



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2021 – 07:07 PM EST

PDB ID : 1D4C
Title : CRYSTAL STRUCTURE OF THE UNCOMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on : 1999-10-03
Resolution : 2.90 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 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) : 2.17.1

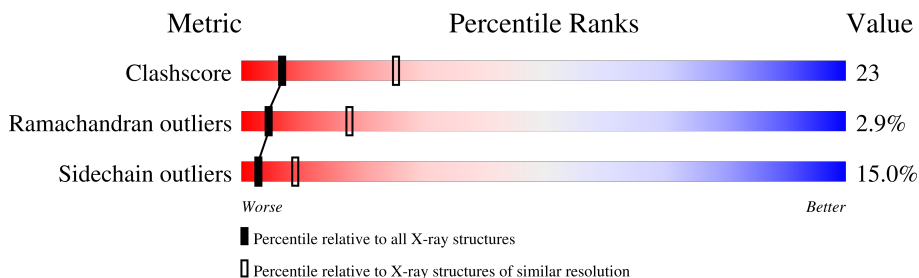
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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	572	51% 35% 12% .
1	B	572	51% 34% 11% ..
1	C	572	51% 33% 13% ...
1	D	572	49% 37% 12% .

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
3	FAD	A	600	X	-	-	-
3	FAD	B	700	X	-	-	-
3	FAD	C	800	X	-	-	-
3	FAD	D	900	X	-	-	-

2 Entry composition [i](#)

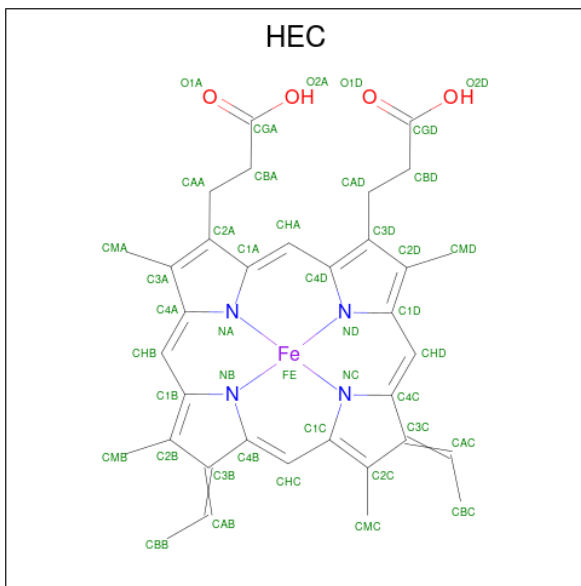
There are 5 unique types of molecules in this entry. The entry contains 17470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME C FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	570	Total 4124	C 2562	N 736	O 807	S 19	0	0	0
1	B	566	Total 4093	C 2542	N 731	O 801	S 19	0	0	0
1	C	568	Total 4099	C 2546	N 733	O 801	S 19	0	0	0
1	D	570	Total 4113	C 2553	N 734	O 807	S 19	0	0	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



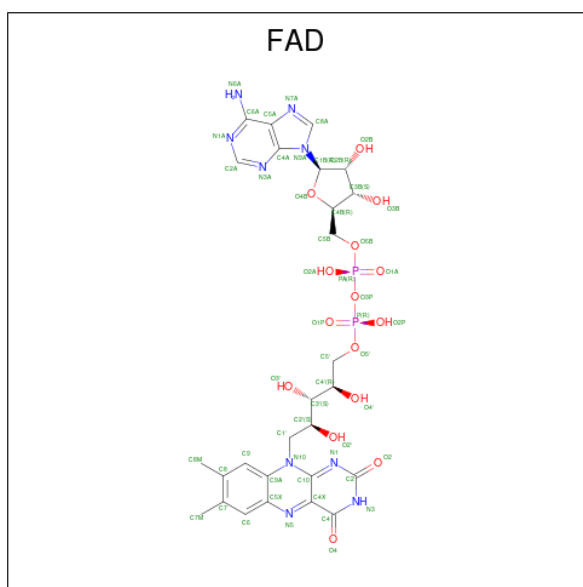
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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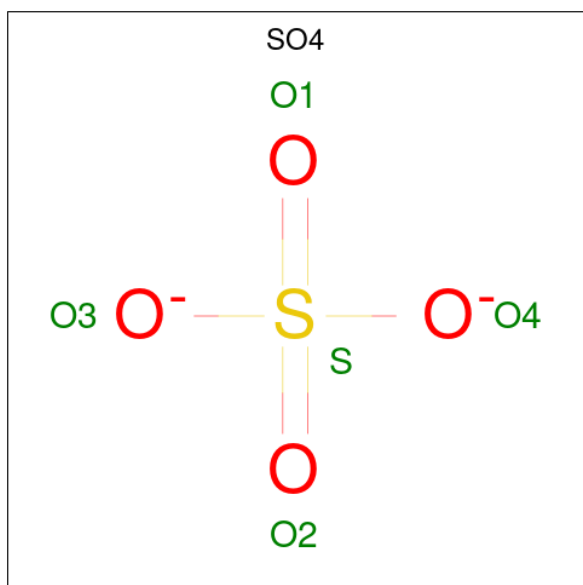
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
3	A	1	Total	53	27	9	15	2	0	0
3	B	1	Total	53	27	9	15	2	0	0
3	C	1	Total	53	27	9	15	2	0	0
3	D	1	Total	53	27	9	15	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

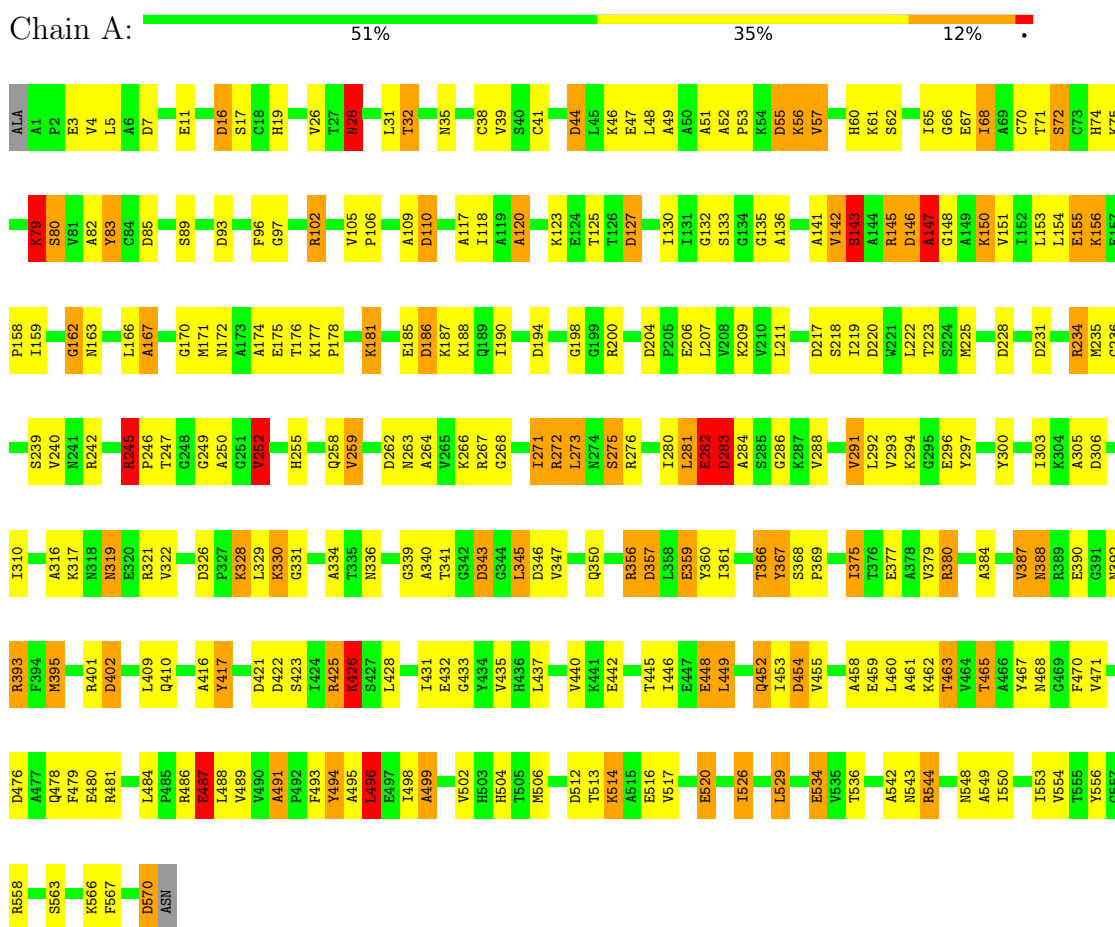
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	29	Total O 29 29	0	0
5	C	30	Total O 30 30	0	0
5	D	19	Total O 19 19	0	0

3 Residue-property plots [i](#)

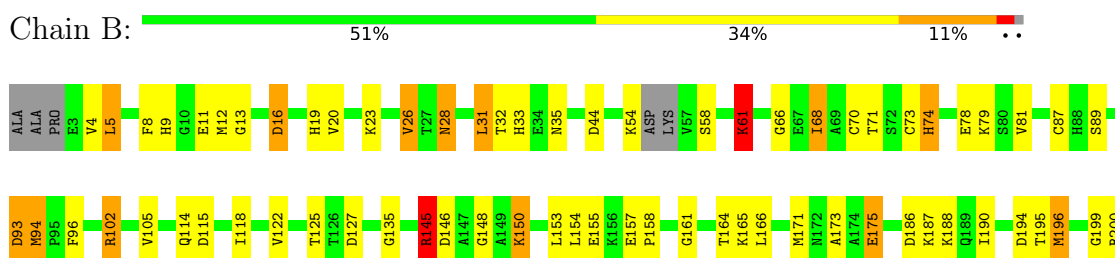
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 216.36Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.7 (15.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17470	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: SO4, HEC, FAD

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	0/4192	2.22	144/5683 (2.5%)
1	B	0.74	7/4159 (0.2%)	1.97	112/5637 (2.0%)
1	C	0.71	3/4166 (0.1%)	2.04	126/5649 (2.2%)
1	D	0.64	1/4179 (0.0%)	1.94	98/5665 (1.7%)
All	All	0.72	11/16696 (0.1%)	2.05	480/22634 (2.1%)

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	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	GLU	CD-OE1	9.81	1.36	1.25
1	C	459	GLU	CD-OE1	9.29	1.35	1.25
1	C	459	GLU	CD-OE2	8.55	1.35	1.25
1	B	476	ASP	CG-OD1	8.47	1.44	1.25
1	B	459	GLU	CD-OE2	7.25	1.33	1.25

The worst 5 of 480 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	ARG	CD-NE-CZ	29.02	164.23	123.60
1	A	267	ARG	CD-NE-CZ	24.00	157.20	123.60
1	A	102	ARG	NE-CZ-NH2	23.33	131.97	120.30
1	D	401	ARG	CD-NE-CZ	21.85	154.19	123.60
1	D	242	ARG	NE-CZ-NH1	20.69	130.65	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Mainchain
1	A	491	ALA	Mainchain,Peptide
1	B	491	ALA	Mainchain,Peptide
1	C	477	ALA	Mainchain
1	C	491	ALA	Mainchain

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	4124	0	4013	179	1
1	B	4093	0	3976	174	0
1	C	4099	0	3977	192	2
1	D	4113	0	3987	210	1
2	A	172	0	121	13	0
2	B	172	0	121	15	0
2	C	172	0	120	15	0
2	D	172	0	121	18	0
3	A	53	0	31	9	0
3	B	53	0	31	8	0
3	C	53	0	31	12	0
3	D	53	0	30	9	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	48	0	0	2	0
5	B	29	0	0	3	0
5	C	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	19	0	0	2	0
All	All	17470	0	16559	786	2

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 23.

