Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 05:34 pm GMT

PDB ID	:	2J7A
Title	:	Crystal structure of cytochrome c nitrite reductase NrfHA complex from Desulfovibrio vulgaris
Authors	:	Rodrigues, M.L.; Oliveira, T.F.; Pereira, I.A.C.; Archer, M.
Deposited on	:	2006-10-06
Resolution	:	2.30 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:

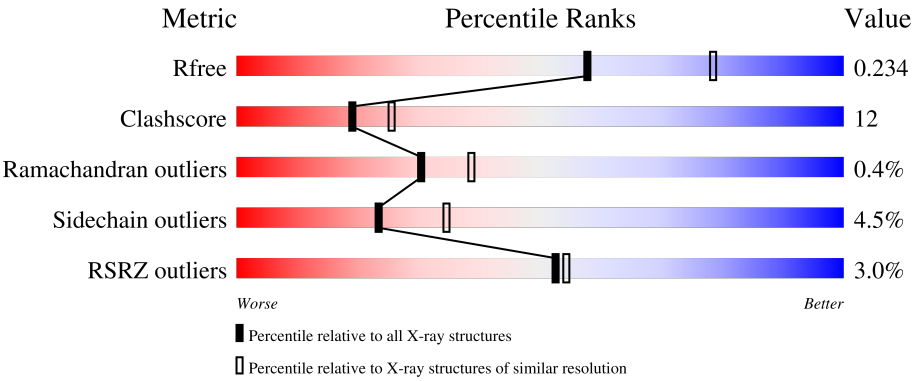
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	500	% 84% 14%
1	B	500	% 82% 16%
1	D	500	84% 14%
1	E	500	3% 81% 15%
1	G	500	% 84% 13%

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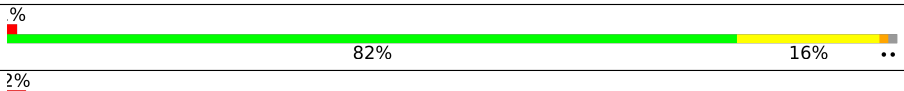
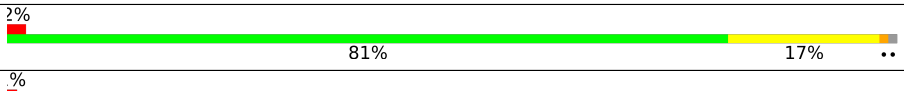
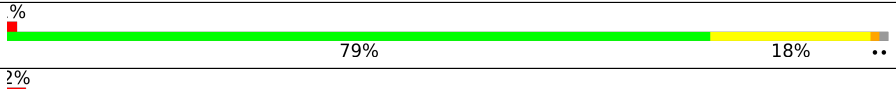
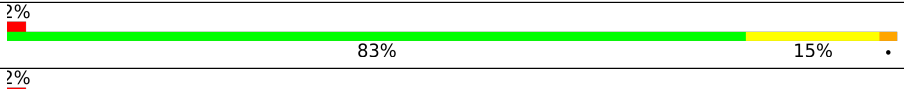
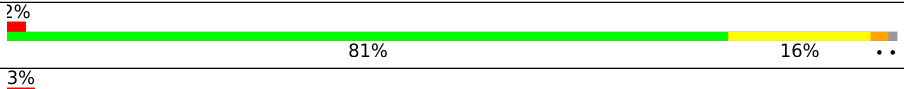
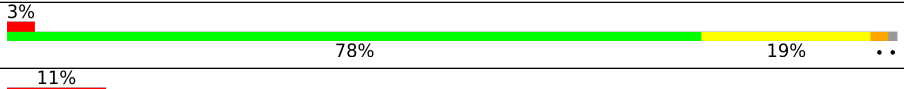
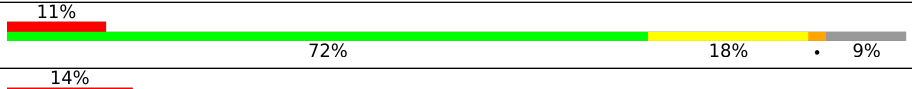
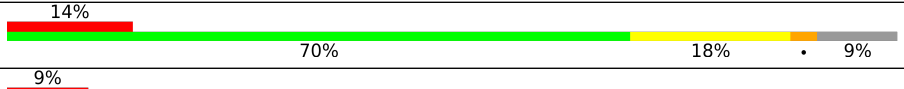
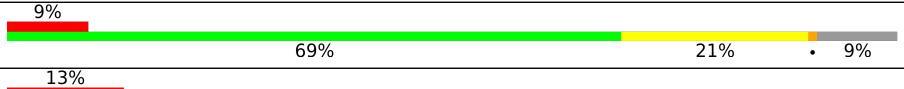
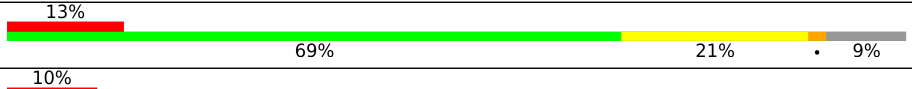
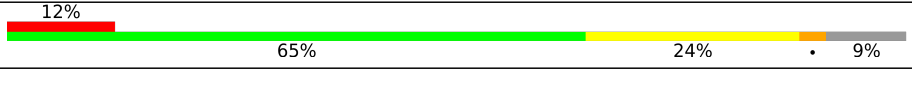
Mol	Chain	Length	Quality of chain
1	H	500	
1	J	500	
1	K	500	
1	M	500	
1	N	500	
1	P	500	
1	Q	500	
2	C	159	
2	F	159	
2	I	159	
2	L	159	
2	O	159	
2	R	159	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 60930 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 NITRITE REDUCTASE NRFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	2	0
			4022	2556	695	742	29			
1	B	498	Total	C	N	O	S	0	1	0
			4032	2560	697	746	29			
1	D	494	Total	C	N	O	S	0	1	0
			4009	2546	693	741	29			
1	E	494	Total	C	N	O	S	0	1	0
			4009	2546	693	741	29			
1	G	494	Total	C	N	O	S	0	1	0
			4008	2545	691	743	29			
1	H	497	Total	C	N	O	S	0	3	0
			4037	2563	694	751	29			
1	J	494	Total	C	N	O	S	0	3	0
			4021	2554	693	745	29			
1	K	496	Total	C	N	O	S	0	0	0
			4014	2549	693	743	29			
1	M	494	Total	C	N	O	S	0	2	0
			4014	2549	693	743	29			
1	N	498	Total	C	N	O	S	0	1	0
			4032	2560	697	746	29			
1	P	494	Total	C	N	O	S	0	1	0
			4007	2544	691	743	29			
1	Q	495	Total	C	N	O	S	0	1	0
			4016	2551	694	742	29			

- Molecule 2 is a protein called CYTOCHROME C QUINOL DEHYDROGENASE NRFH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	145	Total	C	N	O	S	0	1	0
			1094	680	201	197	16			
2	F	145	Total	C	N	O	S	0	1	0
			1093	679	199	199	16			

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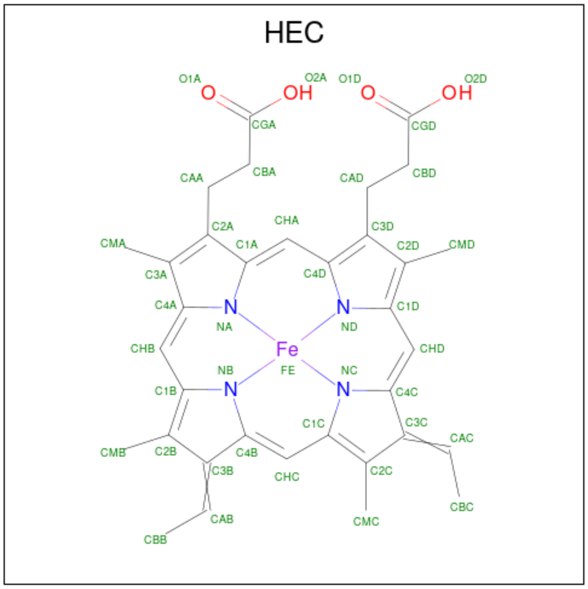
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	145	Total 1087	C 675	N 199	O 197	S 16	0	0	0
2	L	145	Total 1087	C 675	N 199	O 197	S 16	0	0	0
2	O	144	Total 1078	C 669	N 197	O 196	S 16	0	0	0
2	R	145	Total 1087	C 675	N 199	O 197	S 16	0	0	0

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

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

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	E	2	Total Ca 2 2	0	0
4	G	2	Total Ca 2 2	0	0

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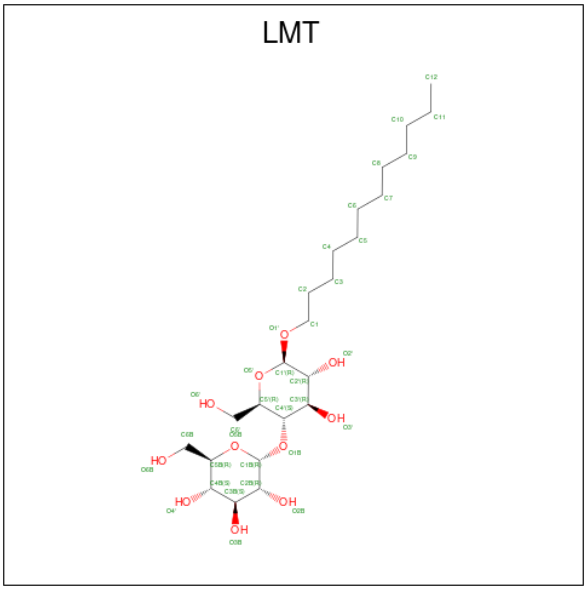
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	2	Total Ca 2 2	0	0
4	J	2	Total Ca 2 2	0	0
4	K	2	Total Ca 2 2	0	0
4	M	2	Total Ca 2 2	0	0
4	N	2	Total Ca 2 2	0	0
4	P	2	Total Ca 2 2	0	0
4	Q	2	Total Ca 2 2	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 35 24 11	0	0
5	F	1	Total C O 35 24 11	0	0
5	I	1	Total C O 35 24 11	0	0
5	L	1	Total C O 35 24 11	0	0

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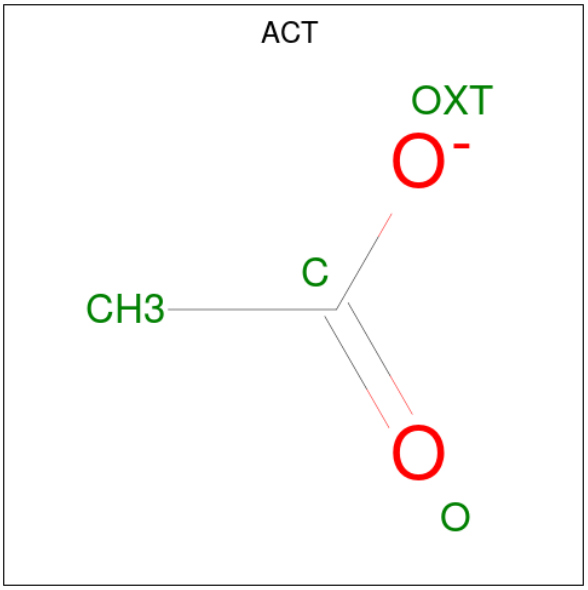
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 35 24 11	0	0
5	R	1	Total C O 35 24 11	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	O	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	201	Total O 201 201	0	0
7	B	188	Total O 188 188	0	0
7	C	50	Total O 50 50	0	0
7	D	170	Total O 170 170	0	0

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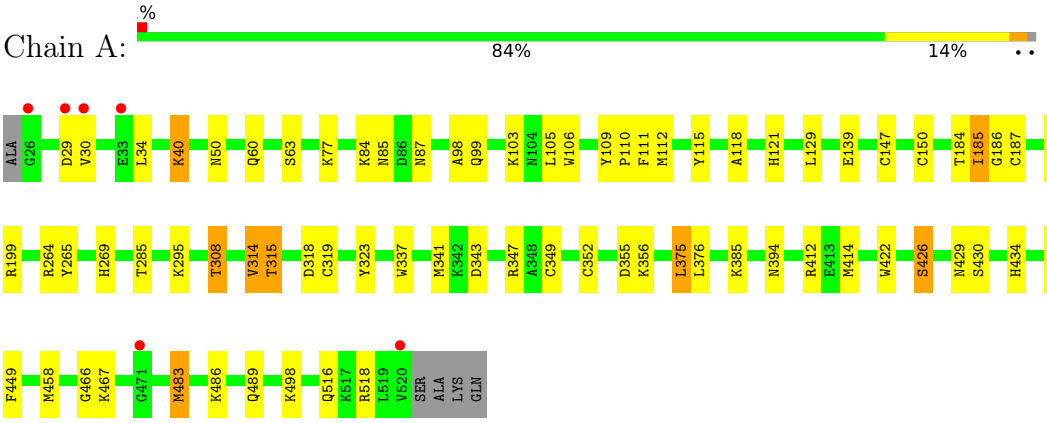
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	155	Total O 155 155	0	0
7	F	42	Total O 42 42	0	0
7	G	160	Total O 160 160	0	0
7	H	194	Total O 194 194	0	0
7	I	40	Total O 40 40	0	0
7	J	168	Total O 168 168	0	0
7	K	106	Total O 106 106	0	0
7	L	43	Total O 43 43	0	0
7	M	203	Total O 203 203	0	0
7	N	206	Total O 206 206	0	0
7	O	50	Total O 50 50	0	0
7	P	173	Total O 173 173	0	0
7	Q	132	Total O 132 132	0	0
7	R	44	Total O 44 44	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.

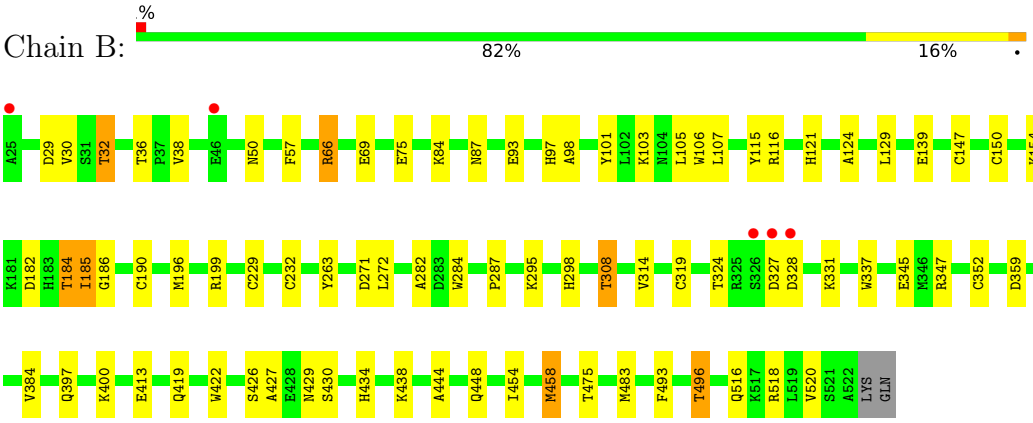
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

Chain A:



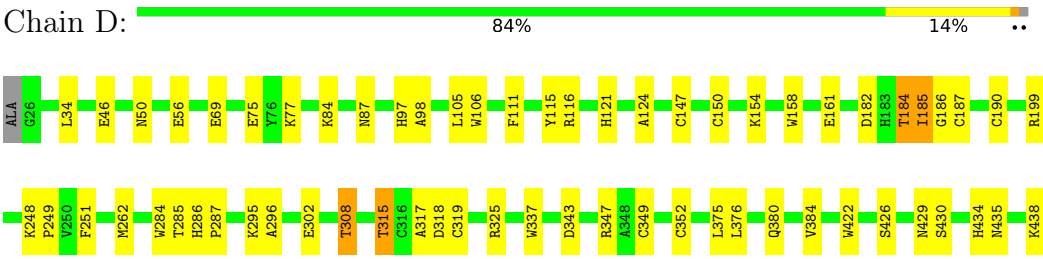
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

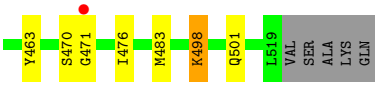
Chain B:



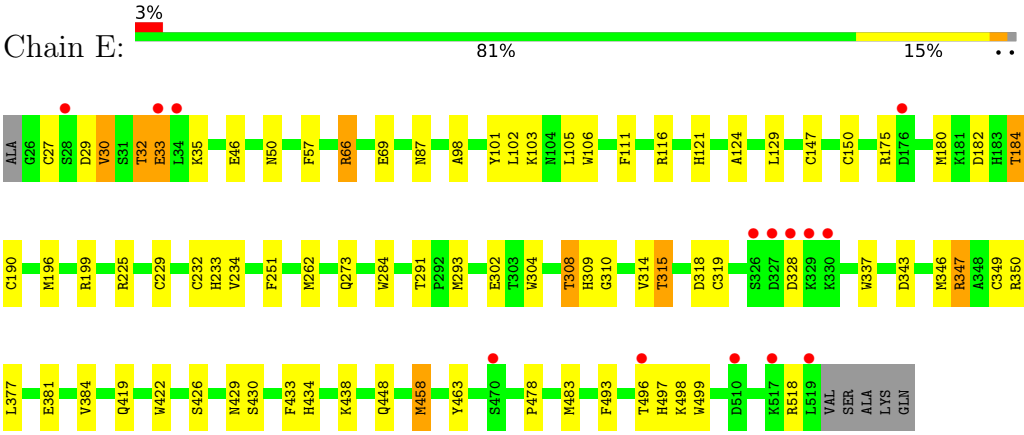
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

Chain D:

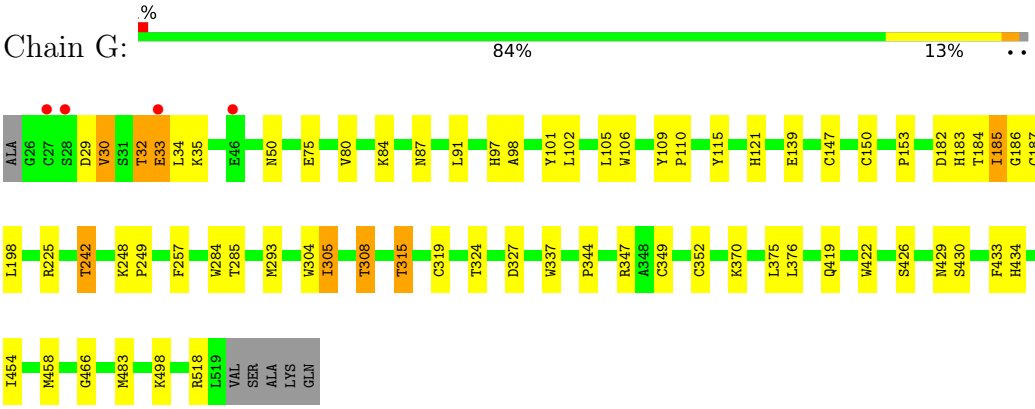




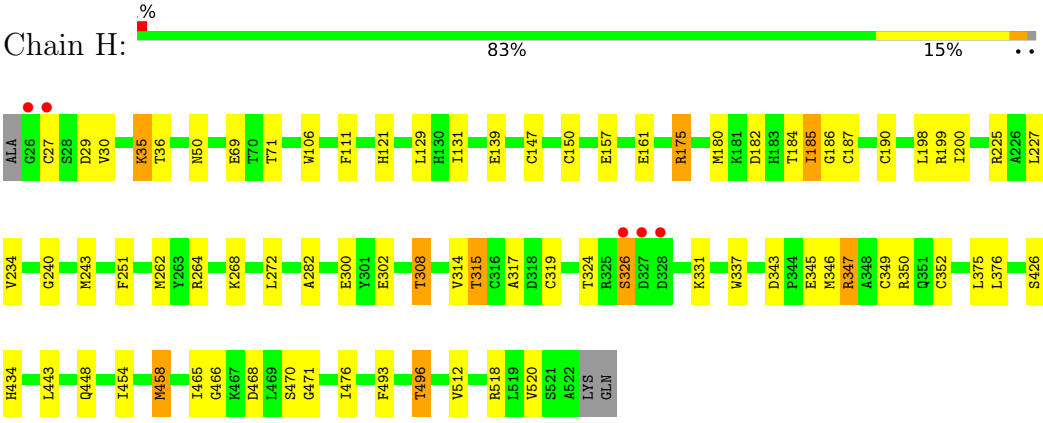
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



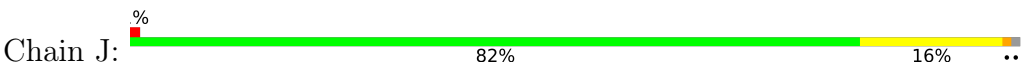
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

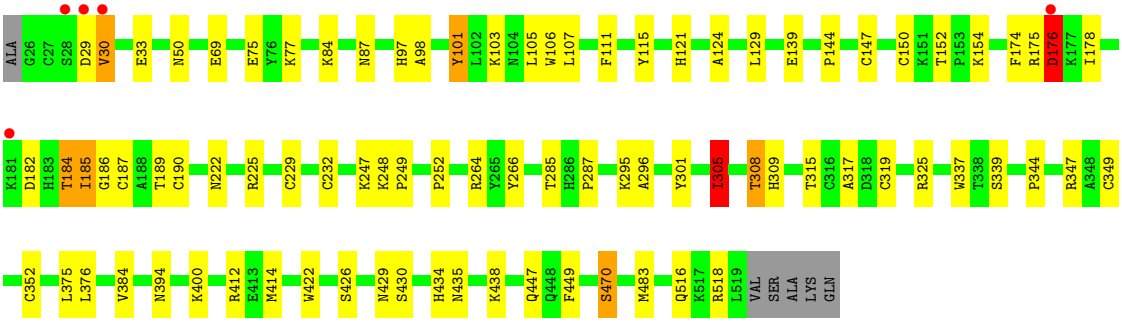


• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

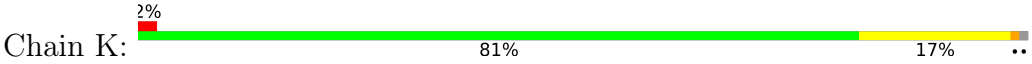


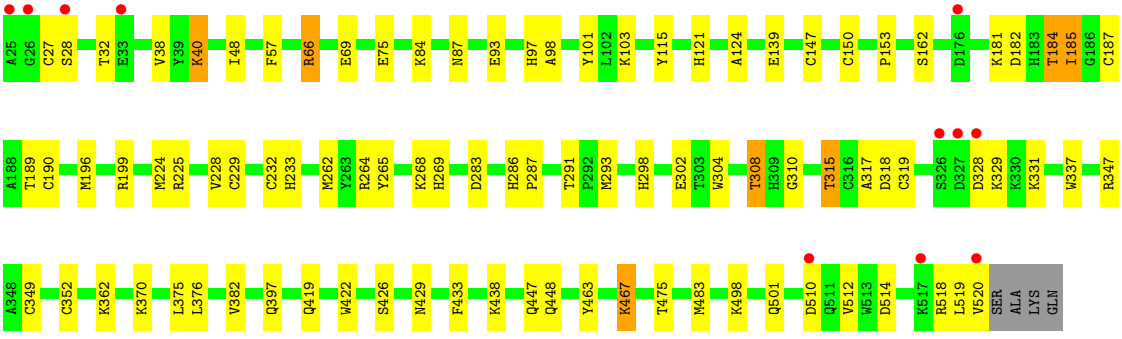
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



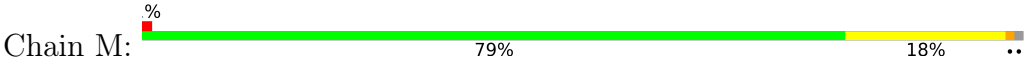


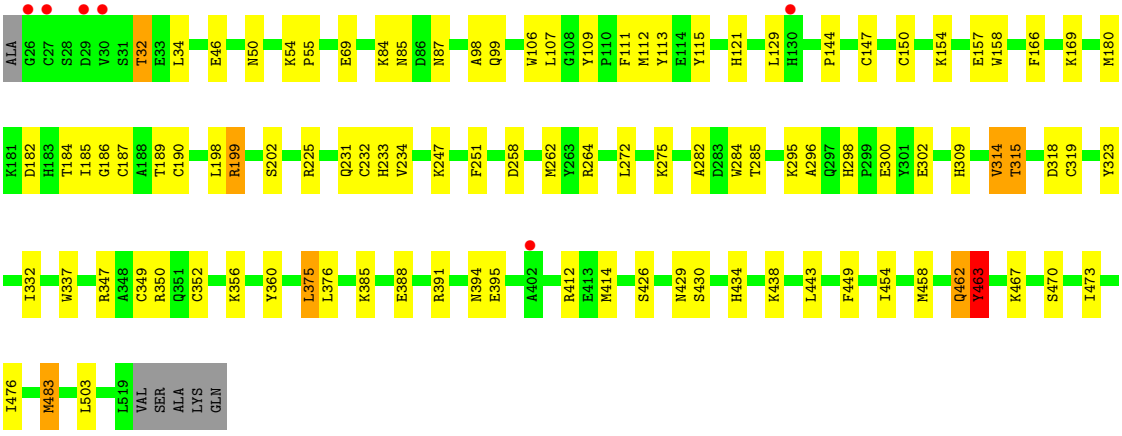
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA



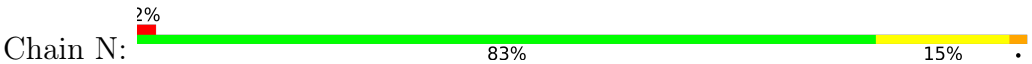


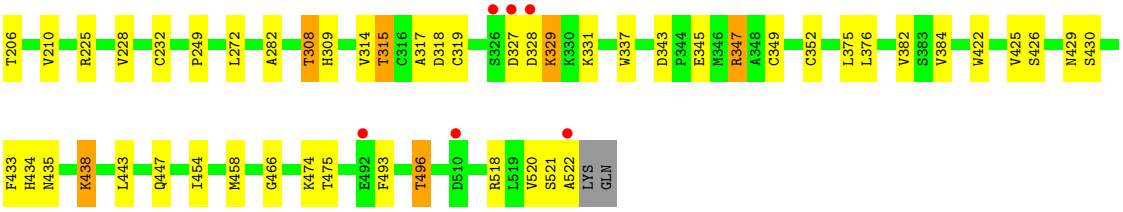
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA





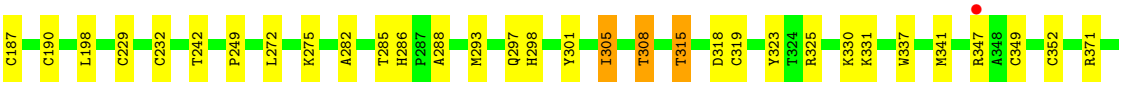
• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

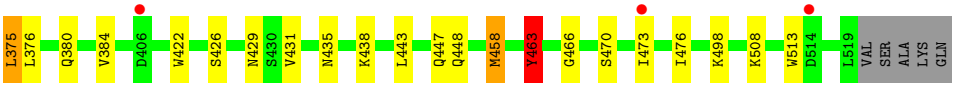




• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

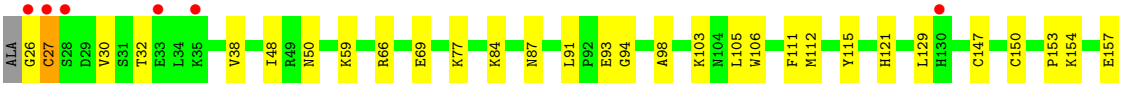
Chain P:

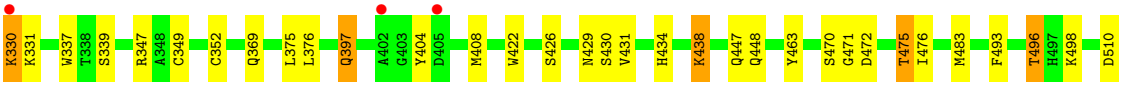


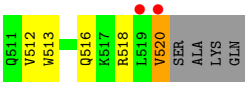


• Molecule 1: CYTOCHROME C NITRITE REDUCTASE NRFA

Chain Q:

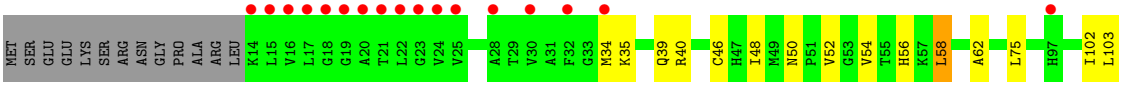






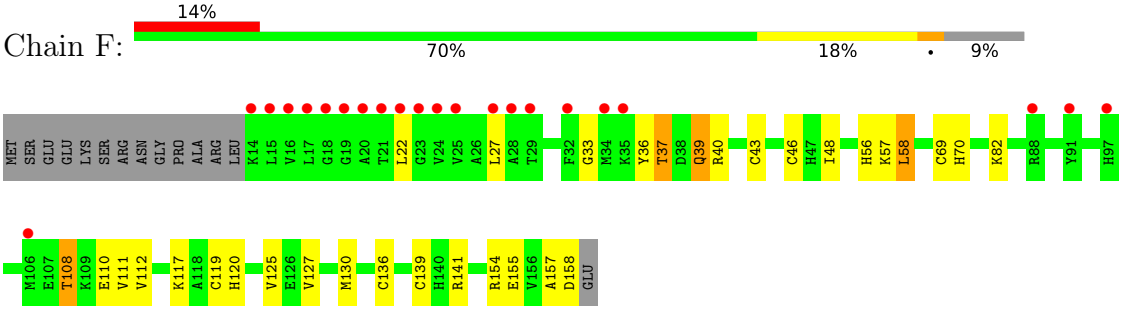
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

Chain C:



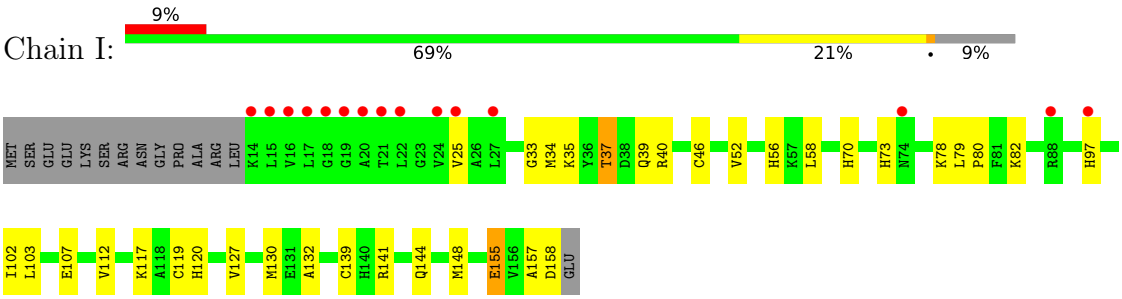
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

Chain F:



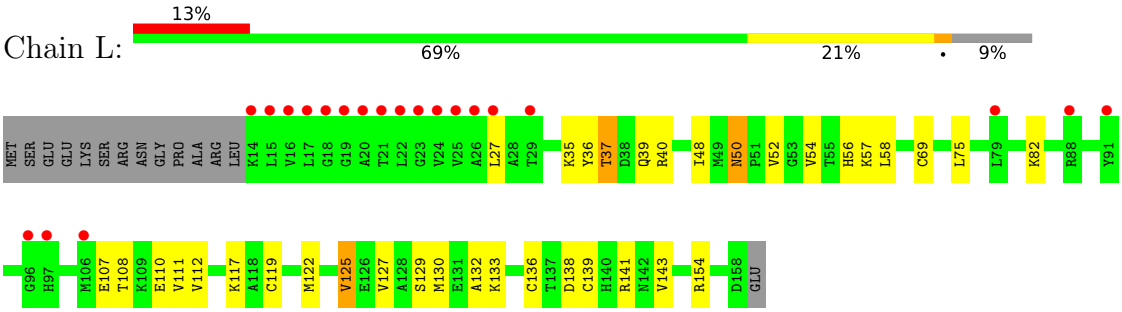
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

Chain I:



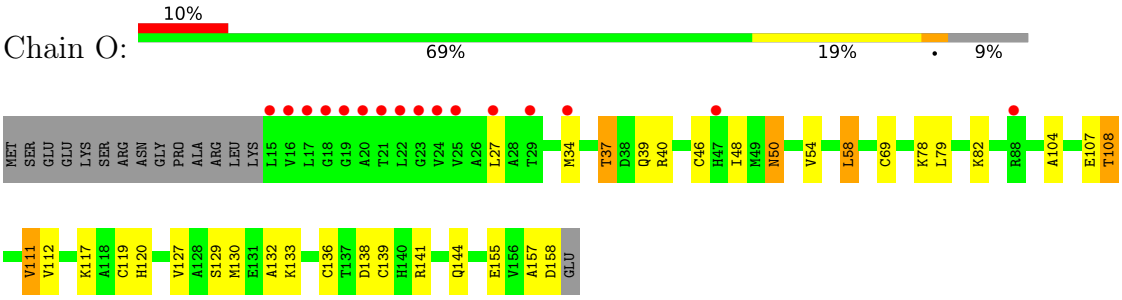
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

Chain L:



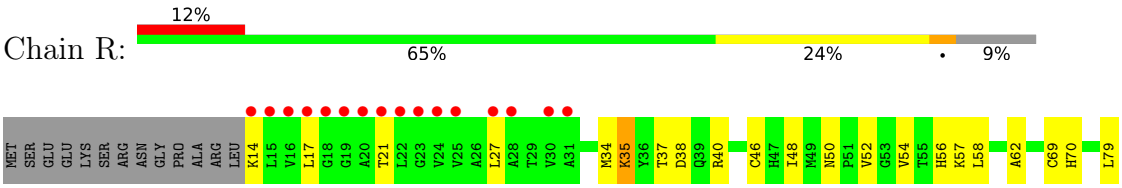
• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

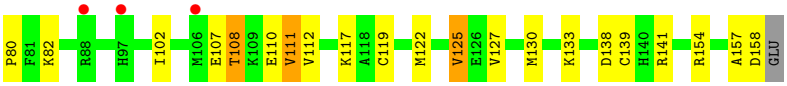
Chain O:



• Molecule 2: CYTOCHROME C QUINOL DEHYDROGENASE NRFH

Chain R:




P80
F81
K82
R88
H97
I102
M106
E107
T108
K109
E110
V111
V112
K117
A118
C119
M122
V125
E126
V127
M130
K133
D138
C139
H140
R141
R154
A157
D158
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.66Å 258.12Å 580.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	288.67 – 2.30 288.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.7 (288.67-2.30) 83.7 (288.67-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.240 0.197 , 0.234	Depositor DCC
R_{free} test set	22270 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	60930	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.81% 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: ACT, CA, LMT, 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	0.56	0/4143	0.65	0/5605
1	B	0.56	0/4150	0.67	1/5616 (0.0%)
1	D	0.55	0/4127	0.65	0/5584
1	E	0.55	0/4127	0.65	0/5584
1	G	0.57	0/4125	0.68	0/5581
1	H	0.55	0/4160	0.66	1/5629 (0.0%)
1	J	0.58	0/4145	0.66	1/5608 (0.0%)
1	K	0.56	0/4128	0.65	0/5586
1	M	0.62	2/4135 (0.0%)	0.68	1/5595 (0.0%)
1	N	0.57	0/4150	0.66	1/5616 (0.0%)
1	P	0.58	0/4124	0.68	2/5580 (0.0%)
1	Q	0.55	0/4134	0.67	1/5594 (0.0%)
2	C	0.51	0/1118	0.73	1/1513 (0.1%)
2	F	0.52	0/1116	0.72	0/1509
2	I	0.50	0/1107	0.68	0/1497
2	L	0.51	0/1107	0.77	0/1497
2	O	0.53	0/1098	0.74	0/1486
2	R	0.47	0/1107	0.69	0/1497
All	All	0.56	2/56301 (0.0%)	0.67	9/76177 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	M	0	3
1	Q	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	462	GLN	C-N	-12.07	1.06	1.34
1	M	463	TYR	C-N	-10.40	1.14	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	463	TYR	O-C-N	5.94	133.30	123.20
1	Q	27	CYS	N-CA-C	5.67	126.31	111.00
1	M	463	TYR	CA-C-N	-5.66	104.89	116.20
1	J	305	ILE	CB-CA-C	-5.65	100.30	111.60
1	B	175	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	H	175	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	N	175	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	P	463	TYR	CA-C-N	-5.08	106.03	116.20
2	C	141	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	VAL	Peptide
1	G	327	ASP	Peptide
1	M	314	VAL	Peptide
1	M	462	GLN	Mainchain
1	M	463	TYR	Mainchain
1	Q	26	GLY	Peptide

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	4022	0	3896	77	0
1	B	4032	0	3896	69	0
1	D	4009	0	3874	64	0
1	E	4009	0	3875	86	0
1	G	4008	0	3874	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	4037	0	3903	90	0
1	J	4021	0	3886	76	0
1	K	4014	0	3882	83	0
1	M	4014	0	3877	78	0
1	N	4032	0	3899	77	0
1	P	4007	0	3870	85	0
1	Q	4016	0	3884	121	0
2	C	1094	0	1095	32	0
2	F	1093	0	1096	47	0
2	I	1087	0	1089	39	0
2	L	1087	0	1090	46	0
2	O	1078	0	1077	45	0
2	R	1087	0	1090	53	0
3	A	215	0	156	36	0
3	B	215	0	154	28	0
3	C	172	0	122	21	0
3	D	215	0	156	38	0
3	E	215	0	157	38	0
3	F	172	0	124	29	0
3	G	215	0	157	44	0
3	H	215	0	157	39	0
3	I	172	0	123	18	0
3	J	215	0	156	38	0
3	K	215	0	157	40	0
3	L	172	0	124	26	0
3	M	215	0	157	41	0
3	N	215	0	157	37	0
3	O	172	0	124	23	0
3	P	215	0	156	40	0
3	Q	215	0	157	50	0
3	R	172	0	124	25	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	2	0	0	0	0
5	C	35	0	46	2	0
5	F	35	0	46	0	0
5	I	35	0	46	3	0
5	L	35	0	46	3	0
5	O	35	0	46	0	0
5	R	35	0	46	0	0
6	C	4	0	3	0	0
6	I	4	0	3	0	0
6	O	4	0	3	0	0
7	A	201	0	0	7	0
7	B	188	0	0	6	0
7	C	50	0	0	0	0
7	D	170	0	0	3	0
7	E	155	0	0	2	0
7	F	42	0	0	1	0
7	G	160	0	0	7	0
7	H	194	0	0	4	0
7	I	40	0	0	1	0
7	J	168	0	0	2	0
7	K	106	0	0	5	0
7	L	43	0	0	5	0
7	M	203	0	0	6	0
7	N	206	0	0	5	0
7	O	50	0	0	3	0
7	P	173	0	0	7	0
7	Q	132	0	0	3	0
7	R	44	0	0	4	0
All	All	60930	0	56056	1278	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 12.

All (1278) 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:K:319:CYS:SG	3:K:1004:HEC:HAC	1.30	1.72
1:N:187:CYS:SG	3:N:1002:HEC:HAB	1.21	1.71
2:L:69:CYS:SG	3:L:1002:HEC:HAC	1.32	1.70
1:K:150:CYS:SG	3:K:1001:HEC:HAC	1.32	1.68
1:J:147:CYS:SG	3:J:1001:HEC:HAB	1.26	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:CYS:SG	3:D:1001:HEC:HAB	1.23	1.66
1:K:190:CYS:SG	3:K:1002:HEC:HAC	1.36	1.66
1:A:147:CYS:SG	3:A:1001:HEC:HAB	1.36	1.66
2:O:136:CYS:SG	3:O:1004:HEC:HAB	1.26	1.66
1:E:229:CYS:SG	3:E:1003:HEC:HAB	1.37	1.64
1:J:150:CYS:SG	3:J:1001:HEC:HAC	1.37	1.63
1:K:147:CYS:SG	3:K:1001:HEC:HAB	1.40	1.61
1:P:150:CYS:SG	3:P:1001:HEC:HAC	1.40	1.57
2:L:136:CYS:SG	3:L:1004:HEC:HAB	1.46	1.56
2:I:46:CYS:SG	3:I:1001:HEC:HAC	1.42	1.55
1:H:187:CYS:SG	3:H:1002:HEC:HAB	1.44	1.53
1:N:147:CYS:SG	3:N:1001:HEC:HAB	1.49	1.50
2:F:69:CYS:SG	3:F:1002:HEC:HAC	1.51	1.50
1:D:352:CYS:SG	3:D:1005:HEC:HAC	1.49	1.50
1:Q:147:CYS:SG	3:Q:1001:HEC:HAB	1.50	1.50
1:E:349:CYS:SG	3:E:1005:HEC:HAB	1.50	1.49
1:P:187:CYS:SG	3:P:1002:HEC:HAB	1.52	1.48
1:Q:190:CYS:SG	3:Q:1002:HEC:HAC	1.52	1.47
1:J:352:CYS:SG	3:J:1005:HEC:HAC	1.55	1.47
1:K:229:CYS:SG	3:K:1003:HEC:HAB	1.55	1.47
1:M:190:CYS:SG	3:M:1002:HEC:HAC	1.55	1.46
1:H:319:CYS:SG	3:H:1004:HEC:HAC	1.56	1.46
1:M:232:CYS:SG	3:M:1003:HEC:HAC	1.55	1.44
1:Q:187:CYS:SG	3:Q:1002:HEC:HAB	1.53	1.44
1:E:147:CYS:SG	3:E:1001:HEC:HAB	1.56	1.44
1:A:187:CYS:SG	3:A:1002:HEC:HAB	1.57	1.44
2:R:46:CYS:SG	3:R:1001:HEC:HAC	1.57	1.43
1:G:187:CYS:SG	3:G:1002:HEC:HAB	1.59	1.43
2:R:69:CYS:SG	3:R:1002:HEC:HAC	1.59	1.43
1:H:147:CYS:SG	3:H:1001:HEC:HAB	1.59	1.43
1:B:147:CYS:SG	3:B:1001:HEC:HAB	1.56	1.42
1:N:349:CYS:SG	3:N:1005:HEC:HAB	1.58	1.42
1:Q:352:CYS:SG	3:Q:1005:HEC:HAC	1.57	1.42
1:B:319:CYS:SG	3:B:1004:HEC:HAC	1.60	1.40
1:M:349:CYS:SG	3:M:1005:HEC:CAB	2.10	1.40
1:B:319:CYS:SG	3:B:1004:HEC:CAC	2.10	1.39
1:Q:150:CYS:SG	3:Q:1001:HEC:HAC	1.61	1.39
2:C:139:CYS:SG	3:C:1004:HEC:CAC	2.11	1.39
1:M:232:CYS:SG	3:M:1003:HEC:CAC	2.11	1.39
1:Q:352:CYS:SG	3:Q:1005:HEC:CAC	2.11	1.39
2:F:69:CYS:SG	3:F:1002:HEC:CAC	2.11	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:CYS:SG	3:N:1001:HEC:CAC	2.12	1.38
1:H:319:CYS:SG	3:H:1004:HEC:CAC	2.10	1.38
1:E:187:CYS:SG	3:E:1002:HEC:HAB	1.63	1.38
1:G:319:CYS:SG	3:G:1004:HEC:CAC	2.11	1.38
1:N:352:CYS:SG	3:N:1005:HEC:HAC	1.63	1.38
1:B:190:CYS:SG	3:B:1002:HEC:CAC	2.11	1.38
1:B:232:CYS:SG	3:B:1003:HEC:CAC	2.11	1.38
1:E:150:CYS:SG	3:E:1001:HEC:HAC	1.61	1.38
2:R:69:CYS:SG	3:R:1002:HEC:CAC	2.12	1.37
1:J:352:CYS:SG	3:J:1005:HEC:CAC	2.12	1.37
1:N:150:CYS:SG	3:N:1001:HEC:HAC	1.61	1.37
1:P:187:CYS:SG	3:P:1002:HEC:CAB	2.11	1.37
2:L:139:CYS:SG	3:L:1004:HEC:CAC	2.13	1.37
1:A:319:CYS:SG	3:A:1004:HEC:CAC	2.12	1.36
2:I:46:CYS:SG	3:I:1001:HEC:CAC	2.11	1.36
1:N:319:CYS:SG	3:N:1004:HEC:CAC	2.12	1.36
1:G:150:CYS:SG	3:G:1001:HEC:CAC	2.12	1.36
1:E:349:CYS:SG	3:E:1005:HEC:CAB	2.12	1.36
1:H:147:CYS:SG	3:H:1001:HEC:CAB	2.13	1.36
1:N:349:CYS:SG	3:N:1005:HEC:CAB	2.14	1.36
1:N:352:CYS:SG	3:N:1005:HEC:CAC	2.14	1.36
2:O:69:CYS:SG	3:O:1002:HEC:HAC	1.65	1.35
1:G:187:CYS:SG	3:G:1002:HEC:CAB	2.13	1.35
1:A:190:CYS:SG	3:A:1002:HEC:CAC	2.15	1.35
2:L:69:CYS:SG	3:L:1002:HEC:CAC	2.12	1.35
1:A:352:CYS:SG	3:A:1005:HEC:HAC	1.64	1.34
1:J:147:CYS:SG	3:J:1001:HEC:CAB	2.13	1.34
1:G:349:CYS:SG	3:G:1005:HEC:CAB	2.13	1.34
1:H:187:CYS:SG	3:H:1002:HEC:CAB	2.13	1.34
1:P:319:CYS:SG	3:P:1004:HEC:CAC	2.15	1.34
1:B:147:CYS:SG	3:B:1001:HEC:CAB	2.16	1.34
1:D:352:CYS:SG	3:D:1005:HEC:CAC	2.16	1.34
1:K:190:CYS:SG	3:K:1002:HEC:CAC	2.16	1.34
1:P:150:CYS:SG	3:P:1001:HEC:CAC	2.14	1.34
1:Q:187:CYS:SG	3:Q:1002:HEC:CAB	2.15	1.34
1:D:150:CYS:SG	3:D:1001:HEC:HAC	1.67	1.33
2:R:139:CYS:SG	3:R:1004:HEC:HAC	1.66	1.33
2:C:139:CYS:SG	3:C:1004:HEC:HAC	1.67	1.33
1:K:349:CYS:SG	3:K:1005:HEC:HAB	1.67	1.33
1:M:147:CYS:SG	3:M:1001:HEC:CAB	2.17	1.33
1:D:150:CYS:SG	3:D:1001:HEC:CAC	2.17	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:CYS:SG	3:G:1005:HEC:CAC	2.16	1.32
1:Q:349:CYS:SG	3:Q:1005:HEC:CAB	2.17	1.32
1:H:352:CYS:SG	3:H:1005:HEC:CAC	2.18	1.31
1:J:187:CYS:SG	3:J:1002:HEC:CAB	2.17	1.31
1:M:352:CYS:SG	3:M:1005:HEC:CAC	2.19	1.31
2:R:119:CYS:SG	3:R:1003:HEC:HAC	1.68	1.31
1:A:187:CYS:SG	3:A:1002:HEC:CAB	2.16	1.31
1:M:147:CYS:SG	3:M:1001:HEC:HAB	1.71	1.31
1:K:147:CYS:SG	3:K:1001:HEC:CAB	2.18	1.31
1:J:187:CYS:SG	3:J:1002:HEC:HAB	1.70	1.30
1:A:319:CYS:SG	3:A:1004:HEC:HAC	1.65	1.30
1:G:147:CYS:SG	3:G:1001:HEC:CAB	2.18	1.30
1:M:187:CYS:SG	3:M:1002:HEC:CAB	2.19	1.30
2:R:139:CYS:SG	3:R:1004:HEC:CAC	2.19	1.30
1:E:352:CYS:SG	3:E:1005:HEC:HAC	1.66	1.30
2:O:139:CYS:SG	3:O:1004:HEC:CAC	2.19	1.29
1:K:229:CYS:SG	3:K:1003:HEC:CAB	2.19	1.29
2:R:46:CYS:SG	3:R:1001:HEC:CAC	2.18	1.29
1:E:150:CYS:SG	3:E:1001:HEC:CAC	2.19	1.29
1:B:232:CYS:SG	3:B:1003:HEC:HAC	1.72	1.28
1:J:190:CYS:SG	3:J:1002:HEC:HAC	1.73	1.28
2:L:139:CYS:SG	3:L:1004:HEC:HAC	1.70	1.28
1:D:319:CYS:SG	3:D:1004:HEC:CAC	2.21	1.28
1:M:190:CYS:SG	3:M:1002:HEC:CAC	2.20	1.28
1:A:349:CYS:SG	3:A:1005:HEC:CAB	2.21	1.27
1:M:352:CYS:SG	3:M:1005:HEC:HAC	1.72	1.27
1:H:190:CYS:SG	3:H:1002:HEC:CAC	2.22	1.27
2:F:46:CYS:SG	3:F:1001:HEC:CAC	2.24	1.26
1:P:349:CYS:SG	3:P:1005:HEC:HAB	1.70	1.26
2:F:46:CYS:SG	3:F:1001:HEC:HAC	1.76	1.26
1:N:319:CYS:SG	3:N:1004:HEC:HAC	1.70	1.25
1:J:319:CYS:SG	3:J:1004:HEC:CAC	2.24	1.25
1:Q:190:CYS:SG	3:Q:1002:HEC:CAC	2.23	1.24
1:Q:232:CYS:SG	3:Q:1003:HEC:CAC	2.25	1.24
1:E:190:CYS:SG	3:E:1002:HEC:CAC	2.24	1.24
1:G:190:CYS:SG	3:G:1002:HEC:CAC	2.25	1.24
1:N:190:CYS:SG	3:N:1002:HEC:CAC	2.26	1.23
1:G:147:CYS:SG	3:G:1001:HEC:HAB	1.75	1.22
1:K:187:CYS:SG	3:K:1002:HEC:HAB	1.79	1.22
1:M:319:CYS:SG	3:M:1004:HEC:CAC	2.26	1.22
1:P:190:CYS:SG	3:P:1002:HEC:CAC	2.28	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:147:CYS:SG	3:P:1001:HEC:CAB	2.28	1.21
1:E:147:CYS:SG	3:E:1001:HEC:CAB	2.27	1.20
1:G:349:CYS:SG	3:G:1005:HEC:HAB	1.79	1.20
1:B:190:CYS:SG	3:B:1002:HEC:HAC	1.78	1.19
1:M:349:CYS:SG	3:M:1005:HEC:HAB	1.75	1.19
1:G:150:CYS:SG	3:G:1001:HEC:HAC	1.79	1.19
1:Q:150:CYS:SG	3:Q:1001:HEC:CAC	2.29	1.19
1:Q:349:CYS:SG	3:Q:1005:HEC:HAB	1.81	1.19
1:H:349:CYS:SG	3:H:1005:HEC:CAB	2.31	1.18
2:O:139:CYS:SG	3:O:1004:HEC:HAC	1.83	1.17
1:J:190:CYS:SG	3:J:1002:HEC:CAC	2.34	1.16
2:C:119:CYS:SG	3:C:1003:HEC:CAC	2.34	1.16
2:F:119:CYS:SG	3:F:1003:HEC:HAC	1.84	1.16
1:M:187:CYS:SG	3:M:1002:HEC:HAB	1.82	1.15
2:O:119:CYS:SG	3:O:1003:HEC:CAC	2.34	1.15
1:D:190:CYS:SG	3:D:1002:HEC:CAC	2.35	1.15
2:R:119:CYS:SG	3:R:1003:HEC:CAC	2.36	1.14
1:K:187:CYS:SG	3:K:1002:HEC:CAB	2.36	1.12
1:H:150:CYS:SG	3:H:1001:HEC:HAC	1.85	1.12
2:F:119:CYS:SG	3:F:1003:HEC:CAC	2.36	1.12
2:L:119:CYS:SG	3:L:1003:HEC:CAC	2.38	1.11
1:M:319:CYS:SG	3:M:1004:HEC:HAC	1.88	1.11
1:G:352:CYS:SG	3:G:1005:HEC:HAC	1.85	1.11
1:H:240:GLY:H	1:H:243:MET:HE2	1.05	1.11
1:E:27:CYS:HB2	2:F:36:TYR:OH	1.47	1.11
1:B:66:ARG:HG2	1:B:66:ARG:HH11	1.11	1.10
1:K:187:CYS:HG	3:K:1002:HEC:HAB	0.99	1.10
1:A:190:CYS:SG	3:A:1002:HEC:HAC	1.91	1.09
1:H:352:CYS:SG	3:H:1005:HEC:HAC	1.86	1.09
2:I:139:CYS:SG	3:I:1004:HEC:HAC	1.86	1.09
1:E:190:CYS:SG	3:E:1002:HEC:HAC	1.87	1.08
1:G:190:CYS:SG	3:G:1002:HEC:HAC	1.91	1.08
1:G:319:CYS:SG	3:G:1004:HEC:HAC	1.82	1.07
1:K:27:CYS:HB2	2:L:36:TYR:OH	1.55	1.07
1:A:347:ARG:HH22	1:D:347:ARG:HD3	1.14	1.07
1:N:190:CYS:SG	3:N:1002:HEC:HAC	1.92	1.06
1:M:352:CYS:HG	3:M:1005:HEC:HAC	0.89	1.05
1:Q:328:ASP:HB3	1:Q:330:LYS:HG2	1.39	1.04
1:A:349:CYS:SG	3:A:1005:HEC:HAB	1.96	1.03
1:D:319:CYS:SG	3:D:1004:HEC:HAC	1.96	1.02
1:A:347:ARG:NH2	1:D:347:ARG:HD3	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:CYS:SG	3:J:1004:HEC:HAC	2.00	1.00
1:P:147:CYS:SG	3:P:1001:HEC:HAB	1.98	1.00
1:B:147:CYS:HG	3:B:1001:HEC:HAB	1.23	0.99
3:R:1002:HEC:HHA	3:R:1002:HEC:HBA1	1.44	0.99
3:O:1002:HEC:HHA	3:O:1002:HEC:HBA1	1.44	0.99
2:F:139:CYS:SG	3:F:1004:HEC:HAC	1.98	0.99
1:E:66:ARG:HG2	1:E:66:ARG:HH11	1.22	0.98
2:I:119:CYS:SG	3:I:1003:HEC:CAC	2.51	0.98
1:D:187:CYS:SG	3:D:1002:HEC:HAB	2.03	0.98
1:H:190:CYS:SG	3:H:1002:HEC:HAC	1.99	0.98
1:A:447:GLN:HE22	1:B:448:GLN:HE21	0.98	0.98
1:H:240:GLY:H	1:H:243:MET:CE	1.78	0.97
2:C:119:CYS:SG	3:C:1003:HEC:HAC	2.03	0.97
1:P:319:CYS:SG	3:P:1004:HEC:HAC	2.01	0.97
2:R:69:CYS:HG	3:R:1002:HEC:HAC	1.26	0.96
1:E:187:CYS:HG	3:E:1002:HEC:HAB	0.80	0.96
1:H:240:GLY:N	1:H:243:MET:HE2	1.79	0.95
2:L:117:LYS:HD3	2:L:130:MET:CE	1.96	0.95
1:E:349:CYS:HG	3:E:1005:HEC:HAB	1.24	0.95
2:O:119:CYS:SG	3:O:1003:HEC:HAC	2.06	0.94
2:L:69:CYS:HG	3:L:1002:HEC:HAC	1.18	0.94
2:L:139:CYS:HG	3:L:1004:HEC:HAC	1.04	0.94
1:Q:232:CYS:SG	3:Q:1003:HEC:HAC	2.06	0.94
1:G:447:GLN:HE22	1:H:448:GLN:HE21	1.17	0.93
1:A:458:MET:CE	1:A:466:GLY:HA2	1.99	0.93
1:K:66:ARG:HG2	1:K:66:ARG:HH21	1.30	0.92
1:Q:328:ASP:HB2	1:Q:330:LYS:NZ	1.84	0.92
1:N:147:CYS:HG	3:N:1001:HEC:HAB	1.25	0.92
1:Q:190:CYS:HG	3:Q:1002:HEC:HAC	0.82	0.92
1:P:447:GLN:HE22	1:Q:448:GLN:HE21	0.97	0.92
1:A:147:CYS:HG	3:A:1001:HEC:HAB	1.22	0.91
2:F:119:CYS:HG	3:F:1003:HEC:HAC	1.35	0.91
2:F:117:LYS:HD3	2:F:130:MET:HE3	1.50	0.91
1:H:147:CYS:HG	3:H:1001:HEC:HAB	1.11	0.91
1:N:349:CYS:HG	3:N:1005:HEC:HAB	1.29	0.91
1:Q:352:CYS:HG	3:Q:1005:HEC:HAC	1.10	0.91
3:L:1002:HEC:HBA1	3:L:1002:HEC:HHA	1.53	0.90
1:P:190:CYS:SG	3:P:1002:HEC:HAC	2.11	0.90
1:D:187:CYS:SG	3:D:1002:HEC:CBB	2.60	0.89
2:I:37:THR:HG22	2:I:82:LYS:NZ	1.86	0.89
1:Q:240:GLY:H	1:Q:243:MET:CE	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:CYS:CB	2:F:36:TYR:OH	2.19	0.89
1:E:187:CYS:HG	3:E:1002:HEC:CAB	1.66	0.89
2:R:117:LYS:HD3	2:R:130:MET:HE3	1.55	0.89
1:K:147:CYS:HG	3:K:1001:HEC:HAB	1.11	0.89
1:D:352:CYS:HG	3:D:1005:HEC:CAC	1.85	0.88
1:H:157:GLU:HG3	7:H:2053:HOH:O	1.71	0.88
2:R:139:CYS:HG	3:R:1004:HEC:HAC	1.33	0.87
1:N:225:ARG:HB3	1:N:315:THR:HG21	1.55	0.86
1:K:229:CYS:HG	3:K:1003:HEC:HAB	1.32	0.86
1:K:27:CYS:CB	2:L:36:TYR:OH	2.24	0.86
1:H:349:CYS:SG	3:H:1005:HEC:HAB	2.17	0.85
2:F:139:CYS:SG	3:F:1004:HEC:CBC	2.65	0.85
1:K:382:VAL:HG11	1:K:447:GLN:HG3	1.59	0.84
1:P:319:CYS:SG	3:P:1004:HEC:CBC	2.66	0.84
1:J:147:CYS:HG	3:J:1001:HEC:HAB	1.41	0.84
1:P:187:CYS:HG	3:P:1002:HEC:CAB	1.67	0.83
1:P:447:GLN:NE2	1:Q:448:GLN:HE21	1.76	0.83
1:Q:349:CYS:HG	3:Q:1005:HEC:HAB	1.38	0.83
1:A:347:ARG:HH22	1:D:347:ARG:CD	1.91	0.83
1:N:458:MET:CE	1:N:466:GLY:HA2	2.09	0.83
2:I:37:THR:HG22	2:I:82:LYS:HZ2	1.42	0.83
2:L:117:LYS:HD3	2:L:130:MET:HE1	1.61	0.83
1:P:447:GLN:HE22	1:Q:448:GLN:NE2	1.75	0.82
1:A:447:GLN:HE22	1:B:448:GLN:NE2	1.76	0.82
1:G:308:THR:HG21	7:G:2156:HOH:O	1.79	0.82
1:G:242:THR:HG22	7:G:2075:HOH:O	1.79	0.82
2:F:69:CYS:HG	3:F:1002:HEC:HAC	1.02	0.81
1:Q:325:ARG:NH2	2:R:102:ILE:HD11	1.94	0.81
1:P:187:CYS:HG	3:P:1002:HEC:HAB	0.77	0.81
1:B:66:ARG:HG2	1:B:66:ARG:NH1	1.88	0.81
1:J:352:CYS:HG	3:J:1005:HEC:CAC	1.90	0.80
1:D:319:CYS:HG	3:D:1004:HEC:HAC	1.44	0.80
2:F:37:THR:HG22	2:F:82:LYS:HZ1	1.47	0.80
1:E:497:HIS:HD2	1:E:499:TRP:H	1.26	0.80
2:I:139:CYS:SG	3:I:1004:HEC:CBC	2.70	0.80
1:G:147:CYS:SG	3:G:1001:HEC:CBB	2.70	0.80
3:F:1002:HEC:HHA	3:F:1002:HEC:HBA1	1.63	0.79
1:Q:328:ASP:HB2	1:Q:330:LYS:HZ3	1.46	0.79
2:R:117:LYS:HD3	2:R:130:MET:CE	2.12	0.79
2:R:119:CYS:HG	3:R:1003:HEC:HAC	1.44	0.79
1:E:33:GLU:HG3	1:E:33:GLU:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:119:CYS:SG	3:L:1003:HEC:HAC	2.20	0.79
1:A:352:CYS:SG	3:A:1005:HEC:C3C	2.71	0.79
1:P:87:ASN:HB3	1:P:98:ALA:HB3	1.64	0.79
1:Q:225:ARG:HB3	1:Q:315:THR:HG21	1.64	0.79
3:K:1003:HEC:HMA3	3:K:1004:HEC:HBA2	1.65	0.78
1:K:225:ARG:HB3	1:K:315:THR:HG21	1.67	0.77
1:D:429:ASN:HB3	3:D:1004:HEC:HAA1	1.64	0.77
1:M:319:CYS:HG	3:M:1004:HEC:HAC	1.48	0.77
1:Q:147:CYS:HG	3:Q:1001:HEC:HAB	0.96	0.77
3:M:1002:HEC:HBC2	3:M:1003:HEC:HBB2	1.67	0.77
1:P:147:CYS:SG	3:P:1001:HEC:CBB	2.73	0.76
1:A:315:THR:HG22	1:A:318:ASP:H	1.50	0.76
1:Q:328:ASP:HB3	1:Q:330:LYS:CG	2.15	0.76
1:D:190:CYS:SG	3:D:1002:HEC:HAC	2.26	0.76
1:G:150:CYS:SG	3:G:1001:HEC:C3C	2.74	0.76
1:D:87:ASN:HB3	1:D:98:ALA:HB3	1.67	0.75
1:Q:121:HIS:ND1	1:Q:337:TRP:CE3	2.53	0.75
1:J:144:PRO:HB3	1:J:247:LYS:HD2	1.68	0.75
1:K:66:ARG:HG2	1:K:66:ARG:NH2	1.99	0.75
1:M:147:CYS:SG	3:M:1001:HEC:CBB	2.75	0.75
2:O:117:LYS:HZ3	2:O:130:MET:HE2	1.51	0.75
1:P:232:CYS:SG	3:P:1003:HEC:C3C	2.74	0.75
1:M:349:CYS:SG	3:M:1005:HEC:CBB	2.75	0.74
2:I:157:ALA:O	2:I:158:ASP:HB2	1.86	0.74
1:P:232:CYS:SG	3:P:1003:HEC:CBC	2.76	0.74
1:B:308:THR:HG21	7:B:2186:HOH:O	1.87	0.74
2:F:37:THR:HG22	2:F:82:LYS:NZ	2.02	0.74
2:O:129:SER:HB3	3:O:1004:HEC:HBB2	1.70	0.74
1:H:225:ARG:HB3	1:H:315:THR:HG21	1.70	0.74
2:R:37:THR:HG23	2:R:82:LYS:NZ	2.02	0.74
2:I:139:CYS:HG	3:I:1004:HEC:HAC	1.53	0.73
1:Q:240:GLY:H	1:Q:243:MET:HE3	1.51	0.73
1:J:376:LEU:HD11	1:J:426:SER:HB2	1.69	0.73
1:B:345:GLU:HB2	1:B:347:ARG:HD2	1.70	0.73
1:H:375:LEU:HD22	1:H:443:LEU:HB3	1.71	0.73
1:Q:240:GLY:H	1:Q:243:MET:HE2	1.54	0.73
1:P:429:ASN:HB3	3:P:1004:HEC:CAA	2.19	0.72
2:R:40:ARG:HE	2:R:56:HIS:HD2	1.34	0.72
2:C:139:CYS:HG	3:C:1004:HEC:HAC	1.53	0.72
1:H:150:CYS:SG	3:H:1001:HEC:CBC	2.76	0.72
1:N:157:GLU:HG3	7:N:2061:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:117:LYS:CD	2:R:130:MET:HE3	2.20	0.72
1:G:139:GLU:OE2	1:G:518:ARG:NH1	2.20	0.72
1:Q:59:LYS:HD3	1:Q:330:LYS:HD3	1.72	0.72
1:A:185:ILE:HG12	3:A:1003:HEC:HBC2	1.71	0.71
1:B:185:ILE:HG12	3:B:1003:HEC:HBC2	1.72	0.71
1:G:447:GLN:NE2	1:H:448:GLN:HE21	1.86	0.71
1:P:349:CYS:SG	3:P:1005:HEC:CBB	2.76	0.71
1:P:448:GLN:HE21	1:Q:447:GLN:HE22	1.36	0.71
2:F:157:ALA:O	2:F:158:ASP:HB2	1.90	0.71
1:P:352:CYS:SG	3:P:1005:HEC:CBC	2.78	0.71
1:E:225:ARG:HB3	1:E:315:THR:HG21	1.72	0.71
1:K:429:ASN:HB3	3:K:1004:HEC:HAA1	1.70	0.71
1:P:105:LEU:HD13	1:P:422:TRP:CZ2	2.26	0.71
1:A:308:THR:HG21	7:A:2197:HOH:O	1.91	0.71
1:G:447:GLN:HE22	1:H:448:GLN:NE2	1.87	0.71
1:P:463:TYR:HH	1:Q:470:SER:HG	1.27	0.71
1:H:493:PHE:O	1:H:496:THR:HB	1.91	0.70
1:N:493:PHE:O	1:N:496:THR:HB	1.90	0.70
1:D:349:CYS:SG	3:D:1005:HEC:CBB	2.77	0.70
1:N:147:CYS:SG	3:N:1001:HEC:CBB	2.79	0.70
1:A:190:CYS:SG	3:A:1002:HEC:CBC	2.79	0.70
1:G:352:CYS:SG	3:G:1005:HEC:C3C	2.79	0.70
1:N:129:LEU:HD12	1:N:180:MET:CE	2.21	0.70
1:G:147:CYS:HG	3:G:1001:HEC:HAB	1.56	0.70
1:D:319:CYS:SG	3:D:1004:HEC:CBC	2.80	0.69
1:A:458:MET:HE1	1:A:466:GLY:HA2	1.74	0.69
1:P:46:GLU:O	1:P:46:GLU:HG3	1.92	0.69
1:H:262:MET:CE	1:H:302:GLU:HG2	2.21	0.69
2:I:119:CYS:SG	3:I:1003:HEC:HAC	2.31	0.69
3:Q:1003:HEC:HMC1	3:Q:1003:HEC:HBC3	1.73	0.69
1:D:458:MET:HE2	1:D:463:TYR:HA	1.75	0.69
1:H:147:CYS:SG	3:H:1001:HEC:CBB	2.80	0.69
2:O:69:CYS:SG	3:O:1002:HEC:CBC	2.80	0.69
1:H:150:CYS:SG	3:H:1001:HEC:C3C	2.81	0.69
1:D:308:THR:HG21	7:D:2167:HOH:O	1.93	0.68
1:H:139:GLU:OE2	1:H:518:ARG:NH2	2.26	0.68
1:J:447:GLN:HE22	1:K:448:GLN:HE21	1.41	0.68
1:K:349:CYS:SG	3:K:1005:HEC:CBB	2.79	0.68
1:D:232:CYS:SG	3:D:1003:HEC:C3C	2.81	0.68
1:K:139:GLU:CD	1:K:518:ARG:HH12	1.96	0.68
1:G:29:ASP:OD1	2:L:39:GLN:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:59:LYS:HE2	1:Q:330:LYS:HZ1	1.58	0.68
1:E:27:CYS:HB2	2:F:36:TYR:HH	1.59	0.68
1:B:352:CYS:SG	3:B:1005:HEC:C3C	2.82	0.68
1:K:232:CYS:SG	3:K:1003:HEC:C3C	2.81	0.68
1:N:232:CYS:SG	3:N:1003:HEC:C3C	2.81	0.68
1:A:349:CYS:SG	3:A:1005:HEC:CBB	2.82	0.68
1:D:185:ILE:HG12	3:D:1003:HEC:HBC2	1.75	0.68
2:O:117:LYS:NZ	2:O:130:MET:HE2	2.08	0.68
1:M:262:MET:CE	1:M:302:GLU:HG2	2.24	0.67
1:E:497:HIS:CD2	1:E:499:TRP:H	2.11	0.67
1:H:190:CYS:SG	3:H:1002:HEC:CBC	2.80	0.67
1:M:157:GLU:HG3	7:M:2060:HOH:O	1.94	0.67
1:J:319:CYS:SG	3:J:1004:HEC:CBC	2.82	0.67
1:Q:325:ARG:NH2	2:R:102:ILE:CD1	2.57	0.67
1:K:498:LYS:O	1:K:501:GLN:HG2	1.93	0.67
3:E:1002:HEC:HBC1	3:E:1003:HEC:HHC	1.77	0.67
2:O:139:CYS:SG	3:O:1004:HEC:C3C	2.83	0.67
1:A:187:CYS:HG	3:A:1002:HEC:CAB	2.07	0.67
1:D:315:THR:HG22	1:D:318:ASP:H	1.61	0.66
1:Q:319:CYS:SG	3:Q:1004:HEC:C3C	2.82	0.66
3:D:1001:HEC:HBC3	3:D:1001:HEC:HMC1	1.76	0.66
1:Q:32:THR:HB	2:R:58:LEU:HD11	1.77	0.66
1:H:331:LYS:HE3	2:I:155:GLU:HG2	1.78	0.66
1:B:190:CYS:SG	3:B:1002:HEC:CBC	2.82	0.66
1:Q:328:ASP:HB2	1:Q:330:LYS:HZ2	1.59	0.66
1:Q:314:VAL:HG22	3:Q:1005:HEC:HBC2	1.76	0.66
2:R:79:LEU:HB2	2:R:80:PRO:HD3	1.76	0.66
1:B:139:GLU:OE1	1:B:518:ARG:NH2	2.29	0.66
1:B:232:CYS:SG	3:B:1003:HEC:C3C	2.83	0.66
1:G:319:CYS:SG	3:G:1004:HEC:CBC	2.83	0.66
1:Q:328:ASP:CB	1:Q:330:LYS:NZ	2.59	0.66
1:D:352:CYS:SG	3:D:1005:HEC:C3C	2.84	0.66
3:R:1002:HEC:HBA1	3:R:1002:HEC:CHA	2.25	0.66
2:L:37:THR:HG23	2:L:82:LYS:NZ	2.11	0.65
1:D:187:CYS:SG	3:D:1002:HEC:C3B	2.83	0.65
1:G:376:LEU:HD11	1:G:426:SER:HB2	1.79	0.65
1:J:232:CYS:SG	3:J:1003:HEC:CBC	2.80	0.65
1:J:470:SER:HG	1:K:463:TYR:HH	1.44	0.65
2:R:40:ARG:HE	2:R:56:HIS:CD2	2.13	0.65
2:F:139:CYS:SG	3:F:1004:HEC:C3C	2.84	0.65
1:H:198:LEU:HD22	1:H:228:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:458:MET:HE3	1:N:466:GLY:HA2	1.78	0.65
2:O:69:CYS:HG	3:O:1002:HEC:HAC	1.59	0.65
1:P:124:ALA:HB3	1:P:184:THR:HG22	1.77	0.65
3:Q:1002:HEC:HBC2	3:Q:1003:HEC:HBB2	1.79	0.65
3:G:1004:HEC:O2A	7:G:2155:HOH:O	2.15	0.65
1:H:429:ASN:HB3	3:H:1004:HEC:CAA	2.27	0.65
1:J:352:CYS:SG	3:J:1005:HEC:C3C	2.85	0.65
2:L:139:CYS:SG	3:L:1004:HEC:C3C	2.84	0.65
1:P:121:HIS:ND1	1:P:337:TRP:CE3	2.64	0.65
1:Q:129:LEU:HD12	1:Q:180:MET:CE	2.26	0.65
1:B:352:CYS:SG	3:B:1005:HEC:CBC	2.81	0.65
1:A:347:ARG:NH2	1:D:347:ARG:CD	2.53	0.65
1:G:33:GLU:HG3	1:G:35:LYS:HE3	1.78	0.64
1:H:349:CYS:SG	3:H:1005:HEC:CBB	2.84	0.64
1:N:458:MET:HE1	1:N:466:GLY:HA2	1.78	0.64
2:R:117:LYS:CE	2:R:130:MET:HE3	2.26	0.64
1:E:429:ASN:HB3	3:E:1004:HEC:CAA	2.27	0.64
1:B:493:PHE:O	1:B:496:THR:HB	1.97	0.64
1:M:352:CYS:SG	3:M:1005:HEC:C3C	2.85	0.64
1:B:121:HIS:ND1	1:B:337:TRP:CE3	2.66	0.64
1:N:129:LEU:HD12	1:N:180:MET:HE2	1.79	0.64
1:N:150:CYS:SG	3:N:1001:HEC:C3C	2.85	0.64
1:H:352:CYS:SG	3:H:1005:HEC:C3C	2.85	0.64
1:M:232:CYS:SG	3:M:1003:HEC:C3C	2.85	0.64
1:Q:106:TRP:CE3	1:Q:111:PHE:HB3	2.33	0.64
1:G:319:CYS:SG	3:G:1004:HEC:C3C	2.85	0.64
2:I:139:CYS:SG	3:I:1004:HEC:C3C	2.84	0.64
1:Q:229:CYS:SG	3:Q:1003:HEC:C3B	2.85	0.64
1:Q:327:ASP:OD1	1:Q:330:LYS:HE3	1.98	0.64
1:E:319:CYS:SG	3:E:1004:HEC:C3C	2.84	0.64
2:R:69:CYS:SG	3:R:1002:HEC:C3C	2.86	0.64
1:H:129:LEU:HD12	1:H:180:MET:CE	2.27	0.63
3:B:1001:HEC:HBC3	3:B:1001:HEC:HMC1	1.81	0.63
3:D:1003:HEC:HMA3	3:D:1004:HEC:HBA2	1.80	0.63
1:M:150:CYS:SG	3:M:1001:HEC:C3C	2.87	0.63
2:O:117:LYS:NZ	2:O:130:MET:CE	2.61	0.63
1:N:29:ASP:OD2	2:O:40:ARG:HD2	1.99	0.63
1:N:382:VAL:HG11	1:N:447:GLN:HG3	1.81	0.63
2:O:108:THR:O	2:O:112:VAL:HG23	1.98	0.63
1:G:454:ILE:O	1:G:458:MET:HG3	1.99	0.63
1:Q:147:CYS:SG	3:Q:1001:HEC:CBB	2.85	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:LYS:HD3	2:L:130:MET:HE2	1.81	0.63
1:M:185:ILE:HG12	3:M:1003:HEC:HBC2	1.79	0.63
2:C:40:ARG:HG3	3:C:1002:HEC:HBB1	1.80	0.62
3:N:1003:HEC:HMA3	3:N:1004:HEC:HBA2	1.79	0.62
2:R:37:THR:HG23	2:R:82:LYS:HZ1	1.62	0.62
1:G:429:ASN:HB3	3:G:1004:HEC:CAA	2.29	0.62
1:J:394:ASN:ND2	1:J:412:ARG:HH22	1.97	0.62
2:F:40:ARG:HG3	3:F:1002:HEC:HBB1	1.81	0.62
1:J:447:GLN:HE22	1:K:448:GLN:NE2	1.96	0.62
1:A:150:CYS:SG	3:A:1001:HEC:C3C	2.85	0.62
1:G:32:THR:HG21	7:L:2004:HOH:O	1.99	0.62
1:J:107:LEU:HD23	1:J:287:PRO:HG2	1.82	0.62
1:K:139:GLU:OE2	1:K:518:ARG:NH1	2.32	0.62
1:P:429:ASN:HB3	3:P:1004:HEC:HAA1	1.80	0.62
1:Q:190:CYS:HG	3:Q:1002:HEC:CAC	1.79	0.62
1:A:319:CYS:SG	3:A:1004:HEC:C3C	2.88	0.62
3:G:1001:HEC:HMC1	3:G:1001:HEC:HBC3	1.82	0.62
1:P:146:THR:HG23	1:P:249:PRO:HD3	1.79	0.62
1:P:352:CYS:SG	3:P:1005:HEC:C3C	2.86	0.62
1:Q:232:CYS:SG	3:Q:1003:HEC:CBC	2.86	0.62
1:N:185:ILE:HG12	3:N:1003:HEC:HBC2	1.82	0.62
1:P:198:LEU:HD11	3:P:1002:HEC:HBD1	1.81	0.62
1:B:190:CYS:SG	3:B:1002:HEC:C3C	2.88	0.62
2:C:48:ILE:HG21	3:C:1001:HEC:HMD3	1.81	0.62
1:G:32:THR:HG22	7:L:2006:HOH:O	1.99	0.62
1:G:349:CYS:SG	3:G:1005:HEC:CBB	2.86	0.62
2:I:73:HIS:HD2	5:I:1005:LMT:O6B	1.82	0.62
2:R:157:ALA:O	2:R:158:ASP:HB2	1.98	0.62
2:R:54:VAL:O	2:R:58:LEU:HD13	2.00	0.61
1:E:66:ARG:HG2	1:E:66:ARG:NH1	2.01	0.61
1:D:470:SER:OG	1:E:463:TYR:OH	2.15	0.61
2:F:69:CYS:HG	3:F:1002:HEC:CAC	1.89	0.61
1:B:429:ASN:HB3	3:B:1004:HEC:HAA1	1.81	0.61
1:E:150:CYS:SG	3:E:1001:HEC:C3C	2.89	0.61
1:N:343:ASP:OD2	1:N:347:ARG:HD3	2.01	0.61
1:D:343:ASP:OD2	1:D:347:ARG:HG2	2.01	0.61
1:M:121:HIS:ND1	1:M:337:TRP:CE3	2.68	0.61
1:N:139:GLU:OE1	1:N:518:ARG:NH2	2.34	0.61
1:H:29:ASP:OD2	2:I:40:ARG:HD2	2.01	0.61
1:N:30:VAL:CG2	2:O:40:ARG:HD3	2.31	0.61
1:N:319:CYS:SG	3:N:1004:HEC:C3C	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:429:ASN:HB3	3:K:1004:HEC:CAA	2.30	0.60
1:P:190:CYS:SG	3:P:1002:HEC:C3C	2.88	0.60
1:E:121:HIS:ND1	1:E:337:TRP:CE3	2.64	0.60
1:E:352:CYS:SG	3:E:1005:HEC:C3C	2.88	0.60
1:H:232:CYS:SG	3:H:1003:HEC:C3C	2.87	0.60
3:M:1005:HEC:HMB1	3:M:1005:HEC:HBB3	1.84	0.60
1:D:190:CYS:SG	3:D:1002:HEC:CBC	2.90	0.60
3:J:1003:HEC:HMA3	3:J:1004:HEC:HBA2	1.84	0.60
1:B:105:LEU:HD13	1:B:422:TRP:CZ2	2.37	0.60
1:E:190:CYS:SG	3:E:1002:HEC:C3C	2.89	0.60
3:H:1003:HEC:HMA3	3:H:1004:HEC:HBA2	1.84	0.60
2:I:37:THR:HG22	2:I:82:LYS:HZ1	1.64	0.60
1:M:199:ARG:HD3	7:M:2074:HOH:O	2.02	0.60
1:Q:59:LYS:HD3	1:Q:330:LYS:CD	2.32	0.60
2:F:39:GLN:HB3	7:F:2001:HOH:O	2.02	0.60
2:L:107:GLU:O	2:L:111:VAL:HG13	2.01	0.60
1:P:308:THR:HG21	7:P:2173:HOH:O	2.01	0.60
1:E:232:CYS:SG	3:E:1003:HEC:C3C	2.86	0.59
1:H:429:ASN:HB3	3:H:1004:HEC:HAA1	1.84	0.59
1:K:87:ASN:HB3	1:K:98:ALA:HB3	1.84	0.59
1:M:376:LEU:HD11	1:M:426:SER:HB2	1.84	0.59
3:Q:1005:HEC:HMB1	3:Q:1005:HEC:HBB3	1.83	0.59
1:K:352:CYS:SG	3:K:1005:HEC:C3C	2.89	0.59
1:Q:376:LEU:HD11	1:Q:426:SER:HB2	1.84	0.59
3:E:1001:HEC:HMC1	3:E:1001:HEC:HBC3	1.83	0.59
1:M:32:THR:HG22	7:R:2012:HOH:O	2.02	0.59
1:M:187:CYS:SG	3:M:1002:HEC:CBB	2.86	0.59
1:M:394:ASN:ND2	1:M:412:ARG:HH22	2.00	0.59
1:N:187:CYS:HG	3:N:1002:HEC:CAB	2.14	0.59
7:G:2090:HOH:O	2:I:132:ALA:HB3	2.02	0.59
1:A:147:CYS:SG	3:A:1001:HEC:CBB	2.85	0.59
1:A:447:GLN:NE2	1:B:448:GLN:HE21	1.83	0.59
1:J:429:ASN:HB3	3:J:1004:HEC:HAA1	1.84	0.59
2:R:48:ILE:HG21	3:R:1001:HEC:HMD3	1.85	0.59
1:K:319:CYS:SG	3:K:1004:HEC:C3C	2.88	0.59
1:H:264:ARG:HG2	1:H:268:LYS:HE3	1.83	0.59
1:A:87:ASN:HB3	1:A:98:ALA:HB3	1.85	0.59
1:D:376:LEU:HD11	1:D:426:SER:HB2	1.84	0.59
1:H:471:GLY:H	1:H:476:ILE:HD11	1.67	0.59
1:N:429:ASN:HB3	3:N:1004:HEC:HAA1	1.85	0.59
2:R:34:MET:SD	2:R:82:LYS:HE2	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:CYS:SG	3:B:1003:HEC:CBB	2.85	0.59
3:B:1003:HEC:HMA3	3:B:1004:HEC:HBA2	1.85	0.59
2:C:139:CYS:SG	3:C:1004:HEC:CBC	2.86	0.59
1:K:121:HIS:ND1	1:K:337:TRP:CE3	2.64	0.59
3:A:1003:HEC:HMA3	3:A:1004:HEC:HBA2	1.85	0.59
1:K:349:CYS:SG	3:K:1005:HEC:C3B	2.89	0.59
3:K:1002:HEC:HBC2	3:K:1003:HEC:HBB2	1.83	0.59
1:B:429:ASN:HB3	3:B:1004:HEC:CAA	2.33	0.58
1:D:105:LEU:HD13	1:D:422:TRP:CZ2	2.37	0.58
1:G:293:MET:HE3	7:G:2078:HOH:O	2.02	0.58
1:N:146:THR:HG23	1:N:249:PRO:HD3	1.84	0.58
1:D:349:CYS:SG	3:D:1005:HEC:C3B	2.91	0.58
1:G:349:CYS:SG	3:G:1005:HEC:C3B	2.90	0.58
3:M:1005:HEC:O2D	2:O:141:ARG:NH2	2.34	0.58
1:N:314:VAL:HG22	3:N:1005:HEC:HBC2	1.84	0.58
2:F:69:CYS:SG	3:F:1002:HEC:C3C	2.91	0.58
1:J:229:CYS:SG	3:J:1003:HEC:CBB	2.84	0.58
1:M:190:CYS:SG	3:M:1002:HEC:C3C	2.92	0.58
1:P:229:CYS:SG	3:P:1003:HEC:C3B	2.90	0.58
1:K:304:TRP:O	1:K:310:GLY:HA3	2.04	0.58
3:E:1001:HEC:HHA	3:E:1001:HEC:O1D	2.03	0.58
2:F:48:ILE:HG21	3:F:1001:HEC:HMD3	1.85	0.58
2:L:117:LYS:CD	2:L:130:MET:CE	2.78	0.58
1:Q:198:LEU:HD11	3:Q:1002:HEC:HBD1	1.85	0.58
1:D:199:ARG:HD3	7:D:2062:HOH:O	2.02	0.58
1:E:352:CYS:SG	3:E:1005:HEC:CBC	2.85	0.58
3:H:1001:HEC:HMC1	3:H:1001:HEC:HBC3	1.86	0.58
1:E:27:CYS:O	1:E:27:CYS:SG	2.62	0.58
1:D:150:CYS:SG	3:D:1001:HEC:C3C	2.92	0.58
3:Q:1004:HEC:HBA1	3:Q:1004:HEC:HMA3	1.86	0.58
1:H:324:THR:O	1:H:331:LYS:HA	2.04	0.57
1:P:146:THR:CG2	1:P:249:PRO:HD3	2.35	0.57
1:Q:147:CYS:HG	3:Q:1001:HEC:CAB	1.82	0.57
1:D:447:GLN:HE22	1:E:448:GLN:HE21	1.52	0.57
2:F:43:CYS:SG	3:F:1001:HEC:CBB	2.85	0.57
1:N:190:CYS:SG	3:N:1002:HEC:C3C	2.92	0.57
1:P:448:GLN:HE21	1:Q:447:GLN:NE2	2.01	0.57
1:E:106:TRP:CE3	1:E:111:PHE:HB3	2.39	0.57
1:K:308:THR:HG21	7:K:2106:HOH:O	2.04	0.57
1:D:248:LYS:HG2	1:D:249:PRO:HD2	1.86	0.57
2:R:119:CYS:SG	3:R:1003:HEC:C3C	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:PHE:O	1:E:496:THR:HG22	2.03	0.57
1:N:429:ASN:HB3	3:N:1004:HEC:CAA	2.34	0.57
1:Q:240:GLY:N	1:Q:243:MET:CE	2.64	0.57
1:D:124:ALA:HB3	1:D:184:THR:HG22	1.85	0.57
3:I:1003:HEC:HMA3	3:I:1004:HEC:HBA2	1.86	0.57
2:O:48:ILE:HG21	3:O:1001:HEC:HMD3	1.86	0.57
1:P:190:CYS:SG	3:P:1002:HEC:CBC	2.91	0.57
1:A:190:CYS:SG	3:A:1002:HEC:C3C	2.91	0.57
2:O:37:THR:CG2	2:O:82:LYS:HZ1	2.18	0.57
3:Q:1002:HEC:HBC1	3:Q:1003:HEC:HHC	1.87	0.57
2:C:136:CYS:SG	3:C:1004:HEC:CBB	2.87	0.57
1:E:262:MET:CE	1:E:302:GLU:HG2	2.35	0.57
3:O:1002:HEC:HHA	3:O:1002:HEC:CBA	2.28	0.57
1:H:314:VAL:HG22	3:H:1005:HEC:HBC2	1.87	0.56
1:K:291:THR:O	1:K:293:MET:HG2	2.05	0.56
1:B:129:LEU:HD12	1:B:180:MET:HE2	1.87	0.56
2:C:35:LYS:HE3	2:C:39:GLN:NE2	2.20	0.56
1:J:87:ASN:HB3	1:J:98:ALA:HB3	1.86	0.56
1:K:66:ARG:HH21	1:K:66:ARG:CG	2.12	0.56
3:M:1002:HEC:HMB1	3:M:1002:HEC:HBB3	1.87	0.56
3:D:1002:HEC:HMC1	3:D:1002:HEC:HBC3	1.88	0.56
1:J:429:ASN:HB3	3:J:1004:HEC:CAA	2.36	0.56
1:K:264:ARG:HG2	1:K:268:LYS:HE3	1.86	0.56
1:K:376:LEU:HD11	1:K:426:SER:HB2	1.87	0.56
1:N:308:THR:HG21	7:N:2203:HOH:O	2.04	0.56
1:N:352:CYS:SG	3:N:1005:HEC:C3C	2.90	0.56
1:P:50:ASN:OD1	1:P:186:GLY:HA3	2.05	0.56
1:Q:352:CYS:SG	3:Q:1005:HEC:C3C	2.93	0.56
1:H:121:HIS:ND1	1:H:337:TRP:CE3	2.69	0.56
1:E:429:ASN:HB3	3:E:1004:HEC:HAA2	1.87	0.56
2:F:40:ARG:HE	2:F:56:HIS:HD2	1.53	0.56
1:H:376:LEU:HD11	1:H:426:SER:HB2	1.87	0.56
1:J:252:PRO:HG3	1:J:266:TYR:OH	2.06	0.56
1:J:308:THR:HG21	7:J:2167:HOH:O	2.05	0.56
1:P:349:CYS:SG	3:P:1005:HEC:C3B	2.93	0.56
1:H:129:LEU:HD12	1:H:180:MET:HE2	1.88	0.56
1:J:84:LYS:HD3	1:J:115:TYR:CE2	2.41	0.56
1:J:121:HIS:ND1	1:J:337:TRP:CE3	2.73	0.56
2:O:119:CYS:SG	3:O:1003:HEC:C3C	2.94	0.56
1:A:50:ASN:OD1	1:A:186:GLY:HA3	2.06	0.56
1:B:397:GLN:NE2	7:B:2146:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:MET:O	1:E:350:ARG:HG3	2.06	0.56
1:E:478:PRO:O	1:E:497:HIS:HE1	1.88	0.56
1:H:139:GLU:CD	1:H:518:ARG:HH22	2.07	0.56
2:I:56:HIS:CE1	3:I:1002:HEC:HMC2	2.40	0.56
1:M:154:LYS:HG2	1:M:158:TRP:CZ2	2.41	0.56
2:F:139:CYS:HG	3:F:1004:HEC:HAC	1.71	0.55
7:G:2090:HOH:O	2:I:132:ALA:CB	2.54	0.55
1:K:150:CYS:SG	3:K:1001:HEC:C3C	2.93	0.55
1:D:435:ASN:ND2	1:D:438:LYS:HE3	2.20	0.55
1:E:433:PHE:CD2	3:E:1004:HEC:HMD2	2.40	0.55
2:F:46:CYS:SG	3:F:1001:HEC:CBC	2.90	0.55
2:F:117:LYS:HD3	2:F:130:MET:CE	2.30	0.55
1:G:352:CYS:HG	3:G:1005:HEC:CAC	2.15	0.55
3:G:1005:HEC:HBC3	3:G:1005:HEC:HMC1	1.88	0.55
1:K:514:ASP:HB2	1:K:519:LEU:HD11	1.88	0.55
3:P:1005:HEC:HMC1	3:P:1005:HEC:HBC3	1.87	0.55
1:A:314:VAL:HG22	3:A:1005:HEC:HBC2	1.89	0.55
2:C:139:CYS:SG	3:C:1004:HEC:C3C	2.92	0.55
2:L:37:THR:HG23	2:L:82:LYS:HZ3	1.70	0.55
1:M:225:ARG:HB3	1:M:315:THR:HG21	1.89	0.55
1:A:394:ASN:ND2	1:A:412:ARG:HH22	2.05	0.55
2:L:119:CYS:SG	3:L:1003:HEC:C3C	2.95	0.55
1:G:225:ARG:HB3	1:G:315:THR:HG21	1.88	0.55
1:N:521:SER:O	1:N:522:ALA:HB3	2.05	0.55
3:Q:1004:HEC:HBA1	3:Q:1004:HEC:CMA	2.36	0.55
1:A:187:CYS:SG	3:A:1002:HEC:C3B	2.94	0.55
1:A:458:MET:HE2	1:A:466:GLY:HA2	1.84	0.55
1:M:262:MET:HE1	1:M:302:GLU:HG2	1.88	0.55
2:I:102:ILE:O	2:I:103:LEU:HD23	2.07	0.54
1:P:470:SER:HG	1:Q:463:TYR:HH	1.53	0.54
1:Q:349:CYS:SG	3:Q:1005:HEC:CBB	2.89	0.54
2:R:139:CYS:SG	3:R:1004:HEC:C3C	2.94	0.54
1:M:319:CYS:SG	3:M:1004:HEC:CBC	2.93	0.54
1:Q:187:CYS:SG	3:Q:1002:HEC:C3B	2.95	0.54
1:A:139:GLU:OE1	1:A:518:ARG:NH1	2.39	0.54
1:M:430:SER:HB3	1:M:434:HIS:CE1	2.42	0.54
2:O:144:GLN:O	2:O:144:GLN:HG2	2.08	0.54
1:A:106:TRP:CE2	1:A:295:LYS:HE2	2.42	0.54
1:B:150:CYS:HB3	1:B:232:CYS:SG	2.48	0.54
2:I:117:LYS:HZ3	2:I:130:MET:HE2	1.73	0.54
1:J:150:CYS:SG	3:J:1001:HEC:C3C	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:1002:HEC:HBC2	3:P:1003:HEC:HBB2	1.90	0.54
1:E:187:CYS:SG	3:E:1002:HEC:CBB	2.89	0.54
1:E:189:THR:HG21	3:E:1003:HEC:HBC3	1.90	0.54
1:H:319:CYS:SG	3:H:1004:HEC:CBC	2.88	0.54
1:J:295:LYS:NZ	1:J:296:ALA:O	2.40	0.54
2:L:117:LYS:CD	2:L:130:MET:HE2	2.38	0.54
1:Q:129:LEU:HD12	1:Q:180:MET:HE3	1.88	0.54
1:G:447:GLN:NE2	1:H:448:GLN:NE2	2.52	0.54
1:K:190:CYS:SG	3:K:1002:HEC:C3C	2.95	0.54
1:Q:349:CYS:SG	3:Q:1005:HEC:C3B	2.94	0.54
1:H:185:ILE:HG12	3:H:1003:HEC:HBC2	1.89	0.54
1:Q:172:ASN:OD1	1:Q:175:ARG:HD2	2.08	0.54
1:D:187:CYS:SG	3:D:1002:HEC:HBB3	2.47	0.53
1:J:248:LYS:HG2	1:J:249:PRO:HD2	1.90	0.53
1:M:198:LEU:HD11	3:M:1002:HEC:HBD1	1.89	0.53
1:H:272:LEU:HD11	1:H:282:ALA:HB2	1.91	0.53
1:M:154:LYS:HE3	7:M:2061:HOH:O	2.09	0.53
1:N:181:LYS:NZ	7:N:2070:HOH:O	2.39	0.53
2:O:136:CYS:SG	3:O:1004:HEC:C3B	2.93	0.53
1:A:315:THR:HG21	7:A:2109:HOH:O	2.07	0.53
7:A:2198:HOH:O	1:B:308:THR:HB	2.07	0.53
2:C:136:CYS:SG	3:C:1004:HEC:C3B	2.93	0.53
3:G:1002:HEC:HMC1	3:G:1002:HEC:HBC3	1.88	0.53
1:J:349:CYS:SG	3:J:1005:HEC:CBB	2.88	0.53
1:K:189:THR:HG21	3:K:1003:HEC:HBC3	1.90	0.53
2:O:157:ALA:O	2:O:158:ASP:HB2	2.08	0.53
3:A:1005:HEC:O2D	2:C:141:ARG:NH2	2.41	0.53
2:I:112:VAL:HG11	3:I:1002:HEC:HMD3	1.90	0.53
1:K:190:CYS:HG	3:K:1002:HEC:CAC	2.18	0.53
1:K:512:VAL:HG22	1:K:520:VAL:HG22	1.91	0.53
1:Q:328:ASP:CB	1:Q:330:LYS:HG2	2.28	0.53
2:C:144:GLN:HG2	2:C:144:GLN:O	2.09	0.53
2:C:46:CYS:SG	3:C:1001:HEC:C3C	2.94	0.53
3:L:1003:HEC:HMC1	3:L:1003:HEC:HBC3	1.90	0.53
1:P:448:GLN:NE2	1:Q:447:GLN:HE22	2.06	0.53
1:H:30:VAL:HG22	2:I:40:ARG:HD3	1.89	0.53
1:H:458:MET:HE3	1:H:466:GLY:HA2	1.91	0.53
1:Q:327:ASP:H	1:Q:330:LYS:HE2	1.73	0.53
1:G:109:TYR:CD1	1:G:110:PRO:HD2	2.44	0.53
1:G:347:ARG:NH2	1:J:347:ARG:HB2	2.24	0.53
3:M:1005:HEC:HMC1	3:M:1005:HEC:HBC3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:150:CYS:SG	3:P:1001:HEC:C3C	2.96	0.53
1:P:175:ARG:HD3	1:P:513:TRP:CD2	2.44	0.53
2:R:70:HIS:CD2	3:R:1002:HEC:NB	2.77	0.53
1:E:433:PHE:CE2	3:E:1004:HEC:HMD2	2.44	0.53
1:M:144:PRO:HB3	1:M:247:LYS:HD3	1.90	0.53
1:P:129:LEU:HD22	1:P:175:ARG:HG3	1.91	0.53
1:Q:493:PHE:O	1:Q:496:THR:HB	2.08	0.53
1:J:129:LEU:HD22	1:J:175:ARG:HG3	1.91	0.52
1:J:232:CYS:SG	3:J:1003:HEC:C3C	2.94	0.52
3:J:1004:HEC:HBC3	3:J:1004:HEC:HMC1	1.91	0.52
1:A:355:ASP:OD2	1:A:356:LYS:NZ	2.36	0.52
1:N:225:ARG:HB3	1:N:315:THR:CG2	2.32	0.52
1:B:272:LEU:HD11	1:B:282:ALA:HB2	1.90	0.52
3:K:1002:HEC:HBC1	3:K:1003:HEC:HHC	1.92	0.52
1:N:121:HIS:ND1	1:N:337:TRP:CE3	2.76	0.52
1:M:429:ASN:HB3	3:M:1004:HEC:HAA1	1.92	0.52
1:Q:352:CYS:HG	3:Q:1005:HEC:CAC	1.91	0.52
1:A:458:MET:HE1	1:A:466:GLY:CA	2.39	0.52
1:D:308:THR:HG22	7:D:2142:HOH:O	2.10	0.52
7:H:2192:HOH:O	2:I:148:MET:HE2	2.10	0.52
1:J:50:ASN:OD1	1:J:186:GLY:HA3	2.10	0.52
2:O:37:THR:CG2	2:O:82:LYS:NZ	2.73	0.52
1:B:103:LYS:HD3	1:B:483:MET:HB3	1.90	0.52
1:G:429:ASN:HB3	3:G:1004:HEC:HAA1	1.91	0.52
1:N:319:CYS:SG	3:N:1004:HEC:CBC	2.88	0.52
1:Q:175:ARG:HD3	1:Q:513:TRP:CD2	2.44	0.52
1:E:187:CYS:SG	3:E:1002:HEC:C3B	2.94	0.52
1:J:124:ALA:HB3	1:J:184:THR:HG22	1.92	0.52
2:L:69:CYS:SG	3:L:1002:HEC:C3C	2.96	0.52
1:A:105:LEU:HD13	1:A:422:TRP:CZ2	2.45	0.52
1:G:458:MET:CE	1:G:466:GLY:HA2	2.40	0.52
3:G:1005:HEC:O2D	2:I:141:ARG:NH2	2.43	0.52
3:E:1002:HEC:HBB3	3:E:1002:HEC:HMB1	1.92	0.52
1:M:109:TYR:O	1:M:112:MET:HG2	2.09	0.52
2:L:132:ALA:HB3	7:L:2031:HOH:O	2.10	0.51
1:N:327:ASP:O	1:N:328:ASP:C	2.48	0.51
2:O:104:ALA:HB1	2:O:108:THR:OG1	2.10	0.51
1:Q:232:CYS:SG	3:Q:1003:HEC:C3C	2.95	0.51
1:B:232:CYS:SG	3:B:1003:HEC:CBC	2.91	0.51
3:B:1005:HEC:HBD1	7:B:2183:HOH:O	2.10	0.51
2:L:50:ASN:O	2:L:54:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:32:THR:CG2	7:R:2012:HOH:O	2.58	0.51
1:E:458:MET:HE2	1:E:463:TYR:HA	1.91	0.51
1:M:429:ASN:HB3	3:M:1004:HEC:CAA	2.40	0.51
1:N:187:CYS:SG	3:N:1002:HEC:C3B	2.95	0.51
1:P:319:CYS:SG	3:P:1004:HEC:C3C	2.94	0.51
2:F:37:THR:CG2	2:F:82:LYS:NZ	2.71	0.51
1:K:27:CYS:HB2	2:L:36:TYR:HH	1.68	0.51
1:N:458:MET:CE	1:N:466:GLY:CA	2.85	0.51
1:N:349:CYS:SG	3:N:1005:HEC:C3B	2.98	0.51
2:O:39:GLN:HG2	1:P:29[B]:ASP:OD2	2.11	0.51
1:P:380:GLN:O	1:P:384:VAL:HG23	2.11	0.51
1:Q:308:THR:HG21	7:Q:2131:HOH:O	2.11	0.51
1:B:376:LEU:HD11	1:B:426:SER:HB2	1.92	0.51
1:E:376:LEU:HD11	1:E:426:SER:HB2	1.92	0.51
1:H:240:GLY:CA	1:H:243:MET:HE2	2.39	0.51
7:P:2009:HOH:O	2:R:130:MET:HB2	2.11	0.51
3:R:1003:HEC:HMA2	3:R:1003:HEC:O2A	2.10	0.51
1:K:467:LYS:O	7:K:2090:HOH:O	2.19	0.51
2:O:117:LYS:HZ2	2:O:130:MET:CE	2.23	0.51
1:Q:50:ASN:OD1	1:Q:186:GLY:HA3	2.10	0.51
2:R:117:LYS:NZ	2:R:130:MET:HE3	2.25	0.51
1:A:376:LEU:HD11	1:A:426:SER:HB2	1.92	0.51
2:C:119:CYS:SG	3:C:1003:HEC:C3C	2.99	0.51
2:I:34:MET:SD	2:I:82:LYS:HE2	2.51	0.51
2:L:40:ARG:HG3	3:L:1002:HEC:HBB1	1.92	0.51
1:B:101:TYR:CG	1:B:384:VAL:HG21	2.46	0.51
1:B:319:CYS:SG	3:B:1004:HEC:C3C	2.95	0.51
1:D:50:ASN:OD1	1:D:186:GLY:HA3	2.10	0.51
1:E:262:MET:HE2	1:E:302:GLU:HG2	1.92	0.51
1:K:328:ASP:O	1:K:329:LYS:HG3	2.10	0.51
1:P:187:CYS:SG	3:P:1002:HEC:CBB	2.91	0.51
1:Q:328:ASP:N	1:Q:330:LYS:HE2	2.26	0.51
1:G:190:CYS:SG	3:G:1002:HEC:C3C	2.97	0.50
1:H:187:CYS:SG	3:H:1002:HEC:C3B	2.96	0.50
3:J:1005:HEC:HMA2	3:J:1005:HEC:O2A	2.11	0.50
1:Q:150:CYS:SG	3:Q:1001:HEC:C3C	2.97	0.50
1:Q:225:ARG:CB	1:Q:315:THR:HG21	2.40	0.50
3:D:1004:HEC:HMC1	3:D:1004:HEC:HBC3	1.94	0.50
1:E:304:TRP:O	1:E:310:GLY:HA3	2.10	0.50
1:J:349:CYS:SG	3:J:1005:HEC:C3B	2.94	0.50
1:Q:48:ILE:HB	1:Q:153:PRO:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:129:LEU:HD13	1:Q:516:GLN:HG2	1.93	0.50
1:B:75:GLU:OE1	1:B:97:HIS:HE1	1.94	0.50
1:B:419:GLN:HA	1:B:422:TRP:CD1	2.47	0.50
1:E:377:LEU:O	1:E:381:GLU:HG3	2.12	0.50
7:G:2134:HOH:O	1:H:375:LEU:HG	2.11	0.50
1:K:362:LYS:HE3	7:K:2061:HOH:O	2.10	0.50
1:P:376:LEU:HD11	1:P:426:SER:HB2	1.93	0.50
1:H:319:CYS:HG	3:H:1004:HEC:CAC	2.16	0.50
1:H:346:MET:O	1:H:350:ARG:HG3	2.11	0.50
1:Q:429:ASN:HB3	3:Q:1004:HEC:HBA2	1.93	0.50
3:D:1002:HEC:HBB3	3:D:1002:HEC:HMB1	1.93	0.50
2:F:136:CYS:SG	3:F:1004:HEC:C3B	2.92	0.50
1:M:375:LEU:HD13	1:M:443:LEU:HB2	1.93	0.50
1:N:345:GLU:HB2	1:N:347:ARG:HD2	1.94	0.50
3:O:1003:HEC:O2A	3:O:1003:HEC:HMA2	2.10	0.50
1:Q:244:GLY:O	7:Q:2050:HOH:O	2.20	0.50
3:C:1004:HEC:CGA	1:D:325:ARG:HH22	2.25	0.50
1:D:190:CYS:SG	3:D:1002:HEC:C3C	2.99	0.50
1:D:429:ASN:HB3	3:D:1004:HEC:CAA	2.38	0.50
1:K:225:ARG:CB	1:K:315:THR:HG21	2.40	0.50
1:Q:66:ARG:HG2	1:Q:66:ARG:HH11	1.76	0.50
1:Q:429:ASN:HB3	3:Q:1004:HEC:HAA1	1.92	0.50
1:E:105:LEU:HD13	1:E:422:TRP:CZ2	2.46	0.50
1:H:106:TRP:CE3	1:H:111:PHE:HB3	2.46	0.50
1:Q:190:CYS:SG	3:Q:1002:HEC:C3C	2.97	0.50
1:H:50:ASN:OD1	1:H:186:GLY:HA3	2.10	0.49
1:J:139:GLU:CD	1:J:518:ARG:HH12	2.14	0.49
1:K:147:CYS:CB	3:K:1001:HEC:HAB	2.39	0.49
1:K:319:CYS:HG	3:K:1004:HEC:CAC	2.20	0.49
1:Q:240:GLY:N	1:Q:243:MET:HE2	2.24	0.49
1:H:129:LEU:HD12	1:H:180:MET:HE1	1.94	0.49
1:N:454:ILE:O	1:N:458:MET:HG3	2.13	0.49
3:N:1001:HEC:HBC3	3:N:1001:HEC:HMC1	1.94	0.49
1:E:101:TYR:CG	1:E:384:VAL:HG21	2.47	0.49
1:P:458:MET:HE3	1:P:466:GLY:N	2.27	0.49
3:A:1002:HEC:HMC1	3:A:1002:HEC:HBC3	1.94	0.49
1:J:430:SER:HB3	1:J:434:HIS:CE1	2.47	0.49
3:L:1004:HEC:HMC1	3:L:1004:HEC:HBC3	1.94	0.49
3:N:1002:HEC:HBC2	3:N:1003:HEC:HBB2	1.93	0.49
1:Q:315:THR:HG22	1:Q:317:ALA:N	2.26	0.49
2:R:37:THR:HG23	2:R:82:LYS:HZ2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LYS:HE3	7:A:2173:HOH:O	2.11	0.49
2:C:56:HIS:CE1	3:C:1002:HEC:HMC2	2.48	0.49
2:F:112:VAL:HG11	3:F:1002:HEC:HMD3	1.92	0.49
3:H:1005:HEC:HMB1	3:H:1005:HEC:HBB3	1.95	0.49
1:M:87:ASN:HB3	1:M:98:ALA:HB3	1.94	0.49
1:Q:105:LEU:HD13	1:Q:422:TRP:CZ2	2.47	0.49
1:B:50:ASN:OD1	1:B:186:GLY:HA3	2.13	0.49
1:D:295:LYS:NZ	1:D:296:ALA:O	2.45	0.49
1:H:232:CYS:SG	3:H:1003:HEC:CBC	2.90	0.49
1:N:376:LEU:HD11	1:N:426:SER:HB2	1.94	0.49
1:Q:240:GLY:N	1:Q:243:MET:HE3	2.21	0.49
1:A:77:LYS:HE2	1:A:429:ASN:O	2.11	0.49
1:A:319:CYS:SG	3:A:1004:HEC:CBC	2.92	0.49
1:B:314:VAL:HG22	3:B:1005:HEC:HBC2	1.95	0.49
1:K:48:ILE:HB	1:K:153:PRO:HB2	1.93	0.49
1:N:124:ALA:HB3	1:N:184:THR:HG22	1.94	0.49
1:N:521:SER:O	1:N:522:ALA:CB	2.60	0.49
2:R:133:LYS:HB3	2:R:138:ASP:HB2	1.93	0.49
1:A:198:LEU:HD11	3:A:1002:HEC:HBD1	1.94	0.49
1:D:319:CYS:HG	3:D:1004:HEC:CAC	2.08	0.49
1:D:447:GLN:HE22	1:E:448:GLN:NE2	2.10	0.49
1:M:202:SER:HB2	1:M:231:GLN:HB3	1.94	0.49
1:Q:472:ASP:HB3	1:Q:475:THR:HG23	1.94	0.49
2:C:50:ASN:O	2:C:54:VAL:HG23	2.13	0.49
2:C:112:VAL:HG11	3:C:1002:HEC:HMD3	1.94	0.49
3:M:1002:HEC:CBC	3:M:1003:HEC:HBB2	2.42	0.49
1:P:109:TYR:O	1:P:112:MET:HB3	2.13	0.49
1:P:229:CYS:SG	3:P:1003:HEC:CBB	2.89	0.49
1:A:430:SER:HB3	1:A:434:HIS:CE1	2.48	0.48
1:B:29:ASP:OD2	2:C:40:ARG:HD2	2.13	0.48
2:C:107:GLU:O	2:C:111:VAL:HG13	2.13	0.48
1:E:185:ILE:O	1:E:186:GLY:O	2.31	0.48
1:H:200:ILE:HD11	1:H:227:LEU:HB3	1.93	0.48
1:J:308:THR:HB	7:K:2105:HOH:O	2.13	0.48
1:N:198:LEU:HD22	1:N:228:VAL:HG11	1.95	0.48
1:P:121:HIS:CD2	3:P:1003:HEC:ND	2.81	0.48
1:A:349:CYS:SG	3:A:1005:HEC:C3B	3.00	0.48
1:J:77:LYS:HE2	1:J:429:ASN:O	2.13	0.48
1:Q:87:ASN:HB3	1:Q:98:ALA:HB3	1.94	0.48
1:A:109:TYR:CD1	1:A:110:PRO:HD2	2.49	0.48
2:C:108:THR:O	2:C:112:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:THR:HG21	3:G:1003:HEC:HBC3	1.95	0.48
2:I:40:ARG:HE	2:I:56:HIS:HD2	1.62	0.48
1:K:433:PHE:HE2	3:K:1004:HEC:HBC2	1.78	0.48
2:L:52:VAL:HG22	7:L:2002:HOH:O	2.12	0.48
1:M:272:LEU:HD11	1:M:282:ALA:HB2	1.95	0.48
1:P:325:ARG:NH1	7:P:2111:HOH:O	2.47	0.48
1:A:30:VAL:CG2	5:C:1005:LMT:H6'1	2.43	0.48
1:A:103:LYS:HD3	1:A:483:MET:HB2	1.94	0.48
1:H:349:CYS:SG	3:H:1005:HEC:C3B	3.01	0.48
1:M:356:LYS:HD2	1:M:360:TYR:CD2	2.48	0.48
1:A:341:MET:HE3	7:A:2023:HOH:O	2.12	0.48
3:C:1002:HEC:HHA	3:C:1002:HEC:HBA1	1.95	0.48
2:L:40:ARG:HE	2:L:56:HIS:HD2	1.61	0.48
1:Q:429:ASN:O	3:Q:1004:HEC:HAA1	2.13	0.48
3:A:1002:HEC:HBC2	3:A:1003:HEC:HBB2	1.96	0.48
2:R:52:VAL:HG23	3:R:1002:HEC:HMB2	1.94	0.48
1:B:331:LYS:HE3	2:C:155:GLU:HG2	1.94	0.48
2:C:102:ILE:O	2:C:103:LEU:HD23	2.13	0.48
1:G:33:GLU:H	1:G:33:GLU:CD	2.17	0.48
1:J:187:CYS:SG	3:J:1002:HEC:C3B	2.98	0.48
1:M:106:TRP:CE3	1:M:111:PHE:HB3	2.49	0.48
2:R:122:MET:O	2:R:125:VAL:HG22	2.14	0.48
1:G:105:LEU:HD13	1:G:422:TRP:CZ2	2.48	0.48
1:H:308:THR:HG21	7:H:2193:HOH:O	2.13	0.48
1:H:331:LYS:HE3	2:I:155:GLU:CG	2.41	0.48
1:K:262:MET:CE	1:K:302:GLU:HG2	2.44	0.48
1:N:331:LYS:HE3	2:O:155:GLU:CG	2.43	0.48
3:N:1003:HEC:C3A	3:N:1004:HEC:HMA3	2.43	0.48
1:Q:429:ASN:HB3	3:Q:1004:HEC:CAA	2.44	0.48
3:A:1003:HEC:HMC1	3:A:1003:HEC:HBC3	1.96	0.48
1:E:225:ARG:CB	1:E:315:THR:HG21	2.42	0.48
1:H:319:CYS:SG	3:H:1004:HEC:C3C	2.98	0.48
1:G:121:HIS:ND1	1:G:337:TRP:CE3	2.82	0.48
1:G:433:PHE:CE2	3:G:1004:HEC:HMD2	2.49	0.48
2:O:117:LYS:HZ2	2:O:130:MET:HE3	1.77	0.48
2:R:40:ARG:HG3	3:R:1002:HEC:HBB1	1.96	0.48
1:D:319:CYS:SG	3:D:1004:HEC:C3C	2.99	0.47
1:G:430:SER:HB3	1:G:434:HIS:CE1	2.49	0.47
1:J:189:THR:HG21	3:J:1003:HEC:HBC3	1.95	0.47
1:B:124:ALA:HB3	1:B:184:THR:HG22	1.95	0.47
1:E:349:CYS:SG	3:E:1005:HEC:C3B	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1005:LMT:H41	5:L:1005:LMT:H72	1.60	0.47
1:Q:236:TYR:CE2	3:Q:1001:HEC:HMC2	2.49	0.47
1:H:262:MET:HE1	1:H:302:GLU:HG2	1.94	0.47
1:Q:471:GLY:H	1:Q:476:ILE:HD11	1.79	0.47
1:G:344:PRO:HD2	1:J:344:PRO:HD3	1.95	0.47
1:P:315:THR:HG22	1:P:318:ASP:H	1.78	0.47
1:Q:91:LEU:HD23	1:Q:94:GLY:O	2.15	0.47
1:M:129:LEU:HD12	1:M:180:MET:CE	2.45	0.47
1:B:147:CYS:SG	3:B:1001:HEC:CBB	2.94	0.47
1:B:319:CYS:SG	3:B:1004:HEC:CBC	2.91	0.47
1:N:206:THR:O	1:N:210:VAL:HG23	2.14	0.47
1:G:80:VAL:HG11	1:G:91:LEU:HD22	1.96	0.47
1:H:190:CYS:SG	3:H:1002:HEC:C3C	3.00	0.47
2:L:143:VAL:HG13	3:L:1002:HEC:HBC2	1.95	0.47
1:M:158:TRP:HB3	1:M:166:PHE:CE1	2.49	0.47
1:N:105:LEU:HD13	1:N:422:TRP:CZ2	2.50	0.47
3:P:1001:HEC:HBB3	3:P:1001:HEC:HMB1	1.96	0.47
1:Q:430:SER:HB3	1:Q:434:HIS:CE1	2.49	0.47
1:Q:512:VAL:HG22	1:Q:520:VAL:HG22	1.97	0.47
1:B:324:THR:O	1:B:331:LYS:HA	2.15	0.47
1:M:166:PHE:HA	1:M:169:LYS:HD2	1.97	0.47
1:P:84:LYS:HD3	1:P:115:TYR:CE2	2.49	0.47
3:P:1005:HEC:O2D	2:R:141:ARG:NH2	2.48	0.47
1:G:458:MET:HE3	1:G:466:GLY:HA2	1.95	0.47
3:H:1002:HEC:HBC3	3:H:1002:HEC:HMC1	1.96	0.47
1:H:345:GLU:HB2	1:H:347:ARG:HD2	1.97	0.47
1:K:32:THR:HG23	2:L:57:LYS:HD3	1.97	0.47
1:K:370:LYS:O	1:K:370:LYS:HG3	2.15	0.47
1:N:57:PHE:CZ	1:N:196:MET:HG3	2.50	0.47
2:R:108:THR:HB	7:R:2015:HOH:O	2.14	0.47
1:G:87:ASN:HB3	1:G:98:ALA:HB3	1.97	0.46
1:G:187:CYS:SG	3:G:1002:HEC:CBB	2.92	0.46
1:H:35:LYS:HD3	1:H:36:THR:O	2.15	0.46
1:J:301:TYR:O	1:J:305:ILE:HG13	2.15	0.46
1:K:185:ILE:HD11	3:K:1003:HEC:HMD2	1.97	0.46
1:K:224:MET:O	1:K:228:VAL:HG22	2.15	0.46
7:P:2006:HOH:O	2:R:130:MET:CE	2.63	0.46
1:Q:129:LEU:O	1:Q:175:ARG:NH2	2.48	0.46
1:Q:328:ASP:CB	1:Q:330:LYS:HZ2	2.24	0.46
2:C:104:ALA:HB1	2:C:108:THR:OG1	2.16	0.46
3:E:1002:HEC:HBC2	3:E:1003:HEC:HBB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:119:CYS:SG	3:F:1003:HEC:C3C	3.03	0.46
1:H:234:VAL:HG21	1:H:251:PHE:CZ	2.50	0.46
1:K:57:PHE:CZ	1:K:196:MET:HG3	2.51	0.46
1:K:75:GLU:OE1	1:K:97:HIS:HE1	1.99	0.46
1:K:84:LYS:HD3	1:K:115:TYR:CE2	2.50	0.46
1:D:106:TRP:CE3	1:D:111:PHE:HB3	2.50	0.46
1:E:50:ASN:OD1	1:E:186:GLY:HA3	2.15	0.46
1:H:225:ARG:HB3	1:H:315:THR:CG2	2.43	0.46
3:I:1004:HEC:HMC1	3:I:1004:HEC:HBC3	1.96	0.46
2:R:46:CYS:SG	3:R:1001:HEC:C3C	2.98	0.46
3:I:1004:HEC:CGA	1:J:325:ARG:HH22	2.28	0.46
1:M:258:ASP:OD1	1:M:438:LYS:HE2	2.16	0.46
1:Q:304:TRP:O	1:Q:310:GLY:HA3	2.16	0.46
1:G:248:LYS:HG2	1:G:249:PRO:HD2	1.97	0.46
1:M:350:ARG:HD3	7:M:2126:HOH:O	2.15	0.46
1:A:375:LEU:HD13	1:A:443:LEU:HB2	1.97	0.46
3:A:1005:HEC:HMB1	3:A:1005:HEC:HBB3	1.97	0.46
2:F:139:CYS:SG	3:F:1004:HEC:HBC3	2.55	0.46
1:K:147:CYS:SG	3:K:1001:HEC:CBB	2.94	0.46
2:L:136:CYS:SG	3:L:1004:HEC:CBB	2.92	0.46
2:C:46:CYS:SG	3:C:1001:HEC:CBC	2.89	0.46
1:J:229:CYS:SG	3:J:1003:HEC:C3B	2.97	0.46
1:P:187:CYS:SG	3:P:1002:HEC:C3B	3.00	0.46
1:B:129:LEU:HD13	1:B:516:GLN:HG3	1.97	0.46
1:E:315:THR:HG22	1:E:318:ASP:H	1.80	0.46
1:E:419:GLN:HA	1:E:422:TRP:CD1	2.51	0.46
1:E:458:MET:CE	1:E:463:TYR:HA	2.46	0.46
3:J:1005:HEC:O2D	2:L:141:ARG:NH2	2.49	0.46
1:K:124:ALA:HB3	1:K:184:THR:HG22	1.98	0.46
1:B:271:ASP:OD2	7:B:2097:HOH:O	2.20	0.46
1:K:315:THR:HG23	1:K:317:ALA:H	1.81	0.46
2:L:112:VAL:HG12	3:L:1003:HEC:HBB1	1.98	0.46
3:O:1004:HEC:HBC3	3:O:1004:HEC:HMC1	1.98	0.46
2:R:112:VAL:HG11	3:R:1002:HEC:HMD3	1.97	0.46
1:A:30:VAL:HG21	5:C:1005:LMT:H6'1	1.98	0.46
1:E:33:GLU:O	1:E:35:LYS:N	2.49	0.46
2:F:108:THR:O	2:F:112:VAL:HG23	2.16	0.46
2:F:157:ALA:O	2:F:158:ASP:CB	2.63	0.46
1:G:150:CYS:HG	3:G:1001:HEC:HAC	1.69	0.46
1:G:419:GLN:HA	1:G:422:TRP:CD1	2.51	0.46
1:H:147:CYS:HG	3:H:1001:HEC:CAB	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:121:HIS:CD2	3:N:1003:HEC:ND	2.84	0.46
1:J:139:GLU:OE2	1:J:518:ARG:NH1	2.45	0.45
1:J:400:LYS:HE3	7:J:2125:HOH:O	2.16	0.45
2:L:112:VAL:HG11	3:L:1002:HEC:HMD3	1.97	0.45
1:N:32:THR:HG21	2:O:58:LEU:HD13	1.98	0.45
1:P:272:LEU:HD11	1:P:282:ALA:HB2	1.98	0.45
1:A:429:ASN:HB3	3:A:1004:HEC:HAA1	1.98	0.45
3:A:1001:HEC:HMC1	3:A:1001:HEC:HBC3	1.98	0.45
1:B:345:GLU:CB	1:B:347:ARG:HD2	2.44	0.45
1:G:30:VAL:HG23	5:I:1005:LMT:H6'1	1.99	0.45
2:L:133:LYS:HB3	2:L:138:ASP:HB2	1.98	0.45
1:N:435:ASN:ND2	1:N:438:LYS:HE2	2.31	0.45
2:O:46:CYS:SG	3:O:1001:HEC:CBC	2.90	0.45
1:Q:129:LEU:HD12	1:Q:180:MET:HE2	1.96	0.45
1:B:139:GLU:CD	1:B:518:ARG:HH21	2.19	0.45
2:F:37:THR:CG2	2:F:82:LYS:HZ2	2.28	0.45
2:F:120:HIS:HB2	3:F:1004:HEC:HMB2	1.98	0.45
3:J:1003:HEC:HBC3	3:J:1003:HEC:HMC1	1.98	0.45
1:Q:352:CYS:SG	3:Q:1005:HEC:CBC	2.95	0.45
3:F:1004:HEC:HBC3	3:F:1004:HEC:HMC1	1.98	0.45
1:K:283:ASP:OD1	7:K:2043:HOH:O	2.21	0.45
1:M:385:LYS:HG3	1:M:473:ILE:HD13	1.97	0.45
1:N:101:TYR:CG	1:N:384:VAL:HG21	2.51	0.45
1:B:106:TRP:CE2	1:B:295:LYS:HE2	2.51	0.45
2:C:40:ARG:NH2	2:C:62:ALA:O	2.50	0.45
1:G:75:GLU:OE1	1:G:97:HIS:HE1	1.99	0.45
1:N:458:MET:HE1	1:N:466:GLY:CA	2.45	0.45
1:E:66:ARG:HH11	1:E:66:ARG:CG	2.08	0.45
1:J:174:PHE:O	1:J:176:ASP:O	2.35	0.45
3:M:1003:HEC:HMA3	3:M:1004:HEC:HBA2	1.97	0.45
1:P:174:PHE:O	1:P:176:ASP:O	2.34	0.45
1:Q:202:SER:HB2	1:Q:231:GLN:HB3	1.99	0.45
1:Q:324:THR:O	1:Q:324:THR:HG23	2.17	0.45
1:A:429:ASN:HB3	3:A:1004:HEC:CAA	2.47	0.45
1:D:75:GLU:OE1	1:D:97:HIS:HE1	2.00	0.45
1:D:77:LYS:HE2	1:D:429:ASN:O	2.17	0.45
1:E:233:HIS:CE1	3:E:1001:HEC:HMD1	2.52	0.45
2:I:144:GLN:O	2:I:144:GLN:HG2	2.16	0.45
1:J:185:ILE:HD11	3:J:1003:HEC:HMD2	1.98	0.45
1:J:319:CYS:SG	3:J:1004:HEC:C3C	3.01	0.45
3:K:1002:HEC:HMB1	3:K:1002:HEC:HBB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:301:TYR:O	1:P:305:ILE:HG13	2.16	0.45
3:P:1001:HEC:HBC3	3:P:1001:HEC:HMC1	1.98	0.45
1:Q:234:VAL:HG21	1:Q:251:PHE:CZ	2.52	0.45
1:A:106:TRP:CE3	1:A:111:PHE:HB3	2.51	0.45
1:E:124:ALA:HB3	1:E:184:THR:HG22	1.99	0.45
1:G:225:ARG:O	1:G:315:THR:HG23	2.17	0.45
1:N:87:ASN:HB3	1:N:98:ALA:HB3	1.98	0.45
1:P:157:GLU:HG3	7:P:2013:HOH:O	2.16	0.45
1:E:430:SER:HB3	1:E:434:HIS:CE1	2.52	0.45
1:A:308:THR:CG2	7:A:2197:HOH:O	2.58	0.45
1:D:84:LYS:HD3	1:D:115:TYR:CE2	2.52	0.45
1:E:121:HIS:HD1	1:E:337:TRP:HE3	1.54	0.45
3:F:1002:HEC:HMB1	3:F:1002:HEC:HBB3	1.98	0.45
1:K:187:CYS:SG	3:K:1002:HEC:C3B	3.03	0.45
3:N:1005:HEC:O2D	7:N:2205:HOH:O	2.21	0.45
2:O:108:THR:HG23	7:O:2048:HOH:O	2.17	0.45
1:G:102:LEU:HD22	1:G:106:TRP:CH2	2.52	0.44
1:J:225:ARG:HB3	1:J:317:ALA:HB3	1.99	0.44
3:M:1004:HEC:HBC3	3:M:1004:HEC:HMC1	2.00	0.44
1:P:173:GLU:O	1:P:177:LYS:HE2	2.17	0.44
1:H:184:THR:O	1:H:185:ILE:C	2.56	0.44
1:H:343:ASP:OD1	1:H:347:ARG:NH1	2.49	0.44
1:H:468:ASP:OD2	7:H:2172:HOH:O	2.21	0.44
1:M:349:CYS:SG	3:M:1005:HEC:C3B	2.97	0.44
2:O:107:GLU:O	2:O:111:VAL:HG13	2.16	0.44
1:Q:59:LYS:HE2	1:Q:330:LYS:NZ	2.31	0.44
1:B:66:ARG:HH11	1:B:66:ARG:CG	2.00	0.44
1:E:33:GLU:O	1:E:33:GLU:CG	2.59	0.44
1:E:87:ASN:HB3	1:E:98:ALA:HB3	1.99	0.44
1:H:458:MET:HE2	1:H:465:ILE:HG13	1.99	0.44
3:J:1005:HEC:HMC1	3:J:1005:HEC:HBC3	1.99	0.44
1:K:40:LYS:HA	1:K:40:LYS:HD3	1.76	0.44
1:M:414:MET:HB3	1:M:449:PHE:O	2.17	0.44
2:O:69:CYS:SG	3:O:1002:HEC:C3C	2.99	0.44
1:D:234:VAL:HG21	1:D:251:PHE:CZ	2.53	0.44
1:B:129:LEU:HD22	1:B:175:ARG:HG3	1.99	0.44
2:F:33:GLY:O	2:F:37:THR:HB	2.16	0.44
1:H:240:GLY:N	1:H:243:MET:CE	2.57	0.44
1:K:150:CYS:HB3	1:K:232:CYS:SG	2.57	0.44
1:K:433:PHE:CD2	3:K:1004:HEC:HMD2	2.52	0.44
1:N:272:LEU:HD11	1:N:282:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG22	2:C:40:ARG:HD3	2.00	0.44
3:D:1005:HEC:HBB3	3:D:1005:HEC:HMB1	1.99	0.44
3:D:1005:HEC:HBA2	3:E:1005:HEC:HBA2	1.99	0.44
1:H:315:THR:HG23	1:H:317:ALA:H	1.82	0.44
1:A:129:LEU:HD13	1:A:516:GLN:HG2	1.98	0.44
2:C:119:CYS:HG	3:C:1003:HEC:HAC	1.79	0.44
1:G:225:ARG:CB	1:G:315:THR:HG21	2.47	0.44
3:G:1004:HEC:HMC1	3:G:1004:HEC:HBC3	2.00	0.44
2:I:117:LYS:NZ	2:I:130:MET:HE2	2.33	0.44
1:K:419:GLN:HA	1:K:422:TRP:CD1	2.53	0.44
3:M:1005:HEC:HMD3	7:N:2139:HOH:O	2.18	0.44
1:N:30:VAL:HG22	2:O:40:ARG:HD3	2.00	0.44
2:O:50:ASN:O	2:O:54:VAL:HG23	2.17	0.44
1:A:60:GLN:NE2	3:A:1002:HEC:HBA2	2.33	0.44
1:A:375:LEU:HD21	1:B:444:ALA:HB1	1.99	0.44
3:A:1005:HEC:O2A	3:A:1005:HEC:HMA2	2.18	0.44
1:D:154:LYS:HG2	1:D:158:TRP:CZ2	2.52	0.44
1:D:232:CYS:SG	3:D:1003:HEC:CBC	2.92	0.44
1:N:50:ASN:OD1	1:N:186:GLY:HA3	2.18	0.44
1:N:315:THR:HG22	1:N:318:ASP:H	1.83	0.44
1:A:323:TYR:O	3:C:1004:HEC:HBD2	2.17	0.44
1:B:298:HIS:H	1:B:427:ALA:HB1	1.83	0.44
1:D:498:LYS:O	1:D:501:GLN:HG2	2.17	0.44
2:I:78:LYS:HE2	2:I:82:LYS:HD2	2.00	0.44
2:I:107:GLU:HB3	7:I:2013:HOH:O	2.18	0.44
1:D:121:HIS:ND1	1:D:337:TRP:CE3	2.85	0.43
1:P:429:ASN:HB3	3:P:1004:HEC:HAA2	1.99	0.43
1:Q:32:THR:HG23	2:R:57:LYS:HD3	2.00	0.43
1:Q:103:LYS:HD3	1:Q:483:MET:HB3	2.00	0.43
1:D:315:THR:HG23	1:D:317:ALA:H	1.82	0.43
1:M:347:ARG:NH2	1:P:347:ARG:HB2	2.34	0.43
2:O:132:ALA:N	7:O:2035:HOH:O	2.49	0.43
1:P:293:MET:HE3	7:P:2142:HOH:O	2.18	0.43
1:E:234:VAL:HG21	1:E:251:PHE:CZ	2.52	0.43
1:G:33:GLU:CG	1:G:35:LYS:HE3	2.46	0.43
2:I:103:LEU:HA	3:I:1002:HEC:HBA2	2.00	0.43
1:J:435:ASN:ND2	1:J:438:LYS:HE3	2.33	0.43
3:O:1002:HEC:HBA1	3:O:1002:HEC:CHA	2.27	0.43
3:B:1002:HEC:HBC2	3:B:1003:HEC:HBB2	2.00	0.43
1:G:84:LYS:HD3	1:G:115:TYR:CE2	2.54	0.43
1:H:343:ASP:CG	1:H:347:ARG:HH11	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:MET:HB3	1:J:449:PHE:O	2.19	0.43
3:N:1002:HEC:HMC1	3:N:1002:HEC:HBC3	1.99	0.43
1:Q:187:CYS:HG	3:Q:1002:HEC:CAB	2.20	0.43
1:Q:404:TYR:O	1:Q:408:MET:HG2	2.18	0.43
2:L:136:CYS:SG	3:L:1004:HEC:C3B	2.99	0.43
2:F:117:LYS:HE2	2:F:130:MET:HG2	2.00	0.43
1:G:190:CYS:SG	3:G:1002:HEC:CBC	2.98	0.43
2:I:120:HIS:HB2	3:I:1004:HEC:HMB2	2.00	0.43
1:H:233:HIS:HB3	1:H:300:GLU:HB2	1.99	0.43
1:H:430:SER:HB3	1:H:434:HIS:CE1	2.54	0.43
3:Q:1003:HEC:HMC1	3:Q:1003:HEC:CBC	2.47	0.43
2:R:56:HIS:CE1	3:R:1002:HEC:HMC2	2.53	0.43
1:E:29:ASP:OD1	2:F:57:LYS:HE3	2.19	0.43
1:E:30:VAL:HG23	2:F:40:ARG:HD3	2.00	0.43
1:J:103:LYS:HD3	1:J:483:MET:HB2	2.00	0.43
1:J:187:CYS:SG	3:J:1002:HEC:CBB	2.97	0.43
1:M:187:CYS:SG	3:M:1002:HEC:C3B	3.02	0.43
2:O:34:MET:SD	2:O:79:LEU:HD23	2.58	0.43
1:P:74:THR:HG21	1:P:341:MET:HB2	2.01	0.43
1:Q:225:ARG:O	1:Q:315:THR:HG23	2.19	0.43
1:J:339:SER:HB2	3:J:1004:HEC:O1A	2.19	0.43
1:Q:369:GLN:HA	1:Q:431:VAL:O	2.19	0.43
1:H:129:LEU:O	1:H:175:ARG:NH2	2.51	0.43
1:H:234:VAL:HG21	1:H:251:PHE:CE2	2.54	0.43
3:I:1003:HEC:HMD3	3:L:1003:HEC:HMD3	2.00	0.43
1:J:105:LEU:HD13	1:J:422:TRP:CZ2	2.54	0.43
1:J:178:ILE:O	1:J:516:GLN:NE2	2.50	0.43
2:L:37:THR:HG23	2:L:82:LYS:HZ1	1.81	0.43
2:L:75:LEU:HD23	5:L:1005:LMT:H81	2.01	0.43
2:L:119:CYS:SG	3:L:1003:HEC:CBC	3.04	0.43
1:B:101:TYR:CD2	1:B:384:VAL:HG21	2.53	0.42
1:E:129:LEU:HD12	1:E:180:MET:HE2	1.99	0.42
1:E:343:ASP:OD2	1:E:347:ARG:NH1	2.51	0.42
2:O:132:ALA:HB3	7:O:2035:HOH:O	2.18	0.42
3:P:1004:HEC:HMC1	3:P:1004:HEC:HBC3	2.01	0.42
1:B:32:THR:OG1	2:C:58:LEU:HD13	2.19	0.42
1:B:84:LYS:HD3	1:B:115:TYR:CE2	2.54	0.42
1:E:103:LYS:HD3	1:E:483:MET:HB3	2.01	0.42
1:E:129:LEU:O	1:E:175:ARG:NH2	2.52	0.42
1:N:315:THR:CG2	1:N:317:ALA:H	2.32	0.42
1:A:308:THR:HB	7:B:2188:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:CYS:SG	3:E:1003:HEC:C3B	3.00	0.42
1:E:497:HIS:CD2	1:E:499:TRP:HB2	2.54	0.42
1:J:222:ASN:O	1:J:315:THR:HG21	2.19	0.42
1:J:315:THR:O	3:J:1004:HEC:HMC3	2.19	0.42
1:M:315:THR:HG22	1:M:318:ASP:H	1.84	0.42
1:M:323:TYR:O	3:O:1004:HEC:HBD2	2.19	0.42
1:Q:319:CYS:SG	3:Q:1004:HEC:CBC	2.91	0.42
2:R:40:ARG:NH2	2:R:62:ALA:O	2.53	0.42
1:A:414:MET:HB3	1:A:449:PHE:O	2.20	0.42
1:B:107:LEU:HD23	1:B:287:PRO:HG2	2.02	0.42
3:B:1002:HEC:HMC1	3:B:1002:HEC:HBC3	2.02	0.42
1:D:380:GLN:O	1:D:384:VAL:HG23	2.19	0.42
1:E:27:CYS:HB3	2:F:36:TYR:OH	2.13	0.42
1:Q:77:LYS:HE2	1:Q:429:ASN:O	2.18	0.42
1:A:121:HIS:ND1	1:A:337:TRP:CE3	2.83	0.42
1:A:486:LYS:O	1:A:489:GLN:HB2	2.19	0.42
2:L:48:ILE:HG21	3:L:1101:HEC:HMD3	2.00	0.42
1:M:50:ASN:OD1	1:M:186:GLY:HA3	2.19	0.42
2:C:117:LYS:HE2	2:C:130:MET:HE2	2.02	0.42
1:E:57:PHE:CZ	1:E:196:MET:HG3	2.55	0.42
3:E:1002:HEC:HBC3	3:E:1002:HEC:HMC1	2.00	0.42
1:K:233:HIS:CE1	3:K:1001:HEC:HMD1	2.54	0.42
1:M:84:LYS:HD3	1:M:115:TYR:CE2	2.55	0.42
1:Q:66:ARG:HG2	1:Q:66:ARG:NH1	2.34	0.42
1:D:286:HIS:HA	1:D:287:PRO:HD3	1.88	0.42
1:G:352:CYS:SG	3:G:1005:HEC:CBC	2.96	0.42
1:M:454:ILE:O	1:M:458:MET:HG3	2.19	0.42
1:G:50:ASN:OD1	1:G:186:GLY:HA3	2.20	0.42
1:K:331:LYS:HB2	1:K:331:LYS:HE2	1.91	0.42
1:M:234:VAL:HG21	1:M:251:PHE:CZ	2.55	0.42
1:P:286:HIS:CE1	1:P:288:ALA:HB3	2.55	0.42
1:Q:175:ARG:HD3	1:Q:513:TRP:CE3	2.53	0.42
1:Q:397:GLN:HA	1:Q:397:GLN:NE2	2.35	0.42
1:D:430:SER:HB3	1:D:434:HIS:CE1	2.55	0.42
1:E:291:THR:O	1:E:293:MET:HG2	2.19	0.42
1:M:391:ARG:O	1:M:395:GLU:HG3	2.20	0.42
7:M:2117:HOH:O	2:O:132:ALA:HB3	2.19	0.42
1:A:118:ALA:HB3	7:A:2195:HOH:O	2.20	0.42
1:E:309:HIS:HB3	1:E:314:VAL:HB	2.02	0.42
1:J:106:TRP:CE3	1:J:111:PHE:HB3	2.55	0.42
2:L:130:MET:HE1	7:L:2020:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1004:HEC:O2A	7:M:2200:HOH:O	2.20	0.42
1:N:328:ASP:O	1:N:329:LYS:HG3	2.20	0.42
1:N:433:PHE:CE2	3:N:1004:HEC:HMD2	2.55	0.42
1:Q:225:ARG:O	1:Q:315:THR:CG2	2.68	0.42
1:A:29:ASP:HB2	2:F:39:GLN:HE21	1.85	0.41
1:B:400:LYS:HD3	7:B:2144:HOH:O	2.20	0.41
1:E:232:CYS:SG	3:E:1003:HEC:CBC	2.92	0.41
1:H:121:HIS:CD2	3:H:1003:HEC:ND	2.87	0.41
1:J:75:GLU:OE1	1:J:97:HIS:HE1	2.02	0.41
1:J:101:TYR:CG	1:J:384:VAL:HG21	2.55	0.41
2:L:107:GLU:O	2:L:107:GLU:HG3	2.20	0.41
1:M:106:TRP:CE2	1:M:295:LYS:HE2	2.55	0.41
1:P:184:THR:O	1:P:185:ILE:C	2.58	0.41
1:P:352:CYS:O	2:R:141:ARG:HD3	2.19	0.41
1:Q:184:THR:O	1:Q:185:ILE:C	2.58	0.41
3:Q:1001:HEC:HMC1	3:Q:1001:HEC:HBC3	2.02	0.41
2:R:107:GLU:O	2:R:111:VAL:HG13	2.20	0.41
1:A:85:ASN:HA	1:A:99:GLN:O	2.20	0.41
1:A:458:MET:CE	1:A:466:GLY:CA	2.84	0.41
1:G:198:LEU:HD11	3:G:1002:HEC:HBD2	2.03	0.41
1:M:233:HIS:HB3	1:M:300:GLU:HB2	2.03	0.41
2:R:35:LYS:O	2:R:38:ASP:HB2	2.21	0.41
1:B:430:SER:HB3	1:B:434:HIS:CE1	2.55	0.41
1:G:375:LEU:HG	1:G:443:LEU:HB3	2.02	0.41
2:I:39:GLN:HG2	1:J:29:ASP:HB3	2.01	0.41
1:K:286:HIS:HA	1:K:287:PRO:HD3	1.86	0.41
1:G:185:ILE:HD11	3:G:1003:HEC:HMD2	2.02	0.41
1:J:152:THR:OG1	1:J:154:LYS:HB2	2.20	0.41
1:M:32:THR:HG21	7:R:2008:HOH:O	2.21	0.41
2:O:119:CYS:HG	3:O:1003:HEC:HAC	1.79	0.41
1:B:263:TYR:OH	1:B:413:GLU:OE2	2.28	0.41
1:H:454:ILE:O	1:H:458:MET:HG3	2.19	0.41
1:J:447:GLN:HE22	1:K:448:GLN:CG	2.33	0.41
2:L:40:ARG:HE	2:L:56:HIS:CD2	2.38	0.41
2:L:122:MET:O	2:L:125:VAL:HG22	2.20	0.41
1:M:189:THR:HG21	3:M:1003:HEC:HBC3	2.01	0.41
1:P:106:TRP:CE3	1:P:111:PHE:HB3	2.55	0.41
1:A:84:LYS:HD3	1:A:115:TYR:CE2	2.56	0.41
2:F:70:HIS:CD2	3:F:1002:HEC:NB	2.89	0.41
1:H:131:ILE:HD13	3:H:1001:HEC:HMA2	2.01	0.41
2:I:79:LEU:HB2	2:I:80:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:388:GLU:HA	1:M:388:GLU:OE1	2.20	0.41
1:P:175:ARG:HD3	1:P:513:TRP:CE3	2.56	0.41
1:E:116:ARG:NH1	7:E:2038:HOH:O	2.49	0.41
1:G:30:VAL:CG2	5:I:1005:LMT:H6'1	2.51	0.41
1:G:304:TRP:CZ3	1:G:305:ILE:HG23	2.55	0.41
1:M:295:LYS:NZ	1:M:296:ALA:O	2.47	0.41
1:M:309:HIS:HB3	1:M:314:VAL:HB	2.03	0.41
1:N:147:CYS:CB	3:N:1001:HEC:HAB	2.42	0.41
1:P:46:GLU:O	1:P:46:GLU:CG	2.65	0.41
1:P:323:TYR:HB3	1:P:331:LYS:HG2	2.03	0.41
1:P:435:ASN:ND2	1:P:438:LYS:HE3	2.36	0.41
1:Q:32:THR:CG2	2:R:57:LYS:HD3	2.50	0.41
1:B:57:PHE:CZ	1:B:196:MET:HG3	2.56	0.41
1:D:262:MET:CE	1:D:302:GLU:HG2	2.51	0.41
3:D:1005:HEC:O2D	2:F:141:ARG:NH2	2.54	0.41
2:F:56:HIS:CE1	3:F:1002:HEC:HMC2	2.55	0.41
3:F:1002:HEC:HBA1	3:F:1002:HEC:CHA	2.43	0.41
1:G:153:PRO:HD2	1:G:183:HIS:O	2.21	0.41
1:G:257:PHE:CB	1:G:305:ILE:HD11	2.50	0.41
1:G:304:TRP:CB	3:G:1004:HEC:HBB2	2.51	0.41
1:J:30:VAL:CG1	5:L:1005:LMT:H6'1	2.51	0.41
1:J:185:ILE:H	1:J:185:ILE:HG13	1.72	0.41
1:K:121:HIS:CD2	3:K:1003:HEC:ND	2.89	0.41
1:K:147:CYS:HG	3:K:1001:HEC:CAB	1.97	0.41
2:L:112:VAL:CG1	3:L:1003:HEC:HBB1	2.51	0.41
3:L:1003:HEC:HMA2	3:L:1003:HEC:O2A	2.21	0.41
1:M:107:LEU:HG	1:M:503:LEU:HD21	2.03	0.41
1:P:330:LYS:HG2	2:R:122:MET:O	2.20	0.41
1:P:371:ARG:HG3	1:P:371:ARG:HH11	1.85	0.41
3:R:1003:HEC:HMA3	3:R:1004:HEC:HBA2	2.02	0.41
1:A:40:LYS:HD3	1:A:40:LYS:C	2.42	0.41
1:A:343:ASP:OD2	1:A:347:ARG:HG3	2.20	0.41
1:G:150:CYS:SG	3:G:1001:HEC:CBC	2.94	0.41
1:G:458:MET:CE	1:G:466:GLY:CA	2.99	0.41
2:I:52:VAL:HG23	3:I:1002:HEC:HMB2	2.02	0.41
3:K:1004:HEC:HMB1	3:K:1004:HEC:HBB3	2.02	0.41
1:P:76:TYR:HB3	1:P:431:VAL:HG21	2.03	0.41
1:Q:303:THR:HA	1:Q:438:LYS:HE3	2.02	0.41
1:G:147:CYS:SG	3:G:1001:HEC:HBB1	2.57	0.41
1:K:184:THR:O	1:K:185:ILE:C	2.60	0.41
1:K:315:THR:HG22	1:K:318:ASP:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:34:MET:SD	2:O:79:LEU:CD2	3.09	0.41
1:Q:129:LEU:HD22	1:Q:175:ARG:HG3	2.02	0.41
1:Q:157:GLU:HG3	7:Q:2032:HOH:O	2.21	0.41
1:B:87:ASN:HB3	1:B:98:ALA:HB3	2.03	0.40
3:D:1002:HEC:HBC1	3:D:1003:HEC:HHC	2.03	0.40
1:H:512:VAL:HG13	1:H:520:VAL:HG22	2.02	0.40
2:I:70:HIS:CE1	3:I:1002:HEC:NA	2.89	0.40
1:M:113:TYR:CE2	1:M:483:MET:HE1	2.57	0.40
1:M:394:ASN:HD22	1:M:412:ARG:HH22	1.68	0.40
1:N:309:HIS:HB3	1:N:314:VAL:HB	2.03	0.40
2:R:117:LYS:NZ	2:R:130:MET:CE	2.84	0.40
1:E:102:LEU:HD23	1:E:102:LEU:HA	1.79	0.40
1:E:308:THR:HG22	7:E:2128:HOH:O	2.20	0.40
2:I:33:GLY:O	2:I:37:THR:HB	2.21	0.40
1:M:54:LYS:HB3	1:M:55:PRO:HD3	2.02	0.40
1:P:75:GLU:OE1	1:P:97:HIS:HE1	2.03	0.40
1:P:375:LEU:HD13	1:P:443:LEU:HB2	2.03	0.40
1:P:473:ILE:H	1:P:473:ILE:HG13	1.67	0.40
1:Q:84:LYS:HD3	1:Q:115:TYR:CE2	2.56	0.40
1:A:265:TYR:O	1:A:269:HIS:HD2	2.03	0.40
1:J:30:VAL:HG22	1:J:30:VAL:O	2.21	0.40
1:K:265:TYR:O	1:K:269:HIS:HD2	2.05	0.40
1:P:297:GLN:O	1:P:298:HIS:C	2.60	0.40
1:Q:233:HIS:CE1	3:Q:1001:HEC:HMD1	2.56	0.40
1:B:454:ILE:O	1:B:458:MET:HG3	2.21	0.40
1:E:32:THR:OG1	2:F:58:LEU:HD13	2.22	0.40
2:I:82:LYS:HB3	2:I:82:LYS:HE3	2.00	0.40
1:J:309:HIS:CE1	3:J:1005:HEC:NA	2.89	0.40
1:K:103:LYS:HD3	1:K:483:MET:HB3	2.03	0.40
1:M:85:ASN:HA	1:M:99:GLN:O	2.21	0.40
1:N:146:THR:CG2	1:N:249:PRO:HD3	2.49	0.40
2:O:120:HIS:HB2	3:O:1004:HEC:HMB2	2.03	0.40
1:P:157:GLU:CG	7:P:2013:HOH:O	2.70	0.40
1:A:109:TYR:O	1:A:112:MET:HG2	2.22	0.40
2:C:52:VAL:HG11	3:C:1002:HEC:C3A	2.51	0.40
1:G:433:PHE:CD2	3:G:1004:HEC:HMD2	2.57	0.40
1:H:262:MET:HE3	1:H:302:GLU:HG2	2.01	0.40
1:N:425:VAL:HG11	1:N:443:LEU:HD11	2.03	0.40
1:N:430:SER:HB3	1:N:434:HIS:CE1	2.56	0.40
2:O:78:LYS:HG2	2:O:82:LYS:HD3	2.03	0.40
2:O:133:LYS:HB3	2:O:138:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:154:LYS:HG2	1:Q:158:TRP:CZ2	2.56	0.40
2:R:79:LEU:HB2	2:R:80:PRO:CD	2.46	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	495/500 (99%)	481 (97%)	13 (3%)	1 (0%)	44	55
1	B	497/500 (99%)	482 (97%)	14 (3%)	1 (0%)	44	55
1	D	493/500 (99%)	478 (97%)	13 (3%)	2 (0%)	30	39
1	E	493/500 (99%)	474 (96%)	17 (3%)	2 (0%)	30	39
1	G	493/500 (99%)	479 (97%)	12 (2%)	2 (0%)	30	39
1	H	498/500 (100%)	483 (97%)	13 (3%)	2 (0%)	30	39
1	J	495/500 (99%)	477 (96%)	16 (3%)	2 (0%)	30	39
1	K	494/500 (99%)	473 (96%)	19 (4%)	2 (0%)	30	39
1	M	494/500 (99%)	477 (97%)	15 (3%)	2 (0%)	30	39
1	N	497/500 (99%)	476 (96%)	19 (4%)	2 (0%)	30	39
1	P	493/500 (99%)	474 (96%)	15 (3%)	4 (1%)	16	20
1	Q	494/500 (99%)	473 (96%)	19 (4%)	2 (0%)	30	39
2	C	144/159 (91%)	139 (96%)	5 (4%)	0	100	100
2	F	144/159 (91%)	138 (96%)	5 (4%)	1 (1%)	19	23
2	I	143/159 (90%)	142 (99%)	1 (1%)	0	100	100
2	L	143/159 (90%)	136 (95%)	7 (5%)	0	100	100
2	O	142/159 (89%)	139 (98%)	3 (2%)	0	100	100
2	R	143/159 (90%)	139 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6795/6954 (98%)	6560 (96%)	210 (3%)	25 (0%)	30 39

