



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 04:17 AM EDT

PDB ID : 2FYN  
Title : Crystal Structure Analysis of the double mutant Rhodobacter Sphaeroides bc1 complex  
Authors : Esser, L.; Xia, D.  
Deposited on : 2006-02-08  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

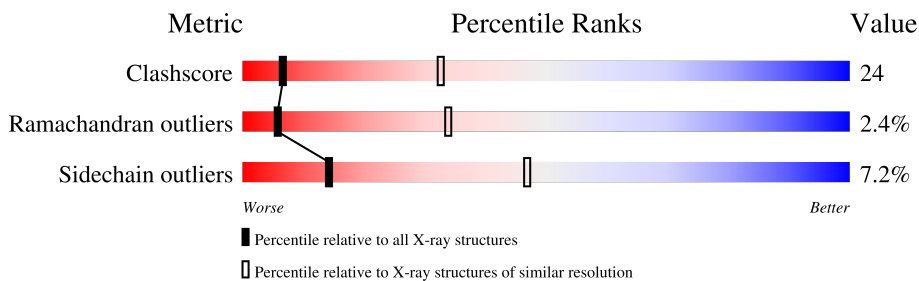
# 1 Overall quality at a glance

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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	59% 34% . .
1	D	445	55% 38% . .
1	G	445	56% 38% . .
1	J	445	53% 39% . .
1	M	445	54% 38% . .
1	P	445	54% 39% . .
2	B	269	59% 31% 5% 5%
2	E	269	52% 37% 6% 5%

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Mol	Chain	Length	Quality of chain		
2	H	269	60%	31%	5%
2	K	269	57%	33%	5% 5%
2	N	269	54%	36%	5% 5%
2	Q	269	49%	40%	6% 5%
3	C	187	61%	28%	6% . .
3	F	187	54%	33%	9% .
3	I	187	52%	37%	7% .
3	L	187	60%	33%	. .
3	O	187	62%	29%	5% .
3	R	187	53%	37%	5% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FES	C	200	-	-	X	-
7	FES	F	200	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 41688 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
			Total	C	N	O	S			
1	A	428	3440	2322	548	555	15	0	0	0
1	D	428	3440	2322	548	555	15	0	0	0
1	G	428	3440	2322	548	555	15	0	0	0
1	J	428	3440	2322	548	555	15	0	0	0
1	M	428	3440	2322	548	555	15	0	0	0
1	P	428	3440	2322	548	555	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02761
A	287	ARG	SER	engineered mutation	UNP Q02761
D	1	MET	-	initiating methionine	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	1	MET	-	initiating methionine	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	1	MET	-	initiating methionine	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	1	MET	-	initiating methionine	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	1	MET	-	initiating methionine	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
			Total	C	N	O	S			
2	B	256	1953	1240	326	374	13	0	0	0
2	E	256	1953	1240	326	374	13	0	0	0
2	H	256	1953	1240	326	374	13	0	0	0
2	K	256	1953	1240	326	374	13	0	0	0
2	N	256	1953	1240	326	374	13	0	0	0
2	Q	256	1953	1240	326	374	13	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	conflict	UNP Q02760
E	98	PRO	ALA	conflict	UNP Q02760
H	98	PRO	ALA	conflict	UNP Q02760
K	98	PRO	ALA	conflict	UNP Q02760
N	98	PRO	ALA	conflict	UNP Q02760
Q	98	PRO	ALA	conflict	UNP Q02760
B	264	HIS	-	expression tag	UNP Q02760
B	265	HIS	-	expression tag	UNP Q02760
B	266	HIS	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	insertion	UNP Q02760
B	269	HIS	-	insertion	UNP Q02760
E	264	HIS	-	insertion	UNP Q02760
E	265	HIS	-	insertion	UNP Q02760
E	266	HIS	-	insertion	UNP Q02760
E	267	HIS	-	insertion	UNP Q02760
E	268	HIS	-	insertion	UNP Q02760
E	269	HIS	-	insertion	UNP Q02760
H	264	HIS	-	insertion	UNP Q02760
H	265	HIS	-	insertion	UNP Q02760
H	266	HIS	-	insertion	UNP Q02760
H	267	HIS	-	insertion	UNP Q02760
H	268	HIS	-	insertion	UNP Q02760
H	269	HIS	-	insertion	UNP Q02760
K	264	HIS	-	insertion	UNP Q02760
K	265	HIS	-	insertion	UNP Q02760
K	266	HIS	-	insertion	UNP Q02760
K	267	HIS	-	insertion	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
K	268	HIS	-	insertion	UNP Q02760
K	269	HIS	-	insertion	UNP Q02760
N	264	HIS	-	insertion	UNP Q02760
N	265	HIS	-	insertion	UNP Q02760
N	266	HIS	-	insertion	UNP Q02760
N	267	HIS	-	insertion	UNP Q02760
N	268	HIS	-	insertion	UNP Q02760
N	269	HIS	-	insertion	UNP Q02760
Q	264	HIS	-	insertion	UNP Q02760
Q	265	HIS	-	insertion	UNP Q02760
Q	266	HIS	-	insertion	UNP Q02760
Q	267	HIS	-	insertion	UNP Q02760
Q	268	HIS	-	insertion	UNP Q02760
Q	269	HIS	-	insertion	UNP Q02760

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

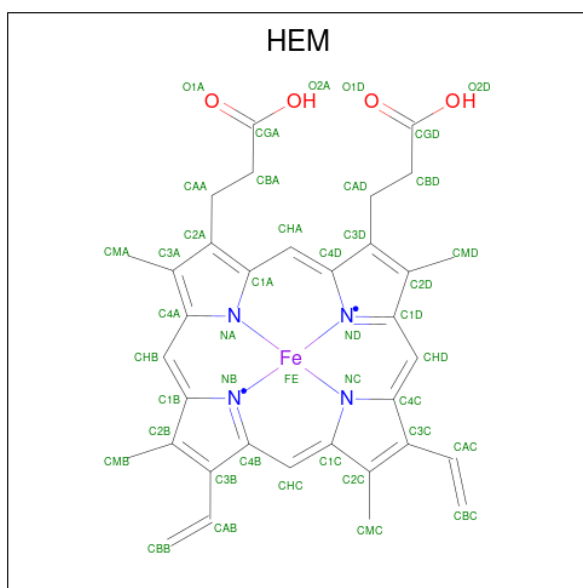
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	179	1340	843	237	254	6	0	0	0
3	F	179	1340	843	237	254	6	0	0	0
3	I	179	1340	843	237	254	6	0	0	0
3	L	179	1340	843	237	254	6	0	0	0
3	O	179	1340	843	237	254	6	0	0	0
3	R	179	1340	843	237	254	6	0	0	0

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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



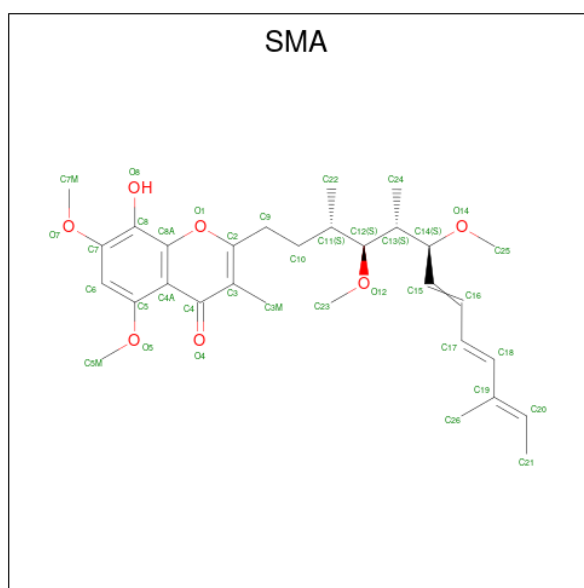
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

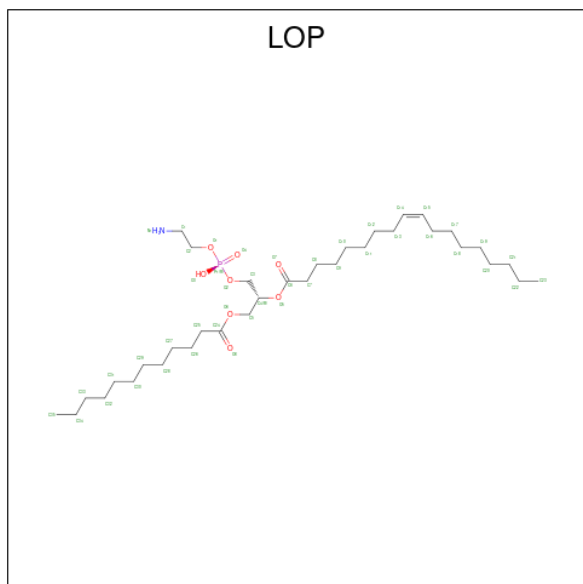
- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



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

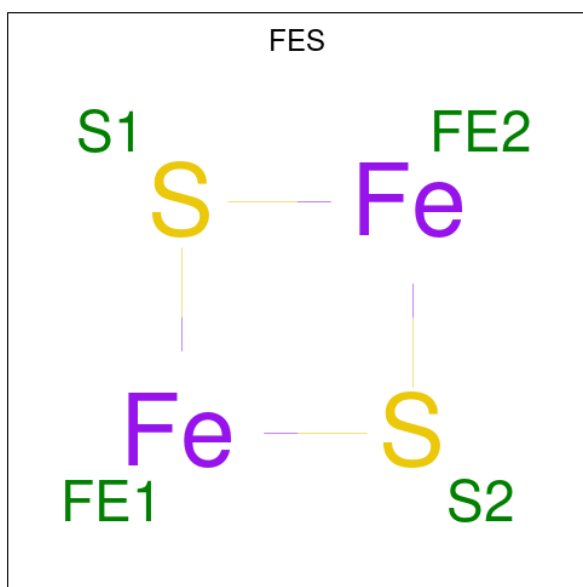


- Molecule 6 is (1R)-2-[[[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

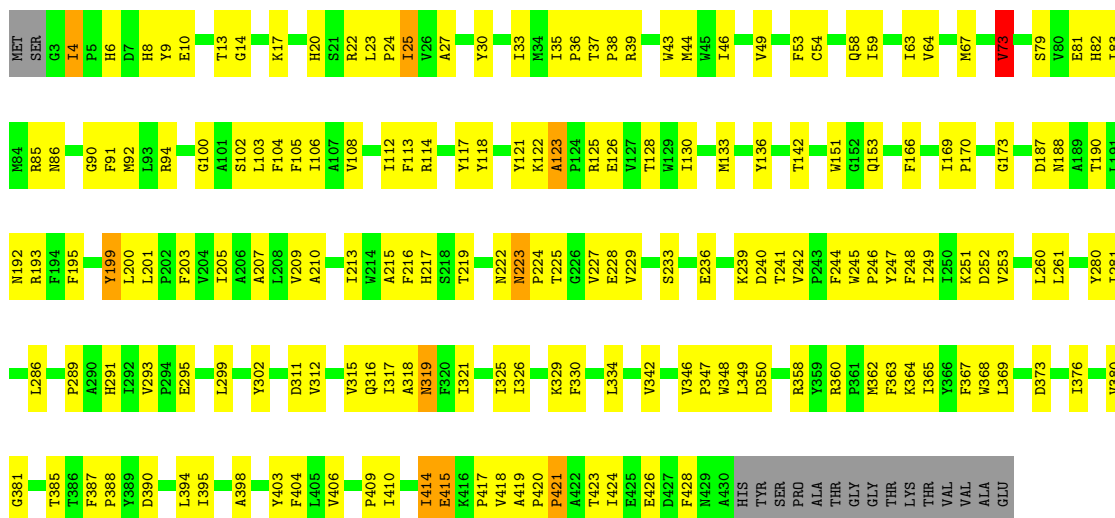


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		
7	I	1	Total	Fe	S	0	0
			4	2	2		
7	L	1	Total	Fe	S	0	0
			4	2	2		
7	O	1	Total	Fe	S	0	0
			4	2	2		
7	R	1	Total	Fe	S	0	0
			4	2	2		