The worst 5 of 786 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)
1:D:18:CYS:SG	2:D:603:HEC:HAC	1.21	1.71
3:B:700:FAD:C2'	3:B:700:FAD:C1'	1.77	1.62
3:D:900:FAD:C2'	3:D:900:FAD:C1'	1.78	1.59
3:A:600:FAD:C1'	3:A:600:FAD:C2'	1.78	1.57
3:C:800:FAD:C2'	3:C:800:FAD:C1'	1.78	1.56

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:OG1	1:C:247:THR:OG1[4_555]	2.12	0.08
1:C:125:THR:OG1	1:D:247:THR:OG1[4_456]	2.15	0.05

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	568/572 (99%)	504 (89%)	51 (9%)	13 (2%)	6	23
1	B	562/572 (98%)	495 (88%)	52 (9%)	15 (3%)	5	19
1	C	566/572 (99%)	482 (85%)	64 (11%)	20 (4%)	3	14
1	D	566/572 (99%)	488 (86%)	61 (11%)	17 (3%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2262/2288 (99%)	1969 (87%)	228 (10%)	65 (3%)	4 18

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	142	VAL
1	A	147	ALA
1	A	454	ASP
1	B	250	ALA

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	409/429 (95%)	350 (86%)	59 (14%)	3 9
1	B	406/429 (95%)	344 (85%)	62 (15%)	2 8
1	C	405/429 (94%)	343 (85%)	62 (15%)	2 8
1	D	407/429 (95%)	346 (85%)	61 (15%)	3 9
All	All	1627/1716 (95%)	1383 (85%)	244 (15%)	3 9

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	506	MET
1	D	376	THR
1	C	224	SER
1	D	350	GLN
1	D	463	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	452	GLN
1	D	452	GLN
1	C	172	ASN
1	D	411	GLN
1	D	336	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](#)

23 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
2	HEC	A	603	1	26,50,50	2.56	5 (19%)	18,82,82	2.34	8 (44%)
2	HEC	D	601	1	26,50,50	2.46	6 (23%)	18,82,82	2.68	7 (38%)
2	HEC	A	602	1	26,50,50	2.23	4 (15%)	18,82,82	3.39	11 (61%)
2	HEC	C	601	1	26,50,50	2.35	4 (15%)	18,82,82	2.81	10 (55%)
3	FAD	A	600	-	51,58,58	1.95	14 (27%)	60,89,89	3.26	23 (38%)
4	SO4	B	714	-	4,4,4	0.50	0	6,6,6	0.49	0
2	HEC	D	604	1	26,50,50	2.25	4 (15%)	18,82,82	2.86	9 (50%)
2	HEC	B	604	1	26,50,50	2.40	4 (15%)	18,82,82	3.04	11 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	D	900	-	51,58,58	1.92	9 (17%)	60,89,89	3.27	22 (36%)
2	HEC	D	603	1	26,50,50	2.48	5 (19%)	18,82,82	1.71	5 (27%)
2	HEC	C	604	1	26,50,50	2.26	5 (19%)	18,82,82	4.69	11 (61%)
4	SO4	C	814	-	4,4,4	0.58	0	6,6,6	0.66	0
3	FAD	B	700	-	51,58,58	1.93	9 (17%)	60,89,89	3.33	29 (48%)
2	HEC	C	603	1	26,50,50	2.42	5 (19%)	18,82,82	2.51	9 (50%)
2	HEC	D	602	1	26,50,50	2.39	4 (15%)	18,82,82	2.61	10 (55%)
2	HEC	B	602	1	26,50,50	2.26	5 (19%)	18,82,82	2.62	7 (38%)
4	SO4	D	914	-	4,4,4	0.48	0	6,6,6	0.69	0
2	HEC	C	602	1	26,50,50	2.53	5 (19%)	18,82,82	3.12	9 (50%)
2	HEC	B	601	1	26,50,50	2.37	4 (15%)	18,82,82	3.06	10 (55%)
3	FAD	C	800	-	51,58,58	1.73	11 (21%)	60,89,89	3.93	24 (40%)
2	HEC	A	601	1	26,50,50	2.72	5 (19%)	18,82,82	3.41	11 (61%)
2	HEC	A	604	1	26,50,50	2.31	5 (19%)	18,82,82	2.83	11 (61%)
2	HEC	B	603	1	26,50,50	2.35	6 (23%)	18,82,82	3.11	9 (50%)

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
2	HEC	A	603	1	-	1/6/54/54	-
2	HEC	D	601	1	-	3/6/54/54	-
2	HEC	A	602	1	-	1/6/54/54	-
3	FAD	A	600	-	2/2/9/9	14/30/50/50	0/6/6/6
2	HEC	C	601	1	-	1/6/54/54	-
3	FAD	D	900	-	2/2/9/9	15/30/50/50	0/6/6/6
2	HEC	B	604	1	-	2/6/54/54	-
2	HEC	D	604	1	-	0/6/54/54	-
2	HEC	D	603	1	-	1/6/54/54	-
2	HEC	C	604	1	-	4/6/54/54	-
2	HEC	C	603	1	-	1/6/54/54	-
3	FAD	B	700	-	2/2/9/9	11/30/50/50	0/6/6/6
2	HEC	D	602	1	-	0/6/54/54	-
2	HEC	B	602	1	-	1/6/54/54	-
2	HEC	C	602	1	-	1/6/54/54	-
2	HEC	B	601	1	-	2/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	800	-	3/3/9/9	12/30/50/50	0/6/6/6
2	HEC	A	601	1	-	3/6/54/54	-
2	HEC	A	604	1	-	0/6/54/54	-
2	HEC	B	603	1	-	0/6/54/54	-

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	C3B-C2B	-9.34	1.31	1.40
2	D	602	HEC	C3B-C2B	-7.87	1.32	1.40
2	C	602	HEC	C3C-C2C	-7.79	1.32	1.40
2	C	602	HEC	C3B-C2B	-7.65	1.32	1.40
2	A	603	HEC	C3C-C2C	-7.64	1.32	1.40

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	FAD	O4B-C4B-C5B	16.51	163.68	109.37
3	C	800	FAD	O5B-C5B-C4B	16.28	165.03	108.99
2	C	604	HEC	CBD-CAD-C3D	14.82	139.81	112.49
3	D	900	FAD	O5B-C5B-C4B	11.50	148.57	108.99
3	D	900	FAD	C5B-C4B-C3B	-10.98	74.02	115.18

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C4'
3	A	600	FAD	C3'
3	B	700	FAD	C4'
3	B	700	FAD	C3'
3	C	800	FAD	C4'

5 of 73 torsion outliers are listed below:

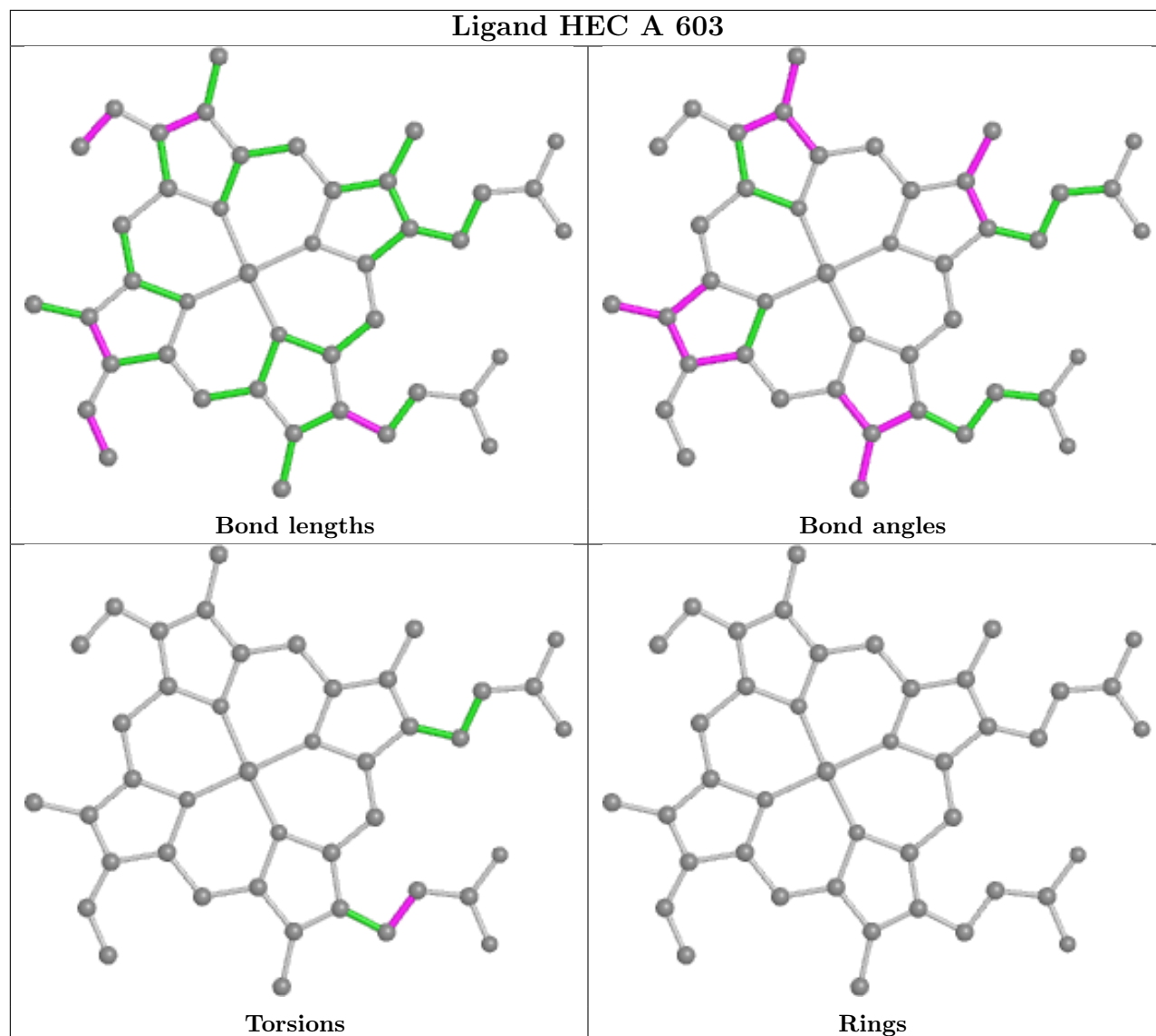
Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C1A-C2A-CAA-CBA
2	A	601	HEC	C3A-C2A-CAA-CBA
2	A	601	HEC	C3D-CAD-CBD-CGD
2	B	601	HEC	C3D-CAD-CBD-CGD
2	B	604	HEC	C2D-C3D-CAD-CBD

