



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 07:53 pm BST

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 wwPDB X-ray Structure Validation Summary 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

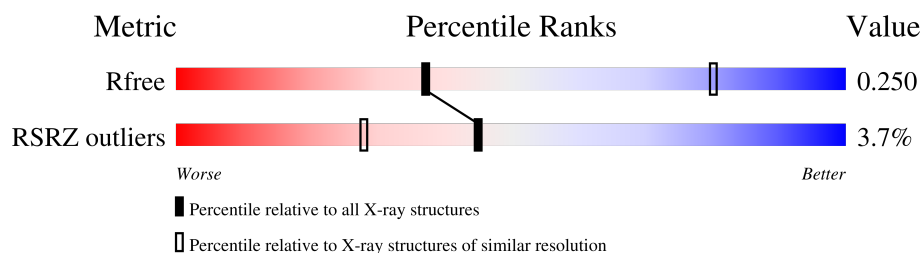
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.

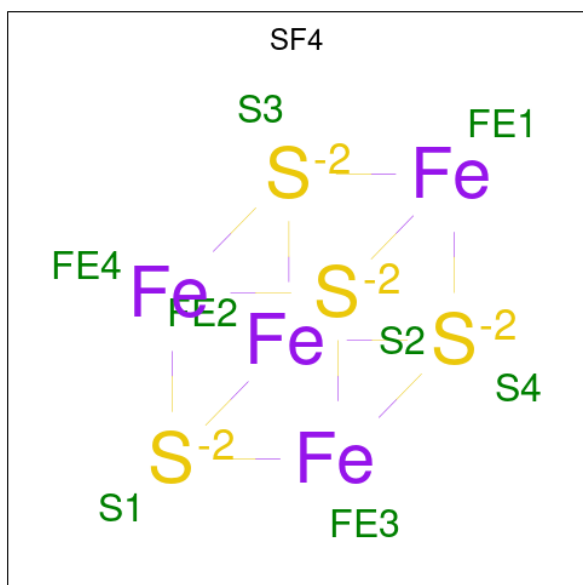
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	D	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	F	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	H	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	J	127	Total	C	N	O	S	0	0	1
			977	603	180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

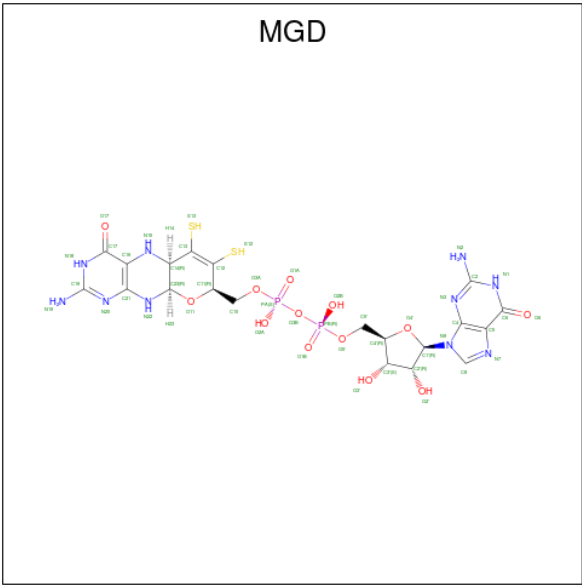


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		

- 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).



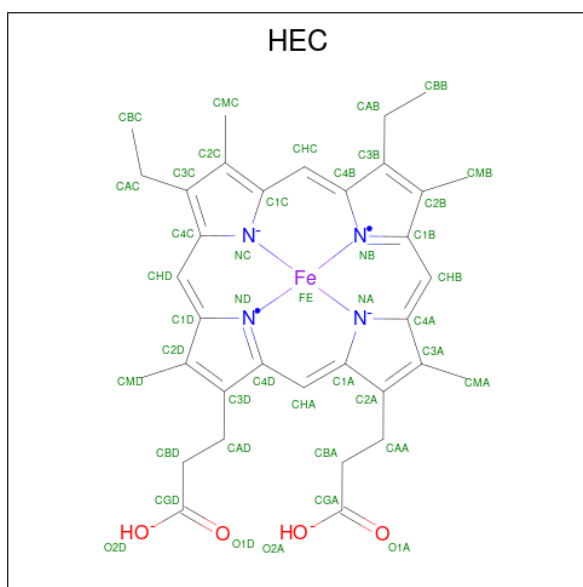
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0

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

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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](#)

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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](#)

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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
3	SF4	M	1801	1	0,12,12	-	-	-		
3	SF4	G	1801	1	0,12,12	-	-	-		
5	MGD	K	1804	4	45,52,52	1.88	11 (24%)	54,81,81	1.88	11 (20%)
3	SF4	E	1801	1	0,12,12	-	-	-		
6	HEC	B	1128	2	50,50,50	1.75	9 (18%)	68,82,82	1.42	8 (11%)
5	MGD	I	1804	4	45,52,52	2.19	17 (37%)	54,81,81	1.68	7 (12%)
6	HEC	N	1128	2	50,50,50	1.52	10 (20%)	68,82,82	1.43	10 (14%)
6	HEC	J	1129	2	50,50,50	1.70	10 (20%)	68,82,82	1.40	11 (16%)
6	HEC	L	1129	2	50,50,50	1.65	9 (18%)	68,82,82	1.40	11 (16%)
5	MGD	G	1803	4	45,52,52	1.95	15 (33%)	54,81,81	1.38	6 (11%)
5	MGD	E	1804	4	45,52,52	1.85	14 (31%)	54,81,81	1.77	8 (14%)
6	HEC	B	1129	2	50,50,50	1.46	10 (20%)	68,82,82	1.25	7 (10%)
6	HEC	J	1128	2	50,50,50	1.59	9 (18%)	68,82,82	1.29	7 (10%)
6	HEC	P	1128	2	50,50,50	1.68	11 (22%)	68,82,82	1.23	8 (11%)
5	MGD	M	1804	4	45,52,52	1.95	12 (26%)	54,81,81	1.77	8 (14%)
6	HEC	H	1128	2	50,50,50	1.47	11 (22%)	68,82,82	1.42	9 (13%)
5	MGD	O	1803	4	45,52,52	2.67	16 (35%)	54,81,81	1.42	8 (14%)
5	MGD	E	1803	4	45,52,52	1.81	14 (31%)	54,81,81	1.50	5 (9%)
6	HEC	D	1128	2	50,50,50	1.70	9 (18%)	68,82,82	1.48	10 (14%)
3	SF4	O	1801	1	0,12,12	-	-	-		
6	HEC	P	1129	2	50,50,50	1.64	9 (18%)	68,82,82	1.47	12 (17%)
5	MGD	M	1803	4	45,52,52	1.88	11 (24%)	54,81,81	1.42	7 (12%)
6	HEC	H	1129	2	50,50,50	1.85	11 (22%)	68,82,82	1.44	11 (16%)
6	HEC	L	1128	2	50,50,50	1.48	8 (16%)	68,82,82	1.28	8 (11%)
6	HEC	F	1128	2	50,50,50	1.61	11 (22%)	68,82,82	1.40	12 (17%)
3	SF4	A	1801	1	0,12,12	-	-	-		
5	MGD	C	1803	4	45,52,52	1.84	11 (24%)	54,81,81	1.42	6 (11%)
3	SF4	I	1801	1	0,12,12	-	-	-		
5	MGD	G	1804	4	45,52,52	2.02	18 (40%)	54,81,81	1.81	8 (14%)
5	MGD	O	1804	4	45,52,52	2.23	16 (35%)	54,81,81	1.82	6 (11%)
3	SF4	C	1801	1	0,12,12	-	-	-		
6	HEC	F	1129	2	50,50,50	1.72	10 (20%)	68,82,82	1.34	9 (13%)
6	HEC	N	1129	2	50,50,50	1.83	12 (24%)	68,82,82	1.39	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	A	1803	4	45,52,52	2.16	14 (31%)	54,81,81	1.47	8 (14%)
6	HEC	D	1129	2	50,50,50	1.60	9 (18%)	68,82,82	1.35	11 (16%)
5	MGD	I	1803	4	45,52,52	2.62	19 (42%)	54,81,81	1.49	8 (14%)
5	MGD	A	1804	4	45,52,52	1.80	10 (22%)	54,81,81	1.76	7 (12%)
5	MGD	C	1804	4	45,52,52	2.00	11 (24%)	54,81,81	1.81	7 (12%)
3	SF4	K	1801	1	0,12,12	-	-	-	-	-
5	MGD	K	1803	4	45,52,52	1.87	14 (31%)	54,81,81	1.46	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	M	1801	1	-	-	0/6/5/5
3	SF4	G	1801	1	-	-	0/6/5/5
5	MGD	K	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	B	1128	2	1/1/3/7	0/14/54/54	-
3	SF4	E	1801	1	-	-	0/6/5/5
5	MGD	I	1804	4	-	7/22/66/66	0/6/6/6
6	HEC	N	1128	2	1/1/3/7	1/14/54/54	-
6	HEC	J	1129	2	1/1/3/7	2/14/54/54	-
5	MGD	G	1803	4	-	5/22/66/66	0/6/6/6
6	HEC	B	1129	2	1/1/3/7	2/14/54/54	-
6	HEC	J	1128	2	1/1/3/7	0/14/54/54	-
5	MGD	E	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	P	1128	2	1/1/3/7	2/14/54/54	-
5	MGD	M	1804	4	-	6/22/66/66	0/6/6/6
6	HEC	H	1128	2	1/1/3/7	2/14/54/54	-
5	MGD	O	1803	4	-	5/22/66/66	0/6/6/6
5	MGD	E	1803	4	-	6/22/66/66	0/6/6/6
6	HEC	D	1128	2	1/1/3/7	2/14/54/54	-
3	SF4	O	1801	1	-	-	0/6/5/5
6	HEC	P	1129	2	1/1/3/7	4/14/54/54	-
6	HEC	H	1129	2	1/1/3/7	2/14/54/54	-
6	HEC	L	1128	2	1/1/3/7	4/14/54/54	-
5	MGD	M	1803	4	-	6/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEC	F	1128	2	1/1/3/7	3/14/54/54	-
3	SF4	A	1801	1	-	-	0/6/5/5
5	MGD	C	1803	4	-	6/22/66/66	0/6/6/6
3	SF4	I	1801	1	-	-	0/6/5/5
5	MGD	G	1804	4	-	6/22/66/66	0/6/6/6
5	MGD	O	1804	4	-	5/22/66/66	0/6/6/6
3	SF4	C	1801	1	-	-	0/6/5/5
6	HEC	F	1129	2	1/1/3/7	2/14/54/54	-
6	HEC	N	1129	2	1/1/3/7	4/14/54/54	-
5	MGD	A	1803	4	-	6/22/66/66	0/6/6/6
6	HEC	D	1129	2	1/1/3/7	4/14/54/54	-
5	MGD	I	1803	4	-	6/22/66/66	0/6/6/6
5	MGD	C	1804	4	-	5/22/66/66	0/6/6/6
5	MGD	A	1804	4	-	5/22/66/66	0/6/6/6
6	HEC	L	1129	2	1/1/3/7	4/14/54/54	-
3	SF4	K	1801	1	-	-	0/6/5/5
5	MGD	K	1803	4	-	6/22/66/66	0/6/6/6

The worst 5 of 381 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
6	N	1129	HEC	C4D-C3D	6.39	1.56	1.45
5	I	1804	MGD	C14-N15	6.32	1.53	1.46
5	M	1804	MGD	C14-N15	6.16	1.53	1.46

The worst 5 of 271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1804	MGD	O11-C23-N22	-8.54	99.79	108.57
5	O	1804	MGD	O11-C23-N22	-8.34	100.00	108.57
5	K	1804	MGD	O11-C23-N22	-8.28	100.06	108.57
5	A	1804	MGD	O11-C23-N22	-8.11	100.23	108.57
5	E	1804	MGD	O11-C23-N22	-7.95	100.40	108.57

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1128	HEC	NA
6	B	1129	HEC	NA
6	D	1128	HEC	NA
6	D	1129	HEC	NA
6	F	1128	HEC	NA

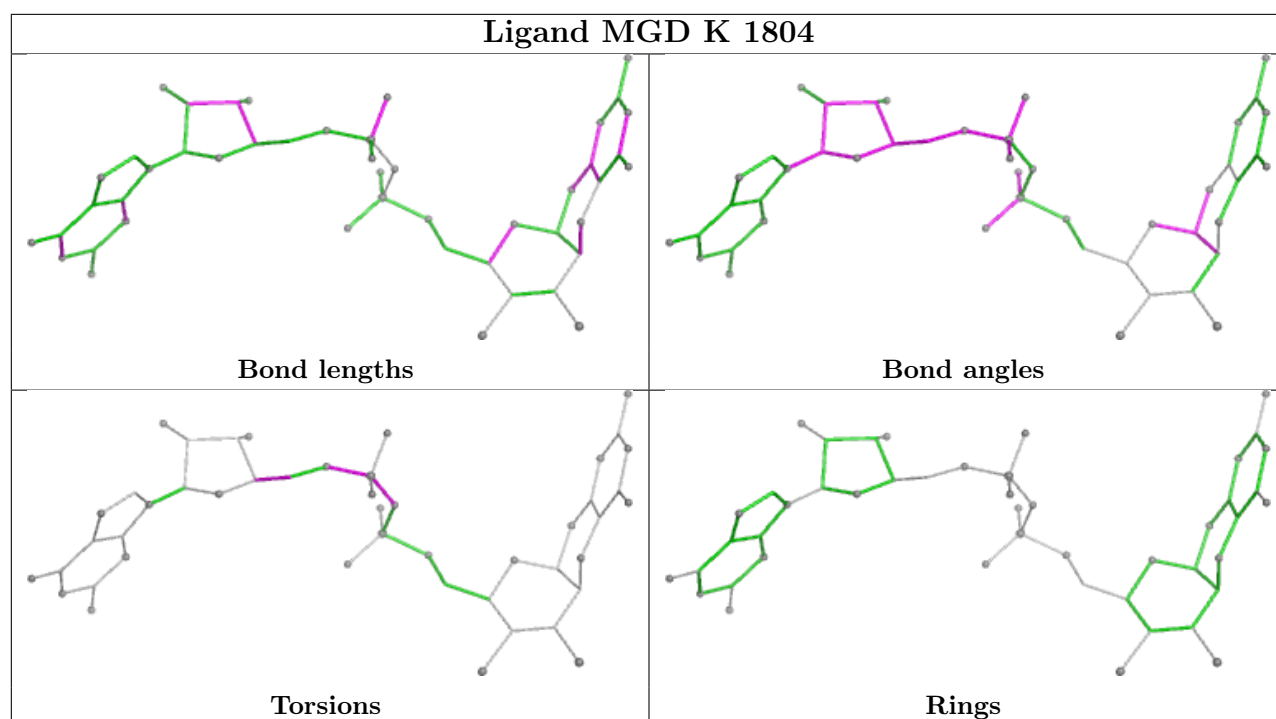
5 of 130 torsion outliers are listed below:

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	1804	MGD	C5'-O5'-PB-O1B
5	A	1804	MGD	C5'-O5'-PB-O2B

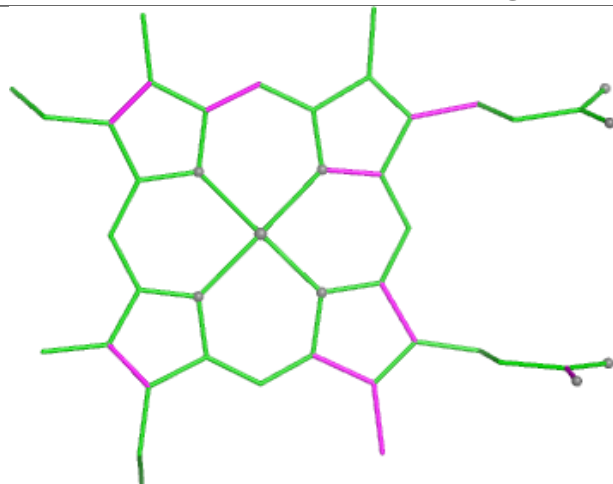
There are no ring outliers.

No monomer is involved in short contacts.

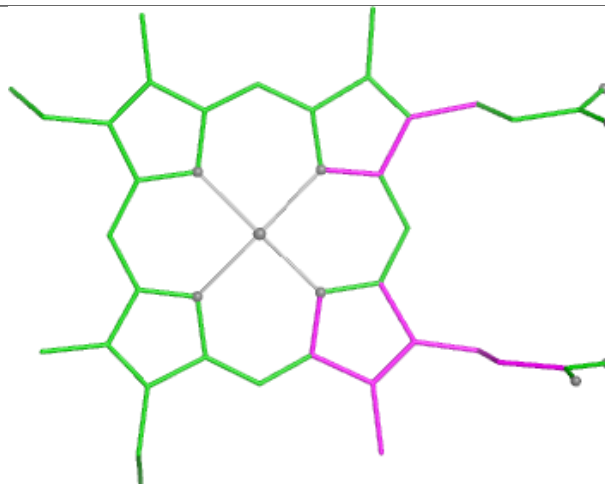
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



