



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 05:01 PM EDT

PDB ID : 2QJY / pdb_00002qjy
Title : Crystal structure of rhodobacter sphaeroides double mutant with stigmatellin and UQ2
Authors : Esser, L.; Xia, D.
Deposited on : 2007-07-09
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
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	:	9.0.015 (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

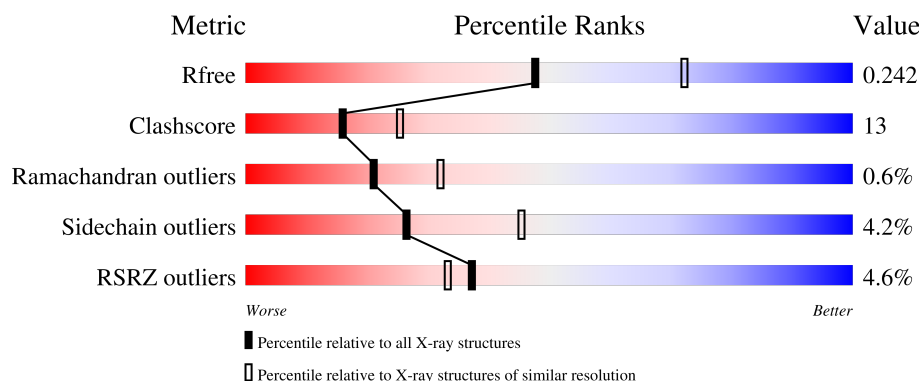
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	445	2% 72% 21% . .
1	D	445	2% 70% 24% . .
1	G	445	2% 70% 23% . .
1	J	445	3% 68% 25% . . .
1	M	445	2% 67% 26% . .

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Mol	Chain	Length	Quality of chain
1	P	445	
2	B	269	
2	E	269	
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	D	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	G	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	J	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	M	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	P	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	engineered mutation	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	287	ARG	SER	engineered mutation	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	N	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	Q	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP Q3IY11
B	265	HIS	-	expression tag	UNP Q3IY11
B	266	HIS	-	expression tag	UNP Q3IY11
B	267	HIS	-	expression tag	UNP Q3IY11
B	268	HIS	-	expression tag	UNP Q3IY11
B	269	HIS	-	expression tag	UNP Q3IY11
E	264	HIS	-	expression tag	UNP Q3IY11
E	265	HIS	-	expression tag	UNP Q3IY11
E	266	HIS	-	expression tag	UNP Q3IY11
E	267	HIS	-	expression tag	UNP Q3IY11
E	268	HIS	-	expression tag	UNP Q3IY11
E	269	HIS	-	expression tag	UNP Q3IY11
H	264	HIS	-	expression tag	UNP Q3IY11
H	265	HIS	-	expression tag	UNP Q3IY11
H	266	HIS	-	expression tag	UNP Q3IY11
H	267	HIS	-	expression tag	UNP Q3IY11
H	268	HIS	-	expression tag	UNP Q3IY11
H	269	HIS	-	expression tag	UNP Q3IY11
K	264	HIS	-	expression tag	UNP Q3IY11
K	265	HIS	-	expression tag	UNP Q3IY11
K	266	HIS	-	expression tag	UNP Q3IY11
K	267	HIS	-	expression tag	UNP Q3IY11
K	268	HIS	-	expression tag	UNP Q3IY11
K	269	HIS	-	expression tag	UNP Q3IY11
N	264	HIS	-	expression tag	UNP Q3IY11
N	265	HIS	-	expression tag	UNP Q3IY11
N	266	HIS	-	expression tag	UNP Q3IY11
N	267	HIS	-	expression tag	UNP Q3IY11
N	268	HIS	-	expression tag	UNP Q3IY11
N	269	HIS	-	expression tag	UNP Q3IY11
Q	264	HIS	-	expression tag	UNP Q3IY11
Q	265	HIS	-	expression tag	UNP Q3IY11

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	266	HIS	-	expression tag	UNP Q3IY11
Q	267	HIS	-	expression tag	UNP Q3IY11
Q	268	HIS	-	expression tag	UNP Q3IY11
Q	269	HIS	-	expression tag	UNP Q3IY11

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	engineered mutation	UNP Q02762
F	135	SER	VAL	engineered mutation	UNP Q02762
I	135	SER	VAL	engineered mutation	UNP Q02762
L	135	SER	VAL	engineered mutation	UNP Q02762
O	135	SER	VAL	engineered mutation	UNP Q02762
R	135	SER	VAL	engineered mutation	UNP Q02762

- Molecule 4 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

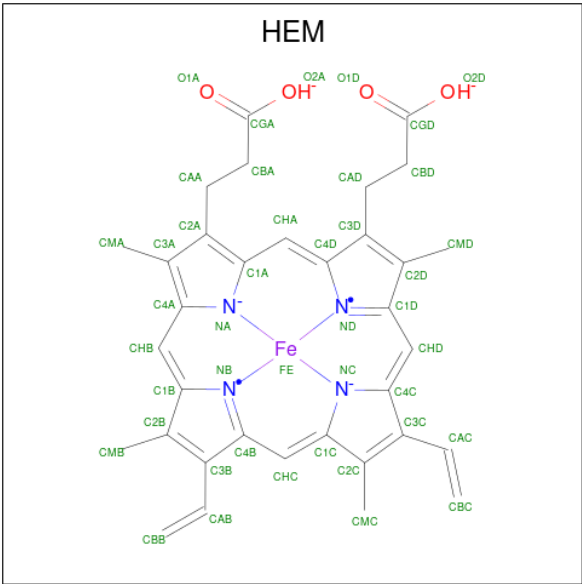
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Sr	0	0
			1	1		
4	B	1	Total	Sr	0	0
			1	1		
4	E	1	Total	Sr	0	0
			1	1		
4	G	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Sr	0	0
			1	1		
4	K	1	Total	Sr	0	0
			1	1		
4	M	1	Total	Sr	0	0
			1	1		
4	N	1	Total	Sr	0	0
			1	1		
4	Q	1	Total	Sr	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



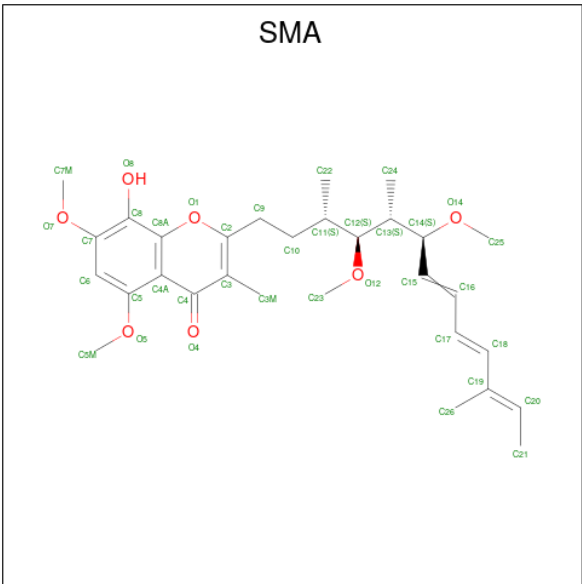
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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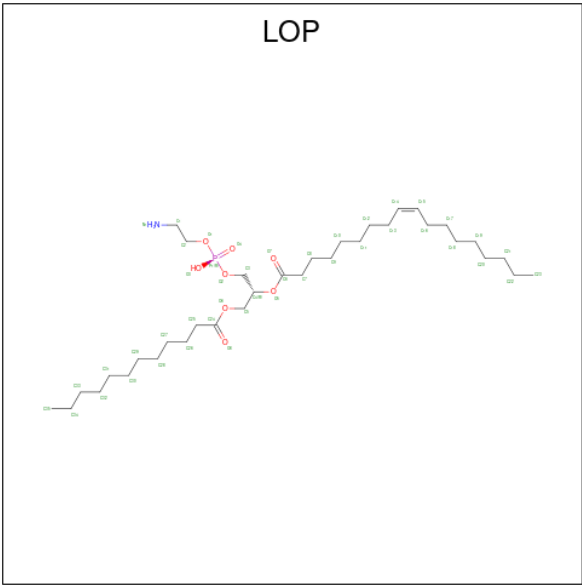
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is STIGMATELLIN A (CCD ID: SMA) (formula: C₃₀H₄₂O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	30	7		
6	D	1	Total	C	O	0	0
			37	30	7		
6	G	1	Total	C	O	0	0
			37	30	7		
6	J	1	Total	C	O	0	0
			37	30	7		
6	M	1	Total	C	O	0	0
			37	30	7		
6	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



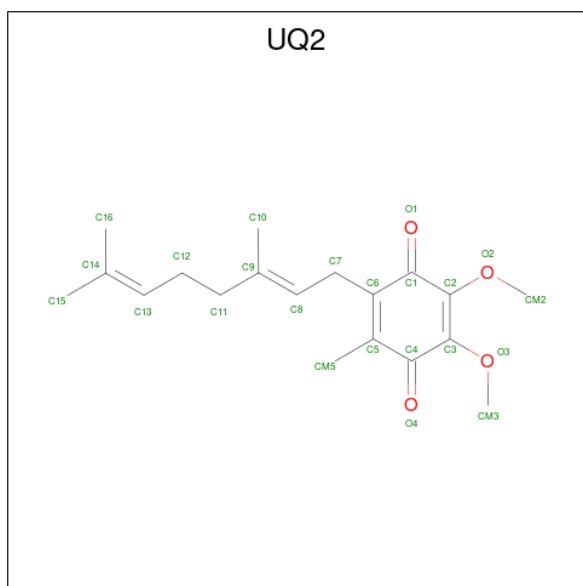
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

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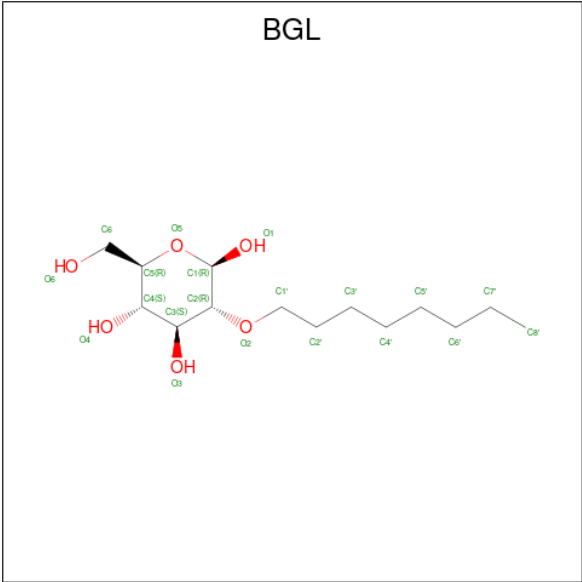
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



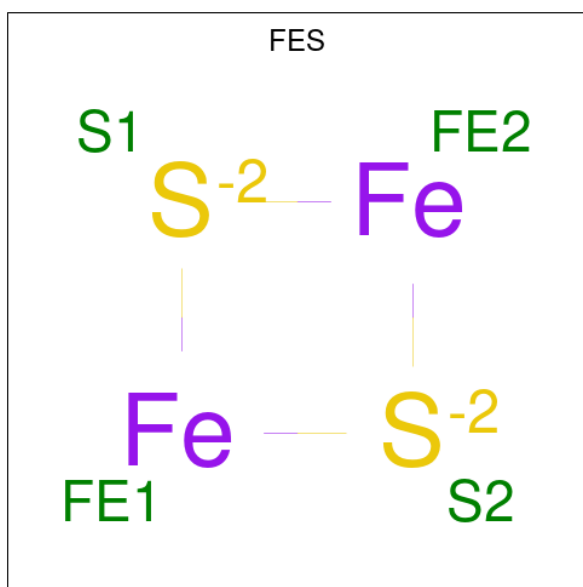
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
8	D	1	Total	C	O	0	0
			23	19	4		
8	G	1	Total	C	O	0	0
			23	19	4		
8	J	1	Total	C	O	0	0
			23	19	4		
8	M	1	Total	C	O	0	0
			23	19	4		
8	P	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			20	14	6		
9	E	1	Total	C	O	0	0
			20	14	6		
9	G	1	Total	C	O	0	0
			20	14	6		
9	K	1	Total	C	O	0	0
			20	14	6		
9	N	1	Total	C	O	0	0
			20	14	6		
9	P	1	Total	C	O	0	0
			20	14	6		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	Fe	S	0	0
			4	2	2		
10	F	1	Total	Fe	S	0	0
			4	2	2		
10	I	1	Total	Fe	S	0	0
			4	2	2		
10	L	1	Total	Fe	S	0	0
			4	2	2		
10	O	1	Total	Fe	S	0	0
			4	2	2		
10	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	I	1	Total	Cl	0	0
			1	1		
11	R	1	Total	Cl	0	0
			1	1		

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	R	1	Total	Na	0	0
			1	1		

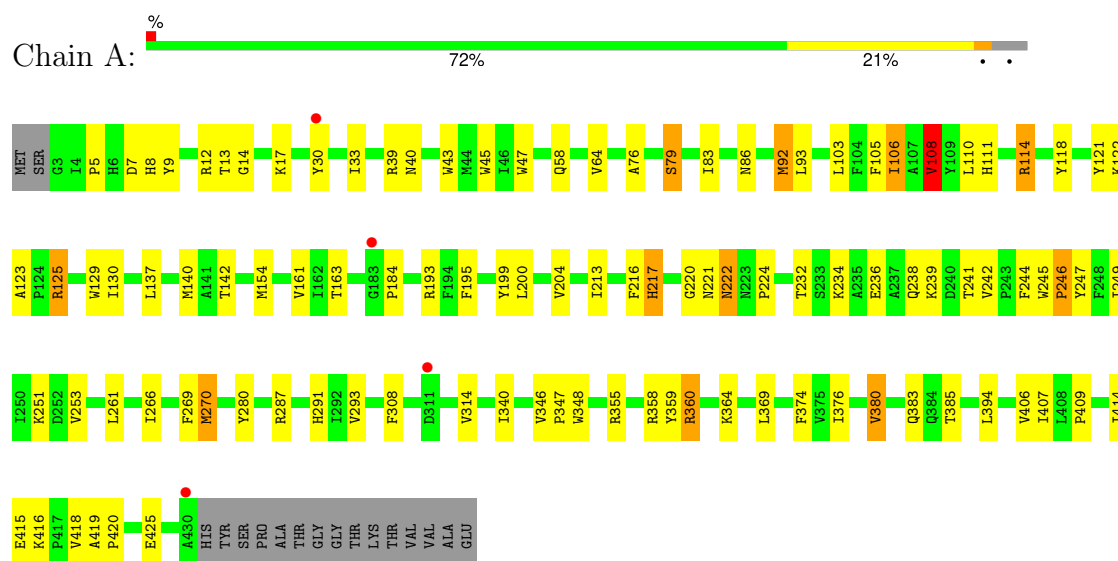
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	73	Total 73	O 73	0	0
13	B	19	Total 19	O 19	0	0
13	C	47	Total 47	O 47	0	0
13	D	64	Total 64	O 64	0	0
13	E	14	Total 14	O 14	0	0
13	F	36	Total 36	O 36	0	0
13	G	68	Total 68	O 68	0	0
13	H	35	Total 35	O 35	0	0
13	I	42	Total 42	O 42	0	0
13	J	55	Total 55	O 55	0	0
13	K	17	Total 17	O 17	0	0
13	L	42	Total 42	O 42	0	0
13	M	34	Total 34	O 34	0	0
13	N	11	Total 11	O 11	0	0
13	O	41	Total 41	O 41	0	0
13	P	60	Total 60	O 60	0	0
13	Q	16	Total 16	O 16	0	0
13	R	24	Total 24	O 24	0	0

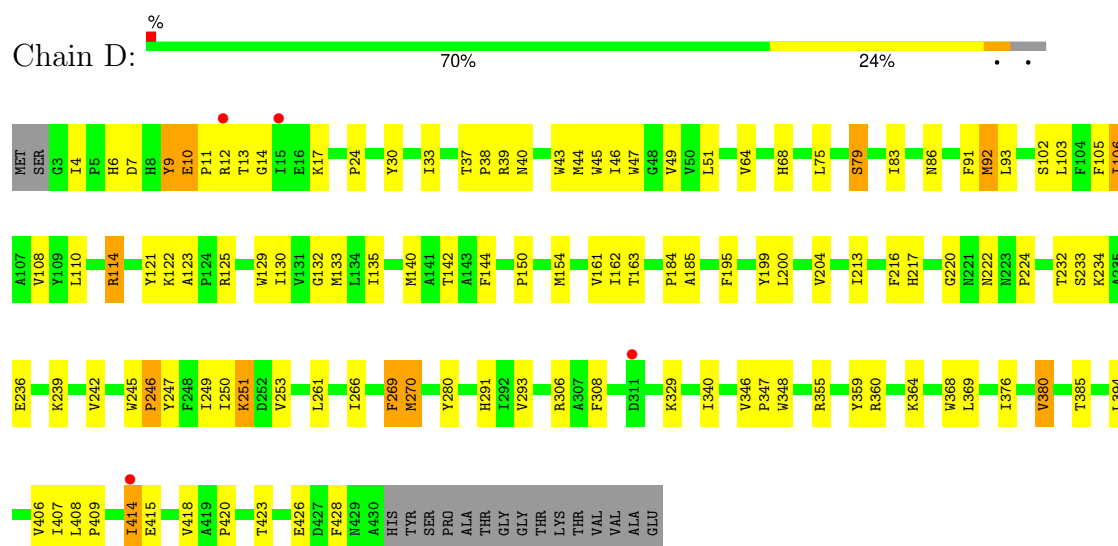
3 Residue-property plots

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

• Molecule 1: Cytochrome b

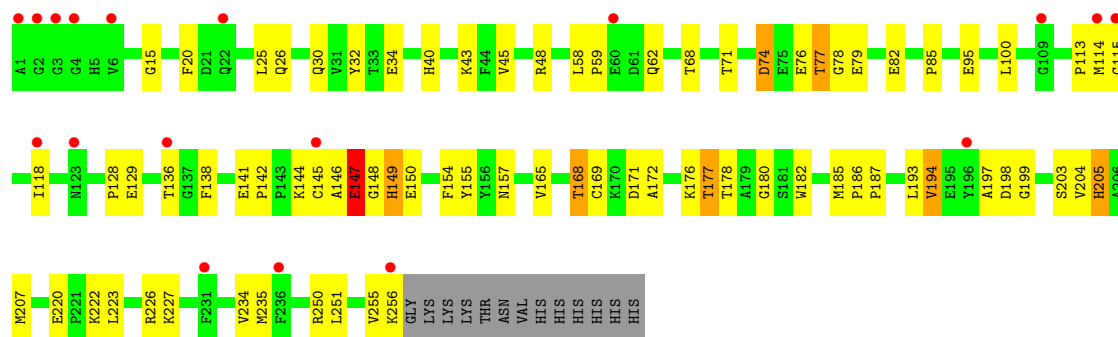


• Molecule 1: Cytochrome b

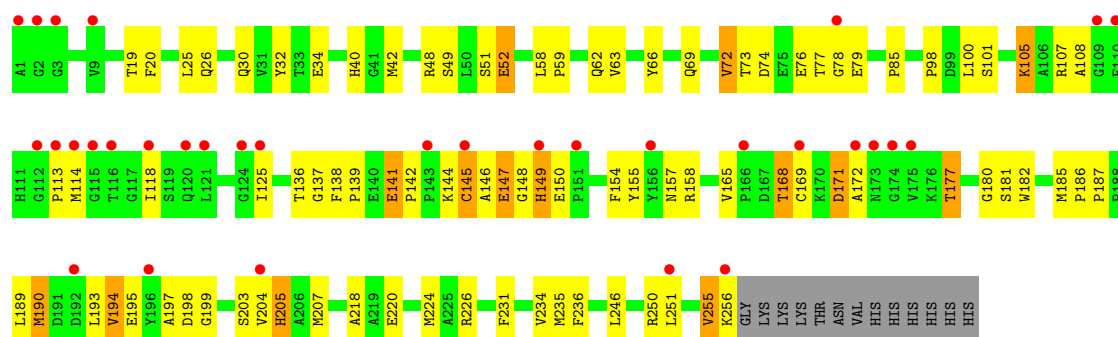


• Molecule 1: Cytochrome b

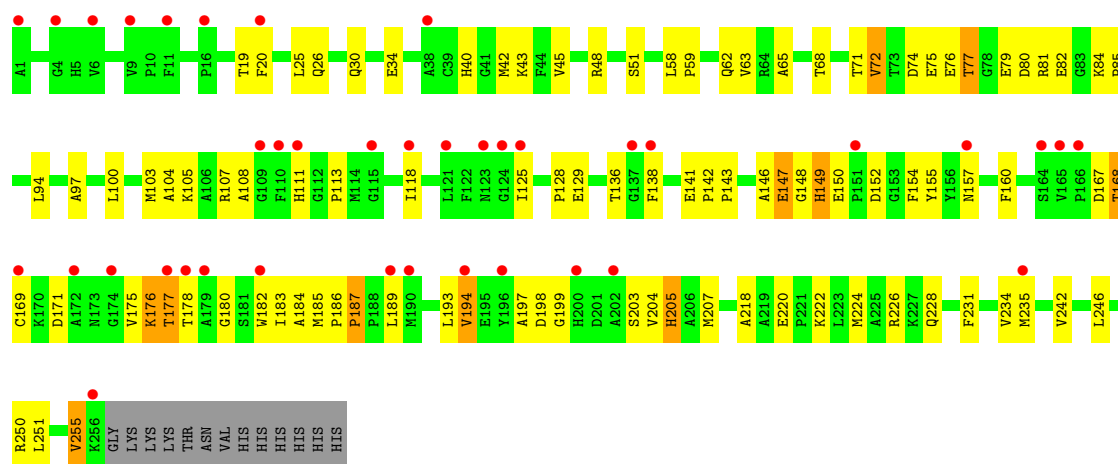




- Molecule 2: Cytochrome c1

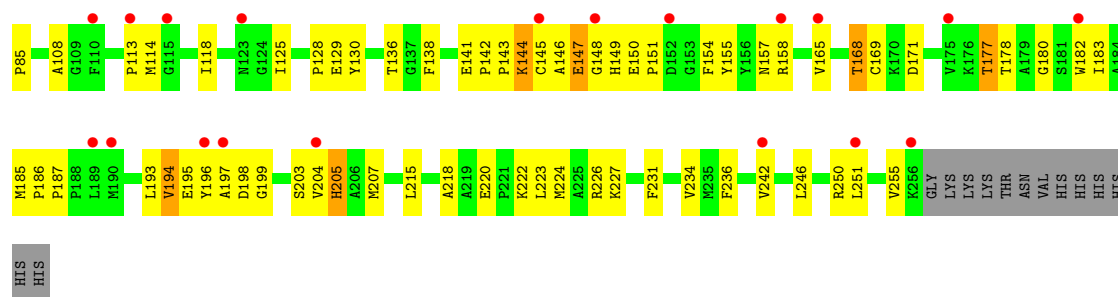


- Molecule 2: Cytochrome c1

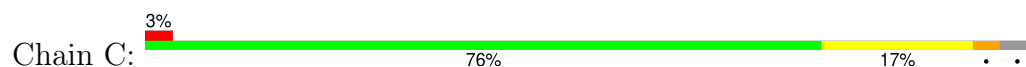


- Molecule 2: Cytochrome c1





- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

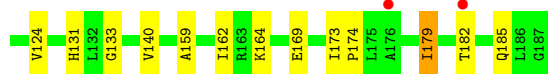
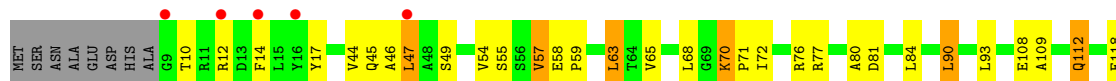


- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

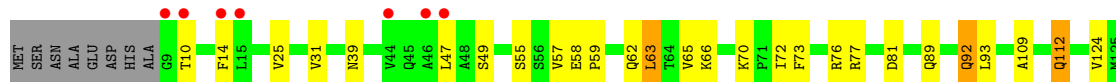
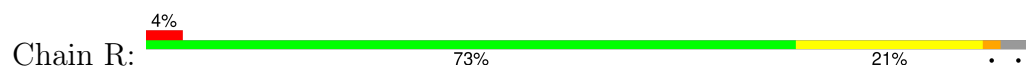




- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	351.89Å 147.04Å 161.31Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 18.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 93.1 (18.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.251 0.225 , 0.242	Depositor DCC
R_{free} test set	9798 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42656	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ2, BGL, HEM, FES, SMA, SR, NA, CL, LOP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/3570	1.03	28/4897 (0.6%)
1	D	0.48	0/3570	1.03	26/4897 (0.5%)
1	G	0.47	0/3570	1.04	31/4897 (0.6%)
1	J	0.48	0/3570	1.04	29/4897 (0.6%)
1	M	0.45	0/3570	1.03	29/4897 (0.6%)
1	P	0.47	0/3570	1.03	31/4897 (0.6%)
2	B	0.44	0/2010	1.03	6/2733 (0.2%)
2	E	0.43	0/2010	1.02	7/2733 (0.3%)
2	H	0.45	0/2010	1.02	7/2733 (0.3%)
2	K	0.42	0/2010	1.01	6/2733 (0.2%)
2	N	0.41	0/2010	1.02	7/2733 (0.3%)
2	Q	0.43	0/2010	0.99	3/2733 (0.1%)
3	C	0.46	0/1370	1.05	6/1866 (0.3%)
3	F	0.48	0/1370	1.05	6/1866 (0.3%)
3	I	0.51	1/1370 (0.1%)	1.14	13/1866 (0.7%)
3	L	0.47	0/1370	1.03	6/1866 (0.3%)
3	O	0.46	0/1370	1.04	5/1866 (0.3%)
3	R	0.45	0/1370	1.05	7/1866 (0.4%)
All	All	0.46	1/41700 (0.0%)	1.03	253/56976 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	44	VAL	CA-C	5.01	1.59	1.52

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	44	VAL	N-CA-C	14.17	123.85	110.53
3	O	133	GLY	N-CA-C	9.60	126.12	114.69
3	R	133	GLY	N-CA-C	9.45	125.94	114.69
3	I	133	GLY	N-CA-C	9.41	125.89	114.69
3	F	133	GLY	N-CA-C	9.17	125.60	114.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TYR	Sidechain
2	E	32	TYR	Sidechain
2	H	32	TYR	Sidechain
2	K	32	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3428	74	0
1	D	3440	0	3428	90	0
1	G	3440	0	3428	96	0
1	J	3440	0	3428	103	0
1	M	3440	0	3428	99	0
1	P	3440	0	3428	82	0
2	B	1953	0	1848	70	0
2	E	1953	0	1848	90	0
2	H	1953	0	1848	74	0
2	K	1953	0	1848	76	0
2	N	1953	0	1848	87	0
2	Q	1953	0	1848	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1340	0	1303	27	0
3	F	1340	0	1303	28	0
3	I	1340	0	1303	29	0
3	L	1340	0	1303	27	0
3	O	1340	0	1303	28	0
3	R	1340	0	1303	28	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	1	0	0	0	0
5	A	86	0	60	7	0
5	B	43	0	30	1	0
5	D	86	0	60	9	0
5	E	43	0	30	1	0
5	G	86	0	60	10	0
5	H	43	0	30	1	0
5	J	86	0	60	15	0
5	K	43	0	30	2	0
5	M	86	0	60	9	0
5	N	43	0	30	3	0
5	P	86	0	60	7	0
5	Q	43	0	30	2	0
6	A	37	0	42	0	0
6	D	37	0	42	0	0
6	G	37	0	42	0	0
6	J	37	0	42	1	0
6	M	37	0	42	0	0
6	P	37	0	42	1	0
7	A	45	0	67	6	0
7	D	45	0	67	2	0
7	G	45	0	67	3	0
7	J	45	0	67	1	0
7	M	45	0	67	3	0
7	P	45	0	67	2	0
8	A	23	0	26	2	0
8	D	23	0	26	2	0
8	G	23	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	23	0	26	1	0
8	M	23	0	26	2	0
8	P	23	0	26	2	0
9	B	20	0	28	1	0
9	E	20	0	28	3	0
9	G	20	0	28	2	0
9	K	20	0	28	2	0
9	N	20	0	28	1	0
9	P	20	0	28	2	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
10	I	4	0	0	0	0
10	L	4	0	0	0	0
10	O	4	0	0	0	0
10	R	4	0	0	0	0
11	I	1	0	0	0	0
11	R	1	0	0	0	0
12	R	1	0	0	0	0
13	A	73	0	0	1	0
13	B	19	0	0	2	0
13	C	47	0	0	0	0
13	D	64	0	0	4	0
13	E	14	0	0	1	0
13	F	36	0	0	0	0
13	G	68	0	0	2	0
13	H	35	0	0	3	0
13	I	42	0	0	0	0
13	J	55	0	0	3	0
13	K	17	0	0	0	0
13	L	42	0	0	1	0
13	M	34	0	0	1	0
13	N	11	0	0	1	0
13	O	41	0	0	1	0
13	P	60	0	0	1	0
13	Q	16	0	0	1	0
13	R	24	0	0	2	0
All	All	42656	0	40992	1093	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1093 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:144:LYS:HA	2:Q:144:LYS:HZ3	1.06	1.14
2:K:139:PRO:HG3	2:K:158:ARG:HH11	1.14	1.12
2:N:77:THR:HG22	2:N:79:GLU:H	1.25	1.02
2:K:194:VAL:HB	2:K:207:MET:HE3	1.42	1.01
2:Q:144:LYS:HA	2:Q:144:LYS:NZ	1.75	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	D	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
1	G	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	J	426/445 (96%)	407 (96%)	18 (4%)	1 (0%)	43	58
1	M	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
1	P	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
2	B	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	10	16
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	10	16
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	10	16
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	6	7
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	6	7
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	16	25
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	21	32
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	21	32
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	7	10
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	11	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	7	10
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	21	32
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	21	32

