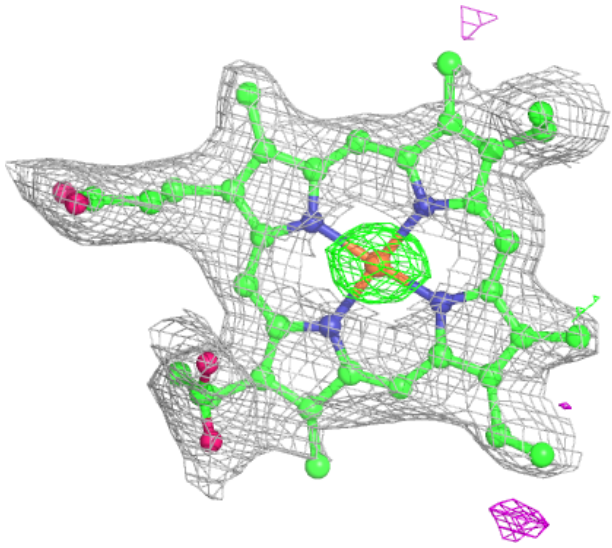


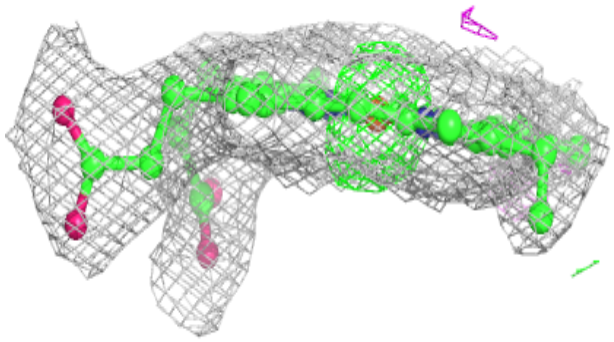


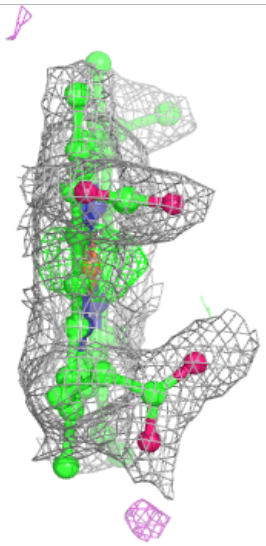


Electron density around HEC A 614:

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

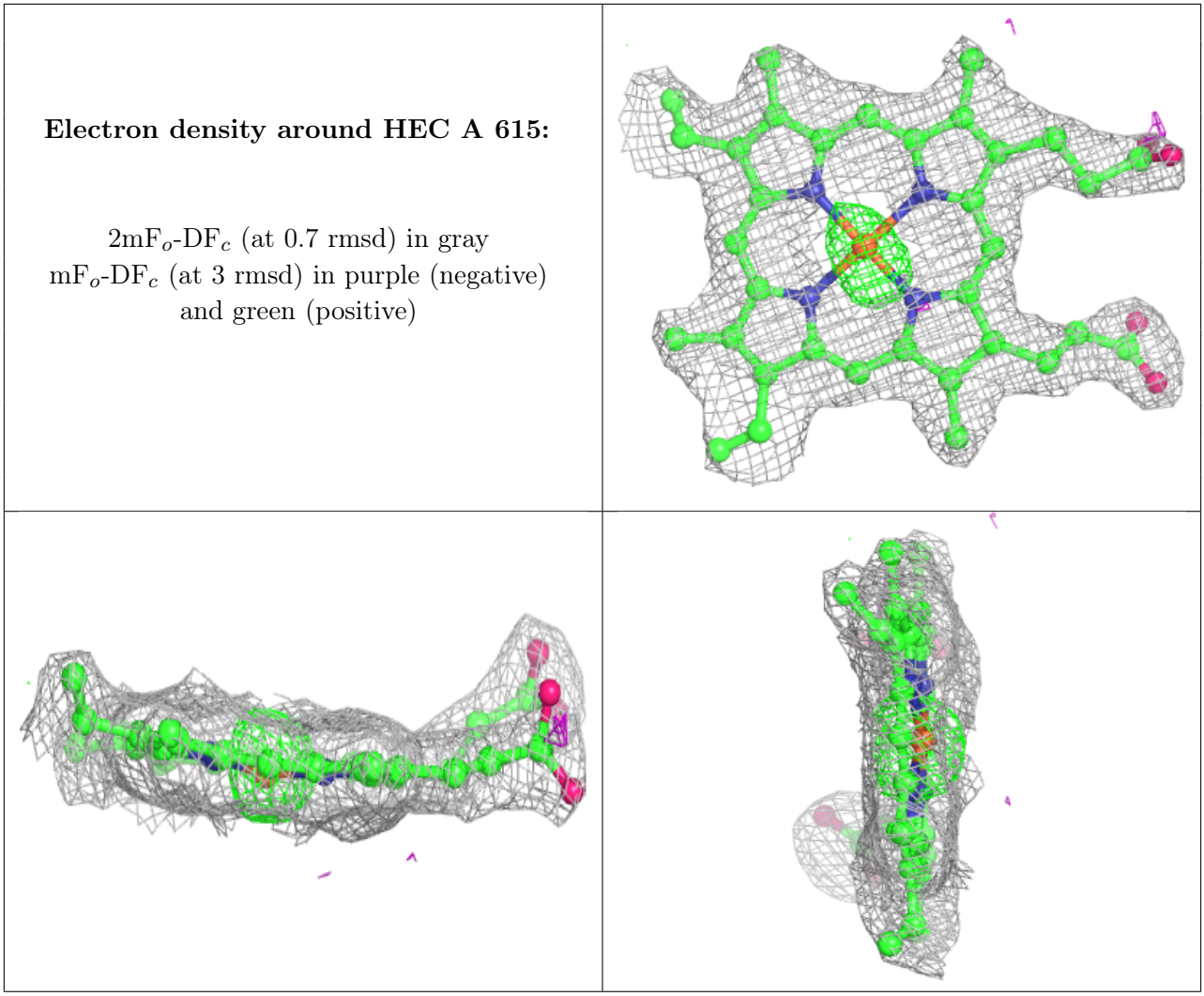






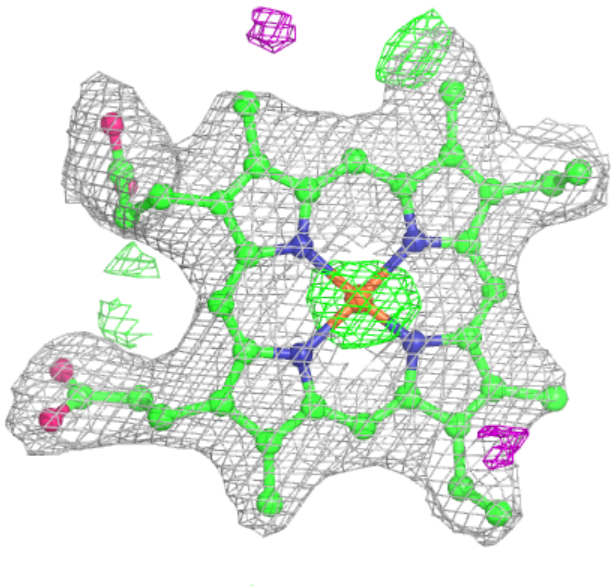
Electron density around HEC A 615:

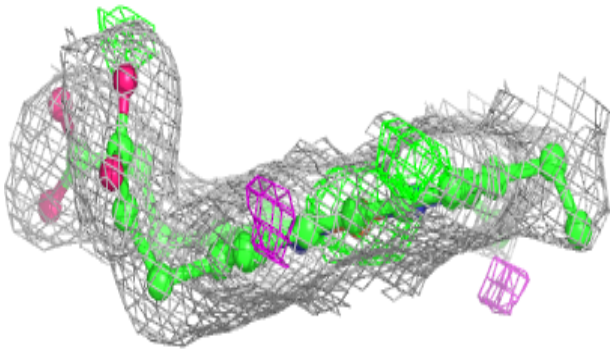
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

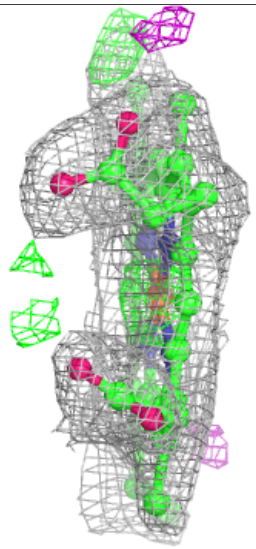


Electron density around HEC A 616:

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

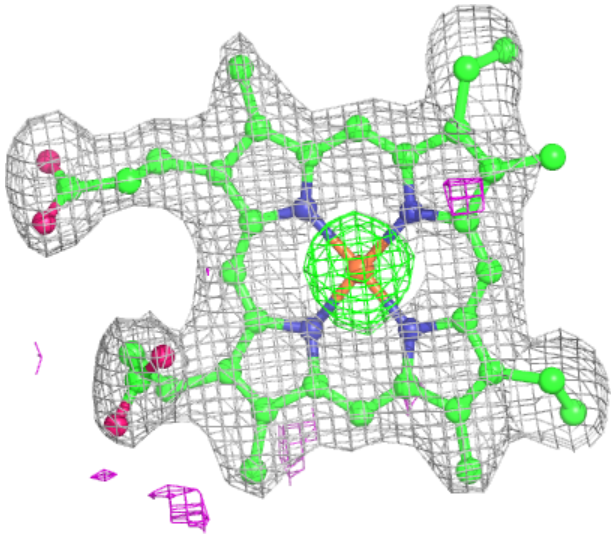


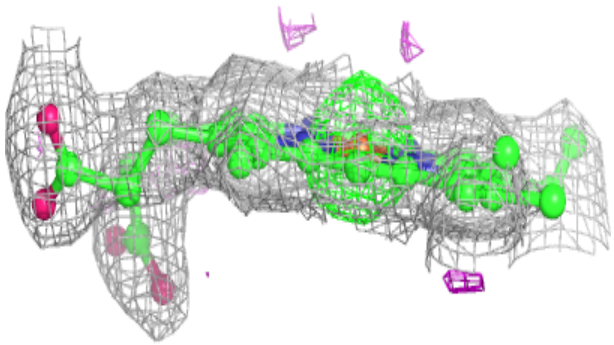


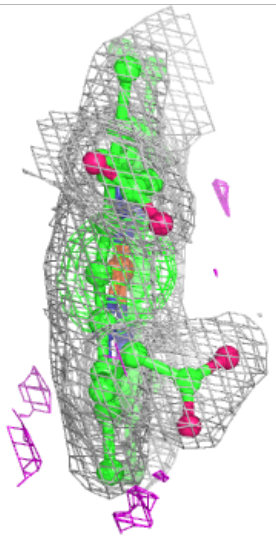


Electron density around HEC A 611:

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

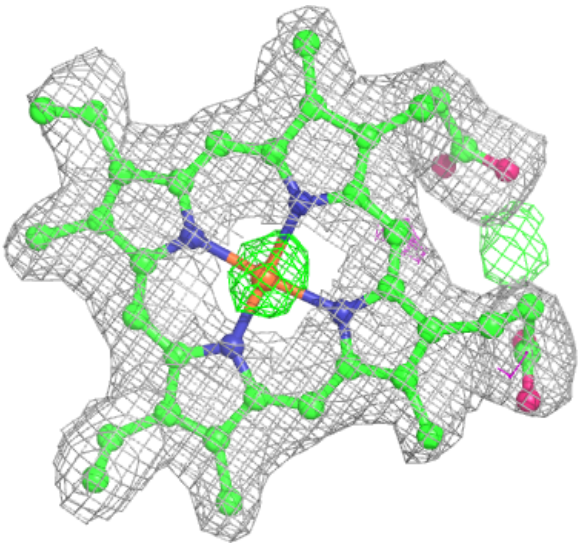


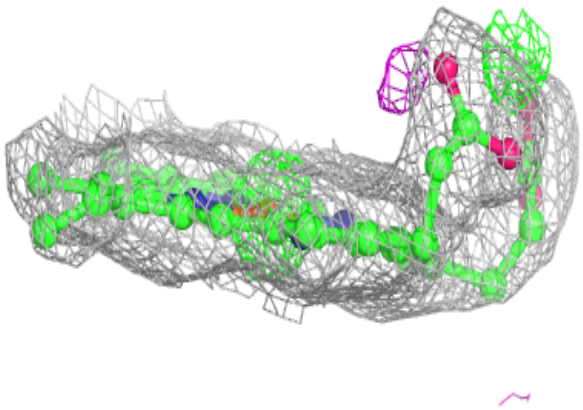


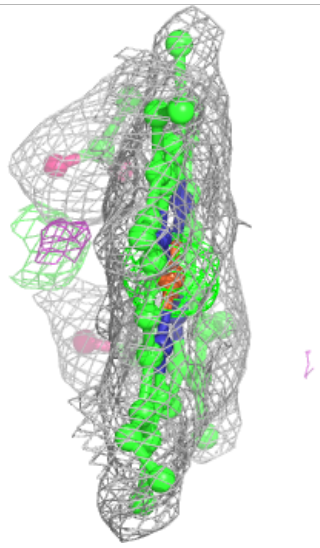


Electron density around HEC A 612:

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

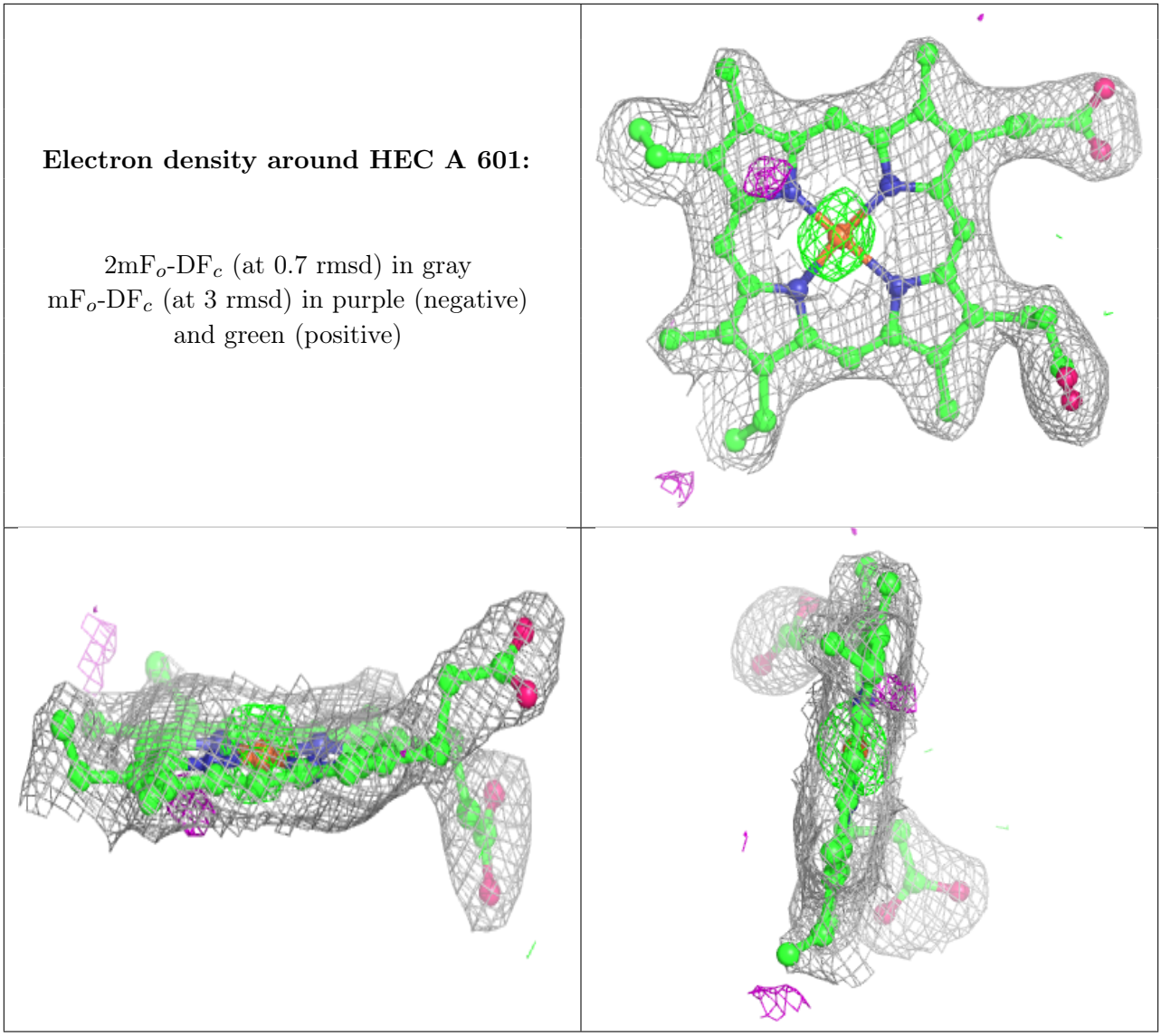






Electron density around HEC A 601:

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



6.5 Other polymers

There are no such residues in this entry.