



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:27 PM EDT

PDB ID : 2FYN / pdb_00002fyn
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

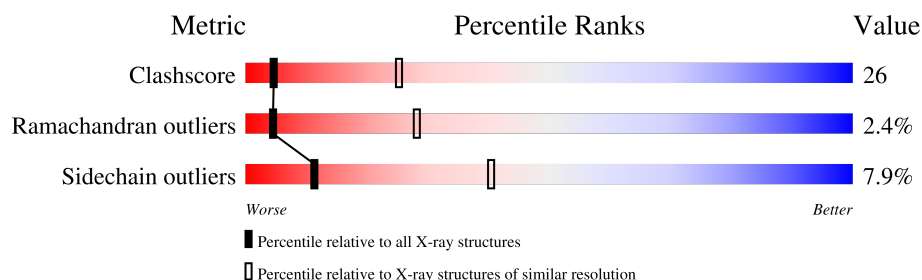
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

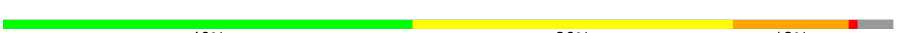
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	D	445	
1	G	445	
1	J	445	
1	M	445	
1	P	445	
2	B	269	
2	E	269	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

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

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
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 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
2	B	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	E	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	H	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
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 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

Continued on next page...

Continued from previous page...

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

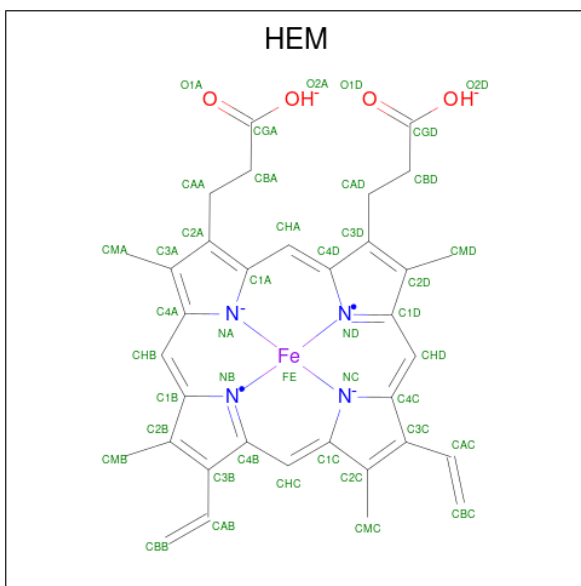
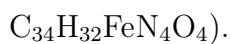
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:



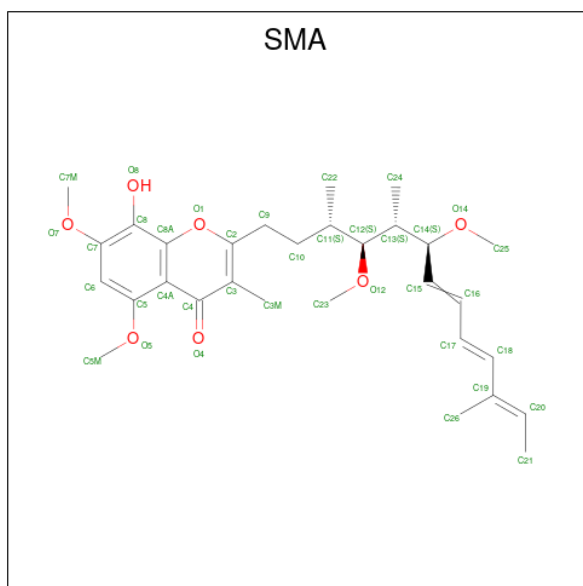
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

Continued on next page...

Continued from previous page...

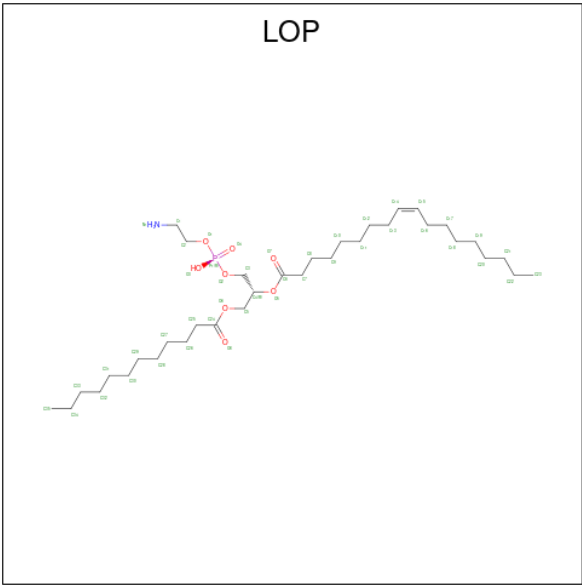
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



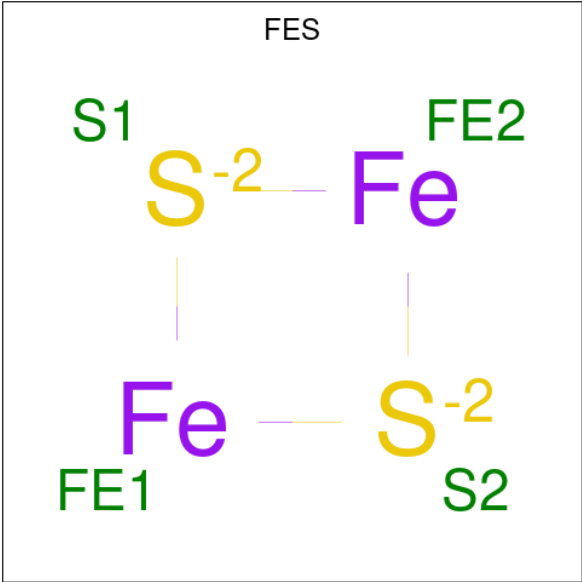
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			37	30 7		
5	D	1	Total	C O	0	0
			37	30 7		
5	G	1	Total	C O	0	0
			37	30 7		
5	J	1	Total	C O	0	0
			37	30 7		
5	M	1	Total	C O	0	0
			37	30 7		
5	P	1	Total	C O	0	0
			37	30 7		

- Molecule 6 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: FES) (formula: Fe₂S₂).



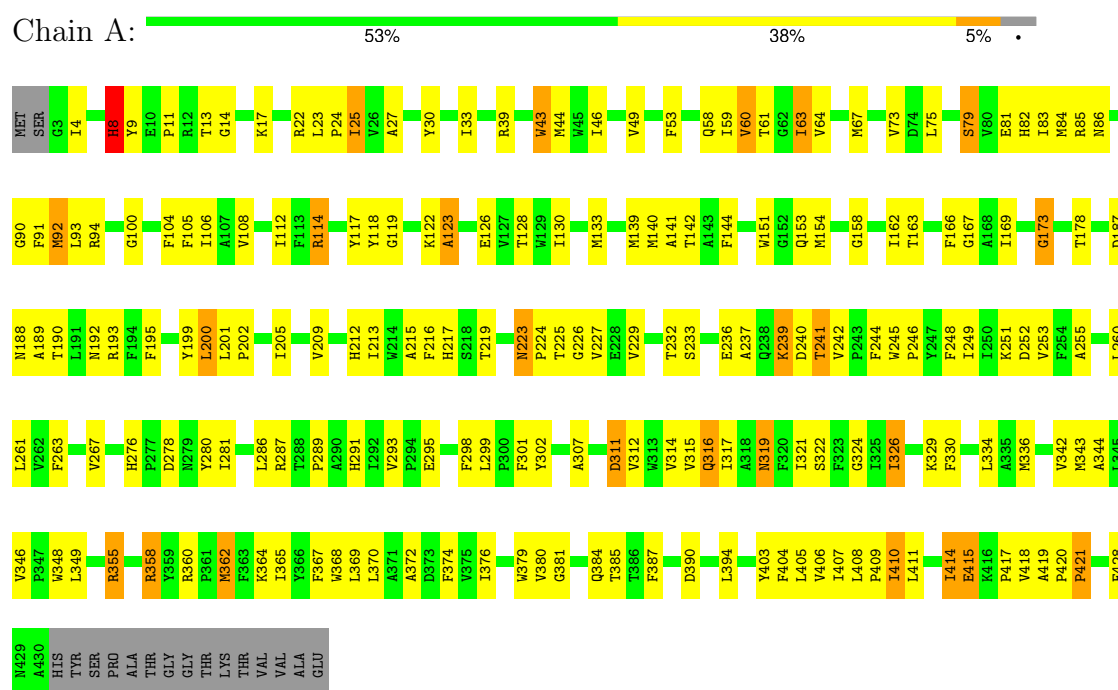
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S		
			4	2	2		
7	I	1	Total	Fe	S		
			4	2	2		
7	L	1	Total	Fe	S	0	0
			4	2	2		
7	O	1	Total	Fe	S		
			4	2	2		
7	R	1	Total	Fe	S		
			4	2	2		

3 Residue-property plots

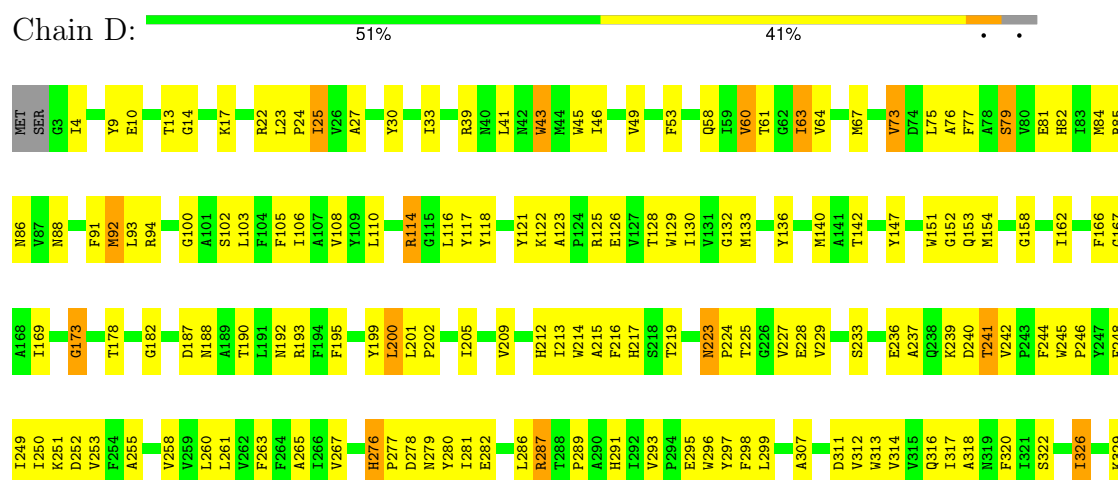
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Cytochrome b

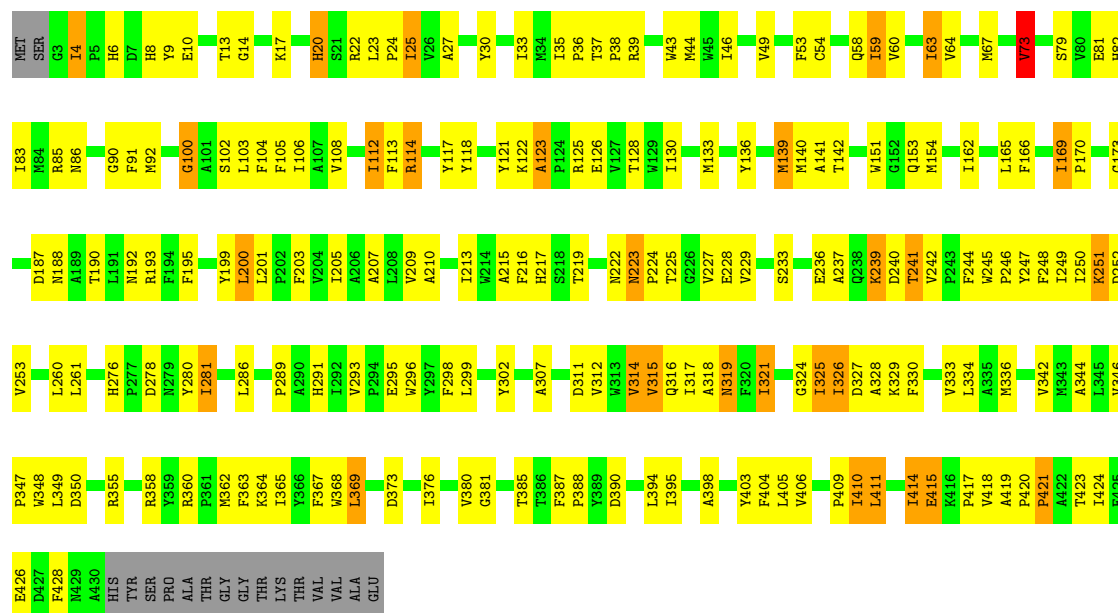


• Molecule 1: Cytochrome b



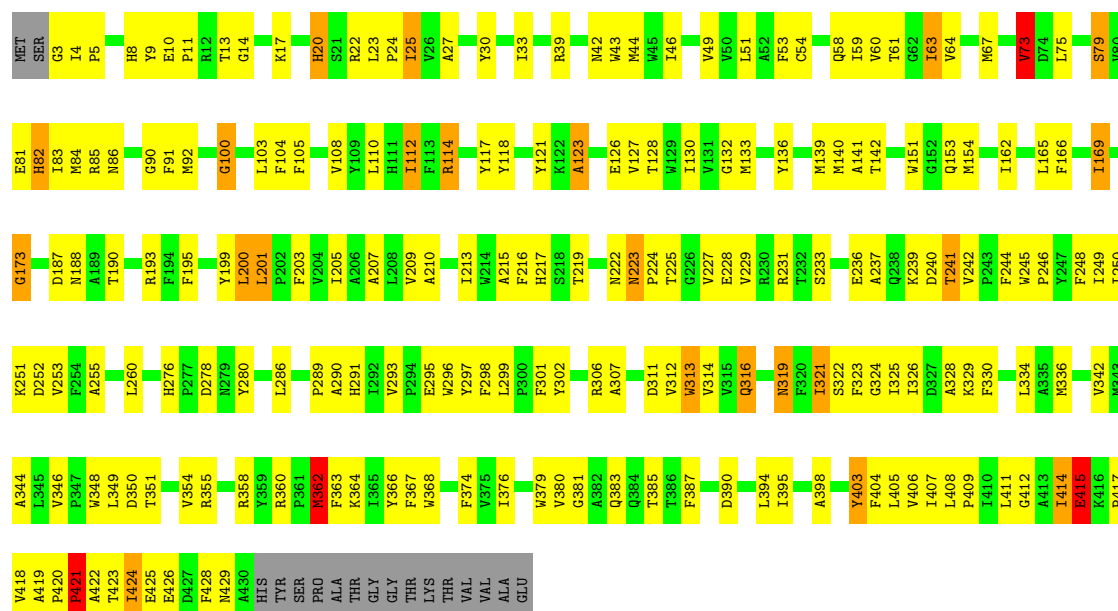
- Molecule 1: Cytochrome b

Chain G: 51% 38% 7% .

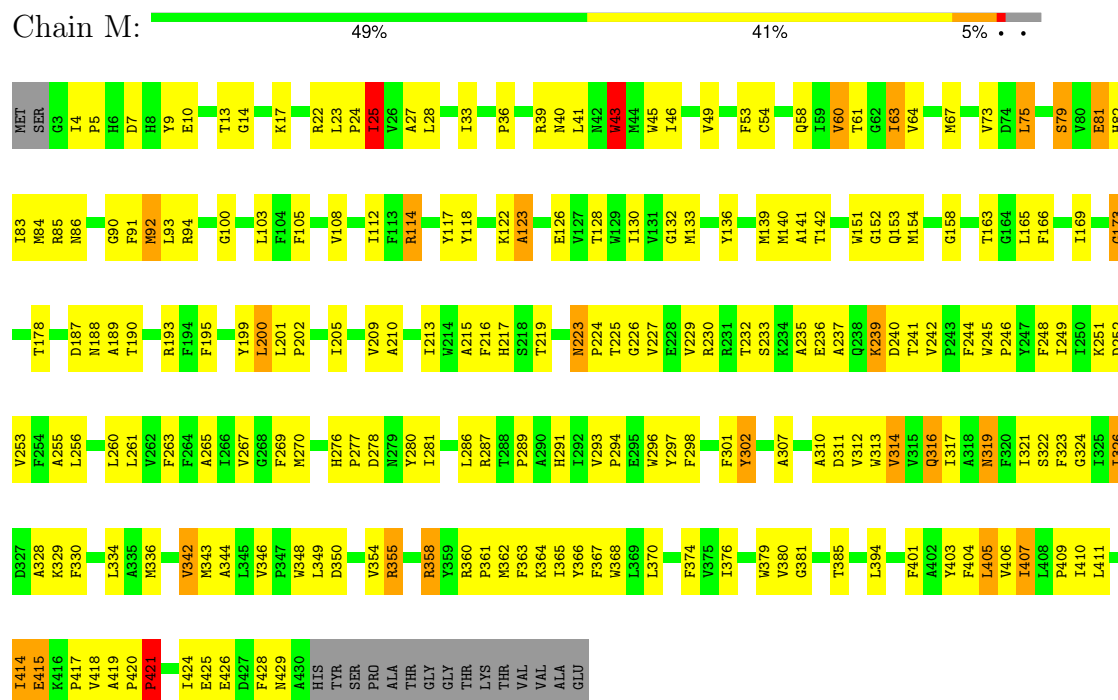


- Molecule 1: Cytochrome b

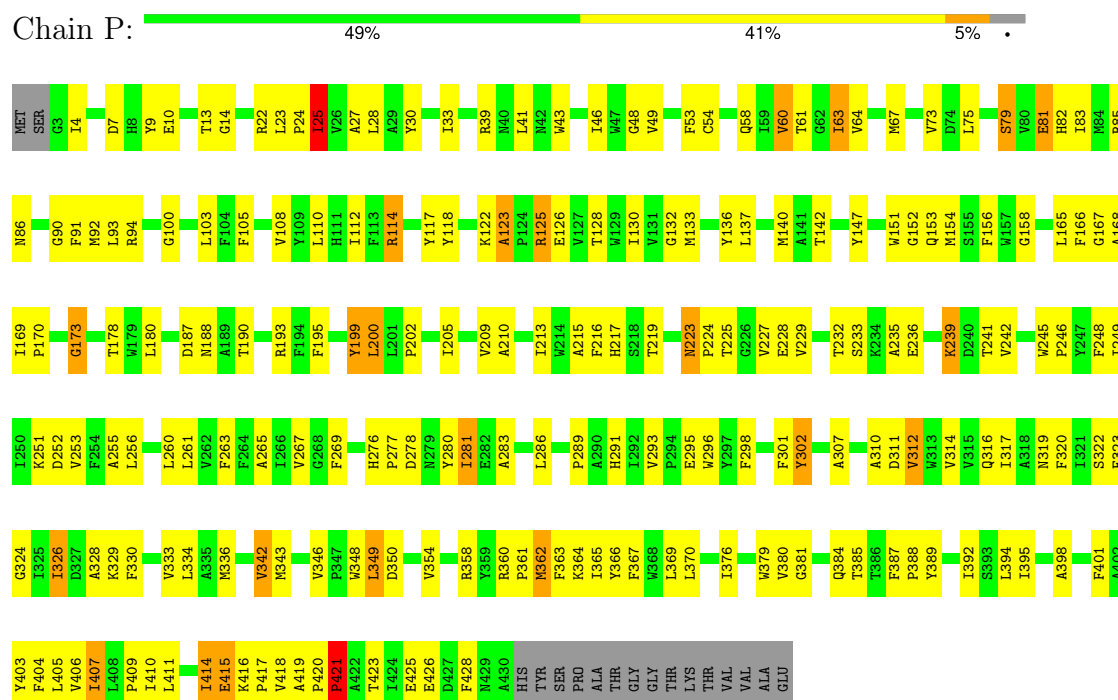
Chain J: 50% 41% 5% . .



