



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 05:53 AM UTC

PDB ID : 1OGY / pdb_00001ogy
Title : Crystal structure of the heterodimeric nitrate reductase from Rhodobacter sphaeroides
Authors : Arnoux, P.; Sabaty, M.; Alric, J.; Frangioni, B.; Guigliarelli, B.; Adriano, J.-M.; Pignol, D.
Deposited on : 2003-05-19
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

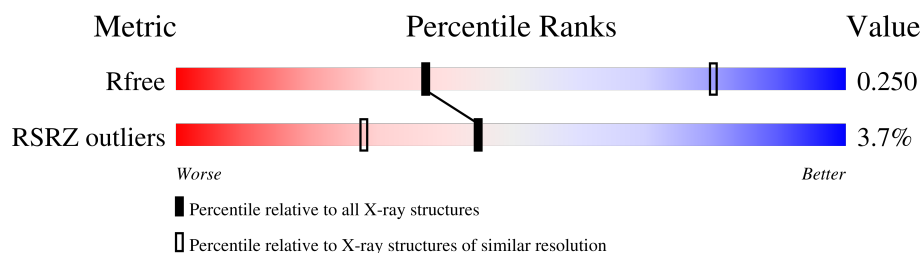
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59336 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 PERIPLASMIC NITRATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	C	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	E	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	G	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	I	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	K	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	M	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	O	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			

- Molecule 2 is a protein called DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE.

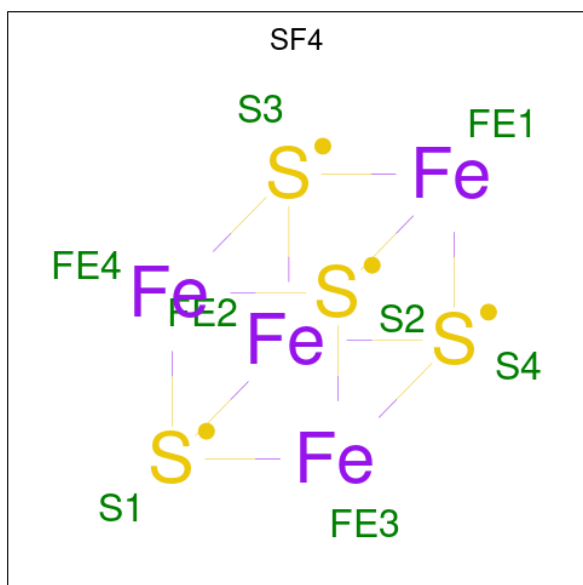
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	D	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	F	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	H	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	J	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	L	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	P	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

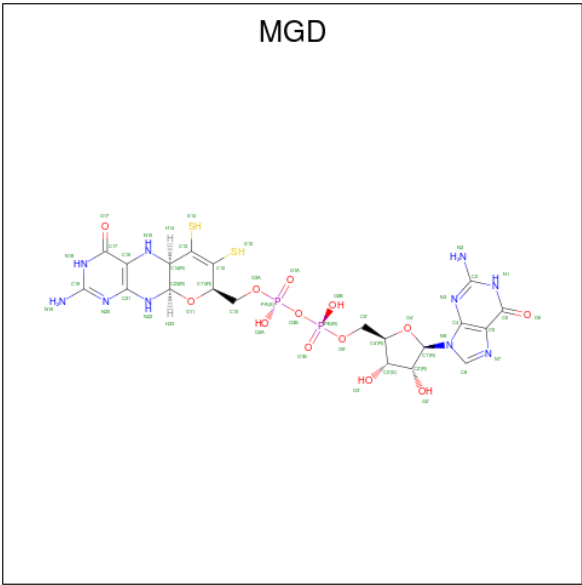


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0
4	G	1	Total Mo 1 1	0	0
4	I	1	Total Mo 1 1	0	0
4	K	1	Total Mo 1 1	0	0
4	M	1	Total Mo 1 1	0	0
4	O	1	Total Mo 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



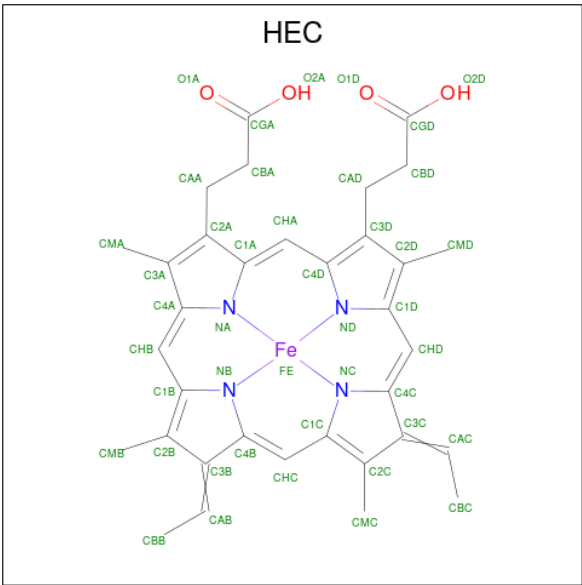
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 225.20Å 154.60Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-3.20) 97.0 (30.00-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.269 0.236 , 0.250	Depositor DCC
R_{free} test set	1348 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	59336	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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
6	HEC	D	1128	2	46,50,50	2.11	15 (32%)	58,82,82	1.93	9 (15%)
3	SF4	M	1801	1	0,12,12	-	-	-		
5	MGD	G	1803	4	47,52,52	2.20	18 (38%)	58,81,81	1.48	7 (12%)
6	HEC	P	1128	2	46,50,50	2.12	13 (28%)	58,82,82	1.72	9 (15%)
5	MGD	E	1803	4	47,52,52	1.84	14 (29%)	58,81,81	1.60	7 (12%)
5	MGD	I	1803	4	47,52,52	2.76	23 (48%)	58,81,81	1.59	9 (15%)
5	MGD	G	1804	4	47,52,52	2.24	19 (40%)	58,81,81	1.86	9 (15%)
5	MGD	M	1803	4	47,52,52	1.98	11 (23%)	58,81,81	1.50	9 (15%)
5	MGD	E	1804	4	47,52,52	2.14	15 (31%)	58,81,81	1.86	9 (15%)
6	HEC	J	1129	2	46,50,50	2.11	13 (28%)	58,82,82	1.87	12 (20%)
3	SF4	A	1801	1	0,12,12	-	-	-		
6	HEC	F	1128	2	46,50,50	2.01	15 (32%)	58,82,82	1.61	10 (17%)
6	HEC	B	1129	2	46,50,50	1.90	11 (23%)	58,82,82	1.55	7 (12%)
6	HEC	B	1128	2	46,50,50	2.08	13 (28%)	58,82,82	1.93	8 (13%)
6	HEC	H	1129	2	46,50,50	2.12	12 (26%)	58,82,82	1.70	9 (15%)
3	SF4	E	1801	1	0,12,12	-	-	-		
3	SF4	K	1801	1	0,12,12	-	-	-		
3	SF4	I	1801	1	0,12,12	-	-	-		
6	HEC	D	1129	2	46,50,50	2.01	13 (28%)	58,82,82	1.60	10 (17%)
5	MGD	C	1804	4	47,52,52	2.17	14 (29%)	58,81,81	1.90	8 (13%)
6	HEC	F	1129	2	46,50,50	2.05	11 (23%)	58,82,82	1.69	7 (12%)
3	SF4	G	1801	1	0,12,12	-	-	-		
3	SF4	C	1801	1	0,12,12	-	-	-		
5	MGD	I	1804	4	47,52,52	2.30	19 (40%)	58,81,81	1.76	8 (13%)
6	HEC	H	1128	2	46,50,50	1.84	13 (28%)	58,82,82	1.79	9 (15%)
6	HEC	J	1128	2	46,50,50	1.95	13 (28%)	58,82,82	1.91	9 (15%)
3	SF4	O	1801	1	0,12,12	-	-	-		
5	MGD	M	1804	4	47,52,52	2.10	14 (29%)	58,81,81	1.84	10 (17%)
5	MGD	C	1803	4	47,52,52	2.07	13 (27%)	58,81,81	1.50	7 (12%)
6	HEC	N	1128	2	46,50,50	1.89	11 (23%)	58,82,82	1.86	10 (17%)
6	HEC	L	1129	2	46,50,50	1.94	12 (26%)	58,82,82	1.76	10 (17%)
5	MGD	K	1804	4	47,52,52	1.98	13 (27%)	58,81,81	1.93	11 (18%)
5	MGD	K	1803	4	47,52,52	2.14	16 (34%)	58,81,81	1.56	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	A	1804	4	47,52,52	1.86	10 (21%)	58,81,81	1.82	7 (12%)
5	MGD	A	1803	4	47,52,52	2.31	16 (34%)	58,81,81	1.55	10 (17%)
5	MGD	O	1803	4	47,52,52	2.88	19 (40%)	58,81,81	1.57	9 (15%)
6	HEC	P	1129	2	46,50,50	2.07	10 (21%)	58,82,82	1.68	9 (15%)
5	MGD	O	1804	4	47,52,52	2.33	17 (36%)	58,81,81	1.95	8 (13%)
6	HEC	L	1128	2	46,50,50	1.93	11 (23%)	58,82,82	1.71	7 (12%)
6	HEC	N	1129	2	46,50,50	2.18	13 (28%)	58,82,82	1.68	8 (13%)

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
6	HEC	D	1128	2	-	4/14/54/54	-
3	SF4	M	1801	1	-	-	0/6/5/5
5	MGD	G	1803	4	-	5/22/66/66	0/6/6/6
6	HEC	P	1128	2	-	4/14/54/54	-
5	MGD	E	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	I	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	M	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	G	1804	4	-	6/22/66/66	0/6/6/6
5	MGD	E	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	J	1129	2	-	4/14/54/54	-
3	SF4	A	1801	1	-	-	0/6/5/5
6	HEC	F	1128	2	-	4/14/54/54	-
6	HEC	B	1129	2	-	4/14/54/54	-
6	HEC	B	1128	2	-	4/14/54/54	-
6	HEC	H	1129	2	-	4/14/54/54	-
3	SF4	E	1801	1	-	-	0/6/5/5
3	SF4	K	1801	1	-	-	0/6/5/5
3	SF4	I	1801	1	-	-	0/6/5/5
6	HEC	D	1129	2	-	4/14/54/54	-
5	MGD	C	1804	4	-	5/22/66/66	0/6/6/6
6	HEC	F	1129	2	-	4/14/54/54	-
3	SF4	G	1801	1	-	-	0/6/5/5
3	SF4	C	1801	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	I	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	H	1128	2	-	4/14/54/54	-
6	HEC	J	1128	2	-	3/14/54/54	-
3	SF4	O	1801	1	-	-	0/6/5/5
5	MGD	M	1804	4	-	6/22/66/66	0/6/6/6
5	MGD	C	1803	4	-	6/22/66/66	0/6/6/6
6	HEC	N	1128	2	-	4/14/54/54	-
6	HEC	L	1129	2	-	4/14/54/54	-
5	MGD	K	1804	4	-	5/22/66/66	0/6/6/6
5	MGD	K	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	A	1804	4	-	5/22/66/66	0/6/6/6
5	MGD	A	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	O	1803	4	-	5/22/66/66	0/6/6/6
6	HEC	P	1129	2	-	4/14/54/54	-
5	MGD	O	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	L	1128	2	-	4/14/54/54	-
6	HEC	N	1129	2	-	6/14/54/54	-

All (450) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1803	MGD	C23-C14	10.24	1.61	1.53
5	I	1803	MGD	C23-C14	8.28	1.60	1.53
5	E	1804	MGD	PB-O3B	7.04	1.67	1.59
5	O	1803	MGD	PB-O3B	6.70	1.66	1.59
6	N	1128	HEC	CAC-C3C	6.62	1.56	1.35
6	N	1129	HEC	CAC-C3C	6.58	1.56	1.35
5	K	1803	MGD	PB-O3B	6.52	1.66	1.59
5	I	1804	MGD	C14-N15	6.51	1.53	1.46
5	G	1804	MGD	PB-O3B	6.38	1.66	1.59
6	P	1129	HEC	CAC-C3C	6.36	1.55	1.35
5	M	1804	MGD	C14-N15	6.34	1.53	1.46
5	C	1804	MGD	C14-N15	6.33	1.53	1.46
6	D	1129	HEC	CAC-C3C	6.32	1.55	1.35
5	O	1803	MGD	C14-N15	6.29	1.53	1.46
5	A	1803	MGD	PB-O3B	6.23	1.66	1.59
5	G	1803	MGD	PB-O3B	6.21	1.66	1.59
5	C	1803	MGD	PB-O3B	6.13	1.66	1.59
6	J	1129	HEC	CAC-C3C	6.13	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1803	MGD	C21-N22	6.11	1.41	1.35
6	B	1129	HEC	CAC-C3C	6.09	1.54	1.35
5	A	1804	MGD	C14-N15	6.04	1.53	1.46
6	P	1128	HEC	CAC-C3C	6.04	1.54	1.35
6	D	1128	HEC	CAC-C3C	6.03	1.54	1.35
6	P	1128	HEC	CAB-C3B	6.00	1.54	1.35
6	F	1128	HEC	CAC-C3C	5.99	1.54	1.35
6	F	1129	HEC	CAC-C3C	5.93	1.54	1.35
6	L	1128	HEC	CAC-C3C	5.92	1.54	1.35
6	B	1128	HEC	CAC-C3C	5.84	1.54	1.35
6	P	1129	HEC	CAB-C3B	5.80	1.53	1.35
5	A	1803	MGD	C23-C14	5.78	1.58	1.53
6	H	1128	HEC	CAC-C3C	5.76	1.53	1.35
6	N	1129	HEC	C4D-C3D	5.73	1.56	1.44
6	H	1129	HEC	CAC-C3C	5.63	1.53	1.35
5	I	1803	MGD	C2'-C3'	5.63	1.68	1.53
6	J	1129	HEC	CAB-C3B	5.55	1.53	1.35
5	I	1803	MGD	C14-N15	5.55	1.52	1.46
5	G	1804	MGD	C14-N15	5.53	1.52	1.46
5	K	1804	MGD	C14-N15	5.44	1.52	1.46
5	O	1804	MGD	C21-N22	5.43	1.41	1.35
5	O	1804	MGD	C14-N15	5.39	1.52	1.46
6	F	1129	HEC	C4D-C3D	5.37	1.55	1.44
5	G	1803	MGD	C14-N15	5.35	1.52	1.46
6	L	1128	HEC	CAB-C3B	5.35	1.52	1.35
5	M	1804	MGD	C21-N22	5.30	1.41	1.35
6	B	1129	HEC	CAB-C3B	5.26	1.52	1.35
6	J	1128	HEC	CAB-C3B	5.25	1.52	1.35
6	L	1129	HEC	CAC-C3C	5.21	1.51	1.35
5	E	1804	MGD	C14-N15	5.14	1.52	1.46
5	I	1803	MGD	C21-N22	5.12	1.40	1.35
6	H	1129	HEC	C1D-C2D	4.97	1.54	1.43
6	N	1129	HEC	CAB-C3B	4.86	1.50	1.35
6	B	1128	HEC	C4D-C3D	4.86	1.54	1.44
6	H	1129	HEC	C4D-C3D	4.85	1.54	1.44
6	J	1128	HEC	CAC-C3C	4.84	1.50	1.35
5	C	1804	MGD	C21-N22	4.77	1.40	1.35
5	C	1803	MGD	C23-C14	4.74	1.57	1.53
6	F	1128	HEC	CAB-C3B	4.74	1.50	1.35
6	D	1128	HEC	C4D-C3D	4.73	1.54	1.44
5	K	1803	MGD	C21-N22	4.72	1.40	1.35
5	M	1803	MGD	C21-N22	4.69	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1129	HEC	CAB-C3B	4.65	1.50	1.35
6	J	1129	HEC	CMD-C2D	4.64	1.60	1.50
6	N	1129	HEC	C1D-C2D	4.63	1.54	1.43
6	D	1128	HEC	CAB-C3B	4.52	1.49	1.35
6	F	1129	HEC	CAB-C3B	4.48	1.49	1.35
5	M	1803	MGD	C23-C14	4.48	1.57	1.53
5	K	1803	MGD	C23-C14	4.47	1.57	1.53
5	C	1804	MGD	C21-N20	4.46	1.43	1.36
6	J	1129	HEC	C1D-C2D	4.44	1.53	1.43
6	H	1128	HEC	CAB-C3B	4.44	1.49	1.35
6	B	1128	HEC	CAB-C3B	4.43	1.49	1.35
6	B	1128	HEC	C1D-C2D	4.42	1.53	1.43
5	A	1803	MGD	PB-O2B	-4.42	1.34	1.55
5	M	1803	MGD	C14-N15	4.36	1.51	1.46
5	E	1804	MGD	C21-N22	4.34	1.40	1.35
5	I	1804	MGD	PB-O3B	4.34	1.64	1.59
6	N	1128	HEC	CAB-C3B	4.33	1.49	1.35
6	D	1129	HEC	CBD-CGD	4.32	1.60	1.50
6	J	1128	HEC	C4D-C3D	4.32	1.53	1.44
5	A	1803	MGD	C21-N22	4.29	1.40	1.35
5	I	1803	MGD	PA-O3B	4.26	1.64	1.59
5	O	1804	MGD	C23-C14	4.25	1.57	1.53
5	C	1804	MGD	PB-O3B	4.22	1.64	1.59
6	H	1129	HEC	CAB-C3B	4.21	1.48	1.35
5	K	1803	MGD	C14-N15	4.20	1.51	1.46
5	I	1803	MGD	PB-O3B	4.16	1.64	1.59
5	C	1803	MGD	C21-N22	4.15	1.39	1.35
6	B	1129	HEC	CMD-C2D	4.12	1.59	1.50
6	P	1128	HEC	C4D-C3D	4.10	1.52	1.44
5	O	1803	MGD	C16-C21	4.10	1.45	1.38
5	E	1803	MGD	C21-N22	4.09	1.39	1.35
6	F	1129	HEC	C1D-C2D	4.09	1.52	1.43
6	P	1129	HEC	CBD-CGD	4.06	1.60	1.50
5	O	1804	MGD	C16-N15	4.02	1.47	1.37
6	D	1128	HEC	C1D-C2D	4.01	1.52	1.43
5	G	1803	MGD	C23-C14	4.00	1.56	1.53
5	I	1804	MGD	C23-C14	4.00	1.56	1.53
5	O	1803	MGD	C16-N15	3.99	1.47	1.37
5	I	1804	MGD	C16-N15	3.98	1.47	1.37
5	A	1803	MGD	C21-N20	3.97	1.42	1.36
6	L	1129	HEC	CAB-C3B	3.96	1.47	1.35
5	I	1803	MGD	O4'-C1'	3.94	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1803	MGD	C21-N22	3.92	1.39	1.35
5	O	1804	MGD	C21-N20	3.89	1.42	1.36
6	P	1128	HEC	C1C-NC	-3.87	1.32	1.39
6	J	1128	HEC	C1D-C2D	3.86	1.52	1.43
5	M	1804	MGD	PB-O3B	3.84	1.63	1.59
5	C	1804	MGD	C16-C21	3.84	1.45	1.38
5	I	1803	MGD	C16-N15	3.83	1.46	1.37
5	K	1804	MGD	C21-N22	3.81	1.39	1.35
6	F	1128	HEC	C4D-C3D	3.81	1.52	1.44
6	L	1129	HEC	CBD-CGD	3.80	1.59	1.50
6	F	1128	HEC	C1C-NC	-3.80	1.32	1.39
6	J	1129	HEC	CBD-CGD	3.77	1.59	1.50
5	O	1804	MGD	C2'-C3'	3.77	1.63	1.53
5	K	1803	MGD	C2'-C3'	3.77	1.63	1.53
5	M	1804	MGD	C16-N15	3.76	1.46	1.37
5	I	1803	MGD	C17-N18	3.75	1.45	1.38
5	G	1804	MGD	C16-N15	3.74	1.46	1.37
5	O	1804	MGD	PB-O3B	3.73	1.63	1.59
5	I	1804	MGD	C2'-C3'	3.73	1.63	1.53
5	C	1803	MGD	C14-N15	3.72	1.50	1.46
6	P	1129	HEC	C4D-C3D	3.69	1.52	1.44
5	K	1804	MGD	C16-N15	3.68	1.46	1.37
5	C	1803	MGD	C16-N15	3.67	1.46	1.37
5	E	1804	MGD	C23-C14	3.66	1.56	1.53
5	M	1803	MGD	C16-N15	3.65	1.46	1.37
6	H	1129	HEC	CBD-CGD	3.63	1.59	1.50
6	P	1129	HEC	C1D-C2D	3.62	1.51	1.43
5	G	1803	MGD	C16-N15	3.62	1.46	1.37
5	C	1804	MGD	C16-N15	3.61	1.46	1.37
6	N	1128	HEC	CMD-C2D	3.59	1.58	1.50
5	A	1804	MGD	C21-N22	3.58	1.39	1.35
5	A	1803	MGD	C17-N18	3.58	1.45	1.38
6	L	1129	HEC	CMD-C2D	3.55	1.58	1.50
6	L	1129	HEC	C4D-C3D	3.54	1.51	1.44
5	E	1803	MGD	C21-N20	3.54	1.41	1.36
5	M	1804	MGD	C23-C14	3.51	1.56	1.53
5	E	1803	MGD	C23-C14	3.51	1.56	1.53
5	G	1804	MGD	C17-N18	3.50	1.45	1.38
5	K	1804	MGD	C21-N20	3.49	1.41	1.36
5	O	1803	MGD	C2'-C3'	3.49	1.62	1.53
6	P	1129	HEC	CMD-C2D	3.48	1.57	1.50
6	L	1129	HEC	C1D-C2D	3.48	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1129	HEC	CBD-CGD	3.47	1.58	1.50
5	A	1803	MGD	C14-N15	3.46	1.50	1.46
6	D	1129	HEC	C4D-C3D	3.46	1.51	1.44
5	I	1804	MGD	C16-C21	3.46	1.44	1.38
5	E	1804	MGD	C16-N15	3.45	1.45	1.37
6	D	1128	HEC	C1C-NC	-3.45	1.33	1.39
5	M	1804	MGD	C2'-C3'	3.44	1.62	1.53
5	O	1804	MGD	C16-C21	3.44	1.44	1.38
5	M	1803	MGD	PB-O3B	3.43	1.63	1.59
5	G	1804	MGD	C21-N20	3.43	1.41	1.36
5	K	1804	MGD	C6-N1	3.43	1.45	1.38
5	G	1803	MGD	C2'-C3'	3.41	1.62	1.53
5	E	1803	MGD	C16-N15	3.39	1.45	1.37
6	D	1129	HEC	CMD-C2D	3.39	1.57	1.50
5	A	1804	MGD	C16-N15	3.39	1.45	1.37
5	G	1803	MGD	PB-O2B	-3.39	1.39	1.55
5	A	1804	MGD	C2'-C3'	3.39	1.62	1.53
5	G	1804	MGD	C21-N22	3.39	1.39	1.35
5	M	1803	MGD	C2'-C3'	3.38	1.62	1.53
6	B	1129	HEC	C1D-C2D	3.36	1.51	1.43
5	A	1803	MGD	PB-O1B	-3.36	1.39	1.50
5	O	1803	MGD	PA-O3B	3.34	1.63	1.59
6	H	1129	HEC	CMD-C2D	3.32	1.57	1.50
5	I	1804	MGD	C2-N2	3.31	1.41	1.34
5	K	1804	MGD	PA-O3B	-3.30	1.55	1.59
5	O	1804	MGD	C5-N7	3.30	1.45	1.39
5	C	1804	MGD	C2'-C3'	3.29	1.62	1.53
5	E	1803	MGD	C2'-C3'	3.27	1.62	1.53
6	B	1128	HEC	CMD-C2D	3.26	1.57	1.50
5	M	1803	MGD	C21-N20	3.24	1.41	1.36
5	M	1803	MGD	PB-O2B	-3.24	1.40	1.55
6	N	1129	HEC	C3B-C2B	-3.24	1.30	1.41
6	H	1129	HEC	C1C-NC	-3.22	1.33	1.39
6	H	1128	HEC	C4D-C3D	3.22	1.51	1.44
5	K	1803	MGD	C16-N15	3.21	1.45	1.37
5	O	1803	MGD	C23-N22	3.21	1.50	1.45
5	I	1804	MGD	C17-N18	3.21	1.44	1.38
6	N	1129	HEC	CMD-C2D	3.20	1.57	1.50
6	J	1128	HEC	CHB-C1B	-3.19	1.32	1.39
6	H	1129	HEC	C3B-C2B	-3.16	1.30	1.41
5	C	1803	MGD	C21-N20	3.16	1.41	1.36
5	M	1804	MGD	C21-N20	3.16	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1803	MGD	PB-O2B	-3.14	1.40	1.55
5	C	1804	MGD	PA-O3B	3.14	1.62	1.59
5	E	1803	MGD	PB-O2B	-3.14	1.40	1.55
5	O	1804	MGD	C17-N18	3.13	1.44	1.38
5	K	1803	MGD	C17-N18	3.13	1.44	1.38
6	H	1128	HEC	C1D-C2D	3.13	1.50	1.43
5	K	1803	MGD	C21-N20	3.12	1.41	1.36
5	I	1804	MGD	C21-N22	3.12	1.38	1.35
5	I	1804	MGD	C21-N20	3.07	1.40	1.36
5	I	1804	MGD	C10-C11	3.07	1.56	1.51
6	L	1128	HEC	C1C-NC	-3.06	1.33	1.39
5	A	1804	MGD	PB-O2B	-3.05	1.41	1.55
5	K	1804	MGD	C3'-C4'	3.04	1.60	1.53
5	E	1803	MGD	PB-O1B	-3.03	1.40	1.50
5	I	1803	MGD	C23-N22	3.03	1.50	1.45
5	A	1803	MGD	C16-N15	3.02	1.45	1.37
6	L	1128	HEC	C4D-C3D	3.02	1.50	1.44
6	P	1128	HEC	CMD-C2D	3.02	1.57	1.50
6	N	1128	HEC	C2A-C3A	-3.01	1.30	1.36
6	F	1129	HEC	CMD-C2D	3.00	1.56	1.50
5	I	1803	MGD	C16-C21	2.98	1.43	1.38
5	K	1804	MGD	C17-N18	2.97	1.44	1.38
6	N	1128	HEC	C3B-C2B	-2.97	1.31	1.41
6	N	1128	HEC	C1C-NC	-2.97	1.34	1.39
6	B	1128	HEC	C3B-C2B	-2.97	1.31	1.41
5	G	1804	MGD	C6-N1	2.95	1.44	1.38
5	G	1804	MGD	C4-N3	2.95	1.41	1.34
6	D	1129	HEC	C1C-NC	-2.94	1.34	1.39
5	C	1803	MGD	C6-N1	2.94	1.44	1.38
6	F	1128	HEC	C3D-C2D	-2.94	1.31	1.38
6	D	1128	HEC	C3D-C2D	-2.93	1.31	1.38
6	J	1128	HEC	C3B-C2B	-2.93	1.31	1.41
6	F	1128	HEC	C1D-C2D	2.92	1.50	1.43
5	O	1803	MGD	C21-N20	2.92	1.40	1.36
5	G	1804	MGD	C2'-C3'	2.91	1.61	1.53
6	J	1129	HEC	CBB-CAB	2.90	1.60	1.49
5	A	1804	MGD	C23-C14	2.89	1.55	1.53
6	N	1129	HEC	C1C-NC	-2.88	1.34	1.39
5	E	1803	MGD	C17-N18	2.86	1.44	1.38
6	P	1129	HEC	C1A-C2A	-2.86	1.40	1.45
5	I	1804	MGD	C3'-C4'	2.85	1.60	1.53
5	O	1804	MGD	C4-N3	2.85	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1128	HEC	C3C-C2C	-2.85	1.31	1.41
5	A	1803	MGD	O17-C17	2.85	1.29	1.23
6	D	1128	HEC	O2D-CGD	-2.82	1.21	1.30
6	N	1129	HEC	CBD-CGD	2.81	1.57	1.50
5	A	1804	MGD	C21-N20	2.81	1.40	1.36
5	K	1803	MGD	C1'-N9	-2.80	1.39	1.47
6	H	1128	HEC	CHB-C1B	-2.79	1.33	1.39
6	F	1128	HEC	C1A-NA	-2.79	1.34	1.39
5	C	1804	MGD	C17-N18	2.78	1.44	1.38
5	I	1804	MGD	C6-N1	2.77	1.44	1.38
5	O	1803	MGD	O11-C11	2.77	1.48	1.43
5	A	1804	MGD	C16-C21	2.77	1.43	1.38
6	L	1129	HEC	C1C-NC	-2.77	1.34	1.39
5	O	1803	MGD	C4-N3	2.76	1.40	1.34
5	I	1803	MGD	C1'-N9	-2.76	1.39	1.47
6	F	1129	HEC	C1C-NC	-2.75	1.34	1.39
5	G	1804	MGD	O4'-C4'	-2.75	1.38	1.45
5	O	1803	MGD	PB-O2B	-2.74	1.42	1.55
5	M	1804	MGD	C3'-C4'	2.74	1.59	1.53
5	E	1803	MGD	O4'-C1'	2.74	1.48	1.42
5	O	1804	MGD	C6-N1	2.74	1.44	1.38
6	P	1128	HEC	C1D-C2D	2.73	1.49	1.43
5	G	1804	MGD	C5-N7	2.73	1.44	1.39
5	E	1804	MGD	C21-N20	2.73	1.40	1.36
6	L	1128	HEC	C3D-C2D	-2.72	1.31	1.38
6	B	1129	HEC	C3B-C2B	-2.72	1.32	1.41
5	O	1804	MGD	C3'-C4'	2.72	1.59	1.53
6	D	1129	HEC	C1D-C2D	2.71	1.49	1.43
6	J	1129	HEC	C4D-C3D	2.71	1.50	1.44
5	I	1803	MGD	C4-N3	2.71	1.40	1.34
6	B	1129	HEC	CBD-CGD	2.70	1.56	1.50
5	E	1804	MGD	C6-N1	2.69	1.43	1.38
5	E	1804	MGD	C17-N18	2.69	1.43	1.38
6	L	1128	HEC	CHB-C1B	-2.69	1.33	1.39
5	O	1803	MGD	O2'-C2'	2.68	1.49	1.43
5	G	1803	MGD	PA-O3B	2.68	1.62	1.59
6	L	1129	HEC	C3B-C2B	-2.68	1.32	1.41
6	B	1128	HEC	O2D-CGD	-2.67	1.22	1.30
5	O	1803	MGD	C2-N1	2.67	1.44	1.37
5	A	1803	MGD	O11-C23	-2.67	1.39	1.43
6	N	1128	HEC	C1D-C2D	2.66	1.49	1.43
6	H	1128	HEC	C3B-C2B	-2.66	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1128	HEC	C1C-NC	-2.66	1.34	1.39
6	D	1129	HEC	C3B-C2B	-2.65	1.32	1.41
5	I	1803	MGD	PB-O2B	-2.65	1.43	1.55
5	G	1804	MGD	C3'-C4'	2.65	1.59	1.53
5	E	1804	MGD	C2'-C3'	2.65	1.60	1.53
6	L	1128	HEC	C4D-ND	-2.65	1.34	1.39
5	I	1804	MGD	C4-N3	2.65	1.40	1.34
5	I	1803	MGD	C21-N20	2.64	1.40	1.36
5	O	1803	MGD	C6-N1	2.64	1.43	1.38
5	I	1803	MGD	O2'-C2'	2.64	1.49	1.43
5	G	1803	MGD	O11-C11	2.63	1.48	1.43
5	E	1803	MGD	C1'-N9	-2.63	1.40	1.47
5	I	1803	MGD	O11-C11	2.61	1.48	1.43
5	A	1803	MGD	C2-N2	2.60	1.40	1.34
5	G	1804	MGD	C16-C21	2.59	1.43	1.38
5	M	1804	MGD	C4-N3	2.59	1.40	1.34
5	G	1803	MGD	C2-N2	2.59	1.40	1.34
6	H	1128	HEC	C3C-C2C	-2.59	1.32	1.41
6	F	1128	HEC	C4D-ND	-2.59	1.34	1.39
6	F	1129	HEC	C3D-C2D	-2.58	1.32	1.38
5	I	1803	MGD	O17-C17	2.58	1.28	1.23
6	J	1128	HEC	C3B-C4B	2.58	1.50	1.46
5	A	1803	MGD	C2'-C3'	2.57	1.60	1.53
6	D	1128	HEC	CHD-C1D	-2.57	1.33	1.39
5	K	1803	MGD	PA-O3B	2.56	1.62	1.59
6	D	1128	HEC	CMD-C2D	2.56	1.56	1.50
6	B	1128	HEC	C1A-NA	-2.55	1.34	1.39
5	M	1804	MGD	C17-N18	2.54	1.43	1.38
5	C	1803	MGD	C4-N3	2.54	1.40	1.34
6	P	1128	HEC	CHD-C1D	-2.54	1.33	1.39
5	G	1803	MGD	C4-N3	2.54	1.40	1.34
6	D	1128	HEC	C3B-C2B	-2.53	1.32	1.41
5	A	1803	MGD	O11-C11	2.53	1.48	1.43
6	F	1128	HEC	C3B-C2B	-2.53	1.32	1.41
5	G	1803	MGD	C6-N1	2.52	1.43	1.38
6	H	1128	HEC	CMD-C2D	2.51	1.55	1.50
5	O	1803	MGD	C17-N18	2.50	1.43	1.38
6	D	1129	HEC	CHD-C1D	-2.49	1.33	1.39
5	I	1803	MGD	C2-N2	2.49	1.40	1.34
5	O	1804	MGD	C10-C11	2.49	1.55	1.51
5	G	1803	MGD	C17-N18	2.49	1.43	1.38
5	C	1804	MGD	C5-N7	2.48	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1128	HEC	CMD-C2D	2.48	1.55	1.50
5	K	1803	MGD	PB-O2B	-2.47	1.43	1.55
5	G	1803	MGD	C21-N20	2.47	1.40	1.36
6	P	1129	HEC	CBB-CAB	2.47	1.58	1.49
5	K	1804	MGD	C4-N3	2.47	1.39	1.34
5	C	1803	MGD	C2'-C3'	2.47	1.60	1.53
5	M	1803	MGD	C17-N18	2.46	1.43	1.38
5	E	1804	MGD	PB-O2B	-2.46	1.43	1.55
5	O	1804	MGD	C2-N2	2.46	1.39	1.34
5	K	1804	MGD	C2'-C3'	2.46	1.60	1.53
5	E	1804	MGD	C1'-N9	-2.44	1.40	1.47
6	B	1129	HEC	CHA-C1A	2.44	1.43	1.38
5	E	1803	MGD	C14-N15	2.44	1.49	1.46
6	L	1128	HEC	CBB-CAB	2.44	1.58	1.49
6	D	1128	HEC	C1A-NA	-2.43	1.35	1.39
6	L	1128	HEC	C1D-C2D	2.42	1.48	1.43
6	N	1128	HEC	C4B-NB	-2.42	1.35	1.39
5	O	1803	MGD	C2-N2	2.41	1.39	1.34
6	N	1129	HEC	C3D-C2D	-2.41	1.32	1.38
5	I	1804	MGD	C2-N1	2.40	1.43	1.37
6	L	1128	HEC	C3B-C2B	-2.40	1.33	1.41
6	H	1128	HEC	CBD-CGD	2.40	1.56	1.50
6	D	1129	HEC	C1A-C2A	-2.40	1.41	1.45
5	G	1803	MGD	O6-C6	2.39	1.28	1.23
6	J	1128	HEC	C3D-C2D	-2.39	1.32	1.38
6	L	1129	HEC	C1A-C2A	-2.38	1.41	1.45
5	M	1804	MGD	PA-O3B	-2.38	1.56	1.59
5	E	1804	MGD	C4-N3	2.38	1.39	1.34
6	F	1128	HEC	C2A-C3A	-2.38	1.31	1.36
5	I	1804	MGD	O2'-C2'	2.37	1.48	1.43
5	C	1804	MGD	PB-O2B	-2.36	1.44	1.55
6	D	1128	HEC	CBB-CAB	2.36	1.58	1.49
6	D	1128	HEC	CHB-C1B	-2.35	1.34	1.39
6	N	1128	HEC	CBB-CAB	2.35	1.58	1.49
6	B	1129	HEC	C4D-C3D	2.35	1.49	1.44
6	J	1128	HEC	CBB-CAB	2.34	1.58	1.49
6	F	1128	HEC	CBD-CGD	2.33	1.56	1.50
6	J	1128	HEC	C3C-C2C	-2.33	1.33	1.41
5	K	1803	MGD	O17-C17	2.32	1.28	1.23
5	K	1804	MGD	PB-O2B	-2.32	1.44	1.55
5	G	1804	MGD	C23-C14	2.32	1.55	1.53
6	P	1128	HEC	C3B-C4B	2.31	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1128	HEC	CBB-CAB	2.31	1.58	1.49
6	J	1129	HEC	C1C-NC	-2.31	1.35	1.39
6	J	1128	HEC	C1C-NC	-2.29	1.35	1.39
5	M	1804	MGD	C16-C21	2.29	1.42	1.38
6	P	1129	HEC	CBD-CAD	2.28	1.59	1.51
5	C	1803	MGD	C17-N18	2.27	1.43	1.38
6	F	1129	HEC	C3B-C2B	-2.27	1.33	1.41
5	I	1803	MGD	O6-C6	2.26	1.27	1.23
5	G	1804	MGD	O17-C17	2.26	1.27	1.23
5	M	1804	MGD	C6-N1	2.26	1.43	1.38
6	L	1129	HEC	C3C-C2C	-2.26	1.33	1.41
5	I	1803	MGD	C2-N1	2.26	1.43	1.37
6	P	1128	HEC	CMB-C2B	2.25	1.55	1.50
5	K	1804	MGD	C16-C21	2.25	1.42	1.38
6	F	1128	HEC	CHB-C1B	-2.25	1.34	1.39
6	P	1128	HEC	CBB-CAB	2.25	1.57	1.49
6	D	1128	HEC	C3C-C2C	-2.25	1.33	1.41
5	C	1804	MGD	C1'-N9	-2.25	1.41	1.47
6	B	1129	HEC	C2A-C3A	-2.24	1.31	1.36
6	P	1128	HEC	C3D-C2D	-2.24	1.33	1.38
5	G	1803	MGD	O17-C17	2.23	1.27	1.23
5	A	1803	MGD	C1'-N9	-2.23	1.41	1.47
5	M	1803	MGD	C2-N2	2.23	1.39	1.34
6	D	1129	HEC	C3C-C2C	-2.23	1.33	1.41
6	H	1129	HEC	C3C-C4C	-2.23	1.42	1.46
6	J	1129	HEC	CHB-C1B	-2.22	1.34	1.39
5	G	1804	MGD	C8-N9	2.22	1.42	1.37
6	N	1129	HEC	CHB-C1B	-2.22	1.34	1.39
6	P	1129	HEC	C1C-NC	-2.22	1.35	1.39
6	P	1128	HEC	C2A-C3A	-2.22	1.32	1.36
5	E	1803	MGD	O11-C23	-2.20	1.40	1.43
5	C	1803	MGD	O11-C11	2.20	1.47	1.43
6	J	1128	HEC	O2D-CGD	-2.19	1.23	1.30
5	I	1804	MGD	C8-N9	2.19	1.42	1.37
5	E	1803	MGD	O17-C17	2.19	1.27	1.23
6	F	1129	HEC	C1A-C2A	-2.19	1.41	1.45
6	J	1129	HEC	CBD-CAD	2.19	1.59	1.51
6	L	1129	HEC	CHD-C1D	-2.19	1.34	1.39
5	E	1804	MGD	C10-C11	2.19	1.54	1.51
5	K	1803	MGD	C2-N2	2.18	1.39	1.34
5	I	1804	MGD	O11-C11	2.18	1.47	1.43
5	C	1803	MGD	C2-N2	2.18	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1128	HEC	CBB-CAB	2.18	1.57	1.49
5	K	1803	MGD	C4-N3	2.17	1.39	1.34
6	F	1128	HEC	C4A-NA	-2.17	1.35	1.39
5	A	1804	MGD	C6-N1	2.17	1.42	1.38
6	B	1128	HEC	CHB-C1B	-2.17	1.34	1.39
5	A	1804	MGD	O3A-C10	2.17	1.52	1.44
6	H	1128	HEC	C3C-C4C	2.17	1.49	1.46
6	H	1128	HEC	CBD-CAD	2.16	1.59	1.51
6	J	1128	HEC	CMD-C2D	2.15	1.55	1.50
6	B	1128	HEC	C3D-C2D	-2.15	1.33	1.38
6	H	1129	HEC	CBB-CAB	2.15	1.57	1.49
6	N	1128	HEC	C4D-C3D	2.15	1.48	1.44
6	D	1129	HEC	CBD-CAD	2.14	1.59	1.51
5	G	1803	MGD	C2-N1	2.14	1.42	1.37
5	G	1804	MGD	C1'-N9	-2.14	1.41	1.47
5	A	1803	MGD	PB-O5'	-2.14	1.51	1.59
5	E	1803	MGD	C6-N1	2.14	1.42	1.38
6	H	1129	HEC	CHB-C4A	-2.14	1.34	1.38
5	M	1804	MGD	PB-O2B	-2.14	1.45	1.55
5	K	1803	MGD	O2'-C2'	2.14	1.48	1.43
5	O	1804	MGD	PB-O2B	-2.13	1.45	1.55
5	E	1804	MGD	C16-C21	2.13	1.42	1.38
6	J	1129	HEC	C3B-C2B	-2.13	1.34	1.41
5	E	1804	MGD	C3'-C4'	2.13	1.58	1.53
5	O	1804	MGD	O3A-C10	2.11	1.52	1.44
5	G	1804	MGD	O3A-C10	2.11	1.52	1.44
6	D	1128	HEC	C4D-ND	-2.10	1.35	1.39
5	I	1803	MGD	C19-N18	2.10	1.42	1.37
6	J	1129	HEC	C1B-NB	2.10	1.43	1.39
6	D	1129	HEC	CHB-C1B	-2.09	1.34	1.39
5	C	1804	MGD	O4'-C4'	-2.09	1.40	1.45
5	O	1803	MGD	C1'-N9	-2.08	1.41	1.47
6	B	1129	HEC	CBB-CAB	2.08	1.57	1.49
5	M	1803	MGD	C1'-N9	-2.08	1.41	1.47
5	G	1804	MGD	C10-C11	2.07	1.54	1.51
6	F	1128	HEC	C3C-C2C	-2.07	1.34	1.41
6	P	1128	HEC	CBD-CAD	2.07	1.59	1.51
5	K	1803	MGD	C23-N22	2.07	1.48	1.45
6	N	1129	HEC	O2D-CGD	-2.06	1.24	1.30
6	N	1129	HEC	CBC-CAC	2.06	1.57	1.49
6	B	1128	HEC	CAA-C2A	2.06	1.56	1.51
5	G	1803	MGD	C1'-N9	-2.06	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1128	HEC	C3C-C4C	2.05	1.49	1.46
6	L	1129	HEC	CBD-CAD	2.05	1.59	1.51
6	B	1129	HEC	C3D-C2D	-2.05	1.33	1.38
6	F	1129	HEC	C2A-C3A	-2.05	1.32	1.36
6	N	1129	HEC	CBB-CAB	2.05	1.57	1.49
6	H	1129	HEC	CBD-CAD	2.05	1.59	1.51
5	K	1804	MGD	O3A-C10	2.04	1.52	1.44
5	I	1804	MGD	O17-C17	2.04	1.27	1.23
5	C	1804	MGD	O3A-C10	2.04	1.52	1.44
5	I	1803	MGD	C19-N19	2.03	1.38	1.34
6	F	1128	HEC	CBD-CAD	2.03	1.59	1.51
6	J	1129	HEC	C3C-C2C	-2.01	1.34	1.41