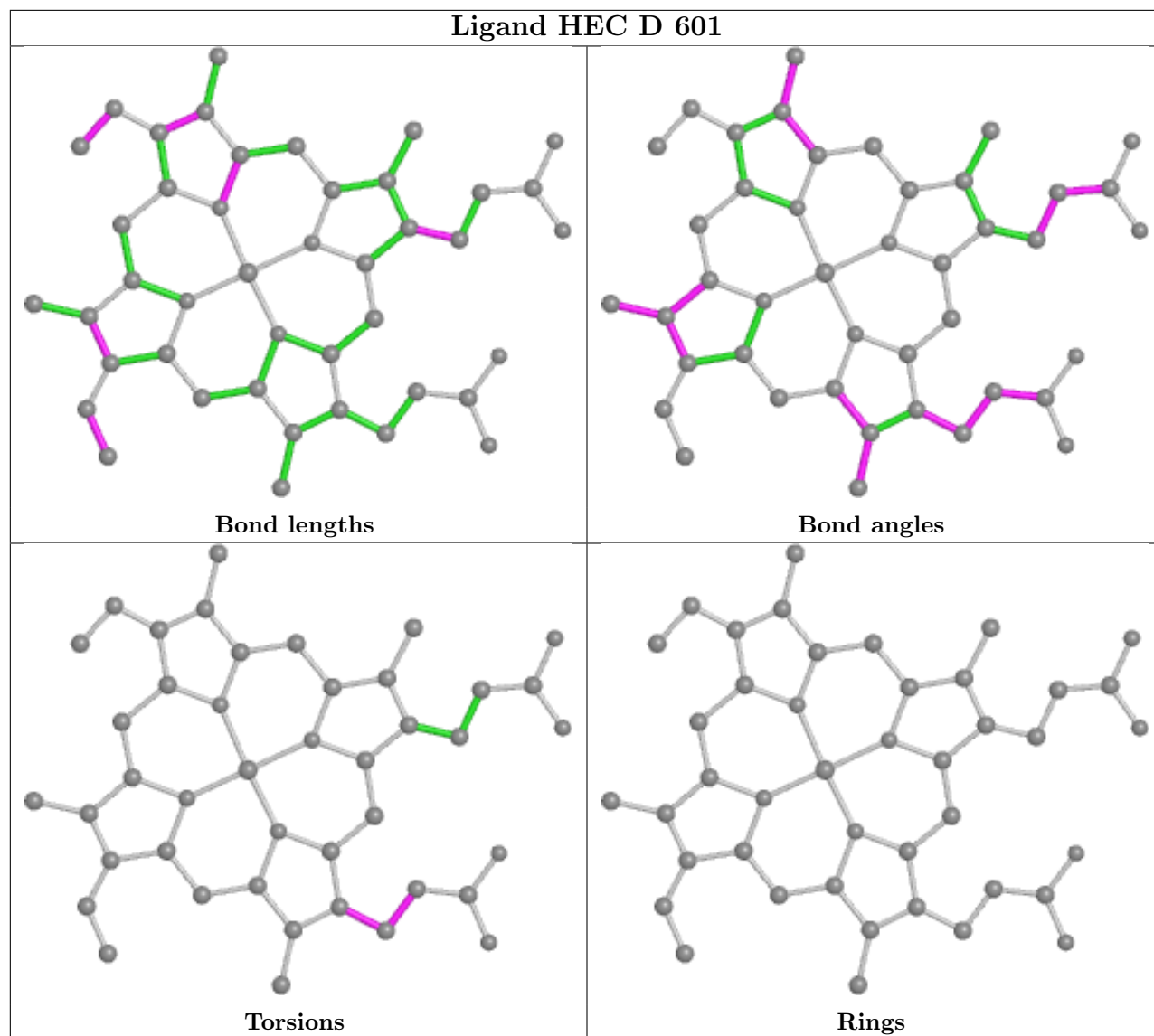
There are no ring outliers.

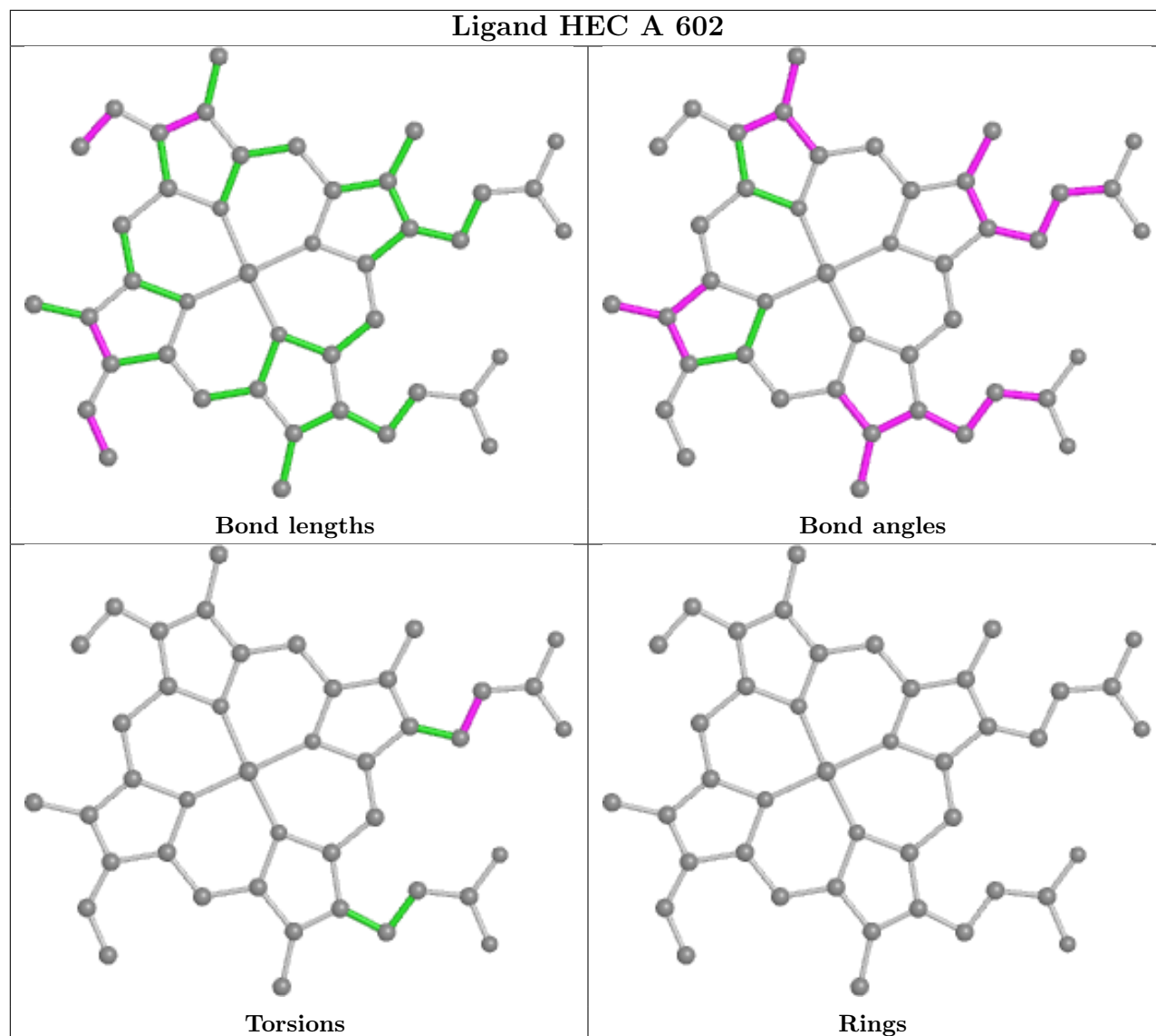
20 monomers are involved in 100 short contacts:

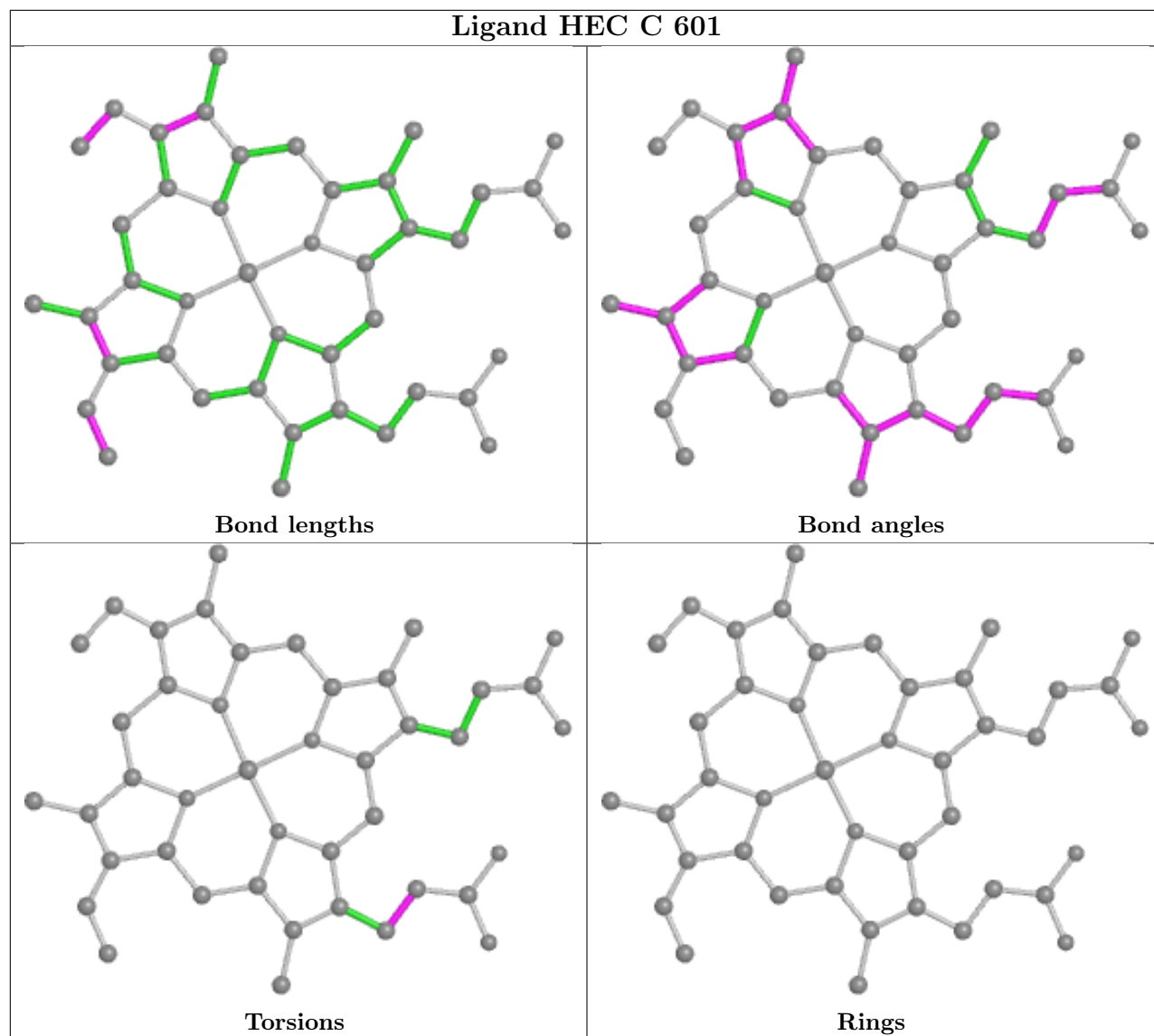
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEC	4	0
2	A	602	HEC	4	0
2	C	601	HEC	5	0
3	A	600	FAD	9	0
4	B	714	SO4	1	0
2	D	604	HEC	2	0
2	B	604	HEC	2	0
3	D	900	FAD	9	0
2	D	603	HEC	5	0
2	C	604	HEC	5	0
3	B	700	FAD	8	0
2	C	603	HEC	1	0
2	D	602	HEC	7	0
2	B	602	HEC	5	0
2	C	602	HEC	4	0
2	B	601	HEC	5	0
3	C	800	FAD	12	0
2	A	601	HEC	6	0
2	A	604	HEC	3	0
2	B	603	HEC	3	0