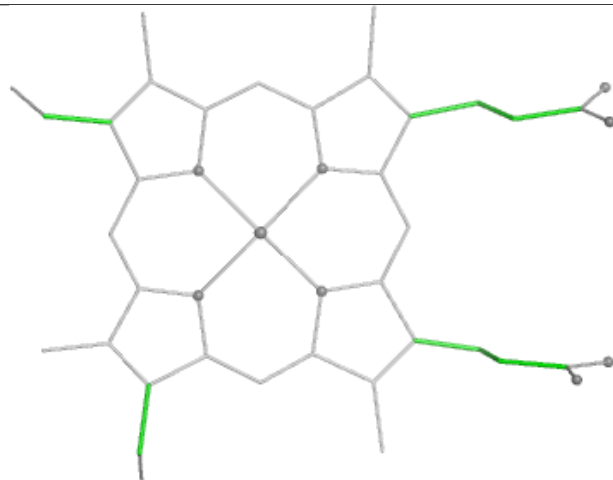
Ligand HEC B 1128



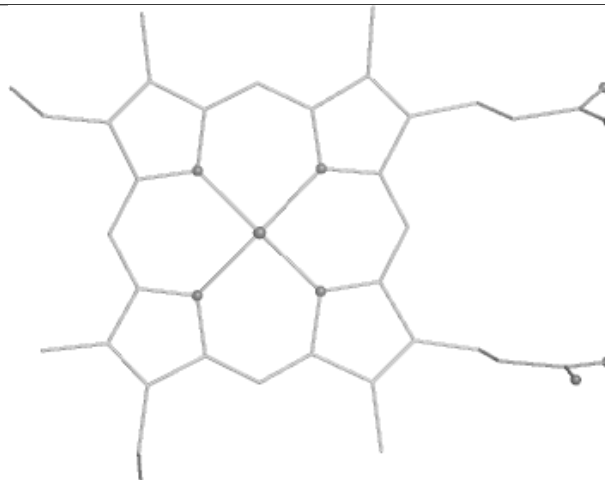
Bond lengths



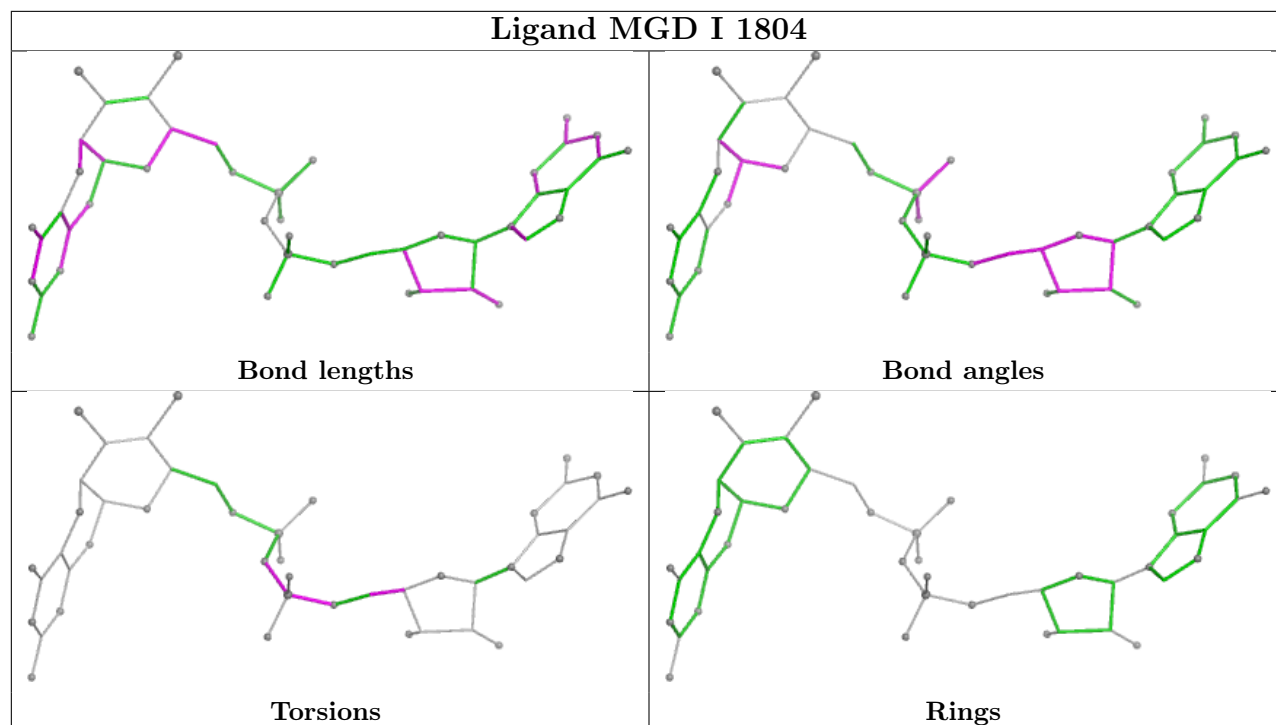
Bond angles

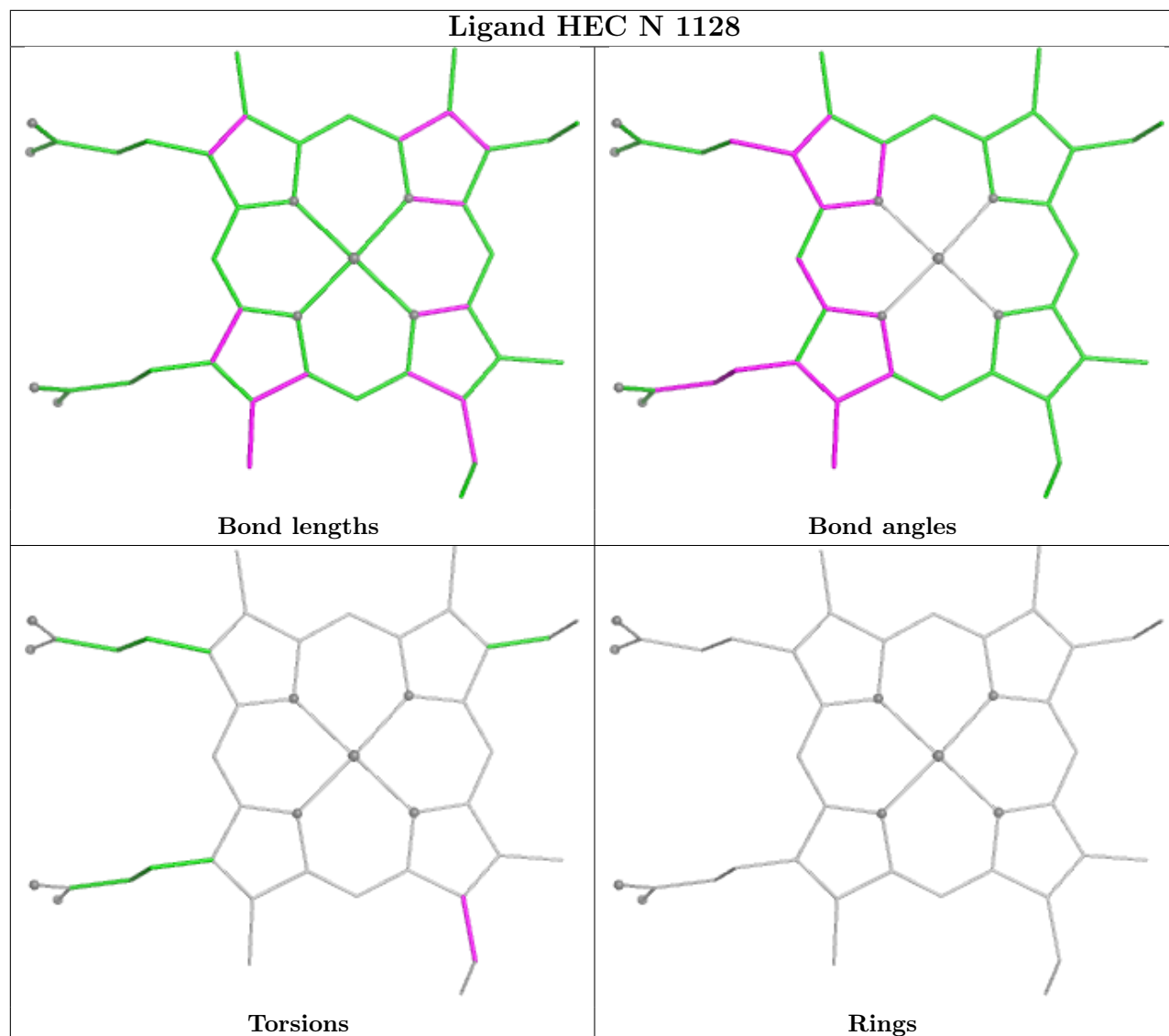


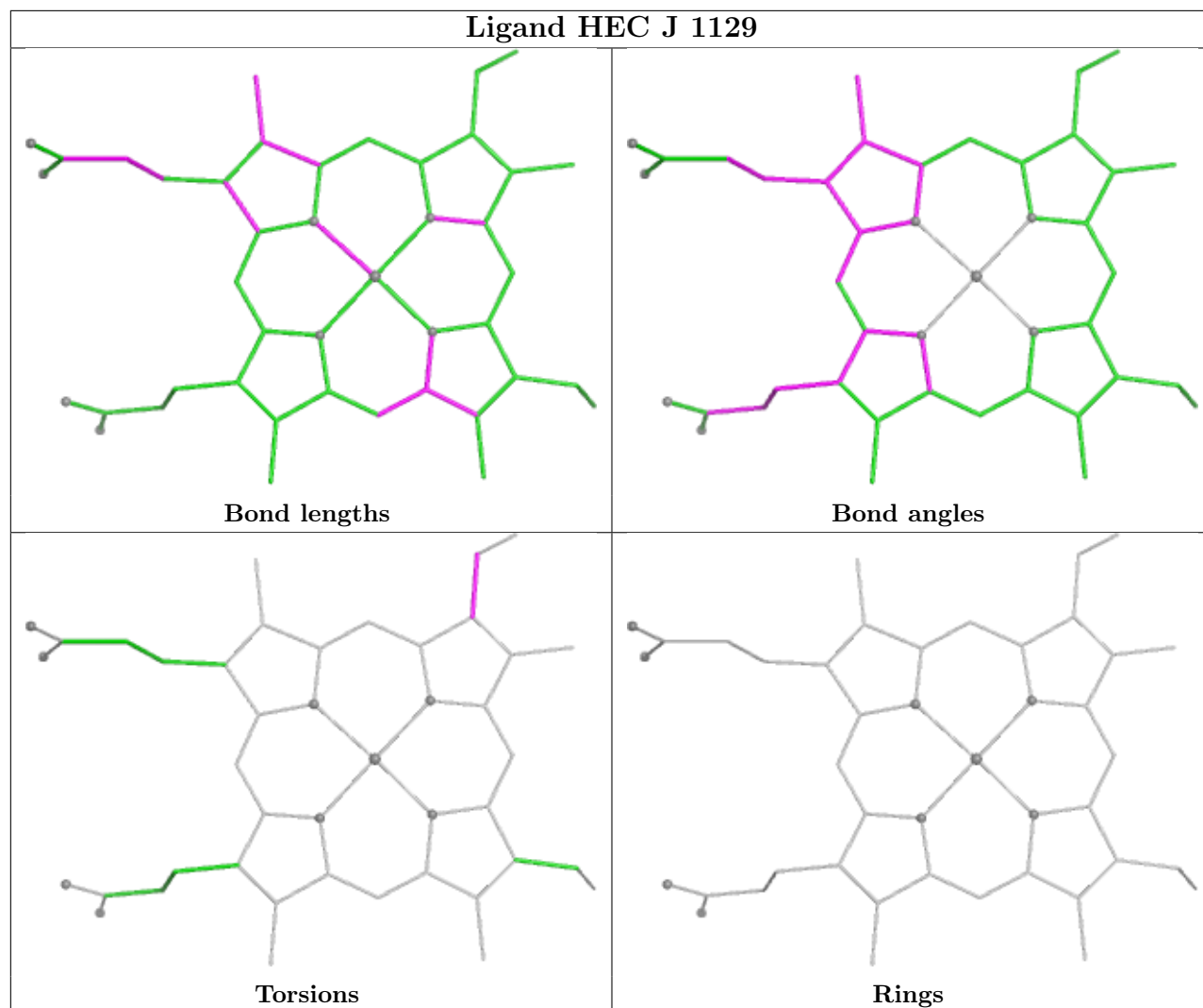
Torsions

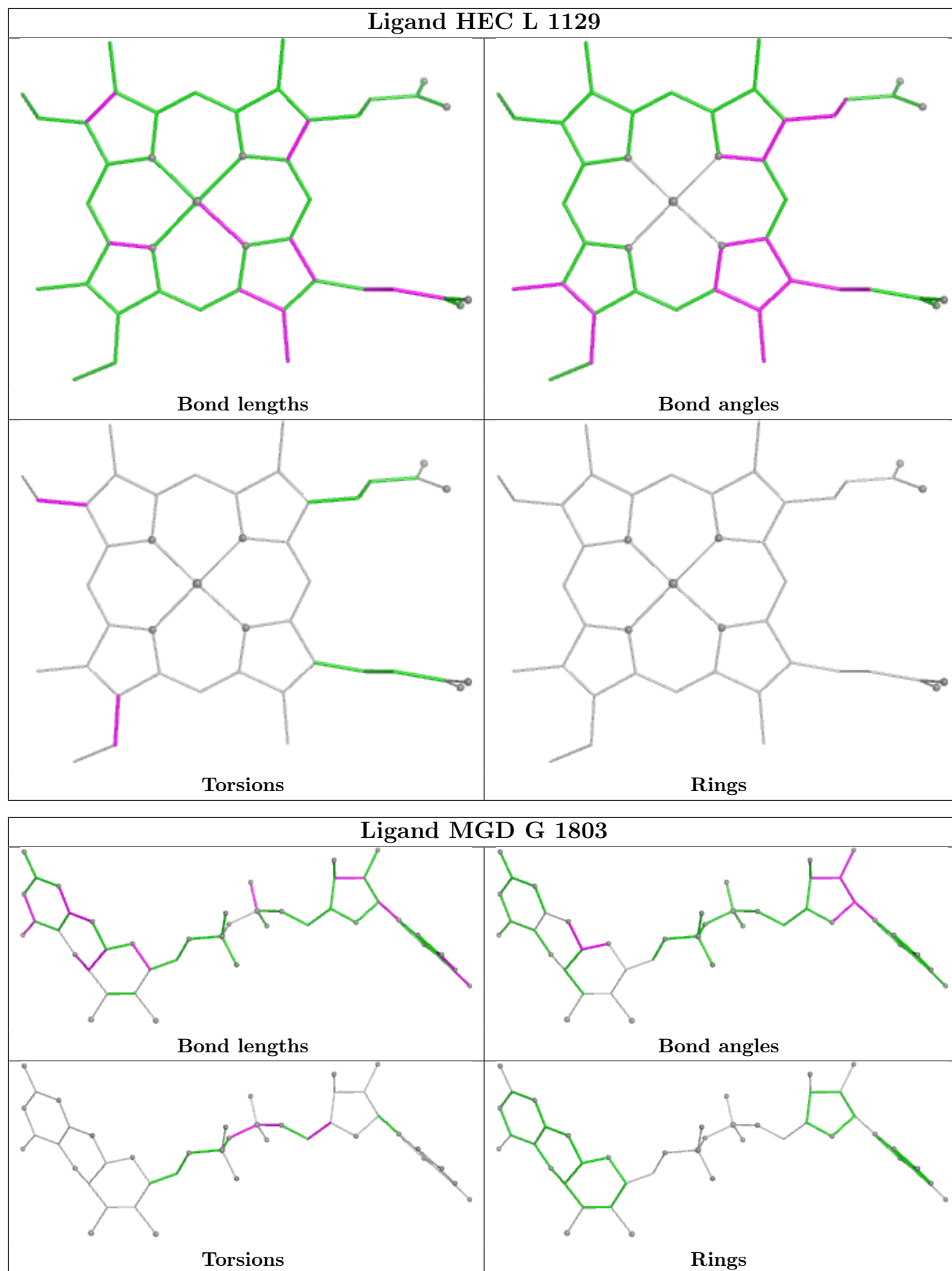


Rings

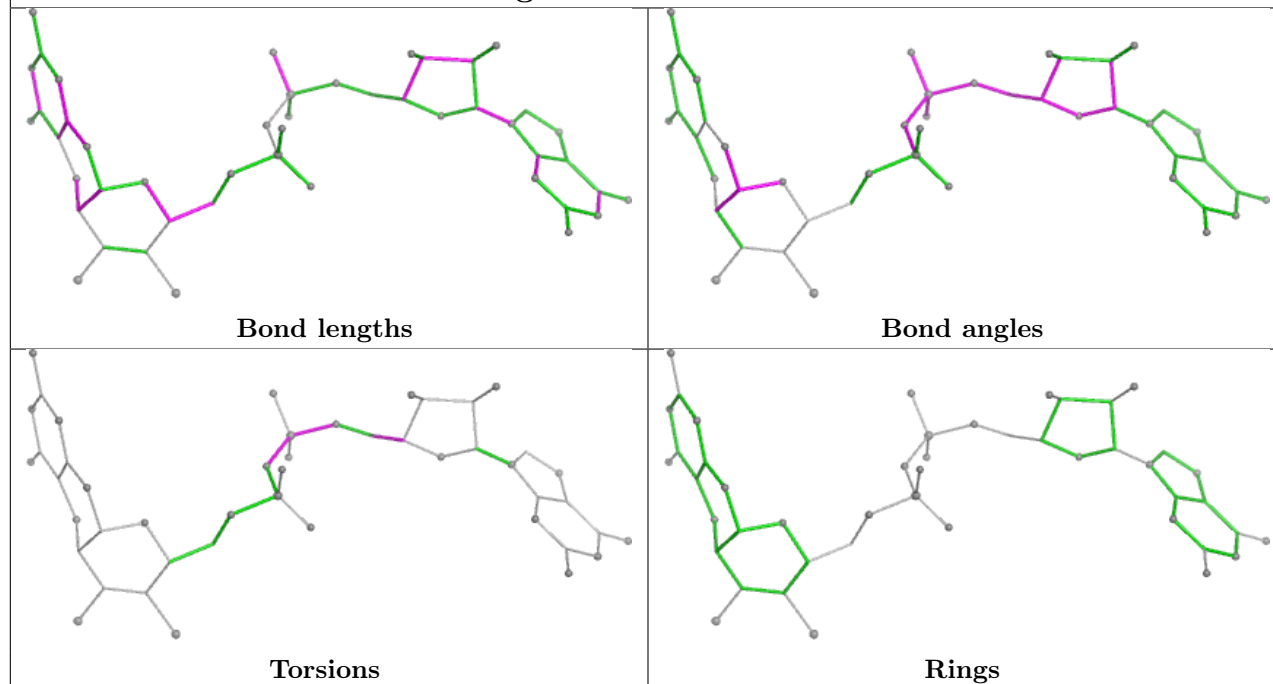




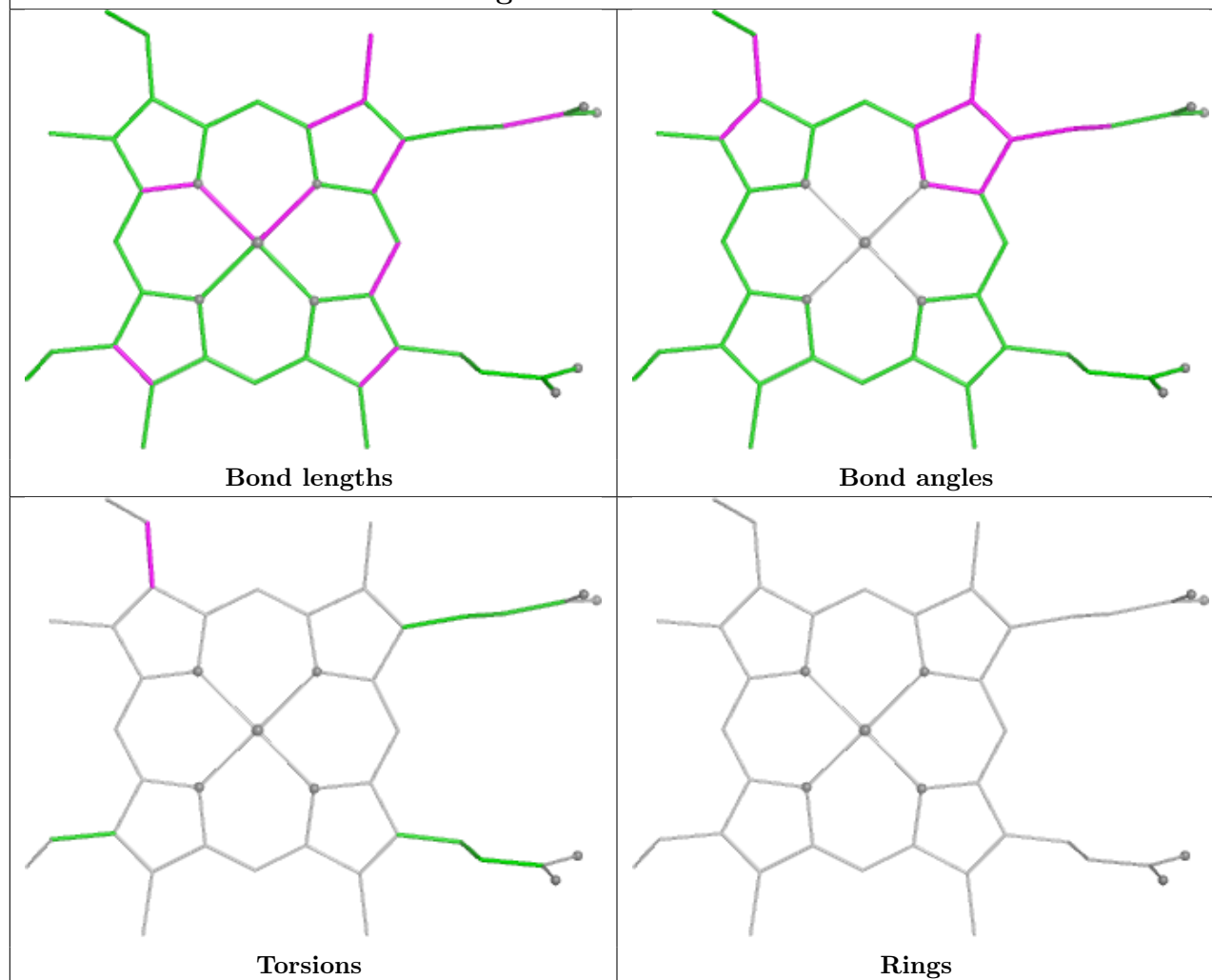


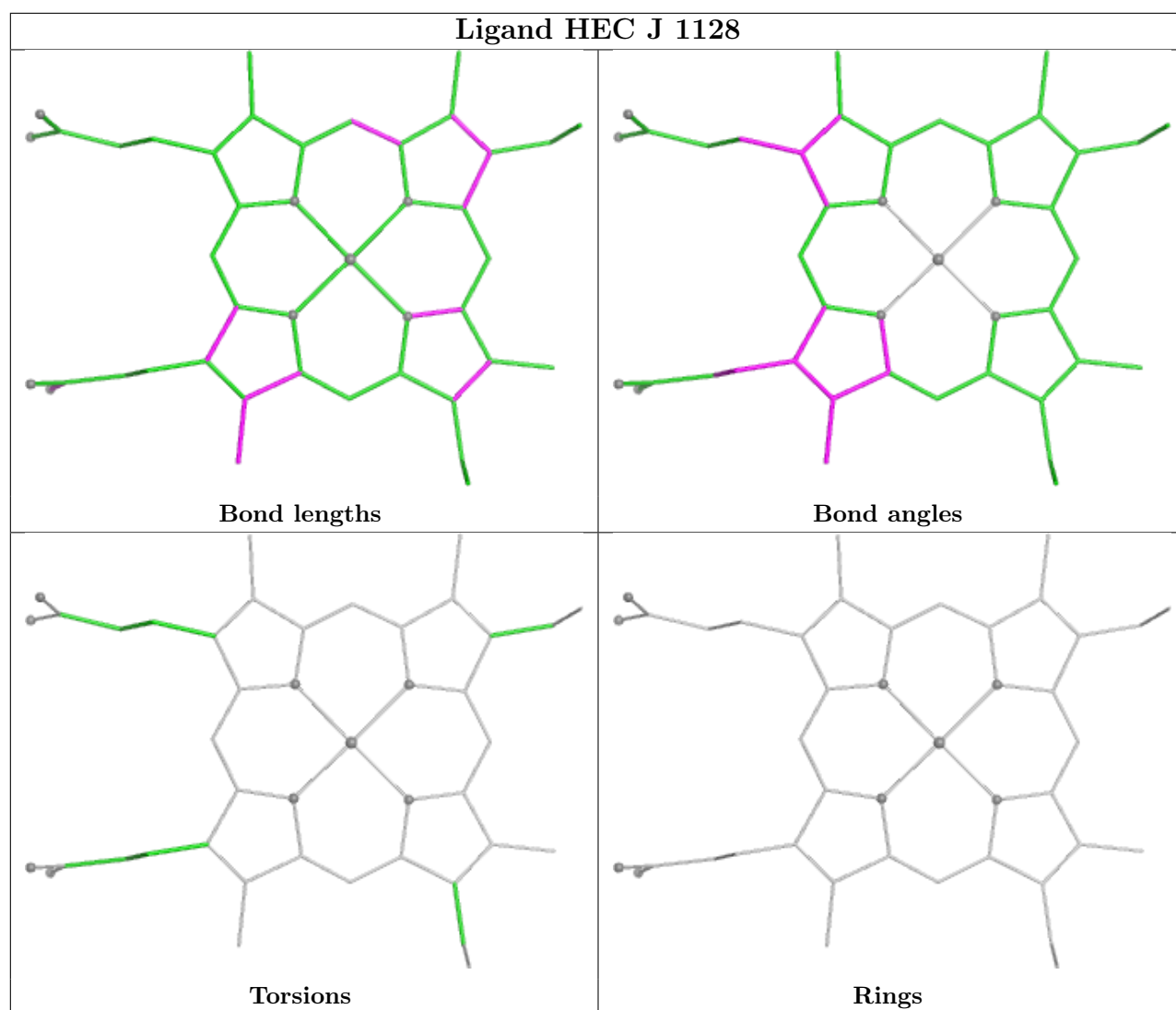


Ligand MGD E 1804

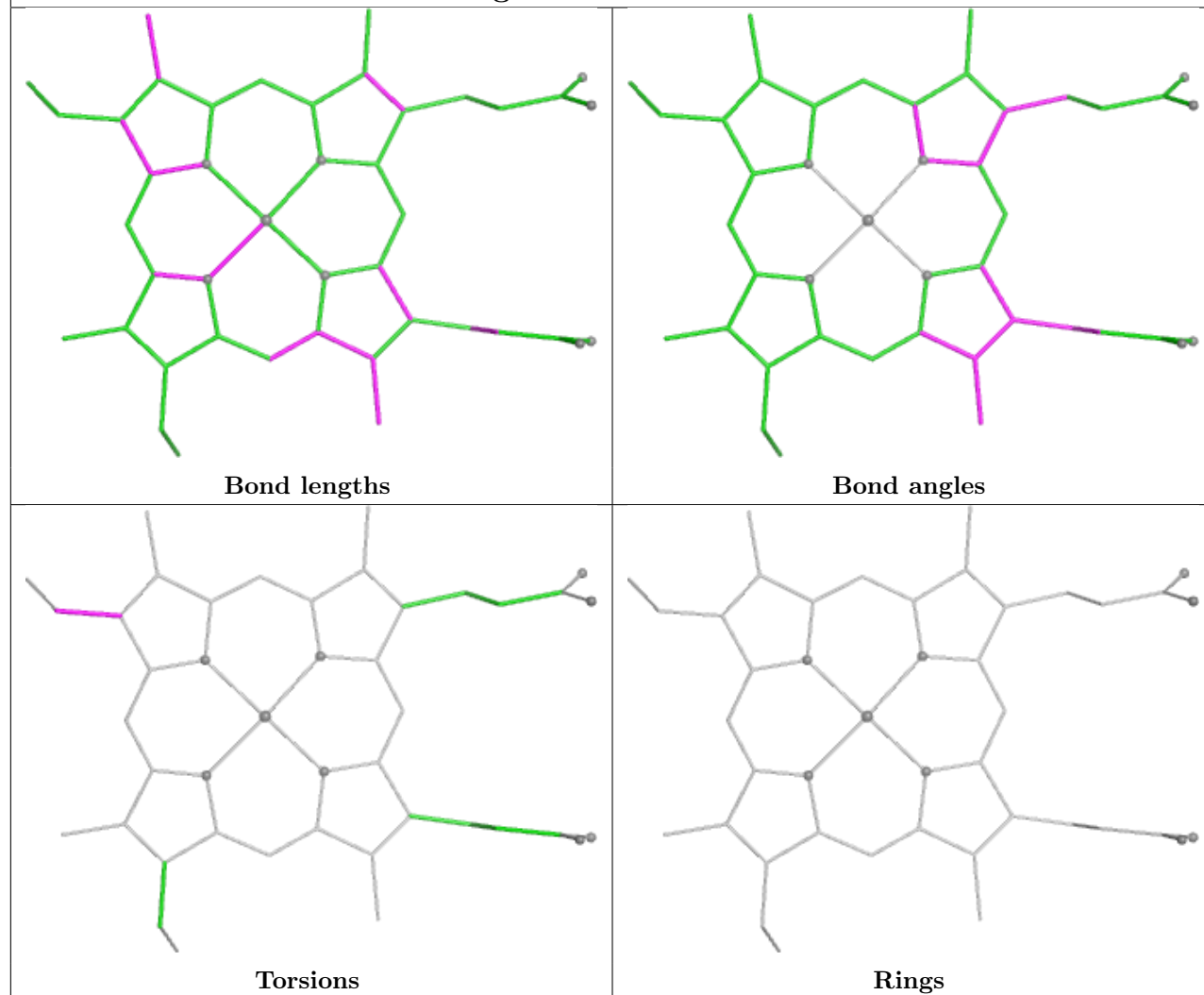


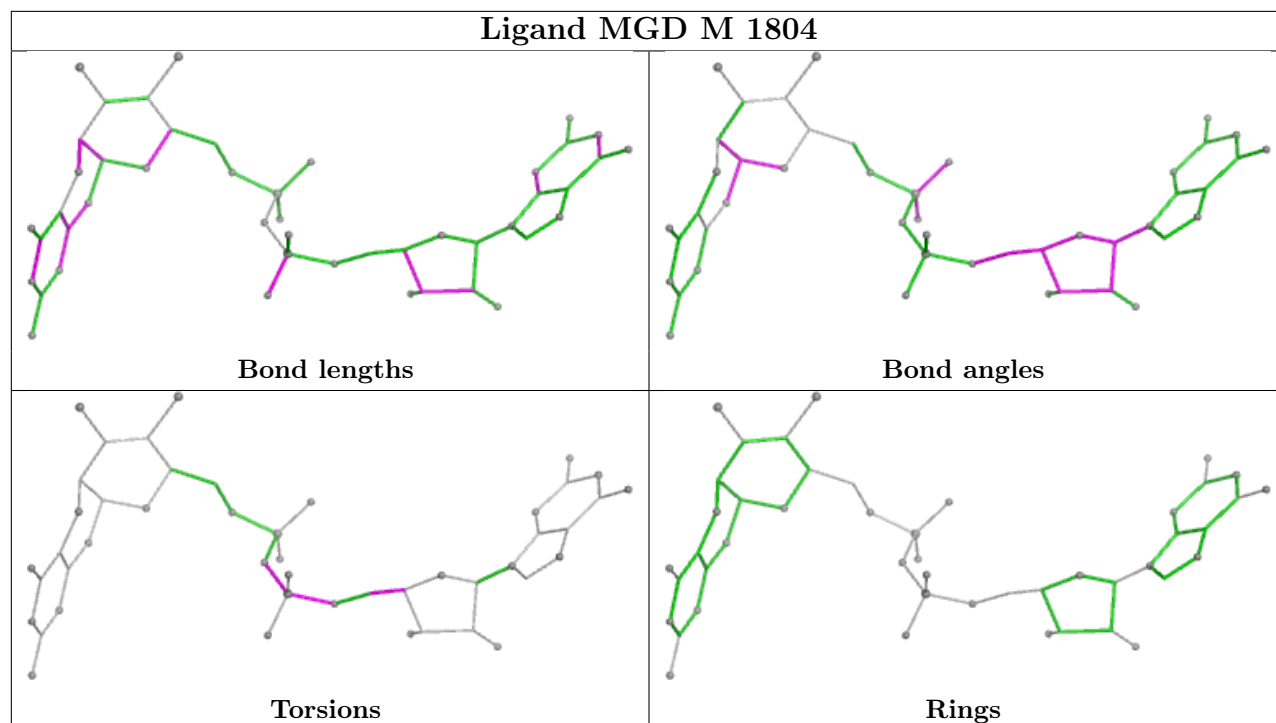
Ligand HEC B 1129