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1804	MGD	O11-C23-N22	-9.72	99.79	108.61
5	O	1804	MGD	O11-C23-N22	-9.49	100.00	108.61
5	K	1804	MGD	O11-C23-N22	-9.42	100.06	108.61
5	A	1804	MGD	O11-C23-N22	-9.23	100.23	108.61
5	E	1804	MGD	O11-C23-N22	-9.04	100.40	108.61
5	M	1804	MGD	O11-C23-N22	-8.97	100.46	108.61
5	G	1804	MGD	O11-C23-N22	-8.49	100.90	108.61
5	I	1804	MGD	O11-C23-N22	-8.35	101.03	108.61
6	N	1128	HEC	CBB-CAB-C3B	-8.20	111.05	127.43
6	L	1128	HEC	CBB-CAB-C3B	-8.05	111.34	127.43
6	D	1128	HEC	CBC-CAC-C3C	-7.93	111.58	127.43
6	J	1128	HEC	CBC-CAC-C3C	-7.73	111.98	127.43
6	H	1129	HEC	CBB-CAB-C3B	-7.56	112.33	127.43
6	J	1128	HEC	CBB-CAB-C3B	-7.54	112.36	127.43
6	B	1128	HEC	CBC-CAC-C3C	-7.40	112.64	127.43
6	B	1128	HEC	CBB-CAB-C3B	-7.34	112.77	127.43
6	J	1129	HEC	CBB-CAB-C3B	-7.21	113.02	127.43
6	P	1128	HEC	CBC-CAC-C3C	-7.13	113.18	127.43
6	H	1128	HEC	CBB-CAB-C3B	-7.02	113.40	127.43
6	F	1129	HEC	CBB-CAB-C3B	-7.01	113.41	127.43
6	N	1129	HEC	CBB-CAB-C3B	-6.56	114.32	127.43
6	D	1128	HEC	CBB-CAB-C3B	-6.52	114.40	127.43
5	G	1804	MGD	O11-C23-C14	-6.46	104.65	108.96
6	F	1128	HEC	CBB-CAB-C3B	-6.40	114.65	127.43
6	L	1129	HEC	CBB-CAB-C3B	-6.34	114.77	127.43
6	P	1128	HEC	CBB-CAB-C3B	-6.14	115.15	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1129	HEC	CBC-CAC-C3C	-6.12	115.20	127.43
5	K	1804	MGD	O11-C23-C14	-6.00	104.97	108.96
6	B	1129	HEC	CBB-CAB-C3B	-5.97	115.50	127.43
6	P	1129	HEC	CBB-CAB-C3B	-5.97	115.50	127.43
6	L	1129	HEC	CBC-CAC-C3C	-5.93	115.59	127.43
6	D	1129	HEC	CBB-CAB-C3B	-5.89	115.67	127.43
5	O	1804	MGD	O11-C23-C14	-5.79	105.10	108.96
6	B	1129	HEC	CBC-CAC-C3C	-5.67	116.10	127.43
6	F	1129	HEC	CBC-CAC-C3C	-5.57	116.29	127.43
5	C	1804	MGD	O11-C23-C14	-5.36	105.39	108.96
5	I	1804	MGD	O11-C23-C14	-5.33	105.41	108.96
5	M	1804	MGD	O11-C23-C14	-5.29	105.43	108.96
6	D	1129	HEC	CBC-CAC-C3C	-5.21	117.01	127.43
6	P	1129	HEC	CBC-CAC-C3C	-5.21	117.02	127.43
5	K	1803	MGD	O4'-C1'-N9	-5.18	96.62	108.36
5	O	1803	MGD	C23-C14-N15	5.05	112.83	107.87
6	H	1128	HEC	CBC-CAC-C3C	-5.05	117.35	127.43
6	N	1129	HEC	CBC-CAC-C3C	-5.00	117.43	127.43
5	E	1803	MGD	O4'-C1'-N9	-4.96	97.12	108.36
5	A	1803	MGD	O4'-C1'-N9	-4.96	97.13	108.36
6	D	1128	HEC	CBD-CAD-C3D	-4.93	98.91	112.53
6	H	1129	HEC	CBC-CAC-C3C	-4.93	117.59	127.43
6	N	1128	HEC	CBC-CAC-C3C	-4.86	117.72	127.43
5	C	1803	MGD	O4'-C1'-N9	-4.78	97.52	108.36
5	E	1804	MGD	O11-C23-C14	-4.78	105.77	108.96
5	G	1803	MGD	O4'-C1'-N9	-4.78	97.53	108.36
5	E	1803	MGD	O11-C23-C14	4.73	112.12	108.96
5	I	1803	MGD	O4'-C1'-N9	-4.70	97.71	108.36
5	O	1803	MGD	O4'-C1'-N9	-4.63	97.87	108.36
5	M	1803	MGD	O4'-C1'-N9	-4.59	97.96	108.36
6	B	1128	HEC	CBD-CAD-C3D	-4.53	100.01	112.53
5	E	1803	MGD	C23-C14-N15	4.50	112.29	107.87
5	A	1804	MGD	O11-C23-C14	-4.40	106.03	108.96
6	L	1129	HEC	C1D-C2D-C3D	4.30	111.74	106.82
6	D	1129	HEC	CMD-C2D-C1D	-4.19	119.04	125.42
6	N	1129	HEC	C1D-C2D-C3D	4.13	111.55	106.82
6	J	1129	HEC	CMD-C2D-C1D	-4.13	119.14	125.42
6	J	1128	HEC	CBD-CAD-C3D	-4.11	101.18	112.53
6	L	1128	HEC	CBC-CAC-C3C	-4.11	119.23	127.43
6	N	1128	HEC	CMD-C2D-C1D	-4.07	119.22	125.42
5	A	1803	MGD	C23-C14-N15	4.05	111.84	107.87
5	K	1803	MGD	C23-C14-N15	4.03	111.82	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1803	MGD	C23-C14-N15	4.02	111.81	107.87
6	J	1128	HEC	C1D-C2D-C3D	3.97	111.36	106.82
6	N	1128	HEC	CBD-CAD-C3D	-3.91	101.71	112.53
6	F	1129	HEC	C1D-C2D-C3D	3.90	111.28	106.82
5	M	1803	MGD	C23-C14-N15	3.86	111.66	107.87
5	M	1803	MGD	O4'-C1'-C2'	-3.85	98.38	106.62
5	I	1803	MGD	C2'-C1'-N9	3.84	123.94	113.25
6	F	1128	HEC	CBC-CAC-C3C	-3.77	119.90	127.43
6	H	1128	HEC	C1D-C2D-C3D	3.75	111.11	106.82
5	C	1803	MGD	C23-C14-N15	3.74	111.54	107.87
6	F	1128	HEC	CBD-CAD-C3D	-3.73	102.23	112.53
6	F	1128	HEC	C1D-C2D-C3D	3.71	111.07	106.82
5	G	1803	MGD	C23-C14-N15	3.71	111.51	107.87
5	E	1803	MGD	O4'-C1'-C2'	-3.70	98.69	106.62
5	A	1803	MGD	C2'-C1'-N9	3.70	123.53	113.25
5	G	1803	MGD	C2'-C1'-N9	3.69	123.53	113.25
5	K	1803	MGD	C2'-C1'-N9	3.67	123.45	113.25
6	D	1129	HEC	C1D-C2D-C3D	3.64	110.98	106.82
6	H	1128	HEC	CMD-C2D-C1D	-3.64	119.88	125.42
6	F	1129	HEC	CAD-C3D-C4D	3.59	131.95	124.94
6	N	1129	HEC	CAD-C3D-C4D	3.58	131.93	124.94
6	P	1129	HEC	CMD-C2D-C1D	-3.58	119.97	125.42
5	M	1803	MGD	C2'-C1'-N9	3.55	123.13	113.25
5	A	1804	MGD	O4'-C1'-C2'	-3.54	99.04	106.62
6	H	1129	HEC	C1D-C2D-C3D	3.53	110.86	106.82
6	P	1129	HEC	C1D-C2D-C3D	3.53	110.86	106.82
5	C	1803	MGD	C2'-C1'-N9	3.50	122.98	113.25
5	C	1803	MGD	O11-C23-C14	3.49	111.29	108.96
5	O	1804	MGD	C23-C14-N15	3.49	111.29	107.87
5	A	1803	MGD	O11-C23-C14	3.48	111.29	108.96
5	E	1803	MGD	C2'-C1'-N9	3.48	122.93	113.25
6	L	1129	HEC	CMD-C2D-C1D	-3.46	120.16	125.42
6	J	1129	HEC	CBA-CAA-C2A	-3.43	103.04	112.53
6	B	1128	HEC	C1D-C2D-C3D	3.38	110.69	106.82
6	B	1129	HEC	C1D-C2D-C3D	3.37	110.68	106.82
6	D	1128	HEC	C1D-C2D-C3D	3.37	110.67	106.82
5	O	1803	MGD	C2'-C1'-N9	3.36	122.59	113.25
6	L	1128	HEC	C1D-C2D-C3D	3.36	110.66	106.82
6	P	1128	HEC	CMD-C2D-C1D	-3.34	120.33	125.42
5	E	1804	MGD	C23-C14-N15	3.29	111.10	107.87
6	P	1129	HEC	CBD-CAD-C3D	3.25	121.52	112.53
5	G	1804	MGD	O5'-C5'-C4'	-3.22	98.04	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1129	HEC	CBD-CAD-C3D	3.21	121.41	112.53
6	L	1128	HEC	CMD-C2D-C1D	-3.19	120.57	125.42
6	P	1129	HEC	C2A-C1A-NA	3.18	113.39	110.32
6	B	1129	HEC	CMD-C2D-C1D	-3.12	120.66	125.42
6	J	1129	HEC	C1D-C2D-C3D	3.11	110.38	106.82
5	I	1804	MGD	O5'-C5'-C4'	-3.11	98.40	108.99
6	H	1129	HEC	CMD-C2D-C1D	-3.09	120.71	125.42
6	J	1128	HEC	CMD-C2D-C1D	-3.07	120.75	125.42
6	L	1129	HEC	CAD-C3D-C4D	3.05	130.90	124.94
5	O	1803	MGD	O4'-C1'-C2'	-3.04	100.11	106.62
5	I	1803	MGD	C2'-C3'-C4'	3.03	108.46	102.61
6	L	1128	HEC	CBD-CAD-C3D	-3.02	104.17	112.53
5	M	1804	MGD	O5'-C5'-C4'	-3.01	98.73	108.99
5	C	1804	MGD	O4'-C4'-C3'	-3.01	99.18	105.15
5	E	1804	MGD	O5'-C5'-C4'	-3.01	98.75	108.99
5	K	1804	MGD	O4'-C1'-C2'	-3.00	100.19	106.62
5	I	1803	MGD	C3'-C2'-C1'	-3.00	95.78	101.46
5	K	1803	MGD	O11-C23-C14	3.00	110.96	108.96
5	C	1804	MGD	O4'-C1'-C2'	-2.97	100.26	106.62
6	P	1128	HEC	C1D-C2D-C3D	2.96	110.21	106.82
5	A	1804	MGD	O4'-C4'-C3'	-2.95	99.29	105.15
5	M	1804	MGD	O4'-C4'-C3'	-2.93	99.34	105.15
6	N	1129	HEC	CMD-C2D-C1D	-2.92	120.97	125.42
6	P	1128	HEC	CBD-CAD-C3D	-2.92	104.47	112.53
5	A	1803	MGD	O4'-C1'-C2'	-2.92	100.37	106.62
6	N	1128	HEC	CAA-C2A-C3A	-2.91	122.42	127.87
6	J	1129	HEC	CBD-CAD-C3D	2.90	120.55	112.53
6	N	1128	HEC	C1D-C2D-C3D	2.89	110.13	106.82
5	O	1804	MGD	O5'-C5'-C4'	-2.88	99.18	108.99
5	I	1803	MGD	O11-C23-C14	2.85	110.87	108.96
5	M	1804	MGD	O4'-C1'-C2'	-2.84	100.54	106.62
5	E	1804	MGD	O4'-C4'-C3'	-2.84	99.52	105.15
6	B	1128	HEC	C2A-C1A-NA	2.81	113.03	110.32
5	O	1803	MGD	O11-C23-N22	-2.79	106.08	108.61
5	O	1804	MGD	O4'-C1'-C2'	-2.78	100.67	106.62
5	I	1803	MGD	O3'-C3'-C4'	-2.77	103.12	111.08
6	L	1129	HEC	C4D-C3D-C2D	-2.77	102.58	106.87
5	O	1804	MGD	O2B-PB-O5'	-2.75	95.11	107.57
6	H	1128	HEC	CBD-CAD-C3D	-2.75	104.94	112.53
5	A	1804	MGD	O2B-PB-O5'	-2.74	95.15	107.57
6	N	1128	HEC	CAA-C2A-C1A	2.73	130.40	124.85
6	J	1129	HEC	C3D-C4D-ND	2.71	113.16	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1804	MGD	O4'-C1'-C2'	-2.70	100.84	106.62
6	J	1129	HEC	C4D-C3D-C2D	-2.70	102.70	106.87
5	G	1804	MGD	O4'-C4'-C3'	-2.67	99.85	105.15
6	B	1129	HEC	CAD-C3D-C4D	2.66	130.14	124.94
6	F	1128	HEC	CMD-C2D-C1D	-2.65	121.39	125.42
6	H	1129	HEC	C2A-C1A-NA	2.63	112.86	110.32
5	K	1803	MGD	O4'-C1'-C2'	-2.62	101.00	106.62
6	B	1129	HEC	CBD-CAD-C3D	2.62	119.77	112.53
5	E	1804	MGD	O2B-PB-O5'	-2.60	95.80	107.57
6	B	1129	HEC	C2D-C1D-ND	-2.58	106.00	110.14
5	G	1804	MGD	O4'-C1'-C2'	-2.57	101.11	106.62
5	O	1804	MGD	O4'-C4'-C3'	-2.56	100.07	105.15
6	H	1128	HEC	CAD-CBD-CGD	2.56	120.46	113.67
5	O	1803	MGD	O11-C23-C14	2.55	110.66	108.96
5	I	1804	MGD	O4'-C4'-C3'	-2.55	100.10	105.15
5	C	1803	MGD	O4'-C1'-C2'	-2.54	101.18	106.62
6	D	1128	HEC	CAD-CBD-CGD	2.51	120.32	113.67
6	D	1129	HEC	CAD-C3D-C4D	2.51	129.83	124.94
5	A	1804	MGD	C2'-C1'-N9	2.49	120.18	113.25
5	G	1803	MGD	O11-C23-N22	-2.49	106.35	108.61
6	P	1129	HEC	C4D-C3D-C2D	-2.47	103.05	106.87
5	K	1804	MGD	O2B-PB-O5'	-2.46	96.40	107.57
5	K	1803	MGD	O11-C23-N22	-2.46	106.38	108.61
6	P	1128	HEC	C2A-C1A-NA	2.46	112.69	110.32
5	K	1803	MGD	C3'-C2'-C1'	-2.45	96.82	101.46
5	K	1804	MGD	O4'-C4'-C3'	-2.45	100.29	105.15
6	L	1129	HEC	CBA-CAA-C2A	-2.45	105.76	112.53
5	K	1804	MGD	O5'-C5'-C4'	-2.44	100.69	108.99
6	B	1128	HEC	CAD-CBD-CGD	2.44	120.12	113.67
6	L	1129	HEC	C2A-C1A-NA	2.42	112.66	110.32
5	C	1803	MGD	O11-C23-N22	-2.42	106.41	108.61
6	J	1129	HEC	C2A-C1A-NA	2.41	112.65	110.32
6	H	1129	HEC	C4D-C3D-C2D	-2.41	103.14	106.87
6	F	1129	HEC	CMD-C2D-C1D	-2.39	121.78	125.42
6	N	1128	HEC	CMD-C2D-C3D	2.37	130.65	125.62
5	I	1803	MGD	O11-C23-N22	-2.35	106.47	108.61
5	M	1804	MGD	C23-C14-N15	2.34	110.17	107.87
5	O	1803	MGD	C3'-C2'-C1'	-2.34	97.03	101.46
5	E	1804	MGD	O4'-C1'-C2'	-2.34	101.61	106.62
6	H	1128	HEC	C2D-C1D-ND	-2.33	106.40	110.14
6	N	1129	HEC	C4D-C3D-C2D	-2.33	103.26	106.87
5	C	1804	MGD	O5'-C5'-C4'	-2.32	101.08	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1128	HEC	CMD-C2D-C1D	-2.30	121.92	125.42
5	M	1804	MGD	C3'-C2'-C1'	-2.29	97.13	101.46
6	D	1128	HEC	CAD-C3D-C4D	2.29	129.41	124.94
6	J	1129	HEC	CMD-C2D-C3D	2.28	130.47	125.62
5	K	1804	MGD	C3'-C2'-C1'	-2.28	97.15	101.46
5	A	1803	MGD	O2'-C2'-C1'	2.28	117.95	110.10
5	A	1803	MGD	O11-C23-N22	-2.28	106.54	108.61
6	F	1128	HEC	C2D-C1D-ND	-2.27	106.50	110.14
6	B	1128	HEC	C2D-C1D-ND	-2.27	106.50	110.14
6	H	1129	HEC	CBD-CAD-C3D	2.26	118.79	112.53
6	N	1129	HEC	C2A-C1A-NA	2.26	112.50	110.32
5	E	1803	MGD	O2'-C2'-C1'	2.26	117.88	110.10
5	M	1804	MGD	O2A-PA-O1A	2.25	122.92	112.44
6	D	1128	HEC	CAA-C2A-C1A	2.25	129.43	124.85
6	D	1129	HEC	CBD-CAD-C3D	2.25	118.75	112.53
5	A	1804	MGD	O5'-C5'-C4'	-2.25	101.34	108.99
6	F	1129	HEC	C4D-C3D-C2D	-2.24	103.40	106.87
6	F	1128	HEC	C2A-C1A-NA	2.24	112.48	110.32
5	G	1804	MGD	O4'-C1'-N9	-2.24	103.29	108.36
5	C	1804	MGD	O2A-PA-O3B	2.23	113.31	107.27
5	G	1803	MGD	C3'-C2'-C1'	-2.23	97.25	101.46
6	D	1129	HEC	C4D-C3D-C2D	-2.22	103.43	106.87
6	J	1128	HEC	C2D-C1D-ND	-2.22	106.59	110.14
6	L	1128	HEC	CAA-C2A-C1A	2.22	129.36	124.85
6	N	1128	HEC	C2D-C1D-ND	-2.21	106.59	110.14
6	P	1129	HEC	C2D-C1D-ND	-2.21	106.61	110.14
6	J	1129	HEC	CAA-CBA-CGA	2.20	119.51	113.67
5	E	1804	MGD	O2A-PA-O3B	2.20	113.22	107.27
5	I	1803	MGD	O2A-PA-O1A	2.20	122.68	112.44
5	K	1804	MGD	O2A-PA-O1A	2.20	122.68	112.44
5	G	1803	MGD	O4'-C1'-C2'	-2.20	101.91	106.62
5	M	1803	MGD	O11-C23-N22	-2.20	106.61	108.61
5	G	1803	MGD	O2'-C2'-C1'	2.19	117.65	110.10
5	C	1804	MGD	C3'-C2'-C1'	-2.19	97.32	101.46
6	F	1128	HEC	CAA-C2A-C1A	2.19	129.30	124.85
5	O	1803	MGD	O4'-C4'-C5'	-2.19	102.33	109.33
6	L	1129	HEC	CBD-CAD-C3D	2.18	118.57	112.53
5	A	1803	MGD	O4'-C4'-C5'	-2.18	102.36	109.33
5	E	1803	MGD	O11-C23-N22	-2.18	106.63	108.61
6	H	1129	HEC	CMA-C3A-C2A	2.18	132.03	126.15
6	H	1128	HEC	CAA-C2A-C1A	2.18	129.28	124.85
6	J	1129	HEC	C2D-C1D-ND	-2.17	106.66	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1804	MGD	O2A-PA-O1A	2.16	122.52	112.44
6	H	1129	HEC	C2D-C1D-ND	-2.16	106.68	110.14
6	F	1128	HEC	CAD-CBD-CGD	2.16	119.38	113.67
5	M	1804	MGD	C2'-C1'-N9	2.15	119.23	113.25
5	K	1804	MGD	C2'-C1'-N9	2.15	119.22	113.25
5	K	1803	MGD	C2'-C3'-C4'	2.15	106.76	102.61
6	H	1128	HEC	C4D-C3D-C2D	-2.14	103.56	106.87
5	O	1804	MGD	O2A-PA-O3B	2.13	113.04	107.27
5	C	1803	MGD	O4'-C4'-C5'	-2.13	102.50	109.33
5	K	1804	MGD	O4'-C1'-N9	-2.13	103.53	108.36
5	E	1804	MGD	O5'-PB-O1B	2.12	117.35	108.94
5	M	1803	MGD	O4'-C4'-C5'	-2.12	102.54	109.33
5	M	1803	MGD	O2'-C2'-C1'	2.12	117.40	110.10
6	P	1128	HEC	CAA-C2A-C1A	2.11	129.14	124.85
5	A	1803	MGD	C3'-C2'-C1'	-2.10	97.49	101.46
5	G	1804	MGD	C23-C14-N15	2.09	109.92	107.87
6	J	1128	HEC	CAD-C3D-C4D	2.09	129.01	124.94
5	I	1804	MGD	O2A-PA-O1A	2.08	122.13	112.44
5	I	1804	MGD	C3'-C2'-C1'	-2.08	97.52	101.46
5	M	1803	MGD	O4'-C4'-C3'	-2.08	101.02	105.15
5	G	1804	MGD	C3'-C2'-C1'	-2.08	97.53	101.46
5	I	1804	MGD	C23-C14-N15	2.07	109.91	107.87
5	A	1803	MGD	C2'-C3'-C4'	2.07	106.61	102.61
6	P	1128	HEC	C4D-C3D-C2D	-2.07	103.67	106.87
6	P	1129	HEC	CMA-C3A-C2A	2.07	131.74	126.15
5	K	1804	MGD	O5'-PB-O1B	2.06	117.11	108.94
6	D	1128	HEC	C4D-C3D-C2D	-2.06	103.68	106.87
6	N	1129	HEC	CBA-CAA-C2A	-2.06	106.84	112.53
6	N	1128	HEC	CAD-CBD-CGD	2.05	119.11	113.67
6	D	1129	HEC	CMD-C2D-C3D	2.05	129.97	125.62
6	J	1128	HEC	CAA-C2A-C1A	2.05	129.01	124.85
5	O	1803	MGD	O2'-C2'-C1'	2.04	117.14	110.10
6	F	1128	HEC	C4D-C3D-C2D	-2.04	103.70	106.87
5	M	1803	MGD	C3'-C2'-C1'	-2.04	97.61	101.46
6	L	1128	HEC	C2D-C1D-ND	-2.03	106.88	110.14
6	J	1128	HEC	CAA-C2A-C3A	-2.03	124.06	127.87
6	L	1129	HEC	C2D-C1D-ND	-2.03	106.88	110.14
6	D	1128	HEC	CMD-C2D-C1D	-2.03	122.33	125.42
6	D	1129	HEC	C2D-C1D-ND	-2.02	106.90	110.14
5	C	1804	MGD	O2B-PB-O5'	-2.01	98.44	107.57
5	M	1804	MGD	O4'-C1'-N9	-2.01	103.81	108.36
6	D	1129	HEC	CMA-C3A-C2A	2.00	131.56	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1128	HEC	CAD-C3D-C4D	2.00	128.85	124.94