• Molecule 1: Cytochrome b

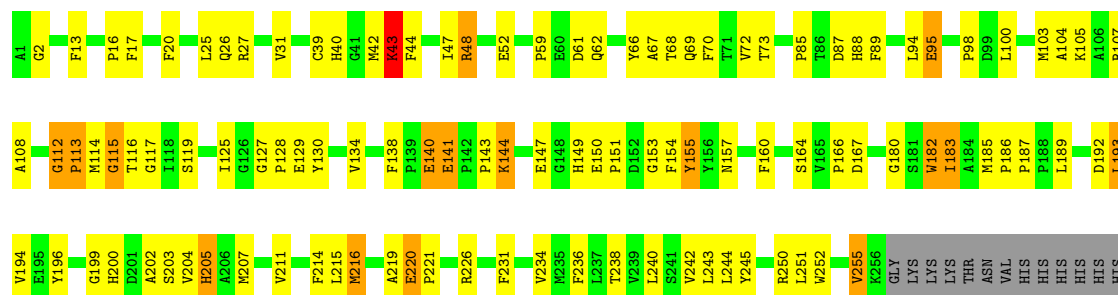


• Molecule 1: Cytochrome b



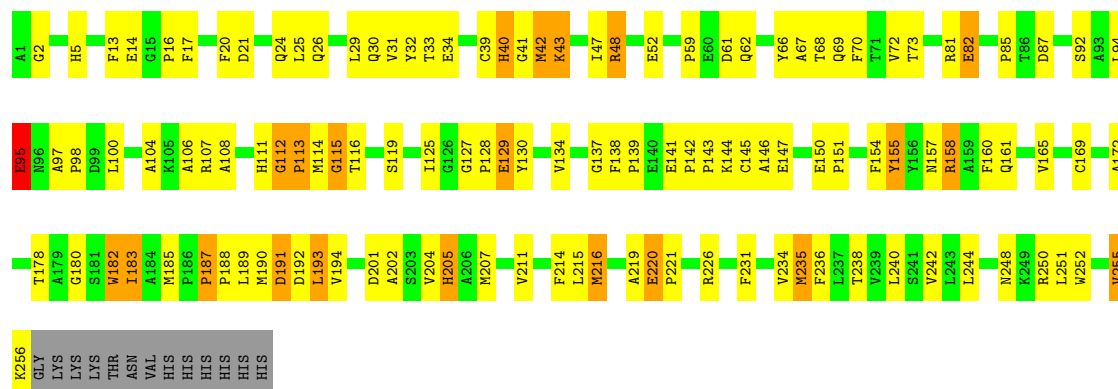
• Molecule 2: Cytochrome c1





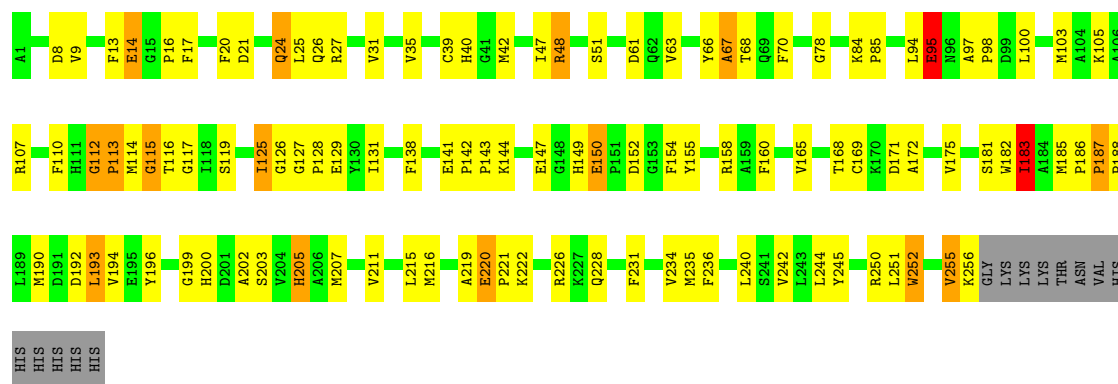
• Molecule 2: Cytochrome c1

Chain E: 49% 38% 8% 5%



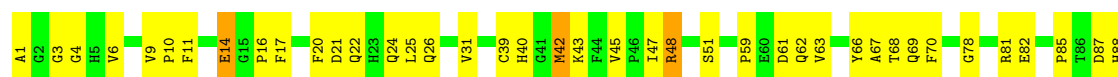
• Molecule 2: Cytochrome c1

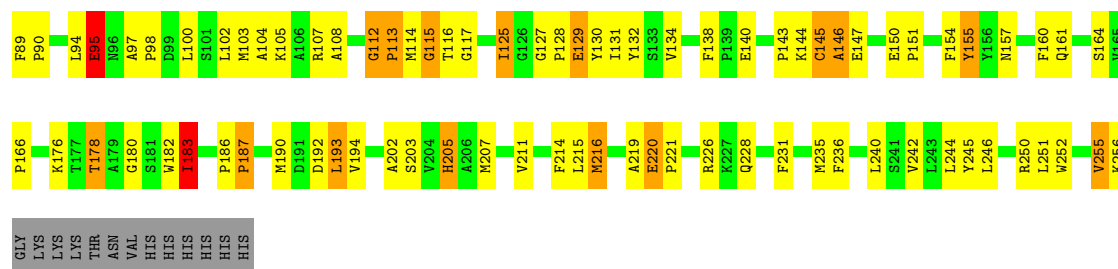
Chain H: 54% 35% 6% 5%



• Molecule 2: Cytochrome c1

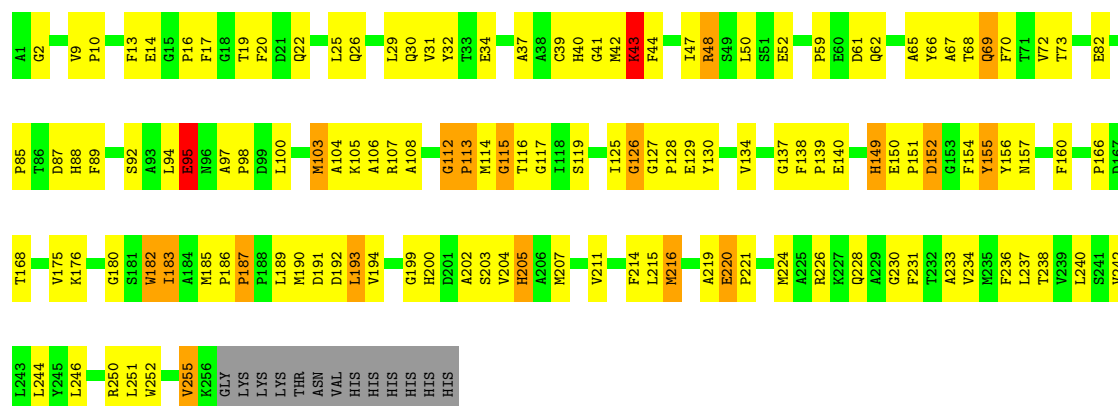
Chain K: 51% 37% 7% 5%





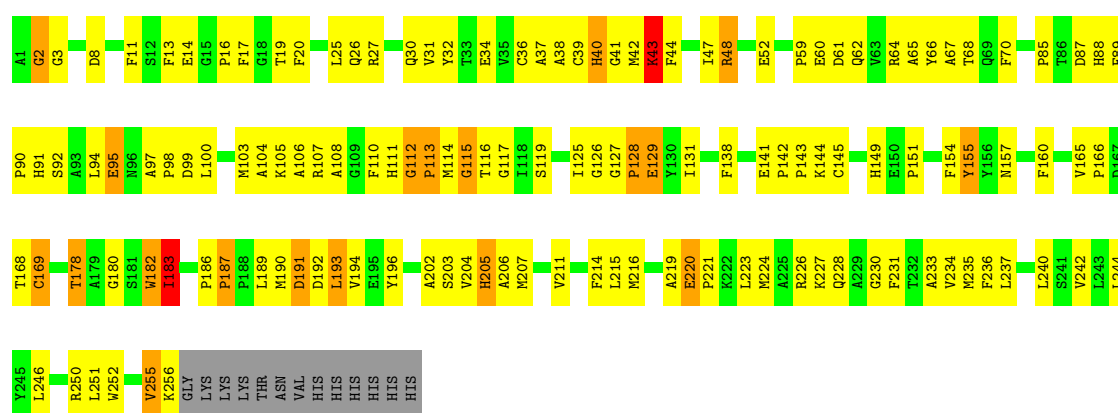
• Molecule 2: Cytochrome c1

Chain N: 46% 41% 7% • 5%



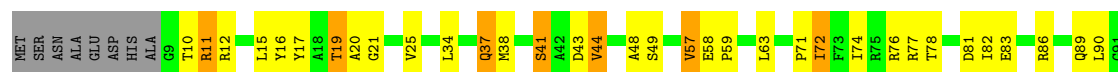
• Molecule 2: Cytochrome c1

Chain Q: 45% 43% 7% • 5%



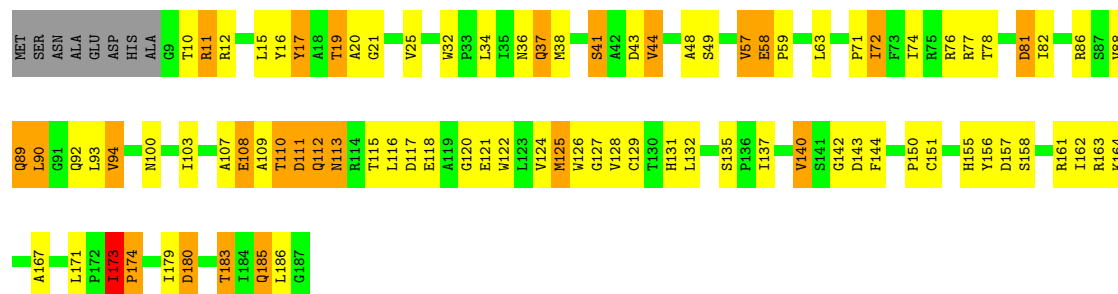
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C: 57% 30% 8% • •

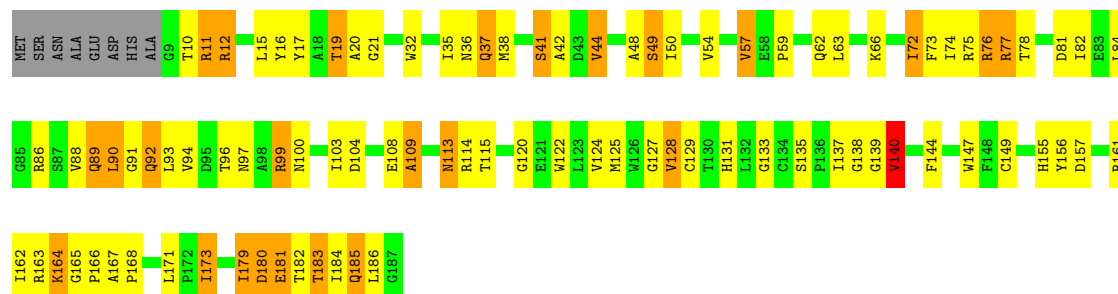




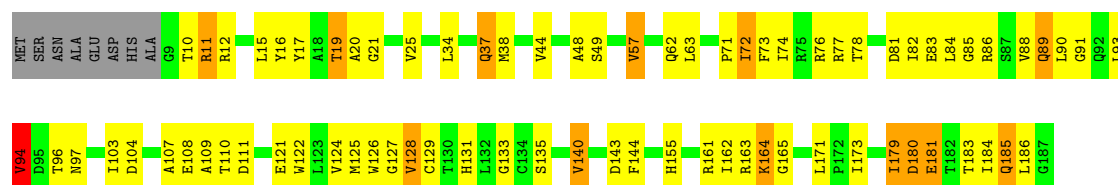
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



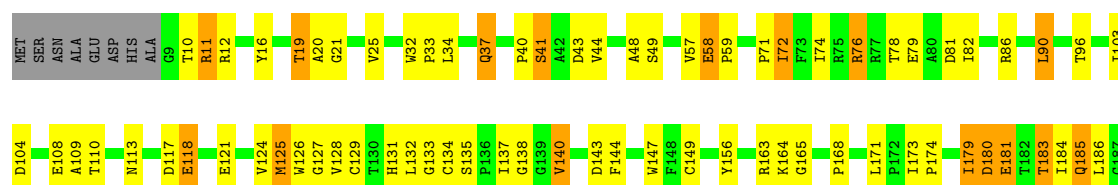
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



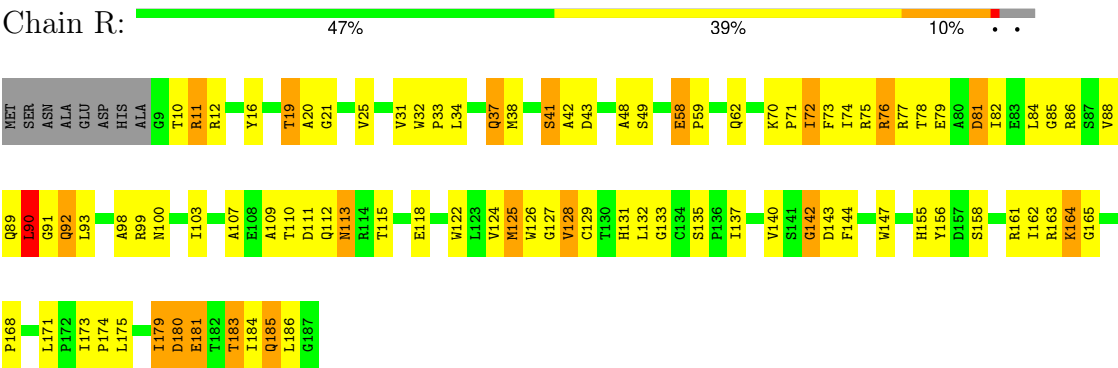
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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



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



4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	41688	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SMA, HEM, FES, 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	0.76	0/3570	1.09	18/4897 (0.4%)
1	D	0.79	0/3570	1.14	22/4897 (0.4%)
1	G	0.81	1/3570 (0.0%)	1.15	21/4897 (0.4%)
1	J	0.75	1/3570 (0.0%)	1.11	17/4897 (0.3%)
1	M	0.70	1/3570 (0.0%)	1.10	25/4897 (0.5%)
1	P	0.74	1/3570 (0.0%)	1.14	28/4897 (0.6%)
2	B	0.69	0/2010	1.11	9/2733 (0.3%)
2	E	0.69	1/2010 (0.0%)	1.16	14/2733 (0.5%)
2	H	0.78	4/2010 (0.2%)	1.15	13/2733 (0.5%)
2	K	0.66	0/2010	1.15	14/2733 (0.5%)
2	N	0.65	0/2010	1.14	18/2733 (0.7%)
2	Q	0.70	0/2010	1.19	17/2733 (0.6%)
3	C	0.86	0/1370	1.24	14/1866 (0.8%)
3	F	0.83	1/1370 (0.1%)	1.23	11/1866 (0.6%)
3	I	0.82	0/1370	1.32	20/1866 (1.1%)
3	L	0.78	0/1370	1.21	13/1866 (0.7%)
3	O	0.77	0/1370	1.23	12/1866 (0.6%)
3	R	0.76	0/1370	1.24	15/1866 (0.8%)
All	All	0.75	10/41700 (0.0%)	1.16	301/56976 (0.5%)

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	139	MET	SD-CE	6.42	1.95	1.79
2	H	14	GLU	CB-CG	6.08	1.70	1.52
2	H	14	GLU	CG-CD	6.07	1.67	1.52
3	F	88	VAL	CA-CB	6.05	1.62	1.54
2	H	190	MET	SD-CE	5.80	1.94	1.79

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	133	GLY	N-CA-C	11.04	125.39	113.58
2	E	14	GLU	N-CA-C	-9.40	97.56	110.35
2	Q	115	GLY	N-CA-C	-9.32	102.28	115.43
1	D	416	LYS	CA-C-N	9.12	129.68	119.92
1	D	416	LYS	C-N-CA	9.12	129.68	119.92

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

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	192	0
1	D	3440	0	3428	186	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3440	0	3428	202	0
1	J	3440	0	3428	200	0
1	M	3440	0	3428	206	0
1	P	3440	0	3428	193	0
2	B	1953	0	1848	106	0
2	E	1953	0	1848	115	0
2	H	1953	0	1848	112	0
2	K	1953	0	1848	117	0
2	N	1953	0	1848	120	0
2	Q	1953	0	1848	137	0
3	C	1340	0	1303	60	0
3	F	1340	0	1303	81	0
3	I	1340	0	1303	73	0
3	L	1340	0	1303	54	0
3	O	1340	0	1303	57	0
3	R	1340	0	1303	79	0
4	A	86	0	60	6	0
4	B	43	0	30	1	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	12	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	4	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

Continued on next page...

Continued from previous page...

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	2139	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 26.