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	GLU
2	E	147	GLU
2	E	190	MET
2	H	77	THR
2	H	147	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/366 (96%)	342 (97%)	11 (3%)	35	57
1	D	353/366 (96%)	345 (98%)	8 (2%)	44	66
1	G	353/366 (96%)	345 (98%)	8 (2%)	44	66
1	J	353/366 (96%)	342 (97%)	11 (3%)	35	57
1	M	353/366 (96%)	343 (97%)	10 (3%)	38	60
1	P	353/366 (96%)	345 (98%)	8 (2%)	44	66
2	B	203/215 (94%)	191 (94%)	12 (6%)	18	31
2	E	203/215 (94%)	191 (94%)	12 (6%)	18	31
2	H	203/215 (94%)	196 (97%)	7 (3%)	32	54
2	K	203/215 (94%)	192 (95%)	11 (5%)	20	35
2	N	203/215 (94%)	193 (95%)	10 (5%)	22	39
2	Q	203/215 (94%)	189 (93%)	14 (7%)	14	24
3	C	138/144 (96%)	131 (95%)	7 (5%)	21	37
3	F	138/144 (96%)	129 (94%)	9 (6%)	15	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	138/144 (96%)	129 (94%)	9 (6%)	15	27
3	L	138/144 (96%)	130 (94%)	8 (6%)	18	32
3	O	138/144 (96%)	128 (93%)	10 (7%)	13	23
3	R	138/144 (96%)	130 (94%)	8 (6%)	18	32
All	All	4164/4350 (96%)	3991 (96%)	173 (4%)	26	45

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	92	MET
1	P	10	GLU
1	M	287	ARG
2	N	177	THR
1	P	421	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	23	HIS
2	Q	62	GLN
2	N	149	HIS
3	O	185	GLN
3	R	45	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 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
8	UQ2	D	1102	-	23,23,23	1.44	5 (21%)	30,31,31	1.17	2 (6%)
5	HEM	M	502	1	50,50,50	1.27	4 (8%)	67,82,82	1.00	3 (4%)
5	HEM	B	301	2	50,50,50	1.36	4 (8%)	67,82,82	1.05	3 (4%)
5	HEM	J	501	1	50,50,50	1.32	4 (8%)	67,82,82	1.03	3 (4%)
6	SMA	J	1004	-	38,38,38	1.99	9 (23%)	47,52,52	1.72	9 (19%)
9	BGL	N	1045	-	20,20,20	1.33	1 (5%)	24,25,25	0.73	0
10	FES	C	200	3	0,4,4	-	-	-	-	-
5	HEM	D	501	1	50,50,50	1.24	2 (4%)	67,82,82	1.03	3 (4%)
5	HEM	G	502	1	50,50,50	1.33	4 (8%)	67,82,82	1.05	3 (4%)
5	HEM	E	301	2	50,50,50	1.29	4 (8%)	67,82,82	1.04	3 (4%)
5	HEM	D	502	1	50,50,50	1.23	4 (8%)	67,82,82	1.02	3 (4%)
10	FES	R	200	3	0,4,4	-	-	-	-	-
9	BGL	P	1046	-	20,20,20	1.18	1 (5%)	24,25,25	0.92	1 (4%)
5	HEM	A	502	1	50,50,50	1.31	3 (6%)	67,82,82	1.04	3 (4%)
10	FES	L	200	3	0,4,4	-	-	-	-	-
8	UQ2	G	1103	-	23,23,23	1.52	5 (21%)	30,31,31	1.09	1 (3%)
6	SMA	G	1003	-	38,38,38	2.08	10 (26%)	47,52,52	1.82	11 (23%)
5	HEM	M	501	1	50,50,50	1.24	4 (8%)	67,82,82	1.01	3 (4%)
5	HEM	Q	301	2	50,50,50	1.30	3 (6%)	67,82,82	1.04	3 (4%)
6	SMA	A	1001	-	38,38,38	2.12	10 (26%)	47,52,52	1.91	14 (29%)
8	UQ2	M	1105	-	23,23,23	1.54	5 (21%)	30,31,31	1.16	3 (10%)
8	UQ2	J	1104	-	23,23,23	1.31	4 (17%)	30,31,31	1.19	3 (10%)
8	UQ2	P	1106	-	23,23,23	1.63	5 (21%)	30,31,31	1.22	5 (16%)
10	FES	O	200	3	0,4,4	-	-	-	-	-
5	HEM	P	502	1	50,50,50	1.25	3 (6%)	67,82,82	1.03	4 (5%)
7	LOP	A	1021	-	44,44,44	0.63	0	47,49,49	1.17	6 (12%)
10	FES	I	200	3	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BGL	E	1042	-	20,20,20	1.03	1 (5%)	24,25,25	0.95	1 (4%)
9	BGL	B	1041	-	20,20,20	1.05	1 (5%)	24,25,25	0.87	1 (4%)
5	HEM	P	501	1	50,50,50	1.27	4 (8%)	67,82,82	1.04	3 (4%)
5	HEM	J	502	1	50,50,50	1.34	4 (8%)	67,82,82	1.05	3 (4%)
7	LOP	J	1024	-	44,44,44	0.65	0	47,49,49	1.24	6 (12%)
9	BGL	K	1044	-	20,20,20	1.00	1 (5%)	24,25,25	1.11	2 (8%)
6	SMA	P	1006	-	38,38,38	2.03	9 (23%)	47,52,52	2.09	14 (29%)
6	SMA	D	1002	-	38,38,38	2.00	9 (23%)	47,52,52	1.89	12 (25%)
6	SMA	M	1005	-	38,38,38	2.07	9 (23%)	47,52,52	1.89	10 (21%)
5	HEM	A	501	1	50,50,50	1.27	3 (6%)	67,82,82	1.02	3 (4%)
7	LOP	P	1026	-	44,44,44	0.62	0	47,49,49	1.18	5 (10%)
8	UQ2	A	1101	-	23,23,23	1.57	6 (26%)	30,31,31	1.19	2 (6%)
10	FES	F	200	3	0,4,4	-	-	-	-	-
7	LOP	G	1023	-	44,44,44	0.72	0	47,49,49	1.16	4 (8%)
5	HEM	N	301	2	50,50,50	1.34	3 (6%)	67,82,82	1.10	3 (4%)
5	HEM	K	301	2	50,50,50	1.33	3 (6%)	67,82,82	1.07	3 (4%)
7	LOP	M	1025	-	44,44,44	0.70	0	47,49,49	1.16	3 (6%)
5	HEM	H	301	2	50,50,50	1.29	3 (6%)	67,82,82	1.11	3 (4%)
5	HEM	G	501	1	50,50,50	1.29	4 (8%)	67,82,82	1.01	3 (4%)
7	LOP	D	1022	-	44,44,44	0.71	0	47,49,49	1.17	5 (10%)
9	BGL	G	1043	-	20,20,20	1.32	1 (5%)	24,25,25	0.75	0

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
8	UQ2	D	1102	-	-	2/15/39/39	0/1/1/1
5	HEM	M	502	1	-	7/14/54/54	-
5	HEM	B	301	2	-	8/14/54/54	-
5	HEM	J	501	1	-	4/14/54/54	-
6	SMA	J	1004	-	-	2/34/34/34	0/2/2/2
9	BGL	N	1045	-	-	0/11/31/31	0/1/1/1
10	FES	C	200	3	-	-	0/1/1/1
5	HEM	D	501	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	G	502	1	-	9/14/54/54	-
5	HEM	E	301	2	-	9/14/54/54	-
5	HEM	D	502	1	-	8/14/54/54	-
10	FES	R	200	3	-	-	0/1/1/1
9	BGL	P	1046	-	-	0/11/31/31	0/1/1/1
5	HEM	A	502	1	-	7/14/54/54	-
10	FES	L	200	3	-	-	0/1/1/1
8	UQ2	G	1103	-	-	5/15/39/39	0/1/1/1
6	SMA	G	1003	-	-	5/34/34/34	0/2/2/2
5	HEM	M	501	1	-	6/14/54/54	-
5	HEM	Q	301	2	-	7/14/54/54	-
6	SMA	A	1001	-	-	5/34/34/34	0/2/2/2
8	UQ2	M	1105	-	-	2/15/39/39	0/1/1/1
8	UQ2	J	1104	-	-	0/15/39/39	0/1/1/1
8	UQ2	P	1106	-	-	4/15/39/39	0/1/1/1
10	FES	O	200	3	-	-	0/1/1/1
5	HEM	P	502	1	-	5/14/54/54	-
7	LOP	A	1021	-	-	12/48/48/48	-
10	FES	I	200	3	-	-	0/1/1/1
9	BGL	E	1042	-	-	0/11/31/31	0/1/1/1
9	BGL	B	1041	-	-	0/11/31/31	0/1/1/1
5	HEM	P	501	1	-	6/14/54/54	-
5	HEM	J	502	1	-	8/14/54/54	-
7	LOP	J	1024	-	-	10/48/48/48	-
9	BGL	K	1044	-	-	0/11/31/31	0/1/1/1
6	SMA	P	1006	-	-	7/34/34/34	0/2/2/2
6	SMA	D	1002	-	-	6/34/34/34	0/2/2/2
6	SMA	M	1005	-	-	8/34/34/34	0/2/2/2
5	HEM	A	501	1	-	3/14/54/54	-
7	LOP	P	1026	-	-	8/48/48/48	-
8	UQ2	A	1101	-	-	6/15/39/39	0/1/1/1
10	FES	F	200	3	-	-	0/1/1/1
7	LOP	G	1023	-	-	11/48/48/48	-
5	HEM	N	301	2	-	8/14/54/54	-
5	HEM	K	301	2	-	8/14/54/54	-
7	LOP	M	1025	-	-	4/48/48/48	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	H	301	2	-	8/14/54/54	-
5	HEM	G	501	1	-	6/14/54/54	-
7	LOP	D	1022	-	-	4/48/48/48	-
9	BGL	G	1043	-	-	0/11/31/31	0/1/1/1

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1003	SMA	O5-C5	7.24	1.48	1.37
6	A	1001	SMA	O5-C5	6.96	1.48	1.37
6	J	1004	SMA	O5-C5	6.64	1.47	1.37
6	D	1002	SMA	O5-C5	6.55	1.47	1.37
6	M	1005	SMA	O7-C7	6.53	1.47	1.37

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1006	SMA	C14-C15-C16	6.09	138.23	125.88
6	P	1006	SMA	O7-C7-C8	4.96	119.71	114.53
6	M	1005	SMA	C5M-O5-C5	-4.94	110.27	117.51
6	A	1001	SMA	O5-C5-C4A	4.79	122.63	115.84
6	A	1001	SMA	O7-C7-C8	4.55	119.29	114.53

There are no chirality outliers.

5 of 221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	HEM	C2B-C3B-CAB-CBB
5	A	502	HEM	C4B-C3B-CAB-CBB
5	D	502	HEM	C2B-C3B-CAB-CBB
5	D	502	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

38 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1102	UQ2	2	0
5	M	502	HEM	6	0
5	B	301	HEM	1	0

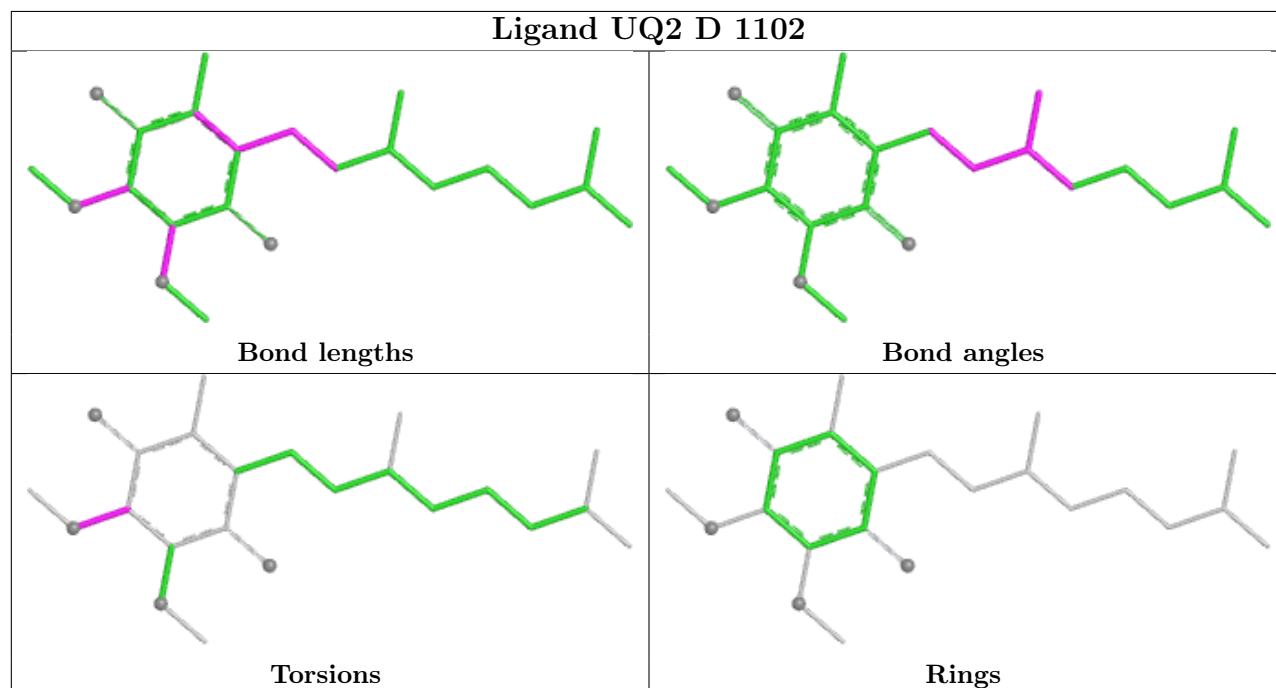
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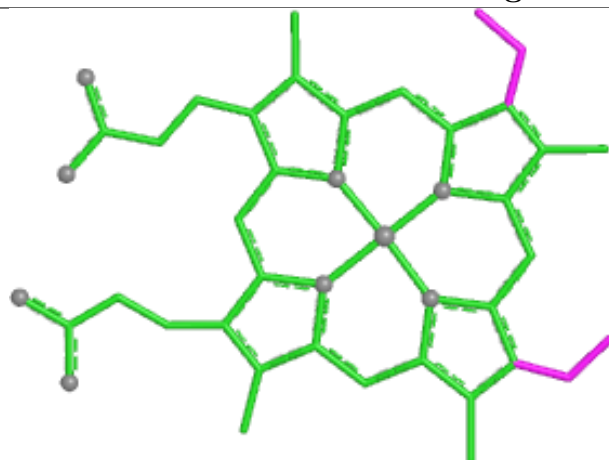
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	501	HEM	9	0
6	J	1004	SMA	1	0
9	N	1045	BGL	1	0
5	D	501	HEM	6	0
5	G	502	HEM	5	0
5	E	301	HEM	1	0
5	D	502	HEM	3	0
9	P	1046	BGL	2	0
5	A	502	HEM	4	0
8	G	1103	UQ2	2	0
5	M	501	HEM	3	0
5	Q	301	HEM	2	0
8	M	1105	UQ2	2	0
8	J	1104	UQ2	1	0
8	P	1106	UQ2	2	0
5	P	502	HEM	3	0
7	A	1021	LOP	6	0
9	E	1042	BGL	3	0
9	B	1041	BGL	1	0
5	P	501	HEM	4	0
5	J	502	HEM	6	0
7	J	1024	LOP	1	0
9	K	1044	BGL	2	0
6	P	1006	SMA	1	0
5	A	501	HEM	3	0
7	P	1026	LOP	2	0
8	A	1101	UQ2	2	0
7	G	1023	LOP	3	0
5	N	301	HEM	3	0
5	K	301	HEM	2	0
7	M	1025	LOP	3	0
5	H	301	HEM	1	0
5	G	501	HEM	5	0
7	D	1022	LOP	2	0
9	G	1043	BGL	2	0

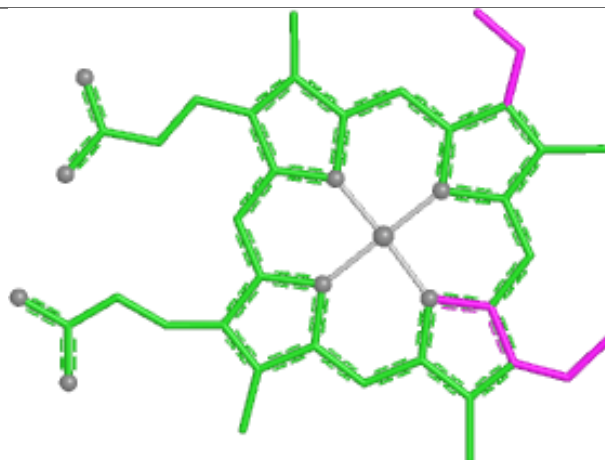
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