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1803	MGD	PA-O3B-PB-O5'
5	A	1803	MGD	C5'-O5'-PB-O1B
5	A	1803	MGD	C5'-O5'-PB-O2B
5	A	1803	MGD	C5'-O5'-PB-O3B
5	A	1804	MGD	C5'-O5'-PB-O1B
5	A	1804	MGD	C5'-O5'-PB-O2B
5	A	1804	MGD	C5'-O5'-PB-O3B
5	C	1803	MGD	PA-O3B-PB-O5'
5	C	1803	MGD	C5'-O5'-PB-O1B
5	C	1803	MGD	C5'-O5'-PB-O2B
5	C	1803	MGD	C5'-O5'-PB-O3B
5	C	1804	MGD	C5'-O5'-PB-O1B
5	C	1804	MGD	C5'-O5'-PB-O3B
5	E	1803	MGD	PA-O3B-PB-O5'
5	E	1803	MGD	C5'-O5'-PB-O1B
5	E	1803	MGD	C5'-O5'-PB-O2B
5	E	1803	MGD	C5'-O5'-PB-O3B
5	E	1804	MGD	C5'-O5'-PB-O1B
5	E	1804	MGD	C5'-O5'-PB-O3B
5	G	1803	MGD	PA-O3B-PB-O5'
5	G	1803	MGD	C5'-O5'-PB-O1B
5	G	1803	MGD	C5'-O5'-PB-O2B
5	G	1803	MGD	C5'-O5'-PB-O3B
5	G	1804	MGD	C5'-O5'-PB-O1B
5	G	1804	MGD	C5'-O5'-PB-O3B
5	I	1803	MGD	PA-O3B-PB-O5'
5	I	1803	MGD	C5'-O5'-PB-O1B
5	I	1803	MGD	C5'-O5'-PB-O2B
5	I	1803	MGD	C5'-O5'-PB-O3B
5	I	1804	MGD	C5'-O5'-PB-O1B
5	I	1804	MGD	C5'-O5'-PB-O2B
5	I	1804	MGD	C5'-O5'-PB-O3B
5	K	1803	MGD	PA-O3B-PB-O5'
5	K	1803	MGD	C5'-O5'-PB-O1B
5	K	1803	MGD	C5'-O5'-PB-O2B
5	K	1803	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
5	K	1804	MGD	C5'-O5'-PB-O1B
5	K	1804	MGD	C5'-O5'-PB-O2B
5	K	1804	MGD	C5'-O5'-PB-O3B
5	M	1803	MGD	C5'-O5'-PB-O1B
5	M	1803	MGD	C5'-O5'-PB-O2B
5	M	1803	MGD	C5'-O5'-PB-O3B
5	M	1804	MGD	C5'-O5'-PB-O1B
5	M	1804	MGD	C5'-O5'-PB-O2B
5	M	1804	MGD	C5'-O5'-PB-O3B
5	O	1803	MGD	PA-O3B-PB-O5'
5	O	1803	MGD	C5'-O5'-PB-O1B
5	O	1803	MGD	C5'-O5'-PB-O2B
5	O	1803	MGD	C5'-O5'-PB-O3B
5	O	1804	MGD	C5'-O5'-PB-O1B
5	O	1804	MGD	C5'-O5'-PB-O2B
5	O	1804	MGD	C5'-O5'-PB-O3B
6	B	1128	HEC	C2B-C3B-CAB-CBB
6	B	1128	HEC	C4B-C3B-CAB-CBB
6	B	1128	HEC	C4C-C3C-CAC-CBC
6	B	1129	HEC	C2B-C3B-CAB-CBB
6	B	1129	HEC	C4B-C3B-CAB-CBB
6	B	1129	HEC	C2C-C3C-CAC-CBC
6	B	1129	HEC	C4C-C3C-CAC-CBC
6	D	1128	HEC	C2B-C3B-CAB-CBB
6	D	1128	HEC	C4B-C3B-CAB-CBB
6	D	1129	HEC	C2B-C3B-CAB-CBB
6	D	1129	HEC	C4B-C3B-CAB-CBB
6	D	1129	HEC	C2C-C3C-CAC-CBC
6	D	1129	HEC	C4C-C3C-CAC-CBC
6	F	1128	HEC	C2B-C3B-CAB-CBB
6	F	1128	HEC	C4B-C3B-CAB-CBB
6	F	1128	HEC	C2C-C3C-CAC-CBC
6	F	1128	HEC	C4C-C3C-CAC-CBC
6	F	1129	HEC	C2B-C3B-CAB-CBB
6	F	1129	HEC	C2C-C3C-CAC-CBC
6	F	1129	HEC	C4C-C3C-CAC-CBC
6	H	1128	HEC	C2B-C3B-CAB-CBB
6	H	1128	HEC	C4B-C3B-CAB-CBB
6	H	1128	HEC	C2C-C3C-CAC-CBC
6	H	1128	HEC	C4C-C3C-CAC-CBC
6	H	1129	HEC	C2C-C3C-CAC-CBC
6	H	1129	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	J	1129	HEC	C2B-C3B-CAB-CBB
6	J	1129	HEC	C2C-C3C-CAC-CBC
6	J	1129	HEC	C4C-C3C-CAC-CBC
6	L	1128	HEC	C2B-C3B-CAB-CBB
6	L	1128	HEC	C4B-C3B-CAB-CBB
6	L	1128	HEC	C2C-C3C-CAC-CBC
6	L	1128	HEC	C4C-C3C-CAC-CBC
6	L	1129	HEC	C2B-C3B-CAB-CBB
6	L	1129	HEC	C4B-C3B-CAB-CBB
6	L	1129	HEC	C2C-C3C-CAC-CBC
6	L	1129	HEC	C4C-C3C-CAC-CBC
6	N	1128	HEC	C2C-C3C-CAC-CBC
6	N	1128	HEC	C4C-C3C-CAC-CBC
6	N	1129	HEC	C2B-C3B-CAB-CBB
6	N	1129	HEC	C4B-C3B-CAB-CBB
6	N	1129	HEC	C2C-C3C-CAC-CBC
6	N	1129	HEC	C4C-C3C-CAC-CBC
6	P	1128	HEC	C2B-C3B-CAB-CBB
6	P	1128	HEC	C4B-C3B-CAB-CBB
6	P	1128	HEC	C2C-C3C-CAC-CBC
6	P	1128	HEC	C4C-C3C-CAC-CBC
6	P	1129	HEC	C2B-C3B-CAB-CBB
6	P	1129	HEC	C4B-C3B-CAB-CBB
6	P	1129	HEC	C2C-C3C-CAC-CBC
6	P	1129	HEC	C4C-C3C-CAC-CBC
6	N	1129	HEC	C4D-C3D-CAD-CBD
5	A	1804	MGD	PA-O3B-PB-O5'
5	C	1804	MGD	PA-O3B-PB-O5'
5	E	1804	MGD	PA-O3B-PB-O5'
5	G	1804	MGD	PA-O3B-PB-O5'
5	I	1804	MGD	PA-O3B-PB-O5'
5	K	1804	MGD	PA-O3B-PB-O5'
5	M	1803	MGD	PA-O3B-PB-O5'
5	M	1804	MGD	PA-O3B-PB-O5'
5	O	1804	MGD	PA-O3B-PB-O5'
6	D	1128	HEC	C4C-C3C-CAC-CBC
6	F	1129	HEC	C4B-C3B-CAB-CBB
6	H	1129	HEC	C4B-C3B-CAB-CBB
6	J	1128	HEC	C4B-C3B-CAB-CBB
6	J	1128	HEC	C4C-C3C-CAC-CBC
6	J	1129	HEC	C4B-C3B-CAB-CBB
6	N	1128	HEC	C4B-C3B-CAB-CBB

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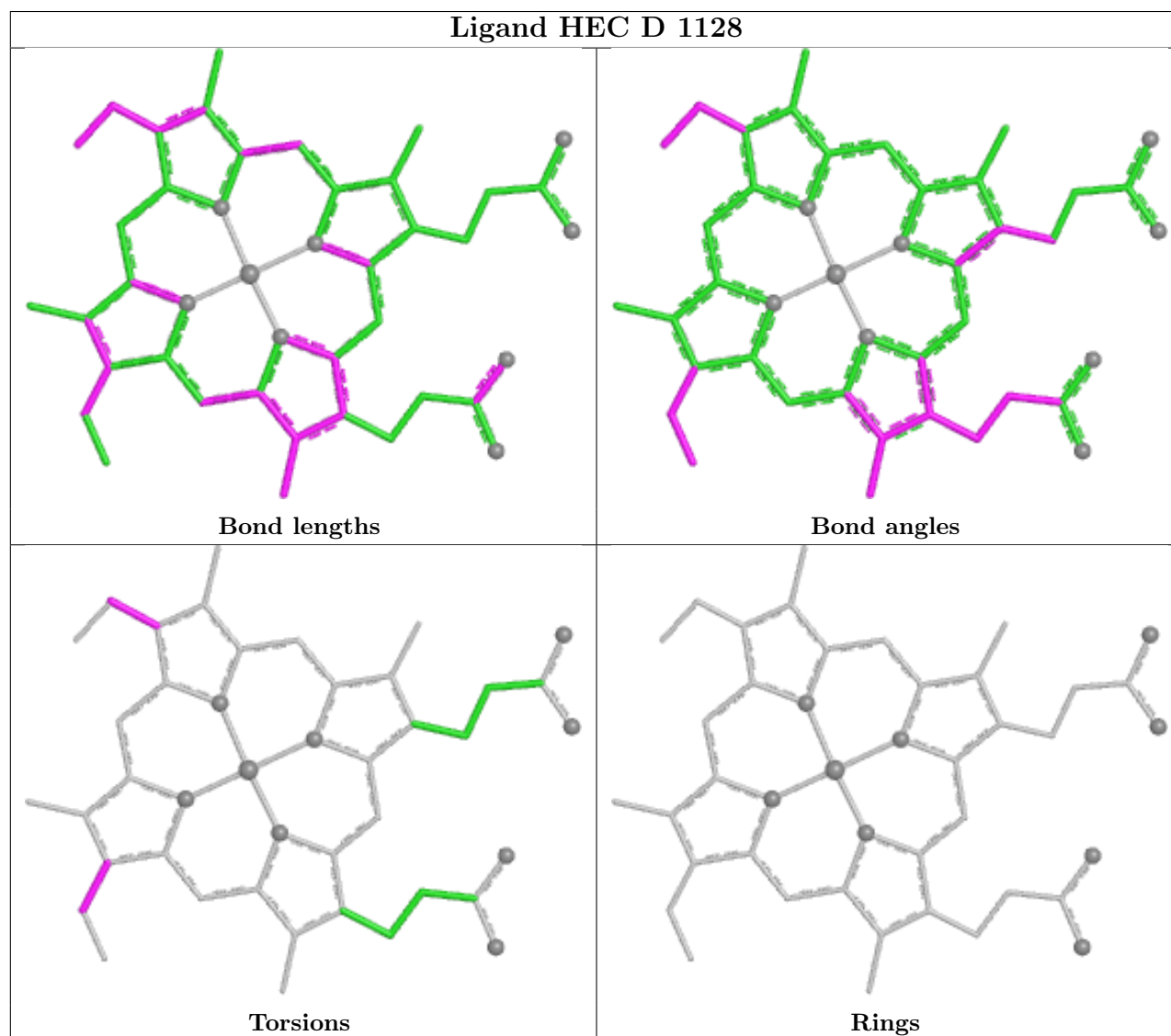
Mol	Chain	Res	Type	Atoms
5	C	1804	MGD	C5'-O5'-PB-O2B
5	E	1804	MGD	C5'-O5'-PB-O2B
5	G	1804	MGD	C5'-O5'-PB-O2B
6	B	1128	HEC	C2C-C3C-CAC-CBC
6	D	1128	HEC	C2C-C3C-CAC-CBC
6	H	1129	HEC	C2B-C3B-CAB-CBB
6	J	1128	HEC	C2B-C3B-CAB-CBB
6	N	1128	HEC	C2B-C3B-CAB-CBB
6	N	1129	HEC	C2D-C3D-CAD-CBD
5	I	1804	MGD	PA-O3B-PB-O1B
5	C	1803	MGD	O4'-C4'-C5'-O5'
5	G	1803	MGD	O4'-C4'-C5'-O5'
5	A	1803	MGD	PA-O3B-PB-O1B
5	C	1803	MGD	PA-O3B-PB-O1B
5	E	1803	MGD	PA-O3B-PB-O1B
5	E	1804	MGD	PA-O3B-PB-O1B
5	G	1804	MGD	PA-O3B-PB-O1B
5	I	1803	MGD	PA-O3B-PB-O1B
5	I	1804	MGD	PA-O3B-PB-O2B
5	K	1803	MGD	PA-O3B-PB-O1B
5	K	1804	MGD	PA-O3B-PB-O1B
5	M	1803	MGD	PA-O3B-PB-O1B
5	M	1804	MGD	PA-O3B-PB-O1B
5	I	1803	MGD	O4'-C4'-C5'-O5'
5	K	1803	MGD	O4'-C4'-C5'-O5'
5	A	1804	MGD	PA-O3B-PB-O2B
5	C	1804	MGD	PA-O3B-PB-O2B
5	E	1804	MGD	PA-O3B-PB-O2B
5	G	1804	MGD	PA-O3B-PB-O2B
5	M	1804	MGD	PA-O3B-PB-O2B
5	O	1804	MGD	PA-O3B-PB-O1B
5	O	1804	MGD	PA-O3B-PB-O2B
5	A	1803	MGD	O4'-C4'-C5'-O5'
5	E	1803	MGD	O4'-C4'-C5'-O5'
5	M	1803	MGD	O4'-C4'-C5'-O5'
5	O	1803	MGD	O4'-C4'-C5'-O5'

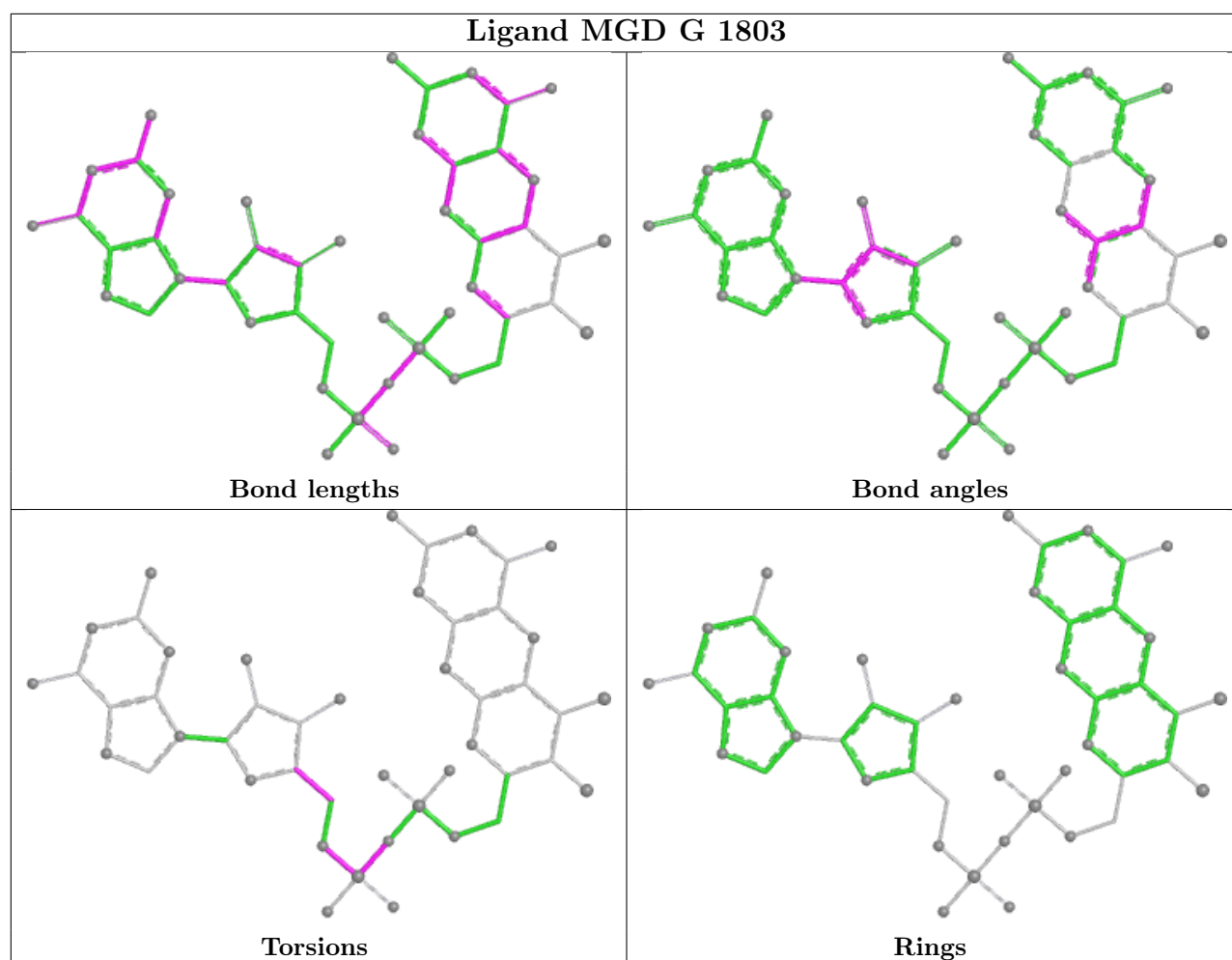
There are no ring outliers.

No monomer is involved in short contacts.

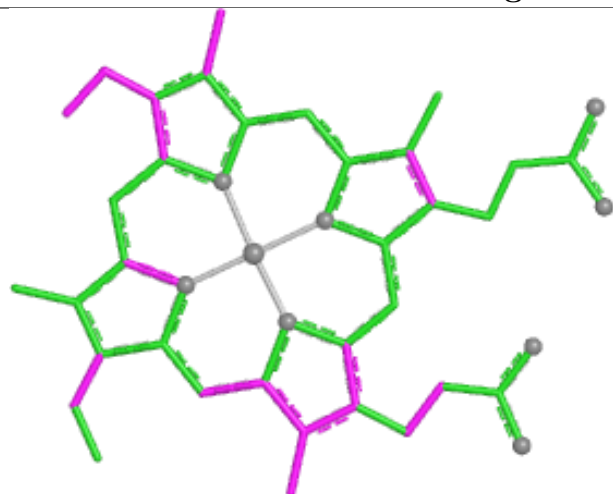
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