The worst 5 of 2139 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%)	9	39
1	D	426/445 (96%)	385 (90%)	37 (9%)	4 (1%)	14	47
1	G	426/445 (96%)	384 (90%)	34 (8%)	8 (2%)	6	33
1	J	426/445 (96%)	379 (89%)	37 (9%)	10 (2%)	5	29
1	M	426/445 (96%)	380 (89%)	38 (9%)	8 (2%)	6	33
1	P	426/445 (96%)	380 (89%)	39 (9%)	7 (2%)	7	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	254/269 (94%)	224 (88%)	23 (9%)	7 (3%)	4	25
2	E	254/269 (94%)	218 (86%)	28 (11%)	8 (3%)	3	22
2	H	254/269 (94%)	220 (87%)	29 (11%)	5 (2%)	6	31
2	K	254/269 (94%)	225 (89%)	21 (8%)	8 (3%)	3	22
2	N	254/269 (94%)	219 (86%)	26 (10%)	9 (4%)	3	20
2	Q	254/269 (94%)	215 (85%)	30 (12%)	9 (4%)	3	20
3	C	177/187 (95%)	153 (86%)	20 (11%)	4 (2%)	5	29
3	F	177/187 (95%)	153 (86%)	18 (10%)	6 (3%)	3	20
3	I	177/187 (95%)	151 (85%)	19 (11%)	7 (4%)	2	17
3	L	177/187 (95%)	151 (85%)	21 (12%)	5 (3%)	4	25
3	O	177/187 (95%)	154 (87%)	19 (11%)	4 (2%)	5	29
3	R	177/187 (95%)	149 (84%)	21 (12%)	7 (4%)	2	17
All	All	5142/5406 (95%)	4532 (88%)	488 (10%)	122 (2%)	4	28

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 ⓘ

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%)	329 (93%)	24 (7%)	14	46
1	D	353/366 (96%)	330 (94%)	23 (6%)	15	47
1	G	353/366 (96%)	327 (93%)	26 (7%)	13	43
1	J	353/366 (96%)	328 (93%)	25 (7%)	13	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	353/366 (96%)	328 (93%)	25 (7%)	13	44
1	P	353/366 (96%)	333 (94%)	20 (6%)	18	51
2	B	203/215 (94%)	193 (95%)	10 (5%)	22	55
2	E	203/215 (94%)	188 (93%)	15 (7%)	13	43
2	H	203/215 (94%)	190 (94%)	13 (6%)	16	48
2	K	203/215 (94%)	190 (94%)	13 (6%)	16	48
2	N	203/215 (94%)	191 (94%)	12 (6%)	18	50
2	Q	203/215 (94%)	191 (94%)	12 (6%)	18	50
3	C	138/144 (96%)	119 (86%)	19 (14%)	3	18
3	F	138/144 (96%)	115 (83%)	23 (17%)	2	11
3	I	138/144 (96%)	120 (87%)	18 (13%)	4	20
3	L	138/144 (96%)	120 (87%)	18 (13%)	4	20
3	O	138/144 (96%)	121 (88%)	17 (12%)	4	22
3	R	138/144 (96%)	120 (87%)	18 (13%)	4	20
All	All	4164/4350 (96%)	3833 (92%)	331 (8%)	11	40

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	60	VAL
1	P	178	THR
1	M	219	THR
2	N	155	TYR
1	P	421	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	8	HIS
3	R	113	ASN
3	L	92	GLN
3	R	39	ASN
1	P	223	ASN

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 ⓘ

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	D	502	1	50,50,50	1.35	4 (8%)	67,82,82	1.13	4 (5%)
5	SMA	D	503	-	38,38,38	2.53	11 (28%)	47,52,52	1.80	11 (23%)
6	LOP	D	504	-	44,44,44	0.73	0	47,49,49	1.38	5 (10%)
6	LOP	M	504	-	44,44,44	0.73	0	47,49,49	1.39	7 (14%)
4	HEM	K	301	2	50,50,50	1.55	7 (14%)	67,82,82	1.08	4 (5%)
5	SMA	J	503	-	38,38,38	1.91	6 (15%)	47,52,52	1.98	11 (23%)
7	FES	O	200	3	0,4,4	-	-	-	-	-
4	HEM	Q	301	2	50,50,50	1.32	3 (6%)	67,82,82	1.05	3 (4%)
5	SMA	G	503	-	38,38,38	1.96	10 (26%)	47,52,52	2.16	10 (21%)
6	LOP	G	504	-	44,44,44	0.78	1 (2%)	47,49,49	1.42	6 (12%)
7	FES	L	200	3	0,4,4	-	-	-	-	-
4	HEM	D	501	1	50,50,50	1.33	4 (8%)	67,82,82	1.08	3 (4%)
6	LOP	A	504	-	44,44,44	0.65	0	47,49,49	1.33	6 (12%)
4	HEM	E	301	2	50,50,50	1.42	5 (10%)	67,82,82	1.05	3 (4%)
4	HEM	H	301	2	50,50,50	1.40	3 (6%)	67,82,82	1.08	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FES	C	200	3	0,4,4	-	-	-		
4	HEM	G	501	1	50,50,50	1.35	5 (10%)	67,82,82	1.07	4 (5%)
4	HEM	M	502	1	50,50,50	1.54	7 (14%)	67,82,82	1.17	4 (5%)
5	SMA	M	503	-	38,38,38	2.15	10 (26%)	47,52,52	2.13	11 (23%)
4	HEM	B	301	2	50,50,50	1.39	4 (8%)	67,82,82	1.08	3 (4%)
4	HEM	J	501	1	50,50,50	1.49	7 (14%)	67,82,82	1.03	3 (4%)
5	SMA	P	503	-	38,38,38	2.21	10 (26%)	47,52,52	1.79	11 (23%)
4	HEM	N	301	2	50,50,50	1.40	4 (8%)	67,82,82	1.11	4 (5%)
7	FES	F	200	3	0,4,4	-	-	-		
4	HEM	P	501	1	50,50,50	1.48	6 (12%)	67,82,82	1.17	3 (4%)
4	HEM	A	501	1	50,50,50	1.40	5 (10%)	67,82,82	1.04	3 (4%)
4	HEM	M	501	1	50,50,50	1.40	5 (10%)	67,82,82	1.07	3 (4%)
6	LOP	J	504	-	44,44,44	0.66	0	47,49,49	1.31	4 (8%)
6	LOP	P	504	-	44,44,44	0.67	1 (2%)	47,49,49	1.34	5 (10%)
4	HEM	A	502	1	50,50,50	1.66	9 (18%)	67,82,82	1.29	7 (10%)
4	HEM	G	502	1	50,50,50	1.54	6 (12%)	67,82,82	1.17	4 (5%)
7	FES	R	200	3	0,4,4	-	-	-		
5	SMA	A	503	-	38,38,38	1.95	8 (21%)	47,52,52	2.07	11 (23%)
7	FES	I	200	3	0,4,4	-	-	-		
4	HEM	J	502	1	50,50,50	1.45	5 (10%)	67,82,82	1.23	5 (7%)
4	HEM	P	502	1	50,50,50	1.48	5 (10%)	67,82,82	1.24	5 (7%)

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	D	502	1	-	8/14/54/54	-
5	SMA	D	503	-	-	4/34/34/34	0/2/2/2
6	LOP	D	504	-	-	5/48/48/48	-
6	LOP	M	504	-	-	6/48/48/48	-
4	HEM	K	301	2	-	8/14/54/54	-
5	SMA	J	503	-	-	8/34/34/34	0/2/2/2
7	FES	O	200	3	-	-	0/1/1/1
4	HEM	Q	301	2	-	11/14/54/54	-
5	SMA	G	503	-	-	7/34/34/34	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LOP	G	504	-	-	8/48/48/48	-
7	FES	L	200	3	-	-	0/1/1/1
4	HEM	D	501	1	-	8/14/54/54	-
6	LOP	A	504	-	-	12/48/48/48	-
4	HEM	E	301	2	-	8/14/54/54	-
4	HEM	H	301	2	-	8/14/54/54	-
7	FES	C	200	3	-	-	0/1/1/1
4	HEM	G	501	1	-	6/14/54/54	-
4	HEM	M	502	1	-	8/14/54/54	-
5	SMA	M	503	-	-	11/34/34/34	0/2/2/2
4	HEM	B	301	2	-	6/14/54/54	-
4	HEM	J	501	1	-	7/14/54/54	-
5	SMA	P	503	-	-	8/34/34/34	0/2/2/2
4	HEM	N	301	2	-	13/14/54/54	-
7	FES	F	200	3	-	-	0/1/1/1
4	HEM	P	501	1	-	9/14/54/54	-
4	HEM	A	501	1	-	4/14/54/54	-
4	HEM	M	501	1	-	12/14/54/54	-
6	LOP	J	504	-	-	12/48/48/48	-
6	LOP	P	504	-	-	4/48/48/48	-
4	HEM	A	502	1	-	8/14/54/54	-
4	HEM	G	502	1	-	9/14/54/54	-
7	FES	R	200	3	-	-	0/1/1/1
5	SMA	A	503	-	-	7/34/34/34	0/2/2/2
7	FES	I	200	3	-	-	0/1/1/1
4	HEM	J	502	1	-	8/14/54/54	-
4	HEM	P	502	1	-	9/14/54/54	-

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SMA	O5-C5	8.05	1.50	1.37
5	M	503	SMA	O5-C5	7.17	1.48	1.37
5	P	503	SMA	O5-C5	6.82	1.48	1.37
5	J	503	SMA	O5-C5	6.82	1.48	1.37
5	P	503	SMA	O7-C7	6.34	1.47	1.37

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	SMA	C5M-O5-C5	-6.73	107.63	117.51
5	G	503	SMA	O7-C7-C8	6.67	121.51	114.53
5	A	503	SMA	O7-C7-C8	5.92	120.72	114.53
5	M	503	SMA	O7-C7-C8	5.58	120.37	114.53
5	G	503	SMA	C5M-O5-C5	-5.30	109.73	117.51

There are no chirality outliers.

5 of 242 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	A	502	HEM	C2C-C3C-CAC-CBC
4	B	301	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

33 monomers are involved in 106 short contacts:

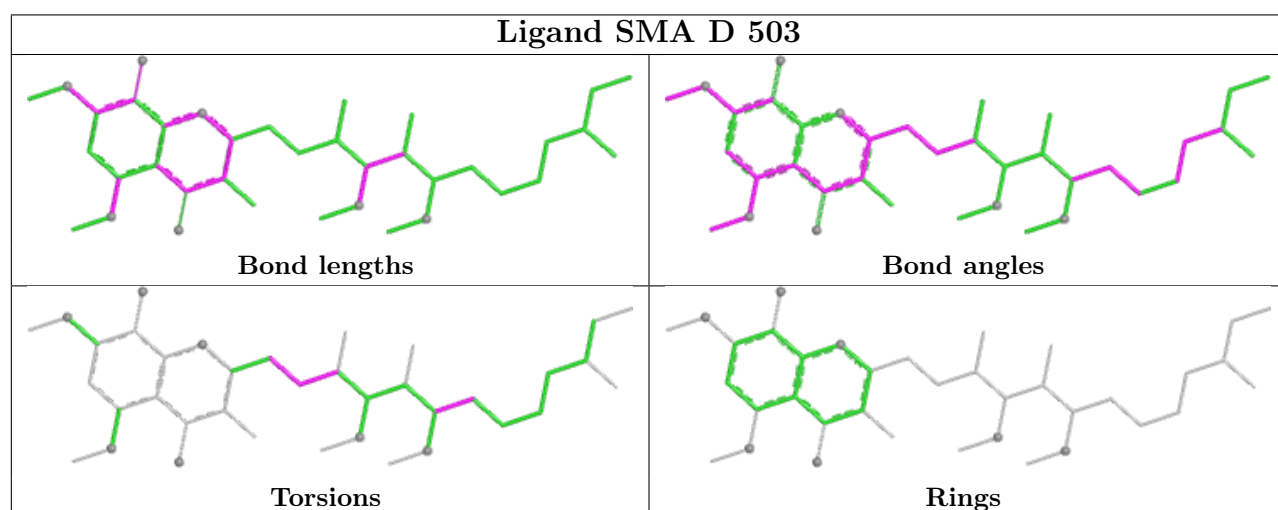
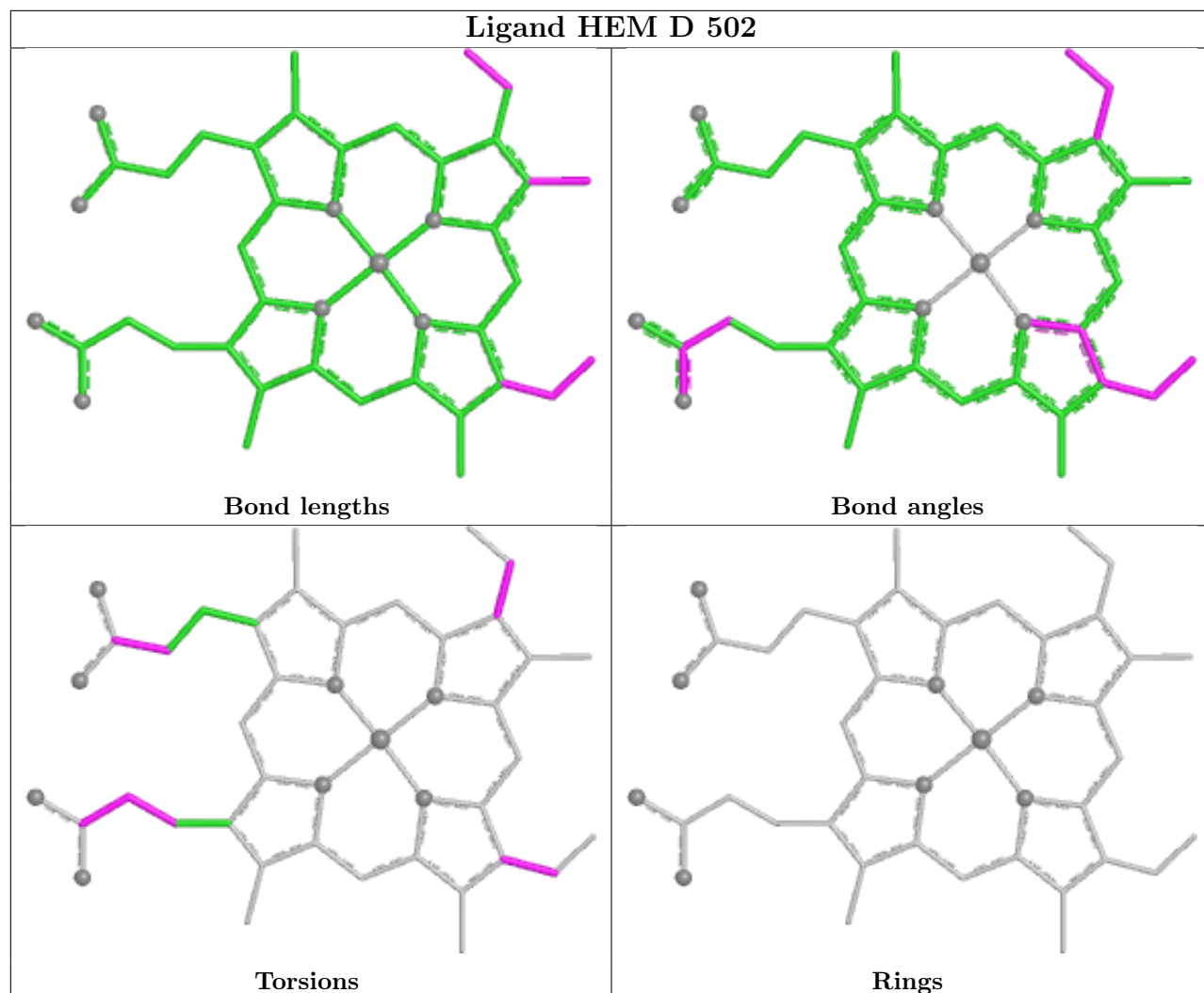
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	HEM	4	0
5	D	503	SMA	1	0
6	D	504	LOP	1	0
6	M	504	LOP	3	0
4	K	301	HEM	1	0
5	J	503	SMA	1	0
7	O	200	FES	1	0
4	Q	301	HEM	1	0
5	G	503	SMA	1	0
6	G	504	LOP	5	0
4	D	501	HEM	8	0
6	A	504	LOP	4	0
4	E	301	HEM	1	0
4	H	301	HEM	2	0
7	C	200	FES	2	0
4	G	501	HEM	8	0
4	M	502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

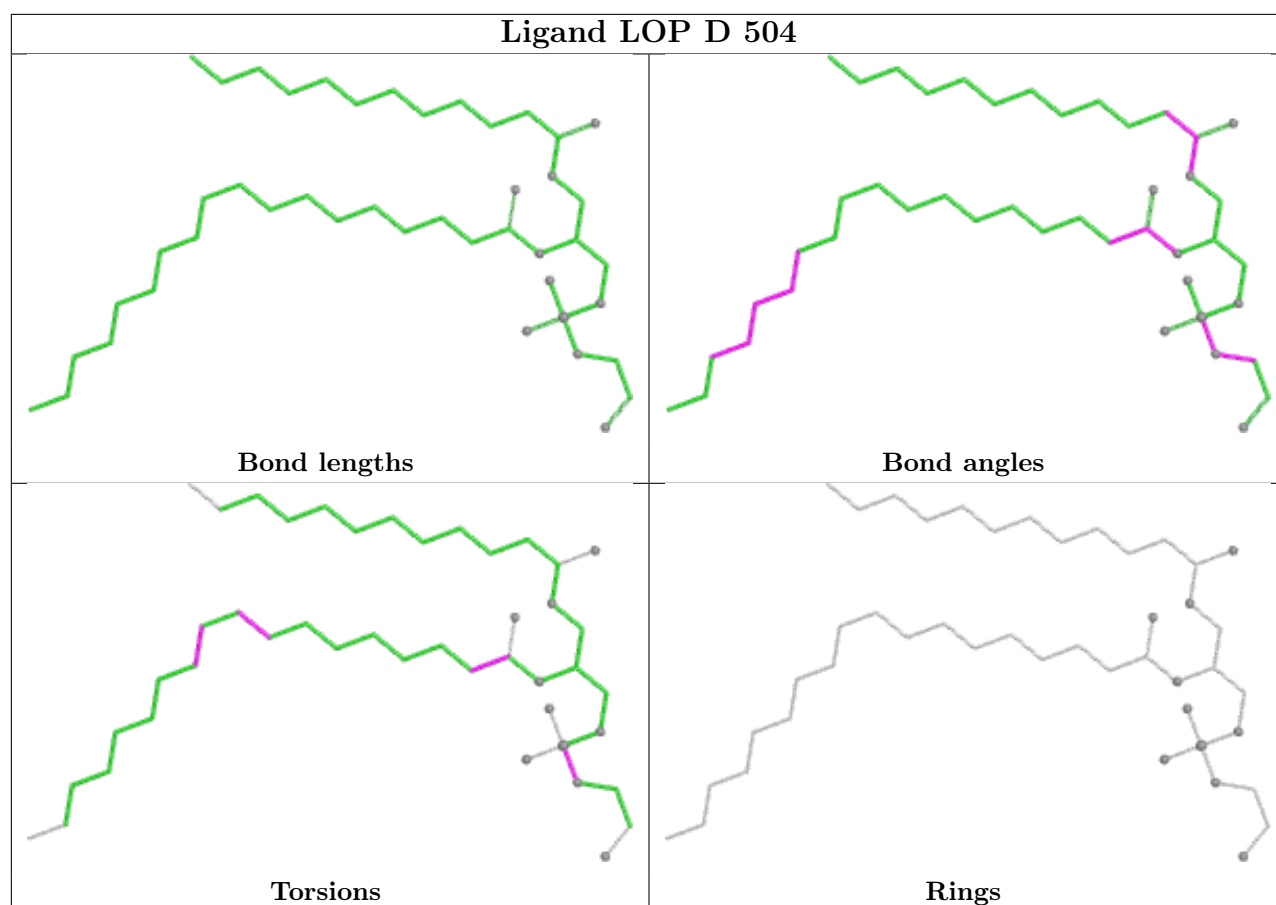
Continued on next page...