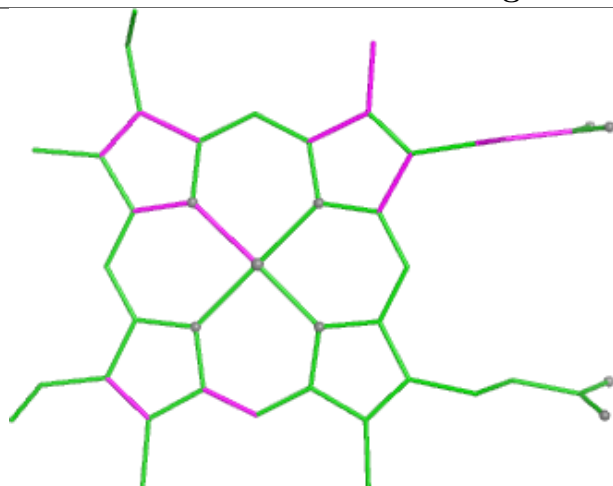


Ligand HEC P 1128

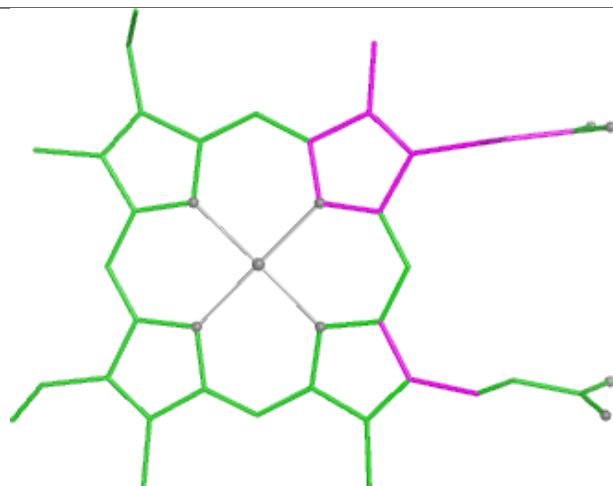




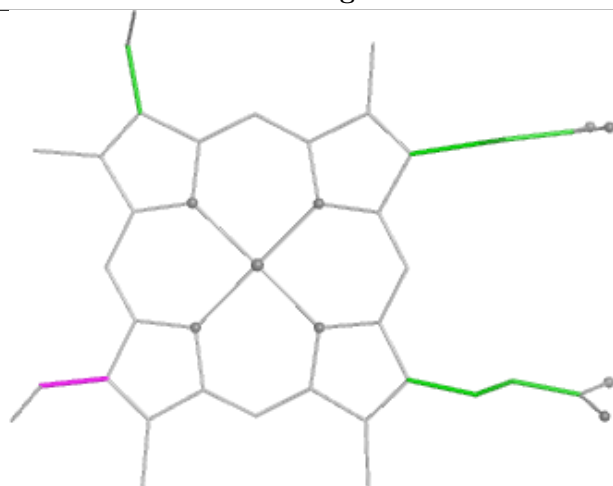
Ligand HEC H 1128



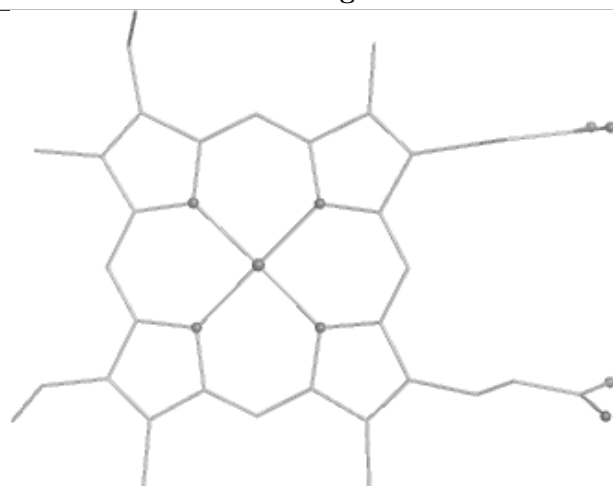
Bond lengths



Bond angles

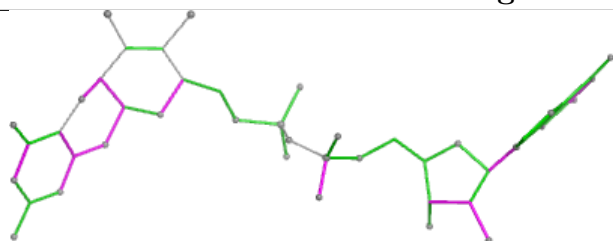


Torsions

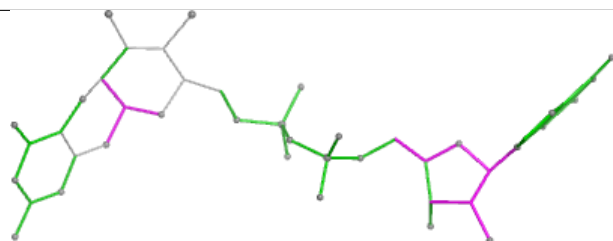


Rings

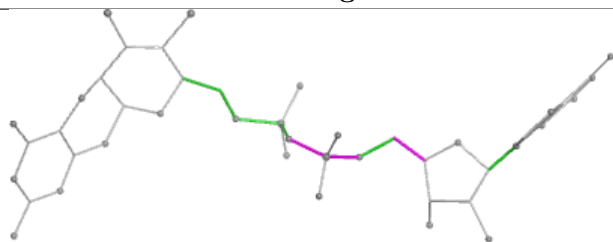
Ligand MGD O 1803



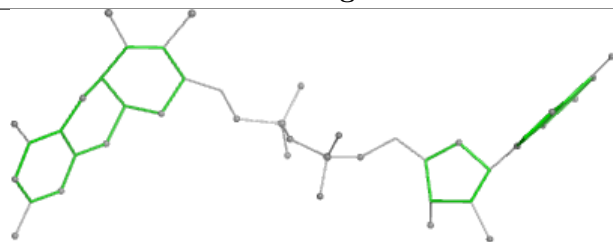
Bond lengths



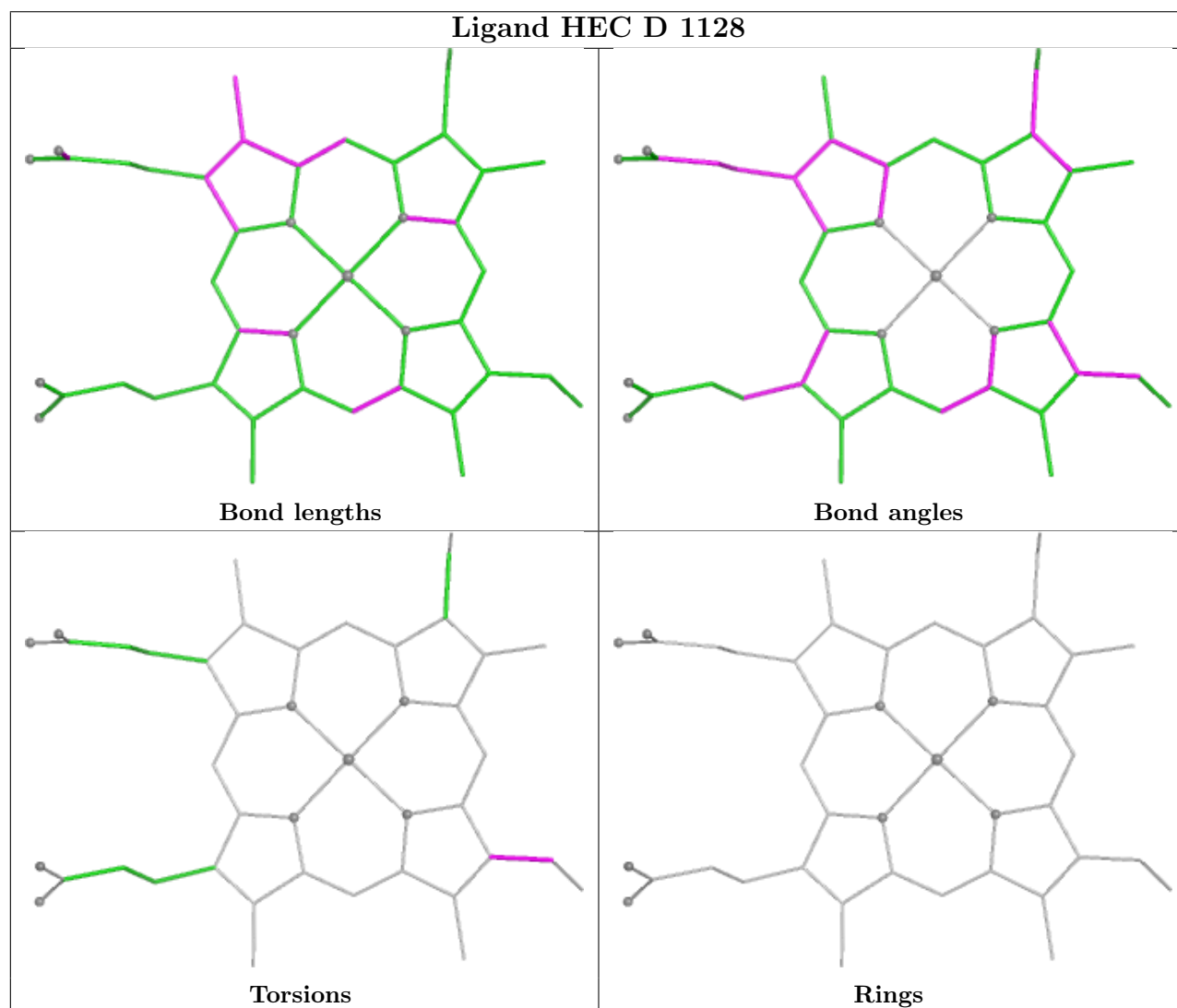
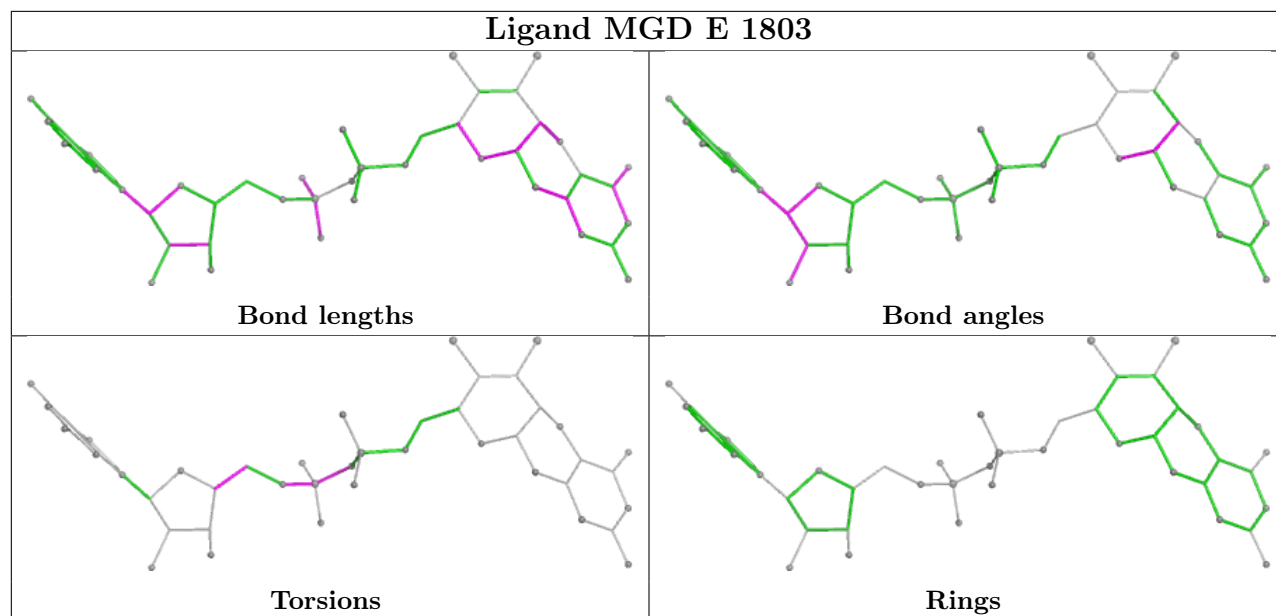
Bond angles