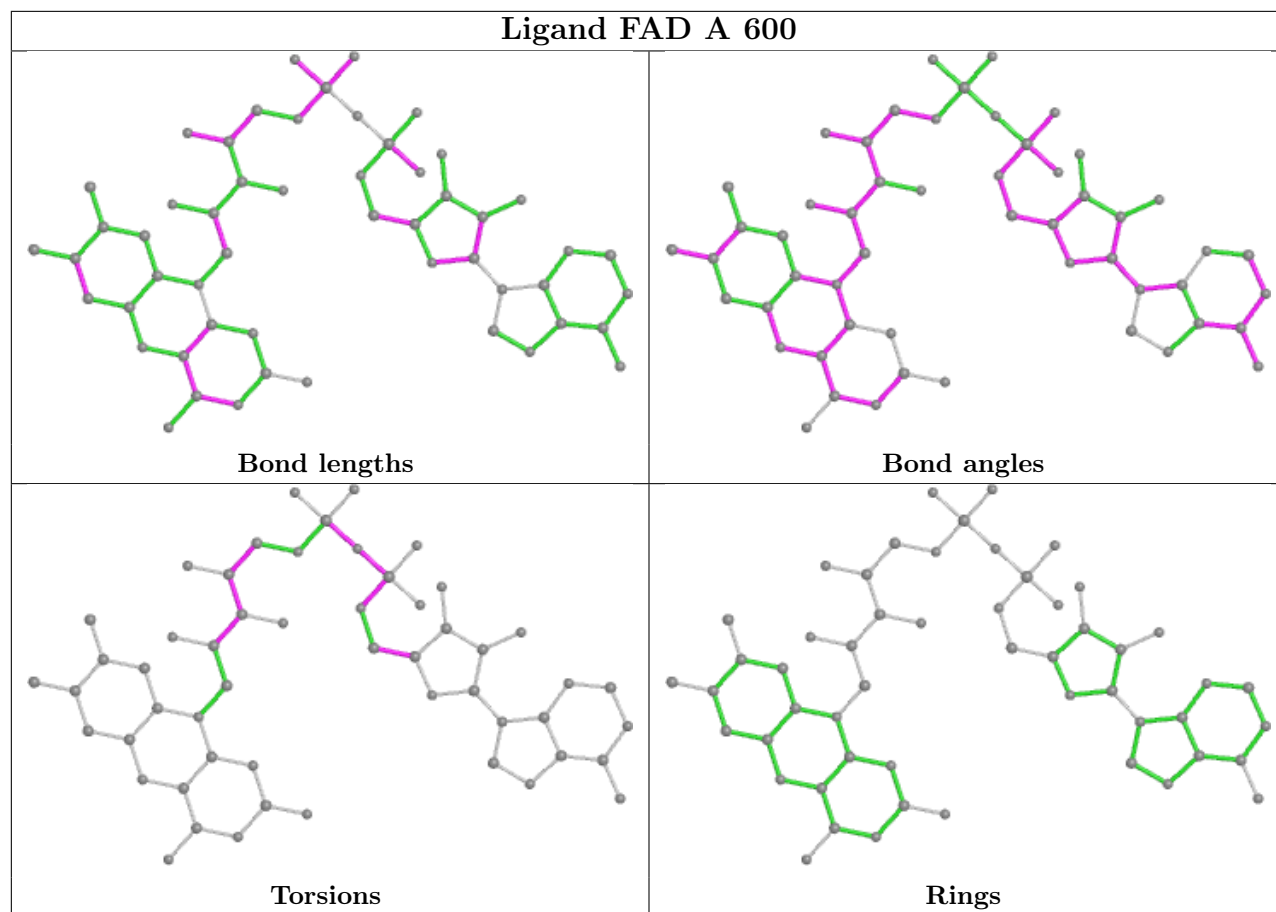
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