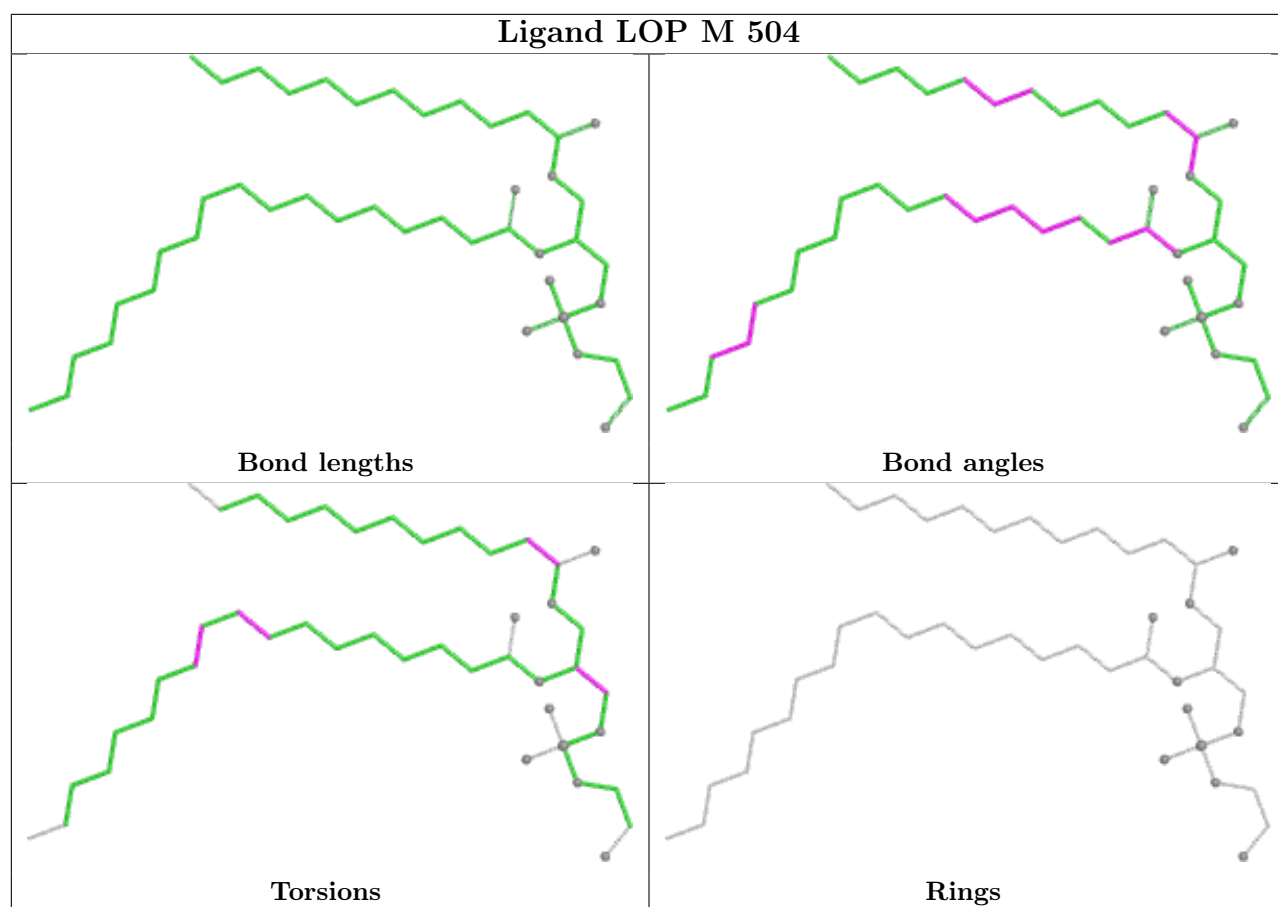
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	200	FES	2	0
4	P	501	HEM	7	0
4	A	501	HEM	3	0
4	M	501	HEM	11	0
6	J	504	LOP	1	0
6	P	504	LOP	1	0
4	A	502	HEM	3	0
4	G	502	HEM	2	0
7	R	200	FES	1	0
5	A	503	SMA	2	0
4	J	502	HEM	7	0
4	P	502	HEM	5	0

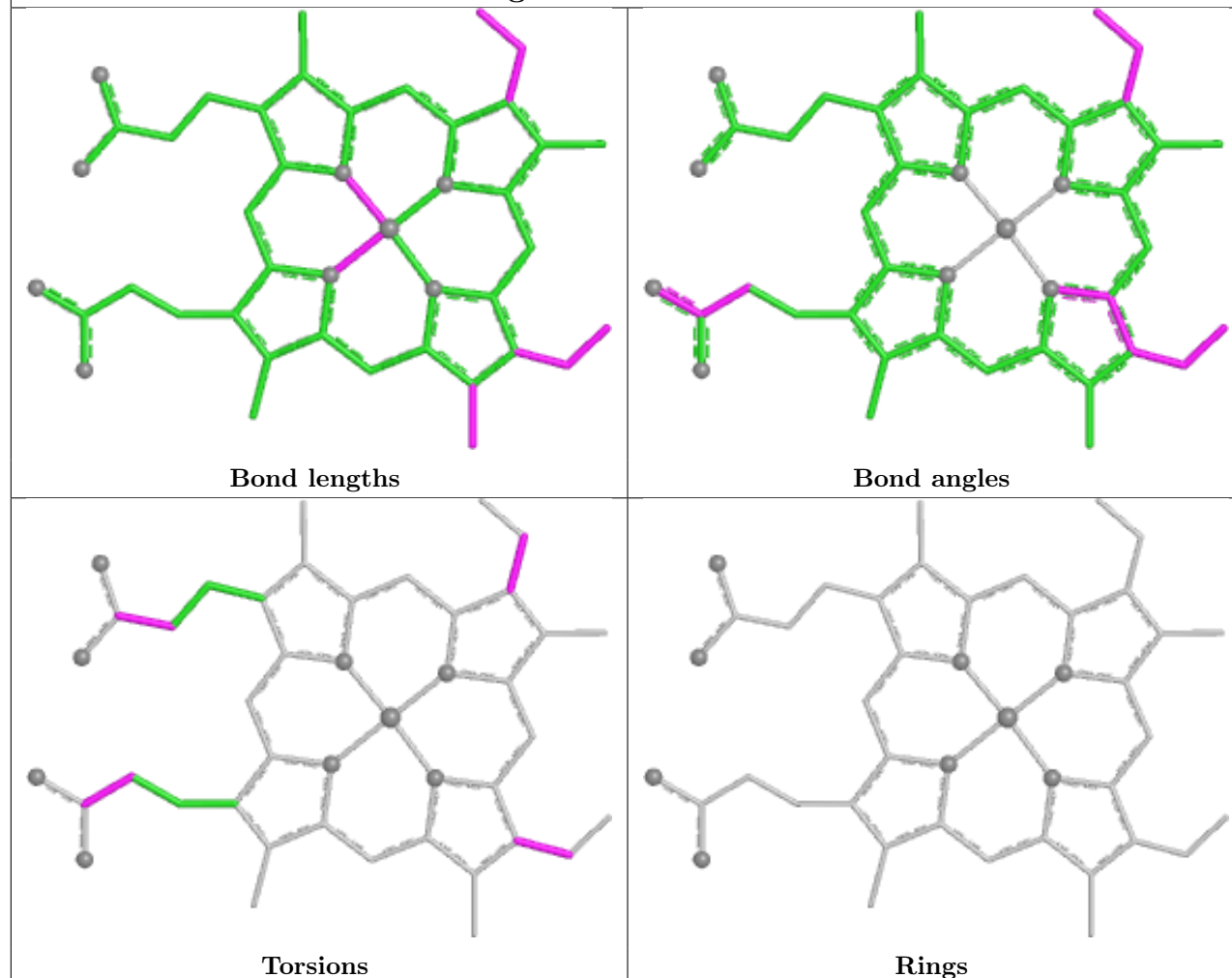
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



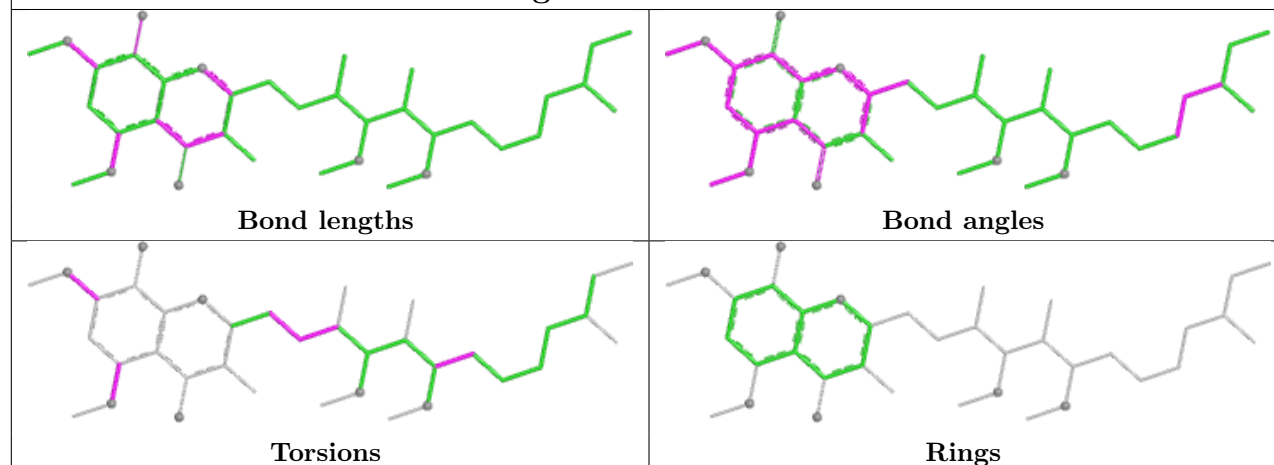


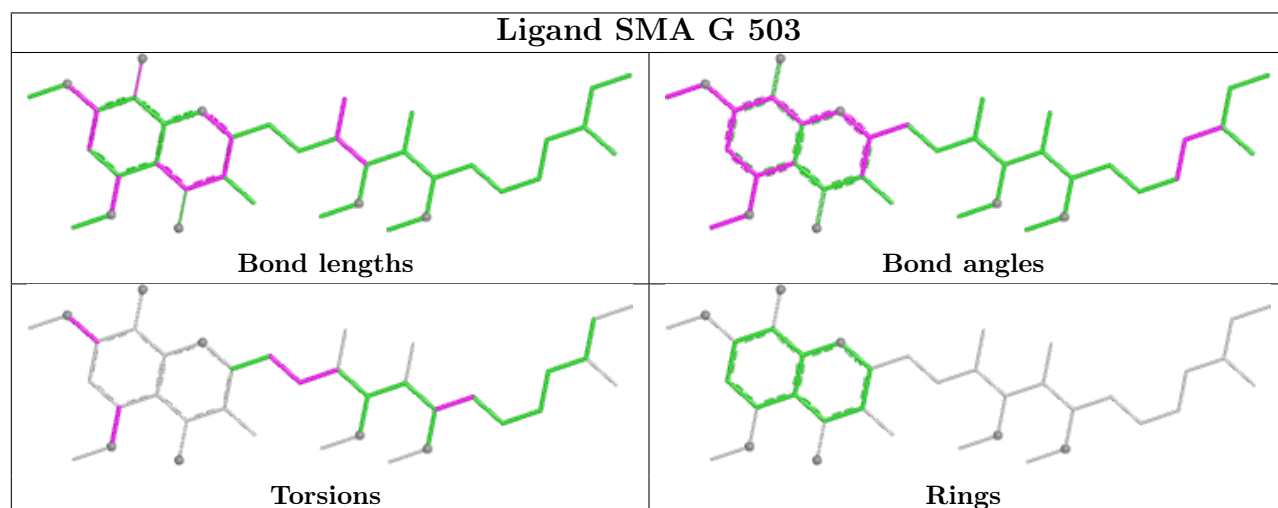
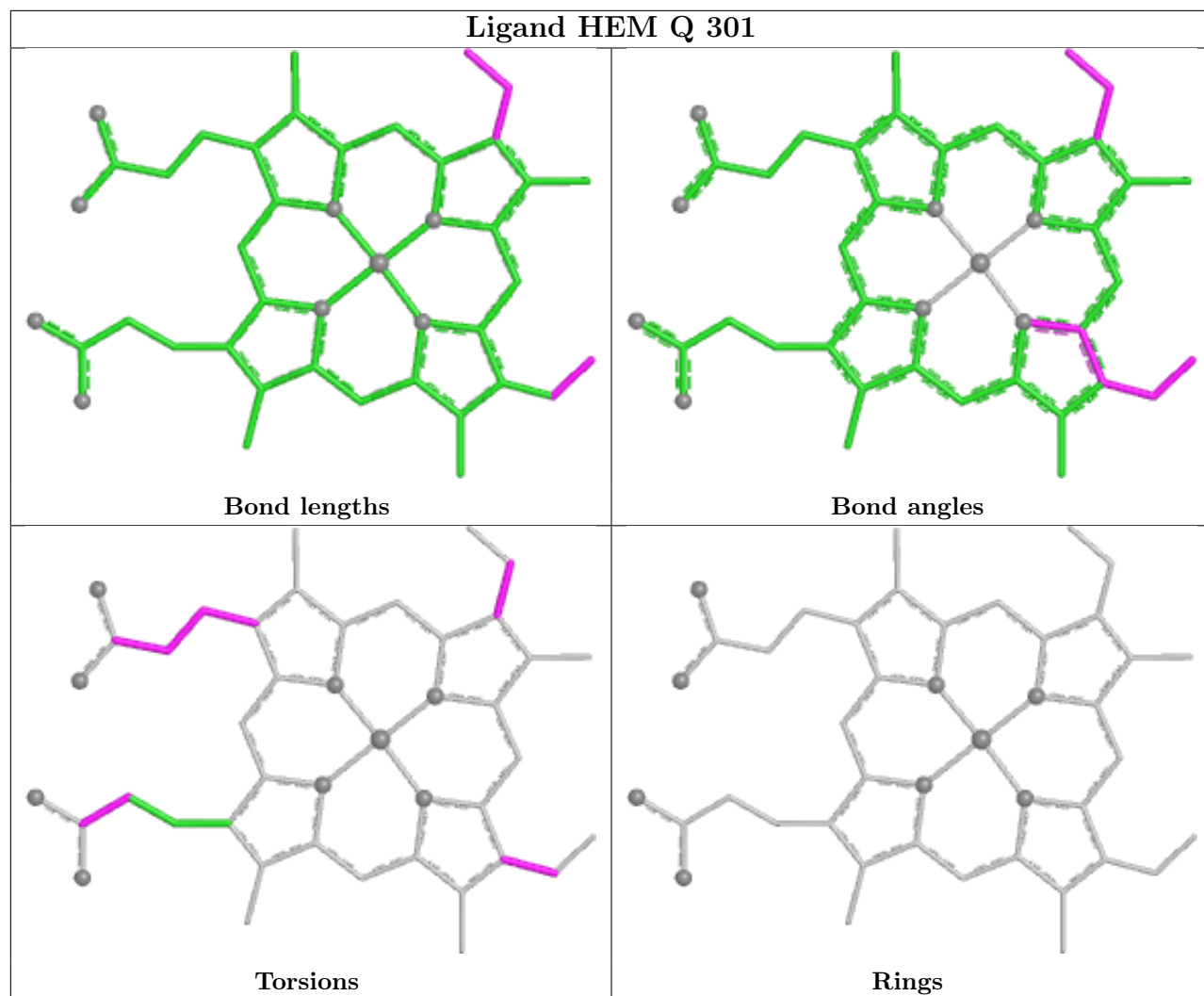