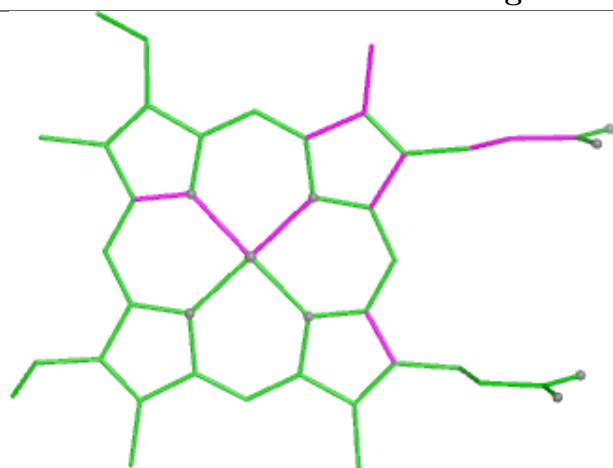
Torsions



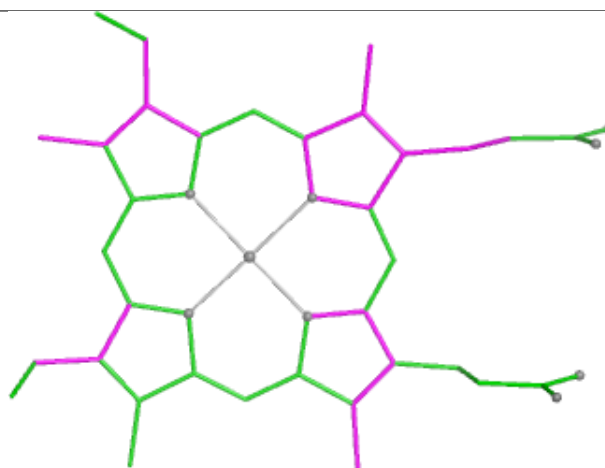
Rings



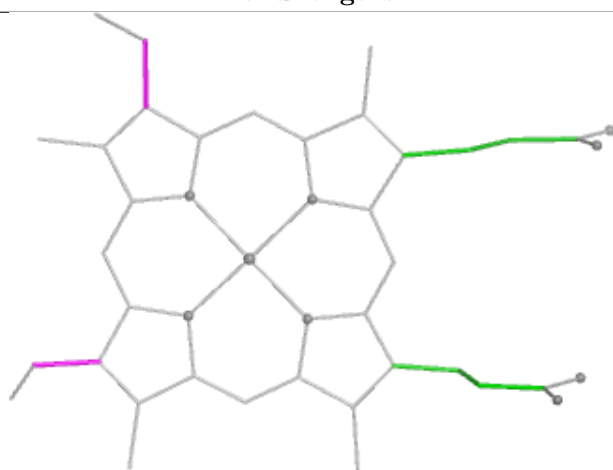
Ligand HEC P 1129



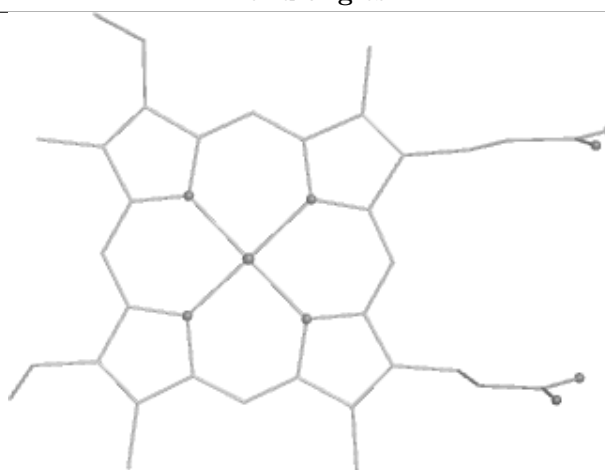
Bond lengths



Bond angles

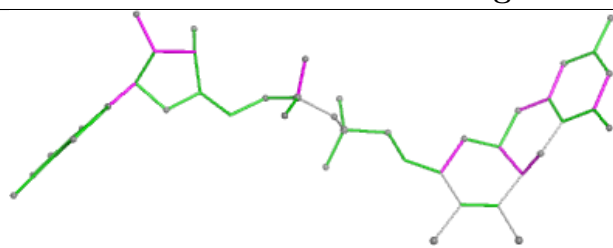


Torsions

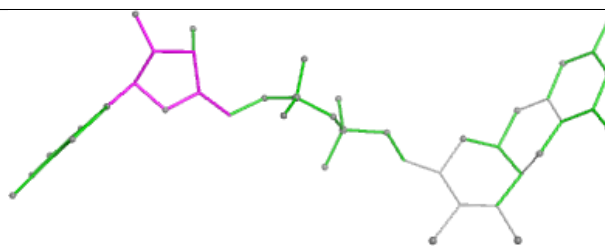


Rings

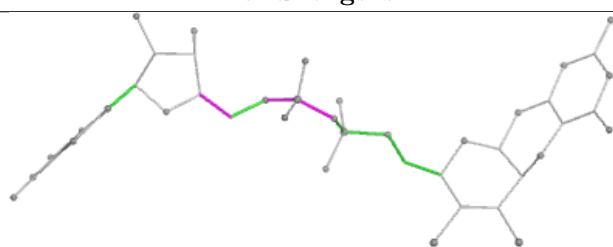
Ligand MGD M 1803



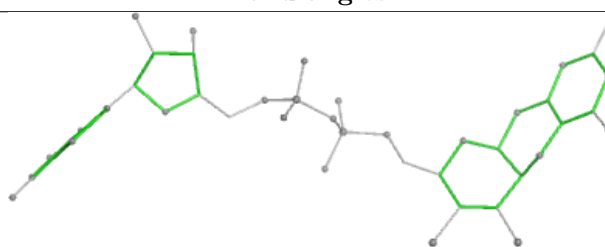
Bond lengths



Bond angles

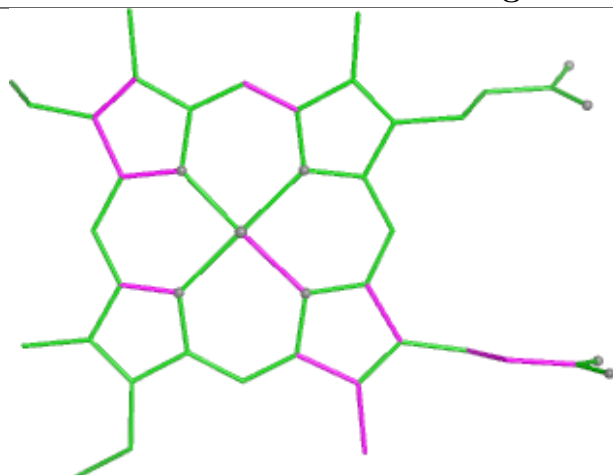


Torsions