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	185	ILE
1	E	186	GLY
1	N	329	LYS
1	J	176	ASP
1	M	463	TYR
1	P	176	ASP
1	Q	185	ILE
1	B	185	ILE
1	K	185	ILE
1	Q	331	LYS
2	F	22	LEU
1	G	185	ILE
1	P	185	ILE
1	P	463	TYR
1	D	185	ILE
1	H	326	SER
1	N	185	ILE
1	D	471	GLY
1	G	30	VAL
1	P	177	LYS
1	A	185	ILE
1	H	185	ILE
1	J	185	ILE
1	M	298	HIS
1	K	298	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	431/432 (100%)	417 (97%)	14 (3%)	34 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	431/432 (100%)	408 (95%)	23 (5%)	19 28
1	D	429/432 (99%)	413 (96%)	16 (4%)	29 43
1	E	429/432 (99%)	409 (95%)	20 (5%)	22 32
1	G	429/432 (99%)	413 (96%)	16 (4%)	29 43
1	H	433/432 (100%)	419 (97%)	14 (3%)	34 50
1	J	431/432 (100%)	418 (97%)	13 (3%)	36 52
1	K	429/432 (99%)	408 (95%)	21 (5%)	21 31
1	M	430/432 (100%)	412 (96%)	18 (4%)	25 37
1	N	431/432 (100%)	415 (96%)	16 (4%)	29 43
1	P	429/432 (99%)	413 (96%)	16 (4%)	29 43
1	Q	430/432 (100%)	408 (95%)	22 (5%)	20 29
2	C	120/131 (92%)	113 (94%)	7 (6%)	17 24
2	F	120/131 (92%)	109 (91%)	11 (9%)	7 9
2	I	119/131 (91%)	112 (94%)	7 (6%)	16 23
2	L	119/131 (91%)	108 (91%)	11 (9%)	7 9
2	O	118/131 (90%)	111 (94%)	7 (6%)	16 23
2	R	119/131 (91%)	107 (90%)	12 (10%)	6 7
All	All	5877/5970 (98%)	5613 (96%)	264 (4%)	23 34

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	40	LYS
1	A	63	SER
1	A	184	THR
1	A	199	ARG
1	A	264	ARG
1	A	285	THR
1	A	308	THR
1	A	315	THR
1	A	375	LEU
1	A	426	SER
1	A	467	LYS
1	A	483	MET
1	A	498	LYS

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Mol	Chain	Res	Type
1	B	32	THR
1	B	36	THR
1	B	38	VAL
1	B	66	ARG
1	B	69	GLU
1	B	93	GLU
1	B	116	ARG
1	B	154	LYS
1	B	182	ASP
1	B	184	THR
1	B	199	ARG
1	B	284	TRP
1	B	308	THR
1	B	327	ASP
1	B	328	ASP
1	B	359	ASP
1	B	370	LYS
1	B	375	LEU
1	B	438	LYS
1	B	458	MET
1	B	475	THR
1	B	496	THR
1	B	520	VAL
2	C	34	MET
2	C	58	LEU
2	C	75	LEU
2	C	110	GLU
2	C	111	VAL
2	C	125	VAL
2	C	127	VAL
1	D	34	LEU
1	D	46	GLU
1	D	56	GLU
1	D	69	GLU
1	D	116	ARG
1	D	161	GLU
1	D	182	ASP
1	D	184	THR
1	D	284	TRP
1	D	285	THR
1	D	308	THR
1	D	315	THR

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Mol	Chain	Res	Type
1	D	375	LEU
1	D	476	ILE
1	D	483	MET
1	D	498	LYS
1	E	30	VAL
1	E	32	THR
1	E	33	GLU
1	E	46	GLU
1	E	66	ARG
1	E	69	GLU
1	E	182	ASP
1	E	184	THR
1	E	199	ARG
1	E	273	GLN
1	E	284	TRP
1	E	308	THR
1	E	315	THR
1	E	328	ASP
1	E	347	ARG
1	E	375	LEU
1	E	438	LYS
1	E	458	MET
1	E	498	LYS
1	E	518	ARG
2	F	27	LEU
2	F	37	THR
2	F	39	GLN
2	F	58	LEU
2	F	108	THR
2	F	110	GLU
2	F	111	VAL
2	F	125	VAL
2	F	127	VAL
2	F	154	ARG
2	F	155	GLU
1	G	32	THR
1	G	33	GLU
1	G	34	LEU
1	G	101	TYR
1	G	182	ASP
1	G	184	THR
1	G	242	THR

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Mol	Chain	Res	Type
1	G	284	TRP
1	G	285	THR
1	G	305	ILE
1	G	308	THR
1	G	315	THR
1	G	324	THR
1	G	370	LYS
1	G	483	MET
1	G	498	LYS
1	H	27	CYS
1	H	35	LYS
1	H	69	GLU
1	H	71	THR
1	H	161	GLU
1	H	182	ASP
1	H	199	ARG
1	H	308	THR
1	H	315	THR
1	H	326	SER
1	H	347	ARG
1	H	458	MET
1	H	470	SER
1	H	496	THR
2	I	25	VAL
2	I	35	LYS
2	I	37	THR
2	I	58	LEU
2	I	97	HIS
2	I	127	VAL
2	I	155	GLU
1	J	30	VAL
1	J	33	GLU
1	J	69	GLU
1	J	101	TYR
1	J	176	ASP
1	J	182	ASP
1	J	184	THR
1	J	264	ARG
1	J	285	THR
1	J	305	ILE
1	J	308	THR
1	J	375	LEU

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Mol	Chain	Res	Type
1	J	470	SER
1	K	28	SER
1	K	38	VAL
1	K	40	LYS
1	K	66	ARG
1	K	69	GLU
1	K	93	GLU
1	K	101	TYR
1	K	162	SER
1	K	181	LYS
1	K	182	ASP
1	K	184	THR
1	K	199	ARG
1	K	308	THR
1	K	315	THR
1	K	347	ARG
1	K	375	LEU
1	K	397	GLN
1	K	438	LYS
1	K	467	LYS
1	K	475	THR
1	K	510	ASP
2	L	27	LEU
2	L	35	LYS
2	L	37	THR
2	L	50	ASN
2	L	58	LEU
2	L	108	THR
2	L	110	GLU
2	L	125	VAL
2	L	127	VAL
2	L	129	SER
2	L	154	ARG
1	M	32	THR
1	M	34	LEU
1	M	46	GLU
1	M	69	GLU
1	M	182	ASP
1	M	184	THR
1	M	199	ARG
1	M	264	ARG
1	M	275	LYS

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Mol	Chain	Res	Type
1	M	284	TRP
1	M	285	THR
1	M	315	THR
1	M	332	ILE
1	M	375	LEU
1	M	467	LYS
1	M	470	SER
1	M	476	ILE
1	M	483	MET
1	N	27	CYS
1	N	30	VAL
1	N	69	GLU
1	N	116	ARG
1	N	182	ASP
1	N	184	THR
1	N	199	ARG
1	N	308	THR
1	N	315	THR
1	N	347	ARG
1	N	375	LEU
1	N	438	LYS
1	N	474	LYS
1	N	475	THR
1	N	496	THR
1	N	520	VAL
2	O	27	LEU
2	O	37	THR
2	O	50	ASN
2	O	58	LEU
2	O	108	THR
2	O	111	VAL
2	O	127	VAL
1	P	34	LEU
1	P	101	TYR
1	P	176	ASP
1	P	182	ASP
1	P	184	THR
1	P	242	THR
1	P	275	LYS
1	P	285	THR
1	P	305	ILE
1	P	308	THR

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Mol	Chain	Res	Type
1	P	315	THR
1	P	375	LEU
1	P	458	MET
1	P	476	ILE
1	P	498	LYS
1	P	508	LYS
1	Q	27	CYS
1	Q	30	VAL
1	Q	38	VAL
1	Q	69	GLU
1	Q	93	GLU
1	Q	112	MET
1	Q	182	ASP
1	Q	199	ARG
1	Q	308	THR
1	Q	329	LYS
1	Q	330	LYS
1	Q	339	SER
1	Q	347	ARG
1	Q	375	LEU
1	Q	397	GLN
1	Q	438	LYS
1	Q	475	THR
1	Q	496	THR
1	Q	498	LYS
1	Q	510	ASP
1	Q	518	ARG
1	Q	520	VAL
2	R	14	LYS
2	R	17	LEU
2	R	21	THR
2	R	27	LEU
2	R	35	LYS
2	R	50	ASN
2	R	108	THR
2	R	110	GLU
2	R	111	VAL
2	R	125	VAL
2	R	127	VAL
2	R	154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	269	HIS
1	A	394	ASN
1	B	97	HIS
1	B	298	HIS
1	B	397	GLN
1	B	448	GLN
2	C	56	HIS
1	D	97	HIS
1	D	269	HIS
1	D	394	ASN
1	D	447	GLN
1	E	269	HIS
1	E	445	GLN
1	E	497	HIS
2	F	39	GLN
2	F	50	ASN
2	F	56	HIS
1	G	97	HIS
1	G	394	ASN
1	G	447	GLN
1	H	298	HIS
2	I	56	HIS
2	I	73	HIS
1	J	97	HIS
1	J	394	ASN
1	J	447	GLN
1	K	97	HIS
1	K	269	HIS
1	K	397	GLN
1	K	448	GLN
2	L	56	HIS
1	M	269	HIS
1	M	394	ASN
1	N	445	GLN
2	O	50	ASN
2	O	56	HIS
1	P	97	HIS
1	P	269	HIS
1	P	447	GLN
1	Q	97	HIS
1	Q	269	HIS
1	Q	397	GLN

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Mol	Chain	Res	Type
1	Q	447	GLN
2	R	50	ASN
2	R	56	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 117 ligands modelled in this entry, 24 are monoatomic - leaving 93 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	L	1003	2	32,50,50	2.22	7 (21%)	24,82,82	1.94	9 (37%)
3	HEC	Q	1002	1	32,50,50	2.35	7 (21%)	24,82,82	1.56	4 (16%)
3	HEC	E	1003	4,1	32,50,50	2.22	7 (21%)	24,82,82	1.64	7 (29%)
3	HEC	N	1005	1	32,50,50	2.24	5 (15%)	24,82,82	1.77	7 (29%)
3	HEC	D	1003	4,1	32,50,50	2.40	9 (28%)	24,82,82	1.39	3 (12%)
6	ACT	C	1006	-	3,3,3	0.78	0	3,3,3	0.88	0
3	HEC	G	1005	1	32,50,50	2.17	7 (21%)	24,82,82	1.86	6 (25%)
3	HEC	P	1001	7,1	32,50,50	2.29	8 (25%)	24,82,82	1.12	1 (4%)
3	HEC	H	1002	1	32,50,50	2.26	6 (18%)	24,82,82	1.63	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	L	1002	2	32,50,50	2.34	6 (18%)	24,82,82	1.62	6 (25%)
3	HEC	G	1001	7,1	32,50,50	2.32	7 (21%)	24,82,82	1.30	3 (12%)
3	HEC	Q	1001	7,1	32,50,50	2.37	8 (25%)	24,82,82	1.18	1 (4%)
3	HEC	A	1004	4,1	32,50,50	2.38	6 (18%)	24,82,82	1.66	4 (16%)
3	HEC	H	1003	4,1	32,50,50	2.32	7 (21%)	24,82,82	1.62	5 (20%)
3	HEC	J	1005	1	32,50,50	2.40	6 (18%)	24,82,82	1.37	3 (12%)
5	LMT	R	1005	-	36,36,36	0.57	0	47,47,47	1.03	2 (4%)
3	HEC	E	1002	1	32,50,50	2.22	7 (21%)	24,82,82	1.54	5 (20%)
3	HEC	N	1001	7,1	32,50,50	2.36	6 (18%)	24,82,82	1.49	4 (16%)
3	HEC	N	1002	1	32,50,50	2.26	7 (21%)	24,82,82	1.58	5 (20%)
3	HEC	F	1001	2	32,50,50	2.32	5 (15%)	24,82,82	1.47	3 (12%)
3	HEC	R	1003	2	32,50,50	2.19	8 (25%)	24,82,82	1.65	6 (25%)
3	HEC	A	1003	4,1	32,50,50	2.37	7 (21%)	24,82,82	1.68	8 (33%)
3	HEC	B	1001	7,1	32,50,50	2.30	8 (25%)	24,82,82	1.31	5 (20%)
3	HEC	D	1001	1	32,50,50	2.34	8 (25%)	24,82,82	1.51	5 (20%)
3	HEC	P	1003	4,1	32,50,50	2.22	6 (18%)	24,82,82	1.59	6 (25%)
3	HEC	K	1004	4,1	32,50,50	2.26	6 (18%)	24,82,82	2.06	8 (33%)
3	HEC	M	1004	4,1	32,50,50	2.17	5 (15%)	24,82,82	2.05	9 (37%)
3	HEC	H	1005	1	32,50,50	2.26	9 (28%)	24,82,82	1.63	4 (16%)
3	HEC	E	1001	7,1	32,50,50	2.38	7 (21%)	24,82,82	1.31	2 (8%)
5	LMT	O	1005	-	36,36,36	0.65	1 (2%)	47,47,47	0.79	1 (2%)
3	HEC	P	1002	1	32,50,50	2.31	6 (18%)	24,82,82	1.65	6 (25%)
3	HEC	C	1003	2	32,50,50	2.17	7 (21%)	24,82,82	1.98	10 (41%)
3	HEC	H	1001	7,1	32,50,50	2.27	6 (18%)	24,82,82	1.48	3 (12%)
3	HEC	R	1004	1,2	32,50,50	2.29	6 (18%)	24,82,82	2.19	7 (29%)
3	HEC	A	1002	1	32,50,50	2.21	6 (18%)	24,82,82	2.00	6 (25%)
6	ACT	O	1006	-	3,3,3	0.71	0	3,3,3	1.29	0
3	HEC	G	1003	4,1	32,50,50	2.31	8 (25%)	24,82,82	1.36	2 (8%)
3	HEC	B	1005	1	32,50,50	2.14	5 (15%)	24,82,82	1.46	4 (16%)
3	HEC	J	1004	4,1	32,50,50	2.18	7 (21%)	24,82,82	1.75	6 (25%)
3	HEC	D	1002	1	32,50,50	2.18	6 (18%)	24,82,82	1.76	5 (20%)
3	HEC	I	1001	2	32,50,50	2.29	6 (18%)	24,82,82	1.55	5 (20%)
5	LMT	I	1005	-	36,36,36	0.58	0	47,47,47	0.90	2 (4%)
3	HEC	K	1005	1	32,50,50	2.21	5 (15%)	24,82,82	1.47	5 (20%)
3	HEC	I	1002	2	32,50,50	2.39	7 (21%)	24,82,82	1.76	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	C	1002	2	32,50,50	2.29	6 (18%)	24,82,82	2.01	11 (45%)
3	HEC	C	1004	1,2	32,50,50	2.22	5 (15%)	24,82,82	1.81	6 (25%)
3	HEC	K	1002	1	32,50,50	2.33	6 (18%)	24,82,82	1.27	2 (8%)
3	HEC	H	1004	4,1	32,50,50	2.27	5 (15%)	24,82,82	1.82	7 (29%)
3	HEC	I	1003	2	32,50,50	2.12	8 (25%)	24,82,82	1.90	9 (37%)
3	HEC	O	1004	1,2	32,50,50	2.35	9 (28%)	24,82,82	2.03	4 (16%)
3	HEC	K	1001	1	32,50,50	2.34	7 (21%)	24,82,82	1.22	2 (8%)
3	HEC	M	1001	1	32,50,50	2.24	5 (15%)	24,82,82	1.49	3 (12%)
5	LMT	C	1005	-	36,36,36	0.56	0	47,47,47	0.83	1 (2%)
3	HEC	A	1005	1	32,50,50	2.29	7 (21%)	24,82,82	2.24	9 (37%)
5	LMT	L	1005	-	36,36,36	0.58	0	47,47,47	0.68	1 (2%)
3	HEC	Q	1005	1	32,50,50	2.22	5 (15%)	24,82,82	1.99	8 (33%)
3	HEC	J	1002	1	32,50,50	2.18	9 (28%)	24,82,82	1.70	7 (29%)
3	HEC	O	1003	2	32,50,50	2.19	7 (21%)	24,82,82	1.69	6 (25%)
3	HEC	Q	1003	4,1	32,50,50	2.29	5 (15%)	24,82,82	1.68	5 (20%)
3	HEC	B	1002	1	32,50,50	2.29	6 (18%)	24,82,82	1.55	5 (20%)
3	HEC	O	1002	2	32,50,50	2.28	6 (18%)	24,82,82	1.90	8 (33%)
3	HEC	L	1004	1,2	32,50,50	2.25	9 (28%)	24,82,82	2.25	5 (20%)
3	HEC	R	1001	2	32,50,50	2.37	6 (18%)	24,82,82	1.95	9 (37%)
3	HEC	M	1003	4,1	32,50,50	2.28	7 (21%)	24,82,82	1.95	7 (29%)
3	HEC	E	1004	4,1	32,50,50	2.24	7 (21%)	24,82,82	1.77	6 (25%)
3	HEC	J	1001	7,1	32,50,50	2.29	7 (21%)	24,82,82	1.40	4 (16%)
3	HEC	N	1003	4,1	32,50,50	2.34	6 (18%)	24,82,82	1.53	5 (20%)
5	LMT	F	1005	-	36,36,36	0.63	0	47,47,47	0.90	2 (4%)
3	HEC	E	1005	1	32,50,50	2.36	8 (25%)	24,82,82	1.57	2 (8%)
3	HEC	M	1005	1	32,50,50	2.34	9 (28%)	24,82,82	1.54	3 (12%)
3	HEC	F	1002	2	32,50,50	2.35	6 (18%)	24,82,82	1.86	10 (41%)
3	HEC	K	1003	4,1	32,50,50	2.34	7 (21%)	24,82,82	1.48	4 (16%)
3	HEC	L	1101	2	32,50,50	2.43	6 (18%)	24,82,82	1.58	5 (20%)
3	HEC	P	1004	4,1	32,50,50	2.15	5 (15%)	24,82,82	1.64	7 (29%)
3	HEC	C	1001	2	32,50,50	2.34	5 (15%)	24,82,82	1.51	4 (16%)
3	HEC	B	1003	4,1	32,50,50	2.27	7 (21%)	24,82,82	1.48	5 (20%)
3	HEC	R	1002	2	32,50,50	2.32	8 (25%)	24,82,82	1.95	8 (33%)
3	HEC	P	1005	1	32,50,50	2.36	8 (25%)	24,82,82	1.68	5 (20%)
3	HEC	O	1001	2	32,50,50	2.39	5 (15%)	24,82,82	1.62	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	G	1004	4,1	32,50,50	2.23	6 (18%)	24,82,82	2.04	8 (33%)
3	HEC	Q	1004	4,1	32,50,50	2.23	6 (18%)	24,82,82	1.49	7 (29%)
3	HEC	A	1001	7,1	32,50,50	2.20	6 (18%)	24,82,82	1.67	5 (20%)
3	HEC	J	1003	4,1	32,50,50	2.42	7 (21%)	24,82,82	1.40	3 (12%)
3	HEC	G	1002	1	32,50,50	2.31	6 (18%)	24,82,82	1.62	3 (12%)
3	HEC	N	1004	4,1	32,50,50	2.23	6 (18%)	24,82,82	1.84	6 (25%)
3	HEC	F	1004	1,2	32,50,50	2.23	9 (28%)	24,82,82	2.09	7 (29%)
6	ACT	I	1006	-	3,3,3	0.71	0	3,3,3	1.12	0
3	HEC	I	1004	1,2	32,50,50	2.11	5 (15%)	24,82,82	1.81	7 (29%)
3	HEC	B	1004	4,1	32,50,50	2.21	5 (15%)	24,82,82	2.02	7 (29%)
3	HEC	D	1004	4,1	32,50,50	2.17	7 (21%)	24,82,82	1.76	7 (29%)
3	HEC	M	1002	1	32,50,50	2.28	6 (18%)	24,82,82	1.60	3 (12%)
3	HEC	F	1003	2	32,50,50	2.29	8 (25%)	24,82,82	1.62	8 (33%)
3	HEC	D	1005	1	32,50,50	2.31	7 (21%)	24,82,82	1.55	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	L	1003	2	-	2/10/54/54	-
3	HEC	Q	1002	1	-	2/10/54/54	-
3	HEC	E	1003	4,1	-	0/10/54/54	-
3	HEC	N	1005	1	-	4/10/54/54	-
3	HEC	D	1003	4,1	-	0/10/54/54	-
3	HEC	G	1005	1	-	4/10/54/54	-
3	HEC	P	1001	7,1	-	2/10/54/54	-
3	HEC	H	1002	1	-	2/10/54/54	-
3	HEC	L	1002	2	-	6/10/54/54	-
3	HEC	G	1001	7,1	-	2/10/54/54	-
3	HEC	Q	1001	7,1	-	2/10/54/54	-
3	HEC	A	1004	4,1	-	2/10/54/54	-
3	HEC	H	1003	4,1	-	0/10/54/54	-
3	HEC	J	1005	1	-	3/10/54/54	-
5	LMT	R	1005	-	-	8/21/61/61	0/2/2/2
3	HEC	E	1002	1	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	N	1001	7,1	-	2/10/54/54	-
3	HEC	N	1002	1	-	2/10/54/54	-
3	HEC	F	1001	2	-	3/10/54/54	-
3	HEC	R	1003	2	-	0/10/54/54	-
3	HEC	A	1003	4,1	-	2/10/54/54	-
3	HEC	B	1001	7,1	-	2/10/54/54	-
3	HEC	D	1001	1	-	2/10/54/54	-
3	HEC	P	1003	4,1	-	0/10/54/54	-
3	HEC	K	1004	4,1	-	2/10/54/54	-
3	HEC	M	1004	4,1	-	1/10/54/54	-
3	HEC	H	1005	1	-	2/10/54/54	-
3	HEC	E	1001	7,1	-	2/10/54/54	-
5	LMT	O	1005	-	-	8/21/61/61	0/2/2/2
3	HEC	P	1002	1	-	2/10/54/54	-
3	HEC	C	1003	2	-	4/10/54/54	-
3	HEC	H	1001	7,1	-	2/10/54/54	-
3	HEC	R	1004	1,2	-	2/10/54/54	-
3	HEC	A	1002	1	-	2/10/54/54	-
3	HEC	G	1003	4,1	-	1/10/54/54	-
3	HEC	B	1005	1	-	2/10/54/54	-
3	HEC	J	1004	4,1	-	2/10/54/54	-
3	HEC	D	1002	1	-	2/10/54/54	-
3	HEC	I	1001	2	-	4/10/54/54	-
5	LMT	I	1005	-	-	8/21/61/61	0/2/2/2
3	HEC	K	1005	1	-	4/10/54/54	-
3	HEC	I	1002	2	-	5/10/54/54	-
3	HEC	C	1002	2	-	6/10/54/54	-
3	HEC	C	1004	1,2	-	4/10/54/54	-
3	HEC	K	1002	1	-	2/10/54/54	-
3	HEC	H	1004	4,1	-	2/10/54/54	-
3	HEC	I	1003	2	-	2/10/54/54	-
3	HEC	O	1004	1,2	-	3/10/54/54	-
3	HEC	K	1001	1	-	2/10/54/54	-
3	HEC	M	1001	1	-	2/10/54/54	-
5	LMT	C	1005	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	1005	1	-	4/10/54/54	-
5	LMT	L	1005	-	-	9/21/61/61	0/2/2/2
3	HEC	Q	1005	1	-	3/10/54/54	-
3	HEC	J	1002	1	-	2/10/54/54	-
3	HEC	O	1003	2	-	2/10/54/54	-
3	HEC	Q	1003	4,1	-	0/10/54/54	-
3	HEC	B	1002	1	-	2/10/54/54	-
3	HEC	O	1002	2	-	6/10/54/54	-
3	HEC	L	1004	1,2	-	2/10/54/54	-
3	HEC	R	1001	2	-	5/10/54/54	-
3	HEC	M	1003	4,1	-	0/10/54/54	-
3	HEC	E	1004	4,1	-	1/10/54/54	-
3	HEC	J	1001	7,1	-	2/10/54/54	-
3	HEC	N	1003	4,1	-	0/10/54/54	-
5	LMT	F	1005	-	-	7/21/61/61	0/2/2/2
3	HEC	E	1005	1	-	3/10/54/54	-
3	HEC	M	1005	1	-	4/10/54/54	-
3	HEC	F	1002	2	-	7/10/54/54	-
3	HEC	K	1003	4,1	-	1/10/54/54	-
3	HEC	L	1101	2	-	3/10/54/54	-
3	HEC	P	1004	4,1	-	1/10/54/54	-
3	HEC	C	1001	2	-	5/10/54/54	-
3	HEC	B	1003	4,1	-	0/10/54/54	-
3	HEC	R	1002	2	-	6/10/54/54	-
3	HEC	P	1005	1	-	4/10/54/54	-
3	HEC	O	1001	2	-	4/10/54/54	-
3	HEC	G	1004	4,1	-	2/10/54/54	-
3	HEC	Q	1004	4,1	-	3/10/54/54	-
3	HEC	A	1001	7,1	-	2/10/54/54	-
3	HEC	J	1003	4,1	-	0/10/54/54	-
3	HEC	G	1002	1	-	6/10/54/54	-
3	HEC	N	1004	4,1	-	2/10/54/54	-
3	HEC	F	1004	1,2	-	4/10/54/54	-
3	HEC	I	1004	1,2	-	0/10/54/54	-
3	HEC	B	1004	4,1	-	2/10/54/54	-
3	HEC	D	1004	4,1	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	M	1002	1	-	2/10/54/54	-
3	HEC	F	1003	2	-	2/10/54/54	-
3	HEC	D	1005	1	-	5/10/54/54	-

All (557) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1004	HEC	C2B-C3B	-7.14	1.33	1.40
3	D	1003	HEC	C2B-C3B	-6.96	1.33	1.40
3	L	1101	HEC	C2B-C3B	-6.95	1.33	1.40
3	L	1002	HEC	C2B-C3B	-6.94	1.33	1.40
3	N	1001	HEC	C2B-C3B	-6.90	1.33	1.40
3	J	1003	HEC	C2B-C3B	-6.83	1.33	1.40
3	F	1002	HEC	C2B-C3B	-6.83	1.33	1.40
3	G	1003	HEC	C2B-C3B	-6.68	1.33	1.40
3	O	1001	HEC	C2B-C3B	-6.58	1.33	1.40
3	A	1004	HEC	C2B-C3B	-6.57	1.33	1.40
3	I	1001	HEC	C2B-C3B	-6.56	1.33	1.40
3	C	1001	HEC	C2B-C3B	-6.53	1.33	1.40
3	R	1001	HEC	C2B-C3B	-6.52	1.33	1.40
3	N	1002	HEC	C2B-C3B	-6.50	1.34	1.40
3	H	1003	HEC	C3C-C2C	-6.47	1.34	1.40
3	N	1005	HEC	C2B-C3B	-6.45	1.34	1.40
3	N	1003	HEC	C2B-C3B	-6.43	1.34	1.40
3	B	1002	HEC	C2B-C3B	-6.34	1.34	1.40
3	Q	1001	HEC	C3C-C2C	-6.31	1.34	1.40
3	M	1003	HEC	C2B-C3B	-6.26	1.34	1.40
3	R	1004	HEC	C2B-C3B	-6.26	1.34	1.40
3	H	1004	HEC	C2B-C3B	-6.25	1.34	1.40
3	J	1005	HEC	C3C-C2C	-6.20	1.34	1.40
3	O	1001	HEC	C3C-C2C	-6.18	1.34	1.40
3	M	1002	HEC	C2B-C3B	-6.13	1.34	1.40
3	E	1001	HEC	C2B-C3B	-6.11	1.34	1.40
3	A	1003	HEC	C3D-C2D	6.11	1.55	1.37
3	C	1002	HEC	C2B-C3B	-6.11	1.34	1.40
3	I	1002	HEC	C2B-C3B	-6.10	1.34	1.40
3	P	1005	HEC	C3C-C2C	-6.09	1.34	1.40
3	R	1002	HEC	C2B-C3B	-6.08	1.34	1.40
3	K	1003	HEC	C2B-C3B	-6.07	1.34	1.40
3	P	1002	HEC	C2B-C3B	-6.04	1.34	1.40
3	I	1002	HEC	C3C-C2C	-6.03	1.34	1.40
3	D	1001	HEC	C3C-C2C	-6.02	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1004	HEC	C2B-C3B	-6.02	1.34	1.40
3	G	1004	HEC	C2B-C3B	-6.02	1.34	1.40
3	P	1001	HEC	C3C-C2C	-5.98	1.34	1.40
3	M	1001	HEC	C3C-C2C	-5.95	1.34	1.40
3	F	1001	HEC	C2B-C3B	-5.95	1.34	1.40
3	J	1003	HEC	C3C-C2C	-5.95	1.34	1.40
3	J	1005	HEC	C2B-C3B	-5.94	1.34	1.40
3	F	1001	HEC	C3C-C2C	-5.94	1.34	1.40
3	Q	1002	HEC	C3D-C2D	5.91	1.55	1.37
3	G	1002	HEC	C2B-C3B	-5.90	1.34	1.40
3	E	1005	HEC	C2B-C3B	-5.87	1.34	1.40
3	D	1005	HEC	C2B-C3B	-5.86	1.34	1.40
3	J	1001	HEC	C2B-C3B	-5.85	1.34	1.40
3	A	1002	HEC	C2B-C3B	-5.84	1.34	1.40
3	Q	1003	HEC	C3C-C2C	-5.83	1.34	1.40
3	M	1005	HEC	C2B-C3B	-5.82	1.34	1.40
3	L	1004	HEC	C2B-C3B	-5.82	1.34	1.40
3	Q	1001	HEC	C2B-C3B	-5.81	1.34	1.40
3	B	1001	HEC	C2B-C3B	-5.80	1.34	1.40
3	N	1004	HEC	C3D-C2D	5.77	1.54	1.37
3	F	1002	HEC	C3C-C2C	-5.76	1.34	1.40
3	A	1003	HEC	C2B-C3B	-5.76	1.34	1.40
3	P	1004	HEC	C2B-C3B	-5.74	1.34	1.40
3	C	1001	HEC	C3C-C2C	-5.74	1.34	1.40
3	O	1002	HEC	C2B-C3B	-5.74	1.34	1.40
3	L	1101	HEC	C3C-C2C	-5.73	1.34	1.40
3	N	1001	HEC	C3D-C2D	5.73	1.54	1.37
3	Q	1005	HEC	C2B-C3B	-5.70	1.34	1.40
3	E	1005	HEC	C3D-C2D	5.68	1.54	1.37
3	G	1002	HEC	C3C-C2C	-5.67	1.34	1.40
3	K	1003	HEC	C3C-C2C	-5.67	1.34	1.40
3	B	1001	HEC	C3D-C2D	5.66	1.54	1.37
3	E	1001	HEC	C3D-C2D	5.65	1.54	1.37
3	H	1001	HEC	C3D-C2D	5.65	1.54	1.37
3	G	1001	HEC	C3C-C2C	-5.65	1.34	1.40
3	H	1001	HEC	C2B-C3B	-5.63	1.34	1.40
3	R	1001	HEC	C3D-C2D	5.63	1.54	1.37
3	Q	1003	HEC	C3D-C2D	5.62	1.54	1.37
3	M	1005	HEC	C3D-C2D	5.61	1.54	1.37
3	K	1004	HEC	C3D-C2D	5.60	1.54	1.37
3	H	1002	HEC	C3D-C2D	5.60	1.54	1.37
3	R	1001	HEC	C3C-C2C	-5.59	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1002	HEC	C3D-C2D	5.58	1.54	1.37
3	L	1101	HEC	C3D-C2D	5.58	1.54	1.37
3	H	1005	HEC	C3D-C2D	5.57	1.54	1.37
3	E	1001	HEC	C3C-C2C	-5.57	1.34	1.40
3	P	1005	HEC	C3D-C2D	5.56	1.54	1.37
3	K	1001	HEC	C3D-C2D	5.56	1.54	1.37
3	Q	1002	HEC	C2B-C3B	-5.55	1.35	1.40
3	D	1002	HEC	C2B-C3B	-5.55	1.35	1.40
3	H	1003	HEC	C3D-C2D	5.55	1.54	1.37
3	B	1004	HEC	C3D-C2D	5.55	1.54	1.37
3	A	1002	HEC	C3D-C2D	5.53	1.54	1.37
3	Q	1002	HEC	C3C-C2C	-5.53	1.35	1.40
3	A	1003	HEC	C3C-C2C	-5.53	1.35	1.40
3	A	1005	HEC	C3C-C2C	-5.52	1.35	1.40
3	M	1004	HEC	C2B-C3B	-5.52	1.35	1.40
3	P	1003	HEC	C2B-C3B	-5.52	1.35	1.40
3	K	1005	HEC	C3D-C2D	5.52	1.54	1.37
3	L	1003	HEC	C3C-C2C	-5.51	1.35	1.40
3	J	1005	HEC	C3D-C2D	5.51	1.54	1.37
3	A	1005	HEC	C3D-C2D	5.51	1.54	1.37
3	J	1004	HEC	C2B-C3B	-5.50	1.35	1.40
3	C	1002	HEC	C3D-C2D	5.50	1.54	1.37
3	D	1003	HEC	C3C-C2C	-5.49	1.35	1.40
3	H	1002	HEC	C3C-C2C	-5.49	1.35	1.40
3	C	1003	HEC	C3D-C2D	5.48	1.53	1.37
3	Q	1004	HEC	C3D-C2D	5.48	1.53	1.37
3	M	1005	HEC	C3C-C2C	-5.48	1.35	1.40
3	A	1004	HEC	C3C-C2C	-5.47	1.35	1.40
3	K	1001	HEC	C2B-C3B	-5.47	1.35	1.40
3	Q	1005	HEC	C3D-C2D	5.47	1.53	1.37
3	B	1003	HEC	C2B-C3B	-5.47	1.35	1.40
3	D	1001	HEC	C2B-C3B	-5.46	1.35	1.40
3	K	1003	HEC	C3D-C2D	5.45	1.53	1.37
3	P	1001	HEC	C3D-C2D	5.44	1.53	1.37
3	R	1002	HEC	C3D-C2D	5.44	1.53	1.37
3	I	1003	HEC	C3D-C2D	5.43	1.53	1.37
3	J	1003	HEC	C3D-C2D	5.42	1.53	1.37
3	F	1003	HEC	C3C-C2C	-5.42	1.35	1.40
3	A	1005	HEC	C2B-C3B	-5.42	1.35	1.40
3	R	1004	HEC	C3D-C2D	5.41	1.53	1.37
3	K	1001	HEC	C3C-C2C	-5.41	1.35	1.40
3	K	1002	HEC	C2B-C3B	-5.40	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1003	HEC	C3D-C2D	5.39	1.53	1.37
3	D	1005	HEC	C3C-C2C	-5.39	1.35	1.40
3	G	1001	HEC	C3D-C2D	5.39	1.53	1.37
3	E	1002	HEC	C3D-C2D	5.39	1.53	1.37
3	L	1004	HEC	C3D-C2D	5.39	1.53	1.37
3	N	1005	HEC	C3D-C2D	5.39	1.53	1.37
3	D	1005	HEC	C3D-C2D	5.38	1.53	1.37
3	I	1004	HEC	C3C-C2C	-5.38	1.35	1.40
3	A	1001	HEC	C3D-C2D	5.38	1.53	1.37
3	H	1005	HEC	C2B-C3B	-5.37	1.35	1.40
3	M	1001	HEC	C2B-C3B	-5.37	1.35	1.40
3	E	1004	HEC	C2B-C3B	-5.37	1.35	1.40
3	J	1001	HEC	C3C-C2C	-5.36	1.35	1.40
3	O	1001	HEC	C3D-C2D	5.35	1.53	1.37
3	O	1002	HEC	C3D-C2D	5.35	1.53	1.37
3	A	1004	HEC	C3D-C2D	5.35	1.53	1.37
3	Q	1001	HEC	C3D-C2D	5.34	1.53	1.37
3	R	1002	HEC	C3C-C2C	-5.34	1.35	1.40
3	F	1001	HEC	C3D-C2D	5.33	1.53	1.37
3	B	1004	HEC	C2B-C3B	-5.33	1.35	1.40
3	R	1003	HEC	C3D-C2D	5.33	1.53	1.37
3	P	1002	HEC	C3C-C2C	-5.33	1.35	1.40
3	P	1005	HEC	C2B-C3B	-5.33	1.35	1.40
3	B	1002	HEC	C3D-C2D	5.33	1.53	1.37
3	E	1003	HEC	C3D-C2D	5.32	1.53	1.37
3	M	1001	HEC	C3D-C2D	5.32	1.53	1.37
3	G	1001	HEC	C2B-C3B	-5.30	1.35	1.40
3	K	1002	HEC	C3C-C2C	-5.30	1.35	1.40
3	J	1001	HEC	C3D-C2D	5.29	1.53	1.37
3	G	1003	HEC	C3D-C2D	5.29	1.53	1.37
3	M	1004	HEC	C3D-C2D	5.29	1.53	1.37
3	H	1004	HEC	C3D-C2D	5.28	1.53	1.37
3	M	1002	HEC	C3D-C2D	5.28	1.53	1.37
3	G	1005	HEC	C3D-C2D	5.28	1.53	1.37
3	F	1004	HEC	C3D-C2D	5.27	1.53	1.37
3	J	1002	HEC	C3C-C2C	-5.27	1.35	1.40
3	O	1002	HEC	C3C-C2C	-5.27	1.35	1.40
3	I	1002	HEC	C3D-C2D	5.26	1.53	1.37
3	A	1001	HEC	C3C-C2C	-5.26	1.35	1.40
3	P	1002	HEC	C3D-C2D	5.26	1.53	1.37
3	O	1003	HEC	C3D-C2D	5.25	1.53	1.37
3	N	1004	HEC	C2B-C3B	-5.25	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1002	HEC	C3D-C2D	5.24	1.53	1.37
3	B	1003	HEC	C3D-C2D	5.24	1.53	1.37
3	P	1003	HEC	C3D-C2D	5.23	1.53	1.37
3	M	1002	HEC	C3C-C2C	-5.23	1.35	1.40
3	M	1003	HEC	C3D-C2D	5.22	1.53	1.37
3	L	1003	HEC	C3D-C2D	5.22	1.53	1.37
3	D	1004	HEC	C3D-C2D	5.22	1.53	1.37
3	G	1002	HEC	C3D-C2D	5.22	1.53	1.37
3	F	1004	HEC	C3C-C2C	-5.22	1.35	1.40
3	E	1004	HEC	C3C-C2C	-5.22	1.35	1.40
3	P	1001	HEC	C2B-C3B	-5.22	1.35	1.40
3	P	1004	HEC	C3D-C2D	5.21	1.53	1.37
3	N	1002	HEC	C3D-C2D	5.20	1.53	1.37
3	C	1001	HEC	C3D-C2D	5.20	1.53	1.37
3	F	1004	HEC	C2B-C3B	-5.18	1.35	1.40
3	E	1005	HEC	C3C-C2C	-5.18	1.35	1.40
3	O	1004	HEC	C3D-C2D	5.18	1.53	1.37
3	K	1004	HEC	C3C-C2C	-5.17	1.35	1.40
3	H	1002	HEC	C2B-C3B	-5.16	1.35	1.40
3	J	1004	HEC	C3D-C2D	5.16	1.53	1.37
3	G	1005	HEC	C3C-C2C	-5.16	1.35	1.40
3	L	1003	HEC	C2B-C3B	-5.15	1.35	1.40
3	I	1001	HEC	C3D-C2D	5.14	1.52	1.37
3	K	1005	HEC	C3C-C2C	-5.13	1.35	1.40
3	B	1004	HEC	C3C-C2C	-5.13	1.35	1.40
3	F	1003	HEC	C3D-C2D	5.13	1.52	1.37
3	C	1004	HEC	C3C-C2C	-5.11	1.35	1.40
3	C	1003	HEC	C2B-C3B	-5.11	1.35	1.40
3	C	1002	HEC	C3C-C2C	-5.11	1.35	1.40
3	G	1004	HEC	C3D-C2D	5.09	1.52	1.37
3	A	1001	HEC	C2B-C3B	-5.09	1.35	1.40
3	B	1001	HEC	C3C-C2C	-5.08	1.35	1.40
3	E	1003	HEC	C3C-C2C	-5.08	1.35	1.40
3	D	1003	HEC	C3D-C2D	5.08	1.52	1.37
3	J	1002	HEC	C3D-C2D	5.08	1.52	1.37
3	B	1005	HEC	C3D-C2D	5.07	1.52	1.37
3	M	1004	HEC	C3C-C2C	-5.07	1.35	1.40
3	E	1004	HEC	C3D-C2D	5.07	1.52	1.37
3	O	1004	HEC	C3C-C2C	-5.06	1.35	1.40
3	K	1005	HEC	C2B-C3B	-5.06	1.35	1.40
3	Q	1005	HEC	C3C-C2C	-5.05	1.35	1.40
3	E	1003	HEC	C2B-C3B	-5.05	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	HEC	C3D-C2D	5.05	1.52	1.37
3	C	1004	HEC	C3D-C2D	5.04	1.52	1.37
3	H	1004	HEC	C3C-C2C	-5.03	1.35	1.40
3	G	1003	HEC	C3C-C2C	-5.03	1.35	1.40
3	N	1005	HEC	C3C-C2C	-5.02	1.35	1.40
3	O	1003	HEC	C2B-C3B	-5.01	1.35	1.40
3	D	1002	HEC	C3D-C2D	5.00	1.52	1.37
3	N	1003	HEC	C3C-C2C	-5.00	1.35	1.40
3	N	1001	HEC	C3C-C2C	-5.00	1.35	1.40
3	F	1002	HEC	C3D-C2D	4.99	1.52	1.37
3	E	1002	HEC	C2B-C3B	-4.95	1.35	1.40
3	Q	1003	HEC	C2B-C3B	-4.95	1.35	1.40
3	R	1004	HEC	C3C-C2C	-4.95	1.35	1.40
3	R	1003	HEC	C3C-C2C	-4.94	1.35	1.40
3	H	1005	HEC	C3C-C2C	-4.93	1.35	1.40
3	F	1003	HEC	C2B-C3B	-4.92	1.35	1.40
3	B	1005	HEC	C2B-C3B	-4.92	1.35	1.40
3	I	1001	HEC	C3C-C2C	-4.90	1.35	1.40
3	Q	1004	HEC	C2B-C3B	-4.89	1.35	1.40
3	C	1003	HEC	C3C-C2C	-4.88	1.35	1.40
3	I	1004	HEC	C3D-C2D	4.87	1.52	1.37
3	P	1003	HEC	C3C-C2C	-4.87	1.35	1.40
3	H	1003	HEC	C2B-C3B	-4.83	1.35	1.40
3	H	1001	HEC	C3C-C2C	-4.83	1.35	1.40
3	L	1002	HEC	C3C-C2C	-4.80	1.35	1.40
3	Q	1004	HEC	C3C-C2C	-4.79	1.35	1.40
3	B	1003	HEC	C3C-C2C	-4.78	1.35	1.40
3	D	1002	HEC	C3C-C2C	-4.76	1.35	1.40
3	N	1004	HEC	C3C-C2C	-4.75	1.35	1.40
3	I	1004	HEC	C2B-C3B	-4.73	1.35	1.40
3	E	1002	HEC	C3C-C2C	-4.71	1.35	1.40
3	G	1005	HEC	C2B-C3B	-4.70	1.35	1.40
3	D	1004	HEC	C3C-C2C	-4.69	1.35	1.40
3	L	1004	HEC	C3C-C2C	-4.68	1.35	1.40
3	G	1004	HEC	C3C-C2C	-4.68	1.35	1.40
3	B	1002	HEC	C3C-C2C	-4.67	1.35	1.40
3	I	1003	HEC	C2B-C3B	-4.67	1.35	1.40
3	O	1003	HEC	C3C-C2C	-4.64	1.35	1.40
3	B	1005	HEC	C3C-C2C	-4.64	1.35	1.40
3	M	1003	HEC	C3C-C2C	-4.60	1.35	1.40
3	K	1004	HEC	C2B-C3B	-4.58	1.36	1.40
3	J	1002	HEC	C2B-C3B	-4.50	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1003	HEC	C2B-C3B	-4.49	1.36	1.40
3	D	1004	HEC	C2B-C3B	-4.39	1.36	1.40
3	E	1002	HEC	CBB-CAB	-4.34	1.33	1.49
3	K	1004	HEC	CBC-CAC	-4.33	1.33	1.49
3	G	1002	HEC	CBB-CAB	-4.27	1.33	1.49
3	Q	1004	HEC	CBC-CAC	-4.24	1.33	1.49
3	M	1004	HEC	CBC-CAC	-4.22	1.33	1.49
3	I	1003	HEC	C3C-C2C	-4.22	1.36	1.40
3	P	1004	HEC	C3C-C2C	-4.21	1.36	1.40
3	J	1001	HEC	CBC-CAC	-4.21	1.33	1.49
3	K	1004	HEC	CBB-CAB	-4.19	1.33	1.49
3	A	1004	HEC	CBC-CAC	-4.19	1.33	1.49
3	J	1004	HEC	C3C-C2C	-4.19	1.36	1.40
3	A	1002	HEC	C3C-C2C	-4.19	1.36	1.40
3	P	1002	HEC	CBC-CAC	-4.14	1.33	1.49
3	R	1002	HEC	CBC-CAC	-4.14	1.34	1.49
3	F	1003	HEC	CBC-CAC	-4.13	1.34	1.49
3	N	1002	HEC	C3C-C2C	-4.10	1.36	1.40
3	A	1002	HEC	CBC-CAC	-4.08	1.34	1.49
3	I	1003	HEC	CBC-CAC	-4.08	1.34	1.49
3	B	1002	HEC	CBB-CAB	-4.07	1.34	1.49
3	F	1002	HEC	CBC-CAC	-4.07	1.34	1.49
3	D	1004	HEC	CBC-CAC	-4.07	1.34	1.49
3	Q	1002	HEC	CBC-CAC	-4.06	1.34	1.49
3	P	1004	HEC	CBC-CAC	-4.05	1.34	1.49
3	J	1002	HEC	CBB-CAB	-4.05	1.34	1.49
3	P	1003	HEC	CBB-CAB	-4.05	1.34	1.49
3	Q	1003	HEC	CBB-CAB	-4.04	1.34	1.49
3	O	1001	HEC	CBC-CAC	-4.04	1.34	1.49
3	K	1001	HEC	CBB-CAB	-4.03	1.34	1.49
3	P	1005	HEC	CBB-CAB	-4.03	1.34	1.49
3	B	1005	HEC	CBC-CAC	-4.03	1.34	1.49
3	Q	1001	HEC	CBB-CAB	-4.03	1.34	1.49
3	O	1002	HEC	CBC-CAC	-4.03	1.34	1.49
3	C	1003	HEC	CBC-CAC	-4.02	1.34	1.49
3	F	1001	HEC	CBC-CAC	-4.02	1.34	1.49
3	K	1002	HEC	CBB-CAB	-4.02	1.34	1.49
3	K	1002	HEC	CBC-CAC	-4.01	1.34	1.49
3	O	1001	HEC	CBB-CAB	-4.00	1.34	1.49
3	E	1001	HEC	CBB-CAB	-4.00	1.34	1.49
3	L	1003	HEC	CBC-CAC	-4.00	1.34	1.49
3	L	1101	HEC	CBC-CAC	-4.00	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1002	HEC	CBC-CAC	-3.99	1.34	1.49
3	J	1004	HEC	CBC-CAC	-3.99	1.34	1.49
3	D	1001	HEC	CBC-CAC	-3.99	1.34	1.49
3	N	1001	HEC	CBC-CAC	-3.99	1.34	1.49
3	G	1004	HEC	CBB-CAB	-3.98	1.34	1.49
3	Q	1002	HEC	CBB-CAB	-3.98	1.34	1.49
3	C	1002	HEC	CBC-CAC	-3.98	1.34	1.49
3	P	1002	HEC	CBB-CAB	-3.97	1.34	1.49
3	H	1005	HEC	CBB-CAB	-3.97	1.34	1.49
3	R	1001	HEC	CBB-CAB	-3.97	1.34	1.49
3	I	1001	HEC	CBC-CAC	-3.96	1.34	1.49
3	G	1005	HEC	CBB-CAB	-3.96	1.34	1.49
3	K	1003	HEC	CBB-CAB	-3.96	1.34	1.49
3	B	1004	HEC	CBC-CAC	-3.96	1.34	1.49
3	D	1003	HEC	CBB-CAB	-3.95	1.34	1.49
3	Q	1005	HEC	CBB-CAB	-3.95	1.34	1.49
3	D	1001	HEC	CBB-CAB	-3.94	1.34	1.49
3	L	1101	HEC	CBB-CAB	-3.94	1.34	1.49
3	G	1001	HEC	CBB-CAB	-3.94	1.34	1.49
3	K	1005	HEC	CBB-CAB	-3.94	1.34	1.49
3	F	1004	HEC	CBC-CAC	-3.94	1.34	1.49
3	A	1002	HEC	CBB-CAB	-3.92	1.34	1.49
3	D	1002	HEC	CBB-CAB	-3.92	1.34	1.49
3	L	1002	HEC	CBB-CAB	-3.92	1.34	1.49
3	R	1002	HEC	CBB-CAB	-3.92	1.34	1.49
3	R	1003	HEC	CBC-CAC	-3.92	1.34	1.49
3	J	1005	HEC	CBB-CAB	-3.91	1.34	1.49
3	M	1002	HEC	CBB-CAB	-3.91	1.34	1.49
3	R	1004	HEC	CBC-CAC	-3.91	1.34	1.49
3	R	1001	HEC	CBC-CAC	-3.91	1.34	1.49
3	K	1001	HEC	CBC-CAC	-3.91	1.34	1.49
3	H	1003	HEC	CBB-CAB	-3.91	1.34	1.49
3	L	1002	HEC	CBC-CAC	-3.90	1.34	1.49
3	M	1001	HEC	CBB-CAB	-3.90	1.34	1.49
3	E	1002	HEC	CBC-CAC	-3.90	1.34	1.49
3	B	1003	HEC	CBB-CAB	-3.90	1.34	1.49
3	P	1004	HEC	CBB-CAB	-3.89	1.34	1.49
3	E	1003	HEC	CBB-CAB	-3.89	1.34	1.49
3	C	1001	HEC	CBC-CAC	-3.89	1.34	1.49
3	E	1005	HEC	CBB-CAB	-3.89	1.34	1.49
3	H	1001	HEC	CBB-CAB	-3.89	1.34	1.49
3	K	1005	HEC	CBC-CAC	-3.89	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1002	HEC	CBC-CAC	-3.88	1.34	1.49
3	D	1005	HEC	CBB-CAB	-3.88	1.34	1.49
3	E	1001	HEC	CBC-CAC	-3.87	1.35	1.49
3	G	1004	HEC	CBC-CAC	-3.87	1.35	1.49
3	C	1001	HEC	CBB-CAB	-3.87	1.35	1.49
3	Q	1004	HEC	CBB-CAB	-3.86	1.35	1.49
3	N	1003	HEC	CBB-CAB	-3.86	1.35	1.49
3	C	1002	HEC	CBB-CAB	-3.86	1.35	1.49
3	J	1001	HEC	CBB-CAB	-3.86	1.35	1.49
3	B	1005	HEC	CBB-CAB	-3.86	1.35	1.49
3	J	1003	HEC	CBC-CAC	-3.85	1.35	1.49
3	N	1004	HEC	CBC-CAC	-3.85	1.35	1.49
3	A	1005	HEC	CBC-CAC	-3.85	1.35	1.49
3	E	1004	HEC	CBC-CAC	-3.85	1.35	1.49
3	H	1004	HEC	CBC-CAC	-3.85	1.35	1.49
3	N	1005	HEC	CBC-CAC	-3.85	1.35	1.49
3	E	1005	HEC	CBC-CAC	-3.84	1.35	1.49
3	N	1001	HEC	CBB-CAB	-3.84	1.35	1.49
3	E	1003	HEC	CBC-CAC	-3.84	1.35	1.49
3	H	1002	HEC	CBC-CAC	-3.83	1.35	1.49
3	E	1004	HEC	CBB-CAB	-3.83	1.35	1.49
3	L	1004	HEC	CBC-CAC	-3.83	1.35	1.49
3	A	1005	HEC	CBB-CAB	-3.83	1.35	1.49
3	I	1002	HEC	CBB-CAB	-3.83	1.35	1.49
3	A	1004	HEC	CBB-CAB	-3.81	1.35	1.49
3	B	1002	HEC	CBC-CAC	-3.81	1.35	1.49
3	M	1001	HEC	CBC-CAC	-3.81	1.35	1.49
3	H	1001	HEC	CBC-CAC	-3.81	1.35	1.49
3	O	1003	HEC	CBC-CAC	-3.81	1.35	1.49
3	H	1005	HEC	CBC-CAC	-3.80	1.35	1.49
3	H	1002	HEC	CBB-CAB	-3.80	1.35	1.49
3	C	1004	HEC	CBC-CAC	-3.80	1.35	1.49
3	Q	1005	HEC	CBC-CAC	-3.80	1.35	1.49
3	G	1005	HEC	CBC-CAC	-3.80	1.35	1.49
3	B	1004	HEC	CBB-CAB	-3.80	1.35	1.49
3	O	1002	HEC	CBB-CAB	-3.80	1.35	1.49
3	A	1003	HEC	CBB-CAB	-3.79	1.35	1.49
3	Q	1001	HEC	CBC-CAC	-3.79	1.35	1.49
3	M	1003	HEC	CBB-CAB	-3.79	1.35	1.49
3	I	1001	HEC	CBB-CAB	-3.79	1.35	1.49
3	J	1003	HEC	CBB-CAB	-3.78	1.35	1.49
3	F	1002	HEC	CBB-CAB	-3.78	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1002	HEC	CBC-CAC	-3.78	1.35	1.49
3	B	1003	HEC	CBC-CAC	-3.77	1.35	1.49
3	P	1001	HEC	CBB-CAB	-3.77	1.35	1.49
3	N	1002	HEC	CBB-CAB	-3.76	1.35	1.49
3	R	1004	HEC	CBB-CAB	-3.76	1.35	1.49
3	I	1003	HEC	CBB-CAB	-3.75	1.35	1.49
3	J	1004	HEC	CBB-CAB	-3.75	1.35	1.49
3	Q	1003	HEC	CBC-CAC	-3.74	1.35	1.49
3	G	1001	HEC	CBC-CAC	-3.73	1.35	1.49
3	D	1005	HEC	CBC-CAC	-3.73	1.35	1.49
3	F	1004	HEC	CBB-CAB	-3.72	1.35	1.49
3	A	1001	HEC	CBC-CAC	-3.72	1.35	1.49
3	F	1001	HEC	CBB-CAB	-3.72	1.35	1.49
3	C	1003	HEC	CBB-CAB	-3.72	1.35	1.49
3	D	1004	HEC	CBB-CAB	-3.72	1.35	1.49
3	N	1005	HEC	CBB-CAB	-3.72	1.35	1.49
3	N	1003	HEC	CBC-CAC	-3.72	1.35	1.49
3	D	1002	HEC	CBC-CAC	-3.71	1.35	1.49
3	H	1004	HEC	CBB-CAB	-3.71	1.35	1.49
3	R	1003	HEC	CBB-CAB	-3.70	1.35	1.49
3	M	1005	HEC	CBC-CAC	-3.70	1.35	1.49
3	J	1002	HEC	CBC-CAC	-3.68	1.35	1.49
3	N	1002	HEC	CBC-CAC	-3.67	1.35	1.49
3	B	1001	HEC	CBB-CAB	-3.67	1.35	1.49
3	F	1003	HEC	CBB-CAB	-3.67	1.35	1.49
3	P	1005	HEC	CBC-CAC	-3.66	1.35	1.49
3	K	1003	HEC	CBC-CAC	-3.65	1.35	1.49
3	A	1001	HEC	CBB-CAB	-3.65	1.35	1.49
3	L	1003	HEC	CBB-CAB	-3.64	1.35	1.49
3	N	1004	HEC	CBB-CAB	-3.63	1.35	1.49
3	M	1004	HEC	CBB-CAB	-3.62	1.35	1.49
3	J	1005	HEC	CBC-CAC	-3.62	1.35	1.49
3	P	1001	HEC	CBC-CAC	-3.62	1.35	1.49
3	M	1003	HEC	CBC-CAC	-3.59	1.36	1.49
3	B	1001	HEC	CBC-CAC	-3.58	1.36	1.49
3	O	1003	HEC	CBB-CAB	-3.58	1.36	1.49
3	D	1003	HEC	CBC-CAC	-3.56	1.36	1.49
3	P	1003	HEC	CBC-CAC	-3.56	1.36	1.49
3	M	1005	HEC	CBB-CAB	-3.55	1.36	1.49
3	L	1004	HEC	CBB-CAB	-3.54	1.36	1.49
3	O	1004	HEC	CBB-CAB	-3.54	1.36	1.49
3	H	1003	HEC	CBC-CAC	-3.53	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1004	HEC	CBB-CAB	-3.52	1.36	1.49
3	I	1004	HEC	CBC-CAC	-3.50	1.36	1.49
3	O	1004	HEC	CBC-CAC	-3.48	1.36	1.49
3	G	1003	HEC	CBB-CAB	-3.46	1.36	1.49
3	C	1004	HEC	CBB-CAB	-3.45	1.36	1.49
3	G	1003	HEC	CBC-CAC	-3.40	1.36	1.49
3	A	1003	HEC	CBC-CAC	-3.34	1.37	1.49
3	D	1004	HEC	CAA-C2A	2.85	1.57	1.52
3	J	1003	HEC	CAD-C3D	2.84	1.56	1.52
3	K	1001	HEC	CAD-C3D	2.81	1.56	1.52
3	P	1001	HEC	CAD-C3D	2.78	1.56	1.52
3	D	1003	HEC	CAD-C3D	2.73	1.56	1.52
3	M	1005	HEC	C4D-ND	2.72	1.41	1.36
3	L	1004	HEC	C4D-ND	2.66	1.41	1.36
3	G	1003	HEC	C1D-ND	2.65	1.41	1.36
3	R	1003	HEC	CAD-C3D	2.65	1.55	1.52
3	D	1004	HEC	CAD-C3D	2.62	1.55	1.52
3	B	1002	HEC	CAD-C3D	2.60	1.55	1.52
3	N	1003	HEC	C4D-ND	2.59	1.41	1.36
3	F	1004	HEC	CAD-C3D	2.58	1.55	1.52
3	F	1003	HEC	CAD-C3D	2.56	1.55	1.52
3	J	1004	HEC	C1C-NC	2.56	1.41	1.36
3	A	1003	HEC	C1D-ND	2.56	1.41	1.36
3	G	1001	HEC	CMC-C2C	2.50	1.57	1.51
3	E	1005	HEC	CAD-C3D	2.49	1.55	1.52
3	D	1001	HEC	CAD-C3D	2.48	1.55	1.52
3	R	1002	HEC	C1D-ND	2.44	1.41	1.36
3	G	1003	HEC	CAD-C3D	2.43	1.55	1.52
3	I	1001	HEC	CAA-C2A	2.42	1.56	1.52
3	G	1004	HEC	CMA-C3A	2.39	1.57	1.51
3	B	1003	HEC	C4D-ND	2.39	1.41	1.36
3	L	1002	HEC	CAD-C3D	2.39	1.55	1.52
3	E	1001	HEC	CAD-C3D	2.38	1.55	1.52
3	B	1003	HEC	C1D-ND	2.37	1.41	1.36
3	J	1004	HEC	CAA-C2A	2.37	1.56	1.52
3	D	1002	HEC	C1D-ND	2.36	1.41	1.36
3	F	1003	HEC	C3C-C4C	2.35	1.47	1.43
3	D	1003	HEC	C4D-ND	2.35	1.41	1.36
3	Q	1002	HEC	CAA-C2A	2.35	1.56	1.52
3	R	1001	HEC	CAD-C3D	2.34	1.55	1.52
3	A	1003	HEC	C4D-ND	2.33	1.41	1.36
3	K	1001	HEC	C3C-C4C	2.32	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1003	HEC	C1D-ND	2.32	1.40	1.36
3	O	1003	HEC	CAA-C2A	2.32	1.56	1.52
3	E	1001	HEC	CAA-C2A	2.31	1.56	1.52
3	J	1003	HEC	C1D-ND	2.31	1.40	1.36
3	L	1004	HEC	C1D-ND	2.29	1.40	1.36
3	H	1002	HEC	C1D-ND	2.28	1.40	1.36
3	D	1005	HEC	C1D-ND	2.27	1.40	1.36
3	P	1003	HEC	CAD-C3D	2.26	1.55	1.52
3	B	1001	HEC	C3C-C4C	2.26	1.47	1.43
3	J	1005	HEC	C3C-C4C	2.26	1.47	1.43
5	O	1005	LMT	O1'-C1'	2.26	1.44	1.40
3	K	1003	HEC	CAD-C3D	2.26	1.55	1.52
3	G	1002	HEC	CAD-C3D	2.26	1.55	1.52
3	D	1003	HEC	C1D-ND	2.26	1.40	1.36
3	Q	1001	HEC	CAD-C3D	2.25	1.55	1.52
3	J	1002	HEC	C1D-ND	2.25	1.40	1.36
3	M	1003	HEC	CAD-C3D	2.25	1.55	1.52
3	F	1002	HEC	C1D-ND	2.24	1.40	1.36
3	P	1002	HEC	C1D-ND	2.24	1.40	1.36
3	N	1002	HEC	C4D-ND	2.24	1.40	1.36
3	H	1003	HEC	C3C-C4C	2.23	1.47	1.43
3	Q	1004	HEC	CAA-C2A	2.22	1.56	1.52
3	N	1004	HEC	C1C-NC	2.22	1.40	1.36
3	E	1002	HEC	CAA-C2A	2.22	1.56	1.52
3	G	1001	HEC	C1D-ND	2.21	1.40	1.36
3	D	1001	HEC	CAA-C2A	2.21	1.56	1.52
3	H	1001	HEC	C4D-ND	2.20	1.40	1.36
3	G	1003	HEC	C4D-ND	2.20	1.40	1.36
3	F	1004	HEC	C4D-ND	2.20	1.40	1.36
3	Q	1001	HEC	C3C-C4C	2.19	1.47	1.43
3	G	1005	HEC	CAD-C3D	2.19	1.55	1.52
3	E	1003	HEC	C1D-ND	2.19	1.40	1.36
3	M	1003	HEC	C1D-ND	2.19	1.40	1.36
3	I	1002	HEC	C2A-C1A	2.19	1.47	1.42
3	H	1005	HEC	CAD-C3D	2.17	1.55	1.52
3	A	1005	HEC	C4B-C3B	2.16	1.47	1.43
3	M	1005	HEC	CMA-C3A	2.16	1.56	1.51
3	K	1002	HEC	CAD-C3D	2.16	1.55	1.52
3	K	1003	HEC	C4D-ND	2.16	1.40	1.36
3	L	1101	HEC	C4D-ND	2.16	1.40	1.36
3	N	1002	HEC	CMC-C2C	2.15	1.56	1.51
3	E	1004	HEC	C4B-C3B	2.15	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1003	HEC	CMB-C2B	2.15	1.56	1.51
3	A	1001	HEC	CMC-C2C	2.14	1.56	1.51
3	P	1005	HEC	CMD-C2D	2.14	1.56	1.51
3	J	1001	HEC	CAD-C3D	2.14	1.55	1.52
3	E	1005	HEC	O1A-CGA	2.14	1.29	1.22
3	D	1005	HEC	CAD-C3D	2.13	1.55	1.52
3	J	1002	HEC	CAD-C3D	2.13	1.55	1.52
3	P	1005	HEC	C1D-ND	2.13	1.40	1.36
3	M	1005	HEC	C3C-C4C	2.13	1.46	1.43
3	L	1003	HEC	C4D-ND	2.12	1.40	1.36
3	O	1003	HEC	CAD-C3D	2.12	1.55	1.52
3	F	1004	HEC	CMD-C2D	2.10	1.56	1.51
3	G	1005	HEC	C4D-ND	2.10	1.40	1.36
3	M	1002	HEC	CAD-C3D	2.09	1.55	1.52
3	C	1003	HEC	CMD-C2D	2.09	1.56	1.51
3	M	1005	HEC	CMC-C2C	2.09	1.56	1.51
3	L	1004	HEC	CMD-C2D	2.09	1.56	1.51
3	R	1002	HEC	C4D-ND	2.09	1.40	1.36
3	E	1005	HEC	CMC-C2C	2.09	1.56	1.51
3	Q	1002	HEC	CMD-C2D	2.08	1.56	1.51
3	A	1002	HEC	CMD-C2D	2.08	1.56	1.51
3	J	1002	HEC	CMC-C2C	2.08	1.56	1.51
3	B	1001	HEC	C1D-ND	2.07	1.40	1.36
3	O	1002	HEC	C1D-ND	2.07	1.40	1.36
3	I	1002	HEC	C3C-C4C	2.07	1.46	1.43
3	K	1004	HEC	CMB-C2B	2.06	1.56	1.51
3	L	1003	HEC	CMD-C2D	2.06	1.55	1.51
3	B	1001	HEC	C4D-ND	2.06	1.40	1.36
3	O	1004	HEC	C1D-ND	2.06	1.40	1.36
3	E	1004	HEC	CAA-C2A	2.06	1.55	1.52
3	L	1004	HEC	CAD-C3D	2.06	1.55	1.52
3	H	1005	HEC	CMA-C3A	2.05	1.56	1.51
3	J	1002	HEC	CMD-C2D	2.05	1.55	1.51
3	I	1003	HEC	C1D-ND	2.05	1.40	1.36
3	P	1001	HEC	C4D-ND	2.05	1.40	1.36
3	D	1001	HEC	CMC-C2C	2.04	1.56	1.51
3	P	1001	HEC	CAA-C2A	2.04	1.55	1.52
3	O	1004	HEC	CMD-C2D	2.04	1.55	1.51
3	C	1002	HEC	C1D-ND	2.04	1.40	1.36
3	A	1005	HEC	CAD-C3D	2.04	1.55	1.52
3	F	1003	HEC	C4D-ND	2.04	1.40	1.36
3	C	1003	HEC	CMB-C2B	2.03	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1004	HEC	C1B-NB	2.03	1.40	1.36
3	Q	1001	HEC	C4D-ND	2.02	1.40	1.36
3	D	1003	HEC	CMD-C2D	2.02	1.55	1.51
3	I	1003	HEC	CAD-C3D	2.02	1.55	1.52
3	I	1003	HEC	CAA-C2A	2.02	1.55	1.52
3	N	1001	HEC	C1D-ND	2.02	1.40	1.36
3	H	1005	HEC	C4D-ND	2.02	1.40	1.36
3	E	1003	HEC	CAA-C2A	2.02	1.55	1.52
3	E	1002	HEC	CMC-C2C	2.01	1.56	1.51
3	J	1001	HEC	CAA-C2A	2.01	1.55	1.52
3	H	1005	HEC	CAA-C2A	2.01	1.55	1.52
3	P	1005	HEC	C4B-C3B	2.01	1.46	1.43
3	A	1004	HEC	CMD-C2D	2.01	1.55	1.51
3	O	1004	HEC	CMA-C3A	2.01	1.56	1.51
3	R	1002	HEC	CAA-C2A	2.00	1.55	1.52
3	R	1003	HEC	CMD-C2D	2.00	1.55	1.51
3	R	1004	HEC	C4D-ND	2.00	1.40	1.36
3	F	1004	HEC	CMB-C2B	2.00	1.56	1.51