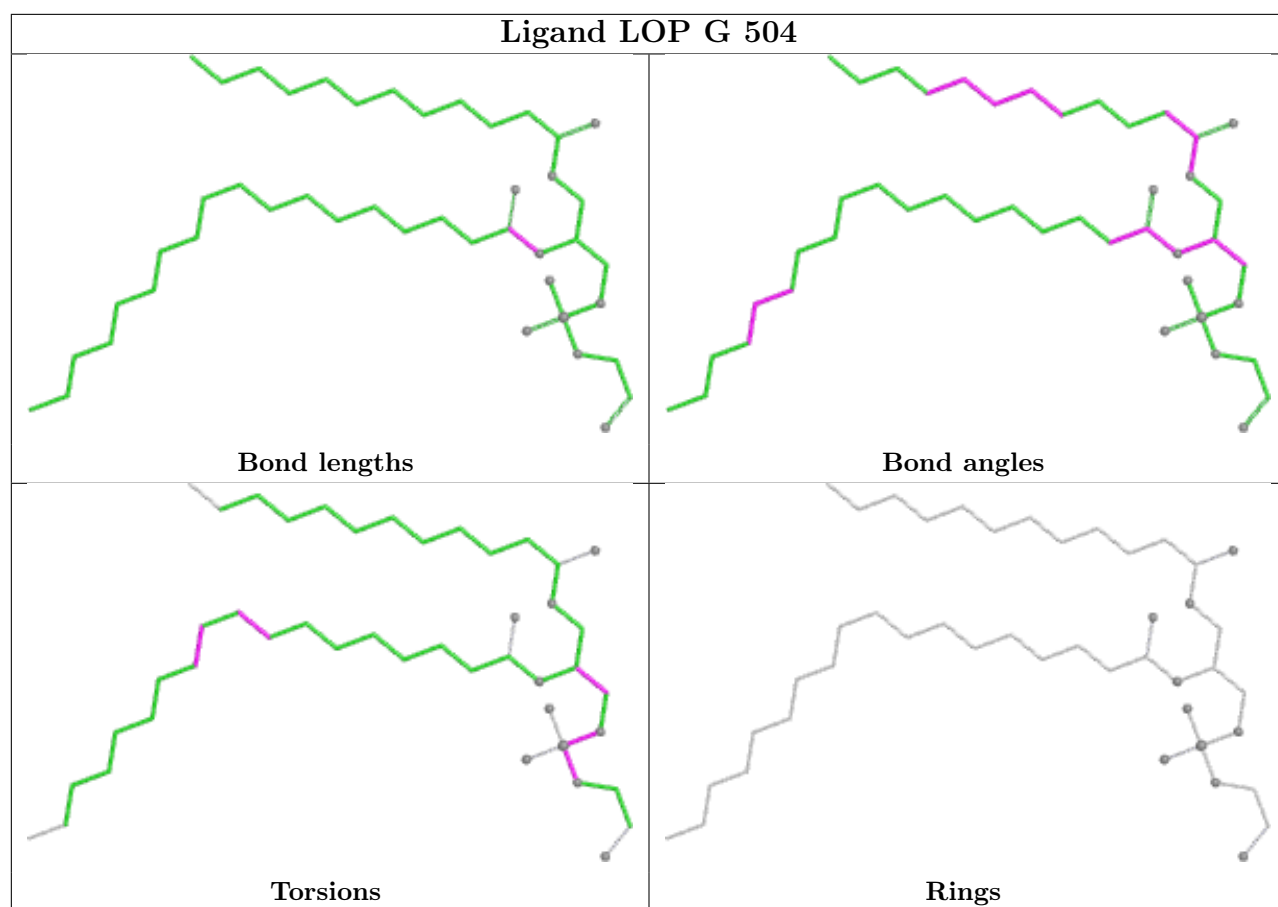
Ligand HEM K 301

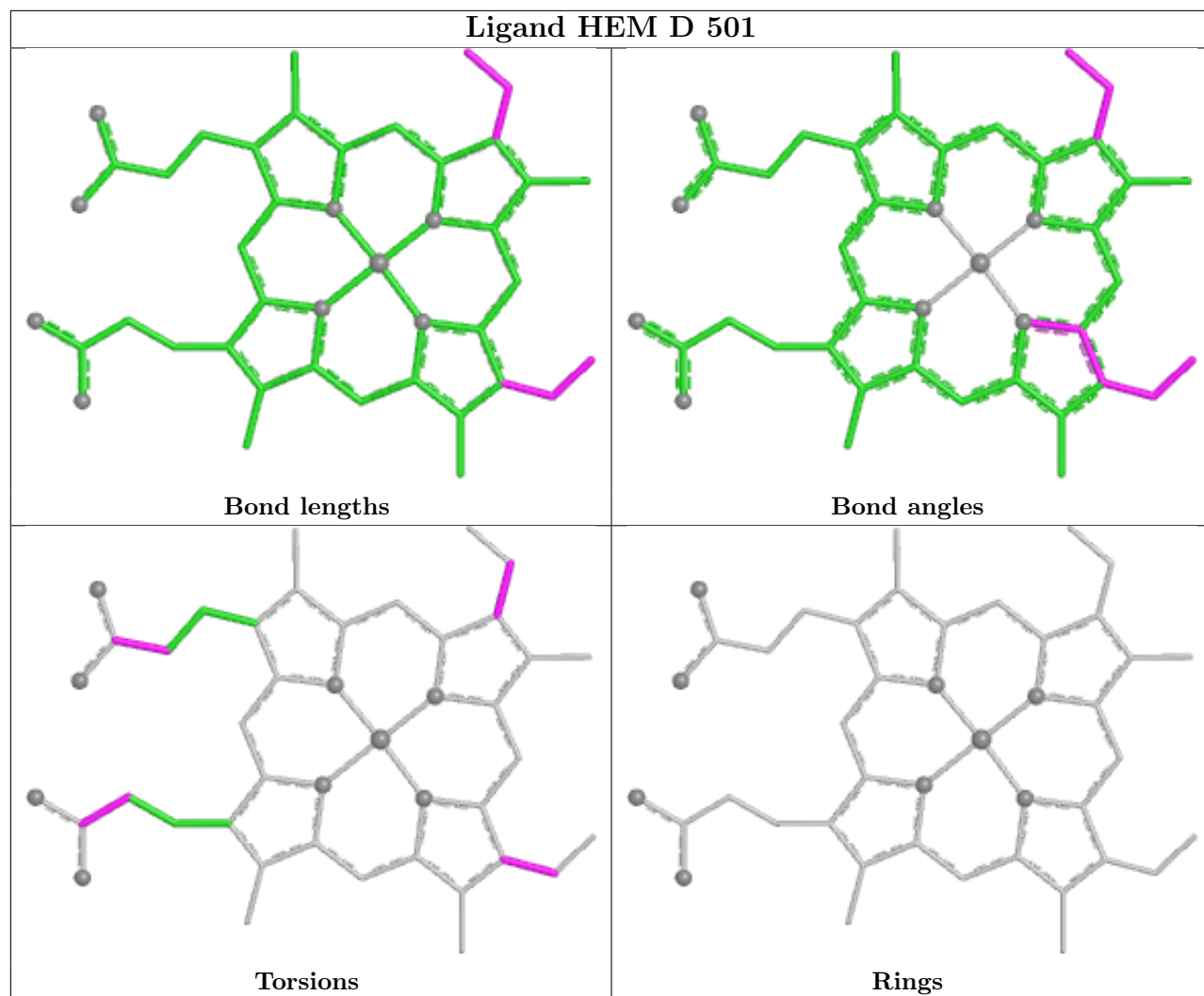


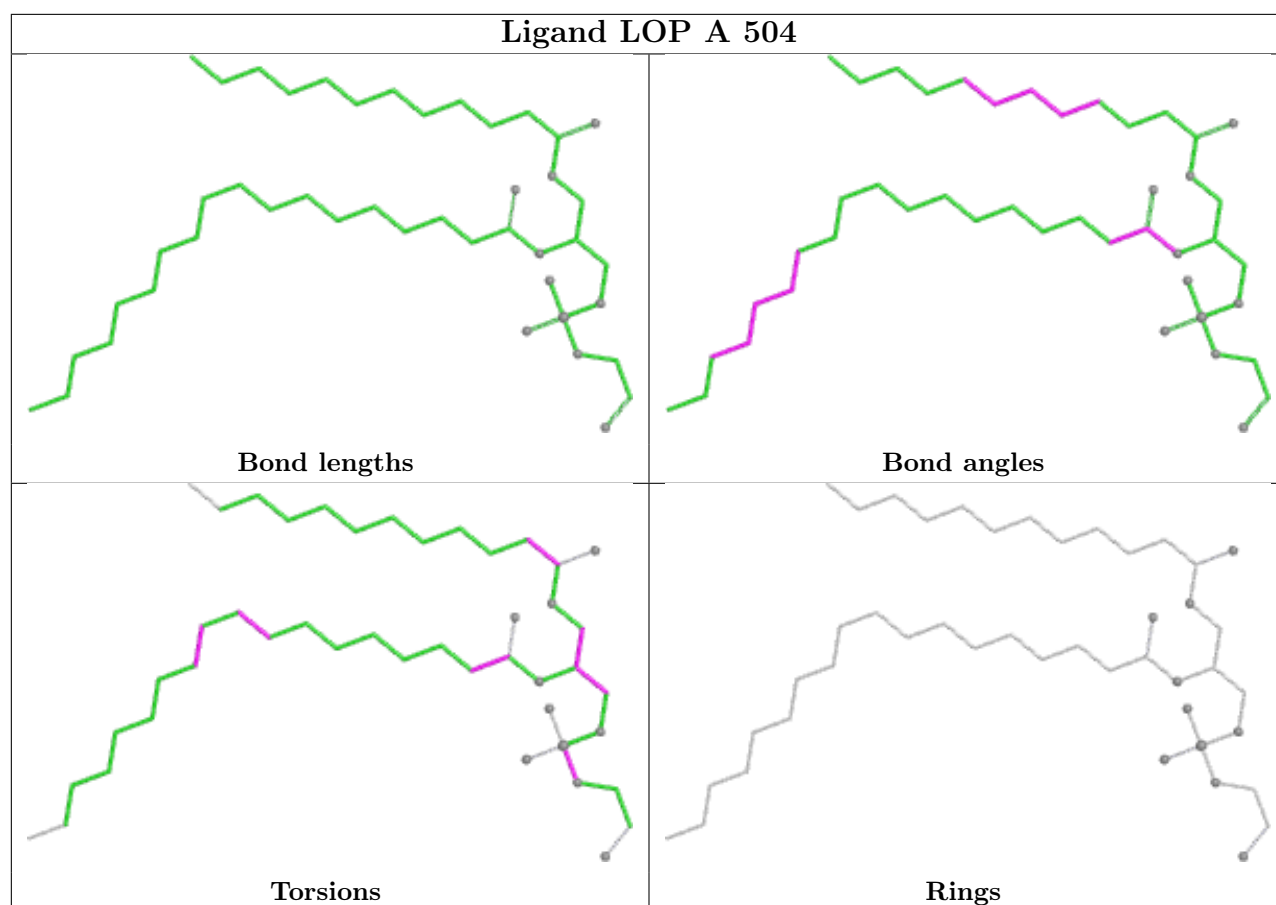
Ligand SMA J 503

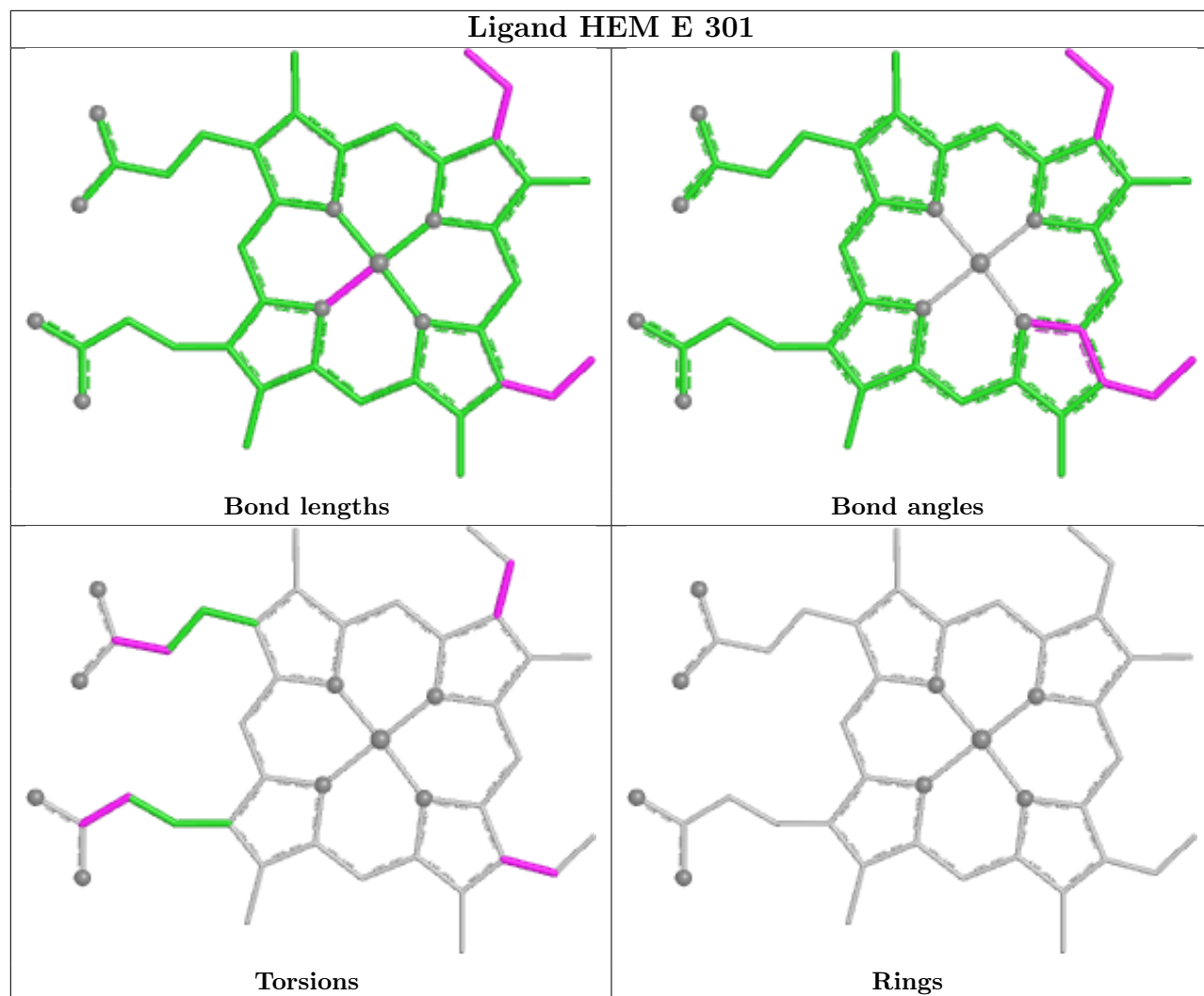


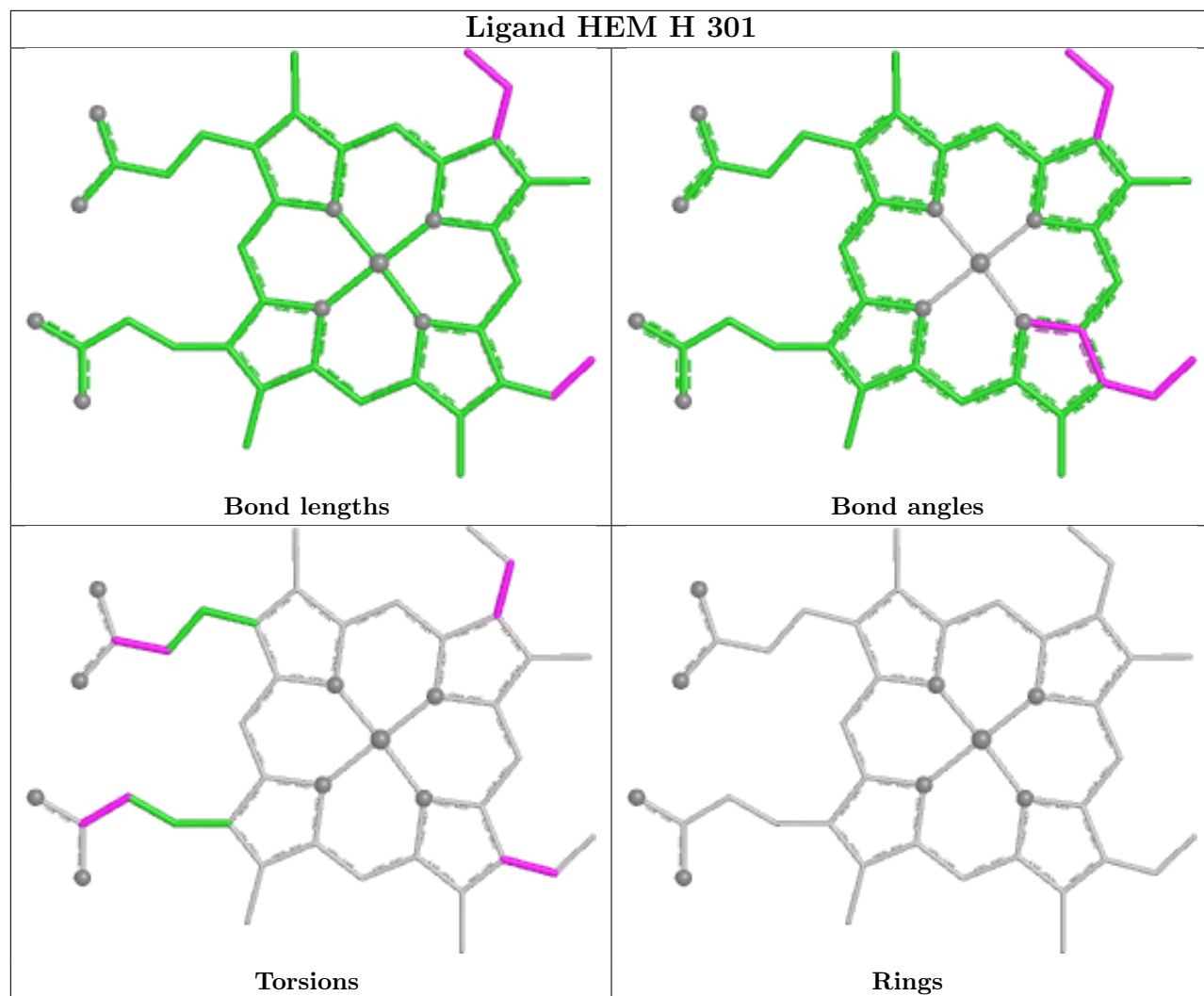


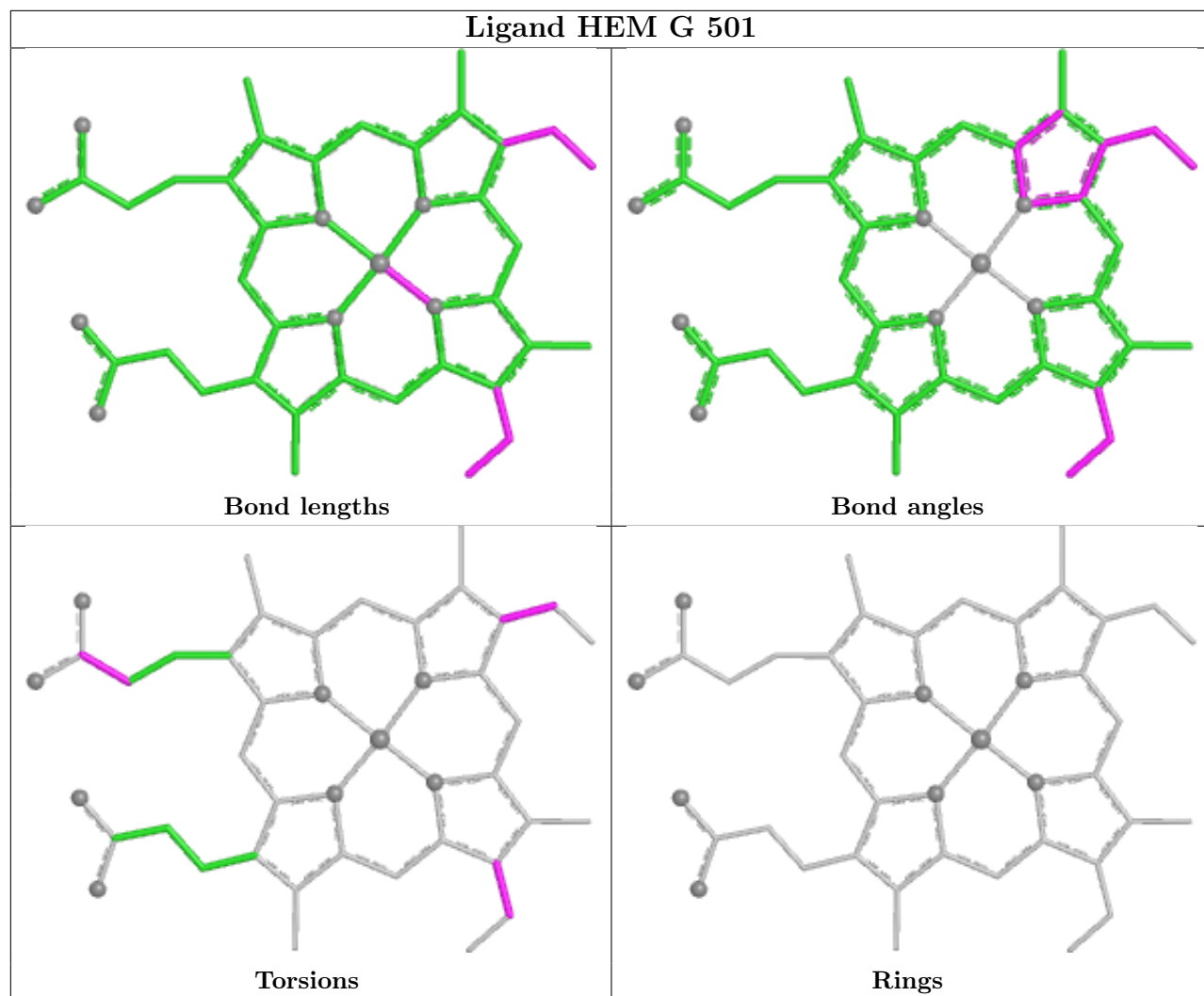




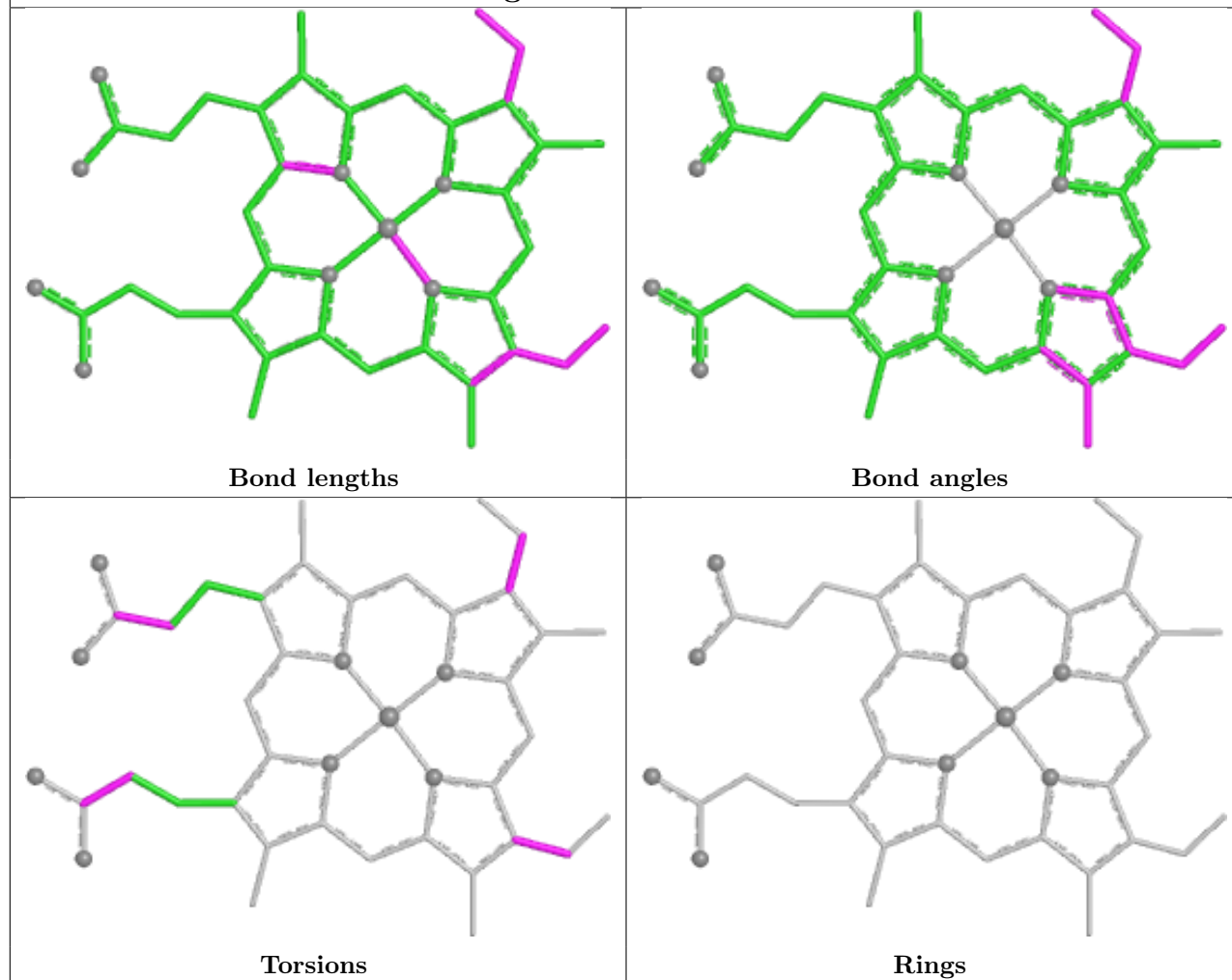




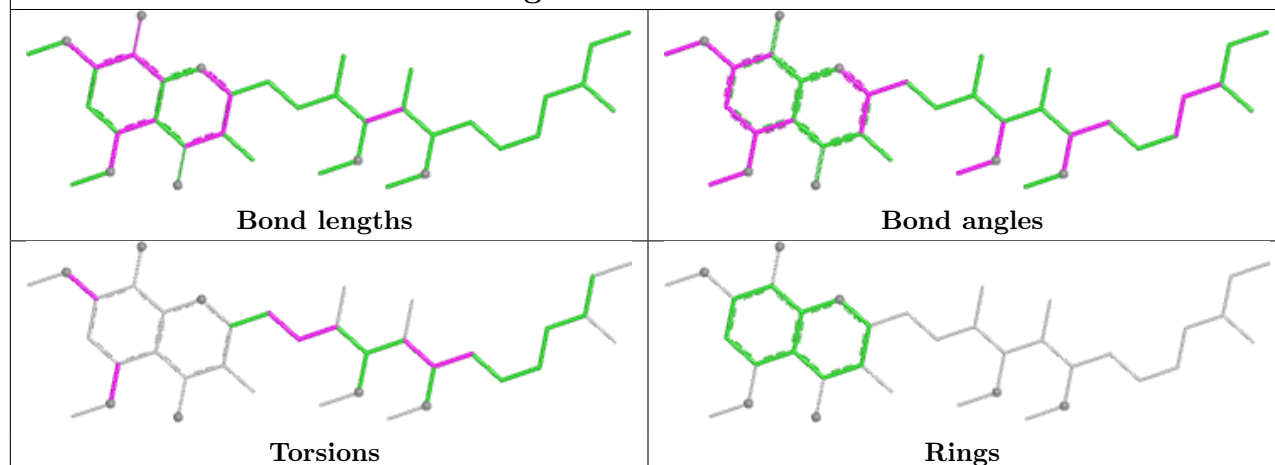


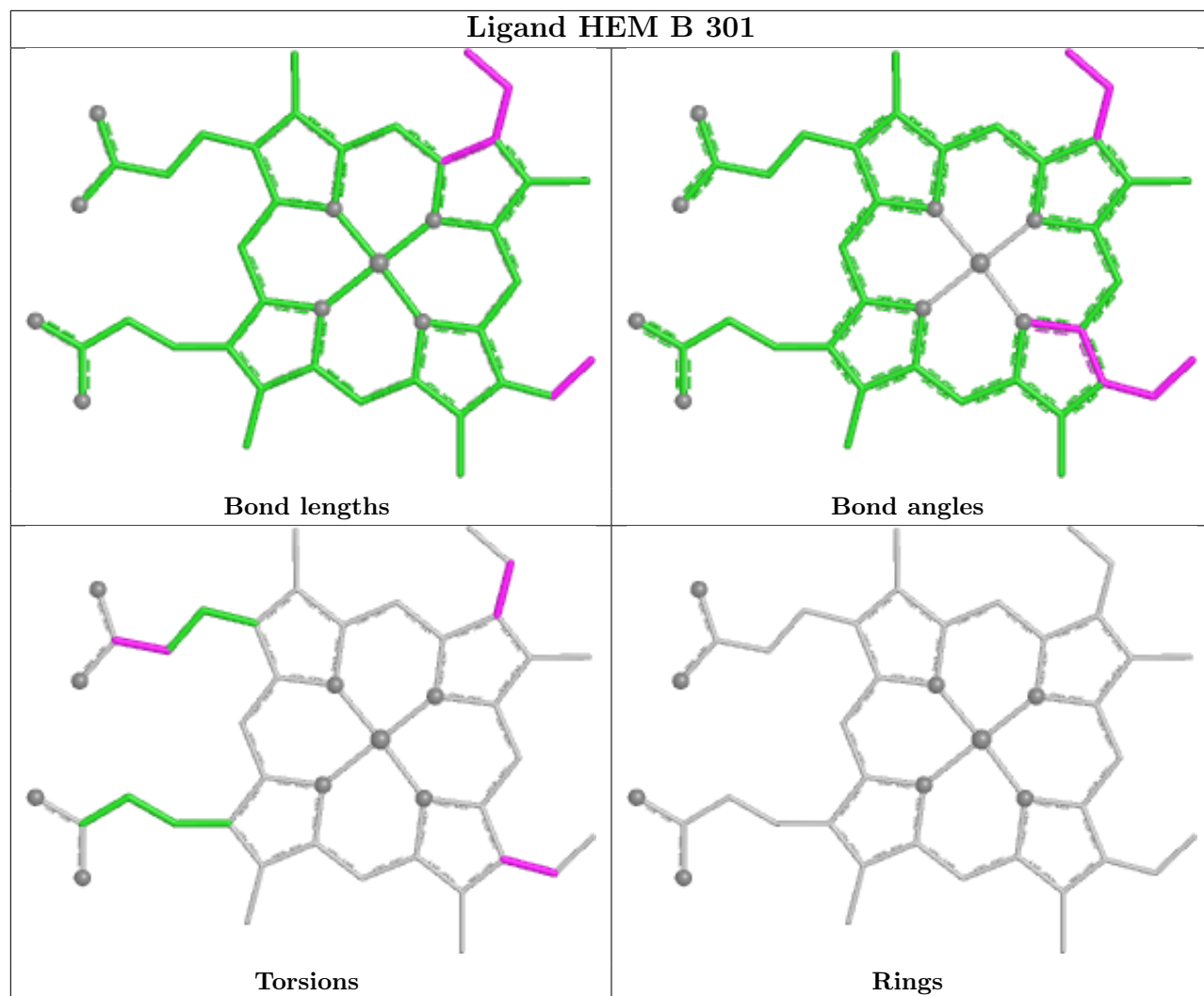