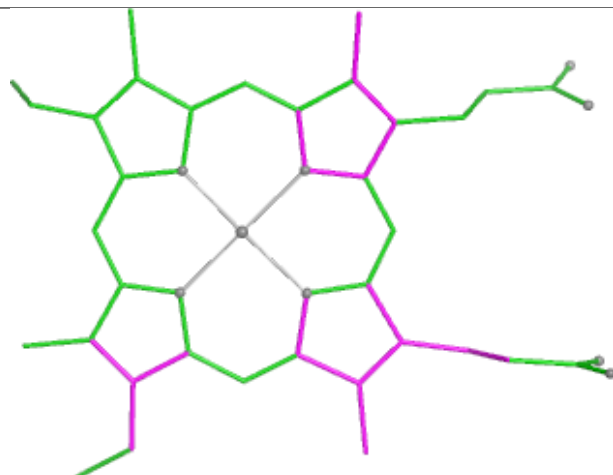


Rings

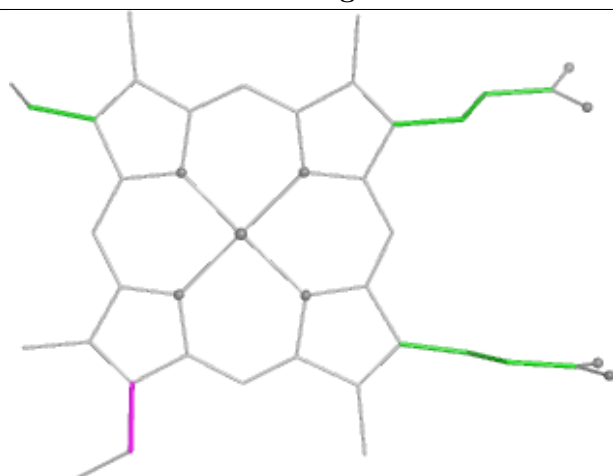
Ligand HEC H 1129



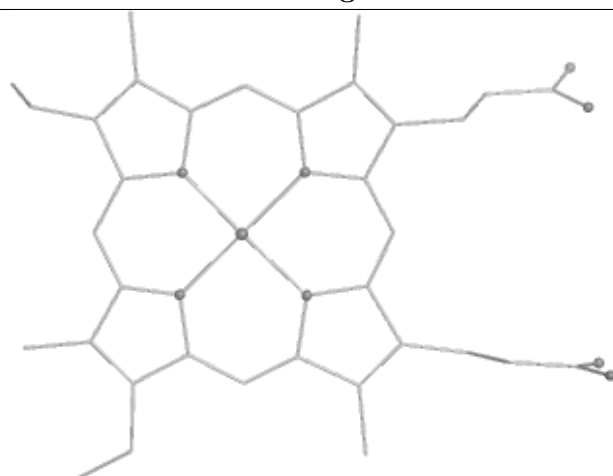
Bond lengths



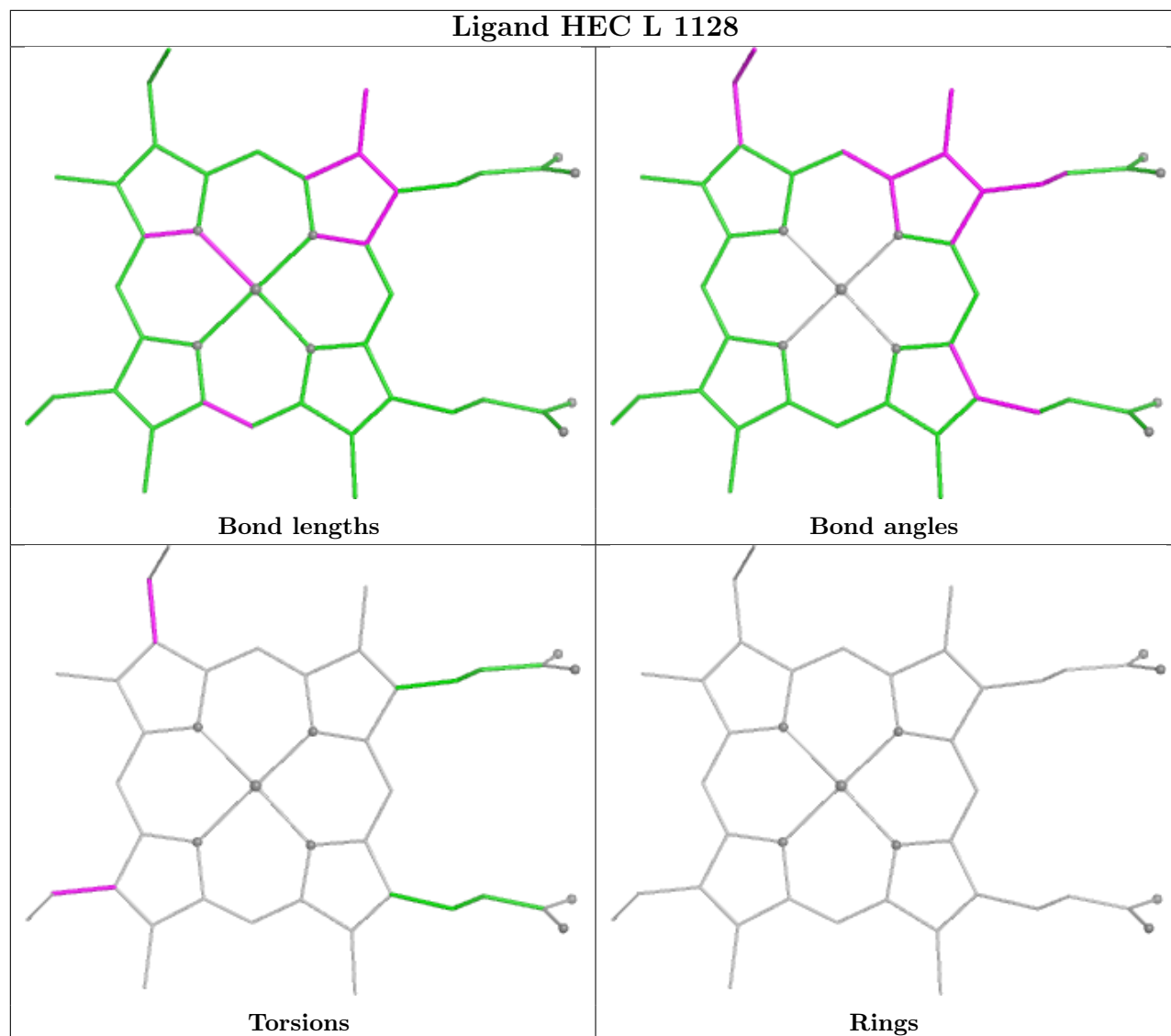
Bond angles

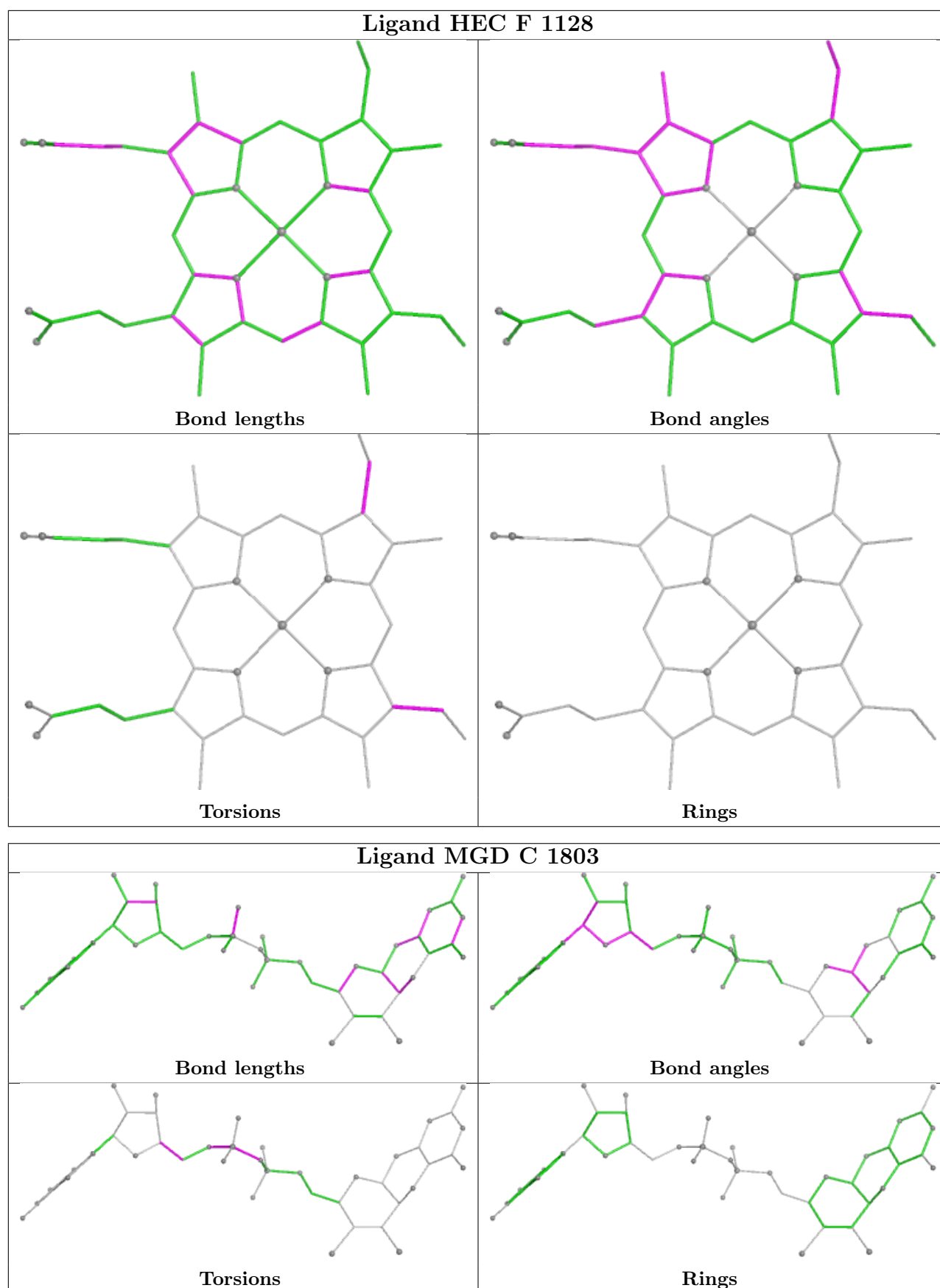


Torsions

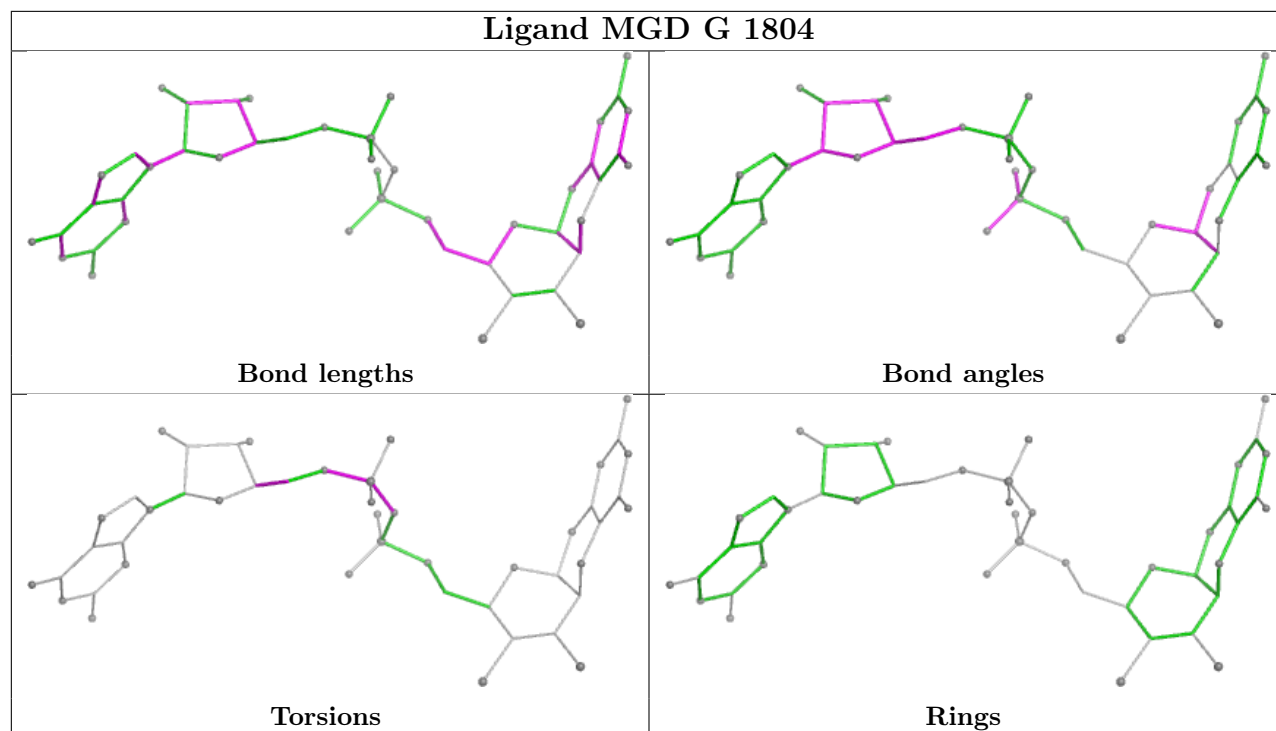


Rings

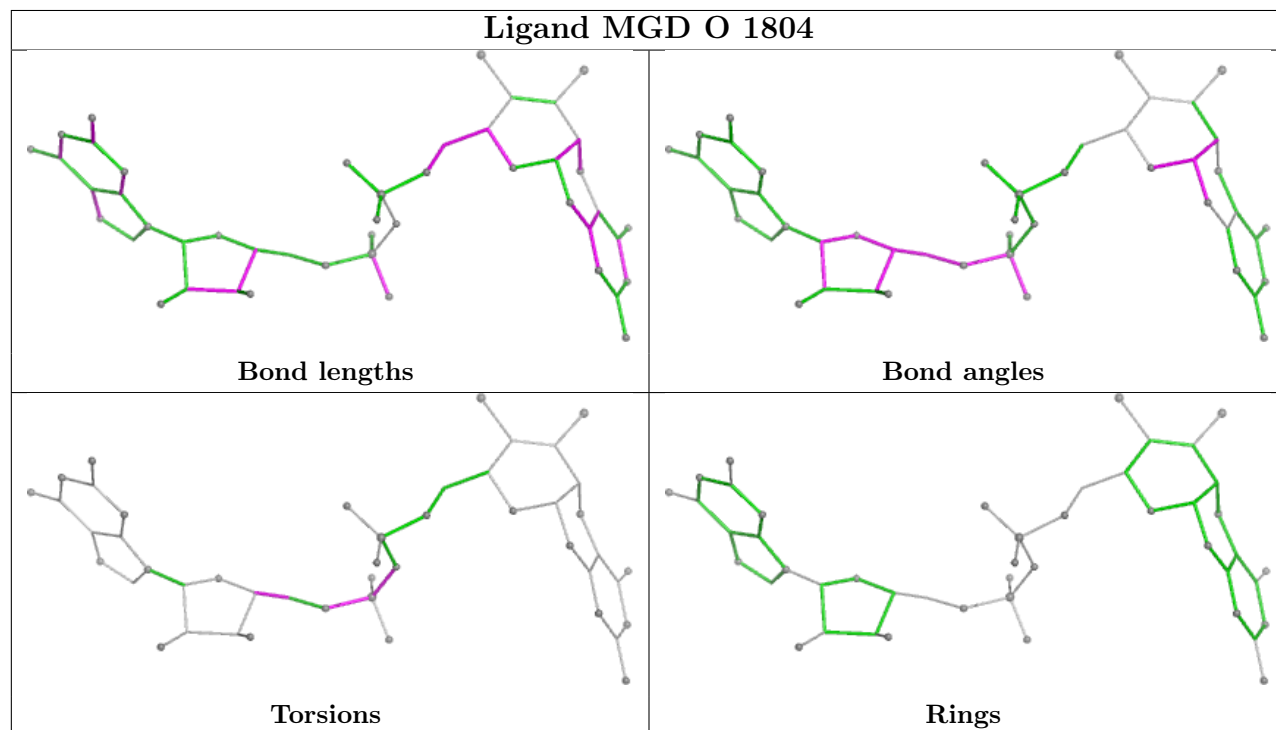


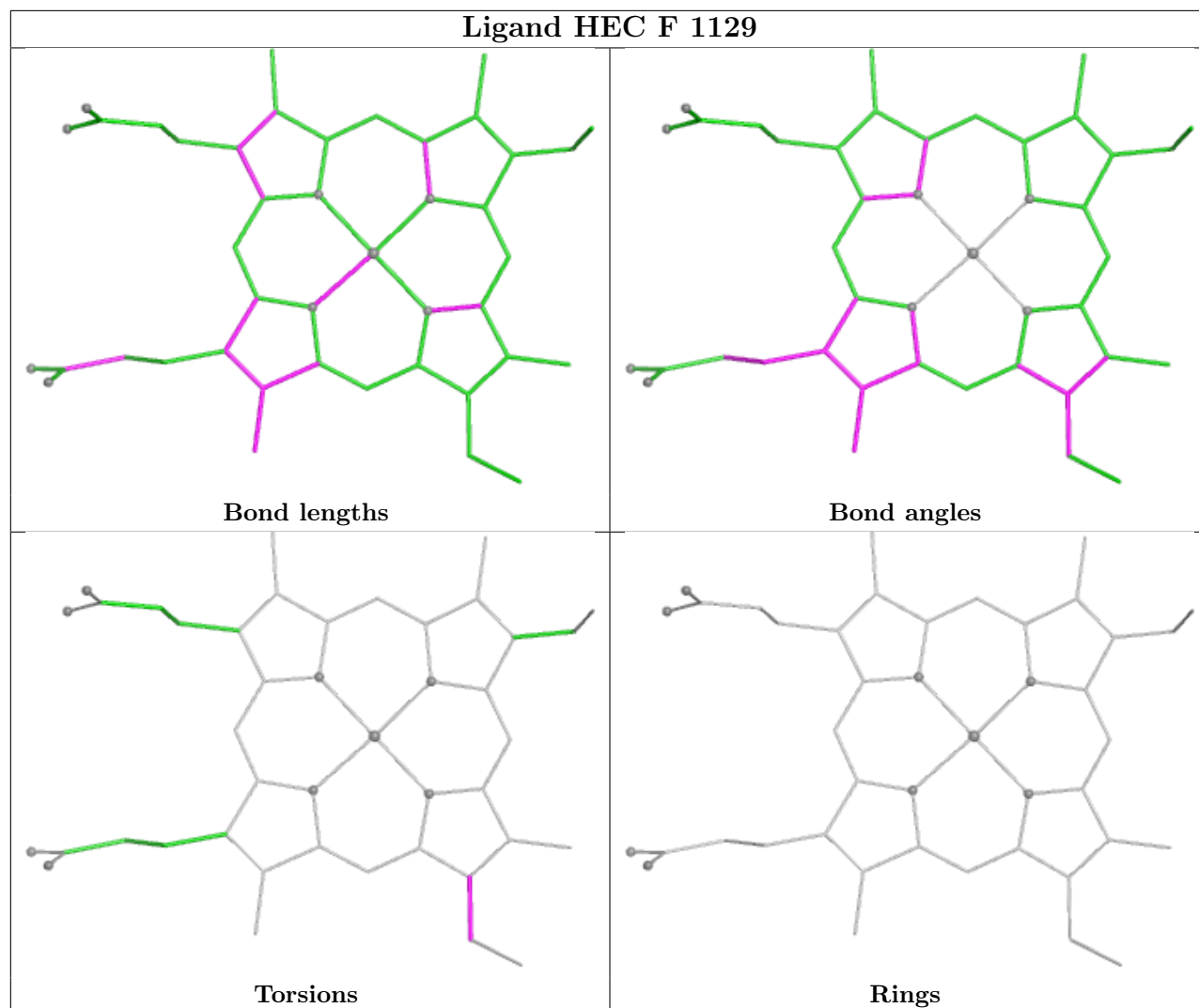


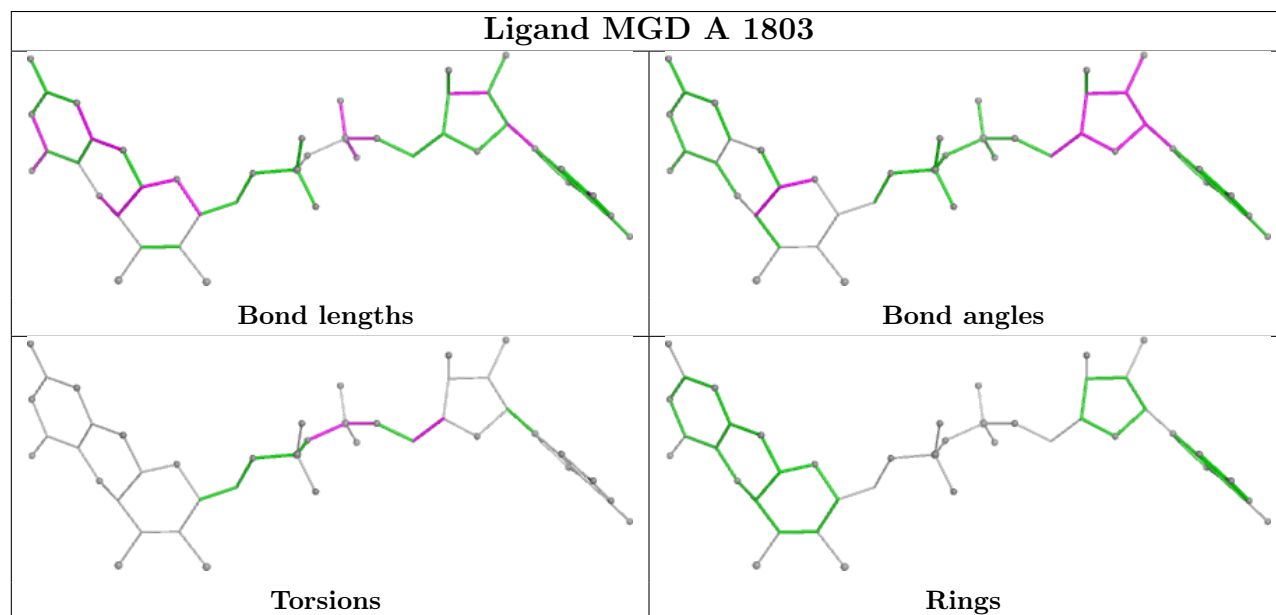
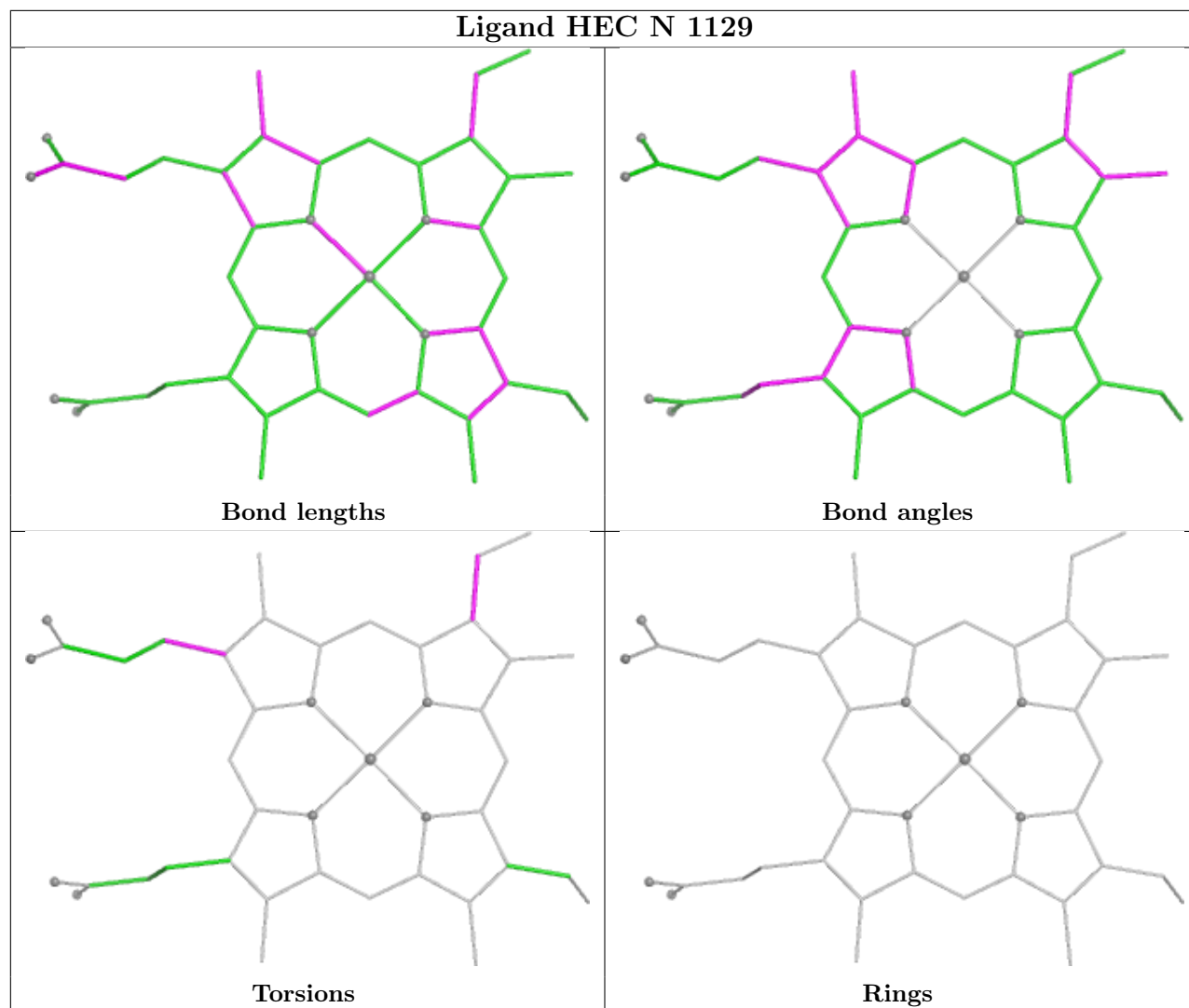
Ligand MGD G 1804