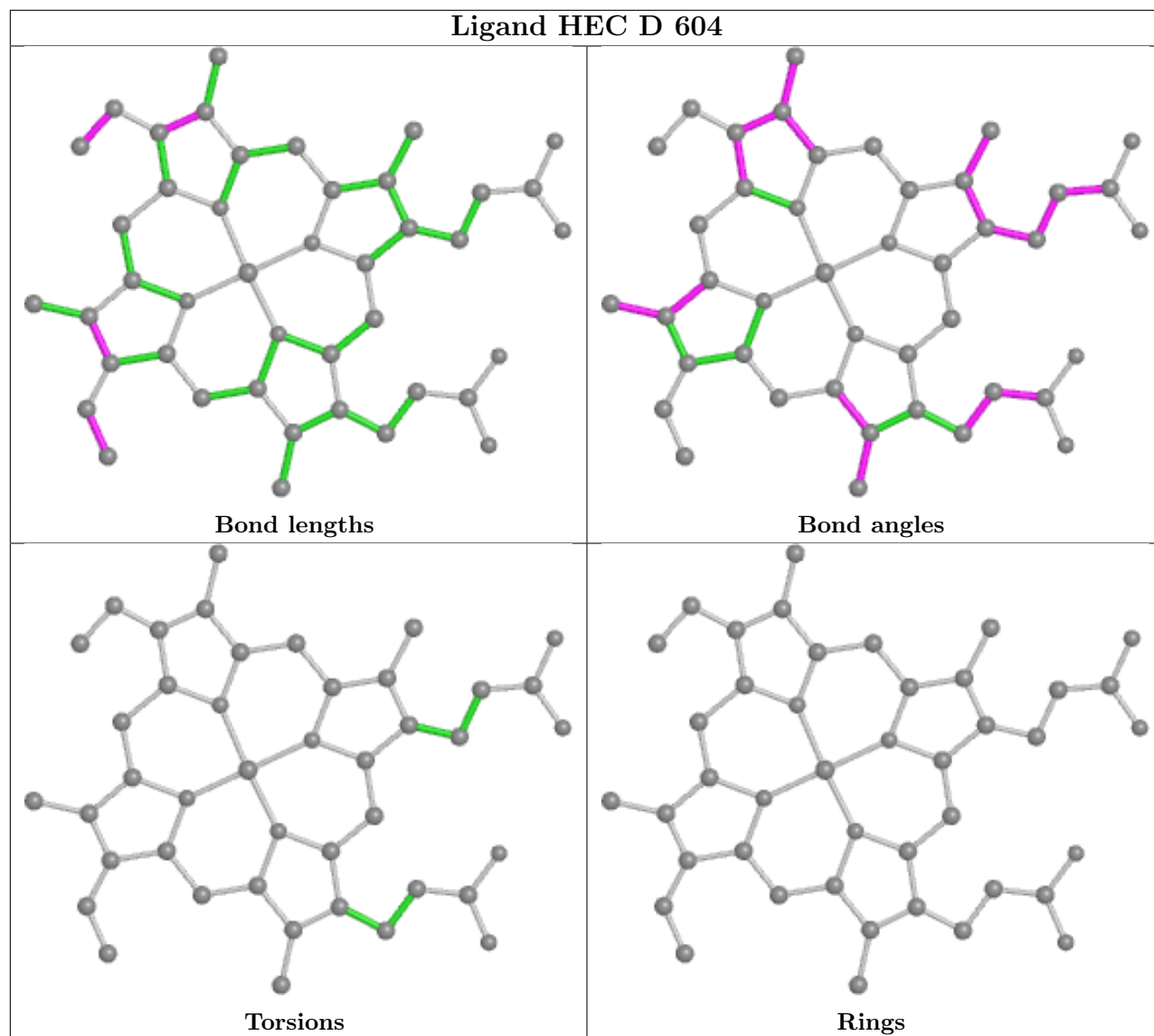


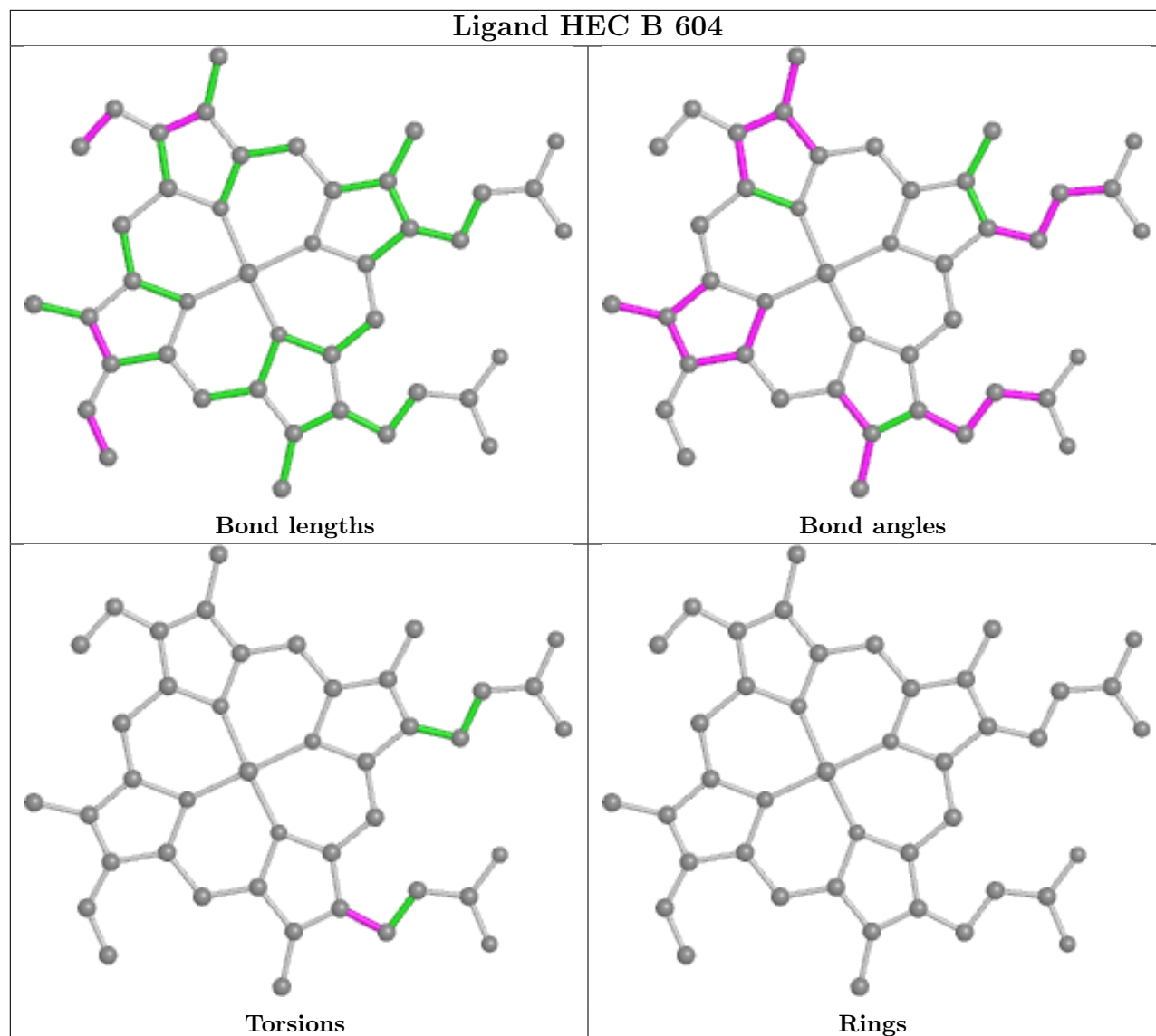


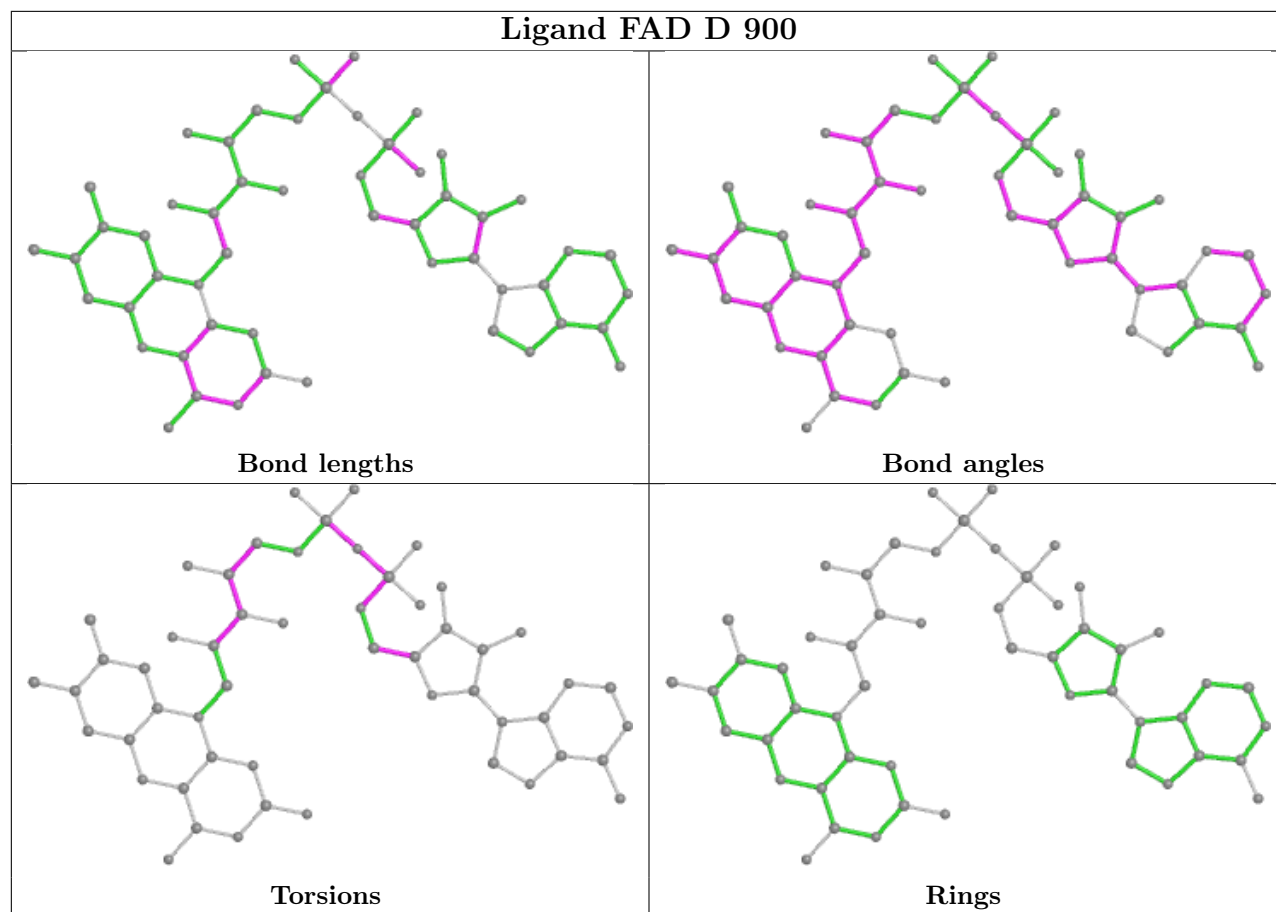


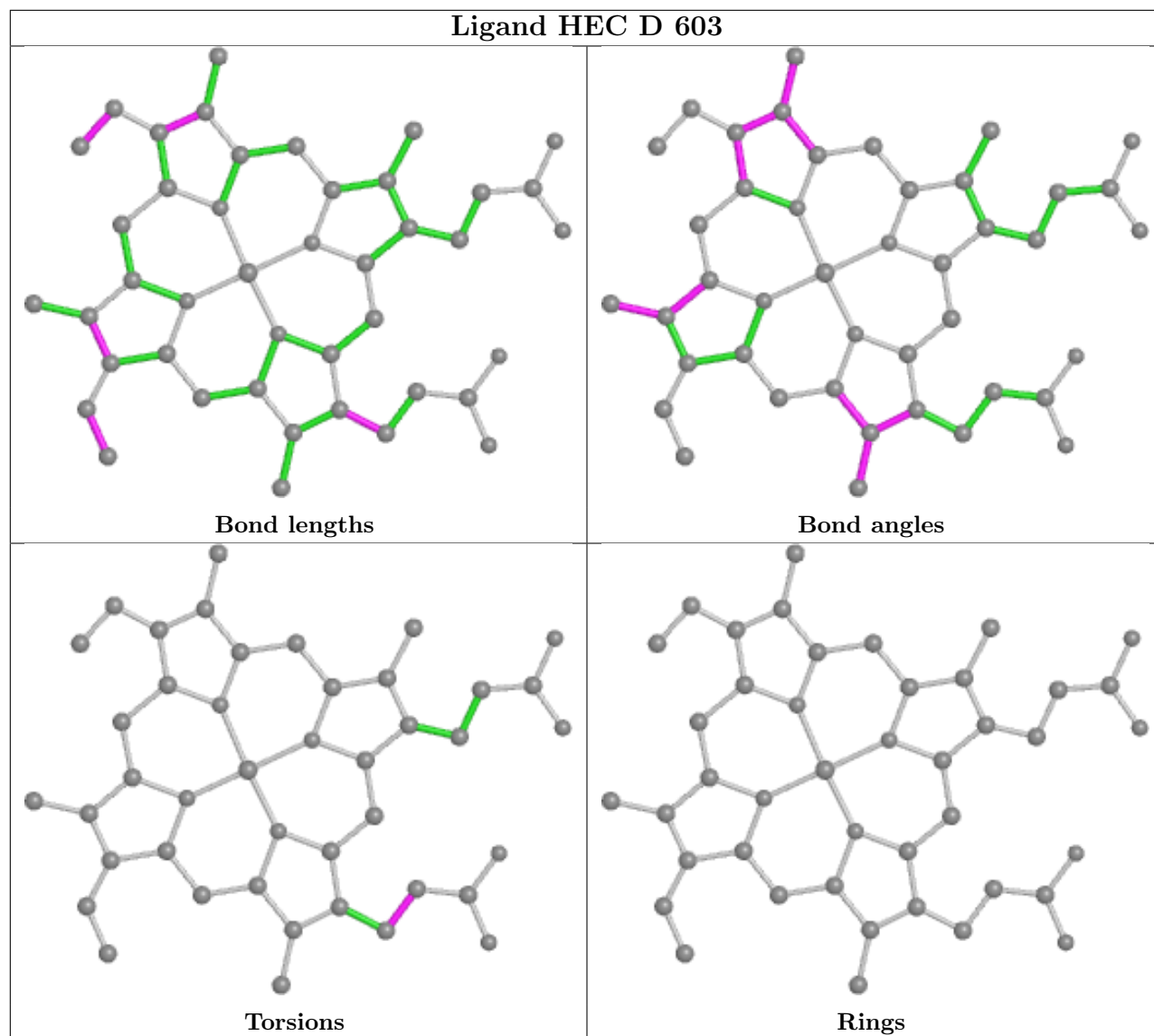