Ligand HEM M 502

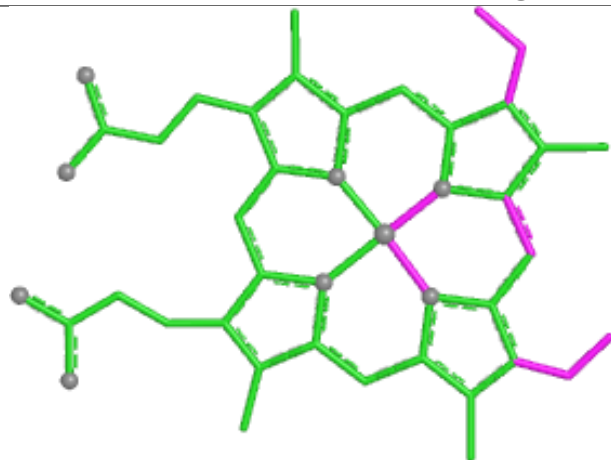


Ligand SMA M 503

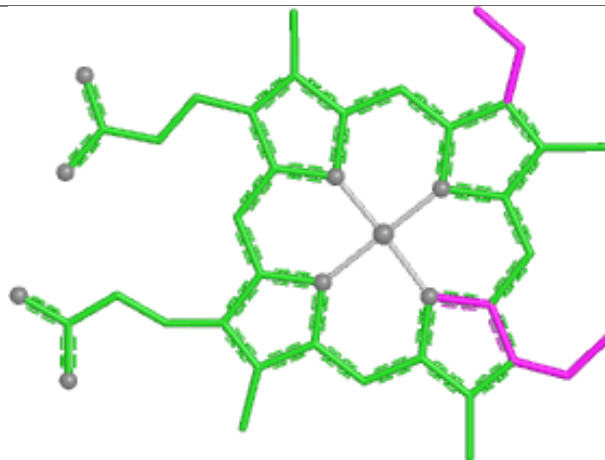




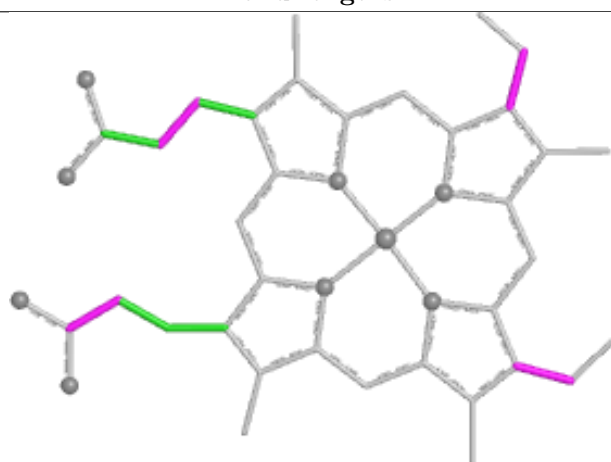
Ligand HEM J 501



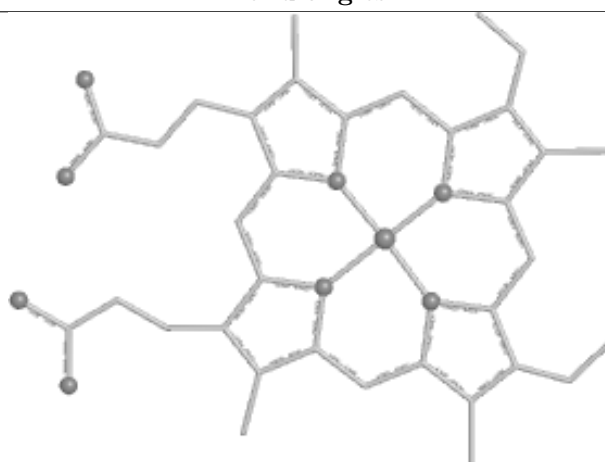
Bond lengths



Bond angles

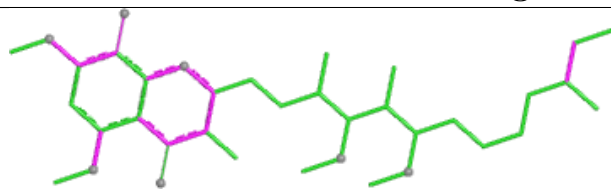


Torsions

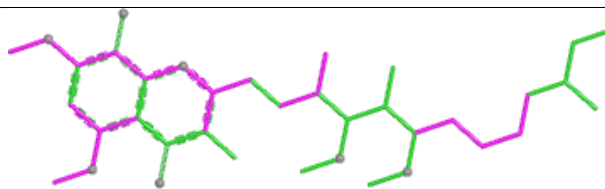


Rings

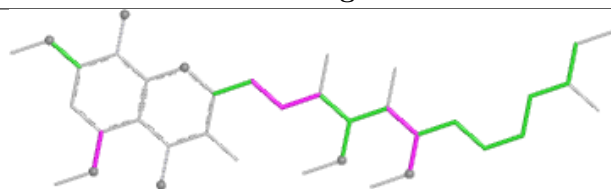
Ligand SMA P 503