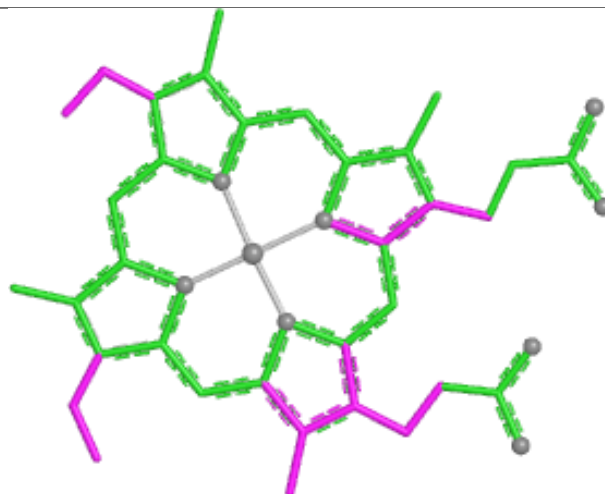




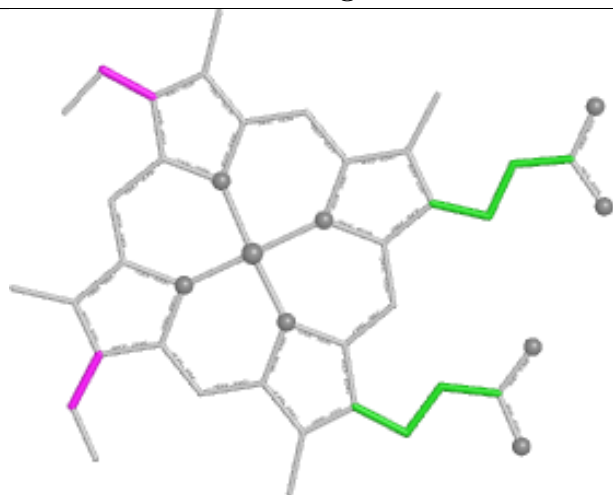
Ligand HEC P 1128



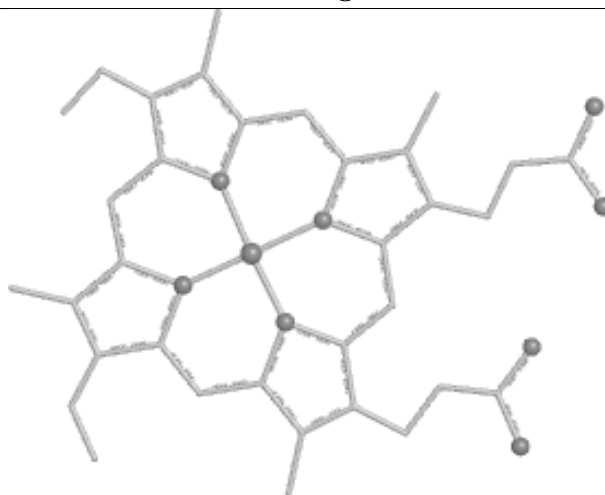
Bond lengths



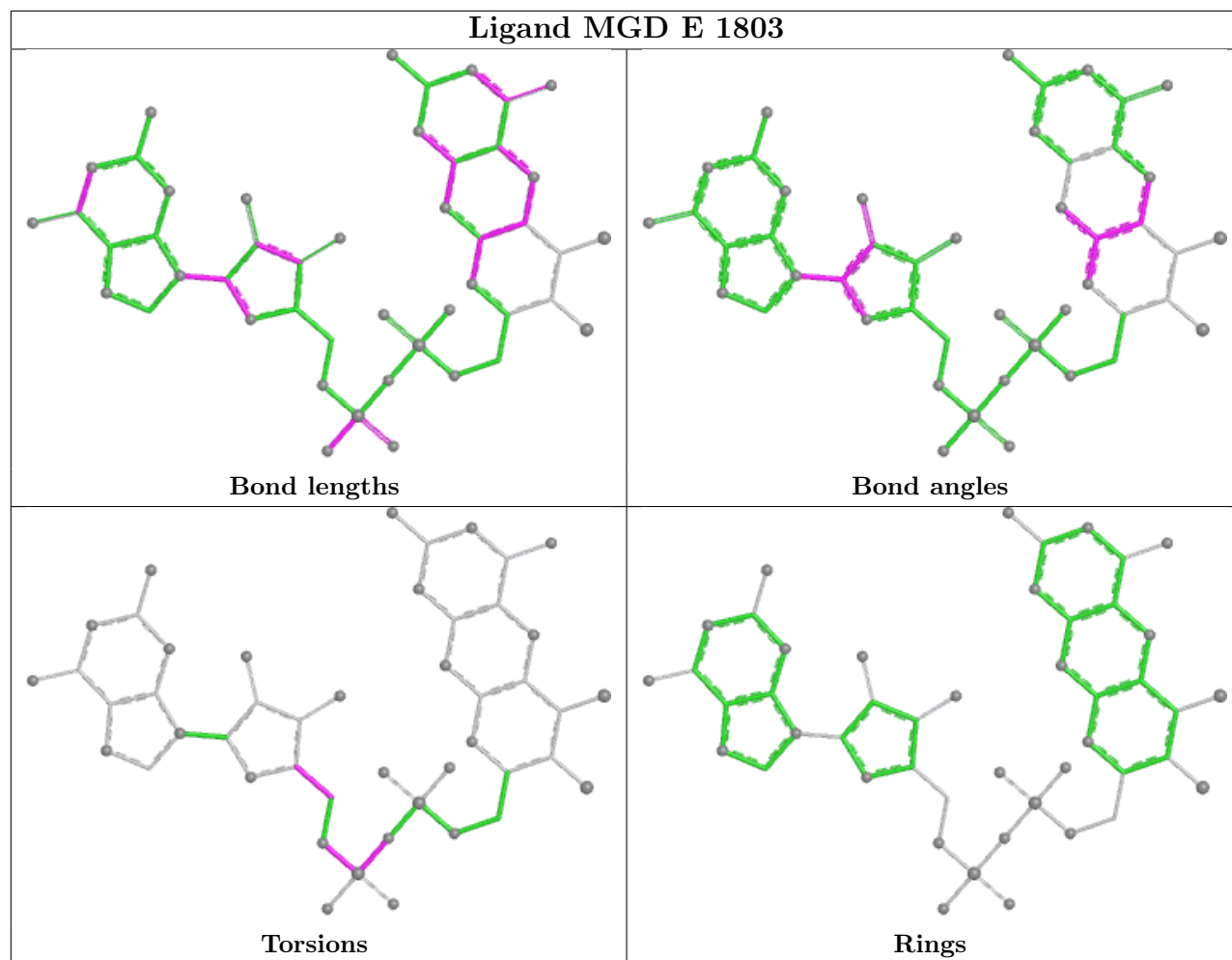
Bond angles

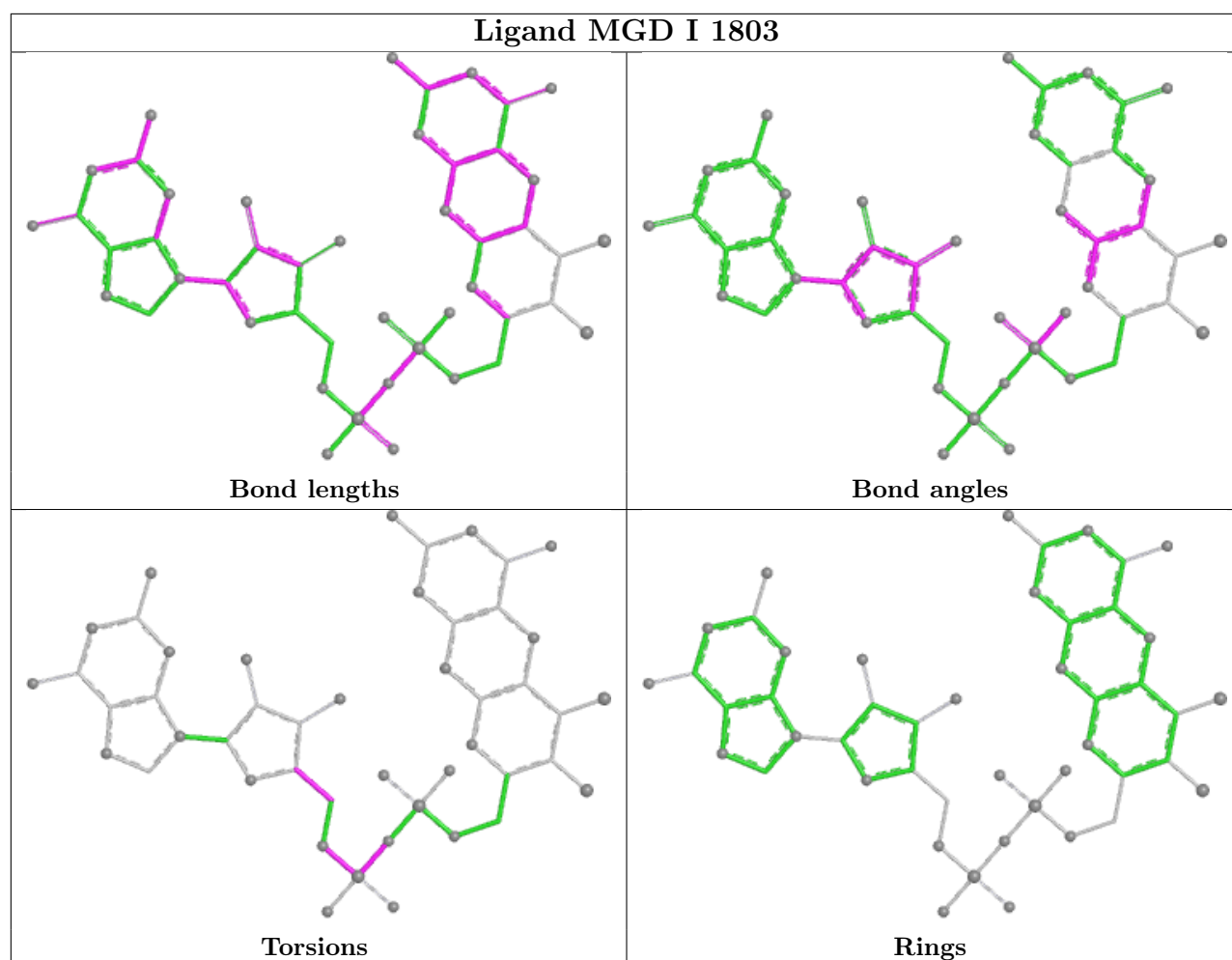


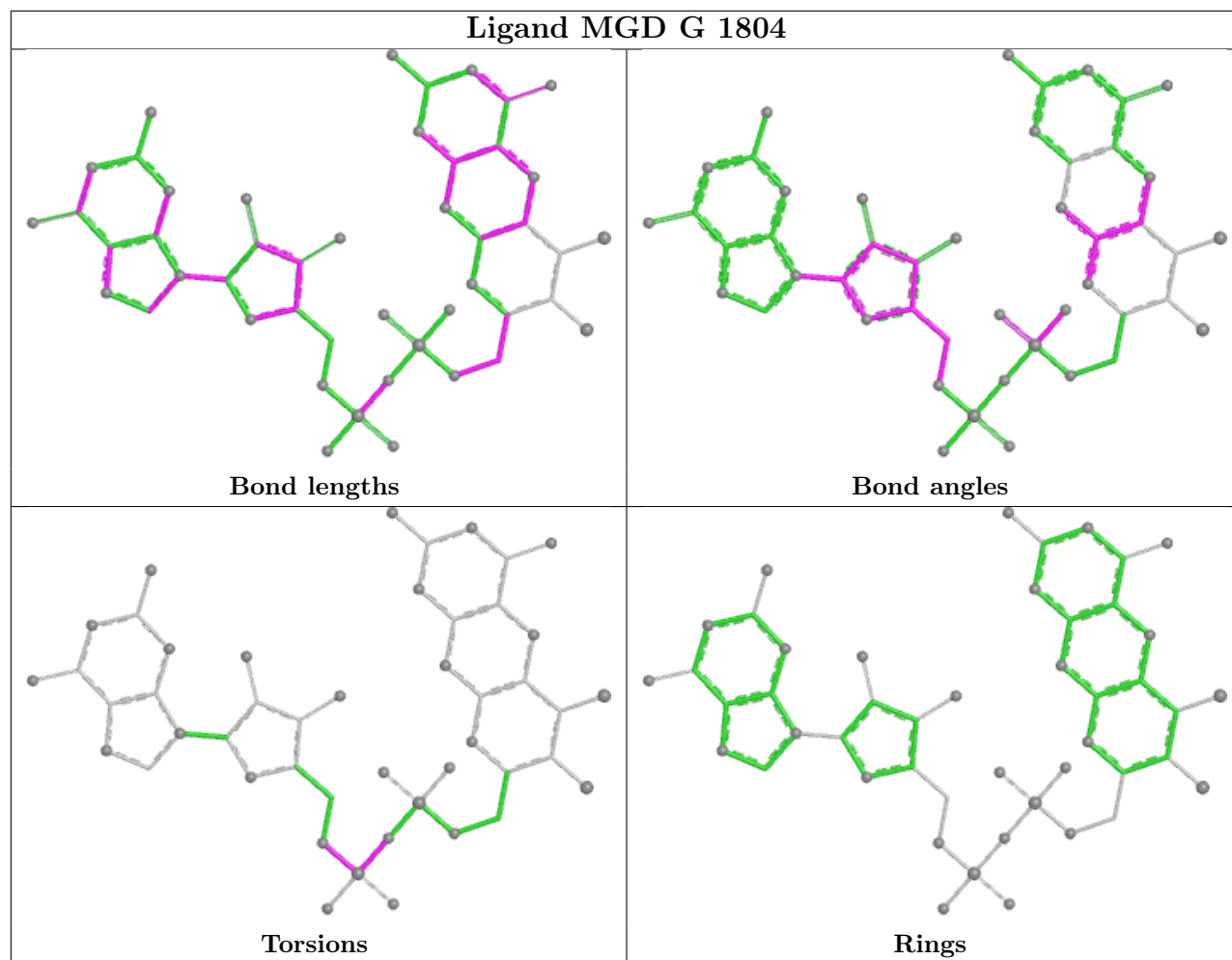
Torsions



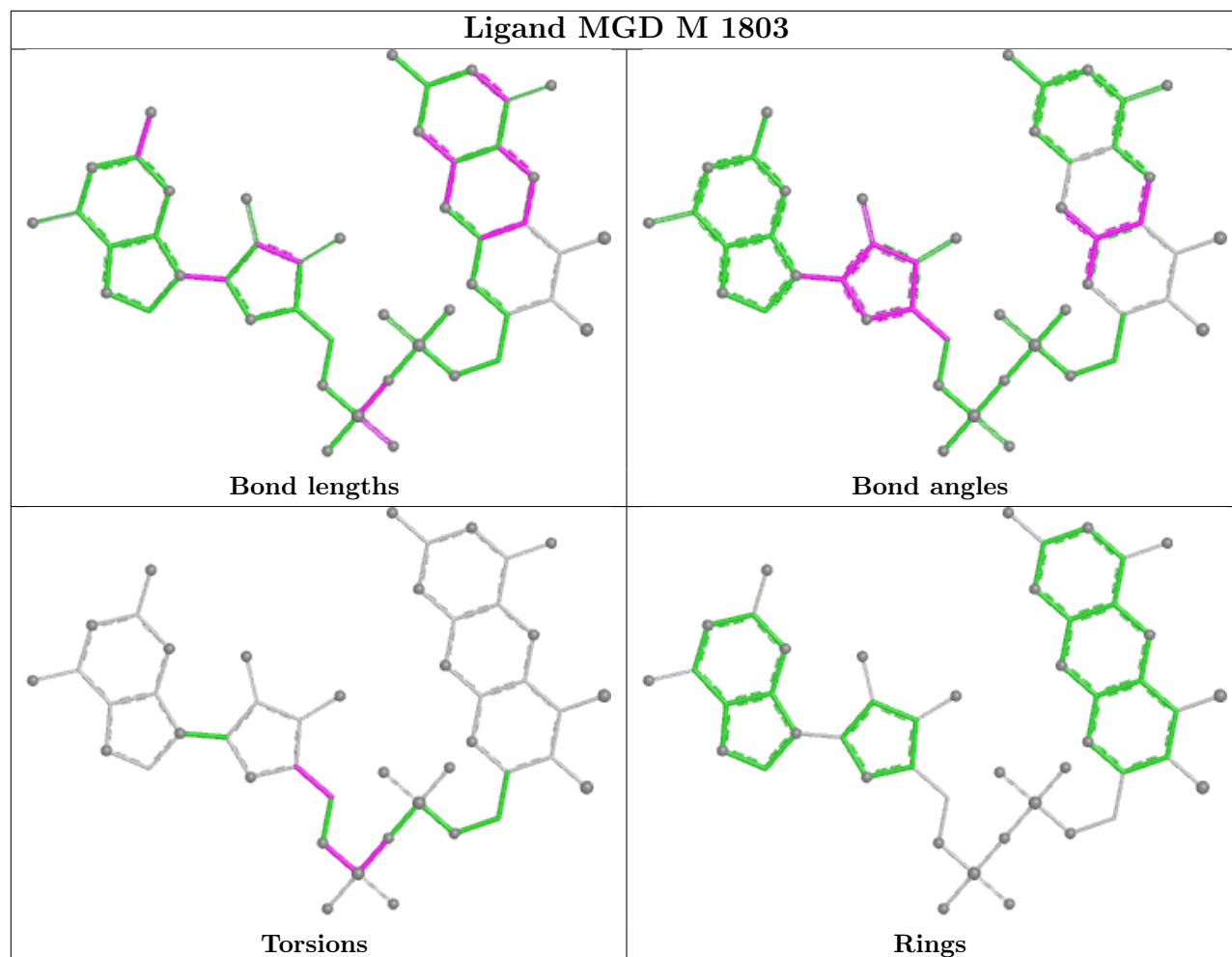
Rings

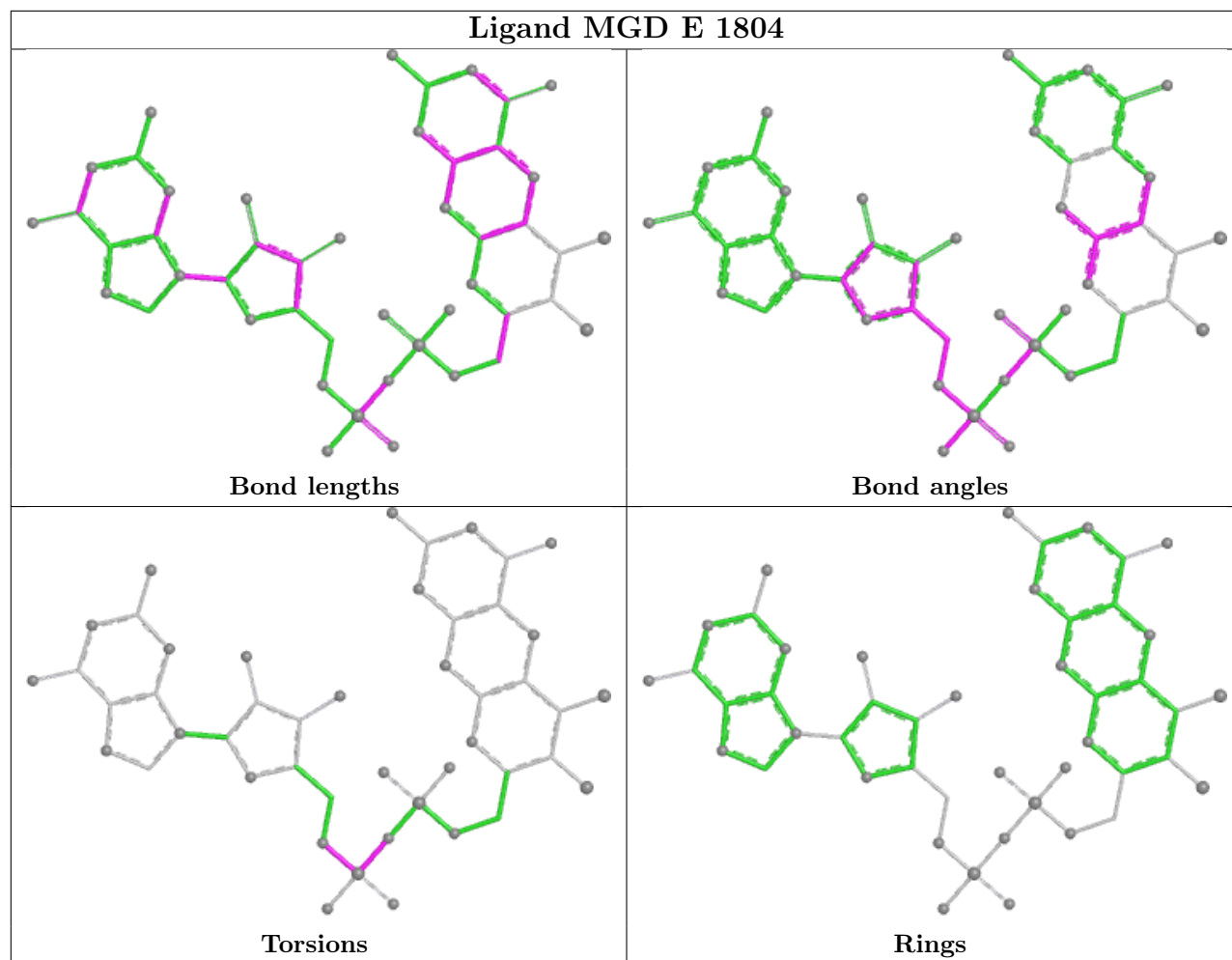




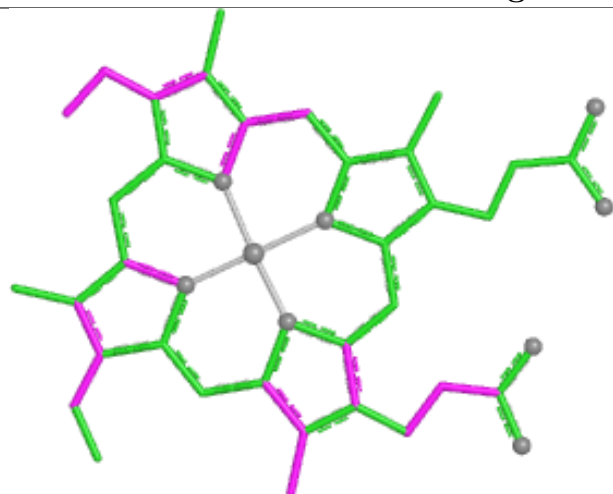


Ligand MGD M 1803

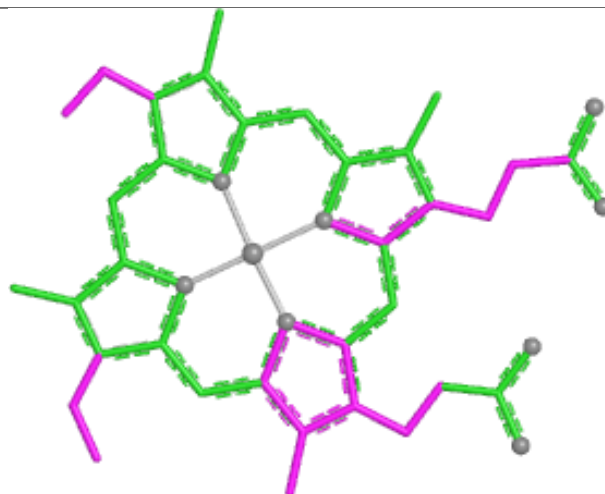




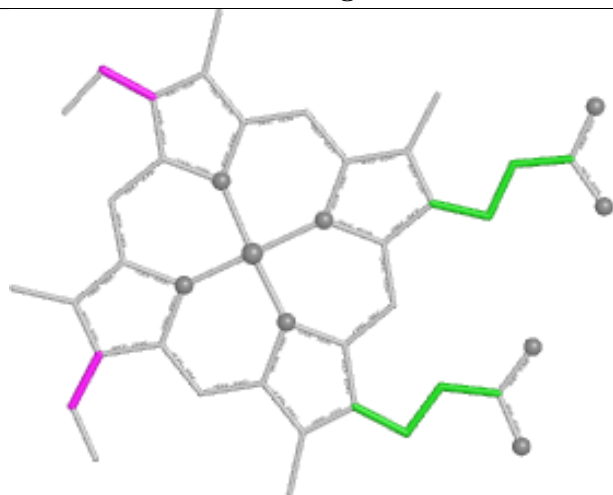
Ligand HEC J 1129



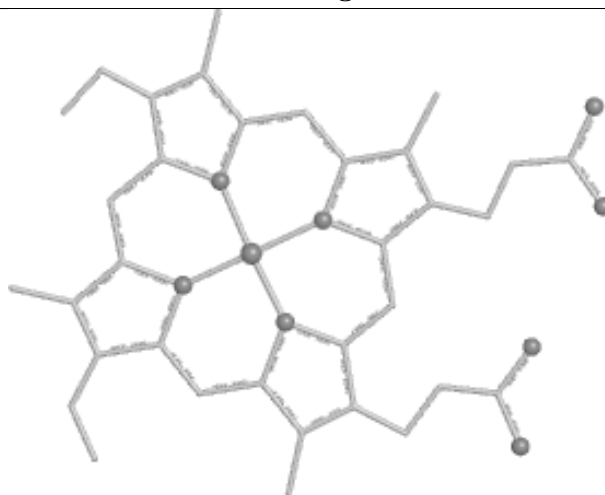
Bond lengths



Bond angles

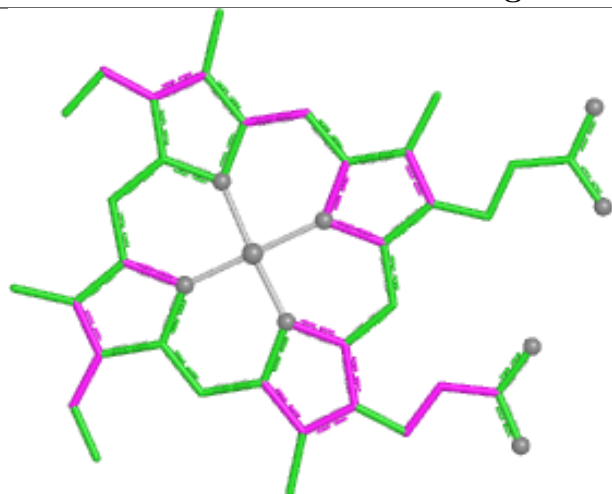


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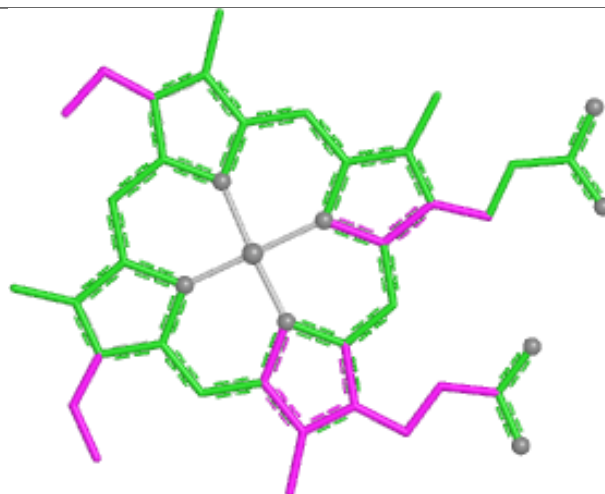


Rings

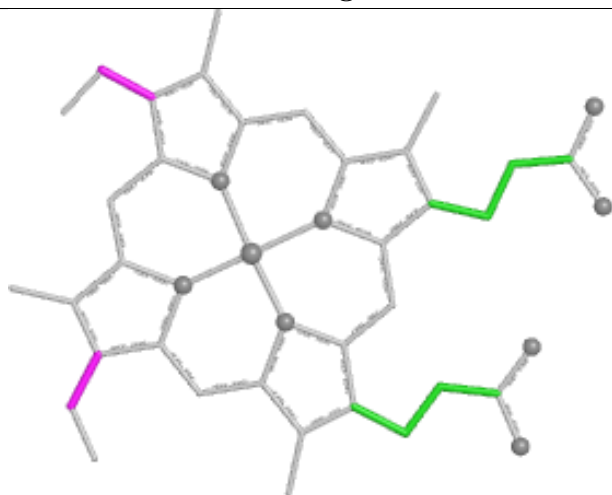
Ligand HEC F 1128



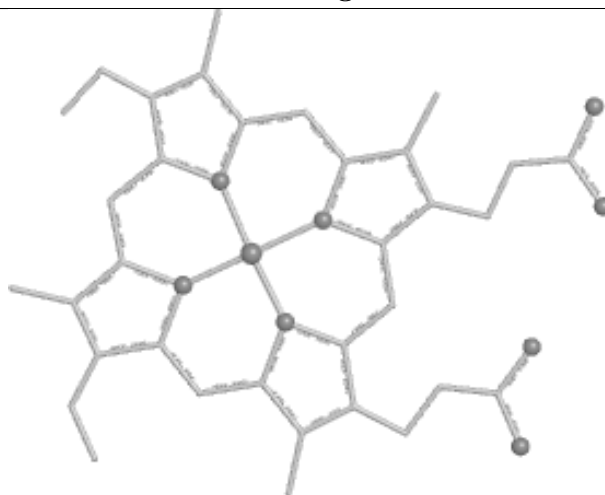
Bond lengths



Bond angles

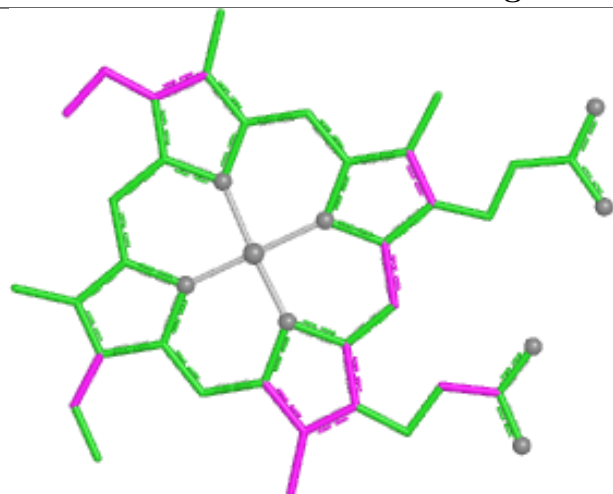


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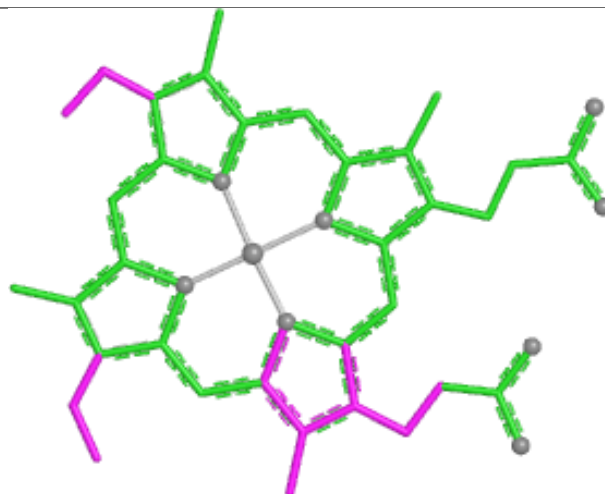


Rings

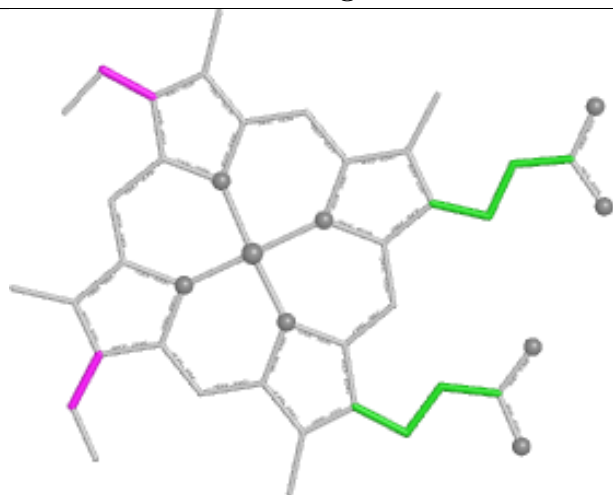
Ligand HEC B 1129



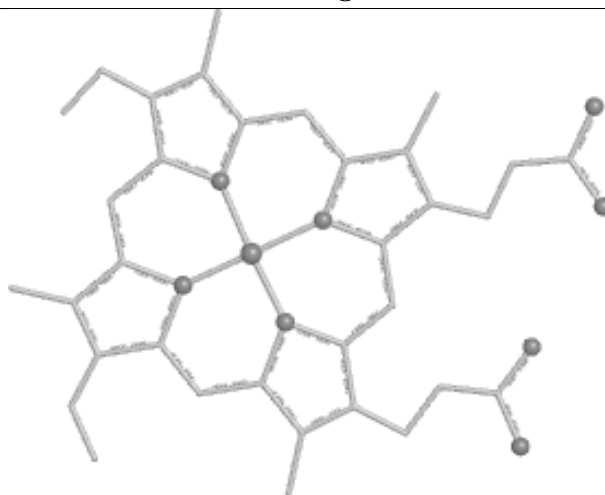
Bond lengths



Bond angles

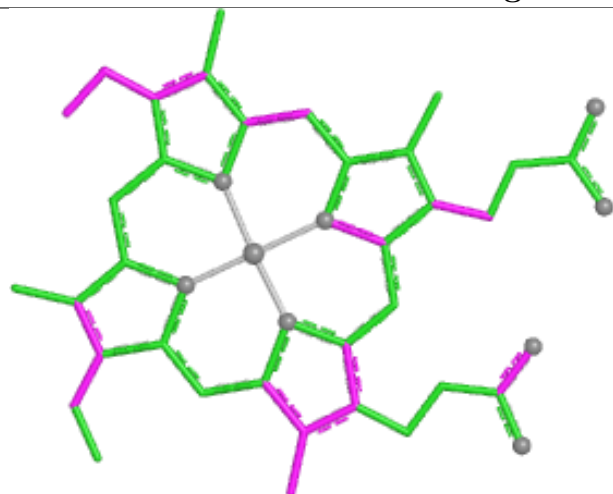


Torsions

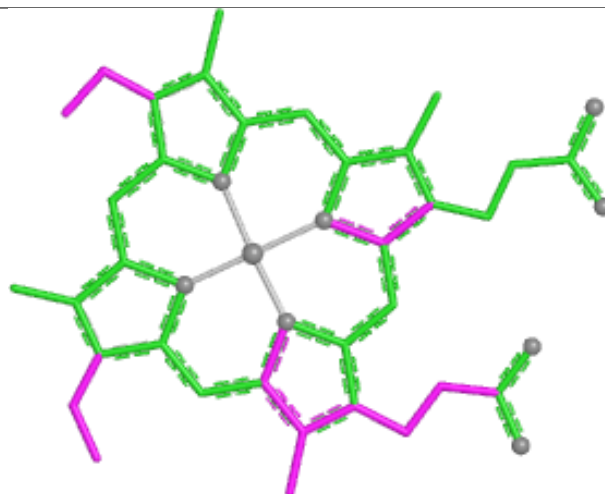


Rings

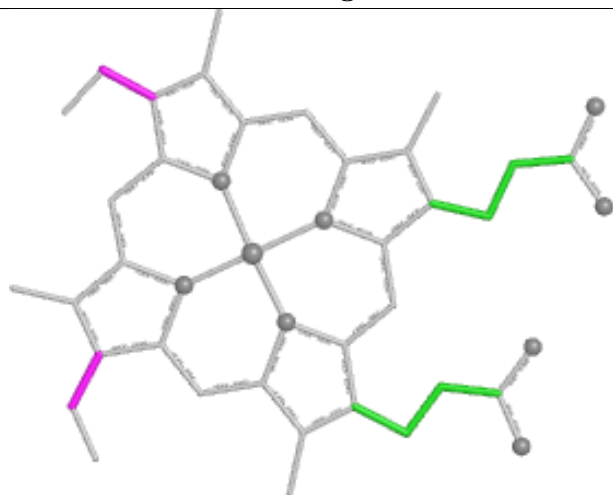
Ligand HEC B 1128



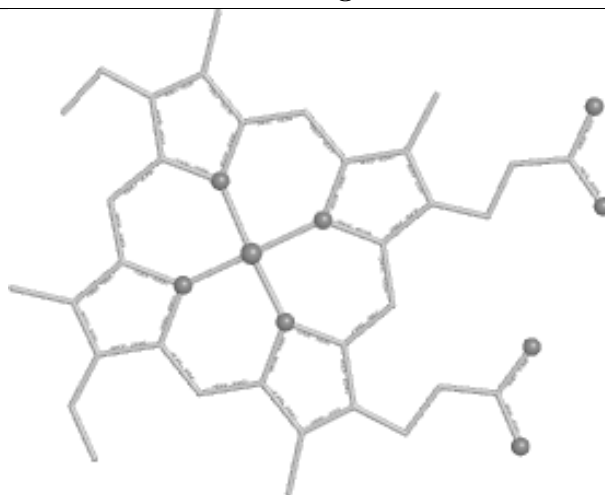
Bond lengths



Bond angles

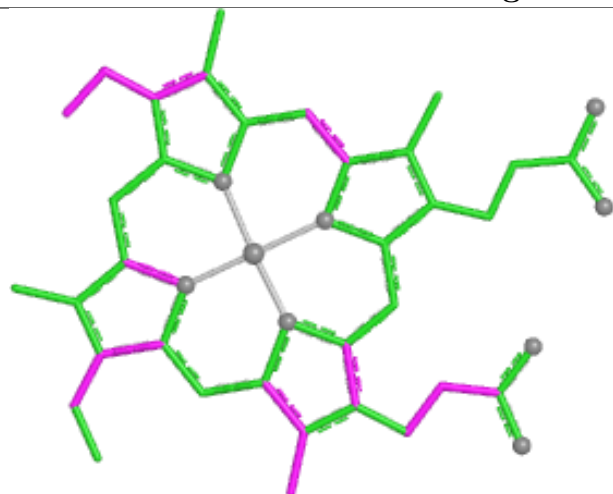


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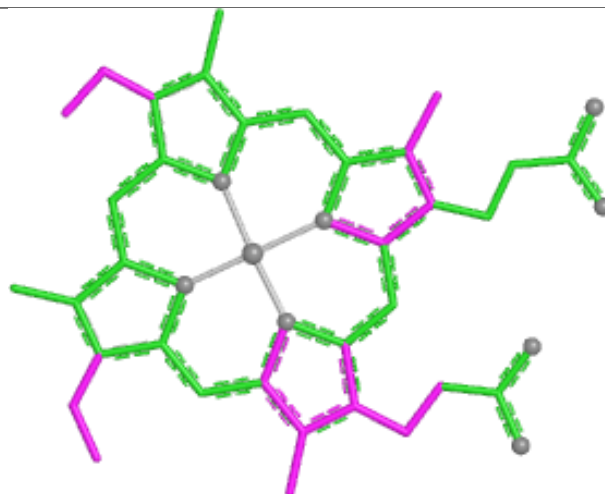


Rings

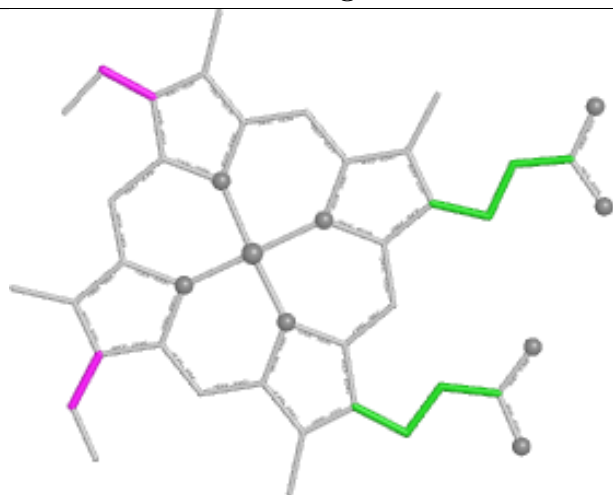
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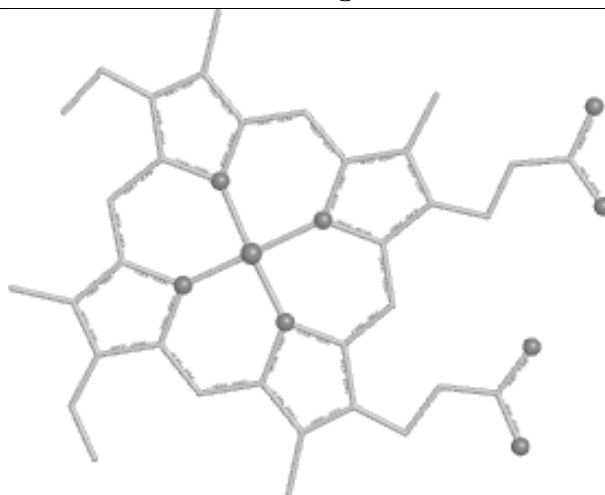
Bond lengths



Bond angles

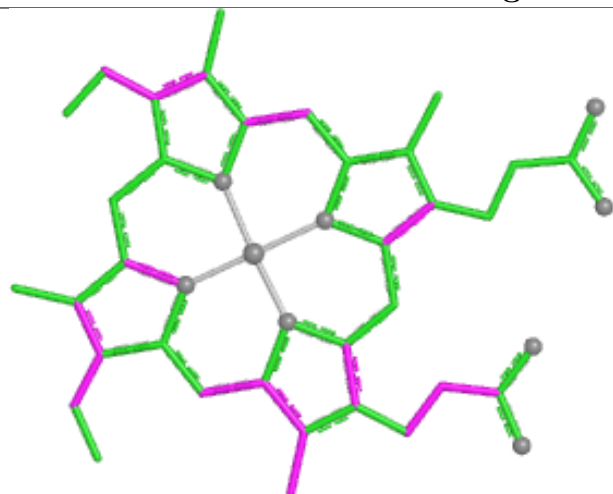


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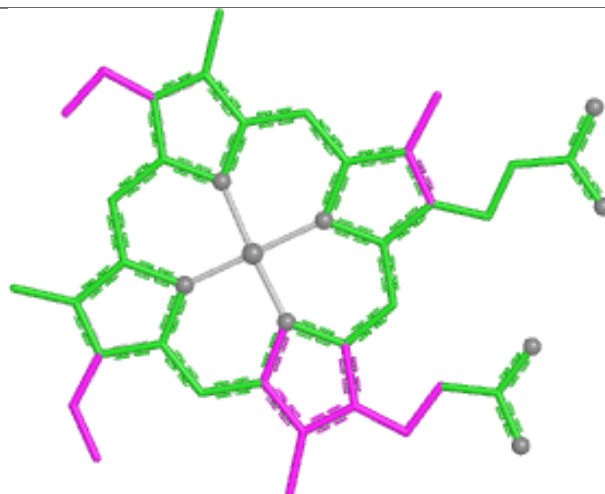