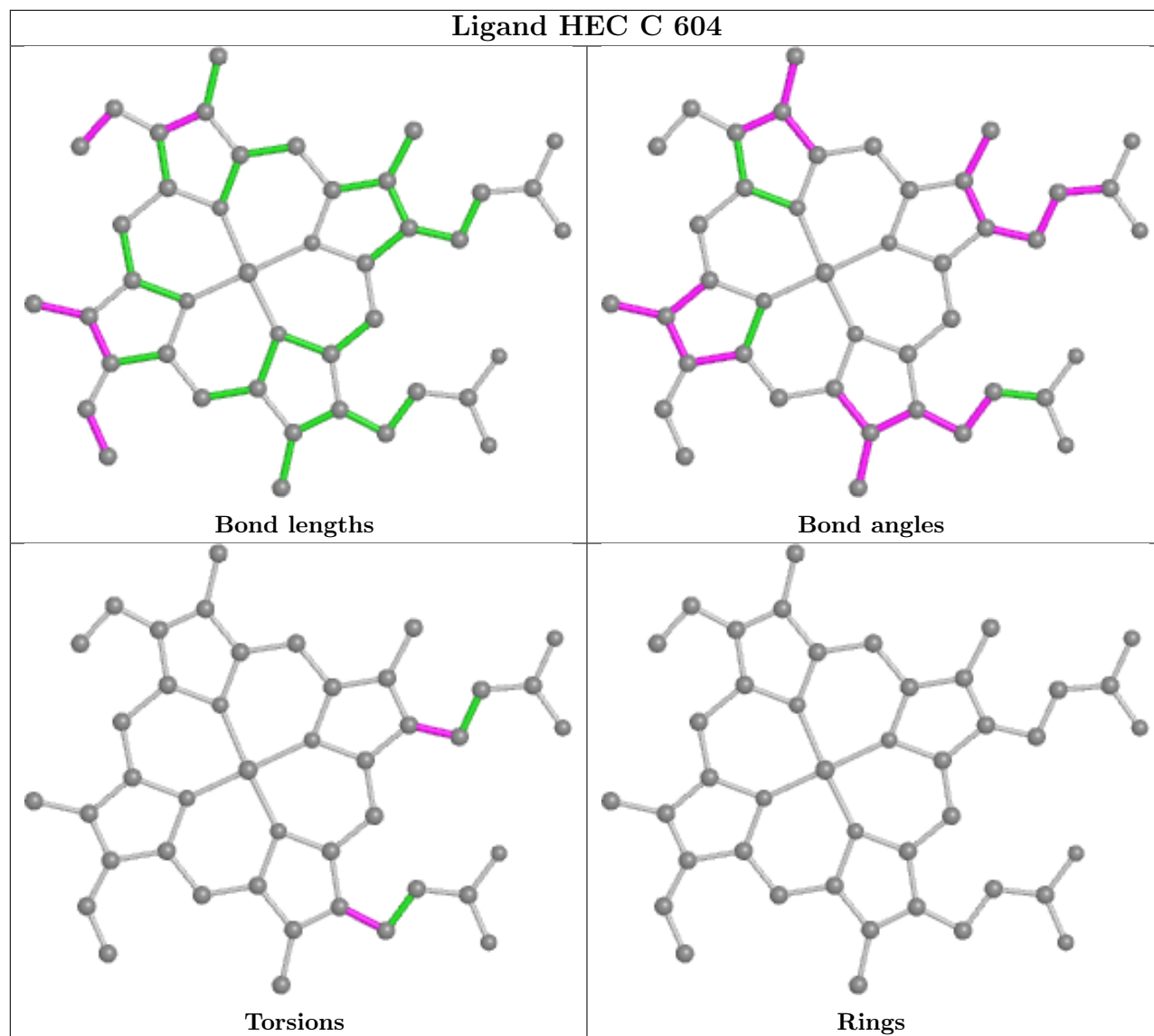


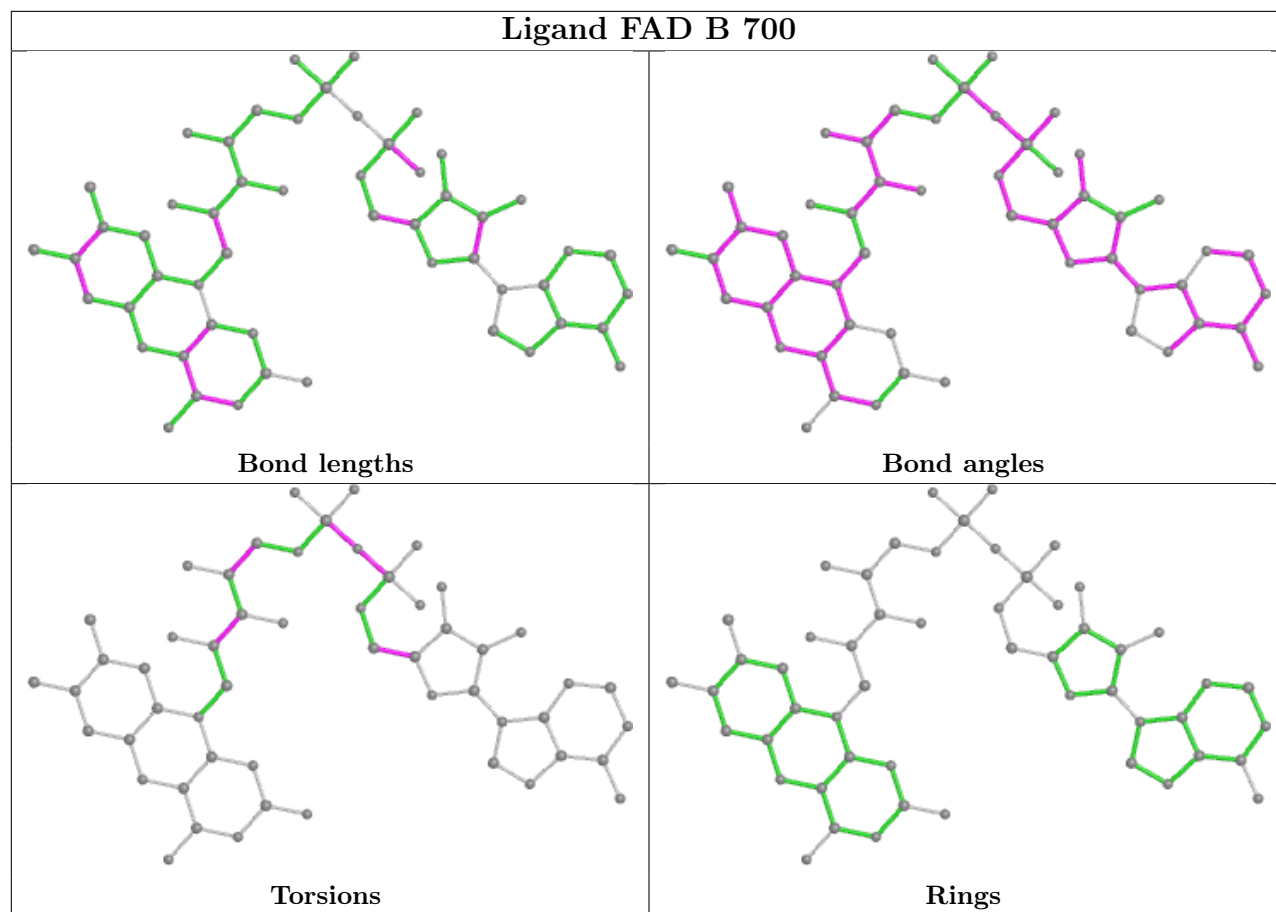


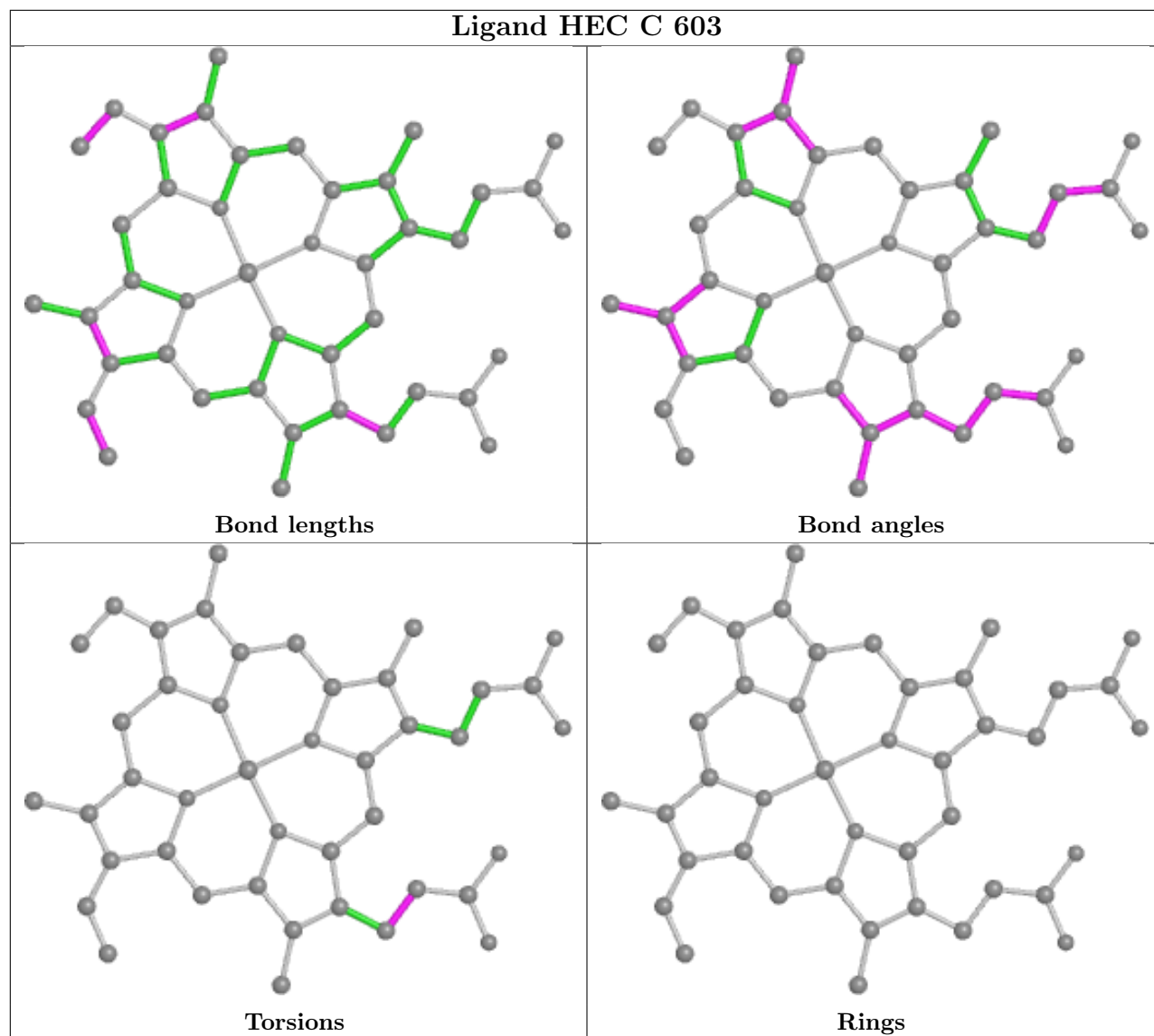


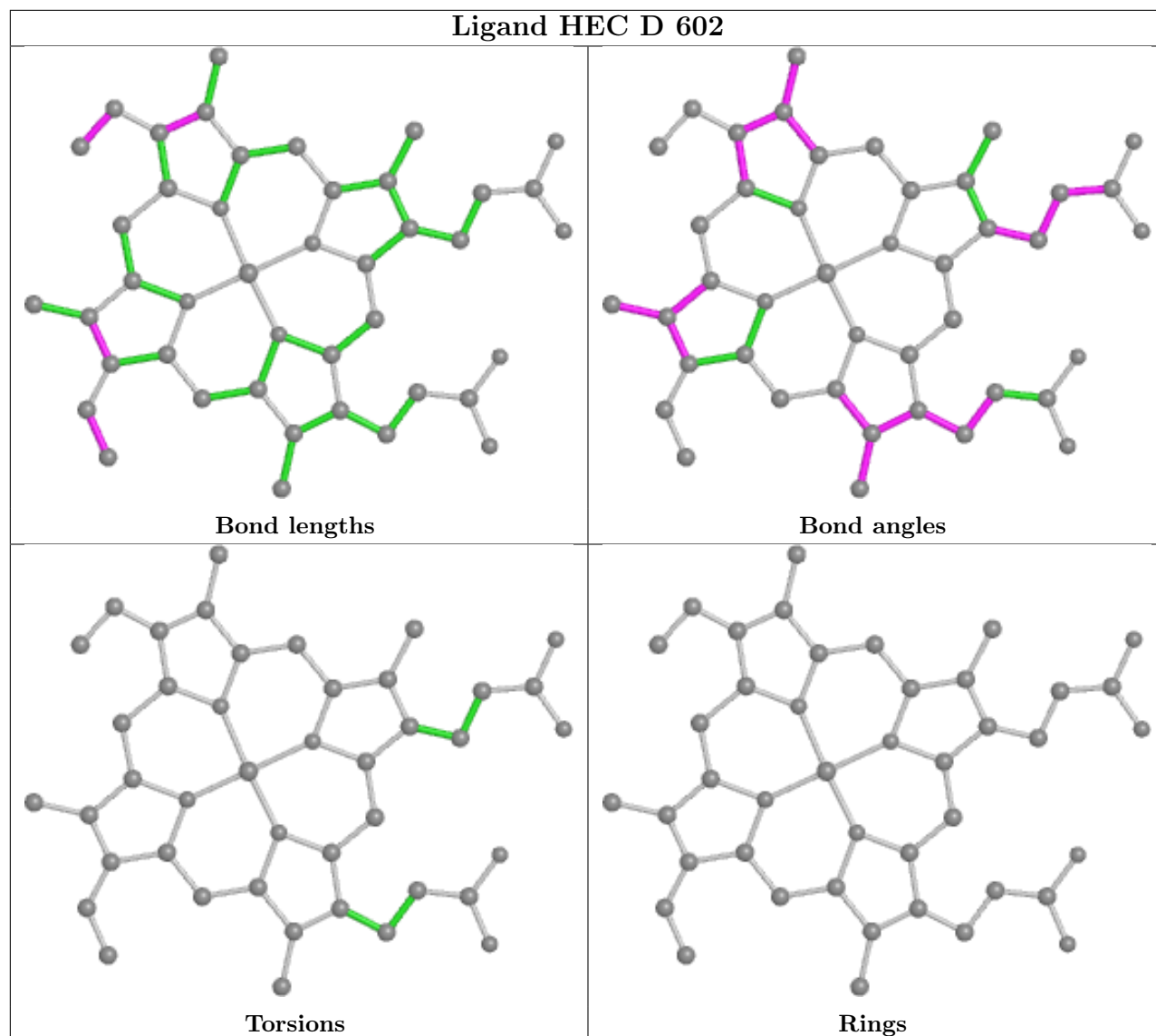


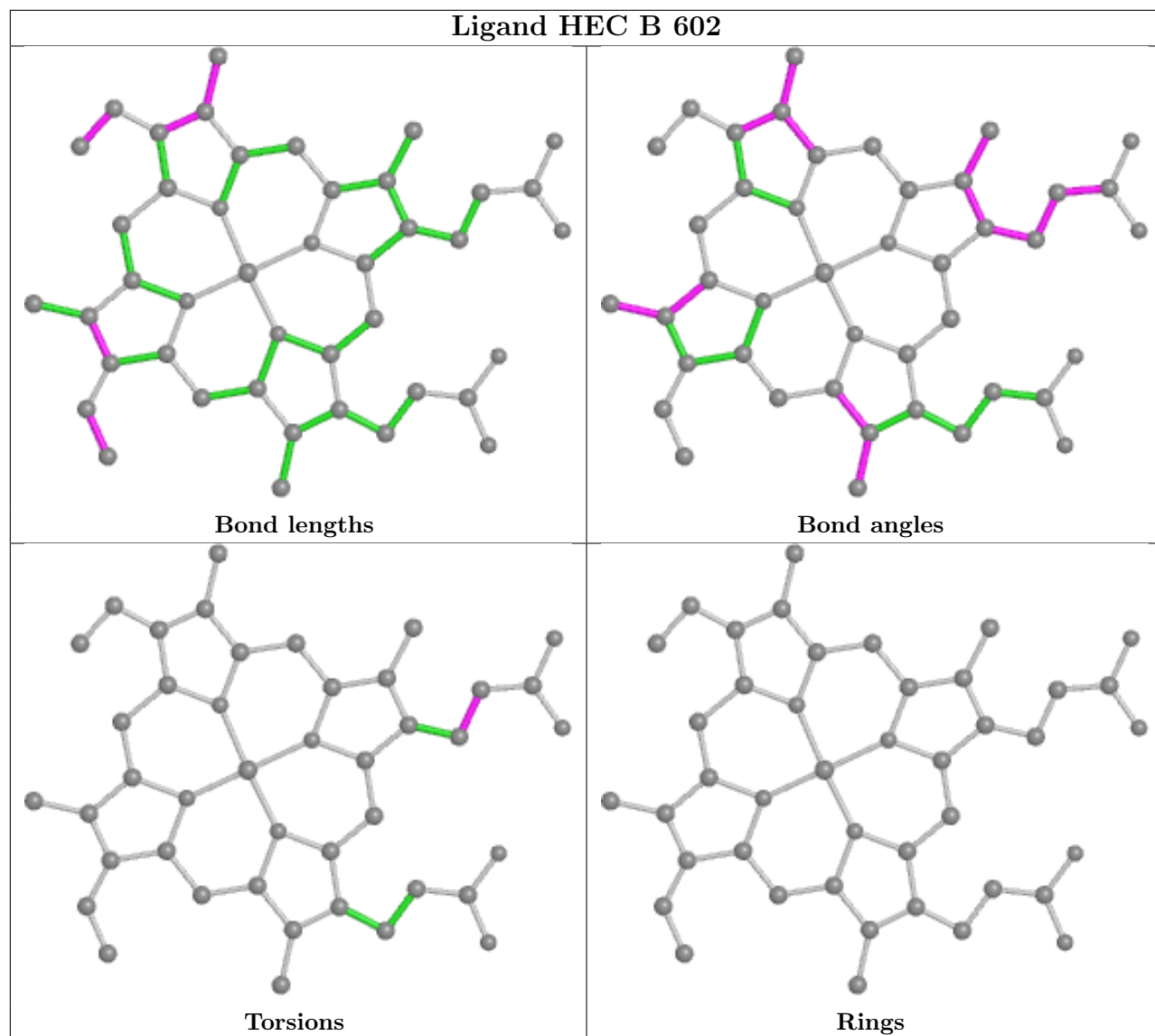