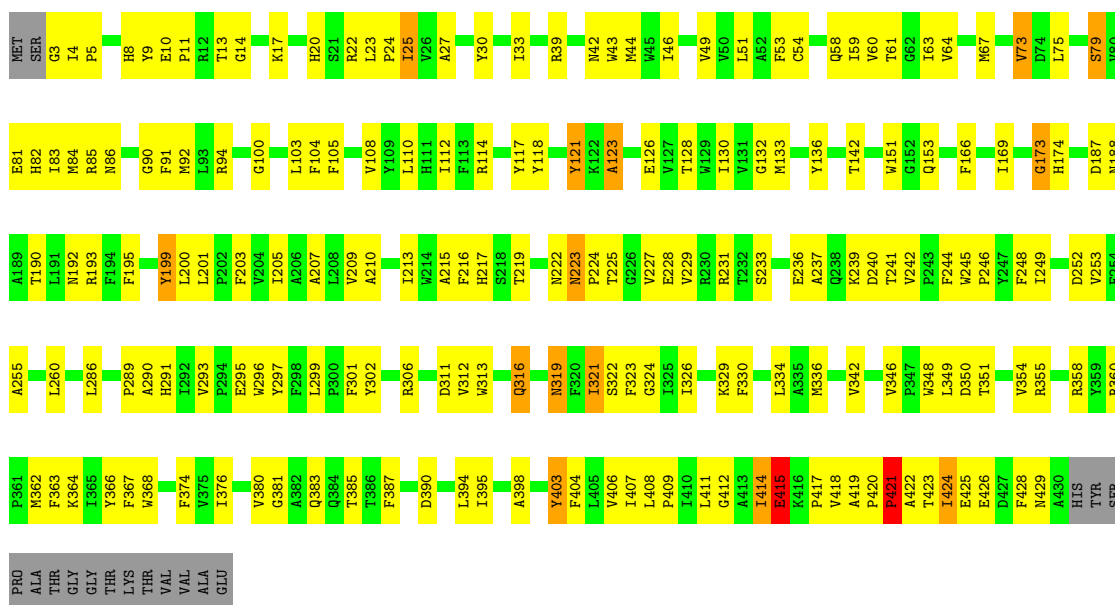




• Molecule 1: Cytochrome b

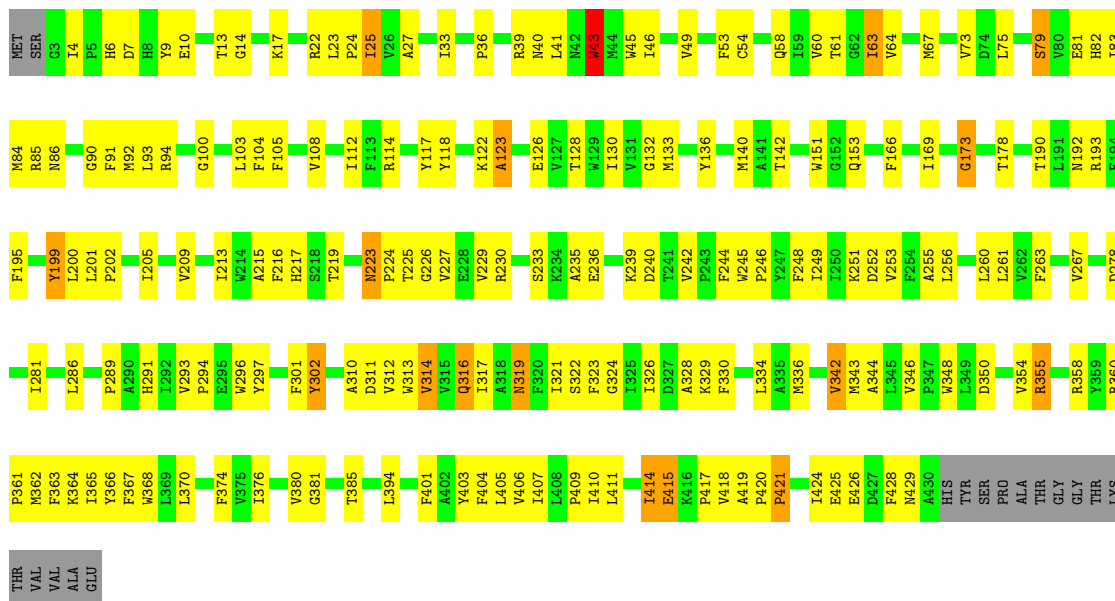


• Molecule 1: Cytochrome b

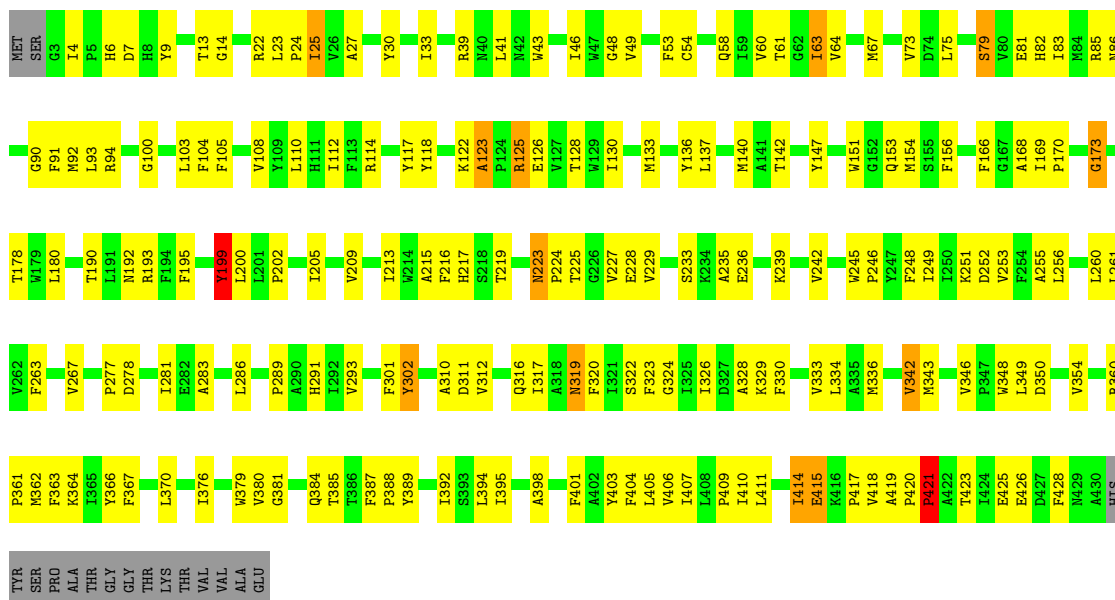


• Molecule 1: Cytochrome b

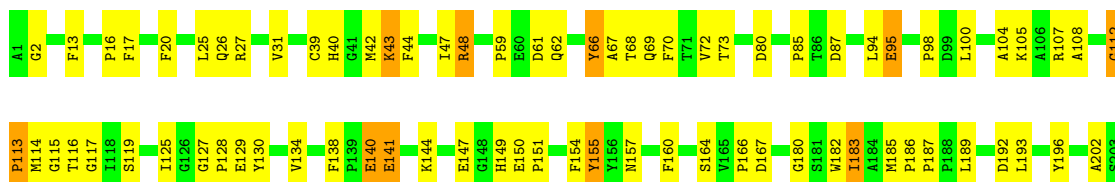




• Molecule 1: Cytochrome b



• Molecule 2: Cytochrome c1



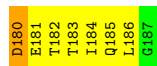
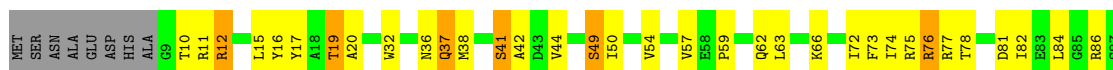






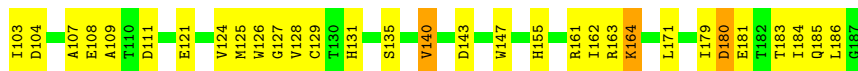
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain I: 52% 37% 7%



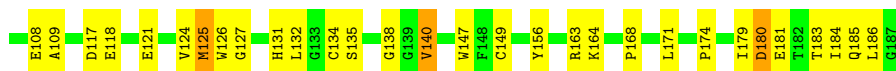
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain L: 60% 33%



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

Chain O: 62% 29% 5%



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

Chain R: 53% 37% 5%





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	351.30Å 147.13Å 160.83Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	18.00 – 3.20	Depositor
% Data completeness (in resolution range)	95.2 (18.00-3.20)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	41688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.65	5/3570 (0.1%)	0.73	0/4897
1	D	0.63	0/3570	0.75	0/4897
1	G	0.66	0/3570	0.76	0/4897
1	J	0.65	2/3570 (0.1%)	0.74	0/4897
1	M	0.60	0/3570	0.72	0/4897
1	P	0.59	0/3570	0.73	0/4897
2	B	0.54	0/2010	0.73	0/2733
2	E	0.59	2/2010 (0.1%)	0.76	1/2733 (0.0%)
2	H	0.67	2/2010 (0.1%)	0.78	3/2733 (0.1%)
2	K	0.58	0/2010	0.74	0/2733
2	N	0.56	0/2010	0.73	0/2733
2	Q	0.57	0/2010	0.78	1/2733 (0.0%)
3	C	0.66	0/1370	0.83	1/1866 (0.1%)
3	F	0.64	0/1370	0.84	1/1866 (0.1%)
3	I	0.65	0/1370	0.89	2/1866 (0.1%)
3	L	0.66	0/1370	0.81	0/1866
3	O	0.60	0/1370	0.83	1/1866 (0.1%)
3	R	0.61	0/1370	0.83	2/1866 (0.1%)
All	All	0.62	11/41700 (0.0%)	0.76	12/56976 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
1	P	0	2
2	E	0	1
2	N	0	1
2	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	14	GLU	CG-CD	10.19	1.67	1.51
2	H	14	GLU	CB-CG	9.76	1.70	1.52
1	A	121	TYR	CE2-CZ	-7.38	1.28	1.38
1	A	121	TYR	CE1-CZ	-7.18	1.29	1.38
1	J	121	TYR	CE1-CZ	-6.93	1.29	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	145	CYS	CA-CB-SG	9.36	130.84	114.00
2	H	14	GLU	OE1-CD-OE2	-7.65	114.12	123.30
2	H	145	CYS	CA-CB-SG	-5.81	103.54	114.00
2	H	183	ILE	CB-CA-C	-5.64	100.32	111.60
3	C	76	ARG	N-CA-C	-5.30	96.69	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	32	TYR	Sidechain
1	M	302	TYR	Sidechain
2	N	32	TYR	Sidechain
1	P	199	TYR	Sidechain
1	P	302	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3428	170	0
1	D	3440	0	3428	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3440	0	3428	183	0
1	J	3440	0	3428	185	0
1	M	3440	0	3428	189	0
1	P	3440	0	3428	175	0
2	B	1953	0	1848	92	0
2	E	1953	0	1848	107	0
2	H	1953	0	1848	102	0
2	K	1953	0	1848	103	0
2	N	1953	0	1848	109	0
2	Q	1953	0	1848	127	0
3	C	1340	0	1303	59	0
3	F	1340	0	1303	74	0
3	I	1340	0	1303	67	0
3	L	1340	0	1303	51	0
3	O	1340	0	1303	54	0
3	R	1340	0	1303	72	0
4	A	86	0	60	7	0
4	B	43	0	30	0	0
4	D	86	0	60	12	0
4	E	43	0	30	1	0
4	G	86	0	60	10	0
4	H	43	0	30	2	0
4	J	86	0	60	17	0
4	K	43	0	30	1	0
4	M	86	0	60	13	0
4	N	43	0	30	2	0
4	P	86	0	60	11	0
4	Q	43	0	30	1	0
5	A	37	0	42	2	0
5	D	37	0	42	1	0
5	G	37	0	42	1	0
5	J	37	0	42	1	0
5	M	37	0	42	2	0
5	P	37	0	42	0	0
6	A	45	0	67	3	0
6	D	45	0	67	1	0
6	G	45	0	67	5	0
6	J	45	0	67	1	0
6	M	45	0	67	3	0
6	P	45	0	67	1	0
7	C	4	0	0	2	0
7	F	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	4	0	0	0	0
7	L	4	0	0	0	0
7	O	4	0	0	1	0
7	R	4	0	0	1	0
All	All	41688	0	40668	1946	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 24.

The worst 5 of 1946 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:157:ASN:HB2	2:Q:183:ILE:HD11	1.30	1.14
2:B:183:ILE:HG23	2:B:185:MET:H	1.12	1.09
1:G:33:ILE:HD11	1:G:249:ILE:HD11	1.32	1.09
1:J:33:ILE:HD11	1:J:249:ILE:HD11	1.31	1.06
1:P:33:ILE:HD11	1:P:249:ILE:HD11	1.37	1.06

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%)	392 (92%)	28 (7%)	6 (1%)	11	46
1	D	426/445 (96%)	385 (90%)	37 (9%)	4 (1%)	17	56
1	G	426/445 (96%)	384 (90%)	34 (8%)	8 (2%)	8	39
1	J	426/445 (96%)	379 (89%)	37 (9%)	10 (2%)	6	34
1	M	426/445 (96%)	380 (89%)	38 (9%)	8 (2%)	8	39
1	P	426/445 (96%)	380 (89%)	39 (9%)	7 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	254/269 (94%)	224 (88%)	23 (9%)	7 (3%)	5	29
2	E	254/269 (94%)	218 (86%)	28 (11%)	8 (3%)	4	26
2	H	254/269 (94%)	220 (87%)	29 (11%)	5 (2%)	7	38
2	K	254/269 (94%)	225 (89%)	21 (8%)	8 (3%)	4	26
2	N	254/269 (94%)	219 (86%)	26 (10%)	9 (4%)	3	24
2	Q	254/269 (94%)	215 (85%)	30 (12%)	9 (4%)	3	24
3	C	177/187 (95%)	153 (86%)	20 (11%)	4 (2%)	6	34
3	F	177/187 (95%)	153 (86%)	18 (10%)	6 (3%)	3	24
3	I	177/187 (95%)	151 (85%)	19 (11%)	7 (4%)	3	21
3	L	177/187 (95%)	151 (85%)	21 (12%)	5 (3%)	5	29
3	O	177/187 (95%)	154 (87%)	19 (11%)	4 (2%)	6	34
3	R	177/187 (95%)	149 (84%)	21 (12%)	7 (4%)	3	21
All	All	5142/5406 (95%)	4532 (88%)	488 (10%)	122 (2%)	6	34

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
2	B	43	LYS
3	C	109	ALA
1	D	414	ILE
1	D	415	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/366 (96%)	332 (94%)	21 (6%)	19	54
1	D	353/366 (96%)	331 (94%)	22 (6%)	18	53
1	G	353/366 (96%)	332 (94%)	21 (6%)	19	54
1	J	353/366 (96%)	329 (93%)	24 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	353/366 (96%)	330 (94%)	23 (6%)	17	51
1	P	353/366 (96%)	330 (94%)	23 (6%)	17	51
2	B	203/215 (94%)	191 (94%)	12 (6%)	19	54
2	E	203/215 (94%)	187 (92%)	16 (8%)	12	43
2	H	203/215 (94%)	192 (95%)	11 (5%)	22	58
2	K	203/215 (94%)	190 (94%)	13 (6%)	17	52
2	N	203/215 (94%)	189 (93%)	14 (7%)	15	49
2	Q	203/215 (94%)	190 (94%)	13 (6%)	17	52
3	C	138/144 (96%)	122 (88%)	16 (12%)	5	24
3	F	138/144 (96%)	118 (86%)	20 (14%)	3	15
3	I	138/144 (96%)	126 (91%)	12 (9%)	10	37
3	L	138/144 (96%)	127 (92%)	11 (8%)	12	42
3	O	138/144 (96%)	126 (91%)	12 (9%)	10	37
3	R	138/144 (96%)	123 (89%)	15 (11%)	6	26
All	All	4164/4350 (96%)	3865 (93%)	299 (7%)	14	47

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	152	ASP
3	R	12	ARG
3	O	12	ARG
1	P	223	ASN
3	F	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	177	GLN
3	O	113	ASN
1	M	222	ASN
2	N	62	GLN
1	P	222	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HEM	A	501	1	41,50,50	1.48	5 (12%)	45,82,82	1.13	3 (6%)
4	HEM	P	502	1	41,50,50	1.76	7 (17%)	45,82,82	1.20	2 (4%)
4	HEM	J	502	1	41,50,50	1.87	7 (17%)	45,82,82	1.17	3 (6%)
4	HEM	A	502	1	41,50,50	1.88	9 (21%)	45,82,82	1.34	6 (13%)
4	HEM	B	301	2	41,50,50	1.51	4 (9%)	45,82,82	1.12	1 (2%)
4	HEM	M	502	1	41,50,50	1.72	7 (17%)	45,82,82	1.19	3 (6%)
4	HEM	J	501	1	41,50,50	1.51	6 (14%)	45,82,82	1.06	2 (4%)
7	FES	C	200	3	0,4,4	-	-	-	-	-
7	FES	I	200	3	0,4,4	-	-	-	-	-
7	FES	F	200	3	0,4,4	-	-	-	-	-
4	HEM	E	301	2	41,50,50	1.59	5 (12%)	45,82,82	1.10	2 (4%)
6	LOP	D	504	-	44,44,44	0.71	0	47,49,49	1.38	5 (10%)
4	HEM	Q	301	2	41,50,50	1.53	4 (9%)	45,82,82	1.11	1 (2%)
6	LOP	J	504	-	44,44,44	0.65	0	47,49,49	1.31	4 (8%)
6	LOP	P	504	-	44,44,44	0.65	1 (2%)	47,49,49	1.34	6 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LOP	A	504	-	44,44,44	0.64	0	47,49,49	1.33	7 (14%)
4	HEM	G	501	1	41,50,50	1.46	5 (12%)	45,82,82	1.04	2 (4%)
5	SMA	G	503	-	38,38,38	1.96	9 (23%)	48,52,52	2.15	10 (20%)
4	HEM	H	301	2	41,50,50	1.54	4 (9%)	45,82,82	1.11	1 (2%)
4	HEM	D	501	1	41,50,50	1.53	5 (12%)	45,82,82	1.01	2 (4%)
5	SMA	J	503	-	38,38,38	1.93	6 (15%)	48,52,52	2.09	10 (20%)
6	LOP	M	504	-	44,44,44	0.71	0	47,49,49	1.38	7 (14%)
4	HEM	K	301	2	41,50,50	1.66	7 (17%)	45,82,82	1.15	3 (6%)
5	SMA	M	503	-	38,38,38	2.16	9 (23%)	48,52,52	2.14	10 (20%)
7	FES	R	200	3	0,4,4	-	-	-	-	-
4	HEM	P	501	1	41,50,50	1.74	7 (17%)	45,82,82	1.08	3 (6%)
5	SMA	A	503	-	38,38,38	1.95	8 (21%)	48,52,52	2.10	14 (29%)
7	FES	L	200	3	0,4,4	-	-	-	-	-
4	HEM	M	501	1	41,50,50	1.47	6 (14%)	45,82,82	1.10	2 (4%)
4	HEM	D	502	1	41,50,50	1.47	5 (12%)	45,82,82	1.19	3 (6%)
4	HEM	N	301	2	41,50,50	1.46	4 (9%)	45,82,82	1.11	2 (4%)
7	FES	O	200	3	0,4,4	-	-	-	-	-
5	SMA	D	503	-	38,38,38	2.55	11 (28%)	48,52,52	1.82	12 (25%)
5	SMA	P	503	-	38,38,38	2.21	10 (26%)	48,52,52	1.81	11 (22%)
4	HEM	G	502	1	41,50,50	1.74	7 (17%)	45,82,82	1.13	3 (6%)
6	LOP	G	504	-	44,44,44	0.77	1 (2%)	47,49,49	1.42	6 (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
4	HEM	A	501	1	-	4/12/54/54	-
4	HEM	P	502	1	-	7/12/54/54	-
4	HEM	J	502	1	-	6/12/54/54	-
4	HEM	A	502	1	-	6/12/54/54	-
4	HEM	B	301	2	-	4/12/54/54	-
4	HEM	M	502	1	-	6/12/54/54	-
4	HEM	J	501	1	-	5/12/54/54	-
7	FES	C	200	3	-	-	0/1/1/1
7	FES	I	200	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	F	200	3	-	-	0/1/1/1
4	HEM	E	301	2	-	6/12/54/54	-
6	LOP	D	504	-	-	6/48/48/48	-
4	HEM	Q	301	2	-	9/12/54/54	-
6	LOP	J	504	-	-	12/48/48/48	-
6	LOP	P	504	-	-	4/48/48/48	-
6	LOP	A	504	-	-	12/48/48/48	-
4	HEM	G	501	1	-	4/12/54/54	-
5	SMA	G	503	-	-	7/34/34/34	0/2/2/2
4	HEM	H	301	2	-	6/12/54/54	-
4	HEM	D	501	1	-	6/12/54/54	-
5	SMA	J	503	-	-	8/34/34/34	0/2/2/2
6	LOP	M	504	-	-	8/48/48/48	-
4	HEM	K	301	2	-	6/12/54/54	-
5	SMA	M	503	-	-	11/34/34/34	0/2/2/2
7	FES	R	200	3	-	-	0/1/1/1
4	HEM	P	501	1	-	7/12/54/54	-
5	SMA	A	503	-	-	7/34/34/34	0/2/2/2
7	FES	L	200	3	-	-	0/1/1/1
4	HEM	M	501	1	-	11/12/54/54	-
4	HEM	D	502	1	-	7/12/54/54	-
4	HEM	N	301	2	-	11/12/54/54	-
7	FES	O	200	3	-	-	0/1/1/1
5	SMA	D	503	-	-	4/34/34/34	0/2/2/2
5	SMA	P	503	-	-	7/34/34/34	0/2/2/2
4	HEM	G	502	1	-	7/12/54/54	-
6	LOP	G	504	-	-	10/48/48/48	-

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SMA	O5-C5	8.20	1.50	1.37
5	M	503	SMA	O5-C5	7.30	1.48	1.37
5	P	503	SMA	O5-C5	6.95	1.48	1.37
5	J	503	SMA	O5-C5	6.95	1.48	1.37
5	P	503	SMA	O7-C7	6.46	1.47	1.37

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	503	SMA	O7-C7-C8	6.91	121.51	114.54
5	A	503	SMA	C5M-O5-C5	-6.56	107.63	117.53
5	A	503	SMA	O7-C7-C8	6.13	120.72	114.54
5	M	503	SMA	O7-C7-C8	5.77	120.37	114.54
5	J	503	SMA	C9-C2-C3	-5.34	119.26	127.07

There are no chirality outliers.