All (466) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1004	HEC	CBA-CAA-C2A	-7.36	100.20	112.60
3	O	1004	HEC	CBA-CAA-C2A	-7.28	100.33	112.60
3	L	1004	HEC	CBA-CAA-C2A	-7.18	100.50	112.60
3	F	1004	HEC	CBA-CAA-C2A	-6.59	101.50	112.60
3	K	1004	HEC	CBA-CAA-C2A	-6.10	102.33	112.60
3	A	1002	HEC	CBD-CAD-C3D	-5.76	102.79	112.62
3	R	1002	HEC	CBD-CAD-C3D	-5.70	102.90	112.62
3	M	1004	HEC	CBA-CAA-C2A	-5.59	103.19	112.60
3	M	1003	HEC	CBA-CAA-C2A	-5.54	103.27	112.60
3	G	1004	HEC	CBA-CAA-C2A	-5.35	103.59	112.60
3	I	1004	HEC	CBA-CAA-C2A	-5.10	104.01	112.60
3	A	1004	HEC	CBA-CAA-C2A	-4.92	104.31	112.60
3	R	1001	HEC	CBD-CAD-C3D	4.86	120.91	112.62
3	D	1002	HEC	CBD-CAD-C3D	-4.83	104.37	112.62
3	C	1004	HEC	CBA-CAA-C2A	-4.77	104.56	112.60
3	Q	1005	HEC	CBD-CAD-C3D	-4.67	104.65	112.62
3	N	1004	HEC	CBA-CAA-C2A	-4.61	104.83	112.60
3	C	1002	HEC	CBD-CAD-C3D	-4.51	104.92	112.62
3	M	1002	HEC	CBD-CAD-C3D	-4.40	105.11	112.62
3	O	1002	HEC	C1D-C2D-C3D	-4.39	103.94	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1005	HEC	CMB-C2B-C1B	-4.37	121.75	128.46
3	B	1004	HEC	CBA-CAA-C2A	-4.34	105.29	112.60
3	G	1002	HEC	CBD-CAD-C3D	-4.32	105.25	112.62
3	L	1004	HEC	CMC-C2C-C1C	-4.28	121.89	128.46
3	F	1002	HEC	CBD-CAD-C3D	-4.23	105.41	112.62
3	C	1002	HEC	C1D-C2D-C3D	-4.21	104.07	107.00
3	H	1003	HEC	CBD-CAD-C3D	-4.18	105.48	112.62
3	A	1005	HEC	CMC-C2C-C1C	-4.14	122.09	128.46
3	J	1004	HEC	CBA-CAA-C2A	-4.13	105.64	112.60
3	A	1005	HEC	CBA-CAA-C2A	-4.01	105.84	112.60
3	C	1003	HEC	C1D-C2D-C3D	-3.94	104.25	107.00
3	Q	1005	HEC	CBA-CAA-C2A	-3.92	106.00	112.60
3	A	1005	HEC	CBD-CAD-C3D	-3.85	106.05	112.62
3	D	1004	HEC	CBA-CAA-C2A	-3.82	106.17	112.60
3	N	1005	HEC	CMC-C2C-C1C	-3.80	122.62	128.46
3	L	1003	HEC	CBA-CAA-C2A	-3.75	106.29	112.60
3	A	1005	HEC	CMB-C2B-C1B	-3.74	122.72	128.46
3	B	1004	HEC	C1D-C2D-C3D	-3.73	104.40	107.00
3	C	1003	HEC	CBD-CAD-C3D	-3.69	106.33	112.62
3	D	1002	HEC	CMC-C2C-C1C	-3.67	122.83	128.46
3	O	1001	HEC	CBD-CAD-C3D	-3.66	106.37	112.62
3	H	1004	HEC	CBA-CAA-C2A	-3.66	106.44	112.60
3	E	1004	HEC	CBA-CAA-C2A	-3.64	106.46	112.60
3	R	1003	HEC	CBA-CAA-C2A	-3.63	106.48	112.60
3	E	1005	HEC	CBA-CAA-C2A	-3.63	106.49	112.60
3	M	1004	HEC	CMC-C2C-C1C	-3.63	122.89	128.46
3	A	1002	HEC	C1D-C2D-C3D	-3.59	104.50	107.00
3	O	1003	HEC	C1D-C2D-C3D	-3.57	104.52	107.00
3	N	1005	HEC	CMC-C2C-C3C	3.54	129.99	125.82
3	N	1002	HEC	CBD-CAD-C3D	-3.47	106.70	112.62
3	B	1004	HEC	CMB-C2B-C1B	-3.46	123.14	128.46
3	P	1004	HEC	CBA-CAA-C2A	-3.45	106.80	112.60
3	G	1004	HEC	C1D-C2D-C3D	-3.44	104.60	107.00
3	A	1001	HEC	C1D-C2D-C3D	-3.43	104.61	107.00
3	J	1004	HEC	CBD-CAD-C3D	-3.43	106.77	112.62
3	O	1002	HEC	CBD-CAD-C3D	-3.43	106.77	112.62
3	M	1005	HEC	CBA-CAA-C2A	-3.43	106.83	112.60
3	G	1005	HEC	CBA-CAA-C2A	-3.42	106.84	112.60
3	I	1003	HEC	C1D-C2D-C3D	-3.41	104.63	107.00
3	M	1005	HEC	CBD-CAD-C3D	-3.40	106.82	112.62
3	Q	1003	HEC	CBD-CAD-C3D	-3.38	106.85	112.62
3	F	1004	HEC	C1D-C2D-C3D	-3.38	104.65	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	1002	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
3	A	1005	HEC	CMC-C2C-C3C	3.37	129.78	125.82
3	R	1001	HEC	CAD-CBD-CGD	-3.35	104.38	113.76
3	E	1004	HEC	CBD-CAD-C3D	-3.33	106.94	112.62
3	C	1004	HEC	CMC-C2C-C1C	-3.33	123.35	128.46
3	Q	1002	HEC	CBD-CAD-C3D	-3.28	107.02	112.62
3	P	1002	HEC	CMB-C2B-C1B	-3.27	123.43	128.46
3	K	1003	HEC	CBA-CAA-C2A	-3.27	107.09	112.60
3	H	1004	HEC	C1D-C2D-C3D	-3.27	104.72	107.00
3	Q	1005	HEC	CMC-C2C-C1C	-3.25	123.47	128.46
3	H	1005	HEC	CMB-C2B-C1B	-3.22	123.52	128.46
3	J	1003	HEC	CBA-CAA-C2A	-3.21	107.19	112.60
3	L	1002	HEC	C2B-C3B-C4B	3.21	109.81	106.35
3	D	1005	HEC	CBD-CAD-C3D	-3.21	107.15	112.62
3	A	1002	HEC	CMB-C2B-C1B	-3.20	123.55	128.46
3	K	1004	HEC	CBD-CAD-C3D	-3.19	107.18	112.62
3	I	1003	HEC	CMC-C2C-C1C	-3.18	123.58	128.46
3	P	1002	HEC	CBD-CAD-C3D	-3.17	107.20	112.62
3	J	1002	HEC	CBD-CAD-C3D	-3.17	107.21	112.62
3	B	1003	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
3	I	1003	HEC	CMB-C2B-C1B	-3.17	123.59	128.46
3	J	1002	HEC	CMB-C2B-C1B	-3.17	123.60	128.46
3	H	1003	HEC	CBA-CAA-C2A	-3.16	107.27	112.60
3	C	1003	HEC	CBA-CAA-C2A	-3.16	107.28	112.60
3	B	1004	HEC	CMB-C2B-C3B	3.14	129.52	125.82
3	E	1003	HEC	CBA-CAA-C2A	-3.13	107.32	112.60
3	L	1003	HEC	CMB-C2B-C3B	3.12	129.49	125.82
3	P	1005	HEC	CBD-CAD-C3D	-3.12	107.30	112.62
3	A	1003	HEC	CBA-CAA-C2A	-3.12	107.35	112.60
3	A	1005	HEC	CMB-C2B-C3B	3.11	129.47	125.82
3	D	1002	HEC	C1D-C2D-C3D	-3.11	104.83	107.00
3	P	1003	HEC	CBD-CAD-C3D	-3.10	107.32	112.62
3	A	1004	HEC	C4C-C3C-C2C	3.10	109.70	106.35
3	A	1001	HEC	CBA-CAA-C2A	-3.09	107.39	112.60
3	D	1004	HEC	C1D-C2D-C3D	-3.09	104.84	107.00
3	I	1003	HEC	CMB-C2B-C3B	3.07	129.43	125.82
3	I	1002	HEC	CBA-CAA-C2A	3.07	117.77	112.60
3	L	1004	HEC	CMC-C2C-C3C	3.06	129.41	125.82
3	O	1002	HEC	CAD-CBD-CGD	-3.05	105.20	113.76
3	H	1002	HEC	CMB-C2B-C1B	-3.04	123.79	128.46
3	F	1002	HEC	C1D-C2D-C3D	-3.04	104.88	107.00
3	B	1005	HEC	CMC-C2C-C1C	-3.02	123.83	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	1004	HEC	C2B-C3B-C4B	3.01	109.61	106.35
3	L	1003	HEC	CMC-C2C-C1C	-3.01	123.83	128.46
3	E	1003	HEC	CBD-CAD-C3D	-3.01	107.48	112.62
3	M	1002	HEC	CMC-C2C-C1C	-3.01	123.84	128.46
3	K	1003	HEC	CMB-C2B-C1B	-3.00	123.86	128.46
3	C	1003	HEC	CMC-C2C-C1C	-3.00	123.86	128.46
3	M	1003	HEC	C4C-C3C-C2C	2.99	109.58	106.35
3	I	1002	HEC	CAA-C2A-C3A	-2.98	118.68	127.25
3	M	1003	HEC	C3C-C4C-NC	-2.98	105.32	110.94
3	L	1003	HEC	C1D-C2D-C3D	-2.97	104.93	107.00
3	H	1002	HEC	CMC-C2C-C1C	-2.96	123.91	128.46
3	N	1003	HEC	CMB-C2B-C1B	-2.96	123.92	128.46
3	Q	1003	HEC	CMC-C2C-C1C	-2.96	123.92	128.46
3	N	1004	HEC	CMC-C2C-C1C	-2.94	123.95	128.46
3	E	1003	HEC	CMC-C2C-C1C	-2.92	123.97	128.46
3	G	1001	HEC	C2B-C3B-C4B	2.92	109.50	106.35
3	G	1005	HEC	CMC-C2C-C1C	-2.92	123.98	128.46
3	M	1001	HEC	C1D-C2D-C3D	-2.92	104.97	107.00
3	B	1002	HEC	CMC-C2C-C1C	-2.91	123.99	128.46
3	D	1003	HEC	CBA-CAA-C2A	-2.91	107.70	112.60
3	Q	1005	HEC	C1D-C2D-C3D	-2.91	104.97	107.00
3	H	1002	HEC	C1D-C2D-C3D	-2.90	104.98	107.00
3	D	1001	HEC	C2B-C3B-C4B	2.90	109.48	106.35
3	C	1004	HEC	C1D-C2D-C3D	-2.89	104.98	107.00
3	C	1001	HEC	C1D-C2D-C3D	-2.89	104.98	107.00
3	O	1003	HEC	C2B-C3B-C4B	2.89	109.47	106.35
3	I	1002	HEC	CBD-CAD-C3D	-2.89	107.69	112.62
3	P	1005	HEC	CMB-C2B-C1B	-2.89	124.03	128.46
3	D	1004	HEC	CMB-C2B-C1B	-2.88	124.03	128.46
3	M	1003	HEC	CMA-C3A-C2A	2.88	130.37	124.94
3	B	1002	HEC	C2B-C3B-C4B	2.88	109.46	106.35
3	E	1002	HEC	C1D-C2D-C3D	-2.87	105.00	107.00
3	M	1004	HEC	CBD-CAD-C3D	-2.87	107.72	112.62
3	G	1005	HEC	CMB-C2B-C3B	2.87	129.19	125.82
3	J	1002	HEC	CMC-C2C-C1C	-2.87	124.06	128.46
3	G	1004	HEC	CMB-C2B-C1B	-2.87	124.06	128.46
3	Q	1004	HEC	CBD-CAD-C3D	-2.86	107.74	112.62
3	R	1003	HEC	C2B-C3B-C4B	2.86	109.44	106.35
3	N	1004	HEC	CMB-C2B-C1B	-2.83	124.11	128.46
3	F	1003	HEC	CBA-CAA-C2A	-2.83	107.83	112.60
3	N	1004	HEC	C1D-C2D-C3D	-2.82	105.04	107.00
3	H	1001	HEC	CMC-C2C-C1C	-2.81	124.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1005	HEC	O2A-CGA-CBA	2.81	123.06	114.03
3	P	1005	HEC	C1D-C2D-C3D	-2.80	105.05	107.00
3	M	1003	HEC	CBD-CAD-C3D	-2.79	107.85	112.62
3	L	1101	HEC	C4C-C3C-C2C	2.79	109.36	106.35
3	Q	1003	HEC	C1D-C2D-C3D	-2.79	105.06	107.00
3	B	1004	HEC	CMC-C2C-C1C	-2.78	124.19	128.46
3	L	1003	HEC	CBD-CAD-C3D	-2.77	107.89	112.62
3	H	1004	HEC	CMC-C2C-C1C	-2.77	124.21	128.46
3	K	1004	HEC	C4C-C3C-C2C	2.76	109.34	106.35
3	H	1004	HEC	CMB-C2B-C1B	-2.76	124.22	128.46
3	G	1003	HEC	C2B-C3B-C4B	2.76	109.33	106.35
3	D	1003	HEC	CMC-C2C-C1C	-2.76	124.23	128.46
5	I	1005	LMT	O1'-C1'-C2'	2.75	112.60	108.30
3	K	1005	HEC	CMC-C2C-C1C	-2.75	124.24	128.46
3	E	1004	HEC	C1D-C2D-C3D	-2.75	105.08	107.00
3	K	1005	HEC	CBA-CAA-C2A	-2.75	107.98	112.60
3	O	1002	HEC	CMB-C2B-C1B	-2.74	124.25	128.46
3	R	1004	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
3	N	1001	HEC	CMC-C2C-C1C	-2.74	124.25	128.46
3	M	1004	HEC	C1D-C2D-C3D	-2.74	105.09	107.00
3	G	1004	HEC	C2B-C3B-C4B	2.73	109.30	106.35
3	O	1001	HEC	C1D-C2D-C3D	-2.72	105.11	107.00
3	Q	1004	HEC	C1D-C2D-C3D	-2.72	105.11	107.00
3	A	1003	HEC	CBD-CAD-C3D	-2.71	107.99	112.62
3	N	1002	HEC	C1D-C2D-C3D	-2.71	105.11	107.00
3	L	1003	HEC	CMB-C2B-C1B	-2.70	124.31	128.46
3	P	1003	HEC	C2B-C3B-C4B	2.69	109.26	106.35
3	I	1004	HEC	CMB-C2B-C1B	-2.68	124.34	128.46
3	C	1003	HEC	CMB-C2B-C1B	-2.68	124.35	128.46
3	M	1004	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
3	I	1002	HEC	O1A-CGA-CBA	-2.67	114.50	123.08
3	A	1004	HEC	C1D-C2D-C3D	-2.67	105.14	107.00
3	D	1002	HEC	CMC-C2C-C3C	2.66	128.95	125.82
3	C	1002	HEC	CAA-C2A-C3A	-2.66	119.61	127.25
3	E	1004	HEC	CMB-C2B-C1B	-2.65	124.39	128.46
3	B	1001	HEC	C3C-C4C-NC	-2.65	105.94	110.94
3	E	1002	HEC	CMB-C2B-C1B	-2.65	124.40	128.46
3	M	1003	HEC	C2B-C3B-C4B	2.64	109.20	106.35
3	J	1004	HEC	C4C-C3C-C2C	2.63	109.19	106.35
3	N	1005	HEC	CMB-C2B-C1B	-2.63	124.42	128.46
3	R	1004	HEC	C1D-C2D-C3D	-2.63	105.17	107.00
3	K	1001	HEC	C4C-C3C-C2C	2.63	109.19	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1004	HEC	CMC-C2C-C3C	2.62	128.90	125.82
3	E	1005	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
3	Q	1002	HEC	C1D-C2D-C3D	-2.62	105.17	107.00
3	K	1004	HEC	C3C-C4C-NC	-2.62	106.00	110.94
3	I	1003	HEC	C2B-C3B-C4B	2.62	109.18	106.35
3	D	1001	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
3	Q	1003	HEC	CMB-C2B-C1B	-2.61	124.45	128.46
3	I	1001	HEC	C1D-C2D-C3D	-2.61	105.18	107.00
3	E	1002	HEC	CMC-C2C-C1C	-2.61	124.45	128.46
3	L	1101	HEC	CMC-C2C-C1C	-2.61	124.45	128.46
3	B	1005	HEC	CMB-C2B-C1B	-2.60	124.46	128.46
3	C	1001	HEC	C2B-C3B-C4B	2.60	109.16	106.35
3	F	1004	HEC	C2B-C3B-C4B	2.60	109.16	106.35
3	H	1005	HEC	CMC-C2C-C1C	-2.60	124.47	128.46
3	C	1004	HEC	CMC-C2C-C3C	2.58	128.86	125.82
5	F	1005	LMT	O1'-C1'-C2'	2.58	112.33	108.30
3	F	1002	HEC	C2B-C3B-C4B	2.58	109.14	106.35
3	J	1002	HEC	CMC-C2C-C3C	2.57	128.84	125.82
3	R	1002	HEC	C1D-C2D-C3D	-2.57	105.21	107.00
3	I	1002	HEC	CMB-C2B-C1B	-2.55	124.54	128.46
3	P	1003	HEC	CBA-CAA-C2A	-2.55	108.30	112.60
3	R	1004	HEC	O1A-CGA-CBA	-2.55	114.89	123.08
3	J	1001	HEC	CMC-C2C-C1C	-2.55	124.55	128.46
5	R	1005	LMT	C3B-C4B-C5B	2.55	114.78	110.24
3	N	1001	HEC	C2B-C3B-C4B	2.55	109.10	106.35
3	N	1005	HEC	CMA-C3A-C2A	2.53	129.71	124.94
3	N	1002	HEC	C2B-C3B-C4B	2.53	109.08	106.35
3	R	1002	HEC	O2A-CGA-CBA	2.52	122.13	114.03
3	D	1002	HEC	CMB-C2B-C1B	-2.50	124.61	128.46
3	E	1001	HEC	C4C-C3C-C2C	2.50	109.05	106.35
3	R	1002	HEC	O1D-CGD-CBD	-2.50	115.06	123.08
3	N	1002	HEC	CBA-CAA-C2A	-2.49	108.41	112.60
3	E	1003	HEC	C2B-C3B-C4B	2.49	109.04	106.35
3	A	1001	HEC	C4C-C3C-C2C	2.48	109.03	106.35
3	Q	1002	HEC	CMB-C2B-C1B	-2.48	124.66	128.46
3	F	1003	HEC	C2B-C3B-C4B	2.47	109.02	106.35
5	I	1005	LMT	C1-O1'-C1'	-2.47	109.74	113.84
3	P	1004	HEC	CMB-C2B-C1B	-2.47	124.66	128.46
3	O	1003	HEC	CBD-CAD-C3D	-2.47	108.40	112.62
3	A	1005	HEC	CMA-C3A-C2A	2.47	129.60	124.94
3	J	1005	HEC	CMB-C2B-C1B	-2.47	124.67	128.46
3	F	1004	HEC	CMC-C2C-C1C	-2.47	124.67	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1004	HEC	CMC-C2C-C1C	-2.46	124.68	128.46
3	B	1003	HEC	CBD-CAD-C3D	-2.46	108.42	112.62
3	B	1001	HEC	C4C-C3C-C2C	2.46	109.01	106.35
3	D	1004	HEC	C4C-C3C-C2C	2.46	109.01	106.35
3	K	1001	HEC	C3C-C4C-NC	-2.45	106.31	110.94
3	J	1001	HEC	CMB-C2B-C1B	-2.45	124.70	128.46
3	D	1004	HEC	CAA-CBA-CGA	2.45	120.62	113.76
3	I	1001	HEC	CAA-CBA-CGA	-2.45	106.90	113.76
3	D	1005	HEC	CMC-C2C-C1C	-2.44	124.71	128.46
5	R	1005	LMT	C1-O1'-C1'	-2.43	109.81	113.84
3	J	1004	HEC	C2B-C3B-C4B	2.43	108.98	106.35
3	P	1003	HEC	CMC-C2C-C1C	-2.43	124.73	128.46
3	G	1004	HEC	C3B-C4B-NB	-2.43	106.36	110.94
3	B	1004	HEC	C4C-C3C-C2C	2.42	108.97	106.35
3	I	1001	HEC	CAD-CBD-CGD	-2.42	106.98	113.76
3	L	1002	HEC	C3B-C4B-NB	-2.42	106.38	110.94
3	A	1003	HEC	C1D-C2D-C3D	-2.41	105.32	107.00
3	J	1004	HEC	C1D-C2D-C3D	-2.41	105.32	107.00
3	R	1001	HEC	CBA-CAA-C2A	-2.41	108.54	112.60
3	R	1001	HEC	CMC-C2C-C1C	-2.41	124.77	128.46
3	J	1002	HEC	C4C-C3C-C2C	2.40	108.95	106.35
3	H	1005	HEC	CMB-C2B-C3B	2.40	128.65	125.82
3	L	1002	HEC	CMC-C2C-C1C	-2.40	124.77	128.46
3	R	1002	HEC	O1A-CGA-CBA	-2.40	115.37	123.08
3	J	1004	HEC	C3B-C4B-NB	-2.40	106.42	110.94
3	O	1004	HEC	CMC-C2C-C1C	-2.40	124.78	128.46
3	P	1005	HEC	O2A-CGA-CBA	2.39	121.72	114.03
3	O	1003	HEC	CMB-C2B-C1B	-2.39	124.78	128.46
3	F	1003	HEC	CMB-C2B-C1B	-2.39	124.79	128.46
3	D	1004	HEC	C3B-C4B-NB	-2.39	106.43	110.94
3	C	1001	HEC	CAD-CBD-CGD	-2.39	107.07	113.76
3	A	1003	HEC	CMC-C2C-C1C	-2.38	124.80	128.46
3	E	1001	HEC	C3C-C4C-NC	-2.38	106.45	110.94
3	I	1004	HEC	CAD-CBD-CGD	-2.38	107.09	113.76
3	L	1004	HEC	CBD-CAD-C3D	-2.36	108.59	112.62
3	N	1003	HEC	CMB-C2B-C3B	2.36	128.60	125.82
3	P	1003	HEC	CMB-C2B-C1B	-2.36	124.84	128.46
3	F	1001	HEC	C4C-C3C-C2C	2.36	108.90	106.35
3	A	1002	HEC	CMB-C2B-C3B	2.35	128.59	125.82
3	B	1003	HEC	CBA-CAA-C2A	-2.35	108.64	112.60
3	A	1001	HEC	CMB-C2B-C1B	-2.35	124.86	128.46
3	I	1004	HEC	C1D-C2D-C3D	-2.34	105.37	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1004	HEC	CMA-C3A-C2A	2.34	129.35	124.94
3	H	1001	HEC	CMB-C2B-C1B	-2.34	124.88	128.46
3	H	1004	HEC	C3C-C4C-NC	-2.33	106.54	110.94
3	D	1001	HEC	C4C-C3C-C2C	2.33	108.87	106.35
3	K	1004	HEC	C2B-C3B-C4B	2.33	108.87	106.35
3	D	1005	HEC	CMB-C2B-C1B	-2.33	124.89	128.46
3	K	1004	HEC	C3B-C4B-NB	-2.33	106.55	110.94
3	G	1002	HEC	CMC-C2C-C1C	-2.32	124.89	128.46
3	K	1004	HEC	CMB-C2B-C1B	-2.31	124.91	128.46
3	J	1002	HEC	CMB-C2B-C3B	2.31	128.54	125.82
3	G	1005	HEC	CBD-CAD-C3D	-2.31	108.68	112.62
3	H	1005	HEC	CBD-CAD-C3D	-2.31	108.68	112.62
3	F	1002	HEC	O2A-CGA-CBA	2.31	121.44	114.03
3	Q	1004	HEC	C3C-C4C-NC	-2.31	106.59	110.94
3	E	1004	HEC	C4C-C3C-C2C	2.31	108.84	106.35
3	H	1004	HEC	C4C-C3C-C2C	2.30	108.84	106.35
3	K	1005	HEC	C3C-C4C-NC	-2.30	106.59	110.94
3	M	1004	HEC	C4C-C3C-C2C	2.30	108.84	106.35
3	B	1005	HEC	CBA-CAA-C2A	-2.30	108.73	112.60
3	L	1003	HEC	O2A-CGA-CBA	2.30	121.41	114.03
3	B	1001	HEC	CBD-CAD-C3D	-2.29	108.71	112.62
3	G	1001	HEC	C1D-C2D-C3D	-2.29	105.40	107.00
3	N	1003	HEC	CMA-C3A-C2A	2.29	129.25	124.94
3	A	1003	HEC	CMB-C2B-C1B	-2.28	124.96	128.46
3	F	1002	HEC	CMC-C2C-C1C	-2.28	124.96	128.46
3	C	1004	HEC	CAD-CBD-CGD	-2.28	107.37	113.76
3	F	1003	HEC	O2A-CGA-CBA	2.28	121.35	114.03
3	D	1005	HEC	CBA-CAA-C2A	-2.28	108.76	112.60
3	Q	1004	HEC	CMB-C2B-C1B	-2.28	124.96	128.46
3	B	1001	HEC	C2B-C3B-C4B	2.28	108.81	106.35
3	O	1003	HEC	CMB-C2B-C3B	2.28	128.50	125.82
3	P	1004	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
3	L	1002	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
3	O	1001	HEC	O1D-CGD-CBD	-2.27	115.80	123.08
3	N	1003	HEC	CMC-C2C-C1C	-2.27	124.98	128.46
3	J	1002	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
3	D	1001	HEC	C3B-C4B-NB	-2.27	106.67	110.94
3	H	1003	HEC	C2B-C3B-C4B	2.26	108.80	106.35
3	L	1002	HEC	CBD-CAD-C3D	-2.26	108.76	112.62
3	R	1002	HEC	C2B-C3B-C4B	2.26	108.79	106.35
3	P	1001	HEC	CMB-C2B-C1B	-2.26	124.99	128.46
3	F	1003	HEC	C3C-C4C-NC	-2.25	106.69	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1005	HEC	CMC-C2C-C3C	2.25	128.47	125.82
3	I	1001	HEC	CMC-C2C-C1C	-2.25	125.01	128.46
3	L	1101	HEC	C3C-C4C-NC	-2.24	106.71	110.94
3	B	1003	HEC	CMB-C2B-C1B	-2.24	125.02	128.46
5	C	1005	LMT	C1'-O5'-C5'	2.24	118.08	113.69
3	Q	1003	HEC	C3B-C4B-NB	-2.24	106.72	110.94
3	K	1005	HEC	CMB-C2B-C1B	-2.24	125.03	128.46
3	R	1003	HEC	CMB-C2B-C1B	-2.24	125.03	128.46
3	N	1005	HEC	CBA-CAA-C2A	-2.24	108.84	112.60
3	A	1002	HEC	C4C-C3C-C2C	2.24	108.77	106.35
3	J	1003	HEC	C1D-C2D-C3D	-2.23	105.44	107.00
3	L	1004	HEC	C1D-C2D-C3D	-2.23	105.44	107.00
3	L	1101	HEC	CAA-CBA-CGA	-2.23	107.51	113.76
3	O	1002	HEC	CMB-C2B-C3B	2.23	128.44	125.82
3	B	1001	HEC	C3B-C4B-NB	-2.23	106.74	110.94
3	G	1001	HEC	C3B-C4B-NB	-2.22	106.75	110.94
3	M	1001	HEC	C4C-C3C-C2C	2.22	108.75	106.35
3	Q	1004	HEC	C4C-C3C-C2C	2.22	108.75	106.35
3	L	1003	HEC	C2B-C3B-C4B	2.22	108.75	106.35
3	B	1004	HEC	C3C-C4C-NC	-2.22	106.76	110.94
3	N	1002	HEC	C3B-C4B-NB	-2.21	106.76	110.94
3	R	1003	HEC	CMB-C2B-C3B	2.21	128.42	125.82
3	A	1005	HEC	O2A-CGA-CBA	2.21	121.14	114.03
3	R	1003	HEC	O2A-CGA-CBA	2.21	121.13	114.03
3	L	1101	HEC	CMB-C2B-C1B	-2.20	125.08	128.46
3	D	1001	HEC	CMB-C2B-C3B	2.20	128.41	125.82
3	L	1002	HEC	CAA-C2A-C3A	-2.20	120.92	127.25
3	N	1005	HEC	CAD-CBD-CGD	-2.20	107.60	113.76
3	R	1003	HEC	CMC-C2C-C1C	-2.20	125.09	128.46
3	H	1003	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
3	Q	1004	HEC	CMC-C2C-C1C	-2.20	125.09	128.46
3	C	1002	HEC	O2A-CGA-CBA	2.19	121.08	114.03
3	K	1003	HEC	CBD-CAD-C3D	-2.19	108.88	112.62
3	E	1003	HEC	C3B-C4B-NB	-2.19	106.81	110.94
3	A	1002	HEC	CMC-C2C-C1C	-2.18	125.11	128.46
3	K	1004	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
3	F	1001	HEC	O1D-CGD-CBD	-2.18	116.08	123.08
3	B	1002	HEC	C3B-C4B-NB	-2.18	106.84	110.94
3	C	1003	HEC	CMB-C2B-C3B	2.17	128.38	125.82
3	R	1001	HEC	C4C-C3C-C2C	2.17	108.69	106.35
3	P	1002	HEC	CMB-C2B-C3B	2.17	128.37	125.82
3	A	1003	HEC	C2B-C3B-C4B	2.17	108.69	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1004	HEC	CAD-CBD-CGD	-2.17	107.68	113.76
3	C	1002	HEC	CBA-CAA-C2A	2.17	116.25	112.60
3	C	1004	HEC	C2B-C3B-C4B	2.16	108.69	106.35
3	P	1004	HEC	CAD-CBD-CGD	-2.16	107.69	113.76
3	C	1003	HEC	O2A-CGA-CBA	2.16	120.98	114.03
3	M	1001	HEC	CMC-C2C-C1C	-2.16	125.14	128.46
3	I	1004	HEC	C2B-C3B-C4B	2.16	108.69	106.35
3	F	1002	HEC	C4C-C3C-C2C	2.16	108.68	106.35
3	F	1003	HEC	CMC-C2C-C1C	-2.16	125.15	128.46
3	O	1001	HEC	CMB-C2B-C1B	-2.15	125.15	128.46
3	G	1005	HEC	C3C-C4C-NC	-2.15	106.88	110.94
3	P	1004	HEC	C4C-C3C-C2C	2.15	108.68	106.35
3	E	1004	HEC	C3C-C4C-NC	-2.15	106.88	110.94
3	D	1004	HEC	C2B-C3B-C4B	2.15	108.67	106.35
3	I	1003	HEC	C3B-C4B-NB	-2.14	106.90	110.94
3	Q	1005	HEC	O1A-CGA-CBA	-2.14	116.20	123.08
3	R	1004	HEC	C2B-C3B-C4B	2.14	108.67	106.35
5	L	1005	LMT	C1'-O5'-C5'	2.14	117.89	113.69
3	G	1004	HEC	C4C-C3C-C2C	2.14	108.66	106.35
3	B	1002	HEC	CBA-CAA-C2A	-2.14	109.00	112.60
3	F	1003	HEC	C4C-C3C-C2C	2.14	108.66	106.35
3	I	1001	HEC	C2B-C3B-C4B	2.14	108.66	106.35
3	C	1002	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
3	A	1004	HEC	C3C-C4C-NC	-2.13	106.92	110.94
3	F	1004	HEC	CMB-C2B-C1B	-2.12	125.20	128.46
3	K	1005	HEC	C4C-C3C-C2C	2.12	108.64	106.35
3	K	1003	HEC	CMC-C2C-C1C	-2.12	125.20	128.46
3	F	1003	HEC	CMB-C2B-C3B	2.12	128.31	125.82
3	A	1003	HEC	C3C-C4C-NC	-2.12	106.95	110.94
3	I	1003	HEC	CMC-C2C-C3C	2.12	128.31	125.82
3	R	1001	HEC	O2A-CGA-CBA	2.11	120.82	114.03
3	G	1002	HEC	CMB-C2B-C1B	-2.11	125.22	128.46
3	F	1002	HEC	O1A-CGA-CBA	-2.11	116.29	123.08
3	D	1003	HEC	C3C-C4C-NC	-2.11	106.96	110.94
3	H	1003	HEC	C3B-C4B-NB	-2.11	106.96	110.94
3	O	1003	HEC	CMC-C2C-C1C	-2.11	125.22	128.46
3	Q	1002	HEC	CMC-C2C-C1C	-2.10	125.24	128.46
3	J	1001	HEC	C2B-C3B-C4B	2.10	108.62	106.35
3	M	1002	HEC	CMB-C2B-C1B	-2.10	125.24	128.46
3	H	1001	HEC	O2A-CGA-CBA	2.10	120.76	114.03
3	J	1005	HEC	C2B-C3B-C4B	2.09	108.61	106.35
3	I	1004	HEC	CMB-C2B-C3B	2.09	128.28	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1002	HEC	C2B-C3B-C4B	2.09	108.61	106.35
3	J	1005	HEC	CMB-C2B-C3B	2.09	128.28	125.82
3	N	1004	HEC	C3B-C4B-NB	-2.09	107.00	110.94
3	R	1004	HEC	O2D-CGD-CBD	2.09	120.74	114.03
3	C	1003	HEC	C2B-C3B-C4B	2.09	108.61	106.35
3	E	1002	HEC	CMB-C2B-C3B	2.09	128.27	125.82
3	O	1004	HEC	CMA-C3A-C2A	2.09	128.88	124.94
3	O	1002	HEC	O1A-CGA-CBA	-2.08	116.39	123.08
3	F	1001	HEC	O2D-CGD-CBD	2.08	120.72	114.03
3	C	1002	HEC	CMC-C2C-C1C	-2.08	125.26	128.46
3	C	1002	HEC	CAD-CBD-CGD	-2.08	107.92	113.76
3	N	1003	HEC	C2B-C3B-C4B	2.08	108.60	106.35
3	O	1002	HEC	C2B-C3B-C4B	2.08	108.60	106.35
3	O	1002	HEC	CMC-C2C-C1C	-2.08	125.27	128.46
3	N	1004	HEC	CBD-CAD-C3D	-2.08	109.07	112.62
3	A	1003	HEC	C4C-C3C-C2C	2.08	108.60	106.35
3	H	1004	HEC	CMB-C2B-C3B	2.08	128.26	125.82
3	C	1002	HEC	O1A-CGA-CBA	-2.08	116.40	123.08
3	F	1002	HEC	C3B-C4B-NB	-2.08	107.02	110.94
3	B	1002	HEC	C1D-C2D-C3D	-2.07	105.55	107.00
3	M	1003	HEC	C3B-C4B-NB	-2.07	107.03	110.94
3	F	1002	HEC	O1D-CGD-CBD	-2.07	116.42	123.08
3	A	1001	HEC	CBD-CAD-C3D	-2.07	109.08	112.62
3	C	1002	HEC	C2B-C3B-C4B	2.07	108.59	106.35
3	F	1002	HEC	C3C-C4C-NC	-2.07	107.03	110.94
3	G	1004	HEC	C3C-C4C-NC	-2.07	107.04	110.94
3	P	1005	HEC	CMB-C2B-C3B	2.07	128.25	125.82
3	Q	1001	HEC	CMB-C2B-C1B	-2.07	125.28	128.46
3	P	1004	HEC	C3B-C4B-NB	-2.07	107.04	110.94
5	O	1005	LMT	O5B-C5B-C4B	2.07	113.45	109.69
3	R	1001	HEC	O1A-CGA-CBA	-2.07	116.44	123.08
3	H	1002	HEC	CMC-C2C-C3C	2.07	128.25	125.82
3	K	1002	HEC	C2B-C3B-C4B	2.07	108.58	106.35
3	E	1003	HEC	C1D-C2D-C3D	-2.07	105.56	107.00
3	M	1005	HEC	CMA-C3A-C2A	2.07	128.84	124.94
5	F	1005	LMT	O5B-C5B-C4B	2.06	113.44	109.69
3	Q	1005	HEC	CMB-C2B-C1B	-2.06	125.29	128.46
3	R	1004	HEC	CMB-C2B-C1B	-2.06	125.29	128.46
3	I	1004	HEC	O1D-CGD-CBD	-2.06	116.46	123.08
3	C	1001	HEC	CBD-CAD-C3D	-2.06	109.11	112.62
3	P	1004	HEC	O2A-CGA-CBA	2.06	120.64	114.03
3	I	1003	HEC	CAD-CBD-CGD	-2.05	108.00	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1002	HEC	C3B-C4B-NB	-2.05	107.07	110.94
3	M	1004	HEC	C3B-C4B-NB	-2.05	107.07	110.94
3	F	1004	HEC	CMB-C2B-C3B	2.05	128.22	125.82
3	B	1005	HEC	O2A-CGA-CBA	2.04	120.60	114.03
3	P	1002	HEC	O1A-CGA-CBA	-2.04	116.52	123.08
3	R	1002	HEC	C3B-C4B-NB	-2.04	107.09	110.94
3	N	1005	HEC	O2A-CGA-CBA	2.04	120.59	114.03
3	N	1001	HEC	CMA-C3A-C2A	2.04	128.78	124.94
3	R	1001	HEC	O2D-CGD-CBD	2.04	120.57	114.03
3	P	1002	HEC	C3B-C4B-NB	-2.04	107.10	110.94
3	B	1003	HEC	CMC-C2C-C3C	2.04	128.21	125.82
3	R	1001	HEC	CMB-C2B-C1B	-2.03	125.34	128.46
3	C	1003	HEC	O1A-CGA-CBA	-2.03	116.56	123.08
3	J	1003	HEC	C2B-C3B-C4B	2.02	108.54	106.35
3	C	1003	HEC	O2D-CGD-CBD	2.02	120.53	114.03
3	A	1005	HEC	C1D-C2D-C3D	-2.02	105.59	107.00
3	C	1002	HEC	CMD-C2D-C3D	2.02	128.74	124.94
3	I	1003	HEC	O2A-CGA-CBA	2.01	120.50	114.03
3	R	1002	HEC	CAD-CBD-CGD	-2.01	108.12	113.76
3	P	1003	HEC	C1D-C2D-C3D	-2.01	105.60	107.00
3	E	1003	HEC	C3C-C4C-NC	-2.01	107.15	110.94
3	M	1004	HEC	C3C-C4C-NC	-2.01	107.15	110.94
3	N	1001	HEC	C1D-C2D-C3D	-2.01	105.60	107.00
3	G	1003	HEC	C3C-C4C-NC	-2.01	107.16	110.94
3	L	1003	HEC	CMC-C2C-C3C	2.00	128.17	125.82
3	J	1001	HEC	CMB-C2B-C3B	2.00	128.17	125.82

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1002	HEC	C1A-C2A-CAA-CBA
3	C	1002	HEC	C3A-C2A-CAA-CBA
3	F	1002	HEC	C1A-C2A-CAA-CBA
3	F	1002	HEC	C3A-C2A-CAA-CBA
3	I	1002	HEC	C1A-C2A-CAA-CBA
3	I	1002	HEC	C3A-C2A-CAA-CBA
3	L	1002	HEC	C1A-C2A-CAA-CBA
3	L	1002	HEC	C3A-C2A-CAA-CBA
3	O	1002	HEC	C1A-C2A-CAA-CBA
3	O	1002	HEC	C3A-C2A-CAA-CBA
3	Q	1004	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	Q	1004	HEC	C3A-C2A-CAA-CBA
3	R	1002	HEC	C1A-C2A-CAA-CBA
3	R	1002	HEC	C3A-C2A-CAA-CBA
5	L	1005	LMT	C4-C5-C6-C7
3	E	1005	HEC	C2A-CAA-CBA-CGA
3	N	1005	HEC	C3D-CAD-CBD-CGD
3	Q	1004	HEC	C2A-CAA-CBA-CGA
5	F	1005	LMT	C6-C7-C8-C9
5	L	1005	LMT	C11-C10-C9-C8
5	O	1005	LMT	C6-C7-C8-C9
5	C	1005	LMT	C6-C7-C8-C9
5	F	1005	LMT	C11-C10-C9-C8
5	L	1005	LMT	C3-C4-C5-C6
5	L	1005	LMT	C6-C7-C8-C9
5	R	1005	LMT	C3-C4-C5-C6
5	C	1005	LMT	C11-C10-C9-C8
5	I	1005	LMT	C5-C6-C7-C8
5	R	1005	LMT	C6-C7-C8-C9
5	L	1005	LMT	C7-C8-C9-C10
5	R	1005	LMT	C7-C8-C9-C10
5	I	1005	LMT	C6-C7-C8-C9
5	O	1005	LMT	C3-C4-C5-C6
5	R	1005	LMT	C1-C2-C3-C4
5	O	1005	LMT	C11-C10-C9-C8
5	C	1005	LMT	C7-C8-C9-C10
5	I	1005	LMT	C2-C3-C4-C5
5	O	1005	LMT	C1-C2-C3-C4
5	F	1005	LMT	C3-C4-C5-C6
5	C	1005	LMT	C4-C5-C6-C7
5	L	1005	LMT	C5-C6-C7-C8
5	F	1005	LMT	C1-C2-C3-C4
5	O	1005	LMT	C4-C5-C6-C7
5	I	1005	LMT	C7-C8-C9-C10
5	L	1005	LMT	O1'-C1-C2-C3
5	R	1005	LMT	C5-C6-C7-C8
5	L	1005	LMT	C1-C2-C3-C4
5	I	1005	LMT	C3-C4-C5-C6
5	R	1005	LMT	C9-C10-C11-C12
5	R	1005	LMT	O1'-C1-C2-C3
5	C	1005	LMT	C3-C4-C5-C6
5	I	1005	LMT	C1-C2-C3-C4
5	C	1005	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	Q	1005	HEC	C2A-CAA-CBA-CGA
5	O	1005	LMT	C4B-C5B-C6B-O6B
5	F	1005	LMT	O1'-C1-C2-C3
3	C	1001	HEC	C3D-CAD-CBD-CGD
3	G	1002	HEC	C3D-CAD-CBD-CGD
3	I	1002	HEC	C3D-CAD-CBD-CGD
3	A	1003	HEC	C2D-C3D-CAD-CBD
3	A	1003	HEC	C4D-C3D-CAD-CBD
3	G	1002	HEC	C2D-C3D-CAD-CBD
3	R	1001	HEC	C2D-C3D-CAD-CBD
5	O	1005	LMT	C2-C3-C4-C5
5	F	1005	LMT	C4'-C5'-C6'-O6'
3	P	1004	HEC	C2A-CAA-CBA-CGA
5	F	1005	LMT	C7-C8-C9-C10
3	H	1002	HEC	CAA-CBA-CGA-O2A
3	M	1002	HEC	CAA-CBA-CGA-O1A
3	O	1003	HEC	CAA-CBA-CGA-O1A
3	I	1001	HEC	CAD-CBD-CGD-O1D
3	D	1004	HEC	CAA-CBA-CGA-O2A
3	B	1002	HEC	CAA-CBA-CGA-O1A
3	G	1002	HEC	CAA-CBA-CGA-O1A
3	K	1004	HEC	CAA-CBA-CGA-O1A
3	D	1005	HEC	C3D-CAD-CBD-CGD
3	E	1004	HEC	C2A-CAA-CBA-CGA
3	K	1003	HEC	C2A-CAA-CBA-CGA
3	L	1002	HEC	CAD-CBD-CGD-O2D
3	O	1001	HEC	CAA-CBA-CGA-O1A
3	O	1001	HEC	CAA-CBA-CGA-O2A
3	Q	1002	HEC	CAA-CBA-CGA-O1A
5	C	1005	LMT	C5-C6-C7-C8
3	E	1002	HEC	CAA-CBA-CGA-O1A
3	H	1002	HEC	CAA-CBA-CGA-O1A
3	J	1004	HEC	CAA-CBA-CGA-O1A
3	A	1002	HEC	CAA-CBA-CGA-O1A
3	C	1001	HEC	CAA-CBA-CGA-O2A
3	N	1002	HEC	CAA-CBA-CGA-O1A
3	A	1004	HEC	CAA-CBA-CGA-O1A
3	B	1004	HEC	CAA-CBA-CGA-O1A
3	D	1004	HEC	CAA-CBA-CGA-O1A
3	E	1002	HEC	CAA-CBA-CGA-O2A
3	F	1004	HEC	CAA-CBA-CGA-O2A
3	H	1004	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	I	1003	HEC	CAA-CBA-CGA-O1A
3	M	1001	HEC	CAA-CBA-CGA-O1A
3	O	1003	HEC	CAA-CBA-CGA-O2A
3	Q	1001	HEC	CAA-CBA-CGA-O1A
3	G	1001	HEC	CAA-CBA-CGA-O1A
3	K	1002	HEC	CAA-CBA-CGA-O1A
3	A	1004	HEC	CAA-CBA-CGA-O2A
3	B	1001	HEC	CAA-CBA-CGA-O1A
3	B	1004	HEC	CAA-CBA-CGA-O2A
3	C	1001	HEC	CAD-CBD-CGD-O1D
3	D	1005	HEC	CAA-CBA-CGA-O1A
3	H	1001	HEC	CAA-CBA-CGA-O1A
3	M	1002	HEC	CAA-CBA-CGA-O2A
3	N	1002	HEC	CAA-CBA-CGA-O2A
3	G	1001	HEC	CAA-CBA-CGA-O2A
3	L	1002	HEC	CAD-CBD-CGD-O1D
3	N	1001	HEC	CAA-CBA-CGA-O1A
5	L	1005	LMT	C9-C10-C11-C12
3	D	1002	HEC	CAA-CBA-CGA-O1A
3	K	1004	HEC	CAA-CBA-CGA-O2A
3	D	1001	HEC	CAA-CBA-CGA-O2A
3	Q	1002	HEC	CAA-CBA-CGA-O2A
3	R	1001	HEC	CAA-CBA-CGA-O1A
3	E	1001	HEC	CAA-CBA-CGA-O1A
3	G	1002	HEC	CAA-CBA-CGA-O2A
3	J	1004	HEC	CAA-CBA-CGA-O2A
3	F	1001	HEC	CAA-CBA-CGA-O2A
3	F	1004	HEC	CAA-CBA-CGA-O1A
3	N	1001	HEC	CAA-CBA-CGA-O2A
3	C	1001	HEC	CAA-CBA-CGA-O1A
3	E	1001	HEC	CAA-CBA-CGA-O2A
3	G	1002	HEC	CAD-CBD-CGD-O1D
3	I	1001	HEC	CAD-CBD-CGD-O2D
3	K	1001	HEC	CAA-CBA-CGA-O1A
3	C	1001	HEC	CAD-CBD-CGD-O2D
3	F	1001	HEC	CAA-CBA-CGA-O1A
3	K	1001	HEC	CAA-CBA-CGA-O2A
3	R	1002	HEC	CAA-CBA-CGA-O2A
3	D	1002	HEC	CAA-CBA-CGA-O2A
3	I	1003	HEC	CAA-CBA-CGA-O2A
3	B	1002	HEC	CAA-CBA-CGA-O2A
3	D	1001	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	1001	HEC	CAA-CBA-CGA-O2A
3	M	1001	HEC	CAA-CBA-CGA-O2A
3	Q	1001	HEC	CAA-CBA-CGA-O2A
3	N	1004	HEC	CAA-CBA-CGA-O1A
3	D	1005	HEC	CAD-CBD-CGD-O2D
3	G	1002	HEC	CAD-CBD-CGD-O2D
3	K	1002	HEC	CAA-CBA-CGA-O2A
3	M	1005	HEC	CAD-CBD-CGD-O2D
3	H	1001	HEC	CAA-CBA-CGA-O2A
3	J	1002	HEC	CAA-CBA-CGA-O1A
3	O	1002	HEC	CAA-CBA-CGA-O2A
3	R	1001	HEC	CAA-CBA-CGA-O2A
3	J	1005	HEC	CAD-CBD-CGD-O1D
3	O	1002	HEC	CAD-CBD-CGD-O2D
3	P	1001	HEC	CAA-CBA-CGA-O2A
3	A	1001	HEC	CAA-CBA-CGA-O2A
3	I	1002	HEC	CAD-CBD-CGD-O2D
3	J	1005	HEC	CAD-CBD-CGD-O2D
3	R	1002	HEC	CAA-CBA-CGA-O1A
3	B	1005	HEC	CAD-CBD-CGD-O2D
3	C	1002	HEC	CAD-CBD-CGD-O2D
3	I	1001	HEC	CAA-CBA-CGA-O2A
3	N	1005	HEC	CAD-CBD-CGD-O2D
3	P	1001	HEC	CAA-CBA-CGA-O1A
3	I	1001	HEC	CAA-CBA-CGA-O1A
3	F	1002	HEC	CAD-CBD-CGD-O2D
3	J	1001	HEC	CAA-CBA-CGA-O2A
3	P	1002	HEC	CAA-CBA-CGA-O1A
3	P	1005	HEC	CAA-CBA-CGA-O1A
3	R	1001	HEC	CAD-CBD-CGD-O2D
5	I	1005	LMT	C9-C10-C11-C12
3	F	1003	HEC	CAA-CBA-CGA-O1A
3	H	1004	HEC	CAA-CBA-CGA-O2A
3	K	1005	HEC	CAD-CBD-CGD-O2D
3	C	1004	HEC	C2A-CAA-CBA-CGA
3	A	1002	HEC	CAA-CBA-CGA-O2A
3	A	1005	HEC	CAD-CBD-CGD-O2D
3	D	1005	HEC	CAA-CBA-CGA-O2A
3	E	1005	HEC	CAD-CBD-CGD-O2D
3	I	1002	HEC	CAD-CBD-CGD-O1D
3	P	1005	HEC	CAD-CBD-CGD-O2D
3	R	1002	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	G	1005	HEC	CAD-CBD-CGD-O2D
3	J	1001	HEC	CAA-CBA-CGA-O1A
3	A	1005	HEC	CAD-CBD-CGD-O1D
3	A	1001	HEC	CAA-CBA-CGA-O1A
3	D	1005	HEC	CAD-CBD-CGD-O1D
3	C	1002	HEC	CAD-CBD-CGD-O1D
3	C	1003	HEC	CAA-CBA-CGA-O1A
3	L	1003	HEC	CAA-CBA-CGA-O1A
3	M	1005	HEC	CAA-CBA-CGA-O1A
3	N	1005	HEC	CAD-CBD-CGD-O1D
3	R	1002	HEC	CAD-CBD-CGD-O1D
5	I	1005	LMT	C4-C5-C6-C7
3	F	1002	HEC	CAD-CBD-CGD-O1D
3	G	1005	HEC	CAD-CBD-CGD-O1D
3	H	1005	HEC	CAD-CBD-CGD-O1D
3	K	1005	HEC	CAD-CBD-CGD-O1D
3	L	1101	HEC	CAA-CBA-CGA-O2A
3	O	1002	HEC	CAD-CBD-CGD-O1D
3	P	1005	HEC	CAD-CBD-CGD-O1D
5	O	1005	LMT	C7-C8-C9-C10
3	B	1005	HEC	CAD-CBD-CGD-O1D
3	C	1004	HEC	CAA-CBA-CGA-O2A
3	E	1005	HEC	CAD-CBD-CGD-O1D
3	H	1005	HEC	CAD-CBD-CGD-O2D
3	M	1005	HEC	CAD-CBD-CGD-O1D
5	R	1005	LMT	C11-C10-C9-C8
3	L	1003	HEC	CAA-CBA-CGA-O2A
3	N	1004	HEC	CAA-CBA-CGA-O2A
3	C	1003	HEC	CAA-CBA-CGA-O2A
3	K	1005	HEC	CAA-CBA-CGA-O1A
3	F	1003	HEC	CAA-CBA-CGA-O2A
3	G	1005	HEC	CAA-CBA-CGA-O1A
3	L	1101	HEC	CAA-CBA-CGA-O1A
3	M	1005	HEC	CAA-CBA-CGA-O2A
3	R	1004	HEC	CAA-CBA-CGA-O1A
3	C	1003	HEC	CAD-CBD-CGD-O2D
3	G	1004	HEC	CAA-CBA-CGA-O1A
3	R	1001	HEC	CAD-CBD-CGD-O1D
3	P	1002	HEC	CAA-CBA-CGA-O2A
3	C	1004	HEC	CAA-CBA-CGA-O1A
3	F	1002	HEC	C3D-CAD-CBD-CGD
3	O	1002	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	P	1005	HEC	CAA-CBA-CGA-O2A
3	C	1004	HEC	CAD-CBD-CGD-O2D
3	G	1005	HEC	CAA-CBA-CGA-O2A
3	Q	1005	HEC	CAD-CBD-CGD-O2D
3	F	1001	HEC	CAD-CBD-CGD-O2D
3	J	1002	HEC	CAA-CBA-CGA-O2A
3	A	1005	HEC	CAA-CBA-CGA-O2A
3	G	1004	HEC	CAA-CBA-CGA-O2A
3	C	1002	HEC	CAA-CBA-CGA-O2A
3	L	1004	HEC	CAD-CBD-CGD-O2D
3	O	1001	HEC	CAD-CBD-CGD-O2D
3	C	1002	HEC	CAA-CBA-CGA-O1A
3	F	1002	HEC	CAA-CBA-CGA-O2A
3	K	1005	HEC	CAA-CBA-CGA-O2A
3	R	1004	HEC	CAA-CBA-CGA-O2A
3	C	1003	HEC	CAD-CBD-CGD-O1D
3	O	1001	HEC	CAD-CBD-CGD-O1D
3	Q	1005	HEC	CAD-CBD-CGD-O1D
3	A	1005	HEC	CAA-CBA-CGA-O1A
3	F	1002	HEC	CAA-CBA-CGA-O1A
3	G	1003	HEC	C2A-CAA-CBA-CGA
3	F	1004	HEC	CAD-CBD-CGD-O1D
3	L	1004	HEC	CAD-CBD-CGD-O1D
3	N	1005	HEC	CAA-CBA-CGA-O1A
3	M	1004	HEC	CAA-CBA-CGA-O1A
3	F	1004	HEC	CAD-CBD-CGD-O2D
3	J	1005	HEC	CAA-CBA-CGA-O1A
3	L	1002	HEC	CAA-CBA-CGA-O2A
3	L	1101	HEC	CAD-CBD-CGD-O2D
3	O	1004	HEC	CAA-CBA-CGA-O1A
3	O	1004	HEC	CAD-CBD-CGD-O2D
3	L	1002	HEC	CAA-CBA-CGA-O1A
3	O	1004	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

87 monomers are involved in 617 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1003	HEC	9	0
3	Q	1002	HEC	12	0
3	E	1003	HEC	7	0
3	N	1005	HEC	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1003	HEC	5	0
3	G	1005	HEC	11	0
3	P	1001	HEC	8	0
3	H	1002	HEC	8	0
3	L	1002	HEC	8	0
3	G	1001	HEC	11	0
3	Q	1001	HEC	10	0
3	A	1004	HEC	7	0
3	H	1003	HEC	5	0
3	J	1005	HEC	10	0
3	E	1002	HEC	12	0
3	N	1001	HEC	8	0
3	N	1002	HEC	8	0
3	F	1001	HEC	5	0
3	R	1003	HEC	6	0
3	A	1003	HEC	4	0
3	B	1001	HEC	5	0
3	D	1001	HEC	5	0
3	P	1003	HEC	6	0
3	K	1004	HEC	9	0
3	M	1004	HEC	9	0
3	H	1005	HEC	9	0
3	E	1001	HEC	8	0
3	P	1002	HEC	12	0
3	C	1003	HEC	4	0
3	H	1001	HEC	10	0
3	R	1004	HEC	5	0
3	A	1002	HEC	12	0
3	G	1003	HEC	2	0
3	B	1005	HEC	4	0
3	J	1004	HEC	10	0
3	D	1002	HEC	11	0
3	I	1001	HEC	2	0
5	I	1005	LMT	3	0
3	K	1005	HEC	4	0
3	I	1002	HEC	5	0
3	C	1002	HEC	5	0
3	C	1004	HEC	9	0
3	K	1002	HEC	11	0
3	H	1004	HEC	8	0
3	I	1003	HEC	4	0
3	O	1004	HEC	9	0

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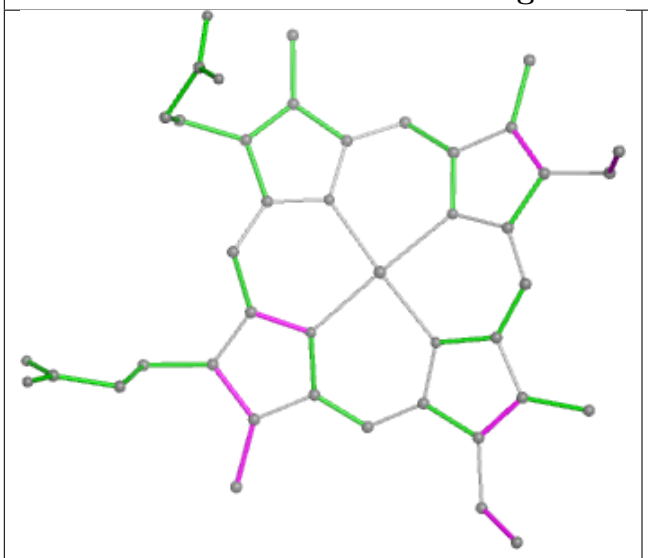
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1001	HEC	9	0
3	M	1001	HEC	4	0
5	C	1005	LMT	2	0
3	A	1005	HEC	10	0
5	L	1005	LMT	3	0
3	Q	1005	HEC	13	0
3	J	1002	HEC	6	0
3	O	1003	HEC	5	0
3	Q	1003	HEC	9	0
3	B	1002	HEC	6	0
3	O	1002	HEC	7	0
3	L	1004	HEC	8	0
3	R	1001	HEC	4	0
3	M	1003	HEC	8	0
3	E	1004	HEC	5	0
3	J	1001	HEC	5	0
3	N	1003	HEC	6	0
3	E	1005	HEC	8	0
3	M	1005	HEC	12	0
3	F	1002	HEC	12	0
3	K	1003	HEC	10	0
3	L	1101	HEC	1	0
3	P	1004	HEC	8	0
3	C	1001	HEC	3	0
3	B	1003	HEC	8	0
3	R	1002	HEC	11	0
3	P	1005	HEC	7	0
3	O	1001	HEC	2	0
3	G	1004	HEC	11	0
3	Q	1004	HEC	8	0
3	A	1001	HEC	5	0
3	J	1003	HEC	8	0
3	G	1002	HEC	9	0
3	N	1004	HEC	9	0
3	F	1004	HEC	8	0
3	I	1004	HEC	8	0
3	B	1004	HEC	7	0
3	D	1004	HEC	10	0
3	M	1002	HEC	11	0
3	F	1003	HEC	4	0
3	D	1005	HEC	9	0

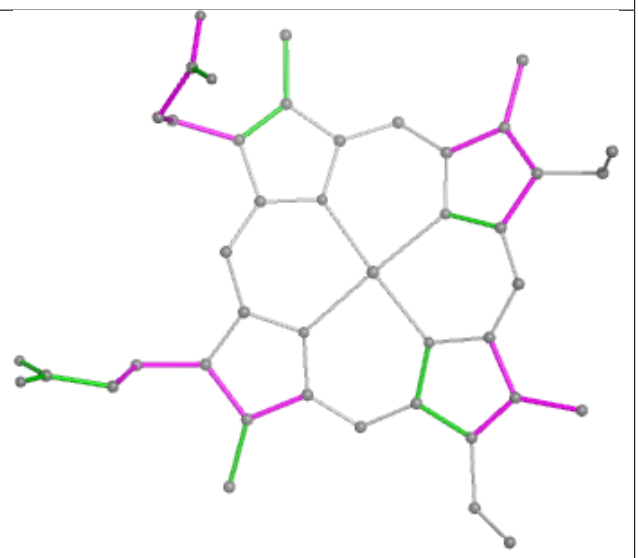
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

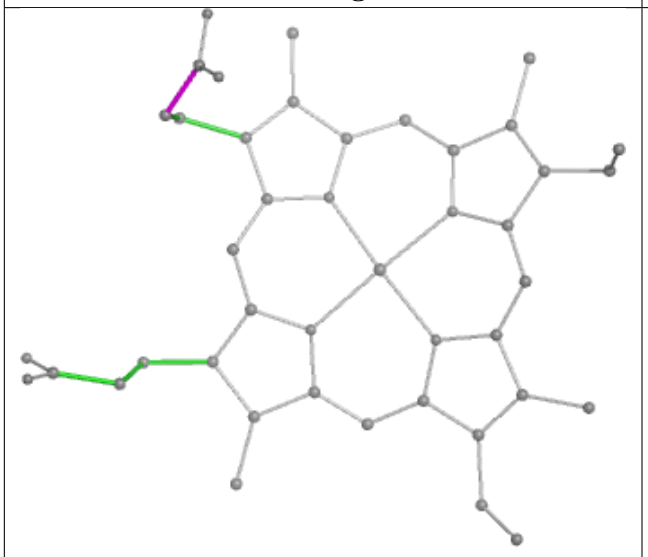
Ligand HEC L 1003



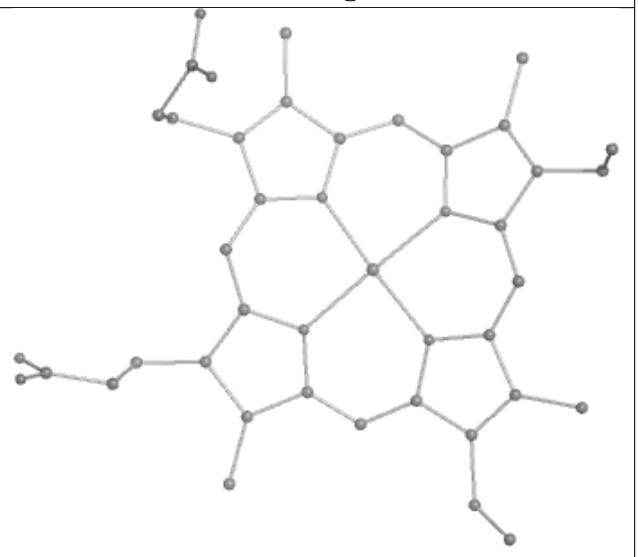
Bond lengths



Bond angles

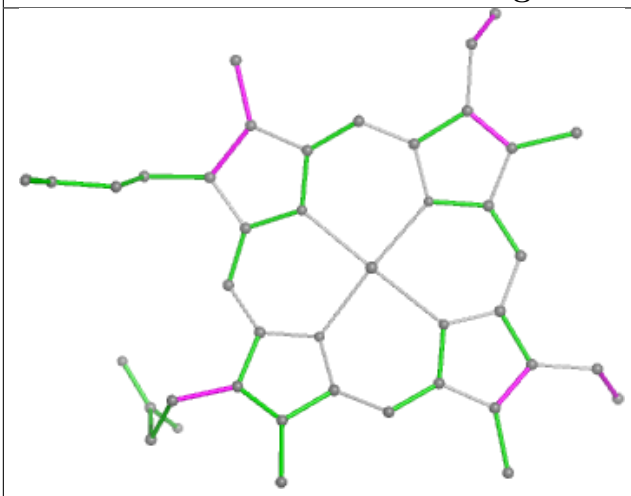


Torsions

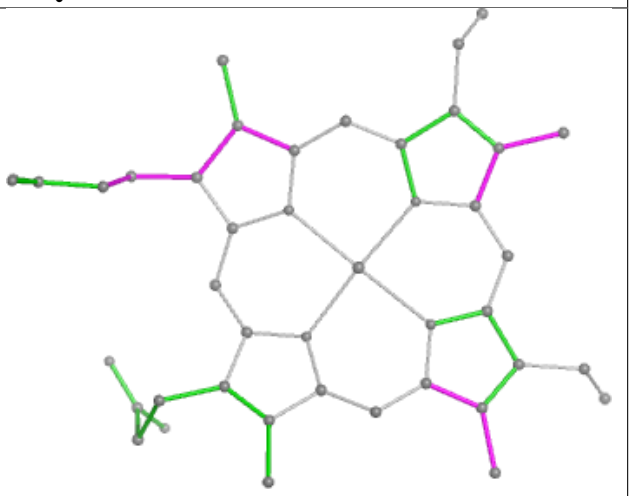


Rings

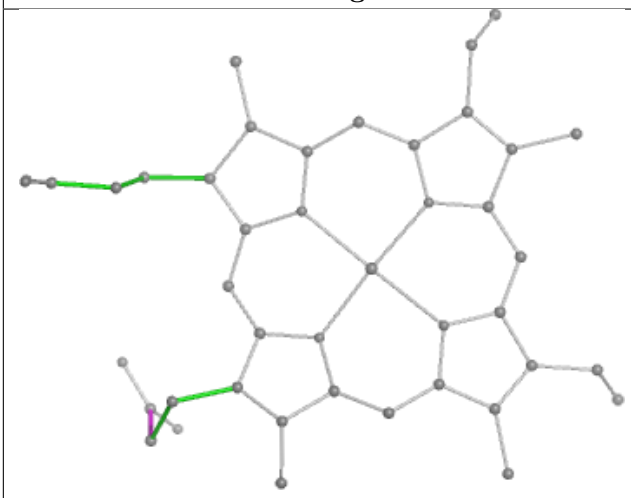
Ligand HEC Q 1002



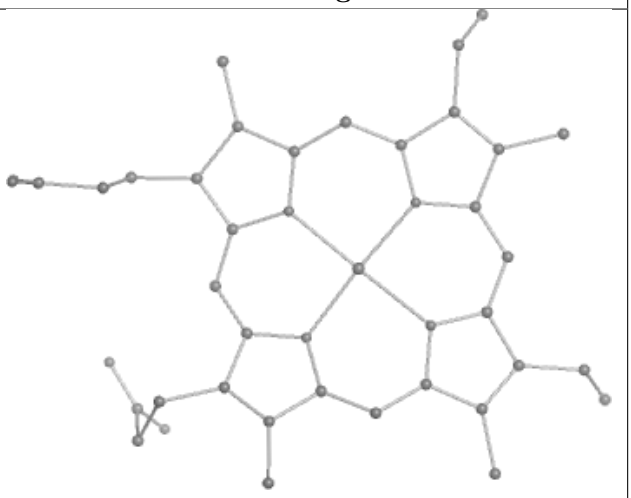
Bond lengths



Bond angles

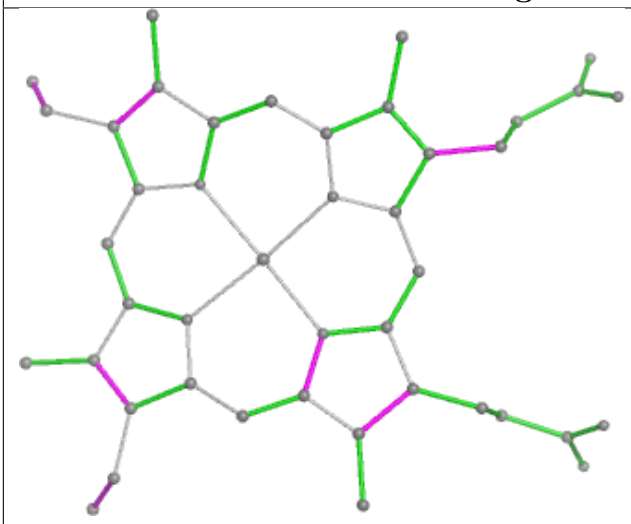


Torsions

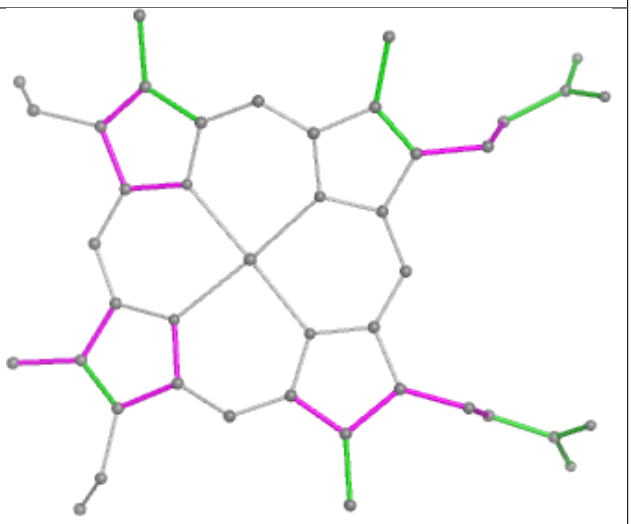


Rings

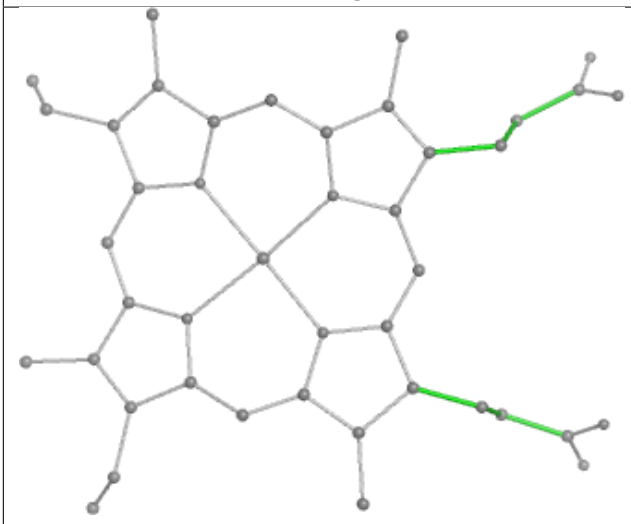
Ligand HEC E 1003



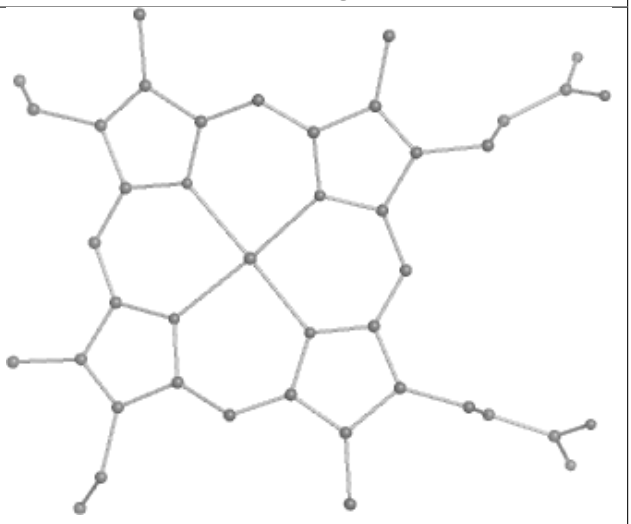
Bond lengths



Bond angles

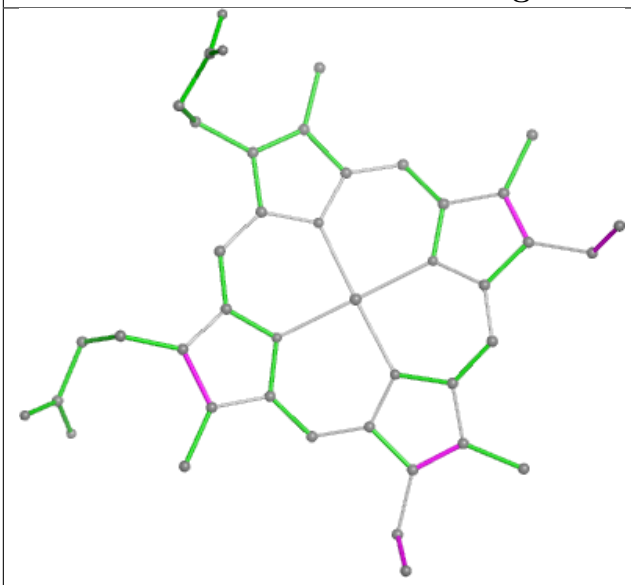


Torsions

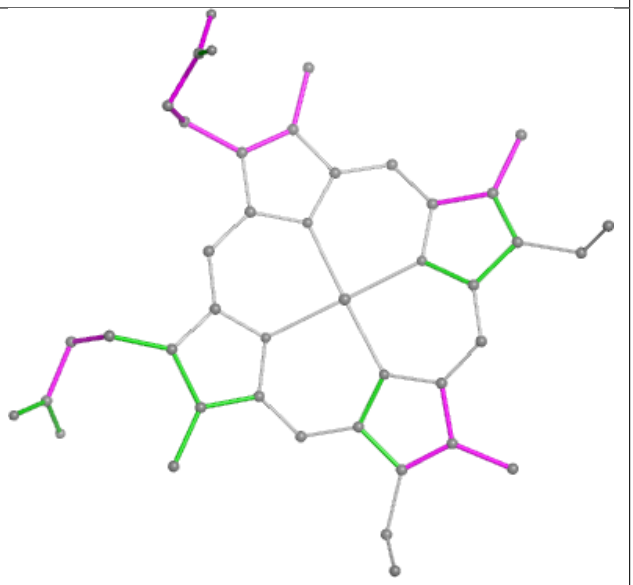


Rings

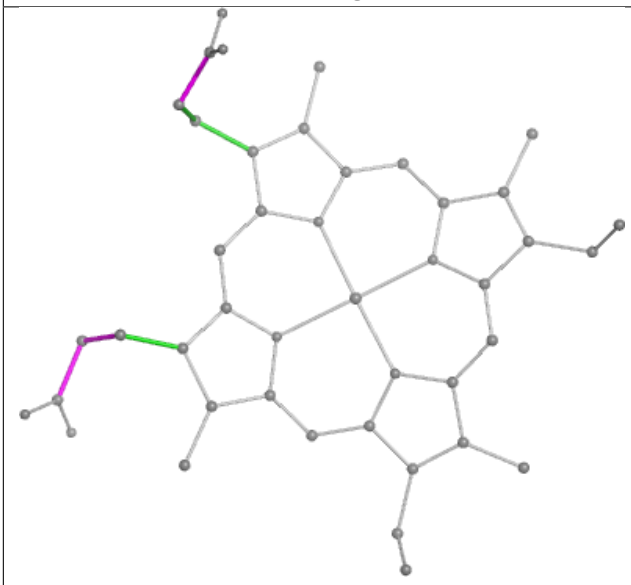
Ligand HEC N 1005



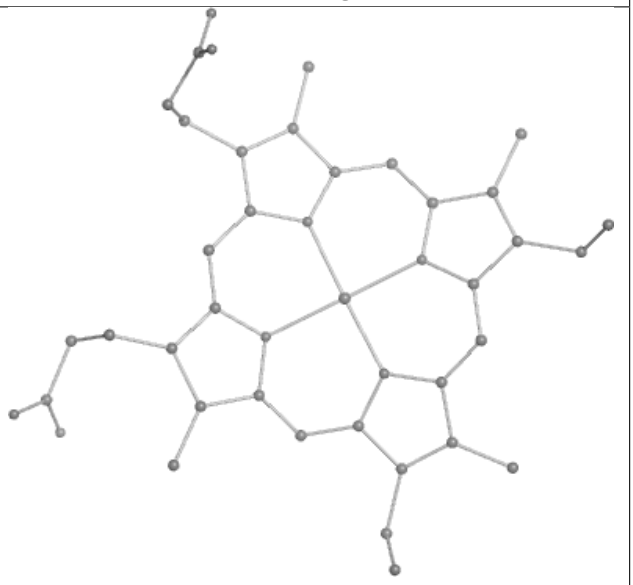
Bond lengths



Bond angles

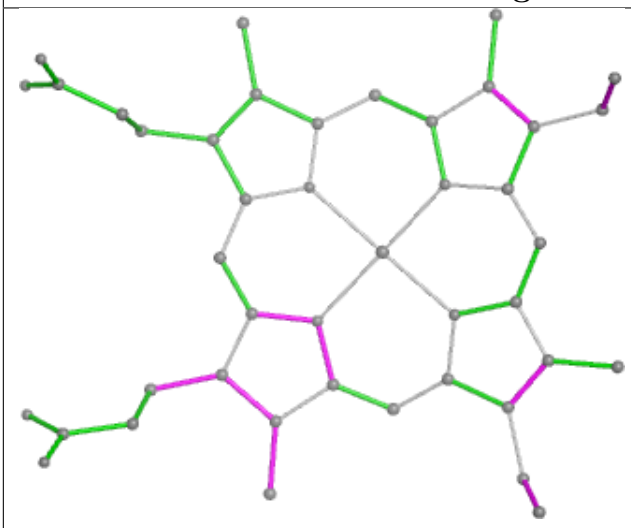


Torsions

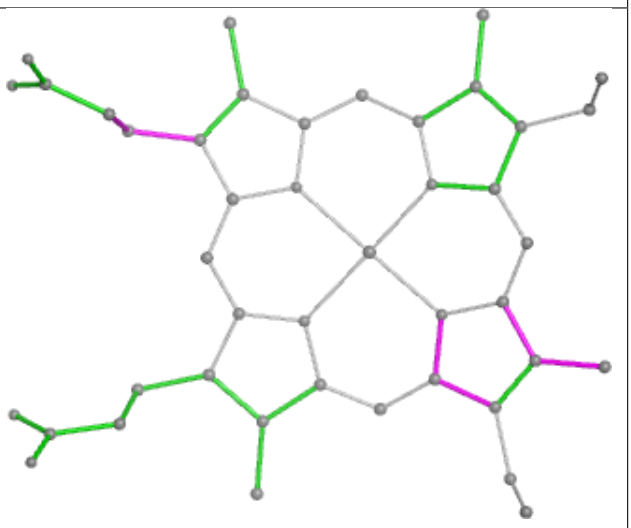


Rings

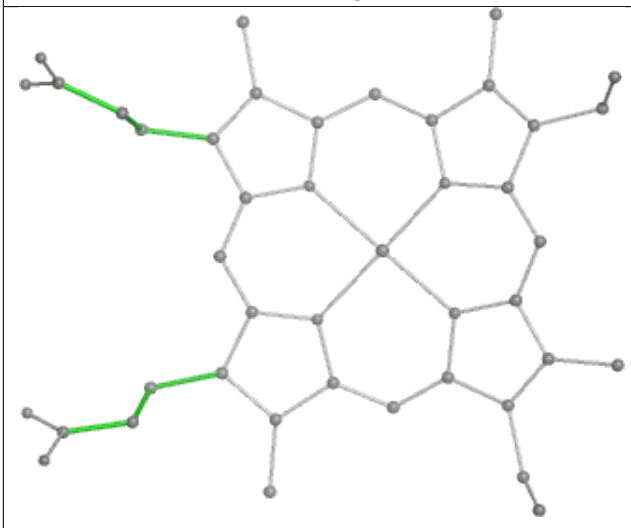
Ligand HEC D 1003



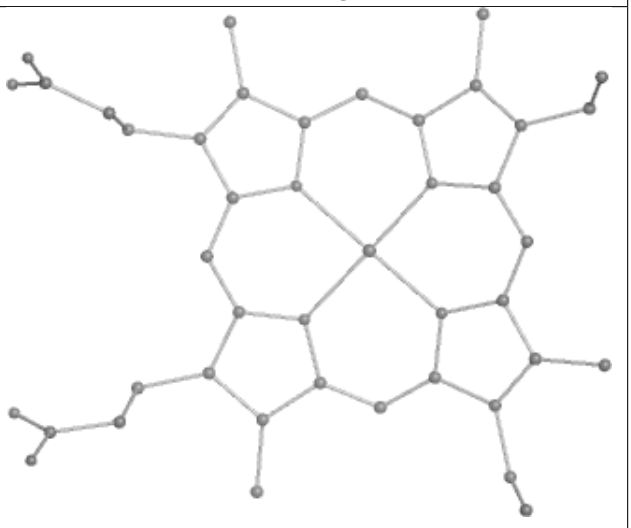
Bond lengths



Bond angles

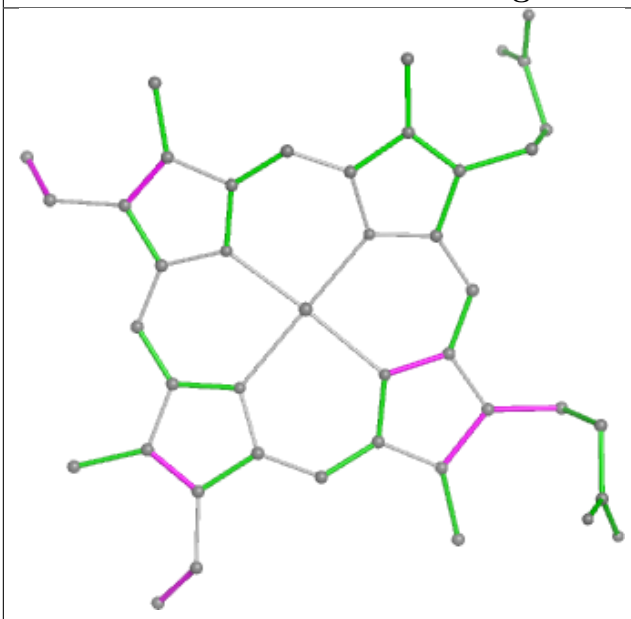


Torsions

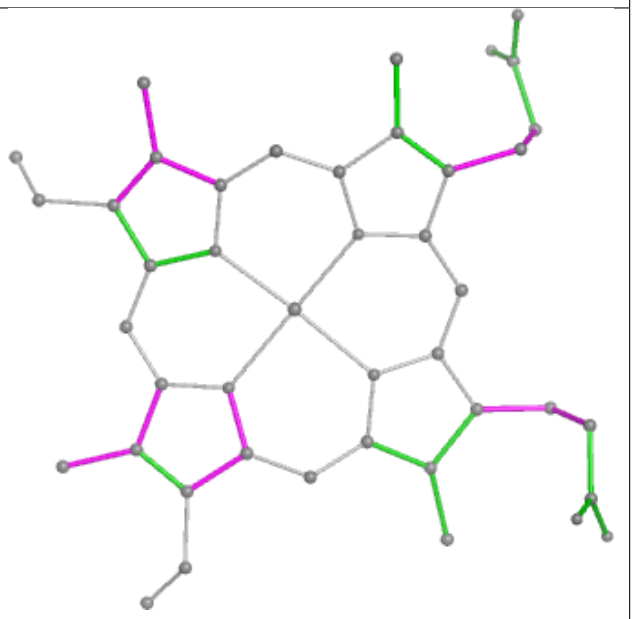


Rings

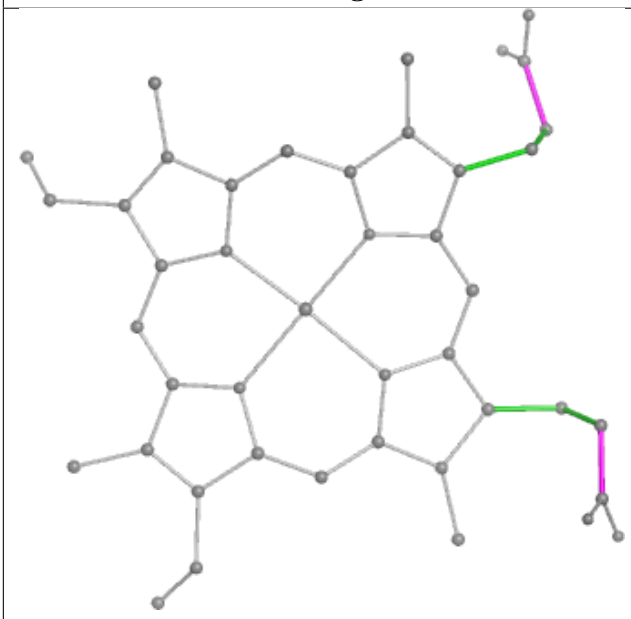
Ligand HEC G 1005



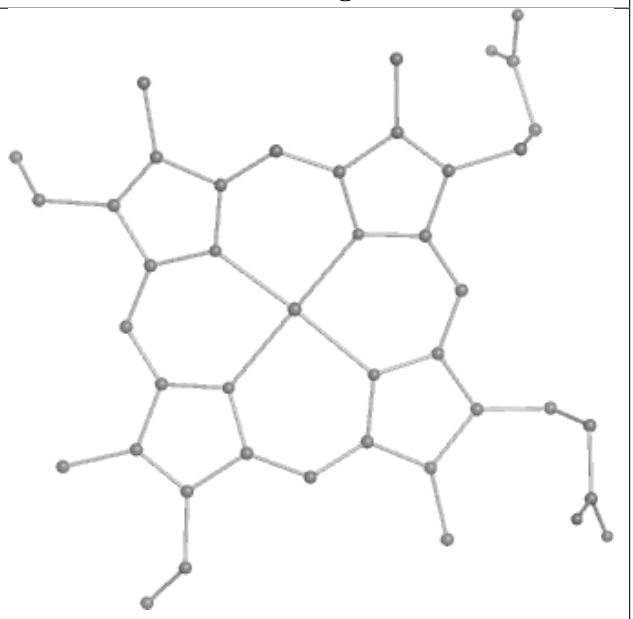
Bond lengths



Bond angles

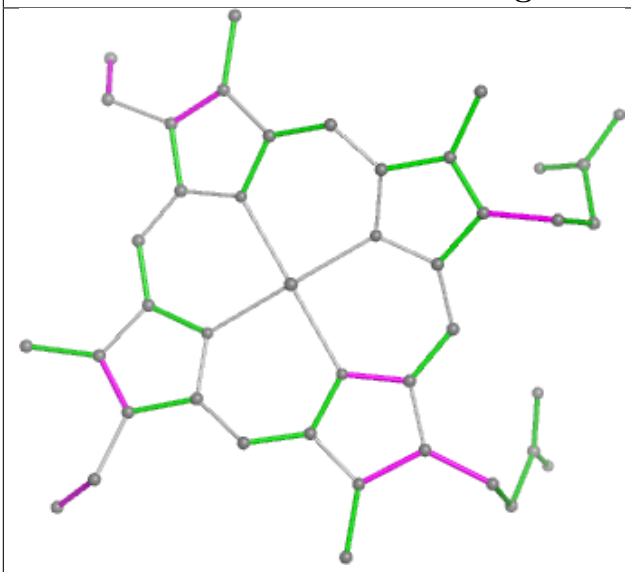


Torsions

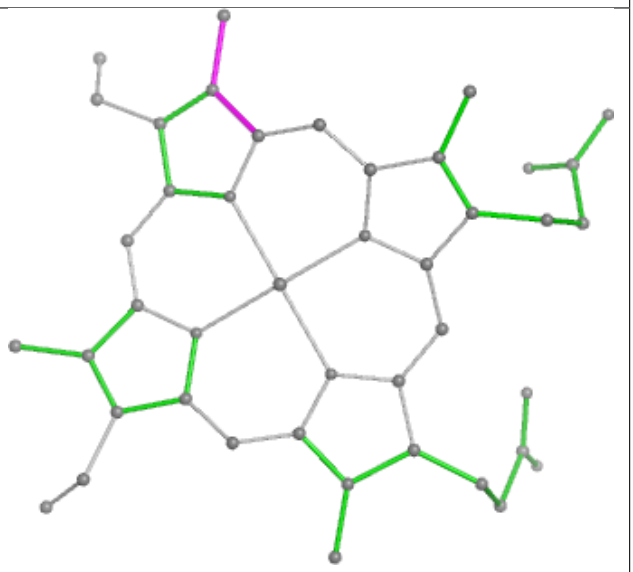


Rings

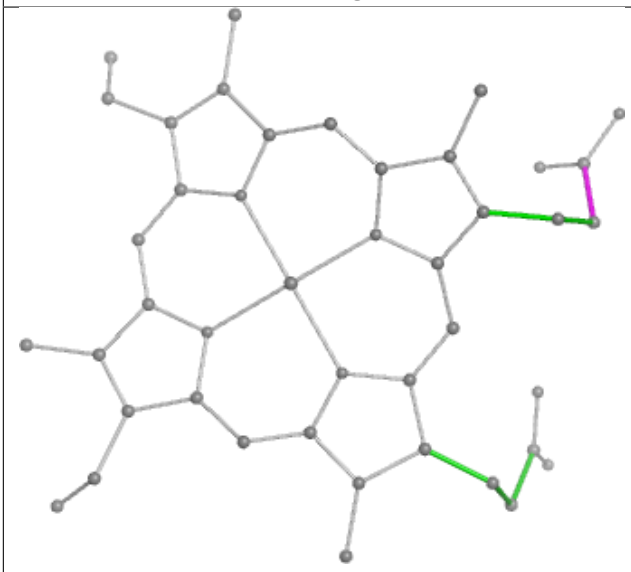
Ligand HEC P 1001



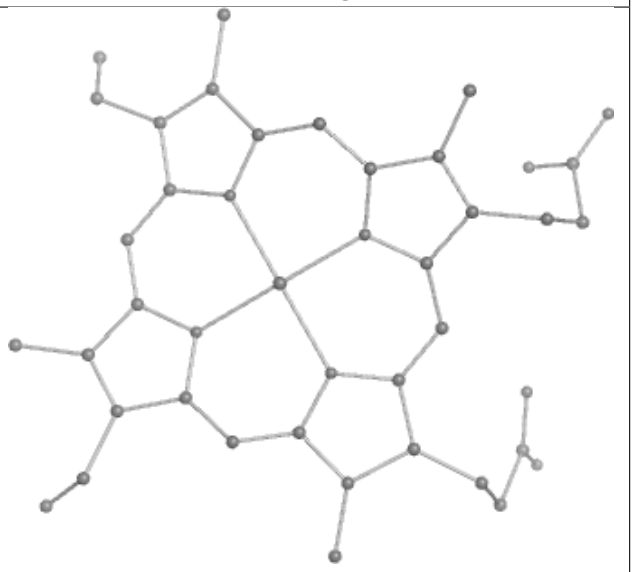
Bond lengths



Bond angles

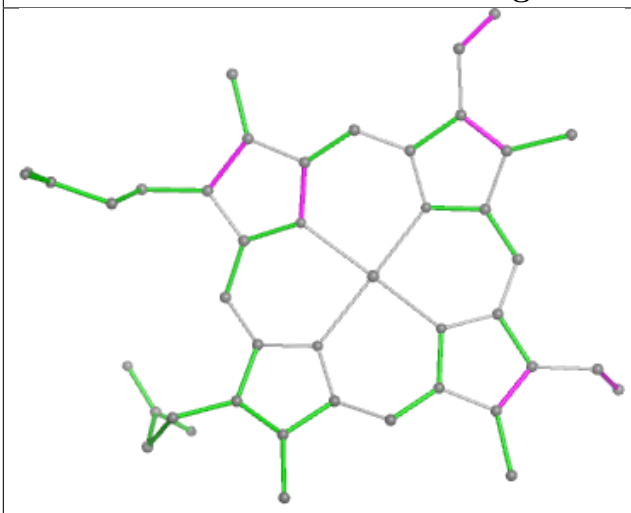


Torsions



Rings

Ligand HEC H 1002



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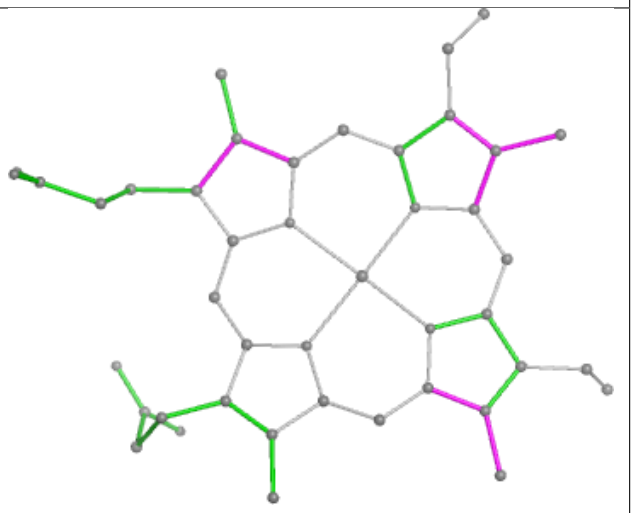
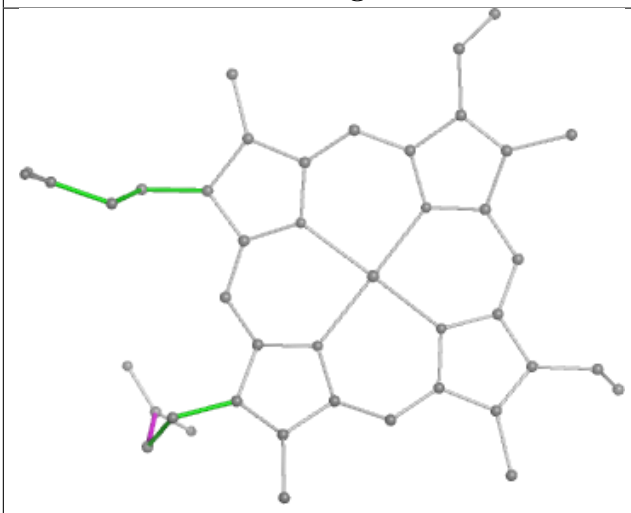
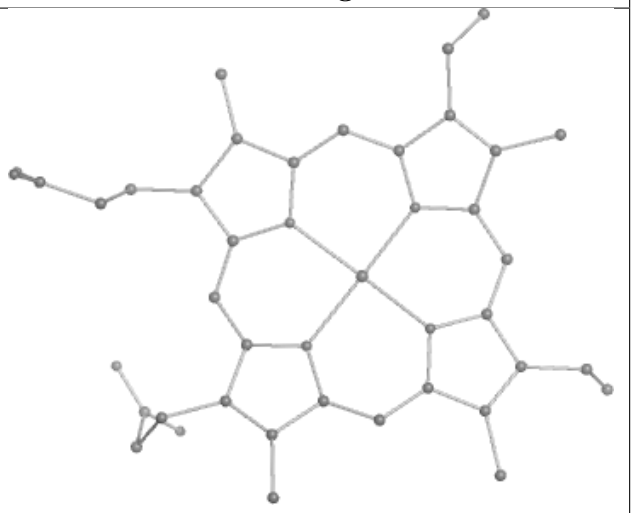


Bond angles

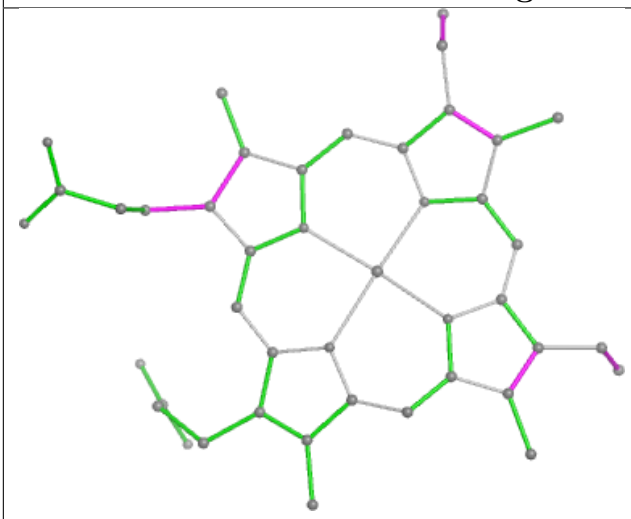


Torsions



Rings

Ligand HEC L 1002



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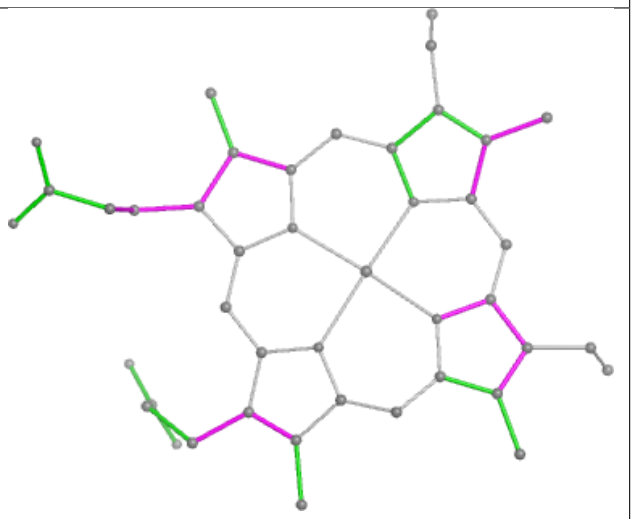
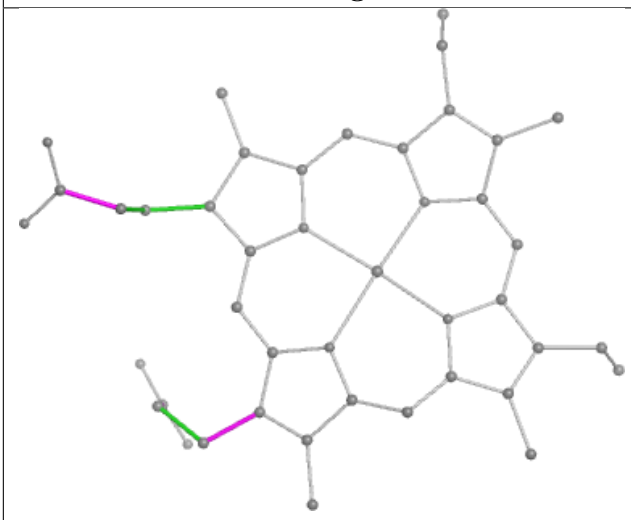


Bond angles



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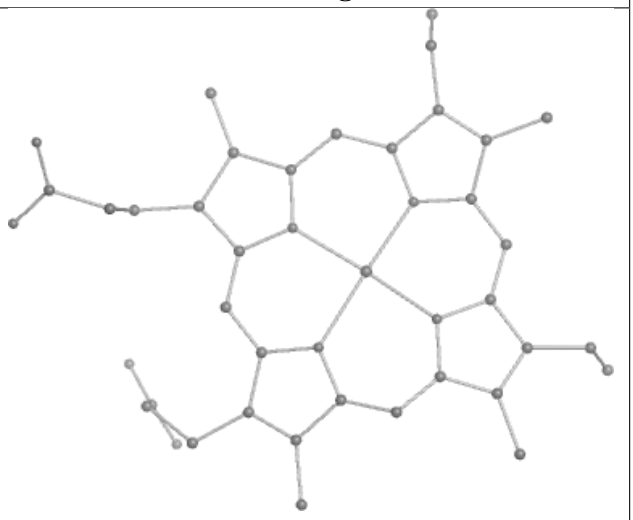
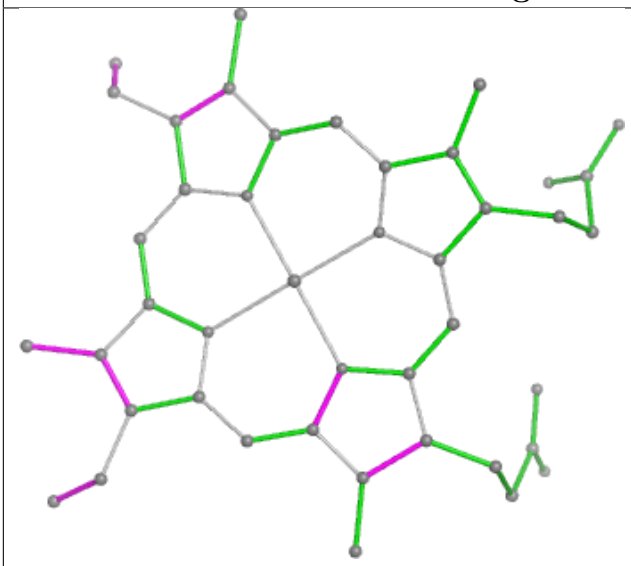


Rings

Ligand HEC G 1001



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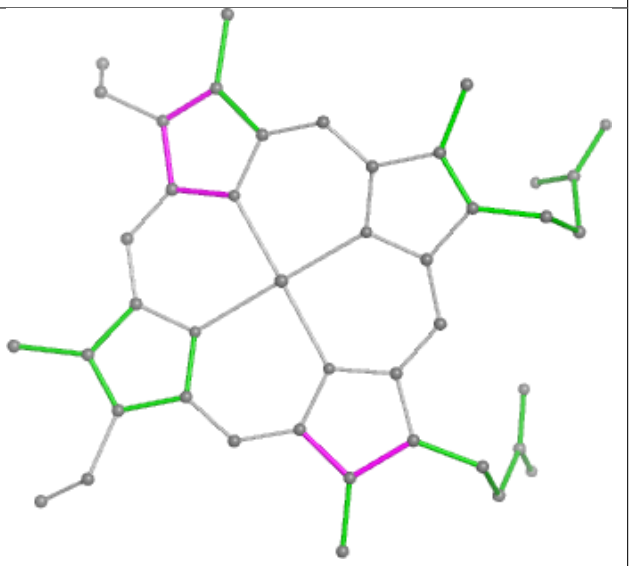
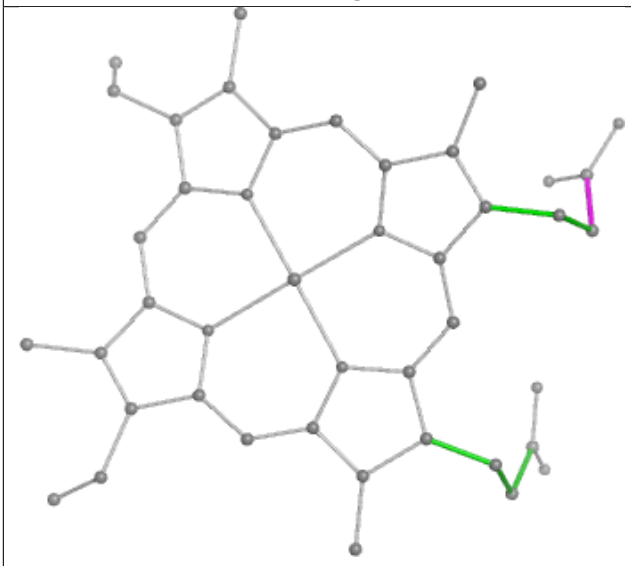
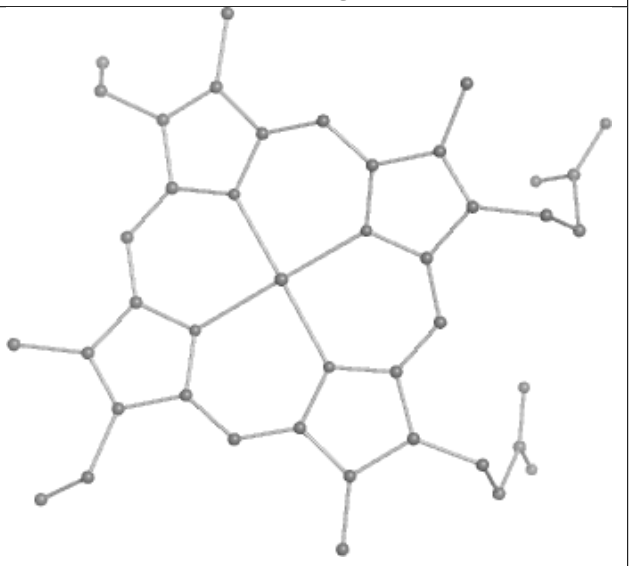


Bond angles

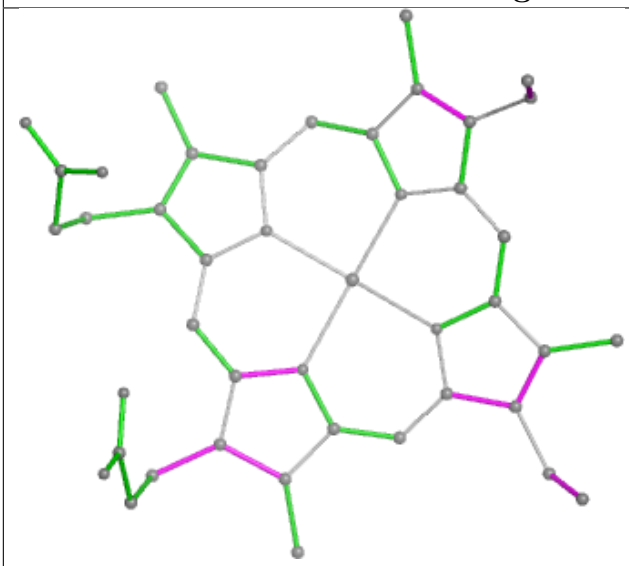


Torsions

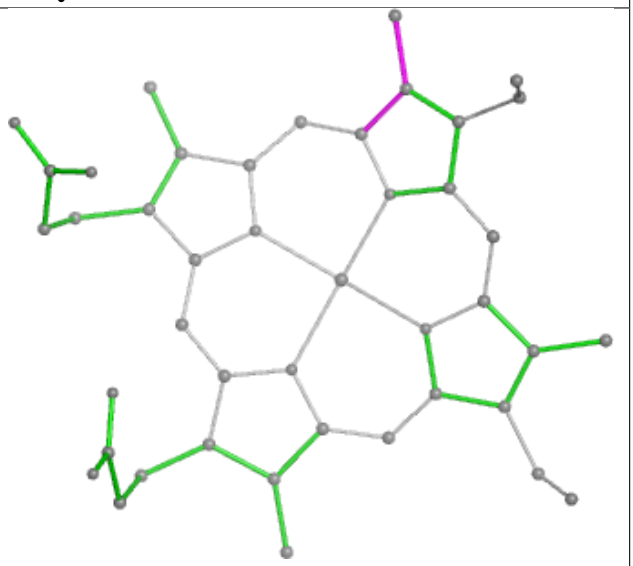


Rings

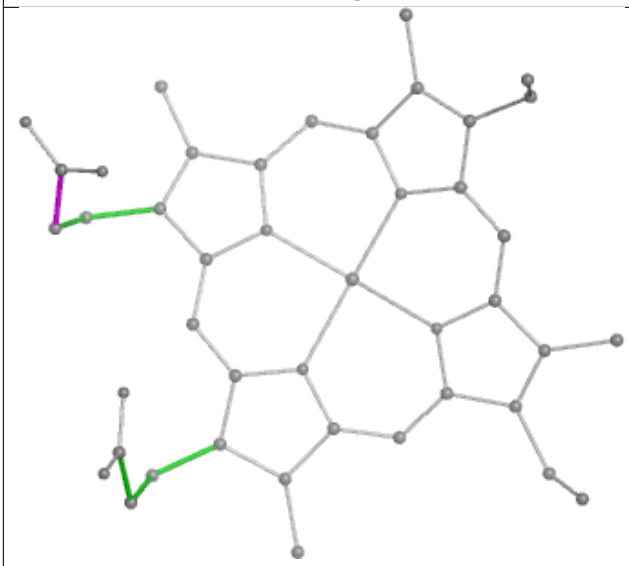
Ligand HEC Q 1001



Bond lengths



Bond angles



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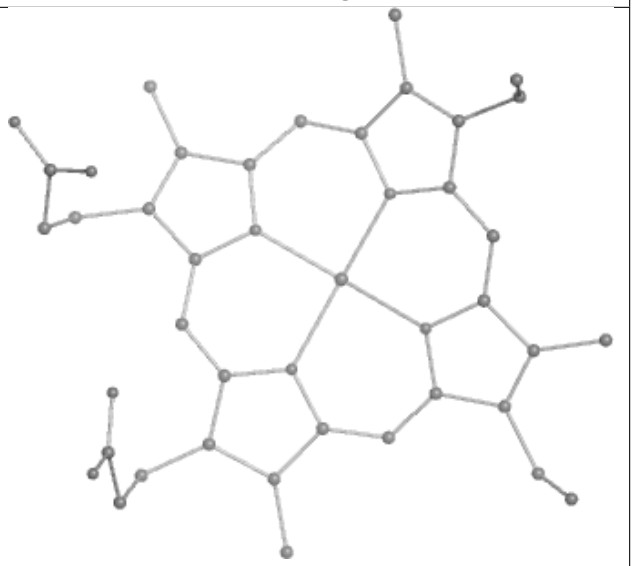
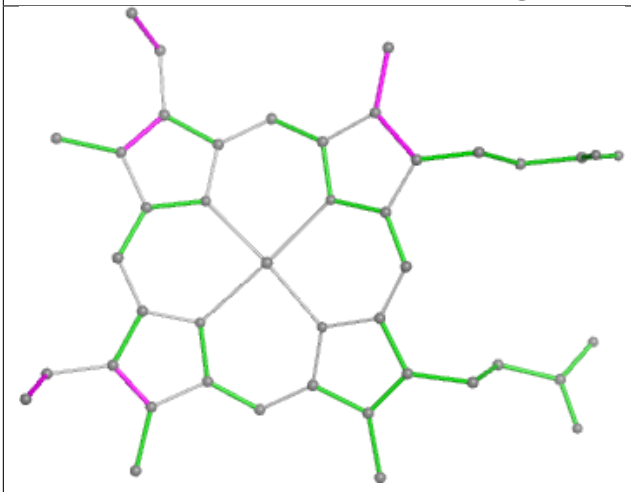


Rings

Ligand HEC A 1004



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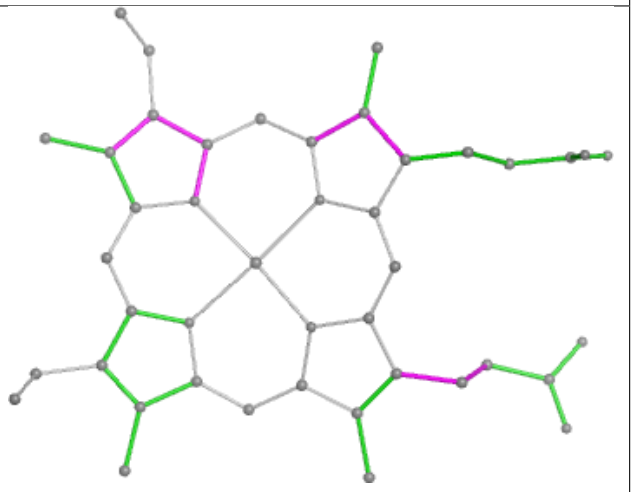
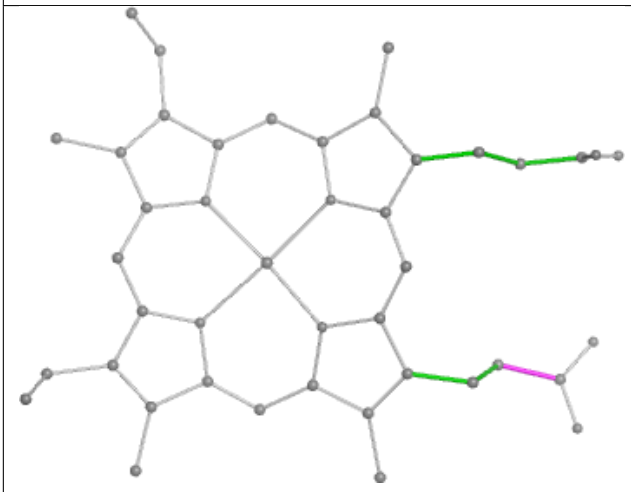


Bond angles



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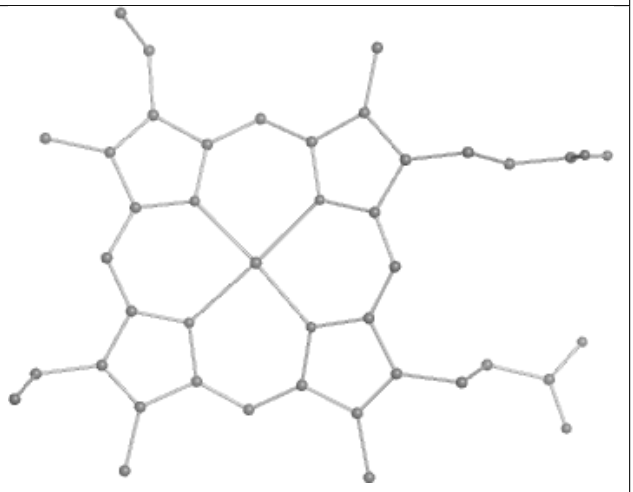
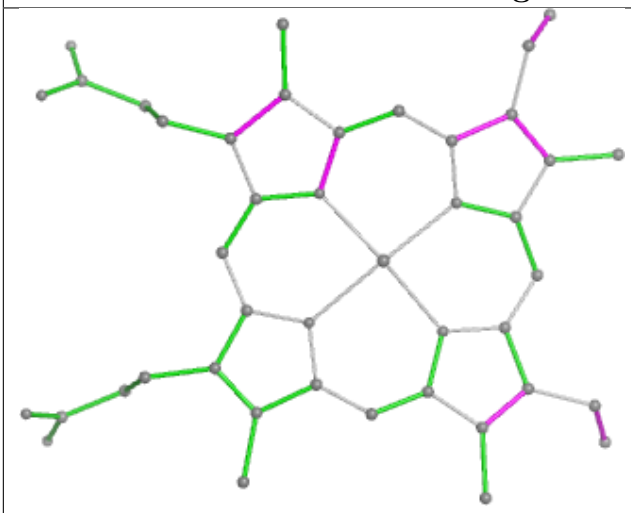
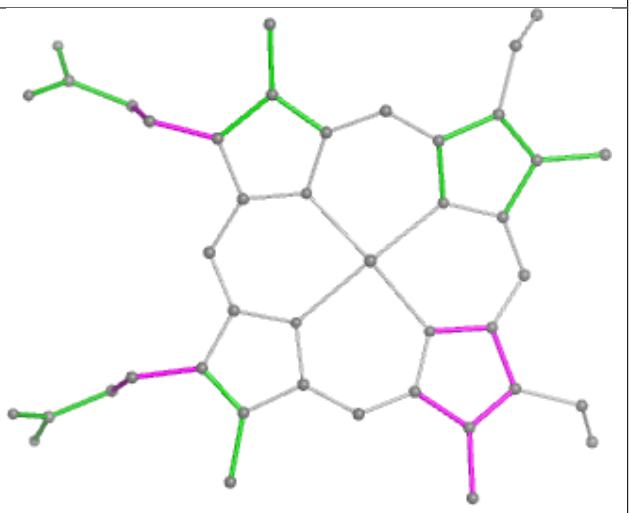


Rings

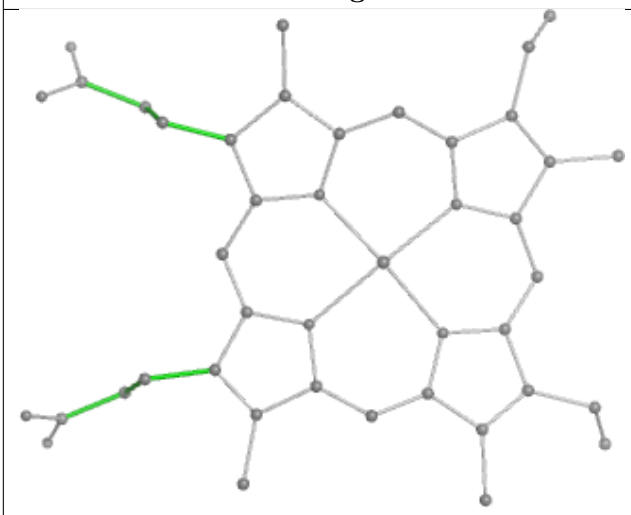
Ligand HEC H 1003



Bond lengths



Bond angles



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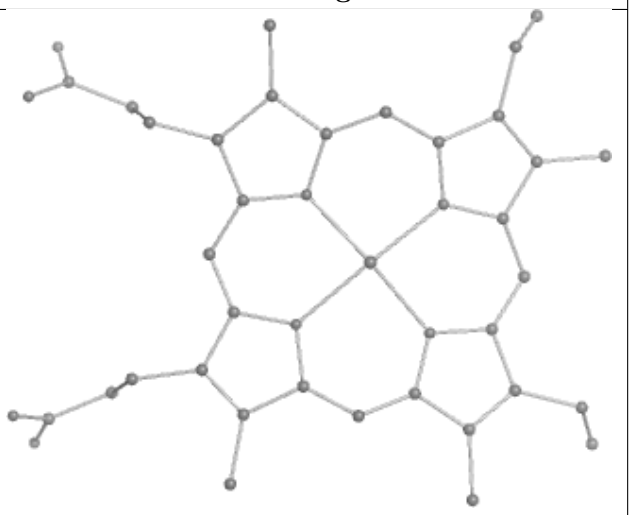
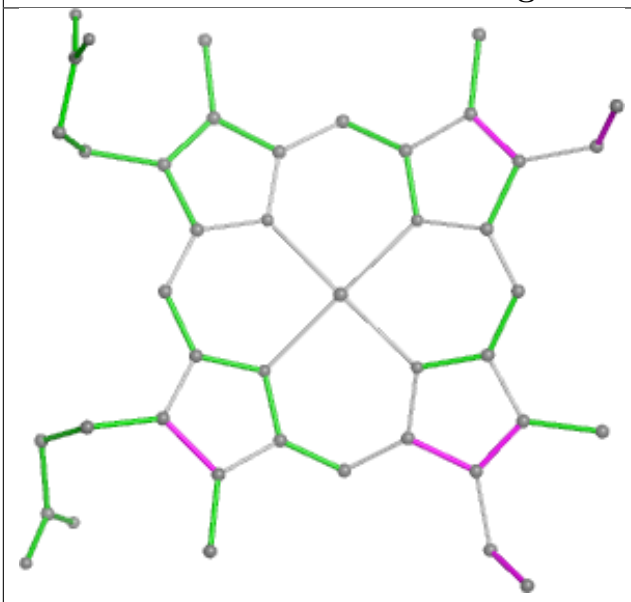


Rings

Ligand HEC J 1005



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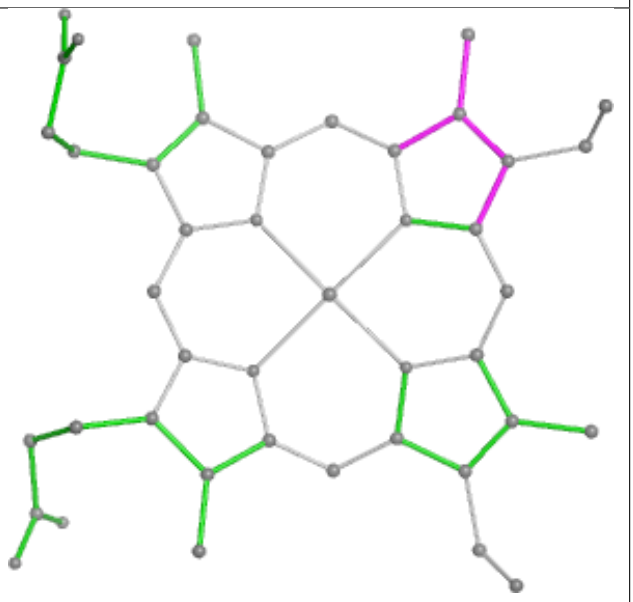
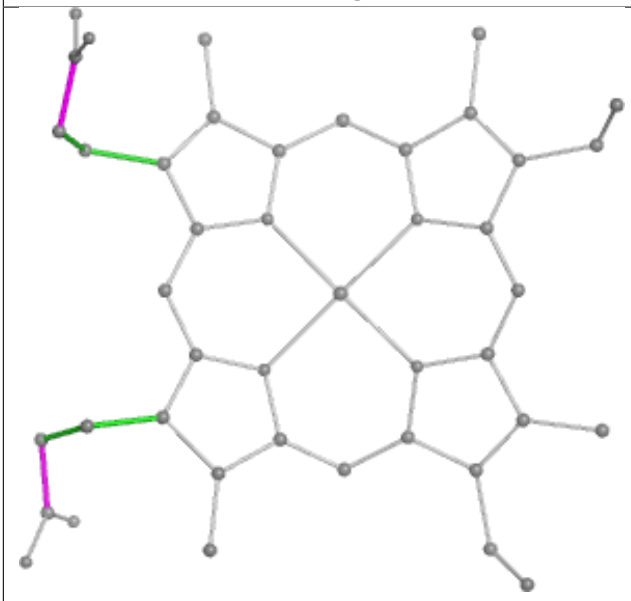
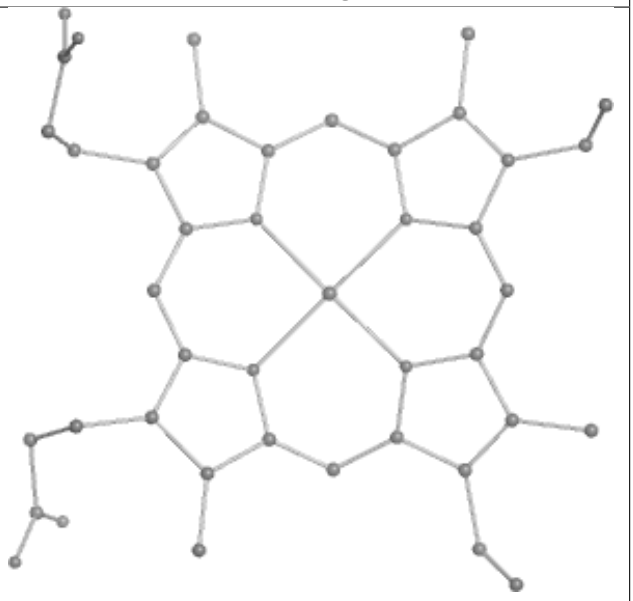


Bond angles

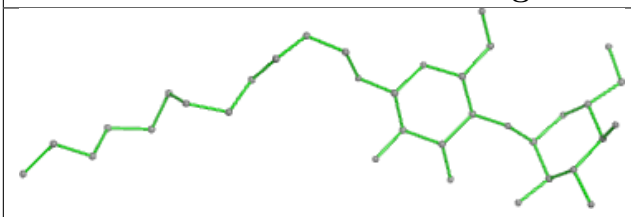


Torsions

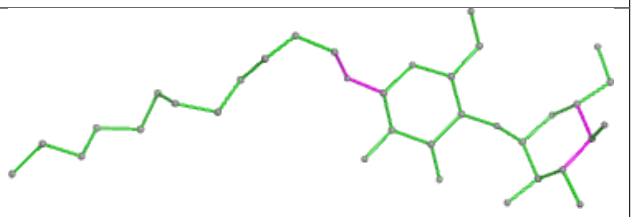


Rings

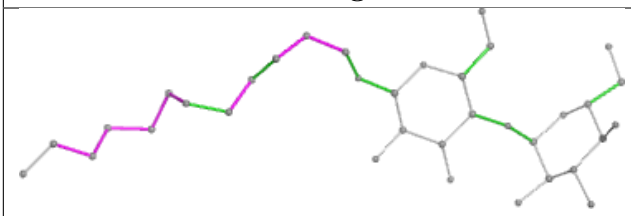
Ligand LMT R 1005



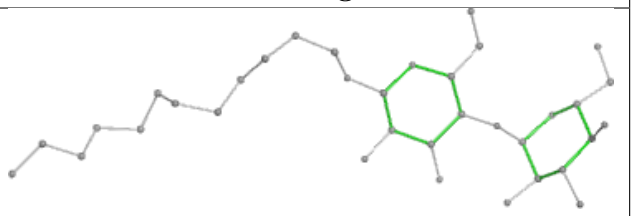
Bond lengths



Bond angles

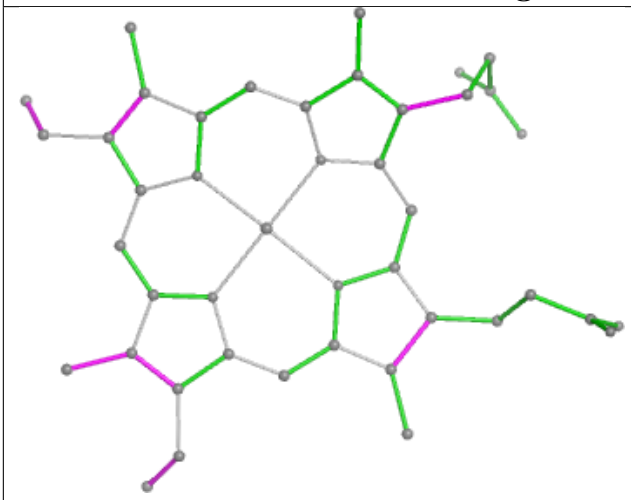


Torsions



Rings

Ligand HEC E 1002



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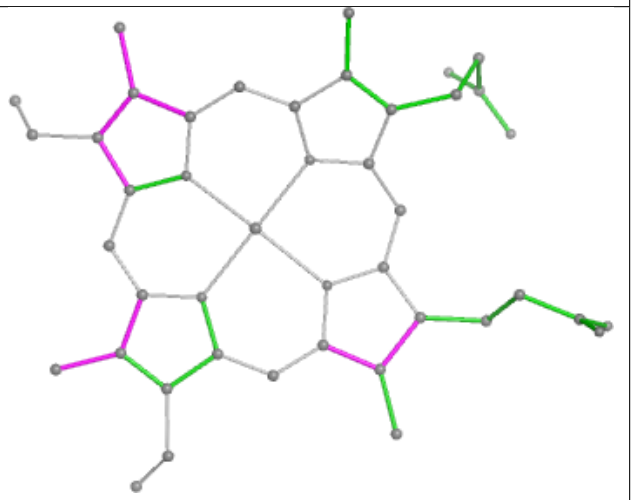
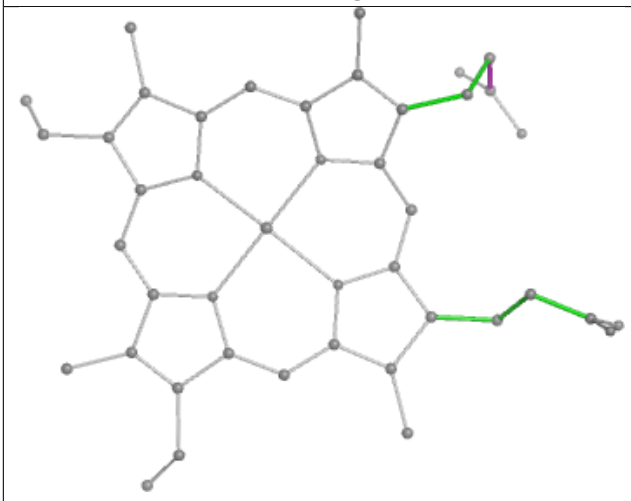
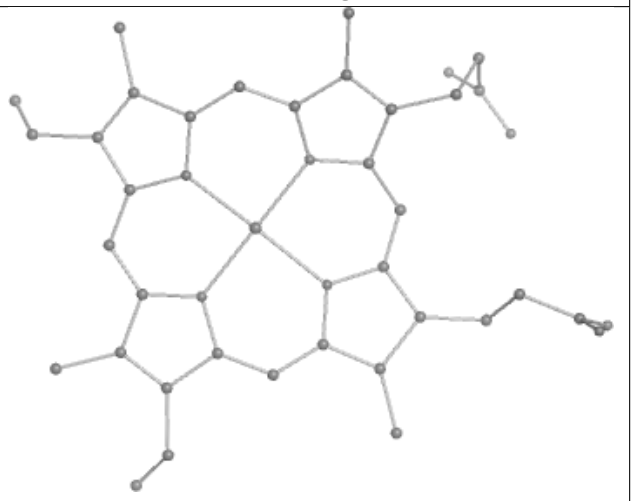