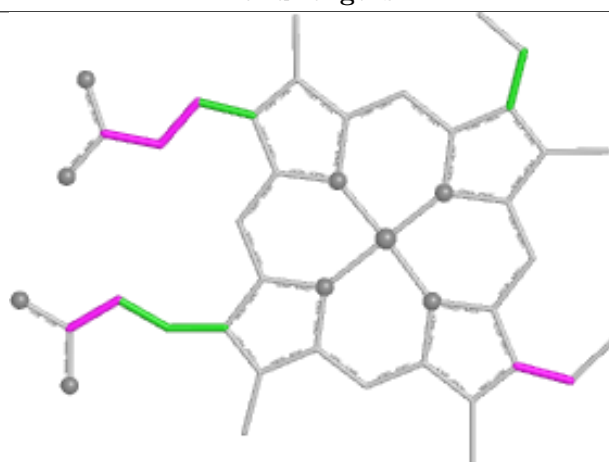


Ligand HEM M 502

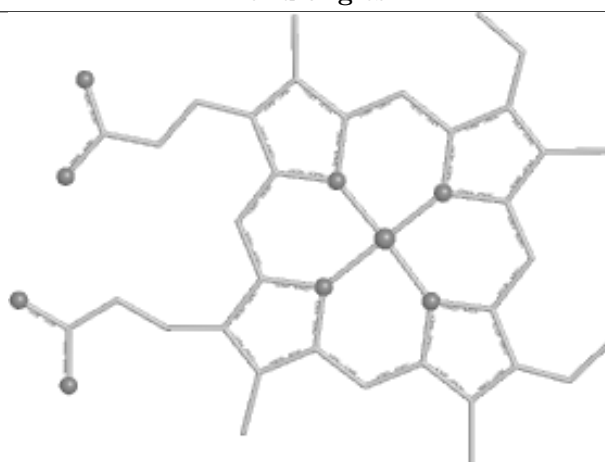
Bond lengths



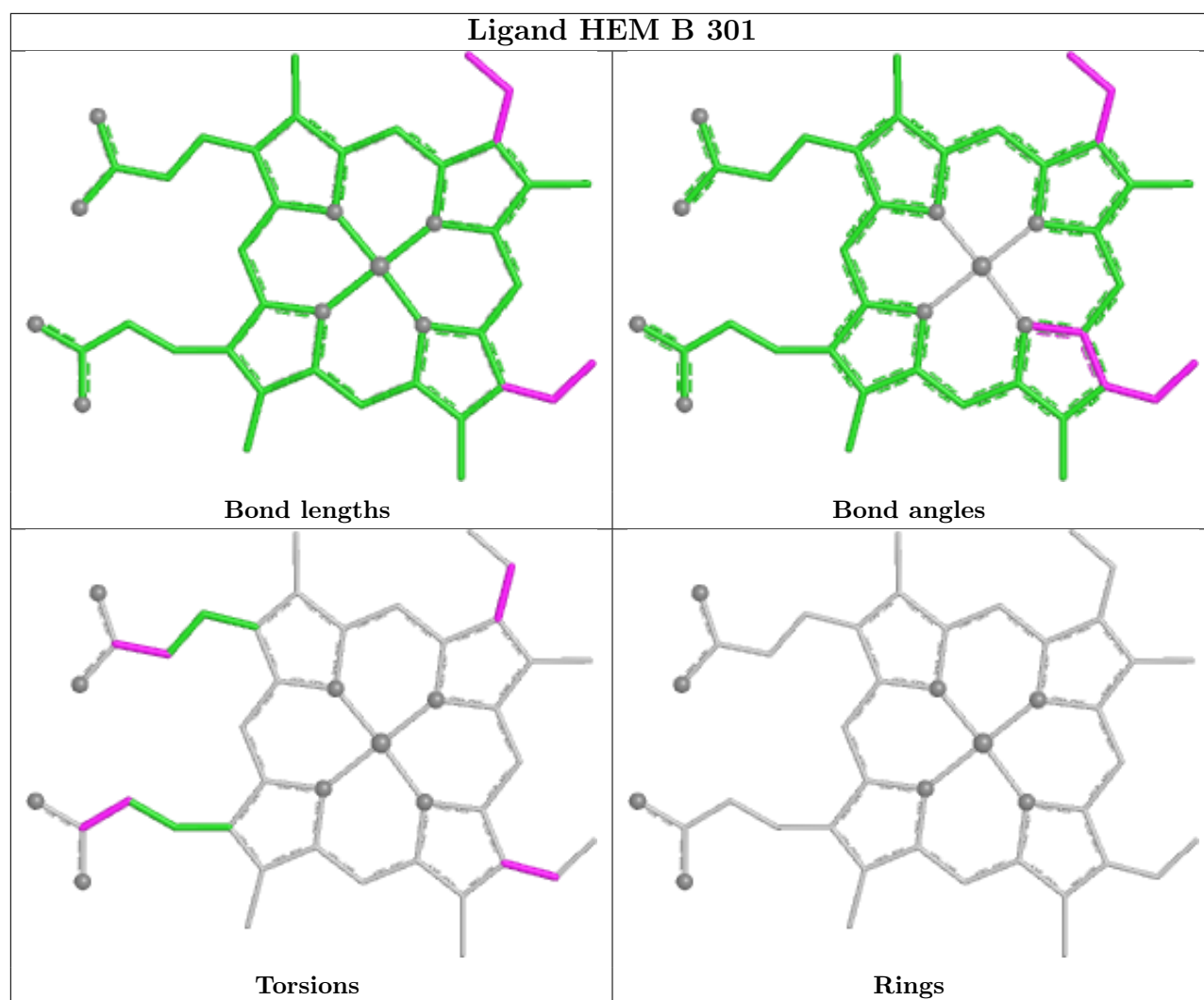
Bond angles



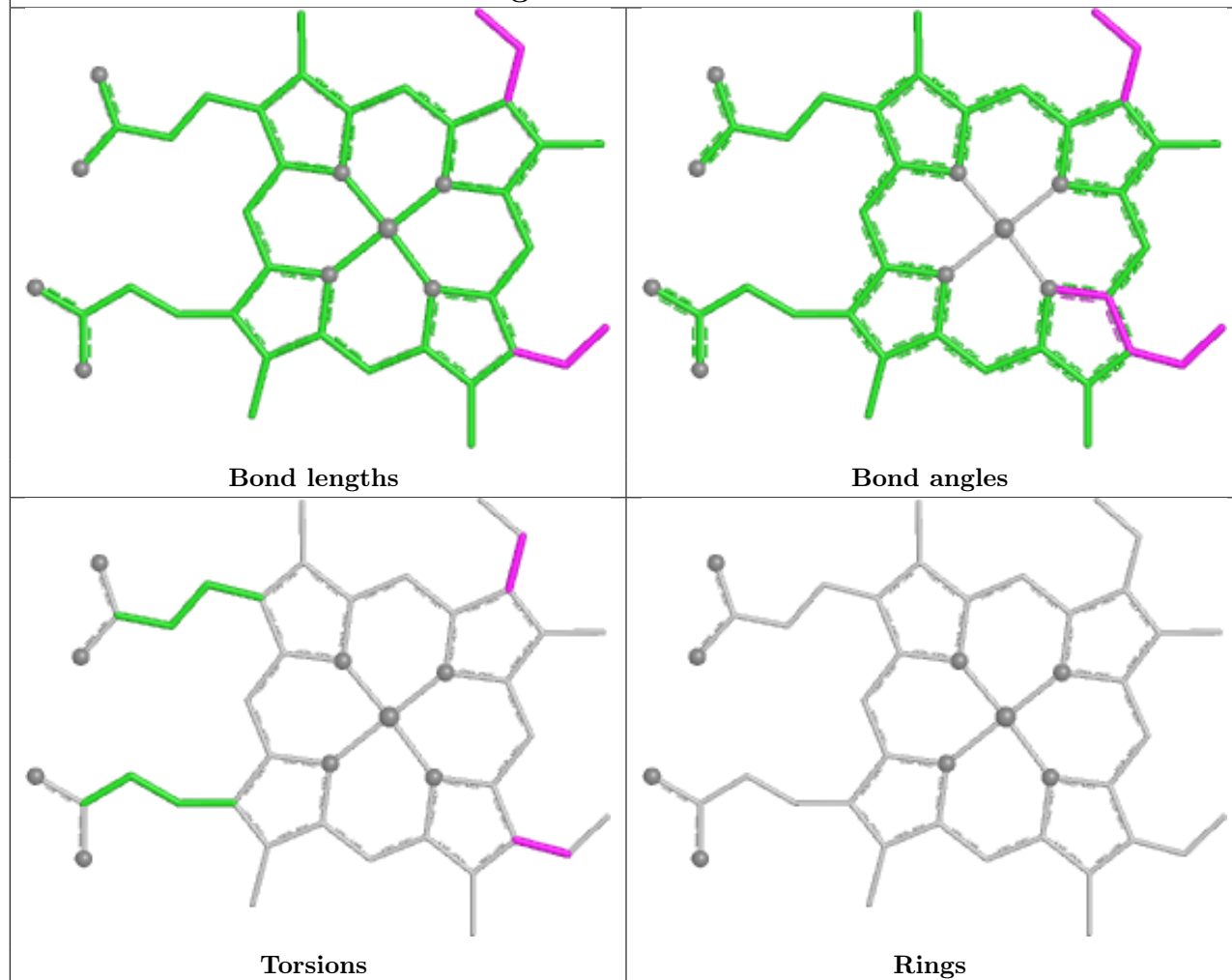
Torsions



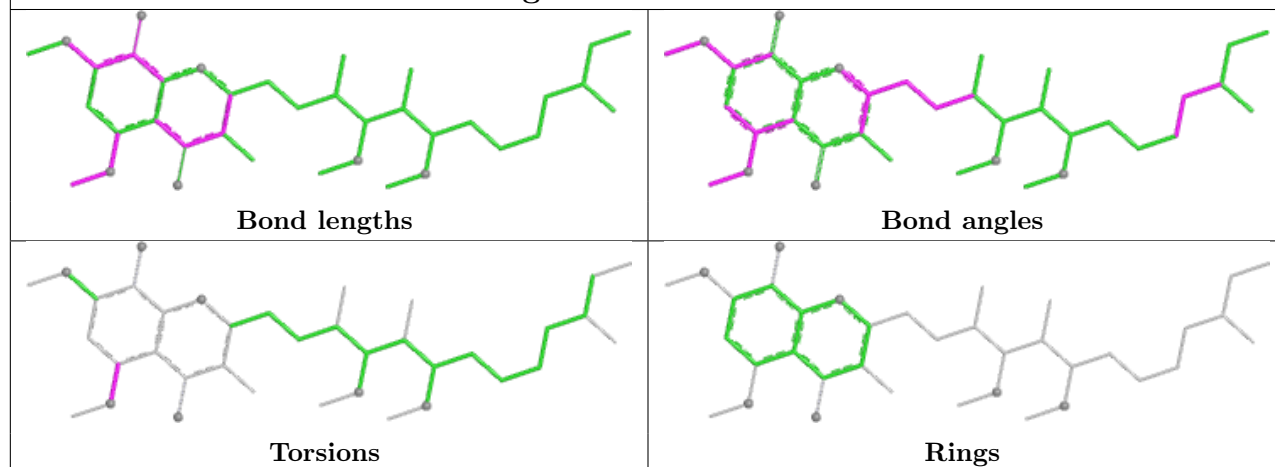
Rings



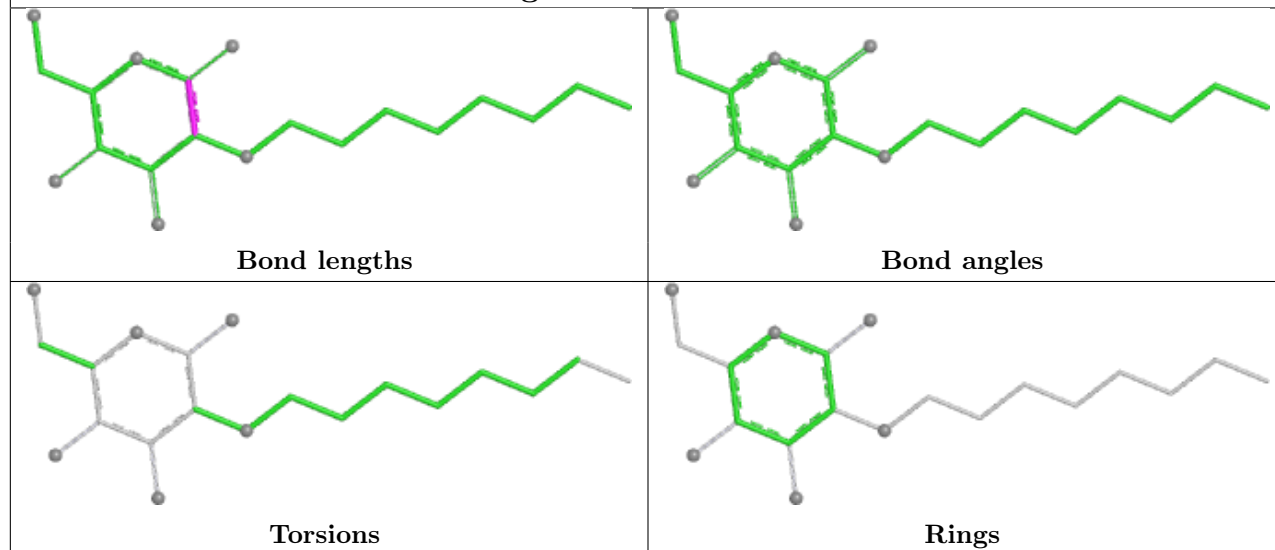
Ligand HEM J 501



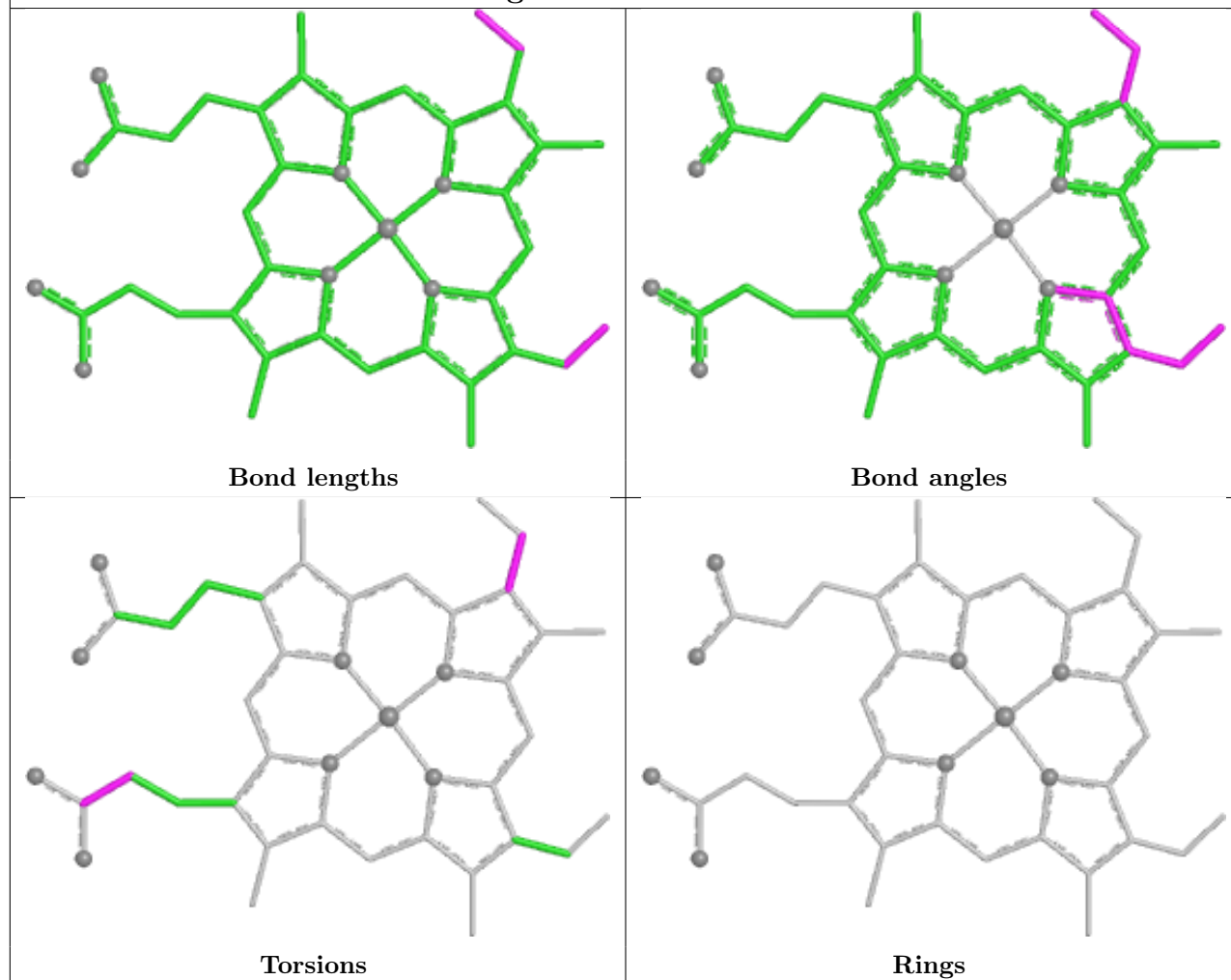
Ligand SMA J 1004

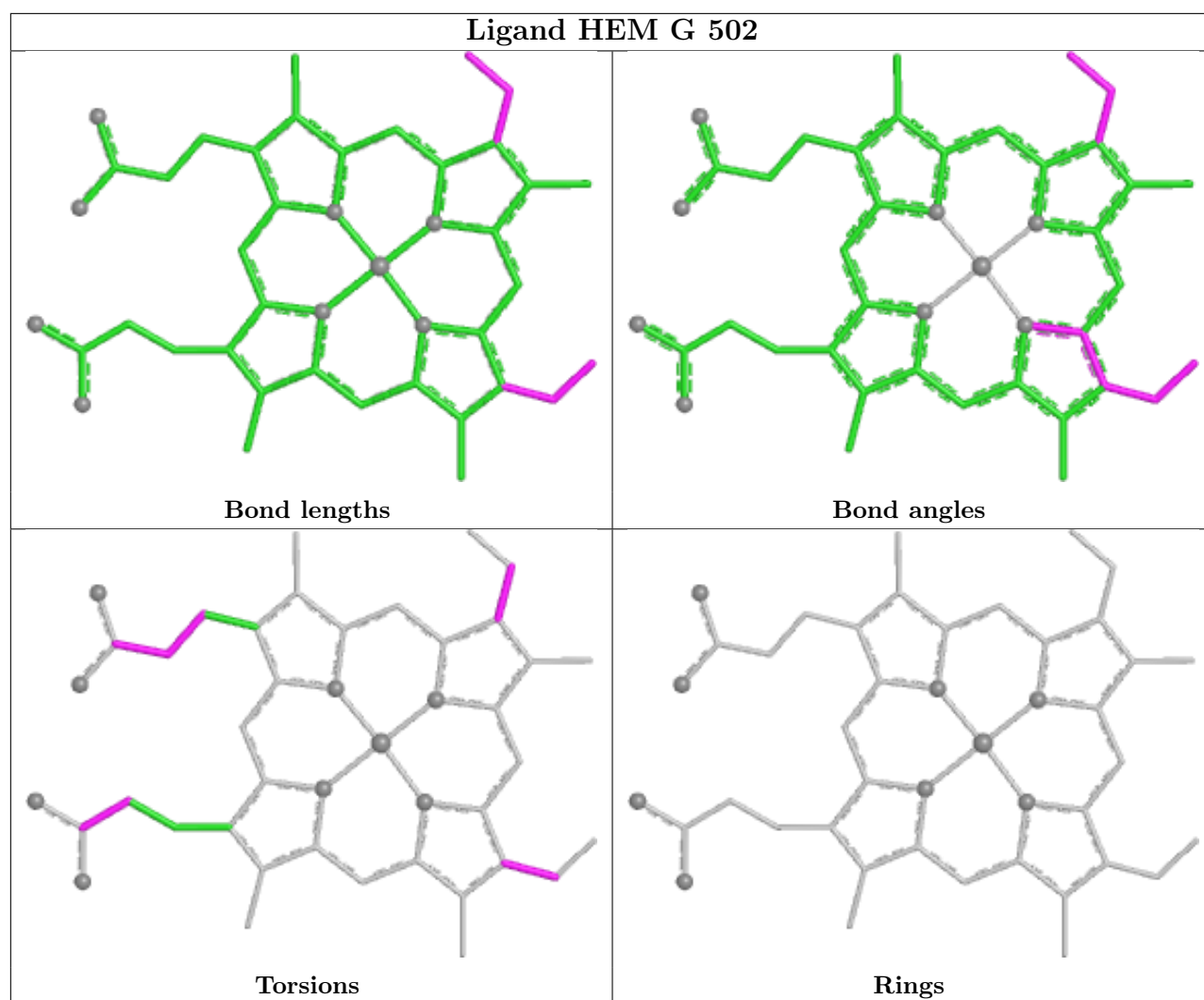


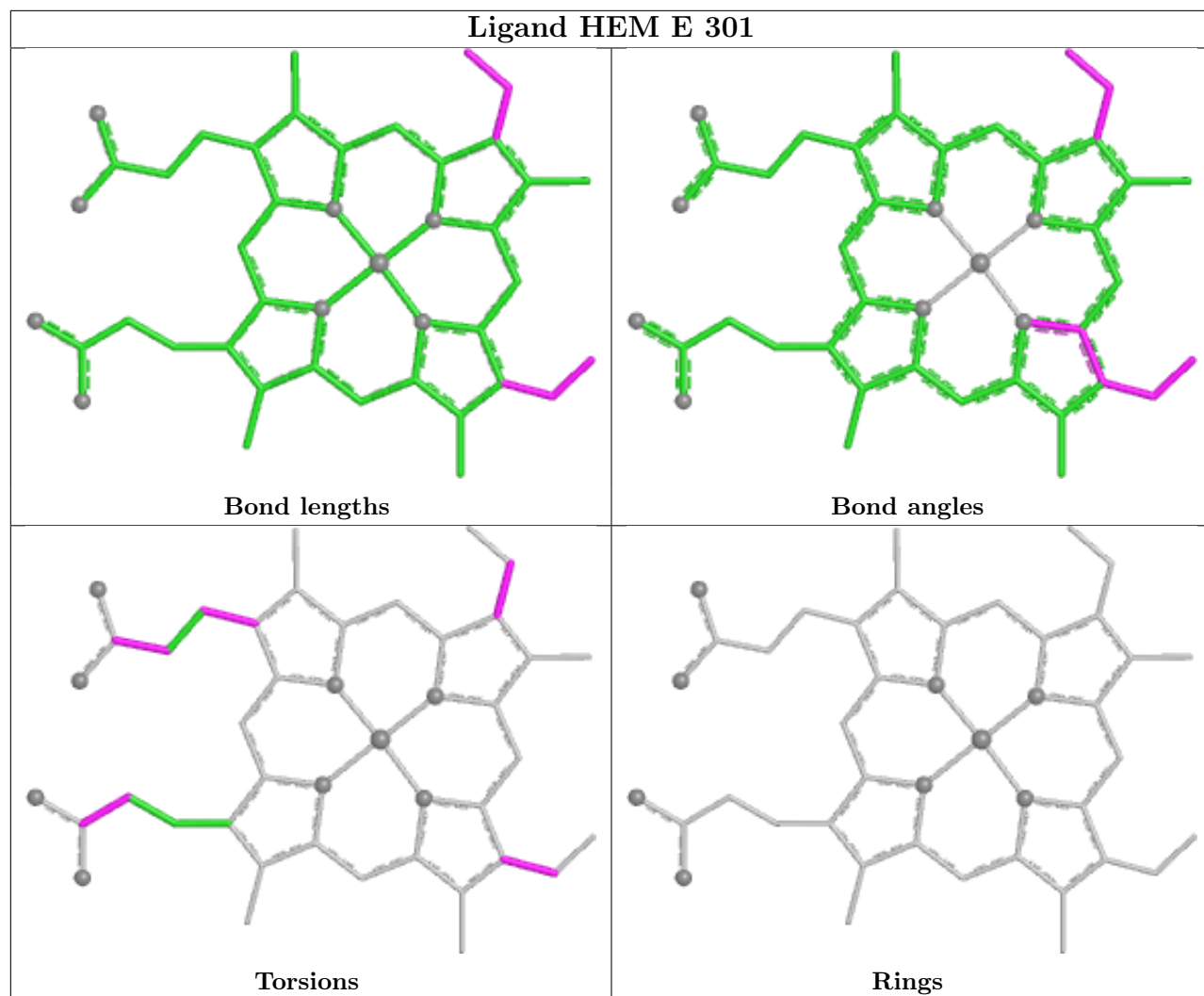
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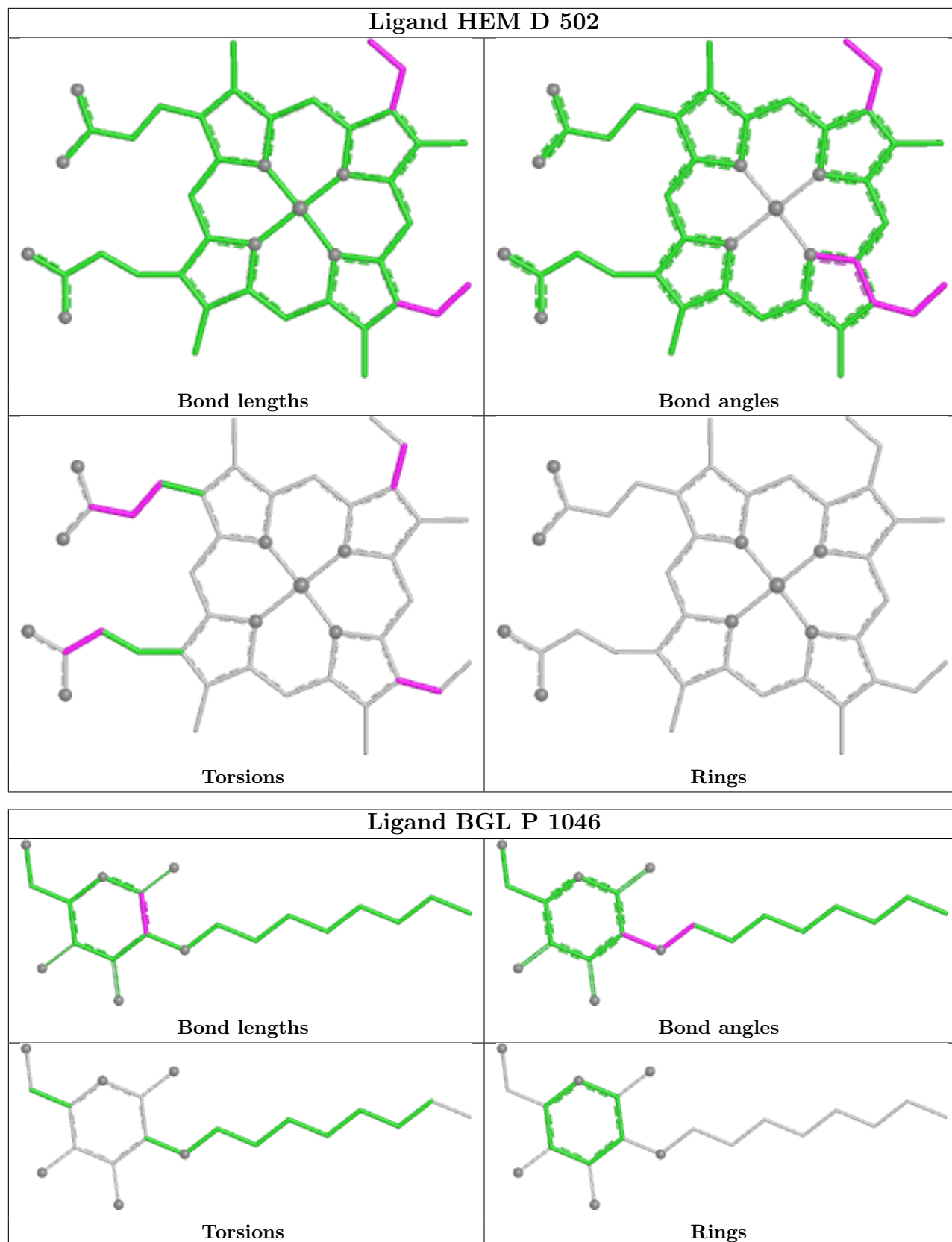


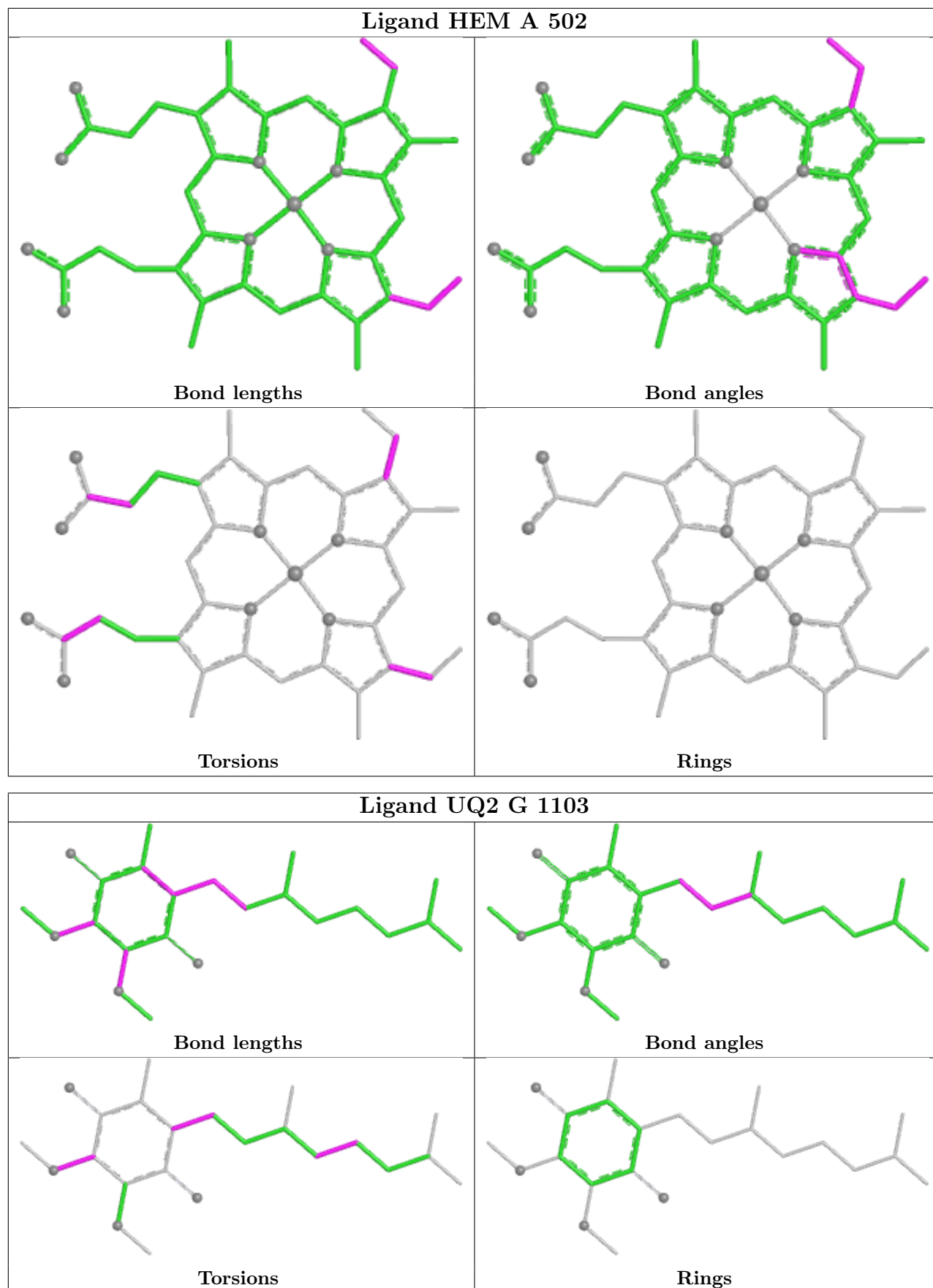
Ligand HEM D 501

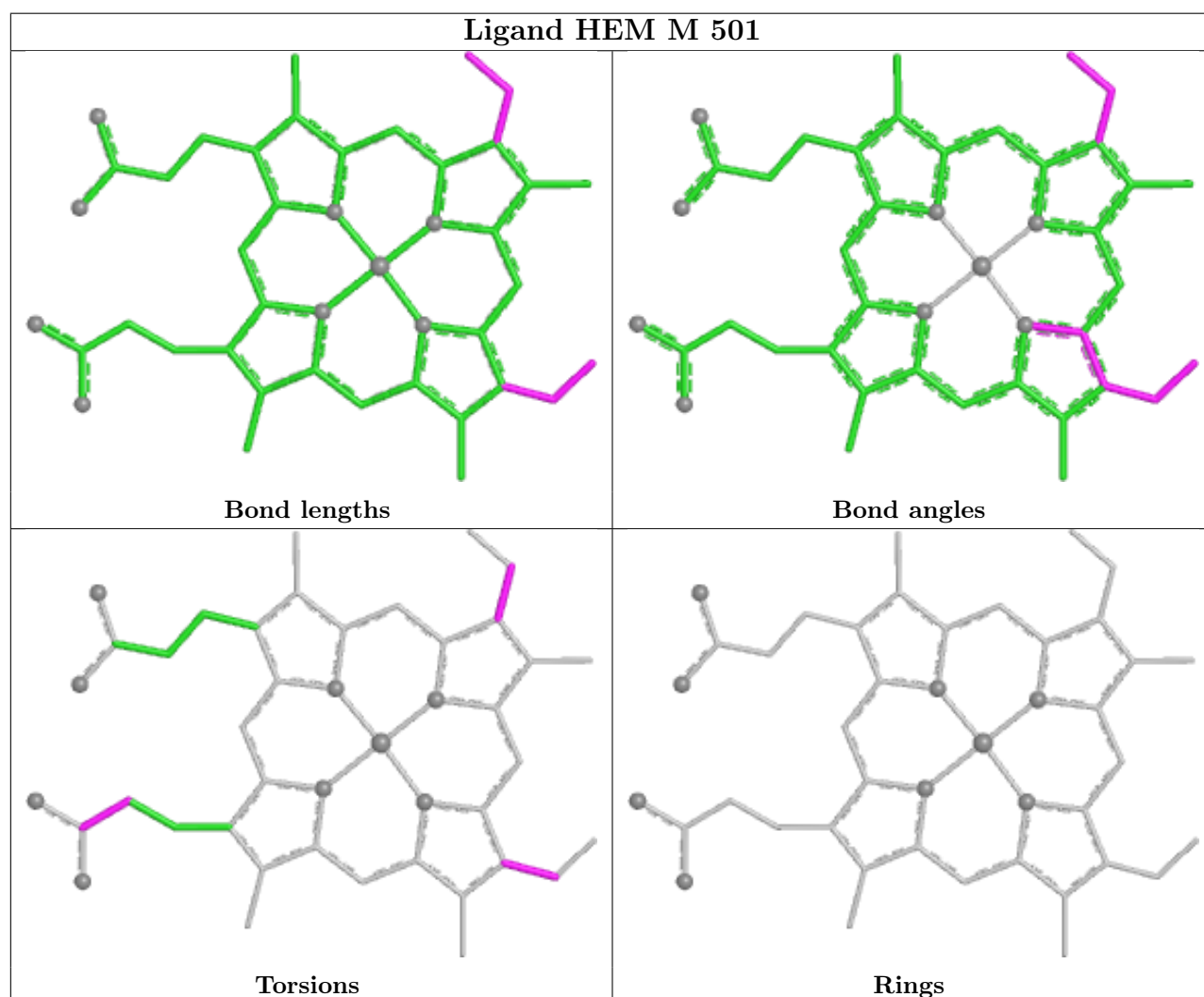
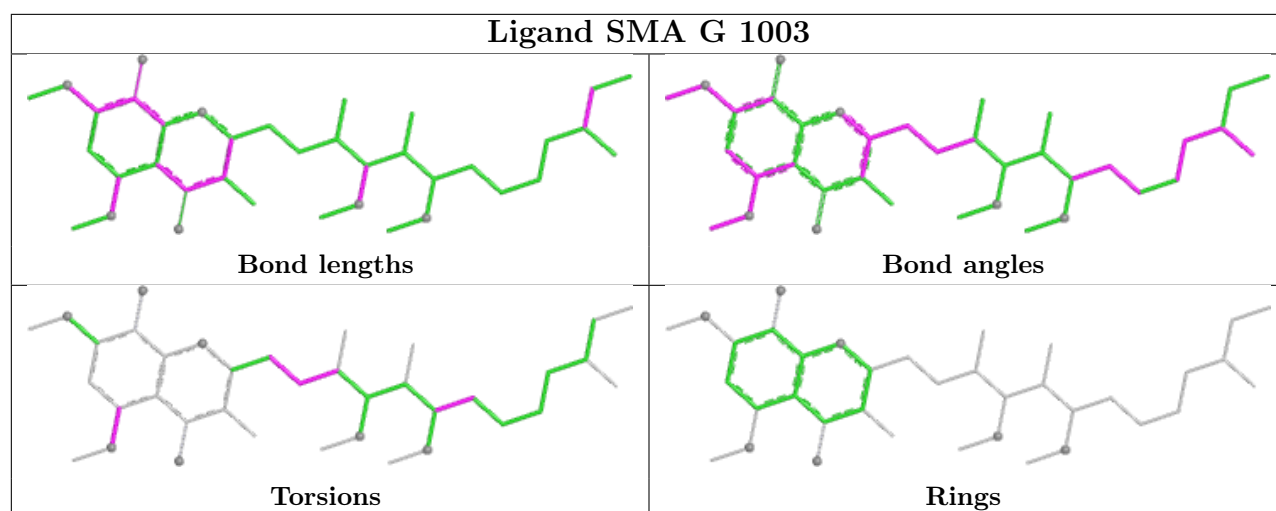


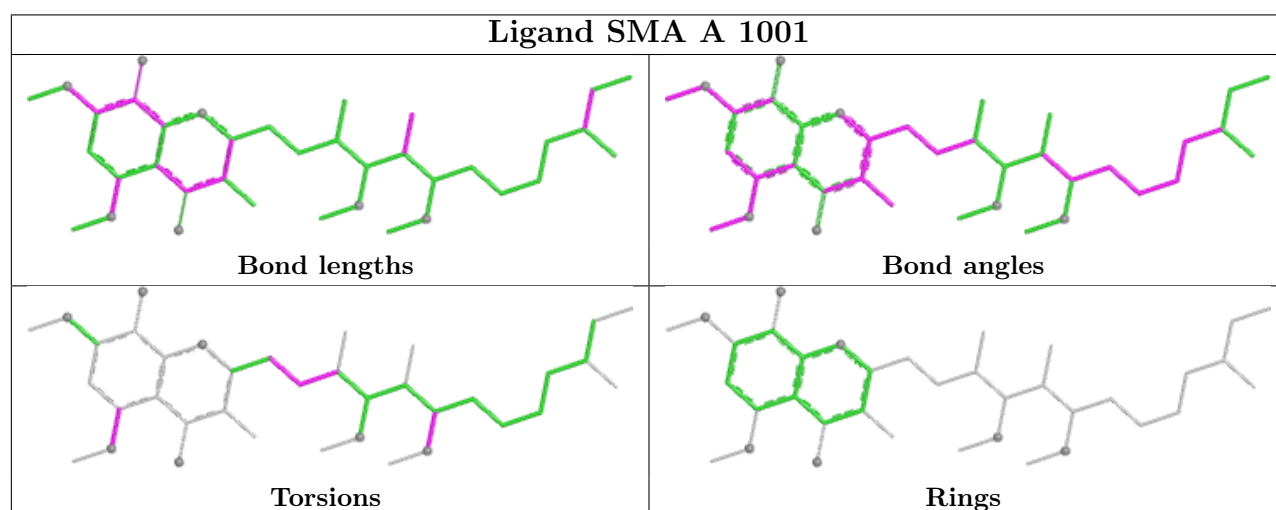
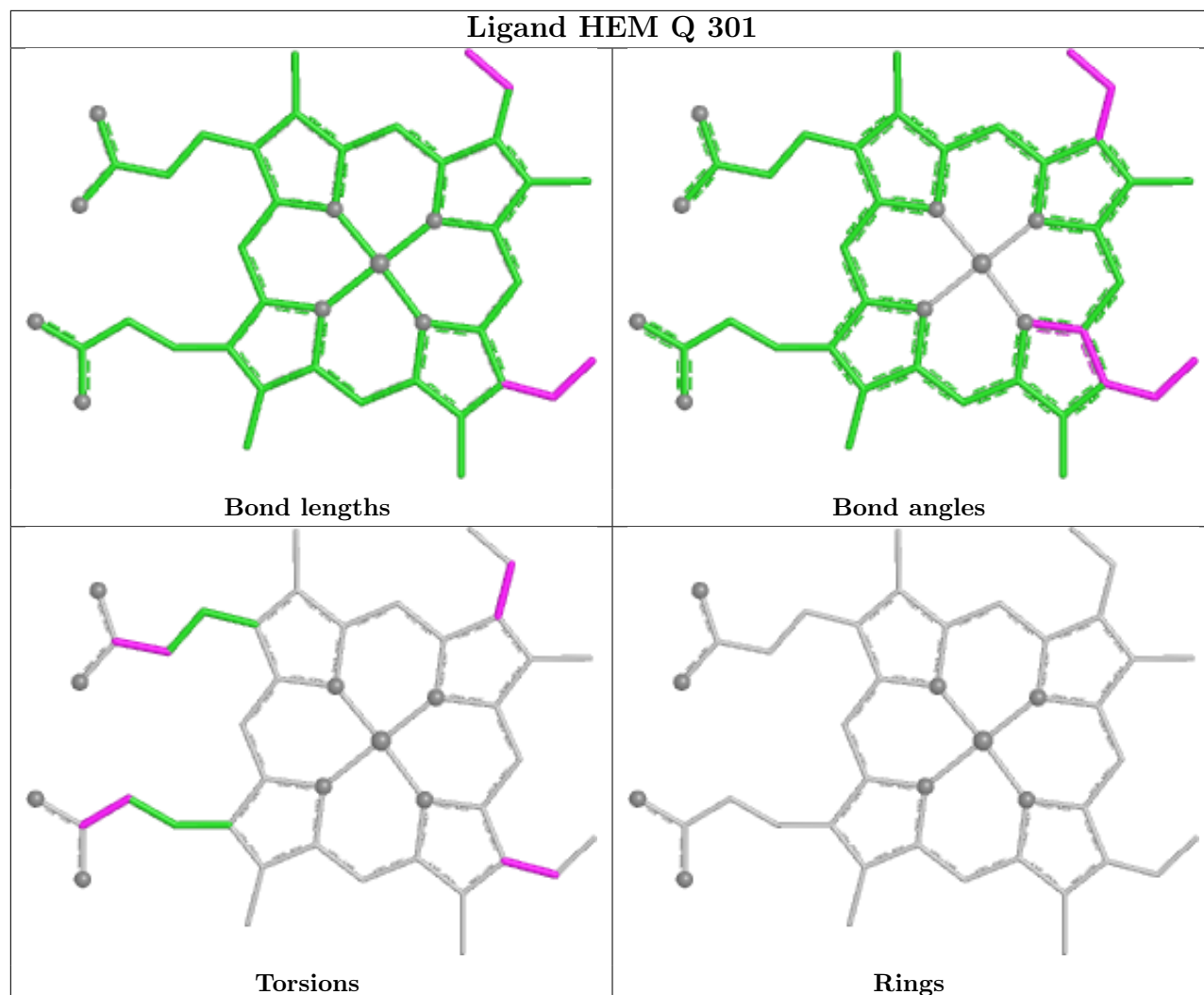