5 of 214 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	HEM	C2B-C3B-CAB-CBB
4	A	502	HEM	C2B-C3B-CAB-CBB
4	A	502	HEM	C4B-C3B-CAB-CBB
4	B	301	HEM	C2B-C3B-CAB-CBB
4	D	501	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

32 monomers are involved in 104 short contacts:

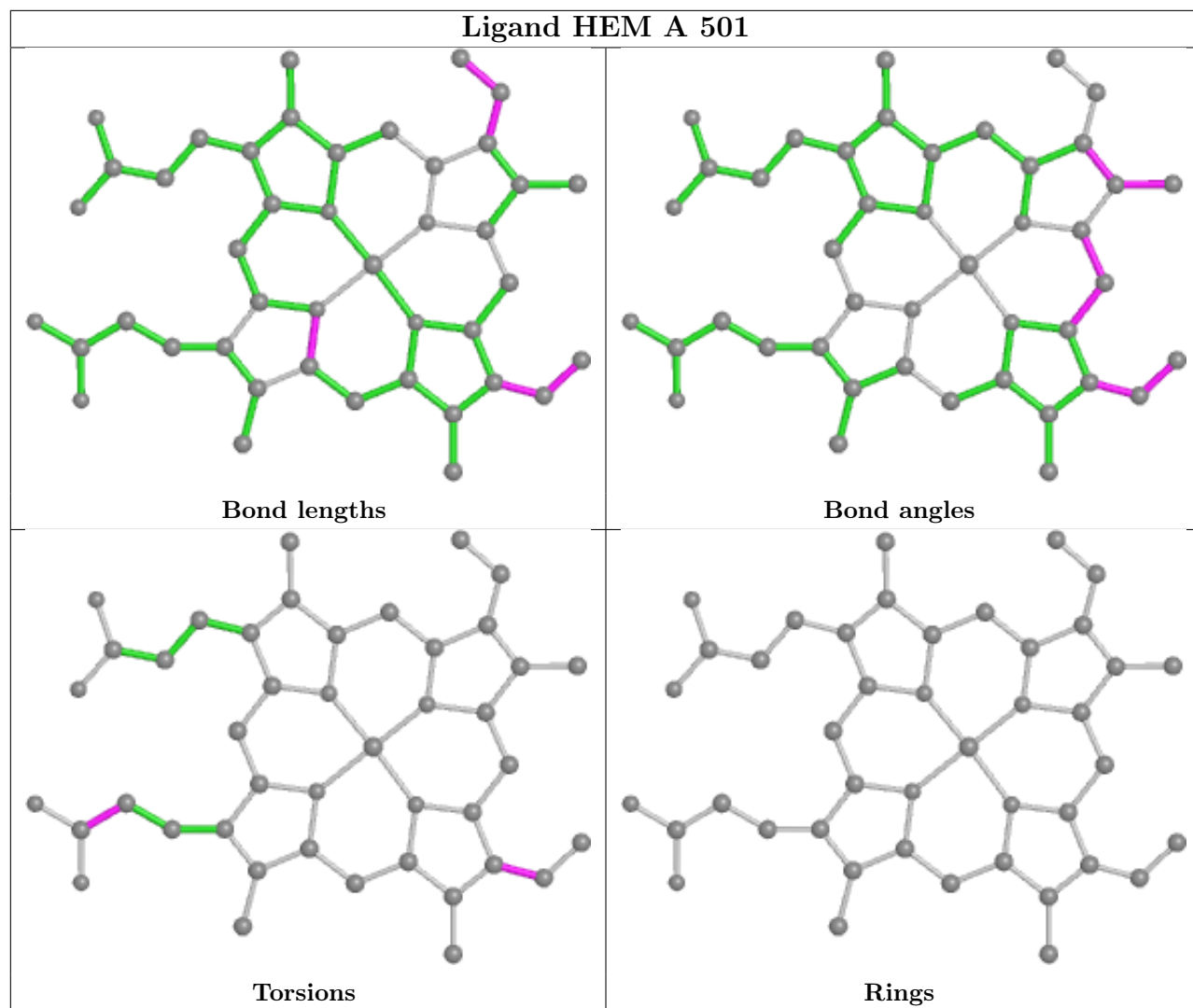
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	HEM	4	0
4	P	502	HEM	5	0
4	J	502	HEM	7	0
4	A	502	HEM	3	0
4	M	502	HEM	2	0
4	J	501	HEM	10	0
7	C	200	FES	2	0
7	F	200	FES	2	0
4	E	301	HEM	1	0
6	D	504	LOP	1	0
4	Q	301	HEM	1	0
6	J	504	LOP	1	0
6	P	504	LOP	1	0
6	A	504	LOP	3	0
4	G	501	HEM	8	0
5	G	503	SMA	1	0
4	H	301	HEM	2	0
4	D	501	HEM	8	0
5	J	503	SMA	1	0
6	M	504	LOP	3	0
4	K	301	HEM	1	0

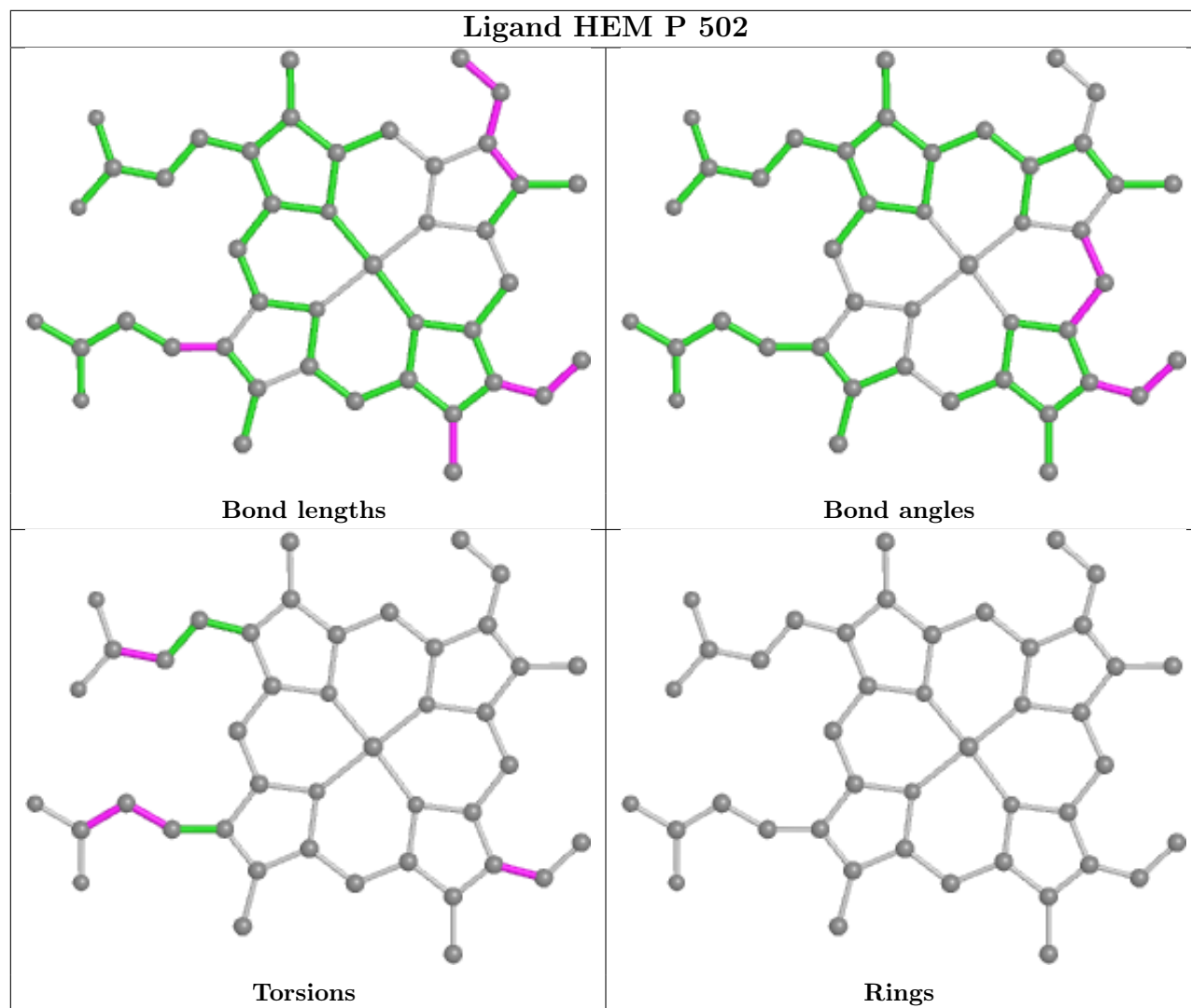
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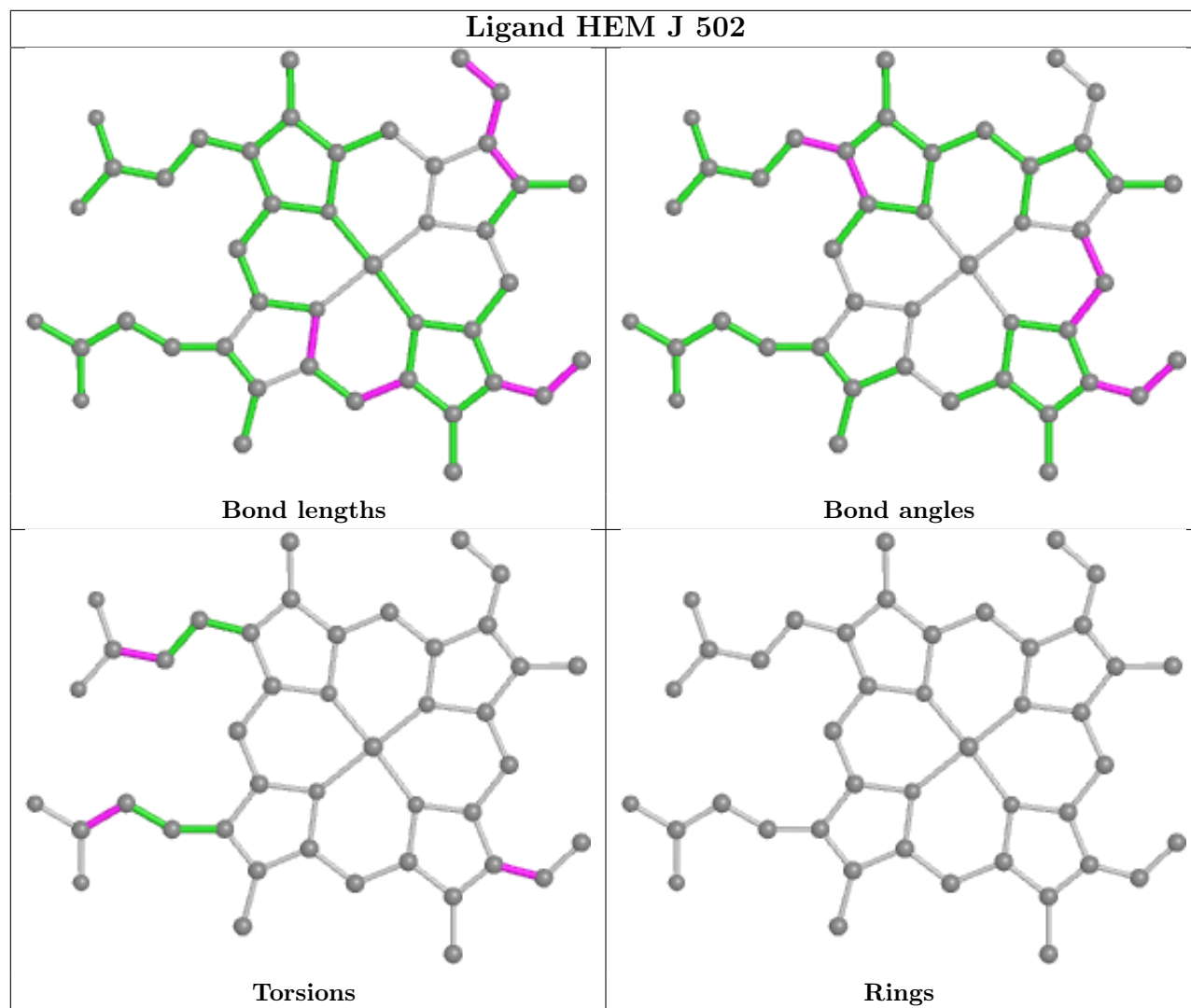
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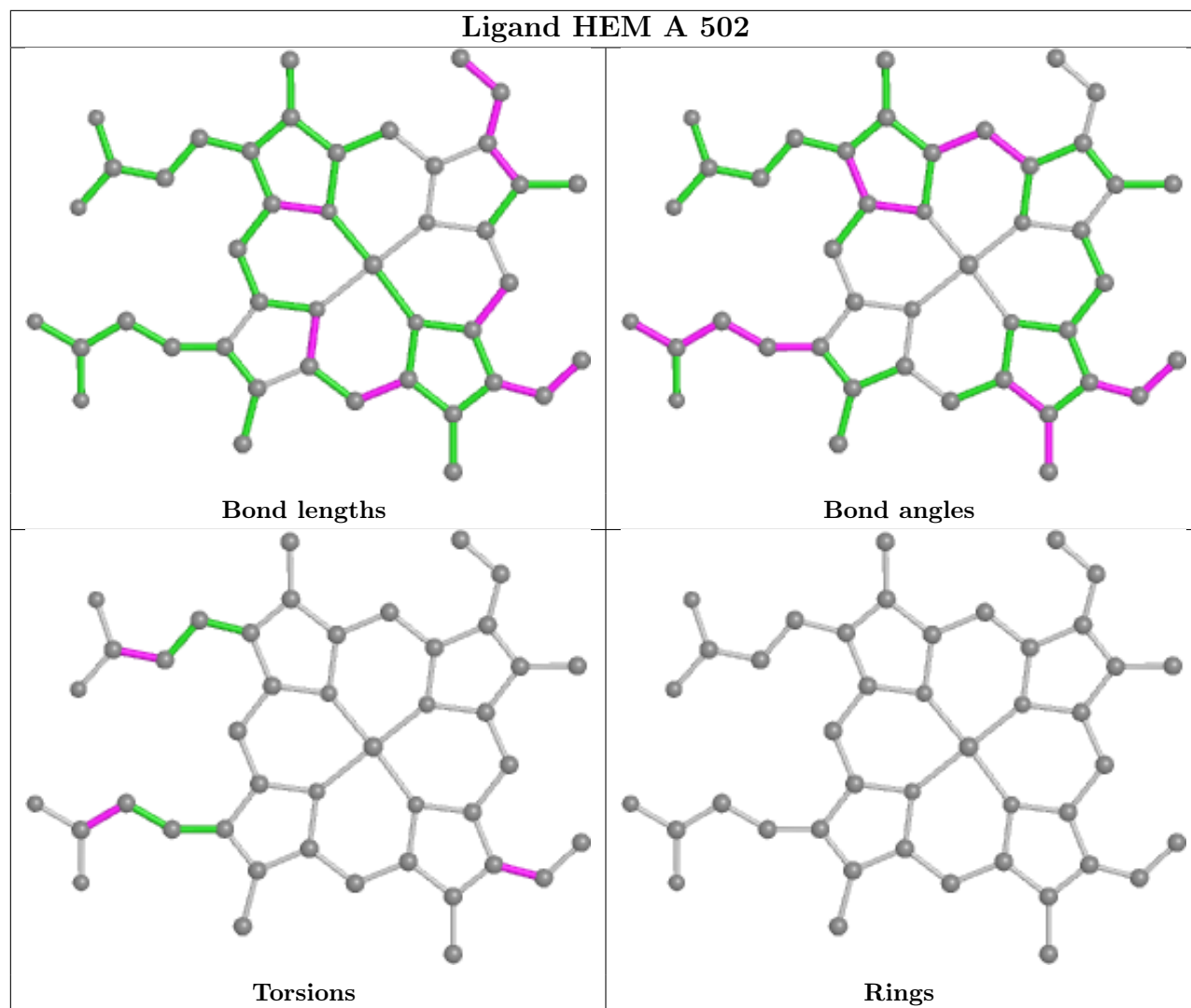
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	503	SMA	2	0
7	R	200	FES	1	0
4	P	501	HEM	6	0
5	A	503	SMA	2	0
4	M	501	HEM	11	0
4	D	502	HEM	4	0
4	N	301	HEM	2	0
7	O	200	FES	1	0
5	D	503	SMA	1	0
4	G	502	HEM	2	0
6	G	504	LOP	5	0

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.