Rings

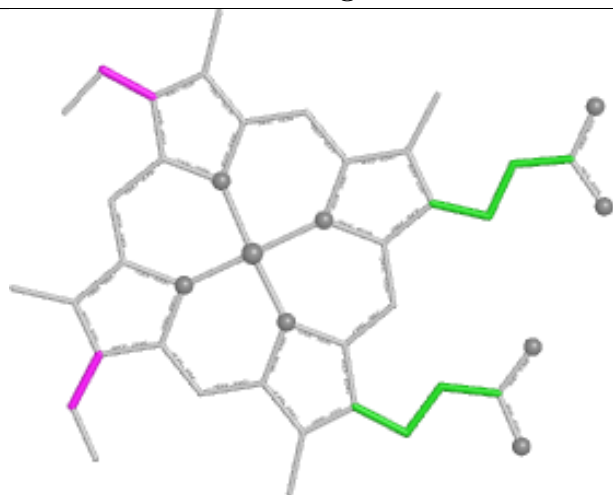
Ligand HEC D 1129



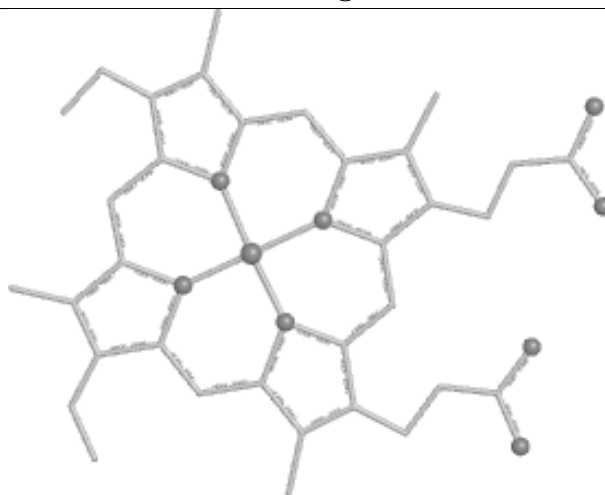
Bond lengths



Bond angles

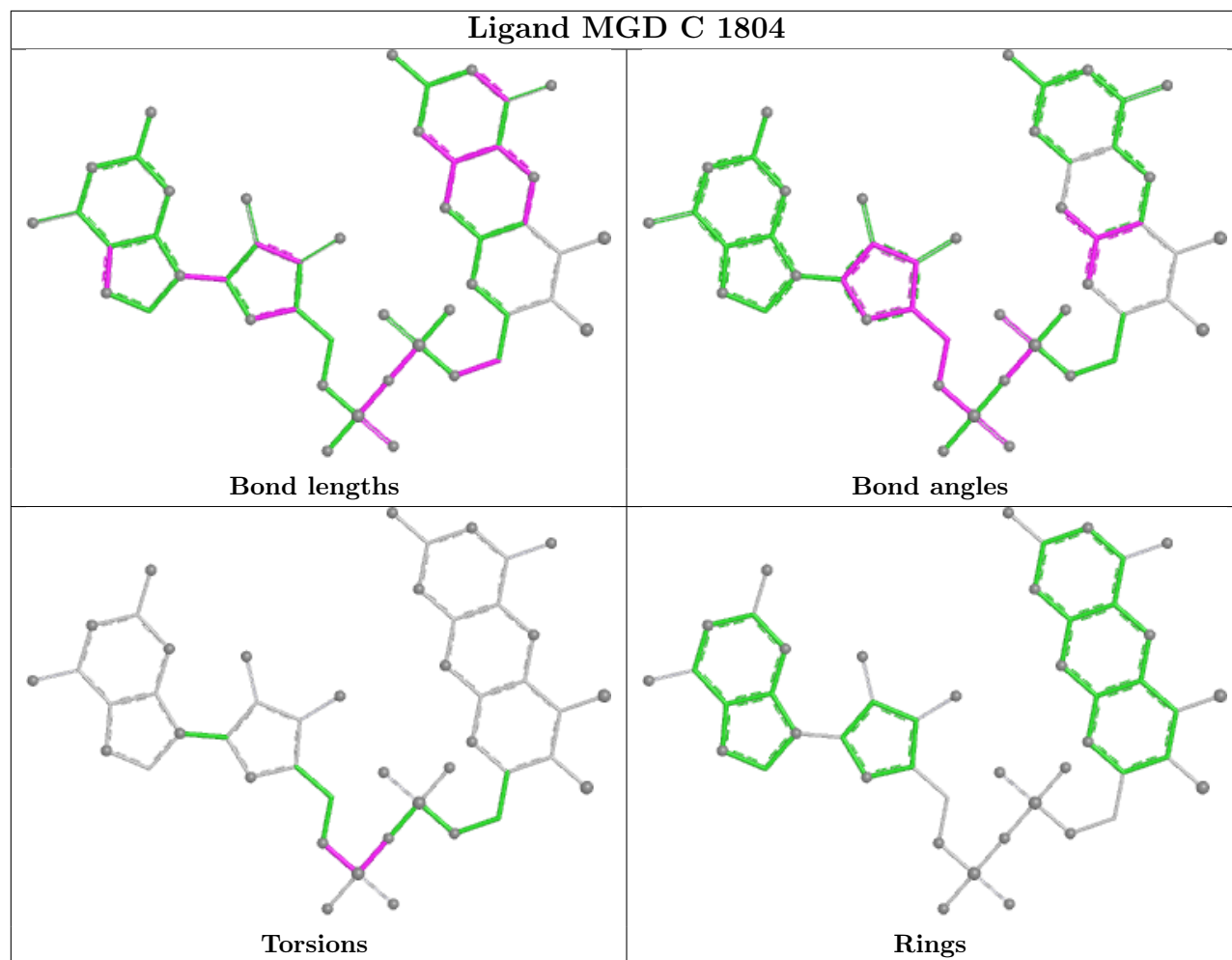


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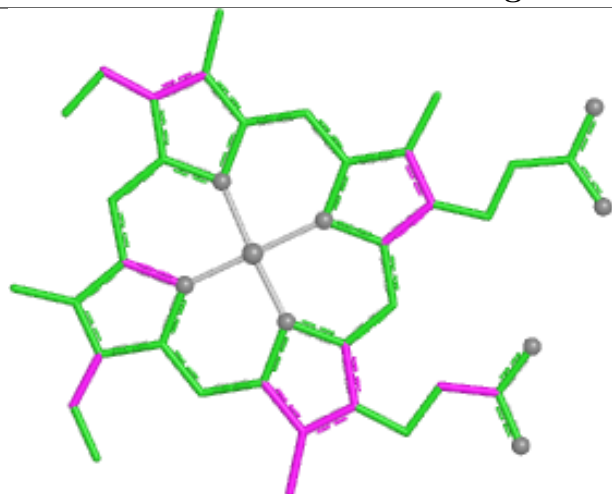


Rings

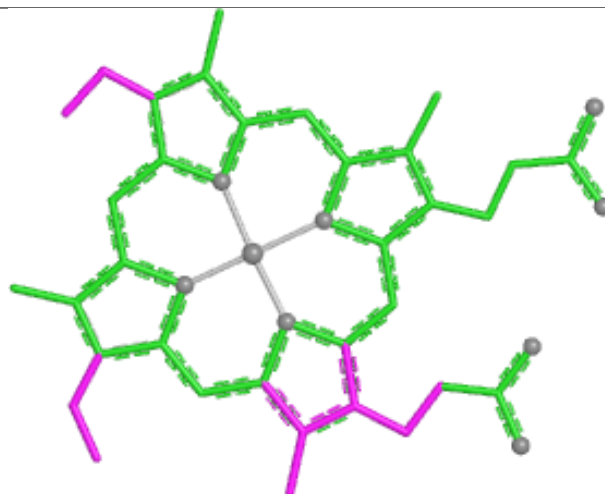
Ligand MGD C 1804



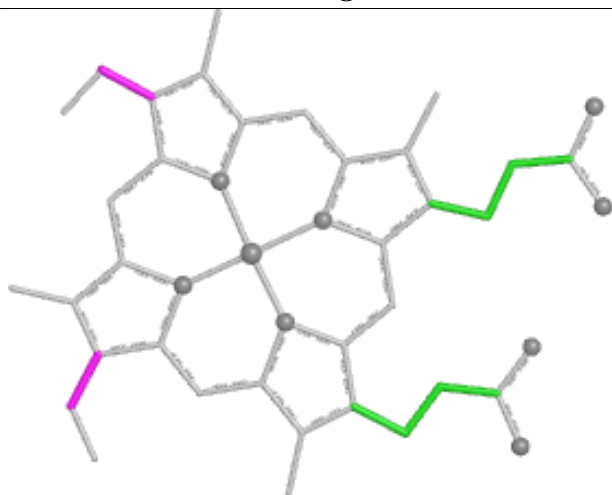
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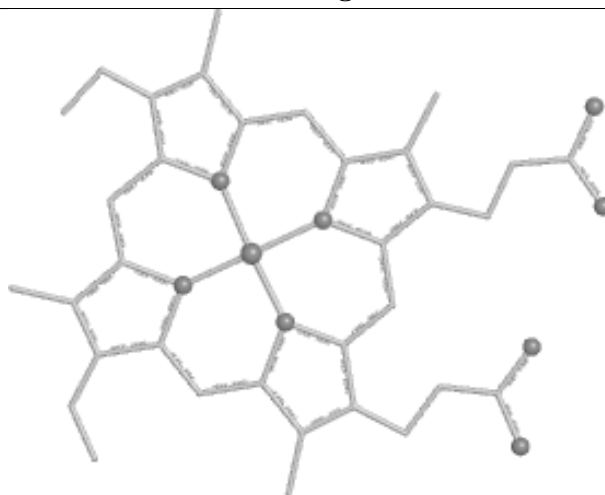
Bond lengths



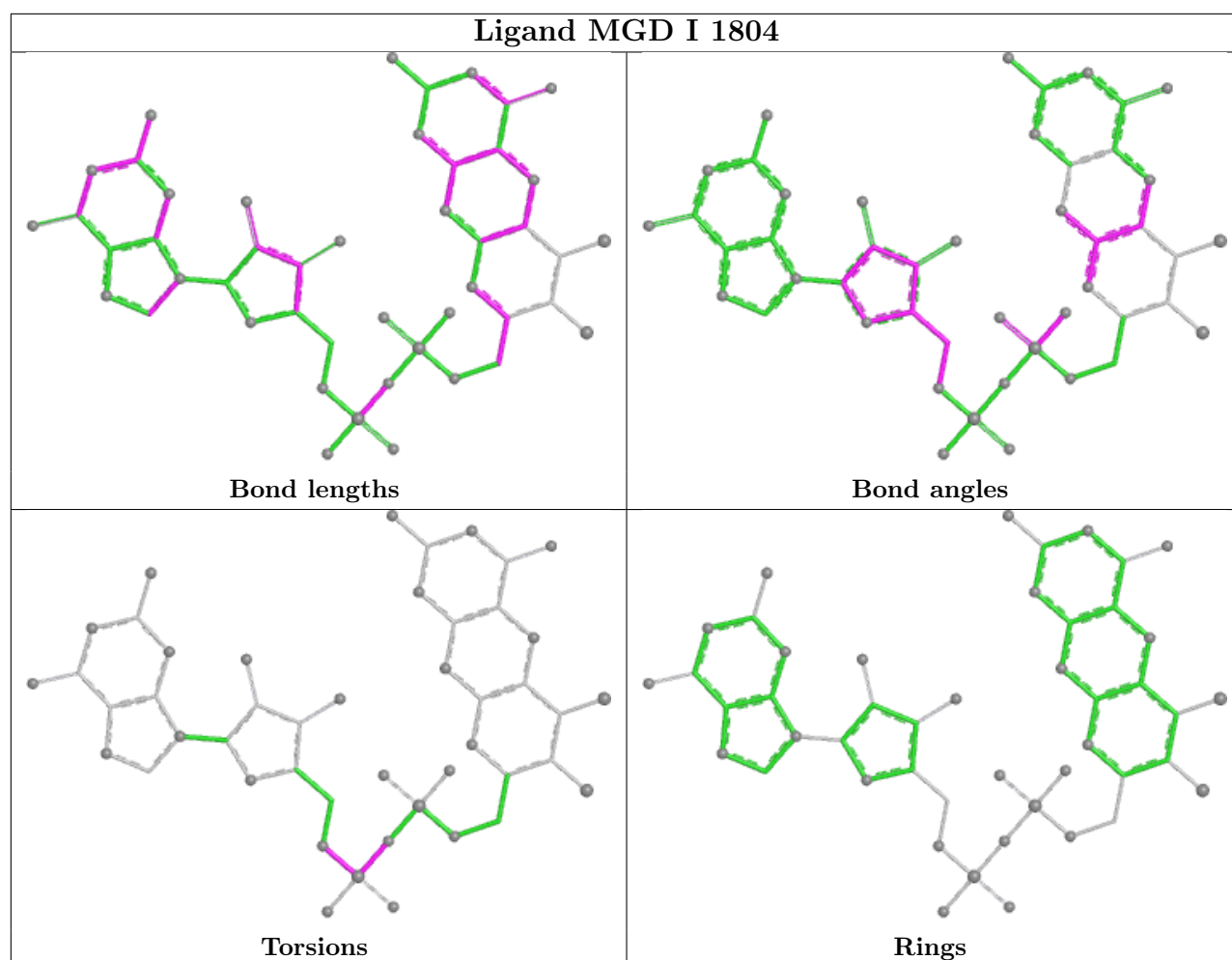
Bond angles



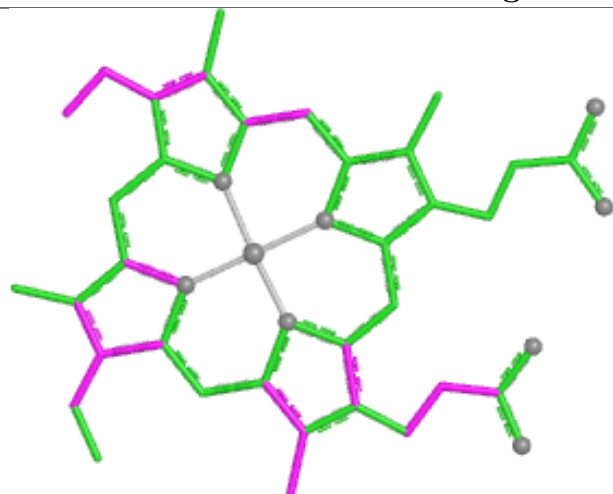
Torsions



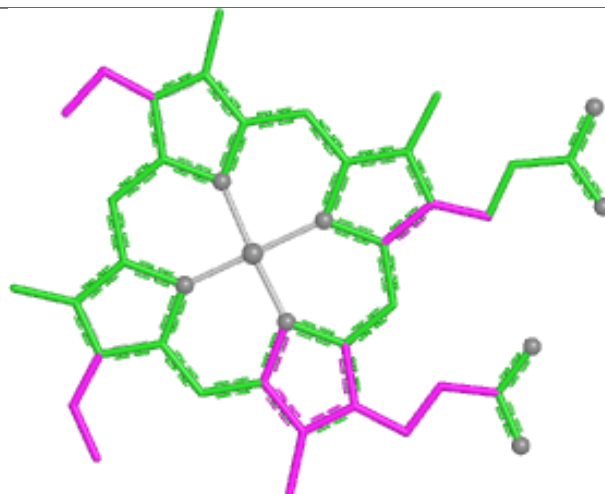
Rings



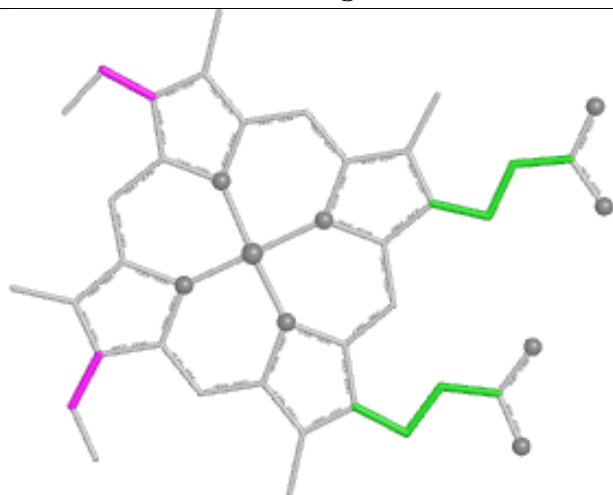
Ligand HEC H 1128



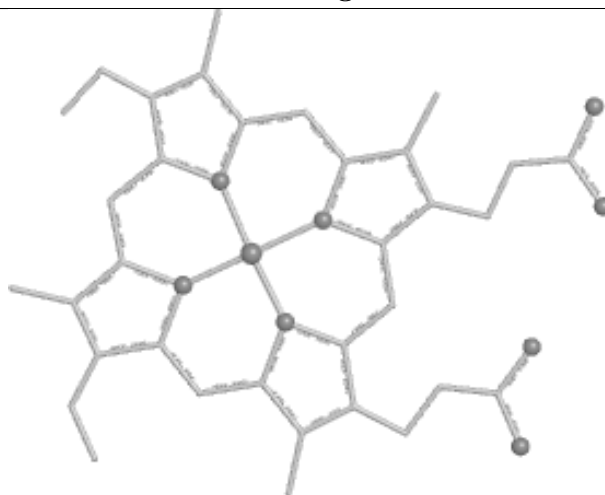
Bond lengths



Bond angles

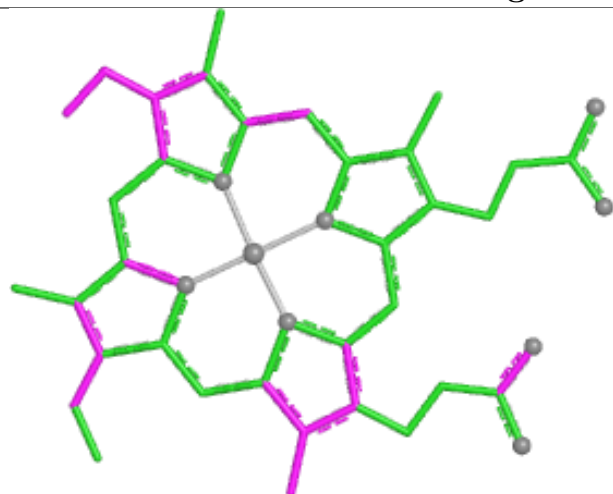


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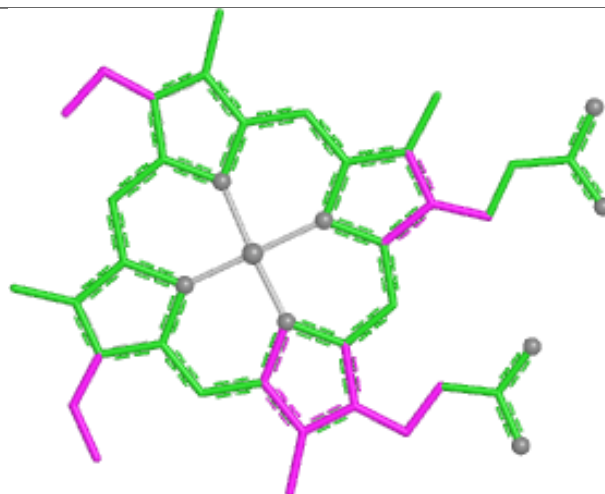


Rings

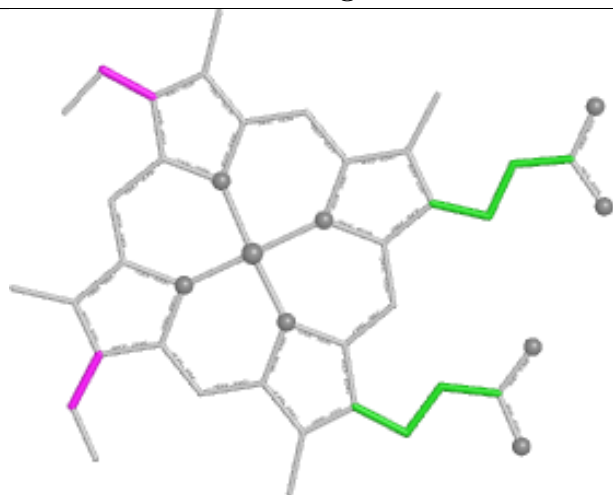
Ligand HEC J 1128



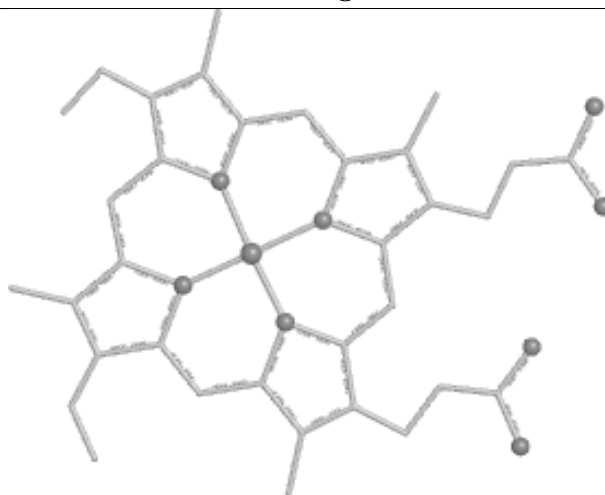
Bond lengths



Bond angles

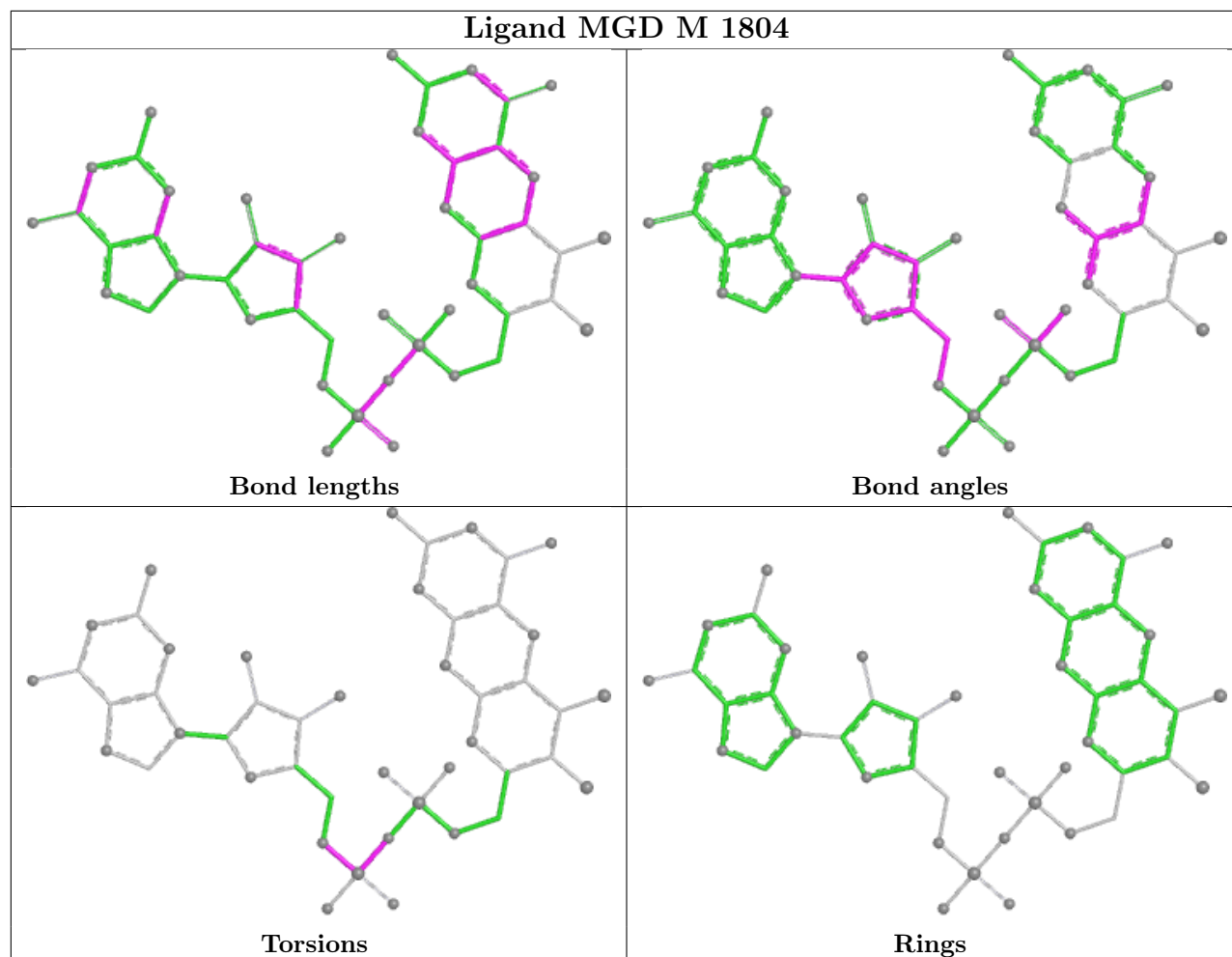


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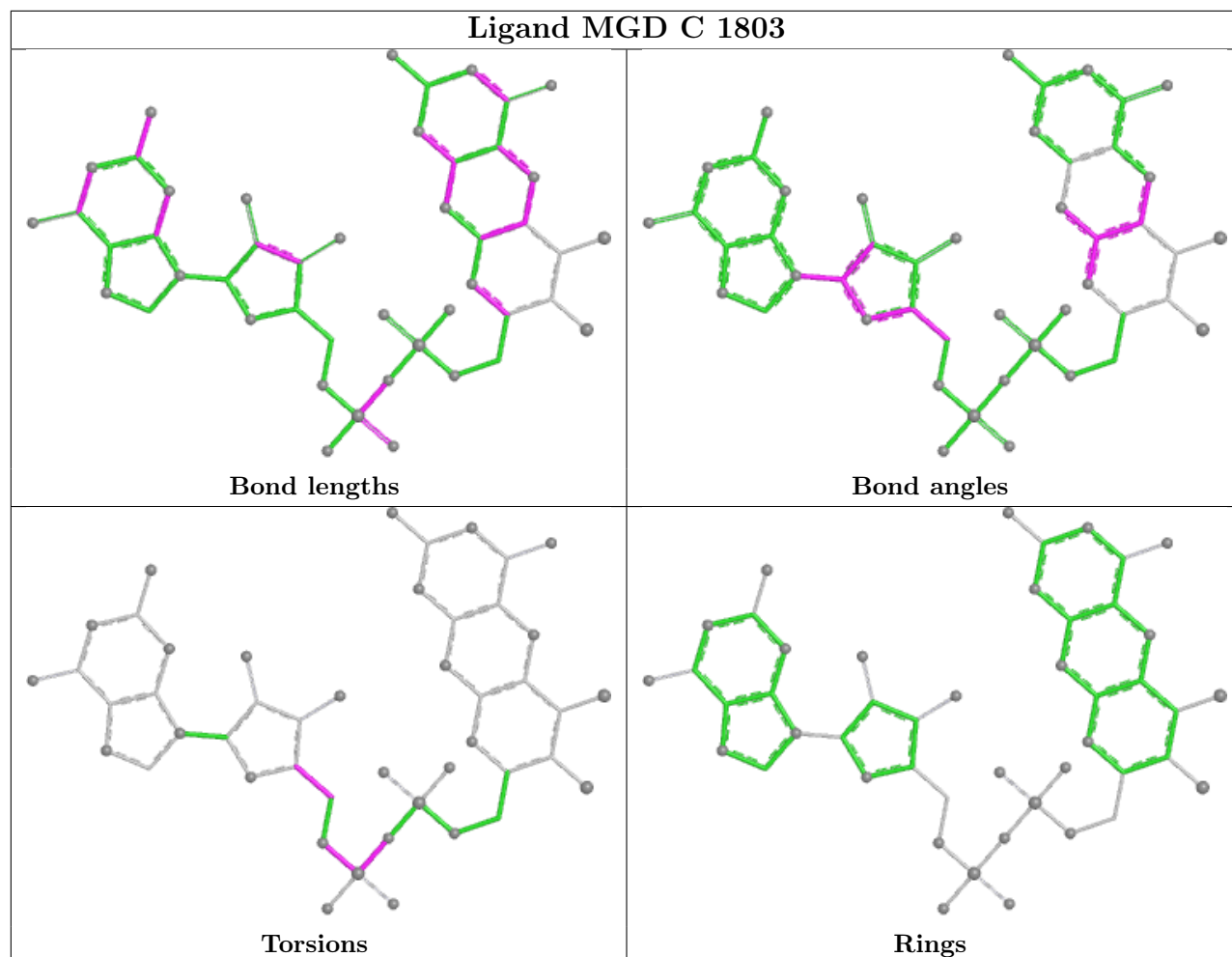


Rings

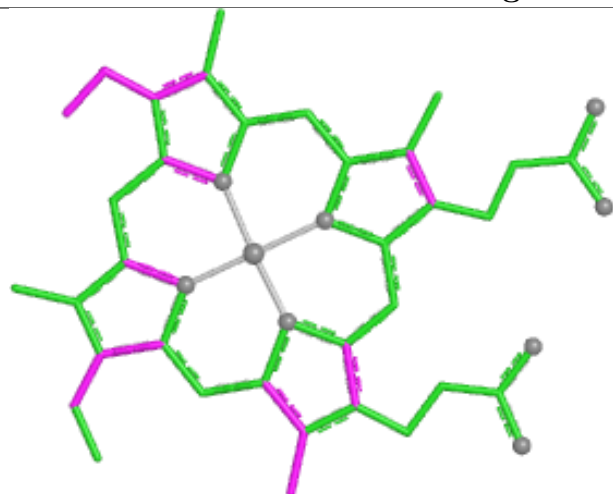
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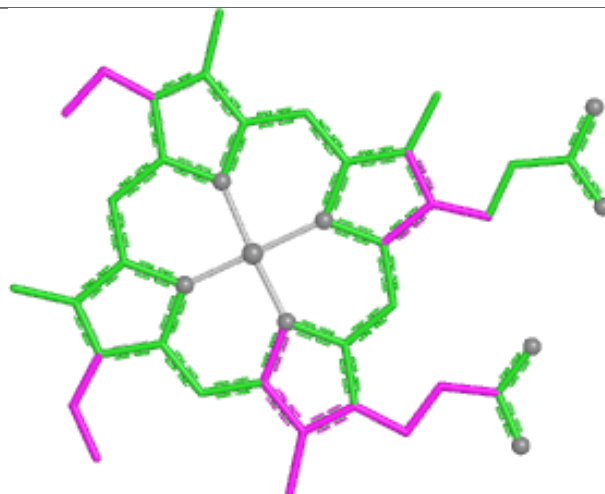
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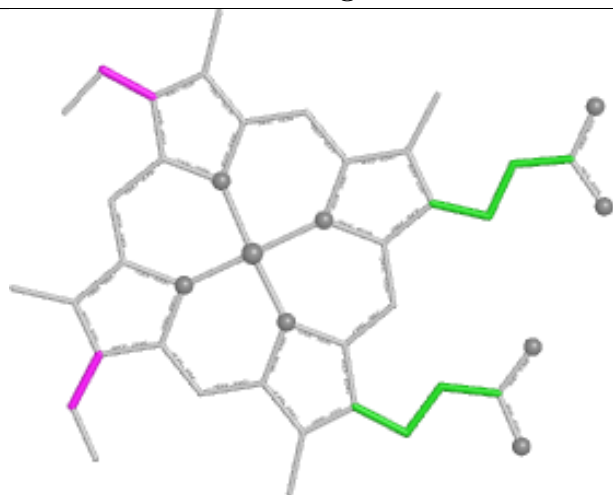
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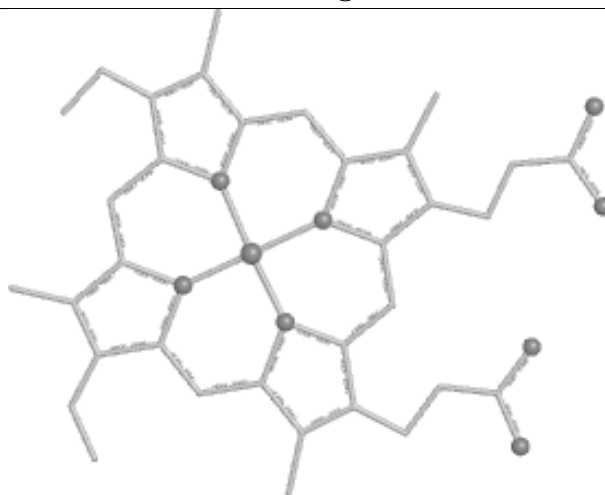
Bond lengths