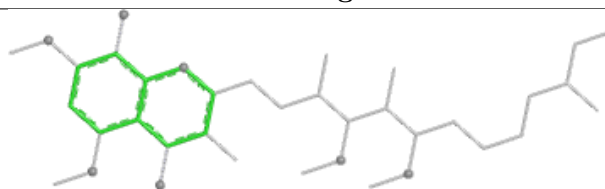
Bond lengths



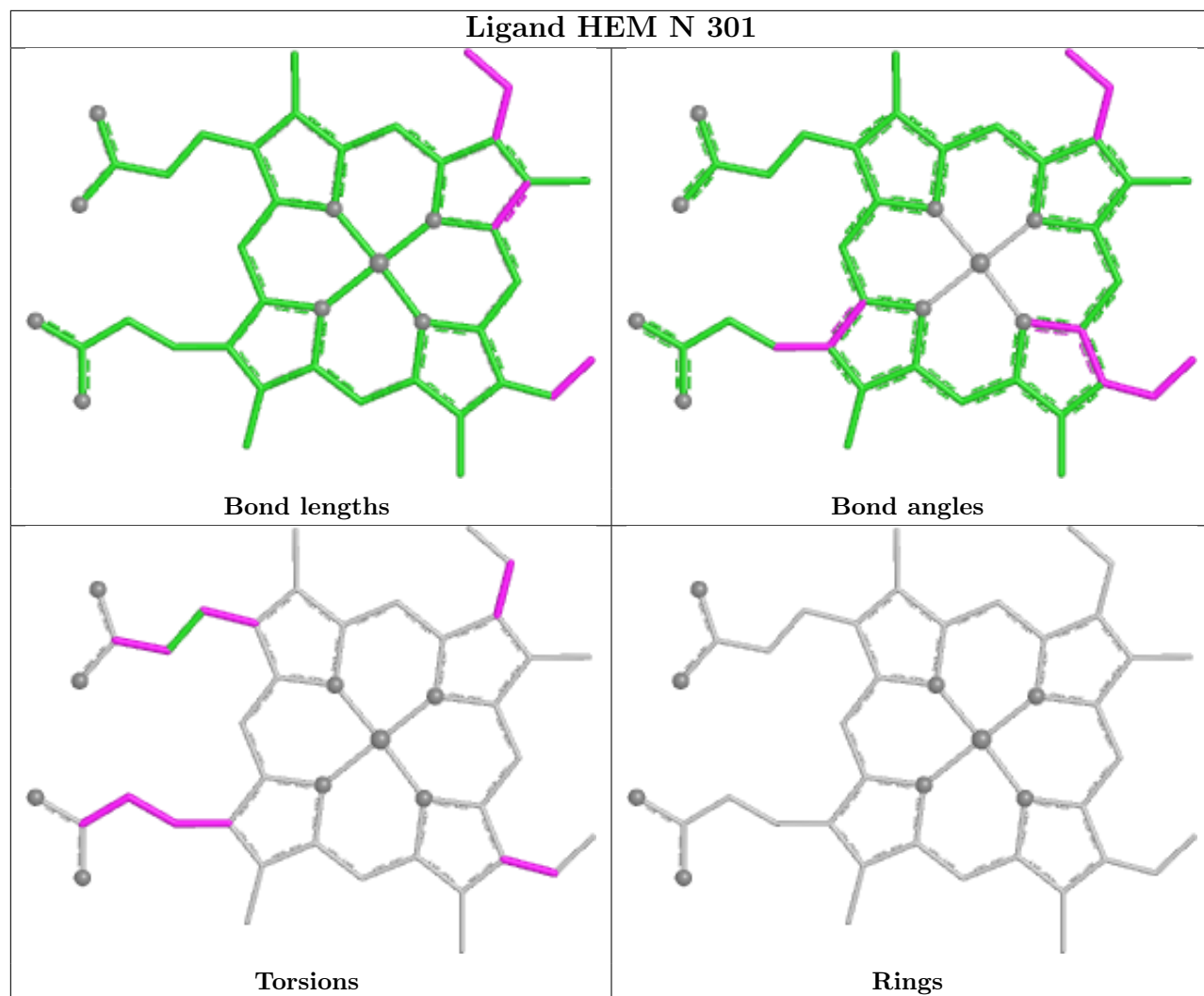
Bond angles

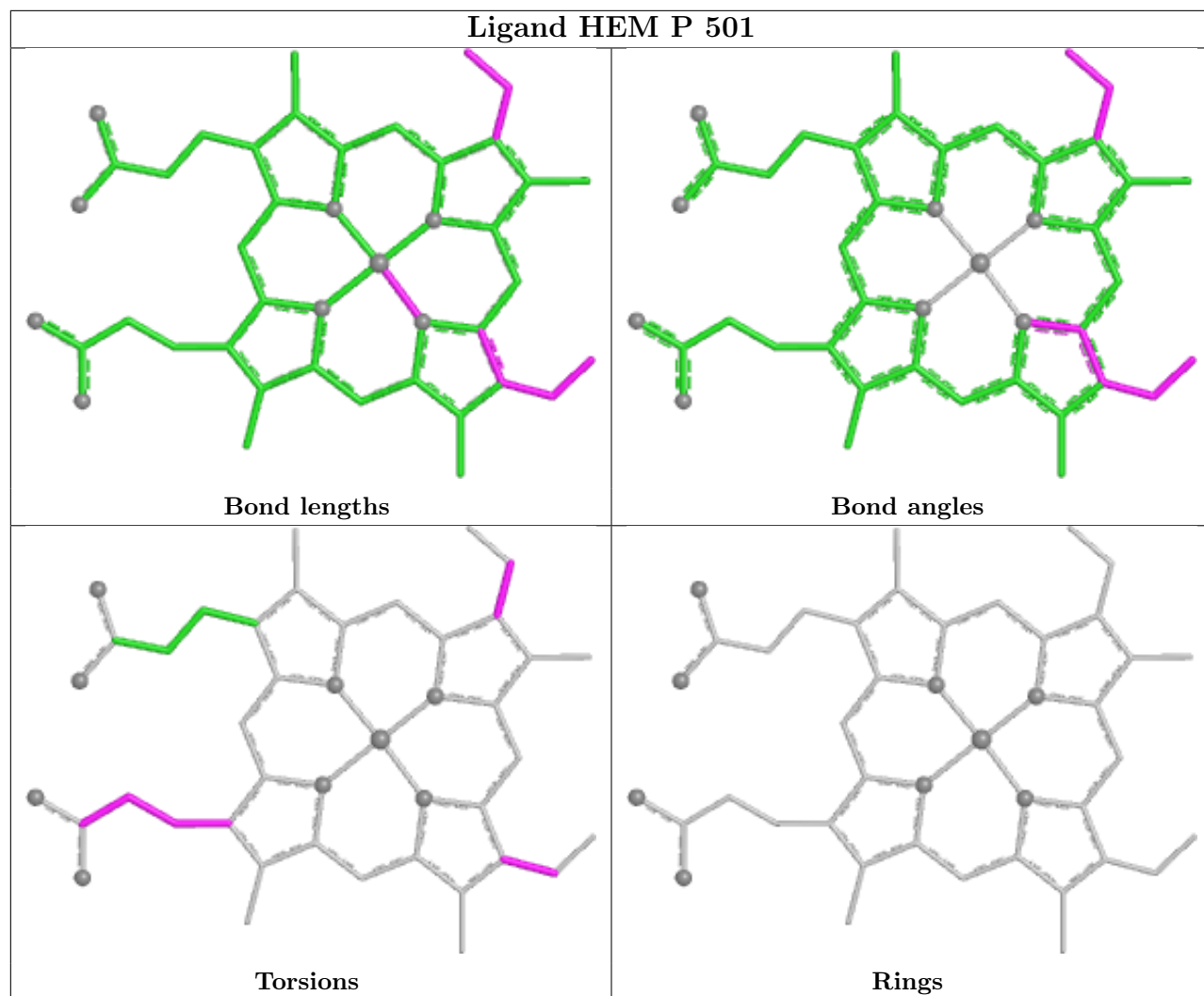


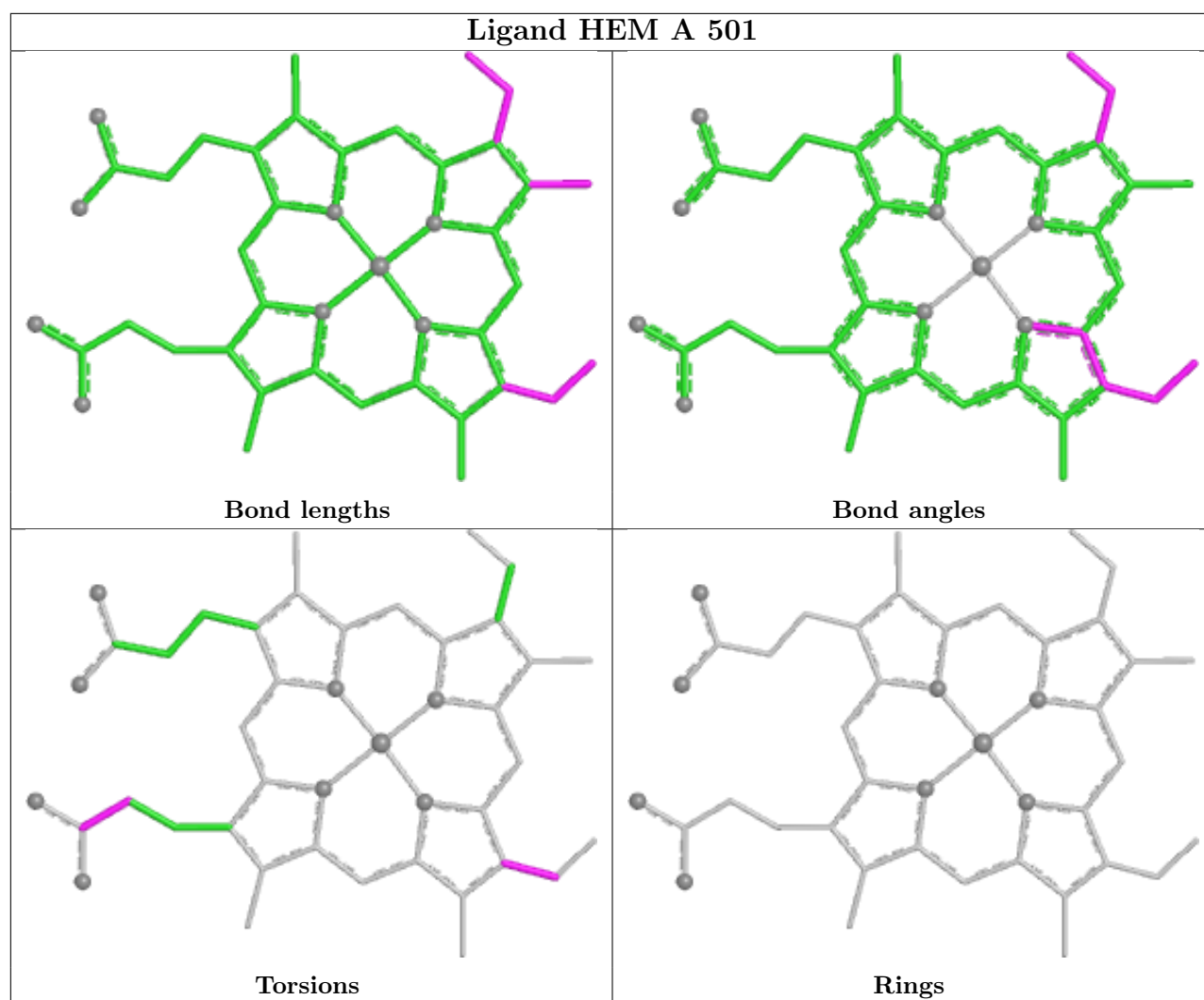
Torsions



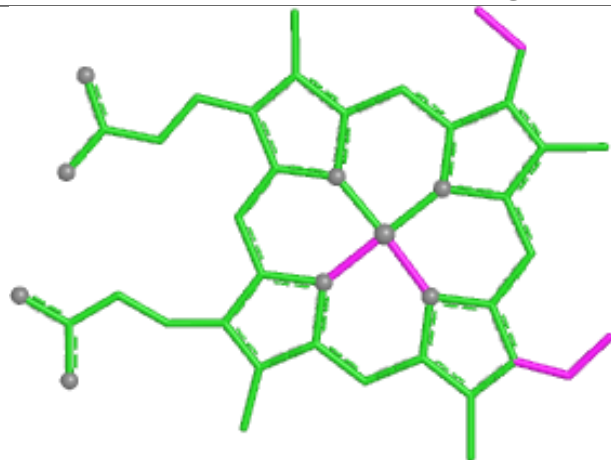
Rings



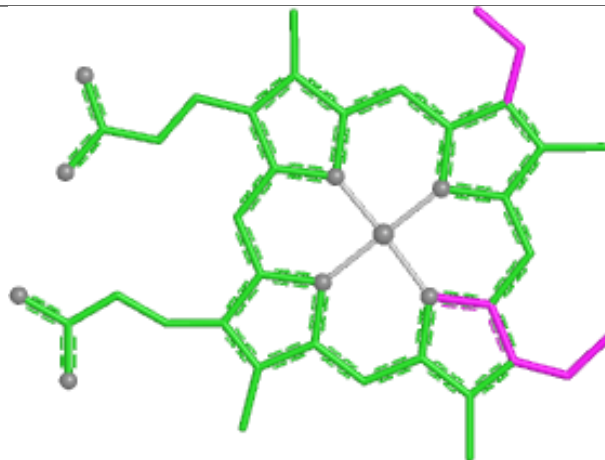




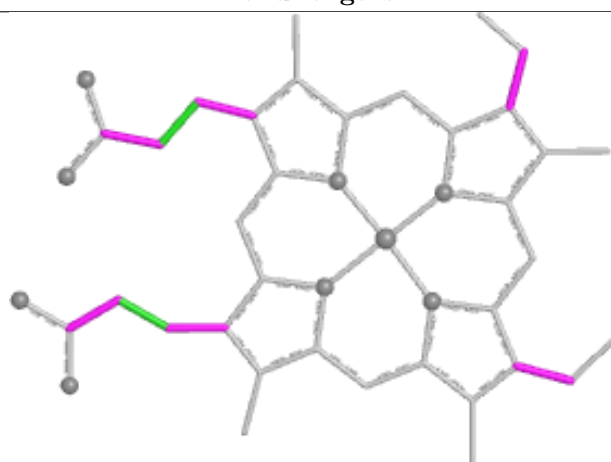
Ligand HEM M 501



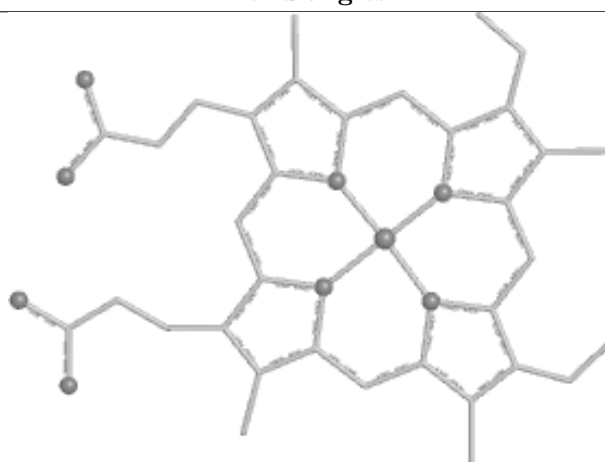
Bond lengths