Bond angles

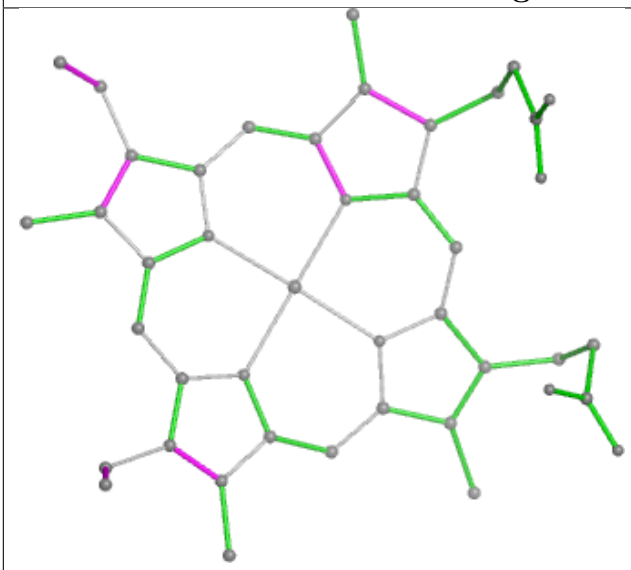


Torsions



Rings

Ligand HEC N 1001



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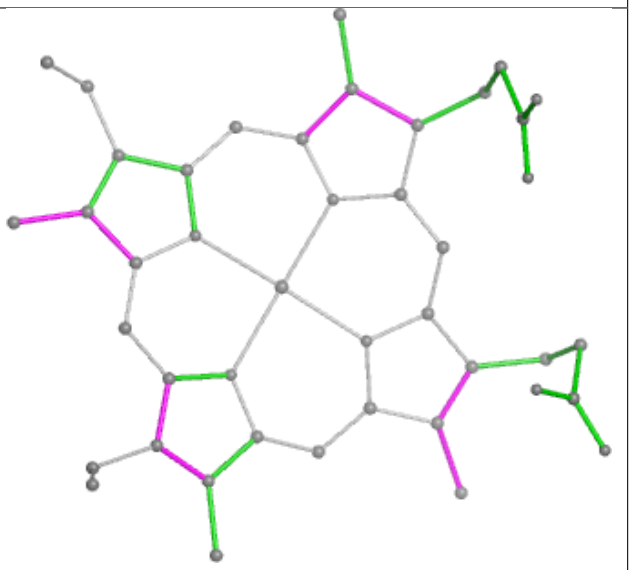
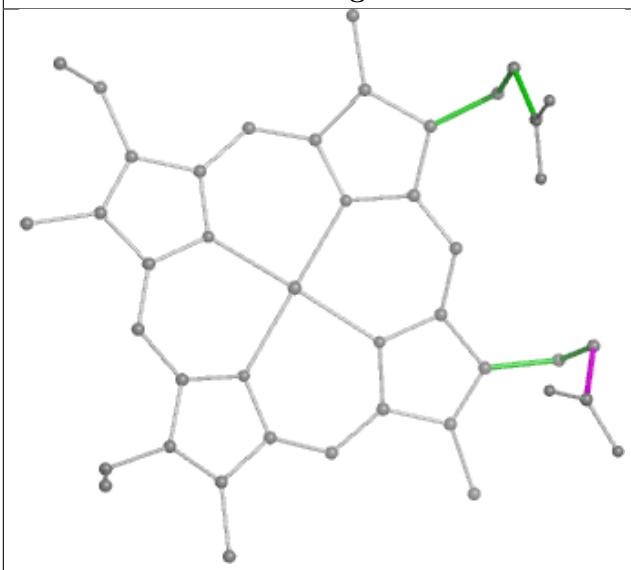
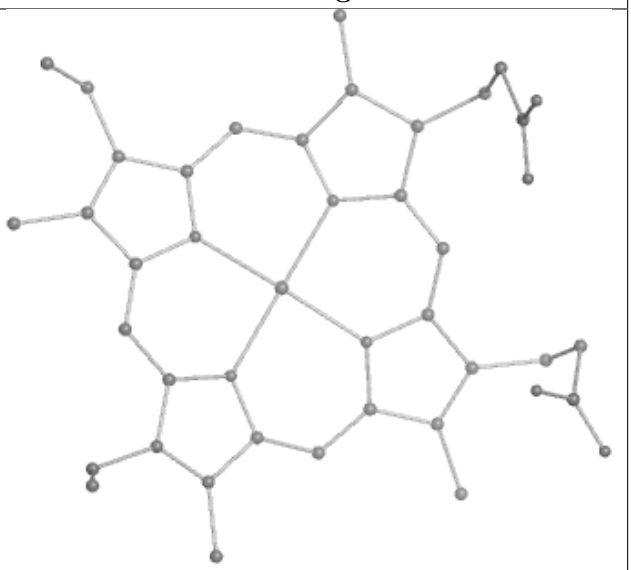


Bond angles

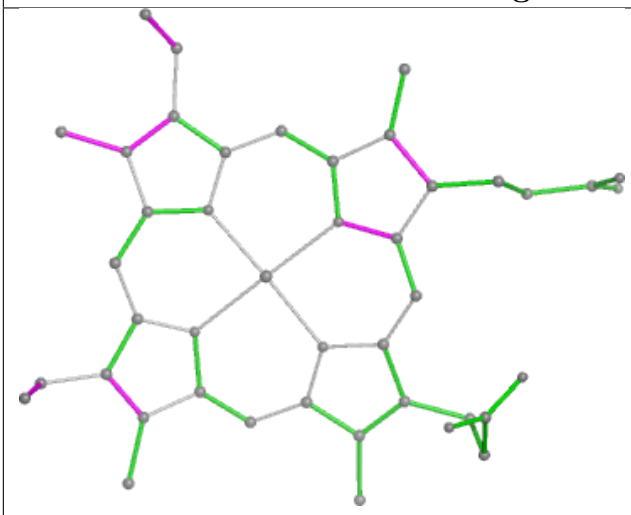


Torsions



Rings

Ligand HEC N 1002



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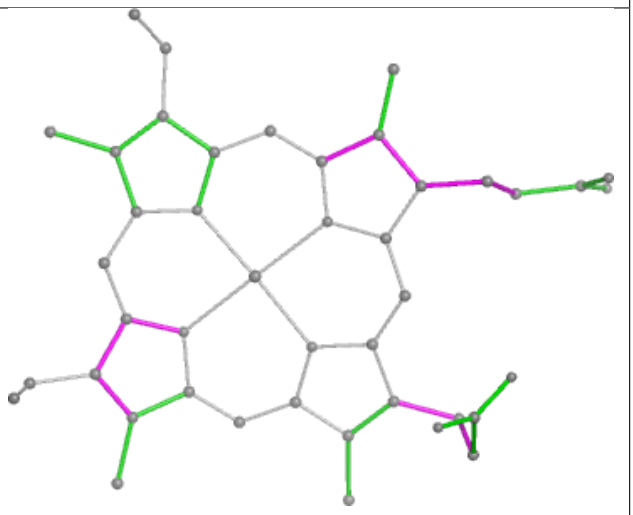
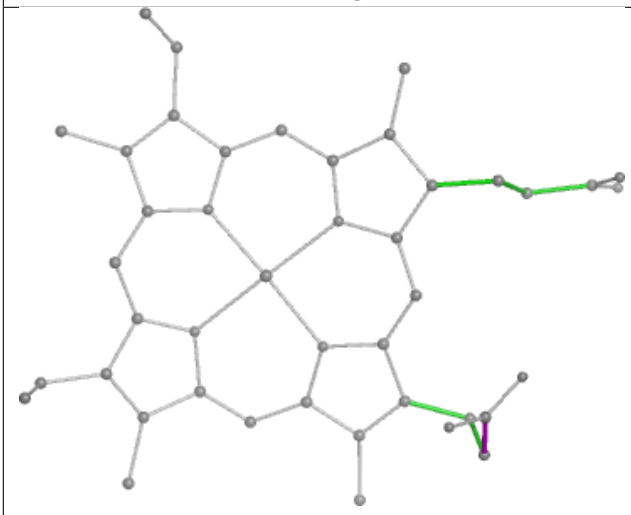
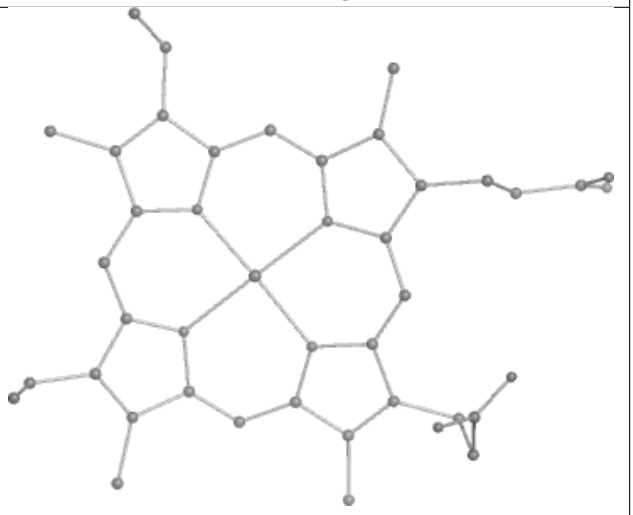


Bond angles

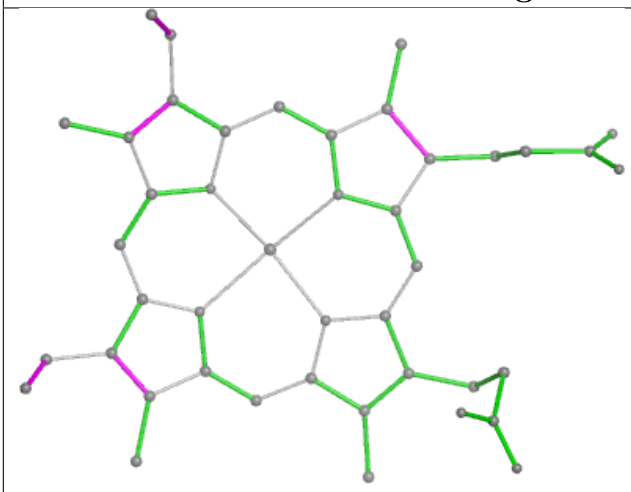


Torsions



Rings

Ligand HEC F 1001



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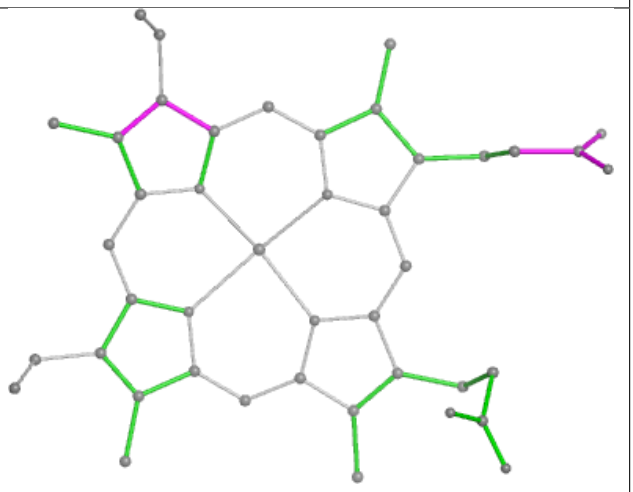
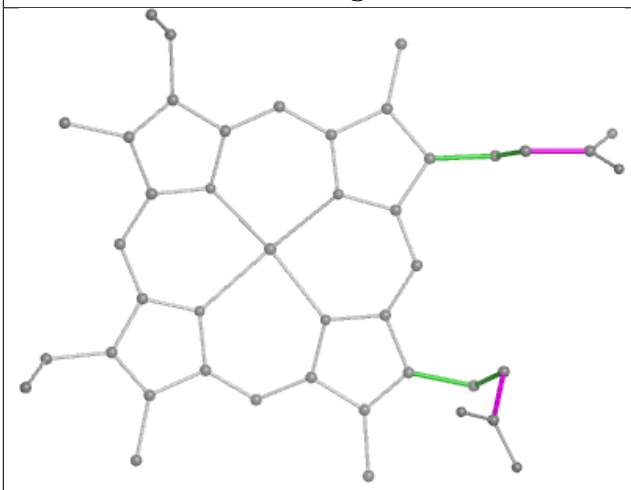
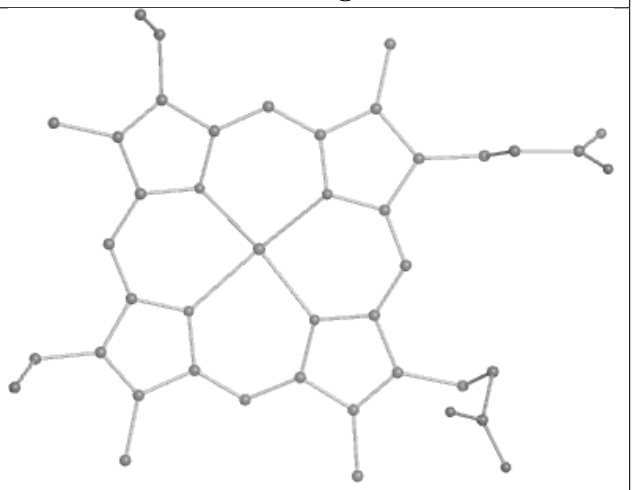


Bond angles

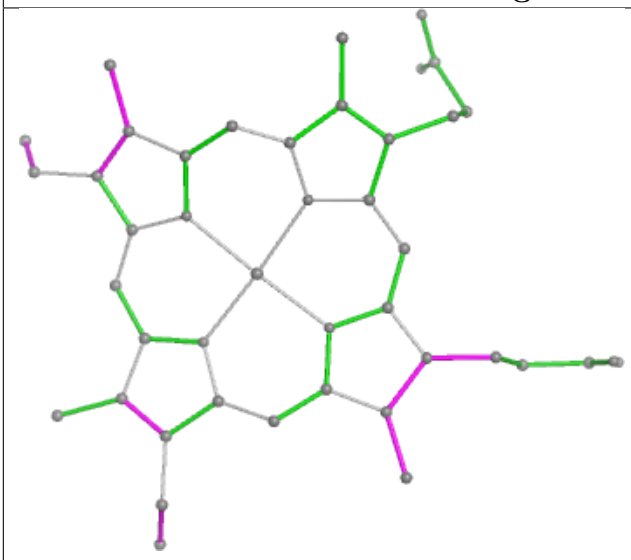


Torsions

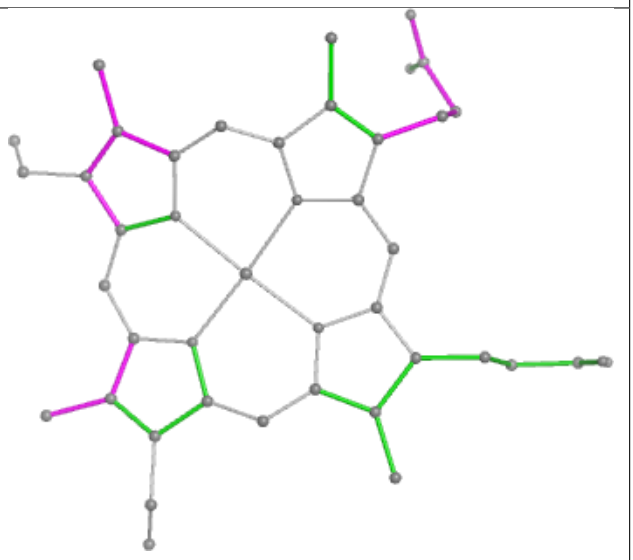


Rings

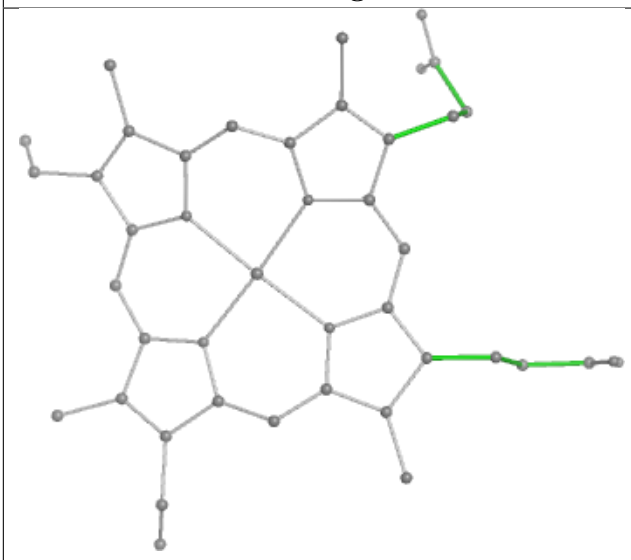
Ligand HEC R 1003



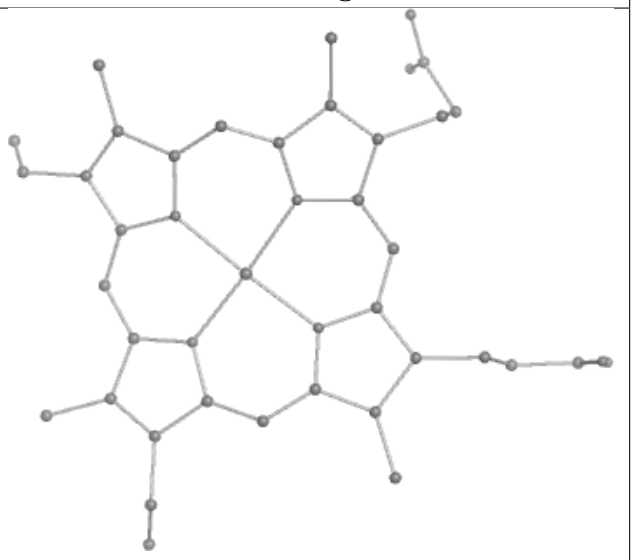
Bond lengths



Bond angles

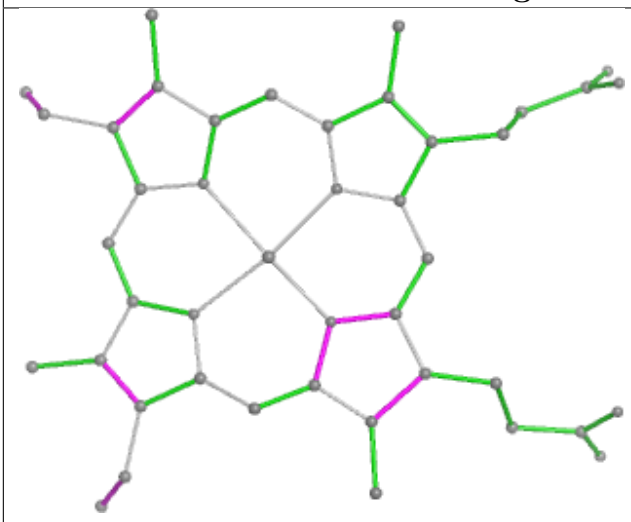


Torsions

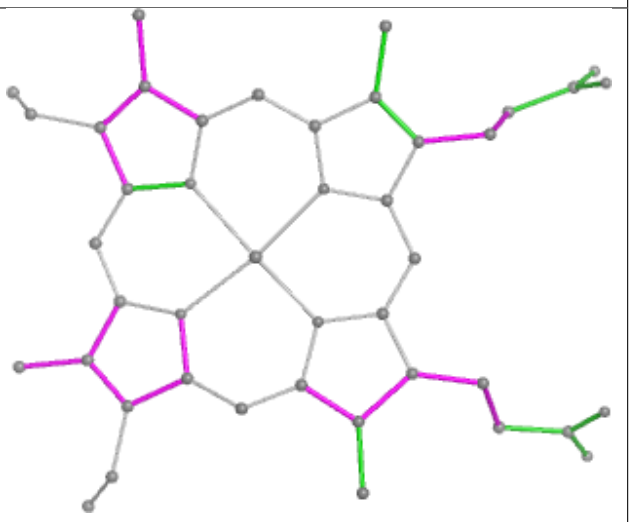


Rings

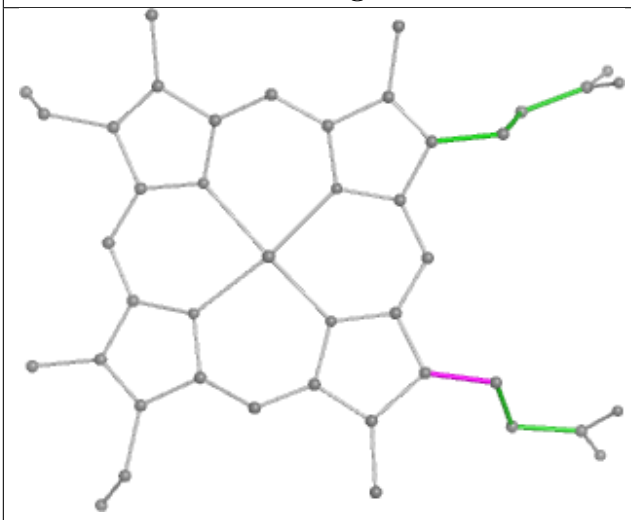
Ligand HEC A 1003



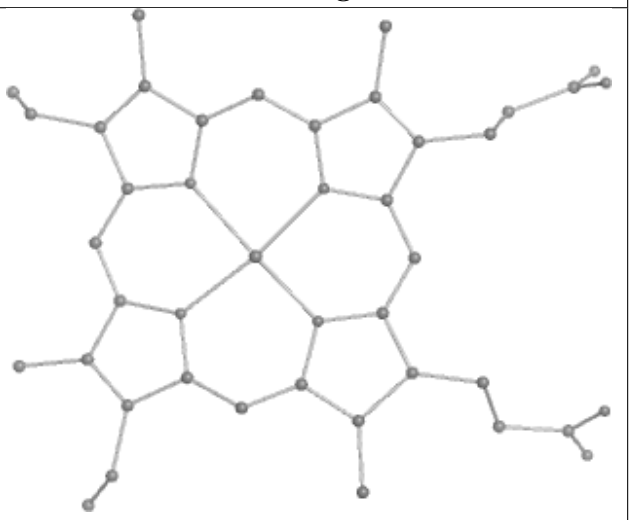
Bond lengths



Bond angles

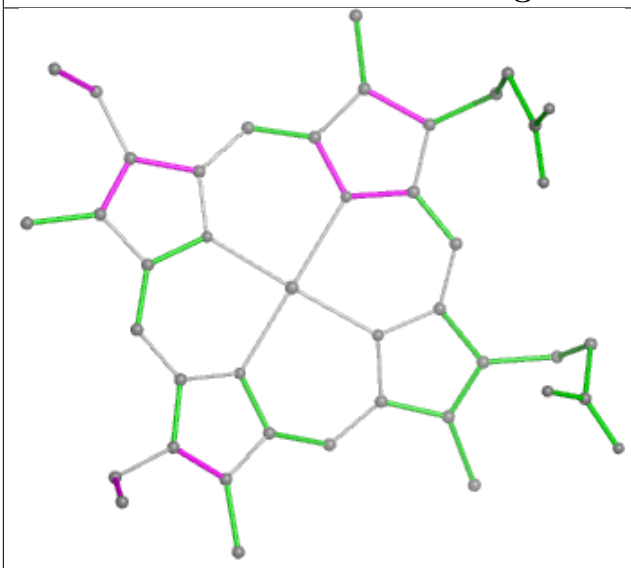


Torsions

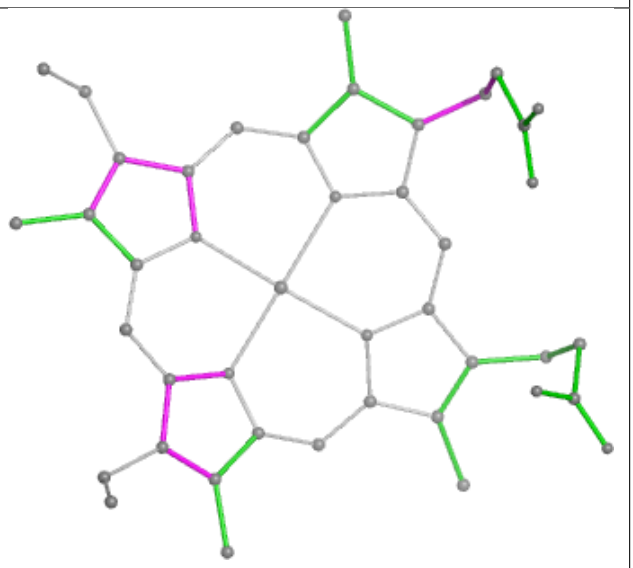


Rings

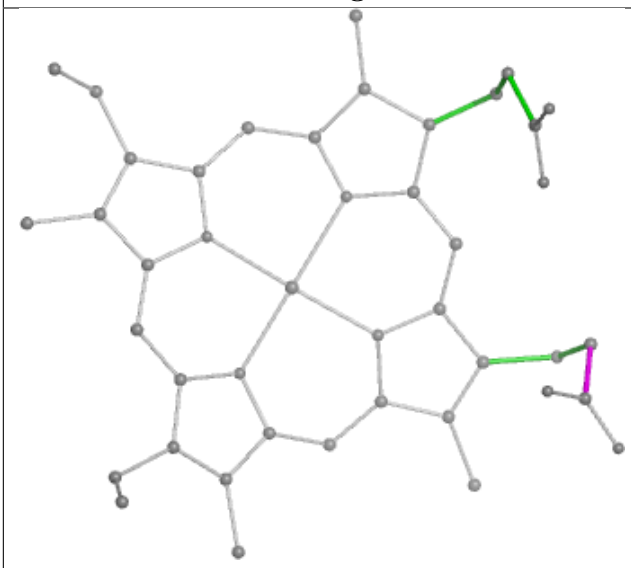
Ligand HEC B 1001



Bond lengths



Bond angles



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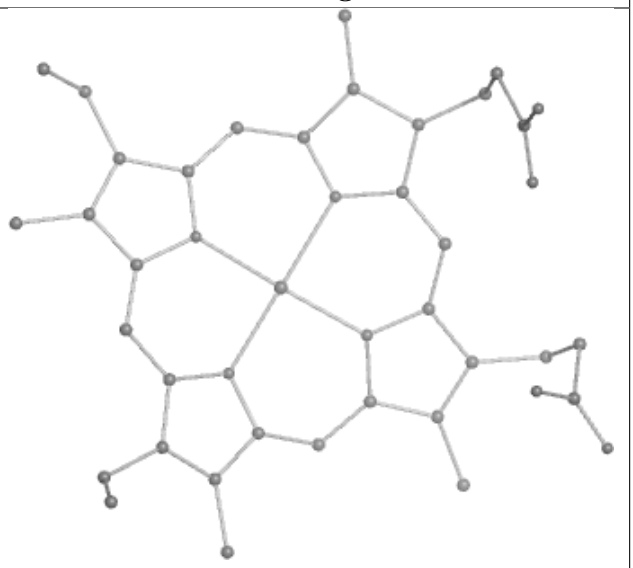
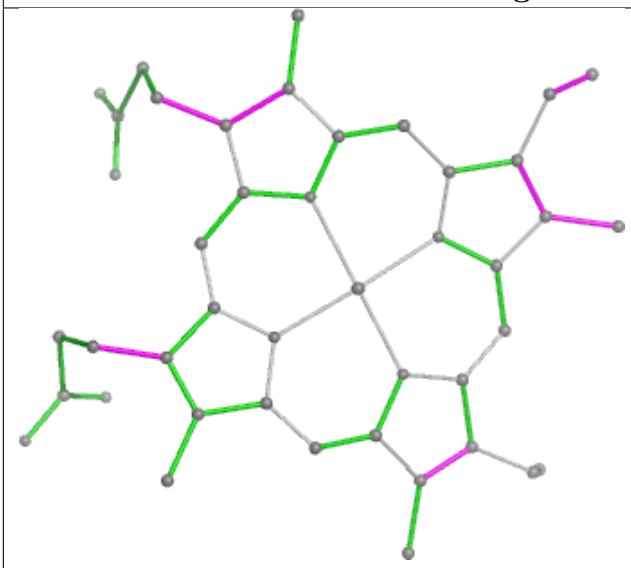


Rings

Ligand HEC D 1001



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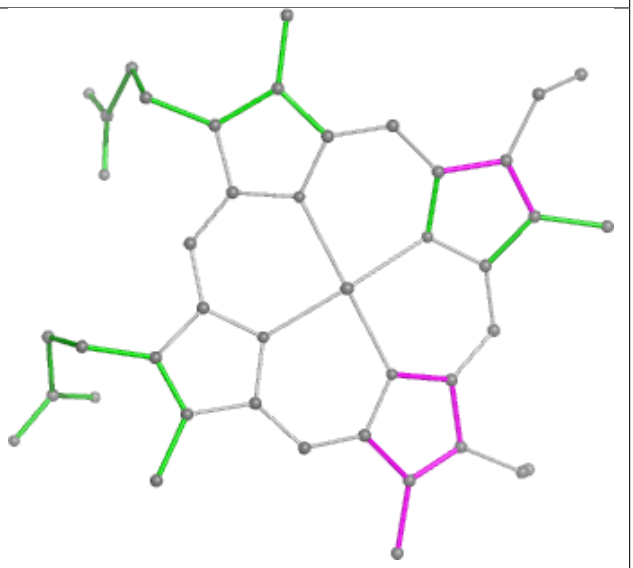
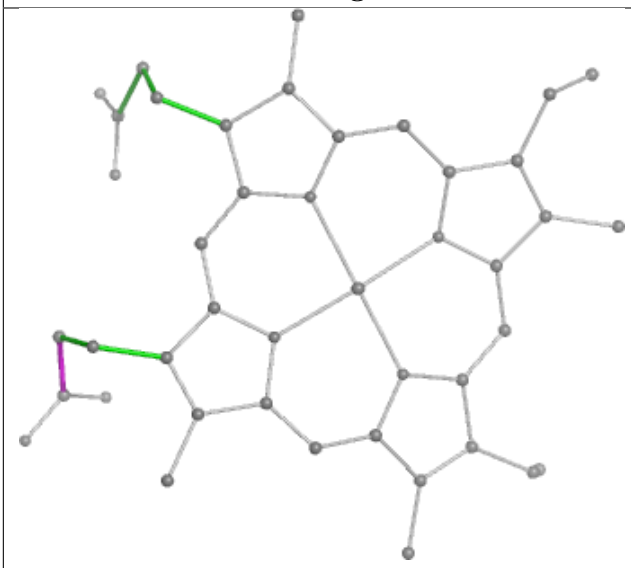
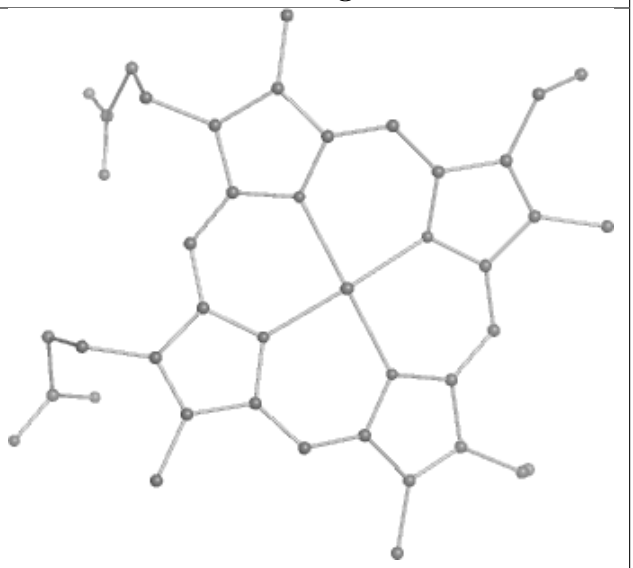


Bond angles

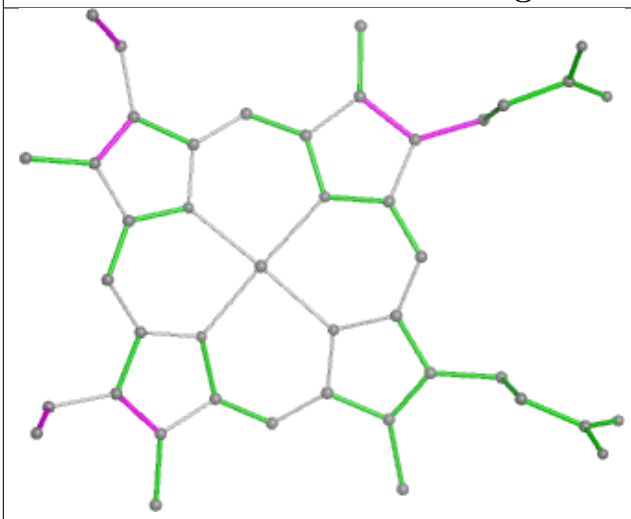


Torsions



Rings

Ligand HEC P 1003



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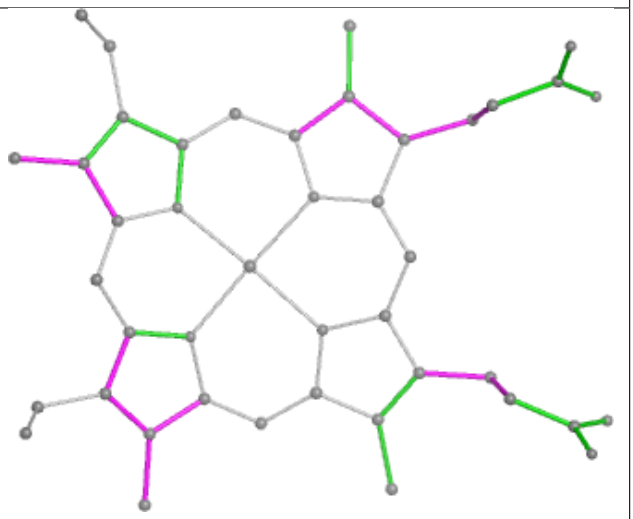
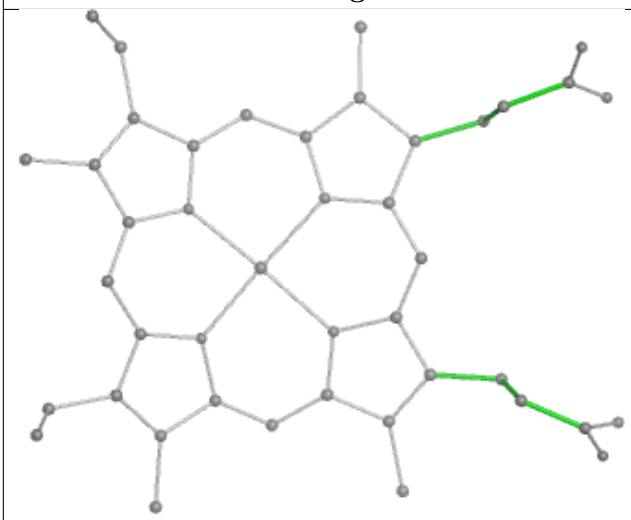
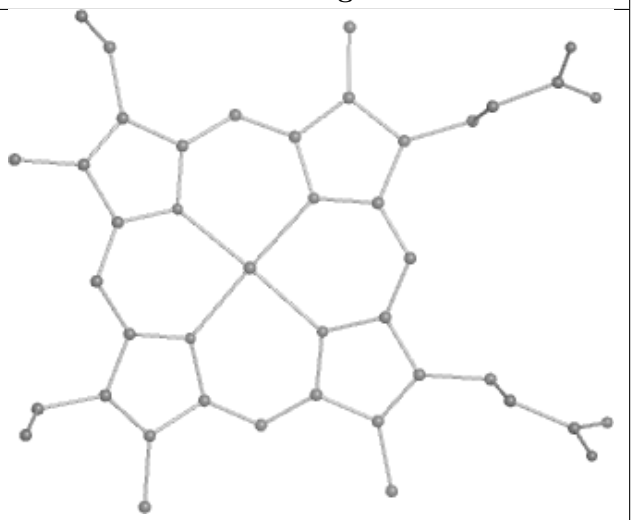


Bond angles

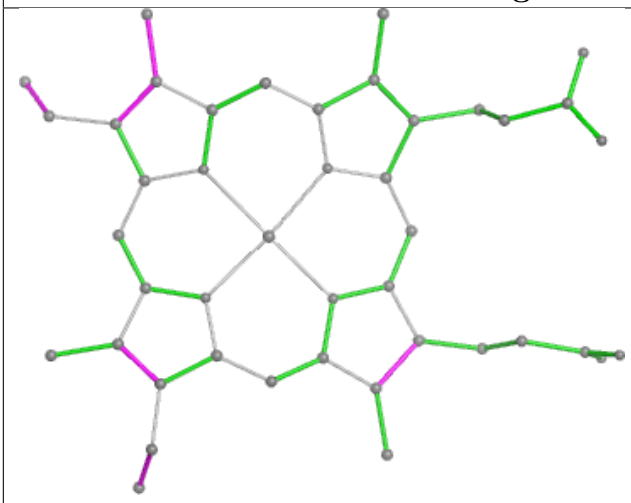


Torsions

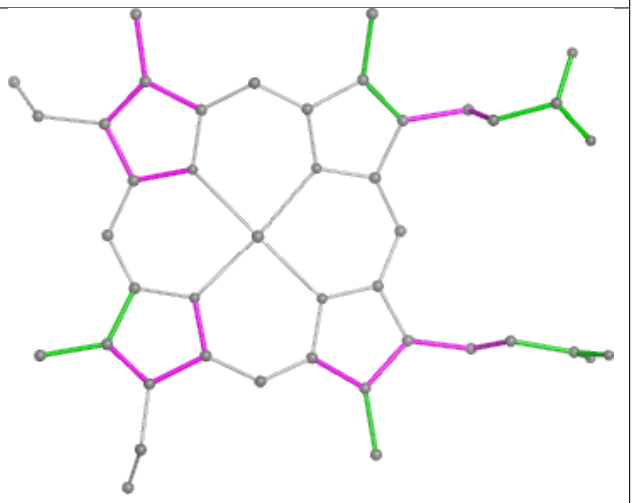


Rings

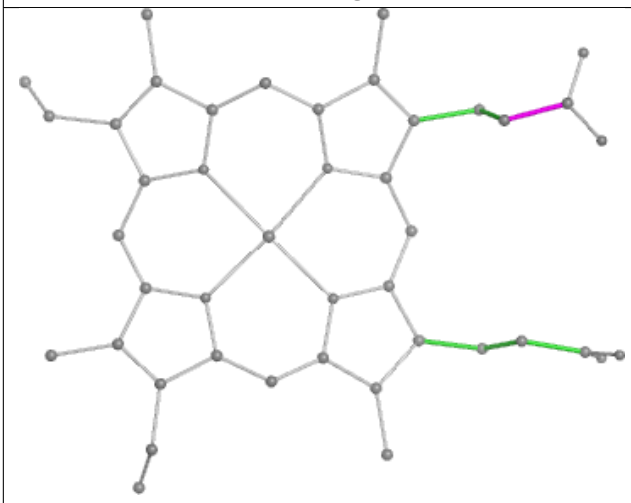
Ligand HEC K 1004



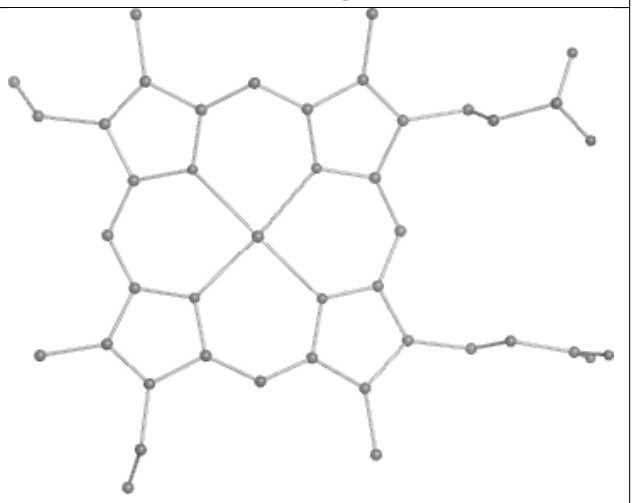
Bond lengths



Bond angles

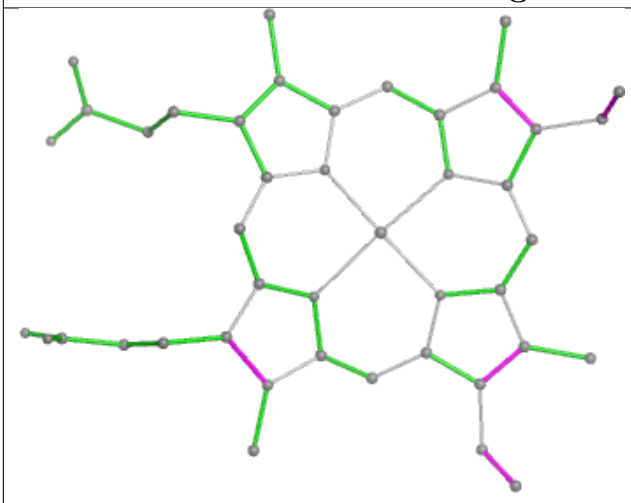


Torsions



Rings

Ligand HEC M 1004



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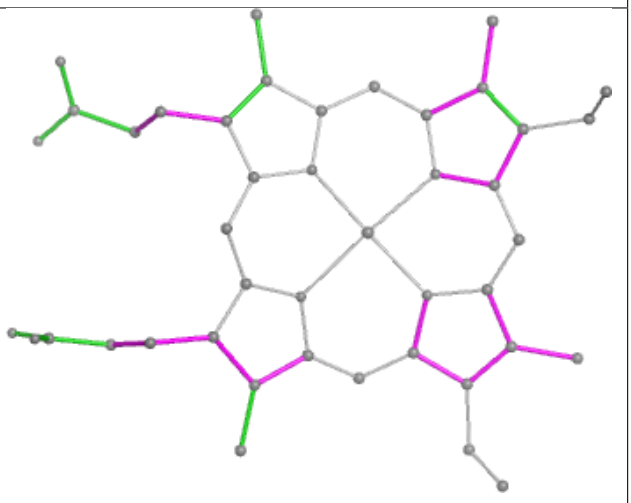
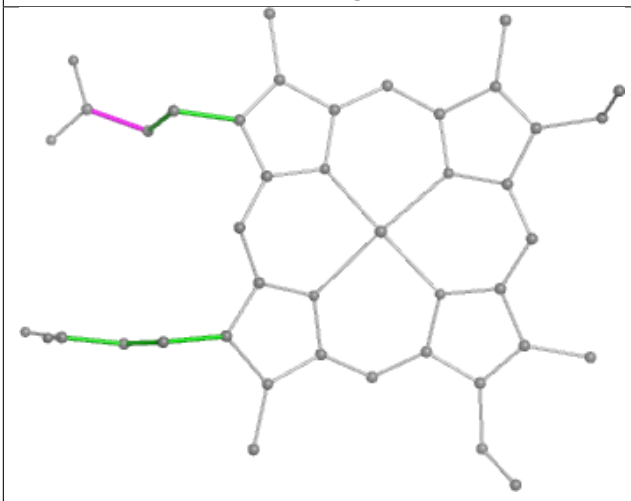
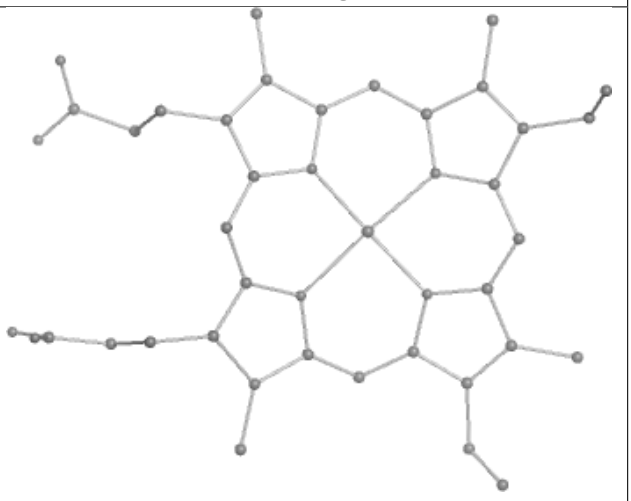


Bond angles

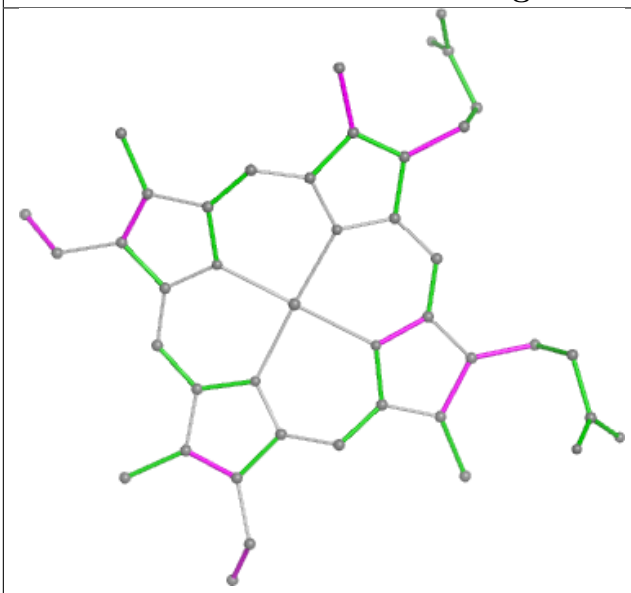


Torsions



Rings

Ligand HEC H 1005



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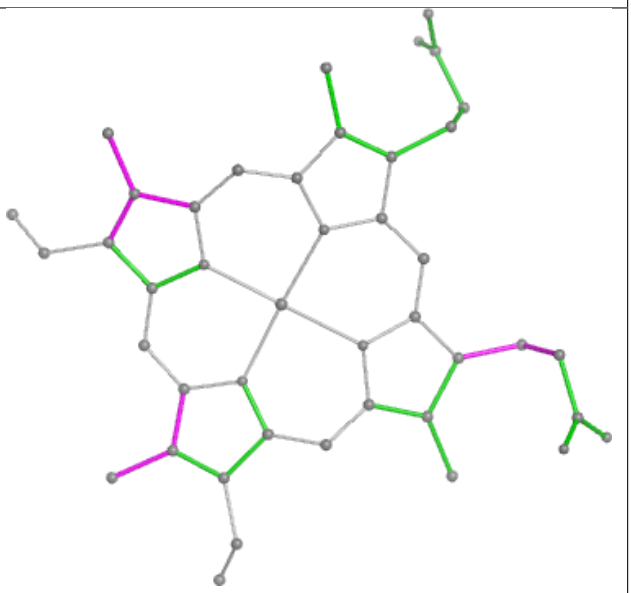
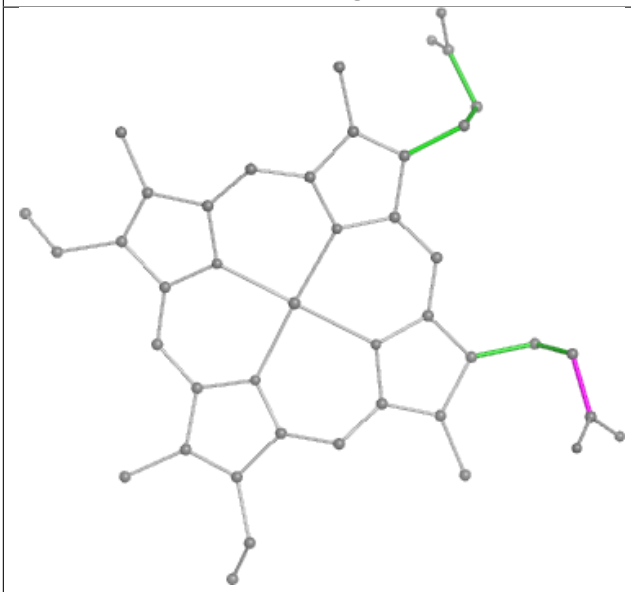


Bond angles



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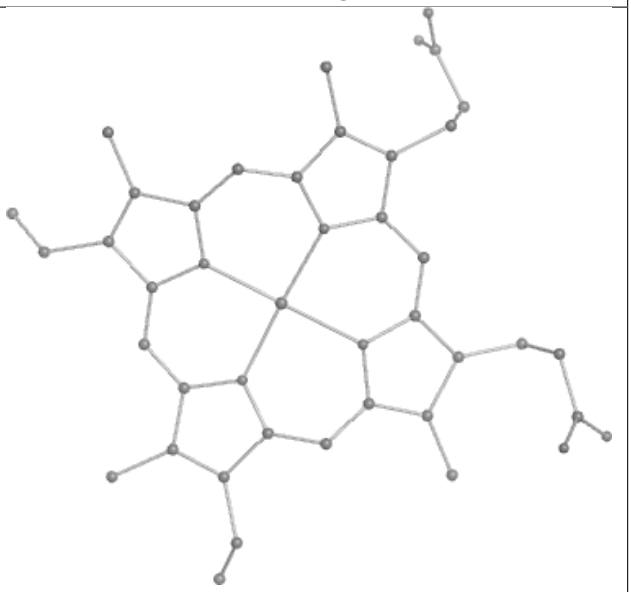
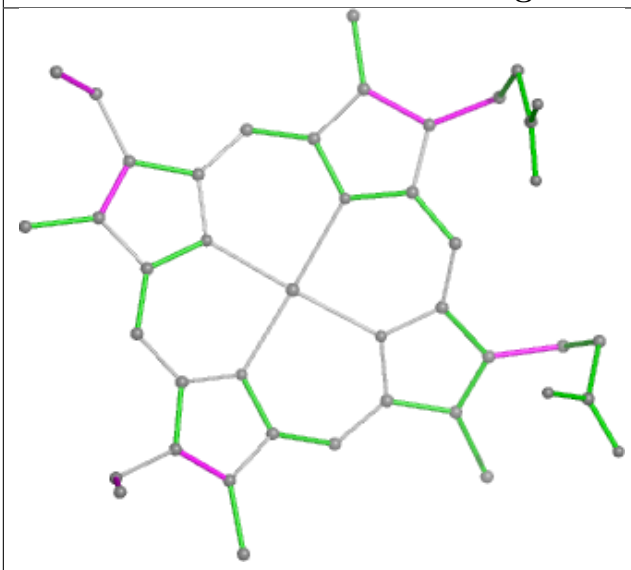


Rings

Ligand HEC E 1001



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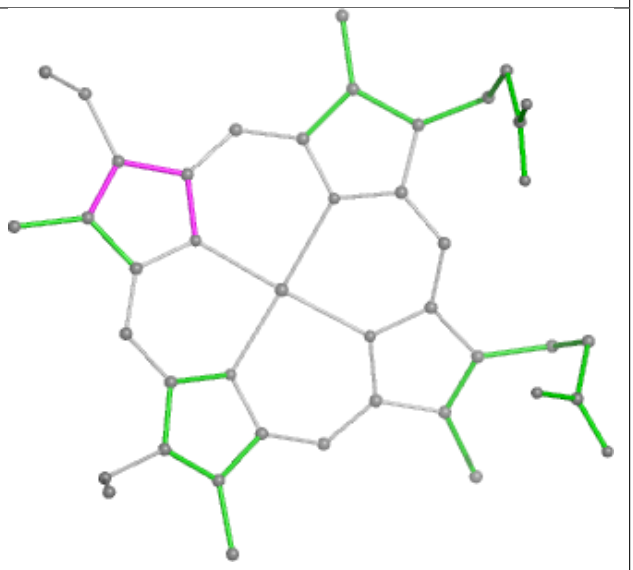
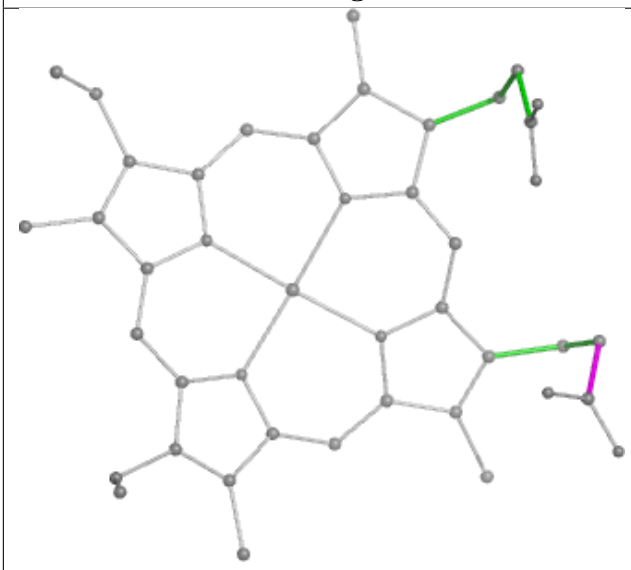
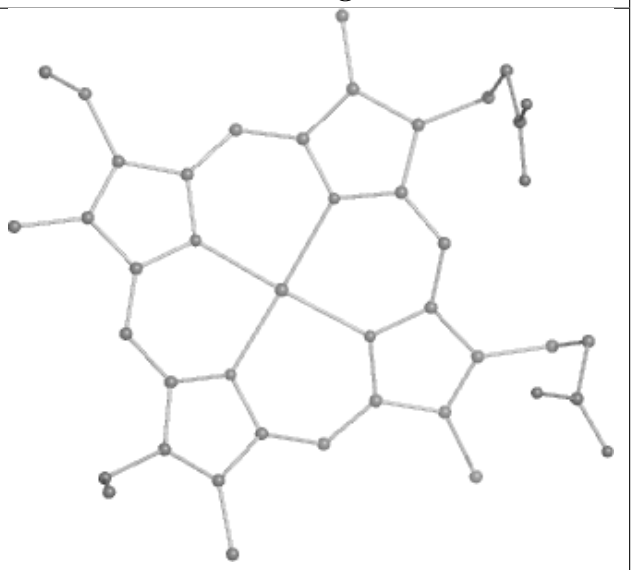


Bond angles

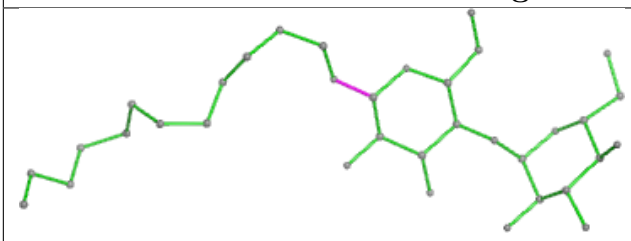


Torsions



Rings

Ligand LMT O 1005



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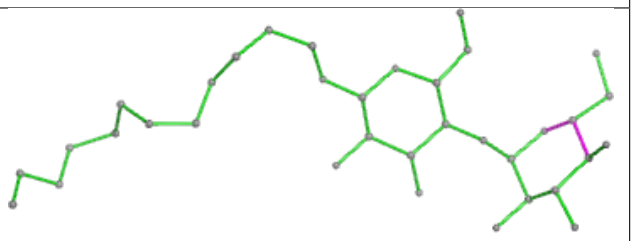
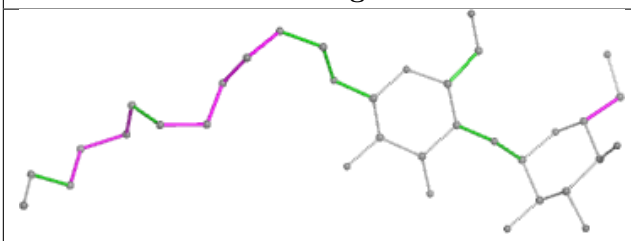
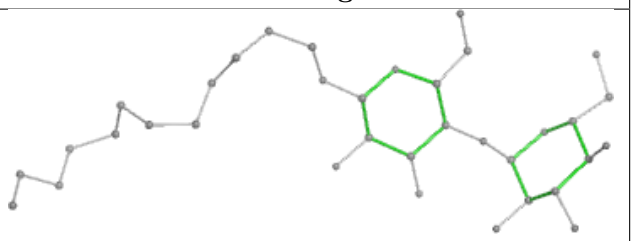


Bond angles

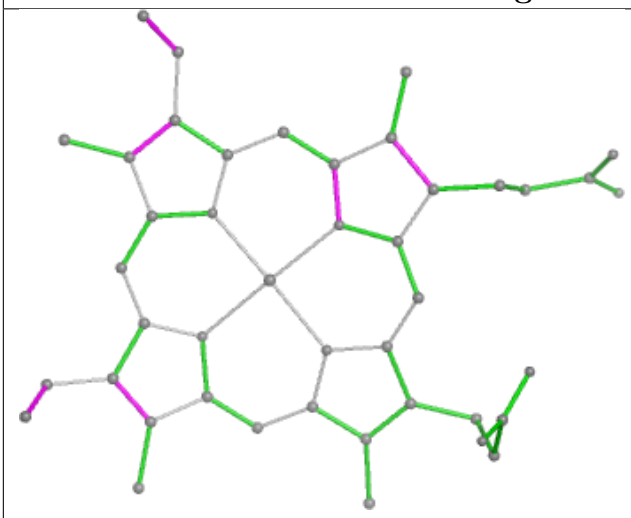


Torsions

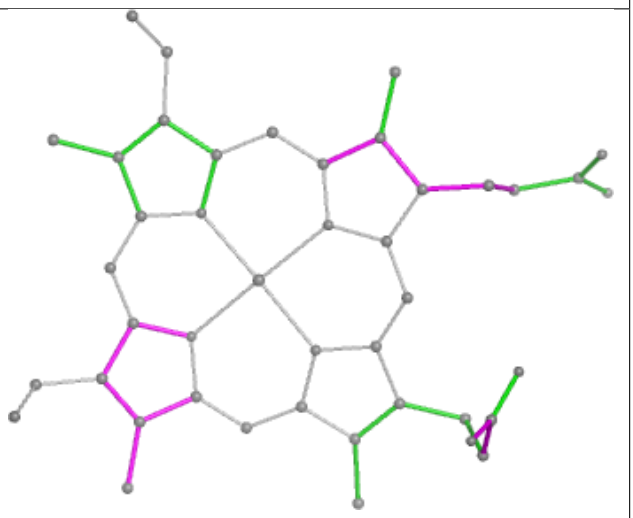


Rings

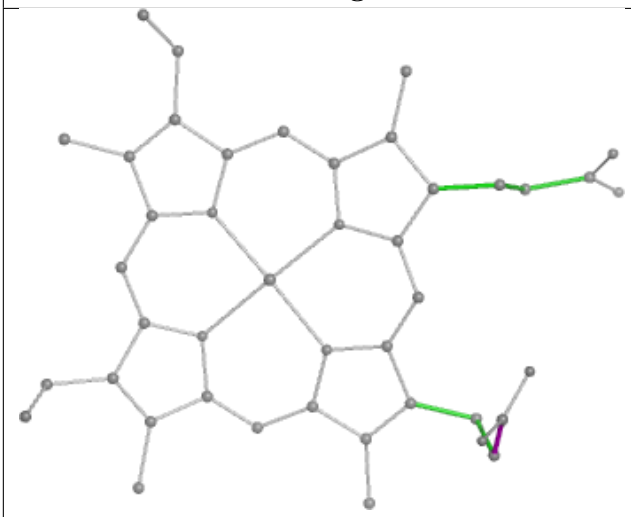
Ligand HEC P 1002



Bond lengths



Bond angles



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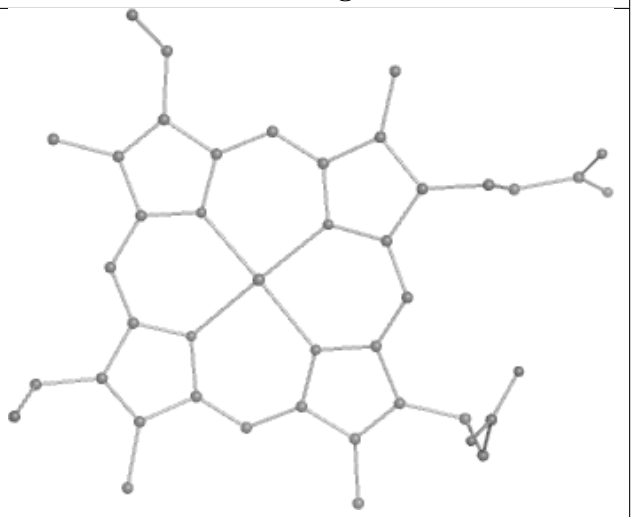
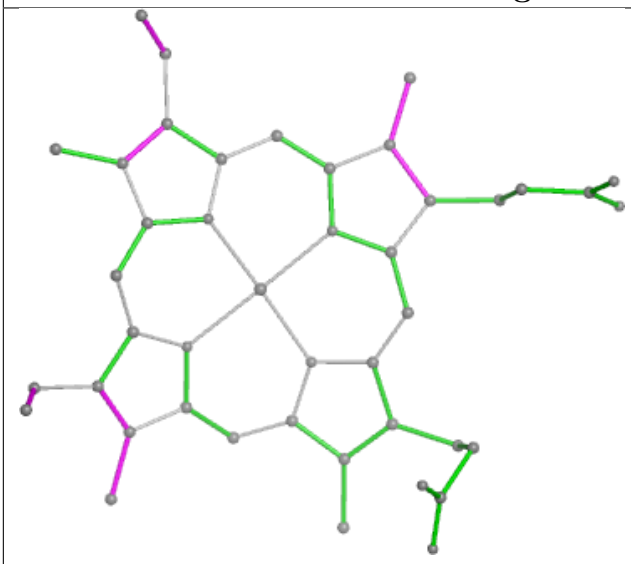
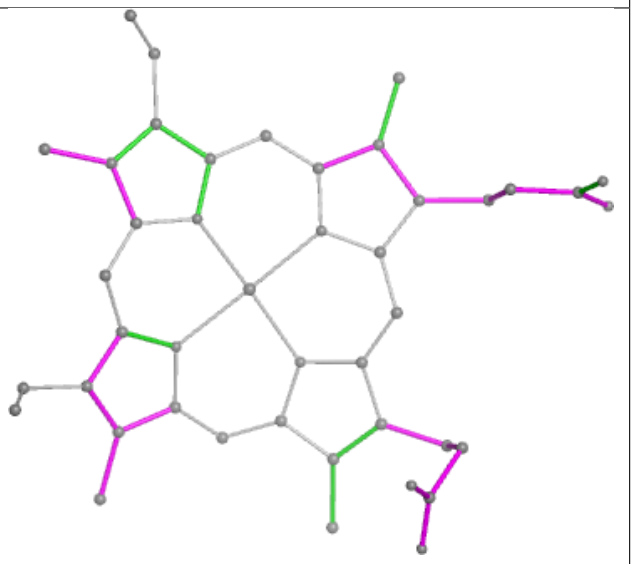


Rings

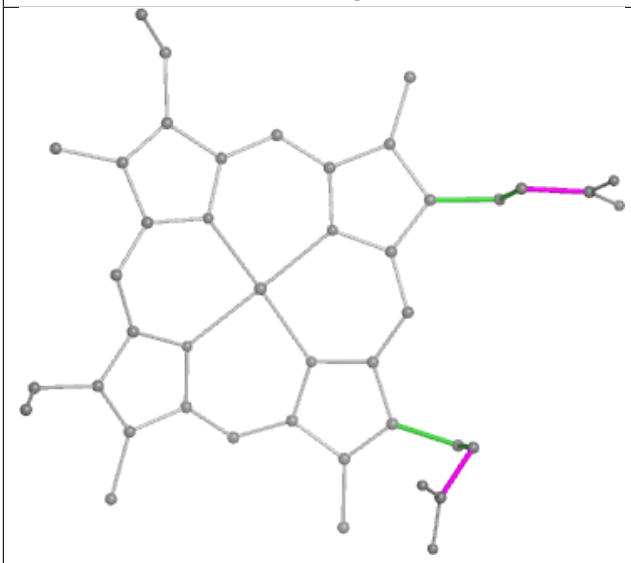
Ligand HEC C 1003



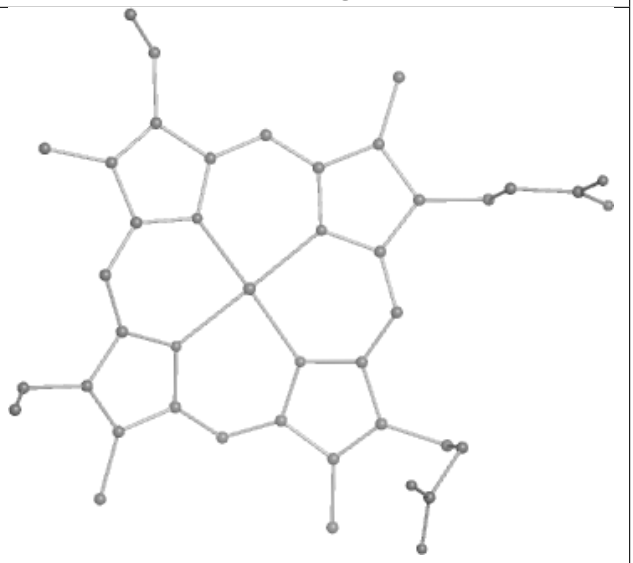
Bond lengths



Bond angles

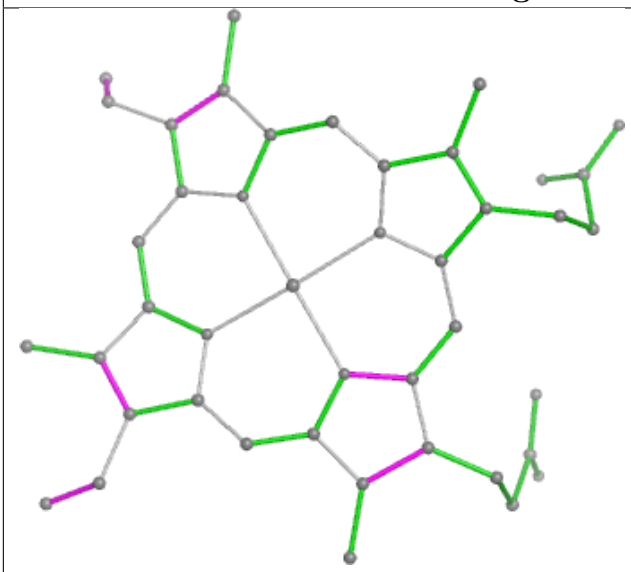


Torsions



Rings

Ligand HEC H 1001



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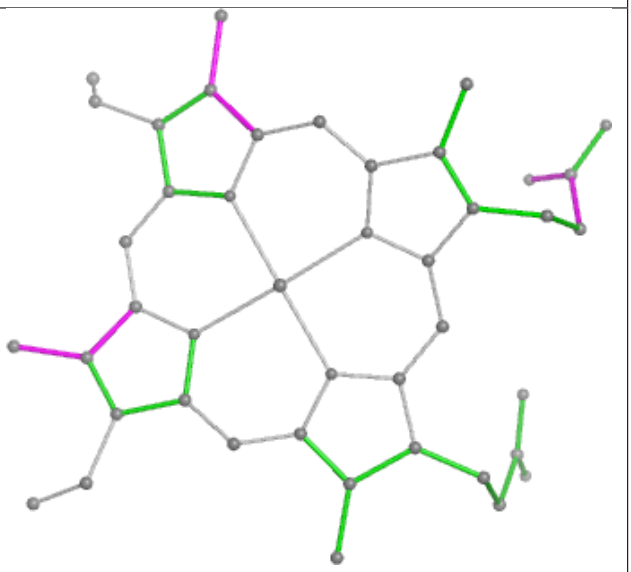
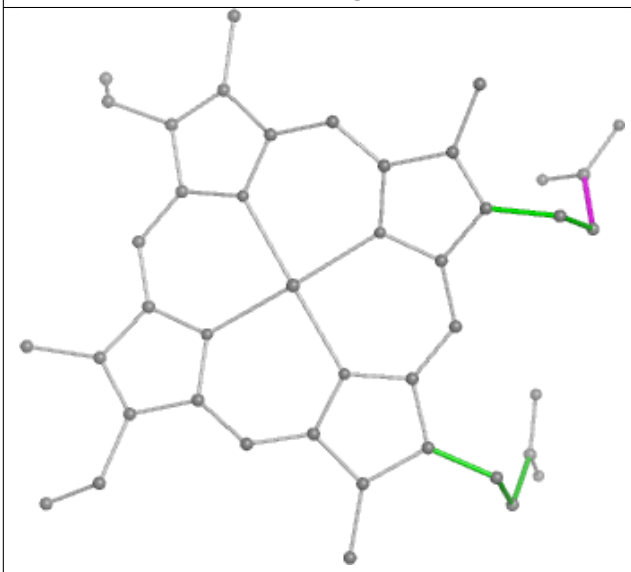


Bond angles



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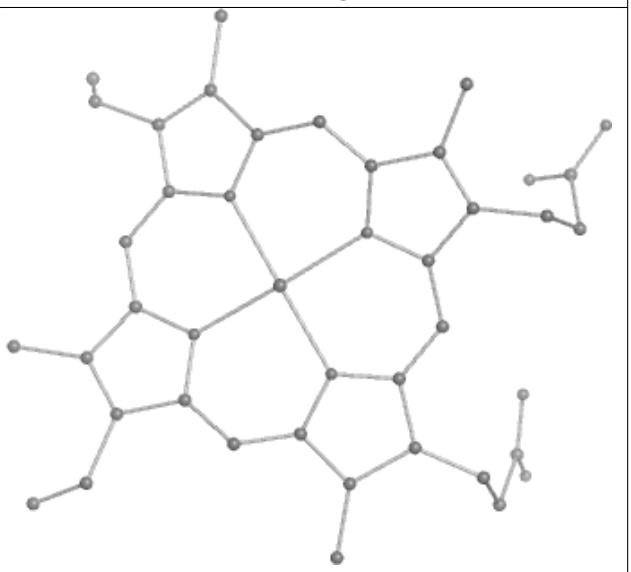
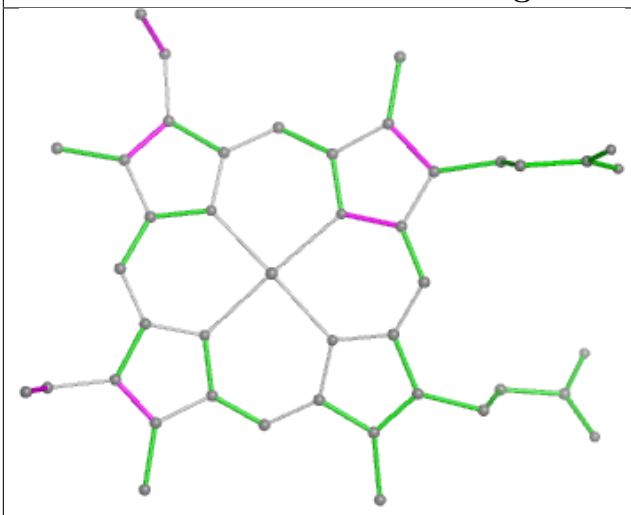


Rings

Ligand HEC R 1004



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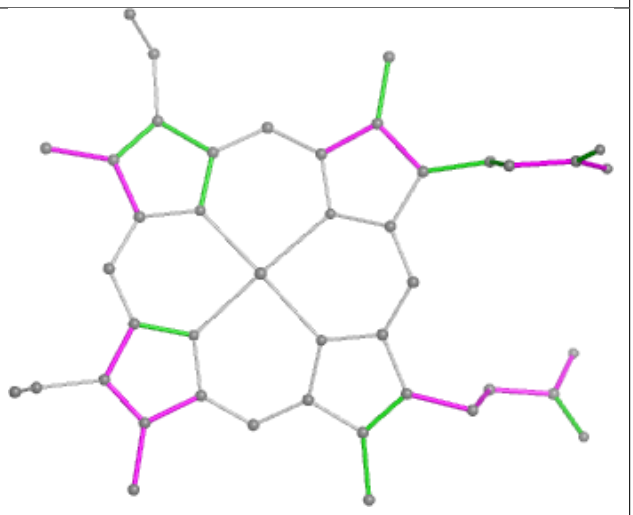
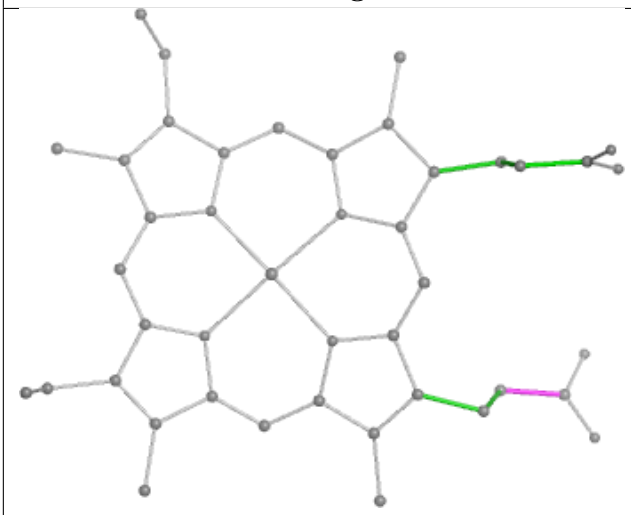
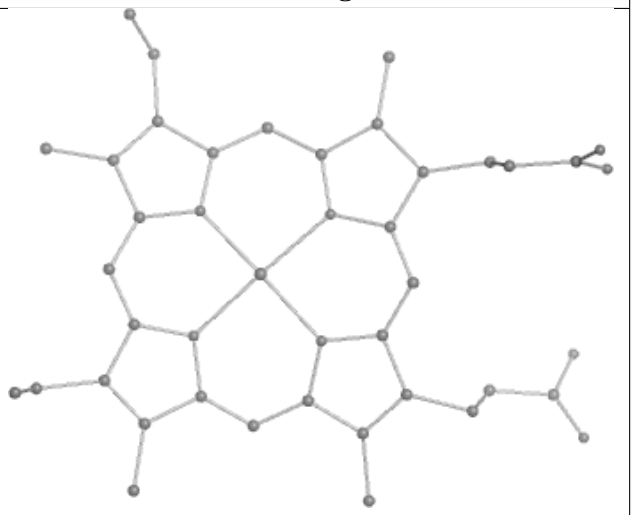


Bond angles

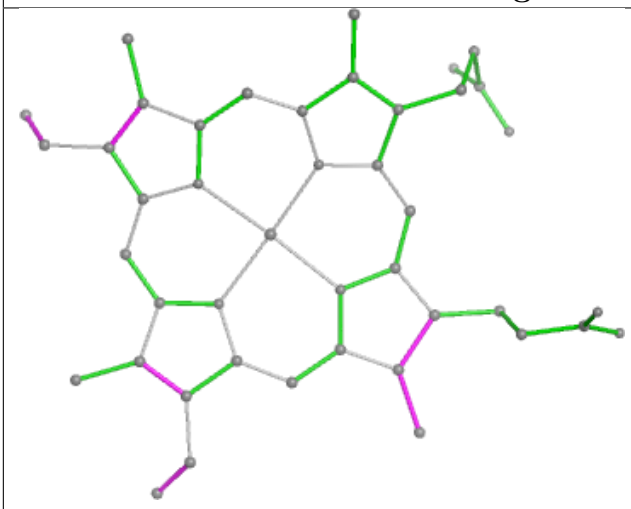


Torsions

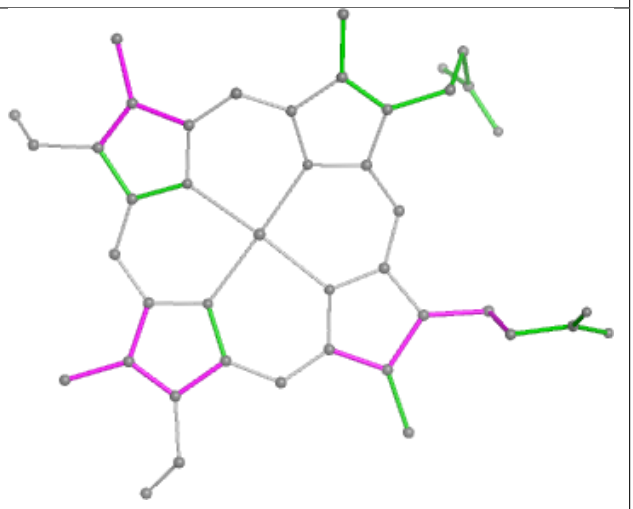


Rings

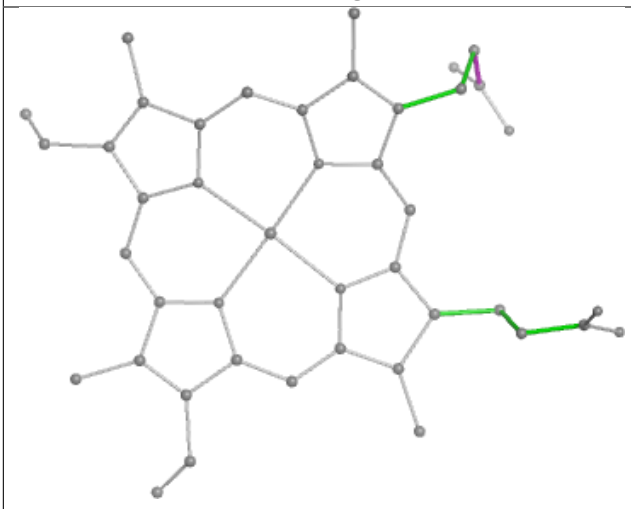
Ligand HEC A 1002



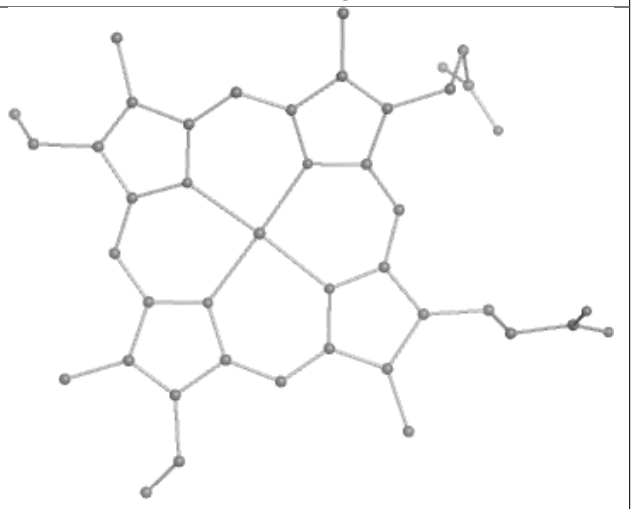
Bond lengths



Bond angles

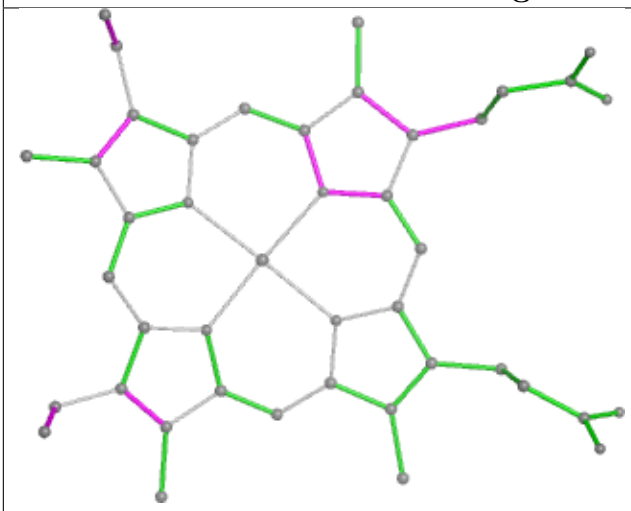


Torsions

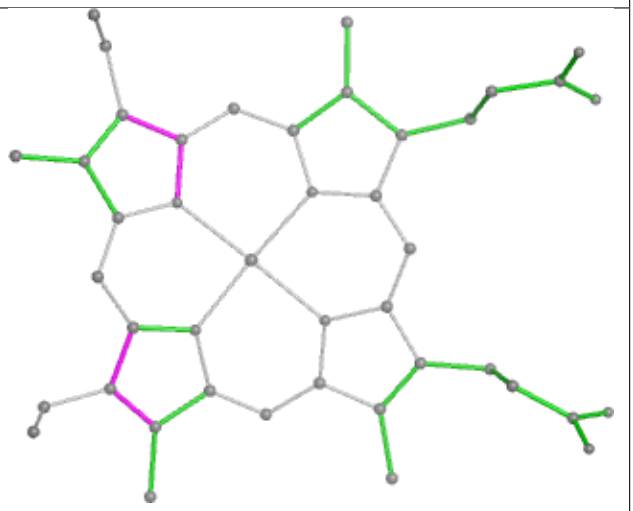


Rings

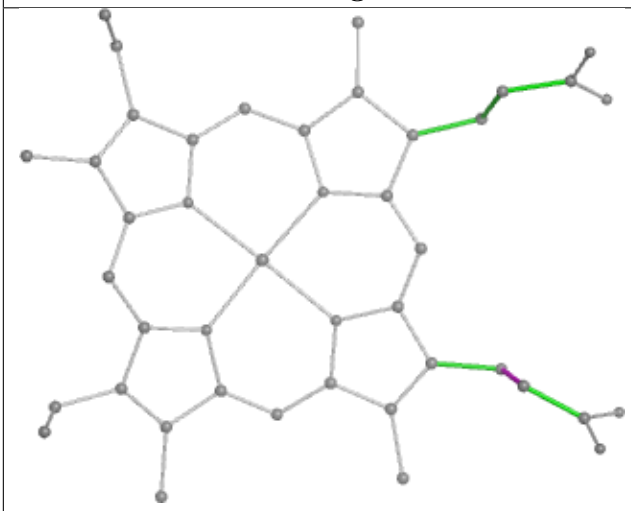
Ligand HEC G 1003



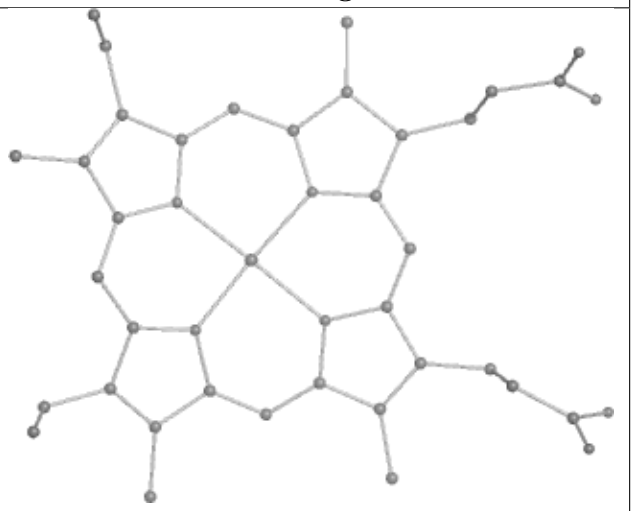
Bond lengths



Bond angles

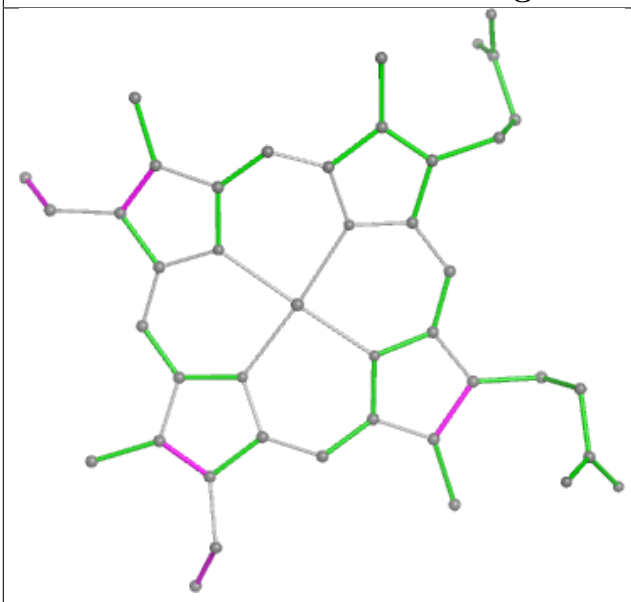


Torsions

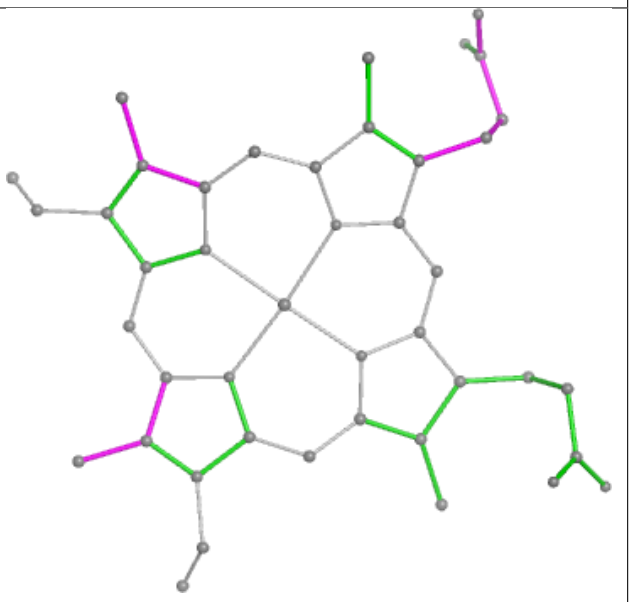


Rings

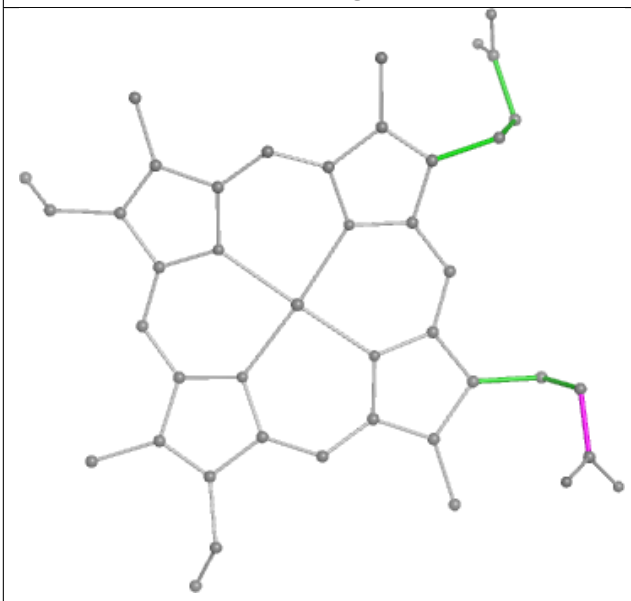
Ligand HEC B 1005



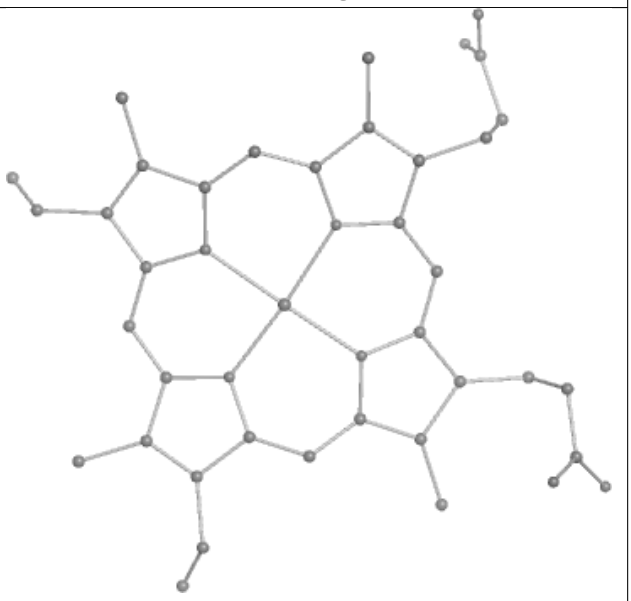
Bond lengths



Bond angles

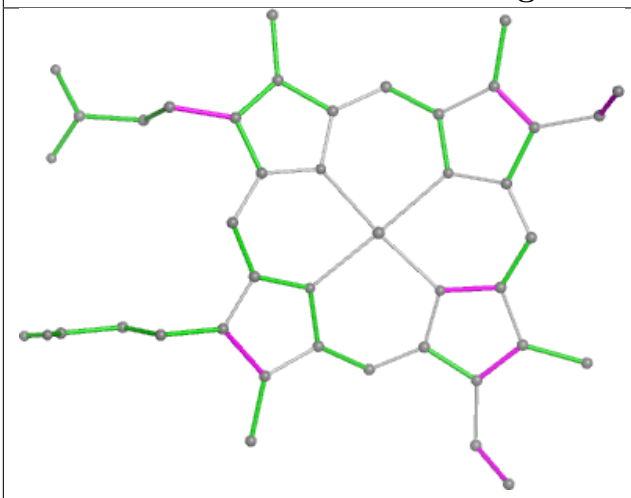


Torsions



Rings

Ligand HEC J 1004



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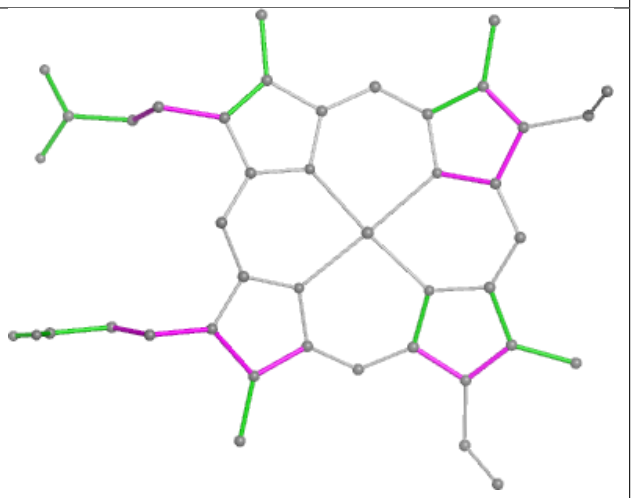

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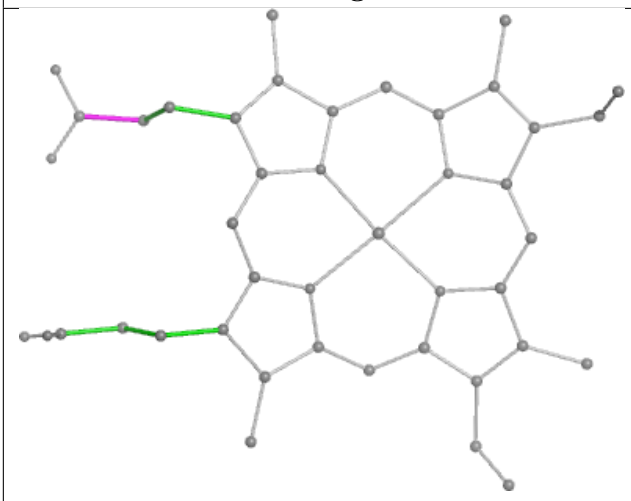

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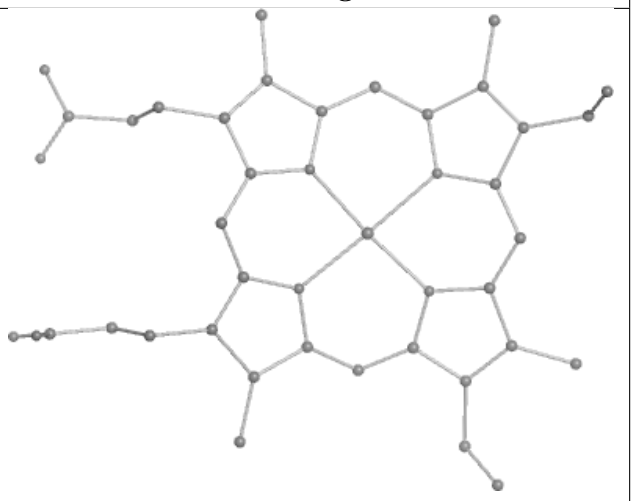
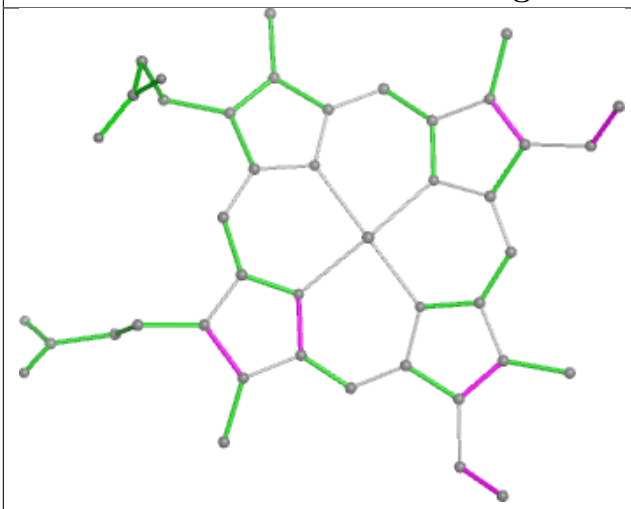


Rings

Ligand HEC D 1002



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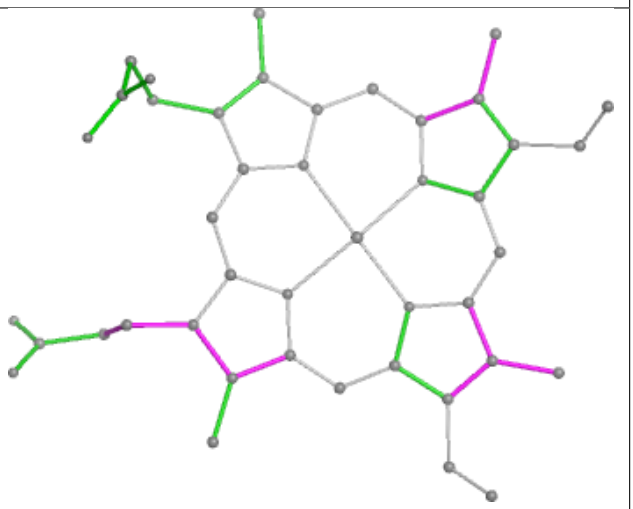
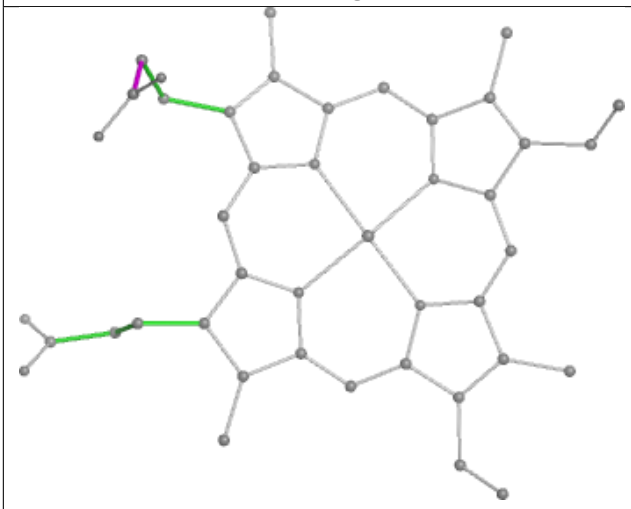


Bond angles



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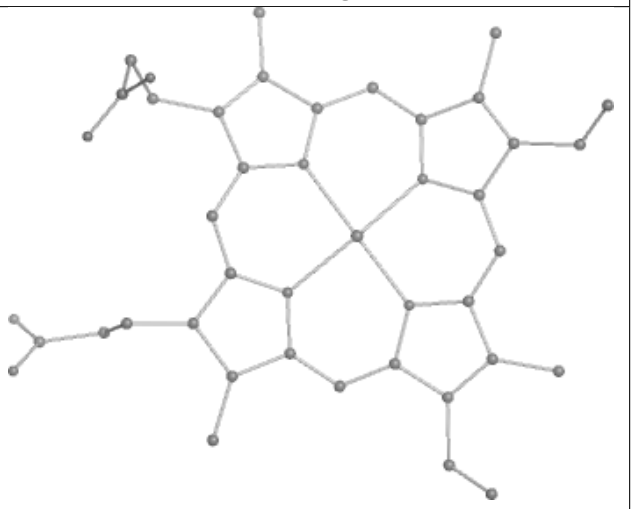
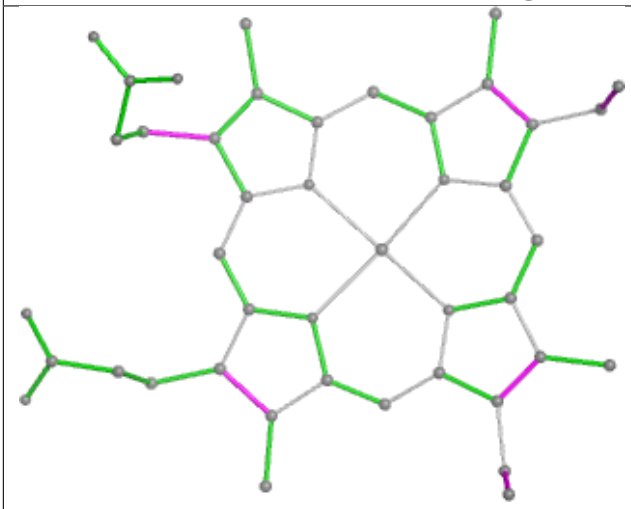


Rings

Ligand HEC I 1001



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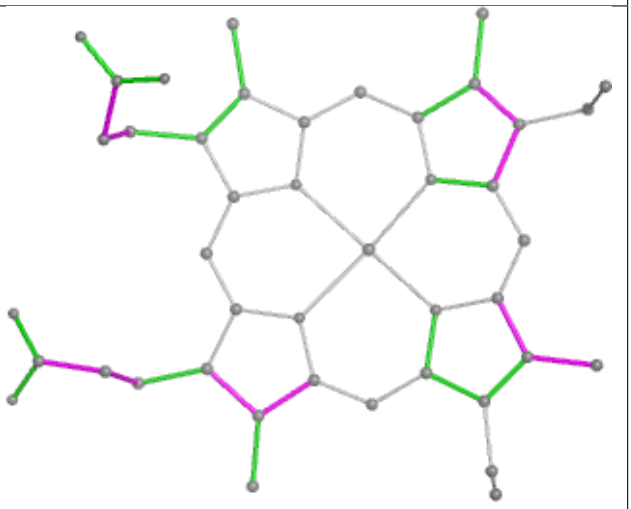

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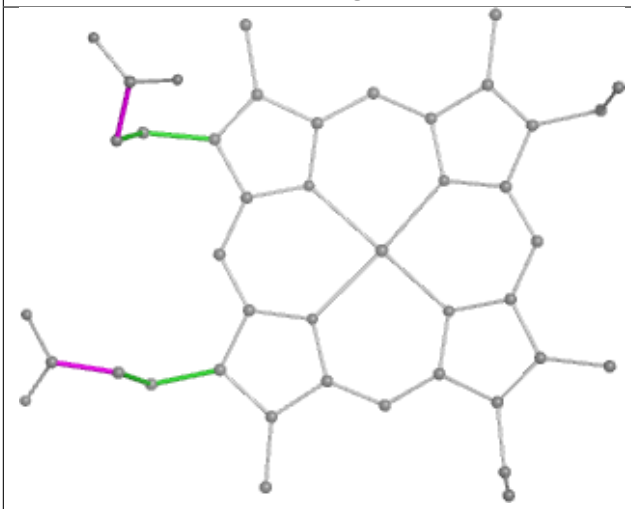

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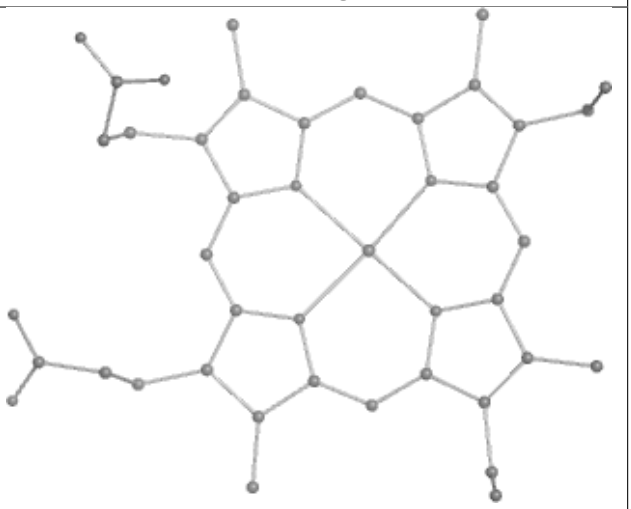
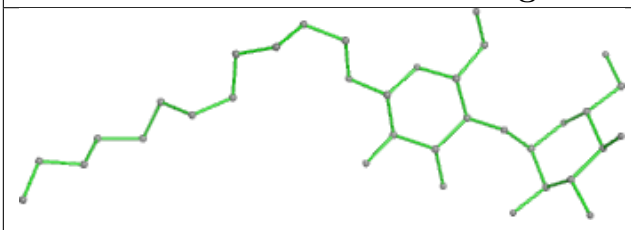


Rings

Ligand LMT I 1005



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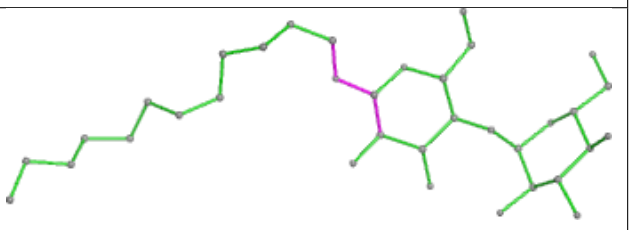
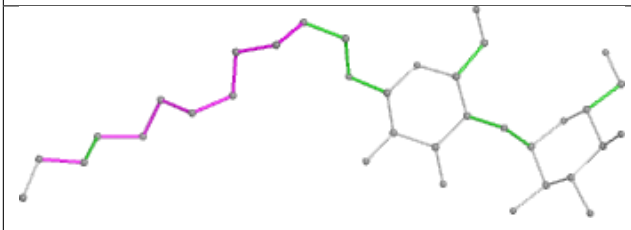


Bond angles



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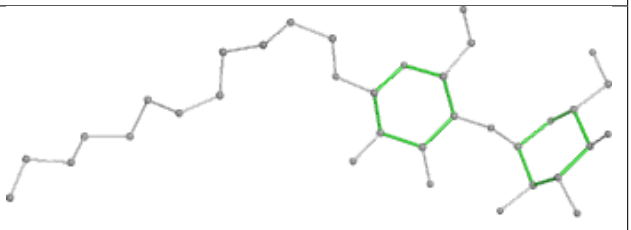
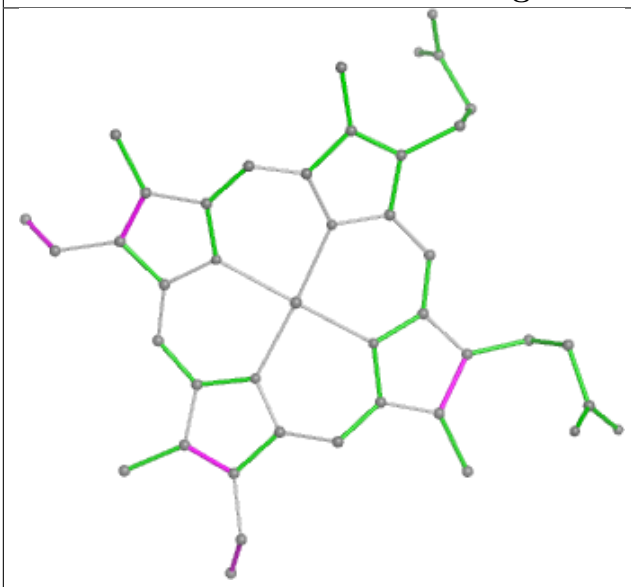


Rings

Ligand HEC K 1005



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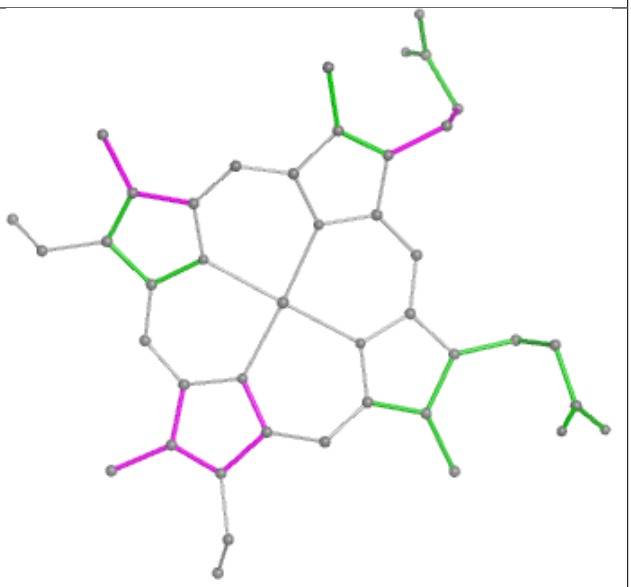

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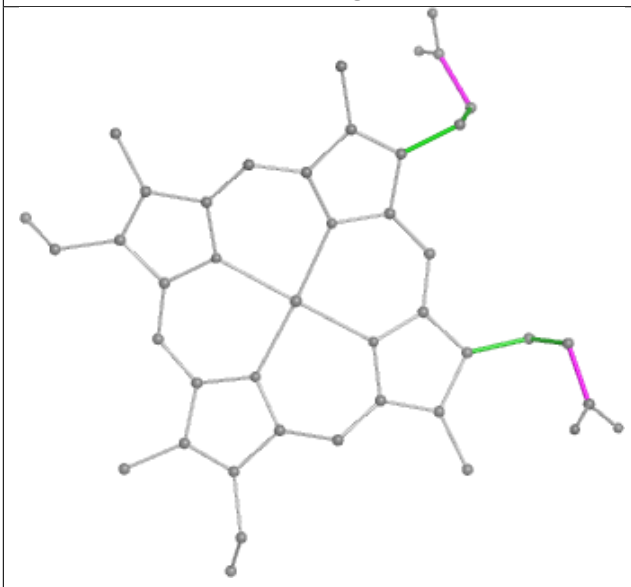

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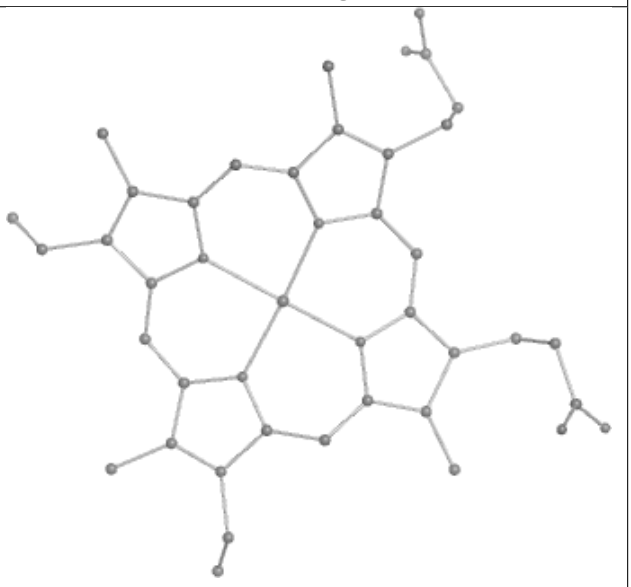
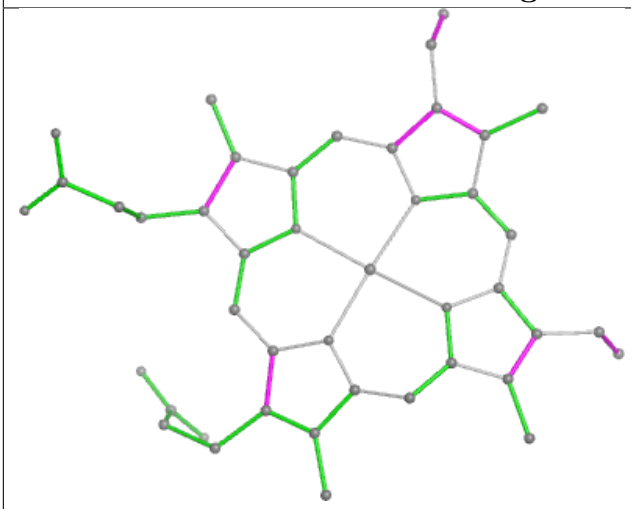


Rings

Ligand HEC I 1002



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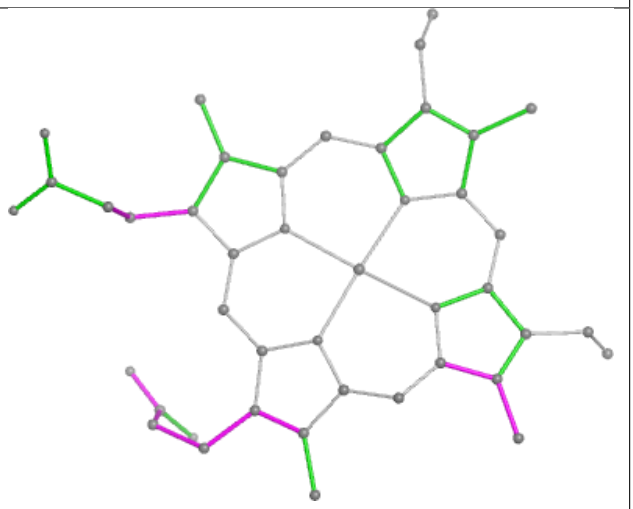
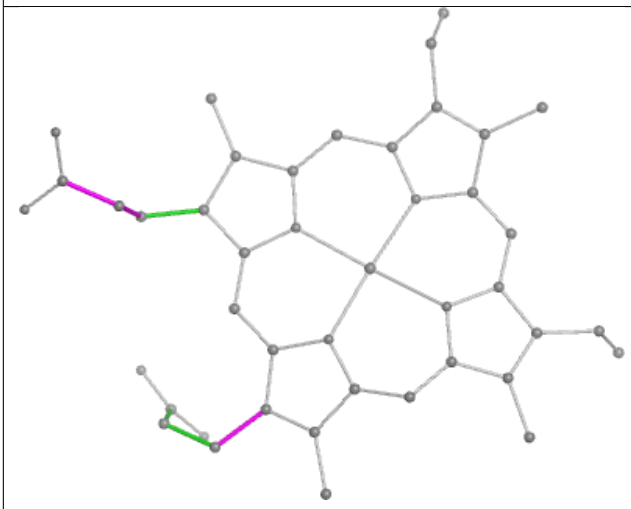


Bond angles



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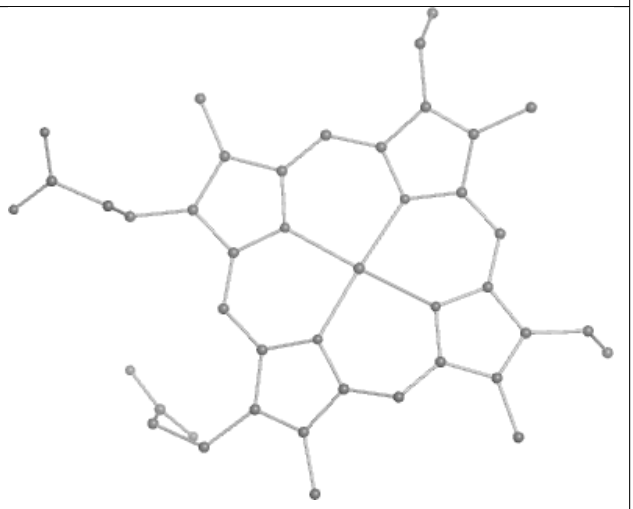
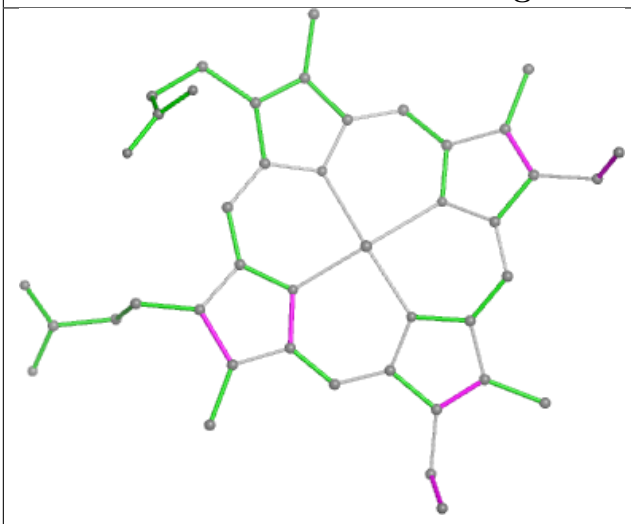


Rings

Ligand HEC C 1002



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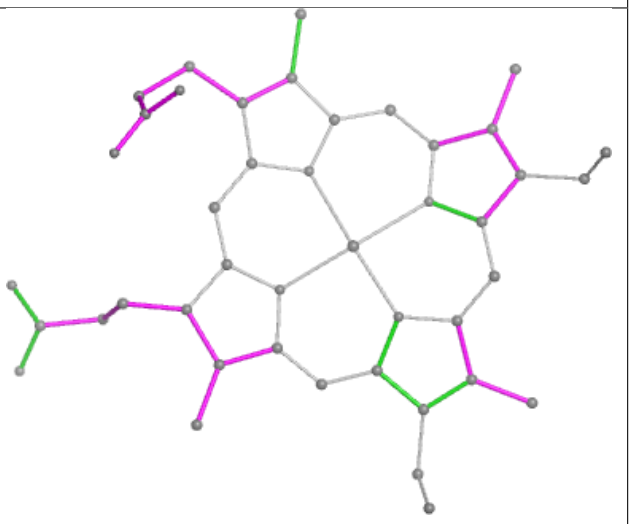
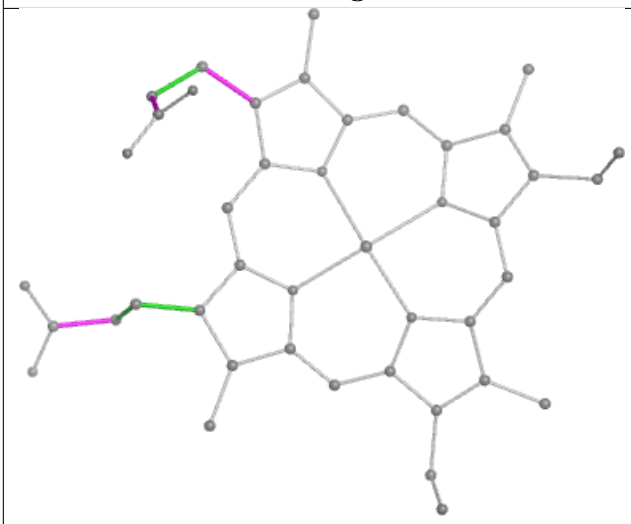


Bond angles



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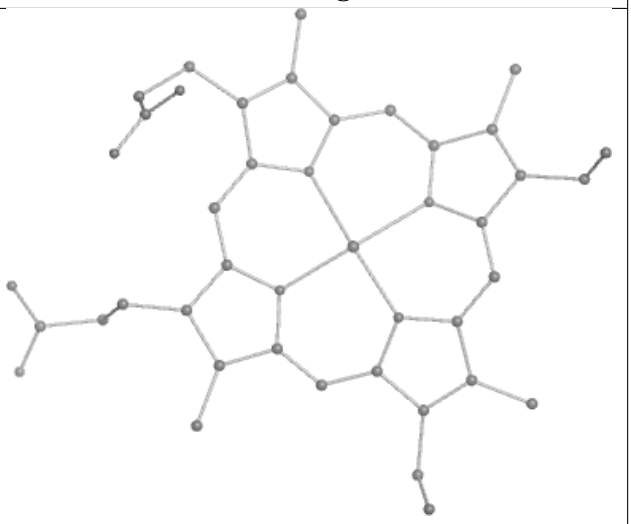
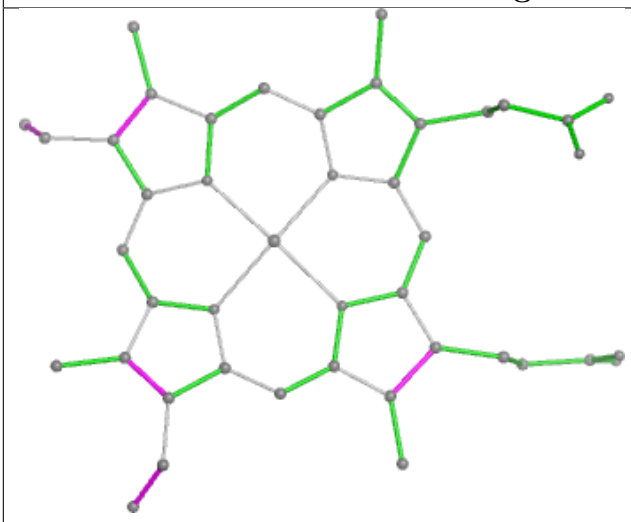