Bond angles

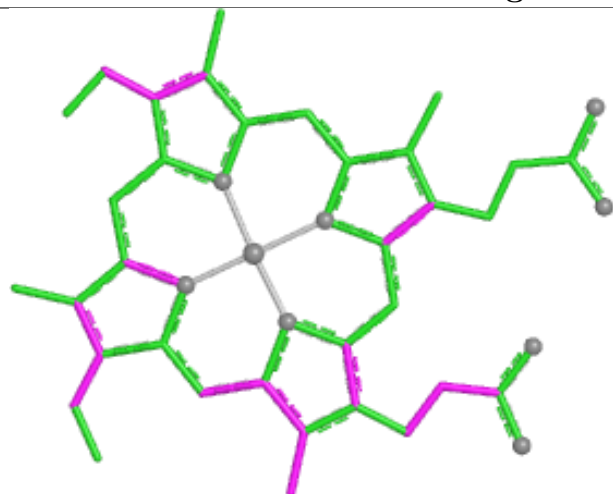


Torsions

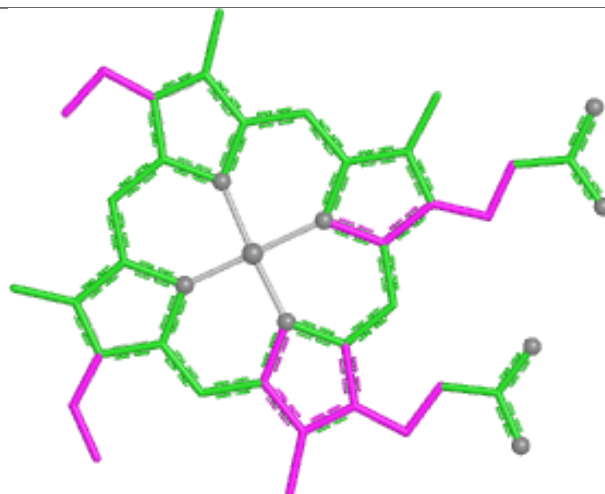


Rings

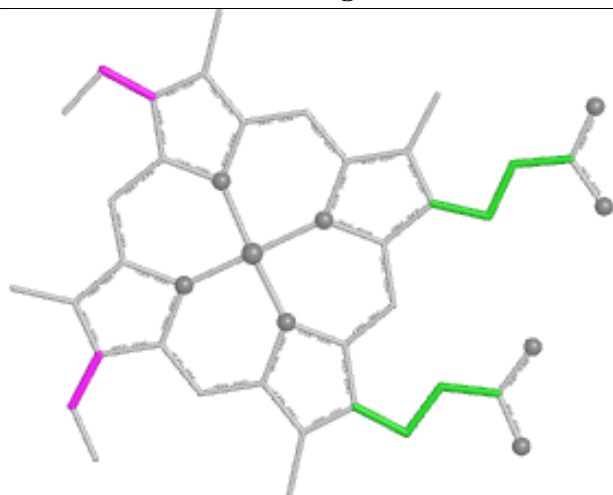
Ligand HEC L 1129



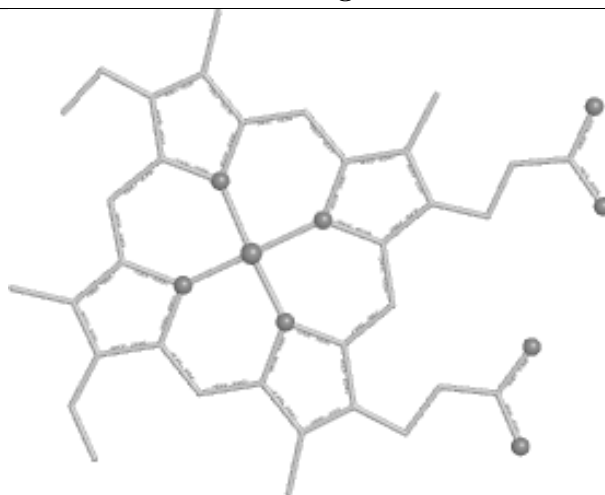
Bond lengths



Bond angles

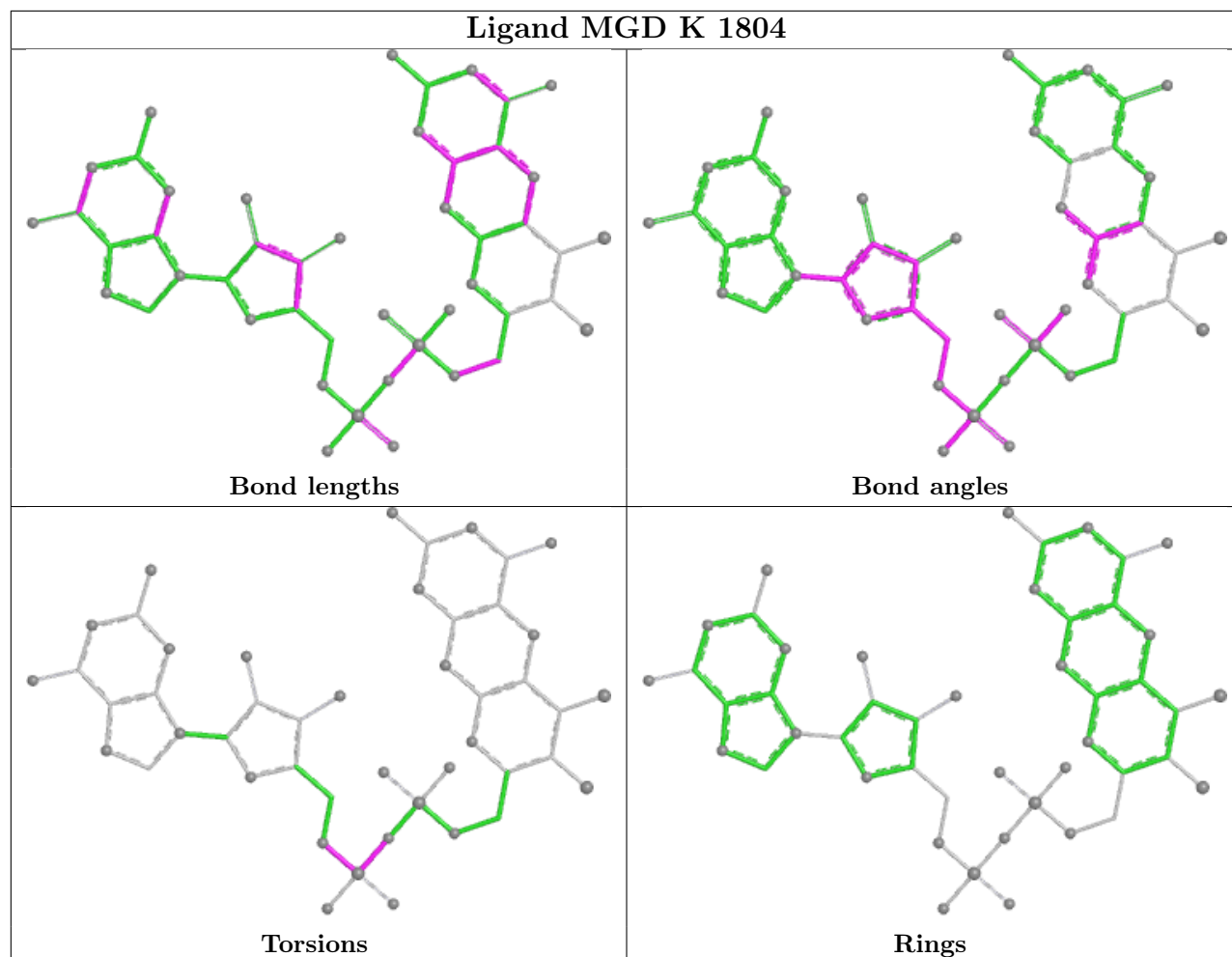


Torsions

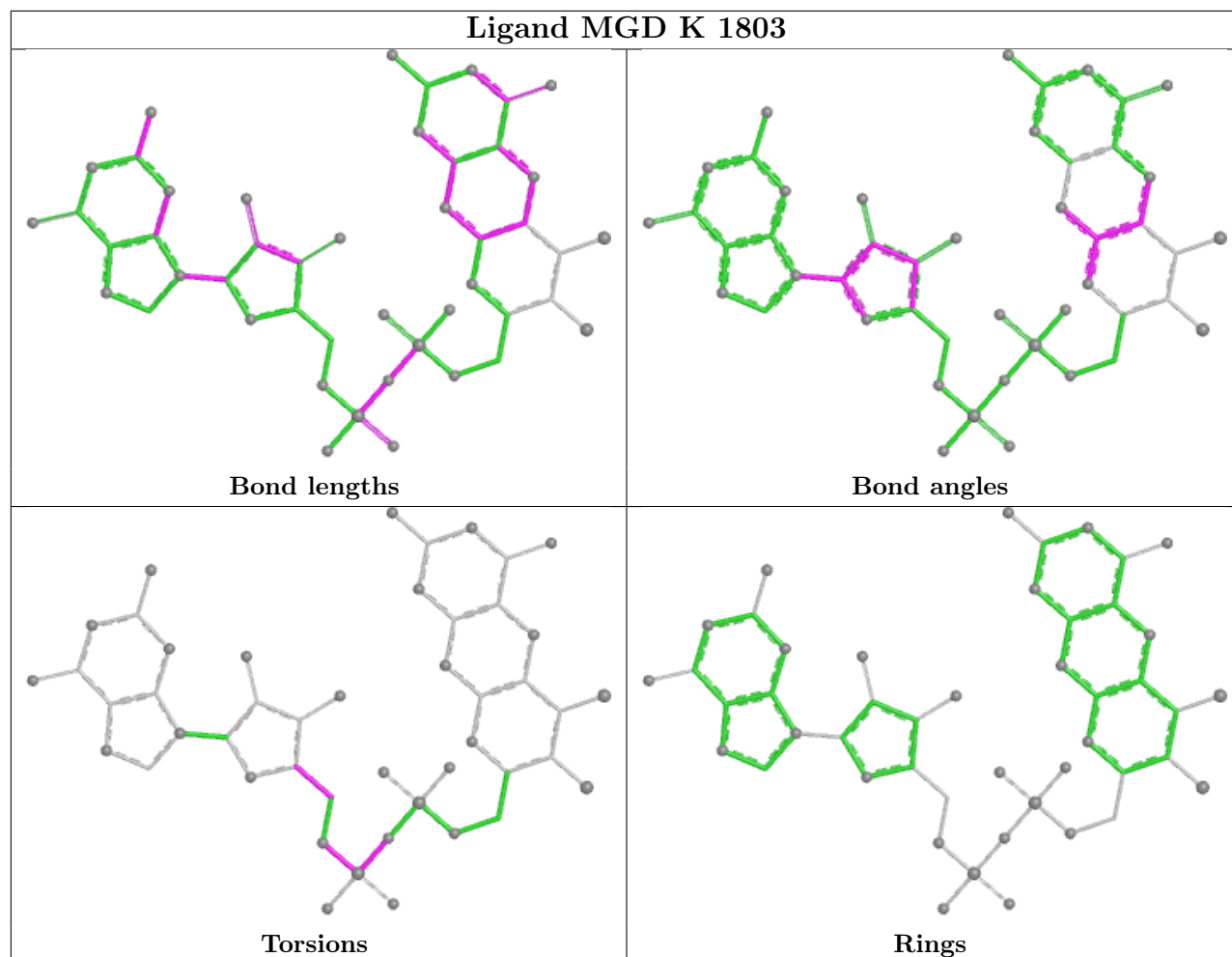


Rings

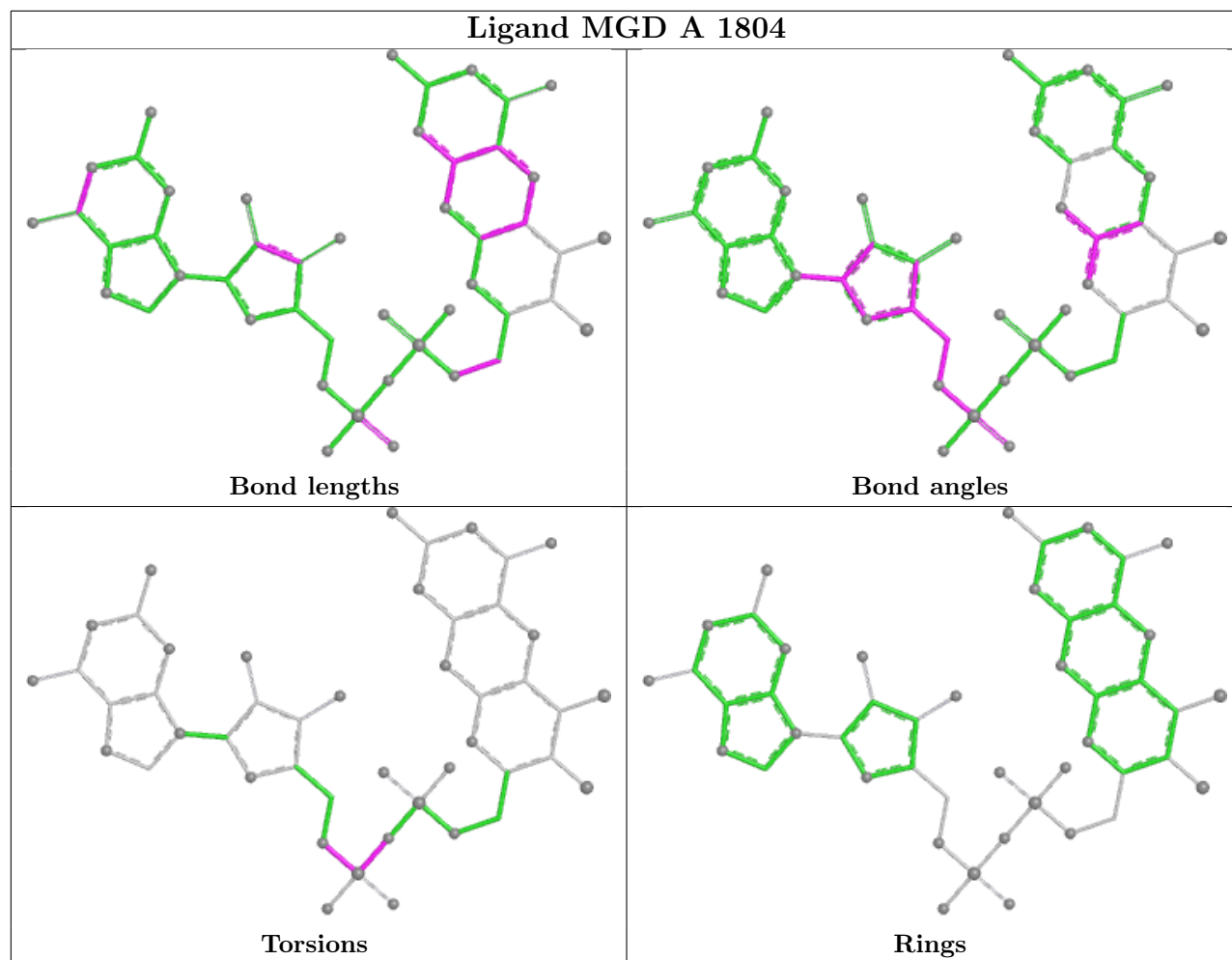
Ligand MGD K 1804



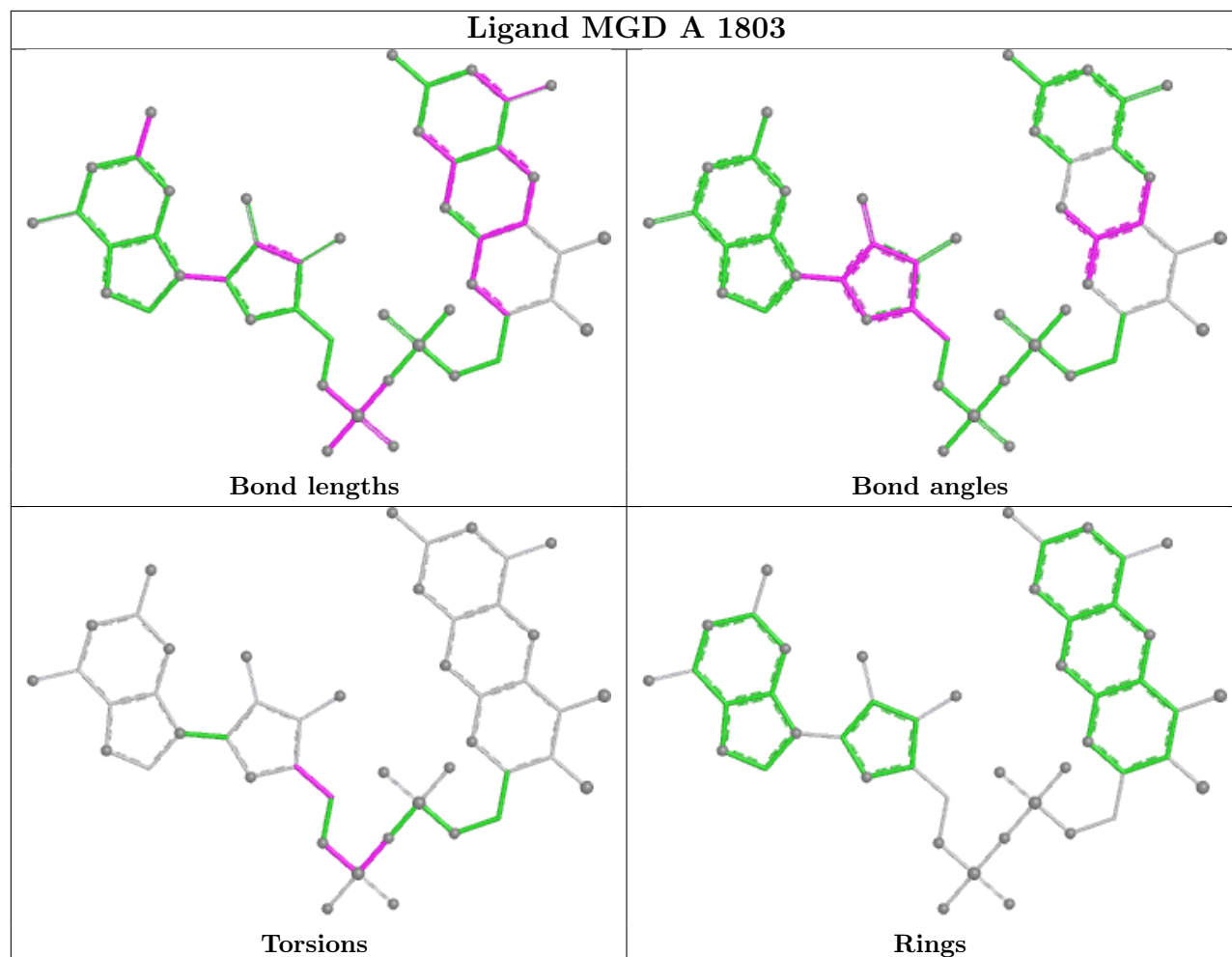
Ligand MGD K 1803



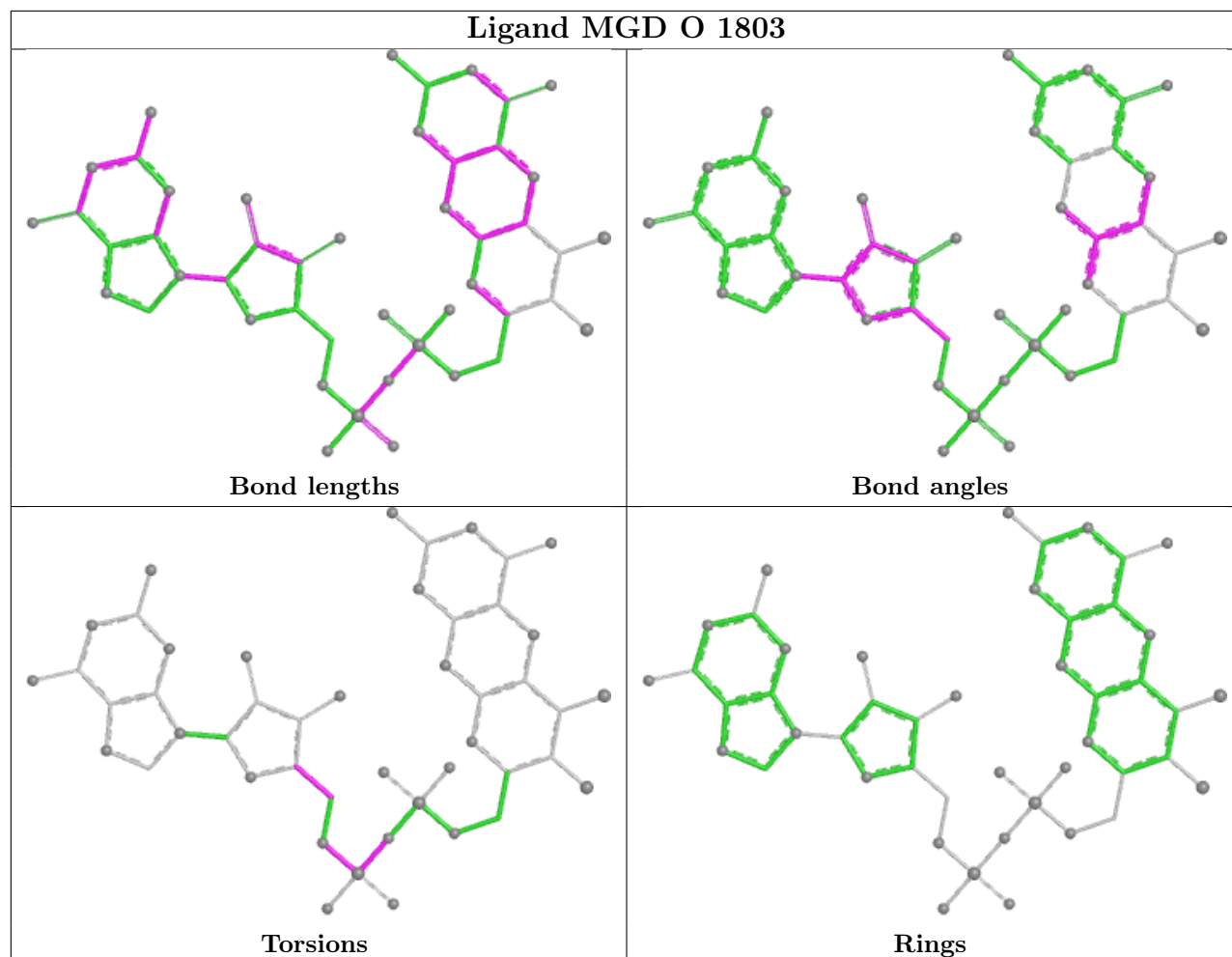
Ligand MGD A 1804



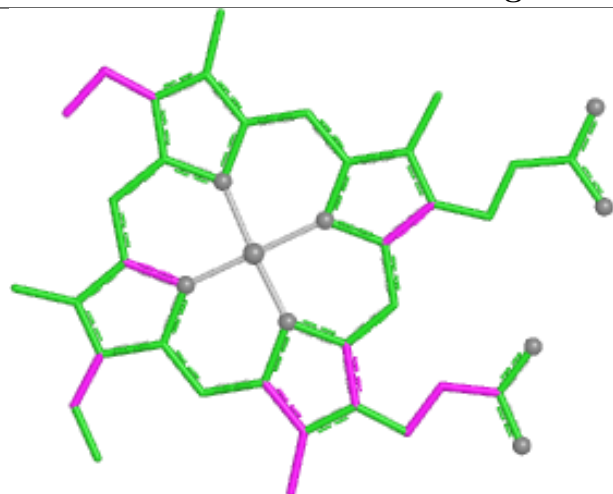
Ligand MGD A 1803



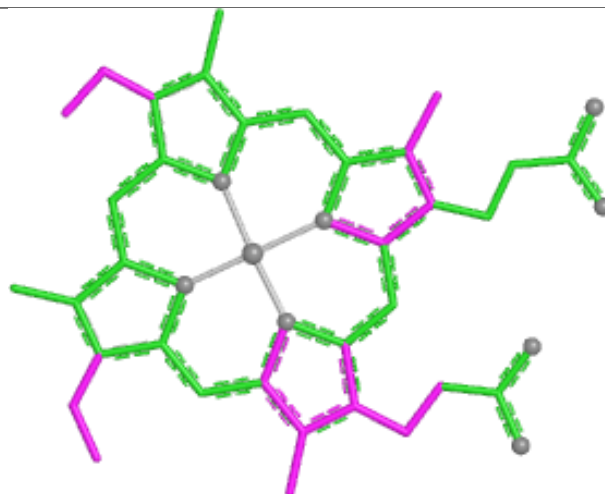
Ligand MGD O 1803



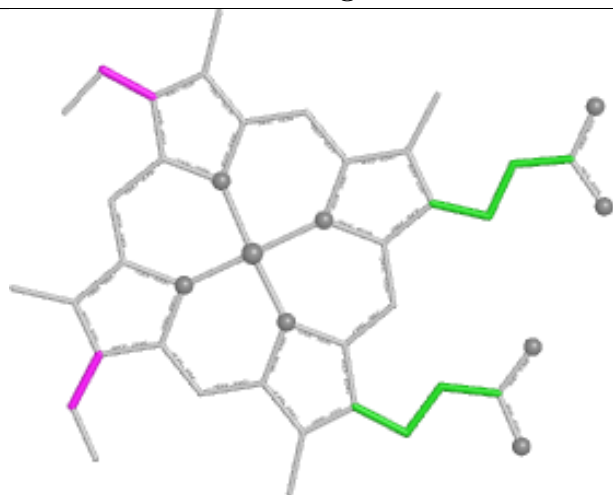
Ligand HEC P 1129



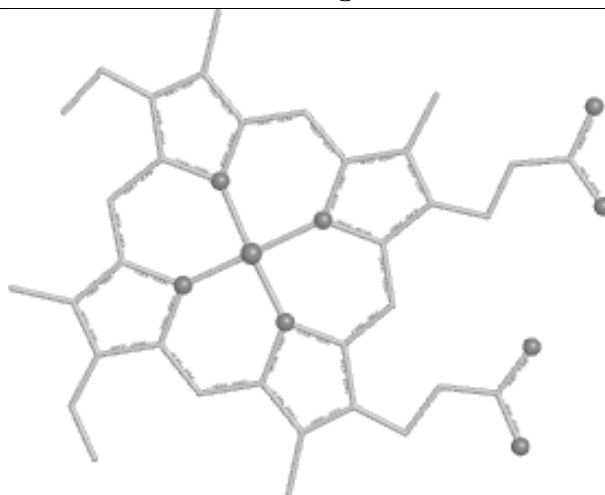
Bond lengths



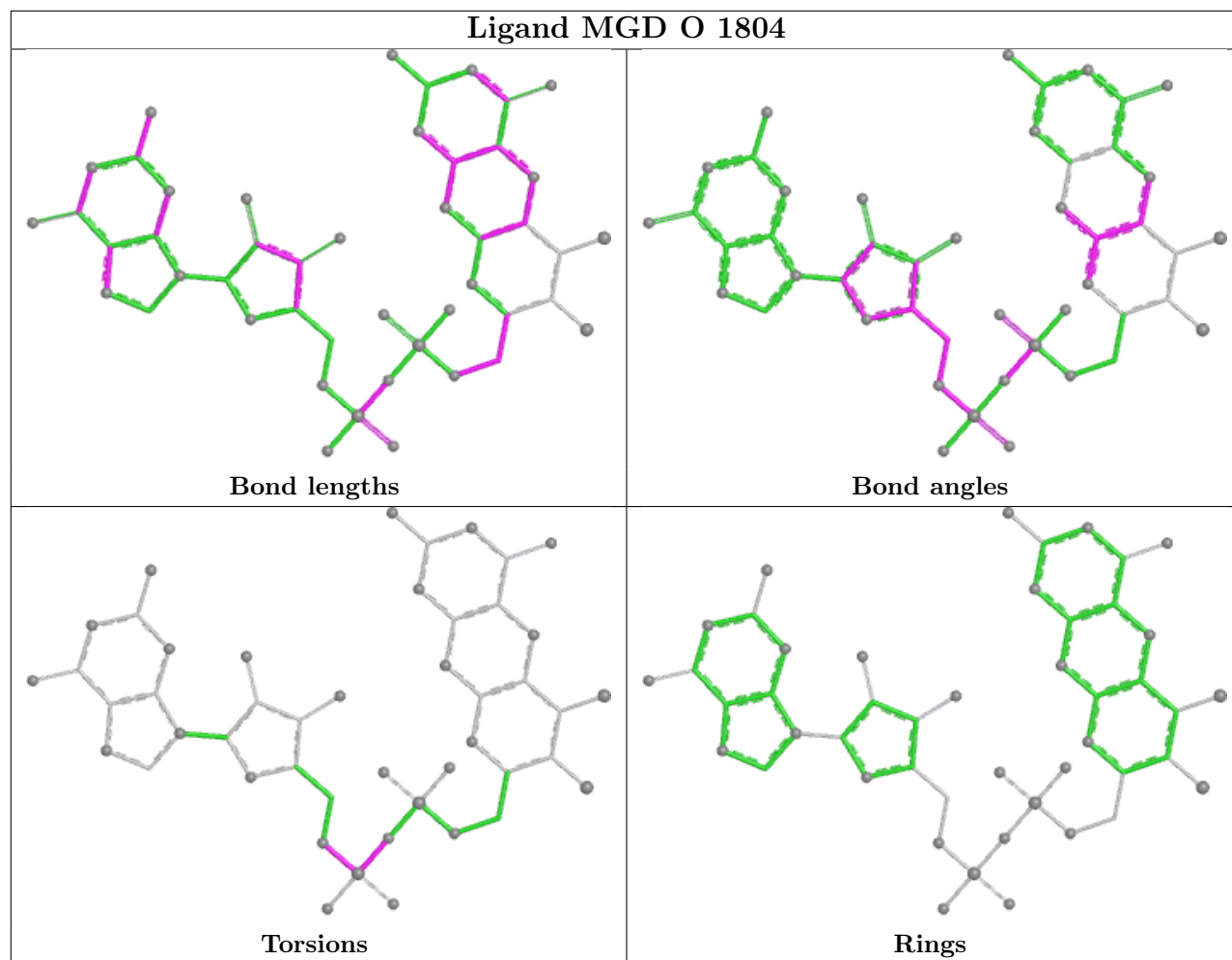
Bond angles



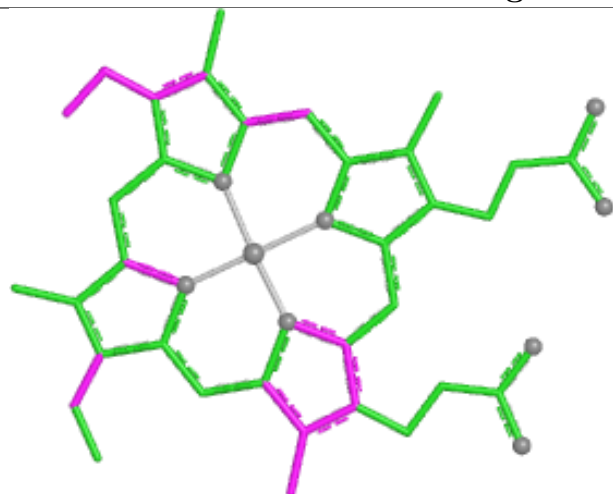
Torsions



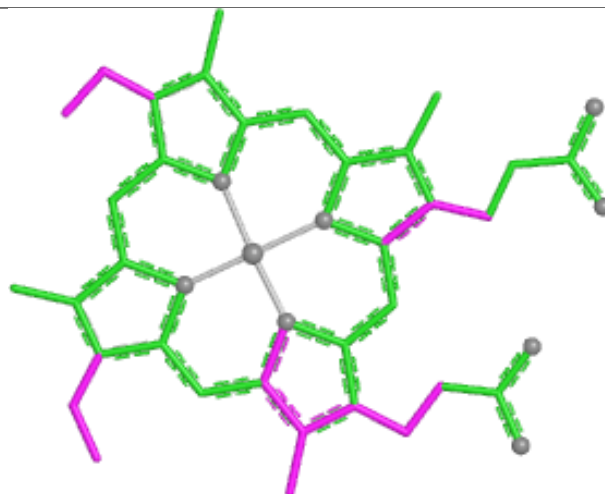
Rings



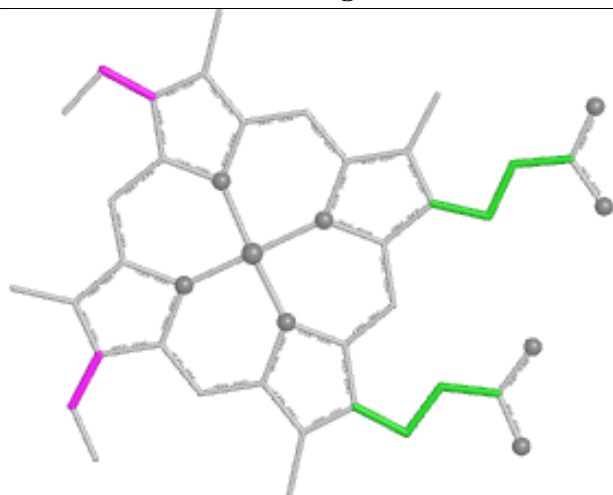
Ligand HEC L 1128



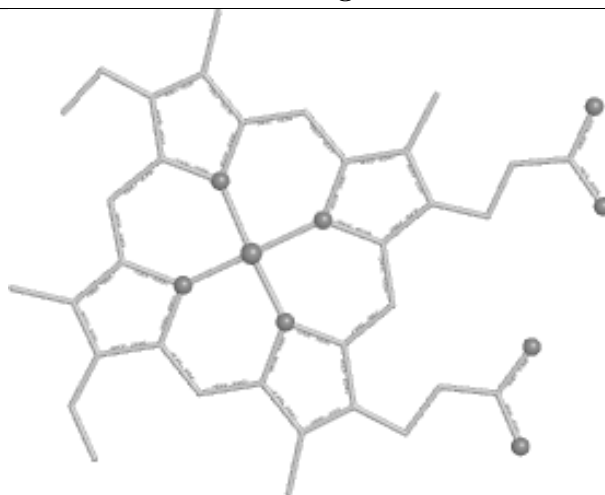
Bond lengths



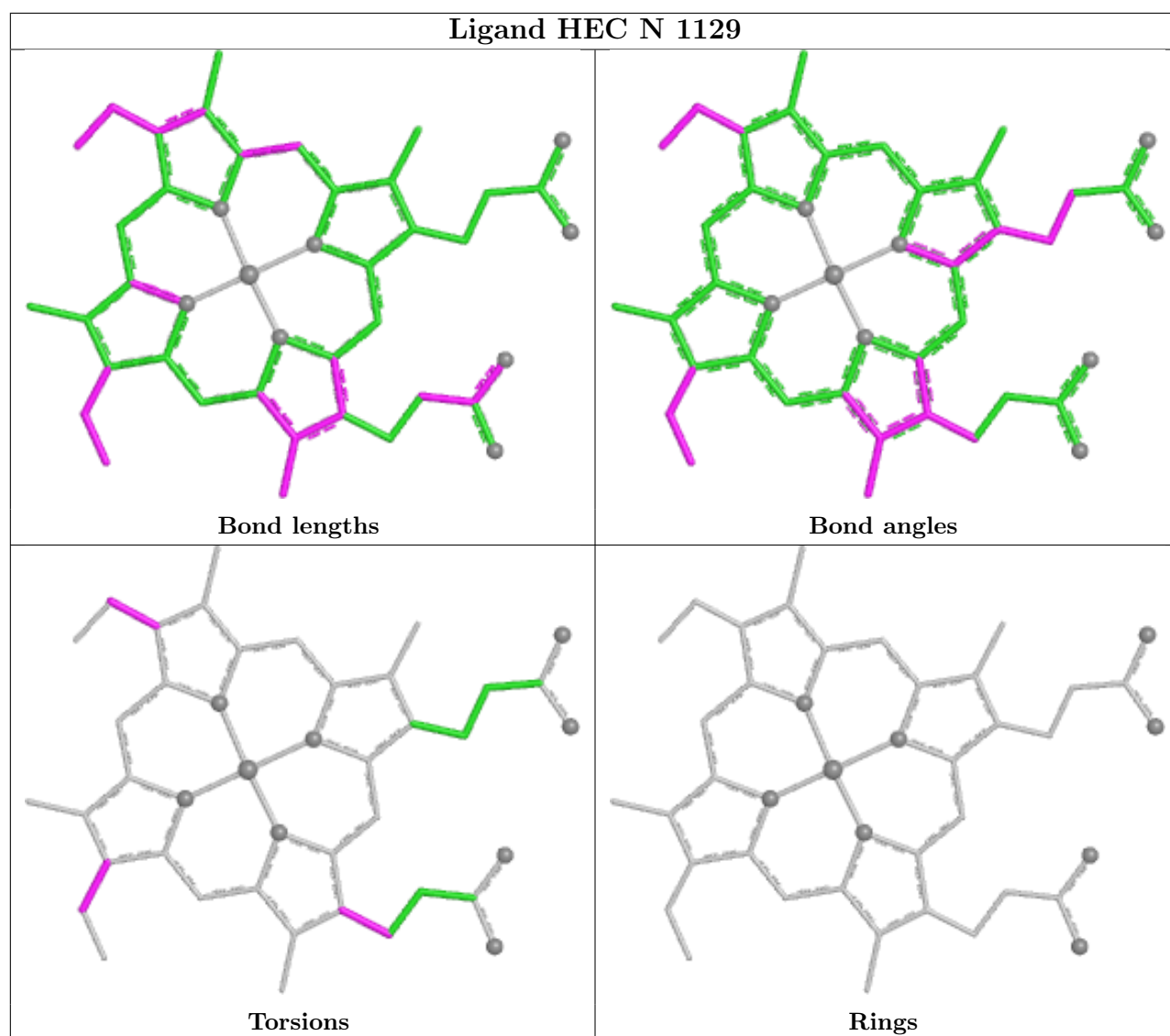
Bond angles



Torsions



Rings



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	790/802 (98%)	0.15	25 (3%)	50	31	10, 24, 60, 88	0
1	C	790/802 (98%)	0.22	21 (2%)	56	36	12, 38, 70, 92	0
1	E	790/802 (98%)	0.16	28 (3%)	47	29	10, 30, 63, 88	0
1	G	790/802 (98%)	0.27	18 (2%)	61	41	12, 44, 73, 92	0
1	I	790/802 (98%)	0.79	36 (4%)	37	23	23, 58, 77, 92	0
1	K	790/802 (98%)	0.29	24 (3%)	52	33	17, 43, 70, 90	0
1	M	790/802 (98%)	0.27	15 (1%)	66	46	13, 42, 70, 91	0
1	O	790/802 (98%)	0.64	32 (4%)	41	25	25, 53, 76, 95	0
2	B	127/130 (97%)	0.44	12 (9%)	14	9	10, 33, 70, 83	0
2	D	127/130 (97%)	0.41	10 (7%)	18	12	14, 38, 75, 87	0
2	F	127/130 (97%)	0.44	13 (10%)	12	8	11, 34, 70, 85	0
2	H	127/130 (97%)	0.44	10 (7%)	18	12	11, 39, 76, 86	0
2	J	127/130 (97%)	0.57	9 (7%)	22	14	18, 47, 82, 93	0
2	L	127/130 (97%)	0.39	6 (4%)	36	23	15, 38, 75, 96	0
2	N	127/130 (97%)	0.44	8 (6%)	26	17	12, 39, 74, 90	0
2	P	127/130 (97%)	0.49	6 (4%)	36	23	19, 44, 76, 89	0
All	All	7336/7456 (98%)	0.36	273 (3%)	45	28	10, 43, 73, 96	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	340	TRP	9.1
1	M	340	TRP	9.0
1	C	340	TRP	8.0
1	A	340	TRP	7.7
1	E	340	TRP	7.6