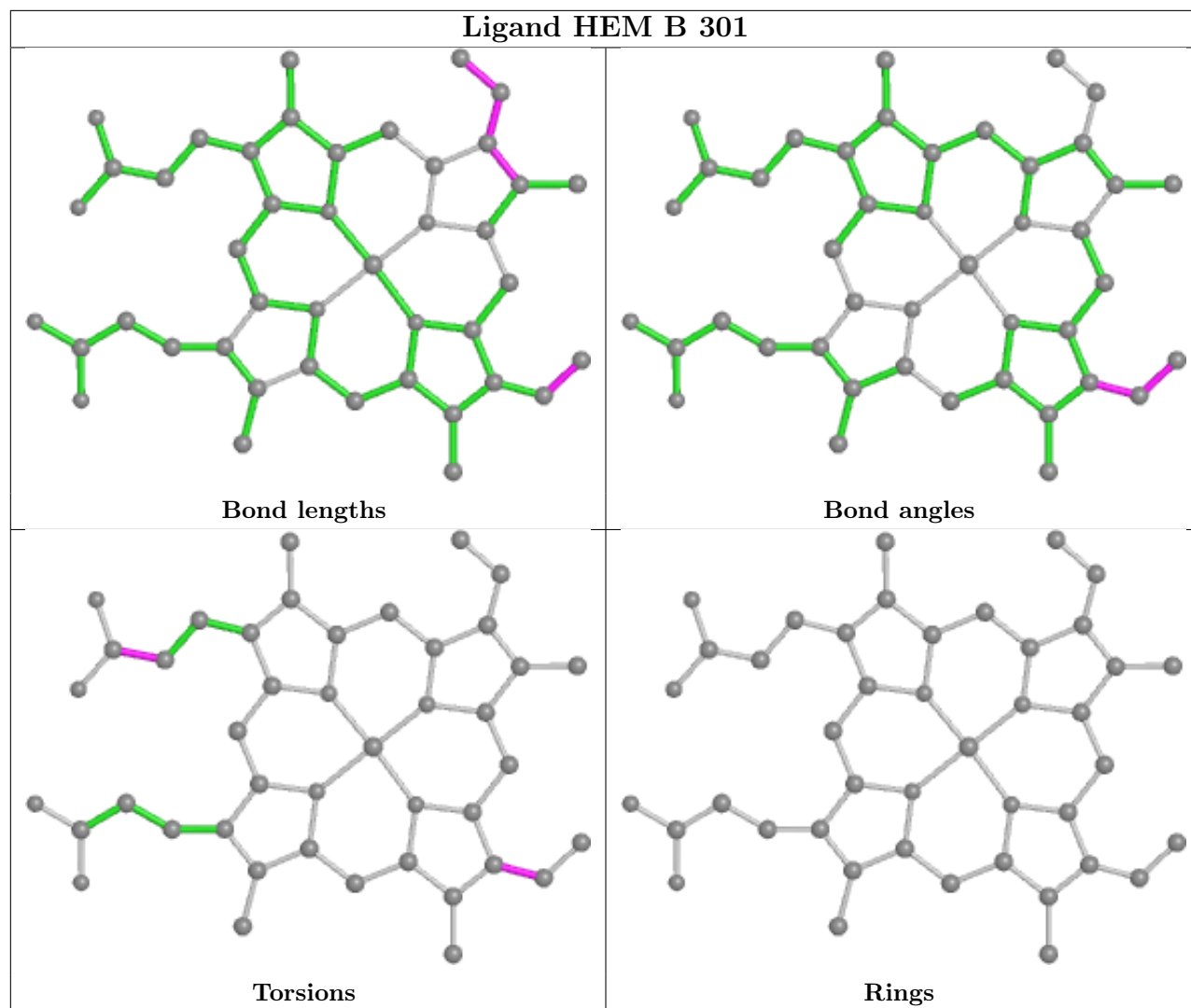


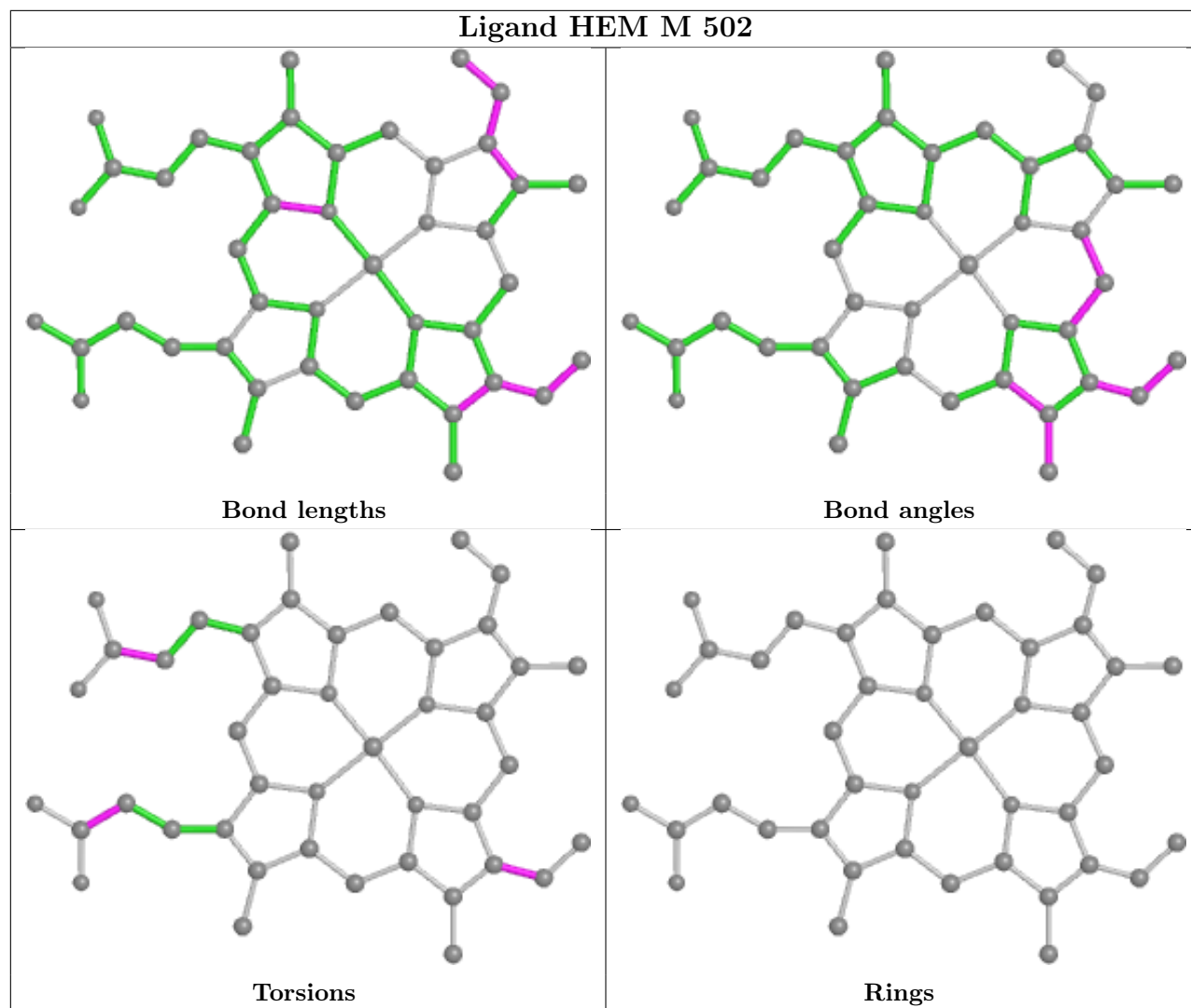


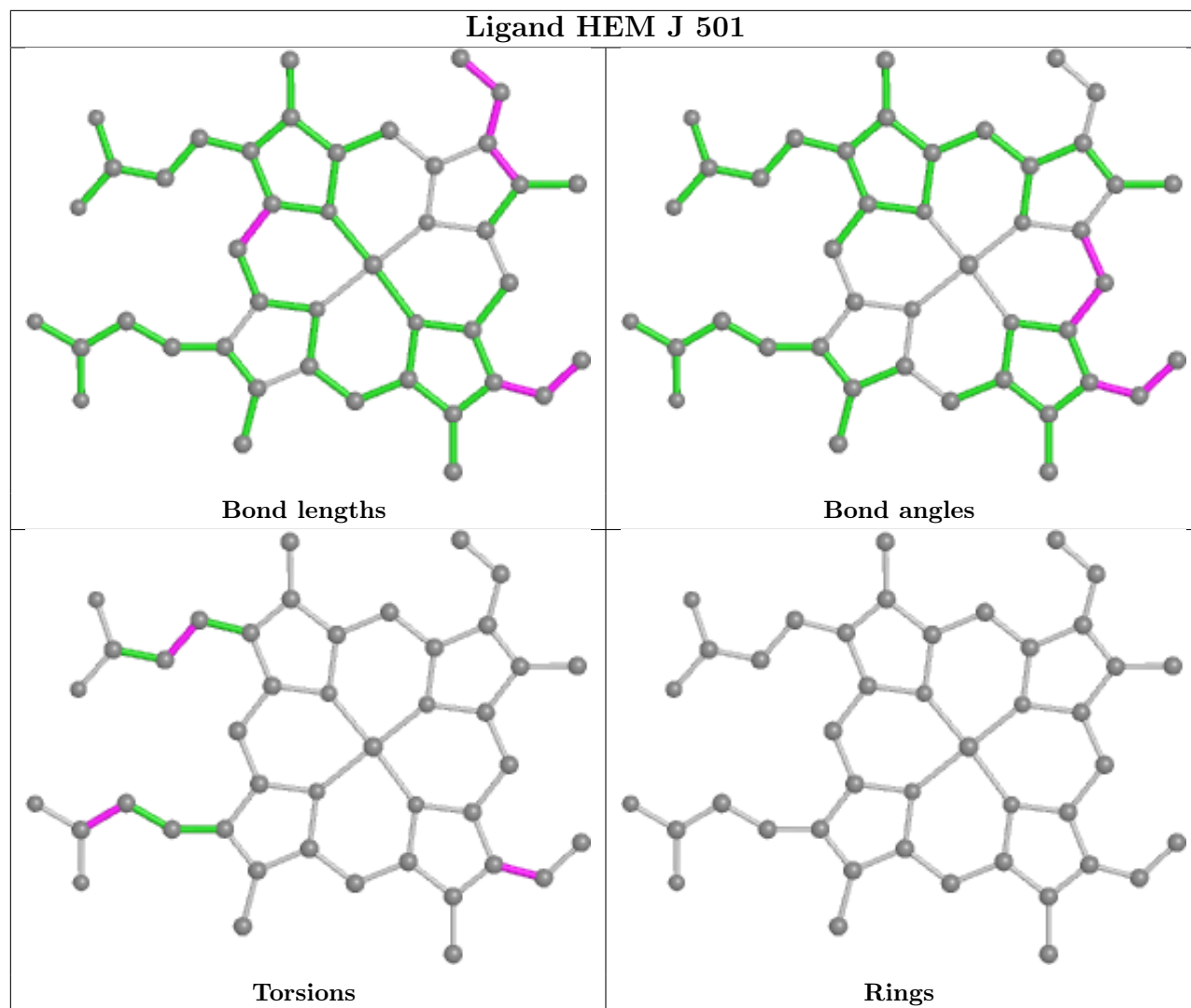


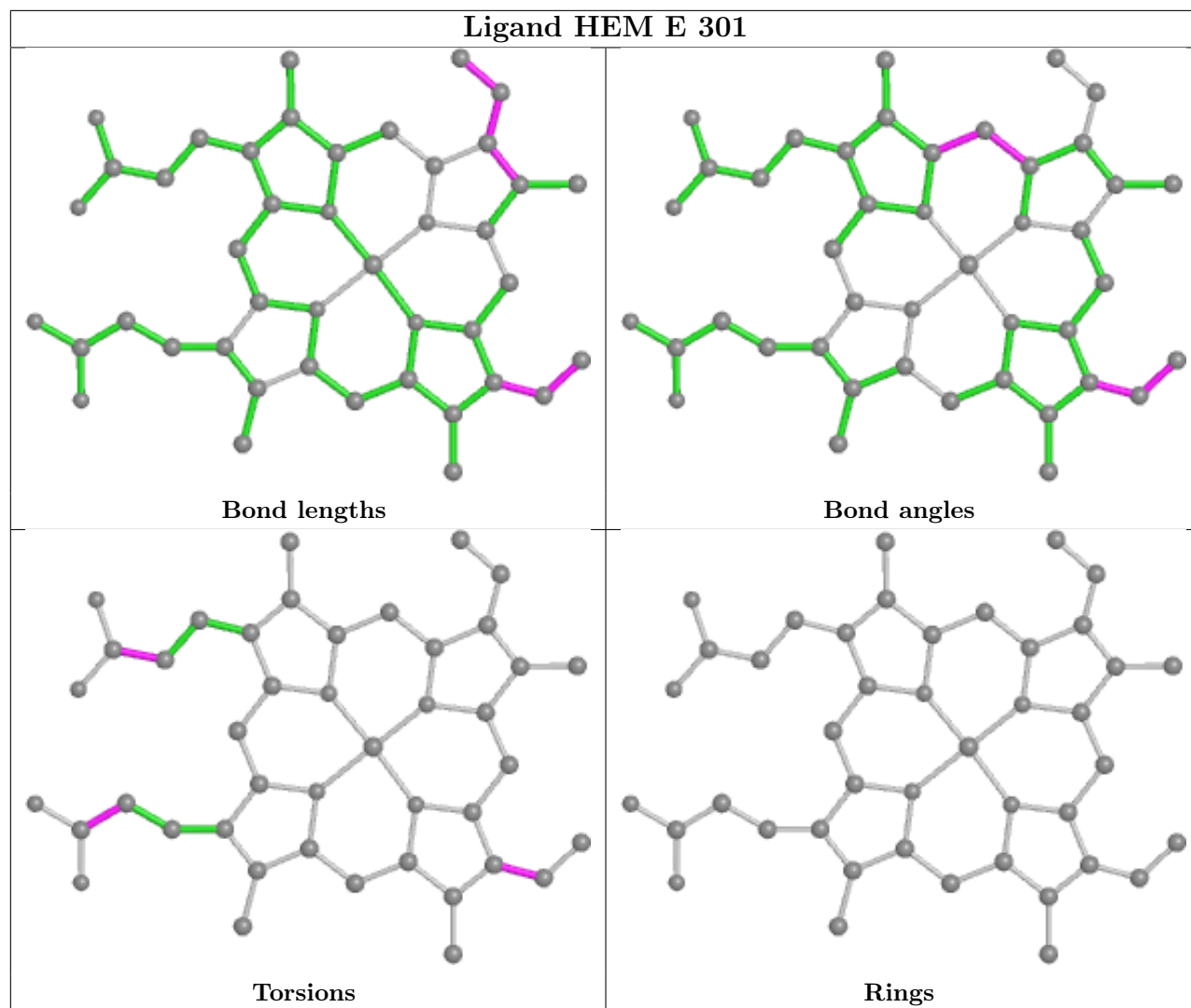