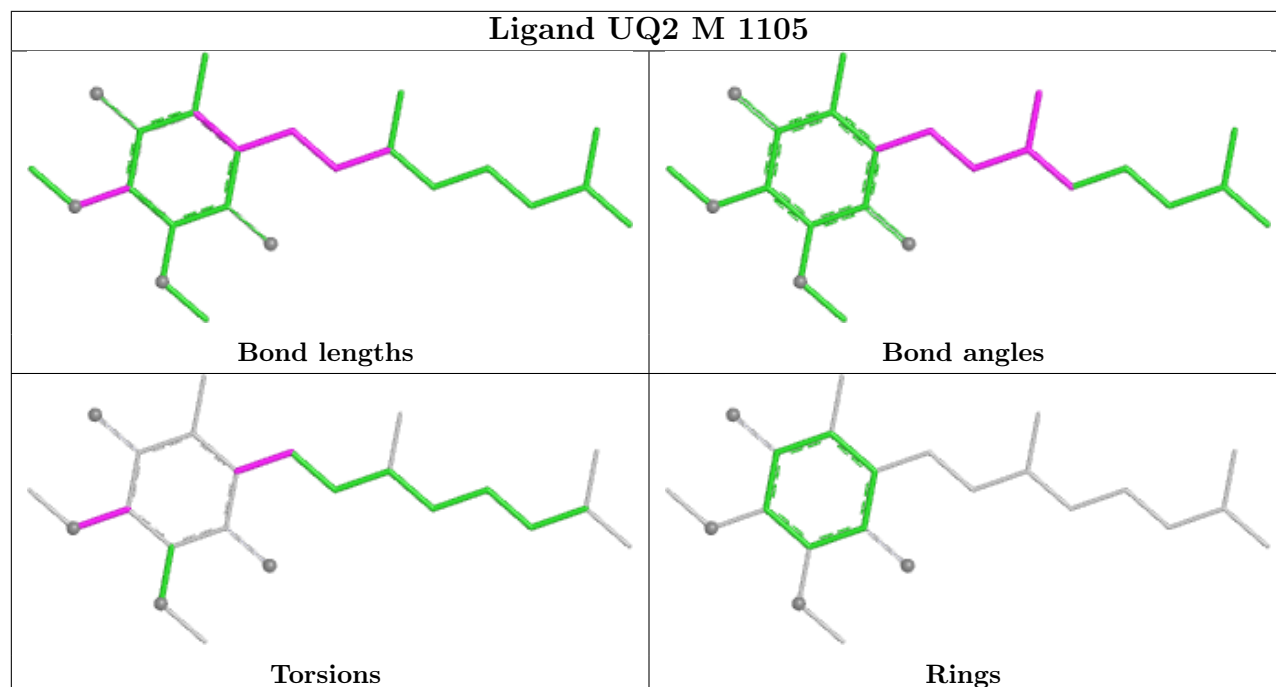




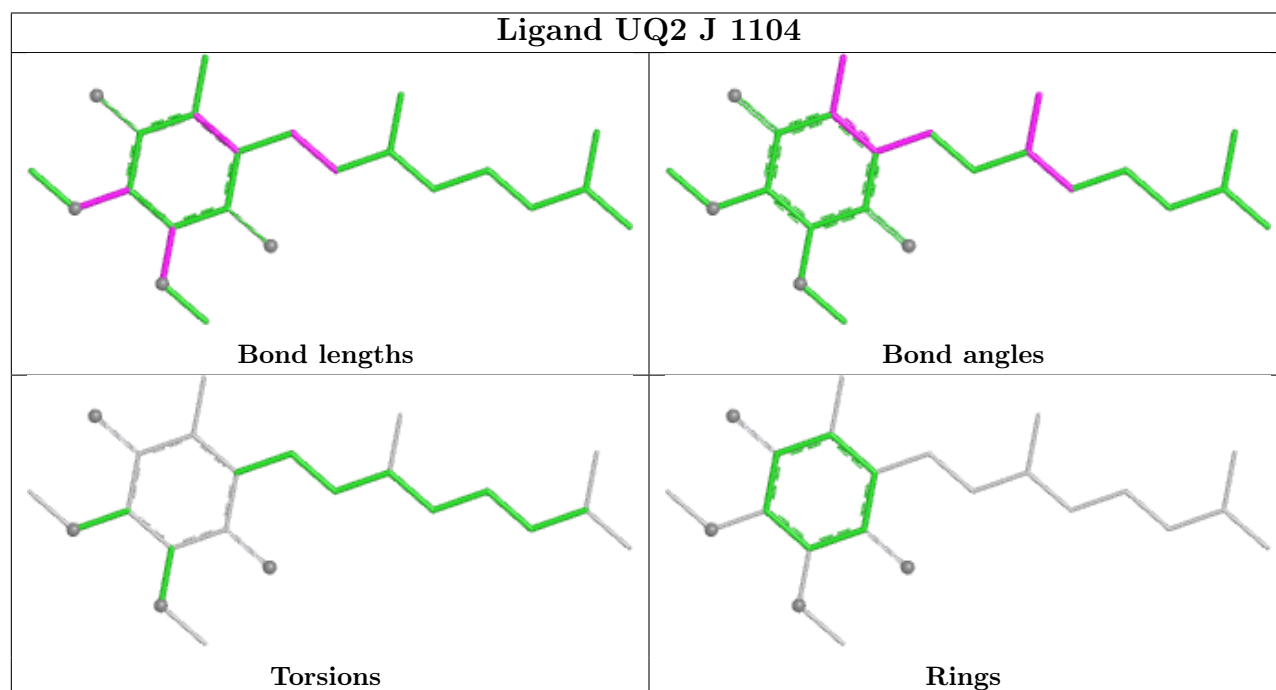




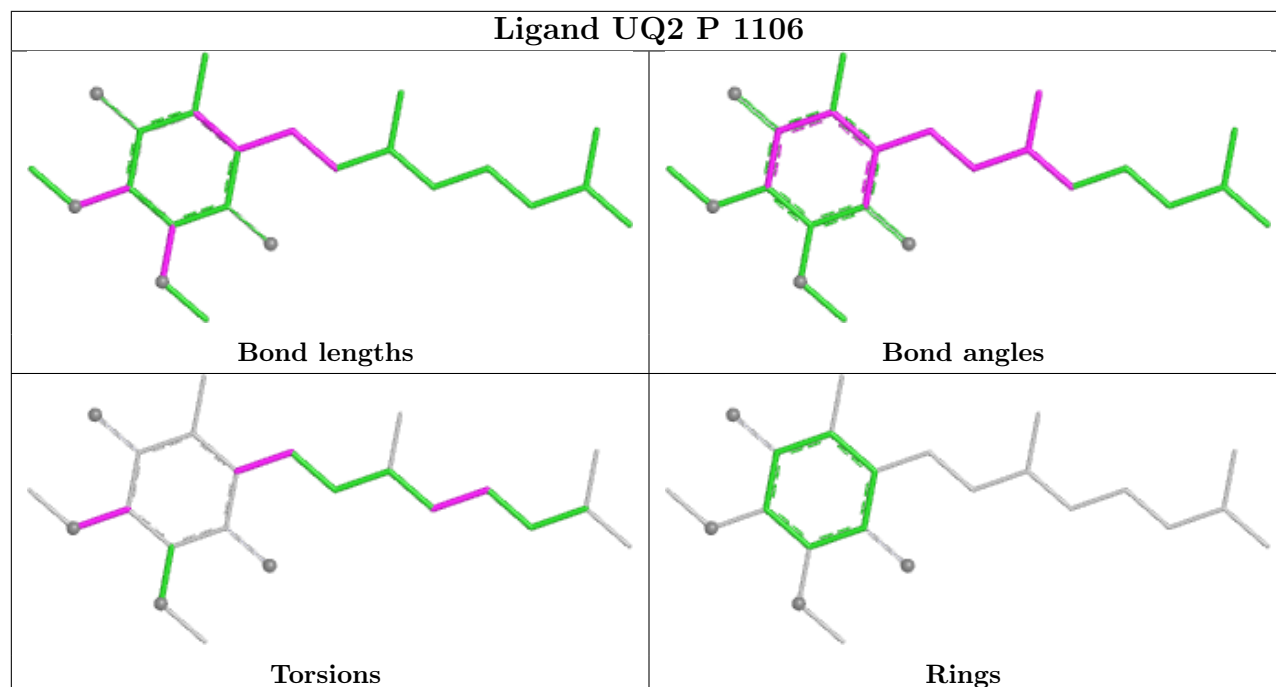
Ligand UQ2 M 1105



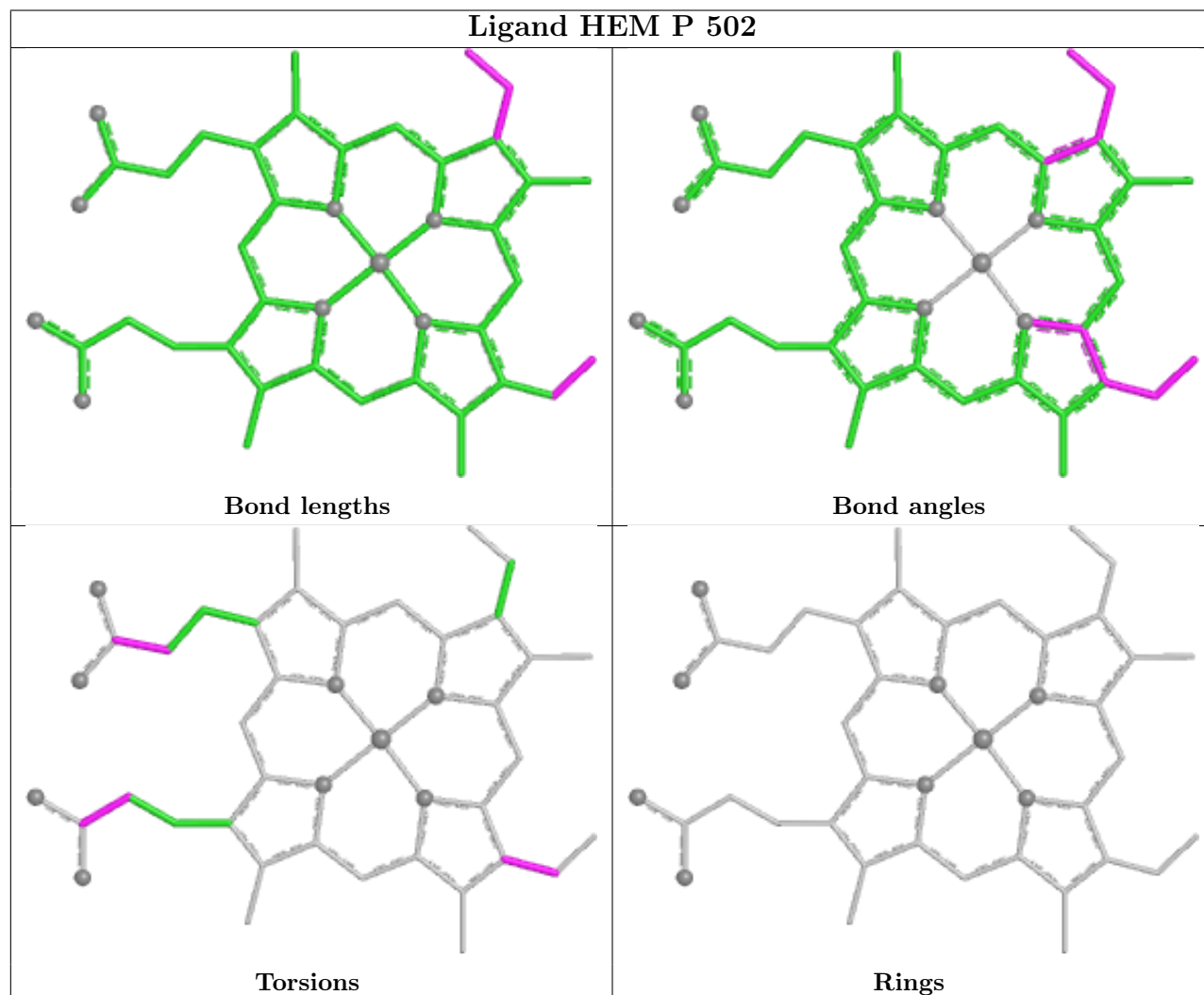
Ligand UQ2 J 1104

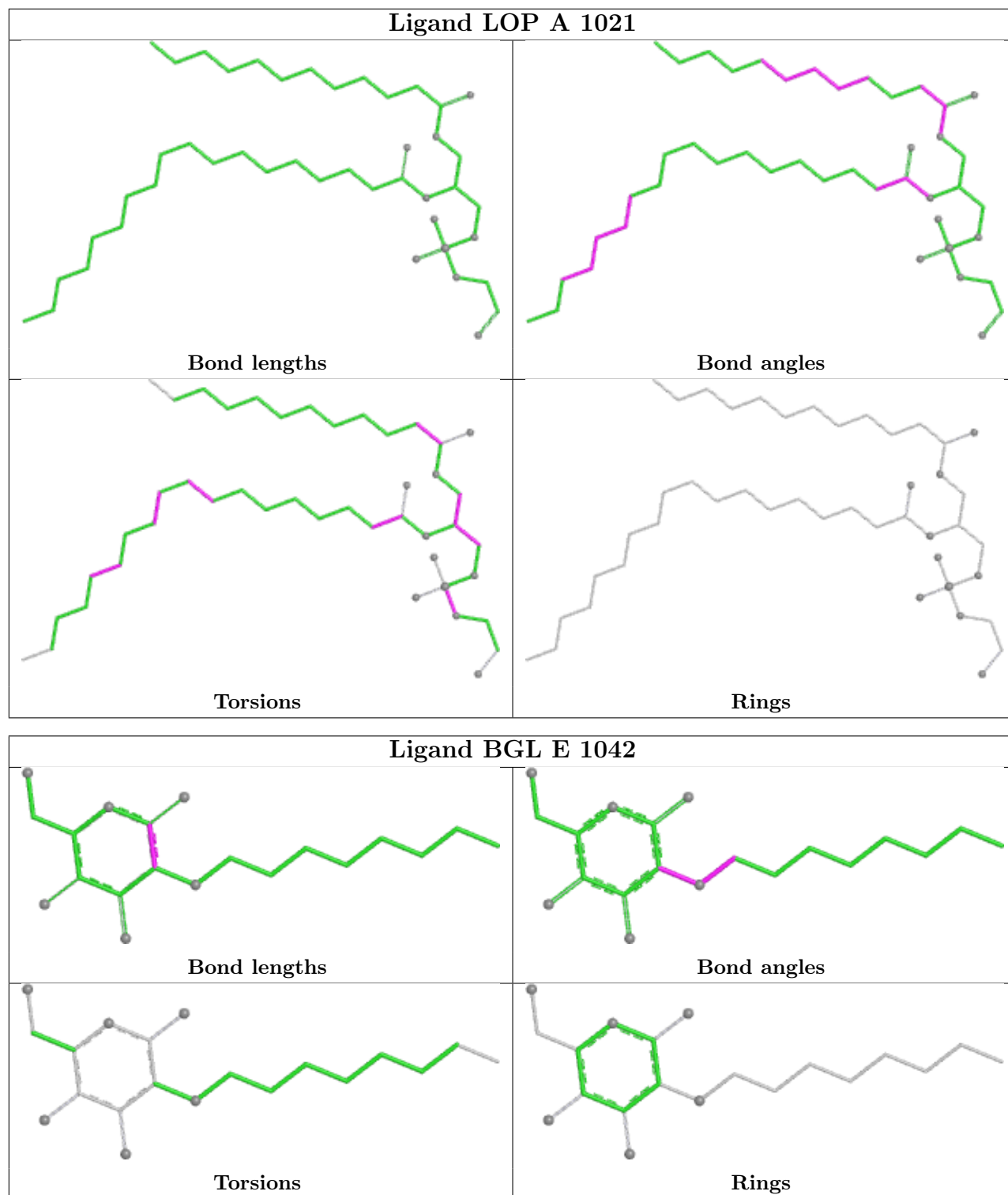


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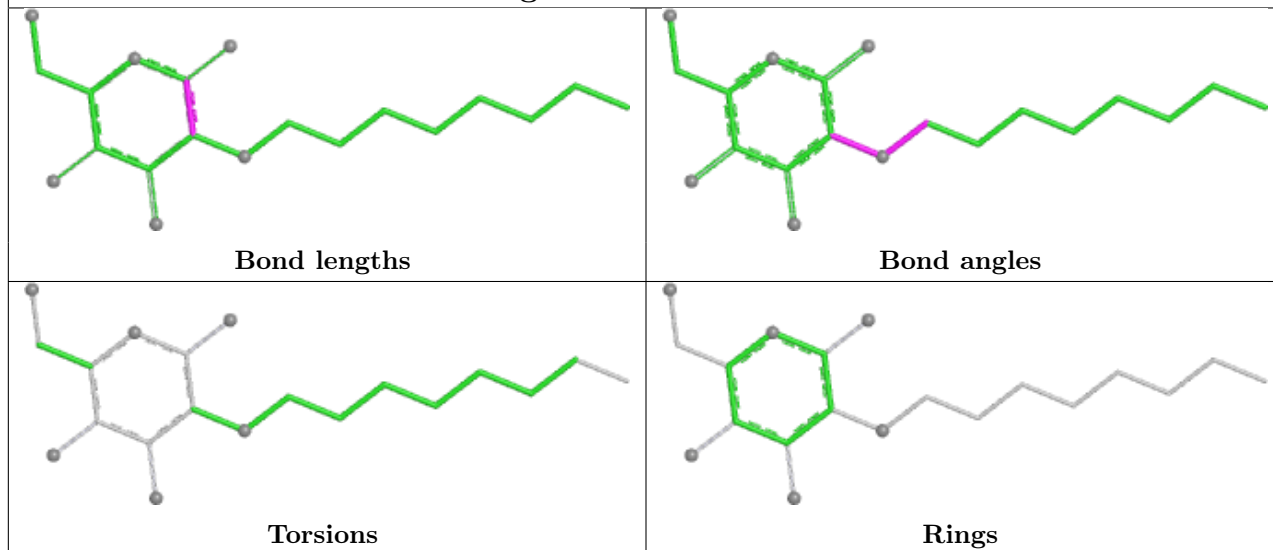


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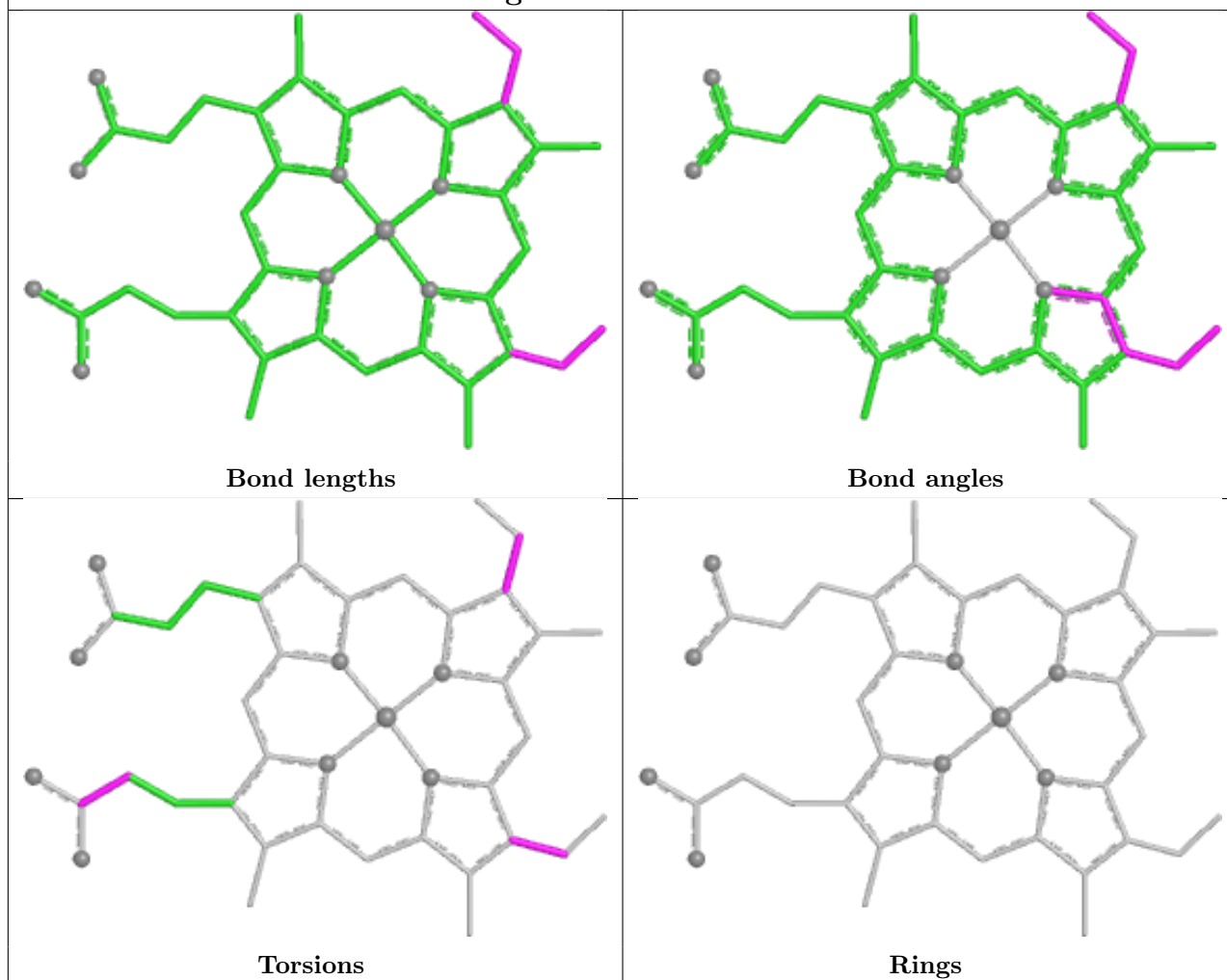