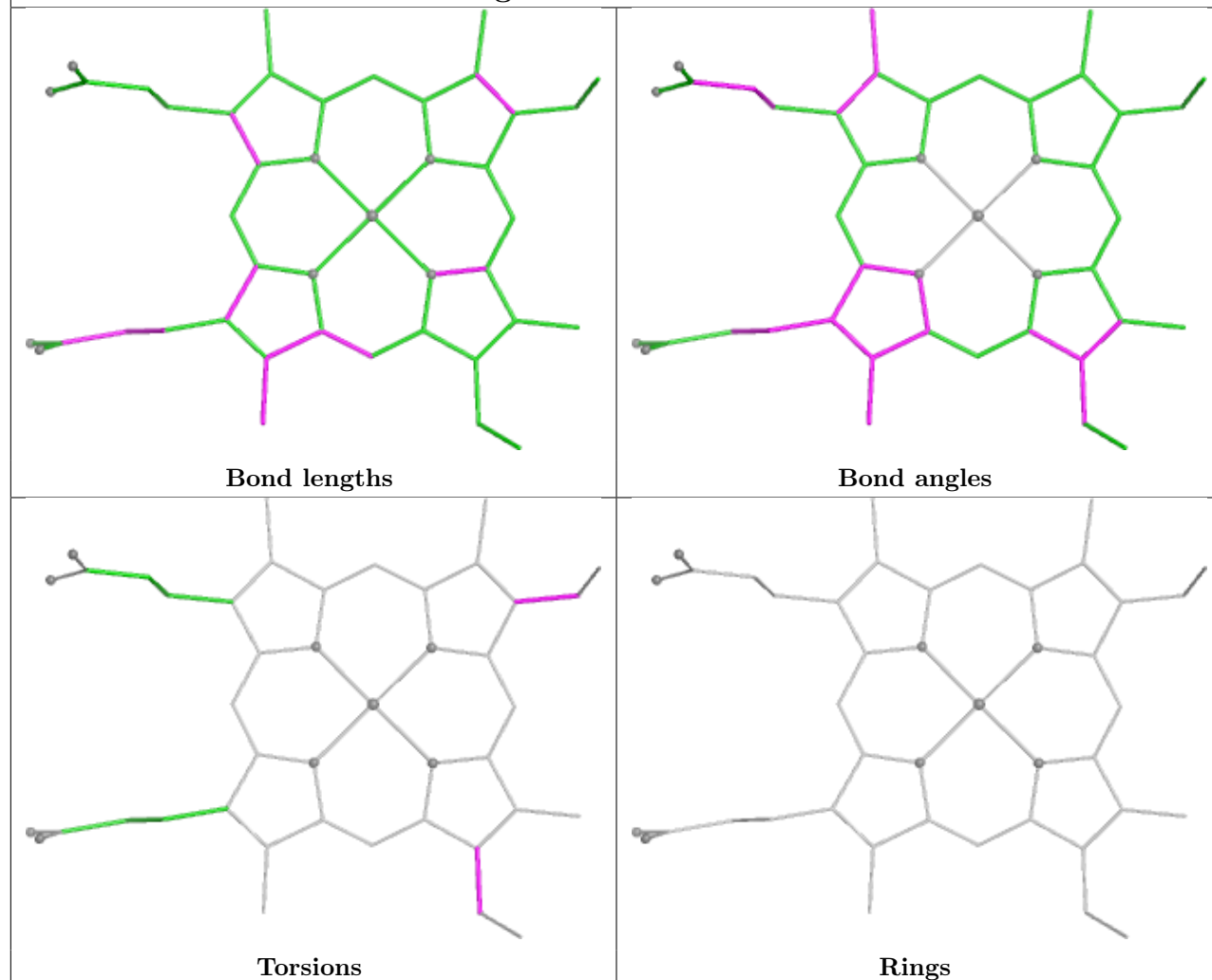
Ligand MGD O 1804



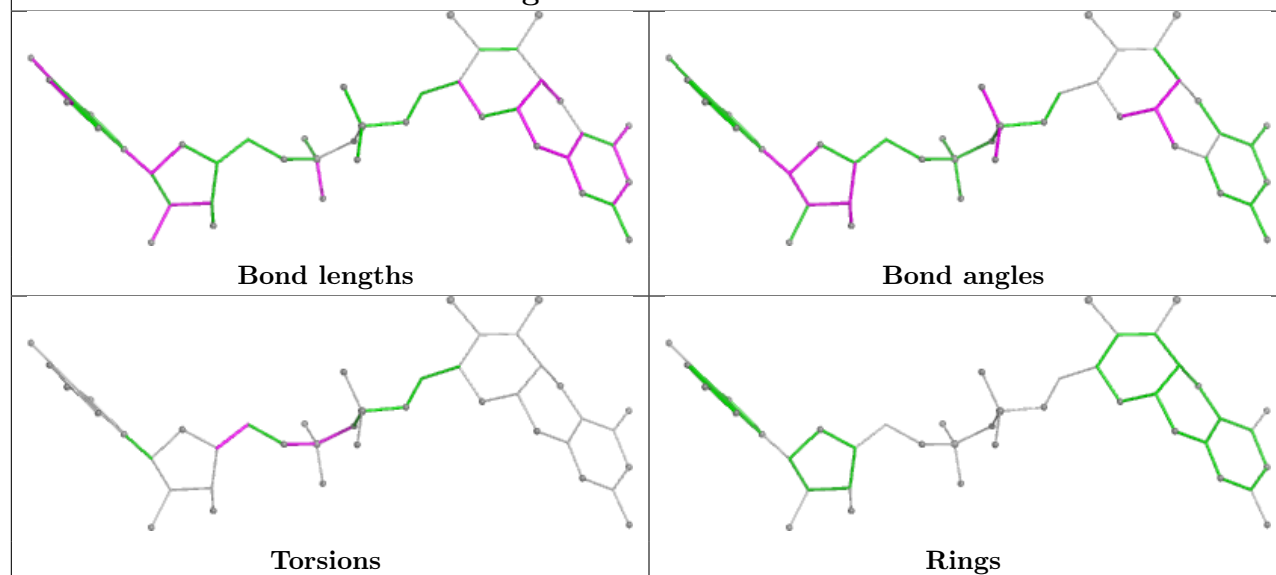




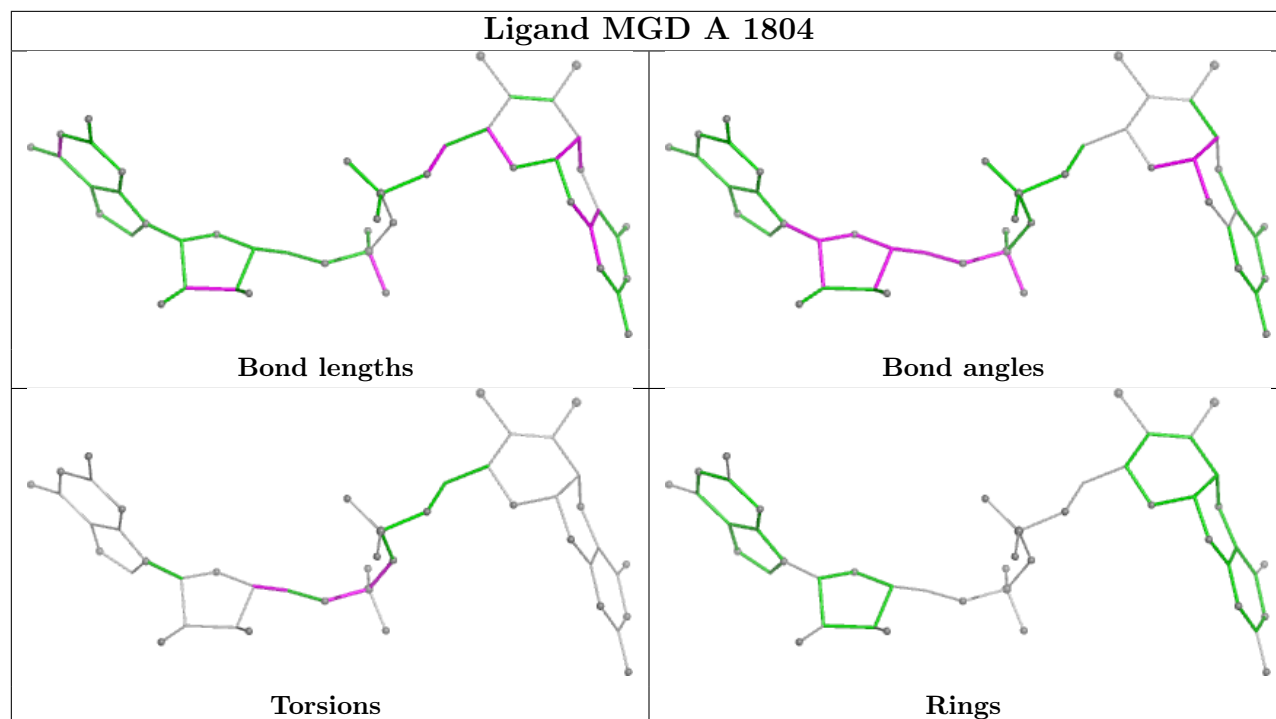
Ligand HEC D 1129



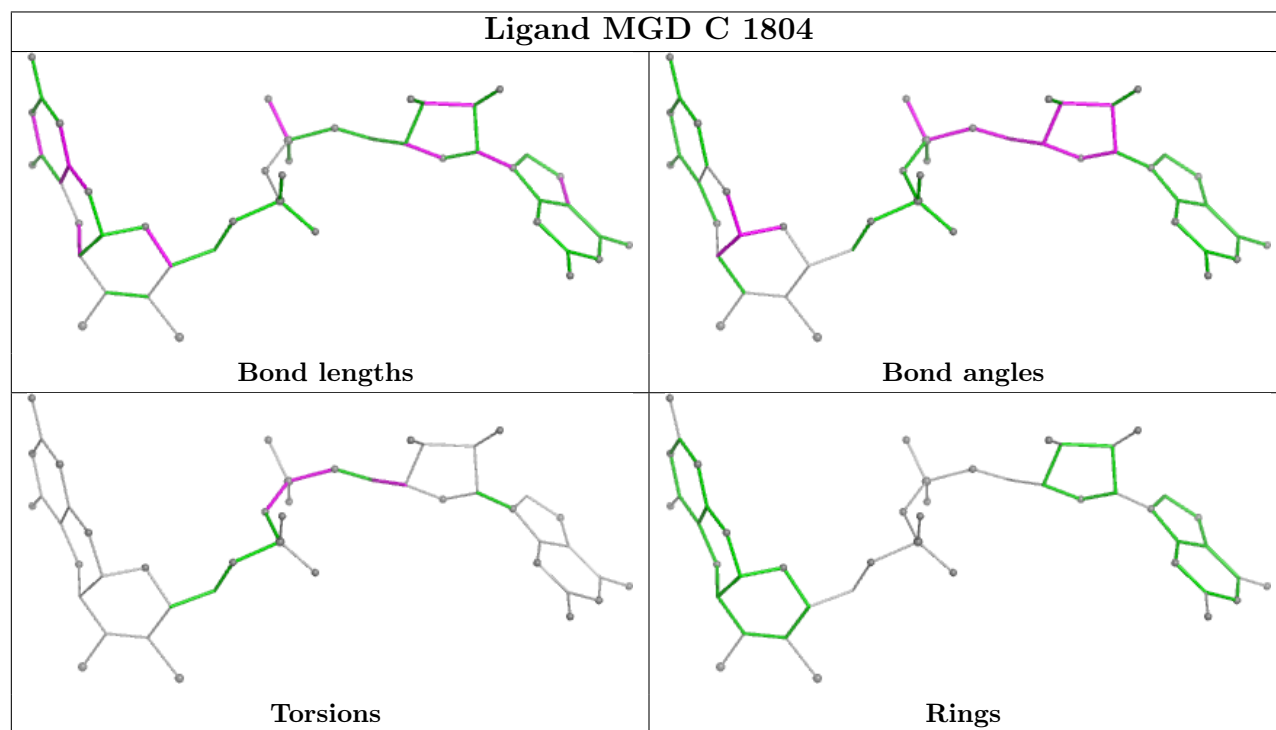
Ligand MGD I 1803

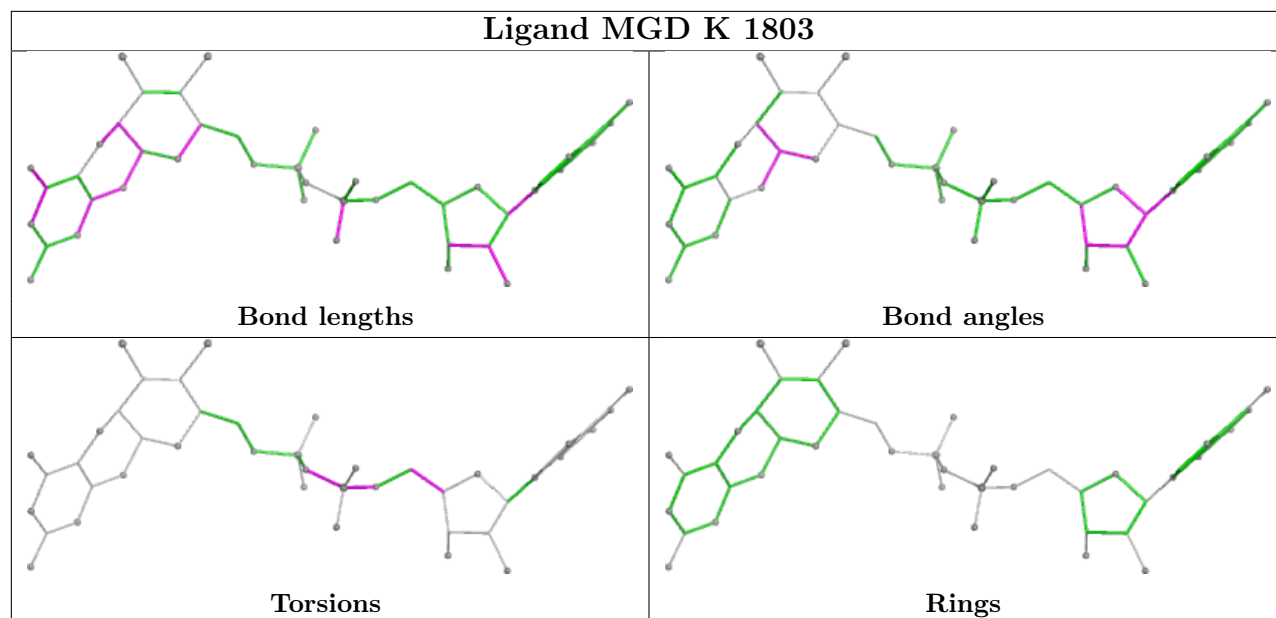


Ligand MGD A 1804



Ligand MGD C 1804





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

The worst 5 of 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

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
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

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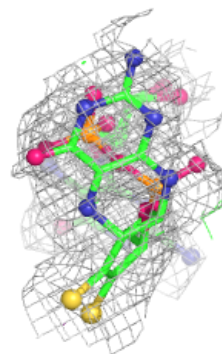
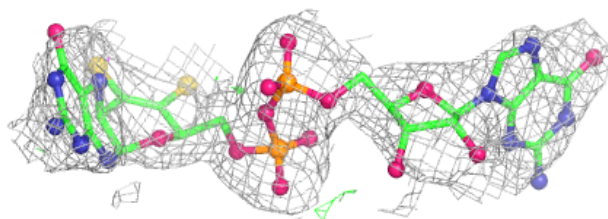
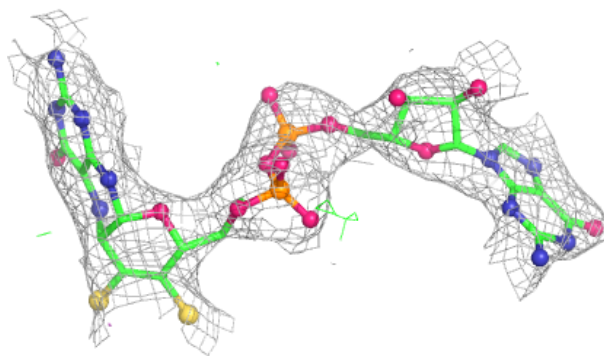
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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

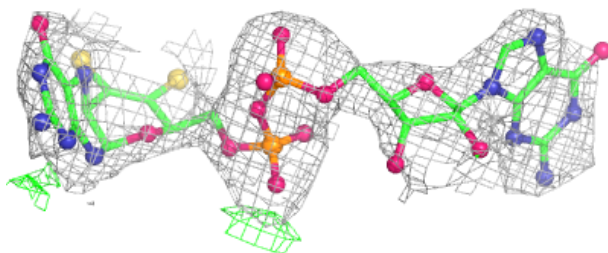
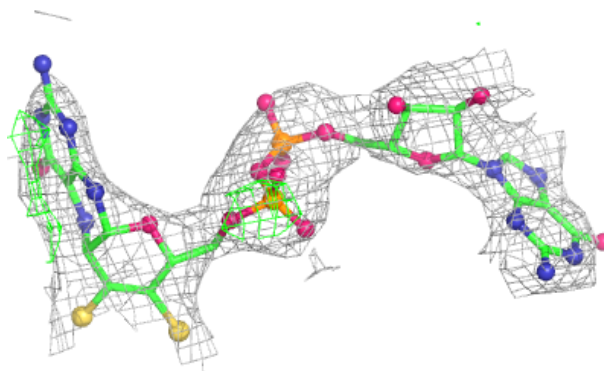
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

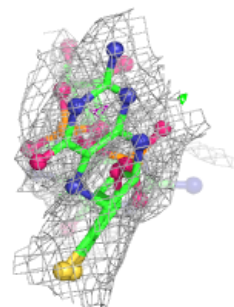
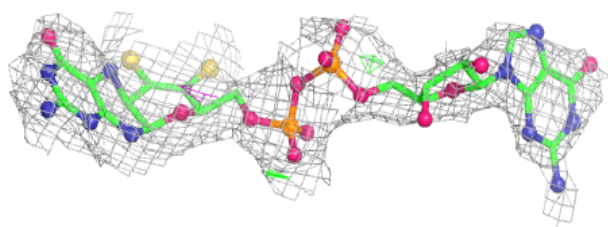
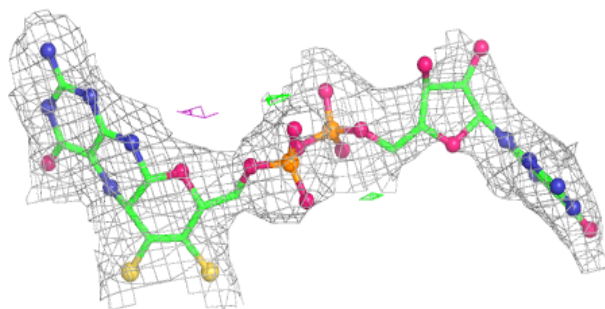
**Electron density around MGD O 1804:**

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

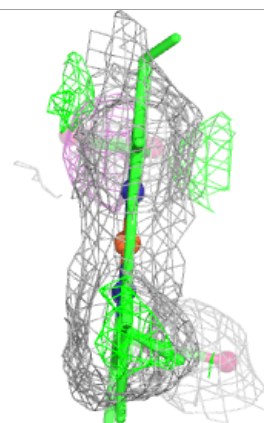
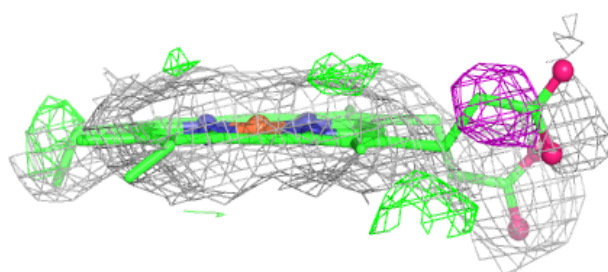
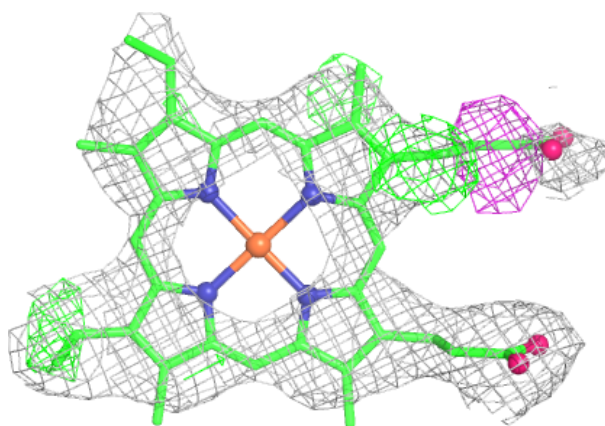


Electron density around MGD I 1803:

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

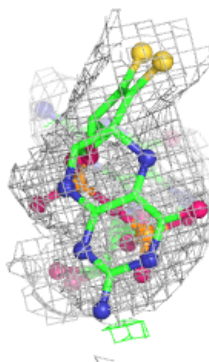
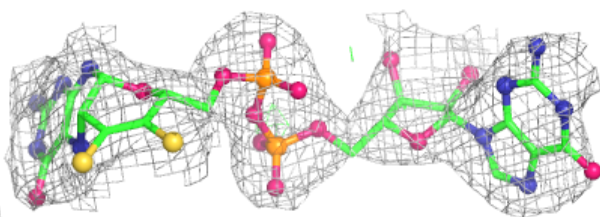
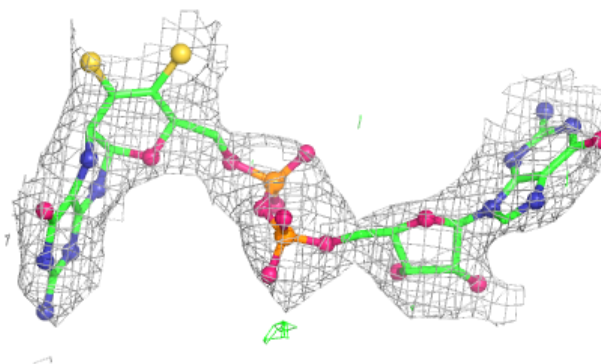
**Electron density around HEC P 1129:**

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

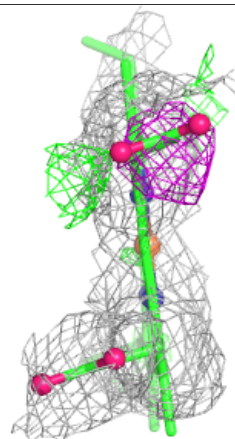
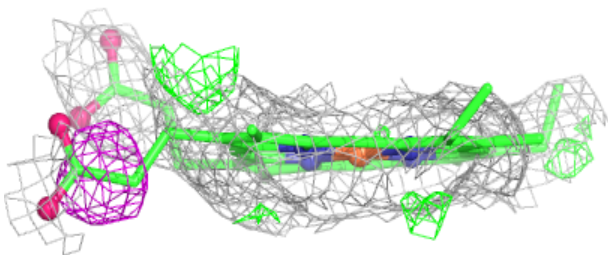
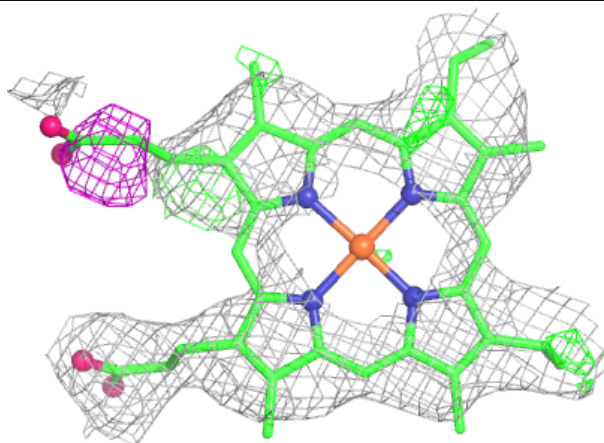


Electron density around MGD K 1804:

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

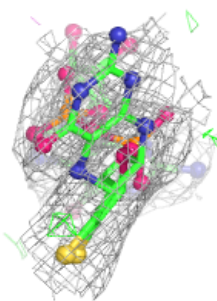
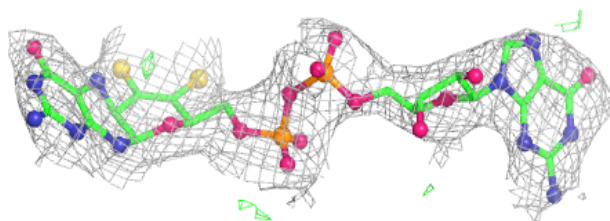
**Electron density around HEC J 1129:**