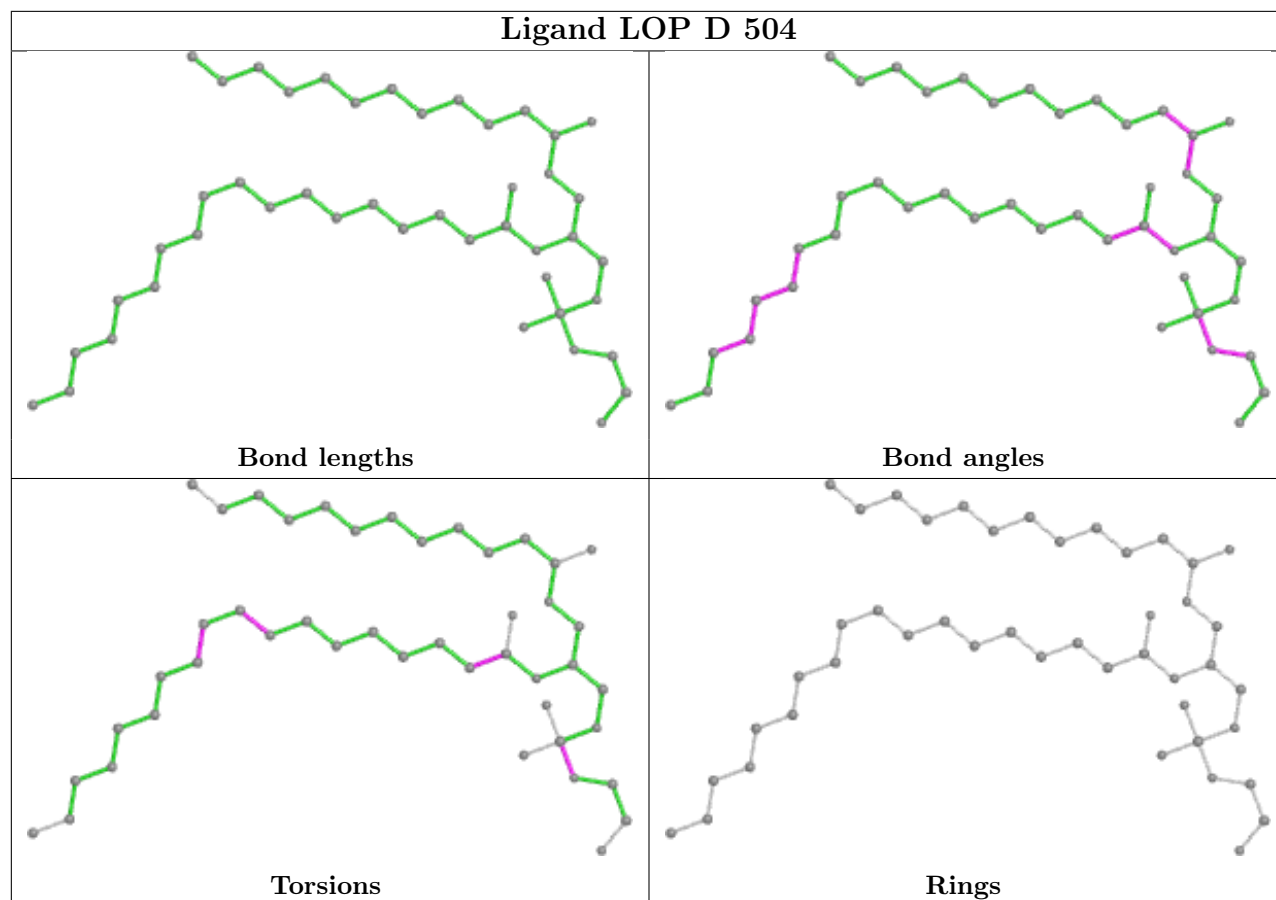


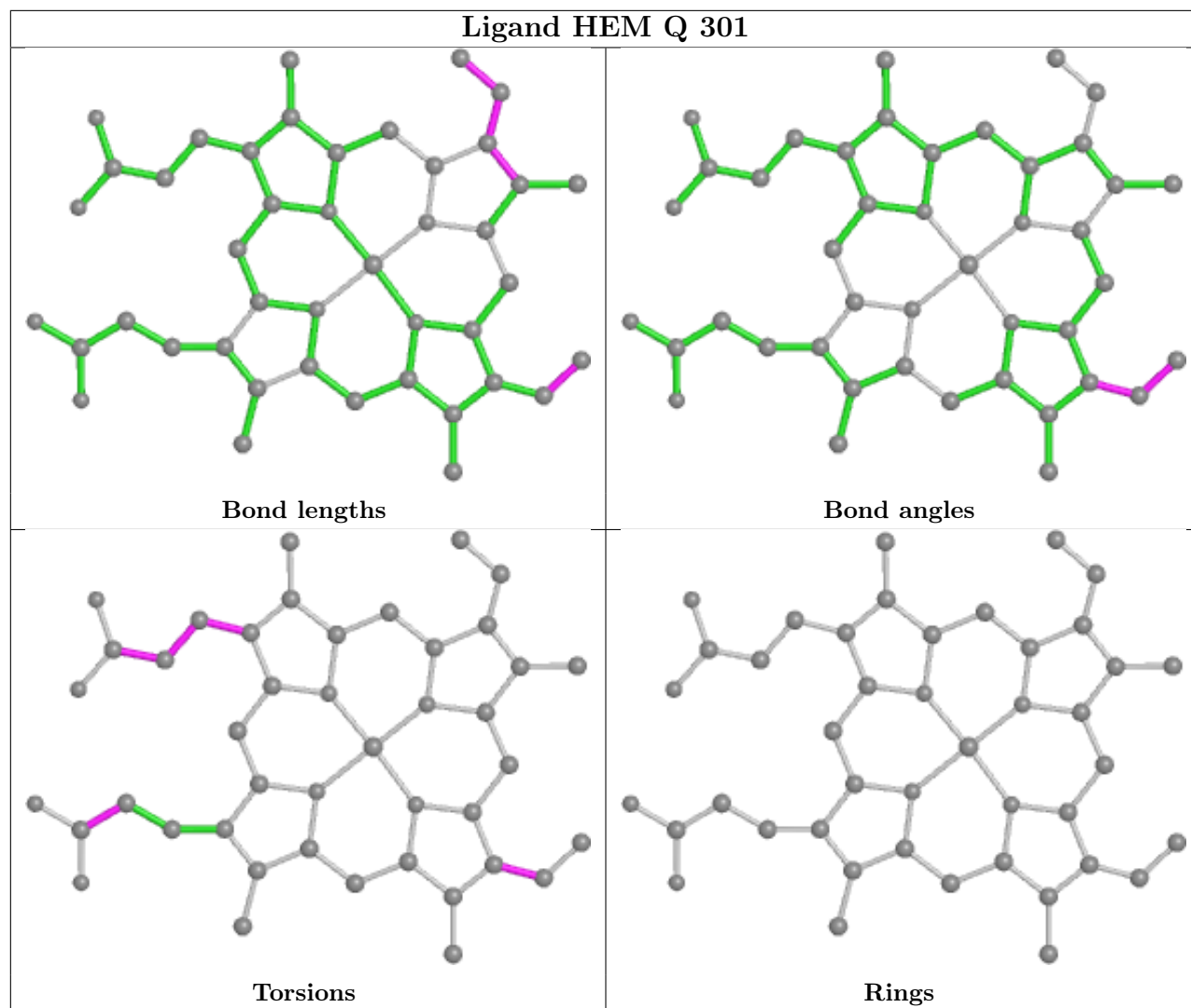


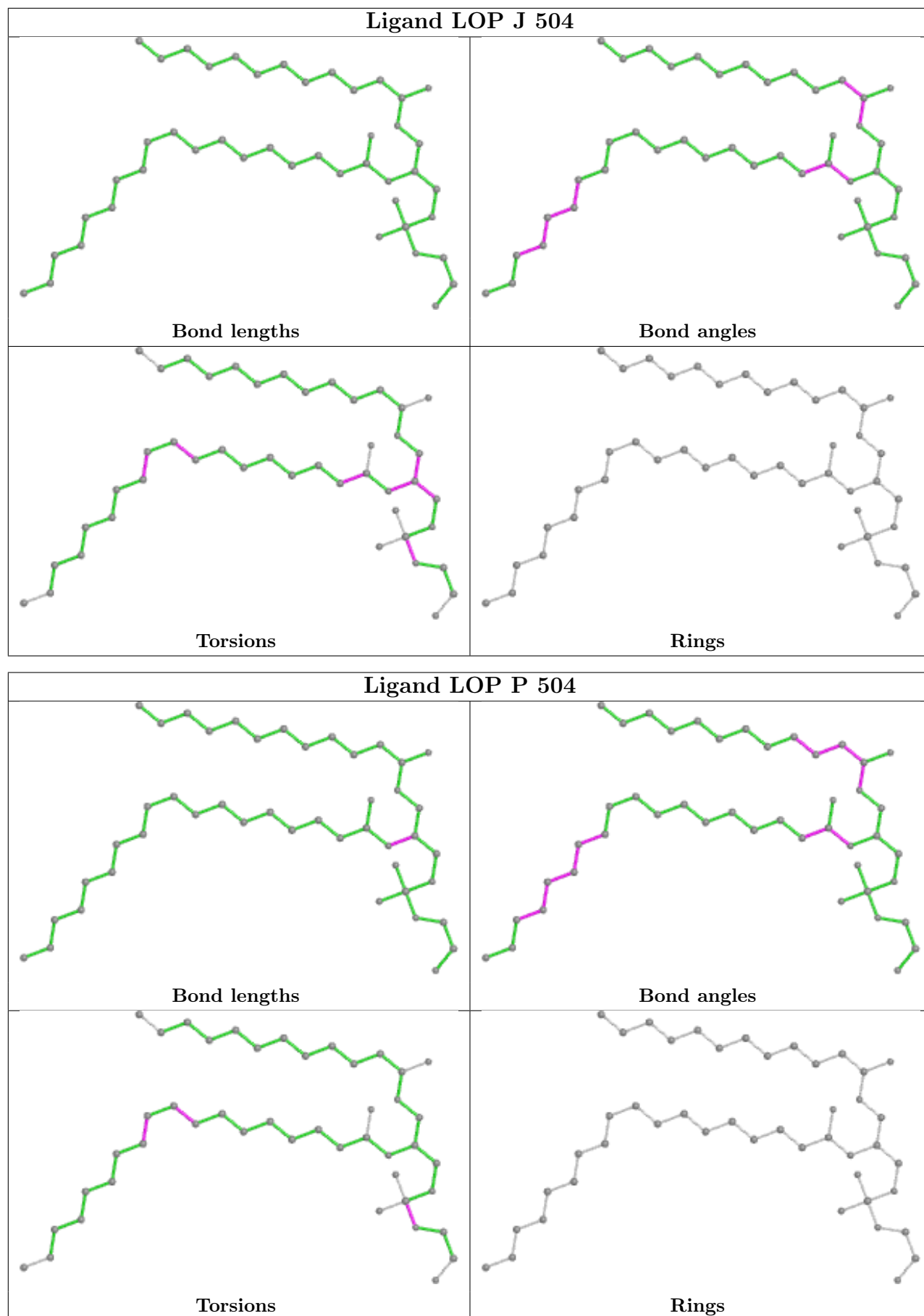


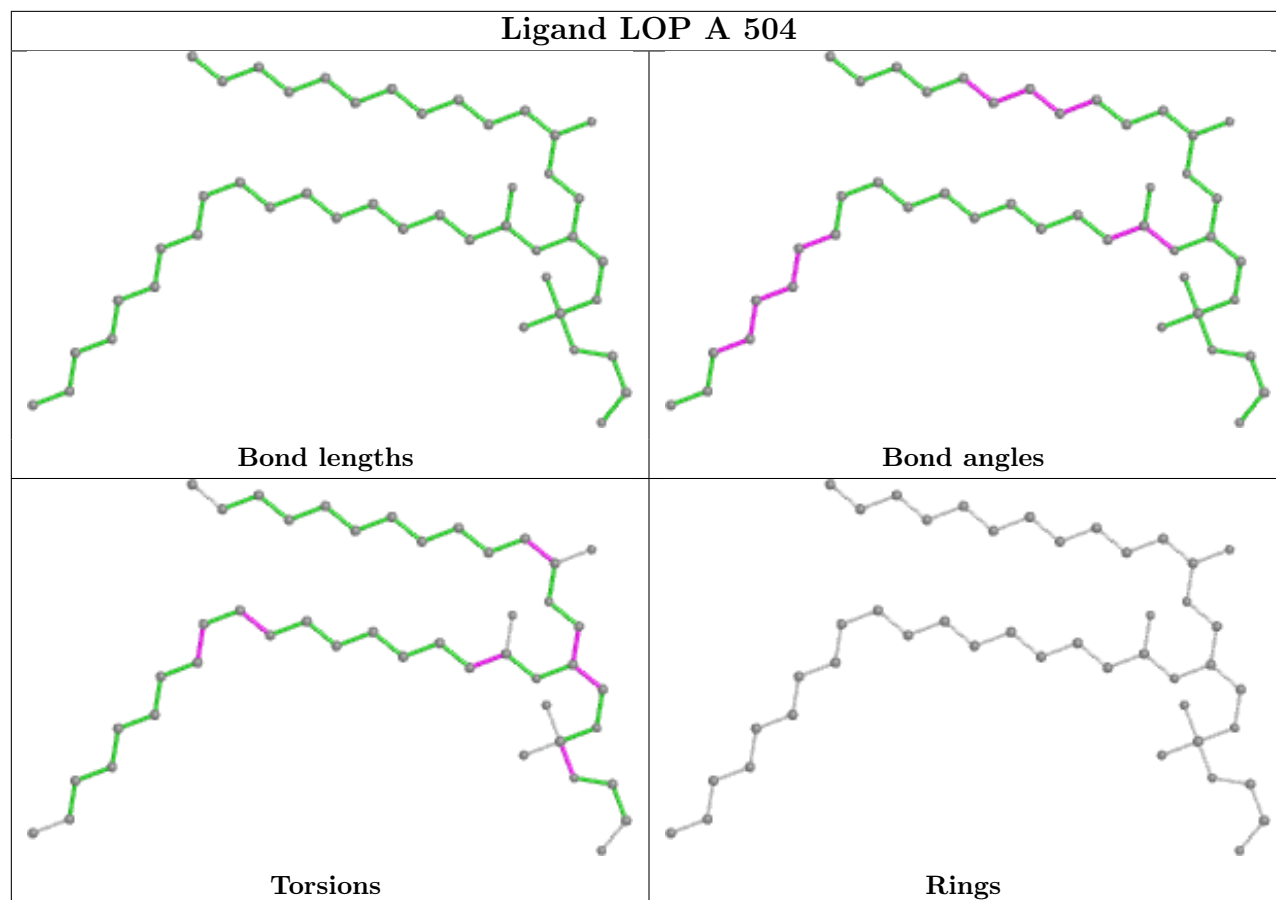