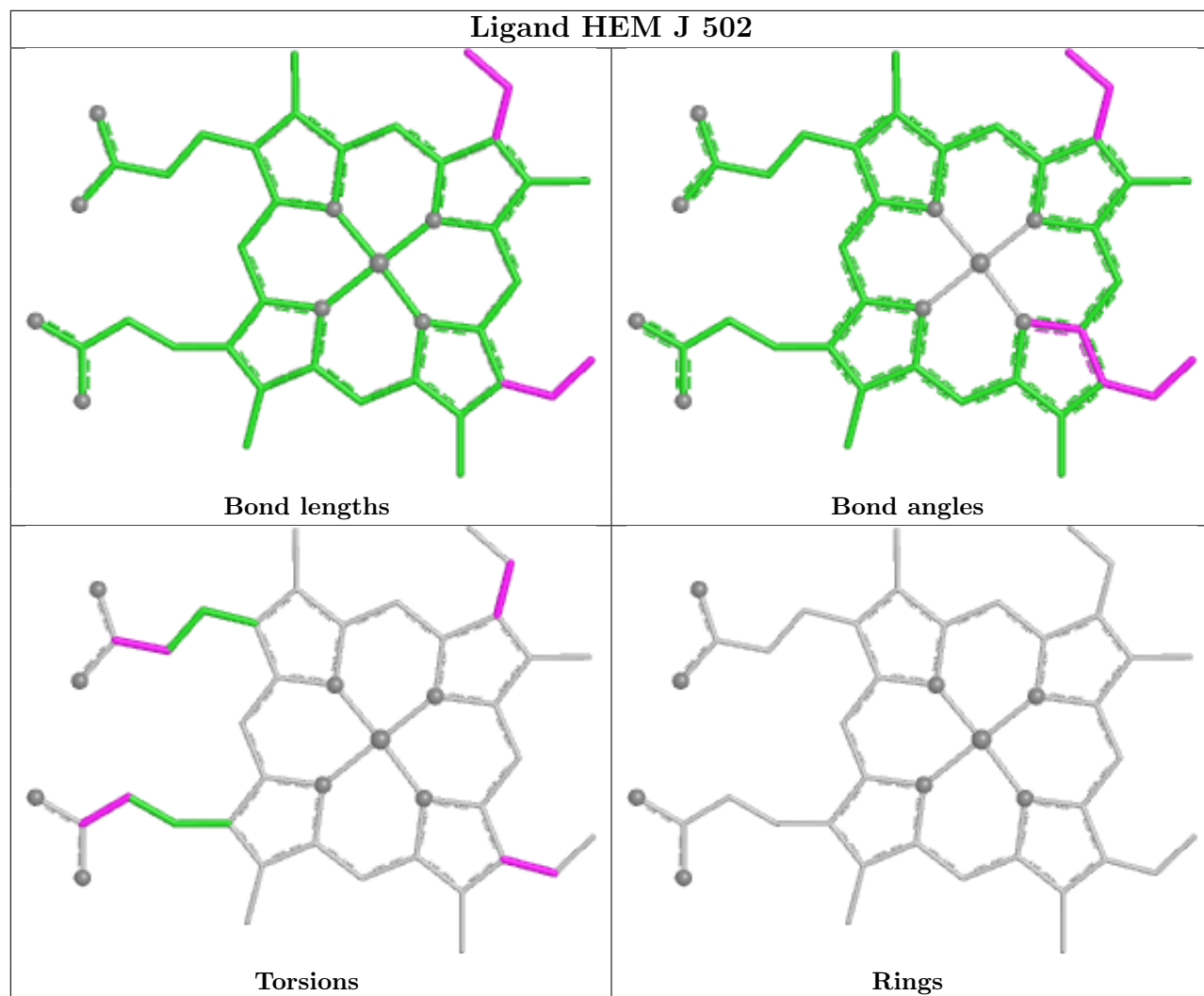


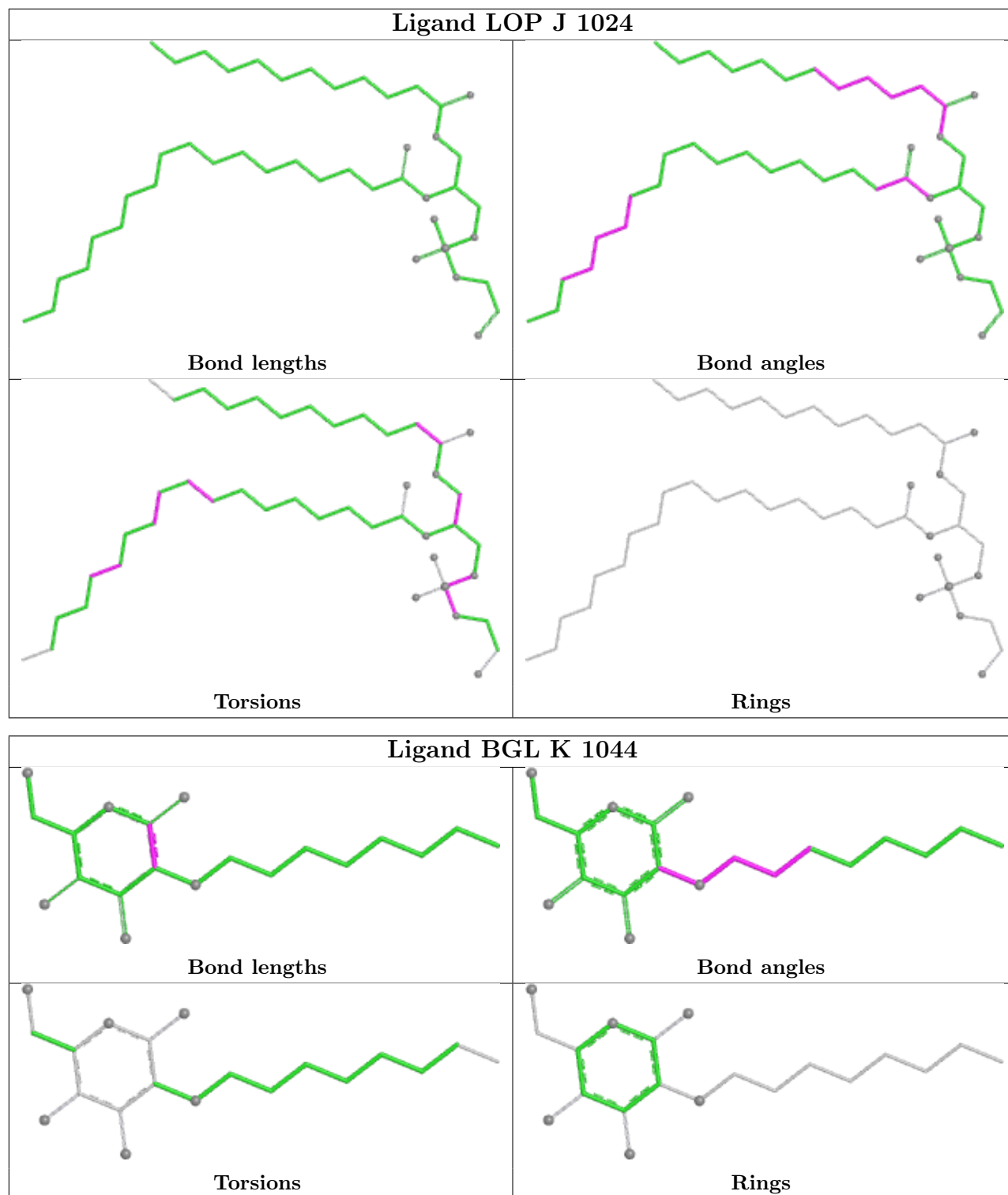
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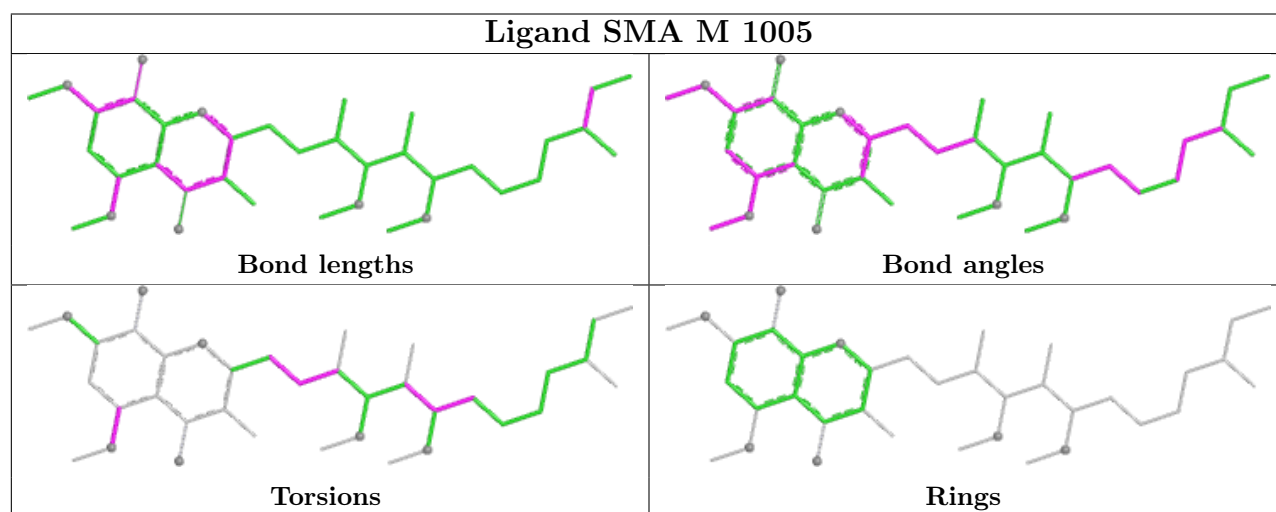
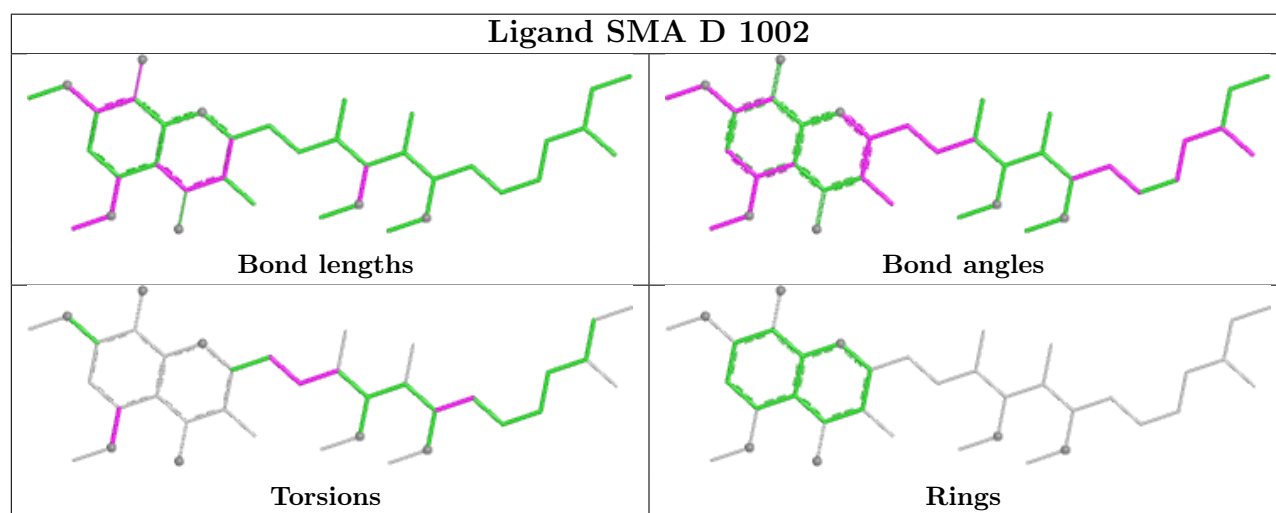
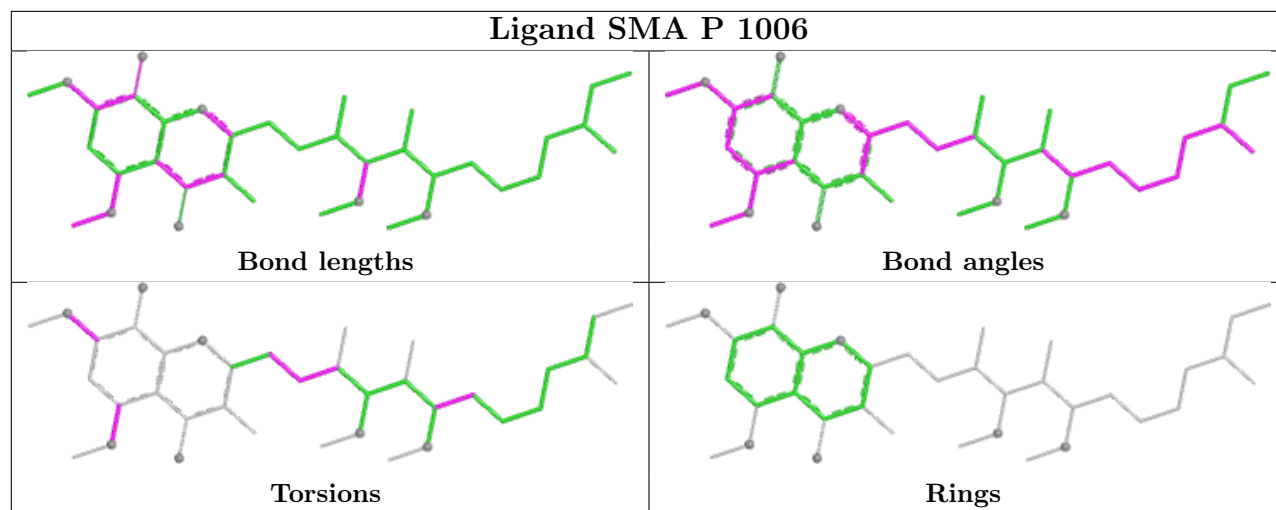


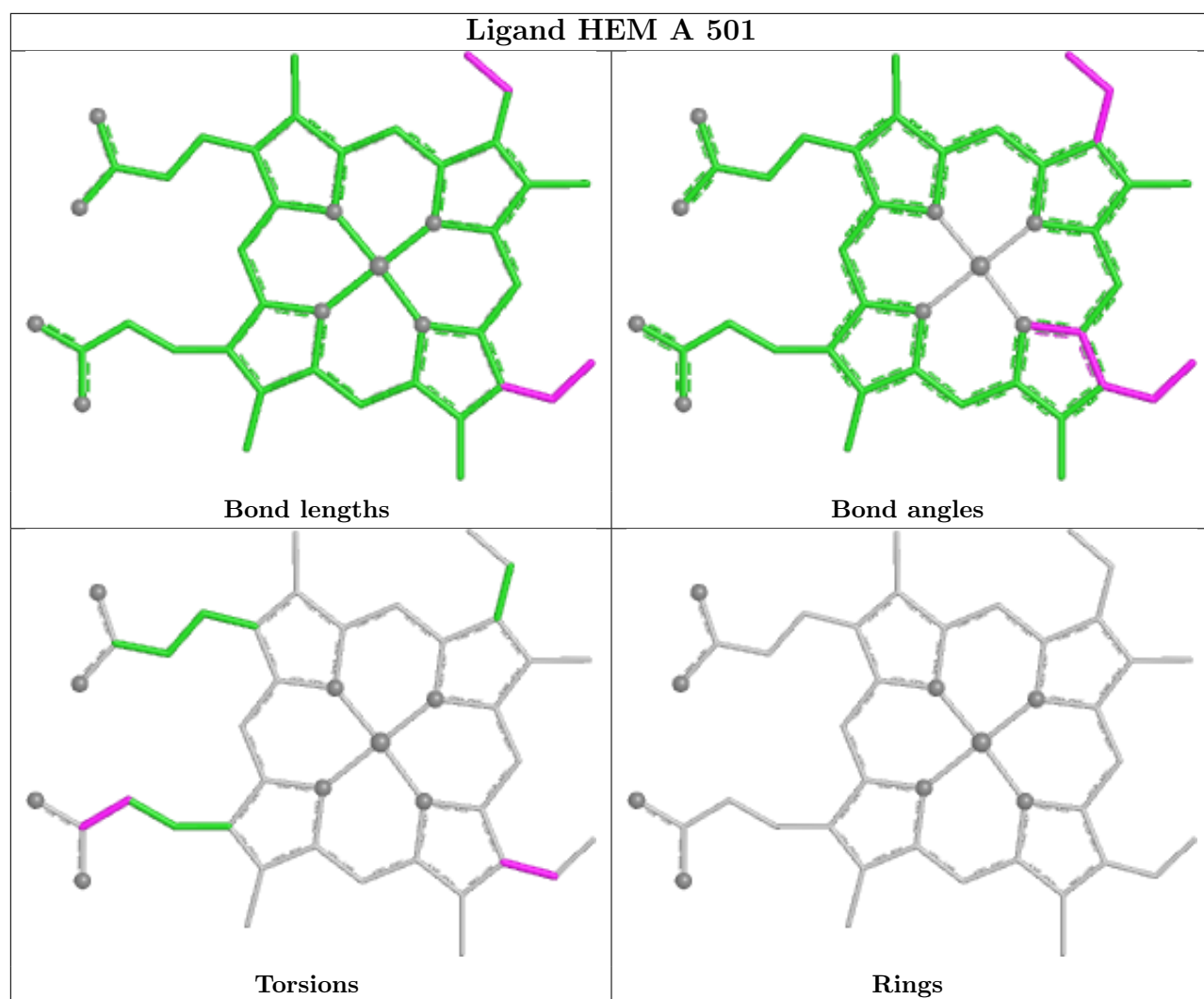
Ligand HEM P 501

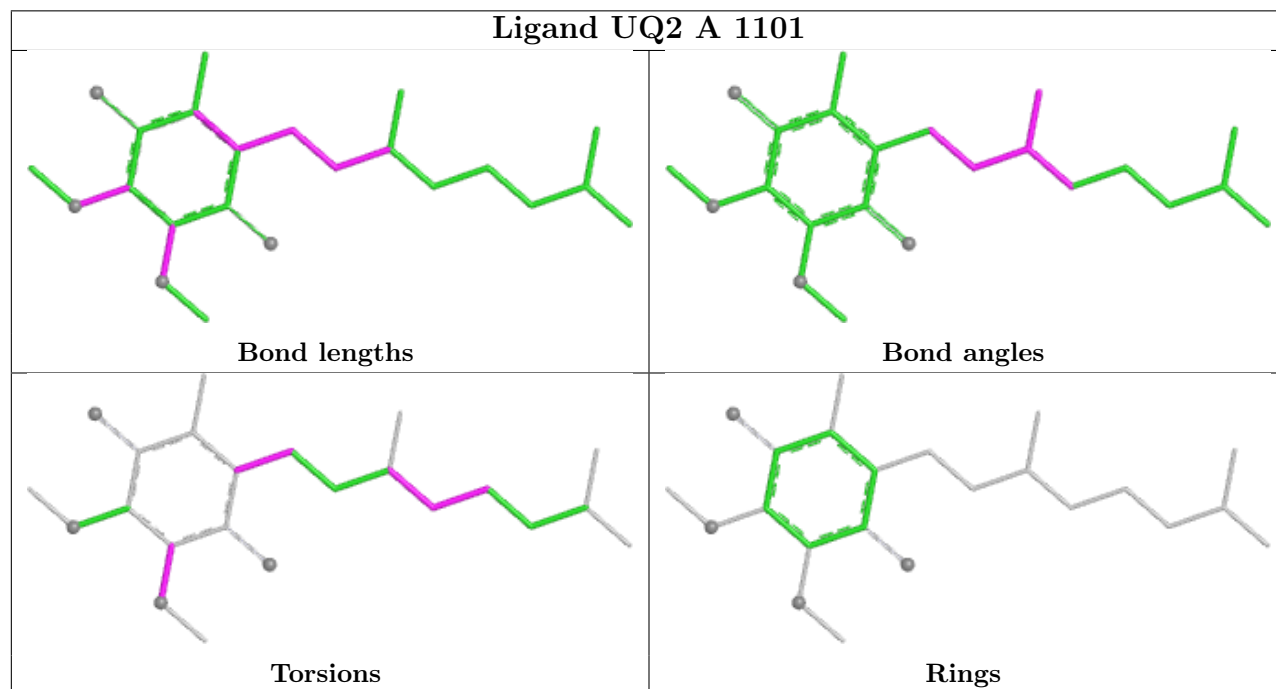
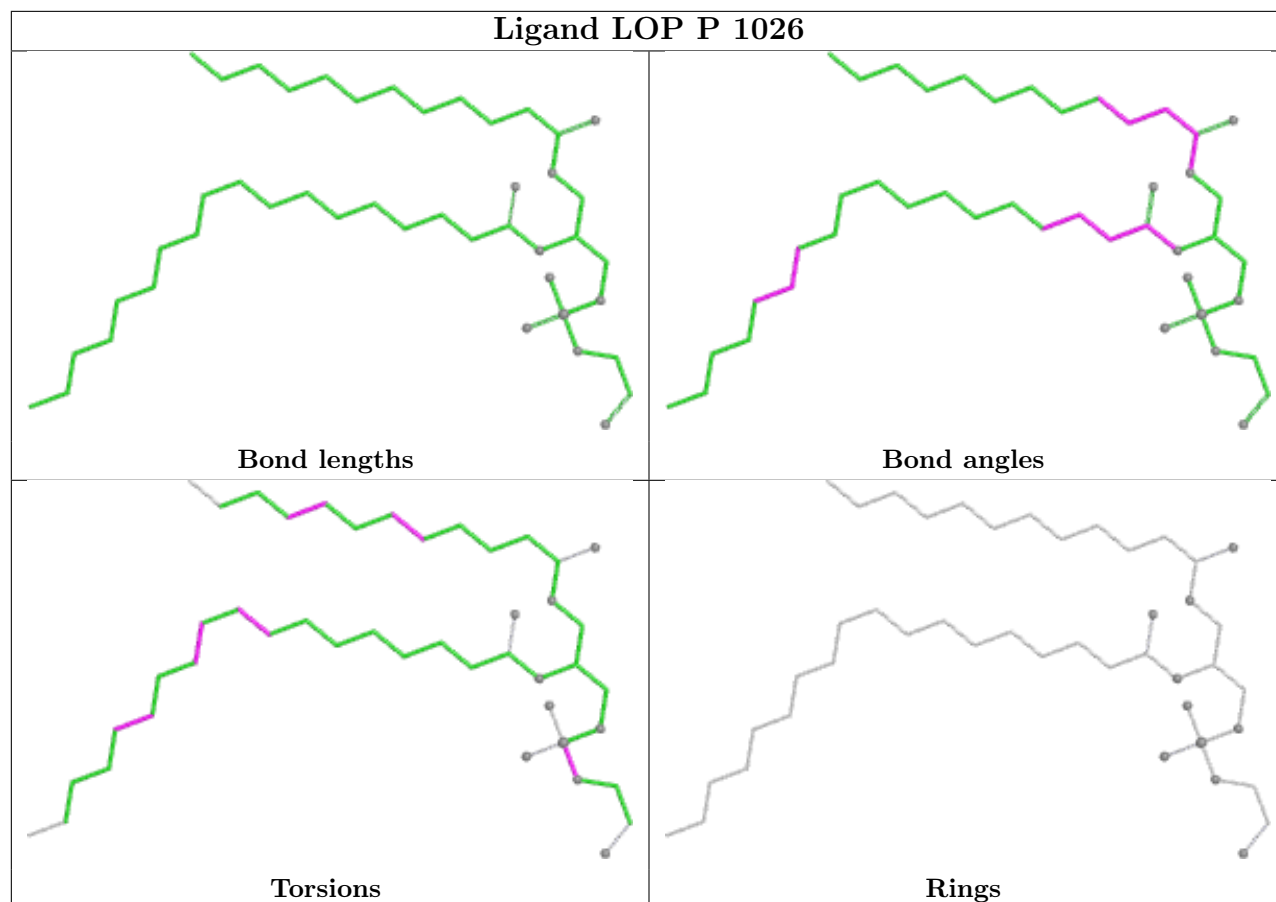