Rings

Ligand HEC C 1004



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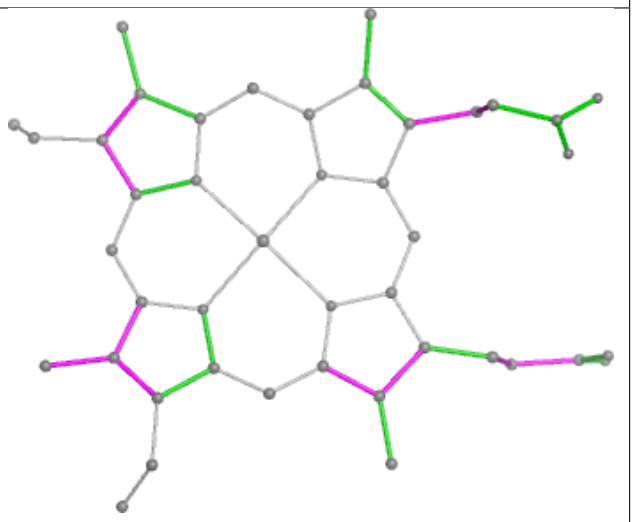
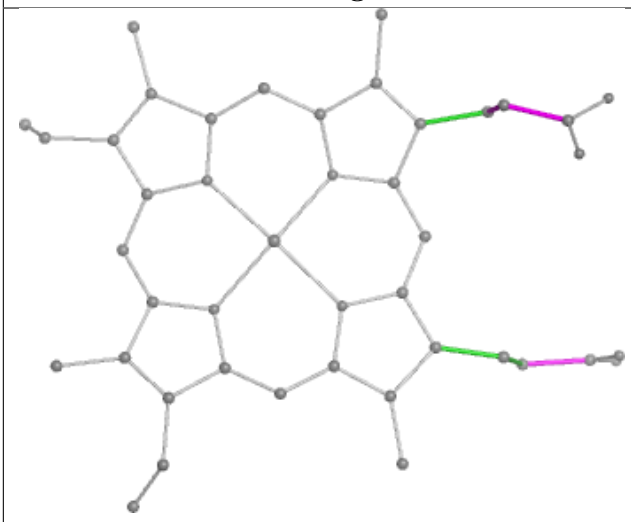


Bond angles



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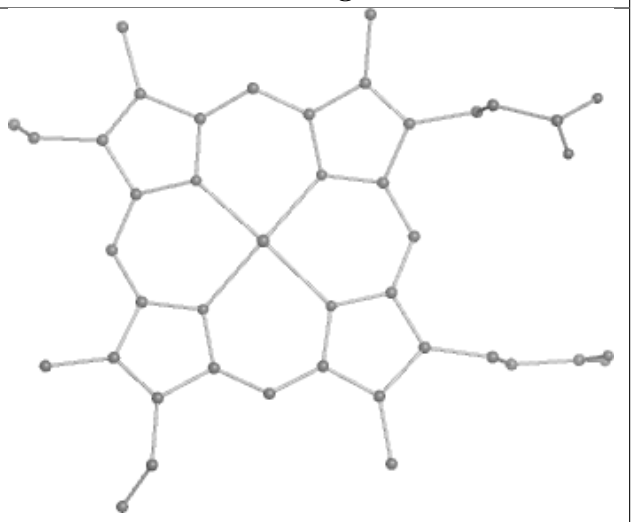
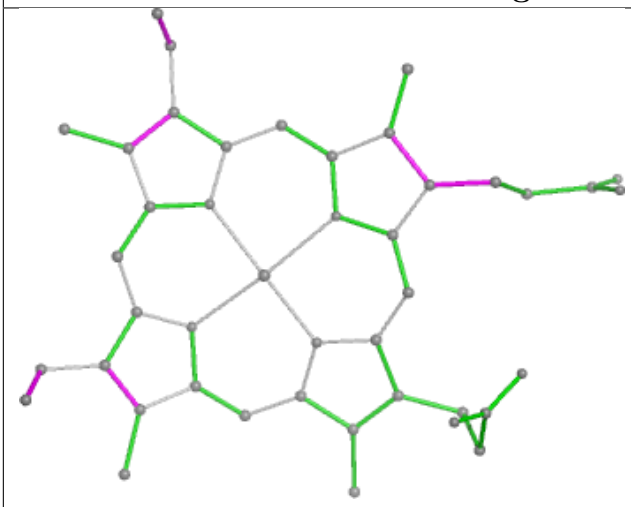


Rings

Ligand HEC K 1002



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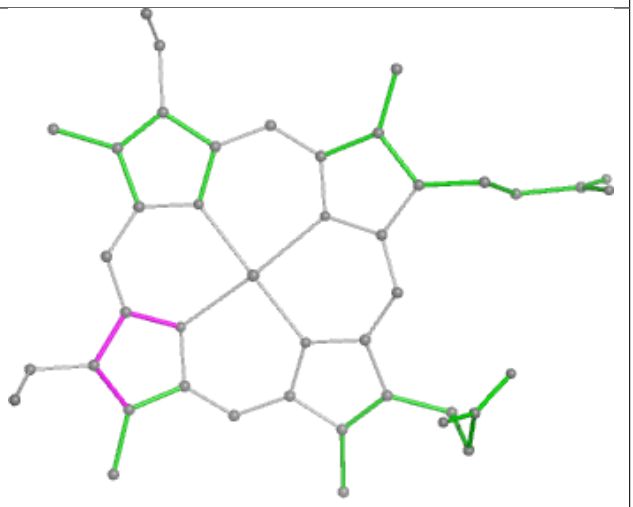
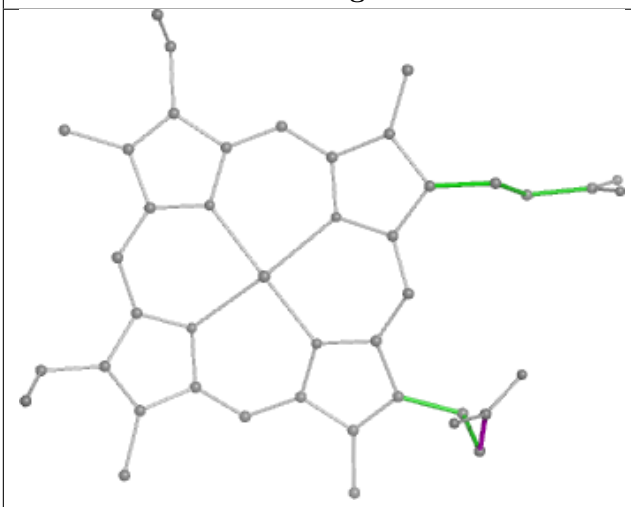


Bond angles



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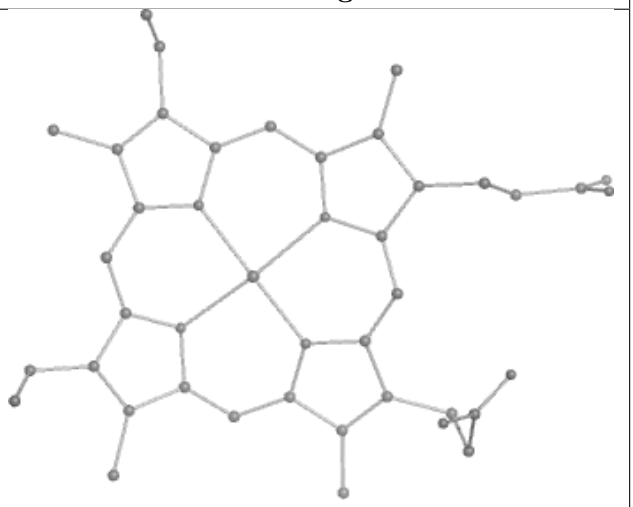
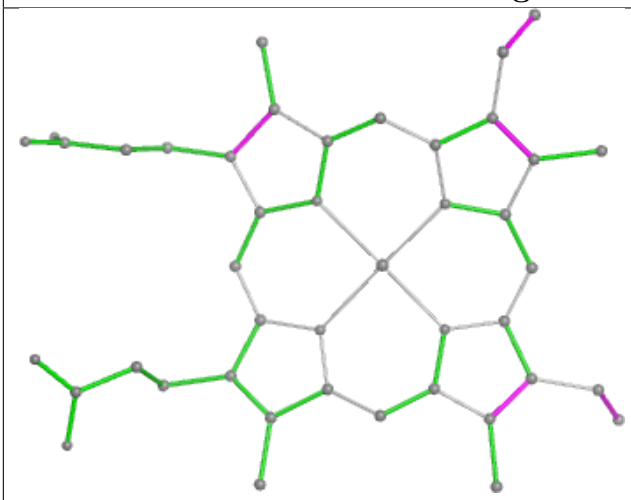


Rings

Ligand HEC H 1004



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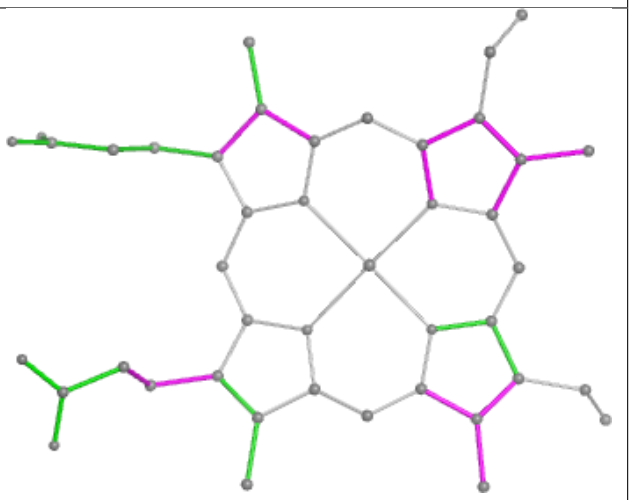
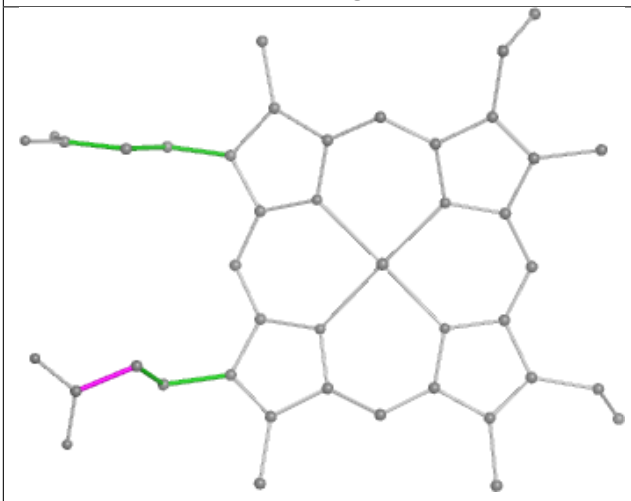
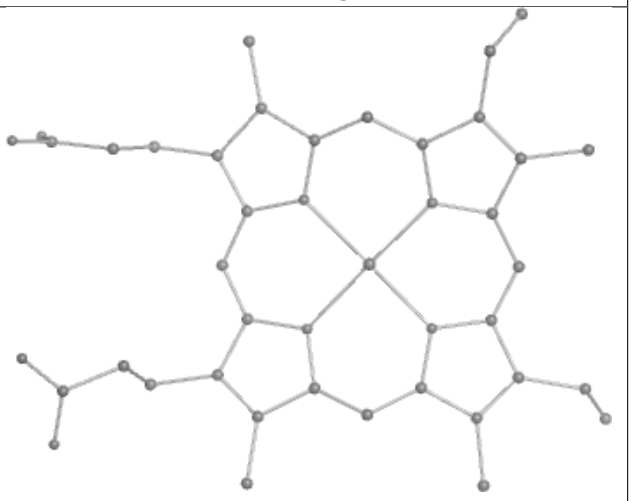


Bond angles

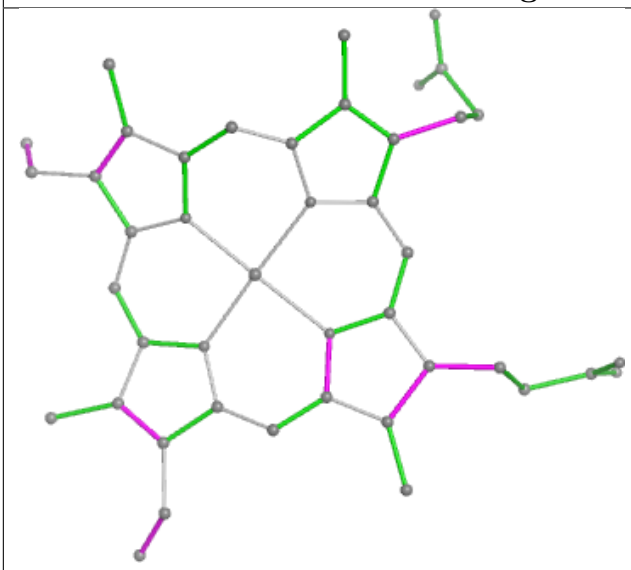


Torsions



Rings

Ligand HEC I 1003



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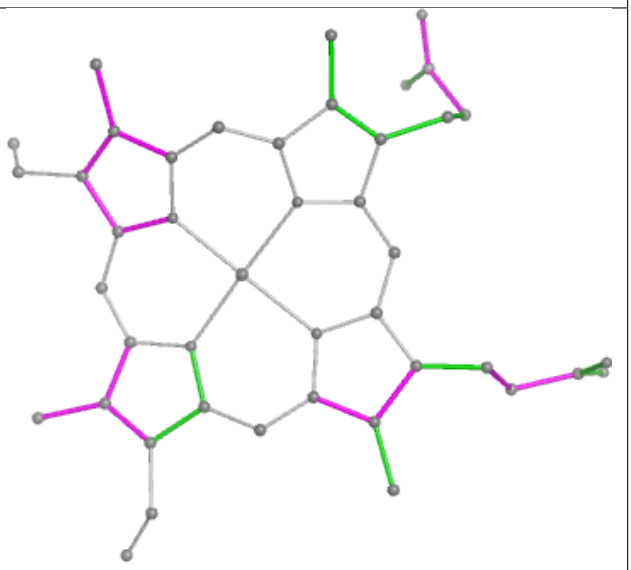
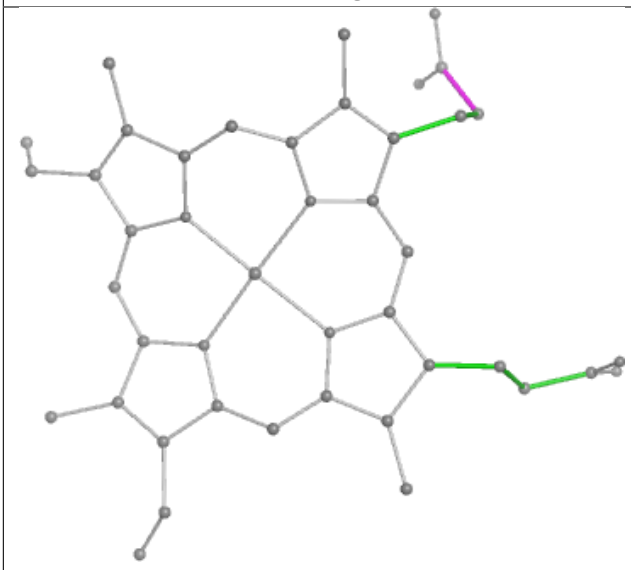


Bond angles



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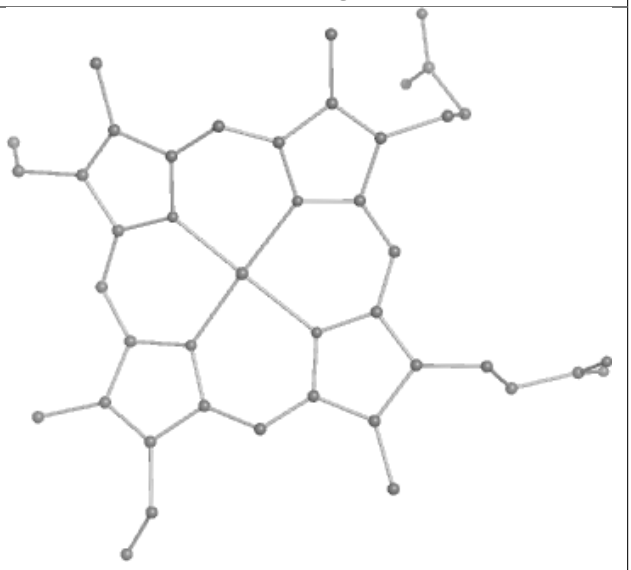
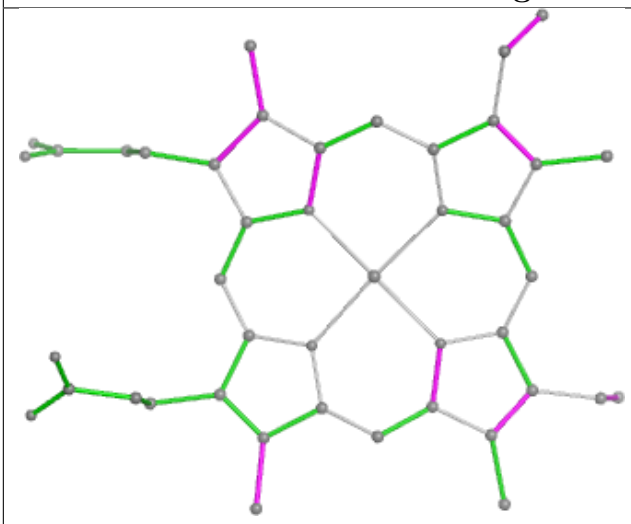
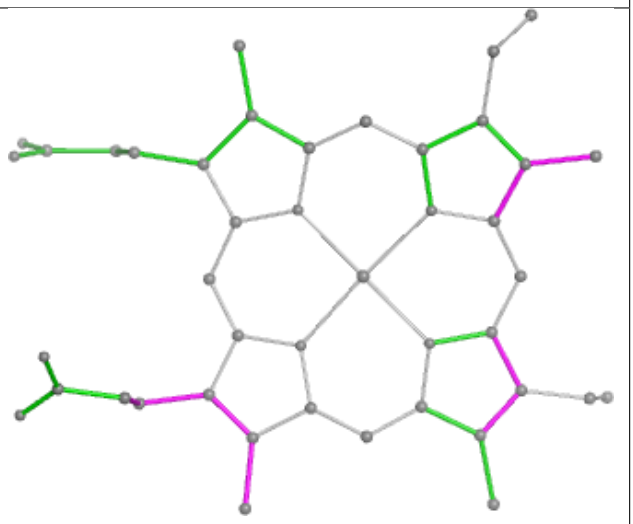


Rings

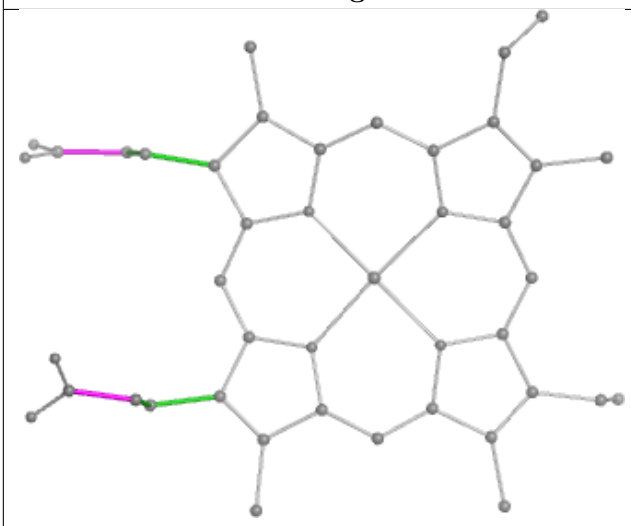
Ligand HEC O 1004



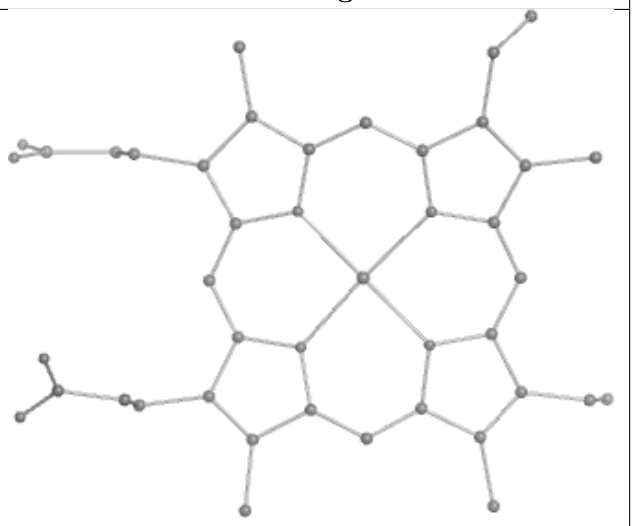
Bond lengths



Bond angles

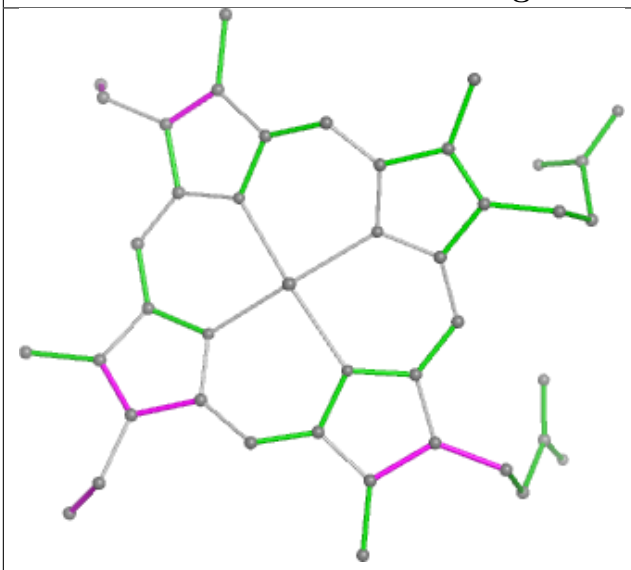


Torsions

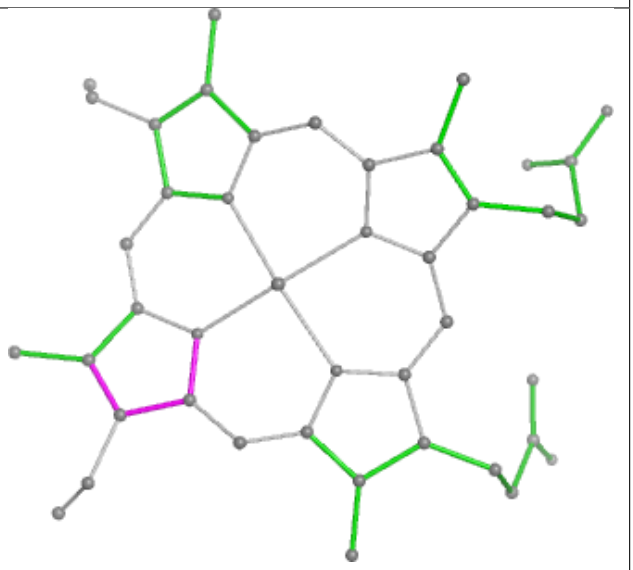


Rings

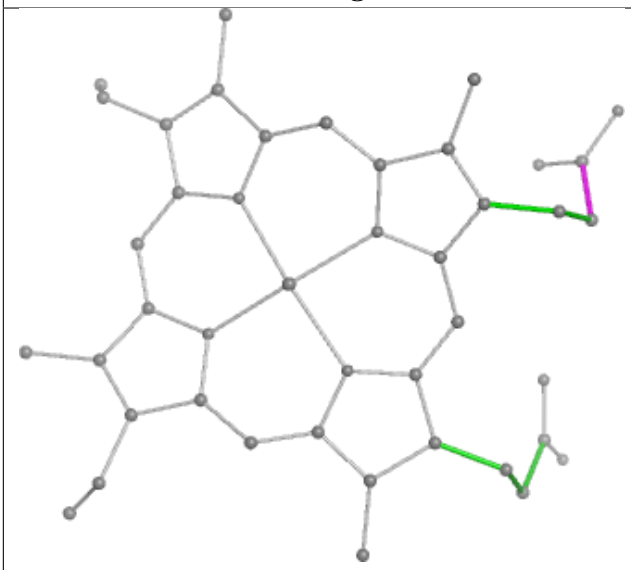
Ligand HEC K 1001



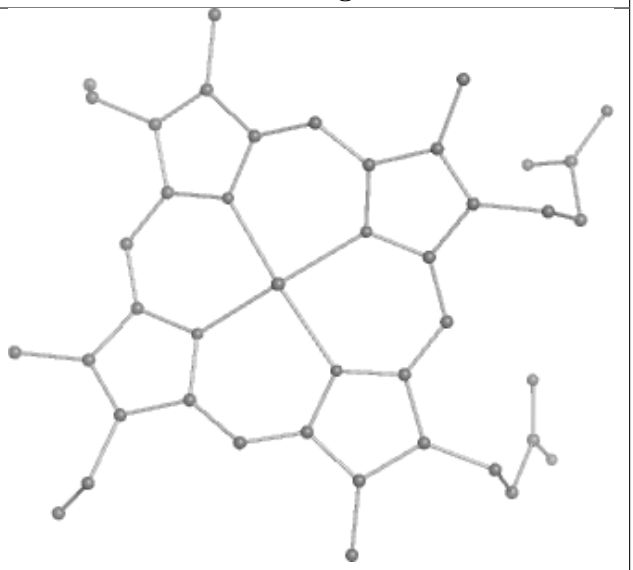
Bond lengths



Bond angles

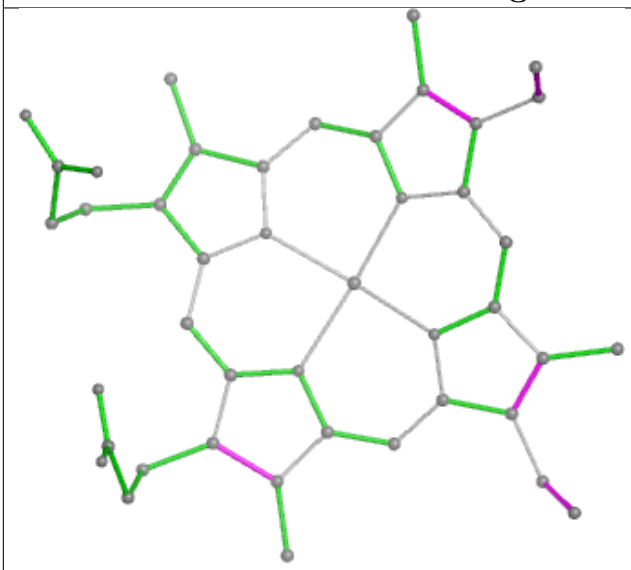


Torsions

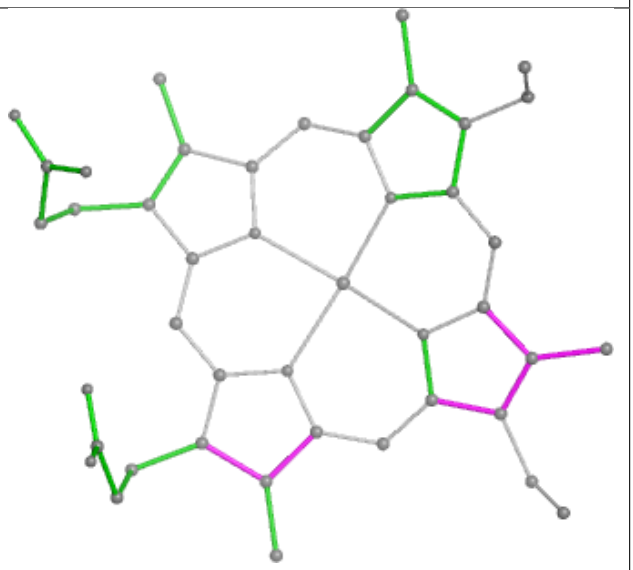


Rings

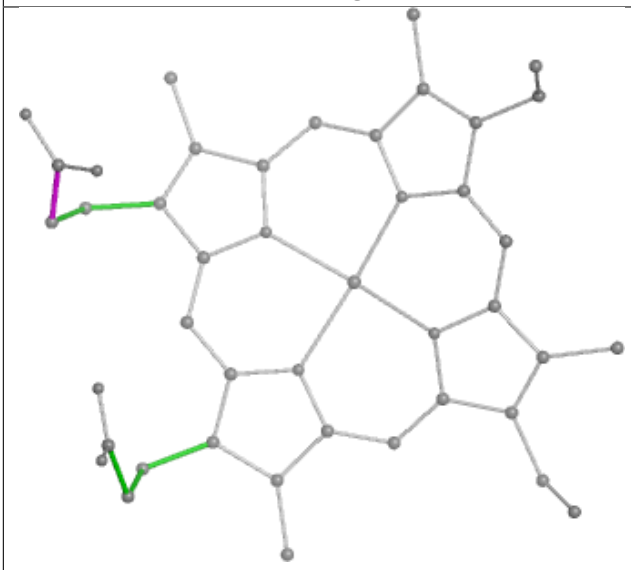
Ligand HEC M 1001



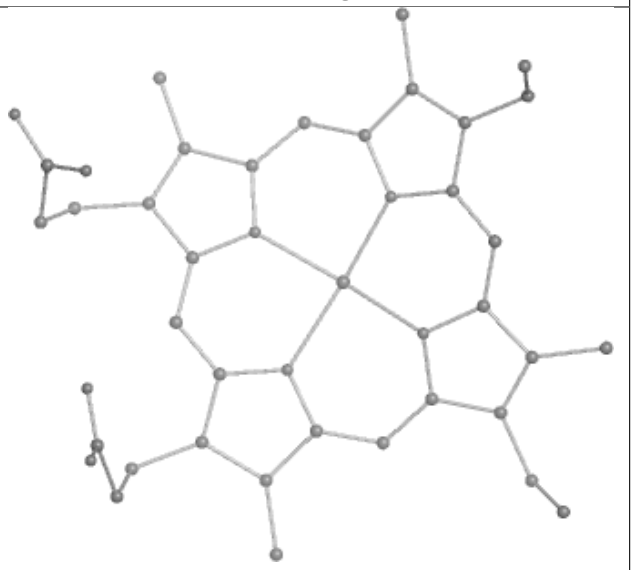
Bond lengths



Bond angles

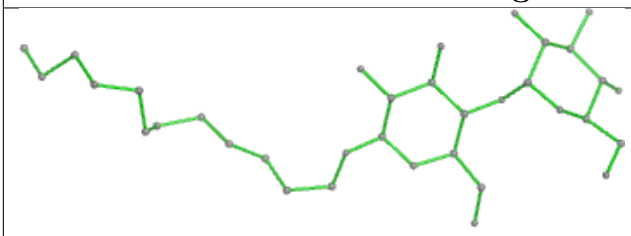


Torsions

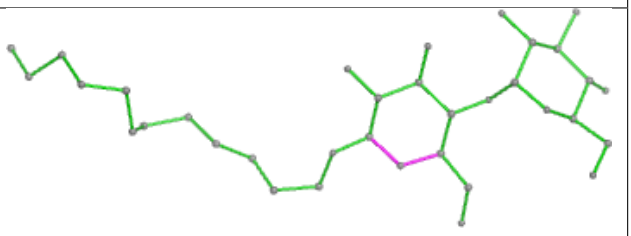


Rings

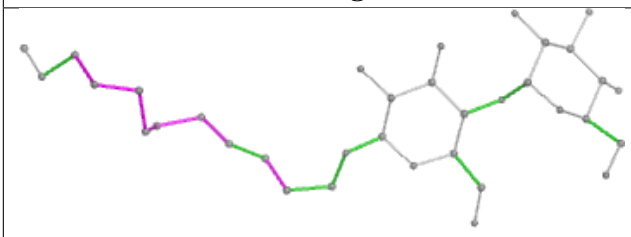
Ligand LMT C 1005



Bond lengths



Bond angles



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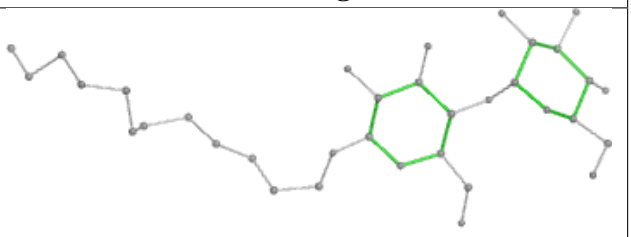
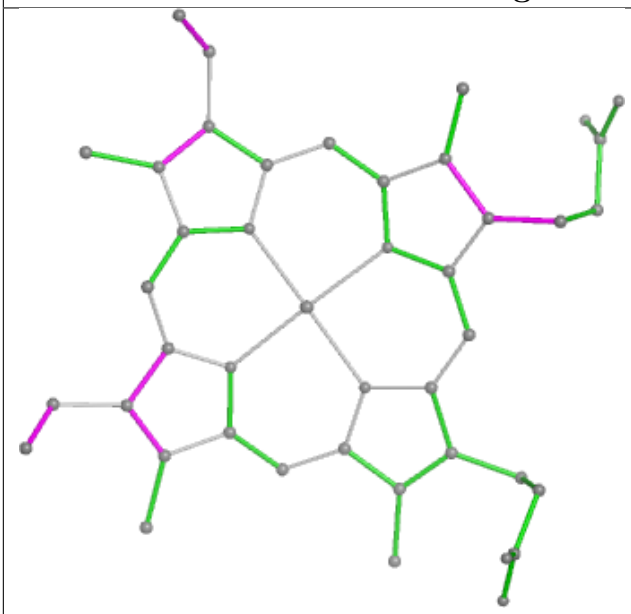


Rings

Ligand HEC A 1005



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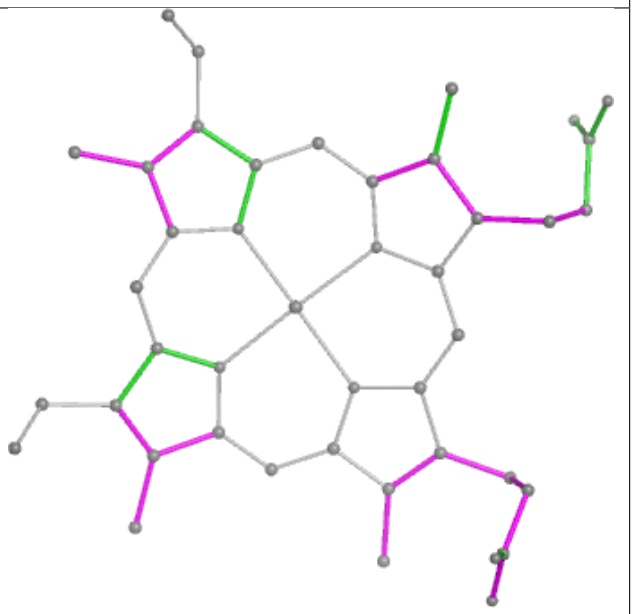
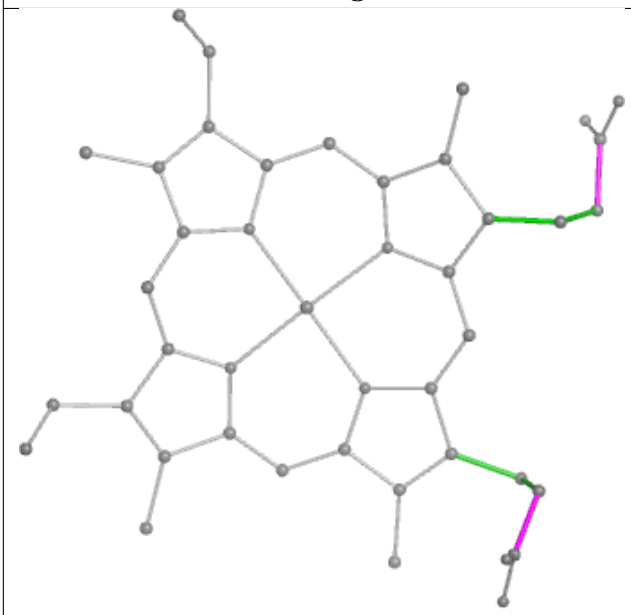
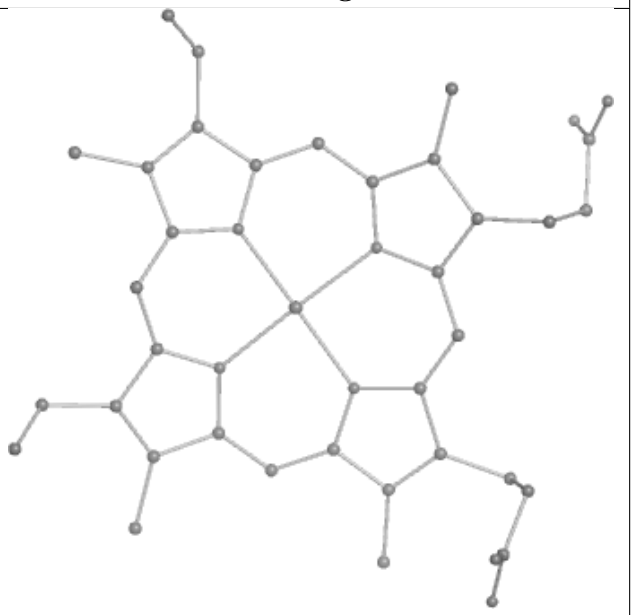


Bond angles

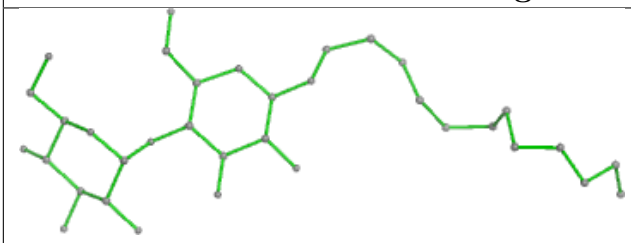


Torsions



Rings

Ligand LMT L 1005



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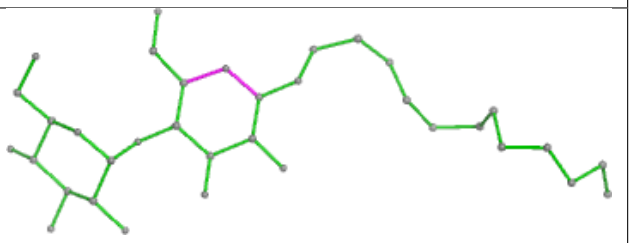
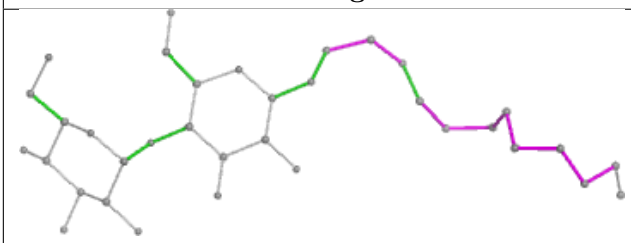


Bond angles



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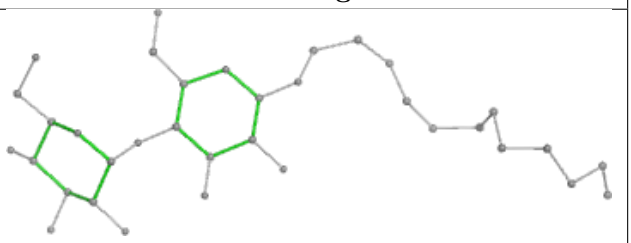
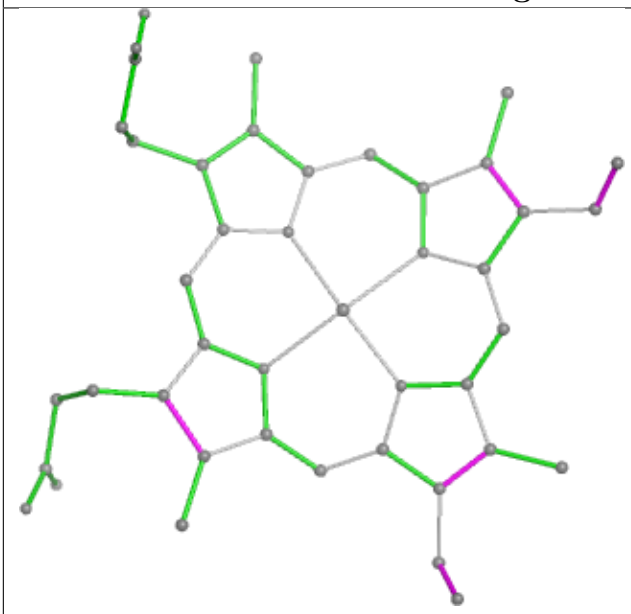
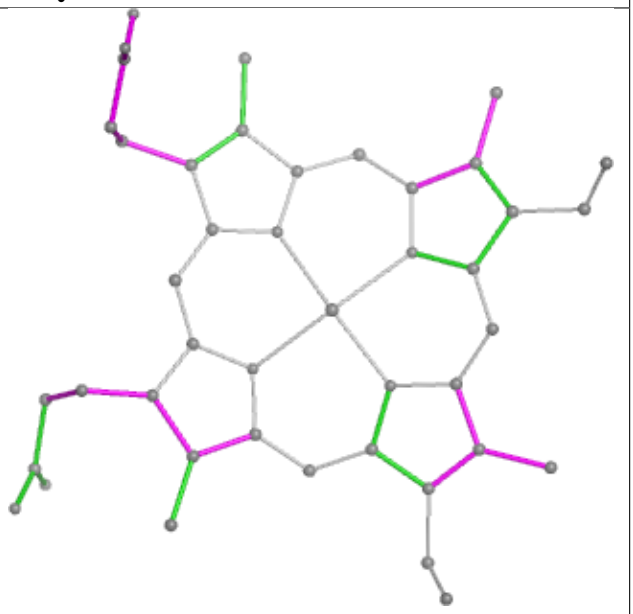


Rings

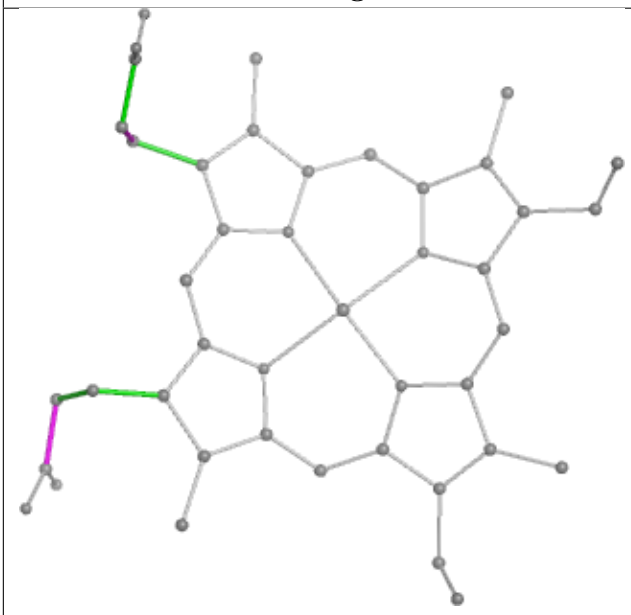
Ligand HEC Q 1005



Bond lengths



Bond angles



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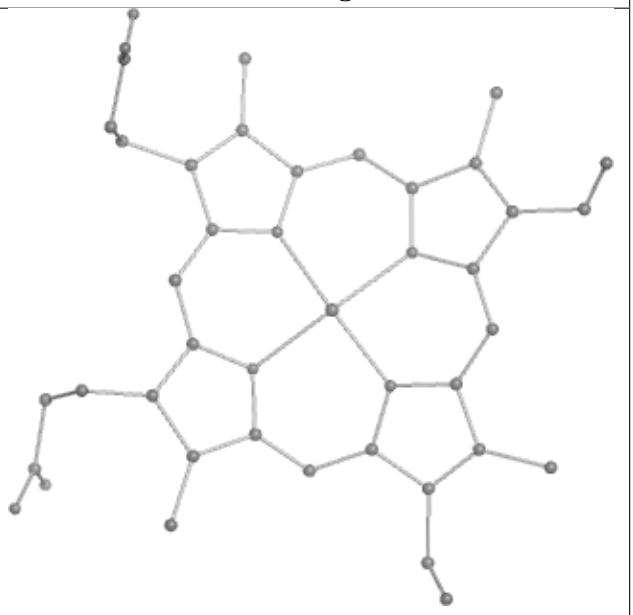
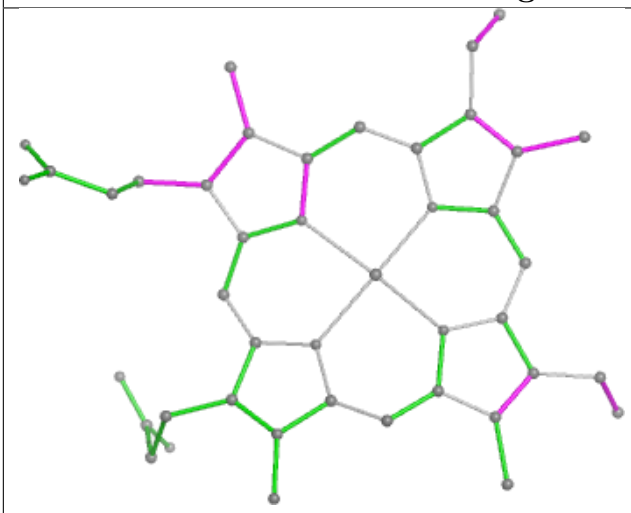


Rings

Ligand HEC J 1002



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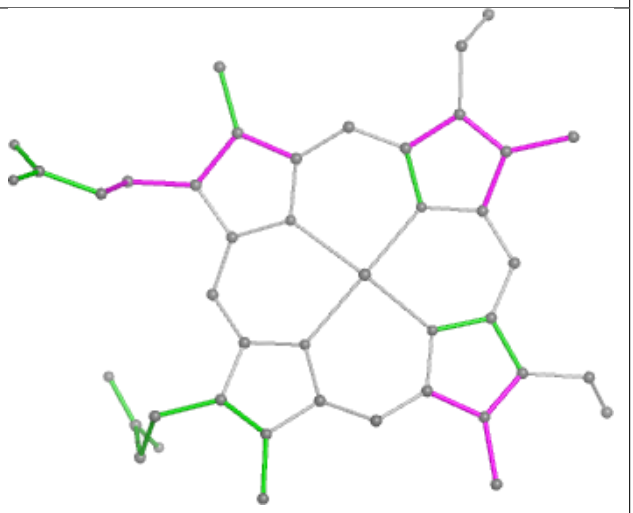
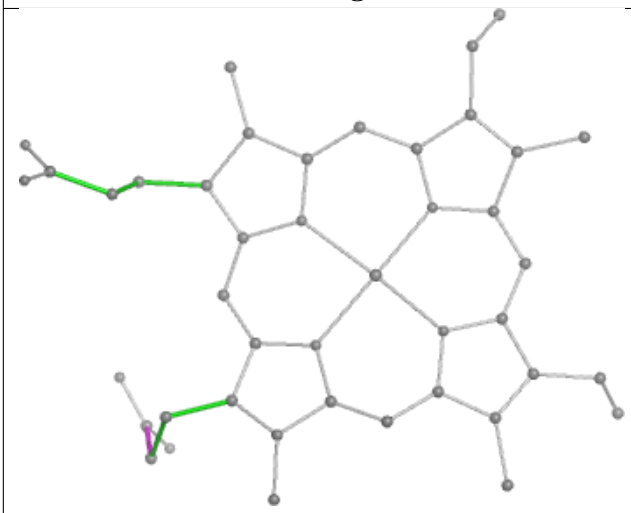


Bond angles



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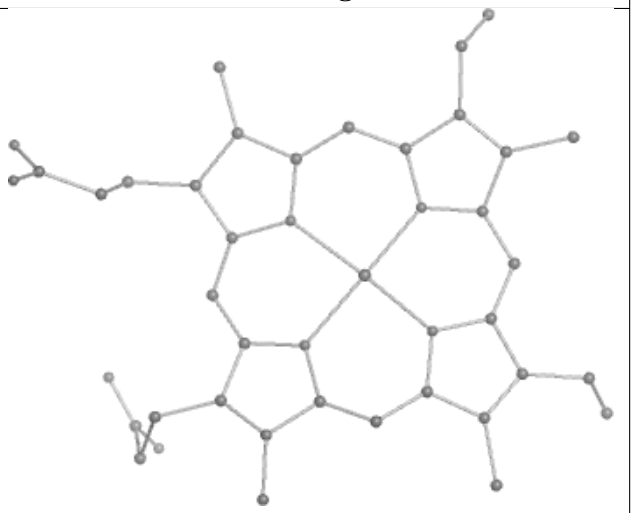
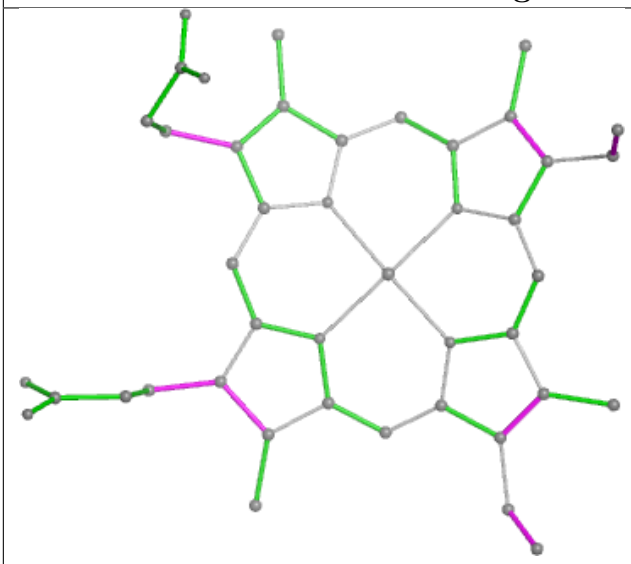


Rings

Ligand HEC O 1003



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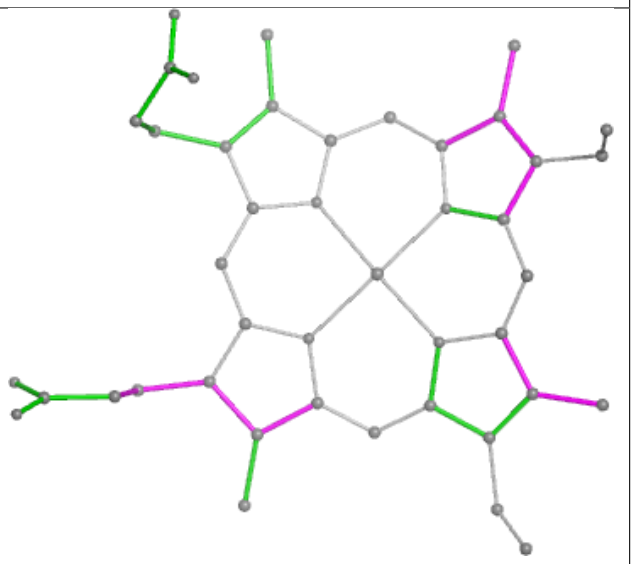
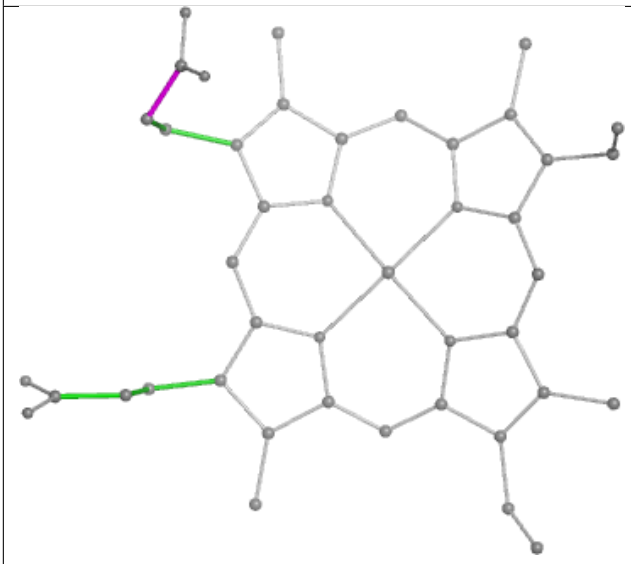


Bond angles



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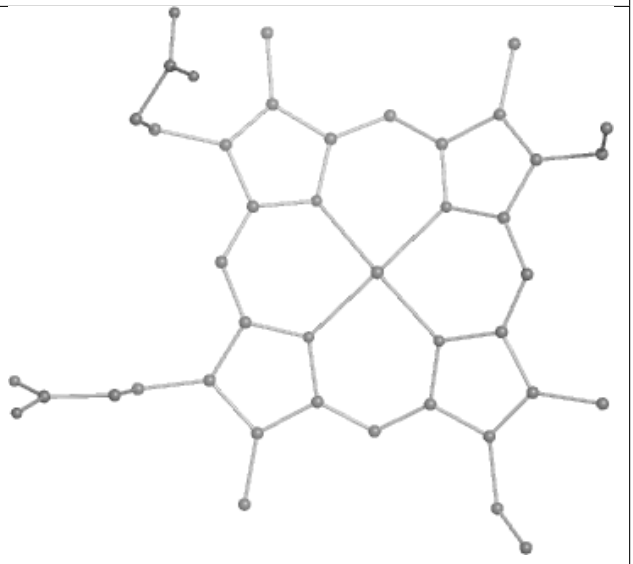
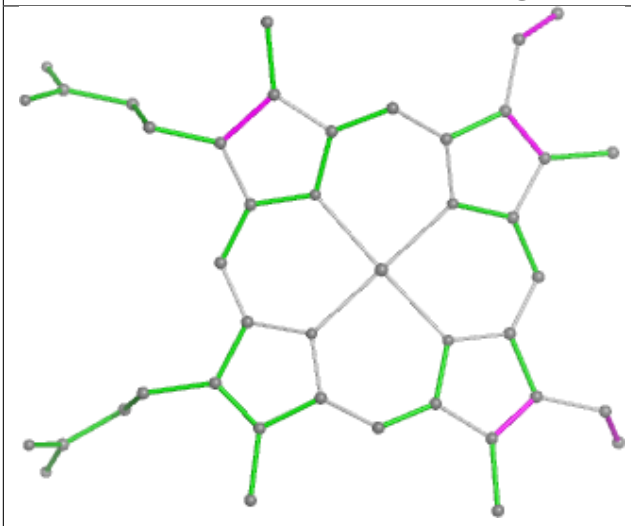


Rings

Ligand HEC Q 1003



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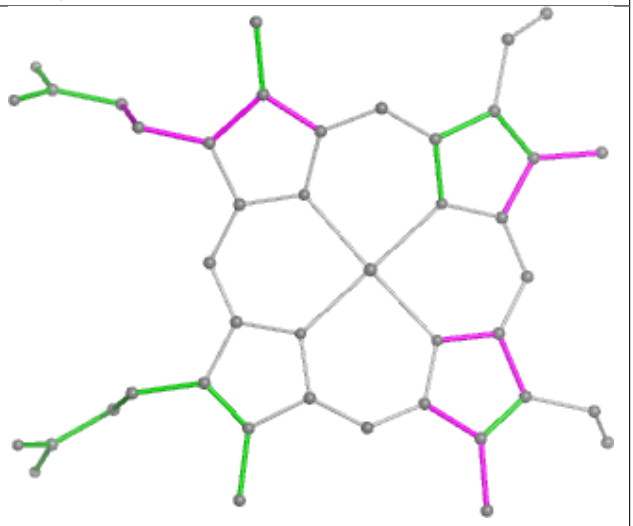
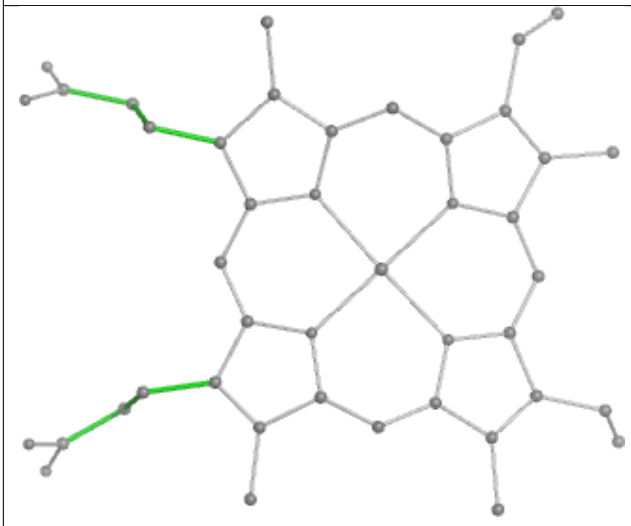


Bond angles



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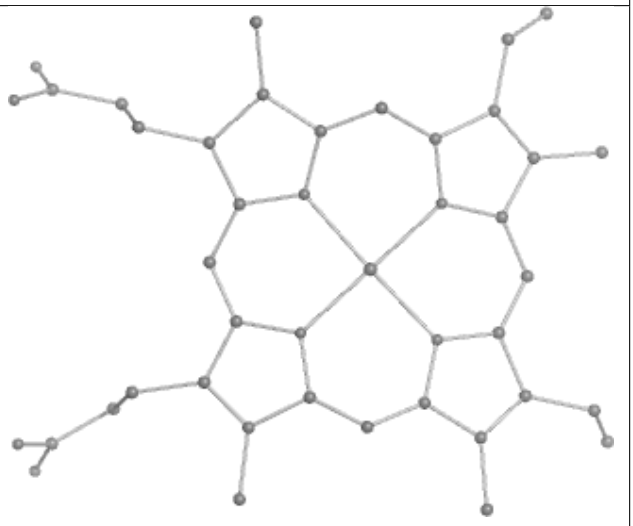
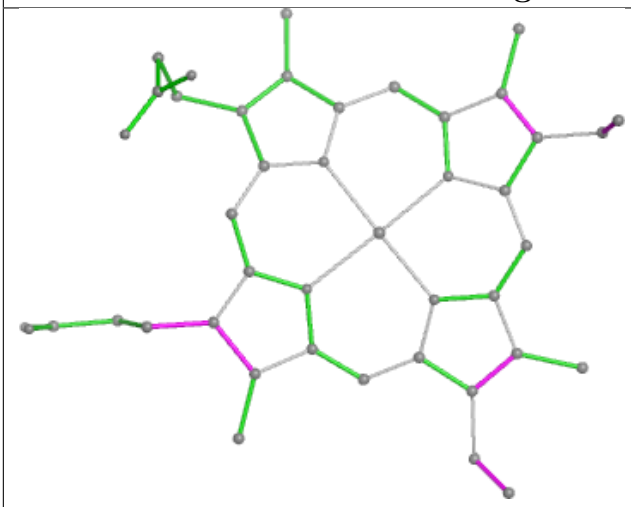


Rings

Ligand HEC B 1002



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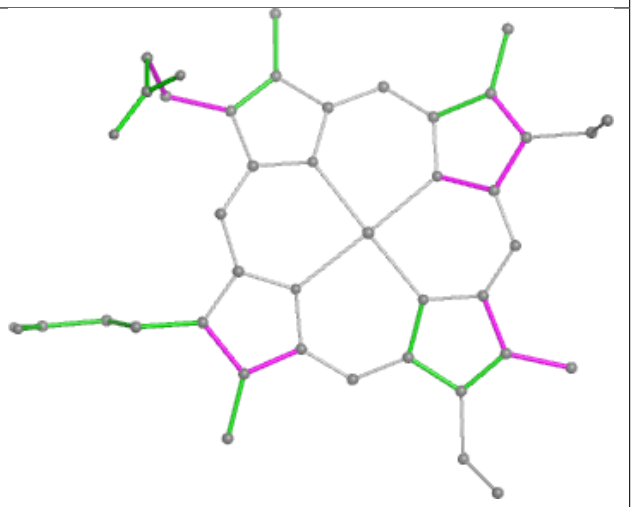
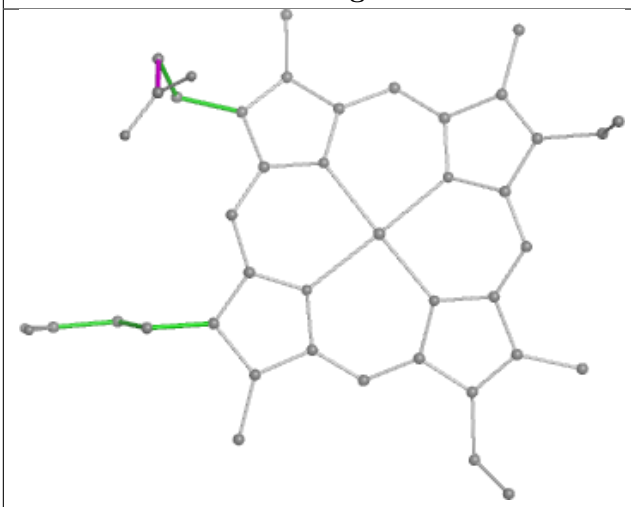
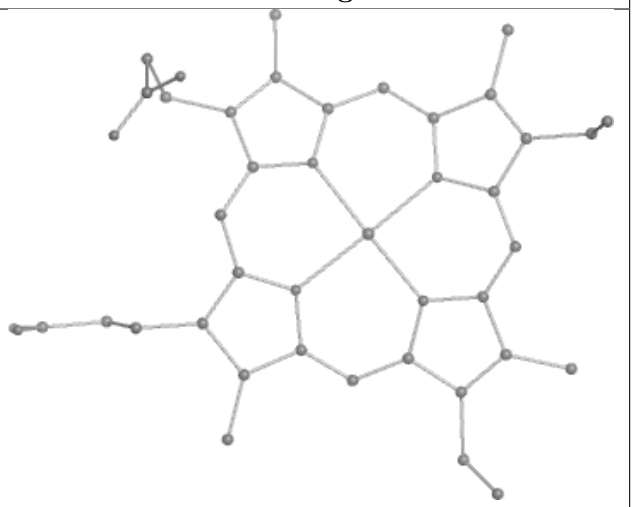


Bond angles

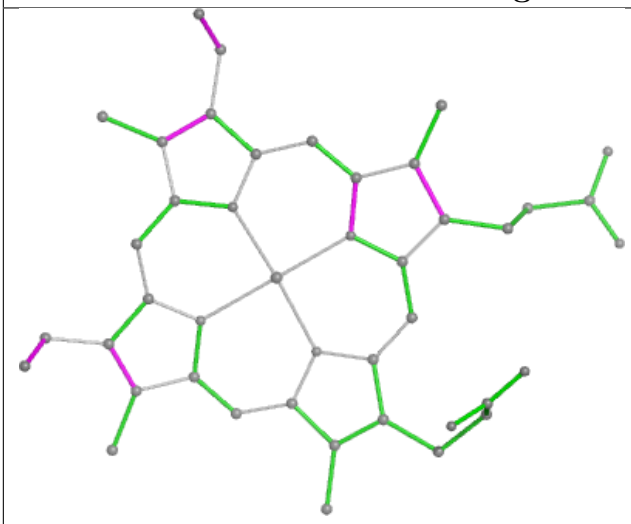


Torsions



Rings

Ligand HEC O 1002



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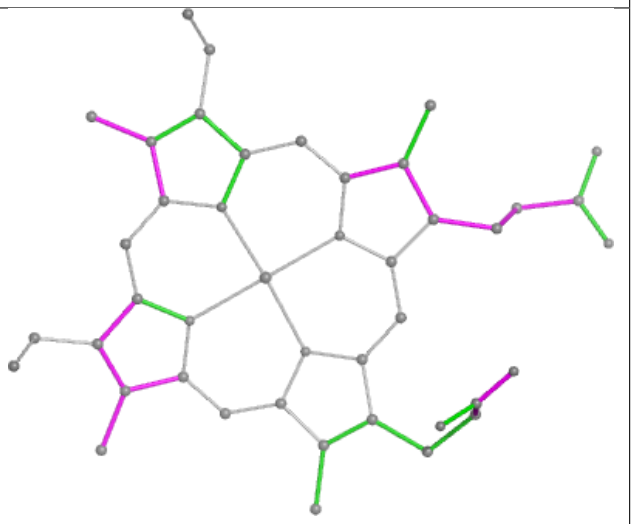
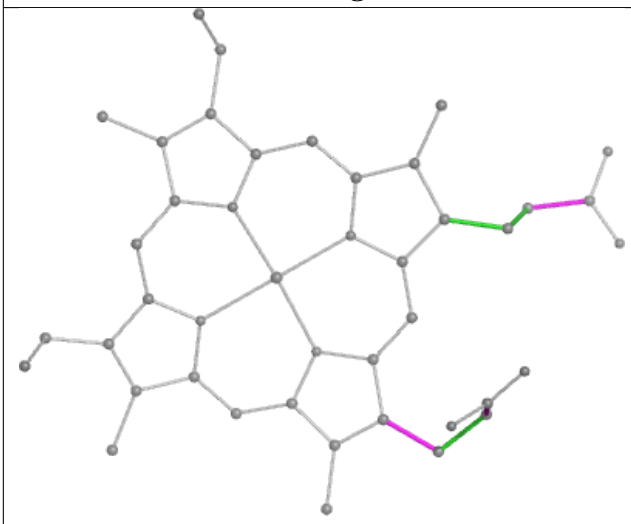
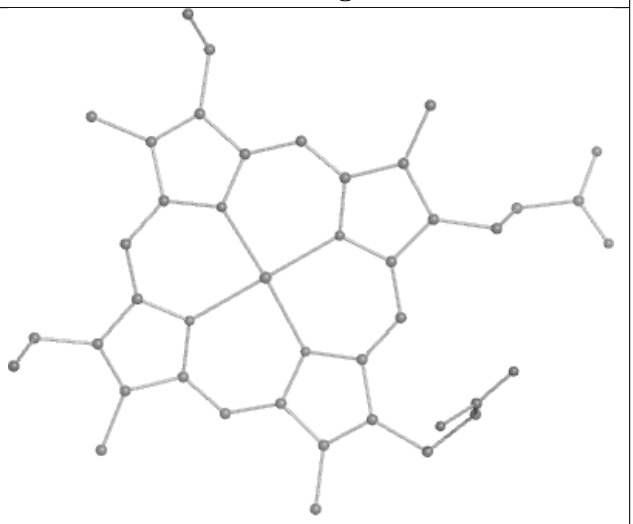


Bond angles

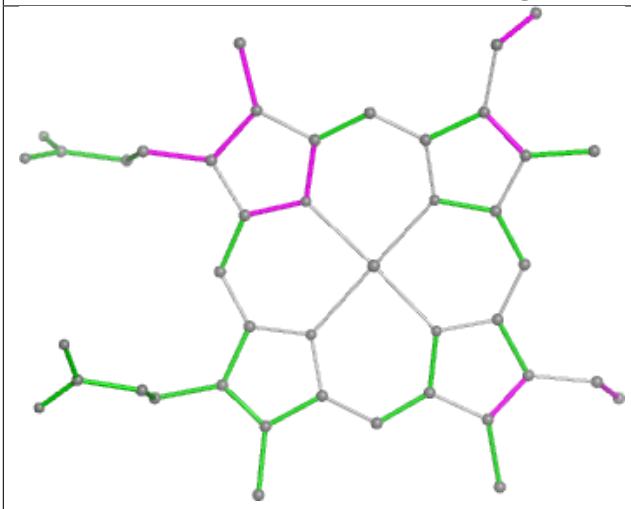


Torsions



Rings

Ligand HEC L 1004



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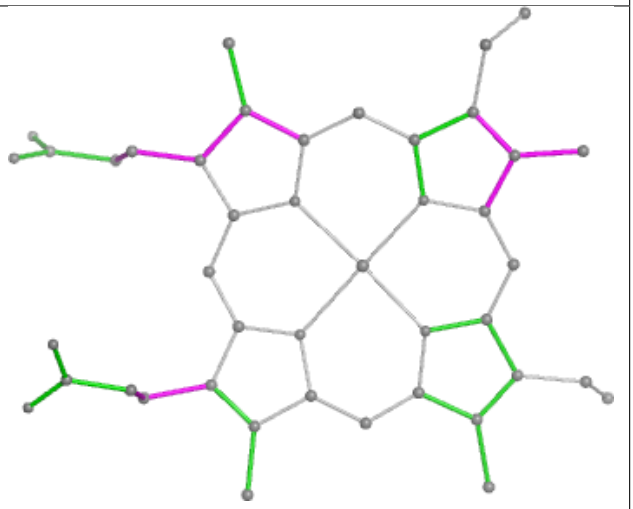
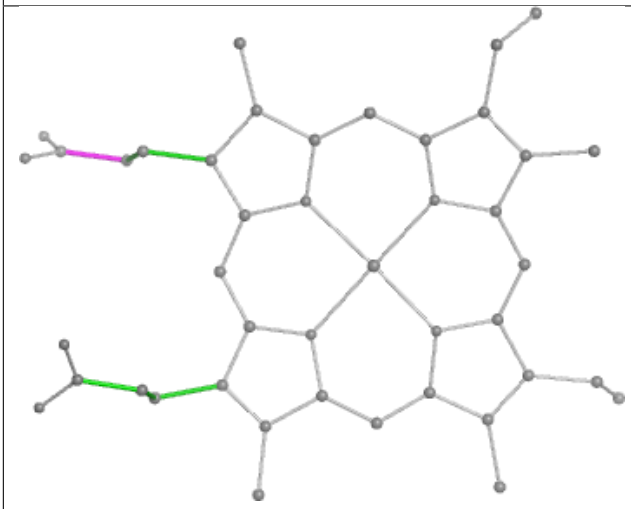
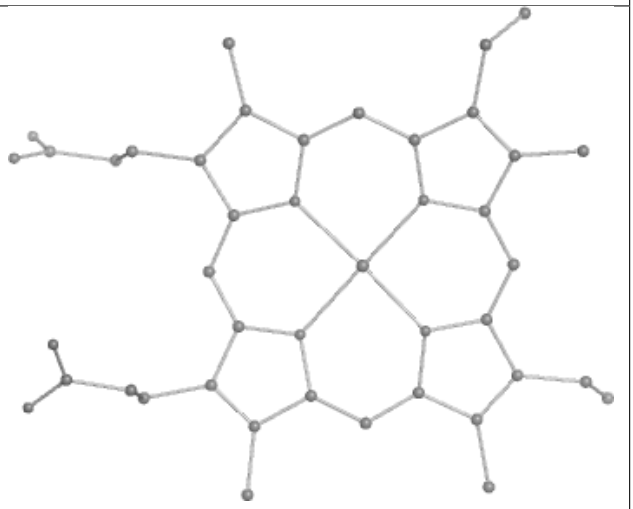


Bond angles

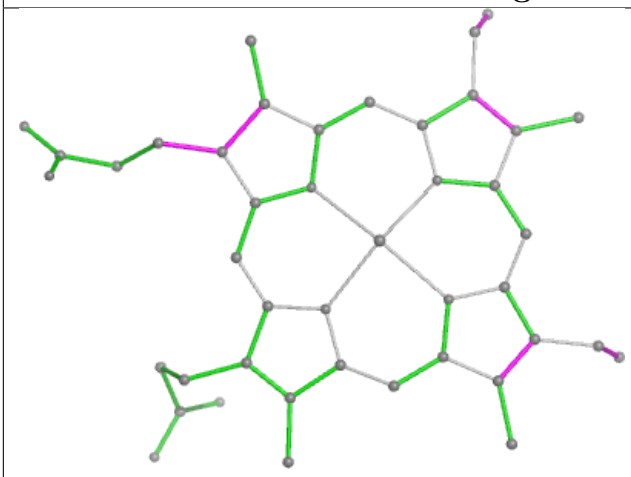


Torsions



Rings

Ligand HEC R 1001



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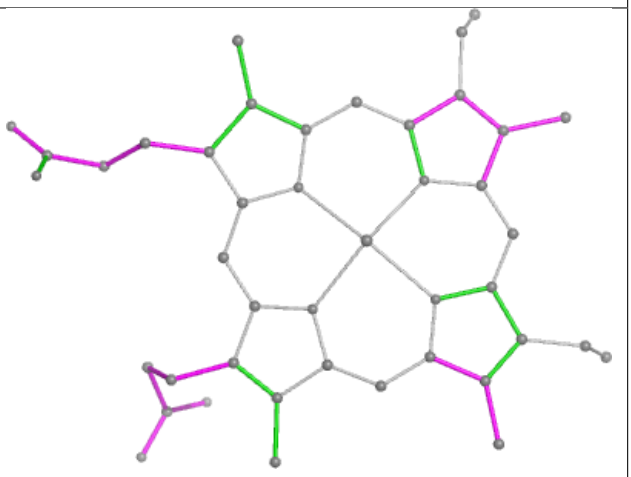
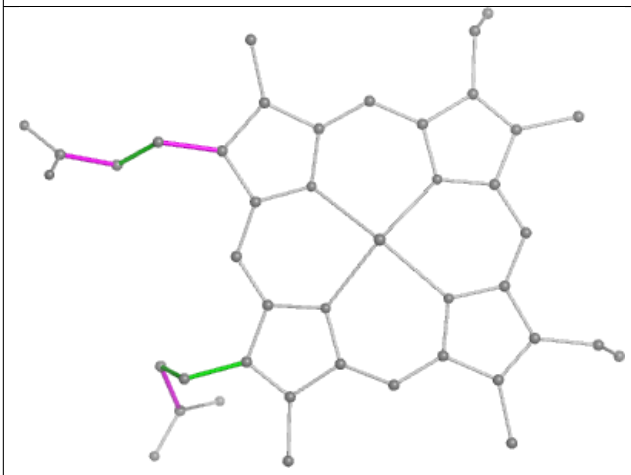
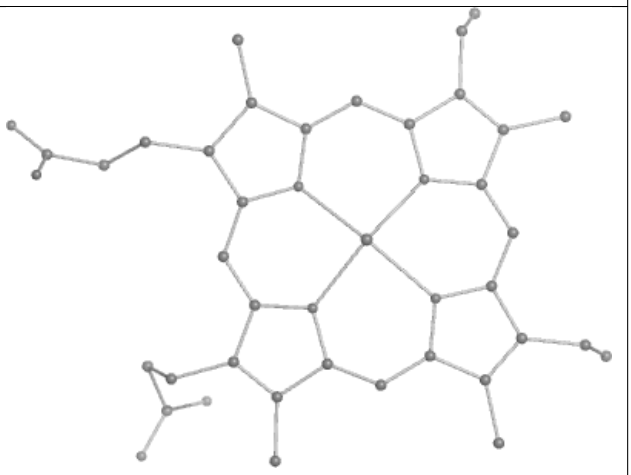


Bond angles

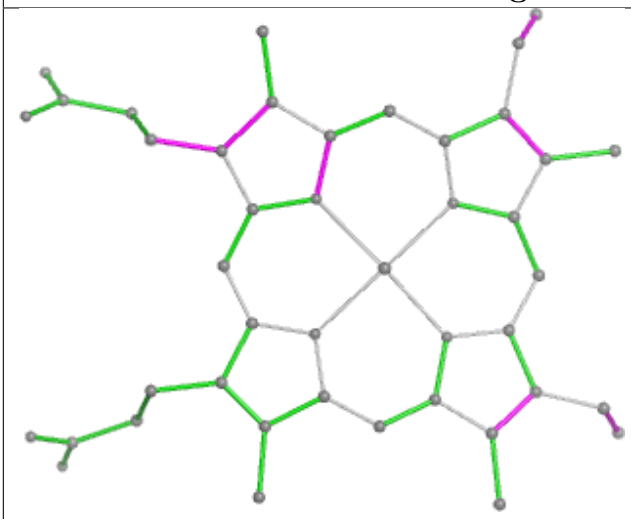


Torsions

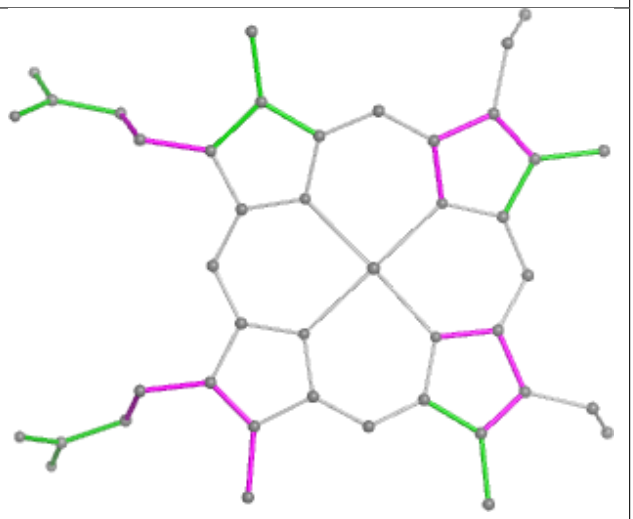


Rings

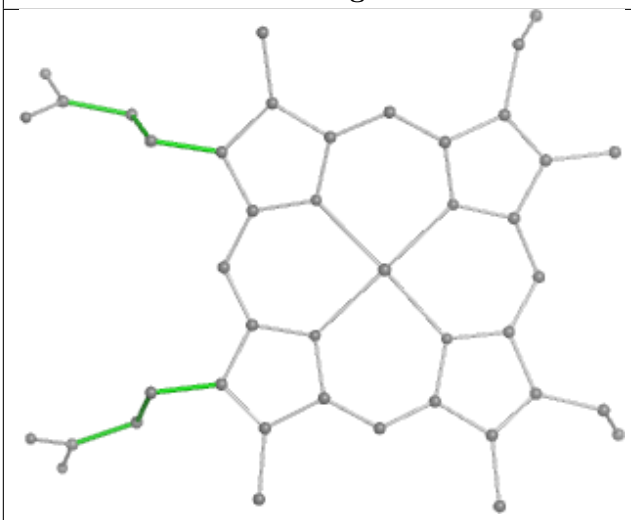
Ligand HEC M 1003



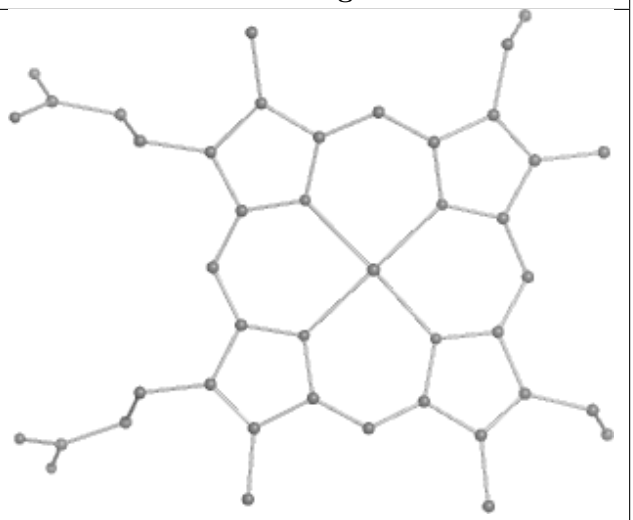
Bond lengths



Bond angles

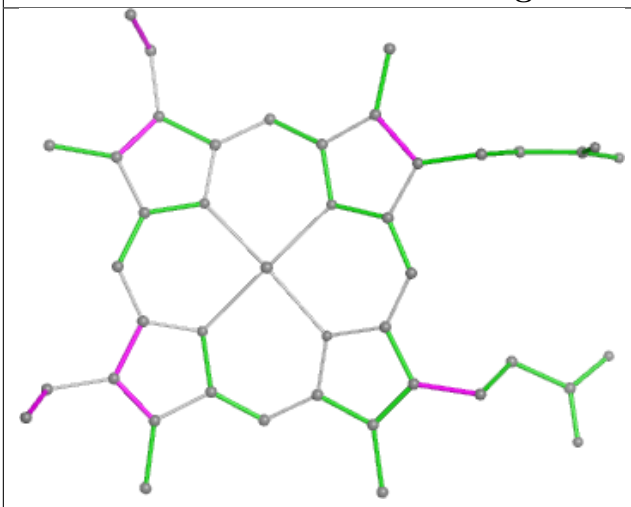


Torsions

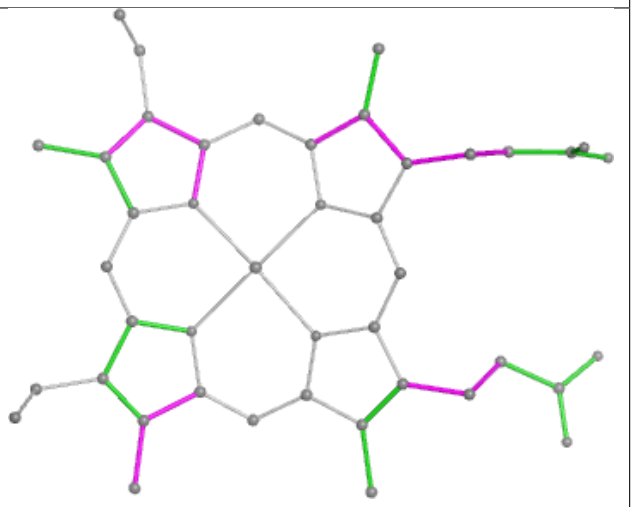


Rings

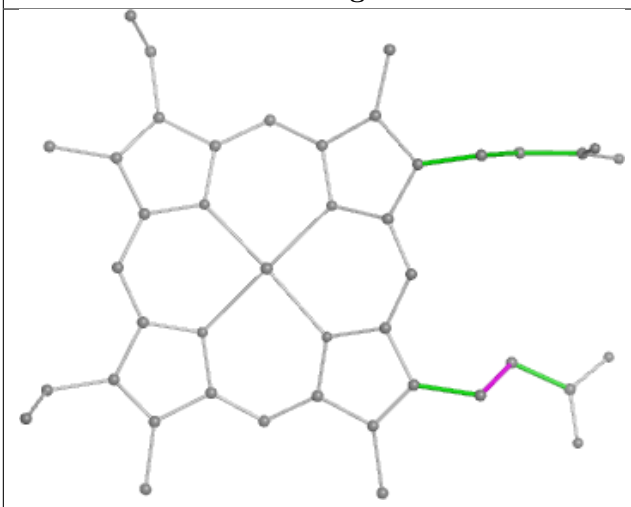
Ligand HEC E 1004



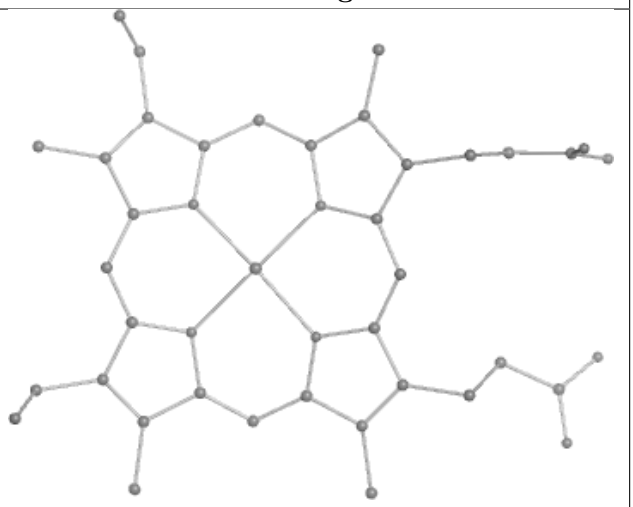
Bond lengths



Bond angles

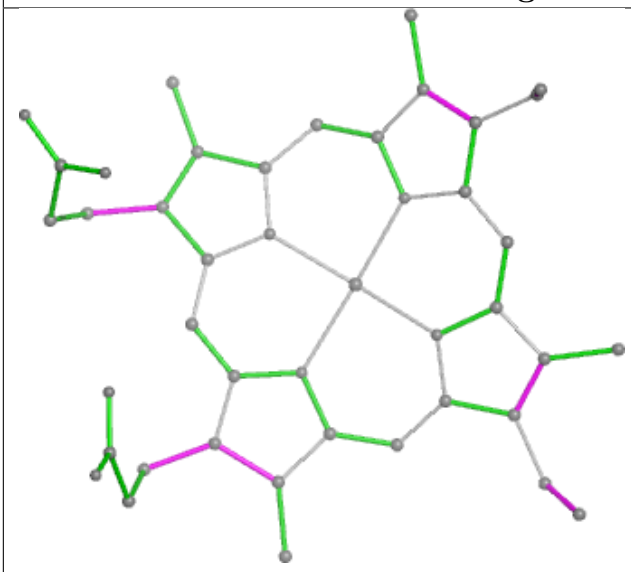


Torsions

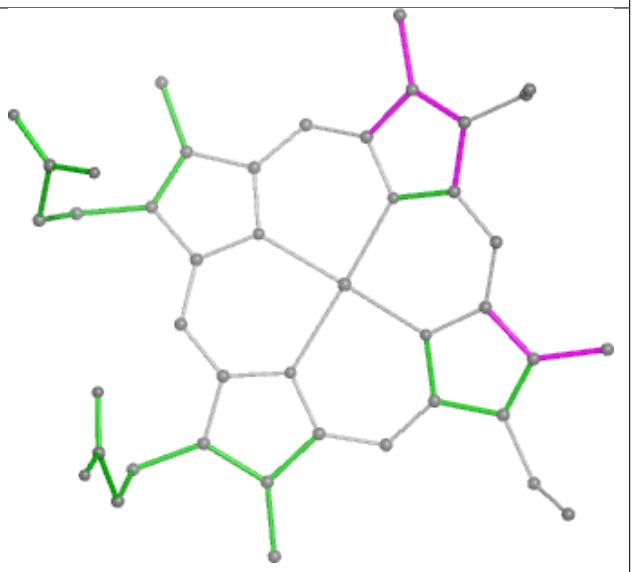


Rings

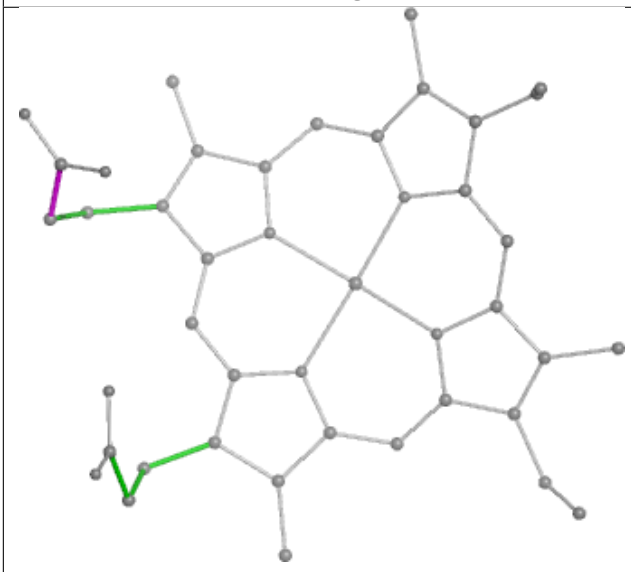
Ligand HEC J 1001



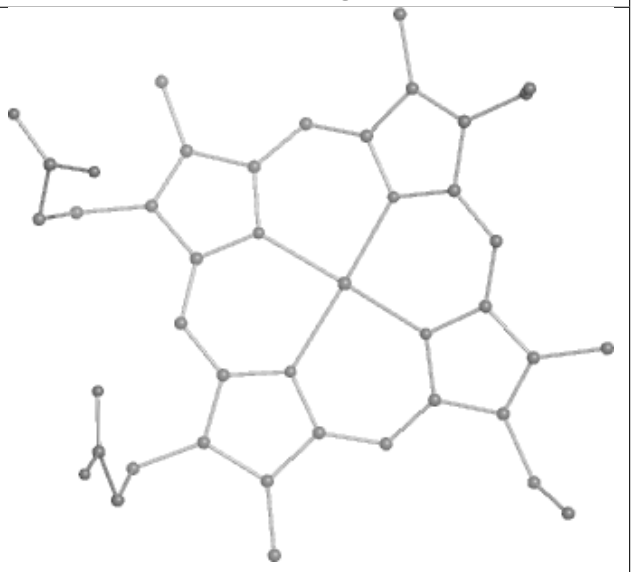
Bond lengths



Bond angles

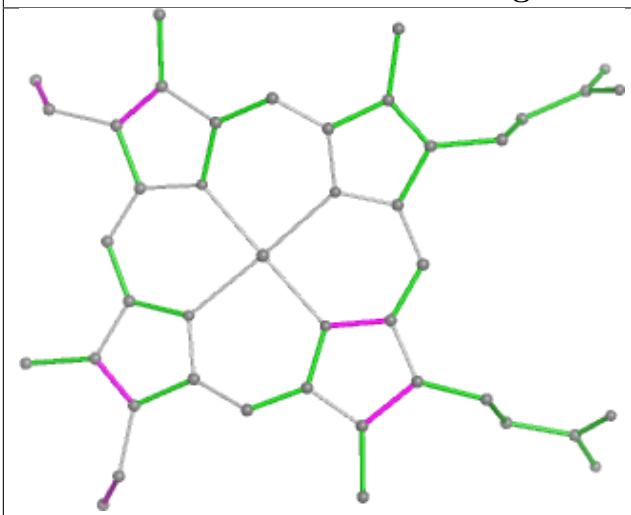


Torsions

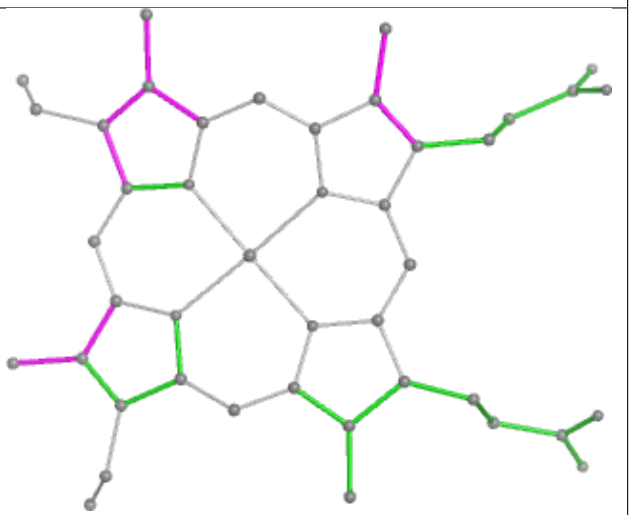


Rings

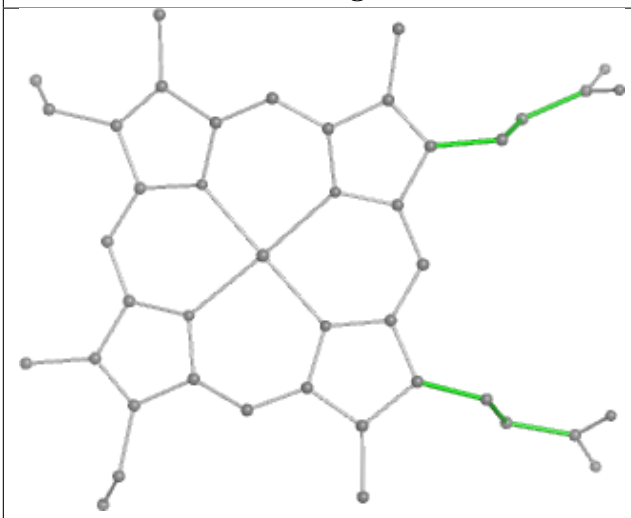
Ligand HEC N 1003



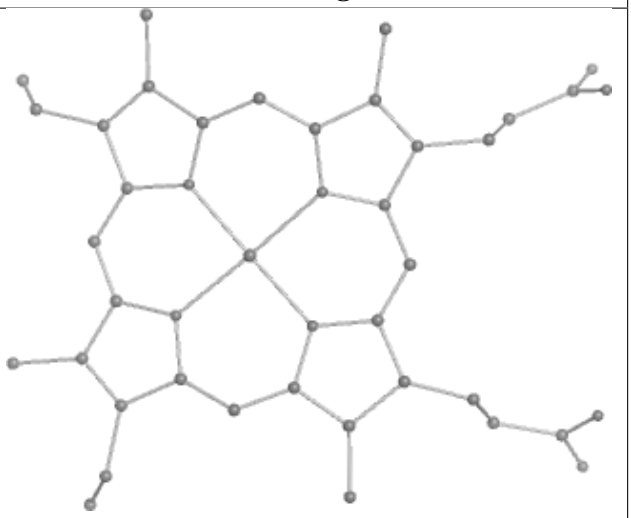
Bond lengths



Bond angles

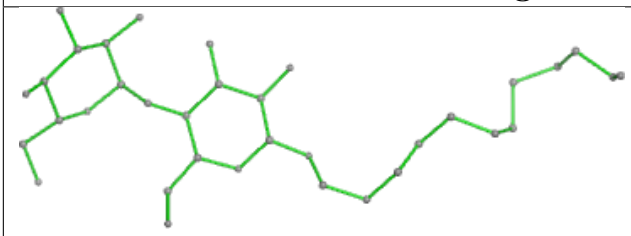


Torsions



Rings

Ligand LMT F 1005



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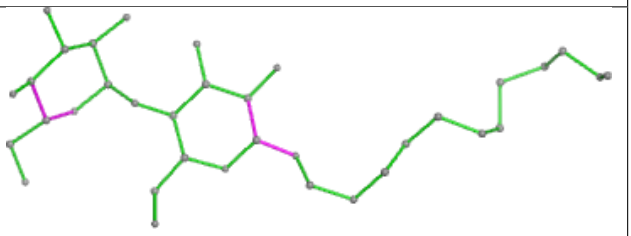
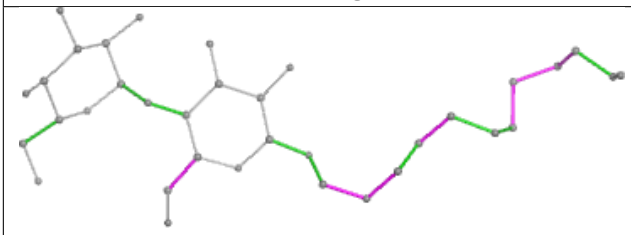
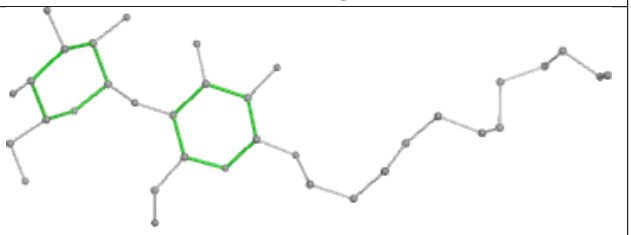


Bond angles

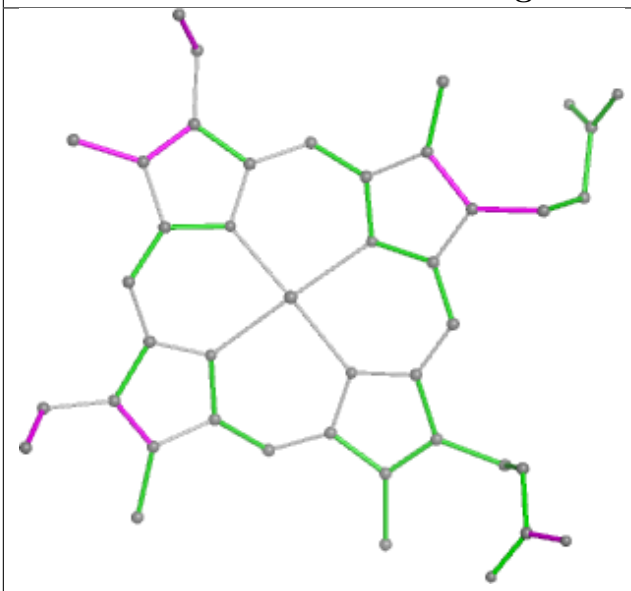


Torsions

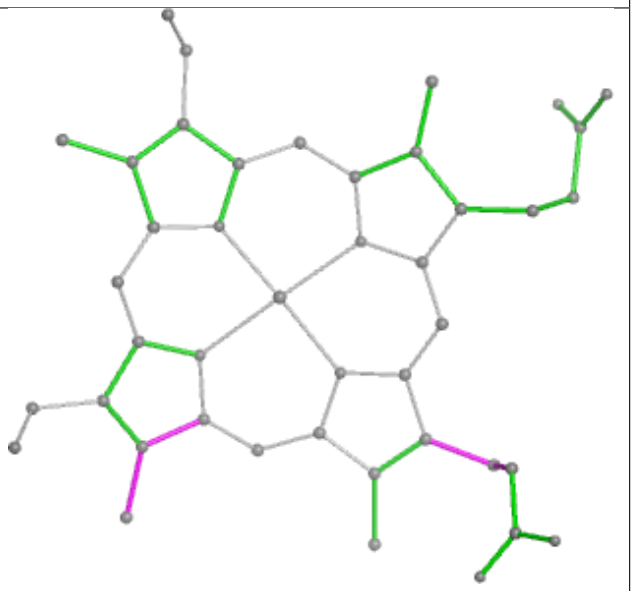


Rings

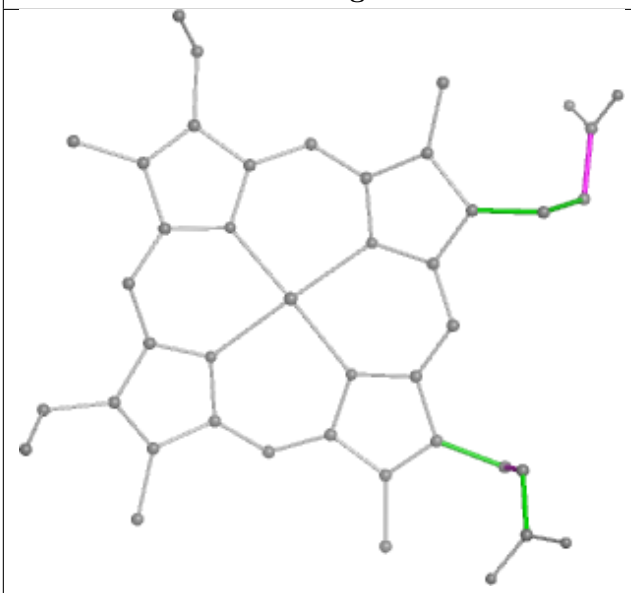
Ligand HEC E 1005



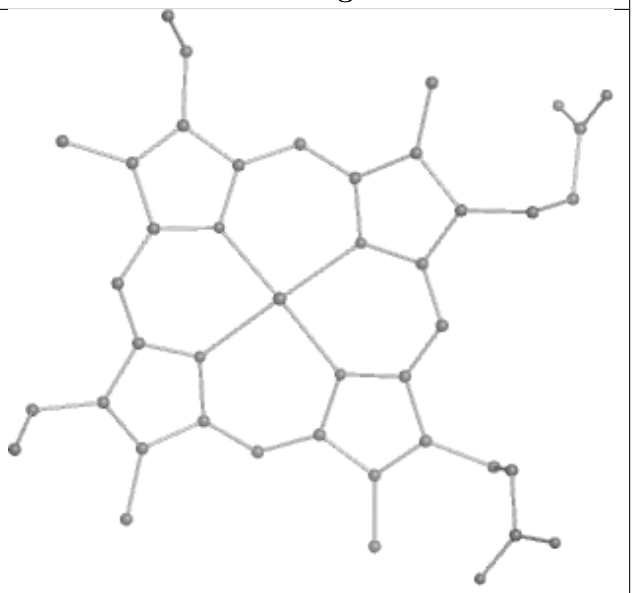
Bond lengths



Bond angles

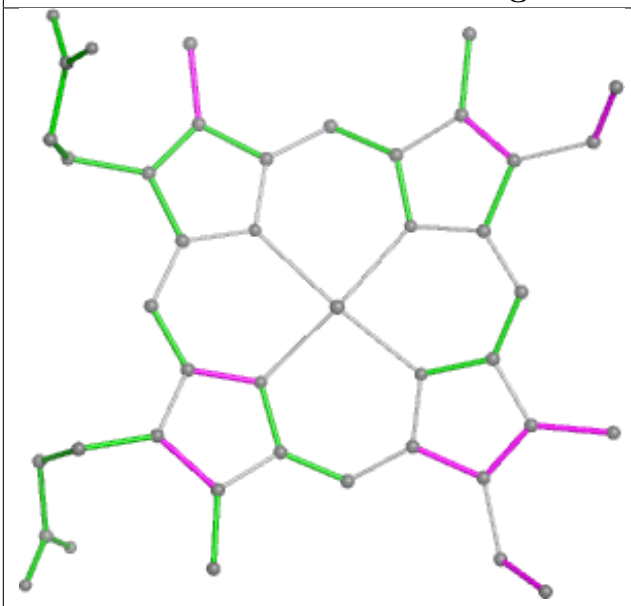


Torsions

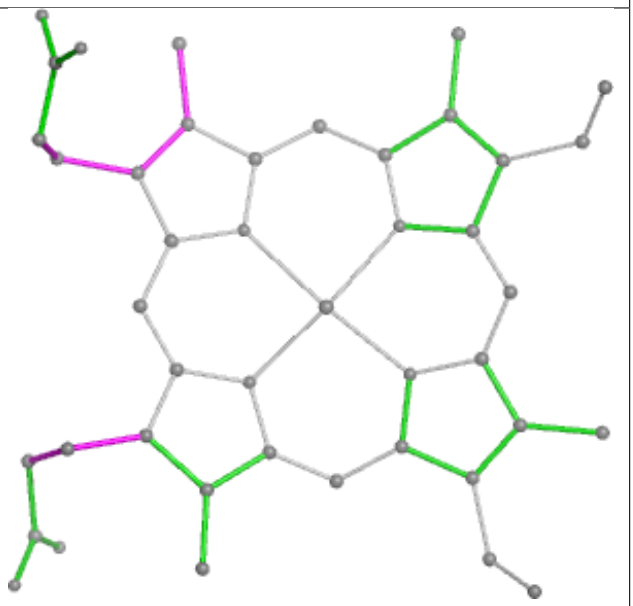


Rings

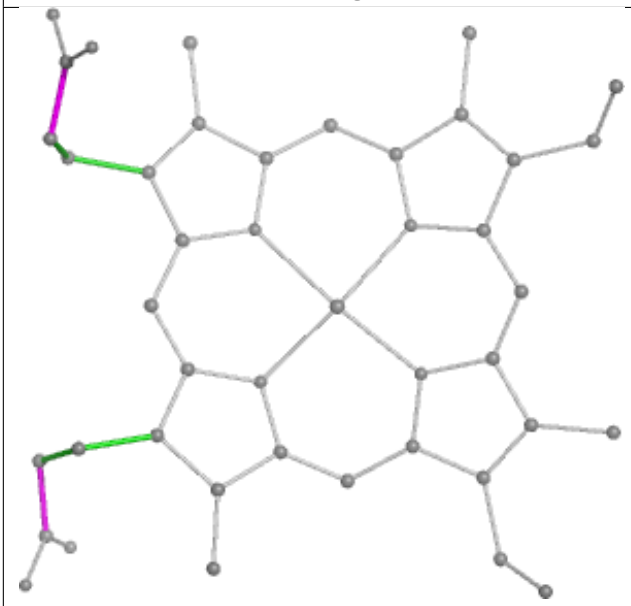
Ligand HEC M 1005



Bond lengths



Bond angles



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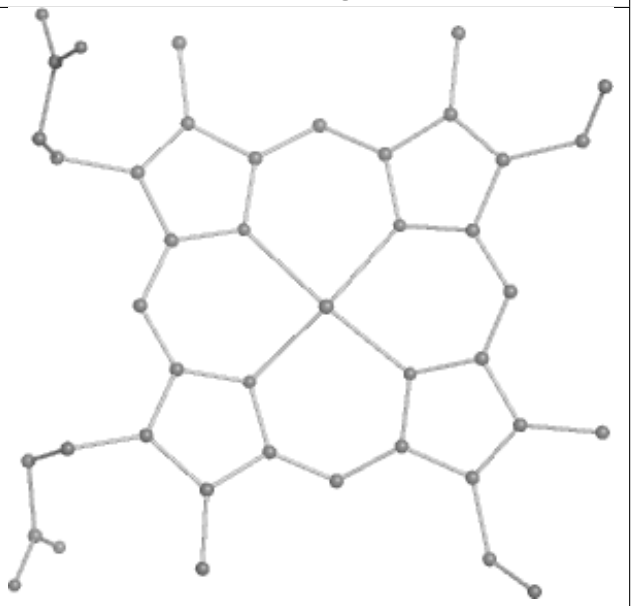
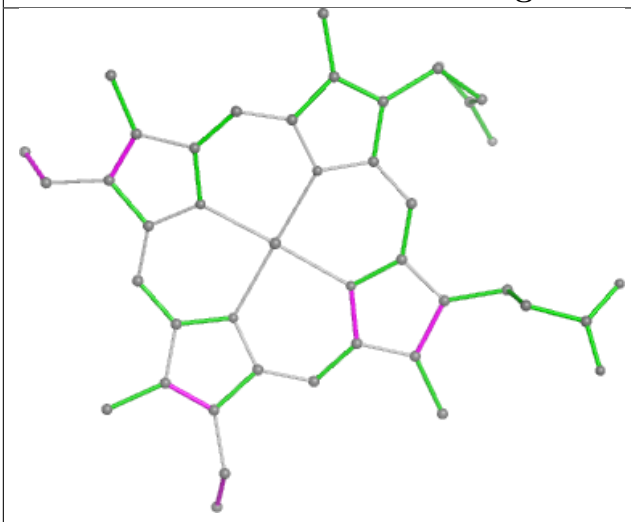


Rings

Ligand HEC F 1002



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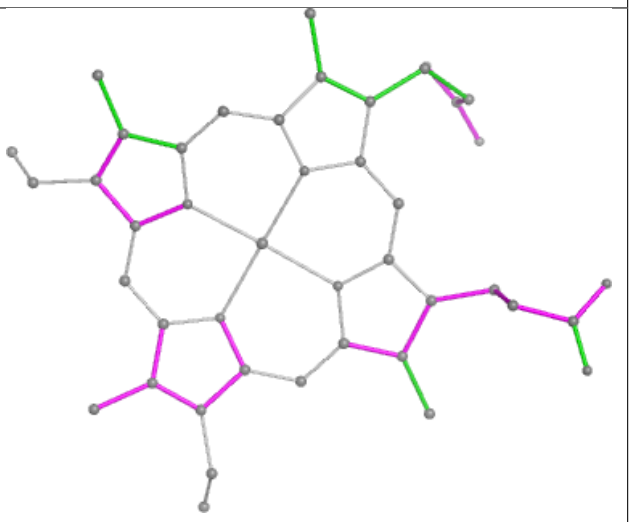
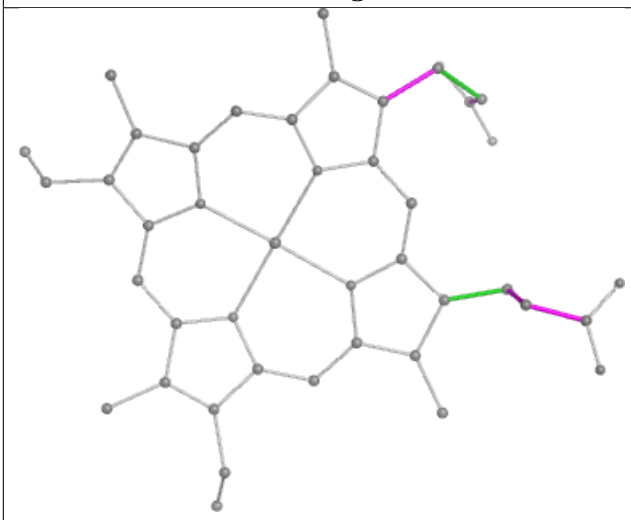
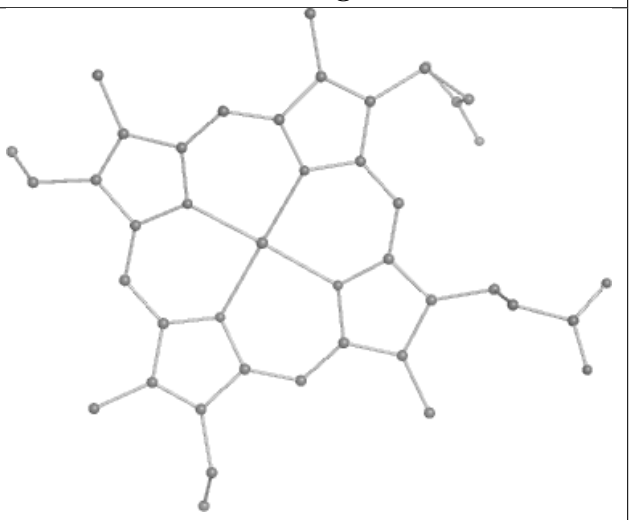


Bond angles

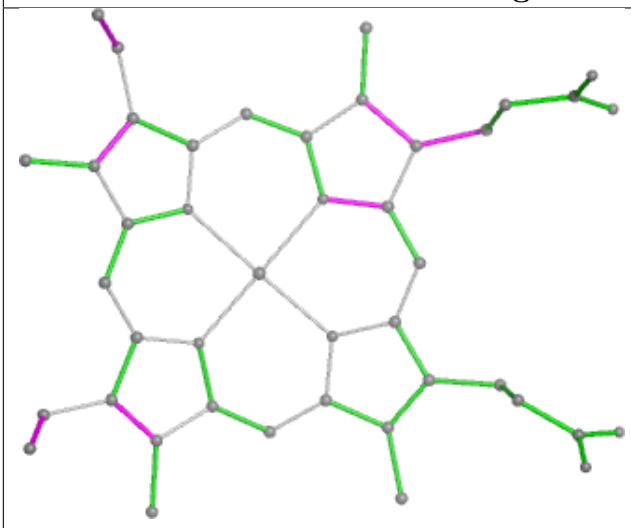


Torsions



Rings

Ligand HEC K 1003



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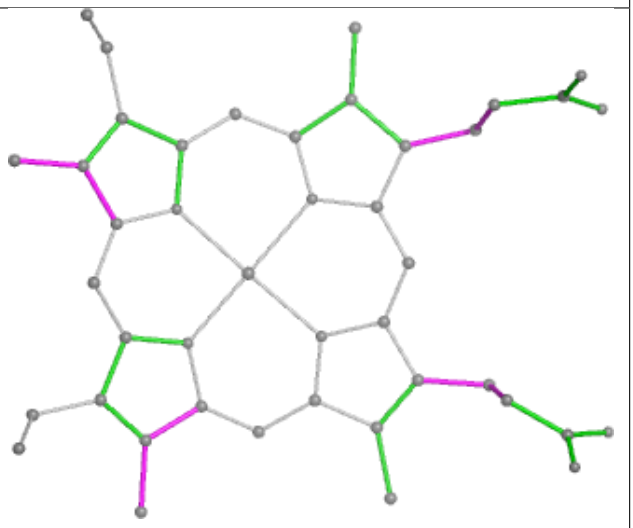
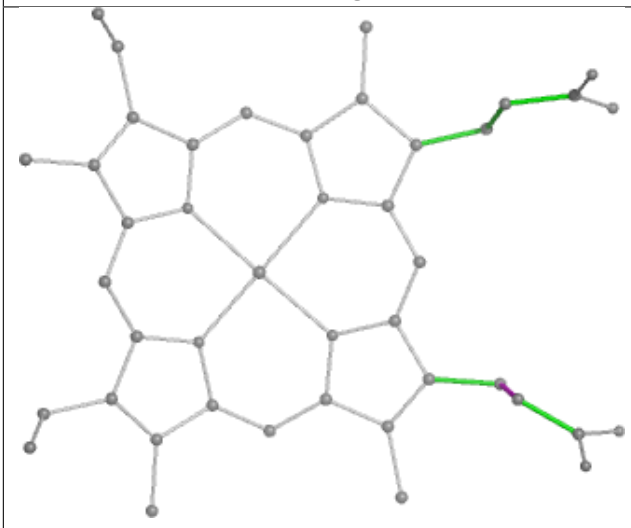
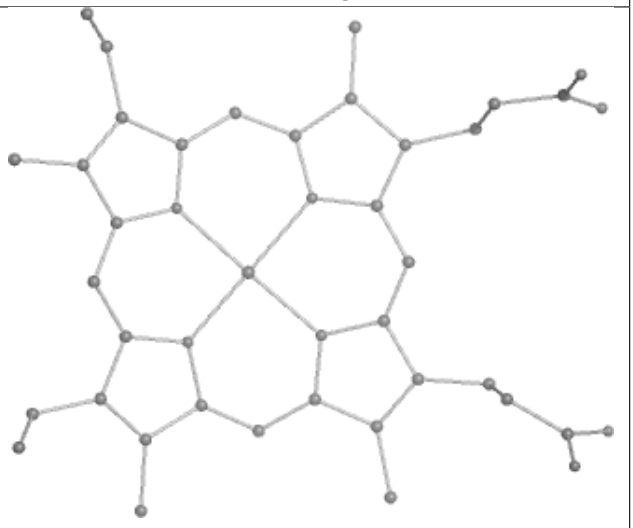


Bond angles

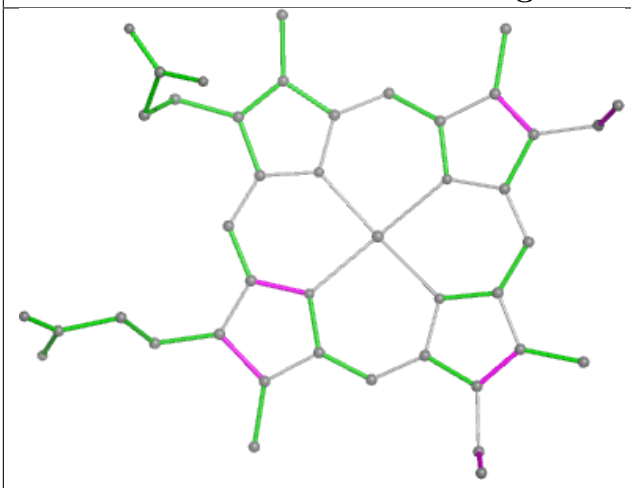


Torsions



Rings

Ligand HEC L 1101



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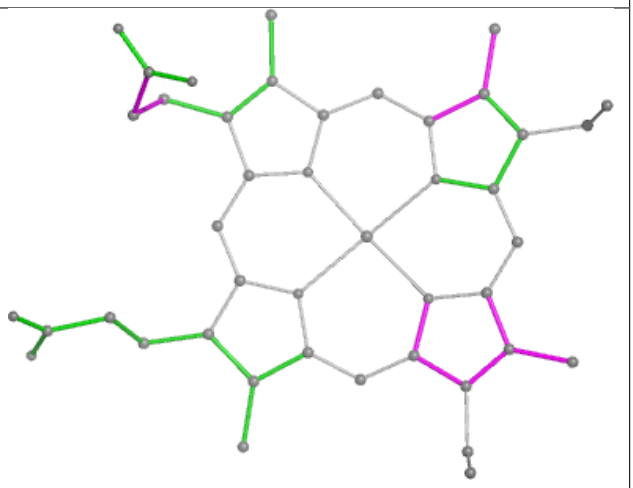
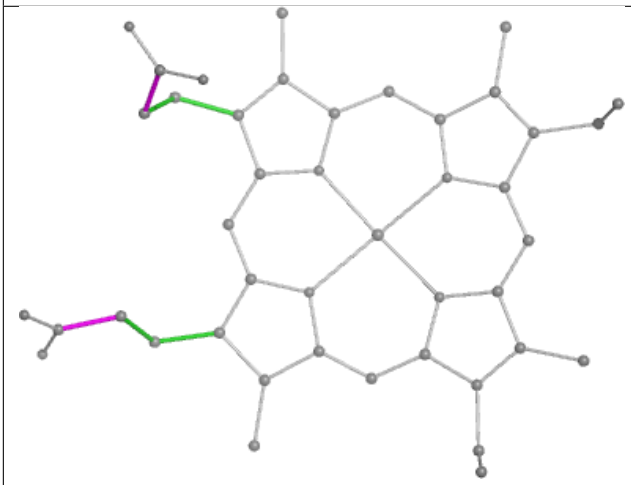
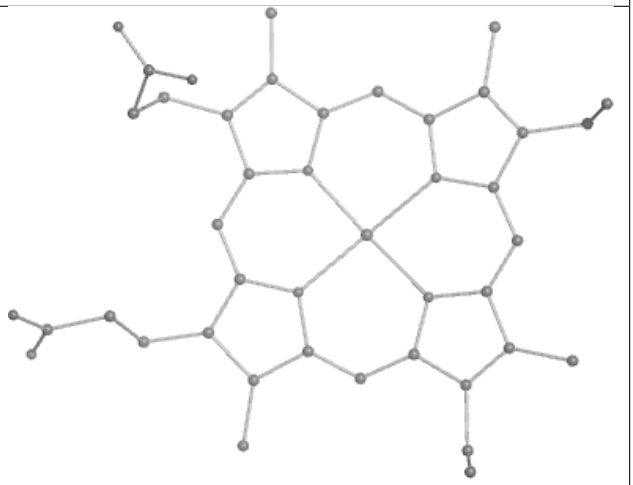