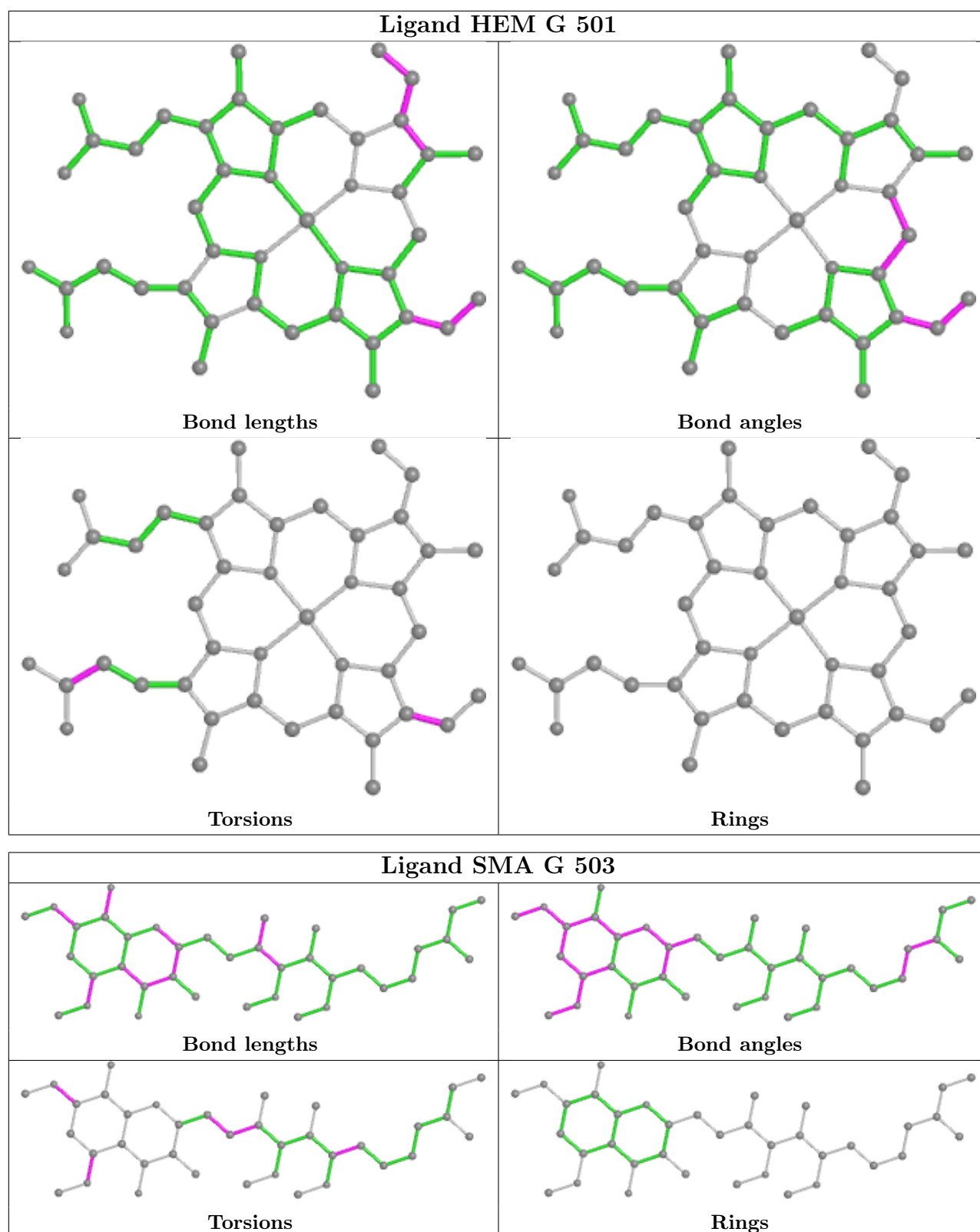


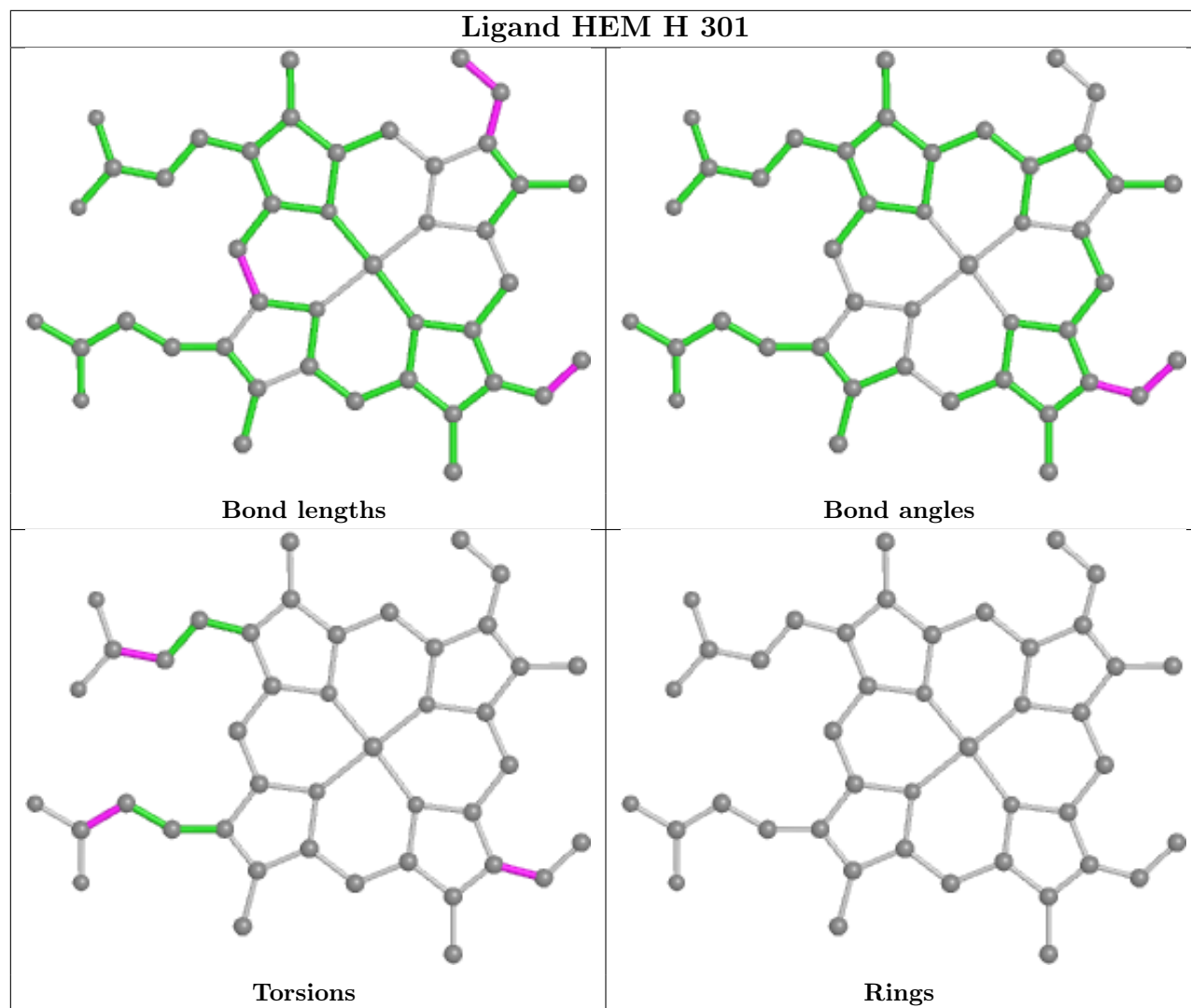


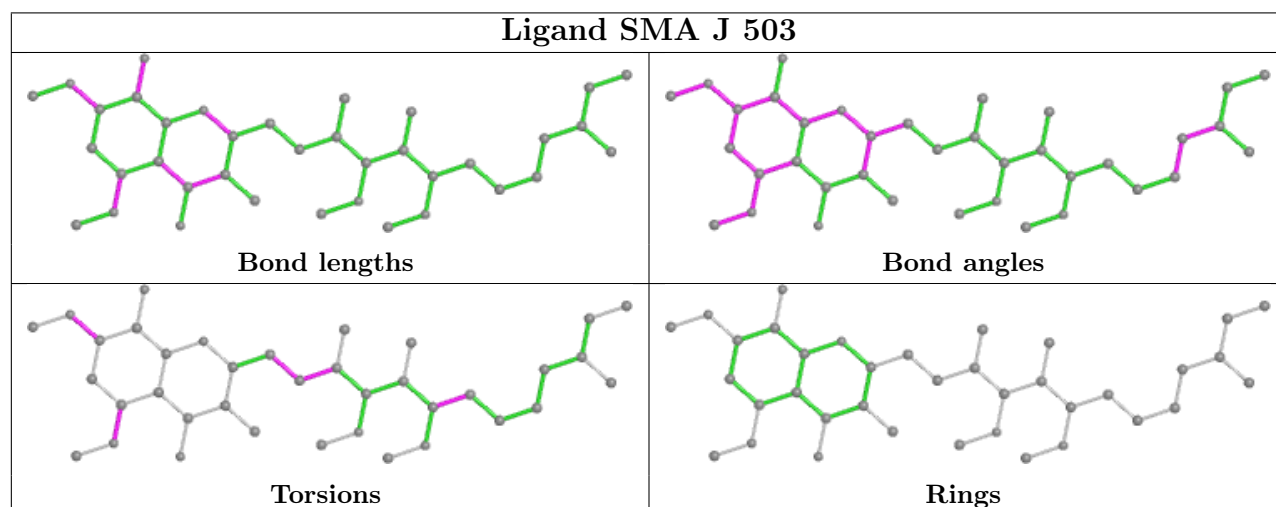
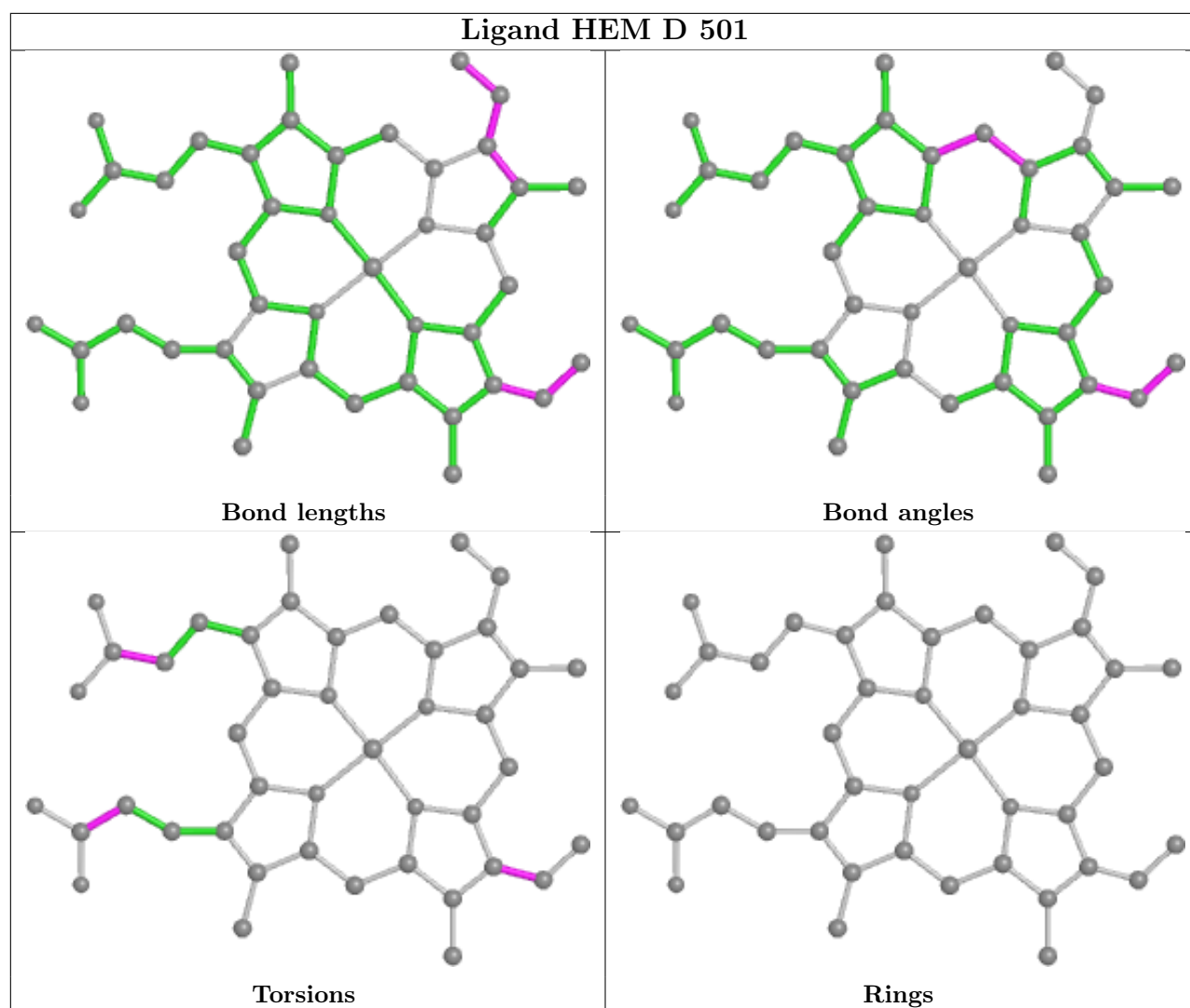