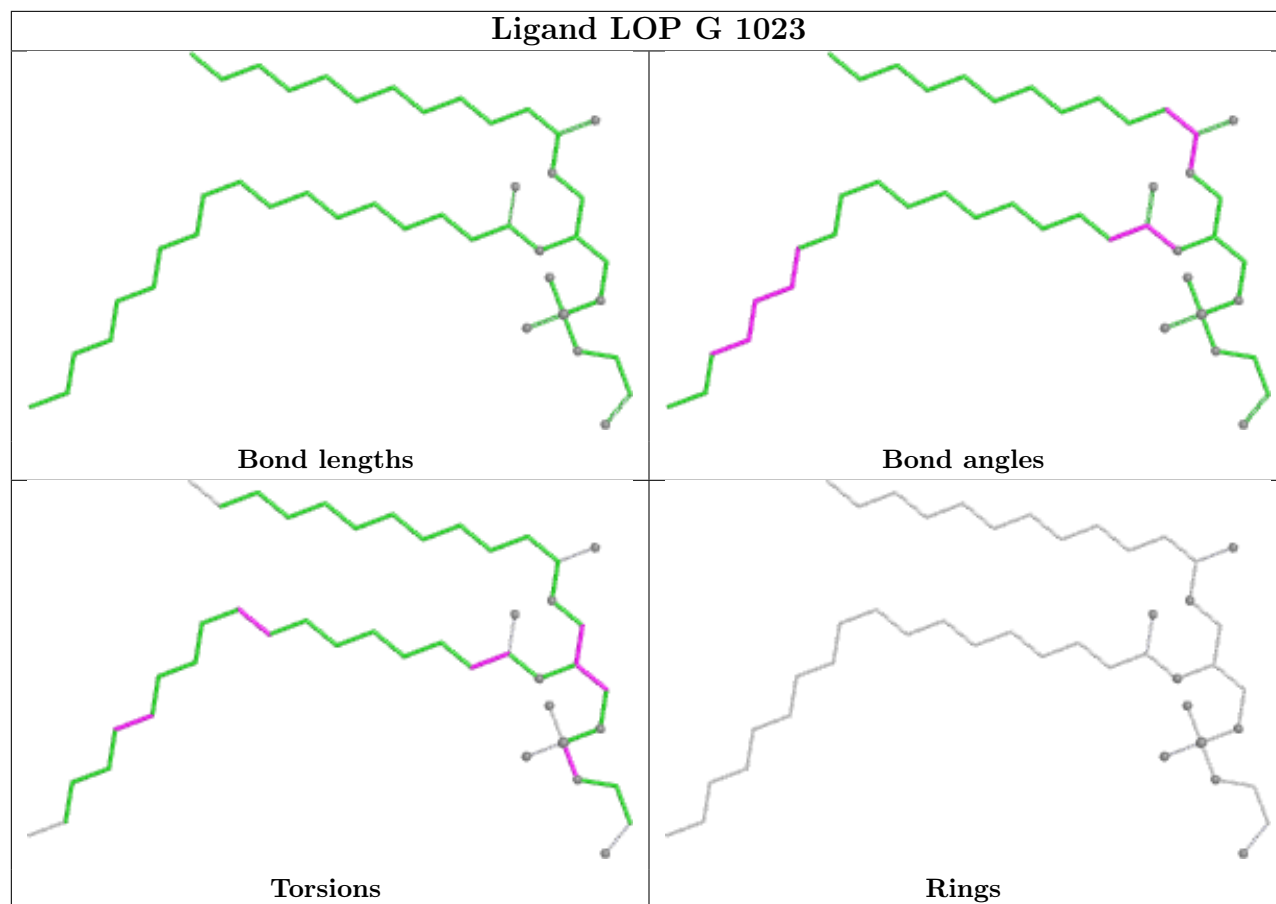


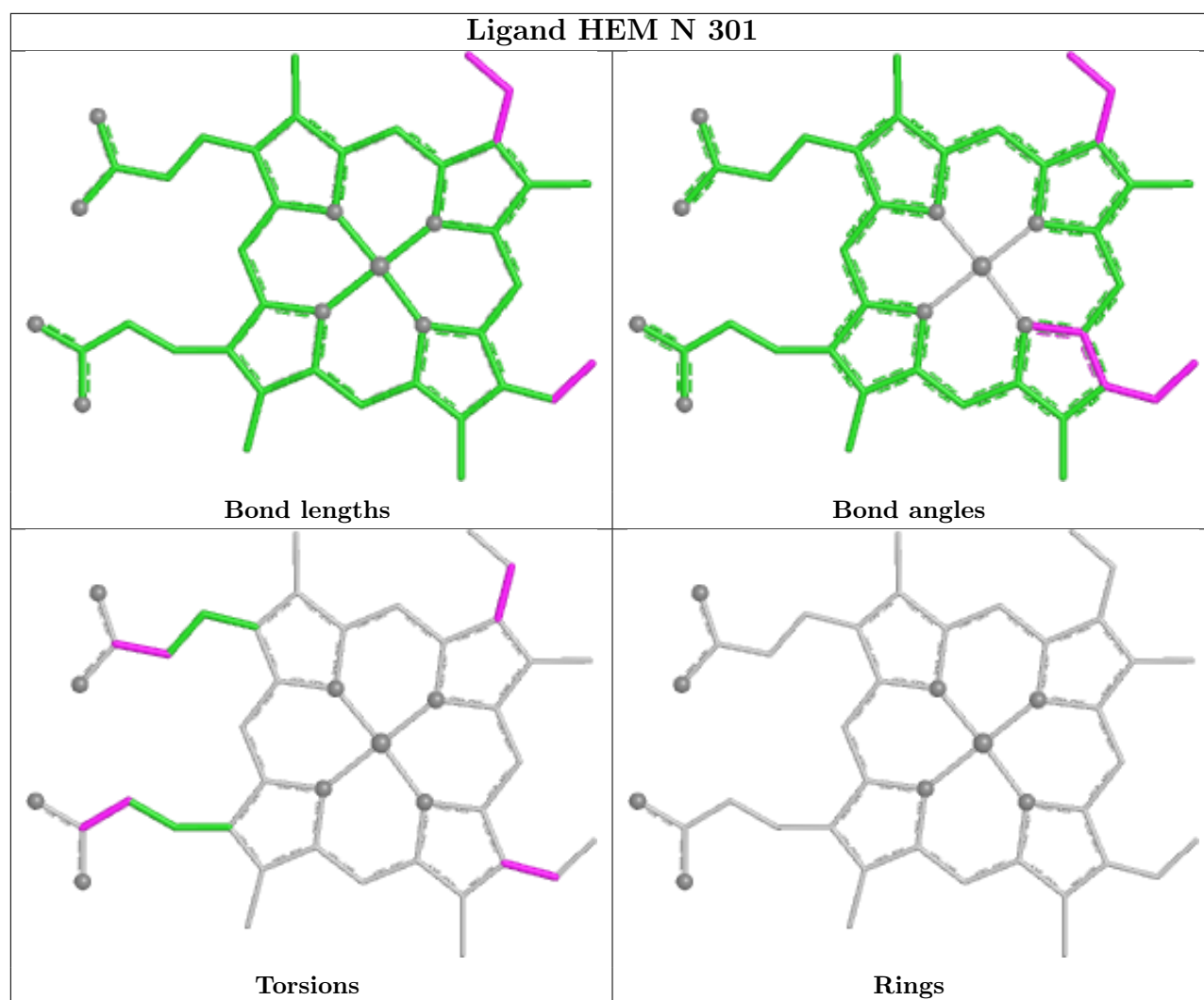


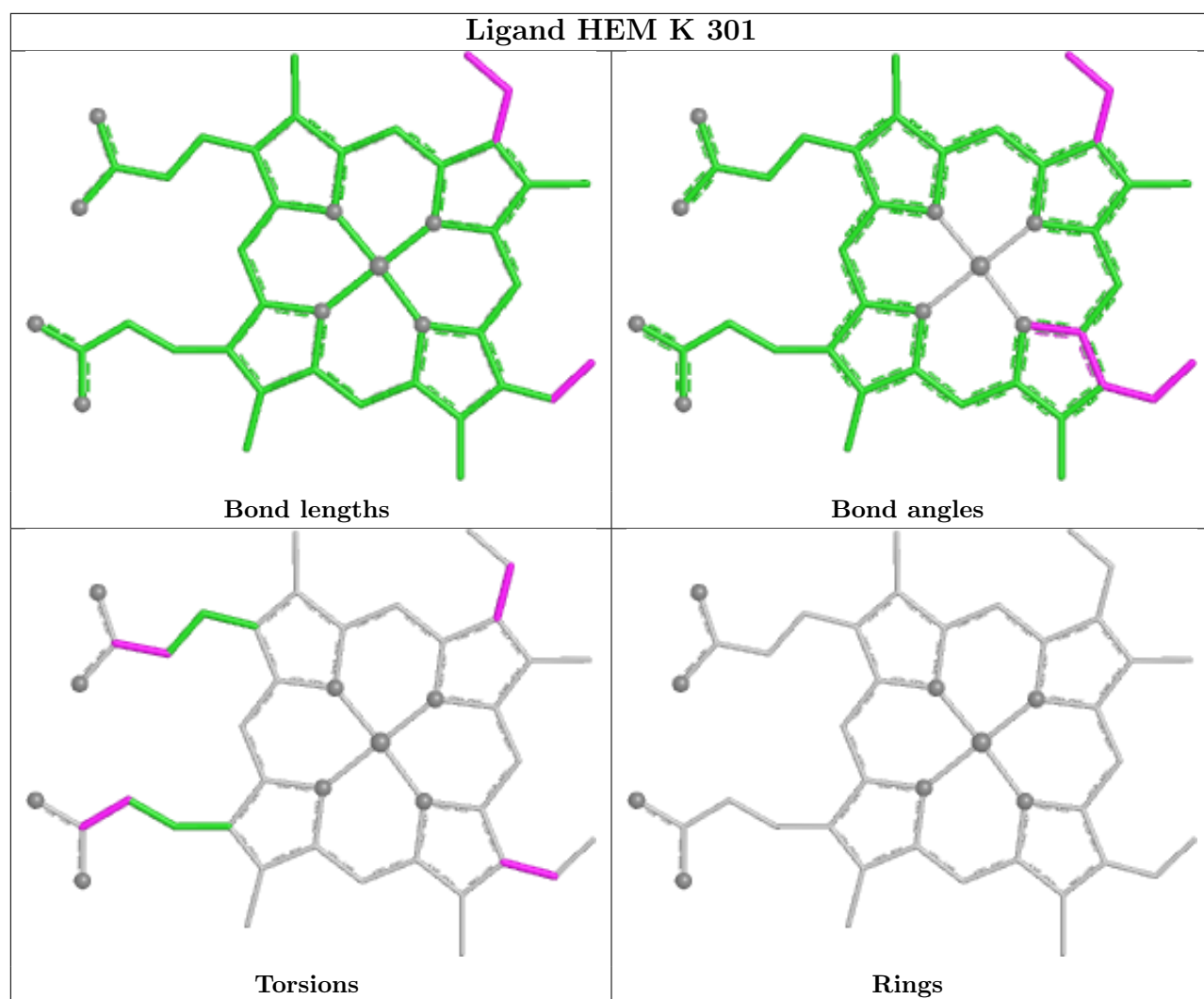


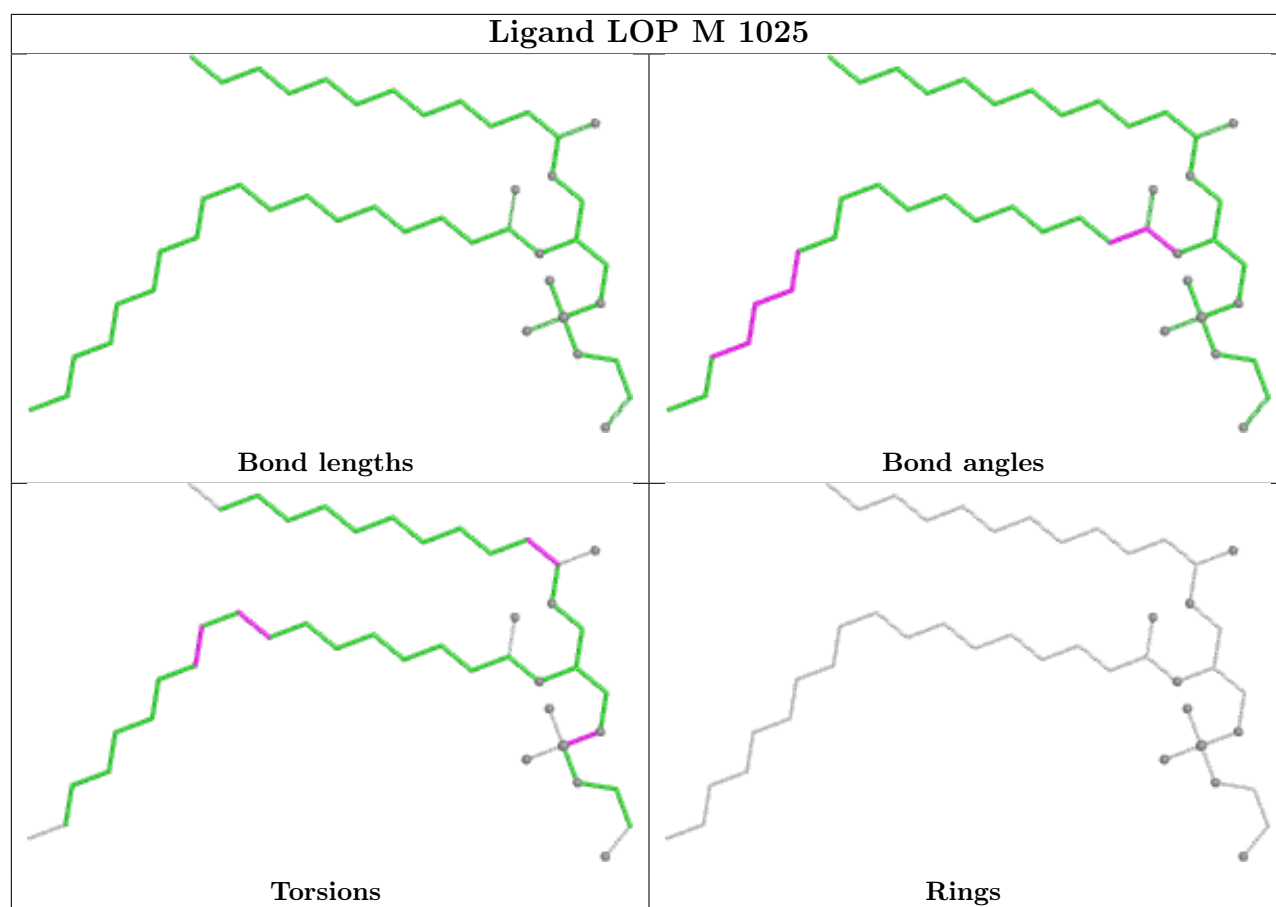


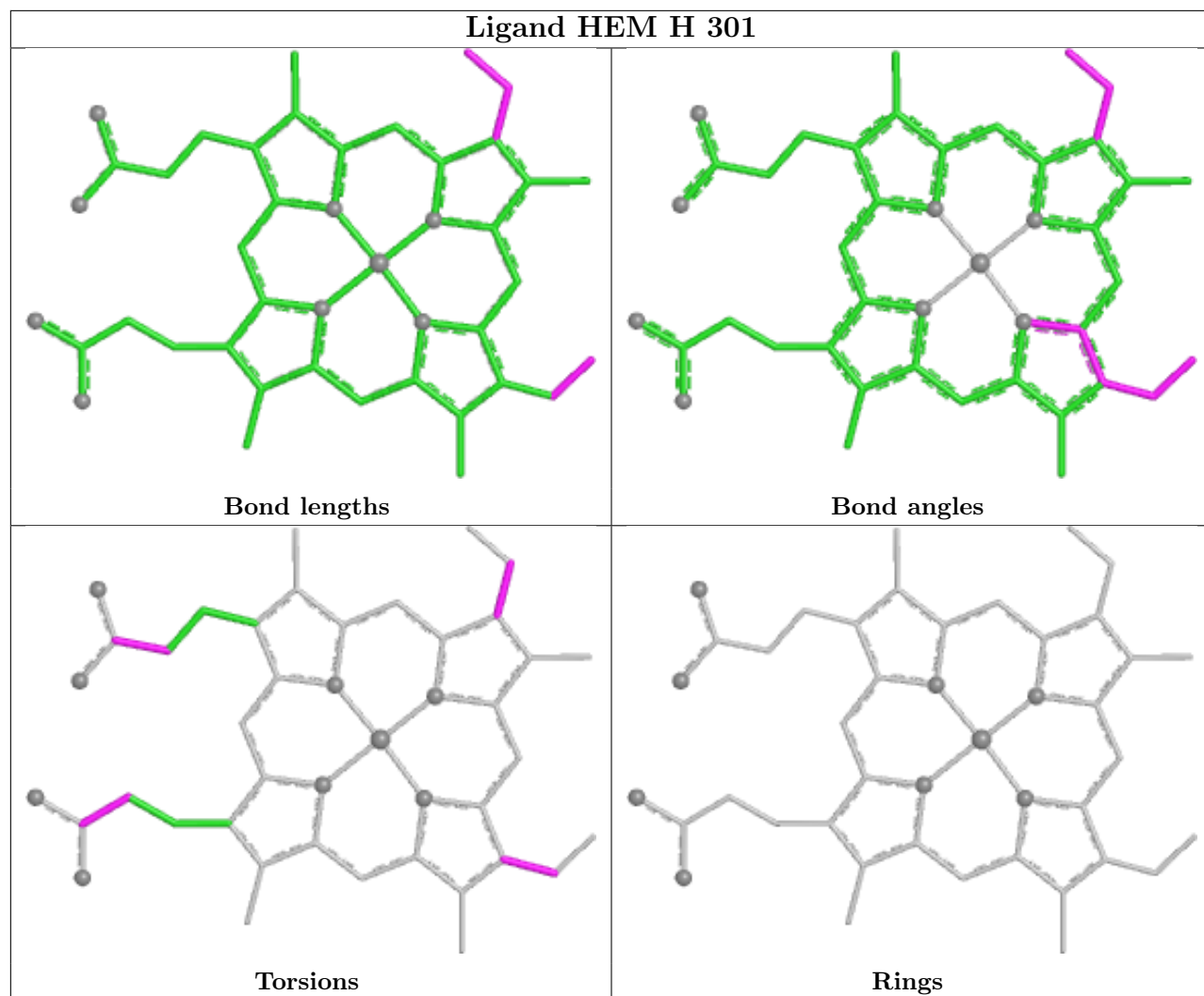


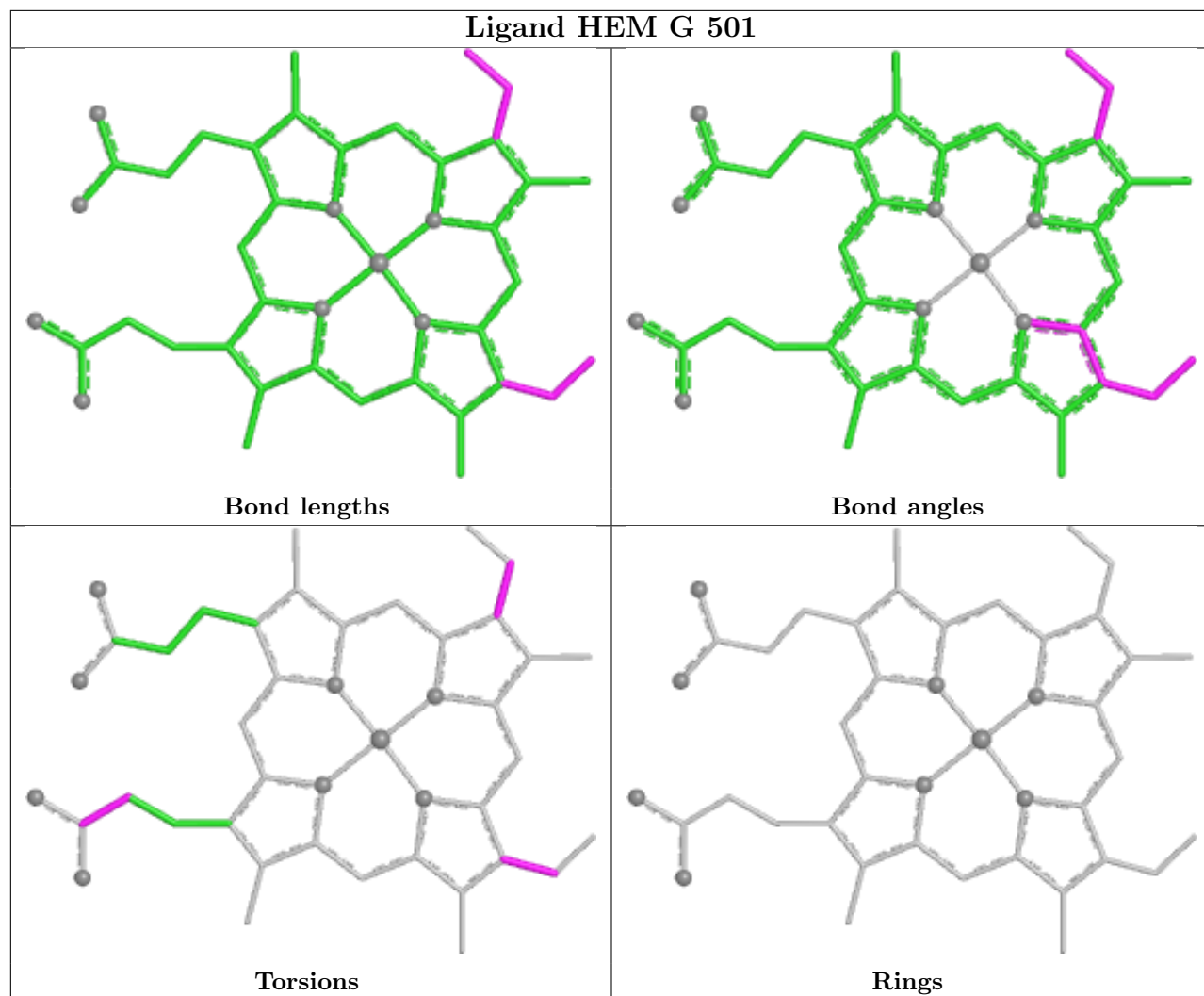


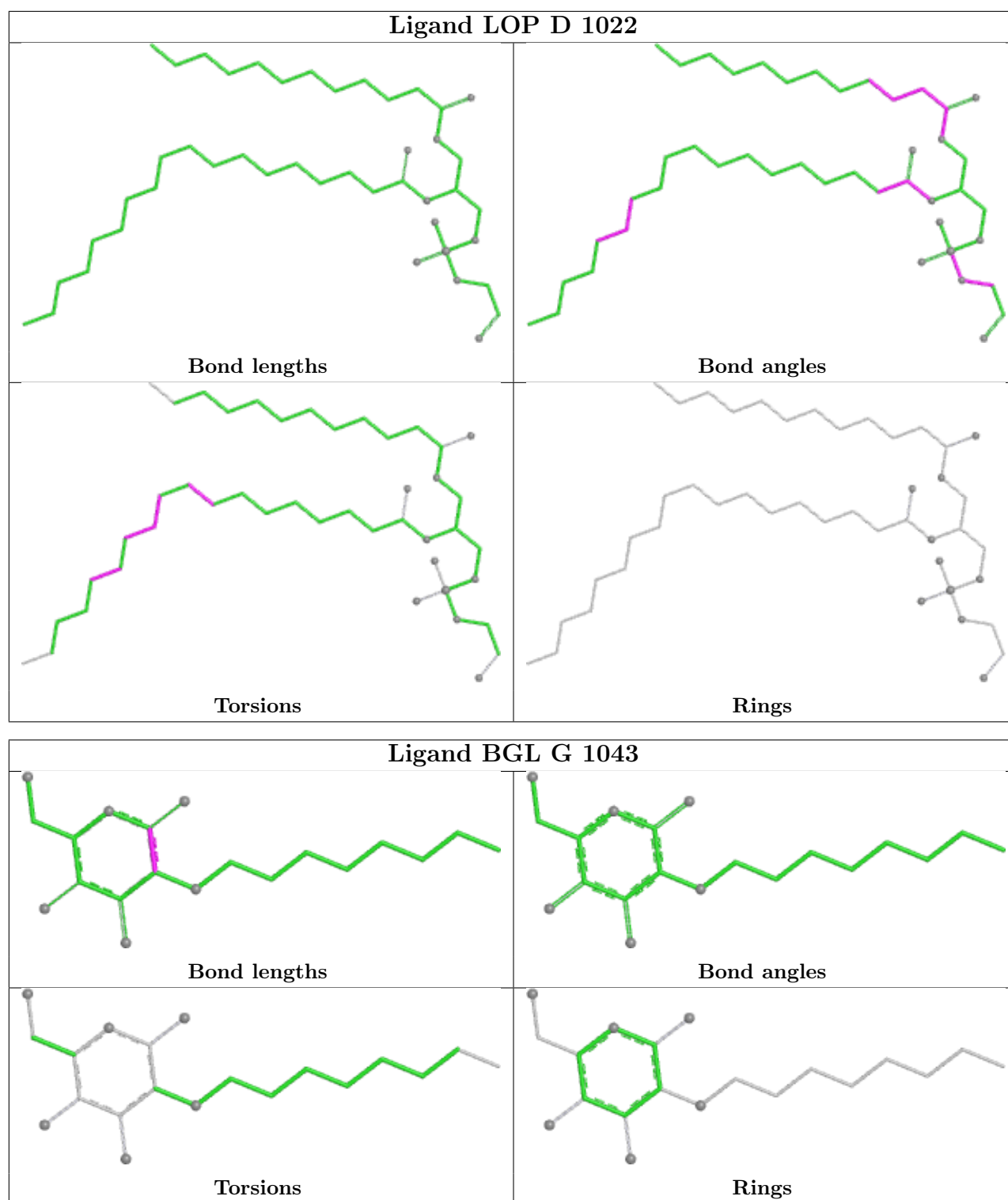












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	428/445 (96%)	-0.02	4 (0%) 81 78	35, 53, 90, 117	0
1	D	428/445 (96%)	0.04	4 (0%) 81 78	35, 53, 93, 124	0
1	G	428/445 (96%)	0.20	8 (1%) 66 62	35, 56, 100, 124	0
1	J	428/445 (96%)	0.39	15 (3%) 47 43	36, 62, 101, 125	0
1	M	428/445 (96%)	0.41	9 (2%) 63 59	38, 67, 107, 130	0
1	P	428/445 (96%)	0.18	9 (2%) 63 59	35, 56, 100, 127	0
2	B	256/269 (95%)	0.62	12 (4%) 36 32	47, 78, 112, 134	0
2	E	256/269 (95%)	0.72	20 (7%) 19 15	50, 80, 117, 133	0
2	H	256/269 (95%)	0.58	18 (7%) 22 19	40, 72, 113, 135	0
2	K	256/269 (95%)	0.91	33 (12%) 7 5	49, 87, 120, 136	0
2	N	256/269 (95%)	1.12	39 (15%) 5 4	59, 95, 121, 135	0
2	Q	256/269 (95%)	0.90	24 (9%) 14 11	51, 87, 119, 134	0
3	C	179/187 (95%)	0.25	6 (3%) 48 44	37, 59, 101, 139	0
3	F	179/187 (95%)	0.26	4 (2%) 62 58	38, 63, 102, 140	0
3	I	179/187 (95%)	0.29	5 (2%) 55 51	41, 58, 105, 139	0
3	L	179/187 (95%)	0.29	12 (6%) 24 20	37, 59, 104, 139	0
3	O	179/187 (95%)	0.34	7 (3%) 43 39	34, 64, 108, 138	0
3	R	179/187 (95%)	0.65	7 (3%) 43 39	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.41	236 (4%) 37 33	34, 66, 112, 140	0

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	109	GLY	5.6
3	I	47	LEU	4.5
2	K	172	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	121	LEU	4.4
2	H	115	GLY	4.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	UQ2	J	1104	23/23	0.57	0.27	107,115,116,117	0
8	UQ2	G	1103	23/23	0.65	0.29	109,116,117,118	0
8	UQ2	A	1101	23/23	0.66	0.25	102,105,108,109	0
8	UQ2	M	1105	23/23	0.68	0.26	112,123,125,125	0
8	UQ2	D	1102	23/23	0.69	0.25	92,98,107,107	0
8	UQ2	P	1106	23/23	0.71	0.25	101,104,107,108	0
9	BGL	N	1045	20/20	0.72	0.22	107,111,113,114	0
7	LOP	M	1025	45/45	0.73	0.20	89,114,123,123	0
7	LOP	J	1024	45/45	0.76	0.18	93,113,125,126	0
9	BGL	B	1041	20/20	0.77	0.22	87,97,101,102	0
9	BGL	K	1044	20/20	0.77	0.19	95,99,101,101	0
7	LOP	G	1023	45/45	0.77	0.19	88,102,112,113	0
9	BGL	P	1046	20/20	0.79	0.18	87,93,95,95	0
7	LOP	P	1026	45/45	0.80	0.18	69,95,99,100	0
9	BGL	G	1043	20/20	0.82	0.21	89,91,101,101	0
7	LOP	A	1021	45/45	0.84	0.16	72,86,94,99	0
9	BGL	E	1042	20/20	0.84	0.17	80,85,102,102	0
7	LOP	D	1022	45/45	0.84	0.15	63,88,98,102	0
4	SR	M	1019	1/1	0.87	0.07	154,154,154,154	0
4	SR	Q	1016	1/1	0.88	0.08	137,137,137,137	0
4	SR	A	1017	1/1	0.89	0.07	114,114,114,114	0

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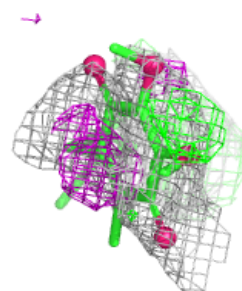
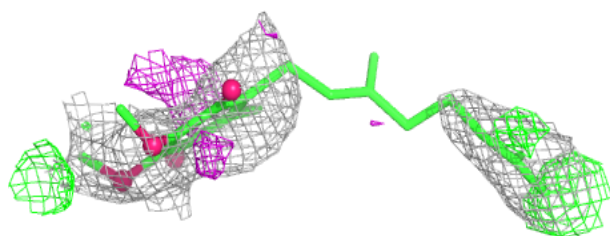
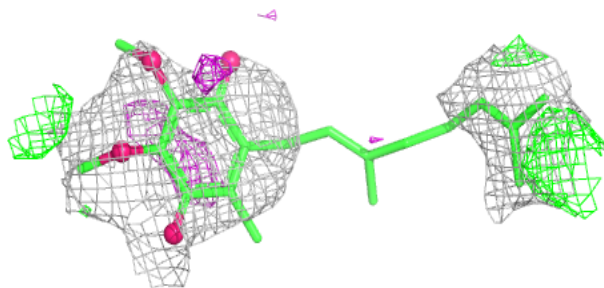
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SR	N	1015	1/1	0.90	0.07	153,153,153,153	0
4	SR	B	1011	1/1	0.91	0.06	132,132,132,132	0
4	SR	K	1014	1/1	0.92	0.05	145,145,145,145	0
4	SR	G	1018	1/1	0.92	0.05	98,98,98,98	0
6	SMA	D	1002	37/37	0.93	0.10	39,44,76,78	0
6	SMA	A	1001	37/37	0.94	0.08	38,47,54,56	0
6	SMA	G	1003	37/37	0.94	0.09	35,43,60,65	0
6	SMA	M	1005	37/37	0.94	0.10	56,66,73,73	0
12	NA	R	2001	1/1	0.94	0.07	62,62,62,62	0
5	HEM	J	501	43/43	0.95	0.13	67,75,79,81	0
6	SMA	P	1006	37/37	0.95	0.09	34,45,76,77	0
11	CL	I	2004	1/1	0.95	0.08	67,67,67,67	0
11	CL	R	2005	1/1	0.95	0.14	67,67,67,67	0
6	SMA	J	1004	37/37	0.95	0.09	40,49,79,85	0
4	SR	H	1013	1/1	0.96	0.05	113,113,113,113	0
4	SR	E	1012	1/1	0.96	0.06	138,138,138,138	0
5	HEM	N	301	43/43	0.96	0.10	65,72,79,84	0
5	HEM	M	501	43/43	0.97	0.10	63,69,75,78	0
5	HEM	E	301	43/43	0.97	0.09	53,62,73,76	0
5	HEM	Q	301	43/43	0.97	0.08	56,65,73,78	0
5	HEM	G	501	43/43	0.97	0.09	50,59,62,62	0
5	HEM	B	301	43/43	0.97	0.09	51,56,70,73	0
5	HEM	K	301	43/43	0.97	0.09	49,55,67,69	0
5	HEM	P	501	43/43	0.98	0.08	48,54,57,57	0
5	HEM	P	502	43/43	0.98	0.08	35,40,49,53	0
5	HEM	G	502	43/43	0.98	0.09	32,36,45,49	0
5	HEM	H	301	43/43	0.98	0.07	33,42,47,50	0
5	HEM	D	501	43/43	0.98	0.08	40,48,53,55	0
5	HEM	J	502	43/43	0.98	0.07	37,41,54,57	0
5	HEM	D	502	43/43	0.98	0.08	32,37,49,58	0
10	FES	O	200	4/4	0.98	0.04	42,43,43,43	0
5	HEM	A	502	43/43	0.98	0.09	32,37,49,49	0
5	HEM	M	502	43/43	0.98	0.08	47,49,59,63	0
5	HEM	A	501	43/43	0.98	0.07	43,47,51,53	0
10	FES	C	200	4/4	0.99	0.03	41,42,42,43	0
10	FES	R	200	4/4	0.99	0.04	55,57,58,58	0
10	FES	F	200	4/4	0.99	0.04	43,43,44,45	0
10	FES	I	200	4/4	0.99	0.04	47,48,48,48	0
10	FES	L	200	4/4	0.99	0.04	40,41,41,42	0

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

orientation to approximate a three-dimensional view.

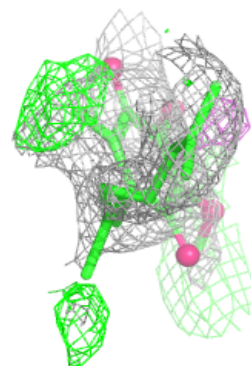
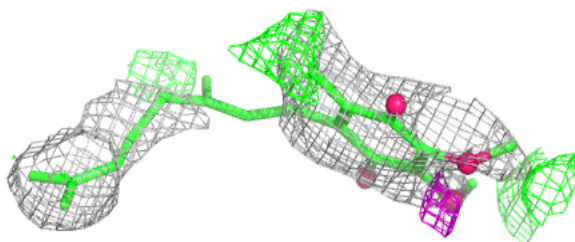
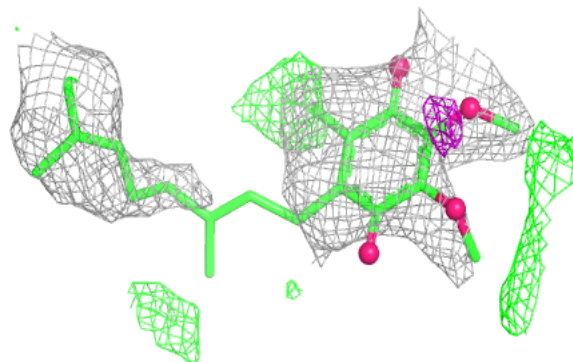
Electron density around UQ2 J 1104:

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



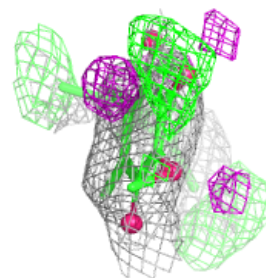
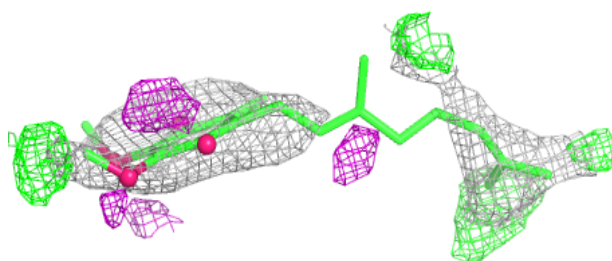
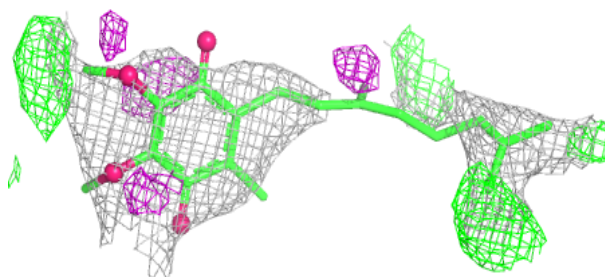
Electron density around UQ2 G 1103:

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

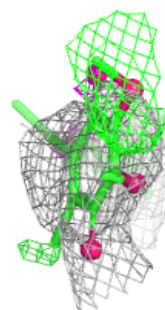
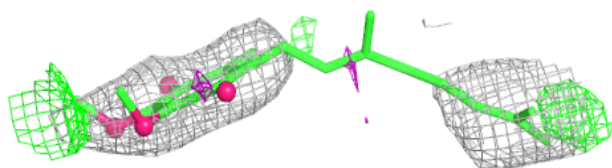
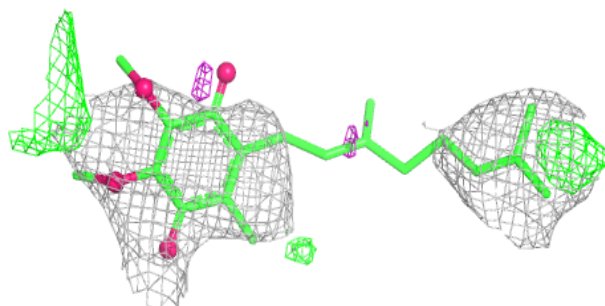


Electron density around UQ2 A 1101:

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

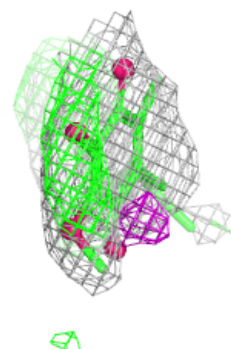
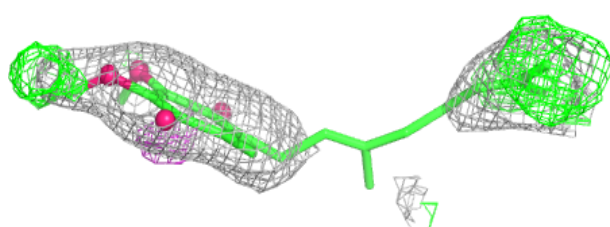
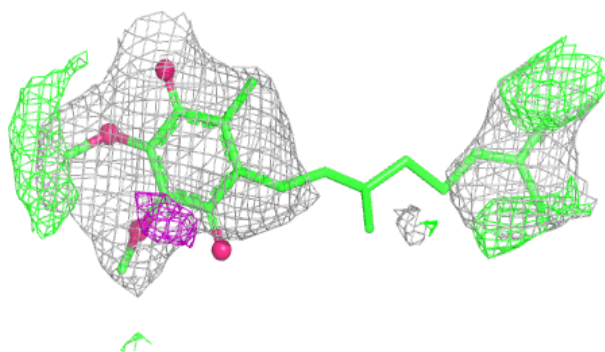
**Electron density around UQ2 M 1105:**

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

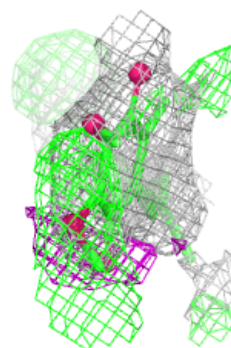
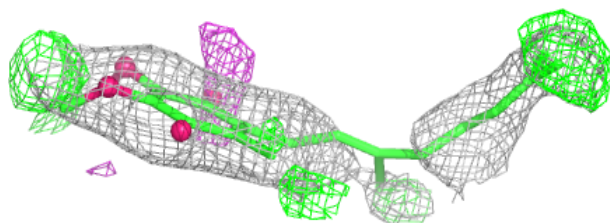
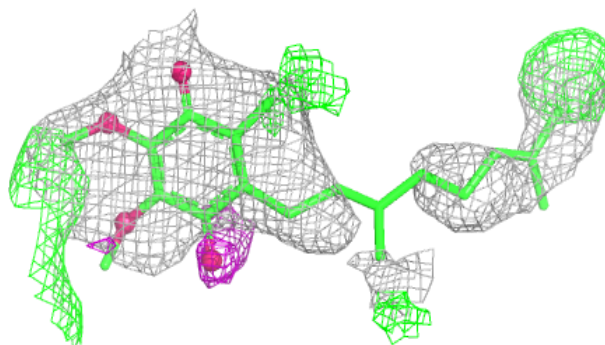


Electron density around UQ2 D 1102:

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

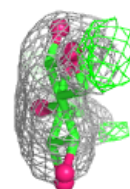
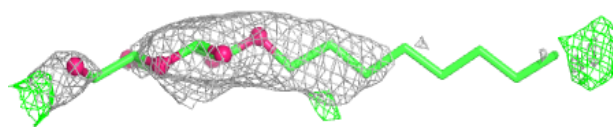
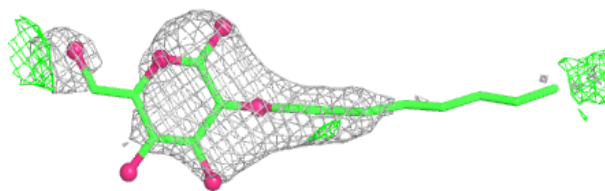
**Electron density around UQ2 P 1106:**