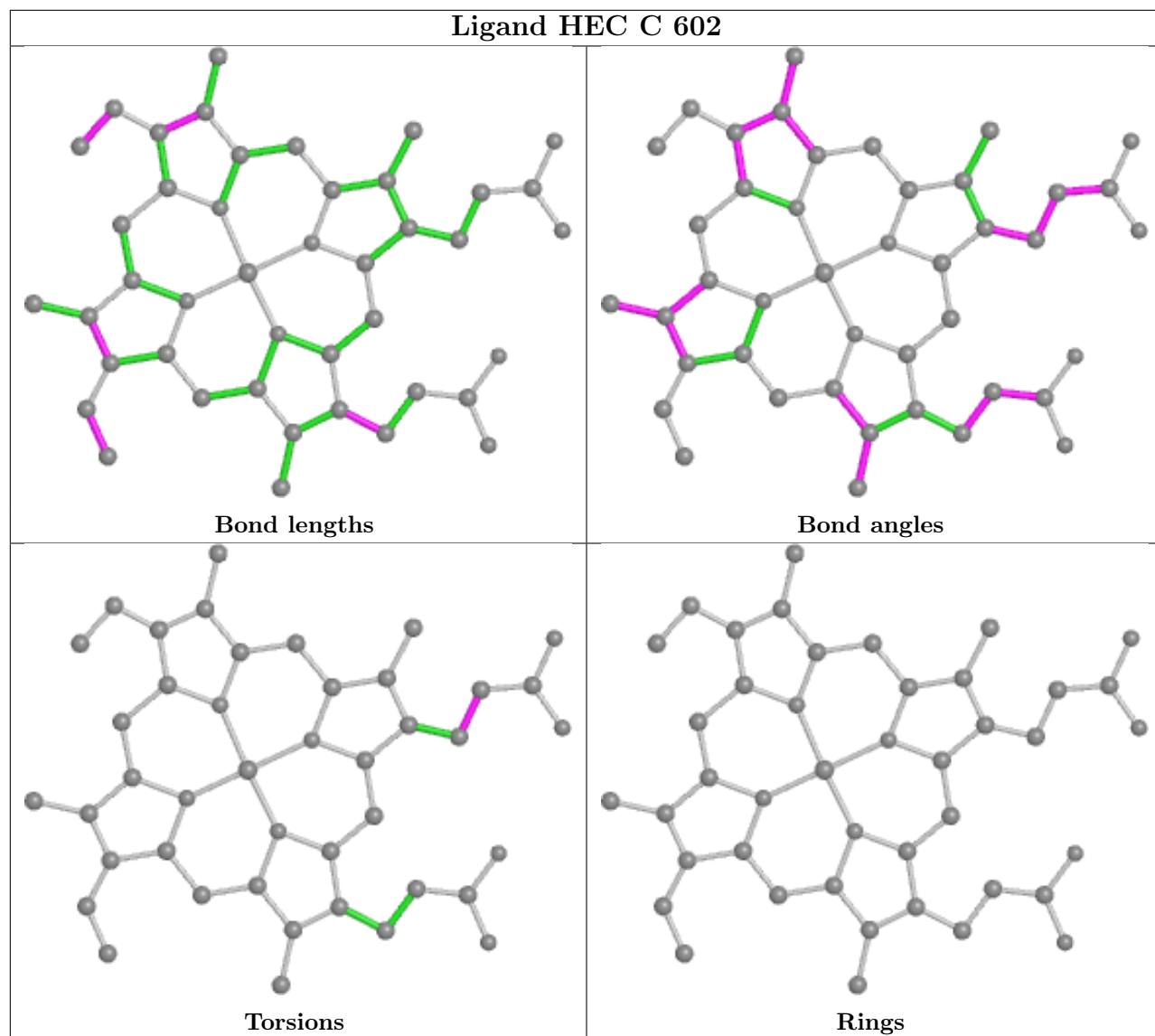


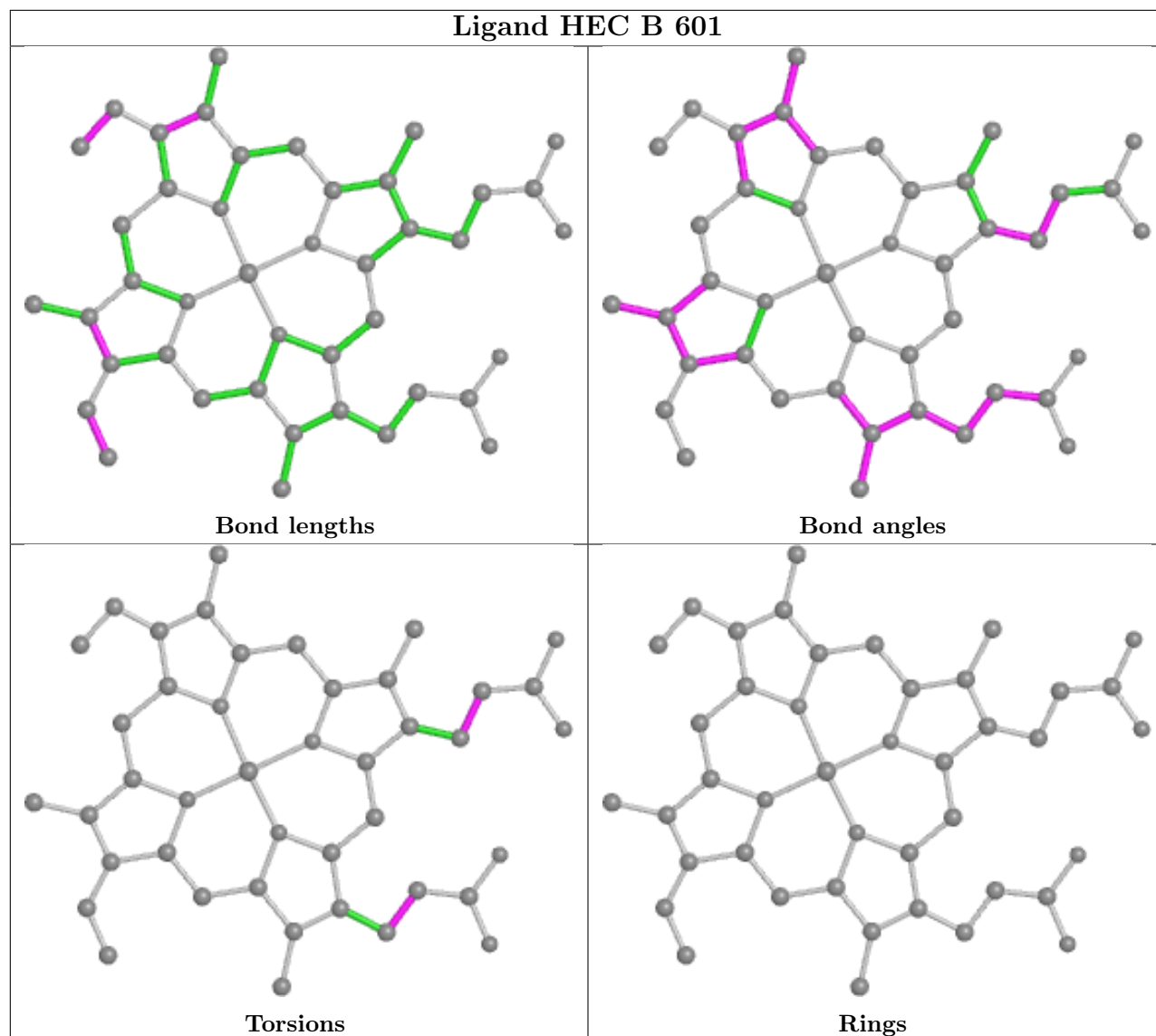


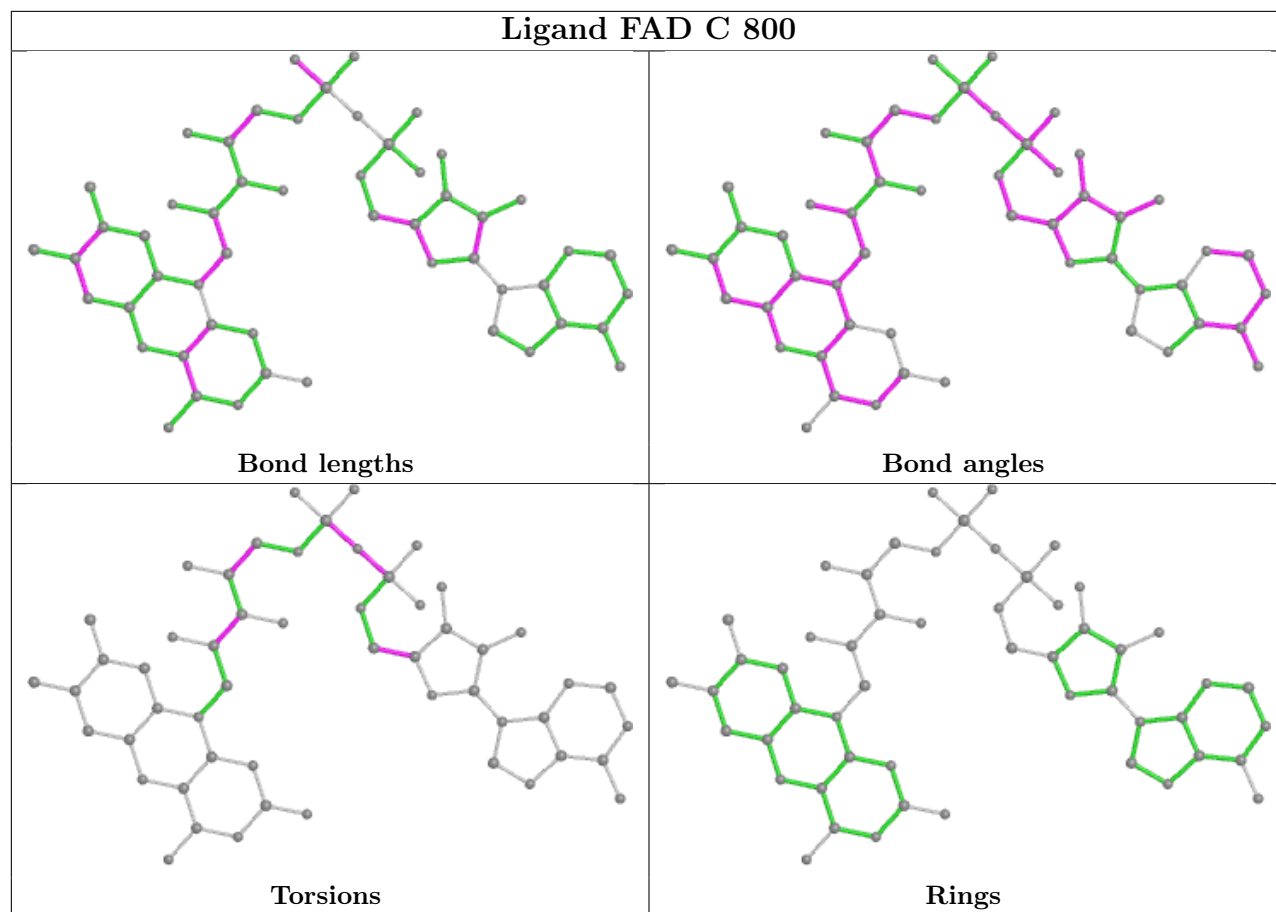


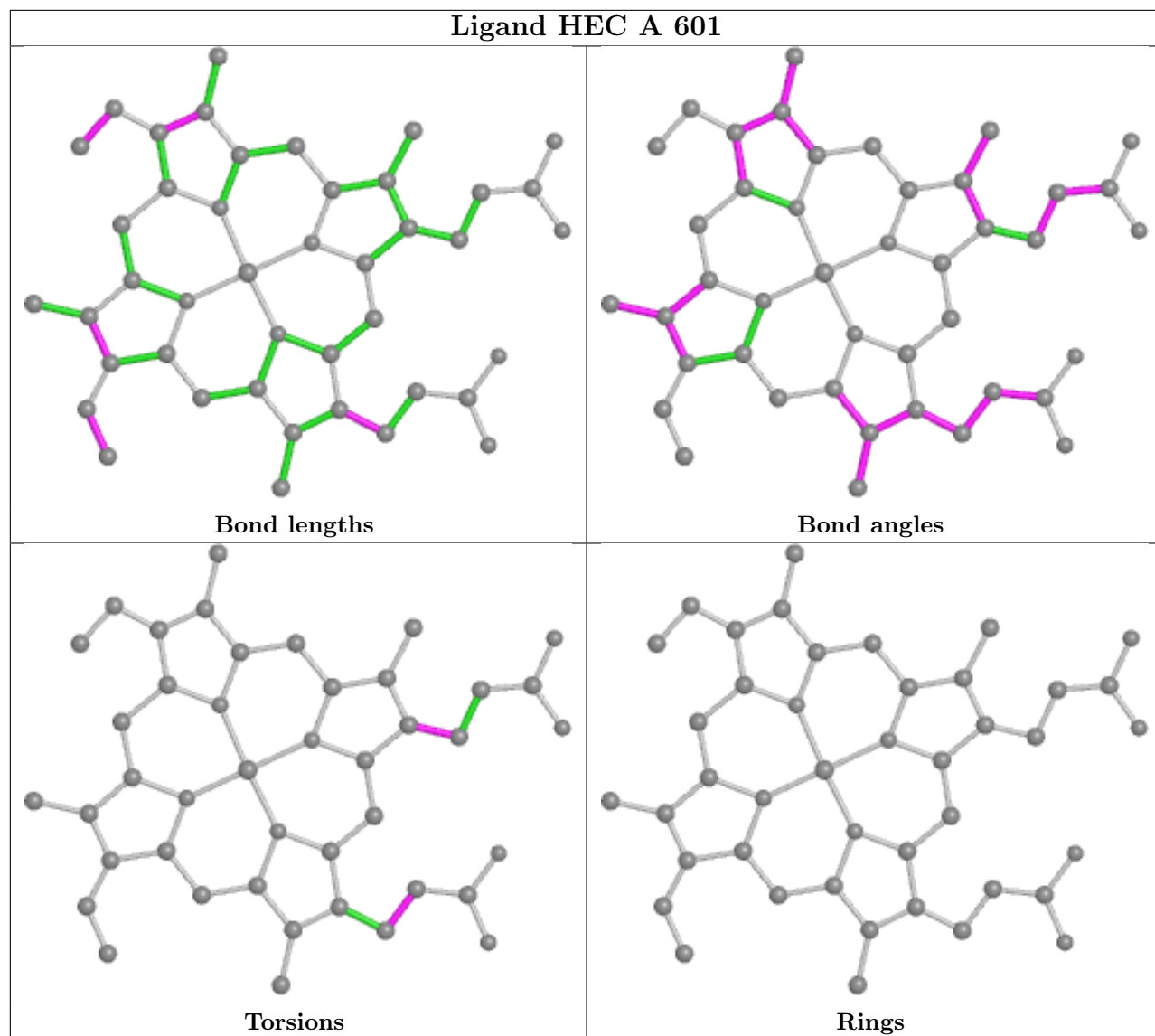