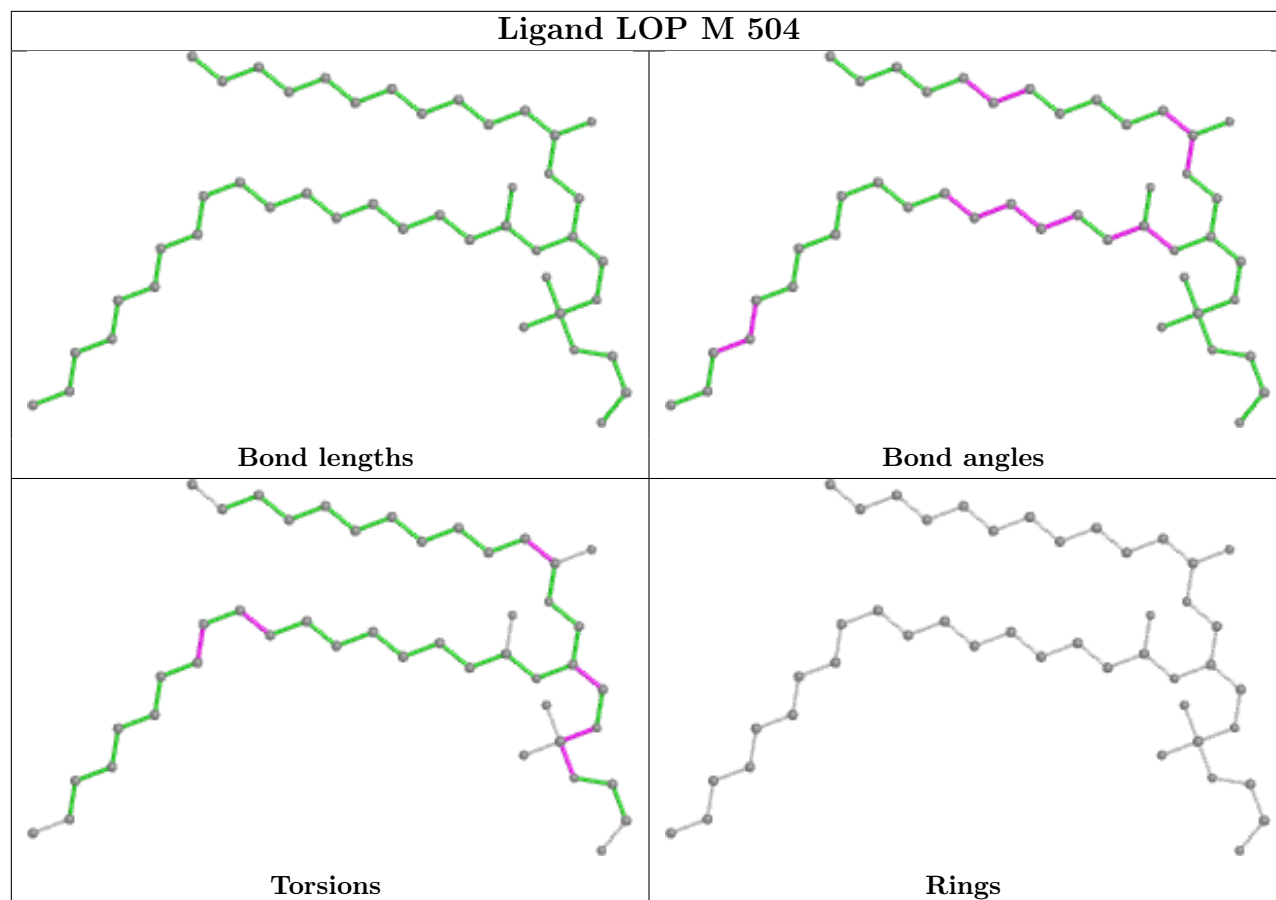


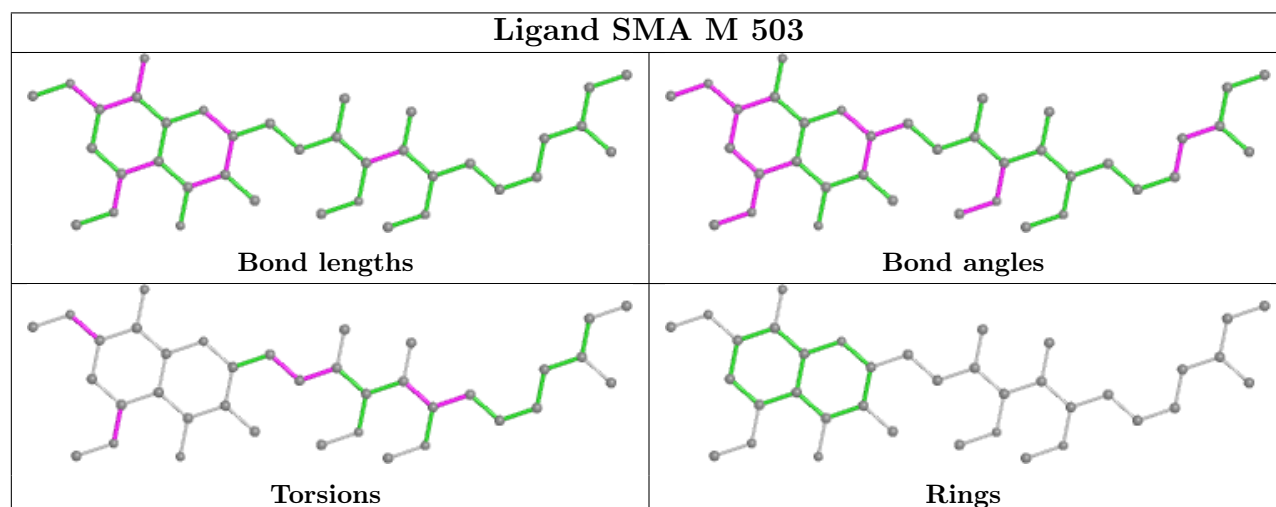
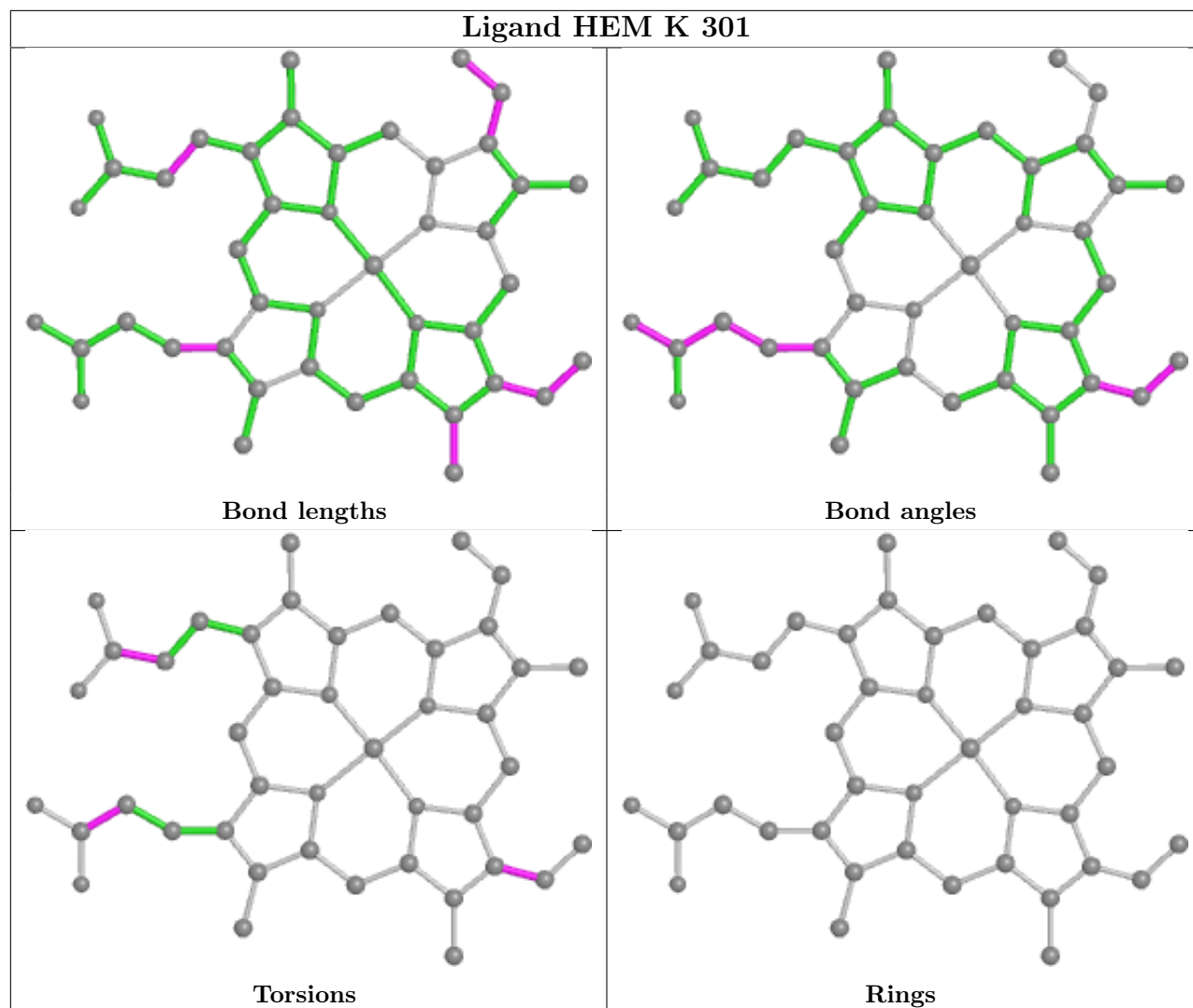


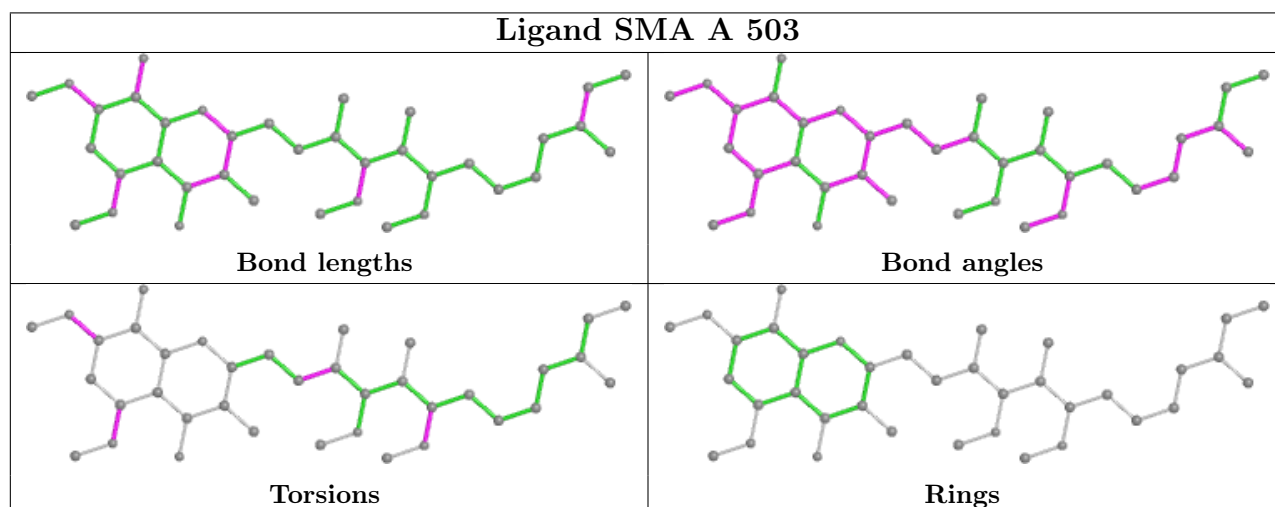
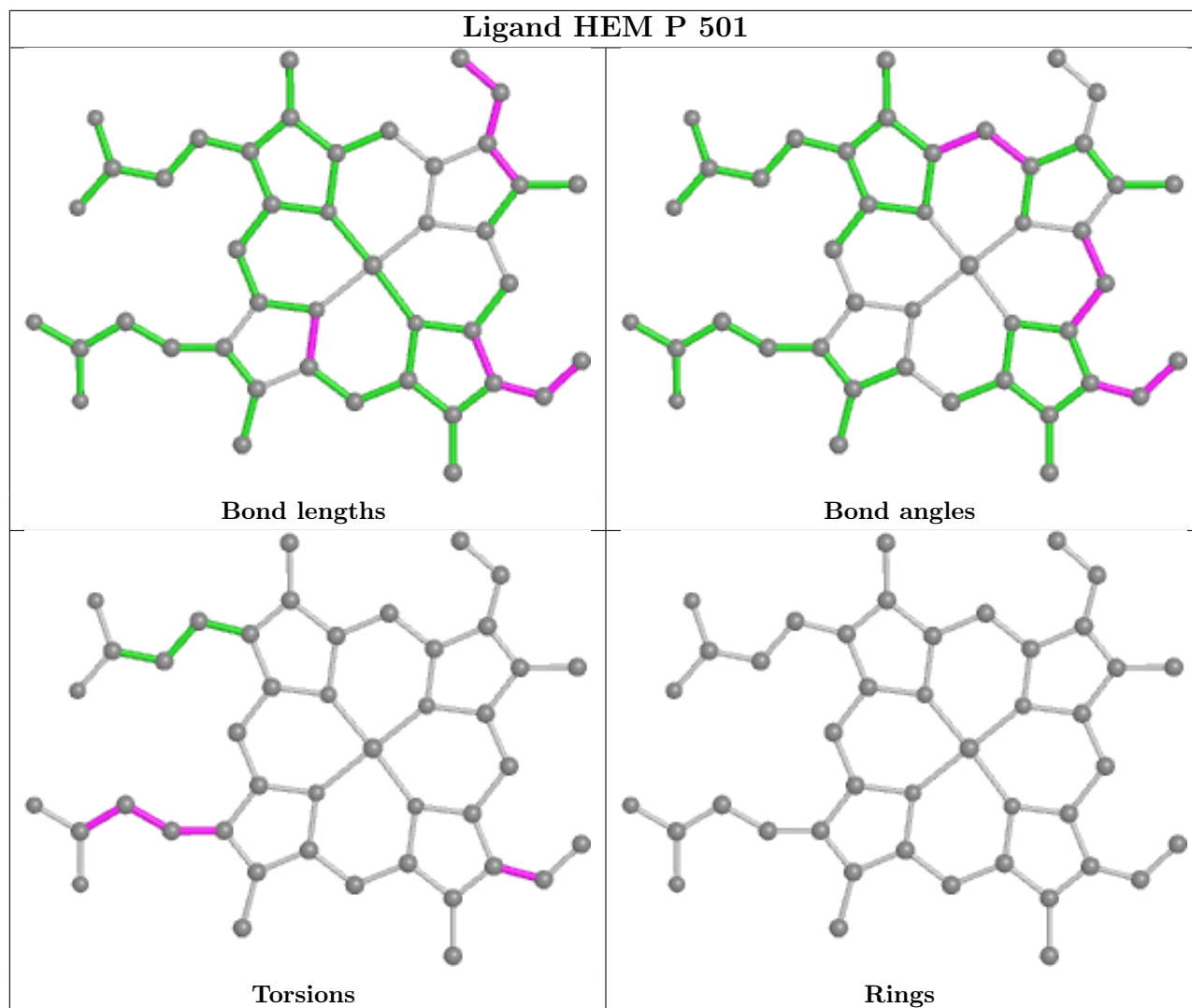