Bond angles

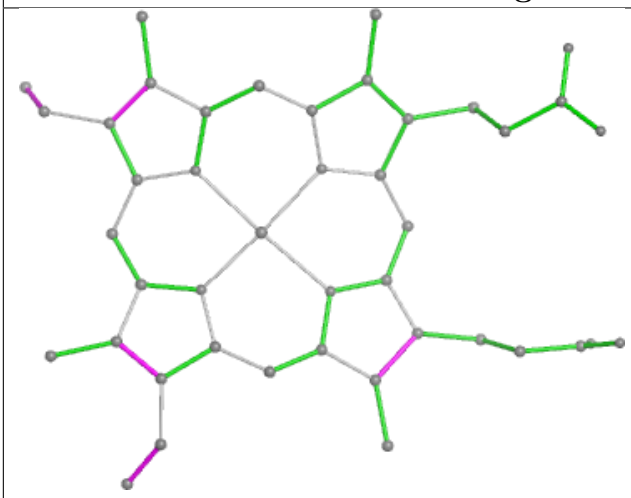


Torsions



Rings

Ligand HEC P 1004



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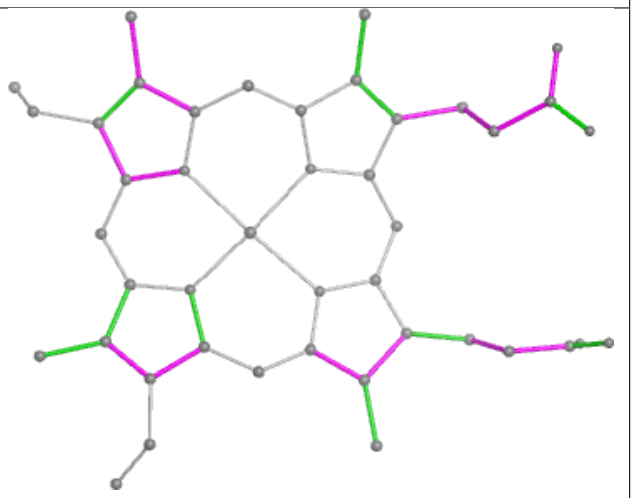
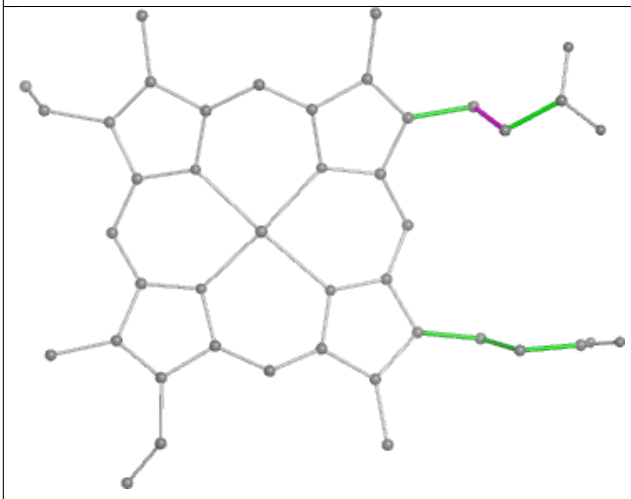
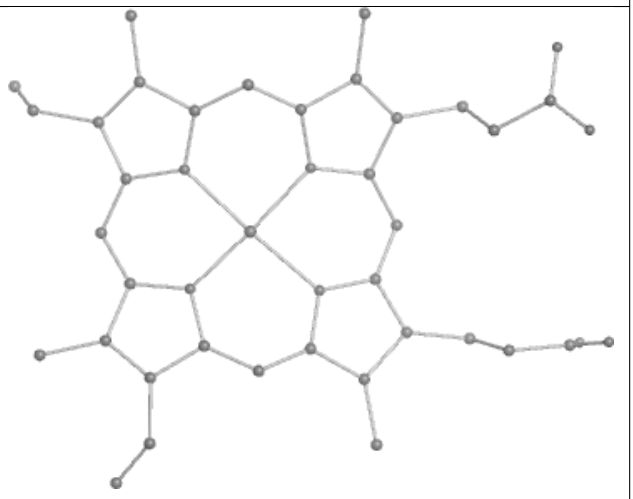


Bond angles

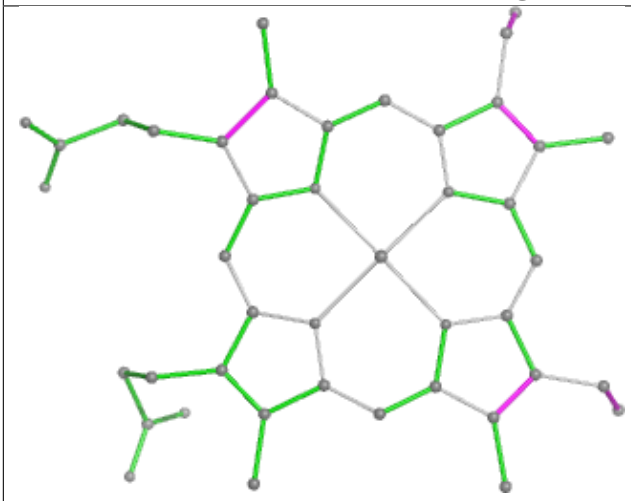


Torsions

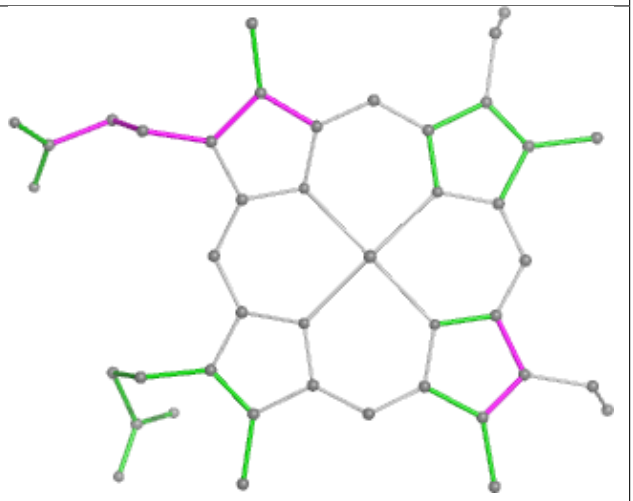


Rings

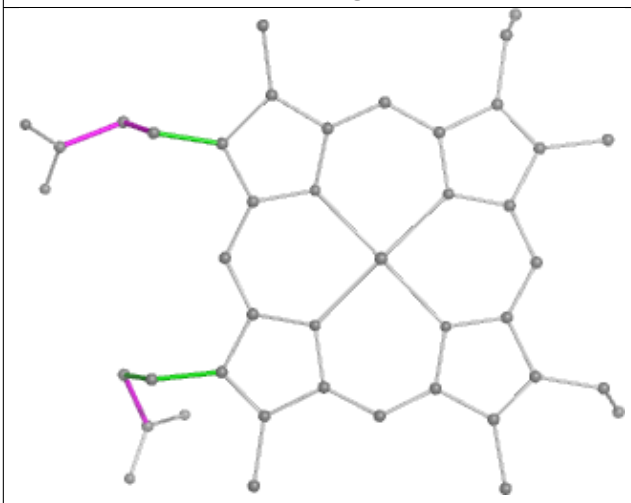
Ligand HEC C 1001



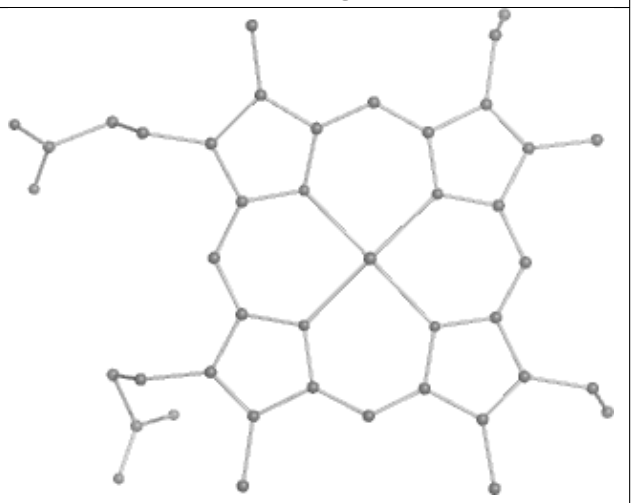
Bond lengths



Bond angles

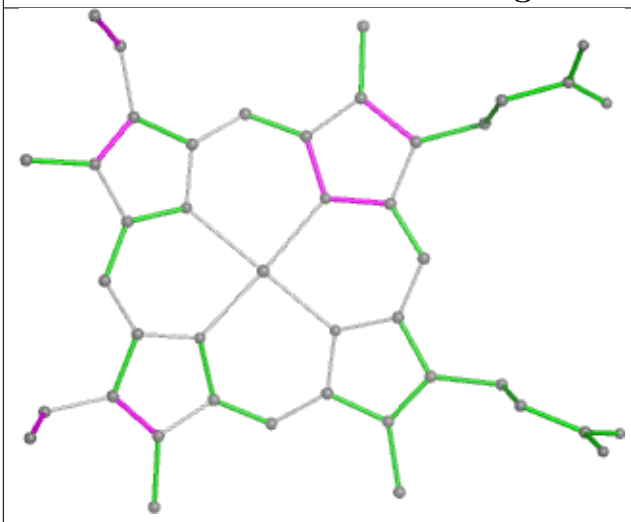


Torsions

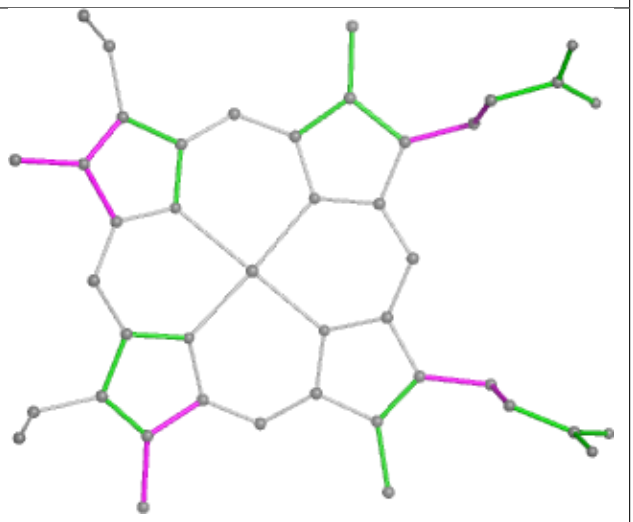


Rings

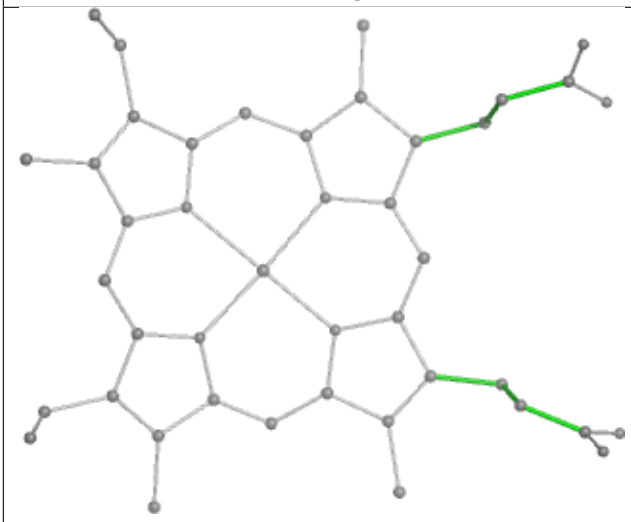
Ligand HEC B 1003



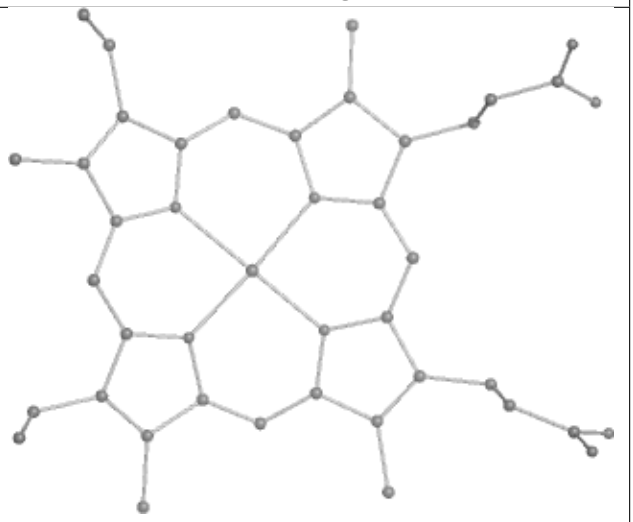
Bond lengths



Bond angles

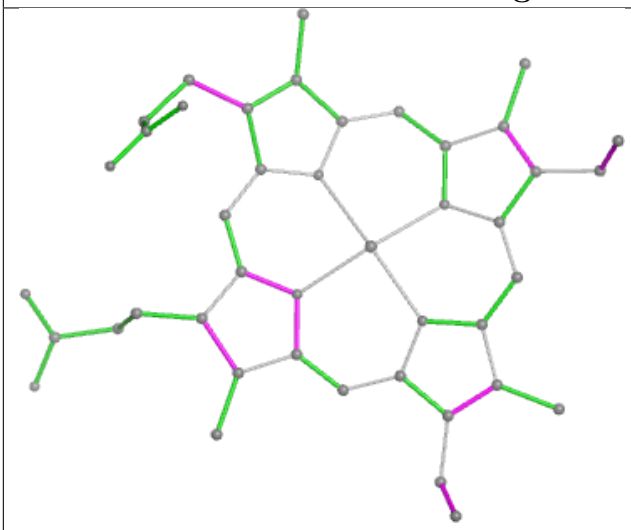


Torsions



Rings

Ligand HEC R 1002



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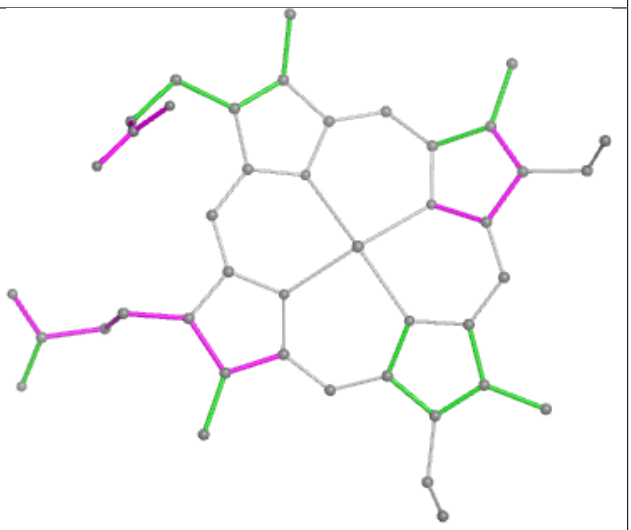
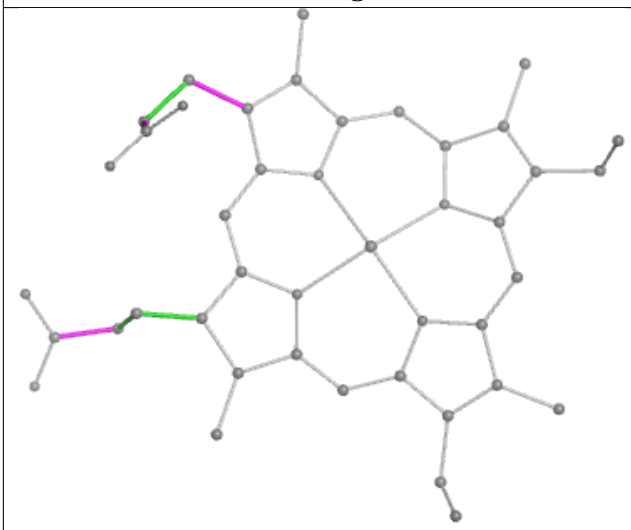
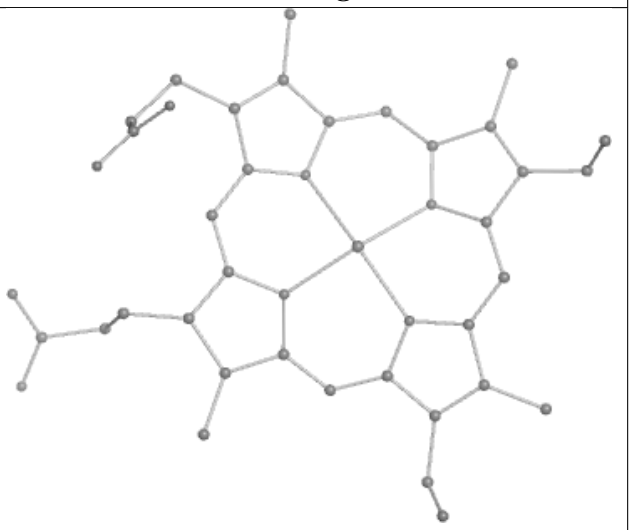


Bond angles

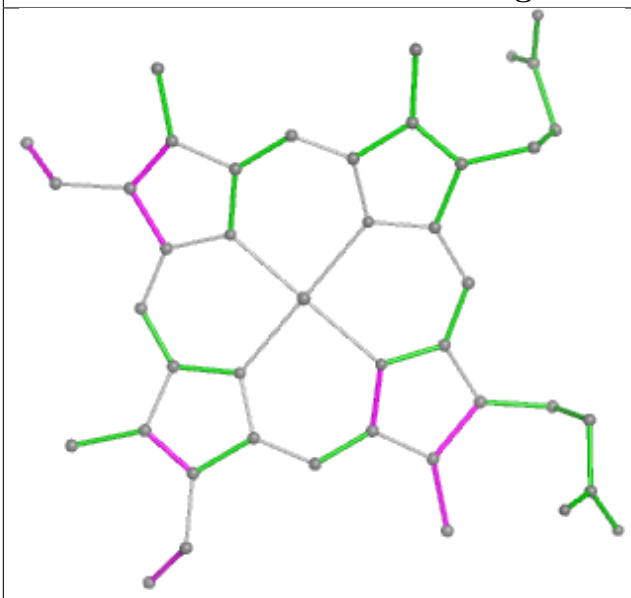


Torsions



Rings

Ligand HEC P 1005



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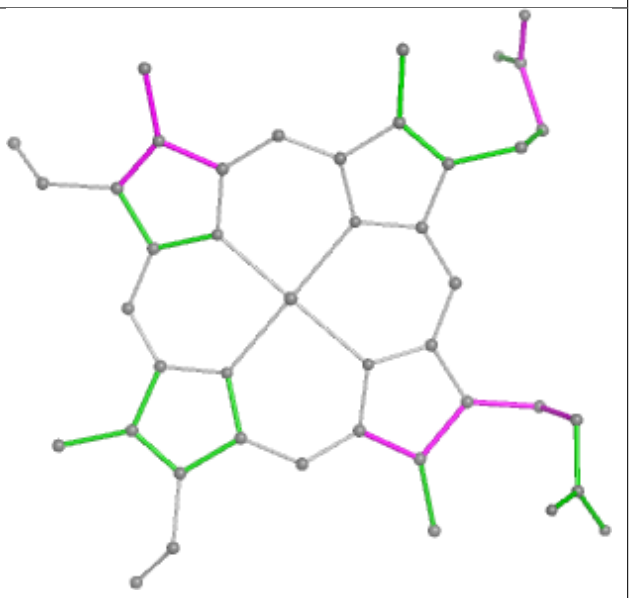
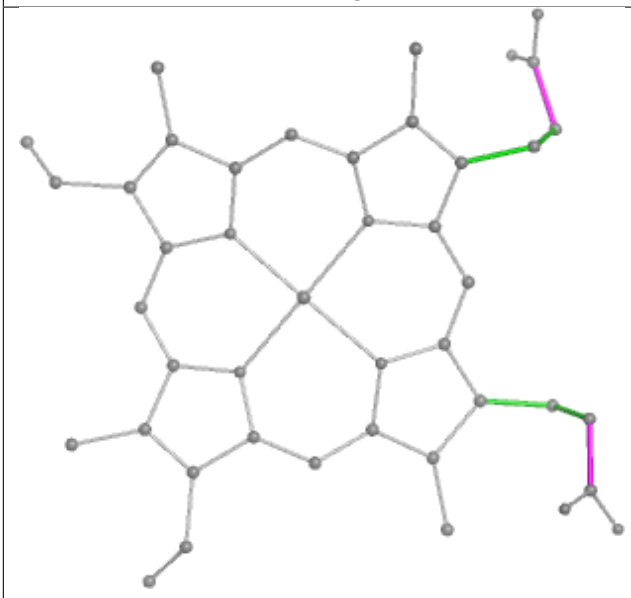
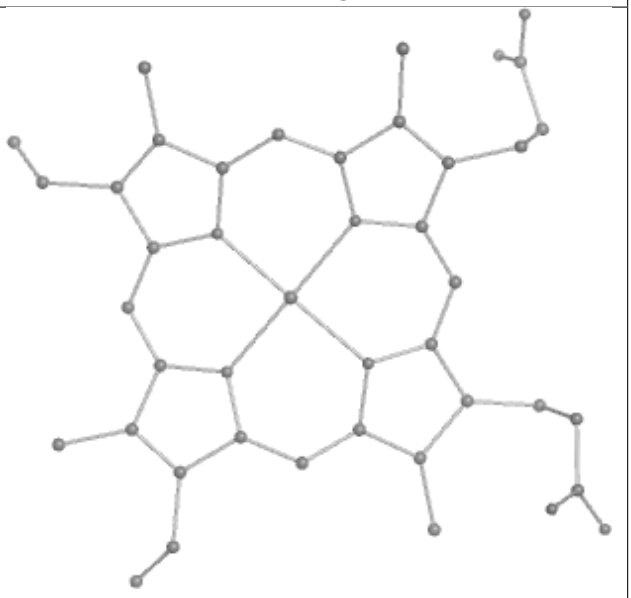


Bond angles

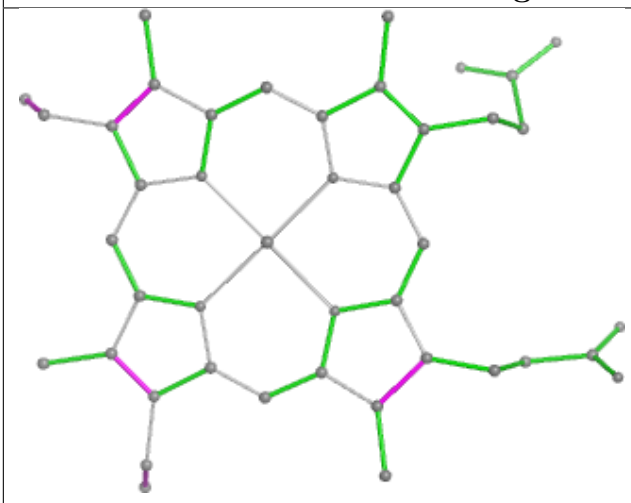


Torsions

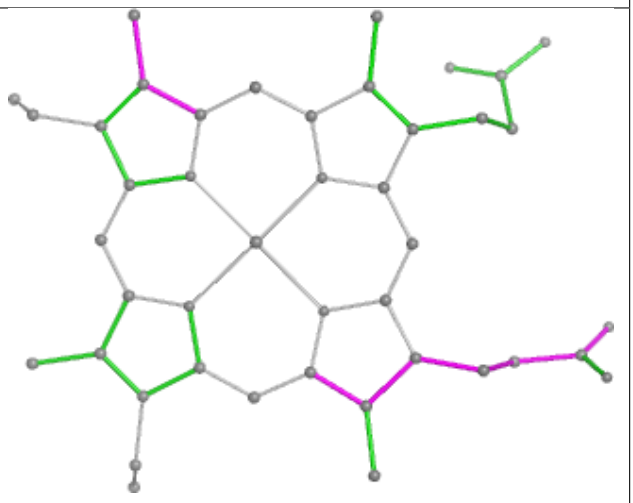


Rings

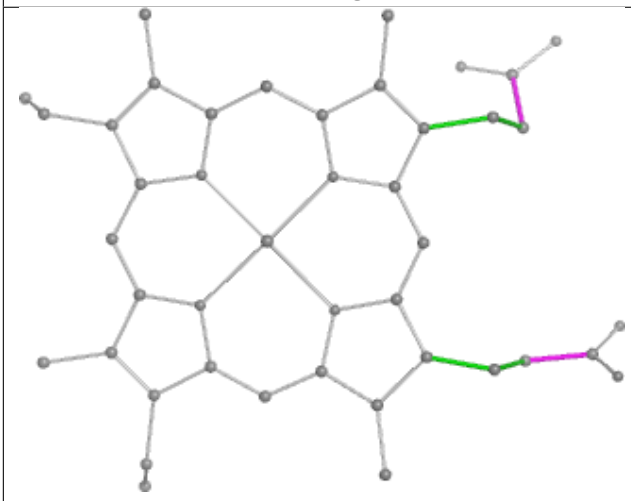
Ligand HEC O 1001



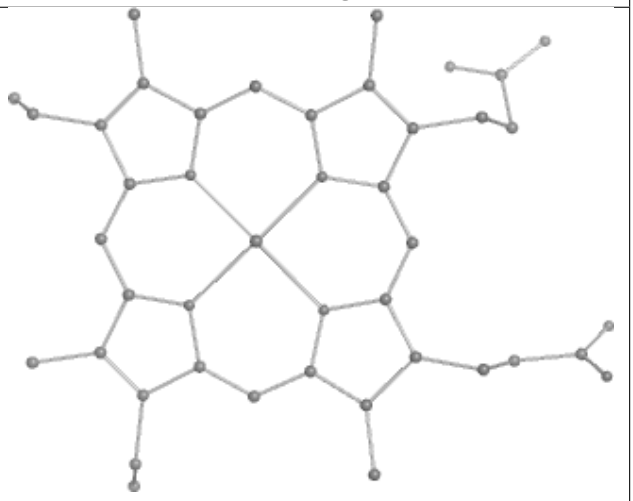
Bond lengths



Bond angles

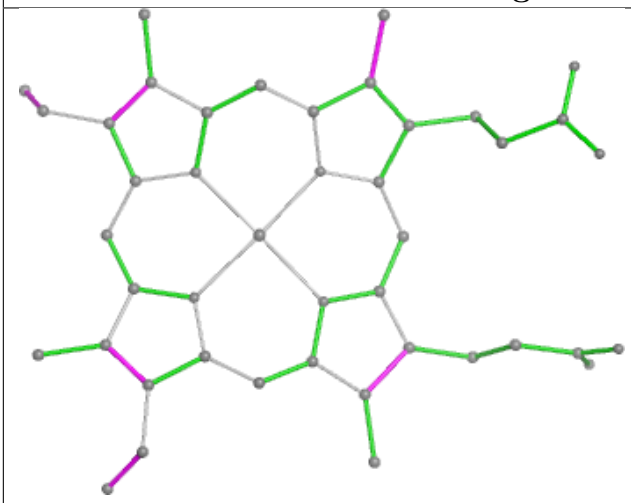


Torsions

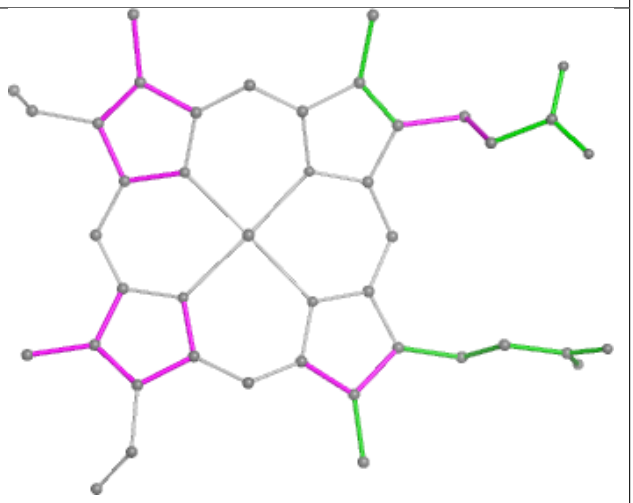


Rings

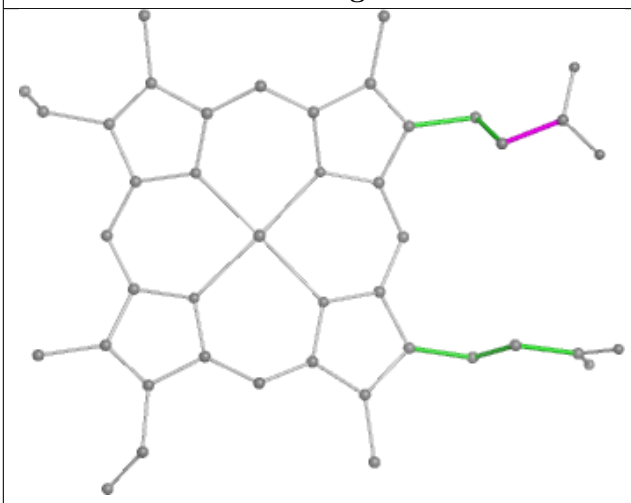
Ligand HEC G 1004



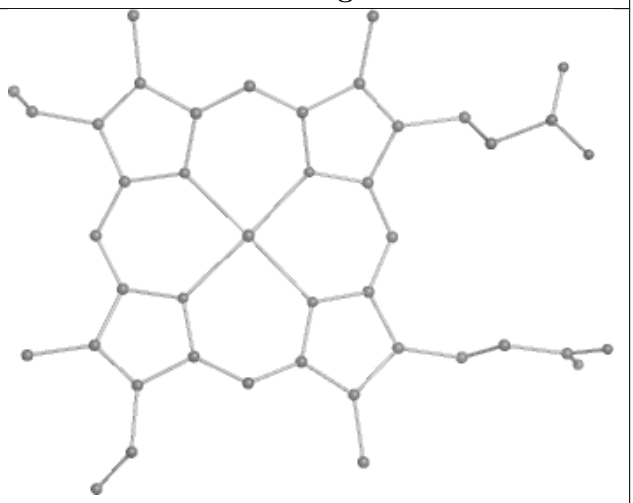
Bond lengths



Bond angles

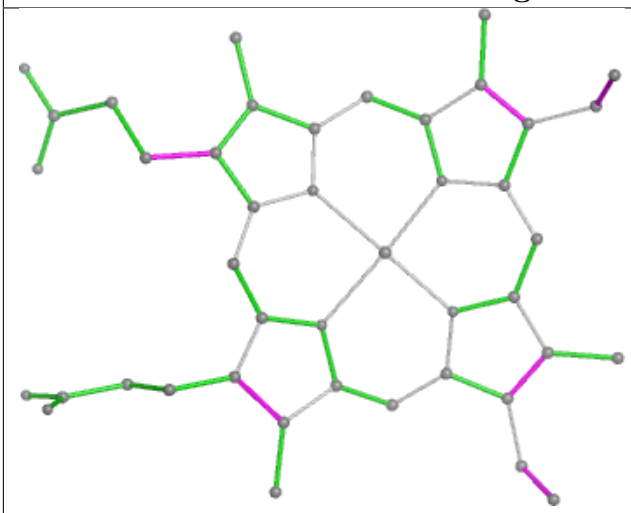


Torsions

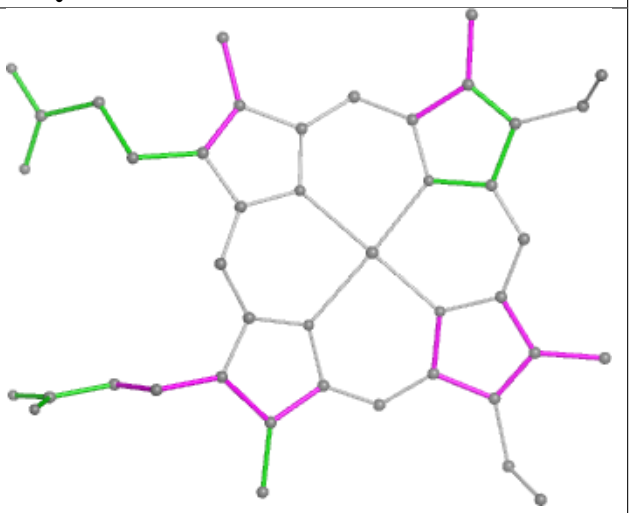


Rings

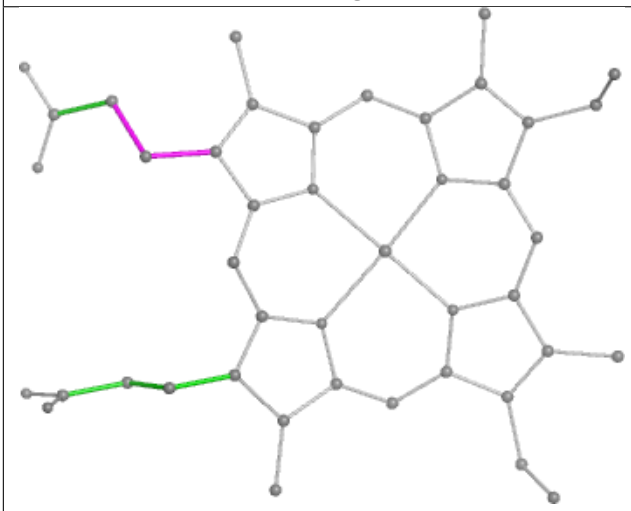
Ligand HEC Q 1004



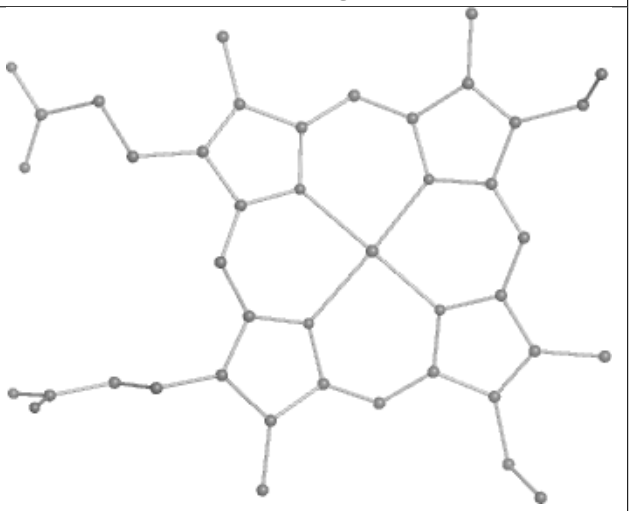
Bond lengths



Bond angles

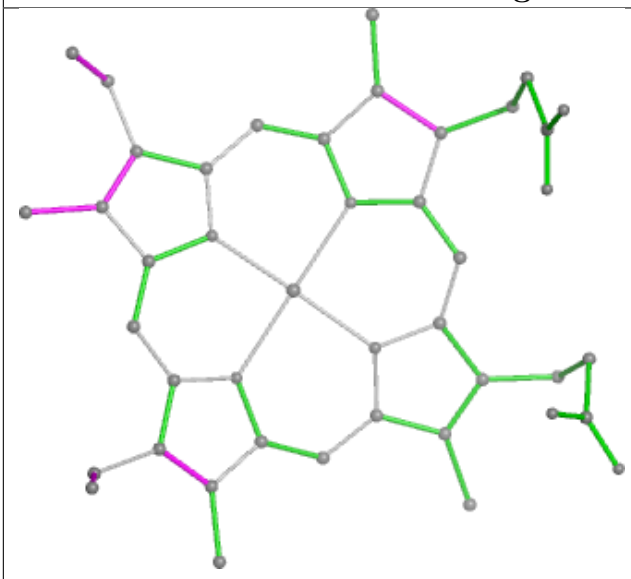


Torsions

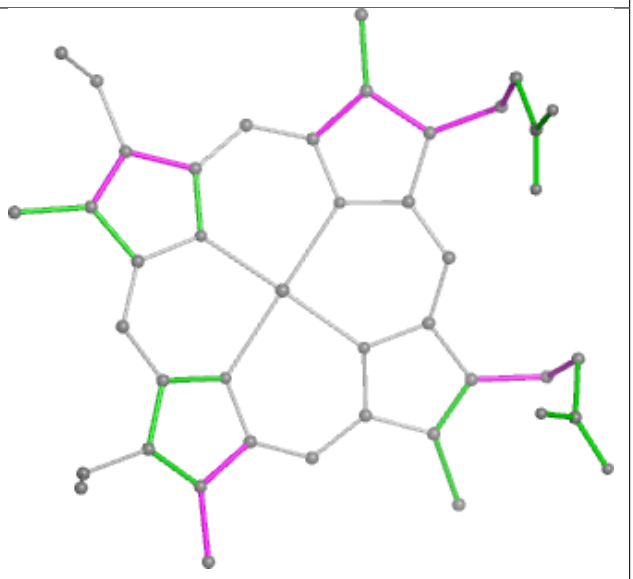


Rings

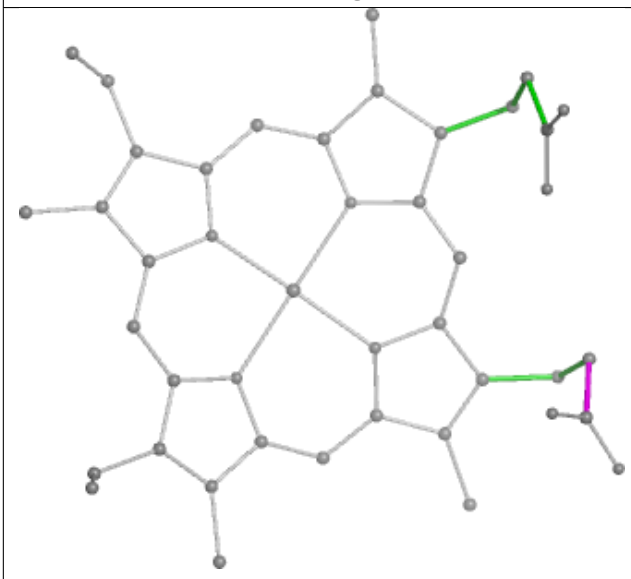
Ligand HEC A 1001



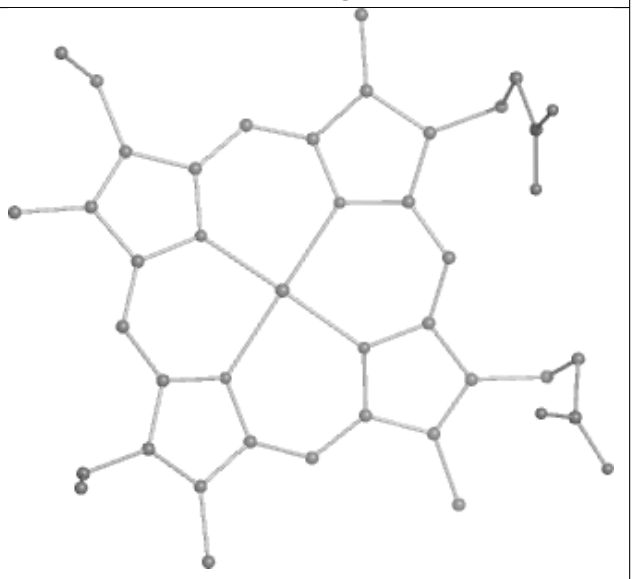
Bond lengths



Bond angles

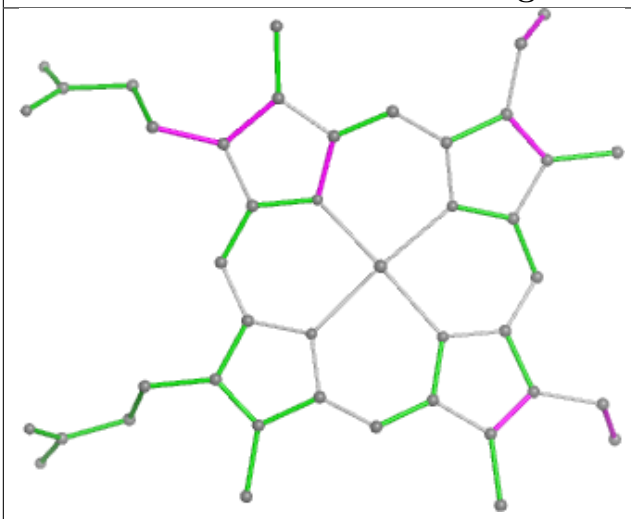


Torsions

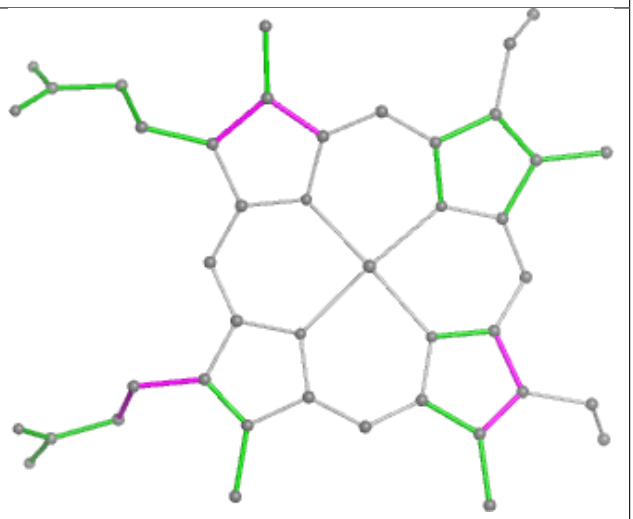


Rings

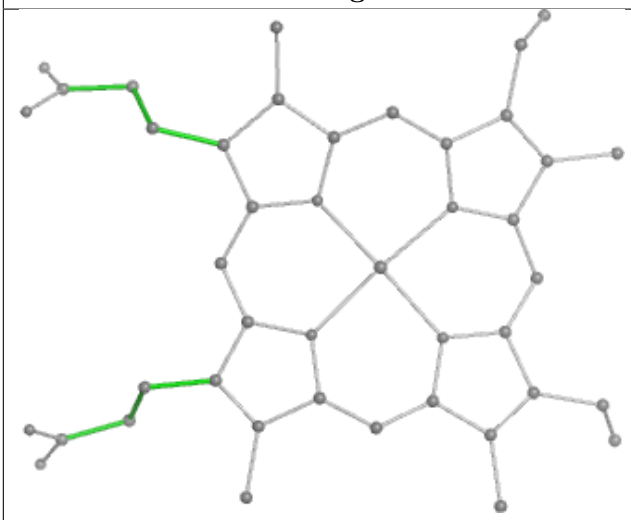
Ligand HEC J 1003



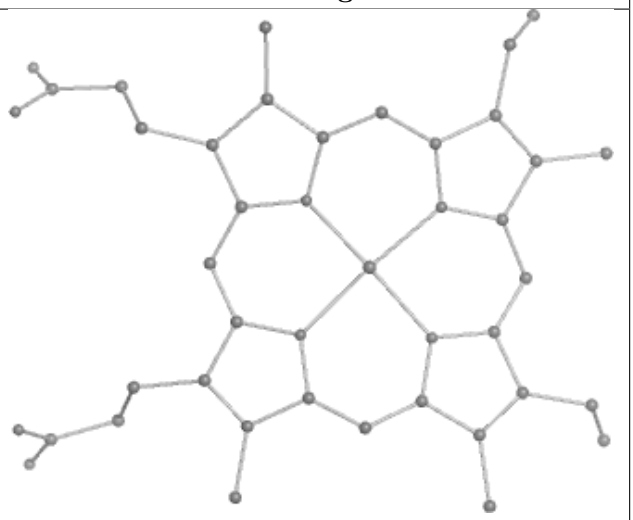
Bond lengths



Bond angles

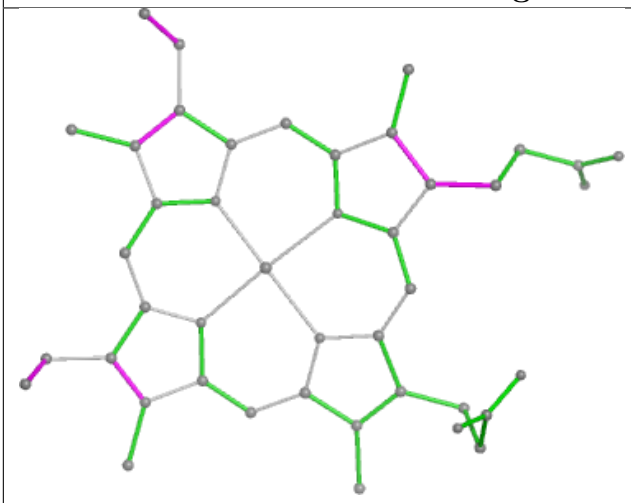


Torsions

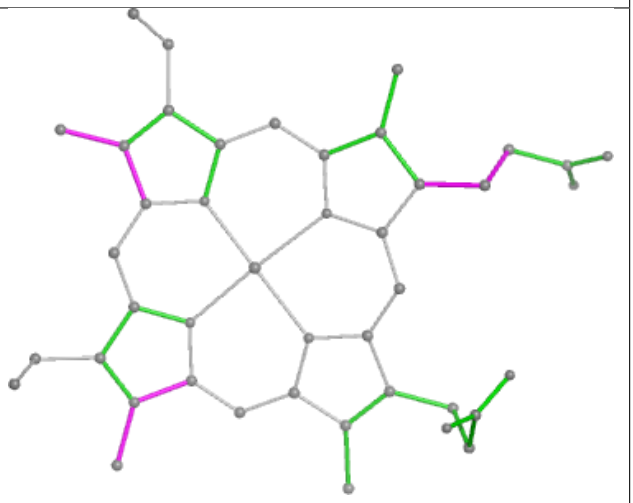


Rings

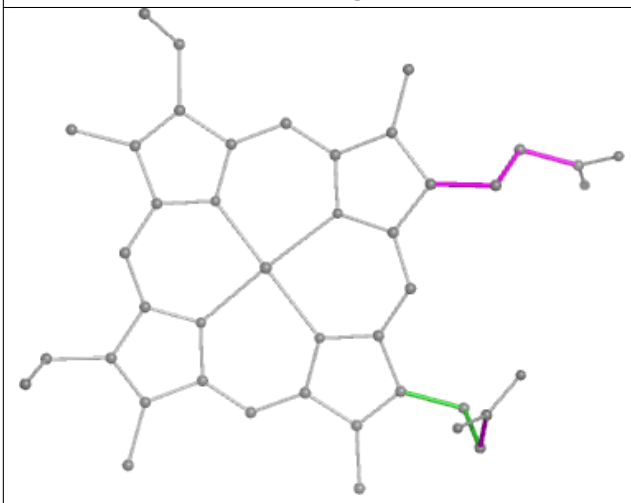
Ligand HEC G 1002



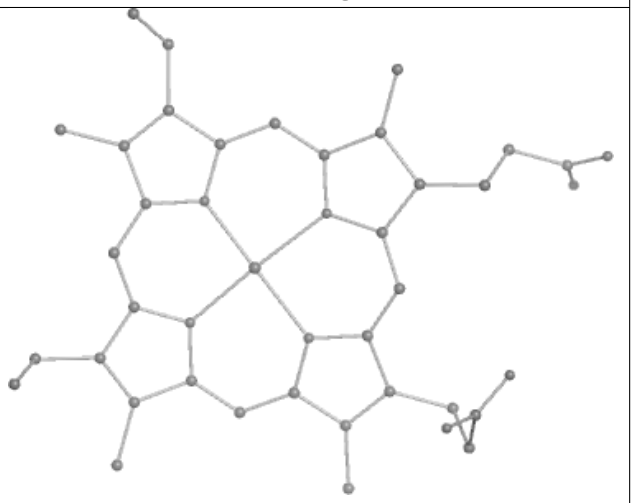
Bond lengths



Bond angles

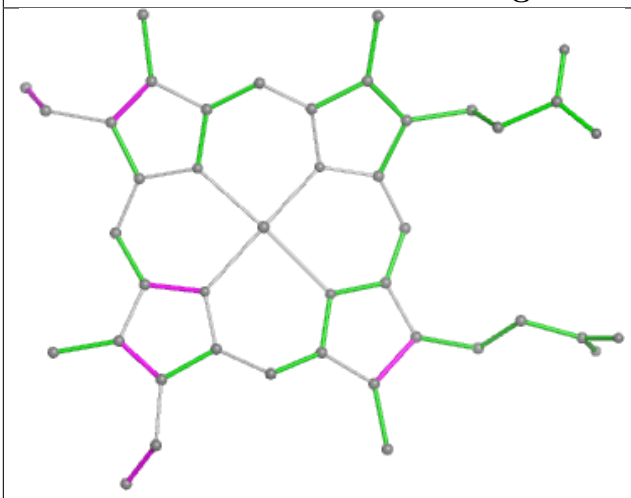


Torsions

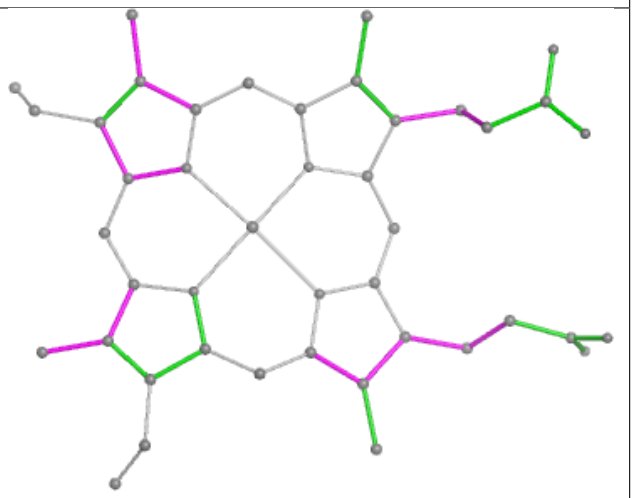


Rings

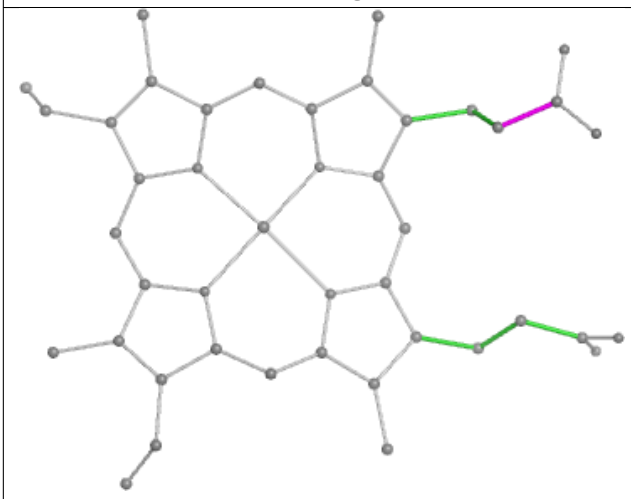
Ligand HEC N 1004



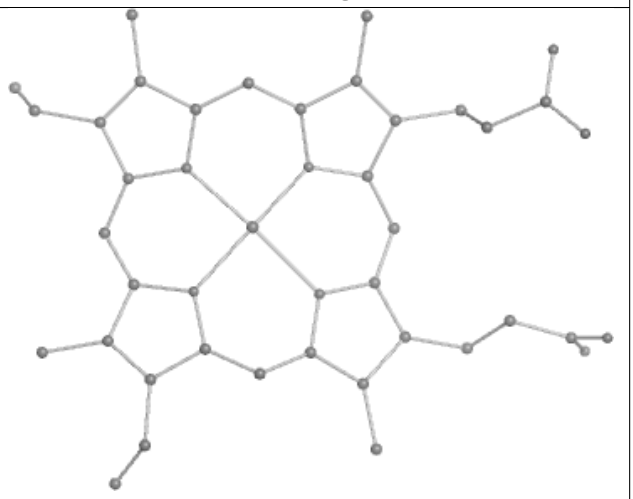
Bond lengths



Bond angles

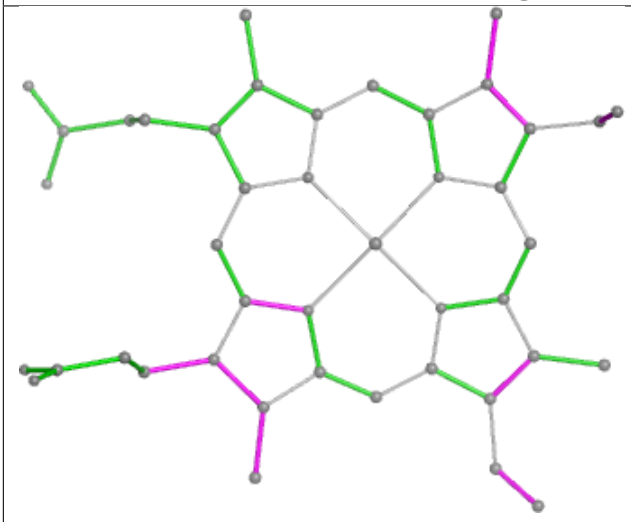


Torsions

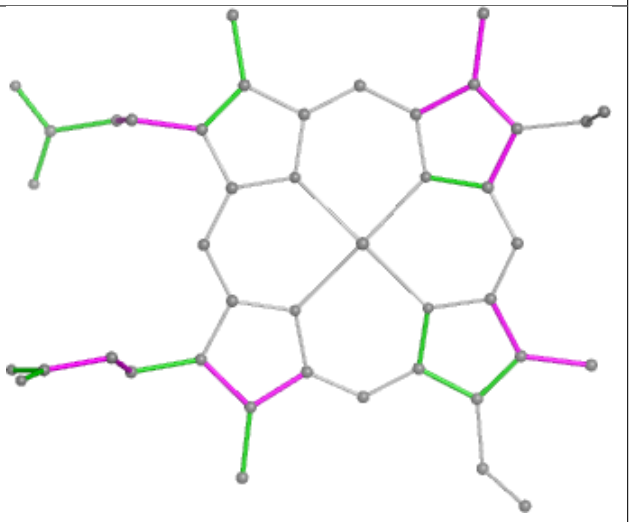


Rings

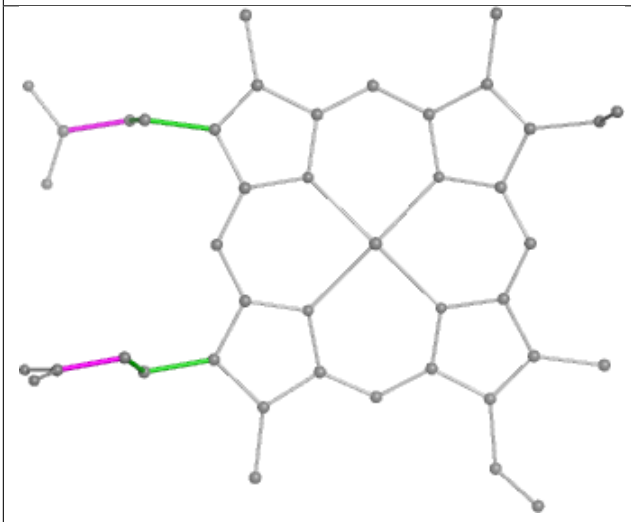
Ligand HEC F 1004



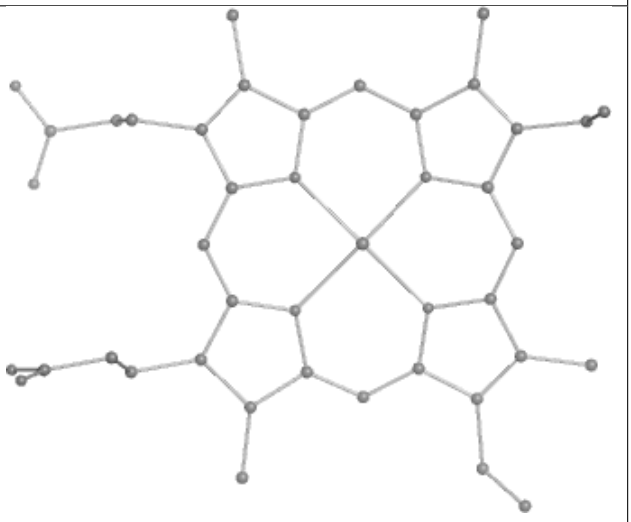
Bond lengths



Bond angles

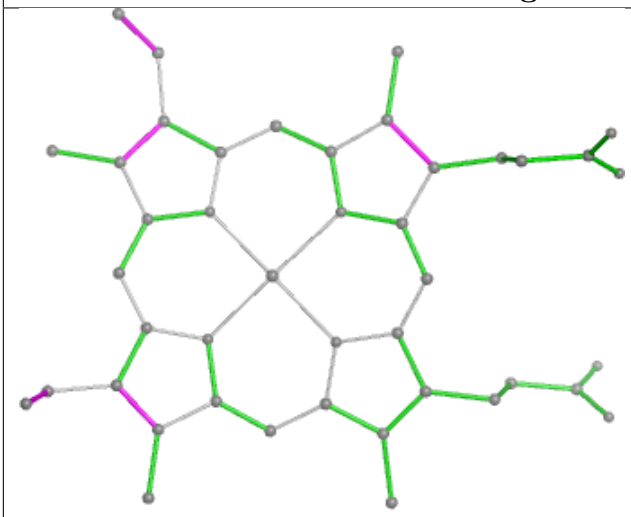


Torsions

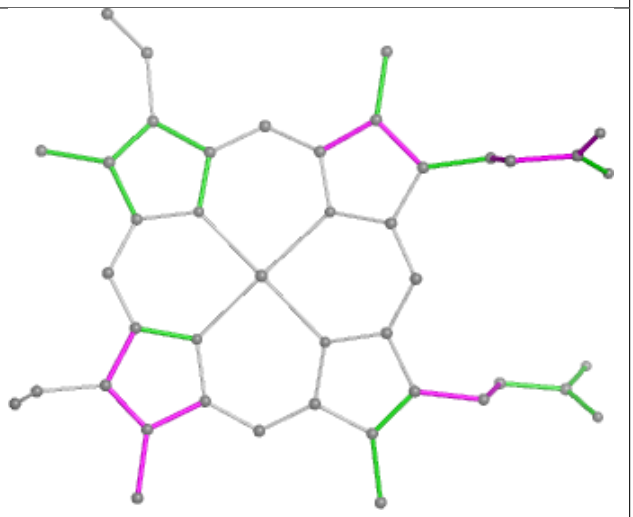


Rings

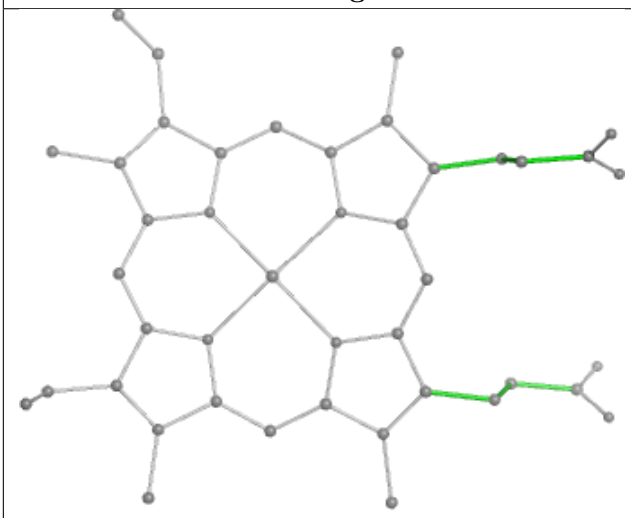
Ligand HEC I 1004



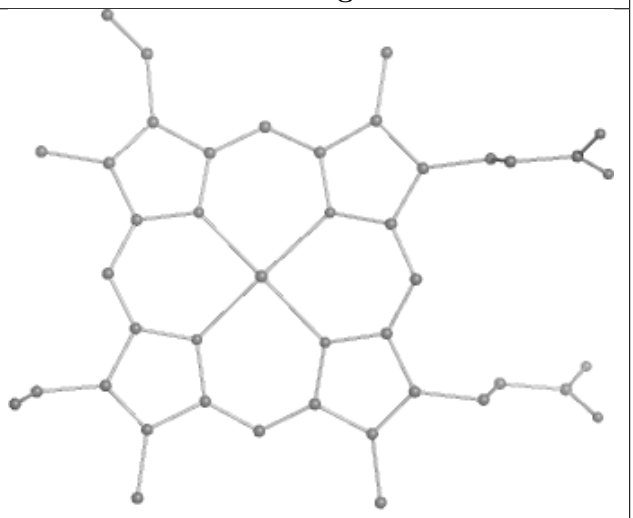
Bond lengths



Bond angles

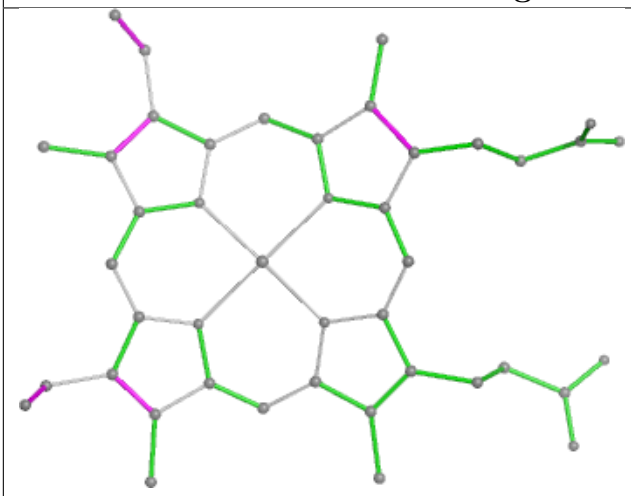


Torsions

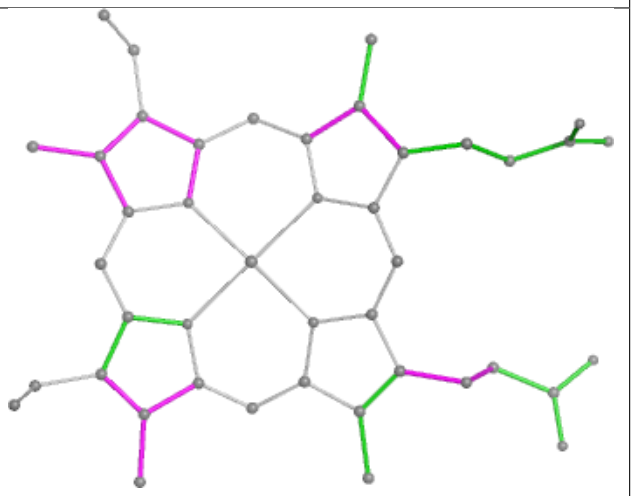


Rings

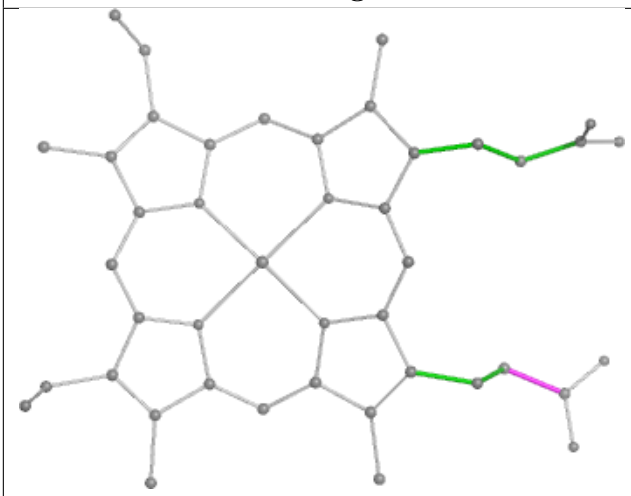
Ligand HEC B 1004



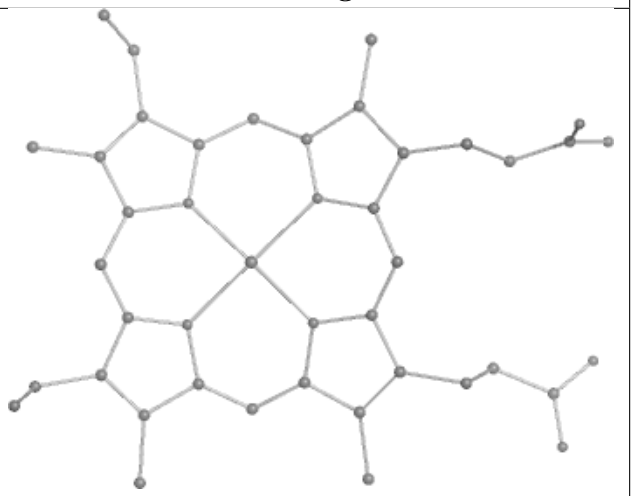
Bond lengths



Bond angles

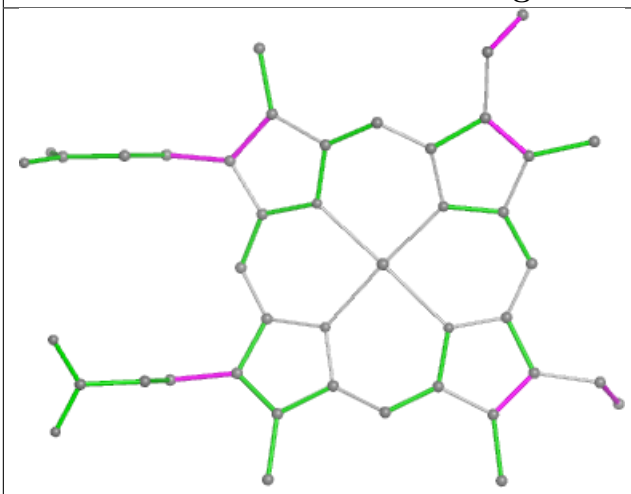


Torsions

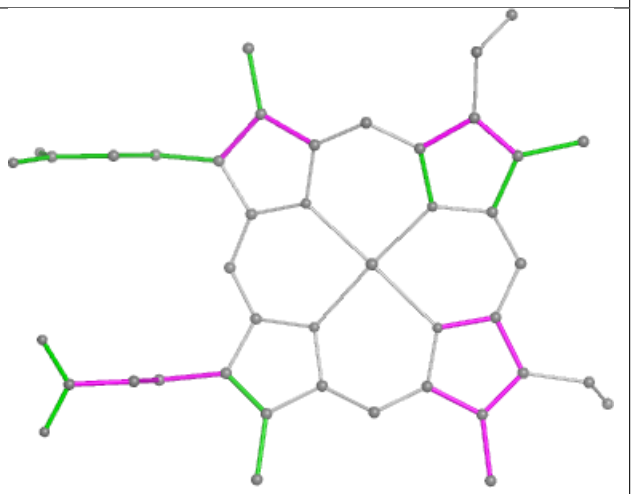


Rings

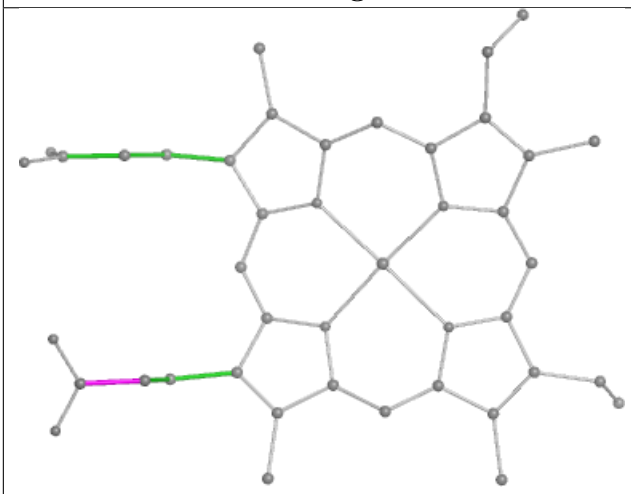
Ligand HEC D 1004



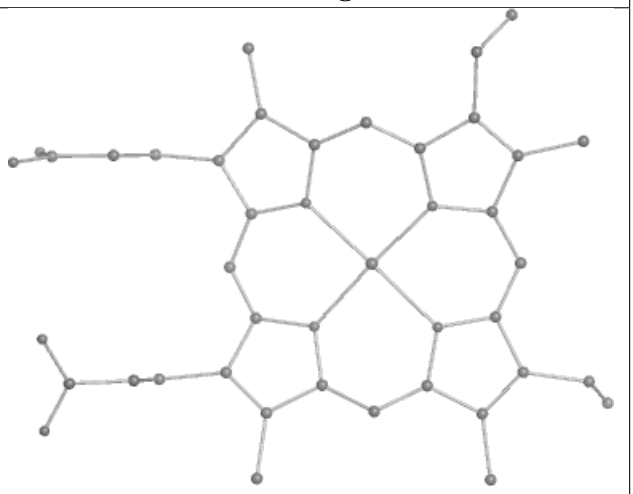
Bond lengths



Bond angles

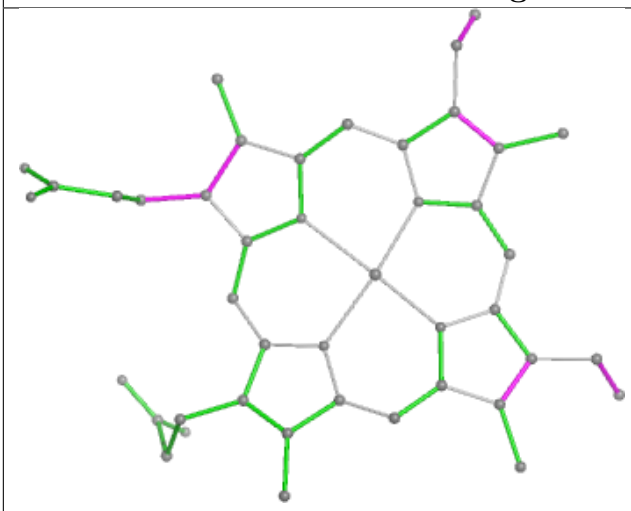


Torsions

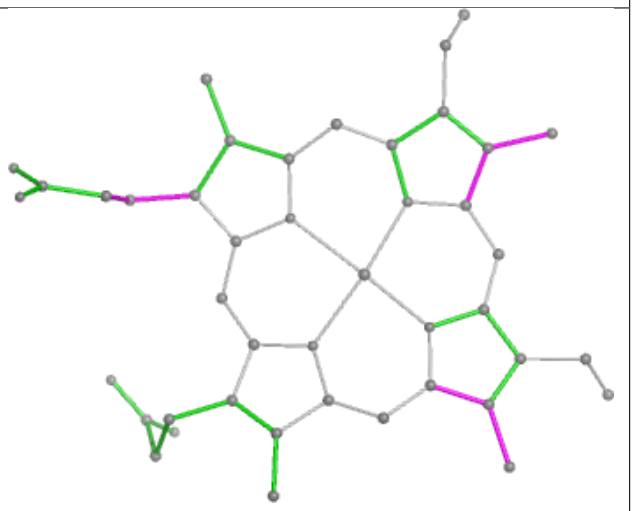


Rings

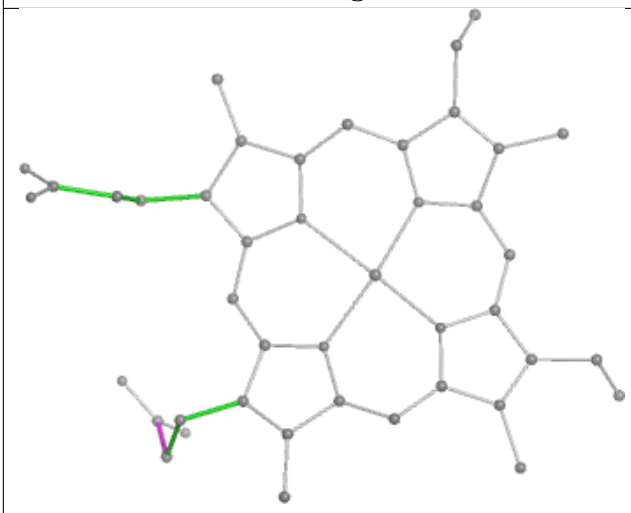
Ligand HEC M 1002



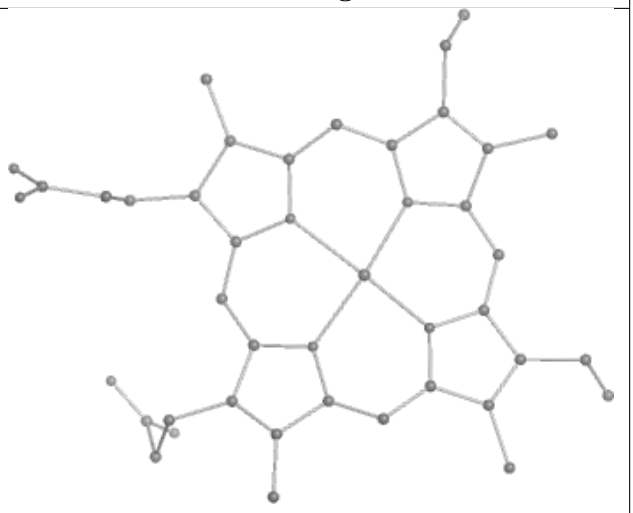
Bond lengths



Bond angles

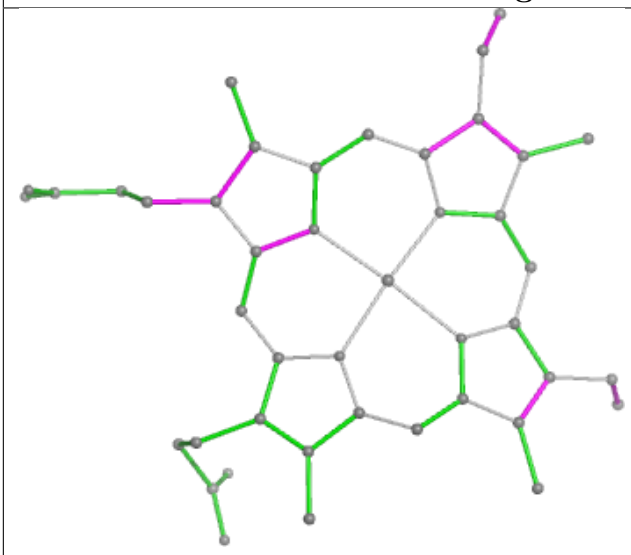


Torsions

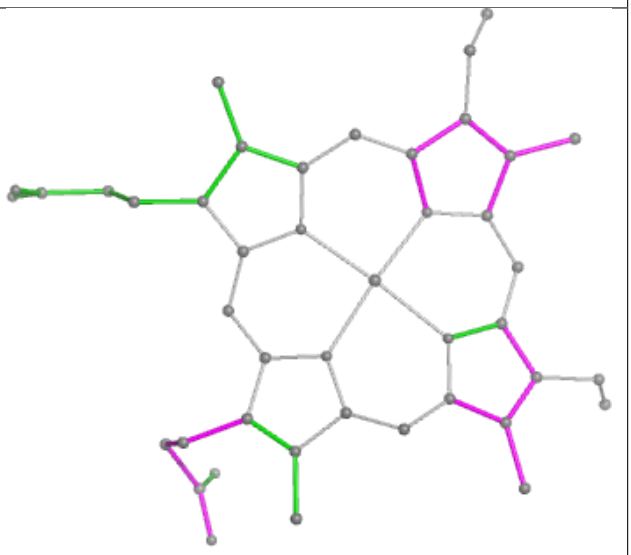


Rings

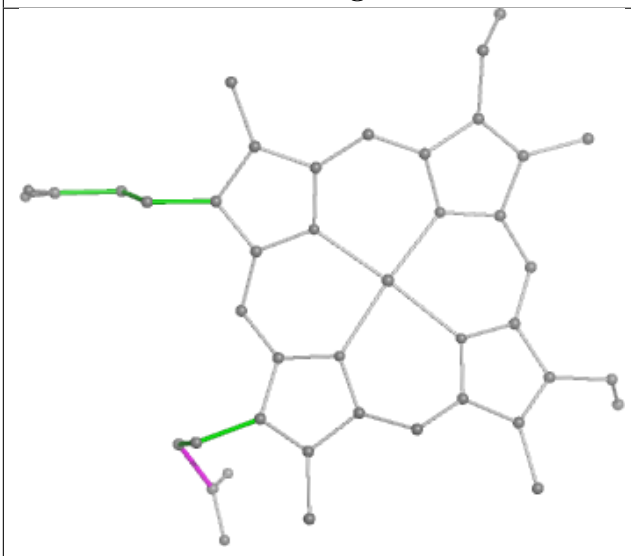
Ligand HEC F 1003



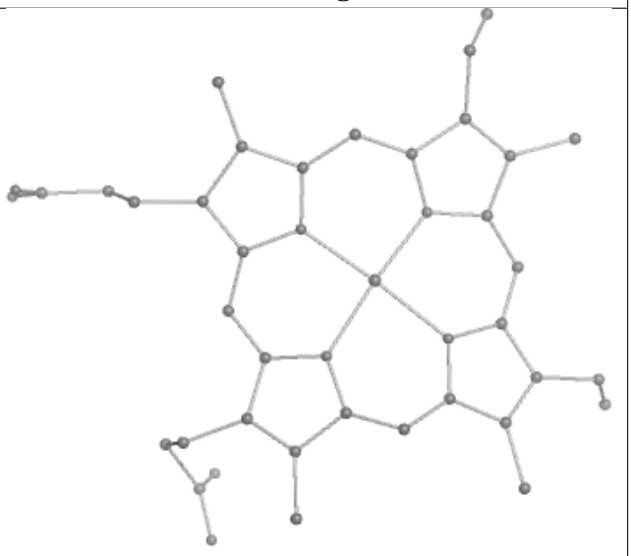
Bond lengths



Bond angles

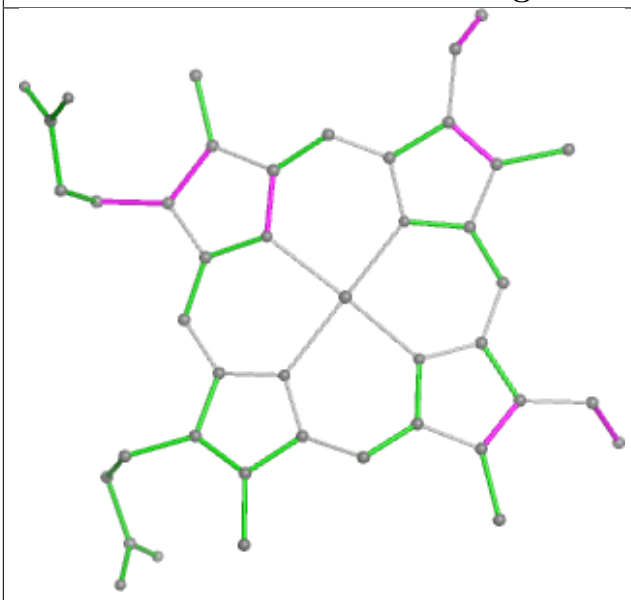


Torsions

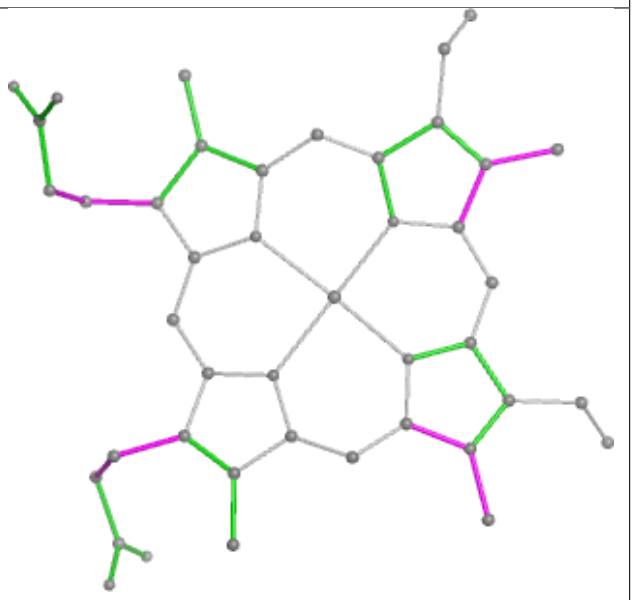


Rings

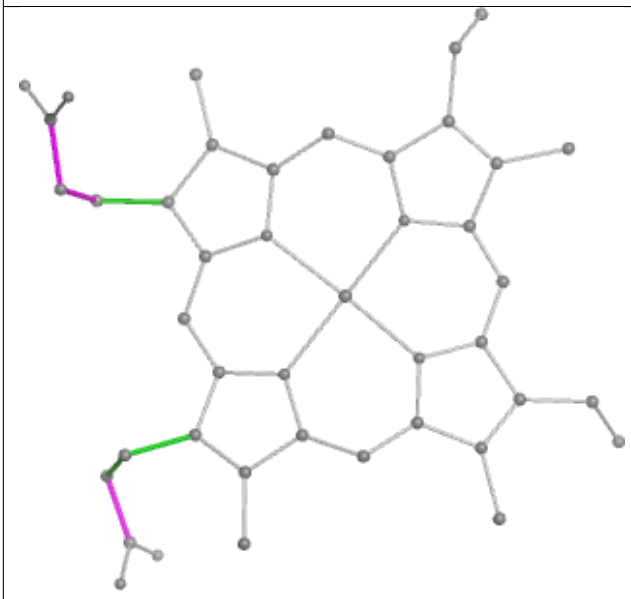
Ligand HEC D 1005



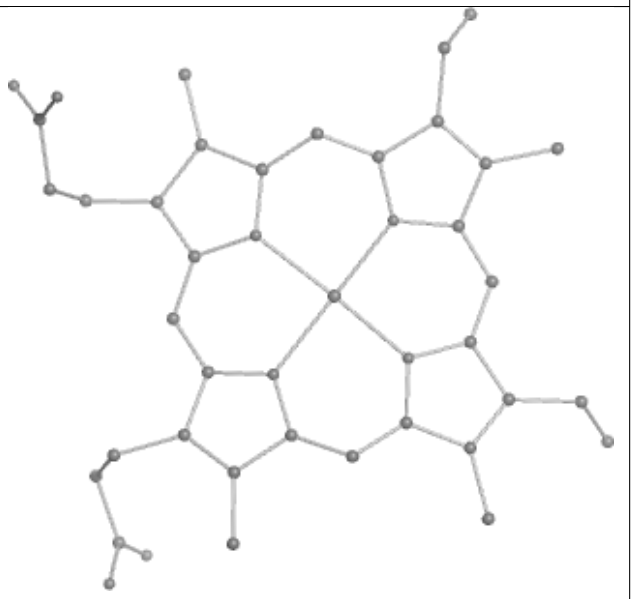
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks

Mol	Chain	Number of breaks
1	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	463:TYR	C	464:GLY	N	1.14
1	M	462:GLN	C	463:TYR	N	1.06

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	495/500 (99%)	-0.29	7 (1%) 73 74	5, 17, 32, 50	2 (0%)
1	B	498/500 (99%)	-0.35	5 (1%) 79 79	5, 16, 33, 52	1 (0%)
1	D	494/500 (98%)	-0.30	1 (0%) 92 92	6, 18, 34, 50	1 (0%)
1	E	494/500 (98%)	-0.10	14 (2%) 55 56	8, 21, 37, 53	1 (0%)
1	G	494/500 (98%)	-0.31	4 (0%) 82 83	6, 17, 32, 50	1 (0%)
1	H	497/500 (99%)	-0.33	5 (1%) 79 79	5, 16, 33, 51	3 (0%)
1	J	494/500 (98%)	-0.22	5 (1%) 79 79	7, 18, 34, 50	3 (0%)
1	K	496/500 (99%)	-0.02	11 (2%) 62 63	9, 21, 38, 53	0
1	M	494/500 (98%)	-0.29	6 (1%) 76 76	5, 17, 32, 50	2 (0%)
1	N	498/500 (99%)	-0.31	10 (2%) 64 66	6, 16, 33, 51	1 (0%)
1	P	494/500 (98%)	-0.19	8 (1%) 70 71	8, 19, 34, 49	1 (0%)
1	Q	495/500 (99%)	-0.04	15 (3%) 52 54	9, 21, 37, 53	1 (0%)
2	C	145/159 (91%)	0.37	18 (12%) 9 10	8, 21, 80, 97	1 (0%)
2	F	145/159 (91%)	0.59	22 (15%) 6 7	8, 26, 80, 96	1 (0%)
2	I	145/159 (91%)	0.38	15 (10%) 13 15	8, 22, 80, 96	0
2	L	145/159 (91%)	0.62	21 (14%) 7 8	11, 27, 81, 96	0
2	O	144/159 (90%)	0.44	16 (11%) 12 13	9, 21, 76, 96	0
2	R	145/159 (91%)	0.61	19 (13%) 8 9	10, 27, 80, 96	0
All	All	6812/6954 (97%)	-0.14	202 (2%) 52 54	5, 19, 38, 97	19 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	15	LEU	8.1
2	O	15	LEU	7.5
2	F	15	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
2	I	15	LEU	7.1
2	R	15	LEU	6.8
2	C	16	VAL	6.7
2	L	16	VAL	6.7
1	M	29	ASP	6.7
2	F	17	LEU	6.6
2	O	16	VAL	6.6
2	C	15	LEU	6.4
2	R	17	LEU	6.2
2	R	14	LYS	6.0
1	A	29	ASP	5.9
2	I	17	LEU	5.9
2	I	14	LYS	5.7
2	O	17	LEU	5.7
2	C	22	LEU	5.4
2	I	16	VAL	5.3
1	E	328	ASP	5.3
2	L	22	LEU	5.1
2	F	22	LEU	5.0
2	I	22	LEU	5.0
1	N	326	SER	5.0
2	C	17	LEU	4.9
2	F	16	VAL	4.9
2	L	17	LEU	4.8
1	Q	327	ASP	4.6
2	R	16	VAL	4.6
1	E	327	ASP	4.5
2	I	20	ALA	4.5
2	L	14	LYS	4.4
1	Q	326	SER	4.4
1	K	326	SER	4.3
2	I	24	VAL	4.3
1	H	327	ASP	4.3
2	C	14	LYS	4.3
2	F	14	LYS	4.2
2	F	19	GLY	4.2
2	F	20	ALA	4.1
2	I	25	VAL	4.1
2	O	24	VAL	4.1
2	F	18	GLY	4.0
1	A	520	VAL	4.0
2	O	25	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	46	GLU	3.9
2	R	22	LEU	3.9
1	Q	520	VAL	3.9
1	P	176	ASP	3.8
2	L	23	GLY	3.8
2	I	21	THR	3.8
2	R	20	ALA	3.8
1	Q	330	LYS	3.8
2	O	22	LEU	3.7
1	K	520	VAL	3.7
2	R	28	ALA	3.7
1	N	327	ASP	3.7
2	L	19	GLY	3.7
2	C	24	VAL	3.7
1	B	326	SER	3.7
2	C	18	GLY	3.6
1	H	326	SER	3.6
2	R	18	GLY	3.6
1	E	176	ASP	3.5
2	I	19	GLY	3.5
2	L	24	VAL	3.5
1	E	326	SER	3.5
2	F	24	VAL	3.5
2	O	18	GLY	3.4
1	H	26	GLY	3.4
2	C	20	ALA	3.4
2	F	34	MET	3.4
2	O	27	LEU	3.3
2	L	88	ARG	3.3
2	R	97	HIS	3.3
1	B	327	ASP	3.3
1	K	327	ASP	3.3
2	R	25	VAL	3.3
1	N	46	GLU	3.2
1	Q	26	GLY	3.2
2	F	21	THR	3.2
1	E	28	SER	3.2
1	Q	405	ASP	3.2
2	I	18	GLY	3.2
1	K	176	ASP	3.2
2	O	20	ALA	3.2
2	C	23	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	328	ASP	3.1
1	H	328	ASP	3.1
2	C	28	ALA	3.1
1	Q	35	LYS	3.1
2	R	24	VAL	3.0
2	R	31	ALA	3.0
2	F	23	GLY	3.0
1	J	176	ASP	3.0
1	Q	329	LYS	3.0
1	N	522	ALA	3.0
2	L	18	GLY	3.0
2	R	106	MET	3.0
2	C	97[A]	HIS	2.9
2	C	21	THR	2.9
2	F	27	LEU	2.9
2	F	25	VAL	2.9
1	Q	519	LEU	2.9
1	E	330	LYS	2.9
2	O	34	MET	2.9
1	A	26	GLY	2.9
1	N	328	ASP	2.9
1	N	25	ALA	2.9
1	G	33	GLU	2.9
1	Q	33	GLU	2.9
2	O	19	GLY	2.8
1	P	514	ASP	2.8
1	G	27	CYS	2.8
1	E	496	THR	2.8
2	F	97	HIS	2.8
2	F	35	LYS	2.8
2	O	88	ARG	2.8
1	A	471	GLY	2.8
2	L	96	GLY	2.8
1	P	406	ASP	2.7
1	P	46	GLU	2.7
2	L	91	TYR	2.7
1	B	328	ASP	2.7
1	Q	130[A]	HIS	2.7
2	R	19	GLY	2.7
1	K	26	GLY	2.6
1	E	33	GLU	2.6
2	F	91	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	R	27	LEU	2.6
2	F	32	PHE	2.6
2	F	28	ALA	2.6
2	L	20	ALA	2.6
2	I	27	LEU	2.6
2	O	21	THR	2.6
1	Q	27	CYS	2.6
1	N	510	ASP	2.6
1	P	473	ILE	2.5
2	L	97	HIS	2.5
1	Q	402	ALA	2.5
1	M	27	CYS	2.5
2	F	88	ARG	2.5
1	K	28	SER	2.5
1	M	26	GLY	2.5
2	L	29	THR	2.5
1	Q	28	SER	2.4
1	H	27	CYS	2.4
2	R	23	GLY	2.4
2	L	27	LEU	2.4
2	L	21	THR	2.4
1	D	471	GLY	2.4
2	C	25	VAL	2.4
1	E	519	LEU	2.4
1	J	181	LYS	2.4
2	C	19	GLY	2.4
2	I	97	HIS	2.4
1	K	25	ALA	2.4
2	R	21	THR	2.3
2	R	88	ARG	2.3
2	C	34	MET	2.3
2	L	106	MET	2.3
1	J	29	ASP	2.3
1	B	46	GLU	2.3
1	B	25	ALA	2.3
2	O	29	THR	2.3
2	R	30	VAL	2.3
1	J	28	SER	2.3
1	E	517	LYS	2.2
1	P	30	VAL	2.2
1	E	470	SER	2.2
1	K	33	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	34	LEU	2.2
1	A	30	VAL	2.2
1	E	329	LYS	2.2
2	O	23	GLY	2.2
2	F	106	MET	2.2
2	F	29	THR	2.2
1	Q	181	LYS	2.2
1	G	28	SER	2.2
1	A	197	GLU	2.2
2	O	47	HIS	2.2
2	L	26	ALA	2.2
1	N	26	GLY	2.1
1	M	130[A]	HIS	2.1
1	J	30	VAL	2.1
1	K	510	ASP	2.1
1	N	492	GLU	2.1
1	K	517	LYS	2.1
2	L	25	VAL	2.1
1	N	27	CYS	2.1
1	A	33	GLU	2.1
1	M	30	VAL	2.1
2	C	30	VAL	2.1
2	I	88	ARG	2.1
1	P	27	CYS	2.1
2	I	74	ASN	2.1
2	L	79	LEU	2.1
1	P	347	ARG	2.0
1	M	402	ALA	2.0
1	E	510	ASP	2.0
2	C	32	PHE	2.0
2	C	106	MET	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
5	LMT	R	1005	35/35	0.78	0.22	41,49,75,75	0
5	LMT	O	1005	35/35	0.81	0.20	38,45,74,75	0
5	LMT	I	1005	35/35	0.82	0.19	36,41,72,73	0
5	LMT	L	1005	35/35	0.82	0.20	40,46,66,67	0
5	LMT	C	1005	35/35	0.83	0.19	36,41,72,73	0
5	LMT	F	1005	35/35	0.83	0.19	37,44,70,71	0
6	ACT	C	1006	4/4	0.86	0.14	34,34,34,34	0
6	ACT	I	1006	4/4	0.86	0.14	38,39,39,39	0
6	ACT	O	1006	4/4	0.89	0.15	32,32,33,33	0
3	HEC	E	1005	43/43	0.94	0.10	11,14,20,24	0
3	HEC	L	1101	43/43	0.94	0.11	23,27,33,36	0
3	HEC	R	1001	43/43	0.94	0.11	22,26,37,42	0
3	HEC	C	1001	43/43	0.94	0.11	17,20,29,34	0
3	HEC	K	1002	43/43	0.95	0.10	18,21,23,24	0
3	HEC	K	1005	43/43	0.95	0.09	9,15,23,26	0
3	HEC	L	1002	43/43	0.95	0.10	16,18,26,29	0
3	HEC	A	1003	43/43	0.95	0.07	2,6,9,12	0
3	HEC	M	1001	43/43	0.95	0.07	3,9,11,12	0
3	HEC	N	1004	43/43	0.95	0.08	2,5,8,13	0
3	HEC	O	1001	43/43	0.95	0.10	17,20,28,34	0
3	HEC	O	1003	43/43	0.95	0.09	8,12,17,20	0
3	HEC	Q	1005	43/43	0.95	0.09	12,15,20,29	0
3	HEC	A	1004	43/43	0.95	0.08	2,5,11,14	0
3	HEC	R	1002	43/43	0.95	0.10	17,20,28,32	0
3	HEC	F	1001	43/43	0.95	0.10	20,24,27,31	0
3	HEC	F	1003	43/43	0.95	0.09	7,10,18,24	0
3	HEC	G	1003	43/43	0.95	0.08	4,7,11,13	0
3	HEC	H	1004	43/43	0.95	0.08	3,6,8,12	0
3	HEC	H	1005	43/43	0.95	0.09	5,8,18,22	0
3	HEC	I	1001	43/43	0.95	0.10	18,21,29,32	0
3	HEC	I	1002	43/43	0.95	0.10	11,15,26,29	0
3	HEC	I	1003	43/43	0.95	0.08	7,12,19,24	0
3	HEC	K	1001	43/43	0.95	0.09	15,19,23,25	0
3	HEC	B	1005	43/43	0.96	0.09	4,8,18,21	0
3	HEC	A	1002	43/43	0.96	0.08	5,9,14,18	0
3	HEC	C	1002	43/43	0.96	0.09	8,13,27,29	0
3	HEC	C	1003	43/43	0.96	0.08	8,11,15,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	I	1004	43/43	0.96	0.08	3,6,16,20	0
3	HEC	J	1001	43/43	0.96	0.07	8,12,16,16	0
3	HEC	J	1002	43/43	0.96	0.08	9,11,16,21	0
3	HEC	J	1003	43/43	0.96	0.07	5,8,12,16	0
3	HEC	J	1004	43/43	0.96	0.08	3,6,13,21	0
3	HEC	J	1005	43/43	0.96	0.08	10,13,19,22	0
3	HEC	C	1004	43/43	0.96	0.08	3,8,17,22	0
3	HEC	D	1002	43/43	0.96	0.07	4,7,13,19	0
3	HEC	K	1003	43/43	0.96	0.08	9,15,17,18	0
3	HEC	K	1004	43/43	0.96	0.08	7,13,21,25	0
3	HEC	D	1005	43/43	0.96	0.08	6,12,18,19	0
3	HEC	E	1001	43/43	0.96	0.08	14,16,18,20	0
3	HEC	L	1003	43/43	0.96	0.08	8,11,16,21	0
3	HEC	L	1004	43/43	0.96	0.08	7,10,19,21	0
3	HEC	E	1002	43/43	0.96	0.08	13,16,19,21	0
3	HEC	E	1003	43/43	0.96	0.08	12,14,16,18	0
3	HEC	M	1002	43/43	0.96	0.08	6,11,13,17	0
3	HEC	M	1003	43/43	0.96	0.07	3,7,12,14	0
3	HEC	M	1004	43/43	0.96	0.07	2,5,14,16	0
3	HEC	M	1005	43/43	0.96	0.07	4,7,16,21	0
3	HEC	N	1001	43/43	0.96	0.08	6,9,12,13	0
3	HEC	N	1002	43/43	0.96	0.08	6,10,12,14	0
3	HEC	N	1003	43/43	0.96	0.08	3,7,8,11	0
3	HEC	E	1004	43/43	0.96	0.08	7,11,14,21	0
3	HEC	N	1005	43/43	0.96	0.09	3,8,21,24	0
3	HEC	A	1005	43/43	0.96	0.07	2,7,16,22	0
3	HEC	O	1002	43/43	0.96	0.09	12,14,23,29	0
3	HEC	B	1001	43/43	0.96	0.08	5,10,13,16	0
3	HEC	O	1004	43/43	0.96	0.08	5,8,20,23	0
3	HEC	P	1001	43/43	0.96	0.09	12,16,21,24	0
3	HEC	P	1002	43/43	0.96	0.08	6,9,17,24	0
3	HEC	P	1003	43/43	0.96	0.07	6,9,12,14	0
3	HEC	P	1005	43/43	0.96	0.08	8,13,18,22	0
3	HEC	Q	1001	43/43	0.96	0.09	13,18,20,22	0
3	HEC	Q	1002	43/43	0.96	0.09	19,21,22,23	0
3	HEC	Q	1003	43/43	0.96	0.09	14,17,20,23	0
3	HEC	F	1002	43/43	0.96	0.10	14,17,27,30	0
3	HEC	B	1002	43/43	0.96	0.08	6,10,15,17	0
3	HEC	F	1004	43/43	0.96	0.08	3,6,16,24	0
3	HEC	R	1003	43/43	0.96	0.08	7,11,17,21	0
3	HEC	R	1004	43/43	0.96	0.07	3,8,16,21	0
3	HEC	G	1001	43/43	0.96	0.07	3,8,11,13	0

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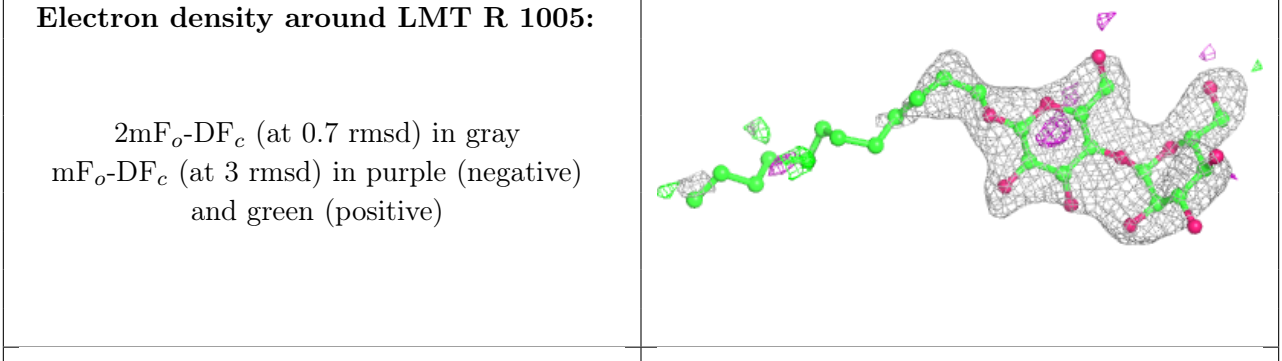
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	G	1002	43/43	0.96	0.09	7,9,14,19	0
3	HEC	B	1003	43/43	0.96	0.08	5,7,9,13	0
3	HEC	G	1004	43/43	0.96	0.07	2,5,12,14	0
3	HEC	G	1005	43/43	0.96	0.07	5,8,12,16	0
3	HEC	H	1001	43/43	0.96	0.08	5,11,13,14	0
3	HEC	H	1002	43/43	0.96	0.08	6,9,14,21	0
3	HEC	H	1003	43/43	0.96	0.08	3,8,10,13	0
3	HEC	B	1004	43/43	0.96	0.07	2,5,7,12	0
3	HEC	D	1001	43/43	0.97	0.08	6,12,16,19	0
3	HEC	A	1001	43/43	0.97	0.07	2,7,12,15	0
3	HEC	D	1003	43/43	0.97	0.07	2,5,8,11	0
3	HEC	Q	1004	43/43	0.97	0.08	7,11,18,19	0
3	HEC	P	1004	43/43	0.97	0.07	5,8,13,18	0
3	HEC	D	1004	43/43	0.97	0.07	2,5,10,16	0
4	CA	Q	1007	1/1	0.98	0.02	20,20,20,20	0
4	CA	H	1007	1/1	0.98	0.02	16,16,16,16	0
4	CA	J	1007	1/1	0.99	0.02	11,11,11,11	0
4	CA	K	1006	1/1	0.99	0.02	16,16,16,16	0
4	CA	K	1007	1/1	0.99	0.03	17,17,17,17	0
4	CA	M	1006	1/1	0.99	0.02	12,12,12,12	0
4	CA	M	1007	1/1	0.99	0.02	14,14,14,14	0
4	CA	N	1007	1/1	0.99	0.02	11,11,11,11	0
4	CA	P	1007	1/1	0.99	0.02	15,15,15,15	0
4	CA	Q	1006	1/1	0.99	0.02	17,17,17,17	0
4	CA	B	1006	1/1	0.99	0.01	11,11,11,11	0
4	CA	B	1007	1/1	0.99	0.02	13,13,13,13	0
4	CA	D	1006	1/1	0.99	0.02	16,16,16,16	0
4	CA	D	1007	1/1	0.99	0.01	11,11,11,11	0
4	CA	E	1006	1/1	0.99	0.02	17,17,17,17	0
4	CA	E	1007	1/1	0.99	0.02	18,18,18,18	0
4	CA	G	1006	1/1	0.99	0.01	13,13,13,13	0
4	CA	G	1007	1/1	0.99	0.03	16,16,16,16	0
4	CA	A	1006	1/1	0.99	0.01	13,13,13,13	0
4	CA	J	1006	1/1	0.99	0.02	13,13,13,13	0
4	CA	A	1007	1/1	1.00	0.01	11,11,11,11	0
4	CA	N	1006	1/1	1.00	0.01	10,10,10,10	0
4	CA	H	1006	1/1	1.00	0.02	11,11,11,11	0
4	CA	P	1006	1/1	1.00	0.01	16,16,16,16	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.