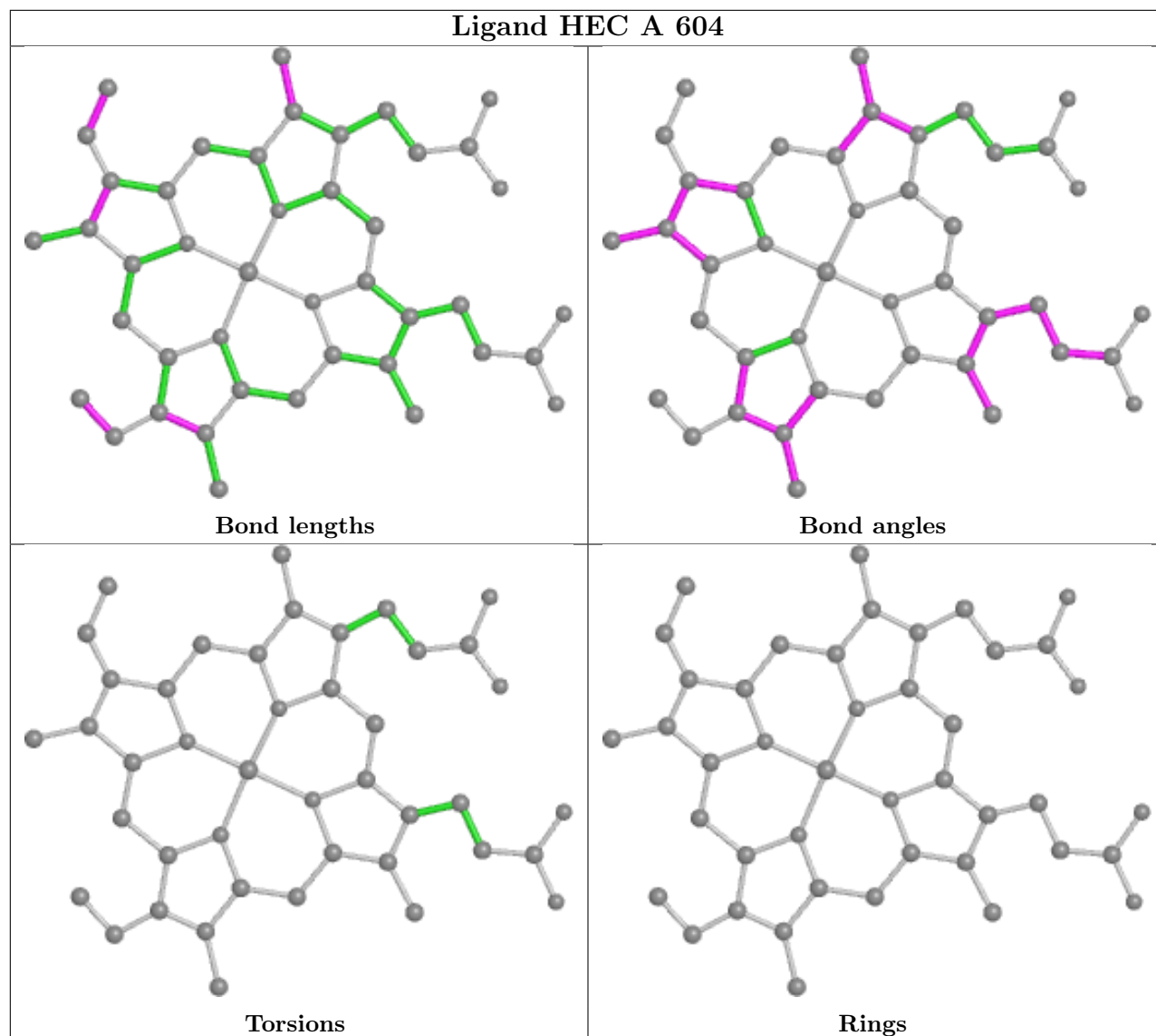


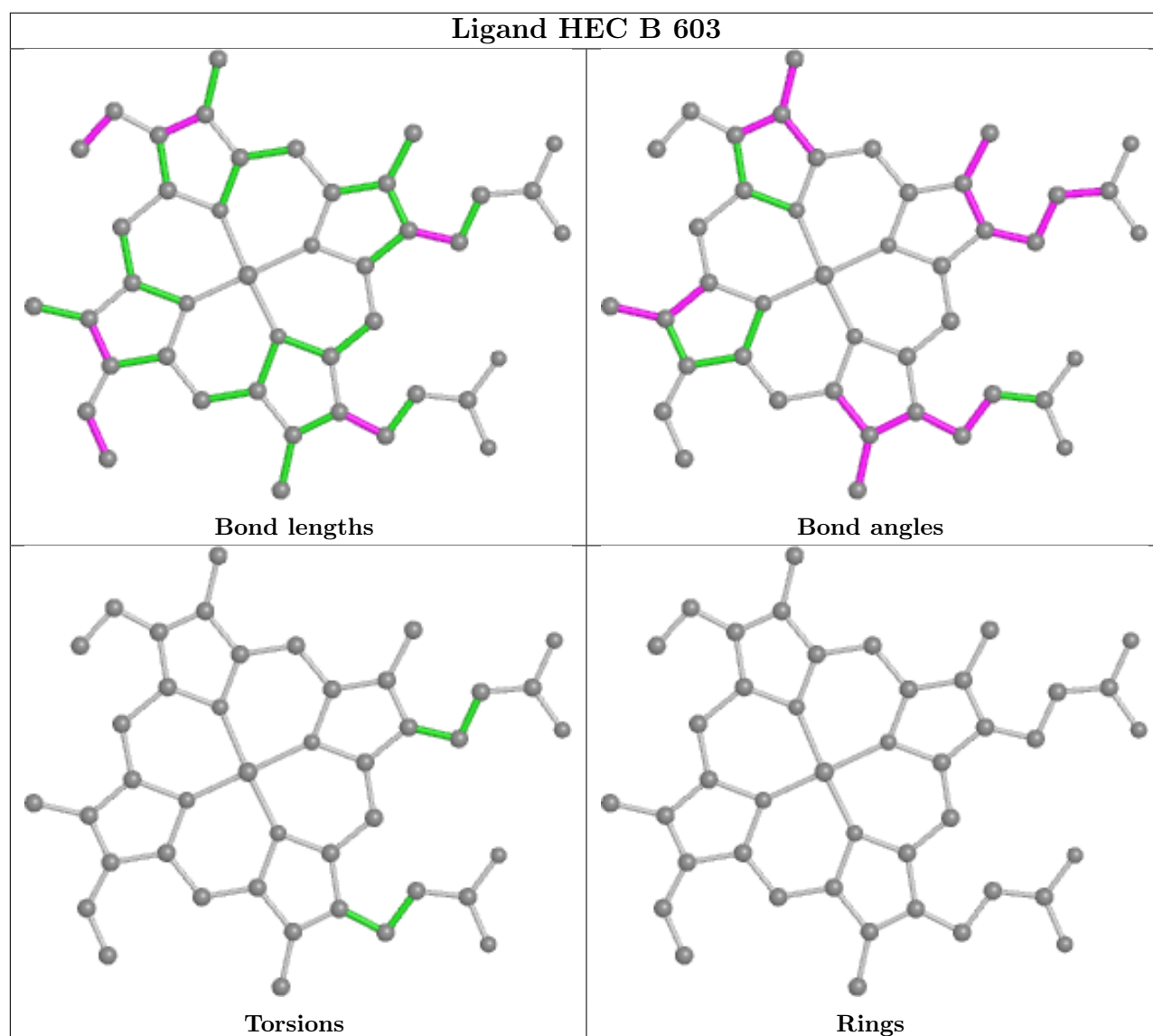












5.7 Other polymers [\(i\)](#)

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.