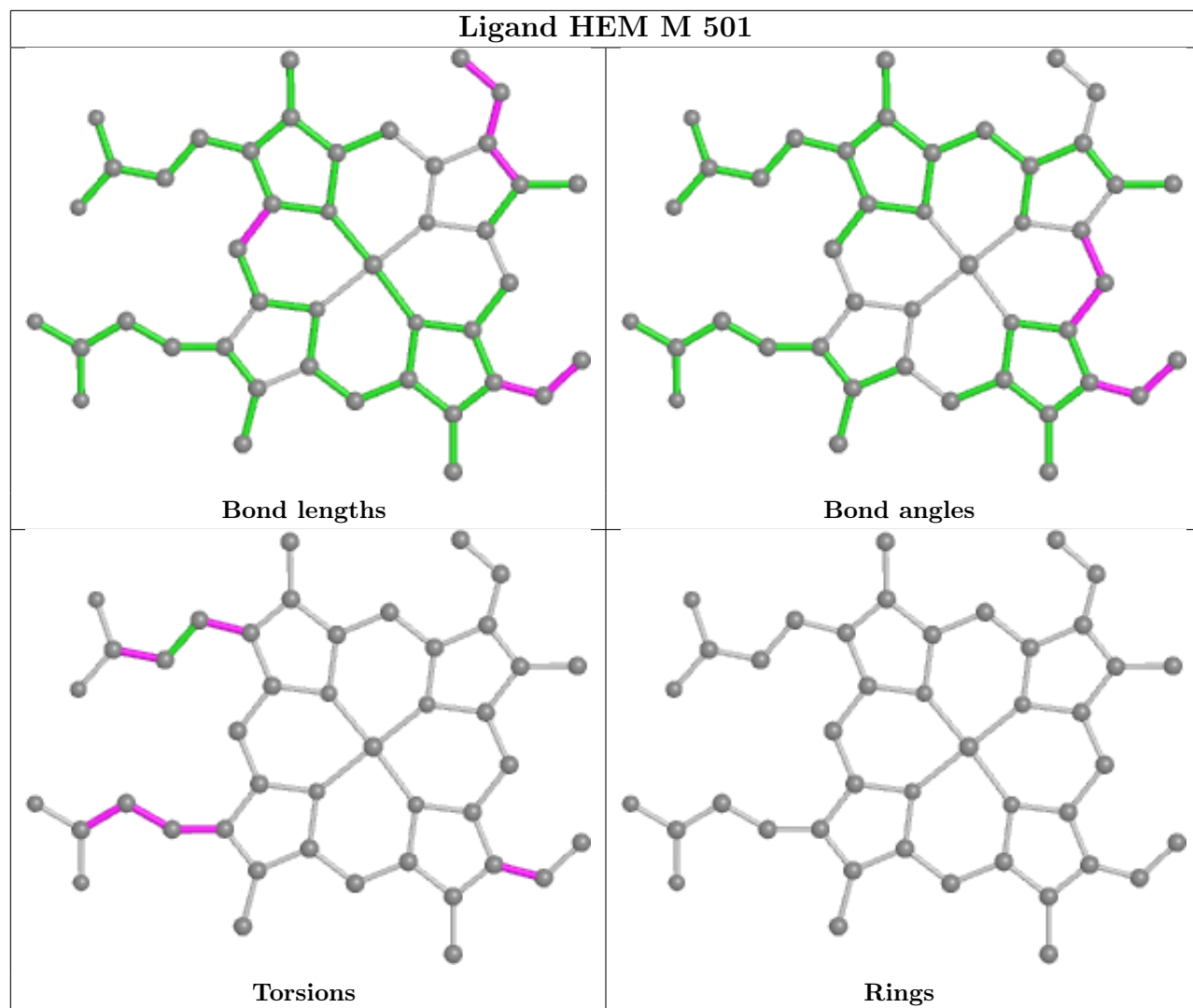


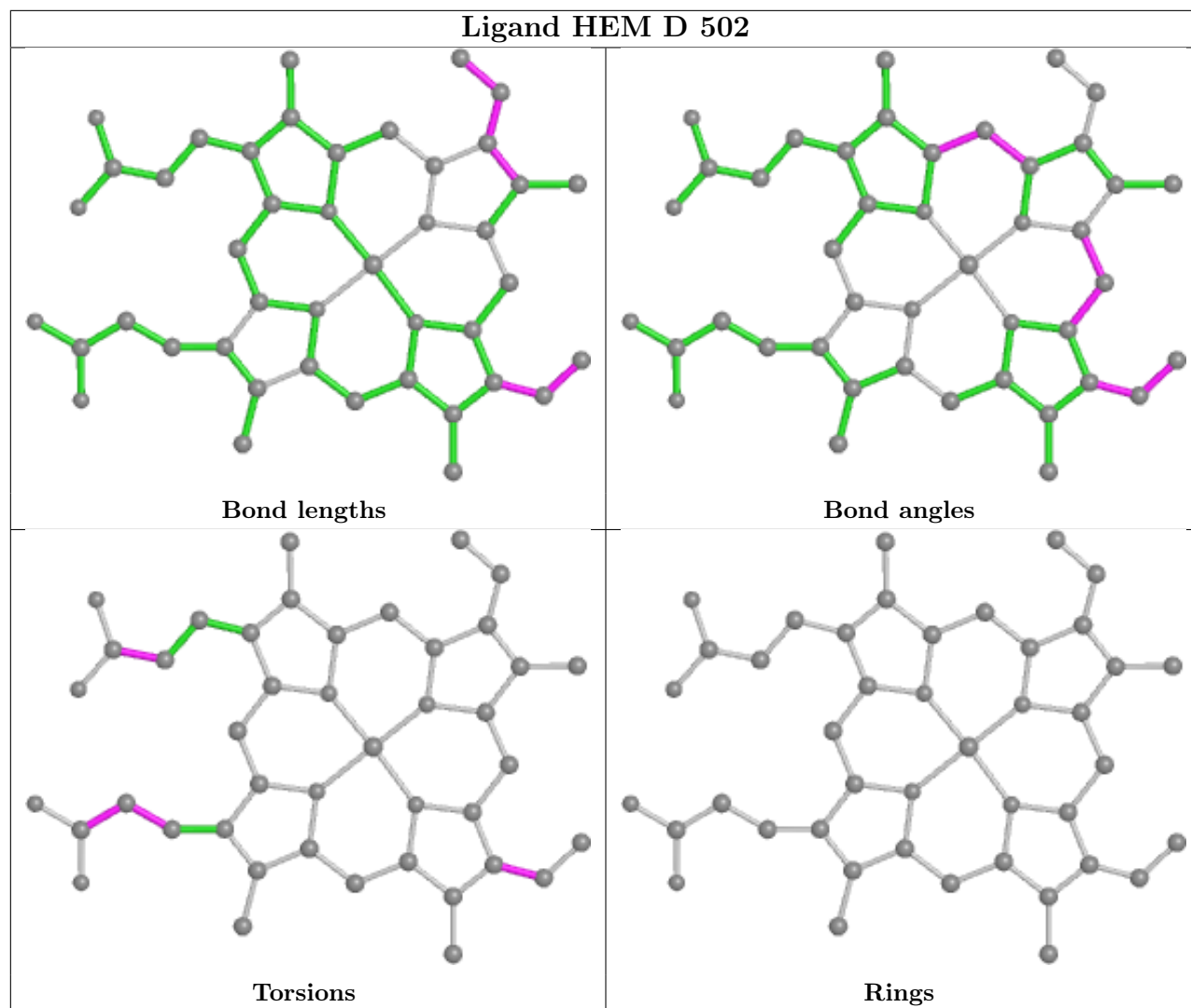




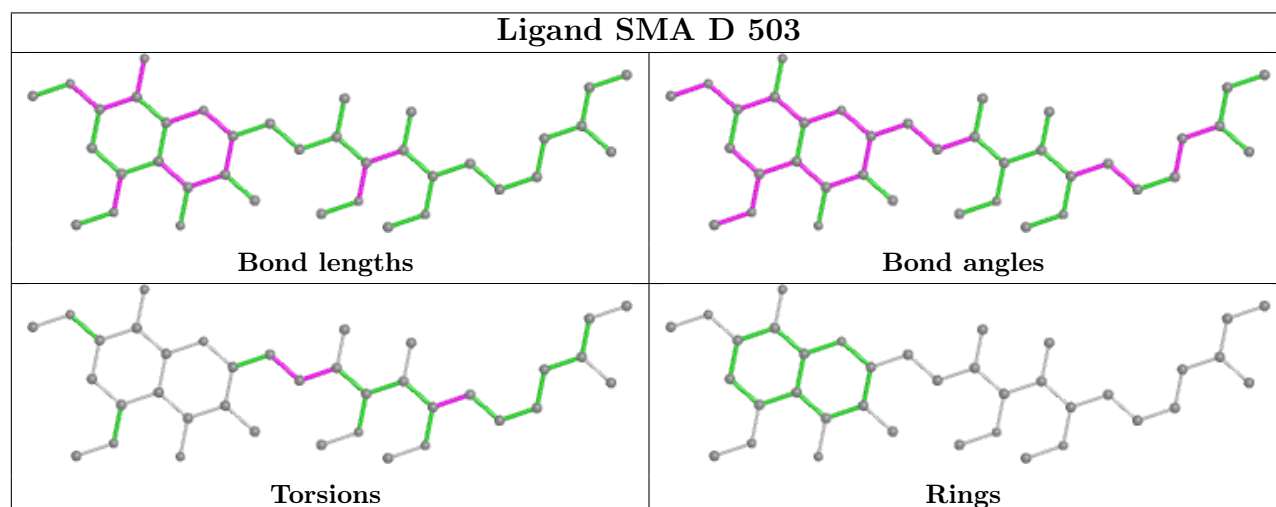
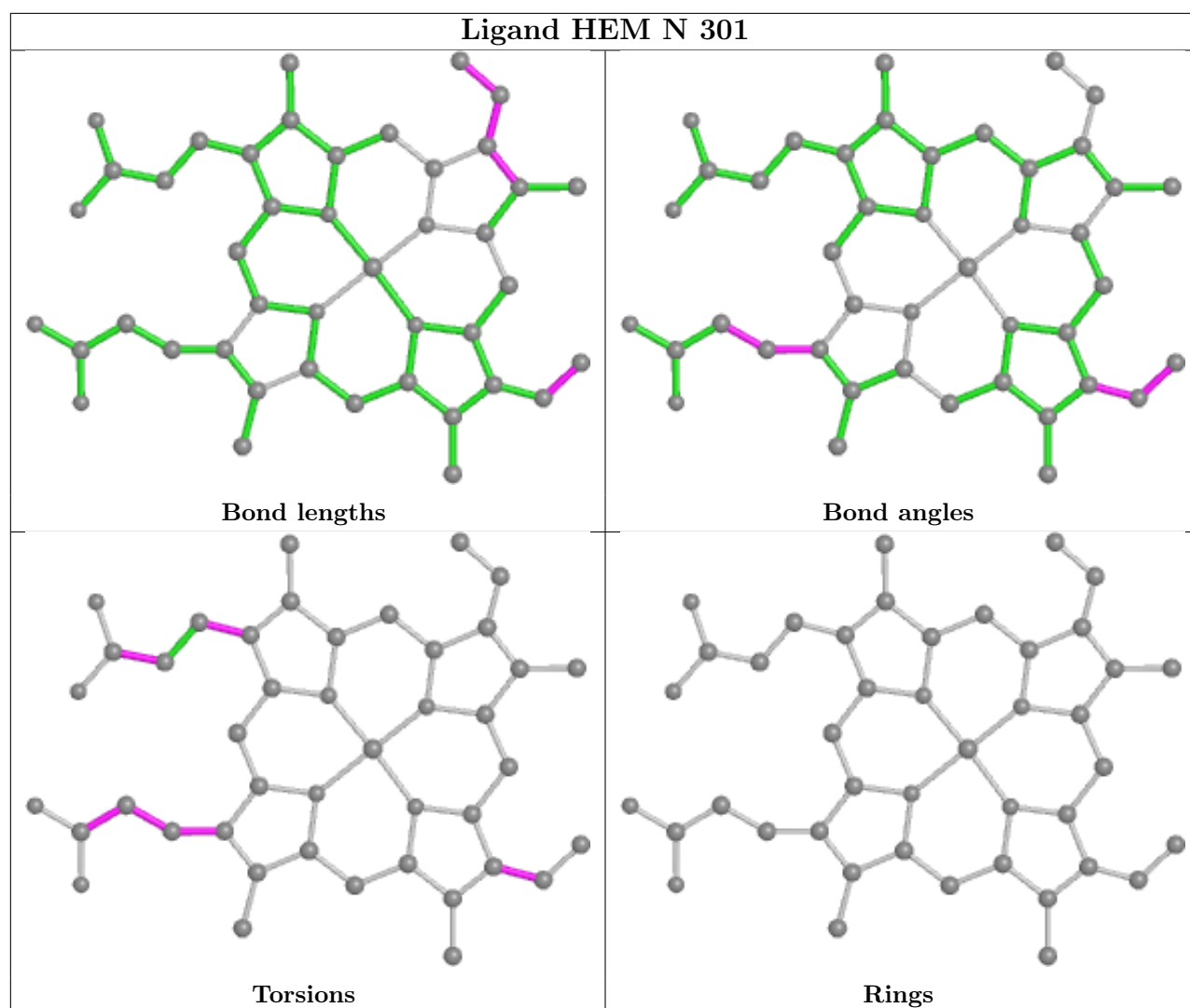


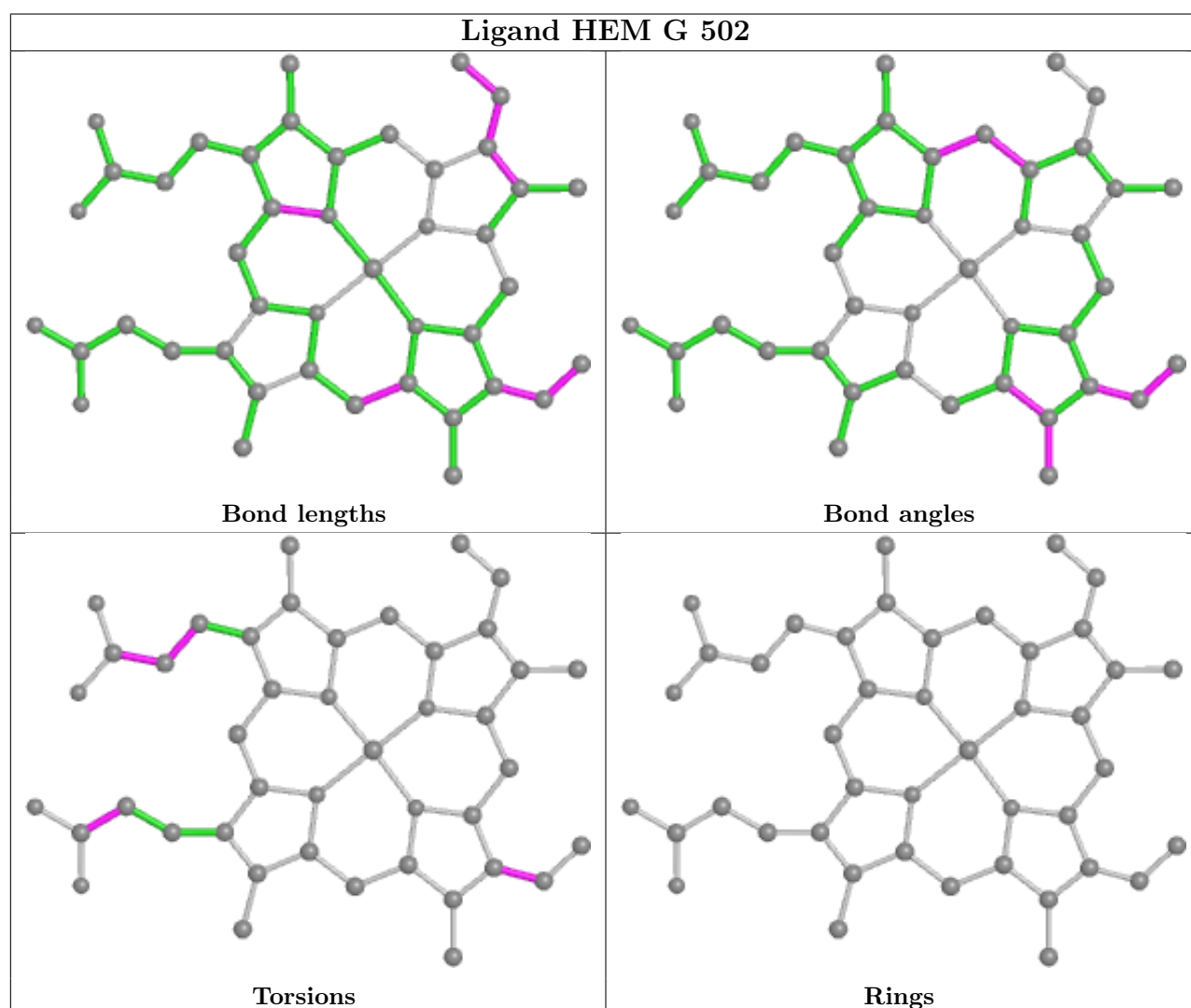
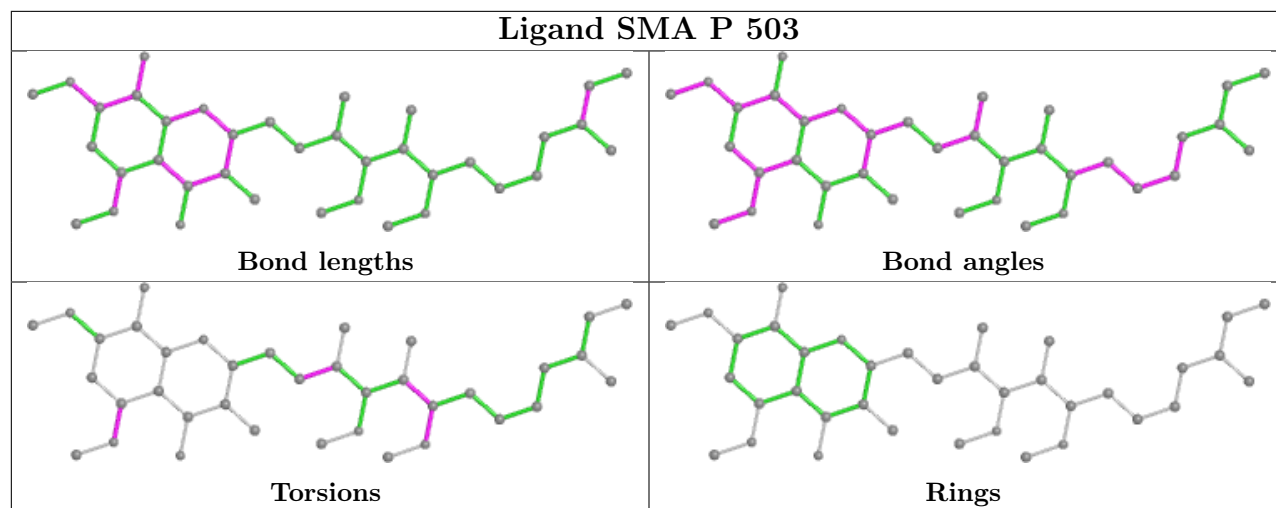


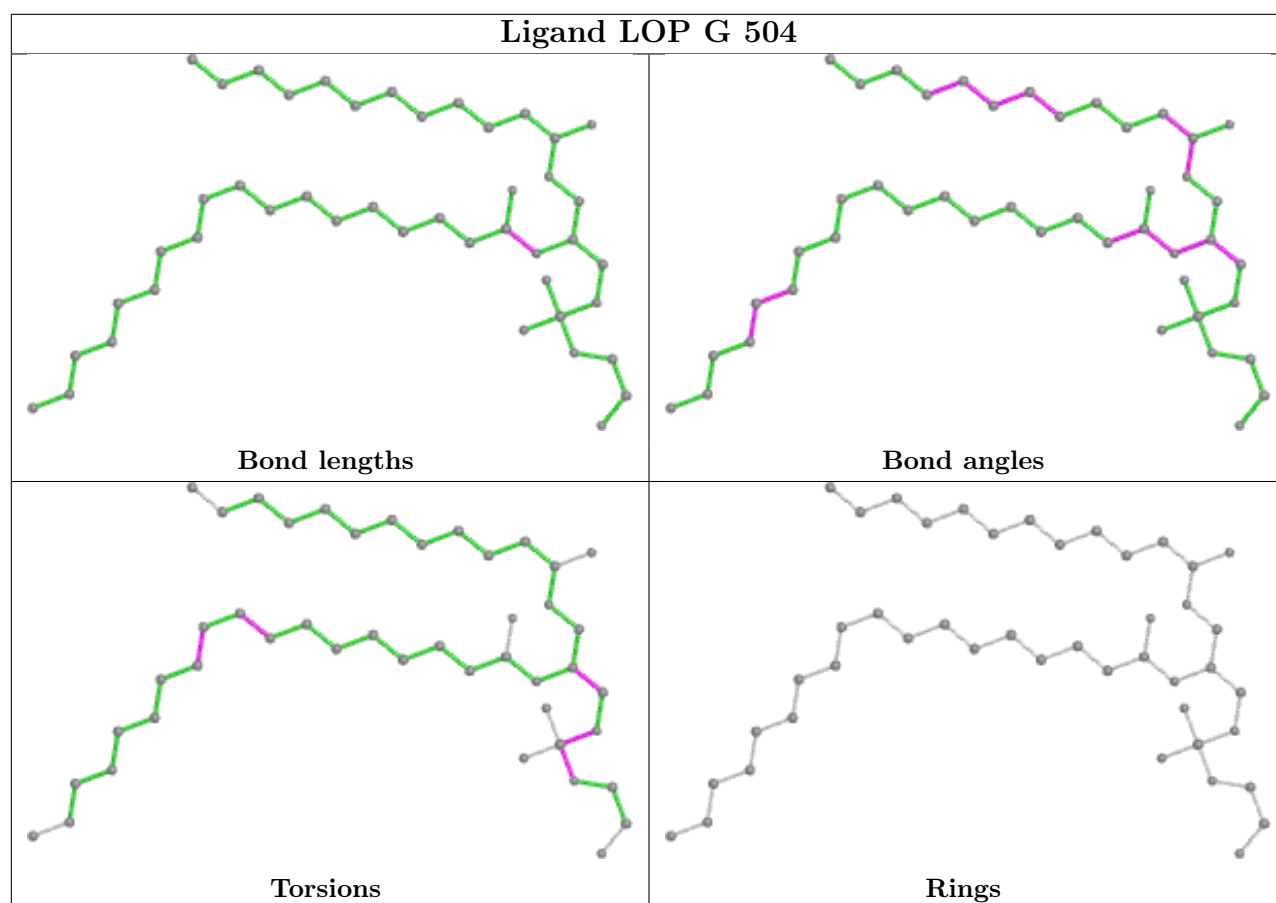












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.