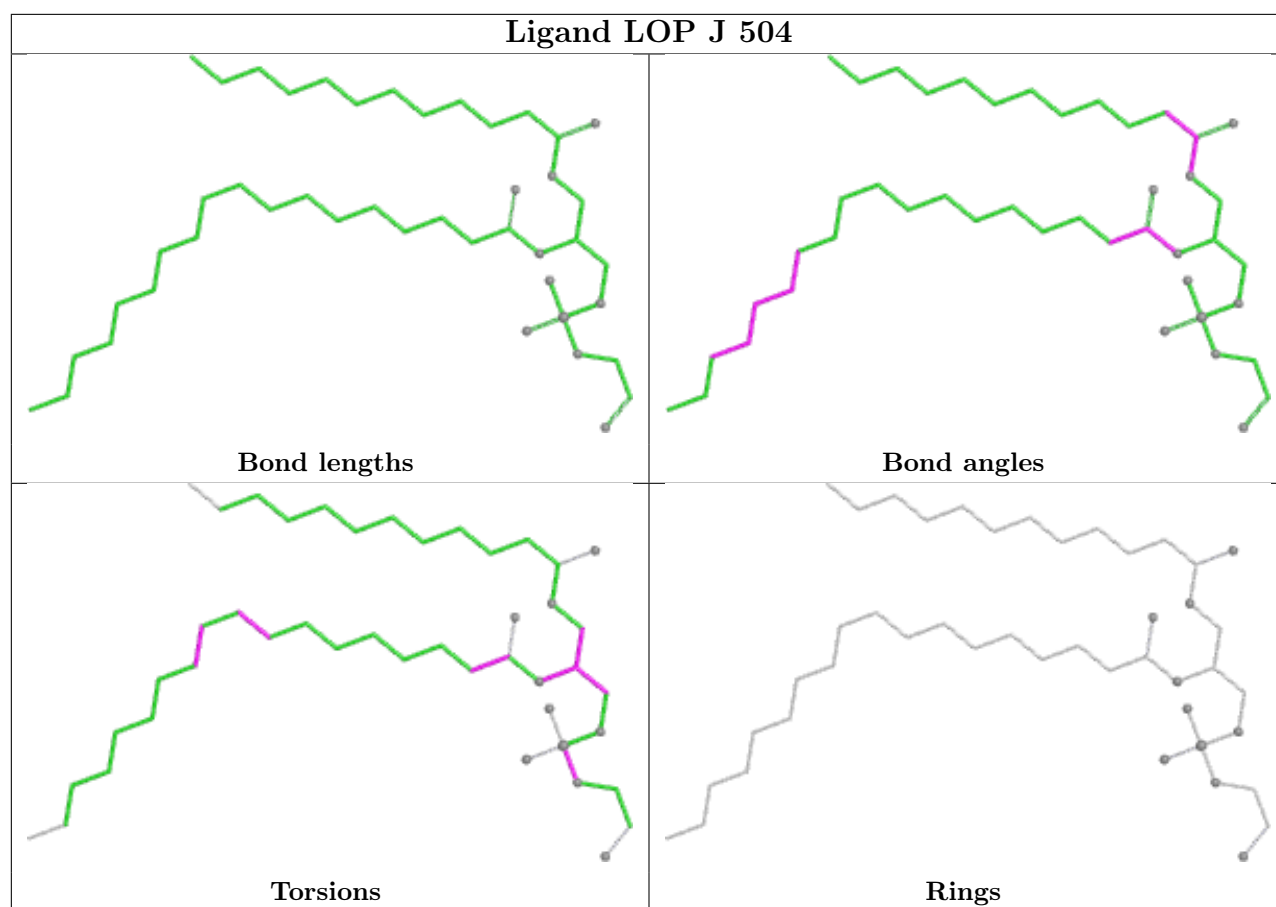
Bond angles

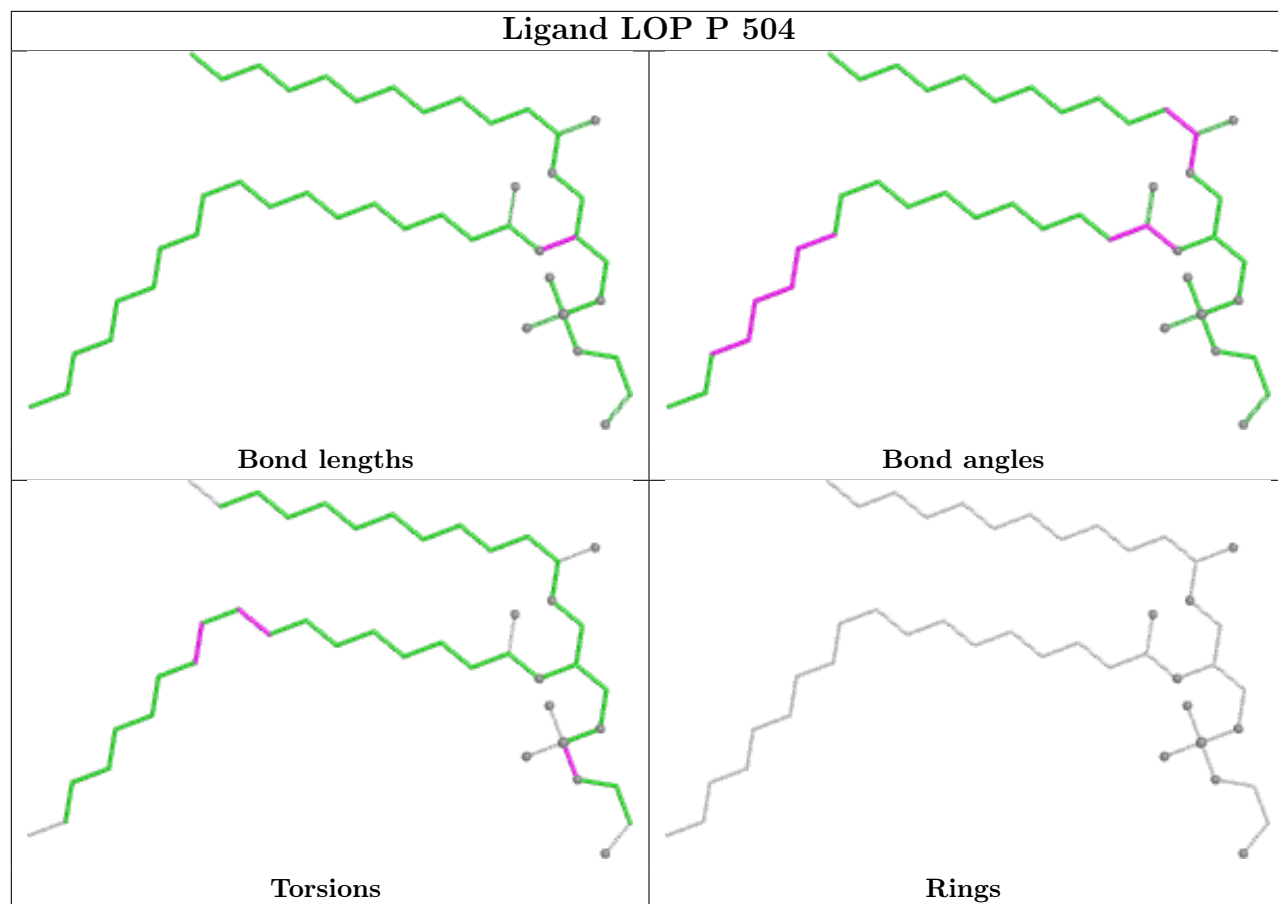


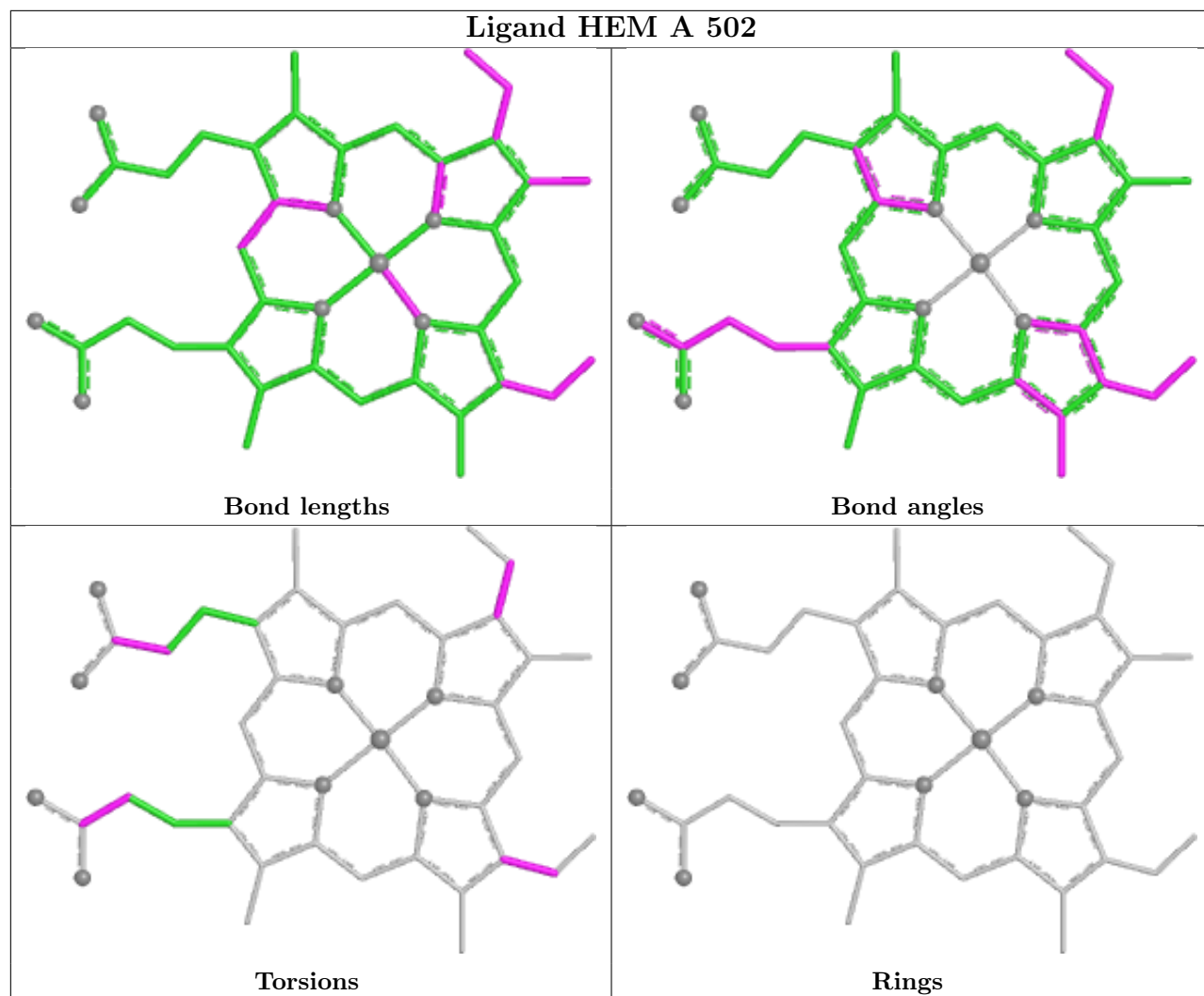
Torsions



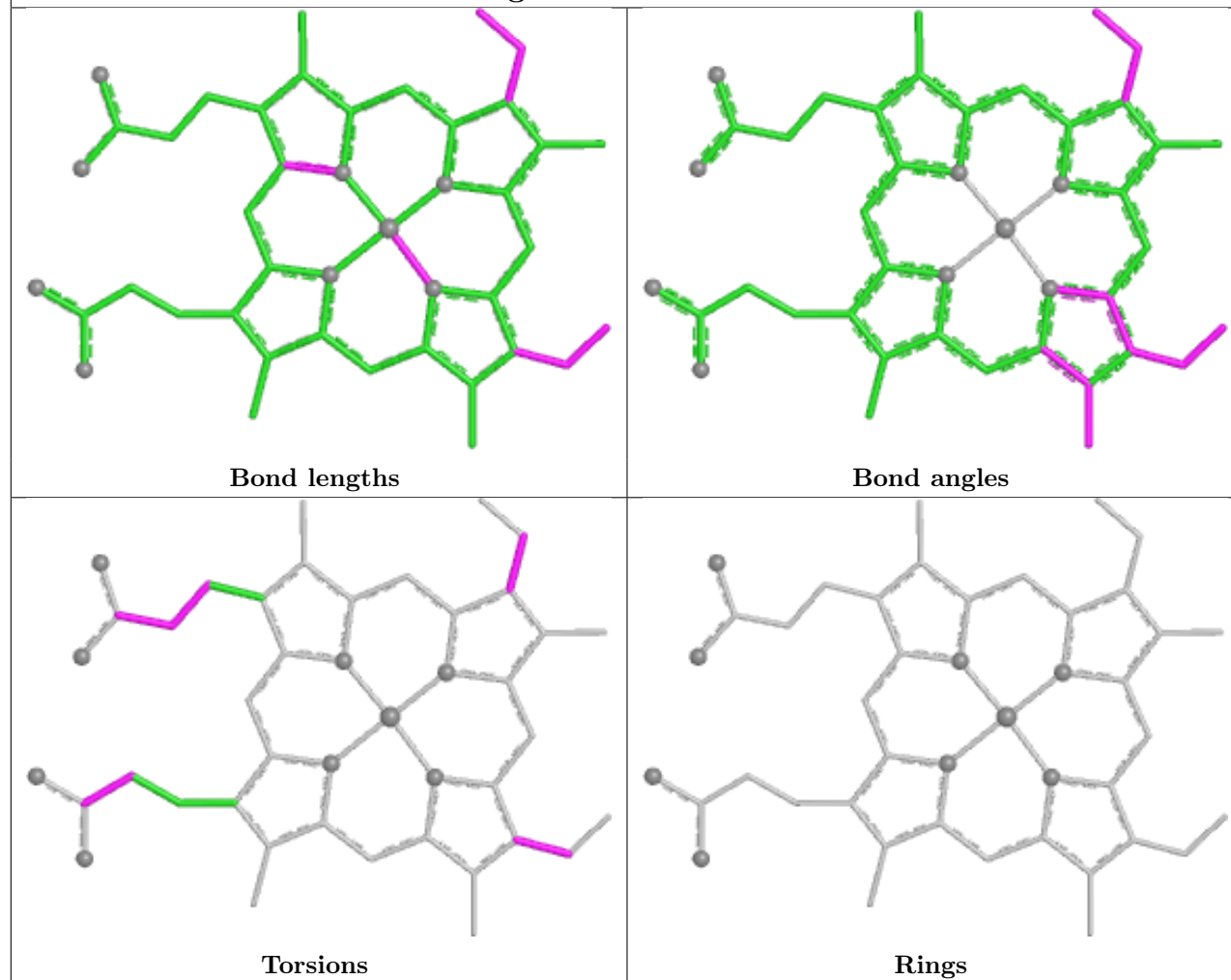
Rings



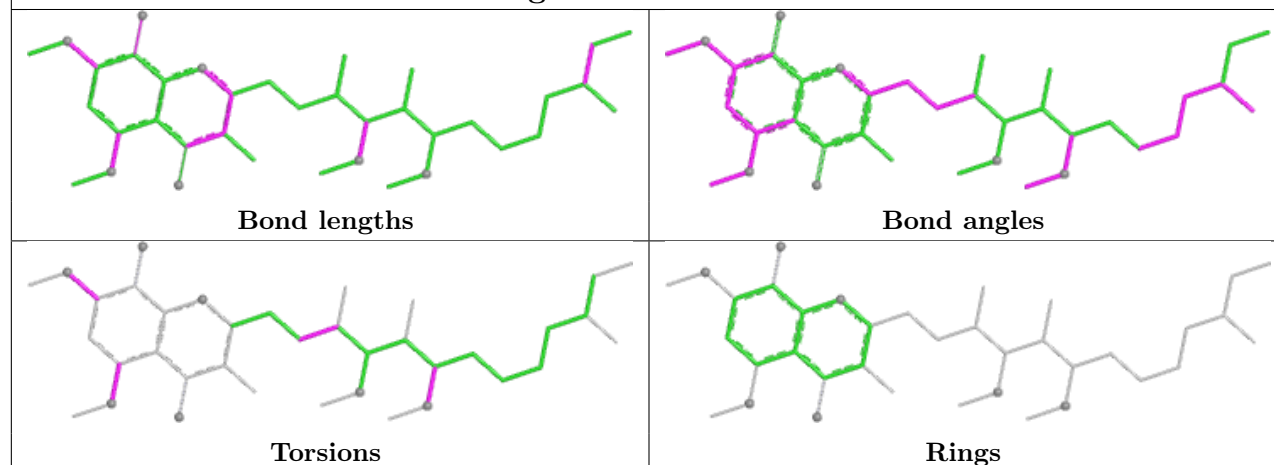


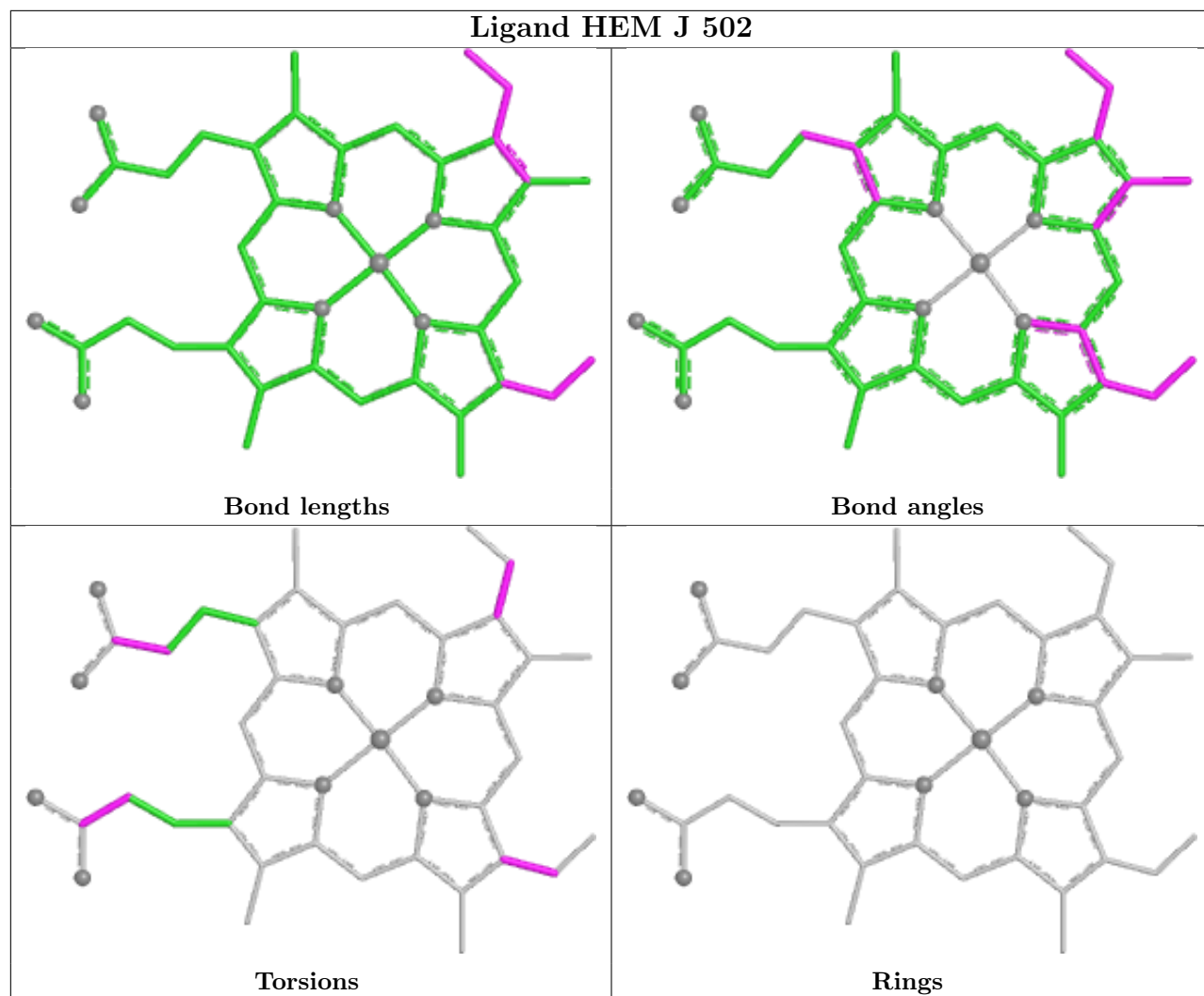


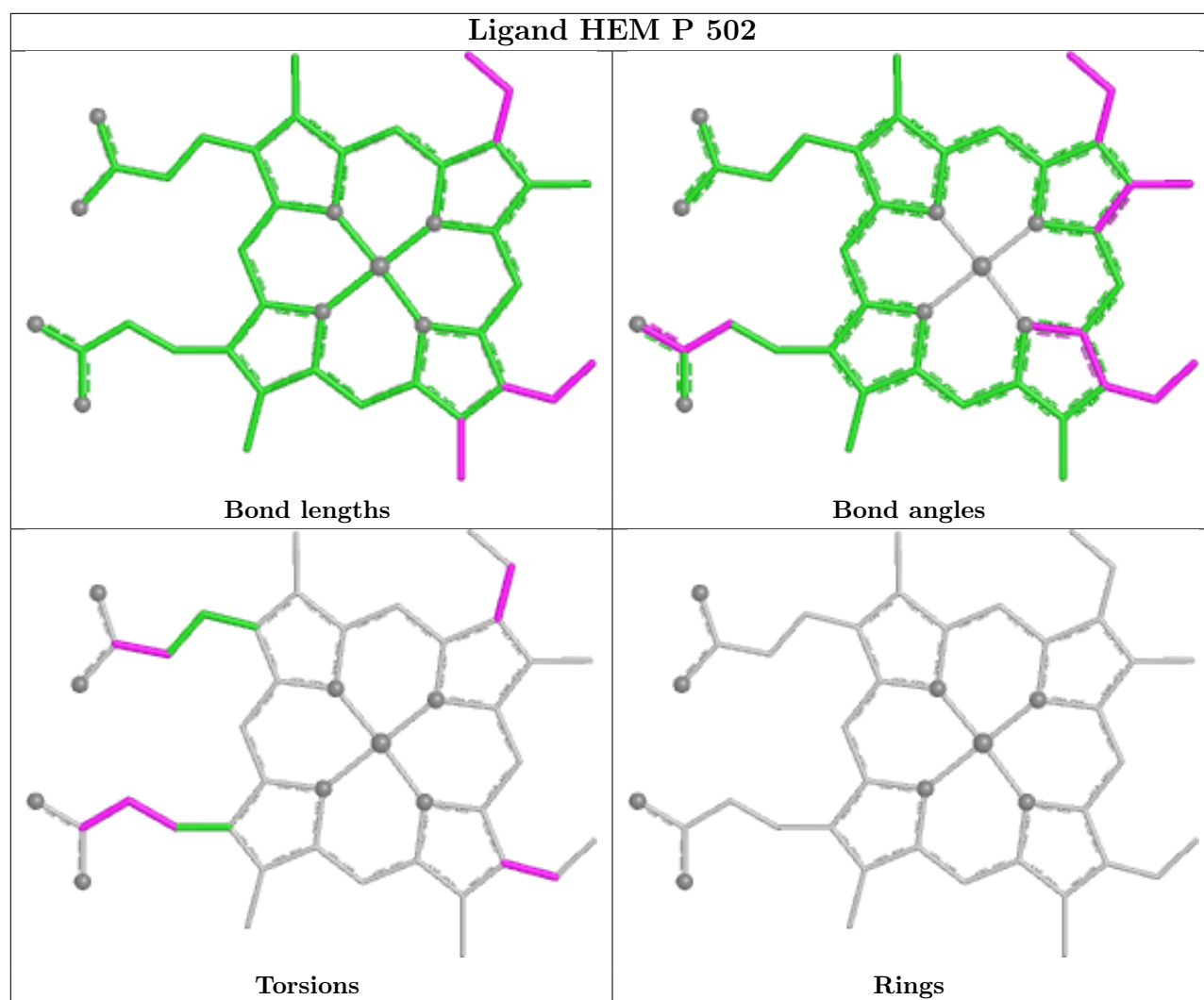
Ligand HEM G 502



Ligand SMA A 503







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.