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

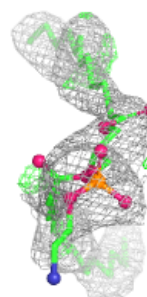
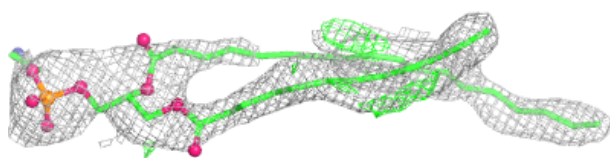
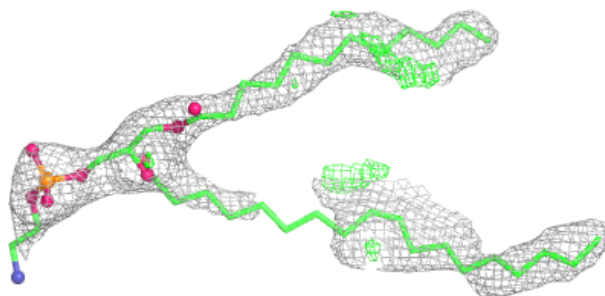


Electron density around BGL N 1045:

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

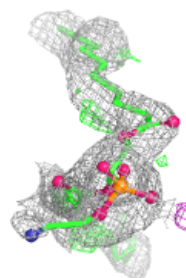
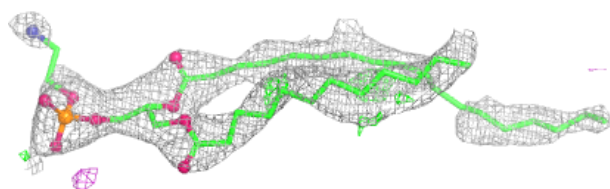
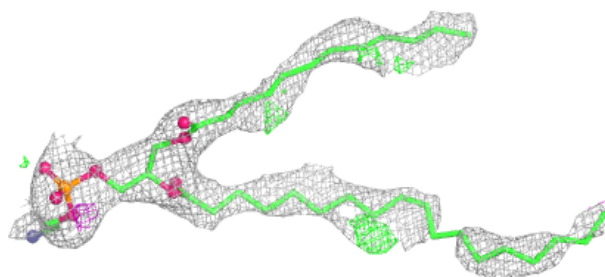
**Electron density around LOP M 1025:**

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

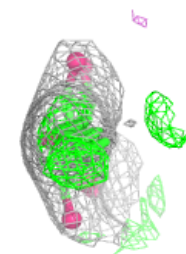
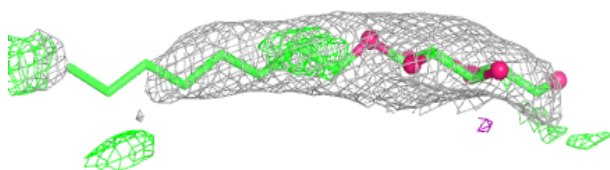
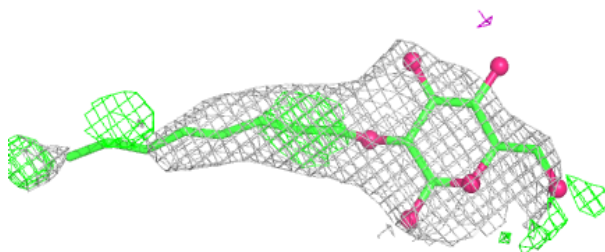


Electron density around LOP J 1024:

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

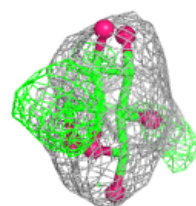
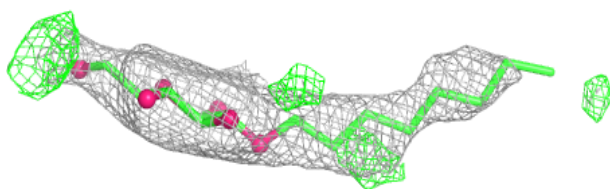
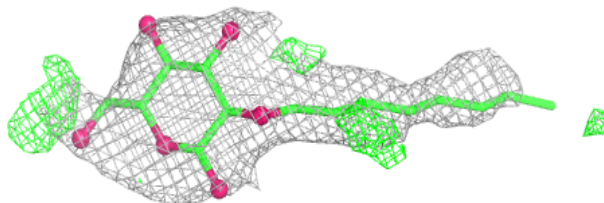
**Electron density around BGL B 1041:**

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

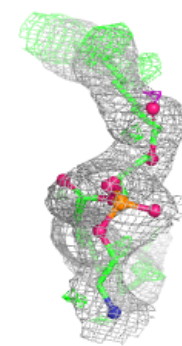
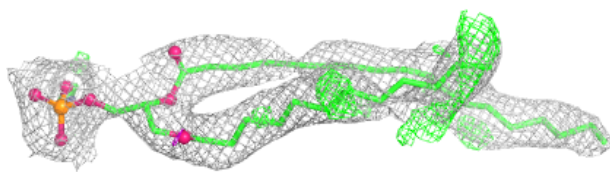
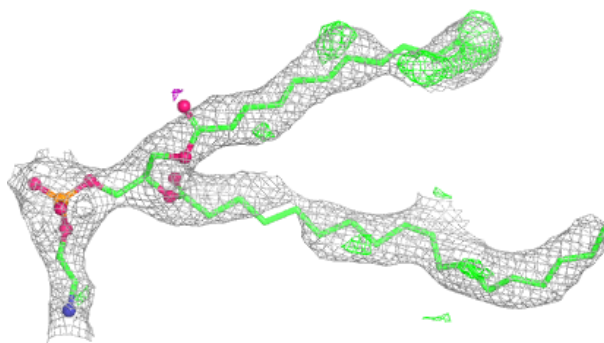


Electron density around BGL K 1044:

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

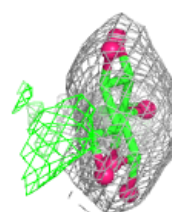
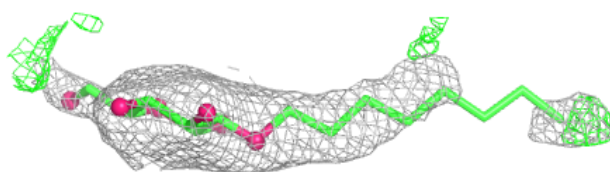
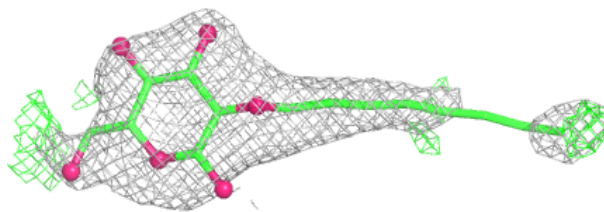
**Electron density around LOP G 1023:**

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

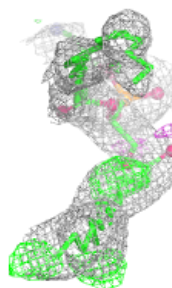
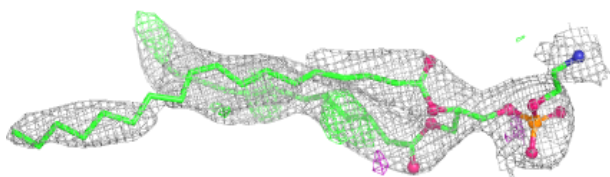
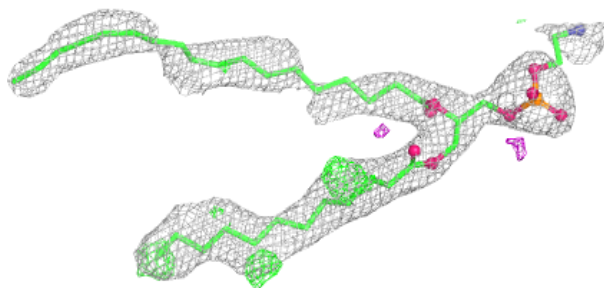


Electron density around BGL P 1046:

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

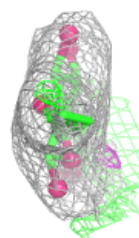
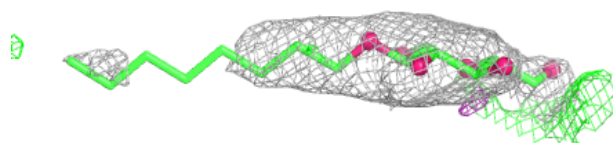
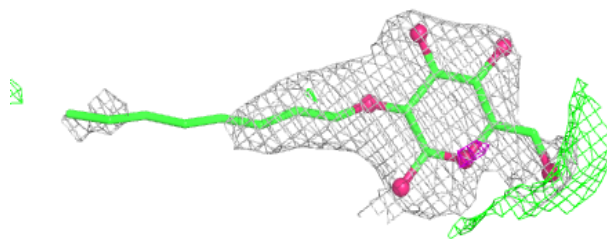
**Electron density around LOP P 1026:**

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

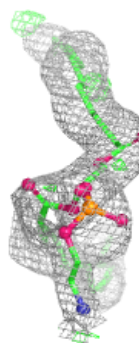
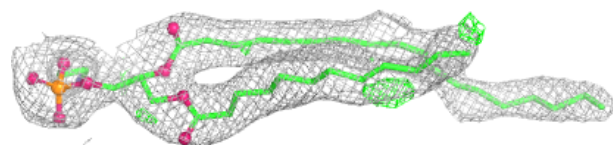
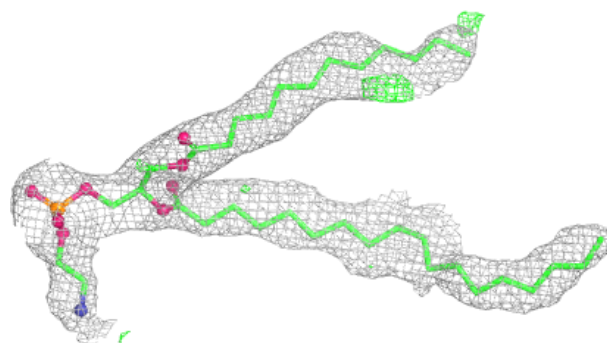


Electron density around BGL G 1043:

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

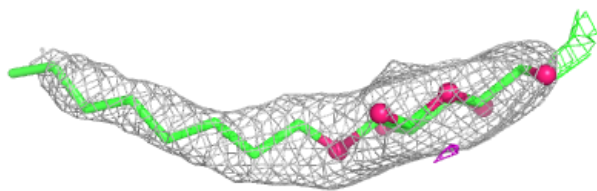
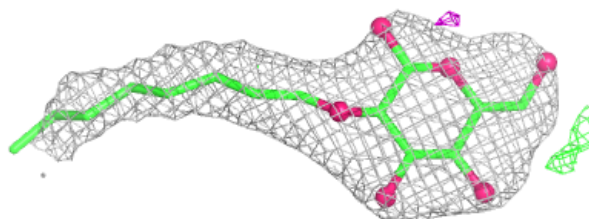
**Electron density around LOP A 1021:**

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

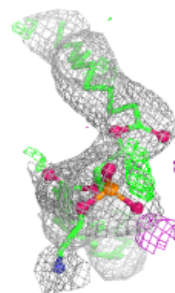
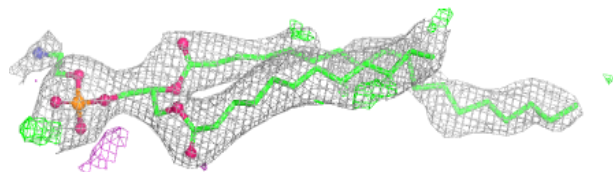
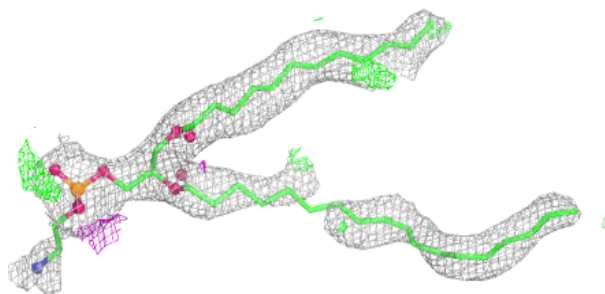


Electron density around BGL E 1042:

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

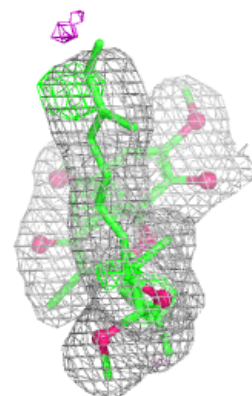
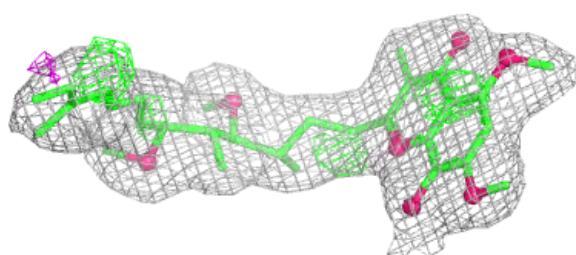
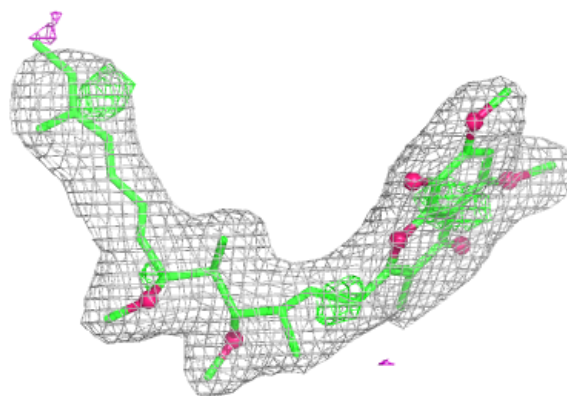
**Electron density around LOP D 1022:**

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

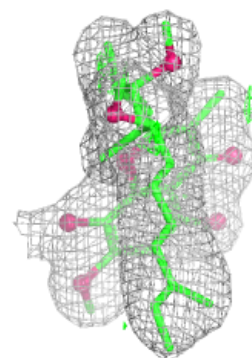
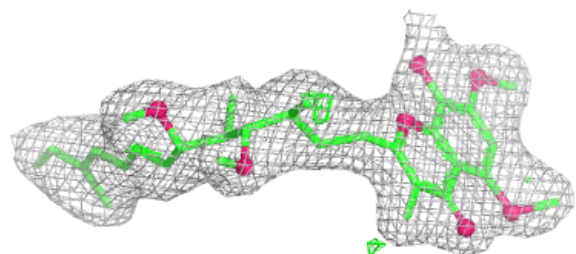
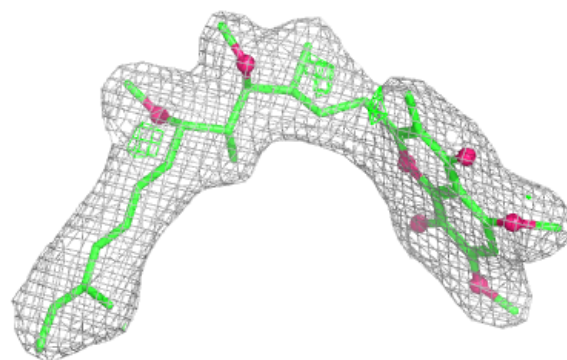


Electron density around SMA D 1002:

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

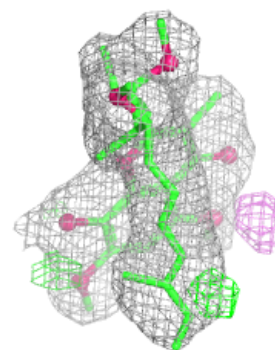
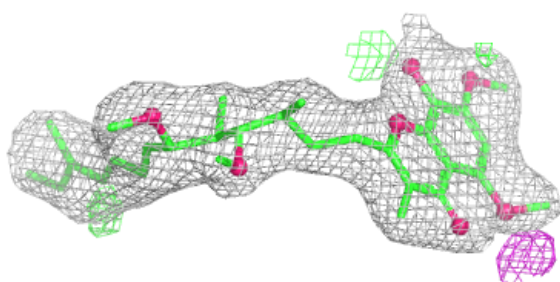
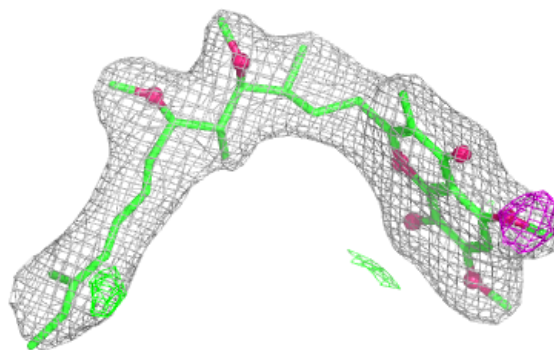
**Electron density around SMA A 1001:**

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

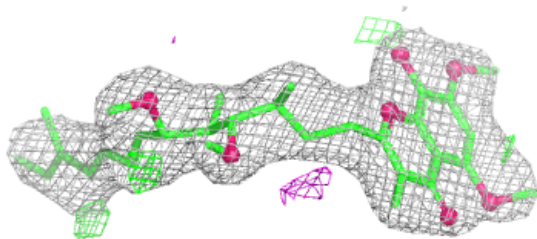
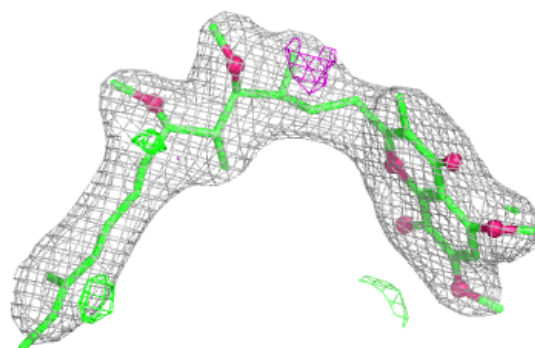


Electron density around SMA G 1003:

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

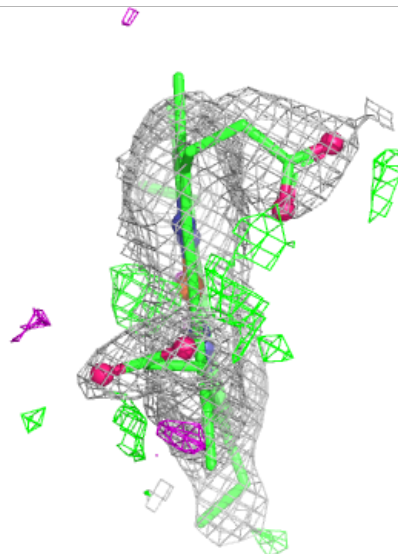
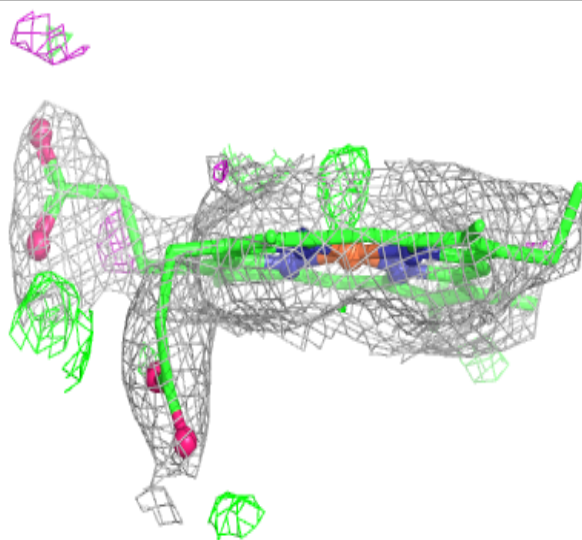
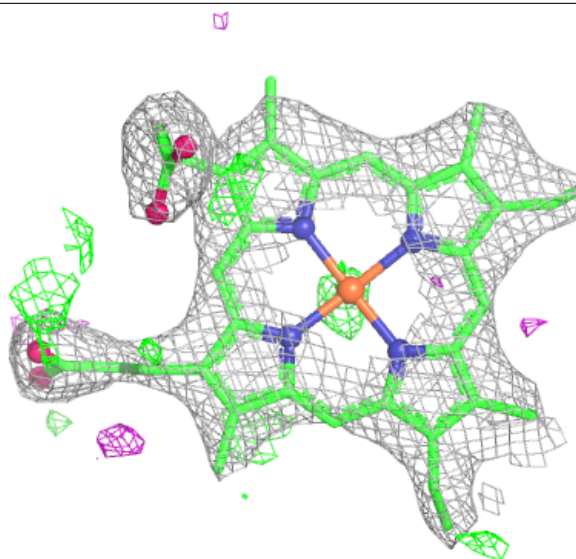
**Electron density around SMA M 1005:**

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



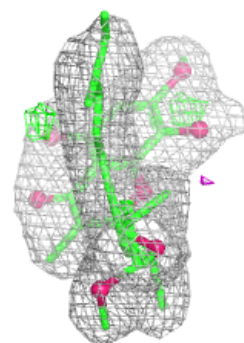
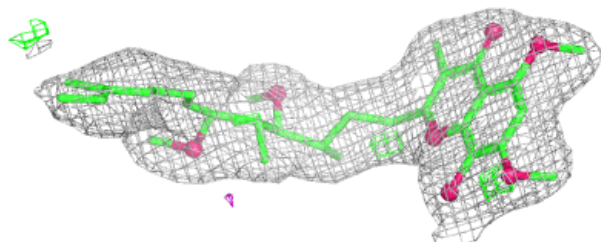
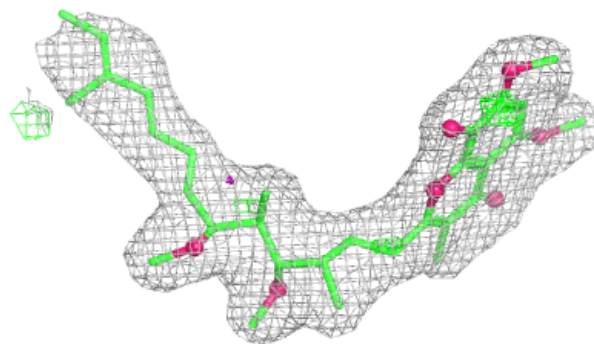
Electron density around HEM J 501:

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

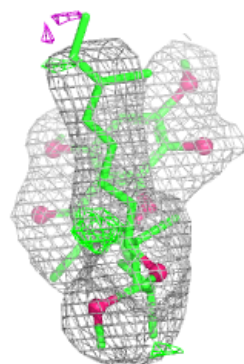
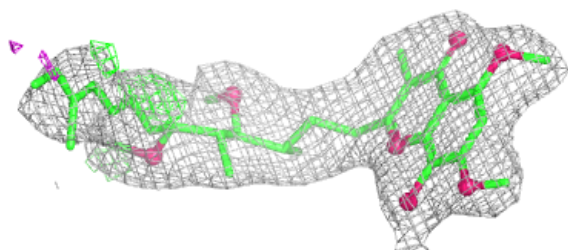
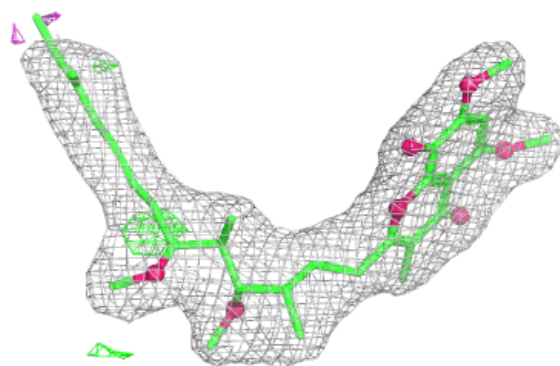


Electron density around SMA P 1006:

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

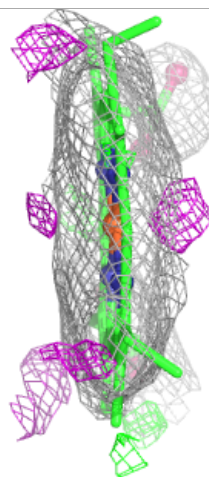
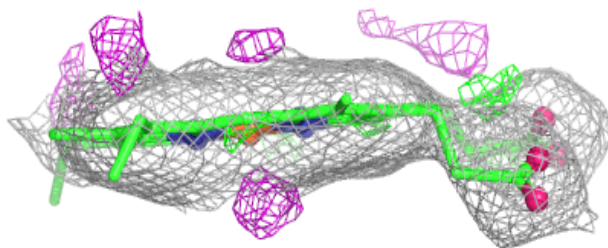
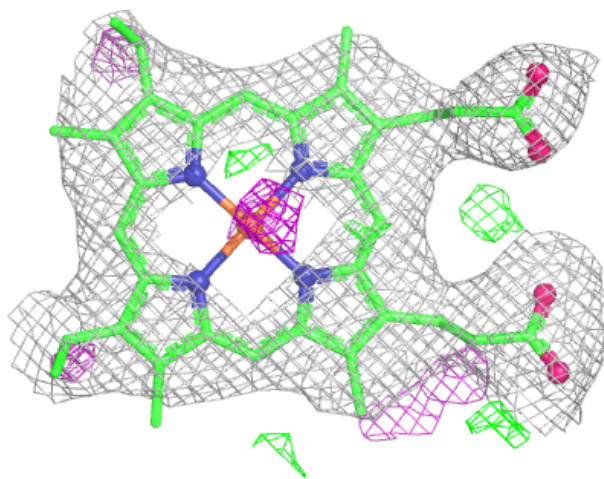
**Electron density around SMA J 1004:**

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



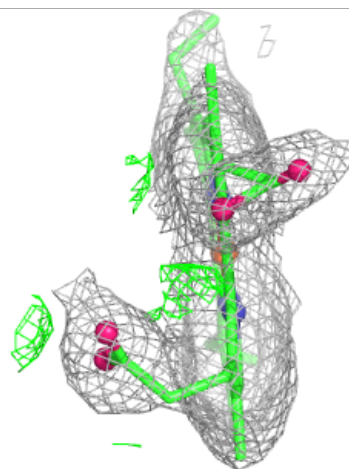
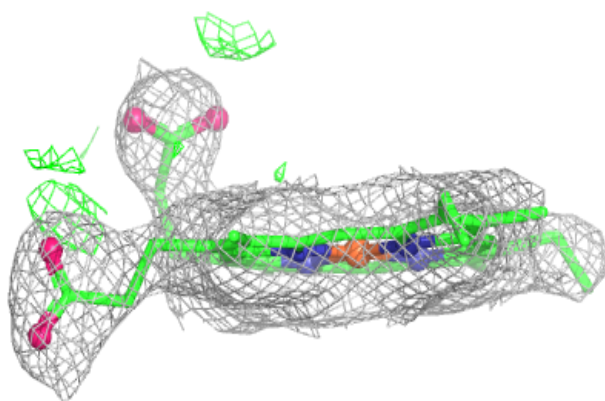
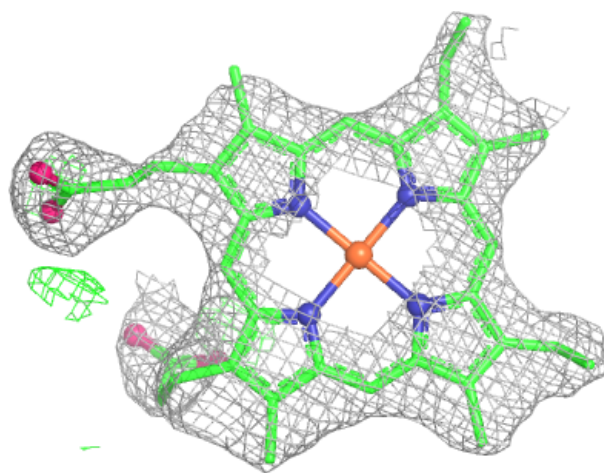
Electron density around HEM N 301:

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



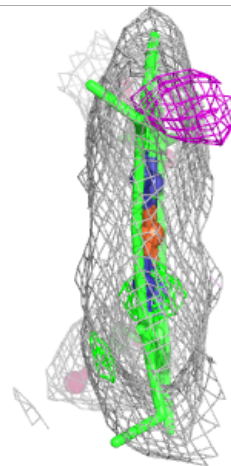
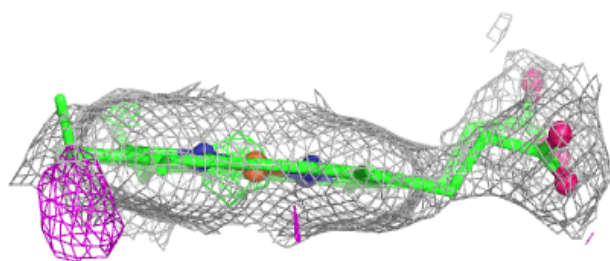
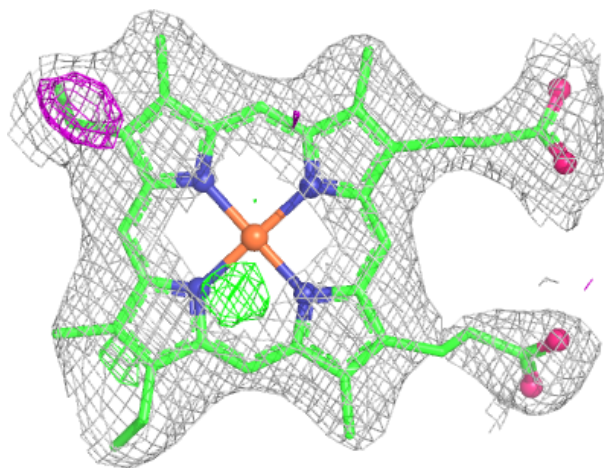
Electron density around HEM M 501:

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



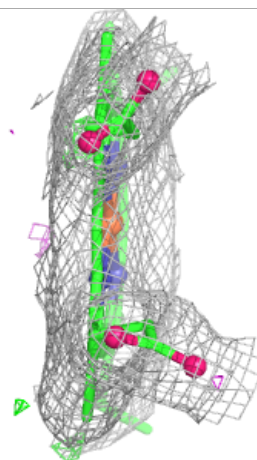
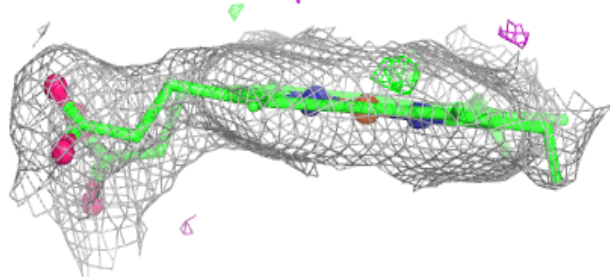
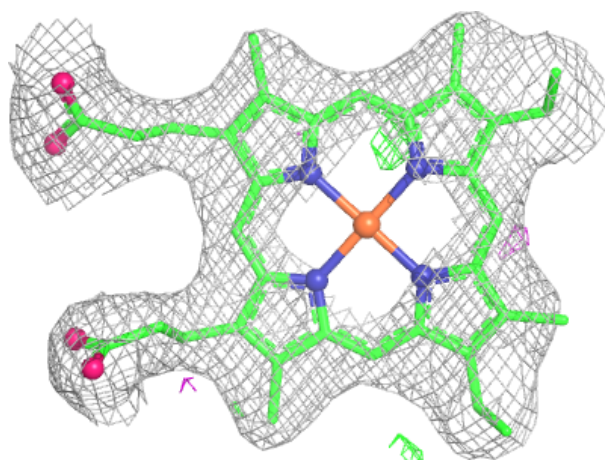
Electron density around HEM E 301:

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



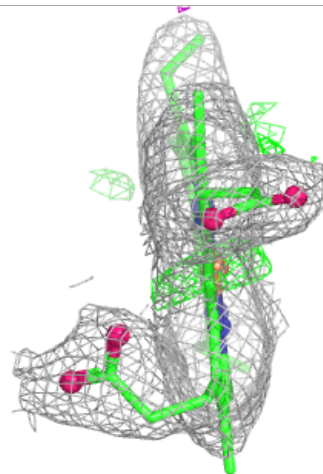
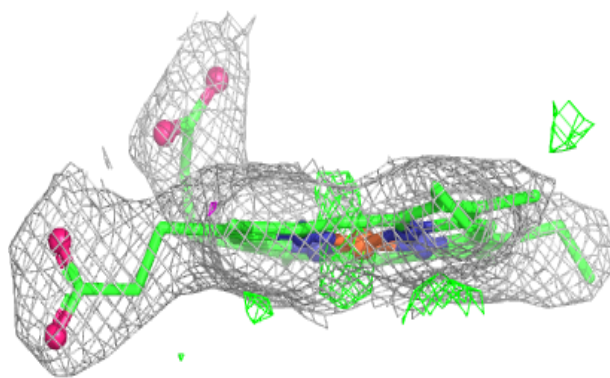
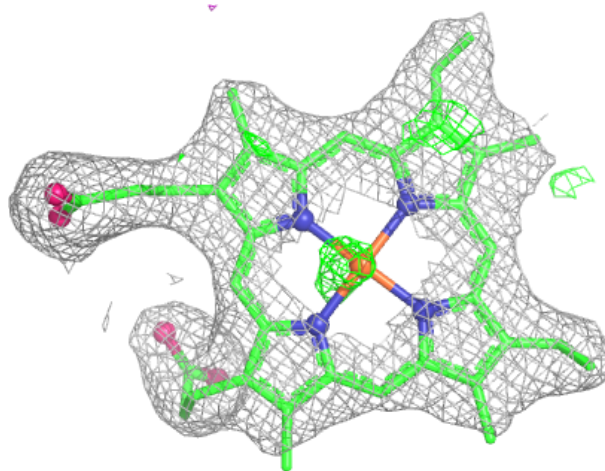
Electron density around HEM Q 301:

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



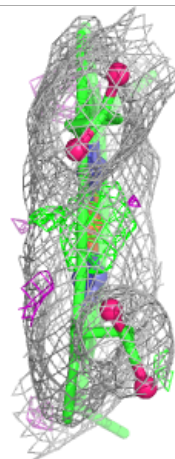
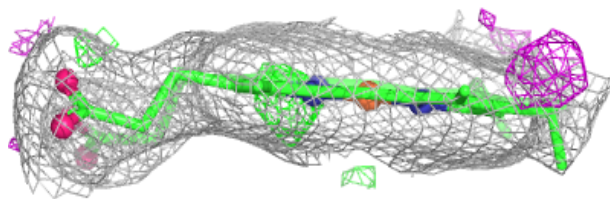
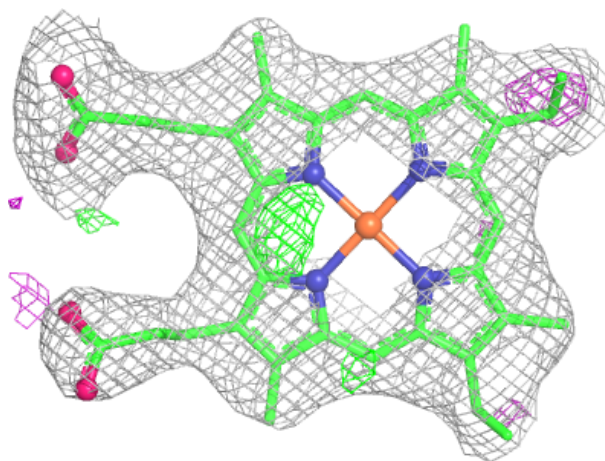
Electron density around HEM G 501:

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



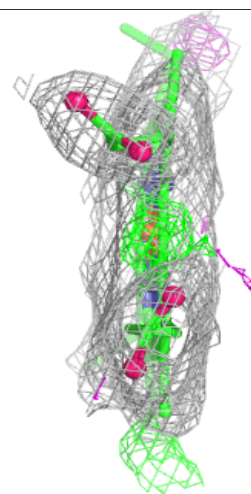
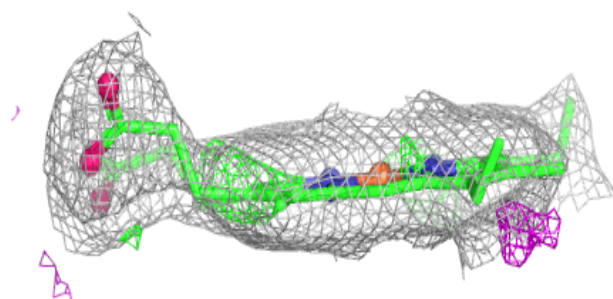
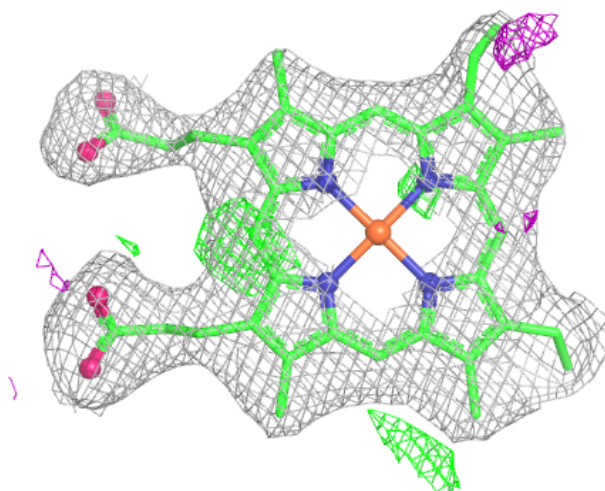
Electron density around HEM B 301:

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



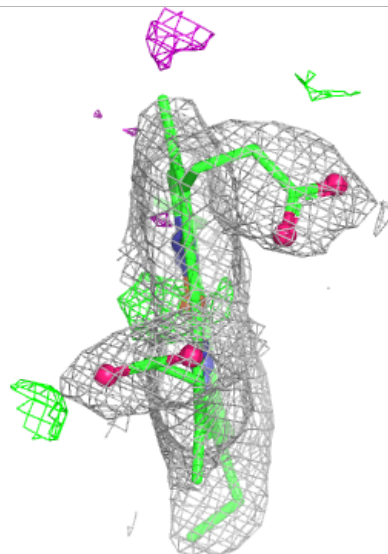
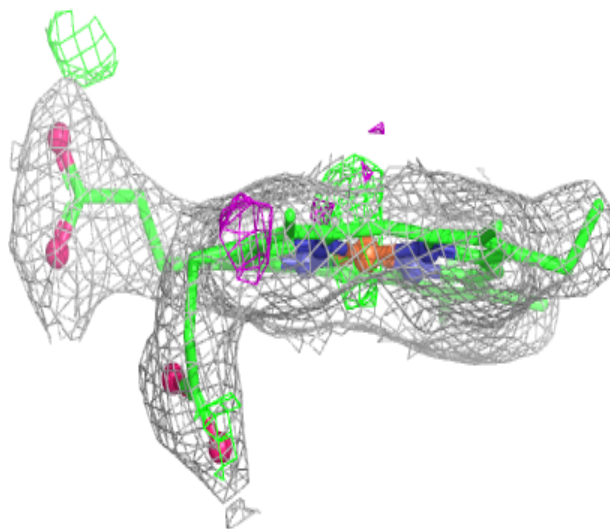
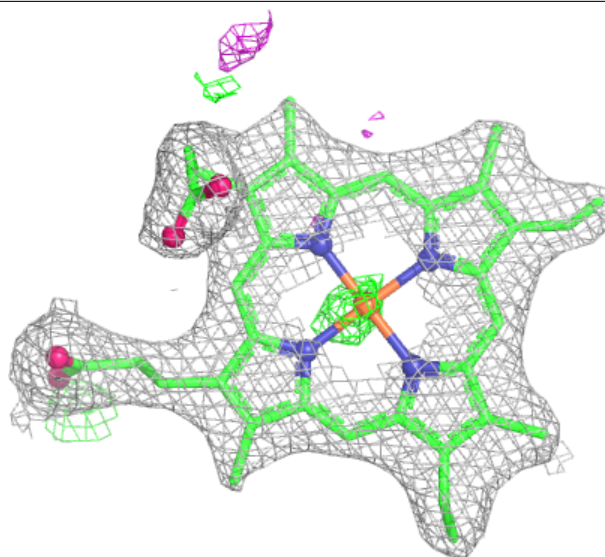
Electron density around HEM K 301:

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



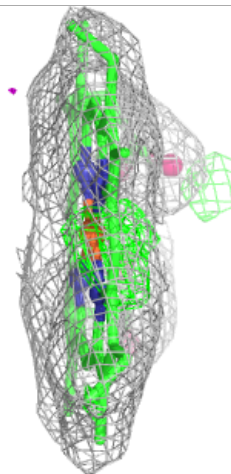
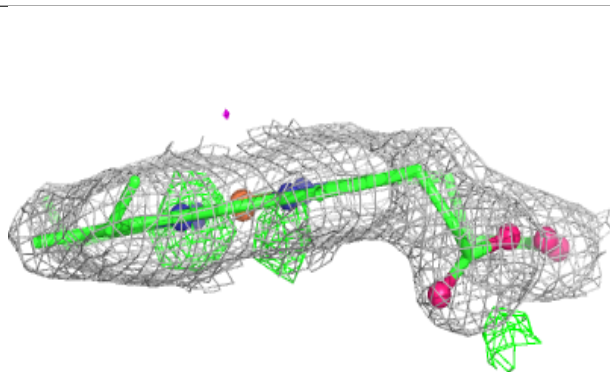
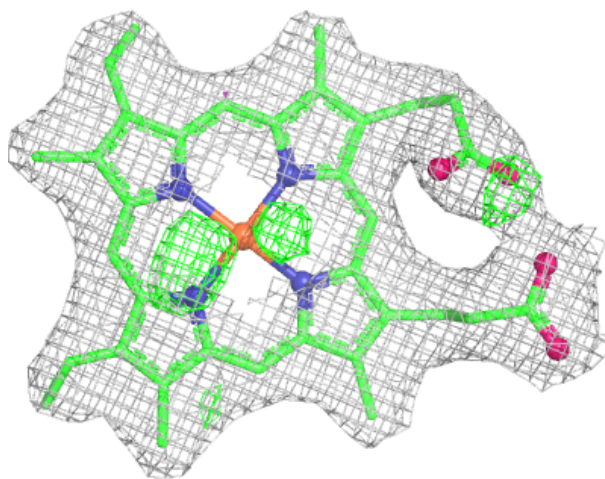
Electron density around HEM P 501:

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



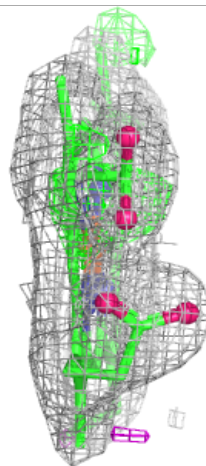
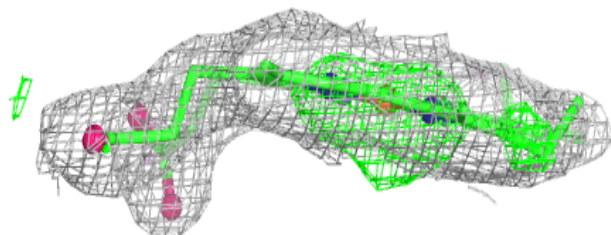
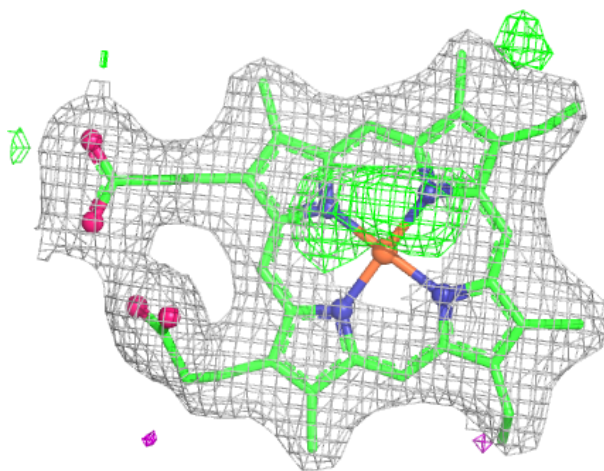
Electron density around HEM P 502:

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



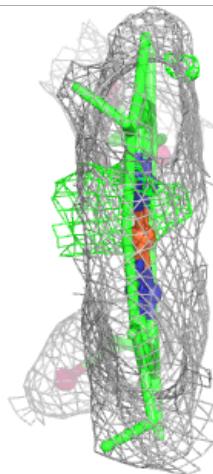
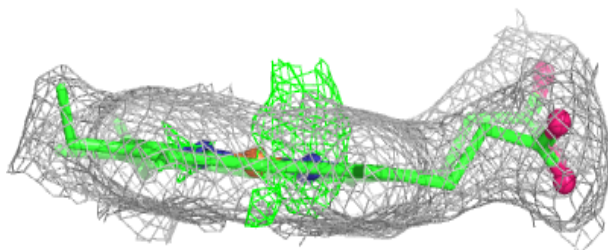
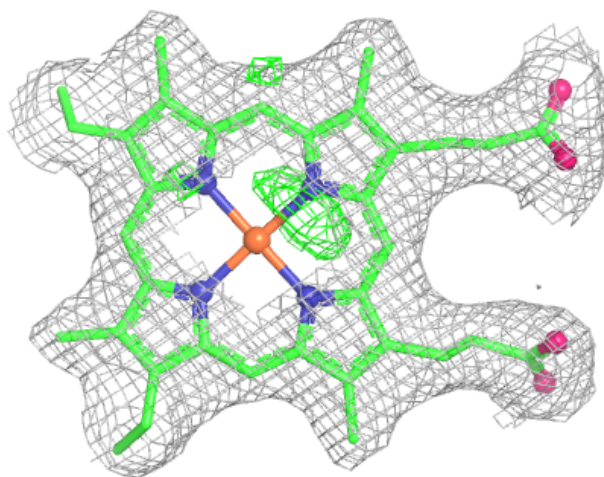
Electron density around HEM G 502:

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



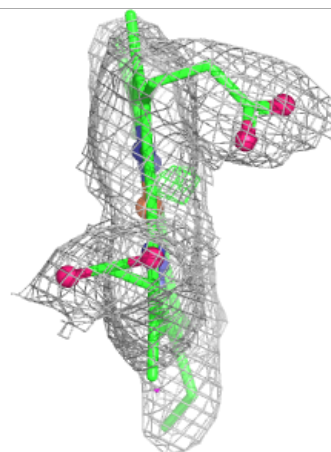
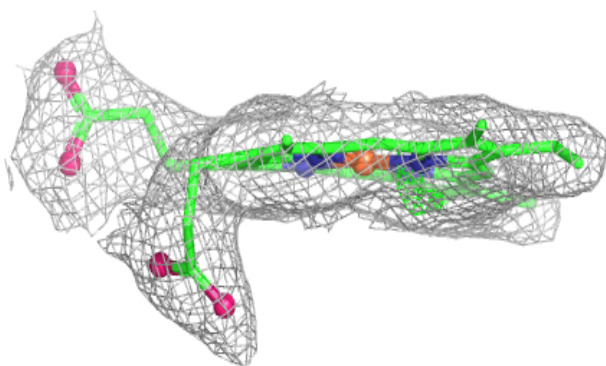
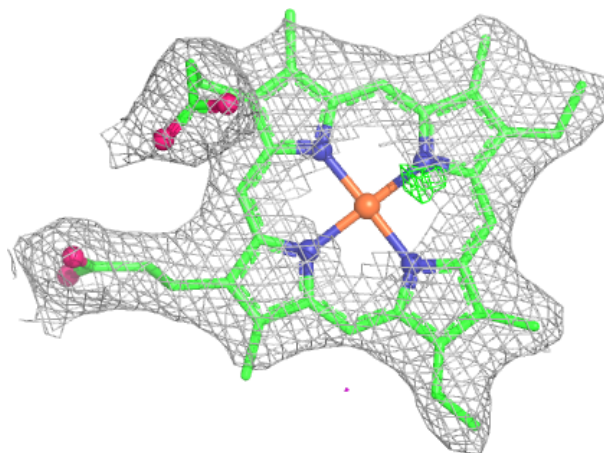
Electron density around HEM H 301:

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



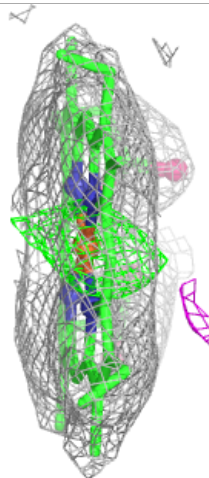
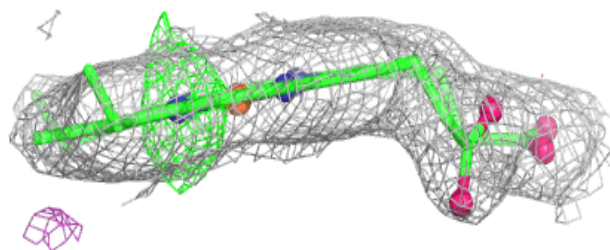
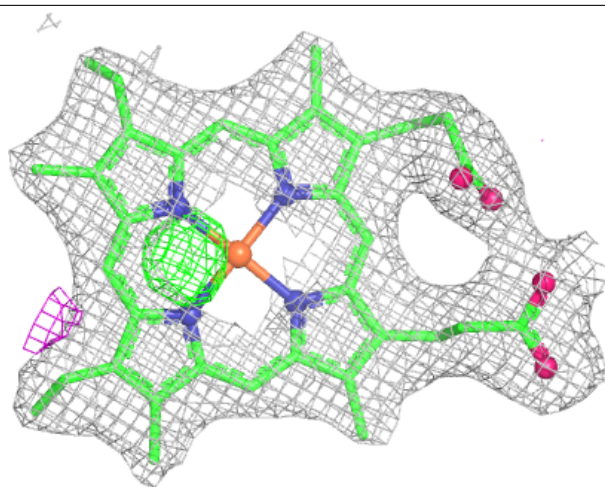
Electron density around HEM D 501:

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



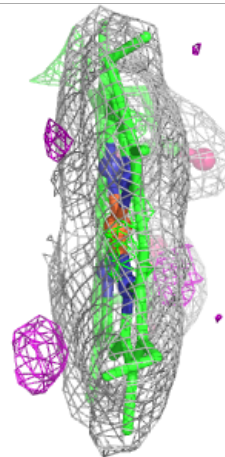
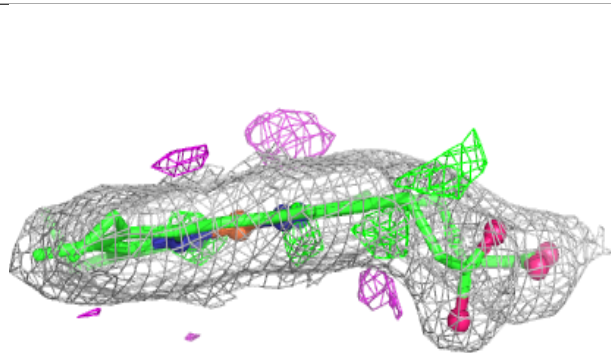
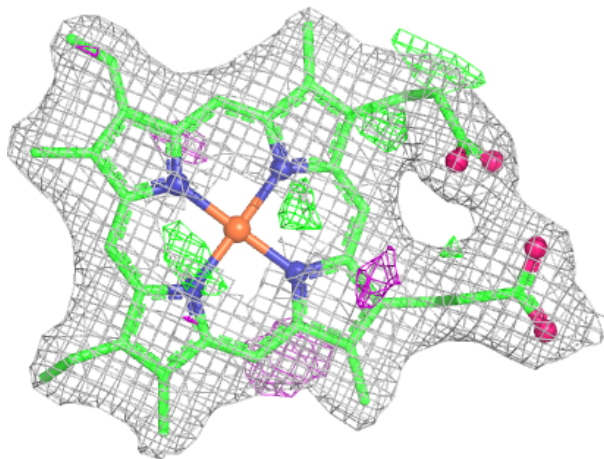
Electron density around HEM J 502:

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



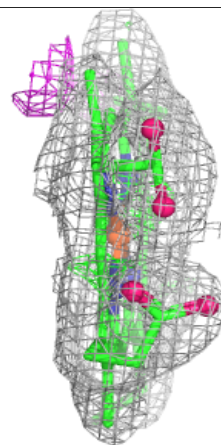
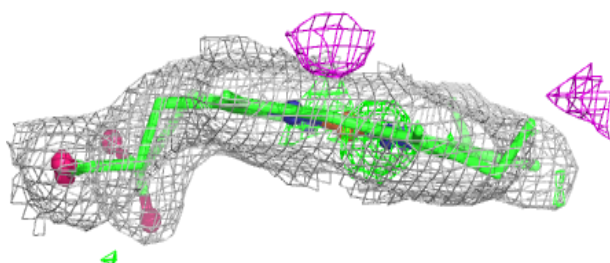
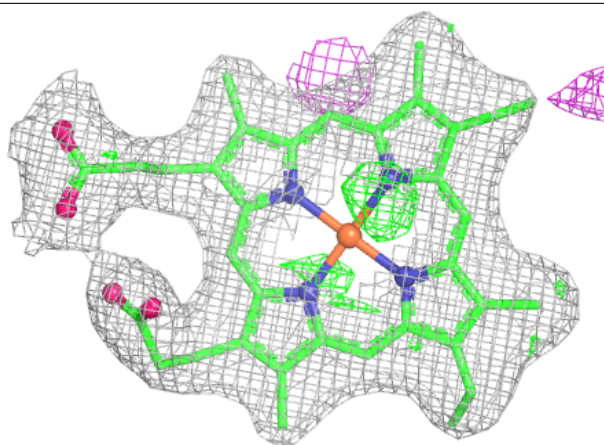
Electron density around HEM D 502:

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



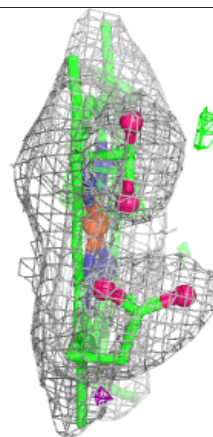
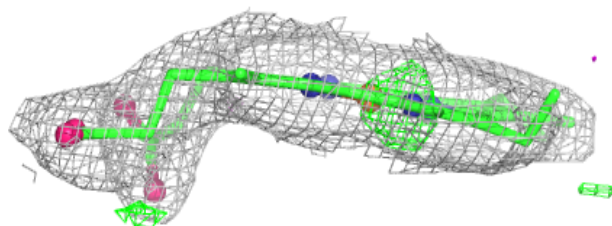
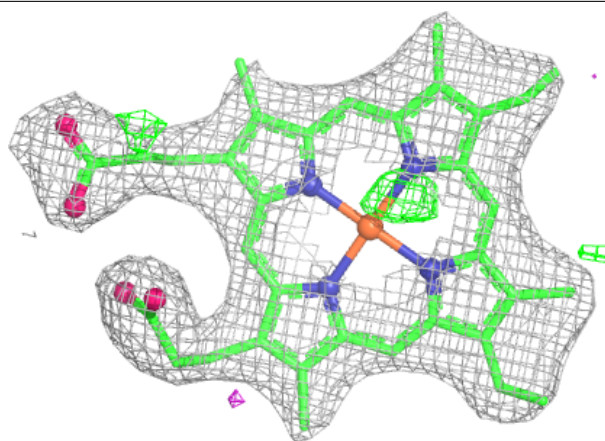
Electron density around HEM A 502:

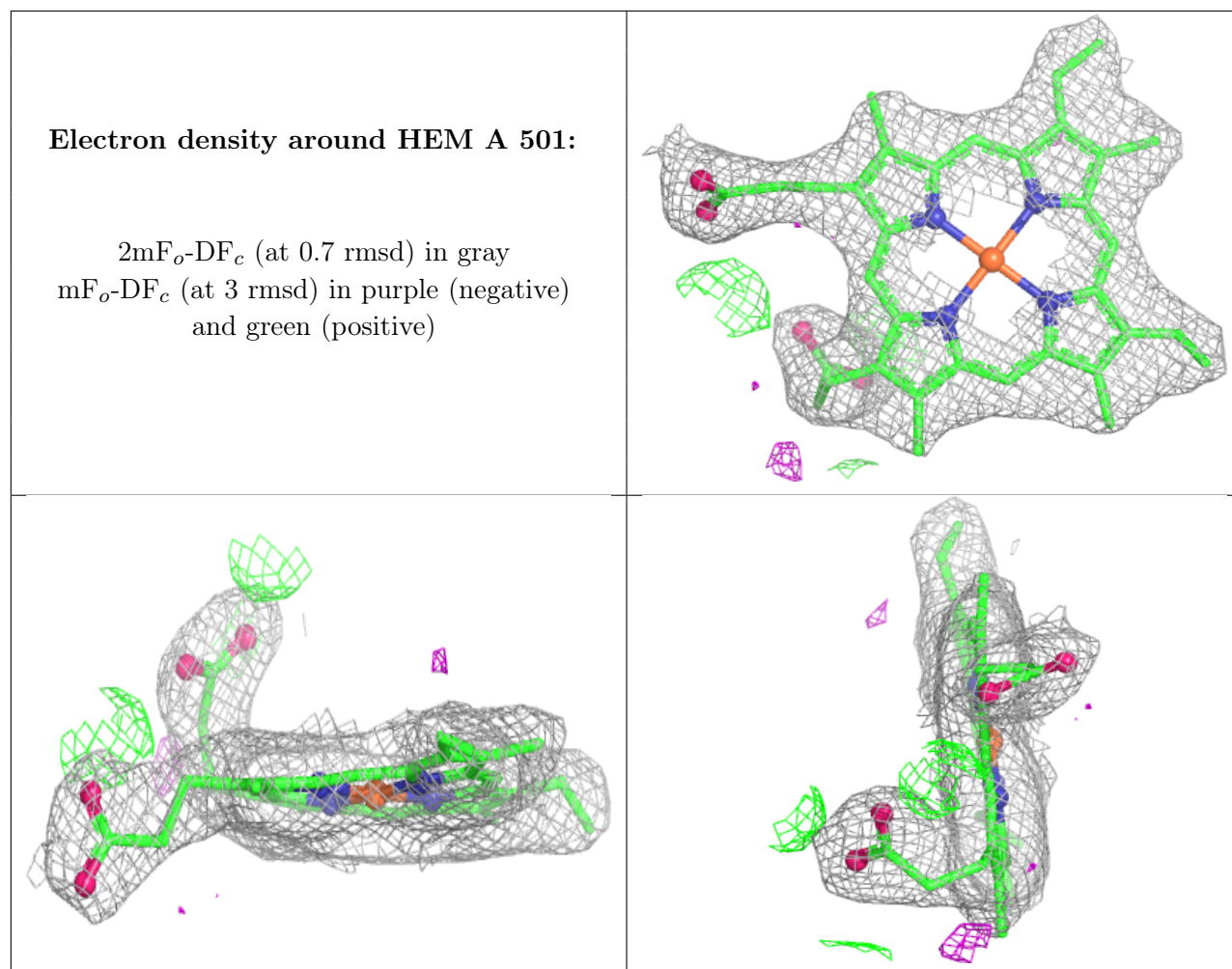
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM M 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.