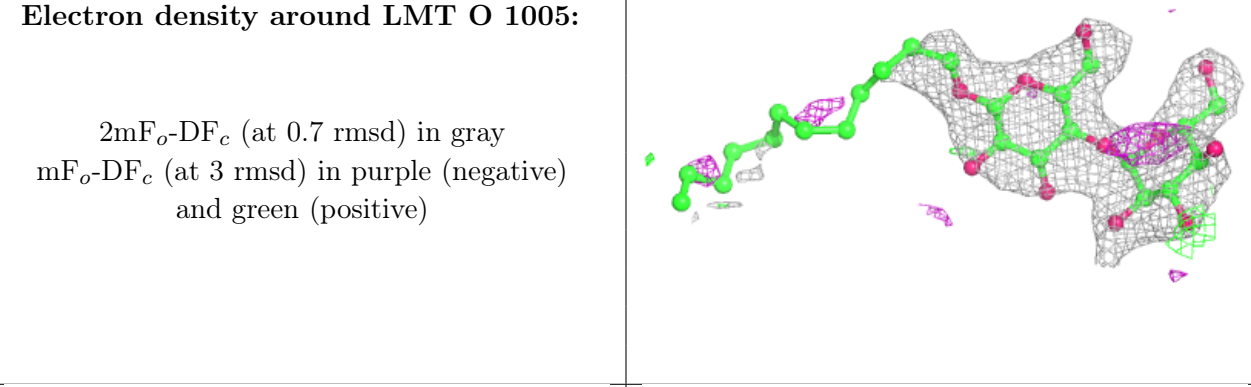
Electron density around LMT R 1005:

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



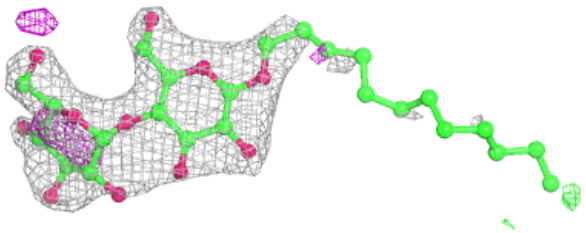
Electron density around LMT O 1005:

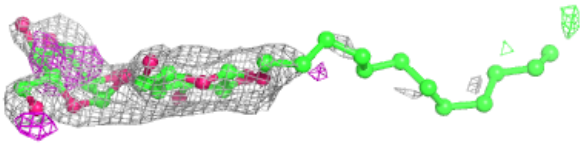
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT I 1005:

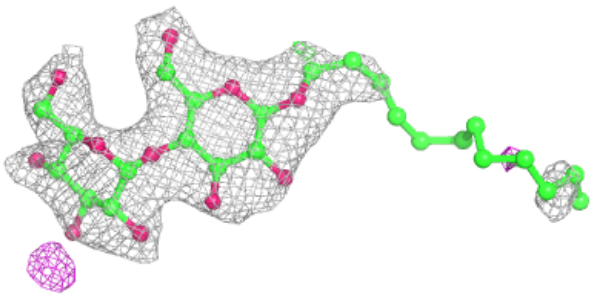
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

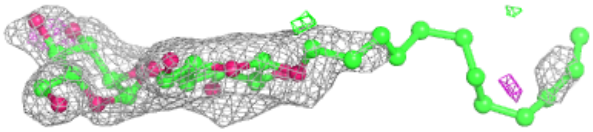




Electron density around LMT L 1005:

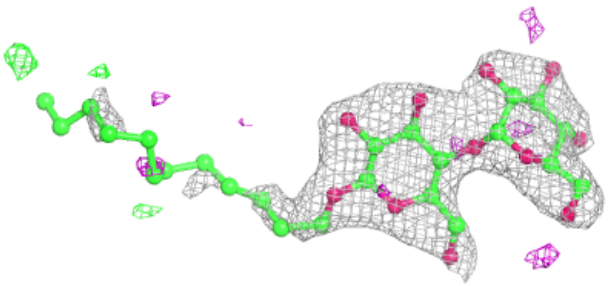
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

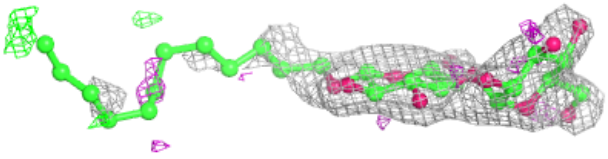


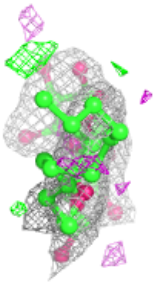


Electron density around LMT C 1005:

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

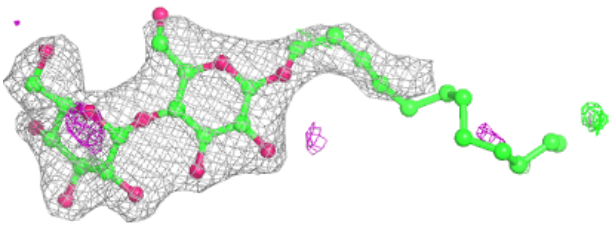


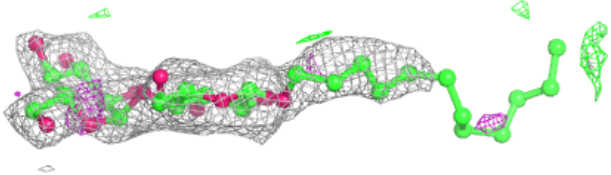


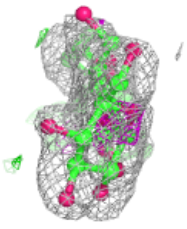


Electron density around LMT F 1005:

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

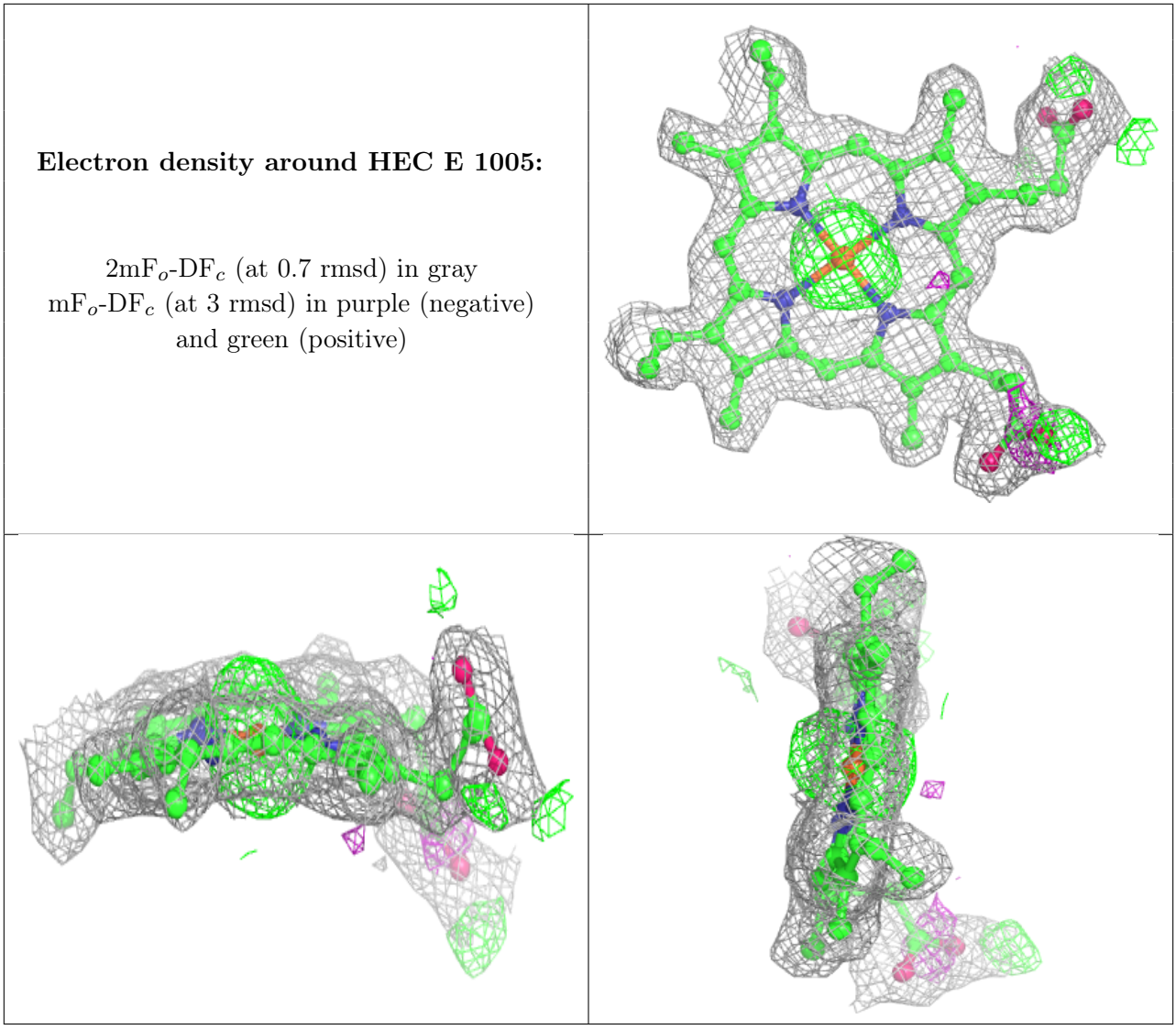






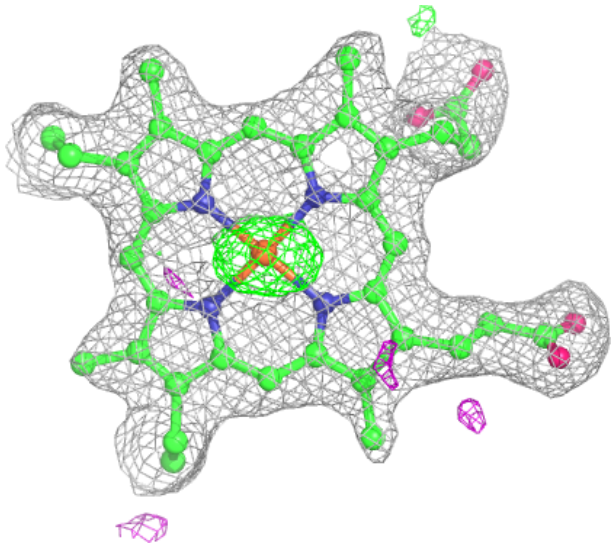
Electron density around HEC E 1005:

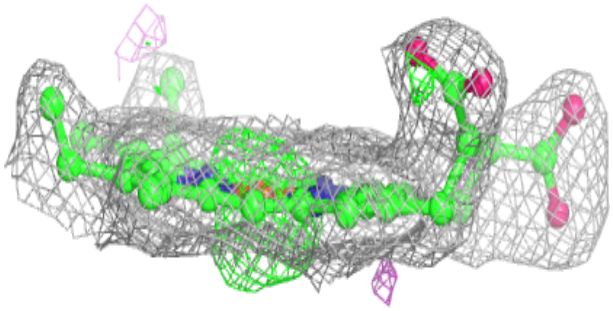
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

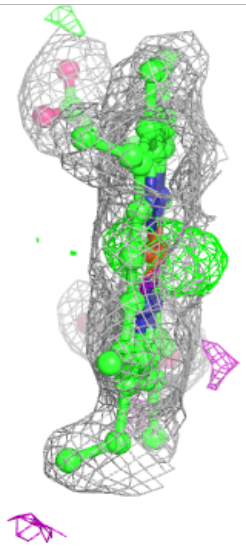


Electron density around HEC L 1101:

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

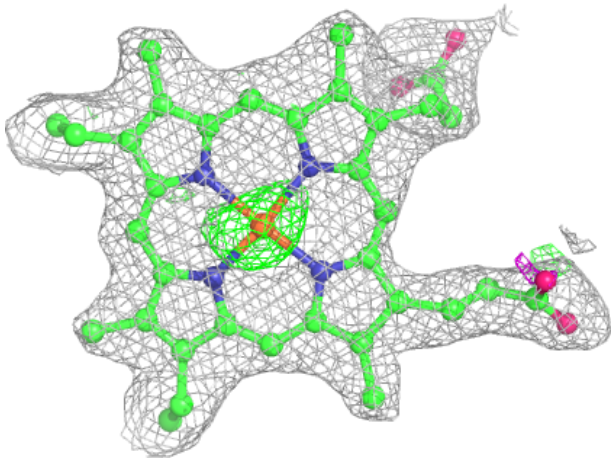


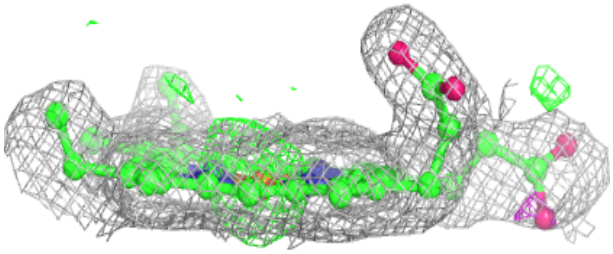


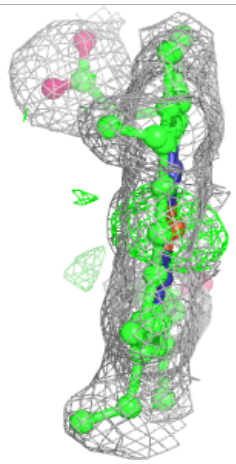


Electron density around HEC R 1001:

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

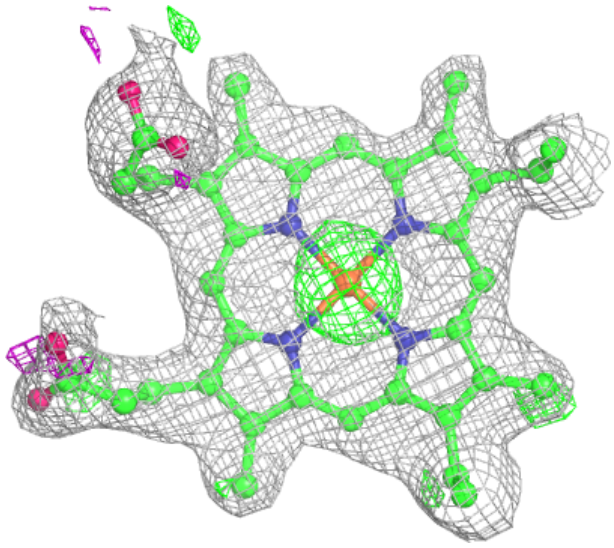


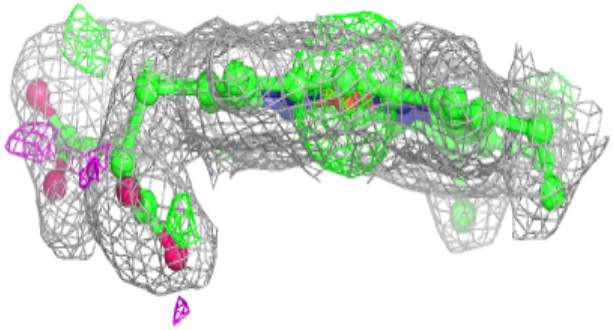


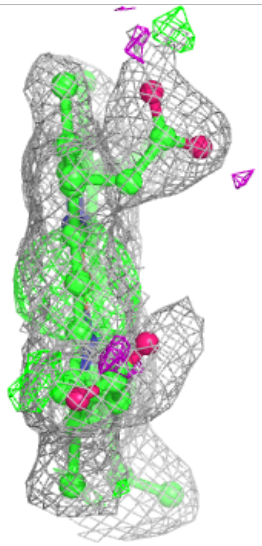


Electron density around HEC C 1001:

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

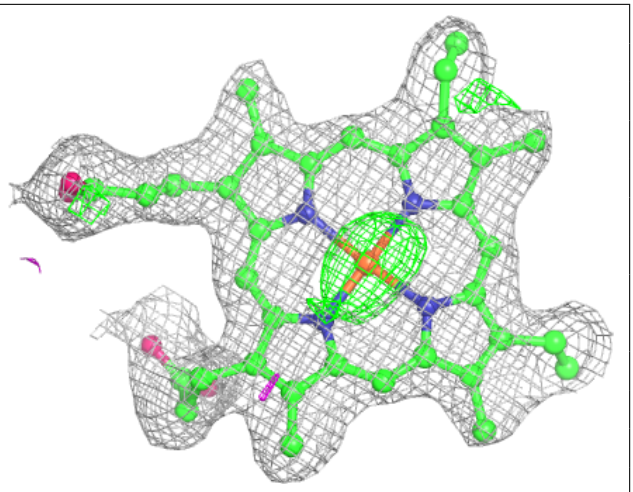


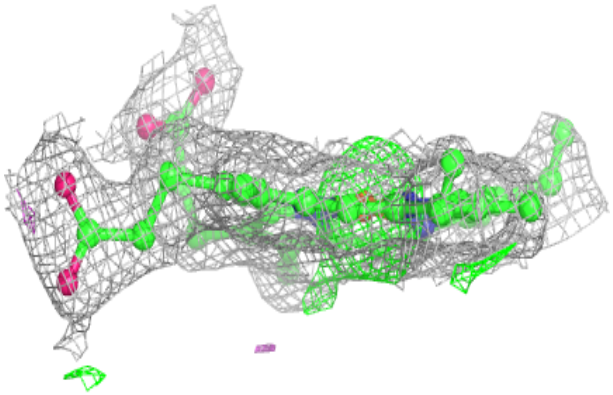


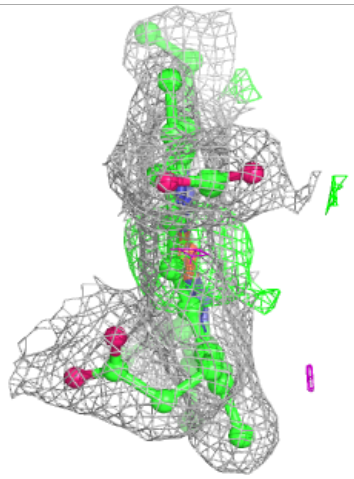


Electron density around HEC K 1002:

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

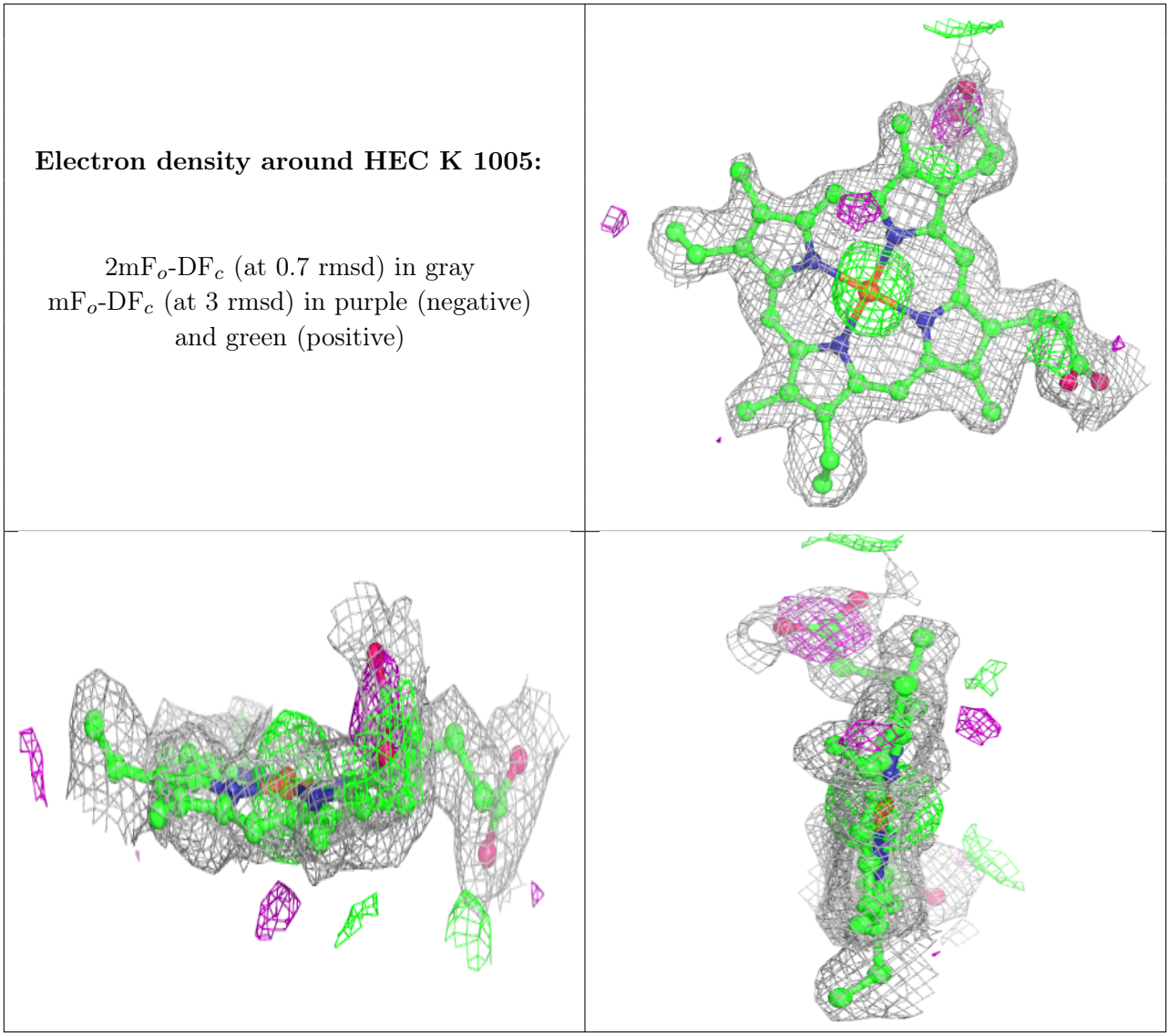






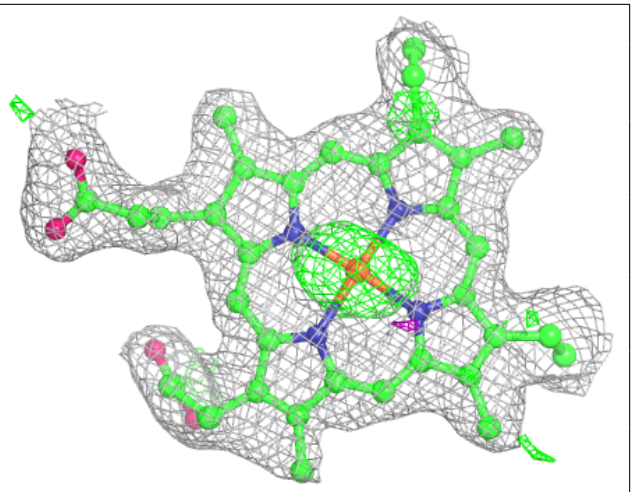
Electron density around HEC K 1005:

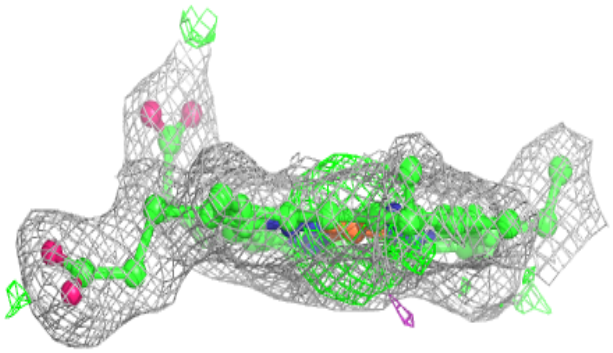
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

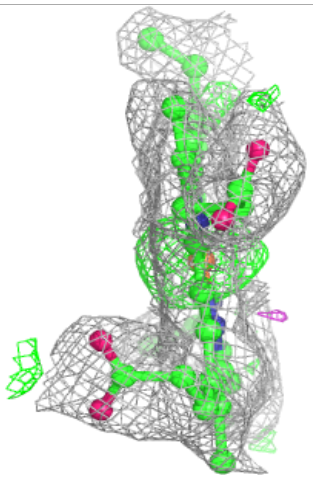


Electron density around HEC L 1002:

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

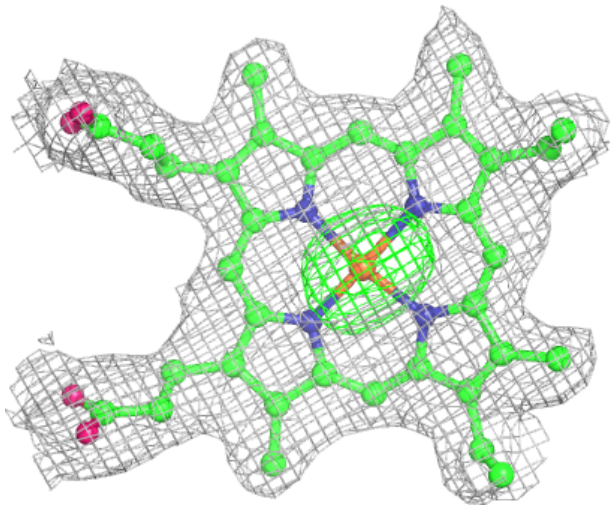


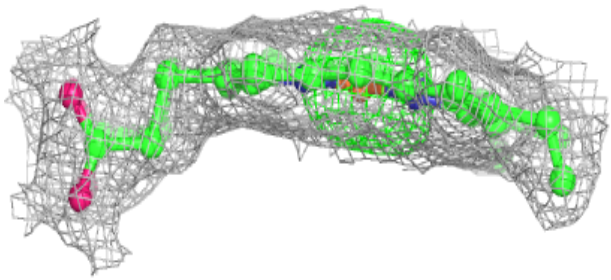


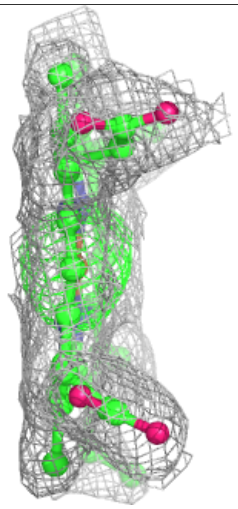


Electron density around HEC A 1003:

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

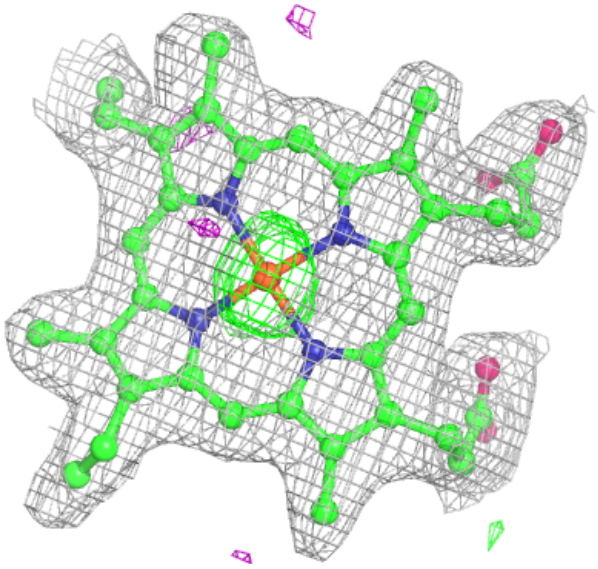


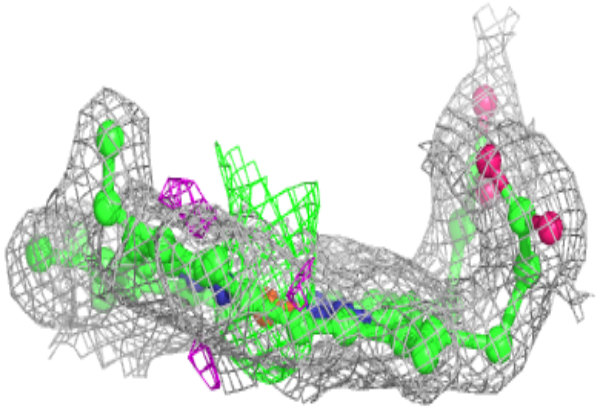


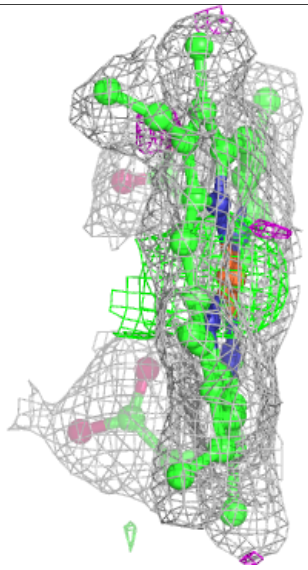


Electron density around HEC M 1001:

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

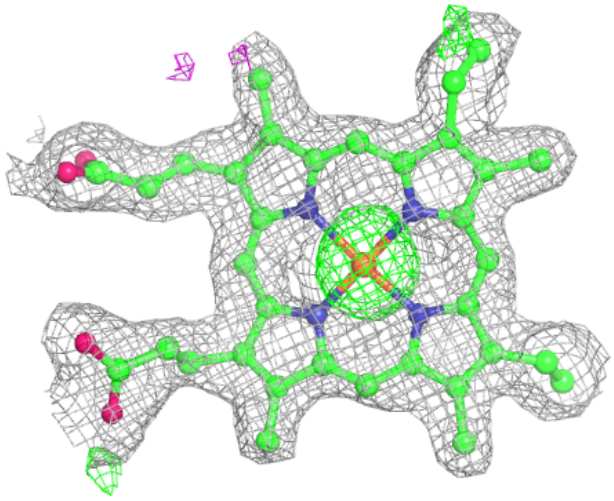


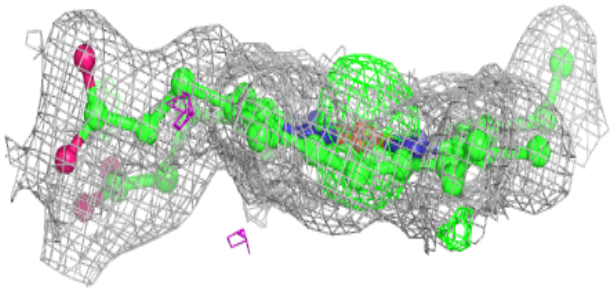


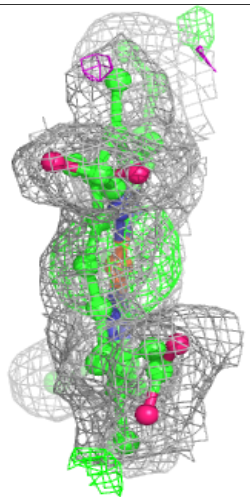


Electron density around HEC N 1004:

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

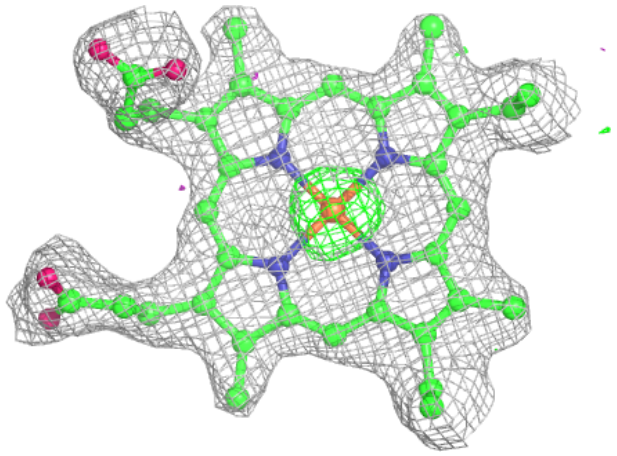


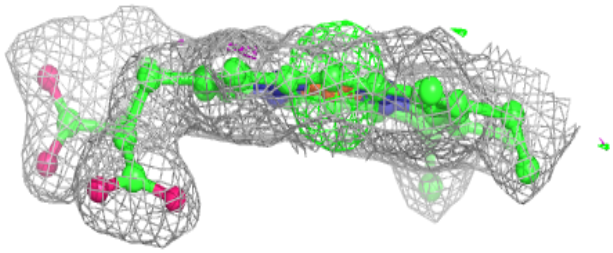


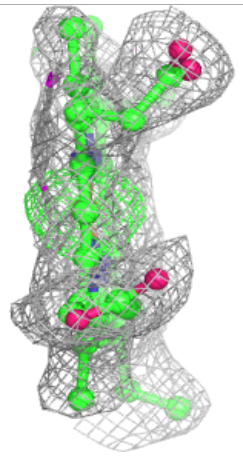


Electron density around HEC O 1001:

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

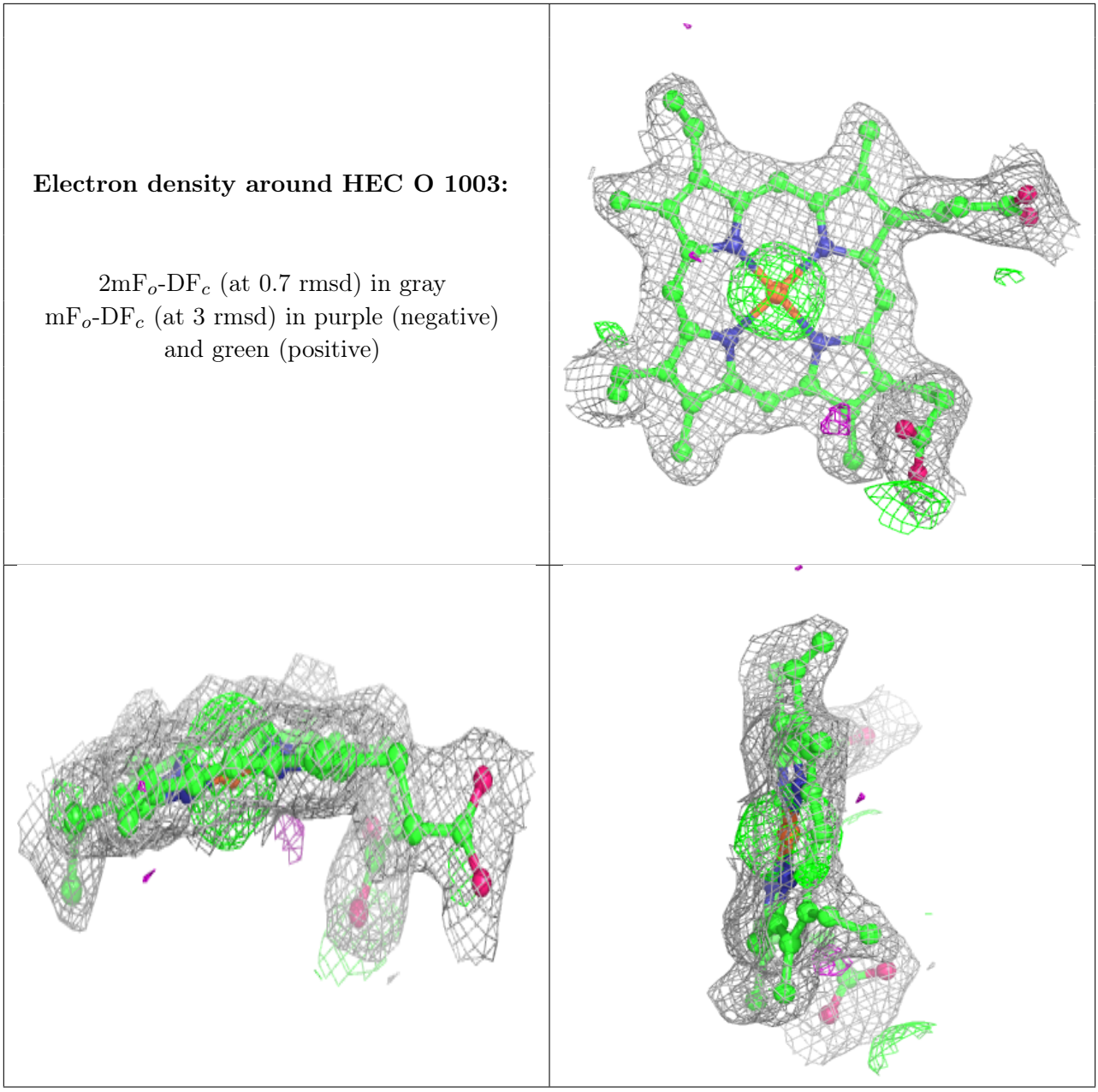






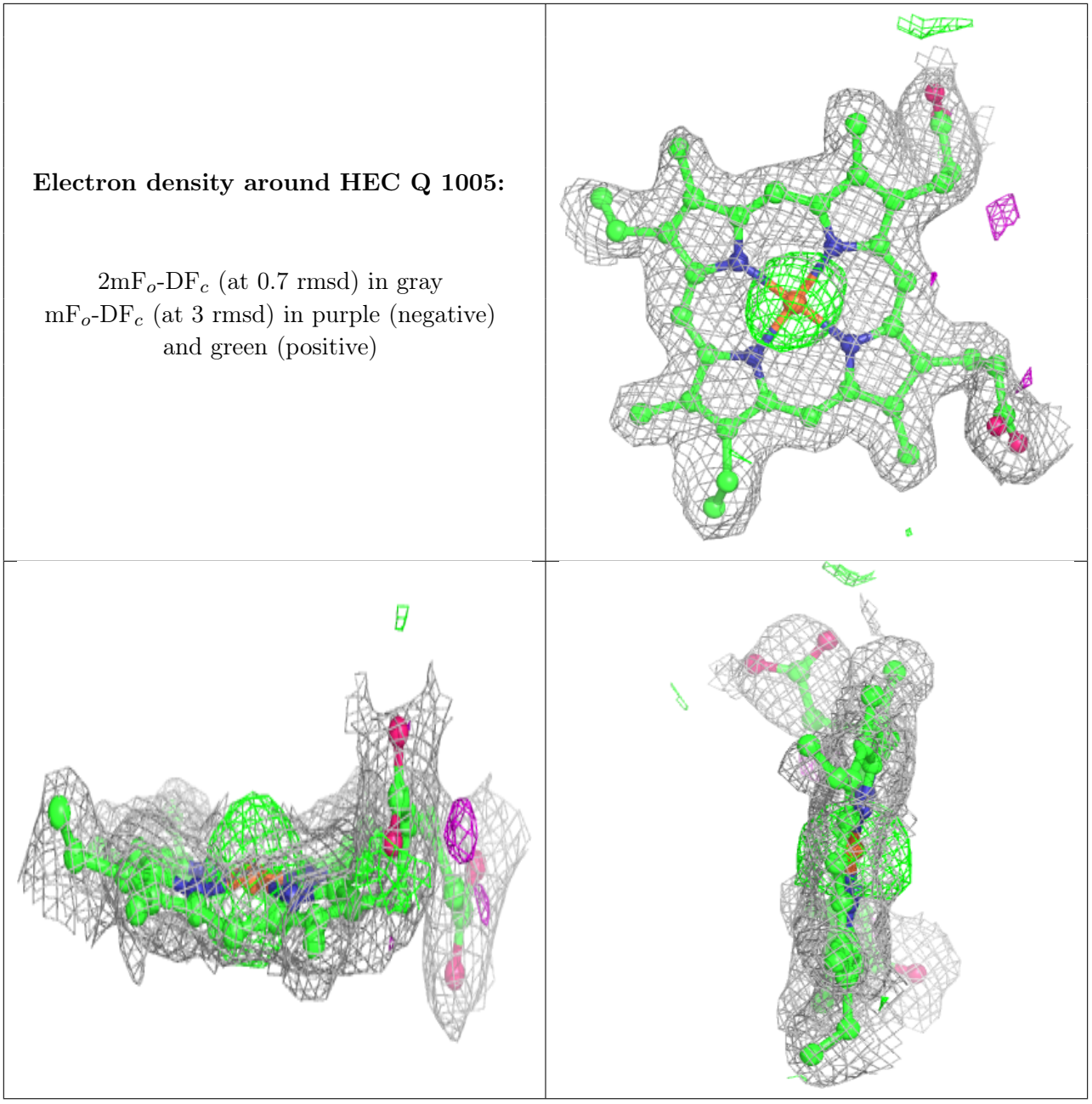
Electron density around HEC O 1003:

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



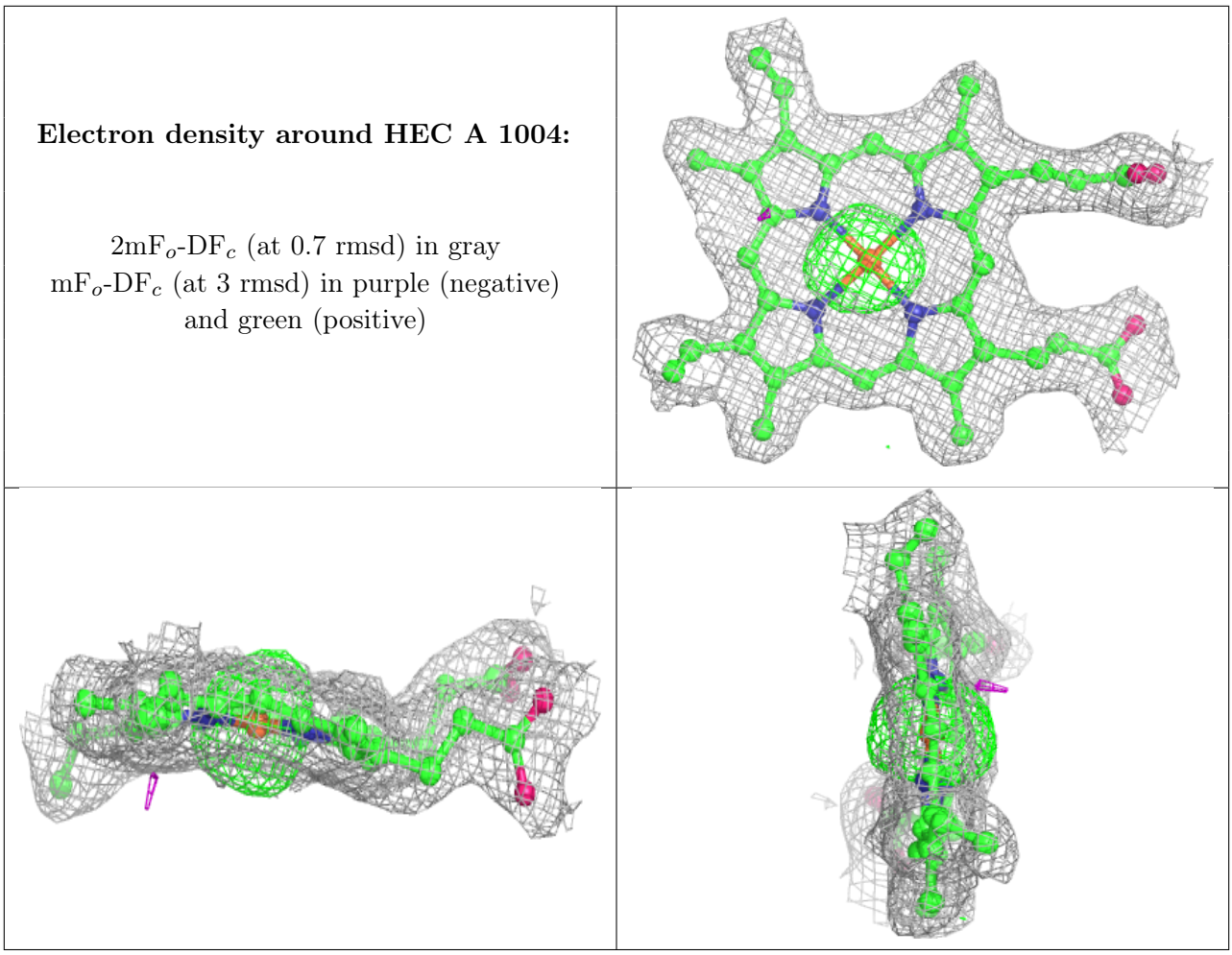
Electron density around HEC Q 1005:

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



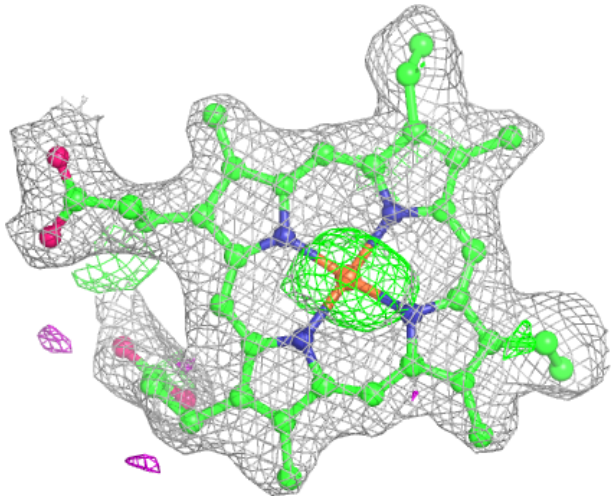
Electron density around HEC A 1004:

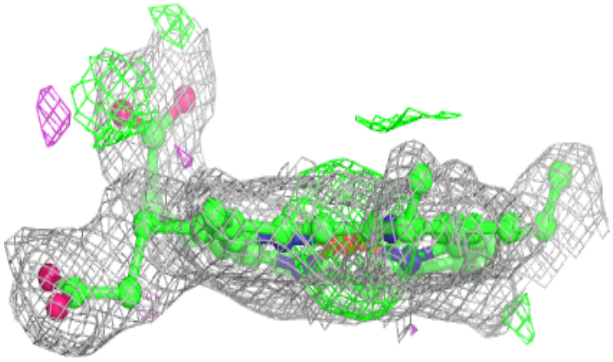
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

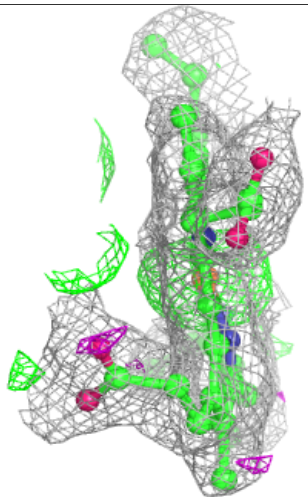


Electron density around HEC R 1002:

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

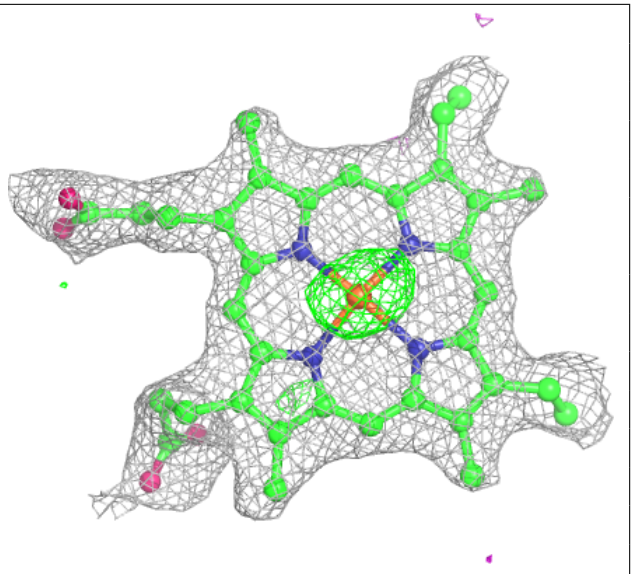


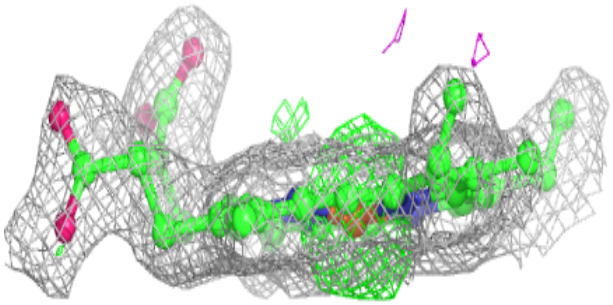


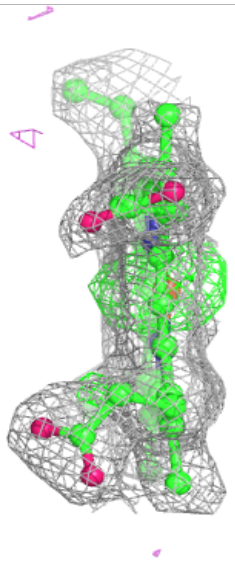


Electron density around HEC F 1001:

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

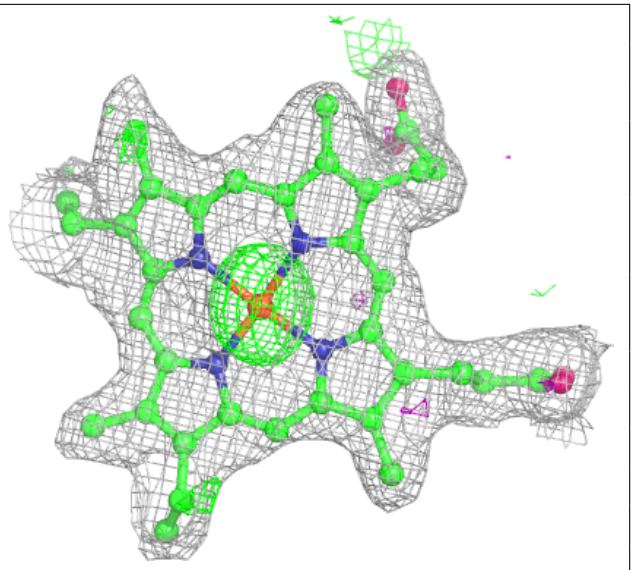


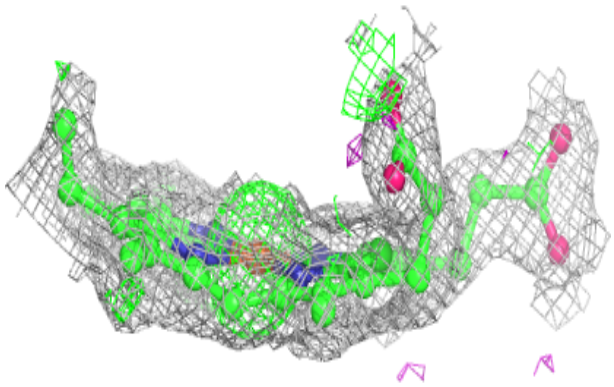


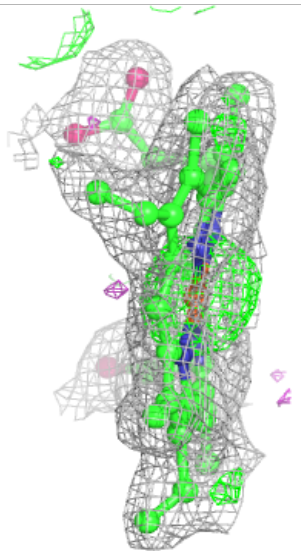


Electron density around HEC F 1003:

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

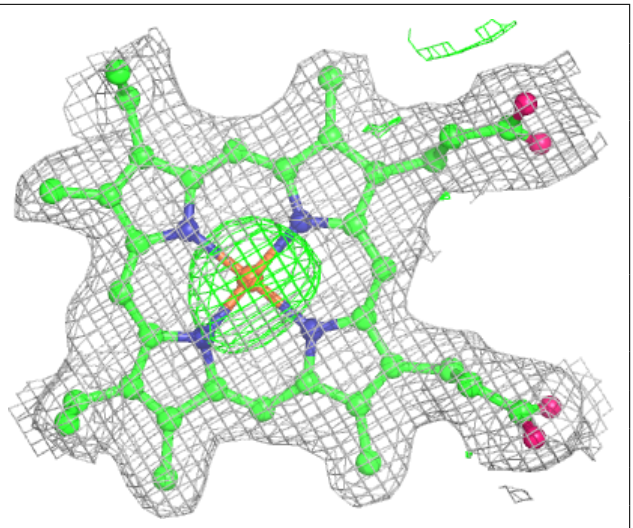


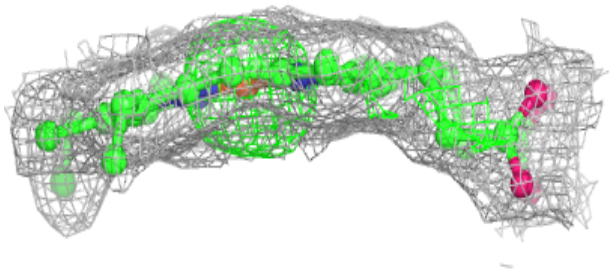


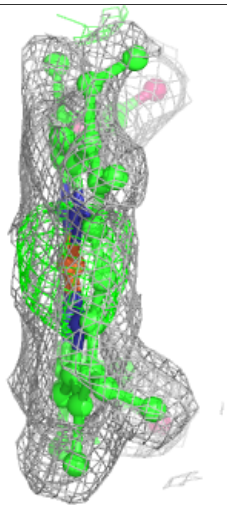


Electron density around HEC G 1003:

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

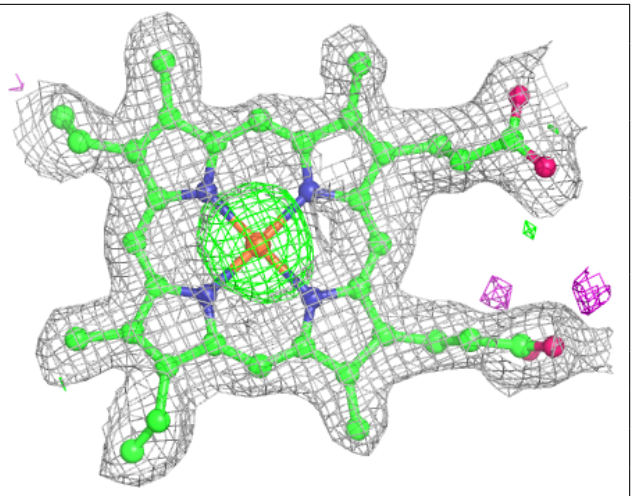


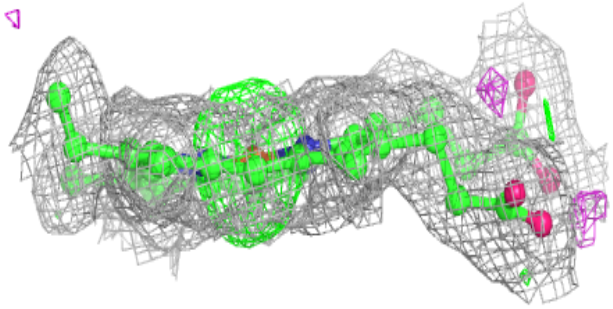


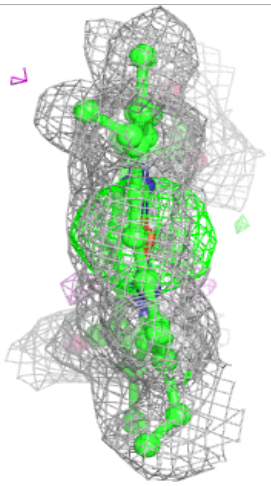


Electron density around HEC H 1004:

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

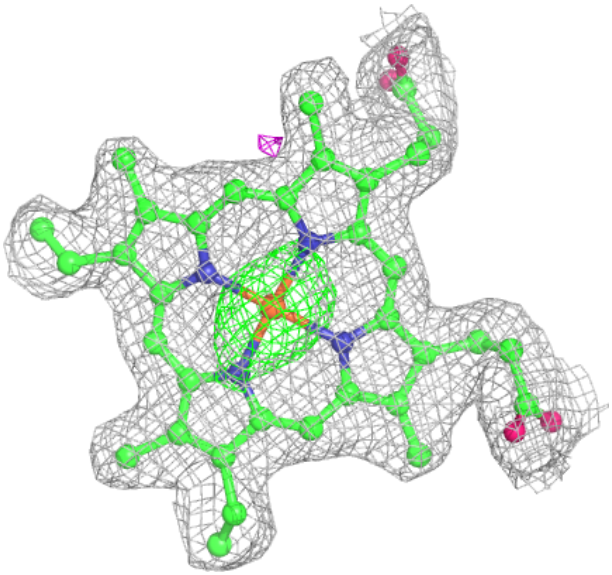


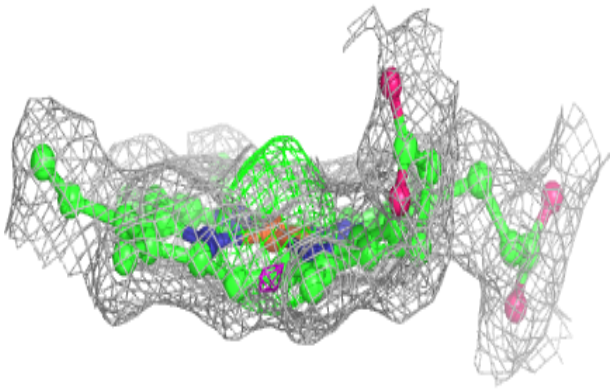


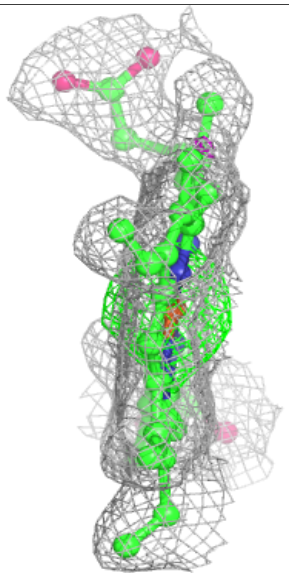


Electron density around HEC H 1005:

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

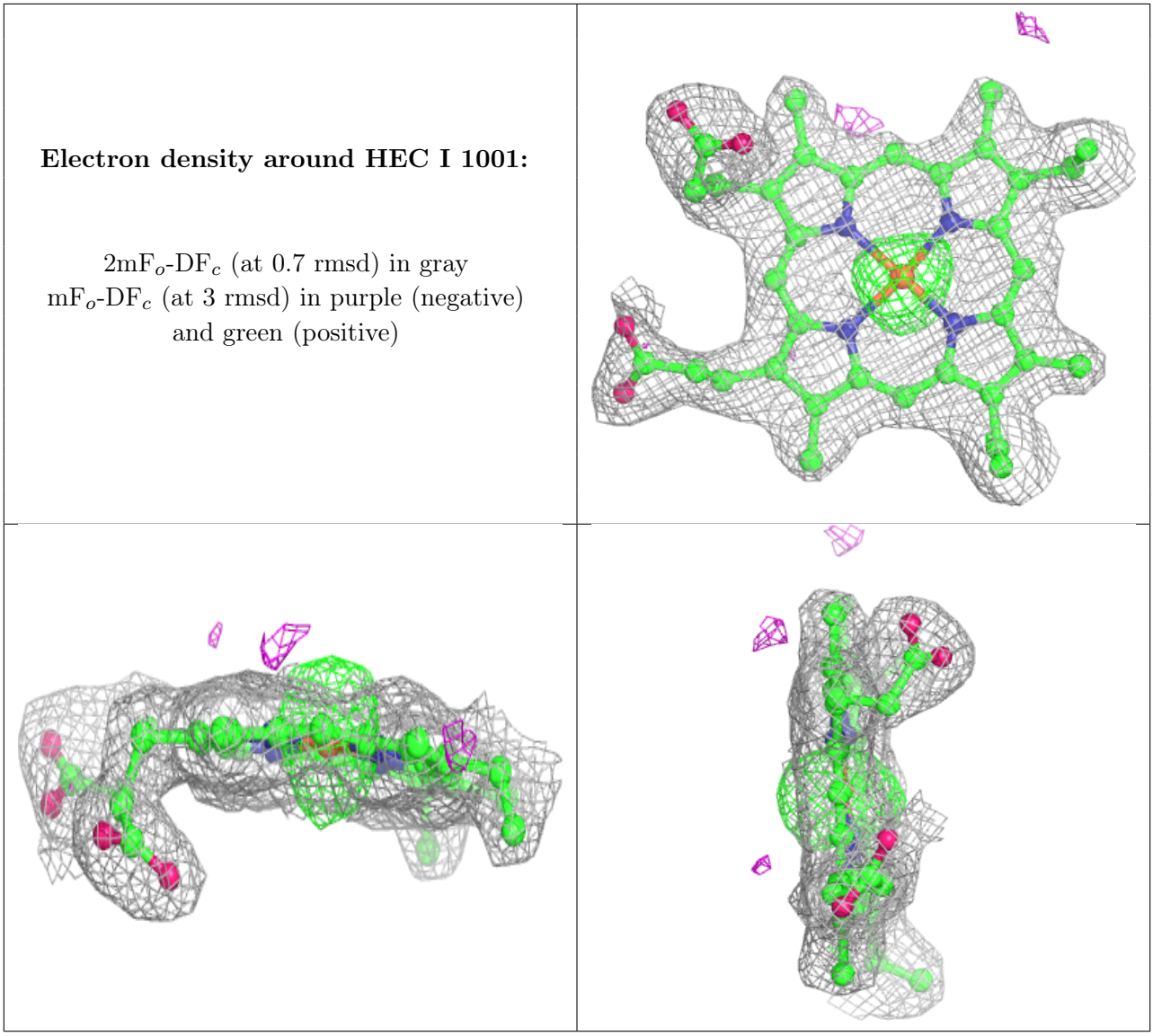






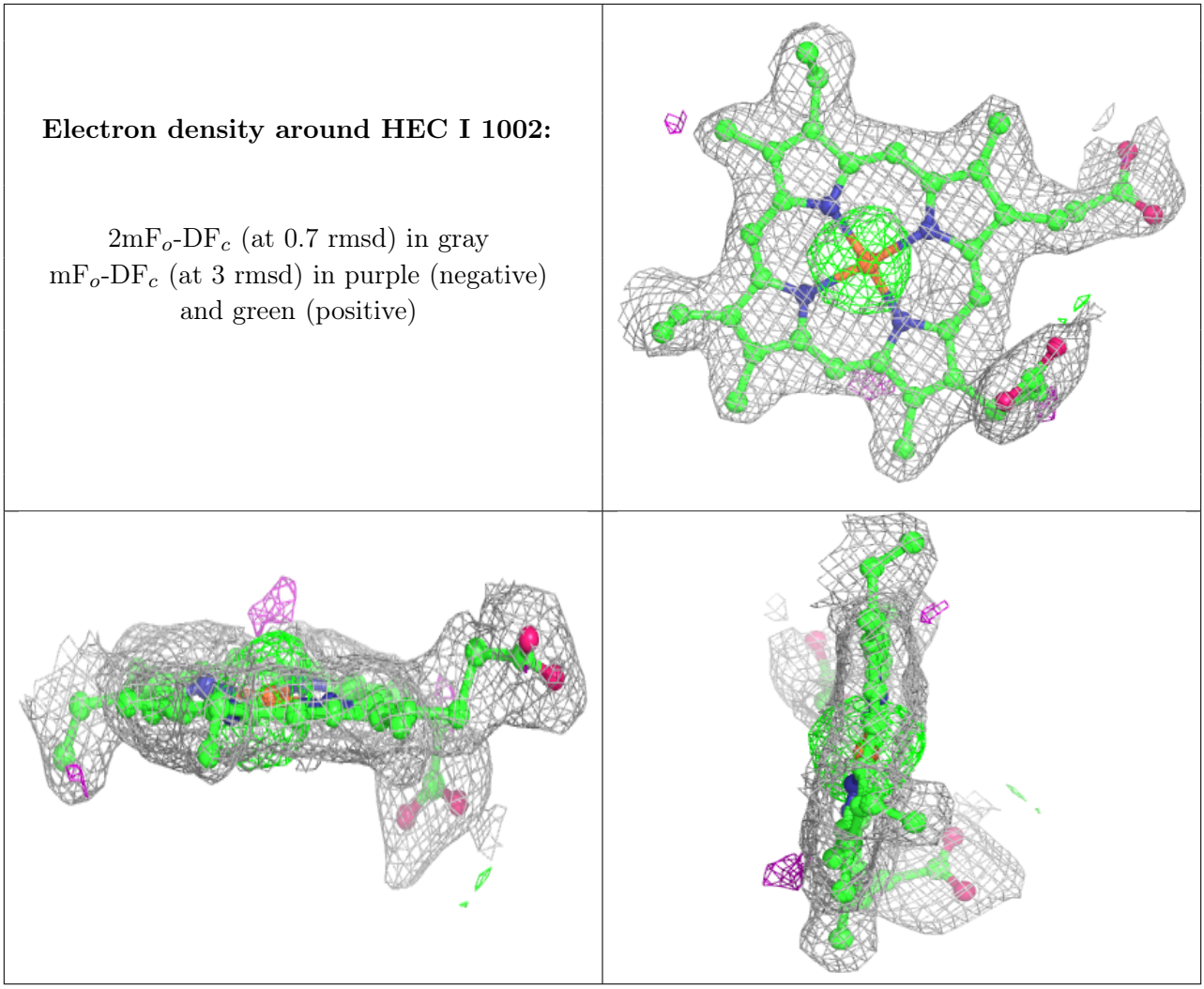
Electron density around HEC I 1001:

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



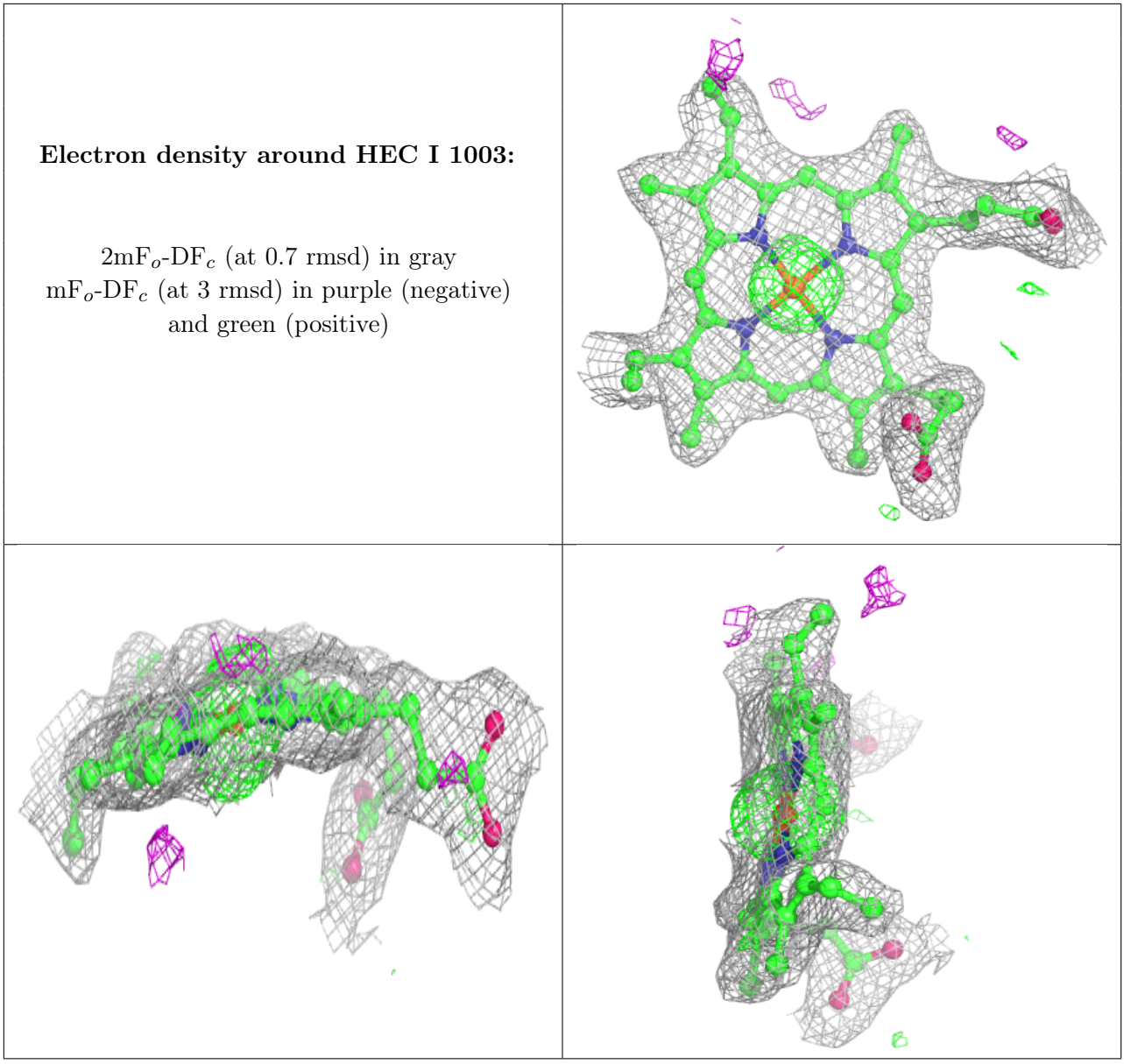
Electron density around HEC I 1002:

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



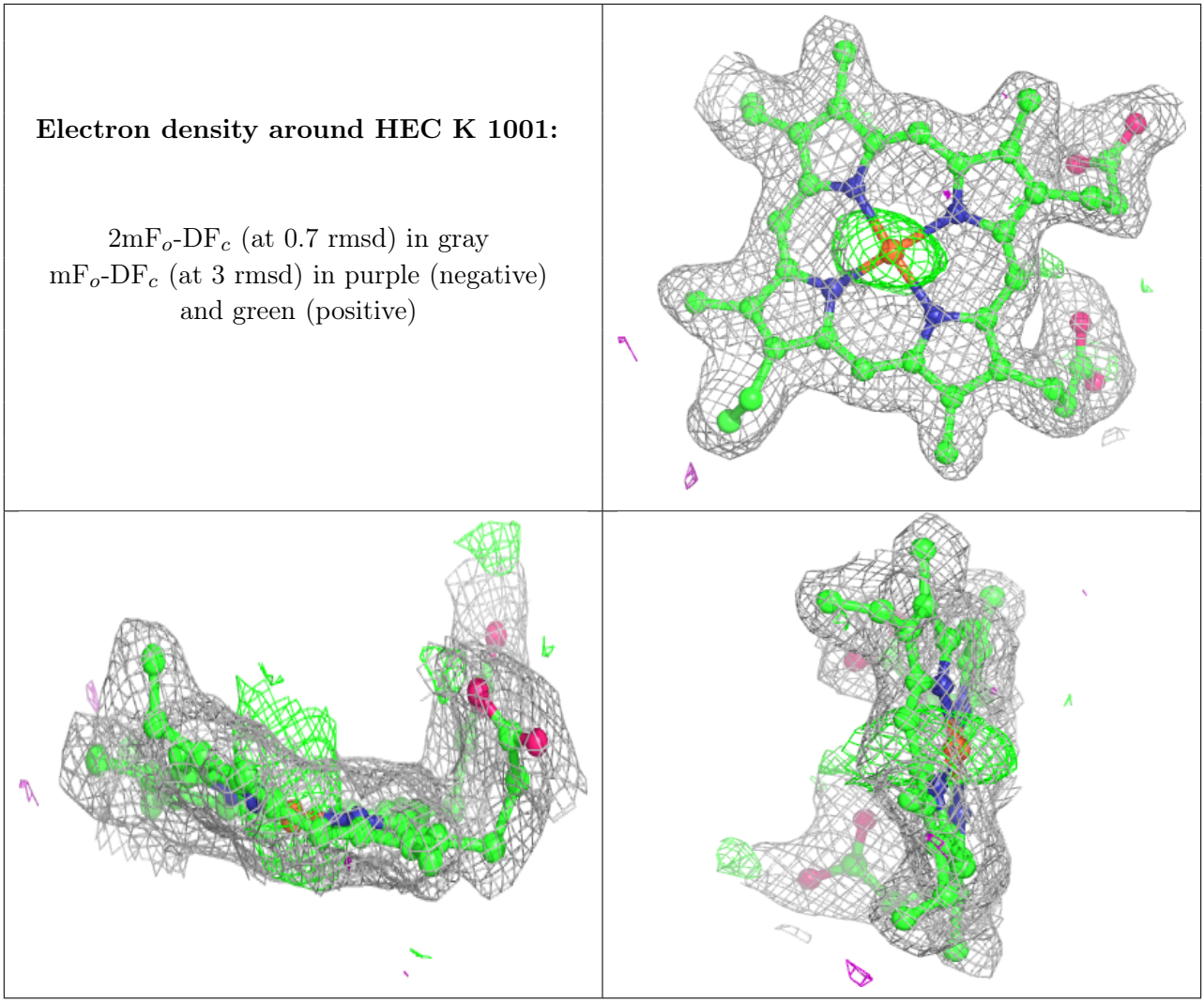
Electron density around HEC I 1003:

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



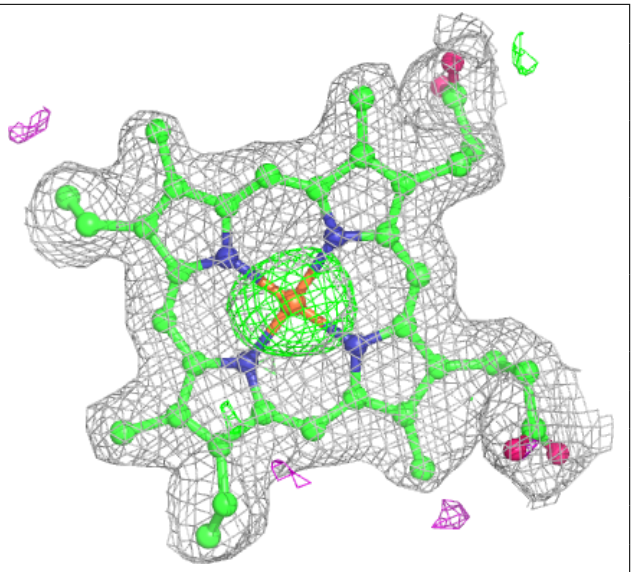
Electron density around HEC K 1001:

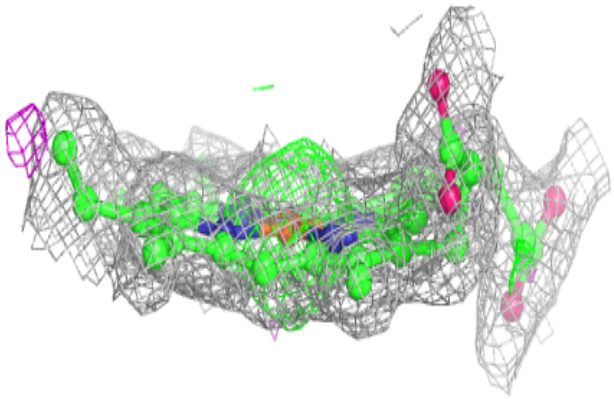
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

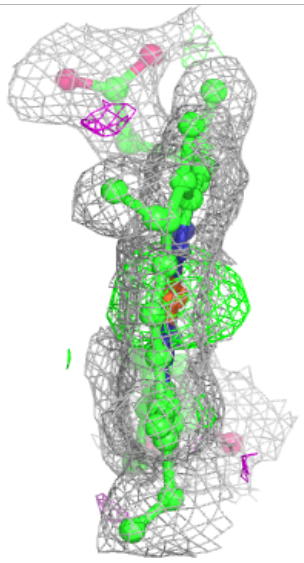


Electron density around HEC B 1005:

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

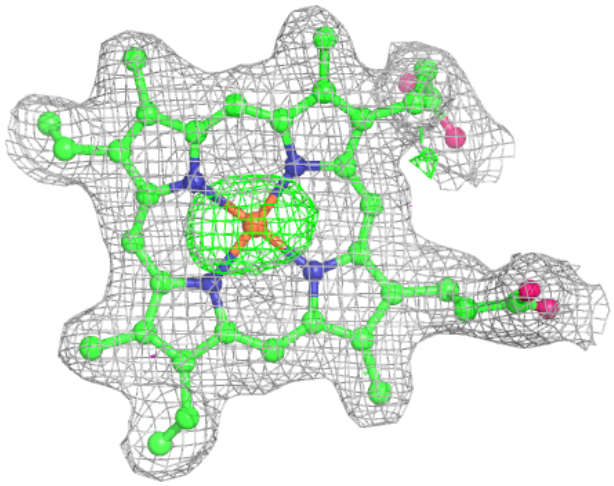


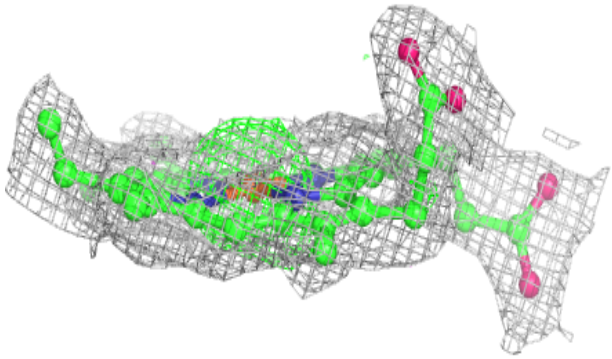


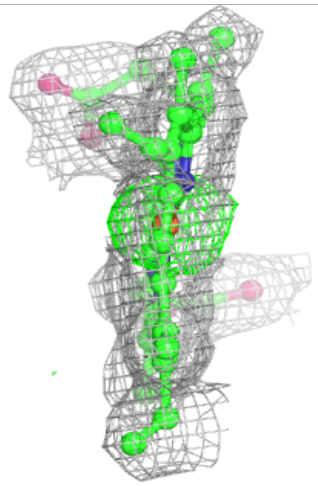


Electron density around HEC A 1002:

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

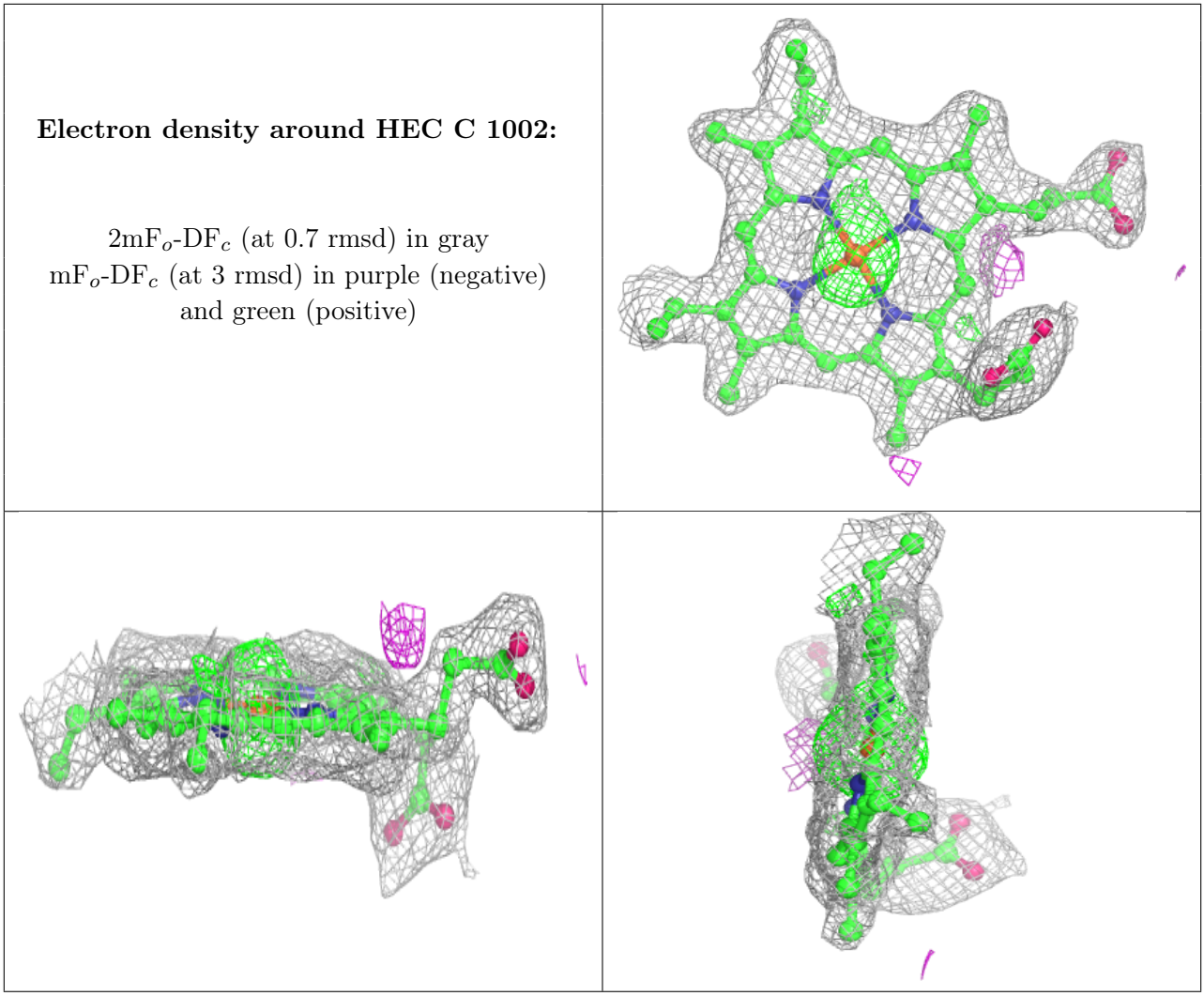






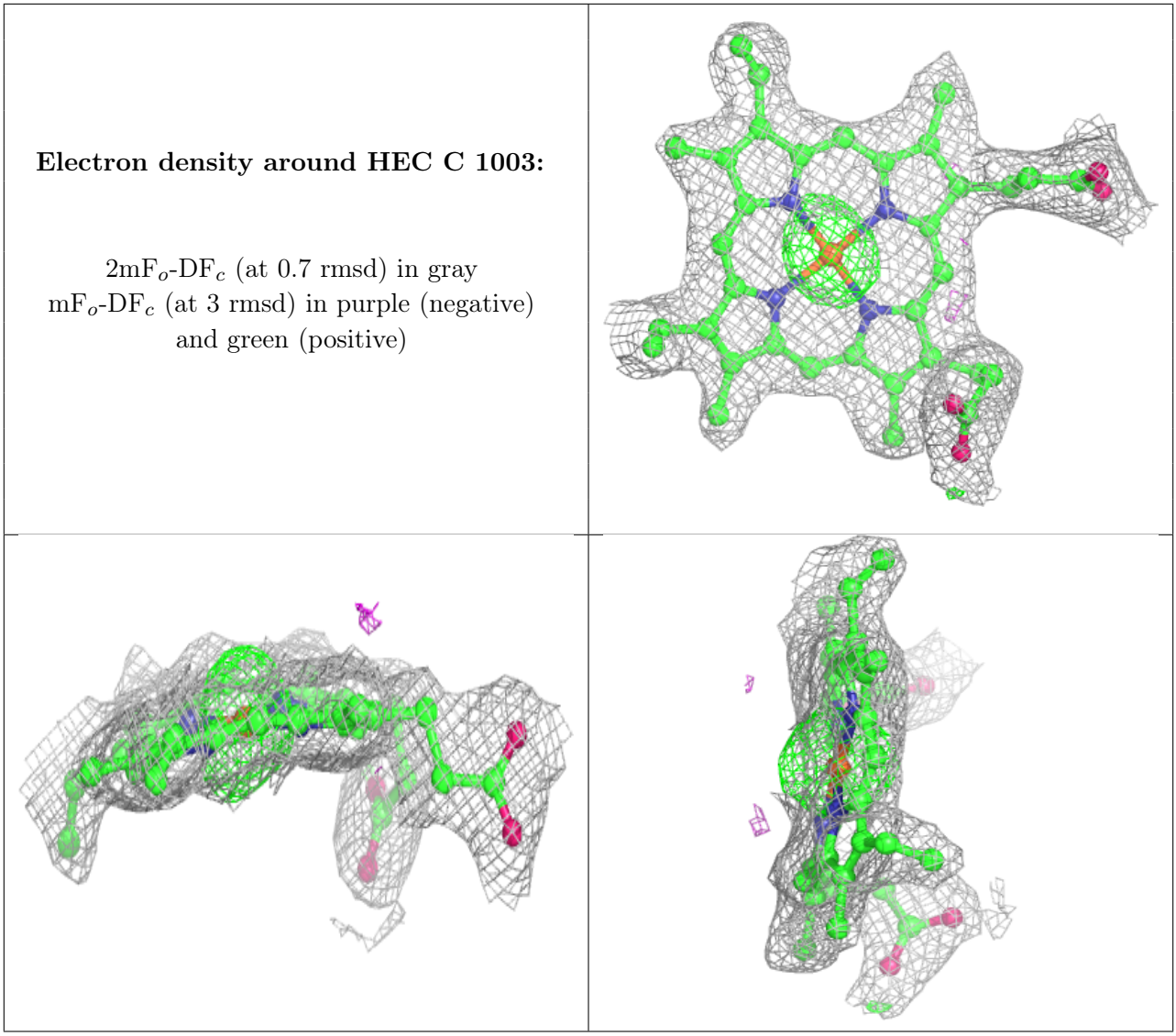
Electron density around HEC C 1002:

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



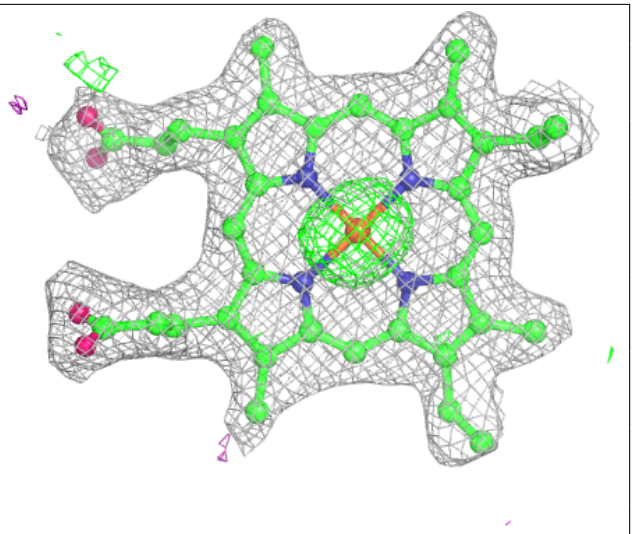
Electron density around HEC C 1003:

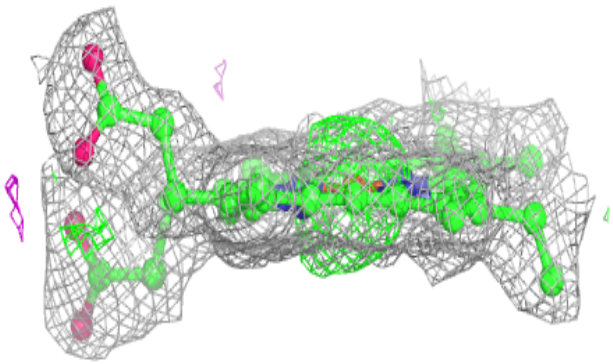
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

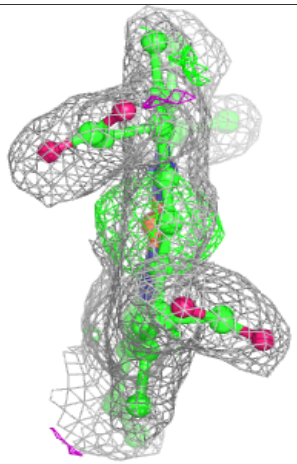


Electron density around HEC I 1004:

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

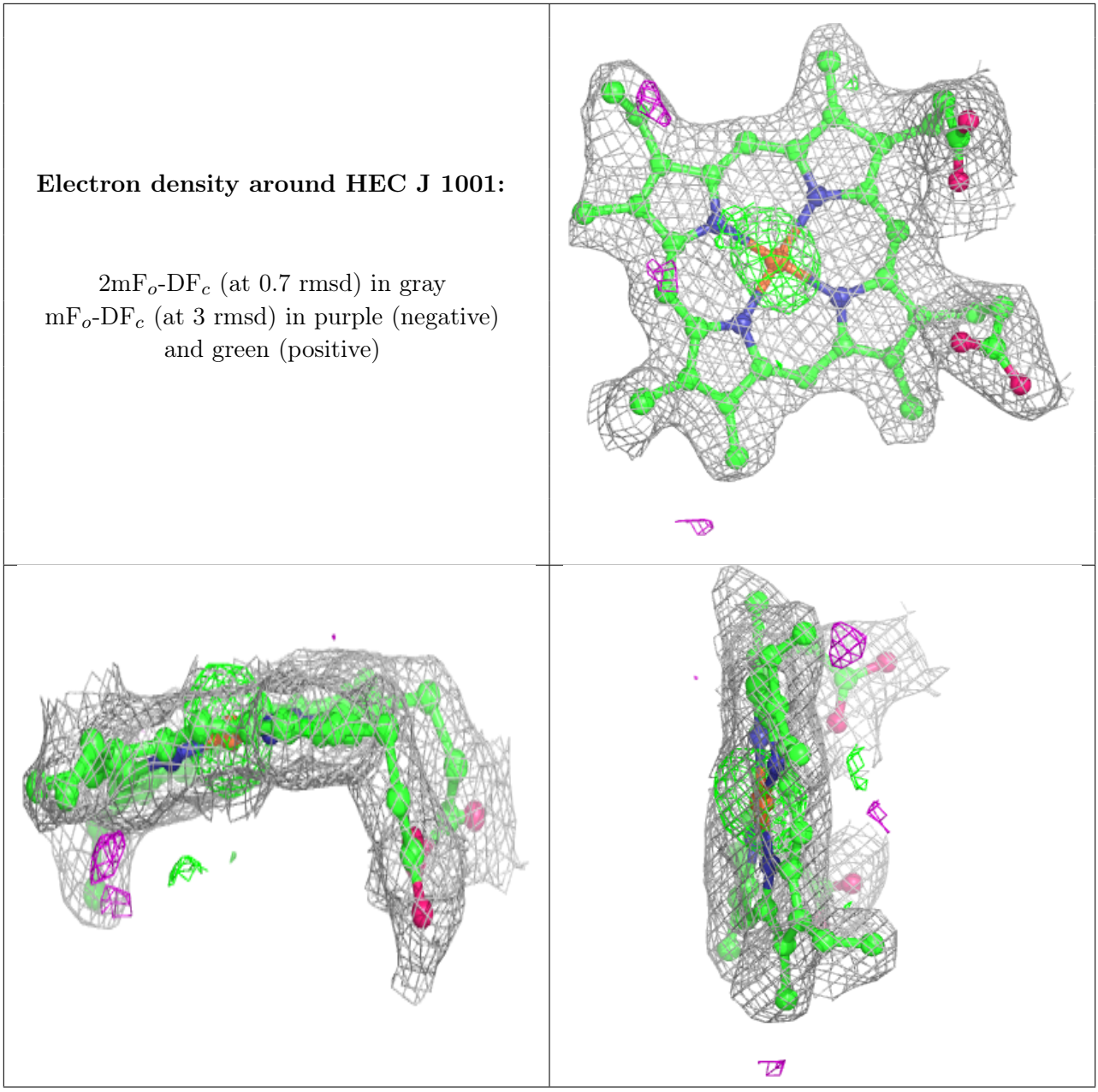






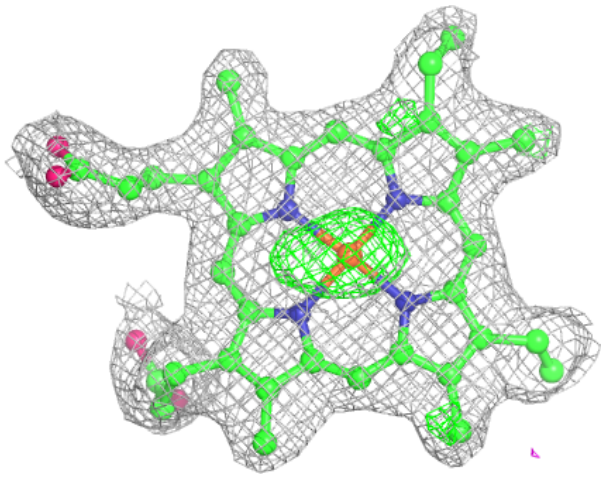
Electron density around HEC J 1001:

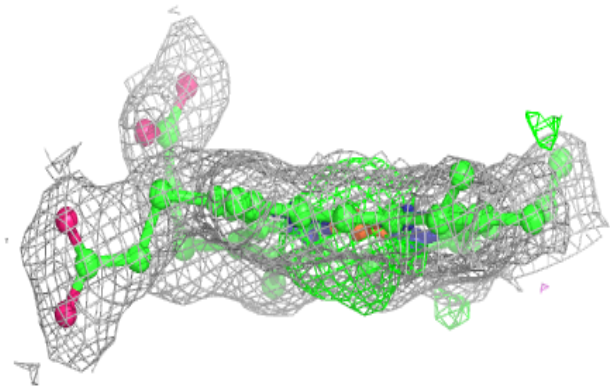
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

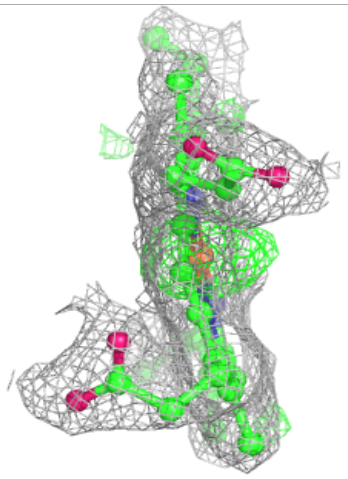


Electron density around HEC J 1002:

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

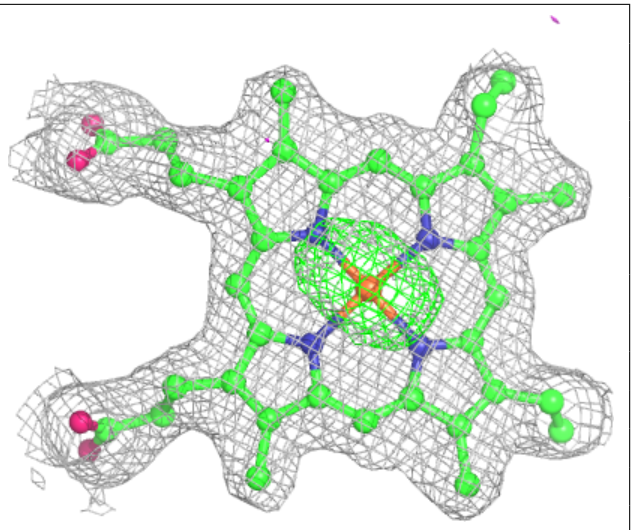


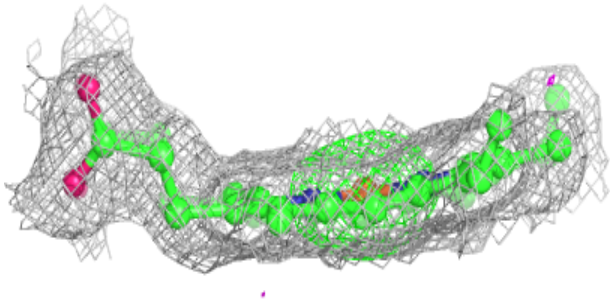


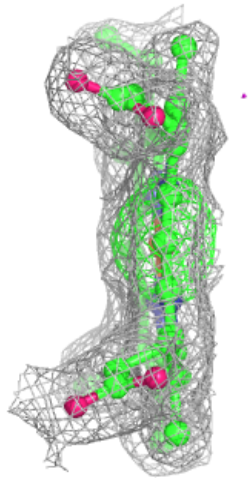


Electron density around HEC J 1003:

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

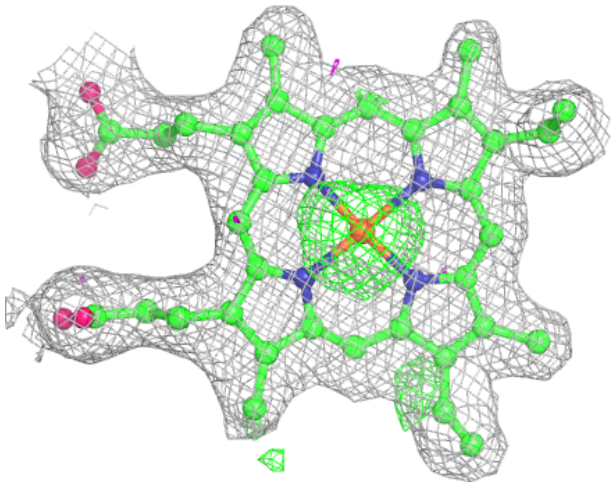


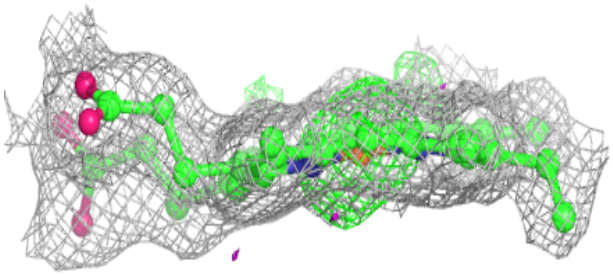


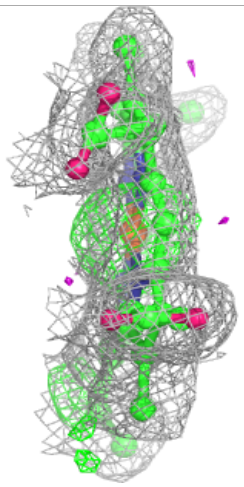


Electron density around HEC J 1004:

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

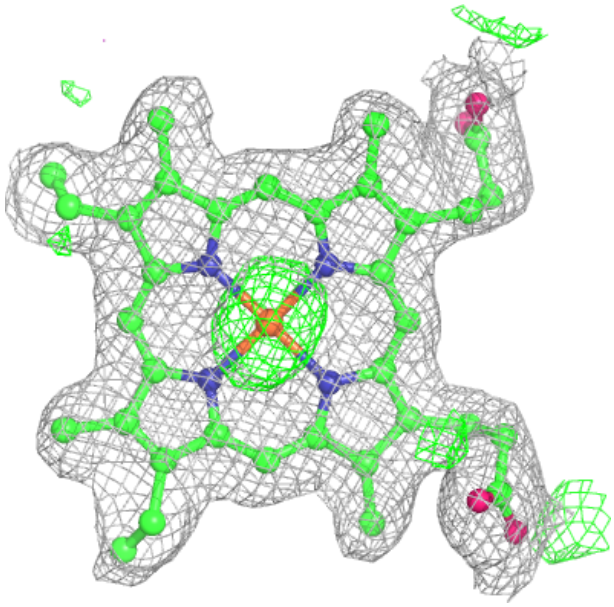


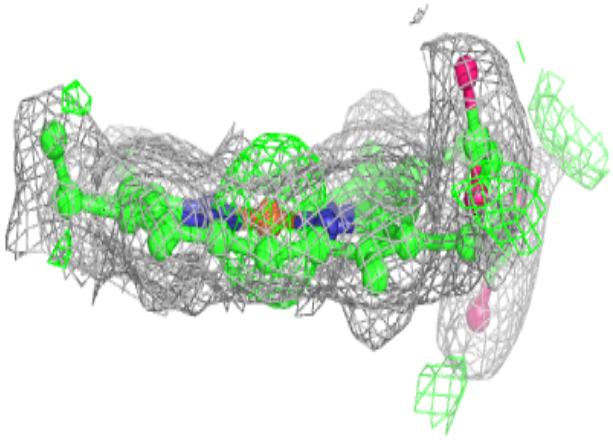


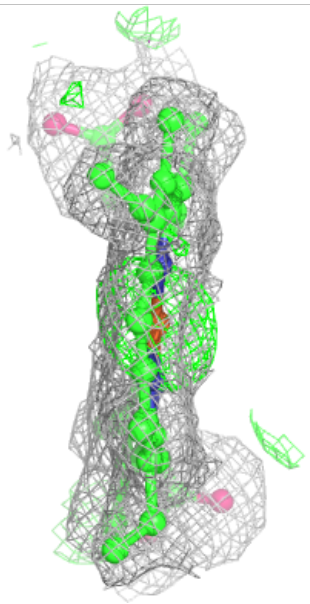


Electron density around HEC J 1005:

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

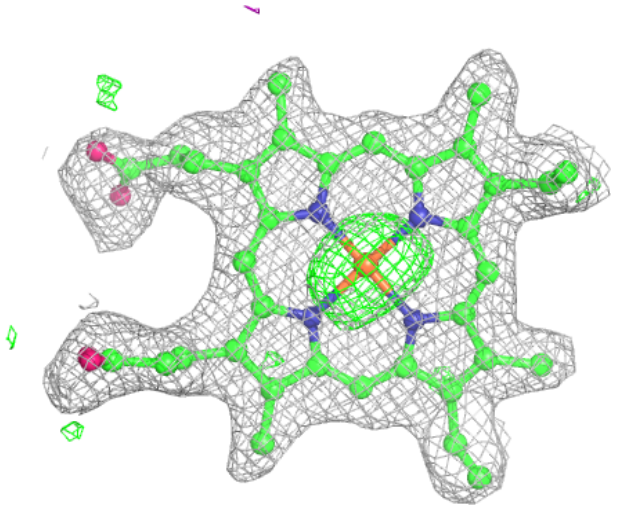


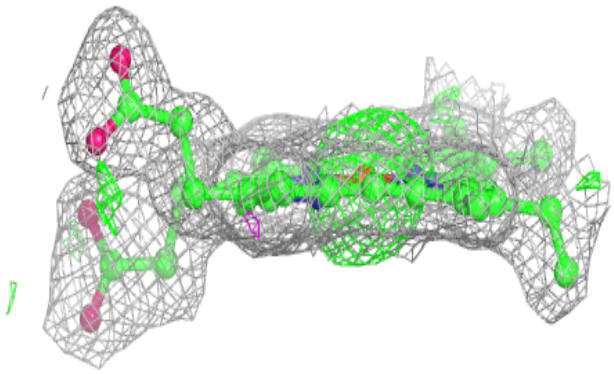


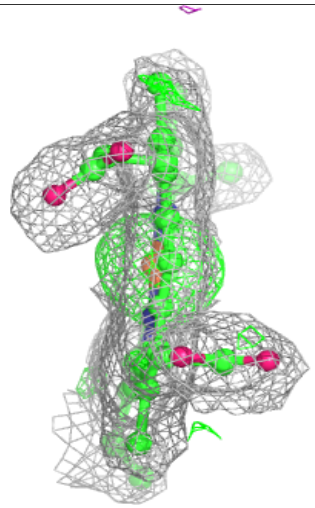


Electron density around HEC C 1004:

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

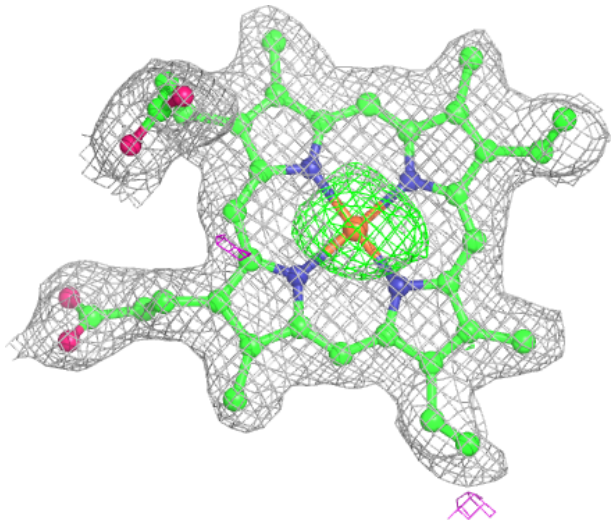


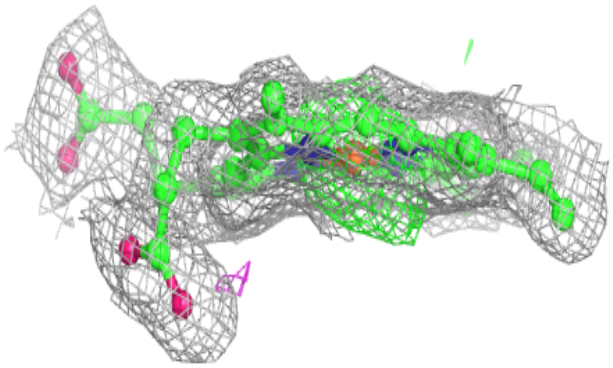


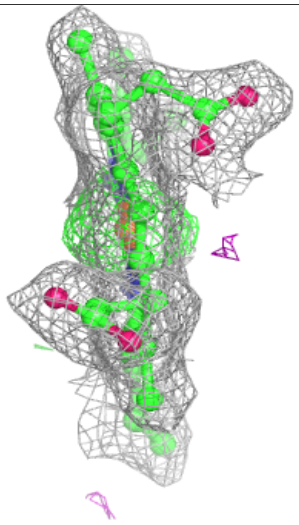


Electron density around HEC D 1002:

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

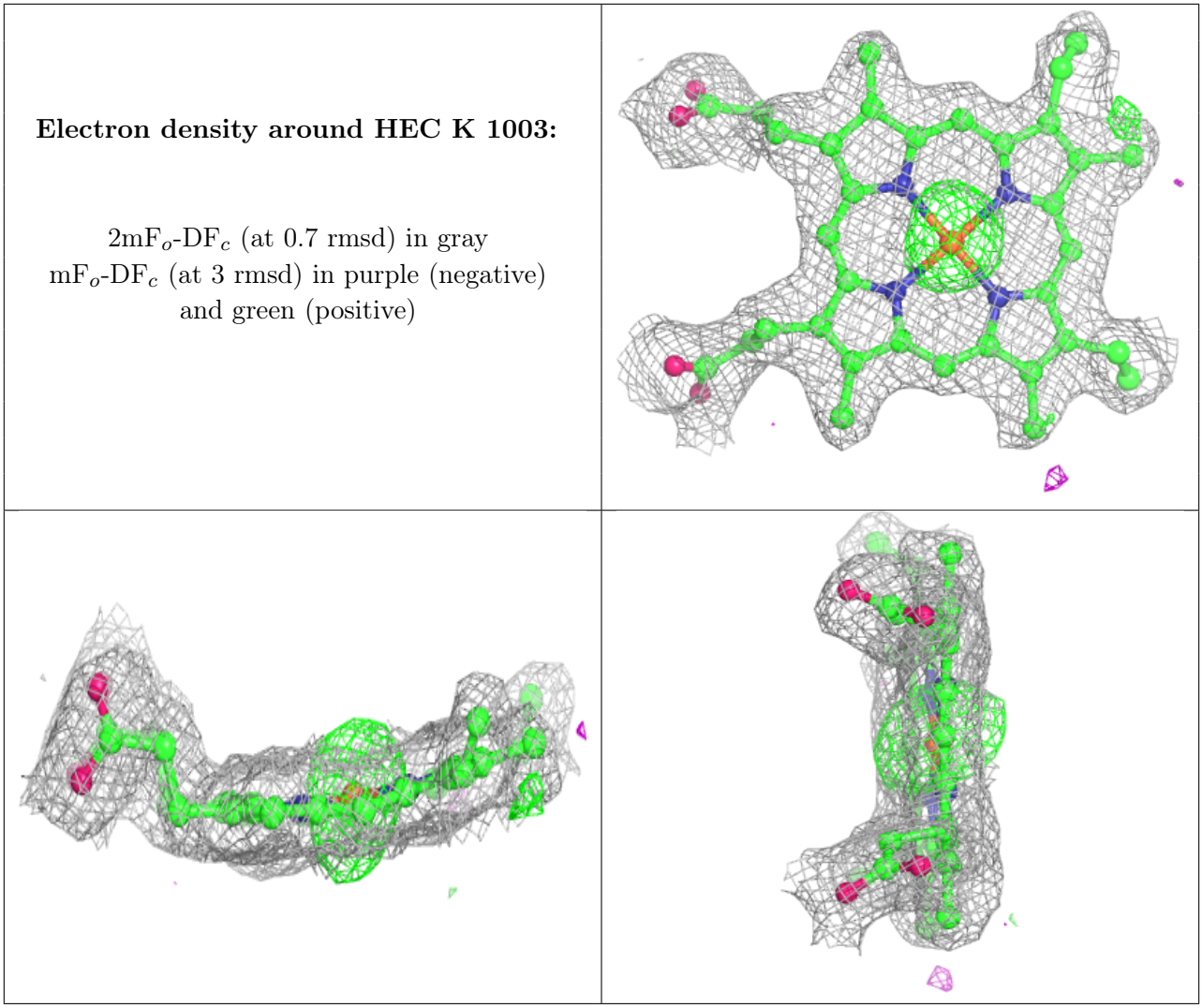






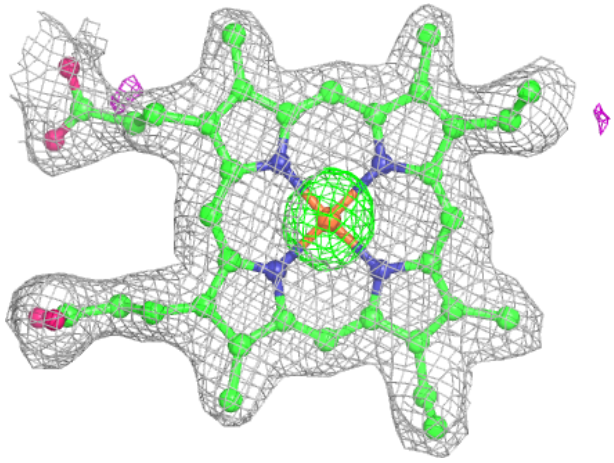
Electron density around HEC K 1003:

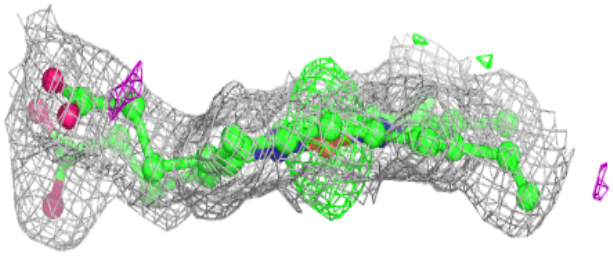
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

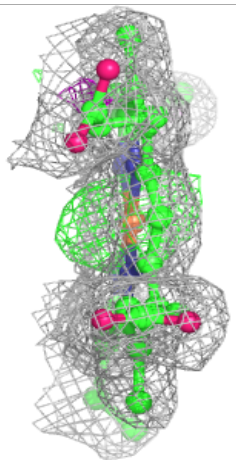


Electron density around HEC K 1004:

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

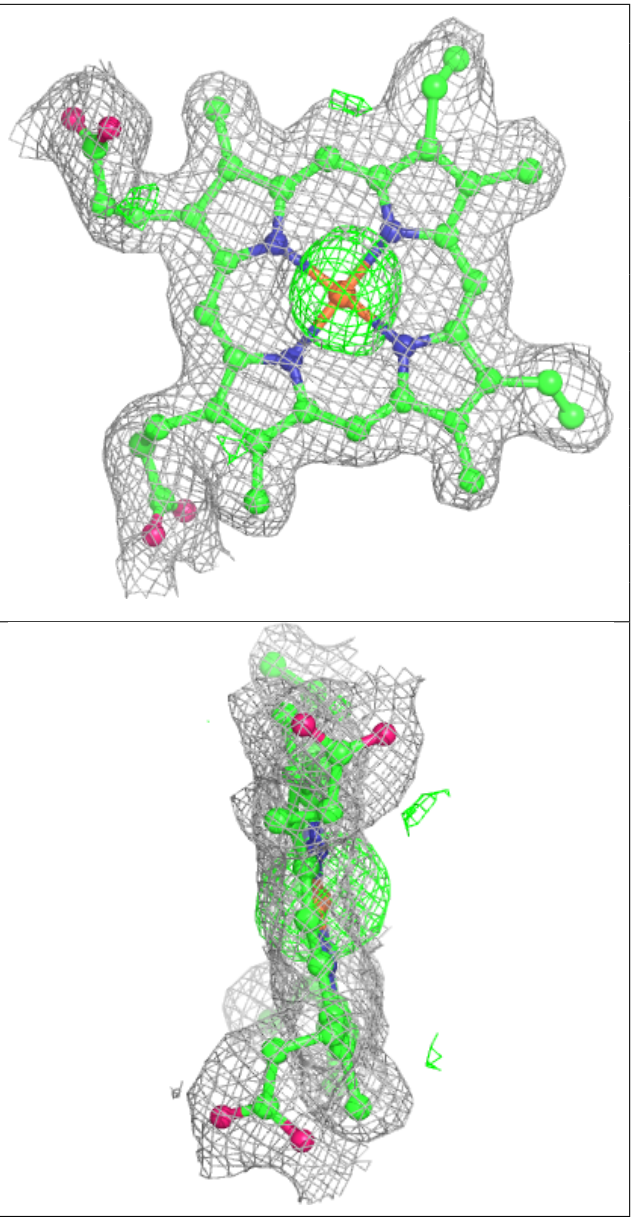


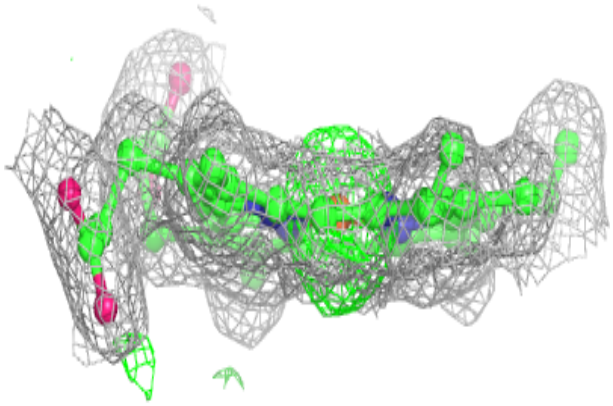




Electron density around HEC D 1005:

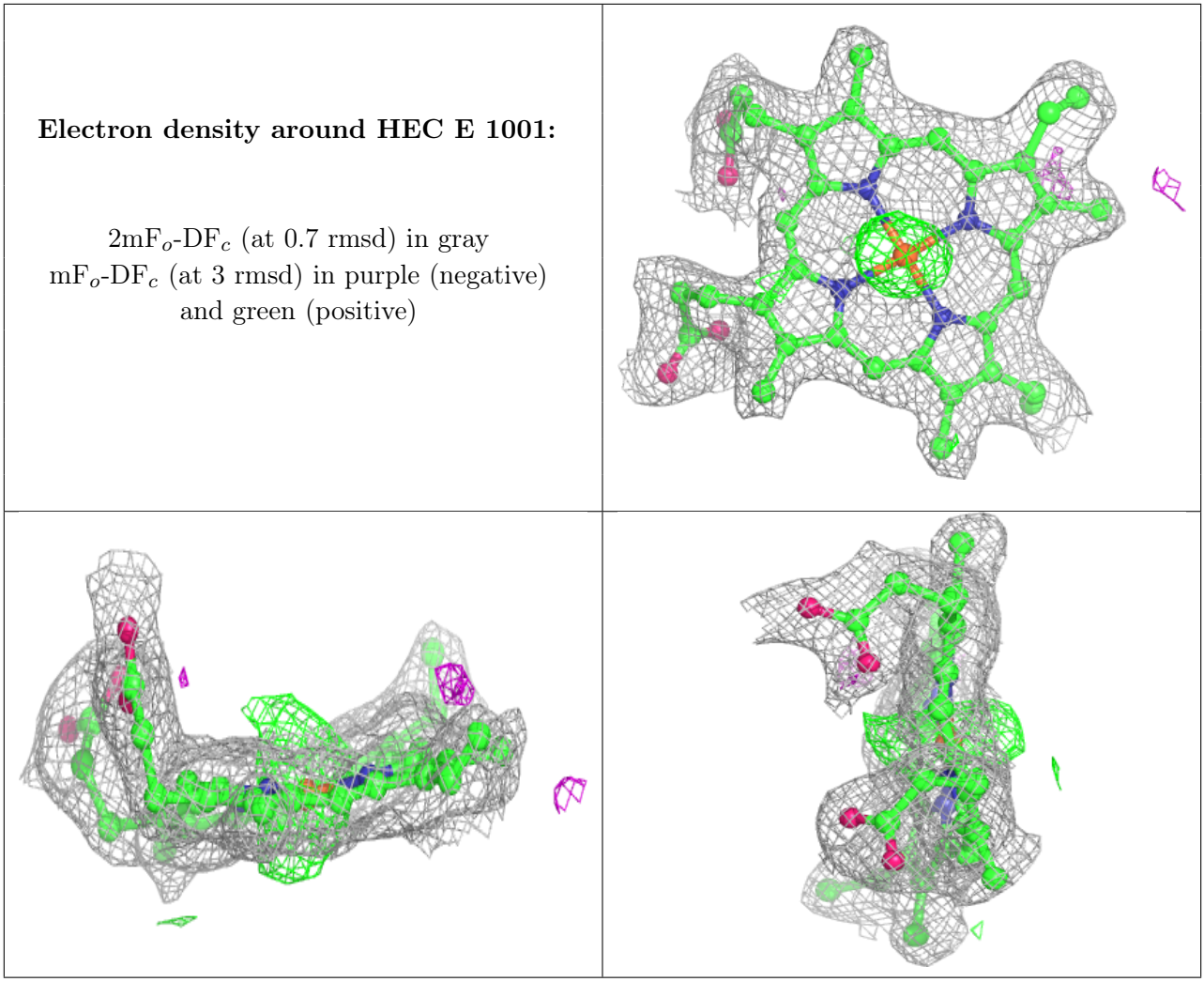
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





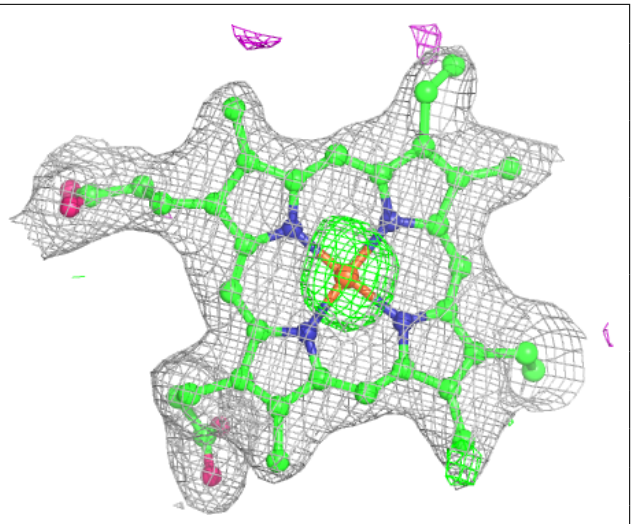
Electron density around HEC E 1001:

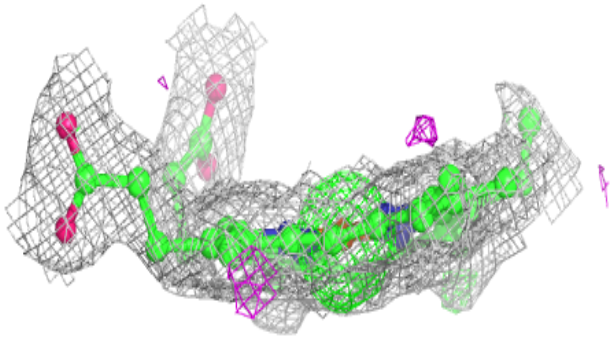
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

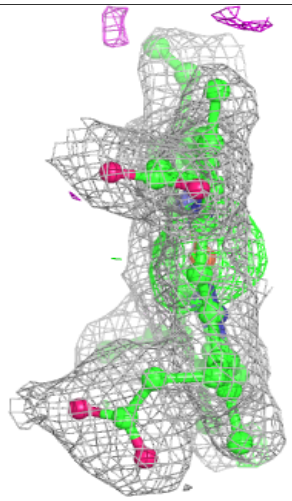


Electron density around HEC L 1003:

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

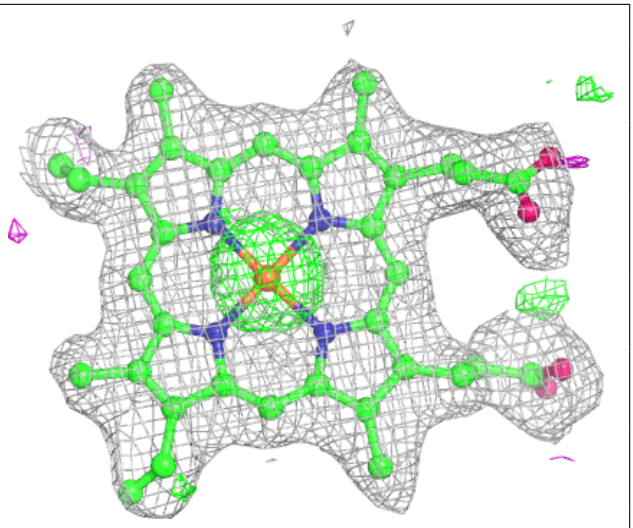


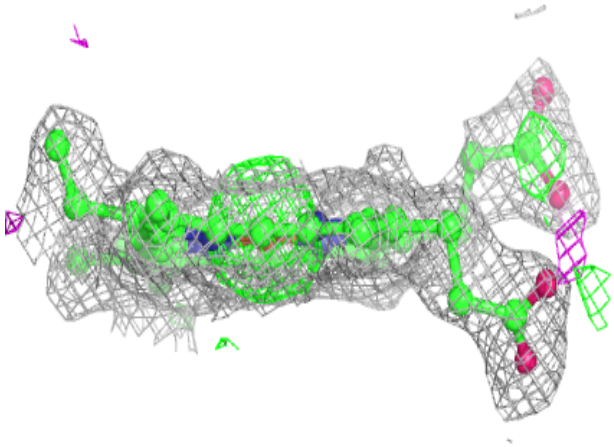


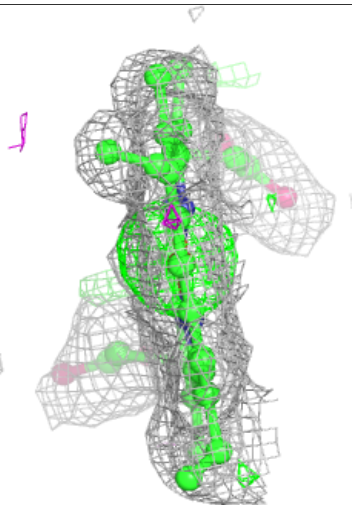


Electron density around HEC L 1004:

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

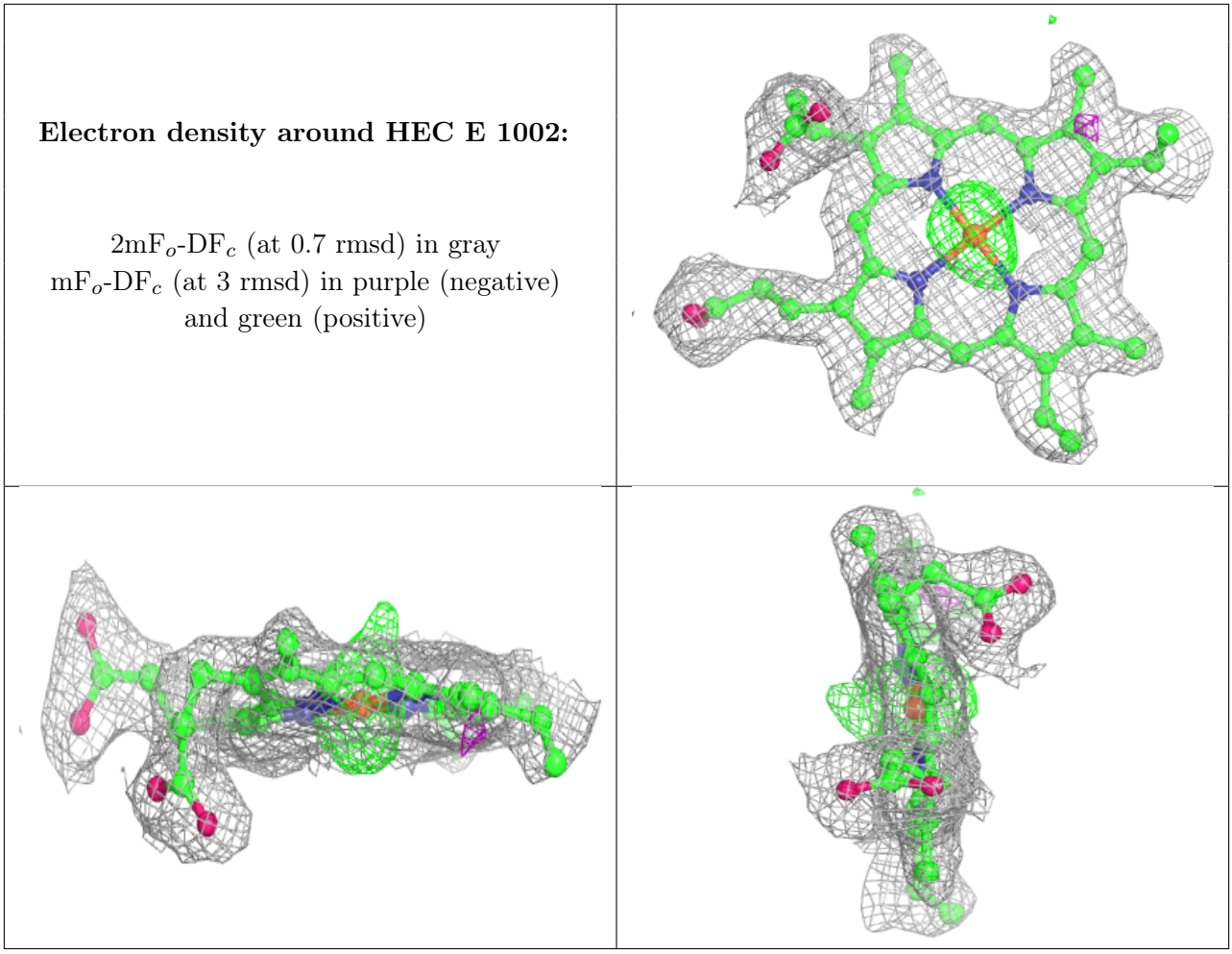






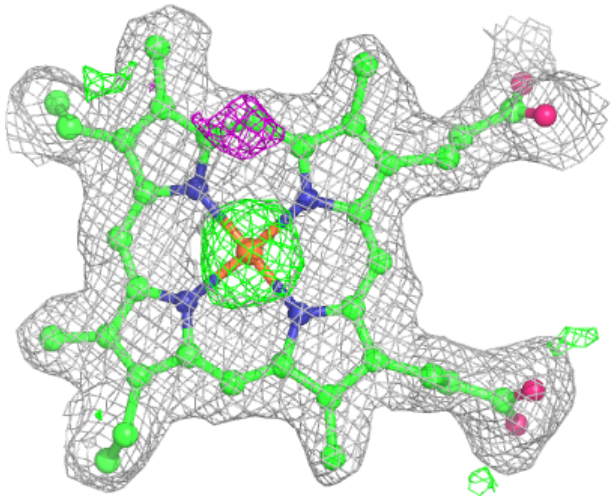
Electron density around HEC E 1002:

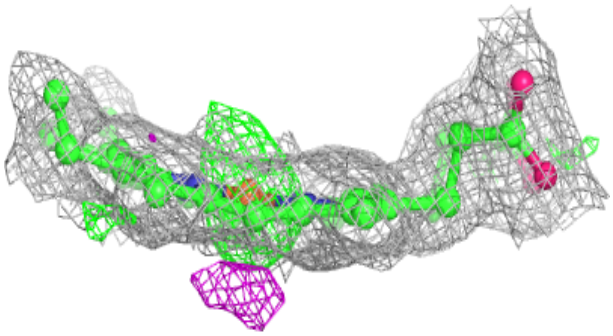
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC E 1003:

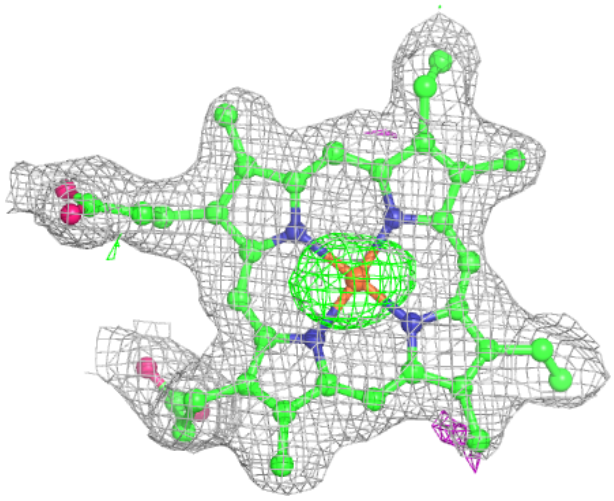
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

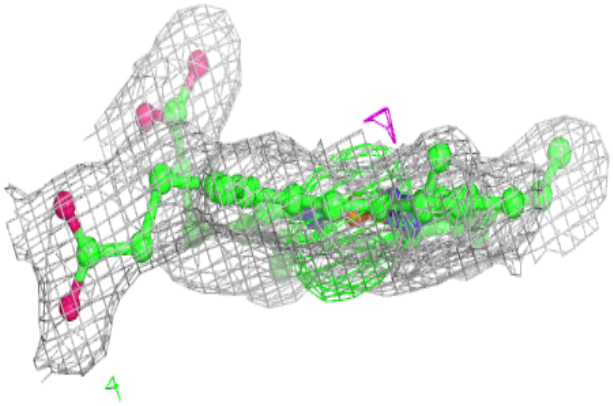


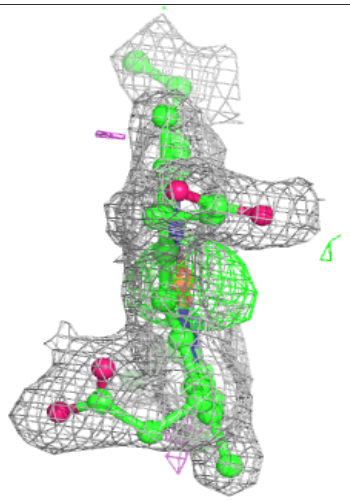


Electron density around HEC M 1002:

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

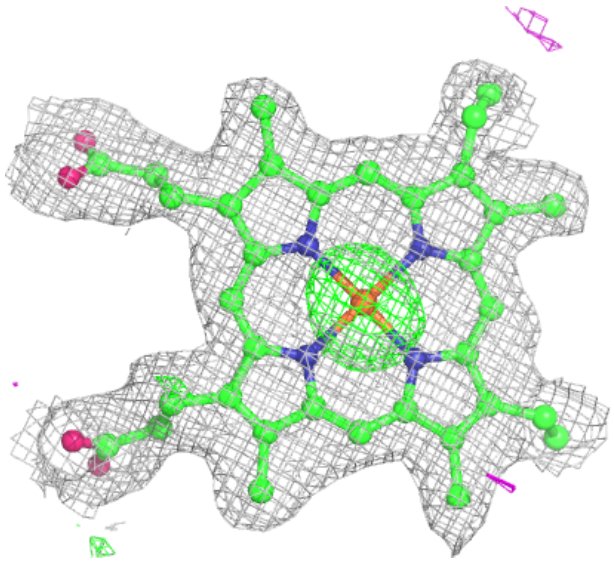


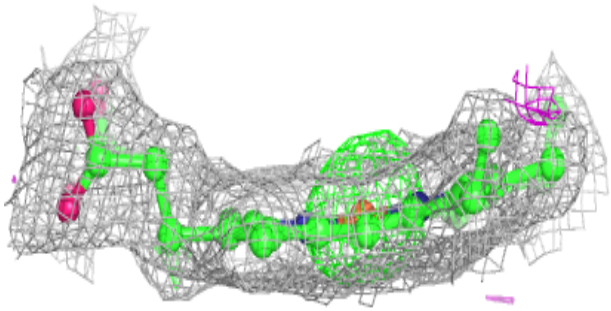


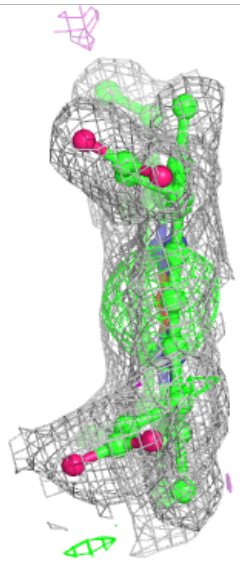


Electron density around HEC M 1003:

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

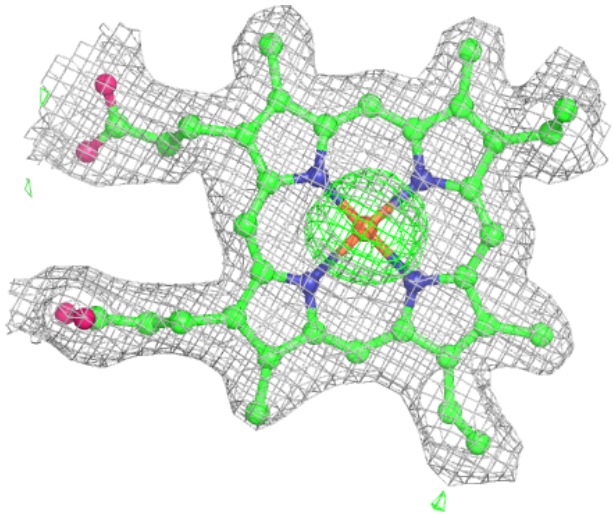


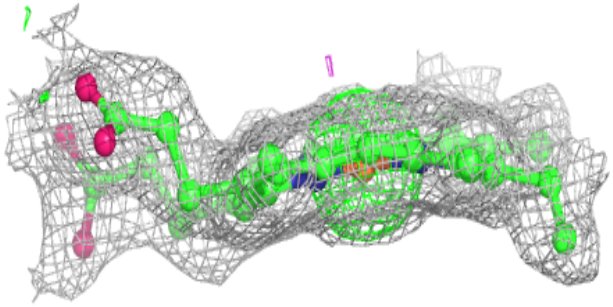


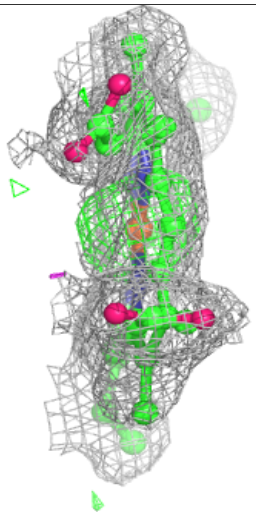


Electron density around HEC M 1004:

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

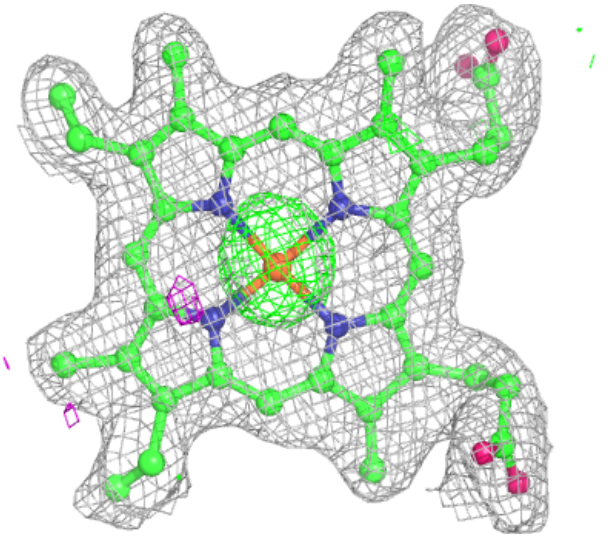


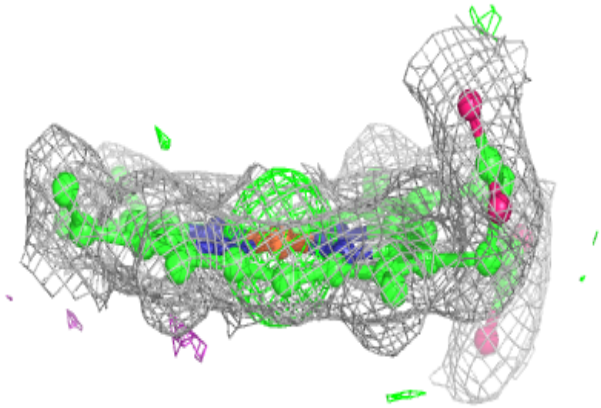


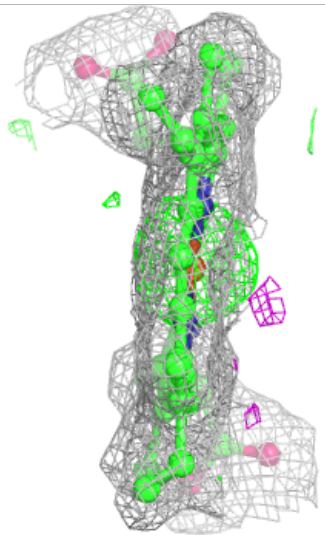


Electron density around HEC M 1005:

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

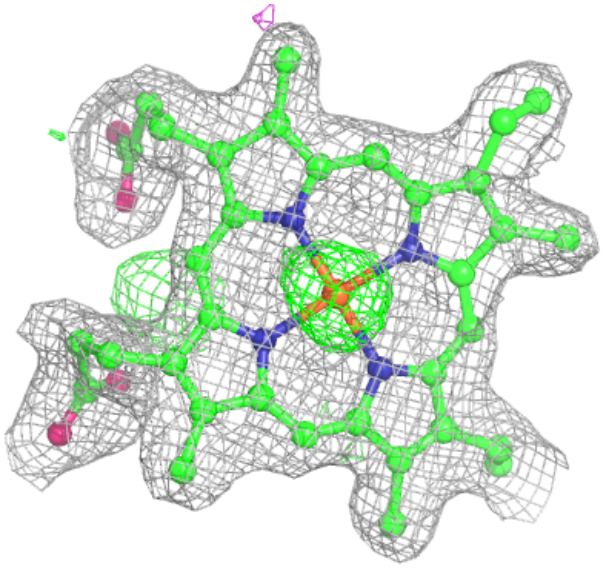


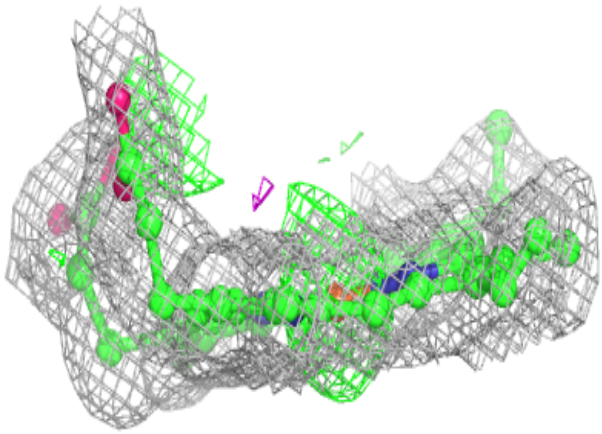


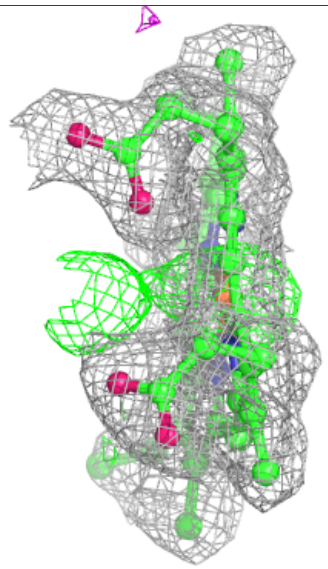


Electron density around HEC N 1001:

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

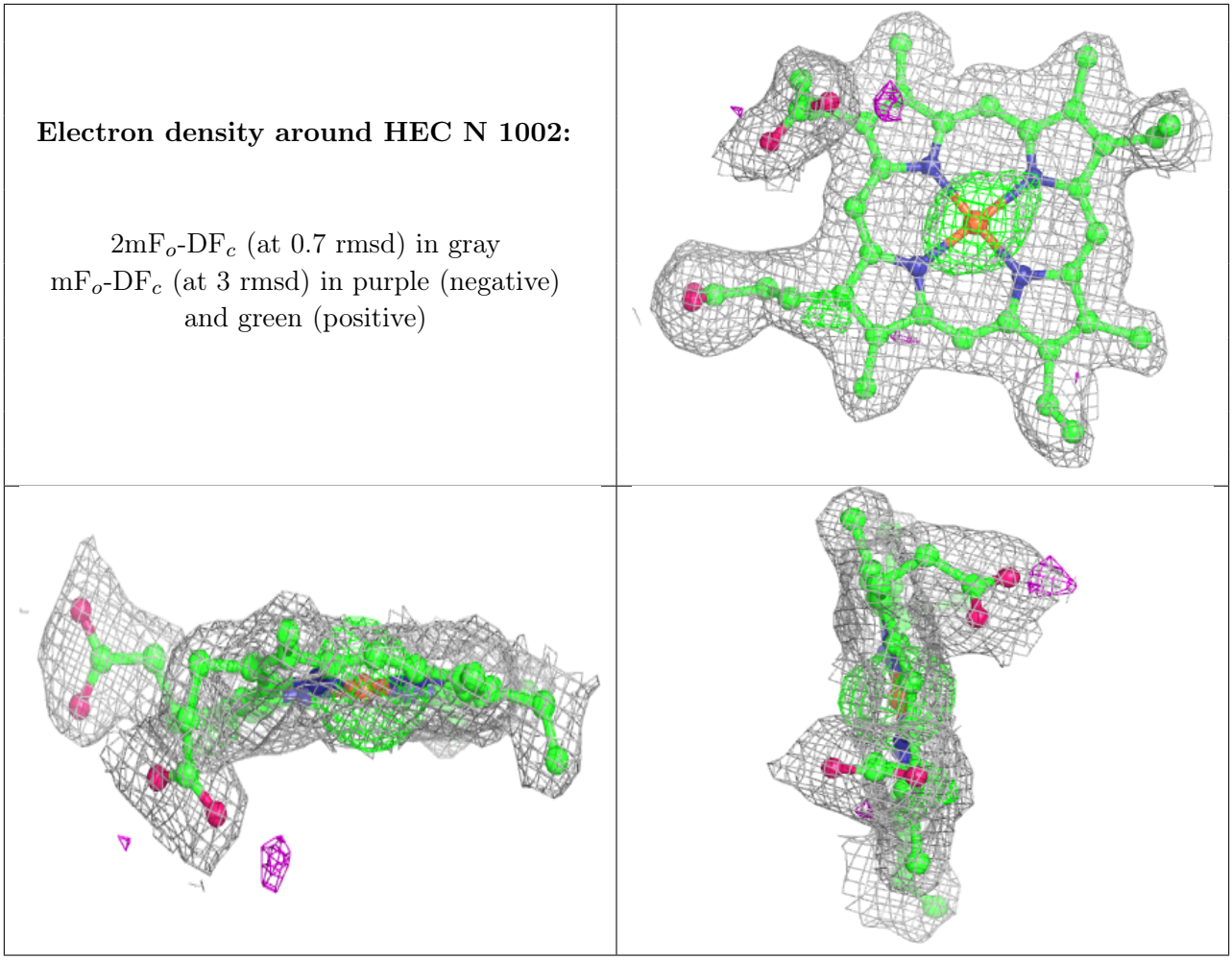






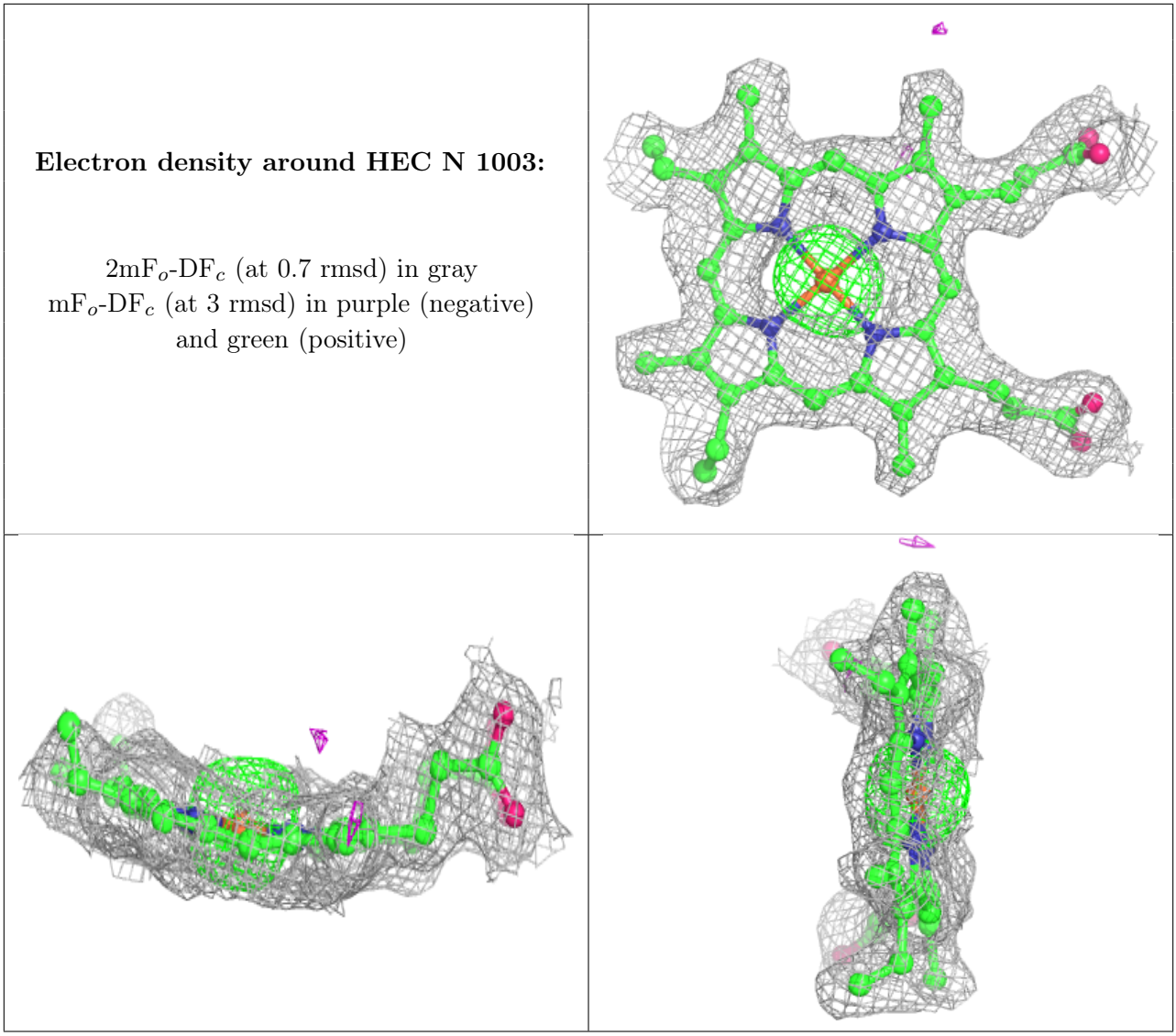
Electron density around HEC N 1002:

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



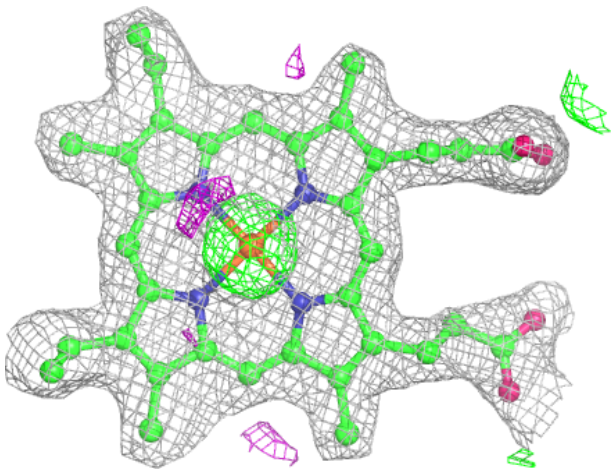
Electron density around HEC N 1003:

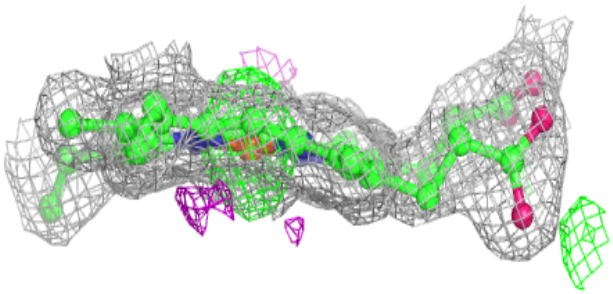
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

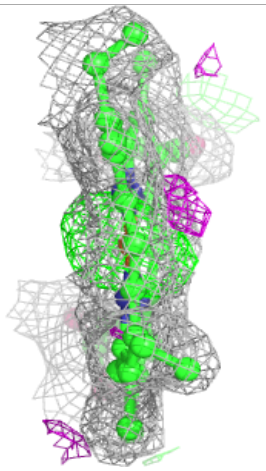


Electron density around HEC E 1004:

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

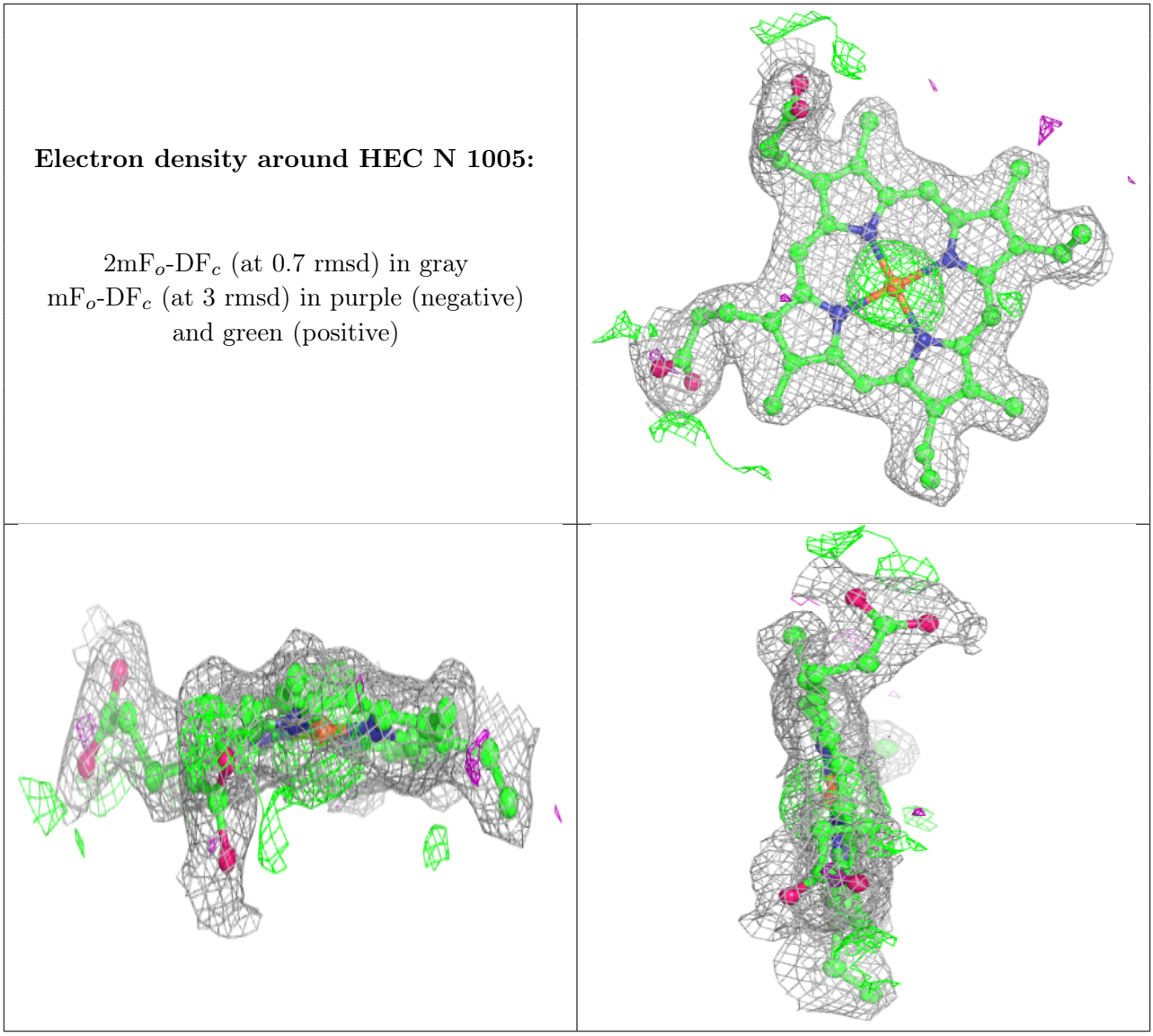






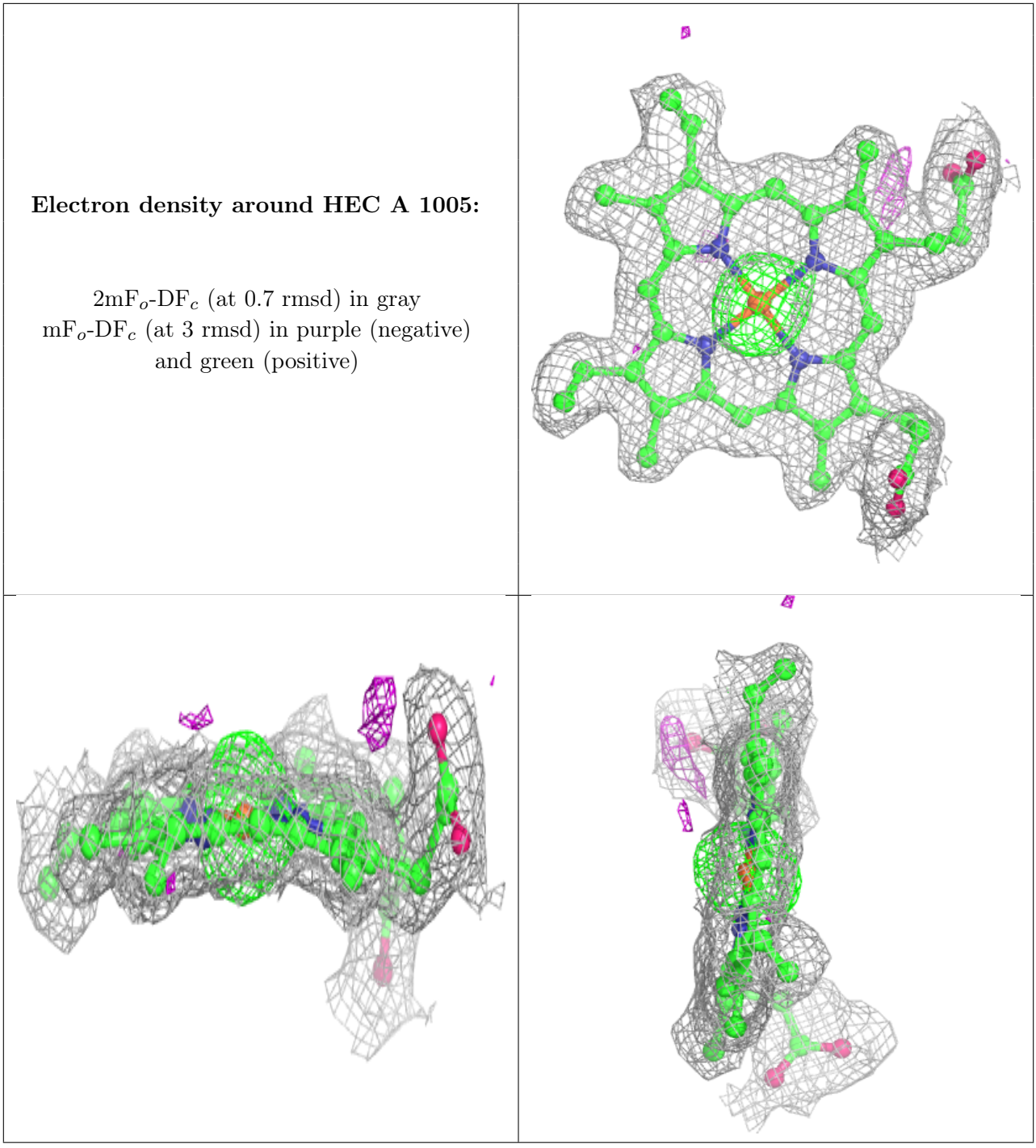
Electron density around HEC N 1005:

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



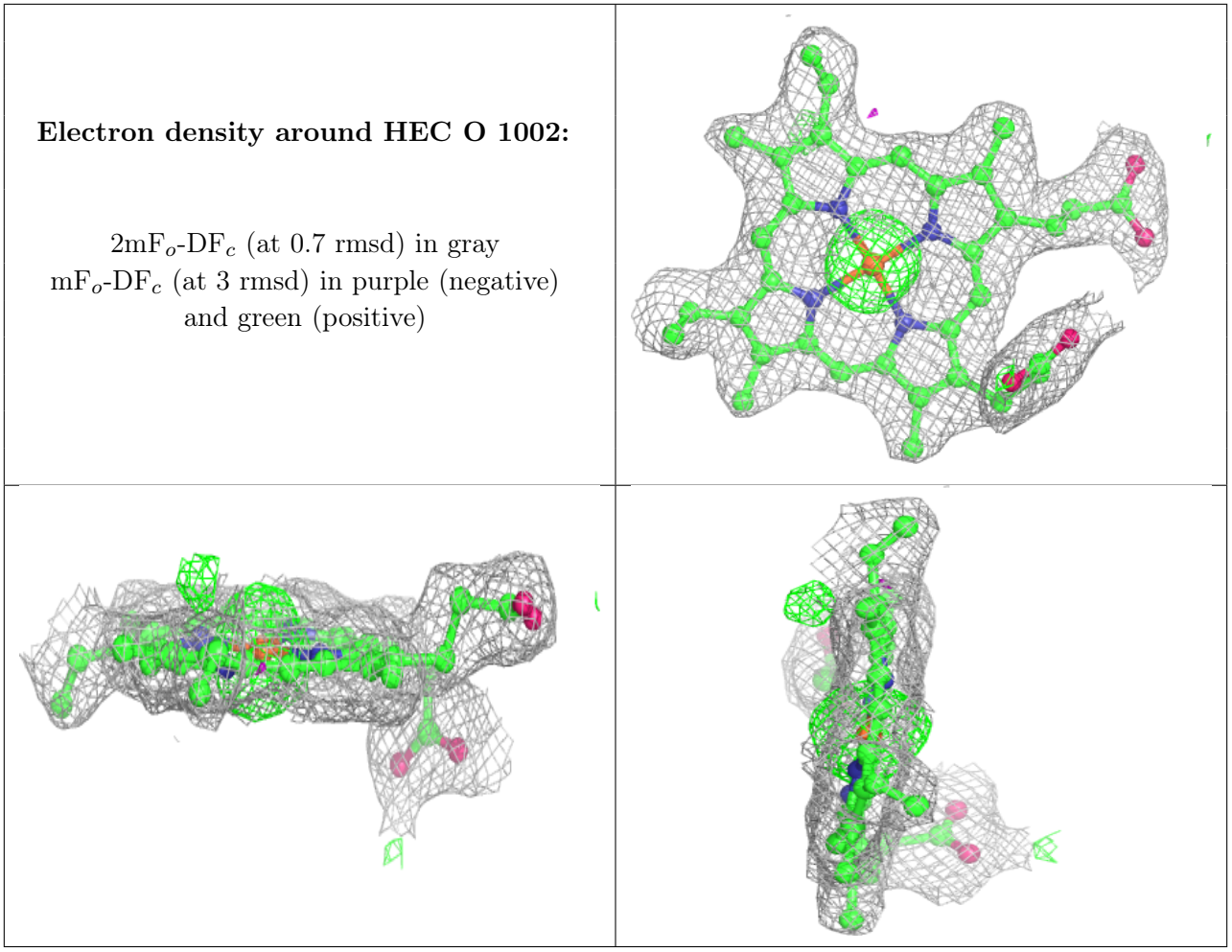
Electron density around HEC A 1005:

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



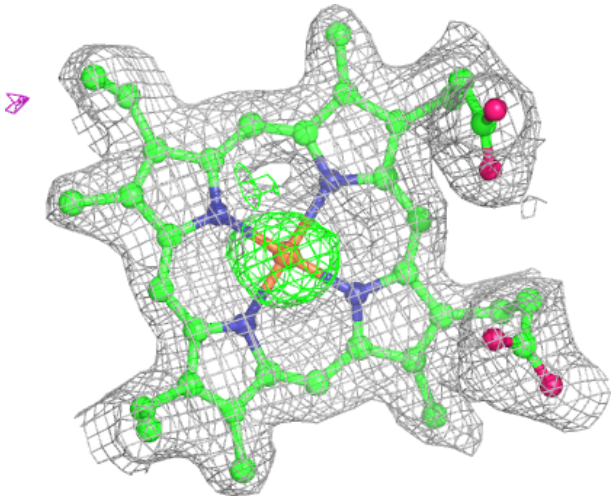
Electron density around HEC O 1002:

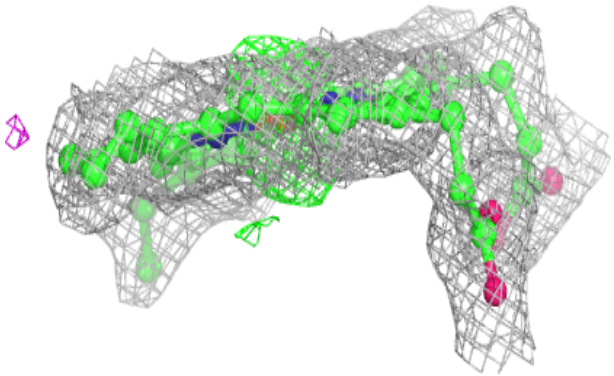
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

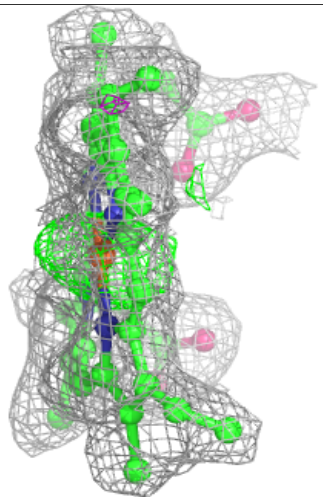


Electron density around HEC B 1001:

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

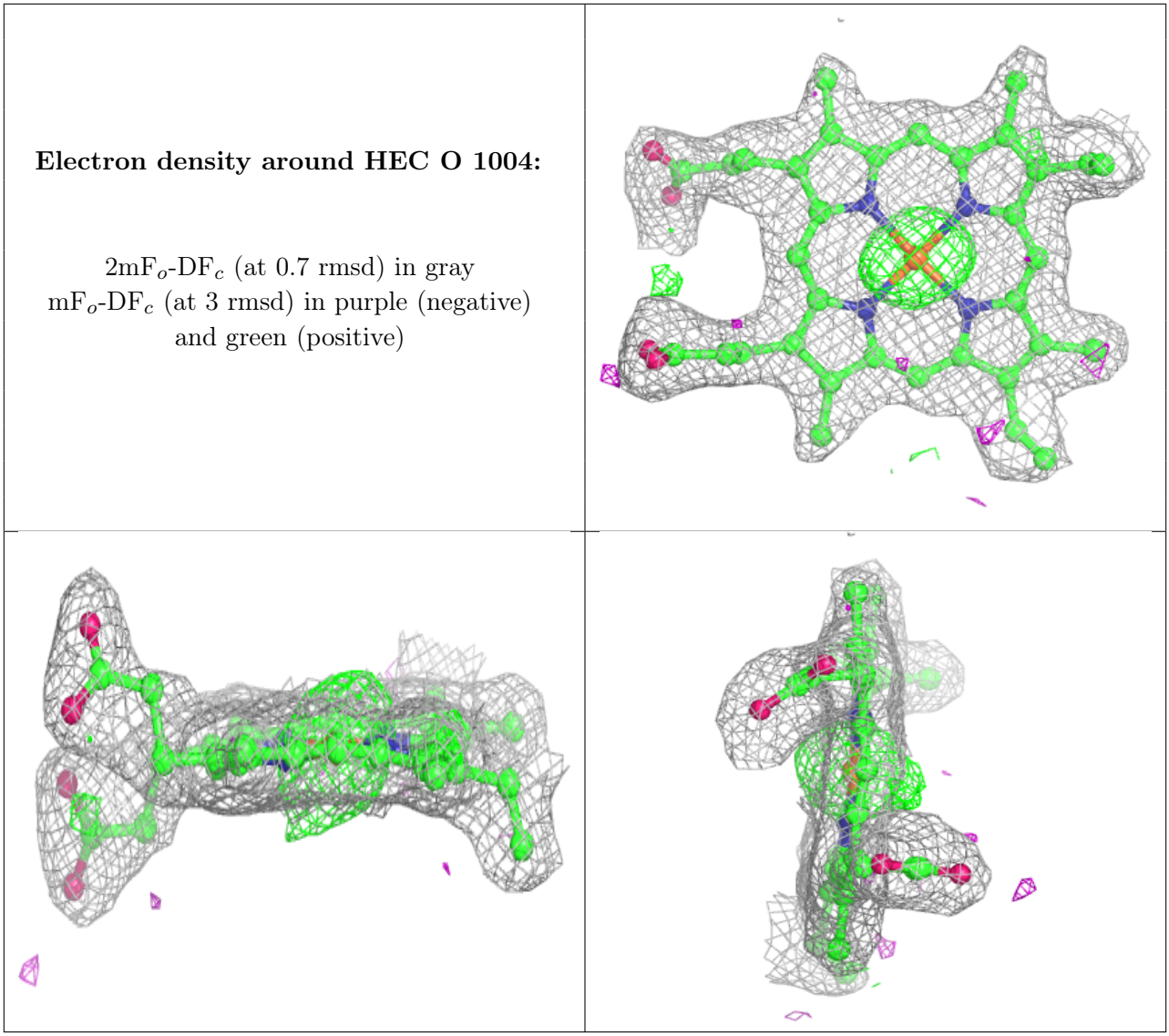






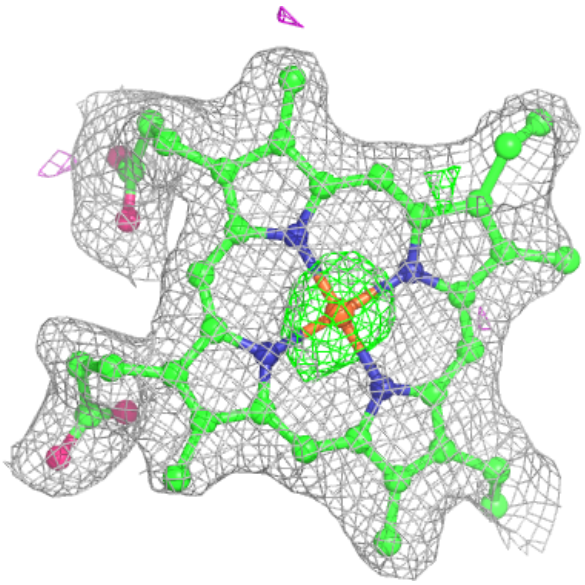
Electron density around HEC O 1004:

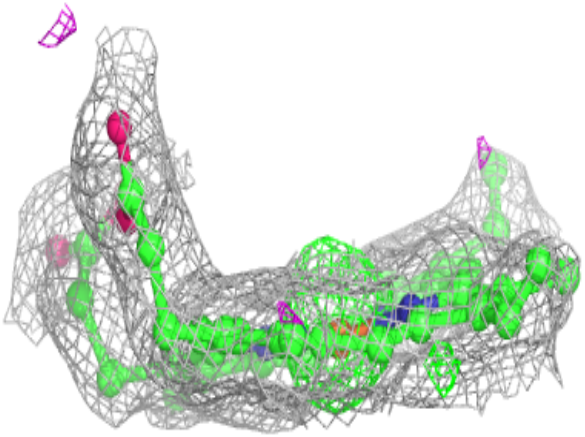
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

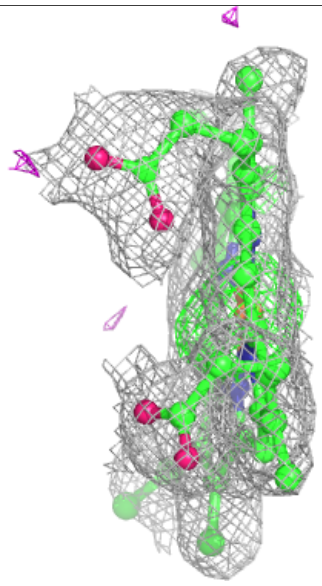


Electron density around HEC P 1001:

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

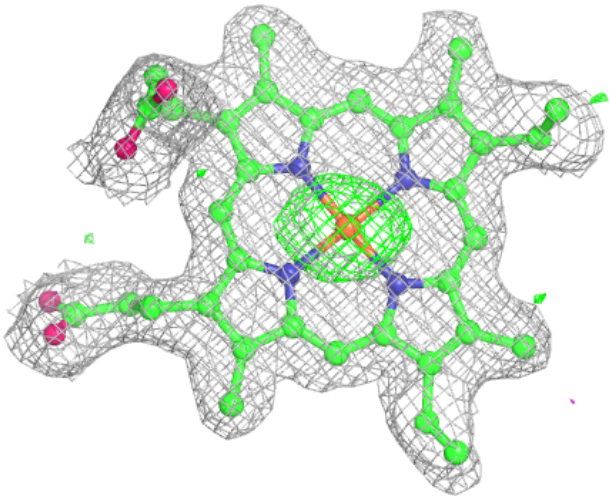


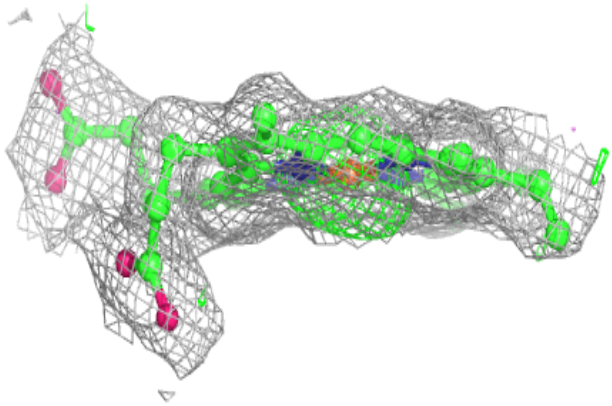


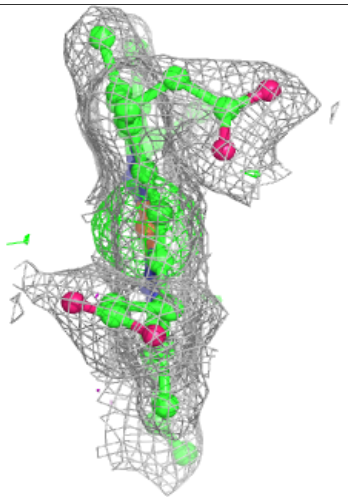


Electron density around HEC P 1002:

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

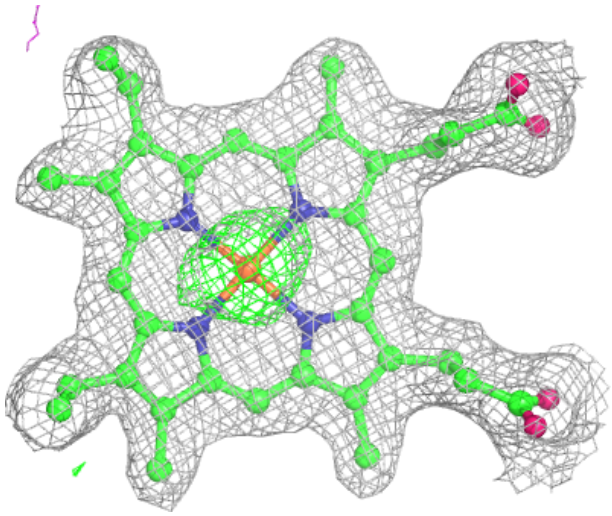


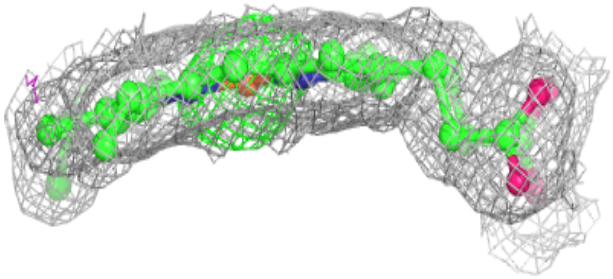


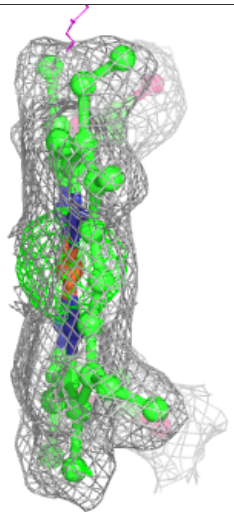


Electron density around HEC P 1003:

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

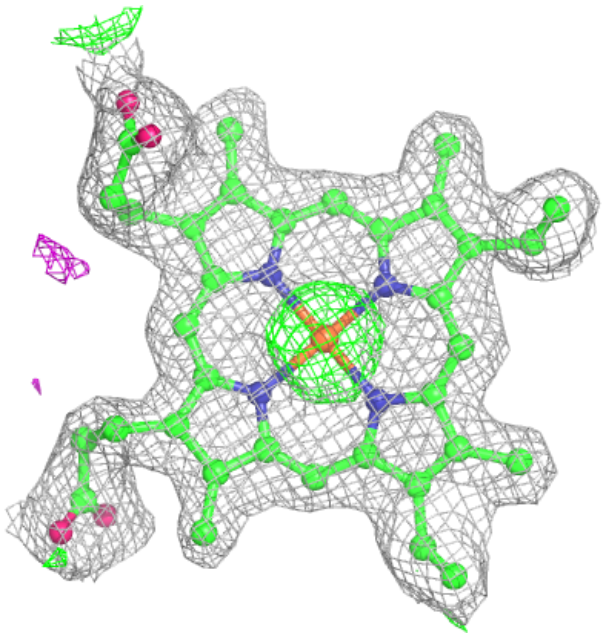


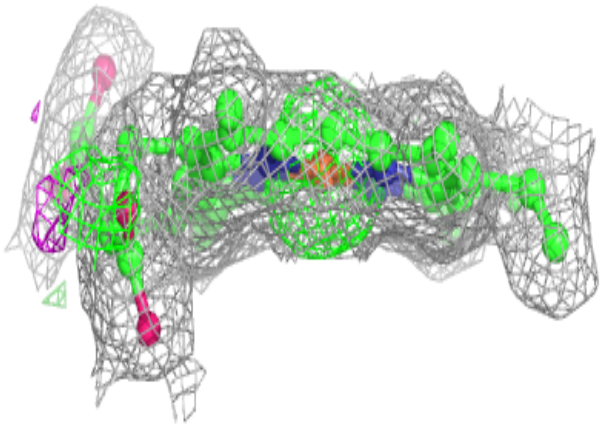


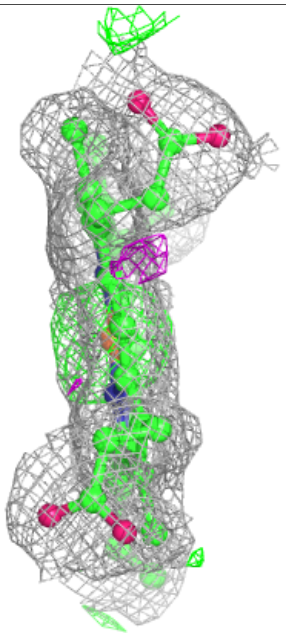


Electron density around HEC P 1005:

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

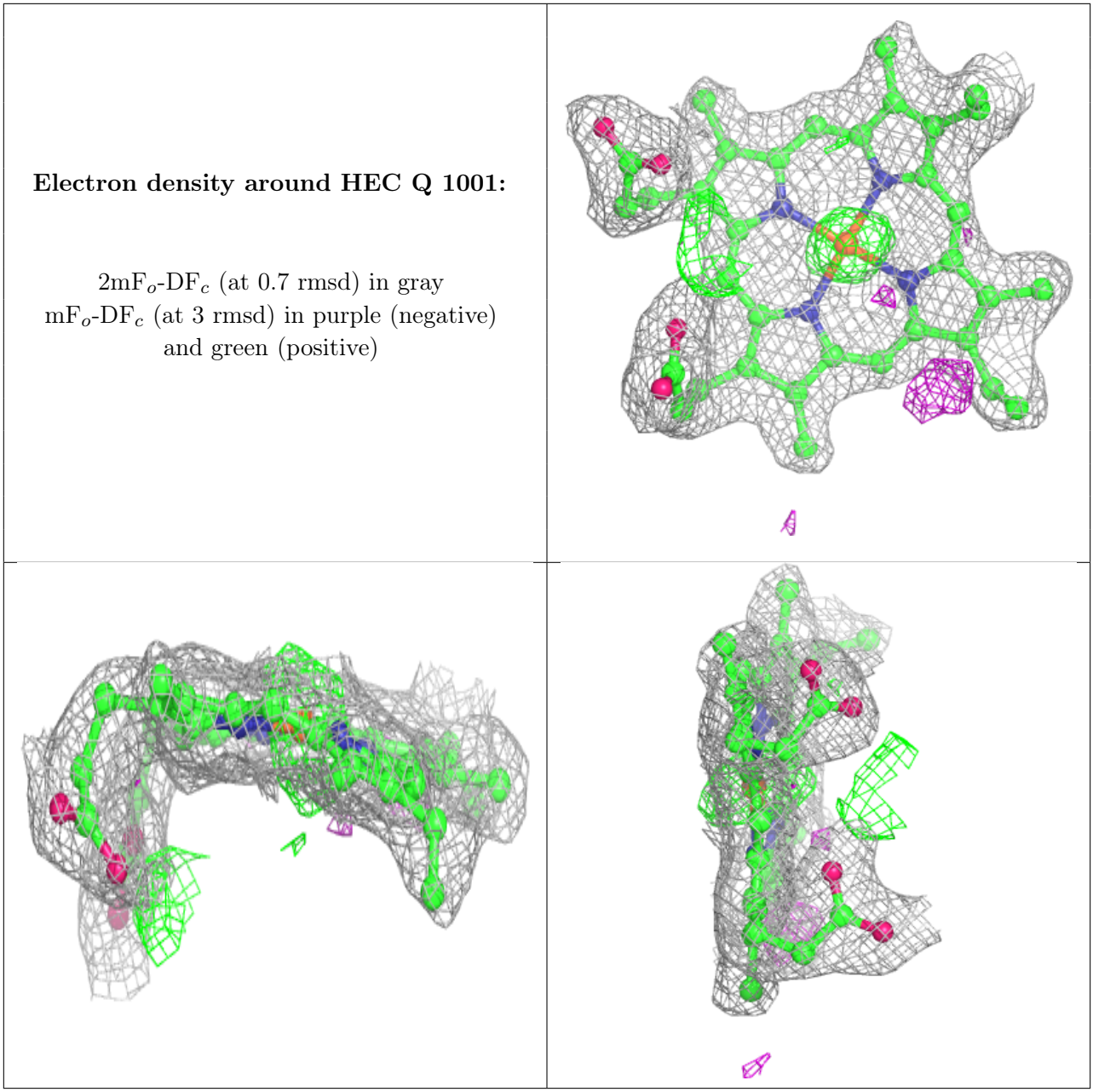






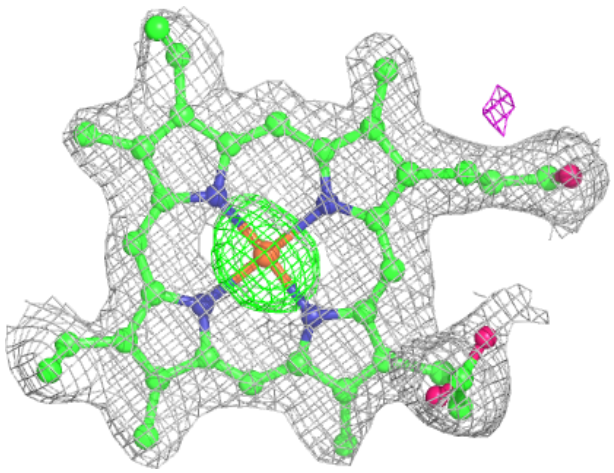
Electron density around HEC Q 1001:

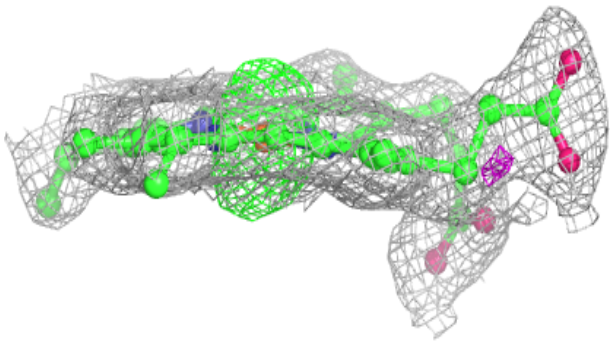
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

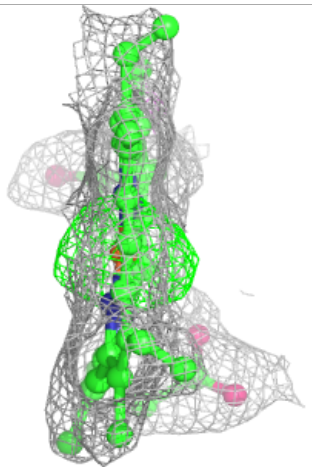


Electron density around HEC Q 1002:

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

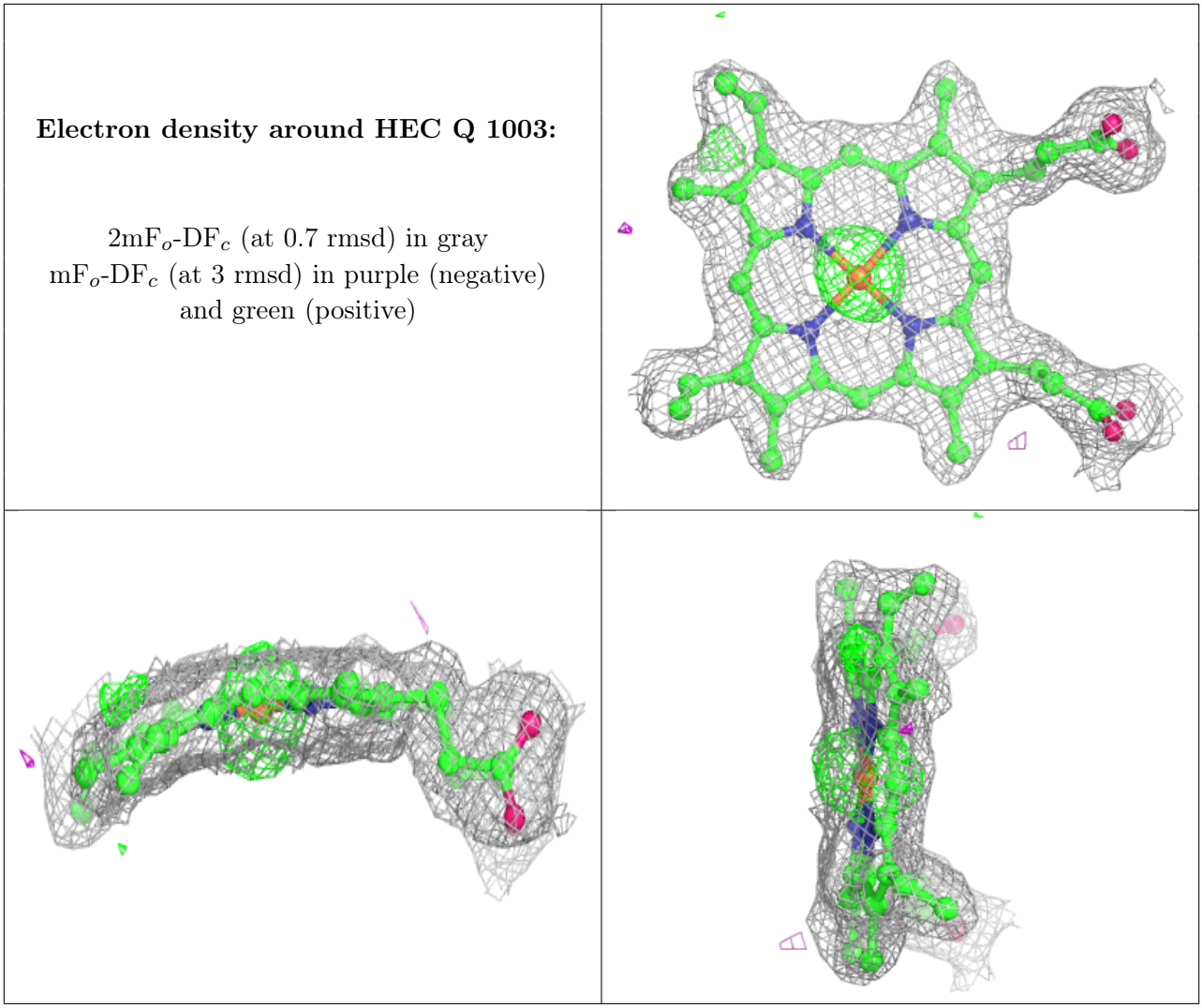






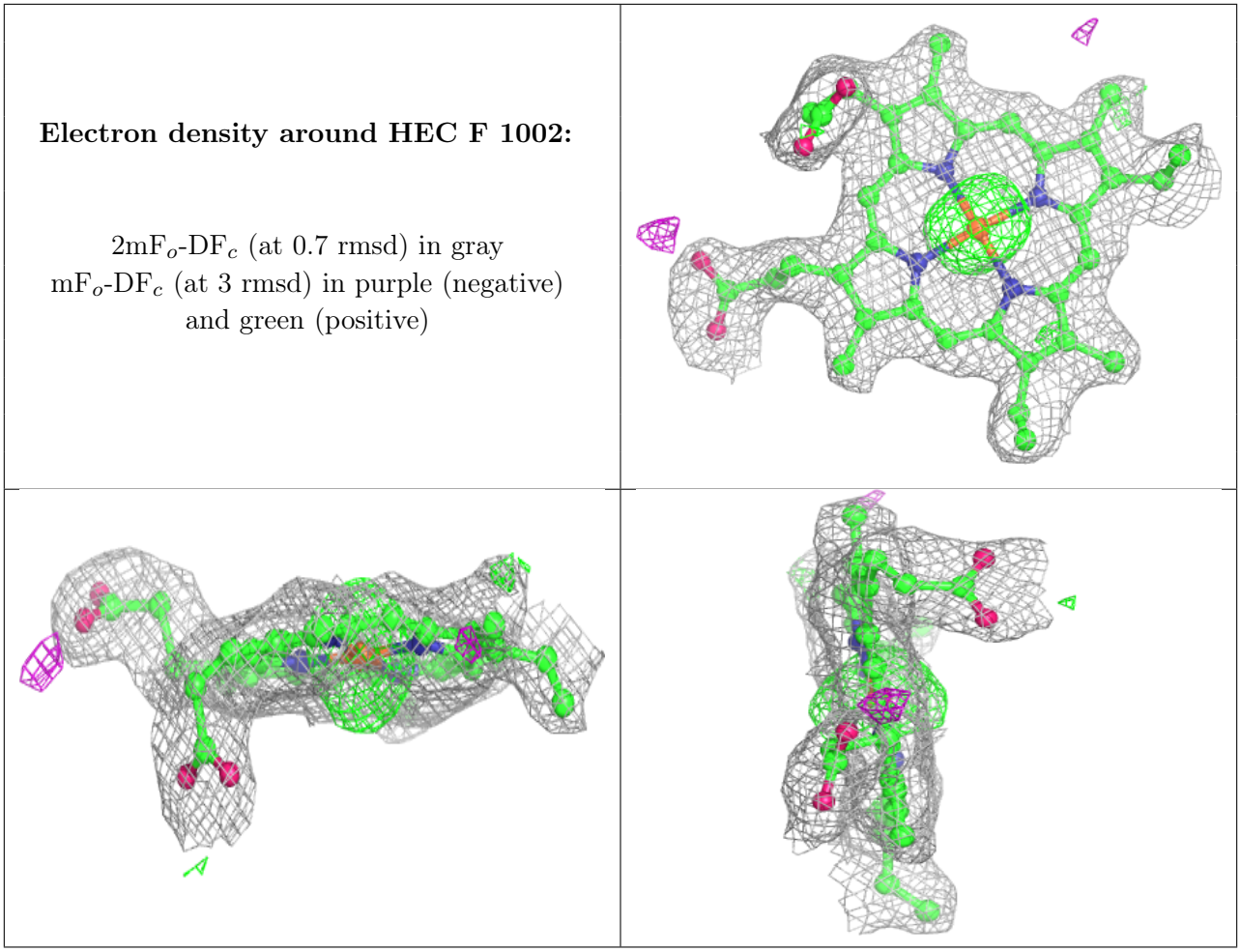
Electron density around HEC Q 1003:

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



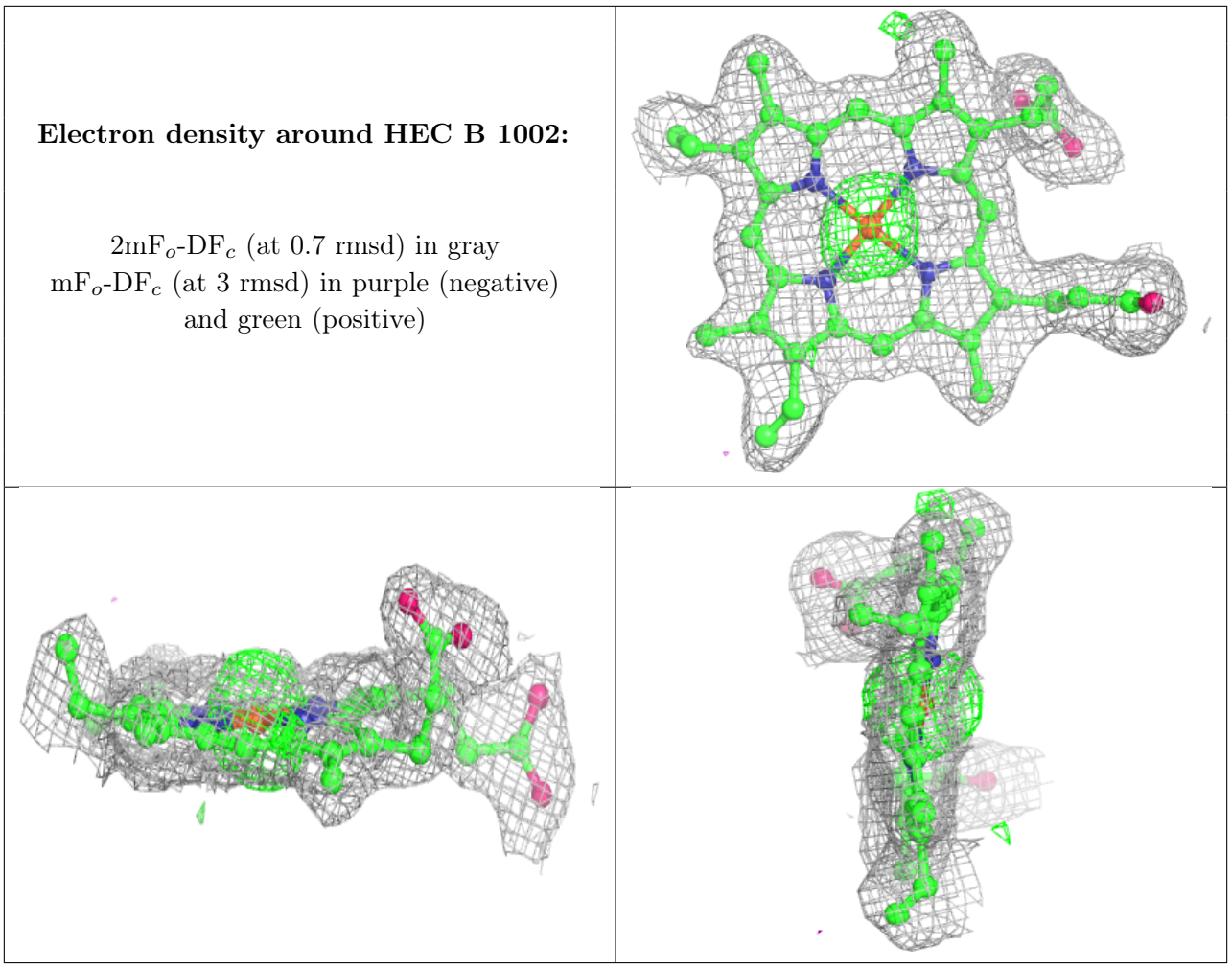
Electron density around HEC F 1002:

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



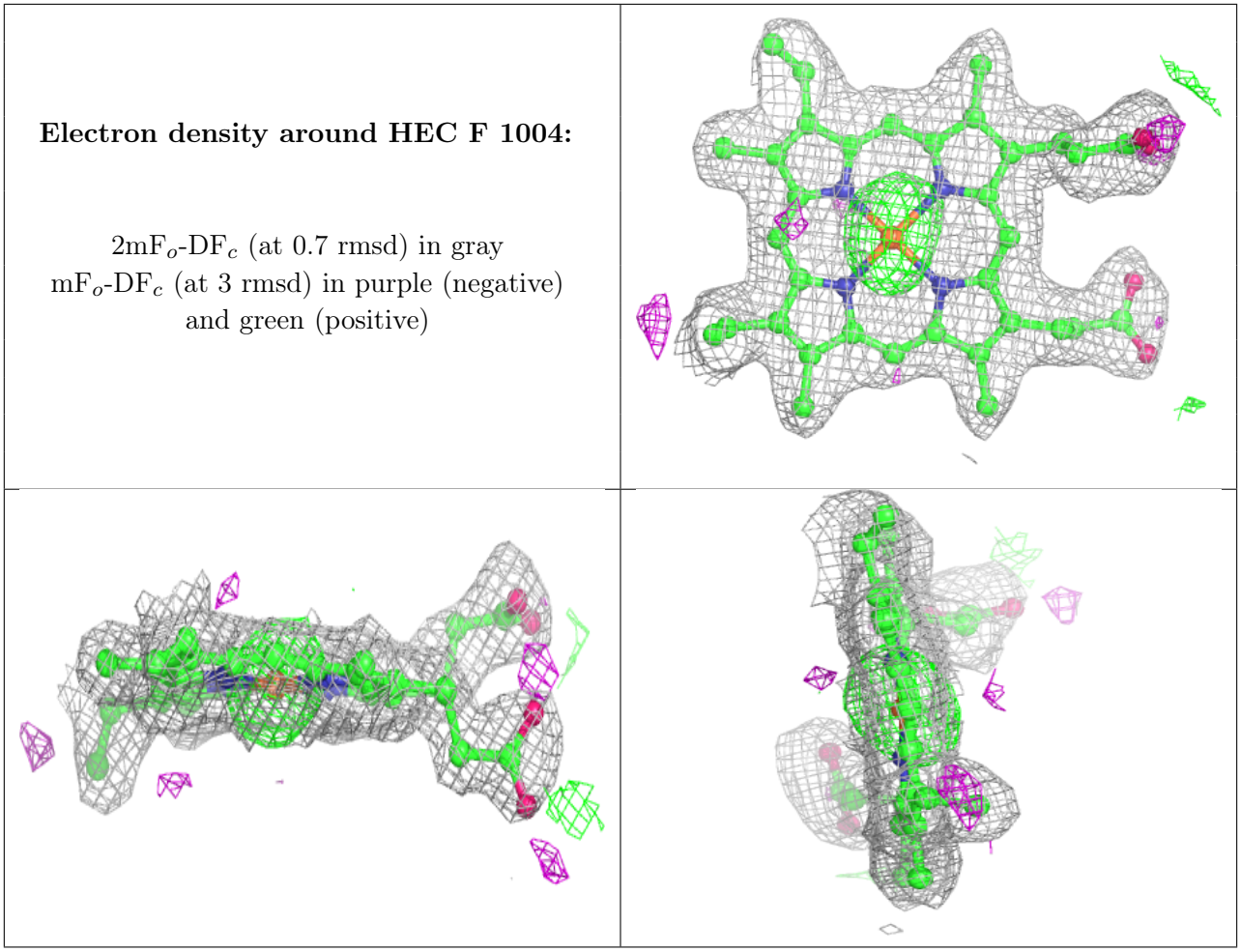
Electron density around HEC B 1002:

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



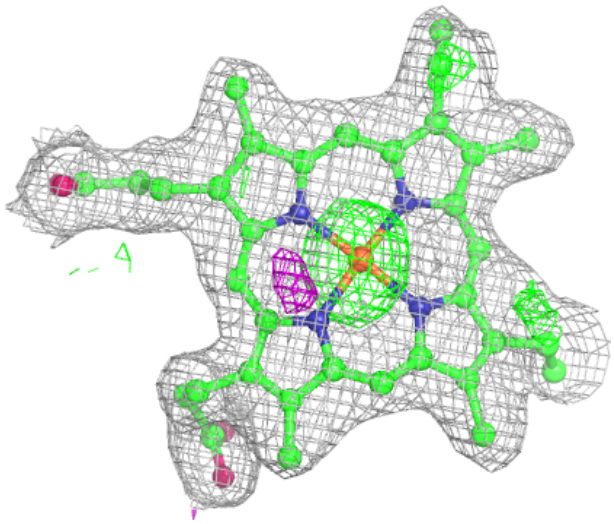
Electron density around HEC F 1004:

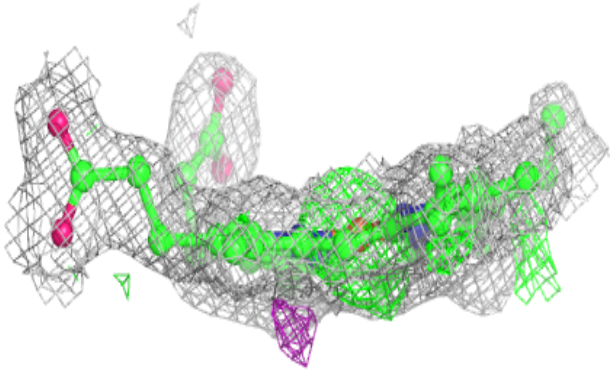
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

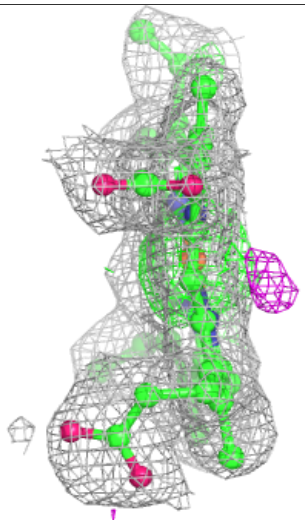


Electron density around HEC R 1003:

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

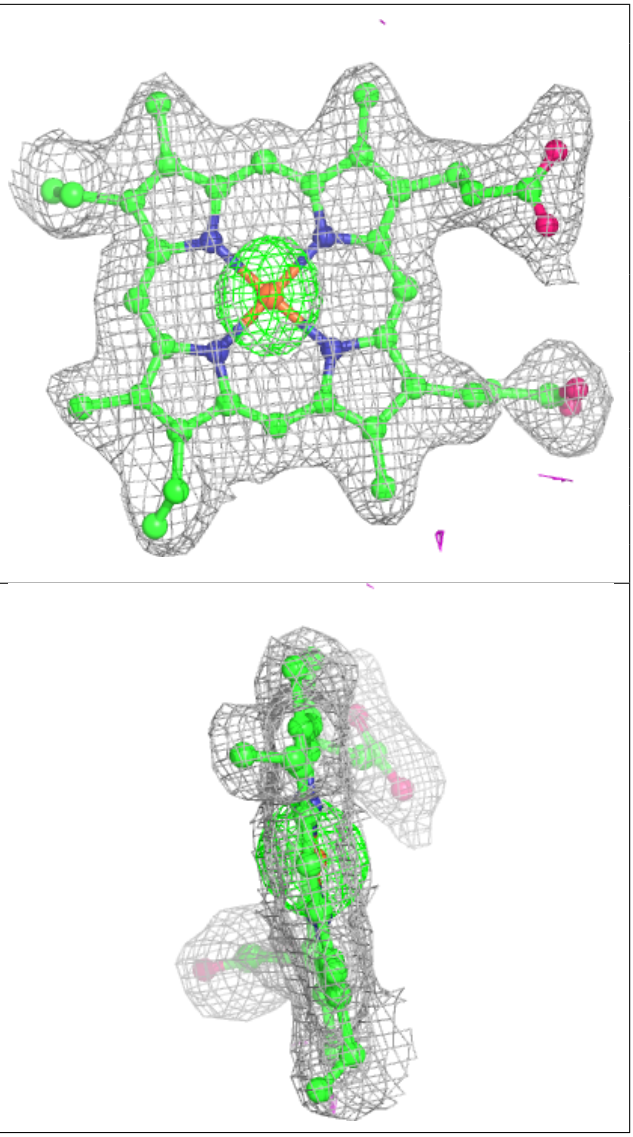


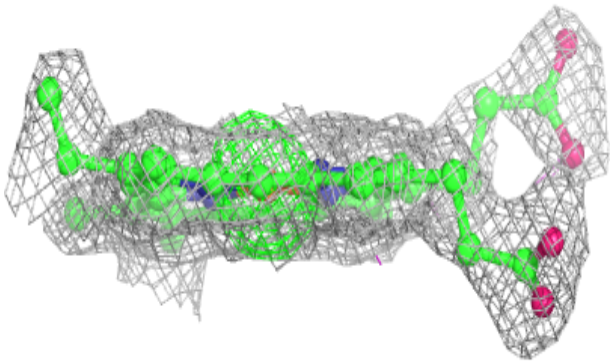




Electron density around HEC R 1004:

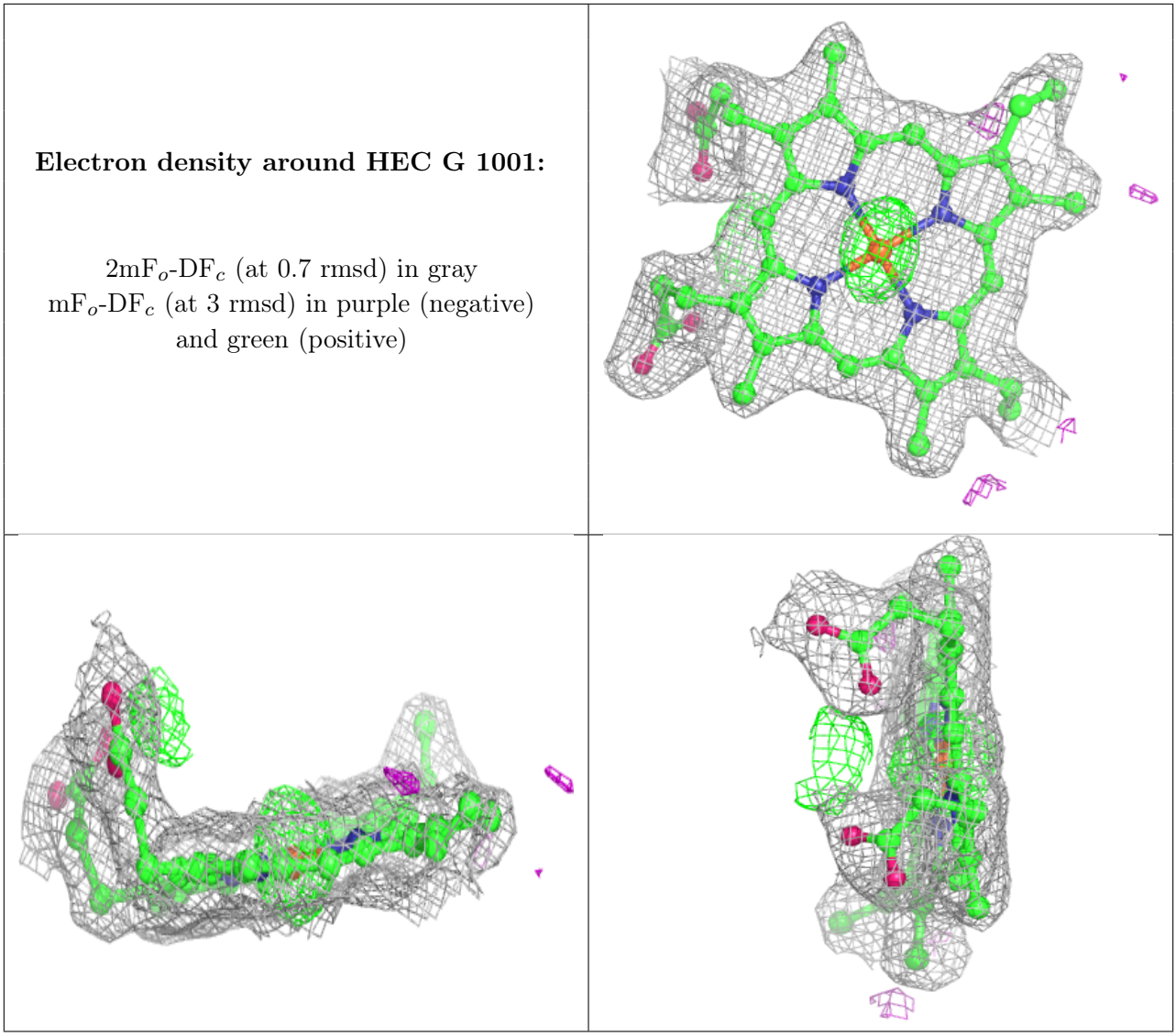
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





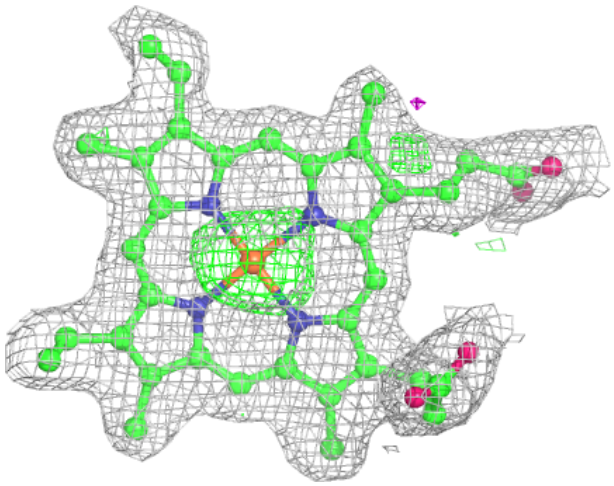
Electron density around HEC G 1001:

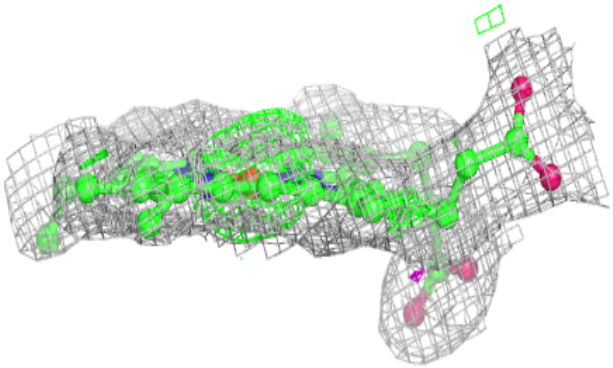
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

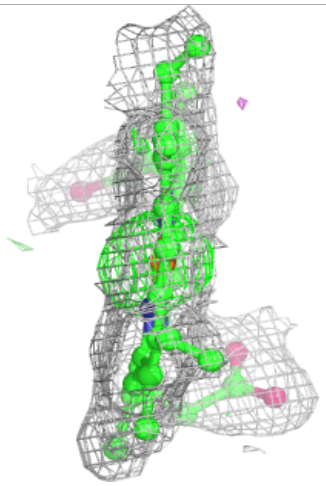


Electron density around HEC G 1002:

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

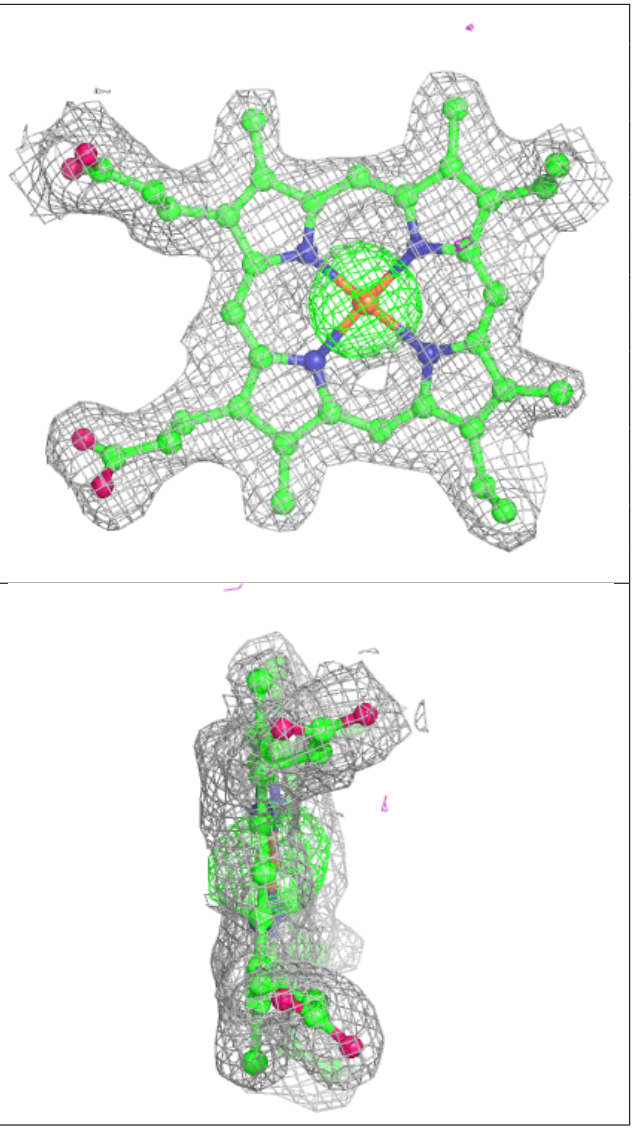






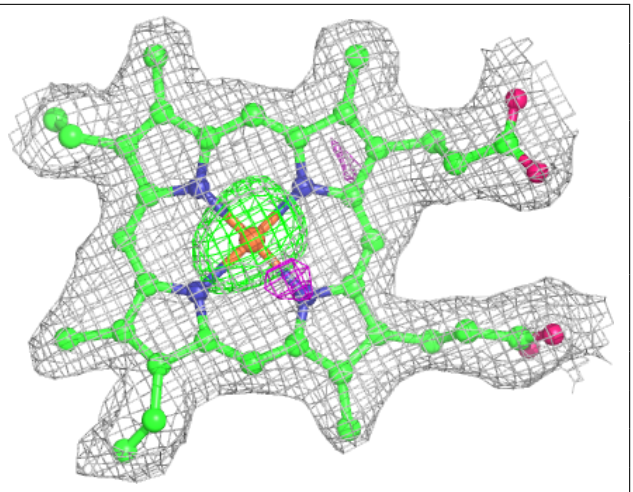
Electron density around HEC B 1003:

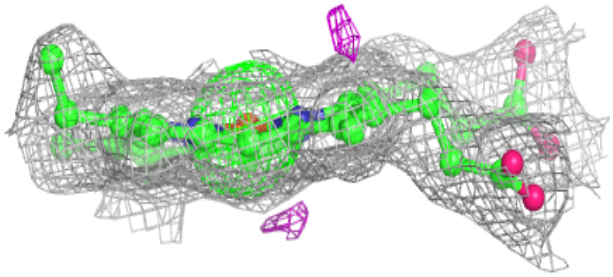
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

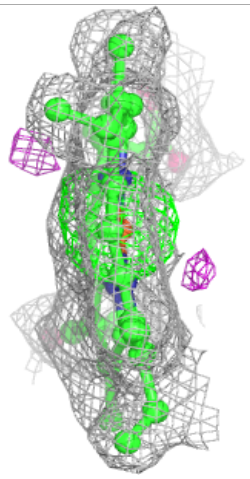


Electron density around HEC G 1004:

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

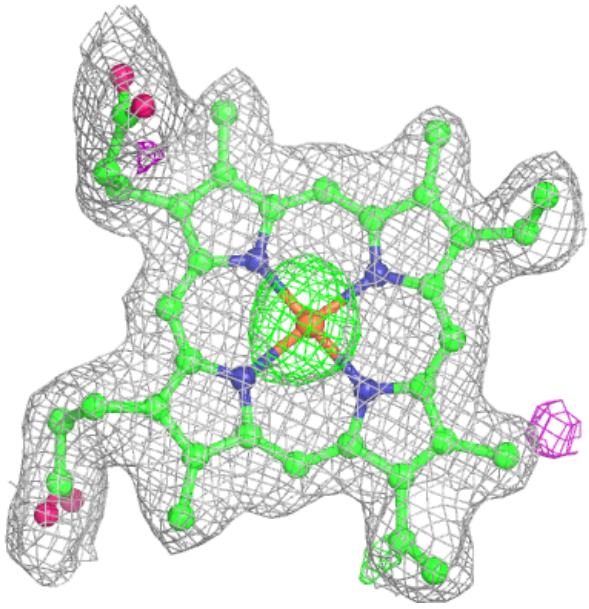


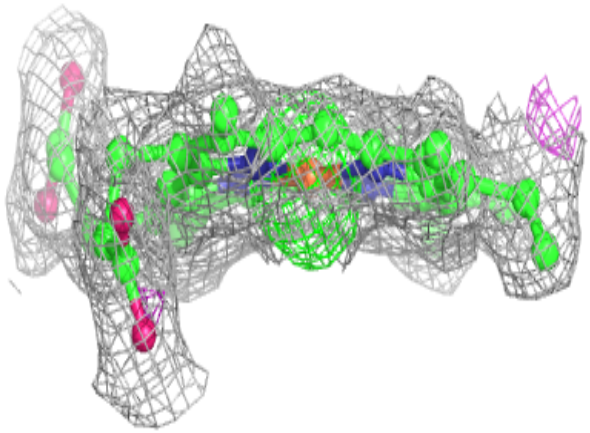


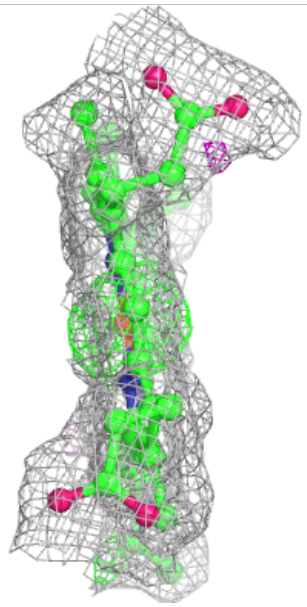


Electron density around HEC G 1005:

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

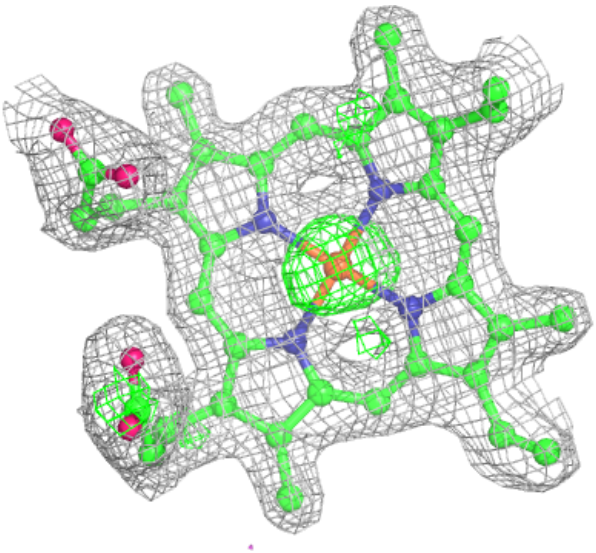


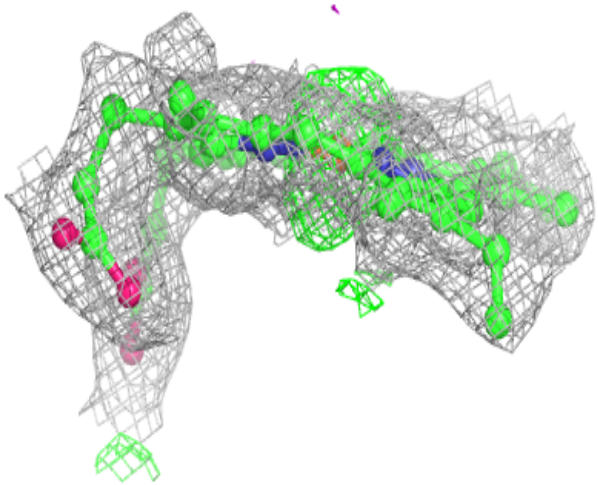


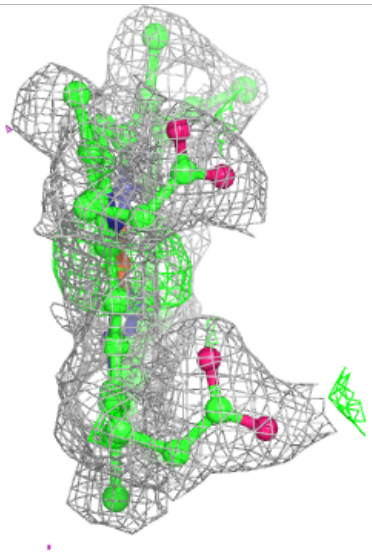


Electron density around HEC H 1001:

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

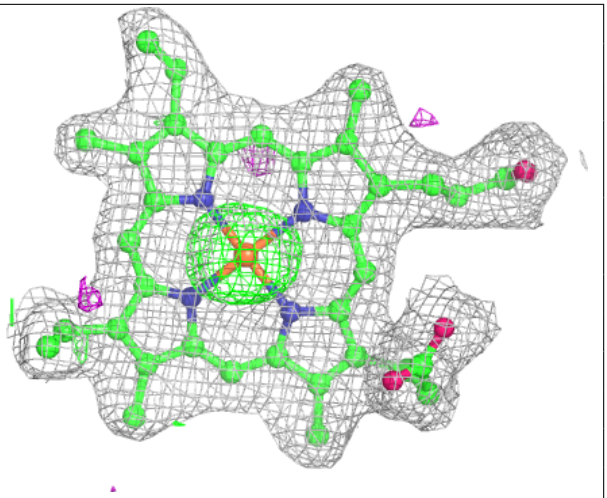


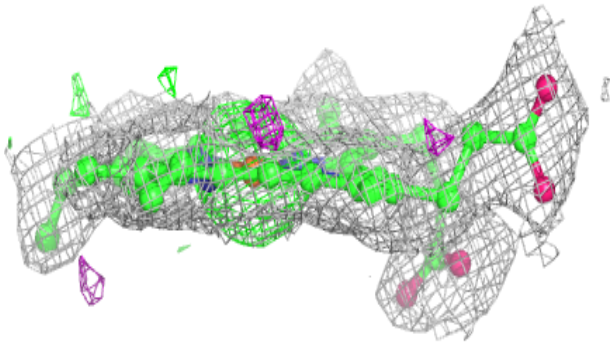


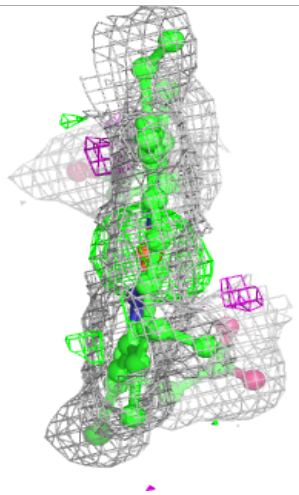


Electron density around HEC H 1002:

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

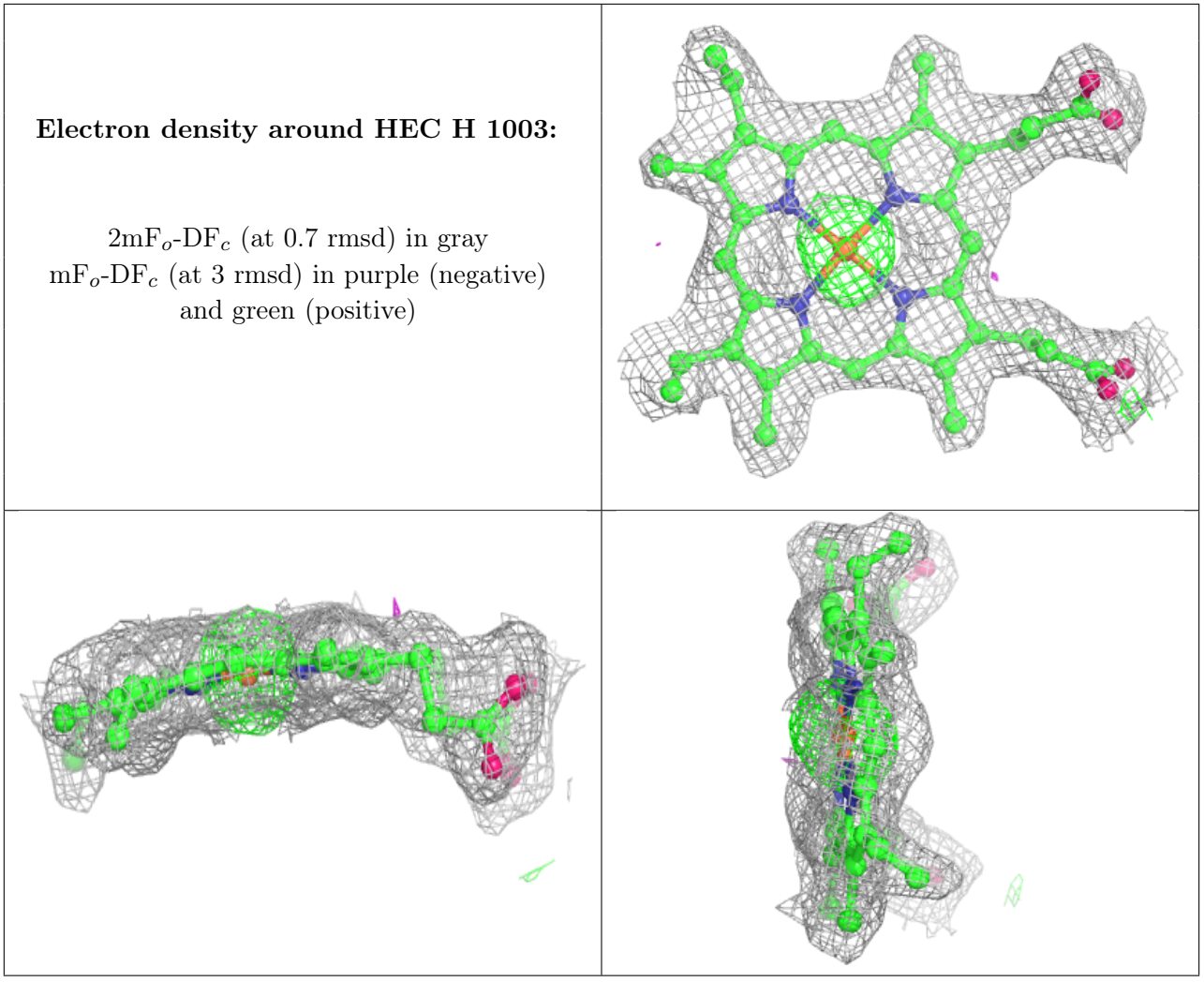






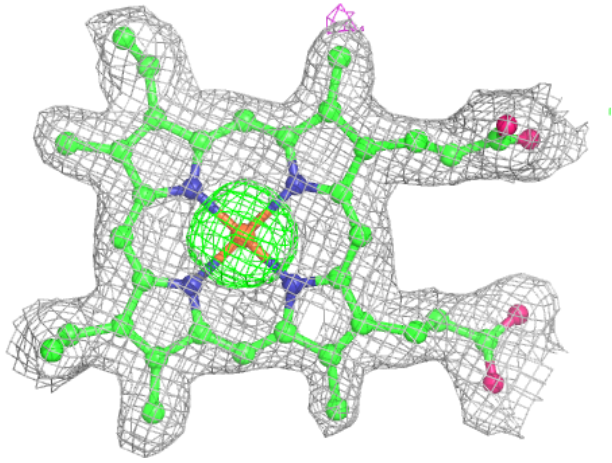
Electron density around HEC H 1003:

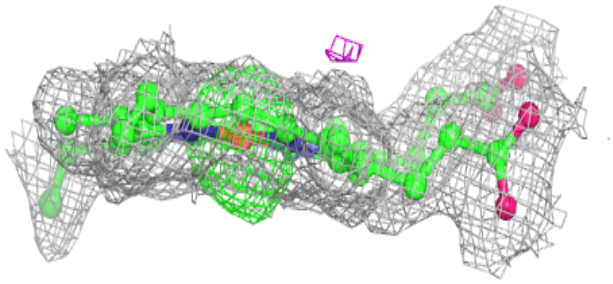
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

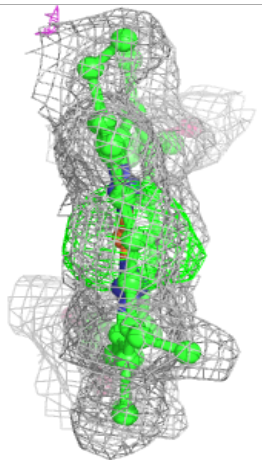


Electron density around HEC B 1004:

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

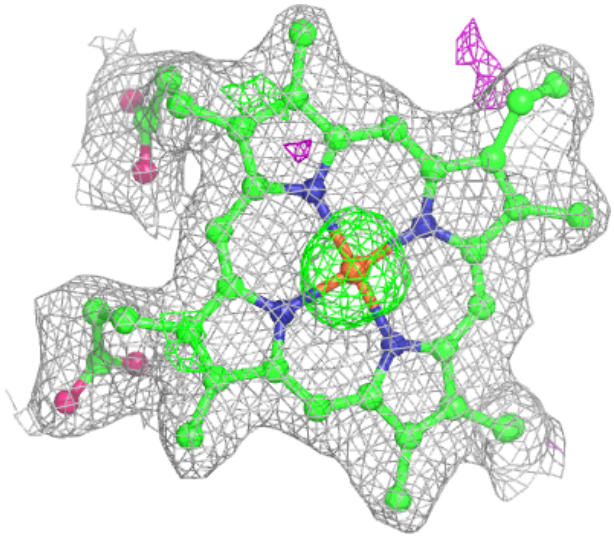


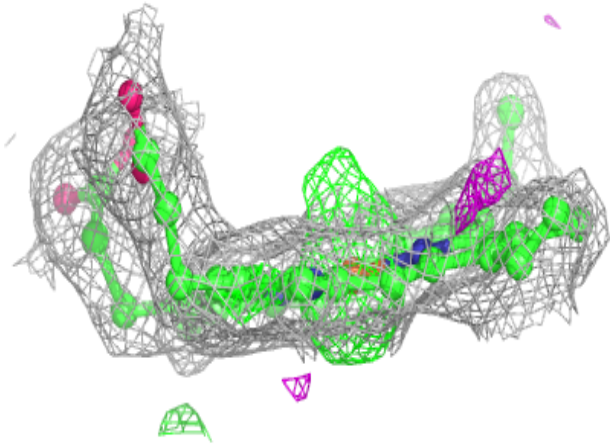




Electron density around HEC D 1001:

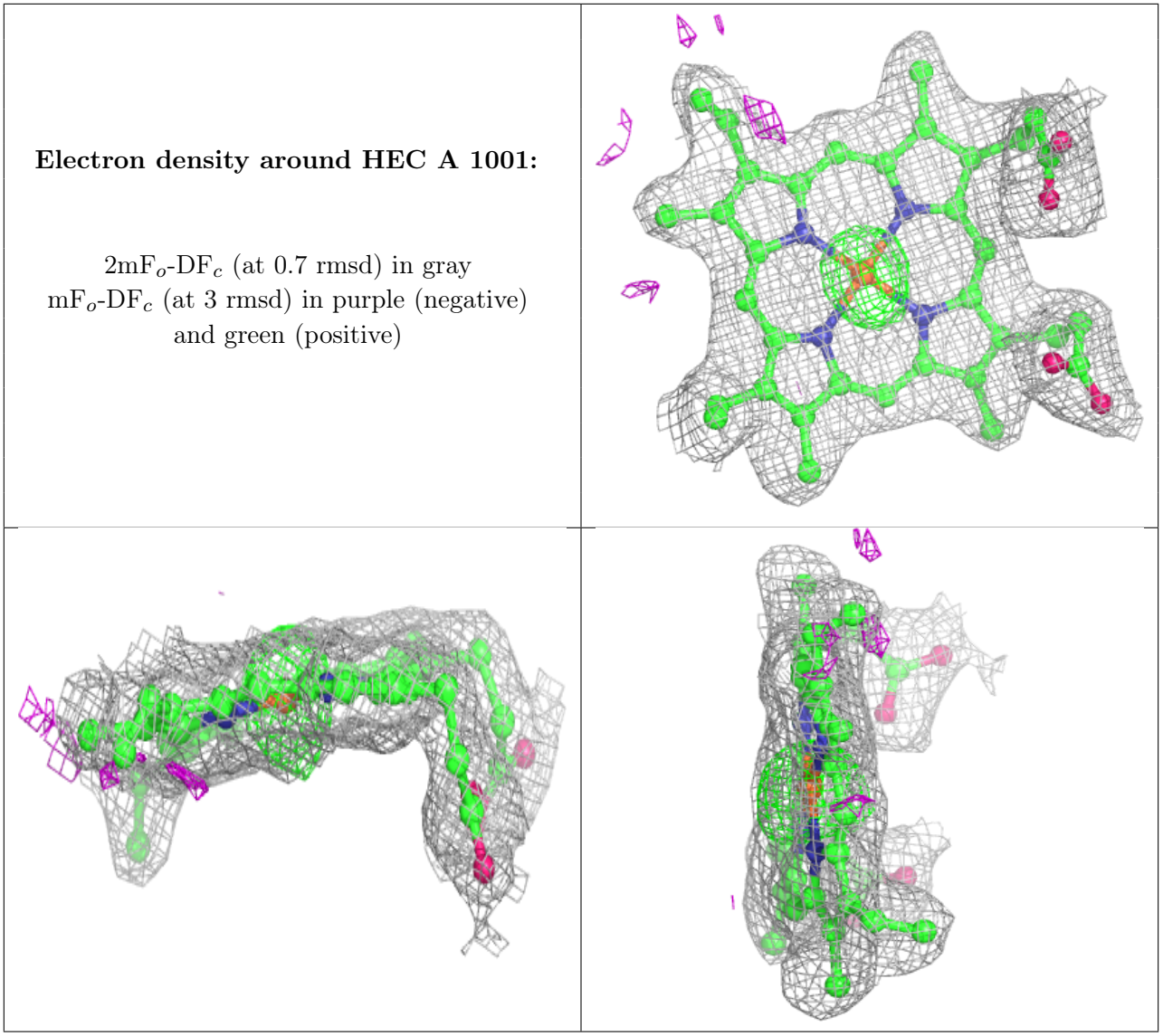
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





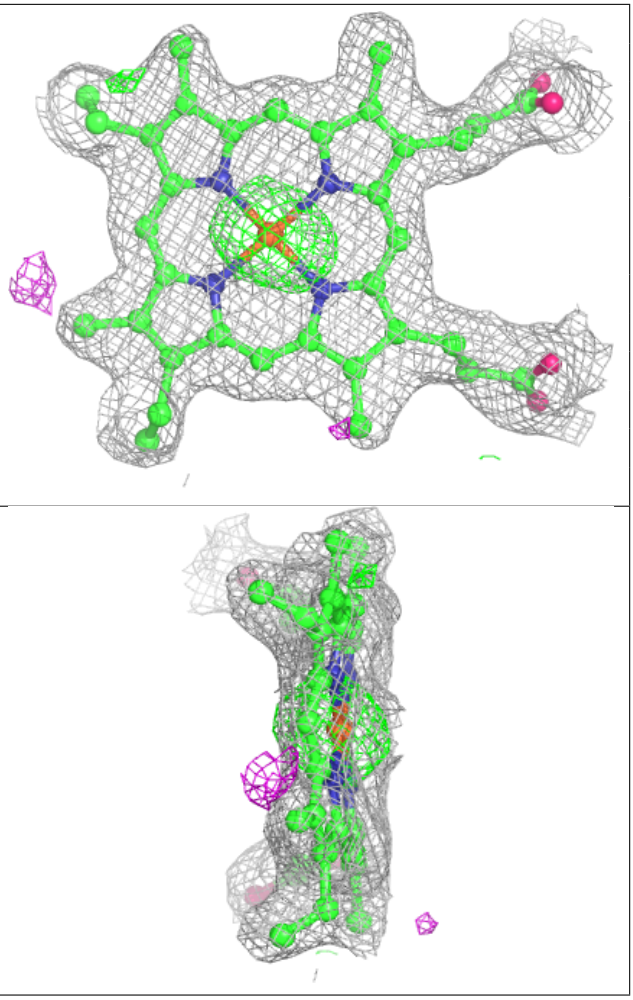
Electron density around HEC A 1001:

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



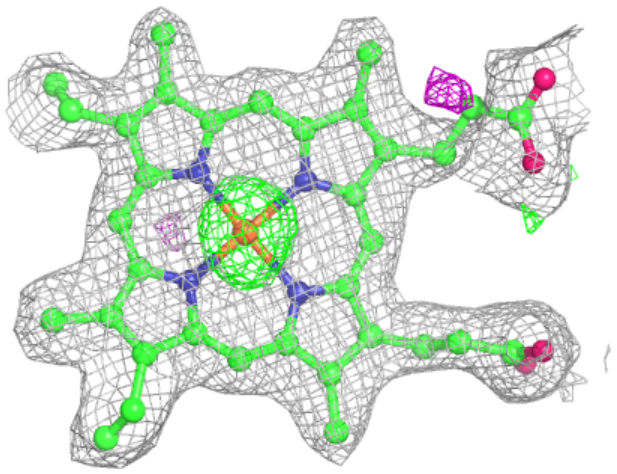
Electron density around HEC D 1003:

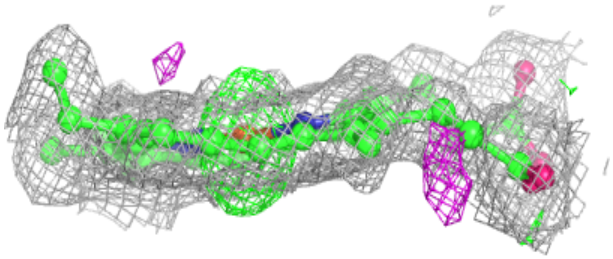
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

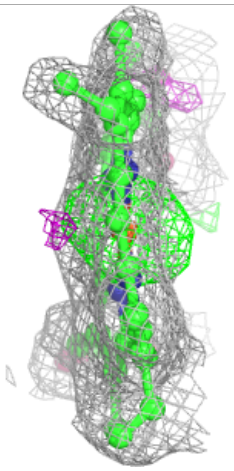


Electron density around HEC Q 1004:

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

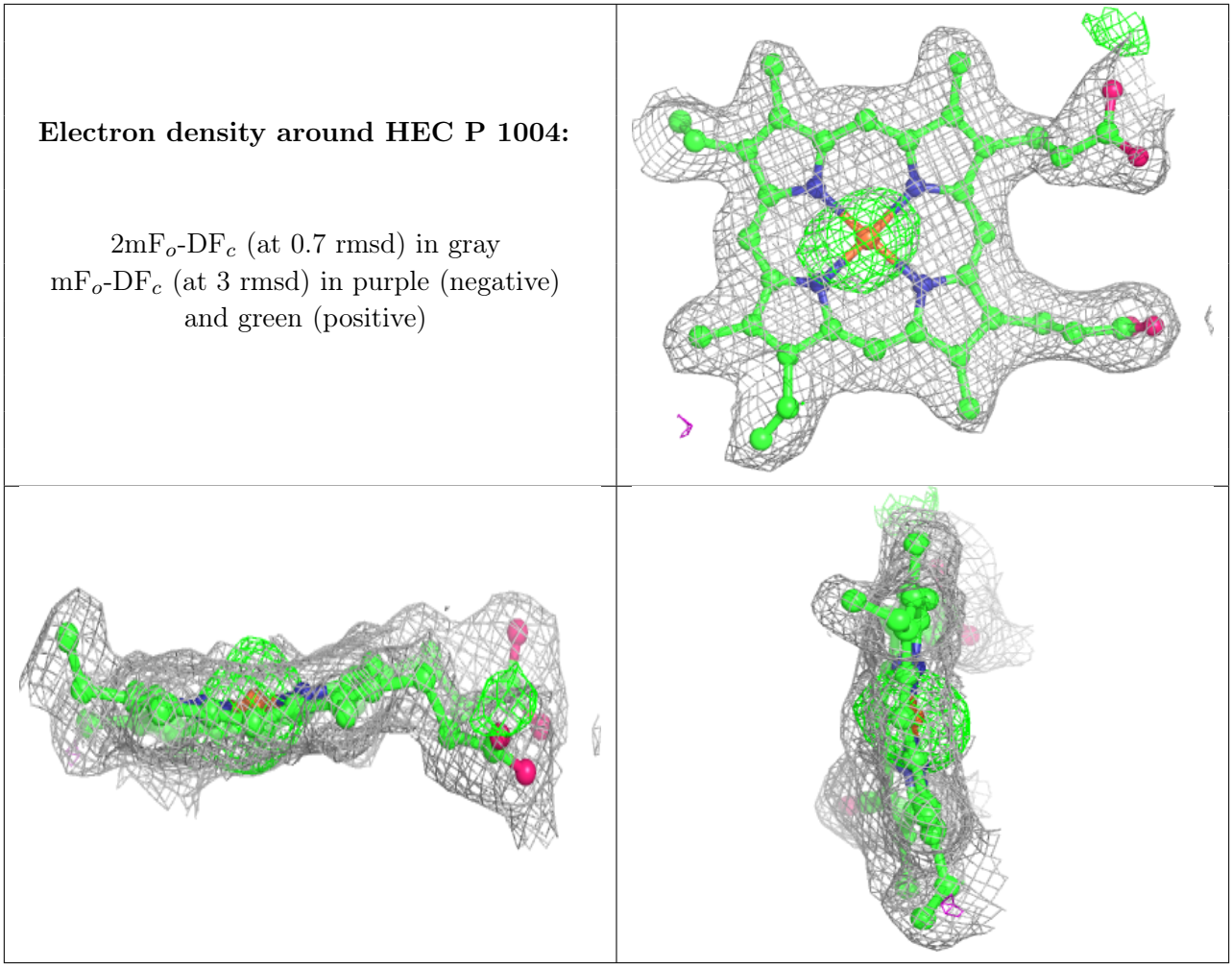






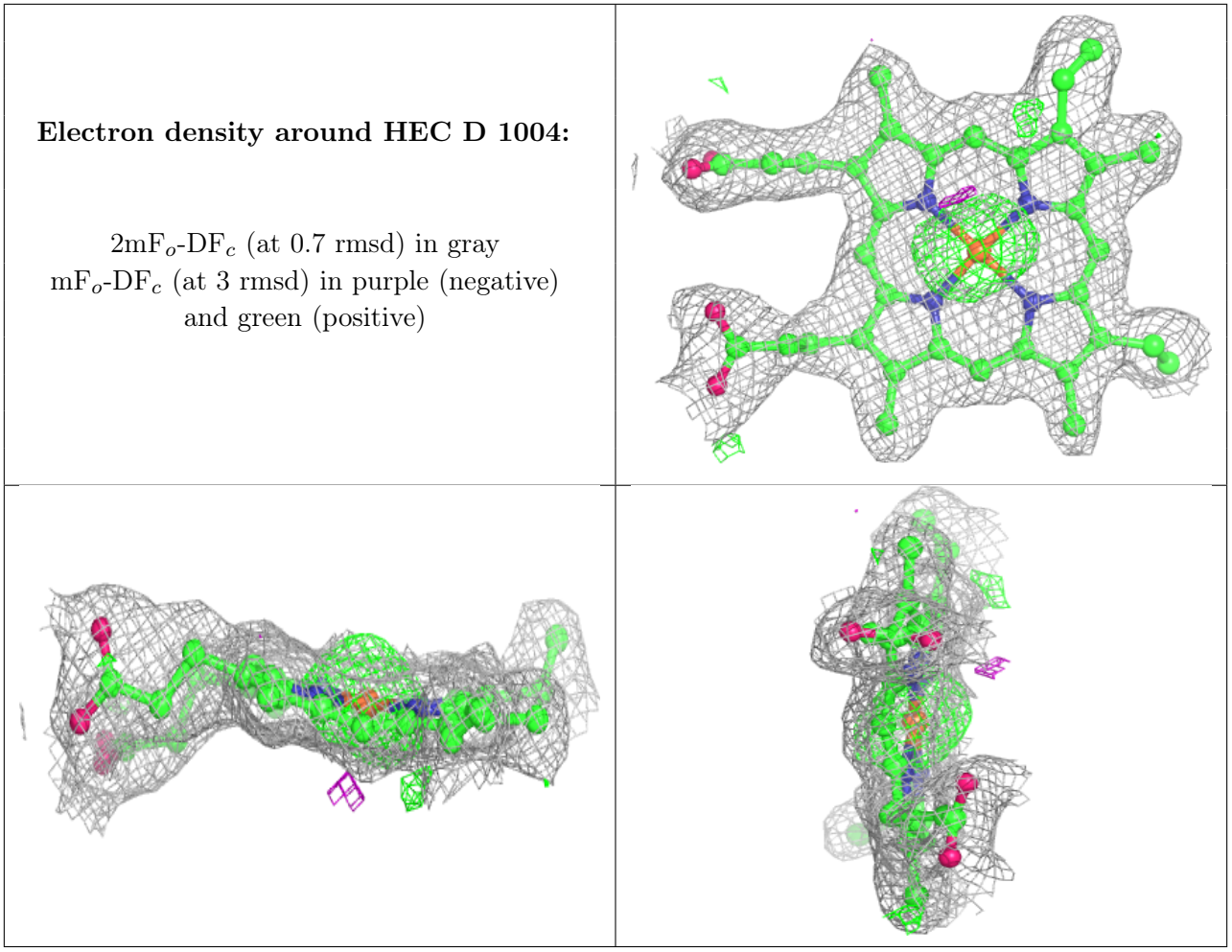
Electron density around HEC P 1004:

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



Electron density around HEC D 1004:

$2mF_o$-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.