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

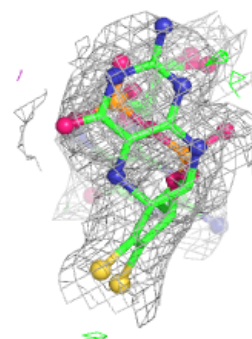
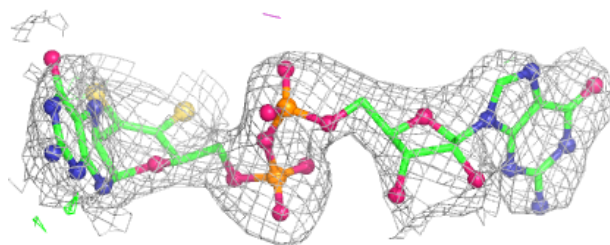
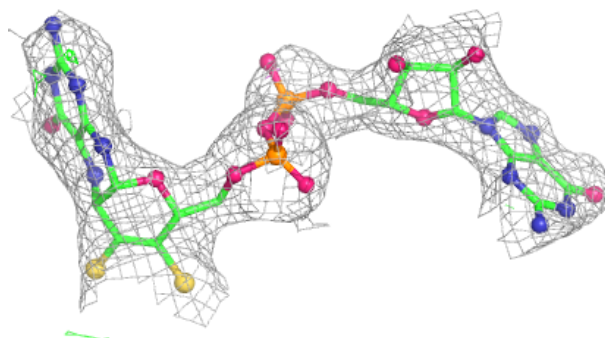


Electron density around MGD O 1803:

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

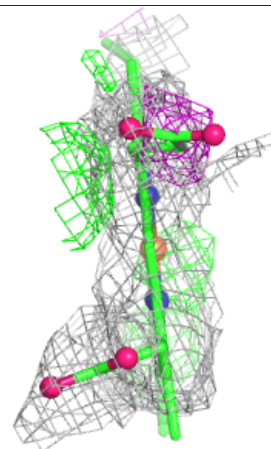
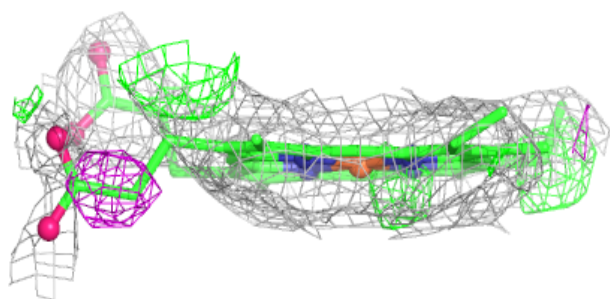
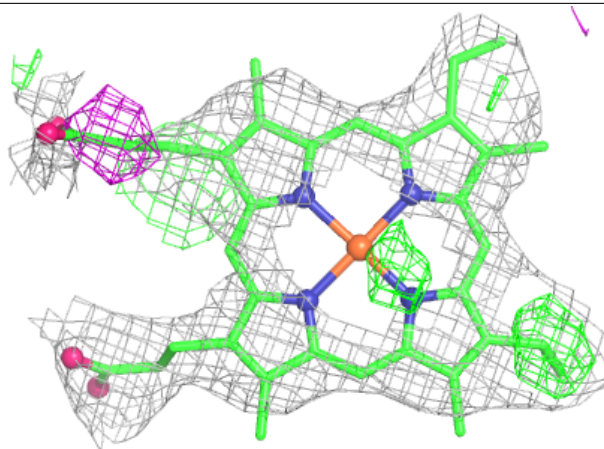
**Electron density around MGD G 1804:**

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



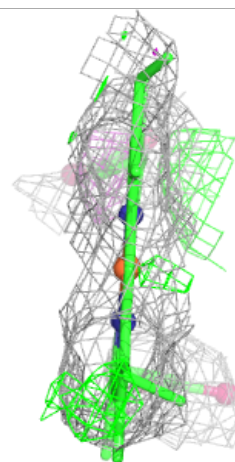
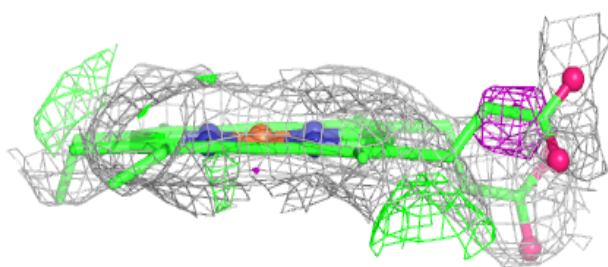
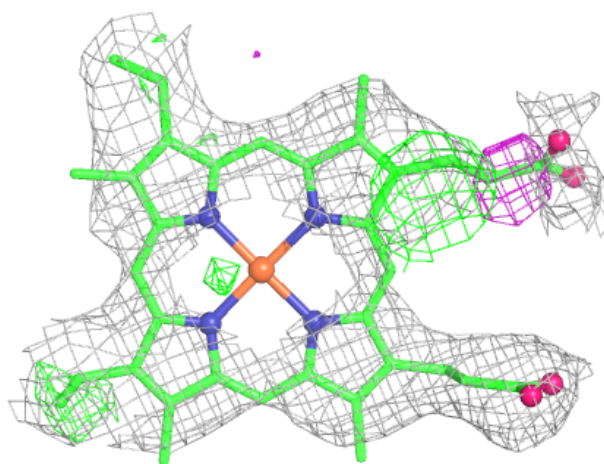
Electron density around HEC L 1129:

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



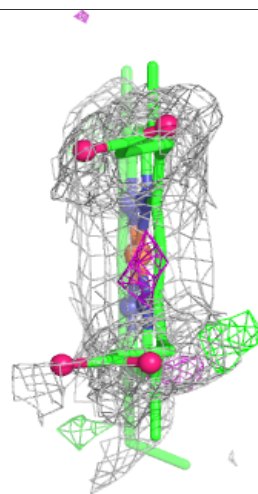
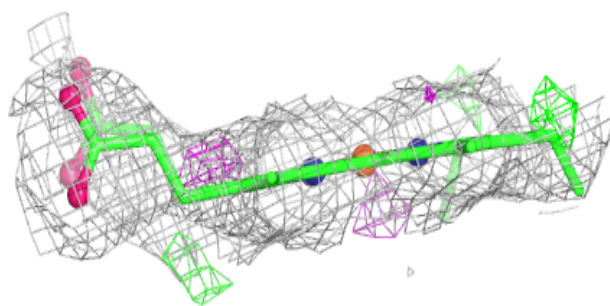
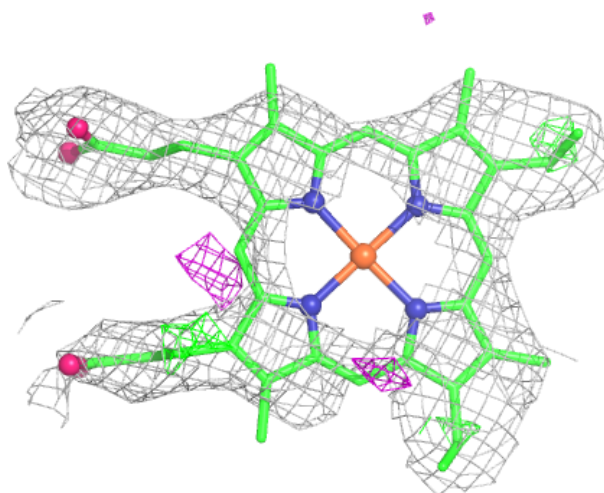
Electron density around HEC N 1129:

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



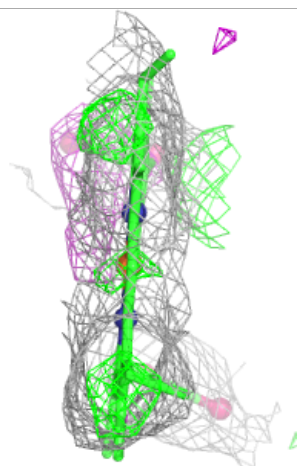
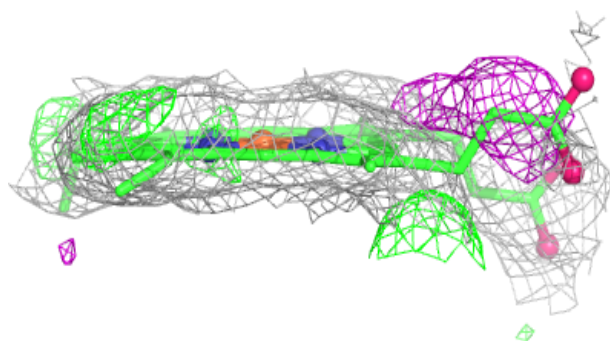
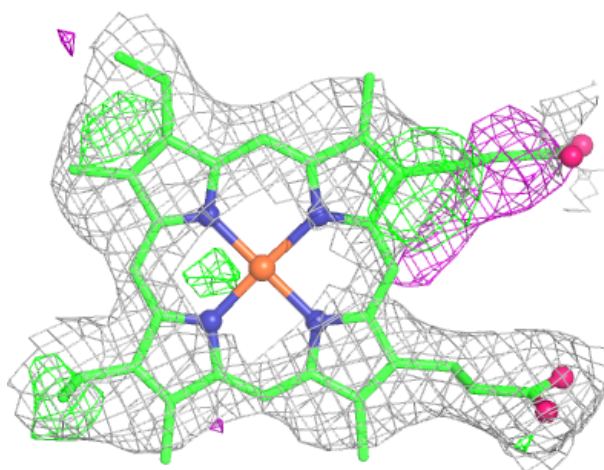
Electron density around HEC P 1128:

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



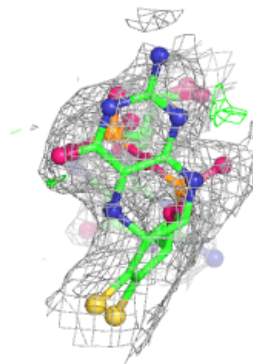
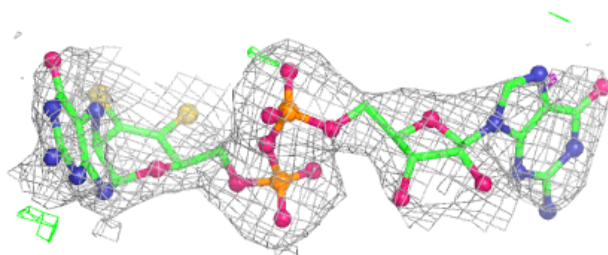
Electron density around HEC H 1129:

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

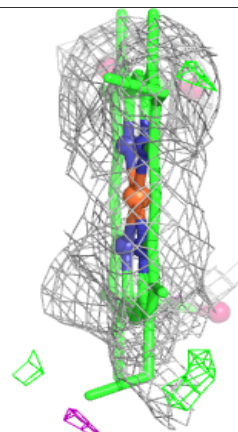
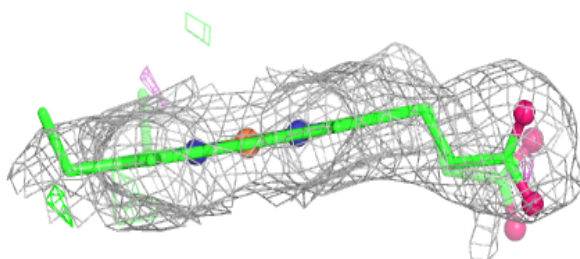
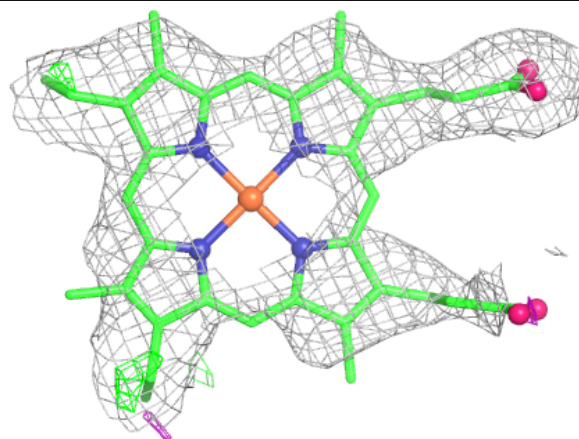


Electron density around MGD C 1804:

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

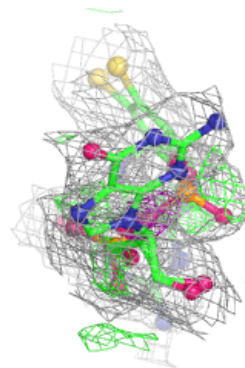
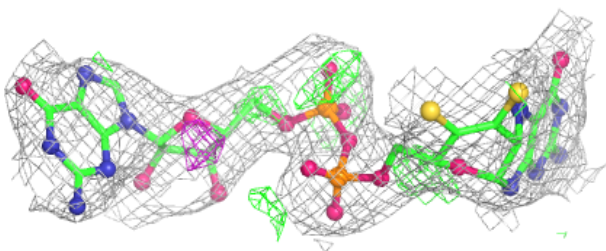
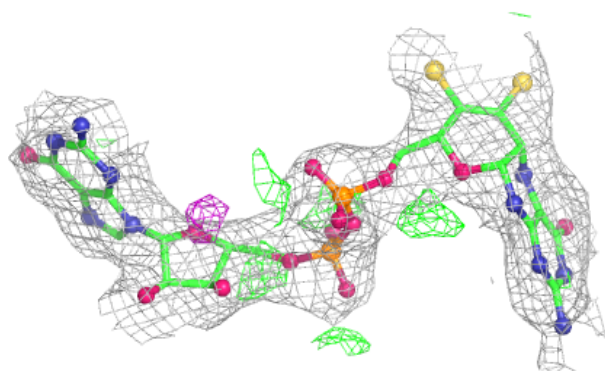
**Electron density around HEC J 1128:**

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



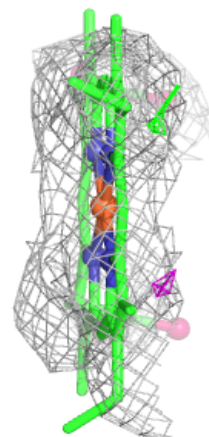
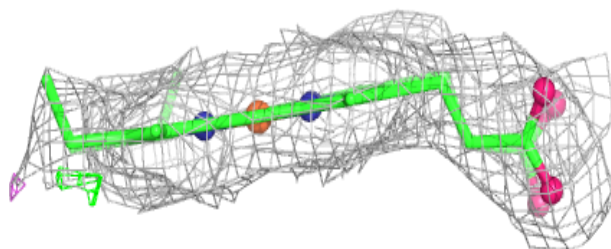
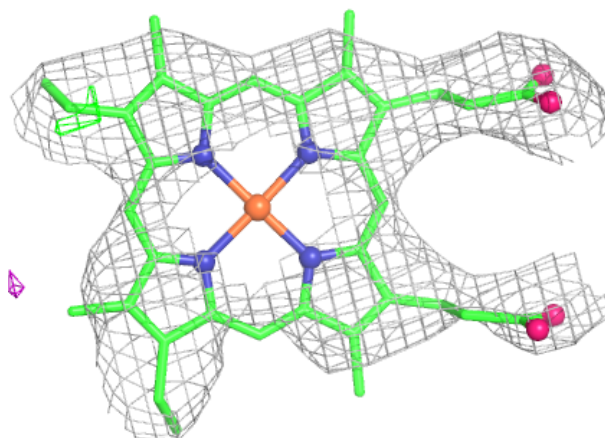
Electron density around MGD E 1804:

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



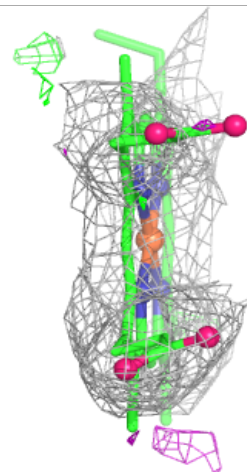
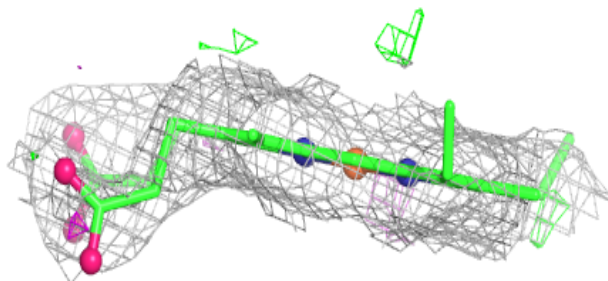
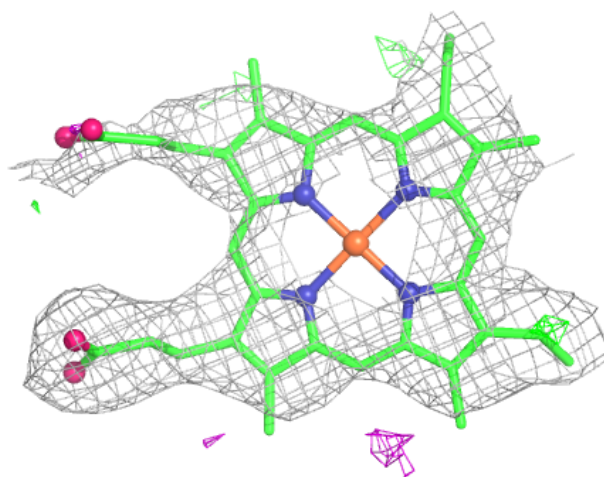
Electron density around HEC L 1128:

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



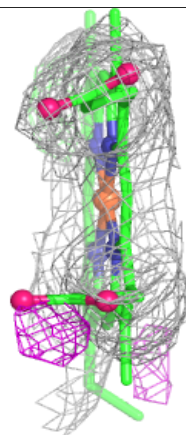
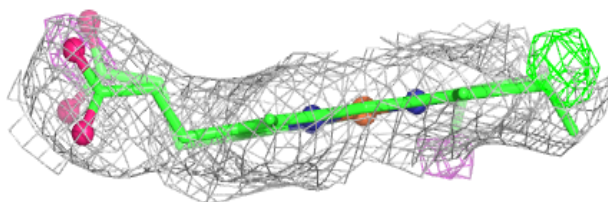
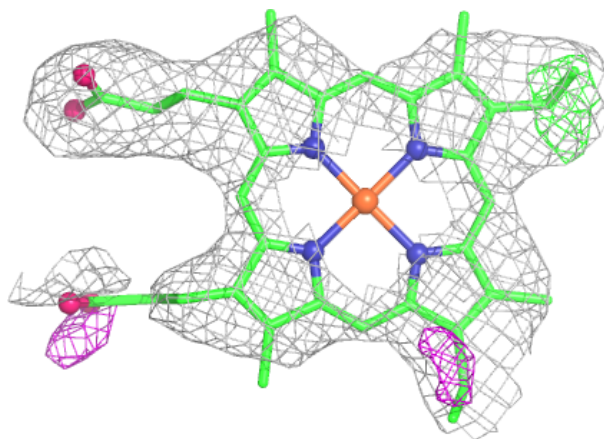
Electron density around HEC D 1128:

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



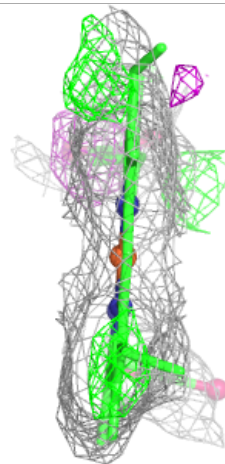
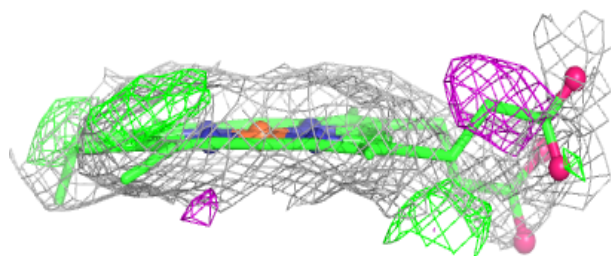
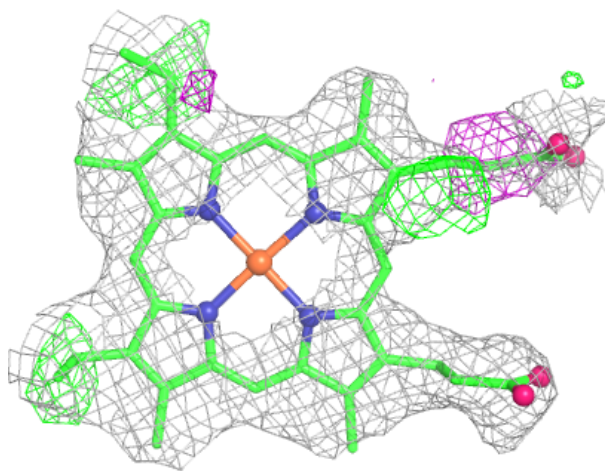
Electron density around HEC F 1128:

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



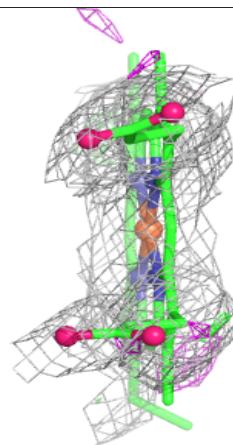
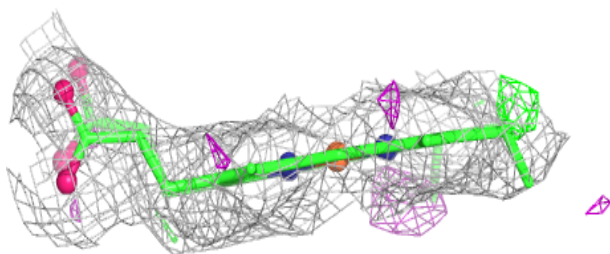
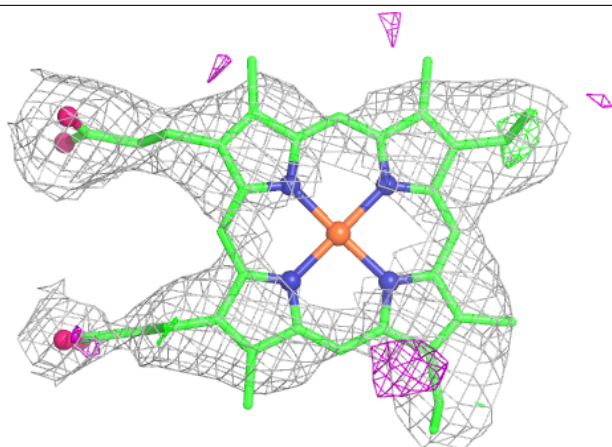
Electron density around HEC F 1129:

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



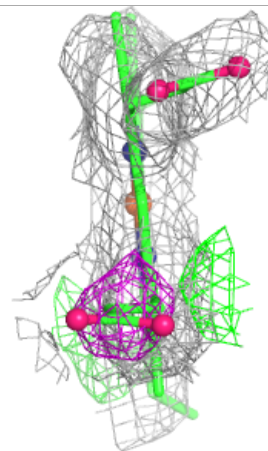
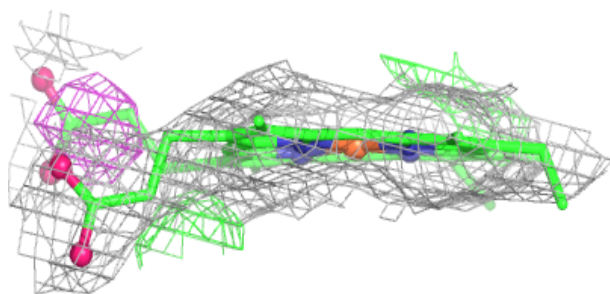
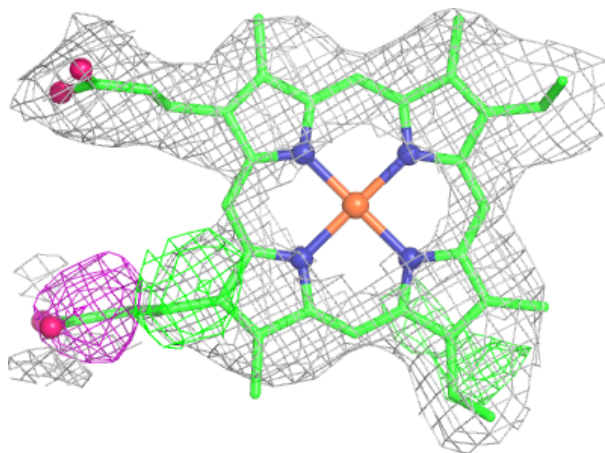
Electron density around HEC H 1128:

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



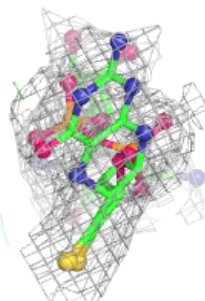
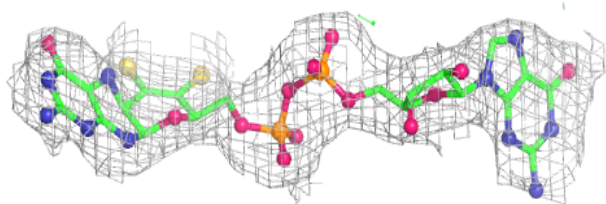
Electron density around HEC D 1129:

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

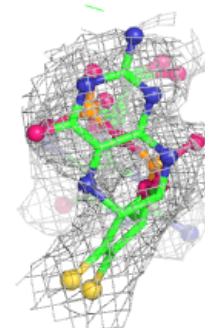
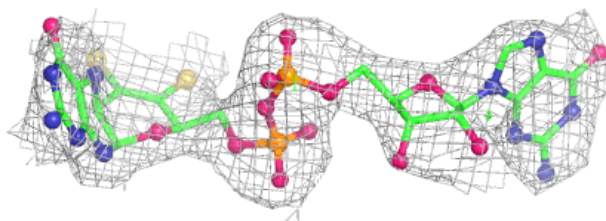


Electron density around MGD M 1803:

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

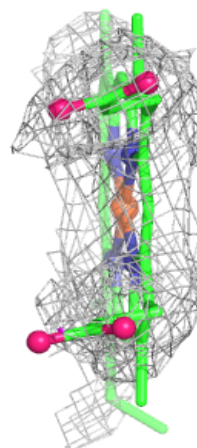
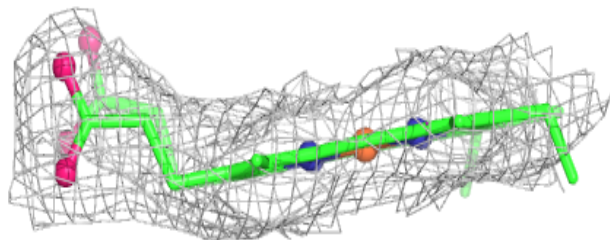
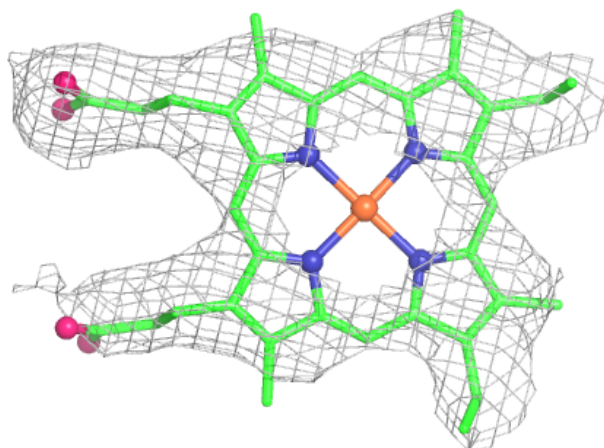
**Electron density around MGD M 1804:**

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



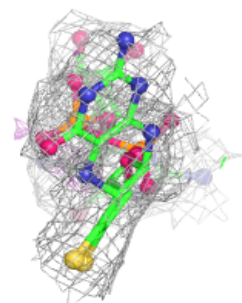
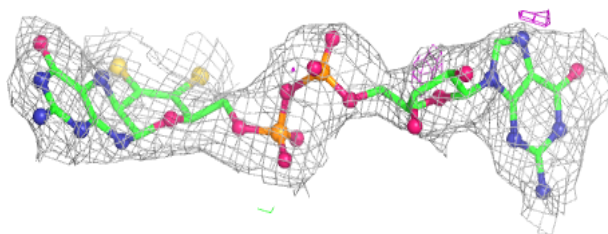
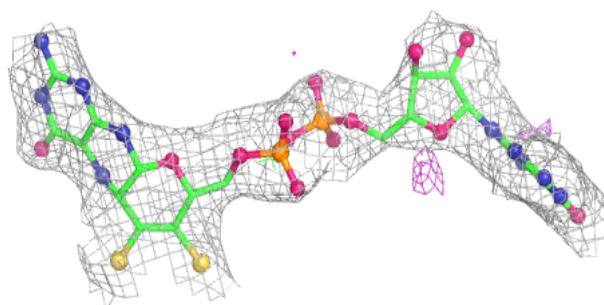
Electron density around HEC N 1128:

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

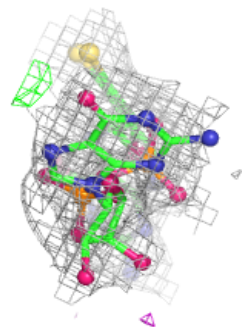
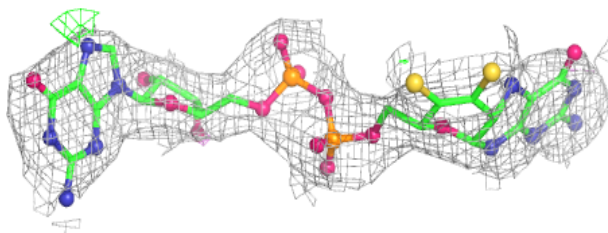
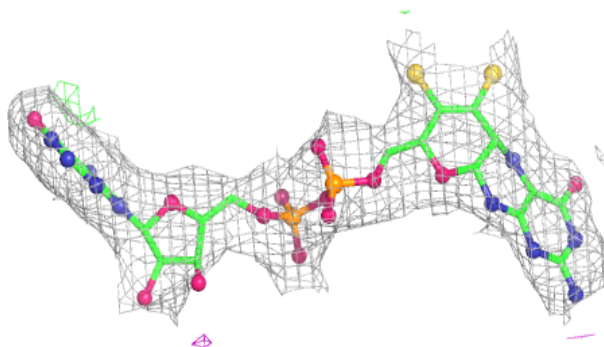


Electron density around MGD C 1803:

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

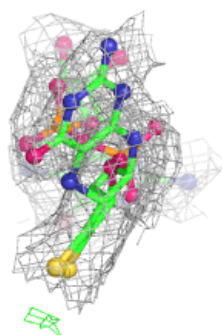
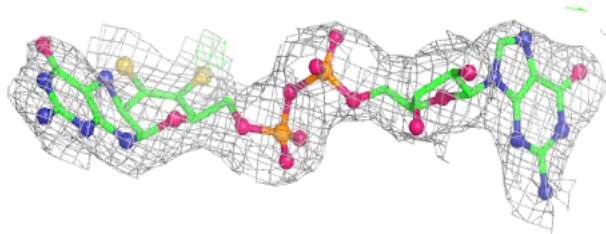
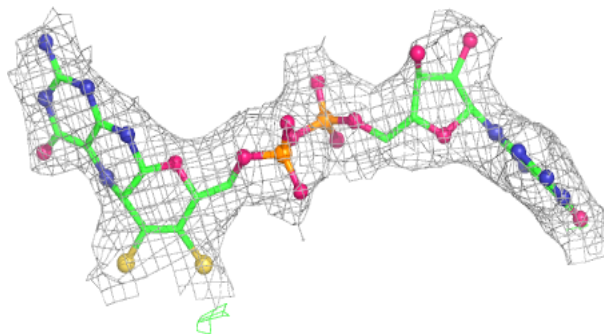
**Electron density around MGD K 1803:**

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

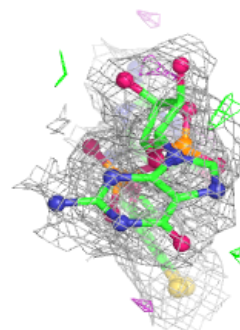
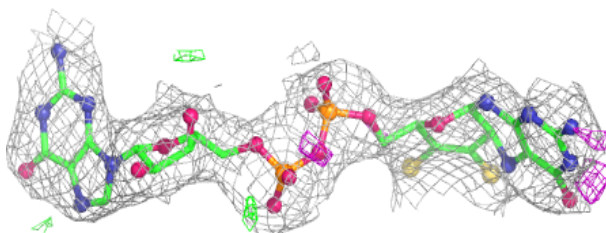
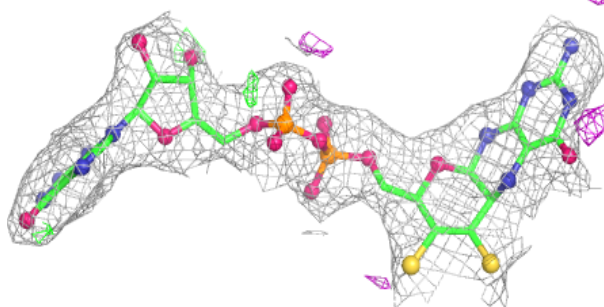


Electron density around MGD G 1803:

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

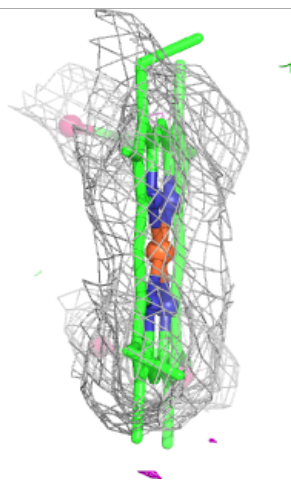
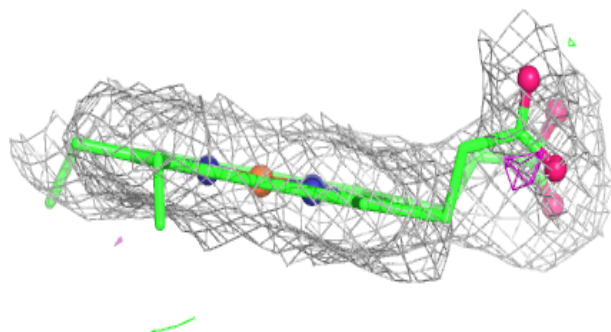
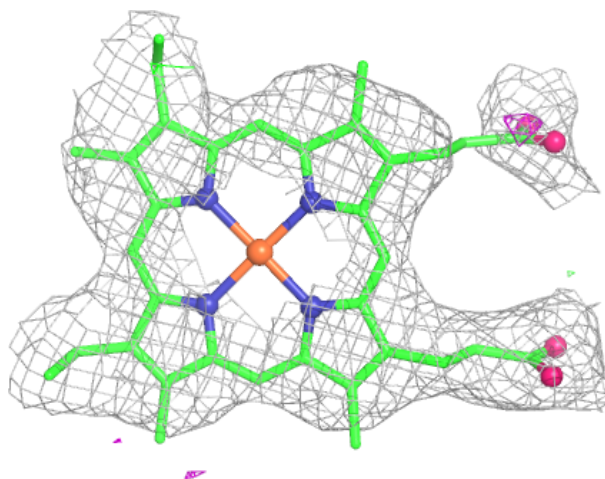
**Electron density around MGD A 1803:**

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



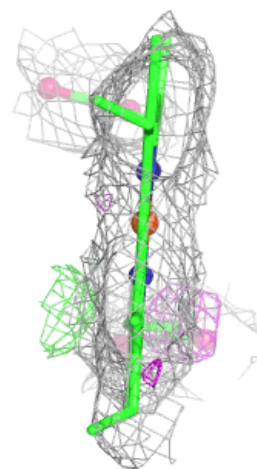
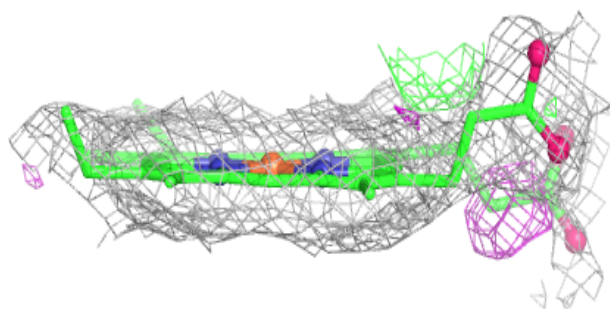
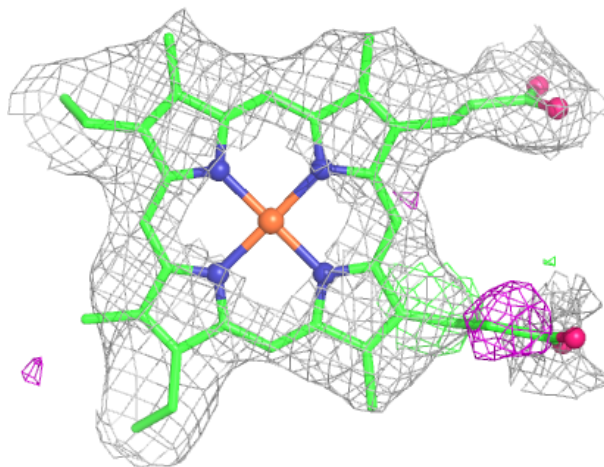
Electron density around HEC B 1128:

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



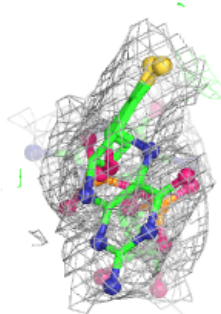
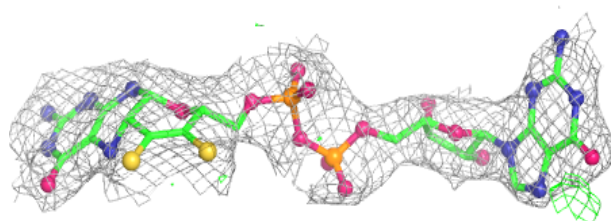
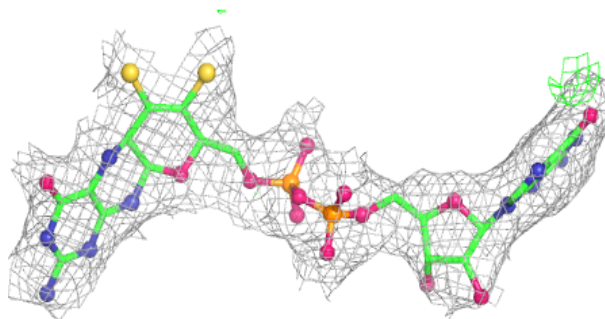
Electron density around HEC B 1129:

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

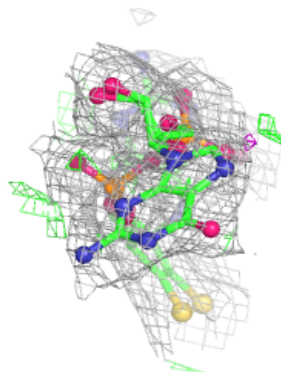
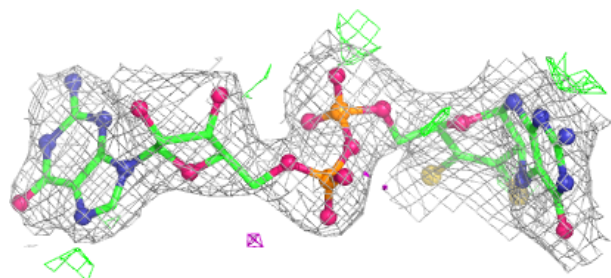
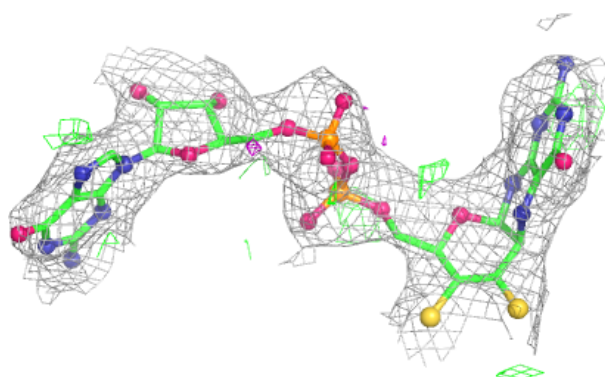


Electron density around MGD E 1803:

$2mF_o-DF_c$ (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.