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Mol	Chain	Res	Type	RSRZ
1	O	340	TRP	7.0
1	G	340	TRP	6.6
1	I	340	TRP	6.2
1	G	801	ALA	5.7
1	A	80	GLY	5.0
1	E	79	ASP	4.8
1	G	80	GLY	4.5
1	E	80	GLY	4.4
1	C	655	GLY	4.3
2	H	2	ASP	4.2
1	A	298	THR	4.1
1	K	80	GLY	4.1
2	L	2	ASP	4.0
1	C	238	ARG	4.0
1	E	801	ALA	3.9
2	J	2	ASP	3.8
1	I	294	ALA	3.7
1	M	418	GLU	3.7
1	K	81	VAL	3.7
2	B	4	PRO	3.7
2	B	14	SER	3.7
2	N	8	GLY	3.6
1	M	79	ASP	3.4
1	C	79	ASP	3.4
1	A	81	VAL	3.3
1	E	299	ASP	3.3
1	M	655	GLY	3.3
2	N	2	ASP	3.3
1	A	801	ALA	3.3
1	G	122	GLY	3.3
1	A	79	ASP	3.2
1	C	801	ALA	3.2
1	G	238	ARG	3.2
1	A	555	SER	3.2
1	C	12	ILE	3.2
1	O	298	THR	3.2
2	N	9	ALA	3.1
1	C	80	GLY	3.1
1	O	555	SER	3.1
2	L	10	ASP	3.1
2	F	5	ARG	3.1
2	L	4	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	3	ALA	3.1
1	G	655	GLY	3.1
1	A	626	GLU	3.1
1	K	411	GLU	3.1
2	H	8	GLY	3.1
2	D	4	PRO	3.1
2	H	3	ALA	3.0
1	M	78	LYS	3.0
2	D	14	SER	3.0
1	M	117	GLY	3.0
1	E	285	ALA	3.0
1	E	418	GLU	2.9
1	A	800	GLU	2.9
1	O	81	VAL	2.9
1	C	87	GLU	2.9
1	M	801	ALA	2.8
1	O	140	PHE	2.8
2	H	9	ALA	2.8
1	A	781	ASP	2.8
1	I	238	ARG	2.8
1	C	117	GLY	2.8
1	E	12	ILE	2.8
1	E	476	GLU	2.8
2	B	7	THR	2.8
1	E	781	ASP	2.8
1	K	801	ALA	2.8
1	E	42	GLY	2.7
1	K	728	ARG	2.7
1	O	12	ILE	2.7
1	C	763	VAL	2.7
1	E	81	VAL	2.7
2	D	6	LEU	2.7
2	J	12	PRO	2.7
2	P	7	THR	2.7
1	O	238	ARG	2.7
2	B	3	ALA	2.7
1	I	81	VAL	2.7
1	A	110	GLU	2.7
1	K	418	GLU	2.7
2	B	6	LEU	2.7
1	E	238	ARG	2.7
2	J	8	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	781	ASP	2.7
2	B	27	ASP	2.7
1	O	550	PRO	2.6
1	C	78	LYS	2.6
1	M	81	VAL	2.6
1	A	280	HIS	2.6
2	N	4	PRO	2.6
1	A	418	GLU	2.6
1	E	298	THR	2.6
1	I	420	TRP	2.6
2	B	123	MET	2.6
1	A	278	PRO	2.6
1	I	171	GLY	2.6
1	A	12	ILE	2.6
1	A	299	ASP	2.6
2	F	2	ASP	2.6
1	O	290	ALA	2.6
1	K	300	PHE	2.5
1	I	550	PRO	2.5
2	H	4	PRO	2.5
1	I	535	GLN	2.5
2	B	2	ASP	2.5
1	K	292	ALA	2.5
2	F	3	ALA	2.5
1	E	272	ILE	2.5
2	B	12	PRO	2.5
2	L	5	ARG	2.5
1	I	474	ASN	2.5
2	D	2	ASP	2.5
1	M	238	ARG	2.5
2	B	8	GLY	2.5
1	I	363	ASN	2.5
1	I	300	PHE	2.5
2	H	7	THR	2.5
1	K	238	ARG	2.5
1	K	282	LEU	2.5
1	O	569	LEU	2.5
1	C	611	GLY	2.5
1	O	548	VAL	2.5
2	H	31	VAL	2.5
1	M	476	GLU	2.5
2	H	5	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	6	LEU	2.5
2	P	75	ILE	2.4
2	F	10	ASP	2.4
1	G	580	ALA	2.4
1	C	800	GLU	2.4
1	O	482	SER	2.4
1	G	79	ASP	2.4
1	M	719	VAL	2.4
1	K	290	ALA	2.4
1	C	85	GLU	2.4
1	O	648	PHE	2.4
1	C	335	ASP	2.4
1	K	719	VAL	2.4
1	C	292	ALA	2.4
1	O	556	ALA	2.4
2	N	5	ARG	2.4
1	C	729	SER	2.4
1	O	234	PRO	2.4
1	E	335	ASP	2.4
1	E	337	ASP	2.4
1	I	104	ALA	2.4
1	I	419	ILE	2.4
2	D	3	ALA	2.4
2	F	108	ALA	2.4
1	O	295	MET	2.4
2	P	11	ARG	2.4
1	G	110	GLU	2.4
1	I	719	VAL	2.4
1	I	80	GLY	2.3
1	I	629	GLY	2.3
2	N	7	THR	2.3
2	J	107	ASN	2.3
1	G	81	VAL	2.3
1	A	77	MET	2.3
1	K	257	ASP	2.3
1	I	449	PHE	2.3
1	A	87	GLU	2.3
1	O	285	ALA	2.3
2	L	14	SER	2.3
2	P	2	ASP	2.3
1	G	116	VAL	2.3
1	I	451	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	80	GLY	2.3
1	K	269	ALA	2.3
1	E	300	PHE	2.3
1	A	281	GLN	2.3
1	I	492	ALA	2.3
1	K	492	ALA	2.3
1	K	655	GLY	2.3
1	O	461	ALA	2.3
1	O	319	SER	2.3
2	F	45	SER	2.3
2	J	45	SER	2.3
1	K	79	ASP	2.3
1	C	77	MET	2.2
1	G	693	GLY	2.2
2	F	4	PRO	2.2
1	I	801	ALA	2.2
1	O	77	MET	2.2
1	O	106	LEU	2.2
2	J	31	VAL	2.2
1	C	208	GLU	2.2
1	G	86	GLY	2.2
1	E	729	SER	2.2
1	A	208	GLU	2.2
1	I	416	ALA	2.2
1	K	615	GLY	2.2
1	O	96	ALA	2.2
2	B	109	GLN	2.2
1	C	447	ILE	2.2
2	D	115	GLU	2.2
2	F	107	ASN	2.2
1	E	611	GLY	2.2
1	O	416	ALA	2.2
1	I	270	THR	2.2
1	I	431	VAL	2.2
1	I	450	TYR	2.2
1	O	116	VAL	2.2
1	E	84	LYS	2.2
1	K	294	ALA	2.2
1	K	386	PHE	2.2
1	I	365	HIS	2.2
1	G	311	THR	2.1
2	J	7	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	6	LEU	2.1
1	A	285	ALA	2.1
1	E	87	GLU	2.1
1	M	796	ALA	2.1
1	A	297	PRO	2.1
2	L	8	GLY	2.1
2	P	4	PRO	2.1
2	F	7	THR	2.1
1	I	447	ILE	2.1
2	F	9	ALA	2.1
1	E	655	GLY	2.1
1	O	629	GLY	2.1
1	C	81	VAL	2.1
2	H	27	ASP	2.1
1	I	70	LEU	2.1
1	K	487	THR	2.1
2	D	7	THR	2.1
2	F	11	ARG	2.1
1	E	289	ALA	2.1
1	O	289	ALA	2.1
1	A	746	GLU	2.1
1	G	615	GLY	2.1
1	K	684	GLU	2.1
1	A	783	ASN	2.1
2	B	107	ASN	2.1
1	I	116	VAL	2.1
1	O	575	VAL	2.1
1	I	124	TRP	2.1
1	K	781	ASP	2.1
1	M	108	LEU	2.1
1	O	554	LEU	2.1
1	I	118	MET	2.1
1	E	559	ALA	2.1
2	N	12	PRO	2.1
1	I	148	ASN	2.1
1	M	141	ARG	2.1
2	N	6	LEU	2.1
1	G	590	HIS	2.1
1	E	492	ALA	2.1
1	O	801	ALA	2.1
1	G	281	GLN	2.1
1	E	551	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	85	GLU	2.1
2	J	4	PRO	2.1
2	D	70	VAL	2.0
1	I	559	ALA	2.0
2	F	121	THR	2.0
1	E	293	GLY	2.0
2	D	8	GLY	2.0
1	O	407	VAL	2.0
1	I	145	LEU	2.0
2	H	14	SER	2.0
1	I	783	ASN	2.0
1	I	151	HIS	2.0
1	A	283	GLN	2.0
1	G	352	VAL	2.0
2	D	128	GLU	2.0
1	I	775	ILE	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MGD	I	1804	47/47	0.89	0.11	47,53,61,64	0
5	MGD	O	1804	47/47	0.89	0.12	46,50,53,54	0
5	MGD	I	1803	47/47	0.90	0.11	34,49,58,61	0
6	HEC	P	1129	43/43	0.91	0.14	23,40,42,43	0
5	MGD	K	1804	47/47	0.92	0.11	24,36,39,42	0
6	HEC	J	1129	43/43	0.92	0.15	32,43,47,50	0
5	MGD	O	1803	47/47	0.92	0.09	37,45,56,57	0

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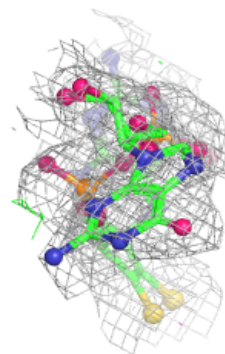
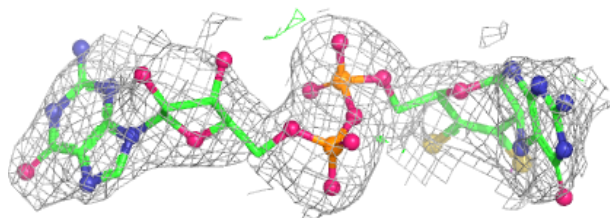
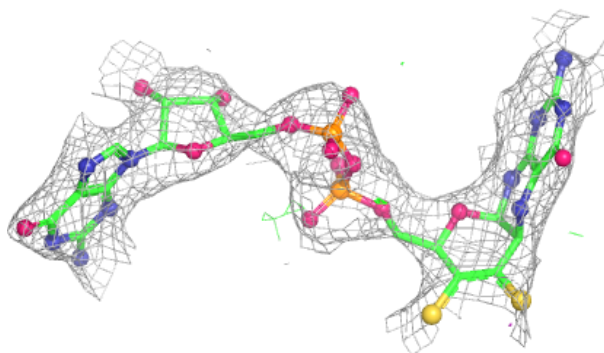
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MGD	G	1804	47/47	0.93	0.10	28,35,39,42	0
6	HEC	L	1129	43/43	0.93	0.16	10,29,44,46	0
6	HEC	N	1129	43/43	0.93	0.14	18,27,41,44	0
6	HEC	P	1128	43/43	0.93	0.14	27,37,49,54	0
6	HEC	H	1129	43/43	0.93	0.15	13,19,42,46	0
5	MGD	C	1804	47/47	0.94	0.10	21,27,39,40	0
6	HEC	J	1128	43/43	0.94	0.12	31,37,50,56	0
5	MGD	E	1804	47/47	0.94	0.10	10,12,20,24	0
6	HEC	L	1128	43/43	0.94	0.11	27,35,44,51	0
6	HEC	D	1128	43/43	0.94	0.12	20,29,44,52	0
6	HEC	F	1128	43/43	0.94	0.12	14,23,47,56	0
6	HEC	F	1129	43/43	0.94	0.14	10,19,38,43	0
6	HEC	H	1128	43/43	0.94	0.12	15,24,38,45	0
6	HEC	D	1129	43/43	0.95	0.13	14,19,48,55	0
5	MGD	M	1803	47/47	0.95	0.08	23,28,34,36	0
5	MGD	M	1804	47/47	0.95	0.09	23,26,30,34	0
6	HEC	N	1128	43/43	0.95	0.11	25,31,43,51	0
5	MGD	C	1803	47/47	0.95	0.09	19,26,32,34	0
5	MGD	K	1803	47/47	0.95	0.08	31,34,36,40	0
5	MGD	G	1803	47/47	0.95	0.08	23,26,36,37	0
4	MO	I	1802	1/1	0.96	0.04	66,66,66,66	0
5	MGD	A	1803	47/47	0.96	0.08	10,12,16,17	0
6	HEC	B	1128	43/43	0.96	0.10	12,15,38,45	0
6	HEC	B	1129	43/43	0.96	0.11	10,16,36,41	0
5	MGD	E	1803	47/47	0.96	0.08	10,17,21,22	0
5	MGD	A	1804	47/47	0.96	0.09	10,10,12,18	0
4	MO	O	1802	1/1	0.97	0.03	62,62,62,62	0
3	SF4	O	1801	8/8	0.97	0.06	29,30,33,33	0
3	SF4	I	1801	8/8	0.97	0.05	34,37,37,39	0
3	SF4	C	1801	8/8	0.99	0.03	10,10,11,12	0
4	MO	A	1802	1/1	0.99	0.02	24,24,24,24	0
4	MO	C	1802	1/1	0.99	0.02	38,38,38,38	0
4	MO	E	1802	1/1	0.99	0.02	28,28,28,28	0
4	MO	G	1802	1/1	0.99	0.03	35,35,35,35	0
3	SF4	G	1801	8/8	0.99	0.04	10,10,12,12	0
4	MO	K	1802	1/1	0.99	0.03	40,40,40,40	0
3	SF4	A	1801	8/8	0.99	0.04	10,10,10,12	0
3	SF4	K	1801	8/8	0.99	0.03	10,10,11,12	0
3	SF4	M	1801	8/8	0.99	0.03	10,10,12,12	0
4	MO	M	1802	1/1	1.00	0.02	39,39,39,39	0
3	SF4	E	1801	8/8	1.00	0.03	10,10,11,12	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.

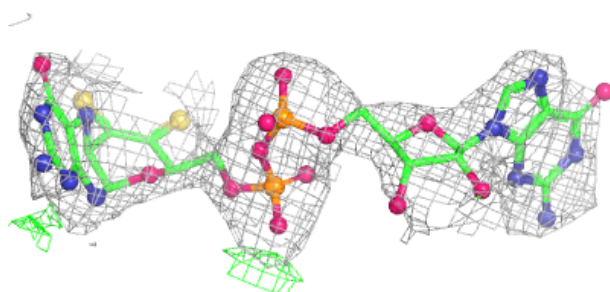
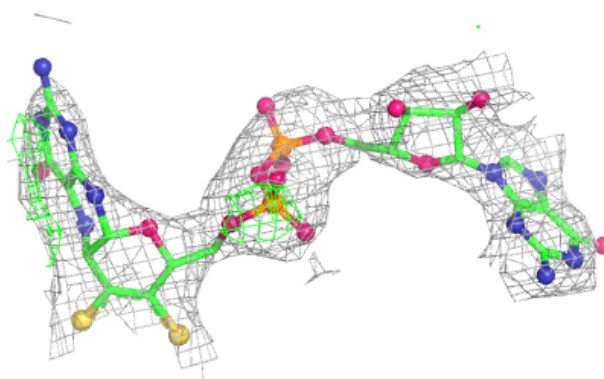
Electron density around MGD I 1804:

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

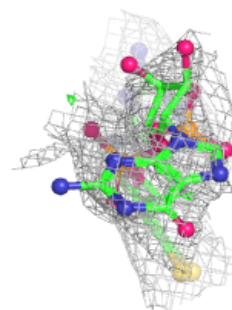
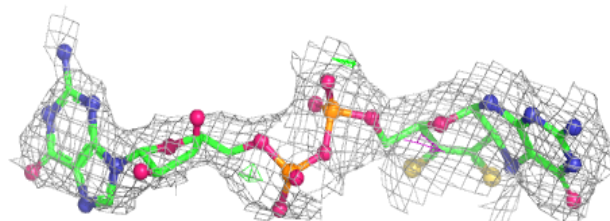
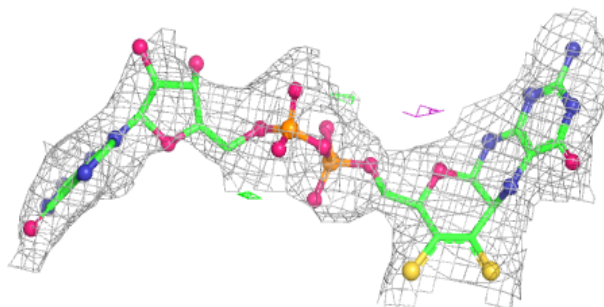


Electron density around MGD O 1804:

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

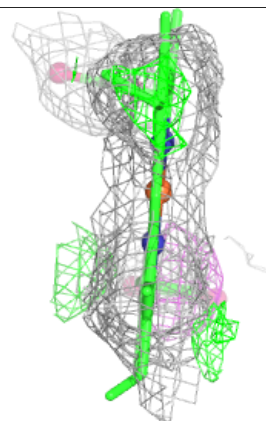
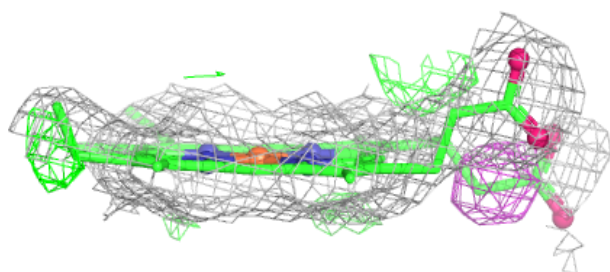
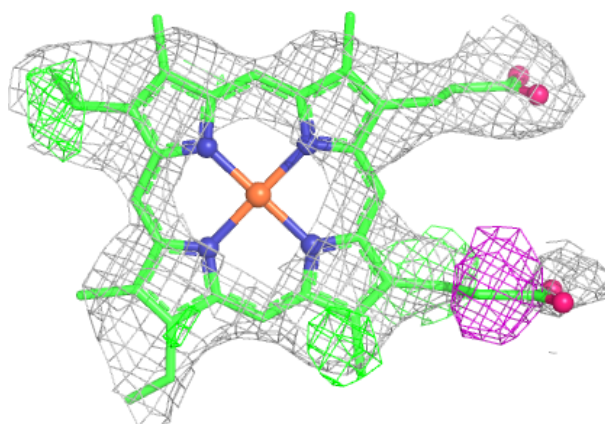
**Electron density around MGD I 1803:**

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

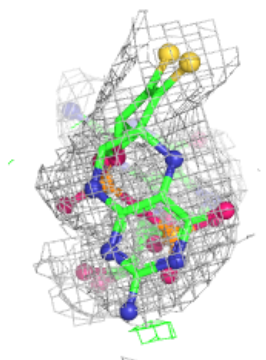
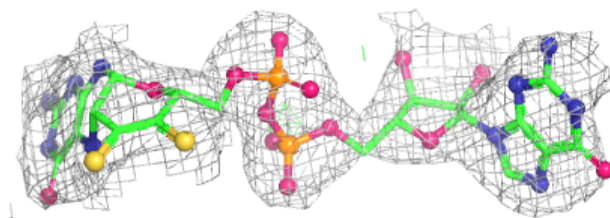
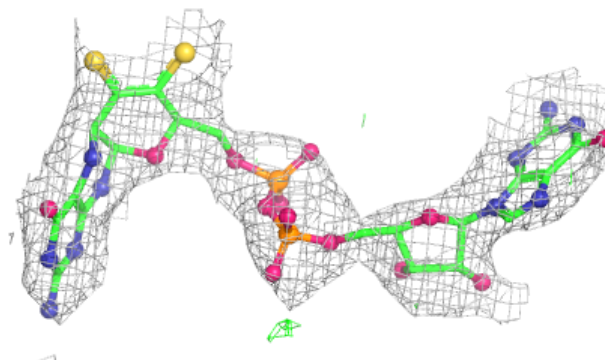


Electron density around HEC P 1129:

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

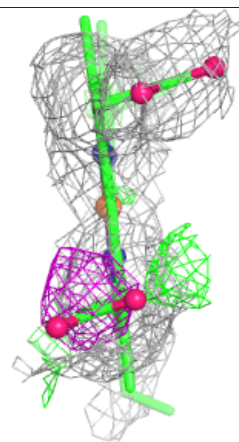
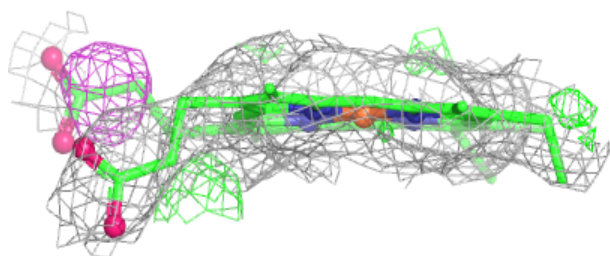
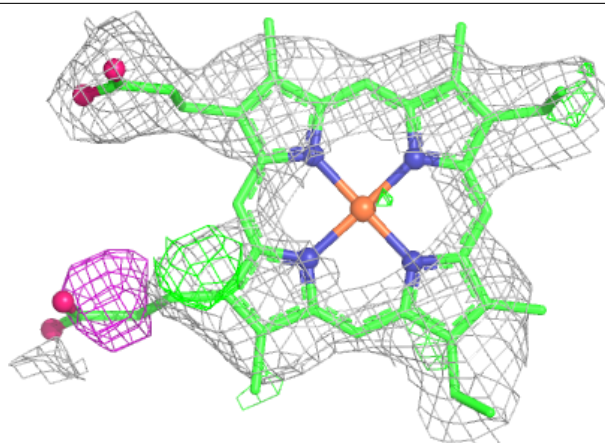
**Electron density around MGD K 1804:**

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

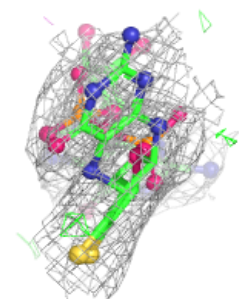
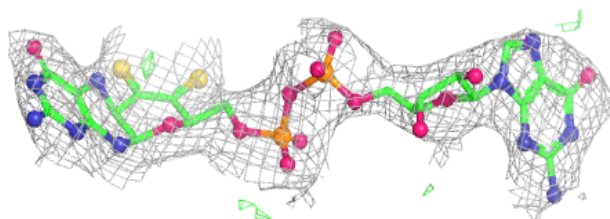


Electron density around HEC J 1129:

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

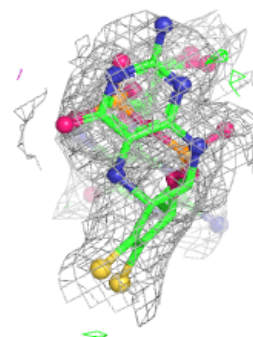
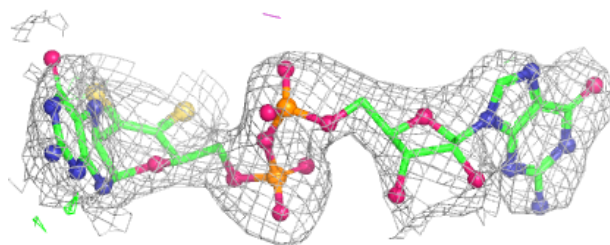
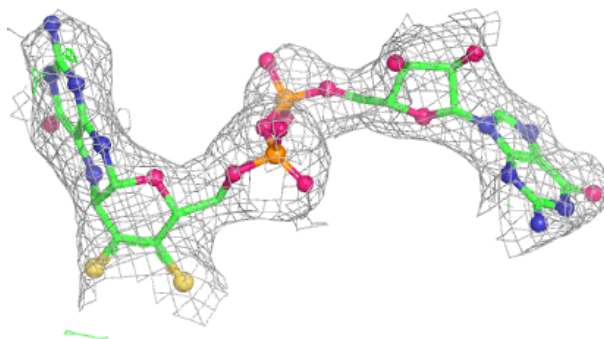
**Electron density around MGD O 1803:**

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

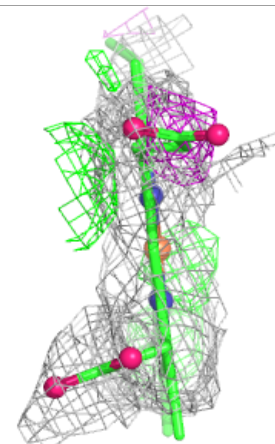
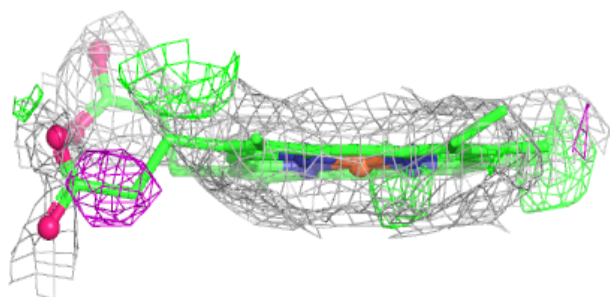
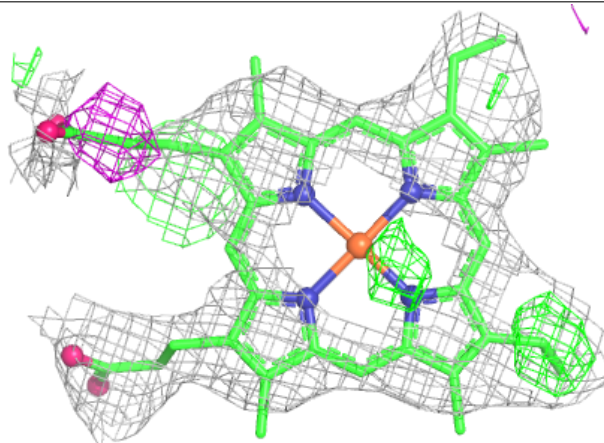


Electron density around MGD G 1804:

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

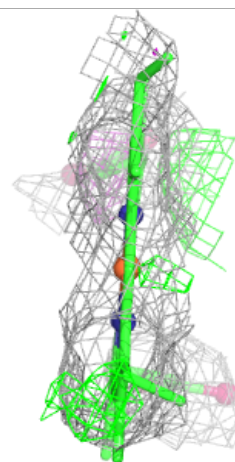
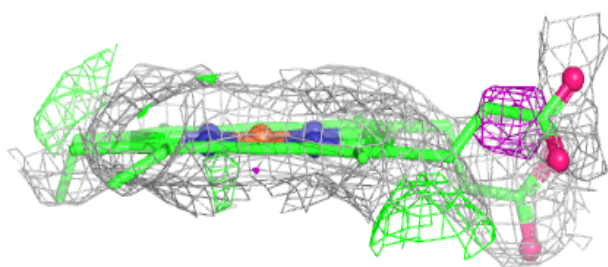
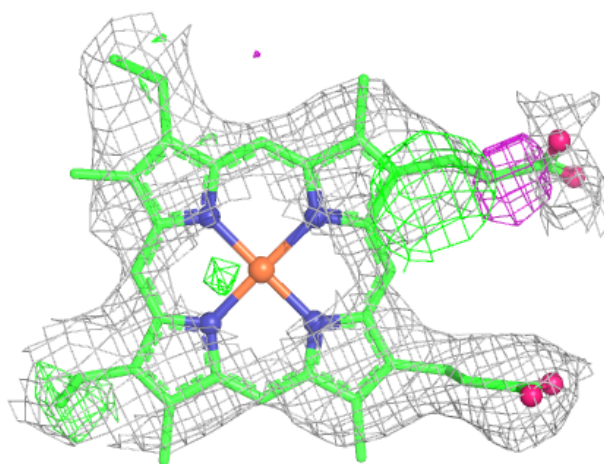
**Electron density around HEC L 1129:**

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



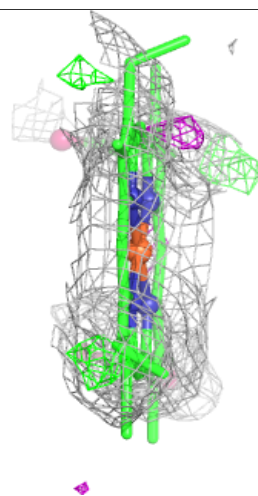
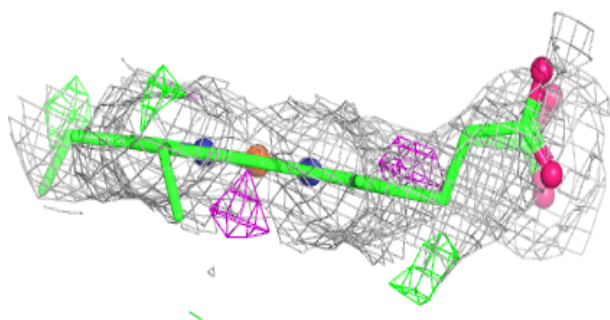
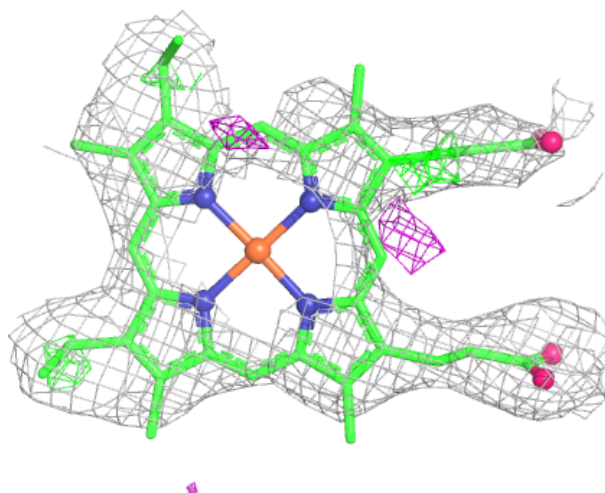
Electron density around HEC N 1129:

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



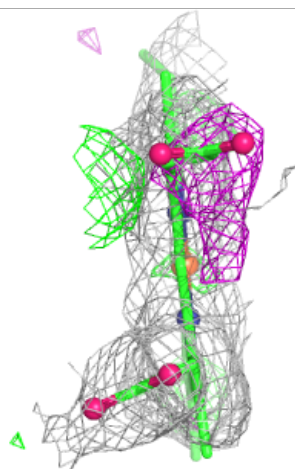
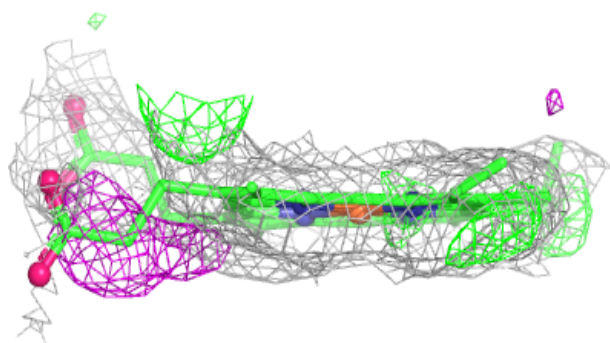
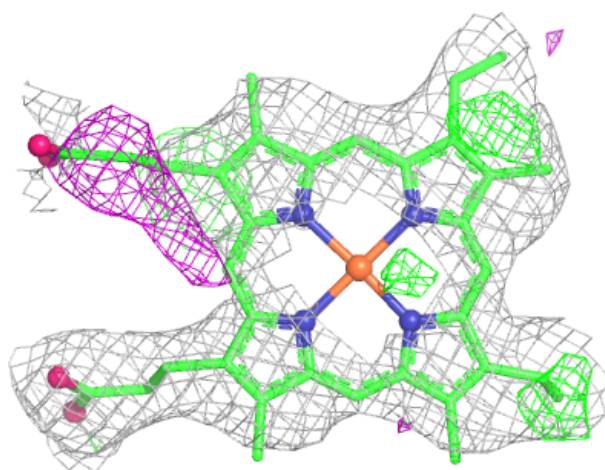
Electron density around HEC P 1128:

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



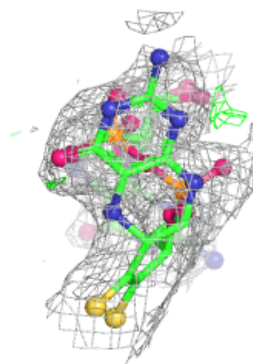
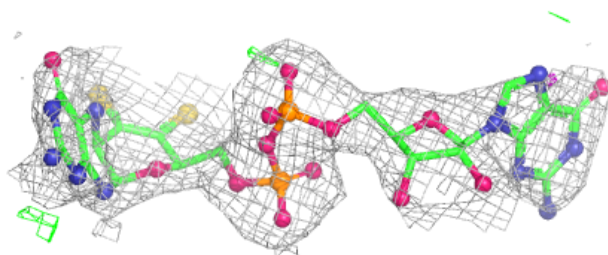
Electron density around HEC H 1129:

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and green (positive)

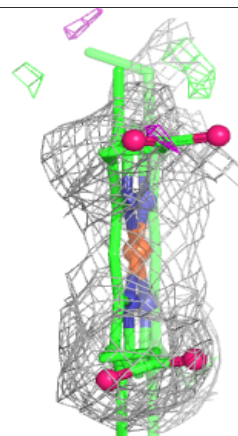
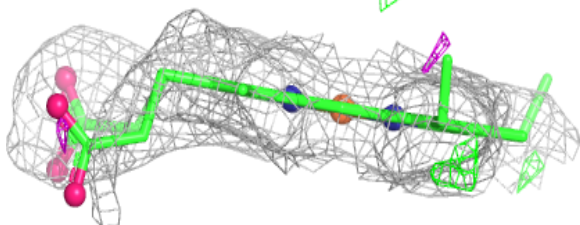
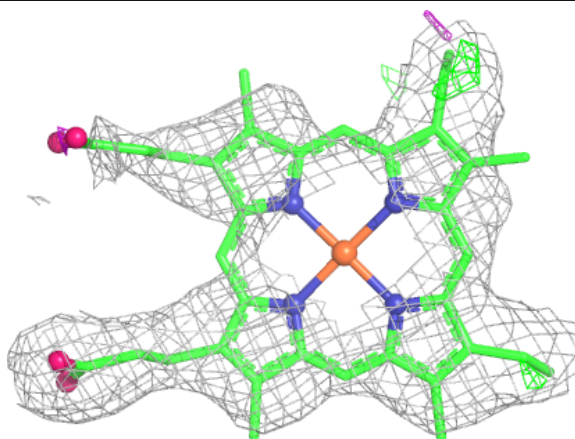


Electron density around MGD C 1804:

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

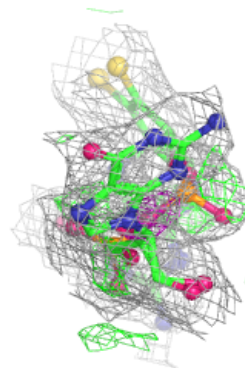
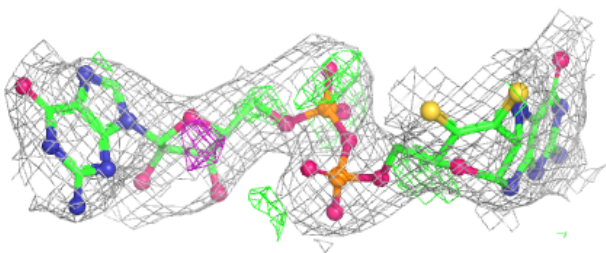
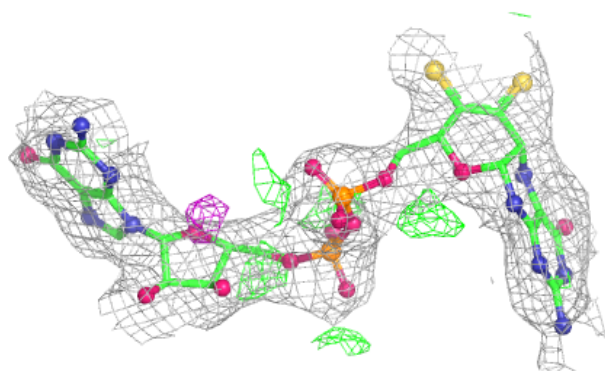
**Electron density around HEC J 1128:**

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



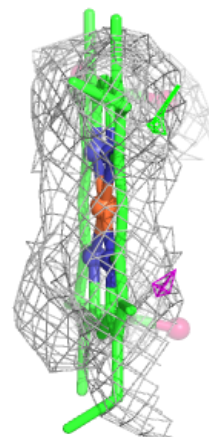
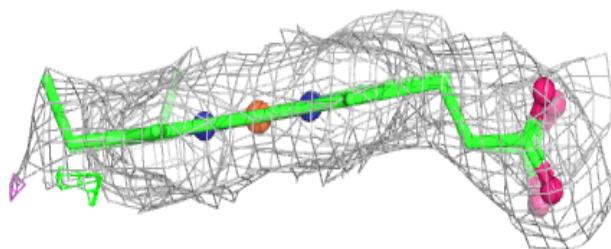
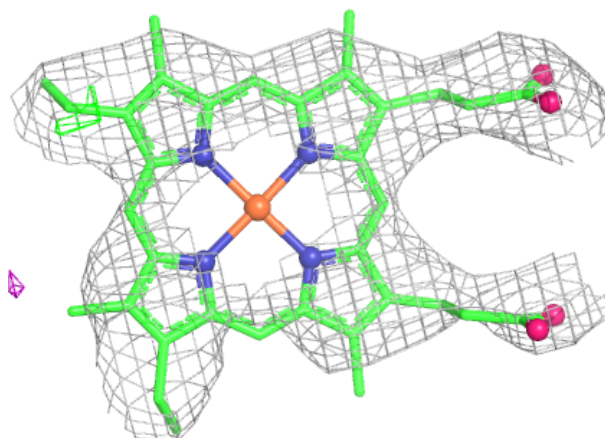
Electron density around MGD E 1804:

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



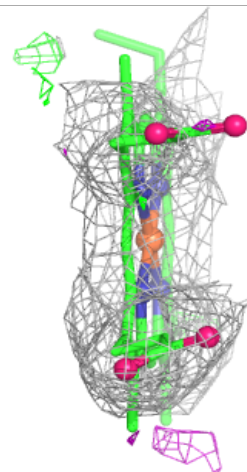
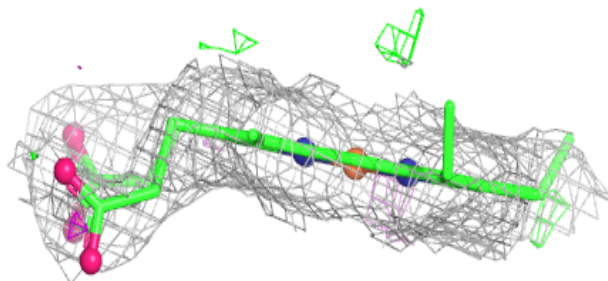
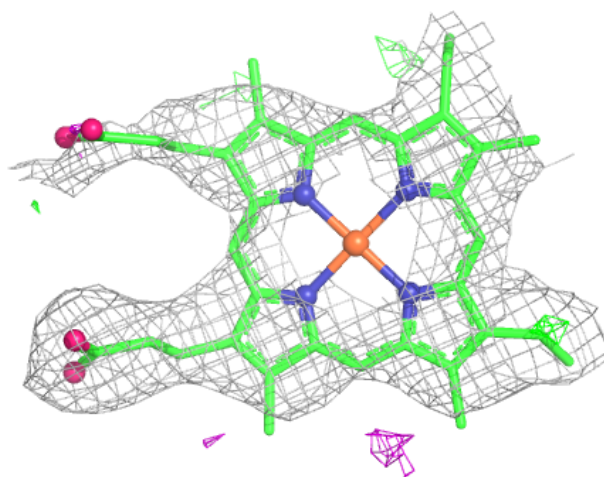
Electron density around HEC L 1128:

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



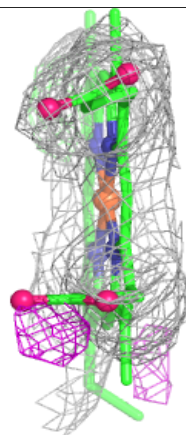
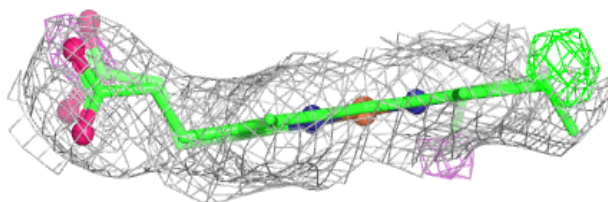
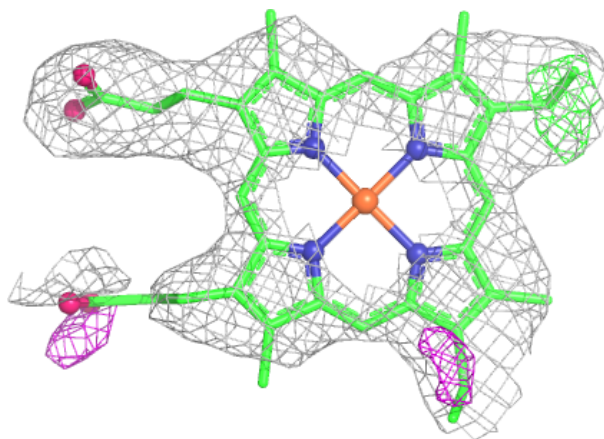
Electron density around HEC D 1128:

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



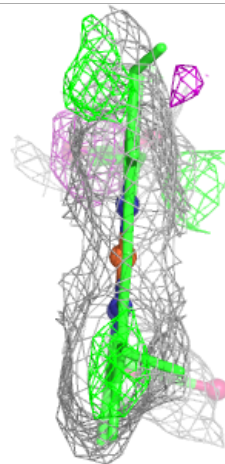
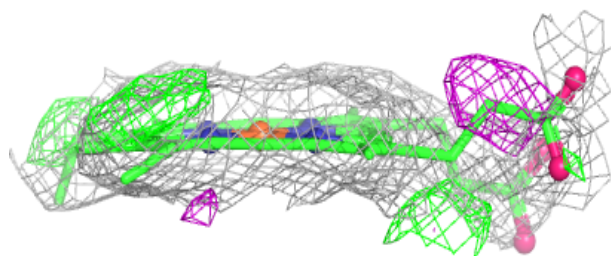
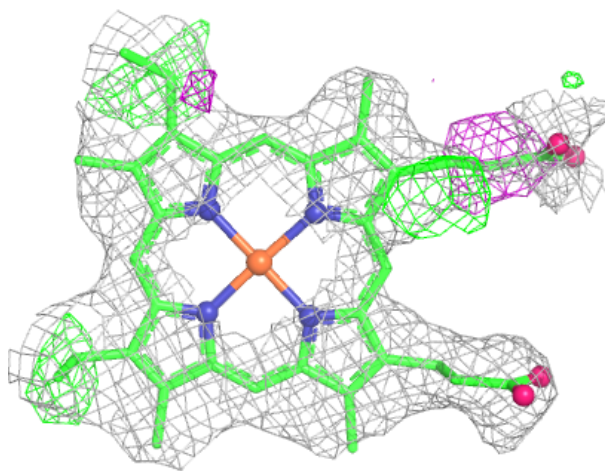
Electron density around HEC F 1128:

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



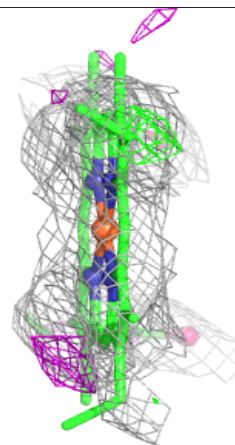
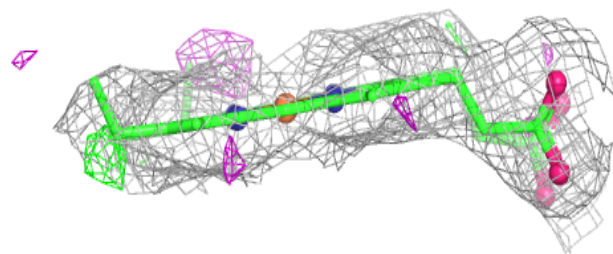
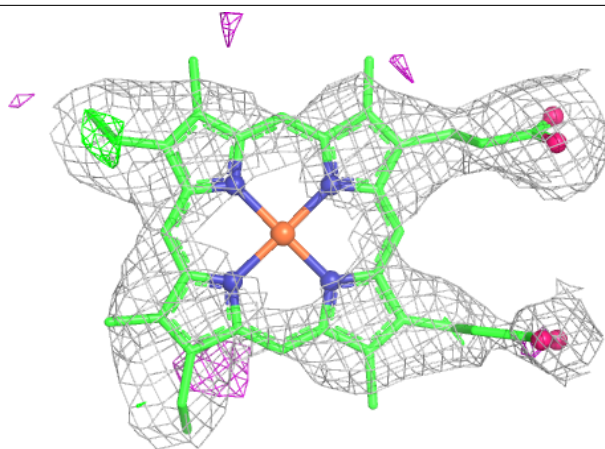
Electron density around HEC F 1129:

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and green (positive)



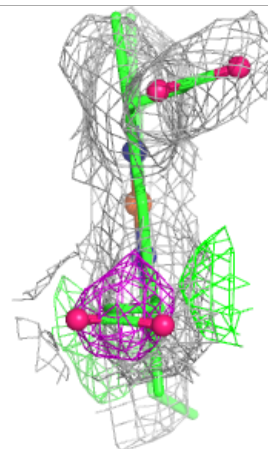
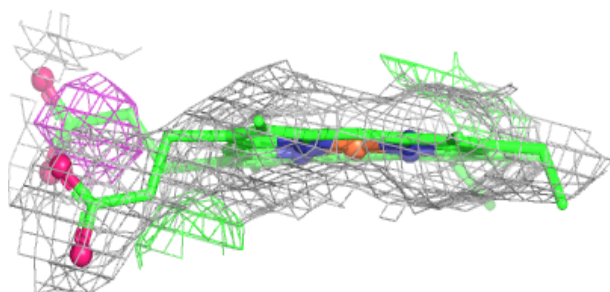
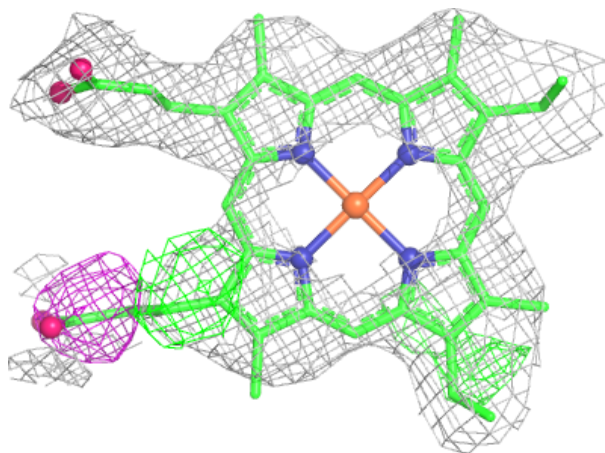
Electron density around HEC H 1128:

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



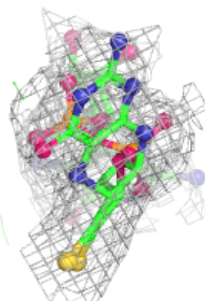
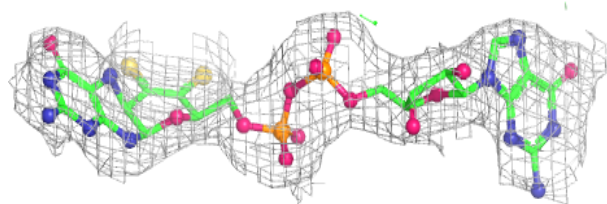
Electron density around HEC D 1129:

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and green (positive)

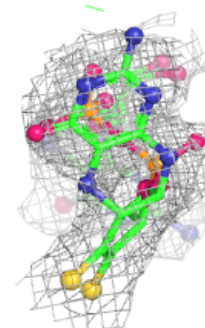
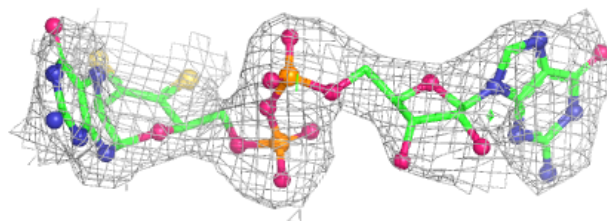


Electron density around MGD M 1803:

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

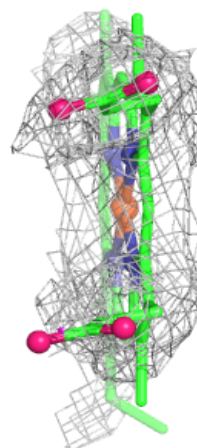
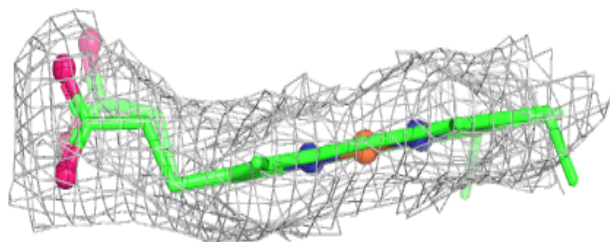
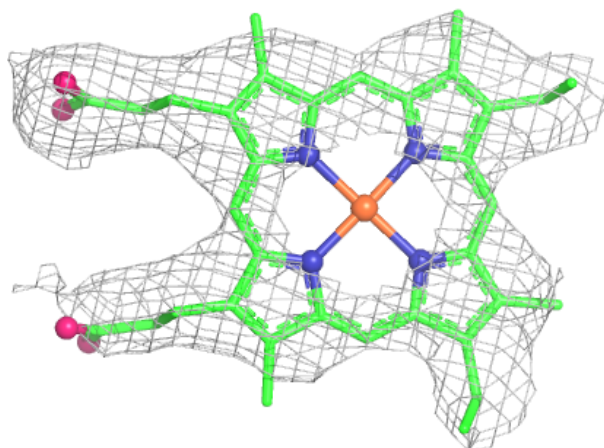
**Electron density around MGD M 1804:**

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



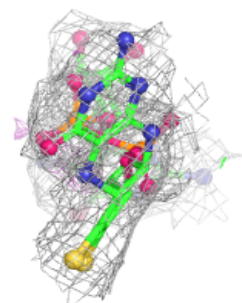
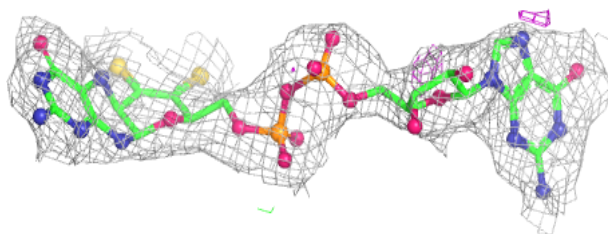
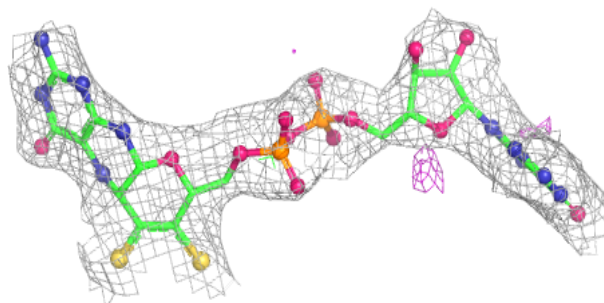
Electron density around HEC N 1128:

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and green (positive)

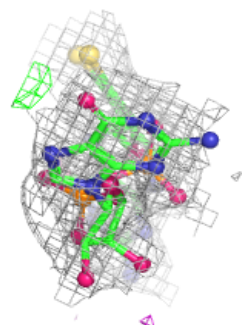
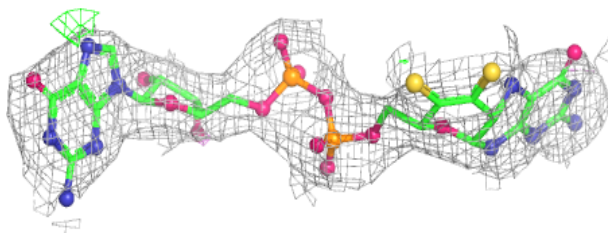
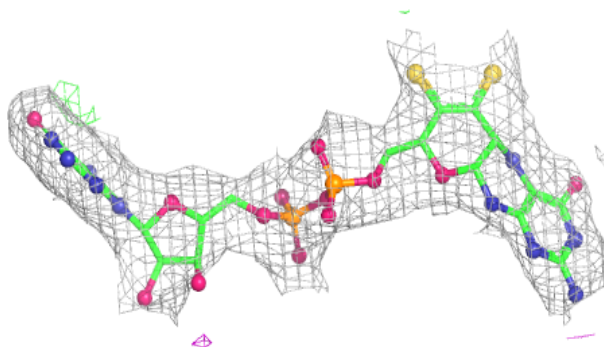


Electron density around MGD C 1803:

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

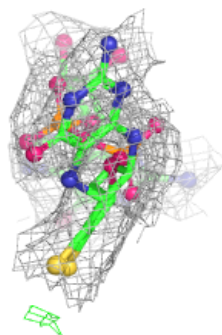
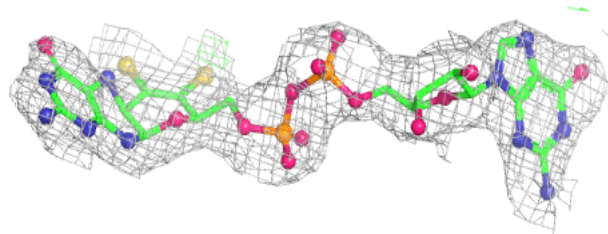
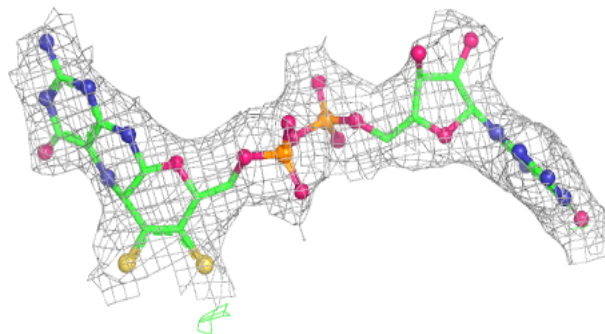
**Electron density around MGD K 1803:**

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

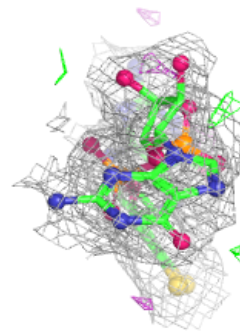
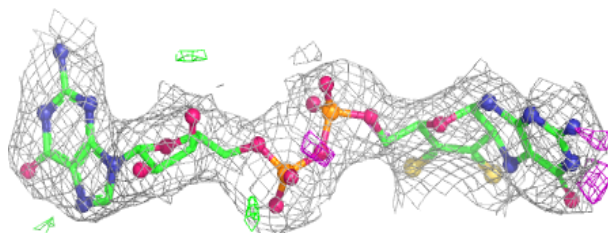


Electron density around MGD G 1803:

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

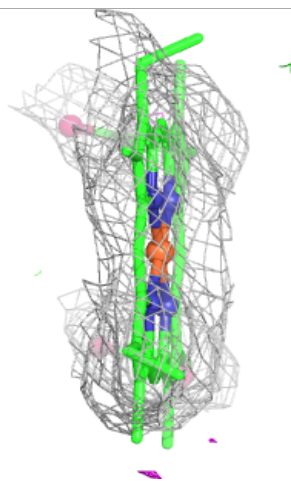
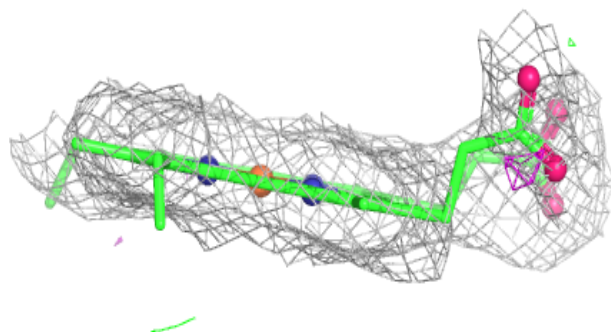
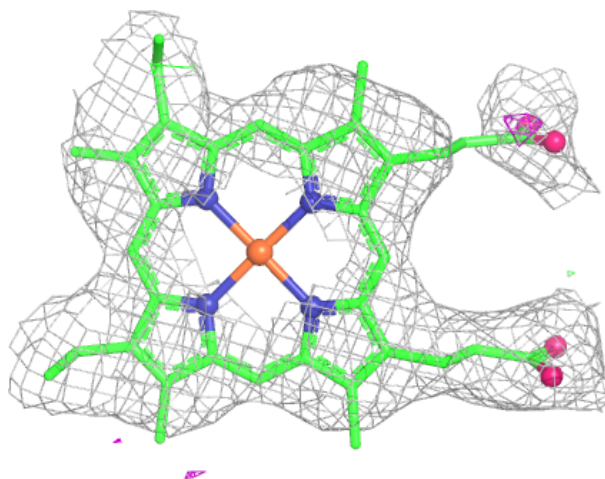
**Electron density around MGD A 1803:**

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



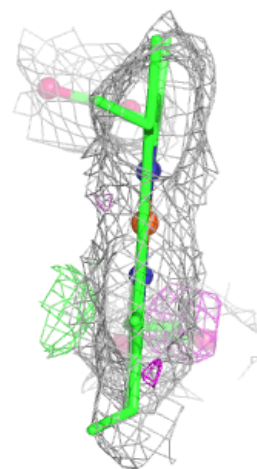
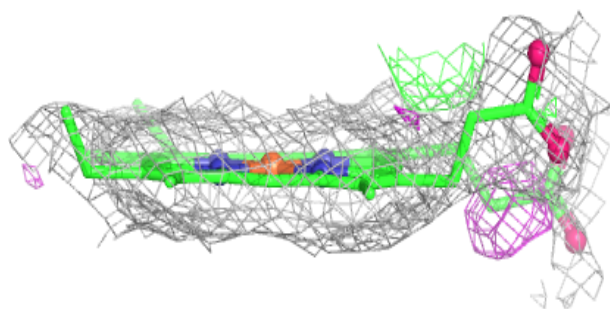
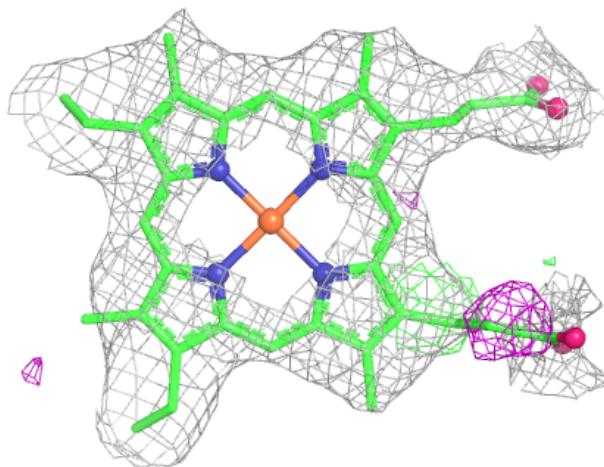
Electron density around HEC B 1128:

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



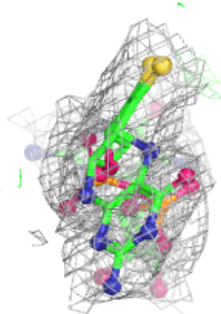
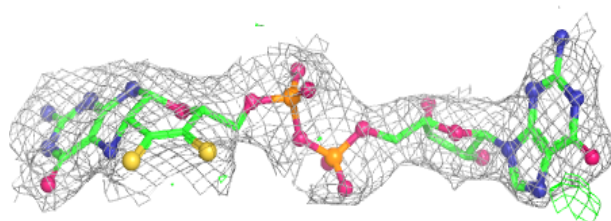
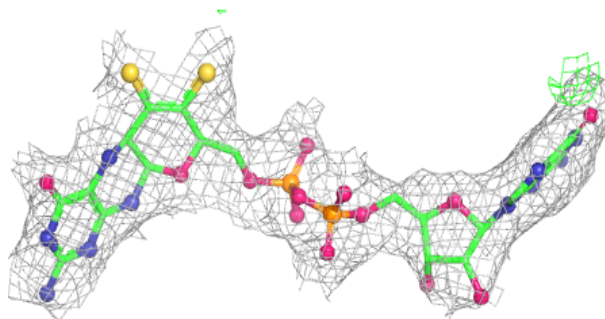
Electron density around HEC B 1129:

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

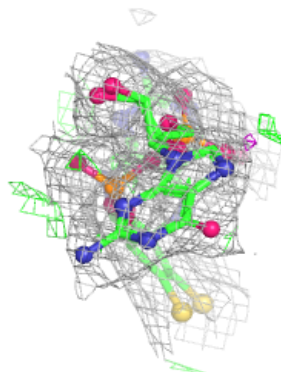
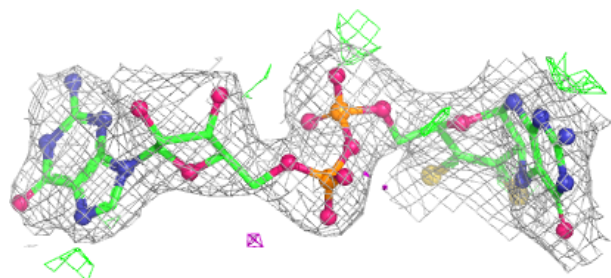
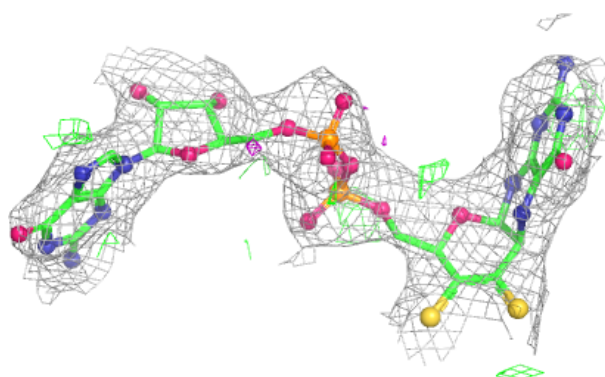


Electron density around MGD E 1803:

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

**Electron density around MGD A 1804:**

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



5.5 Other polymers [i](#)

There are no such residues in this entry.